

## **Metabolomic profiles associated with a mouse model of antipsychotic-induced food intake and weight gain**

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## Supplementary data legends

**Supplemental figure 1. Pathway analysis of the plasma metabolites associated with antipsychotic hyperphagia.** Pathway analysis conducted using Metaboanalyst software determined a significant number of hits related to arachidonic acid metabolism, steroid hormone biosynthesis and retinol metabolism.

**Supplemental Table 1. Plasma metabolites detected in control, olanzapine, minocycline, and co-treated (olanzapine and minocycline) mice.** 7140 metabolites were detected in the plasma, comprising 396 identified metabolites and 6744 unknown metabolites.

**Supplemental Table 2. Differential analysis of plasma metabolite abundance between groups.** Differential analysis revealed that 1188 metabolites were significantly changed between OLZ vs CON adjusted p value < 0.3. Relative abundance is also calculated for these metabolites in OLZ vs MO (minocycline + Olanzapine), and MINO vs CON.

**Supplemental Table 3. All plasma metabolites significantly associated with antipsychotic hyperphagia.** To identify metabolites that are specifically associated with AP-induced hyperphagia and weight gain, we applied another set of filters: metabolites that were significantly changed with OLZ treatment compared with CON and these metabolites should not be differentially changed between CON vs MINO, which revealed 389 plasma metabolites significantly associated with antipsychotic hyperphagia.

**Supplemental Table 4. Known plasma metabolites significantly associated with antipsychotic hyperphagia.** Known metabolites that were significantly changed with OLZ treatment compared with CON and these metabolites should not be differentially changed between CON vs MINO. This revealed 19 'known' metabolites.

**Supplemental Table 5. Hypothalamic metabolites detected in control, olanzapine, minocycline, and co-treated (olanzapine and minocycline) mice.** In the hypothalamus, we detected a total of 414 metabolites of which 92 were identified and 322 unclassified metabolites.

**Supplemental Table 6. Differential analysis of hypothalamic metabolite abundance between groups.** Differential analysis revealed that 151 metabolites were significantly changed between OLZ vs CON adjusted p value < 0.3. Relative abundance changes is also calculated for these metabolites in OLZ vs MO (minocycline + Olanzapine), and MINO vs CON.

**Supplemental Table 7. Hypothalamic metabolites significantly associated with antipsychotic hyperphagia.** To identify hypothalamic metabolites that are specifically associated with AP-induced hyperphagia and weight gain, we applied the same filter that we used with plasma metabolites (metabolites that were significantly changed with OLZ treatment compared with CON and these metabolites should not be differentially changed between CON vs MINO). This revealed just one metabolite, indoxylsulfuric acid, that was increased by ~2 fold by OLZ treatment compared with CON and OLZ+MINO normalized levels to CON range.







# Supplemental Table 1

Method	Polarity	m/z	RT	ID	C1	C3	C5	C8	O1	O3	O4	O7	O8	M3	M4	M5	M7	M8	MO3	MO4	MO6	MO7	MO8
EIC	Negative	361.2390	3.80	10,11-DiHDDPA [M-H]	110184	94077	102473	250633	79260	80414	82353	88574	100228	154956	96746	95581	123335	71017	81914	133165	88521	149821	65229
EIC	Negative	343.2279	5.28	10,11-EdDPA [M-H]	307369	304542	167076	384531	228046	243992	243992	221258	502024	227783	182563	309862	114576	114576	233941	458258	384426	201796	292606
EIC	Negative	405.2286	2.00	11-Deoxycortisol [M-H]	0	583097	0	0	159367	222279	459364	0	625694	178216	698963	211385	629796	683482	544959	761257	413262	190151	461931
EIC	Negative	337.2383	3.90	11,12-diHTeT [M-H]	394053	305195	300908	598182	269664	411109	274073	269089	406023	257789	347372	355557	212602	212602	281677	405750	299566	399014	212327
EIC	Negative	397.2579	3.81	11,12-diHTeT [M-H+Ac]	246940	169357	237856	137822	122945	261919	122873	86014	247555	141080	135823	242367	262580	192182	79062	572075	425369	437263	200877
EIC	Negative	319.2281	5.45	11,12-EdT [M-H]	409944	347010	220438	474101	395948	412782	421246	267554	343136	282133	313681	498086	405410	267669	413398	555876	644020	379165	498565
EIC	Negative	377.2330	4.03	11,12-diHTeT [M-H+Ac]	581939	349440	709340	774783	472266	350655	349718	842371	371712	670836	339541	361298	292263	708137	413855	239672	447549	805997	388531
EIC	Negative	353.2279	2.36	11,12-dk-PGF2a [M-H]	352459	294089	285867	323664	281297	321238	333971	419842	308889	231889	262544	297207	286420	284884	282448	463914	318036	302551	275656
EIC	Negative	367.2122	2.17	11d-TX82 [M-H]	280279	205823	361691	241957	105891	137845	168911	124117	111229	280946	158659	196841	158053	147621	173522	263293	156342	184688	217451
EIC	Negative	379.2473	4.92	12-HETE [M-H+Acetate]	316550	209749	440310	458570	272391	294330	325413	437362	422860	318987	266955	359057	366044	315267	226561	786899	364161	536981	226755
EIC	Negative	351.2170	3.55	12-OPDA [M-H+Acetate]	326032	265838	717338	766239	578074	390240	563329	939637	506509	568493	297563	396430	321213	380111	197433	240935	380275	676547	359927
EIC	Negative	313.2387	3.45	12,13 diHOME [M-H]	2293626	1433159	4154629	10339952	2448478	2156194	3397563	4715300	3806153	3811524	2073877	3709062	3225590	2513523	756373	3453222	2973423	5695206	1554121
EIC	Negative	295.2279	5.17	12,13 EpOME [M-H]	3600487	2097970	3806851	3952462	2430621	2749700	3400897	3265680	5406491	2480827	1836364	3168216	2935760	1749715	1843098	4102327	3456429	3657575	2657606
EIC	Negative	393.2289	3.43	12oxo LTB4 [M-H+Acetate]	511034	181441	387946	207588	92947	110817	124642	93555	117542	394254	91218	134938	111296	136804	102034	339775	140645	73454	147798
EIC	Negative	335.2228	5.04	12S-HpETE [M-H]	684173	376716	779392	686146	358103	328528	444355	616736	283003	764117	367760	478575	359353	352320	378257	283003	481707	913556	352238
EIC	Negative	343.2277	4.74	13 HDoHE [M-H]	644289	760434	433657	1096856	977887	647536	934441	493652	1721460	570382	509098	581068	865579	304057	752222	1189581	991742	665905	700153
EIC	Negative	295.2279	4.50	13-HODE [M-H]	4299983	1414617	4299983	5397009	3304521	2306281	2392174	5549218	4517201	2293929	1579536	1900332	1903457	2858088	662475	1821840	2155996	4238027	1700218
EIC	Negative	293.2125	4.59	13-oxoODE [M-H]	1152010	713182	1119246	1396739	1184329	935833	1369207	1086325	1660993	828983	700391	889075	933859	918433	651246	3203894	1130518	1312126	940928
EIC	Negative	361.2390	3.70	13,14-DiHDDPA [M-H]	136600	128017	140606	377107	136191	112493	123524	132660	139045	148106	126360	151524	196159	85963	95238	139055	139588	214994	135496
EIC	Negative	393.2288	2.89	13,14-dihydro-15-keto	1692485	944831	1625943	1110748	955533	393628	1566346	868082	1061549	1465596	1154254	1639381	2034402	1088530	947341	1030424	1396181	2003007	1369552
EIC	Negative	353.2328	2.64	13,14-dihydro-15-keto	287184	132597	199242	147278	258989	179873	149545	84361	201672	136981	120197	136800	93851	125393	83631	135349	142443	167362	111333
EIC	Negative	297.1692	1.70	13,14-dihydro-15-keto	0	90745	0	0	41176	167912	27938	0	36148	0	88262	30102	24226	22182	35067	77628	72508	0	84317
EIC	Negative	343.2278	5.17	13,14-EdPPA [M-H]	442502	475915	246608	703643	354724	519568	515253	316876	497797	354759	354724	383966	526645	264319	439964	682563	536793	314393	456932
EIC	Negative	293.2125	3.98	13(S) HTeT [M-H]	306257	207431	620617	2153305	442437	278021	367266	993831	646225	593477	309508	541801	505702	279223	147801	459789	438611	960926	196983
EIC	Negative	353.2312	4.03	13(S) HTeT [M-H+Acetate]	382256	377393	988953	2275723	764250	542475	638451	1612416	1275105	990811	499698	874345	760474	260008	136296	882683	594087	1385124	272657
EIC	Negative	353.2312	4.14	13(S) HTeT [M-H+Acetate]	1542332	1280941	2846920	3188959	2091430	1446516	1734070	353117	2244691	2299384	1366411	1404617	1401719	2529408	991760	1168974	1923854	3193435	1728637
EIC	Negative	309.2074	4.12	13S-HpETE [M-H]	1447036	826542	1933968	790240	704944	1070858	684083	1495917	359340	1432233	643030	832797	528110	1328063	1077536	449221	659903	1593211	1125808
EIC	Negative	395.2439	3.32	14,15-diHETE [M-H+Acetate]	2057452	987304	2602963	3154710	599781	653017	947956	1359623	887347	1521060	928264	1450383	1377365	1004703	824984	1266172	1467590	1799418	937305
EIC	Negative	381.2625	5.71	15-oxoEDE [M-H+Acetate]	384013	395660	1060273	1009331	759630	492719	693906	1144626	898832	607471	325316	443574	447547	380839	322274	370276	466702	792041	364013
EIC	Negative	395.2441	2.92	15-epi-PGA1 [M-H+Acetate]	2328182	2725766	1650420	129116	2572673	2242925	136995	2992421	135174	171020	150917	144463	2511359	1947553	2753180	118918	2319562	2760071	2429857
EIC	Negative	379.2472	4.62	15-HETE [M-H+Acetate]	565953	345499	1000039	1134207	556696	403331	591110	1142900	657384	1063251	598084	620984	634938	625082	186682	672206	622146	1117980	511670
EIC	Negative	317.2124	4.14	15(S) HEPE [M-H]	20792812	18380351	21203246	19235856	7055493	4661397	11604355	7836969	10939718	11994421	12324922	19866059	19268476	13022391	1717709	16502979	16657888	13171287	11401453
EIC	Negative	377.2332	4.14	15(S) HEPE [M-H+Acetate]	875000	755831	959645	811631	349178	300705	502441	425053	508450	543675	821569	779515	531042	785155	710235	631672	562366	488630	
EIC	Negative	315.1967	4.16	15d PGA2 [M-H]	2090173	862850	3082886	2274975	479086	905458	925508	859998	770614	3083649	1463601	1328996	1481537	1103210	473741	1214231	1425080	1648407	1372481
EIC	Negative	393.2288	3.23	15d PGD2 [M-H+Acetate]	181896	139276	214516	206588	131807	106397	178664	141971	215728	159677	120657	152183	145289	125204	115362	158750	152535	150537	149280
EIC	Negative	315.1967	4.02	15d PGJ2 [M-H]	16241493	7544009	32205244	18498521	4789559	3653307	10586273	9297297	7402762	12333125	12060375	11555030	15603887	8744897	4215823	1105622	11903671	14782492	21605182
EIC	Negative	351.2180	2.28	15R-PGD2 [M-H]	788133	389797	748197	921068	148577	254640	264825	242077	234271	1259627	333869	411468	386479	413367	310527	418353	432120	625347	583142
EIC	Negative	343.2279	4.64	16,17-DiHODE [M-H]	1530218	1287601	351523	4471771	1323118	1278769	1031396	1319222	5374942	6202483	730855	1611331	1278769	1160111	1641366	1131156	5390500	3685756	1987571
EIC	Negative	379.2477	4.34	16-HETE [M-H+Acetate]	434730	571357	425587	361568	429488	624809	482912	416416	734406	478962	665502	576791	533837	413139	194724	642003	699368	271766	618311
EIC	Negative	361.2390	3.63	16,17-DiHDDPA [M-H]	317293	350832	352401	941011	371263	167149	292527	387799	309768	538065	429992	601407	184341	258992	184341	258992	343914	526057	1995252
EIC	Negative	319.2279	4.31	17-HETE [M-H]	5056180	1138791	5168089	3479636	669300	876685	1182069	803452	708298	4899975	1438793	1369692	1723464	1240760	1080644	1392681	1729462	2396035	1237051
EIC	Negative	379.2480	4.40	17-HETE [																			

fpHILIC	Positive	241.1292	3.19	ANSERINE	6317116	3952579	3364399	5090608	3165917	5322522	3428434	2837730	3752768	3623189	3991477	4152607	4115541	3929855	3834844	5100988	3256326	4812912	3331111
fpHILIC	Negative	187.0378	2.71	ARABITOL(M+Cl)RIBITC	2917426	1949397	2218371	3444990	2283702	2975423	2433880	2911692	3613314	2484500	1993545	2211263	2382474	1865425	1440727	2564448	2273650	2718796	1995515
EIC	Negative	311.2957	6.72	ARACHIDATE[M+H]	6494117	10616147	8403271	12905934	14284889	9371361	13138705	10595053	8954705	12805066	12732307	16705353	10670212	13623811	13198990	7567970	12934813	15138816	11255206
EIC	Negative	303.2327	6.44	Arachidonic Acid [M+H]	279097984	286350250	74770048	308100898	272181760	240106265	305291285	296875285	273160024	199873177	266454207	273219723	291855651	234738924	241612353	281442482	281256126	23527673	270570187
EIC	Negative	303.2327	6.58	Arachidonic Acid [M+H]	2100065	3063116	1586917	3011277	3780460	3251577	4057548	2929640	2266028	2430767	3943136	4025696	4338848	3511353	3654571	4131778	4952532	3968987	3698437
fpHILIC	Negative	131.0463	3.50	ASPARAGINE	12893349	6797381	8569788	6763466	4573566	4841557	3869839	5573223	3800565	8282181	6826062	7131154	7161180	6778168	12941841	8296191	5358340	9419360	3452519
fpHILIC	Positive	133.0605	3.50	ASPARAGINE	12846199	10654547	11954843	7263961	5490428	6332984	5959176	6741955	6347364	9251476	7288003	7907089	8987410	10829127	14980068	10079335	7349610	10835011	8772231
fpHILIC	Negative	113.0357	3.50	ASPARAGINE(M+H2O-H)	1722506	889920	1280494	1053317	662456	760243	625874	876086	637181	1529235	1400394	1110687	1117921	1129987	2045107	1374557	859417	1511322	551525
EIC	Negative	407.2805	2.75	β-Muricholic Acid [M+H]	169281174	19474887	198073416	100097636	30051720	39170150	20002242	151853885	37012646	5853435	299348	110109	6630086	447054	113141	90532	65572	3922362	542283
EIC	Negative	467.3020	2.75	β-Muricholic Acid [M+H]	77307030	9343046	86292364	44953376	14348556	17484424	9095656	71806776	17342814	2809515	341060	225885	3032147	399553	268196	205585	219834	1954376	534134
EIC	Negative	339.3269	6.86	Behenic Acid [M+H]	128890	163904	136114	192930	158334	171559	208990	163856	157665	245209	221247	350244	231549	253726	261656	167803	246622	333741	224047
fpHILIC	Negative	116.0717	2.28	BETAINE	7882849	3905292	6183611	5480663	4164353	5467874	4392542	5442712	2831511	5429602	3292554	3717558	3354480	2254425	3374708	3574619	3432685	5689481	2423437
fpHILIC	Positive	118.0863	2.28	BETAINE	1197446912	856638080	1077841920	970940992	922274496	1021024640	939321792	1027562496	732770752	1008540224	804361792	844726592	809894336	612896192	746776704	776748416	813261440	977769024	663242944
fpHILIC	Positive	140.0681	2.28	BETAINE(M+Na)	1657798	3112809	3317566	3387178	3094878	3786097	2694902	3458880	1754455	2842474	1921976	2291579	2359401	2214164	2668413	2171347	1660126	3711379	1360877
fpHILIC	Negative	225.0993	3.63	CARNOSINE	2608349	1271185	1697302	2046413	1117139	1413814	1078333	888614	707238	1924403	1585195	1648291	1545421	983667	1044095	1425717	1118335	1002640	1076657
fpHILIC	Positive	227.1134	3.63	CARNOSINE	8446045	3889466	4491539	5913339	2775701	5532052	3759743	2389121	3859266	5258414	4606140	5083266	5081354	3801713	3348933	5622241	3865312	3366945	5501348
fpHILIC	Positive	249.0955	3.63	CARNOSINE(M+Na)	978852	518241	709660	903040	476875	556635	489436	467177	385235	888570	716013	741594	707317	472049	485601	666741	492721	514050	577095
EIC	Negative	391.2859	3.68	Chenodeoxycholic acid	23690433	1137086	36650252	5955779	3258109	1946589	3384821	10523079	1266596	418387	16264	44732	174821	0	20084	0	298726	79676	
EIC	Negative	451.3070	3.68	Chenodeoxycholic acid	67123118	3270221	106807504	18238944	9991295	5765890	9986023	31003785	3836998	1125647	79134	84425	470817	72409	68122	84759	38790	873505	151506
fpHILIC	Negative	191.0197	4.72	CITRATE	139428784	93197952	96307032	115063464	106547232	143562208	100517312	98689088	119337632	91292784	96558808	98500064	99044648	99422136	88094200	120587600	92102672	103995624	95811264
fpHILIC	Negative	213.0017	4.72	CITRATE (M+Na-2H)	546853	578444	538485	688860	621380	571942	586110	641885	667429	652330	698799	609261	681761	689180	710985	618667	630240	632462	723587
fpHILIC	Positive	236.9983	4.71	CITRATE(M+2Na-H)	878112	1007371	992789	1148327	1131496	1138396	1254517	1297759	1250876	1265376	1268862	1268858	1399844	1288979	1304413	1365508	1385786	1224407	
fpHILIC	Positive	215.0161	4.71	CITRATE(M+Na)	1578021	1086213	1328043	1853349	1939899	2771902	1627818	1419514	1854878	1330146	1624279	1244551	1270457	1420212	972667	2286170	1189397	1558260	1243830
fpHILIC	Positive	176.1026	3.71	CITRULLINE	63703408	56758932	64275536	65868912	72690504	88680928	79811728	63848400	69098224	62754060	56473324	64741752	54878736	44534568	64566720	68590416	49969252	53232748	48261684
fpHILIC	Negative	174.0883	3.71	CITRULLINE	16926856	13622335	13972847	12944227	15362122	17464784	14450564	12923574	11404907	12541884	12894065	12084766	11697424	9591678	14052641	13999587	12366599	12673760	11127372
fpHILIC	Negative	196.0704	3.72	CITRULLINE (M+Na-2H)	628637	706523	727332	679623	6567123	651375	634752	657496	666037	629632	675534	730361	614733	701049	703968	643663	641659	553117	
fpHILIC	Positive	202.0663	3.72	CITRULLINE(M+2Na-H)	568566	651310	688258	704453	772695	634475	644545	756895	565885	834261	761908	764454	746488	661163	728735	671161	721430	764077	629111
fpHILIC	Positive	198.0856	3.72	CITRULLINE(M+Na)	12874030	13213772	13942743	13801182	14904485	14640567	14517182	13902787	14317192	14106111	13561146	14341663	13759940	12095453	15190483	14277701	12488013	13441811	12132001
EIC	Negative	345.0705	1.87	CORTEXOLONE [M+H]	40254	175719	0	0	58284	100438	137084	0	205386	0	201247	73045	225907	220428	188373	291716	126189	0	206443
EIC	Negative	405.2285	1.87	CORTEXOLONE (M+H+Ac)	13827269	47507340	2250432	3559977	11235558	20517681	35246986	2212124	50981536	1737051	5561763	17074820	54872334	58984682	46116788	60480451	34060787	4302583	42522583
EIC	Negative	361.2018	1.45	CORTISOL [M+H]	0	31250	0	0	116111	44387	79700	0	69268	0	40429	0	21692	162454	80463	80398	26488	0	132913
fpHILIC	Negative	130.0622	3.36	CREATINE	8920123	8032879	4421572	3826605	6681534	8688202	6355983	6001655	8501108	3493709	4511170	6260162	7443535	6505364	7459436	9385311	6438643	6410756	3740799
fpHILIC	Positive	132.0768	3.37	CREATINE	905958272	807127872	548336768	50986368	632487040	837678720	603247872	708904704	737437056	477395456	525010016	641353024	736034240	771633856	785265152	868057472	619840640	769910064	481608416
fpHILIC	Positive	154.0596	3.37	CREATINE(M+Na)	1074096	1520606	993972	929638	1401770	1730106	1041304	1362034	1586639	803707	1154215	1278578	1364018	1712766	1405494	1542811	1380042	1370213	1027222
fpHILIC	Negative	242.0786	2.61	CYTIDINE	802499	422705	325700	794990	402394	662700	461389	501664	404632	466125	307714	617814	478013	369214	444571	810671	460941	525590	624559
fpHILIC	Positive	244.0919	2.62	CYTIDINE	12768348	8711554	5861432	12636649	7915307	13371811	7816389	8088312	12292029	8409480	6687174	11965852	9347790	6753963	8054861	12060288	7189578	9517051	7112551
fpHILIC	Negative	278.0548	2.61	CYTIDINE(M+Cl)	2642578	1716414	1206037	2478733	1692305	2560751	1860725	2035956	2129171	1400997	2059250	2019822	1597483	1874675	2010218	1830753	2017026	1702599	
fpHILIC	Positive	266.0732	2.61	CYTIDINE(M+Na)	1774218	1307568	953544	2080553	1397684	2072617	1304759	1434804	2088950	1442631	1102125	1926592	1562198	1094208	1259585	1992065	1293706	1513412	1366366
fpHILIC	Positive	112.0507	2.22	CYTOSINE	10664462	8099069	10767831	11903500	9125440	11568850	8319314	9596635	10268833	1066465	10344922	10357358	9872386	8229079	6563972	8982356	7245700	8397223	8396331
fpHILIC	Positive	159.0274	2.05	D-GLUCURONOLACTON	2633330	1184890	3218257	527901	7017837	5985480	2556776	617601	4641355	836051	38670	48402	4530093	4977155	0	54319	5994378	66166	0
fpHILIC	Positive	162.0756	3.18	D-MANNOSAMINE[M+H]	914632	735359	972185	914546	806629	1043300	974304	797687	771152	782898	743711	704526	749777	615699	731183	688680	695389	891618	668631
fpHILIC	Negative	229.0117	4.03	D-RIBOSE-5-PHOSPHAT	1135162	373902	219271	300856	663912	824540	527752	298857	1069304	204798	229450	540808	460608	702979	467262	570991	1191701	510996	715395
EIC	Negative	367.2120	1.32	d16-D PGF1α [M+H]	469748	101249	0	0	24449	36054	51034	0	28425	179986	108102	75121	64373	104465	46655	89819	109604	0	64871
EIC	Negative	391.2859	3.85	Deoxycholic Acid [M+H]	180539560	32030821	166167883	125196938	52062801	40074616	54557476	122977693	15999898	58831555	5953162	3491762	5037061	160435	1029400	1790295	839702	1388791	9023240
EIC	Negative	451.3069	3.85	Deoxycholic Acid [M+H]	43479769	8118852	42206422	31015428	12812877	10288544	14228485	2910											

EIC	Negative	335.2231	3.32	EIC_171	2673538	1169098	3137382	2480717	530521	606435	957268	1011401	474746	1877509	994787	1368732	1263349	1223011	1050985	1240207	1621477	1614961	1174766
EIC	Negative	337.2383	3.73	EIC_181	351590	237810	347843	686234	328855	316747	292905	386339	287076	464120	256601	404361	351858	163986	206308	399163	287459	496863	176921
EIC	Negative	337.2382	3.54	EIC_182	634861	408395	677888	1751911	524664	530552	596919	736105	629998	827198	519749	930662	762831	250328	330776	629937	623937	1006354	285654
EIC	Negative	341.2334	3.69	EIC_184	976933	402623	989957	642891	546527	608659	816788	1068580	168493	575431	372692	469362	319598	183500	259528	263785	219583	788424	342401
EIC	Negative	343.2277	4.42	EIC_193;EIC_195	542395	602545	319821	710064	562665	475637	616113	335029	1126065	469053	462388	565900	671010	215074	620983	978298	742474	458626	611652
EIC	Negative	343.2277	4.20	EIC_198;EIC_201	1800099	1707986	1626050	4858218	1707811	1669193	1454534	2022361	2631937	2760554	1649230	3433258	2496957	971435	1301699	2402991	2031041	2572346	1300091
EIC	Negative	295.2279	4.37	EIC_200	7600328	5319601	11868138	9516957	8132087	7033492	7916484	10062917	7858021	6645544	5086729	5490204	5462019	109277753	3305389	9499134	7596666	10238852	6780080
EIC	Negative	295.2279	4.43	EIC_200;EIC_21	5868100	3741927	10522118	5638066	5031159	4415555	6123265	6380718	5475788	4830318	3883324	3941239	3338253	8185164	2355467	7277939	5308954	7836805	4331652
EIC	Negative	349.2023	1.73	EIC_219	4661361	1121679	2632369	2818422	203349	345970	408317	330478	365585	5717463	1145128	895127	614021	992223	2696777	672411	854037	351055	835096
EIC	Negative	295.2279	4.60	EIC_22	1814263	1242153	2793288	2098844	1476053	1505184	2403587	1803080	1783972	1459831	1056914	1237674	1127736	1850811	842572	3085360	2050788	2107796	1259174
EIC	Negative	351.2180	2.69	EIC_232;EIC_237;EIC_2	1269165	592287	1742809	707783	323741	357170	542365	447053	342040	826993	541355	706468	719023	567057	647001	539880	521454	903129	692049
EIC	Negative	351.2180	1.99	EIC_233;EIC_249	1240954	2002709	883624	450273	577744	823106	956532	0	826293	960124	1907250	1767383	1199103	1336586	1247557	2136947	2166815	0	1667854
EIC	Negative	295.2279	4.87	EIC_24	1758142	1223342	2681576	2048385	1850019	1634064	1810269	2745009	2479887	1434098	1183958	1268345	1477835	2777201	775516	1427006	1695083	2398377	1532683
EIC	Negative	295.2279	4.23	EIC_25	1149653	773847	1771176	2506718	1065347	941476	1106316	1623156	1364437	1236935	759763	1075993	949548	1072596	575745	1821045	1032673	1841128	756012
EIC	Negative	353.2343	3.25	EIC_251;EIC_256;EIC_2	82265	50695	122171	55776	75020	118529	55370	66294	101434	54678	40748	42777	46989	39443	35463	3035833	55351	95609	50039
EIC	Negative	353.2322	3.31	EIC_251;EIC_265	184205	159102	180669	190372	186965	178831	176301	619625	167680	166780	10478	155937	164252	153508	150369	3083900	182311	163674	154416
EIC	Negative	353.2055	4.76	EIC_277	24162	0	358595	0	0	181549	0	0	0	0	77689	208603	0	328747	101199	35556	0	622842	0
EIC	Negative	295.2279	3.92	EIC_29	4355107	2833948	7837475	32728570	5934848	4237401	5177897	13505552	10547096	9029549	4894902	10786102	8421024	2089140	2453830	12700316	6715084	14602457	3229498
EIC	Negative	297.2436	4.72	EIC_31	6765881	5291685	14916543	18029994	11225066	8268788	9321963	16933909	13253614	9886977	5680328	8179057	8162908	8436309	3488445	10952324	8526313	13389325	5843028
EIC	Negative	363.2530	3.78	EIC_312	188964	72611	152430	59842	133174	54967	33222	11516	46190	58773	41548	174571	0	38304	46964	481940	40551	71855	69873
EIC	Negative	363.2553	3.79	EIC_312	208443	138793	196069	564609	185477	163088	144547	227530	214969	310168	152295	182090	212987	112316	92886	206691	186210	296295	85317
EIC	Negative	365.1975	2.01	EIC_315	0	82273	0	0	0	0	0	0	0	0	81057	108200	71661	52858	101426	105545	36372	0	105486
EIC	Negative	299.1878	2.57	EIC_32	883040	77085	604590	1048908	73587	98743	106217	663709	53721	724641	85247	88049	80991	56535	100727	78715	73440	737070	71629
EIC	Negative	299.1880	2.49	EIC_32	79673	499498	43582	89403	547183	651773	591208	60944	517940	73529	668815	884291	687057	330754	611587	714156	646607	78154	40780
EIC	Negative	375.2173	2.91	EIC_328;EIC_332;EIC_3	7457627	4877275	9229228	6705362	2905285	2570058	4312582	2578429	3050684	7207804	4968992	5839924	5067730	5126322	4100040	5829202	5441222	4707553	3238359
EIC	Negative	299.2591	5.44	EIC_33	1842977	1539795	1350476	1451152	2487107	2496631	1916251	1877615	1710715	1233811	1181899	1069900	1407122	1462059	1577666	1929276	13670027	1826091	197439
EIC	Negative	299.2591	5.50	EIC_33	1497490	1181801	3633108	3046581	2311495	1759553	2158629	4027523	2801719	2048264	1288801	1297498	1667995	1678430	822133	1423725	1187704	2543997	1396947
EIC	Negative	299.2592	5.37	EIC_33	5103601	3825379	10326756	13335019	5078186	3473148	5002087	10435433	6876145	5357375	3041570	3386209	3931515	6054609	2994770	2893625	4506673	9156559	4742954
EIC	Negative	299.2591	5.36	EIC_33	1986408	1754053	10927021	14024105	2348181	1989892	5002087	10740308	7390547	5357375	3041570	1579739	3931515	2465127	2994770	2893625	1994961	9534463	4742954
EIC	Negative	375.2172	3.76	EIC_340	451381	292059	621130	337972	203589	212671	332867	296710	227275	275984	196848	310042	297781	303902	210327	321854	298258	423708	1860000
EIC	Negative	377.2333	2.64	EIC_346	0	77908	0	0	102364	89578	137957	0	99497	0	60080	68314	61960	47794	70038	89804	72938	76446	75423
EIC	Negative	391.2135	2.15	EIC_352	1353176	376558	1429942	594509	318174	722010	105904	131491	911314	406329	590108	379105	599793	505039	608404	310377	723011	121660	324769
EIC	Negative	391.2136	2.48	EIC_356	331987	891958	0	1141773	875013	910392	1081200	0	915759	623557	891712	915469	983075	998739	964810	889005	1023292	377117	1073529
EIC	Negative	289.1810	3.77	EIC_4	284245	194640	393113	238032	216737	193256	296053	306614	64155	365190	289301	280445	184479	168938	195875	79683	149056	263116	120349
EIC	Negative	307.1936	2.26	EIC_41;EIC_42	0	210838	44762	0	109843	0	155992	205643	97801	309343	0	200301	177395	31486	19914	167443	38214	263113	30758
EIC	Negative	309.2074	3.68	EIC_51;EIC_58	922156	938972	922363	1593730	1292200	834852	1491311	1394720	1706642	968164	680727	996371	878243	797690	726278	1008581	1074276	1178738	1000156
EIC	Negative	309.2073	3.61	EIC_51;EIC_59	964863	876440	1056768	1578506	1209746	1385745	1391639	1543824	856580	1209287	992977	794792	728626	979187	711329	754442	1052981	1009288	96794
EIC	Negative	309.2072	3.37	EIC_55	303533	245577	295801	481708	351291	282196	366121	442105	523621	239205	207988	334926	245905	222028	212668	333580	288451	324968	259191
EIC	Negative	309.2074	3.80	EIC_58	12694305	3365429	16848273	11980314	3717569	3801183	3710269	10912164	3076735	19543624	3408964	4346705	3433061	8241886	6748073	2706653	4662310	14392047	5825451
EIC	Negative	291.1967	3.99	EIC_6	102125	68735	101414	97142	94993	68820	103292	96269	156016	82525	68071	71347	78055	72935	56800	102475	95362	120955	82195
EIC	Negative	311.2230	3.23	EIC_61;EIC_64;EIC_66	1133502	996137	1372220	1572841	1426964	962420	1830818	1367103	1038948	835820	1169337	1032442	917867	842874	1355161	1210315	1265325	1210227	1210227
EIC	Negative	311.2229	3.30	EIC_61;EIC_64;EIC_67	1972991	1540887	2116138	2288030	2286455	1828469	2704432	1941396	5304684	1498612	1273156	1950604	1736700	1621262	1229432	6502351	2122896	2394020	2085420
EIC	Negative	311.2229	2.92	EIC_62	1434912	512646	1621077	2267828	669030	680872	1050939	1176049	818334	1606756	446462	656091	882620	670382	277282	743279	907958	1564755	474824
EIC	Negative	311.2229	3.08	EIC_62;EIC_66	734475	508125	739498	752113	691001	607976	923544	718108	979489	561308	428711	646795	525544	454392	390387	1338620	617975	654694	561849
EIC	Negative	311.2229	4.35	EIC_63;EIC_68	14278944	4139812	17807795	18188107	6042277	4593753	6260993	15952954	5280500	23451307	4671745	5877099	5814179	8153851	7981772	4160074	6495203	24077019	6091536
EIC	Negative	313.2388	3.32	EIC_71;EIC_73;EIC_74	3766900	2024915	7914021	31227329	4761730	3620259	5564348	11363710	8363841	8597089	3986055	8600092	7539058	2068100	899658	7399676	5778599	12024925	1746547
EIC	Negative	313.2385	3.14	EIC_74	878304	318929	846428	724049	349046	463988	526279	463988	552003	559371	336979	497316	494960						

EIC	Negative	535.4738	6.53	FAHFA_535.472635	828676	964767	1561079	1908255	1336773	975744	1521206	1640030	2110758	1152335	1708533	1262644	2028019	1739100	1125314	1904472	1802115	1475008	1231771
EIC	Negative	551.5055	6.58	FAHFA_551.503935	348927	524916	539367	708087	653040	514298	758482	651422	1223786	485612	515838	433020	728929	640579	562100	804136	826015	593567	598012
EIC	Negative	555.4425	6.70	FAHFA_555.441335	459393	422278	359720	444545	633171	434503	598725	509544	326679	530863	538837	482345	414509	505207	617052	398058	285350	395287	514046
EIC	Negative	555.4419	6.29	FAHFA_555.441335	9570693	14766058	24793610	39684589	26034000	12257067	19370727	24767516	29814918	13357126	9023753	11752323	21188987	89927669	5180990	12589050	17023208	18779303	9731877
EIC	Negative	555.4425	6.63	FAHFA_555.441335	879748	498814	579175	737430	934985	675398	1186601	1025358	561384	830534	723595	778572	564951	575882	1077681	1113880	772826	692438	1057696
EIC	Negative	559.4750	6.67	FAHFA_559.4756985	5172547	4565304	4977899	5432464	6700649	6638626	7174838	8654638	5298701	6521293	5203234	4966325	4906250	4825792	6014084	6348631	4942807	5661293	8667804
EIC	Negative	559.4731	6.70	FAHFA_559.472635	3216574	2574719	2834299	3247388	4670858	2985951	4401367	3996244	3130072	2552178	3739868	3206551	2556596	3552833	4213877	2901938	1996239	3024509	3373329
EIC	Negative	559.4716	6.47	FAHFA_559.472635	41032510	50348298	49668699	61463355	52734342	40329612	50976624	50027661	70087557	56875709	43680081	49238649	50771921	42528403	43455701	52571024	52975365	65580414	45727432
EIC	Negative	563.5049	6.65	FAHFA_563.503935	431548	784583	1301943	1509593	1053029	1159390	1154639	1293432	1750446	3737555	597523	833328	4121735	780299	512477	1026099	886230	905020	583137
EIC	Negative	563.5048	6.55	FAHFA_563.503935	7407676	6651239	9529378	10826528	10132700	6314883	11101477	9853144	12991891	8238243	20056592	13422782	25674191	12498565	12365450	12413109	15129949	22940103	10340876
EIC	Negative	581.4579	6.41	FAHFA_581.456985	1484208	2619907	4246049	6677966	4119208	2411683	5194352	4796085	6315357	2105610	1976146	4191010	3507951	1459217	1052427	3176067	3117396	3682277	1374520
EIC	Negative	583.4726	6.46	FAHFA_583.472635	2463625	3803153	2281561	5603873	4358645	3333092	4613225	3762936	5208319	3335669	3504930	4127379	4177896	3191943	3274958	4480807	4342154	3707727	3590445
EIC	Negative	587.5083	6.84	FAHFA_587.503935	95017	94614	59194	74095	84711	62697	51805	44766	354664	35813	68807	73281	87691	62514	79633	84335	238089	80406	66056
EIC	Negative	589.5218	6.57	FAHFA_589.519585	1521514	2151945	2052888	3926272	2398655	2952980	2966923	3987116	3536102	1689063	4104044	3005855	2829055	1848439	2325312	3955778	2614369	4678196	2295317
EIC	Negative	593.5530	6.71	FAHFA_593.550885	191490	386715	343781	516015	425962	299724	486250	416041	385223	91478	308920	364027	304265	280377	205951	334626	290869	326187	203447
EIC	Negative	603.4430	6.37	FAHFA_603.441335	298415	41626	407401	125925	49428	0	136693	65580	221597	124101	59088	75083	52244	0	123910	162596	135959	119929	
EIC	Negative	607.4730	6.64	FAHFA_607.472635	30935076	33399766	1476807	39029194	32408575	23624528	36103507	29308851	33218461	16356160	27480407	29955877	35515719	20215258	19746415	32567700	31083886	24077173	28365746
EIC	Negative	619.5682	6.44	FAHFA_619.566535	749063	805070	1083774	1471349	1410092	1083774	1100432	1320474	1193292	1135888	2646068	1276311	964885	1072160	1629012	1724097	1108266	22077136	681024
EIC	Negative	631.4727	6.44	FAHFA_631.472635	2842897	5503640	2319215	8121231	4453821	2613036	3436910	4566163	6538985	2317104	2809748	2468181	5091809	1574338	1705640	4903486	3066673	2855624	2463544
EIC	Negative	277.2174	6.29	GAMMA-LINOLENATE [M-]	259445398	334155311	491897270	678757171	48646456	29268918	386815542	479804996	563340058	312079828	239928283	281701676	428415830	232686808	167898290	306540235	377969995	406482534	245664416
EIC	Negative	337.2327	6.29	GAMMA-LINOLENATE [M-]	0	547758	0	0	0	58734	0	881101	961291	0	434250	0	592705	441030	0	522010	765232	0	0
fpHILIC	Negative	195.0510	3.11	GLUCONATE	21164068	17612336	12994808	16134800	25703544	34287940	28567742	14126324	29128876	15589673	21883266	25153206	19660160	20165750	22397164	24640004	23256956	12348842	17327818
fpHILIC	Negative	259.0231	4.35	GLUCOSE 6-PHOSPHATE	504939	224863	108276	236685	235381	481234	174557	154529	304693	177435	143146	284670	206700	241928	181199	512457	365611	283296	322143
fpHILIC	Negative	193.0351	3.92	GLUCURONATE	2035132	1500301	1334746	1690109	1684470	2293761	1287790	1174372	1678493	1597437	1058221	1594653	1191904	1270611	1491711	1929126	1475601	1855687	1786952
fpHILIC	Negative	229.0117	3.90	GLUCURONATE [M-CI]	3052424	1411931	1890019	1716775	1975485	2467613	1964698	1231983	1604188	896641	887682	1002781	2278989	1910830	395260	846986	3774681	1083310	708185
fpHILIC	Positive	130.0498	3.47	GLUTAMINE[M-H2O+H]	135620608	99550528	117003168	117488536	98255928	103656328	96699312	98774168	16264952	106611888	106944576	9376324	93868256	84208352	113740040	90700560	99826344	107863928	92925176
fpHILIC	Negative	145.0619	3.47	GLUTAMINE	175012512	115482760	145489840	126490824	106152768	113358816	110111424	109731248	100659616	124580016	110586216	111500136	110135104	87360104	140132304	104944240	107288560	137916528	79366040
fpHILIC	Positive	147.0763	3.47	GLUTAMINE	524928832	393783168	470730008	465122080	395777184	410887680	394788320	382990272	429661632	419904472	424219168	392478816	386596320	348605344	447007688	367112576	447433376	434528896	373632832
fpHILIC	Negative	127.0513	3.47	GLUTAMINE [M-H2O+H]	5399490	3609923	4122449	4140890	3356536	3525554	3405654	3579921	3049477	3871420	3565726	3483246	3405531	2703501	4443388	3219687	3619082	4027338	2407960
fpHILIC	Negative	167.0442	3.47	GLUTAMINE [M+Na-2H]	1438585	1256255	1405155	1286944	1179280	1199714	1309834	1188582	1168504	1347333	1167121	1210429	1191924	1034656	1532426	1232476	1233553	1355284	921714
fpHILIC	Positive	169.0581	3.45	GLUTAMINE[M+Na]	10063963	10013392	12825250	12456639	11412187	11650433	11092460	12818326	10502452	11655612	12209981	11606783	11109990	10248242	11837445	11476983	10992460	12293636	7957108
EIC	Negative	448.3079	2.97	Glycochenodeoxycholi	1052932	103950	103205	472139	23652	0	84146	611602	33783	6079248	108149	64892	401875	0	0	0	0	66065	14262
EIC	Negative	464.3024	2.13	GLYCCHOLATE [M-H]	13292092	805388	52118404	18816324	1193151	1020663	1055534	37266458	2197983	6079248	108149	64892	401875	773353	200504	62248	388789	11709119	336516
EIC	Negative	448.3081	2.09	Glycosodeoxycholic	859183	79394	1975707	871635	987805	83078	118191	1897538	124144	0	0	0	0	0	0	0	0	0	0
EIC	Negative	309.2799	6.64	Gondolic Acid [M-H]	13345937	23594155	25508340	36772030	349789594	26221225	30794298	30884730	34412069	26623116	27129561	52549012	36397494	29732540	27473345	50993991	36492277	42637035	27101759
EIC	Negative	369.3010	6.64	Gondolic Acid [M-H+Ac	377966	504170	350250	685591	492408	624594	595280	761126	640961	526063	407551	532420	443310	539629	468592	725358	568109	528691	708990
fpHILIC	Positive	118.0612	3.65	GUANIDINOACETATE	19563672	8084588	15277096	29573390	7837655	14806788	9242879	2161600	18005528	8971783	9524854	8751040	6561233	9395342	9028141	10539670	25728484	9076654	666666
EIC	Negative	267.2332	6.50	HEPTADECANOIC ACID	5612460	6618146	9586990	11463829	8495894	7597134	10206950	13275517	13147013	7993157	9203369	10734016	12312832	10532607	8985185	12926012	12443561	13040542	8591502
EIC	Negative	269.2488	6.58	HEPTADECANOATE [M-]	5976396	5951186	5753221	8181426	8428891	6793088	8656190	8844424	13030570	8903976	8937029	8053889	110108695	11299862	7758679	12025890	12237307	19824412	11631162
fpHILIC	Positive	156.0766	3.32	HISTIDINE	167834416	82345752	167047376	113778480	58880908	74912208	67887792	97924728	59043308	141947648	84814224	95998940	76073120	91765128	119627408	75880568	71227472	143647840	92484800
fpHILIC	Positive	178.0533	3.41	HISTIDINE[M+Na]	2211689	2052228	3990285	2623440	2050784	1840138	1695165	2086813	3588623	2281382	2269062	1832663	3012580	21067375	1619538	1866584	2029244	3066691	2714810
EIC	Negative	267.0462	0.57	HOMOCYSTEINE [M-H]	49561	48608	139705	368897	99190	64124	109830	128000	677510	251785	90062	103822	231868	16147	54498	245947	87308	164586	48122
EIC	Negative	335.2231	3.94	HXK3 [M-H]	367595	282910	206013	713880	244162	302185	245909	420049	1417039	188934	199163	390488	848331	674479	241887	559702	1473750	948048	639912
fpHILIC	Negative	108.0125	3.39	HYPOTAURINE	2147646	744667	1075875	1603066	694960	2030282	447721	1473318	299650	1247462	303925	796184	324125	388616	224971	1081192	175012	1356274	1029079
fpHILIC	Positive	110.0273	3.38																				

EIC	Negative	269.2125	4.75	Novel EIC_1	1291290	1234596	2067090	1857813	1985678	1589034	1848629	2322468	2345999	1366703	1129953	1314313	1333454	1374252	1084035	1828301	1297793	1645224	1353187
EIC	Negative	345.2438	4.94	Novel EIC_13;Novel EIC	371544	197414	176989	704750	178427	240874	186492	275767	906272	209630	145543	311177	620743	322658	230608	379604	813626	611084	257145
EIC	Negative	345.2435	5.29	Novel EIC_14;Novel EIC	548980	113311	127789	955570	117573	127000	181522	277789	479592	121618	106081	342845	413020	171075	240350	276246	572502	686051	230942
EIC	Negative	347.2595	5.22	Novel EIC_23	232017	62335	149776	184975	77674	93585	82179	141122	125091	196414	79551	148194	109084	39709	84805	187400	174882	159312	109184
EIC	Negative	347.2594	5.60	Novel EIC_24;Novel EIC	460451	202150	172781	1097916	254289	323128	240676	437815	943785	186183	178330	586068	816027	460585	327151	451750	1235621	1166548	374008
EIC	Negative	365.2694	5.67	Novel EIC_33	404818	214271	420429	367242	246161	186780	263095	321122	233187	345389	189944	181237	188451	157162	239517	234308	176039	305574	180932
EIC	Negative	295.1541	5.18	Novel EIC_4	213562	168075	0	357414	267998	0	288191	280447	0	0	202867	0	212066	259846	0	0	187376	187115	0
EIC	Negative	295.1588	5.18	Novel EIC_4	224982	185609	295589	442528	284477	234441	321056	315431	338980	212707	204841	224929	313688	155859	147271	184679	229434	315427	172292
EIC	Negative	309.1710	2.73	Novel EIC_6	2801515	3941745	1932157	2478474	3291824	3155036	3580132	2759325	3185264	3308664	3851194	3413713	4055231	3443620	4128913	2871559	3869595	3956003	4165219
EIC	Negative	325.2371	4.92	Novel EIC_9	278205	127213	371415	374752	190353	144152	166749	351869	126609	301364	148418	179422	177794	166996	142326	178112	211806	498298	123790
fpHLIC	Positive	204.1226	2.32	O-ACETYL CARNITINE	252386896	289114848	337102784	504985258	291623424	369159808	385057824	324496576	625402816	304302816	401348608	391777440	434942464	168504864	198548672	523925248	267362464	338750656	230938064
fpHLIC	Positive	202.1086	2.31	O-ACETYL CARNITINE	296554	323650	353225	509159	296454	349652	393416	367303	595019	331915	418960	413682	472251	198048	232442	499507	271154	363682	220963
EIC	Negative	384.3127	6.36	Oleoyl Ethanolamide [M-H]	3255840	2913322	2436172	3994120	3300164	3542223	3513855	3344328	2379535	1995769	2316541	2505368	2372227	1492576	2023407	2258012	2047602	2328169	1612335
EIC	Negative	355.2853	6.39	OLEOYL-GLYCEROL [M-H]	937275	683770	1220901	986196	335144	306059	153402	141159	0	484771	80254	403895	459765	200380	200679	425228	392000	710840	209625
EIC	Negative	415.3060	6.44	OLEOYL-GLYCEROL [M-H]	45278836	27232203	8769027	21627335	17309883	26429824	28771337	25698067	13492916	21996242	29327089	15208911	19861602	29931830	30916522	10037265	26329033	14399644	17030251
fpHLIC	Negative	145.0141	3.88	OXOGLUTARATE	1598343	1213601	1875250	2581616	944016	1407106	1347403	2246129	904006	2507589	1227150	171747	900463	1991018	2082764	754681	1224245	2067082	1229374
fpHLIC	Positive	176.0690	3.50	P-OCTOPAMINE(M+Na)	2216851	1155050	2046980	3253482	36722249	3130153	2668658	3618098	1026305	3848465	3978365	4024449	3934593	0	2982839	3759838	3990629	3053717	684946
fpHLIC	Negative	341.1091	3.53	PALATINOSE;SUCROSE	2391539	49419260	29723630	3460413	4510216	5428136	18158210	8550205	37537600	2343553	1545875	4043746	4998860	44063472	4079867	3333763	1159565	4607508	187939216
fpHLIC	Negative	377.0860	3.53	PALATINOSE(M+Cl);SUC	145414	1790201	1233869	251128	341053	488085	999855	404065	1403898	156745	139472	347326	483139	1398442	332628	232346	738638	301909	4360407
fpHLIC	Negative	363.0904	3.55	PALATINOSE(M+Na-2H)	75374	710722	619765	127855	154053	164232	466583	247988	150460	16745	127855	138063	161892	754228	134184	107009	314061	159604	0
fpHLIC	Positive	365.1048	3.53	PALATINOSE(M+Na);SUC	2589430	14167190	12673654	3409331	3750562	4091804	102730506	6903117	13452089	2373143	1666290	3791091	3891149	0	3798218	3190543	7905948	4469640	9856480
EIC	Negative	253.2170	6.42	PALMITOLEIC ACID [M-H+H]	145406976	152334531	303893616	329755900	250528675	173611384	313063040	284474688	339027817	194282115	146740383	198662525	236811715	123373036	125394296	202712497	224613497	236853067	109395604
EIC	Negative	313.2385	6.39	PALMITOLEATE [M-H+H]	37307512	17588604	36869444	29376092	24460200	18469254	1711714	1965191	2021416	25644950	14404268	1254815	13456887	11830691	682320	13913844	15027454	19157098	13006392
EIC	Negative	313.2386	6.52	Palmitoleic Acid [M-H+H]	941549	1112505	1313023	1857017	1779123	1653452	1678865	2819674	2618616	1820108	1479744	1472840	1473803	1822854	1277631	1600214	1590344	2946277	1365255
EIC	Negative	358.2962	6.24	Palmitoyl Ethanolamid	2907898	2082838	2409014	3136362	2624664	3436454	2616987	2866191	15025490	2272712	2649762	2554176	2018348	1591867	1942082	2130220	2260016	2405308	1939961
EIC	Negative	331.1919	2.41	PGAS [M-H]	7488365	5176897	9741816	6505689	2240233	2369159	3909225	2254822	1185794	5537973	4383962	6842155	4117065	5000011	5852902	4561861	4838942	4537788	4082024
EIC	Negative	391.2135	2.43	PGAS [M-H+Acetate]	1910363	1233439	2036905	1685753	559219	689205	984069	681275	519111	1136659	963560	1722210	1569279	1168605	1454926	1072904	1170708	1481619	1175442
EIC	Negative	353.2326	2.23	PGDI [M-H]	220087	104675	184486	236104	105140	215575	130647	181303	156377	199443	91344	122200	161670	186972	115342	134228	272914	295222	98999
EIC	Negative	351.2811	1.48	PGDI [M-H+Acetate]	884669	1359779	946410	282933	534848	658474	1096461	0	712584	387119	1148232	1341157	1357411	1196976	1310044	1743687	1364113	271618	1089511
EIC	Negative	411.2388	1.48	PGD2 [M-H+Acetate]	1095958	2042671	789835	783201	711296	951546	1384320	0	855863	360457	1406978	1729666	1710621	1514575	1682807	223767	1716306	293958	1316432
EIC	Negative	367.2128	2.37	PGG2 [M-H]	251774	91300	269945	150401	63264	87475	111811	134678	75979	169727	90914	118224	135777	98422	90026	134959	118891	66318	106685
fpHLIC	Negative	164.0716	2.06	PHENYLALANINE	85071552	47952824	61533752	36995976	34888080	51645988	39199472	32726562	40509432	51417020	41358944	47102824	39774052	57090140	65162700	44499320	35708948	52378744	46773232
fpHLIC	Positive	166.0859	2.06	PHENYLALANINE	483868864	276771392	378964288	2463966176	225403120	283886752	243844768	237151472	260669648	317115232	267492752	285804192	233358352	374641152	409788192	290270880	211712800	341046816	270318464
fpHLIC	Negative	210.0284	3.97	PHOSPHOCREATINE	1096835	290313	239993	427946	288192	576263	439691	350858	369557	310137	348611	495988	351163	402097	330438	635983	432423	590768	380772
fpHLIC	Positive	212.0427	3.97	PHOSPHOCREATINE	2115027	803229	483350	994406	761085	1499832	1040752	759217	870967	646650	822870	1172110	832951	982397	774445	1490461	1028219	1364658	927255
fpHLIC	Positive	130.0863	2.71	PIPECOLATE	12485032	14812108	9729421	16489753	14302058	18409794	13865738	7896523	12165471	8890542	14140082	12525613	15618387	7732377	12165973	17617362	13564453	9852160	9265333
fpHLIC	Negative	114.0560	2.79	PROLINE	16625191	16468868	12510500	6168700	7480513	11201414	6004681	6682575	9525250	9375107	16655019	6822012	16774652	27086158	8479343	8111995	1212195	13982244	9265333
fpHLIC	Positive	116.0707	2.79	PROLINE	873386112	791868224	752803968	549392568	609956184	775746624	528468352	575783680	538934800	637772864	673619456	559630236	8234745280	1015801984	607444232	588987762	725147488	769967488	9265333
fpHLIC	Positive	160.0341	2.79	PROLINE(M+2Na-H)	1085123	1182008	1125899	956178	686697	805188	492526	63082	541400	861602	797780	898152	733006	1384994	1358610	856477	771182	1173358	1138538
fpHLIC	Positive	138.0521	2.79	PROLINE(M+Na)	1722691	2145443	2101572	1371169	1518684	1711814	1017405	1338748	1175473	1844835	1890256	2100958	1334042	2822664	2436060	1420410	1579286	1913806	2109335
fpHLIC	Positive	151.0866	0.98	PYRIDOXAMINE[M-H+2C]	632753	607725	276421	203146	899055	992000	567797	30164	0	46020	32503	0	0	43319	462082	0	46065	0	0
fpHLIC	Negative	104.0354	3.62	SERINE	37373420	21773034	26605544	23226048	13815662	14502344	12576777	16295856	13025245	23399998	18482700	21213318	20555774	18819268	30305386	23516894	17125850	30442232	15207836
fpHLIC	Positive	106.0501	3.61	SERINE	189593626	15950545	15708095	11685174	10542176	127937495	9379645	112737379	9379645	16083645	14856634	154531513	15046096	16322972	23937090	17707608	14837737	14561895	15038502
fpHLIC	Positive	88.0398	3.61	SERINE(M+2Na-H)	524336	512821	495055	401543	266442	368662	351177	297888	349804	423298	396457	413337	407715	454470	682642	471354	347926	432837	424585
fpHLIC	Positive	150.0134	3.62	SERINE(M+2Na-H)	481058	508272	612491	614079	599608	438510	464714	695908	416534	708712	681953	570692	624607	491290	642456	625602	5		



fpHILIC	Positive	118.0862	2.70	VALINE	189461264	226060384	198742560	151577840	173969760	235383408	196479616	146329952	158744288	182998896	246969584	242085520	209265616	310406752	333916032	209335728	184898144	178683760	248191360
fpHILIC	Negative	152.0484	2.71	VALINE (M+Cl)	291197	411555	425810	318034	364498	436629	401274	370351	343034	403326	459022	432626	394596	545982	603897	313273	430525	306001	479412
EIC	Negative	299.1348	1.14	unknown	44817	24121	30517	20623	73496	45322	55743	53792	56405	53842	87820	32767	37656	68449	43605	43338	37573	37503	48431
EIC	Negative	298.2834	6.67	unknown	310342	411479	365462	689813	619642	643453	617651	710669	856333	685383	512170	702710	635797	581158	468894	627413	639032	697075	708500
EIC	Negative	297.1847	1.03	unknown	87124	56778	77038	56965	163798	128783	131215	117848	140897	112032	156592	85086	87795	139771	113751	107190	87570	101410	109547
EIC	Negative	357.1557	0.90	unknown	567901	389588	488026	377744	937670	851545	886401	739437	924738	589158	778447	613416	519264	845386	722030	171758	552978	602861	792702
EIC	Negative	439.3378	6.79	unknown	550877	963413	698823	885118	975374	1438666	1130949	1341690	1233746	816359	584061	659079	795904	612891	614414	749354	653043	105906	1149428
EIC	Negative	434.3358	5.79	unknown	445626	695775	708697	492492	1244558	1098772	1241566	1112405	1155192	438682	808239	513443	332272	986310	898089	835259	1090498	1521321	872584
EIC	Negative	358.1596	0.90	unknown	104960	73868	93951	75297	184849	135509	170960	133234	175611	113593	151734	112555	100384	163742	141380	135191	111527	123733	149121
EIC	Negative	433.3328	5.79	unknown	1583630	2326125	2336340	1781906	4214336	3577431	4115998	3929269	3979814	1456982	2691434	1802762	1206482	3491957	2998686	2943842	3550478	4960632	2894699
EIC	Negative	253.1235	3.23	unknown	242207	276492	241764	314555	330613	358311	371491	408318	381550	394232	229109	259075	266084	264442	289546	297060	293337	335669	343861
EIC	Negative	449.1739	3.46	unknown	269602	112711	130500	109947	386293	282496	308589	243479	264330	213506	286817	201133	162221	344813	242804	238747	160800	249357	339472
EIC	Negative	450.1772	3.29	unknown	167144	93168	95123	76036	307049	214250	236930	187912	215815	133581	187466	139167	118741	244907	174667	188585	128997	196649	253251
EIC	Negative	297.1349	0.92	unknown	348958	235376	290142	212882	829628	678397	681519	449399	736623	499535	814729	364594	415116	711425	438497	509354	403444	504860	625722
EIC	Negative	440.3828	6.79	unknown	218040	291600	216367	267094	292259	422296	347018	411531	407552	264878	187150	198071	266865	245503	322983	225615	208647	352255	355173
EIC	Negative	425.2560	1.21	unknown	50388	93664	52623	74391	177441	275554	164419	215629	241329	49650	57165	62713	56595	61136	137012	90857	142916	144529	130288
EIC	Negative	367.9042	3.33	unknown	0	0	0	0	145138	96728	87924	99760	55476	0	0	0	10600	76726	43883	73214	101221	67029	
EIC	Negative	451.1724	3.29	unknown	272552	134292	148730	128648	414553	309816	320498	242597	299713	208223	281714	205837	176643	340106	241360	266369	169547	268021	330357
EIC	Negative	297.2797	6.67	unknown	1425990	2063365	1742492	3427826	2995072	2976513	2919126	3338736	3985260	3211956	2329386	3555199	2913269	2758294	2203087	2930341	3121178	3551428	3119455
EIC	Negative	449.1741	3.35	unknown	316616	121778	201866	161645	367607	465631	347716	461162	620203	453514	267100	238831	337726	262617	372274	337726	262617	426587	564712
EIC	Negative	370.8956	3.33	unknown	60682	29876	48972	18117	397943	254767	230331	265439	139058	25194	34459	18165	19835	43429	207508	105210	183621	240087	175983
EIC	Negative	487.2727	1.20	unknown	24073	56248	28341	42926	103249	159730	113802	59661	33737	30812	39372	38250	28741	40610	84435	63320	78635	74717	74852
EIC	Negative	451.1724	3.15	unknown	158511	74953	97449	81987	244783	175414	176914	140669	175522	118427	170737	136486	116173	237508	136407	173422	123025	158495	236070
EIC	Negative	258.9080	0.58	unknown	5360	26315	0	39183	47204	79182	103269	140091	111125	69678	102611	107574	107969	46479	84514	86125	109646	125073	65630
EIC	Negative	369.9016	3.33	unknown	0	0	0	0	157307	102152	86210	107800	52969	17664	10438	0	8885	11283	86233	30100	75974	88287	69482
fpHILIC	Positive	117.1021	2.66	unknown	78003	0	0	0	1464803	1701790	1142943	828640	625021	0	36457	0	57283	0	893334	865980	1234075	621188	1172382
EIC	Negative	474.2210	3.46	unknown	547207	293078	277763	194629	1013486	750924	724637	531614	67824	408825	709475	462981	371255	846730	572806	653689	424882	532219	801572
EIC	Negative	368.8983	3.33	unknown	161663	83352	157363	42474	1410181	697532	655745	733733	380168	78788	86445	77749	75887	82450	612661	333974	536727	685926	482111
EIC	Negative	366.9008	3.33	unknown	154426	85258	134751	49793	1151960	725300	644409	737878	385469	87366	88266	76755	68922	88305	603531	288513	515394	668832	513205
EIC	Negative	449.1738	3.29	unknown	746965	349250	405718	314595	1098012	857868	908396	845494	546828	730880	572597	460762	936447	672305	716809	499251	743400	933182	
EIC	Negative	643.4252	2.78	unknown	264464	396317	337658	388153	1432100	757724	1253936	1379386	1049419	114791	235705	164848	90405	1293461	67429	1094874	328165	1937919	895743
EIC	Negative	473.2178	3.46	unknown	1856939	978686	989293	658275	3562719	2465774	2543202	1773437	2327480	1436736	2531519	1592096	1334003	3017065	2000820	2162635	1333114	1852770	2718015
EIC	Negative	282.2520	6.66	unknown	3610920	4580718	6244073	8259298	5879463	7125767	6948838	7849973	10411226	5730108	5470785	6741416	9498906	6676482	5779968	7885359	7387244	7780951	5562788
EIC	Negative	450.1774	3.15	unknown	106602	70568	61238	46565	184381	133308	135579	98918	131020	86159	130027	105076	84128	162981	105580	138534	76197	117369	153482
fpHILIC	Negative	242.0864	1.03	unknown	965303	877885	810327	1086155	1203151	1066996	1037232	933433	1189144	941746	819817	765896	908262	666869	734063	886794	929692	819743	494187
EIC	Negative	349.3287	2.79	unknown	2352812	2789278	2260139	2035511	8227691	4215752	6623272	8401478	7913402	2608838	3769332	1129607	4492956	7292433	3779759	7541147	2307727	993283	4310180
EIC	Negative	473.2178	3.41	unknown	2573063	1297341	1372053	905324	4703404	3358135	3255297	2298853	2911043	1682169	3050796	1962863	1718233	3822745	2571406	2843149	1807246	2215280	3679960
EIC	Negative	402.3054	2.67	unknown	1019253	420462	352327	363331	1063520	533036	527293	349740	536030	67907	539862	152076	355053	402390	310011	440051	928499	789036	320254
EIC	Negative	474.2212	3.15	unknown	785033	499957	446404	389002	1523194	1150196	1099806	803542	1112706	632534	1054257	798183	666300	1339064	863764	1120797	678246	841930	1494104
EIC	Negative	379.2129	0.84	unknown	25373	28410	31046	28000	99320	68929	78864	107409	59579	20159	26117	27624	22372	21233	61933	49945	34876	102469	43070
EIC	Negative	529.2768	4.82	unknown	412812	408709	345031	312278	412812	408709	345031	312278	412812	408709	345031	312278	412812	408709	553046	553697	514063	406346	774206
EIC	Negative	343.1702	4.42	unknown	368154	514061	352962	359527	609837	591275	628083	668466	553007	411374	414353	405284	415034	379958	486134	507891	474016	529662	607120
EIC	Negative	474.2210	3.41	unknown	716368	368775	387105	249750	1373996	941044	950213	647287	853829	499045	841922	586326	4109544	1090544	736256	813710	529018	630244	1023449
EIC	Negative	330.3048	4.48	unknown	57791	142073	121484	73692	187560	318421	183406	236229	196355	49742	0	64731	51415	49381	229794	134169	48279	298881	154312
EIC	Negative	450.2424	2.79	unknown	499455	673848	601951	503115	1863994	976283	1561568	2001440	614147	901925	246418	999071	1689800	865918	1774411	532381	2415531	974702	
EIC	Negative	295.1539	2.93	unknown	195202	193508	205488	791717	473012	276204	397830	513182	962023	361955	219404	323919	432851	129065	140337	369898	79680	504098	128634
EIC	Negative	412.3521	6.71	unknown	411204	589261	435756	556876	671937	686679	868292	822134	584899	481199	408973	552098	914210	545853	524939	551211	568791	727114	
EIC	Negative	473.2178	3.35	unknown	2251903	1513364	1010576	864201	6111656	4341282	4078255	2940219	4089386	1189504	3360721	2130367	1946661	4261489	3349682	3258445	2043142	3051688	4120821
EIC	Negative	474.2210	3.35	unknown	643164	426915	312084	244652	1775937	1268113	1173336	890421	1181005	382219	938552	647712	555899	118899					

fpHILIC	Negative	241.0831	1.03	unknown	8425455	7002569	7247959	9926228	10845545	10312342	8634412	7633372	10515620	8486437	6307129	6600940	8477054	6235940	6150014	7145732	8450771	7575480	4495982
EIC	Negative	433.3171	4.74	unknown	202846	172810	186476	267517	286396	317776	221647	356761	311816	269064	137607	136977	185150	180664	215987	192642	156712	164801	293516
EIC	Negative	492.3423	3.24	unknown	84188	123837	80590	68268	192458	182427	159709	73615	11547	125925	116996	174343	206127	167612	136759	89503	118591		
EIC	Negative	482.3155	6.22	unknown	566266	809099	572451	699062	858316	862047	685992	856833	856432	497044	542559	515026	442908	606805	446620	397699	575975	598326	629148
fpHILIC	Negative	345.1542	0.47	unknown	767033	360526	676315	173951	10719394	852738	797951	674015	1047348	468039	690017	767909	494901	253173	638728	1030785	596763	544030	305064
EIC	Negative	270.2159	4.30	unknown	175940	127574	193564	197656	211424	171646	270452	226357	207090	172483	138674	127778	155847	151571	116532	235805	178840	200675	127185
EIC	Negative	475.2680	1.71	unknown	296710	243281	218559	67808	672139	255158	699001	555917	380624	75193	25087	27517	31395	87021	65871	79671	32686	101521	79226
EIC	Negative	433.3180	4.84	unknown	289675	241572	218503	315583	396379	491428	281658	365171	503551	331381	206726	245272	250350	336408	334823	336824	188956	188331	503880
EIC	Negative	432.4205	7.14	unknown	49751	68370	40295	58438	86827	76182	68324	67887	112808	82000	37133	86030	49540	54189	61656	67564	60138	67804	44296
EIC	Negative	483.3076	2.67	unknown	136851	0	0	0	214813	113059	92150	38963	86200	37524	106407	19965	94439	107186	55104	64863	150708	131704	55406
EIC	Negative	300.2626	5.44	unknown	336724	322810	302587	380004	493376	488936	375269	360170	340711	210389	231933	212588	277788	311257	292809	438972	239624	349225	301042
EIC	Negative	424.2436	0.85	unknown	94844	149349	97368	84753	208103	225240	128096	127835	110657	109725	133684	56458	204438	105213	120107	200912	98030	184210	77609
EIC	Negative	491.3381	3.24	unknown	291777	392944	233596	209463	610650	572800	461014	427331	784138	249865	338896	399032	411189	557609	628879	515759	422834	286304	382361
EIC	Negative	269.0877	2.27	unknown	33158	64956	0	80796	274575	381001	316866	134223	237863	98224	18081	63587	61210	64798	99545	194130	243869	119093	259632
fpHILIC	Positive	175.0221	2.48	unknown	357879	270611	251745	57399	490923	618274	324501	188993	430198	212688	0	0	353164	698802	0	0	503581	63410	0
EIC	Negative	558.4613	6.67	unknown	2062532	1886065	2013027	2140354	2698981	2732807	3134347	3426294	2148027	2616862	2112174	1978836	1938538	1955448	2354703	2547882	2030488	2261232	3530302
EIC	Negative	628.5624	6.59	unknown	169442	138633	165467	229334	251710	215411	329529	308321	555539	335377	155105	55941	206884	542306	229849	327722	277318	224667	351575
fpHILIC	Negative	304.1041	2.30	unknown	486130	461344	453857	400951	740913	716280	606711	413745	398824	598653	500989	380588	716390	605336	688154	465581	700713	352032	0
fpHILIC	Positive	508.3765	0.58	unknown	928887	1196932	954278	1169703	1294071	1308563	1262092	917124	1262240	1055219	1318057	1215010	1283151	706131	1120238	1037529	1068480	1040042	1077527
EIC	Negative	474.2212	3.00	unknown	552608	560428	376639	523124	927203	968522	932238	698754	1007387	867261	596125	525776	624797	884287	747825	790406	751944	791781	1071917
EIC	Negative	641.5725	6.55	unknown	0	1095154	1291131	2106608	2141553	1913819	1821906	2141897	3613518	3022172	0	0	4588105	0	0	3342823	3607571	0	0
EIC	Negative	295.2643	6.60	unknown	2987501	3492194	4121720	6518134	4730565	4146649	4795468	4579134	4030901	5105181	5721077	4237567	3548520	6375736	6265473	6456755	4716108		
EIC	Negative	627.5574	6.58	unknown	309166	233770	265227	488885	572264	543540	508904	732397	1379179	509596	377633	273267	377626	701705	378748	558843	530187	453959	855383
EIC	Negative	604.2968	2.20	unknown	0	0	0	43512	145191	146300	240772	0	186874	0	0	151179	125469	109404	143719	185107	0	218019	
EIC	Negative	269.1403	2.11	unknown	166134	174418	195229	251024	233498	322352	361755	345889	257787	302094	153676	150881	160607	160267	179325	203411	251981	374300	245242
EIC	Negative	325.1127	0.71	unknown	0	0	0	0	68980	95478	100126	215581	39119	0	0	0	0	70210	46879	54975	196416	48205	
EIC	Negative	335.2233	1.54	unknown	0	56780	150681	0	161422	402296	162853	319210	182117	0	31518	9181	10891	52269	53834	60470	129262	463887	99268
EIC	Negative	441.2527	1.11	unknown	13932	41514	0	13635	77312	179544	75078	26298	72526	0	13096	5492	0	5321	27676	0	22261	24657	31940
EIC	Negative	494.2167	0.76	unknown	374463	293295	556235	353659	421253	400170	747151	643561	392021	522007	455344	339280	179454	183460	379550	312485	423438	205235	231100
EIC	Negative	283.1011	2.74	unknown	126697	96501	65478	92530	381987	656597	489643	217639	368018	201703	98475	93520	96670	93848	154794	283683	387021	118978	377802
fpHILIC	Positive	142.9384	4.50	unknown	249947	351580	414680	393764	378965	440944	437981	446667	417017	580184	477743	429752	415380	445692	434094	411831	392614	436897	377389
EIC	Negative	327.1632	3.41	unknown	151913	190031	171732	546611	743898	1174654	933099	638516	680985	523772	218943	219148	205356	237410	312151	581964	716120	771526	763405
EIC	Negative	308.2679	6.57	unknown	4154468	4764432	4910728	6355316	6326979	5202188	6933265	7105234	9292802	5656531	6851932	7854383	7077267	6009453	4962911	5087147	6536977	10823704	6553695
EIC	Negative	394.2685	1.71	unknown	583477	298802	412156	89670	918299	273275	926273	850986	551230	174551	42323	36681	40223	92825	95009	70084	57505	288593	77037
EIC	Negative	454.2903	1.71	unknown	844799	431736	642988	108243	1285799	395837	1322530	1218921	824577	189976	65556	64725	61094	153027	105716	100378	83421	368104	105669
fpHILIC	Positive	836.6094	0.43	unknown	2315147	2387643	1681636	2049399	3098427	2897617	2744378	2266204	2734689	1862664	2242515	2459309	2302543	2461317	2311593	2926059	2680374	2128861	2301167
fpHILIC	Positive	155.0096	2.73	unknown	624238	639966	668769	1120430	667519	926390	1183410	1176315	489590	690866	1382887	675647	166200	609686	609686	1382887	675647	764022	592268
EIC	Negative	301.1804	3.58	unknown	276996	235247	632923	791845	442841	283730	690980	674380	891921	738497	340948	252579	223377	166200	334305	377963	539331	231932	156440
EIC	Negative	433.3175	4.60	unknown	407366	298837	321092	437642	477383	550790	406265	563737	478055	260456	346920	385668	464856	457351	625701	278466	185641	591144	0
EIC	Negative	401.3024	2.67	unknown	4441873	1744123	1374558	1560241	4505651	2294653	2281833	1238885	2026616	1968668	2329544	633089	2318878	1764560	1294854	1877168	3916607	3235268	1391951
fpHILIC	Negative	117.0710	0.54	unknown	801822	266786	961311	1156444	2224838	437311	1875210	822605	2554967	1589877	0	168753	172993	0	0	357443	149887	1223831	0
fpHILIC	Positive	199.0890	3.71	unknown	797912	807854	878428	866408	975426	1004134	1015300	856329	893302	889172	907359	954199	832160	786218	967897	932738	852754	819563	818732
fpHILIC	Negative	133.9917	0.88	unknown	500513	1174177	1773910	2740799	2607836	2487714	2442811	2291897	3130496	3513646	2015935	3857520	1174558	2529063	712339	1570771	2111169	1483313	2626527
EIC	Negative	324.1432	3.43	unknown	95467	98589	122803	187157	158483	117073	138066	171112	207690	174896	125309	187188	160146	70247	68534	134422	128069	168892	84609
EIC	Negative	449.3279	3.34	unknown	2150111	3707054	2038289	1641058	4901364	474010	4847195	3478544	4973871	1361162	2833382	2231553	2455168	1934439	4145682	4973871	4405302	2976159	3761762
EIC	Negative	509.7611	6.23	unknown	0	31086	59416	0	82811	112384	160704	422613	218372	154722	179028	127042	123046	80170	90756	102378	135456	196692	174351
fpHILIC	Negative	105.0442	0.96	unknown	137208	174336	312738	578133	392428	331084	295527	348384	862507	778826	647196	328613	314792	259329	363132	464983	195917	334149	176725
EIC	Negative	393.2656	1.71	unknown	2297125	1225465	1472910	314042	410311	1135632	3626913	3363471	1800788	491225	143395	152639	125289	461394	354356	225968	220793	637327	292928
EIC	Negative	403.3059	6.51	unknown	386808	244100	431918	762600	527304	550551	475663	778013	889756	547128	164850	445663	533568	703827	609139	638085	582028	633021	738608
EIC	Negative	379.2130	0.97	unknown	74069	63029</																	

EIC	Negative	425.3637	6.58	unknown	1275780	1077950	1162607	1646768	1592219	1121332	1516492	1659036	2316612	1561913	1236298	873332	1330456	758872	965636	1303202	928093	955526	920480	
EIC	Negative	461.1948	3.11	unknown	82132	63323	31860	62614	96075	67603	75032	82009	82312	71787	76983	70184	57545	86915	77360	110321	61258	52287	79840	
EIC	Negative	511.9545	2.67	unknown	115475	108936	105643	105643	191136	109959	169961	187212	124201	104864	130734	70900	92013	134392	146729	141786	104552	152033	118377	
fpHILIC	Negative	273.0771	1.15	unknown	174274	169661	144707	246754	408552	280902	311596	189004	364129	298929	181428	265964	610145	248045	128009	240729	262606	159234	201021	
EIC	Negative	459.2725	3.01	unknown	650266	371070	625867	0	1790543	239848	1507431	360508	403208	202440	97408	95082	109851	153032	130424	128949	120156	311510	152410	
EIC	Negative	378.2739	2.27	unknown	441847	1041275	1287756	489356	4236674	1189404	3421125	3571150	843220	206900	38679	161045	0	0	230783	0	0	482720	601562	
EIC	Negative	377.2703	2.27	unknown	5516179	4147737	5126436	1971411	16282239	4607660	13720251	14385437	3349279	117366	552622	602455	579021	252835	826064	761694	470905	1786652	2122685	
EIC	Negative	393.1729	5.49	unknown	231889	174488	205036	289954	311296	405674	261556	262322	348285	244692	186213	193759	155124	196384	182655	355000	281517	342350	296667	
EIC	Negative	524.3312	2.24	unknown	0	34805	0	0	117957	22211	92473	96534	47503	35567	25075	31902	15983	33208	40833	70237	26330	143052	56452	
EIC	Negative	439.2975	2.27	unknown	237897	162894	264522	43224	526670	150525	428053	467921	134105	0	17449	24444	26296	7767	32304	27354	16485	59747	78746	
EIC	Negative	460.2768	3.28	unknown	134705	145970	250878	104268	454605	74013	675833	382584	427502	0	0	0	0	0	0	0	13559	0	72754	
EIC	Negative	437.2912	2.12	unknown	1056065	1179731	908504	480016	4772489	1017231	6576887	3617362	2729694	733001	268965	176858	245568	164325	0	272861	372935	382360	827751	520380
EIC	Negative	616.3425	1.06	unknown	166068	37329	79596	18996	165025	131634	167133	159047	36583	7105	0	0	0	0	0	0	0	17624	0	
EIC	Negative	333.1115	0.90	unknown	193230	91536	168595	117481	257195	261076	233435	162690	285681	1286304	244953	170039	153775	400451	207965	212727	151449	192773	343879	
EIC	Negative	378.2738	2.12	unknown	407648	489959	384422	236256	1918773	389727	2588453	1521970	1048453	255005	0	49231	31412	0	0	0	44136	400942	46293	
EIC	Negative	423.2394	0.85	unknown	281939	576948	372661	327317	689786	735557	463499	517365	350694	356247	469579	169840	608727	462495	475530	673537	354878	621024	321001	
fpHILIC	Positive	244.1100	2.71	unknown	538522	658065	386262	427007	807816	695765	602195	609676	634492	339373	502102	621162	699021	761848	576926	582844	652210	582674	624372	
EIC	Negative	438.2946	2.27	unknown	969613	729595	954799	381947	2980136	844348	2412219	2670397	588541	205149	118822	126385	106862	49428	176249	135594	94519	340781	368710	
EIC	Negative	299.1880	3.71	unknown	233460	123363	210280	403653	276701	219218	230855	355843	518029	282135	169653	277543	263432	199236	170199	306545	222016	370054	154417	
EIC	Negative	297.1532	4.30	unknown	313605	228779	274437	623303	828272	1647339	807210	692792	846585	536538	298592	370297	270852	338482	405575	899330	806993	887343	681105	
fpHILIC	Negative	103.4001	0.96	unknown	34496960	29620530	43569808	90194496	65964784	36133388	53039560	47299372	133893896	51053232	98013040	55152924	61028868	37286716	51293472	97796840	24881346	51762516	26546764	
EIC	Negative	437.2910	2.27	unknown	3434961	2679597	3368096	1852587	10714078	3000278	8621206	9444734	2139348	730315	341175	370831	317191	188936	502721	505663	294163	1199254	1363498	
EIC	Negative	319.1908	1.26	unknown	26921	17947	36755	24887	110620	60296	92841	32194	21865	27658	18577	0	3686	7955	74393	23359	32725	26951	19394	
EIC	Negative	404.2162	1.74	unknown	147512	307158	135134	177117	309723	271347	326622	344718	268317	178161	318942	119709	263306	268980	247306	468194	275119	113393	320901	
EIC	Negative	459.2729	3.28	unknown	530144	534876	742371	353926	1572671	247430	2495508	1443844	1475116	0	50927	59464	62416	0	12460	102703	0	13723	258695	
EIC	Negative	467.2965	5.91	unknown	415473	640173	465909	556539	667334	737122	487187	604208	638104	403246	435816	450329	368390	509862	344620	361653	471581	399252	428319	
EIC	Negative	338.2361	2.15	unknown	408976	416985	327323	398993	448109	428363	493363	534452	450260	461281	430042	476644	442978	451881	437315	427947	460249	412867	453015	
EIC	Negative	534.3324	4.98	unknown	545001	669549	439117	691970	633155	647106	554516	628348	850366	515335	478150	625606	432531	776808	544046	483029	595321	503270	554821	
EIC	Negative	453.2864	1.71	unknown	2861503	1921251	1875061	525018	4569004	1447723	5825011	5446328	2843310	687724	185753	204636	226889	464566	444294	364728	288864	1231351	465877	
fpHILIC	Negative	131.0463	2.86	unknown	2307393	1695939	1891302	0	2607461	3900726	2099285	2130163	2485000	3057351	2151260	2479317	2164535	2270467	3683748	2629267	2793797	2114628	1413011	
fpHILIC	Positive	810.6008	0.43	unknown	32552266	38707156	30792644	34803348	48487276	42860000	44526092	46632872	33289980	35937588	36803888	42384604	38008792	38813240	37453892	38702408	50427196	39910196	38745068	
fpHILIC	Negative	123.9888	1.15	unknown	170135	273382	242594	348172	618646	477638	513941	281603	546342	481017	315111	479394	966519	360735	215617	365814	424492	264600	372048	
fpHILIC	Negative	125.0247	0.95	unknown	644226	604782	626840	1408548	583351	984460	955142	968499	1898872	1040526	785815	615600	910073	1270500	578975	1455189	833907	1037623	520087	
EIC	Negative	404.9993	0.49	unknown	662453	463941	549663	541653	1185044	614439	941587	707007	524492	670427	474082	378513	568416	2942241	749014	448999	518939	510761	576994	
EIC	Negative	403.1721	3.43	unknown	359920	373063	388603	782391	559127	445215	549472	657938	80756	616556	515101	742608	630302	236099	277924	589661	555794	680974	289551	
EIC	Negative	486.0073	0.49	unknown	961082	715634	781326	774562	1481149	895698	1307971	1011427	7246345	952818	651493	595406	766239	3202322	1053887	628452	772561	784558	812512	
fpHILIC	Negative	125.0357	1.03	unknown	21238222	17519168	17204456	24143998	22964984	24525250	21252382	17454582	2263378	19776170	15267138	17232308	18518026	14248706	14482947	17009698	18626038	15996444	11709621	
fpHILIC	Negative	870.5852	0.42	unknown	5918061	5961727	4638980	5354569	8967381	7562357	7635710	7083609	5002703	6544508	6236603	7507766	7103513	5851599	7479993	6342959	9149750	6179635	6493559	
EIC	Negative	453.2822	5.23	unknown	18434413	23135709	16727334	23729381	25125802	24255678	21022296	20827748	29572252	15873500	18478169	18854923	16525653	23381001	16093798	18218251	20074659	15839216	18490951	
EIC	Negative	375.2558	3.13	unknown	1249217	1811620	1812463	734197	7897756	872547	14623296	6436491	7305688	48484	153669	145891	176182	42650	63900	339206	50795	71236	1055100	
EIC	Negative	542.2741	1.70	unknown	0	142849	60497	100380	103905	199150	162876	107704	0	41576	135810	102910	89642	99321	99750	95223	93433	114045	0	
EIC	Negative	615.3389	1.06	unknown	467328	95751	232451	58451	452483	362097	476092	444305	103471	24220	6283	0	8022	0	0	0	0	51240	11479	
fpHILIC	Positive	905.5927	0.37	unknown	1120162	1150890	1011129	1439938	1521059	1161421	1063877	1412798	1060962	1705004	1466784	1273440	1360333	1215693	1184966	1344975	1372290	1194079	1594545	
fpHILIC	Positive	813.6127	0.43	unknown	1753435	2155829	1663357	1803253	2478508	2313835	2444178	2547359	1754953	2114692	2034153	1963068	2092197	2250696	1899110	1697170	2731549	2001443	1928570	
EIC	Negative	334.2834	6.59	unknown	388604	440153	448167	572091	477138	646260	802930	661947	555730	628155	609031	575466	654515	552562	416676	427924	685389	711200	571107	
fpHILIC	Negative	104.0435	0.96	unknown	1554028	1358201	1937374	4089907	3066058	1615396	2490736	2179955	6279208	2245743	4755344	2673963	2789012	1861166	2300777	3776796	1368000	2398625	1147310	
EIC	Negative	508.3387	2.83	unknown	48471	225614	85601	0	614762	138764	561685	395333	317025	80868	197524	253136	133781	235946	275166	281464	248385	259680	233925	
EIC	Negative	586.3626	1.24	unknown	0	0	56308	25621	135267	0	127975	67952	251892	0	6572	0	125535	0	7102	0	0	0	0	
EIC	Negative	452.2790	5.23	unknown	75981857	97309791	68773881	99270563	105257987	101784565	87272884	86915695	123											

fpHILIC	Positive	387.1901	3.71	unknown	500686	407569	362602	499121	576472	724222	557336	456886	548805	414230	462735	460829	468963	412762	488307	486421	557597	455564	425039
fpHILIC	Negative	110.9758	0.94	unknown	2085331	1027813	951693	611976	4641911	2393880	4301840	1209754	2209361	451075	464428	646637	698788	832940	773699	1979780	786169	903697	1067197
EIC	Negative	383.2996	5.63	unknown	0	0	0	0	305751	264185	284187	0	0	0	0	0	0	121327	203788	0	256446	0	0
EIC	Negative	322.9959	0.49	unknown	399888	318852	333429	358873	758076	397409	540237	443882	364095	400347	320788	242331	331787	2381938	431451	256212	350561	323213	350581
fpHILIC	Positive	197.0892	3.07	unknown	435727	255203	258134	249408	669108	1052916	419187	270136	664951	179473	246504	216177	199453	195132	428120	679542	276867	622432	241737
EIC	Negative	446.3787	6.70	unknown	250461	141085	186697	344919	260182	254640	309264	286454	521150	220152	352103	301602	429822	265784	283064	276958	276411	294621	370493
EIC	Negative	463.2555	2.72	unknown	57406	147560	68487	247283	215772	226376	182520	159272	294029	128423	171588	262965	210760	195793	232819	216865	199113	144833	200886
EIC	Negative	425.2561	0.73	unknown	103961	178415	144064	245078	401179	238969	304778	412045	186096	150920	226007	181947	318863	118079	252304	323880	231102	414694	126633
EIC	Negative	333.2709	6.53	unknown	690982	695141	659132	1252795	779217	1169540	1203389	1951647	1284251	1053621	1471590	1175562	1405619	1192816	989070	1240180	1347199	127220	874027
EIC	Negative	361.2022	1.63	unknown	3095854	2999375	1627736	923135	3586685	11064485	3517744	3252118	4230294	1985623	3245554	980899	4271500	6276229	3365524	8376153	1390005	5060395	3156525
EIC	Negative	535.1625	1.63	unknown	0	82263	0	0	74329	199900	69416	0	65090	0	61585	0	83638	84882	46180	100819	17503	42753	45997
fpHILIC	Positive	308.0907	3.62	unknown	200315	401079	306706	465493	882569	1654612	1137146	477071	656303	415025	582274	812300	815148	642673	528362	663650	986304	709651	783729
EIC	Negative	520.2324	0.98	unknown	161014	137870	208329	166569	170293	165958	280434	204402	231568	257251	234305	119136	70340	99420	163787	149655	180949	64325	115670
EIC	Negative	527.2379	2.14	unknown	0	251761	214650	136586	343765	287599	406576	213101	302487	0	0	0	0	0	0	36321	0	0	0
EIC	Negative	459.2735	2.12	unknown	62753	281710	155115	0	874819	224713	1051712	379122	538437	43675	72924	52183	49818	62492	73924	107600	112309	172285	109573
EIC	Negative	360.2994	6.60	unknown	478534	451998	338974	450305	539475	578145	825143	613585	583731	706336	536437	743032	596218	422929	340049	465798	626686	897046	564473
EIC	Negative	329.1521	3.08	unknown	0	0	0	0	415471	457964	601996	0	0	0	386903	316919	419224	570774	430633	0	0	234309	0
EIC	Negative	423.2394	0.73	unknown	138474	609519	212682	207153	1258778	490006	932298	718313	529080	220345	418039	81224	295764	220043	393061	753636	581980	695537	260479
EIC	Negative	338.2365	3.54	unknown	0	84878	0	0	106086	108450	0	173190	138490	174683	108610	177817	136913	57017	73594	0	0	65303	0
EIC	Negative	337.2327	3.11	unknown	0	156600	0	0	158758	154474	154293	165860	163112	198283	161631	151163	0	155363	0	0	151264	207621	0
EIC	Negative	507.3332	2.83	unknown	2552263	693127	379332	108893	1921207	379882	1802562	1047124	914029	276711	598367	776526	388827	777066	850414	899107	835675	815173	660461
fpHILIC	Positive	200.0536	2.05	unknown	233476	158872	372086	57845	748842	601156	252626	132977	55887	0	0	492162	535391	0	0	653954	0	0	0
EIC	Negative	378.2743	3.01	unknown	1707579	790968	2069289	344616	4191438	534392	3306106	3328961	784756	398713	0	81033	121698	131159	97515	93724	108954	566297	135613
EIC	Negative	454.2848	5.23	unknown	3184827	4011670	2858506	4183840	4411043	4236575	3599649	5011890	5011890	2777718	3189828	3346182	2891455	4005556	2798744	3211227	355431	2765467	3174188
EIC	Negative	337.2328	4.99	unknown	0	270735	0	0	261531	173743	271297	413144	250294	0	273737	0	0	306044	421617	0	252523	0	251367
EIC	Negative	393.2652	1.97	unknown	0	158507	0	0	477045	615392	815029	0	327226	0	0	0	11044	29378	18603	41461	0	0	51401
EIC	Negative	454.1863	0.69	unknown	42048	46803	80263	58030	58666	60910	108471	110679	56711	60281	74482	58888	31755	21848	64339	47518	70162	40840	25907
EIC	Negative	538.2430	1.14	unknown	51353	50420	41456	31231	50416	68487	98991	88709	43716	74922	57764	83809	62984	50693	43429	56903	63724	44711	63816
EIC	Negative	377.2705	3.01	unknown	6849964	2881137	8117411	1560765	16374780	1792073	13253134	13197395	3325833	1661760	603727	606734	556875	1004339	795625	731276	703626	2424224	1038171
EIC	Negative	319.2786	4.00	unknown	323457	314222	297382	277888	337209	316912	295021	309696	294220	255893	294761	289017	305043	291022	292634	301833	339664	271976	292969
EIC	Negative	495.3111	6.17	unknown	0	376841	63947	109851	491159	355624	502268	256729	416016	124529	381055	200695	346628	301642	474380	405441	251389	323236	329529
EIC	Negative	428.3172	6.53	unknown	613845	397716	620979	675712	419442	1350908	1138891	977741	1348997	1055130	853229	764520	599914	659270	584820	1138974	713209	985080	402008
EIC	Negative	457.2581	3.14	unknown	100998	156053	137224	51352	558478	73212	1019207	34426	0	0	10268	0	0	487751	0	41861	0	0	80936
EIC	Negative	431.3018	4.91	unknown	913001	596012	561035	856603	832107	1123035	666726	1116962	1151229	892744	513045	582166	678028	844613	819160	796119	694305	629579	1033978
EIC	Negative	251.1323	3.91	unknown	2497912	973497	771710	434638	3216230	870636	2354783	599554	607047	781525	960747	197584	1615136	823646	599534	646262	2106821	1036295	2174182
EIC	Negative	322.9959	0.55	unknown	26714	85949	70947	92836	148254	84628	144889	175028	91288	26115	68416	89810	96073	209832	80785	63867	93472	104772	24676
EIC	Negative	503.2872	4.46	unknown	491327	842254	514506	500285	648907	1202725	771624	591171	646242	663616	657597	642296	756587	764897	708666	537821	705698	493609	762268
EIC	Negative	343.1388	1.56	unknown	37872	74239	90650	0	88301	78479	103354	76717	95050	0	215970	124708	97314	297897	53703	108847	51026	0	74578
EIC	Negative	588.3332	4.33	unknown	330729	416828	323162	366144	475741	551889	571578	452667	378698	359537	413928	472717	448754	366889	459657	508891	493016	366576	440507
EIC	Negative	437.2911	3.01	unknown	4506119	1984833	5590438	1014100	11320256	1227311	8736390	8738373	2252801	1122958	424028	440607	389506	684041	553538	494570	498490	1625851	687229
EIC	Negative	438.2945	3.01	unknown	1255267	541575	1945418	292138	3159235	327775	2394370	2400798	651818	138406	118885	119891	113462	183548	171714	143333	137508	460115	208532
EIC	Negative	376.1823	2.58	unknown	0	0	0	0	505138	0	519997	0	265731	0	0	0	0	0	0	0	938714	0	0
EIC	Negative	238.9941	0.49	unknown	641722	454165	446566	472503	1134672	614208	811934	582457	435104	579662	495560	356984	484397	4518316	642564	385286	464416	473408	522733
EIC	Negative	584.3837	6.12	unknown	6109743	8079850	6309920	6804799	7444001	8279997	8044376	7521628	6787180	802112	7244483	7641064	7330095	7232816	6887556	6592108	7558472	6290332	7353689
EIC	Negative	437.2913	3.28	unknown	54451	56567	74917	34747	160160	11054	200530	10668	10151	0	0	0	0	0	0	0	13319	25994	0
EIC	Negative	602.3293	3.03	unknown	109999	116905	108997	152341	126739	113704	232325	128756	224672	158151	115849	98357	112564	101775	97634	122062	252205	174563	82396
EIC	Negative	485.0032	0.49	unknown	6529242	5186458	5551518	6046197	11135987	6596298	9034341	7018673	5420401	7105714	5362132	4223011	5842623	24212895	7537644	4760690	5739450	6047762	6084504
EIC	Negative	466.3939	5.91	unknown	1625335	2394845	1940009	2212153	2561360	2834383	1948290	2289270	2424908	1482911	1626885	1465290	1326235	1978845	1330836	1374065	1821298	1469103	1715826
EIC	Negative	363.2371	6.71	unknown	571819	610901	545225	1231120	866872	964431	927773	935665	947106	944659	1145765	1258919	1108081	732986	836764	852844	870949	1051294	675115
EIC	Negative	602.3469	4.33	unknown	88928706	108341821	83277891	93864055	109980137	126042556	125153093	103487644	99204798	92079987	106571907	111037316	110210115	95323913	106862189	110605837	120935029	93753580	106371504
EIC	Negative	520.2323	0.89	unknown	51810	56504	54768	608															



EIC	Negative	370.1592	2.11	unknown	1094857	800845	805091	1285042	1387322	1150012	1327201	968951	1407524	917265	957009	1084190	1065439	438828	1200538	1647736	866756	993983	395293
fpHILIC	Positive	146.0268	1.03	unknown	375937	3517176	1696518	1752012	3441121	3640029	5478687	2009130	3845618	1804840	3695265	2928015	4753615	2127038	2548747	2770600	3638161	2176939	2364707
EIC	Negative	455.2875	5.23	unknown	396920	495894	374220	592029	588087	572767	457163	491858	686121	334144	427643	384079	361478	537291	385290	412037	506388	352559	405206
EIC	Negative	415.1975	2.89	unknown	0	0	0	0	239197	177139	0	0	0	0	0	0	0	0	0	0	0	0	0
EIC	Negative	320.9970	0.49	unknown	4733616	3809739	3886146	3976500	8398567	4424558	6692016	4830681	3634116	4966277	3803217	3016742	4016251	27384709	5515885	3359795	3629625	4100557	4268437
fpHILIC	Negative	196.0542	3.11	unknown	1324192	1133377	828906	1058113	1660901	2242641	1850733	936487	1832291	919031	1487761	1609063	1291601	1268338	1485683	1669594	1536924	811216	1142051
EIC	Negative	443.2056	1.63	unknown	173618	212886	0	0	272661	830358	262480	0	322290	155698	251034	90554	337873	486786	268503	661718	115981	230385	268367
EIC	Negative	526.2844	4.37	unknown	2659742	8166625	2207172	3986108	6328279	7185615	5597193	3652738	6663802	2431384	4228424	3877369	3862809	5354701	4660582	4754567	5293862	2575758	3813282
EIC	Negative	365.2383	1.44	unknown	0	232635	0	0	404555	344561	319396	0	344240	0	238899	165527	410823	312074	473091	524164	205936	0	167764
EIC	Negative	649.0093	0.48	unknown	5036310	3894609	4044930	4473738	7987371	4592730	6907966	5215624	3961649	5179914	3800988	3139792	4326680	10611934	5069045	3598414	4052668	4562260	4395955
fpHILIC	Positive	222.0787	3.71	unknown	269544	222558	153149	518493	384790	421525	341963	209106	1097047	245936	311454	345153	504965	355051	336252	609004	438355	354059	196688
EIC	Negative	525.2818	4.37	unknown	12727054	32444282	11429691	20076195	33347350	36667705	28445022	19142019	34024119	12154491	22611950	20149233	19361871	28676850	23532987	24271693	27273141	13354632	19701748
EIC	Negative	494.9585	0.47	unknown	260116	187766	241075	183880	426209	227652	289106	234167	183435	211667	184477	124903	170477	783760	205604	111257	204196	214419	218289
EIC	Negative	535.2865	4.98	unknown	140016	167387	134712	163691	191250	171020	153419	169286	250278	127277	152624	156769	128351	190014	160582	145336	157027	140691	143413
EIC	Positive	473.2184	2.64	unknown	236393	140277	0	93442	330987	263951	288340	103005	249299	144157	213268	180012	168980	327417	194424	265871	169049	162168	334078
fpHILIC	Positive	503.2950	0.50	unknown	169180	2222823	1267385	1238801	2458437	2520004	2303689	1647601	1787891	1013182	1734500	1904250	1625852	1975191	1960079	1254125	2382362	1153196	1452675
EIC	Negative	311.1690	5.48	unknown	11399861	9491800	10649245	17346935	20057202	34548104	19936697	14758089	18791899	11846524	10555757	10896945	8047154	10981613	11435744	18635097	16470278	16943772	18023339
EIC	Negative	568.0091	0.48	unknown	989478	768582	826579	902810	1659783	960761	1413898	1077643	760119	1046679	797578	599768	862872	2684463	1085089	609438	841197	928149	862623
EIC	Negative	500.9785	0.49	unknown	316109	225444	172454	215139	1100065	338448	617238	362728	180606	411343	209823	118454	205190	11333609	446785	152239	196978	229875	268533
EIC	Negative	542.3738	5.61	unknown	653195	875253	638694	798108	798705	867232	687307	676617	877475	639771	797080	728634	691410	685055	672752	626458	671386	603075	761452
EIC	Negative	502.2846	4.46	unknown	3534810	5995362	3367633	3804632	6266185	7477712	5877047	4072281	4985928	3241271	4788391	4701069	3625904	6028193	5147115	4057467	5431902	3485990	4917880
EIC	Negative	306.9825	0.55	unknown	0	69055	63792	95967	143220	54237	144468	184932	88179	91567	71764	73526	234759	79481	58114	94852	98929	0	0
EIC	Negative	353.3072	6.65	unknown	180605	222534	270743	517089	368198	610868	438300	445193	399033	265539	277524	384841	438120	339870	299415	416933	369539	341039	241435
EIC	Negative	649.3909	5.89	unknown	228407	314267	190074	217601	299041	370538	303575	215780	353335	186077	304314	262971	286733	237097	290799	282154	267787	174262	310696
fpHILIC	Positive	414.1385	3.11	unknown	796088	835811	817454	955561	949469	877651	1030511	1047530	250006	858190	1036869	1024746	858508	642651	958837	860444	719800	876663	591395
fpHILIC	Positive	205.1263	2.32	unknown	24324086	27911430	31926762	50164962	28999138	36491964	37189420	31323462	61243800	28790964	38534020	38805920	42880560	16208464	20023408	15288516	25479196	33909488	22722120
EIC	Negative	393.2653	1.66	unknown	392350	253210	0	0	383160	778099	811298	234369	285406	0	24612	12757	20648	7603	35685	27587	20343	101693	31699
fpHILIC	Negative	361.2026	0.47	unknown	412751	380293	450626	181503	547290	1297929	393108	461634	469305	267517	358917	72649	427100	527246	224327	728832	212512	595105	394337
fpHILIC	Positive	432.2375	0.41	unknown	33501580	36296516	31011192	38184436	49437532	40011400	3707952	36385024	47517988	40068324	32112678	36757996	41053968	33884696	23296266	30581062	32750244	41050500	25641078
EIC	Negative	281.1738	5.18	unknown	1656099	1657657	2331547	2873324	2176252	2067704	2302244	2332535	2888522	1594748	1779625	1805688	2167425	1632844	1572558	1705674	1807066	2503997	1683306
EIC	Negative	524.2786	4.37	unknown	41230109	105453348	37090907	64944913	108409312	118480387	93356993	61960846	110825963	39833373	74947054	66365034	63293849	92057818	78634118	78773167	88513012	43910551	64451733
fpHILIC	Negative	306.0764	3.63	unknown	311887	325143	260819	422260	732629	1350575	890221	394312	413256	350090	473434	814350	646231	413465	443038	558663	833212	690719	671656
EIC	Negative	530.4295	6.63	unknown	2379366	1328149	1332752	1697122	2498690	1366549	3418928	3190487	2035619	2168784	1641394	1709307	1200198	1799772	2699064	3230665	1841166	1140078	2779975
EIC	Negative	413.2464	3.01	unknown	157013	90198	169232	34816	389729	41762	298662	275578	47042	21666	0	13568	15843	0	11689	0	45490	0	0
EIC	Negative	425.2561	1.11	unknown	207794	241030	237340	466048	877579	560578	579841	482110	316606	314401	351163	139017	541446	304537	648048	658204	419408	641309	320019
EIC	Negative	564.3668	5.84	unknown	269085	335547	250111	297203	353892	407803	331374	275419	365626	185417	335776	253362	248261	219153	274097	287523	264291	205855	258111
EIC	Negative	312.1722	5.48	unknown	2311927	1826693	2165265	3420252	3898933	6838911	3936300	2923457	3743519	2232447	2073078	2117527	1592631	2202052	2258732	3611049	3205863	3264612	3466652
EIC	Negative	356.2472	2.15	unknown	2123656	2700530	2403076	2635146	2666252	2750882	2431550	6243788	2693285	2557101	2877783	2586492	2673806	2537000	2634774	2677749	2380722	2736500	0
EIC	Negative	241.1808	3.87	unknown	740358	999176	1345225	7062012	2700491	1431021	2579788	2815313	2649341	2366213	1304831	2248111	2761230	485112	471378	2677645	1648882	3387283	565023
EIC	Negative	388.9040	0.55	unknown	16886	82795	63797	118535	174009	167685	278943	93567	53867	90259	74979	104566	247641	107185	54284	114421	125353	49239	0
fpHILIC	Positive	236.0717	3.14	unknown	1037307	1127721	1149903	982140	1285725	1130042	1127469	1238332	1119095	1119947	1094063	1286208	1245829	1172961	1146233	1047461	1195596	1195596	0
fpHILIC	Negative	401.1996	0.35	unknown	204132	325123	358128	584887	1024468	714773	657451	531142	669602	650007	602618	987566	383339	634365	424213	441872	860037	316042	556611
EIC	Negative	426.2597	1.11	unknown	59903	60318	61216	116705	224160	139470	144769	119470	81225	163705	93735	45825	146863	85650	154832	117958	104442	156381	85653
fpHILIC	Negative	375.1144	3.12	unknown	445010	311651	230691	294158	466802	618123	486539	282270	596417	301900	405433	508577	320079	324955	411429	475722	413228	198440	314866
EIC	Negative	501.2819	4.46	unknown	18384070	32084121	17749572	20499614	33415594	38856194	31735745	21797471	26429737	17006889	24909689	23429952	19652651	30196366	27732639	21271783	29125493	18390573	26333345
EIC	Negative	313.1668	5.48	unknown	608327	511560	596685	944864	1049779	1852346	1063056	770282	1011693	637395	543630	587741	442921	622274	613934	1005034	894086	884581	957232
EIC	Negative	480.2021	0.70	unknown	77225	97547	101512	97123	90369	84053	155659	135244	114459	101074	143952	92825	61417	55297	89572	103373	106609	62555	61676
EIC	Negative	312.1722	5.29	unknown	3536203	3244222	3438527	6724480	7750916	17411070	8422861	5853145	7										

fpHILIC	Positive	524.3714	0.55	unknown	149534192	195521696	162359776	181950000	223913008	243475072	204715216	190427968	162722656	188444192	184146528	218472624	212826496	192437216	208379152	179028048	217347568	203409312	194948544
fpHILIC	Negative	207.0137	0.49	unknown	909668	2123044	1832319	4473416	4423875	3657822	3734070	3065500	4756280	4887753	2858153	5938354	1480988	3479010	1513421	1751661	3768916	1887931	4127364
EIC	Negative	638.2853	3.73	unknown	17428	108168	54751	60426	129633	101883	113852	85841	242094	60078	118505	69618	144575	221723	104444	211121	159806	68873	109658
EIC	Negative	336.2624	1.95	unknown	0	62607	0	0	87476	135974	128264	0	283337	0	0	0	14989	16347	17572	33683	17661	0	20597
EIC	Negative	337.2051	6.42	unknown	6404301	4638684	4121401	4806718	11924909	3641673	12198550	6360689	6316986	4638766	4825518	2087454	5465609	3026057	2333023	4315623	1080274	8129798	4985256
EIC	Negative	492.3420	3.59	unknown	172055	157429	294382	98439	358789	86536	348464	504589	240743	51514	78241	128112	68111	258748	143448	124169	169990	146606	142596
EIC	Negative	335.2232	1.95	unknown	0	289635	0	0	293014	571553	585455	0	1263755	0	113029	108538	65887	135590	77527	158390	86741	0	78869
EIC	Negative	556.3526	5.09	unknown	13075369	13362885	12845200	13041709	13142451	13395571	13511564	13763957	13728679	12662217	14191777	13453088	12496695	14770850	13616654	13634195	13034472	12882681	13656200
EIC	Negative	459.2731	2.27	unknown	350311	228676	338722	188584	752225	204903	594850	153750	193905	153750	159656	29927	33929	14927	45068	42667	29179	221579	141954
EIC	Negative	307.1561	3.00	unknown	923155	699707	838462	612009	833779	945425	926468	891744	705166	740237	209569	704001	202609	0	716918	247136	0	0	422896
EIC	Negative	458.1687	0.69	unknown	76494	55936	51986	27691	65773	80202	59887	161483	65075	85912	23257	126419	109422	46010	64427	62935	94061	79932	90825
EIC	Negative	242.1841	3.87	unknown	114516	167488	207846	1080636	393766	224329	428544	431194	1033071	361551	199692	339245	437245	77350	88308	409662	255027	542213	91007
EIC	Negative	346.1591	2.02	unknown	1182670	1286640	567859	854595	2113953	1948228	2000421	869332	2167183	510333	1486482	1740793	1447561	691865	1908395	2363239	1335157	297939	712997
fpHILIC	Positive	766.5734	0.43	unknown	774581	832976	936399	625556	1067608	949687	831582	1388805	868587	669337	791951	622468	662335	844928	796391	878471	728483	1055914	943004
fpHILIC	Positive	175.1070	3.04	unknown	1064657	541892	628366	688283	1322931	2652286	872706	593647	1398650	367179	364363	383409	403416	512928	835241	1216834	549037	1690448	575133
EIC	Negative	438.2491	2.06	unknown	72475	329956	0	0	354490	335539	357594	204461	355590	75726	288648	378870	262494	303510	303510	240534	300441	128245	325267
fpHILIC	Positive	174.1125	2.06	unknown	423826	688743	386976	512288	839043	765621	696842	587376	485555	494518	627813	656061	567324	715432	470111	495922	665165	403246	660642
EIC	Negative	543.2963	6.12	unknown	4445392	4853533	4020551	4299446	4797397	4771168	4939279	4400985	4388710	4119988	4478675	4861135	4636863	4557878	3972734	4914352	4504373	4782952	5277198
EIC	Negative	453.2821	4.98	unknown	3151125	4720736	3043823	3908579	4436783	4896485	3547418	3427585	5162858	2683319	3188973	3459998	2807245	4659546	3150931	2833784	3512875	2751539	3496518
EIC	Negative	592.3282	3.24	unknown	472819	828663	325450	592275	963107	1198268	623164	1894589	308070	722637	1279574	815355	866694	971273	971273	994939	751112	438261	721165
fpHILIC	Negative	257.2393	0.38	unknown	3901992	6310427	7302804	9706385	6593283	6394289	7325652	7916905	10490113	5242444	5078171	6458009	6857800	4754760	4428446	6241790	5953568	6274052	5630088
EIC	Negative	354.1752	3.46	unknown	92127	135833	70547	264150	220932	134497	239260	134497	239260	168344	99541	665215	62873	92386	353886	165322	132782	92150	121509
EIC	Negative	318.1098	1.96	unknown	0	224893	0	0	675766	674661	414506	0	213790	0	265449	73680	77136	56062	202124	196318	74985	0	44860
EIC	Negative	561.4788	6.88	unknown	0	0	444602	0	773888	485384	0	577826	521452	0	0	0	0	0	0	459954	438268	0	0
EIC	Negative	595.4957	6.59	unknown	393357	403765	345392	421272	494199	381054	679385	528158	874476	405494	492037	317095	415891	492562	485110	635376	454643	348441	596648
EIC	Negative	487.0023	0.49	unknown	725809	524371	585221	629382	1141479	632451	963247	692348	521472	707811	528641	421527	507379	2402985	721448	487072	575210	569536	609682
EIC	Negative	409.2610	1.77	unknown	68393	46752	371723	113268	306554	484058	230869	673818	154275	41768	259696	226660	324130	301661	187560	324934	219391	0	215147
fpHILIC	Negative	142.0509	1.05	unknown	230363	106040	200109	1679591	481091	482007	448447	370984	1528634	536700	320735	331804	560086	96996	119141	698217	219705	270988	86719
EIC	Negative	255.0664	1.82	unknown	0	8405	14418	0	239193	0	324944	28254	207821	0	53352	59061	63776	61048	0	189151	246760	0	211983
fpHILIC	Negative	126.0391	1.03	unknown	1293124	1055995	920054	1370583	1180503	1424354	1319440	1037206	1405818	1190847	961513	992098	1165230	892272	835594	1171862	1046361	903161	706408
fpHILIC	Negative	525.2823	0.50	unknown	1319827	2901201	775166	1216648	3375705	3274367	3109190	1175318	3606417	744433	2087454	2223711	2028837	2262249	2538161	2064342	2564800	774906	1978745
EIC	Negative	423.2393	1.44	unknown	0	144648	0	0	411156	318442	272130	0	93785	0	155335	28354	267399	159257	232987	237014	182720	0	159931
EIC	Negative	379.2475	1.65	unknown	85482	66080	0	0	168916	111027	279458	0	206206	0	10592	13448	10479	18562	20448	26611	15306	0	20427
EIC	Negative	515.2436	1.03	unknown	234581	435253	220444	0	276313	420338	610128	476225	311162	331371	393335	550431	435398	421871	308947	299545	365581	337178	528341
fpHILIC	Negative	233.9844	0.98	unknown	2605982	2633926	1246123	1403593	3902001	3682260	2831574	1861567	2320615	0	0	32626	0	0	0	48991	0	0	35018
EIC	Negative	319.2273	3.12	unknown	102277	113718	564508	125345	244165	207397	436432	751359	624288	95009	129919	82415	121211	347640	175150	309093	127909	447238	121530
EIC	Negative	570.3686	5.76	unknown	2023489	3029713	1981237	2058558	2813254	3253256	2671543	2435884	2273243	1767875	2535766	2537063	2483249	2535213	2530108	2428751	2599533	1943074	2574635
EIC	Negative	413.1944	3.35	unknown	0	0	0	0	747179	779240	1388322	188946	848337	0	2169299	0	0	1029191	0	0	0	1855019	0
EIC	Negative	527.2865	4.38	unknown	356854	971311	365160	542412	968073	1056639	817708	577314	0	389638	671513	750085	510922	886395	698569	699133	756237	451934	519105
EIC	Negative	339.1453	1.47	unknown	0	31380	0	0	83672	77902	66390	0	76768	0	41207	32561	17680	63250	67600	63888	45758	0	86591
EIC	Negative	452.2790	4.98	unknown	13206764	19482518	12735922	16421329	18425810	20355324	15396755	14374611	21391489	11221015	13583142	14293331	11499112	19484311	12852157	11597264	14923598	11363505	14276414
EIC	Negative	536.4780	6.53	unknown	304875	414553	575926	730877	507913	366914	603693	662410	811547	680441	628983	567426	1124916	664677	405701	701630	686525	630026	418160
EIC	Negative	595.3459	3.60	unknown	145230	255309	140492	174978	287821	256444	296772	231511	563098	160992	238622	257299	229096	308554	251275	288828	239775	161162	212001
EIC	Negative	504.3067	4.93	unknown	213019	419517	273843	133259	424041	492158	360090	728267	281257	172071	317092	209588	285849	408626	340263	184767	332676	243278	342436
EIC	Negative	310.0651	1.56	unknown	64417	109019	0	0	132236	142445	132075	72594	0	125200	0	97679	88003	136291	153609	74256	106628	0	132621
EIC	Negative	246.1137	2.13	unknown	0	0	0	0	302891	333258	24717	0	0	0	25554	12945	45244	0	10521	6985	0	82624	
EIC	Negative	300.1606	2.09	unknown	228227	175526	211907	204604	248429	203711	227687	307129	189242	137372	123125	138692	147945	153389	145177	201672	187641	234202	132033
EIC	Negative	366.2372	1.86	unknown	251800	221089	0	0	548908	419455	318860	0	231136	0	305448	154048	424681	252149	423221	485700	237742	0	174417
fpHILIC	Positive	904.5886	0.37	unknown	2150223	2190362	1956724	2623361	2800214	2019882	2035265	2475884	2961497	3058277	2584756	2156465	2408391	2218260	2216062	2361685	2515551	2204234	2733388
EIC	Negative	336.9715	0.49	unknown	77653	49166	0	55719	375392	78319	154457	78590	39806	73745	46836	0</							

fpHILIC	Positive	144.1016	2.10	unknown	866735	643038	778540	565869	1859341	3366187	8279463	1050442	1177826	381451	455987	520080	773139	621883	463347	598920	1077104	1275684	519865
fpHILIC	Positive	144.1016	3.00	unknown	1655641	1773822	1104174	1600947	1789661	2426004	1751238	1420567	4512995	1076385	1514348	1611948	1615705	1164045	1091435	2220345	1441565	1062186	998014
fpHILIC	Negative	325.1842	0.35	unknown	10890265	20989900	25090110	39847396	63849424	60168364	40264660	32495958	43473452	42945208	37887652	61419744	20582350	43088256	25569990	27849688	47561652	22909424	32511324
fpHILIC	Negative	253.2171	0.38	unknown	28209720	47890892	92818904	139741312	86220272	65544596	90715776	111944384	143237024	55477444	38575316	59299696	95214960	29340732	31988336	70352568	71100120	74723824	38948352
fpHILIC	Negative	236.1876	0.35	unknown	2145656	4216097	5203436	8304714	12401732	12094673	7713679	6784144	9038379	8930438	7818347	12306834	4082622	8746384	5429261	5766744	9100402	4627466	6653352
EIC	Negative	567.3864	5.89	unknown	2388359	3745179	2506985	2824560	3899423	4666247	3564306	2514849	3812336	2171152	3849470	3364189	3140128	2680357	3363116	3176394	2927955	2008803	3447187
EIC	Negative	320.2311	3.11	unknown	20968	13642	135334	19446	50433	53541	89260	177632	122366	20232	324403	13347	34815	81077	45932	71938	33292	109995	31460
EIC	Negative	600.2598	2.20	unknown	117207	148005	64149	172265	187209	180523	309650	160862	262649	390327	242924	148444	76148	128928	158997	161942	208624	179581	153049
fpHILIC	Positive	834.5991	0.43	unknown	7814408	14662769	7801957	9153496	15125794	13061650	11838332	10090936	14692669	8942419	12756032	11330644	11450972	12765594	10793742	15092683	15276289	9668831	12391036
EIC	Negative	527.4474	6.98	unknown	2365644	1813124	605879	808235	958765	4391109	1768550	3913740	1877842	1071612	993140	1812370	948627	1352868	644623	1138913	959692	670233	1602740
EIC	Negative	281.0218	1.19	unknown	54882	47329	43186	48495	64508	61416	68573	44007	50177	51898	57537	53621	52442	119421	58814	46572	51197	42502	60031
EIC	Negative	364.2216	1.89	unknown	0	81539	0	0	142909	438405	140548	0	145951	0	140208	158605	163416	96048	156612	261225	130606	0	80706
EIC	Negative	228.0412	1.72	unknown	8749	87054	0	0	101681	72268	157919	36419	98345	12457	119188	124008	135939	101427	46976	142840	69501	0	64937
fpHILIC	Positive	417.2171	0.41	unknown	656116	639080	527841	642451	1085620	901873	871334	850683	2067090	672943	728317	710917	836610	777015	393495	642966	618158	781105	510426
fpHILIC	Negative	311.1685	0.35	unknown	11229351	21398570	23812776	41248672	60364592	61647952	39688244	33075618	42592540	42220156	37972248	61027464	19841994	42212736	24205786	25884614	50726496	23443148	31055502
EIC	Negative	429.3014	3.73	unknown	0	0	0	0	0	344517	334375	0	0	423492	0	127232	0	0	0	0	0	0	213377
EIC	Negative	361.2024	5.18	unknown	0	0	0	0	1281453	1321320	0	0	0	0	0	1321367	0	1398971	0	0	0	0	0
EIC	Negative	525.4891	6.58	unknown	131776	166619	47952	171627	162610	126387	263032	192500	449189	135711	185584	107703	310044	110093	268720	240465	163934	295374	0
EIC	Negative	528.4509	6.98	unknown	902692	699613	236326	305176	354901	1685273	676126	1515983	721573	399283	381102	679172	360209	513800	245452	439871	380234	251464	628872
EIC	Negative	501.2819	1.98	unknown	0	0	0	0	0	311374	291745	0	0	0	374826	0	0	0	0	0	0	0	0
EIC	Negative	375.2483	3.14	unknown	0	0	0	0	0	27710	0	5579766	6583254	0	37643	143205	162194	36795	51636	58918	81060	75116	0
EIC	Negative	527.2869	4.54	unknown	924317	1717597	795017	1300530	1703015	1794756	1748650	1111631	1803140	832348	1181527	1389857	1206116	1490787	1445704	1801402	1376220	1011481	1294984
EIC	Negative	390.2942	6.43	unknown	8665932	7770323	7556979	10608422	10163407	10703957	8726439	8342089	10915191	10362621	6926441	7611077	8023737	10125748	9267149	8349749	7824517	7171495	12353582
EIC	Negative	365.2337	5.83	unknown	0	0	0	0	0	754170	0	0	643816	0	0	0	0	0	0	0	0	0	0
EIC	Negative	438.2983	5.76	unknown	668850	979506	660183	731288	997790	1148421	721194	727791	1088617	607989	770121	946092	695714	964359	773275	787286	859135	631573	897081
EIC	Negative	295.1544	3.00	unknown	295365	291820	276697	293367	306286	288855	345261	338011	286433	271627	264210	272690	293199	252098	261001	288572	308244	331647	308761
EIC	Negative	258.1137	2.12	unknown	0	0	0	0	9383	0	669527	1177060	46239	0	0	24710	33126	42594	5143	6070	7505	0	125745
fpHILIC	Negative	103.0038	3.85	unknown	862316	774458	644634	1490553	895848	1169112	2547152	668436	2199545	730136	653999	727804	723961	676704	607569	1561161	605315	829671	802938
EIC	Negative	265.0484	1.19	unknown	3583527	3858131	3294645	3175797	3835220	4465336	4525391	3933399	3845506	3705512	4196476	4197813	3738877	4150466	4057655	3642225	4223870	2893797	4326639
EIC	Negative	256.1927	2.20	unknown	186771	207680	74062	234859	250479	264415	236404	244856	278333	198339	182687	260827	1783439	180471	3012097	196357	258279	224237	0
EIC	Negative	372.3122	6.35	unknown	1086028	1339834	743364	740661	1194010	1143056	1131656	1316737	933699	593400	897331	769754	834176	859076	903933	672104	931591	860178	1156907
EIC	Negative	345.1560	2.02	unknown	6496006	7221511	3345364	3882695	11763705	11008357	11093533	3919908	11773897	3180342	8422583	9663647	7445208	4322179	10587979	12852656	7544275	2007953	3959398
EIC	Negative	526.2845	4.54	unknown	6397483	12192401	5487845	7813658	12062564	11958100	10791407	7974443	12295288	5940202	9237278	8224097	8607026	10342967	8694065	7283664	9612543	6287783	8859122
EIC	Negative	368.1431	1.78	unknown	62074	44474	64995	0	64600	67853	63713	63235	57559	81080	50770	63681	53967	28218	63915	78513	53630	0	34802
EIC	Negative	243.1965	3.43	unknown	1155120	794911	2597578	2403120	2481387	1628154	2064941	3369180	2448902	1505097	880080	1319830	1105351	673591	322862	884523	1109173	1737549	0
EIC	Negative	356.2518	2.35	unknown	796470	1062847	930588	921887	1006651	1038126	1153077	977998	1029521	996668	1058028	1008002	1055780	856213	850739	1033011	1017018	881748	1157726
EIC	Negative	266.0518	1.19	unknown	568327	593013	506152	480953	589196	700595	703868	509792	608691	569076	655712	640904	567868	636669	613338	568545	632743	447709	660028
EIC	Negative	423.2762	1.97	unknown	0	112395	0	0	248941	237281	383723	0	308452	0	0	0	0	0	0	0	0	0	12050
fpHILIC	Positive	526.2928	0.50	unknown	3102482	6834279	2165262	3558148	6593205	6604423	6585852	3663643	2602180	4736509	4906140	4672911	5893375	4285418	46523471	6200251	2094555	4045648	0
EIC	Negative	569.3659	5.76	unknown	9812948	14501108	9616552	10223184	13807365	16068931	12938095	11848191	11088371	8656153	12405391	12913050	12040072	12767551	12182862	11660641	12764583	9296263	12573793
EIC	Negative	369.1558	2.11	unknown	5309901	3936425	3794018	6435860	6848214	5661137	6586625	4497074	6824088	4326506	4755458	5379787	5191014	2178799	6014019	3796649	4385874	4351308	1988238
EIC	Negative	618.3423	3.74	unknown	129015	190479	126263	132636	187705	219163	210576	161655	243823	94502	178177	247234	207030	211102	178090	219011	195695	135494	185961
fpHILIC	Negative	255.0630	0.43	unknown	0	0	0	0	0	833109	1128043	0	0	514015	41287	903310	61570	69142	0	0	0	0	107696
EIC	Negative	498.2628	3.82	unknown	0	1909982	0	847227	1662632	1352867	1103474	806850	3367152	539669	875380	505095	822072	2379016	1036989	1153171	1354630	656355	864475
EIC	Negative	648.3869	5.89	unknown	675287	987542	689528	784845	1006947	1194639	973240	672504	1187229	649675	994475	899764	921627	758742	934032	1182297	932357	849830	578864
EIC	Negative	475.2244	3.00	unknown	132514	113864	39143	102659	211937	185145	266600	90975	115215	156913	133993	128923	121555	188409	153449	159377	151048	108959	219434
EIC	Negative	616.3027	5.23	unknown	0	0	0	0	0	169980	0	0	0	0	235212	0	0	0	0	0	0	0	307194
EIC	Negative	571.3706	5.76	unknown	326973	430978	298649	318642	409146	523880	415445	328387	347923	260247	395770	405344	373829	381839	422533	391995	412420	390845	374867
fpHILIC	Negative	279.1234	0.97	unknown	1094199	487849	506680	511142	1106946	1511628	957208	707338	636523	708474	855768	842639	798438	1009413	796063	859226	1016535	994875	579212
EIC	Negative	516.3233	5.61	unknown	326761	424061	331682	413753	386730	431661	312996	345404	471302	338379									

