Supplementary Information for

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

*Ramesh Jagannathan**

International Medical Cannabis Association, Toronto, Ontario, M1S 5E8, CANADA

Column1	Positive/Negative/Cannabis Metabolite	log S	log D	Papp
	468 Metabolites and positive & negative controls			
P1	Acetorphine	-4.388	1.338	-4.913
P2	Allylprodine	-3.957	2.778	-4.508
P3	Anileridine	-4.566	2.702	-4.944
P4	Benzethidine	-4.719	2.935	-4.688
P5	Betameprodine	-3.557	2.845	-4.507
P6	Bezitramide	-5.754	3.255	-4.807
P7	Butyrfentanyl	-5.413	3.396	-4.653
P8	Carfentanil	-4.865	2.873	-4.68
P9	Clonitazene	-5.47	2.732	-4.59
P10	Cocaine	-2.929	1.141	-4.498
P11	Codeine	-2.299	0.787	-4.446
P12	Codoxime	-3.473	0.46	-5.13
P13	Desomorphine	-3.503	0.969	-4.55
P14	Dextromoramide	-4.68	2.965	-4.583
P15	Diampromide	-4.746	2.81	-4.558
P16	Diethylthiambutene	-5.485	2.828	-4.563
P17	Difenoxin	-5.804	1.127	-5.187
P18	Ethanol	1.285	-0.026	-4.267
P19	Ethylmethylthiambutene	-4.482	2.823	-4.55
P20	Etonitazene	-5.476	1.52	-4.64
P21	Etorphine	-3.842	1.531	-5.078
P22	Fentanyl	-5.127	3.196	-4.623
P23	Heroin	-3.257	0.63	-4.487
P24	Hydrocodone	-3.133	1.261	-4.482
P25	Hydromorphone	-3.017	0.683	-4.707
P26	Isomethadone	-4.318	2.952	-4.543
P27	Ketobemidone	-2.956	1.009	-4.488
P28	Levomoramide	-4.68	2.965	-4.583
P29	Meperidine	-2.76	2.019	-4.465
P30	Morphine	-2.769	0.015	-5.212
P31	Morphine–n–oxide (morphine oxide)	-2.818	-0.082	-5.182
P32	Oxycodone	-2.258	0.472	-4.768
P33	Oxymorphone (dihydrohydroxymorphinone)	-2.55	-0.185	-5.176
P34	Propiram	-3.125	2.477	-4.469
P35	Acetylmethadol	-4.841	3.247	-4.584
P36	AH-7921	-4.566	2.611	-4.569
P37	Alphameprodine	-3.557	2.845	-4.507
P38	Alphaprodine	-3.375	2.556	-4.498
P39	Dextropropoxyphene	-4.726	3.072	-4.568

P40	Phenadoxone	-4.756	3.035	-4.567
P41	Phenampromide	-3.769	2.635	-4.492
P42	Phenazocine	-5.122	1.566	-4.804
P43	Phenomorphan	-5.29	1.969	-4.949
P44	Phenoperidine	-4.799	2.659	-4.884
P45	Piminodine	-5.048	2.877	-4.939
P46	Piritramide	-4.664	3.209	-5.076
P47	Proheptazine	-3.536	2.837	-4.534
P48	Properidine	-3.314	2.526	-4.455
P49	Racemethorphan	-3.867	1.77	-4.591
P50	Etoxeridine	-2.321	1.554	-4.718
P51	Remifentanil	-3.316	1.303	-4.499
P52	Sufentanil	-4.895	2.917	-4.675
P53	Thebacon	-3.238	1.301	-4.466
P54	Thebaine	-3.101	1.52	-4.486
P55	Thiofentanyl	-4.932	2.926	-4.602
P56	Tilidine	-3.466	2.472	-4.482
P57	Trimeperidine	-3.563	2.876	-4.493
P58	U-47700	-4.513	2.606	-4.582
P59	MT-45	-5.628	3.642	-4.76
P60	Lysergide	-3.387	2.241	-4.561
P61	Midomafetamine	-2.011	1.763	-4.449
P62	Methaqualone	-3.325	2.45	-4.181
P63	Mescaline	-1.779	0.453	-4.525
E1	N -arachidonoylethanolamine	-4.962	3.362	-4.946
E2	2-arachidonoyl glycerol.	-5.393	3.307	-5.037
E3	Dihomo- g -linolenoylethanolamide	-4.844	3.557	-4.932
E4	Docosatetraenoylethanolamide	-5.37	3.718	-4.943
E5	Arachidonylglyceryl ether	-5.379	3.73	-5.039
E6	N -arachidonoyl dopamine	-6.378	2.103	-5.129
E7	N -oleoyl dopamine	-5.815	2.201	-5.131
E8	Oleamide	-4.673	3.464	-4.604
E9	O -arachidonoylethanolamine	-4.873	3.515	-4.78
P64	Nicotine	-0.989	1.664	-4.461
N1	Acetate	1.141	-0.645	-4.344
N2	Biotin	-2.606	-0.935	-5.205
N3	Choline	0.718	0.023	-4.761
N4	Glucose	0.57	0.433	-5.783
N5	Glutamate	-0.789	-1.452	-5.114
N6	Histidine	-0.91	-1.506	-5.411
N7	Isoleucine	-0.834	-1.209	-4.967

N8	Lactate	0.918	-0.981	-4.445
N9	Leucine	-0.865	-1.225	-4.963
N10	Lysine	-0.401	-1.651	-5.432
N11	Methionine	-0.692	-1.317	-5.029
N12	Phenylalanine	-1.318	-1.385	-4.854
N13	Pyruvate	0.919	-0.828	-4.385
N14	Riboflavin	-3.517	0.864	-6.003
N15	Thiamine	-2.656	0.546	-5.171
N16	Tryptophan	-2.21	-1.255	-5.187
N17	Tyrosine	-1.824	-1.848	-5.305
N18	Valine	-0.248	-1.239	-5.04
T	THC	-3.5	2.007	-4.746
C1	1,1-Dimethylhydrazine	1.132	-0.1	-4.254
C2	1,2,3,4-Tetramethylbenzene	-4.146	2.469	-4.275
C3	1,2-Diethylbenzene	-3.466	2.323	-4.257
C4	1,3,5-Triazine-2,4,6-triamine	-1.486	-0.16	-5.474
C5	1,3-Dichlorobenzene	-3.113	2.516	-4.188
C6	1,4-Diethylbenzene	-3.728	2.365	-4.255
C7	1-Butanol	-0.029	0.415	-4.268
C8	1-Butoxy-2-Propanol	-0.366	1.378	-4.398
C9	Hexan-1-ol	-1.21	1.546	-4.25
C10	Undecan-1-ol	-3.641	2.982	-4.357
C11	2,2,5-Trimethylhexane	-5.04	2.827	-4.332
C12	2,3,4-Trimethylpentane	-4.675	2.623	-4.304
C13	2,4,6-Trimethylphenol	-2.031	0.697	-4.496
C14	2,4-Ditert-butylphenol	-4.025	1.563	-4.604
C15	2,6-Diethylpyrazine	-1.007	1.635	-4.24
C16	2,5-Dimethylpyrazine	-0.025	1.152	-4.195
C17	Butan-2-one	0.346	1.24	-4.227
C18	2-Butoxyethanol	0.679	0.34	-4.338
C19	1-(2-Chlorophenyl)Ethenone	-2.292	1.874	-4.181
C20	1,3-Dimethyl-2-Vinyl Benzene	-3.755	2.423	-4.225
C21	2-Ethoxyethanol	0.883	-0.245	-4.367
C22	2-Ethyl-1-hexanol	-2.184	1.997	-4.299
C23	2-Ethyl Toluene	-3.23	2.111	-4.188
C24	2-Formyl-Delta-9-Tetrahydrocannabinol	-5.499	1.941	-4.896
C25	2-Geranyl-5-Hydroxy-3-n-Pentanyl-1,4-Benzoquinone	-5.543	1.793	-4.775
C26	2-Heptanone	-1.489	1.897	-4.237
C27	2-Hydroxy-Acetophenone	-1.379	0.155	-4.465
C28	2-Isopropyl-3-methyl-pyrazine	-1.279	1.83	-4.286
C29	2-Methylaziridine	0.933	0.041	-4.296

C30	2-Methylnaphthalene	-3.796	2.712	-4.14
C31	2-Methyl-1H-imidazole	0.673	0.085	-4.205
C32	2-Methyl-Propanamine	0.647	0.366	-4.327
C33	2-Methylpentane	-3.725	2.284	-4.297
C34	2-Nitropropane	-0.401	-0.053	-4.27
C35	2-Phenoxy Ethanol	-0.755	0.155	-4.348
C36	3-(1-Methyl Ethyl)-Phenol Carbamate	-3.14	2.131	-4.387
C37	3-(3-Hydroxy Phenyl)-2-Propenoic acid, methyl ester	-2.208	-0.231	-4.738
C38	3,4,5,6-Tetrahydro-7-hydroxy-a,a-2-trimethyl-9-n-propyl-2,6-methano-2H-1-Benzoxocin-5-methanol	-4.282	1.43	-4.839
C39	3,4,5-Trimethylphenol	-2.051	0.628	-4.485
C40	3,4,5-Trimethylhex-1-ene	-4.321	2.626	-4.314
C41	3-Ethyl Toulene	-3.214	2.103	-4.183
C42	3-Ethyl-O-xylene	-3.938	2.424	-4.238
C43	3-Hydroxy-Delta-4,5-Cannabichromene	-5.119	1.741	-4.907
C44	3-Isopropyl Benzaldehyde	-2.303	2.084	-4.235
C45	3-Methyl Acetophenone	-2.051	1.716	-4.167
C46	3-Methyl Heptane	-5.097	2.829	-4.323
C47	3-methylcyclopent-2-en-1-one	-0.1	1.426	-4.122
C48	3-Methyl Pentane	-3.659	2.296	-4.296
C49	3-Methyl-5-(1-Methyl Ethyl)-Phenol Methyl Carbamate	-3.286	2.418	-4.393
C50	3-Pentanol	-0.249	1.486	-4.298
C51	4,5-Dihydroxy-2,3,6-Trimethoxy-9,10-Dihydrophenanthrene	-3.65	0.991	-4.882
C52	4,7-Dimethoxyphenanthrene-1,2,5-triol	-4.039	1.026	-5.055
C53	4-Acetoxy Cannabichromene	-5.608	1.93	-4.858
C54	4-Acetoxy-2-geranyl-5-hydroxy-3-n-pentylphenol	-5.948	1.762	-5.058
C55	4-Carene	-4.36	2.483	-4.309
C56	4-Ethoxy-3-anisaldehyde	-2.154	0.888	-4.299
C57	4-Hydroxy-2,3,6,7-tetramethoxy-9,10dihydrophenanthrene	-3.885	1.039	-4.812
C58	4-Methoxy-Couramin	-2.321	0.331	-4.255
C59	4-Methyl Decane	-6.047	2.965	-4.429
C60	4-Methylpyrimidine	0.574	0.422	-4.138
C61	4-Methyl Guaiacol	-1.068	0.415	-4.566
C62	4-Methyl Phenyl ethyl amine	-1.504	1.469	-4.318
C63	4-Pyridinamine	-0.994	1	-4.203
C64	4-Terpinyl Delta-9-tetrahydrocannabinolate	-6.078	2.452	-5.043
C65	4-Terpenyl Cannabinolate	-5.889	2.312	-4.984

C66	5-Acetoxy-6-Geranyl-3n -Pentyl-1,4-Benzoquinone	-5.968	3.351	-4.62
C67	5-Acetyl-4-Hydroxycannabigerol	-5.977	1.731	-5.059
C68	5-Ethenyl-2-Methylpyridine	-1.487	1.708	-4.109
C69	5-Methoxy Cannabigerolic acid	-5.948	1.689	-5.059
C70	5-Methyl-4-Pentyl-Biphenyl-2,2,6-Triol	-4.764	1.305	-4.974
C71	5-Methylindane	-3.406	2.146	-4.206
C72	5-Octanolide	-1.68	2.048	-4.22
C73	6,7-cis -Epoxycannabigerol	-5.126	1.342	-5.123
C74	6,7-cis-Epoxycannabigerolic acid	-5.126	1.342	-5.123
C75	6a-R-Cannabichromanone B	-4.686	1.008	-4.937
C76	6a-R-Cannabichromanone C	-4.685	0.92	-4.667
C77	6-Metiltetrapterol A	-5.615	1.476	-5.288
C78	6-Prenylapigenin	-5.128	1.169	-5.039
C79	7,8-Dehydro-10-O-ethylcannabitriol	-4.801	1.904	-5.047
C80	7,8-Dihydrocannabinol	-4.416	1.996	-4.721
C81	7-Hydroxy Cannabichromane	-4.935	1.857	-4.916
C82	7-Hydroxy cannabinol	-5.313	1.705	-4.963
C83	7-Methoxy Cannabispiranone	-3.643	1.528	-4.427
C84	7-R-Cannabicoumarononic acid	-5.389	1.186	-4.938
C85	8,9-Dihydroxy-delta-6a-tetrahydrocannabinol	-4.777	1.405	-4.946
C86	8-Hydroxy cannabinolic acid	-5.562	1.169	-5.1
C87	8-Hydroxyl cannabinol	-5.326	1.716	-4.955
C88	8a-Hydroxy-Delta-9-tetrahydrocannbinol	-4.59	1.836	-4.94
C89	8-oxo-Delta-9-tetrahydrocannbinol	-4.769	1.783	-4.718
C90	9,10-Anhydrocannabitriol	-5.076	2.087	-4.739
C91	9,10-Dihydro-2,3,5,6-Tetramethoxyphenanthrene-1,4-dione	-3.218	0.999	-4.447
C92	9 β ,10 β -Epoxyhexahydrocannabinol	-4.982	2.063	-4.766
C93	10 α -Hydroxy-Delta- 9,11 -Hexahydrocannabinol	-4.629	1.802	-4.938
C94	10-Ethoxy-9-hydroxy-delta-6a-Tetrahydrocannabinol	-5.241	2.04	-5.052
C95	10-Hydroxy-9-oxo-Delta-8-Tetrahydrocannabinol	-4.814	1.31	-4.882
C96	10-O-Ethyl bis-nor Cannabitriol	-4.795	1.856	-5.012
C97	10-Oxo-delta-6a-Tetrahydrocannabinol (OTHC)	-4.8	1.788	-4.722
C98	11-Acetoxy-Delta-8-Tetrahydrocannbinoic acid	-5.502	1.502	-5.122
C99	11-Acetoxy-Delta- 9 -Tetrahydrocannabinolic acid A	-5.502	1.484	-5.12
C100	Abnormal Cannabigerol	-5.432	2.006	-4.918
C101	Acetaldehyde	1.207	-0.078	-4.213
C102	Acetamide	1.399	-0.211	-4.449
C103	Acetic acid	1.083	-1.245	-4.353

C104	Acetone	1.036	0.281	-4.233
C105	Acetyl abnormal hydrocannabigeroquinol	-5.948	1.762	-5.058
C106	Acetyl cannabigeroquinol	-5.968	3.351	-4.62
C107	Acrolein	0.675	0.075	-4.166
C108	Acetophenone	-1.414	1.646	-4.144
C109	Alloaromadendrene	-5.662	2.88	-4.458
C110	Alpha-Bisabolol	-4.398	2.929	-4.422
C111	α-Bulnescene	-5.88	2.927	-4.459
C112	α-Cadinene	-5.85	2.988	-4.453
C113	a-Cadinyl Delta-9-tetrahydrocannabinolate	-5.96	2.776	-5.067
C114	Alpha-Cannabispiranol	-3.564	0.784	-4.754
C115	Alpha-Cedrene	-5.729	2.952	-4.439
C116	Alpha-Cis-Bergamotene	-5.864	2.99	-4.461
C117	Alpha- Copaene	-5.667	2.919	-4.435
C118	Alpha-Cubebene	-5.705	2.928	-4.435
C119	Alpha-Eudesmol	-4.177	2.908	-4.447
C120	Alpha-Guaiene	-5.88	2.932	-4.453
C121	Alpha-Gurjunene	-5.822	2.914	-4.462
C122	Alpha-Humulene	-6.518	3.059	-4.412
C123	Alpha-Ionol	-3.279	2.745	-4.357
C124	Alpa-Linilenic acid	-4.829	1.55	-4.729
C125	Alpha-Longipinene	-5.853	2.96	-4.436
C126	Alpha-Methyl-Cinnamaldehyde	-2.273	1.92	-4.149
C127	Alpha-Phellandrene	-4.116	2.714	-4.308
C128	Alpha-Pinene	-4.577	2.745	-4.326
C129	Alpha-Selinene	-5.89	2.954	-4.456
C130	Alpha-Terpinyl Delta-9-tetrahydrocannabinolate	-6.058	2.437	-5.044
C131	Alpha-Terpinene	-4.289	2.802	-4.324
C132	Alpha-Terpineol	-1.961	2.214	-4.344
C133	Alpha-Thujene	-4.516	2.733	-4.324
C134	Alpha-Trans-Bergamotene	-5.864	2.99	-4.461
C135	Alpha-Ylangene	-5.667	2.919	-4.435
C136	Amorfrutin-3	-4.591	0.596	-5.085
C137	Amorfrutin-4	-6.664	1.618	-5.146
C138	Amorfrutin-A	-5.311	1.093	-4.928
C139	Amorfrutin-B	-6.529	1.746	-5.148
C140	Anethole	-3.074	1.455	-4.158
C141	Anhydrocannabimovone	-4.686	1.781	-4.756
C142	Anhydrocannabisativine	-3.497	2.697	-4.727
C143	Anthopogochromenic acid	-4.897	1.17	-4.848
C144	Anthopogocyclolic acid	-4.559	0.78	-4.832

C145	Apigenin	-3.595	0.487	-4.985
C146	Arachidin-3	-5.14	1.373	-5.016
C147	Araphyn-1	-5.405	1.522	-4.876
C148	Araphyn-3	-3.834	0.834	-5.568
C149	Araphyn-4	-4.019	0.893	-5.233
C150	Aristolene	-5.878	2.919	-4.446
C151	Aromadendrene	-5.662	2.88	-4.458
C152	Benzaldehyde	-1.186	1.396	-4.103
C153	Benzonitrile	-1.422	1.393	-4.092
C154	Benzophenone	-3.054	2.475	-4.095
C155	Benzphentamine	-4.033	2.911	-4.315
C156	Benzyl acetate	-1.714	1.537	-4.197
C157	Benzyl Alcohol	-0.522	1.219	-4.144
C158	Benzyl formate	-1.461	1.388	-4.197
C159	Benzyl Nitrile	-2.474	1.506	-4.085
C160	Beta-Cannabispiranol	-3.564	0.784	-4.574
C161	Beta-Caryophyllene oxide	-4.273	2.866	-4.413
C162	Beta-Caryophyllene	-5.871	2.933	-4.45
C163	Beta-Cedrene	-5.738	2.932	-4.438
C164	Beta-Elemene	-5.548	2.937	-4.445
C165	Beta-Eudesmol	-4.196	2.938	-4.438
C166	Beta-fenchol (Beta-Fenchyl Alcohol)	-2.222	2.029	-4.382
C167	Beta-Fenchyl-Delta-9-tetrahydrocannabinolate	-6.049	2.514	-5.062
C168	Betahistine	-0.735	0.777	-4.223
C169	Beta-Irone	-3.928	2.788	-4.391
C170	Beta-phellandrene	-4.138	2.655	-4.31
C171	Beta-Pinene	-4.428	2.708	-4.326
C172	Beta-Selinene	-5.91	2.927	-4.449
C173	β-sitosteryl-3-O-b-D-glucopyranoside-2'-O-palmitate	-5.549	4.523	-5.088
C174	Betazole	-0.006	-0.046	-4.44
C175	Bis-nor-cannabichromanone	-4.583	1.193	-4.657
C176	Bis-nor-cannabielsoic acid B	-4.833	0.862	-5.017
C177	Bis-nor-cannabielsoin	-4.504	1.379	-4.824
C178	Bis-nor-cannabitriol	-4.808	1.357	-4.988
C179	Borneol	-2.307	2.026	-4.388
C180	Bornyl Delta-9-tetrahydrocannabinolate	-5.939	2.988	-5.055
C181	Butane	-2.833	1.663	-4.229
C182	Butyl formate	-0.999	0.951	-4.214
C183	Gamma-Cadinyl Cannabigerolate	-5.64	2.588	-5.207
C184	Calarene	-5.888	2.908	-4.447
C185	Camphene	-4.42	2.71	-4.326

