Supplementary Information for

Identification of psychoactive metabolites from *Cannabis sativa*, its smoke and other phytocannabinoids using machine learning and multivariate methods

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Column1	Positive/Negative/Cannabis Metabolite	AlogP	apol	naAromAtom
	468 Metabolites and positive & negative controls			
P1	Acetorphine	0.8863	75.96775	6
P2	Allylprodine	1.6988	51.05382	6
P3	Anileridine	3.4358	61.1942	12
P4	Benzethidine	3.6685	63.323	12
P5	Betameprodine	0.6922	49.29382	6
P6	Bezitramide	4.6735	81.90138	21
P7	Butyrfentanyl	2.321	63.48579	12
P8	Carfentanil	2.3857	66.84979	12
P9	Clonitazene	5.6538	58.72024	15
P10	Cocaine	0.5592	48.23065	6
P11	Codeine	1.408	49.18865	6
P12	Codoxime	0.6615	57.41303	6
P13	Desomorphine	0.6077	46.62665	6
P14	Dextromoramide	1.8415	69.14138	12
P15	Diampromide	3.327	58.6322	12
P16	Diethylthiambutene	4.5621	49.06265	10
P17	Difenoxin	4.8927	71.7542	18
P18	Ethanol	-0.1076	8.322758	0
P19	Ethylmethylthiambutene	4.3117	45.96907	10
P20	Etonitazene	5.1034	64.1962	15
P21	Etorphine	0.7238	70.31217	6
P22	Fentanyl	2.609	60.3922	12
P23	Heroin	1.5712	57.40624	6
P24	Hydrocodone	1.099	49.18865	6
P25	Hydromorphone	0.848	46.09507	6
P26	Isomethadone	3.1637	56.86541	12
P27	Ketobemidone	1.6366	43.10665	6
P28	Levomoramide	1.8415	69.14138	12
P29	Meperidine	2.2159	43.10665	6
P30	Morphine	1.157	46.09507	6
P31	Morphine–n–oxide (morphine oxide)	0.7519	46.89707	6
P32	Oxycodone	0.6599	49.99065	6
P33	Oxymorphone (dihydrohydroxymorphinone)	0.4089	46.89707	6
P34	Propiram	-0.4678	48.93182	6
P35	Acetylmethadol	2.8914	63.854583	12
P36	AH-7921	2.0966	50.191446	6
P37	Alphameprodine	0.6922	49.293825	6
P38	Alphaprodine	1.3684	46.200239	6
P39	Dextropropoxyphene	3.7425	60.760997	12

P40	Phenadoxone	2.7697	62.520997	12
P41	Phenampromide	0.4425	50.258618	6
P42	Phenazocine	4.0178	58.625411	12
P43	Phenomorphan	2.6783	63.478997	12
P44	Phenoperidine	3.0007	63.322997	12
P45	Piminodine	3.5126	64.28779	12
P46	Piritramide	0.9936	75.392962	12
P47	Proheptazine	1.624	49.293825	6
P48	Properidine	1.9154	46.200239	6
P49	Racemethorphan	1.0902	50.251825	6
P50	Etoxeridine	1.5456	53.991411	6
P51	Remifentanil	0.5019	60.080204	6
P52	Sufentanil	1.9017	65.42779	11
P53	Thebacon	1.1813	54.844239	6
P54	Thebaine	1.7266	50.948653	6
P55	Thiofentanyl	2.1764	58.438618	11
P56	Tilidine	2.5192	47.960239	6
P57	Trimeperidine	1.9013	49.293825	6
P58	U-47700	1.5722	50.191446	6
P59	MT-45	1.9428	65.777376	12
P60	Lysergide	2.1491	55.971825	9
P61	Midomafetamine	1.4423	32.065895	6
P62	Methaqualone	3.847	40.497102	16
P63	Mescaline	1.5245	34.201481	6
E1	N -arachidonoylethanolamine	0.4318	66.095341	0
E2	2-arachidonoyl glycerol.	0.4648	69.026134	0
E3	Dihomo- g -linolenoylethanolamide	-0.9624	67.428927	0
E4	Docosatetraenoylethanolamide	-0.1442	72.282513	0
E5	Arachidonylglyceryl ether	0.0906	69.55772	0
E6	N -arachidonoyl dopamine	2.5303	80.124513	6
E7	N -oleoyl dopamine	-1.0763	77.938099	6
E8	Oleamide	-2.7377	56.919755	0
E9	O -arachidonoylethanolamine	0.6859	66.095341	0
P64	Nicotine	0.0243	29.1351	6
N1	Acetate	-0.9077	7.124379	0
N2	Biotin	-1.2457	35.77469	0
N3	Choline	-1.5741	20.0371	0
N4	Glucose	-2.5134	23.37352	0
N5	Glutamate	-2.3176	18.44234	0
N6	Histidine	-1.0384	21.46514	5
N7	Isoleucine	-1.2501	21.93231	0

N8	Lactate	-1.4837	11.01997	0
N9	Leucine	-0.3183	21.93231	0
N10	Lysine	-2.7491	23.6991	0
N11	Methionine	-0.7303	21.73872	0
N12	Phenylalanine	0.5898	25.87872	6
N13	Pyruvate	-1.1715	9.686379	0
N14	Riboflavin	-0.7277	52.46786	14
N15	Thiamine	-1.4538	40.55748	11
N16	Tryptophan	0.8833	31.16552	9
N17	Tyrosine	0.4498	26.68072	6
N18	Valine	-0.5739	18.83872	0
T	THC	1.8987	58.56779	6
C1	1,1-Dimethylhydrazine	-0.3777	11.054344	0
C2	1,2,3,4-Tetramethylbenzene	3.7748	26.935102	6
C3	1,2-Diethylbenzene	2.1322	26.935102	6
C4	1,3,5-Triazine-2,4,6-triamine	-1.1065	15.880758	6
C5	1,3-Dichlorobenzene	3.4136	17.587172	6
C6	1,4-Diethylbenzene	2.1322	26.935102	6
C7	1-Butanol	-0.9734	14.50993	0
C8	1-Butoxy-2-Propanol	-1.115	24.592688	0
C9	Hexan-1-ol	-1.5494	20.697102	0
C10	Undecan-1-ol	-2.9894	36.165032	0
C11	2,2,5-Trimethylhexane	2.4471	29.17586	0
C12	2,3,4-Trimethylpentane	1.2792	26.082274	0
C13	2,4,6-Trimethylphenol	3.1486	24.643516	6
C14	2,4-Ditert-butylphenol	4.4908	40.111446	6
C15	2,6-Diethylpyrazine	-0.0312	24.281516	6
C16	2,5-Dimethylpyrazine	0.7045	18.094344	6
C17	Butan-2-one	-0.1678	13.176344	0
C18	2-Butoxyethanol	-1.1043	21.499102	0
C19	1-(2-Chlorophenyl)Ethenone	2.3617	21.729551	6
C20	1,3-Dimethyl-2-Vinyl Benzene	3.3541	25.601516	6
C21	2-Ethoxyethanol	-0.2385	15.31193	0
C22	2-Ethyl-1-hexanol	-1.2606	26.884274	0
C23	2-Ethyl Toluene	2.4673	23.841516	6
C24	2-Formyl-Delta-9-Tetrahydrocannabinol	2.3006	62.88979	6
C25	2-Geranyl-5-Hydroxy-3-n-Pentanyl-1,4-Benzoquinone	1.7063	59.36979	0
C26	2-Heptanone	-1.0318	22.457102	0
C27	2-Hydroxy-Acetophenone	1.4299	21.018344	6
C28	2-Isopropyl-3-methyl-pyrazine	1.0445	24.281516	6
C29	2-Methylaziridine	-0.4079	11.047551	0

C30	2-Methylnaphthalene	3.2246	26.02793	10
C31	2-Methyl-1H-imidazole	0.1589	13.240758	5
C32	2-Methyl-Propanamine	0.2837	15.474723	0
C33	2-Methylpentane	0.5918	19.895102	0
C34	2-Nitropropane	0.6002	12.651551	0
C35	2-Phenoxy Ethanol	1.4016	22.35193	6
C36	3-(1-Methyl Ethyl)-Phenol Carbamate	2.2417	32.065895	6
C37	3-(3-Hydroxy Phenyl)-2-Propenoic acid, methyl ester	1.9065	26.67393	6
C38	3,4,5,6-Tetrahydro-7-hydroxy-a,a-2-trimethyl-9-n-propyl-2,6-methano-2H-1-Benzoxocin-5-methanol	1.7344	54.516204	6
C39	3,4,5-Trimethylphenol	3.0212	24.643516	6
C40	3,4,5-Trimethylhex-1-ene	1.5472	27.842274	0
C41	3-Ethyl Toulene	2.4673	23.841516	6
C42	3-Ethyl-O-xylene	2.9535	26.935102	6
C43	3-Hydroxy-Delta-4,5-Cannabichromene	1.87	59.36979	6
C44	3-Isopropyl Benzaldehyde	2.0065	26.403516	6
C45	3-Methyl Acetophenone	2.0561	23.30993	6
C46	3-Methyl Heptane	-0.3724	26.082274	0
C47	3-methylcyclopent-2-en-1-one	0.6409	16.696344	0
C48	3-Methyl Pentane	-0.34	19.895102	0
C49	3-Methyl-5-(1-Methyl Ethyl)-Phenol Methyl Carbamate	2.7279	35.159481	6
C50	3-Pentanol	-0.9841	17.603516	0
C51	4,5-Dihydroxy-2,3,6-Trimethoxy-9,10-Dihydrophenanthrene	3.0872	45.932274	12
C52	4,7-Dimethoxyphenanthrene-1,2,5-triol	3.194	41.505102	14
C53	4-Acetoxy Cannabichromene	3.2217	65.025376	6
C54	4-Acetoxy-2-geranyl-5-hydroxy-3-n-pentylphenol	3.3654	66.358962	6
C55	4-Carene	1.4126	28.268688	0
C56	4-Ethoxy-3-anisaldehyde	2.0618	28.00752	6
C57	4-Hydroxy-2,3,6,7-tetramethoxy-9,10dihydrophenanthrene	3.2108	49.02586	12
C58	4-Methoxy-Couramin	2.3806	25.340344	10
C59	4-Methyl Decane	-0.6928	35.363032	0
C60	4-Methylpyrimidine	0.56	15.000758	6
C61	4-Methyl Guaiacol	2.1598	22.35193	6
C62	4-Methyl Phenyl ethyl amine	1.6777	25.608309	6
C63	4-Pyridinamine	0.0602	15.000758	6
C64	4-Terpinyl Delta-9-tetrahydrocannabinolate	3.2437	90.200478	6
C65	4-Terpenyl Cannabinolate	4.4531	87.533306	12

C66	5-Acetoxy-6-Geranyl-3n -Pentyl-1,4-Benzoquinone	1.7414	65.025376	0
C67	5-Acetyl-4-Hydroxycannabigerol	3.3654	66.358962	6
C68	5-Ethenyl-2-Methylpyridine	1.6946	21.181137	6
C69	5-Methoxy Cannabigerolic acid	3.335	66.358962	6
C70	5-Methyl-4-Pentyl-Biphenyl-2,2,6-Triol	2.3811	48.755446	12
C71	5-Methylindane	1.8414	25.601516	6
C72	5-Octanolide	-1.2074	25.019102	0
C73	6,7-cis -Epoxycannabigerol	1.3057	60.97379	6
C74	6,7-cis-Epoxycannabigerolic acid	1.3057	60.97379	6
C75	6a-R-Cannabichromanone B	0.5919	59.640204	6
C76	6a-R-Cannabichromanone C	0.3617	56.546618	6
C77	6-Metiltetrapterol A	5.5002	66.575032	18
C78	6-Prenylapigenin	5.0943	51.212274	16
C79	7,8-Dehydro-10-O-ethylcannabitriol	1.6178	65.025376	6
C80	7,8-Dihydrocannabinol	2.3465	57.234204	6
C81	7-Hydroxy Cannabichromane	2.4105	60.703376	6
C82	7-Hydroxy cannabinol	3.0955	56.702618	12
C83	7-Methoxy Cannabispiranone	1.2986	43.90186	6
C84	7-R-Cannabicoumarononic acid	1.2904	61.400204	9
C85	8,9-Dihydroxy-delta-6a-tetrahydrocannabinol	0.8747	60.17179	6
C86	8-Hydroxy cannabinolic acid	2.5818	60.066618	12
C87	8-Hydroxyl cannabinol	3.0955	56.702618	12
C88	8a-Hydroxy-Delta-9-tetrahydrocannbinol	1.3256	59.36979	6
C89	8-oxo-Delta-9-tetrahydrocannbinol	1.3517	58.036204	6
C90	9,10-Anhydrocannabitriol	1.5756	58.036204	6
C91	9,10-Dihydro-2,3,5,6-Tetramethoxyphenanthrene-1,4-dione	0.7574	48.494274	6
C92	9 β ,10 β -Epoxyhexahydrocannabinol	1.3518	59.36979	6
C93	10 α -Hydroxy-Delta- 9,11 -Hexahydrocannabinol	1.0823	59.36979	6
C94	10-Ethoxy-9-hydroxy-delta-6a-Tetrahydrocannabinol	1.468	66.358962	6
C95	10-Hydroxy-9-oxo-Delta-8-Tetrahydrocannabinol	1.3564	59.36979	6
C96	10-O-Ethyl bis-nor Cannabitriol	1.5272	63.265376	6
C97	10-Oxo-delta-6a-Tetrahydrocannabinol (OTHC)	1.5291	58.036204	6
C98	11-Acetoxy-Delta-8-Tetrahydrocannbinoic acid	1.0904	68.389376	6
C99	11-Acetoxy-Delta- 9 -Tetrahydrocannabinolic acid A	0.8008	68.389376	6
C100	Abnormal Cannabigerol	3.5977	59.901376	6
C101	Acetaldehyde	-0.1825	6.989172	0
C102	Acetamide	-0.6249	8.755965	0
C103	Acetic acid	-0.2299	7.791172	0

C104	Acetone	-0.244	10.082758	0
C105	Acetyl abnormal hydrocannabigeroquinol	3.3654	66.358962	6
C106	Acetyl cannabigeroquinol	1.7414	65.025376	0
C107	Acrolein	0.4084	8.749172	0
C108	Acetophenone	1.5699	20.216344	6
C109	Alloaromadendrene	2.1549	42.403032	0
C110	Alpha-Bisabolol	2.7502	44.538618	0
C111	α-Bulnescene	2.3639	42.403032	0
C112	α-Cadinene	2.407	42.403032	0
C113	a-Cadinyl Delta-9-tetrahydrocannabinolate	3.6129	104.334822	6
C114	Alpha-Cannabispiranol	0.2825	42.14186	6
C115	Alpha-Cedrene	2.4838	42.403032	0
C116	Alpha-Cis-Bergamotene	2.7484	42.403032	0
C117	Alpha- Copaene	1.7635	42.403032	0
C118	Alpha-Cubebene	1.6446	42.403032	0
C119	Alpha-Eudesmol	1.5816	44.538618	0
C120	Alpha-Guaiene	2.3416	42.403032	0
C121	Alpha-Gurjunene	2.5253	42.403032	0
C122	Alpha-Humulene	4.1708	42.403032	0
C123	Alpha-Ionol	2.1533	38.351446	0
C124	Alpa-Linilenic acid	-0.0979	53.28779	0
C125	Alpha-Longipinene	1.8331	42.403032	0
C126	Alpha-Methyl-Cinnamaldehyde	2.396	25.06993	6
C127	Alpha-Phellandrene	1.7112	28.268688	0
C128	Alpha-Pinene	1.5162	28.268688	0
C129	Alpha-Selinene	2.6017	42.403032	0
C130	Alpha-Terpinyl Delta-9-tetrahydrocannabinolate	3.2437	90.200478	6
C131	Alpha-Terpinene	1.8841	28.268688	0
C132	Alpha-Terpineol	1.1223	30.404274	0
C133	Alpha-Thujene	1.6288	28.268688	0
C134	Alpha-Trans-Bergamotene	2.7484	42.403032	0
C135	Alpha-Ylangene	1.7635	42.403032	0
C136	Amorfrutin-3	3.4803	56.973032	12
C137	Amorfrutin-4	5.6333	67.21179	12
C138	Amorfrutin-A	4.6521	56.171032	12
C139	Amorfrutin-B	5.8843	70.305376	12
C140	Anethole	2.6925	26.403516	6
C141	Anhydrocannabimovone	1.2081	58.036204	6
C142	Anhydrocannabisativine	-2.2091	66.535341	0
C143	Anthopogochromenic acid	4.2052	49.557446	6
C144	Anthopogocyclolic acid	3.0253	49.557446	6

C145	Apigenin	3.3727	37.07793	16
C146	Arachidin-3	4.1537	49.18186	12
C147	Araphyn-1	4.2937	48.37986	12
C148	Araphyn-3	2.7985	52.119446	12
C149	Araphyn-4	2.9385	51.317446	12
C150	Aristolene	1.6486	42.403032	0
C151	Aromadendrene	2.1549	42.403032	0
C152	Benzaldehyde	1.5894	17.122758	6
C153	Benzonitrile	1.7089	16.753965	6
C154	Benzophenone	3.2342	30.34993	12
C155	Benzphentamine	3.5388	45.022653	12
C156	Benzyl acetate	1.6046	24.11193	6
C157	Benzyl Alcohol	1.2255	18.456344	6
C158	Benzyl formate	1.5258	21.018344	6
C159	Benzyl Nitrile	1.7437	19.847551	6
C160	Beta-Cannabispiranol	0.2825	42.14186	6
C161	Beta-Caryophyllene oxide	1.9144	43.205032	0
C162	Beta-Caryophyllene	3.2289	42.403032	0
C163	Beta-Cedrene	1.8851	42.403032	0
C164	Beta-Elemene	3.2309	42.403032	0
C165	Beta-Eudesmol	0.6981	44.538618	0
C166	Beta-fenchol (Beta-Fenchyl Alcohol)	1.0088	30.404274	0
C167	Beta-Fenchyl-Delta-9-tetrahydrocannabinolate	2.4863	87.106892	6
C168	Betahistine	0.5837	24.281516	6
C169	Beta-Irone	2.1914	40.111446	0
C170	Beta-phellandrene	1.5645	28.268688	0
C171	Beta-Pinene	1.3695	28.268688	0
C172	Beta-Selinene	1.7182	42.403032	0
C173	β-sitosteryl-3-O-b-D-glucopyranoside-2'-O-palmitate	-3.7356	155.38537	0
C174	Betazole	-0.4358	18.101137	5
C175	Bis-nor-cannabichromanone	1.9998	52.651032	6
C176	Bis-nor-cannabielsoic acid B	2.0669	56.546618	6
C177	Bis-nor-cannabielsoin	2.4532	53.182618	6
C178	Bis-nor-cannabitriol	1.2123	57.078204	6
C179	Borneol	0.9432	30.404274	0
C180	Bornyl Delta-9-tetrahydrocannabinolate	3.4159	104.334822	6
C181	Butane	-0.4734	13.70793	0
C182	Butyl formate	-0.6731	17.07193	0
C183	Gamma-Cadinyl Cannabigerolate	4.5973	108.761994	6
C184	Calarene	2.3854	42.403032	0
C185	Camphene	1.3875	28.268688	0

C186	Cannabichromanone (CBCF)	0.8811	57.078204	6
C187	Cannabichromaonone D	2.0924	58.036204	6
C188	Cannabichromene (CBC)	3.3266	58.56779	6
C189	Cannabichromenic acid (CBCA)	2.8129	61.93179	6
C190	Cannabichromevarin (CBCV)	3.9026	52.380618	6
C191	Cannabichromevarinic acid (CBCVA)	3.3889	55.744618	6
C192	Cannabicitran	1.64	58.56779	6
C193	Cannabicoumaronone	1.5493	58.036204	9
C194	Cannabicyclol (CBL)	2.0193	58.56779	6
C195	Cannabicyclolic acid (CBLA)	1.7604	61.93179	6
C196	Cannabicyclovarin (CBLV)	2.7227	52.380618	6
C197	Cannabidiol (CBD)	2.5816	58.56779	6
C198	Cannabidiolic acid (CBDA)	2.3227	61.93179	6
C199	Cannabidiol monomethylether (CBDM)	2.8326	61.66138	6
C200	Cannabidiorcol (CBD-C1)	3.9739	46.193446	6
C201	Cannabidivarin (CBDV)	3.1576	52.380618	6
C202	Cannabidivarinic acid (CBDVA)	2.8987	55.744618	6
C203	Cannabielsoic acid B (CBEA-B)	1.4909	62.73379	6
C204	Cannabielsoic acid A (CBEA-A)	1.4909	62.73379	6
C205	Cannabielsoin (CBE)	1.7498	59.36979	6
C206	Cannabiflavin B	5.3327	55.10786	16
C207	Cannabifuran (CBF)	3.0632	55.900618	13
C208	Cannabigerol (CBG)	3.5977	59.901376	6
C209	Cannabigerolic acid monomethylether (CBGAM)	3.335	66.358962	6
C210	Cannabigerolic acid (CBGA)	3.084	63.265376	6
C211	Cannabigerol monomethylether (CBGM)	3.8487	62.994962	6
C212	Cannabigeroquinone	2.1627	58.56779	0
C213	Cannabigerovarin (CBGV)	4.0463	53.714204	6
C214	Cannabigerovarinic acid (CBGVA)	3.66	57.078204	6
C215	Cannabiglendol	1.6004	54.516204	6
C216	Cannabimovone	0.8871	57.078204	6
C217	Cannabinerol	3.5977	59.901376	6
C218	Cannabinerolic acid	3.084	63.265376	6
C219	Cannabinodiol (CBND)	3.5192	55.900618	12
C220	Cannabinodivarin (CBVD)	4.0952	49.713446	12
C221	Cannabinol methylether (CBNM)	3.4865	58.994204	12
C222	Cannabinol (CBN)	3.2355	55.900618	12
C223	Cannabinol-C2 (CBN-C2)	4.2927	46.61986	12
C224	Cannabinol-C4 (CBN-C4)	3.5235	52.807032	12
C225	Cannabinolic acid (CBNA)	2.7218	59.264618	12
C226	Cannabiorcol (CBN-C1)	4.5004	43.526274	12

C227	Cannabiorcicchromene	4.7189	46.193446	6
C228	Cannabiorcicchromenic acid	4.3326	49.557446	6
C229	Cannabiorcicitran	3.1597	46.193446	6
C230	Cannabiorcicyclol	3.539	46.193446	6
C231	Cannabiorcicyclolic acid	3.0253	49.557446	6
C232	Cannabioxepane	3.2899	53.233446	13
C233	Cannabiripsol (CBR)	0.4579	61.505376	6
C234	Cannabissativine	-3.3243	68.670927	0
C235	Cannabisin-A	5.737	88.45979	28
C236	Cannabisin-B	5.0918	89.793376	24
C237	Cannabisin-C	5.3428	92.886962	24
C238	Cannabisin-D	5.5938	95.980548	24
C239	Cannabispirone	1.175	40.808274	6
C240	Cannabitriol (CBT)	0.8091	60.17179	6
C241	Cannabitriolvarin (CBTV)	1.5251	53.182618	6
C242	Cannabivarin (CBV)	3.8115	49.713446	12
C243	Cannflavin A	6.4375	69.242204	16
C244	Cannflavin B	5.2053	55.10786	16
C245	Cannflavin C	6.4375	69.242204	16
C246	Carbofuran	2.5928	34.627895	6
C247	Carmagerol	0.9936	62.838962	6
C248	Carvacrol	2.5933	27.737102	6
C249	Carvone	1.5954	27.737102	0
C250	CBDA-THC ester	4.1699	119.967994	12
C251	Cedryl acetate	1.7364	50.194204	0
C252	Cetyl Alcohol	-4.4294	51.632962	0
C253	Chiricanine B	3.9259	52.275446	12
C254	Chlorocannabiorcicchromenic acid	5.1244	51.070653	6
C255	Chrysoeriol	3.4837	40.973516	16
C256	cis-2-Pinanol	0.8417	30.404274	0
C257	cis-Beta-Farnesene	4.3258	42.403032	0
C258	cis-Gamma-Bisabolene	3.953	42.403032	0
C259	cis-Ocimene	3.2403	28.268688	0
C260	cis-Sabinene Hydrate	0.9414	29.602274	0
C261	Citronellyl acetate	1.8432	37.393446	0
C262	Citronellolformate	1.7644	34.29986	0
C263	Compound-2	-0.1732	60.97379	6
C264	Compound-3	0.6173	59.640204	6
C265	compound-4	2.0924	58.036204	6
C266	Confluentin	5.9511	60.32779	6
C267	Cumene	2.2471	23.841516	6