EIC	Negative	225.0917	2.86	unknown	115268	94754	193237	120642	305785	247085	115645	216499	299071	207395	148369	373620	348488	138381	93336	155159	304695	328480	229041	
fpHILIC	Negative	303.0595	2.48	unknown	827308	166733	300147	39304	606817	704282	417082	149647	508485	154654	0	0	431560	482336	0	0	691262	0	0	
fpHILIC	Positive	160.0794	3.71	unknown	1042268	868677	978052	1010501	1137205	1402102	1295650	965511	1012902	1019647	903561	0	1147225	852348	712882	960096	996772	774311	927965	755457
EIC	Negative	309.1711	5.20	unknown	4101150	0	2469894	0	4134445	0	3724174	2356477	0	0	2734720	0	2847721	0	0	0	0	4159772	0	2386656
fpHILIC	Negative	165.0403	2.96	unknown	4728657	3402449	2660990	3417830	4638569	5473687	5520055	3135269	4958819	3269227	3920512	4228516	3688422	3907628	4488581	5094485	4967342	3527293	3895335	
EIC	Negative	226.1446	2.00	unknown	0	139801	0	0	273185	353201	248121	0	153058	0	263279	528191	254069	134141	282936	260591	286521	0	136862	
EIC	Negative	441.2131	1.81	unknown	142101	141351	86162	0	193528	205325	171135	96775	67805	0	114298	104398	124288	80372	116618	76742	124488	0	100894	
EIC	Negative	363.2553	1.97	unknown	0	184569	0	0	310661	508545	1123480	0	730333	0	17964	29603	0	50234	0	0	0	0	68596	
EIC	Negative	419.1912	3.74	unknown	22486	105597	200947	50094	121243	29901	335545	264004	61849	69579	207465	33415	13727	48140	30472	0	14102	16731	0	
EIC	Negative	227.0380	1.71	unknown	242685	644158	187933	139524	799317	546878	1100871	281652	691987	215572	868475	946158	1066336	738924	287075	1084626	546035	69116	498870	
EIC	Negative	541.3712	5.61	unknown	3205364	4652329	3247572	3861459	3950772	4284620	3658232	3563776	4386187	3215523	3974259	3600201	3652832	3540045	3633517	3377516	3509930	3178143	4019765	
fpHILIC	Negative	213.9981	0.97	unknown	17174702	14047676	10495868	4877611	19738434	28264534	14425637	10198725	9830976	117433	113821	110357	176781	96121	103723	143722	104286	77363	84603	
EIC	Negative	343.1401	1.49	unknown	0	73422	0	0	83749	99798	126049	0	140578	0	406693	237921	110118	501235	54801	155760	68229	0	128180	
EIC	Negative	319.1903	3.31	unknown	532895	149770	176877	148910	363299	417649	743946	833927	107402	26956	24623	28489	27056	25857	22007	18492	18319	32796	0	
EIC	Negative	585.3867	6.12	unknown	928510	1246821	937027	1123830	1156754	1262724	1262327	1224389	1058114	947508	1138146	1179346	1146360	1141956	1026838	1048469	1203270	1000933	1119362	
EIC	Negative	509.3503	3.28	unknown	113854	307161	337901	70718	326507	281103	236477	136220	422738	101596	257004	177058	233822	303939	487417	322822	247678	134027	201663	
EIC	Negative	288.1632	1.35	unknown	26434	192151	0	0	272101	260324	239492	0	343564	0	264410	210310	290318	82164	266008	398367	245991	0	107069	
fpHILIC	Negative	894.5845	0.42	unknown	1337398	2234315	993378	1348792	2639508	2145219	1991389	1296658	2204104	1447962	1832254	1907673	2059288	1924032	1927664	2133800	2307001	1302937	1859114	
EIC	Negative	271.2281	4.51	unknown	1104974	451073	1114827	1083510	1271445	1191294	868727	1447736	1184881	701364	510637	604003	583785	738941	405945	683888	662999	1060890	647571	
EIC	Negative	338.2366	3.12	unknown	0	218223	0	0	220387	210924	0	210981	199378	230470	198348	221727	203384	217969	226893	223717	12591	0	219359	
EIC	Negative	473.2830	3.86	unknown	0	0	0	0	2659583	0	0	1392527	107676	486465	308789	107517	0	99792	180964	78011	270913	783196	0	
fpHILIC	Negative	158.1183	2.32	unknown	286711	285569	298301	420092	269941	413809	402074	293891	549864	283804	378065	365272	396853	144854	247743	498880	283422	288281	208793	
fpHILIC	Negative	192.0667	0.89	unknown	7791774	9165460	3883374	2927496	14074583	25208370	14703781	4936683	5796495	913443	1919042	2460571	1362037	1978947	1978198	4696941	1855170	1049104	1750115	
EIC	Negative	566.3829	5.89	unknown	7719086	11993544	8089133	8926632	12290574	14779503	11310417	7560335	12131741	6957177	12268668	10475917	9796877	8405901	10656633	10026082	9227258	6253226	10845128	
fpHILIC	Negative	149.0457	2.80	unknown	1979957	2093331	1535408	1636512	2289356	3917101	3546074	1579202	2824234	2233968	3200617	3522880	3050156	3031222	2233513	2743113	3161558	2048688	2879950	
EIC	Negative	359.1840	3.65	unknown	7483842	7808994	7367314	7225555	7627382	7500867	8843012	8107008	2181196	7471960	7311819	7728826	7067062	7353540	7264443	7348474	6763233	7490357	8055314	
EIC	Negative	299.1877	1.98	unknown	0	1121010	0	0	103487	147525	117639	0	168779	0	201794	139835	175549	141758	117735	217041	108730	0	88152	
EIC	Negative	438.2941	5.75	unknown	500275	606314	455295	714013	903103	1058743	684122	479418	1067811	496670	613059	434406	377333	925245	432755	1058731	793846	594301	531266	
fpHILIC	Negative	312.1721	0.35	unknown	2281535	4234609	4655105	9366607	12159847	12069089	7875151	6314243	8449711	8280721	7484640	12191054	4296798	5888574	4862063	5064599	9483581	4732670	6526260	
EIC	Negative	378.9949	1.19	unknown	130664	135767	136805	123642	129547	140590	133111	142050	137274	125653	131831	133776	136879	124572	132952	126531	133480	120656	131016	
fpHILIC	Negative	387.1850	0.35	unknown	372011	657194	651445	1095533	1960520	1634860	1140849	921635	1087951	1309775	1075742	1734168	601649	1333536	746897	833092	1337760	669241	1080727	
EIC	Negative	491.2430	1.82	unknown	480736	124289	239636	0	519470	979736	648599	40183	136045	0	0	7639	9706	18801	0	0	22736	0	27988	
EIC	Negative	453.2822	1.71	unknown	238420	1530183	0	421067	0	4720206	4284700	2316549	556061	0	163063	177205	6532	360559	297240	238478	890196	369378	0	
EIC	Negative	257.2271	6.24	unknown	273771	816985	399064	1007818	1492119	494746	1036981	496335	2021082	227044	472481	80740	189831	535623	456567	1133918	1150999	442967	247541	
EIC	Negative	582.4618	6.41	unknown	641640	937272	1694677	16613081	1647340	973390	1461593	1761603	3701333	921099	793991	1523297	1321120	956041	615552	1161089	1285896	1409450	628121	
fpHILIC	Negative	183.0121	0.35	unknown	131401	335312	347940	510565	828947	774615	549962	449985	544748	657077	632822	836362	300975	550472	364365	359857	668110	298273	416249	
EIC	Negative	241.1078	0.82	unknown	250302	299677	259488	238540	259518	263436	323876	220780	217882	220720	231630	258077	226594	302674	302674	275811	259348	263149	255681	
fpHILIC	Positive	161.0915	2.96	unknown	977704	1372089	675451	745728	12190847	1654675	1489281	738516	1557414	524384	563382	714827	658040	886014	861733	1067079	929798	761464	905024	
EIC	Negative	367.2393	6.53	unknown	866606	1079107	786447	826211	721420	1800836	1416084	886088	928673	1821299	884258	854543	536803	582858	1019459	546476	577539	563546	0	
fpHILIC	Positive	138.0489	2.07	unknown	1085639	79631	333825	0	1027518	734290	283241	35271	704331	79629	0	0	489090	707594	0	0	1081396	0	0	
EIC	Negative	321.0442	1.43	unknown	0	71697	0	0	78176	275412	84579	0	46679	0	81112	94401	93908	92857	116817	67182	73680	0	76920	
fpHILIC	Positive	136.0421	2.47	unknown	346664	280029	241394	377704	546898	290597	416203	268735	920667	317349	393191	341063	462845	230160	306379	622317	348261	402968	211648	
fpHILIC	Positive	131.0813	3.72	unknown	553018	340886	441600	460170	518276	675586	470209	506841	470209	412016	373184	433354	425261	361064	559320	496798	433808	61988	455811	
EIC	Negative	337.1415	3.43	unknown	135953	116902	193843	927629	358977	276391	402901	519954	724035	571237	341868	691598	559948	155581	175425	497173	457679	775679	184263	
EIC	Negative	495.3696	2.83	unknown	261506	420585	362383	214760	458120	256072	510777	445810	400523	622273	329141	339895	234319	611530	479201	357546	428145	401794	364375	
EIC	Negative	347.0515	1.19	unknown	537875	596525	521819	485583	593403	689911	677982	498308	589623	558370	635176	621741	591389	621451	619264	575754	634982	420931	648071	
EIC	Negative	495.3696	3.37	unknown	510003	367812	378337	623641	544490	510954	417157	788744	572764	277106	459112	471491	499840	382214	760137	589491	295298	495411	377046	
EIC	Negative	461.2908	2.47	unknown	84808	28914	125305	35816	192036	29068	66403	355282	133667	72104	38377	34621	29763	106129	114414	77400	67783	391040	91890	
EIC	Negative	462.1128	1.48	unknown	0	56614	0	0	139657	335218	1060641	0	70346	0	181260	102035	81261	77483	23870	93566	131444	0	36812	
EIC	Negative	393.2653	2.62	unknown	256145	34587	0	0	127906	0	331355	278955	218097	0	0	0								



EIC	Negative	463.3425	6.61	unknown	1174838	666470	190939	320252	3557657	2073331	2525574	1645817	3881024	183262	621670	1456345	2493568	3472684	1843942	2110988	3425171	1205273	2385444
EIC	Negative	415.2164	1.56	unknown	37620	603514	0	122837	1044150	33475	890479	44671	1935928	0	0	0	15292	0	0	0	0	0	84867
EIC	Negative	593.4788	6.57	unknown	1958444	1239978	1172356	1370726	1697193	1873787	1814319	2730658	1434787	2409126	1911489	1969460	1886520	1977405	1770269	1590780	1828987	2122254	
EIC	Negative	564.5084	6.65	unknown	180310	309880	542779	645590	428303	466531	435510	491388	697931	284157	235011	355176	613243	346469	210455	473058	318445	372210	226825
fpHILIC	Positive	112.0870	4.47	unknown	2030117	4911722	1885583	5163625	3243265	7171675	2137201	5019560	8655113	2335992	3446974	4415662	6331440	4470103	4737413	6481293	4291787	5713219	4697952
fpHILIC	Positive	222.0583	0.57	unknown	2364999	2682288	1000008	1366440	2882960	5909890	2152651	1663048	4031535	0	0	0	0	0	0	0	0	0	0
fpHILIC	Negative	524.2783	0.50	unknown	4484048	10223448	2263319	3552335	10046995	9491353	9649853	3929237	12428929	2441886	6487890	7063633	6443088	7286598	7169715	6562376	8408240	2228600	5990923
EIC	Negative	524.2786	4.54	unknown	109056373	215185054	92208702	139615952	206036691	198834741	185581365	137855306	210726939	96596188	134395955	136818376	146850131	169174770	152307114	126425230	162983274	11212470	151037626
EIC	Negative	629.3659	4.26	unknown	0	0	0	1503199	1692067	1931390	0	1237601	1711719	0	0	0	0	0	0	0	0	0	0
EIC	Negative	272.2315	4.51	unknown	183821	54738	187900	165594	213129	214785	134288	241697	193888	142042	53229	58368	117508	138006	0	0	0	0	0
EIC	Negative	510.3589	3.57	unknown	29489	180438	31694	0	144576	183863	136239	31082	237977	0	145004	113931	131990	144460	184002	166365	117094	29330	98061
EIC	Negative	604.2911	2.20	unknown	0	207491	0	43963	168314	175707	281729	62890	224522	314181	174786	201069	181434	141488	127925	164373	219219	106606	252828
EIC	Negative	569.3659	5.50	unknown	1347852	1979071	1259985	1517012	1847162	2077740	1745909	1634276	1495378	1175649	1613136	1669895	1637469	1610869	1526627	1380003	1524603	1177854	1579615
EIC	Negative	291.1600	2.53	unknown	56847	45408	77103	28521	59860	53386	81161	99264	33155	32522	44620	34614	45662	46177	29519	45518	32973	108611	53668
fpHILIC	Negative	224.1292	0.45	unknown	495565	514146	594541	416029	592128	818066	603688	344874	506108	489554	1092905	991725	667597	1076302	411391	476749	598954	241156	590356
fpHILIC	Negative	339.1997	0.35	unknown	5238671	10699347	12432930	20114202	32788824	27584660	19510650	16248549	22808396	21111794	19338822	32193374	10055731	21759554	13185659	12550427	28617324	10646271	15882926
EIC	Negative	483.0908	1.48	unknown	0	12802	0	0	48307	105060	348367	0	0	0	63271	34163	0	27243	0	32921	45748	0	9069
EIC	Negative	437.2458	2.06	unknown	361242	1027361	0	0	1107011	1012695	1075807	420442	907026	249477	879661	1045238	753201	755512	816467	756693	904950	306708	948032
EIC	Negative	272.1693	2.16	unknown	1738858	1257628	1209277	3347512	1990317	1285814	2070951	2130777	3016797	1922326	1204817	1265048	1901811	386882	1085223	2763940	1324195	2937204	646481
EIC	Negative	566.0064	0.55	unknown	149904	470495	266413	519136	693456	293221	650525	1198758	336524	142519	387959	448288	566058	704830	362455	342667	510427	534407	104429
EIC	Negative	379.2480	1.74	unknown	499511	155221	178103	0	344129	682095	663403	58258	399902	0	15174	15534	21755	18789	16562	19204	15297	0	16921
EIC	Negative	327.1458	1.33	unknown	84277	95738	0	0	133294	129491	131212	0	88312	0	391532	233786	150012	521371	70219	156026	70424	0	112540
EIC	Negative	649.0095	0.55	unknown	95698	283785	175238	255874	374316	159049	396774	813886	195512	143502	249232	295014	364216	401041	205317	141313	318109	293744	70235
fpHILIC	Positive	528.3037	0.50	unknown	543331	527754	388132	426183	611985	631348	587457	352691	658405	228521	466478	590597	408821	452317	409967	326898	516735	227683	339025
EIC	Negative	337.2327	3.73	unknown	0	216274	0	0	291744	298720	0	343397	0	411533	244931	0	343853	161097	0	367791	271689	0	182523
EIC	Negative	303.2333	4.96	unknown	197255	143722	176827	352407	221031	277966	263055	256832	291994	184345	214775	198533	248423	99604	161504	249131	155266	193566	146141
fpHILIC	Positive	147.0220	2.99	unknown	529272	923623	782691	1064974	1694410	7049561	1909346	477340	1143408	586888	1019879	1536343	1362219	586892	1258743	1865514	1739155	1174352	1475320
EIC	Negative	250.1120	1.48	unknown	0	24090	0	0	31936	41713	47672	0	70339	0	32786	38820	50322	16168	27451	57247	37588	0	12539
EIC	Negative	560.4752	6.47	unknown	16100565	20244144	20007801	21031247	21233151	16915104	21075544	19993470	28746470	22659715	17296264	19740478	20476921	16602435	17269345	21252793	21216175	26265733	18359967
EIC	Negative	442.0726	2.09	unknown	47416	111686	0	0	77008	178471	190186	64243	217179	0	234935	0	31575	95601	196208	314975	0	0	150338
EIC	Negative	321.2913	3.99	unknown	554374	562570	572962	537672	595921	593738	561151	574515	529589	543660	577206	529404	524748	511473	518612	561876	560357	539267	559600
EIC	Negative	500.9273	4.20	unknown	208784	274965	193207	236077	276105	295671	239820	201636	271218	181186	263869	230796	246245	275987	265870	253391	226877	192172	214421
EIC	Negative	283.1023	2.25	unknown	0	112188	0	0	17162	145255	89929	177567	52037	109421	38578	28340	23888	135859	117333	38633	0	0	37505
EIC	Negative	269.1402	2.24	unknown	163342	148376	192762	284122	188451	210506	240552	395036	236385	312722	119716	148597	138535	126927	142503	182720	163453	371041	208511
EIC	Negative	343.1780	6.05	unknown	129665	98900	164278	122597	146437	133552	222418	222975	78794	185061	125643	18899	18620	0	105462	186280	18620	0	430925
EIC	Negative	227.1651	2.82	unknown	114300	120204	241340	122338	176397	226175	196446	236115	146395	146542	156692	272387	218951	103195	145308	175316	162420	193024	122988
EIC	Negative	349.0490	0.57	unknown	46951	76229	159754	408293	129757	59428	131827	126588	165626	146542	99791	112738	236510	12695	68526	240703	55041	214361	662434
fpHILIC	Positive	526.3767	0.55	unknown	8916989	10690752	9517607	11133795	13683256	13506429	11115681	10898899	9274754	10926128	10795809	12597934	11471977	10902567	11898953	9343181	12500886	11284911	11050815
EIC	Negative	371.1397	2.85	unknown	0	87019	0	0	123347	87371	87371	0	43736	136984	129543	122443	117634	55290	99886	92805	169547	0	49736
EIC	Negative	250.0259	1.93	unknown	0	8751	0	0	109726	86715	99953	0	79442	0	163951	142209	143013	160197	44936	85681	137829	0	101416
EIC	Negative	453.2865	1.66	unknown	316976	200943	117639	0	261112	548565	636276	0	226116	0	0	0	0	24620	401028	25668	74759	19037	
EIC	Negative	346.2029	3.39	unknown	545550	390441	585717	409566	552808	533000	600255	730062	360581	522887	473463	413363	406860	403204	488418	422373	404400	537389	379185
EIC	Negative	295.2643	6.66	unknown	190984	248613	365105	536588	341685	395934	337010	346428	496752	314247	294578	434937	404439	342442	288774	398435	365868	490129	300787
EIC	Negative	416.2659	1.90	unknown	0	36659	0	0	61391	59081	68755	0	146789	0	59279	56481	64028	22805	34607	85764	51587	0	28606
fpHILIC	Negative	213.0099	0.97	unknown	34677116	27642664	22345810	10184652	38861712	54237204	28975176	19796590	19152020	242055	239877	259304	280972	208402	268795	289867	156033	108467	235553
EIC	Negative	299.2531	5.99	unknown	0	0	0	0	0	0	751591	0	225831	581260	260933	599595	564833	0	89397	180834	0	0	687063
EIC	Negative	546.3176	5.77	unknown	362501	555864	347492	411792	498340	546690	482992	450822	402266	330424	456707	434743	444935	434345	426375	406247	466475	364782	434071
EIC	Negative	527.2963	4.72	unknown	241788	581926	265759	305671	619573	614299	426635	356026	770480	274918	435764	381008	364756	814632	569764	434811	496225	287398	442880
EIC	Negative	373.3152	6.35	unknown	239138	451568	200745	211064	450161	302618	433019	455863	285770	211139	275560	287259	379704	245239	238364	304464	352216	318641	434691
fpHILIC	Negative	181.0870	0.61	unknown	2213339	2376599	4427739	2623586	3871170	2651816	3505635	4225128	3064823	8934986	8366548	7530375	4814309	5978010	1105312	3567067	1978202	2252232	2081183
EIC	Negative	50																					

fpHILIC	Positive	151.1438	2.08	unknown	7008461	6000321	5632095	1056206	6673479	52756648	17974854	731279	4632397	1174339	13974185	7544043	38264616	0	3524041	3655692	2370514	904789	7360060
fpHILIC	Positive	351.1978	3.71	unknown	2083180	1293539	1342842	1098926	1717485	2299828	1928289	1226869	1234795	1046736	1172478	1295907	1219933	852276	1402210	1544628	1093321	1114492	974260
fpHILIC	Positive	416.2150	0.41	unknown	3645518	3765876	3326833	3684636	5492656	5260463	3709966	3963732	11635628	3797517	3594067	3951653	4806115	4635632	2722328	3414819	3846859	4175420	2742695
EIC	Negative	544.3217	5.77	unknown	922905	1396607	974983	1069452	1327874	1400754	1277599	1101402	1115557	872361	1163090	1140276	1125823	1085507	1035641	1107566	1120243	957489	1110662
EIC	Negative	305.1748	3.63	unknown	229900	199018	257670	294579	183323	221068	302095	425632	336216	320061	119794	221718	286082	131752	168938	209456	229481	248947	152885
EIC	Negative	602.3468	4.72	unknown	18940376	22873485	17057184	19131752	23584018	25604522	27822043	21586397	19071649	17418108	20866380	24343343	23159678	18416937	20572309	19203991	22171982	16201820	20558627
EIC	Negative	292.0114	0.55	unknown	26912	123428	116553	129950	110492	88099	151451	234111	112977	61447	109883	127459	121448	50018	93145	113302	151079	157128	64892
EIC	Negative	460.2752	5.12	unknown	52150	0	0	0	0	0	173458	243133	0	0	0	0	0	0	0	161219	0	0	
fpHILIC	Positive	152.1473	2.08	unknown	480584	331982	362130	132701	436770	347984	1246765	30009	354404	47418	858646	531770	2500296	0	265695	228208	151123	0	605337
fpHILIC	Negative	132.0452	0.96	unknown	1094599	826614	690212	397326	1128446	2006386	866245	740732	666296	0	0	0	0	0	0	30129	0	0	0
EIC	Negative	363.2180	1.89	unknown	359386	317220	0	0	600764	1631485	502862	0	542520	0	532100	645436	687414	387255	642156	1087950	575556	0	330219
EIC	Negative	429.1953	1.92	unknown	0	121320	0	0	382781	83636	187338	0	187244	0	106313	100883	126070	122163	150179	126548	121652	0	106248
EIC	Negative	455.0134	0.55	unknown	272790	749033	684307	798323	663814	512543	839781	1777566	848684	420269	769501	848478	856301	294249	641012	557962	988698	1007622	335972
fpHILIC	Positive	370.2947	0.60	unknown	2557553	2074874	3105647	6384294	3192759	3576829	3638179	3730537	5979772	2962094	2215117	2493397	3008383	794845	1458648	3731710	1828952	2818931	1886718
fpHILIC	Negative	278.2206	0.38	unknown	2900248	4054886	4932572	6442316	4611038	3619718	4232610	6002612	7771099	3550254	3066009	3667761	4839971	2203612	3237473	2947332	4068507	3607466	3456177
EIC	Negative	564.3663	4.99	unknown	398732	547712	367989	464080	634160	613428	519491	335436	573779	385957	509978	501949	511256	363656	558956	529216	461655	341075	461769
fpHILIC	Negative	500.2784	0.51	unknown	8016202	12662830	5866781	5534536	12596603	13936532	12009148	6759629	10373419	4903021	9200402	9275060	8177341	11144386	11811210	6946667	11661153	4668688	10819332
fpHILIC	Negative	618.3403	0.62	unknown	722136	729513	920209	720058	684420	1276304	930209	983028	749431	630269	806516	924069	875674	672688	655850	690018	827938	560631	935639
fpHILIC	Negative	142.5059	0.44	unknown	791217	1098603	1497147	1372914	902739	1079683	1652739	1406199	1286379	1772814	1269120	1279448	1331626	897642	824728	932003	1350353	1076676	1159034
EIC	Negative	502.2942	4.93	unknown	3397511	6302075	3935557	3471065	6446460	8132025	5781460	3856844	4278823	2667020	4790394	3341963	3417472	5680494	5111848	3103578	5009039	3181928	4556497
fpHILIC	Positive	77.0796	2.09	unknown	744399	679794	648990	312731	796179	2905760	1443193	172295	761079	230925	1808669	983666	2222004	52539	458357	578495	442246	245843	951027
EIC	Positive	385.1877	2.17	unknown	45173	175751	36045	101572	137603	86585	175539	106994	263920	38501	124602	103370	119111	156891	159369	191282	104683	125260	106008
EIC	Negative	540.2733	2.82	unknown	338500	675609	304833	291597	550440	855758	461300	364853	1068007	416915	438439	622897	453400	406003	657463	771874	830252	257487	737511
fpHILIC	Positive	155.0536	2.44	unknown	1181348	674440	2225072	2093743	1593411	2505393	1066860	2791478	5634451	1654410	1059607	3046558	3581137	2848346	762451	2034580	2262077	1496138	839619
EIC	Negative	401.2184	1.99	unknown	0	541643	0	0	562640	860495	984542	0	820694	0	630388	685158	490300	280733	629353	566195	444989	0	336184
EIC	Negative	318.2672	3.43	unknown	614268	651709	567532	523806	607497	631977	615191	608407	851238	530413	614209	635342	600047	583270	616616	558772	596078	527801	617658
EIC	Negative	445.2958	3.08	unknown	2801659	1173773	1482294	1016546	1687249	1964528	1536452	3060325	2790479	1131012	734134	1387568	1157494	2021547	1669163	1305018	1275548	227830	1132540
EIC	Negative	564.2584	1.64	unknown	232341	253655	0	0	186530	287828	378087	228417	292944	251013	283220	353753	306613	188096	145070	0	287317	49487	312677
EIC	Negative	557.3570	6.10	unknown	63020	1210460	175583	0	909678	1751435	0	0	0	0	0	0	0	0	0	0	0	0	0
fpHILIC	Negative	263.0650	1.04	unknown	626069	627094	441686	878303	742094	729731	607501	515031	717011	643542	514585	514147	583172	434320	463226	490166	590469	528167	392758
fpHILIC	Positive	281.1383	0.41	unknown	510261	536795	430286	503719	755710	722478	502097	637664	1899439	575111	493515	714698	710089	626782	384343	511210	463334	579001	362404
fpHILIC	Positive	129.0261	3.13	unknown	531110	706973	628175	739255	771245	825916	784694	750161	618875	601801	735374	694074	622419	472020	566636	774043	558925	596869	519117
EIC	Negative	283.1111	3.08	unknown	332533	438464	374005	508835	418517	567282	508794	508835	373012	472029	371982	368548	415932	419421	443840	442114	480371	319812	482922
fpHILIC	Positive	221.1211	1.65	unknown	0	5277987	2349047	2963015	2352119	6195674	3642545	1680864	3787849	2383514	3957465	3862241	0	3435193	5397758	5043328	1526264	2627239	0
EIC	Negative	602.3469	4.89	unknown	3953987	5152724	4057117	4103957	4986301	5769757	4842156	3806874	3781695	4541854	5691035	5217371	4338065	4470760	4311711	5402458	3997668	5357797	0
fpHILIC	Positive	192.0736	3.10	unknown	220104	379467	301240	389260	359915	424169	290319	253557	704175	286944	346306	350190	352298	284797	375635	398343	328542	254434	262524
EIC	Negative	509.3498	1.86	unknown	69313	65906	0	0	98749	81326	75871	0	92628	0	68408	58871	60197	97568	93335	63834	0	60512	
EIC	Negative	454.2847	4.98	unknown	564762	827055	535711	729831	752860	838536	607105	593138	905115	489482	516086	614882	495503	864460	512991	467572	631591	486663	597026
EIC	Negative	499.2650	3.99	unknown	334223	1422246	0	0	376598	1288020	826980	803885	463192	2737447	270528	81430	702909	1693019	89892	74843	970157	333839	727554
EIC	Negative	253.1062	1.37	unknown	0	148391	0	0	247421	182847	316480	0	390948	0	189551	210883	217749	122322	153927	199612	233145	0	163123
EIC	Negative	255.2230	6.42	unknown	2676693	3020414	5620203	6290844	5375450	4063736	5675892	5453652	6040881	4354675	3379719	5180920	5506747	2457747	2420632	6040881	5657438	4377734	2614218
EIC	Negative	299.0957	2.76	unknown	68128	288481	51342	42404	361540	268021	437294	85543	127243	15720	275486	190258	91675	112309	295008	232700	115482	39224	78448
EIC	Negative	423.0376	1.19	unknown	145102	156756	138921	151446	173192	189621	186667	167037	156419	165419	173760	161956	174194	171296	149761	197316	173216	147578	198945
EIC	Negative	391.1975	1.97	unknown	0	350823	0	0	593684	469562	585815	0	363276	0	403913	313581	337990	126246	298829	461339	37386	0	243913
fpHILIC	Negative	79.9573	0.97	unknown	3233037	2836972	2324265	1178047	4018140	5576484	2798867	1853253	1753216	115226	110111	143041	117103	73841	118641	138096	96322	140006	136688
EIC	Negative	262.1123	2.05	unknown	0	195219	0	0	204297	196568	213497	0	221461	0	182348	183019	193982	246153	209051	203250	234771	0	178855
EIC	Negative	302.2206	6.25	unknown	9146689	27076286	10889743	31751814	30852609	15827001	23294888	16702742	5209691	14384853	15378779	12290984	28939707	17066151	15034262	26006435	24582045	13433720	11042575
EIC	Negative	246.1533	1.67	unknown	782930	992206	665297	2490615	1329447	1661345	1567104	796811	2699791	1473954	1634728	1269538	2106690	371963	1339735	2224197	1454481	1726432	584093
EIC	Negative	354.2277	2.72	unknown	418935	543850	517534	415284	474516	546062	528229	465221	595710	415444	553239	536986	564993	586268	581641	498216	524455	452588	

EIC	Negative	487.1907	4.08	unknown	132987	147809	123787	198179	181289	153012	197091	165346	251112	233339	158059	197411	187699	83995	99965	200196	183565	209023	100814	
EIC	Negative	359.1902	3.65	unknown	7243091	0	7208673	7314741	7100793	7034703	7557623	7550868	8214069	0	0	0	0	0	0	0	0	0	0	7512612
fpHILIC	Negative	277.0595	1.04	unknown	1207305	854213	914206	1096207	1221454	1370408	799227	1033018	811055	694498	640932	642298	629354	584294	632077	691172	636900	438967	0	
EIC	Negative	233.1185	2.23	unknown	80208	51586	34308	80609	59357	50917	52425	96800	104410	69729	38580	53387	51543	36455	43189	54616	60722	80630	71098	
fpHILIC	Negative	405.0291	4.72	unknown	933852	583210	807527	887693	895472	1234838	793901	879403	1046066	866627	729744	778288	854908	915162	767548	1009558	842790	931898	729075	
EIC	Negative	244.1999	3.59	unknown	171450	48996	88894	89554	142368	163777	91781	140194	91016	71357	59678	54892	58115	62812	30727	55899	59296	83051	60704	
EIC	Negative	352.2193	3.55	unknown	70003	58960	179964	52056	143687	87432	112295	188725	94652	162211	65245	73807	64462	97893	48160	53559	88568	147617	69365	
fpHILIC	Negative	351.0565	4.50	unknown	578170	411902	233057	421216	565818	875029	533615	327766	1156348	223430	476568	725597	759094	731445	713556	761106	861819	277684	402342	
EIC	Negative	303.0913	1.97	unknown	0	107737	0	0	172735	106793	159223	0	110618	0	139685	89663	84040	72353	144220	131827	77200	0	52594	
fpHILIC	Negative	243.0334	0.50	unknown	0	282775	454903	189865	394283	262076	550804	372840	140446	192539	763894	407972	315034	520184	0	204100	273599	186563	346525	
fpHILIC	Positive	130.0608	2.51	unknown	248649	246867	148517	267696	276779	450523	283411	159172	558473	198718	336977	432976	407910	281766	329123	535937	311183	183267	261929	
EIC	Negative	241.1439	3.24	unknown	112268	113249	91688	89083	120891	114290	118467	97684	112377	105577	110055	118109	103980	100600	132375	153934	109766	0	123643	
EIC	Negative	569.3659	5.62	unknown	1554370	2600049	1617061	1767795	2405183	3173852	2248569	2049628	2038309	1295033	1944056	1964418	2466315	2190293	2561541	2075987	2172656	1172410	2047520	
fpHILIC	Positive	129.0657	2.57	unknown	1100822	448137	922473	1157077	981530	881008	840109	736810	1217876	1335094	744766	677640	698080	750931	764058	716691	1091812	1108603	628688	
fpHILIC	Positive	638.3359	0.40	unknown	854881	1221673	858487	949492	1007456	1176613	882492	1233060	2091222	881799	958706	933027	1286261	1271474	580799	883539	963448	816608	1066065	
EIC	Negative	633.5094	6.43	unknown	4057194	5682982	3123209	7211298	6190308	4068446	4977802	5073348	7439062	2369934	2321529	2756146	4354600	2545044	1920969	2326202	3407727	3343091	3491278	
fpHILIC	Positive	249.1069	1.80	unknown	451535	1262769	1101538	1636933	1214465	1528489	1397251	1214520	1560159	1398955	1441500	1243128	1667228	1035206	1255753	1414913	1167956	1167640	1039707	
EIC	Negative	379.1561	6.46	unknown	494880	958146	541296	923630	703204	601879	5056334	6390586	449452	680686	494526	781703	559226	788591	606385	668768	572382	600683	539373	
EIC	Negative	381.2296	0.79	unknown	189668	177579	216739	599489	316770	762789	327054	1182752	155104	202365	296129	223126	121361	117401	667105	292507	214117	1135282	269574	
EIC	Negative	301.2656	5.59	unknown	412514	29991	157690	114936	332243	453641	172146	218340	147011	202365	296129	223126	121361	117401	667105	292507	214117	1135282	269574	
EIC	Negative	402.2225	1.99	unknown	0	136315	0	0	123743	183073	216827	0	182195	0	145650	155445	80880	89755	123679	145874	128612	0	96612	
EIC	Negative	506.3231	5.17	unknown	582616	573592	505182	530532	596862	772424	721332	578978	627209	502373	742289	585799	571053	595489	670204	627600	6562694	477688	567035	
EIC	Negative	602.3390	3.73	unknown	159780	761606	247640	286868	637390	480487	527974	372236	1010599	257389	465473	282920	537359	866171	428435	776921	596731	264554	392141	
EIC	Negative	251.1292	1.99	unknown	0	239153	0	0	233078	300708	204131	0	261387	0	224500	235147	253776	183563	176204	322564	255027	0	164535	
EIC	Negative	357.2523	2.15	unknown	398925	757464	447464	669771	653242	655366	750298	628321	634791	650368	614418	650899	527385	622930	619935	556400	633131	480380	557545	
fpHILIC	Negative	301.2173	0.38	unknown	2187440	4995062	3595959	4644469	5399841	2842588	4747932	2777947	12655842	2473651	2799136	2472343	5474768	2512716	2104977	4047261	4331247	2519334	2511284	
EIC	Negative	430.9688	0.55	unknown	170111	261436	325113	298251	253791	193115	323480	514834	335711	189923	294074	301424	326903	54546	245897	256075	348594	400334	159022	
EIC	Negative	509.3487	1.94	unknown	0	195873	0	0	376622	76434	346337	0	230732	0	103604	162835	79503	130617	267928	258588	137306	0	151393	
EIC	Negative	522.8085	6.49	unknown	1524403	2020791	1723769	1847741	2677131	1642823	1861441	2198421	1720120	1328664	1891777	1815489	1910067	1415573	1482796	1626803	2305937	2592496	2009566	
EIC	Negative	473.2830	3.70	unknown	0	0	61002	0	24594	636532	0	452775	0	37512	10653	21411	11196	23718	20636	24059	0	96499	19678	
EIC	Negative	443.8600	1.34	unknown	12462	72679	0	0	59332	85151	73986	0	99238	0	67727	56888	80603	77869	61782	80123	56226	0	48353	
EIC	Negative	316.1224	1.97	unknown	0	290890	0	0	231161	204161	190988	0	634927	0	234938	240770	557728	165296	224722	692761	242631	0	69264	
EIC	Negative	497.3065	5.57	unknown	434912	411910	411735	321683	423232	433920	421820	503850	313839	398357	324836	249756	258459	274249	294364	258343	357611	406064	351939	
EIC	Negative	323.1842	4.08	unknown	3349607	3073628	3879343	7289798	4856024	3938474	5306632	4857357	8686171	6242639	4696922	6044049	5654808	1784792	2603589	5144051	5028383	6486756	2242031	
EIC	Negative	564.2695	1.63	unknown	0	32764	0	0	29521	234786	304354	0	240875	0	239979	287019	323230	29298	36154	0	39222	0	259263	
fpHILIC	Positive	168.0766	3.17	unknown	357916	183522	201166	135576	189600	875576	408030	163830	193444	145486	167513	247491	185844	213762	175366	622585	307071	240819	297760	
EIC	Negative	247.1552	0.97	unknown	19262	13711	62219	10018	54262	11338	28172	58994	17164	16476	28905	54962	15984	13166	16174	23102	17910	9572	17082	
fpHILIC	Negative	197.0819	2.78	unknown	447877	425269	434112	1953924	834613	1040550	1406233	815441	1771238	1104798	1113650	1517206	1736445	169889	490470	1994650	724258	722046	237010	
EIC	Negative	312.2264	3.08	unknown	165309	99608	146156	160853	145109	136907	186853	146071	184154	1061194	1061194	103512	96897	77328	72699	124694	131710	117334	0	
fpHILIC	Negative	213.0227	0.38	unknown	1622968	975157	2650580	1834539	2056719	4427563	2284377	2644766	1189675	1796103	1536001	1959338	2138834	1657221	1475813	1692824	1798205	1569405	5684729	
EIC	Negative	383.2553	1.58	unknown	800983	1004920	666726	700190	969618	968311	946243	744172	983411	780079	956091	951284	1100666	916095	922515	972559	974630	550699	948474	
EIC	Negative	321.1689	3.43	unknown	2818558	2579776	2995099	6668811	4271056	3293595	4095156	4537305	5770246	4618405	3343717	5293397	4607333	1563065	2012797	3954610	3721753	5421596	1938416	
fpHILIC	Positive	602.1880	3.15	unknown	929431	935928	997919	858202	941609	1044439	977232	1196585	1004238	1027437	137805	1004238	1027437	880318	834912	894710	823706	830759	1079802	
EIC	Negative	301.0726	2.33	unknown	39668	141875	100285	0	98805	77146	133837	122107	40795	0	94215	0	16648	15022	58696	290177	0	0	53779	
EIC	Negative	330.2077	3.98	unknown	436695	267487	433686	382485	444811	299226	415131	459575	376505	368547	306759	321992	292883	280839	312684	321412	293954	370211	264195	
EIC	Negative	324.2186	4.00	unknown	171073	178813	137540	111428	176802	145969	168310	200800	133501	154017	143520	124971	133804	114826	161963	126957	164106	183198	152312	
EIC	Negative	619.0206	0.55	unknown	66997	283992	203584	242612	187742	140020	280697	687981	268982	121668	271599	294899	307274	47985	190796	158506	351906	358814	90323	
EIC	Negative	423.3495	6.72	unknown	83574	127566	169761	137128	232169	742469	137365	132026	96843	147008	157847	218115	81736	70636	123798	129394	0	266823	134548	
EIC	Negative	581.3654	4.34	unknown	990224	1784120	707576	581369	837487	1691545	727778	1621992	985798	1493364	871659	2611196	887788	812837	824343	868137	1529281	1478209	784398	
fpHILIC	Negative	383.0997	3.32	unknown	451573	230826	257563	319054	335638	523284	2199													

EIC	Negative	300.2626	5.59	unknown	3545022	416905	1385387	825175	2742888	3606904	1386978	1906266	1128087	506975	643317	418974	452202	607476	214534	407795	486860	876697	533685
EIC	Negative	291.0368	1.59	unknown	383855	827493	75855	55036	1056563	1929961	1020317	89595	365620	54711	862726	165041	73536	36956	460031	567975	54099	45521	42446
EIC	Negative	429.1956	1.77	unknown	168048	123210	126828	0	563273	38421	299928	178479	93357	65604	70552	121603	134396	144597	209569	0	115457	0	615470
fpHILIC	Positive	249.1514	2.46	unknown	486541	305470	336460	1051141	297025	415111	518610	288430	1657247	495303	509240	470445	493720	109253	239148	735893	245243	480698	237699
fpHILIC	Positive	548.2982	0.40	unknown	408550	478618	224445	268881	561132	757549	471481	507418	4158072	135858	338465	609499	875223	862597	306883	418444	381832	485224	527501
EIC	Negative	299.2591	5.59	unknown	107852944	1954890	6935775	3952005	13590901	17969868	6970958	9717642	5652751	2853229	3100761	1969007	2242045	2974110	1409563	2184621	2561464	4365512	2567200
fpHILIC	Negative	191.0566	2.94	unknown	50555	180438	99370	361827	293790	193822	15058769	265362	187445	113344	40967	69371	76959	191104	63304	169599	790164	422433	132382
fpHILIC	Negative	131.0596	0.49	unknown	2015014	1315599	1316183	1672666	2214389	2297034	1885818	995647	2091430	1787495	1910629	2273986	1348751	842080	2160962	1598714	1071853	1357161	975460
fpHILIC	Negative	160.0981	2.31	unknown	358959	307407	418509	575424	325379	450475	448133	346970	712498	359535	441464	452185	543407	187714	267631	634308	2811754	357475	281820
fpHILIC	Negative	152.0294	2.48	unknown	2715577	1532931	1737705	543494	1830380	2446486	1601239	960388	1994208	1098338	80278	0	1602501	3472449	0	67926	2540269	351226	116734
EIC	Negative	308.1598	3.00	unknown	201279	126358	140490	104175	156266	182823	155653	161405	135201	145658	131905	133846	113827	87307	124957	125321	21722	116622	91784
EIC	Negative	310.2108	3.68	unknown	204307	192851	165860	316445	259928	166597	288133	249588	364794	214779	148690	207560	173881	156748	157552	204194	238827	204885	195576
fpHILIC	Positive	134.0639	2.86	unknown	776651	393674	466193	608000	635291	977532	601601	397845	555886	459720	486825	543743	457449	601420	1038757	526158	491785	511100	294450
EIC	Negative	634.3347	4.17	unknown	2368520	2955800	2530424	2214730	2697809	2740611	2985458	2585531	3089480	2251161	2631872	2616052	2866481	2960897	2639975	2839619	2519585	2256977	2500108
fpHILIC	Positive	248.1487	2.46	unknown	4057309	2260916	2876578	8978147	2752974	3563200	3687251	2534627	12953754	3802728	3921356	3596028	4147721	1130765	1889564	6448228	2374494	4172708	1863218
EIC	Negative	411.2255	3.14	unknown	0	50331	23764	14663	0	0	374621	0	190769	0	0	15710	0	0	0	28423	16113	0	0
EIC	Negative	406.1895	4.08	unknown	118081	95664	97351	199306	138293	134108	161152	140510	191809	172245	134978	170218	167150	50438	81102	159557	151418	187952	68974
EIC	Negative	295.1544	2.85	unknown	1894611	1118567	1157028	2137799	1834281	1487975	1741141	1787073	1803227	1188658	1825686	1588849	793275	872936	1370041	1473631	2615182	810411	0
EIC	Negative	432.3194	4.17	unknown	112888	80894	138508	106414	100132	147655	119441	183730	97050	103318	108090	111102	84679	104707	110080	94316	106220	180828	62776
EIC	Negative	303.0877	1.96	unknown	0	0	0	0	160526	96666	0	0	105754	0	0	124505	82495	0	131214	124611	15085	0	0
fpHILIC	Positive	796.5815	0.44	unknown	955955	1193986	808262	1069377	1242498	1190109	1009887	1152882	902580	892519	858947	937517	858659	1018262	933146	909492	1234287	952393	949773
EIC	Negative	243.1965	3.59	unknown	1048239	314895	571965	543702	850042	1055424	512581	885865	548761	345951	370251	337571	321441	397217	250804	101607	362735	568221	367077
fpHILIC	Negative	821.5733	0.44	unknown	1459053	1364261	1257458	1119257	1484598	1157921	1089656	1209811	1632923	1243494	1368322	1559266	1251095	1327677	1511329	1049237	1502355	1055670	1323109
EIC	Negative	580.3623	5.40	unknown	164405787	167785930	169021492	155175970	166586720	185259651	171487030	172462465	160323384	149057615	174945315	179454923	172978005	163447155	170214195	160831664	173732745	159809650	180156772
fpHILIC	Negative	264.1088	2.31	unknown	415266	350970	489405	644485	356322	532288	533214	404774	791315	404119	535315	543043	556745	196900	311455	729877	347599	477665	347732
EIC	Negative	580.2681	3.98	unknown	129562	300437	94581	130382	289026	173479	168633	124352	602194	100783	149166	95238	152159	351239	152905	602194	251903	0	166460
EIC	Negative	494.2596	1.98	unknown	321719	306143	446497	278646	206719	410921	346150	647815	466440	268132	289640	295619	290869	963832	430934	163220	322443	283159	314863
EIC	Negative	266.1400	2.17	unknown	702665	1579514	487707	1015619	1016497	1022558	971945	847874	5502216	756146	1021133	997999	1776384	1547067	1121999	3043772	1898254	872236	638787
EIC	Negative	356.1904	4.11	unknown	865537	942725	552358	1835942	1194219	1165803	1674605	899255	1666227	1004161	948887	1325119	1536203	428503	899948	1839784	1442433	1136490	661767
EIC	Negative	601.3347	3.73	unknown	647443	3140014	803628	1138985	2520637	1806199	2170778	1251588	4252529	919915	1806408	1100333	2195464	3569080	1553926	3096294	2495184	924062	1587027
fpHILIC	Negative	249.1857	0.38	unknown	866605	1144756	1800622	4189845	1738177	1197448	2091835	2973043	3434432	1727242	1028409	1984000	1975744	792752	710856	1179101	2291891	2351164	1113872
EIC	Negative	587.3582	4.08	unknown	0	0	80233	355998	158300	111746	160634	148418	326769	210862	121437	210066	188471	0	20245	158307	156972	275828	15282
EIC	Negative	261.0744	2.09	unknown	166728	322395	0	36368	305347	298812	325794	200216	322802	1599100	309191	34816	171306	223013	287838	346279	91062	35793	260965
fpHILIC	Negative	303.2336	0.37	unknown	38868348	73059488	48898488	77960808	68095424	71616920	82647336	52972260	87542496	45988124	55008484	77274912	69511088	43888116	58164776	55731528	78535176	58446548	63663628
EIC	Negative	537.0172	0.55	unknown	158305	498512	433541	467294	374910	1169722	670266	511431	1169722	420283	485499	526487	559054	204657	385679	314986	610608	638799	187314
fpHILIC	Positive	805.6237	0.46	unknown	535795	270106	358359	424067	446085	506788	473373	480432	331846	601124	343284	479514	262145	259055	418838	375472	398758	467007	528766
EIC	Negative	453.2821	1.83	unknown	143661	3192022	0	0	0	0	10382678	2373001	1914239	0	0	114681	221086	0	200029	168596	164644	0	424817
fpHILIC	Negative	187.0030	2.48	unknown	1214483	595461	787223	207493	822598	957110	739306	444546	775673	957967	0	0	804795	1608548	0	0	1005026	186285	70126
EIC	Negative	512.9719	0.55	unknown	131561	208812	222343	231690	174345	140056	214375	450577	228243	114244	215539	249484	256161	20515	191365	204432	255920	300666	110874
EIC	Negative	600.3314	3.73	unknown	1923634	9414003	2441818	3417572	7398003	5299382	6345658	3792002	12522052	2696545	5272640	3324457	6624765	10680561	4696836	9263756	7167185	2634721	4713979
EIC	Negative	278.1843	3.46	unknown	0	207118	0	0	0	0	0	0	0	0	0	179163	0	0	0	0	0	0	219622
EIC	Negative	321.1743	3.45	unknown	2597461	0	0	0	4030478	0	0	0	0	0	0	0	0	124707	1880615	210805	189315	0	263402
EIC	Negative	240.1604	2.91	unknown	0	0	0	0	0	782240	0	0	0	0	0	345885	0	0	440864	0	0	0	0
EIC	Negative	325.1946	4.65	unknown	0	0	0	0	0	0	0	0	273995	314494	0	0	0	0	0	183778	0	0	0
EIC	Negative	555.3682	4.17	unknown	0	0	0	0	0	0	691106	0	0	389098	72426	0	647625	664396	548083	0	0	0	0
EIC	Negative	555.3682	4.24	unknown	0	0	0	0	0	0	406377	0	0	0	0	0	338170	336639	343094	0	0	0	0
EIC	Negative	609.3879	4.04	unknown	0	0	0	0	0	0	0	0	108465	266054	0	0	21983	0	101150	0	0	0	0
EIC	Negative	415.2113	6.04	unknown	0	0	0	0	0	440666	0	0	0	648175	44703	0	639418	46038	49134	0	0	0	380821
EIC	Negative	229.0538	1.91	unknown	0	345241	0	0	302212	208546	326385	0	351235	0	441292	356165	319026	365948	264684	362509	274330	0	218886
fpHILIC	Positive	171.0760	1.60	unknown	134457	270519	920691	0	1484855	0	243027	0	2694365	1087995	0	0	1918735	1606922	0	0	1375496	962429	1328720
fpHILIC	Positive	204.1336	2.61	unknown	941148	855701	668396	883022	995093	2081116	966128	784396	1262859	1030893	1608998	1360256							



EIC	Negative	328.2820	4.45	unknown	2264003	2161904	2058505	2262709	2275172	2181542	2167777	2227375	2178363	2164088	2254487	2291895	2223291	1907753	2066365	2190814	2136381	2365425	2018738
fpHILIC	Negative	361.1251	3.34	unknown	782067	675652	831387	948227	794417	919268	920736	841116	866218	844425	922949	712881	913164	445338	717910	606519	881518	700901	615532
fpHILIC	Positive	141.0626	1.84	unknown	10848311	5165684	5810342	7830783	8280533	13117774	8818261	7997405	7188232	6809500	6786098	6772473	5939592	4882633	7440140	11650471	6532104	7197580	5468628
EIC	Negative	489.2834	2.13	unknown	2742446	5060488	2297304	3379176	4673415	4347905	4919498	2982642	3657036	1309567	114029	120658	241655	24286	28791	285373	28514	941109	146166
fpHILIC	Positive	314.1231	3.89	unknown	670574	52051	0	0	285848	1115191	258819	242879	0	0	0	40811	0	258223	0	62946	0	322667	0
fpHILIC	Negative	344.1535	0.37	unknown	754729	996053	546709	1668259	626789	1052121	1003221	717997	2439471	561956	997742	1360703	1359591	717729	1175321	2320701	788694	423777	645220
EIC	Negative	581.3655	5.40	unknown	51853750	52855053	53320517	49250268	532599488	58724173	54429519	54314852	50538363	47115723	55686310	56762243	54735441	52046034	53478183	50830622	54877312	50721316	57129381
fpHILIC	Negative	611.1453	4.51	unknown	559387	244321	125375	270778	462671	735830	308046	238411	410469	217687	211845	390772	275834	351162	329200	381178	472528	362014	489241
EIC	Negative	255.1138	1.46	unknown	0	395289	0	0	345076	355019	360056	0	303929	0	373220	420038	361902	195596	250254	431733	283356	0	242412
EIC	Negative	315.2282	1.61	unknown	474496	405246	139353	0	390498	355776	622793	260581	395290	267966	364904	346399	442021	353235	369370	442593	368196	110848	603524
fpHILIC	Positive	173.0206	3.86	unknown	934874	997581	624468	686452	960144	1486161	874650	470991	744088	493448	685727	689335	636806	571049	754836	998917	850850	703636	838853
EIC	Negative	226.1891	5.57	unknown	450663	695604	1841256	3054334	1732640	862137	1385671	2199806	2957908	924264	478878	837817	1349869	316589	200881	1028260	1113769	1532239	459056
EIC	Negative	370.1685	2.21	unknown	67679	148148	64348	25505	121324	132034	118041	66610	118169	42321	107421	101354	107856	93172	134354	165459	106298	47087	93017
EIC	Negative	415.1975	1.45	unknown	0	520137	0	0	412205	563670	335536	0	524522	0	345409	452902	121077	257662	645503	344739	0	186582	0
EIC	Negative	612.3316	4.26	unknown	324638	609198	310116	364579	468223	573059	449647	401545	551379	394023	597667	473553	484278	466373	454523	559991	585210	329174	481322
EIC	Negative	327.2181	2.10	unknown	152418	68899	113919	62314	53991	110531	1305398	59148	99148	53153	50946	93104	86043	69787	52203	264368	82007	60671	749621
EIC	Negative	333.1314	3.23	unknown	0	76376	163310	124128	276388	233179	131098	203566	164089	265881	103350	116940	193759	154911	99193	58493	128518	149058	164126
EIC	Negative	487.1900	1.43	unknown	0	10451	0	0	99005	101334	46217	0	80251	0	24181	24752	78727	67673	81308	42664	41082	0	69574
fpHILIC	Negative	229.0538	0.37	unknown	633482	1044695	646910	216966	596009	693002	947002	673241	1063745	542555	936371	845708	667074	1135248	683040	730178	774736	598327	592651
EIC	Negative	552.2736	2.62	unknown	0	450140	0	0	402638	50287	4594	305334	401967	0	78428	385866	492024	409172	496620	81287	516017	0	87455
fpHILIC	Positive	711.0675	2.94	unknown	4659810	4794773	4649117	4850314	4854071	4844498	5135498	4540428	5479438	5035383	5092741	5431904	5364586	4473423	4752016	5226715	4688497	4784358	4905318
fpHILIC	Negative	82.9542	0.95	unknown	3190927	5884038	9807159	13411159	12332045	72513504	7751550	6625725	10283822	21767332	10717677	35815624	70673536	36444096	9588975	13851277	11477009	25417052	16854372
fpHILIC	Positive	427.0948	4.29	unknown	1191189	1612359	477766	863345	1692050	2275476	1790083	664279	1869072	774075	1440845	1880609	1666582	1707561	1858801	1717089	1710037	773106	1558291
EIC	Negative	552.5000	6.35	unknown	419006	453461	443369	623111	512088	584611	630543	566692	456089	213055	230624	304359	334999	274292	224609	2588150	295605	287340	267416
EIC	Negative	227.1285	1.20	unknown	97272	99590	116953	135425	105773	82837	134996	130715	137727	87548	71029	110793	125749	64883	74401	86153	101096	130492	100013
EIC	Negative	462.9630	3.75	unknown	946419	1344295	842851	1075622	1178596	1350878	1178712	930952	1397661	771247	1187305	979836	1065588	1008930	1205746	1200190	1018042	936937	920342
fpHILIC	Negative	102.0561	2.58	unknown	872482	398869	820329	1058869	827304	985553	772092	714349	924309	956880	629290	584261	623782	585661	646963	656684	896219	813286	539480
fpHILIC	Negative	164.0644	2.45	unknown	666041	871046	530418	324888	1012178	958312	1209538	501028	1191532	496206	1181932	1182918	1172634	929676	923582	1001644	989708	651286	1042632
EIC	Negative	648.3173	1.94	unknown	0	183974	0	0	202511	222556	267615	0	181276	0	17324	242727	143745	162991	182594	191422	205664	0	221711
fpHILIC	Positive	373.1799	3.72	unknown	4276864	3604983	3932783	3565204	4314885	4266759	4519786	3657245	3109401	3275847	3552808	3542490	3173350	2540342	4038480	3803150	3150555	3639507	2897155
EIC	Negative	499.9343	4.20	unknown	403012	529427	359084	431086	490870	495029	472028	379589	482789	340358	449417	412270	439300	470987	446643	461647	414057	364897	387614
EIC	Negative	243.1603	2.96	unknown	231287	217858	394743	329754	215965	252820	359658	549575	335994	378674	165115	355932	336670	158016	164093	248185	272637	350153	210397
EIC	Negative	317.1635	1.87	unknown	171895	86285	0	0	112018	166458	82283	0	432159	0	118909	132232	171855	130139	142156	127252	101666	0	57738
EIC	Negative	256.1637	3.03	unknown	78781	87418	100448	76343	57482	68350	113805	169529	108173	115617	53716	93134	78609	55502	45285	60396	75129	97534	63772
fpHILIC	Negative	84.9513	0.95	unknown	1274905	2134074	3539754	4505086	4287086	25684282	2731812	2204958	4642504	7490390	3596014	12904656	25296660	12902903	3240653	4895754	3901222	8892982	5885043
EIC	Negative	461.2902	2.12	unknown	55654	24456	68001	102086	59617	70951	24463	155487	96624	97909	31759	42646	49912	92938	62453	29834	43611	152843	37793
fpHILIC	Negative	177.0411	0.95	unknown	318800	284612	260858	431251	362494	338046	398567	245500	445038	670736	403742	315697	263473	261094	384164	506872	291883	261697	241933
fpHILIC	Positive	104.0709	2.57	unknown	59679132	34281272	52371348	81902936	59924872	79993992	57030504	58425608	62400652	48414148	34315392	37925816	36201380	30238928	34569156	44572024	39291648	43208116	44657628
EIC	Negative	594.9786	0.55	unknown	54780	160334	183757	146461	131499	169723	324586	481210	169923	581240	176922	183384	179144	0	122119	119972	223360	226514	567820
fpHILIC	Positive	105.4070	2.57	unknown	2712785	1481819	2456009	3695168	2834150	3793448	2762434	2582275	2671824	2307060	1575189	1768593	1504330	1374602	1519373	1938941	1884491	1942344	2042516
EIC	Negative	475.2672	2.25	unknown	370793	61314	452332	0	322183	22101	199030	1855695	227797	0	0	0	0	0	0	0	0	0	27199
EIC	Negative	353.2314	4.39	unknown	132334	60800	412832	329496	270818	157499	239467	515163	356414	242632	95225	165349	218793	91362	47887	187135	178046	315945	109584
EIC	Negative	382.9622	0.57	unknown	14158	0	38618	68619	10167	13172	19652	22533	176383	0	14708	9208	48049	0	7934	62571	0	23008	15527
EIC	Negative	567.3174	2.81	unknown	1246740	575339	1213340	453738	1540801	705933	1622879	757517	231884	265758	104414	47193	86875	0	14960	33459	16551	92729	206468
EIC	Negative	379.2478	6.20	unknown	272753	249957	93288	83701	155225	221015	166577	1040825	144028	408925	144028	242070	208021	187156	194256	183463	177005	123588	237393
EIC	Negative	324.1876	4.08	unknown	626104	552977	711801	1309782	893890	713023	948856	895910	1181117	1054408	829652	1046924	980919	320720	479266	928315	936094	1131983	392819
EIC	Negative	374.3713	0.55	unknown	53491	125246	133341	174642	118100	68698	151042	263714	136627	87937	129661	144271	143013	67561	123796	98760	161736	183353	69565
EIC	Negative	225.1857	3.47	unknown	218855	217451	253755	546019	299365	377140	347401	314967	486285	238555	271275	314890	287559	104031	178030	302572	194945	230005	159892
fpHILIC	Positive	142.0690	1.84	unknown	703144	325540	384614	461241	516728	889946	530897	489802	446853	424485	395417	421829	357347	303143	475536	719685	397165		

EIC	Negative	602.3467	4.14	unknown	193096	534655	294220	260761	389216	444047	432444	360702	461220	255086	475466	339401	405774	517827	335628	489640	409552	223530	356693
EIC	Negative	227.1066	1.56	unknown	63481	121492	56077	0	126258	139629	141305	48811	0	47650	118714	107955	100449	80806	143746	71243	100857	0	126417
EIC	Negative	454.2901	1.82	unknown	4033873	887470	1622645	0	2722819	4800875	2873631	776939	656267	0	38013	40743	76578	63208	65223	48965	33578	0	122193
EIC	Negative	360.0064	1.19	unknown	166543	171876	139349	129530	159935	184677	187899	141684	144992	145724	169966	161028	140463	157832	158285	139997	160915	126150	166951
EIC	Negative	600.3314	3.90	unknown	10299395	36786816	11115332	13623679	28152415	18869326	23773838	15680550	43890716	11237700	19306115	13236980	25918955	37759168	16433892	26583596	26100522	11984872	18793115
EIC	Negative	357.2589	2.01	unknown	5052043	12557884	4643284	367245	12713129	12517393	12943660	3973445	9820778	4174520	11950117	11812527	10170425	9325685	11530209	11781635	11561091	3587872	11524728
EIC	Negative	496.3049	5.57	unknown	1600706	1500709	1585424	1424082	1607282	1656964	1490057	1959071	1357273	1425155	1296587	999372	1144806	1182406	1194055	1086645	1425804	1527697	1305472
fpHILIC	Negative	511.4732	0.38	unknown	268878	798055	1294969	232192	1088091	884657	1380061	1558978	1781079	642844	319848	723987	1026075	285275	268956	654052	1092669	1082934	451575
EIC	Negative	420.9404	0.67	unknown	11766	59039	55718	55284	44786	29097	52160	114107	54065	32951	46321	61492	66229	5069	38063	43577	66970	76034	24615
EIC	Negative	356.2472	2.06	unknown	2793733	3791437	2559609	2235857	3657704	3698427	3738355	2456239	3369418	2509254	3493033	3581914	3391603	3286313	3451518	3588392	3448338	2044934	3496574
EIC	Negative	635.3419	2.65	unknown	0	75463	0	0	77959	81459	135667	0	72764	0	68559	90812	80141	77262	53136	82762	101535	0	120389
EIC	Negative	540.3315	5.10	unknown	862636	1008367	896130	898921	960611	981583	959340	915933	904281	923543	957049	8993213	916835	965588	946876	923252	901619	898081	936641
fpHILIC	Negative	144.0666	0.95	unknown	2038691	1462775	1487917	7173666	2654207	4517630	3493536	2154787	6275974	2236695	2578878	2873847	3370614	878705	1696735	5079379	2451859	1172695	901628
EIC	Negative	581.3572	4.35	unknown	1542826	416518	1714933	1487986	1518091	1688697	1632695	1663069	1659003	1950500	1817697	1604589	1598117	1902802	1499710	1527847	1635430	1481282	1871740
fpHILIC	Negative	101.0608	0.49	unknown	666174	543475	439593	583127	662028	847327	702515	357208	870394	628426	734715	976761	511829	329086	928107	720303	454701	367301	426730
fpHILIC	Positive	267.0082	1.61	unknown	122278	288821	0	451863	782503	441296	533462	0	737643	0	327425	562038	661310	710749	560339	519294	0	636790	0
EIC	Negative	535.2500	1.30	unknown	176729	98689	0	0	176744	171579	292456	0	150769	249664	150851	125949	53156	98536	125528	114376	154722	0	97569
EIC	Negative	338.1743	4.08	unknown	89182	65486	102668	270248	132179	112703	168436	149043	135917	162849	133597	179919	167819	7629	0	152583	136406	183909	0
EIC	Negative	298.1723	3.38	unknown	77605	131078	156937	423202	247835	160615	232955	221807	307514	166541	129279	254108	185155	73033	61489	130986	138561	303560	84446
EIC	Negative	249.0380	0.89	unknown	75944	93689	29642	26302	130217	99817	67534	63289	204555	63829	5580	70148	73964	77028	170882	37813	54760	170747	0
EIC	Negative	325.2658	4.73	unknown	561210	591779	493203	638334	599729	596478	560120	566766	574524	558684	580763	531958	536072	511846	550500	580076	526356	555564	546466
EIC	Negative	437.2868	5.74	unknown	1166510	1392593	1152380	1238128	1365567	1651062	1058181	1214800	1287702	921592	1096088	1062305	1083251	1249549	960043	1087205	1205142	1032306	1233438
fpHILIC	Positive	764.5318	0.38	unknown	346781	359035	269986	301127	388279	201850	243317	443490	561216	260126	210524	241988	213674	507802	209717	170254	287058	229190	206069
EIC	Positive	601.3247	3.90	unknown	3536528	12347248	3744896	4678882	9548784	6281375	7972347	5199631	14634124	3737860	6437402	4412593	8640206	12529423	5515038	8907029	2608138	4040625	6405299
EIC	Negative	552.3320	2.72	unknown	577033	0	0	0	337928	0	438952	0	281993	0	451759	306647	296516	0	0	0	285966	0	0
EIC	Negative	328.2932	6.65	unknown	158617	203671	233384	477960	273290	360382	420960	265550	246275	249836	387044	385040	272195	289850	256978	276220	320580	159808	0
EIC	Negative	498.9309	4.20	unknown	4129565	5522543	3790409	4708942	5107177	5400461	4756296	5034688	3652856	4933178	4566893	5052048	4806941	4948635	4830183	4368433	3777879	4096476	0
EIC	Negative	554.2740	1.77	unknown	809318	795605	745976	493145	551321	789081	1070132	1095786	619656	1177988	793055	1011015	723184	868985	491407	558112	631741	0	1020510
fpHILIC	Negative	327.2330	0.37	unknown	32716214	73663672	40384904	107444320	65692220	50759880	72651832	54733804	107106444	51203184	42856004	46553164	73541752	28933730	43375664	64539172	61572868	53455152	43472300
fpHILIC	Positive	156.0420	2.30	unknown	0	564953	557269	625268	606334	628207	548851	802720	240189	513560	453806	439732	465547	365669	548662	243853	130447	516955	179825
EIC	Negative	420.1147	1.67	unknown	0	91764	0	96738	87160	109965	88556	0	142759	40237	88896	75031	125736	17093	69499	95094	68522	62822	39596
EIC	Negative	363.2540	3.11	unknown	420065	95211	197688	27867	278074	106902	556948	79543	407798	17748	21949	18825	24804	23492	22532	13348	17994	17399	26785
fpHILIC	Negative	155.0098	1.97	unknown	1914468	1604034	1676728	2023921	2038056	2902587	2554059	2016012	1282826	1866582	1783512	1838974	1676489	1899891	2203912	1666795	2282886	2040576	1839645
EIC	Negative	630.3782	4.27	unknown	0	0	0	0	0	246355	184175	0	0	0	0	0	0	0	0	0	0	0	0
fpHILIC	Positive	215.1390	1.66	unknown	0	259436	204916	406882	226245	574410	159051	244755	317016	301133	340206	199444	198926	256112	341248	225436	193461	167681	0
fpHILIC	Negative	289.0688	2.77	unknown	278918	134209	160904	238940	299043	749101	215165	125314	100105	248586	295269	403522	121625	0	190513	146737	175410	191286	97761
fpHILIC	Negative	130.0590	0.49	unknown	21108112	16502648	16286704	16856042	20212794	24157010	20249252	10863980	25279060	19086146	20232368	24014904	15641117	10733741	25054636	17858858	12921660	11761450	12188534
EIC	Negative	297.1688	3.38	unknown	523210	867835	1100935	2671085	1628236	997515	1412932	1534321	1955034	1096139	793576	1352498	1142253	465218	373235	912797	955651	1962504	510088
fpHILIC	Positive	127.0500	2.74	unknown	1476074	945387	1127197	1399874	992050	1677308	1236365	1880755	1371388	1241210	893881	1294636	1115399	1196435	835098	1565417	1438289	1517482	107480
EIC	Negative	476.2718	1.82	unknown	692953	208024	230978	0	469759	744730	543095	34899	133042	0	6739	0	16025	7098	15612	9844	16207	0	35403
EIC	Negative	516.2472	1.03	unknown	0	105455	0	0	69494	101367	139818	0	70721	89238	95271	128960	92043	95251	79219	71048	81699	0	108917
fpHILIC	Negative	192.0666	0.61	unknown	17130956	20580484	9008398	6275455	24873676	51069000	21091468	9284894	11339575	1396118	3978957	3820710	2383723	3574037	2858755	4592358	3897922	1852020	3351004
EIC	Negative	251.1269	3.23	unknown	377956	581093	1626476	1626476	959742	559323	867818	736534	1117950	956400	495122	821916	712471	430276	351193	572606	706390	742279	541290
EIC	Negative	381.1648	3.46	unknown	187038	64750	144086	91322	118616	130858	162825	273644	59975	167450	70641	102728	88645	83178	102569	104799	104801	221087	63101
EIC	Negative	602.3382	3.90	unknown	804096	2858097	879758	1022739	2129067	1452834	1777923	1231952	3287505	926276	1604663	1059522	1997369	2791377	1342976	2077322	2054345	1035913	1439404
EIC	Negative	540.2733	3.10	unknown	485054	483838	263908	372672	458975	586661	388188	324652	813360	356850	355807	468015	385000	330485	517332	511814	562810	124906	524172
EIC	Negative	283.1030	0.57	unknown	145736	74489	308605	557961	156416	131193	192198	183864	1185292	775811	161249	133021	304171	57129	72367	369732	100741	285731	162144
EIC	Negative	580.3623	5.17	unknown	7599180	9749969	81691353	7376012	87580101	106620533	105893560	84366132	78079349	67927230	99042912	99250348	91175401	96785742	98787692	89224813	9464968	72919833	94974114
fpHILIC	Positive	115.0636	1.80	unknown	1747090	1407393	1418193	1674235	1599030	2088228	1814173	1405467	1802035	1520780	1602412								

EIC	Negative	328.2360	6.41	unknown	66443948	111560428	92281229	149884830	109969306	99632978	123468896	111028148	126869670	88049030	85779607	93168312	110545863	62591953	74818460	97712562	106570536	91240134	73916854
fpHILIC	Positive	233.1579	1.83	unknown	1345933	2256905	1709549	1677123	1745295	3095813	2370206	1568914	1582392	1070840	2136833	2065942	1860629	3151748	1556308	2257825	1695897	1151990	1615629
fpHILIC	Positive	190.1630	4.65	unknown	1079502	523766	408501	935699	870535	892660	789419	626088	1112411	611417	670595	808396	829673	731270	1029787	875605	846375	557618	744041
EIC	Negative	540.2736	3.44	unknown	211069	224657	80183	122827	177646	266551	155712	112080	349505	153964	138649	205092	137573	138397	199139	218148	257750	79396	241320
EIC	Negative	529.3010	4.17	unknown	0	0	81566	0	0	0	0	0	391317	0	365574	0	0	0	0	0	0	345794	0
EIC	Negative	608.9910	0.55	unknown	312023	1625031	1275242	1767896	1020568	857238	1415951	277886	1466309	465676	1416646	1770434	1762296	57220	947916	1034572	1680902	1768246	399357
fpHILIC	Negative	277.2172	0.38	unknown	12885396	18894370	27203476	41722568	26918814	17876900	24131362	26718798	3995308	18517540	14654418	19787326	23569852	11557058	14177434	15589179	21949066	21681624	16567714
EIC	Negative	358.2080	5.81	unknown	116527	311260	186000	696781	388827	181094	269829	340510	660787	175690	202702	162239	314521	134509	140358	236376	356031	191329	106343
fpHILIC	Negative	239.0165	3.87	unknown	947505	2528010	473297	731700	1507339	2784722	2646857	623941	3484681	495123	2737188	1883571	3619751	1982680	3321791	1897944	2378304	678400	1953505
EIC	Negative	570.3687	5.50	unknown	286052	391821	279649	316670	359928	401384	343291	328330	296100	243458	348330	352359	329471	343004	314517	290450	318233	249698	352189
EIC	Negative	321.2061	2.88	unknown	406750	140031	128347	130418	218690	433958	303451	253300	103959	32762	37771	26825	26936	24778	33550	31630	32965	32525	27814
fpHILIC	Negative	628.3253	0.54	unknown	6855852	13574518	62471125	71244412	10887976	11446018	11086338	6612682	12953935	6938522	12529831	9889809	11320655	9039957	9499987	12551374	11994434	5430054	12199889
EIC	Negative	291.0368	2.17	unknown	52424	97671	126492	31296	68537	181334	119005	41223	24380	30857	235033	64129	0	0	84212	117707	0	0	0
EIC	Negative	388.8248	0.52	unknown	186787	117700	162441	151059	253329	143513	177440	151057	128797	188040	157191	119267	157976	370378	187658	112188	118662	147375	153664
fpHILIC	Negative	115.0402	0.44	unknown	2107383	3224022	5602420	5431533	2974323	3661563	5413852	4704476	4224624	5532155	4313629	4353094	4487072	2876362	2873756	3806124	4662326	3834824	3730652
EIC	Negative	315.1249	2.05	unknown	0	80683	83988	0	135309	118040	170059	0	13025	0	36069	0	0	0	183342	112221	104851	0	90008
fpHILIC	Positive	729.5887	0.47	unknown	425370	470084	361749	376669	552283	348905	411124	319058	626799	442577	442745	345062	358863	501505	438841	461189	522826	416716	396942
EIC	Negative	271.2281	4.66	unknown	3598476	2972024	10692136	10551480	8108157	5196468	6417696	12152642	9454848	6228982	3305599	4966363	4404419	4193839	2037044	3855850	4748938	7609810	4986933
EIC	Negative	473.2831	6.83	unknown	95598	107435	99283	111502	94067	108153	148721	118914	81282	58771	87851	62946	74990	65768	23042	62709	26662	52300	29113
EIC	Negative	253.1446	1.92	unknown	0	283785	0	0	217801	123149	279356	0	379870	0	211603	175612	303036	172511	199573	269816	218973	0	140667
EIC	Negative	280.1197	3.22	unknown	61765	36352	118975	51205	134782	58082	71496	137847	50952	85098	53114	14289	9896	34545	148085	9137	46908	87420	32075
fpHILIC	Positive	104.1073	4.07	unknown	285827552	193999568	214999376	180055290	203876448	259605792	238174832	216200768	204526016	182276992	144960384	183762304	153304512	138076864	201599920	215368480	166120896	211435216	195510384
EIC	Negative	391.1513	0.74	unknown	174857	131289	88614	94049	131017	118826	132216	150434	145494	123551	108290	133159	120095	105847	138919	119360	129632	105595	132366
EIC	Negative	523.2661	4.03	unknown	114848	534604	121301	203406	361404	411645	306130	163735	437028	187740	378876	322564	388746	508075	369759	272712	378679	22285	370020
EIC	Negative	538.2452	1.27	unknown	371649	371695	241507	105141	397748	498853	647239	45742	326525	497942	311986	499104	430645	299289	255804	374899	371936	0	383117
EIC	Negative	357.2051	5.81	unknown	527571	1365528	857419	3050116	1492626	815253	1232093	1396851	2918604	928865	795287	687869	1489241	604807	726661	1094695	1418671	817965	517470
EIC	Negative	315.2328	6.39	unknown	1747166	6351818	2859393	6464028	4665169	4456841	5755302	2595327	15787898	3949779	4525350	2385556	5532704	3475289	2581644	4661508	4637287	2810698	3480185
EIC	Negative	415.1975	1.87	unknown	701856	2440865	0	0	1560410	731604	1945265	0	4586470	0	1215242	1070837	1775141	1402198	1936410	3365738	1223937	0	1003219
EIC	Negative	379.2482	3.12	unknown	141268	68975	160935	85447	82483	94311	121211	169075	175702	312619	90851	95178	98831	118977	92098	137507	101317	136336	103999
EIC	Negative	605.3660	4.80	unknown	6723319	14600435	10286573	7845575	12207987	14648471	13598401	9079758	9364243	8133968	15171725	11328466	12305378	11233473	11221435	12306022	13928386	6192010	11997372
EIC	Negative	381.2627	5.59	unknown	1190229	136199	456823	201813	753101	1037296	404462	582722	317164	185818	204832	162495	147611	201492	107656	127204	163595	259956	164188
fpHILIC	Positive	362.1192	2.08	unknown	593051	45244	201909	41586	297611	453535	230641	0	327565	0	0	0	279972	300494	0	0	346424	0	0
EIC	Negative	231.1758	2.65	unknown	172040	228269	273393	245329	286970	197965	268480	348108	152678	261322	229527	186830	155733	177472	168671	138950	152902	366729	327024
EIC	Negative	372.2401	1.87	unknown	133847	101810	0	0	131234	143036	129947	0	189991	0	121839	148659	127582	63762	58682	98673	96699	0	93823
EIC	Negative	285.2075	3.47	unknown	0	102385	280577	182968	47511	193917	243952	341981	73910	227943	117400	168872	60474	110696	135769	69646	141394	268960	75789
EIC	Negative	347.1870	2.44	unknown	584344	2090083	597294	883526	1179478	925309	2223605	1708344	1231203	891230	265827	2505859	2158591	1782644	2284116	2224883	1759130	288719	293194
EIC	Negative	399.1701	4.08	unknown	198644	177090	220053	478854	300722	248506	307746	316832	415510	396883	328016	387167	335173	98577	153983	328574	324809	493120	191963
EIC	Negative	310.0722	0.69	unknown	71472	5306	0	4064	0	11805	0	154765	73825	4147	15489	0	20289	74705	17510	31810	42933	24927	17031
EIC	Negative	307.0315	1.26	unknown	461536	729079	70394	35853	846478	1040800	666251	28456	382904	506227	118317	51121	18429	311816	232860	42778	0	34982	0
fpHILIC	Positive	133.0730	2.45	unknown	554762	203135	584765	490164	337584	642005	200291	670821	1234712	472300	330369	730452	734674	746327	191005	465249	706464	412068	342070
EIC	Negative	374.2572	1.81	unknown	1034407	1075520	962694	0	957634	1037986	1084294	790773	555871	979350	925296	1035985	973040	970480	1010710	1032182	0	976787	0
EIC	Negative	241.1808	4.39	unknown	3745139	830441	2427949	3456933	3255855	4199601	2188552	3331216	2342939	2041783	1046609	1309703	1347810	659119	443874	954289	1277762	2786624	710648
fpHILIC	Positive	639.3408	0.40	unknown	349096	391444	405992	375074	338969	452474	364962	327132	326751	345747	475867	486026	398244	242918	443874	336245	398244	338723	401018
EIC	Negative	296.1580	2.85	unknown	307760	190088	211035	301351	290276	237996	272123	250911	311801	311710	197169	298173	262671	125992	148142	210848	238859	406298	117611
EIC	Negative	320.1566	4.90	unknown	78061	91453	0	0	191311	93345	21645	0	0	0	0	0	0	0	0	91493	0	0	0
fpHILIC	Negative	308.0982	3.20	unknown	652808	466331	532480	697371	850967	885741	645100	438788	615188	528460	639394	499291	501081	408719	533999	655381	545286	556551	610096
fpHILIC	Positive	259.1134	3.32	unknown	4899200	11222589	4979366	4387583	8001451	986221	11001331	4850632	956438	3544609	8611073	9931514	7432874	7259803	7361684	9877002	7881716	5285608	10226306
fpHILIC	Positive	544.3386	0.56	unknown	144401184	142307840	184467184	148212904	144076160	169291632	188346168	163894768	114308776	133892392	132433536	164431848	150639904	121547464	129724608	128941096	159466096	145421680	141910944
EIC	Negative	594.3777	5.75	unknown	369661	470646	378707	302000	446076	549738	549037	460672	376442	239131	40704</								

EIC	Negative	304.1173	1.81	unknown	85763	51953	0	0	64131	144221	71100	0	35764	0	55680	89227	77382	40467	86668	79076	92634	0	38878
fpHILIC	Negative	305.0681	4.52	unknown	452090	238038	121176	205175	308904	558818	242259	198256	280659	178929	149419	307654	0	239925	225544	283970	385435	264157	354632
fpHILIC	Positive	114.0988	1.80	unknown	486195	423762	398617	403928	360775	541417	459563	361367	468025	384128	415236	442732	449934	306575	336823	459282	390133	334711	320500
EIC	Negative	397.1551	3.43	unknown	159103	171402	197457	507408	277542	219963	274884	331640	396806	318553	281001	402340	328810	108649	151701	269630	269742	440039	138088
fpHILIC	Negative	310.1288	2.70	unknown	238550	262295	592104	164487	414588	275658	335000	421351	260142	312105	526849	369634	305562	432779	108528	277590	186660	156069	223477
EIC	Negative	327.2907	6.65	unknown	743919	822423	1111322	2243462	1218435	1601832	1347830	1607366	1278177	1104917	1116639	1667153	1703491	949688	985368	1165443	1242882	1354002	772797
EIC	Negative	500.2789	4.64	unknown	168351504	213584558	158801883	165319160	199871990	208721496	193056103	171062162	173252379	129589405	164398571	157099119	152766540	197209026	175662575	116630141	187964440	153523112	184786715
EIC	Negative	442.0091	1.19	unknown	123164	126380	107881	97030	122166	131958	126470	101141	113173	112587	122442	121215	118792	119266	115339	102664	117913	90859	127083
EIC	Negative	272.2315	4.66	unknown	605832	584911	1944406	1924343	1462117	917323	1050735	2254454	1739771	1095389	603854	938648	742561	692995	367452	668035	858140	1339821	637577
EIC	Negative	269.1402	2.34	unknown	373823	207239	43374	88596	266542	213055	244372	130039	337145	127101	153117	49813	219984	95401	108075	199520	40817	89482	66925
EIC	Negative	583.3811	5.40	unknown	0	0	0	1677999	0	1941029	0	1851288	0	1578695	0	0	1753281	0	1637309	0	0	0	0
fpHILIC	Positive	288.1915	2.29	unknown	541522	520765	447639	707175	652750	549538	522406	507350	569403	578660	400079	480352	676200	386746	231457	429252	467400	664984	434686
fpHILIC	Negative	841.5428	0.44	unknown	159392	325545	212724	140934	296993	287894	393963	150926	682797	209240	309231	317909	342951	328313	314225	346888	296925	89552	263056
EIC	Negative	255.1604	1.94	unknown	66587	178223	0	0	165913	243452	165910	0	176297	0	176751	267665	283123	149141	203850	221641	151844	0	133382
fpHILIC	Positive	115.0697	1.80	unknown	6901747	5718647	5540251	6289859	5729195	7698963	6595799	5620990	6831304	5707622	6457380	6114718	6789690	5071783	5757405	6960401	5302193	5604775	5181598
fpHILIC	Positive	828.5493	0.43	unknown	73689	571508	260739	355594	515073	359054	456886	233947	571486	333424	382807	479583	606406	438967	395288	480529	401081	296303	414852
EIC	Negative	604.3628	4.90	unknown	2957451	4221865	3724941	2610157	3645775	5377367	4301868	3845592	2291949	2393688	4108623	2963556	3107437	3317190	3454458	3039017	3594698	2182743	3522837
EIC	Negative	438.2490	3.17	unknown	170336	161771	174617	172386	173363	174390	171191	173661	174390	167379	197536	177420	172450	1660357	170570	164859	169801	170035	170672
EIC	Negative	269.1374	2.12	unknown	56412	77687	170117	0	132092	99819	0	314305	0	260615	0	0	44658	0	0	0	0	0	342216
fpHILIC	Positive	164.0731	2.73	unknown	690136	281391	242907	780470	496270	497328	472898	356533	801038	513178	423163	316833	395136	177116	320595	665274	323256	5211776	237955
EIC	Negative	548.2644	1.28	unknown	66089	106343	0	0	90549	78378	131040	0	105854	72698	92148	86164	106287	75373	80363	87428	108762	0	118791
fpHILIC	Negative	233.9133	2.09	unknown	602298	1133172	585704	285520	602897	573751	1839105	965341	182451	383523	299802	1273739	834751	1293214	45991	535347	149815	366149	148708
EIC	Negative	578.2732	1.87	unknown	458599	371055	0	0	318740	438013	683396	0	369718	0	416289	487249	431834	312444	347261	309864	419520	0	517522
EIC	Negative	430.1989	1.41	unknown	0	353216	0	0	365834	26476	360433	0	139657	0	200355	144242	183975	115544	336399	286564	99693	0	71369
EIC	Negative	263.1294	2.04	unknown	131546	145381	338867	94924	216768	270170	263427	249356	31833	171925	244342	220339	176162	105736	200039	154744	164719	97837	112350
EIC	Negative	372.1855	2.64	unknown	71748	619744	147298	492565	584141	895942	647278	118445	403183	452875	567794	624742	561388	508294	663287	708325	515968	80960	437738
EIC	Negative	464.3102	6.03	unknown	385896	549922	376222	462854	576841	590054	424469	400584	432106	110947	430715	435024	384227	428290	445437	396318	458807	365158	519323
EIC	Negative	272.2314	5.12	unknown	121005	138165	315147	313783	236777	158297	210350	338311	270057	170947	711129	119859	179636	194135	66668	207045	144282	288458	119319
EIC	Negative	522.2627	4.02	unknown	485434	1704906	408535	737581	1193830	1331869	943122	526827	1473935	556614	1312919	976495	1247422	1605223	1172245	951509	1295071	545122	1142122
EIC	Negative	503.2995	4.45	unknown	0	59850	0	0	997073	0	0	0	598056	422724	0	609346	550788	0	0	60546	0	43120	696969
EIC	Negative	607.3717	4.80	unknown	272870	516370	362956	267431	454458	520592	466683	320806	319535	296143	568595	400827	430288	398634	403963	419689	520513	227266	418124
EIC	Negative	630.3782	4.93	unknown	0	695224	0	0	1602415	1107577	0	0	1052665	1406859	0	0	484867	0	529973	0	0	0	995969
fpHILIC	Negative	302.2201	0.38	unknown	379707	1181445	1027392	1395901	973454	583866	1141396	373775	3424782	720645	677629	644741	1173195	551082	630351	1059593	906988	710124	551581
EIC	Negative	365.0326	2.04	unknown	324016	316427	487156	109417	182817	693960	990252	0	109638	265492	516579	253295	85308	156408	30425	272929	270329	134240	475336
EIC	Negative	254.2203	6.42	unknown	19000073	27846856	53621314	59120330	42855439	32022594	42421449	50869456	60501767	33920239	25577959	35541974	41957820	21988831	19658806	35890008	39095290	14844635	19381106
fpHILIC	Positive	151.0477	3.46	unknown	554078	574961	594411	601187	597234	569675	695085	666418	563374	593104	620112	654578	653172	418603	547491	611029	638688	630211	0
fpHILIC	Positive	321.2012	2.30	unknown	5968768	4163284	7871962	10376188	5509790	6554985	7507921	8702761	7866764	5678904	4286457	4200576	5832563	2368789	4844713	5872572	2439492	6847630	2048633
EIC	Negative	335.1536	3.43	unknown	287085	238545	333461	876588	446305	320145	437369	543776	657993	548344	339126	545660	493770	152798	199933	431157	384400	560450	169715
EIC	Negative	322.1723	3.43	unknown	521296	473108	580448	1219833	688795	605638	730302	807539	1022418	803263	667699	956361	866287	282592	364628	710290	681407	1086491	356178
EIC	Negative	387.0262	0.54	unknown	5298966	14012276	11737952	16002640	10039294	8288553	12550915	23312081	12187588	6186052	1119787	14301235	15468548	5762143	9104292	898676	1390880	15022746	5154523
EIC	Negative	353.2002	5.50	unknown	2351757	1117471	1368252	1468766	2246094	856602	1182209	1333916	872961	1333916	1707518	749181	786005	648665	1344517	2108101	1494632	1195360	0
EIC	Negative	299.2527	4.62	unknown	471116	193559	179274	312971	162858	308747	227882	1033953	189254	667962	408153	441347	463823	552145	201126	372204	497091	147456	388967
EIC	Negative	392.2639	6.44	unknown	4547887	4187834	1327688	3485930	2792533	3903842	4874795	7117486	4904661	3151301	4029412	2059468	2833983	3408227	3298360	3312597	3333500	1982761	2212883
EIC	Negative	501.2819	4.64	unknown	47290073	60593287	44499575	47176474	56577468	59609138	55405847	48348014	48543791	37465543	44606758	44916815	42935516	56390632	49639248	33269753	5320722	43916833	52565888
EIC	Negative	300.2626	5.71	unknown	1019786	973594	2956000	2840350	2027478	1385296	2018703	3272635	2365274	1530572	924504	1188281	1330225	994904	498927	397925	1232801	2291723	987979
EIC	Negative	375.2481	5.49	unknown	0	257592	25350	0	145454	0	239970	183934	275999	0	0	173156	0	0	0	210606	0	0	253704
EIC	Negative	271.2282	5.12	unknown	718495	655073	1749804	1640711	1170037	936211	1091660	1861301	1507779	919312	657656	751234	867556	1032054	610696	955960	808725	1523470	820854
EIC	Negative	231.2108	6.16	unknown	48026	45056	36418	336344	157971	17171	145308	177468	165935	60072	36826	130909	96320	0	144670	76619	171207	42914	0
EIC	Negative	272.2314	4.22	unknown	304129	311874	917352	931698	703494	468071	555376	1096284	758703	458518	298979	364230	387641	432708	182266	376118	435332	679667	380202
fpHILIC	Negative	26																					



fpHILIC	Negative	175.0441	3.81	unknown	340281	226858	226932	232029	203024	396261	151317	156305	705531	176119	181567	326443	214159	194523	181622	202523	225762	255035	193201
fpHILIC	Positive	87.0796	3.36	unknown	586463	623077	278389	253698	395818	664077	514194	347888	438946	322939	315096	453144	498030	644184	487258	536737	352827	479054	287045
EIC	Negative	299.2593	6.48	unknown	4576471	10410487	11985808	11778183	11443757	11421478	7304999	16494675	8013258	6995091	4964486	5061996	5046449	8039051	5422724	3052924	4963356	9302209	829465
EIC	Negative	353.2132	4.22	unknown	168597	162171	409930	409287	321683	221271	262364	477617	234309	210466	147694	179157	188644	225516	111386	163675	193990	306539	163859
EIC	Negative	503.2870	4.64	unknown	1287923	1706554	1106546	1206433	1483592	1608012	1538374	1229325	1345167	973401	1336683	1130856	1115831	1440913	1267356	852546	1363491	1127407	1304720
EIC	Negative	337.1693	4.08	unknown	413316	355942	488907	1250406	653332	508963	730667	674682	1010173	814010	640747	802582	826117	219257	290312	734248	681864	900295	258164
EIC	Negative	469.0291	0.54	unknown	2849583	71382862	595733	8201409	4880786	4193618	6098606	11974744	5945300	3303280	5636015	7051441	7564093	3103898	4273237	4261993	6958979	7361554	2595041
EIC	Negative	371.1891	5.81	unknown	113615	284433	157563	662915	307313	159239	235724	255705	621181	189185	149844	144604	363598	114942	146975	240782	297588	157934	1084126
fpHILIC	Positive	455.1799	2.62	unknown	1906427	1249114	1023832	1414848	1545558	1731731	1380878	1600878	2188059	1532351	1061293	1763601	1668622	1046914	1053294	2036889	1909055	1619662	1071129
fpHILIC	Positive	307.0831	4.52	unknown	388058	151509	81704	197222	291094	620941	203035	146292	276598	151020	178495	311350	174629	272149	189444	278450	281817	249197	325648
EIC	Negative	349.2385	2.25	unknown	170144	0	188317	171210	103083	120818	80536	484629	497920	110412	0	0	0	0	0	0	0	469441	0
EIC	Negative	629.3659	4.78	unknown	2748733	4206098	2400651	2638354	3634729	3042706	3312382	2832031	4372278	2383256	3670554	2758344	2794956	2854993	2531987	2685441	3151188	2130227	3108117
EIC	Negative	251.2015	6.28	unknown	5014556	7119835	8628276	16011932	9833643	7853688	10864865	10186582	12432189	7948753	5704132	9283970	10609802	4338826	4414317	6754360	7542501	10003519	5311264
fpHILIC	Positive	190.1429	2.82	unknown	323355	488868	293199	405470	354902	631523	282963	162243	804380	378506	351031	409906	462702	303861	357130	512859	368125	315407	308666
fpHILIC	Positive	534.2936	0.90	unknown	282980	453273	430779	321419	409963	505104	640019	224670	467391	248238	373047	406750	379131	355821	387664	395756	300588	196329	338165
fpHILIC	Negative	165.0555	0.57	unknown	10805295	2189300	2419653	1688705	5056176	19908718	2370850	1522517	2164094	2321714	1964072	2114897	1809671	2986075	2799424	1542405	1566311	2253822	1848958
fpHILIC	Negative	132.4748	0.54	unknown	654394	287353	190641	341797	440851	391426	321348	117755	442978	177515	305888	310258	264825	248153	429256	211294	184197	118549	254172
fpHILIC	Negative	271.2278	0.39	unknown	0	1821260	4594227	5860128	3006040	3121304	2895988	4610733	4452030	3548310	2186911	3225104	2779212	2094645	1320882	2804115	2462310	4214241	2454579
fpHILIC	Positive	781.5547	0.44	unknown	1034233	2311756	1550764	1676720	1639500	1703105	2148785	1503208	2854769	1234385	1658464	1567938	2000318	2616721	1747443	2003759	1753726	1202124	1606075
EIC	Negative	300.2627	5.51	unknown	311460	259435	682333	622914	496186	325915	389908	852334	246172	384920	578131	279470	284426	330674	167979	264626	296932	524641	255959
EIC	Negative	598.3732	5.46	unknown	8106720	7698278	8551115	7619898	8726361	8302334	8601255	10001342	5742072	7837681	7448362	6463620	6928022	6842384	7536317	5840779	7205882	7815508	6431246
fpHILIC	Negative	299.0984	3.34	unknown	705201	539757	597051	624976	682999	657064	695674	594711	605097	571882	596217	646804	571136	384745	538341	594175	710582	559377	540851
EIC	Negative	327.1633	1.83	unknown	0	23209	0	165116	134398	0	0	0	0	0	0	0	0	0	0	0	0	0	69842
EIC	Negative	397.2048	6.23	unknown	97890	216426	155315	258321	161760	123075	149589	185276	486235	210901	163028	94903	223091	131819	114726	394913	230437	136709	112731
EIC	Negative	435.2327	4.13	unknown	240744	211608	421239	502062	379096	254804	371837	575600	370423	492517	228511	239675	218043	423798	168460	189818	310366	526798	297795
EIC	Negative	301.2659	5.71	unknown	118932	111687	351496	340545	230301	156496	229169	391936	287635	707076	106859	140130	134914	121002	60093	112324	150553	265999	138160
fpHILIC	Negative	310.1134	3.32	unknown	998668	1148569	820117	2491503	1404915	2508662	1119451	1269654	1428733	1521372	1760381	1572582	1570971	732966	1005314	1515448	1794785	1512609	1409216
EIC	Negative	632.4754	6.44	unknown	1353601	1837760	826942	3804821	2064410	1229640	2226569	2064754	2965573	1157854	1348482	1125010	2452533	837703	846790	2236455	1486936	1321205	1079672
fpHILIC	Positive	190.9925	4.01	unknown	276818	421143	505438	371387	386247	252174	428729	657008	376831	546377	529237	225039	254213	685672	713264	198111	271649	394041	358066
EIC	Negative	389.0306	0.54	unknown	143505	356878	295356	388464	249997	209337	290574	601967	286698	144774	278946	337000	181076	154585	211921	225761	351636	380448	113518
EIC	Negative	599.3781	3.16	unknown	407327	350592	378427	424354	394657	503631	416120	484193	272015	382175	352936	435384	352026	239146	327791	327328	401310	478860	342153
fpHILIC	Negative	295.2274	0.39	unknown	1856855	1797972	3389772	4491974	3099130	2236323	3076267	3286371	3487290	2493490	1619219	2415189	1816752	2354699	1474531	2707508	2380704	4215994	1798394
fpHILIC	Positive	320.1239	3.47	unknown	977715	700456	783886	1029105	1139238	1085606	944578	1068772	767706	2909938	1101348	1179967	1058825	892436	1023237	1024567	933721	1105196	477829
EIC	Negative	417.2042	1.87	unknown	28623	116101	0	69517	39130	37724	0	197694	0	65161	54058	63240	95651	84814	127485	46862	0	42195	
EIC	Negative	288.2260	6.35	unknown	236220	256450	536852	674061	391922	506224	378605	509622	328083	436660	250346	413357	309679	228655	173543	301945	400695	449278	231612
fpHILIC	Positive	371.2992	0.60	unknown	677761	250093	908426	1315930	647322	864176	730178	940744	1276702	623611	639294	535568	907638	0	235278	735231	561695	582381	151577
EIC	Negative	351.2163	5.06	unknown	87555	61442	101708	247767	120012	97146	107969	139123	169490	164261	54632	72127	51804	34835	123003	139752	140359	43942	
EIC	Negative	391.1749	2.85	unknown	500423	1280480	276313	550607	643067	965906	652162	799259	381476	1243919	1236695	814437	439499	600172	762630	574061	716814	940718	326135
EIC	Negative	605.3555	5.31	unknown	0	1938334	0	0	1581428	0	2198200	0	0	0	0	0	0	0	0	912899	0	0	0
fpHILIC	Positive	220.1174	1.65	unknown	0	51940016	22024240	28259054	23277452	57460720	36245272	0	38888924	23364996	38507824	37610184	32350848	33341476	51340200	50996372	15798013	23301850	0
EIC	Negative	606.3784	5.50	unknown	5254512	8588420	6933758	5693985	7609802	11874125	7868372	6711212	4842624	4840239	8667315	7500210	6707696	6968040	6632922	5946835	7435700	4550279	8178127
EIC	Negative	630.3782	5.28	unknown	2901278	3134337	2732899	2794510	3623278	4548473	4139793	2888780	2137950	2160115	3924800	3828800	2775714	2316232	3233923	2672015	3458887	2311088	3296479
fpHILIC	Positive	273.1206	2.29	unknown	0	520438	925816	688675	524200	618571	525195	851556	363923	274188	406477	200076	324060	160275	233491	271408	0	572080	0
EIC	Negative	316.2570	4.03	unknown	548505	554505	28682	1896055	855129	765427	844609	1149590	971721	761395	524732	898625	838074	671471	360109	1513009	726416	1304147	22114
fpHILIC	Positive	257.1508	2.29	unknown	2106079	5608421	7440330	10328407	10178366	9595215	6050910	9152170	3696466	4160075	4201882	4380364	8659962	9312639	9518342	6682865	1232834	6332949	1588887
EIC	Negative	526.2845	4.71	unknown	853224	1904408	830096	214403	2129345	2116661	321243	272787	2388664	760717	1526523	164480	1101294	2325761	1612519	1206133	1638285	830056	1348011
EIC	Negative	608.3942	5.49	unknown	341109	605186	240029	424342	488214	852964	559049	374599	351345	387512	430232	35806	366021	545260	344660	197051	161820	182079	582677
EIC	Negative	508.3380	3.38	unknown	100955	58365	125188	80672	92805	100604	82805	142110	55727	21679	42178	44444	48348	60115	66243	51855	41662	113708	33682
fpHILIC	Positive	133.0738	3.36																				