C186	Cannabichromanone (CBCF)	-4.746	1.403	-4.747
C187	Cannabichromaonone D	-4.834	2.196	-4.577
C188	Cannabichromene (CBC)	-4.98	1.968	-4.728
C189	Cannabichromenic acid (CBCA)	-5.643	1.581	-5.02
C190	Cannabichromevarin (CBCV)	-4.991	1.86	-4.65
C191	Cannabichromevarinic acid (CBCVA)	-5.398	1.399	-4.962
C192	Cannabicitran	-4.956	2.471	-4.576
C193	Cannabicoumaronone	-4.956	2.209	-4.563
C194	Cannabicyclol (CBL)	-4.547	1.964	-4.767
C195	Cannabicyclolic acid (CBLA)	-5.446	1.323	-5.066
C196	Cannabicyclovarin (CBLV)	-4.545	1.741	-4.687
C197	Cannabidiol (CBD)	-5.258	1.864	-4.923
C198	Cannabidiolic acid (CBDA)	-5.8	1.466	-5.072
C199	Cannabidiol monomethylether (CBDM)	-5.463	1.991	-4.863
C200	Cannabidiorcol (CBD-C1)	-4.499	1.519	-4.827
C201	Cannabidivarin (CBDV)	-5.119	1.714	-4.892
C202	Cannabidivarinic acid (CBDVA)	-5.064	1.299	-5.04
C203	Cannabielsoic acid B (CBEA-B)	-5.256	1.268	-5.066
C204	Cannabielsoic acid A (CBEA-A)	-5.25	1.279	-5.076
C205	Cannabielsoin (CBE)	-4.817	1.805	-4.961
C206	Cannabiflavin B	-5.192	1.205	-5.056
C207	Cannabifuran (CBF)	-6.03	1.811	-4.701
C208	Cannabigerol (CBG)	-5.507	1.989	-4.936
C209	Cannabigerolic acid monomethylether (CBGAM)	-5.948	1.689	-5.059
C210	Cannabigerolic acid (CBGA)	-5.891	1.558	-5.077
C211	Cannabigerol monomethylether (CBGM)	-5.554	2.059	-4.836
C212	Cannabigeroquinone	-5.212	3.269	-4.532
C213	Cannabigerovarin (CBGV)	-4.929	1.855	-4.884
C214	Cannabigerovarinic acid (CBGVA)	-5.512	1.388	-5.045
C215	Cannabiglendol	-4.424	1.409	-4.832
C216	Cannabimovone	-4.573	1.233	-4.995
C217	Cannabinerol	-5.507	1.989	-4.936
C218	Cannabinerolic acid	-5.891	1.558	-5.077
C219	Cannabinodiol (CBND)	-5.934	1.798	-4.91
C220	Cannabinodivarin (CBVD)	-5.523	1.643	-4.862
C221	Cannabinol methylether (CBNM)	-5.999	2.334	-4.565
C222	Cannabinol (CBN)	-5.086	1.861	-4.718
C223	Cannabinol-C2 (CBN-C2)	-4.887	1.545	-4.624
C224	Cannabinol-C4 (CBN-C4)	-5.274	1.766	-4.711
C225	Cannabinolic acid (CBNA)	-5.682	1.257	-4.997
C226	Cannabiorcol (CBN-C1)	-4.855	1.45	-4.608

C227	Cannabiorcicchromene	-4.422	1.617	-4.643
C228	Cannabiorcicchromenic acid	-4.914	1.147	-4.853
C229	Cannabiorcicitran	-4.58	1.895	-4.482
C230	Cannabiorcicyclol	-4.442	1.412	-4.611
C231	Cannabiorcicyclolic acid	-4.542	0.771	-4.829
C232	Cannabioxepane	-6.022	2.177	-4.549
C233	Cannabiripsol (CBR)	-4.751	1.397	-4.945
C234	Cannabissativine	-2.87	1.929	-5.535
C235	Cannabisin-A	-4.773	1.453	-6.344
C236	Cannabisin-B	-4.32	1.173	-6.537
C237	Cannabisin-C	-4.464	1.283	-6.418
C238	Cannabisin-D	-4.711	1.529	-6.224
C239	Cannabispirone	-3.584	0.946	-4.523
C240	Cannabitriol (CBT)	-4.755	1.407	-4.941
C241	Cannabitriolvarin (CBTV)	-4.246	1.651	-4.616
C242	Cannabivarin (CBV)	-5.37	1.685	-4.654
C243	Cannflavin A	-5.846	1.834	-5.192
C244	Cannflavin B	-5.192	1.205	-5.056
C245	Cannflavin C	-5.747	1.785	-5.168
C246	Carbofuran	-2.756	0.483	-4.447
C247	Carmagerol	-4.888	1.514	-5.113
C248	Carvacrol	-2.04	1.171	-4.534
C249	Carvone	-2.063	2.07	-4.258
C250	CBDA-THC ester	-5.379	2.803	-5.211
C251	Cedryl acetate	-4.374	3	-4.458
C252	Cetyl Alcohol	-6.646	3.544	-4.476
C253	Chiricanine B	-4.817	1.573	-4.621
C254	Chlorocannabiorcicchromenic acid	-5.494	1.312	-4.918
C255	Chrysoeriol	-3.602	0.664	-5.106
C256	cis-2-Pinanol	-2.085	1.991	-4.378
C257	cis-Beta-Farnesene	-6.607	3.021	-4.402
C258	cis-Gamma-Bisabolene	-6.416	2.984	-4.416
C259	cis-Ocimene	-4.438	2.76	-4.294
C260	cis-Sabinene Hydrate	-4.554	2.786	-4.326
C261	Citronellyl acetate	-3.332	2.768	-4.328
C262	Citronellolformate	-3.113	2.152	-4.304
C263	Compound-2	-4.81	1.094	-4.948
C264	Compound-3	-4.876	0.992	-4.785
C265	compound-4	-4.834	2.196	-4.577
C266	Confluentin	-5.596	1.956	-4.828
C267	Cumene	-3.392	2.367	-4.284

C268	Cuminaldehyde	-2.439	2.132	-4.223
C269	Daurichromenic acid	-6.075	1.66	-5.096
C270	Delta-9-tetrahydrocannabiorcolic acid (THCA-C1)	-4.633	1.051	-4.809
C271	Decanal	-3.545	3.085	-4.294
C272	Decarboxyamorfrutin A	-5.041	1.753	-4.767
C273	Decarboxyamorfrutin B	-6.863	2.159	-5
C274	Dehydrocannabifuran (DCBF)	-6.056	1.782	-4.678
C275	Delta-3-Carene	-4.382	2.753	-4.304
C276	Delta-7-cis-Isotetrahydrocannabivarin	-4.708	1.8	-4.673
C277	Delta-7-trans-Isotetrahydrocannabinol	-3.753	1.973	-4.738
C278	Delta-8-tetrahydrocannabinol (Δ8-THC)	-3.723	2.011	-4.746
C279	Delta-8-tetrahydrocannabinolic acid (Δ8-THCA)	-5.434	1.593	-5.029
C280	Delta-9-cis-tetrahydrocannabivarin	-4.708	1.845	-4.677
C281	Delta-9-nor-tetrahydrocannbinolic acid	-5.52	1.548	-5.016
C282	Delta-9-nor-tetrahydrocannbinol	-4.555	1.945	-4.739
C283	Delta-9-Tetrahydrocannabinol-C4	-4.345	1.936	-4.744
C284	Delta-9-tetrahydrocannabiorcol (THC-C1)	-4.471	1.609	-4.636
C285	Delta-9-tetrahydrocannabinolic acid A (THCA-A)	-5.434	1.593	-5.029
C286	Delta-9-tetrahydrocannabinolic acid B (THCA-B)	-5.43	1.595	-5.01
C287	Delta-9-tetrahydrocannabinolic acid-C4 (THCA-C4)	-5.351	1.483	-4.994
C288	Delta-Cadinene	-5.888	2.963	-4.458
C289	Demethylamorfrutin A	-5.303	0.804	-4.992
C290	Demethyldecarboxyamorfrutin A	-4.979	1.481	-4.866
C291	Deprenyl O-methyl cannbigerolic acid	-4.581	1.12	-4.872
C292	Desmodianone A	-5.97	1.848	-5.24
C293	Desmodianone C	-6.187	1.853	-5.436
C294	Desmodianone D	-4.895	1.773	-5.29
C295	Desmodianone E	-5.699	1.846	-5.252
C296	Diacetone alcohol	0.57	0.346	-4.269
C297	Dibutyl phthalate	-4.392	2.671	-4.401
C298	Diethyl Phthalate	-2.396	1.799	-4.403
C299	Dimethylbenzylcarbinyl acetate	-2.83	2.236	-4.261
C300	Dimethylsulfone	0.442	-0.335	-4.321
C301	Dimethylsulfide	-0.595	1.036	-4.207
C302	Dodecane	-7.341	3.003	-4.426
C303	Dothiepin Sulfoxide	-4.596	2.857	-4.415
C304	Durene	-4.242	2.47	-4.279
C305	Dyclocaine	-4.154	1.717	-4.526
C306	epi-Bornyl Delta-9-tetrahydrocannabinolate	-6.041	2.522	-5.059
C307	Estragole	-2.749	1.278	-4.132
C308	Ethylacetate	-0.045	0.166	-4.253

C309	Ethylenediamine	1.035	-0.18	-4.451
C310	Ethylene oxide	1.105	-0.069	-4.216
C311	Ethylenimine	0.891	-0.065	-4.242
C312	Eudesmyl-Cannabigerolate	-5.671	2.652	-5.183
C313	Eugenol	-1.868	0.77	-4.551
C314	Eugenyl acetate	-2.608	0.909	-4.366
C315	Fenchone	-2.04	2.309	-4.336
C316	Fenchyl Alcohol	-2.222	2.029	-4.382
C317	Ferruginene A	-4.962	1.423	-5
C318	Ferruginene B	-4.968	1.419	-4.991
C319	Ferruginene C	-5.576	1.644	-5.047
C320	Formic acid	0.85	-0.769	-4.522
C321	Furfural	-0.106	1.193	-4.143
C322	Furfurylmethylamphetamine	-3.612	2.11	-4.337
C323	Gamma-curcumene	-6.4	2.996	-4.458
C324	Gamma-eudesmol	-4.363	2.94	-4.428
C325	Gamma-Gurjunene	-5.897	2.933	-4.459
C326	Gamma-Hexalactone	-0.617	1.676	-4.214
C327	Gamma-Muurolene	-5.878	2.942	-4.459
C328	Gamma-Terpinene	-4.24	2.799	-4.324
C329	Glepidotin C	-4.205	1.142	-4.979
C330	Globulol	-3.686	2.733	-4.424
C331	Grossamide	-4.928	1.792	-6.171
C332	Guajol	-0.73	0.151	-4.514
C333	Heli-Cannabigenol	-6.795	2.064	-5.05
C334	Heptanal	-1.895	1.899	-4.233
C335	Hexadecane	-8.358	3.7	-4.45
C336	Hexahydrocannabinol	-4.149	1.905	-4.75
C337	Hexanal	-1.271	1.646	-4.215
C338	Hexanoic acid, methyl ester	-1.932	1.371	-4.219
C339	Hexanoic acid, propyl ester	-2.813	2.274	-4.231
C340	Hexestrol	-4.461	1.473	-4.83
C341	Hordenine	-1.305	0.622	-4.613
C342	Hydroxy Heli-Cannabigerol	-6.92	1.906	-5.134
C343	Ipsdienol	-2.448	2	-4.305
C344	Isoamyl alcohol	-0.476	1.214	-4.327
C345	Isobornyl acetate	-2.626	2.688	-4.359
C346	Isobornyl thiocyanoacetate	-3.354	2.813	-4.385
C347	Isobutane	-2.852	1.564	-4.299
C348	Isobutyraldehyde	0.072	0.59	-4.242
C349	Isobutyrophenone	-2.417	2.046	-4.207

C350	Isocannabitrol	-4.958	1.484	-4.952
C351	Isocyanatomethane	0.904	-0.163	-4.218
C352	Isodurene	-4.135	2.513	-4.267
C353	Isoeugenol	-2.237	1.039	-4.551
C354	Isolimonene	-4.142	2.679	-4.321
C355	Isoprene	-2.066	1.64	-4.223
C356	Isoquinoline	-1.575	1.78	-4.064
C357	Kaempferol	-3.427	0.273	-5.074
C358	Limonene oxide	-1.359	1.972	-4.441
C359	Limonene	-4.142	2.791	-4.329
C360	Linalool	-2.147	2.333	-4.297
C361	Linalyl acetate	-3.212	2.892	-4.252
C362	Linoleic acid	-4.998	1.596	-4.706
C363	Longifolene	-5.821	2.947	-4.43
C364	Luteolin	-3.502	0.302	-5.123
C365	Machaeridiol A	-6.6	1.814	-5.024
C366	Machaeridiol B	-6.53	1.744	-5.126
C367	Machaeridiol C	-6.399	1.712	-5.159
C368	Machaeridiol D	-5.821	1.677	-5.165
C369	m-Cymene	-3.63	2.628	-4.31
C370	Methacrolein	-0.014	0.498	-4.208
C371	Methacrylic anhydride	-1.415	1.172	-4.25
C372	Methyl acetate	0.606	-0.114	-4.265
C373	Methyl acetylsalicylate	-2.198	1.203	-4.342
C374	Methyl anthranilate	-1.738	0.847	-4.458
C375	Methyl Benzoate	-1.674	1.366	-4.166
C376	Methyl carbamate	0.868	-0.512	-4.446
C377	Methyl heptadienone	-1.857	1.783	-4.219
C378	Methyl heptanoate	-2.218	1.59	-4.256
C379	Methyl Hydrazine	1.196	-0.067	-4.249
C380	Methyl isoeugenol	-2.576	1.496	-4.325
C381	Methyl Salicylate	-2.055	-0.883	-4.762
C382	Methyl valerate	-1.317	1.109	-4.226
C383	Methylene Chloride	-0.962	1.348	-4.208
C384	Methylen-bis-Delta-9-tetrahydrocannabinol	-5.955	3.193	-5.219
C385	Methylisohexenyl ketone	-1.998	2.128	-4.232
C386	m-Tert-Butyl Phenol	-2.006	1.162	-4.517
C387	Myrcene	-4.364	2.704	-4.276
C388	Nerol	-2.763	2.416	-4.303
C389	Nerolidol	-4.297	3.001	-4.42
C390	Nitrobenzene	-1.595	1.345	-4.174

C391	Nonanal	-3.129	2.713	-4.263
C392	Nonane	-5.691	2.939	-4.308
C393	nor-Cannabidiol	-5.132	1.779	-4.915
C394	nor-Cannabinol	-5.274	1.766	-4.711
C395	nor-Cannabivarin	-4.887	1.545	-4.624
C396	N-p-Coumaroyltyramine	-3.391	0.715	-5.072
C397	N-trans-feruloyltyramine	-3.569	0.737	-5.17
C398	Octanal	-2.383	2.239	-4.243
C399	o-Cymene	-3.741	2.578	-4.31
C400	o-Dimethyl Hydroquinone	-1.117	0.887	-4.313
C401	O-Guaiacol	-0.73	0.151	-4.514
C402	Oleic acid	-5.074	1.613	-4.697
C403	O-Methyl Cannabigerol	-5.554	2.059	-4.836
C404	O-Methyl Acetophenone	-2.035	1.723	-4.164
C405	O-Pentyl-cannabidiol	-6	2.366	-4.947
C406	O-Pentyl-Delta-9-tetrahydrocannbinol	-6.549	2.839	-4.686
C407	O-Propyl-cannabidiol	-5.779	2.149	-4.896
C408	O-Propyl-Delta-9-tetrahydrocannbinol	-6.143	2.635	-4.689
C409	Orientin	-3.326	-0.084	-6.422
C410	O-Xylene	-2.817	1.947	-4.215
C411	P-Acetanisole	-1.922	0.856	-4.2
C412	P-Aminotoluene	-1.108	1.43	-4.33
C413	P-Cymene	-3.775	2.671	-4.318
C414	Pentadecane	-8.831	3.585	-4.447
C415	Pentamethylbenzene	-4.159	2.668	-4.303
C416	Pentanal	-0.791	1.387	-4.216
C417	Perillaldehyde	-2.198	2.154	-4.272
C418	Perrottetinene	-6.407	2.019	-4.898
C419	Perrottetinenic acid	-6.196	1.644	-5.212
C420	P-ethyl Toulene	-3.171	2.116	-4.185
C421	Phenol	-0.157	0.023	-4.27
C422	Phenylethyl alcohol	-0.876	1.297	-4.172
C423	Piperidine	0.235	0.541	-4.194
C424	Piperonal	-1.681	1.248	-4.246
C425	P-Methyl Acetophenone	-2.304	1.727	-4.163
C426	Propanal	0.686	0.292	-4.2
C427	Propofol	-3.381	1.506	-4.675
C428	Propanoic acid,anhydride	-1.017	0.646	-4.274
C429	Propylamine	0.92	0.265	-4.318
C430	Propylene Glycol	1.099	-0.448	-4.754
C431	P-Tert-Butylphenol	-2.125	1.189	-4.507

C432	P-Xylene	-2.834	1.951	-4.225
C433	Quercetin	-3.534	0.142	-6.168
C434	rac-6'-Epoxycannbigerol	-5.464	1.93	-4.99
C435	rac-6'-Epoxycannbigerolic acid	-5.577	1.48	-5.098
C436	Radulanin A	-4.647	1.468	-4.729
C437	Radulanin H	-4.68	0.836	-4.878
C438	Radulanin I	-4.679	1.358	-4.718
C439	Radulanin J	-4.99	1.942	-4.644
C440	Radulanin K	-4.793	0.635	-4.909
C441	Radulanin L	-4.51	1.272	-4.881
C442	Rhododaurichromanic A	-5.603	1.664	-5.099
C443	Roughanic acid	-4.467	1.34	-4.649
C444	Sabinene	-4.389	2.717	-4.322
C445	Salicyladehyde	-0.872	-0.274	-4.399
C446	Sativene	-5.71	2.929	-4.432
C447	Sesquicannabigerol	-6.42	2.263	-5.112
C448	Stearidonic acid	-4.813	1.49	-4.713
C449	Styrene	-2.632	1.917	-4.124
C450	Tert-butyl alcohol	0.798	0.229	-4.275
C451	Terpinolene	-4.273	2.839	-4.274
C452	tert-butyl-benzene	-3.714	2.58	-4.251
C453	Tetrahydrocannabinol epoxide	-4.982	2.063	-4.766
C454	Tetrahydrozoline	-2.792	2.239	-4.302
C455	Thymol	-1.986	1.209	-4.534
C456	Toluene	-2.385	1.767	-4.161
C457	Trans-alpha-farnesene	-6.071	3.053	-4.407
C458	Trans-Archidin-1	-5.575	1.276	-5.34
C459	Trans-Archidin-2	-5.12	1.184	-4.977
C460	Trans-gamma-bisabolene	-6.416	2.984	-4.416
C461	Trans-ocimene	-4.348	2.76	-4.294
C462	Tridecane	-7.482	3.027	-4.427
C463	Tyramine	-1.094	-0.131	-4.686
C464	Undecane	-7.038	2.973	-4.4
C465	Valencene	-5.972	2.927	-4.458
C466	Verbenone	-2.14	1.971	-4.334
C467	Vitexin	-3.37	-0.144	-6.317
C468	N-trans-caffeoyltyramine	-3.49	0.483	-5.465

	Metabolites after MDS using CDK (165) (used for MDS using ADMET)			
		log S	log D	Papp
C19	1-(2-chlorophenyl)ethenone	-2.292	1.874	-4.181
C24	2-Formyl-Delta-9-Tetrahydrocannabinol	-5.499	1.941	-4.896
C25	2-Geranyl-5-Hydroxy-3-n-Pentanyl-1,4-Benzoquinone	-5.543	1.793	-4.775
C38	3,4,5,6-tetrahydro-7-hydroxy-a,a-2-trimethyl-9-n-propyl-2,6-methano-2H-1-Benzoxocin-5-methanol	-4.282	1.43	-4.839
C43	3-Hydroxy-Delta-4,5-Cannabichromene	-5.119	1.741	-4.907
C45	3-Methyl Acetophenone	-2.051	1.716	-4.167
C51	4,5-Dihydroxy-2,3,6-Trimethoxy-9,10-Dihydrophenanthrene	-3.65	0.991	-4.882
C53	4-Acetoxy Cannabichromene	-5.608	1.93	-4.858
C54	4-Acetoxy-2-geranyl-5-hydroxy-3-n-pentylphenol	-5.948	1.762	-5.058
C57	4-hydroxy-2,3,6,7-tetramethoxy-9,10dihydrophenanthrene	-3.885	1.039	-4.812
C66	5-acetoxy-6-geranyl-3n -pentyl-1,4-benzoquinone	-5.968	3.351	-4.62
C70	5-Methyl-4-Pentyl-Biphenyl-2,2,6-Triol	-4.764	1.305	-4.974
C75	6a-R-Cannabichromanone B	-4.686	1.008	-4.937
C79	7,8-Dehydro-10-O-ethylcannabitriol	-4.801	1.904	-5.047
C80	7,8-dihydrocannabinol	-4.416	1.996	-4.721
C81	7-Hydroxy Cannabichromane	-4.935	1.857	-4.916
C82	7-hydroxy cannabinol	-5.313	1.705	-4.963
C83	7-Methoxy Cannabispiranone	-3.643	1.528	-4.427
C84	7-R-Cannabicoumarononic acid	-5.389	1.186	-4.938
C88	8a-Hydroxy-Delta-9-tetrahydrocannbinol	-4.59	1.836	-4.94
C89	8-oxo-Delta-9-tetrahydrocannbinol	-4.769	1.783	-4.718
C90	9,10-Anhydrocannabitriol	-5.076	2.087	-4.739
C92	9 β ,10 β -Epoxyhexahydrocannabinol	-4.982	2.063	-4.766
C93	10 α -Hydroxy-Delta- 9,11 -hexahydrocannabinol	-4.629	1.802	-4.938
C94	10-Ethoxy-9-hydroxy-delta-6a-tetrahydrocannabinol	-5.241	2.04	-5.052
C95	10-Hydroxy-9-oxo-Delta-8-tetrahydrocannabinol	-4.814	1.31	-4.882
C96	10-O-Ethyl bis-nor cannabitriol	-4.795	1.856	-5.012
C97	10-Oxo-delta-6a-tetrahydrocannabinol (OTHC)	-4.8	1.788	-4.722
C100	abnormal cannabigerol	-5.432	2.006	-4.918
C105	acetyl abnormal hydrocannabigeroquinol	-5.948	1.762	-5.058
C114	Alpha-Cannabispiranol	-3.564	0.784	-4.754
C123	Alpha-Ionol	-3.279	2.745	-4.357
C124	Alpa-Linilenic acid	-4.829	1.55	-4.729