C268	Cuminaldehyde	2.0065	26.403516	6
C269	Daurichromenic acid	5.5648	63.69179	6
C270	Delta-9-tetrahydrocannabiorcolic acid (THCA-C1)	3.0321	49.557446	6
C271	Decanal	-2.1223	31.73786	0
C272	Decarboxyamorfrutin A	5.1658	52.807032	12
C273	Decarboxyamorfrutin B	6.398	66.941376	12
C274	Dehydrocannabifuran (DCBF)	3.7716	54.567032	13
C275	Delta-3-Carene	2.1434	28.268688	0
C276	Delta-7-cis-Isotetrahydrocannabivarin	3.0263	52.380618	6
C277	Delta-7-trans-Isotetrahydrocannabinol	2.4503	58.56779	6
C278	Delta-8-tetrahydrocannabinol (Δ8-THC)	2.0609	58.56779	6
C279	Delta-8-tetrahydrocannabinolic acid (Δ8-THCA)	1.6398	61.93179	6
C280	Delta-9-cis-tetrahydrocannabivarin	2.6021	52.380618	6
C281	Delta-9-nor-tetrahydrocannbinolic acid	2.4429	60.598204	6
C282	Delta-9-nor-tetrahydrocannbinol	2.7018	57.234204	6
C283	Delta-9-Tetrahydrocannabinol-C4	2.1867	55.4742	6
C284	Delta-9-tetrahydrocannabiorcol (THC-C1)	3.291	46.193446	6
C285	Delta-9-tetrahydrocannabinolic acid A (THCA-A)	1.5124	61.93179	6
C286	Delta-9-tetrahydrocannabinolic acid B (THCA-B)	1.5124	61.93179	6
C287	Delta-9-tetrahydrocannabinolic acid-C4 (THCA-C4)	1.8004	58.838204	6
C288	Delta-Cadinene	2.2115	42.403032	0
C289	Demethylamorfrutin A	4.4011	53.077446	12
C290	Demethyldecarboxyamorfrutin A	4.7874	49.713446	12
C291	Deprenyl O-methyl cannbigerolic acid	2.1028	52.224618	6
C292	Desmodianone A	5.5913	69.242204	12
C293	Desmodianone C	5.735	70.57579	12
C294	Desmodianone D	4.4114	69.242204	12
C295	Desmodianone E	4.1634	69.242204	12
C296	Diacetone alcohol	-0.0853	20.16552	0
C297	Dibutyl phthalate	0.3286	46.03745	6
C298	Diethyl Phthalate	2.0602	33.6631	6
C299	Dimethylbenzylcarbinyl acetate	2.5083	33.39269	6
C300	Dimethylsulfone	-0.2206	12.02476	0
C301	Dimethylsulfide	0.7952	10.42076	0
C302	Dodecane	-2.7774	38.45662	0
C303	Dothiepin Sulfoxide	2.8277	52.24465	12
C304	Durene	3.7748	26.9351	6
C305	Dyclocaine	0.2744	52.38741	6
C306	epi-Bornyl Delta-9-tetrahydrocannabinolate	3.0646	90.20048	6
C307	Estragole	2.8139	26.40352	6
C308	Ethylacetate	0.2715	13.97834	0

C309	Ethylenediamine	-1.4766	11.05434	0
C310	Ethylene oxide	-0.1309	6.989172	0
C311	Ethylenimine	-0.3972	7.953965	0
C312	Eudesmyl-Cannabigerolate	4.9875	105.6684	6
C313	Eugenol	2.6739	27.20552	6
C314	Eugenyl acetate	2.709	32.8611	6
C315	Fenchone	1.2557	29.07069	0
C316	Fenchyl Alcohol	1.0088	30.40427	0
C317	Ferruginene A	2.9177	61.93179	6
C318	Ferruginene B	3.4229	61.93179	6
C319	Ferruginene C	3.7495	61.12979	6
C320	Formic acid	-0.3087	4.697586	0
C321	Furfural	1.1422	13.07117	5
C322	Furfurylmethylamphetamine	3.0916	40.97107	11
C323	Gamma-curcumene	3.512	42.40303	0
C324	Gamma-eudesmol	1.2945	44.53862	0
C325	Gamma-Gurjunene	2.6467	42.40303	0
C326	Gamma-Hexalactone	-0.6314	18.83193	0
C327	Gamma-Muurolene	2.2603	42.40303	0
C328	Gamma-Terpinene	2.4017	28.26869	0
C329	Glepidotin C	3.6156	50.51545	12
C330	Globulol	1.2587	44.53862	0
C331	Grossamide	5.7825	95.98055	24
C332	Guajol	1.6736	19.25834	6
C333	Heli-Cannabigenol	6.0196	63.84779	12
C334	Heptanal	-1.2583	22.4571	0
C335	Hexadecane	-3.9294	50.83096	0
C336	Hexahydrocannabinol	1.4701	59.90138	6
C337	Hexanal	-0.9703	19.36352	0
C338	Hexanoic acid, methyl ester	-0.7667	23.2591	0
C339	Hexanoic acid, propyl ester	-1.0941	29.44627	0
C340	Hexestrol	2.5264	47.95345	12
C341	Hordenine	2.0192	29.50389	6
C342	Hydroxy Heli-Cannabigerol	5.8796	64.64979	12
C343	Ipsdienol	2.3273	29.07069	0
C344	Isoamyl alcohol	-0.1638	17.60352	0
C345	Isobornyl acetate	1.3223	36.05986	0
C346	Isobornyl thiocyanoacetate	1.8361	41.15307	0
C347	Isobutane	1.0124	13.70793	0
C348	Isobutyraldehyde	0.5419	13.17634	0
C349	Isobutyrophenone	2.2943	26.40352	6

C350	Isocannabitrol	0.747	63.26538	6
C351	Isocyanatomethane	-0.8688	7.422379	0
C352	Isodurene	3.7748	26.9351	6
C353	Isoeugenol	2.4251	27.20552	6
C354	Isolimonene	2.232	28.26869	0
C355	Isoprene	1.8614	14.13434	0
C356	Isoquinoline	1.7687	21.60755	10
C357	Kaempferol	3.1053	37.87993	16
C358	Limonene oxide	0.4229	29.87269	0
C359	Limonene	2.1424	28.26869	0
C360	Linalool	2.4692	30.40427	0
C361	Linalyl acetate	2.8483	36.05986	0
C362	Linoleic acid	-0.9485	54.62138	0
C363	Longifolene	1.8468	42.40303	0
C364	Luteolin	3.2327	37.87993	16
C365	Machaeridiol A	5.0453	62.5142	12
C366	Machaeridiol B	4.9053	63.3162	12
C367	Machaeridiol C	5.1725	61.98262	15
C368	Machaeridiol D	3.7233	62.78462	15
C369	m-Cymene	2.7333	26.9351	6
C370	Methacrolein	0.9615	11.84276	0
C371	Methacrylic anhydride	2.0932	23.15393	0
C372	Methyl acetate	0.0211	10.88476	0
C373	Methyl acetylsalicylate	1.5898	27.47593	6
C374	Methyl anthranilate	1.0755	22.78514	6
C375	Methyl Benzoate	1.6947	21.01834	6
C376	Methyl carbamate	0.0183	9.557965	0
C377	Methyl heptadienone	1.6634	22.88352	0
C378	Methyl heptanoate	-1.0547	26.35269	0
C379	Methyl Hydrazine	-0.9136	7.960758	0
C380	Methyl isoeugenol	2.6761	30.2991	6
C381	Methyl Salicylate	1.5547	21.82034	6
C382	Methyl valerate	-0.4787	20.16552	0
C383	Methylene Chloride	1.0729	7.453586	0
C384	Methylen-bis-Delta-9-tetrahydrocannabinol	4.1968	118.8956	12
C385	Methylisohexenyl ketone	1.5927	24.2171	0
C386	m-Tert-Butyl Phenol	3.0904	27.7371	6
C387	Myrcene	3.0936	28.26869	0
C388	Nerol	2.3397	30.40427	0
C389	Nerolidol	3.7014	44.53862	0
C390	Nitrobenzene	2.4212	16.59797	6

C391	Nonanal	-1.8343	28.64427	0
C392	Nonane	-1.9134	29.17586	0
C393	nor-Cannabidiol	2.8696	55.4742	6
C394	nor-Cannabinol	3.5235	52.80703	12
C395	nor-Cannabivarin	4.2927	46.61986	12
C396	N-p-Coumaroyltyramine	3.0619	44.76148	12
C397	N-trans-feruloyltyramine	3.1729	48.65707	12
C398	Octanal	-1.5463	25.55069	0
C399	o-Cymene	2.7333	26.9351	6
C400	o-Dimethyl Hydroquinone	1.9246	22.35193	6
C401	O-Guaiacol	1.801	19.25834	6
C402	Oleic acid	-2.3427	55.95496	0
C403	O-Methyl Cannabigerol	3.8487	62.99496	6
C404	O-Methyl Acetophenone	2.0561	23.30993	6
C405	O-Pentyl-cannabidiol	1.9292	74.03572	6
C406	O-Pentyl-Delta-9-tetrahydrocannbinol	1.7614	75.79572	6
C407	O-Propyl-cannabidiol	2.5052	67.84855	6
C408	O-Propyl-Delta-9-tetrahydrocannbinol	2.3374	69.60855	6
C409	Orientin	0.8412	59.11786	16
C410	O-Xylene	2.8024	20.74793	6
C411	P-Acetanisole	1.6809	24.11193	6
C412	P-Aminotoluene	1.697	19.42114	6
C413	P-Cymene	2.7333	26.9351	6
C414	Pentadecane	-3.6414	47.73738	0
C415	Pentamethylbenzene	4.261	30.02869	6
C416	Pentanal	-0.6823	16.26993	0
C417	Perillaldehyde	1.308	27.7371	0
C418	Perrottetinene	4.448	62.5142	12
C419	Perrottetinenic acid	4.1891	65.8782	12
C420	P-ethyl Toulene	2.4673	23.84152	6
C421	Phenol	1.69	15.36276	6
C422	Phenylethyl alcohol	1.4811	21.54993	6
C423	Piperidine	-1.2612	17.23472	0
C424	Piperonal	1.6123	20.48676	6
C425	P-Methyl Acetophenone	2.0561	23.30993	6
C426	Propanal	-0.1063	10.08276	0
C427	Propofol	2.5242	33.92427	6
C428	Propanoic acid,anhydride	-0.0424	19.63393	0
C429	Propylamine	-0.975	12.38114	0
C430	Propylene Glycol	-0.9081	12.21834	0
C431	P-Tert-Butylphenol	3.0904	27.7371	6

C432	P-Xylene	2.8024	20.74793	6
C433	Quercetin	2.9653	38.68193	16
C434	rac-6'-Epoxycannbigerol	2.568	60.70338	6
C435	rac-6'-Epoxycannbigerolic acid	2.0543	64.06738	6
C436	Radulanin A	4.4331	48.37986	12
C437	Radulanin H	4.0468	51.74386	12
C438	Radulanin I	3.5328	48.37986	12
C439	Radulanin J	3.5137	47.04627	12
C440	Radulanin K	2.749	47.31669	12
C441	Radulanin L	4.0383	49.18186	12
C442	Rhododaurichromanic A	4.3849	63.69179	6
C443	Roughanic acid	0.4781	47.10062	0
C444	Sabinene	1.0301	28.26869	0
C445	Salicyladehyde	1.4494	17.92476	6
C446	Sativene	1.7772	42.40303	0
C447	Sesquicannabigerol	4.8299	74.03572	6
C448	Stearidonic acid	1.2963	51.9542	0
C449	Styrene	2.3817	19.41434	6
C450	Tert-butyl alcohol	0.5733	14.50993	0
C451	Terpinolene	2.7208	28.26869	0
C452	tert-butyl-benzene	3.2304	26.9351	6
C453	Tetrahydrocannabinol epoxide	1.3518	59.36979	6
C454	Tetrahydrozoline	0.7261	35.74869	6
C455	Thymol	2.5933	27.7371	6
C456	Toluene	2.3162	17.65434	6
C457	Trans-alpha-farnesene	4.4725	42.40303	0
C458	Trans-Archidin-1	4.0137	49.98386	12
C459	Trans-Archidin-2	4.6474	50.51545	12
C460	Trans-gamma-bisabolene	3.953	42.40303	0
C461	Trans-ocimene	3.2403	28.26869	0
C462	Tridecane	-3.0654	41.5502	0
C463	Tyramine	1.0515	23.31672	6
C464	Undecane	-2.4894	35.36303	0
C465	Valencene	2.676	42.40303	0
C466	Verbenone	1.2447	27.7371	0
C467	Vitexin	0.9812	58.31586	16
C468	N-trans-caffeoyltyramine	2.9219	45.56348	12

	Metabolites from Machine Learning Methods (330) (used for MDS using CDK)			
		AlogP	apol	naAromAtom
C2	1,2,3,4-tetramethylbenzene	3.7748	26.935102	6
C3	1,2-diethylbenzene	2.1322	26.935102	6
C5	1,3-dichlorobenzene	3.4136	17.587172	6
C6	1,4-diethylbenzene	2.1322	26.935102	6
C11	2,2,5-trimethylhexane	2.4471	29.17586	0
C13	2,4,6-trimethylphenol	3.1486	24.643516	6
C14	2,4-ditert-butylphenol	4.4908	40.111446	6
C15	2,6-diethylpyrazine	-0.0312	24.281516	6
C19	1-(2-chlorophenyl)ethenone	2.3617	21.729551	6
C20	1,3-dimethyl-2-vinyl-benzene	3.3541	25.601516	6
C23	2-Ethyl Toluene	2.4673	23.841516	6
C24	2-Formyl-Delta-9-Tetrahydrocannabinol	2.3006	62.88979	6
C25	2-Geranyl-5-Hydroxy-3-n-Pentanyl-1,4-Benzoquinone	1.7063	59.36979	0
C27	2-Hydroxy-Acetophenone	1.4299	21.018344	6
C28	2-isopropyl-3-methyl-pyrazine	1.0445	24.281516	6
C30	2-methylnaphthalene	3.2246	26.02793	10
C35	2-Phenoxy Ethanol	1.4016	22.35193	6
C36	3-(1-Methyl Ethyl)-Phenol Carbamate	2.2417	32.065895	6
C37	3-(3-Hydroxy Phenyl)-2-Propenoic acid, methyl ester	1.9065	26.67393	6
C38	3,4,5,6-tetrahydro-7-hydroxy-a,a-2-trimethyl-9-n-propyl-2,6-methano-2H-1-Benzoxocin-5-methanol	1.7344	54.516204	6
C39	3,4,5-trimethylphenol	3.0212	24.643516	6
C40	3,4,5-trimethylhex-1-ene	1.5472	27.842274	0
C41	3-Ethyl Toulene	2.4673	23.841516	6
C42	3-Ethyl-O-xylene	2.9535	26.935102	6
C43	3-Hydroxy-Delta-4,5-Cannabichromene	1.87	59.36979	6
C44	3-Isopropyl Benzaldehyde	2.0065	26.403516	6
C45	3-Methyl Acetophenone	2.0561	23.30993	6
C46	3-Methyl Heptane	-0.3724	26.082274	0
C49	3-Methyl-5-(1-Methyl Ethyl)-Phenol Methyl Carbamate	2.7279	35.159481	6
C51	4,5-Dihydroxy-2,3,6-Trimethoxy-9,10-Dihydrophenanthrene	3.0872	45.932274	12
C52	4,7-dimethoxyphenanthrene-1,2,5-triol	3.194	41.505102	14
C53	4-Acetoxy Cannabichromene	3.2217	65.025376	6
C54	4-Acetoxy-2-geranyl-5-hydroxy-3-n-pentylphenol	3.3654	66.358962	6
C55	4-Carene	1.4126	28.268688	0

C56	4-Ethoxy-3-anisaldehyde	2.0618	28.00752	6
C57	4-hydroxy-2,3,6,7-tetramethoxy-9,10dihydrophenanthrene	3.2108	49.02586	12
C58	4-Methoxy-Couramin	2.3806	25.340344	10
C59	4-Methyl Decane	-0.6928	35.363032	0
C61	4-Methyl Guaiacol	2.1598	22.35193	6
C62	4-Methyl Phenyl ethyl amine	1.6777	25.608309	6
C64	4-Terpinyl Delta-9-tetrahydrocannabinolate	3.2437	90.200478	6
C65	4-Terpenyl Cannabinolate	4.4531	87.533306	12
C66	5-acetoxy-6-geranyl-3n -pentyl-1,4-benzoquinone	1.7414	65.025376	0
C67	5-Acetyl-4-hydroxycannabigerol	3.3654	66.358962	6
C68	5-ethenyl-2-methylpyridine	1.6946	21.181137	6
C70	5-Methyl-4-Pentyl-Biphenyl-2,2,6-Triol	2.3811	48.755446	12
C71	5-methylindane	1.8414	25.601516	6
C72	5-Octanolide	-1.2074	25.019102	0
C75	6a-R-Cannabichromanone B	0.5919	59.640204	6
C76	6a-R-Cannabichromanone C	0.3617	56.546618	6
C79	7,8-Dehydro-10-O-ethylcannabitriol	1.6178	65.025376	6
C80	7,8-dihydrocannabinol	2.3465	57.234204	6
C81	7-Hydroxy Cannabichromane	2.4105	60.703376	6
C82	7-hydroxy cannabinol	3.0955	56.702618	12
C83	7-Methoxy Cannabispiranone	1.2986	43.90186	6
C84	7-R-Cannabicoumarononic acid	1.2904	61.400204	9
C85	8,9-Dihydroxy-delta-6a-tetrahydrocannabinol	0.8747	60.17179	6
C87	8-hydroxyl cannabinol	3.0955	56.702618	12
C88	8a-Hydroxy-Delta-9-tetrahydrocannbinol	1.3256	59.36979	6
C89	8-oxo-Delta-9-tetrahydrocannbinol	1.3517	58.036204	6
C90	9,10-Anhydrocannabitriol	1.5756	58.036204	6
C91	9,10-dihydro-2,3,5,6-tetramethoxyphenanthrene-1,4-dione	0.7574	48.494274	6
C92	9 β ,10 β -Epoxyhexahydrocannabinol	1.3518	59.36979	6
C93	10 α -Hydroxy-Delta- 9,11 -hexahydrocannabinol	1.0823	59.36979	6
C94	10-Ethoxy-9-hydroxy-delta-6a-tetrahydrocannabinol	1.468	66.358962	6
C95	10-Hydroxy-9-oxo-Delta-8-tetrahydrocannabinol	1.3564	59.36979	6
C96	10-O-Ethyl bis-nor cannabitriol	1.5272	63.265376	6
C97	10-Oxo-delta-6a-tetrahydrocannabinol (OTHC)	1.5291	58.036204	6
C98	11-Acetoxy-Delta-8-tetrahydrocannbinoic acid	1.0904	68.389376	6
C99	11-Acetoxy-Delta- 9 -tetrahydrocannabinolic acid A	0.8008	68.389376	6
C100	abnormal cannabigerol	3.5977	59.901376	6
C105	acetyl abnormal hydrocannabigeroquinol	3.3654	66.358962	6

C106	Acetyl cannabigeroquinol	1.7414	65.025376	0
C108	Acetophenone	1.5699	20.216344	6
C109	Alloaromadendrene	2.1549	42.403032	0
C110	Alpha-Bisabolol	2.7502	44.538618	0
C111	α-bulnescene	2.3639	42.403032	0
C112	α-cadinene	2.407	42.403032	0
C113	a-Cadinyl Delta-9-tetrahydrocannabinolate	3.6129	104.334822	6
C114	Alpha-Cannabispiranol	0.2825	42.14186	6
C115	Alpha-Cedrene	2.4838	42.403032	0
C116	Alpha-Cis-Bergamotene	2.7484	42.403032	0
C117	Alpha- Copaene	1.7635	42.403032	0
C118	Alpha-Cubebene	1.6446	42.403032	0
C119	Alpha-Eudesmol	1.5816	44.538618	0
C120	Alpha-Guaiene	2.3416	42.403032	0
C121	Alpha-Gurjunene	2.5253	42.403032	0
C122	Alpha-Humulene	4.1708	42.403032	0
C123	Alpha-Ionol	2.1533	38.351446	0
C124	Alpa-Linilenic acid	-0.0979	53.28779	0
C125	Alpha-Longipinene	1.8331	42.403032	0
C126	Alpha-Methyl-Cinnamaldehyde	2.396	25.06993	6
C127	Alpha-Phellandrene	1.7112	28.268688	0
C128	Alpha-Pinene	1.5162	28.268688	0
C129	Alpha-Selinene	2.6017	42.403032	0
C130	Alpha-Terpinyl Delta-9-tetrahydrocannabinolate	3.2437	90.200478	6
C131	Alpha-Terpinene	1.8841	28.268688	0
C132	Alpha-Terpineol	1.1223	30.404274	0
C133	Alpha-Thujene	1.6288	28.268688	0
C134	alpha-trans-bergamotene	2.7484	42.403032	0
C135	Alpha-Ylangene	1.7635	42.403032	0
C139	Amorfrutin-B	5.8843	70.305376	12
C140	Anethole	2.6925	26.403516	6
C141	Anhydrocannabimovone	1.2081	58.036204	6
C142	anhydrocannabisativine	-2.2091	66.535341	0
C146	Arachidin-3	4.1537	49.18186	12
C147	Araphyn-1	4.2937	48.37986	12
C149	Araphyn-4	2.9385	51.317446	12
C150	Aristolene	1.6486	42.403032	0
C151	Aromadendrene	2.1549	42.403032	0
C152	benzaldehyde	1.5894	17.122758	6
C153	Benzonitrile	1.7089	16.753965	6
C154	Benzophenone	3.2342	30.34993	12

C155	benzphentamine	3.5388	45.022653	12
C157	Benzyl Alcohol	1.2255	18.456344	6
C158	benzyl formate	1.5258	21.018344	6
C159	Benzyl Nitrile	1.7437	19.847551	6
C160	Beta-Cannabispiranol	0.2825	42.14186	6
C161	Beta-Caryophyllene oxide	1.9144	43.205032	0
C162	Beta-Caryophyllene	3.2289	42.403032	0
C163	Beta-Cedrene	1.8851	42.403032	0
C164	Beta-Elemene	3.2309	42.403032	0
C165	Beta-Eudesmol	0.6981	44.538618	0
C167	beta-Fenchyl-Delta-9-tetrahydrocannabinolate	2.4863	87.106892	6
C169	Beta-Irone	2.1914	40.111446	0
C170	beta-phellandrene	1.5645	28.268688	0
C171	Beta-Pinene	1.3695	28.268688	0
C172	Beta-Selinene	1.7182	42.403032	0
C175	Bis-nor-cannabichromanone	1.9998	52.651032	6
C177	Bis-nor-cannabielsoin	2.4532	53.182618	6
C178	Bis-nor-cannabitriol	1.2123	57.078204	6
C180	Bornyl Delta-9-tetrahydrocannabinolate	3.4159	104.334822	6
C184	Calarene	2.3854	42.403032	0
C185	Camphene	1.3875	28.268688	0
C186	Cannabichromanone (CBCF)	0.8811	57.078204	6
C187	Cannabichromaonone D	2.0924	58.036204	6
C188	Cannabichromene (CBC)	3.3266	58.56779	6
C189	Cannabichromenic acid (CBCA)	2.8129	61.93179	6
C190	Cannabichromevarin (CBCV)	3.9026	52.380618	6
C191	Cannabichromevarinic acid (CBCVA)	3.3889	55.744618	6
C192	Cannabicitran	1.64	58.56779	6
C193	cannabicoumaronone	1.5493	58.036204	9
C194	Cannabicyclol (CBL)	2.0193	58.56779	6
C195	Cannabicyclolic acid (CBLA)	1.7604	61.93179	6
C196	Cannabicyclovarin (CBLV)	2.7227	52.380618	6
C197	Cannabidiol (CBD)	2.5816	58.56779	6
C199	Cannabidiol monomethylether (CBDM)	2.8326	61.661376	6
C200	Cannabidiorcol (CBD-C1)	3.9739	46.193446	6
C201	Cannabidivarin (CBDV)	3.1576	52.380618	6
C204	Cannabielsoic acid A (CBEA-A)	1.4909	62.73379	6
C205	Cannabielsoin (CBE)	1.7498	59.36979	6
C206	cannabiflavin B	5.3327	55.10786	16
C207	Cannabifuran (CBF)	3.0632	55.900618	13
C208	Cannabigerol (CBG)	3.5977	59.901376	6

C211	Cannabigerol monomethylether (CBGM)	3.8487	62.994962	6
C212	cannabigeroquinone	2.1627	58.56779	0
C213	Cannabigerovarin (CBGV)	4.0463	53.714204	6
C215	Cannabiglendol	1.6004	54.516204	6
C216	cannabimovone	0.8871	57.078204	6
C217	cannabinerol	3.5977	59.901376	6
C219	Cannabinodiol (CBND)	3.5192	55.900618	12
C220	Cannabinodivarin (CBVD)	4.0952	49.713446	12
C221	Cannabinol methylether (CBNM)	3.4865	58.994204	12
C222	Cannabinol (CBN)	3.2355	55.900618	12
C223	Cannabinol-C2 (CBN-C2)	4.2927	46.61986	12
C224	Cannabinol-C4 (CBN-C4)	3.5235	52.807032	12
C226	Cannabiorcol (CBN-C1)	4.5004	43.526274	12
C227	cannabiorcicchromene	4.7189	46.193446	6
C229	cannabiorcicitran	3.1597	46.193446	6
C230	cannabiorcicyclol	3.539	46.193446	6
C231	cannabiorcicyclolic acid	3.0253	49.557446	6
C232	cannabioxepane	3.2899	53.233446	13
C233	Cannabiripsol (CBR)	0.4579	61.505376	6
C239	cannabispirone	1.175	40.808274	6
C240	Cannabitriol (CBT)	0.8091	60.17179	6
C241	Cannabitriolvarin (CBTV)	1.5251	53.182618	6
C242	Cannabivarin (CBV)	3.8115	49.713446	12
C243	cannflavin A	6.4375	69.242204	16
C244	cannflavin B	5.2053	55.10786	16
C245	cannflavin C	6.4375	69.242204	16
C246	carbofuran	2.5928	34.627895	6
C247	carmagerol	0.9936	62.838962	6
C248	Carvacrol	2.5933	27.737102	6
C250	Carvone	1.5954	27.737102	0
C251	Cedryl acetate	1.7364	50.194204	0
C253	Chiricanine B	3.9259	52.275446	12
C256	cis-2-pinanol	0.8417	30.404274	0
C257	cis-beta-farnesene	4.3258	42.403032	0
C258	cis-gamma-bisabolene	3.953	42.403032	0
C259	cis-ocimene	3.2403	28.268688	0
C260	cis-sabinene hydrate	0.9414	29.602274	0
C261	Citronellyl acetate	1.8432	37.393446	0
C262	Citronellolformate	1.7644	34.29986	0
C263	compound-2	-0.1732	60.97379	6
C264	Compound-3	0.6173	59.640204	6