EIC	Negative	526.2947	5.07	unknown	3912706	2312995	3612867	4026577	4436174	7292780	4788923	3670326	1349348	2654057	3630547	4983947	1699049	2686066	4540498	1474576	3103281	2587937	3069811
EIC	Negative	243.1965	3.23	unknown	412051	346555	1068403	1008448	752552	559346	611417	1167675	843740	605854	385486	428619	414156	535570	172474	354491	475106	841483	437735
EIC	Negative	560.3314	6.23	unknown	665804	705196	731194	772925	806757	788785	757803	722345	701776	715641	787999	762306	728566	745312	701507	716349	730366	744766	682238
EIC	Negative	271.2281	4.29	unknown	751764	579830	1119721	1418132	1019253	814762	842749	1410385	1047283	828801	600454	656840	760795	736959	536271	930739	741589	1121218	674855
EIC	Negative	308.0679	1.55	unknown	2066907	2286928	1447118	772827	2575625	2899852	2682661	1041727	682100	1285582	2543182	2093307	1679659	1765155	2698125	1512417	2077209	975249	2536639
EIC	Negative	606.3776	4.79	unknown	296750	250403	0	316665	2575872	3155720	0	372466	169321	0	372466	0	279496	0	0	0	269265	0	0
EIC	Negative	325.2010	3.09	unknown	346711	336955	499064	644883	549629	362758	445288	620161	505319	446810	311870	371462	383369	516875	235769	324630	408944	552781	365459
EIC	Negative	387.1084	1.39	unknown	321293	361455	0	0	213792	245077	473223	0	241924	0	95081	126840	286915	88593	58221	218610	171179	0	275697
EIC	Negative	428.1904	0.69	unknown	100197	114942	75828	62642	64433	79202	103607	157189	80960	75933	102052	133175	96953	80300	88711	77601	79645	98797	90803
EIC	Negative	558.3329	6.11	unknown	2632310	2907580	2570041	2820660	2648695	2768914	2930133	2794947	2645323	2646075	2653574	2873135	2837558	2672979	2516776	2567671	2756627	2591107	2812137
fpHILIC	Negative	163.0402	1.77	unknown	759283	369924	350128	194633	401505	708585	659800	208422	152279	260371	445898	252892	229672	291636	302278	198812	256475	820897	249149
fpHILIC	Positive	163.0797	3.75	unknown	279967	339593	279426	207589	314134	632042	317665	135034	254926	172903	343786	268004	325285	625340	258360	309611	280427	179427	251955
EIC	Negative	507.3332	1.99	unknown	0	220958	0	0	287839	570520	147785	0	132380	0	215040	301889	177337	202887	259238	158080	203912	0	108488
EIC	Negative	516.2734	3.30	unknown	561188	356669	394194	0	297500	598664	261711	412976	395055	487476	242079	380172	227784	238059	370565	346536	525262	0	545898
fpHILIC	Positive	381.0783	3.53	unknown	105331	702467	175959	165990	261390	246404	577079	391886	628518	194437	136022	235739	260435	716689	216336	181607	425894	234499	632342
fpHILIC	Negative	189.0349	2.71	unknown	940958	582462	734893	1180989	755197	882010	866688	941464	970505	938670	744057	795773	806070	685402	451387	846029	848038	928277	623340
EIC	Negative	296.2313	4.49	unknown	395429	290819	875772	1151800	681224	446230	492599	1148296	917314	487945	331350	409187	361754	570151	127588	401846	389730	853102	340302
EIC	Negative	425.3074	6.58	unknown	239207	670290	1147811	439265	982930	294573	354777	914599	974348	5119883	785445	272582	907635	206643	339118	602545	514440	489894	198632
EIC	Negative	627.3504	4.43	unknown	53603895	69128127	53774986	55055661	62967034	59941779	64465307	55287518	63111057	53384643	66527980	60053884	60896149	58590223	58179703	60265750	57831881	51590502	59737895
EIC	Negative	382.3418	6.72	unknown	125545	164654	201710	337708	194139	219081	271403	164663	178597	169442	268700	248678	140124	194008	211232	229475	268236	140309	0
fpHILIC	Positive	158.0268	1.02	unknown	351113	200557	376339	222610	249866	494871	157386	313133	601339	161200	272681	280483	263193	376302	220424	227204	408054	257516	204120
EIC	Negative	320.2260	5.66	unknown	0	0	0	0	0	203766	228701	0	0	0	162834	258080	0	0	0	0	205718	0	0
fpHILIC	Positive	202.1181	2.40	unknown	4430570	3151245	3683662	3995291	3891399	6002427	3337912	3969827	3112547	3700112	4797456	3695187	3475055	2606365	2906107	3324090	4100800	2506121	3479177
EIC	Negative	327.2255	6.22	unknown	108225	352079	111212	472072	324009	245342	211832	160564	470716	173919	318960	185102	441796	161273	194726	629943	309355	212956	184194
fpHILIC	Negative	242.1844	0.38	unknown	607831	640635	495553	3276068	889301	789321	1390342	1134131	2514766	1382961	808699	1208493	1443015	180368	298122	1045468	1323825	2193071	247778
EIC	Negative	275.1269	3.25	unknown	81936	90332	86335	173286	89355	100928	97757	100938	156880	102962	77079	149988	149312	73212	75021	118480	120266	98384	75553
fpHILIC	Negative	217.0175	0.77	unknown	1070744	304852	428675	214716	425736	1132002	386112	384891	530991	86824	32478	82541	105279	226933	141879	173970	81736	170433	0
EIC	Negative	473.2881	2.76	unknown	603128	619171	555738	714370	1006149	539788	1168180	295541	257108	227319	0	0	0	0	0	0	90840	83502	0
EIC	Negative	523.3841	5.80	unknown	0	169746	0	0	348159	0	0	0	0	0	0	98239	195323	0	0	84280	0	121287	18539
EIC	Negative	283.2427	6.41	unknown	3707619	6666150	5160749	8576713	6482801	5819981	5806074	6631986	7284998	5072646	4970955	5825570	6666388	4606377	4233841	5856070	6377789	5952471	4156870
fpHILIC	Negative	429.3003	0.40	unknown	1177682	467443	1406895	519394	668587	670684	843328	1426897	1067858	524566	473745	438094	393402	1204866	629832	438354	576029	737286	568226
EIC	Negative	377.1798	1.90	unknown	193906	455474	0	0	206620	320292	367832	0	191473	0	307512	217541	99028	0	320017	396330	199483	0	149678
fpHILIC	Negative	222.0263	0.59	unknown	627285	816196	207068	468783	337204	1465459	516152	278462	175865	596696	1465520	611717	560741	499893	308412	537955	0	1021434	0
EIC	Negative	253.1446	2.00	unknown	267244	453703	200372	122842	436391	347840	404046	0	500534	155944	332533	321973	400950	277947	330245	615175	408395	0	236880
EIC	Negative	326.2720	5.20	unknown	261619	228361	225599	255932	255400	261844	228276	264524	241599	253325	236627	253935	94250	266339	243722	44399	261531	30208	32058
EIC	Negative	602.3388	4.14	unknown	43694	95037	114433	165052	142658	431673	127074	0	0	0	0	328433	388461	475809	96698	0	0	96229	0
EIC	Negative	232.8893	0.66	unknown	26348	72525	93648	85375	66835	52355	67756	119081	77165	60113	68422	89450	28316	56453	54476	81751	96657	53105	0
fpHILIC	Positive	232.1539	1.83	unknown	11887471	17966620	14221863	13440093	14361327	24781862	18844606	11738198	12835019	0	17721650	16927182	15470689	26557990	13363095	16930703	13372223	9541811	12945118
fpHILIC	Positive	127.0502	1.03	unknown	1053972	561811	842749	1017017	938172	1012570	688995	665823	968758	635014	438519	459929	490552	396734	432972	524787	509253	455914	275667
fpHILIC	Negative	619.2891	0.50	unknown	3318748	3658057	2727293	2678036	3386982	4468000	4254425	2584801	3938606	2155868	4110283	4449310	3967200	3093531	3512078	3975872	4015624	2046850	4326257
EIC	Negative	291.1220	3.08	unknown	79283	186636	135109	183295	194857	87751	137567	192939	89696	96943	177032	266206	66206	78219	247867	115705	121613	47012	17032
EIC	Negative	276.2050	6.16	unknown	208482	228776	302540	1154153	532141	373570	583112	592811	608178	310943	205660	375427	397605	70044	189968	337603	308600	473986	180675
EIC	Negative	299.2590	6.00	unknown	600814	613935	849458	801409	729202	708063	762678	804810	643899	550121	566981	624277	610403	740405	505440	6489564	638388	742542	740766
fpHILIC	Negative	200.1738	0.40	unknown	813214	578562	1196426	1761179	1035744	743938	724340	1071245	1871612	740883	506294	620189	797447	512149	384549	691005	722213	949128	665028
EIC	Negative	253.1446	2.36	unknown	956402	677001	1002381	1164983	753854	848175	1000029	1302574	887292	1362592	644800	660033	631820	614618	691074	774666	735879	1214415	838570
EIC	Negative	484.3647	6.02	unknown	1360397	1368879	1304501	2909051	1604246	1764859	1822209	1577936	2443061	1245168	1543802	1680716	1954888	668888	1203799	2148324	1192237	1379285	992583
EIC	Negative	316.8898	0.66	unknown	19949	94757	113377	103825	74499	19703	80540	61213	86897	62123	85989	95064	121222	21732	57625	97985	109445	136209	52199
EIC	Negative	552.3321	4.04	unknown	4432121	8149139	4549633	1281205	6017666	7560236	8204842	6414307	3902462	4424311	6011250	7399179	6344512	7420451	7184957	5683207	6832183	4017399	5904306
fpHILIC	Positive	804.5516	0.44	unknown	1006671	2818905	1325505	1625346	1826697	2190775	2469627	1467867	2477540	1310029	2044274	2334019	3044197	2158476	2052525	2483500	2391592	175589	1863864
EIC	Negative	635.3377																					

fpHILIC	Negative	328.2363	0.37	unknown	7922750	19612596	9110410	26857354	16137965	11911823	15675947	14667008	24501590	12067491	10263071	10524747	18225682	7106261	10562353	15391818	14585811	12543941	9745140
fpHILIC	Negative	92.0434	1.74	unknown	334641	1017071	1080497	1367485	971187	1090733	1035062	875393	1219955	925427	787752	1031351	966754	640695	625208	1171554	864401	1118340	800011
fpHILIC	Negative	270.1712	0.41	unknown	1130315	641358	1081558	765838	674198	958793	914027	864667	1253372	1269061	950029	1021577	840741	564928	612950	756136	839214	1156566	837310
EIC	Negative	595.3806	6.00	unknown	1445098	1918826	1434819	3171622	1591762	2450783	2227714	1468507	1044802	1060218	1327100	1493218	1282735	1171281	1482536	1008977	1291877	906312	1284991
EIC	Negative	335.1865	2.49	unknown	1357761	330497	581428	382090	748859	643272	892834	1403031	212175	1220409	273267	326210	243008	295001	374945	271544	351247	1123100	431068
EIC	Negative	418.3730	3.75	unknown	272027	390095	238753	292204	307613	348520	327380	258861	326357	219495	327426	266645	313038	289687	325356	332400	288362	257623	251062
EIC	Negative	463.9059	6.24	unknown	1455745	2343160	1182381	2907306	1620161	2975225	2072795	1893583	2163035	2025764	3790706	1469982	1856192	4625532	2306899	1124923	3440924	1259679	2147716
fpHILIC	Negative	539.3033	0.38	unknown	317987	474242	1307522	1679989	923598	876024	931100	1292300	1173442	617907	468761	726254	674468	250977	181687	292185	914812	1165572	796032
EIC	Negative	527.2984	5.06	unknown	1234128	666362	1105381	1208140	1168912	2204986	1353069	1095584	392208	754635	1057427	1524818	531679	849428	1279829	404318	895677	812769	862341
EIC	Negative	310.1746	5.20	unknown	0	320994	421471	0	713230	0	396308	0	448353	0	0	225145	0	0	0	0	0	0	416300
fpHILIC	Positive	150.0545	0.97	unknown	302988	388564	144313	158972	422399	463982	400716	116569	282267	255953	586434	488734	386235	372752	536865	341200	363403	215615	0
fpHILIC	Positive	763.5924	0.44	unknown	452005	394265	381702	259719	427584	385932	271888	407881	435558	377819	538934	386438	352572	543590	356393	354540	310830	303636	301320
fpHILIC	Positive	245.0955	2.61	unknown	1062792	778425	565356	1363642	791337	1263764	770259	794468	1201528	820770	584933	1083046	935538	717522	669995	1154466	671904	923748	740065
fpHILIC	Negative	369.1558	0.47	unknown	713288	422405	466940	1038662	677201	798506	727429	559201	675533	554123	571249	570692	562737	223983	554420	849765	509050	653419	224810
EIC	Negative	431.3180	5.26	unknown	299308	61517	507409	198940	277105	144465	266784	501259	163872	116544	77501	101934	99822	112146	142986	105361	110186	236193	127151
EIC	Negative	301.1658	1.60	unknown	92435	168418	168548	0	138968	47146	142823	191058	166853	126487	102393	73260	73117	77277	69780	61684	78430	56879	128515
EIC	Negative	276.2050	5.81	unknown	1729428	4308784	2786722	12465517	5350691	2595227	4176416	4682624	10150539	2772047	2432684	2224274	5052000	1883443	2158347	3550285	4793661	2729687	1569854
fpHILIC	Negative	147.0300	3.97	unknown	16165833	8599044	10062224	16745211	12970774	17355014	13016778	11232698	11837419	8486015	2832574	8915153	9389089	8373961	9627336	10556342	10661743	12034780	9359498
fpHILIC	Positive	197.1011	5.40	unknown	1229763	1254003	972320	975404	1125046	1256403	1172874	976890	1204999	887478	1198021	1186068	1217534	1111966	1514881	1150182	887485	972028	1096365
fpHILIC	Positive	227.1250	1.80	unknown	27517252	20187306	20602202	26651420	21628300	31516220	26115820	21011746	25940060	24711172	2829586	22966058	26505310	17985766	22432112	29635742	22127286	21649574	18387006
EIC	Negative	463.9667	3.75	unknown	102899	130662	70284	103198	122965	116649	109140	84374	106847	78095	118441	97669	91469	99377	111023	127425	90818	95941	77048
fpHILIC	Positive	264.1497	3.37	unknown	1908170	1207218	439536	287117	674720	1092122	822019	965538	1325364	281576	484010	628529	1135203	1125624	1308762	609435	878693	368313	0
EIC	Negative	568.3623	4.78	unknown	0	0	503960	339148	423534	0	397741	296595	360706	0	0	0	456058	0	0	0	0	0	417557
EIC	Negative	366.9415	3.64	unknown	327090	565307	354714	448510	520358	524867	485180	345132	480442	3525273	492721	459970	565598	487643	547179	317123	407546	363731	448497
fpHILIC	Negative	279.9955	0.98	unknown	1210841	1157642	972763	878935	1509110	1844447	1689220	524302	326969	0	0	0	0	0	0	0	0	0	0
EIC	Negative	244.1999	3.23	unknown	68059	52943	178832	158528	120534	92436	103793	178376	124741	104181	71997	71583	72464	88028	27449	58151	85678	124901	78015
EIC	Negative	435.2326	4.03	unknown	57383	21893	107255	240698	105784	63455	69187	184469	144110	120369	31927	88973	90960	30024	14774	106088	76215	187729	0
EIC	Negative	290.8484	0.66	unknown	43916	112302	162836	143366	116180	60322	106875	203823	139639	100122	114793	123325	157794	42870	83991	92028	136095	169815	94727
EIC	Negative	307.1655	3.16	unknown	936800	446595	923156	765667	854035	462841	792348	1200363	590884	864394	357765	348752	412052	341370	467035	488239	550201	214495	321787
EIC	Negative	373.2058	3.94	unknown	60237	0	412139	26623	44838	336968	198908	28053	45183	38304	32973	336321	365151	251401	86803	235998	54581	73611	162021
EIC	Negative	379.2472	4.72	unknown	515700	394253	1019793	1140966	833136	574253	716253	1112737	882449	756800	476813	617834	573213	646313	167983	736317	595800	848888	470496
EIC	Negative	275.2016	5.81	unknown	8717824	21739927	14025785	62472529	27060828	13059648	21116356	23034657	50943855	14009608	12231552	11392167	25121787	9356231	10804597	17563606	24188286	13859154	7762502
fpHILIC	Negative	165.0555	1.62	unknown	149814	0	535174	511472	1220665	240676	0	613437	0	413317	0	0	300346	0	602611	0	485944	708174	478788
EIC	Negative	247.1703	4.79	unknown	1008459	2053129	1962818	8904323	3030126	1368430	2327742	3127158	7522922	2331713	1166623	1443760	3777195	821012	672852	2885866	2962766	2839906	1026656
fpHILIC	Negative	174.0123	4.59	unknown	2130206	1670039	1668406	1825211	1772846	2345632	1926923	1525790	1684933	1679445	1792432	1672900	1687812	1522652	1467284	1766446	1490688	1683400	1702485
EIC	Negative	299.2234	2.87	unknown	70836	72704	109597	101992	117011	84273	67915	141347	52783	127944	71679	60674	63961	55201	45411	52643	68727	134647	66437
EIC	Negative	305.1749	3.44	unknown	1057150	370011	772495	268305	659435	602449	801860	648718	203953	316664	173470	495350	170901	336807	481772	182546	400329	273056	144310
EIC	Negative	252.1306	3.23	unknown	54808	79625	108333	187433	137656	74055	122126	92716	142831	69240	68599	116351	80718	50906	48340	81954	90313	80385	86194
EIC	Negative	571.2871	2.74	unknown	419443	297190	271644	327436	326019	349312	261233	362170	0	0	0	0	0	0	0	0	0	0	0
EIC	Negative	458.3494	5.67	unknown	756978	565430	587854	1178804	615490	723391	576143	728592	1102443	573931	626144	586000	696933	305107	500740	706387	381450	510939	349126
EIC	Negative	227.0900	1.25	unknown	72326	29099	35554	60900	37311	48209	52318	29099	30101	34071	36824	34701	45864	46662	35197	32556	40380	26565	24856
EIC	Negative	609.3876	5.74	unknown	352429	447281	395416	288535	393965	530796	461852	390512	215432	282764	368989	361480	282612	269961	283523	233468	348495	276598	363642
EIC	Negative	286.2103	5.79	unknown	28432	36072	76263	167642	125720	32343	85415	54153	0	0	0	69907	56473	12183	0	33321	33696	78388	20913
EIC	Negative	628.3531	4.43	unknown	12240520	15323859	12033404	12565585	13971551	13665235	14200904	12199214	14060299	12156844	14948833	13656600	13805568	13212215	13254149	13633678	13446956	11700829	13374312
EIC	Negative	361.1659	1.76	unknown	324378	408958	319110	323269	364210	334620	410079	335954	344472	329184	356695	495223	592609	416197	411281	464794	393660	0	366322
fpHILIC	Positive	789.6135	0.44	unknown	1826080	1626748	2050544	1838191	1982801	1900507	1716363	2453090	1333472	2065130	2159518	1850662	1440687	2299464	1960002	1424825	1883888	1504289	1760149
EIC	Negative	367.2436	6.43	unknown	4125254	0	5068332	6476867	5112098	5740210	0	7733875	5358982	6023207	3555268	4685516	5369749	3983709	3487248	4611122	4002111	2142367	5360547
EIC	Negative	283.1291	2.18	unknown	398963	272323	271366	321763	300734	423315	336230	285943	232070	390398	199124	260593	213393	184692	255115	246149	245129	369760	233188
fpHILIC	Negative	148.0335	3.97	unknown	856914	506949	520462	936637	702609	954234	706630	615358	622924	547738	49								

EIC	Negative	409.2865	4.44	unknown	0	387679	442122	512907	0	243069	472088	516401	547360	0	31659	37376	0	0	0	0	0	0	194941	94611
EIC	Negative	435.0356	2.09	unknown	77818	151675	0	0	120054	114611	111436	0	100450	0	89986	12575	44397	57128	73233	83075	0	0	0	56701
EIC	Negative	305.1774	3.46	unknown	1015241	340605	739778	433531	627585	545138	739338	1002850	240045	597788	270416	462756	314473	318649	425894	355666	355168	752188	268386	
EIC	Negative	603.4632	5.82	unknown	67936	209444	122636	510841	204366	154031	260850	226408	381187	89704	102681	62167	171364	107095	132424	62338	196379	0	52501	
EIC	Negative	278.1841	3.32	unknown	0	199535	0	324387	0	369261	269632	0	10337	0	262658	382407	0	0	0	0	0	0	284714	0
EIC	Negative	256.0698	2.42	unknown	130631	37830	455786	68927	690309	65602	65089	68096	73399	1314362	103180	167371	72705	74854	8886	46270	67800	173321	84577	
fpHILIC	Negative	305.2492	0.37	unknown	7308564	13572176	13399585	13122711	11086642	11200185	13286101	11991991	13170069	10157987	1074064	10849193	10930309	1701118	8490821	7641659	11975655	10668283	9916221	
fpHILIC	Negative	337.2050	0.35	unknown	860952	401571	313747	412602	1113748	274242	662088	244052	110279	751580	427776	364946	629585	340310	304004	401722	522149	455089	432364	
EIC	Negative	559.3376	6.11	unknown	745501	865678	747936	908381	817009	827867	900394	796657	774453	805239	815133	917415	833021	865448	821880	764032	853197	715268	812946	
EIC	Negative	360.1536	2.09	unknown	2765737	1926263	1163496	232557	1823306	1878469	1979918	1702638	1954405	1298068	2038880	12104	474055	1052062	1399884	3724687	73974	418236	1052447	
EIC	Negative	288.2052	6.21	unknown	75928	108223	111637	192633	148171	111842	120530	158768	114056	146971	88071	107241	129164	20733	56633	127179	109250	128464	69401	
fpHILIC	Positive	511.3583	0.59	unknown	1320609	1505558	1215357	1239707	1375860	1765273	1589925	1296178	1351212	1249651	1376730	1313628	1709398	1211149	1500155	1323790	1500109	12379825	1499304	
EIC	Positive	268.1272	2.93	unknown	170028	239481	88927	77371	149263	218444	187820	85925	115387	136181	152353	135748	129652	160079	192525	158975	130058	88896	104192	
fpHILIC	Positive	112.0507	2.61	unknown	6033146	4267182	3035410	6500643	4050499	5820295	3938005	4316576	6112507	4367403	2825918	5407199	4608123	3463926	3786644	6408438	3594985	4364396	3470995	
EIC	Negative	306.2413	6.44	unknown	648209	821298	126879	1151781	836825	581274	597092	705824	885004	590935	625173	700576	712658	607965	596501	650491	705774	740625	633682	
EIC	Negative	556.3526	4.84	unknown	8555075	10767773	8452339	8686026	9081617	9126343	9278696	8705943	10307848	8300008	9788665	9517261	9460787	9766580	9732586	9470885	8896957	7542648	9690848	
EIC	Negative	634.3356	4.04	unknown	253231	526879	239142	132695	380503	472520	450271	250955	248179	275638	416680	434335	367074	431140	475314	303485	415534	240473	354622	
EIC	Negative	300.2627	6.48	unknown	963423	1985599	2243544	2417378	2307256	1328855	1468930	3263085	1637794	786281	637357	1052332	1684334	1569463	786281	622213	993159	1863300	154522	
EIC	Negative	630.3690	4.93	unknown	1308539	752222	1156808	1314074	1110008	2013725	1656642	1220049	301310	775609	1104550	1402509	702372	517258	1132145	548002	961677	856321	1002434	
fpHILIC	Negative	280.0519	2.61	unknown	857099	559376	415284	815305	555724	828052	538484	639163	585694	606480	478049	856342	782419	484003	606480	658350	622731	663338	567479	
EIC	Negative	359.1503	2.09	unknown	12655604	8519135	5192382	1184771	8108874	8289235	8818078	7721607	8871301	540228	9033383	111311	2071811	4789466	6376304	16629339	605401	11472012	4486005	
EIC	Negative	266.1842	3.31	unknown	459354	158304	390231	0	283825	272112	293256	358657	332808	364339	283193	130865	188895	260534	175914	444820	152800	158990	0	
fpHILIC	Negative	160.0332	3.84	unknown	461562	358444	442713	364806	387527	697680	397546	414921	248157	284292	548437	309120	296262	1493281	426282	304204	314104	290358	523903	
EIC	Negative	272.0649	1.64	unknown	160255	25928	0	0	24202	115556	64519	0	177771	0	206454	202354	77175	33885	0	30259	57930	27621	88818	
EIC	Negative	311.1861	2.50	unknown	138196	101261	119812	217347	110041	99893	163233	164328	173671	138098	74562	89387	136275	82249	67084	194693	125162	190890	77628	
EIC	Negative	504.3153	5.65	unknown	842331	1386339	1064142	277003	1157744	2076242	1134342	968772	519956	429200	599522	1502661	1143099	592752	914726	726599	1368838	0	0	
EIC	Negative	287.0567	1.04	unknown	136047	45089	172540	46068	160863	181722	101327	49494	322695	112505	201882	354767	108945	56548	14498	36351	77120	115310	116572	
EIC	Negative	298.2470	4.72	unknown	1314416	1050748	2864168	3641175	2241317	1628712	1872121	3394946	2642843	2022327	1169606	1753706	1644684	1773209	727892	2110515	1728482	2665408	1170109	
EIC	Negative	594.3777	6.00	unknown	4432370	5919117	4513978	3973612	4773324	7335721	6730006	4516931	3215180	3278757	4156943	4680333	4018301	3638836	4690287	3332119	3939447	2817517	4020675	
fpHILIC	Negative	225.1863	0.39	unknown	694878	5759202	10387520	20633700	12423045	6028466	11576698	9834046	1312639	7385522	3277902	8073364	7123040	2813954	2319590	6451487	7123730	8971966	4800954	
fpHILIC	Positive	571.4280	0.41	unknown	469119	139752	133521	272529	695000	182718	302048	205319	419515	403697	397519	572671	170493	379609	343321	290908	568399	208096	287476	
fpHILIC	Positive	201.0865	2.59	unknown	829102	465882	748815	818707	626344	1027845	695330	877297	415857	650700	654215	665361	524404	625517	568198	775154	531089	596767	563908	
fpHILIC	Negative	495.1908	3.51	unknown	91000	796103	471478	137838	218764	203113	412921	280091	699748	1381706	191006	182561	212391	666079	182408	167697	328020	153017	949399	
EIC	Negative	456.4143	6.35	unknown	944332	861150	1833639	2375145	1363787	878838	1874374	1914826	1469604	1317905	613572	1242292	779618	477516	430497	595084	903603	1188443	517722	
EIC	Negative	435.2698	5.41	unknown	208367	409941	203001	482163	58841	227646	194278	783412	294535	307883	135433	363904	454684	401099	65962	144329	159262	172333	0	
EIC	Negative	390.1955	5.79	unknown	102446	147938	214744	374359	255421	136201	230754	217858	230976	175927	91546	260953	175674	81629	30051	118186	138736	188501	94982	
fpHILIC	Negative	153.0444	0.52	unknown	3388743	2078635	1438495	366728	2023286	1865122	2072128	1921300	2476144	1611340	2027123	0	597100	1128028	1263917	3761436	2711376	284354	1500274	
EIC	Negative	331.1902	5.58	unknown	1238970	1526302	2154846	5298512	2334070	1434194	2166011	2809626	4092930	2182167	1207133	2105800	2499774	937558	1008313	1983728	1934648	2682013	1304496	
fpHILIC	Negative	149.0279	0.78	unknown	496004	324909	314944	180701	1219609	981189	139802	208612	125344	182612	225344	222892	580945	411990	96304	3000410	200410	191854	432346	
EIC	Negative	552.3342	4.04	unknown	4503874	7865543	4681447	3731500	6544401	7705164	8895311	4689239	4295048	4630448	6937214	7297927	6605395	7337967	7645255	5568800	7240078	4236861	9500819	
EIC	Negative	319.2711	3.30	unknown	235747	271612	241548	236884	245014	247859	233209	271451	243309	230072	247839	273469	247839	229167	256971	236920	242835	218058	246267	
EIC	Negative	569.3659	5.55	unknown	1613104	1930896	1484670	1584614	1841090	2224983	2037336	1656705	1415150	1261280	1491253	1622431	1691209	1423852	1864006	1446332	1529784	1076007	1558928	
EIC	Negative	630.3691	4.78	unknown	703264	1151278	566521	642699	833565	565612	632956	851600	828860	611000	828860	692765	611480	768900	577630	682216	723678	490279	675091	
EIC	Negative	273.1245	3.38	unknown	19464	50136	88585	179970	97943	58734	77478	93084	103700	72118	44600	78573	63725	26325	12283	71315	52010	110294	21447	
EIC	Negative	322.1776	5.79	unknown	139218	253897	319977	579801	390168	214946	387708	341997	366239	249728	145405	343255	291334	94273	84391	262089	196952	286730	113702	
EIC	Negative	325.2026	3.00	unknown	246062	148394	319593	500958	288998	219121	239514	421398	349028	352163	174995	318088	266935	116441	89326	240443	261503	442829	128071	
fpHILIC	Negative	327.1453	0.57	unknown	357783	316182	987650	148256	349146	409796	365820	562164	405889	207614	974399	665899	417903	991197	108272	522559	272802	188428	523160	
EIC	Negative	319.2785	3.76	unknown	261953	314220	249418	285448	289645	300739	277452	262612	274537	286472	278048	281202	267631	278033	258436	282630	284063	277491	291379	
EIC	Negative	255.1969	3.69	unknown	397636	379252																		

fpHILIC	Positive	323.1264	4.19	unknown	1305656	341995	254451	122859	587646	1324803	450194	101814	240068	50840	92198	132083	67463	437848	85710	147916	55706	227801	49295
EIC	Negative	309.1526	3.78	unknown	789828	263684	687741	307625	474578	467400	499556	1021169	116096	0	357865	274977	230911	147381	308295	236428	293370	645679	365420
EIC	Negative	235.1705	3.05	unknown	360808	380108	345921	338341	337750	334276	394037	361920	321028	0	335132	335775	336522	342395	321274	400288	346941	356327	348692
fpHILIC	Positive	395.1617	3.72	unknown	669572	592082	644442	575492	738076	597465	589591	577667	560768	616153	580082	568632	551488	397155	669587	558120	552338	590104	410072
EIC	Negative	303.2249	4.96	unknown	190393	0	0	0	0	0	0	237543	0	0	171893	193192	174600	121763	86876	0	0	0	146980
fpHILIC	Negative	136.0165	0.52	unknown	1072258	712508	667593	129336	646850	703752	925806	600881	973643	740544	770475	0	220632	394937	384924	1179612	59991	135717	562927
EIC	Negative	503.2984	5.13	unknown	1922339	2587377	1757499	1479969	2384649	2560550	2117175	1684759	637800	1905740	1807960	1387358	1373045	2302040	1524745	767536	1698377	1213711	1766624
EIC	Negative	588.3326	4.52	unknown	802901	870121	743662	743271	802477	833632	737828	785382	894249	740082	863332	810234	860065	796085	797797	815465	740429	768179	816387
EIC	Negative	352.2207	3.47	unknown	55480	21148	68255	21485	80262	58418	59826	146897	121255	85145	57819	84966	77480	21846	21463	76729	56706	137578	23453
EIC	Negative	285.2073	2.37	unknown	528563	261926	392838	421670	379782	420619	391545	545289	218638	370819	209781	290280	223218	180065	194759	244674	223586	471056	205039
EIC	Negative	562.3844	2.71	unknown	1023529	397515	710575	570990	622641	1266604	572197	564809	444251	547111	470842	519101	632565	653703	430634	486825	590962	666883	500649
EIC	Negative	252.2046	6.28	unknown	904534	1260894	1983430	2763649	1758442	1412543	1941373	1811577	2222888	1574161	978817	1645331	2037580	791115	819114	1148987	1372734	1839947	961354
EIC	Negative	490.1993	1.03	unknown	96381	62526	75439	38725	57668	77639	100461	83736	69046	161812	70733	82783	68150	116182	52921	56781	52064	69028	139187
fpHILIC	Negative	129.0193	4.58	unknown	10697994	8248063	8294852	9614712	8999072	11609105	9246608	7341168	9320008	7134938	8858671	8278941	8185928	7898191	7671312	9417301	7974378	8501163	7434358
EIC	Negative	375.2168	5.02	unknown	239779	319864	267992	720993	392296	362778	418513	381446	500706	376511	315324	468804	406230	218295	235490	388131	346973	470635	187021
EIC	Negative	609.3650	4.04	unknown	449010	39887	615716	207752	174222	106563	93167	1047962	108589	293256	1047962	16284	52565	107169	115039	21942	108282	348693	98059
fpHILIC	Positive	292.0725	2.43	unknown	504402	238432	1062424	143221	722033	586334	236891	55145	477573	143267	0	701844	740074	0	0	0	1015190	0	0
EIC	Negative	629.4762	6.17	unknown	516164	554326	604630	2459497	825900	768937	1487543	1114737	487565	443207	499909	662312	240937	361701	340293	655838	569409	252268	0
EIC	Negative	459.1509	1.48	unknown	0	842973	0	0	370839	378783	390254	0	338008	0	353376	288685	354804	382512	416704	293631	330105	0	226469
EIC	Negative	460.1545	1.48	unknown	0	185541	0	0	83754	84681	84558	0	79085	0	71900	86239	81931	90250	67191	81217	0	0	0
EIC	Negative	243.1794	1.85	unknown	1900683	989935	492209	0	1053644	1309841	1286769	0	927351	0	846147	800475	952315	781813	862083	1493873	874015	0	1069766
EIC	Negative	367.1401	1.78	unknown	261323	186435	206867	314189	276165	331779	299459	74238	274102	264597	235228	280019	283048	150813	283291	385836	249148	0	128100
EIC	Negative	322.1442	2.51	unknown	212121	112962	197036	170244	176183	133935	165300	276063	118908	176813	95882	112682	104249	100563	121828	118700	108594	192518	87463
fpHILIC	Negative	193.0242	4.72	unknown	2098778	1460524	1397997	1743133	1542582	2090956	1522782	1455647	1786144	1422226	1432553	1470109	1436515	1493447	1253158	1892401	1397819	1520139	1407218
EIC	Negative	568.3626	5.55	unknown	5391718	6267623	5128172	5235829	6013102	7206981	6636191	5634432	4831953	4084208	4984648	5499284	5459920	4623975	6056321	4701260	4966584	3572438	4866386
EIC	Negative	394.2622	6.44	unknown	2089748	1331919	527310	1084556	947629	1329386	1591038	1532871	1068298	1103711	1212768	613649	939227	1121367	1165755	651258	1192743	705463	714546
fpHILIC	Negative	227.2016	0.39	unknown	21927522	25714652	59758540	75810808	42874628	29223602	43582996	59401480	54174992	34852992	20557826	30622552	35871612	18030686	13975875	25999374	34000880	47306688	2454862
fpHILIC	Positive	564.3314	0.40	unknown	2719790	3096371	2096640	2223331	2707703	2168952	2456173	2782865	3171588	1614628	2357421	2523043	4435697	3710014	1012041	2711440	2277825	1819031	4675252
EIC	Negative	283.1919	3.46	unknown	14850843	4282461	11490539	7647764	8725350	7910534	10146010	15038661	3616473	9391998	3917768	6485776	4515368	4200027	5398993	5286911	5193366	11326929	3442740
EIC	Negative	293.2125	3.46	unknown	135065	105171	206662	392497	165957	120938	180174	248385	345821	280804	120050	248560	194987	80915	90599	336150	185518	246577	124091
EIC	Negative	256.2000	3.69	unknown	81937	58222	41081	235042	139419	73717	134935	123897	122634	129301	69759	120839	107465	35054	21702	102738	107165	138277	36162
fpHILIC	Negative	255.2329	0.38	unknown	224955440	343397216	461329568	582365440	376129408	343023264	379646080	426973824	522734688	286097248	284759136	353196928	389244576	279387104	256241216	335271232	342267328	357533696	325501408
EIC	Negative	366.2665	5.93	unknown	211386	0	0	0	0	20956	0	0	224870	0	167586	0	0	0	0	0	0	0	0
fpHILIC	Positive	131.0892	2.71	unknown	820460	975098	702653	1071078	956182	1239589	953106	628912	828286	642062	1124279	810955	927312	490503	670446	1020415	1017817	740370	641668
EIC	Negative	301.2661	4.40	unknown	239177	168163	215653	211488	221000	215657	211054	212677	211054	213335	172287	187026	217557	185973	204220	230765	159153	216017	184649
EIC	Negative	311.1648	3.67	unknown	290698	276145	340192	301336	119814	839038	203856	169009	77264	282372	285833	389671	489707	292628	136112	338332	241454	352376	297837
EIC	Negative	284.9514	3.46	unknown	2605401	759963	2097452	1357173	1560380	1412548	1772074	2677272	612280	1707431	724401	1152366	797863	760282	965113	652280	935076	2027722	605668
fpHILIC	Negative	848.5942	0.43	unknown	1560601	1198881	1382080	1301425	1409889	1506118	1035654	617082	977075	1330312	1211482	1395721	1050190	1349291	1415712	1004547	1266047	1251355	1398279
EIC	Negative	485.3033	2.88	unknown	260682	23623	229081	38124	67053	62861	412600	52107	931615	19418	30870	37005	22752	56836	32319	53288	14815	225622	24011
fpHILIC	Positive	309.1285	3.48	unknown	1420191	1481713	1517223	1418616	1238152	1356688	1610547	1337293	1319310	1511502	1229197	948948	1352794	689436	1232315	1065984	1426746	1568816	1110897
EIC	Negative	330.2522	6.49	unknown	13907329	3819816	11912751	27235358	13153525	13468292	12453039	20042810	11590786	14607104	12907367	11180306	10133475	7209274	10922170	10055406	9482019	22310220	11804713
EIC	Negative	351.2166	5.19	unknown	206577	364795	332160	1076041	521429	317530	482193	494827	617448	355553	357058	669776	446761	172026	168691	382666	366743	664980	192709
EIC	Negative	489.2839	2.74	unknown	205645	2016451	3215548	2931060	2893557	3397146	1756222	3454630	3295870	582821	0	0	727710	47535	0	0	0	0	431341
EIC	Negative	252.2049	6.31	unknown	490874	840104	1420327	1301291	1438438	557005	1332676	1303799	1456002	915742	675660	1116787	0	352283	0	560269	926501	1549720	0
EIC	Negative	427.2711	0.91	unknown	143047	42100	128143	248096	69272	177724	61101	298009	42515	154762	63806	59095	74251	43088	53607	111630	64645	250513	51149
EIC	Negative	393.1727	3.20	unknown	124290	51141	76340	96393	62176	115964	87942	108276	41808	43688	47177	0	0	0	0	0	40053	0	41082
EIC	Negative	251.1322	3.39	unknown	112539	165948	0	0	0	0	240830	0	301066	0	145922	0	0	0	0	0	0	0	154204
fpHILIC	Negative	153.0307	2.64	unknown	417264	370354	315127	501927	395318	534620	397468	308198	348706	417783	506053	391824	406727	265111	389303	341351	411863	323901	316387
EIC	Negative	271.0615	1.64	unknown	840151	160966	425041	0	131143	653877	358922	92864	1110947	318740	1215961	1179548	400724	226700	53181	157849	267947	255876	447741
EIC	Negative	228.2047																					

EIC	Negative	359.2960	6.24	unknown	0	446170	473199	775580	586743	805407	591699	0	331195	507053	619924	602141	0	0	481563	489794	512898	0	0
EIC	Negative	396.3123	5.83	unknown	137740	167785	135850	162109	147537	171413	153010	139179	137320	122059	144507	146246	150658	181404	155161	146619	153068	129089	140560
fpHILIC	Positive	383.1152	3.16	unknown	846746	896177	917222	1029707	947121	957899	895443	946792	943368	973785	820753	952063	953202	742287	905795	863294	874087	775951	817735
EIC	Negative	227.2014	6.35	unknown	75122258	97313091	170436732	212991060	133726823	103908780	121232610	178442943	152849058	94235738	61413931	95063444	103112096	58829834	45634266	78815298	85681503	131038409	74253104
EIC	Negative	631.3817	5.49	unknown	3068160	2743447	2574129	2701057	2958308	3350334	3154232	2697365	2178534	1890750	2865810	2636429	1964995	1731694	1956475	1538424	2166731	1924086	2623279
fpHILIC	Negative	267.2328	0.38	unknown	3001711	4265727	6365380	7951901	4568555	3750683	5121410	6737265	6692151	3394782	3296424	3936634	5871614	2882715	2187101	4333353	4157062	4914749	3473405
EIC	Negative	251.1921	5.58	unknown	338008	499315	609985	7764784	720870	421408	612382	871556	1287058	567156	311133	597055	678813	283920	269456	544665	588189	487985	355584
EIC	Negative	630.3685	4.43	unknown	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
EIC	Negative	305.1738	4.91	unknown	1657124	1996239	3076396	7417007	4225469	1844093	3582401	3510820	4132667	2474169	3174589	2960522	2552787	996808	748631	2020257	2213693	3517995	1253833
EIC	Negative	303.1574	4.34	unknown	261187	155021	277176	497795	319924	229218	438445	305274	337860	299860	211455	368622	394231	45822	118740	259441	222428	423985	100314
fpHILIC	Negative	488.1795	3.51	unknown	492842	3059485	2557427	571691	708203	802929	1830731	1096155	2771035	467606	439549	721489	757723	0	666096	511557	1194321	693121	0
fpHILIC	Negative	181.0870	0.96	unknown	672176	604114	1644321	513484	1080363	527606	1016599	780078	602427	1400534	1882137	1449445	941731	1132645	236788	626566	289019	432902	399301
fpHILIC	Negative	501.3952	0.36	unknown	1293307	1236913	1473555	996732	1571965	948103	1613088	1120297	1259681	931573	1164929	988855	937774	1009132	1438107	1370195	722138	992776	916513
fpHILIC	Negative	112.0516	1.80	unknown	8541685	6244391	6566967	8151410	6402431	9351515	7369960	6304341	7709298	6959581	7659322	7016937	7598294	5645068	7330535	8224784	7192747	6844468	6150990
fpHILIC	Negative	487.1782	3.52	unknown	2048647	15741919	12420957	2459468	2991668	3526757	9124012	4987148	13798916	1458823	1049384	3057774	3304245	0	2770541	1818093	5844300	3033769	0
fpHILIC	Negative	281.2486	0.37	unknown	288683040	424136544	594543616	699828864	445140288	412217824	530359776	524745984	621440000	362279616	311728544	437793824	461788352	269496000	309970912	397594048	426658944	507640928	323202400
EIC	Negative	249.1860	3.42	unknown	623525	241251	590678	542262	428202	289126	465251	655075	489193	458436	275990	333873	285278	176997	281134	342137	241905	420682	225850
EIC	Negative	555.3503	4.84	unknown	41855302	52799354	42548495	42129997	44251470	43640436	45375732	41824832	49011031	40288270	47797308	47384194	46138110	47627906	47217785	45831674	43321572	36931327	41788776
EIC	Negative	542.3118	1.80	unknown	141044	90801	138672	0	107941	113729	94933	103319	69912	96239	94452	140444	93956	110291	107588	71374	89314	0	91016
EIC	Negative	359.3002	6.24	unknown	670984	631322	533498	970479	726525	1053128	694267	657174	374574	644938	811182	686968	452492	349375	613782	852509	579130	543900	447228
fpHILIC	Negative	282.2513	0.37	unknown	58672376	81310880	123478520	137908144	898989352	80722936	107374968	104277064	118960416	72192112	61252992	89170688	91303080	53521692	63540040	75255176	87267664	100519376	66019748
EIC	Negative	323.2502	6.37	unknown	0	1894834	3264384	0	1515910	1574234	0	2233026	0	1597780	0	0	1090746	0	964137	0	1090746	0	1667114
EIC	Negative	573.4754	6.35	unknown	623388	705865	881064	767026	732686	685524	835662	778299	723270	488788	383378	561205	763750	417733	391191	467644	534275	462192	753338
EIC	Negative	510.3536	2.87	unknown	934214	58646	677348	176026	184709	62387	178579	1380806	144997	1308006	56660	66586	43827	107046	109483	67580	73249	697159	80114
EIC	Negative	630.3781	5.49	unknown	8123222	7637954	6952851	7473354	8410756	8889299	8596182	7472397	5608590	5188123	7904729	7470716	5527911	4833224	5484692	4358234	6274288	5250177	6904647
EIC	Negative	495.2792	3.58	unknown	365487	746258	486348	332149	1177146	161484	629470	347691	666877	739594	618769	270072	591207	678498	688654	620092	567609	668228	408185
fpHILIC	Positive	203.0522	3.16	unknown	19468550	21818064	21204866	24619702	22499134	20621178	21611102	22629064	21272504	21789562	20293934	22364814	22253742	17296014	20921160	20420638	20315646	18482602	17927294
EIC	Negative	230.2102	6.35	unknown	179235	11741	251025	380661	213281	191025	113108	256327	341250	257004	549534	174619	119537	60393	48510	120605	70465	185186	55805
EIC	Negative	243.1965	3.09	unknown	3794450	3842358	6797768	7968280	6273303	4003464	4853859	7824335	5388636	5607255	3484755	4091473	4097297	5991145	2305139	3298715	4629489	6509321	4198169
EIC	Negative	474.2629	3.93	unknown	662728	873068	707243	901484	788081	924624	826590	665273	643796	424283	716627	464738	473608	1129091	909413	536057	763715	646632	734872
fpHILIC	Negative	140.9194	2.12	unknown	2420671	2877814	2214243	2938649	2545394	3070934	2701372	2507026	2600388	2338544	2971125	2756788	2608102	2481934	2412268	2313417	2665607	2328842	2595314
EIC	Negative	285.2350	3.57	unknown	75402	77889	66912	80577	73005	71329	72594	89628	64925	72094	78906	71771	83172	78290	76035	70748	73702	77364	64803
EIC	Negative	257.2272	6.38	unknown	801418	1075787	516981	1396745	920124	1578368	1083400	783066	906212	74091	836640	1490528	1280847	424491	910724	960798	1167223	1056498	819660
EIC	Negative	345.1745	5.58	unknown	312788	401836	482843	1200754	586673	308386	492791	647802	929796	565879	305431	559639	635670	225771	229863	530667	433331	644716	313329
EIC	Negative	319.1589	4.91	unknown	401677	431608	682992	1618640	929037	433329	774342	746749	900896	578381	302711	659549	527115	231547	181503	423737	417638	763765	278764
EIC	Negative	239.1652	3.77	unknown	724209	701122	738495	2762974	1374967	632823	1322313	1241059	1756606	1147898	991475	1306194	1462624	333584	472568	1224840	903833	1736023	317928
EIC	Negative	548.4692	5.78	unknown	206433	301920	443264	0	598189	550384	544634	0	0	598189	2034763	469525	343646	115663	82470	255186	303279	468425	150424
EIC	Negative	242.1841	4.08	unknown	5258257	4483187	6848687	24757514	9353713	7342978	10720525	9892652	15114658	11991761	8398033	12933921	12125980	2661992	3886998	10167453	9888732	153148238	3305893
EIC	Negative	325.2009	3.00	unknown	135515	165987	268179	635716	256723	238944	236854	301853	11991761	917118	331912	248126	113740	66378	66780	207712	462439	113542	787674
EIC	Negative	303.1589	3.22	unknown	326507	110489	231530	160192	193875	184323	254548	292810	54534	249007	108926	146434	114162	115250	190738	138968	155796	261938	714964
fpHILIC	Negative	149.0244	0.57	unknown	1011627	673104	699064	360010	624896	585333	1059412	683774	592259	4616785	458333	485124	297919	709233	709233	363967	396749	496362	104030
EIC	Negative	587.3455	3.23	unknown	170175	180924	169034	180598	192719	195952	168466	182231	168711	144781	171742	157663	166218	159676	175121	162597	169036	159500	183615
fpHILIC	Positive	322.2047	2.30	unknown	1009488	718517	1281526	2013638	729430	1094071	1069757	1583550	1161097	1047617	532953	732485	940993	384052	698808	9057292	393941	1014430	360688
fpHILIC	Negative	130.0228	4.58	unknown	541158	479673	481334	567933	489798	626754	566746	407882	467537	386636	455831	490686	472334	424414	410946	589837	458208	466669	415673
EIC	Negative	237.1132	1.80	unknown	152849	106706	127994	0	121079	97850	109106	90032	101333	90249	85726	78435	97673	43310	102062	142373	75754	0	5323
EIC	Negative	434.2370	6.30	unknown	3400060	1493662	2122415	3805133	1944733	3911814	3117253	2966240	997549	1823142	1203254	2888060	1837895	1066097	2221508	1334603	1662142	3017740	1262669
EIC	Negative	263.0020	1.91	unknown	10426559	6309526	1803424	1217312	6129383	4718447	1389813	6072760	1575664	7288097	7342114	9182516	8371327	6221256	6697547	7995514	6965140	530482	6619089
fpHILIC	Negative	142.9171	2.12	unknown	2276529	2858803	2166973	2849068	2356534	3169033	2658719												

EIC	Negative	309.2716	6.57	unknown	941549	1032386	584111	813658	1042676	676755	830670	809611	1136368	1159386	1269488	944322	802755	788927	922834	529598	852816	1330908	866945
fpHILIC	Positive	494.3237	0.61	unknown	12558132	13374523	13519752	10626311	10638983	11511624	15583880	10203929	9215732	9662322	12716031	13597259	14911869	12740216	12848489	11510890	12990120	10145471	9752411
EIC	Negative	530.2327	4.84	unknown	3011856	3109271	2940142	3056672	2893738	2759387	2921292	2953777	3125080	2867333	2216031	2939058	3048752	2924031	2997453	3117862	2887977	2648247	3042575
EIC	Negative	228.9854	0.55	unknown	486578	118993	147603	340720	104783	363650	177718	77335	104189	238347	162910	173337	116441	93169	139893	227174	79593	170478	212132
EIC	Negative	254.1480	2.27	unknown	1160791	691104	913390	1267820	713354	629751	552575	807175	587887	1148424	429724	507385	639005	412471	481590	579509	574909	1083301	377918
EIC	Negative	236.1373	4.12	unknown	66163	48538	67930	148172	49904	35044	50153	77970	36967	75055	38179	34871	71465	7879	30718	75429	40124	72413	31866
EIC	Negative	236.1375	4.23	unknown	225273	107933	195736	310980	84652	101597	93886	154467	67001	61351	78772	125251	125415	15827	88871	107217	78007	160284	68305
EIC	Negative	138.1529	4.60	unknown	235162	63186	34197	646073	67469	146439	131030	225671	83277	258961	75321	235487	220891	0	59810	135525	116587	28979	52669
EIC	Negative	621.4017	6.22	unknown	2396633	775130	2200423	1577074	1083580	534530	689865	2439941	777730	1839172	799374	841654	728709	686067	848483	958084	747121	2365736	618804
EIC	Negative	470.0325	0.48	unknown	7537529	7769606	8407015	8542689	6794546	7273543	7711572	7734563	8375282	7978871	7733839	7598014	8149986	2861459	7399664	7784801	7740623	7810850	7205103
fpHILIC	Negative	548.1718	3.35	unknown	1978329	1694149	2053814	1916817	1614428	1682243	1516597	1917917	1704250	2030011	1803357	1755334	1600877	1486168	1691567	1521039	1626430	1798087	1820444
EIC	Negative	576.5632	0.64	unknown	133977	55571	131684	103245	106869	80687	71383	49733	80561	210309	51455	30053	63816	127680	60060	60272	44126	89806	136042
fpHILIC	Positive	262.1645	2.26	unknown	2403175	2180602	2207504	2009000	1942072	2806617	2305985	1623381	2218345	2167810	2435450	2455747	2396874	1779958	2317761	2388815	1618583	2270776	2332068
EIC	Negative	542.6502	0.52	unknown	279199	0	236787	181731	225885	137457	147925	0	121479	275975	65960	28048	90589	288761	116213	102143	43553	163805	208873
fpHILIC	Negative	311.2957	0.37	unknown	1160201	1286144	2015993	2087278	1513435	816033	1059770	822938	861104	1387020	947264	1866820	846417	1242413	719953	755833	878028	1685821	1048499
fpHILIC	Negative	126.0031	3.22	unknown	11878660	8707358	8136858	9729491	8941034	10052182	7919053	7670858	8693443	8328052	7514225	8764977	9028724	7119384	7852020	9441520	8721170	9377237	8020119
fpHILIC	Positive	148.0037	3.23	unknown	2043724	2305235	2326571	2473480	2076614	2427761	2023926	1934737	2377688	1966396	1860117	2265651	2117944	2007163	2066824	2367309	2315101	2111019	2083577
EIC	Negative	366.7784	0.52	unknown	213989	87080	176476	187344	224835	163553	168806	48144	172060	279416	72594	73349	143645	651295	157416	133095	101096	148352	241952
EIC	Negative	285.2073	3.87	unknown	31835648	9057790	39934108	38550908	12635130	12018841	14166488	32738961	12603487	42346903	10920967	13332545	12113989	13643782	10999529	10441659	12680231	40439754	9984270
EIC	Negative	325.2658	4.47	unknown	660716	524243	600991	507562	569002	541925	569078	589881	495850	625113	569078	607095	504973	636393	567925	597607	553773	6403937	531797
EIC	Negative	271.1748	2.44	unknown	1233852	626868	926504	978470	800896	867976	764550	914789	921394	1171051	961533	909620	792305	772488	826556	782018	929405	1141771	608027
EIC	Negative	295.2279	4.02	unknown	8204428	4320367	12772488	13904183	6799708	5261201	5563977	13661754	5743983	10059401	4961641	5397202	4442584	10704805	5707158	3793130	6842866	14596553	6648586
fpHILIC	Negative	386.0329	4.81	unknown	1714584	198195	989293	1004661	241382	277957	178834	929194	214604	1209432	171235	229612	186731	290146	202499	241730	228422	886924	290550
EIC	Negative	388.0295	0.48	unknown	8734527	9042173	10018986	9975367	7970347	8612997	9317661	9081584	9396183	9427590	8599654	8746114	9290789	4506052	8733553	9251539	9104069	8865442	8624028
EIC	Negative	608.3942	6.23	unknown	1295248	1015416	1277070	1030206	874713	1228792	1063029	999104	816325	863291	997474	1209614	869643	930575	1276510	982821	907984	865313	973108
EIC	Negative	578.3467	4.35	unknown	151756064	176065269	165496008	145053712	152612678	164204309	149169611	156790082	153235615	147270092	180785899	162308184	158743125	185084309	153585928	152253779	150577003	150191950	173352908
fpHILIC	Negative	250.1448	0.41	unknown	866061	435059	279806	1086193	664828	912707	664470	407172	295388	644185	750611	1048235	710053	346017	657815	737790	59876	412476	556713
EIC	Negative	528.2853	4.04	unknown	135426	255159	145487	158440	175377	227947	218853	148744	127654	113767	194342	222746	207700	201775	202943	165809	216069	124865	182075
EIC	Negative	387.2125	3.22	unknown	165443	239658	169051	150926	219865	165597	159342	179348	147563	143006	156916	150964	158363	143503	179145	165148	169689	163603	199070
EIC	Negative	253.1445	2.06	unknown	288842	314224	211702	200998	251839	222392	292314	173321	274939	241507	181480	230986	280516	235984	323765	328838	299015	124830	144819
EIC	Negative	387.0262	0.48	unknown	79293181	81029760	90198001	89641813	71665741	77587249	81718424	82077852	84401501	86181970	81459905	78419184	83872180	39853981	77759097	82583882	80536198	80947481	77990813
fpHILIC	Negative	305.0737	3.21	unknown	3687637	2906637	2786754	3343888	2864183	3172453	2714924	2700421	30057208	3300512	2865652	2888259	2740743	2459044	2928467	2830124	2710066	3411695	2720794
EIC	Negative	339.2539	3.96	unknown	99352	48768	73150	156601	47798	51882	85224	75462	762981	7198030	2417755	2122928	2544032	1975893	1835946	2305443	3717748	1789756	
EIC	Negative	286.2108	3.87	unknown	5504873	1626494	7251502	6930687	2312605	2138384	2558127	5896048	2212473	7629281	1819030	2417755	2122928	2544032	7536247	7349369	7449659	9392817	7049185
EIC	Negative	299.2530	4.40	unknown	8841917	8381730	8687390	9141525	8470441	7010709	7301344	8284397	7628422	8680614	7069345	7101331	7537428	7261755	6480335	259262	719400	174507	470808
EIC	Negative	429.2860	4.32	unknown	1198963	445805	576065	785875	219479	519614	367097	559334	589751	851783	499505	328180	370602	313996	6480335	259262	719400	174507	470808
EIC	Negative	469.0291	0.48	unknown	55263884	58361996	64032983	63963230	49182861	54329926	58225470	57832579	60566334	60617400	58015747	56369156	59802382	21743349	54707786	58563663	5765081	57159839	54447740
fpHILIC	Negative	146.0458	2.32	unknown	4166872	2335396	2297644	3109304	2661257	3721694	2130634	2063714	2722313	3243351	3355884	3448551	2734160	2317547	3067251	2865583	2483738	2368786	2610976
EIC	Negative	287.2232	3.21	unknown	353372	169797	443577	701951	787363	317104	234055	407173	2702133	3373351	249912	330088	271652	417661	137383	347252	281389	504207	248595
EIC	Negative	337.2327	2.06	unknown	638962	652400	562891	4442580	597219	585942	650379	450982	572908	539766	638206	634589	540227	541113	575039	694484	643593	404193	579171
EIC	Negative	504.3067	4.35	unknown	1091989	1293007	1179627	1108530	1017141	1185034	11478624	1045753	1240383	1376690	1626480	1159542	1451948	1092535	1045753	1119542	1153460	930461	1341012
EIC	Negative	373.1418	1.82	unknown	720152	415183	721408	0	355733	230515	378069	433708	269062	0	469482	452711	499800	205237	265354	693334	439453	0	282326
EIC	Negative	254.1762	3.07	unknown	170067	121891	140183	207869	127158	169841	152543	124118	102877	155587	140690	179958	142908	111784	139139	163046	144645	133966	101438
EIC	Negative	295.1818	3.71	unknown	962060	0	1033923	0	0	0	1017349	0	833058	474911	0	499903	457020	547601	569357	0	0	0	
EIC	Negative	235.1705	2.95	unknown	242579	223826	219010	221354	229188	202832	246422	218409	205890	220158	217191	210515	221151	199955	217281	236336	222261	208970	227773
EIC	Negative	551.0325	0.48	unknown	40416975	43578156	48758948	47556003	35659600	40647501	42304302	43362618	44919504	44974243	43184916	41483112	45133129	12436091	39685627	43930813	42105173	42630777	40461420
EIC	Negative	266.1483	2.62	unknown	739306	527975	1002725	404646	521485	826569	376029	725065	180304	1098732	614456	413722	327133	810563	603506	250692	361946	8555	



EIC	Negative	574.7641	0.52	unknown	444764	405148	656346	630428	339062	426555	347079	390989	551595	413633	422206	395428	440192	59554	362329	515053	372908	486082	346679
EIC	Negative	283.2283	6.22	unknown	391319	290270	405760	633424	252353	209087	273386	279716	322363	278184	278302	402152	471452	210806	210965	359828	257241	297976	229607
EIC	Negative	275.1655	0.89	unknown	65741	0	83045	69536	0	74752	0	0	0	0	0	82654	0	0	99860	0	54617	0	0
EIC	Negative	341.2699	4.28	unknown	66599	35911	144073	482779	61401	75094	79090	203077	105577	125552	98260	127211	137242	38017	48157	130573	87544	223486	42124
EIC	Negative	373.0102	0.48	unknown	626836	626964	685994	629688	574383	636477	592235	581893	724458	696039	632950	683056	569683	314876	624995	609056	684098	687697	550618
EIC	Negative	458.8488	0.52	unknown	405883	475812	594340	646052	391003	482579	444364	420668	530824	417053	496008	466796	486208	107387	419619	522563	462338	520653	378580
EIC	Negative	578.3467	4.89	unknown	13903598	18679352	18709044	12980088	13645377	17591921	16947030	15094941	11957886	13066879	18214431	18719663	15445291	20100508	14887064	16291006	14267273	13833008	20723213
EIC	Negative	325.6600	4.98	unknown	1453191	1433745	1425588	1639498	1473663	1351685	1384792	194212	1418128	1495113	1390591	1420064	1457528	1308854	1487821	1482044	1441983	1486149	1338607
EIC	Negative	317.1146	0.92	unknown	784423	502269	973849	911422	422455	332333	576246	760398	317387	970319	670631	546796	624745	247326	356765	545412	387583	905924	250886
EIC	Negative	295.1552	2.43	unknown	1958828	1473643	1523829	1546905	1493526	1331050	1401652	1556248	1504313	1537362	1447733	1454310	1636610	1363688	1345789	1743568	1416023	1482378	1414097
EIC	Negative	256.1638	2.37	unknown	169732	78533	142936	147427	73552	103625	76684	108720	47001	141394	62781	82456	72362	58550	84108	71303	58408	142105	60241
EIC	Negative	263.1291	2.28	unknown	1003656	331766	1222294	352754	235175	432393	235978	624090	87333	1149762	269219	301386	129753	393228	362932	134911	179783	629882	333683
EIC	Negative	502.6319	0.63	unknown	272023	198590	565195	382477	213414	249388	184387	139160	314100	688228	193684	173486	221254	97938	166933	240472	164996	267242	278963
EIC	Negative	329.2877	4.97	unknown	366183	378284	347583	394258	370745	358287	363130	368527	355826	372045	357214	366943	375358	334633	365148	387208	375136	383205	335931
EIC	Negative	637.3536	5.27	unknown	809516	757919	693311	730538	665721	556801	680146	684934	694173	744471	673738	709725	723230	669968	720112	668468	638138	632699	677344
EIC	Negative	312.2630	6.50	unknown	194335	174493	392380	877853	217456	149369	249311	245294	219333	338615	473997	318492	318161	61011	122927	294753	253365	301344	121036
EIC	Negative	286.7722	0.52	unknown	262724	65563	206804	134917	258964	158171	117687	76738	125806	406210	78585	68681	96566	1408565	116356	140649	42429	125048	325358
fpHILIC	Positive	193.0949	3.13	unknown	631616	873378	845230	749496	760734	812812	703157	836781	746511	602120	752363	901211	665839	929866	795932	746510	725464	766072	855949
fpHILIC	Positive	499.3497	0.60	unknown	2332852	3173672	2357815	2554551	2519797	2530184	2893930	2028613	2754934	2165598	3082441	2899088	3389052	3085156	281390	3019523	2296226	2068909	2748635
fpHILIC	Positive	148.0794	3.47	unknown	30663828	22273982	25872270	26871026	21599718	22741054	22731554	22576062	25747088	23615502	23266796	21382192	21824688	19508372	24905168	21168046	25762802	24118900	21440974
fpHILIC	Negative	182.0538	1.76	unknown	2098955	885205	1044764	1434885	842607	511066	847920	867310	857241	1470811	1024859	1085504	969380	1262584	923982	950261	991180	1268122	879278
EIC	Negative	347.2593	6.22	unknown	330555	155115	221959	354301	135633	227037	135421	227490	310736	256772	123339	216564	186097	67187	154977	243619	257218	215299	183447
EIC	Negative	339.9407	0.52	unknown	249165	259829	279252	334289	229744	236049	285300	324787	268983	379024	263425	316105	294850	75620	236604	275690	304987	296417	255770
EIC	Negative	557.3563	5.09	unknown	1940142	2000536	1888977	2031327	1881032	1940998	1950109	2034164	2085274	1829034	2201889	2026243	1897535	2184051	2053777	2064718	1824544	1912544	2196296
fpHILIC	Negative	369.1096	3.20	unknown	1107723	1172848	1330493	1303715	1049058	1051115	998229	1124452	1126794	1245484	1193490	1170582	977361	969016	1228179	1002847	986516	1189443	1039544
EIC	Negative	319.1897	5.15	unknown	598883	348278	1051326	1319715	175767	88396	124029	240452	146318	636835	159734	1360458	202099	171079	99896	132101	90818	209300	228825
EIC	Negative	251.1288	2.74	unknown	346038	355307	190681	508513	331800	255621	194247	169391	197998	507500	164746	187661	233426	107189	200482	271091	181452	411055	106115
EIC	Negative	370.9448	0.55	unknown	662449	155946	260530	469092	158666	474513	213995	91319	152646	335097	220555	207267	168288	75885	89861	297459	109200	203832	308387
EIC	Negative	555.2726	5.62	unknown	2868821	2277168	2752383	3055926	2081660	1643951	1917729	2024765	1570796	2503869	1487157	1430121	1921882	1545591	1599621	1571877	1938596	2871828	1430231
EIC	Negative	265.1087	2.22	unknown	83558	60090	69636	81652	56230	53288	57327	92208	53559	101777	56299	65823	46139	52361	52361	47596	84545	65071	0
fpHILIC	Negative	124.0150	2.98	unknown	488720	458978	447018	549582	338323	531295	357396	270322	300945	417798	331796	283165	423945	156414	298054	403360	409066	393850	327958
EIC	Negative	252.1606	2.64	unknown	6757879	4565252	3457509	7616593	5360087	8557234	5373789	3922453	3709610	4726606	6096739	6424270	4992008	2290439	7422372	6295179	6707878	3938900	3070077
fpHILIC	Positive	495.3270	0.61	unknown	3862228	3432979	3350190	2909829	3305700	2954329	3742574	2569212	2700818	2659423	2874009	3845052	3513110	3281184	3338094	3154038	3947265	2729040	2402743
EIC	Negative	464.2785	4.89	unknown	891521	1003133	1126265	637070	733819	1045278	812212	850659	414291	643417	739177	733861	561906	1278746	849589	442667	707074	851182	1079167
fpHILIC	Positive	273.0462	2.70	unknown	310144	316759	238552	394951	324099	346755	319513	175136	288161	283404	318257	347580	251587	158340	294768	229582	201419	238769	517855
fpHILIC	Positive	785.5869	0.43	unknown	16461353	15852007	17753570	13994723	11979605	13241882	12971873	14005408	10591790	13894232	13543558	12997641	11499192	17261466	13103127	11269436	11416118	14262029	13942623
EIC	Negative	349.2011	4.37	unknown	302710	223983	4400415	498245	1400415	345484	178534	339472	340248	537899	292154	523899	406224	81657	91169	365096	308282	864844	1791621
EIC	Negative	440.2470	6.09	unknown	117603	127396	103551	251239	77729	69178	85022	131895	144174	177660	134859	51025	120906	167836	95893	55513	146484	139486	80518
EIC	Negative	579.3498	4.89	unknown	4425173	5814786	6010027	4091145	4359847	5587532	5319955	4654125	3788645	4048850	5751012	5813791	4940528	6328526	4679377	40107620	4521834	4372257	6581287
EIC	Negative	508.9095	0.55	unknown	297038	75063	187331	237281	91945	231758	132926	13145	135577	179935	108686	98143	103941	0	92719	153204	72928	105978	169915
EIC	Negative	616.2505	1.03	unknown	143727	78952	222583	126234	71298	43185	103712	128838	100973	69349	82963	130649	42566	69349	82963	130649	42566	154279	38820
EIC	Negative	363.2549	5.88	unknown	1724510	1066615	1985881	1841208	1172676	703597	880059	1703826	914798	2309989	1165533	793032	902700	909707	1137400	944338	901495	1663043	834505
EIC	Negative	323.2501	5.21	unknown	13721538	3635866	3488901	3725221	3554376	3523852	3252366	3628280	3266778	3487599	3422186	3266726	3438761	3060643	3458513	3713837	3417338	3568193	3409155
EIC	Negative	381.2567	4.40	unknown	609371	523623	537230	426032	559163	425163	453723	525735	475207	660371	812590	468373	531132	481924	494460	497533	460122	584406	450893
fpHILIC	Negative	819.5577	0.43	unknown	9442158	9017557	7922106	6323034	7140362	6310956	5747288	6563615	8891174	6685028	8128024	7258093	6506452	9839019	8114044	6031667	6001800	5893849	9300685
fpHILIC	Positive	733.5567	0.44	unknown	482551	512852	748722	494172	384107	427257	345995	496784	603134	475727	507278	511522	445111	810525	431805	347238	542197	543889	437216
fpHILIC	Negative	844.5689	0.43	unknown	6724470	5848757	6695599	5989928	5031394	5307939	4826395	4939410	4342763	5198301	5024956	5186035	4915164	5728442	5507340	4291978	4690753	5017179	5548590
EIC	Negative	566.3472	5.16	unknown	380813	428715	365678	367876	447700	433667	437408	381584	349538	359043	445374								

EIC	Negative	406.2534	5.66	unknown	124568	146051	118744	187212	127398	132984	138803	119160	111916	135874	133768	145398	165241	113380	137287	135409	127394	145761	101085
EIC	Negative	319.1556	3.15	unknown	524942	138649	544246	448634	171204	199456	246201	388138	94856	507086	176053	248993	169457	116515	152712	136086	177080	484596	178846
EIC	Negative	501.3013	3.81	unknown	480914	180871	512308	1105082	233890	346918	421638	603031	566627	603015	351109	338487	636161	31632	205078	426132	431463	1167720	0
EIC	Negative	297.1718	2.53	unknown	473390	191349	406940	212029	103577	164683	143101	314024	71527	350106	177705	118551	118528	156632	106468	83690	86289	381658	160325
EIC	Negative	374.2913	3.22	unknown	556427	671549	572542	759689	687749	677359	566574	623136	649921	672901	679054	645208	649230	556920	585840	828778	610032	612855	654277
fpHILIC	Negative	160.0615	1.66	unknown	158126	3004156	0	3751226	0	4304793	2808077	0	0	0	4363097	4766060	0	0	3095805	4211376	0	0	0
fpHILIC	Positive	240.1014	1.67	unknown	613457	693216	720367	745652	457871	578105	647946	550950	653014	658758	712152	675302	646710	507356	621920	746077	445149	585717	568706
fpHILIC	Negative	195.9262	4.55	unknown	1192816	1003057	1006201	1094570	824163	1136359	916965	931982	1031313	1267355	966433	1031377	1018739	935505	1132326	1031687	853702	935293	1022341
EIC	Negative	263.1654	3.90	unknown	191137	93182	332122	153842	104744	86058	122750	174394	78130	223167	134944	116610	109611	106644	96873	70751	86266	216241	111724
EIC	Negative	504.3134	4.00	unknown	0	0	332808	706393	15614	0	0	0	0	593648	0	0	0	0	16050	0	0	0	0
EIC	Negative	313.2027	2.41	unknown	198612	71585	210124	114906	65824	83701	69251	144439	48731	165044	74631	73263	59037	56695	68917	69915	68323	141921	74501
EIC	Negative	352.1751	2.44	unknown	312751	133682	160114	234796	177668	176790	148832	261387	194574	196322	162715	178304	144947	141822	167248	136853	154430	410351	117835
EIC	Negative	319.2640	5.88	unknown	836974	519072	933253	881320	569075	343715	452739	807072	462846	1112129	593151	396242	463359	452055	591106	467535	445296	799170	407924
EIC	Negative	326.2001	3.09	unknown	266717	114235	185013	332038	164749	215918	145444	215918	131597	235246	94434	230386	176240	222577	161418	159206	181207	238832	141298
EIC	Negative	480.8962	0.52	unknown	1086799	1274974	1203691	1431196	798095	1012915	1099617	1331154	1197005	951871	12107052	1371088	1248701	161422	970054	1080872	1172785	1250395	1122480
fpHILIC	Negative	594.3404	0.62	unknown	2059432	2597943	2918702	1838329	1704206	2720560	2039387	2066176	1547004	1623707	2316047	2224835	2070491	2336195	1865490	1657817	1632563	2161396	3052824
EIC	Negative	278.1839	3.13	unknown	675875	347757	581242	478240	0	471358	433959	498332	0	565150	499582	555223	394927	0	518161	0	432104	494169	0
EIC	Negative	255.1604	2.45	unknown	512691	291748	525664	593296	303481	333183	303637	300174	303825	99381	247417	337208	356281	259156	272962	343053	287254	566863	234636
EIC	Negative	327.2727	4.01	unknown	382116	324556	301314	316862	329552	337768	345895	316073	303825	292992	616544	326754	307146	333994	308632	355717	332777	356702	326987
fpHILIC	Negative	146.0651	3.47	unknown	9257249	5925570	7639285	6729111	5707488	6262063	6108204	6077079	508110	6860115	6029740	6287811	5693778	4535227	7357454	5795120	6601910	7407164	4323179
EIC	Negative	636.3501	5.27	unknown	2301463	2241621	2132761	2077572	1976310	1750952	2010747	2070603	2181598	2159809	2176032	2277798	2238818	2084484	2241206	2177548	2011782	1800949	2052299
fpHILIC	Positive	229.1546	2.03	unknown	3993114	3128676	2243111	3865372	2524413	3644919	2870750	1682911	3062717	2800184	2890989	3324907	3050500	2120547	2731292	4412447	2260597	2605097	2192951
fpHILIC	Positive	175.1190	5.38	unknown	54862160	52207740	37747520	40414576	44586832	57423480	46470476	36142392	42173936	33076006	43138776	46869676	50216416	44944368	65776228	56984972	53129420	34685776	41088288
EIC	Negative	579.3498	4.49	unknown	7582616	8806299	10334847	7146087	6913476	7781443	7067400	7346153	6853409	7101495	8958405	7915550	7263904	10456002	7164884	7375416	6459795	7280663	8777204
fpHILIC	Positive	343.1889	2.39	unknown	1007906	806349	822116	755562	829248	838390	946968	695717	719265	871999	957966	833051	881852	876423	881079	1819916	781813	980790	689596
fpHILIC	Positive	247.1279	3.02	unknown	1679955	720430	772216	867321	708465	10450768	695079	438890	578320	764072	900821	926341	796284	776995	885993	913542	688508	616505	886449
fpHILIC	Positive	148.0734	3.48	unknown	3828256	3268924	3461595	3592235	2787761	3445419	2853660	2878994	3576112	3413552	3523607	2826389	3058265	2423909	3800380	3047880	3357592	3228874	2953011
EIC	Negative	299.2313	4.60	unknown	365489	227512	563107	400413	316659	320088	530391	346135	353633	301219	214075	242303	231903	362804	200140	618206	407592	436643	235371
EIC	Negative	478.2843	4.68	unknown	9523400	10109178	10148086	8018106	7687468	9468654	7403413	8172865	5778246	7114843	8233044	7505998	6248732	18086498	8679091	4394815	7553552	9262907	9832776
EIC	Negative	241.0506	2.39	unknown	5509545	4126674	5158407	5774095	3691900	3951830	4124509	5122375	3565658	5379195	3786147	4053182	3966248	4089158	3973475	3964881	3927933	5330594	3909157
EIC	Negative	313.1197	1.06	unknown	373386	162628	226698	258361	137749	140227	162159	313302	153017	318730	155086	212829	190611	152376	152015	198053	175299	279877	130098
EIC	Negative	637.3536	5.04	unknown	708466	497787	603111	598294	463755	411899	556333	621342	606764	709660	475708	547856	509541	522083	554702	539176	528551	658367	465471
fpHILIC	Positive	787.6059	0.43	unknown	20134682	19738960	24368056	19585688	20083122	18671686	17544124	24263556	15452994	20386776	20788256	18493914	16185466	233103242	19775330	16479713	19430524	22369636	21087972
EIC	Negative	327.1601	1.83	unknown	375149	477258	283789	0	184439	155985	209944	26574	306589	0	139516	168860	147576	138903	215990	405890	218455	0	72045
EIC	Negative	417.2278	4.56	unknown	738052	572793	851394	656514	487752	481929	331528	508941	578767	687324	404187	659884	427135	441860	351019	581360	505578	643995	384999
fpHILIC	Positive	330.1760	2.70	unknown	312355	406882	396712	276009	333287	335858	390468	292495	349646	315426	337533	345835	373967	541637	325178	326573	312105	863514	420662
fpHILIC	Positive	311.1229	3.54	unknown	1139469	726153	826907	740143	562070	957720	564813	560270	515637	905284	830329	513935	479198	740319	613635	557480	610700	333484	587214
EIC	Negative	288.1637	2.64	unknown	483504	134958	0	37474	56390	186254	291138	0	111975	42234	192197	203619	189346	111148	191354	153728	235058	0	86924
EIC	Negative	429.2862	3.34	unknown	649545	258688	361358	524887	173748	273688	427313	358403	401225	842122	224935	262416	282971	407446	462245	262416	282971	221380	221025
EIC	Negative	331.1193	3.46	unknown	1604121	1527714	1666496	1636756	1269377	1108789	1447857	1495426	1325384	1759184	1455056	1465765	1400081	1292698	1684984	1618335	1114081	1343557	1019043
fpHILIC	Negative	274.1409	4.35	unknown	536791	477231	297632	337790	390407	700859	350944	487580	279527	322847	588838	569473	376101	472870	500863	567631	308630	290668	310643
fpHILIC	Negative	207.0144	4.21	unknown	3703655	1207904	452390	1843927	1990607	2841979	1650892	761485	2187214	537982	1005837	2684197	1820429	1309785	1700346	2923384	2238518	1279910	1609044
fpHILIC	Positive	496.2795	0.60	unknown	2019528	2521235	1915187	1947212	2116079	1945732	2102332	1671717	1196951	2428735	2291321	2677977	2448165	2491657	2531084	2346691	1541971	22108974	0
fpHILIC	Positive	302.2149	0.61	unknown	2369099	683112	1327203	2248761	807822	886314	1256742	1436084	803519	1284986	1108937	976509	971143	190961	702566	1056523	897078	2211766	499463
EIC	Negative	376.8464	0.52	unknown	615695	531268	835412	824825	529318	605410	513599	354323	617017	682338	523447	496450	542890	167919	472546	609387	500020	578189	548822
EIC	Negative	476.2785	4.68	unknown	205372816	208704751	219450424	172033686	160200475	203634827	154771155	175795069	120219310	156547436	173991869	157927214	134334018	227747963	185281078	91559791	164337636	191756651	209486576
EIC	Negative	450.9511	0.55	unknown	674472	233974	339100	582373	167321	570953	290480	93194	187301	327152	284662	302428	201786	74374	230423	380316	162216	261858	314793
EIC	Negative	478.2943	5.54	unknown	84125669	100424174	86610179	69395287	80373980	102621218	75913593	76212527	51506499	57397689	64551								

EIC	Negative	541.3347	4.46	unknown	2630817	2270438	2159754	2194357	1957249	2050256	1838791	1870242	2242105	2240327	2129713	2219234	2112580	2120189	2049360	2492385	1829375	2009385	1986004
EIC	Negative	406.2604	5.21	unknown	507806	426017	424370	416023	447098	466719	431636	469646	372165	465921	476539	428693	469613	417232	469364	463251	421101	464425	459259
fpHILIC	Positive	144.0805	2.07	unknown	731933	314911	486786	342203	315387	278367	304519	275158	282260	361808	354056	302266	279175	505039	463306	284033	257616	363814	196692
fpHILIC	Positive	263.1687	2.25	unknown	234919	430467	247586	310099	340086	279377	360292	265683	281197	248928	310681	381505	277651	228687	260134	351474	260451	387242	330663
fpHILIC	Negative	172.0250	3.88	unknown	570228	420444	627932	867274	310827	427700	486696	692176	431309	242531	289896	659559	763084	0	468898	674605	405634		
EIC	Negative	229.1442	2.10	unknown	224328	204785	250650	208132	182599	189749	222117	200285	207121	309802	259206	244127	363528	116720	217164	229370	275221	168813	153714
EIC	Negative	275.1620	0.89	unknown	68459	110656	92297	71184	58612	80041	71752	83478	46275	58432	57584	85241	68721	50759	62042	104370	369958	58730	66089
EIC	Negative	288.9420	0.55	unknown	546104	100409	172649	306810	91020	346706	145002	32542	151147	284646	138120	129781	56196	90496	129360	197947	78564	127797	265222
fpHILIC	Positive	205.0816	3.85	unknown	2054918	716866	890604	1903973	751185	1275998	754835	777663	751551	914289	840029	953140	966977	599767	716067	1128738	986737	881836	780847
fpHILIC	Negative	144.1112	0.45	unknown	437019	283538	564020	555001	395854	391380	319651	385623	336465	397846	280053	396339	307541	310388	300033	375572	404949	513383	312693
EIC	Negative	380.8154	0.65	unknown	245014	92535	131107	249837	58750	177972	96418	46134	66533	143728	102624	118341	89828	33057	73078	115986	60514	84958	130295
fpHILIC	Positive	149.0456	2.48	unknown	683622	691615	737077	351952	380350	589068	377312	344847	340344	495853	503136	515464	375069	719760	479056	329257	412604	433413	465422
fpHILIC	Positive	520.3403	0.60	unknown	383323168	394942528	478174720	355023648	308324064	378886464	362608896	369770560	269561568	315178016	418279584	398481536	364397472	432863744	313779456	304237568	339842368	386536480	418069600
EIC	Negative	1089555	345752	880932	900255	327177	393318	433933	660455	287503	1170034	341414	487818	405001	347293	372338	399569	329565	820681	272574			
EIC	Negative	265.1449	2.62	unknown	4381507	3669588	8535314	2640378	3748459	4998491	2627988	3695371	1099045	6121300	3642555	2987307	1469264	4831987	3936227	1816127	2134855	5210852	3781549
fpHILIC	Positive	786.5998	0.43	unknown	42646264	42913056	50660840	40849884	40872592	41489220	35732548	53250992	31655394	45369668	43645212	39972444	34432196	52140028	42958136	35096156	38668760	48381000	46903976
fpHILIC	Negative	98.9559	4.56	unknown	3955875	3138924	3398721	3618799	2690449	3595319	2268681	3042052	3528826	4068587	3042351	3337558	3618174	2851810	3649809	3747586	2674768	3134571	3221347
fpHILIC	Negative	211.1705	0.39	unknown	1509351	871057	1714589	2924184	1022728	1068639	1224144	1311917	1775628	816990	1547100	1790917	572541	788750	1123985	1264703	2268891	675505	
EIC	Negative	325.2745	5.83	unknown	1137906	1143003	2309572	2564048	1582879	951782	1145782	1812983	1176161	1186133	1297162	1257092	1265017	1672282	1385233	808451	1224455	3232858	1228078
fpHILIC	Negative	200.1292	0.45	unknown	3112916	1748013	2159471	3290297	1674920	2369819	2195872	1602598	1932933	2690108	1922236	2323457	3937368	875708	1968948	2819329	1939084	2505984	984774
EIC	Negative	318.1789	1.78	unknown	199267	107340	185313	82755	52779	82151	117384	66258	37961	125963	133017	173616	172581	82909	72089	140138	101490	0	59198
fpHILIC	Positive	163.1153	2.92	unknown	53660316	53508776	47381936	32754484	30817130	49173984	41359608	31680352	25115956	36206436	45152368	44980592	35758012	36586228	42020368	33268290	33153284	34650228	44914288
EIC	Negative	585.0388	0.49	unknown	1520411	1652953	1921429	1822714	1376473	1514835	1582546	1640203	1699892	1669542	1737491	1562996	1773582	110695	1531876	1745417	1655459	1674429	1559887
EIC	Negative	253.2075	5.12	unknown	351665	164650	620249	292126	162611	178707	234879	439173	47619	380021	189223	185795	164342	209587	176682	103363	171259	419349	241931
fpHILIC	Positive	221.0911	2.61	unknown	1597110	1873872	1729694	1114255	1584665	1680455	1777836	1212756	1316716	1344593	1793162	1584663	1608889	1976125	1970694	1686570	1252555	1497676	1520833
fpHILIC	Negative	181.0597	1.76	unknown	20142916	9158250	111331978	15206214	8424294	16350900	8197744	8503857	8081664	14714568	10239509	11163426	9861841	12447211	9329286	8903216	10849468	13351408	9487965
EIC	Negative	318.1182	0.92	unknown	149921	98911	177631	167331	77468	68933	98878	136102	72573	141008	113630	101775	108283	45137	82436	98791	85524	156226	52396
EIC	Negative	540.3312	4.46	unknown	9302815	8260009	7717826	7551285	6822036	6922773	6609199	6798309	7528062	7648048	7520437	7645928	7793271	7305010	7512231	8923693	6036177	6879503	6780900
fpHILIC	Negative	194.9274	4.55	unknown	84022248	70252064	72543080	78856672	57682008	74823952	62112668	65838444	70490512	85447184	63962320	70830632	77033424	65640920	75902560	79096824	59235336	63976876	68510096
fpHILIC	Positive	293.1452	3.47	unknown	1121845	666057	808635	794836	737260	741760	726134	770673	748496	876102	836831	679803	797376	690223	979590	689498	761355	928716	544762
EIC	Negative	378.8184	0.65	unknown	148939	54733	77503	145503	34223	113288	56799	16532	43710	94669	60869	72361	51597	20339	43649	71828	34258	50855	76774
EIC	Negative	247.1703	3.84	unknown	203046	244327	137976	147136	195360	176479	186579	173278	161756	140166	205060	180911	203518	148753	178174	153802	179894	193081	231963
EIC	Negative	372.8115	0.52	unknown	1043796	837733	1348957	1244933	806377	899152	790924	628677	1074639	1132619	825363	830028	853793	198146	796599	998840	747128	974899	887556
fpHILIC	Negative	196.9233	4.55	unknown	7445866	6162219	6332557	6915964	5076767	6391476	5364101	5776647	6208817	7417636	5297311	6197246	6585361	5975611	6599829	6981664	5039400	5614366	5994871
EIC	Negative	345.2104	6.31	unknown	4179148	13122685	15331457	11138244	5199947	12352622	6143649	11101238	9920617	11342802	20514748	15849263	5495648	8860131	15412079	18090920	5772243	6224978	7525863
fpHILIC	Negative	97.9595	4.56	unknown	624266	561410	562030	609397	475067	630525	525965	503185	528714	702998	530258	502422	568155	462340	576184	647344	496989	526267	552295
EIC	Negative	257.1760	2.83	unknown	287350	202088	290814	269819	219759	269670	232082	275336	156871	315966	182746	317346	299329	137524	183533	216557	218096	396364	196261
fpHILIC	Positive	806.5683	0.43	unknown	42863012	76773720	41393884	51206274	50755044	50160710	47898896	39013060	74052000	43375764	65420536	58861048	63355756	60544148	50604868	69423384	58319928	35497288	11127800
EIC	Negative	450.2632	4.06	unknown	871974	1322233	1179081	751477	1041766	1028592	867526	724273	728749	128789	1038222	932719	726943	939767	1268886	1048995	893766	957144	1397267
fpHILIC	Negative	166.0132	2.98	unknown	734693	409194	663101	637145	435547	472526	359980	389385	368888	571303	449372	464605	498822	256147	396093	358918	485981	498887	388613
fpHILIC	Negative	304.1302	0.93	unknown	514136	402953	317585	381820	317585	318204	423233	358937	404239	364762	326800	351265	341626	410703	334238	328049	421888	330858	
fpHILIC	Negative	183.5558	0.44	unknown	18943132	18255506	17402424	13360260	15265789	13307121	11234166	12746728	18403352	14599579	16859006	14531310	14291114	19891282	16544258	13481533	13708244	11799348	19034628
EIC	Negative	556.3009	4.36	unknown	839384	797631	883302	877043	802018	696816	751624	817043	685874	787899	854021	861308	815897	796944	830273	632808	712722	863696	785448
fpHILIC	Positive	279.1000	2.97	unknown	5256625	2679299	4529694	2588100	2189403	2670938	2782004	2478035	2644615	3687842	4295438	2550224	3495867	5053840	4791288	628979	3783678	1735814	2478180
EIC	Negative	466.2209	0.88	unknown	169150	231307	117981	84703	108420	127296	133536	118892	116018	116018	194649	175834	151444	155469	121241	146755	103124	116359	183117
EIC	Negative	478.8991	0.52	unknown	1129949	1283362	1215254	1495708	862881	1022407	1070729	1302788	1255848	932865	1250181	1384976	1295866	117341	957446	1128606	1266119	1223141	1192291
EIC	Negative	232.8893	0.52	unknown	969488	676527	1131882	1002526	785007	723775	652278	522004	829006	1139831	647411	627680							

EIC	Negative	448.1698	0.71	unknown	682479	580772	798567	321002	463919	564141	586763	341325	484805	760895	619657	482297	486349	821789	507352	469851	404172	285909	920934
EIC	Negative	436.6609	0.62	unknown	85113	65686	114849	85953	75666	66850	61881	46310	85908	131396	62251	59734	60983	44846	55694	72662	48514	67099	113209
fpHILIC	Negative	554.3087	0.60	unknown	2094129	2500717	1932844	1790738	1675369	1838551	2100386	1683861	1735862	1869012	1845295	2297722	2143183	1984091	2178790	1991790	19212780	1514767	1988602
EIC	Negative	440.7698	0.65	unknown	95458	47057	55063	100901	22357	73374	42603	28299	29767	62515	52750	55068	40624	8590	31227	55451	27188	40854	53730
EIC	Negative	371.1422	3.94	unknown	206499	167223	269775	149331	106301	261949	188455	158800	143272	121419	187437	258245	263639	223826	92282	226379	186437	268270	138920
EIC	Negative	531.2732	5.75	unknown	2434145	3181633	1998810	2321195	3197289	1633180	3139883	2199014	1375588	1692457	2170244	2382078	2243130	2673895	2383815	1413349	3120663	3228443	2129700
EIC	Negative	249.1126	3.07	unknown	14203	55169	32287	112335	62324	67366	17560	15860	68081	74707	45600	89731	44059	41687	26152	58068	73788	68814	19895
EIC	Negative	263.1654	3.31	unknown	260410	242686	270097	301924	199429	185847	206478	214166	155224	254794	229093	212765	238114	164328	172313	198836	184632	219095	247716
fpHILIC	Negative	196.9316	4.56	unknown	1355634	1085519	1161172	1197046	936210	1159413	911691	1068496	1132181	1411472	1099599	1133078	1265411	1023444	1215731	1214119	1006522	985650	1197174
fpHILIC	Positive	343.1641	3.39	unknown	1695127	1636039	1079391	1030365	1307720	1418310	1143639	1172056	1406606	936253	1068717	1439742	1431713	1792042	1525428	1464750	1233801	1698780	942058
EIC	Negative	250.1448	2.24	unknown	1136666	611596	549780	1535966	669980	1184918	695745	578164	532395	852011	795618	910246	682311	294761	1079109	939959	877592	603492	399285
EIC	Negative	619.0205	0.48	unknown	242947	306383	284062	314669	253807	272163	261669	307143	322894	308944	288123	329413	289212	49838	239216	315104	352822	329158	273702
EIC	Negative	318.7466	0.61	unknown	104993	70031	112950	104199	87270	81184	67206	50937	93639	135934	68071	59783	80978	74179	64173	71610	72458	82062	114770
EIC	Negative	446.1721	0.71	unknown	1954194	1662116	2275655	946577	1306276	1650947	1673510	934702	1402974	2164649	1768025	1403701	1402885	2344531	1463771	1315878	1141250	885248	2620462
EIC	Negative	447.1756	0.71	unknown	391455	321807	442072	178771	249724	320977	327429	181300	268796	422834	333015	276025	267646	450196	288362	252463	218475	171926	506330
EIC	Negative	519.1675	1.87	unknown	43329	365089	0	0	65758	144810	149437	207587	0	228211	86027	221432	172730	166995	179976	112726	0	145918	
EIC	Negative	619.3472	2.85	unknown	332807	964480	1075252	686010	366471	720018	475704	605402	266979	972764	881040	605987	277314	91215	496529	519803	573692	565840	441919
fpHILIC	Positive	167.0483	3.24	unknown	6010418	5450413	4464935	4633675	4083561	5024510	3538748	3140111	3594710	3385319	3932692	4299980	3547298	4042542	4680705	4333110	4552029	4060657	
EIC	Negative	366.2728	6.01	unknown	201904	140223	222689	161158	134717	83202	141434	168909	123336	201178	137767	117283	104859	131740	161039	178801	103057	134743	118041
EIC	Negative	505.2078	1.15	unknown	164496	131033	121032	67381	80853	117984	164198	45878	121466	122181	88829	146292	99021	75998	96198	142069	172629	80104	65459
EIC	Negative	274.1848	2.48	unknown	1163381	200957	649458	1538850	280092	230945	351391	1419665	500284	1069554	221411	358888	286019	74642	189842	352488	261242	1680835	198680
fpHILIC	Negative	147.0663	3.47	unknown	1056363	673873	868267	764074	670313	674118	606061	582503	567338	839896	674037	699661	651975	533703	832364	540428	588325	869795	430025
fpHILIC	Negative	291.0385	2.69	unknown	1115317	247244	132522	131411	187872	387486	0	173095	343315	73143	82831	203659	182198	161465	82684	306350	249605	344758	182810
EIC	Negative	635.0444	0.48	unknown	1359243	1445440	1644945	1622353	1134272	1305670	1327648	1469255	1554348	1477313	1430074	1513552	84216	1379160	1538299	1345493	1551355	1296673	
EIC	Negative	260.7875	0.61	unknown	172515	133390	200817	176501	180589	139905	142163	103124	175966	259139	127049	113381	137179	204453	136467	134869	134016	154696	323683
fpHILIC	Negative	309.1083	3.54	unknown	726318	363274	426283	397090	279590	148719	245975	331874	234201	439999	268747	234200	240293	312463	318232	244025	317105	486731	248864
EIC	Negative	325.2384	5.94	unknown	570127	337041	1441177	601833	344692	0	432455	908474	0	645908	432223	530011	354464	338002	273968	0	322572	738870	466956
EIC	Negative	242.1841	3.53	unknown	238615	162683	324371	305066	151322	179553	179518	211522	152806	245448	190701	282224	266488	176612	149495	193496	179371	278364	134356
fpHILIC	Negative	357.0292	3.01	unknown	559048	493372	549956	613589	399990	414505	403609	434307	445469	667474	427004	384097	457831	407593	391331	404628	474040	533885	439852
EIC	Negative	299.2592	4.34	unknown	0	5600672	5056496	4970579	5236493	0	0	0	0	0	0	0	0	0	0	0	0	5600907	0
EIC	Negative	475.2665	3.99	unknown	1320997	1592166	1750083	906644	1078938	1715215	965830	1226881	646415	759142	1311871	862809	731300	2633706	1307135	400878	1094949	1284861	1938276
EIC	Negative	476.6699	3.99	unknown	235219	313351	362057	192494	226940	341540	205544	233122	130501	170565	276649	186372	177819	497074	253373	85089	243881	253890	380871
EIC	Negative	570.3424	2.89	unknown	182052	228067	165117	130506	140070	107012	0	136229	130566	1036229	126993	156170	137270	343036	163953	183464	138031	0	241379
EIC	Negative	570.3417	3.94	unknown	400416	330554	337203	292325	311502	401531	345189	340789	231287	389452	450777	393939	280770	425351	433335	311148	271325	304255	426894
fpHILIC	Positive	173.0916	2.59	unknown	1513751	1374785	1018829	901548	943802	1705187	1126775	360819	1038198	1156341	1345487	823914	1177730	1683896	1215663	624314	1181364	855168	
fpHILIC	Negative	203.0678	3.86	unknown	723789	274992	317226	562244	242231	447358	230733	260960	250200	320800	278083	278142	287513	192162	256415	383469	306508	331519	256734
EIC	Negative	135.1620	2.01	unknown	979369	816613	860948	406387	603987	969807	1398400	0	866899	1264457	1135640	489649	541617	1062471	702870	0	0	0	0
fpHILIC	Negative	358.1694	0.93	unknown	890381	328198	640306	924704	377795	353237	389052	822870	745073	537768	268241	435592	416647	400375	436414	615559	559446	908808	362468
EIC	Negative	380.6992	0.62	unknown	99898	82809	141209	96883	95421	74400	81782	52559	71463	52559	73493	66602	79443	90716	71643	75299	68663	84184	135433
fpHILIC	Negative	571.3445	0.62	unknown	878809	944589	593678	661869	560403	930218	738109	610465	1024185	700095	832649	769137	893144	787851	1005429	918603	782779	571128	807590
fpHILIC	Negative	125.0066	3.22	unknown	1605081	1134842	961849	1334921	1016021	1290270	1040987	1013556	1042547	1073775	1089425	1230662	1133656	1042547	1100754	1475015	1148033	1185318	1075672
fpHILIC	Positive	328.1602	2.78	unknown	6021232	5481088	6308594	4498547	5143956	5483098	4425707	5081931	4469692	5206993	5978399	5599274	5182233	6098532	5093180	5012627	4965361	5597993	5769622
fpHILIC	Positive	792.5925	0.43	unknown	677792	764690	1032787	860168	850039	803136	611989	828069	630324	760748	831707	757103	799603	680326	645412	1028152	840756	817902	759210
EIC	Negative	301.2385	3.28	unknown	148379	81960	320489	139747	218636	147183	75970	175055	63287	152633	118386	102268	113326	108795	91731	191368	130133	256723	60578
EIC	Negative	345.1714	1.53	unknown	289583	241424	0	289492	146262	184795	121089	0	69177	0	139055	213606	119207	163416	119813	161390	72324	0	118669
EIC	Negative	299.2592	4.40	unknown	0	7626982	8054837	7985151	7889285	0	0	0	0	0	0	0	0	0	0	0	0	8475975	0
fpHILIC	Negative	409.2351	0.61	unknown	3786327	5375044	3097774	4150198	3757244	4001725	3629729	3096207	4944257	3719511	5449861	4484941	4777755	4623173	4771780	4307461	3994326	3285252	4526963
fpHILIC	Positive	344.1325	2.99	unknown	458060	415715	672440	402656	274597	367545	258971	193298	155164	304946	259260	251205	279970	201332	276759	216942	279154	358049	212422
EIC	Negative	424.2475	3.95	unknown	592535	656321	815449	522289	460278	753807	514279	591676	345617	478558	566057	608025	368804	1222221	516970	323783	539273	675927	820494
EIC																							

EIC	Negative	410.1712	3.94	unknown	466382	386923	728564	343519	212671	677039	423414	323370	277248	249680	460279	626771	688572	513047	189936	463675	476584	633973	306904	
EIC	Negative	578.3460	3.68	unknown	0	5433857	3448319	127807	118890	111653	222527	5125620	0	91333	103201	4199488	4578946	3765600	0	75739	114267	576784	77960	
EIC	Negative	286.9446	0.55	unknown	872706	160036	269481	459512	142388	559090	202412	155034	0	459750	210041	209405	559090	153290	138381	230917	314143	72506	182523	423600
EIC	Negative	282.1798	3.03	unknown	185771	64003	149960	165722	61431	73849	71302	109301	56213	222622	61466	100575	72907	66421	70334	69066	67312	146956	49128	
EIC	Negative	257.1760	2.36	unknown	357316	166432	339556	338619	194389	239278	244942	283551	219289	292854	221167	293002	283195	183115	228235	304699	206206	366490	173377	
fpHILIC	Positive	128.0176	3.23	unknown	4752617	4177390	3220444	3555959	2911449	4033249	2614989	2376250	3473573	2608844	2491471	3041849	3238444	2794687	3127300	3924745	3209017	3558128	2869557	
EIC	Negative	293.1741	5.18	unknown	208256	144739	169835	505321	207411	161801	180305	205462	256739	235848	181166	213376	348422	62729	133171	403003	199283	257065	103289	
fpHILIC	Negative	161.0563	2.94	unknown	744071	286936	190410	275421	192751	542840	178104	197605	266207	256121	238244	348686	244002	214869	200874	322558	349947	286983	326777	
EIC	Negative	476.2785	4.47	unknown	76972350	91444216	87094888	66126309	69381394	102600825	66585162	74772189	48274252	62754981	81783098	65642011	53945263	116117014	96436954	47370388	74207780	78288018	95809161	
fpHILIC	Negative	245.1137	3.03	unknown	531653	342121	334954	255216	287065	566659	287564	244432	255993	294524	369429	375772	309313	348203	464464	333747	336850	242287	403067	
EIC	Negative	255.0929	0.75	unknown	144227	68972	53498	179352	63657	206370	175959	0	46418	81186	116101	155943	121413	164663	97000	146990	93954	73721	122423	
EIC	Negative	620.5429	0.64	unknown	101920	52592	156641	113362	51907	69283	57349	44671	85191	176203	53575	37055	65124	0	35640	71487	31075	80573	115729	
EIC	Negative	477.2815	4.47	unknown	20271228	23487179	22825407	17297280	18293321	26819409	17546386	19517860	12441627	16799080	21346072	17196054	14283766	30466156	25081037	12405469	19353272	20607557	25195161	
fpHILIC	Positive	318.1296	3.39	unknown	298936	270352	454440	408731	244756	239499	377091	279736	156463	558553	389226	270313	374533	145180	337957	136757	299598	315149	318153	
fpHILIC	Positive	177.1232	3.39	unknown	794317	386772	758269	667439	387030	519317	464018	488393	365496	517824	416161	561729	396053	439120	445134	484069	405302	628588	450910	
EIC	Negative	478.2844	4.47	unknown	3592097	4755542	4120563	3171947	3306923	4970058	3173660	3509472	2382874	2949177	3786161	3207870	2523711	5410651	4478987	2295541	3752781	3821669	4474125	
fpHILIC	Negative	595.3438	0.62	unknown	732414	709430	976122	566452	634857	816268	608554	724225	442398	612732	796123	732683	589767	840723	603818	625217	683566	676867	916145	
fpHILIC	Positive	149.0595	2.06	unknown	2094140	1165616	1665184	1188837	1113898	1173865	1088996	1112606	1192788	1341338	1190345	1391463	1001016	1670561	1624907	1136862	858393	1398501	1061619	
EIC	Negative	251.0924	2.53	unknown	194894	166818	140286	216400	162380	153718	165435	148609	141124	194216	152020	139803	162634	152758	169862	146172	161942	209588	150628	
EIC	Negative	322.2440	5.22	unknown	1401733	1264063	1285769	1384223	1259788	1154342	1173245	1327292	1325275	1299268	1239134	1174118	1190423	1232866	1399177	1277424	1337158	1322728		
EIC	Negative	490.7658	0.52	unknown	813239	495034	952611	843264	508288	580772	458931	463958	681897	835459	466604	426793	515099	57045	432216	615583	535755	599741	709127	
EIC	Negative	464.1822	0.71	unknown	313126	269255	376280	151428	212089	263020	271184	151667	279086	227857	263020	274740	379316	239495	221858	194112	144698	425310		
EIC	Negative	320.7431	0.62	unknown	178095	126620	212647	176623	174225	131428	134837	92322	184898	257831	130653	106253	137151	141411	123978	140389	125593	152306	238741	
EIC	Negative	373.2022	3.94	unknown	231244	196332	466340	226534	116908	388742	202220	184184	146948	136532	205714	361187	398229	278250	90439	249825	261734	323846	174956	
EIC	Negative	330.2523	6.50	unknown	13907329	8399113	19176256	27235558	570727	17055422	12453039	986951	11590786	14607104	12202137	871720	10133475	703937	836327	10055406	12548342	22310220	756638	
fpHILIC	Negative	336.0522	2.99	unknown	1629343	1064299	1343894	1363504	865533	1070425	879471	917993	1006358	1437724	930845	880616	932479	920235	924450	842515	1026823	1311299	884605	
EIC	Negative	344.2176	3.63	unknown	338356	84867	470008	70781	38274	112352	59811	220840	33135	211974	54219	134935	42457	112144	60710	19323	87211	170076	169256	
fpHILIC	Positive	127.0211	3.23	unknown	647376	558716	445517	484507	375084	492557	377959	356869	431391	314164	339519	445467	434594	433689	426577	565731	392524	461772	372405	
EIC	Negative	550.7204	0.52	unknown	545766	310873	729242	788081	401736	408259	472247	283961	519282	638030	426963	446834	600749	0	393259	407720	410006	531161	471940	
fpHILIC	Negative	126.0112	3.23	unknown	1702345	1174844	1182775	1362503	1011988	1319166	1044969	1054243	1195399	1090432	1120345	1131258	1115599	938543	1211034	1228400	1156130	1461052	1086246	
EIC	Negative	438.6577	0.62	unknown	85924	77094	134361	97824	85677	72025	72409	53591	94428	154665	66122	59247	74796	52723	64761	73576	62803	81278	130614	
EIC	Negative	582.6385	0.52	unknown	534548	226970	537682	632954	316309	448205	275389	95714	480782	701173	217150	220020	267441	0	163730	430722	239193	388138	544661	
EIC	Negative	523.3650	3.15	unknown	152706	114656	126288	108204	104663	100436	101708	151410	180782	610158	118689	105317	84372	73518	112966	145685	106829	154470	101755	
EIC	Negative	253.1446	2.68	unknown	3976801	6490650	3686580	4945227	4734985	2265114	4555817	2660394	7727679	3409150	3739124	3811267	5546613	5422439	5496144	7799518	3563939	3399774	3334005	
fpHILIC	Positive	210.0951	2.38	unknown	602246	335620	228020	288390	303938	462154	359175	149786	212433	300842	494942	478515	464598	370497	401706	358821	281908	241075	342568	
EIC	Negative	365.6923	5.92	unknown	899656	687093	1153004	842404	637184	483319	730255	916409	642376	1062548	633779	590226	547252	613782	914136	858946	518369	817425	620597	
EIC	Negative	346.2138	6.31	unknown	931035	2786047	3112032	2282156	1063291	2500540	1179220	2122152	2032920	2422912	4167276	3192900	1195227	1811827	3176297	1683598	2028878	1300926	1643309	
fpHILIC	Positive	248.1116	3.18	unknown	681801	248154	221069	434691	279201	403315	264635	207446	450260	249609	332968	320324	347496	373559	249301	542875	301060	358503	304320	
fpHILIC	Negative	857.5180	0.38	unknown	1939142	1387752	1212475	2275543	1265861	956944	768889	1432116	2119183	1432116	1557055	1441056	833767	1542719	1228966	1420457	1557109	1294419	1066619	
EIC	Negative	234.8865	0.59	unknown	263451	211816	329227	257632	240061	207890	212432	171427	265390	319323	216898	203766	227017	227891	202803	237490	184084	232944	343880	
EIC	Negative	253.1810	3.45	unknown	143638	88064	182500	134926	113094	93038	113094	97004	132955	77954	143105	84192	68263	98574	103022	127743	143102	177943	348370	
fpHILIC	Positive	875.1299	3.32	unknown	1113313	788963	1084933	1138570	1016413	954685	609338	786197	890603	907160	664475	977487	878841	986540	1214430	1007692	564938	783053	1094718	
EIC	Negative	511.3641	3.13	unknown	143605	53362	110479	59991	105696	93281	93281	93281	93281	907645	57121	36303	33996	46986	65014	50254	55839	142325	51839	
fpHILIC	Positive	244.0790	3.16	unknown	3732045	4534697	4858377	5062489	4428119	4194749	0	4607154	4002664	4283765	4215127	4181502	4361154	3479620	3817696	3820484	3748540	4062444	3443292	
EIC	Negative	492.7622	0.52	unknown	587302	359600	755214	635033	432167	452306	362978	67842	385229	381861	402824	73929	73929	383691	516164	426018	483196	589379		
EIC	Negative	241.1808	3.52	unknown	1604395	1006799	2069910	2004960	968841	1157117	1138297	1335263	1004875	1503401	1222903	1744613	1655258	1129778	996079	1232532	1201256	1820666	896488	
EIC	Negative	366.3461	6.85	unknown	51441	86231	69466	127773	57566	90832	76001	79796	83787	122756	118231	118900	70142	189706	77083	92063	821235	140279	68115	
fpHILIC	Positive	923.5700	3.18	unknown	845977	598610	908108	951370	700514	772005	616989	774587	558449	8117730	729525	634821	772500	1201696	833073	7528				

fpHILIC	Positive	508.3393	0.60	unknown	1131688	1233239	1470111	984678	1283024	1406390	1153126	1107553	825301	1057764	1346359	1261745	1140753	0	1216605	1161521	1567949	1163705	1276408
fpHILIC	Positive	194.0441	2.98	unknown	1551524	1076680	1196618	724981	762322	681816	721683	1135852	697666	963382	554828	590551	656867	986281	1196841	673785	709419	9991010	843434
fpHILIC	Positive	417.1870	2.61	unknown	1665075	1958495	1976842	1224989	1563671	1452235	1733148	1306282	1282881	1470281	2068540	2005741	1740996	2002832	2141436	1671614	1235884	1513174	1558908
EIC	Negative	360.2468	3.28	unknown	136473	56335	100515	45091	47484	63714	67979	126868	61683	91716	68474	74444	48375	279764	77221	16812	92738	160344	59992
EIC	Negative	307.1895	3.88	unknown	1533217	659115	2107263	1934334	845055	763040	1022824	1836228	975263	2853840	783237	1052485	875647	871922	767255	773972	953015	2824814	707575
fpHILIC	Positive	191.1205	3.25	unknown	1726001	419744	882705	1356888	613630	611987	396708	562432	661987	1541502	604305	615918	544840	349254	381302	763680	543670	1096522	369886
EIC	Negative	272.7954	0.64	unknown	321443	158153	492607	354551	253885	287948	247482	180711	334449	181557	229990	196601	251269	181762	210061	278443	196167	286522	475484
EIC	Negative	462.1661	0.68	unknown	92610	74830	56528	26844	41091	57174	63053	58211	630493	74437	61482	73358	63341	85964	59650	56404	50015	47687	100023
fpHILIC	Negative	322.9883	2.05	unknown	4476081	2774474	2620344	5978185	2083586	1181813	3348709	4601259	690898	4554316	3132922	2809122	5792207	7269472	5429274	1251722	6048429	3674417	2807193
EIC	Negative	305.2483	5.87	unknown	128083	123136	144031	141347	99663	93957	103151	115904	84144	143983	108279	126105	113302	104340	119918	105489	119518	113805	92533
EIC	Negative	332.7515	0.64	unknown	71674	41972	85490	64916	45212	55332	45377	36303	62982	111816	47696	38648	46605	25062	41799	47881	35769	61471	85184
EIC	Negative	317.1757	3.22	unknown	138184	120302	151579	174165	180006	103466	123305	120660	148477	145388	119158	118507	148684	96192	97098	234540	122051	130304	86193
EIC	Negative	327.2545	5.67	unknown	844582	628093	1170639	1019514	776782	690481	628732	1046239	580825	823607	650055	837564	718363	518520	484630	1114587	761517	1265656	506001
EIC	Negative	272.7954	0.64	unknown	389492	209216	474230	346502	252894	275039	232210	174828	327184	581550	220614	197659	245455	211493	201127	273263	191465	285158	450188
EIC	Negative	283.2282	5.95	unknown	706965	670522	725691	837027	457786	391875	425232	425214	341486	375927	377204	544988	552630	425859	544527	524911	391274	413194	392708
EIC	Negative	294.8425	0.52	unknown	1341485	732983	1492741	1235306	9111070	932232	763916	1567108	793733	702556	1567108	793733	702556	1567108	793733	702556	1567108	793733	702556
EIC	Negative	614.4147	2.73	unknown	162688	144060	268732	609212	340449	246376	229963	249723	158916	523083	498739	239105	216287	427508	105417	0	282297	634267	338854
fpHILIC	Positive	233.0777	2.69	unknown	859828	674829	504844	935729	588723	823985	476840	535720	523083	495685	576455	462693	467631	578825	516653	468265	503223	1134617	
EIC	Negative	427.1798	2.32	unknown	449812	1013390	323171	0	397418	32044	741740	0	763861	1421213	27335	0	1143129	32879	1061005	74569	10662	73456	929609
EIC	Negative	414.1987	3.34	unknown	133586	631442	188254	0	196028	234389	77974	208452	700766	114153	503427	57195	51060	670353	51060	670353	0	143819	183419
EIC	Negative	254.1762	3.02	unknown	312722	239000	226919	310999	247226	290103	286902	223539	127568	282757	271504	356147	291526	224657	306862	302628	305340	231110	211907
EIC	Negative	359.2441	3.28	unknown	677109	252400	522588	270359	273991	323211	316915	611411	293506	412889	274345	322428	275997	1255444	341717	193601	474752	794136	274145
EIC	Negative	271.1921	4.38	unknown	750801	391755	1159372	546791	352886	297457	388432	754908	196162	669027	393626	449691	324412	563336	397436	274947	327398	689591	522395
EIC	Negative	477.3592	5.96	unknown	0	62689	47932	56920	60857	54460	54460	54460	45329	18856	89345	67236	55701	85738	38128	64927	58578	0	87834
EIC	Negative	378.7017	0.62	unknown	97493	90248	139978	100419	98319	77853	79918	54443	103256	160380	75699	67008	79036	69185	75846	83886	68385	91217	141240
EIC	Negative	243.1602	4.11	unknown	428350	394385	577786	326375	207490	257842	377443	281227	271545	250935	186555	433890	508440	280809	266419	340975	336537	374993	254543
fpHILIC	Negative	182.0319	3.17	unknown	541680	252475	424956	431020	202941	257942	287796	311644	320282	461176	294300	292326	284585	293228	289381	214030	400566	348562	284707
fpHILIC	Positive	201.0652	2.61	unknown	387933	505098	453868	259266	308910	503132	370456	212217	255675	281840	417190	350704	338295	422818	415515	503956	300535	281456	338189
fpHILIC	Negative	237.1497	0.39	unknown	2377974	1618267	2439035	3800571	1830260	1451239	2126771	1579232	2414953	2527282	1579603	1814834	2751832	1023368	1986851	250877	2332869	2688000	1024615
EIC	Negative	298.1850	2.57	unknown	4658480	74545	2633011	5516733	96464	75624	81647	3388090	55934	3235961	77288	142354	127592	37673	96339	83391	89943	3770257	52557
EIC	Negative	262.7844	0.61	unknown	289605	228364	346131	291966	294736	223733	232422	143804	288576	408125	205664	191584	233991	325543	225268	223717	218405	259640	392157
fpHILIC	Negative	78.9589	4.07	unknown	1268871	615852	450933	1630183	555934	1230729	556854	380320	306249	776830	691325	1162656	662691	361860	368491	1077277	724698	720204	488617
EIC	Negative	385.2382	5.88	unknown	255050	140526	253158	262620	141647	107486	130366	156250	107486	163848	123389	143411	124477	169479	169479	152842	145125	292936	125267
EIC	Negative	286.2108	4.43	unknown	205345	238668	219662	227831	110719	131745	192211	183015	174888	132972	197063	218163	204427	169861	225896	207630	148433	181893	125128
EIC	Negative	561.3006	5.54	unknown	763827	635874	696738	615349	626921	653447	552794	660347	520575	600318	576145	596102	517458	762720	622169	707432	649800	712617	714137
EIC	Negative	564.5813	0.63	unknown	130767	65764	187842	139575	65668	79050	64977	31398	107831	2121078	66128	60534	75871	0	58040	64991	17870	97646	151191
fpHILIC	Positive	223.1066	2.95	unknown	1479198	1140170	1165037	994511	1029050	1107191	745333	827831	1142565	879769	695955	792282	1161706	1168447	1168447	161072	989502	1381368	867477
fpHILIC	Negative	277.0859	2.96	unknown	3063384	2032265	3144457	1813448	1439783	1959974	1786747	2021396	1979628	2890128	3127527	1613299	2609799	4134942	3732766	388676	2742289	1380360	2021405
EIC	Negative	352.8014	0.52	unknown	830399	350121	831970	661415	445599	503890	440314	288730	566907	102962	361319	443820	564213	255705	407630	566907	286632	447282	812562
EIC	Negative	366.2728	5.92	unknown	249089	173406	254430	191809	156187	99857	182073	236031	149010	745537	184165	165553	134054	141151	225631	215645	126380	206664	145824
EIC	Negative	290.8484	0.59	unknown	440602	371239	558831	432430	415250	343285	345424	308869	472468	246761	372497	339362	401018	372445	335352	407780	306587	427869	629862
EIC	Negative	245.1580	5.24	unknown	878099	195929	1064522	838870	110228	289423	185485	567106	102778	612687	216799	212321	97042	0	200094	329531	29673	722635	120986
EIC	Negative	227.1652	3.97	unknown	129952	89375	151037	544080	89375	151037	544080	89375	151037	544080	89375	151037	544080	89375	69907	218128	115427	185878	426666
fpHILIC	Positive	270.0726	2.74	unknown	1237890	1178765	1001550	640415	751629	1445100	958051	345148	576294	617498	827276	722346	653966	637202	1211470	1026123	650467	893214	776322
fpHILIC	Negative	185.1183	0.40	unknown	2107239	1430751	2114604	1728744	1124966	1382605	1600537	1266637	1659357	1382605	1525592	1515945	1583903	1752341	1598047	1146702	1769499	1542034	
EIC	Negative	644.3571	3.22	unknown	283261	84737	143739	137155	83923	184351	113264	110259	60563	147021	105086	199361	76423	49461	119663	99392	142469	80645	175588
EIC	Negative	292.8455	0.52	unknown	2727474	1616943	3123892	2655679	1940243	1889370	1587615	1130681	2192491	3224585	1604387	1472529	1710354	1174970	1591120	2061569	144112	2108161	2668034
EIC	Negative	395.1842	3.94	unknown	3964317	3143141	4997580	2678113	1496904	4564775	3344199	2825471	2509524	2133509	3442631	4500560	4906347	3925298	1776470	389107	3737499	4820965	2823904
EIC	Negative	313.1813	3.94	unknown	55113004	42331097	88084235	43233224	23570039														