C126	Alpha-Methyl-Cinnamaldehyde	-2.273	1.92	-4.149
C139	Amorfrutin-B	-6.529	1.746	-5.148
C140	Anethole	-3.074	1.455	-4.158
C141	Anhydrocannabimovone	-4.686	1.781	-4.756
C146	Arachidin-3	-5.14	1.373	-5.016
C147	Araphyn-1	-5.405	1.522	-4.876
C160	Beta-Cannabispiranol	-3.564	0.784	-4.574
C175	Bis-nor-cannabichromanone	-4.583	1.193	-4.657
C177	Bis-nor-cannabielsoin	-4.504	1.379	-4.824
C178	Bis-nor-cannabitriol	-4.808	1.357	-4.988
C186	Cannabichromanone (CBCF)	-4.746	1.403	-4.747
C187	Cannabichromaonone D	-4.834	2.196	-4.577
C188	Cannabichromene (CBC)	-4.98	1.968	-4.728
C189	Cannabichromenic acid (CBCA)	-5.643	1.581	-5.02
C190	Cannabichromevarin (CBCV)	-4.991	1.86	-4.65
C191	Cannabichromevarinic acid (CBCVA)	-5.398	1.399	-4.962
C192	Cannabicitran	-4.956	2.471	-4.576
C193	cannabicoumaronone	-4.956	2.209	-4.563
C194	Cannabicyclol (CBL)	-4.547	1.964	-4.767
C195	Cannabicyclolic acid (CBLA)	-5.446	1.323	-5.066
C196	Cannabicyclovarin (CBLV)	-4.545	1.741	-4.687
C197	Cannabidiol (CBD)	-5.258	1.864	-4.923
C199	Cannabidiol monomethylether (CBDM)	-5.463	1.991	-4.863
C200	Cannabidiorcol (CBD-C1)	-4.499	1.519	-4.827
C201	Cannabidivarin (CBDV)	-5.119	1.714	-4.892
C204	Cannabielsoic acid A (CBEA-A)	-5.25	1.279	-5.076
C205	Cannabielsoin (CBE)	-4.817	1.805	-4.961
C207	Cannabifuran (CBF)	-6.03	1.811	-4.701
C211	Cannabigerol monomethylether (CBGM)	-5.554	2.059	-4.836
C212	cannabigeroquinone	-5.212	3.269	-4.532
C213	Cannabigerovarin (CBGV)	-4.929	1.855	-4.884
C215	Cannabiglendol	-4.424	1.409	-4.832
C217	cannabinerol	-5.507	1.989	-4.936
C219	Cannabinodiol (CBND)	-5.934	1.798	-4.91
C220	Cannabinodivarin (CBVD)	-5.523	1.643	-4.862
C221	Cannabinol methylether (CBNM)	-5.999	2.334	-4.565
C222	Cannabinol (CBN)	-5.086	1.861	-4.718
C223	Cannabinol-C2 (CBN-C2)	-4.887	1.545	-4.624
C224	Cannabinol-C4 (CBN-C4)	-5.274	1.766	-4.711
C226	Cannabiorcol (CBN-C1)	-4.855	1.45	-4.608
C227	cannabiorcicchromene	-4.422	1.617	-4.643

C229	cannabiorcicitran	-4.58	1.895	-4.482
C230	cannabiorcicyclol	-4.442	1.412	-4.611
C231	cannabiorcicyclolic acid	-4.542	0.771	-4.829
C232	cannabioxepane	-6.022	2.177	-4.549
C239	cannabispirone	-3.584	0.946	-4.523
C241	Cannabitriol (CBT)	-4.246	1.651	-4.616
C242	Cannabitriolvarin (CBTV)	-5.37	1.685	-4.654
C246	Cannabivarin (CBV)	-2.756	0.483	-4.447
C251	Cedryl acetate	-4.374	3	-4.458
C253	Chiricanine B	-4.817	1.573	-4.621
C256	cis-2-pinanol	-2.085	1.991	-4.378
C261	Citronellyl acetate	-3.332	2.768	-4.328
C262	Citronellolformate	-3.113	2.152	-4.304
C263	compound-2	-4.81	1.094	-4.948
C264	Compound-3	-4.876	0.992	-4.785
C265	compound-4	-4.834	2.196	-4.577
C266	Confluentin	-5.596	1.956	-4.828
C268	Cuminaldehyde	-2.439	2.132	-4.223
C270	Delta-9-tetrahydrocannabiorcolic acid (THCA-C1)	-4.633	1.051	-4.809
C272	Decarboxyamorfrutin A	-5.041	1.753	-4.767
C273	Decarboxyamorfrutin B	-6.863	2.159	-5
C274	Dehydrocannabifuran (DCBF)	-6.056	1.782	-4.678
C276	Delta-7-cis-Isotetrahydrocannabivarin	-4.708	1.8	-4.673
C277	Delta-7-trans-Isotetrahydrocannabinol	-3.753	1.973	-4.738
C278	Delta-8-tetrahydrocannabinol (Δ8-THC)	-3.723	2.011	-4.746
C279	Delta-8-tetrahydrocannabinolic acid (Δ8-THCA)	-5.434	1.593	-5.029
C280	Delta-9-cis-tetrahydrocannabivarin	-4.708	1.845	-4.677
C281	Delta-9-nor-tetrahydrocannbinolic acid	-5.52	1.548	-5.016
C282	Delta-9-nor-tetrahydrocannbinol	-4.555	1.945	-4.739
C283	Delta-9-Tetrahydrocannabinol-C4	-4.345	1.936	-4.744
C284	Delta-9-tetrahydrocannabiorcol (THC-C1)	-4.471	1.609	-4.636
C285	Delta-9-tetrahydrocannabinolic acid A (THCA-A)	-5.434	1.593	-5.029
C286	Delta-9-tetrahydrocannabinolic acid B (THCA-B)	-5.43	1.595	-5.01
C287	Delta-9-tetrahydrocannabinolic acid-C4 (THCA-C4)	-5.351	1.483	-4.994
C290	Demethyldecarboxyamorfrutin A	-4.979	1.481	-4.866
C297	Dibutyl phthalate	-4.392	2.671	-4.401
C298	Diethyl Phthalate	-2.396	1.799	-4.403
C299	Dimethylbenzylcarbinyl acetate	-2.83	2.236	-4.261
C305	Dyclocaine	-4.154	1.717	-4.526
C307	Estragole	-2.749	1.278	-4.132
C313	Eugenol	-1.868	0.77	-4.551

C314	Eugenyl acetate	-2.608	0.909	-4.366
C315	Fenchone	-2.04	2.309	-4.336
C317	Ferruginene A	-4.962	1.423	-5
C318	Ferruginene B	-4.968	1.419	-4.991
C319	Ferruginene C	-5.576	1.644	-5.047
C329	Glepidotin C	-4.205	1.142	-4.979
C333	Heli-Cannabigenol	-6.795	2.064	-5.05
C336	Hexahydrocannabinol	-4.149	1.905	-4.75
C339	Hexanoic acid, propyl ester	-2.813	2.274	-4.231
C341	Hordenine	-1.305	0.622	-4.613
C342	Hydroxy Heli-Cannabigerol	-6.92	1.906	-5.134
C349	Isobutyrophenone	-2.417	2.046	-4.207
C350	Isocannabitrol	-4.958	1.484	-4.952
C353	Isoeugenol	-2.237	1.039	-4.551
C358	Limonene oxide	-1.359	1.972	-4.441
C361	linoleic acid	-3.212	2.892	-4.252
C362	Longifolene	-4.998	1.596	-4.706
C365	Machaeridiol A	-6.6	1.814	-5.024
C366	Machaeridiol B	-6.53	1.744	-5.126
C367	Machaeridiol C	-6.399	1.712	-5.159
C368	Machaeridiol D	-5.821	1.677	-5.165
C380	Methyl isoeugenol	-2.576	1.496	-4.325
C386	m-Tert-Butyl Phenol	-2.006	1.162	-4.517
C393	nor-cannabidiol	-5.132	1.779	-4.915
C394	nor-cannabinol	-5.274	1.766	-4.711
C395	nor-cannabivarin	-4.887	1.545	-4.624
C396	N-p-Coumaroyltyramine	-3.391	0.715	-5.072
C397	N-trans-feruloyltyramine	-3.569	0.737	-5.17
C402	oleic acid	-5.074	1.613	-4.697
C403	O-Methyl Cannabigerol	-5.554	2.059	-4.836
C405	O-Pentyl-cannabidiol	-6	2.366	-4.947
C407	O-Propyl-cannabidiol	-5.779	2.149	-4.896
C411	p-acetanisole	-1.922	0.856	-4.2
C417	Perillaldehyde	-2.198	2.154	-4.272
C418	Perrottetinene	-6.407	2.019	-4.898
C419	Perrottetinenic acid	-6.196	1.644	-5.212
C427	Propofol	-3.381	1.506	-4.675
C434	rac-6'-Epoxycannbigerol	-5.464	1.93	-4.99
C435	rac-6'-Epoxycannbigerolic acid	-5.577	1.48	-5.098
C436	Radulanin A	-4.647	1.468	-4.729
C437	Radulanin H	-4.68	0.836	-4.878

C438	Radulanin I	-4.679	1.358	-4.718
C440	Radulanin K	-4.793	0.635	-4.909
C441	Radulanin L	-4.51	1.272	-4.881
C448	stearidonic acid	-4.813	1.49	-4.713
C453	Tetrahydrocannabinol epoxide	-4.982	2.063	-4.766
C454	Tetrahydrozoline	-2.792	2.239	-4.302
C455	Thymol	-1.986	1.209	-4.534
C459	Trans-Archidin-2	-5.12	1.184	-4.977
C466	Verbenone	-2.14	1.971	-4.334
	468 Metabolites and positive & negative controls			
Pgp-In	HIA	F20%	F30%	PPB
0.732	0.528	0.281	0.3	79
0.911	0.713	0.363	0.534	85
0.873	0.72	0.508	0.44	94
0.858	0.583	0.529	0.371	92
0.884	0.702	0.347	0.547	75
0.933	0.74	0.487	0.531	96
0.966	0.808	0.236	0.269	94
0.964	0.621	0.42	0.37	94
0.506	0.699	0.7	0.624	93
0.725	0.598	0.531	0.626	69
0.222	0.722	0.59	0.507	54
0.249	0.443	0.408	0.455	67
0.055	0.786	0.588	0.343	62
0.713	0.785	0.627	0.547	90
0.83	0.799	0.434	0.515	93
0.26	0.797	0.504	0.553	82
0.768	0.726	0.559	0.623	89
0.018	0.821	0.613	0.764	9
0.398	0.795	0.546	0.586	83
0.675	0.589	0.526	0.521	94
0.362	0.577	0.397	0.255	79
0.935	0.818	0.194	0.164	93
0.5	0.607	0.087	0.094	73
0.332	0.736	0.617	0.584	55
0.063	0.768	0.656	0.457	53
0.268	0.809	0.664	0.663	89
0.411	0.776	0.325	0.575	72

0.713	0.785	0.627	0.547	90
0.579	0.756	0.46	0.682	65
0.042	0.759	0.607	0.171	51
0.056	0.432	0.395	0.246	53
0.33	0.615	0.437	0.5	50
0.062	0.627	0.196	0.129	43
0.794	0.705	0.458	0.431	70
0.646	0.742	0.635	0.738	90
0.252	0.84	0.751	0.61	91
0.884	0.702	0.347	0.547	75
0.782	0.702	0.347	0.493	59
0.83	0.75	0.562	0.632	90
0.702	0.776	0.478	0.662	90
0.797	0.825	0.367	0.509	83
0.736	0.775	0.199	0.249	92
0.74	0.757	0.289	0.225	87
0.826	0.289	0.59	0.212	92
0.86	0.7	0.543	0.456	93
0.8	0.816	0.531	0.567	94
0.81	0.689	0.355	0.442	83
0.455	0.687	0.457	0.734	69
0.492	0.748	0.179	0.183	75
0.734	0.438	0.411	0.356	59
0.903	0.516	0.38	0.402	77
0.947	0.734	0.459	0.321	93
0.418	0.63	0.188	0.412	67
0.455	0.732	0.446	0.466	69
0.898	0.81	0.3	0.214	93
0.59	0.745	0.555	0.462	75
0.637	0.698	0.44	0.529	76
0.316	0.833	0.767	0.642	85
0.702	0.808	0.547	0.532	77
0.726	0.844	0.387	0.364	72
0.251	0.755	0.605	0.65	53
0.205	0.85	0.697	0.638	86
0.222	0.674	0.647	0.704	36
0.735	0.667	0.468	0.374	88
0.7	0.413	0.298	0.346	88
0.741	0.667	0.468	0.348	87
0.741	0.667	0.468	0.365	89
0.647	0.499	0.31	0.326	85

0.852	0.623	0.36	0.439	86
0.825	0.623	0.36	0.386	86
0.515	0.759	0.682	0.349	84
0.519	0.641	0.443	0.302	90
0.251	0.842	0.776	0.773	40
0.024	0.629	0.617	0.647	9
0.08	0.433	0.63	0.469	34
0.01	0.199	0.336	0.525	10
0.029	0.292	0.589	0.507	23
0.024	0.349	0.497	0.585	26
0.012	0.669	0.701	0.721	11
0.049	0.767	0.793	0.707	32
0.029	0.567	0.543	0.606	15
0.02	0.732	0.794	0.745	33
0.07	0.589	0.83	0.694	20
0.036	0.641	0.747	0.637	23
0.099	0.798	0.847	0.78	46
0.026	0.528	0.494	0.637	19
0.515	0.243	0.417	0.463	60
0.242	0.571	0.191	0.207	77
0.094	0.769	0.823	0.683	62
0.023	0.708	0.744	0.641	50
0.013	0.745	0.803	0.717	26
0.922	0.82	0.206	0.141	97
0.013	0.735	0.804	0.807	12
0.026	0.899	0.784	0.842	69
0.169	0.904	0.686	0.777	70
0.013	0.846	0.815	0.846	26
0.127	0.874	0.78	0.877	67
0.083	0.94	0.782	0.77	71
0.075	0.793	0.45	0.433	42
0.229	0.683	0.333	0.521	46
0.085	0.795	0.218	0.258	54
0.085	0.795	0.218	0.175	70
0.189	0.741	0.723	0.661	66
0.032	0.769	0.723	0.731	64
0.024	0.831	0.635	0.671	70
0.047	0.744	0.516	0.595	89
0.03	0.938	0.726	0.786	38
0.027	0.954	0.767	0.867	24
0.066	0.8	0.716	0.692	40

0.192	0.663	0.352	0.395	38
0.122	0.877	0.834	0.819	67
0.177	0.912	0.787	0.845	65
0.087	0.656	0.383	0.574	15
0.122	0.816	0.326	0.505	59
0.283	0.918	0.764	0.78	68
0.949	0.791	0.348	0.315	93
0.685	0.66	0.437	0.357	93
0.22	0.773	0.602	0.429	60
0.061	0.83	0.725	0.763	54
0.043	0.908	0.719	0.731	41
0.038	0.79	0.794	0.768	10
0.397	0.942	0.774	0.624	66
0.016	0.885	0.773	0.821	9
0.018	0.759	0.844	0.804	39
0.164	0.757	0.704	0.764	59
0.021	0.68	0.647	0.734	29
0.284	0.609	0.497	0.514	44
0.367	0.554	0.572	0.587	69
0.359	0.824	0.785	0.459	63
0.593	0.788	0.455	0.415	90
0.015	0.831	0.635	0.662	63
0.231	0.771	0.727	0.708	67
0.625	0.939	0.771	0.737	65
0.315	0.903	0.745	0.81	71
0.637	0.783	0.354	0.36	92
0.379	0.929	0.808	0.764	66
0.456	0.945	0.806	0.829	66
0.198	0.754	0.592	0.539	64
0.256	0.796	0.703	0.881	47
0.06	0.79	0.696	0.78	59
0.258	0.554	0.572	0.534	76
0.04	0.818	0.603	0.711	49
0.166	0.614	0.633	0.59	74
0.246	0.619	0.633	0.501	77
0.778	0.625	0.265	0.373	92
0.774	0.528	0.387	0.385	88
0.253	0.862	0.763	0.699	68
0.57	0.778	0.721	0.761	49
0.117	0.689	0.661	0.607	76
0.472	0.778	0.598	0.531	59

0.192	0.754	0.592	0.443	66
0.022	0.954	0.754	0.877	17
0.066	0.778	0.671	0.622	47
0.136	0.793	0.847	0.786	60
0.045	0.88	0.799	0.758	34
0.974	0.669	0.229	0.257	90
0.958	0.662	0.245	0.326	91
0.925	0.586	0.276	0.37	91
0.853	0.585	0.397	0.339	88
0.214	0.96	0.766	0.817	50
0.797	0.538	0.408	0.387	89
0.538	0.668	0.459	0.359	89
0.167	0.898	0.696	0.794	69
0.425	0.789	0.522	0.634	54
0.566	0.512	0.393	0.303	88
0.566	0.512	0.393	0.303	88
0.72	0.659	0.376	0.292	91
0.766	0.667	0.441	0.344	89
0.694	0.545	0.582	0.344	93
0.628	0.511	0.536	0.369	92
0.61	0.639	0.36	0.314	92
0.831	0.822	0.214	0.378	93
0.79	0.736	0.385	0.307	93
0.66	0.75	0.404	0.345	90
0.389	0.818	0.553	0.64	72
0.905	0.676	0.459	0.408	93
0.537	0.636	0.36	0.315	93
0.547	0.564	0.436	0.399	90
0.659	0.74	0.405	0.381	90
0.848	0.773	0.358	0.235	94
0.898	0.802	0.365	0.247	95
0.693	0.781	0.375	0.326	94
0.717	0.734	0.595	0.58	76
0.838	0.78	0.47	0.297	92
0.745	0.761	0.348	0.279	94
0.7	0.655	0.382	0.341	94
0.7	0.583	0.399	0.267	93
0.839	0.636	0.442	0.431	89
0.854	0.801	0.327	0.319	95
0.841	0.481	0.3	0.24	91
0.915	0.481	0.3	0.217	91

0.664	0.706	0.44	0.344	88
0.039	0.812	0.742	0.759	14
0.015	0.797	0.884	0.723	9
0.012	0.824	0.733	0.604	12
0.022	0.789	0.731	0.598	30
0.774	0.528	0.387	0.385	88
0.925	0.586	0.276	0.37	91
0.072	0.784	0.711	0.639	28
0.132	0.946	0.81	0.869	51
0.486	0.796	0.707	0.652	75
0.635	0.885	0.513	0.455	86
0.412	0.792	0.681	0.507	76
0.358	0.874	0.767	0.567	76
0.986	0.669	0.229	0.24	88
0.088	0.76	0.453	0.455	67
0.193	0.861	0.737	0.628	74
0.457	0.834	0.686	0.468	79
0.484	0.844	0.701	0.624	75
0.557	0.872	0.736	0.598	75
0.183	0.901	0.471	0.609	78
0.425	0.792	0.681	0.566	76
0.458	0.799	0.709	0.604	74
0.198	0.792	0.707	0.646	74
0.203	0.863	0.65	0.48	84
0.307	0.805	0.568	0.396	88
0.236	0.841	0.713	0.541	75
0.205	0.93	0.803	0.734	59
0.142	0.864	0.764	0.606	75
0.154	0.83	0.727	0.66	68
0.171	0.877	0.711	0.54	76
0.984	0.674	0.231	0.229	89
0.089	0.855	0.767	0.7	76
0.232	0.872	0.509	0.605	69
0.131	0.851	0.704	0.626	68
0.457	0.834	0.686	0.468	79
0.484	0.844	0.701	0.624	75
0.774	0.489	0.463	0.437	93
0.764	0.517	0.41	0.41	89
0.724	0.505	0.509	0.446	92
0.904	0.529	0.412	0.442	91
0.44	0.846	0.738	0.65	67

0.637	0.789	0.438	0.384	95
0.443	0.711	0.536	0.357	78
0.329	0.574	0.439	0.493	91
0.128	0.587	0.507	0.552	82
0.328	0.531	0.542	0.465	90
0.129	0.617	0.581	0.535	90
0.169	0.618	0.557	0.617	88
0.269	0.512	0.501	0.439	84
0.337	0.512	0.501	0.526	89
0.397	0.868	0.734	0.613	76
0.486	0.796	0.707	0.652	75
0.126	0.927	0.782	0.847	42
0.047	0.916	0.79	0.888	45
0.114	0.911	0.751	0.837	75
0.198	0.879	0.429	0.453	85
0.238	0.829	0.709	0.386	41
0.074	0.858	0.658	0.681	43
0.457	0.799	0.705	0.643	37
0.234	0.898	0.782	0.774	50
0.088	0.76	0.453	0.455	67
0.254	0.776	0.573	0.631	79
0.251	0.766	0.675	0.576	76
0.218	0.858	0.731	0.641	74
0.33	0.849	0.713	0.53	73
0.205	0.897	0.476	0.596	79
0.08	0.849	0.414	0.577	63
0.985	0.687	0.268	0.258	88
0.206	0.905	0.794	0.736	28
0.645	0.858	0.765	0.587	82
0.22	0.855	0.761	0.641	74
0.214	0.825	0.673	0.675	69
0.158	0.881	0.701	0.552	75
0.961	0.409	0.296	0.309	79
0.038	0.689	0.705	0.666	15
0.526	0.683	0.412	0.424	92
0.274	0.647	0.463	0.433	87
0.523	0.766	0.454	0.453	93
0.699	0.612	0.406	0.451	85
0.099	0.877	0.343	0.579	63
0.977	0.692	0.201	0.23	88
0.033	0.775	0.72	0.781	57

0.349	0.724	0.588	0.548	34
0.969	0.551	0.325	0.281	84
0.356	0.868	0.734	0.705	76
0.174	0.847	0.7	0.714	69
0.848	0.71	0.449	0.34	93
0.923	0.797	0.438	0.383	93
0.76	0.829	0.258	0.386	94
0.693	0.58	0.352	0.413	92
0.628	0.827	0.32	0.472	92
0.568	0.574	0.39	0.491	92
0.875	0.832	0.515	0.387	90
0.936	0.802	0.586	0.363	91
0.702	0.792	0.363	0.349	95
0.658	0.567	0.436	0.361	93
0.551	0.788	0.409	0.463	90
0.858	0.703	0.467	0.292	88
0.771	0.555	0.439	0.288	88
0.941	0.776	0.489	0.296	93
0.433	0.697	0.549	0.457	86
0.756	0.698	0.515	0.4	88
0.659	0.548	0.481	0.367	88
0.402	0.654	0.426	0.368	89
0.601	0.57	0.412	0.349	89
0.675	0.772	0.416	0.36	94
0.812	0.485	0.532	0.424	92
0.757	0.82	0.43	0.402	92
0.665	0.706	0.44	0.377	89
0.797	0.538	0.408	0.387	89
0.6	0.529	0.405	0.342	87
0.879	0.78	0.449	0.403	92
0.749	0.795	0.665	0.34	91
0.492	0.706	0.44	0.452	88
0.454	0.529	0.405	0.419	87
0.569	0.791	0.48	0.423	92
0.545	0.541	0.532	0.423	88
0.665	0.706	0.44	0.377	89
0.6	0.529	0.405	0.342	87
0.723	0.691	0.467	0.349	88
0.561	0.642	0.544	0.408	87
0.965	0.776	0.447	0.391	93
0.765	0.807	0.327	0.326	93