C265	compound-4	2.0924	58.036204	6
C266	Confluentin	5.9511	60.32779	6
C267	Cumene	2.2471	23.841516	6
C268	Cuminaldehyde	2.0065	26.403516	6
C270	Delta-9-tetrahydrocannabiorcolic acid (THCA-C1)	3.0321	49.557446	6
C271	Decanal	-2.1223	31.73786	0
C272	Decarboxyamorfrutin A	5.1658	52.807032	12
C273	Decarboxyamorfrutin B	6.398	66.941376	12
C274	Dehydrocannabifuran (DCBF)	3.7716	54.567032	13
C275	Delta-3-Carene	2.1434	28.268688	0
C276	Delta-7-cis-Isotetrahydrocannabivarin	3.0263	52.380618	6
C277	Delta-7-trans-Isotetrahydrocannabinol	2.4503	58.56779	6
C278	Delta-8-tetrahydrocannabinol (Δ8-THC)	2.0609	58.56779	6
C279	Delta-8-tetrahydrocannabinolic acid (Δ8-THCA)	1.6398	61.93179	6
C280	Delta-9-cis-tetrahydrocannabivarin	2.6021	52.380618	6
C281	Delta-9-nor-tetrahydrocannbinolic acid	2.4429	60.598204	6
C282	Delta-9-nor-tetrahydrocannbinol	2.7018	57.234204	6
C283	Delta-9-Tetrahydrocannabinol-C4	2.1867	55.4742	6
C284	Delta-9-tetrahydrocannabiorcol (THC-C1)	3.291	46.193446	6
C285	Delta-9-tetrahydrocannabinolic acid A (THCA-A)	1.5124	61.93179	6
C286	Delta-9-tetrahydrocannabinolic acid B (THCA-B)	1.5124	61.93179	6
C287	Delta-9-tetrahydrocannabinolic acid-C4 (THCA-C4)	1.8004	58.838204	6
C288	Delta-Cadinene	2.2115	42.403032	0
C290	Demethyldecarboxyamorfrutin A	4.7874	49.713446	12
C293	Desmodianone C	5.735	70.57579	12
C294	Desmodianone D	4.4114	69.242204	12
C295	Desmodianone E	4.1634	69.242204	12
C297	Dibutyl phthalate	0.3286	46.03745	6
C298	Diethyl Phthalate	2.0602	33.6631	6
C299	Dimethylbenzylcarbinyl acetate	2.5083	33.39269	6
C303	Dothiepin Sulfoxide	2.8277	52.24465	12
C304	Durene	3.7748	26.9351	6
C305	Dyclocaine	0.2744	52.38741	6
C306	epi-Bornyl Delta-9-tetrahydrocannabinolate	3.0646	90.20048	6
C307	Estragole	2.8139	26.40352	6
C312	Eudesmyl-Cannabigerolate	4.9875	105.6684	6
C313	Eugenol	2.6739	27.20552	6
C314	Eugenyl acetate	2.709	32.8611	6
C315	Fenchone	1.2557	29.07069	0
C317	Ferruginene A	2.9177	61.93179	6
C318	Ferruginene B	3.4229	61.93179	6

C319	Ferruginene C	3.7495	61.12979	6
C322	Furfurylmethylamphetamine	3.0916	40.97107	11
C323	gamma-curcumene	3.512	42.40303	0
C324	gamma-eudesmol	1.2945	44.53862	0
C325	Gamma-Gurjunene	2.6467	42.40303	0
C327	gamma-muurolene	2.2603	42.40303	0
C328	Gamma-Terpinene	2.4017	28.26869	0
C329	Glepidotin C	3.6156	50.51545	12
C330	Globulol	1.2587	44.53862	0
C332	guajol	1.6736	19.25834	6
C333	Heli-Cannabigenol	6.0196	63.84779	12
C334	Heptanal	-1.2583	22.4571	0
C336	Hexahydrocannabinol	1.4701	59.90138	6
C339	Hexanoic acid, propyl ester	-1.0941	29.44627	0
C341	Hordenine	2.0192	29.50389	6
C342	Hydroxy Heli-Cannabigerol	5.8796	64.64979	12
C349	Isobutyrophenone	2.2943	26.40352	6
C350	Isocannabitrol	0.747	63.26538	6
C252	Isodurene	3.7748	26.9351	6
C353	Isoeugenol	2.4251	27.20552	6
C354	Isolimonene	2.232	28.26869	0
C356	Isoquinoline	1.7687	21.60755	10
C358	Limonene oxide	0.4229	29.87269	0
C359	Limonene	2.1424	28.26869	0
C361	Linalyl acetate	2.8483	36.05986	0
C362	linoleic acid	-0.9485	54.62138	0
C363	Longifolene	1.8468	42.40303	0
C365	Machaeridiol A	5.0453	62.5142	12
C366	Machaeridiol B	4.9053	63.3162	12
C367	Machaeridiol C	5.1725	61.98262	15
C368	Machaeridiol D	3.7233	62.78462	15
C369	m-cymene	2.7333	26.9351	6
C373	Methyl acetylsalicylate	1.5898	27.47593	6
C380	Methyl isoeugenol	2.6761	30.2991	6
C384	Methylen-bis-Delta-9-tetrahydrocannabinol	4.1968	118.8956	12
C386	m-Tert-Butyl Phenol	3.0904	27.7371	6
C389	Nerolidol	3.7014	44.53862	0
C391	Nonanal	-1.8343	28.64427	0
C392	Nonane	-1.9134	29.17586	0
C393	nor-cannabidiol	2.8696	55.4742	6
C394	nor-cannabinol	3.5235	52.80703	12

C395	nor-cannabivarin	4.2927	46.61986	12
C396	N-p-Coumaroyltyramine	3.0619	44.76148	12
C397	N-trans-feruloyltyramine	3.1729	48.65707	12
C398	Octanal	-1.5463	25.55069	0
C399	o-cymene	2.7333	26.9351	6
C400	o-dimethyl hydroquinone	1.9246	22.35193	6
C401	O-Guaiacol	1.801	19.25834	6
C402	oleic acid	-2.3427	55.95496	0
C403	O-Methyl Cannabigerol	3.8487	62.99496	6
C404	O-Methyl Acetophenone	2.0561	23.30993	6
C405	O-Pentyl-cannabidiol	1.9292	74.03572	6
C406	O-Pentyl-Delta-9-tetrahydrocannbinol	1.7614	75.79572	6
C407	O-Propyl-cannabidiol	2.5052	67.84855	6
C408	O-Propyl-Delta-9-tetrahydrocannbinol	2.3374	69.60855	6
C410	o-xylene	2.8024	20.74793	6
C411	p-acetanisole	1.6809	24.11193	6
C412	p-aminotoluene	1.697	19.42114	6
C413	P-Cymene	2.7333	26.9351	6
C415	Pentamethylbenzene	4.261	30.02869	6
C417	Perillaldehyde	1.308	27.7371	0
C418	Perrottetinene	4.448	62.5142	12
C419	Perrottetinenic acid	4.1891	65.8782	12
C420	P-ethyl Toulene	2.4673	23.84152	6
C422	Phenylethyl alcohol	1.4811	21.54993	6
C424	Piperonal	1.6123	20.48676	6
C425	P-Methyl Acetophenone	2.0561	23.30993	6
C427	Propofol	2.5242	33.92427	6
C434	rac-6'-Epoxycannbigerol	2.568	60.70338	6
C435	rac-6'-Epoxycannbigerolic acid	2.0543	64.06738	6
C436	Radulanin A	4.4331	48.37986	12
C437	Radulanin H	4.0468	51.74386	12
C438	Radulanin I	3.5328	48.37986	12
C439	Radulanin J	3.5137	47.04627	12
C440	Radulanin K	2.749	47.31669	12
C441	Radulanin L	4.0383	49.18186	12
C443	roughanic acid	0.4781	47.10062	0
C444	Sabinene	1.0301	28.26869	0
C446	Sativene	1.7772	42.40303	0
C447	sesquicannabigerol	4.8299	74.03572	6
C448	stearidonic acid	1.2963	51.9542	0
C449	Styrene	2.3817	19.41434	6

C451	Terpinolene	2.7208	28.26869	0
C452	tert-butyl-benzene	3.2304	26.9351	6
C453	Tetrahydrocannabinol epoxide	1.3518	59.36979	6
C454	Tetrahydrozoline	0.7261	35.74869	6
C455	Thymol	2.5933	27.7371	6
C456	Toluene	2.3162	17.65434	6
C457	trans-alpha-farnesene	4.4725	42.40303	0
C458	trans-Archidin-1	4.0137	49.98386	12
C459	trans-Archidin-2	4.6474	50.51545	12
C460	trans-gamma-bisabolene	3.953	42.40303	0
C461	trans-ocimene	3.2403	28.26869	0
C465	Valencene	2.676	42.40303	0
C466	Verbenone	1.2447	27.7371	0
	Metabolites after MDS using ADMET (112) (used for HCA and Scaffold analysis)			
		ALogP	apol	naAromAtom
C19	1-(2-chlorophenyl)ethenone	2.3617	21.729551	6
C24	2-Formyl-Delta-9-Tetrahydrocannabinol	2.3006	62.88979	6
C38	3,4,5,6-tetrahydro-7-hydroxy-a,a-2-trimethyl-9-n-propyl-2,6-methano-2H-1-Benzoxocin-5-methanol	1.7344	54.516204	6
C43	3-Hydroxy-Delta-4,5-Cannabichromene	1.87	59.36979	6
C45	3-Methyl Acetophenone	2.0561	23.30993	6
C51	4,5-Dihydroxy-2,3,6-Trimethoxy-9,10-Dihydrophenanthrene	3.0872	45.932274	12
C53	4-Acetoxy Cannabichromene	3.2217	65.025376	6
C54	4-Acetoxy-2-geranyl-5-hydroxy-3-n-pentylphenol	3.3654	66.358962	6
C57	4-hydroxy-2,3,6,7-tetramethoxy-9,10dihydrophenanthrene	3.2108	49.02586	12
C66	5-acetoxy-6-geranyl-3n -pentyl-1,4-benzoquinone	1.7414	65.025376	0
C75	6a-R-Cannabichromanone B	0.5919	59.640204	6
C79	7,8-Dehydro-10-O-ethylcannabitriol	1.6178	65.025376	6
C80	7,8-dihydrocannabinol	2.3465	57.234204	6
C81	7-Hydroxy Cannabichromane	2.4105	60.703376	6
C82	7-hydroxy cannabinol	3.0955	56.702618	12
C83	7-Methoxy Cannabispiranone	1.2986	43.90186	6
C84	7-R-Cannabicoumarononic acid	1.2904	61.400204	9
C88	8a-Hydroxy-Delta-9-tetrahydrocannbinol	1.3256	59.36979	6
C89	8-oxo-Delta-9-tetrahydrocannbinol	1.3517	58.036204	6
C90	9,10-Anhydrocannabitriol	1.5756	58.036204	6
C92	9 β ,10 β -Epoxyhexahydrocannabinol	1.3518	59.36979	6

C93	10 α -Hydroxy-Delta- 9,11 -hexahydrocannabinol	1.0823	59.36979	6
C94	10-Ethoxy-9-hydroxy-delta-6a-tetrahydrocannabinol	1.468	66.358962	6
C95	10-Hydroxy-9-oxo-Delta-8-tetrahydrocannabinol	1.3564	59.36979	6
C96	10-O-Ethyl bis-nor cannabitriol	1.5272	63.265376	6
C97	10-Oxo-delta-6a-tetrahydrocannabinol (OTHC)	1.5291	58.036204	6
C105	acetyl abnormal hydrocannabigeroquinol	3.3654	66.358962	6
C114	Alpha-Cannabispiranol	0.2825	42.14186	6
C139	Amorfrutin-B	5.8843	70.305376	12
C141	Anethole	1.2081	58.036204	6
C160	Beta-Cannabispiranol	0.2825	42.14186	6
C175	Bis-nor-cannabichromanone	1.9998	52.651032	6
C177	Bis-nor-cannabielsoin	2.4532	53.182618	6
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C191	Cannabichromevarinic acid (CBCVA)	3.3889	55.744618	6
C193	cannabicoumaronone	1.5493	58.036204	9
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C215	Cannabiglendol	1.6004	54.516204	6
C219	Cannabinodiol (CBND)	3.5192	55.900618	12
C220	Cannabinodivarin (CBVD)	4.0952	49.713446	12
C221	Cannabinol methylether (CBNM)	3.4865	58.994204	12
C222	Cannabinol (CBN)	3.2355	55.900618	12
C223	Cannabinol-C2 (CBN-C2)	4.2927	46.61986	12
C224	Cannabinol-C4 (CBN-C4)	3.5235	52.807032	12
C226	Cannabiorcol (CBN-C1)	4.5004	43.526274	12
C227	cannabiorcicchromene	4.7189	46.193446	6
C230	cannabiorcicyclol	3.539	46.193446	6
C231	cannabiorcicyclolic acid	3.0253	49.557446	6
C232	cannabioxepane	3.2899	53.233446	13
C239	cannabispirone	1.175	40.808274	6
C241	Cannabitriolvarin (CBTV)	1.5251	53.182618	6

C242	Cannabivarin (CBV)	3.8115	49.713446	12
C246	carbofuran	2.5928	34.627895	6
C263	compound-2	-0.1732	60.97379	6
C264	Compound-3	0.6173	59.640204	6
C265	compound-4	2.0924	58.036204	6
C266	Confluentin	5.9511	60.32779	6
C268	Cuminaldehyde	2.0065	26.403516	6
C270	Delta-9-tetrahydrocannabiorcolic acid (THCA-C1)	3.0321	49.557446	6
C273	Decarboxyamorfrutin B	6.398	66.941376	12
C274	Dehydrocannabifuran (DCBF)	3.7716	54.567032	13
C276	Delta-7-cis-Isotetrahydrocannabivarin	3.0263	52.380618	6
C277	Delta-7-trans-Isotetrahydrocannabinol	2.4503	58.56779	6
C278	Delta-8-tetrahydrocannabinol (Δ8-THC)	2.0609	58.56779	6
C279	Delta-8-tetrahydrocannabinolic acid (Δ8-THCA)	1.6398	61.93179	6
C280	Delta-9-cis-tetrahydrocannabivarin	2.6021	52.380618	6
C281	Delta-9-nor-tetrahydrocannbinolic acid	2.4429	60.598204	6
C282	Delta-9-nor-tetrahydrocannbinol	2.7018	57.234204	6
C283	Delta-9-Tetrahydrocannabinol-C4	2.1867	55.4742	6
C284	Delta-9-tetrahydrocannabiorcol (THC-C1)	3.291	46.193446	6
C285	Delta-9-tetrahydrocannabinolic acid A (THCA-A)	1.5124	61.93179	6
C286	Delta-9-tetrahydrocannabinolic acid B (THCA-B)	1.5124	61.93179	6
C287	Delta-9-tetrahydrocannabinolic acid-C4 (THCA-C4)	1.8004	58.838204	6
C317	Ferruginene A	2.9177	61.93179	6
C318	Ferruginene B	3.4229	61.93179	6
C319	Ferruginene C	3.7495	61.12979	6
C333	Heli-Cannabigenol	6.0196	63.84779	12
C336	Hexahydrocannabinol	1.4701	59.90138	6
C342	Hydroxy Heli-Cannabigerol	5.8796	64.64979	12
C350	Isocannabitrol	0.747	63.26538	6
C365	Machaeridiol A	5.0453	62.5142	12
C366	Machaeridiol B	4.9053	63.3162	12
C367	Machaeridiol C	5.1725	61.98262	15
C368	Machaeridiol D	3.7233	62.78462	15
C393	nor-cannabidiol	2.8696	55.4742	6
C394	nor-cannabinol	3.5235	52.80703	12
C395	nor-cannabivarin	4.2927	46.61986	12
C405	O-Pentyl-cannabidiol	1.9292	74.03572	6
C407	O-Propyl-cannabidiol	2.5052	67.84855	6
C418	Perrottetinene	4.448	62.5142	12
C419	Perrottetinenic acid	4.1891	65.8782	12
C427	Propofol	2.5242	33.92427	6

C435	rac-6'-Epoxycannbigerolic acid	2.0543	64.06738	6
C436	Radulanin A	4.4331	48.37986	12
C437	Radulanin H	4.0468	51.74386	12
C438	Radulanin I	3.5328	48.37986	12
C440	Radulanin K	2.749	47.31669	12
C441	Radulanin L	4.0383	49.18186	12
C453	Tetrahydrocannabinol epoxide	1.3518	59.36979	6
C454	Tetrahydrozoline	0.7261	35.74869	6
C455	Thymol	2.5933	27.7371	6
	468 Metabolites and positive & negative controls			
naAromAtom	nAromBond	nAtom	bpol	C1SP2
6	6	68	46.94824	1
6	6	46	32.18417	2
12	12	54	34.8038	1
12	12	56	38.473	1
6	6	45	32.18417	1
21	22	69	43.49862	1
12	12	56	37.71421	1
12	12	59	40.58821	2
15	16	50	32.09976	1
6	6	43	30.68535	2
6	6	43	28.76935	0
6	6	51	34.92297	1
6	6	41	26.85335	0
12	12	61	41.81662	1
12	12	52	35.5278	1
10	10	40	29.49735	2
18	18	60	34.2078	1
0	0	9	6.559242	0
10	10	37	27.31093	2
15	16	57	39.0618	1
6	6	63	41.88783	0
12	12	53	35.5278	1
6	6	50	34.78776	2
6	6	43	29.72735	0
6	6	40	25.62493	0
12	12	50	32.45459	0
6	6	39	25.89535	0
12	12	61	41.81662	1

6	6	39	27.81135	1
6	6	40	24.66693	0
6	6	41	24.96493	0
6	6	44	29.72735	0
6	6	41	25.62493	0
6	6	45	33.56818	3
12	12	57	38.743417	1
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6	6	45	32.184175	1
6	6	42	29.997761	1
12	12	54	36.557003	1
12	12	55	36.557003	0
6	6	46	33.341382	1
12	12	51	31.496589	0
12	12	55	33.683003	0
12	12	56	36.557003	1
12	12	57	38.31021	1
12	12	66	42.087038	1
6	6	45	32.184175	1
6	6	42	29.997761	1
6	6	45	31.226175	0
6	6	50	36.286589	1
6	6	55	41.275796	3
11	11	57	41.91021	2
6	6	48	33.829761	1
6	6	44	30.685347	0
11	11	50	35.621382	2
6	6	43	29.997761	1
6	6	45	32.184175	1
6	6	43	29.808554	1
12	12	58	38.942624	0
9	10	49	32.908175	2
6	6	29	20.890105	0
16	17	33	19.562898	2
6	6	32	23.672519	0
0	0	62	42.066659	1
0	0	65	44.415866	1
0	0	64	44.253073	1
0	0	68	46.439487	1
0	0	66	45.64428	0
6	6	73	46.439487	1

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0	0	55	38.560245	1
0	0	62	42.662659	1
6	6	26	18.6049	2
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0	0	32	23.00731	1
0	0	21	17.9449	0
0	0	24	15.03448	0
0	0	18	10.95966	2
5	5	20	12.11686	2
0	0	22	14.50969	1
0	0	11	7.382035	1
0	0	22	14.50969	1
0	0	24	14.9429	1
0	0	20	14.60328	1
6	6	23	12.32328	1
0	0	9	6.153621	1
14	15	47	29.06014	2
11	11	35	24.82452	3
9	10	27	14.07648	2
6	6	24	12.32328	1
0	0	19	12.32328	1
6	6	53	34.71221	0
0	0	12	8.745656	0
6	6	24	15.304898	0
6	6	24	15.304898	0
6	6	15	8.539242	0
6	6	12	5.212828	0
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0	0	29	21.86414	0
0	0	26	19.677726	0
6	6	22	13.118484	0
6	6	37	24.050554	0
6	6	22	15.758484	2
6	6	16	11.385656	2
0	0	13	9.703656	0
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0	0	27	19.677726	0
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6	6	56	35.67021	2
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0	0	22	16.262898	0
6	6	18	9.703656	0
6	6	22	15.758484	2
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0	0	20	15.304898	0
0	0	13	8.908449	0
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6	6	29	19.932105	0
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6	6	50	32.525796	0
6	6	22	13.118484	0
0	0	27	19.677726	1
6	6	21	13.118484	0
6	6	24	15.304898	0
6	6	54	34.71221	1
6	6	23	14.076484	1
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0	0	20	15.304898	0
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0	0	18	13.118484	0
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14	16	35	19.136898	0
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6	6	61	40.043038	1
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6	6	23	13.551691	0
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6	6	61	40.043038	1
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6	6	56	35.67021	1
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16	17	43	22.551726	0
6	6	59	38.814624	0
6	6	51	32.525796	0
6	6	56	36.898624	0
12	12	50	30.339382	0
6	6	39	26.65414	0
9	10	55	36.357796	2
6	6	55	34.71221	0
12	12	53	31.297382	1
12	12	50	30.339382	0
6	6	54	34.71221	0
6	6	52	33.483796	0
6	6	52	34.441796	0
6	6	42	29.257726	0
6	6	54	36.62821	0
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6	6	58	38.814624	1
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6	6	62	40.730624	2
6	6	55	34.982624	0

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6	6	38	23.78014	0
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0	0	39	26.236968	0
0	0	42	28.423382	0
0	0	39	26.236968	1
0	0	39	26.236968	0
0	0	39	26.236968	0
0	0	36	24.050554	0
0	0	50	33.75421	1
0	0	39	26.236968	0
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0	0	39	26.236968	1
6	6	82	55.077522	1
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0	0	29	19.677726	0
0	0	26	17.491312	0
0	0	39	26.236968	0
0	0	39	26.236968	0
12	12	50	29.110968	2
12	12	59	33.75421	1
12	12	49	29.110968	1
12	12	62	37.856624	1
6	6	23	15.034484	0
6	6	52	33.483796	1

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12	12	41	21.86414	0
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12	12	24	11.89007	0
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6	6	21	13.80607	1
6	6	16	8.745656	0
6	6	18	11.619656	0
6	6	16	8.312449	0
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0	0	39	26.236968	1
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6	6	52	32.525796	1
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0	0	17	13.80607	0

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6	6	52	35.399796	0
6	6	53	34.71221	0
6	6	56	35.67021	1
6	6	47	30.339382	0
6	6	50	31.297382	1
6	6	53	36.62821	0
9	10	52	35.399796	1
6	6	53	34.71221	0
6	6	56	35.67021	1
6	6	47	30.339382	0
6	6	53	32.79621	1
6	6	56	33.75421	2
6	6	56	36.89862	1
6	6	41	24.050554	1
6	6	47	28.423382	1
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6	6	57	35.67021	2
6	6	57	35.67021	2
6	6	54	34.71221	1
16	17	47	26.65414	0
13	15	49	30.339382	0
6	6	55	34.982624	0
6	6	61	40.043038	1
6	6	58	35.940624	1
6	6	58	39.085038	0
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6	6	52	31.567796	1
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6	6	55	34.982624	0
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13	15	45	27.882554	1
6	6	57	36.898624	0
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28	29	74	36.03221	2
24	24	76	38.218624	2
24	24	79	42.321038	2
24	24	82	46.423452	2
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6	6	55	34.71221	0
6	6	48	30.339382	0
12	12	43	25.966554	0
16	17	60	35.399796	0
16	17	47	26.65414	0
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0	0	25	16.262898	1
12	12	108	68.196006	2
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6	6	54	35.399796	0

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6	6	54	34.71221	0
6	6	21	13.118484	0
6	6	23	14.076484	1
6	6	57	35.67021	1
6	6	44	26.924554	1
0	0	31	22.82214	1
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6	6	53	34.71221	1
6	6	53	34.71221	0
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6	6	47	30.339382	0
6	6	54	33.483796	2
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6	6	56	35.67021	1
6	6	53	33.483796	1
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6	6	42	29.79855	2
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6	6	30	20.36531	1
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0	0	9	8.839242	0
0	0	38	28.42338	0
12	12	43	29.31535	0
6	6	24	15.3049	0
6	6	48	34.37059	0

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6	6	23	15.03448	1
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6	6	24	15.03448	1
6	6	29	20.0949	2
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6	6	56	34.71221	1
6	6	55	32.79621	2
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5	5	11	7.246828	2
11	11	36	24.66693	1
0	0	39	26.23697	0
0	0	42	28.42338	0
0	0	39	26.23697	1
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0	0	26	17.49131	0
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0	0	19	14.07648	1
0	0	23	18.1789	1
0	0	29	22.55173	1
12	12	42	24.05055	0
6	6	27	18.3781	0
12	12	57	32.79621	0
0	0	27	17.49131	2
0	0	18	13.11848	0
0	0	34	24.73814	1
0	0	36	26.58493	1