EIC	Negative	323.0540	2.39	unknown	586950	220158	470472	645395	190583	201102	216795	493563	183489	641974	190734	202576	195502	199797	194099	208428	197886	643129	207069
EIC	Negative	278.1766	3.13	unknown	764219	369120	617126	532570	390675	514172	455967	520456	198210	598499	525779	593192	426769	439521	580732	331650	486790	516539	430892
EIC	Negative	120.1278	2.54	unknown	1249748	831742	851548	757874	636597	583321	612708	546041	437174	961956	715323	756841	680853	623762	762787	882158	567069	548175	420262
EIC	Negative	552.2846	3.83	unknown	241436	493792	352099	402068	314359	378778	432356	331655	401998	278356	500679	539522	428053	445996	454705	466613	391604	342392	445011
EIC	Negative	584.3053	4.00	unknown	153088	75737	88936	230534	85265	130769	137466	159357	113329	298269	118564	146826	157135	0	73262	110527	169011	325292	29469
EIC	Negative	305.1384	3.83	unknown	453466	600947	543196	764448	489121	412728	628665	396088	642529	593436	549320	694273	727110	356118	653389	771297	525203	648775	307974
EIC	Negative	237.1495	4.23	unknown	13946833	14262919	17299296	18728529	11681281	6242858	11459658	10102679	11731973	12597162	9905694	6630642	14234586	7672797	11401439	15804678	9366003	15388275	5934869
fpHILIC	Positive	176.1276	2.47	unknown	633646	596201	751423	555968	506575	508035	567122	468367	579093	575858	784871	736425	665873	560436	586890	750923	502022	509058	622956
EIC	Negative	314.2419	5.99	unknown	146025	107140	245577	147705	50277	90859	53488	54292	126145	70303	69429	125856	111313	62582	68104	76787	83688	137972	57652
EIC	Negative	593.2872	3.10	unknown	251406	47615	192907	192550	88394	162715	115664	182895	0	158196	79163	117853	105866	50213	133885	98303	68282	195402	125928
EIC	Negative	505.4998	7.44	unknown	61017	29687	79421	106179	60083	39226	46413	81737	46797	46077	25363	81954	54531	40755	63285	67705	46689	96120	36606
fpHILIC	Negative	152.9958	2.94	unknown	590887	446452	540158	480089	429852	617729	458052	396729	374589	659261	739883	658972	519819	387526	528556	545546	535985	523462	444433
EIC	Negative	305.1746	2.36	unknown	1047888	499026	1130777	928195	239958	375582	565668	603104	282381	547748	275947	405117	823973	226708	616968	379988	203865	692273	448650
EIC	Negative	331.1309	1.28	unknown	281261	111241	97835	123404	70370	141615	9411	104429	153235	152984	177040	194493	93458	99918	183693	139562	0	85909	0
EIC	Negative	435.1072	3.65	unknown	524238	632129	514072	560443	534286	589064	580989	616771	560224	599114	705657	637351	662606	626463	701985	596722	562280	761083	643367
EIC	Negative	278.1765	3.46	unknown	381887	222688	274311	154788	203062	272878	200745	287945	64339	260309	189838	254696	168717	155216	316735	126830	260741	232766	229178
EIC	Negative	319.1532	4.23	unknown	1347694	1370783	1620855	1706063	1116406	620489	973012	978074	1220664	1212640	978633	941157	1320187	764404	1109409	1482514	896407	1488663	586681
EIC	Negative	631.2418	2.47	unknown	2807499	1201428	1790133	3080267	1198508	176195	1482404	2012489	1376609	1613080	1434882	1416753	1813921	713766	951376	1786210	1320348	2594122	1044991
fpHILIC	Negative	473.3634	0.37	unknown	1448733	1241979	1278726	1224273	1071144	892253	1355940	1065940	989829	1333701	850914	968548	1113241	975256	1560679	1649922	858077	1145827	882292
EIC	Negative	344.7309	0.52	unknown	275774	27680	192028	89160	162670	90468	77356	32676	31307	262670	93099	62006	818725	83926	101807	81707	271195	0	0
EIC	Negative	268.8010	0.64	unknown	1906842	1027411	2269122	1691051	1221264	1270155	1087185	860712	1567147	2891131	1067175	968314	1220781	1039847	985988	1315840	921348	1414463	2178691
EIC	Negative	475.2667	3.81	unknown	326529	498610	461811	274725	352169	650004	319144	339005	204094	253374	488785	289919	235454	967075	572688	202497	390846	352301	598078
fpHILIC	Positive	197.0893	3.11	unknown	435727	300027	291978	229408	0	581683	302591	222692	357450	221633	285596	284284	228617	251825	335325	397850	281103	345622	303122
fpHILIC	Positive	203.1020	2.71	unknown	611717	346647	234686	175444	174500	393403	91661	59391	144992	190135	241071	289012	177478	419157	277046	195161	157208	96199	25524
EIC	Negative	530.8041	0.52	unknown	1295684	572472	1291466	958659	719845	773265	587716	1205499	885717	1564773	574944	488231	583395	377466	581883	846584	444142	750771	1320825
EIC	Negative	266.1399	2.25	unknown	241620	363368	55871	776304	509357	364198	225246	577041	259665	370451	228682	454405	164161	316790	616387	536975	210010	86219	0
EIC	Negative	397.1997	3.76	unknown	2696147	1637469	2920251	1845865	1030965	1359104	1985788	1653600	1294708	1336030	1302985	1964517	2244688	1627472	1286764	1895859	1777665	2304421	1063206
EIC	Negative	236.1050	2.90	unknown	194514	130799	78117	88402	129784	86350	91367	105699	107857	83709	140798	95916	134392	89013	143082	90427	138493	86696	134117
EIC	Negative	400.6813	0.64	unknown	149105	77970	201375	136303	75280	97677	73768	61757	126497	235628	75459	71302	90227	34373	62919	100135	61535	108566	161939
fpHILIC	Positive	169.0944	5.22	unknown	3563220	4288105	3288131	2787788	2889760	3853950	3187785	2341128	3346854	2722581	3843034	3846731	3651063	3537702	4374931	3601981	3247555	3048960	3506373
EIC	Negative	534.9526	0.55	unknown	257662	140783	163774	301334	69504	280467	132388	93011	66333	130336	166542	198248	127747	0	155575	195739	106218	155014	118169
EIC	Negative	526.2444	0.69	unknown	78446	133998	85195	65769	53045	75874	86826	107296	42356	47948	105165	114357	104866	50950	78657	64056	66123	128910	78364
fpHILIC	Positive	189.1228	2.90	unknown	5667066	3160201	2826510	2789911	2846456	3517961	2263601	1851733	2445375	3052352	2754679	2765944	2191515	2482409	3738962	3208473	2550104	2914105	2307570
EIC	Negative	279.1581	4.08	unknown	18574	79774	120331	468047	16266	112951	170956	164741	16621	21394	144729	22869	16995	57316	24941	178869	19593	258861	66143
EIC	Negative	448.6673	0.64	unknown	104429	54130	147990	92555	57801	69708	53816	36533	80555	174118	52406	64636	64436	17937	47101	66638	15993	70994	109333
EIC	Negative	637.3536	5.14	unknown	402081	239278	341116	330900	290856	197217	225788	368619	341667	463562	305855	234564	291786	273820	281226	303390	316004	414549	307301
EIC	Negative	329.1762	2.32	unknown	577212	360777	962520	330900	267231	153686	378904	394398	202664	432620	315592	239880	153644	119649	196499	390797	288181	625299	296700
fpHILIC	Positive	129.0658	3.40	unknown	2905380	1864601	3213195	5378559	2504299	1981235	2088558	2033705	2122270	7905241	2050794	1793518	1898133	1220460	2232324	1982620	2156755	2789994	2549887
fpHILIC	Negative	242.9968	4.05	unknown	917165	380737	348063	1125876	386021	411448	468177	433817	608411	2909487	473181	340751	330815	234615	428414	357237	710683	537336	0
EIC	Negative	292.8456	0.59	unknown	554843	470892	721820	536172	499832	406869	438145	354512	603256	971731	463416	392230	461811	461842	404045	494001	382054	516881	826880
EIC	Negative	240.1604	2.66	unknown	5330573	2035338	2663904	7730030	2444782	5788366	3319152	4126014	3122649	3122649	4967764	4392834	935938	4022454	990600	4507989	4236707	1549318	0
fpHILIC	Negative	285.1021	3.62	unknown	501717	313239	400254	442576	260294	250622	251240	347252	258939	379943	324756	329174	305692	175898	369695	330405	257411	428831	170103
fpHILIC	Positive	247.1740	1.65	unknown	567974	301514	397333	342281	199985	418008	218124	175537	266163	385794	382595	263338	271847	484172	503359	315011	166411	181283	302954
fpHILIC	Negative	191.0579	0.86	unknown	749082	546710	533327	636192	379271	523319	445422	481435	424109	587103	652449	724420	475763	763220	918480	0	415556	663348	572331
EIC	Negative	592.3280	2.68	unknown	484947	469579	405890	291631	411206	478437	491849	320510	434671	377469	487214	579245	0	504558	417568	526410	456064	255821	781253
EIC	Negative	266.8039	0.64	unknown	1190986	646434	1415428	1049273	741716	796660	674556	526279	973465	1769042	672914	596024	765136	631921	606424	811862	577114	869768	1370935
EIC	Negative	238.1529	4.23	unknown	2174249	2263536	2714915	2954970	1846604	990932	1768689	1549851	1808855	1972903	1531516	1562503	1189773	1222691	1755018	2503946	1534049	2399578	905445
EIC	Negative	398.2030	3.76	unknown	609673	391174	725983	484668	252735	349429	496004	415202	307668	338691	300844	455371	546426	429755	319352	467048	418827	601802	272138
fpHILIC	Positive	117.0568	2.61	unknown	440286	497111	373414	298339	378938														



fpHILIC	Negative	134.0176	4.15	unknown	6520198	5588658	5158013	5221971	5572376	5260573	5045346	4800073	3582166	6340485	5125540	4862573	3300504	6392188	7655927	3962708	4935217	6113941	5239745
fpHILIC	Negative	269.0546	2.69	unknown	6787334	5484466	4522731	6741536	4940711	6955863	6218804	3484550	3310141	4090377	2993949	5118482	3205588	3956012	6092520	3601405	4029370	3842719	11037411
EIC	Negative	580.2925	2.63	unknown	4412231	60781	3898989	3847091	78436	96545	4356648	407319	4291971	170167	186212	106083	404620	404620	230904	122799	156016	5175907	153648
EIC	Negative	313.1455	2.22	unknown	532891	227604	587499	373644	167837	345725	375831	413031	452483	407306	196837	609027	355102	331394	131712	348582	323259	728637	487353
EIC	Negative	297.1692	2.52	unknown	393172	157725	369462	0	0	147680	56669	92492	142021	139414	0	140973	309463	102500	73247	61381	39171	94142	128755
EIC	Negative	504.1308	0.71	unknown	178131	117803	187411	61955	111198	129564	108570	43523	123412	215636	125628	91672	106570	218683	97770	104229	74490	49534	266327
EIC	Negative	528.6739	0.52	unknown	431932	206200	664965	420335	237497	310658	227420	107862	443094	587727	138253	198679	112443	0	157085	379358	165694	351965	455123
fpHILIC	Negative	259.0634	0.37	unknown	1402923	3181938	2060936	1073668	1363760	1441049	2590890	2140900	1520205	1294611	3738248	4228248	2185096	4001812	3190978	1913802	1368470	1228341	2412679
EIC	Negative	279.1583	4.44	unknown	2731759	613412	1478442	2185055	710723	690877	890876	1354286	321832	1378955	641141	1344710	1082736	345185	756221	926016	664388	1746496	4762493
EIC	Negative	388.7126	0.64	unknown	262365	138908	356918	239412	148015	169747	139885	105974	221206	419890	143466	122619	161216	74370	123488	170723	116616	187621	306611
EIC	Negative	338.2363	2.06	unknown	250406	271373	133331	131405	179512	197962	194623	101559	178417	110490	195673	189477	274377	256185	222257	195449	228059	122048	214068
EIC	Negative	358.2516	5.78	unknown	347255	266985	322772	367133	262181	247356	301839	351402	261542	383416	320603	274357	291271	245876	310833	266750	326401	409278	328506
fpHILIC	Positive	146.1174	2.05	unknown	806584	761129	913705	886091	612391	549948	877911	455640	909256	610898	871115	954680	1050841	679477	551807	1003104	903032	910622	557777
fpHILIC	Negative	163.1127	0.40	unknown	1883328	970633	1319041	2070864	656415	1086336	876793	1368616	495431	1520759	685438	1172390	863512	477203	1217393	1094936	765725	1450485	643310
EIC	Negative	512.2735	2.08	unknown	12513956	2817486	9728611	0	1418204	1649946	1962511	0	1115823	4619764	2444656	223697	1396761	1864994	1736196	3566820	524921	0	1267004
fpHILIC	Negative	369.0614	1.99	unknown	1814556	740266	749300	2112518	616245	503032	976014	1160383	2467917	1437596	1260499	1157188	2296977	1754236	1685300	909291	2002347	1255535	756628
EIC	Negative	259.1915	2.62	unknown	289328	204338	528575	848386	272840	381743	309378	385588	359383	848395	337635	453753	470138	541779	173565	362345	381535	669997	386583
EIC	Negative	352.3297	6.74	unknown	174195	160870	171616	228616	210920	147816	165800	147813	124487	219185	205317	280479	148160	133694	195213	163043	174572	304149	147056
fpHILIC	Negative	317.0356	2.67	unknown	59039376	8551389	6531750	6814504	7992450	18954404	2723071	11781235	20284924	7008732	5325468	17875974	12261237	15055651	5368623	15759388	16812818	21672856	11746658
EIC	Negative	386.7160	0.64	unknown	491235	270733	648315	452557	295450	321684	264540	195079	421890	804912	281952	246092	312891	149481	232332	331811	219588	367993	583231
EIC	Negative	412.7570	0.52	unknown	293994	135796	389423	296411	195950	226370	175658	82833	261555	390986	176118	181286	229749	65031	160560	224755	152489	247939	305276
fpHILIC	Positive	217.1294	3.42	unknown	986468	789169	825908	286111	737344	989213	704434	740634	757297	791835	769891	851129	615752	998871	1066462	887592	591809	926444	794607
EIC	Negative	442.6774	0.64	unknown	359425	195361	525031	371803	215961	242161	198971	156549	317941	629098	209336	187603	239884	105283	173857	250406	164483	284439	438028
EIC	Negative	298.2470	4.92	unknown	740987	525931	1207699	1400523	719544	769564	769560	1111546	1212012	669481	564388	902060	941051	629775	333129	2190694	881621	1331278	574672
fpHILIC	Positive	300.1992	0.98	unknown	2789896	1416914	1941097	2940159	1369741	1589940	1711964	1656357	1354762	2164196	1577374	1726604	2066797	699483	1615396	1772053	1871024	2607482	1040555
EIC	Negative	382.7227	0.64	unknown	234950	121632	291042	202979	129850	141743	123162	91973	185807	356638	123668	106665	139367	69616	101435	155772	100333	152726	270432
EIC	Negative	357.1346	3.17	unknown	381519	168515	113699	15561	131628	102444	142177	86491	87158	72062	161438	6965	20306	46330	82857	496475	7750	10449	41002
EIC	Negative	517.2774	3.11	unknown	179565	116668	0	75406	142612	63493	0	87655	0	68685	115108	72759	88122	100676	75555	142672	0	124787	
EIC	Negative	310.2107	4.12	unknown	306415	153700	386157	170284	139912	219836	141911	288091	59403	286353	129904	164480	96884	250603	219806	83330	134252	312370	336916
fpHILIC	Positive	253.0318	3.23	unknown	814883	530784	346119	572074	392852	627091	328974	313286	486878	818377	328129	437981	497223	339088	456056	596070	437584	575398	435453
EIC	Negative	419.1128	0.46	unknown	160322	147138	63740	72720	77905	142631	101868	93127	71755	87855	114906	88192	131660	83992	178948	147565	62097	79011	99020
fpHILIC	Positive	204.1337	3.59	unknown	759071	471930	548839	567048	545753	634654	442733	466082	518368	606042	639600	603728	582085	431489	641864	702655	551355	596722	539909
EIC	Negative	526.6770	0.52	unknown	682330	310537	623653	761627	149886	598800	381090	147141	564165	879080	271341	272568	423396	0	337703	600782	230471	507206	734238
EIC	Negative	506.1271	0.71	unknown	116388	76734	127408	46295	70906	85510	80968	33615	79760	152457	87192	61855	73329	155294	69399	64308	54259	35056	185020
EIC	Negative	510.9076	0.55	unknown	307107	67122	171447	246888	95751	220432	99859	0	83068	196301	123493	124990	62221	0	83452	191944	34551	95722	174969
EIC	Negative	444.6737	0.64	unknown	414050	218009	577902	402285	241548	295988	220238	158248	353618	704123	222784	207190	263505	111182	184588	276986	182197	309719	481947
EIC	Negative	309.1709	3.49	unknown	175380	144124	149505	227500	137246	115344	145727	127500	145720	145456	153532	201151	130822	154556	163844	143416	224043	164646	164646
EIC	Negative	446.6702	0.64	unknown	254669	136821	358492	251403	146332	173609	137446	98674	218832	426043	138475	126857	161168	59838	116273	173251	114161	193846	309770
EIC	Negative	524.6803	0.52	unknown	613017	266314	640606	271403	334772	427683	304838	160183	504681	0	243867	152510	300953	0	243867	103568	136883	472440	665956
fpHILIC	Positive	143.0485	3.24	unknown	3552471	3623280	2868696	2665348	2112811	3150838	2023846	1761860	2778689	1888829	1952131	2473694	2883542	2285428	2569062	3285168	2566570	2917861	2445311
EIC	Negative	297.2436	4.92	unknown	3809228	5267482	5920274	6991476	3594677	3891166	5946713	5968173	5182722	1531897	2726353	4340260	4555462	3221326	1748690	10918691	4417483	6880287	2704360
fpHILIC	Positive	488.1764	3.18	unknown	1035160	1035500	853215	796916	899523	879178	887976	714827	835431	760685	1184742	1142366	1130784	1012024	1129626	994722	940306	802968	1047399
EIC	Negative	551.2511	1.11	unknown	176093	128770	196493	151032	81818	75315	137387	62497	102554	160183	130434	147975	162316	77269	87210	145326	118627	107228	77279
EIC	Negative	392.2226	2.15	unknown	322152	101922	558586	231310	101479	213047	120508	213320	87614	105687	169755	122024	212528	152331	233809	133104	246175	124587	120583
fpHILIC	Negative	93.0455	2.67	unknown	1051229	166921	120556	127623	131755	189647	53387	102508	403343	128535	100996	354759	327777	329451	109706	305405	306748	429628	201744
fpHILIC	Negative	188.1029	3.17	unknown	1629320	1675443	2127972	1712996	1421283	1315152	1908357	1727489	1526427	2221193	1355269	1260079	1494355	1528393	1962601	1507287	1730858	2205594	1806903
EIC	Positive	411.1082	0.69	unknown	174684	113386	106356	83672	8061	131304	86296	75462	75427	175727	107954	101493	90802	123886	117025	158277	74409	77167	99369
EIC	Negative	257.1760	3.11	unknown	341778	215745	315157	203742	189429	198664	230312	202249	198912	205683	207869	311275	379273	250637	195445	246749	241311	273862	232408
EIC	Negative	343.2495	3.84	unknown	130959	90037																	

EIC	Negative	266.1454	3.72	unknown	215106	86101	163231	200693	97111	112033	121656	112790	49923	172818	87948	154197	143055	42530	108489	113781	96941	198101	65616
fpHILIC	Negative	233.0777	3.94	unknown	545883	351609	289041	285325	253106	409938	230327	217018	253640	306072	301374	306500	308845	291063	362086	344566	321059	285708	298176
fpHILIC	Positive	158.0443	2.71	unknown	817141	557463	765961	837399	420455	613739	333879	697111	313602	669530	551999	718784	597327	589770	550265	643239	412245	692860	528416
EIC	Negative	562.5862	0.64	unknown	239235	121945	379683	268351	123350	142869	119261	98847	496634	413259	121836	112750	140966	0	97875	153013	95094	185323	276568
EIC	Negative	341.2112	5.01	unknown	215517	140741	238690	287645	144468	136268	164297	164297	164297	228234	172657	171611	125179	112756	180512	161300	146892	256115	139395
EIC	Negative	285.2073	4.43	unknown	1013363	1327958	1169340	1268679	787159	719964	967986	618996	618996	963466	944773	1235970	1180349	963297	1201152	1131899	945988	1015720	812382
EIC	Negative	556.3723	2.91	unknown	209058	532546	692861	1681510	341993	881459	454723	0	115311	0	557983	1281410	981658	142113	646703	484282	580546	0	420030
fpHILIC	Positive	257.3070	2.69	unknown	1000010	756972	599799	6073702	743116	858311	770906	513682	476135	696994	433011	788006	543803	614248	726682	586850	719130	554103	1394673
EIC	Negative	135.1563	3.65	unknown	673070	622712	604707	508240	585324	543951	530707	672978	490122	436497	627860	509827	595780	499044	583836	594883	652929	786276	726294
fpHILIC	Negative	135.0184	4.15	unknown	1490830	1219728	1294532	1201338	1301973	1170926	1237529	1135434	866878	1372122	1184915	1165278	815690	1529946	1775850	977257	1199667	1627089	1186436
fpHILIC	Positive	262.1275	3.12	unknown	917749	774980	325342	584829	615024	810961	529537	393309	574885	365558	414543	627050	479170	478835	505435	1119679	547626	458452	833039
EIC	Negative	502.3032	4.00	unknown	6005134	3146342	5076528	11069661	3309122	5417799	6247853	6805017	4960546	9800415	5928620	6339447	7274126	1317771	3948740	5343995	7324424	12772777	2306049
EIC	Negative	549.3048	2.34	unknown	312496	104284	410878	131475	54129	87811	90633	235730	25785	262401	93406	87373	57989	130094	86585	39126	38924	296220	125045
EIC	Negative	448.2571	2.48	unknown	264629	93738	386646	965934	128587	252162	237774	672837	143038	743023	198705	320865	404695	49755	124709	65371	397889	1006078	107074
EIC	Negative	354.7988	0.52	unknown	277708	155303	251123	242146	139648	180619	195808	95433	247624	325108	149268	131491	170547	76555	168358	247438	129736	202631	271123
EIC	Negative	317.1146	0.78	unknown	847285	716161	1203223	1214782	599858	376833	755538	847363	386236	884923	117346	732578	846048	340237	462684	789532	576555	1368561	322335
fpHILIC	Negative	270.0583	2.70	unknown	602517	462787	385252	632214	419998	656853	500092	300039	312972	423827	273370	513922	298459	379698	507110	316316	366900	349627	1061530
fpHILIC	Positive	207.1123	2.07	unknown	3518824	2362070	3032326	2089468	1980703	2199452	2342326	2437441	2327531	2980481	2237479	2369864	2098931	3069240	3520454	2524308	1951472	3000049	2414010
EIC	Negative	273.1722	1.84	unknown	95352	61198	50286	0	54819	102043	41660	0	31250	0	43833	62520	68518	69922	67549	76112	62098	0	67279
fpHILIC	Positive	302.2146	0.97	unknown	2238108	1038722	1704438	2610299	1032109	1108192	1367973	1376003	1110115	1161928	1316573	1503020	1630165	518339	1076186	1605653	1427839	2290443	72450
EIC	Negative	258.2158	6.09	unknown	127064	80358	135882	110414	26494	81369	87743	80743	34192	64641	51463	88293	93602	59439	82242	92319	73594	83026	27340
EIC	Negative	299.1873	2.31	unknown	259819	108338	267254	208473	93003	159474	136064	231270	80440	344840	131431	141997	156973	98448	125179	12302	130793	326631	123858
EIC	Negative	130.1664	2.40	unknown	286126	173882	223002	211830	159606	136596	151798	256078	150848	237189	183386	155254	187362	138169	189895	140811	188052	315465	182535
EIC	Negative	313.2027	2.66	unknown	738943	337821	758435	364835	295658	382811	198158	344458	105114	675004	248466	474312	216565	266719	229930	105188	257837	547222	339296
EIC	Negative	464.7238	0.52	unknown	348669	138151	457717	338815	323293	243462	99670	90473	359382	462101	173838	73257	205237	0	161077	251189	145570	294521	368530
EIC	Negative	500.6365	0.64	unknown	283938	152710	421212	288912	153143	180872	148186	241378	505240	157541	141324	180891	59436	119548	119548	191168	120567	129421	1476292
fpHILIC	Negative	138.0390	2.67	unknown	3755719	617303	448570	438946	522430	1253876	163602	717472	1292214	438884	361265	1168772	759376	1085091	358873	1036316	1093605	1469340	746063
EIC	Negative	470.7155	0.52	unknown	525761	174468	394060	414419	248738	259468	248205	108243	342363	512802	194152	182589	245624	56007	186536	336822	205350	278722	430718
EIC	Negative	558.5952	0.64	unknown	199720	108309	315371	211643	108971	133895	106516	84554	183150	358615	107868	98733	128694	38820	90271	145236	96248	159633	243958
EIC	Negative	464.3102	3.11	unknown	228033	16000	276027	179994	37349	34133	12881	404102	39893	311831	41756	35002	35157	51306	35328	16197	42633	153398	0
EIC	Negative	466.7210	0.52	unknown	798471	408336	785108	871667	525205	555584	346476	232854	487850	1037723	466853	395429	463280	0	383868	422881	354854	578680	802334
EIC	Negative	317.1146	1.05	unknown	141333	84746	151919	170122	81668	57725	89706	111588	53639	114538	93712	86165	100391	49911	59031	98260	73064	192993	47422
fpHILIC	Positive	147.0452	2.06	unknown	1341896	637047	835358	508764	485266	515575	597854	470725	645342	735000	589638	669034	545223	917154	924701	629717	539684	788325	717577
EIC	Negative	464.2058	0.76	unknown	191345	477463	229644	167955	211181	299917	302054	300875	142673	180943	298840	400017	449940	274001	263160	218777	221964	343568	453461
EIC	Negative	385.2016	4.90	unknown	420477	564317	561809	613626	560308	482697	514899	500766	419238	582817	628026	629669	633317	688064	641047	628776	607937	564882	517630
fpHILIC	Positive	157.0969	2.79	unknown	2938967	2374955	2436268	1987523	2068224	2163835	1905761	1950708	1778113	1969419	1897777	2159473	1756620	2292073	2726065	2206750	2137993	2292343	2428260
fpHILIC	Positive	175.0705	2.70	unknown	2949365	2177094	2936973	3086846	1825591	2053525	1401498	2061101	2515417	2432730	2004079	1904132	2411499	2085550	2649710	1279740	2297365	2217926	2482610
EIC	Negative	343.2116	3.64	unknown	1958893	406365	2483634	590642	257585	696408	472120	1020414	150541	1123324	311874	621255	278423	668327	472015	195235	425005	1304507	711726
EIC	Negative	529.3324	4.98	unknown	3051735	1745573	2839537	7360093	1553481	2879664	3167724	3452374	2793951	5868984	3132753	3037821	4066239	505314	2095662	2903461	3674814	7003981	907642
fpHILIC	Positive	480.3079	0.50	unknown	2175710	2584604	2180749	1464627	2030197	2443072	2152899	1667082	1197330	1259102	1966829	2345605	1364753	2918801	2182355	2553368	2205312	1646326	2728219
fpHILIC	Positive	376.0506	3.23	unknown	1545034	979300	622440	946321	575566	987676	488227	463213	890491	564048	457856	736153	755419	589020	643597	1111210	791368	911353	622591
EIC	Negative	501.3010	4.00	unknown	18979268	9331346	16082186	36016684	10085624	17148976	19974188	21512897	15720848	32135195	19318099	20097191	23844662	3206403	11335872	16962295	23980147	42335338	6585401
fpHILIC	Positive	367.1644	3.62	unknown	1824534	1000211	1218379	1184165	711389	800829	634659	944279	626472	1274592	893340	920502	742485	854562	1109690	780492	672408	1235191	567169
EIC	Negative	331.1541	3.27	unknown	276678	200542	411435	138399	124708	190826	107868	196025	68784	307623	174253	172548	103265	216979	221394	80378	129772	211969	181375
EIC	Negative	474.2736	2.97	unknown	538433	200502	599220	1075880	231291	345757	451099	870364	612843	1036400	357619	322790	667387	53030	224394	368816	566801	1722809	127673
EIC	Negative	227.1478	2.33	unknown	294412	191927	122473	219571	81973	250731	98428	108796	50891	195427	120226	152582	99159	59236	192043	105980	158072	160158	91995
EIC	Negative	502.6136	0.64	unknown	352624	193225	538151	359223	196635	226132	179449	135500	305266	655139	194125	169232	215125	73733	158177	237576	157056	273864	424149
fpHILIC	Positive	117.0739	2.79	unknown	48807904	44935664	42474920	31037900	35048736	44933384	31510628	31895312	30281012	45488324	36719388	38313480	31547514	46167368	57224404	34223612	31903996	40546762	42642560

fpHILIC	Positive	251.0363	3.23	unknown	9917971	6401878	4575019	6401041	4488959	7218657	3742967	3308875	5430356	3898008	3600665	5538111	5438614	4632097	4890155	7565218	5161616	6898893	4700111
fpHILIC	Positive	168.0914	2.06	unknown	2423598	1434803	1929147	1272830	1215780	1545093	1253155	1208111	1393257	1663274	1545206	1518409	1232548	1870578	1996688	1495653	1243268	1842209	1412380
fpHILIC	Positive	188.0699	2.61	unknown	53747232	68844856	55036104	35632484	47491884	65621600	61678004	37736504	41584944	45783840	62640648	59087084	52875616	72353456	85041424	61047680	50423716	52206280	58231456
EIC	Negative	385.2606	3.72	unknown	231224	103504	164297	98412	91074	103798	111686	194527	89724	129076	124279	88290	87689	502433	152986	36341	183413	230419	110701
EIC	Negative	405.2532	5.21	unknown	235474	192444	247315	187317	158949	171309	191281	218687	144176	202601	214001	198236	203714	184970	234748	224636	197180	214476	197578
EIC	Negative	493.3544	3.74	unknown	177297	232009	144180	127810	161242	231200	153548	152795	125514	152609	320572	167077	197209	216644	242069	215847	204209	128893	204988
EIC	Negative	373.2374	6.09	unknown	367806	405578	327847	277433	377102	324504	319357	343897	267417	277599	352342	274966	353774	289453	377850	367210	398095	406761	423252
fpHILIC	Negative	287.0521	2.94	unknown	1820334	905848	866540	1168827	792903	1489359	743203	747893	1013147	967785	725456	1321716	1079896	1191455	1186861	940312	1360876	1181680	1118406
EIC	Negative	323.2587	4.92	unknown	149730	74686	225375	267319	84462	113969	78177	182670	175634	1811704	70940	150428	190989	60723	86455	235598	149970	176804	119080
EIC	Negative	556.2656	3.99	unknown	272371	340598	312595	167287	219644	347627	182892	238144	74063	168197	269471	169956	155516	469593	278048	97470	241376	278195	389890
fpHILIC	Positive	118.0651	2.06	unknown	1710203	911938	1439428	875743	746705	1021297	845392	796535	872679	1086579	952397	1067100	768843	1280365	1395840	943647	787742	1172256	880678
EIC	Negative	343.2123	3.53	unknown	390946	346829	317799	252362	165119	358025	285001	259504	343168	211417	270350	374979	341003	378341	359605	312577	228038	386589	420226
EIC	Negative	329.1762	2.18	unknown	8490063	7498679	9579260	8632289	3210235	9817426	8140541	5063969	7598570	8128563	5506637	11906276	9777581	6245439	3462465	9037196	6944857	13866268	8282892
EIC	Negative	383.2442	3.27	unknown	92775	46025	94022	41371	33902	51419	34014	71045	29680	63709	42444	33571	36815	126981	48152	34427	49567	98901	35323
EIC	Negative	498.2527	0.99	unknown	187585	147585	167294	0	120945	0	191576	107594	156312	128453	0	119313	103718	158251	0	120267	103646	126584	
fpHILIC	Positive	130.0647	2.61	unknown	844168	1041102	987926	577431	720532	967717	830213	637132	702796	753908	908407	872223	816108	1077316	1194279	919255	769424	753536	1038323
fpHILIC	Negative	190.0541	0.86	unknown	11391603	7726395	7186241	7435453	4946636	7914984	5814306	6495255	4847815	8129984	9403721	8864499	6573986	10310047	12408937	0	62389624	9806524	8818914
EIC	Negative	475.2851	3.40	unknown	2234329	957869	2124579	5886702	1290885	2200780	2325319	3687797	1973061	1575036	2324527	2341515	3226011	336012	1036336	1493510	3173224	7464278	742350
EIC	Negative	503.2020	4.00	unknown	1941306	1188164	1546717	3391041	1060402	1654700	1942769	2085207	1508317	3040947	1870145	1976784	2265006	485770	1191629	1664067	2370051	4033322	748040
EIC	Negative	476.2887	3.40	unknown	567806	262917	562336	1698610	385394	602987	632229	977817	547642	1555391	614000	647841	974613	96184	306245	440923	852975	2018379	198452
EIC	Negative	445.2960	3.15	unknown	735365	145129	740152	810057	139214	202573	152043	509732	172289	792980	139046	179679	167399	132652	146277	151117	159347	836362	133954
EIC	Negative	548.3014	2.34	unknown	988250	266371	1556318	487455	184516	245681	225400	755534	84817	845267	296587	262892	147391	455865	295373	459660	175479	790120	410611
EIC	Negative	390.0345	0.48	unknown	158395	160836	127203	213252	177564	150788	133535	168182	138054	206032	178993	180352	205883	66855	184756	226501	173064	189889	158920
EIC	Negative	428.1827	2.67	unknown	203010	182966	237366	169416	87358	118502	194299	116553	142729	736127	139746	229564	206825	167479	155273	171679	164553	176789	131187
fpHILIC	Positive	503.3145	0.37	unknown	953042	441236	912515	2943862	594169	854423	1132963	1275550	1025920	2231121	1064857	1008864	1489950	130544	461308	831210	1280217	2984203	375284
EIC	Negative	618.3421	3.52	unknown	1890765	1303780	1236456	1124732	1039922	1867475	1297177	1268602	1188188	1379807	1227231	1998010	1329784	778382	1347821	1726234	1983374	852560	2185086
EIC	Negative	582.3779	5.40	unknown	11009165	11319746	11281464	10569416	11388373	12785521	0	11695239	10868501	9745265	11743905	11938786	11650252	11132011	11495170	10628412	11802729	10672930	12201275
EIC	Negative	299.2235	5.09	unknown	1223000	1244859	1178314	1418097	812817	754180	852089	977895	826597	804726	938481	1212749	1082105	1105545	1244120	1077962	1011397	953880	842468
EIC	Negative	621.4015	5.65	unknown	0	0	393952	0	23353	36144	105537	32188	0	0	0	0	23377	0	239739	0	0	0	0
fpHILIC	Negative	263.4022	2.61	unknown	405082	515092	508861	304627	343100	282838	456461	195921	186291	307476	528950	281232	416028	328774	623462	277987	285059	271247	322964
EIC	Negative	314.2056	2.66	unknown	80068	74007	91264	0	55590	102511	39061	63944	35951	91339	48533	92288	49809	58884	69466	37771	60036	108379	85668
EIC	Negative	349.2389	3.57	unknown	84034	47794	79518	97324	18900	25356	17322	20644	18975	58332	24354	29783	19345	25913	15675	24069	25561	39521	18321
fpHILIC	Positive	189.1343	4.87	unknown	893557	655075	372894	502903	410424	457623	357224	345428	813191	587303	456936	508517	413444	605114	933607	709506	434853	318792	507861
EIC	Negative	412.3436	6.03	unknown	1286790	543081	561981	981757	608815	430537	995773	496296	631723	456956	587227	412451	490310	453132	593711	775407	453563	443203	1590186
EIC	Negative	333.2075	4.12	unknown	475737	124048	621934	364323	205117	207138	198967	353237	219991	563685	219991	221238	197670	243003	207595	197630	234403	444627	244297
EIC	Negative	608.6791	0.52	unknown	597556	438567	807916	882699	363981	436002	528660	228596	558563	680054	393587	493669	516934	49481	418831	497431	404583	673241	845570
EIC	Negative	616.5513	0.64	unknown	69744	36188	113872	81648	40449	37967	47396	36047	21855	66434	37667	38621	46446	0	30359	51535	33066	60362	84634
EIC	Negative	319.2278	5.99	unknown	242401	163957	536799	222382	128585	144160	150159	249769	70607	281857	194362	202355	140767	226095	124545	116180	169999	293221	202821
EIC	Negative	611.4305	4.14	unknown	179992	140215	399196	461666	119819	88207	151050	196671	176215	182867	110849	170948	150193	193614	137067	140643	188813	256245	170331
fpHILIC	Positive	190.0862	2.06	unknown	1410368	738153	1219365	781055	748487	733193	714273	660563	653814	1086590	848511	775213	683530	1110752	1088764	764092	627183	1014198	789656
EIC	Negative	290.2942	6.39	unknown	23490398	8814691	16698076	11612293	6997074	12300406	0	7805044	0	13674160	10925420	10025642	0	15514145	12851578	4906484	9470733	0	5873667
EIC	Negative	289.1448	1.81	unknown	395502	239851	473349	0	82498	189305	237336	99226	176654	139540	218216	324816	292208	200525	222642	288962	203189	0	244637
EIC	Negative	425.2195	2.22	unknown	305314	96015	217565	280044	85409	148984	109300	266897	26724	248451	64538	127133	81002	78114	121843	69804	148750	295615	143024
fpHILIC	Negative	292.2325	4.07	unknown	1372972	447480	163502	3088254	424568	749033	377705	92802	173246	684395	830801	2219060	695366	157474	115090	1629616	767127	736216	315795
EIC	Negative	401.1570	4.23	unknown	233649	165948	237302	287371	156086	172271	146251	174214	77469	221120	129541	131210	127293	103736	184256	226363	123232	249285	101072
fpHILIC	Negative	215.0671	2.63	unknown	1660693	277019	181486	281322	332401	790836	1166506	259509	586712	176527	236377	602705	443213	557636	227629	650235	505348	747478	421629
EIC	Negative	280.1888	3.65	unknown	1092191	1183023	938855	1087079	1091070	921353	907777	1060071	805815	992156	1111710	1021105	1204532	936808	1160590	1031320	1058526	1326242	1280158
fpHILIC	Positive	70.0657	2.79	unknown	13522982	12863025	11985989	8782025	9822269	12188199	8762266	9130400	4843968	9708024	10562862	10770667	8939799	12768138	15892755	9860055	9638961	11407807	12373809
fpHILIC	Negative	132.0302</																					

EIC	Negative	411.1846	3.76	unknown	1229231	714690	1498377	840668	438141	606560	835148	662881	599479	594079	582176	877973	1009429	703116	538735	922051	789033	1157909	484065	
EIC	Negative	366.2492	6.43	unknown	445787	0	0	393703	3533099	0	0	0	2831033	0	0	2947288	3072767	2928843	2261603	2728921	0	0	2892896	0
EIC	Negative	348.8067	0.52	unknown	736386	343875	809424	582840	438675	494401	345627	293664	539613	986763	332559	382311	431406	183858	388039	551398	421550	414890	840559	
fpHILIC	Positive	74.0607	3.18	unknown	4881388	6608911	4335106	3545065	4247158	6258499	4904559	3293108	4295677	3717385	6005735	6036134	6295798	6340630	7462750	5760403	5000292	4272037	5984306	
EIC	Negative	142.1859	3.76	unknown	346337	178556	406320	216474	310500	167854	235813	194871	143953	167191	150532	242191	273833	205414	146600	255557	217810	331154	124944	
EIC	Negative	257.2124	6.09	unknown	766069	466230	750843	684475	256928	332257	378187	447806	251949	379017	310722	473257	553588	353673	505618	401698	404332	488387	270723	
EIC	Negative	366.2502	6.39	unknown	3261268	1440407	3986759	3111232	1042797	2115541	0	2538655	0	2681061	1933144	1787969	718847	2252777	2015104	1190056	1867400	977997	1019893	
EIC	Negative	390.2944	6.44	unknown	2987253	685338	7556979	10608422	398202	370983	8726439	13732025	497201	344110	6926441	0	0	10125748	9267149	0	7824571	0	12353582	
fpHILIC	Negative	261.0416	2.61	unknown	1305480	1636488	1239462	855076	1136277	1197466	1429393	912613	929625	1101360	1387404	1431310	1220709	1617496	1834153	1151600	1184452	1324368	1463215	
EIC	Negative	271.1919	3.81	unknown	776051	650187	869149	986542	447720	462076	485336	684656	398092	801996	506424	643676	639206	569342	707673	618550	493895	791173	466283	
EIC	Negative	464.2785	4.67	unknown	107628	179357	167764	110108	135968	195330	158230	136512	41770	109167	142289	176737	119548	252639	216413	125562	190506	108108	188954	
fpHILIC	Negative	165.0751	2.06	unknown	8470731	4667219	5913404	3694527	3405368	5037692	3786232	3375125	4361287	4966282	4046909	4584747	3944481	5682982	6605959	4247598	3663485	5458199	4827150	
fpHILIC	Positive	352.1695	2.70	unknown	1182244	1107992	1080662	1218451	1223265	1554136	1189598	513757	534354	882671	680206	1083117	691964	1066104	1562526	639585	739749	786960	2560649	
EIC	Negative	378.1743	3.31	unknown	819273	190969	1559600	613997	64941	262390	114274	785151	37071	853624	206595	270083	218577	505922	139389	65791	302263	530123	533890	
EIC	Negative	457.3663	4.94	unknown	364743	89518	145452	135316	249283	97878	160919	100639	131277	112203	126687	82941	121472	117379	82925	113232	436997	193070	93907	
EIC	Negative	344.9032	0.56	unknown	618876	75777	231532	255197	101066	292747	102579	25677	106084	356126	106084	90610	100277	96552	112528	178795	59066	113377	331160	
fpHILIC	Negative	447.3481	0.37	unknown	1092529	716867	772877	783196	704914	660503	929176	691501	564215	712871	938333	673437	682205	733246	1084547	1237042	618852	713120	761774	
EIC	Negative	291.1603	1.64	unknown	932715	485677	906104	199191	190676	506676	542680	286408	400050	616513	428454	731437	618817	383062	259796	529432	379304	711933	515462	
EIC	Negative	504.3064	4.00	unknown	357755	186046	100328	643036	200907	321062	81127	457273	317930	538153	392138	406157	460931	11882	0	353336	447073	811490	102798	
EIC	Negative	300.2261	5.09	unknown	245434	268202	197356	258959	167163	140579	156193	188355	169245	159135	200641	249784	196027	239809	237060	163899	191662	189672	0	
fpHILIC	Negative	240.1600	0.40	unknown	1219301	587181	243150	3714052	418053	1652721	439272	492357	113041	711944	602356	915297	793364	0	665390	860161	1175654	901259	274556	
EIC	Negative	285.2075	5.00	unknown	401640	363618	355124	258290	307986	298660	374936	289660	267651	339144	307499	299550	331948	248624	371349	367151	381408	478187	408984	
fpHILIC	Positive	219.0971	3.60	unknown	2883774	3130248	1728629	1730198	2293610	3277131	2108687	1319767	2188662	2402636	2711357	2256554	2695405	2662600	4091315	2126245	2495724	1573817	3646090	
fpHILIC	Negative	251.0176	3.23	unknown	957695	590648	373640	547792	355653	634403	341527	323048	438426	412367	289663	542008	503545	371612	517339	623516	456997	580993	427415	
fpHILIC	Positive	208.1162	2.07	unknown	569984	313842	262998	305852	301644	283774	246230	316088	264058	351947	300057	288689	244532	346767	388025	311303	205711	506846	347535	
EIC	Negative	518.2965	2.91	unknown	348908	193643	399878	1070146	236353	231917	330259	487596	262050	339144	364759	388684	458435	0	338293	329978	421422	582233	49421	
EIC	Negative	368.1480	0.71	unknown	266628	236579	315039	140439	154071	203301	170736	217827	115768	226527	207160	168192	129615	262358	261389	132031	174391	237446	269408	
EIC	Negative	365.3810	6.16	unknown	689837	408722	742824	567134	484492	285237	557779	587776	387403	634814	528999	538018	412042	610981	612738	678680	428476	651495	456233	
fpHILIC	Positive	189.0730	2.61	unknown	6575481	7946746	6285214	4140833	5193336	7081296	7346361	4447943	4987314	5172600	6981593	6941935	6332786	8424554	9662155	7272630	5866294	6635428	684285	
fpHILIC	Positive	103.0544	2.06	unknown	4075781	2123376	3142789	1948592	1706153	2127311	1866044	1771297	2199047	2525656	2068407	2306576	1823962	3020556	3413596	2308323	1764220	2683601	2098880	
EIC	Negative	233.1545	3.87	unknown	838169	1920389	1127489	989823	1712542	859455	1893909	915267	1541950	867675	1466999	1340859	1974428	1625780	1412611	1872696	1439702	1603354	2269681	
fpHILIC	Positive	131.0491	2.06	unknown	1530703	819158	1396489	811861	608086	773817	672173	750730	753408	1016064	840435	871500	661777	1286324	1161989	802680	626614	1117491	827656	
EIC	Negative	582.3779	5.17	unknown	5169292	6651469	5602451	4926176	6086826	7503235	0	5726749	5159622	4597187	6516755	6808780	6200480	6459735	6601338	5918099	6247950	4966005	6303279	
fpHILIC	Positive	157.0604	2.58	unknown	2108202	2253376	1851823	2136919	1382911	3766544	1671809	1406901	1040623	2097477	2694796	2821563	2459981	2741512	2358989	1930644	2346142	1740341	3209434	
fpHILIC	Positive	206.1001	2.61	unknown	19316124	25797492	20392010	12618395	17708398	21732432	21386632	13348977	14852347	16655352	22539092	13185334	18404618	26058946	29907802	21925998	18502970	20665206	20953612	
EIC	Negative	340.2568	5.50	unknown	231517	129458	338482	289332	144287	133365	150953	217432	130981	223032	148498	177993	182865	162952	135701	143882	189156	372952	130379	
fpHILIC	Positive	146.0596	2.61	unknown	1932966	2387415	1853998	1083467	1557373	2349464	2021740	1146909	1246645	2253061	1800000	1676548	2378795	2755492	1322659	1620841	1664827	2030817	0	
EIC	Negative	408.7626	0.52	unknown	871325	490483	867340	622049	429023	483677	525775	284639	598681	1125768	436546	490647	646234	151063	343434	53676	427884	635916	963642	
EIC	Negative	255.1067	0.46	unknown	201678	191989	61508	720451	115074	139098	98597	80766	81004	132247	111539	121758	128729	222745	80736	167931	71005	98309	100379	
fpHILIC	Positive	161.0916	3.18	unknown	776395	1019787	702180	679355	626590	865816	820232	478194	738644	613986	1039113	1108033	1152551	1061744	962290	936503	913798	643188	966127	
EIC	Negative	584.6361	0.52	unknown	656221	337182	1041375	761712	395358	443665	344977	0	666242	958158	289307	252111	418898	0	275660	573055	171904	508436	783807	
fpHILIC	Positive	252.1071	3.17	unknown	1793534	1929164	1377179	1219787	1067647	1226119	1519944	751863	921195	1553123	1387027	1041588	1585237	870760	1780116	1253943	1331530	1319373	1191991	
fpHILIC	Positive	86.0969	2.40	unknown	16473507	15210351	13797540	9331021	12432841	19638938	14757697	7148772	13114822	13102543	15589304	15657600	14624502	18255806	29607108	17279738	11347014	10611682	15817623	
fpHILIC	Positive	72.0814	2.71	unknown	16138675	18541480	17309728	12862034	14191101	19367876	15962148	11975274	12764700	14820449	19485528	19889494	17729670	24586230	28374696	16738744	14354030	13856609	19843867	
EIC	Negative	511.2706	2.08	unknown	19714873	8248542	15302173	3409371	3235455	4079895	5604198	2642314	3022586	8868461	6019005	515551	3021245	5410636	5148176	10688014	1413392	2379039	3693879	
fpHILIC	Negative	166.0770	2.06	unknown	551917	254335	300419	199057	183210	260133	222829	183275	320413	262840	211797	243134	172341	306899	336919	218770	222851	316351	261302	
fpHILIC	Negative	353.0898	3.20	unknown	528760	492098	411408	718157	421839	687867	563515	362761	529893	447334	540036	507708	552218	982132	624570	811390	534639	616127	632727	
fpHILIC	Positive	377.1735	2.06	unknown	1490349	728164	0	8077																

EIC	Negative	299.1879	2.81	unknown	124913	123463	126507	109080	89023	144580	124651	89695	96349	215214	131911	209985	224205	128844	140877	130788	157431	146532	113767
fpHILIC	Positive	118.0742	2.78	unknown	3392169	3399640	3169609	2213202	2404110	2906126	2248364	2182342	2425086	2710949	2627613	2525499	2389927	3448961	4214834	2367504	2359293	2902908	3590663
EIC	Negative	257.1759	2.16	unknown	335225	152741	199052	129295	129295	124218	171084	121379	282784	194095	124218	226849	154436	303145	176023	139930	162726	233162	226387
fpHILIC	Positive	117.0670	2.79	unknown	3269522	2988318	2783624	2121545	2230126	2889536	1919521	2004023	2042665	2418545	2355210	2623436	2037477	3163464	4121928	2350579	2095154	2576497	2912425
EIC	Negative	507.3690	4.41	unknown	673269	457968	615157	575854	499363	288255	587298	4042665	743596	606694	504398	455623	328988	548602	631583	479587	664822	438766	
EIC	Negative	493.3542	4.09	unknown	292231	532615	330339	183245	433834	236848	424453	253873	393488	238465	384847	306242	336096	391748	617728	511118	325574	257749	498922
EIC	Negative	318.2156	3.91	unknown	1001243	428225	1665968	782927	306893	252621	751704	619100	690024	670208	543823	747732	900640	491345	249235	598966	620683	943694	368988
EIC	Negative	618.3422	3.06	unknown	2451730	1696941	1536868	1433407	1151620	2576785	1571488	1713918	1724993	1883242	1579142	2822560	1768574	1001763	1811306	2531449	2826448	1166977	2760587
fpHILIC	Positive	190.0763	2.61	unknown	436386	648974	448911	283471	411989	479261	499368	279591	321553	477542	478391	498555	532193	774751	485050	390266	419499	496603	
fpHILIC	Negative	249.0217	3.23	unknown	10785753	6503601	4461743	6774648	4204925	7509266	4043331	3531277	5453608	4432945	3473234	5776985	5795756	4506027	5238161	8079462	5442288	7487202	5190281
EIC	Negative	624.3313	3.94	unknown	2073473	7872412	1652445	2958694	4172769	4477691	4044116	1944429	4374541	3159605	7721329	5093304	6018205	5167570	5243912	5107033	5300222	2194394	6315381
EIC	Negative	594.3423	2.53	unknown	321854	270950	351960	197891	269090	335263	326472	181607	299684	269988	354509	332331	228002	312212	323876	382845	349020	213461	527532
fpHILIC	Positive	159.1124	2.70	unknown	1886595	2282745	1985220	1525349	1957689	2024771	1975769	1580511	1559859	1917389	2867630	2315197	2180300	3178881	2968436	2180522	1986580	1786903	2657154
EIC	Negative	296.1873	3.28	unknown	183286	23226	87114	124987	39738	108501	20201	86102	17161	95396	63201	87683	55468	33606	85811	41088	69237	96644	53085
EIC	Negative	628.3727	3.94	unknown	754447	468227	2109291	469485	185025	1573654	559326	404371	243587	210969	663332	1323234	2227260	902985	146709	916786	873093	1461527	378673
EIC	Negative	383.1827	3.87	unknown	161711	63440	211023	303511	81844	147691	285451	1748626		210969	125048	166501	148758	146488	112298	126617	134459	524533	130980
EIC	Negative	411.1846	2.91	unknown	5736494	5467617	5551879	3745877	3461044	5249789	3563609	3976291	6018114	5612840	6020397	5598664	5363574	4945273	5614477	5669039	4909981	4335652	
EIC	Negative	333.2075	3.80	unknown	2340001	1093963	2714023	2097720	995188	1161449	1281192	1639378	2080560	1185981	1453173	1715988	1141985	1150570	1360304	1437830	2600129	1415354	
fpHILIC	Positive	207.1028	2.61	unknown	1422974	1797505	1456682	858629	1197167	1449839	1744150	951512	978209	1250857	1572449	1546883	1331247	1820655	2316489	1598206	1180703	1344080	1611699
fpHILIC	Positive	509.2871	0.37	unknown	1092154	1083482	901834	770649	1039358	469086	854303	882900	406114	713190	9304376	806978	705357	1072331	1003270	398068	1050037	1188531	1015700
EIC	Negative	346.9010	0.56	unknown	579033	76005	169173	247163	104031	296150	71960	11913	83841	318944	75827	69650	85461	67853	101716	154673	38800	123037	305800
EIC	Negative	507.2727	5.84	unknown	25837857	25124210	21815747	18856338	20199813	11106348	17454791	21680803	8593398	16355489	18367100	16243942	15282856	25922884	23421761	9580070	19614475	29332307	18815663
EIC	Negative	312.2264	4.35	unknown	2847522	809498	3501335	3712247	1307874	949387	1255450	3117793	1085878	4764946	970166	1215443	1182803	1581634	1602017	825215	1295151	1949166	1178164
fpHILIC	Positive	198.0865	2.36	unknown	3209424	2657987	2856004	2619971	1972818	2988556	1734257	1964640	1762055	2626629	3114727	2256342	2597913	4306440	2474117	2757069	2770563	1906368	3393106
fpHILIC	Positive	171.0953	2.83	unknown	1829455	1630978	1150643	1119234	1295770	1489236	1069716	922136	1864036	1130135	1243318	1233358	1354996	1559490	2388291	1882299	1503750	1287498	1413881
fpHILIC	Negative	168.0277	3.66	unknown	459463	406143	369984	431205	354665	456356	327989	396385	369078	485992	391334	479372	385214	429294	447251	519556	534687	523254	406220
EIC	Negative	508.2763	5.84	unknown	7034995	6822871	5886169	5042392	5469493	3016441	4698799	5963383	2346119	4383629	4825907	4365832	4168160	7100184	6338411	2592580	5323487	7989046	5196502
fpHILIC	Positive	170.0919	2.83	unknown	24571946	23760600	14458396	15762170	17795866	20465716	16166531	11762041	24748676	15351748	16722984	17482172	19144630	20062026	32211332	27583356	19788942	17668324	18841936
fpHILIC	Positive	526.3135	0.37	unknown	640996	596896	460932	431882	557753	268962	484365	507226	229983	378767	526147	451330	433400	624760	556409	266465	597712	627623	561419
EIC	Negative	551.2846	3.47	unknown	1047543	633555	2340919	685092	526382	410213	703262	1154013	284931	1278621	715248	661337	392914	474576	541747	441456	493330	1845761	611299
EIC	Negative	394.2321	2.90	unknown	434235	208812	468965	311994	165726	100383	372380	339734	262474	438874	307258	410923	480671	255716	230365	258190	314595	469873	312716
EIC	Negative	365.6963	6.19	unknown	907816	535639	1078556	731183	858655	288549	675204	854992	517804	1146638	642718	475097	462451	602975	913276	803391	581933	769945	665023
EIC	Negative	339.2536	5.50	unknown	1068242	692984	1589467	1311620	693034	599949	663881	1083229	516933	1800112	694713	909247	779066	703395	661356	610082	844911	1786559	645809
EIC	Negative	330.1794	2.34	unknown	121495	65835	189856	167439	36848	78240	80168	75552	51814	59285	55810	114869	117241	64222	46529	79692	63157	169016	54372
fpHILIC	Positive	371.1465	2.47	unknown	706034	457227	325505	331175	280061	520189	246399	200116	29816	309923	531106	555652	328464	315947	498298	380216	299692	345894	425651
fpHILIC	Negative	112.9373	5.36	unknown	1189308	288615	1034115	350088	421906	567950	509611	136807	376468	106540	232746	79672	194990	184258	1466810	92425	450470	291740	
fpHILIC	Positive	119.0894	2.71	unknown	9897502	12208442	10384224	7822908	9127781	12502308	10642647	7837961	9569269	13362746	12948661	10970619	16746202	18324240	11017250	9977321	9915728	13125149	
fpHILIC	Positive	218.0914	2.62	unknown	682884	839556	727148	516826	625878	717335	709467	446570	539158	611662	710037	681659	606603	920187	1065634	834698	625485	639179	727064
fpHILIC	Negative	263.0918	2.06	unknown	1475462	337918	296698	167528	223495	591989	207983	174327	244056	205889	413204	163567	250651	232384	240186	218895	659794	310799	
EIC	Negative	642.3007	5.54	unknown	386647	307018	364424	297837	313771	293788	266788	333560	304494	379644	337390	338589	284744	378953	367068	343535	375692	404822	355597
fpHILIC	Positive	309.1467	2.78	unknown	847964	801881	690131	543556	548961	654293	476689	744624	369760	349624	689760	576102	723932	763355	712233	613818	641142	842266	
EIC	Negative	589.2761	5.84	unknown	1016457	966933	865948	748033	831908	440863	668856	333240	662205	699408	612735	653569	1044842	923836	369497	816613	1611798	762710	
fpHILIC	Negative	509.2879	0.38	unknown	2030234	2187889	2097045	1944138	1463364	1682428	1617095	1010312	1324699	1273388	17482172	19144630	2145402	2079111	1270016	1715929	2581553	1896934	
EIC	Negative	570.2976	3.10	unknown	138866	98281	152579	92812	51586	125118	54187	130871	114050	141764	104240	148263	104899	72893	113222	137257	110159	68087	182506
EIC	Negative	316.1998	3.76	unknown	7038017	3971962	9168600	4850001	2433068	3424207	4785168	3942233	2967400	3630325	1865558	5219576	5667253	3992586	2961714	5212620	4479316	6966138	2926326
fpHILIC	Positive	148.1097	5.22	unknown	922529	1057852	873396	599467	689798	995125	799132	489689	786347	675872	1076867	1154514	1066745	961531	1321959	985056	832253	774120	921614
EIC	Negative	299.2235	4.44	unknown	1294257	538953	1639853	1315066	669643	788031	698857	1262250	576476	1430722	662424	817730	619719	816378	655235	1264218	821473	1774157	673781
EIC	Negative	555.3885	3.65	unknown	247																		

fpHILIC	Negative	218.0406	2.94	unknown	2070859	2372125	2884668	2078749	1881462	2056395	1658468	2132988	1791050	2639520	1776201	2183593	1967203	1963907	2638600	2001690	2557135	3233660	1951042
EIC	Negative	293.2487	4.99	unknown	259379	112842	259690	181674	116837	78806	123753	197681	137184	346390	123994	144703	122926	138791	197657	192053	122326	231129	108520
fpHILIC	Negative	275.0215	4.15	unknown	628859	183923	230860	357468	251678	330890	169808	121518	46145	337943	241190	198789	75454	226852	290957	144062	159503	434558	169143
EIC	Negative	357.2060	4.05	unknown	531937	291448	509545	740780	370189	298454	258907	414850	347641	1017463	310313	315697	285373	302060	335364	305477	472260	1721999	365771
EIC	Negative	625.3344	3.94	unknown	725660	2865248	612709	1032568	1466690	1599372	645556	562192	1137727	1137727	2754193	1851430	2097084	1834433	1886222	1621921	1956415	783460	2302120
EIC	Negative	509.2789	5.84	unknown	1364576	1354292	1185703	1024443	1089382	594527	948502	1135500	489272	901234	1004904	936797	850520	1439220	1229887	526643	1102652	1573988	1118334
EIC	Negative	618.3422	3.25	unknown	2302528	1613612	1525599	1666336	1158499	2519267	1434433	1691820	1565422	2016026	1545961	2709363	1689058	969317	1808673	2547297	2168592	1090023	2784342
fpHILIC	Positive	300.1188	3.16	unknown	1003827	1384234	896768	770008	975502	1105432	1097592	922539	902423	1046732	1726843	1431757	1350475	1411668	1695152	1335867	1036429	1093872	1366429
fpHILIC	Positive	144.1016	2.19	unknown	589618	510941	390335	569804	788397	0	421167	964058	446810	448198	628891	562362	388750	502763	857156	649086	457347	370468	675368
EIC	Negative	285.2073	4.37	unknown	497783	320779	571971	583435	243969	222129	398661	335449	333578	351287	338327	545053	595648	391882	383487	457861	391289	432390	336821
fpHILIC	Positive	122.0698	3.18	unknown	884145	1092683	797048	761070	817369	1040221	871915	624653	858380	714419	1088124	963131	1171767	1121228	1339970	1104871	959837	803896	1292315
EIC	Negative	318.1428	2.35	unknown	326059	152458	476105	463795	88872	139373	159294	357548	88132	280438	137981	251316	211478	178560	289110	205506	178407	297122	117934
EIC	Negative	363.2008	3.74	unknown	2689993	231159	563425	6502531	121471	315405	186982	118860	99004	0	1196967	226350	97195	49642	129446	297322	167047	305768	199792
fpHILIC	Positive	133.1049	2.40	unknown	14457123	14122018	12267772	8633252	11134102	16466432	13037744	6800494	12246001	12847524	14240488	14703525	13079928	16855024	25617728	16260124	10313482	10332789	15505828
EIC	Negative	619.3471	3.06	unknown	795142	572347	507700	465960	378292	843294	525985	551070	546533	652447	518201	926248	565710	337018	617713	845010	942748	395991	914309
EIC	Negative	495.1974	2.67	unknown	103880	172017	127490	153877	117672	103485	161014	107819	142795	130120	146133	222812	208363	181128	147229	153250	180131	187805	160142
EIC	Negative	135.1250	2.15	unknown	249001	215786	276821	292574	133725	137803	153268	228828	92740	176065	120654	270791	226957	227481	273872	225685	173544	167126	137736
EIC	Negative	507.2727	5.59	unknown	10194286	14172119	10098083	9185049	13407117	7053370	11295298	11529177	5333440	8671492	11753157	9551059	7872443	15764723	16855773	7103653	14093389	14003994	11684361
EIC	Negative	332.1952	2.67	unknown	5453347	4452023	5506200	5027146	2043969	2579197	4544706	2920461	3618287	3929139	3529574	5974381	5694484	4782401	3575397	4372973	4564525	4646580	3436410
EIC	Negative	367.1685	2.67	unknown	256082	245374	507169	89426	208509	147169	208509	147158	208511	208511	191682	236231	256529	220735	165580	216208	197364	186033	189610
fpHILIC	Positive	157.0798	3.32	unknown	11282682	5375450	11040516	7432561	4097376	5112137	4744253	6055331	4167064	9654556	5417475	6666693	5322983	6240166	7904535	5173464	4176313	9190466	5854390
fpHILIC	Positive	174.0599	2.71	unknown	663942	485624	533792	489375	458873	434728	308487	487304	226739	551890	424845	4565650	356759	556595	547873	562373	329867	502881	484235
EIC	Negative	479.2028	3.61	unknown	160822	167845	299922	206180	80628	116988	161123	129379	9414	148238	183033	228550	257904	186506	106379	169103	167046	177762	150782
EIC	Negative	528.1782	3.19	unknown	787239	237009	347465	595287	317061	199325	249600	716548	299340	4599885	338450	354347	387078	156847	233389	643878	442898	664207	285030
fpHILIC	Positive	258.0747	2.52	unknown	795053	697458	466486	630660	493564	903803	473632	448874	657173	610627	812902	858044	596989	648546	805927	807115	569079	815123	911034
EIC	Negative	519.3686	6.70	unknown	426490	797203	446281	334397	396811	482306	437218	209410	289590	326597	1312761	807161	738135	896732	771366	461006	308181	388017	500106
EIC	Negative	422.2299	5.92	unknown	3564531	3298966	2715958	2295244	2753935	2388673	1749619	1879877	1429815	1509649	3241217	2737907	3056995	2771885	3311000	2881494	2702457	2478059	2028339
fpHILIC	Positive	130.0864	5.21	unknown	16150545	21310190	15246231	13074269	13989051	18061788	15211785	8828678	12390357	12744620	18698798	21726256	19202362	17541428	24827352	19444786	14314744	14296635	17176858
fpHILIC	Positive	361.1444	2.47	unknown	3096188	2322049	2309296	1323580	5654812	2147005	1451043	1587888	1692970	1601460	2265857	2411059	2227498	2885928	2709830	2092856	1676480	227348	2502623
EIC	Negative	355.1400	1.62	unknown	1646296	1406479	993107	172646	107428	1109314	559504	1083247	467506	992644	836627	912813	502237	2057097	1340431	492933	843820	926196	1215011
fpHILIC	Positive	107.0494	2.06	unknown	828713	455675	751717	385474	353885	473292	396053	416791	362505	596219	410424	492472	350966	626973	740371	587717	401766	623436	409906
EIC	Negative	332.9485	0.52	unknown	153677	0	92655	0	48131	67653	0	73163	219476	51480	0	0	58222	0	72012	0	0	177139	0
EIC	Negative	258.1799	2.09	unknown	191796	149601	205627	154072	83434	153273	124722	70969	92952	145487	135913	214529	225916	146349	156154	212288	146731	72659	104940
EIC	Negative	410.7598	0.52	unknown	690112	393641	671362	743016	327711	398367	459580	222152	456442	893370	396812	389611	492737	119593	373434	444765	334429	564544	743297
EIC	Negative	384.1853	3.19	unknown	409911	77602	575962	382017	76231	93354	94131	30268	209647	411300	26288	137619	137912	144739	98010	141971	412126	147969	0
EIC	Negative	357.2301	3.84	unknown	2171566	360247	2755811	794329	310532	550536	405013	1189697	63948	1374084	284983	595179	324791	461398	412961	148930	390338	1724129	651199
EIC	Negative	289.1449	1.88	unknown	753854	582721	0	0	264213	526336	518836	0	549685	694627	799419	664357	349243	699192	610012	0	0	558681	0
EIC	Negative	421.2265	5.92	unknown	15324260	13994598	11840955	10173110	11709975	10173548	7403877	8079392	6231468	6733419	14289429	11883451	13129763	12038966	14274506	12328698	11477516	10644066	8886110
EIC	Negative	508.2763	5.59	unknown	2723325	3955939	2780397	2416660	3638687	1945690	3076907	3064401	3076907	3057071	3196385	2572330	2121509	4257537	4551497	1891196	3816701	3913103	3184442
EIC	Negative	313.2386	5.99	unknown	776460	551454	1314955	712360	213394	388449	245093	181556	605630	294308	366487	630694	521158	359236	317878	380725	504856	712668	244849
fpHILIC	Negative	157.0504	0.97	unknown	769377	997618	1093558	564133	716692	609537	613905	403172	812126	71728	1821126	490844	633727	476970	404106	393907	391489	1906653	377483
fpHILIC	Negative	298.1141	3.16	unknown	42170100	56314656	40682136	35806804	39045728	45999044	52713300	39701372	39342520	42943132	74104760	66888928	56525800	62823572	71295064	60688756	46876224	42605156	65376096
fpHILIC	Negative	173.0567	2.71	unknown	9663102	7000558	7715302	7514074	5526219	6352408	4291455	7234836	3177674	7015775	6569377	6457585	5940073	7784485	7649646	71928032	5292831	7259098	7042361
fpHILIC	Positive	383.2015	3.22	unknown	403779	297983	367707	506663	205064	410904	212546	181929	251890	3802629	375790	426180	420610	466016	253689	353257	247380	412164	402893
EIC	Negative	259.0647	1.77	unknown	1005996	2766650	811960	87410	952652	1010428	1969202	1136513	618060	0	3314819	3592002	1583888	3327758	2798420	1656761	1118263	0	1959603
fpHILIC	Positive	123.0438	2.95	unknown	5456581	4339021	5248326	3282703	2943476	3465632	2753725	3185871	3076147	4386672	3027268	2896572	2979519	4368035	4592880	3351176	3631238	5413628	3471584
EIC	Negative	500.2888	3.41	unknown	2323666	1131527	2214450	5012789	1362207	1842114	1935956	3050682	1917113	4345390	2226049	2052722	2989131	4339971	1433398	2131746	3108294	5967378	769804
EIC	Negative	433.2212	1.78	unknown</																			

fpHILIC	Negative	200.0154	2.96	unknown	371030	512237	327769	165929	220642	443973	328545	246901	320385	209427	336794	408070	369916	731195	470138	235069	409197	350380	632857
fpHILIC	Negative	190.0541	0.61	unknown	32952584	21256540	24283652	23001388	14074455	19650720	16224852	15582322	12556415	16800272	22868370	20044974	14167829	19991208	27822568	14584969	18040304	22319860	22225066
fpHILIC	Positive	87.1002	2.40	unknown	1017756	819863	679283	537298	720786	1106128	763319	378662	704845	808194	26883070	899601	860573	937315	1885665	931798	624383	612423	585765
fpHILIC	Positive	119.0835	2.71	unknown	678470	771751	752360	503821	724178	844766	703751	508817	558355	695308	986437	1000378	779518	1188875	1248330	875946	811368	597389	960281
fpHILIC	Negative	335.1296	3.34	unknown	1325716	753262	1174269	889513	558336	652596	602596	780806	526119	6709297	863008	869519	764020	952517	1083803	725495	589848	986101	817516
fpHILIC	Positive	156.0777	3.61	unknown	93859464	46294484	60937708	58217520	29960100	41817528	31366394	39735924	35248428	67092962	38232404	41439996	35946296	40705552	56917880	43154040	34558944	61408680	43664988
EIC	Negative	392.2169	2.67	unknown	176292	119930	174306	143906	74484	71350	144796	47972	115079	116470	100591	172093	170214	65844	109705	124304	1405758	136164	99703
EIC	Negative	310.2108	3.80	unknown	2540688	685739	3385677	2415253	736044	761914	751607	2165469	629855	4083446	704792	869826	678477	1619922	1329378	556232	882910	2873165	1151116
EIC	Negative	227.1652	2.62	unknown	182628	273634	196136	183119	299643	181189	122447	196679	331812	354263	362390	291919	155773	219210	359742	345180	157733	374816	226180
EIC	Negative	589.4474	4.14	unknown	198540	167034	453452	440429	94227	75186	134099	187550	143781	218703	103650	179508	183227	230283	142155	124105	192718	237302	122563
EIC	Negative	423.2266	5.92	unknown	1162244	1059003	898789	765597	850340	747495	561972	618414	451674	505243	1054195	880468	987446	878163	1084321	950543	889602	778313	649870
fpHILIC	Negative	201.1131	0.61	unknown	1003294	1176996	848137	1834515	601377	1878809	904107	1064463	1405181	1683819	2088929	1953082	2965516	1175332	1584119	2409929	1298102	1494489	1105536
fpHILIC	Positive	111.0748	3.33	unknown	503575	223938	601936	398142	237816	237576	364619	324173	185092	572796	340848	275125	325410	305118	438741	227909	243987	455200	453833
EIC	Negative	406.7654	0.52	unknown	439044	229310	431144	305650	271475	342440	171703	70880	395299	585930	296751	237403	261167	0	280777	363611	182572	374816	486780
EIC	Negative	320.9970	0.68	unknown	129009	166759	187337	118954	107761	104467	116777	127388	99894	158940	137589	128072	162292	155792	140325	168634	129348	168910	143173
fpHILIC	Positive	165.0542	2.95	unknown	23106582	17161544	23791170	14762781	12948536	14154799	12001328	13008197	13343301	19272474	11353236	12170436	12431084	19324486	19277438	13192857	16693209	22286650	16947332
EIC	Negative	643.3460	3.15	unknown	286185	400603	189372	229755	213719	389322	222424	215011	407397	295009	331498	424829	339898	184579	306741	527674	455300	157385	509327
EIC	Negative	369.1736	2.90	unknown	0	0	445710	0	0	351100	0	0	0	0	0	388701	0	0	0	0	0	474493	0
fpHILIC	Negative	278.1247	2.57	unknown	327074	703243	624346	310969	308118	528932	831648	257818	208514	523810	662800	572502	498976	561001	893341	384463	498095	456285	653483
fpHILIC	Positive	102.0373	2.47	unknown	1404219	1758962	1430231	725208	935441	1412174	826806	840426	806693	919438	1172495	1239280	1060573	2194214	1457672	1003351	1429295	1205961	1740967
fpHILIC	Negative	137.0356	1.01	unknown	1527715	660345	455231	518597	745615	787036	315711	700460	1172980	1167666	732181	816528	862409	1143276	713084	885328	1476203	1441824	517581
EIC	Negative	283.1531	3.31	unknown	379871	441892	237164	200338	375512	313072	314112	311217	238531	252014	338624	353225	337934	337452	432014	344242	447053	371877	505126
fpHILIC	Negative	204.0860	2.61	unknown	4517851	5719065	4655108	2888145	3916412	4627120	5163000	3233347	3541776	732035	5339578	4905185	4287693	6034595	7441778	5525132	4399416	4814835	5539436
fpHILIC	Positive	253.1146	2.79	unknown	723867	751424	903538	841672	664382	720082	471960	644968	720485	770201	795668	854590	616048	829106	1103895	648802	687232	961151	960269
EIC	Negative	594.3423	2.43	unknown	1041070	856688	1482650	848846	479630	791327	659023	1126684	392857	373278	888894	899404	668827	1683839	825271	489903	697594	1308637	1438394
EIC	Negative	330.1794	2.42	unknown	238173	249440	373397	195345	158409	151915	122697	91004	508956	143613	173434	192100	188561	178561	173574	181875	165750	187681	202602
EIC	Negative	570.2952	3.10	unknown	135754	92518	153747	96963	51586	118926	65910	130871	95629	142348	104838	149533	104899	76539	98292	127133	106684	68087	227203
fpHILIC	Negative	896.9057	3.78	unknown	702476	204232	37687	1063657	119705	328773	0	821423	769838	146371	372064	500263	1442680	177375	206066	191123	1351077	743646	273543
EIC	Negative	618.3423	2.71	unknown	2823477	2355167	1534413	1801657	1401188	3400554	2212233	1886550	2461851	3366092	2526025	4037739	2655564	1332134	2585707	3333704	3787092	1713410	4002015
EIC	Negative	427.1797	3.24	unknown	84630	46865	90432	73615	20079	31833	32446	27328	20893	58251	33919	36655	28164	26475	26230	30084	43587	28929	39299
fpHILIC	Negative	155.0463	2.59	unknown	1305434	1215486	1109403	1238334	711582	1765602	938085	809196	552460	1194482	1644080	1617443	1677045	1544387	1274072	965197	1602740	920673	1730460
fpHILIC	Positive	131.0906	2.30	unknown	5814940	4348916	4809612	2855842	3874862	5437142	4633048	2111818	3843015	4804167	4836933	5215613	3895199	5692208	10350652	4773115	3627779	3439764	4885705
fpHILIC	Positive	131.0896	5.22	unknown	1125161	1578045	1056194	862539	855965	1200854	992492	5962363	867376	803580	1262517	1527152	1344811	1198912	1682880	1398725	920839	974187	1157902
fpHILIC	Negative	299.1175	3.16	unknown	4919415	6419202	4796674	4030048	4483212	5247518	5983895	4325711	4732878	4874781	8596126	8220688	6805421	7331079	8412997	6976083	5545222	5246221	7531583
EIC	Negative	239.1287	2.33	unknown	425816	206582	302614	510330	211063	267258	72425	106294	374300	274690	191470	242399	313600	127480	259272	321420	196553	397378	1375759
EIC	Negative	332.1952	2.17	unknown	1244631	789601	1328909	1225137	401386	376260	598771	497053	457186	1091404	517817	778947	568070	513389	487367	794021	541254	656431	688515
EIC	Negative	409.2248	2.48	unknown	173321	172770	0	121368	68590	134978	81391	0	0	0	81654	160841	134914	123798	100862	137496	139651	116891	113007
fpHILIC	Negative	155.0655	3.34	unknown	2442274	1438174	2407172	1506229	1182408	1303005	1052325	1252411	987193	1673650	1339391	1382530	1208383	1769108	2135644	1328836	1100042	1762070	1550180
EIC	Negative	378.9556	0.67	unknown	87866	101169	130390	84098	71248	85098	81074	81074	81074	81074	81074	81074	81074	81074	88212	113462	84352	110114	104109
fpHILIC	Positive	317.2113	0.39	unknown	1194342	800486	1696550	1072410	359856	646497	728534	647607	492697	902928	744719	983131	1009799	680230	470098	888420	935671	943083	692318
fpHILIC	Positive	120.0300	3.18	unknown	400302	504713	296935	287640	341217	271574	391958	329251	487834	507791	573036	548210	541721	573036	548210	541721	573036	548210	541721
EIC	Negative	345.1712	3.77	unknown	456962	611403	579489	364527	190856	233246	423670	174779	204253	772664	380184	522615	514300	249855	342166	396575	313354	247440	379080
EIC	Negative	373.2960	4.92	unknown	82593	244931	524608	318017	83060	26363	69936	171545	102833	151315	169878	136991	114048	66162	107693	263035	52451	263035	52451
fpHILIC	Positive	157.0796	3.61	unknown	6208549	3036894	4210267	3910353	1955823	2580641	2093879	2676814	2720257	4327655	2612762	2376252	2391271	2675667	3723554	2953554	2298227	3894399	2992016
EIC	Negative	389.1923	3.88	unknown	88651	65012	110131	119927	71053	93360	78574	145247	109189	126611	82644	139707	93305	110393	82511	96423	101213	307224	93843
EIC	Negative	581.2886	3.41	unknown	279442	134908	270246	457057	139250	232059	230172	330268	245313	531078	271581	242314	334879	55329	174651	277574	345486	714489	101741
EIC	Negative	374.2059	3.94	unknown	71077	62870	119061	79182	21094	97518	55055	28589	25631	27795	62574	87338	101520	75249	21829	75761	79777	91244	43878
fpHILIC	Positive	119.4040	2.94	unknown	2749857	2188461	2612335	1866572	1325451	1523512	1374958	1523066	1553814	2205620	1402285	1455885	1437170	2					



fpHILIC	Positive	104.0529	2.46	unknown	10317424	10552874	8745997	4061318	5496007	9099711	6087006	5438370	6163786	5796204	7895153	9193613	7102168	15201949	10817158	6791311	7000285	8393424	11861309
EIC	Negative	413.1947	2.67	unknown	1406271	1229648	1146796	1321639	623298	744967	1239856	756593	994675	1080866	1029370	1558045	1766526	1332923	1022514	1211762	1255484	13704709	1262907
EIC	Negative	262.1166	2.87	unknown	494549	183389	969533	311475	136299	234227	199026	439112	68586	722323	261279	366536	182345	321767	238165	122205	251461	612495	172931
EIC	Negative	407.2439	1.51	unknown	682929	1703482	713346	1073336	928033	1191230	1123497	508529	1121043	769930	2254952	734658	1899613	2032097	1111762	2339374	763990	1227840	1333130
EIC	Negative	516.2735	2.60	unknown	836949	489449	843798	0	341151	171030	355624	0	515191	0	363968	494858	393831	280253	519703	519255	911517	0	808402
EIC	Negative	329.1762	2.42	unknown	1016986	1122400	1795251	860693	631949	656140	550487	364089	660360	628268	736728	900225	845604	817811	769419	834840	719928	793555	863545
EIC	Negative	642.3422	3.06	unknown	1276430	1676811	879146	995476	1114447	1658523	1241700	783655	1808250	1277982	1589348	1879246	1393987	859110	1510720	2227316	2216185	728053	2514473
EIC	Negative	379.1777	3.31	unknown	187726	39178	377995	129589	21325	52608	16687	179667	13271	196509	48684	77033	63396	138321	36116	17763	75575	134350	130969
fpHILIC	Positive	158.0813	3.32	unknown	691168	372336	749844	388196	250560	276985	316856	452172	228400	360297	483309	426500	335133	412088	476949	315638	329650	564108	436981
EIC	Negative	258.1798	2.24	unknown	257486	74789	199404	283853	67700	120355	63493	122707	97857	283566	99421	133471	114550	149566	106667	114793	95223	226653	114151
EIC	Negative	362.1685	2.59	unknown	78153	224816	0	68637	99210	108058	172940	0	128793	0	70841	230183	328025	406670	210720	214724	27395	0	201279
fpHILIC	Positive	360.1966	5.21	unknown	510951	646193	456302	439105	457859	519511	493535	401565	0	477753	578755	575994	533621	495958	558315	559167	568061	459407	466858
EIC	Negative	334.2109	3.53	unknown	388484	211374	625315	323818	109127	112463	204717	174620	109518	220646	144689	189500	229722	122295	164034	189944	174352	242258	220583
EIC	Negative	375.2175	3.61	unknown	402707	238074	826939	389812	113931	192572	302323	230376	148662	837345	333760	411517	480426	328006	136669	270337	334736	347157	290154
EIC	Negative	237.0224	1.77	unknown	182043	177319	174619	92463	137787	181634	161803	86794	161827	145147	165875	221923	300283	182126	146044	229608	485995	0	157235
EIC	Negative	642.3422	3.20	unknown	711667	783492	409210	466033	378156	481907	443341	603833	370150	313491	632120	448308	509668	641608	474748	264306	459366	807580	736569
EIC	Negative	643.3458	2.68	unknown	474488	541639	289754	334675	305066	603833	370150	313491	632120	448308	509668	641608	474748	264306	459366	807580	736569	232371	812758
EIC	Negative	345.1709	2.45	unknown	1095505	2515818	1115093	950585	1167245	2071300	1858656	500526	1248937	763650	2522945	3048013	3667397	2644142	3381911	2421194	2373250	774472	594259
fpHILIC	Negative	181.0712	2.95	unknown	2725116	1904407	2374904	1537298	1319724	1542349	1424242	1599968	1440106	2162293	1212314	1469413	1285457	2512447	2571169	1355613	1675819	2666862	1976336
EIC	Negative	333.2075	3.68	unknown	1507431	1100494	1601440	1976988	624525	449064	811442	1424900	767627	464056	449028	352534	669622	951766	625451	1054778	1064778	802750	1976336
fpHILIC	Positive	134.1003	4.83	unknown	652268	517566	507520	441866	446842	545707	528157	397935	545258	521012	442159	478709	487584	581832	885471	538490	834773	613454	575471
EIC	Negative	303.1603	3.97	unknown	104362	89653	132138	107443	454532	49625	62381	49625	399529	90774	139229	120811	75231	72351	139639	69390	71262	70645	0
EIC	Negative	257.1760	2.24	unknown	1564549	368180	1292471	1798952	429643	709692	398472	810180	562294	1791161	506524	846140	776535	932323	646191	713575	589429	1432833	693656
EIC	Negative	329.2332	3.49	unknown	226734	139174	238622	172852	101968	101968	123472	124078	307946	158562	167480	117703	108660	106503	195020	245550	221188	143083	0
EIC	Negative	427.1797	2.67	unknown	728764	637222	634241	579484	291223	349689	606961	450751	491655	546728	564797	817882	773192	661533	520918	605377	702269	719718	520356
EIC	Negative	643.3461	3.20	unknown	262756	291859	152444	170190	142548	281946	163677	291357	256913	232868	329556	230804	112246	214048	383892	331792	122649	394728	0
fpHILIC	Positive	106.0490	2.46	unknown	419296	571463	404759	195812	350322	474472	279925	248259	291625	256313	300836	466754	318444	696932	490003	395723	389603	481912	548919
EIC	Negative	468.7190	0.52	unknown	745899	385895	758767	803085	347416	375852	449769	251495	502911	987724	377475	331906	450622	131738	353067	635813	311772	574372	829594
EIC	Negative	352.2214	1.83	unknown	363376	112913	298013	0	37831	63264	76626	78146	59761	0	109954	151121	108408	110759	91015	121540	110096	0	120219
fpHILIC	Positive	409.1855	2.61	unknown	7572457	10573501	7453878	3080569	6604584	6504635	7994075	4179901	4914646	4990663	10082755	7510446	7200840	10128518	13139208	7793568	5890716	7244097	8253022
EIC	Negative	336.2265	3.16	unknown	187022	96601	172761	153666	73521	68142	84993	100275	77656	131434	78050	128698	107651	83027	69455	82543	148016	192669	76910
EIC	Negative	319.1910	3.21	unknown	189261	375704	208860	410512	158207	94137	119661	177631	109864	143014	98632	173900	137355	124899	271261	223873	134943	161781	137535
fpHILIC	Positive	247.1072	1.07	unknown	3678982	1964889	3049326	3395347	1913109	1887104	2158799	2575631	1363304	2396630	2219373	2101574	1847442	2607508	3592381	3293257	1835417	3470760	1760734
EIC	Negative	543.2982	2.55	unknown	749116	0	1463705	505375	0	51201	0	274398	6466	417504	0	0	0	0	0	0	0	468071	0
EIC	Negative	517.2963	2.91	unknown	1276126	537385	1652974	3522350	750194	669591	1102733	1562259	1149360	3219416	1206830	1251708	1594046	841317	894485	1701302	3545768	395934	0
fpHILIC	Negative	89.0438	3.35	unknown	479658	492653	352118	306736	326571	424116	344291	270913	365998	334191	421951	451152	409652	532011	636981	495192	406088	517823	385825
EIC	Negative	414.1981	2.67	unknown	322538	309676	279129	266848	164420	183126	304735	151276	252551	241540	266848	392683	306714	294475	253088	306714	294475	344764	265428
EIC	Negative	261.0593	1.77	unknown	42879	130846	21906	34933	42966	44634	90428	49244	7711	18916	146770	159984	82733	143834	122104	7711	46881	0	87796
EIC	Negative	367.8767	0.70	unknown	36411	115449	97530	94033	54989	57844	76392	47504	100412	95963	94665	31341	31341	89263	103315	100852	211487	6567	0
fpHILIC	Positive	133.0971	4.83	unknown	12483398	9398154	9165286	8065170	8065170	9748197	9695656	7632147	9943539	9545827	7963622	8514269	9321136	10709811	17390548	9987741	14781347	11305517	10272433
EIC	Negative	429.1957	2.89	unknown	253515	223888	186586	205326	129779	71653	335981	300698	249864	300698	334292	384319	249558	258160	214164	200416	256800	422727	308877
fpHILIC	Positive	183.0841	2.95	unknown	22742172	16587837	21762190	13853333	12287987	13711382	10499830	12643647	12094068	16948474	11081804	11509106	11353022	18864368	21428618	12958029	14874262	21421134	15959496
fpHILIC	Positive	102.0915	5.23	unknown	866490	1395501	1357173	934437	1077248	1330677	1372437	670513	925565	1081922	1518557	1973675	1420149	1539061	2072647	1717164	1179254	1114999	1526465
fpHILIC	Positive	222.1223	1.65	unknown	0	725552	309811	343343	335424	0	459071	213914	527658	337688	493082	481083	409412	406865	615135	620702	325012	300956	313108
EIC	Negative	413.2001	4.28	unknown	720828	166188	932488	451360	91385	76973	173984	237451	123608	847562	261838	276223	276226	209912	119248	179170	256374	244921	196442
fpHILIC	Positive	110.0714	3.32	unknown	10838697	4769521	11115893	6820697	3533283	4264527	4645719	5258302	5314273	1238358	5330117	5140220	4889230	5498199	6619391	4826844	4145191	8554849	5908110
fpHILIC	Positive	197.1014	3.14	unknown	915449	915747	1461463	810586	522782	763884	890684	763267	580522	915439	744983	816862	801469	1032068	971033	816764	871170	1238195	1093367
EIC	Negative	596.3579	3.57	unknown	233951	1586738	1742715	1045964	781425	1985871	1060526	1388542	1212662	2035710	1354572	2413114	1395067	826413	1638287	2173704	2054710	977052	226948
EIC	Negative	331.1919	2.17	unknown	5806725	3548670	616																

EIC	Negative	352.2213	1.78	unknown	410375	170801	286131	44778	57093	99835	99392	78939	91000	398460	159509	194626	151613	159441	102916	172834	159205	0	177609
fpHILIC	Negative	465.3042	0.34	unknown	14548842	11850517	14316771	11402863	11475429	7275297	6942948	10185777	10834840	13573942	10208086	11330406	8703099	15284959	14756198	13506718	11039811	15458611	12425493
EIC	Negative	463.2080	5.66	unknown	460895	345292	578519	381587	312647	281976	329209	410719	356394	475532	367988	373216	489081	356290	332723	488899	473574	609305	527691
EIC	Negative	315.1967	3.62	unknown	15516278	10734086	27972466	16676917	5081582	7956736	13260849	9693171	6196153	13308006	13466495	18730269	21136405	13506136	6481126	12377548	13476448	16308586	12096468
fpHILIC	Positive	231.1331	2.79	unknown	6995822	7139894	6000397	4038578	4174322	6112032	3482097	3126848	3512357	4978355	5412944	5356872	4092707	6949891	8317959	4264395	4658766	5999895	6143332
EIC	Negative	286.0891	0.70	unknown	25689	75625	60302	44839	33809	36558	49976	72681	33482	31546	60507	62112	64658	25535	59863	66860	60982	109266	29192
EIC	Negative	594.3426	3.10	unknown	5224935	3541869	4326624	2695906	1712083	4581376	2189480	3350364	3336905	4304860	3701640	5430882	3241717	2757471	3671186	4624803	4257462	2506334	6800082
fpHILIC	Negative	217.1076	0.40	unknown	652503	801612	366897	0	302648	785208	0	314058	218401	535238	47782	652971	0	1146081	988383	129113	239445	266330	712443
EIC	Negative	297.2074	5.11	unknown	558749	216571	597372	369702	127555	192750	286786	287941	276296	302245	261566	470741	358367	321082	216178	230909	379457	598956	263703
EIC	Negative	631.2416	2.38	unknown	184619	111711	295653	385291	103546	55128	150738	122998	136490	166037	137971	144863	180363	84518	85271	173347	114616	350728	97096
fpHILIC	Positive	91.0588	3.33	unknown	1835877	2186132	1479488	1279489	1265591	1718722	1312747	1304319	1335974	1743952	1901452	1840395	1888632	2238586	2673734	1952959	1643164	1877655	1872018
EIC	Negative	396.2463	3.32	unknown	518991	239040	607323	724308	155062	156125	250956	311996	216731	394397	252706	343142	346864	244828	228983	318738	361614	434452	231814
EIC	Negative	316.1998	3.62	unknown	3431782	2427397	6235827	3593001	1087996	1728641	2961773	2149572	1338547	2900469	2982196	4012671	4621015	3026159	1476526	2755337	2948390	3569426	2653276
EIC	Negative	257.1760	3.23	unknown	826728	441523	993379	824818	273785	349277	453799	453414	280047	634121	429311	736009	764572	472715	505549	562430	472949	641704	433051
EIC	Negative	362.1978	4.14	unknown	401402	319914	532501	336200	294599	212483	266245	232681	213218	253348	261505	234218	256567	213395	252937	378139	411013	473429	246279
EIC	Negative	262.0687	0.56	unknown	103397	88550	117842	78211	65643	62160	60240	60966	62160	92595	57736	82651	67433	53686	87725	66149	76762	148128	83575
fpHILIC	Positive	299.2002	0.38	unknown	485363	441055	781684	529837	215809	221928	414964	226973	328905	312338	426673	582933	483885	314062	291061	407687	462501	359730	151801
fpHILIC	Negative	245.0931	1.07	unknown	5153748	3281992	4144338	5108986	2877553	2911032	3388431	4017551	2158194	3823472	3468141	3175663	2664779	3624911	5685609	5368348	2998158	5243213	2906686
EIC	Negative	383.1477	3.52	unknown	1030221	1006686	1226322	1022871	315734	532519	628800	467052	474711	557844	802828	1303889	1102279	640262	778413	870436	605998	625073	618861
fpHILIC	Negative	164.0386	2.96	unknown	2165568	1338649	2306873	918782	1794910	2576285	1734137	1709798	2343038	3052530	3035701	1748150	5628061	3638523	1794666	2536740	2349137	4376514	
fpHILIC	Positive	149.0265	2.97	unknown	750258	640967	406668	198790	388524	538667	399919	397455	435645	279164	434681	470666	381793	1299216	997770	279836	504853	489607	854672
fpHILIC	Positive	166.0526	2.98	unknown	24710502	22171280	16290550	7041184	13576360	21062820	12701570	11101663	16263117	12703321	13518002	19487796	11918234	40846680	29325310	12631277	18923036	17865800	29430894
fpHILIC	Positive	90.0554	3.33	unknown	55668472	67962784	44409136	39852328	38119412	53567964	38800588	37774268	37454852	49223302	53441928	56729648	51167140	62142264	82118528	55359716	47366012	56257200	58662368
EIC	Negative	364.2133	2.78	unknown	258400	134657	257947	80664	121434	190546	147862	199546	189128	186213	155335	164827	142649	141739	107848	126463	323663	330855	182494
EIC	Negative	348.1904	2.46	unknown	822874	415115	963550	592756	233094	164423	410225	384185	237308	521448	305043	471700	412752	335253	422879	424413	339737	564541	320957
fpHILIC	Positive	105.0563	2.46	unknown	561395	538489	454267	178600	268760	427825	258762	236627	300707	277207	412039	362660	339749	666349	469256	339275	311553	393506	652415
EIC	Negative	297.1863	5.49	unknown	1639192	651412	1960740	936956	768075	491758	735988	591468	613741	897329	921081	1028552	1278686	781082	734887	1256446	367992	1018710	1270128
fpHILIC	Positive	120.0900	2.70	unknown	667122	1087283	793044	582611	679726	829902	764536	531542	583458	842571	1044057	939742	794772	1159799	1414387	853849	821177	689571	1143711
EIC	Negative	557.3835	4.07	unknown	62083	34063	129986	251634	44520	21199	61780	26564	70915	87383	57021	66558	76684	0	84280	73410	137914	31558	
fpHILIC	Negative	577.3080	0.80	unknown	227677	216794	235054	109301	198573	173817	265877	176453	139318	148376	228165	223979	137484	187434	214357	0	259020	668386	245735
EIC	Negative	277.1807	2.33	unknown	0	90144	171252	286583	33319	62463	44622	58727	36228	147948	140024	279465	95635	65078	82995	82960	92173	22090	62279
fpHILIC	Positive	134.1059	2.30	unknown	818616	799555	661071	568659	724140	843094	862895	172148	613866	481687	772636	777282	713335	972586	1809451	654824	581849	510671	114123
EIC	Negative	406.1995	2.31	unknown	216505	415627	227722	305733	187521	250003	351946	243126	279621	855568	371939	572322	540403	417271	430838	379055	411017	362996	330410
fpHILIC	Positive	394.0711	2.97	unknown	295047	332601	525669	273880	207978	132529	179533	301293	262853	389917	263414	231592	218802	298180	342519	208691	323011	407007	298390
EIC	Negative	359.2213	5.65	unknown	838855	595750	1000319	611420	489504	516442	580824	574349	521999	645974	880112	548538	707656	496513	505020	707755	748611	1114743	834100
EIC	Negative	381.1467	2.31	unknown	963304	631784	837594	695884	222237	361851	474833	423150	426559	613446	528271	839167	688797	576875	625857	529294	565907	545991	514539
EIC	Negative	508.2275	1.33	unknown	1210299	543161	296458	535102	433198	581492	0	323247	323247	715586	399158	570936	525520	543886	533988	735141	818858	0	497756
EIC	Negative	371.1996	3.32	unknown	146145	62381	170887	238185	43064	52164	70404	97668	65512	127802	67803	85604	87259	59528	61470	124945	106439	128946	57874
EIC	Negative	243.1601	3.46	unknown	57177	84746	84114	42542	78512	81271	47085	60758	42320	70400	52621	74027	67779	55423	70920	100885	50340	133901	96171
EIC	Negative	411.1844	3.62	unknown	551267	418177	1032179	640888	182252	325027	487505	364086	261492	430982	498285	753417	843227	549684	261224	479742	512663	626552	490563
fpHILIC	Negative	74.0247	3.17	unknown	534545	926038	606094	470788	523236	689233	624266	510213	580800	505821	1224989	964115	1118443	1038094	1038094	975272	758283	606515	905617
fpHILIC	Negative	118.1029	1.64	unknown	1179071	36099700	17843088	18025330	127929318	0	23934602	13328595	29917450	18858536	26152116	26157310	23282960	23829958	31139520	30608575	21244700	18128276	19267592
EIC	Negative	266.8039	0.52	unknown	2302886	561549	1794888	1195783	962931	935918	645241	680073	559793	3931659	557943	856764	638581	1435559	731918	1058860	462141	871394	2895362
EIC	Negative	316.1633	3.49	unknown	58780	59565	72715	68667	24604	18970	24472	22222	13995	33035	30045	43088	31606	7454	36517	56508	26644	11855	209970
EIC	Negative	343.0446	0.69	unknown	67109	138899	141058	102341	73802	74868	88020	116160	70163	84761	113240	117228	132033	63606	113159	127155	120957	181292	69669
EIC	Negative	503.2845	4.93	unknown	3254720	6222376	3887451	0	6300551	0	5610891	0	0	0	4574587	0	3176987	0	4987060	0	4940611	3080177	4419638
EIC	Negative	255.1444	2.67	unknown	4562135	7624035	4301495	5552380	4985860	534470	5131374	2978629	2399058	4057136	4220684	4483646	1367463	6233072	6300538	8769911	917664	3686337	3781391
fpHILIC	Negative	580.3256	0.60	unknown	57012828	62773876	65509536	48844288	0	58530432	54542788	44727256	48791196	63411580	0	54350132	67691784	52455724	0	53575556	5156		

fpHILIC	Positive	292.1486	2.70	unknown	514994	531969	637623	616807	426861	570625	313299	414777	214155	508332	593064	492806	433985	593695	687518	632032	386310	598821	579934
EIC	Negative	300.2052	5.65	unknown	9028866	6472232	11325960	6888062	5543756	5622327	6286150	6757603	6190260	7114101	6851752	6560993	8667847	6004670	5667299	8582242	8796570	12325333	9843256
EIC	Negative	259.6074	2.14	unknown	355931	976075	486003	52522	499285	619385	578990	523175	326434	273311	601527	6599907	4193805	1890613	1252535	700073	486557	1595354	7541625
EIC	Negative	643.3464	3.27	unknown	292815	302343	171437	188460	135965	316919	152052	147520	309846	273448	245991	350743	257049	128475	234196	419304	386719	122860	418030
fpHILIC	Negative	91.0551	0.52	unknown	908954	659361	681430	148161	317428	676948	388124	203901	319885	571028	513185	631583	439426	1031649	936416	355927	423595	500623	620772
fpHILIC	Positive	393.1673	2.97	unknown	1719068	835989	1048659	529799	700050	676662	366105	1401733	832256	1335306	464577	548849	521528	2449447	1766739	469448	865862	1645948	1174000
EIC	Negative	351.2179	1.79	unknown	1820465	762702	1361496	327824	262302	470547	484061	283994	381261	1768292	721691	885972	671779	713155	456515	818516	705691	0	824248
EIC	Negative	306.1773	2.22	unknown	553690	302347	431178	407437	111934	165382	228178	199501	166944	320389	177704	380012	331767	237548	236793	293789	238777	318762	211559
EIC	Negative	299.2019	5.65	unknown	41033974	29618836	53336445	31703879	25321600	25479531	28629071	30931264	26897608	33083752	31380743	29855725	39288400	27435060	25907008	39845383	40019635	55914068	44831466
EIC	Negative	362.1978	3.76	unknown	522358	491968	1083930	498546	348285	230427	296511	233033	185961	286405	371890	321966	236120	219636	307203	437233	407635	558191	219450
EIC	Negative	405.1922	2.31	unknown	914962	1609966	818161	1296335	786579	1053914	1366230	725400	1286294	1276754	1506050	2375536	2091688	1712656	1796061	1503550	1677801	1421179	1385887
fpHILIC	Negative	246.0969	1.07	unknown	689175	433470	593247	721954	396705	380891	453890	521345	282323	538828	473091	435724	326538	543637	751548	700277	456074	748681	379892
EIC	Negative	316.1998	2.91	unknown	66505910	44173621	84795032	64701862	26376957	24018790	40899243	27085406	27744585	63389361	45382700	56570830	48826544	46707070	38361687	51501217	51276979	43852895	33158736
EIC	Negative	313.1815	3.38	unknown	425761	1519172	1078373	1158284	1094539	352025	285420	511521	413252	412384	511506	448742	419382	607211	1098443	1703214	633432	287762	245167
EIC	Negative	391.2134	2.05	unknown	6512031	3864239	7456786	4217550	2033329	2443378	2888960	1530501	1349595	4412344	2604405	2808485	2036997	2559098	2915848	4016836	2859463	2465237	3056613
fpHILIC	Positive	107.0534	3.61	unknown	684605	505476	565793	368711	366433	469232	388101	521438	439595	539202	452148	514622	451695	520962	819701	525921	489585	400106	609527
EIC	Negative	303.1518	3.52	unknown	299940	266024	357578	322069	88164	148421	184517	137857	118140	179863	201035	383207	321540	200002	217688	250109	178243	211110	156008
EIC	Negative	595.3458	2.36	unknown	1355594	800665	1146332	774377	377717	1035584	499401	173214	1336646	1336646	815412	1279859	668993	552313	801331	1111285	1033419	799240	1575259
EIC	Negative	270.7981	0.52	unknown	2333292	630677	1961096	1251404	992306	995391	673044	559310	1072067	3457821	620108	483737	684221	1481895	695075	1132401	732100	853277	3071160
EIC	Positive	315.1967	2.91	unknown	305203592	202280964	384623799	293705531	119500671	109388359	186701809	122551384	125670487	289042175	209664515	257723055	223467150	211930706	175028041	234140018	235001105	18987724	150042920
EIC	Negative	311.1861	3.72	unknown	193297	116050	245235	131216	69311	109217	136347	77053	100953	1136660	148204	246171	235699	164797	101915	163861	160378	162031	150409
EIC	Negative	516.2738	2.74	unknown	1050011	653133	951044	0	473000	965974	408927	0	683538	0	622669	726651	260825	547228	720540	798583	1207072	0	1071455
EIC	Negative	411.1799	2.18	unknown	421839	530271	401187	636884	205206	359962	413941	366061	355516	622713	208178	726521	296576	289951	139462	672978	322469	962087	725861
fpHILIC	Positive	243.1031	1.64	unknown	0	533090	243842	324063	0	337695	161155	996123	255701	442527	418022	370040	326115	108100	486943	257288	236384	233981	
fpHILIC	Positive	84.0814	5.24	unknown	5530722	7893586	7046519	4622084	5404844	6933182	5518727	3335459	4866953	5286650	7333780	9483593	7097356	7346557	10465010	8955888	6024316	5749705	7831831
EIC	Negative	392.2169	2.06	unknown	1532473	861306	1882299	10612050	415030	5017125	652753	338377	366790	893593	579169	812824	627039	664945	700426	797677	660486	660813	593739
EIC	Negative	345.1711	2.31	unknown	21195100	36357254	17303411	28953113	15739835	23588875	30514941	16940022	25858273	28681537	31191636	50689996	44399947	36568531	38951015	32894403	35157678	32608117	29665110
EIC	Negative	376.2209	2.91	unknown	1858919	1197178	2173928	1830249	720538	710568	684149	745833	1793548	1793548	1201961	1562446	1329559	1228937	1010115	1426477	1333333	1287192	884226
EIC	Negative	347.1869	2.46	unknown	3498304	1840765	3977461	2606614	1001089	975358	1898344	1407464	1025080	2049097	1355934	2123242	1805297	1525502	1861747	1936795	1503983	3386131	1462044
fpHILIC	Negative	74.0247	3.61	unknown	3029175	1613786	1867527	2352099	1088728	1372526	1209708	1422778	1236570	1767249	1435116	1758791	1377623	1337098	1930581	1996211	1656943	2363011	1577833
fpHILIC	Negative	117.0751	2.70	unknown	1724916	1950396	1534267	932664	1310483	1811285	1438577	948197	1096109	1266878	1677615	1790398	1468654	2428779	3073864	1672748	1466996	1378657	2348411
EIC	Negative	285.0856	0.70	unknown	182926	469595	368253	327545	225805	227176	288010	456759	186614	203917	378655	404969	404419	155232	380734	416624	399754	727684	154683
EIC	Negative	435.2030	1.14	unknown	46565	58167	44638	97287	26743	32746	48984	19769	56000	31324	48071	75332	83666	38380	50841	71353	78249	27597	49352
EIC	Negative	356.1540	2.53	unknown	582576	305307	697990	482129	315749	417224	402774	471530	248568	717617	456320	553873	503907	618711	625412	512260	605816	566219	483531
EIC	Negative	315.1602	3.36	unknown	469816	601169	438873	465149	265245	319783	276887	420401	317124	276487	350084	635704	595721	430095	594084	635517	431068	382027	365188
fpHILIC	Negative	180.0336	0.56	unknown	507612	277313	454060	397529	340899	479406	374981	199059	429953	180182	367547	384653	525537	358825	304449	731341	461041	739846	151556
EIC	Negative	251.1269	2.75	unknown	96467	298478	43352	507956	242103	100867	76796	0	42853	180182	367547	384653	525537	358825	304449	731341	461041	739846	151556
EIC	Negative	346.1742	2.31	unknown	4601210	8149260	3665425	6571831	3488000	5218125	3688931	5653912	6624321	6919884	11163866	9896708	8136190	8526691	7298988	7782460	7208288	6661020	
fpHILIC	Positive	346.1540	2.61	unknown	688486	623890	564233	452816	504150	610825	451417	504515	610825	358161	658937	395867	692515	615587	455457	515686	596991	669610	
EIC	Negative	334.2108	2.81	unknown	324377	244526	608054	241531	175527	201268	330212	183994	197519	627174	306131	314694	305931	268988	260770	279704	371207	396027	343911
EIC	Negative	311.1657	3.47	unknown	98669	111435	156674	169710	65442	86194	62774	83540	123236	83121	39450	115236	98129	122392	98902	70216	95512		
EIC	Negative	388.7124	0.52	unknown	487399	145363	574361	296678	223558	274300	123652	28337	305161	774284	106907	95695	144450	226438	151295	295274	118171	226052	652886
fpHILIC	Negative	147.0493	3.66	unknown	1553566	844769	722765	841154	536450	1018369	494737	607622	762194	483185	792032	624460	613185	837729	1009252	1048281	1276542	825610	
EIC	Negative	594.3426	3.00	unknown	4230798	2922281	3168885	2143428	1246225	3882251	1640409	2630442	2668346	3858636	3010371	4516623	2665642	2059635	2921130	3992040	3631008	2109461	5600025
EIC	Negative	316.1999	2.26	unknown	0	270813	0	318806	299246	281928	0	0	0	0	353853	385843	146503	349417	0	322941	0	207307	
fpHILIC	Negative	146.0459	3.67	unknown	28093212	13839049	12876397	14339232	9528889	17244656	9499051	11109562	11271459	14261254	8448241	14964627	11139966	11495973	15195157	17870262	18641996	22417784	14720120
fpHILIC	Positive	87.1003	2.31	unknown	757829	1049626	610001	231107	674872	719052	563930	0	524053	524285	166162	918562	665418	888540	1701738	648939	451634	177815	785302
EIC	Negative	395.1897	5.65	unknown	1489391	1109253	1983105	1106558	963683	9													