0.5	0.77	0.444	0.401	90
0.759	0.792	0.408	0.356	93
0.714	0.564	0.436	0.346	92
0.212	0.759	0.444	0.406	81
0.62	0.829	0.385	0.425	90
0.485	0.574	0.439	0.488	91
0.58	0.828	0.534	0.564	72
0.311	0.782	0.443	0.507	80
0.248	0.587	0.507	0.443	83
0.829	0.806	0.513	0.51	90
0.603	0.598	0.443	0.3	92
0.523	0.516	0.471	0.387	71
0.432	0.386	0.432	0.472	88
0.75	0.408	0.437	0.375	88
0.847	0.479	0.489	0.393	88
0.816	0.532	0.509	0.391	89
0.098	0.796	0.523	0.491	70
0.561	0.636	0.36	0.318	93
0.644	0.726	0.412	0.403	94
0.626	0.78	0.417	0.397	92
0.934	0.515	0.435	0.411	92
0.812	0.485	0.532	0.424	92
0.878	0.515	0.435	0.413	92
0.444	0.6	0.505	0.603	62
0.639	0.569	0.438	0.334	86
0.023	0.805	0.594	0.628	80
0.167	0.853	0.72	0.619	70
0.973	0.59	0.342	0.311	86
0.411	0.783	0.474	0.478	78
0.085	0.795	0.218	0.175	74
0.856	0.709	0.538	0.527	96
0.45	0.606	0.538	0.504	92
0.586	0.498	0.635	0.495	89
0.154	0.839	0.395	0.653	59
0.411	0.727	0.645	0.457	79
0.646	0.832	0.685	0.564	79
0.101	0.761	0.718	0.554	71
0.261	0.853	0.688	0.588	67
0.385	0.7	0.498	0.333	73
0.467	0.7	0.498	0.485	69
0.814	0.657	0.431	0.329	90

0.85	0.667	0.441	0.323	89
0.923	0.797	0.438	0.383	93
0.811	0.835	0.359	0.401	93
0.086	0.921	0.793	0.884	57
0.16	0.929	0.808	0.828	60
0.713	0.586	0.396	0.455	91
0.506	0.6	0.448	0.358	89
0.539	0.768	0.562	0.416	70
0.621	0.764	0.584	0.512	93
0.867	0.771	0.464	0.493	91
0.713	0.821	0.385	0.419	91
0.19	0.847	0.723	0.627	69
0.596	0.838	0.3	0.457	94
0.735	0.838	0.3	0.343	96
0.845	0.82	0.206	0.288	97
0.889	0.577	0.345	0.251	94
0.867	0.818	0.275	0.274	94
0.887	0.557	0.417	0.332	91
0.918	0.794	0.337	0.316	94
0.921	0.818	0.275	0.191	96
0.631	0.811	0.363	0.373	82
0.889	0.577	0.345	0.251	94
0.807	0.651	0.327	0.252	94
0.886	0.571	0.385	0.255	93
0.432	0.861	0.7	0.602	77
0.444	0.448	0.526	0.42	91
0.24	0.633	0.529	0.522	87
0.506	0.534	0.439	0.393	90
0.903	0.568	0.493	0.363	91
0.802	0.532	0.452	0.388	89
0.698	0.576	0.545	0.411	85
0.807	0.585	0.496	0.307	88
0.04	0.715	0.625	0.577	35
0.592	0.653	0.502	0.414	83
0.507	0.669	0.57	0.482	65
0.451	0.787	0.711	0.542	65
0.018	0.671	0.676	0.797	21
0.024	0.736	0.703	0.704	31
0.076	0.762	0.588	0.46	69
0.773	0.832	0.668	0.696	84
0.021	0.899	0.784	0.9	69

0.904	0.662	0.388	0.421	86
0.978	0.686	0.246	0.207	88
0.369	0.83	0.721	0.586	57
0.14	0.756	0.628	0.397	9
0.014	0.239	0.723	0.777	12
0.016	0.777	0.666	0.725	16
0.018	0.734	0.776	0.707	10
0.979	0.631	0.315	0.295	85
0.202	0.769	0.648	0.538	63
0.611	0.773	0.717	0.522	73
0.139	0.841	0.643	0.715	65
0.08	0.849	0.414	0.577	63
0.636	0.719	0.472	0.341	91
0.653	0.716	0.479	0.396	91
0.738	0.698	0.459	0.315	90
0.039	0.803	0.7	0.6	11
0.16	0.808	0.646	0.836	28
0.215	0.841	0.562	0.425	87
0.506	0.832	0.685	0.576	80
0.363	0.904	0.462	0.501	78
0.286	0.792	0.681	0.517	76
0.314	0.764	0.536	0.731	33
0.436	0.858	0.705	0.609	76
0.112	0.853	0.691	0.7	76
0.345	0.619	0.494	0.466	89
0.441	0.824	0.356	0.513	77
0.893	0.508	0.51	0.35	88
0.06	0.772	0.672	0.748	44
0.608	0.691	0.443	0.468	88
0.539	0.768	0.562	0.476	59
0.076	0.762	0.588	0.46	71
0.843	0.83	0.342	0.288	95
0.527	0.774	0.592	0.547	56
0.308	0.744	0.549	0.425	47
0.247	0.741	0.443	0.257	56
0.073	0.789	0.525	0.636	84
0.097	0.724	0.559	0.609	51
0.515	0.662	0.453	0.422	89
0.217	0.79	0.62	0.499	59
0.065	0.774	0.555	0.63	48
0.419	0.78	0.454	0.354	66

0.399	0.714	0.472	0.369	75
0.021	0.769	0.723	0.753	54
0.057	0.796	0.737	0.711	43
0.124	0.924	0.798	0.784	60
0.674	0.608	0.393	0.291	92
0.018	0.767	0.763	0.728	17
0.047	0.899	0.784	0.852	70
0.152	0.779	0.662	0.605	72
0.144	0.871	0.759	0.587	74
0.061	0.788	0.728	0.653	58
0.053	0.938	0.662	0.651	50
0.28	0.47	0.575	0.492	91
0.309	0.81	0.605	0.583	48
0.218	0.844	0.676	0.607	75
0.311	0.79	0.579	0.445	71
0.544	0.709	0.603	0.427	75
0.316	0.794	0.453	0.312	86
0.211	0.857	0.735	0.57	75
0.366	0.438	0.557	0.462	92
0.696	0.682	0.438	0.512	89
0.749	0.655	0.436	0.491	90
0.813	0.681	0.443	0.438	89
0.85	0.689	0.519	0.367	89
0.281	0.905	0.781	0.823	70
0.069	0.799	0.733	0.681	33
0.141	0.661	0.59	0.524	46
0.063	0.753	0.707	0.588	10
0.565	0.702	0.732	0.683	50
0.252	0.8	0.808	0.668	42
0.304	0.862	0.791	0.721	37
0.044	0.619	0.718	0.691	11
0.036	0.769	0.726	0.592	66
0.32	0.745	0.517	0.37	53
0.011	0.699	0.848	0.795	16
0.349	0.775	0.695	0.754	70
0.175	0.813	0.832	0.671	47
0.296	0.744	0.609	0.44	41
0.022	0.701	0.671	0.724	42
0.936	0.654	0.364	0.246	88
0.289	0.751	0.711	0.583	67
0.1	0.78	0.543	0.537	80

0.297	0.749	0.715	0.519	70
0.209	0.77	0.452	0.469	74
0.586	0.797	0.512	0.421	85
0.063	0.788	0.707	0.834	39
0.539	0.768	0.562	0.416	60
0.076	0.762	0.588	0.46	64
0.854	0.698	0.515	0.339	88
0.759	0.792	0.408	0.356	93
0.5	0.77	0.444	0.401	90
0.443	0.646	0.584	0.529	86
0.617	0.577	0.561	0.425	91
0.539	0.768	0.562	0.443	63
0.338	0.876	0.767	0.781	72
0.16	0.786	0.7	0.895	43
0.06	0.772	0.672	0.748	44
0.275	0.794	0.453	0.264	85
0.879	0.78	0.449	0.403	92
0.322	0.922	0.8	0.779	62
0.943	0.754	0.466	0.285	89
0.987	0.762	0.401	0.373	91
0.935	0.754	0.466	0.315	91
0.985	0.762	0.401	0.413	92
0.511	0.263	0.494	0.334	76
0.083	0.916	0.795	0.875	66
0.316	0.839	0.765	0.616	49
0.045	0.936	0.918	0.883	48
0.119	0.905	0.781	0.829	70
0.076	0.762	0.588	0.46	71
0.027	0.899	0.784	0.869	67
0.461	0.783	0.686	0.594	49
0.348	0.855	0.687	0.633	70
0.907	0.801	0.323	0.319	94
0.945	0.563	0.416	0.336	92
0.206	0.94	0.782	0.766	65
0.018	0.846	0.621	0.686	45
0.202	0.823	0.617	0.616	43
0.018	0.754	0.693	0.677	36
0.306	0.736	0.595	0.631	41
0.21	0.945	0.806	0.76	58
0.102	0.81	0.718	0.746	30
0.151	0.805	0.594	0.626	90

0.066	0.651	0.58	0.599	37
0.019	0.619	0.798	0.785	26
0.01	0.601	0.439	0.591	20
0.034	0.78	0.543	0.615	80
0.043	0.943	0.799	0.915	56
0.314	0.438	0.557	0.493	95
0.738	0.694	0.443	0.389	92
0.646	0.557	0.419	0.315	89
0.361	0.757	0.42	0.5	94
0.576	0.447	0.44	0.465	92
0.561	0.762	0.432	0.534	89
0.913	0.758	0.584	0.603	89
0.665	0.462	0.561	0.506	92
0.589	0.669	0.431	0.476	92
0.657	0.58	0.405	0.384	93
0.307	0.805	0.568	0.438	88
0.121	0.846	0.692	0.638	69
0.062	0.787	0.689	0.698	43
0.495	0.871	0.741	0.597	75
0.719	0.706	0.44	0.351	88
0.295	0.805	0.568	0.473	89
0.169	0.913	0.763	0.836	47
0.013	0.763	0.636	0.62	38
0.185	0.833	0.699	0.677	75
0.097	0.877	0.766	0.832	60
0.838	0.78	0.47	0.297	92
0.442	0.818	0.731	0.699	62
0.088	0.805	0.594	0.674	80
0.076	0.946	0.804	0.919	50
0.375	0.727	0.645	0.526	79
0.104	0.492	0.528	0.492	90
0.174	0.607	0.542	0.467	89
0.646	0.832	0.685	0.564	79
0.101	0.761	0.718	0.554	71
0.076	0.762	0.588	0.46	71
0.038	0.551	0.511	0.568	46
0.076	0.762	0.588	0.46	68
0.544	0.877	0.709	0.539	76
0.272	0.819	0.685	0.704	64
0.476	0.263	0.494	0.287	77
0.419	0.472	0.441	0.462	88

	Metabolites after MDS using CDK (165) (used for MDS using ADMET)			
Pgp-In	HIA	F20%	F30%	PPB
0.122	0.877	0.834	0.819	67
0.949	0.791	0.348	0.315	93
0.685	0.66	0.437	0.357	93
0.593	0.788	0.455	0.415	90
0.637	0.783	0.354	0.36	92
0.456	0.945	0.806	0.829	66
0.166	0.614	0.633	0.59	74
0.778	0.625	0.265	0.373	92
0.774	0.528	0.387	0.385	88
0.117	0.689	0.661	0.607	76
0.925	0.586	0.276	0.37	91
0.538	0.668	0.459	0.359	89
0.72	0.659	0.376	0.292	91
0.61	0.639	0.36	0.314	92
0.831	0.822	0.214	0.378	93
0.79	0.736	0.385	0.307	93
0.66	0.75	0.404	0.345	90
0.389	0.818	0.553	0.64	72
0.905	0.676	0.459	0.408	93
0.848	0.773	0.358	0.235	94
0.898	0.802	0.365	0.247	95
0.693	0.781	0.375	0.326	94
0.838	0.78	0.47	0.297	92
0.745	0.761	0.348	0.279	94
0.7	0.655	0.382	0.341	94
0.7	0.583	0.399	0.267	93
0.839	0.636	0.442	0.431	89
0.854	0.801	0.327	0.319	95
0.664	0.706	0.44	0.344	88
0.774	0.528	0.387	0.385	88
0.088	0.76	0.453	0.455	67
0.203	0.863	0.65	0.48	84
0.307	0.805	0.568	0.396	88
0.205	0.93	0.803	0.734	59
0.904	0.529	0.412	0.442	91

0.44	0.846	0.738	0.65	67
0.637	0.789	0.438	0.384	95
0.129	0.617	0.581	0.535	90
0.169	0.618	0.557	0.617	88
0.088	0.76	0.453	0.455	67
0.526	0.683	0.412	0.424	92
0.523	0.766	0.454	0.453	93
0.699	0.612	0.406	0.451	85
0.848	0.71	0.449	0.34	93
0.923	0.797	0.438	0.383	93
0.76	0.829	0.258	0.386	94
0.693	0.58	0.352	0.413	92
0.628	0.827	0.32	0.472	92
0.568	0.574	0.39	0.491	92
0.875	0.832	0.515	0.387	90
0.936	0.802	0.586	0.363	91
0.702	0.792	0.363	0.349	95
0.658	0.567	0.436	0.361	93
0.551	0.788	0.409	0.463	90
0.858	0.703	0.467	0.292	88
0.941	0.776	0.489	0.296	93
0.433	0.697	0.549	0.457	86
0.756	0.698	0.515	0.4	88
0.601	0.57	0.412	0.349	89
0.675	0.772	0.416	0.36	94
0.757	0.82	0.43	0.402	92
0.879	0.78	0.449	0.403	92
0.749	0.795	0.665	0.34	91
0.492	0.706	0.44	0.452	88
0.569	0.791	0.48	0.423	92
0.665	0.706	0.44	0.377	89
0.723	0.691	0.467	0.349	88
0.561	0.642	0.544	0.408	87
0.965	0.776	0.447	0.391	93
0.765	0.807	0.327	0.326	93
0.5	0.77	0.444	0.401	90
0.759	0.792	0.408	0.356	93
0.212	0.759	0.444	0.406	81
0.62	0.829	0.385	0.425	90
0.58	0.828	0.534	0.564	72
0.311	0.782	0.443	0.507	80

0.248	0.587	0.507	0.443	83
0.829	0.806	0.513	0.51	90
0.098	0.796	0.523	0.491	70
0.644	0.726	0.412	0.403	94
0.626	0.78	0.417	0.397	92
0.444	0.6	0.505	0.603	62
0.411	0.783	0.474	0.478	78
0.856	0.709	0.538	0.527	96
0.154	0.839	0.395	0.653	59
0.385	0.7	0.498	0.333	73
0.467	0.7	0.498	0.485	69
0.814	0.657	0.431	0.329	90
0.85	0.667	0.441	0.323	89
0.923	0.797	0.438	0.383	93
0.811	0.835	0.359	0.401	93
0.16	0.929	0.808	0.828	60
0.506	0.6	0.448	0.358	89
0.621	0.764	0.584	0.512	93
0.867	0.771	0.464	0.493	91
0.713	0.821	0.385	0.419	91
0.596	0.838	0.3	0.457	94
0.735	0.838	0.3	0.343	96
0.845	0.82	0.206	0.288	97
0.889	0.577	0.345	0.251	94
0.867	0.818	0.275	0.274	94
0.887	0.557	0.417	0.332	91
0.918	0.794	0.337	0.316	94
0.921	0.818	0.275	0.191	96
0.631	0.811	0.363	0.373	82
0.889	0.577	0.345	0.251	94
0.807	0.651	0.327	0.252	94
0.886	0.571	0.385	0.255	93
0.24	0.633	0.529	0.522	87
0.592	0.653	0.502	0.414	83
0.507	0.669	0.57	0.482	65
0.451	0.787	0.711	0.542	65
0.904	0.662	0.388	0.421	86
0.369	0.83	0.721	0.586	57
0.202	0.769	0.648	0.538	63
0.611	0.773	0.717	0.522	73
0.139	0.841	0.643	0.715	65

0.636	0.719	0.472	0.341	91
0.653	0.716	0.479	0.396	91
0.738	0.698	0.459	0.315	90
0.345	0.619	0.494	0.466	89
0.608	0.691	0.443	0.468	88
0.843	0.83	0.342	0.288	95
0.247	0.741	0.443	0.257	56
0.097	0.724	0.559	0.609	51
0.515	0.662	0.453	0.422	89
0.124	0.924	0.798	0.784	60
0.674	0.608	0.393	0.291	92
0.152	0.779	0.662	0.605	72
0.309	0.81	0.605	0.583	48
0.544	0.709	0.603	0.427	75
0.316	0.794	0.453	0.312	86
0.696	0.682	0.438	0.512	89
0.749	0.655	0.436	0.491	90
0.813	0.681	0.443	0.438	89
0.85	0.689	0.519	0.367	89
0.349	0.775	0.695	0.754	70
0.1	0.78	0.543	0.537	80
0.854	0.698	0.515	0.339	88
0.759	0.792	0.408	0.356	93
0.5	0.77	0.444	0.401	90
0.443	0.646	0.584	0.529	86
0.617	0.577	0.561	0.425	91
0.275	0.794	0.453	0.264	85
0.879	0.78	0.449	0.403	92
0.943	0.754	0.466	0.285	89
0.935	0.754	0.466	0.315	91
0.316	0.839	0.765	0.616	49
0.348	0.855	0.687	0.633	70
0.907	0.801	0.323	0.319	94
0.945	0.563	0.416	0.336	92
0.151	0.805	0.594	0.626	90
0.738	0.694	0.443	0.389	92
0.646	0.557	0.419	0.315	89
0.361	0.757	0.42	0.5	94
0.576	0.447	0.44	0.465	92
0.561	0.762	0.432	0.534	89
0.665	0.462	0.561	0.506	92

0.589	0.669	0.431	0.476	92
0.295	0.805	0.568	0.473	89
0.838	0.78	0.47	0.297	92
0.442	0.818	0.731	0.699	62
0.088	0.805	0.594	0.674	80
0.174	0.607	0.542	0.467	89
0.272	0.819	0.685	0.704	64
	468 Metabolites and positive & negative controls			
VD	BBB	A2-In	A2-Subs	A4-In
0.963	0.962	0.072	0.384	0.34
1.001	0.984	0.031	0.483	0.108
0.952	0.962	0.095	0.297	0.38
0.85	0.981	0.078	0.33	0.063
1.004	0.978	0.014	0.505	0.016
0.521	0.811	0.068	0.466	0.253
0.838	0.972	0.097	0.42	0.137
0.617	0.962	0.036	0.146	0.133
0.195	0.899	0.672	0.558	0.619
0.417	0.97	0.145	0.475	0.164
1.198	0.994	0.037	0.429	0.051
0.372	0.89	0.039	0.443	0.089
1.089	0.995	0.054	0.322	0.037
0.784	0.984	0.049	0.476	0.246
0.725	0.882	0.285	0.527	0.33
1.362	0.961	0.647	0.592	0.122
0.242	0.771	0.028	0.362	0.121
-0.34	0.962	0.039	0.718	0
1.276	0.965	0.778	0.65	0.186
0.485	0.828	0.427	0.552	0.709
1.112	0.969	0.064	0.332	0.342
0.32	0.962	0.048	0.398	0.055
0.663	0.992	0.055	0.442	0.042
1.11	0.995	0.043	0.432	0.037
0.932	0.99	0.037	0.198	0.022
1.308	0.962	0.056	0.569	0.014
-0.096	0.976	0.047	0.541	0.022
0.784	0.984	0.049	0.476	0.246
0.757	0.994	0.104	0.369	0.014

0.917	0.984	0.035	0.316	0.044
0.349	0.862	0.049	0.372	0.127
0.872	0.994	0.035	0.444	0.027
0.719	0.987	0.03	0.318	0.02
0.497	0.955	0.134	0.682	0.203
1.643	0.962	0.193	0.608	0.034
0.463	0.995	0.436	0.643	0.209
1.004	0.978	0.014	0.505	0.016
0.992	0.985	0.021	0.407	0.009
1.096	0.962	0.107	0.546	0.066
0.917	0.884	0.04	0.605	0.081
0.709	0.97	0.128	0.51	0.093
1.281	0.98	0.087	0.4	0.17
1.03	0.97	0.073	0.404	0.304
0.84	0.941	0.041	0.328	0.085
0.822	0.985	0.264	0.373	0.077
1.22	0.962	0.027	0.44	0.264
1.03	0.99	0.023	0.415	0.04
0.877	0.978	0.076	0.484	0.003
1.087	1	0.034	0.716	0.069
0.81	0.955	0.052	0.404	0.028
0.195	0.985	0.028	0.288	0.046
0.956	0.976	0.072	0.408	0.32
1.074	0.989	0.062	0.438	0.074
1.231	1	0.092	0.531	0.085
0.879	0.973	0.103	0.5	0.135
1.18	0.967	0.089	0.355	0.118
1.042	0.985	0.093	0.429	0.012
0.585	0.98	0.526	0.607	0.585
1.276	0.974	0.038	0.56	0.323
1.33	0.98	0.339	0.698	0.458
0.418	0.957	0.811	0.601	0.766
0.315	0.991	0.601	0.68	0.07
0.296	0.772	0.065	0.44	0.039
0.088	0.97	0.307	0.326	0.158
-0.282	0.965	0.705	0.297	0.139
-0.06	0.97	0.51	0.332	0.209
0.017	0.97	0.51	0.332	0.209
0.017	0.962	0.636	0.356	0.129
-0.265	0.842	0.485	0.422	0.811
-0.256	0.842	0.681	0.46	0.84