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0	0	13	9.703656	1
6	6	23	14.07648	0
6	6	58	36.89862	1
0	0	7	5.557621	0
6	6	24	15.3049	0
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0	0	26	17.49131	1
0	0	13	8.745656	2
10	11	17	8.972449	2
16	17	31	13.80607	0
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0	0	26	17.49131	1
0	0	29	19.67773	1
0	0	34	24.73814	2
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0	0	39	26.23697	1
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12	12	55	30.6098	1
15	16	53	30.33938	1
15	16	54	32.25538	0
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0	0	26	20.36531	1
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6	6	19	11.61966	1
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0	0	5	3.026414	0
12	12	107	69.42442	0
0	0	23	16.2629	0
6	6	25	15.3049	0
0	0	26	17.49131	2

0	0	29	19.67773	0
0	0	42	28.42338	1
6	6	14	6.722035	0
0	0	28	20.63573	1
0	0	29	21.86414	0
6	6	50	30.6098	1
12	12	46	28.15297	0
12	12	40	23.78014	0
12	12	38	20.20252	1
12	12	42	24.30493	1
0	0	25	18.44931	1
6	6	24	15.3049	0
6	6	20	14.76407	0
6	6	17	10.66166	0
0	0	54	38.12704	1
6	6	58	39.08504	0
6	6	20	11.89007	0
6	6	68	45.64428	1
6	6	69	47.56028	1
6	6	62	41.27145	1
6	6	63	43.18745	1
16	17	52	26.65414	0
6	6	18	10.93207	0
6	6	21	13.80607	0
6	6	17	9.178863	0
6	6	24	15.3049	0
0	0	47	34.98262	0
6	6	27	17.49131	0
0	0	16	11.89007	1
0	0	25	16.2629	2
12	12	54	32.5258	0
12	12	57	33.4838	1
6	6	21	13.11848	0
6	6	13	6.559242	0
6	6	19	10.93207	0
0	0	17	12.68528	0
6	6	17	11.34924	1
6	6	20	11.89007	0
0	0	10	7.517242	1
6	6	31	19.67773	0
0	0	19	14.76407	2

0	0	13	9.178863	0
0	0	13	8.745656	0
6	6	25	15.3049	0
6	6	18	10.93207	0
16	17	32	13.80607	0
6	6	56	36.89862	0
6	6	59	37.85662	1
12	12	41	23.78014	0
12	12	44	24.73814	1
12	12	41	23.78014	0
12	12	39	23.50973	0
12	12	39	20.36531	1
12	12	42	23.78014	0
6	6	57	35.67021	1
0	0	44	29.38138	1
0	0	26	17.49131	1
6	6	15	7.517242	1
0	0	39	26.23697	1
6	6	68	43.72828	0
0	0	48	31.5678	1
6	6	16	8.745656	1
0	0	15	10.93207	0
0	0	26	17.49131	0
6	6	24	15.3049	0
6	6	54	36.62821	0
6	6	31	19.47131	1
6	6	25	15.3049	0
6	6	15	8.745656	0
0	0	39	26.23697	1
12	12	43	21.86414	0
12	12	44	24.05055	0
0	0	39	26.23697	0
0	0	26	17.49131	1
0	0	41	30.6098	0
6	6	21	11.36528	0
0	0	35	26.23697	0
0	0	39	26.23697	1
0	0	25	16.2629	0
16	17	51	26.65414	0
12	12	39	20.20252	1

	Metabolites from Machine Learning Methods (330) (used for MDS using CDK)			
naAromAtom	nAromBond	nAtom	bpol	C1SP2
6	6	24	15.3049	0
6	6	24	15.3049	0
6	6	12	5.212828	0
6	6	24	15.3049	0
0	0	29	21.86414	0
6	6	22	13.11848	0
6	6	37	24.05055	0
6	6	22	15.75848	2
6	6	17	9.030449	0
6	6	22	13.11848	1
6	6	21	13.11848	0
6	6	56	35.67021	2
0	0	54	34.71221	0
6	6	18	9.703656	0
6	6	22	15.75848	2
10	11	21	10.93207	0
6	6	20	12.84807	0
6	6	29	19.93211	0
6	6	23	13.80607	1
6	6	50	32.5258	0
6	6	22	13.11848	0
0	0	27	19.67773	1
6	6	21	13.11848	0
6	6	24	15.3049	0
6	6	54	34.71221	1
6	6	23	14.07648	1
6	6	20	11.89007	0
0	0	26	19.67773	0
6	6	32	22.11852	0
12	12	40	25.42573	0
14	16	35	19.1369	0
6	6	59	39.77262	1
6	6	61	40.04304	1
0	0	26	17.49131	0
6	6	25	17.90848	1
12	12	43	29.52814	0
10	11	21	13.53566	1

0	0	35	26.23697	0
6	6	20	12.84807	0
6	6	23	13.55169	0
6	6	82	55.07752	1
12	12	78	50.70469	1
0	0	59	39.77262	1
6	6	61	40.04304	1
6	6	18	11.15886	2
12	12	43	24.05055	0
6	6	22	13.11848	0
0	0	24	18.1789	1
6	6	54	34.4418	1
6	6	51	33.21338	0
6	6	59	38.81462	0
6	6	51	32.5258	0
6	6	56	36.89862	0
12	12	50	30.33938	0
6	6	39	26.65414	0
9	10	55	36.3578	2
6	6	55	34.71221	0
12	12	50	30.33938	0
6	6	54	34.71221	0
6	6	52	33.4838	0
6	6	52	34.4418	0
6	6	42	29.25773	0
6	6	54	36.62821	0
6	6	54	34.71221	1
6	6	61	41.00104	0
6	6	54	34.71221	0
6	6	58	38.81462	1
6	6	52	33.4838	0
6	6	62	40.73062	2
6	6	62	40.73062	2
6	6	55	34.98262	0
6	6	61	40.04304	1
0	0	59	39.77262	1
6	6	17	9.703656	0
0	0	39	26.23697	1
0	0	42	28.42338	0
0	0	39	26.23697	1
0	0	39	26.23697	0

6	6	95	63.82318	1
6	6	38	23.78014	0
0	0	39	26.23697	0
0	0	39	26.23697	0
0	0	39	26.23697	0
0	0	39	26.23697	0
0	0	42	28.42338	0
0	0	39	26.23697	1
0	0	39	26.23697	0
0	0	39	26.23697	0
0	0	36	24.05055	0
0	0	50	33.75421	1
0	0	39	26.23697	0
6	6	21	11.89007	1
0	0	26	17.49131	0
0	0	26	17.49131	0
0	0	39	26.23697	1
6	6	82	55.07752	1
0	0	26	17.49131	0
0	0	29	19.67773	0
0	0	26	17.49131	0
0	0	39	26.23697	0
0	0	39	26.23697	0
12	12	62	37.85662	1
6	6	23	15.03448	0
6	6	52	33.4838	1
0	0	63	45.66466	1
12	12	42	21.86414	0
12	12	41	21.86414	0
12	12	45	24.05055	0
0	0	39	26.23697	0
0	0	39	26.23697	1
6	6	14	7.517242	1
6	6	13	6.126035	0
12	12	24	11.89007	0
12	12	39	24.93735	0
6	6	16	8.745656	0
6	6	18	11.61966	0
6	6	16	8.312449	0
6	6	38	23.78014	0
0	0	40	28.15297	1

0	0	39	26.23697	1
0	0	39	26.23697	1
0	0	39	26.23697	3
0	0	42	28.42338	1
6	6	79	52.89111	1
0	0	37	25.00855	0
0	0	26	17.49131	1
0	0	26	17.49131	1
0	0	39	26.23697	2
6	6	47	30.06897	1
6	6	48	30.33938	1
6	6	52	32.5258	1
6	6	95	63.82318	1
0	0	39	26.23697	0
0	0	26	17.49131	1
6	6	52	34.4418	0
6	6	52	35.3998	0
6	6	53	34.71221	0
6	6	56	35.67021	1
6	6	47	30.33938	0
6	6	50	31.29738	1
6	6	53	36.62821	0
9	10	52	35.3998	1
6	6	53	34.71221	0
6	6	56	35.67021	1
6	6	47	30.33938	0
6	6	53	32.79621	1
6	6	56	36.89862	1
6	6	41	24.05055	1
6	6	47	28.42338	1
6	6	57	35.67021	2
6	6	54	34.71221	1
16	17	47	26.65414	0
13	15	49	30.33938	0
6	6	55	34.98262	0
6	6	58	39.08504	0
0	0	53	34.71221	0
6	6	49	30.6098	0
6	6	50	32.5258	0
6	6	52	31.5678	1
6	6	55	34.98262	0

12	12	49	28.42338	1
12	12	43	24.05055	1
12	12	52	34.4418	0
12	12	49	30.33938	0
12	12	40	23.78014	0
12	12	46	28.15297	0
12	12	37	21.59373	0
6	6	41	25.96655	0
6	6	41	27.88255	0
6	6	41	25.96655	0
6	6	44	26.92455	1
13	15	45	27.88255	1
6	6	57	36.89862	0
6	6	36	22.55173	0
6	6	55	34.71221	0
6	6	48	30.33938	0
12	12	43	25.96655	0
16	17	60	35.3998	0
16	17	47	26.65414	0
16	17	60	35.3998	0
6	6	31	21.84811	0
6	6	59	37.16904	0
6	6	25	15.3049	0
0	0	25	16.2629	1
0	0	47	33.4838	1
12	12	45	27.88255	0
0	0	29	19.67773	0
0	0	39	26.23697	2
0	0	39	26.23697	0
0	0	26	17.49131	1
0	0	28	19.67773	0
0	0	36	26.92455	1
0	0	33	24.73814	0
6	6	56	36.62821	0
6	6	54	35.3998	0
6	6	52	35.3998	0
6	6	54	34.71221	0
6	6	21	13.11848	0
6	6	23	14.07648	1
6	6	44	26.92455	1
0	0	31	22.82214	1

12	12	46	28.15297	0
12	12	59	36.89862	0
13	15	47	28.15297	1
0	0	26	17.49131	0
6	6	47	30.33938	1
6	6	53	34.71221	1
6	6	53	34.71221	0
6	6	56	35.67021	1
6	6	47	30.33938	0
6	6	54	33.4838	2
6	6	51	32.5258	1
6	6	50	32.5258	0
6	6	41	25.96655	0
6	6	56	35.67021	1
6	6	56	35.67021	1
6	6	53	33.4838	1
0	0	39	26.23697	0
12	12	43	24.05055	0
12	12	62	35.67021	0
12	12	60	35.3998	0
12	12	60	35.3998	0
6	6	42	29.79855	2
6	6	30	21.0529	2
6	6	30	20.36531	1
12	12	43	29.31535	0
6	6	24	15.3049	0
6	6	48	34.37059	0
6	6	82	55.07752	1
6	6	23	15.03448	1
6	6	97	64.09359	1
6	6	24	15.03448	1
6	6	29	20.0949	2
0	0	27	18.44931	0
6	6	56	34.71221	2
6	6	56	34.71221	1
6	6	55	32.79621	2
11	11	36	24.66693	1
0	0	39	26.23697	0
0	0	42	28.42338	0
0	0	39	26.23697	1
0	0	39	26.23697	1

0	0	26	17.49131	0
12	12	44	24.05055	1
0	0	42	28.42338	0
6	6	17	10.66166	0
12	12	56	32.79621	0
0	0	22	16.2629	1
6	6	55	36.89862	0
0	0	29	22.55173	1
6	6	27	18.3781	0
12	12	57	32.79621	0
6	6	23	14.07648	0
6	6	58	36.89862	1
6	6	24	15.3049	0
6	6	24	15.03448	0
0	0	26	17.49131	1
10	11	17	8.972449	2
0	0	28	21.32331	0
0	0	26	17.49131	1
0	0	34	24.73814	2
0	0	52	35.94062	1
0	0	39	26.23697	1
12	12	54	30.6098	1
12	12	55	30.6098	1
15	16	53	30.33938	1
15	16	54	32.25538	0
6	6	24	15.3049	0
6	6	24	16.68007	2
6	6	27	19.1369	0
12	12	107	69.42442	0
6	6	25	15.3049	0
0	0	42	28.42338	1
0	0	28	20.63573	1
0	0	29	21.86414	0
6	6	50	30.6098	1
12	12	46	28.15297	0
12	12	40	23.78014	0
12	12	38	20.20252	1
12	12	42	24.30493	1
0	0	25	18.44931	1
6	6	24	15.3049	0
6	6	20	14.76407	0

6	6	17	10.66166	0
0	0	54	38.12704	1
6	6	58	39.08504	0
6	6	20	11.89007	0
6	6	68	45.64428	1
6	6	69	47.56028	1
6	6	62	41.27145	1
6	6	63	43.18745	1
6	6	18	10.93207	0
6	6	21	13.80607	0
6	6	17	9.178863	0
6	6	24	15.3049	0
6	6	27	17.49131	0
0	0	25	16.2629	2
12	12	54	32.5258	0
12	12	57	33.4838	1
6	6	21	13.11848	0
6	6	19	10.93207	0
6	6	17	11.34924	1
6	6	20	11.89007	0
6	6	31	19.67773	0
6	6	56	36.89862	0
6	6	59	37.85662	1
12	12	41	23.78014	0
12	12	44	24.73814	1
12	12	41	23.78014	0
12	12	39	23.50973	0
12	12	39	20.36531	1
12	12	42	23.78014	0
0	0	44	29.38138	1
0	0	26	17.49131	1
0	0	39	26.23697	1
6	6	68	43.72828	0
0	0	48	31.5678	1
6	6	16	8.745656	1
0	0	26	17.49131	0
6	6	24	15.3049	0
6	6	54	36.62821	0
6	6	31	19.47131	1
6	6	25	15.3049	0
6	6	15	8.745656	0

0	0	39	26.23697	1
12	12	43	21.86414	0
12	12	44	24.05055	0
0	0	39	26.23697	0
0	0	26	17.49131	1
0	0	39	26.23697	1
0	0	25	16.2629	0
	Metabolites after MDS using ADMET (112) (used for HCA and Scaffold analysis)			
naAromAtom	nAromBond	nAtom	bpol	C1SP2
6	6	17	9.030449	0
6	6	56	35.67021	2
6	6	50	32.5258	0
6	6	54	34.71221	1
6	6	20	11.89007	0
12	12	40	25.42573	0
6	6	59	39.77262	1
6	6	61	40.04304	1
12	12	43	29.52814	0
0	0	59	39.77262	1
6	6	54	34.4418	1
6	6	59	38.81462	0
6	6	51	32.5258	0
6	6	56	36.89862	0
12	12	50	30.33938	0
6	6	39	26.65414	0
9	10	55	36.3578	2
6	6	54	34.71221	0
6	6	52	33.4838	0
6	6	52	34.4418	0
6	6	54	36.62821	0
6	6	54	34.71221	1
6	6	61	41.00104	0
6	6	54	34.71221	0
6	6	58	38.81462	1
6	6	52	33.4838	0
6	6	61	40.04304	1
6	6	38	23.78014	0
12	12	62	37.85662	1
6	6	52	33.4838	1
6	6	38	23.78014	0

6	6	47	30.06897	1
6	6	48	30.33938	1
6	6	52	32.5258	1
6	6	52	34.4418	0
6	6	52	35.3998	0
6	6	56	35.67021	1
6	6	50	31.29738	1
9	10	52	35.3998	1
6	6	56	35.67021	1
6	6	47	30.33938	0
6	6	53	32.79621	1
6	6	56	36.89862	1
6	6	41	24.05055	1
6	6	47	28.42338	1
6	6	57	35.67021	2
6	6	54	34.71221	1
13	15	49	30.33938	0
6	6	50	32.5258	0
12	12	49	28.42338	1
12	12	43	24.05055	1
12	12	52	34.4418	0
12	12	49	30.33938	0
12	12	40	23.78014	0
12	12	46	28.15297	0
12	12	37	21.59373	0
6	6	41	25.96655	0
6	6	41	25.96655	0
6	6	44	26.92455	1
13	15	45	27.88255	1
6	6	36	22.55173	0
6	6	48	30.33938	0
12	12	43	25.96655	0
6	6	31	21.84811	0
6	6	56	36.62821	0
6	6	54	35.3998	0
6	6	52	35.3998	0
6	6	54	34.71221	0
6	6	23	14.07648	1
6	6	44	26.92455	1
12	12	59	36.89862	0
13	15	47	28.15297	1

6	6	47	30.33938	1
6	6	53	34.71221	1
6	6	53	34.71221	0
6	6	56	35.67021	1
6	6	47	30.33938	0
6	6	54	33.4838	2
6	6	51	32.5258	1
6	6	50	32.5258	0
6	6	41	25.96655	0
6	6	56	35.67021	1
6	6	56	35.67021	1
6	6	53	33.4838	1
6	6	56	34.71221	2
6	6	56	34.71221	1
6	6	55	32.79621	2
12	12	56	32.79621	0
6	6	55	36.89862	0
12	12	57	32.79621	0
6	6	58	36.89862	1
12	12	54	30.6098	1
12	12	55	30.6098	1
15	16	53	30.33938	1
15	16	54	32.25538	0
6	6	50	30.6098	1
12	12	46	28.15297	0
12	12	40	23.78014	0
6	6	68	45.64428	1
6	6	62	41.27145	1
12	12	54	32.5258	0
12	12	57	33.4838	1
6	6	31	19.67773	0
6	6	59	37.85662	1
12	12	41	23.78014	0
12	12	44	24.73814	1
12	12	41	23.78014	0
12	12	39	20.36531	1
12	12	42	23.78014	0
6	6	54	36.62821	0
6	6	31	19.47131	1
6	6	25	15.3049	0

	468 Metabolites and positive & negative controls			
C2SP2	C3SP2	C1SP3	C2SP3	C3SP3
6	2	4	7	3
6	1	3	3	2
10	2	5	3	0
10	2	7	2	0
5	1	4	3	2
16	2	4	5	0
11	1	4	6	0
11	1	4	4	1
11	1	6	1	0
5	1	0	6	1
6	2	1	5	1
5	2	2	6	1
4	2	1	7	1
10	2	8	2	1
11	1	4	3	0
7	1	5	1	0
15	3	3	3	0
0	0	2	0	0
7	1	3	1	0
11	1	8	1	0
6	2	3	7	3
11	1	4	5	0
6	2	3	5	1
5	2	1	6	1
5	2	1	6	1
11	2	3	1	1
6	1	3	3	0
10	2	8	2	1
5	1	4	2	0
6	2	1	5	1
6	2	1	5	1
5	2	1	6	1
5	2	1	6	1
3	0	5	5	0
10	2	3	4	0

5	1	1	5	1
5	1	4	3	2
5	1	4	2	2
10	2	3	2	2
11	2	6	3	0
6	0	5	5	0
9	3	4	4	1
9	3	2	8	1
10	2	5	4	0
11	1	6	3	0
10	2	5	6	1
5	1	4	3	2
5	1	4	3	0
4	2	1	7	1
5	1	8	2	0
6	0	4	4	1
9	0	5	4	1
6	2	2	5	1
7	3	1	4	0
9	0	4	5	0
7	1	2	3	0
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3	0	0	0	0
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13	4	2	1	0
14	5	3	3	0
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4	2	3	0	1
2	2	2	2	1
8	9	7	13	4
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0	0	2	14	0
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2	4	4	5	0
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4	2	2	0	1
7	5	5	4	1
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11	6	5	3	1
9	4	5	2	5
10	5	5	2	4
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4	2	4	4	0
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5	1	3	1	1
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0	0	2	0	0
0	0	2	0	0
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2	2	3	2	1
9	4	1	4	0
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5	1	1	1	0
11	5	3	5	0
2	2	2	2	0
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0	0	3	0	1
0	0	2	0	1
6	1	2	0	1
4	3	4	6	4
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2	4	4	0	0
7	1	1	0	0

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13	2	0	0	0
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2	1	3	2	1
2	1	4	2	1
4	0	1	12	0
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13	2	0	0	0
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11	3	3	3	4
4	2	3	0	1
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3	2	4	4	1
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7	5	4	3	1

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2	0	1	14	0
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4	2	2	0	0
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4	2	3	0	1
5	1	1	0	0
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10	4	2	3	0
2	4	4	5	0
3	2	3	1	0
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1	2	3	5	2
2	1	3	1	2
12	3	1	5	0
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	Metabolites from Machine Learning Methods (330) (used for MDS using CDK)			
C2SP2	C3SP2	C1SP3	C2SP3	C3SP3
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4	2	2	2	0

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3	3	3	0	0
4	2	6	0	0
2	0	2	2	0
6	1	1	0	0
4	3	2	0	0
4	2	2	1	0
4	5	4	5	3
6	4	4	7	0
6	1	1	0	0
2	0	3	0	1
7	3	1	0	0
6	0	2	0	0
5	1	2	0	1
7	1	0	0	0
4	2	4	5	4
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1	0	4	0	3
4	2	2	1	0
3	3	3	1	0
6	3	3	7	1
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4	2	3	0	1
8	4	0	2	0
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7	3	5	6	1
6	4	5	7	0
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8	4	0	2	0
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4	2	2	1	0
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7	7	7	7	3
6	4	5	7	0
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6	4	6	5	2
5	5	4	6	1
5	3	4	8	1
7	5	4	4	1
5	2	0	6	0
4	4	4	6	2
4	4	4	7	2
7	5	4	4	1
5	3	4	6	3
6	3	4	5	3
4	4	4	7	2
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6	4	4	7	0
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2	2	4	5	2
0	3	3	5	3
2	2	4	3	4
5	5	8	10	8
4	2	0	7	0
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2	2	4	4	2
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1	1	4	3	5
1	1	4	5	3
0	3	3	5	3

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4	2	4	4	0
3	1	4	3	1
6	0	1	10	0
1	1	4	4	3
6	2	1	0	0
3	1	3	1	2
1	1	3	2	2
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1	1	3	2	2
2	2	4	4	2
1	1	4	3	5
10	6	3	5	0
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13	3	2	0	1
11	3	2	2	1
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14	5	3	3	0
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2	2	2	2	1
0	0	5	5	4
11	3	2	2	1
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3	3	3	4	0
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0	0	3	3	3
1	1	5	3	1
1	1	4	3	1
6	2	4	7	2
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8	4	5	4	1
5	1	2	0	1
4	2	2	0	1
4	4	4	2	3
0	0	1	8	0
10	4	2	3	0
11	5	3	5	0
7	6	3	4	0
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4	3	3	5	3
4	3	3	7	3
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4	4	4	6	3

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9	4	5	2	5
10	5	5	2	4
4	2	4	4	0
4	2	4	0	0
5	1	3	1	1
10	4	2	1	0
2	4	4	0	0
6	1	5	6	0
4	4	7	10	4
6	1	0	1	0
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6	1	1	1	0
1	0	3	3	1
4	4	3	6	3
6	3	4	4	4
5	5	3	5	2
8	1	2	2	0
3	3	4	4	1
0	2	4	6	2
1	2	3	4	4
1	2	3	4	4
2	2	3	2	1
9	4	1	4	0
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6	0	0	0	0
11	5	3	5	0
0	0	1	5	0
4	2	4	7	4
0	0	3	5	0

5	1	1	1	0
11	5	3	5	0
6	1	2	0	1
4	3	4	6	4
2	4	4	0	0
7	1	1	0	0
2	1	2	2	2
5	2	0	0	0
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1	2	2	3	1
2	1	4	2	1
4	0	1	12	0
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11	4	2	3	3
11	4	2	3	3
11	4	2	3	3
11	3	3	3	4
4	2	3	0	1
5	1	1	0	0
7	1	1	0	0
8	8	8	13	6
5	1	3	0	0
3	2	4	4	1
0	0	1	7	0
0	0	2	7	0
5	4	3	5	2
7	5	4	3	1
7	5	4	1	1
12	2	1	1	0
12	2	1	1	0
0	0	1	6	0
4	2	3	0	1
6	0	0	0	0
6	0	0	0	0
2	0	1	14	0
6	4	4	7	0
5	2	2	0	0
5	4	5	9	2
5	4	6	8	3
5	4	5	7	2
5	4	6	6	3

4	2	2	0	0
6	1	1	0	0
5	1	1	0	0
4	2	3	0	1
1	5	5	0	0
1	2	1	3	1
10	4	3	4	3
9	5	3	4	3
4	2	2	1	0
5	1	1	1	0
5	1	0	0	0
5	2	2	0	0
4	2	4	0	2
5	3	4	8	1
4	4	4	8	1
10	4	2	3	0
9	5	2	3	0
9	3	2	3	1
11	3	1	1	2
10	4	1	1	2
10	4	2	3	0
6	0	1	8	0
0	1	2	3	2
0	1	3	4	5
7	5	5	9	0
8	0	1	8	0
6	1	0	0	0
1	3	3	3	0
5	1	3	0	0
4	2	4	7	4
4	2	2	3	1
4	2	3	0	1
5	1	1	0	0
4	3	4	3	0
13	3	2	0	1
10	4	2	3	0
2	4	4	5	0
3	2	3	1	0
1	2	3	5	2
2	1	3	1	2

	Metabolites after MDS using ADMET (112) (used for HCA and Scaffold analysis)			
C2SP2	C3SP2	C1SP3	C2SP3	C3SP3
6	1	1	0	0
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4	2	4	5	4
6	3	3	7	1
5	2	2	0	0
8	4	0	2	0
7	3	5	6	1
6	4	5	7	0
8	4	0	2	0
6	4	5	7	0
6	3	4	5	2
6	4	6	5	2
5	5	4	6	1
5	3	4	8	1
7	5	4	4	1
5	2	0	6	0
4	4	4	6	2
5	3	4	6	3
6	3	4	5	3
4	4	4	7	2
4	2	4	7	4
4	3	3	7	3
4	4	6	7	2
5	3	4	6	3
4	3	6	4	4
5	4	4	6	2
6	4	5	7	0
4	2	0	7	0
10	6	3	5	0
5	3	3	6	3
4	2	0	7	0
6	3	4	3	2
4	3	3	5	3
4	3	4	4	4
6	2	4	6	2