EIC	Negative	384.7182	0.52	unknown	959013	218263	1090168	641837	337434	506364	315798	112144	505036	1534107	258272	261375	317869	290531	303266	541474	170600	458417	1266033
EIC	Negative	397.1322	3.52	unknown	322527	320571	391214	318792	91709	168114	190256	133342	142099	175810	238484	433173	359800	197503	248228	284021	197772	197307	193049
EIC	Negative	327.2545	5.91	unknown	381162	187798	676872	419080	87727	192845	91837	150870	187889	168116	154412	397035	346255	170036	318341	246286	260628	341861	101233
fpHILIC	Negative	222.0772	1.66	unknown	0	3111345	4623249	5104309	1692394	2867389	1549584	3241383	1206213	5440330	1778183	1630095	1636285	3198443	4271205	2323171	2349419	5247539	2128823
fpHILIC	Negative	328.7566	0.52	unknown	1250012	330969	916227	927489	431900	670591	422608	201112	516204	1961005	398309	313002	494886	496640	401991	482423	298728	298728	1656853
EIC	Negative	301.2082	5.65	unknown	1106013	804885	1400539	821287	647476	690456	755076	785038	731540	874311	842272	767671	1026436	665088	704001	1055519	1133711	1506620	1187288
EIC	Negative	478.2942	4.47	unknown	0	4271364	0	0	0	0	0	0	2260376	0	0	0	0	0	0	0	0	3499686	0
fpHILIC	Negative	88.0405	3.35	unknown	13390293	14754238	9503386	6698962	8741776	12033700	8270515	6776288	9334667	9056281	10723665	12722251	11135240	14702920	19016698	14435862	10645272	13999637	11852456
fpHILIC	Positive	168.0487	2.97	unknown	1067044	1106046	910003	359574	649975	974130	534156	432327	708462	640623	721075	832365	494337	1690789	1378713	688389	844491	834878	1366623
fpHILIC	Negative	345.1717	0.43	unknown	2099654	2163273	2234216	2380885	948853	1348540	1492750	985430	1443236	1400261	1771266	2799886	2968080	1825513	1945434	1821123	2196617	1897181	1791543
EIC	Negative	302.1481	3.52	unknown	2278188	1998559	2666157	2134726	616798	1114465	1277521	891626	897467	1187389	1570924	2885567	2338914	1358316	1635099	1843711	1368570	1344437	1255523
fpHILIC	Positive	121.0644	2.95	unknown	473385	375833	492411	327600	284472	305073	212667	295149	340067	354359	268421	318310	336041	314262	477988	340192	423462	637119	355358
fpHILIC	Negative	142.0510	1.66	unknown	0	997823	725531	614364	827316	0	834080	495814	438214	604805	1132045	1052293	747819	1186795	901503	1087300	624155	665775	756394
fpHILIC	Negative	219.1068	1.64	unknown	0	3796944	1845689	1909446	1612076	0	1989452	1467439	2951579	1899377	2897564	2815153	2239618	2326998	3101475	3566888	2125063	1836008	1865776
fpHILIC	Positive	133.1049	2.30	unknown	14245406	13383800	11020977	6252206	9255211	13513545	10759890	4267698	11059766	9043719	14171335	13076236	10877273	19419616	31219054	11916366	10041112	6989872	15919696
EIC	Negative	585.4164	3.76	unknown	63772	29998	176983	119789	0	29859	35851	46830	10724	151383	31571	36010	18281	16931	11003	19528	36436	66550	58539
fpHILIC	Positive	308.1141	3.18	unknown	634696	751802	477982	472165	439470	550557	445950	398054	499465	471281	722749	788638	709297	856165	910745	684612	639607	512355	891034
EIC	Negative	642.3422	3.02	unknown	814548	1464270	547539	852465	635820	1243727	722609	511826	1203362	979063	1264546	1560115	1335864	858266	1152663	1831848	1457373	568432	1704146
EIC	Negative	236.0651	0.47	unknown	114965	65023	84728	64274	32343	60746	32894	31129	57963	9871	35874	76660	50250	60133	73596	66261	34522	86848	74396
EIC	Negative	275.1656	2.55	unknown	1182164	632953	1081043	945793	346959	348115	558568	569557	336405	638706	669531	875413	901244	548800	634896	644087	759346	665609	666527
EIC	Negative	313.1197	1.69	unknown	763626	556394	506252	1051816	454877	324536	481955	607134	385764	864601	594925	691711	633959	397156	407140	831366	646459	1257812	384082
EIC	Negative	495.1973	2.24	unknown	414634	104062	367900	627900	316771	46279	29693	71804	194013	626673	47115	95685	59663	75685	59703	68220	68215	344922	81105
EIC	Negative	329.1761	3.30	unknown	768123	438561	1092974	730888	217200	351057	424648	377811	244589	596800	562275	760995	898215	509174	379681	497580	557115	618045	475506
EIC	Negative	562.3144	2.30	unknown	180211	0	1168110	923113	0	0	0	493577	0	701554	0	0	0	0	0	0	0	773014	0
EIC	Negative	397.2001	4.03	unknown	1020648	477328	1745215	883345	317223	405492	623779	548890	584292	759903	606487	644609	863141	562003	299619	673380	712918	823387	1323938
fpHILIC	Positive	151.0615	2.46	unknown	16125790	17418898	13467339	7027089	8575195	14006917	9295621	8945233	9506387	9871456	1253959	14714678	11341183	24229104	18735154	11448090	12776681	14922112	21266850
EIC	Negative	379.1946	2.07	unknown	431509	268360	632805	1681378	65540	75651	140655	61925	112912	898396	402994	107998	0	130849	256643	33432	230485	66773	0
EIC	Negative	446.6708	0.52	unknown	557003	101725	720351	208275	256926	146125	0	310873	0	875985	130657	110863	166540	93404	98522	278033	95700	224712	754416
EIC	Negative	512.2689	1.26	unknown	1021202	33913	9189348	5384922	88752	53184	45588	9816737	128044	840795	89858	50476	57084	137340	133170	75450	74770	15592876	80533
EIC	Negative	313.1196	1.84	unknown	3861145	2062800	983843	84318	1858301	453828	1773845	553342	1426044	304197	2592231	2774187	2552387	471000	1504715	3862742	2624944	0	1532898
fpHILIC	Negative	206.0821	0.74	unknown	1721701	714152	952486	700048	492412	969215	511573	538528	552975	937179	788548	932254	621046	1291936	1723331	889013	643899	939084	635450
EIC	Negative	367.2439	6.39	unknown	5150994	2400854	6449790	0	1592782	3645664	1707454	503106	0	3973069	3146991	2707873	1336298	3626454	3317328	1873800	3306120	1666877	1577708
EIC	Negative	347.1869	2.17	unknown	1453395	1167655	1261366	1151945	302601	577889	624913	421916	448976	1210717	364358	1015113	711199	690165	502809	816167	588348	1032585	806194
fpHILIC	Positive	117.0659	3.12	unknown	1968669	1711819	2265795	2977909	1159329	1578295	1911683	1740821	1278644	2569811	1759956	1575659	2132812	1712391	1580207	2621338	2615456	2995290	2281800
fpHILIC	Negative	135.0273	2.46	unknown	1922248	1987569	1596364	785665	988385	1394121	987891	1121061	1438559	1121061	1491411	1680150	1141440	2751645	2062520	1021274	1251506	1529703	2520013
EIC	Negative	507.2243	0.91	unknown	103190	51870	89491	35799	18691	23408	67104	27771	43082	69193	37072	64918	49368	49275	50279	67986	80086	39698	46111
fpHILIC	Negative	207.0858	0.58	unknown	1507053	850993	996491	522613	365907	1275137	612687	665284	960324	1026682	995565	833439	1384349	1613703	1026875	655888	1192467	931130	0
fpHILIC	Positive	150.0481	2.46	unknown	2425476	2267209	1987422	963678	971993	2007156	1452256	1001336	1435995	1257171	1836320	2221220	1590581	3558360	2677564	1621701	1592966	2167538	2786830
EIC	Negative	336.2266	2.06	unknown	677170	233131	779399	397172	100827	141391	167804	148329	903821	232364	254769	338237	323674	193213	237171	323674	338237	217966	312271
EIC	Negative	492.2743	3.15	unknown	614278	273631	465153	245470	119956	388449	127511	292203	184998	420997	235737	329607	184703	282096	346189	191430	357641	315228	549582
fpHILIC	Positive	388.1803	3.54	unknown	126163	2601891	1443698	173542	413855	235895	926436	513855	419234	47983	241347	202081	1957953	192240	156111	523468	216246	4542514	0
EIC	Negative	258.1799	3.23	unknown	121400	74654	151697	136413	37923	51506	74692	61808	44396	97646	62071	114104	115067	63703	91580	92438	75632	102638	66154
EIC	Negative	362.2373	3.50	unknown	575771	0	481185	0	0	345732	553806	0	0	388721	494553	614576	44842	0	485504	0	743861	196341	
EIC	Negative	643.3459	3.01	unknown	277861	517997	172937	277795	221147	441885	232914	199804	417778	356878	440759	550650	475563	314878	415401	635893	528934	224100	594626
EIC	Negative	491.4381	3.82	unknown	715531	576043	816682	326013	416248	403092	402033	416248	403092	395012	614759	758470	593278	867103	717923	565991	569520	719188	361476
EIC	Negative	261.0411	0.69	unknown	309284	575262	513350	343379	284211	302763	330916	323257	247546	370062	438139	446769	488095	344020	472235	553806	421492	596097	316935
EIC	Negative	263.0378	0.69	unknown	102424	180622	160702	109943	89386	97649	109419	100349	85254	114141	142634	142058	167080	111720	157748	180912	132080	190896	102914
fpHILIC	Positive	133.0314	2.46	unknown	41567892	42036852	34255160	16582389	21207120	34208232	23639334	20236146	23181256	23986258	32374096	37427686	28741206	59253740	45145188	26905014	28887524	34938064	58540068
EIC	Negative	327.1605	4.23	unknown	527448	725410	612282	867485	276720	278367	337410</												

fpHILIC	Positive	153.0567	2.46	unknown	812444	840836	643140	334156	481609	668183	461161	437342	494442	504704	596830	757584	576437	1323984	1022791	665235	651460	721630	1054752
EIC	Negative	491.3379	2.99	unknown	1590198	1689786	1612088	1201103	887744	1168696	1063485	1020122	903609	2438156	1643418	1888719	1159125	1100794	2515157	2188184	1103932	1519900	843456
EIC	Negative	492.3419	2.99	unknown	523294	540317	529405	371977	317825	403470	350585	1020122	903609	772408	540199	583857	373252	367606	815214	709095	399465	473824	282385
EIC	Negative	291.0700	2.85	unknown	8453470	10213803	9900042	2876951	7107255	6434407	9402505	6198033	2721048	8747647	11962118	10683457	7486333	16455828	15135460	5721777	7020670	8314395	15148763
EIC	Negative	318.2063	2.91	unknown	973957	617316	1137629	788566	330954	279570	498887	328115	363069	850153	511712	778648	631589	718352	470501	680673	687945	622746	452002
EIC	Negative	292.0732	2.85	unknown	1413126	1795724	1629051	495512	1216820	1212594	1640082	1003311	477885	1500663	2045657	1818068	1265135	2786464	2587586	982291	1208345	1413133	2597740
EIC	Negative	282.0733	4.35	unknown	260992	64075	165622	748419	47182	59029	69251	105255	178642	198878	150367	218651	164853	0	66455	236819	119004	283046	40363
fpHILIC	Positive	312.1102	2.50	unknown	570093	661868	492071	273472	284288	550660	436390	372116	341880	472766	460049	501901	409283	922870	789824	368509	520089	674912	870226
EIC	Negative	413.1739	2.91	unknown	1220367	1054777	1543953	1844396	939703	963109	1710501	1160645	1329647	2390686	1934268	2411444	2168216	2100337	1718498	2334814	2297355	1978436	1582124
EIC	Negative	639.4113	3.82	unknown	470391	0	504476	418334	12095	0	392085	0	514589	35224	27039	0	0	0	0	19083	0	637238	0
EIC	Negative	319.1219	2.38	unknown	161776	51722	96657	26803	33074	61250	23181	41998	33879	83020	46011	56539	49312	115849	89880	35410	61255	61030	66615
EIC	Negative	375.1200	1.11	unknown	39086	23446	41280	67236	25696	13038	25393	41674	17680	20360	34257	42696	58375	19177	26345	54167	36944	61517	21928
EIC	Negative	314.1230	1.85	unknown	594592	317394	146837	0	275393	172029	266901	0	223685	0	425914	422476	418271	248865	248046	611649	416186	0	250620
fpHILIC	Positive	389.1837	3.54	unknown	0	452263	225847	0	33220	145188	48568	309320	0	561897	0	0	0	347992	0	60194	107645	0	705309
EIC	Negative	414.1808	2.91	unknown	237603	215002	345318	410772	205071	186366	375806	288314	275841	150324	470728	544163	464795	458549	402016	496787	497201	406828	367710
EIC	Negative	323.1058	1.08	unknown	57575	50407	144655	74494	17899	60895	70200	107064	54025	150324	72210	67232	161288	114561	106131	73998	116047	167898	129771
EIC	Negative	348.1907	1.38	unknown	493195	396910	0	131124	242657	250182	0	137593	0	329090	437366	386233	294554	310113	430054	270555	0	259238	0
EIC	Negative	332.1952	2.24	unknown	12801968	4605775	13261539	7757880	1996767	1904714	4089429	3426634	2318384	8848340	3840937	5835300	5364093	4146316	3734459	4170788	2524834	8155786	2863105
EIC	Negative	302.1841	2.63	unknown	208001	220364	552072	287755	138421	200653	272972	0	110383	261560	253501	431873	337071	300603	260584	322564	347392	73037	177285
EIC	Negative	483.2725	6.19	unknown	2098376	2858716	2446926	2010470	2268764	1598948	1949249	2273202	716719	1919679	2994662	2372633	1658626	4153109	4191456	1313955	2480147	3359680	3159293
fpHILIC	Negative	250.0929	3.17	unknown	299327	536849	397021	276155	224913	406943	393206	226149	269951	484205	375764	368970	391546	380636	702451	443884	437340	449262	459103
EIC	Negative	595.3822	4.13	unknown	359578	171840	245027	353301	203585	142546	101256	749150	164781	872785	710703	264932	231083	321931	4702712	2117581	518091	793813	319379
fpHILIC	Negative	263.1138	0.95	unknown	1819144	905301	2199687	720237	709435	1826762	1013222	1655550	675705	1361400	1407178	2222267	1427479	1354699	382453	2331483	452929	1293700	581090
EIC	Negative	330.1794	3.12	unknown	738218	858749	581626	755147	266333	903204	393855	176583	337999	532521	821435	1302687	1329282	808084	929833	655609	171257	449779	656756
fpHILIC	Positive	134.0349	2.46	unknown	2052056	2291992	1690819	942003	1068430	1870734	1187547	958852	1253033	1359670	1680310	1776904	1371508	3099548	2633093	1501983	1489162	1721046	3089916
EIC	Negative	329.1761	3.24	unknown	417483	630202	565259	892121	168784	132479	140597	265826	93028	360748	278878	209318	182240	100564	303143	433740	170007	157054	252471
fpHILIC	Negative	438.2166	1.64	unknown	0	622207	217581	241380	263767	0	193987	126829	486363	226722	442790	432214	322476	346392	621105	532336	265273	155415	186829
fpHILIC	Negative	329.2324	0.48	unknown	711523	190838	602973	111458	139786	434674	366871	158849	345248	398972	120382	281669	202361	262475	107611	1219164	307551	416193	326598
EIC	Negative	492.3425	3.82	unknown	217318	181650	224453	98203	121890	132206	125685	119689	88578	278429	202183	247986	184788	276689	324243	181639	192812	237014	123505
EIC	Negative	331.1919	2.24	unknown	57488586	20796503	60682694	34192863	8924176	8507416	18379029	15122975	10362656	39721957	17431980	26393464	23815838	18585788	16884552	18589865	15826769	36629970	12908238
EIC	Negative	273.2074	2.43	unknown	101296	33303	139301	91163	57198	61309	27236	100186	24663	101502	33586	33746	32999	22813	38800	223591	46576	107686	29629
EIC	Negative	374.1442	1.82	unknown	196496	86186	152366	0	100080	48212	52308	0	52955	0	100969	117684	107013	47357	74619	157015	106883	0	79857
EIC	Negative	594.3424	2.27	unknown	481929	377774	482696	343854	213477	487466	237818	364480	405101	609797	419914	623942	309244	292041	411258	675005	521083	362188	852726
EIC	Negative	313.1816	3.61	unknown	346057	357841	932549	1250208	203180	152158	288411	316328	321752	275420	224956	293269	303466	209713	142585	288827	276834	263322	1149626
fpHILIC	Positive	291.0695	0.37	unknown	6067893	3939994	9044914	3373955	2645363	2423552	3858733	4255118	1627502	5118732	4422731	4708580	3336328	5858170	5720192	16217023	2909359	6982773	6729107
EIC	Negative	500.6353	0.52	unknown	692497	122373	820668	452223	214648	354358	150820	0	470568	1183343	149780	142887	203866	0	135320	338886	102613	301162	916129
fpHILIC	Positive	152.0622	2.46	unknown	1099288	1099422	951578	437273	617791	876121	621160	629947	621600	9391547	1017900	805154	1659321	1378839	839669	838673	964671	169189	0
EIC	Negative	347.1869	1.38	unknown	1841990	1821449	0	608851	1085443	1114596	0	618953	0	1525180	2032555	1714600	1323432	1462495	1812992	1273132	0	1138253	0
EIC	Negative	371.2017	2.52	unknown	497358	217640	422670	397739	113981	110956	111278	485328	205797	282512	202720	242804	228944	161634	209712	289122	215972	270217	202075
EIC	Negative	427.1796	2.46	unknown	375812	150615	358182	437236	57557	110366	113799	86836	82799	545814	184497	201217	213175	168841	168550	151188	173108	67849	188484
EIC	Negative	409.1691	2.88	unknown	405241	389316	397183	426798	182986	138599	239775	310179	204598	285923	268324	265012	308045	263628	383217	308045	263628	383217	254318
EIC	Negative	328.2574	5.91	unknown	97890	46042	132543	83771	23579	43165	37896	18450	65980	39758	40210	81593	70388	37874	61197	56114	71215	83408	41907
EIC	Negative	370.0164	0.50	unknown	418761	221858	208414	274037	130998	135082	138103	139102	318988	148437	179517	127637	48827	142715	330593	274027	197397	240030	0
EIC	Negative	353.1669	0.85	unknown	51672	41794	507703	16444	40847	58479	89074	49220	73851	120975	72349	101536	74176	109494	115700	26558	309975	41982	23867
EIC	Negative	316.1999	4.02	unknown	3523306	1617225	7088185	4045862	1017640	1346772	2245407	2058955	1684573	2746849	2186417	2554277	3392531	1987689	958659	2648734	2584251	3189978	4738687
fpHILIC	Negative	311.1122	2.43	unknown	589040	987082	488722	391174	533563	661491	700499	624749	714417	637258	1385532	1464207	735661	1446732	1027690	1273300	652342	860266	1568999
EIC	Negative	392.1070	0.47	unknown	526273	791178	460496	309804	282930	625715	356126	189999	244939	393361	634978	758479	690874	466759	982033	722271	441180	413399	270268
fpHILIC	Positive	215.0695	3.30	unknown	758461	665809	351820	327188	287913	422112	217883	135843	290530	299320	343789	475433	382310	366971	511029	506340	264736	542889	430431
EIC	Negative	317.1757	1.82	unknown	260925	101172	284850	0	20670	62667	50469	0	24968	0	44532	80563	62328	56076	72203	68372	5074		

EIC	Negative	332.1952	2.57	unknown	678088	751925	713821	475104	289811	287810	411782	113813	247135	1009077	786932	886274	591511	576369	355083	594427	716346	511519	138287
fpHILIC	Positive	297.1848	0.50	unknown	692761	184801	858570	401424	51301	66287	158794	140996	156789	338871	96439	220531	230568	115769	166277	83176	186174	378495	171228
EIC	Negative	241.0873	2.50	unknown	156770	111839	196385	107992	58247	141524	93579	95865	25098	143229	127643	212431	228464	136059	56234	163831	231756	441308	163492
EIC	Negative	604.3629	4.32	unknown	6615367	8078800	6352122	6997652	8239092	1630522	1176116	7673590	1032689	765693	7906507	1004661	8088664	7022885	7979388	8206085	9106481	764615	7950123
EIC	Negative	362.1979	2.18	unknown	1509307	2541154	1845119	1414161	1061035	370140	979976	572089	1036666	1286456	626902	1553579	910609	632450	1065233	2122905	1516466	1579292	637363
EIC	Negative	506.6292	0.52	unknown	663519	97208	733765	410739	208437	323647	145494	0	356302	1135753	136457	34966	152028	123929	138404	292169	99724	294755	955753
EIC	Negative	396.2471	2.52	unknown	617950	298742	573852	576935	127926	145484	228739	186262	175749	627133	296296	382913	355814	324510	199722	340846	282046	394489	271574
EIC	Negative	269.1762	3.81	unknown	530097	262179	565832	321685	167861	163022	305119	249648	176876	314148	258589	462403	515286	329200	236662	315357	352690	592229	323989
fpHILIC	Negative	347.1862	0.61	unknown	2140757	1108121	1632466	2510625	707604	867915	764665	735105	909411	2229096	1261594	1648246	1258968	924758	1260584	1989293	1621760	1290715	1067879
EIC	Negative	334.2108	1.80	unknown	432327	123141	283125	0	39171	29529	70860	27423	37598	438096	95404	102370	54545	94293	386517	108601	113737	0	92291
EIC	Negative	440.6790	0.52	unknown	282061	36804	332575	242050	97791	118770	31983	0	174862	484781	29775	81738	62973	0	33243	167326	40056	142480	366745
EIC	Negative	299.1653	2.99	unknown	5511847	2940737	9794825	6173154	1275353	1989662	2734594	1672650	1779063	3960767	3628947	4870494	3905599	3088958	2692748	4289608	3788619	3357501	2209133
fpHILIC	Positive	274.0890	3.15	unknown	639991	1579869	917742	633916	612691	886710	854295	613996	588857	1101125	1034786	1059433	964733	1197053	1685125	983886	1109377	1108206	1269716
EIC	Negative	332.1952	3.24	unknown	838979	475465	1160051	891887	198201	190644	307307	205189	178292	636536	295201	430156	360531	232622	263107	426516	329971	536888	313741
EIC	Negative	275.0601	2.33	unknown	71774	169797	262999	38294	94082	227254	108574	59725	72579	195865	455680	439061	199818	451061	342952	191436	132418	92968	214671
EIC	Negative	258.2426	6.54	unknown	207253	217915	158474	329650	168760	186437	197599	158994	306171	368983	406519	285063	400308	273880	231594	410331	401691	347319	377112
fpHILIC	Negative	164.0433	0.51	unknown	722660	440872	539080	381674	253895	753430	326288	182900	356435	578965	507317	571624	400843	1248778	1018973	443520	496345	582382	712530
fpHILIC	Positive	344.1849	4.83	unknown	493370	376712	193827	140629	152675	184254	165087	159370	207877	280294	206777	165603	173755	525221	788868	362891	296183	147978	320512
EIC	Negative	642.5975	0.52	unknown	275880	80483	438670	331676	165538	224011	101258	0	427383	100949	78164	122909	0	78166	172148	75646	197439	331580	
EIC	Negative	348.1904	2.68	unknown	308578	187260	375778	252909	94071	126930	168807	136575	109412	247416	158504	237804	260110	192481	287160	211208	196290	233846	179704
EIC	Negative	336.2265	2.51	unknown	13094569	6216816	11192925	11155177	2550733	2848984	5088622	3703638	3402459	11667212	5845750	8071036	7087726	6723008	4165927	6819405	5730700	8423032	5595070
EIC	Negative	398.2028	4.02	unknown	232181	107697	424094	186882	77740	150796	116521	104582	172109	145481	168487	207070	142161	85927	178193	155968	220276	292765	
EIC	Negative	501.3012	3.76	unknown	441575	42226	156999	415490	73810	188551	108844	252247	196426	449712	219251	159758	286173	31632	101441	206867	306974	817692	0
EIC	Negative	632.2962	3.10	unknown	84366	56970	97538	65655	36577	86375	34852	86346	80205	93418	109212	78271	73091	91563	120551	112011	72022	167954	
EIC	Negative	392.2172	2.43	unknown	448182	303201	471920	407785	135569	185532	329352	182065	138793	315768	235428	435915	395758	357837	360976	281071	312141	365096	379499
EIC	Negative	491.3379	2.90	unknown	2764365	2072413	2862636	1778917	2214720	3115955	1092260	1367018	939707	4780111	2896812	4722451	2908559	4717952	4184104	2319768	3420280	3604194	1741785
EIC	Negative	275.1656	2.14	unknown	1141625	905261	2651059	2112626	350968	690615	776405	498624	759096	2516863	1098194	2666536	1037201	1037681	707269	1121263	1296847	1270281	984539
EIC	Negative	348.1902	1.78	unknown	292501	96619	236142	87540	24540	40433	44905	32281	82541	382242	102442	90240	63204	78298	59934	70763	59653	0	116116
EIC	Negative	492.2327	1.93	unknown	1135930	1674452	1717524	525694	1437654	1171804	2117886	0	1159425	1143574	1607359	2243320	1976256	2238491	1881711	2625974	3692941	0	2128655
EIC	Negative	560.5912	0.52	unknown	889054	154682	1143048	629359	200582	390898	167621	0	566280	1490302	144701	123175	180501	0	181719	385297	98966	306428	1337424
EIC	Negative	335.2232	2.06	unknown	3208558	940789	3393971	1882465	401188	682408	703919	826015	711775	4205317	1077360	1062370	1069698	1350686	756339	935420	1617103	1087670	1450685
EIC	Negative	634.4110	2.91	unknown	842600	348231	1127691	669080	181982	107056	320774	142724	183171	833536	343932	473014	499038	384296	241918	449104	448580	345778	160395
EIC	Negative	296.1852	3.28	unknown	172382	0	0	0	0	97066	0	0	0	84625	0	76965	0	0	83168	0	0	0	87715
EIC	Negative	492.3420	2.90	unknown	836372	635020	828573	514073	676060	972516	303524	429411	311384	1448771	906156	1415998	889685	1500203	1338635	673778	1091950	1124903	515035
fpHILIC	Negative	172.0979	0.59	unknown	10766249	9983647	7206208	5281037	5526636	11126112	6167706	2938585	5534225	1790104	1185799	9052722	7106318	10388216	24339886	9942607	5509938	5345439	10017599
EIC	Negative	318.2157	4.89	unknown	2326293	832679	2910198	1819115	463822	339379	727578	791397	485002	3268810	1091816	936752	650567	710295	442511	1087566	1427150	1035645	960265
fpHILIC	Negative	150.0126	4.37	unknown	717313	597301	353734	508917	167862	711629	110366	287699	119822	107330	120861	63890	1808713	1206309	148348	196528	240651	674248	1480792
EIC	Negative	411.1853	4.02	unknown	298425	132979	591793	311056	92656	110035	200442	153924	123558	225154	178094	191444	286246	158412	76579	214140	220646	285186	406025
EIC	Negative	448.3515	6.54	unknown	1514345	817049	1114464	1244553	1201635	864292	1324778	1263059	1241499	1974385	2038698	1041895	1648961	1867098	3032683	2526601	1331350	1474620	2057576
EIC	Negative	335.2232	2.51	unknown	59014202	27961316	50851402	50501125	11570085	12789344	22887651	16927765	15279563	52392291	26573302	36664648	32298966	30226777	18823069	31027752	25914558	39093680	25666981
EIC	Negative	345.1711	2.46	unknown	2235302	2122511	1963752	2026742	1021542	1790684	1662403	1141449	2161355	2086468	2669193	3330146	2333259	2928090	2077097	2164089	2625343	2920254	
EIC	Negative	367.1687	2.43	unknown	278237	150594	276808	210145	92422	82647	119951	86560	63987	178894	127899	190601	165215	155618	172004	166638	138735	137724	175213
EIC	Negative	315.1602	3.49	unknown	230034	233869	325524	270922	91373	86462	114050	68367	83921	163404	126691	204601	152778	116673	155682	240050	151519	119660	120823
EIC	Negative	427.1739	2.31	unknown	490797	1205394	330747	1152354	461104	587072	887994	753664	853489	1810536	804279	1424784	1364123	983528	1221465	974404	948940	2037923	1103884
EIC	Negative	395.2441	2.52	unknown	2659770	1210226	2223060	2231245	532343	609718	923506	695299	2549396	1165092	1575968	1360929	1359201	1359201	823550	1427710	1169437	1645776	1140871
EIC	Negative	273.1495	2.64	unknown	168817	88359	185668	87352	44664	64283	99767	0	65938	103643	92772	137879	169365	114096	59272	69695	115180	143831	72928
fpHILIC	Positive	334.0916	2.49	unknown	280837	386853	189451	109867	131578	301549	199950	112685	157215	237463	306432	247243	218761	554968	414598	199290	234988	308455	447743
EIC	Negative	325.1619	0.50	unknown	288737	333447	142143	107840	155387	218304	95506	66237	156024	156221	283316	307606	254709	79514	388541	358035	152511	131892	199801
EIC	Negative	400.2190	4.14	unknown	434229	361446	385658	358456	139352	12													

fpHILIC	Negative	383.1218	2.95	unknown	648705	394655	500009	270954	236832	197734	214952	295515	254374	438305	196989	279845	245771	623637	658498	215333	314613	606044	413192
fpHILIC	Negative	316.1998	0.44	unknown	2556892	1272537	4117182	2881375	520963	689405	1065322	687881	845880	2162383	1370154	1822527	1678748	1248702	967679	1528549	1645298	1567938	1303208
EIC	Negative	407.2439	2.20	unknown	0	2121517	0	4049376	1393998	922606	2366843	0	2414100	3508462	2958079	1213691	2554852	2218908	1668811	3046200	1496269	1498817	2393224
EIC	Negative	336.2265	3.32	unknown	586711	250621	693174	569095	119432	133162	216937	224069	103939	400275	217597	281275	281534	257120	235738	288485	355617	331462	262116
EIC	Negative	628.5039	6.76	unknown	154720	133714	120677	167767	149672	121126	155581	131895	161622	254336	374310	216275	282909	342840	291445	261887	319731	149797	382116
EIC	Negative	395.1842	2.88	unknown	647453	701803	490755	562735	377386	256385	368540	318908	248051	480911	392347	497935	499432	546329	705022	674103	675614	453622	395156
EIC	Negative	335.2153	2.90	unknown	653884	299110	571626	404574	174381	0	394776	294335	305743	0	411797	503719	600354	372959	283519	454182	398008	582217	445708
EIC	Negative	507.2244	2.08	unknown	241339	145474	333067	112508	94555	149657	216458	0	126354	171408	196150	417277	398260	192980	243202	323614	266069	110356	234153
fpHILIC	Negative	305.1428	0.60	unknown	4566534	2405595	3827408	4035873	2909376	2931965	3407495	4326452	2852460	6336068	5124681	6176995	5046346	5555996	4259402	4664017	6222604	11538601	3747571
EIC	Negative	451.1516	2.24	unknown	43476	14134	182527	166097	15133	9990	40100	94512	30370	203156	31563	49209	39130	43265	35723	46447	33533	206229	30301
EIC	Negative	411.1805	3.12	unknown	402264	476210	341684	407448	138666	372899	221904	99704	150007	364312	433712	606382	563640	469988	477015	375690	425404	253204	291200
EIC	Negative	546.2809	2.55	unknown	609738	0	1022007	491032	0	0	382536	22219	253086	0	0	9685	0	0	0	0	10157	740196	0
EIC	Negative	399.2156	4.88	unknown	881828	333996	1100042	628107	168731	108922	299547	282779	190670	1227605	432012	371825	272957	282591	160126	461727	528644	386813	410771
EIC	Negative	481.2183	4.14	unknown	344207	289298	276653	246739	102187	114169	179561	108389	152882	190470	199936	298991	280787	209118	317032	275828	259849	178607	190773
EIC	Negative	442.6767	0.52	unknown	697418	159821	1009455	519466	31247	345263	235214	38999	462861	1216843	163302	146691	269012	0	163876	412367	126362	340174	1031498
EIC	Negative	313.1814	2.89	unknown	17723829	13500599	19370701	16257297	6365153	4070485	7633011	6518614	4599663	11922725	7224893	10587671	9680088	8799320	10319117	136660542	13305171	10288593	6818254
EIC	Negative	332.1952	2.41	unknown	1581371	1169700	2176411	1405518	462710	531920	918119	497802	506780	1220875	1564920	922728	1113937	1310161	1011033	1065171	984316	1075637	0
EIC	Negative	400.2189	4.28	unknown	398569	169134	409419	303500	68322	47342	117481	450569	137471	450569	213794	1936182	232316	131627	111274	165653	208502	206507	189988
EIC	Negative	314.1846	2.89	unknown	3933189	3012204	4187821	3563445	1388392	885617	1675583	1932801	1008888	2619928	1611899	2286720	2091220	1962098	2283225	2973308	2882403	2243855	1480080
EIC	Negative	347.1869	1.59	unknown	928835	428851	918421	694990	163136	208714	311326	195319	185696	532949	433346	396445	332111	352940	490251	340352	212485	366660	0
EIC	Negative	415.1206	2.91	unknown	139386	97585	196564	195753	47072	49458	79859	49460	63106	92286	189431	236177	143844	119296	110327	166667	96148	101575	66644
EIC	Negative	493.3468	2.90	unknown	134390	176788	226775	48148	137806	220708	63905	123776	85807	308988	187728	153457	291640	357724	180465	264330	252428	129436	0
fpHILIC	Negative	256.0806	3.00	unknown	362114	239552	224482	159338	279653	289775	257938	217772	56174	274660	283072	219133	175838	342885	550285	296485	361894	291630	565549
EIC	Positive	329.1761	4.71	unknown	8250871	6335363	9281332	7361538	3079908	2864187	4679138	3481954	4008401	5001494	5121459	8905134	8097420	6029255	8395595	8516619	5978987	5316056	5773969
EIC	Negative	431.2100	2.52	unknown	2188498	879841	1594725	1534141	362919	398254	694579	528463	466451	1812850	806420	1096071	987371	938488	601280	954062	776240	1478321	792603
EIC	Negative	315.1967	3.31	unknown	4734872	3994118	12148226	9287713	3101155	1603888	14204386	1437630	2116127	6026021	5753933	5892898	2390419	3538217	2623351	4284150	5724928	2638325	2913287
EIC	Negative	241.0558	0.68	unknown	73092	62359	68545	35059	40997	44023	33999	19561	44167	73510	47644	57798	63731	113483	65732	90291	52423	53562	81963
EIC	Negative	387.1805	2.10	unknown	121224	104841	40931	43041	34428	66051	100119	0	50082	47076	76515	150954	141054	78229	101837	133390	97729	55357	83857
EIC	Negative	633.4074	2.91	unknown	3904710	1824757	6026683	3620201	920682	780893	1607178	945807	719989	3825605	2011542	2828035	2231026	2130565	1409823	2616423	2324059	1969218	1050919
fpHILIC	Negative	627.4995	0.36	unknown	952949	1929736	1469361	2062511	789196	799022	964389	828775	825232	1632923	2804694	1271306	1751303	3693857	1261168	1256415	2371840	864963	2176933
EIC	Negative	249.1498	2.53	unknown	753315	43141	307241	56404	35899	41275	44968	45489	33624	79616	49362	46818	59030	59935	43706	43393	153715	72144	66777
EIC	Negative	267.1614	4.37	unknown	665420	516503	790747	294223	121005	263601	396861	341401	167196	342306	497933	655327	757502	462394	722044	543187	413288	349237	414605
EIC	Negative	361.1442	3.98	unknown	74442	217286	104126	269903	84271	18802	69133	111228	78584	76282	89447	105342	85477	101981	180703	203088	121731	106675	74143
EIC	Negative	459.1865	3.92	unknown	638768	176534	501929	1429399	45843	63530	64622	63297	63236	1196855	270587	53933	0	123762	238607	0	185017	22484	0
EIC	Negative	309.1036	0.47	unknown	422838	638308	343324	266949	45843	254727	412002	331239	312972	138616	483161	583364	562312	408288	841049	633222	370048	359166	426860
fpHILIC	Positive	363.1534	2.94	unknown	1213443	734983	1262637	515520	386331	499347	327455	408691	357968	804133	381973	373720	417536	844084	962106	434716	625471	1041286	692944
EIC	Negative	557.2967	0.95	unknown	244249	71946	260045	227511	60407	62807	55043	62807	55043	80143	87525	41714	56835	68093	45779	83660	143861	92105	111917
fpHILIC	Negative	187.0723	2.48	unknown	2590279	2603202	1720143	2002145	1209446	2147625	974350	1744907	1518503	2116532	2449133	2295106	1340031	3463562	4907559	1605101	1584373	2298443	4029348
EIC	Negative	499.2283	2.52	unknown	305126	174937	0	151054	92527	148940	0	109106	329929	169663	202404	200475	194577	128204	109106	166213	200854	159418	0
fpHILIC	Negative	351.2181	0.97	unknown	1495092	858499	1613503	1403264	311709	431756	693063	596668	536620	1301975	789318	794263	943581	691788	736734	1117120	985315	1107325	882283
EIC	Negative	524.2944	4.21	unknown	880317	703177	1342470	635614	321444	215487	639813	360125	1370886	639067	685204	900038	734655	412384	423867	988407	359762	1124636	0
EIC	Negative	417.2263	2.52	unknown	3295371	1403006	2191128	2283717	609869	659754	1165867	889023	806230	3165764	1325364	1758512	1570977	1485653	1002030	1482974	1295492	2706547	1375172
fpHILIC	Negative	73.0296	1.68	unknown	0	2908138	1998916	2695115	1708235	0	1940689	1552307	2435162	2456248	2992725	2478775	2404442	2907341	4667172	3200344	1819352	2644663	2266548
EIC	Negative	500.2049	3.21	unknown	124987	63950	108135	51165	60449	47131	50609	60877	31501	116280	67898	120498	66231	76714	53173	77406	67117	209533	72035
EIC	Negative	303.1603	2.48	unknown	214624	256982	218047	158661	95180	197576	152199	145435	110146	263250	282353	437883	441805	218706	350956	287046	239156	253330	210307
fpHILIC	Positive	191.0818	1.85	unknown	886105	0	0	285529	46587	78925	0	273101	743363	37708	35031	329403	382485	832626	127762	98008	1234628	443825	286169
EIC	Negative	545.2726	2.57	unknown	2101130	27810	3322688	1514155	24359	28577	31367	1216746	63240	824666	12204	28719	46135	44534	49007	52879	32494	2452593	31814
EIC	Negative	595.2744	2.48	unknown	179988	41834	330929	197512	36309	37549	20560	123576	59161	289406	39101	26056	50887	57489	33860	86966	57617	302339	52408
EIC	Negative	362.1975	3.63	unknown	148599	87942	503089	199227	48931	65072	81972	67214	72138	72484	52173	89672	93141	88745	33212				



EIC	Negative	266.1482	1.73	unknown	225792	211906	338964	32039	79104	152511	50656	141479	73361	218172	138473	165145	78394	540061	266034	63912	187361	122972	345127
fpHILIC	Positive	188.1390	4.89	unknown	608610	1681511	844982	750557	582034	746097	983606	646096	857372	1466991	1297926	1156658	1029522	2420338	2369755	1267222	1540805	792188	1604855
EIC	Negative	414.1986	2.24	unknown	930836	216354	807440	642038	352792	75040	243512	0	234962	686191	137584	245130	139958	171635	221878	217354	195576	875903	3040954
EIC	Negative	493.2444	3.08	unknown	665996	219692	745286	343559	103007	121698	190946	180299	80214	294179	123814	94290	336090	115128	304454	189351	154620	328326	379393
EIC	Negative	339.1361	1.32	unknown	55862	0	0	0	0	0	0	0	69371	0	0	43665	93964	102598	0	0	139142	0	0
EIC	Negative	316.2572	3.81	unknown	785681	434829	850208	455522	379525	730433	373047	290186	679871	440099	364589	626239	690636	523858	265165	1581879	1167971	1294727	613097
fpHILIC	Negative	115.0594	2.78	unknown	967624	884766	698569	334744	449243	196162	313836	396761	314815	581755	550222	610245	378005	907270	1673636	503828	513470	681914	830671
EIC	Negative	334.2109	3.04	unknown	1044303	527734	1258995	868421	196531	229557	282872	326171	163710	775671	409851	618982	434986	517890	357946	554279	507653	480706	505979
EIC	Negative	627.5000	6.76	unknown	245005	311420	261665	368251	257070	258779	292514	300253	386361	560470	683608	511737	633328	801288	628375	581907	710522	364555	711712
fpHILIC	Positive	191.0836	2.23	unknown	266816	524906	385380	211417	268055	422842	312731	272734	346755	382475	354792	493235	379928	1406658	700437	402888	471524	482292	1204279
EIC	Negative	481.3126	5.55	unknown	294438	209631	616169	122436	544116	0	176550	0	55499	0	90778	0	121589	644605	485261	0	479071	0	595894
EIC	Negative	227.1007	0.47	unknown	364991	522278	283656	210738	196198	373493	239364	132616	174807	280860	421666	535374	509565	425180	706659	533797	319701	313922	371858
EIC	Negative	376.1779	2.24	unknown	119623	144677	109623	89496	66152	21244	43263	0	61806	81228	52972	92543	84579	50359	72961	123359	108528	34748	48771
EIC	Negative	241.1556	1.52	unknown	7457609	6164595	34809275	15670420	11280370	7844997	10338987	23256634	5893934	25849287	9302933	7555219	35893832	12486696	19370552	7038325	26004970	50508467	15374320
EIC	Negative	242.1590	1.52	unknown	1073447	845962	4688577	2225857	1545501	1103100	1413113	3296123	813330	3581751	1331828	1042265	5004859	1748057	2781458	969795	3674934	6950018	2131340
EIC	Negative	314.1845	3.68	unknown	563567	399285	992076	1168161	228656	213148	447027	432004	223442	723601	559935	647193	915759	433939	244398	525263	546954	601357	1202850
EIC	Negative	533.3860	3.37	unknown	162722	99966	612532	2268621	69439	50928	115878	59837	72507	910744	126355	220799	112430	77220	0	135850	204835	230654	176623
EIC	Negative	393.2287	2.55	unknown	1120254	577781	733420	917198	195636	253645	351715	218434	703250	800997	1417711	648096	463706	557768	421926	623132	589335	455792	526511
EIC	Negative	280.1178	1.32	unknown	55127	6099	0	0	13824	0	0	74032	0	17003	45313	104855	106141	0	7701	152311	0	17958	
EIC	Negative	374.2996	4.92	unknown	0	68222	139252	79995	15957	0	22481	16612	10204	18561	19718	53251	24044	22927	0	18199	70563	0	0
EIC	Negative	401.1247	1.87	unknown	4520722	2638102	5615559	0	1393919	1797855	3030148	0	1861051	550751	1968139	3593408	3836243	2788794	1573694	4668723	4331126	0	5862322
EIC	Negative	554.3160	2.97	unknown	641979	0	3163203	3161247	0	0	0	2335101	0	2599154	120834	0	137644	180506	168358	0	0	4522838	79470
EIC	Negative	440.1471	1.63	unknown	211523	76656	0	0	92561	38790	101640	0	77033	64411	124116	126348	139626	54278	68085	198628	117545	160302	88884
EIC	Negative	499.2017	3.21	unknown	445319	256834	374253	169334	233558	157094	167224	230571	126318	449305	266650	445250	230160	295612	178669	304484	268147	832623	287240
EIC	Negative	291.1966	3.68	unknown	277555	174644	211274	427852	81834	100335	117060	95145	77689	344738	241467	227507	184579	160140	141842	196467	176756	248713	202387
EIC	Negative	402.1282	1.87	unknown	1045855	660723	1297474	0	327306	446318	694088	0	428944	0	435572	874320	879292	632027	377189	1117541	1009500	0	1383917
EIC	Negative	445.3239	5.52	unknown	223941	72850	549864	113667	38854	48027	40040	168647	34342	251754	96392	85501	73718	121515	30916	92871	74308	442435	36855
EIC	Negative	413.1948	2.24	unknown	3221345	850324	3114585	2579121	1427426	267871	1007690	0	996121	2818424	556733	939211	665875	737369	905541	860824	832605	3633518	1357826
fpHILIC	Negative	355.1402	1.38	unknown	342352	192597	0	0	85209	301340	39561	0	71673	0	138713	147546	79653	782468	481659	88108	140889	0	310878
EIC	Negative	252.0875	1.74	unknown	421217	237934	141394	0	145925	1229402	74625	83219	87091	195489	180599	119901	87688	406404	550498	112648	170414	191381	185261
EIC	Negative	314.1845	3.16	unknown	0	204541	291205	318262	123051	56534	0	78109	174291	257773	246141	0	103988	154581	205432	178529	0	0	0
EIC	Negative	301.1802	3.15	unknown	613935	259813	926449	707639	78606	122598	172496	101574	884365	332770	276775	336337	266445	123174	325964	443251	226737	273216	0
EIC	Negative	306.0526	2.47	unknown	636057	330407	1802316	329783	102700	130936	198953	292967	804847	3097618	308958	381932	404276	426438	397618	469691	513778	469629	304562
EIC	Negative	494.2489	3.08	unknown	180848	59993	196647	127403	28798	12674	60111	61019	10007	99220	28109	11890	90069	28183	81504	38582	31604	101471	103186
EIC	Negative	339.2654	6.07	unknown	0	96851	0	0	115040	0	0	0	0	0	0	129907	0	0	0	0	0	237583	0
EIC	Negative	309.1744	3.48	unknown	0	0	0	224376	0	0	0	142048	0	112859	0	0	0	136936	156570	0	0	0	0
EIC	Negative	332.1952	2.75	unknown	1484796	3404662	1001128	2518412	1716179	2490304	3810791	692592	1706209	4551371	3765791	4986059	5593116	4034315	3805278	37520856	3164430	6639558	4429053
EIC	Negative	313.1815	3.68	unknown	2655918	1854396	4741684	5381589	1112702	957514	2070199	1542200	1058717	3417125	2441790	2982481	3871008	1819372	933992	2393952	2611934	2681392	5333793
EIC	Negative	265.1449	1.73	unknown	1290256	1423355	2083526	365874	455513	940935	324962	756728	447501	1296751	1166707	9409334	3180043	1642763	431607	1108210	482945	204899	204899
EIC	Negative	364.2135	3.05	unknown	856451	390082	2015773	664947	241297	281014	352735	388567	342267	710287	4479515	630245	519779	418560	219944	502101	1337286	801087	481385
EIC	Negative	363.2004	3.92	unknown	15119669	4405569	11886795	34504401	1075702	1978481	1869547	1152444	26080128	6135584	1096760	654351	141966	2222556	6931487	673799	5078543	851340	851340
EIC	Negative	390.2400	3.40	unknown	343517	1716191	2703354	2783240	972213	1449354	1147458	1282658	565753	1946554	2070434	1166339	1343225	677455	1218156	3150383	1576249	3930289	1402771
EIC	Negative	394.2319	2.55	unknown	291567	137711	194504	289452	64224	64222	55826	52874	201739	108094	156995	109583	150098	119690	73291	151115	146236	133554	137122
EIC	Negative	403.1322	1.86	unknown	120151	112346	294414	0	63971	77740	119652	0	82180	0	102743	156812	151156	118034	73399	195026	186993	0	263063
EIC	Negative	331.1918	2.75	unknown	6282374	15350519	4965971	11012341	3590009	10946140	16917638	3234694	7513409	20567497	16787887	22404854	24627294	17657829	17094842	15704414	14045718	30209789	19461128
EIC	Negative	323.2502	4.92	unknown	0	0	188648	0	0	83216	153197	0	0	0	0	0	0	0	0	0	122558	0	167421
fpHILIC	Negative	351.2179	0.61	unknown	6088249	3042124	4992715	6570985	1071411	1737145	1842690	2118660	1790046	6948437	3265446	3231605	3306362	2656928	2778732	3927876	4059087	4049601	3127161
EIC	Negative	449.2568	2.48	unknown	0	15489	63326	248919	0	58130	61142	92028	42601	228441	64764	104387	136505	17798	52635	9059	127256	305848	37909
EIC	Negative	365.1989	3.92	unknown	994719	288615	796322	2341097	67046	124789	92065	136404	72738	1755329	443920	80860	70501	0	167698	466222	16270	327054	58753
EIC	Negative	461.3280	3.41	unknown	132151	36114	327626	27552	23767	0	151974	9708	164348	59131	23199	9422	25745	38667	83999	35024	219244	13301	0
EIC	Negative	315.1967	4.30	unknown	1066732	700762	1741897	1699262	242367	185496	317589	319447	225673										

EIC	Negative	521.2758	3.58	unknown	101485	85936	229525	146837	47641	30215	79816	63735	53111	143884	128411	115092	155718	98614	54777	83200	133331	113008	221319	
EIC	Negative	533.3024	2.79	unknown	2158825	39480	2983523	2259615	0	0	33980	1169330	79183	956805	0	0	51841	73019	0	0	0	2830604	0	
EIC	Negative	382.7211	0.52	unknown	400148	104330	458774	2296920	0	155312	1104336	34891	243924	656561	101195	97489	109894	0	115368	241508	76917	202592	566374	
EIC	Negative	350.2055	1.73	unknown	1062123	244300	590215	646501	50204	86051	90113	74271	90862	1223309	264397	197211	140488	234020	132568	211712	200111	129030	187469	
fpHILIC	Positive	163.0597	2.91	unknown	474941	184246	277951	63148	85399	114431	225874	67474	0	106564	68748	116205	0	703638	439681	69763	76522	208260	297399	
EIC	Negative	399.2155	3.35	unknown	6030361	4007671	6551669	5147542	1373251	1487227	2631123	1477910	1670335	7965181	4873822	3864261	3545139	4400441	2115893	4284282	4341917	3360092	5066198	
EIC	Negative	459.1873	3.71	unknown	110419	26012	62687	284728	0	25407	0	15097	0	289190	56684	11439	0	0	21026	42160	11958	15390	0	
EIC	Negative	632.2974	3.00	unknown	72455	41015	0	62763	22399	71078	13440	25094	68510	94245	71566	112917	73870	70078	75352	91037	94969	66567	120767	
EIC	Negative	493.2794	3.03	unknown	163033	32758	70084	48486	0	86511	0	20414	0	52255	25757	78184	23572	20091	68208	21504	0	29233	120477	
EIC	Negative	389.2911	6.44	unknown	36037224	34703508	31677198	45834044	43112692	1716724	36073268	2006466	2030173	1659776	29528754	34153096	33038382	1988467	38333440	36841880	33061908	28463296	53675936	
EIC	Negative	273.1493	2.16	unknown	2159297	1225343	4117040	2997803	125312	673679	531134	462452	290644	2100717	1174666	2739157	1114061	896364	776650	877767	1511481	436964	1072958	
EIC	Negative	418.2307	2.52	unknown	823180	342427	561189	534109	154570	150824	276392	74587	195351	776219	329222	405227	374535	373800	242309	381501	307588	672282	309715	
EIC	Negative	265.1480	1.73	unknown	0	1245112	49170	323795	392475	0	283634	24880	412545	0	26399	977718	834758	0	0	0	0	0	2094644	
EIC	Negative	400.2192	3.36	unknown	1463945	968827	1505977	1322867	329404	379273	621786	345391	394678	1919109	1158907	942528	841026	1088705	508164	1045939	1025462	823391	1265444	
EIC	Negative	334.2082	2.01	unknown	187055	245053	0	36868	94562	204167	0	51777	174088	302876	365812	138087	74357	209744	174242	209401	100897	179670	0	
EIC	Negative	378.2377	3.35	unknown	1172742	418021	1382032	921163	177099	220723	356428	252879	240337	1979043	687558	358745	475791	591837	311668	599994	680132	491547	738729	
EIC	Negative	243.1604	1.52	unknown	99600	105367	560288	234833	169513	122543	172047	299805	84203	295904	152941	121492	568141	205923	317897	117960	398738	842260	244405	
EIC	Negative	557.3350	2.28	unknown	377298	0	1499109	1134560	0	0	1093407	9761	0	1347831	0	0	43200	50260	53284	21571	0	0	2436518	0
EIC	Negative	317.2123	2.91	unknown	8632346	5773508	11217143	0	3407450	0	3630454	0	5044236	0	0	6497301	6137784	5039640	6721895	0	0	0	4319357	
fpHILIC	Positive	85.0288	2.92	unknown	690048	424691	378737	147067	128756	167032	284731	290765	98506	294502	256155	267898	278842	884399	770361	264726	262061	296230	625913	
EIC	Negative	423.2219	3.92	unknown	1340476	393348	1039818	3027263	84514	132040	166725	183974	79260	2190626	590120	108048	59480	0	213823	658761	67225	453524	89756	
EIC	Negative	399.2288	2.32	unknown	11681634	4777645	8814762	1208464	1243972	1560286	2367613	1892833	1523369	3825813	6211485	4422935	3699167	5420332	2690919	4396785	5349431	6464436	857137	
EIC	Negative	433.2002	2.51	unknown	606683	229008	501694	695817	149739	174499	344065	265621	238976	1040894	440926	618216	563569	528527	330573	569891	444782	924507	428864	
EIC	Negative	314.1846	2.82	unknown	154998	353620	290509	623850	122772	102461	145511	100497	101952	270142	204947	290272	241442	201514	282691	262286	261000	161022	365345	
EIC	Negative	364.2036	3.92	unknown	3529997	1035798	2833536	8277669	225006	352906	405731	421952	229466	6249043	1569315	246730	140601	19807	538781	1747337	161475	1109290	223624	
EIC	Negative	519.2860	2.54	unknown	807776	0	1026846	549277	0	0	278895	0	0	0	0	0	0	0	0	0	0	0	650248	0
EIC	Negative	429.1955	2.32	unknown	1482853	466737	1003110	1581961	196211	157577	299528	366164	199183	2437112	526914	429897	420343	542221	302480	436898	525749	1028098	549883	
EIC	Negative	522.3520	2.33	unknown	144610	59070	173079	572942	15751	11847	25301	33787	33787	367602	52880	52420	45196	24210	23518	45680	52180	122380	18975	
EIC	Negative	316.1997	3.30	unknown	1066998	847652	2644292	2000281	672474	330024	175030	332475	200294	1429680	1285231	1294408	533636	771019	575896	950084	1239292	594698	621981	
EIC	Negative	239.2015	4.44	unknown	301231	68685	334595	180605	27263	61900	126978	110517	87081	168914	133614	230901	227026	186195	119387	140561	209488	358833	140304	
EIC	Negative	494.2490	2.18	unknown	648536	193191	0	108267	91623	245192	0	99680	1933221	198031	162756	122270	228511	90690	315434	403488	0	465732	0	
EIC	Negative	534.3020	2.79	unknown	455797	10421	501617	460529	0	0	274931	26035	221840	11866	0	0	0	15267	0	15777	0	14406	0	
EIC	Negative	531.2997	2.79	unknown	22240738	53926	27900599	21458019	59907	83994	109685	11906674	416931	9396633	111432	88355	253002	285952	1810899	78731	89662	29077542	123205	
EIC	Negative	342.2732	6.06	unknown	0	0	224098	0	0	160920	0	0	0	0	0	0	0	0	0	0	0	200232	0	
EIC	Negative	511.3643	2.86	unknown	178187	69287	0	56373	74739	68761	64348	0	14557	133981	61116	55001	47543	62442	63235	87730	71938	244207	56130	
EIC	Negative	627.4999	6.86	unknown	89478	287294	116815	283135	105809	108112	187582	89108	155082	291708	701595	267747	451272	965636	268501	247297	430451	101876	479283	
EIC	Negative	531.2832	0.89	unknown	161770	5371	188985	179601	33149	25857	346212	15022	13941	590456	5260	12480	0	14648	5585	11103	1019434	9183	0	
EIC	Negative	364.2134	3.22	unknown	568641	192237	1956237	721078	111385	170484	181596	186884	195081	209670	191426	270683	264870	206670	115272	264640	1047017	366414	209612	
fpHILIC	Positive	202.1086	0.57	unknown	890251	885429	164761	141914	353106	797020	255960	0	398267	840563	611927	486472	317641	10117792	2245586	473875	466036	646330	640133	
EIC	Negative	583.3806	5.19	unknown	158161	0	247465	796449	0	332239	0	867261	912193	196201	0	0	0	0	194609	975924	294263	814690	1033503	
EIC	Negative	565.3028	3.69	unknown	87853	135768	354143	222745	122774	56380	80479	515285	293355	240196	179751	177751	0	0	0	0	0	350561	0	
EIC	Negative	552.2981	2.43	unknown	87643	0	229883	74586	0	0	146874	0	161842	0	0	0	0	0	0	0	0	0	0	
EIC	Negative	409.2225	1.73	unknown	3832646	905438	2069217	2083733	90619	140763	218103	105553	210282	4651915	807830	588970	351197	684077	303346	571976	556937	0	508246	
EIC	Negative	479.3745	5.33	unknown	2057292	1406788	1637182	2024314	704653	963479	699844	1055773	815642	2866550	2890776	1989160	1713886	1682916	1853289	2432313	1908843	2375195	1587208	
EIC	Negative	503.2983	4.03	unknown	1842698	997167	1607227	631921	181675	273992	55575	34291	173819	0	0	67716	485770	0	1127566	0	92074	143504	712331	
EIC	Negative	507.1702	2.44	unknown	341773	70701	42023	164932	9309	24044	29112	20819	30314	218157	57189	57095	31170	56690	24739	43603	58032	101908	43980	
fpHILIC	Positive	317.2124	0.44	unknown	4788285	1711637	7606033	4637844	574754	594832	1258896	892430	858011	8350926	2137096	2259541	1687500	1620230	891552	1676145	2736486	1756921	3011447	
EIC	Negative	593.6695	4.04	unknown	112951	60386	89148	76547	55571	47835	43780	120388	60225	199289	161108	119927	126675	77911	103383	132391	138861	319168	96340	
EIC	Negative	427.1984	3.84	unknown	0	91701	277402	158398	0	91482	183947	249306	0	285385	100068	154799	190907	911684	201595	253858	111338	513439	185533	
EIC	Negative	343.2132	3.10	unknown	512015	187133	205957	157181	260193	227521	260029	158590	233213	183062	192173	683106	408656	248398	201285	1181459	969994	226597	183661	
EIC	Negative	533.2901	2.51	unknown	319373	92380	190980	47401	57473	36821	90644	0	57084	208157	103115	102146	104916	90949	68874	115793	92538	195618	114234	
EIC	Negative	373.0721	2.85																					

EIC	Negative	319.2189	3.36	unknown	4145495	1496297	5505340	3527075	461160	557132	916500	570305	607783	7208026	2259302	1678176	1503866	1944440	720851	1762966	1975625	1520985	2135190
EIC	Negative	371.2440	4.04	unknown	168080	96542	92012	80503	148085	92418	115064	62287	106864	91581	96529	386344	198554	106948	68303	618639	483109	111890	92554
EIC	Negative	556.3324	2.28	unknown	936629	23924	4826355	3470246	0	0	3142117	64525	4534195	120894	73431	151028	192734	186122	75362	97651	7971598	72161	
EIC	Negative	352.2213	1.60	unknown	1120260	368193	520965	152564	74102	117209	128321	0	95431	921698	265409	213870	146820	223458	169533	273886	320243	0	324506
EIC	Negative	400.2191	3.77	unknown	401505	158356	515195	694909	73960	88655	108692	122316	83607	860115	313750	237189	224068	207529	103956	193682	277845	197936	480117
EIC	Negative	593.8875	3.63	unknown	1014857	556083	1384815	1033905	229210	285836	473730	436238	139875	1966217	1236376	898297	998783	682416	251210	600430	992485	831357	1475329
EIC	Negative	311.2124	3.36	unknown	133065984	53155091	177553786	107588994	15730004	17476157	32955443	17783407	18794620	251039758	73891464	55161274	46228487	62470846	24598967	61410410	66855315	46116022	74405608
EIC	Negative	318.2156	3.36	unknown	29454914	11776013	3931866	23570309	3475234	3847270	7302487	3937756	4137000	54895049	16150368	12174842	10192811	13666595	5374465	13636419	14902720	10101839	16388836
EIC	Negative	444.9849	0.49	unknown	7176350	6115632	8270621	7883594	283136	333742	352215	320997	8931442	8169813	591456	6914850	8293524	2342659	5422472	314359	6209151	7941434	7350455
EIC	Negative	437.1702	3.36	unknown	194535	119367	224853	267729	44387	71587	109172	75092	83518	583334	265583	187932	192954	229488	101107	239491	232196	177800	273811
fpHLIC	Negative	401.1302	3.53	unknown	65269	1176524	711074	78709	132481	132035	384288	197149	933016	55474	0	93220	100903	987799	113005	81146	279590	95345	4249991
EIC	Negative	377.2334	3.36	unknown	4443342	1603505	5739765	3599706	590964	555108	1039391	578205	577611	7692979	2318087	1799558	1420045	1968674	779650	1915532	2214407	1489039	2503229
EIC	Negative	577.3015	5.25	unknown	389775	1207284	295406	651554	421019	675426	495230	311546	386913	701653	1520210	1227333	2349904	1013297	1175276	1162396	1311805	933607	1671864
EIC	Negative	307.1944	3.52	unknown	0	294418	643079	0	0	0	0	216159	734097	275007	270786	0	0	103726	0	0	486844	0	0
fpHLIC	Negative	343.1139	3.52	unknown	69132	1512180	875759	125214	165002	193953	526241	268159	1255192	85942	56217	164663	152030	1350423	142560	109693	375797	183661	5772100
EIC	Negative	417.2266	2.62	unknown	371813	284241	422639	298276	71727	100450	143436	0	83517	714790	300129	219932	224554	265210	144206	207059	354745	0	388875
EIC	Negative	318.2155	3.05	unknown	379114	106613	861680	327497	77975	54986	87860	98827	72051	976050	315975	121751	158157	162318	92621	206551	269670	323614	185091
EIC	Negative	557.3354	2.39	unknown	459689	25608	26411920	3161525	15499	8765	0	1402135	36294	3181297	107212	97277	115741	202452	155144	71476	70790	3670986	59020
EIC	Negative	334.2109	2.32	unknown	12532996	5265640	9282483	12610844	1370369	1657307	2626669	2236417	1682535	21710495	6597181	4792480	3801336	6260234	3027137	4786893	6115751	6654404	5778729
EIC	Negative	294.1792	6.03	unknown	0	676944	0	909916	0	0	0	673121	0	0	0	0	0	966847	0	0	991396	0	0
EIC	Negative	320.2215	3.36	unknown	420706	143540	506299	300725	37397	46843	83167	45051	56712	726129	191480	156374	116210	159253	61956	190772	175050	119108	198379
EIC	Negative	556.3324	2.39	unknown	1401055	87272	7216068	9464196	41830	32442	25484	4117973	109194	9353239	339522	260851	324959	620716	446554	108493	236461	10995895	171767
EIC	Negative	418.2306	2.56	unknown	452588	203915	176023	324995	57342	72907	87607	74587	57499	697611	238203	167906	149176	232601	107418	183616	250755	101062	330898
EIC	Negative	394.2317	2.32	unknown	2356084	1002981	1773670	2447566	2725504	304963	488417	425430	298389	4227455	1345522	937130	722920	1824808	571099	923697	1133833	1284943	1084529
fpHLIC	Negative	196.0285	1.65	unknown	0	1145388	0	738515	0	0	930748	0	0	0	0	0	0	1963276	1480126	1119332	0	0	0
EIC	Negative	298.1827	5.23	unknown	1989241	734497	2848051	1556203	421934	283591	586919	541874	317103	2413936	1315053	1257879	1639458	938190	461359	1129501	1345220	1001525	2097499
EIC	Negative	393.2286	2.32	unknown	9792298	4062238	7413516	10023741	1083550	1281572	2026913	1654430	1271201	17152084	5288002	3781332	3040465	4813064	2300221	3670972	4692837	5376029	4511147
EIC	Negative	416.2288	6.31	unknown	503860	1607918	223916	89780	810653	1341184	78614	373994	353807	177217	152661	193988	254595	356913	191013	3640298	325204	2188686	1989814
EIC	Negative	392.2172	2.48	unknown	319786	274850	179915	350946	277433	14535	0	23540	205774	275075	283352	0	0	294223	273586	304983	0	16724	
EIC	Negative	415.2256	6.31	unknown	2156457	7147602	1127041	734511	3654924	551862	453050	1557153	1872704	841464	695306	7009029	1272665	1473746	773709	15638416	1261286	9815596	9315981
EIC	Negative	364.2038	3.72	unknown	538734	135867	347127	1407586	0	69944	35099	0	29221	1455436	254035	46305	0	0	40224	203641	0	79995	56002
EIC	Negative	381.2565	5.44	unknown	164350	118693	0	0	0	165134	0	0	0	0	0	0	0	0	112519	203519	0	0	151380
EIC	Negative	297.1865	5.23	unknown	9352001	3582844	13002719	6649572	1613882	1313690	2944177	2304619	1375002	10990205	6023978	5758637	7347202	4298937	2104112	5030012	6383456	4198167	9340088
fpHLIC	Negative	342.1124	3.53	unknown	331284	6949079	4239270	471153	728478	791619	2505636	1167524	5196321	345728	227588	629058	621502	6237731	565510	466857	1536621	668371	26198768
EIC	Negative	333.1356	2.96	unknown	322726	25367	396131	45095	12955	21285	10756	10756	66400	36432	0	65812	0	259483	0	0	40496	0	31284
EIC	Negative	297.1720	3.84	unknown	115983	77681	116210	77649	20231	33590	53821	0	52557	84300	96023	117954	162665	103583	151309	101181	80999	51374	69550
EIC	Negative	385.2383	5.69	unknown	902730	309776	745539	469160	254171	184615	274215	501470	136787	860037	708855	490884	336014	389516	1012502	171896	591289	953551	490873
EIC	Negative	471.3448	5.84	unknown	301353	106497	520615	318083	26117	84214	66701	114604	58114	398483	167770	211476	134244	69933	409957	168555	157144	100263	165482
EIC	Negative	433.2210	1.60	unknown	359463	136649	0	0	25810	0	0	31759	274071	108607	109188	67333	96462	73458	105451	146179	0	140654	0
EIC	Negative	534.3884	3.37	unknown	66888	51103	206847	800469	0	12737	20863	33613	37397	315125	73423	98909	36412	15531	0	51976	71234	105436	71096
EIC	Negative	554.3152	2.79	unknown	1663266	0	3786176	7863643	120092	131700	0	4637974	328163	4723282	526450	443310	371720	701076	610641	371160	474607	12294836	448439
EIC	Negative	317.2122	3.05	unknown	1493576	582539	3918054	1528109	263587	296903	382293	354452	325170	4301725	1443349	582194	790967	711557	429143	869334	1188153	1302010	882061
EIC	Negative	318.2157	4.53	unknown	1124233	357302	1554061	909948	235376	100874	317103	147840	182325	2116299	582344	672675	193426	400884	136228	599955	789076	569888	589531
EIC	Negative	629.3853	2.89	unknown	1565274	815366	2111879	1542715	301522	89719	413202	268650	127253	1603966	493237	774204	631783	657962	548137	1023147	1006631	642489	379081
EIC	Negative	555.3184	2.79	unknown	605721	15087	1322960	2793058	29256	34427	0	1514896	123376	3037514	969417	743153	656248	866275	489465	717793	960584	440586	1164718
EIC	Negative	546.3193	3.25	unknown	1236729	0	2786954	1367831	0	0	830655	28839	1687445	167445	11356	0	30093	33682	0	0	0	2492023	9705
EIC	Negative	336.2265	2.62	unknown	2080878	844068	2206113	1444343	188021	290204	391324	175814	250902	3037514	969417	743153	656248	866275	489465	717793	960584	440586	1164718
EIC	Negative	415.1919	3.36	unknown	586961	81688	792802	674142	132006	138185	273900	175223	177470	1873072	661531	517626	445106	634721	239629	615315	631481	418883	714999
EIC	Negative	309.0626	0.49	unknown	628240	326521	0	0	0	0	238508	0	0	0	0	0	0	236951	0	0	367221	0	330574
EIC	Negative	635.4327	4.14	unknown	451170	309122	495547	343052	46601	42963	131897	74800	77237	178807	135868	404888	337205	141860	306225	252312	218252	177098	150306
EIC																							

EIC	Negative	393.2286	2.44	unknown	9955067	2385420	10599369	6452590	556385	766513	1197225	935004	918612	17463809	3599208	2364954	1772343	3416825	1015307	2881799	3496602	3433995	3161406	
EIC	Negative	334.2109	2.44	unknown	14797171	3491393	15763421	9489561	859059	1054326	1792861	1401598	1382805	25683097	5388526	3433050	2557040	5163482	1565924	4398188	5339182	4926429	4638357	
fpHLIC	Positive	360.1497	3.53	unknown	794857	22525682	13514578	1255584	1835191	2240935	8260221	3176757	17786320	905324	588544	1964193	2023313	20852010	1706093	1468073	4455295	1737214	98346760	
EIC	Negative	315.2538	3.45	unknown	192801	0	299552	953131	0	0	0	0	0	87141	79606	167920	1015629	967489	1012069	0	0	985508	923893	1013525
EIC	Negative	445.2007	3.92	unknown	1110018	356665	786502	2240266	13863	118535	24859	82256	87414	2065974	322072	75336	25363	0	108515	519752	16967	363886	57615	
EIC	Negative	630.3858	2.89	unknown	778953	422187	983330	733733	117146	17448	203571	115102	78938	539602	184815	375064	282873	236017	255086	502618	506418	310594	166959	
EIC	Negative	354.2352	3.31	unknown	63774	52338	70667	53839	46113	72131	58045	59388	57832	51513	69396	69971	63878	14829	53298	724393	62975	55928	65085	
EIC	Negative	314.2420	6.40	unknown	7431503	3443869	7254149	409892	286087	3804534	443805	429838	415640	5070975	2997314	2989659	2680032	136083	3553015	2741176	2924481	5798679	2665662	
EIC	Negative	413.2003	3.77	unknown	551277	244183	960064	968055	77631	99799	150887	140841	114652	1556200	500596	357601	342293	355576	129826	132709	460773	178917	918142	
EIC	Negative	394.2318	2.44	unknown	2419040	587221	2656593	1561386	135945	182605	291508	227396	218911	4213260	872418	582755	424740	845042	239921	714332	883303	883384	783226	
EIC	Negative	314.1845	1.88	unknown	0	326213	0	0	0	454586	0	0	0	0	0	0	0	0	503875	487640	518504	0	0	
EIC	Negative	469.3320	5.49	unknown	790758	255987	1161561	833690	114948	121034	121983	181203	108064	1264931	410543	528821	335768	254580	923187	337008	309928	194437	412776	
EIC	Negative	469.2961	6.00	unknown	1106541	1090291	1368720	1480701	215321	107731	239994	206994	143217	835913	555139	683243	251186	389268	580729	933045	237111	987966	338862	
fpHLIC	Positive	599.2869	0.35	unknown	80857	135985	408483	249959	86870	70197	106033	206045	61356	446051	225587	249247	122840	230268	64565	130349	256460	1291636	46127	
fpHLIC	Positive	171.0760	1.64	unknown	174647	1470022	0	1622308	0	0	1704657	0	0	0	1919947	1994448	0	1606922	2201375	2818002	734943	0	0	
EIC	Negative	516.3085	3.75	unknown	3584329	15939	4492251	2759386	0	35090	29408	1076937	59613	1379306	38109	11569	64252	96775	50473	0	13522	3953753	54578	
EIC	Negative	397.2513	2.56	unknown	418572	203265	353215	330110	35096	49958	64153	26675	28861	716576	169780	108455	122469	139460	95816	134430	168633	56470	241650	
EIC	Negative	429.1960	2.44	unknown	2078783	424324	1997862	1397869	106954	120432	121639	216841	197078	3249886	632098	214193	258276	586774	117917	509305	617665	832330	521261	
EIC	Negative	633.4078	3.76	unknown	888959	0	114773	1113458	0	0	188576	0	0	0	0	0	15303	47267	0	298048	0	345073	0	
EIC	Negative	313.1815	3.43	unknown	713647	407150	1145333	1148133	131743	158658	174532	181524	167798	2293685	1092304	667588	369170	572653	294189	444485	645117	137814	1221217	
EIC	Negative	407.2061	1.92	unknown	0	138995	0	0	82387	39516	0	0	49971	0	138520	146465	265630	74811	162078	133989	171741	0	123758	
EIC	Negative	318.2156	3.77	unknown	3548826	1616349	5819517	6285135	503648	560432	995138	739925	620268	9393547	2985526	2084266	1996597	2067352	732901	1519407	2801821	1229340	5579801	
EIC	Negative	322.1778	3.43	unknown	480669	453569	525062	0	0	574817	0	0	0	0	612925	0	0	0	338350	0	633562	982394	51762	
EIC	Negative	431.1845	2.44	unknown	604861	109046	665043	586269	54975	65695	101443	147149	85811	2670571	331437	216633	168379	338870	127803	319129	363104	479239	301831	
EIC	Negative	335.2232	2.56	unknown	37198661	12423423	24884391	26558503	2513936	3677927	4955763	2561336	2953817	57790513	1498578	9929221	8849383	12917015	6553237	10949034	14454893	6257207	20427009	
EIC	Negative	628.3532	4.93	unknown	0	8576817	0	0	0	0	3422330	0	0	0	0	0	8760829	0	0	0	0	0	12094239	
EIC	Negative	336.2265	2.56	unknown	8312192	2742705	5495568	5925994	543857	815325	1117306	544226	650798	12849892	3307182	2154759	1953429	2862810	1441381	2415213	3214406	1401549	4506395	
EIC	Negative	335.0233	2.14	unknown	123132	72890	156386	0	72726	279921	42618	0	10179	96425	634417	319838	158423	142556	68098	164341	837073	80443	125466	
EIC	Negative	634.4181	3.76	unknown	367518	107372	1070902	555712	17365	39047	75063	50995	40460	500818	118061	158398	165699	145123	58583	141093	199666	139964	255599	
EIC	Negative	397.1999	6.36	unknown	0	131135	571390	0	228999	0	0	0	41532	392233	286283	0	241587	0	171509	256662	216734	320044	0	
EIC	Negative	495.3694	3.73	unknown	88128	83467	94288	164273	47197	85067	50902	75855	39323	508645	298485	132217	96952	138726	156659	259379	125796	395898	130064	
EIC	Negative	410.2258	1.73	unknown	963749	210667	488960	689843	21791	24816	12595	64758	31087	1312625	192172	180013	109684	178060	78301	169519	151846	0	156072	
EIC	Negative	334.2180	2.26	unknown	555174	155736	2894221	3516130	256543	70140	542987	277364	83741	8616442	171952	1030414	661589	1434798	493961	166349	146466	1365081	2276579	
EIC	Negative	316.1999	3.46	unknown	1657681	760786	2240968	2648608	190394	183177	302385	257296	304180	4629709	1333763	970240	765699	874029	339685	769310	1116823	482441	2066216	
EIC	Negative	633.4164	3.76	unknown	1007460	239782	1891035	1319819	40631	38128	123125	76158	1004382	314506	399040	407955	295533	0	71683	317121	446077	406567	576584	
EIC	Negative	559.4022	3.36	unknown	184400	56850	199575	120317	0	18112	20141	0	139249	1615130	64207	56368	24496	55131	0	31750	80461	0	27139	
EIC	Negative	369.1855	2.33	unknown	804883	319947	673176	787340	41315	86906	34228	75660	1684868	20897710	6043273	4287382	3565041	4124357	1510201	3334131	5178036	2012171	9506921	
EIC	Negative	315.1967	3.45	unknown	7399665	3385179	10144624	12471082	845875	859785	1688468	1089782	1286812	20897710	6043273	4287382	3565041	4124357	1510201	3334131	5178036	2012171	9506921	
EIC	Negative	509.2386	1.59	unknown	1556164	395343	1457695	633651	272179	0	453491	0	0	4242346	633687	470659	2672243	2437056	256996	909277	1480439	956822	1012803	
EIC	Negative	395.2441	2.56	unknown	10737298	3595226	6748250	7713670	684603	1012327	1323534	633586	809796	16746074	4274874	2672243	2437056	3573652	1831234	3153613	4093872	1788873	5948379	
EIC	Negative	417.2264	2.56	unknown	1809515	809290	635148	1075700	184813	251949	333575	0	0	2793282	973289	618647	875529	462038	1641783	6665131	916828	523085	1017644	
EIC	Negative	479.2650	2.33	unknown	1322025	295653	2719707	2854078	75554	97575	127891	157929	89274	4594125	646262	386967	217542	310747	107711	389384	441367	470125	669885	
EIC	Negative	528.3011	2.36	unknown	1412204	7399	2330039	5369256	32397	32373	0	2719472	78976	5309966	123444	77232	123273	158112	158112	88228	147454	10358379	105678	
EIC	Negative	431.3015	3.03	unknown	0	141630	0	0	0	0	0	0	143372	0	59041	134862	131942	0	0	142839	127752	145374	130529	
EIC	Negative	397.2000	6.23	unknown	0	206377	166105	0	194668	0	0	0	0	0	127430	0	219950	0	100907	290803	194546	163394	0	
EIC	Negative	315.1825	2.36	unknown	615076	112535	92454	89700	155936	98806	163923	101693	109717	86483	155843	294461	52750	227961	215640	465986	1604869	99665	97596	
EIC	Negative	396.2471	2.56	unknown	2624333	869739	1579205	1859322	166805	254332	308656	108315	196542	4155022	1059679	660307	614440	853201	435790	768067	1009416	434491	1442181	
EIC	Negative	470.2991	6.00	unknown	351607	345360	457284	488919	74068	0	89249	65930	26174	285043	167788	225853	76714	107066	185449	314917	101099	314258	99241	
EIC	Negative	397.2000	3.46	unknown	555977	307054	742696	807019	74511	70792	141930	85747	99578	1570166	495704	348891	287922	363591	136489	273123	445055	163963	863049	
EIC	Negative	335.2230	2.32	unknown	1839443	186328	1409057	1815244	100430	129032	142289	377141	254190	0	969460	691944	560589	0	495277	719732	890217	1082461	859241	
EIC	Negative	377.2337	3.77	unknown	784192	170802	1382020	1465741	130383</															





EIC	Negative	403.2491	3.78	unknown	204517	242218	240241	234920	226074	240747	248200	245503	240905	210241	183784	217686	230532	227021	244251	240247	216866	253950	255669
EIC	Negative	355.2432	2.35	unknown	469998	503350	421434	130457	446269	478152	497944	466272	464457	451041	465683	489186	478385	461440	489891	491959	485982	411927	492298
EIC	Negative	398.9667	3.09	unknown	118035	193145	112766	107032	154043	156857	158100	95646	171065	107977	186166	150103	174887	146878	179208	174887	143816	110267	133502
EIC	Negative	369.1915	2.71	unknown	535412	398617	248013	326213	353494	401109	378544	579824	387547	494152	344999	369168	384822	395449	430354	303860	447211	447956	491593
EIC	Negative	306.2521	6.50	unknown	4880112	8442364	7383492	10686355	8155410	7427013	9970169	9277789	9277839	7279491	10916329	8913068	9855206	8020363	8224504	8001896	11224788	9039869	8944949
EIC	Negative	356.2472	2.48	unknown	2919432	3657704	2201597	2722219	3763772	3534958	3619616	3728545	3624573	3624889	3685622	3645485	3679958	3839868	3778243	3538998	3707112	3618272	3893954
fpHILIC	Positive	302.0705	3.39	unknown	319848	490514	545422	5572920	513990	545264	552426	530263	467509	675879	496039	474411	512714	466556	516360	528611	579932	463874	518579
fpHILIC	Negative	178.0752	0.94	unknown	1909941	1960316	1750585	1651470	1976577	1710699	1843465	1946185	1973417	1818610	1939493	1706416	1664812	1956027	2027543	2050752	1841743	1685033	1937854
fpHILIC	Positive	177.0659	0.96	unknown	593175	543624	306060	395975	1047908	1243529	728312	381797	957125	624584	1048830	706493	893577	538549	1012042	920485	1203778	306836	931927
EIC	Negative	540.2730	2.71	unknown	551618	526597	303541	348400	422408	723976	365543	378241	954488	452292	392107	563860	387430	332013	495227	689278	780498	231641	676759
EIC	Negative	358.2625	2.35	unknown	3294868	3593779	3121402	3282894	3410718	3428078	3738474	3439263	3474158	3181630	3614800	3541473	3519684	3580548	3564247	3483023	3670496	3227242	3730292
EIC	Negative	535.2869	5.23	unknown	483301	468141	436578	510771	518173	402466	457955	577674	567439	528164	424002	507842	440186	522057	487727	511322	501489	555394	494547
fpHILIC	Positive	133.0799	3.37	unknown	40373180	36694776	24584342	23011768	29421860	37514816	26654468	31839122	32885296	21552510	24215452	29311344	33118436	35060372	35510652	38773112	27787442	36303444	21634336
EIC	Negative	283.0614	2.17	unknown	303226	325358	271978	316079	296432	287532	308717	359096	303867	351789	251922	324577	295171	339381	271110	335511	207990	338472	356416
EIC	Negative	320.2856	4.00	unknown	617045	631603	595160	564092	633441	605727	600369	590498	590511	578579	599871	579822	586605	588165	597251	610539	658353	600728	587950
EIC	Negative	441.1884	3.65	unknown	612700	672834	510961	615671	641629	602922	576829	665511	669227	647599	618411	627788	601042	611953	610959	613370	577931	723874	666904
EIC	Negative	309.0628	1.55	unknown	608366	708220	444652	317446	819379	929412	796617	340834	204104	442045	810567	653342	528724	534345	855257	466995	649901	341936	813826
EIC	Negative	502.3992	6.59	unknown	1125002	1132656	1045180	1112392	1597405	1073207	2147885	1678600	2545181	1433207	1365838	1108547	1057233	1570580	1877124	2479978	1388476	1059080	2044185
EIC	Negative	365.2334	0.91	unknown	36114	59639	19770	32754	78362	84605	54850	44655	56633	26898	68440	20309	69773	80975	85437	106023	31796	55862	43957
fpHILIC	Positive	235.0798	3.14	unknown	1726674	2184128	1836542	1721070	1933748	1706723	1897362	2056193	2039225	1686780	2008466	1988947	2218270	2144213	2015796	1746407	1898184	1892203	3230623
EIC	Negative	552.2709	4.72	unknown	1298600	1449582	1081564	1214879	2490362	2684138	1834251	1868554	2836012	1429475	2216046	2100600	1664929	3013664	2347148	2804238	1885102	1596327	3230623
fpHILIC	Positive	136.0392	0.95	unknown	571695	633921	274518	302265	985454	1325769	720842	341102	983004	501440	918237	739443	479875	957244	921658	1222594	343437	967479	
EIC	Negative	320.2856	3.75	unknown	586924	597312	567036	558752	606633	585336	557815	586026	548620	565198	589780	560216	560983	557862	582481	583416	556550	600009	599478
EIC	Negative	647.2346	1.85	unknown	174770	97105	0	91100	62546	153347	0	77220	0	0	119343	119382	130596	73333	95181	135942	93670	0	64546
EIC	Negative	554.3473	5.47	unknown	6146279	9460952	6181041	7203029	7990235	8228526	7662010	6538423	10389907	6940574	9622117	9106951	9325528	9604708	8861363	8696197	8149799	5963677	9686904
EIC	Negative	337.2328	2.48	unknown	1837162	1849785	1557664	1847368	1967312	1803494	1985965	1804628	1837201	1927169	1894327	1936051	1915998	1998385	1927979	1837563	1929437	1793497	2043521
fpHILIC	Positive	142.9384	4.62	unknown	365826	399502	410322	434914	458970	484291	513941	471992	510451	503324	633213	470201	489057	456442	511208	473242	517473	484143	487493
fpHILIC	Positive	134.0808	3.15	unknown	802907	634638	513206	397649	717444	988293	804279	354082	382164	516185	715223	600114	616185	472352	793912	810037	552368	704191	425194
EIC	Negative	528.2733	4.82	unknown	1277112	1227834	1007509	1035417	2341952	2442946	1720422	1860475	1574281	1191761	1782451	1860189	1318272	2041256	1961475	1954623	1762484	1602713	2800887
fpHILIC	Positive	134.0808	3.36	unknown	3649530	3528567	2154352	1933583	2511526	3588422	2737924	2823033	3281621	2038559	2194832	2835810	3041785	3162081	3556322	3636540	2684881	3384119	1896436
EIC	Negative	192.0338	2.68	unknown	482024	556879	428909	561328	557306	686046	549727	482265	409577	498690	525975	552215	503032	558655	515828	594973	615117	461506	536449
EIC	Negative	341.0343	1.19	unknown	800220	319595	269542	280570	301632	371484	349203	259564	293111	289008	465958	336342	292201	332192	324253	268136	324210	307153	374887
EIC	Negative	280.0222	1.19	unknown	81447	82431	83392	89431	91830	94639	90292	87572	98574	79584	123893	97103	87794	88744	91347	82038	88868	90542	104877
EIC	Negative	506.3231	5.40	unknown	1535961	1627914	1516306	1407811	1579975	1690566	1438392	1671046	1474916	1414643	1470221	1662891	1602294	1419630	1567162	1544059	1603593	1571765	1686532
EIC	Negative	421.2253	0.86	unknown	344345	1144708	399255	381892	1480257	1699632	1169993	1871193	1432098	1360473	169271	733560	1222807	898568	1945373	1158634	1205465	1554146	
fpHILIC	Negative	221.1819	0.42	unknown	206289	631098	168215	294125	443051	372192	184580	118091	1410657	149701	216381	372758	909372	333031	335648	861320	271802	205309	895458
EIC	Negative	322.6719	6.53	unknown	5419706	5664689	5430692	9568074	6045562	9323355	9383389	8572974	9464156	8106695	1103261	9038858	10366107	9368268	7985898	8895760	10366753	9496993	678354
EIC	Negative	427.2713	1.07	unknown	37678	67726	60971	96205	81677	108861	59638	68221	52358	82200	78436	43989	94821	60416	77205	101105	55741	108497	33469
EIC	Negative	395.2441	2.93	unknown	1990925	2288617	1490033	1544406	2042422	1956387	1852259	2491718	1938268	2591231	2312821	1767541	2118549	1656523	2279135	1982687	2039467	2412749	2419245
fpHILIC	Positive	449.0766	4.29	unknown	371695	514154	198553	300454	543713	629583	532817	249455	585970	280651	465005	558305	611664	623337	604121	618964	566538	282810	1519497
EIC	Negative	534.2823	5.23	unknown	1910342	1593220	1642525	2042657	1974955	1617661	1688967	2042021	2063800	1907277	1690087	1839556	1675319	1962203	1818907	1911064	1878281	2111476	1843928
fpHILIC	Negative	558.3308	0.60	unknown	3612882	4131781	2848237	3138096	3810978	3432246	3373626	3312035	4530729	3253028	4092870	3860268	4094957	3757005	3951279	4203561	3568589	2538432	4355756
EIC	Negative	135.2513	3.44	unknown	970424	1032004	957804	921851	1042707	1030095	1007526	1016040	963039	822552	946372	1037452	1151473	1066640	914418	1128476	1020293	1062202	
fpHILIC	Positive	234.0768	3.14	unknown	21679124	26734658	24904478	23128458	26447202	22876672	24560252	25980778	24925550	26086018	27080294	26129484	26106356	28377216	27950452	25139918	24360114	24046254	25758180
EIC	Negative	297.2436	5.66	unknown	2754088	1984092	2314170	2004018	2482510	2702477	2165871	2296231	2588568	1926010	1994340	2212092	2219515	2505516	1804810	3211764	2331348	2725301	2406918
EIC	Negative	237.0766	1.86	unknown	133038	143699	0	0	135643	126593	125067	0	123156	0	115459	121870	112419	126398	130133	129489	129035	0	132138
EIC	Negative	226.1193	1.81	unknown	138445	163496	413506	0	118436	168073	195726	350132	122761	334110	190440	185755	435537	222675	278265	165922	378368	0	249300
fpHILIC	Positive	258.1095	3.32	unknown	47834332	120580872																	

fpHILIC	Positive	184.0737	3.68	unknown	7261435	4802447	3296431	5441937	5718998	8983337	4868197	4000154	5428157	3487946	3624435	6731425	4060351	3970699	5173772	7038304	5655527	6335233	5870453
fpHILIC	Positive	224.1119	2.53	unknown	473528	334682	259696	373274	346938	463257	311868	263999	501787	278791	367468	423659	421540	304593	397976	480854	216641	365910	445715
fpHILIC	Positive	148.0964	2.65	unknown	1708708	1976781	1931575	2219460	2416507	2519712	1916066	1288946	2377836	2383952	2286855	2506709	2268743	2066422	2547246	2491573	1796400	2013595	2028424
EIC	Negative	621.2952	5.33	unknown	399372	3219505	2309198	3015751	3794866	4836397	4342038	3198467	4001666	2356982	4447630	4615355	5001878	4710357	3885822	4392439	4313940	3195079	5089661
fpHILIC	Negative	130.0228	0.76	unknown	79496	730195	119277	51859	426682	576652	111086	83742	33574	74513	67899	319507	90725	72689	292100	303435	64308	282871	332072
EIC	Negative	361.1953	6.22	unknown	28205	298088	0	328711	172256	178088	190661	59576	303759	154185	205776	183238	237341	137005	160677	200337	219091	177590	179733
EIC	Negative	346.1591	1.92	unknown	0	211035	0	0	356963	358780	391950	0	293838	362080	262169	862054	264801	271235	448551	396171	375243	0	233893
EIC	Negative	319.1539	4.91	unknown	351437	0	0	0	400239	0	207950	0	0	0	0	0	0	0	0	415217	0	0	0
EIC	Negative	382.2967	5.78	unknown	1693562	1713796	1708568	2240685	1903362	2070502	2024991	2200774	1775253	1935792	2046580	1889085	1989127	1589473	1985251	1892088	2242490	2380633	1857609
fpHILIC	Negative	165.0403	3.19	unknown	5391668	4015530	3272984	5300110	4546126	6450810	6284696	3826049	5588175	3890095	5472910	5742929	4925308	6635170	4771767	6594855	6032729	4729394	5585442
EIC	Negative	492.1835	2.72	unknown	823054	1022228	1004201	879785	926659	1017905	1163145	893056	913626	888901	1059286	992477	1146669	1107506	1118371	1078949	1080700	788148	1036144
EIC	Negative	427.3207	6.62	unknown	821602	400102	681415	893328	507849	584907	1236597	989144	508340	593270	706026	531387	618652	640304	640304	1043671	650310	649729	989994
fpHILIC	Positive	389.1795	3.34	unknown	355133	1227486	297745	229735	723020	968365	798729	260743	779812	121520	487862	675849	641857	962053	721201	1046850	643025	430169	825932
EIC	Positive	480.3082	5.30	unknown	783562	1230851	1472147	1117814	905571	1189551	1189757	1209357	1080916	1045496	918347	1232526	870760	2148259	1633966	1212602	1316853	657949	1688567
EIC	Negative	298.2469	5.66	unknown	553569	410742	454713	429566	501885	537216	393575	485512	518499	386663	399997	445380	478977	502571	377113	629184	464170	576587	485567
EIC	Negative	268.1556	2.28	unknown	478081	369343	355648	572447	452320	432696	520118	354239	534173	115651	432424	496281	469065	304898	551913	594741	387485	542108	277727
EIC	Negative	250.1448	2.30	unknown	1650521	1405725	728812	1671599	1650215	2470614	1666445	819544	980727	1717767	1176106	1612404	1941089	1516230	916192	1862790	1990176	1587987	1377878
EIC	Negative	245.1757	3.08	unknown	68894	74396	79298	79298	108690	66306	99626	117291	109700	97976	92083	122471	91732	98047	118065	94835	127680	105356	75458
EIC	Negative	344.2315	4.74	unknown	141073	155163	80513	252535	232410	136556	206179	111791	398072	133518	132682	143638	195000	46304	197630	296552	254399	160534	209905
EIC	Negative	443.1565	2.05	unknown	1509082	4916774	1435811	1153794	3875641	4269225	4343424	921446	3366378	1924906	4127528	3462396	4028022	4687860	5300197	4035094	4237946	958206	2915336
fpHILIC	Positive	104.0709	3.03	unknown	7143600	10056730	7203646	14000275	10718520	8881030	7340426	7065207	12295511	6794799	10616970	7224964	6840526	7609128	8443105	10564196	10650668	11208530	7286316
EIC	Positive	334.1637	2.64	unknown	248167	212735	168135	252114	260022	375447	225207	139870	175319	273391	277048	283585	215157	114237	342402	290657	298991	131586	142897
EIC	Negative	306.2521	6.57	unknown	280998	413874	292924	471358	457882	462138	549269	479099	602291	426985	598033	517238	702618	380502	477120	420694	626520	599868	528918
EIC	Negative	437.2459	2.15	unknown	248541	923473	235005	466723	846231	346456	808962	415796	873735	648363	305433	932357	282158	649204	402965	865603	448042	582657	1030749
EIC	Negative	239.1288	2.81	unknown	2953803	3802920	2246064	2274588	3595228	4068086	4016281	2491985	3279630	3482752	5004553	3056552	3406302	3750339	3736347	3902095	3667514	3000113	3824536
EIC	Negative	410.2640	1.88	unknown	193880	181886	0	0	178346	356874	134318	0	120265	0	270161	228137	290517	182605	177129	235973	165907	0	243833
EIC	Negative	289.1236	3.79	unknown	280961	325430	267580	299758	286761	295851	299084	296308	288611	275034	285922	293989	308461	303965	305220	312753	304321	305527	304787
EIC	Negative	409.2607	1.29	unknown	147603	85881	23996	0	111415	418402	84228	0	84729	219347	154415	161714	101186	137403	200133	86251	146148	0	295882
fpHILIC	Negative	135.0298	2.95	unknown	104463200	82146112	48396156	67554736	11796296	113023080	116406760	8730176	143457056	49557732	68662744	103952752	89533784	130326384	149534128	100333192	126608944	99949616	126732792
EIC	Negative	528.3073	4.33	unknown	689759	796208	582289	567127	646262	811974	832156	657925	668241	625329	693155	740250	673366	586247	695135	746067	1084745	679262	566274
EIC	Negative	619.3466	3.37	unknown	574167	486788	210998	190515	341684	818949	445466	531483	470335	117437	421753	752152	488602	101961	548876	670325	687759	91829	721978
EIC	Negative	444.1593	2.05	unknown	347508	1119666	331318	216541	870854	966707	977578	120242	785793	276061	928129	754608	981822	1038698	1272578	903655	922812	147373	638688
fpHILIC	Negative	303.0586	2.99	unknown	1050187	541418	271302	463291	781122	547002	736739	545590	1023496	322124	339756	536607	493702	507948	663571	1029347	991487	643565	796625
EIC	Negative	374.2572	1.43	unknown	0	764781	0	0	750288	760822	758395	0	969420	0	745869	734668	759145	786135	786265	737543	798017	0	748030
EIC	Negative	265.1481	4.60	unknown	12337519	8145373	6458934	12988198	22164619	8161774	10681223	5385874	9986019	7589326	4645069	7922366	6832678	5739859	5144700	15376665	19898174	8875343	9596780
fpHILIC	Negative	158.0823	0.61	unknown	3458972	3508020	2748970	3434231	3390595	6979323	4188167	1627036	4077304	2124621	2887031	3389327	3715124	2824404	7921915	4941993	3598590	1950964	7895579
EIC	Negative	449.3279	2.93	unknown	1358900	2366466	1159259	940018	2563660	1849400	2481693	1632462	4077304	2124621	2887031	3389327	3715124	2824404	7921915	4941993	3598590	1950964	7895579
EIC	Negative	637.5357	4.87	unknown	728588	688128	645418	653001	672705	597602	681885	683280	733980	739351	683032	697258	713422	666892	714615	759813	709314	687696	656103
EIC	Negative	582.3779	6.26	unknown	95421077	92907853	98832937	98993128	100315507	97942784	97916488	98989186	101195688	101713056	10546004	111116738	100772512	99095223	99683887	108682237	102229619	106722595	102556630
fpHILIC	Negative	75.0088	0.99	unknown	5215589	3609970	2293433	3527811	6286309	5067443	6727734	4534932	8632596	2406899	3412118	5774811	5114117	6602071	7496547	5554930	7606300	4973549	7106667
EIC	Negative	279.1252	1.97	unknown	0	39945	0	0	57106	49019	64015	0	33968	0	33968	47554	44232	40660	90750	60597	0	42564	
EIC	Negative	409.2608	1.88	unknown	532750	732306	0	0	727198	1295075	577272	0	471748	0	1029073	899459	1146438	754386	678789	914280	678010	0	949195
EIC	Negative	588.4014	2.85	unknown	0	225726	199050	688996	484277	334991	302923	222970	519864	196573	177774	348193	478545	177207	151153	559528	495841	566390	182625
EIC	Negative	347.1274	0.89	unknown	71947	59850	66103	75530	65622	81117	73951	57955	71057	86705	55344	60241	65601	80123	65600	67984	69894	78643	84643
EIC	Negative	582.2826	4.47	unknown	556167	491016	489197	524465	532572	403886	477941	507910	672346	564439	467676	485073	481084	573625	546096	604787	558939	584836	430113
EIC	Negative	327.1812	2.28	unknown	313770	201499	360303	205459	233185	266248	223413	405105	129995	371710	159524	291497	148883	324797	203210	189343	186221	558829	183469
EIC	Negative	268.2365	6.50	unknown	1093488	1251044	1862749	2195886	1854436	1396507	2020360	2453819	2476953	1535064	1712137	2005491	2316187	1955542	1651744	2405131	2025080	2506031	1748864
fpHILIC	Positive	243.0518	2.63	unknown	745603	2124634	1891247	1225443	1515682	1684938	1862163	1335161	1345830	1358901	1821944	1636347	1484931	1726519	2017725	1484851	1479901	1501060	1674110
fpHILIC	Negative	205.0352	0.96	unknown	847652	5																	



EIC	Negative	227.1285	1.00	unknown	70342	73985	67210	71647	68743	71841	71279	73172	64692	66369	72493	75387	68980	68419	70834	75334	76494	80413	68893
EIC	Negative	240.1323	2.81	unknown	381527	552496	298453	392385	527598	594521	582909	358920	476845	497778	729961	542045	516682	542870	543786	591092	556654	470107	542900
fpHILIC	Negative	160.0615	1.61	unknown	185581	0	2275990	0	2826103	195932	541132	2019171	2616208	2909964	324969	0	3064907	3185108	0	3068474	2374294	3291270	3291270
EIC	Negative	422.1593	3.11	unknown	532409	389224	479359	388205	532384	498383	540307	440404	576412	475050	494934	455562	473709	651750	495217	668654	468651	479772	633502
EIC	Negative	528.3216	3.87	unknown	997927	2143147	1014573	1139420	1570430	2010704	1821382	1297698	1498956	1434631	1964594	2087536	1892959	2195358	1997996	1759032	1674192	1603446	1698029
EIC	Negative	266.1517	4.60	unknown	1693230	1179456	893313	1835537	3192292	1089044	1492697	767506	1387740	1012129	642716	1171013	957664	809993	733042	2116450	2906201	1328357	1363907
EIC	Negative	424.1563	3.11	unknown	178885	138525	162171	132187	173056	179052	190817	152453	210383	147772	160873	151060	161178	221037	194887	239652	156989	156356	211730
EIC	Negative	412.2708	4.04	unknown	614595	722145	430994	451494	608361	577788	574356	717288	576701	577539	679429	585109	635523	483880	713012	487585	681178	677393	697730
EIC	Negative	269.1406	2.72	unknown	547118	573097	368846	424400	546508	563979	614543	546392	532647	692762	516189	464497	538892	511158	614417	493845	589217	632156	665522
fpHILIC	Negative	182.0456	0.47	unknown	2513888	1246067	1538800	2496021	2308880	3998720	3717276	1053442	1014981	2752395	2471384	3784726	1837967	675216	1576716	1864364	2298103	1468923	5715281
fpHILIC	Negative	259.1298	2.69	unknown	2428954	2601414	2123303	1214919	2307529	3563528	2209252	981829	1465929	1779272	2535464	2463927	1789634	2844575	4380984	1754469	1602960	1224116	2293120
fpHILIC	Negative	867.5579	0.43	unknown	3847182	5497277	3277674	3258144	4818583	4355643	4029582	3275627	6327088	3803357	5557441	5217264	5720858	4876459	5234667	6050984	4863610	2907742	5339962
fpHILIC	Negative	391.2860	0.38	unknown	759852	334500	565886	667633	761464	722716	651971	421866	265411	799648	568936	672835	266218	430069	613811	602630	386840	962360	458617
EIC	Negative	429.3342	3.69	unknown	1282693	536040	318850	422608	1453507	740084	690743	324056	561191	518821	673482	292564	607927	536202	359833	572468	1768562	882793	454829
EIC	Negative	382.3773	6.94	unknown	72705	73857	71011	76010	102970	71217	72233	96812	108163	109889	62758	169400	73268	82981	68264	66482	84831	182647	81698
EIC	Negative	511.3642	1.91	unknown	0	124509	0	176210	142663	117151	142663	0	148616	0	116512	169400	117394	113408	206423	217812	94031	0	108698
EIC	Negative	431.2953	3.03	unknown	109436	173824	121329	123248	137610	131214	127470	149654	167632	115152	151150	139530	151776	138716	133326	148368	155571	166687	161494
EIC	Negative	329.1520	2.78	unknown	1861990	1637052	1484456	1324779	1700201	1539415	2118947	1621025	1479222	1601927	1767770	1944261	1681694	2048256	1789872	2016676	1663300	2308713	2308713
EIC	Negative	383.1834	6.31	unknown	143520	0	636840	501131	190278	425868	227189	540377	481420	521424	823862	601111	303535	501715	632045	400359	340652	334194	295438
EIC	Negative	421.1558	3.11	unknown	2510752	1898289	2158030	1840777	2500023	2452731	2585367	2063054	2794566	2036691	2113042	2246298	3006958	2525638	3252089	2208832	2299212	3024699	3024699
fpHILIC	Negative	177.0226	0.89	unknown	1636219	1592723	1344040	1345558	1585303	2961206	1759044	1145990	1508866	1549832	2048850	1924600	1968310	1925335	1837709	2652948	1734131	1454245	1945715
EIC	Negative	429.3342	3.69	unknown	156031	156528	72800	189939	143536	234300	128143	185033	163448	259875	191478	160643	184264	131097	199374	206594	147221	173286	191219
EIC	Negative	642.3423	3.47	unknown	168472	292503	119877	151479	235606	259459	267039	124218	286673	134715	257588	234022	210569	162269	215556	292430	280076	109970	361784
EIC	Negative	245.0819	1.02	unknown	53329	56837	56753	47028	53078	52286	62131	56334	47005	67596	53598	61434	56578	54148	60167	61825	57160	56879	55032
EIC	Negative	610.3375	2.01	unknown	316609	677041	348542	0	572428	621874	700829	124693	493919	0	740606	817758	342940	463873	505086	665409	595645	0	877728
fpHILIC	Negative	103.0038	0.99	unknown	3859386	2596895	1538897	2468622	4212023	3825045	4220743	3416659	5679790	1703628	2522246	3907104	3884282	4705401	5143336	3858386	5312848	3624978	5020869
fpHILIC	Negative	143.0714	0.43	unknown	663858	495239	572907	828020	623921	571976	744616	479700	578265	602182	628420	824097	999024	495925	437406	964670	856125	538039	428741
EIC	Negative	301.0720	1.80	unknown	230412	816059	503090	0	548516	523252	768179	373859	456872	193733	712255	147947	117694	155156	383352	1982615	63490	0	443596
EIC	Negative	345.1713	5.57	unknown	277969	363909	171428	165832	521128	277982	0	262955	152578	490860	29118	86713	593314	0	479226	183281	644328	0	306652
EIC	Negative	264.9975	1.92	unknown	0	268620	0	0	252061	205728	271827	0	281755	0	332056	32191	386341	395086	114026	294417	372823	0	106652
EIC	Negative	413.3013	1.97	unknown	0	147915	0	0	152834	126278	102273	0	117604	0	176374	103291	125666	107055	136217	131732	134865	0	134205
EIC	Negative	299.1143	1.43	unknown	0	222824	0	0	216541	192354	209481	0	200721	0	232970	199223	240910	188791	237105	182791	237652	0	224626
EIC	Negative	357.1686	3.72	unknown	240500	418256	170863	159758	407296	271545	209455	267499	310716	118279	167852	223295	530243	143306	267203	287423	229931	254322	492082
fpHILIC	Positive	399.1436	3.78	unknown	756610	487532	398489	578145	517285	879750	518514	412589	541271	561508	584071	712105	517046	573193	560899	608373	624820	664917	632813
EIC	Negative	325.3112	6.75	unknown	468754	522166	458199	659475	969010	641472	686632	614742	568410	612792	694444	809598	624842	501365	844784	730236	684577	1118788	528005
EIC	Negative	281.2383	6.47	unknown	9442809	10838308	10036869	10102782	10065027	9015881	10664561	11184995	12574848	11447480	10312832	11540411	11496745	10930411	10258377	11784642	11968313	13535157	10154943
EIC	Negative	381.3747	6.94	unknown	242789	243915	261299	273718	387743	261954	274322	344589	310716	118279	167852	223295	530243	143306	267203	287423	229931	254322	492082
EIC	Negative	280.2353	6.47	unknown	83921490	95825064	89129946	89894661	89950141	78626823	92630181	99208223	110253731	100021111	91137397	98827568	101743676	97105613	8899632	102840268	106510196	120504908	88875262
fpHILIC	Negative	152.0546	1.01	unknown	385779	473713	270672	177871	714214	697657	233071	574646	617777	585287	514357	576837	412441	699949	574665	901810	227094	763072	763072
EIC	Negative	275.2316	3.84	unknown	203807	228566	195379	199928	243381	227254	197583	198786	210391	203238	243392	225069	221671	205418	246992	225250	222910	239806	227254
EIC	Negative	397.1998	2.91	unknown	4493853	5423076	4073533	4656338	4774366	4672853	5569470	4403647	5137868	43171237	5436612	5363106	5293742	5675691	5351216	5139626	5325277	5240542	5291456
EIC	Negative	293.2489	6.52	unknown	465897	556197	766945	1114838	668525	645618	732416	927255	1044850	754735	874509	815267	1033014	893053	773566	873796	1031085	941030	718201
EIC	Negative	239.1077	3.33	unknown	118210	132966	125783	136921	133226	154150	135512	121407	111923	141074	133842	164022	145096	155134	141890	157762	131873	147934	147934
EIC	Negative	320.1261	3.84	unknown	2839718	3979601	2620787	3870695	3857850	3980031	3768637	3193376	4219859	3500407	4007226	3733466	3793133	4373727	4341839	4371864	3794619	3829560	4226442
EIC	Negative	359.1244	0.84	unknown	200708	127421	105727	179726	150844	171254	164145	217003	177255	128408	115606	129713	200124	169894	159003	229722	212417	182042	182042
fpHILIC	Positive	216.0552	3.63	unknown	717573	692845	454691	541319	637230	943812	861091	525233	1012903	483523	529863	699860	667850	895286	740654	746396	926811	824735	1068744
EIC	Negative	326.3143	6.75	unknown	111767	126466	117226	148166	228846	144393	149566	178852	139303	137516	155003	198652	146102	120455	198667	151868	159774	266338	133921
EIC	Negative	252.1718	1.14	unknown	258259	255511	210942	181680	215372	193715	250729	288011	232171	213876	275343	243324	283399	207725	278136	199628	272505	266461	253294
EIC	Negative	321.2307	3.84	unknown	488148	62																	

EIC	Negative	491.3380	2.82	unknown	376569	869218	341617	538040	807479	825988	605386	602765	827247	677097	919003	697713	831045	908844	867484	833371	691399	767079	868106
fpHILIC	Negative	133.0346	2.95	unknown	1403565	847080	554171	821322	1373384	1248259	1229135	948084	1523401	540008	628627	1212411	1042461	1570311	1692854	1308766	1328621	1125971	1486675
EIC	Negative	253.1566	0.98	unknown	157362	180092	137767	128350	143868	132843	166990	198668	153235	144730	172672	161173	123843	151126	193659	135086	186406	185229	173962
EIC	Negative	248.1326	0.78	unknown	147700	159029	140119	137397	161337	221490	208766	123226	120130	153587	201956	336876	262004	193804	123156	293949	175822	125343	251244
EIC	Negative	339.1792	2.09	unknown	57410	84510	0	41399	61115	85188	98044	0	67684	51357	57234	144145	150340	86464	77321	103184	88661	0	76040
EIC	Negative	380.2489	5.86	unknown	166259	122952	176069	187341	102968	177361	146652	189213	214451	189103	133780	198788	160178	94240	128811	286225	205856	163650	160047
EIC	Negative	567.5557	6.63	unknown	3425895	7246630	6958497	1803467	12264689	8392431	10525522	13175753	14398281	10569310	10876396	12926619	9807582	16560722	12929684	12924800	16902453	11519102	10448066
EIC	Negative	450.3312	2.93	unknown	364096	702043	347725	300357	747843	531629	689262	480405	599986	295856	565659	543901	553359	550200	832671	722756	717464	496336	589882
EIC	Negative	412.2709	4.09	unknown	283317	317917	220364	209229	268473	262657	281594	331799	244437	288927	345502	263858	267620	234660	332020	224809	344263	285090	344638
fpHILIC	Positive	235.1283	3.70	unknown	389990	447822	311356	294798	453976	467555	364535	294617	325647	348612	459772	403341	317426	566639	493717	462616	396212	310141	439531
EIC	Negative	407.1470	2.85	unknown	92201	152645	209355	239676	133044	206357	171932	194226	120267	306175	288262	205450	123129	100514	184775	173297	212862	248800	71310
EIC	Negative	430.1744	2.03	unknown	278895	340665	338339	224221	301533	402797	566330	134827	278998	266856	468058	710111	422187	333395	380266	573384	475251	127552	302562
fpHILIC	Positive	219.0756	2.62	unknown	691775	750178	746033	508798	638913	765295	830419	561312	693749	589233	766725	741490	818700	914504	968566	772690	611059	726956	772112
EIC	Negative	430.3375	3.69	unknown	344764	127429	35551	105392	367212	203221	161059	76750	151297	136822	169558	80907	157907	131581	91988	164849	460043	226859	115369
fpHILIC	Positive	248.0945	3.40	unknown	272265	217389	50654	658971	347296	379976	256948	172735	410331	468734	299382	266246	417880	92747	291938	491597	501806	271488	175302
EIC	Negative	612.8336	0.86	unknown	472696	1967955	860435	815571	1346835	2155132	891498	967696	696902	601468	1534006	1138599	1440936	1122158	1936371	1324529	1781253	979489	677585
EIC	Negative	276.1888	3.72	unknown	788816	2137861	501098	628144	2146931	773888	1421041	872777	1910549	406440	778325	1023146	1646592	779909	1322753	1552111	1264279	1045262	2695711
EIC	Negative	423.1532	3.11	unknown	910632	661828	701809	626812	861875	707434	804922	861875	956864	508820	809587	724330	753287	1024039	889765	1219883	754397	776509	1048571
EIC	Negative	385.1784	3.11	unknown	116619	91887	89484	114115	152174	127791	131940	88784	170585	97571	108982	108796	143891	156711	133919	164280	125651	142886	176011
fpHILIC	Negative	175.0726	2.74	unknown	314399	254129	176624	273689	251421	585985	274088	423511	289983	217380	423511	393153	343424	496318	720204	398930	324257	197210	502516
fpHILIC	Negative	230.1036	2.74	unknown	764598	658667	440684	576551	506951	927502	538819	385313	758559	493950	666210	654459	613355	550261	710187	874854	708170	453388	703727
EIC	Negative	251.1483	2.30	unknown	198385	199997	72972	230942	247336	354215	217914	93508	144313	448160	266620	274693	221441	137645	265606	285088	236811	219743	163563
EIC	Negative	425.2561	0.86	unknown	93596	117939	100121	147684	202471	303134	140902	220118	130593	180604	152804	91325	148120	118057	187655	184023	157733	428434	168655
EIC	Negative	371.2440	5.69	unknown	255735	263490	202860	191740	221517	198390	224904	272210	237009	240637	268869	229944	275939	224857	248062	191359	272850	286291	263284
fpHILIC	Positive	159.0911	2.61	unknown	11171388	13886672	12809254	9971223	11736143	1478389	13850490	10252377	10208445	11632699	14172910	13741187	12475249	15238026	15497219	14367478	11900292	12693830	12818812
EIC	Negative	613.3353	0.86	unknown	178289	757878	339929	309581	509581	809584	337464	356582	339929	439800	607741	440247	528293	411958	728447	497801	670250	359683	267901
EIC	Negative	365.1978	2.58	unknown	216303	142862	0	111314	87462	180631	206074	20021	158721	88814	141424	272423	247637	143300	80778	198522	150110	84621	212570
EIC	Negative	389.1975	2.18	unknown	0	54559	41652	52111	37744	83445	63242	34663	73257	30413	37411	85867	74024	57051	26079	74147	62445	104257	58449
fpHILIC	Positive	124.0587	0.92	unknown	1234051	1674336	342471	963290	2164961	2293291	1875094	646957	2784827	746297	2051522	2248737	1811505	1840132	2605095	2614869	2127197	1244180	2281217
EIC	Negative	502.2714	3.87	unknown	567739	1004175	509869	604843	784526	952200	938509	556486	748706	711765	947538	1035487	864184	1083968	997785	863486	854261	854829	862183
EIC	Negative	396.3926	7.00	unknown	90206	82331	83368	97671	145989	72641	75336	102835	123788	124826	74421	157668	78302	117685	112762	88351	110403	183376	84830
EIC	Negative	310.1663	2.77	unknown	475156	531427	252216	304675	606810	498405	484582	506052	475749	493710	579293	505139	708229	450200	576761	458149	605421	584675	638681
EIC	Negative	344.2887	6.63	unknown	86437	157362	125272	192065	175816	179146	263155	222575	255308	98850	204165	244927	241255	289586	225077	190957	130638	274845	219945
fpHILIC	Negative	178.0510	0.93	unknown	3311755	2907221	2938052	983269	2339728	5039052	2811913	2001641	2055605	1388990	3222163	2842388	2651647	3684211	4150551	2407635	2398180	2618808	6431120
EIC	Negative	598.2549	4.64	unknown	274248	387278	374112	520054	600715	558683	651440	711110	579677	579677	574533	585811	663259	677354	765480	565731	754231	727830	4939229
EIC	Negative	237.1088	2.78	unknown	535853	648806	251878	329121	666430	568634	771684	498262	636210	505562	746519	691785	695717	626493	746791	634669	748177	607196	768915
EIC	Negative	327.2180	2.23	unknown	425427	225833	382277	256046	516551	244608	489781	302561	489759	316551	621148	619533	378275	167754	605994	587022	531268	493092	
EIC	Negative	270.2159	5.73	unknown	123685	129439	116509	148550	153251	146339	139007	119443	116513	129616	112983	117147	124118	109484	107957	224616	147752	133612	139610
EIC	Negative	339.3181	6.71	unknown	146866	215589	147929	252754	300317	213641	240124	192631	247324	192631	247324	296379	297806	235788	296255	280576	279728	279612	171406
EIC	Negative	275.1656	3.72	unknown	4304593	11327164	2587285	3409496	11303664	4048755	7466679	4547668	10193316	2241536	4260343	5278033	8893228	4141503	7207107	8218080	6708718	5636736	14278294
EIC	Negative	415.1976	6.06	unknown	0	0	0	0	0	0	0	0	0	0	0	0	0	0	361427	0	489661	0	0
EIC	Negative	569.5419	6.63	unknown	289001	615370	556133	1224966	1071064	705057	859799	1075332	1176914	888866	851008	1172160	800291	1547566	1014173	1084281	1449081	1033710	895701
EIC	Negative	447.2058	3.11	unknown	449976	400192	316152	313975	523889	488038	519678	357445	584078	374492	476885	447397	443379	613598	494852	685866	460093	448363	681562
EIC	Negative	416.3009	2.64	unknown	420581	515902	419040	584036	570035	659626	673570	490840	586245	532318	726629	695528	756218	1053181	706345	739940	723009	483567	687624
fpHILIC	Negative	125.0179	3.34	unknown	719989	491915	471331	500808	536143	596781	630333	466233	583518	500616	522857	493347	547072	690312	691014	485174	669668	660749	598465
fpHILIC	Positive	125.0710	2.84	unknown	290722	415605	273028	274379	318188	350294	340535	268553	533803	246381	348791	324307	458355	266572	491204	461204	397764	316051	364359
fpHILIC	Positive	190.0505	0.96	unknown	1430821	1054814	802727	670161	1018684	1859217	1193237	553919	437284	716801	1141582	973381	758911	952814	1637796	990719	1037109	818712	1193401
EIC	Negative	380.2083	2.28	unknown	232323	181609	162162	232392	164919	145041	166992	324069	166386	269657	176561	138848	183849	138819	196359	164446	197253	318777	209083
fpHILIC	Negative	478.2937	0.51	unknown	2944274	3567916	2382294	1454782	3173763	3754482													