-0.137	0.986	0.968	0.215	0.061
-0.082	0.978	0.832	0.337	0.116
0.817	0.996	0.169	0.85	0.022
-0.624	0.986	0.068	0.304	0
-0.693	0.962	0.013	0.186	0.011
0.025	0.428	0.001	0.444	0
-0.5	0.787	0	0.082	0
-0.722	0.882	0.001	0.024	0.001
-0.548	0.989	0.004	0.128	0.015
-0.673	0.946	0.002	0.102	0.001
-0.738	0.958	0.013	0.294	0.001
-0.667	0.988	0.007	0.034	0.001
-0.578	0.822	0.005	0.092	0.002
-0.594	0.958	0.004	0.024	0.002
-0.643	0.995	0.009	0.077	0.002
-0.741	0.98	0.092	0.348	0.001
-0.664	0.23	0.168	0.38	0.286
-0.134	0.576	0.34	0.401	0.119
-0.575	1	0.028	0.151	0.027
-0.473	0.856	0.008	0.016	0.011
-0.599	0.973	0.002	0.058	0.001
1.494	0.878	0.273	0.37	0.364
-0.034	0.949	0.025	0.514	0.001
0.986	0.997	0.793	0.7	0.007
0.956	1	0.87	0.674	0.005
-0.242	0.974	0.018	0.438	0.001
-0.14	1	0.956	0.726	0.005
0.952	0.997	0.317	0.598	0.002
-0.112	0.941	0.137	0.462	0.002
-0.002	0.925	0.167	0.4	0.012
-0.043	0.941	0.191	0.412	0.004
0.224	0.941	0.191	0.412	0.004
0.415	0.99	0.006	0.47	0.011
0.35	0.978	0.01	0.572	0.001
0.284	0.944	0.138	0.408	0.013
0.884	0.705	0.168	0.38	0.024
0.511	1	0.644	0.546	0.091
0.273	1	0.37	0.636	0.001
-0.235	0.989	0.19	0.41	0
-0.103	0.944	0.167	0.382	0.005
-0.367	0.995	0.729	0.788	0.006

0.745	0.996	0.484	0.682	0.03
-0.31	0.933	0.033	0.464	0.002
0.062	0.863	0.098	0.406	0.01
0.768	1	0.899	0.64	0.047
0.321	0.892	0.279	0.416	0.712
-0.144	0.579	0.185	0.374	0.164
-0.07	0.992	0.768	0.342	0.003
-0.303	0.942	0.473	0.622	0.003
0.432	0.994	0.075	0.636	0.017
0.142	0.955	0.018	0.518	0.006
0.722	0.988	0.989	0.586	0.029
0.05	0.993	0.233	0.599	0.011
0.145	0.984	0.048	0.376	0.005
0.239	0.995	0.036	0.518	0.003
-0.491	0.921	0.103	0.44	0.011
-0.006	0.989	0.782	0.558	0.004
-0.044	0.918	0.408	0.73	0.28
-0.634	0.781	0.796	0.586	0.041
0.746	0.824	0.113	0.402	0.286
0.383	0.895	0.63	0.488	0.027
0.374	0.99	0.045	0.546	0.019
0.751	0.996	0.927	0.58	0.102
1.001	1	0.924	0.668	0.038
0.421	0.695	0.166	0.379	0.467
0.258	0.956	0.757	0.715	0.207
0.07	0.981	0.914	0.56	0.024
0.302	0.978	0.176	0.45	0.011
-0.158	0.995	0.193	0.652	0.003
0.237	0.968	0.03	0.566	0.002
0.042	0.854	0.313	0.552	0.155
-0.157	0.939	0.026	0.5	0.002
0.324	0.871	0.773	0.554	0.028
-0.152	0.923	0.956	0.528	0.284
-0.017	0.694	0.439	0.318	0.5
-0.144	0.578	0.658	0.306	0.302
0.541	0.997	0.022	0.554	0.051
-0.059	0.963	0.888	0.536	0.042
0.506	0.89	0.584	0.504	0.086
-0.365	0.918	0.983	0.732	0.175
0.473	0.989	0.219	0.38	0.034
0.049	0.981	0.653	0.702	0.107

-0.05	0.828	0.523	0.424	0.039
0.801	0.755	0.199	0.498	0.103
-0.391	0.979	0.674	0.672	0.646
-0.152	0.714	0.221	0.414	0.681
-0.042	0.574	0.384	0.487	0.804
-0.241	0.773	0.358	0.408	0.271
-0.175	0.635	0.615	0.34	0.354
0.473	0.986	0.732	0.592	0.019
-0.131	0.29	0.246	0.352	0.216
0.475	0.606	0.782	0.446	0.467
0.94	0.997	0.914	0.538	0.023
-0.537	1	0.05	0.5	0.007
-0.372	0.162	0.086	0.346	0.174
-0.372	0.162	0.086	0.346	0.174
-0.289	0.517	0.089	0.444	0.438
-0.379	0.634	0.224	0.44	0.299
-0.13	0.414	0.336	0.45	0.83
-0.542	0.297	0.82	0.354	0.541
0.501	0.692	0.257	0.384	0.588
1.135	0.81	0.528	0.392	0.515
0.686	0.831	0.228	0.364	0.443
0.622	0.784	0.451	0.464	0.572
0.689	0.99	0.338	0.678	0.201
-0.425	0.587	0.216	0.404	0.345
0.44	0.65	0.206	0.378	0.59
-0.536	0.29	0.376	0.392	0.344
0.704	0.805	0.671	0.442	0.537
0.926	0.842	0.164	0.328	0.357
0.592	0.903	0.132	0.424	0.306
0.824	0.774	0.223	0.398	0.431
0.142	0.903	0.411	0.732	0.253
0.952	0.899	0.234	0.412	0.53
0.85	0.814	0.205	0.354	0.332
0.579	0.71	0.17	0.41	0.564
0.122	0.623	0.161	0.447	0.667
0.762	0.783	0.176	0.446	0.53
0.404	0.75	0.295	0.46	0.542
-0.314	0.519	0.206	0.351	0.48
-0.303	0.433	0.197	0.303	0.395
0.498	0.618	0.567	0.274	0.395
-0.352	0.982	0.115	0.536	0.004

-0.562	0.989	0.032	0.28	0
-0.639	0.96	0.011	0.168	0
-0.263	0.991	0.03	0.368	0
-0.144	0.578	0.658	0.306	0.302
-0.241	0.773	0.358	0.408	0.271
-0.266	0.979	0.119	0.546	0.017
-0.092	0.995	0.634	0.46	0.001
0.584	0.984	0.213	0.5	0.112
0.403	0.858	0.064	0.262	0.06
0.425	0.976	0.28	0.45	0.081
0.489	0.911	0.052	0.544	0.028
-0.264	0.586	0.178	0.385	0.652
0.659	0.878	0.211	0.402	0.063
0.643	0.968	0.048	0.544	0.061
0.465	0.968	0.03	0.326	0.061
0.661	0.968	0.082	0.488	0.057
0.648	0.936	0.097	0.514	0.071
0.46	0.97	0.032	0.39	0.122
0.428	0.98	0.291	0.446	0.017
0.634	0.982	0.275	0.492	0.07
0.453	0.995	0.131	0.604	0.048
0.397	0.973	0.018	0.472	0.039
-0.79	0.891	0.47	0.154	0.006
0.649	0.997	0.052	0.428	0.125
0.022	0.975	0.5	0.54	0.019
0.438	0.96	0.037	0.599	0.008
0.581	0.997	0.043	0.598	0.051
0.42	0.986	0.059	0.506	0.04
-0.236	0.781	0.24	0.393	0.677
0.423	0.995	0.187	0.618	0.01
0.311	0.965	0.105	0.402	0.022
0.548	0.981	0.035	0.57	0.007
0.465	0.968	0.03	0.326	0.061
0.661	0.968	0.082	0.488	0.057
-0.767	0.307	0.162	0.394	0.383
-0.502	0.157	0.209	0.326	0.229
-0.29	0.268	0.308	0.334	0.202
-0.287	0.243	0.254	0.362	0.341
0.438	0.986	0.89	0.668	0.185
0.47	0.932	0.225	0.412	0.34
0.131	0.946	0.124	0.402	0.322

-0.109	0.154	0.046	0.26	0.134
-0.441	0.556	0.055	0.28	0.119
-0.578	0.464	0.987	0.408	0.931
-0.184	0.422	0.644	0.484	0.704
0.042	0.817	0.5	0.59	0.343
-0.217	0.315	0.288	0.311	0.344
-0.202	0.662	0.164	0.365	0.104
0.633	0.989	0.09	0.641	0.084
0.584	0.984	0.213	0.5	0.112
-0.141	0.987	0.842	0.58	0.006
0.189	0.985	0.878	0.608	0.005
0.259	0.989	0.361	0.346	0.004
1.437	0.983	0.345	0.674	0.072
-0.42	0.992	0.542	0.293	0.005
-0.042	0.993	0.16	0.766	0.002
-0.391	0.978	0.768	0.486	0.024
0.345	0.985	0.958	0.542	0.039
0.659	0.878	0.211	0.402	0.063
0.603	0.988	0.093	0.388	0.044
0.432	0.99	0.15	0.524	0.068
0.589	0.975	0.049	0.502	0.086
0.445	0.98	0.048	0.38	0.06
0.376	0.981	0.028	0.402	0.118
0.31	0.972	0.017	0.292	0.006
-0.152	0.847	0.25	0.478	0.71
0.485	0.971	0.381	0.806	0.028
0.398	0.949	0.134	0.47	0.014
0.395	0.976	0.082	0.575	0.006
0.506	0.996	0.034	0.522	0.032
0.365	0.991	0.043	0.484	0.025
-0.703	0.415	0.061	0.304	0.437
0.14	0.588	0.063	0.56	0.037
0.108	0.51	0.168	0.434	0.299
-0.365	0.482	0.06	0.296	0.181
0.658	0.84	0.083	0.39	0.342
0.515	0.784	0.141	0.438	0.336
0.307	0.995	0.004	0.246	0.004
-0.277	0.749	0.196	0.434	0.737
0.114	0.996	0.126	0.526	0.001
-0.503	0.981	0.756	0.43	0.051
-0.523	0.255	0.179	0.344	0.708

0.632	0.987	0.09	0.59	0.057
0.457	0.995	0.013	0.468	0.022
0.062	0.787	0.24	0.48	0.292
0.511	0.923	0.302	0.428	0.46
0.859	0.724	0.233	0.326	0.469
-0.187	0.356	0.119	0.29	0.25
0.888	0.761	0.15	0.36	0.386
-0.108	0.393	0.075	0.29	0.166
1.072	0.983	0.311	0.468	0.281
0.727	0.909	0.283	0.526	0.418
1.014	0.926	0.215	0.356	0.462
-0.473	0.687	0.124	0.32	0.399
0.976	0.937	0.134	0.398	0.373
0.582	0.696	0.312	0.337	0.299
-0.458	0.226	0.149	0.3	0.24
0.927	0.612	0.267	0.396	0.378
0.426	0.689	0.276	0.321	0.127
0.53	0.733	0.19	0.385	0.208
-0.482	0.248	0.09	0.306	0.152
-0.349	0.452	0.096	0.29	0.273
-0.347	0.456	0.089	0.354	0.368
0.674	0.816	0.137	0.356	0.438
-0.207	0.413	0.627	0.436	0.506
0.964	0.494	0.85	0.562	0.788
0.471	0.665	0.494	0.326	0.238
-0.131	0.29	0.246	0.352	0.216
-0.445	0.196	0.214	0.292	0.131
0.678	0.696	0.484	0.392	0.554
0.042	0.916	0.521	0.362	0.14
0.544	0.721	0.303	0.36	0.175
-0.45	0.23	0.122	0.282	0.081
0.753	0.783	0.151	0.382	0.298
0.041	0.772	0.142	0.374	0.207
0.471	0.665	0.494	0.326	0.238
-0.445	0.196	0.214	0.292	0.131
0.748	0.41	0.663	0.492	0.618
0.707	0.46	0.539	0.514	0.548
1.158	0.921	0.747	0.514	0.88
1.26	0.661	0.686	0.45	0.72
1.159	0.75	0.758	0.418	0.581
1.254	0.661	0.689	0.454	0.68

-0.481	0.227	0.384	0.416	0.473
1.083	0.706	0.716	0.444	0.38
0.825	0.569	0.156	0.302	0.317
-0.142	0.21	0.058	0.272	0.074
1.079	0.984	0.18	0.496	0.101
0.914	0.912	0.178	0.326	0.251
-0.478	0.611	0.064	0.308	0.113
0.858	0.929	0.89	0.584	0.81
0.467	0.743	0.162	0.336	0.286
0.241	0.862	0.053	0.39	0.321
-0.613	0.415	0.826	0.3	0.746
-0.613	0.3	0.182	0.302	0.696
-0.431	0.2	0.123	0.386	0.714
-0.292	0.2	0.111	0.404	0.611
0.481	0.943	0.312	0.536	0.098
0.329	0.555	0.184	0.374	0.471
0.834	0.858	0.286	0.486	0.457
1.236	0.703	0.637	0.468	0.676
-0.116	0.399	0.443	0.44	0.652
-0.207	0.413	0.627	0.436	0.506
-0.105	0.454	0.481	0.442	0.596
-0.261	0.985	0.376	0.62	0.054
0.261	0.567	0.219	0.382	0.442
0.549	0.663	0.648	0.466	0.098
0.065	0.987	0.106	0.575	0.025
-0.569	0.116	0.131	0.434	0.824
0.011	0.936	0.055	0.406	0.015
0.142	0.941	0.191	0.412	0.004
0.612	0.966	0.546	0.482	0.208
-0.223	0.205	0.05	0.254	0.132
-0.399	0.478	0.939	0.514	0.869
0.369	0.993	0.023	0.42	0.043
0.447	0.918	0.11	0.246	0.064
0.426	0.975	0.301	0.31	0.029
0.383	0.986	0.109	0.406	0.008
0.607	0.969	0.022	0.476	0.01
-0.051	0.92	0.32	0.175	0.024
-0.205	0.838	0.127	0.26	0.047
-0.079	0.765	0.112	0.434	0.367
-0.429	0.749	0.263	0.438	0.332
0.511	0.923	0.302	0.428	0.46

0.587	0.574	0.154	0.302	0.554
0.605	0.994	0.133	0.77	0.048
0.259	0.951	0.538	0.639	0.044
-0.22	0.213	0.069	0.274	0.212
-0.159	0.476	0.07	0.322	0.053
0.052	0.98	0.831	0.336	0.033
0.978	0.683	0.634	0.436	0.401
0.566	0.645	0.487	0.45	0.543
0.794	0.447	0.802	0.496	0.644
532	0.997	0.078	0.538	0.059
1.171	0.828	0.22	0.47	0.231
1.274	0.81	0.307	0.434	0.323
1.458	0.913	0.281	0.412	0.415
-0.164	0.531	0.161	0.334	0.291
1.301	0.893	0.194	0.406	0.264
-0.21	0.627	0.126	0.386	0.353
1.115	0.91	0.202	0.448	0.43
1.388	0.878	0.257	0.382	0.302
1.058	0.857	0.188	0.348	0.138
-0.164	0.531	0.161	0.334	0.291
-0.195	0.506	0.148	0.286	0.246
-0.17	0.531	0.15	0.332	0.242
0.484	0.958	0.055	0.606	0.038
-0.725	0.162	0.228	0.292	0.109
0.56	0.652	0.565	0.38	0.088
-0.073	0.317	0.319	0.336	0.095
-0.144	0.302	0.137	0.346	0.716
-0.261	0.517	0.214	0.376	0.55
0.131	0.615	0.187	0.346	0.699
0.037	0.594	0.129	0.412	0.467
-0.262	0.978	0.011	0.29	0.002
-0.443	0.995	0.98	0.641	0.022
-0.499	0.994	0.991	0.578	0.006
-0.024	0.993	0.136	0.322	0.035
-0.427	0.973	0.014	0.552	0.002
-0.225	0.99	0.104	0.598	0.004
0.33	0.994	0.593	0.356	0.005
1.239	0.981	0.29	0.887	0.114
0.984	0.997	0.838	0.558	0.005
0.711	0.989	0.968	0.752	0.033
-0.2	0.867	0.179	0.421	0.706

0.492	0.996	0.843	0.61	0.295
-0.445	0.989	0.596	0.313	0.001
0.03	0.715	0.004	0.466	0.004
-0.206	0.992	0.012	0.51	0.001
0.108	0.983	0.008	0.534	0
-0.575	0.543	0.18	0.354	0.692
0.092	0.938	0.75	0.466	0.235
-0.224	0.992	0.828	0.51	0.258
0.262	0.99	0.01	0.482	0.019
0.31	0.972	0.017	0.292	0.006
0.146	0.684	0.057	0.37	0.388
0.193	0.683	0.096	0.326	0.649
0.147	0.55	0.074	0.337	0.277
-0.597	0.956	0.084	0.37	0.002
-0.376	0.995	0.907	0.58	0.003
1.19	0.976	0.637	0.686	0.232
0.456	0.983	0.129	0.394	0.04
0.418	0.969	0.071	0.426	0.063
0.433	0.952	0.13	0.504	0.019
-0.488	0.993	0.085	0.434	0.01
0.463	0.941	0.041	0.536	0.061
0.421	0.988	0.224	0.66	0.019
0.265	0.657	0.206	0.442	0.138
0.565	0.967	0.097	0.432	0.068
-0.265	0.37	0.16	0.483	0.829
-0.144	0.968	0.685	0.673	0.013
0.355	0.625	0.454	0.396	0.202
-0.132	0.98	0.831	0.336	0.033
0.284	0.994	0.593	0.356	0.005
1.081	0.917	0.208	0.388	0.238
-0.154	0.98	0.766	0.348	0.021
-0.472	0.992	0.787	0.333	0.008
-0.35	0.995	0.887	0.274	0.052
0.64	0.726	0.413	0.35	0.252
0.572	0.71	0.05	0.53	0.017
0.103	0.295	0.308	0.312	0.487
0.076	0.844	0.067	0.266	0.026
-0.065	0.962	0.001	0.462	0.001
-0.089	0.984	0.005	0.295	0.008
-0.255	0.936	0.034	0.355	0.069
0.2	0.985	0.02	0.588	0.001

-0.268	0.964	0.17	0.526	0.009
0.121	0.992	0.239	0.518	0.004
0.398	0.737	0.13	0.332	0.45
-0.488	0.94	0.123	0.574	0.007
0.988	0.994	0.716	0.526	0.06
-0.017	0.808	0.826	0.492	0.077
0.388	0.964	0.108	0.48	0.007
-0.006	0.984	0.103	0.46	0.004
0.521	0.994	0.882	0.614	0.305
-0.977	0.264	0.983	0.358	0.743
0.273	0.992	0.026	0.384	0.03
0.389	0.986	0.384	0.542	0.015
0.239	0.934	0.044	0.292	0.06
-0.068	0.952	0.055	0.246	0.021
-0.782	0.956	0.909	0.106	0.007
0.585	0.994	0.053	0.388	0.052
-0.934	0.464	0.968	0.412	0.867
0.313	0.77	0.605	0.452	0.154
-0.088	0.735	0.663	0.494	0.315
0.162	0.621	0.765	0.498	0.274
0.375	0.652	0.402	0.42	0.24
0.884	0.98	0.443	0.69	0.236
-0.262	0.967	0.427	0.408	0.009
-0.548	0.947	0.359	0.336	0.003
-0.522	0.979	0.168	0.382	0
-0.602	0.994	0.972	0.728	0.012
-0.277	0.98	0.912	0.618	0.08
-0.366	0.989	0.875	0.438	0.008
-0.595	0.974	0.108	0.309	0.002
-0.103	0.947	0.095	0.308	0.001
-0.474	0.992	0.846	0.341	0.014
-0.112	0.937	0.032	0.476	0.014
0.205	0.982	0.869	0.596	0.087
-0.736	0.922	0.866	0.612	0.015
-0.5	0.992	0.698	0.375	0.004
-0.294	0.987	0.028	0.564	0.002
-0.181	0.92	0.296	0.394	0.42
-0.015	0.954	0.101	0.25	0.005
0.476	0.74	0.154	0.464	0.06
0.367	0.934	0.095	0.262	0.022
0.233	0.769	0.034	0.256	0.005

0.422	0.928	0.058	0.26	0.194
-0.509	0.993	0.431	0.466	0.006
-0.077	0.98	0.831	0.336	0.033
0.288	0.994	0.593	0.356	0.005
0.573	0.696	0.284	0.348	0.24
1.254	0.661	0.689	0.454	0.68
1.159	0.75	0.758	0.418	0.581
0.248	0.717	0.611	0.292	0.197
0.278	0.514	0.668	0.455	0.55
-0.072	0.98	0.831	0.336	0.033
0.91	0.992	0.559	0.88	0.126
-0.055	1	0.87	0.807	0.014
-0.144	0.968	0.685	0.673	0.013
-0.845	0.908	0.968	0.118	0.006
0.678	0.696	0.484	0.392	0.554
0.065	0.992	0.822	0.732	0.007
0.553	0.58	0.308	0.37	0.411
0.75	0.962	0.334	0.476	0.585
0.652	0.58	0.279	0.386	0.438
0.861	0.962	0.305	0.496	0.616
-1.016	0.391	0.125	0.264	0.068
0.555	1	0.819	0.794	0.016
-0.009	0.975	0.936	0.682	0.01
0.455	0.968	0.248	0.368	0.114
0.887	0.98	0.202	0.59	0.073
0.285	0.994	0.593	0.356	0.005
0.972	0.997	0.889	0.614	0.014
-0.147	0.98	0.652	0.398	0.033
0.047	0.971	0.288	0.466	0.047
0.937	0.807	0.277	0.394	0.301
-0.291	0.377	0.181	0.33	0.418
0.753	0.994	0.716	0.452	0.045
-0.095	0.912	0.225	0.398	0.005
0.114	0.948	0.492	0.56	0.005
0.264	0.991	0.022	0.57	0.001
-0.249	0.979	0.971	0.54	0.473
0.018	0.976	0.896	0.462	0.003
-0.252	0.969	0.2	0.53	0.004
1.07	0.962	0.159	0.874	0.047
-0.589	0.994	0.203	0.431	0
0.179	0.937	0.058	0.46	0.003