7	2	4	6	2
6	4	4	6	1
6	4	4	4	1
5	3	4	6	2
3	3	4	6	4
4	2	4	4	4
5	4	3	6	2
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3	4	3	7	3
4	3	3	7	3
7	5	4	4	1
4	2	4	5	4
7	6	3	4	0
7	6	3	2	0
7	5	4	4	1
7	5	4	4	1
7	5	4	1	1
7	5	4	3	1
7	5	4	0	1
7	3	4	2	1
4	2	4	2	4
3	3	4	2	4
7	6	3	4	0
5	2	0	6	0
4	4	4	5	2
7	5	4	2	1
5	1	2	1	1
6	2	4	7	2
7	2	4	6	2
7	2	4	6	2
8	4	5	4	1
4	2	2	0	1
4	4	4	2	3
11	5	3	5	0
7	6	3	4	0
4	3	3	5	3
4	3	3	7	3
5	3	4	6	3
4	4	4	6	3

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4	5	4	4	3
5	4	4	4	3
5	3	4	5	3
5	3	4	2	3
4	4	4	6	3
4	4	4	6	3
4	4	4	5	3
4	4	3	6	3
6	3	4	4	4
5	5	3	5	2
11	5	3	5	0
4	2	4	7	4
11	5	3	5	0
4	3	4	6	4
11	4	2	3	3
11	4	2	3	3
11	4	2	3	3
11	3	3	3	4
5	4	3	5	2
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10	4	3	4	3
9	5	3	4	3
4	2	4	0	2
4	4	4	8	1
10	4	2	3	0
9	5	2	3	0
9	3	2	3	1
10	4	1	1	2
10	4	2	3	0
4	2	4	7	4
4	2	2	3	1
4	2	3	0	1
	468 Metabolites and positive & negative controls			
nHBDon	nHBAcc	nAtomLC	nAtomP	nAtomLAC

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0	4	5	6	2
0	3	4	6	3
0	3	5	12	4
0	3	5	9	4
0	5	4	9	3
0	2	5	12	2
0	5	4	9	0
1	2	2	8	0
1	3	5	8	2
1	1	0	8	0
0	4	5	6	4
0	3	9	9	3
0	1	6	12	4
1	4	5	6	4
1	1	3	0	0
0	1	6	12	4
0	2	5	12	2
2	3	5	8	5
0	3	4	9	3
0	4	3	10	0
0	2	2	8	0
1	2	0	8	0
0	2	8	6	6
1	2	4	7	3
0	4	5	6	4
0	3	5	6	0
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1	3	2	8	0
2	3	0	8	0
0	4	6	9	3
0	3	9	6	7
1	3	4	9	0
0	3	4	6	3
0	3	4	6	3
0	3	9	6	4
0	3	7	6	7
0	3	6	9	3

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1	1	2	7	2
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1	4	5	7	3
1	5	5	6	4
0	3	4	6	3
0	3	5	6	0
0	1	2	7	0
1	5	6	6	2
0	7	5	9	3
0	4	4	9	3
0	3	3	8	0
0	2	2	8	0
0	3	4	9	3
0	3	5	6	0
0	3	4	6	3
0	3	4	9	0
0	2	2	6	2
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1	1	4	8	3
0	1	0	17	0
1	1	3	9	2
2	3	24	3	20
2	4	24	3	20
2	3	24	3	20
2	3	26	3	22
2	3	24	2	20
3	2	23	8	20
3	2	21	8	18
1	2	19	3	18
1	3	24	3	20
0	2	0	6	0
0	2	3	3	0
3	5	6	4	5
1	1	5	0	2
5	6	2	0	0
2	5	7	3	5
3	4	4	5	3
2	3	6	3	5
1	3	4	3	3
2	3	6	3	5

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2	3	7	3	4
2	3	4	6	3
0	3	4	5	3
5	6	6	16	5
2	4	3	7	2
3	3	4	9	3
3	3	4	7	3
2	3	5	3	4
1	0	5	8	5
1	2	3	2	0
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0	0	2	6	0
3	6	0	9	0
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1	1	7	0	6
1	1	12	0	11
0	0	6	0	6
0	0	5	0	5
1	0	0	7	0
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0	2	0	6	0
0	1	4	2	4
1	2	8	0	4
0	1	3	8	0
0	0	2	8	0
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1	1	7	0	7
0	0	2	6	0
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1	3	8	9	8
0	1	7	2	7
1	1	3	9	0
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0	0	2	6	0
2	1	5	10	5
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0	1	3	8	0
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2	0	2	17	0
3	0	2	19	0
1	1	5	13	5
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1	0	2	17	0
0	0	2	12	0
0	0	10	0	10
0	2	0	6	0
1	0	2	8	0
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1	2	5	11	5
1	2	5	17	5
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2	1	8	11	8
0	1	2	8	0
2	2	8	11	8
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3	3	5	11	5
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3	1	0	14	0
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1	0	5	12	5
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3	2	5	10	5
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2	0	5	15	5
2	1	5	8	5
1	1	5	8	5
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0	4	2	18	0
1	1	5	8	5
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0	1	4	10	3
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0	0	0	2	0
0	0	3	2	0
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1	1	3	2	0
0	0	3	2	0
0	0	5	2	5
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3	2	8	11	8
2	2	4	11	4
2	2	8	11	8
0	0	3	9	3
1	1	5	8	5
2	5	7	3	7
2	2	5	13	5
2	2	3	11	0
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4	2	4	16	4
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0	1	3	6	2
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0	0	0	2	0
0	0	3	2	0
1	1	3	2	0
1	1	0	0	0
1	2	5	11	5
1	2	4	6	2
0	1	4	6	4
0	0	3	4	0
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0	0	3	2	0
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1	2	4	10	4
3	3	3	11	3
2	1	3	8	3
3	2	3	8	3
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1	2	5	11	5
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0	2	7	3	4
2	2	8	11	8
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1	0	5	10	5
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0	1	5	10	5
1	0	5	8	5
2	2	5	11	5

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3	2	5	11	5
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3	2	8	11	8
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8	4	5	26	2
8	4	5	13	2

7	4	5	13	2
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3	0	2	21	0
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0	0	3	0	0
0	2	11	3	8
0	2	11	3	8
2	3	6	10	5
1	3	5	10	5
0	1	5	12	5
1	0	9	10	9
0	0	3	6	0
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2	0	8	8	8
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0	0	16	0	16
1	0	5	8	5
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3	0	8	8	8
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3	2	5	8	5
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4	0	0	21	0
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1	2	19	3	18
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8	5	2	21	0
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1	1	0	7	0
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0	1	3	4	0
1	0	2	8	2
2	2	3	11	2
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1	0	0	7	0
1	1	3	6	2
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0	1	2	10	0
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0	1	4	2	3
1	0	3	7	0
0	3	7	5	3
1	1	4	0	3
2	2	4	0	3
1	0	3	7	3
0	0	0	6	0
5	0	0	22	0
2	1	5	8	5
3	3	5	11	5
1	0	2	8	2
2	2	3	11	2
1	0	2	8	2
0	0	2	16	2
2	2	3	19	2
2	0	2	8	2

2	2	5	11	5
1	2	17	3	16
0	0	3	2	0
1	1	2	9	0
0	0	3	2	0
2	0	12	8	12
1	2	19	3	18
0	0	2	8	0
1	1	3	0	3
0	0	3	2	0
0	0	3	6	3
1	1	5	8	5
1	2	0	6	0
1	0	3	7	0
0	0	0	6	0
0	0	12	4	12
4	0	4	20	4
3	0	4	8	4
0	0	7	2	7
0	0	8	4	8
0	0	13	0	13
2	1	3	7	2
0	0	11	0	11
0	0	3	2	0
0	1	0	4	0
7	5	2	20	0
4	2	6	13	3
	Metabolites from Machine Learning Methods (330) (used for MDS using CDK)			
nHBDon	nHBAcc	nAtomLC	nAtomP	nAtomLAC
0	0	0	6	0
0	0	2	6	0
0	0	0	6	0
0	0	2	6	0
0	0	6	0	6
1	0	0	7	0
1	0	3	7	0
0	2	2	6	0
0	1	3	8	0
0	0	2	8	0

0	0	2	6	0
1	1	5	10	5
1	3	8	9	8
1	1	3	9	0
0	2	3	6	0
0	0	0	10	0
1	1	4	7	2
1	2	4	10	0
1	2	5	12	3
2	1	3	8	3
1	0	0	7	0
0	0	6	2	6
0	0	2	6	0
0	0	2	6	0
2	1	5	10	5
0	1	3	8	0
0	1	3	8	0
0	0	7	0	7
1	2	4	10	0
2	0	2	17	0
3	0	2	19	0
1	1	5	13	5
2	1	8	11	8
0	0	0	2	0
0	1	3	10	0
1	0	2	17	0
0	0	2	12	0
0	0	10	0	10
1	0	2	8	0
1	1	3	6	2
1	2	5	11	5
1	2	5	17	5
0	4	8	11	8
2	1	8	11	8
0	1	2	8	0
3	0	5	15	5
0	0	0	6	0
0	2	3	3	3
2	3	5	10	5
1	3	5	10	5
2	2	5	12	5

1	0	5	12	5
2	1	5	8	5
2	0	5	15	5
0	1	2	8	0
1	3	5	13	5
3	2	5	10	5
2	0	5	15	5
2	1	5	8	5
1	1	5	8	5
1	1	5	10	5
0	4	2	18	0
1	1	5	8	5
2	1	5	8	5
2	2	5	10	5
2	1	5	8	5
2	2	4	8	3
1	1	5	12	5
2	4	5	11	5
2	4	5	11	5
2	0	8	8	8
2	1	8	11	8
0	4	8	11	8
0	1	3	8	0
0	0	0	2	0
1	1	7	2	7
0	0	3	2	0
0	0	3	2	0
1	2	5	11	5
2	1	2	8	0
0	0	0	2	0
0	0	5	2	5
0	0	3	2	0
0	0	3	2	0
1	1	3	2	0
0	0	3	2	0
0	0	0	2	0
0	0	0	2	0
1	1	4	2	4
1	2	19	3	18
0	0	0	2	0
0	1	4	10	3

0	0	3	4	0
0	0	0	2	0
0	0	3	2	0
1	2	5	11	5
0	0	3	4	0
1	1	3	2	0
0	0	3	2	0
0	0	5	2	5
0	0	3	2	0
2	2	8	11	8
0	0	3	9	3
1	1	5	8	5
2	5	7	3	7
3	0	4	19	4
2	0	4	18	4
4	2	4	16	4
0	0	0	2	0
0	0	0	2	0
0	1	2	8	0
0	1	2	8	0
0	1	2	14	0
0	1	4	6	3
1	1	2	6	0
0	2	4	6	0
0	1	3	6	2
2	1	2	8	0
0	1	0	2	0
0	0	0	2	0
0	0	0	2	0
0	0	3	2	0
1	1	3	2	0
1	2	5	11	5
0	1	4	6	4
0	0	3	4	0
0	0	0	2	0
0	0	3	2	0
1	2	4	10	4
2	1	3	8	3
3	2	3	8	3
1	2	5	11	5
0	0	0	2	0

0	0	0	2	0
1	2	5	10	5
0	1	5	12	5
1	0	5	10	5
2	2	5	13	5
1	0	5	10	5
2	2	5	13	5
0	0	5	8	5
0	1	5	10	5
1	0	5	8	5
2	2	5	11	5
1	0	3	8	3
2	0	5	8	5
1	0	5	8	5
2	0	3	8	3
2	0	3	8	3
3	3	5	11	5
2	1	5	8	5
3	0	4	21	4
1	0	5	14	5
2	0	8	8	8
1	0	8	8	8
0	2	8	8	8
2	0	8	8	8
2	1	3	8	3
3	2	4	8	4
2	0	8	8	8
2	0	5	16	5
2	0	3	16	3
0	0	5	14	5
1	0	5	14	5
1	0	2	14	2
1	0	4	14	4
1	0	0	14	0
1	0	5	10	5
0	0	0	8	0
1	0	0	8	0
2	2	3	11	0
0	0	5	16	5
3	2	5	8	5
1	1	2	8	0

3	2	5	10	5
2	2	3	9	3
1	0	3	14	3
3	0	8	21	8
3	0	4	21	4
3	0	8	21	8
1	2	4	11	0
4	2	8	8	8
1	0	3	7	0
0	1	3	4	0
0	2	3	3	0
1	1	2	16	2
1	1	0	0	0
0	0	12	4	12
0	0	7	2	7
0	0	8	4	8
0	0	3	0	0
0	2	11	3	8
0	2	11	3	8
2	3	6	10	5
1	3	5	10	5
0	1	5	12	5
1	0	9	10	9
0	0	3	6	0
0	1	3	8	0
2	2	3	11	0
0	1	11	2	10
1	0	4	8	4
1	0	8	8	8
1	0	5	16	5
0	0	0	2	0
1	0	3	8	3
1	0	5	8	5
1	0	5	8	5
2	2	5	11	5
1	0	3	8	3
2	2	4	11	4
1	0	4	8	4
1	0	4	8	4
1	0	0	8	0
2	2	5	11	5

2	2	5	11	5
2	2	4	11	4
0	0	3	2	0
2	0	4	8	4
4	1	8	11	8
3	1	0	11	0
3	1	0	11	0
0	4	7	12	4
0	4	5	12	0
0	2	5	6	3
0	2	5	16	3
0	0	0	6	0
0	2	5	9	4
1	2	5	11	5
0	0	3	7	3
2	2	8	11	8
1	0	3	8	3
0	1	3	10	3
0	1	0	2	0
3	2	7	8	7
3	2	7	8	7
3	1	7	8	7
0	1	4	6	3
0	0	7	4	7
1	1	3	2	0
0	0	3	2	0
0	0	3	2	0
0	0	3	2	0
3	1	4	8	4
1	1	0	0	0
1	0	2	8	0
2	0	8	8	8
0	1	8	2	7
1	0	5	8	5
0	2	10	3	6
1	1	4	7	2
3	0	8	8	8
0	1	4	8	3
3	2	5	8	5
0	0	0	6	0
1	0	3	10	3

0	0	3	2	0
0	1	0	10	0
0	2	0	0	0
0	0	3	2	0
0	2	9	3	8
1	2	19	3	18
0	0	0	2	0
2	0	3	16	2
3	0	3	17	2
2	0	3	17	0
2	1	0	17	0
0	0	3	6	0
0	3	4	12	0
0	0	3	10	3
2	0	5	8	5
1	0	3	7	3
1	1	12	2	12
0	1	10	2	9
0	0	9	0	9
2	0	4	8	4
1	0	4	14	4
1	0	2	14	2
3	2	6	12	3
3	2	6	13	3
0	1	9	2	8
0	0	3	6	0
0	0	2	8	0
1	0	2	8	0
1	2	19	3	18
1	0	8	8	8
0	1	3	8	0
1	0	6	8	5
0	0	6	8	5
1	0	5	8	5
0	0	5	8	5
0	0	0	6	0
0	1	3	9	0
1	1	0	7	0
0	0	3	6	0
0	0	0	6	0
0	1	3	4	0

1	0	2	8	2
2	2	3	11	2
0	0	2	6	0
1	1	3	6	2
0	1	2	10	0
0	1	3	8	0
1	0	3	7	0
2	1	5	8	5
3	3	5	11	5
1	0	2	8	2
2	2	3	11	2
1	0	2	8	2
0	0	2	16	2
2	2	3	19	2
2	0	2	8	2
1	2	17	3	16
0	0	3	2	0
0	0	3	2	0
2	0	12	8	12
1	2	19	3	18
0	0	2	8	0
0	0	3	2	0
0	0	3	6	3
1	1	5	8	5
1	2	0	6	0
1	0	3	7	0
0	0	0	6	0
0	0	12	4	12
4	0	4	20	4
3	0	4	8	4
0	0	7	2	7
0	0	8	4	8
0	0	3	2	0
0	1	0	4	0
	Metabolites after MDS using ADMET (112) (used for HCA and Scaffold analysis)			
nHBDon	nHBAcc	nAtomLC	nAtomP	nAtomLAC
0	1	3	8	0
1	1	5	10	5
2	1	3	8	3

2	1	5	10	5
0	1	3	8	0
2	0	2	17	0
1	1	5	13	5
2	1	8	11	8
1	0	2	17	0
0	4	8	11	8
2	3	5	10	5
2	2	5	12	5
1	0	5	12	5
2	1	5	8	5
2	0	5	15	5
0	1	2	8	0
1	3	5	13	5
2	1	5	8	5
1	1	5	8	5
1	1	5	10	5
1	1	5	8	5
2	1	5	8	5
2	2	5	10	5
2	1	5	8	5
2	2	4	8	3
1	1	5	12	5
2	1	8	11	8
2	1	2	8	0
2	2	8	11	8
1	1	5	8	5
2	1	2	8	0
1	2	4	10	4
2	1	3	8	3
3	2	3	8	3
1	2	5	10	5
0	1	5	12	5
2	2	5	13	5
2	2	5	13	5
0	1	5	10	5
2	2	5	11	5
1	0	3	8	3
2	0	5	8	5
1	0	5	8	5
2	0	3	8	3

2	0	3	8	3
3	3	5	11	5
2	1	5	8	5
1	0	5	14	5
2	1	3	8	3
2	0	5	16	5
2	0	3	16	3
0	0	5	14	5
1	0	5	14	5
1	0	2	14	2
1	0	4	14	4
1	0	0	14	0
1	0	5	10	5
1	0	0	8	0
2	2	3	11	0
0	0	5	16	5
1	1	2	8	0
2	2	3	9	3
1	0	3	14	3
1	2	4	11	0
2	3	6	10	5
1	3	5	10	5
0	1	5	12	5
1	0	9	10	9
0	1	3	8	0
2	2	3	11	0
1	0	8	8	8
1	0	5	16	5
1	0	3	8	3
1	0	5	8	5
1	0	5	8	5
2	2	5	11	5
1	0	3	8	3
2	2	4	11	4
1	0	4	8	4
1	0	4	8	4
1	0	0	8	0
2	2	5	11	5
2	2	5	11	5
2	2	4	11	4
3	2	7	8	7

3	2	7	8	7
3	1	7	8	7
2	0	8	8	8
1	0	5	8	5
3	0	8	8	8
3	2	5	8	5
2	0	3	16	2
3	0	3	17	2
2	0	3	17	0
2	1	0	17	0
2	0	4	8	4
1	0	4	14	4
1	0	2	14	2
1	0	6	8	5
1	0	5	8	5
1	0	2	8	2
2	2	3	11	2
1	0	3	7	0
3	3	5	11	5
1	0	2	8	2
2	2	3	11	2
1	0	2	8	2
2	2	3	19	2
2	0	2	8	2
1	1	5	8	5
1	2	0	6	0
1	0	3	7	0
	468 Metabolites and positive & negative controls			
MLogP	nRotB	nSmallRings	nAromRings	nRingBlocks
3.77	6	7	1	1
3.11	6	2	1	2
3.44	7	3	2	3
3.55	9	3	2	3
3	5	2	1	2
4.21	8	5	4	4
3.66	8	3	2	3
3.55	9	3	2	3
2.89	8	3	3	2
2.78	5	4	1	2

3	1	5	1	1
2.89	4	5	1	1
3	0	5	1	1
3.77	7	4	2	4
3.44	9	2	2	2
2.89	6	2	2	2
4.1	7	4	3	4
1.57	0	0	0	0
2.78	5	2	2	2
3.11	10	3	3	2
3.66	4	7	1	1
3.55	7	3	2	3
3.11	4	5	1	1
3	1	5	1	1
2.89	0	5	1	1
3.55	7	2	2	2
2.78	3	2	1	2
3.77	7	4	2	4
2.78	4	2	1	2
2.89	0	5	1	1
2.78	0	5	1	1
2.89	1	5	1	1
2.78	0	5	1	1
2.78	6	2	1	2
3.66	9	2	2	2
2.67	5	2	1	2
3	5	2	1	2
2.89	4	2	1	2
3.55	9	2	2	2
3.66	7	3	2	3
3	6	2	1	2
3.66	3	4	2	2
3.88	3	5	2	2
3.55	8	3	2	3
3.55	9	3	2	3
3.88	7	4	2	4
3	4	2	1	2
2.89	4	2	1	2
3.22	1	4	1	1
2.89	9	2	1	2
2.89	10	2	1	2

3.33	9	3	2	3
3.11	3	5	1	1
3.11	2	5	1	1
3.22	7	3	2	3
3	5	2	1	2
3	4	2	1	2
2.67	4	2	1	2
3.88	5	4	2	4
3.22	4	4	2	1
2.34	3	2	1	1
2.89	1	3	3	2
2.23	5	1	1	1
3.55	17	0	0	0
3.55	18	0	0	0
3.55	18	0	0	0
3.77	19	0	0	0
3.66	18	0	0	0
4.1	18	1	1	1
3.88	19	1	1	1
3.22	15	0	0	0
3.55	17	0	0	0
2.34	1	2	1	2
1.46	0	0	0	0
1.9	5	2	0	1
1.79	2	0	0	0
1.46	1	1	0	1
1.46	4	0	0	0
1.57	3	1	1	1
1.79	3	0	0	0
1.46	1	0	0	0
1.79	3	0	0	0
1.68	5	0	0	0
1.57	4	0	0	0
2.12	3	1	1	1
1.46	1	0	0	0
2.23	5	3	3	1
2.12	4	2	2	2
2.23	3	2	2	1
2.01	3	1	1	1
1.68	2	0	0	0
3.55	4	3	1	1

1.46	0	0	0	0
2.56	0	1	1	1
2.56	2	1	1	1
1.13	0	1	1	1
1.9	0	1	1	1
2.56	2	1	1	1
1.79	2	0	0	0
2.01	5	0	0	0
2.01	4	0	0	0
2.56	9	0	0	0
2.45	3	0	0	0
2.34	2	0	0	0
2.34	0	1	1	1
2.89	2	1	1	1
2.12	2	1	1	1
1.9	0	1	1	1
1.79	1	0	0	0
1.9	5	0	0	0
2.12	1	1	1	1
2.56	1	1	1	1
1.68	3	0	0	0
2.23	5	0	0	0
2.45	1	1	1	1
3.66	5	3	1	1
3.44	9	1	0	1
2.12	4	0	0	0
2.12	1	1	1	1
2.12	1	1	1	1
1.68	0	1	0	1
2.67	0	2	2	1
1.68	0	1	1	1
1.79	0	0	0	0
2.12	2	0	0	0
1.46	1	0	0	0
2.12	3	1	1	1
2.34	4	1	1	1
2.23	3	1	1	1
3.22	3	3	1	1
2.34	0	1	1	1
2.45	3	0	0	0
2.45	1	1	1	1

2.56	1	1	1	1
3.44	8	2	1	1
2.45	2	1	1	1
2.34	1	1	1	1
2.34	4	0	0	0
2.01	0	1	0	1
2.12	2	0	0	0
2.45	4	1	1	1
1.9	2	0	0	0
2.78	3	3	2	1
2.67	2	3	3	1
3.55	9	2	1	1
3.55	11	1	1	1
2.56	0	2	0	1
2.23	4	1	1	1
2.89	4	3	2	1
2.23	1	2	2	1
2.67	7	0	0	0
1.79	0	1	1	1
2.12	1	1	1	1
2.34	2	1	1	1
1.79	0	1	1	1
4.54	8	4	1	2
4.54	8	4	2	2
3.55	11	1	0	1
3.55	11	1	1	1
2.23	1	1	1	1
3.55	11	1	1	1
3.11	5	2	2	2
2.56	0	2	1	1
2.12	2	1	0	1
3.22	10	2	1	2
3.22	10	2	1	2
3.22	7	2	1	1
3.11	7	2	1	1
3.66	1	5	3	2
3.11	3	3	3	2
3.55	6	3	1	1
3.55	4	3	1	1
3.44	7	2	1	1
3.44	4	3	2	1

2.89	2	3	1	1
3.33	8	3	2	1
3.33	4	3	1	1
3.33	5	3	2	1
3.44	4	3	2	1
3.44	4	3	1	1
3.44	4	3	1	1
3.44	4	4	1	1
2.78	4	3	1	1
3.44	4	4	1	1
3.44	4	3	1	1
3.55	6	3	1	1
3.44	4	3	1	1
3.44	4	3	1	1
3.44	4	3	1	1
3.44	8	3	1	1
3.44	8	3	1	1
3.55	9	1	1	1
1.57	0	0	0	0
1.46	0	0	0	0
1.46	0	0	0	0
1.68	0	0	0	0
3.55	11	1	1	1
3.55	11	1	0	1
1.68	1	0	0	0
2.23	1	1	1	1
3.11	0	3	0	1
3	4	1	0	1
3.11	1	2	0	1
3.11	1	2	0	1
5.09	8	5	1	2
2.78	1	3	1	1
3.11	0	4	0	1
3.11	3	3	0	1
3.11	1	5	0	1
3.11	1	3	0	1
3	1	2	0	1
3.11	1	2	0	1
3.11	0	3	0	1
3.11	0	0	0	1
2.78	2	1	0	1