EIC	Negative	293.1541	4.05	unknown	362398	458669	268011	257802	405318	346258	304535	343340	283768	267913	302582	265283	327115	250008	368142	380039	359911	403659	401710
EIC	Negative	236.1050	2.78	unknown	3479044	4103413	2104311	2409339	3948777	3570630	4958731	3192833	3837984	3223684	4891683	4044669	4550858	3934670	4771411	3845527	4723863	3843368	4993880
EIC	Negative	269.1761	2.66	unknown	87153	147158	91384	107327	98406	165288	105597	122116	107484	158394	168804	181840	186267	77004	117986	154815	164614	114267	129168
EIC	Negative	293.1762	2.78	unknown	885300877	104552788	35886893	59624776	104910929	92817219	123366257	79855168	99993757	85213213	126581390	104240113	117810089	100643480	120820425	992170664	119570247	100315475	129823247
EIC	Negative	474.2630	3.81	unknown	0	1923851	1691276	1039515	1315247	2519471	1262415	1376548	719321	1080321	1866131	1144405	944354	3711928	2153413	719556	1492010	1392829	2426449
EIC	Negative	298.2470	5.03	unknown	539977	373234	760522	567274	625525	579643	591308	583258	738007	423068	353032	508773	521351	411640	257530	1505600	580897	841779	362331
EIC	Negative	377.1970	0.90	unknown	145411	224186	130776	97593	244928	141365	124782	116961	136066	127055	164095	52136	214785	311866	220058	228827	106957	131080	183673
fpHILIC	Positive	242.6414	4.20	unknown	603597	234525	154162	259294	602190	611149	473682	438010	886635	230224	263498	522256	440191	611743	1036271	470982	609095	466938	623643
EIC	Negative	297.2436	5.03	unknown	2701722	1777803	3550406	286475	3295723	2805048	3091653	3018870	3618190	2119251	1600772	2668008	2437892	2165461	1385058	7600901	2809038	4261514	1989372
EIC	Negative	579.3586	3.65	unknown	1074108	1216278	754723	735485	1070760	1018970	939056	1161291	1012980	937365	1024913	938640	1083383	796668	1202767	1076359	1078992	1235328	1321015
EIC	Negative	395.3892	7.00	unknown	236451	213470	244617	258139	324182	255884	232891	326484	408366	454776	198877	545700	221901	338735	309307	236691	357340	626644	236520
fpHILIC	Negative	279.0540	2.95	unknown	399114	193545	46801	174578	387466	332958	382793	244166	593792	91522	135836	334857	276441	477049	594721	340532	492194	368778	419642
EIC	Negative	365.2340	1.77	unknown	251995	328169	185448	631604	793689	277693	588861	715810	539005	358189	484687	262887	569605	1936896	1178957	981315	512613	0	657178
fpHILIC	Negative	102.0561	3.03	unknown	995406	834269	890474	1188240	1331371	934242	1000386	738105	1959903	961742	1560366	1007100	1021189	932627	1119033	1662347	1576210	1589297	867715
fpHILIC	Positive	160.1329	2.96	unknown	69678944	59590404	51109288	45771852	70402216	91207784	74919728	49400124	63519296	58867008	121679432	79574968	95540744	71634432	79901440	94308668	78789952	55010992	91357400
EIC	Negative	541.2760	2.82	unknown	119650	207518	0	98304	164855	265817	149483	0	324184	124260	124621	191382	153425	118446	209024	223469	255094	127221	218945
EIC	Negative	533.4012	4.98	unknown	0	0	277826	0	114507	0	0	210444	0	0	0	193704	0	122428	0	106907	115760	0	149117
EIC	Negative	259.1666	0.85	unknown	124459	141938	136221	104369	126445	116395	137623	194166	102648	120766	158831	127268	188762	124634	164743	131785	177380	169802	131368
EIC	Negative	370.1880	2.77	unknown	160961	257543	73688	127324	247892	257513	232161	274160	256147	242309	273705	243454	251861	280989	219628	313446	294247	343065	
EIC	Negative	640.2980	4.32	unknown	308502	232130	135966	493365	449672	463315	541365	504612	544620	592557	509615	570961	495296	592557	577746	580225	617258	498159	
fpHILIC	Positive	280.0917	3.31	unknown	1828990	7688727	3530649	2574935	6051391	6716171	7280412	3509166	6565693	2667947	6263389	8365348	5889917	8736132	6307947	7751131	6334162	4801709	926371
fpHILIC	Positive	288.0740	3.58	unknown	623574	597577	398343	606209	434009	711176	574023	376560	534657	514220	467788	462783	710723	386213	477216	71878	680300	625855	509971
fpHILIC	Negative	202.0510	1.03	unknown	25569276	24330660	26155692	15394558	20784154	29745900	20532988	20190474	23595128	24762142	23889098	20813462	20344502	34302128	28423072	26981586	27491546	24221416	24670082
fpHILIC	Negative	168.0778	2.84	unknown	1135649	1946963	1483562	1293748	1764220	1893253	1580465	1190956	2179448	1540078	1768467	1779921	1766701	1068440	1514307	2482481	2421226	1795204	1666598
EIC	Negative	273.1246	1.43	unknown	0	94596	0	97535	71545	92962	0	87572	0	113025	102686	96912	139232	92800	96750	108512	0	103645	
fpHILIC	Negative	303.1029	2.25	unknown	738132	201962	132356	96588	272006	156661	154836	154489	347233	61580	108125	325939	201956	161550	535790	294010	395045	274927	0
EIC	Negative	331.1305	1.43	unknown	0	55607	0	98304	71132	53885	73649	0	64089	0	75097	84921	102766	62858	99218	79237	0	60773	
fpHILIC	Positive	161.1360	2.96	unknown	6002888	5349173	4632056	4254888	6247912	7166512	6647505	4179520	5649813	4963571	10139296	6934616	8314632	6219475	6769250	7515028	7307075	5063092	7682221
EIC	Negative	235.1705	5.07	unknown	692792	403625	388529	607879	649926	621595	732964	684559	755380	413083	379027	626780	705592	550452	750008	850065	847271	703671	818832
EIC	Negative	340.1526	1.85	unknown	147303	88738	0	0	160973	215588	213237	0	159117	0	162845	145272	187212	154898	173083	298898	179214	0	212909
EIC	Negative	287.2232	2.83	unknown	136301	147810	452326	273578	342708	320992	172341	441604	171033	363449	181805	185414	228888	194600	218624	507815	256553	523235	166082
fpHILIC	Negative	151.0513	1.01	unknown	4712569	5881986	2147374	3419208	7850953	9464513	7172906	3113918	7881182	5241257	8783524	6703786	7939764	5788775	9165814	7805479	11318270	2993506	9697990
fpHILIC	Negative	137.0243	0.52	unknown	1878485	1298251	2924232	960734	1273132	2345046	2094430	1293729	1280555	1235711	2070000	1551434	2035206	1422302	1252276	1429656	2219653	2878873	1797740
EIC	Negative	509.3496	2.42	unknown	118664	67665	197657	132942	313449	271625	227210	122950	248833	270594	169573	164108	56213	250028	347809	281069	165853	506972	68626
EIC	Negative	590.2848	4.24	unknown	211995	238674	306317	267337	291453	351669	421524	328818	280232	316513	269942	466989	470915	428081	452089	362525	381735	373096	368030
EIC	Negative	270.2523	6.58	unknown	1150140	1179017	1111880	1542923	1589348	1324657	1639095	1697475	2431089	1511491	1841915	1447589	1884660	2063753	1437435	2205519	2221481	1944109	2867749
EIC	Negative	558.2816	4.68	unknown	1928944	1455264	1645128	1979123	1861589	1352169	1678177	2091519	2368480	1820094	1797321	2044330	1626402	2133886	1994370	2073400	2234545	1440228	1470028
EIC	Negative	527.2021	3.11	unknown	146043	175209	105223	144114	218594	212073	216908	121337	250856	130518	196750	176546	176993	287757	222204	281262	205407	182668	291170
EIC	Negative	366.2659	4.91	unknown	220879	187858	143340	152121	135368	175661	188387	210629	159218	156029	191842	173273	203272	159554	212947	190153	227497	239821	123032
EIC	Negative	294.2156	4.59	unknown	220756	141479	200033	243911	218027	211418	251315	183294	323472	164680	148665	165808	163312	174254	75526	658710	213717	254578	176793
EIC	Negative	267.2331	6.57	unknown	183244	198488	253385	306070	267127	212139	338892	454824	264495	334483	334562	427650	321574	381852	400574	418334	455656	290624	0
EIC	Negative	459.8077	1.63	unknown	34664	0	0	79891	227614	113824	0	100421	44104	117190	173753	91000	271807	55206	146043	88619	0	0	0
fpHILIC	Positive	281.0949	3.31	unknown	220817	786723	331818	252880	6931970	598052	655399	559797	224796	491125	725475	537948	836811	595374	744008	587606	425576	807772	0
EIC	Negative	333.1558	2.04	unknown	0	194726	0	194209	117886	230119	187448	150182	394356	200376	501800	315691	177762	496013	252826	400831	250020	0	353481
EIC	Negative	505.3170	2.27	unknown	108862	98335	102794	92423	108862	98335	102794	92423	108862	110059	117537	136452	39399	152068	147609	142574	108379	257389	91446
EIC	Negative	310.2833	6.64	unknown	3063909	5291063	5813677	8145237	7678589	5762476	7023043	6883004	7873572	5837475	6017662	11627464	8186138	6411381	6119472	11300504	8238980	9405354	9568002
EIC	Negative	312.2264	3.30	unknown	377736	306759	422468	459992	473618	363211	560895	372940	746810	297465	253568	377849	347171	335651	249985	1302587	442493	492293	494189
EIC	Negative	582.2821	4.64	unknown	1562323	1240036	1287822	1338525	1310384	1087009	1268007	1293899	1733767	1615752	1425223	1398375	1687458	1228006	1639449	1657482	1610474	1532615	1362398
EIC	Negative	367.3493	6.79																				

fpHILIC	Negative	738.5213	0.35	unknown	243210	452466	375896	608779	700483	306376	427517	349013	881468	483530	648656	590081	578582	2092521	435763	736816	801508	518397	671900
fpHILIC	Negative	326.0751	2.24	unknown	689375	564215	360385	563766	1059957	831517	987630	723733	1259995	424240	582654	895817	940096	1020694	1189372	1448436	1021901	947668	1133833
EIC	Negative	242.0515	0.53	unknown	273416	133066	202660	269726	355339	324334	208274	171363	250216	522664	172410	143779	175342	86478	337676	206274	369982	232163	410161
EIC	Negative	293.1765	3.74	unknown	266700	194535	112939	109361	205447	187083	183750	324348	183219	165004	139912	221638	295982	195445	205595	169423	209200	246118	457746
EIC	Negative	580.2931	1.98	unknown	242611	354358	0	239021	423520	559472	520113	1148892	0	795117	679092	1032188	1424516	1215050	766043	882610	0	620619	
EIC	Negative	444.2244	1.99	unknown	0	195750	0	0	158497	144060	162714	0	152357	0	214121	166342	178902	156516	184299	142645	193068	0	214437
EIC	Negative	421.2517	2.72	unknown	177017	284321	179537	351735	361463	321471	247233	308676	342369	258069	334765	329838	348006	355809	395189	397643	359118	375340	356564
fpHILIC	Positive	446.1584	3.31	unknown	470318	986180	484387	376599	692570	815517	752940	517376	634815	421309	723717	834552	667491	837784	686047	1062468	727549	624253	963825
EIC	Negative	288.1490	1.13	unknown	142449	98145	110739	94430	107553	110513	121090	130603	125885	161909	140363	115331	148353	156106	143831	114904	135123	172138	191455
EIC	Negative	577.3509	3.65	unknown	13622942	15175267	8686909	9261835	12917508	11483964	10937667	13611069	10323362	10647762	12082689	11654826	12441993	9976374	14229483	12754132	12930092	15260990	15482294
EIC	Negative	287.1175	0.99	unknown	87842	65712	75831	66633	70602	64094	72372	85253	71747	92816	80352	70434	84754	93544	82187	68717	83516	84855	115323
EIC	Negative	323.1842	5.94	unknown	0	0	0	0	0	0	0	230745	0	0	396157	0	432133	0	0	275493	0	0	0
EIC	Negative	397.1797	1.63	unknown	0	0	0	0	28753	85902	12673	0	31240	0	32325	0	37556	53969	24885	67802	13828	43404	99539
EIC	Negative	301.1660	5.18	unknown	442884	559422	435725	461828	541251	501817	556842	406403	502131	448830	553457	547247	516878	620344	620400	661023	528291	534993	655552
EIC	Negative	307.1926	3.02	unknown	72840	55117	0	52084	67205	67143	90615	68180	95972	63490	46358	63420	103721	94342	44232	202074	73300	80793	66340
EIC	Negative	642.3149	4.79	unknown	105901	178970	230785	212079	252138	290178	321123	260835	254220	242685	350433	307021	373201	264261	306124	392738	395113	231493	332024
EIC	Negative	345.1572	2.89	unknown	201050	866631	66627	442993	620466	879481	727029	211040	914840	352997	873740	1272365	1279106	633981	1230366	1978183	748799	254045	414001
fpHILIC	Positive	132.0803	2.61	unknown	1122011	1453912	1190387	823679	1087233	1424931	1596090	757495	916788	1040080	1574553	1293471	1180382	1721904	1800316	1257516	1243686	1254470	1428487
EIC	Negative	594.5562	6.63	unknown	568075	1452767	1640367	2577898	2454357	1583452	1946751	2026789	2247885	1621617	1691509	3163220	2043456	1824609	1802360	2822197	3703644	2559543	1646400
EIC	Negative	630.3207	0.86	unknown	240470	534209	383792	307209	481959	778399	266925	210074	466925	412717	437647	303983	423329	771887	626401	266925	510278	315262	461818
EIC	Negative	344.1539	2.89	unknown	478461	4399266	715230	1243139	3252548	4747619	3986064	1270060	7337554	1944404	4671449	6041119	6871068	3538842	6620265	10649119	4130122	1252668	2263546
EIC	Negative	642.3422	2.89	unknown	548495	723583	137336	269339	475083	824780	506734	244051	295629	429637	519754	549415	695532	623588	623588	723451	695422	300260	1465165
EIC	Negative	631.3212	0.86	unknown	148091	311571	211072	170147	279596	441406	152039	132664	147285	215883	251021	182888	254873	449670	370480	262725	299534	183273	271529
EIC	Negative	255.1604	3.91	unknown	499063	508596	377364	320859	486035	405879	388974	460162	319499	598554	410492	394630	448582	340195	488150	443641	462498	554745	540268
EIC	Negative	417.1195	1.61	unknown	523727	456680	830770	280497	295736	415428	815156	550912	550798	354466	549678	846269	673136	620022	504311	820736	762097	550136	537885
fpHILIC	Negative	230.0740	2.95	unknown	240409	330617	268134	192311	318600	432557	376027	221980	303329	301346	663401	401283	256355	302787	324031	515707	409399	281528	466145
EIC	Negative	313.1197	1.99	unknown	990483	1779875	739040	803557	1667361	1028580	1826420	729418	1306324	0	2180419	2147002	2275086	1005819	1201295	3200474	1943796	267690	1307844
fpHILIC	Negative	119.9763	0.81	unknown	460499	449318	451509	514823	539080	507679	540816	580451	541268	483951	492887	552868	547711	504628	583610	0	727902	1453905	512841
EIC	Negative	339.2366	4.38	unknown	359457	347686	251365	206312	332972	256041	332966	318912	228360	277242	35057	256309	360563	269635	336931	310776	351818	391187	389616
EIC	Negative	610.3377	1.92	unknown	0	289176	0	0	240372	267945	303354	0	253036	0	326665	359191	361038	306761	258798	307147	288042	0	439223
EIC	Negative	375.1795	2.78	unknown	1956628	3920463	1256421	1194764	3692983	3465669	4192217	2117043	3612621	3856169	4491795	4391741	4158092	3852708	4601066	3615821	4459609	3465350	4591715
EIC	Negative	455.2564	1.81	unknown	50653	396933	255903	337763	0	366044	0	366044	223930	253468	399285	405213	435816	404998	406632	428192	453629	0	427076
fpHILIC	Negative	125.9949	1.94	unknown	430069	449076	400664	623648	452120	568447	431092	378022	597565	656005	743988	660615	645274	556558	701628	669828	608961	446341	526267
EIC	Negative	373.2372	5.83	unknown	511446	547388	389633	371072	520541	467204	399564	521962	357311	355420	468478	403071	456896	370119	524498	522050	550136	598675	560393
fpHILIC	Positive	738.5325	0.34	unknown	57898	113747	89076	119800	113747	89076	119800	99622	183323	156269	178237	188664	589443	94189	159343	223662	173536	192627	0
EIC	Negative	397.1795	0.86	unknown	85389	188081	96587	81750	303461	117840	323467	163675	398042	138292	247401	37981	149113	406617	182988	422453	204916	235519	343276
EIC	Negative	276.1970	2.86	unknown	282841	352907	175598	259948	294634	305616	264174	358216	287951	285724	356121	264771	358976	301686	402248	282323	393015	368615	567674
EIC	Negative	592.2995	4.85	unknown	441521	454430	599234	698053	646362	656510	766271	748232	765297	805343	726369	778709	895005	826214	894281	878613	853013	910683	825996
EIC	Negative	587.3596	2.78	unknown	9629680	9502912	4951276	5221207	10459740	8104980	14542450	8563795	5212356	6850518	14206900	10666965	13175524	9895793	10432741	9388798	13579329	9530429	15414803
EIC	Negative	321.0442	2.18	unknown	920046	1223314	1340488	288224	710868	732728	1399184	445417	1295309	437163	945897	1747396	1263553	1178276	1159711	1697249	1230911	419232	1076193
fpHILIC	Positive	221.0912	2.42	unknown	1093790	548066	231837	249098	833021	668982	807454	342484	603634	219603	470210	689368	580737	936566	1219364	609090	690418	539548	931185
EIC	Negative	588.3629	2.78	unknown	3852533	3693490	1863569	1973403	3867076	3058232	5457418	3293233	3490235	2543716	5398814	3867783	4873035	3734346	5322822	3508797	5061850	3588978	8801504
EIC	Negative	340.3303	6.80	unknown	516343	628944	649068	619411	670526	762728	620845	762728	734735	734735	734735	734735	828667	839928	525503	832542	625084	1085597	834986
fpHILIC	Negative	171.0413	2.73	unknown	261841	463871	267684	174704	361361	637703	316141	205119	221635	323215	551993	307910	330295	909277	617942	362339	281555	289053	574687
EIC	Negative	592.3278	2.83	unknown	311303	582789	223471	227034	476663	511725	554062	358656	473843	411336	599206	719939	385933	707371	757975	678348	559677	278080	889202
EIC	Negative	339.3269	6.80	unknown	2109256	2616782	2630257	2554710	2733306	3109760	2525741	3181319	2266334	3013215	3104039	3906675	2575094	3409960	3375467	2222616	3399566	4493645	3424995
EIC	Negative	401.2250	3.84	unknown	356999	1041212	318712	717902	835574	981180	739226	593881	951454	770463	1005048	904947	928983	932645	934657	966798	1065334	1058148	998291
EIC	Negative	614.1851	3.83	unknown	73889	169715	132190	193315	172074	188553	249313	161671	226825	173120	305410	323542	243273	278574	272062	271812	227475	186990	258237
EIC	Negative	278.2838	3.65	unknown	97906233	105484845	78874286	68893516	96290802	86280139	83697934	98361753	71414625	76518609	92432581	84570417							

EIC	Negative	424.2713	4.25	unknown	757114	699286	584707	506969	668336	591325	663295	798334	569642	612450	731065	643909	764988	660287	812636	669337	885774	900311	858334
fpHILIC	Negative	103.0041	1.68	unknown	11561584	46563808	32439944	43695860	26382714	53564352	31397194	25560862	45362272	40336460	47401992	39575096	38806200	44402772	72425280	51761516	26778844	41478344	36145556
EIC	Negative	279.0642	2.50	unknown	442312	337575	149318	224003	324498	315146	307271	380948	307221	579079	332451	307941	331347	362431	360952	344477	335497	670798	342427
EIC	Negative	424.2713	4.18	unknown	802097	933428	651504	594954	792773	732095	790815	1017853	708838	742897	920504	768517	998327	766934	965136	784877	1063298	1183911	1081659
EIC	Negative	643.3456	2.89	unknown	175779	329495	0	155046	208895	285319	181652	82758	376552	122852	64443	170533	173948	211544	250564	264947	253286	157906	540061
EIC	Negative	552.2827	2.60	unknown	417736	457392	269958	0	240507	345972	405211	345346	398206	378852	495788	391513	498868	404763	552736	359390	547235	443633	485774
EIC	Negative	272.0965	1.61	unknown	137227	252151	0	114760	114570	221857	273281	211052	0	33524	231525	323714	224420	160140	360046	329403	202377	0	182473
fpHILIC	Positive	249.1071	3.69	unknown	465543	742105	299737	387710	498942	961698	551933	348580	414219	350298	1003898	986745	807815	761320	707688	912040	672979	441424	724217
EIC	Negative	516.2732	2.89	unknown	319030	276048	0	0	231131	401072	211157	0	281750	0	173673	257081	197559	195276	324728	269926	369784	0	473444
EIC	Negative	288.1318	1.92	unknown	0	113112	0	0	54509	125138	109614	0	93999	0	94823	166328	148216	109738	120395	143150	107274	0	112770
EIC	Negative	345.2073	2.18	unknown	281858	537555	257408	360638	985991	1163838	1304694	1979165	1739760	397340	737362	89858	793360	2578581	1168581	2772243	425597	2414282	2280914
EIC	Negative	592.2995	5.05	unknown	402012	414184	571180	654297	506119	559682	618073	730313	732479	738337	651128	784055	752253	802480	724006	784883	804107	917631	747289
EIC	Negative	477.7391	0.84	unknown	218807	507414	177671	229767	304573	772648	173833	185030	151576	166546	278862	238689	260219	275506	632564	592868	316941	265336	201680
EIC	Negative	314.1796	1.88	unknown	431847	371407	0	0	426462	540186	426912	0	316160	0	468377	440313	544303	192884	659835	608606	579809	0	314881
EIC	Negative	279.1865	3.65	unknown	11712725	12456188	9458281	8352586	11535332	10210918	9709312	0	11879803	8579323	9441220	10902669	10119145	11023189	8997899	12570797	11575483	13264737	14190221
EIC	Negative	628.3532	4.78	unknown	0	11944372	0	0	0	0	0	0	12406813	6520055	0	0	7807093	0	7152326	0	0	0	8567123
fpHILIC	Negative	124.9914	1.93	unknown	18408396	19497436	18159146	29049690	19651032	25553762	20668342	17615270	25793236	30763636	32927038	29634750	29221876	25775922	34812348	30719384	26374882	21625344	24966936
EIC	Negative	457.1821	2.78	unknown	103863	464940	0	0	447403	401916	452842	183956	491211	379519	542413	454953	514022	466150	577448	442614	516461	395551	539201
EIC	Negative	338.2342	4.07	unknown	1673921	1773899	1303038	1009037	1659277	1458113	1495890	1758110	1244520	1355120	1725002	1449662	1743397	1530786	2025148	1515465	1882219	1935451	2297070
fpHILIC	Positive	169.0686	0.96	unknown	221161	235454	175237	208728	353819	362694	320949	191685	209319	196353	379319	243865	314133	413132	403132	302756	275554	259448	688271
EIC	Negative	309.1710	2.94	unknown	547497	789884	534542	445385	827874	765558	728930	614624	568201	511262	191713	831167	908783	809693	952126	812726	1026281	632480	1021681
EIC	Negative	322.0472	2.18	unknown	135945	213264	209088	43233	127022	126531	247537	63043	230757	61152	169265	33120	227475	199384	200614	281428	225363	90806	211283
fpHILIC	Negative	121.0296	0.90	unknown	2091073	1229347	1644048	1428918	1920246	2173081	1098374	1979703	1909938	1807238	984873	1812408	1941381	1615267	1646611	3298500	2276541	2288055	1807964
fpHILIC	Negative	126.9873	1.93	unknown	825333	856524	776099	1294434	877932	1181807	1004673	780336	1121020	1373258	1599666	1391414	1385821	1202256	1647942	1434099	1179172	984132	1394532
EIC	Negative	398.2266	4.23	unknown	204428	207998	140952	155235	191888	154188	167038	205890	187921	161108	209591	184116	230696	162537	205452	137278	270776	257771	223218
EIC	Negative	608.4777	6.44	unknown	13574221	21815452	306710	16271358	14262255	10756504	15440462	12551470	19914846	7136556	20923252	12597022	15599622	15665798	15104970	23392012	22960728	10310511	21139480
EIC	Negative	437.2459	2.48	unknown	371798	380825	150414	128997	411297	372866	313749	539267	414870	793620	421435	415018	411951	450426	425403	419388	418400	918556	433010
EIC	Negative	364.1840	1.92	unknown	0	117282	0	0	65277	153157	157596	0	109276	0	162573	268615	262840	180052	175199	147378	173431	0	122875
EIC	Negative	478.2413	0.84	unknown	172084	288254	98767	139568	174002	397882	96424	121255	114043	128812	192974	135948	147772	141988	334604	308890	186082	214164	110036
EIC	Negative	556.3526	3.65	unknown	762086	0	527688	0	942385	799711	0	527318	576096	742084	0	0	552533	0	941188	951055	1006033	0	0
EIC	Negative	435.3486	6.56	unknown	711229	347450	416374	651503	504785	534155	474295	588395	928428	722124	1086420	572474	741741	647643	796641	810903	558764	901571	821761
fpHILIC	Negative	121.0409	0.92	unknown	198759	271286	44030	168766	377610	438498	332655	114233	537626	143878	373377	467368	375627	300968	477858	611807	454437	292821	476604
EIC	Negative	311.2231	2.49	unknown	168964	71618	139391	81119	83838	138052	157707	104209	144286	81951	72481	89623	88362	97654	73872	366481	150986	116731	106096
EIC	Negative	420.2511	2.72	unknown	561122	1091462	714051	1264413	1184626	1093517	1034766	1096012	1136621	882334	1102545	1297830	3137373	1368989	1342726	1419996	1482254	1344895	1559084
EIC	Negative	434.2664	2.73	unknown	825144	245246096	798153	266955520	264950832	252985152	250338016	1605137	241320672	778528	244475888	251994128	321506528	298873184	318576768	317784640	326280800	0	344295744
EIC	Negative	463.3072	2.14	unknown	86565	17991	119430	90324	93867	27881	12375	494597	87180	227557	8960	31537	26766	62407	59554	41984	42758	732295	48980
EIC	Negative	605.4810	6.84	unknown	209056	146587	145737	0	191402	158218	250287	284957	158218	250287	203221	279043	233389	223244	212597	228512	166100	208597	208597
EIC	Negative	431.1394	3.80	unknown	172298	186651	154379	185077	196644	247544	171259	230124	162610	136266	145176	210072	236699	259854	209746	277683	277646	275016	263634
fpHILIC	Negative	401.1116	2.69	unknown	178295	597216	479194	256121	353076	419706	719025	472460	635628	348272	463595	503669	625470	443703	568020	396940	496820	0	0
EIC	Negative	282.1717	2.50	unknown	346885	400874	201788	219956	334032	302487	334308	404714	292363	394127	394755	343274	356282	384901	378864	338301	436129	538304	467340
EIC	Negative	402.2300	3.84	unknown	191106	334130	110303	178116	195162	264118	253430	176582	385058	391720	178156	333819	289329	319703	345112	370676	345027	321021	304444
fpHILIC	Negative	247.0933	3.69	unknown	325552	451586	223184	231640	358375	549171	307396	210969	221500	197022	513140	579214	471021	465284	434061	551520	407317	259232	449712
fpHILIC	Negative	346.1615	2.97	unknown	804488	783926	1046203	510368	1627695	1545341	1251341	1203010	373960	719238	1089116	1298676	1141777	991045	1132876	1481778	1330063	1529337	2217343
EIC	Negative	229.1809	2.65	unknown	156757	185035	120581	143806	199244	160911	185849	157708	182275	152327	180465	186847	215945	148022	151784	399415	209638	210662	179785
EIC	Negative	581.2969	1.98	unknown	0	119250	0	0	134728	167616	180259	0	381638	0	229416	207080	317485	448378	374229	246085	294368	0	208599
EIC	Negative	298.1664	2.15	unknown	187379	190905	158202	109145	228597	316092	194329	163869	170576	145196	425906	275909	375750	411273	408063	329960	340148	107024	210203
fpHILIC	Positive	282.1183	3.18	unknown	1243799	1772028	1142150	1032556	1027641	1655261	1971803	813001	998982	1145233	1933389	1488544	2051314	1318084	1933264	1776593	1742432	1276038	1688025
EIC	Negative	328.8034	0.65	unknown	56248	49518	76711	90102	83467	99248	100686	95067	145611	160724	121381	121463	141442	62715	111077	153325	118035	144368	155680
EIC	Negative	370.1593	1.87	unknown	73602	25343	0	0	98816	77755	79508	0	0	0	86771	62165	62255	28821	80817				

fpHILIC	Positive	126.1026	3.89	unknown	3181328	2232678	1097932	4052905	2122772	4190363	1193658	3492738	4174806	1923593	2136961	3749901	5651532	4938377	2271021	3838248	6843486	4742020	2689885
EIC	Negative	635.3386	2.65	unknown	0	93831	0	0	69675	79203	122050	0	40852	0	78177	94354	75042	68700	88818	90303	101335	0	138515
EIC	Negative	642.3421	3.39	unknown	708570	851698	435626	450524	480600	896707	538491	476106	938773	662392	771747	934108	727230	431991	681911	1162592	1031413	350225	1252446
EIC	Negative	320.2261	4.40	unknown	0	0	113730	106697	163980	0	230333	0	25720	131419	291145	370087	29647	0	0	0	55284	513674	0
fpHILIC	Negative	240.0628	2.61	unknown	536346	871897	687345	338833	598052	661421	796078	535823	475235	622665	908551	767064	717638	957541	1291234	728201	760152	668749	680872
EIC	Negative	284.2588	6.56	unknown	236128	236819	321772	351913	335126	265265	369463	330485	834668	278656	555864	437785	690979	465007	486711	356994	487185	615895	456767
EIC	Negative	282.2520	6.56	unknown	24968769	26475446	32478072	35683096	35299490	27647978	0	0	8526442	4558746	6699389	0	0	0	0	0	0	0	0
EIC	Negative	293.1762	6.03	unknown	0	0	0	0	0	0	0	8526442	4558746	6699389	0	0	0	0	0	0	0	0	0
EIC	Negative	362.2373	4.96	unknown	0	0	0	0	0	0	0	102294	182929	0	0	121034	101070	97345	0	0	0	0	256627
fpHILIC	Negative	737.5231	0.35	unknown	445161	1184838	1073375	1307866	1660180	339177	1267487	874562	2310669	1225706	1741414	1641852	1600879	6281102	1267639	1978308	2227817	1636229	1623052
fpHILIC	Negative	163.0247	2.90	unknown	1057741	813850	527014	584635	769504	863703	979767	552282	1111216	453111	472528	835426	795098	1102606	1202140	1160951	1279501	893903	1276465
EIC	Negative	534.7828	1.29	unknown	81633	268323	0	0	204076	307391	107682	0	98993	125720	190886	214254	213840	176036	362527	219157	282909	0	113504
EIC	Negative	307.0648	1.95	unknown	3418020	14621570	3209874	522052	12134324	10537693	14707507	999324	5502674	2978548	14715839	16073362	16242425	14746399	22437186	12641999	12379693	675007	11635288
EIC	Negative	565.5146	6.55	unknown	621759	550419	791775	1179338	1522087	592049	1267213	1175259	1038768	782096	2395920	1104882	3604448	986842	1467806	985165	1604053	2718631	853565
EIC	Negative	363.1810	1.92	unknown	0	537659	0	0	216094	727626	652685	0	516011	0	702263	1143333	1159330	843470	791970	702443	778141	0	608777
EIC	Negative	436.2718	2.72	unknown	5755334	9685663	5555507	10599610	10949602	10468911	10079299	7724508	9473294	7865903	9489212	10242341	12637502	12583882	12786648	13528707	13771651	12826952	13623886
EIC	Negative	509.3497	3.04	unknown	97857	120351	97994	67600	194983	152872	218874	196802	202092	144280	199215	66416	127242	156558	271810	352301	243387	177949	274158
fpHILIC	Negative	119.0542	3.17	unknown	1462325	2199777	1472834	1230312	1484934	1950358	2036709	1593453	1708227	1742270	2541093	2719006	2522635	2964572	3183688	2703784	1887707	1836782	2768400
EIC	Negative	624.3314	3.79	unknown	376601	1869984	359948	691533	1034020	1530503	1099516	453644	1128878	763665	2162221	1458499	1828809	1454156	1553186	1815400	1673993	539103	1605569
EIC	Negative	308.0680	1.95	unknown	580892	2491218	381483	0	2134568	1800175	2514732	0	946846	0	2547298	2788167	2788537	2571784	3829535	2168989	2174048	0	1987158
EIC	Negative	642.3422	2.68	unknown	1242532	1478269	777652	893328	908478	1676606	1075365	844919	1875247	1327881	1054699	1762483	1331591	717469	1331417	2312538	2033705	618550	2485573
EIC	Negative	625.3343	3.79	unknown	135233	708962	135852	250613	360373	578287	389227	412255	269917	769635	544721	686890	502674	578938	649127	606789	222104	578288	0
EIC	Negative	608.3592	5.27	unknown	360593	266709	129216	220090	280326	251065	348434	285841	434363	174132	193001	296121	401302	379849	428834	413795	498430	317450	557794
EIC	Negative	305.1432	3.83	unknown	413567	267774	489523	729502	434480	343331	590636	35191	573293	533200	252228	611524	782166	328842	592076	754915	457071	624949	294040
EIC	Negative	619.3462	2.71	unknown	932457	769139	517445	568461	459784	1099061	782405	681851	839907	1109306	811258	1324093	921618	478499	889294	1177325	1327380	588923	1360793
fpHILIC	Negative	530.3031	0.59	unknown	389437	723065	125106	162457	472245	417950	378763	408141	539921	0	516649	494836	582206	567915	295921	542177	343242	1462684	426898
EIC	Negative	412.1849	2.18	unknown	45402	112099	44769	191095	55072	81117	99728	100135	140544	0	61567	152809	65382	11419	50059	130218	65692	233088	181300
fpHILIC	Negative	216.0308	0.94	unknown	89795	42244	0	39398	1564380	2596727	1587934	789690	867055	0	0	92710	57383	106558	3133112	1832484	1664996	1516971	1869455
EIC	Negative	435.2692	2.72	unknown	35600416	59501464	33881568	64543632	66163013	62962490	61079633	46925835	56553599	48977085	56967452	63249607	75836000	75164021	78894481	82380667	85026665	77287807	83719727
EIC	Negative	434.2662	2.72	unknown	133715964	224162548	127945177	244092324	250169495	238566553	230640004	177227416	214337834	183736556	216561506	236283591	286733634	286587986	29954211	311000377	323583378	293434789	314379058
EIC	Negative	358.2161	2.72	unknown	198197	202312	89250	259785	266147	262688	297048	197832	245468	203753	231851	242613	370382	372191	320716	328655	425330	326541	365158
EIC	Negative	642.3422	2.79	unknown	821719	2205509	634904	735636	1104360	1999628	1157952	677493	2132293	1449274	1677882	2124173	1446220	874306	1541780	2469255	2393449	710895	2710783
EIC	Negative	376.2513	2.72	unknown	2190708	3684685	2001982	4134713	4092047	3895656	4008643	2877501	3626578	2950598	3598888	3837603	5007510	4679871	4894725	5111537	5452019	5050020	5199671
fpHILIC	Negative	200.0414	2.46	unknown	396955	679818	463872	255675	566603	589217	726332	372542	659535	480558	964909	1014001	697988	828602	1035204	691642	665693	620703	1038129
EIC	Negative	375.2481	2.72	unknown	15659271	26260095	14552206	29167356	30101434	27243394	21332206	25529812	21564400	28605075	27822525	34761403	33843518	335768642	37419513	38771519	35266262	36955342	0
fpHILIC	Negative	488.1621	3.66	unknown	67524	203720	246555	40237	44946	66818	262023	83274	584093	0	0	88930	40058	305060	53947	51575	98088	135353	1131400
EIC	Negative	618.3422	2.63	unknown	450806	519379	297149	321348	416844	808980	556146	522239	467315	557837	861780	563215	323210	675151	974246	960289	225079	967589	0
fpHILIC	Negative	136.0331	2.83	unknown	1006636	800263	555984	584412	726043	1075012	630414	654040	747272	719588	697014	753641	698858	1590074	1119702	1141869	1045826	869322	134447
EIC	Negative	505.3170	2.62	unknown	0	151099	0	171736	119794	162244	113428	0	75319	164044	123791	157565	300512	162359	146074	143514	172152	0	978786
EIC	Negative	643.3459	3.06	unknown	451825	577608	323231	360765	407070	574738	463929	275350	631347	440206	567175	669438	505557	299494	544831	798489	801951	256500	885240
EIC	Negative	608.3191	3.87	unknown	619626	1808765	531143	621008	1243429	1459834	724891	1109239	2025057	2086790	2017134	2321198	2133870	1815439	1561695	1855665	0	0	0
EIC	Negative	271.1096	1.46	unknown	0	64914	0	86241	93111	95658	0	107967	0	78385	85703	100841	88635	96648	238219	106720	0	95191	
EIC	Negative	539.2318	1.91	unknown	0	125432	0	0	116010	125236	126460	0	115758	0	127998	127598	94231	90011	164704	193491	179811	0	141044
EIC	Negative	491.3382	2.67	unknown	117236	105377	51349	36981	96681	120009	109976	83173	60497	250708	155718	155462	102982	504365	177234	112088	133221	117950	120241
EIC	Negative	384.1854	1.87	unknown	76290	207117	0	0	49023	115884	177767	0	217955	0	233360	84661	242471	228852	196383	237649	153715	0	200214
EIC	Negative	390.0709	1.95	unknown	0	120682	0	0	107475	81078	120991	0	40160	0	120465	131547	138752	124038	195150	99589	92054	0	104831
EIC	Negative	374.2452	2.72	unknown	64973897	110174015	60818535	120982160	122963251	116903392	115204410	87490531	105882244	91101432	106582625	117042910	144144242	143566576	150858238	156370851	162354174	145076560	156981388
EIC	Negative	481.3329	6.52	unknown	369862	661846	420028	714573	1370275	877741	1841059	804119	1166854	446321	1152141	767031	846162	1262741	1813031	1385230	1388542	497382	3448718
EIC	Negative	614.5445	6.54	unknown	3533906	2133393	1466118	4248585	2628706	2462858	3149728	6083157	4291940	4480181	4321853	4061381	682665	6834624	4369404	5013032	609662	4332521	5899565
fpHILIC																							

EIC	Negative	251.1268	2.54	unknown	0	0	0	74675	632486	0	0	40522	0	481837	442611	0	0	0	495953	46623	0	435735	
EIC	Negative	466.2442	2.44	unknown	0	355505	0	0	313590	267327	288396	302328	303755	422018	427034	324909	430028	328181	429940	320893	419067	555493	426644
EIC	Negative	381.2291	0.86	unknown	47018	59486	75295	72595	170924	196760	146496	265630	71038	75010	110209	95763	45130	79198	289499	194951	187132	380015	189513
EIC	Negative	500.2791	3.42	unknown	328369	1001409	2059447	0	1206879	0	0	2779900	0	0	0	1940231	2738091	30837	1297972	1814305	2716995	0	0
EIC	Negative	292.1566	2.36	unknown	42802	101194	0	135253	71906	122093	73461	71492	53259	147863	114812	122994	147838	78777	126856	129941	129417	103757	83745
EIC	Negative	618.3442	2.48	unknown	300397	339405	102638	154585	246633	575865	294449	341987	339939	466747	348548	601332	361524	243750	437902	623077	628145	293318	650203
EIC	Negative	322.9961	1.19	unknown	0	64653	81189	105072	6710	0	154275	194275	143689	166091	0	181302	169149	184113	16841	184556	180164	186761	138882
EIC	Negative	285.0723	0.98	unknown	21982	0	10133	38987	35446	28538	54872	64391	53257	41056	16364	53853	54952	38214	77063	64704	100711	51803	53101
EIC	Negative	376.1604	3.65	unknown	106081	97908	310180	143632	233250	236793	176431	271161	267099	149996	297252	239871	336444	252483	373771	332212	351328	305685	377328
EIC	Negative	431.3176	3.86	unknown	141416	218465	143287	123749	313885	360527	337963	424632	278572	310568	394501	297259	215653	213683	565335	652292	293926	692233	317148
EIC	Negative	237.1085	2.07	unknown	0	0	0	0	0	0	0	0	309850	0	0	0	0	0	455754	0	0	0	0
EIC	Negative	487.2319	1.87	unknown	172398	722088	0	0	215197	331103	556769	0	803052	0	836465	297277	850160	887617	723394	832041	568517	0	687368
EIC	Negative	434.2662	2.88	unknown	1779740	3545382	2113371	3686670	4516726	3982953	3311969	3094940	2939446	2041317	2811776	2933678	4431483	4663929	4786771	5570035	5935589	4640186	5414900
EIC	Negative	375.2167	4.74	unknown	42847	38840	45831	53597	61778	37478	61121	77472	52935	55656	0	38115	0	28738	27432	275821	40851	47109	39397
EIC	Negative	327.1636	4.22	unknown	0	0	0	0	252561	261856	79961	0	206527	258981	0	0	0	0	133143	351345	407417	298318	0
EIC	Negative	374.2452	2.88	unknown	846529	1645777	1014240	1722905	1238880	1881370	1557963	1455449	1359888	974848	1341879	1387424	2126060	2199655	2322409	2707549	2790590	2081929	2566484
fpHILIC	Positive	155.0789	4.84	unknown	320950	337349	272935	203617	258495	260367	359467	211003	342201	380318	281059	295921	354328	360841	574273	336623	531249	314301	379543
EIC	Negative	389.0681	1.95	unknown	0	636466	0	0	495700	417753	572657	0	235212	0	657039	693998	707899	634456	968088	530622	524609	0	546796
EIC	Negative	618.3421	2.85	unknown	426402	674662	318774	245058	571117	959579	664409	347823	677786	490539	681918	990897	642493	497991	900339	1051243	1116309	364515	1378561
EIC	Negative	349.0388	1.99	unknown	0	253789	243047	0	115529	500708	233702	0	121786	0	773146	300721	184094	69545	299966	682632	0	419378	0
EIC	Negative	363.2096	3.91	unknown	0	0	0	0	969106	0	1751989	0	1033025	0	0	1063242	0	138632	0	0	0	4781601	840111
fpHILIC	Negative	280.1039	3.18	unknown	637391	1257517	752475	594822	872196	1200154	1215668	585537	622864	672250	1469753	1394827	1474871	1107393	1826859	1254648	1245210	956047	1498888
EIC	Negative	436.2719	2.87	unknown	75747	155318	132007	153830	183168	178858	142862	120378	121621	93380	119304	136552	191352	193835	190410	237016	264224	200328	229347
EIC	Negative	304.1591	1.88	unknown	193123	123888	0	0	85469	152077	113218	0	63511	0	135842	207438	134495	249908	153395	164327	136010	0	168541
EIC	Negative	407.2347	1.87	unknown	515051	2032393	0	0	470965	1036682	1499448	0	2167898	0	2711502	835664	2405136	2481069	1966574	2570727	1418296	0	1822917
EIC	Negative	331.1913	1.47	unknown	0	441337	0	202207	368763	192098	434843	0	423902	0	326059	426172	476160	587270	571518	707027	431720	0	421813
EIC	Negative	472.2214	2.72	unknown	1046785	1626475	1272307	2592332	2705769	2887278	3225798	2412125	3241916	3058212	3540543	3570873	4196787	4100441	4386137	4351435	4424499	4350746	4276243
EIC	Negative	510.2909	6.36	unknown	936773	1213600	1449595	1253817	1325456	1322730	1488951	1822506	1110992	1343311	1725455	175441	1416574	3045515	2801045	1213333	1824272	2700941	2120872
EIC	Negative	435.2692	2.88	unknown	475825	899973	579073	985529	1169715	1039321	908076	774303	744480	574928	744423	822623	1187070	1180923	1272190	1501797	1573279	1182119	1464106
EIC	Negative	395.1842	5.66	unknown	0	1064905	0	1109095	954418	76728	1066162	0	1068942	1249230	1248283	1161712	1478274	1021540	0	1567502	1553923	0	1695144
EIC	Negative	241.0506	1.40	unknown	0	0	0	0	0	0	0	0	0	0	0	0	0	0	50136	88783	114817	0	94319
EIC	Negative	294.1821	3.30	unknown	0	0	0	0	726980	0	0	0	0	0	0	5944	4100	0	0	0	453006	649114	0
EIC	Negative	289.1812	5.08	unknown	448503	481946	535386	446418	746562	378887	646975	602880	692999	348957	620256	479668	887008	408323	854671	1008161	1214625	617625	958073
fpHILIC	Negative	233.0570	0.96	unknown	436994	191319	67482	76660	324168	141253	322605	87074	366849	115054	129903	292553	218773	476071	663572	218349	321249	221763	459673
EIC	Negative	406.2318	1.87	unknown	3507397	12097781	0	575203	2859547	5145967	8991646	539064	13102389	868451	14147563	4286540	13999305	15194804	11714465	15307117	8683955	0	10867956
EIC	Negative	330.2368	2.01	unknown	409030	196370	204622	0	209526	663319	424295	137098	299127	0	176037	285281	239623	167360	151629	1920624	304300	0	258407
EIC	Negative	383.1813	1.87	unknown	248144	846895	0	0	297607	405696	694341	0	947343	0	1006608	424613	1023842	1102546	893924	1109077	647186	0	919865
fpHILIC	Negative	264.9424	4.61	unknown	655704	269548	59967	151824	420532	703901	233957	212434	475207	107468	105828	530442	371801	543451	343057	948255	657506	531187	635355
fpHILIC	Negative	197.0314	1.73	unknown	0	584761	657704	930659	916556	0	954179	101492	1088989	868636	584848	748333	742004	938776	971392	851923	1341664	1289013	1446119
fpHILIC	Negative	144.0456	0.57	unknown	7385458	2136413	1275941	1610257	3744880	3687505	4756926	2991814	3803665	1259104	2298237	5112258	3091370	6517663	6332166	4165937	6624647	5402164	6447134
EIC	Negative	463.1444	1.87	unknown	0	208800	0	0	42562	100437	164621	0	202616	0	91424	281287	290222	270216	214937	233313	174647	0	162422
EIC	Negative	642.3422	2.59	unknown	881901	1442099	353087	604513	766024	1649651	776293	472540	1601464	984176	1349147	1766897	1276639	637693	1201366	2239635	1959519	440000	2230236
EIC	Negative	382.1876	1.87	unknown	176083	623579	0	0	180435	282717	461516	0	640034	0	649789	335594	722156	817108	610644	747704	455932	0	539944
EIC	Negative	381.1842	1.87	unknown	655419	2568102	0	0	706721	1224863	2016770	0	2810822	0	2938518	1099278	3050475	3367008	2694181	3238515	1941405	0	2537691
EIC	Negative	408.2476	1.51	unknown	0	420780	0	375781	210949	313618	289393	0	289630	0	585479	206282	487341	553724	268978	565937	185185	345921	361961
fpHILIC	Positive	228.1958	0.49	unknown	1101888	876240	1134405	1395718	891391	832901	1105003	923800	1121317	1565922	629143	1685555	2625708	529581	1326362	1125521	1938113	1894444	1275171
EIC	Negative	344.2315	4.64	unknown	408386	323571	55486	1030310	307487	304633	281229	301599	1227978	173068	176231	406512	960537	432000	401377	729709	1243683	869612	520792
EIC	Negative	388.2429	4.60	unknown	465908	784841	393776	517548	638523	685291	591305	515984	571641	320711	590385	634131	938568	888512	913922	1019515	1041902	633092	1075603
EIC	Negative	294.0968	1.08	unknown	0	12264	0	50518	3920	21366	3341	62432	64944	0	22811	43046	92519	81413	5373	20036	134281	64342	19437
EIC	Negative	370.2319	1.81	unknown	113989	60941	0	0	72013	131529	0	167738	437453	0	88591	278296	437188	514727	85220	94302	936608	0	83387
EIC	Negative	425.2765	1.67	unknown	25650	72506	0	0	80407	65938	69254	20354	75450	49678	79677	66227	74895	66053	74361	201023	89937	52040	72567
EIC	Negative	511.4731	6.54	unknown	3269671	4255423	4199197	7008315	5371197	3304241	5507724	6480638	7765070	6									

EIC	Negative	374.2452	2.94	unknown	664734	1086153	791576	1366484	1469565	1294358	1081973	1160563	1059364	760274	946037	1256409	1585648	1650658	1775035	2058147	2245278	1845954	2145064
EIC	Negative	613.5415	6.54	unknown	5134043	4835236	6890793	10563427	6525653	5784589	7930283	8607938	10253212	22088720	10321956	9125815	16417277	16128293	10225443	12504376	16428257	11228442	14625204
EIC	Negative	518.2877	2.94	unknown	84980	79392	62047	62047	78809	210660	41876	445933	63677	76829	0	63672	5266	2450	266750	79783	63534	908944	83943
EIC	Negative	434.2663	2.94	unknown	1445662	2215782	1687816	2785439	3143090	2698536	2244287	2318580	2116593	1615530	2096260	2519320	3346752	3434922	3739064	4366966	4567448	3829452	4392720
EIC	Negative	389.1982	3.11	unknown	0	91921	0	18221	29879	105767	42247	0	44581	15767	80916	157347	132628	74532	100146	81648	83272	20723	86394
EIC	Negative	294.2156	4.74	unknown	105197	127919	147518	214804	166403	145959	180576	157536	221558	135643	100467	127505	113252	102907	112705	874303	159116	184570	130680
EIC	Negative	408.2472	2.20	unknown	0	408369	0	1126323	469342	293364	699282	147504	527183	881493	748780	320658	656705	589524	431026	784029	389196	1194361	614783
fpHILIC	Positive	188.0345	2.98	unknown	2012126	2189684	1533622	435089	1997702	2047720	1007860	1754348	1977676	1349605	1403059	1666020	1332005	7196896	5134088	1315959	2063937	2177690	4068990
EIC	Negative	443.1672	2.59	unknown	0	0	0	0	56055	0	65813	0	51211	0	75244	94844	139893	82974	88085	52138	81620	0	69498
EIC	Negative	573.2321	1.93	unknown	0	426877	0	0	377748	321425	568997	0	323687	0	408431	601601	523522	562086	503097	630249	974279	0	57962
EIC	Negative	408.2395	1.87	unknown	57040	141682	0	0	0	84649	148385	0	232260	0	204438	0	246827	249699	221320	275465	140904	0	147965
EIC	Negative	471.3480	6.54	unknown	977287	549675	754995	1105692	877531	663085	1008137	1078650	1008619	1907781	1480890	760709	1018805	1568463	1913229	2276041	1024892	1180683	1436033
EIC	Negative	391.1740	2.73	unknown	237042	280540	108676	136792	263585	214062	325161	159557	193673	420510	254948	280487	304634	322419	426208	227203	418411	479028	401986
fpHILIC	Positive	304.0993	3.16	unknown	269193	989773	417730	369171	440624	664877	699282	365565	468504	534943	874877	1006101	943030	1002246	1091288	784186	775119	689399	1117869
EIC	Negative	435.2409	4.03	unknown	0	0	0	0	97765	0	0	0	0	123136	0	0	0	0	0	0	0	165500	0
EIC	Negative	346.1740	2.45	unknown	256707	530579	264663	220058	255570	466822	418706	290551	291739	185578	580789	677287	828003	564321	759614	556907	544595	942620	114153
EIC	Negative	335.1405	2.27	unknown	0	0	0	0	0	0	275430	0	0	0	0	110475	0	0	0	0	0	467174	0
EIC	Negative	411.1997	2.60	unknown	88376	63442	0	0	63568	134998	30519	0	47930	0	81066	59131	41071	170235	132406	38303	135272	0	163884
EIC	Negative	329.2337	2.01	unknown	2621228	1046127	874101	611334	1008584	2825485	2199322	521837	1625242	758981	789420	1495374	1191844	1009416	905883	9403001	1901566	607386	1221001
EIC	Negative	433.2213	1.48	unknown	0	255528	0	0	129429	117234	206420	0	171196	0	212724	244775	220338	260439	340488	248011	0	214773	0
EIC	Negative	472.3509	6.54	unknown	340574	235210	277445	355827	337912	247802	331919	374002	359605	552837	520058	253845	383752	431310	736651	795055	357960	459331	471120
EIC	Negative	490.3260	2.87	unknown	0	75275	0	0	57275	145200	86417	0	61235	201224	114650	112466	90302	105774	156440	108766	105575	123305	102244
EIC	Negative	628.3973	2.68	unknown	101159	243677	139809	201887	228485	126126	199484	90413	292493	79149	144383	181127	316045	330721	327955	597594	273184	174337	235442
EIC	Negative	528.3215	5.42	unknown	0	0	0	0	0	0	1594783	0	0	0	0	0	0	0	0	1152011	0	0	1602242
EIC	Negative	447.3483	6.54	unknown	4878675	2555609	3544045	3696406	4168949	2846396	4419189	4140887	4009104	6041930	6556937	3389765	5393858	6218828	9412820	8620355	4551196	4958159	6309580
EIC	Negative	428.1767	2.31	unknown	52492	306793	64245	223953	122317	151647	188064	226070	190661	489260	246920	403629	328247	304921	304786	253711	243744	482222	230516
EIC	Negative	301.0598	0.70	unknown	18542	42225	32856	35243	37161	41357	56149	53624	33409	49435	69941	71963	73724	78438	82133	85807	81387	97963	36324
fpHILIC	Positive	303.2315	0.37	unknown	295106	143736	103231	980821	120703	196687	109774	443742	967468	110744	185188	466579	1046864	592865	170806	209523	1455667	980814	366615
EIC	Negative	451.2654	4.06	unknown	0	284706	0	0	102705	362127	0	96675	169382	0	246564	209041	178821	465173	284410	236083	229338	207293	314381
EIC	Negative	379.1412	0.60	unknown	11926	0	0	0	37686	0	7242	0	94981	104073	0	66884	114886	63157	0	0	25403	102734	0
fpHILIC	Positive	192.1596	0.59	unknown	3495045	1719963	1795606	3654699	7115196	2129285	2399805	2698491	4122164	1934989	4600083	4802553	3231586	2169515	12475827	3736803	10551953	2673543	2685182
fpHILIC	Positive	251.1025	0.50	unknown	556533	105945	62694	196677	359919	261667	597223	316415	466788	110884	87704	367982	433721	711362	858721	233748	802821	571440	1037889
EIC	Negative	417.3226	6.55	unknown	15724501	8889110	10888284	16048001	17038663	15999903	14673391	20657738	25579516	26082990	25935190	20794314	30065995	33854257	33888290	26090991	25964213	34240454	45026711
EIC	Negative	387.1464	2.97	unknown	32559	43019	0	24582	64073	52350	53565	57280	51490	65880	109535	112511	103108	128536	105244	105657	120437	87349	744722
EIC	Negative	348.2631	5.60	unknown	120578	32961	40155	246810	83964	77491	40682	96764	222127	51604	20401	124824	204231	127697	116818	114371	314802	301844	78228
EIC	Negative	574.2347	1.93	unknown	0	133873	0	0	120928	94183	171763	0	90461	0	138032	206056	156066	194396	150487	207086	313095	0	179168
EIC	Negative	598.3077	6.32	unknown	63362	169774	302569	248951	254108	476778	351651	449359	307517	395159	553488	526430	593427	421621	981185	386265	612495	877666	0
fpHILIC	Negative	223.0750	2.81	unknown	199540	182988	232479	196067	245641	560978	264387	203086	384795	197518	224203	322983	615671	197098	106592	2064897	263787	311949	213388
fpHILIC	Negative	133.0508	1.00	unknown	308027	341809	336063	369489	418922	484341	267326	355527	293710	389382	501918	442999	398206	1072694	534035	437305	722824	574000	979425
EIC	Negative	333.2200	5.72	unknown	0	406800	0	0	573047	464062	488544	0	465005	0	263793	294354	418642	397231	316164	1862640	312130	642557	427871
EIC	Negative	300.1685	1.92	unknown	0	215829	0	0	103548	149970	195621	0	90125	0	269885	354798	302234	228895	276025	905792	237817	0	193532
EIC	Negative	639.5575	6.55	unknown	21079025	9773642	12650727	19838170	20118860	17911856	17016775	19484049	35501663	28073512	33964156	25276385	46857760	43845019	39826672	29979489	32219340	46247394	49112033
EIC	Negative	409.2608	1.16	unknown	23291	13882	19949	0	46243	30010	41229	68838	50853	50853	24032	24237	15871	37308	84740	48007	73716	230078	158121
EIC	Negative	443.1837	1.87	unknown	196674	518832	0	0	214239	419868	763625	0	1162105	0	1295190	400408	1450850	1426583	1150372	1543454	868319	0	1074431
EIC	Negative	418.3260	6.55	unknown	3974656	2333256	2675285	4068136	4293480	3986187	3651262	5195810	6162061	6728263	7578637	5329722	7715182	8658105	8649115	6740887	6715584	8656772	11674210
EIC	Negative	449.1948	1.48	unknown	0	49369	0	0	47286	64699	101255	0	64880	0	106167	111668	147093	98206	123985	162041	119653	0	99969
EIC	Negative	640.5612	6.55	unknown	9056136	4270666	5652907	8423234	8576747	7552535	7448495	8394838	15461905	12515420	17488586	10946554	20579354	19303543	17612710	13238147	14084629	20332066	21104589
EIC	Negative	409.2609	1.41	unknown	0	41279	0	0	266334	237083	183733	0	187051	0	161505	162403	54956	220531	427738	301013	535665	0	287947
fpHILIC	Negative	305.1432	0.90	unknown	1556632	1027879	1328494	1340222	1385544	1126208	1296336	1499892	1133297	1913079	1575661	1880030	1521712	1753319	1510931	3036757	1895032	3989654	1336672
EIC	Negative	329.2389	6.06	unknown	0	359600	0	0	0	0	867887	0	0	0	368949	0	0	0	427789	244132	276408	638642	0
EIC	Negative	512.2635	2.38	unknown	0	73657	0	0	32272	30074	58146	0	124081	460671	65023	34922	66835	80976	221388	95315	64980	0	66642



EIC	Negative	447.2058	1.92	unknown	0	470244	0	0	179823	184577	200555	0	201141	0	380337	362165	269156	297899	304621	528359	444801	0	290211
EIC	Negative	306.1462	2.97	unknown	250776	252826	273284	279366	389950	318220	387684	289714	416738	484237	741345	866952	721521	943939	699682	789498	979398	738013	496493
EIC	Negative	433.2214	1.98	unknown	0	246378	0	0	85498	107404	158155	0	104789	0	214418	221426	137080	148497	168728	271621	287162	0	214550
EIC	Negative	305.1431	2.97	unknown	1554841	1544463	1597431	1720644	2410061	1994085	2368572	1653166	2462162	3104566	4599261	5267304	4489725	5640429	4450312	4748770	5802576	4522711	3088531
EIC	Negative	434.2237	1.92	unknown	0	364517	0	0	143199	137507	156923	0	164267	0	314695	2529306	225261	239713	242882	395672	366624	0	246133
EIC	Negative	423.2260	3.91	unknown	46435	27813	0	0	91548	138827	52462	165214	88611	0	531786	84829	24874	0	0	593092	82231	421358	19537
EIC	Negative	483.2365	4.76	unknown	161238	41267	0	366668	32653	49466	0	205968	375075	21791	95440	239535	387424	294825	166674	106180	482054	526082	107477
EIC	Negative	251.1322	3.31	unknown	0	0	0	0	0	115025	0	0	0	0	0	0	123306	0	0	101465	139485	0	0
EIC	Negative	412.2424	1.99	unknown	0	189704	0	0	49945	97827	93954	0	107667	0	191921	179470	113734	83475	103195	278756	197884	0	159535
EIC	Negative	448.2731	3.02	unknown	162583	87134	162700	331670	140365	115343	270135	232776	259256	172227	223876	308248	434195	61978	54892	555175	536080	485113	547048
fpHILIC	Positive	404.1774	4.66	unknown	385110	63649	0	214123	42850	110152	0	253461	729497	0	49017	335581	454840	780583	117324	100502	1288681	607589	326937
EIC	Negative	325.2658	5.83	unknown	1053251	0	0	0	1457354	0	0	0	1102166	1186517	1228175	0	0	0	1361452	775840	0	2173302	1202837
EIC	Negative	361.2013	3.54	unknown	345490	169162	142475	629698	76136	247968	46791	436146	1026191	41968	213714	627072	961800	1080850	220619	162873	1800057	1568262	201384
EIC	Negative	448.2797	3.02	unknown	0	266515	151551	376493	350554	271611	305453	110362	308833	0	244390	354586	495980	435420	439924	657712	612453	570892	634508
EIC	Negative	433.2212	1.92	unknown	0	1543926	0	0	562336	569821	656399	0	649588	0	1256685	1202000	917056	1029001	1083358	1682439	1508239	0	1039432
EIC	Negative	580.3622	4.53	unknown	2461359	2308647	1865130	2255878	15055338	1549282	2020427	1584922	2095975	1616980	1809578	2211171	2231565	1906737	15277646	2022195	14796695	14717400	1877729
EIC	Negative	526.2845	5.06	unknown	0	0	0	0	3822612	0	0	1326455	2351558	3525434	0	0	0	4252170	1285772	2872855	0	3041508	
fpHILIC	Negative	319.2276	0.38	unknown	1533081	884822	754092	5223019	1095040	1490434	917547	2443092	4891384	662254	1245090	2963014	6224401	3916574	1652489	1562688	11370218	7262106	2335896
fpHILIC	Negative	115.0039	0.83	unknown	842564	1748616	1164794	951208	1362030	1743370	878961	871459	853775	736588	834214	1176760	1168168	1057974	1163126	1887228	1625811	2119593	5946747
EIC	Negative	319.1599	3.13	unknown	0	14323	0	0	161069	54016	67223	0	80218	94430	464988	0	169666	50243	133567	139630	124672	159564	430757
EIC	Negative	319.2280	3.84	unknown	0	0	0	11536961	0	0	0	10742769	12211002	0	13254241	0	0	0	12807031	13063435	13073225	0	12557610
EIC	Negative	261.0220	1.95	unknown	0	87357	0	0	68274	84071	75412	0	79343	0	81927	99682	152679	88843	74692	115079	415765	0	96913
EIC	Negative	644.3514	2.67	unknown	0	0	0	0	103479	96263	0	0	0	74247	47154	173417	131464	0	0	0	213269	0	247169
EIC	Negative	439.2258	6.22	unknown	228398	445575	96245	126551	509791	934904	136885	310040	392946	209372	184768	1004289	333142	237674	219992	2576868	312395	1158751	1023199
EIC	Negative	440.2297	6.22	unknown	42124	103859	0	36867	137997	225718	36114	73718	115387	55138	0	264681	83116	60410	55422	677402	83546	300167	251660
EIC	Negative	492.3421	3.19	unknown	78208	63892	79868	53809	73239	83718	70175	88099	68477	259107	174527	196853	101984	79767	241648	252990	109846	221376	627929
EIC	Negative	491.3381	3.19	unknown	280406	206200	266665	177343	223410	272877	205844	242695	217040	761556	513650	603105	329115	254401	755012	781170	309244	689318	231597
EIC	Negative	321.2342	4.76	unknown	809634	290549	0	2337982	222674	447446	259568	1229778	2173200	0	393931	1347914	2881081	2078143	700177	560718	4852779	3611969	596897
EIC	Negative	279.1968	3.54	unknown	2773068	1360117	298375	8478730	495603	2736846	211330	5168821	11227278	613202	2518799	7242601	11069322	12647701	2119106	1981807	2283990	18713170	1599416
EIC	Negative	441.2524	0.88	unknown	21271	52716	30714	25923	164287	152557	108026	69758	108624	62095	109187	77710	53280	84532	216751	217322	316796	344487	290839
EIC	Negative	280.2000	3.54	unknown	507709	263825	76218	1370252	104815	496487	47693	897996	2137974	135444	489398	1320344	2117518	2360894	471210	407491	4345839	3464838	329259
EIC	Negative	328.1846	2.19	unknown	32331	0	0	0	0	106384	0	51941	0	0	0	0	0	0	0	276950	0	111439	0
fpHILIC	Negative	259.0906	3.16	unknown	67290	267825	39311	0	129846	209286	126221	63285	99852	74623	304169	375648	272409	557380	494640	324948	188837	150183	384792
EIC	Negative	320.2312	4.76	unknown	5832006	2297050	507973	17278146	1627731	3117386	1586759	8857965	16462577	1124978	3491684	9968528	21638369	15773773	5348044	4169274	36098360	27919501	4466747
EIC	Negative	449.1948	1.92	unknown	0	262761	0	0	150465	169347	239078	0	221741	0	438257	347874	361475	396780	618625	567470	0	0	362029
EIC	Negative	577.3016	5.05	unknown	122847	577339	128716	329880	332943	560852	347511	217125	331828	525916	1209937	814954	1356474	693173	919412	955471	1118496	557812	936205
EIC	Negative	429.1684	2.75	unknown	0	0	0	0	107668	152155	258085	0	127842	268044	253449	363591	428705	358245	269684	275815	234853	504598	335282
EIC	Negative	309.1546	3.58	unknown	0	0	0	0	0	47702	0	87623	0	0	0	0	0	0	0	107216	141621	91727	0
EIC	Negative	307.1587	4.43	unknown	185968	493947	122469	162522	447474	598138	185982	173427	3522699	240609	141661	81246	199640	286388	395238	117489	5254598	6467779	271277
EIC	Negative	322.2371	4.76	unknown	80452	27814	0	263168	0	47738	0	156172	219867	0	43203	152188	332314	233152	93842	52758	520933	325147	90861
EIC	Negative	355.2054	4.76	unknown	403668	131461	30606	1094524	114814	192090	105300	528892	971905	95236	175696	611783	1339336	911642	296222	275749	2204411	1808491	323171
EIC	Negative	432.2108	1.02	unknown	22330	0	17887	20726	0	11288	22407	0	0	28852	0	183700	197359	0	307143	268659	16024	21850	16465
EIC	Negative	299.2530	5.50	unknown	0	0	0	0	0	1961860	0	0	0	1880055	1234660	0	1462121	0	795826	1374076	1571242	0	1354572
EIC	Negative	290.1433	1.87	unknown	0	10091	0	0	0	88226	23010	0	0	0	31925	26775	35562	12405	0	140458	119623	0	30868
EIC	Negative	417.2053	4.76	unknown	29073	0	0	302992	25025	29909	0	295588	410120	0	85424	239658	550192	379771	155829	119286	858088	738767	122300
EIC	Negative	345.2103	2.19	unknown	0	21326	0	0	0	1047406	0	134626	0	352308	0	0	30112	0	1017276	60762	0	0	2067407
EIC	Negative	427.1798	2.75	unknown	81114	366115	0	111010	179080	209037	355434	0	191820	506174	464988	554464	586342	399239	404158	369762	417050	869134	450904
EIC	Negative	539.3045	3.73	unknown	0	0	0	0	0	61767	0	0	0	0	0	117442	0	0	169187	0	0	0	111110
fpHILIC	Negative	185.0277	0.47	unknown	160864	234250	129845	107249	234184	527284	493347	70603	360960	68645	0	254130	1100454	223801	139907	533730	3025044	205418	716879
fpHILIC	Positive	399.2507	0.40	unknown	213800	162517	269662	507152	454615	283301	432553	1751394	625944	329717	3240050	1262312	547583	313482	675568	510372	635166	3064443	5034909
EIC	Negative	555.3913	6.54	unknown	520736	287894	241037	566993	526892	485878	404606	661993	501661	508373	871877	402879	853781	979515	958410	1507106	901536	2212869	1653183
EIC	Negative	493.2447	1.92	unknown	0	354461	0	0	26035	68672	448509	0	51932	0	433372	93432	197996	203823	112142	420685	640322	0	500347
EIC	Negative	619.3459	2.48	unknown	0	68543	0	0	0	41657	102240	76059	38092	0	121596	0	0	49328	35223	20586			

EIC	Negative	299.2530	5.44	unknown	0	0	0	0	0	0	1829173	0	0	1201852	1094773	0	1364912	0	1497038	2157756	1293294	0	1678463
EIC	Negative	258.1796	3.76	unknown	177004	2432171	24120	22057	1921761	2332915	91198	60841	30454	18324	68646	1628712	136645	31500	252467	3987210	93085	8260824	3562147
EIC	Negative	257.1760	3.76	unknown	1090033	15737708	216034	208610	12326718	14561214	567910	371698	200612	176590	384553	10539708	893686	154909	1620743	25622957	579450	52825975	2230225
fpHILIC	Positive	148.0965	3.19	unknown	770835	890873	469792	543174	778773	977879	876010	477466	1466531	1826204	3737082	5642697	2091261	376540	1303127	6128623	655697	6670909	2242626
EIC	Negative	259.1813	3.76	unknown	18722	293808	0	0	234455	274221	0	0	0	0	0	188871	0	0	33608	504548	0	973287	413847
fpHILIC	Negative	530.2781	0.61	unknown	569098	48133	1382275	904635	35947	34120	43802	2821245	83971	1001463	43879	0	0	251343	102395	95070	0	11527478	0
EIC	Negative	410.2636	1.10	unknown	19967	13447	27377	5776	47815	35420	20231	14796	31231	57613	67261	54101	30013	101682	102467	70484	130544	145704	163910
EIC	Negative	409.2607	1.10	unknown	65855	50615	85074	30620	179913	125003	69533	70191	123972	187169	242284	193849	116966	385808	419791	220356	510054	609583	648323
EIC	Negative	532.2819	1.96	unknown	0	0	0	0	0	0	0	0	83539	0	55194	47071	81703	211329	126955	78236	90614	0	70760
EIC	Negative	582.2815	1.99	unknown	0	0	0	0	0	0	0	54447	0	0	0	0	72462	0	121763	85741	0	0	63408
EIC	Negative	355.2051	3.32	unknown	0	71314	0	0	70928	58774	0	0	69571	0	0	0	181154	63973	0	144935	63349	995837	0
EIC	Negative	573.3794	3.76	unknown	17980	227294	0	0	129628	183931	0	0	0	0	0	188775	0	0	513929	0	1283758	255712	
EIC	Negative	639.4646	4.76	unknown	239053	39605	0	2086575	0	43315	0	624644	1836961	0	101258	683756	3378542	1800215	192828	127448	10436623	5691403	123652
EIC	Negative	415.2259	2.44	unknown	0	0	0	0	0	0	0	415211	0	0	0	0	0	0	915039	0	1859408	0	0
EIC	Negative	367.1592	2.13	unknown	0	0	0	0	123552	0	0	8567	0	0	66687	0	0	0	35281	40214	0	62311	761954
EIC	Negative	530.2798	1.95	unknown	0	29014	0	0	57964	32308	41967	311363	228980	349639	426197	379608	717632	2167504	1242339	713394	746387	1443527	654082
fpHILIC	Negative	155.0351	3.75	unknown	463669	122772	160474	168237	396588	97226	205192	93318	185988	815476	275763	105888	135907	224310	696706	152222	4426145	706458	1096642
EIC	Negative	464.3097	2.14	unknown	0	0	0	0	60689	0	0	0	0	0	97392	0	0	664461	172432	0	0	0	279268
EIC	Negative	325.2018	2.58	unknown	296430	334395	105078	281030	476931	638276	287676	158902	451012	232403	261095	200149	215383	200832	280233	15061403	193466	213009	269235
EIC	Negative	612.2817	1.59	unknown	0	0	0	0	54507	0	8483	0	105883	0	42066	80370	45467	407459	394051	459028	246312	0	302423
EIC	Negative	532.2813	1.26	unknown	86105	0	228548	112726	0	0	0	455878	16666	349731	0	0	0	0	0	0	0	4280321	0
EIC	Negative	345.2105	2.51	unknown	0	0	0	0	18635	0	31306	0	75755	0	0	192356	0	0	689198	0	0	0	450340
EIC	Negative	455.2407	2.34	unknown	0	0	0	0	0	8701	33080	0	0	45477	178907	19658	0	194168	8892	0	14211	373016	0
EIC	Negative	321.2340	6.21	unknown	0	0	0	0	0	0	0	0	151112	0	0	0	0	0	442248	0	595967	0	464245
EIC	Negative	613.2883	1.59	unknown	0	0	0	0	10614	0	0	0	26178	0	0	9403	10200	122759	130514	157622	82215	0	92591
fpHILIC	Positive	101.0600	3.56	unknown	36658	0	157025	36528	91680	95688	62801	0	0	972154	454745	635665	411123	0	554628	462163	402688	1519414	874135
EIC	Negative	531.2847	1.95	unknown	0	30833	0	0	0	0	0	0	56626	0	198068	132738	222632	656806	427538	246638	268985	0	219656
EIC	Negative	486.1887	0.73	unknown	0	0	0	0	0	5099	0	0	0	67360	127777	168378	126806	97411	35204	107539	155735	97115	59832
EIC	Negative	337.2297	2.15	unknown	1293341	0	1142007	1330533	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
EIC	Negative	577.3347	3.65	unknown	12547811	14623181	8661424	0	0	0	0	0	0	0	0	0	12454176	0	0	0	0	0	0
EIC	Negative	636.4365	4.28	unknown	174510	0	280580	113906	0	0	0	0	0	273489	47633	0	39551	0	0	0	0	0	0
EIC	Negative	531.3323	4.13	unknown	220405	0	139615	43813	0	0	0	0	0	72234	0	0	0	0	0	0	0	0	0
EIC	Negative	507.3280	2.44	unknown	528136	273202	53447	0	0	0	0	0	0	0	248226	0	0	0	0	0	0	0	0
EIC	Negative	499.2853	1.98	unknown	0	2923784	0	0	0	0	0	0	0	0	0	0	8953628	0	0	0	0	0	0
EIC	Negative	416.2011	5.67	unknown	0	100262	0	0	0	0	0	0	0	0	0	110472	0	0	0	0	0	0	0
EIC	Negative	430.3048	5.65	unknown	0	498303	341950	0	0	0	0	0	0	0	493104	0	0	0	0	0	0	0	0
EIC	Negative	597.3053	1.50	unknown	0	55901	0	0	0	0	0	0	0	0	430756	285714	1652890	1169784	0	0	0	0	0
EIC	Negative	280.2002	3.65	unknown	0	0	0	1063057	0	0	0	0	0	0	0	0	1131901	851993	0	0	0	0	0
EIC	Negative	412.2786	4.04	unknown	0	0	0	410406	0	0	0	0	0	535430	646822	541877	0	0	0	0	0	0	0
EIC	Negative	251.1322	2.40	unknown	141766	81572	0	0	0	0	0	0	0	0	0	0	0	0	0	79134	0	0	0
EIC	Negative	426.1848	0.69	unknown	93945	0	0	0	0	0	0	0	0	0	0	0	0	80523	0	0	0	0	92117
EIC	Negative	359.2205	6.10	unknown	98531	0	180400	33248	0	0	0	0	0	298552	26729	19639	0	0	0	0	29839	65270	
EIC	Negative	313.1547	2.22	unknown	0	0	0	0	0	0	0	0	0	348664	0	487043	0	257762	102434	0	0	0	0
EIC	Negative	280.2001	3.79	unknown	0	0	0	231836	0	0	0	0	0	0	0	116630	82300	0	0	0	147196	0	0
EIC	Negative	357.1702	5.65	unknown	0	0	0	0	0	0	0	0	0	121401	0	135701	0	0	0	168920	0	0	0
EIC	Negative	634.4106	3.76	unknown	0	0	818605	481990	0	0	0	0	0	0	128457	0	0	130783	0	125443	0	45966	0
EIC	Negative	460.1901	3.92	unknown	190950	55118	119550	411150	0	0	0	0	0	325603	88266	0	0	0	19912	84883	0	72418	0
EIC	Negative	293.1019	2.56	unknown	0	0	0	0	0	0	0	0	0	0	0	115332	120565	0	98534	90853	0	0	0
EIC	Negative	357.1675	5.65	unknown	0	169021	109221	0	0	0	0	0	0	0	0	0	0	0	0	0	0	193897	0
EIC	Negative	488.2276	2.70	unknown	0	0	0	0	0	0	0	0	0	0	97698	0	99205	0	0	95039	0	0	114531
EIC	Negative	371.1814	2.44	unknown	210914	42984	214285	154035	0	0	0	0	0	400930	13656	0	8696	91595	0	57048	76653	0	81952
EIC	Negative	299.1877	5.23	unknown	0	0	0	0	0	0	0	0	0	288179	0	150968	180380	0	22521	115287	0	93541	0
EIC	Negative	401.2309	3.36	unknown	0	0	257595	207248	0	0	0	0	0	0	222478	170154	0	0	0	0	0	0	240498
EIC	Negative	396.1867	0.71	unknown	0	159929	183609	0	0	0	0	0	0	149225	160392	140434	0	146930	0	0	103317	0	161099
EIC	Negative	345.1558	5.58	unknown	0	0	0	0	0	0	0	0	0	0	0	532095	0	213748	0	0	0	0	283129
EIC	Negative	268.1926	3.44	unknown	316578	0	0	0	0	0	0	0	0	0	0	0	0	0	103847	200833	0	0	0
EIC	Negative	422.2188	3.11	unknown	138494	0	694971	200376	0	0	0	0	0	0	0	0	0	0	0	0	264055	60987	0
EIC	Negative	395.1842	6.09	unknown	281411	0	557227	196428	0	0	0	0	0	745879	0	124376	0	0	0	94977	116426	0	117678
EIC	Negative	345.1559	3.76	unknown	0	0	0	0	0	0	0	0	0	0	0	486823	490381	232229	0	0	0	0	343778
EIC	Negative	320.2313	3.36	unknown	0	0	0	307126	0	0	0	0	0	705222	0	0	154431	0	160049	0	0	0	188440
EIC	Negative	451.1650	3.14	unknown	0	77280	0	0	0	0	0	0	0	0	0	13951	107611	0	0	0	0	141256	227359
EIC	Negative	329.2390	3.80	unknown	0	0	595889	429457	0	0	0	0	0	0	0	0	0	163334	214375	0	0	0	0
EIC	Negative	251.1322	2.56	unknown	1321653	609978	0	158672	0	0	0	0	0	44256	0	0	450442	0	0				



EIC	Negative	452.3106	3.22	unknown	511707	32858	412860	255059	34993	82955	50245	202706	10596	139273	0	0	0	0	0	0	0	17275	0	
EIC	Negative	452.3115	3.85	unknown	12500025	2288886	12071434	9023591	3761123	2913166	4059911	8337524	988900	4220950	62995	150691	119280	0	0	0	0	0	876856	38218
EIC	Negative	390.2735	3.20	unknown	1331477	107528	1718424	848651	216802	114989	280540	737630	0	224722	8105	0	0	0	0	0	0	41088	24092	
EIC	Negative	505.2573	2.13	unknown	4517902	1363523	4957453	3025177	2108840	2262132	3279751	4969178	1736904	621617	34920	37477	107804	0	27326	116602	8183	452754	63237	
EIC	Negative	449.2907	3.00	unknown	3728261	111259	8828782	2801637	258695	346692	351927	2079708	0	0	0	0	0	0	0	0	0	0	143990	
fpHILIC	Negative	189.0117	0.43	unknown	2317818	1062387	2584827	1095841	367495	152526	1473387	1982785	1164991	0	0	0	0	89892	79930	73205	0	0	88366	
EIC	Negative	394.2957	3.85	unknown	825451	158964	821490	619122	232991	215941	322793	600481	87635	302465	0	46725	0	0	0	0	0	42944	25429	
EIC	Negative	633.4763	3.86	unknown	378403	18975	616282	1955681	284501	107275	301982	813646	179298	262887	0	0	22338	0	0	0	0	80026	0	
EIC	Negative	506.2605	2.14	unknown	1166052	337414	1250285	844740	572227	618273	850437	1393039	475055	190434	0	0	29298	0	0	32470	0	144701	10073	
EIC	Negative	469.3078	2.13	unknown	8738159	3191672	8203709	4795084	3045323	3567016	3992949	5548080	2105167	875341	85263	37026	213419	11544	26756	129580	19553	677115	25624	
EIC	Negative	389.2697	3.00	unknown	1637571	0	3564997	1137765	128244	140166	72768	859345	41334	0	0	0	0	0	0	0	0	59959	0	
fpHILIC	Negative	107.0501	0.43	unknown	2359583	1110629	2184612	856397	166960	145468	1727719	2162534	1109957	0	78425	49621	0	68138	67138	71138	0	43438	0	
EIC	Negative	389.2700	3.28	unknown	2650544	121720	2249488	908816	112136	238699	243500	595523	37387	137413	36238	9188	32876	34040	29223	0	0	0	30890	
EIC	Negative	468.3050	2.13	unknown	46385934	16879676	42053915	25044284	16426741	18480050	20803842	31047572	10948082	4743522	420796	262868	841661	84846	228007	678673	109447	3582029	383444	
EIC	Negative	467.3017	2.13	unknown	161573266	57965065	148575193	87525683	56998722	63405424	72553886	106614434	38078761	16446815	1482122	956138	2992697	322190	848977	2358111	423833	12262732	1383108	
EIC	Negative	407.2806	2.13	unknown	53859988	18767360	47326297	28157673	17835885	20455829	23424661	34817585	12275413	5408037	506948	261210	934243	13357	244804	773056	103504	4056079	428311	
EIC	Negative	587.4309	3.87	unknown	730098	101839	1472740	2119626	355392	156043	356114	986427	156842	330569	19984	0	20472	0	0	0	0	88114	15997	
EIC	Negative	391.2858	3.22	unknown	841356	45074	886313	466602	85122	97335	89101	360720	33273	208776	0	0	0	0	0	0	0	35216	0	
EIC	Negative	408.2841	2.13	unknown	14258769	4874563	12205035	7391329	4772419	5345361	6089321	9202571	3196412	1392157	136289	92061	224607	29250	76350	219861	31571	1088124	109198	
EIC	Negative	569.3340	1.67	unknown	15126073	3719507	12282905	6496923	3808124	2817640	6305168	6092245	1685427	562651	95030	37397	146587	0	28133	207857	7038	790839	60452	
EIC	Negative	429.2602	3.85	unknown	5168500	378018	4706647	2612358	735012	525094	790866	2388095	186698	783789	51640	55962	67852	0	0	0	0	155827	106784	
EIC	Negative	410.2906	2.30	unknown	302963	84248	347610	154561	124737	89960	48725	41831	0	0	0	10576	0	0	0	0	0	37019	0	
EIC	Negative	390.2737	3.61	unknown	6382509	276667	5479240	2562767	873187	419281	1061778	2383261	199815	782959	72959	16271	68367	0	0	0	0	166262	131612	
EIC	Negative	425.2917	2.30	unknown	227793	44582	277929	153481	94156	70587	191408	46553	53621	0	0	0	0	0	0	0	0	28363	0	
fpHILIC	Negative	189.0034	0.43	unknown	10188801	5060900	10299471	5112439	1181807	574858	7292280	9677816	5084169	274396	305528	376419	165271	361416	463343	348948	207401	73393	360598	
EIC	Negative	405.2645	2.94	unknown	2385080	111608	1472340	190503	115784	288599	241392	605046	91566	33357	0	14065	0	0	11389	8645	0	20132	43472	
EIC	Negative	464.3023	1.65	unknown	6241626	273197	16244964	2167296	582115	314935	187057	17689399	708136	758081	16979	0	138942	71919	37468	0	54010	1142047	29859	
EIC	Negative	428.2648	3.85	unknown	3945084	278904	3465666	1956676	548774	379871	856961	1772820	195710	620678	63966	29953	63985	0	20467	0	0	113315	94234	
EIC	Negative	427.2624	3.85	unknown	14998076	1099466	13192025	6955917	2038305	1543807	2183354	6842139	561495	2363138	229840	133541	202749	0	60217	76011	0	437862	304125	
EIC	Negative	357.1743	2.68	unknown	1572825	746932	1146318	749466	603536	605602	801240	979839	213071	0	0	0	0	0	0	0	0	213828	0	
EIC	Negative	389.2697	3.61	unknown	24042126	1123512	20780898	9782324	3146585	1650262	3967566	8889829	762984	3019598	242612	40872	221646	0	0	109895	0	617329	509802	
fpHILIC	Negative	187.0069	0.42	unknown	245826224	124481496	231948112	119652992	21432316	16225096	177414000	244036656	123695200	4917355	5169553	6737707	5398946	10105297	11089251	8124074	5334265	4488520	10331717	
EIC	Negative	453.3139	3.85	unknown	2276258	422333	2128907	1590066	618683	491137	733072	1512197	186683	778553	42489	0	0	0	0	0	0	17294	68039	
EIC	Negative	449.2416	3.85	unknown	670008	154315	524469	607507	252180	181256	224563	561197	97068	310090	48564	14954	15292	0	0	0	0	69666	21470	
fpHILIC	Negative	188.0105	0.43	unknown	18924908	9386558	16923106	8388057	1453195	1430539	12819858	17217400	8911777	321153	491645	406920	678208	656664	684274	382148	396945	777022	0	
EIC	Negative	360.1931	3.02	unknown	13333759	6250074	13579536	6409525	5921184	4719570	7157975	10003009	2041855	104081	47463	56014	105696	40447	40402	53858	0	15290	2021295	
EIC	Negative	359.1901	3.02	unknown	64168303	29916887	64516997	30791673	28174638	22673059	34148850	47791510	9634197	482435	165989	192022	442292	192007	133265	114740	162222	211461	9584873	
EIC	Negative	467.2021	2.52	unknown	14290631	930929	14836712	3507963	1202172	1493778	1232534	6249345	758729	1001445	0	0	163105	0	0	0	0	625592	0	
EIC	Negative	444.2608	2.30	unknown	3011075	384357	3008276	1262856	599853	438742	437345	1992564	285026	520008	32142	22936	59737	0	10440	0	0	187621	75129	
EIC	Negative	361.1888	3.27	unknown	3661187	0	629431	394041	1292204	0	2000348	1038301	100545	323384	126470	0	118014	259418	0	0	0	190908	219180	
EIC	Negative	385.1327	3.33	unknown	231800	119607	339503	310283	50128	64653	77101	180961	75353	0	0	0	0	0	0	0	0	0	34215	
EIC	Negative	361.1891	3.02	unknown	4109345	1913386	4328612	2052387	1785370	1492459	2192094	3122757	617235	84542	0	13509	37048	30842	47765	9642	30341	22002	598689	
EIC	Negative	445.2547	2.30	unknown	3856037	452995	3963417	1650179	795088	564674	578181	2618639	383419	686740	41186	26331	0	0	0	0	0	291354	93486	
EIC	Negative	443.2570	2.30	unknown	10793837	1368687	11314085	4733263	2256162	1592265	1745368	7455653	1116876	1831052	87896	73336	242191	27097	45527	49753	20244	757610	233387	
EIC	Negative	478.3183	2.36	unknown	1301318	30763	3095141	85400	57288	61670	55183	2447401	119036	236410	0	12045	0	0	0	0	0	222429	0	
EIC	Negative	359.1905	2.78	unknown	8661351	0	11551195	3702420	4852799	3811523	5161948	4217135	1413923	0	0	0	0	0	0	0	0	1683709	0	
EIC	Negative	360.1936	2.79	unknown	1865485	992451	2298942	844367	896776	772293	992331	886192	264225	0	0	0	0	0	0	0	0	0	34437	
EIC	Negative	427.2626	3.05	unknown	812763	83091	893260	500831	87721	67412	99192	265597	0	274607	0	0	0	0	0	0	0	37381	8760	
EIC	Negative	453.3131	3.05	unknown	436415	44415	509256	280050	73326	38143	72510	154820	10955	143377	0	0	0	0	0	0	0	31466	0	
EIC	Negative	452.3111	3.05	unknown	2375387	233071	2926857	1588443	293338	183100	392321	927234	130650	823033	39912	0	7748	0	0	0	0	127165	46315	
EIC	Negative	392.2891	3.85	unknown	47216682	8424179	44185560	33078257	13711111	10605208	14604074	32284433	4222137	15844051	1558705	915829	1366051	50336	253144	495213	215638	3543068	2373898	
EIC	Negative	393.2925	3.85	unknown	7671077	1287537	7003386	5078497	2237718	1679359	2287313	5184662	653230	2467640	253652	154234	198463	0	48482	66627	17465	616981	379501	
EIC	Negative	393.2921	3.05	unknown	8																			

EIC	Negative	499.2933	2.78	unknown	147629554	38694	112910139	144732587	40699	88854	74338	91229074	196091	29397292	57102	69820	103706	152787	98364	20047	69112	10830334	55997
EIC	Negative	634.4336	2.31	unknown	1356868	29852	897079	529842	54078	98403	54225	472724	38030	132480	0	0	0	0	0	0	0	86757	0
EIC	Negative	505.2574	2.30	unknown	5426199	507545	7060413	4693724	1363491	951315	1099755	8160051	766879	2572212	62445	74549	155472	33652	29596	40310	27997	1232045	172968
EIC	Negative	409.2868	2.30	unknown	2649951	543956	2862269	1578440	938048	662307	667211	2120727	438460	914683	56747	40091	90409	11490	25150	12593	7469	405792	139539
EIC	Negative	478.3182	1.70	unknown	361461	107967	245227	52245	114216	103991	78712	332418	70638	69443	0	0	0	0	0	0	0	67363	25670
EIC	Negative	485.2577	3.12	unknown	466270	10773	405664	308891	39810	0	23662	332818	0	558761	0	0	0	0	0	0	0	53683	0
EIC	Negative	506.2599	2.29	unknown	1554548	138724	1906043	1250131	343434	266975	277944	2169404	213859	726749	22812	14127	45451	43400	43431	0	38393	325564	50766
EIC	Negative	446.2576	2.15	unknown	578650	145904	681524	253363	208257	213772	37495	310159	63401	32040	23984	32324	29461	22906	15467	36676	10067	43240	12171
EIC	Negative	500.2912	2.83	unknown	46306892	0	35033798	45972172	0	0	2680315	28742867	2513794	9542520	887883	415053	0	129126	214926	225196	0	3403042	1046190
EIC	Negative	413.1952	4.15	unknown	113500	0	823245	0	283038	256218	0	329213	466459	0	28164	0	33791	0	0	129408	0	0	0
EIC	Negative	473.2884	3.85	unknown	4528160	2263328	4024433	4324164	3338120	2838557	3327449	4286427	1625346	3646960	545328	336491	464365	0	112206	192321	105842	1065293	847797
EIC	Negative	446.2584	2.30	unknown	902312	102865	990983	392771	215693	163891	163659	732537	113894	211416	29483	28359	45033	23161	28909	31005	24148	100185	36196
EIC	Negative	499.2933	2.23	unknown	6695365	521097	13884617	10627995	539972	347044	300914	8484642	510053	5579617	174779	62625	106513	139787	129474	90631	77847	1079884	272489
fpHILIC	Negative	172.9913	0.47	unknown	75228528	6266413	8492568	1410112	4105731	54134684	2855738	5140785	4616784	1490997	1070834	2680031	2907292	1518505	1222298	4685797	1600545	1766243	2259279
EIC	Negative	359.1901	3.33	unknown	8400778	3681088	10570663	2818109	2600905	2285329	2368902	3811578	729305	357292	141185	133711	120082	147536	74388	47986	62496	199390	1585311
EIC	Negative	436.3143	5.17	unknown	2180382	149681	2065843	1000704	300566	135783	199676	897603	90751	760856	53567	0	28920	0	0	0	0	181415	108010
EIC	Negative	502.3990	5.80	unknown	0	94892	70723	759447	223435	0	137713	136154	326197	95905	23650	101996	126879	0	0	0	110516	38233	0
EIC	Negative	474.2631	2.88	unknown	0	0	0	0	0	0	0	0	0	0	0	0	0	0	48347	29766	0	0	0
EIC	Negative	319.1535	3.13	unknown	88882	133147	51563	417124	0	0	363856	79450	56488	29695	227237	161730	0	44602	0	0	0	36100	0
EIC	Negative	407.2442	1.89	unknown	0	104422	0	0	33827	845313	19336	0	20492	0	2372924	706658	21500	61373	0	0	84075	0	0
EIC	Negative	376.2939	5.17	unknown	994644	54676	861711	447254	135724	58626	61648	385260	0	313565	30053	31048	0	0	0	0	0	79303	39268
fpHILIC	Negative	171.0564	0.95	unknown	1368533	251960	981431	832684	737647	879303	652596	1229190	443821	0	48554	128970	95401	112093	282096	146244	110560	43615	148111
fpHILIC	Positive	251.0481	0.95	unknown	1687993	209792	1107172	1122825	775978	1007360	724184	1155601	431310	0	53022	741042	59940	74883	300859	117044	150991	50980	134763
EIC	Negative	507.2612	2.30	unknown	198962	0	313854	240987	81266	64512	17863	358349	23341	146854	23341	18150	0	15819	0	0	0	69655	0
EIC	Negative	389.2696	3.12	unknown	7642161	266298	7568494	5090620	496813	373332	405644	4483526	189523	9549560	228261	0	181257	0	0	0	0	962729	210662
EIC	Negative	449.2899	3.12	unknown	10040036	307819	10380785	6650140	623710	423085	605000	5852950	252327	12869751	322009	99675	0	0	0	0	0	1262525	288233
EIC	Negative	390.2733	3.12	unknown	2038765	87959	2044388	1351812	137661	109887	124725	1511117	53504	2528086	80712	31671	61407	0	0	0	0	256069	66894
EIC	Negative	450.2942	3.12	unknown	2911634	107256	3037188	1887566	194793	118417	155034	1707678	73061	3798522	84406	17411	69440	0	0	0	0	367613	98320
EIC	Negative	375.1848	2.77	unknown	1693507	218730	1023196	1065422	0	0	1738526	0	3483853	0	4103770	185389	379106	0	0	0	0	375289	0
EIC	Negative	480.2782	3.61	unknown	2768038	54835	1503176	649435	53177	43840	62667	1190946	52178	640077	0	0	0	0	0	0	0	361129	0
EIC	Negative	477.2820	3.02	unknown	356812	0	275110	154853	0	91056	180547	24111	131825	203177	0	421634	307489	0	0	0	0	94112	0
EIC	Negative	596.5278	6.36	unknown	328841	279959	209205	780922	289151	339928	257498	132807	195859	138917	136144	156640	97555	0	0	96004	0	172145	0
EIC	Negative	339.2654	5.50	unknown	0	629665	1545002	1325282	681822	596983	0	1009763	506936	0	0	0	0	0	0	619196	0	0	0
EIC	Negative	362.1883	3.03	unknown	0	339524	0	392115	0	262698	0	134918	111621	0	0	0	0	0	0	0	0	120263	0
EIC	Negative	406.2678	5.20	unknown	435728	0	0	0	363485	0	0	411138	0	0	0	0	0	0	0	0	0	0	98277
EIC	Negative	630.3781	4.79	unknown	639648	1018689	558227	111890	0	147083	792287	629321	1002253	155844	807935	628749	0	686068	0	0	627148	0	0
EIC	Negative	462.3162	3.06	unknown	95456	14896	341460	375792	42346	406649	30957	106649	20539	105750	26096	7760	0	0	0	0	0	69285	0
EIC	Negative	472.2765	3.12	unknown	286645	0	276925	214827	14880	31707	15473	190792	0	0	0	0	0	0	0	0	0	62280	0
EIC	Negative	390.2735	3.28	unknown	715771	66014	627828	243622	60055	77344	84079	176438	33481	52072	23470	12683	30227	25376	25995	17326	14134	15353	35444
EIC	Negative	452.3821	5.79	unknown	51160	245979	518849	2658440	958335	41234	736133	524839	692610	257555	94956	598124	244524	25543	0	50429	243300	394046	78220
fpHILIC	Positive	166.0718	2.68	unknown	126575	400910	432213	600592	395985	386184	367049	456886	334369	210727	252942	523694	356747	224614	210403	62133	149690	0	72760
EIC	Negative	448.3512	4.91	unknown	16814	15779	114494	675857	150361	0	101956	126784	159853	60552	0	79768	52538	0	0	14490	17137	108935	0
EIC	Negative	333.2074	6.06	unknown	0	0	4958356	7641276	4458263	2433231	3786455	4673007	0	3397865	2359798	2923676	3626416	182485	1916841	0	140040	0	2056184
EIC	Negative	553.4480	5.81	unknown	169720	324955	390350	935760	493827	323252	708730	409082	376637	227424	194327	204151	223078	125466	87115	68750	243270	140225	81925
EIC	Negative	381.1717	3.35	unknown	473104	200123	597460	188127	149110	129140	132074	236095	66220	0	0	15947	17200	10723	12555	26722	24959	23053	107076
EIC	Negative	481.2810	3.61	unknown	847588	11657	482894	204628	15558	0	22099	356733	14062	193901	0	0	0	0	0	0	0	111944	0
EIC	Negative	446.2576	2.19	unknown	499299	36024	636761	170125	51486	41994	41765	340904	46044	48340	23984	32324	21154	24680	16336	36676	21756	43240	26624
EIC	Negative	524.2948	3.29	unknown	401502	0	349012	385209	41101	45791	60693	303008	296008	331819	43397	37547	30240	346783	35067	39006	47241	46088	42757
EIC	Negative	483.2979	3.75	unknown	2391076	7916	2133441	175484	79911	58667	58008	1270067	71439	881318	28235	16887	19720	0	12448	12919	0	372136	35505
EIC	Negative	471.2731	3.12	unknown	1065057	26473	978399	727873	0	0	12932	703179	16431	1422058	54747	8987	49669	0	0	0	0	167024	44049
EIC	Negative	473.2827	3.06	unknown	158919	238297	1857170	182630	265314	180561	72829	217477	72783	154572	51909	0	0	0	0	0	14573	0	45864
EIC	Negative	482.2943	3.76	unknown	7987796	127091	6926436	4149599	234670	174594	169493	4151586	202614	2881332	86465	63090	58590	45851	63716	59662	49269	1196636	68546
EIC	Negative	365.2463	6.39	unknown	0	7030993	19074970	14292722	0	9818884	5439546	0	0	9545785	7934966	0	0	0	0	0	0	0	4646216
EIC	Negative	500.2289	0.71	unknown	165060	38112	69742	89829	20465	123501	38919	20972	21694	58505	23693	18976	12937	23854	0	0	0	20182	44549
fpHILIC	Positive																						

EIC	Negative	269.1576	5.06	unknown	294481	184392	224820	242858	163597	293678	173268	242195	109702	123127	82490	0	0	0	32039	131579	0	224480	0
EIC	Negative	323.2502	5.67	unknown	0	119812	163790	143779	0	119787	102155	114061	0	93780	0	0	0	0	0	0	0	136354	0
EIC	Negative	481.2096	1.78	unknown	314875	23163	324253	181959	64417	85513	75654	362402	26331	234651	49977	96113	90815	105146	48628	73961	0	21596	
EIC	Negative	351.1806	2.26	unknown	587086	83895	222995	112072	127279	142206	174076	450506	45204	285230	56821	74915	52619	47578	40482	54618	70248	126873	95396
EIC	Negative	403.3227	4.01	unknown	961736	0	507142	79321	0	0	0	208782	0	137191	0	0	0	0	0	0	0	86594	0
EIC	Negative	341.2698	6.42	unknown	2007707	1940136	2802397	1777000	1286560	1085571	1023786	1380046	1433558	928944	700937	879620	1104310	498865	684602	455541	889608	295056	258196
EIC	Negative	245.1579	4.23	unknown	118528	0	0	349505	66894	81345	87465	96413	0	156011	0	0	0	0	0	0	0	141218	0
EIC	Negative	601.4479	5.58	unknown	107558	166217	183483	1289648	141868	94174	272788	321144	398458	229834	184458	103593	235314	105199	145575	0	236128	97439	43562
EIC	Negative	641.4795	6.39	unknown	983529	1334280	1518898	2048167	1527632	1132740	1277345	1974734	923589	855694	529503	534626	739967	312113	404461	553276	536470	821630	504688
EIC	Negative	239.0672	2.98	unknown	479189	251731	106777	283082	255634	247924	145228	131319	377816	174528	244274	110241	109086	147125	112442	127577	86174	81776	90159
EIC	Negative	469.3308	4.91	unknown	91055	106390	252396	1558558	450487	111417	295524	291988	396132	172065	24616	227353	167641	0	14226	103148	123168	385674	39974
EIC	Negative	342.2016	3.13	unknown	586305	22524	426544	59958	26056	0	321701	0	298304	298304	120706	39204	96744	49804	0	53262	46969	0	0
EIC	Negative	642.4849	6.39	unknown	449143	607669	679401	1389645	673334	374703	780229	780328	376707	447080	300476	214865	527138	117136	192466	308673	266007	340317	202416
EIC	Negative	227.1909	5.79	unknown	373547	591131	834332	2214817	1176627	478532	1010148	909816	1009683	612248	367888	904212	588950	0	0	489548	555464	684345	290639
EIC	Negative	605.4798	6.17	unknown	1294998	2257296	2643172	6107035	2121613	1961583	2916430	2779970	2674634	1305204	1351055	1087730	1882871	1151237	1148406	718573	1686096	1208912	750997
EIC	Negative	469.3283	4.91	unknown	91055	114783	264006	1558558	450209	106093	303601	268449	210672	155588	52705	237795	192088	20916	14226	102236	145448	291001	51093
EIC	Negative	471.2729	3.44	unknown	228290	39876	230152	216307	65953	61113	91393	117175	32605	104430	25535	63569	69814	0	0	49310	114613	0	0
EIC	Negative	226.1891	5.94	unknown	142248	249910	474285	1504952	622940	254387	465540	438375	579200	164850	185256	479659	295518	95866	65339	215164	272024	395869	128882
EIC	Negative	298.2469	6.42	unknown	1700483	1071276	1828017	5094482	1449870	1080719	1410817	2353891	2382319	727077	1011734	1512688	1101617	342882	301860	1180671	721217	1390663	463828
EIC	Negative	482.2797	3.60	unknown	259124	24258	159611	78848	11915	14243	13841	117595	0	12015	9114	20931	21937	9391	10196	9575	43401	0	0
EIC	Negative	226.1891	5.79	unknown	3059192	5075105	7488186	19783076	10555207	4543795	9300046	7475911	9065627	5249470	2957636	8224434	5160415	1596821	1467054	3978999	4619154	6470186	2481009
fpHILIC	Positive	345.1765	2.25	unknown	3549333	1463595	2844755	4001458	2090220	2429479	2204358	2943961	2648146	2338248	1428711	1684702	1940109	758111	797062	1207575	963343	2157793	489617
EIC	Negative	225.1857	5.79	unknown	12054969	19949845	30048293	80136298	42479812	18074450	36654392	30994634	35674628	21096274	12106214	32902549	20539649	6463513	5783072	15837768	18354927	25893450	9854883
EIC	Negative	354.0363	2.09	unknown	261539	311787	110778	57761	229400	212345	182890	163911	163911	82110	169111	16059	85440	117370	137258	159726	37002	0	107467
EIC	Negative	551.3218	2.65	unknown	339971	193515	126683	49634	157269	186492	133626	248028	43214	68993	85185	81660	96222	0	83353	83880	86937	0	105868
EIC	Negative	225.1875	5.94	unknown	582398	984327	1875498	6036464	2610946	12012962	1864822	1802455	2217190	1154167	648187	1957913	1135144	377372	285885	872949	1064085	1706340	551097
EIC	Negative	225.1759	4.91	unknown	91849	95997	171355	525718	251626	102931	176851	204768	239687	123669	75061	165635	139980	63538	21434	93583	110502	204227	30102
fpHILIC	Negative	363.0737	3.29	unknown	0	1882307	1528286	669310	489902	1107283	278070	277061	534990	127706	776005	381758	344186	166711	261685	871757	0	135239	0
EIC	Negative	307.1893	5.94	unknown	181431	279765	550711	1601777	751235	298061	548732	527243	681096	345517	212903	589736	348861	106790	87387	260564	347616	479809	153245
EIC	Negative	606.4823	6.17	unknown	529997	844187	1195966	2346321	871505	786578	1094893	1018512	0	1585312	0	0	1668956	465120	258260	764726	522843	299353	0
EIC	Negative	608.3946	5.74	unknown	0	2638735	2498923	1875178	0	3141606	2524691	2224656	0	0	74298	117220	0	0	0	101262	68144	155173	30785
EIC	Negative	500.3824	5.58	unknown	0	74006	120675	784881	126172	0	49638	174041	397097	89387	22731	74298	117220	0	0	0	0	0	0
EIC	Negative	297.2435	6.42	unknown	7357680	4455338	9124433	24791343	7649814	5655634	6603349	11832435	11290473	7357959	4908749	7498601	5997666	1725214	1886025	5947397	3545082	6785110	2345326
EIC	Negative	503.2994	4.64	unknown	0	1608051	0	0	0	1539660	0	1253375	964298	1227370	1151541	1116240	0	0	0	0	0	0	1342761
EIC	Negative	431.3379	3.38	unknown	0	64556	195955	1745347	216708	99298	179911	197795	351662	160623	69523	160553	131631	25766	12372	65459	84227	324134	16406
EIC	Negative	324.0088	1.26	unknown	64225	50675	68490	37708	47200	48934	36545	62805	33836	53413	21553	16914	21547	28311	25944	42043	17354	0	25202
fpHILIC	Positive	346.1796	2.25	unknown	487044	325465	734361	607928	293447	619428	248214	419428	432537	441066	180656	387237	330270	138676	223309	122972	78718	354723	62011
EIC	Negative	361.1844	3.00	unknown	0	1928452	4186348	1971698	0	1480467	0	0	0	0	15750	13140	12646	61285	48390	0	13726	600186	0
EIC	Negative	591.3199	1.24	unknown	882388	30917	1882510	329701	37921	141535	77075	692082	65000	1807703	56141	41090	65678	0	114099	70119	0	192437	118788
EIC	Negative	514.2855	0.99	unknown	827221	25418	3973898	4134008	56880	26398	0	4591785	104083	2736873	128528	0	0	0	0	0	0	2279071	68781
EIC	Negative	434.3364	5.44	unknown	230035	46868	451385	143310	150448	56453	29893	292562	38539	0	149944	0	35640	0	0	45149	199778	34573	0
fpHILIC	Negative	175.0246	3.29	unknown	48492	46060900	28378534	12525967	15011176	30954256	8771110	5998194	12093366	17203260	21932962	9510860	11548569	3712577	6604527	26450484	1913005	2411713	279011
EIC	Negative	314.2058	3.25	unknown	195623	60077	195075	76469	99783	94270	111159	243450	25127	146822	55607	41583	43911	38327	36670	27084	38205	111376	71081
EIC	Negative	455.4106	6.35	unknown	1906962	2689038	5774895	7195745	4266803	2853962	3673893	6288514	4908992	2492294	1946622	4363194	2684664	1160619	1507694	1908808	1896643	3817885	1773212
EIC	Negative	360.1934	3.65	unknown	1598401	0	1576982	1541572	0	1717048	1619934	0	0	0	0	0	0	0	0	0	0	0	1658272
EIC	Negative	604.3628	4.52	unknown	14242704	358649	13601586	14049583	13489967	13888372	14142702	0	13667018	13044895	13668725	0	0	13376744	0	0	13534026	0	13950299
EIC	Negative	309.1972	5.79	unknown	88587	103437	133735	332788	189079	98631	176167	146955	163426	130137	0	173062	99520	0	23686	93899	94872	112683	61633
fpHILIC	Negative	176.0281	3.30	unknown	0	3411375	1817171	874954	1062814	2256599	585537	421360	857391	1205877	1547080	677466	820245	284790	505144	1921866	0	210662	0
EIC	Negative	450.3313	2.87	unknown	1808221	119067	1419863	414111	282681	44507	309716	2846413	272262	489340	40025	91121	78694	185301	145242	97371	117973	1466158	91118
EIC	Negative	449.3279	2.87	unknown	6184458	443470	4700424	1306997	942393	117953	1115909	9472380	963228	1806695	151452	331643	232723	643531	505695	364959	397634	4853612	340457
fpHILIC	Negative	174.0169	3.29	unknown	0	4672963	3900302	2429738	2532200	4150892	1784201	1287474	2161281	2841997	3273373	1921075	2085565	878590	1433496	3892412	0	725619</	