-0.363	0.733	0.001	0.448	0
0.498	0.742	0.145	0.43	0.052
0.541	0.995	0.514	0.55	0.009
-1.56	0.264	0.968	0.364	0.846
0.695	0.739	0.232	0.346	0.376
-0.314	0.278	0.113	0.342	0.245
0.941	0.767	0.72	0.478	0.305
-0.438	0.356	0.568	0.344	0.365
0.992	0.778	0.338	0.44	0.276
0.952	0.986	0.573	0.574	0.26
-0.73	0.642	0.133	0.368	0.162
0.681	0.813	0.655	0.496	0.5
-0.237	0.279	0.042	0.28	0.238
-0.827	0.891	0.47	0.154	0.006
0.495	0.983	0.029	0.518	0.015
-0.333	0.878	0.86	0.47	0.023
0.632	0.96	0.016	0.432	0.024
0.118	0.665	0.468	0.332	0.338
-0.751	0.891	0.294	0.15	0.004
0.191	0.992	0.663	0.594	0.01
-0.134	0.986	0.004	0.402	0.002
0.442	0.993	0.732	0.588	0.005
0.815	0.993	0.078	0.558	0.006
0.952	0.899	0.234	0.412	0.53
1.065	0.985	0.034	0.733	0.069
0.522	0.568	0.55	0.556	0.118
0.369	0.997	0.486	0.68	0.01
0.457	0.978	0.128	0.382	0.027
-0.525	0.713	0.447	0.5	0.5
0.288	0.289	0.423	0.3	0.303
0.426	0.975	0.301	0.31	0.029
0.383	0.986	0.109	0.406	0.008
0.296	0.994	0.593	0.356	0.005
0.265	0.064	0.034	0.426	0.106
0.377	0.994	0.593	0.356	0.005
0.429	0.983	0.119	0.546	0.034
0.164	0.996	0.035	0.508	0.035
-0.982	0.236	0.189	0.264	0.069
-0.13	0.505	0.583	0.284	0.676

	Metabolites after MDS using CDK (165) (used for MDS using ADMET)			
VD	BBB	A2-In	A2-Subs	A4-In
-0.367	0.995	0.729	0.788	0.006
0.321	0.892	0.279	0.416	0.712
-0.144	0.579	0.185	0.374	0.164
0.746	0.824	0.113	0.402	0.286
0.421	0.695	0.166	0.379	0.467
0.07	0.981	0.914	0.56	0.024
0.324	0.871	0.773	0.554	0.028
-0.017	0.694	0.439	0.318	0.5
-0.144	0.578	0.658	0.306	0.302
0.506	0.89	0.584	0.504	0.086
-0.241	0.773	0.358	0.408	0.271
0.475	0.606	0.782	0.446	0.467
-0.289	0.517	0.089	0.444	0.438
0.501	0.692	0.257	0.384	0.588
1.135	0.81	0.528	0.392	0.515
0.686	0.831	0.228	0.364	0.443
0.622	0.784	0.451	0.464	0.572
0.689	0.99	0.338	0.678	0.201
-0.425	0.587	0.216	0.404	0.345
0.926	0.842	0.164	0.328	0.357
0.592	0.903	0.132	0.424	0.306
0.824	0.774	0.223	0.398	0.431
0.952	0.899	0.234	0.412	0.53
0.85	0.814	0.205	0.354	0.332
0.579	0.71	0.17	0.41	0.564
0.122	0.623	0.161	0.447	0.667
0.762	0.783	0.176	0.446	0.53
0.404	0.75	0.295	0.46	0.542
0.498	0.618	0.567	0.274	0.395
-0.144	0.578	0.658	0.306	0.302
0.659	0.878	0.211	0.402	0.063
0.397	0.973	0.018	0.472	0.039
-0.79	0.891	0.47	0.154	0.006
0.022	0.975	0.5	0.54	0.019
-0.287	0.243	0.254	0.362	0.341
0.438	0.986	0.89	0.668	0.185

0.47	0.932	0.225	0.412	0.34
-0.184	0.422	0.644	0.484	0.704
0.042	0.817	0.5	0.59	0.343
0.659	0.878	0.211	0.402	0.063
0.108	0.51	0.168	0.434	0.299
0.658	0.84	0.083	0.39	0.342
0.515	0.784	0.141	0.438	0.336
0.062	0.787	0.24	0.48	0.292
0.511	0.923	0.302	0.428	0.46
0.859	0.724	0.233	0.326	0.469
-0.187	0.356	0.119	0.29	0.25
0.888	0.761	0.15	0.36	0.386
-0.108	0.393	0.075	0.29	0.166
1.072	0.983	0.311	0.468	0.281
0.727	0.909	0.283	0.526	0.418
1.014	0.926	0.215	0.356	0.462
-0.473	0.687	0.124	0.32	0.399
0.976	0.937	0.134	0.398	0.373
0.582	0.696	0.312	0.337	0.299
0.927	0.612	0.267	0.396	0.378
0.426	0.689	0.276	0.321	0.127
0.53	0.733	0.19	0.385	0.208
-0.347	0.456	0.089	0.354	0.368
0.674	0.816	0.137	0.356	0.438
0.964	0.494	0.85	0.562	0.788
0.678	0.696	0.484	0.392	0.554
0.042	0.916	0.521	0.362	0.14
0.544	0.721	0.303	0.36	0.175
0.753	0.783	0.151	0.382	0.298
0.471	0.665	0.494	0.326	0.238
0.748	0.41	0.663	0.492	0.618
0.707	0.46	0.539	0.514	0.548
1.158	0.921	0.747	0.514	0.88
1.26	0.661	0.686	0.45	0.72
1.159	0.75	0.758	0.418	0.581
1.254	0.661	0.689	0.454	0.68
1.083	0.706	0.716	0.444	0.38
0.825	0.569	0.156	0.302	0.317
1.079	0.984	0.18	0.496	0.101
0.914	0.912	0.178	0.326	0.251
-0.478	0.611	0.064	0.308	0.113

0.858	0.929	0.89	0.584	0.81
0.481	0.943	0.312	0.536	0.098
0.834	0.858	0.286	0.486	0.457
1.236	0.703	0.637	0.468	0.676
-0.261	0.985	0.376	0.62	0.054
0.011	0.936	0.055	0.406	0.015
0.612	0.966	0.546	0.482	0.208
0.369	0.993	0.023	0.42	0.043
-0.051	0.92	0.32	0.175	0.024
-0.205	0.838	0.127	0.26	0.047
-0.079	0.765	0.112	0.434	0.367
-0.429	0.749	0.263	0.438	0.332
0.511	0.923	0.302	0.428	0.46
0.587	0.574	0.154	0.302	0.554
0.259	0.951	0.538	0.639	0.044
-0.159	0.476	0.07	0.322	0.053
0.978	0.683	0.634	0.436	0.401
0.566	0.645	0.487	0.45	0.543
0.794	0.447	0.802	0.496	0.644
1.171	0.828	0.22	0.47	0.231
1.274	0.81	0.307	0.434	0.323
1.458	0.913	0.281	0.412	0.415
-0.164	0.531	0.161	0.334	0.291
1.301	0.893	0.194	0.406	0.264
-0.21	0.627	0.126	0.386	0.353
1.115	0.91	0.202	0.448	0.43
1.388	0.878	0.257	0.382	0.302
1.058	0.857	0.188	0.348	0.138
-0.164	0.531	0.161	0.334	0.291
-0.195	0.506	0.148	0.286	0.246
-0.17	0.531	0.15	0.332	0.242
0.56	0.652	0.565	0.38	0.088
-0.443	0.995	0.98	0.641	0.022
-0.499	0.994	0.991	0.578	0.006
-0.024	0.993	0.136	0.322	0.035
0.711	0.989	0.968	0.752	0.033
0.492	0.996	0.843	0.61	0.295
0.092	0.938	0.75	0.466	0.235
-0.224	0.992	0.828	0.51	0.258
0.262	0.99	0.01	0.482	0.019
0.146	0.684	0.057	0.37	0.388

0.193	0.683	0.096	0.326	0.649
0.147	0.55	0.074	0.337	0.277
0.265	0.657	0.206	0.442	0.138
0.355	0.625	0.454	0.396	0.202
1.081	0.917	0.208	0.388	0.238
-0.35	0.995	0.887	0.274	0.052
0.572	0.71	0.05	0.53	0.017
0.103	0.295	0.308	0.312	0.487
0.121	0.992	0.239	0.518	0.004
0.398	0.737	0.13	0.332	0.45
-0.017	0.808	0.826	0.492	0.077
0.273	0.992	0.026	0.384	0.03
-0.068	0.952	0.055	0.246	0.021
-0.782	0.956	0.909	0.106	0.007
0.313	0.77	0.605	0.452	0.154
-0.088	0.735	0.663	0.494	0.315
0.162	0.621	0.765	0.498	0.274
0.375	0.652	0.402	0.42	0.24
0.205	0.982	0.869	0.596	0.087
0.476	0.74	0.154	0.464	0.06
0.573	0.696	0.284	0.348	0.24
1.254	0.661	0.689	0.454	0.68
1.159	0.75	0.758	0.418	0.581
0.248	0.717	0.611	0.292	0.197
0.278	0.514	0.668	0.455	0.55
-0.845	0.908	0.968	0.118	0.006
0.678	0.696	0.484	0.392	0.554
0.553	0.58	0.308	0.37	0.411
0.652	0.58	0.279	0.386	0.438
-0.009	0.975	0.936	0.682	0.01
0.047	0.971	0.288	0.466	0.047
0.937	0.807	0.277	0.394	0.301
-0.291	0.377	0.181	0.33	0.418
1.07	0.962	0.159	0.874	0.047
0.695	0.739	0.232	0.346	0.376
-0.314	0.278	0.113	0.342	0.245
0.941	0.767	0.72	0.478	0.305
-0.438	0.356	0.568	0.344	0.365
0.992	0.778	0.338	0.44	0.276
-0.73	0.642	0.133	0.368	0.162
0.681	0.813	0.655	0.496	0.5

-0.751	0.891	0.294	0.15	0.004
0.952	0.899	0.234	0.412	0.53
1.065	0.985	0.034	0.733	0.069
0.522	0.568	0.55	0.556	0.118
0.288	0.289	0.423	0.3	0.303
0.164	0.996	0.035	0.508	0.035
	468 Metabolites and positive & negative controls			
A4-Subs	C9-In	C9-Subs	C19-In	C19-Subs
0.326	0.373	0.272	0.199	0.434
0.522	0.054	0.549	0.103	0.733
0.788	0.159	0.202	0.28	0.714
0.706	0.083	0.153	0.173	0.69
0.522	0.021	0.458	0.055	0.723
0.706	0.181	0.328	0.205	0.542
0.854	0.03	0.169	0.286	0.693
0.831	0.095	0.188	0.433	0.687
0.622	0.398	0.46	0.558	0.703
0.852	0.1	0.149	0.076	0.46
0.928	0.056	0.132	0.061	0.172
0.812	0.112	0.296	0.065	0.3
0.8	0.032	0.645	0.056	0.456
0.542	0.257	0.345	0.379	0.516
0.738	0.519	0.378	0.404	0.601
0.618	0.192	0.503	0.54	0.509
0.598	0.065	0.312	0.026	0.536
0.634	0.001	0.404	0.019	0.31
0.722	0.247	0.641	0.418	0.639
0.618	0.313	0.571	0.524	0.732
0.272	0.261	0.339	0.131	0.522
0.94	0.011	0.126	0.266	0.733
0.704	0.136	0.288	0.073	0.334
0.954	0.049	0.206	0.07	0.206
0.964	0.03	0.912	0.054	0.354
0.852	0.123	0.489	0.077	0.643
0.886	0.016	0.924	0.039	0.908
0.542	0.257	0.345	0.379	0.516
0.88	0.041	0.132	0.152	0.854
0.914	0.05	0.76	0.044	0.304

0.735	0.118	0.54	0.054	0.464
0.964	0.041	0.233	0.114	0.456
0.972	0.031	0.53	0.077	0.592
0.71	0.067	0.321	0.055	0.619
0.92	0.194	0.603	0.205	0.531
0.666	0.121	0.48	0.374	0.596
0.522	0.021	0.458	0.055	0.723
0.282	0.009	0.437	0.048	0.697
0.902	0.344	0.197	0.25	0.566
0.624	0.116	0.529	0.227	0.691
0.754	0.074	0.266	0.203	0.591
0.664	0.083	0.259	0.11	0.71
0.584	0.131	0.447	0.101	0.702
0.748	0.073	0.165	0.145	0.736
0.736	0.117	0.198	0.248	0.586
0.604	0.047	0.263	0.056	0.468
0.358	0.023	0.381	0.057	0.667
0.8	0.046	0.325	0.102	0.791
0.866	0.024	0.916	0.054	0.89
0.792	0.041	0.15	0.06	0.704
0.773	0.055	0.266	0.214	0.609
0.916	0.315	0.249	0.394	0.703
0.732	0.105	0.207	0.134	0.302
0.75	0.061	0.304	0.132	0.458
0.904	0.058	0.293	0.44	0.719
0.744	0.077	0.262	0.41	0.67
0.522	0.036	0.366	0.214	0.683
0.642	0.083	0.387	0.373	0.552
0.51	0.099	0.402	0.233	0.644
0.942	0.078	0.116	0.146	0.569
0.62	0.331	0.637	0.463	0.734
0.893	0.682	0.304	0.263	0.754
0.528	0.022	0.652	0.066	0.59
0.166	0.286	0.752	0.1	0.262
0.152	0.404	0.736	0.245	0.268
0.16	0.293	0.753	0.1	0.25
0.16	0.293	0.753	0.1	0.25
0.296	0.427	0.519	0.24	0.332
0.446	0.941	0.75	0.777	0.536
0.462	0.957	0.753	0.777	0.548
0.046	0.048	0.535	0.11	0.192

0.18	0.293	0.604	0.362	0.238
0.876	0.008	0.903	0.087	0.892
0.036	0.001	0.391	0.045	0.166
0.176	0.021	0.392	0.053	0.364
0.15	0.001	0.301	0.003	0.266
0.008	0.001	0.403	0.023	0.15
0.034	0.002	0.412	0.007	0.084
0.22	0.009	0.35	0.043	0.102
0.052	0.004	0.346	0.022	0.16
0.028	0.002	0.44	0.035	0.208
0.028	0.004	0.358	0.016	0.158
0.008	0.003	0.35	0.024	0.082
0.024	0.004	0.327	0.035	0.1
0.036	0.005	0.317	0.024	0.158
0.112	0.002	0.43	0.072	0.16
0.404	0.163	0.41	0.07	0.362
0.468	0.089	0.445	0.096	0.26
0.176	0.019	0.4	0.058	0.182
0.184	0.014	0.471	0.02	0.11
0.039	0.002	0.354	0.014	0.154
0.86	0.45	0.969	0.612	0.794
0.264	0.001	0.341	0.024	0.461
0.332	0.005	0.491	0.291	0.74
0.388	0.006	0.691	0.233	0.854
0.052	0.001	0.224	0.022	0.236
0.376	0.023	0.532	0.534	0.572
0.358	0.026	0.512	0.233	0.636
0.252	0.009	0.516	0.048	0.362
0.18	0.018	0.47	0.054	0.472
0.252	0.029	0.582	0.048	0.35
0.252	0.029	0.582	0.048	0.35
0.182	0.055	0.34	0.03	0.394
0.118	0.009	0.382	0.035	0.432
0.194	0.033	0.573	0.291	0.516
0.452	0.057	0.497	0.346	0.482
0.416	0.034	0.465	0.091	0.5
0.352	0	0.447	0.017	0.624
0.138	0.001	0.436	0.037	0.282
0.282	0.012	0.507	0.036	0.416
0.514	0.041	0.68	0.708	0.494
0.566	0.014	0.525	0.317	0.714

0.366	0.008	0.325	0.013	0.346
0.174	0.064	0.551	0.065	0.346
0.454	0.053	0.643	0.566	0.85
0.696	0.619	0.791	0.661	0.638
0.458	0.368	0.458	0.5	0.444
0.098	0.026	0.656	0.12	0.25
0.356	0.039	0.549	0.397	0.378
0.32	0.019	0.476	0.072	0.587
0.074	0.006	0.342	0.079	0.274
0.306	0.114	0.714	0.427	0.678
0.344	0.002	0.423	0.028	0.53
0.09	0.031	0.245	0.183	0.308
0.124	0.036	0.484	0.102	0.526
0.1	0.025	0.418	0.208	0.426
0.466	0.137	0.507	0.335	0.619
0.572	0.079	0.547	0.265	0.576
0.394	0.096	0.613	0.358	0.428
0.64	0.371	0.462	0.494	0.53
0.256	0.008	0.508	0.217	0.528
0.178	0.036	0.44	0.157	0.478
0.452	0.078	0.423	0.782	0.734
0.48	0.051	0.584	0.649	0.772
0.64	0.492	0.626	0.486	0.614
0.51	0.078	0.537	0.375	0.72
0.362	0.054	0.481	0.643	0.392
0.144	0.103	0.523	0.174	0.454
0.434	0.005	0.487	0.104	0.682
0.21	0.02	0.425	0.056	0.412
0.392	0.136	0.462	0.358	0.46
0.172	0.007	0.433	0.02	0.35
0.65	0.063	0.628	0.181	0.708
0.416	0.364	0.702	0.373	0.49
0.556	0.607	0.581	0.558	0.42
0.49	0.707	0.507	0.316	0.438
0.385	0.015	0.314	0.157	0.5
0.54	0.149	0.659	0.552	0.596
0.622	0.046	0.53	0.194	0.602
0.444	0.056	0.914	0.199	0.752
0.078	0.171	0.572	0.132	0.436
0.438	0.002	0.376	0.116	0.657
0.3	0.156	0.742	0.436	0.624

0.39	0.028	0.549	0.245	0.716
0.172	0.09	0.449	0.258	0.368
0.664	0.65	0.72	0.637	0.502
0.608	0.751	0.515	0.883	0.47
0.512	0.39	0.437	0.532	0.384
0.504	0.701	0.614	0.354	0.482
0.486	0.003	0.594	0.061	0.628
0.444	0.521	0.547	0.139	0.454
0.55	0.759	0.697	0.875	0.688
0.58	0.062	0.429	0.564	0.822
0.53	0.011	0.39	0.205	0.712
0.448	0.349	0.506	0.1	0.41
0.448	0.349	0.506	0.1	0.41
0.636	0.398	0.685	0.436	0.53
0.602	0.388	0.75	0.457	0.548
0.602	0.617	0.399	0.765	0.706
0.47	0.198	0.601	0.267	0.531
0.616	0.55	0.582	0.547	0.662
0.659	0.5	0.682	0.772	0.728
0.604	0.542	0.624	0.555	0.548
0.618	0.772	0.683	0.821	0.666
0.682	0.078	0.56	0.121	0.596
0.556	0.481	0.571	0.188	0.455
0.65	0.441	0.666	0.427	0.686
0.562	0.647	0.571	0.486	0.506
0.62	0.792	0.712	0.887	0.68
0.732	0.478	0.799	0.594	0.682
0.752	0.582	0.806	0.725	0.68
0.687	0.443	0.684	0.435	0.698
0.604	0.176	0.45	0.4	0.704
0.73	0.535	0.765	0.367	0.694
0.786	0.393	0.757	0.414	0.67
0.701	0.5	0.657	0.391	0.718
0.686	0.5	0.688	0.683	0.686
0.744	0.43	0.636	0.455	0.705
0.697	0.448	0.635	0.433	0.719
0.626	0.489	0.634	0.234	0.454
0.644	0.507	0.643	0.23	0.508
0.412	0.694	0.567	0.391	0.502
0.036	0.005	0.401	0.113	0.372
0.042	0	0.235	0.017	0.172

0.024	0	0.376	0.007	0.15
0.044	0	0.275	0.054	0.21
0.49	0.707	0.507	0.316	0.438
0.512	0.39	0.437	0.532	0.384
0.048	0.01	0.55	0.134	0.25
0.274	0.017	0.468	0.315	0.382
0.556	0.032	0.422	0.158	0.526
0.53	0.065	0.398	0.336	0.426
0.428	0.046	0.467	0.295	0.596
0.462	0.026	0.461	0.199	0.642
0.658	0.64	0.679	0.622	0.56
0.67	0.025	0.581	0.167	0.608
0.586	0.038	0.349	0.175	0.588
0.48	0.061	0.387	0.299	0.452
0.641	0.031	0.378	0.105	0.652
0.492	0.08	0.28	0.202	0.53
0.659	0.073	0.337	0.331	0.508
0.456	0.019	0.412	0.125	0.572
0.553	0.069	0.352	0.33	0.644
0.59	0.043	0.493	0.367	0.704
0.575	0.04	0.392	0.219	0.556
0.072	0.034	0.883	0.021	0.196
0.565	0.052	0.459	0.269	0.608
0.358	0.038	0.619	0.351	0.678
0.37	0.023	0.358	0.236	0.664
0.467	0.013	0.475	0.286	0.652
0.659	0.02	0.45	0.215	0.64
0.738	0.667	0.702	0.796	0.518
0.4	0.006	0.417	0.084	0.598
0.494	0.043	0.424	0.488	0.488
0.404	0.012	0.283	0.183	0.586
0.48	0.061	0.387	0.299	0.452
0.641	0.031	0.378	0.105	0.652
0.518	0.439	0.538	0.162	0.522
0.498	0.465	0.369	0.172	0.534
0.522	0.375	0.522	0.279	0.54
0.542	0.532	0.447	0.259	0.514
0.382	0.062	0.769	0.344	0.752
0.541	0.404	0.644	0.593	0.506
0.46	0.186	0.326	0.087	0.404
0.56	0.229	0.473	0.215	0.406