3.22	13	0	0	0
3.11	0	5	0	1
2.45	2	1	1	1
2.56	1	1	0	1
2.56	0	3	0	1
3.11	1	2	0	1
4.54	8	4	1	2
2.56	1	1	0	1
2.45	1	1	0	1
2.56	1	2	0	1
3.11	3	3	0	1
3.11	1	5	0	1
3.22	8	2	2	2
3.77	9	2	2	2
3.33	7	2	2	2
3.88	10	2	2	2
2.45	2	1	1	1
3.44	6	3	1	1
3.22	6	1	0	1
3	4	2	1	1
3	1	4	1	1
2.56	1	3	3	2
3.22	4	2	2	2
3.33	4	2	2	2
3	5	2	2	2
3.11	5	2	2	2
3.11	0	3	0	1
3.11	0	3	0	1
2.12	1	1	1	1
2.12	0	1	1	1
2.78	2	2	2	2
3.22	5	2	2	2
2.23	3	1	1	1
2.12	1	1	1	1
2.12	3	1	1	1
2.23	1	1	1	1
2.78	1	3	1	1
3	0	2	0	1
3.11	0	1	0	1
3.11	0	4	0	1
3.11	3	1	0	1

3	1	2	0	1
2.45	0	3	0	1
4.43	7	6	1	2
2.12	3	1	1	1
2.89	2	1	0	1
2.56	1	1	0	1
2.56	0	3	0	1
3.11	1	2	0	1
6.3	25	5	0	2
1.68	2	1	1	1
3.11	5	2	1	1
3.11	4	3	1	1
3.22	3	3	1	1
3.22	2	3	1	1
2.45	0	3	0	1
5.09	8	5	1	2
1.9	1	0	0	0
1.79	4	0	0	0
5.2	14	3	1	2
3.11	0	3	0	1
2.56	0	3	0	1
3.22	7	2	1	1
3.44	4	2	1	1
3.55	7	2	1	1
3.44	8	2	1	1
3.33	5	2	1	1
3.22	6	2	1	1
3.55	4	4	1	1
3.44	7	3	2	1
3.55	4	4	1	1
3.44	5	4	1	1
3.33	2	4	1	1
3.55	6	2	1	2
3.44	7	2	1	2
3.66	7	2	1	2
3.11	2	2	1	2
3.33	4	2	1	2
3.22	5	2	1	2
3.33	6	3	1	1
3.33	6	3	1	1
3.44	5	3	1	1

3.11	4	3	3	2
3.55	5	3	3	1
3.55	9	1	1	1
3.55	11	1	1	1
3.44	10	1	1	1
3.66	10	1	1	1
3.55	9	1	0	1
3.33	7	1	1	1
3.22	8	1	1	1
3.22	3	3	1	1
3.22	6	2	1	2
3.55	9	1	1	1
3.44	10	1	1	1
3.55	6	2	2	2
3.33	4	2	2	2
3.66	5	3	2	1
3.55	4	3	2	1
3.22	1	3	2	1
3.44	3	3	2	1
3.44	5	3	2	1
3.11	0	3	2	1
3.11	3	2	1	1
3	4	2	1	1
3.11	0	4	1	1
3.11	0	4	1	1
3	1	4	1	1
3.55	4	4	3	1
3.33	4	3	1	1
3.11	6	1	0	1
4.1	11	5	5	4
4.1	11	5	4	4
4.21	12	5	4	4
4.32	13	5	4	4
2.78	1	3	1	1
3.33	4	3	1	1
3.22	2	3	1	1
3.33	2	3	2	1
3.66	7	3	3	2
3.11	4	3	3	2
3.66	7	3	3	2
2.34	3	2	1	1

3.33	10	1	1	1
2.45	1	1	1	1
2.45	1	1	0	1
5.42	14	5	2	3
3.11	2	4	0	1
3.11	14	0	0	0
3.33	3	3	2	2
2.89	4	2	1	1
2.56	2	3	3	2
2.45	0	3	0	1
3.11	7	0	0	0
3.11	3	1	0	1
2.56	3	0	0	0
2.56	1	2	0	1
2.56	7	0	0	0
2.45	7	0	0	0
3.22	8	2	1	1
3.22	8	2	1	1
3.44	4	2	1	1
3.66	6	2	1	1
2.45	1	1	1	1
2.45	2	1	1	1
3.55	7	2	1	1
3	1	3	1	1
2.45	8	0	0	0
3.44	6	2	2	2
3.99	9	2	2	2
3.55	5	3	3	1
2.56	0	2	0	1
3.33	3	3	1	1
3.55	5	3	1	1
3.55	4	3	1	1
3.44	5	3	1	1
3.33	2	3	1	1
3.44	4	3	1	1
3.55	3	3	1	1
3.44	3	3	1	1
3.11	0	3	1	1
3.44	5	3	1	1
3.44	5	3	1	1
3.33	4	3	1	1

3.11	1	2	0	1
3.22	6	2	2	2
3.33	5	2	2	2
3	8	1	1	1
3.66	4	4	2	2
3.66	6	3	2	2
3.66	1	6	2	2
3.66	1	5	2	2
1.9	2	0	0	0
2.78	10	1	1	1
2.34	6	1	1	1
2.56	4	1	1	1
1.35	0	0	0	0
1.57	0	0	0	0
2.78	9	0	0	0
3.22	3	3	2	1
2.56	0	1	1	1
3.11	8	2	1	2
4.54	7	6	1	2
2.45	3	1	1	1
1.68	2	0	0	0
1.46	1	0	0	0
1.57	0	1	0	1
1.57	0	1	0	1
5.09	13	3	1	2
2.34	3	1	1	1
2.45	5	1	1	1
2.45	0	3	0	1
2.45	0	3	0	1
3.44	5	3	1	1
3.44	4	3	1	1
3.55	6	2	1	2
1.35	0	0	0	0
1.79	1	1	1	1
2.89	5	2	2	2
3.11	4	1	0	1
3	1	2	0	1
3.11	1	2	0	1
1.9	1	1	0	1
3.11	1	2	0	1
2.56	1	1	0	1

3.22	6	2	2	2
3	0	3	0	1
4.32	14	5	4	4
2.01	1	1	1	1
3.88	8	2	2	2
2.12	5	0	0	0
3.22	13	0	0	0
3.55	4	3	1	1
2.01	4	0	0	0
2.01	5	0	0	0
2.23	7	0	0	0
3.22	5	2	2	2
2.34	3	1	1	1
3.77	8	2	2	2
2.45	4	0	0	0
1.9	2	0	0	0
2.56	2	3	0	1
2.45	4	3	0	1
1.9	0	0	0	0
1.79	1	0	0	0
2.45	2	1	1	1
3.44	4	3	1	1
1.46	0	0	0	0
2.56	0	1	1	1
2.34	2	1	1	1
2.56	1	1	0	1
2.01	1	0	0	0
2.34	0	2	2	1
2.45	1	3	3	2
2.34	1	3	0	2
2.56	1	1	0	1
2.45	4	0	0	0
2.56	6	0	0	0
3.22	14	0	0	0
3.11	0	4	0	1
2.45	1	3	3	2
3.88	4	3	2	3
3.77	4	3	2	3
3.77	3	4	3	3
3.66	1	5	3	2

2.56	1	1	1	1
1.79	1	0	0	0
2.01	4	0	0	0
1.57	1	0	0	0
2.12	4	1	1	1
2.01	2	1	1	1
2.12	2	1	1	1
1.35	1	0	0	0
2.23	2	0	0	0
2.12	6	0	0	0
1.35	0	0	0	0
2.45	3	1	1	1
2.01	2	1	1	1
1.9	4	0	0	0
1.35	0	0	0	0
5.75	10	6	2	2
2.23	3	0	0	0
2.45	1	1	1	1
2.56	4	0	0	0
2.45	4	0	0	0
3	7	0	0	0
1.79	1	1	1	1
2.34	7	0	0	0
2.45	6	0	0	0
3.44	5	2	1	2
3.44	3	3	2	1
3.22	1	3	2	1
2.89	6	2	2	2
2.89	7	2	2	2
2.23	6	0	0	0
2.56	1	1	1	1
2.12	2	1	1	1
2.01	1	1	1	1
3.22	15	0	0	0
3.66	10	1	1	1
2.34	1	1	1	1
4.1	11	2	1	2
4.21	9	3	1	1
3.88	9	2	1	2
3.99	7	3	1	1
2.56	3	4	3	3

2.34	0	1	1	1
2.23	2	1	1	1
2.12	0	1	1	1
2.56	1	1	1	1
3.11	12	0	0	0
2.67	0	1	1	1
1.9	3	0	0	0
2.45	2	1	0	1
3.88	3	4	2	2
3.77	4	4	2	2
2.45	1	1	1	1
2.01	0	1	1	1
2.23	2	1	1	1
1.9	0	1	0	1
2.01	1	2	1	1
2.34	1	1	1	1
1.68	1	0	0	0
2.67	2	1	1	1
1.79	4	0	0	0
1.68	1	0	0	0
1.57	1	0	0	0
2.45	1	1	1	1
2.34	0	1	1	1
2.34	1	3	3	2
3.44	9	2	1	2
3.33	10	2	1	2
3.33	3	3	2	2
3.22	4	3	2	2
3.33	3	4	2	2
3.33	3	4	2	2
3.11	3	4	2	2
3.22	3	3	2	2
3.55	4	4	1	1
3	11	0	0	0
2.56	1	2	0	1
2.01	1	1	1	1
3.11	1	5	0	1
4.1	12	1	1	1
3.22	12	0	0	0
2.34	1	1	1	1
1.79	0	0	0	0

2.56	0	1	0	1
2.56	1	1	1	1
3.44	4	4	1	1
2.67	1	3	1	2
2.45	1	1	1	1
2.23	0	1	1	1
3.11	6	0	0	0
3.11	4	2	2	2
3.22	5	2	2	2
3.11	3	1	0	1
2.56	3	0	0	0
2.89	10	0	0	0
2.12	2	1	1	1
2.67	8	0	0	0
3.11	1	2	0	1
2.45	0	3	0	1
2.67	3	4	3	3
2.78	6	2	2	2
	Metabolites from Machine Learning Methods (330) (used for MDS using CDK)			
MLogP	nRotB	nSmallRings	nAromRings	nRingBlocks
2.56	0	1	1	1
2.56	2	1	1	1
1.9	0	1	1	1
2.56	2	1	1	1
2.45	3	0	0	0
2.34	0	1	1	1
2.89	2	1	1	1
2.12	2	1	1	1
2.12	1	1	1	1
2.56	1	1	1	1
2.45	1	1	1	1
3.66	5	3	1	1
3.44	9	1	0	1
2.12	1	1	1	1
2.12	1	1	1	1
2.67	0	2	2	1
2.12	3	1	1	1
2.34	4	1	1	1
2.23	3	1	1	1

3.22	3	3	1	1
2.34	0	1	1	1
2.45	3	0	0	0
2.45	1	1	1	1
2.56	1	1	1	1
3.44	8	2	1	1
2.45	2	1	1	1
2.34	1	1	1	1
2.34	4	0	0	0
2.45	4	1	1	1
2.78	3	3	2	1
2.67	2	3	3	1
3.55	9	2	1	1
3.55	11	1	1	1
2.56	0	2	0	1
2.23	4	1	1	1
2.89	4	3	2	1
2.23	1	2	2	1
2.67	7	0	0	0
2.12	1	1	1	1
2.34	2	1	1	1
4.54	8	4	1	2
4.54	8	4	2	2
3.55	11	1	0	1
3.55	11	1	1	1
2.23	1	1	1	1
3.11	5	2	2	2
2.56	0	2	1	1
2.12	2	1	0	1
3.22	7	2	1	1
3.11	7	2	1	1
3.55	6	3	1	1
3.55	4	3	1	1
3.44	7	2	1	1
3.44	4	3	2	1
2.89	2	3	1	1
3.33	8	3	2	1
3.33	4	3	1	1
3.44	4	3	2	1
3.44	4	3	1	1
3.44	4	3	1	1

3.44	4	4	1	1
2.78	4	3	1	1
3.44	4	4	1	1
3.44	4	3	1	1
3.55	6	3	1	1
3.44	4	3	1	1
3.44	4	3	1	1
3.44	4	3	1	1
3.44	8	3	1	1
3.44	8	3	1	1
3.55	9	1	1	1
3.55	11	1	1	1
3.55	11	1	0	1
2.23	1	1	1	1
3.11	0	3	0	1
3	4	1	0	1
3.11	1	2	0	1
3.11	1	2	0	1
5.09	8	5	1	2
2.78	1	3	1	1
3.11	0	4	0	1
3.11	3	3	0	1
3.11	1	5	0	1
3.11	1	3	0	1
3	1	2	0	1
3.11	1	2	0	1
3.11	0	3	0	1
3.11	0	0	0	1
2.78	2	1	0	1
3.22	13	0	0	0
3.11	0	5	0	1
2.45	2	1	1	1
2.56	1	1	0	1
2.56	0	3	0	1
3.11	1	2	0	1
4.54	8	4	1	2
2.56	1	1	0	1
2.45	1	1	0	1
2.56	1	2	0	1
3.11	3	3	0	1
3.11	1	5	0	1

3.88	10	2	2	2
2.45	2	1	1	1
3.44	6	3	1	1
3.22	6	1	0	1
3.22	4	2	2	2
3.33	4	2	2	2
3.11	5	2	2	2
3.11	0	3	0	1
3.11	0	3	0	1
2.12	1	1	1	1
2.12	0	1	1	1
2.78	2	2	2	2
3.22	5	2	2	2
2.12	1	1	1	1
2.12	3	1	1	1
2.23	1	1	1	1
2.78	1	3	1	1
3	0	2	0	1
3.11	0	1	0	1
3.11	0	4	0	1
3.11	3	1	0	1
3	1	2	0	1
4.43	7	6	1	2
2.89	2	1	0	1
2.56	1	1	0	1
2.56	0	3	0	1
3.11	1	2	0	1
3.11	5	2	1	1
3.22	3	3	1	1
3.22	2	3	1	1
5.09	8	5	1	2
3.11	0	3	0	1
2.56	0	3	0	1
3.22	7	2	1	1
3.44	4	2	1	1
3.55	7	2	1	1
3.44	8	2	1	1
3.33	5	2	1	1
3.22	6	2	1	1
3.55	4	4	1	1
3.44	7	3	2	1

3.55	4	4	1	1
3.44	5	4	1	1
3.33	2	4	1	1
3.55	6	2	1	2
3.66	7	2	1	2
3.11	2	2	1	2
3.33	4	2	1	2
3.33	6	3	1	1
3.44	5	3	1	1
3.11	4	3	3	2
3.55	5	3	3	1
3.55	9	1	1	1
3.66	10	1	1	1
3.55	9	1	0	1
3.33	7	1	1	1
3.22	3	3	1	1
3.22	6	2	1	2
3.55	9	1	1	1
3.55	6	2	2	2
3.33	4	2	2	2
3.66	5	3	2	1
3.55	4	3	2	1
3.22	1	3	2	1
3.44	3	3	2	1
3.11	0	3	2	1
3.11	3	2	1	1
3.11	0	4	1	1
3.11	0	4	1	1
3	1	4	1	1
3.55	4	4	3	1
3.33	4	3	1	1
2.78	1	3	1	1
3.33	4	3	1	1
3.22	2	3	1	1
3.33	2	3	2	1
3.66	7	3	3	2
3.11	4	3	3	2
3.66	7	3	3	2
2.34	3	2	1	1
3.33	10	1	1	1
2.45	1	1	1	1

2.45	1	1	0	1
3.11	2	4	0	1
3.33	3	3	2	2
2.45	0	3	0	1
3.11	7	0	0	0
3.11	3	1	0	1
2.56	3	0	0	0
2.56	1	2	0	1
2.56	7	0	0	0
2.45	7	0	0	0
3.22	8	2	1	1
3.22	8	2	1	1
3.44	4	2	1	1
3.66	6	2	1	1
2.45	1	1	1	1
2.45	2	1	1	1
3	1	3	1	1
2.45	8	0	0	0
3.44	6	2	2	2
3.99	9	2	2	2
3.55	5	3	3	1
2.56	0	2	0	1
3.33	3	3	1	1
3.55	5	3	1	1
3.55	4	3	1	1
3.44	5	3	1	1
3.33	2	3	1	1
3.44	4	3	1	1
3.55	3	3	1	1
3.44	3	3	1	1
3.11	0	3	1	1
3.44	5	3	1	1
3.44	5	3	1	1
3.33	4	3	1	1
3.11	1	2	0	1
3.33	5	2	2	2
3.66	6	3	2	2
3.66	1	6	2	2
3.66	1	5	2	2
2.78	10	1	1	1
2.34	6	1	1	1

2.56	4	1	1	1
3.22	3	3	2	1
2.56	0	1	1	1
3.11	8	2	1	2
4.54	7	6	1	2
2.45	3	1	1	1
5.09	13	3	1	2
2.34	3	1	1	1
2.45	5	1	1	1
2.45	0	3	0	1
3.44	5	3	1	1
3.44	4	3	1	1
3.55	6	2	1	2
2.89	5	2	2	2
3.11	4	1	0	1
3	1	2	0	1
3.11	1	2	0	1
3.11	1	2	0	1
2.56	1	1	0	1
3.22	6	2	2	2
3	0	3	0	1
2.01	1	1	1	1
3.88	8	2	2	2
2.12	5	0	0	0
3.55	4	3	1	1
2.23	7	0	0	0
2.34	3	1	1	1
3.77	8	2	2	2
2.45	2	1	1	1
3.44	4	3	1	1
2.56	0	1	1	1
2.34	2	1	1	1
2.56	1	1	0	1
2.34	0	2	2	1
2.34	1	3	0	2
2.56	1	1	0	1
2.56	6	0	0	0
3.22	14	0	0	0
3.11	0	4	0	1
3.88	4	3	2	3
3.77	4	3	2	3

3.77	3	4	3	3
3.66	1	5	3	2
2.56	1	1	1	1
2.12	4	1	1	1
2.45	3	1	1	1
5.75	10	6	2	2
2.45	1	1	1	1
3	7	0	0	0
2.34	7	0	0	0
2.45	6	0	0	0
3.44	5	2	1	2
3.44	3	3	2	1
3.22	1	3	2	1
2.89	6	2	2	2
2.89	7	2	2	2
2.23	6	0	0	0
2.56	1	1	1	1
2.12	2	1	1	1
2.01	1	1	1	1
3.22	15	0	0	0
3.66	10	1	1	1
2.34	1	1	1	1
4.1	11	2	1	2
4.21	9	3	1	1
3.88	9	2	1	2
3.99	7	3	1	1
2.34	0	1	1	1
2.23	2	1	1	1
2.12	0	1	1	1
2.56	1	1	1	1
2.67	0	1	1	1
2.45	2	1	0	1
3.88	3	4	2	2
3.77	4	4	2	2
2.45	1	1	1	1
2.23	2	1	1	1
2.01	1	2	1	1
2.34	1	1	1	1
2.67	2	1	1	1
3.44	9	2	1	2
3.33	10	2	1	2

3.33	3	3	2	2
3.22	4	3	2	2
3.33	3	4	2	2
3.33	3	4	2	2
3.11	3	4	2	2
3.22	3	3	2	2
3	11	0	0	0
2.56	1	2	0	1
3.11	1	5	0	1
4.1	12	1	1	1
3.22	12	0	0	0
2.34	1	1	1	1
2.56	0	1	0	1
2.56	1	1	1	1
3.44	4	4	1	1
2.67	1	3	1	2
2.45	1	1	1	1
2.23	0	1	1	1
3.11	6	0	0	0
3.11	4	2	2	2
3.22	5	2	2	2
3.11	3	1	0	1
2.56	3	0	0	0
3.11	1	2	0	1
2.45	0	3	0	1
	Metabolites after MDS using ADMET (112) (used for HCA and Scaffold analysis)			
MLogP	nRotB	nSmallRings	nAromRings	nRingBlocks
2.12	1	1	1	1
3.66	5	3	1	1
3.22	3	3	1	1
3.44	8	2	1	1
2.34	1	1	1	1
2.78	3	3	2	1
3.55	9	2	1	1
3.55	11	1	1	1
2.89	4	3	2	1
3.55	11	1	0	1
3.22	7	2	1	1

3.55	6	3	1	1
3.55	4	3	1	1
3.44	7	2	1	1
3.44	4	3	2	1
2.89	2	3	1	1
3.33	8	3	2	1
3.44	4	3	1	1
3.44	4	3	1	1
3.44	4	4	1	1
3.44	4	4	1	1
3.44	4	3	1	1
3.55	6	3	1	1
3.44	4	3	1	1
3.44	4	3	1	1
3.44	4	3	1	1
3.55	11	1	1	1
2.78	1	3	1	1
3.88	10	2	2	2
3.44	6	3	1	1
2.78	1	3	1	1
3.11	5	2	1	1
3.22	3	3	1	1
3.22	2	3	1	1
3.22	7	2	1	1
3.44	4	2	1	1
3.44	8	2	1	1
3.22	6	2	1	1
3.44	7	3	2	1
3.44	5	4	1	1
3.33	2	4	1	1
3.55	6	2	1	2
3.66	7	2	1	2
3.11	2	2	1	2
3.33	4	2	1	2
3.33	6	3	1	1
3.44	5	3	1	1
3.55	5	3	3	1
3.22	3	3	1	1
3.55	6	2	2	2
3.33	4	2	2	2
3.66	5	3	2	1

3.55	4	3	2	1
3.22	1	3	2	1
3.44	3	3	2	1
3.11	0	3	2	1
3.11	3	2	1	1
3.11	0	4	1	1
3	1	4	1	1
3.55	4	4	3	1
2.78	1	3	1	1
3.22	2	3	1	1
3.33	2	3	2	1
2.34	3	2	1	1
3.22	8	2	1	1
3.22	8	2	1	1
3.44	4	2	1	1
3.66	6	2	1	1
2.45	2	1	1	1
3	1	3	1	1
3.99	9	2	2	2
3.55	5	3	3	1
3.33	3	3	1	1
3.55	5	3	1	1
3.55	4	3	1	1
3.44	5	3	1	1
3.33	2	3	1	1
3.44	4	3	1	1
3.55	3	3	1	1
3.44	3	3	1	1
3.11	0	3	1	1
3.44	5	3	1	1
3.44	5	3	1	1
3.33	4	3	1	1
3.44	5	3	1	1
3.44	4	3	1	1
3.55	6	2	1	2
3.88	8	2	2	2
3.55	4	3	1	1
3.77	8	2	2	2
3.44	4	3	1	1
3.88	4	3	2	3
3.77	4	3	2	3

3.77	3	4	3	3
3.66	1	5	3	2
3.44	5	2	1	2
3.44	3	3	2	1
3.22	1	3	2	1
4.1	11	2	1	2
3.88	9	2	1	2
3.88	3	4	2	2
3.77	4	4	2	2
2.67	2	1	1	1
3.33	10	2	1	2
3.33	3	3	2	2
3.22	4	3	2	2
3.33	3	4	2	2
3.11	3	4	2	2
3.22	3	3	2	2
3.44	4	4	1	1
2.67	1	3	1	2
2.45	1	1	1	1
	468 Metabolites and positive & negative controls			
nAromBlocks	nRings3	nRings4	nRings5	nRings6
1	0	0	1	6
1	0	0	0	2
2	0	0	0	3
2	0	0	0	3
1	0	0	0	2
3	0	0	1	4
2	0	0	0	3
2	0	0	0	3
2	0	0	1	2
1	0	0	1	2
1	0	0	1	4
1	0	0	1	4
1	0	0	1	4
2	0	0	1	3
2	0	0	0	2
2	0	0	2	0
3	0	0	0	4

0	0	0	0	0
2	0	0	2	0
2	0	0	1	2
1	0	0	1	6
2	0	0	0	3
1	0	0	1	4
1	0	0	1	4
1	0	0	1	4
2	0	0	0	2
1	0	0	0	2
2	0	0	1	3
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1	0	0	1	4
1	0	0	1	4
1	0	0	1	4
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1	0	0	0	2
2	0	0	0	2
2	0	0	0	3
1	0	0	0	2
2	0	0	0	4
2	0	0	0	5
2	0	0	0	3
2	0	0	0	3
2	0	0	0	4
1	0	0	0	1
1	0	0	0	2
1	0	0	0	4
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2	0	0	1	2
1	0	0	1	4
1	0	0	1	4
2	0	0	1	2
1	0	0	0	2
1	0	0	0	2
1	0	0	0	2

2	0	0	0	4
1	0	0	1	3
1	0	0	1	1
2	0	0	0	3
1	0	0	0	1
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
1	0	0	0	1
1	0	0	0	1
0	0	0	0	0
0	0	0	0	0
1	0	0	1	1
0	0	0	0	0
0	0	0	2	0
0	0	0	0	0
0	0	0	0	1
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0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
1	0	0	0	1
0	0	0	0	0
1	0	0	0	3
2	0	0	1	1
1	0	0	1	1
1	0	0	0	1
0	0	0	0	0
1	0	0	0	3
0	0	0	0	0
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
0	0	0	0	0

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0	0	0	0	0
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
0	0	0	0	0
0	0	0	0	0
1	0	0	0	1
1	0	0	0	1
0	0	0	0	0
0	0	0	0	0
1	0	0	0	1
1	0	0	0	3
0	0	0	0	1
0	0	0	0	0
1	0	0	0	1
1	0	0	0	1
0	1	0	0	0
1	0	0	0	2
1	0	0	1	0
0	0	0	0	0
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1	0	0	0	1
1	0	0	0	1
1	0	0	0	3
1	0	0	0	1
0	0	0	0	0
1	0	0	0	1
1	0	0	0	1
1	0	0	0	2
1	0	0	0	1
1	0	0	0	1
0	0	0	0	0
0	0	0	1	0
0	0	0	0	0