EIC	Negative	520.6001	0.64	unknown	86008	33269	95186	69280	83244	59156	56243	23779	43235	159839	10017	16728	23550	124272	0	24414	13996	10545	97895
EIC	Negative	311.1528	3.38	unknown	72344	106987	196700	437436	186102	123125	164532	171939	239196	139133	93677	165698	135848	32907	28430	126518	120588	214879	0
EIC	Negative	417.0284	1.26	unknown	388790	323603	442966	124434	226279	234997	219615	266813	151542	242964	202323	29346	87272	141686	124358	263582	58582	11245	153728
EIC	Negative	311.1659	3.21	unknown	249487	171605	177657	278056	147621	291251	129986	137388	65040	92881	113478	35390	36543	0	90735	175495	25124	114406	24537
EIC	Negative	293.1393	2.23	unknown	139390	33920	225938	39544	59444	37111	84506	224255	137336	231954	177839	34365	43285	24088	29266	64625	45936	117876	42154
EIC	Negative	632.4972	6.28	unknown	1040073	1154995	1348077	2526985	820551	923099	1188000	1404488	1337491	824257	781375	443386	916016	904133	761037	288081	948274	794104	392187
EIC	Negative	420.1383	1.06	unknown	61587	209815	82393	66170	45254	32072	89117	0	146024	0	0	0	0	0	0	0	0	0	157527
EIC	Negative	331.1914	4.93	unknown	1479546	527591	1537848	1038297	804482	557573	918343	1496655	353664	1133039	556737	395217	422736	329631	405640	0	391441	1047878	485105
EIC	Negative	499.0997	1.26	unknown	300790	323412	384699	88994	244446	230891	127318	268846	183821	208518	230900	5295	101058	191860	150622	254024	44493	0	202868
fpHILIC	Negative	215.1650	0.39	unknown	567497	869900	1586733	3955744	1504595	1021144	1235852	1678137	1799905	1219172	630080	1179907	1036495	405216	226076	764388	853346	1629172	619444
EIC	Negative	313.2748	6.01	unknown	230765	213765	498563	562382	195997	126289	176624	516771	270162	136251	120278	117276	160788	114638	84279	122609	126539	280162	116036
EIC	Negative	447.3125	3.59	unknown	335788	43344	335585	82019	55766	56229	39242	169528	30973	50243	11093	13300	10807	35787	29532	30079	30784	92743	16486
EIC	Negative	543.4623	6.35	unknown	331587	164926	224078	1038752	163382	221719	102588	241840	283632	227357	205162	266616	273823	0	0	221137	89603	212780	51579
EIC	Negative	323.2594	6.37	unknown	1285132	1201697	2744475	4563697	2162899	2288295	1614422	3068129	1559122	2143100	970869	1246558	1481866	779217	545568	1390944	983322	2351353	810731
EIC	Negative	244.1999	3.81	unknown	200874	153466	503479	706932	321895	252833	320750	601082	392593	313431	193269	240687	225777	210620	90502	174115	199751	439601	171593
EIC	Negative	225.1857	6.03	unknown	327108	683748	1057805	3575410	1455468	645773	1049499	1237269	1529307	891436	483675	1068429	826506	280773	186438	465316	847766	1504623	384430
EIC	Negative	243.1965	3.81	unknown	1247395	1038218	3217983	4368684	2094064	1631405	2070782	3652059	2542275	2090888	1198752	1555346	1389817	1378662	581796	1086184	1317969	2869693	1032610
fpHILIC	Positive	344.2790	0.61	unknown	1171198	851492	1127631	2625706	1000009	1127631	1158348	1152769	1158348	1634202	697276	1101134	997740	418776	585894	656074	1150715	633640	1363640
EIC	Negative	381.1597	4.91	unknown	84402	88276	149389	373144	208434	79850	154944	174545	216483	127962	66908	153610	115067	47862	27389	102852	100048	191338	58051
EIC	Negative	294.2157	5.46	unknown	157020	108450	184398	485042	212382	121073	143006	252332	342235	156774	102636	120461	118779	49629	61648	121951	126780	231524	74641
EIC	Negative	342.2372	3.62	unknown	377817	139078	441558	255611	168932	226375	296789	431936	88325	264956	118213	172785	116528	64197	108200	118058	85721	271610	114325
EIC	Negative	631.4953	6.28	unknown	2266747	2401260	3218288	5892637	1754377	2143084	2785350	3327034	3063606	2040343	1923565	1063144	2082134	1952802	1834182	79130	2289777	1633821	1022300
EIC	Negative	325.2021	3.36	unknown	643010	304443	689866	476506	472459	465142	515333	732678	150722	474376	251589	278350	206747	150070	204240	186619	209016	461801	286380
EIC	Negative	307.1892	6.03	unknown	115819	221521	359887	1035415	494825	220763	343179	362037	475814	313508	156604	354007	320269	90489	68201	166051	319721	434663	105860
EIC	Negative	289.2174	6.36	unknown	864486	897071	1020271	1923639	817340	1074213	949230	1492476	977414	480632	584607	785649	789738	422590	631119	570509	591714	709073	563438
EIC	Negative	594.3425	2.35	unknown	4951037	98086	3606532	3109429	1436694	3825925	1778396	3550396	2704702	486334	3013112	4866385	2599605	233418	127591	4145678	124732	3087147	208279
EIC	Negative	283.1450	5.79	unknown	97058	91451	138691	222827	150668	59158	143280	114704	161795	110632	59930	151291	98065	29328	21722	85400	96640	113804	46858
EIC	Negative	363.2295	5.83	unknown	1866985	1889151	1811867	1971795	1507343	1863620	2452718	1723024	1656193	1484782	1835641	982559	1568588	2322689	2198221	121404	1845305	0	1192347
EIC	Negative	272.9448	1.21	unknown	193902	122934	156404	124025	111235	35689	27890	54378	21677	37537	23077	22221	19167	22044	30224	48693	16278	35520	15372
EIC	Negative	297.2075	3.74	unknown	575825	262537	568388	296255	331648	427620	430960	576233	230716	374183	180282	308988	296466	200601	191296	253769	190957	400441	128095
EIC	Negative	510.2478	1.12	unknown	1433539	557438	2308064	1068154	813067	945205	1476903	1629763	1021428	1829534	1195980	642184	268915	648411	797991	670002	764162	541228	665767
EIC	Negative	324.2625	6.37	unknown	378463	258988	648807	1007696	523399	351036	485900	503979	513102	336710	233603	353414	333542	230038	162335	333954	297418	363963	233497
EIC	Negative	377.1807	2.55	unknown	1552317	613353	1815120	934546	304691	524814	475235	645367	229066	0	0	0	372762	0	0	372762	0	905526	0
EIC	Negative	387.2542	2.82	unknown	298940	64802	527132	78430	79145	53031	83339	304994	79420	158189	45494	54570	35605	74879	55398	29840	45816	179468	42307
EIC	Negative	553.2752	3.12	unknown	236794	12143	162365	33486	0	0	171439	26642	320758	0	171439	0	15441	0	9751	10978	0	99435	16184
fpHILIC	Negative	170.1266	0.43	unknown	421982	311399	508646	954395	527215	305724	368654	513598	647475	393689	366985	511118	353526	125024	192854	232921	250478	465148	251065
EIC	Negative	479.3374	2.97	unknown	260476	12739	230082	77763	9746	12165	33332	342923	0	0	28603	64842	0	0	0	0	0	252424	0
EIC	Negative	592.2515	1.12	unknown	117580	60196	193737	93662	74617	85083	131216	166348	97853	173434	109143	66786	36067	61530	73809	63283	73460	55988	62125
EIC	Negative	511.3995	4.07	unknown	14178	0	55543	239400	56664	31142	47760	95366	95839	16343	26836	43228	76945	12887	0	51298	19473	123896	0
EIC	Negative	251.1654	4.07	unknown	190738	69498	259950	157640	89506	122954	109641	207146	49355	219097	102325	139143	133204	127870	61964	39703	56687	96124	91146
EIC	Negative	506.6207	0.63	unknown	119210	65056	180909	93973	59421	68037	55682	15615	91574	0	4714	91247	240485	18798	0	4714	19247	0	17773
EIC	Negative	419.1349	1.06	unknown	259073	925806	350428	275921	175547	130775	357981	13795	613290	0	0	0	5953	0	0	16608	5270	0	751193
EIC	Negative	625.2130	2.08	unknown	317348	206166	203476	0	77668	130282	110046	0	49212	0	133687	0	26419	78373	77702	78691	0	0	64304
EIC	Negative	247.1073	4.88	unknown	197800	333338	373881	1600070	501023	243856	404161	568036	964062	414196	510222	317977	492582	113493	100235	404473	406563	545878	155070
EIC	Negative	387.2756	5.99	unknown	7985182	5920876	7484828	7829693	3839232	3923599	6882420	7044663	4831627	4054505	5001692	2690674	5198639	7245136	4998504	4831627	4598628	3035076	2487410
EIC	Negative	625.3606	3.15	unknown	339778	24713	356761	116467	132280	47593	65134	514260	70171	179284	49463	12919	30743	57215	73028	47219	73555	256302	49817
fpHILIC	Positive	456.1912	2.23	unknown	846708	371886	715911	740658	475424	484590	354653	486286	585438	481763	399084	506116	461638	303959	232695	334317	276198	346757	252200
EIC	Negative	363.2546	5.18	unknown	414724	168263	340770	282763	252737	247938	231524	336419	196410	288743	154859	187480	154264	104225	105835	169793	109716	243399	138153
EIC	Negative	251.2015	6.31	unknown	2726161	4512901	7487843	17216134	8571413	4105383	7308736	6881233	8081847	5109964	3454262	6113883	5096427	2331677	1364307	3075162	5543635	8584028	2784392
EIC	Negative	607.3820	5.01	unknown	969810	1346007	1031631	856804	0	0	1168039	0	0	36864	0	995413	0	1054327	0	0	0	741614	0
EIC</																							

EIC	Negative	429.2490	2.39	unknown	1204264	430225	985908	924428	663385	674529	601740	1537044	167531	802583	251475	272106	181409	315064	273546	167390	271477	1226204	363192
EIC	Negative	630.3781	5.13	unknown	756967	219134	498635	0	352655	0	470949	480611	0	0	0	397603	38114	111215	289683	102549	44617	387794	0
EIC	Negative	250.1893	5.26	unknown	249733	258967	406133	1061060	403211	175744	300444	495695	553244	287351	149845	210838	321297	104582	138377	195071	285664	433319	166569
EIC	Negative	285.1987	3.34	unknown	271800	0	280408	229451	90050	75761	91462	236104	75757	432385	0	93850	73397	84044	67558	0	73097	219432	0
EIC	Negative	313.2748	6.12	unknown	86485	103450	231255	271143	134209	72027	130963	234058	197170	128172	47340	98896	133103	51635	45851	107078	91615	180566	49885
EIC	Negative	393.3012	6.43	unknown	4241434	3586228	5813549	4339999	3580637	1690331	3470105	5190064	3092787	3888732	1829920	1327143	1884727	1685378	2099287	2407361	2426744	1844420	1998364
EIC	Negative	619.4931	6.29	unknown	500826	726135	614394	574498	648351	585096	715367	698485	412654	55769	402504	123664	482273	502053	590266	217259	477316	272497	382849
fpHILIC	Positive	352.2451	2.29	unknown	3957881	468558	2196233	1327886	890147	1365189	719873	1047697	163487	976742	252836	362343	425953	161205	793785	491909	117505	1262230	0
EIC	Negative	293.1398	1.77	unknown	2241571	1487055	1659444	425941	1639058	822072	1356702	1436708	631594	1950498	786782	796234	594554	943498	1080391	912639	460768	0	1114013
EIC	Negative	273.2342	4.02	unknown	108045	95188	308756	981330	230632	185277	197622	548725	396435	303401	162526	296751	261378	99265	29020	265403	171613	450329	76465
EIC	Negative	249.1860	5.26	unknown	1336391	1316500	2390404	6189870	2247785	927643	1736339	2813392	3342580	1734210	924756	1274869	1835670	778291	817931	1267583	1661736	2412263	913370
EIC	Negative	270.1793	3.10	unknown	318272	81285	189307	129469	129095	133577	160406	270316	63867	149940	57820	82400	65844	62285	88888	83784	82042	171672	58042
EIC	Negative	291.1025	2.21	unknown	151334	140154	211019	163710	129322	113458	147814	218725	142365	121286	89544	85319	68855	54403	82366	84481	83356	143106	88189
EIC	Negative	648.3875	5.79	unknown	196828	467403	265767	243417	315702	349009	261957	272508	282004	99854	245822	187326	185862	194331	177347	189636	247045	114312	222136
EIC	Negative	268.2002	3.44	unknown	348265	237687	832437	809473	541625	362568	410874	799898	441932	505026	224271	348457	337683	410784	113031	233541	385945	632284	276232
EIC	Negative	412.2788	5.46	unknown	1831550	1544380	1564134	2087475	1089147	1203462	1832124	1261253	1509209	1258184	1541406	666894	1103768	1578534	1770275	280555	1325990	529975	530049
EIC	Negative	354.2350	4.03	unknown	73924	94497	183552	468854	158481	103122	135348	309008	243299	184391	101248	180333	149833	66713	15685	155782	128510	255760	55432
EIC	Negative	339.1795	2.39	unknown	34041	45144	79109	54908	50179	69666	55528	55304	27915	31600	30039	35620	39504	39799	21438	38478	26901	37889	0
EIC	Negative	333.2049	6.06	unknown	2634557	3205219	5194925	8199274	5165963	2630690	4134294	4939022	5493546	3700031	2655826	3042497	3745162	1951788	2096548	2473519	3151328	4475167	2211760
EIC	Negative	411.2756	5.73	unknown	1674066	1245155	1572654	5128380	363634	704618	1215179	2092323	1155311	1708559	537990	1346728	1933158	1759501	0	1412605	0	571344	0
fpHILIC	Negative	402.1010	0.97	unknown	284018	348786	558996	478689	365900	195208	277380	357700	273625	120335	160912	134139	137002	123552	142648	160255	124030	414636	106814
EIC	Negative	279.1590	4.28	unknown	124002	179299	185253	546884	304013	190775	232306	207542	321122	242445	120491	206764	104361	69918	157977	196334	259031	127264	0
fpHILIC	Negative	280.1401	2.30	unknown	3290731	2185687	4227312	2114630	2345442	3041519	2790065	1936026	1719045	3406129	1543382	1343286	1752765	1212786	1690483	944406	1588260	2682824	732273
EIC	Negative	447.3491	4.83	unknown	265986	39885	588894	1540983	168561	188169	304320	538520	304320	458421	52269	241745	280306	0	26762	64006	177748	522597	43969
fpHILIC	Positive	137.0456	2.43	unknown	5189035	1114892	8228001	648230	3473628	2838702	1535668	605422	2861422	842784	114232	62780	4348725	3770120	0	63538	0	7187571	57573
EIC	Negative	269.1762	3.10	unknown	1867852	462747	1123918	768329	1076657	760588	1529475	318028	958566	345514	489913	378560	391629	545073	475271	464391	1049113	310139	0
EIC	Negative	250.1893	5.68	unknown	371846	541409	910174	2733192	1044401	555202	793390	1010205	1371668	697546	425412	834786	733700	244888	226347	511446	793733	1195951	356595
EIC	Negative	551.3238	3.55	unknown	572068	738631	606387	636138	756886	564782	631893	492578	477927	526974	599559	631474	570603	569719	570468	521857	519432	0	161393
EIC	Negative	342.2371	3.69	unknown	241833	99630	239730	158615	112674	118636	179308	223000	46631	168864	77673	96422	72290	45398	61985	63157	66264	169147	76061
EIC	Negative	397.2228	6.51	unknown	112554	98091	451856	451344	276002	105078	0	83185	602945	304294	384547	109925	281662	54032	85590	254041	221211	63264	65496
EIC	Negative	391.2861	6.39	unknown	5481023	3546600	4986900	4501543	3256071	2675273	2571768	4002503	1571232	3715085	2617304	1659741	1796960	685636	2449632	1491056	1936563	1832682	1400875
EIC	Negative	433.3329	5.44	unknown	856223	133339	1429536	459490	509043	209186	224123	949704	208217	506893	126271	139003	103238	158287	173421	141720	180542	671408	193879
EIC	Negative	448.3171	4.05	unknown	1016422	72224	845051	287558	58867	101883	110639	445861	64080	323784	54129	51054	54235	140981	55563	14639	58102	306682	44684
EIC	Negative	464.3023	2.45	unknown	923957	0	1261741	678299	102113	222587	0	1725151	105171	32247	0	0	0	5622	1392968	0	5622	1392968	0
EIC	Negative	319.2220	4.29	unknown	4640990	1060134	4884373	734596	229632	813950	1089481	490336	0	4512700	458694	1614733	329199	408153	222604	300609	404047	443630	332816
fpHILIC	Positive	455.1818	2.23	unknown	4153546	1478302	2795455	3235968	1676489	2079020	1523825	1868253	2397853	2188290	1830555	2089677	1790433	1095150	964528	1443230	1108372	1484245	1206508
EIC	Negative	415.2110	5.67	unknown	876437	438132	824711	698282	665095	484715	576080	657157	530746	657157	391316	493555	404481	335285	365776	419099	400404	542151	323944
EIC	Negative	365.2275	5.83	unknown	708982	748058	676048	763131	606998	770739	897229	681335	679721	558658	727801	413908	605536	832027	793762	0	731733	369586	473710
EIC	Negative	419.3168	2.97	unknown	152449	0	146585	63186	8930	0	20920	0	0	0	0	0	0	0	0	0	0	162830	0
fpHILIC	Positive	69.0454	0.95	unknown	484137	760297	608595	352325	474479	385829	395781	229714	236924	249371	269470	130912	145244	232162	221773	261996	220269	211974	206479
fpHILIC	Positive	460.2698	0.40	unknown	3822787	2645492	2444374	2556330	3177535	2746609	2356125	2521691	3401749	2429663	2093497	2427495	2494771	2131666	1438192	1896389	1796896	2429251	1502495
EIC	Negative	387.2756	5.83	unknown	13678795	15313858	13222057	13518143	11212696	15109409	20294946	13111255	1710459	9827503	13756211	6458564	11337553	18172857	16358779	3752140	13684285	5074958	7774598
EIC	Negative	625.4811	6.41	unknown	387427	308019	485601	1539399	612634	201588	492117	627977	1003796	552021	472671	329088	539693	115642	670897	359161	735752	152909	0
EIC	Negative	251.2015	6.06	unknown	43752752	53050435	86427131	162296814	80868970	41449959	66289329	83264971	99011416	55944455	38210157	48826992	61802482	30006368	31493716	41880441	53735961	80578431	34645108
EIC	Negative	291.1276	3.89	unknown	175781	189018	313106	285232	201232	164527	281982	359780	359780	230683	145063	286220	625493	100296	97818	171777	211853	202939	121491
EIC	Negative	489.3230	4.27	unknown	5520290	1375150	6256163	3442575	1851580	1785572	2250491	5759206	2189070	2279703	1228800	1444905	1244939	2756531	1711338	1091194	1420268	3583729	1240808
EIC	Negative	279.1583	4.60	unknown	355419	541022	1038830	2092610	913920	357076	975211	928517	1180800	809966	351178	883829	732545	218263	200848	561012	680957	1055491	352573
EIC	Negative	355.2133	3.61	unknown	367497	92510	284932	130114	0	29859	0	29859	0	149308	78140	102387	67102	56957	73574	0	96573	0	0
EIC	Negative	577.3506	2.91	unknown	313851	170821	293489	435565	116020	277222	117390	118427	0	269678	73259	289792	230582	0	184339	94482	79392</		



EIC	Negative	411.2754	5.46	unknown	7447854	6089325	6024853	8164242	1444196	4666294	6727550	4875568	5921111	5190127	6070035	2562884	4312465	6123887	7169799	1099346	5214171	1977678	2162121	
fpHILIC	Negative	484.2738	0.46	unknown	1051345	0	1832755	1737800	0	0	0	3086059	0	1105677	0	0	0	0	0	0	0	0	2065543	0
EIC	Negative	244.1999	3.00	unknown	309423	226013	587539	1478437	487949	345106	398921	894556	590726	589178	312789	558758	450707	117745	93665	379437	369646	827267	149494	
EIC	Negative	269.1762	2.92	unknown	536759	84222	391151	257495	157422	190487	170942	272160	151195	341147	103833	161263	112027	87974	111897	117615	91097	232649	77725	
EIC	Negative	444.1910	3.26	unknown	62286	69077	71960	214389	11271	80466	47937	35421	22303	72517	36065	26601	11584	7747	38746	80097	13526	0	251718	
EIC	Negative	314.2418	6.38	unknown	5651504	2901304	5818493	4431561	3857876	2982985	4292496	6749938	2101483	3899225	2451557	2389548	2180183	1793369	2476144	2236110	2337400	4207348	2145718	
EIC	Negative	393.2589	6.44	unknown	9336188	6207880	2242120	4932579	4130178	5735690	6909588	6744200	3103711	4699390	5866225	2720290	3939876	5349651	4837909	2157774	4578307	3039381	3306600	
EIC	Negative	334.2108	5.67	unknown	3071011	1445132	2978681	2452294	2024287	1544492	1995147	2932768	1539717	2140078	1286027	1387463	1321621	1082868	1227417	1184818	1232213	2038025	1050591	
EIC	Negative	630.3501	3.90	unknown	0	483808	154653	186224	0	132824	371838	136965	103287	126779	159495	0	27884	65986	480759	57546	25292	25350	166583	242102
EIC	Negative	437.2907	6.20	unknown	17085576	6287392	11071505	24863419	4900613	5054590	5252207	12912766	8350172	9398981	5302988	2989670	5727261	6128363	5742555	2302379	5788101	7349899	3394032	
EIC	Negative	271.2281	4.03	unknown	5272897	4560071	16272474	47940624	11893512	8179565	9415012	28251870	19290084	14830210	7624512	14258891	12701426	3645091	1881558	13639944	9336421	22877605	4218276	
EIC	Negative	629.3662	5.12	unknown	3287967	913886	2231067	2504673	1541402	2208850	2055924	2125751	338049	1425826	1145351	1673460	864090	546046	1203068	455352	1082540	1669744	1172598	
EIC	Negative	541.3410	3.92	unknown	563949	22128	2397636	1297449	31635	0	1525267	22700	905841	23267	21717	21310	72569	70412	29027	20618	946994	0	0	
EIC	Negative	583.4929	6.42	unknown	8661649	12576420	10145866	14521306	13093745	11802531	6733589	10695580	14204331	10874786	935153	7697771	10970569	8084970	6359422	7970176	7427479	8808213	7624692	
EIC	Negative	272.2314	4.02	unknown	1009204	832618	2778901	8352971	2077710	1447028	1711976	5102833	3463060	2597694	1350052	2535319	2263260	643973	349358	2408663	1714773	4103245	749733	
EIC	Negative	329.2330	4.05	unknown	466155	260107	551525	456398	325984	301919	316141	444117	316141	390284	191617	237701	228801	167506	176182	168080	201080	291184	213264	
EIC	Negative	632.3939	6.09	unknown	474487	539017	430424	321722	425380	622953	504798	374344	278045	297188	396299	359671	337405	256364	324174	226361	316583	250460	375935	
fpHILIC	Positive	234.1440	2.50	unknown	805893	431872	387927	881939	499159	542072	390254	549625	650407	517184	519862	276746	501078	179006	327535	524188	370705	274047	248955	
EIC	Negative	385.2271	3.29	unknown	331145	52474	463893	927893	41981	42938	39877	123823	43736	259708	12091	212575	47587	39357	45049	28236	46161	78659	0	
EIC	Negative	502.2946	5.13	unknown	7014199	10381541	6871217	5180213	9041237	9335374	7575243	6026649	3955518	6508217	5043632	4789132	8016565	5290844	2857627	6436273	4339562	6795107	0	
EIC	Negative	300.2626	5.25	unknown	413202	354940	963202	1812050	603454	465835	547594	1279108	790955	616970	347650	628592	539149	470635	180229	580607	414946	942533	382797	
fpHILIC	Negative	559.4728	0.37	unknown	1879888	1921965	3655425	3869433	2747745	1601809	2289407	2355071	3281032	16469925	1520217	2176134	1787894	1316562	1611630	1501437	1603455	2019386	1593312	
EIC	Negative	438.2941	6.12	unknown	6342095	4798799	492784	9507360	4551740	6663674	5693233	5527689	5972761	4976556	4938865	2854197	3705743	4420503	5598564	2161624	5674525	2822176	3023107	
EIC	Negative	319.2279	3.36	unknown	3770608	0	0	3187172	0	490994	559257	0	490994	559257	0	2112354	1535557	0	0	0	0	1334321	0	
EIC	Negative	300.1684	3.12	unknown	21567	12936	25409	200392	101469	0	9833	110990	9550	16360	8615	0	10724	0	0	14316	11276	132105	0	
EIC	Negative	337.2044	3.16	unknown	378833	115512	376422	181219	140645	187853	91046	259348	32868	239015	95438	118159	42823	49359	136807	61484	133435	0	152493	
EIC	Negative	279.1605	2.39	unknown	1076035	574560	834057	798949	679713	1035419	856114	970821	241155	853557	458635	578475	474646	399010	580892	350472	574305	585660	485982	
EIC	Negative	265.1811	3.69	unknown	319634	374805	363750	1774516	556935	371779	501533	546276	1132793	957357	330087	397268	610660	197402	168038	548558	468196	706077	227950	
EIC	Negative	579.2262	2.92	unknown	519117	276374	159170	240021	129627	218625	107095	315651	141443	424278	144741	166045	186365	48420	87478	136239	61733	303192	33878	
fpHILIC	Negative	284.1001	2.28	unknown	1330715	1170751	1311107	914257	986548	1216872	1001693	711212	700694	1187374	703220	644900	864211	519406	539380	447314	827952	898917	451514	
EIC	Negative	243.1965	4.65	unknown	2055635	2899105	4679192	15185516	5414785	3369931	4962605	5623973	7068209	5586228	2744606	4834370	4539549	1484616	1178040	3496910	3821555	7851520	1704260	
EIC	Negative	628.3628	5.12	unknown	9098642	2573010	6143616	6742600	4248086	5903239	5840549	896207	4008529	3325108	4819518	2436415	1520720	3203284	1333263	3012238	4726264	3435352	0	
EIC	Negative	440.3104	6.35	unknown	597214	820435	816199	1020067	621016	860566	702955	683955	828443	778162	684787	452227	450440	696046	641739	103472	629181	480223	467132	
EIC	Negative	269.2125	3.74	unknown	1576778	816803	2601957	2469425	1748236	1273689	1576982	2870583	1483565	665800	873343	1153833	1157604	952187	628244	1160266	1172623	2248787	913612	
EIC	Negative	270.2159	5.19	unknown	423330	581235	825766	2691090	1149418	5861138	926112	920231	1330401	195010	603005	1086382	822437	285662	248860	697671	672434	1404129	323460	
EIC	Negative	430.3046	4.27	unknown	2594495	745742	3015547	1648681	1021240	957103	1065008	2730953	1069588	1170843	575130	783304	629378	1373701	884466	635292	704759	1866229	990915	
EIC	Negative	416.2114	5.67	unknown	218629	113540	214909	174307	141954	119071	143954	226994	106138	106747	118824	110610	106367	98217	110361	114475	110610	124127	970025	
EIC	Negative	279.2234	6.29	unknown	7118742	7399854	10917204	15183376	11093891	6563814	8356655	10803921	12520763	6900215	9547453	7694923	5305494	3870912	6876145	8282935	9097763	7742973	0	
EIC	Negative	447.3129	4.05	unknown	3274078	310686	2561497	960237	273835	427893	351359	1550906	262944	1212910	192501	213167	448108	247515	167004	184910	254299	1139693	1407253	
EIC	Negative	266.1846	3.69	unknown	40389	64324	91808	390519	102007	69528	88080	96349	202000	106674	65198	70099	108012	30950	30659	92425	85365	133145	41392	
EIC	Negative	348.1914	6.06	unknown	153666	188659	275357	453828	236669	125180	228622	183236	160311	121865	160311	210865	106627	97301	139729	171147	247105	118814	0	
EIC	Negative	511.3063	4.27	unknown	1415421	611166	1535189	1032175	681237	724435	845434	1614209	740860	701402	502665	606134	509423	877797	655806	431455	554243	969723	554422	
EIC	Negative	325.0019	1.26	unknown	6433679	5156853	6177297	3604459	3888255	3789622	3754061	4135063	3203105	4564356	3397115	1139206	2382322	2803283	2664326	3527233	1687554	1996721	2979245	
EIC	Negative	437.2907	6.12	unknown	23079924	17786820	15207782	33502704	15924624	23746981	20359145	19444545	21378163	17619791	15883146	10342918	13124648	15719536	20461872	7549218	20423256	10315032	10667389	
EIC	Negative	301644	14.1974	3.74	unknown	301644	141974	473371	434326	293913	512897	282380	319408	1678226	202125	198219	173972	113004	218274	208446	1083052	170007	0	
EIC	Negative	565.4469	4.14	unknown	57978	46178	282315	334844	144021	75754	131751	372725	138326	150485	57931	59111	65197	192002	196409	43050	115328	298003	115794	
fpHILIC	Positive	236.1686	2.28	unknown	9998151	3638727	8072779	6271562	5072919	6234539	4660713	6908636	2337336	5743314	4052324	3130039	3424944	1627727	3845669	3047547	2468077	6459702	1592313	
EIC	Negative	463.3444	5.22	unknown	433154	0	219975	46082	0	0	102563	0	63498	0	242114	427589	461384	217500	26409	0	0	44750	0	
EIC	Negative	266.1844																						

EIC	Negative	273.2073	2.36	unknown	521331	145261	419161	448019	271753	332837	256414	623238	137310	526920	136414	163433	141068	93722	137227	147175	210823	488519	151952
fpHILIC	Negative	498.2898	0.44	unknown	57871648	1114611	73275488	88571296	1108062	1487736	1883424	68525880	3040223	36730376	1181197	1024233	1971105	1894498	1511511	1017314	1363793	4809900	1280809
EIC	Negative	239.2015	6.35	unknown	872575	1001780	2147466	1451232	1043837	1175207	1541945	1651400	962707	732141	975424	1309844	740311	416684	1022534	1102901	1336012	915022	0
EIC	Negative	337.2139	5.68	unknown	471921	161366	348239	430822	200350	148718	199566	278477	252398	261983	193385	158411	182321	282696	217666	34562	182411	169698	153866
EIC	Negative	325.0019	1.41	unknown	581634	1347719	0	0	843975	875519	781141	0	542929	0	904486	149623	410718	620614	485298	847242	236082	0	569884
EIC	Negative	597.2296	1.96	unknown	0	124311	0	0	30981	43107	115908	0	0	0	173400	65998	98688	17445	18124	56337	44667	0	14458
EIC	Negative	343.8252	5.82	unknown	106125	90899	135474	465899	184128	66108	218402	120200	148536	141302	72036	169927	198412	27872	86670	70654	122992	177347	61091
EIC	Negative	301.2657	5.38	unknown	110398	83274	280705	320550	130187	57816	125943	254022	177157	130970	66656	127399	108372	156589	58850	44216	96225	214679	111039
EIC	Negative	300.9577	1.25	unknown	416267	261908	382481	266174	193912	159896	156821	198005	151194	297862	138242	68665	95311	150809	110468	126333	70991	150000	148367
EIC	Negative	319.2275	3.96	unknown	438621	0	602687	1774346	506895	346558	435054	806054	616081	715289	359739	682666	570607	0	471903	385161	1053992	0	0
EIC	Negative	540.3376	3.93	unknown	1633091	131894	7543868	4069398	157416	52675	63859	4598456	173784	2730419	157401	159341	163381	312895	251508	171092	150938	2809367	175496
EIC	Negative	429.2860	3.73	unknown	495029	284322	534715	341761	265730	284548	404091	377561	353905	487159	396797	131616	196034	408913	360485	104036	331733	165049	227802
EIC	Negative	251.2015	5.80	unknown	315389	429524	757563	1316072	728961	466874	615802	912301	801089	518200	385913	575703	651712	337943	297663	458053	556449	783665	392152
fpHILIC	Negative	670.3730	0.54	unknown	1021559	298692	501749	0	299914	346945	385285	139086	550929	0	426250	0	65290	269183	107459	579609	0	0	388732
EIC	Negative	568.0678	1.26	unknown	1464789	1394013	1530690	933443	1065096	968716	1046694	1129972	960993	1212833	999706	225377	664374	794870	794670	980412	448756	513317	920207
EIC	Negative	271.2281	6.35	unknown	19613268	11590651	21630409	4846104	15988647	17469753	15688630	20047482	20088957	16965355	12946519	18926555	15136803	6789210	6440425	17145834	11152821	18934760	9491349
EIC	Negative	500.1029	1.26	unknown	74896	87365	114092	23704	65760	70088	69733	0	55618	64264	61926	0	21992	54359	37650	73243	14585	0	59359
EIC	Negative	242.1841	3.82	unknown	140682	202346	201031	907014	341021	216614	262946	289702	534889	364233	203865	294678	276195	107899	92125	241931	231841	494600	104412
EIC	Negative	235.1338	3.97	unknown	161961	127812	234362	631170	204298	131612	212651	265532	297303	270731	123611	201855	211595	75786	75940	180680	150461	296219	83747
EIC	Negative	299.2592	5.25	unknown	1943541	1730384	4699885	11079545	3031889	2102759	2793466	6651657	3891926	3276850	1956483	3245582	2847690	2323289	1064351	3069982	2281325	4683094	1987452
EIC	Negative	272.2315	6.35	unknown	3426097	2062643	3767409	8766704	2815857	3126207	2702680	3582805	3644991	3095700	2375110	3294645	2705496	1239559	1101690	3057113	1973595	3405716	1716096
EIC	Negative	523.3292	2.46	unknown	287624	35573	456726	230300	38668	85076	68544	58544	35212	313987	42242	40601	35552	60539	51976	35846	44109	482406	31341
fpHILIC	Negative	223.1703	0.39	unknown	4339681	3047194	6974932	13867830	5357696	4347734	6212667	6563548	5953082	6400800	2923116	6546050	5557190	1099285	2030941	3235063	5194698	7147808	2581118
fpHILIC	Positive	235.1649	2.28	unknown	94304776	35476624	73098192	55152416	43967456	57581780	41132560	6376384	22889136	54688660	24850214	27720346	28826584	14688727	31592438	26532842	26540024	61603976	16539002
fpHILIC	Negative	187.1341	0.41	unknown	3200682	1387488	2641801	4431181	2200016	3204851	2153333	2360765	2292109	24323291	1229455	2014258	2003321	1401658	1256283	1635022	1688811	2619279	1478905
EIC	Negative	239.1653	2.25	unknown	570532	271265	617823	957294	394176	351602	446720	697603	541798	645050	286737	398079	357646	140118	210400	429839	247145	675838	166308
EIC	Negative	297.2436	4.52	unknown	3508333	2030131	10212497	34816343	6429336	4432925	5623635	18234081	10925161	9017520	4715858	11340752	8816223	2284768	857299	9545858	5565335	14098722	2398361
EIC	Negative	414.2940	6.17	unknown	86087236	96979381	81159144	110162719	69994648	88803355	98296621	80521717	18716140	67518712	89010633	49512511	67273031	83187172	90043031	35802353	79012214	141037989	49915367
EIC	Negative	607.3817	5.85	unknown	877288	1195102	906465	722663	1003986	1435079	1298953	820146	380272	622258	969979	877784	769428	619468	836622	512089	813730	524398	829777
EIC	Negative	237.1495	2.22	unknown	664862	358989	540178	999190	457710	463047	678949	669874	495187	673048	338391	527599	516817	138491	297959	520647	329213	603267	218070
EIC	Negative	252.1320	2.54	unknown	203260	96669	164411	109361	101154	116582	161800	176775	94325	130944	80488	69890	68714	75045	71035	83561	69865	149064	90027
EIC	Negative	291.1967	4.29	unknown	272032	304134	299701	1140857	349769	261396	334599	396791	828668	372601	220320	246944	477969	137374	165504	472312	339625	427757	142235
EIC	Negative	268.2000	4.37	unknown	564406	657497	910964	3624477	1165213	714865	853245	1072625	1592499	1080720	614093	1194814	880242	326967	318856	751369	744261	170762	329005
EIC	Negative	490.3259	4.27	unknown	1783647	476218	2036975	1090091	641144	646642	747150	1804523	664013	751895	416608	453883	475730	974195	622244	439362	488281	1203727	459471
EIC	Negative	504.2994	5.13	unknown	358642	557697	334336	299862	418689	476564	409844	321693	288158	185915	454760	273962	442625	299508	161746	361540	223933	319821	0
fpHILIC	Negative	329.2497	0.37	unknown	10399700	7837418	12878024	20952898	7945118	10022139	10094753	11139261	14511024	10029115	661892	9472610	9150772	3869333	5808609	6386634	8686268	1064304	6992187
EIC	Negative	258.1798	3.00	unknown	500643	156379	240620	196965	212664	246223	250146	289660	167162	277971	117656	180955	138488	120197	189336	117247	132402	210023	112131
EIC	Negative	413.2911	6.17	unknown	335130417	378599278	312913782	426766988	276293192	344477427	377865620	310284522	305331119	261321798	344430175	190371126	263271813	324220719	351150379	138572006	307714424	161009747	196305326
EIC	Negative	270.2159	4.05	unknown	421848	420757	960433	1701542	755695	607398	1304452	563711	1304452	668668	541899	663297	579687	251489	663297	600911	978106	442721	0
fpHILIC	Negative	253.0176	0.58	unknown	1241876	1234839	1546357	600929	1069252	2372199	1156200	1116924	464117	874151	1140837	934608	516597	1028903	1346928	634345	555111	864754	1026148
EIC	Negative	251.1654	2.52	unknown	562635	493366	659447	1303149	356925	510374	589655	541510	616997	448060	1243830	480839	149147	382543	291500	299156	469899	629403	0
fpHILIC	Negative	195.1390	0.40	unknown	2563306	1263566	3013902	5073973	2173859	1756881	2617738	2973072	2871619	2156031	1605967	2342008	2351653	653425	1001545	1684237	1847344	3188465	1147778
EIC	Negative	263.2017	6.07	unknown	158069	232884	197153	459204	231898	165045	224051	222913	294388	184441	149181	218832	236272	108075	167399	180838	185427	148465	135326
EIC	Negative	273.2342	6.35	unknown	393132	208249	388674	998159	335656	359680	297646	368362	415939	342768	242269	408356	298466	142931	133157	348766	200893	406121	188074
EIC	Negative	502.2945	5.44	unknown	510472	459371	421710	338331	407438	547513	453660	265576	306050	252337	224735	365689	0	312700	124516	371031	366221	310159	0
EIC	Negative	254.1762	3.17	unknown	111989	71228	117452	449664	86213	98252	102202	133157	202725	116374	92622	119533	126092	0	62951	139769	98947	146037	0
EIC	Negative	343.2879	5.83	unknown	57248	24262	313962	474327	188867	125408	166413	245627	143291	0	102356	179691	199212	54804	58367	102044	141840	301306	21894
EIC	Negative	378.8434	0.52	unknown	135591	119020	187906	196745	90696	100473	170932	128583	142835	150531	123855	116584	128101	50836	121044	0	99794	123022	

EIC	Negative	247.1703	5.39	unknown	276534	154873	260841	934114	322502	250447	400902	483069	318059	414800	205005	381885	451526	65120	160082	323235	228323	472639	123747
fpHILIC	Positive	401.3458	0.59	unknown	1060111	804567	932055	1778829	811994	832212	888030	832440	1279922	716824	733685	715823	1148636	524882	672790	1040412	696387	811746	202567
EIC	Negative	330.2370	3.80	unknown	126252	49009	116114	91595	57429	94978	62265	115363	22845	82713	40418	47919	43324	32167	38684	44497	50885	82588	43516
EIC	Negative	237.1859	5.85	unknown	226270	337587	377137	1511878	4887739	269674	331665	458054	729618	449714	232297	305739	660094	118885	111798	492524	433815	497523	145021
EIC	Negative	570.0723	1.25	unknown	105039	102796	103472	61608	66033	66838	72527	49124	102796	85291	71277	19263	50098	59653	54195	74652	37352	0	67868
EIC	Negative	314.0529	2.41	unknown	144474	99381	173636	125504	82159	81420	91094	183561	50451	120266	117535	82850	45574	16749	70240	72120	33804	140918	44104
fpHILIC	Negative	180.0748	0.48	unknown	4946335	1830360	2280380	639779	1925813	2230611	2386008	2393673	2738400	2506953	2583704	275817	1252534	1310920	1680600	4680027	242095	658542	1379422
EIC	Negative	399.2763	6.25	unknown	483226	283550	364318	406605	261537	303725	343222	372152	259484	312262	387894	221206	278872	275658	341744	172902	279044	176067	170888
EIC	Negative	527.2983	5.23	unknown	2722947	857625	1726211	1861840	1569545	2322310	1955411	1700259	4739677	1169922	1302872	1915853	681863	847120	1432006	375553	1181863	1382558	1332313
EIC	Negative	555.2803	1.77	unknown	327313	302425	366539	292538	94762	284825	418863	342728	329574	486120	297860	315061	241276	271942	81008	184833	226701	0	377582
EIC	Negative	623.4355	6.31	unknown	369812	945629	1147921	1083086	675292	833249	423601	910643	1095717	685092	967500	857005	359565	433528	681641	549895	720150	542398	424867
EIC	Negative	364.2129	6.41	unknown	3684288	5843763	4193842	4896897	4992972	4888764	6130560	4585280	4273805	3782903	4070371	4623172	3995011	3058874	3109589	4182504	4175445	3454976	3512249
EIC	Negative	249.1498	3.21	unknown	576318	226536	652365	380270	306622	342820	193375	472675	106240	525557	257714	150243	118387	0	206633	141996	82134	494375	128911
EIC	Negative	605.3660	5.13	unknown	813306	845605	852976	596549	629051	696055	751842	878645	431492	523395	656549	467428	579300	485106	476074	468790	560057	497353	54139
EIC	Negative	523.3288	2.85	unknown	256295	293664	651565	1151813	320118	301476	305022	484209	363841	675137	330591	337443	177263	63632	109585	234334	252340	666470	54139
EIC	Negative	543.4638	4.13	unknown	65876	36564	254447	313606	120051	59855	90529	283311	126580	165842	40846	51767	55041	167319	14104	36519	98759	267397	87955
EIC	Negative	479.3384	3.43	unknown	793132	587026	1277553	1820816	2083086	1226026	2188121	2976608	5490471	3414057	1394849	4046267	3003509	232242	302557	2148050	2045046	5557631	310799
EIC	Negative	399.2544	5.95	unknown	151982	341267	115809	351590	221878	252359	132650	590971	717050	171050	172774	193698	482098	146360	192881	226376	199436	123748	135129
EIC	Negative	241.1808	3.07	unknown	4406545	1894670	5227629	8753114	3743397	3575270	4270157	5716151	3879312	4819262	2890125	4574877	4063113	1770885	1685169	3477505	2935024	6039820	1592872
EIC	Negative	283.1919	3.90	unknown	784722	375015	724799	757021	543276	484738	623969	780275	546280	590204	357556	481618	371474	216892	358083	382136	313367	735127	1296849
EIC	Negative	531.3320	3.74	unknown	430668	54299	705504	108617	89678	49794	50138	248010	57085	201956	43465	37108	14360	37189	36076	20455	44382	226383	40127
EIC	Negative	227.1652	3.47	unknown	178601	157783	265079	917313	294091	176773	320156	374107	514669	347219	218857	357046	351788	105844	104504	326655	249704	485028	108156
EIC	Negative	283.1921	4.83	unknown	328979	146382	415945	744323	241421	248188	297606	408934	166536	417041	194677	273073	309414	115680	120081	153160	193492	430964	116917
EIC	Negative	265.1481	2.62	unknown	0	3106860	0	2042635	3169427	0	2233457	0	955941	0	0	2552354	1284163	0	0	1567854	0	0	3170900
fpHILIC	Negative	151.0401	0.52	unknown	687945216	305392160	289129408	81141120	294068128	315022112	384826944	316810048	453634016	323896288	339952544	2264593	97656424	202012784	208686112	669749952	43309780	91504664	30297888
EIC	Negative	300.2626	5.38	unknown	1016646	756812	2093179	2655514	1035847	657689	987514	2125490	1392246	1031886	595276	681874	741265	1208745	563533	561983	762455	1714403	971914
fpHILIC	Negative	197.1546	0.41	unknown	8257199	2778161	5892637	11277799	4074439	4720874	4692571	6151330	3855338	4388535	2276990	4671450	4119327	1531831	2691067	2905592	2923578	6732657	2304286
EIC	Negative	228.1686	3.47	unknown	16159	26359	47750	155458	53022	40418	62604	60009	84734	50105	38636	57585	64242	21457	21375	80758	43197	78066	21285
EIC	Negative	273.1723	3.27	unknown	47891	37843	73809	45741	23841	62864	79667	64848	98374	53100	69105	92617	72966	42079	24669	42050	51170	68301	60416
EIC	Negative	477.0439	1.25	unknown	131302	131678	131533	118222	96945	83351	91666	88697	87714	119531	92629	47783	70509	71417	84947	80352	60123	28950	81484
EIC	Negative	319.1588	4.83	unknown	527185	265660	734990	1002990	464473	451791	588780	726606	346346	742231	312480	504993	535777	132588	207239	403826	406645	714292	199134
fpHILIC	Negative	87.0453	0.92	unknown	1090676	608632	1526227	1146657	751913	842169	663491	1026968	797540	728611	556074	759930	606613	545431	50507	643028	648366	668171	594273
EIC	Negative	338.2702	6.38	unknown	544157	353646	613324	1940430	409697	362123	515873	620715	663017	446325	309257	533838	528092	173080	218038	574590	344124	589024	202053
EIC	Negative	243.1421	4.24	unknown	200333	97196	194591	183268	115434	149724	129002	153267	70118	139379	99405	104569	71996	26954	78247	124054	35409	173438	51854
fpHILIC	Negative	280.2358	0.38	unknown	51006864	65372852	100794704	116234264	76634176	65694072	76400872	83825664	105224600	59180368	49059492	69248824	70039056	42264040	47442832	58727764	68102728	76332488	55239196
fpHILIC	Negative	152.0434	0.52	unknown	61112420	26959610	24602762	6764659	25413560	26704418	34651976	28531902	39216628	27982972	2945480	203175	8502363	17683856	18220174	58960812	38722144	8273880	26590532
EIC	Negative	312.2264	5.98	unknown	509978	178627	674895	422710	301155	201750	357313	718918	113269	471457	2385950	202440	157353	139111	180325	150579	178923	588349	172479
EIC	Negative	502.2845	5.13	unknown	6753310	9250428	6552233	0	8697547	0	7271668	0	0	6179720	0	0	0	0	0	0	5895318	0	6095034
EIC	Negative	439.2965	6.12	unknown	1123177	999094	786534	1659243	849237	1074187	10330028	1013070	977710	875688	754811	531343	658933	772663	1241083	389523	1021582	507108	553653
EIC	Negative	288.1616	2.64	unknown	482669	212299	488667	469744	364007	412207	606661	102325	414928	311165	205312	206333	157498	133430	112675	230508	560258	290018	
EIC	Negative	242.1841	3.07	unknown	668051	296479	835114	1387558	576344	564311	691824	605264	764669	465848	719913	635809	276577	238463	547956	407023	1002312	249093	
EIC	Negative	463.3071	2.46	unknown	2694739	223890	3977161	2131464	319959	576324	230894	5640208	340413	2674304	328972	330303	196156	340475	242923	185948	267375	4573014	184198
EIC	Negative	449.3284	4.15	unknown	2108234	102523	1571228	642255	113456	85415	103031	62908	764498	847495	631823	91334	63866	76448	93452	54144	622639	646669	53046
EIC	Negative	271.1746	5.90	unknown	224557	114159	212862	293060	84797	105929	82877	170757	150485	141905	93155	44990	66856	0	66780	135678	0	200901	44019
EIC	Negative	287.2231	2.96	unknown	154745	154038	598520	2513971	656411	379669	596068	1227881	1068315	804619	331938	767765	870110	97637	109013	1052805	571601	1117016	105248
EIC	Negative	480.3417	3.43	unknown	227011	184157	399309	5759525	649985	477540	691272	872683	1691739	985205	488414	1239721	938414	95100	100616	680854	626221	1795841	99410
EIC	Negative	303.1574	4.59	unknown	67092	68302	140177	387686	105024	198447	131646	132892	102780	194020	48906	160183	134977	42393	41399	112366	86779	227814	0
EIC	Negative	383.2912	5.63	unknown	317124	235843	429943	744944	340344	265248	310842	438256	438098	300339	206334	244845	343447	124257	205831	268869	279009	395112	201753
fpHILIC	Negative	111.0201	1.36	unknown	23259306	19039550	19305102	28579316	21154208	24109976	20827160	168332											

EIC	Negative	239.2015	6.30	unknown	1291484	1604605	2933354	3775831	2445302	1524247	1945382	2699773	2802199	1906016	1381659	1665410	2197511	1552419	735580	1645763	2114524	2627208	1573785
fpHILIC	Negative	279.2328	0.38	unknown	253796960	336813792	502389312	602385344	384532768	321965536	388183744	424285760	537096640	293701344	259603520	354625952	352635232	209661760	247406464	295808992	334460512	402334528	286287328
fpHILIC	Negative	321.1368	0.95	unknown	1153850	407959	904403	414251	438857	501151	347999	452980	516628	505331	246988	400051	310758	298717	347307	319921	234243	336135	254103
EIC	Negative	271.2281	6.04	unknown	4735611	8946325	9836324	12960213	8554290	7446873	7573119	10935772	8355059	7597762	5245246	6156008	6107848	6312923	4430237	5435665	6270455	9676987	6854891
EIC	Negative	526.2928	5.23	unknown	8684689	2914809	5814386	6485497	4951179	7124560	5381287	5400022	1449372	3836345	4388509	5978495	2320487	2740423	4973932	1422449	3420367	4408653	4424681
EIC	Negative	111.2228	5.98	unknown	2544066	845076	3307989	2071803	1546017	930508	1759867	3610089	567904	2447630	1137777	1023887	836444	696208	851207	762396	929010	2963757	912887
fpHILIC	Negative	117.0043	0.57	unknown	800866	637568	1052395	871158	760869	861818	736391	881409	717989	975367	712562	967214	644779	507447	540777	685146	562107	625615	580525
EIC	Negative	270.1795	3.19	unknown	93160	31631	68129	37516	47548	45336	52823	67360	19382	32823	25389	29158	30900	21656	41264	31923	32134	53393	19046
EIC	Negative	429.3011	4.20	unknown	1674073	703860	1707542	1242469	656383	876636	650820	1584147	910773	970787	569782	639803	539354	965572	708815	523409	693155	1064888	558852
EIC	Negative	391.2439	6.17	unknown	8921615	9767381	8988411	11933212	7121046	8646657	10209277	8607936	8611264	7794182	9249382	5612243	7078120	8725456	9821201	4143397	8408180	5086825	5691950
EIC	Negative	304.0911	1.26	unknown	1209324	1241576	1579615	374704	1146838	1217188	1279715	1139018	893325	1115402	1177422	98313	547720	1059859	867920	1871796	290422	195016	1172722
fpHILIC	Negative	565.5183	0.37	unknown	255190	1417692	1597684	2344288	914897	894183	1218398	1055103	1501804	683482	276877	1206422	747038	472632	637129	1021019	739879	1226620	657720
EIC	Negative	242.1842	2.97	unknown	244890	111360	353370	355793	210334	178543	173445	362534	179803	349662	148962	207830	144374	204569	71417	111777	169567	336828	157644
EIC	Negative	323.1844	3.82	unknown	98362	143726	136436	539865	214720	144212	176975	186506	335697	254000	142937	199184	176495	79411	75247	158089	164288	329834	84486
EIC	Negative	309.1341	1.58	unknown	541276	379735	307489	168998	256027	200227	253445	259880	125323	414648	159494	207227	188471	220503	181100	201686	131640	105094	220542
EIC	Negative	508.3386	2.43	unknown	183775	87890	103318	179681	179681	291764	67441	136621	61403	198355	82795	136629	75750	84218	130636	80457	107649	173900	72814
fpHILIC	Negative	199.1708	0.40	unknown	4160819	4705679	9250367	12333026	6646800	4848846	5961417	8372530	9861151	5297360	3607596	4707981	6482524	3684080	3272900	5117215	5746645	6898587	4567012
fpHILIC	Positive	426.3571	0.54	unknown	5270700	3998937	5426003	9724309	4897880	5127436	6209160	4905671	927162	4807857	4752849	5419543	7032957	2032155	3646239	6650209	3718191	5348352	2955065
EIC	Negative	556.4314	3.43	unknown	141603	96675	155181	580733	221099	160251	301256	215601	297999	130036	162608	253873	236829	86435	99979	234348	188977	309169	86336
EIC	Negative	269.1716	3.19	unknown	480386	159506	390257	227397	340572	253399	243026	306977	98719	130036	134406	210727	172760	131597	198198	202391	170751	299113	122871
EIC	Negative	263.1654	2.44	unknown	546553	232785	486839	319617	333318	313974	416766	443697	155375	384571	215049	214069	210350	202657	280720	184544	230218	382265	200646
EIC	Negative	287.2016	6.08	unknown	312541	223545	370783	831294	364114	274358	464642	517451	395610	480077	264449	399095	373251	107284	177152	396260	287264	363249	166381
EIC	Negative	495.3696	4.04	unknown	827841	475896	635519	690384	547015	666014	555265	778859	260685	515754	436046	340742	304501	277290	442409	381574	465115	565457	306135
EIC	Negative	272.2314	6.04	unknown	813949	1590486	1758358	2203534	1513450	1732605	1332463	1998854	1470934	1312641	938611	1083881	1059102	1105659	763625	980630	1123135	1713151	1236420
EIC	Negative	389.2464	6.17	unknown	26469405	28063694	26032210	34855007	20075796	25117169	29225674	26450041	25053159	22556924	26651464	16134804	20164686	25440308	28978529	12208757	24194902	14889202	16456705
EIC	Negative	606.3783	5.74	unknown	30329745	35645786	39953925	45510681	30059228	48199109	34215516	29569444	17742987	2540007	30734925	27221914	23531058	22652029	24289890	18973357	25526500	22050954	29417013
EIC	Negative	313.2387	2.36	unknown	108477	50718	72788	148388	63729	64932	68793	124236	91705	94178	38572	82767	67975	52904	31918	84437	59048	99122	44631
EIC	Negative	305.1738	4.83	unknown	3175744	2150422	3848622	4524871	2679158	2614881	3328242	3752217	2345700	3573238	2215317	3526396	3444197	983167	1560983	1788991	2516115	3428006	1680588
fpHILIC	Positive	318.1904	2.51	unknown	715903	368218	684847	825873	511068	507790	651004	432580	818895	817357	450013	395511	599512	206132	625989	607202	323566	456189	245763
EIC	Negative	325.2658	5.20	unknown	1137992	1069345	252019	211226	0	83108	1029646	1100449	1013395	209687	1069445	1026417	1068834	995147	1064554	189127	1029198	123652	0
EIC	Negative	507.3334	2.43	unknown	568892	323476	399160	298395	527284	879555	200027	450333	198351	609154	305359	406141	221242	233972	433839	245762	316895	558834	190137
EIC	Negative	300.2277	6.06	unknown	1531232	474419	1755891	1184483	778151	551933	820172	1761593	235995	1231510	635054	526763	507857	414766	545235	288721	513583	1230107	632438
EIC	Negative	369.2278	2.96	unknown	39136	23943	64570	162555	65066	48701	74842	92177	84655	64177	44125	67011	84655	25731	14603	89369	66765	85916	193475
EIC	Negative	305.0933	1.26	unknown	175972	192057	217199	82201	168674	182037	199034	147888	134904	179037	186277	16532	89356	170947	128124	291751	48693	0	175774
EIC	Negative	361.2602	5.49	unknown	11857121	3907217	8736186	8718686	4569348	3832417	6636349	4636219	4013377	6387087	880662	3352009	4018000	6706681	78070078	5071418	2360946	2079219	0
EIC	Negative	553.4128	3.44	unknown	22469	34568	89523	1174424	106838	75958	137552	222739	250266	152901	0	178422	144987	30390	0	152334	146376	315628	0
EIC	Negative	347.2594	5.02	unknown	163871	95521	198843	522232	134403	142835	140522	187888	462277	123136	195331	136332	85819	91707	149245	108613	278429	60843	0
fpHILIC	Negative	202.0722	3.59	unknown	859852	546893	515709	534487	502557	946523	402496	162041	310886	462277	842954	329748	343251	297460	459371	361342	344101	217779	419673
EIC	Negative	301.2030	2.52	unknown	492363	135863	498536	190547	498536	251787	260368	66410	611863	611863	129521	110687	133300	131947	82218	128952	454866	152647	0
EIC	Negative	283.1921	2.43	unknown	1369418	454350	1248349	956593	707550	734883	861970	1449016	411124	1045033	471330	533690	493089	436257	525515	468688	476188	1380422	379279
EIC	Negative	407.0050	1.26	unknown	384394	320673	347651	270791	253938	262974	239784	232011	239784	239784	234607	127360	204016	203228	194454	232025	163877	166281	207890
EIC	Negative	604.3629	5.31	unknown	6346832	5850611	7696383	5033695	4817834	6213632	6570719	6352991	2614770	4917229	5279159	4684442	4445577	3912302	4261509	2977597	4822700	4028045	4527227
EIC	Negative	239.1652	3.43	unknown	28096702	25116158	36278687	141320581	47522065	35841925	49662019	56314711	78795022	60403521	38144485	66553224	57454444	15147582	17336783	47945978	45733337	79023903	18104438
EIC	Negative	323.1850	3.07	unknown	322414	178788	353514	651348	338671	326450	376968	459130	316784	395191	257244	504886	344640	173468	171497	304350	275654	510995	149152
EIC	Negative	330.1794	1.78	unknown	875428	390033	825989	405919	219476	152613	380413	163725	362975	523399	243581	257308	234049	256383	220696	341756	279960	0	151086
fpHILIC	Positive	276.1432	3.07	unknown	2059296	1142071	1178493	1601884	1597891	1607325	1238590	819993	1213568	1165297	1233994	556613	571424	448409	1029754	964828	1235063	669326	1137260
EIC	Negative	607.3816	5.74	unknown	10265892	12146918	11605992	84959152	10152198	14256099	11617444	10018946	6014195	7401256	10356836	9150479	7991831	7608813	8320524	6505744	8812590	6852878	10023462
EIC	Negative	275.1427	3.43	unknown	172947	14																	

fpHILIC	Negative	159.1027	0.46	unknown	1552329	1423470	1952618	4470849	1747495	1949784	1701601	1821703	2589104	1940717	1347516	1793194	1768703	985250	932679	1853257	1499330	2377687	1129939
EIC	Negative	307.2053	4.14	unknown	203327	169259	488905	484868	294900	195122	243958	528285	308247	311243	170952	224149	223224	367399	157876	142450	280877	448248	218251
EIC	Negative	434.0306	1.25	unknown	235839	227043	237169	224556	166696	153313	162260	219626	157129	189738	155461	82778	171115	132851	135183	142151	106474	148054	150816
EIC	Negative	237.1494	2.96	unknown	168162	102954	184648	362014	137715	140354	172084	185307	186982	183686	118860	174623	156812	92068	93992	132901	130198	200562	96076
EIC	Negative	335.1865	3.72	unknown	714873	231080	728947	519331	334442	409717	398902	743271	116105	493669	239722	313036	223823	152162	235858	217424	227600	685545	225316
EIC	Negative	275.1269	3.07	unknown	367578	259967	290858	494141	363807	312394	386688	289311	248720	361195	290780	342289	312718	133472	248644	338377	272884	194610	133933
EIC	Negative	273.2342	6.04	unknown	102689	178414	202976	249973	176791	156015	157976	209046	159560	143109	114100	132508	117135	143614	87596	119044	129869	273118	153268
EIC	Negative	525.3431	2.23	unknown	394579	61977	612316	220201	103513	82074	71981	609063	89035	226522	47746	46539	28304	60676	55049	83926	64169	505449	51992
fpHILIC	Negative	179.0757	2.29	unknown	612686	309946	522364	466833	376614	474969	408982	486849	256831	70514	329316	324675	275633	306850	315668	274082	488497	210674	
EIC	Negative	253.1809	3.52	unknown	688462	408589	1282478	2931266	202452	215163	240308	474605	190356	1104835	295674	809552	336883	234091	149166	174307	132343	303578	294844
fpHILIC	Negative	178.0721	2.28	unknown	9159164	4383589	7423321	6472381	5259473	6924410	5498712	6448726	3415836	6358814	3646678	4426360	4035589	2677725	4028585	4277908	3969034	6724764	2962721
EIC	Negative	550.3207	3.55	unknown	1988513	2378355	1918569	2137040	1936636	1940052	2229575	1727329	1603539	1706589	2060420	2198289	1928652	1973971	2009273	1750661	1745181	267576	1751879
EIC	Negative	252.2048	5.80	unknown	66990	75358	135625	270588	123721	92874	105992	140861	139168	89364	67706	115222	117172	58045	50583	76540	110889	159009	83581
EIC	Negative	291.1220	3.36	unknown	403096	238355	290261	650549	300681	373075	370874	562358	225677	204973	228293	411611	454689	138821	281048	258243	186731	581475	154130
EIC	Negative	299.2240	6.06	unknown	8107041	2606973	9318454	6437823	4083662	2741212	4043261	9761348	1216866	6777465	3491364	2812332	2692497	2200280	2894312	1614638	2839532	6586498	3503161
fpHILIC	Positive	132.0654	1.76	unknown	1756934	841190	855510	1642424	1115388	1277144	934497	912132	1016773	1281959	1208325	1276118	996609	0	821555	1035267	680089	916654	742284
fpHILIC	Negative	101.0608	0.61	unknown	14560357	4010825	12756654	8122239	2454743	8715102	2104053	9375632	7715956	4638486	5114392	4502097	4056900	5520849	5340449	3291441	5393452	4518888	5157558
EIC	Negative	389.2910	6.39	unknown	100402104	37037716	70601856	0	29641972	51374132	33808212	33114106	0	59229984	45929294	41647916	0	62881492	54069252	0	3855592	0	24734394
fpHILIC	Positive	147.1202	2.96	unknown	2088916	1279101	1722420	2213526	1003602	1168451	1139365	1328192	1195042	1090251	1290400	1158861	1138157	861237	888926	1036348	954294	1171359	609277
EIC	Negative	249.1860	3.36	unknown	461824	135356	340893	290885	181736	193032	204223	329886	159481	301688	195450	135458	107410	155354	130034	152085	338637	97818	
EIC	Negative	505.3515	4.08	unknown	509963	400015	793815	526344	1400295	854968	1641754	1496346	2874374	2079756	1155590	2266212	2135097	140444	313088	1555059	1534680	2980214	230768
EIC	Negative	353.2699	6.52	unknown	719529	539217	1189209	2016676	856849	613911	954892	1202744	574703	807234	626241	626241	575554	571444	576621	661725	656802	820025	582586
fpHILIC	Positive	298.1137	2.15	unknown	1019994	479634	571051	875828	578461	986178	691728	456432	671631	624205	651000	720273	681035	396379	546506	727355	491251	542043	402046
EIC	Negative	262.2639	5.49	unknown	2479974	867082	1872867	1811864	956455	782975	1418345	961364	860228	1347178	1247884	692351	819396	1489764	1725325	213885	11801423	494386	471971
EIC	Negative	299.1650	3.24	unknown	333438	357660	417790	305636	114039	217935	197997	137012	127344	115800	185652	278845	124229	36626	160692	192365	102190	100318	85055
EIC	Negative	284.1954	3.56	unknown	491793	196649	427169	315925	295642	281379	357387	493734	126556	344704	180211	284126	216329	193073	234210	225613	222200	403706	159402
EIC	Negative	496.3732	4.04	unknown	242142	161524	199367	229685	154943	206717	166976	244498	89592	184135	155116	90715	83763	98524	128051	116408	165882	189230	88461
EIC	Negative	605.3351	3.04	unknown	289130	50121	387255	239078	80662	57543	89042	196947	91651	213867	51507	43823	53246	130490	77797	45117	59658	307172	56736
EIC	Negative	294.2156	3.98	unknown	67447	34977	122431	434716	100616	69221	72594	205476	125064	119252	70149	111688	110247	54751	30886	93869	83573	208748	42342
fpHILIC	Negative	115.0401	0.57	unknown	136700448	119156136	158913376	165116112	121298592	153127968	149396880	142838592	145474176	146566608	148512864	173978720	182081444	81449856	101780800	121912136	110292504	134556048	102468256
EIC	Negative	276.1278	3.33	unknown	130829	102498	0	110619	98932	100997	98350	0	29249	0	0	0	98365	11703	98354	108829	55499	0	0
EIC	Negative	237.1495	3.01	unknown	248699	128667	201406	300223	174467	197553	193515	187838	158181	185286	127699	170859	150431	89104	138227	155050	130109	213785	93081
fpHILIC	Negative	268.2361	0.38	unknown	589550	755272	1375105	1617879	889190	698638	929172	1298880	815862	572330	727229	1200883	580796	375933	959268	906290	813812	709218	797818
fpHILIC	Negative	167.1078	0.43	unknown	1205889	586381	1029923	1406264	854134	683388	760094	793691	877064	924242	659806	939342	874173	437804	437024	616824	693941	888858	547100
EIC	Negative	439.3071	6.35	unknown	2155618	2859861	2979868	2309789	1529421	3060131	2287794	2897219	1581045	1881877	2717701	1100289	1624602	2486434	2374216	912541	2242670	1575912	2026320
EIC	Negative	258.1503	3.69	unknown	194527	94880	197582	194097	135091	107529	124844	201554	113488	163438	97638	90358	78549	78553	105375	112415	87111	162548	80401
EIC	Negative	480.2999	4.84	unknown	1137421	0	0	0	0	0	1289559	0	0	0	0	0	0	0	0	0	0	1035424	0
EIC	Negative	294.2157	5.02	unknown	417377	475778	446293	1043096	606762	580662	732331	685375	790394	590374	473371	776991	638765	334236	413198	619110	496930	882482	316936
EIC	Negative	295.2277	6.22	unknown	463700	485088	620751	1044498	590542	433694	468101	576351	698590	454325	392140	496333	446504	250118	357689	434085	666160	342700	
EIC	Negative	447.4915	6.36	unknown	1475341	1103635	1607635	166392	1055105	862671	968037	652506	534715	920225	673756	628669	494388	465984	387828	745341	607423	750259	785947
fpHILIC	Negative	275.1082	3.86	unknown	541205	235200	362697	406864	265584	340408	280502	290420	247348	518122	302684	181159	263994	142229	337755	142299	185574	221995	186600
EIC	Negative	530.3582	2.92	unknown	130381	45340	289191	789274	131922	44959	188299	124949	214897	314288	113670	202684	164392	0	187805	150681	229161	0	
EIC	Negative	238.1529	2.37	unknown	802100	405374	719164	687835	450572	429263	528758	329042	0	746677	366848	445480	394068	353186	406221	356683	328075	599699	348547
EIC	Negative	298.1849	5.49	unknown	382731	162350	445766	261255	156457	0	193395	128785	0	181094	165092	0	0	157148	0	0	0	228329	0
EIC	Negative	329.1761	1.78	unknown	3810595	1737842	3613495	1668327	984743	675255	1714254	619718	1575153	2441666	1115582	1140060	1036008	1195551	1005219	1506542	1261594	0	713862
EIC	Negative	310.1745	3.09	unknown	583539	159801	400560	191425	281931	199559	346622	469516	101713	295560	126650	159937	124595	123057	226774	197367	172595	426910	104287
EIC	Negative	269.1370	2.34	unknown	476665	239395	511548	1566398	511548	226133	262402	809728	396075	735766	158466	229400	275764	114738	113862	233342	186015	939188	158041
fpHILIC	Positive	267.0574	2.66	unknown	951409	881091	966345	1643764	1010284	1262583	952660	1031864	1200229	1079550	1075281	1067615	976324	607059	892531	1061018	994921	697142	757354
EIC	Negative	244.1896	4.08	unknown	61309	40505	81324	236418	79882	68177	95276	91087	131418	11									

EIC	Negative	409.2970	6.18	unknown	659789	477658	697185	788828	727029	351934	442703	580554	429688	626469	405558	366188	368447	462748	471161	449572	358986	417613	366890
EIC	Negative	254.1481	2.89	unknown	555159	149713	353210	226046	164975	202535	226968	255297	111516	344465	113646	188694	134413	159155	166722	100300	112018	270975	133876
EIC	Negative	336.0378	0.55	unknown	346800	157381	146853	456670	110951	106253	238044	126949	112913	148591	196141	268413	169678	119285	138821	129807	114107	177041	128730
fpHILIC	Negative	156.0455	0.96	unknown	2452923	9078809	8808009	3470334	2819608	4445902	2347839	2887544	2513912	5419332	4556717	2461789	2672119	3856049	2757595	3245234	2033733	2811129	1398774
EIC	Negative	284.1955	2.43	unknown	249971	82456	180862	126792	128792	140928	139283	265769	68517	119323	776517	91712	83634	66594	91389	78841	89798	271899	79456
EIC	Negative	463.3423	4.00	unknown	546488	0	315016	71368	0	0	0	118143	0	61340	0	0	0	0	0	0	0	96467	0
EIC	Negative	251.1289	2.55	unknown	1629874	726213	984011	650111	713909	685580	885199	1109477	465120	882996	571086	502685	557331	462091	497842	609370	510846	1023226	509997
EIC	Negative	498.2901	2.62	unknown	351632538	2939172	578220678	343794427	0	0	473261571	19366122	287936582	6494129	7558728	12712107	0	9903433	4993071	7478349	373459006	6627883	6627883
EIC	Negative	376.2788	6.13	unknown	345415	146790	175794	280996	140802	119088	185730	111126	150153	121874	123915	105074	133119	137300	167385	88165	124595	103457	93996
EIC	Negative	538.3219	3.00	unknown	85056	0	270949	174641	0	0	0	484106	0	94239	0	0	0	16694	23438	0	0	372420	0
fpHILIC	Positive	400.3415	0.56	unknown	3704165	2484644	3622390	6003168	3100800	2944898	3347512	3298396	5027791	3206571	3210918	3604104	3749112	1592937	2390828	4123141	2494704	3409480	2075297
EIC	Negative	271.2281	4.14	unknown	20483139	17188090	46267782	52608585	29540404	19578419	24830462	51674028	31870785	31525479	18419657	20491870	21335665	36995595	13914362	15902611	27298287	47980153	23786252
fpHILIC	Negative	169.0771	0.97	unknown	380975	925663	1023395	385273	287505	507395	233644	258569	292066	600515	416998	253601	296700	391928	300990	344217	238489	266608	142316
EIC	Negative	284.1954	3.79	unknown	224890	67165	179048	126477	106348	108556	129777	218920	57012	155448	60092	98862	70628	76221	103966	58697	81944	190913	72526
EIC	Negative	306.1770	4.83	unknown	561809	390561	664956	825683	461125	465243	593461	644819	402541	642970	359096	662048	596017	188568	328749	386665	468622	637016	280802
EIC	Negative	306.1769	2.36	unknown	206149	113888	223821	191430	10159	17907	130006	136130	67007	115631	11221	84111	160060	49818	16171	67007	45048	9377	133339
EIC	Negative	242.1841	3.20	unknown	354876	193464	567195	606998	276282	345705	293774	417854	318111	452176	248928	395875	330883	396033	157920	205604	284443	465947	238828
fpHILIC	Negative	325.0451	0.98	unknown	320068	593445	546332	1033926	901172	0	712038	712038	814804	851273	363032	898286	1427942	891118	235873	479816	443656	737415	315848
fpHILIC	Positive	586.2732	0.38	unknown	2768523	2669585	4771065	4868651	2254595	1701946	2185452	3547785	1910860	4319211	3085957	2485191	2980788	921793	1141731	2382435	1320767	3683629	976339
EIC	Negative	608.3945	6.34	unknown	8822702	6713557	6877630	4963168	5222408	8494497	7820309	6158472	4351614	5175794	5300742	6147382	5491099	5059835	6555154	4663569	4701749	4531590	5818008
fpHILIC	Positive	239.1640	0.45	unknown	804584	435388	919209	961815	674938	547816	770522	785211	425452	803418	488632	583025	652196	304713	444790	552244	415333	731905	479552
EIC	Negative	283.1920	3.56	unknown	2825429	1084147	2516308	1736024	1637958	1596511	1987343	2654126	708877	1912832	1011525	1522473	1268515	1107477	1302199	1223337	1286848	2304669	922339
EIC	Negative	502.2947	5.24	unknown	1141150	945996	942091	701180	1095803	1193164	858872	924335	462155	628826	653466	618070	513674	899023	817888	351803	774283	833152	941869
EIC	Negative	271.0929	0.55	unknown	290565	74413	101050	139904	59221	201311	87937	0	28707	178740	182055	185741	167162	219030	143750	144466	208824	705421	193360
fpHILIC	Negative	110.9758	2.96	unknown	559082	191892	1154513	449197	282699	233574	262266	743088	197969	718740	182055	185741	167162	219030	143750	144466	208824	705421	193360
EIC	Negative	281.1763	3.22	unknown	5330127	1694294	3873392	2424362	2825713	2759169	3688781	4317230	678073	3226671	1666228	2149887	1676265	1741127	2493310	1725374	2242988	3834868	1461167
EIC	Negative	240.2048	6.35	unknown	160569	147746	409506	371416	223847	140373	186411	275468	255933	212367	138096	195155	212762	200516	45732	204690	226582	227327	183867
fpHILIC	Negative	270.2519	0.37	unknown	993410	988294	1517687	1666489	1010472	1294105	1138165	1293452	1430236	997003	796227	1217705	1144643	1009123	835116	1006770	1104447	981123	1135073
EIC	Negative	412.2790	5.73	unknown	431021	321065	413049	1277219	175478	188783	325448	541608	29425	426412	417373	167190	370113	485951	432611	62951	398660	216036	141545
EIC	Negative	269.1761	3.34	unknown	569916	370470	422891	310575	309858	421298	338851	253556	545836	364726	264236	425800	484993	374873	339367	462688	335186	250831	146923
fpHILIC	Positive	113.0539	2.22	unknown	553227	358170	461411	575238	348530	554438	343732	464338	504860	493581	413300	452584	456162	405275	336703	423178	324454	377876	358366
fpHILIC	Positive	548.3698	0.54	unknown	3932834	3349640	4289689	3151042	3320290	4275461	3667317	3491179	2134572	8202715	3218449	2992491	2591387	2648721	2708827	2116701	3085475	2786307	3187772
EIC	Negative	268.2002	3.56	unknown	365563	195592	665419	608809	277287	295165	227458	559469	218369	1521057	218263	251919	185582	469497	98413	103465	237672	582278	274950
EIC	Negative	241.1809	4.08	unknown	33809135	28855861	43697679	157642868	58655283	44713267	67818167	62672064	95933225	76524529	53851357	81419807	77506030	16518569	24761770	65180040	62320859	98084084	20901473
EIC	Negative	484.3734	4.08	unknown	257058	210392	528006	6183181	852658	468164	1223381	1002400	2294361	1423005	740033	1198225	1543668	84471	149289	1081085	1015004	2452700	107048
EIC	Negative	322.2477	6.22	unknown	301270	132605	335663	537044	216312	197094	122502	299039	193248	330602	144229	190512	166624	96527	93030	152548	131472	352151	116983
EIC	Negative	328.0002	1.25	unknown	613735	578484	675605	407240	592867	631735	614572	508989	571948	591649	602270	244741	508136	598652	576720	697226	395973	219432	574255
fpHILIC	Positive	440.2058	3.12	unknown	472972	182353	189470	547286	221220	578852	163000	121690	204102	245629	226643	225137	274205	68872	171936	289203	244391	169353	186778
EIC	Negative	479.3374	3.30	unknown	749146	54844	86503	382187	0	522512	0	0	42023	0	0	0	0	42023	0	0	0	501746	0
EIC	Negative	445.2958	2.86	unknown	946523	397412	763292	715982	392971	451735	437761	869997	507351	711776	345709	381838	312171	660245	424968	255030	391522	794902	325478
EIC	Negative	269.0878	0.65	unknown	519225	171510	215232	664465	86981	482040	250329	114557	120448	127295	245853	296808	216564	44486	136931	213574	122044	209611	150488
EIC	Negative	419.3165	3.07	unknown	272293	0	214921	65197	12056	11409	12085	279571	12096	70999	0	0	12082	9087	0	0	9438	251216	0
EIC	Negative	581.0430	0.55	unknown	548629	496484	318631	1105424	242623	761788	586854	384042	244419	265167	543211	733004	486302	135578	378731	460428	337315	400740	253008
fpHILIC	Positive	232.1399	3.97	unknown	665697	512802	384137	675226	456151	664947	399466	372999	413855	436840	418094	445712	511791	340803	395231	362705	403115	291698	449830
EIC	Negative	283.1939	3.63	unknown	1384541	417067	1121111	866119	646738	700952	774172	1160349	280733	911185	369150	606960	450023	452159	542289	463377	484957	1055023	392603
EIC	Negative	277.1808	2.85	unknown	4889033	10601614	10828848	8134771	5548163	7773199	5889559	7677415	3351593	10288534	9886657	6271581	3206144	2744899	5101374	4602285	5596768	8111170	1532759
EIC	Negative	354.2347	4.14	unknown	295011	250176	548532	321791	631175	445443	321791	631175	445443	4998254	248524	241362	246177	482579	199846	198479	359805	630252	328363
EIC	Negative	299.2591	4.63	unknown	0	325435	848726	1110471	587216	0	520390	0	524520	0	0	0	0	0	380319	0	0	966875	0
EIC	Negative	505.0078	0.55	unknown	256973	63267	52204	158842	0	222345	72435	0	45938	71142	99259	60600	0	62256</					

EIC	Negative	407.2928	5.10	unknown	2434356	246145	519508	982252	363621	196858	298304	428281	420919	421815	216820	293058	284806	192867	233049	264331	271717	520673	132194
EIC	Negative	309.1710	2.85	unknown	10594785	21912611	24222740	17471736	12372544	16688764	12892448	16281796	7721092	22924449	20747721	13606738	7514712	6632260	11343385	10136016	12021042	16910460	4574816
EIC	Negative	320.2314	5.66	unknown	184279	163188	207946	643805	223828	219699	231216	317049	389463	256151	177095	295513	98574	98574	157095	267582	205531	390655	130726
fpHILIC	Positive	127.0979	5.42	unknown	3814637	3575607	2296300	2489268	2838797	3635705	3338285	2220289	2708181	1786617	2271663	2461375	2657415	2571175	4330420	2635091	1478353	1679615	2167648
fpHILIC	Negative	298.1419	3.48	unknown	1750416	1297062	1648930	1776570	1627901	1733526	1414783	1727261	1273643	1744138	1681913	1719262	1736758	1267117	1538133	1552561	1669494	1724749	0
EIC	Negative	377.2329	5.53	unknown	261518	285246	394674	851413	473217	332229	395592	395146	546405	521915	310826	485014	458477	175838	205191	300054	426762	628269	225811
EIC	Negative	241.1808	3.20	unknown	2369471	1205752	3579957	3836356	1802617	1962798	1802609	2740905	2015711	2835198	1630621	2505937	2052693	2522212	990185	1331738	1653576	2864884	1575374
EIC	Negative	233.0424	1.25	unknown	192754	173511	157219	149794	168743	173735	184339	149600	157729	175284	192612	106756	158515	153183	164826	175930	148958	32863	173624
fpHILIC	Positive	585.2701	0.37	unknown	7647882	7241932	13204343	13777293	5946069	4896655	6067090	9729743	5517474	11709050	8801712	6898748	8090993	705250	3044603	6649715	3601867	10785249	2763524
EIC	Negative	239.1652	2.91	unknown	3833906	2511479	2510949	6087932	1996612	4931816	2419888	1970986	1028441	2720491	2169664	4387048	4476897	2401268	2824018	1660312	1922850	2294394	1607812
EIC	Negative	506.3264	6.39	unknown	2661141	3070283	2625516	2099542	2053632	3051310	1950617	2222630	1254871	1472546	1303353	1810528	975198	1744093	1397006	1503886	1187281	1800857	2906315
EIC	Negative	311.1772	2.85	unknown	431869	617307	613289	470748	380212	478513	366823	489028	195942	643132	564690	390978	227751	193073	311244	263537	360700	500449	160179
EIC	Negative	355.0106	1.19	unknown	73059	68705	54211	44104	50499	52703	48809	46536	47346	57670	42695	40725	42187	35193	40452	33239	33569	61025	37114
EIC	Negative	449.3281	3.74	unknown	4709887	616122	8491566	1370123	792086	441779	426406	2541227	584314	2140249	366771	307422	238213	461736	363654	404541	410324	2445461	376166
EIC	Negative	295.2279	5.53	unknown	4026258	4687660	6145499	14975376	7826284	5274498	6434875	6537885	8354439	7517605	4772889	7605876	6316591	2995725	3354541	4784174	6294927	10573599	3801499
EIC	Negative	337.2137	5.49	unknown	1068524	338845	750237	829993	421357	320075	528230	423929	406284	647446	529485	296014	401365	609795	741074	812074	476637	276623	180297
fpHILIC	Positive	510.3555	0.59	unknown	4791543	5345612	4348803	4676826	5232834	5615582	4771569	4593423	3603735	4088493	4559877	4679246	4672960	4266631	5181100	4939741	4693457	5108428	0
EIC	Negative	499.2932	2.60	unknown	104379958	890169	174039083	102404763	33069	12548	140533913	0	86062794	1978188	2230345	0	3057384	1540970	0	111478449	1592474	0	
EIC	Negative	445.3329	4.06	unknown	132067	12725	315145	84037	0	84037	0	146393	0	126721	17793	20763	0	12899	13309	0	81157	15196	0
EIC	Negative	500.2913	2.61	unknown	32223428	241920	54246976	32118693	30630	12428	48958	4442816	0	27612082	624781	692825	1228702	0	935099	484337	724493	34621887	513609
EIC	Negative	443.2411	3.49	unknown	162474	93860	135038	403726	110715	119272	103210	169231	124983	245459	107409	137595	171995	29248	49585	128427	101909	218090	27791
EIC	Negative	319.2640	5.96	unknown	486264	407742	538045	507159	416263	268652	336716	432086	34758	583833	398536	250283	278596	197970	397608	286868	254661	364973	210911
fpHILIC	Positive	794.6088	0.43	unknown	1531860	1475069	1613438	1952598	1371058	1430519	1212965	1718203	1640698	1232325	1357400	1138156	1089298	1078385	1106300	1236413	1260526	1388046	1193420
EIC	Negative	240.2044	6.30	unknown	241278	273773	445718	773805	437843	226678	318616	443452	426564	341391	235054	280748	371830	279508	81825	296163	387488	533728	254515
EIC	Negative	583.0304	1.19	unknown	71932	84419	71203	53074	63909	70538	62189	49410	54243	60721	52248	50519	51945	42248	47657	41357	51255	48883	62786
EIC	Negative	281.1765	3.45	unknown	812541	284292	743728	464801	465070	422961	571439	806149	188837	548677	283279	452319	337264	341106	400152	308837	390689	715642	243968
EIC	Negative	316.1999	5.64	unknown	686062	429663	635762	687994	568182	398476	421008	624674	472424	584817	487957	464265	437390	449003	422268	393367	417729	491955	360448
fpHILIC	Positive	169.0352	2.98	unknown	741323	451327	662115	870045	391197	524184	186036	340643	379703	466662	637461	509019	133299	238275	238275	426564	390902	331923	270639
EIC	Negative	388.2791	5.91	unknown	625790	244679	436812	446008	252944	312159	365149	265328	193809	344356	367683	213032	239907	390403	473042	19365	331614	194502	147968
fpHILIC	Negative	88.0121	1.03	unknown	9456632	6195359	5128376	3490089	4409488	6244990	6950319	1449020	1237496	4274014	5716139	3473912	2096358	4639194	4380392	4563785	1928944	3358961	2804112
EIC	Negative	407.2809	5.32	unknown	466427	375460	525977	376734	460015	303824	436619	441662	412352	429223	364556	297456	334488	324727	385391	397826	324469	333339	284501
EIC	Negative	346.2470	5.83	unknown	255069	289452	298952	778716	294399	290669	310386	395917	704045	378368	277719	236720	510727	185198	155156	365119	398496	401014	167153
EIC	Negative	285.2435	4.74	unknown	558877	516530	1107911	1266257	842808	560441	635749	700875	704087	728425	449792	560024	538375	797045	445332	551540	570482	1119219	638311
EIC	Negative	265.1811	3.39	unknown	476989	179090	573285	417047	237038	299346	258698	474504	157539	455421	238903	334267	238598	241779	184633	160607	182074	431354	240543
EIC	Negative	339.2177	3.08	unknown	111275	45115	157463	75039	46966	62266	66419	88661	75039	87844	46966	33435	37272	26215	35905	55127	21373	83115	42542
fpHILIC	Positive	232.0914	3.35	unknown	511481	284197	420332	443331	424594	299245	330076	371318	358665	315427	454135	278605	260289	319851	0	310326	343222	404398	441348
EIC	Negative	278.1840	2.85	unknown	841132	1958731	2027589	1471377	1009541	1440893	1399664	627439	2013147	185013	1503515	1286035	595471	499769	970134	851081	1038371	1503426	324751
EIC	Negative	419.0227	1.19	unknown	82908	79562	54392	62224	55043	63910	49006	44342	35637	54154	49597	48561	29988	36548	38326	37721	36018	60287	36241
EIC	Negative	526.3154	4.05	unknown	664082	740424	635867	518310	50545	720077	652386	568016	535399	559894	581932	613823	569536	606051	491762	506001	491762	448233	407738
EIC	Negative	526.3154	3.64	unknown	2866034	3124893	3048715	2960253	2423798	3608757	3327332	2629917	2452408	2608236	2753064	3219338	2746947	3808417	2827870	2609321	2303715	2171872	2310521
fpHILIC	Negative	360.1230	3.34	unknown	3706960	3281150	3547248	4130820	3628468	3604156	3898922	3226699	3250642	3310279	3919218	3549484	3597755	1933647	2985622	2839537	3183934	3021542	2793608
EIC	Negative	527.3190	3.64	unknown	725149	828938	931114	782873	661733	1013253	939292	751647	178628	741294	745055	906868	757347	971166	744200	736918	585072	769315	602927
EIC	Negative	635.5241	6.46	unknown	17462892	15294210	10982586	13249806	9367818	11822821	15085570	13927618	11039027	15540230	12567732	8151865	10610017	16816430	13759115	4956909	14789225	11356571	6707661
fpHILIC	Positive	487.1773	2.61	unknown	2119036	797477	410937	2092656	827685	1421382	629770	765837	1984292	929843	333285	312421	1000247	490242	507349	1695991	712458	1113525	710727
EIC	Negative	501.2928	2.61	unknown	7429882	51751	11733309	6870601	72735	43988	9000	9787516	38137	5742286	143212	156959	218212	254473	194509	117022	123514	7767320	141914
fpHILIC	Negative	232.0512	2.92	unknown	381616	464266	427983	413482	312931	552269	387505	368659	259323	409319	578777	510834	382345	287663	299520	353897	325113	331440	276789
EIC	Negative	644.3552	3.78	unknown	117683	12246	31290	77372	28829	66695	31795	46167	24797	49832	20610	71848	0	14421	41935	33677	39345	0	52578
fpHILIC	Positive	223.1692	0.37	unknown	677144	444011	825577	778168	529108	415831	562194	629559	391482	556733	409070	508678	399223	377868	399861	374182	35		

EIC	Negative	359.2206	6.30	unknown	3507741	2702638	3747857	3065577	3190465	2318695	3287806	3120255	2810355	3024320	2263609	2359371	2775485	2303972	1769597	2711978	2828471	2799538	2447737
EIC	Negative	395.2440	3.45	unknown	177586	136463	313433	511663	159164	173696	263834	339695	323953	241438	168115	268115	228112	187000	94282	248385	223499	371863	138001
EIC	Negative	451.3447	6.51	unknown	500494	530994	636321	816199	538223	382243	597150	506168	588937	626270	527419	532725	493471	331368	419384	534712	505565	446318	327453
fpHILIC	Positive	701.5586	0.48	unknown	1840866	2118972	1697155	2033773	1961204	1582951	1338830	1666573	2341282	1639807	1716288	1578410	1712840	1705661	1555111	1608029	1587739	1298444	1546167
EIC	Negative	463.3066	6.09	unknown	475201	0	0	1054992	0	0	0	0	0	0	0	0	0	0	0	0	0	536339	0
fpHILIC	Positive	231.0978	3.86	unknown	618919	243722	458431	416555	298905	341121	336959	292641	293769	429867	326441	226386	337672	237781	323862	201009	311447	230987	264958
EIC	Negative	563.4309	6.70	unknown	79936	67616	115478	189921	117081	103760	113848	84694	152416	98418	122109	88170	97257	102274	102274	86833	54805	101487	86785
EIC	Negative	412.2787	5.59	unknown	1153241	841378	980192	1727443	476942	561561	868397	831358	721606	906158	1063988	390871	698356	1038334	1149694	188711	918384	332359	372622
EIC	Negative	310.1745	2.85	unknown	1981006	4158429	4240761	3123930	2308387	317936	2441674	3014742	1431891	4254729	3888174	2551166	1435592	1223133	2246066	1948423	2292605	323784	860330
EIC	Negative	439.0101	1.19	unknown	600073	555511	472211	422113	397904	421651	429921	379111	351277	397318	345142	326395	288369	296214	317256	284810	295029	467061	336963
EIC	Negative	319.2277	2.15	unknown	387809	0	367196	0	0	0	0	458709	0	0	459152	404120	0	422159	0	0	392781	0	
EIC	Negative	315.8959	0.52	unknown	98875	115877	147696	138186	107269	123841	120971	107754	136886	99271	103529	109035	106889	40091	94667	106703	97356	124623	88248
EIC	Negative	264.1689	3.06	unknown	448834	367642	395574	314955	317635	407991	353189	411419	215389	309589	303654	329588	328159	252966	291656	286207	266646	344455	273508
EIC	Negative	458.9978	1.19	unknown	199098	199243	196430	175449	149042	137584	143866	166193	144891	154804	127140	119148	124101	116012	117097	114585	116346	173759	114594
EIC	Negative	345.2436	5.83	unknown	1002153	1272729	1256654	3165200	1137116	1189712	1333493	1609336	1985621	1644884	1123025	922800	2026631	812778	700490	1477447	1598912	1718865	735113
EIC	Negative	287.1659	4.94	unknown	37262	50964	77136	197145	54973	24274	68800	78450	0	0	0	24104	84987	0	11428	72939	42014	87656	0
EIC	Negative	358.0100	1.19	unknown	190159	159128	143413	127687	119244	128911	128843	107715	102427	130160	104170	98337	84297	86700	90290	81387	80219	150782	101341
EIC	Negative	297.1241	3.43	unknown	150939	147034	202873	539730	236214	182185	230005	292559	337050	321730	206031	314255	266285	97069	110723	233912	201064	416713	135114
EIC	Negative	323.1848	3.20	unknown	224253	118166	299310	379473	177891	200639	171894	285071	206762	275888	162531	217027	176090	220989	101795	186797	164421	294953	148144
fpHILIC	Negative	285.2708	0.37	unknown	2522831	3181194	3171808	4239514	3300171	3436760	3239482	3130252	2647815	3212719	3017019	3379521	2569985	2673409	2022808	2444328	2634361	3197584	323073
EIC	Negative	315.1967	5.64	unknown	2955337	1983492	2950138	2956464	2941869	1675094	2023346	2796599	2129182	2839995	2156151	2094183	2155786	1864458	1834671	1906709	1968480	2183444	1661879
EIC	Negative	648.3470	4.77	unknown	297944	237880	264288	199518	229732	228709	268018	236452	152687	263922	119627	199270	199270	199270	244221	241737	133675	152321	194105
EIC	Negative	238.1528	3.60	unknown	110706	69305	120821	174014	78233	85073	96660	112552	59317	90905	82873	104903	100365	43628	63653	83763	61677	111658	50696
EIC	Negative	415.2437	6.12	unknown	431408	221031	289937	617964	222426	329933	320990	301282	377297	429847	277932	154932	243417	240139	344242	344300	382333	285173	178791
fpHILIC	Negative	89.0131	1.03	unknown	1850649	1311747	1069228	820836	870789	1240350	1344269	291761	244090	823595	1316549	633474	472465	976140	913036	977669	369108	560034	614989
EIC	Negative	282.1798	3.22	unknown	967459	330168	685332	405020	502379	483496	638303	771714	132630	569188	276850	392609	335159	302458	445704	340635	431765	689157	271268
EIC	Negative	515.2876	1.50	unknown	0	4735905	287233504	219313072	7610405	9055201	3380116	411822464	49251946	340532512	12225758	6834510	64390080	36729820	19382873	9121758	15079081	359891952	11085849
fpHILIC	Negative	243.0622	2.65	unknown	15198453	12751750	12328033	18522126	13574961	17232436	14633676	11261107	12947646	16155539	16607228	14745769	14172063	8270405	14021023	12365342	13272043	10075137	10297265
EIC	Negative	314.2421	3.32	unknown	1035551	741801	1873716	6594999	1249932	1023141	1428969	2591697	1969386	1960417	1128529	20077560	1834110	745224	495905	1761909	1485396	2715220	664593
fpHILIC	Negative	297.2436	0.39	unknown	2626494	2053406	5514902	8172422	3372114	2677241	3844128	5024866	36481195	3153443	2089918	3817660	3012453	3017793	1759377	4140581	3621331	4834122	2373001
fpHILIC	Positive	160.0965	2.71	unknown	2532251	1549994	2189136	2654107	1332271	2480974	1737643	2029401	2163526	2061402	2237786	2163709	1750247	1426654	1437300	2109033	1418542	2170352	1284984
fpHILIC	Positive	251.1024	0.96	unknown	3293522	1279400	2224174	3685919	2209462	2467441	1756956	1584744	1616479	2346368	2374591	2173848	2192384	1790200	1331280	2068991	1584299	2192880	1151748
EIC	Negative	417.0367	0.55	unknown	2355440	1375011	1251304	3306365	873485	2606050	1754580	969848	840311	1162540	1665319	2023976	1383624	638894	1197553	1568207	930591	1387728	1007950
fpHILIC	Negative	359.1195	3.34	unknown	26471036	23045224	25683850	28673164	24714362	24368254	27524196	25100706	23572940	2471027	27264494	22778162	24767636	13842757	21161274	21713564	23347486	2265980	19968530
EIC	Negative	367.2142	4.14	unknown	91196	81780	189915	113788	171388	77766	187182	124090	130916	79658	83373	84117	146694	106602	163546	70271	71761	106602	101360
EIC	Negative	554.3374	4.17	unknown	3134375	4610465	3604091	2986469	3455003	3809213	4454074	3103455	3987826	2653483	3472368	3663257	4095641	4061012	3558729	3705359	3153154	2697242	3130253
EIC	Negative	235.2657	4.15	unknown	202744	206669	199328	199994	199976	200733	190298	176917	169337	165430	176317	176450	174743	176450	173110	160337	177476	156925	159785
fpHILIC	Positive	831.5723	0.43	unknown	1286176	2364012	2305663	1684181	1977417	2360016	2506298	1773307	1355409	1173067	2053070	2026144	1965964	1885382	1530925	1821246	1860626	1262019	2174319
EIC	Negative	297.2436	6.27	unknown	4976633	5937773	9276877	24278629	9900755	6333294	9557475	10700820	12271779	11446867	6558148	10694572	9027802	3686949	3689234	2209814	9308046	1720577	4772396
fpHILIC	Positive	265.1762	1.66	unknown	56513	817145	418537	467157	336350	732252	466508	245822	502687	384076	603781	580788	343179	543955	579415	585389	230332	272533	313125
EIC	Negative	294.1793	3.29	unknown	1083313	706996	1064864	942994	841938	511683	710452	627932	1124217	629920	630607	552998	464851	759089	986988	485854	717940	452363	
EIC	Negative	335.0337	0.55	unknown	3419767	1714355	1566417	4319237	1119758	3577704	2247286	1179519	1050785	1517794	2023742	2504130	1723478	897362	1545158	2089217	1245646	1715035	1369545
EIC	Negative	379.2473	4.51	unknown	315394	187730	608359	1682774	386405	335053	936759	649502	626427	331403	693548	518067	224589	182742	653758	391333	783580	227846	
EIC	Negative	606.3688	5.01	unknown	5930138	8106892	6691896	5477187	6968399	7508375	7361821	6144696	5482500	5150421	7583701	6546046	6944077	6360285	5629956	555910	6641640	4140813	8609658
fpHILIC	Positive	371.1671	1.81	unknown	1113307	512540	872940	1326651	6182507	905408	576001	774541	1070823	667791	742738	635435	400051	631077	741339	548894	759902	466924	742781
EIC	Negative	416.3004	6.25	unknown	962211	583426	799156	972343	352732	578678	572163	730222	513494	647776	711794	464246	517103	677969	674870	59125	561663	570867	519202
EIC	Negative	245.1552	4.23	unknown	133068	75090	197344	399605	71362	78329	99757	157149	85692	171793	72680	104285	149291	24273	41998	88834	97292	148559	58937
fpHILIC	Negative	310.2833	0.37	unknown	1577561	2566790	3563020	7315332	3362005	2271494	2432741	2283728	2299011	2185474	1807725	3720714	2539588	1374732	16277				



EIC	Negative	440.0129	1.19	unknown	129139	130245	104637	92693	91933	95468	89509	75418	81892	100218	75873	74614	72339	74703	67484	63542	67015	102625	80197
EIC	Negative	285.2073	4.09	unknown	4433611	1413510	3687500	2464210	2260879	2747064	2489435	3779239	498302	2694798	1282818	2201349	1480683	1456318	2066094	1171766	1713787	3991433	1382333
EIC	Negative	409.2821	4.72	unknown	729597	847945	660784	653227	828966	680887	728679	700041	717356	787909	657675	700269	744617	626931	665347	732490	636990	607676	612168
EIC	Negative	414.2489	6.12	unknown	272745	199991	165093	374027	131906	210826	159893	210662	252872	243842	155457	105665	139748	155910	209156	110524	231503	157654	115304
EIC	Negative	263.1654	3.06	unknown	2552601	1972020	2126071	1738180	1770669	2211085	2055098	2253763	1168019	1736584	1707062	1805447	1840388	1390261	1640969	1587054	1588878	1902949	1580784
EIC	Negative	274.1047	0.61	unknown	117143	38142	66016	52541	35730	47477	36433	25498	39954	70848	37545	25784	33961	27801	38902	26113	34533	28063	34424
fpHILIC	Positive	546.3526	0.55	unknown	17810554	21087640	22580520	18365130	19692816	22227824	22406690	19651786	16206614	17455912	20973064	19385070	21095920	17362990	15795507	16498022	20558690	15442801	19704342
EIC	Negative	313.1197	1.25	unknown	882574	316965	587021	600051	322604	364406	364738	659825	398252	656360	342402	431487	414264	383719	353226	459877	414755	297256	325503
fpHILIC	Positive	119.0836	2.28	unknown	4363163	2826480	4405076	3489530	3203498	3549188	3071149	3781207	2719587	3591710	3237852	2765021	2860915	2170062	2604871	2562060	2939350	3901557	2319109
EIC	Negative	295.2279	4.09	unknown	1196562	1103435	2134152	4575432	1740320	1343387	1553686	2671921	2063285	1754999	1232304	1907209	1635089	1073199	692574	2311623	1756424	2509843	963624
fpHILIC	Negative	144.0456	0.96	unknown	581744	328776	331624	270353	400955	387166	417653	249393	204436	201135	299720	246541	200868	340367	413402	235259	276396	228877	304782
EIC	Negative	516.2731	3.42	unknown	502036	281652	367598	361695	235776	490284	192658	353826	332142	355820	231488	301655	190558	203280	297903	262884	436120	0	413978
EIC	Negative	607.3712	5.01	unknown	979122	1443886	1087342	834884	1123811	1254290	1185797	1005713	897569	848596	1299474	1018607	1013841	1054915	903050	945305	1128784	755783	1074761
EIC	Negative	579.3498	4.74	unknown	16279552	20844888	19387687	14220115	16333479	18007721	18775571	15989137	13928394	13785145	18900562	17538764	15118765	18266269	14875040	13990336	13002162	12841492	18309668
EIC	Negative	570.3420	3.26	unknown	190334	125078	170487	125223	115337	210131	121877	158025	35112	167572	151313	161113	33564	157917	143096	43177	93401	121970	161650
EIC	Negative	418.0401	0.55	unknown	299013	152918	139233	432842	107662	325653	206540	85741	137970	186284	246260	178220	90722	153688	195958	123140	164734	129023	
EIC	Negative	598.3734	5.31	unknown	1236132	1203721	1277595	1102161	1128818	1109181	1218104	1413901	744665	1101410	1058855	899160	892448	927971	1074273	781163	1101741	1122816	873723
EIC	Negative	257.1760	2.90	unknown	7921887	2375161	5614553	4182541	2265861	2395851	2626974	3586815	1653946	6731816	2183656	2710230	1890947	2004458	2065136	2116648	1829452	3485172	1514661
EIC	Negative	578.3467	4.74	unknown	52150384	65805283	61475042	45091787	51313156	57415961	59362053	50002208	43359132	49320326	58462167	55592855	48116414	56991638	47504507	44332832	41517968	40431747	5021565
EIC	Negative	433.3331	4.16	unknown	134799	73110	116850	154236	114848	142732	99568	142287	75422	170103	83771	79653	69425	23067	66535	91498	425673	7906925	90965
EIC	Negative	265.1811	2.82	unknown	216653	155142	362262	268033	182126	231155	202481	305022	164888	309808	174756	229257	158039	216557	158224	138833	130771	330144	205507
EIC	Negative	442.2965	5.95	unknown	120682	138661	299333	477694	150682	176643	134841	279644	213585	308087	174756	104553	165438	117555	109560	126635	143365	325466	130540
EIC	Negative	567.3505	4.77	unknown	2164042	2915374	2469020	1571531	2112566	2738995	2952724	1979743	1474587	1826877	2107176	2543548	2039730	2242163	2412882	2083728	1769853	1505036	2170694
EIC	Negative	305.1747	3.34	unknown	1029930	202645	1120812	746773	329558	254608	342544	715713	281594	1383140	2466174	304022	248158	275510	253470	222998	253447	726551	242621
EIC	Negative	258.2158	3.48	unknown	59117	36106	83432	127189	56036	42449	56558	87437	34558	70534	47602	65369	50163	24782	38394	51156	49558	86932	36338
EIC	Negative	444.6736	0.63	unknown	261384	230052	597112	416672	241935	288919	228283	168150	361000	738335	236454	210222	272123	112970	182264	158825	188939	305972	301968
EIC	Negative	516.6092	0.64	unknown	96457	37555	103033	71644	86595	95973	59748	40589	61132	161866	39415	29912	49775	141335	44611	37985	29839	58512	100842
EIC	Negative	284.1954	3.34	unknown	2118873	368087	2282012	1597890	602932	584463	679281	1848763	501817	2657282	464093	624074	529346	514847	486708	415554	497036	1575222	427635
fpHILIC	Positive	263.0732	3.15	unknown	703539	497336	450766	634709	485874	635624	379759	405452	588694	494117	417008	483941	405435	410662	387552	557846	440652	429141	389725
EIC	Negative	361.1659	3.38	unknown	615647	110554	589561	287085	270293	307532	372766	724445	59747	453200	187735	217781	154332	167699	253911	125054	250077	636577	267303
EIC	Negative	482.6955	0.52	unknown	218060	58213	186904	172013	226878	149460	155833	79093	84299	264344	67255	80906	106662	327606	100968	102090	57276	128388	208075
EIC	Negative	540.3314	3.75	unknown	612907	44224	2100030	781511	60209	55925	31268	1651086	44719	0	63475	65771	49161	100117	76269	72278	63234	137988	50458
EIC	Negative	344.1546	2.83	unknown	1667411	0	1618741	3598426	49337	0	1586646	0	1855515	0	0	0	0	0	0	0	0	1422654	24341
EIC	Negative	599.2525	0.84	unknown	136099	98748	195129	151738	65694	39778	100837	115140	53140	123556	103106	80128	114235	26938	45530	74773	49019	131755	30360
EIC	Negative	323.1851	2.97	unknown	164180	83234	182846	188366	137874	132737	113196	190609	83234	128866	90509	144500	143621	77982	79865	116695	216029	124969	
fpHILIC	Negative	332.2676	0.37	unknown	1212764	1322858	1662320	2762476	1273747	1356110	1691269	1761052	1268422	1776489	1069459	1769554	1531363	879463	1186121	819372	1363731	1805828	1333443
EIC	Negative	265.1811	3.31	unknown	1993312	914886	2209122	2747777	1248859	1426963	1378178	19692349	911771	2071728	1162966	1965839	1497976	776421	914693	1278355	871167	1980432	850627
EIC	Negative	265.1811	2.88	unknown	274099	128277	268375	405137	166773	205727	161524	258243	133637	322906	147045	249741	183429	113404	114398	128314	140515	313883	122843
fpHILIC	Negative	557.4577	0.35	unknown	3504167	3400369	3357100	2683361	3596489	2630053	3269440	3115753	2590231	2590231	2427241	1885919	2134872	3122715	1633711	1976897	2329101	2472774	
fpHILIC	Negative	239.0773	3.34	unknown	959828	858442	918962	895974	871424	858770	922467	842057	781643	784104	749172	651400	811253	722851	710768	729932	922338	757000	673130
fpHILIC	Negative	279.0383	2.65	unknown	630858	566431	526016	480984	685813	689384	595366	488470	681172	673916	637916	580663	370047	565375	508460	605312	438677	416171	
EIC	Negative	319.2640	6.03	unknown	253395	203865	275451	247241	234867	178985	161629	255372	186149	296728	212622	139460	166353	161764	214928	163105	176258	210021	137998
EIC	Negative	377.9976	1.19	unknown	131000	119131	113033	104647	89220	88238	90447	75565	94059	96760	73425	70959	72277	66656	70794	64362	69940	109004	74170
EIC	Negative	568.3515	4.77	unknown	459588	573882	518049	367254	458300	540984	610752	440591	315495	395862	468897	517538	460078	487823	528864	495883	350760	301195	423469
EIC	Negative	361.1846	3.26	unknown	3842994	3010442	4329677	10412952	1517784	2864255	2285661	1078949	776382	373454	1766650	1086254	507043	285262	2037020	2893917	799660	1187297	651100
EIC	Negative	243.1276	6.19	unknown	1001950	777961	857815	689220	814155	782637	725707	1032193	412808	644738	655688	860466	614139	525595	692702	691620	598158	753373	610557
EIC	Negative	296.2951	3.71	unknown	196929	82227	190117	125116	125655	103106	154268	196587	77305	632628	87820	120136	89921	86615	104903	102096	99541	193765	82506
EIC	Negative	293.2124	3.77	unknown	873580	672517	1195816	807419	867500	842618	988319	972912	671503	838162	582594	514235	496421	1448041	339837	641652	815803	1382925	679479
EIC	Negative	426.7345</																					