0.588	0.18	0.472	0.195	0.413
0.37	0.12	0.631	0.124	0.412
0.526	0.239	0.618	0.105	0.478
0.562	0.162	0.638	0.171	0.624
0.522	0.533	0.442	0.087	0.458
0.542	0.416	0.485	0.129	0.574
0.613	0.023	0.339	0.17	0.566
0.556	0.032	0.422	0.158	0.526
0.182	0.031	0.485	0.267	0.562
0.402	0.053	0.371	0.261	0.576
0.13	0.06	0.343	0.322	0.268
0.934	0.144	0.251	0.189	0.879
0.196	0.021	0.383	0.441	0.356
0.716	0.004	0.369	0.17	0.53
0.204	0.124	0.472	0.62	0.57
0.324	0.129	0.424	0.494	0.57
0.67	0.025	0.581	0.167	0.608
0.628	0.029	0.283	0.083	0.653
0.631	0.018	0.442	0.224	0.652
0.656	0.019	0.392	0.094	0.652
0.482	0.027	0.377	0.229	0.466
0.639	0.072	0.35	0.217	0.524
0.437	0.005	0.208	0.151	0.404
0.706	0.645	0.699	0.665	0.582
0.502	0.003	0.587	0.028	0.834
0.542	0.034	0.391	0.353	0.436
0.468	0.014	0.343	0.077	0.672
0.537	0.009	0.357	0.126	0.61
0.631	0.021	0.415	0.127	0.646
0.565	0.356	0.337	0.09	0.266
0.418	0.009	0.473	0.037	0.498
0.598	0.244	0.561	0.492	0.59
0.619	0.159	0.384	0.166	0.474
0.696	0.19	0.502	0.349	0.652
0.726	0.302	0.631	0.463	0.711
0.444	0.003	0.265	0.1	0.38
0.714	0.686	0.655	0.758	0.46
0.156	0.009	0.49	0.081	0.424
0.114	0.138	0.664	0.463	0.506
0.582	0.662	0.436	0.589	0.49
0.618	0.017	0.315	0.131	0.49

0.479	0.011	0.397	0.201	0.632
0.594	0.431	0.723	0.427	0.546
0.676	0.46	0.671	0.701	0.648
0.6	0.604	0.591	0.669	0.528
0.526	0.409	0.522	0.335	0.418
0.592	0.417	0.486	0.599	0.516
0.54	0.242	0.405	0.257	0.424
0.755	0.378	0.562	0.62	0.729
0.594	0.464	0.656	0.595	0.526
0.716	0.437	0.73	0.542	0.659
0.654	0.336	0.591	0.273	0.515
0.696	0.267	0.595	0.484	0.649
0.597	0.319	0.795	0.426	0.692
0.576	0.288	0.65	0.2	0.494
0.651	0.43	0.752	0.389	0.636
0.522	0.174	0.633	0.237	0.634
0.572	0.158	0.68	0.374	0.67
0.556	0.15	0.513	0.157	0.498
0.63	0.277	0.507	0.21	0.472
0.696	0.257	0.495	0.236	0.536
0.724	0.33	0.616	0.397	0.662
0.51	0.273	0.674	0.419	0.589
0.624	0.779	0.601	0.888	0.724
0.434	0.699	0.572	0.47	0.532
0.444	0.521	0.547	0.139	0.454
0.4	0.5	0.489	0.133	0.456
0.526	0.738	0.624	0.457	0.564
0.432	0.367	0.495	0.467	0.512
0.416	0.5	0.466	0.389	0.532
0.398	0.309	0.373	0.091	0.486
0.616	0.401	0.487	0.414	0.532
0.491	0.218	0.554	0.428	0.394
0.434	0.699	0.572	0.47	0.532
0.4	0.5	0.489	0.133	0.456
0.562	0.744	0.711	0.881	0.59
0.536	0.562	0.635	0.863	0.582
0.662	0.726	0.664	0.944	0.712
0.636	0.763	0.649	0.926	0.72
0.588	0.726	0.539	0.853	0.592
0.646	0.716	0.626	0.926	0.742
0.588	0.632	0.516	0.625	0.546

0.564	0.492	0.55	0.759	0.726
0.588	0.381	0.453	0.608	0.496
0.516	0.164	0.429	0.263	0.386
0.736	0.166	0.398	0.587	0.72
0.663	0.273	0.527	0.551	0.636
0.626	0.145	0.466	0.248	0.461
0.696	0.768	0.599	0.902	0.71
0.76	0.373	0.737	0.322	0.676
0.506	0.211	0.353	0.056	0.484
0.45	0.569	0.518	0.735	0.444
0.492	0.451	0.515	0.417	0.47
0.58	0.427	0.576	0.338	0.526
0.578	0.406	0.575	0.338	0.502
0.612	0.061	0.629	0.113	0.558
0.687	0.393	0.671	0.372	0.664
0.744	0.256	0.491	0.626	0.688
0.614	0.624	0.569	0.911	0.72
0.522	0.447	0.556	0.403	0.567
0.51	0.273	0.674	0.419	0.589
0.512	0.507	0.538	0.445	0.568
0.674	0.077	0.495	0.332	0.508
0.462	0.731	0.553	0.308	0.562
0.41	0.388	0.571	0.565	0.754
0.432	0.025	0.484	0.304	0.548
0.62	0.652	0.601	0.614	0.556
0.465	0.022	0.275	0.141	0.296
0.252	0.029	0.582	0.048	0.35
0.706	0.159	0.495	0.682	0.616
0.456	0.256	0.451	0.281	0.312
0.38	0.212	0.782	0.332	0.593
0.521	0.013	0.294	0.166	0.449
0.21	0.085	0.436	0.177	0.274
0.53	0.074	0.447	0.371	0.484
0.316	0.007	0.555	0.143	0.478
0.436	0.014	0.252	0.074	0.574
0.14	0.091	0.285	0.244	0.27
0.132	0.131	0.407	0.209	0.348
0.6	0.449	0.648	0.287	0.546
0.604	0.469	0.727	0.469	0.496
0.676	0.46	0.671	0.701	0.648
0.586	0.556	0.402	0.575	0.472

0.576	0.076	0.519	0.192	0.881
0.51	0.082	0.544	0.261	0.759
0.514	0.321	0.389	0.242	0.38
0.65	0.16	0.621	0.224	0.548
0.034	0.183	0.696	0.329	0.392
0.546	0.438	0.587	0.676	0.696
0.564	0.615	0.495	0.655	0.644
0.55	0.653	0.647	0.862	0.592
0.556	0.02	0.383	0.289	0.584
0.676	0.312	0.504	0.495	0.686
0.705	0.479	0.606	0.547	0.702
0.734	0.535	0.911	0.64	0.708
0.73	0.418	0.748	0.339	0.612
0.818	0.281	0.844	0.56	0.766
0.732	0.451	0.656	0.375	0.586
0.75	0.482	0.819	0.639	0.738
0.856	0.388	0.91	0.612	0.79
0.761	0.238	0.764	0.465	0.748
0.73	0.418	0.748	0.339	0.612
0.701	0.354	0.741	0.279	0.556
0.734	0.363	0.694	0.339	0.608
0.492	0.077	0.411	0.15	0.698
0.476	0.268	0.418	0.184	0.562
0.458	0.232	0.455	0.569	0.686
0.408	0.345	0.617	0.14	0.476
0.616	0.509	0.345	0.554	0.53
0.714	0.544	0.351	0.34	0.634
0.661	0.48	0.414	0.426	0.613
0.759	0.345	0.56	0.343	0.756
0.12	0.006	0.317	0.103	0.17
0.39	0.242	0.518	0.905	0.44
0.394	0.197	0.419	0.686	0.338
0.474	0.087	0.426	0.487	0.377
0.112	0.008	0.396	0.081	0.42
0.128	0.011	0.429	0.14	0.378
0.082	0.055	0.666	0.137	0.382
0.932	0.042	0.621	0.092	0.845
0.228	0.002	0.458	0.135	0.614
0.584	0.5	0.361	0.109	0.698
0.732	0.582	0.713	0.5	0.592
0.36	0.143	0.736	0.605	0.804

0.116	0.006	0.295	0.071	0.196
0.044	0.002	0.338	0.014	0.274
0.1	0.003	0.413	0.036	0.376
0.114	0.001	0.268	0.006	0.31
0.646	0.685	0.457	0.72	0.428
0.45	0.165	0.955	0.414	0.678
0.476	0.189	0.858	0.438	0.468
0.548	0.006	0.262	0.059	0.653
0.437	0.005	0.208	0.151	0.404
0.676	0.262	0.48	0.25	0.556
0.662	0.448	0.462	0.389	0.492
0.492	0.187	0.605	0.126	0.544
0.012	0.009	0.341	0.139	0.15
0.29	0.047	0.465	0.518	0.58
0.848	0.425	0.33	0.532	0.838
0.464	0.053	0.453	0.176	0.466
0.636	0.127	0.342	0.464	0.496
0.422	0.026	0.387	0.109	0.516
0.424	0.004	0.28	0.102	0.627
0.498	0.042	0.467	0.157	0.65
0.426	0.028	0.512	0.133	0.654
0.498	0.322	0.516	0.274	0.712
0.635	0.045	0.264	0.17	0.421
0.6	0.554	0.514	0.621	0.514
0.378	0.019	0.71	0.239	0.614
0.488	0.482	0.389	0.544	0.638
0.034	0.183	0.696	0.329	0.392
0.082	0.055	0.666	0.137	0.382
0.753	0.385	0.774	0.542	0.724
0.03	0.168	0.686	0.329	0.408
0.088	0.042	0.704	0.26	0.272
0.058	0.128	0.453	0.44	0.212
0.454	0.76	0.484	0.231	0.525
0.706	0.021	0.585	0.012	0.665
0.522	0.617	0.478	0.339	0.516
0.144	0.078	0.438	0.069	0.308
0.174	0.004	0.401	0.018	0.386
0.447	0.006	0.261	0.049	0.347
0.42	0.048	0.286	0.109	0.299
0.07	0.005	0.439	0.049	0.42
0.056	0.014	0.445	0.095	0.412

0.28	0.027	0.467	0.414	0.424
0.7	0.541	0.738	0.529	0.638
0.086	0.009	0.44	0.152	0.394
0.236	0.008	0.409	0.305	0.606
0.39	0.059	0.656	0.328	0.598
0.266	0.011	0.361	0.092	0.462
0.142	0.006	0.418	0.226	0.32
0.184	0.032	0.449	0.209	0.466
0.428	0.203	0.644	0.109	0.272
0.432	0.036	0.268	0.094	0.552
0.554	0.007	0.791	0.245	0.63
0.244	0.163	0.401	0.218	0.314
0.192	0.055	0.377	0.223	0.25
0.062	0.104	0.979	0.038	0.214
0.559	0.031	0.39	0.116	0.549
0.328	0.071	0.496	0.124	0.542
0.636	0.17	0.521	0.333	0.664
0.67	0.266	0.486	0.434	0.666
0.606	0.333	0.503	0.544	0.752
0.658	0.289	0.578	0.565	0.674
0.524	0.044	0.504	0.553	0.818
0.076	0.006	0.464	0.197	0.274
0.142	0.009	0.382	0.078	0.212
0.106	0.001	0.4	0.038	0.168
0.528	0.152	0.766	0.313	0.306
0.408	0.03	0.337	0.39	0.323
0.384	0.088	0.403	0.369	0.372
0.052	0	0.267	0.014	0.242
0.106	0.011	0.439	0.094	0.204
0.084	0.051	0.718	0.26	0.256
0.062	0.001	0.259	0.02	0.34
0.362	0.025	0.593	0.342	0.63
0.444	0.065	0.524	0.49	0.406
0.09	0.014	0.634	0.26	0.28
0.116	0.006	0.472	0.157	0.274
0.77	0.449	0.855	0.604	0.736
0.108	0.006	0.356	0.09	0.2
0.37	0.105	0.552	0.31	0.49
0.146	0.025	0.462	0.15	0.264
0.262	0.012	0.322	0.035	0.266
0.266	0.365	0.354	0.22	0.3

0.266	0.13	0.486	0.244	0.582
0.034	0.183	0.696	0.329	0.392
0.082	0.055	0.666	0.137	0.382
0.597	0.253	0.734	0.426	0.692
0.646	0.716	0.626	0.926	0.742
0.588	0.726	0.539	0.853	0.592
0.466	0.379	0.556	0.471	0.418
0.532	0.375	0.656	0.458	0.498
0.034	0.183	0.696	0.329	0.392
0.732	0.381	0.551	0.543	0.857
0.368	0.004	0.653	0.256	0.754
0.378	0.019	0.71	0.239	0.614
0.03	0.069	0.957	0.045	0.18
0.526	0.738	0.624	0.457	0.564
0.428	0.06	0.626	0.639	0.38
0.635	0.5	0.687	0.47	0.554
0.722	0.607	0.706	0.692	0.625
0.629	0.5	0.712	0.47	0.626
0.71	0.605	0.725	0.692	0.677
0.352	0.049	0.456	0.064	0.37
0.392	0.011	0.504	0.309	0.824
0.302	0.045	0.749	0.414	0.568
0.294	0.05	0.394	0.142	0.566
0.458	0.181	0.542	0.373	0.784
0.082	0.055	0.666	0.137	0.382
0.26	0.003	0.399	0.199	0.624
0.024	0.101	0.628	0.329	0.43
0.52	0.035	0.616	0.312	0.604
0.76	0.332	0.729	0.634	0.754
0.73	0.472	0.611	0.373	0.626
0.366	0.282	0.509	0.637	0.638
0.304	0.044	0.276	0.101	0.366
0.344	0.017	0.342	0.215	0.634
0.238	0.007	0.288	0.012	0.37
0.444	0.08	0.49	0.525	0.611
0.256	0.071	0.442	0.52	0.398
0.106	0.007	0.483	0.134	0.426
0.814	0.045	0.929	0.281	0.886
0.1	0.002	0.442	0.08	0.244
0.148	0.004	0.385	0.034	0.394
0.096	0.001	0.342	0.005	0.318

0.532	0.102	0.474	0.257	0.282
0.266	0.015	0.495	0.191	0.746
0.4	0.049	0.303	0.109	0.425
0.565	0.454	0.561	0.429	0.579
0.52	0.348	0.494	0.204	0.512
0.63	0.587	0.518	0.816	0.736
0.636	0.596	0.494	0.486	0.564
0.706	0.419	0.478	0.665	0.682
0.72	0.29	0.41	0.712	0.74
0.55	0.242	0.413	0.231	0.444
0.626	0.588	0.605	0.847	0.712
0.624	0.293	0.397	0.196	0.461
0.072	0.034	0.883	0.021	0.196
0.616	0.008	0.402	0.075	0.69
0.308	0.283	0.475	0.328	0.443
0.529	0.015	0.306	0.052	0.6
0.484	0.74	0.575	0.47	0.532
0.068	0.028	0.881	0.021	0.208
0.276	0.01	0.737	0.146	0.57
0.08	0.011	0.296	0.063	0.27
0.496	0.049	0.54	0.531	0.61
0.382	0.024	0.356	0.262	0.616
0.73	0.535	0.765	0.367	0.694
0.722	0.049	0.358	0.094	0.682
0.498	0.337	0.643	0.49	0.8
0.308	0.013	0.336	0.301	0.832
0.32	0.049	0.431	0.145	0.44
0.474	0.083	0.579	0.126	0.648
0.492	0.362	0.583	0.354	0.532
0.53	0.074	0.447	0.371	0.484
0.316	0.007	0.555	0.143	0.478
0.082	0.055	0.666	0.137	0.382
0.514	0.049	0.614	0.06	0.454
0.082	0.055	0.666	0.137	0.382
0.657	0.039	0.365	0.188	0.568
0.473	0.015	0.317	0.233	0.694
0.326	0.049	0.503	0.061	0.31
0.436	0.317	0.516	0.357	0.454

	Metabolites after MDS using CDK (165) (used for MDS using ADMET)			
A4-Subs	C9-In	C9-Subs	C19-In	C19-Subs
0.514	0.041	0.68	0.708	0.494
0.696	0.619	0.791	0.661	0.638
0.458	0.368	0.458	0.5	0.444
0.64	0.371	0.462	0.494	0.53
0.64	0.492	0.626	0.486	0.614
0.362	0.054	0.481	0.643	0.392
0.65	0.063	0.628	0.181	0.708
0.556	0.607	0.581	0.558	0.42
0.49	0.707	0.507	0.316	0.438
0.622	0.046	0.53	0.194	0.602
0.512	0.39	0.437	0.532	0.384
0.55	0.759	0.697	0.875	0.688
0.636	0.398	0.685	0.436	0.53
0.616	0.55	0.582	0.547	0.662
0.659	0.5	0.682	0.772	0.728
0.604	0.542	0.624	0.555	0.548
0.618	0.772	0.683	0.821	0.666
0.682	0.078	0.56	0.121	0.596
0.556	0.481	0.571	0.188	0.455
0.732	0.478	0.799	0.594	0.682
0.752	0.582	0.806	0.725	0.68
0.687	0.443	0.684	0.435	0.698
0.73	0.535	0.765	0.367	0.694
0.786	0.393	0.757	0.414	0.67
0.701	0.5	0.657	0.391	0.718
0.686	0.5	0.688	0.683	0.686
0.744	0.43	0.636	0.455	0.705
0.697	0.448	0.635	0.433	0.719
0.412	0.694	0.567	0.391	0.502
0.49	0.707	0.507	0.316	0.438
0.67	0.025	0.581	0.167	0.608
0.575	0.04	0.392	0.219	0.556
0.072	0.034	0.883	0.021	0.196
0.358	0.038	0.619	0.351	0.678
0.542	0.532	0.447	0.259	0.514

0.382	0.062	0.769	0.344	0.752
0.541	0.404	0.644	0.593	0.506
0.526	0.239	0.618	0.105	0.478
0.562	0.162	0.638	0.171	0.624
0.67	0.025	0.581	0.167	0.608
0.598	0.244	0.561	0.492	0.59
0.696	0.19	0.502	0.349	0.652
0.726	0.302	0.631	0.463	0.711
0.594	0.431	0.723	0.427	0.546
0.676	0.46	0.671	0.701	0.648
0.6	0.604	0.591	0.669	0.528
0.526	0.409	0.522	0.335	0.418
0.592	0.417	0.486	0.599	0.516
0.54	0.242	0.405	0.257	0.424
0.755	0.378	0.562	0.62	0.729
0.594	0.464	0.656	0.595	0.526
0.716	0.437	0.73	0.542	0.659
0.654	0.336	0.591	0.273	0.515
0.696	0.267	0.595	0.484	0.649
0.597	0.319	0.795	0.426	0.692
0.651	0.43	0.752	0.389	0.636
0.522	0.174	0.633	0.237	0.634
0.572	0.158	0.68	0.374	0.67
0.696	0.257	0.495	0.236	0.536
0.724	0.33	0.616	0.397	0.662
0.624	0.779	0.601	0.888	0.724
0.526	0.738	0.624	0.457	0.564
0.432	0.367	0.495	0.467	0.512
0.416	0.5	0.466	0.389	0.532
0.616	0.401	0.487	0.414	0.532
0.434	0.699	0.572	0.47	0.532
0.562	0.744	0.711	0.881	0.59
0.536	0.562	0.635	0.863	0.582
0.662	0.726	0.664	0.944	0.712
0.636	0.763	0.649	0.926	0.72
0.588	0.726	0.539	0.853	0.592
0.646	0.716	0.626	0.926	0.742
0.564	0.492	0.55	0.759	0.726
0.588	0.381	0.453	0.608	0.496
0.736	0.166	0.398	0.587	0.72
0.663	0.273	0.527	0.551	0.636

0.626	0.145	0.466	0.248	0.461
0.696	0.768	0.599	0.902	0.71
0.612	0.061	0.629	0.113	0.558
0.744	0.256	0.491	0.626	0.688
0.614	0.624	0.569	0.911	0.72
0.674	0.077	0.495	0.332	0.508
0.465	0.022	0.275	0.141	0.296
0.706	0.159	0.495	0.682	0.616
0.521	0.013	0.294	0.166	0.449
0.14	0.091	0.285	0.244	0.27
0.132	0.131	0.407	0.209	0.348
0.6	0.449	0.648	0.287	0.546
0.604	0.469	0.727	0.469	0.496
0.676	0.46	0.671	0.701	0.648
0.586	0.556	0.402	0.575	0.472
0.51	0.082	0.544	0.261	0.759
0.65	0.16	0.621	0.224	0.548
0.546	0.438	0.587	0.676	0.696
0.564	0.615	0.495	0.655	0.644
0.55	0.653	0.647	0.862	0.592
0.676	0.312	0.504	0.495	0.686
0.705	0.479	0.606	0.547	0.702
0.734	0.535	0.911	0.64	0.708
0.73	0.418	0.748	0.339	0.612
0.818	0.281	0.844	0.56	0.766
0.732	0.451	0.656	0.375	0.586
0.75	0.482	0.819	0.639	0.738
0.856	0.388	0.91	0.612	0.79
0.761	0.238	0.764	0.465	0.748
0.73	0.418	0.748	0.339	0.612
0.701	0.354	0.741	0.279	0.556
0.734	0.363	0.694	0.339	0.608
0.458	0.232	0.455	0.569	0.686
0.39	0.242	0.518	0.905	0.44
0.394	0.197	0.419	0.686	0.338
0.474	0.087	0.426	0.487	0.377
0.584	0.5	0.361	0.109	0.698
0.36	0.143	0.736	0.605	0.804
0.45	0.165	0.955	0.414	0.678
0.476	0.189	0.858	0.438	0.468
0.548	0.006	0.262	0.059	0.653