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0	0	0	0	0
2	0	0	0	3
1	0	0	0	3
1	0	0	0	2
1	0	0	0	1
0	1	0	0	1
1	0	0	0	1
2	0	0	0	3
1	0	0	0	2
0	0	0	0	0
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	4
2	0	0	0	4
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1	1	0	0	1
1	1	0	0	1
1	0	0	0	2
1	0	0	0	2
3	0	0	0	5
2	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	2
2	0	0	0	3
1	0	0	1	2
1	0	0	1	2
1	0	0	0	3
2	0	0	0	3
2	0	0	0	3
1	0	0	0	3
1	0	0	0	3

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1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
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0	0	0	0	1
0	0	0	0	0
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0	1	0	1	0
0	0	0	0	1
0	0	0	1	0
0	0	0	0	2
1	0	0	0	5
1	0	0	1	2
0	0	0	2	1
0	0	1	0	2
0	0	1	0	4
0	1	0	1	1
0	0	0	0	2
0	0	0	1	0
0	1	0	1	0
0	0	0	0	0
0	0	0	0	1
0	0	0	0	0
0	0	1	0	2
1	0	0	0	1
0	0	0	0	1
0	0	1	0	2
0	0	0	0	2
1	0	0	0	4

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0	0	1	0	2
0	0	1	0	4
2	0	0	0	2
2	0	0	0	2
2	0	0	0	2
2	0	0	0	2
1	0	0	0	1
1	0	0	2	1
0	0	0	0	1
1	0	0	0	2
1	0	1	1	2
2	0	0	0	3
2	0	0	0	2
2	0	0	0	2
2	0	0	0	2
2	0	0	0	2
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0	1	0	1	0
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1	0	0	1	2
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0	0	1	0	0
0	0	0	2	1
0	0	0	0	1
0	0	0	0	2
0	0	0	2	1
1	0	0	2	4
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0	0	0	0	1
0	0	1	0	2

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1	0	0	0	2
1	0	0	1	2
1	0	0	1	2
1	0	0	0	3
0	0	0	2	1
1	0	0	0	5
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0	0	0	0	0
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0	1	0	0	2
0	0	0	2	1
1	0	0	0	2
1	0	0	0	2
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1	0	0	1	2
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1	0	0	0	1
0	0	0	0	1

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1	0	0	0	1
0	0	0	0	1
2	0	0	0	5
0	0	0	2	1
0	0	0	0	0
2	0	0	0	3

1	0	0	0	2
2	0	0	0	3
0	0	1	0	2
0	0	0	0	0
0	0	0	0	1
0	0	0	0	0
0	1	0	1	0
0	0	0	0	0
0	0	0	0	0
1	0	0	0	2
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1	0	0	0	1
1	0	0	0	1
1	0	0	0	2
1	0	0	0	3
0	0	0	0	0
2	0	0	0	2
2	0	0	0	2
1	0	0	1	2
0	1	0	0	1
1	0	0	0	3
1	0	0	0	3
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2	0	0	0	2
2	0	0	0	2
1	0	0	0	1
2	0	0	0	4
2	0	0	0	3
2	0	1	1	4

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1	0	0	0	1
1	0	0	0	2
1	0	0	2	4
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0	0	0	0	0
0	0	0	0	0
0	1	0	0	0
0	1	0	0	0
1	0	0	0	3
1	0	0	0	1
1	0	0	0	1
0	0	0	2	1
0	0	0	2	1
1	0	0	1	2
1	0	0	1	2
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1	0	0	1	0
2	0	0	1	1
0	0	0	0	1
0	0	0	0	2
0	0	0	1	0
0	0	0	1	0
0	0	0	0	2
0	0	0	0	1
2	0	0	0	2
0	1	0	1	0
4	0	0	1	4
1	0	0	0	1
2	0	0	0	2
0	0	0	0	0
0	0	0	0	0

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2	0	0	0	2
1	0	0	0	1
2	0	0	0	2
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0	0	0	0	0
0	0	0	2	1
0	0	0	2	1
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0	0	0	0	0
1	0	0	0	1
1	0	0	0	3
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1	0	0	0	1
0	0	0	0	1
0	0	0	0	0
1	0	0	0	2
2	0	0	0	3
0	2	0	0	1
0	0	0	0	1
0	0	0	0	0
0	0	0	0	0
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2	0	0	0	3
2	0	0	0	3
2	0	0	1	3
2	0	0	1	4
1	0	0	0	1
0	0	0	0	0
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1	0	0	0	1
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0	0	0	0	0

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1	0	0	0	1
1	0	0	0	1
0	0	0	0	0
0	0	0	0	0
2	0	0	0	6
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1	0	0	0	1
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1	0	0	0	1
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0	0	0	0	0
1	0	0	0	2
2	0	0	0	3
2	0	0	0	3
2	0	0	0	2
2	0	0	0	2
0	0	0	0	0
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1	0	0	0	1
1	0	0	0	2
1	0	0	0	3
1	0	0	0	2
1	0	0	0	3
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1	0	0	0	1
1	0	0	0	1
0	0	0	0	0
1	0	0	0	1
0	0	0	0	0
0	0	0	0	1

2	0	0	0	4
2	0	0	0	4
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
0	0	0	0	1
1	0	0	1	1
1	0	0	0	1
0	0	0	0	0
1	0	0	0	1
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
1	0	0	0	1
1	0	0	0	1
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2	1	0	0	3
2	1	0	0	3
2	0	0	0	2
1	0	1	1	2
0	0	0	0	0
0	1	0	1	0
1	0	0	0	1
0	0	0	2	2
1	0	0	0	1
0	0	0	0	0
1	0	0	0	1
0	0	0	0	0
0	0	0	0	1
1	0	0	0	1
1	1	0	0	3
1	0	0	1	2
1	0	0	0	1
1	0	0	0	1
0	0	0	0	0
2	0	0	0	2

2	0	0	0	2
0	0	0	0	1
0	0	0	0	0
0	0	0	0	0
1	0	0	0	1
0	0	0	0	0
0	0	0	0	2
0	0	1	0	2
2	0	0	0	4
2	0	0	0	2
	Metabolites from Machine Learning Methods (330) (used for MDS using CDK)			
nAromBlocks	nRings3	nRings4	nRings5	nRings6
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
0	0	0	0	0
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	3
0	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	2
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	3
1	0	0	0	1
0	0	0	0	0
1	0	0	0	1

1	0	0	0	1
1	0	0	0	2
1	0	0	0	1
1	0	0	0	1
0	0	0	0	0
1	0	0	0	1
2	0	0	0	3
1	0	0	0	3
1	0	0	0	2
1	0	0	0	1
0	1	0	0	1
1	0	0	0	1
2	0	0	0	3
1	0	0	0	2
0	0	0	0	0
1	0	0	0	1
1	0	0	0	1
1	0	0	0	4
2	0	0	0	4
0	0	0	0	1
1	0	0	0	1
1	0	0	0	1
2	0	0	0	2
1	0	0	1	1
0	0	0	0	1
1	0	0	0	2
1	0	0	0	2
1	0	0	0	3
1	0	0	0	3
1	0	0	0	2
2	0	0	0	3
1	0	0	1	2
1	0	0	1	2
1	0	0	0	3
2	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	1	0	0	3
1	0	0	0	3
1	1	0	0	3
1	0	0	0	3

1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	1
1	0	0	0	1
0	0	0	0	1
1	0	0	0	1
0	1	0	1	0
0	0	0	0	1
0	0	0	1	0
0	0	0	0	2
1	0	0	0	5
1	0	0	1	2
0	0	0	2	1
0	0	1	0	2
0	0	1	0	4
0	1	0	1	1
0	0	0	0	2
0	0	0	1	0
0	1	0	1	0
0	0	0	0	0
0	0	0	0	1
0	0	0	0	0
0	0	1	0	2
1	0	0	0	1
0	0	0	0	1
0	0	1	0	2
0	0	0	0	2
1	0	0	0	4
0	0	0	0	1
0	0	0	0	1
0	1	0	1	0
0	0	1	0	2
0	0	1	0	4
2	0	0	0	2
1	0	0	0	1
1	0	0	2	1
0	0	0	0	1

2	0	0	0	2
2	0	0	0	2
2	0	0	0	2
0	1	0	0	2
0	1	0	1	0
1	0	0	0	1
1	0	0	0	1
2	0	0	0	2
2	0	0	0	2
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	1	2
0	1	1	0	0
0	0	1	0	0
0	0	0	2	1
0	0	0	0	1
0	0	0	0	2
1	0	0	2	4
0	0	0	0	1
0	0	0	0	1
0	0	1	0	2
0	0	0	0	2
1	0	0	0	2
1	0	0	1	2
1	0	0	0	3
1	0	0	0	5
0	1	0	0	2
0	0	0	2	1
1	0	0	0	2
1	0	0	0	2
1	0	0	0	2
1	0	0	0	2
1	0	0	0	2
1	0	0	0	2
1	0	0	0	4
1	0	0	1	2
1	0	1	1	2
1	0	1	1	2
1	0	1	1	2
1	0	0	0	2

1	0	0	0	2
1	0	0	0	2
1	0	0	0	2
1	0	0	1	2
1	0	0	1	2
2	0	0	0	3
1	0	0	1	2
1	0	0	0	1
1	0	0	0	1
0	0	0	0	1
1	0	0	0	1
1	0	0	1	2
1	0	0	1	1
1	0	0	0	1
2	0	0	0	2
2	0	0	0	2
2	0	0	0	3
2	0	0	0	3
2	0	0	0	3
2	0	0	0	3
2	0	0	0	3
1	0	0	0	2
1	0	0	0	4
1	0	1	1	2
1	0	1	1	2
1	0	0	1	2
1	0	0	0	3
1	0	0	1	2
1	0	0	0	3
1	0	0	0	3
2	0	0	0	3
2	0	0	0	3
2	0	0	0	3
2	0	0	0	3
1	0	0	1	1
1	0	0	0	1
1	0	0	0	1
0	0	0	0	1
0	0	0	2	1
2	0	0	0	3
0	0	1	0	2

0	0	0	0	0
0	0	0	0	1
0	0	0	0	0
0	1	0	1	0
0	0	0	0	0
0	0	0	0	0
1	0	0	0	2
1	0	0	0	2
1	0	0	0	2
1	0	0	0	2
1	0	0	0	1
1	0	0	0	1
1	0	0	0	3
0	0	0	0	0
2	0	0	0	2
2	0	0	0	2
1	0	0	1	2
0	1	0	0	1
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
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1	0	0	0	3
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1	0	0	0	3
1	0	0	0	3
0	0	0	0	2
2	0	0	0	2
2	0	0	0	3
2	0	1	1	4
2	0	0	0	5
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
2	0	0	0	2
1	0	0	0	1
1	0	0	0	2

1	0	0	2	4
1	0	0	0	1
1	0	0	0	3
1	0	0	0	1
1	0	0	0	1
0	0	0	2	1
1	0	0	1	2
1	0	0	1	2
1	0	0	0	2
2	0	0	1	1
0	0	0	0	1
0	0	0	0	2
0	0	0	1	0
0	0	0	0	2
0	0	0	0	1
2	0	0	0	2
0	1	0	1	0
1	0	0	0	1
2	0	0	0	2
0	0	0	0	0
1	0	0	0	3
0	0	0	0	0
1	0	0	0	1
2	0	0	0	2
1	0	0	0	1
1	0	0	0	3
1	0	0	0	1
1	0	0	0	1
0	0	0	0	1
1	0	0	0	2
0	2	0	0	1
0	0	0	0	1
0	0	0	0	0
0	0	0	0	0
0	0	0	2	1
2	0	0	0	3
2	0	0	0	3
2	0	0	1	3
2	0	0	1	4
1	0	0	0	1
1	0	0	0	1

1	0	0	0	1
2	0	0	0	6
1	0	0	0	1
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
1	0	0	0	2
2	0	0	0	3
2	0	0	0	3
2	0	0	0	2
2	0	0	0	2
0	0	0	0	0
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
0	0	0	0	0
1	0	0	0	1
1	0	0	0	1
1	0	0	0	2
1	0	0	0	3
1	0	0	0	2
1	0	0	0	3
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
1	0	0	0	1
0	0	0	0	1
2	0	0	0	4
2	0	0	0	4
1	0	0	0	1
1	0	0	0	1
1	0	0	1	1
1	0	0	0	1
1	0	0	0	1
1	1	0	0	1
1	1	0	0	1
2	0	0	0	2
2	0	0	0	2
2	1	0	0	3
2	1	0	0	3

2	1	0	0	3
2	0	0	0	2
0	0	0	0	0
0	1	0	1	0
0	0	0	2	2
1	0	0	0	1
0	0	0	0	0
1	0	0	0	1
0	0	0	0	1
1	0	0	0	1
1	1	0	0	3
1	0	0	1	2
1	0	0	0	1
1	0	0	0	1
0	0	0	0	0
2	0	0	0	2
2	0	0	0	2
0	0	0	0	1
0	0	0	0	0
0	0	0	0	2
0	0	1	0	2
	Metabolites after MDS using ADMET (112) (used for HCA and Scaffold analysis)			
nAromBlocks	nRings3	nRings4	nRings5	nRings6
1	0	0	0	1
1	0	0	0	3
1	0	0	0	3
1	0	0	0	2
1	0	0	0	1
2	0	0	0	3
1	0	0	0	2
1	0	0	0	1
2	0	0	0	3
0	0	0	0	1
1	0	0	0	2
1	0	0	0	3
1	0	0	0	3
1	0	0	0	2
2	0	0	0	3

1	0	0	1	2
1	0	0	1	2
1	0	0	0	3
1	0	0	0	3
1	1	0	0	3
1	1	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	1
1	0	0	1	2
2	0	0	0	2
1	0	0	2	1
1	0	0	1	2
1	0	0	0	2
1	0	0	1	2
1	0	0	0	3
1	0	0	0	2
1	0	0	0	2
1	0	0	0	2
1	0	0	0	2
1	0	0	1	2
1	0	1	1	2
1	0	1	1	2
1	0	0	0	2
1	0	0	0	2
1	0	0	0	2
1	0	0	0	2
1	0	0	1	2
1	0	0	1	2
1	0	0	1	2
1	0	0	1	2
2	0	0	0	2
2	0	0	0	2
2	0	0	0	3
2	0	0	0	3
2	0	0	0	3
2	0	0	0	3
2	0	0	0	3

1	0	0	0	2
1	0	1	1	2
1	0	1	1	2
1	0	0	1	2
1	0	0	1	2
1	0	0	0	3
2	0	0	0	3
1	0	0	1	1
1	0	0	0	2
1	0	0	0	2
1	0	0	0	2
1	0	0	0	2
1	0	0	0	1
1	0	0	0	3
2	0	0	0	2
1	0	0	1	2
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	0	3
1	0	0	1	2
1	0	0	1	2
1	0	0	0	2
2	0	0	0	2
1	0	0	0	3
2	0	0	0	2
1	0	0	0	3
2	0	0	0	3
2	0	0	0	3
2	0	0	1	3
2	0	0	1	4
1	0	0	0	2
2	0	0	0	3

2	0	0	0	3
1	0	0	0	2
1	0	0	0	2
2	0	0	0	4
2	0	0	0	4
1	0	0	0	1
1	1	0	0	1
2	0	0	0	2
2	0	0	0	2
2	1	0	0	3
2	1	0	0	3
2	0	0	0	2
1	1	0	0	3
1	0	0	1	2
1	0	0	0	1
	468 Metabolites and positive & negative controls			
nRings7	TopoPSA	MW	nB	nBase
0	68.23	453.2515	38	1
0	29.54	287.1885	22	1
0	55.56	352.2151	28	1
0	38.77	367.2147	29	1
0	29.54	275.1885	21	1
0	71.03	492.2525	41	1
0	23.55	350.2358	28	1
0	49.85	394.2256	31	1
0	64.2	386.151	29	1
1	55.84	303.1471	24	1
0	41.93	299.1521	26	1
0	80.59	372.1685	31	1
0	32.7	271.1572	24	1
0	32.78	392.2464	32	1
0	23.55	324.2202	25	1
0	59.72	291.1115	20	1
0	64.33	424.2151	35	1
0	20.23	46.04186	2	0
0	59.72	277.0959	19	1
0	73.43	396.2161	31	1
0	62.16	411.241	35	1

0	23.55	336.2202	27	1
0	65.07	369.1576	31	1
0	38.77	299.1521	26	1
0	49.77	285.1365	25	1
0	20.31	309.2093	24	1
0	40.54	247.1572	19	1
0	32.78	392.2464	32	1
0	29.54	247.1572	19	1
0	52.93	285.1365	25	1
0	72.75	301.1314	26	1
0	59	315.1471	27	1
0	70	301.1314	26	1
0	36.44	275.1998	21	1
0	29.54	353.2355	27	1
0	32.34	328.1109	22	1
0	29.54	275.1885	21	1
0	29.54	261.1729	20	1
0	29.54	339.2198	26	1
0	29.54	351.2198	28	1
0	23.55	274.2045	21	1
0	23.47	321.2093	27	1
0	23.47	347.2249	30	1
0	49.77	367.2147	29	1
0	41.57	366.2307	29	1
0	73.36	430.2733	35	2
1	29.54	275.1885	21	1
0	29.54	261.1729	20	1
0	12.47	271.1936	23	1
0	59	321.194	24	1
0	76.15	376.1998	28	1
0	61.02	386.2028	29	1
0	48	341.1627	29	1
0	30.93	311.1521	27	1
0	51.79	342.1766	26	1
0	29.54	273.1729	21	1
0	29.54	275.1885	21	1
0	23.55	328.1109	22	1
0	6.48	348.2565	29	2
0	39.34	323.1998	27	1
0	30.49	193.1103	15	1
0	34.89	250.1106	21	0

0	53.71	211.1208	15	1
0	49.33	347.2824	24	0
0	66.76	378.277	26	0
0	49.33	349.2981	24	0
0	49.33	375.3137	26	0
0	49.69	364.2977	25	0
0	69.56	439.3086	32	0
0	69.56	417.3243	30	0
0	43.09	281.2719	19	0
0	52.32	347.2824	24	1
0	16.13	162.1157	13	1
0	40.13	59.0133	3	0
0	103.73	244.0882	17	0
0	20.23	104.1075	6	2
0	110.38	180.0634	12	0
0	103.45	146.0453	9	1
0	92	155.0695	11	1
0	63.32	131.0946	8	1
0	60.36	89.02387	5	0
0	63.32	131.0946	8	1
0	89.34	146.1055	9	2
0	88.62	149.051	8	1
0	63.32	165.079	12	1
0	57.2	87.00822	5	0
0	161.56	376.1383	29	0
0	104.15	265.1123	19	1
0	79.11	204.0899	16	1
0	83.55	181.0739	13	1
0	63.32	117.079	7	1
0	29.46	314.2246	25	0
0	29.26	60.06875	3	0
0	0	134.1096	10	0
0	0	134.1096	10	0
0	116.73	126.0654	9	0
0	0	145.969	8	0
0	0	134.1096	10	0
0	20.23	74.07316	4	0
0	29.46	132.115	8	0
0	20.23	102.1045	6	0
0	20.23	172.1827	11	0
0	0	128.1565	8	0

0	0	114.1409	7	0
0	20.23	136.0888	10	0
0	20.23	206.1671	15	0
0	25.78	136.1	10	0
0	25.78	108.0687	8	0
0	17.07	72.05751	4	0
0	29.46	118.0994	7	0
0	17.07	154.0185	10	0
0	0	132.0939	10	0
0	29.46	90.06808	5	0
0	20.23	130.1358	8	0
0	0	120.0939	9	0
0	46.53	354.2195	28	0
0	54.37	330.2195	24	0
0	17.07	114.1045	7	0
0	37.3	136.0524	10	0
0	25.78	136.1	10	0
0	21.94	57.05785	4	1
0	0	142.0783	12	0
0	28.68	82.0531	6	0
0	26.02	73.08915	4	1
0	0	86.10955	5	0
0	43.14	89.04768	5	0
0	29.46	138.0681	10	0
0	38.33	193.1103	14	0
0	46.53	178.063	13	0
0	49.69	304.2038	24	0
0	20.23	136.0888	10	0
0	0	126.1409	8	0
0	0	120.0939	9	0
0	0	134.1096	10	0
0	49.69	330.2195	25	0
0	17.07	148.0888	11	0
0	17.07	134.0732	10	0
0	0	114.1409	7	0
0	17.07	96.05751	7	0
0	0	86.10955	5	0
0	38.33	207.1259	15	0
0	20.23	88.08882	5	0
0	68.15	302.1154	24	0
0	79.15	286.0841	23	0

0	55.76	372.2301	28	0
0	66.76	374.2457	27	0
0	0	136.1252	11	0
0	35.53	180.0786	13	0
0	57.15	316.1311	25	0
0	39.44	176.0473	14	0
0	0	156.1878	10	0
0	25.78	94.0531	7	0
0	29.46	138.0681	10	0
0	26.02	135.1048	10	1
0	38.91	94.0531	7	0
0	55.76	494.3396	39	0
0	55.76	490.3083	39	0
0	60.44	372.2301	27	0
0	66.76	374.2457	27	0
0	12.89	119.0735	9	0
0	66.76	374.2457	27	0
0	60.69	286.1569	22	0
0	0	132.0939	11	0
0	26.3	142.0994	10	0
0	90.29	362.2093	27	0
0	90.29	362.2093	27	0
0	83.83	360.1937	27	0
0	80.67	346.178	26	0
0	96.22	432.1573	36	0
0	90.9	338.1154	27	0
0	58.92	372.2301	29	0
0	29.46	312.2089	25	0
0	49.69	332.2351	25	0
0	49.69	326.1882	26	0
0	35.53	260.1412	21	0
0	76.74	372.1937	29	0
0	69.92	346.2144	27	0
0	86.99	370.178	29	0
0	49.69	326.1882	26	0
0	49.69	330.2195	26	0
0	46.53	328.2038	26	0
0	41.99	328.2038	27	0
0	71.06	330.1103	26	0
0	41.99	330.2195	27	0
0	49.69	330.2195	26	0

0	58.92	374.2457	29	0
0	49.69	330.2195	26	0
0	58.92	360.2301	28	0
0	46.53	328.2038	26	0
0	93.06	416.2199	32	0
0	93.06	416.2199	32	0
0	40.46	316.2402	23	0
0	17.07	44.02621	2	0
0	43.09	59.03711	3	0
0	37.3	60.02113	3	0
0	17.07	58.04186	3	0
0	66.76	374.2457	27	0
0	60.44	372.2301	27	0
0	17.07	56.02621	3	0
0	17.07	120.0575	9	0
1	0	204.1878	17	0
0	20.23	222.1984	16	0
1	0	204.1878	16	0
0	0	204.1878	16	0
0	55.76	562.4022	45	0
0	49.69	248.1412	20	0
1	0	204.1878	17	0
0	0	204.1878	16	0
0	0	204.1878	17	0
0	0	204.1878	17	0
0	20.23	222.1984	17	0
1	0	204.1878	16	0
1	0	204.1878	17	0
0	0	204.1878	15	0
0	20.23	194.1671	14	0
0	37.3	278.2246	19	0
2	0	204.1878	17	0
0	17.07	146.0732	11	0
0	0	136.1252	10	0
0	0	136.1252	11	0
0	0	204.1878	16	0
0	55.76	494.3396	39	0
0	0	136.1252	10	0
0	20.23	154.1358	11	0
0	0	136.1252	11	0
0	0	204.1878	16	0

0	0	204.1878	17	0
0	86.99	356.1624	27	0
0	77.76	394.2144	30	0
0	66.76	340.1675	26	0
0	66.76	408.2301	31	0
0	9.23	148.0888	11	0
0	46.53	328.2038	26	0
0	61.44	363.2886	27	2
0	66.76	302.1518	23	0
0	66.76	302.1518	25	0
0	90.9	270.0528	22	0
0	60.69	296.1412	23	0
0	40.46	280.1463	22	0
0	101.15	330.1467	25	0
0	80.92	314.1518	24	0
0	0	204.1878	17	0
1	0	204.1878	17	0
0	17.07	106.0419	8	0
0	23.79	103.0422	8	0
0	17.07	182.0732	15	0
0	3.24	239.1674	19	1
0	26.3	150.0681	11	0
0	20.23	108.0575	8	0
0	26.3	136.0524	10	0
0	23.79	117.0578	9	0
0	49.69	248.1412	20	0
0	12.53	220.1827	18	0
0	0	204.1878	16	0
1	0	204.1878	17	0
0	0	204.1878	15	0
0	20.23	222.1984	17	0
0	20.23	154.1358	12	0
0	55.76	480.324	39	0
0	24.92	136.1	10	1
0	17.07	206.1671	15	0
0	0	136.1252	10	0
0	0	136.1252	11	0
0	0	204.1878	16	0
0	105.45	814.6687	62	0
0	54.7	111.0796	8	1
0	63.6	316.1675	24	0

0	86.99	346.178	27	0
0	49.69	302.1882	24	0
0	69.92	332.1988	26	0
0	20.23	154.1358	12	0
0	55.76	562.4022	45	0
0	0	58.07825	3	0
0	26.3	102.0681	6	0
0	66.76	578.4335	44	0
0	0	204.1878	17	0
0	0	136.1252	11	0
0	63.6	332.1988	25	0
0	35.53	328.2038	26	0
0	29.46	314.2246	24	0
0	66.76	358.2144	27	0
0	29.46	286.1933	22	0
0	66.76	330.1831	25	0
0	18.46	314.2246	26	0
0	39.44	328.2038	26	0
0	29.46	314.2246	26	0
0	66.76	358.2144	29	0
0	29.46	286.1933	24	0
0	40.46	314.2246	24	0
0	77.76	358.2144	27	0
0	29.46	328.2402	25	0
0	40.46	258.162	20	0
0	40.46	286.1933	22	0
0	77.76	330.1831	25	0
0	86.99	374.2093	29	0
0	86.99	374.2093	29	0
0	49.69	330.2195	26	0
0	100.13	368.126	29	0
0	33.37	310.1933	25	0
0	40.46	316.2402	23	0
0	66.76	374.2457	27	0
0	77.76	360.2301	26	0
0	29.46	330.2559	24	0
0	34.14	314.2246	23	0
0	40.46	288.2089	21	0
0	77.76	332.1988	24	0
0	49.69	304.2038	24	0
0	77.76	332.1988	25	0