EIC	Negative	315.1601	3.29	unknown	305731	283463	407960	374609	268298	188864	234069	258726	248113	490345	288235	264719	227291	184250	328439	190661	183465	251754	117244
EIC	Negative	311.2010	5.27	unknown	944561	1102304	973924	1542277	0	0	0	1418507	0	1068292	1269499	1268385	1214839	1292630	1268994	0	0	0	0
EIC	Negative	529.2903	4.17	unknown	377817	502932	401887	383199	381389	406321	484387	436300	480595	384620	406659	411777	431020	511681	428763	402280	381411	358460	387445
EIC	Negative	253.1446	2.89	unknown	3550653	1029618	2219306	1357362	1016841	1297303	1413684	1664217	711017	2093735	731958	1156420	833635	892829	1127221	832945	867085	1783823	849799
fpHILIC	Negative	306.2521	0.37	unknown	1634905	3295080	2895866	3556772	2387812	2859768	2985144	2399958	3072660	3292628	2583327	2409165	2781234	1524912	2107034	1995602	2649322	2876233	2636047
fpHILIC	Negative	173.0091	4.58	unknown	31245084	25812978	25301750	29573402	27296468	34122464	27840914	21755594	28733000	21198906	96146386	23911766	25203094	23519164	22635910	29203292	23953534	25643860	23704914
EIC	Negative	227.1652	3.60	unknown	173564	87059	178758	139950	102714	121004	116142	139930	96549	166757	271265	151871	154976	50919	77161	121616	939534	1546169	59234
EIC	Negative	280.1613	4.45	unknown	418244	71435	243402	341031	149745	69302	160403	203148	54040	189321	78293	152698	144928	52640	80479	140541	67254	281962	0
fpHILIC	Negative	114.0197	0.59	unknown	5673831	6191681	6757223	3777712	2990360	5329401	6765931	1780297	1220849	5970265	5164596	3364324	1945597	4718623	3980431	4272726	1284622	3005733	2760692
EIC	Negative	330.9579	1.19	unknown	182096	156921	133999	130798	123683	120557	115632	113796	113104	141380	108350	104906	93446	89887	103280	91777	82002	149487	99231
fpHILIC	Negative	558.4603	0.36	unknown	1347358	1402285	1291919	1013406	1594609	1165751	1337556	1166392	857987	877782	1042406	1029916	761083	829229	1408833	1151975	1002633	939356	983755
fpHILIC	Negative	293.1144	2.73	unknown	1769676	998957	1246480	934804	976704	1724352	1101774	913559	993015	1393235	991741	1157706	834179	1238458	1339336	880876	927069	1043278	926392
EIC	Negative	245.1580	5.01	unknown	182378	100242	206976	228194	110995	114949	92070	157947	44418	163456	95199	86216	81356	18465	83706	149976	45753	166790	20456
EIC	Negative	475.9986	0.55	unknown	75587	68696	73184	146487	28026	107943	82309	32038	51241	47577	78360	87185	78572	0	63580	105791	27324	0	73847
fpHILIC	Negative	282.1182	2.82	unknown	1560910	1060067	1023369	1707873	1219409	1919701	1142958	1067519	1128601	1029026	1230531	1248684	1315135	967616	968918	1272828	1185948	1386403	998961
EIC	Negative	471.2196	0.71	unknown	511600	777663	853866	468778	485642	588463	76236	841849	429614	510570	812449	704573	619192	408251	614312	479590	593307	646085	506473
EIC	Negative	239.1339	4.05	unknown	177030	86870	188563	247843	85777	108920	115210	133820	68542	137146	88094	134635	127717	43067	76529	89865	89953	149034	54552
EIC	Negative	475.2835	4.68	unknown	1253006	1314683	1314851	974009	940731	1220656	879110	1122392	624725	921761	1015488	990431	757251	1536079	1103503	0	874893	1154419	1166241
EIC	Negative	450.3313	3.74	unknown	1391368	177326	2566472	401352	232372	128288	119871	752661	175018	663150	120783	99463	67046	135796	117208	138647	127836	765212	115705
EIC	Negative	434.2368	5.63	unknown	2728047	2507030	1969877	3796454	2014690	1841690	2231899	1923235	2670362	3087377	1947143	1848519	2843644	907867	1577038	2494778	1821461	2531017	1168544
fpHILIC	Negative	202.9978	2.98	unknown	3261211	3024775	3406365	3998115	2147717	3004320	2767997	1930420	2354827	2920377	3005346	2510444	3218496	1032832	1617931	2263371	2260157	2779136	2041694
EIC	Negative	308.8195	0.52	unknown	357946	177594	251637	223474	397742	218288	227822	152008	416232	194622	118385	119982	206311	1296397	199582	154677	154266	237239	312472
EIC	Negative	278.1476	3.87	unknown	625024	623407	397247	604688	418423	316640	391169	391368	493151	394287	1253908	631413	624975	360518	315962	387305	296932	444996	361288
EIC	Negative	296.2313	4.09	unknown	232290	217858	410759	911484	341582	272999	303533	507590	383550	376948	240770	364572	377732	211376	147610	442574	364627	490174	176108
EIC	Negative	250.1893	3.29	unknown	382117	278654	409917	399565	277432	185952	267104	275812	227995	437159	268250	223673	207182	184876	288958	226125	175671	240660	177780
fpHILIC	Negative	244.0656	2.65	unknown	16780649	10226163	33665623	43050154	20562076	11438906	17406373	38735321	19154512	26930295	13637844	16002392	15343342	20777271	13976288	11677555	18591576	36960645	15251076
fpHILIC	Negative	114.0055	1.92	unknown	1414005	1278976	1149467	1804889	1334987	1592648	1474101	1060867	1177643	1588415	1569906	1334885	1360699	780222	1333680	1293696	1340947	1105296	985229
fpHILIC	Negative	114.0354	1.92	unknown	5891754	2023804	2380156	9567101	3027250	3304002	3055148	2143355	5849867	4347980	3964700	371258	4197836	1346921	2728464	6567812	2638655	2136106	1357138
fpHILIC	Negative	384.1849	0.59	unknown	1122620	387118	654646	816048	374094	234871	248429	673075	266138	677282	180026	485412	394961	295502	203627	126842	351386	715708	217836
EIC	Negative	333.1712	3.02	unknown	275281	144785	308712	218961	176458	133840	235881	239481	89078	652444	138194	143348	112062	105774	132158	111307	102042	346842	94321
fpHILIC	Positive	730.5366	0.45	unknown	521224	617479	630720	736033	339225	545891	619792	501387	341939	378903	505618	357553	511398	703168	427100	320586	444602	459489	460480
EIC	Negative	283.1919	3.34	unknown	12176979	2106981	12813028	8969354	3263764	3131823	3893135	8203990	2912104	14713830	2628826	3628918	2998855	2956802	2770778	2302200	2835352	8944555	2407121
EIC	Negative	288.1902	2.42	unknown	191065	74329	214683	102926	70334	70185	102926	44444	187889	78612	82189	74898	75671	73120	15676	80850	151213	76159	0
EIC	Negative	336.1900	3.72	unknown	161861	55852	157431	116146	70057	88182	80362	152005	22842	106064	53252	62609	54059	32709	57380	55514	51098	161326	47047
fpHILIC	Negative	226.1448	0.41	unknown	1788247	717721	795033	1854133	886273	1647853	1108402	953946	790268	1137472	875792	1376839	1133457	315414	1089913	1016757	1060320	1052539	633751
fpHILIC	Negative	216.0986	2.59	unknown	3714719	2044372	3277821	3407448	2931702	3895191	3038983	3009379	1663132	3043276	2554731	2529257	2379849	2725570	2435910	3078055	2480020	2690623	2412096
EIC	Negative	552.3314	3.96	unknown	8862766	14738162	10187350	8539213	10172000	11485133	9134254	11335323	8177197	10865253	11726196	12225351	14725538	11900181	11442447	9899300	7863671	9325763	0
fpHILIC	Negative	245.0778	2.01	unknown	1251306	778007	702747	1387976	926895	1366403	936457	680981	945476	971814	1032496	983239	854363	511407	780397	1170504	970204	764822	696647
fpHILIC	Positive	833.5862	0.43	unknown	2886122	5769390	2673665	2851207	3740967	3959837	464560	2915390	3190708	2529114	3634152	3527901	3863800	3313674	3787876	3940381	3368258	2259595	306942
EIC	Negative	344.2314	4.97	unknown	309986	408966	341640	1263398	393952	351232	392368	520399	361761	516303	402075	437150	589041	201924	282486	569084	385295	585647	241997
fpHILIC	Negative	167.0210	2.98	unknown	176452656	153122240	176614080	190393344	110795944	147085120	137182488	93586544	110722448	146013600	136019072	125725304	144646720	55936532	83744568	111944224	120426488	129692488	95659094
EIC	Negative	630.3782	4.43	unknown	309434	0	323566	0	0	0	321882	283765	0	0	0	0	0	0	0	0	0	239749	307341
EIC	Negative	282.7780	0.52	unknown	247423	74278	194854	125979	282072	117760	133025	33644	94753	322551	39186	36551	86671	1248990	108142	88900	34579	98197	267584
EIC	Negative	289.1447	1.76	unknown	229542	98969	324660	108325	28370	84667	81071	99226	29118	147033	88668	101911	101038	75082	47729	81739	79174	0	82891
EIC	Negative	474.9950	0.55	unknown	815523	495150	479513	1148443	299506	949952	607018	324376	316807	688883	181733	689542	464097	79630	441088	653688	344342	485257	335145
fpHILIC	Negative	198.0715	2.92	unknown	2699911	3023496	2741805	2372508	2192178	3180800	2379168	2313855	1571667	2613936	3102919	3268184	2463879	1940955	2057644	2133083	1952776	2220921	2164612
EIC	Negative	311.9930	0.55	unknown	145318	30626	40663	157940	51803	124465	82086	11578	22294	72258	75328	50788	30868	16236	74124	72517	18334	39207	59842
EIC	Negative	360.2676	6.36	unknown	991527	613020	1127793	1540492	845004	815611	972550	1378812	1000562	929129	864607	921							

fpHILIC	Negative	291.1312	3.47	unknown	4312681	2484462	3112150	2798587	2440759	2728824	2215492	2508075	2074561	2708263	2519776	2698675	2368695	1735608	3105560	2387552	2316100	3110728	0
EIC	Negative	239.1653	2.74	unknown	623032	332524	744839	733143	451209	368851	381811	518306	308418	1245433	310821	400032	336418	623141	157696	150347	358496	862950	321531
fpHILIC	Positive	702.5610	0.48	unknown	896253	915284	799491	876262	818434	746471	593818	836674	1068614	805418	803962	790406	761060	928434	811150	1068614	749570	629532	72628
EIC	Negative	241.1808	3.15	unknown	1226445	881310	1614630	2131266	1294926	1606081	1481666	1269282	1592811	1102459	1876485	1905908	1355084	908577	1323824	1438773	166228	965018	
fpHILIC	Negative	289.0793	3.38	unknown	767714	204137	329439	473394	219422	591879	138598	111632	332063	73730	249895	141581	110831	35779	382323	185943	493444	359523	
fpHILIC	Negative	195.1010	2.97	unknown	1378661	1100737	1069940	1329413	1068574	1467041	1148016	538766	1213664	1065894	1289841	1514651	1074953	319994	976586	1453548	1066962	692480	773428
EIC	Negative	461.2908	6.09	unknown	9284084	11397159	8013130	27378009	4572642	1719304	5764008	10561882	10613438	11721026	11568468	3401668	10943707	11168729	7796542	3348445	9847656	1166544	6225316
EIC	Negative	391.2439	6.24	unknown	1288832	515099	8811693	1259265	431042	395340	563861	787820	659283	873265	695292	372591	586348	662658	742264	188430	506607	813165	341814
EIC	Negative	411.1798	1.78	unknown	327287	191008	298140	111859	111103	75226	188403	0	155128	244016	121723	143063	110588	126502	100623	190508	121584	0	71562
fpHILIC	Positive	808.5810	0.43	unknown	27496506	30193594	23060724	23147580	23454950	26460218	28449452	23144480	21962158	19938434	23742776	25981562	24174590	23259934	23750416	23121598	24505920	18827248	22699072
EIC	Negative	268.2001	3.77	unknown	419883	204580	473235	322367	207286	222081	234135	348105	111213	342365	207781	220610	180080	164953	189770	147917	135811	371729	181669
EIC	Negative	296.1951	3.52	unknown	260428	84641	194861	114733	108266	131500	137073	160074	44382	128235	68631	120957	64089	72228	82544	63672	81140	231824	72472
EIC	Negative	292.9957	1.19	unknown	174737	156455	141994	135273	110761	111170	106913	127468	105080	132111	99392	93932	83801	82757	93259	80963	90534	152898	95837
EIC	Negative	394.9893	0.55	unknown	495896	214433	237950	559251	182776	478325	267411	143929	146649	204724	282509	314306	213703	62576	219924	312945	164144	235528	183274
EIC	Negative	637.2281	1.03	unknown	47633	27499	73836	60373	24157	15038	41582	45765	14406	35621	44185	37248	44408	14389	25736	17127	18207	52997	15008
EIC	Negative	307.2272	5.68	unknown	139205	61802	152852	186604	71443	66248	146140	56721	66248	137159	57849	47072	83591	21156	44015	58937	63769	176883	23294
fpHILIC	Negative	605.4052	0.36	unknown	1162996	1111640	1165415	798051	929489	932968	1069852	1277483	750213	515647	852953	929039	948944	1365283	1159566	956564	708347	770755	950431
EIC	Negative	287.1868	2.42	unknown	1138761	364729	1308404	722691	937429	392557	621962	1083410	145638	1169547	475228	485168	349105	349747	419896	253886	329607	928916	489618
EIC	Negative	389.2464	6.24	unknown	3805716	1603220	2774274	3779675	1040089	1277948	1515361	2275042	2020600	2733352	2182107	1118122	1676590	2119272	2315891	672120	1619670	1815966	1034721
EIC	Negative	556.9982	0.55	unknown	418536	319574	294587	722647	207944	611777	239392	235305	214645	400456	523914	353302	22883	275517	362334	271406	316733	2104375	
fpHILIC	Positive	468.3080	0.61	unknown	7234198	4351224	5986040	5017381	4396845	5118755	5765714	5340488	4239441	4622772	4370079	4099672	4736678	5007304	5081123	4559819	4092928	5049184	4032947
EIC	Negative	488.2276	0.71	unknown	298064	454624	511094	290494	288885	352639	456162	512771	286358	300708	507526	434810	361288	239432	379843	282898	357348	309716	314496
EIC	Negative	264.8976	0.65	unknown	339207	132638	134492	280475	78552	260845	141489	66248	82385	159122	147271	154866	115389	48532	102888	151912	79219	99236	145170
EIC	Negative	296.2313	4.37	unknown	1504209	1169720	2400576	1945355	1689218	1480899	1649748	2164987	1575914	1307654	1071305	1053210	1086542	2251609	695903	2037536	1959422	2079125	1469594
EIC	Negative	325.2021	3.21	unknown	275197	128979	332299	230169	166357	142863	187627	293158	123045	242169	72466	147301	136097	124137	133919	148164	139099	297624	121458
EIC	Negative	259.1369	2.67	unknown	107551	35758	65825	65856	61453	68623	64733	95017	0	53630	35598	46282	33593	15306	55606	64223	47904	75425	23596
EIC	Negative	437.3276	6.39	unknown	1324331	761978	1286110	1029596	689193	483204	740682	1005303	136322	804286	629579	463257	514425	567226	642339	526491	541158	609629	491960
EIC	Negative	364.2577	6.03	unknown	688242	657227	775802	714836	734046	487303	516053	712154	599114	870155	683400	451363	501109	504029	698679	467903	574052	633422	432866
fpHILIC	Negative	91.0041	1.74	unknown	13006488	29188672	32070286	39799228	27621822	31001936	29773582	24785534	31667878	27058202	23561434	31579332	27761084	18416046	18835110	32436268	2551586	32060856	2451220
fpHILIC	Negative	283.2642	0.37	unknown	105968360	147370176	162834448	168016832	155205648	127696628	145729104	122019248	114836856	124983608	103378312	148941568	103959668	124561416	98332888	99494144	121759968	136244416	156522080
EIC	Negative	283.1921	3.00	unknown	242078	147472	213410	386418	217132	236767	299920	234927	209459	298627	206135	319622	345936	133110	155643	254667	215064	330809	151791
fpHILIC	Negative	78.9189	2.10	unknown	5796470	6094952	4817775	5410248	4954481	7217190	5417956	4496697	5608559	5002112	5995137	5273211	5845199	5543158	5633869	4748074	5264366	4595392	5273593
EIC	Negative	446.3358	6.51	unknown	1033026	1071435	1407103	1585776	1602976	605767	1330381	1427252	1158979	1332717	1254082	833547	840972	691240	1101906	1409357	914299	915385	807847
EIC	Negative	289.1060	3.18	unknown	885899	404932	678942	1904681	430944	505450	520847	691890	262554	753106	381551	525234	560819	175410	452823	425949	339657	710855	294584
fpHILIC	Positive	832.5822	0.43	unknown	6371620	10148059	5222020	5733040	7127114	8004460	8753523	5430243	5499145	5026182	7029384	7180423	7112663	6711797	6966167	6499145	7336474	4121224	6354144
EIC	Negative	512.9608	4.37	unknown	913037	1172910	896282	1212770	983250	986265	1060783	981788	1008940	829499	928028	850564	891140	885448	973487	1043568	807943	1024563	781452
fpHILIC	Negative	193.0132	2.98	unknown	3877479	3428431	2661258	4279092	2846696	4569144	3434367	1589978	2699042	3719476	3970235	3122459	880594	3402765	4403361	2639755	2015846	2023282	
fpHILIC	Positive	204.0560	3.16	unknown	1201577	1466366	1443584	1607818	1442187	1339411	1415418	1393552	1389984	1458607	1381872	1265126	1489422	1203881	1311174	1365104	1248801	1373121	1160573
fpHILIC	Negative	332.0028	2.05	unknown	558437	759178	722347	601743	662971	672203	601880	601880	601880	652323	640091	691365	357115	303140	652323	292898	393822	477118	286263
fpHILIC	Positive	219.1340	3.32	unknown	574890	285942	151035	200574	177154	286545	232125	64936	75586	192060	251556	328709	84512	197369	252758	261021	70597	63469	124330
EIC	Negative	317.2028	2.99	unknown	0	0	0	259666	60671	61492	0	34329	0	0	0	0	0	0	0	0	200386	0	0
EIC	Negative	253.1439	3.79	unknown	784164	841211	739287	790191	766020	716975	959678	672467	755328	567084	772228	870556	836769	841281	844206	715195	585021	716849	712385
fpHILIC	Negative	158.0400	2.97	unknown	1154477	1019917	908298	1106067	901285	1089601	927971	1045478	851358	707371	1014090	842733	861698	189403	823629	1003489	755204	495608	620815
EIC	Negative	246.9022	1.19	unknown	169444	87205	126284	92965	80587	73446	67761	54754	65516	137587	50943	48213	43305	82853	42951	51243	36507	93112	92091
EIC	Negative	338.9371	0.52	unknown	3146530	4367897	4302741	5004598	3284943	3616312	4145375	4972988	4308380	3635656	4235366	4550498	4546384	1937972	3396167	3667221	4351653	4513530	2863544
EIC	Negative	610.6760	0.52	unknown	295981	252409	479827	545302	269784	329357	309902	154071	539737	414811	261839	266906	333923	0	224070	292003	280091	357218	328582
fpHILIC	Negative	219.0451	2.99	unknown	2656161	2087730	3516449	1956741	1077077	2261593	2407054	856684	517178	1205755	1081837	1899940	1607705	0	1038802	1389205	1138994	1751177	1489913
EIC	Negative	406.2966	5.77	unknown	321842	404247	297738	374064	393856	376067	360369	304995	265054	297504	35241	270608	3						

EIC	Negative	237.1495	3.49	unknown	143832	59576	141287	187191	66140	81192	92198	113196	46952	113100	53628	99044	83798	38005	61035	63754	57320	152436	37828
EIC	Negative	553.3346	4.24	unknown	8727865	11114114	8203213	7056937	9153923	10611284	12314262	7587574	6777794	7090394	9332622	10756093	10142709	10646159	10430991	7704811	9165396	1717621	8802941
EIC	Negative	321.2444	6.22	unknown	1323800	640140	1455809	2439109	740506	855566	623081	1135766	776261	1464071	650564	941330	746221	411214	437807	648457	645324	1653038	465467
EIC	Negative	528.2855	3.96	unknown	291913	415463	335445	261841	294228	349381	368429	277474	339700	269708	319272	367381	355645	419970	333650	361462	285407	269052	270419
EIC	Negative	235.1339	4.12	unknown	385000	261277	461175	944065	308646	235499	317458	468147	204096	438856	191164	202482	419371	88626	171803	442662	256119	500297	94212
EIC	Negative	340.9345	0.52	unknown	2002644	2804536	2778677	3276263	2190496	2293557	2658572	3276614	2734855	2322164	2719370	2867401	2804876	775971	2220405	2438131	2851149	2879706	1886522
EIC	Negative	458.6535	0.64	unknown	105684	58350	112544	84236	111613	26877	69757	44200	75357	183705	44299	37286	64190	213679	56647	54267	32426	69534	130414
EIC	Negative	480.2998	5.09	unknown	2226842	2357976	0	0	2379587	0	0	0	0	0	2521151	0	0	0	0	0	0	2221041	0
EIC	Negative	286.7725	0.64	unknown	179674	68314	154883	117266	185946	112789	120161	75122	106175	271091	71836	50979	87107	714953	94392	81579	68096	110953	205464
EIC	Negative	313.2387	6.21	unknown	226707	114451	399453	180524	137917	36397	137414	277450	85142	216292	117270	191093	58059	57692	73315	97375	84794	270539	103761
EIC	Negative	248.1370	3.70	unknown	69704	57525	148090	58287	66337	106960	111254	114598	0	147669	138176	107198	51408	70138	85559	61216	69584	119951	36541
fpHILIC	Negative	171.1391	0.42	unknown	3292160	2507721	5371245	5226317	3423119	3214635	2832643	3166549	3553713	3477521	2710566	3306524	3698037	2934866	2274903	3049538	3276743	3645840	2883775
EIC	Negative	500.2274	0.81	unknown	141018	192947	146473	88786	107523	153246	166548	177936	91794	121839	152560	150941	161683	108796	135989	118736	133085	124949	138718
EIC	Negative	247.1340	3.69	unknown	401288	272334	898997	367853	371615	604657	582305	674663	116650	835995	819168	626695	256174	374743	485747	361107	426731	720511	203159
EIC	Negative	329.2333	6.05	unknown	1048525	415954	1116313	815791	399064	287171	389475	869925	217207	854327	392861	310775	363188	271727	454389	242164	285952	625736	414579
EIC	Negative	238.1460	2.16	unknown	124467	87239	77402	306019	85382	93624	94775	75376	92660	129534	84121	172203	84625	51187	80671	93054	91941	111808	72169
EIC	Negative	285.2072	2.28	unknown	122316	69471	127357	80859	82316	86064	102870	75272	75736	92660	56695	83935	76514	62894	53716	100601	66652	109469	74631
EIC	Negative	311.9939	1.19	unknown	103956	93622	88610	87892	81388	84519	89348	93181	79307	80861	86229	75752	77078	72566	76371	68602	73947	107511	68614
EIC	Negative	634.3348	3.96	unknown	627737	1011643	644641	575851	777513	804317	904796	653712	827527	620285	775910	840355	850881	1043440	919459	828199	716153	550631	698426
EIC	Negative	552.3313	4.24	unknown	29123374	37289486	28179852	23873428	30434928	35287638	41057897	25504885	2156427	23865246	31918226	36428756	34212434	36437380	34950744	25717915	30999377	24043419	29753094
fpHILIC	Positive	141.0539	2.67	unknown	1105104	271498	80679	161878	209947	474059	0	258805	436922	158067	74561	350321	243149	349822	47298	318956	306535	416835	208912
fpHILIC	Negative	168.0244	2.98	unknown	9669978	8683618	9676929	11285640	6089937	8054700	7389834	5297628	5872444	6200062	7409801	7008146	7589817	3042908	4722958	6106222	7065607	7394809	5330230
EIC	Negative	570.3417	4.05	unknown	2314717	2416954	2101681	1989949	1818879	2300406	1890286	2127134	1441722	2101312	1985547	1933761	1896083	1736222	1714070	1828994	1823130	1789930	2114932
EIC	Negative	312.9867	0.55	unknown	582784	211095	226870	560892	144223	495385	241267	118463	140106	250765	258980	185312	46686	216894	293913	136888	199655	219970	0
EIC	Negative	229.1810	3.83	unknown	123991	90888	135601	305963	94698	78639	95390	109672	118201	146085	76833	98514	145318	54656	58825	143154	93284	116351	53702
EIC	Negative	339.2123	5.49	unknown	358691	130633	289757	325663	152519	125816	218305	186203	151345	250262	179455	113235	180562	228274	284285	64526	202006	116550	114560
fpHILIC	Negative	235.0811	1.89	unknown	737688	213077	510950	499070	224936	488442	320813	410317	455051	404151	366649	616519	208177	280216	202910	514822	168149	466501	428821
EIC	Negative	470.2164	0.82	unknown	76741	98774	110167	56890	60573	79417	101647	85581	78756	108386	66730	67575	69619	82521	65399	70032	70632	80937	80837
EIC	Negative	338.2415	3.54	unknown	140271	103708	138886	390312	121943	119019	119843	178089	156735	177457	109289	196669	152476	61263	82010	136743	111805	245474	76480
EIC	Negative	284.7750	0.64	unknown	269796	97240	229380	179544	277448	158128	174074	105373	162367	491190	105499	83148	128003	1048194	142983	126110	92599	158422	320410
fpHILIC	Positive	186.1123	2.36	unknown	796666	973846	806057	860133	801426	833568	839420	675790	916199	1008676	1068862	941786	1016629	786639	618047	986527	829725	558844	821580
fpHILIC	Negative	239.0774	3.19	unknown	675237	734642	751162	942997	683687	676485	836592	605430	658427	634989	735697	571767	695584	390430	598477	591994	716164	782446	614012
EIC	Negative	616.4305	2.72	unknown	315571	210258	197921	601619	318410	203445	241815	224897	261654	372820	195055	247289	288511	111938	146153	286725	273349	365820	101694
EIC	Negative	578.3390	4.01	unknown	2927340	3890580	2966512	3349669	3146451	3392449	3846098	3178931	2951228	2529015	3820439	3913471	3215422	3450718	3357374	3232110	3111435	2464832	3351693
EIC	Negative	389.2728	5.84	unknown	567579	547377	587352	660432	156887	168027	748928	632102	158895	2320467	497579	153958	165460	591454	633745	637445	148171	475930	142422
EIC	Negative	286.2474	4.74	unknown	106223	81729	213382	221660	134786	85428	123429	238945	132187	123817	78983	84009	105892	139304	87230	85319	129490	237256	131988
EIC	Negative	502.2845	5.24	unknown	1100323	924387	944824	0	901846	0	803616	0	0	0	631099	0	0	0	0	0	742354	0	859592
EIC	Negative	316.2572	3.54	unknown	161099	158367	157131	160446	160886	163080	154075	146513	149343	148467	145984	146709	155124	142570	144419	150460	146968	142330	141822
EIC	Negative	248.8995	1.19	unknown	105042	54906	80508	57449	51230	46916	44017	53996	52130	32380	42152	26136	52829	67114	52829	2470	25374	55876	61114
fpHILIC	Positive	157.0749	2.61	unknown	1215391	1367324	1186565	1033447	1074021	1475213	1304342	928573	1003229	1037746	1402534	1205343	1062447	1240779	1228636	1041928	1301348	1089205	1063139
fpHILIC	Positive	760.5779	0.44	unknown	22934636	25387116	23908926	19226456	20901790	19709264	18279486	20215376	27668799	18671904	23210516	21868918	19192314	28839220	22420734	18874560	19589230	16674183	22788944
EIC	Negative	310.9892	0.55	unknown	1811844	605143	742548	1616113	497368	1548781	764959	325703	415703	775726	768826	827610	586817	310001	657389	942879	424698	613052	701164
EIC	Negative	244.1998	4.13	unknown	63976	61845	69179	69393	63976	61845	69179	73160	69393	71201	58653	72765	73575	57762	69401	63803	90554	43284	43284
EIC	Negative	275.1268	3.48	unknown	167447	99159	124951	141880	105874	80923	84668	89587	41479	124802	75782	91498	83242	54787	77460	90793	54340	110477	45406
EIC	Negative	296.9919	1.19	unknown	420892	426183	388577	377124	385254	398955	394003	385620	381116	388577	396640	391100	359705	371675	371343	351831	373675	359733	372240
EIC	Negative	318.8873	0.52	unknown	756665	731796	1095653	1127670	751521	793744	805420	693445	963636	792637	740175	808320	864116	321997	739064	813971	721061	880094	614571
EIC	Negative	251.1323	3.18	unknown	355339	0	0	0	0	282141	0	0	0	0	0	0	410058	0	0	0	265342	0	0
EIC	Negative	581.2410	2.93	unknown	1981133	1179066	1002934	1514658	501999	1031321	604992	1725324	385828	2973568	904377	1140000	1109187	169505	350509	1181576	517431	1594646	352368
fpHILIC	Negative	80.9169	2.10	unknown	5687029	6476060	5036893	5961009	4995333	7158834	5607138	4623500	5662901	5135114	6287215	5867647	6310368	5704582	5838500	4749240	5422366	4861904	5512702
EIC	Negative</																						

EIC	Negative	258.9312	0.52	unknown	1349943	1589103	1815562	2094668	1380903	1420654	1506263	1579646	1641895	1388683	1540320	1548420	1610959	695769	1370033	1469530	1472263	1680940	1132168
EIC	Negative	237.1495	4.69	unknown	836325	236083	898131	881413	295790	454997	362364	578814	193648	618998	271617	569425	423423	101005	288649	287156	342796	639182	226676
EIC	Negative	398.8929	0.52	unknown	1218796	1623102	1875928	2108954	1278671	1521618	1569558	1577773	1710791	1329723	1596646	1696650	1634412	497810	1340477	1710236	1572536	1688971	1063441
EIC	Negative	300.2566	4.40	unknown	1906802	1753036	1778316	1739286	1814431	1562566	1527524	1718432	1691683	1833229	1423304	1431283	1608591	1578089	1530097	1500234	1551702	1764503	1522495
fpHILIC	Positive	276.1549	4.03	unknown	957357	344799	511881	1062036	469745	598908	469745	400292	562896	516856	797709	851211	526309	323921	338553	713941	390436	363153	447135
EIC	Negative	268.0978	1.76	unknown	101472	77439	145953	99004	60569	73659	60823	55584	69914	96458	73731	80433	82329	111689	98033	70075	74018	0	61365
EIC	Negative	277.1555	4.08	unknown	0	0	0	1065283	0	0	395001	412024	562194	461453	325784	473162	475657	0	0	394570	350274	551738	0
EIC	Negative	363.2545	6.03	unknown	2688011	2690105	3159541	2975963	2978323	1907768	2061278	2950733	2404241	3584187	2844099	1816399	2113219	2161811	2917969	2001938	2337578	2564535	1831464
fpHILIC	Negative	582.3404	0.58	unknown	18305818	20945290	18954646	12989921	15672723	20518288	21496966	15612538	15128867	12953465	18965544	19751158	17445396	17069846	19568376	16219472	16796432	12638768	18588328
EIC	Negative	343.1543	2.84	unknown	240774	337923	254507	163081	271019	218240	310419	90723	147224	126755	143916	243639	144088	200554	321142	253911	143336	43489	221548
fpHILIC	Positive	131.0531	3.47	unknown	7743326	5660131	6650137	6350943	5745405	6024646	5923773	6157616	6239970	5936638	6140627	5796029	5340475	5018245	6474518	4941637	6099349	6118190	4902959
EIC	Negative	1837.215	2.38	unknown	1837215	2338936	1820487	1493593	1891847	2220444	2529323	1698592	1441188	1533580	1962006	2280375	2119957	2267378	2292480	1571727	1953764	1575904	1884213
fpHILIC	Negative	182.0318	3.03	unknown	2445789	1428632	1440867	1675770	1129646	1148513	956741	1208585	1191205	1563704	1184565	1043965	1116733	1099824	1247846	996897	1169939	1035872	894889
fpHILIC	Positive	358.1633	3.47	unknown	2819409	1888881	2480313	2646259	2230605	2328876	2382898	2768048	2403803	2653747	2659292	2296246	2446606	1994463	2658400	2548778	2300763	2582510	1408020
EIC	Negative	256.9340	0.52	unknown	2003816	2381305	2762636	3142147	2163800	2244063	2324956	2430118	2524547	2142400	2335964	2401761	2410344	1055027	2117815	2363367	2329477	2538843	1744177
EIC	Negative	361.2389	5.27	unknown	696040	455123	715863	726907	490916	374696	542009	417716	859814	297150	324271	368968	264658	494671	349017	336418	326212	231390	0
EIC	Negative	326.2217	6.21	unknown	765667	2725178	760525	2792022	1736726	1537670	1455990	1041349	2778171	1306993	1861373	1467594	2758086	1173032	1502586	2090335	1901825	1286168	1337695
EIC	Negative	486.6876	0.52	unknown	164807	29643	163930	0	139884	93816	0	97608	0	194677	58594	0	76308	215076	51732	49780	257324	30158	156749
EIC	Negative	256.8834	0.62	unknown	121314	49634	32730	78642	35434	118258	61833	18844	33704	42099	64230	64360	48944	32409	59158	73587	33900	34559	53422
EIC	Negative	251.1268	3.18	unknown	415518	314530	525361	441470	346921	297112	413506	350831	171733	321045	329495	349068	511772	200390	312674	330115	283759	360668	213336
fpHILIC	Positive	761.5842	0.44	unknown	7139867	8331139	7556628	6917559	7112125	5996955	6423026	6861097	8948146	6078820	7426649	7317849	6668295	8859416	7468799	6262444	7091169	5522027	7232476
EIC	Negative	452.9477	0.55	unknown	420307	140309	207775	363636	114508	380095	192690	88725	119859	919637	185941	200905	158925	27528	141938	240323	113367	151547	203836
EIC	Negative	284.1954	2.67	unknown	70267	46871	48063	89450	38644	62927	57632	64413	43919	105926	64860	116089	74560	58963	48088	58943	55899	47102	44104
EIC	Negative	516.2736	3.11	unknown	650860	338521	400735	480815	237716	513106	217289	442291	349512	496790	248320	338722	270523	222139	347255	327469	474814	0	522275
EIC	Negative	400.6941	0.64	unknown	108734	58101	118430	84004	124796	71316	80107	46858	72540	192601	45046	36039	59926	289304	65016	59553	41458	77714	132158
EIC	Negative	571.3451	4.05	unknown	684699	701429	603909	618578	551916	682658	567207	625519	426483	628023	588033	583233	578276	498055	518243	538605	583619	532746	539594
EIC	Negative	265.1811	2.99	unknown	400336	220885	467966	587440	288356	369031	354390	427652	240017	494711	299089	532678	425364	225318	234655	354986	251383	550259	205498
EIC	Negative	596.8132	0.52	unknown	480198	683648	845960	988609	524854	673725	660501	629886	808708	783847	755392	759821	762498	0	565370	746226	672141	733707	418665
fpHILIC	Positive	106.1110	4.07	unknown	648541	498220	471650	395026	373151	531501	528722	472718	372530	385762	267884	321925	349372	297515	524595	526322	334236	412730	370653
EIC	Negative	386.2374	5.75	unknown	4460559	2437845	3925388	6324819	2228678	2518606	2459382	3112789	2634885	3682629	2475708	2751223	2538050	1698842	1941293	2643678	2121551	3979416	1653652
EIC	Negative	287.1868	2.46	unknown	947351	303459	1048549	675531	409984	388276	487121	1090865	173205	1042744	403099	406220	346470	346706	359474	288874	354723	969130	458390
EIC	Negative	571.3450	4.18	unknown	4303352	4012269	3906674	4044177	3339140	3999165	3538346	3975959	2810688	4088616	3881140	3449663	3396931	2952049	2800110	3453160	3388303	3593550	3605994
EIC	Negative	634.3345	4.23	unknown	1367962	1430809	1190528	943500	1299759	1276087	1572033	1089109	1106862	7070817	1340130	1481360	1522019	1593278	1576535	1088792	1166696	1060474	1196479
EIC	Negative	356.2172	3.26	unknown	406547	75297	440672	841017	80608	123663	123222	250064	29235	273826	64753	108472	62408	81035	73915	29541	68710	316680	89979
fpHILIC	Positive	782.5682	0.43	unknown	81311248	94635952	81127816	18131860	72673336	73059496	72851776	91005296	67151640	78715832	78400448	76300464	90854856	67701664	72443888	77611784	63109884	83137664	0
EIC	Negative	339.2539	3.83	unknown	94110	81283	178361	460579	60664	94521	76141	170851	110152	164846	99677	155117	136626	43238	36476	127437	88480	185970	50978
EIC	Negative	284.7750	0.52	unknown	408102	109296	311301	113007	397340	240719	209842	91158	178307	103017	140858	146760	2121643	167177	167312	77643	190527	507969	0
fpHILIC	Negative	182.8247	2.10	unknown	697112	1100155	885346	948344	672406	746892	648829	928430	599982	1142733	905791	858283	612245	1136699	1096492	286640	706222	577699	769535
fpHILIC	Negative	269.2486	0.37	unknown	4060133	5860224	6752783	7580689	6182097	4734293	5562824	6367801	4712459	4306710	5272385	5475789	4291966	4104772	6037802	5160162	5292955	5903772	6147830
EIC	Negative	457.1721	3.26	unknown	133826	135071	173406	442695	62996	117849	82246	40075	33345	159483	77524	49483	19182	8321	88768	126597	43825	47284	15105
EIC	Negative	570.3417	4.18	unknown	14688244	13531302	13232176	13726111	11418494	13335958	11605781	13412004	9566463	13547040	13092752	11570324	11687660	10067954	9627544	11291522	11337871	12275518	12183640
EIC	Negative	337.2328	2.15	unknown	1704757	1502139	1423958	1665160	1533040	1476893	1609414	1505349	1472142	1499866	1476863	1558925	1481742	1487295	1460483	1452536	1517455	1299050	1530374
EIC	Negative	577.3347	4.01	unknown	13705935	18151230	13489229	15338190	13406625	14704075	17307855	15028763	13372471	10799561	17041248	18398447	14754738	15932822	14994885	14096628	14559527	11112310	1586547
EIC	Negative	324.5560	4.01	unknown	377396	356352	326463	293696	356589	0	345996	12597	328680	317674	306069	323828	316982	341410	330217	0	0	351762	316046
fpHILIC	Positive	224.1188	2.72	unknown	620840	520827	828656	972723	547204	547513	768783	578241	394112	924279	413157	473369	548284	277053	484377	490462	584028	716621	436074
EIC	Negative	342.2731	6.20	unknown	754267	541010	1122925	1059777	504176	387694	563398	566356	461810	528246	446348	583139	551801	363604	334721	466301	467764	862598	329911
fpHILIC	Negative	157.0366	2.97	unknown	24738772	21909210	19905114	24463130	17039328	25508022	20372286	9582873	17114652	18164308	21444108	22394824	18968772	5525035	19303838	23779088	16258658	12578000	13776961
EIC	Negative	577.3347	3.91	unknown	3393976	5074447	5172705	3345767	3547														

EIC	Negative	335.1415	3.65	unknown	645414	640326	480198	537287	566585	498637	559162	600945	592327	633655	545181	558868	506386	516865	534204	530090	373081	643405	627218
EIC	Negative	570.9313	0.55	unknown	76468	75790	92048	112093	69435	19594	88659	134285	94081	43619	67296	69612	79242	0	51159	107402	92475	139513	0
EIC	Negative	281.1765	2.93	unknown	765906	159623	584982	418603	189567	199301	193190	376429	158275	748107	138988	194400	152912	185972	229459	142532	167075	380019	155148
EIC	Negative	315.2090	6.47	unknown	2987879	2783311	2828772	3240623	2795256	2625800	2391532	2518183	2165869	2890077	2336094	2146091	2143998	2210631	2357846	2388311	2275355	2493436	2508476
EIC	Negative	439.2618	2.35	unknown	8484156	385132	684068	899831	351807	373755	359758	1083717	2166161	948797	332718	346056	341367	310664	344706	346226	328109	1018329	367153
EIC	Negative	276.1305	3.33	unknown	135692	119295	88791	113945	119319	107780	102202	113138	54186	96222	102554	102447	110180	56630	99932	117564	73113	112194	75288
EIC	Negative	298.2108	3.82	unknown	406598	122447	537934	455722	191213	190185	193993	400694	196598	486122	158407	185189	160780	197812	151106	154353	189816	490847	142795
EIC	Negative	291.1965	3.23	unknown	168864	118128	153272	294289	117249	133480	146587	180613	133700	187899	125768	180008	173967	113929	114247	140180	148624	190008	92039
fpHILIC	Positive	230.0956	3.34	unknown	10496189	6227775	8161470	8978708	8102839	7671957	7716241	8056787	8341155	8371518	6916965	6754102	7313328	8321460	8018217	5750756	8002922	8260671	8375699
EIC	Positive	461.2908	6.00	unknown	11479961	22526932	10015840	35744784	10511666	21765913	14303984	13567986	21345421	21965695	23880029	7868379	17692498	19949010	20805648	7838748	25380814	9623141	14826780
EIC	Negative	343.0627	0.50	unknown	307601	248208	340255	240586	191003	220743	257948	220767	328476	290178	260388	225935	209001	0	196003	276946	216265	253710	231254
EIC	Negative	399.1175	0.83	unknown	65257	65241	121298	113218	51764	30229	80330	84195	40590	77047	77462	69229	82983	15387	34808	61055	54931	99932	25875
EIC	Negative	576.3314	3.91	unknown	10798178	16207639	16495186	10419022	11132266	14839962	11969634	12236321	7624738	8597675	14071757	11612849	10832806	19489138	10731994	7852659	10433132	10780498	15899639
fpHILIC	Negative	218.0519	2.99	unknown	548073	403229	861372	316299	202542	416959	495272	175969	146890	262828	317489	324313	263193	112684	187568	260845	261156	341493	334650
EIC	Negative	280.1887	3.78	unknown	238878	94844	156869	0	102032	149732	106898	160218	61752	157195	99684	135714	0	0	146146	111259	0	200230	102109
EIC	Negative	598.8083	0.52	unknown	292741	444961	558003	559463	322256	422904	380716	412837	509511	498260	434244	454647	480686	0	333780	475729	423655	476757	249422
EIC	Negative	255.1604	2.37	unknown	942665	451621	850489	882906	449287	669090	477582	711340	303018	849121	332740	507186	476026	396335	507810	418536	379015	855032	374970
EIC	Negative	602.3469	4.52	unknown	1917986254	191602547	180110021	187803116	183787164	188792978	192400595	182918750	175485655	185411363	200983154	188987559	180805149	193049840	176330732	183840269	174701506	190179998	
EIC	Negative	579.3437	4.01	unknown	470848	641943	529692	562895	480308	557693	610922	542687	488549	387705	537087	730647	556599	638680	534285	482728	555435	383545	629645
fpHILIC	Positive	219.1418	2.04	unknown	1593298	1611733	1797718	1267888	1163626	1907984	1285342	1155871	1167361	959733	1506662	1411571	1012469	1799230	1755527	1085542	59154	1063965	1581435
EIC	Negative	240.1685	3.03	unknown	111473	96200	206970	159854	93468	105908	96149	138918	99704	518663	88236	103599	94542	190511	63859	63254	104613	174584	109192
EIC	Negative	566.3470	4.94	unknown	1075205	1359322	1135022	879899	1092287	1275842	1290881	983052	608592	934623	1192303	1154753	1055865	1000556	1265339	608950	937498	761269	1206779
fpHILIC	Negative	326.1278	3.42	unknown	1361472	1072343	1264023	1534206	1050785	948891	1017536	1162431	1037104	1175491	1097503	1089507	1038580	813665	948471	1052837	941511	1245326	849520
fpHILIC	Positive	197.0880	2.93	unknown	583323	619797	587496	476488	418134	724098	539640	490035	321533	523380	683463	632291	537604	381634	520437	537470	474282	442037	433706
EIC	Negative	604.3350	4.52	unknown	14688276	14098235	13968243	14041059	13689244	14806530	13927909	14985305	14154828	13371341	13790545	15332405	14016320	13658646	14337397	12974265	14599378	12785090	14418239
EIC	Negative	528.3064	4.52	unknown	1788712	1724117	1635815	1508404	1468059	1498451	1516535	1882006	1423908	1563786	1623229	12975058	1171801	1607815	1662720	1520316	1570543	1252554	1524696
EIC	Negative	562.9574	5.02	unknown	556219	674486	582559	699138	553698	644189	598543	596650	616643	500750	597419	590090	539745	569985	630851	639563	549406	597775	490113
EIC	Negative	239.1652	3.02	unknown	711676	608919	1252931	1068547	586159	624768	571787	944013	660897	998888	589158	639720	542225	1265246	401814	415373	663082	1064851	727901
EIC	Negative	371.1350	1.62	unknown	231562	264793	314345	0	127306	360283	425377	245530	103802	262663	234893	193716	122247	527942	300867	125208	117585	116302	269826
EIC	Negative	325.2183	6.21	unknown	3056075	11368396	3033191	11314347	6712417	6202671	5895218	4249401	11108488	5336746	7488260	5930366	11310621	4639158	6129476	8521772	7161819	5180871	5580689
EIC	Negative	402.2952	6.29	unknown	304922	329030	361356	123460	45104	362549	369314	156170	43992	257803	285424	196437	194081	340962	422419	0	311711	61230	149399
EIC	Negative	311.2593	6.50	unknown	1007123	764099	1761020	3977868	974061	726447	1079552	1379291	1028628	1617436	1923516	1633483	1418198	465008	538057	1239946	1084093	1540435	615282
EIC	Negative	264.1322	2.28	unknown	194623	66857	125559	49634	54075	80457	45435	109466	9731	82216	52621	61473	8988	77266	66257	9731	19832	112757	82600
fpHILIC	Positive	231.0982	3.34	unknown	1216125	932554	1003244	1121605	998295	1032319	887469	1020365	877114	1198388	1017033	794673	886664	830985	910644	709476	893316	1070038	1074860
fpHILIC	Positive	290.1347	3.34	unknown	1456075	309511	639439	1330516	623452	375605	390586	567255	679720	979720	510709	391683	299357	270551	330720	765634	655623	610611	487826
EIC	Negative	269.1403	1.69	unknown	219349	437891	220692	255902	275815	150283	254574	158970	424295	175164	204577	208345	287422	270724	281336	393717	182945	185100	176365
EIC	Negative	284.1955	3.11	unknown	150613	83472	119839	106249	96374	108218	91505	136808	102748	191062	104239	107695	103934	94775	89274	110261	98294	138213	80094
fpHILIC	Negative	547.1688	3.36	unknown	8447710	8215375	9611043	10085469	7601032	7354564	7553384	9621601	7906915	9509900	8642050	8465705	7749760	7429106	7262000	7573921	7404467	8398244	7956001
fpHILIC	Positive	204.1537	4.46	unknown	1274488	7671037	765238	1205229	1112426	798602	594739	993844	1118145	905445	878201	1011786	590164	10216834	1010122	796857	726743	801187	1085688
EIC	Negative	323.1854	3.40	unknown	1202323	503098	997838	499502	527070	681785	658661	681845	180428	769857	515285	817276	495521	328439	458864	404022	461152	890871	427858
fpHILIC	Positive	732.5513	0.44	unknown	1215050	1341227	1242698	1133975	981706	875534	947022	1020544	932637	1183634	839854	1094690	976773	1467447	1010700	783686	1136711	1090392	1018567
EIC	Negative	269.0878	0.55	unknown	12464953	2584103	3960873	7501519	2060505	8009707	3871065	1409182	2047556	7323508	3576368	3724322	2634036	2093737	2629798	3651077	1861220	2774021	5922685
EIC	Negative	572.3480	4.18	unknown	928597	826976	845122	840110	768685	834263	715653	851834	743794	818384	684855	737897	629161	602898	602898	655981	703079	776427	529295
EIC	Negative	237.1495	4.60	unknown	1742922	539403	2024373	3906620	707912	856982	976529	1404008	576298	1610280	711620	1304523	1338371	275358	492795	886609	841328	1733787	439325
EIC	Negative	409.2819	4.45	unknown	577795	433697	477711	528102	397695	240725	587882	582021	534318	533302	446603	468778	543728	385862	398197	551652	432536	543000	343862
fpHILIC	Positive	522.3547	0.58	unknown	98566416	108538352	111105256	87689360	87601248	103948328	116650664	96483872	70867744	83344440	97383001	111294098	95047760	93238736	101401728	85234480	92866672	87395584	93812952
EIC	Negative	326.2550	5.88	unknown	245482	121281	297313	985267	143055	120702	144132	238432	208534	625554	134841	216909	189105	77834	99868	205244	160391	324518	86674
fpHILIC	Negative	254.0157	2.39	unknown	1110878	458791	662465																

EIC	Negative	270.0913	0.55	unknown	1304086	270691	409062	771961	210625	833226	432786	142352	214413	761890	362176	405229	253045	204102	280077	391529	211022	292199	613875
EIC	Negative	531.3066	4.84	unknown	790775	869882	811337	858198	775067	737051	808957	852029	828021	792807	803255	780535	800810	797976	808749	856414	758419	711661	768693
EIC	Negative	428.2649	4.05	unknown	201772	172340	189602	147501	197611	131325	170872	210726	184661	601156	170872	158310	201908	151916	182163	115046	187671	184184	138261
EIC	Negative	567.3506	4.94	unknown	328115	405724	330385	268466	333910	384802	393545	273023	188450	268162	387137	363909	315708	304590	371615	278340	300183	240795	344913
EIC	Negative	324.2560	4.99	unknown	359389	329570	293666	379664	326899	0	310370	327405	301179	328890	320895	320339	287721	265673	313761	0	323961	327222	279364
EIC	Negative	488.8975	3.47	unknown	94325	84057	69477	120973	79458	701176	99735	53963	74894	83958	85872	79048	68648	71395	62007	95969	79282	76358	55641
fpHLIC	Negative	304.0706	3.21	unknown	39120944	29145194	29107830	33610020	30432572	31159962	29311688	29121542	31096252	30721932	2480476	29490462	28939432	24656926	28869756	31699112	27787806	31723584	27460000
fpHLIC	Positive	140.0471	2.66	unknown	2110597	500654	353391	441425	339129	926380	115646	509511	1057045	282077	279338	977313	531736	620590	223272	719995	571153	876867	487816
EIC	Negative	471.0346	0.49	unknown	1769743	1902914	2041612	2062111	1583366	1925668	1872895	1922988	2002918	1956653	1885640	1815018	1902947	184027	1797235	1807559	1835875	1754807	1732646
EIC	Negative	605.3556	4.52	unknown	2546160	2358774	2215820	2202315	2217577	2409075	2340597	2375520	2192152	2222565	2302025	2337774	2293288	2247514	2354363	2167757	2367227	2074915	2301300
fpHLIC	Positive	84.0448	3.47	unknown	8691995	5132679	6116416	5537776	5530097	5775566	4965677	5782375	5507454	5666002	5401772	5947497	4696299	4643280	6360982	5270036	5009897	5914243	4362429
fpHLIC	Positive	140.0528	2.66	unknown	21131312	3460528	2651062	2982741	2941855	8233851	885585	3870604	9214042	2405900	2094005	7399680	4404511	5058377	1926418	5674790	4994776	7997674	3966459
EIC	Negative	298.2470	4.41	unknown	2376699	1864580	2171576	2206365	2153341	1999582	1989760	2253953	1919781	2330429	1886215	1921238	2001794	1872396	2020199	1917339	2009002	2286018	1853366
EIC	Negative	354.0044	1.19	unknown	78922	83401	73686	76660	69266	72005	68420	72093	64174	65831	67412	67077	64642	59869	69439	62417	66803	78268	61316
fpHLIC	Positive	762.5909	0.44	unknown	1623236	1880344	1651841	1747138	1780979	1432698	1600246	1725827	2146040	1506964	2023194	1942600	1633828	2190310	1784661	1501094	1951075	1406741	1865624
EIC	Negative	529.3531	2.92	unknown	258725	211821	211821	2219030	298156	531167	394216	361448	598048	685838	236265	478186	618400	122999	104324	555958	385222	600313	163873
EIC	Negative	365.1977	2.53	unknown	125611	89685	146000	92201	57083	88162	117946	66804	89809	93048	79570	125027	125000	69017	55772	103923	85021	82810	83049
fpHLIC	Positive	164.1164	2.92	unknown	4319605	4249476	4162037	2775118	2391258	2998863	3424267	2944918	1977717	3523487	3582388	3558120	2940783	2882563	3236200	1966419	2286770	2648244	3559587
EIC	Negative	336.7163	0.62	unknown	199806	115702	179589	129076	142328	119258	109187	73056	132010	216727	94739	71657	95312	195538	86418	108747	75738	109472	189240
EIC	Negative	261.1507	2.83	unknown	449182	223777	613070	622850	191246	303108	249329	438198	175946	678828	204236	232456	174747	114602	257590	182456	155757	494500	182125
fpHLIC	Positive	131.0499	3.48	unknown	717072	461110	639572	661900	411718	349132	597583	611130	422717	603124	554681	314813	546844	447103	664860	339580	569915	338338	408213
fpHLIC	Positive	133.2277	4.56	unknown	559963	480901	525339	661900	617998	384370	800991	404107	438300	545601	682704	511255	515500	522698	408796	537977	501229	379459	536155
fpHLIC	Negative	147.0185	4.03	unknown	626982	438933	551211	624720	386174	421503	463288	570454	337569	636248	469844	361446	305322	535746	575362	263294	314629	592235	388346
fpHLIC	Negative	325.1254	3.43	unknown	11156044	8638204	9722128	10735243	8073156	7873679	7873679	8992657	7857256	8916621	8414931	9073790	7917995	5756748	8906402	7945318	7748302	8915602	6792405
EIC	Negative	355.2130	3.32	unknown	1144937	224926	1100170	558313	278506	379469	431431	782543	111069	790505	198657	372048	191293	198574	242525	100221	221090	1110620	264422
fpHLIC	Positive	269.1069	1.79	unknown	0	66379	72444	687263	43795	48318	112117	389349	110138	75943	141758	75751	1682405	414073	32113	65545	466810	93859	32156
fpHLIC	Positive	759.5728	0.44	unknown	48908028	56493532	54776980	42440028	41302056	39121400	34176212	39664884	56129968	38882092	57606848	42221552	40172048	63294436	42139096	38566460	36248728	34789060	54420296
EIC	Negative	484.6909	0.52	unknown	221664	64982	262344	168721	285778	144219	130493	0	181808	299130	90994	28950	188007	117903	146056	84629	158455	220445	106384
EIC	Negative	289.1060	3.11	unknown	263729	88288	178524	320539	88303	162973	125852	203508	36552	216441	74431	142491	127387	136313	77214	86855	219393	85229	107834
EIC	Negative	317.2491	5.27	unknown	287044	216429	315672	267111	225442	66922	191090	240951	173589	3681709	196427	165949	134801	106973	206937	166619	162586	236654	107596
fpHLIC	Negative	528.2943	0.61	unknown	834334	690635	731400	738472	722677	678302	689138	789204	560355	705952	709136	788018	588797	679243	931336	709689	548649	543279	639614
fpHLIC	Negative	820.5682	0.44	unknown	4450455	4432211	4218020	3057956	3834043	3072688	3455279	3414418	4836706	3468816	3798485	3527177	3685264	4586266	4300450	3353320	3608087	2921241	4076384
EIC	Negative	451.2654	4.27	unknown	868765	1207006	1084930	771775	965701	1247569	940852	802640	660261	615824	1010754	867740	713271	1373921	848123	975086	693909	914079	198384
fpHLIC	Negative	187.1087	2.91	unknown	1468776	1373621	1403085	1355828	1133263	1832202	1082842	829287	1233639	1420335	1314607	1281453	1041744	775008	1164090	1427581	1154411	1337888	862588
EIC	Negative	253.1446	2.27	unknown	7101838	4441075	5966420	9261316	4623431	4015793	3573307	5449246	3886224	7542055	2652676	3236451	4036645	2655756	3129991	4992036	3642228	6841741	2554514
fpHLIC	Negative	763.5598	0.48	unknown	644502	1133564	684964	691384	955096	683962	757358	474505	953438	578996	887119	685119	619644	661766	843941	824087	654363	546765	887931
EIC	Negative	280.1625	2.39	unknown	211638	94034	145034	111844	150531	189138	51640	183957	161900	129322	101357	51890	93534	101357	101357	51890	93534	111727	89049
EIC	Negative	342.7334	0.52	unknown	249506	63893	231834	125472	171794	135043	124496	22169	133234	71722	47138	27760	74119	931890	83324	106798	34201	104729	292224
EIC	Negative	396.1779	0.71	unknown	139738	184717	217957	95769	110402	136431	161944	121919	119214	183273	192252	167085	121797	162652	129476	114059	117212	106355	171784
EIC	Negative	402.6897	0.64	unknown	125154	54212	112429	86723	113852	76869	76006	46477	70722	201420	55353	38324	63664	314795	66535	54598	44727	78033	133538
EIC	Negative	639.4113	4.03	unknown	0	0	207175	186558	0	0	214979	0	0	0	0	0	0	0	0	0	0	211505	0
EIC	Negative	241.1808	3.98	unknown	604417	443488	719822	1373013	599141	492858	170941	787318	0	668907	134135	184388	646581	335431	321299	0	539994	809640	346280
EIC	Negative	342.2655	6.06	unknown	197295	144025	240637	270176	141983	135281	165533	160585	231372	161562	143438	168331	170648	134336	128105	202755	180581	204400	105018
EIC	Negative	546.2505	1.12	unknown	157479	81004	269670	187773	82589	51604	113037	141356	61582	135070	135003	113796	133411	40647	75214	89825	72217	169800	35919
EIC	Negative	516.2967	4.18	unknown	397455	316933	341408	360515	279474	345285	281323	324494	251352	361758	347499	282063	286278	263293	240627	271336	307425	330665	302467
fpHLIC	Positive	121.0394	2.66	unknown	4090791	585959	442094	523469	567580	1452889	167295	377743	1645216	510714	403740	1360175	823226	1005642	424213	1054264	930693	1411409	677478
EIC	Negative	438.2487	6.00	unknown	612375	1012401	557255	1451253	573533	956260	693627	749943	899475	1135572	1087317	466430	878818	941996	976667	463213	117070	550265	739552
fpHLIC	Positive	391.1017	3.37	unknown	3387399	2852449	4964039	4521680	3873378	3146686	3354235	4036599	3185033	4986786	3849763	3354946	3553089	3056458	2942313	3090277	3661121	4604334	3387557
EIC	Negative																						







EIC	Negative	452.3107	2.57	unknown	7323037	614585	5194416	1710272	774139	730387	1341688	1833731	397724	139921	0	0	24947	0	13130	0	0	0	0
EIC	Negative	473.2881	2.84	unknown	1501401	529307	1148540	809054	446839	944235	867334	980082	399614	0	0	0	0	0	0	0	0	0	11861
fpHILIC	Positive	350.1368	2.66	unknown	1928109	350497	276624	324452	325732	772579	74457	468832	977478	277540	187516	641610	467506	0	102599	577545	653517	879642	392890
EIC	Negative	287.1077	3.54	unknown	231832	252920	239858	245869	224069	242691	248512	230210	218700	241245	236653	233987	249306	220063	233837	223365	219554	249588	232429
EIC	Negative	289.1236	3.59	unknown	458807	422400	396408	430672	384558	427321	419821	408507	380299	396276	398400	395067	408050	365960	395144	417067	394376	373819	430788
fpHILIC	Negative	157.0869	0.40	unknown	2177473	1576344	2945793	2159084	1519634	2400816	1945650	1671270	2139405	2747442	1430857	2171726	2537194	1509349	1557743	2242818	1721933	2836118	1274372
EIC	Negative	254.1761	3.37	unknown	1445566	473680	757957	2372758	296273	953643	407926	650868	682328	1050864	630352	950218	677889	226471	398951	825193	511036	904845	337563
fpHILIC	Negative	245.0430	3.06	unknown	1395337	804292	660967	959999	898925	1065991	1104515	822159	661136	844086	840196	1138825	642539	682571	994547	961252	792428	984796	799759
EIC	Negative	466.1816	0.70	unknown	116913	111947	144862	65375	92542	109015	123764	82260	96100	128926	114411	109940	91333	134647	92794	90176	95187	66559	156833
EIC	Negative	320.2674	5.88	unknown	205221	121435	211985	200245	127614	74269	110950	187089	109939	256196	135634	102079	109938	100644	129193	98089	112094	176501	91476
fpHILIC	Positive	772.5830	0.43	unknown	1481241	1501744	1494854	1274140	1159636	1483145	1082996	1623623	1119049	1156555	1297547	1085264	1081700	1707108	1269876	1069803	1218248	1355940	1528395
EIC	Negative	270.1713	2.44	unknown	8343937	4073950	6041642	6422950	5259518	5567375	4956798	6042432	5899286	7440735	6381234	5767152	5061348	5081903	5429269	4957915	5856595	7190057	4179802
EIC	Negative	328.2820	4.97	unknown	1746609	1790522	1648696	1811969	1769195	1610245	1663982	1741205	1609629	1648811	1663665	1660789	1617385	1581631	1654655	1705488	1708799	1733888	1559073
fpHILIC	Negative	868.5672	0.43	unknown	4692850	4567322	3240507	3678244	4195975	4556507	4252354	3712111	3099361	3201777	3732274	4381594	4359137	3796184	4194804	3960751	4615525	3248379	3722242
EIC	Negative	634.0388	0.48	unknown	5303502	5682192	6324528	6241299	4518598	5207927	5512413	5641357	5874999	5671606	5539480	5382598	5852927	1313956	4918113	5707710	5502145	5497021	5033236
fpHILIC	Negative	386.2373	0.36	unknown	818203	582274	1048942	1740613	500439	695426	483579	689969	692267	715639	514188	657330	554785	312441	446866	604048	566353	1090267	343211
EIC	Negative	312.2542	6.29	unknown	696897	375083	844610	2185234	526931	419027	513254	659903	756659	592218	433559	635762	700370	315646	331628	855393	574556	776366	328450
fpHILIC	Negative	581.3289	0.59	unknown	18144482	20222258	20950244	15457464	14702417	20562982	17475858	16837634	14503083	15450852	19423570	19630196	16665942	21438138	15513204	14834660	16116686	15253073	22098720
EIC	Negative	295.1194	2.22	unknown	152255	96732	165635	199827	85345	78534	95423	98800	81455	201934	100758	108775	85086	55885	108144	81231	59652	120279	68876
EIC	Negative	557.3569	4.84	unknown	1311654	1603385	1382475	1266273	1347625	1257292	1432368	1291819	1479848	1196370	1358135	1492646	1410446	1420673	1436838	1390575	1388334	1107260	1465575
EIC	Negative	339.0966	0.85	unknown	112313	102798	159667	150407	94224	67858	118685	127224	63996	138836	100242	124867	108802	45927	73238	88960	87816	172483	48114
EIC	Negative	295.1919	3.52	unknown	1301278	393871	985338	544825	534975	619055	716437	888954	217396	683837	353166	636446	387736	380156	509914	328949	422459	1358180	348893
fpHILIC	Positive	513.3373	0.61	unknown	1215698	651182	1177969	649705	610787	801237	734221	913318	603316	965432	642176	716159	322580	715138	817044	952009	742574	826378	314719
fpHILIC	Negative	266.1513	0.35	unknown	994435	1580098	4212425	3656420	4233657	2077413	1598028	1420947	1073395	2549510	2199083	1797418	2271352	1338707	1696131	2766095	3205155	1161454	1553690
fpHILIC	Negative	309.2800	0.37	unknown	7106327	10670731	16012353	15284279	11529938	9185068	11277193	10033638	9095214	8774260	7210107	14142572	10404389	6011099	7582101	11684591	8490179	15055205	8209276
fpHILIC	Positive	280.1034	2.97	unknown	527652	349912	538349	327271	289556	318162	405111	263534	256740	409656	480663	221938	391657	199686	551580	55224	428540	169728	326351
EIC	Negative	570.3418	2.42	unknown	5232662	3846191	4067529	4656260	3198353	4033240	3395653	4269972	3161356	4234625	3959994	4005705	3355531	2955193	3335305	3308693	3308772	4484962	3601258
EIC	Negative	382.8119	0.65	unknown	167165	70370	83598	163977	46368	114982	65759	47088	50237	94112	76992	74320	62347	18361	55345	83409	40395	63967	81213
EIC	Negative	338.7139	0.62	unknown	180592	101587	168817	122343	127660	108454	99896	67576	117756	210679	84738	73705	87440	179665	79673	100288	70315	96326	174581
fpHILIC	Negative	146.0177	4.03	unknown	3344886	2393991	2915533	3462054	2239399	2179034	2288745	3456676	1855313	3281470	2419137	1779296	1598735	3007892	3265079	1560865	1855355	3277502	2059926



180000	180001	180002	180003	180004	180005	180006	180007	180008	180009	180010	180011	180012	180013	180014	180015	180016	180017	180018	180019	180020	180021	180022	180023	180024	180025	180026	180027	180028	180029	180030	180031	180032	180033	180034	180035	180036	180037	180038	180039	180040	180041	180042	180043	180044	180045	180046	180047	180048	180049	180050	180051	180052	180053	180054	180055	180056	180057	180058	180059	180060	180061	180062	180063	180064	180065	180066	180067	180068	180069	180070	180071	180072	180073	180074	180075	180076	180077	180078	180079	180080	180081	180082	180083	180084	180085	180086	180087	180088	180089	180090	180091	180092	180093	180094	180095	180096	180097	180098	180099	180100
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unknown	482.153	1.659125202	0.52864421	0.00807672	0.11108499	1.26493167	0.93905479	1.38815325	0.47482242	-0.48913089	-0.73087376	0.00234534	0.05699795	0.00700224	-0.72380061	0.00233858	-0.62099809	1.0391815	-0.18381	0.13337715	0.0094572	0.76969173	-0.7802810	0.93466481	-0.120818	-17.594708	
unknown	482.308	1.62765457	0.47790031	0.02084683	0.2431211	1.27088477	1.13893451	0.4200311	0.2149475	-0.2149475	0.7912036	0.0028678	0.0028678	0.0706271	0.7628768	0.7628768	0.0113918	-0.6111818	1.101891	-0.048679	0.0702744	0.0662029	0.7197742	-0.498791	0.870222	-0.101368	
unknown	255.262	1.08574077	-0.59314761	0.07707876	-0.78802037	0.57862717	-0.78802037	0.64472827	-0.83876727	0.42825237	-0.1762179	0.00280809	0.0706271	1.0298122	0.1613986	1.063577	0.7520623	-0.1013918	1.0857408	0.0028081	0.0028081	0.0028081	0.0028081	0.0028081	0.0028081	0.0028081	-13.30761
unknown	188.736	1.2097787	0.77482226	0.02208794	0.10133196	0.82622266	0.5466622	0.42748662	0.27088021	0.42748662	0.27088021	0.0132016	0.0132016	0.0132016	0.0132016	0.0132016	0.0132016	0.0132016	1.2097788	0.0132016	0.0132016	0.0132016	0.0132016	0.0132016	0.0132016	-0.738187	
unknown	175.148882	0.49217976	0.00881134	0.02374149	1.2012805	0.30804079	0.30804079	0.51073769	0.10738108	-0.0737381	0.00281225	0.00281225	0.00281225	0.00281225	0.00281225	0.00281225	0.00281225	0.00281225	1.7514889	0.00281225	0.00281225	0.00281225	0.00281225	0.00281225	0.00281225	-0.170737	
unknown	227.8646	1.13023236	0.01696664	0.0164248	-0.82090064	0.63207974	0.63207974	0.50766281	0.00880064	0.00880064	0.00880064	0.00880064	0.00880064	0.00880064	0.00880064	0.00880064	0.00880064	0.00880064	1.2278647	0.00880064	0.00880064	0.00880064	0.00880064	0.00880064	0.00880064	-0.809208	
unknown	140.074	1.11771715	0.73025282	0.00980085	0.00722166	1.0030976	0.96027768	0.5641076	0.00736166	-0.87593628	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.4007401	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.827896	
unknown	102.611	0.62444138	0.00243092	0.00560055	0.00243092	0.17164799	0.17164799	0.17164799	0.17164799	0.17164799	0.17164799	0.17164799	0.17164799	0.17164799	0.17164799	0.17164799	0.17164799	0.17164799	1.0261101	0.00243092	0.00243092	0.00243092	0.00243092	0.00243092	0.00243092	-0.774764	
unknown	139.424	1.39841422	0.55242887	0.00480022	0.00480022	0.51410727	0.48779728	0.61308817	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.3942401	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	-0.500348	
unknown	349.2	1.26028449	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.3492000	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.878798	
unknown	271.23	1.34641402	0.00808072	0.00148827	0.00808072	0.00808072	0.00808072	0.00808072	0.00808072	0.00808072	0.00808072	0.00808072	0.00808072	0.00808072	0.00808072	0.00808072	0.00808072	0.00808072	1.2712300	0.00148827	0.00148827	0.00148827	0.00148827	0.00148827	0.00148827	-0.284209	
unknown	226.338	1.20897767	0.79038771	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.2263380	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.960604	
unknown	421.025	1.01114107	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.0111411	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.785428	
unknown	408.066	1.15884551	0.46432125	0.01088121	0.01088121	1.2000361	1.2000361	0.46432125	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	1.1588456	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	-0.488414	
unknown	437.317	1.16028708	0.64830026	0.01088121	0.01088121	1.2144776	1.2144776	0.64830026	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	1.1602871	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	0.01088121	-0.538468	
unknown	409.003	1.2603777	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.2603778	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.900203	
unknown	483.802	1.00488728	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.0048873	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.790355	
unknown	138.481	1.00488728	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.3848101	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.178193	
unknown	137.474	1.39841422	0.81574828	0.00903701	0.00903701	0.00903701	0.00903701	0.81574828	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	1.3747401	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	-0.205741	
unknown	807.361	1.45440517	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	1.4544052	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	0.00480022	-0.778617	
unknown	157.076	1.30884293	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.5707601	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.330357	
unknown	303.131	1.23069784	0.62531614	0.00280809	0.00280809	0.00280809	0.00280809	0.62531614	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.2306979	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.431888	
unknown	136.076	1.50879277	0.44023226	0.00903701	0.00903701	0.00903701	0.00903701	0.44023226	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	1.3607601	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	0.00903701	-0.760169	
unknown	479.208	1.2793851	0.45423028	0.00280809	0.00280809	0.00280809	0.00280809	0.45423028	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.2793852	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.437146	
unknown	155.075	1.31266791	0.45423028	0.00280809	0.00280809	0.00280809	0.00280809	0.45423028	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.5507501	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.388278	
unknown	338.275	1.2793851	0.60313056	0.00280809	0.00280809	0.00280809	0.00280809	0.60313056	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.3382750	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.210222	
unknown	445.111	1.440514	0.57670788	0.00280809	0.00280809	0.00280809	0.00280809	0.57670788	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.4405141	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.282029	
unknown	308.475	1.30483807	0.52713204	0.00280809	0.00280809	0.00280809	0.00280809	0.52713204	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.3048381	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.282029	
unknown	481.311	1.42621878	0.44230888	0.00280809	0.00280809	0.00280809	0.00280809	0.44230888	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.4262189	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.182039	
unknown	486.696	1.30718166	0.40236024	0.00280809	0.00280809	0.00280809	0.00280809	0.40236024	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.3071817	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.762376	
unknown	119.166	1.53297782	0.64962022	0.00280809	0.00280809	0.00280809	0.00280809	0.64962022	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	1.1916601	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	0.00280809	-0.197878	
unknown	255.262	1.30718166	0.40236024	0.00280809	0.00280809	0.00280809	0.00280809	0.40236024	0.00280809	0.00280809																	

# Supplemental table 4

DLZ vs CON									
ID	m/z	statistic_OvC	dm_OvC	pvalue_OvC	adj_pval_OvC	fold_change_imputed_OvC	log2_fold_change_imput_ed_OvC	fold_change_imputed_scaled_OvC	log2_fold_change_imputed_scaled_OvC
116-TXB2 [M-H]	367.2122	-5.35067446	-0.8803872	0.0010815	0.02720363	0.475700298	-1.071876155	0.528203565	-0.520850563
15(5) HEPE [M-H]	317.2124	-5.21607731	-1.038881753	0.001230507	0.038328362	0.441117278	-1.180765826	0.486823068	-1.088530563
15(5) HEPE [M-H+Acetate]	377.2322	-6.325572287	-0.962707732	0.000394353	0.025604563	0.457935038	-1.126785139	0.506468887	-0.981451743
15B-PG2 [M-H]	351.2128	-6.228623102	-1.41516662	0.000435056	0.026402395	0.321548752	-1.626898063	0.358466085	-1.4800381411
17(18) EpETE [M-H]	317.2124	-3.641146032	-1.575115524	0.008274505	0.112753035	0.275824207	-1.858179016	0.31092087	-1.685380636
20cooh AA [M-H]	333.2075	-3.479398588	-0.924878494	0.010275834	0.1291112	0.465005437	-1.151828373	0.504038047	-0.988801118
8-iso-PGA1 [M-H]	335.2232	-8.120514417	-2.403329614	8.24E-05	0.017507073	0.161519702	-2.629523207	0.181300852	-2.463542383
8-iso-PGA2 [M-H+Acetate]	395.2441	-9.683481292	-2.375632867	2.64E-05	0.016446553	0.163497599	-2.612849334	0.182596019	-2.453277284
8-iso-PGA2 [M-H+Acetate]	393.2288	-8.563889321	-2.079593988	5.89E-05	0.016446553	0.188501762	-2.332776284	0.222422877	-2.168622915
8(9)-EpETE [M-H]	317.2124	-4.340096024	-1.529660053	0.003797778	0.073706376	0.290120013	-1.785278274	0.326021287	-1.616963928
ASPARAGINE	133.0605	-2.977728398	-0.582348143	0.02581009	0.184860554	0.577697195	-0.791614606	0.633500653	-0.658581989
CITRULLINE	176.1026	4.661421136	0.429688822	0.002310647	0.054200457	1.194316521	0.256185234	1.318489724	0.398886327
Docosatrienoic Acid [M-H]	335.2958	2.60909045	0.679911369	0.03490662	0.245666463	1.318881333	0.399347963	1.461344667	0.449271579
Palmitoleic Acid [M-H+Acetate]	313.2386	3.572389654	0.933298617	0.00967905	0.119217362	1.673192926	0.743601804	1.843624897	0.882511013
PGA3 [M-H]	331.1919	-6.208265981	-1.30577215	0.000441685	0.026405285	0.357391034	-1.484786769	0.398285901	-1.328110643
PGA3 [M-H+Acetate]	391.2135	-6.40255056	-1.153895919	0.00036639	0.024987604	0.399959106	-1.320205998	0.444468223	-1.169849718
SERINE	104.0354	-4.77928356	-0.748540613	0.00013948	0.049746038	0.515449756	-0.95696389	0.569274762	-0.812802653
SERINE[M+2Q+H]	88.0398	-2.464654888	-0.386963421	0.043169789	0.086166	0.675979325	-0.564948972	0.739769966	-0.44851365
Tyrosine Acid [M-H+Acetate]	411.3483	5.225814203	0.872408464	0.00121802	0.038228202	1.604698802	0.682302532	1.752592271	0.809490401

M0v0									
statistic_M	dm_M0v0	pvalue_M0	adj_pval_M	imputed_scaled	log2_fold_c	fold_change	log2_fold_c	fold_change	log2_fold_c
3.64746686	0.62395912	0.0056264	0.08668786	1.53596721	0.61914742	1.65198367	0.72419855		
3.68435184	0.81122724	0.00618028	0.09461138	1.71881026	0.7814103	1.84565211	0.88413065		
3.78912142	0.17774139	0.00531849	0.08785991	1.63192413	0.70657398	1.75075869	0.80798025		
5.07671887	0.0345191	0.0098104	0.04774127	2.07068482	1.00101998	2.21871717	1.15089164		
2.92534178	1.04452952	0.01913411	0.17270636	2.06726045	1.04772016	2.2254246	1.15408062		
2.49272226	0.62193951	0.03786338	0.23944854	1.55080849	0.63302054	1.67051506	0.74029299		
4.19178385	1.65231758	0.00303036	0.07179053	2.81913366	1.49525137	3.0591004	1.61107044		
3.30189181	1.36323015	0.02108217	0.12714389	2.84475863	1.50830625	3.10959562	1.63672086		
2.74426602	1.24775295	0.02528197	0.1381335	2.79309756	1.48186397	3.04239575	1.60220783		
2.34902091	0.74029043	0.05465227	0.20807339	1.70282841	0.78793932	1.83302396	0.87227272		
3.79354822	0.72526204	0.00528503	0.08785991	1.68621896	0.75379189	1.80775077	0.85419579		
-2.7705654	-0.3905228	0.02427549	0.194609	0.76075424	-0.3944876	0.81608004	-0.2932174		
-1.7899974	-0.4806696	0.0531185	0.08786091	0.7194382	-0.4700415	0.77322821	-0.3710252		
-2.6884624	-0.5242182	0.02754221	0.20470748	0.67565863	-0.6566136	0.72893768	-0.4611301		
5.31275675	0.9718403	0.00080527	0.04269255	1.90497028	0.92978849	2.0439526	1.03136174		
5.40014152	0.9226252	0.00060591	0.04061469	1.85139033	0.8886091	1.98012884	0.98595978		
3.42654604	0.88915419	0.00900304	0.11470966	1.66565085	0.75167059	1.76926724	0.82315138		
2.49484415	0.51232169	0.0374003	0.23944854	1.44393084	0.53000164	1.55178985	0.6339332		
-1.5522878	-0.5063333	0.00748442	0.10231843	0.70256021	-0.5098062	0.75588805	-0.40379283		

MINO vs CON									
statistic_Mv	dm_MvC	pvalue_Mv	adj_pval_M	imputed_scaled	log2_fold_c	fold_change	log2_fold_c	fold_change	log2_fold_c
-1.9074320	-0.345607	0.09812708	0.48809108	0.69162285	-0.5319426	0.83221515	-0.26497315		
-1.0993003	-0.2165545	0.3080011	0.67534471	0.76849183	-0.3798982	0.91873231	-0.1222835		
-1.3359907	-0.2462157	0.22334924	0.61943033	0.74877151	-0.4174025	0.89692937	-0.1569493		
-0.7217383	-0.2776868	0.49385225	0.76821474	0.78880971	-0.3436644	0.95187198	-0.07116061		
-0.1733323	-0.0971664	0.86729594	0.94560399	0.89632812	-0.1578011	1.09248676	0.12761529		
-0.2553106	-0.0817701	0.80582231	0.92643993	0.83564286	-0.2590416	1.01541168	0.0206647		
-0.7871123	-0.3664964	0.45703363	0.74883513	0.76103733	-0.393904	0.92188009	-0.117349		
-0.6058438	-0.3101203	0.5637872	0.80205641	0.83680802	-0.2570309	1.01282725	0.03838813		
-0.5209555	-0.3159753	0.61450562	0.83097556	0.919561	-0.209828	1.11212398	0.15331763		
-1.0051091	-0.4903669	0.34827614	0.69479002	0.67605107	-0.5647959	0.82191235	-0.2826425		
-0.2335305	-0.0554793	0.82203184	0.91199556	0.82828436	-0.2718019	0.98800725	-0.0718189		
0.64384809	0.0433333	0.54018754	0.7903383	0.90462814	-0.1446032	1.08263311	0.11454442		
1.74644704	0.51719665	0.12423259	0.35380578	1.1600749	0.46168097	1.42702659	0.13012118		
2.9267301	0.9257942	0.022127	0.30919845	1.27695463	0.35270277	1.5331941	0.61654035		
-1.4262389	-0.2700143	0.19683715	0.59578827	0.71611731	-0.4817322	0.86466659	-0.2097341		
-1.0122475	-0.1982749	0.34512255	0.69848379	0.76483131	-0.38773	0.92121008	-0.1183978		
-1.3348318	-0.1862451	0.2263861	0.61978339	0.75183844	-0.4115059	0.91680216	-0.1493171		
0.06492255	0.01008251	0.95005084	0.98447878	0.7426877	-0.1938512	1.04060531	0.05742229		
1.03428496	0.20911261	0.33540662	0.69185437	1.00746168	0.01072497	1.19668091	0.25785243		

# Supplemental table 5

Method	Polarity	m/z	RT	ID	C1	C3	C5	C7	C8	O1	O3	O4	O7	O8	M3	M4	M5	M7	M8	M03	M04	M06	M07	M08
EC	Negative	379.2473	4.84	11-HETE [MH+Acetate]	72853	89665	80417	58396	95688	57633	51243	42503	48360	50825	38532	41536	37873	45162	59025	40361	49784	61398	60789	135614
EC	Negative	411.4447	4.84	11-HETE [MH+Acetate]	87826	114447	102391	80663	106639	60666	52063	59154	60666	59154	37223	40638	39163	40638	59154	40638	90127	90127	143276	143276
EC	Negative	317.2122	4.03	11(S)HEPE [MH]	71956	16309	30753	21450	13092	82355	84500	64659	77854	76165	103046	80679	80845	98580	82107	71262	65129	67622	67622	76739
EC	Negative	379.2481	4.92	12-HETE [MH+Acetate]	118385	386639	209271	187399	192322	195140	102522	110878	114758	117177	140124	100735	75976	119649	246237	138589	90975	104555	104555	342481
EC	Negative	377.2315	5.03	12-oxoETE [MH+Acetate]	69375	242374	130955	88732	113666	95613	84329	65922	71286	76289	87975	64878	65010	75628	312943	113262	60815	67195	126902	307998
EC	Negative	397.2559	4.50	12,13-diHETE [MH+Acetate]	2603518	6181385	433984	171217	137006	4951335	3102600	171000	24435	395819	0	150435	115285	16063	25493	103073	932456	330286	330286	2175997
EC	Negative	381.2653	5.71	15-oxoETE [MH+Acetate]	0	0	89096	88703	0	0	175106	181761	0	0	150435	115285	16063	25493	103073	0	61037	121397	0	0
EC	Negative	379.2485	4.71	15-HETE [MH+Acetate]	99201	297872	267184	119397	175929	160137	74545	97914	91844	99581	107332	75990	42735	84824	194803	103764	6030	83767	243640	608536
EC	Negative	377.2314	4.60	17(18)EETE [MH+Acetate]	49020	123953	147362	92713	68846	88021	29908	54399	61501	58401	37389	61742	26379	56329	36440	57815	66721	12397	129602	245270
EC	Negative	70.847	5.0	5-oxoETE [MH+Acetate]	51629	127588	65330	59025	58305	58305	58305	58305	58305	58305	58305	58305	58305	58305	58305	58305	58305	58305	58305	58305
EC	Negative	377.2314	5.32	5-oxoETE [MH+Acetate]	39838	254917	170259	78730	209627	79624	75098	38499	71507	70848	83737	74817	9869	77367	326606	1000283	25517	68401	155501	129040
EC	Negative	379.2482	5.66	5,6-EET [MH+Acetate]	119229	153311	138009	105172	158670	122258	88244	90569	95147	92300	93959	70010	79184	93083	87091	122724	74875	74722	123860	116741
EC	Negative	411.2377	2.01	8-iso-15-keto-PGF2alpha [MH+Acetate]	110247	153401	127405	180289	239415	229848	142267	142833	112106	110079	118829	125222	79284	132431	167630	119778	192892	147973	31425	920478
EC	Negative	397.2559	4.50	8,9-diHETE [MH+Acetate]	127306	127306	127306	127306	127306	127306	127306	127306	127306	127306	127306	127306	127306	127306	127306	127306	127306	127306	127306	127306
EC	Negative	379.2485	5.03	9-HETE [MH+Acetate]	191799	502652	493618	256066	312266	363924	219685	25570	270225	304412	283403	221897	180737	298111	367525	318761	182719	112285	536655	1049780
EC	Negative	193.2124	4.74	9-oxoODE [MH]	193214	973111	1422291	366504	781399	900880	2161158	1164928	800754	819313	323791	340940	226177	113081	207217	152174	447443	236821	258856	1491987
EC	Negative	313.2388	5.34	9,10-diHOME [MH]	108006	207477	199720	173237	134061	184607	120240	122487	129563	139902	126770	121693	107174	123374	213001	126424	117148	111174	188138	252180
EC	Negative	291.2599	4.50	11-HOME [MH]	539870	1216113	890988	2161158	1164928	1164928	1164928	1164928	1164928	1164928	1164928	1164928	1164928	1164928	1164928	1164928	1164928	1164928	1164928	1164928
EC	Negative	277.2171	6.53	alpha-Ionic Acid [M-H]	293577	1064741	1306473	676105	3401971	966618	304126	132342	1873055	2560654	1812899	363601	759510	1865368	703435	2696818	163546	173146	1793017	2195265
EC	Negative	331.2646	6.53	Adrenic Acid [M-H]	2604120	20312897	9236304	5760444	25212705	9106530	4526257	12304997	7600828	15179631	12893152	3510129	6162598	13240123	5412051	14232569	875968	2240337	26006113	1834400
gHILIC	Positive	106.0616	3.74	AMINOMIDPATE	94215	1275856	2054923	760122	751398	701222	691335	1032869	6780111	1311832	1490089	603570	1289992	1902809	868954	1731931	556732	897350	187495	241854
gHILIC	Positive	144.0655	3.75	AMINOMIDPATE (MH2OH)	79794	675400	1268907	379015	472329	365803	238303	403992	435991	795951	803364	236118	564599	1187848	901785	228372	321466	1089135	1249592	3342893
EC	Negative	311.2956	6.72	ARACHIDATE [MH]	1019500	5244927	3118107	2381789	4908374	3547641	2668055	2501242	3883590	3164425	3836669	1478859	1936524	3420172	2230422	4937915	3219292	1898558	3282992	3342893
EC	Negative	339.3266	6.85	Behenic Acid [M-H]	11645	78911	62174	25996	82152	47962	26181	44475	55249	59814	60890	0	25254	70256	0	97392	0	0	84280	59094
EC	Negative	266.0892	0.56	DEOXYGLUCOSINE [MH]	70035	307186	437087	222341	355184	414255	119577	138886	156709	408161	421728	251970	446272	442872	155148	53374	171293	79028	57093	52026
EC	Negative	271.0618	0.56	DEOXYGLUCOSINE (MH+Acetate)	47763	197617	289788	144712	248483	246129	195780	289788	289788	289788	289788	289788	289788	289788	289788	289788	289788	289788	289788	289788
EC	Negative	272.0646	0.51	DEOXYURIDINE [MH]	104030	359664	516847	694806	212375	109578	109578	382064	638583	472271	825059	1353338	452141	654290	249119	506464	175990	321064	410451	71380
EC	Negative	329.3237	2.79	EC_124,EC_126	175253	319787	197088	161930	248004	200864	150533	153313	155477	147740	141157	131659	156251	144558	192331	211265	239186	137908	20007	33884
EC	Negative	329.2336	2.79	EC_125,EC_126,EC_129	207393	330690	227639	389644	473446	473446	163754	259922	240761	193660	176253	158690	175729	207499	289999	250502	327400	184865	296327	13887
EC	Negative	329.2336	2.79	EC_125,EC_126,EC_129	107975	150074	107975	150074	107975	150074	107975	150074	107975	150074	107975	150074	107975	150074	107975	150074	107975	150074	107975	150074
EC	Negative	329.2338	2.52	EC_128	47076	211638	93055	70578	118752	213615	45033	60861	63746	48107	57181	48524	44929	63130	106687	70397	78840	55285	101953	205510
EC	Negative	333.2075	2.55	EC_138	63725	145973	101568	72616	412852	246238	38561	64233	100313	81813	738446	75711	80389	130499	97348	52041	96798	652929	303141	
EC	Negative	333.2076	2.55	EC_138,EC_140,EC_145	60062	84622	63834	31176	212057	211566	25771	37810	51126	45094	711267	47017	52388	74966	65893	51722	35635	63271	323140	187422
EC	Negative	291.2124	4.43	EC_16,EC_18,EC_19	72108	77119	77119	77119	77119	77119	77119	77119	77119	77119	77119	77119	77119	77119	77119	77119	77119	77119	77119	77119
EC	Negative	293.2124	4.54	EC_16,EC_18	95129	174171	1494891	399112	774125	1041036	164633	279435	202356	310242	312166	48468	238543	133368	228784	142137	460460	232069	238409	1417452
EC	Negative	295.2280	4.43	EC_20,EC_21	953059	2056546	2887137	1197375	4412013	1373788	1290491	1383503	872999	677831	562587	1200908	914811	950545	1254700	532864	2662350	408844		unchanged
EC	Negative	295.2280	4.40	EC_20,EC_21	739059	1348005	1600306	679811	799352	1070153	571919	571029	643499	655386	471109	367025	221153	574086	678489	290904	1162655	2628416		unchanged
EC	Negative	294.2280	4.40	EC_21	2898437	4422049	4422049	4422049	4422049	4422049	4422049	4422049	4422049	4422049	4422049	4422049	4422049	4422049	4422049	4422049	4422049	4422049	4422049	4422049
EC	Negative	295.2280	5.02	EC_23,EC_30	574799	2705465	2237574	934920	1265391	1144745	842764	811011	778963	851757	929663	690231	597107	892404	3687262	1160253	623268	758663	1968098	3781786
EC	Negative	353.2341	3.24	EC_251,EC_256,EC_260,EC_265	32475	73059	87537	44593	72327	62107	40626	60209	54927	70984	61335	46783	39431	57450	60403	63721	93936	58063	116204	150021
EC	Negative	359.2208	3.78	EC_294,EC_296	110430	121120	21497	123904	338764	338764	102565	156213	143366	80211	241749	52346	118858	98055	124168	152786	79389	16		



EIC	Negative	320.2262	4.76	0	0	77470	0	255893	0	0	0	466107	301644	0	0	0	0	0	0	0	0	0	68592	0	0	0	0
PHLIC	Negative	208.1187	1.72	160664	55634	81814	708447	87797	7133564	80709	72000	0	92224	0	0	0	36063	5567896	0	0	0	96660	1673500	0	0	0	163837
EIC	Negative	141.9571	1.44	141957	108123	108123	69445	69445	69445	69445	69445	69445	100423	64021	61274	0	61274	150273	56077	0	0	926187	1222674	150273	0	0	161764
PHLIC	Negative	404.1042	3.54	90460	216977	216977	158531	512682	4893753	62799	42000	42000	47962	63980	0	0	138604	220760	312287	0	0	129678	70535	130527	354746	495972	
EIC	Negative	247.9723	0.64	0	40539	0	0	0	23600	0	0	25242	67947	43422	0	0	50370	0	0	0	0	26402	0	0	0	19837	
EIC	Negative	511.1734	3.46	30152	78485	78485	21857	21865	36996	15510	15275	22549	366764	9813	103746	15403	27130	152482	0	0	17420	20894	185378	17294	46912		
PHLIC	Negative	103587	10.64	103587	74664	235676	105927	118892	58369	78219	60893	107933	5313	60893	57372	37158	60893	57372	37158	60893	57372	37158	60893	57372	37158	60893	
EIC	Negative	397.2002	3.62	0	29353	31339	19676	58261	191982	18930	23786	26441	30742	70349	17004	16517	45366	23446	32909	0	0	26645	59619	0	0	19837	
EIC	Negative	512.1776	3.15	44216	26520	108210	18958	27051	38952	23308	29803	19919	387072	24102	148316	22228	19715	233236	0	0	21733	25560	254894	19379	75634		
EIC	Negative	511.1740	3.15	155189	89506	205659	75584	88450	137836	60573	83528	17552	1526681	79229	578793	89506	84780	863539	0	0	74847	78882	303269	70227	269500		
EIC	Negative	451.2002	0.64	0	41304	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	153475	0	0	0	41184	
EIC	Negative	307.1506	3.15	35952	83475	109659	43771	97606	701646	27983	56111	77689	60893	67152	40756	32671	38576	34422	73444	42388	59811	100725	104257	425512	0		
EIC	Negative	511.1740	2.93	37158	26793	90175	29311	7468	28970	18855	20351	27549	300240	23222	104475	16219	29198	164772	0	0	24762	26035	181794	26931	62613		
EIC	Negative	461.1822	4.15	0	98872	0	0	0	1130964	0	0	0	930224	0	0	0	1977120	0	0	0	0	0	0	0	0	95719	
PHLIC	Negative	307.1545	3.03	8824	74868	0	0	0	8824	0	0	0	0	0	0	0	10045	0	0	0	0	15707	0	0	0	0	
EIC	Negative	307.1545	3.14	0	72053	0	0	0	598855	0	0	0	0	0	0	0	15887	0	0	0	0	0	0	0	0	0	
PHLIC	Negative	245.9359	0.40	2139373	300621	110222	2118296	127493	94459	9465712	597522	0	0	0	0	0	4366766	291240	104281	343756	97094	1320323	983413	0	0	504888	
PHLIC	Negative	165.9966	0.58	0	947704	8940959	730067	1557482	0	0	0	0	0	0	0	0	348850	0	0	0	0	229936	0	0	0	80818	
EIC	Negative	301.1744	2.72	175553	1730038	1633216	1914706	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	344645	
EIC	Negative	283.8419	2.43	0	59407	505061	60263	188371	0	0	0	0	0	0	0	0	5114	3993	44485	0	0	88224	30670	104720	83407	85000	
PHLIC	Positive	87.1003	4.46	150398	0	608618	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	248232	0	0	0	0	
EIC	Negative	342.2655	6.60	0	8288	194699	309323	0	0	0	0	0	0	0	0	0	0	87767	0	0	0	176834	0	0	0	7950	
EIC	Negative	370.2061	2.53	0	24295	157052	54751	66513	0	0	0	0	0	0	0	0	19464	17954	0	0	0	49325	24895	128958	312095	0	
EIC	Negative	321.2386	5.05	0	0	179497	122595	0	0	0	0	0	0	0	0	0	0	0	0	0	0	273305	0	0	0	0	
EIC	Negative	321.2386	4.85	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114662	0	0	0	0	
EIC	Negative	370.2059	2.67	0	8288	134585	44482	51233	0	0	0	0	0	0	0	0	0	0	0	0	0	179491	0	0	0	0	
EIC	Negative	365.0074	2.01	0	86425	53920	34013	57379	0	0	0	0	0	0	0	0	0	0	0	0	0	42790	0	0	0	37480	
EIC	Negative	403.3066	3.99	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	181329	
EIC	Negative	349.2791	4.99	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	155181	
EIC	Negative	349.2791	5.87	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	49507	
EIC	Negative	628.3134	4.93	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	182611	
EIC	Negative	356.2269	4.89	0	0	8167	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	93265	
PHLIC	Negative	150.0018	0.52	76530	1011929	12446676	1241035	2354853	0	0	105238	0	0	0	0	0	1262004	0	0	0	1043950	3489	0	0	0	93344	
EIC	Negative	232.0047	1.54	0	80145	521600	137594	220802	0	0	10185	2651	0	0	0	0	136818	11254	71240	0	0	5198	0	0	0	26336	
EIC	Negative	329.6414	2.72	12114	120292	428722	125264	1485046	4104	15787	3904	0	4300	3527	185453	14201	63685	5985	7622	10057	57881	34768	0	0	34768		
EIC	Negative	331.0087	2.44	0	175872	171262	94254	192557	0	0	0	0	0	0	0	0	0	0	0	0	0	14020	0	0	0	15970	
EIC	Negative	309.0264	2.44	0	144942	313797	136465	234426	0	0	3853	3219	5812	24940	0	0	23273	131324	0	0	0	35253	2778	0	0	12642	
PHLIC	Negative	343.9953	3.59	44996	3664486	32114998	2790369	3587524	88331	0	432084	61071	921113	60404	492392	303352	3728501	0	0	0	1802911	42169	108498	1835438	3097086		
EIC	Negative	249.0051	2.44	0	99499	9147223	0	0	0	0	4277	4639	16995	0	0	0	10052	92098	0	0	0	312	0	0	0	7958	
EIC	Negative	249.0051	2.44	20364	594858	1100428	690174	954676	0	0	24069	136819	160571	0	0	0	512684	74251	0	0	0	119096	4859	149759	145438	6585	
PHLIC	Negative	344.9972	3.59	0	531928	4369988	361416	496899	0	0	87983	52205	88769	0	0	0	77270	36691	482202	0	0	243363	140225	240369	455927	0	
PHLIC	Negative	112.0042	0.96	0	231466	574110	106602	195499	0	0	73039	0	0	0	0	0	61306	0	0	0	0	53962	0	0	0	118095	
PHLIC	Negative	112.0042	0.96	0	231466	574110	106602	195499	0	0	73039	0	0	0	0	0	61306	0	0	0	0	53962	0	0	0	118095	
PHLIC	Positive	346.0085	3.59	38390	451837	5601130	457239	499513	0	0	29621	37808	48480	101279	0	0	238293	37893	405979	0	0	187949	0	0	0	203600	
PHLIC	Negative	192.0037	0.53	1639636	0	326070	162624	2055021	0	0	61013	103967	127660	0	0	0	269781	1037711	104756	270273	314682	2537689	240695	363152	0	533805	
EIC	Negative	359.0148	0.95	3807911	16326	19711	77064	103128	31090	296127	51637	16469	0	0	0	0	15040	320063	9534	9261	46586	11498	1218019	108764	9665	0	
EIC	Negative	282.3163	6.46	0	5374782	5374782	2703811	1023234	6278981	168235	308683	333637	445207	0	0	0	5057762	224168	331973	0	0	4554068	512078	378457	14584722	437023	
PHLIC	Negative	144.0301	0.97	85453	1006580	4305427	766419	1107882	64579	353242	74266	107222	69133	46955	252249	96906	586082	40002	272136	92971	150350	378624	469908	0	0	469908	
EIC	Negative	401.2340	5.47	0	96911	96623	69005	118789	23857	0	0	22885	0	0	0	0	39216	16740	0	0	0	15457	13013	31783	50421	54102	
EIC	Negative	356.1428	3.16	208118	135466	109166	151025	153647	47375	0	0	0	0	0	0	0	0	0	0	0	0	32658	32064	0	0	76821	
EIC	Negative	370.1264	2.70	90784	270793	52736	143464	216704	0	0	80178	44341	64925	0	0	0	51889	0	0	0	0	325353	88564	74988	412795	17786	
EIC	Negative	333.2123	4.92	0	55416	56060	26632	27089	0	0	5589	0	0	0	0	0	0	0	0	0	0	30691	0	0	0	141088	
EIC	Negative	359.1027	1.68	184533	133885	94254	149270	136830	0	0	37694	11444	33829	0	0	0	26984	30727	0	0	0	34266	17486	75359	79739	50113	
EIC	Negative	441.0173	0.45	1723786	33582	24085	66012	46686	47717	103170	41227	35116	0	0	0	0	20396	246503	33690	13855	46323	22292	544680	69313	29206	21305	
EIC	Negative	252.0025	0.91	0	51116	1610516	16653011	2343729	239060	0	0	0	0	0</													



EC	Negative	366.0332	0.46	1020705	29981	45203	86767	65317	57167	180970	76324	44416	23640	28558	231316	57914	26206	71235	22142	351044	72509	42792	30325
EC	Negative	293.1764	3.53	341469	365492	361122	370711	421395	140485	107642	98358	117257	113060	98627	140402	133670	141627	118014	106415	155667	152196	176322	148981
PHILIC	Negative	6768117	4044786	2514708	1912924	1329264	8708157	6052620	1701038	305664	901207	805624	969520	171277	812721	790124	1654021	2281051	1683448	1724049	3605207	3765114	3610007
EC	Negative	293.1423	3.59	142426	406620	71639	42029	44547	44186	31075	41787	51925	52442	51168	23254	26162	56664	38697	28209	51070	73663	44894	32752
EC	Negative	332.2680	6.54	1046374	346148	3068085	2187315	10121717	190628	1456339	190628	221518	257502	210629	1384374	2446998	4297860	2096679	4360874	300840	759371	393754	264627
EC	Negative	582.3778	5.17	431299	1265529	0	0	1127824	0	898180	0	1792617	0	1792617	0	1491894	0	349637	0	349637	0	1862199	0
EC	Negative	109976	4.13	109976	41296	46072	23013	23013	20213	20144	31393	36189	35619	22862	17416	19195	18822	41851	39607	54607	15853	18180	34527
EC	Negative	458.9955	0.46	315841	329542	243764	359980	315427	278735	501824	237474	218744	184187	209572	721252	209508	226051	221641	269734	2566216	347581	140159	204829
EC	Negative	481.2967	2.62	1502357	429184	256996	142815	164116	169347	239776	159871	104601	143307	341684	221177	81324	202625	119187	197795	290020	274593	121464	84664
EC	Negative	540.0005	0.46	540802	50998	33381	73363	53865	50769	1010210	42303	35901	20855	13475	130487	35813	33510	18826	22501	341083	65140	28277	22605
EC	Negative	249.1792	2.98	839283	870555	853289	843485	916920	814020	5176	41680	76426	41680	268657	279555	336702	355899	332043	270075	322429	421122	415999	410884
EC	Negative	349.2053	6.30	597112	540960	1021557	1112480	1410183	425147	138670	142955	316333	555129	219821	156796	6806920	1147634	15554593	33904	261912	196087	93161	422000
EC	Negative	1202.208	1.5258	196898	196898	214045	235212	82229	31750	25178	66016	107660	424819	113917	230722	147724	224472	3061603	68747	50240	17863	112447	79831
EC	Negative	375.1792	2.98	369628	351967	323283	333792	375757	111043	128866	110161	121171	120939	92403	113815	150519	142691	121515	117841	122425	106072	109509	156590
PHILIC	Negative	244.0463	1.00	0	447543	0	76757	521061	0	49334	65564	245158	0	42215	0	457344	0	822118	0	32697	44206	84767	394078
EC	Negative	313.0724	2.48	63541	11695	26322	0	12909	26252	0	3604	9923	0	6223	3363	0	580936	3045	16135	8509	0	82867	329629
PHILIC	Positive	259.1282	2.73	0	593686	0	37609	1391433	39327	67202	155264	203708	249524	30511	80792	127987	1120004	0	311321	34190	112154	900080	348527
EC	Negative	293.1762	2.98	4425462	4860063	4662392	4511112	4934434	1787847	1655975	1413145	1698772	1737077	1434033	1439577	1775877	1855027	1685369	1482515	1661152	2189211	2231404	2269758
EC	Negative	358.2630	1.99	6465904	110173	6370551	6993864	104670	105877	105958	6577284	100797	6261158	6121117	6492679	106454	6218146	102522	104024	6480877	4890546	6524903	6524903
EC	Negative	317.1398	3.76	706567	877728	529911	529911	746448	231885	334946	205748	266782	279050	203992	185953	272343	235234	244291	326641	189010	218273	382092	365026
EC	Negative	425.0648	1.68	179767	140948	135398	50575	337115	84362	57781	57709	75027	27057	50912	63319	44505	97528	63574	540079	52967	57514	60719	152550
EC	Negative	294.1792	2.98	839283	870555	853289	843485	916920	814020	5176	41680	76426	41680	268657	279555	336702	355899	332043	270075	322429	421122	415999	410884
EC	Negative	270.6327	2.83	33205	16904	36150	67853	0	0	28856	0	29136	0	0	0	0	135854	0	0	0	32208	154412	0
EC	Negative	318.1431	3.75	144376	172102	102749	148385	149204	53142	67886	44647	53241	55054	43908	40719	55621	47775	51267	60085	41555	62038	82389	78131
EC	Negative	354.2371	2.25	13181	116139	209938	118496	183839	47312	31383	64774	65893	69570	85234	28892	51383	92039	60632	0	22945	34921	189318	293844
EC	Negative	530.2800	1.46	0	18285	0	57938	29313	0	0	0	28994	0	43761	23230	26639	10450	54447	51557	23150	14501	58948	59486
EC	Negative	457.9984	0.46	441475	51578	35004	65219	84258	50532	83714	42289	50946	23985	33721	109364	35198	38377	29365	42476	343565	67967	25429	38077
EC	Negative	251.1323	2.08	145839	86855	69522	0	99282	61548	40198	0	0	0	72229	0	76839	72844	0	54018	0	108753	106079	0
EC	Negative	249.1496	5.30	1411172	3578094	2417678	1937607	3344360	983568	800046	679311	1388786	1196807	920194	489383	974304	1086303	937161	1449974	384553	998903	1834143	1661494
EC	Negative	250.678	2.54	162068	61326	415476	320239	179236	135909	112300	77532	117428	77532	161605	181189	104815	161605	181189	104815	231074	6183	165055	287375
PHILIC	Positive	173.0355	2.46	977452	440180	258611	101647	268760	101647	268760	101647	175064	118750	225539	295124	487849	151805	355591	272430	181260	170279	399862	234577
PHILIC	Positive	399.2504	0.41	10029129	3435685	2739995	11748206	3493370	3827315	1940588	2650906	1874697	11196831	6848720	1803751	4981860	3021510	1804810	15665010	2536488	1748812	2229853	3842490
PHILIC	Negative	199.0377	1.81	4043707	1413543	1239968	6144711	2491083	971251	3675129	397579	1120748	3076861	779036	1217496	1734626	1791781	1778391	615792	2316944	1682207	3842490	3842490
PHILIC	Negative	375.2155	4.74	13409	81983	128384	30821	68712	78520	0	0	0	15680	15109	0	10310	0	5482	11728	0	0	111686	336766
PHILIC	Positive	400.2334	0.41	824700	2337831	871855	577882	2525986	670051	820508	413305	495348	479930	2255089	819710	380732	1152605	562064	424560	3211385	560051	322266	364480
EC	Negative	238.9912	1.68	2999118	284011	220143	96224	565496	203003	95248	91792	136401	100859	100859	157528	152101	100859	157528	152101	183515	105488	137648	247894
EC	Negative	237.0990	1.68	705533	683481	519636	239408	1365834	484104	238224	215345	330408	226590	315560	632042	219304	380861	377974	1933286	275302	328334	547973	613382
EC	Negative	431.3015	3.03	176649	136652	142767	142633	128303	0	153934	0	0	0	0	0	139298	142605	148795	105981	0	0	156639	136210
EC	Negative	236.0961	1.68	6354966	632068	4836475	1713852	1119326	4341319	2226264	1905071	3040355	2004742	2846670	5781088	2058612	3463563	1477596	17758403	2471153	3059012	4958021	5649585
EC	Negative	357.1084	5.36	69992	79620	43456	17248	109560	0	37686	99709	0	79687	0	63141	10716	69382	18250	0	19343	85353	71606	0
PHILIC	Positive	453.3253	0.40	3762601	0	2226632	1723224	20060752	0	1952391	1044409	1075638	0	2140110	210386	2221187	2297865	2128115	1939929	1352832	0	2203942	0
PHILIC	Positive	201.0519	1.81	103971	533535	433546	1807803	742534	316566	501520	146075	299885	329072	816742	284095	392279	595374	280094	617104	205782	756624	1364233	1364233
EC	Negative	513.2727	1.70	67092	24269	247657	424928	610261	29529	7298	11007	489887	68826	214501	31443	66579	35344	140191	146200	27325	76007	1391889	237880
EC	Negative	255.0660	2.42	3319066	44924	99718	56140	45461	98979	30556	36899	46982	26896	124688	25366	66989	1554493	46011	18949	41162	44700	118949	104034
PHILIC	Positive	140.0530	2.47	1091436	493661	192809	62621	196310	93982	327486	235194	158202	97989	113703	438557	455078	202831	300139	355124	91802	101097	472354	226104
EC	Negative	512.2692	1.70	178801	58799	836946	1392076	2046265	80165	42394	48829	1651694	222121	710345	1000309	208181	175156	460672	472026	75005	269975	4702221	780016
EC	Negative	379.2480	5.96	127829	551741	411270	166067	345832	165550	137371	139601	138966	1473247	138434	110912	107937	143890	566556	221972	108030	2101567	2101567	713104
EC	Negative	362.2915	3.47	218031	3116163	209734	402667	290248	227000	99888	95479	137315	94046	138700	71220	117061	112992	132747	110063	92829	221005	167133	139562
PHILIC	Positive	176.0912	2.63	77148	517331	2023359	72465	550045	195726	178417	391155	289340	420115	102368	240646	266014	714589	139540	483304	1514739	161342	486592	686513
EC	Negative	298.2469	5.96	219958	1187610	918494	345046	812844	374140	277603													



294.1792	-7.3801856	-1.2243773	0.000151865	0.000704972	0.35710137	-1.485594	0.38235694	-1.38700802	0.622684386	0.140247993	0.550824655	0.868511102	1.182065378	0.24130983	0.971434809	-0.0481810912	-6.11470097	-1.108671	0.000484025	0.008203368	0.360408885	-1.477201523	0.403553308	-1.309161683	
412.2137	2.0923237	0.4580205	0.077695568	0.210251897	1.18441047	0.24418915	1.12382754	0.181201216	-1.421351151	-0.368561773	0.184799209	0.67909986	0.790093881	-0.33994006	0.71496392	-0.48405753	1.472811875	0.34871205	0.18403498	0.44473217	0.19552211	-0.012738041	1.044814346	0.062643535	
331.0413	-2.6673686	-0.8715955	0.031212008	0.103958497	0.45953508	-1.1217531	0.49725076	-1.007954524	0.6698784	0.19232864	0.521797159	0.856999201	1.198367129	0.261069956	0.911532794	-0.133835333	-1.914923258	-0.533915808	0.097052218	0.305387874	0.540257505	-0.888280887	0.579387174	-0.787400347	
383.2207	-2.4147858	-0.9818762	0.046846609	0.142542427	0.46887406	-1.0927076	0.45481405	-1.195653268	0.77741246	0.160981517	0.786497196	0.94622983	1.305703503	0.384882574	0.959549005	-0.059571607	-2.666482251	-1.328909081	0.032163314	0.152668228	0.368195158	-1.441457441	0.349710263	-0.515789372	
399.2504	-3.330241	-1.0850189	0.038888119	0.122515096	0.33688887	-1.4791351	0.44346284	-1.17953561	0.17031276	0.134120776	0.869023079	0.99823252	1.73344239	0.793556661	1.117883503	1.09826721	-0.718763887	-0.376581077	0.495573051	0.759867583	0.633130608	-0.654874533	0.613770644	-0.70422845	
318.1431	-0.0647075	-1.0979472	0.004787313	0.025417935	0.38558066	-1.3748954	0.42029974	-1.24430563	0.643203404	0.131731406	0.53808786	0.862071616	1.18333842	0.242857266	0.845120954	-0.24277026	-5.182528995	-1.182653316	0.001277325	0.016450297	0.336776235	-1.570132223	0.369765186	-1.435138695	
248.1496	-4.283706	-1.1037321	0.008468973	0.01228976	0.17626537	-1.4102236	0.42022388	-1.250730609	0.35588847	0.099214421	0.82621255	0.86199369	1.251604779	0.228848577	0.85641758	-0.223080257	-4.821084288	-1.108771399	0.002219104	0.019793179	0.327749684	-1.60483808	0.376610692	-1.408804336	
359.2208	2.3547973	1.2929861	0.050765884	0.150608711	1.83359797	0.87655331	1.86592387	0.898980204	-0.35496641	-0.072388173	0.826524838	0.959044444	0.97104774	0.442385819	0.728022786	-0.39961083	2.009444667	0.064493051	0.283777379	1.617167781	0.693469366	1.498946238	0.683763556	-0.585706356	
403.2701	-3.7280814	-0.8047314	0.007389717	0.03318127	0.47729955	-1.0670331	0.48612593	-1.046597992	0.39642022	0.09852828	0.702001898	0.956912137	1.139295994	0.180223616	0.982376148	-0.025335848	-2.212828214	-0.667617141	0.062535298	0.236838809	0.498987714	-1.000254543	0.567143484	-0.81821432	
262.2915	-3.8883005	-0.7873762	0.006003352	0.029830253	0.50569961	-0.9836474	0.52449319	-0.91112322	0.339230943	0.098749438	0.742096465	0.963971151	1.117579953	0.160379465	0.954972921	-0.067011773	-3.249702253	-0.812247446	0.001386606	0.016247176	0.442034841	-1.174507935	0.47632302	-1.070264648	
402.2334	-2.7189473	-1.0596555	0.02897215	0.098500078	0.36579683	-1.4508855	0.46178645	-1.114702244	0.88078046	0.071284517	0.931432065	0.99823252	1.70000208	0.765432923	2.106555273	1.074200748	-0.655846602	-0.338482932	0.532878763	0.78715701	0.656848512	-0.606806757	0.65782882	-0.60421706	
11 HETE (M)	379.2473	-3.6538141	-0.4903534	0.00815176	0.0356667	0.9190735	-0.7565567	0.65063066	-0.621408349	0.521734437	0.146454871	0.61897951	0.9222782	1.306811277	0.388279129	0.95999488	-0.68890347	-3.598714612	-0.570725258	0.008754804	0.054679124	0.524732986	-0.93034661	0.616802861	-0.71108713
250.1328	-3.8825445	-1.0717315	0.006031164	0.028028052	0.3810321	-1.3030092	0.42464287	-1.22975637	0.192197711	0.057731865	0.852376432	0.99823252	1.22083011	0.287486808	0.811332828	-0.266501813	-4.375850986	-1.222474603	0.003120797	0.027543478	0.319182005	-1.644225004	0.368116108	-1.441766863	
459.2144	-1.9380917	-0.4885116	0.091751381	0.24173852	0.58434949	-0.7759966	0.64218088	-0.638948395	0.377959399	0.110026417	0.713291848	0.95925058	1.318103134	0.399597366	0.915711282	-0.124202229	-1.98805091	-1.207311335	0.153940622	0.41206366	0.55622615	-0.845477411	0.702389502	-0.509656813	
298.2469	-1.8341048	-0.7993066	0.026054206	0.026048051	0.4034248	-1.0996189	0.49423245	-1.058472737	0.224833841	0.036247231	0.827740653	0.99823252	1.12494383	0.204799207	0.82604871	-0.26004871	-0.703781819	-0.444429509	0.304299181	0.76399611	0.63867675	-0.802996652	0.839646412	-0.252488895	
5 HETE (M)	379.2471	-2.885611	-0.5629334	0.02026759	0.07152622	0.56961706	-0.8119157	0.63218472	0.118811397	0.039797609	0.9008154	0.99823252	1.24896435	0.349638313	0.863947613	-0.21098426	-1.57807512	-0.45977915	0.15956113	0.416487311	0.59183159	-0.756741391	0.718984474	-0.490246692	
379.248	-2.3812824	-0.8645235	0.048794054	0.145972127	0.40361335	-1.3089542	0.49431109	-1.04560881	0.132412891	0.022611596	0.897927879	0.99823252	1.129185466	0.17528272	0.812690651	-0.29921221	-0.950202577	-0.539244288	0.373370216	0.461292423	0.598416376	-0.75010135	0.796514938	-0.328226676	
250.081	-3.6876306	-2.9928673	0.007949683	0.029493088	0.15515788	-2.6881911	0.18379794	-2.361408646	0.004893372	0.020402058	0.99973187	1.06822363	0.909139972	1.051410873	0.147195992	-1.570447184	-1.19046211	0.009091481	0.055802886	0.237314662	-1.075127464	0.23899519	-1.126898827	-1.126898827	
297.2436	-1.8630027	-0.7912706	0.104748663	0.262680925	0.40737849	-1.2955454	0.49613756	-1.021187296	0.078464883	0.012029136	0.93988445	0.99823252	1.17297229	0.812477787	0.239640748	-0.711668273	-0.445320461	0.499693198	0.760217003	0.616123094	-0.698709482	0.838357495	-0.254265221		
379.2482	-3.999885	-0.2628135	0.06427414	0.14445123	0.6946407	-0.5267	0.75053996	-0.413999972	-0.370550946	-0.042216784	0.720951538	0.95925058	1.049977094	0.070074566	0.790820788	-0.3385773	-5.417812247	-0.32022902	0.00989026	0.01417546	0.620967409	-0.897633997	0.682890207	-0.55027945	
383.2955	-4.1049511	-0.6306651	0.006446744	0.02454702	0.41486919	-0.8839835	0.37015944	-0.816267975	-0.179454314	-0.050160051	0.862201352	0.99823252	1.04039398	0.907692801	0.890486312	-0.187011773	-1.640593384	-0.917837316	0.008211894	0.053119095	0.423902882	-1.238033011	0.441739179	-1.178731001	
249.0051	-1.9631129	-2.461557	0.096377446	0.234849422	0.10683082	-3.2266002	0.11862253	-3.075550051	-0.850384277	-0.172178025	0.419833104	0.787264591	0.741839397	-0.430827936	0.508493702	-0.97393652	-0.438129051	-0.53757346	0.674484993	0.851489828	0.332761519	-1.58776018	0.391760697	-1.351954228	

# Supplemental table 7

		OvsC								MOvsO								MvsC										
ID	m/z	statistic_Ov	pvalue_Ovs	adj_pval_Ov	imputed_	fold_change	log2_fold_c	fold_change	log2_fold_c	imputed_	fold_change	log2_fold_c	fold_change	log2_fold_c	imputed_	fold_change	log2_fold_c	fold_change	log2_fold_c	imputed_	fold_change	log2_fold_c	fold_change	log2_fold_c	imputed_	fold_change	log2_fold_c	statOvsC*st
		sc	dm_OvsC	C	sc	OvsC	uted_OvsC	caled_OvsC	_OvsC	OvsO	dm_MOvsO	vsO	OvsO	MOvsO	O	O	_MOvsO	sc	dm_MvsC	sc	vsC	MvsC	uted_MvsC	caled_MvsC	_MvsC	atMOvsO	atMvsO	
Indoxylsulfuric Acid	212.0026	3.26995577	1.97532396	0.01367516	0.05291694	2.94820047	1.55983463	3.89616608	1.96205517	-5.3113854	-2.5872711	0.00071845	0.25576977	0.18986632	-2.3969441	0.1059176	-3.2389857	-0.9062644	-0.4389892	0.3940197	0.67749755	0.53099033	-0.9132425	0.57305314	-0.8032592	-17.367995		