0	40.46	316.2402	23	0
0	77.76	360.2301	26	0
0	40.46	310.1933	24	0
0	40.46	282.162	22	0
0	18.46	324.2089	26	0
0	29.46	310.1933	25	0
0	29.46	268.1463	22	0
0	29.46	296.1776	24	0
0	66.76	354.1831	28	0
0	29.46	254.1307	21	0
0	29.46	258.162	20	0
0	66.76	302.1518	23	0
0	18.46	258.162	22	0
0	29.46	258.162	22	0
0	66.76	302.1518	25	0
1	22.37	306.162	26	0
0	69.92	348.2301	27	0
0	84.83	381.2991	28	2
0	179.58	594.2002	48	0
0	179.58	596.2159	48	0
0	168.58	610.2315	49	0
0	157.58	624.2472	50	0
0	46.53	246.1256	20	0
0	69.92	346.2144	27	0
0	49.69	302.1882	24	0
0	29.46	282.162	23	0
0	100.13	436.1886	34	0
0	100.13	368.126	29	0
0	100.13	436.1886	34	0
0	47.56	221.1052	17	0
0	80.92	350.2457	25	0
0	20.23	150.1045	11	0
0	17.07	150.1045	11	0
0	105.45	686.4183	54	0
1	26.3	264.2089	21	0
0	20.23	242.261	16	0
0	38.69	310.1569	25	0
0	66.76	336.1128	24	0
0	100.13	300.0634	24	0
0	20.23	154.1358	12	0
0	0	204.1878	14	0

0	0	204.1878	15	0
0	0	136.1252	9	0
0	0	138.1409	11	0
0	26.3	198.162	13	0
0	26.3	184.1463	12	0
0	83.83	362.2093	27	0
0	80.67	360.1937	27	0
0	35.53	328.2038	26	0
0	29.46	326.2246	25	0
0	0	120.0939	9	0
0	17.07	148.0888	11	0
0	66.76	370.2144	28	0
0	66.76	302.1518	24	0
0	17.07	156.1514	10	0
0	29.46	296.1776	23	0
0	29.46	364.2402	28	0
0	33.37	308.1776	25	0
0	0	136.1252	11	0
0	29.46	286.1933	23	0
0	29.46	314.2246	25	0
0	29.46	314.2246	25	0
0	66.76	358.2144	28	0
0	29.46	286.1933	23	0
0	66.76	356.1988	28	0
0	29.46	312.2089	25	0
0	29.46	300.2089	24	0
0	29.46	258.162	21	0
0	66.76	358.2144	28	0
0	66.76	358.2144	28	0
0	66.76	344.1988	27	0
0	0	204.1878	16	0
0	77.76	326.1518	25	0
0	40.46	282.162	22	0
0	66.76	306.1831	22	0
0	96.22	436.1886	35	0
0	107.22	438.2042	34	0
0	96.22	436.1886	37	0
0	96.22	436.1886	36	0
0	37.3	116.0837	7	0
0	52.6	278.1518	20	0
0	52.6	222.0892	16	0

0	26.3	192.115	14	0
0	42.52	94.00885	4	0
0	25.3	62.01902	2	0
0	0	170.2035	11	0
1	39.52	311.1344	24	1
0	0	134.1096	10	0
0	29.54	289.2042	22	1
0	55.76	494.3396	40	0
0	9.23	148.0888	11	0
0	26.3	88.05243	5	0
0	52.04	60.06875	3	2
0	12.53	44.02621	3	0
0	21.94	43.0422	3	1
0	66.76	564.4179	43	0
0	29.46	164.0837	12	0
0	35.53	206.0943	15	0
0	17.07	152.1201	12	0
0	20.23	154.1358	12	0
0	69.92	358.2144	28	0
0	69.92	358.2144	28	0
0	60.69	342.2195	26	0
0	37.3	46.00548	2	0
0	30.21	96.02113	7	0
0	16.38	229.1467	18	1
0	0	204.1878	15	0
0	20.23	222.1984	17	0
1	0	204.1878	16	0
0	26.3	114.0681	8	0
0	0	204.1878	16	0
0	0	136.1252	10	0
0	60.69	298.1569	23	0
1	20.23	222.1984	18	0
0	146.58	624.2472	50	0
0	29.46	124.0524	9	0
0	40.46	350.2246	27	0
0	17.07	114.1045	7	0
0	0	226.2661	15	0
0	29.46	316.2402	25	0
0	17.07	100.0888	6	0
0	26.3	130.0994	8	0
0	26.3	158.1307	10	0

0	40.46	270.162	21	0
0	23.47	165.1154	12	1
0	60.69	366.2195	28	0
0	20.23	152.1201	10	0
0	20.23	88.08882	5	0
0	26.3	196.1463	15	0
0	75.39	253.1136	18	0
0	0	58.07825	3	0
0	17.07	72.05751	4	0
0	17.07	148.0888	11	0
0	69.92	360.2301	28	0
0	29.43	57.02146	3	0
0	0	134.1096	10	0
0	29.46	164.0837	12	0
0	0	136.1252	10	0
0	0	68.0626	4	0
0	12.89	129.0578	11	0
0	111.13	286.0477	23	0
0	25.06	168.115	14	0
0	0	136.1252	10	0
0	20.23	154.1358	10	0
0	26.3	196.1463	13	0
0	37.3	280.2402	19	0
1	0	204.1878	17	0
0	111.13	286.0477	23	0
0	40.46	348.2089	28	0
0	60.69	364.2038	29	0
0	53.6	362.1882	30	0
0	62.83	378.1831	32	0
0	0	134.1096	10	0
0	17.07	70.04186	4	0
0	43.37	154.063	10	0
0	26.3	74.03678	4	0
0	52.6	194.0579	14	0
0	52.32	151.0633	11	0
0	26.3	136.0524	10	0
0	52.32	75.03203	4	0
0	17.07	124.0888	8	0
0	26.3	144.115	9	0
0	38.05	46.0531	2	0
0	18.46	178.0994	13	0

0	46.53	152.0473	11	0
0	26.3	116.0837	7	0
0	0	83.95336	2	0
0	58.92	640.4492	52	0
0	17.07	126.1045	8	0
0	20.23	150.1045	11	0
0	0	136.1252	9	0
0	20.23	154.1358	10	0
0	20.23	222.1984	15	0
0	43.14	123.032	9	0
0	17.07	142.1358	9	0
0	0	128.1565	8	0
0	40.46	300.2089	23	0
0	29.46	296.1776	24	0
0	29.46	268.1463	22	0
0	69.56	283.1208	22	0
0	78.79	313.1314	24	0
0	17.07	128.1201	8	0
0	0	134.1096	10	0
0	18.46	138.0681	10	0
0	29.46	124.0524	9	0
0	37.3	282.2559	19	0
0	29.46	330.2559	24	0
0	17.07	134.0732	10	0
0	29.46	384.3028	29	0
0	18.46	396.3028	31	0
0	29.46	356.2715	27	0
0	18.46	368.2715	29	0
0	201.28	448.1006	35	0
0	0	106.0783	8	0
0	26.3	150.0681	11	0
0	26.02	107.0735	8	0
0	0	134.1096	10	0
0	0	212.2504	14	0
0	0	148.1252	11	0
0	17.07	86.07316	5	0
0	17.07	150.1045	11	0
0	29.46	348.2089	29	0
0	66.76	392.1988	32	0
0	0	120.0939	9	0
0	20.23	94.04186	7	0

0	20.23	122.0732	9	0
0	12.03	85.08915	6	1
0	35.53	150.0317	12	0
0	17.07	134.0732	10	0
0	17.07	58.04186	3	0
0	20.23	178.1358	13	0
0	43.37	130.063	8	0
0	26.02	59.0735	3	1
0	40.46	76.05243	4	0
0	20.23	150.1045	11	0
0	0	106.0783	8	0
0	131.36	302.0427	24	0
0	52.99	332.2351	25	0
0	90.29	376.225	28	0
1	29.46	280.1463	23	0
1	66.76	324.1362	26	0
0	29.46	280.1463	24	0
0	18.46	278.1307	24	0
0	66.76	308.1049	26	0
1	49.69	296.1412	24	0
0	66.76	370.2144	30	0
0	37.3	250.1933	17	0
0	0	136.1252	11	0
0	37.3	122.0368	9	0
1	0	204.1878	17	0
0	40.46	384.3028	28	0
0	37.3	276.2089	19	0
0	0	104.0626	8	0
0	20.23	74.07316	4	0
0	0	136.1252	10	0
0	0	134.1096	10	0
0	41.99	330.2195	27	0
0	24.39	200.1313	17	2
0	20.23	150.1045	11	0
0	0	92.0626	7	0
0	0	204.1878	14	0
0	80.92	312.1362	24	0
0	60.69	298.1569	23	0
0	0	204.1878	15	0
0	0	136.1252	9	0
0	0	184.2191	12	0

0	46.25	137.0841	10	1
0	0	156.1878	10	0
0	0	204.1878	16	0
0	17.07	150.1045	12	0
0	181.05	432.1056	34	0
0	89.79	299.1158	23	0
	Metabolites from Machine Learning Methods (330) (used for MDS using CDK)			
nRings7	TopoPSA	MW	nB	nBase
0	0	134.1096	10	0
0	0	134.1096	10	0
0	0	145.969	8	0
0	0	134.1096	10	0
0	0	128.1565	8	0
0	20.23	136.0888	10	0
0	20.23	206.1671	15	0
0	25.78	136.1	10	0
0	17.07	154.0185	10	0
0	0	132.0939	10	0
0	0	120.0939	9	0
0	46.53	354.2195	28	0
0	54.37	330.2195	24	0
0	37.3	136.0524	10	0
0	25.78	136.1	10	0
0	0	142.0783	12	0
0	29.46	138.0681	10	0
0	38.33	193.1103	14	0
0	46.53	178.063	13	0
0	49.69	304.2038	24	0
0	20.23	136.0888	10	0
0	0	126.1409	8	0
0	0	120.0939	9	0
0	0	134.1096	10	0
0	49.69	330.2195	25	0
0	17.07	148.0888	11	0
0	17.07	134.0732	10	0
0	0	114.1409	7	0
0	38.33	207.1259	15	0
0	68.15	302.1154	24	0

0	79.15	286.0841	23	0
0	55.76	372.2301	28	0
0	66.76	374.2457	27	0
0	0	136.1252	11	0
0	35.53	180.0786	13	0
0	57.15	316.1311	25	0
0	39.44	176.0473	14	0
0	0	156.1878	10	0
0	29.46	138.0681	10	0
0	26.02	135.1048	10	1
0	55.76	494.3396	39	0
0	55.76	490.3083	39	0
0	60.44	372.2301	27	0
0	66.76	374.2457	27	0
0	12.89	119.0735	9	0
0	60.69	286.1569	22	0
0	0	132.0939	11	0
0	26.3	142.0994	10	0
0	83.83	360.1937	27	0
0	80.67	346.178	26	0
0	58.92	372.2301	29	0
0	29.46	312.2089	25	0
0	49.69	332.2351	25	0
0	49.69	326.1882	26	0
0	35.53	260.1412	21	0
0	76.74	372.1937	29	0
0	69.92	346.2144	27	0
0	49.69	326.1882	26	0
0	49.69	330.2195	26	0
0	46.53	328.2038	26	0
0	41.99	328.2038	27	0
0	71.06	330.1103	26	0
0	41.99	330.2195	27	0
0	49.69	330.2195	26	0
0	58.92	374.2457	29	0
0	49.69	330.2195	26	0
0	58.92	360.2301	28	0
0	46.53	328.2038	26	0
0	93.06	416.2199	32	0
0	93.06	416.2199	32	0
0	40.46	316.2402	23	0

0	66.76	374.2457	27	0
0	60.44	372.2301	27	0
0	17.07	120.0575	9	0
1	0	204.1878	17	0
0	20.23	222.1984	16	0
1	0	204.1878	16	0
0	0	204.1878	16	0
0	55.76	562.4022	45	0
0	49.69	248.1412	20	0
1	0	204.1878	17	0
0	0	204.1878	16	0
0	0	204.1878	17	0
0	0	204.1878	17	0
0	20.23	222.1984	17	0
1	0	204.1878	16	0
1	0	204.1878	17	0
0	0	204.1878	15	0
0	20.23	194.1671	14	0
0	37.3	278.2246	19	0
2	0	204.1878	17	0
0	17.07	146.0732	11	0
0	0	136.1252	10	0
0	0	136.1252	11	0
0	0	204.1878	16	0
0	55.76	494.3396	39	0
0	0	136.1252	10	0
0	20.23	154.1358	11	0
0	0	136.1252	11	0
0	0	204.1878	16	0
0	0	204.1878	17	0
0	66.76	408.2301	31	0
0	9.23	148.0888	11	0
0	46.53	328.2038	26	0
0	61.44	363.2886	27	2
0	60.69	296.1412	23	0
0	40.46	280.1463	22	0
0	80.92	314.1518	24	0
0	0	204.1878	17	0
1	0	204.1878	17	0
0	17.07	106.0419	8	0
0	23.79	103.0422	8	0

0	17.07	182.0732	15	0
0	3.24	239.1674	19	1
0	20.23	108.0575	8	0
0	26.3	136.0524	10	0
0	23.79	117.0578	9	0
0	49.69	248.1412	20	0
0	12.53	220.1827	18	0
0	0	204.1878	16	0
1	0	204.1878	17	0
0	0	204.1878	15	0
0	20.23	222.1984	17	0
0	55.76	480.324	39	0
0	17.07	206.1671	15	0
0	0	136.1252	10	0
0	0	136.1252	11	0
0	0	204.1878	16	0
0	63.6	316.1675	24	0
0	49.69	302.1882	24	0
0	69.92	332.1988	26	0
0	55.76	562.4022	45	0
0	0	204.1878	17	0
0	0	136.1252	11	0
0	63.6	332.1988	25	0
0	35.53	328.2038	26	0
0	29.46	314.2246	24	0
0	66.76	358.2144	27	0
0	29.46	286.1933	22	0
0	66.76	330.1831	25	0
0	18.46	314.2246	26	0
0	39.44	328.2038	26	0
0	29.46	314.2246	26	0
0	66.76	358.2144	29	0
0	29.46	286.1933	24	0
0	40.46	314.2246	24	0
0	29.46	328.2402	25	0
0	40.46	258.162	20	0
0	40.46	286.1933	22	0
0	86.99	374.2093	29	0
0	49.69	330.2195	26	0
0	100.13	368.126	29	0
0	33.37	310.1933	25	0

0	40.46	316.2402	23	0
0	29.46	330.2559	24	0
0	34.14	314.2246	23	0
0	40.46	288.2089	21	0
0	49.69	304.2038	24	0
0	77.76	332.1988	25	0
0	40.46	316.2402	23	0
0	40.46	310.1933	24	0
0	40.46	282.162	22	0
0	18.46	324.2089	26	0
0	29.46	310.1933	25	0
0	29.46	268.1463	22	0
0	29.46	296.1776	24	0
0	29.46	254.1307	21	0
0	29.46	258.162	20	0
0	18.46	258.162	22	0
0	29.46	258.162	22	0
0	66.76	302.1518	25	0
1	22.37	306.162	26	0
0	69.92	348.2301	27	0
0	46.53	246.1256	20	0
0	69.92	346.2144	27	0
0	49.69	302.1882	24	0
0	29.46	282.162	23	0
0	100.13	436.1886	34	0
0	100.13	368.126	29	0
0	100.13	436.1886	34	0
0	47.56	221.1052	17	0
0	80.92	350.2457	25	0
0	20.23	150.1045	11	0
0	17.07	150.1045	11	0
1	26.3	264.2089	21	0
0	38.69	310.1569	25	0
0	20.23	154.1358	12	0
0	0	204.1878	14	0
0	0	204.1878	15	0
0	0	136.1252	9	0
0	0	138.1409	11	0
0	26.3	198.162	13	0
0	26.3	184.1463	12	0
0	83.83	362.2093	27	0

0	80.67	360.1937	27	0
0	35.53	328.2038	26	0
0	29.46	326.2246	25	0
0	0	120.0939	9	0
0	17.07	148.0888	11	0
0	66.76	302.1518	24	0
0	17.07	156.1514	10	0
0	29.46	296.1776	23	0
0	29.46	364.2402	28	0
0	33.37	308.1776	25	0
0	0	136.1252	11	0
0	29.46	286.1933	23	0
0	29.46	314.2246	25	0
0	29.46	314.2246	25	0
0	66.76	358.2144	28	0
0	29.46	286.1933	23	0
0	66.76	356.1988	28	0
0	29.46	312.2089	25	0
0	29.46	300.2089	24	0
0	29.46	258.162	21	0
0	66.76	358.2144	28	0
0	66.76	358.2144	28	0
0	66.76	344.1988	27	0
0	0	204.1878	16	0
0	40.46	282.162	22	0
0	107.22	438.2042	34	0
0	96.22	436.1886	37	0
0	96.22	436.1886	36	0
0	52.6	278.1518	20	0
0	52.6	222.0892	16	0
0	26.3	192.115	14	0
1	39.52	311.1344	24	1
0	0	134.1096	10	0
0	29.54	289.2042	22	1
0	55.76	494.3396	40	0
0	9.23	148.0888	11	0
0	66.76	564.4179	43	0
0	29.46	164.0837	12	0
0	35.53	206.0943	15	0
0	17.07	152.1201	12	0
0	69.92	358.2144	28	0

0	69.92	358.2144	28	0
0	60.69	342.2195	26	0
0	16.38	229.1467	18	1
0	0	204.1878	15	0
0	20.23	222.1984	17	0
1	0	204.1878	16	0
0	0	204.1878	16	0
0	0	136.1252	10	0
0	60.69	298.1569	23	0
1	20.23	222.1984	18	0
0	29.46	124.0524	9	0
0	40.46	350.2246	27	0
0	17.07	114.1045	7	0
0	29.46	316.2402	25	0
0	26.3	158.1307	10	0
0	23.47	165.1154	12	1
0	60.69	366.2195	28	0
0	17.07	148.0888	11	0
0	69.92	360.2301	28	0
0	0	134.1096	10	0
0	29.46	164.0837	12	0
0	0	136.1252	10	0
0	12.89	129.0578	11	0
0	25.06	168.115	14	0
0	0	136.1252	10	0
0	26.3	196.1463	13	0
0	37.3	280.2402	19	0
1	0	204.1878	17	0
0	40.46	348.2089	28	0
0	60.69	364.2038	29	0
0	53.6	362.1882	30	0
0	62.83	378.1831	32	0
0	0	134.1096	10	0
0	52.6	194.0579	14	0
0	18.46	178.0994	13	0
0	58.92	640.4492	52	0
0	20.23	150.1045	11	0
0	20.23	222.1984	15	0
0	17.07	142.1358	9	0
0	0	128.1565	8	0
0	40.46	300.2089	23	0

0	29.46	296.1776	24	0
0	29.46	268.1463	22	0
0	69.56	283.1208	22	0
0	78.79	313.1314	24	0
0	17.07	128.1201	8	0
0	0	134.1096	10	0
0	18.46	138.0681	10	0
0	29.46	124.0524	9	0
0	37.3	282.2559	19	0
0	29.46	330.2559	24	0
0	17.07	134.0732	10	0
0	29.46	384.3028	29	0
0	18.46	396.3028	31	0
0	29.46	356.2715	27	0
0	18.46	368.2715	29	0
0	0	106.0783	8	0
0	26.3	150.0681	11	0
0	26.02	107.0735	8	0
0	0	134.1096	10	0
0	0	148.1252	11	0
0	17.07	150.1045	11	0
0	29.46	348.2089	29	0
0	66.76	392.1988	32	0
0	0	120.0939	9	0
0	20.23	122.0732	9	0
0	35.53	150.0317	12	0
0	17.07	134.0732	10	0
0	20.23	178.1358	13	0
0	52.99	332.2351	25	0
0	90.29	376.225	28	0
1	29.46	280.1463	23	0
1	66.76	324.1362	26	0
0	29.46	280.1463	24	0
0	18.46	278.1307	24	0
0	66.76	308.1049	26	0
1	49.69	296.1412	24	0
0	37.3	250.1933	17	0
0	0	136.1252	11	0
1	0	204.1878	17	0
0	40.46	384.3028	28	0
0	37.3	276.2089	19	0

0	0	104.0626	8	0
0	0	136.1252	10	0
0	0	134.1096	10	0
0	41.99	330.2195	27	0
0	24.39	200.1313	17	2
0	20.23	150.1045	11	0
0	0	92.0626	7	0
0	0	204.1878	14	0
0	80.92	312.1362	24	0
0	60.69	298.1569	23	0
0	0	204.1878	15	0
0	0	136.1252	9	0
0	0	204.1878	16	0
0	17.07	150.1045	12	0
	Metabolites after MDS using ADMET (112) (used for HCA and Scaffold analysis)			
nRings7	TopoPSA	MW	nB	nBase
0	17.07	154.0185	10	0
0	46.53	354.2195	28	0
0	49.69	304.2038	24	0
0	49.69	330.2195	25	0
0	17.07	134.0732	10	0
0	68.15	302.1154	24	0
0	55.76	372.2301	28	0
0	66.76	374.2457	27	0
0	57.15	316.1311	25	0
0	60.44	372.2301	27	0
0	83.83	360.1937	27	0
0	58.92	372.2301	29	0
0	29.46	312.2089	25	0
0	49.69	332.2351	25	0
0	49.69	326.1882	26	0
0	35.53	260.1412	21	0
0	76.74	372.1937	29	0
0	49.69	330.2195	26	0
0	46.53	328.2038	26	0
0	41.99	328.2038	27	0
0	41.99	330.2195	27	0
0	49.69	330.2195	26	0

0	58.92	374.2457	29	0
0	49.69	330.2195	26	0
0	58.92	360.2301	28	0
0	46.53	328.2038	26	0
0	66.76	374.2457	27	0
0	49.69	248.1412	20	0
0	66.76	408.2301	31	0
0	46.53	328.2038	26	0
0	49.69	248.1412	20	0
0	63.6	316.1675	24	0
0	49.69	302.1882	24	0
0	69.92	332.1988	26	0
0	63.6	332.1988	25	0
0	35.53	328.2038	26	0
0	66.76	358.2144	27	0
0	66.76	330.1831	25	0
0	39.44	328.2038	26	0
0	66.76	358.2144	29	0
0	29.46	286.1933	24	0
0	40.46	314.2246	24	0
0	29.46	328.2402	25	0
0	40.46	258.162	20	0
0	40.46	286.1933	22	0
0	86.99	374.2093	29	0
0	49.69	330.2195	26	0
0	33.37	310.1933	25	0
0	49.69	304.2038	24	0
0	40.46	310.1933	24	0
0	40.46	282.162	22	0
0	18.46	324.2089	26	0
0	29.46	310.1933	25	0
0	29.46	268.1463	22	0
0	29.46	296.1776	24	0
0	29.46	254.1307	21	0
0	29.46	258.162	20	0
0	29.46	258.162	22	0
0	66.76	302.1518	25	0
1	22.37	306.162	26	0
0	46.53	246.1256	20	0
0	49.69	302.1882	24	0
0	29.46	282.162	23	0

0	47.56	221.1052	17	0
0	83.83	362.2093	27	0
0	80.67	360.1937	27	0
0	35.53	328.2038	26	0
0	29.46	326.2246	25	0
0	17.07	148.0888	11	0
0	66.76	302.1518	24	0
0	29.46	364.2402	28	0
0	33.37	308.1776	25	0
0	29.46	286.1933	23	0
0	29.46	314.2246	25	0
0	29.46	314.2246	25	0
0	66.76	358.2144	28	0
0	29.46	286.1933	23	0
0	66.76	356.1988	28	0
0	29.46	312.2089	25	0
0	29.46	300.2089	24	0
0	29.46	258.162	21	0
0	66.76	358.2144	28	0
0	66.76	358.2144	28	0
0	66.76	344.1988	27	0
0	69.92	358.2144	28	0
0	69.92	358.2144	28	0
0	60.69	342.2195	26	0
0	40.46	350.2246	27	0
0	29.46	316.2402	25	0
0	60.69	366.2195	28	0
0	69.92	360.2301	28	0
0	40.46	348.2089	28	0
0	60.69	364.2038	29	0
0	53.6	362.1882	30	0
0	62.83	378.1831	32	0
0	40.46	300.2089	23	0
0	29.46	296.1776	24	0
0	29.46	268.1463	22	0
0	29.46	384.3028	29	0
0	29.46	356.2715	27	0
0	29.46	348.2089	29	0
0	66.76	392.1988	32	0
0	20.23	178.1358	13	0
0	90.29	376.225	28	0

1	29.46	280.1463	23	0
1	66.76	324.1362	26	0
0	29.46	280.1463	24	0
0	66.76	308.1049	26	0
1	49.69	296.1412	24	0
0	41.99	330.2195	27	0
0	24.39	200.1313	17	2
0	20.23	150.1045	11	0