0.676	0.262	0.48	0.25	0.556
0.662	0.448	0.462	0.389	0.492
0.492	0.187	0.605	0.126	0.544
0.498	0.322	0.516	0.274	0.712
0.488	0.482	0.389	0.544	0.638
0.753	0.385	0.774	0.542	0.724
0.058	0.128	0.453	0.44	0.212
0.706	0.021	0.585	0.012	0.665
0.522	0.617	0.478	0.339	0.516
0.28	0.027	0.467	0.414	0.424
0.7	0.541	0.738	0.529	0.638
0.39	0.059	0.656	0.328	0.598
0.432	0.036	0.268	0.094	0.552
0.192	0.055	0.377	0.223	0.25
0.062	0.104	0.979	0.038	0.214
0.636	0.17	0.521	0.333	0.664
0.67	0.266	0.486	0.434	0.666
0.606	0.333	0.503	0.544	0.752
0.658	0.289	0.578	0.565	0.674
0.362	0.025	0.593	0.342	0.63
0.37	0.105	0.552	0.31	0.49
0.597	0.253	0.734	0.426	0.692
0.646	0.716	0.626	0.926	0.742
0.588	0.726	0.539	0.853	0.592
0.466	0.379	0.556	0.471	0.418
0.532	0.375	0.656	0.458	0.498
0.03	0.069	0.957	0.045	0.18
0.526	0.738	0.624	0.457	0.564
0.635	0.5	0.687	0.47	0.554
0.629	0.5	0.712	0.47	0.626
0.302	0.045	0.749	0.414	0.568
0.52	0.035	0.616	0.312	0.604
0.76	0.332	0.729	0.634	0.754
0.73	0.472	0.611	0.373	0.626
0.814	0.045	0.929	0.281	0.886
0.565	0.454	0.561	0.429	0.579
0.52	0.348	0.494	0.204	0.512
0.63	0.587	0.518	0.816	0.736
0.636	0.596	0.494	0.486	0.564
0.706	0.419	0.478	0.665	0.682
0.55	0.242	0.413	0.231	0.444

0.626	0.588	0.605	0.847	0.712
0.068	0.028	0.881	0.021	0.208
0.73	0.535	0.765	0.367	0.694
0.722	0.049	0.358	0.094	0.682
0.498	0.337	0.643	0.49	0.8
0.492	0.362	0.583	0.354	0.532
0.473	0.015	0.317	0.233	0.694
	468 Metabolites and positive & negative controls			
D6-In	D6-Subs	T1/2	CL	hERG
0.536	0.626	1.753	1.856	0.478
0.574	0.49	1.574	2.144	0.876
0.699	0.563	1.812	1.932	0.98
0.715	0.588	1.855	1.875	0.982
0.504	0.499	1.64	2.134	0.849
0.592	0.383	2.186	1.346	0.966
0.755	0.278	1.627	1.776	1
0.747	0.288	1.702	1.684	0.968
0.613	0.407	1.896	1.425	0.861
0.508	0.395	0.866	2.155	0.655
0.53	0.994	1.418	2.631	0.26
0.503	0.756	1.495	1.668	0.248
0.562	0.868	1.647	2.458	0.443
0.631	0.512	2.193	1.761	0.978
0.684	0.344	1.801	1.732	0.994
0.696	0.639	2.154	1.513	0.69
0.692	0.469	2.032	1.55	0.98
0.12	0.469	1.411	1.3	0.354
0.702	0.679	2.142	1.552	0.648
0.619	0.483	1.59	2.031	0.873
0.535	0.681	1.777	2.178	0.433
0.761	0.172	1.479	1.678	0.998
0.472	0.71	1.398	1.916	0.152
0.463	0.965	1.47	2.442	0.341
0.45	0.907	1.207	2.644	0.304
0.614	0.465	2.97	1.124	0.962
0.468	0.584	1.097	2.281	0.487
0.631	0.512	2.193	1.761	0.978
0.418	0.681	1.772	1.804	0.52

0.475	0.957	0.904	2.924	0.194
0.397	0.724	0.98	2.326	0.229
0.634	0.946	1.5	2.09	0.191
0.562	0.768	1.023	2.406	0.163
0.683	0.445	1.501	1.629	0.659
0.48	0.59	2.735	1.722	0.99
0.62	0.544	1.652	1.749	0.726
0.504	0.499	1.64	2.134	0.849
0.452	0.39	1.53	2.173	0.751
0.701	0.185	2.077	1.921	0.96
0.405	0.562	2.524	1.45	0.958
0.769	0.38	1.692	1.884	0.857
0.764	0.652	2.109	2.045	0.915
0.724	0.655	2.103	2.14	0.9
0.693	0.566	1.793	2.008	0.974
0.698	0.583	1.866	1.82	0.994
0.708	0.442	2.084	1.927	0.976
0.521	0.356	1.544	2.145	0.849
0.388	0.53	1.639	2.016	0.637
0.958	0.968	1.769	2.526	0.881
0.712	0.574	1.464	1.937	0.775
0.696	0.296	1.555	1.688	0.548
0.698	0.128	1.772	1.785	0.992
0.518	0.906	1.512	2.15	0.443
0.611	0.8	1.587	2.198	0.525
0.729	0.223	1.757	1.894	0.97
0.512	0.303	1.614	2.521	0.805
0.373	0.353	1.594	2.193	0.849
0.65	0.439	1.617	1.858	0.702
0.895	0.674	2.193	1.778	0.904
0.862	0.621	2.091	2.015	0.855
0.918	0.984	1.281	1.9	0.135
0.221	0.167	2.171	1.095	0.313
0.451	0.697	1.451	1.784	0.133
0.238	0.536	1.813	1.558	0.693
0.264	0.478	1.85	1.552	0.616
0.212	0.508	1.788	1.522	0.649
0.212	0.508	1.872	1.474	0.681
0.41	0.471	2.013	1.61	0.635
0.471	0.643	1.852	1.623	0.702
0.468	0.627	1.669	1.707	0.655

0.142	0.437	1.701	1.395	0.471
0.247	0.512	1.762	1.377	0.705
0.588	0.873	1.497	1.868	0.215
0.044	0.167	1.582	0.908	0.4
0.144	0.358	0.969	1.341	0.113
0.061	0.526	1.522	1.599	0.265
0.062	0.428	1.129	1.139	0.207
0.11	0.308	1.331	0.748	0.104
0.137	0.234	0.764	1.403	0.051
0.114	0.228	1.412	1.075	0.091
0.117	0.225	1.417	0.862	0.266
0.097	0.262	1.517	1.065	0.089
0.062	0.402	1.336	1.11	0.02
0.087	0.345	1.224	0.904	0.048
0.149	0.42	0.974	1.438	0.103
0.141	0.191	1.481	0.866	0.319
0.256	0.332	1.034	1.558	0.317
0.385	0.304	1.253	1.681	0.249
0.22	0.585	0.776	1.553	0.196
0.174	0.522	0.717	1.919	0.127
0.101	0.255	1.42	1.138	0.119
0.529	0.182	2.964	1.442	0.657
0.223	0.608	1.672	1.189	0.34
0.418	0.581	1.79	1.796	0.333
0.544	0.392	1.759	1.825	0.291
0.103	0.258	1.631	1.408	0.18
0.643	0.603	1.588	1.17	0.316
0.68	0.404	1.783	1.766	0.287
0.189	0.376	1.503	1.674	0.28
0.257	0.545	1.455	1.545	0.129
0.285	0.385	1.796	1.807	0.265
0.285	0.385	1.622	2.274	0.373
0.253	0.505	1.842	1.862	0.348
0.155	0.545	1.854	1.869	0.394
0.209	0.593	1.607	2.034	0.304
0.373	0.553	1.55	2.48	0.497
0.306	0.244	1.639	1.524	0.19
0.194	0.384	1.583	1.401	0.261
0.049	0.229	1.665	1.475	0.365
0.228	0.459	1.372	1.479	0.146
0.178	0.273	1.304	1.327	0.256

0.478	0.509	1.747	1.694	0.287
0.167	0.416	1.52	1.299	0.143
0.432	0.422	1.772	2.076	0.293
0.533	0.412	1.727	1.665	0.292
0.542	0.37	2.276	1.557	0.636
0.492	0.386	1.799	1.375	0.617
0.068	0.344	1.809	1.629	0.271
0.159	0.27	1.185	1.888	0.217
0.347	0.408	1.634	1.517	0.224
0.168	0.556	1.329	1.569	0.308
0.565	0.672	2.036	1.641	0.262
0.334	0.488	1.094	1.627	0.303
0.118	0.404	1.738	1.541	0.385
0.268	0.437	1.858	1.592	0.396
0.11	0.221	1.557	1.02	0.321
0.608	0.544	1.288	1.675	0.15
0.347	0.547	1.006	1.841	0.188
0.228	0.508	0.963	1.574	0.169
0.502	0.317	1.994	2.054	0.477
0.246	0.645	1.555	1.936	0.297
0.316	0.535	1.861	1.88	0.328
0.763	0.554	1.694	1.659	0.292
0.473	0.435	1.756	1.757	0.333
0.548	0.401	1.96	1.82	0.626
0.448	0.486	1.502	1.605	0.209
0.142	0.409	1.428	1.608	0.236
0.344	0.546	1.863	1.867	0.366
0.12	0.318	1.246	1.45	0.324
0.173	0.526	1.837	1.603	0.398
0.262	0.545	0.978	1.868	0.299
0.156	0.506	1.758	1.691	0.358
0.518	0.704	1.632	1.897	0.518
0.486	0.793	1.91	1.919	0.416
0.455	0.402	1.927	1.788	0.605
0.446	0.491	1.802	1.713	0.58
0.29	0.42	1.931	1.841	0.315
0.319	0.735	0.977	1.875	0.135
0.459	0.602	1.807	1.88	0.533
0.439	0.825	1.347	1.802	0.247
0.4	0.542	1.794	2.019	0.343
0.572	0.367	1.033	1.421	0.233

0.346	0.828	1.171	1.675	0.199
0.65	0.767	1.747	1.94	0.149
0.538	0.341	0.847	1.304	0.154
0.485	0.33	2.006	1.463	0.478
0.542	0.394	1.999	1.718	0.609
0.4	0.373	1.7	1.434	0.574
0.481	0.524	1.651	1.716	0.554
0.414	0.509	1.308	1.586	0.187
0.468	0.605	1.814	1.934	0.539
0.562	0.601	1.961	2.146	0.599
0.561	0.729	1.812	1.72	0.261
0.207	0.327	1.465	1.298	0.204
0.454	0.493	1.695	2.125	0.447
0.454	0.493	1.695	2.125	0.447
0.487	0.351	1.612	1.964	0.42
0.435	0.339	1.546	1.667	0.445
0.393	0.298	1.88	1.8	0.48
0.4	0.491	1.934	2.217	0.462
0.53	0.313	1.867	1.606	0.497
0.552	0.358	2.746	1.363	0.656
0.472	0.428	2.065	1.654	0.653
0.526	0.412	2.277	2.029	0.571
0.322	0.672	1.942	1.986	0.592
0.466	0.34	1.992	1.922	0.486
0.534	0.417	1.96	1.751	0.433
0.507	0.436	1.978	1.957	0.469
0.573	0.467	2.32	1.998	0.591
0.492	0.305	2.46	1.738	0.566
0.452	0.32	2.317	1.616	0.626
0.558	0.356	2.291	1.592	0.524
0.387	0.519	1.491	1.889	0.442
0.531	0.31	2.347	1.749	0.468
0.474	0.297	2.356	1.741	0.59
0.541	0.37	1.937	1.614	0.445
0.458	0.376	2.124	1.87	0.439
0.519	0.365	2.106	1.864	0.453
0.461	0.254	2.27	1.49	0.606
0.5	0.422	1.93	2.061	0.356
0.491	0.371	1.949	2.063	0.366
0.492	0.558	1.993	1.602	0.669
0.085	0.287	1.502	1.146	0.359

0.018	0.154	1.344	0.912	0.365
0.018	0.183	1.413	0.949	0.38
0.042	0.121	1.689	1.221	0.421
0.446	0.491	1.802	1.713	0.58
0.4	0.373	1.7	1.434	0.574
0.133	0.333	1.349	1.145	0.32
0.096	0.154	1.569	1.552	0.222
0.264	0.395	1.949	1.985	0.323
0.359	0.539	1.584	2.073	0.445
0.26	0.436	1.835	1.859	0.319
0.365	0.493	1.878	1.849	0.33
0.491	0.325	1.991	1.34	0.496
0.474	0.696	1.801	2.441	0.428
0.388	0.389	2.003	1.978	0.334
0.282	0.462	2.024	1.844	0.365
0.334	0.519	1.991	2.025	0.33
0.38	0.459	2.047	1.995	0.329
0.369	0.331	1.628	2.288	0.34
0.286	0.48	1.829	1.853	0.314
0.283	0.452	1.952	1.982	0.322
0.369	0.466	1.92	1.782	0.443
0.328	0.441	1.563	2.152	0.317
0.142	0.584	1.728	1.203	0.608
0.365	0.463	2.011	2.021	0.335
0.295	0.339	1.618	1.426	0.2
0.329	0.452	1.784	1.721	0.316
0.353	0.541	1.883	1.807	0.336
0.362	0.4	1.871	1.853	0.34
0.493	0.316	2.023	1.454	0.468
0.411	0.579	1.782	1.689	0.298
0.394	0.525	1.715	2.015	0.29
0.29	0.544	1.876	1.86	0.315
0.282	0.462	2.024	1.844	0.365
0.334	0.519	1.991	2.025	0.33
0.541	0.586	1.535	2.042	0.508
0.499	0.474	1.838	1.863	0.553
0.503	0.611	1.695	2.126	0.607
0.483	0.599	1.864	1.821	0.598
0.523	0.85	1.525	1.65	0.242
0.458	0.487	2.138	1.752	0.607
0.378	0.312	1.715	1.604	0.649

0.36	0.359	1.774	2.209	0.504
0.314	0.369	1.568	2.108	0.304
0.611	0.488	1.331	1.885	0.598
0.378	0.571	1.872	2.017	0.552
0.502	0.557	1.962	1.868	0.717
0.437	0.547	1.257	2.167	0.344
0.58	0.572	1.401	2.127	0.431
0.347	0.454	2.039	2.026	0.327
0.264	0.395	1.949	1.985	0.323
0.299	0.278	1.521	1.534	0.216
0.509	0.323	1.552	1.559	0.21
0.038	0.112	1.946	1.193	0.198
0.791	0.265	2.076	2.006	0.722
0.244	0.34	1.452	1.216	0.156
0.675	0.521	1.402	1.79	0.229
0.436	0.295	1.23	1.177	0.161
0.713	0.497	1.687	1.443	0.2
0.474	0.696	1.801	2.441	0.428
0.32	0.373	1.927	2.069	0.32
0.362	0.392	1.876	1.853	0.338
0.333	0.442	1.986	2.014	0.331
0.268	0.44	1.879	1.414	0.403
0.32	0.328	1.617	2.295	0.335
0.228	0.396	1.725	2.375	0.361
0.477	0.329	1.975	1.603	0.473
0.532	0.605	1.341	1.835	0.151
0.265	0.315	1.688	1.766	0.339
0.338	0.447	1.738	1.712	0.296
0.3	0.434	1.793	1.854	0.332
0.308	0.41	1.846	1.862	0.328
0.389	0.332	2.16	0.849	0.581
0.424	0.556	1.023	1.82	0.119
0.399	0.366	1.643	2.143	0.517
0.429	0.345	1.431	1.985	0.371
0.491	0.395	1.921	1.891	0.562
0.501	0.371	1.971	2.013	0.408
0.148	0.334	1.65	2.36	0.347
0.479	0.286	1.985	1.278	0.508
0.137	0.462	1.809	1.495	0.37
0.157	0.51	1.517	1.011	0.192
0.505	0.508	1.974	1.329	0.465

0.325	0.358	2.203	2.031	0.327
0.237	0.497	1.827	1.874	0.334
0.433	0.276	1.75	2.01	0.483
0.462	0.431	2.267	1.676	0.67
0.475	0.386	2.353	1.685	0.708
0.445	0.374	1.87	2.133	0.523
0.447	0.374	2.23	1.919	0.731
0.427	0.326	1.737	2.18	0.548
0.561	0.35	2.452	1.705	0.508
0.471	0.34	2.178	1.867	0.682
0.536	0.368	2.47	1.984	0.447
0.503	0.4	1.929	1.967	0.354
0.517	0.376	2.256	2.23	0.469
0.511	0.423	2.391	1.483	0.66
0.459	0.425	1.958	1.986	0.476
0.512	0.58	2.525	1.468	0.762
0.384	0.456	1.984	1.936	0.546
0.483	0.416	2.217	1.737	0.646
0.429	0.378	1.81	2.027	0.48
0.463	0.388	1.654	1.994	0.378
0.507	0.392	1.664	1.944	0.371
0.511	0.388	2.068	1.705	0.57
0.391	0.614	1.879	2.039	0.43
0.618	0.583	2.718	1.999	0.687
0.451	0.559	1.983	1.563	0.669
0.468	0.605	1.814	1.934	0.539
0.472	0.488	1.67	1.972	0.465
0.461	0.66	2.069	1.532	0.752
0.368	0.393	1.823	1.075	0.578
0.416	0.529	1.894	1.786	0.702
0.445	0.432	1.548	2.08	0.494
0.533	0.375	1.984	2.031	0.444
0.358	0.334	1.68	1.99	0.466
0.451	0.559	1.983	1.563	0.669
0.472	0.488	1.67	1.972	0.465
0.539	0.563	2.42	1.73	0.694
0.5	0.568	2.208	1.965	0.662
0.644	0.565	2.672	1.842	0.814
0.627	0.483	2.736	1.852	0.647
0.585	0.481	2.428	2.186	0.629
0.619	0.505	2.603	2.01	0.653

0.518	0.405	1.99	1.901	0.562
0.476	0.513	2.333	2.081	0.554
0.402	0.419	1.885	1.94	0.607
0.337	0.329	1.734	2.221	0.512
0.4	0.396	2.276	2.077	0.484
0.389	0.447	2.036	2.475	0.382
0.32	0.364	1.578	2.107	0.318
0.686	0.545	2.503	1.902	0.755
0.464	0.299	1.837	1.901	0.423
0.37	0.364	1.632	1.74	0.506
0.562	0.551	2.4	1.18	0.608
0.556	0.542	2.205	1.183	0.61
0.516	0.601	2.227	1.243	0.618
0.515	0.601	2.182	1.308	0.626
0.294	0.605	1.795	2.039	0.331
0.493	0.383	1.87	1.702	0.447
0.533	0.406	1.865	1.737	0.621
0.602	0.494	2.451	2.169	0.638
0.395	0.588	2.107	1.737	0.56
0.391	0.614	1.879	2.039	0.43
0.421	0.57	2.141	1.751	0.548
0.406	0.57	0.874	1.881	0.241
0.519	0.512	1.757	1.934	0.469
0.455	0.634	1.313	2.16	0.294
0.245	0.388	1.694	1.506	0.249
0.49	0.367	2.181	1.123	0.589
0.236	0.215	1.725	1.365	0.347
0.285	0.385	1.734	2.24	0.466
0.436	0.582	2.108	1.938	0.755
0.344	0.325	1.728	1.91	0.533
0.576	0.645	1.111	1.952	0.314
0.194	0.466	1.67	2.286	0.345
0.217	0.532	1.86	1.417	0.477
0.336	0.535	1.78	1.787	0.471
0.236	0.551	1.88	1.645	0.299
0.263	0.581	1.895	1.969	0.344
0.212	0.41	1.553	1.292	0.346
0.202	0.382	1.68	1.255	0.348
0.469	0.354	1.677	2.069	0.408
0.429	0.3	1.704	1.729	0.411
0.462	0.431	2.267	1.676	0.67

0.407	0.403	2.158	1.519	0.697
0.749	0.543	1.843	1.627	0.291
0.312	0.407	1.524	1.534	0.215
0.35	0.336	1.909	2	0.527
0.32	0.297	1.824	2.195	0.428
0.212	0.491	1.643	2.02	0.337
0.577	0.772	2.102	1.876	0.822
0.545	0.728	2.082	1.539	0.78
0.577	0.586	2.573	1.853	0.653
0.358	0.735	1.936	1.805	0.32
0.504	0.359	2.375	1.91	0.625
0.526	0.359	2.792	1.509	0.667
0.537	0.36	2.898	1.456	0.657
0.476	0.313	2.097	1.98	0.467
0.509	0.225	2.613	1.865	0.635
0.482	0.361	2.006	1.938	0.457
0.528	0.335	2.754	1.455	0.645
0.524	0.204	2.775	1.674	0.655
0.383	0.331	2.222	2.007	0.509
0.476	0.313	2.097	1.98	0.467
0.441	0.331	2.143	1.956	0.441
0.466	0.305	2.029	1.968	0.471
0.44	0.437	1.899	1.865	0.325
0.52	0.456	1.673	2.116	0.53
0.576	0.662	1.947	1.956	0.706
0.479	0.603	1.512	2.167	0.536
0.372	0.258	1.865	1.772	0.46
0.438	0.345	2.074	1.607	0.436
0.353	0.292	1.775	1.936	0.385
0.35	0.25	1.953	1.756	0.398
0.096	0.276	1.734	1.507	0.247
0.324	0.359	1.147	1.764	0.617
0.082	0.25	1.075	1.751	0.209
0.389	0.284	1.411	1.287	0.242
0.083	0.177	1.726	0.833	0.382
0.115	0.473	1.794	0.914	0.402
0.275	0.515	1.767	1.961	0.396
0.742	0.672	2.433	1.653	0.97
0.226	0.558	1.77	1.781	0.333
0.914	0.674	1.802	1.892	0.873
0.47	0.322	2.011	1.577	0.481

0.695	0.92	1.449	1.703	0.244
0.086	0.308	1.538	1.073	0.293
0.07	0.561	1.712	1.375	0.233
0.089	0.536	1.624	1.316	0.368
0.154	0.678	1.546	1.618	0.319
0.467	0.355	2.016	1.291	0.475
0.559	0.943	1.041	1.766	0.216
0.361	0.769	0.87	1.838	0.263
0.156	0.252	1.761	1.877	0.35
0.228	0.396	1.725	2.375	0.361
0.419	0.434	1.857	1.783	0.436
0.472	0.43	1.852	1.918	0.425
0.391	0.476	2.196	1.73	0.576
0.036	0.316	1.32	0.894	0.371
0.29	0.324	0.899	1.276	0.2
0.796	0.439	1.629	2.092	0.471
0.375	0.558	1.786	1.785	0.477
0.324	0.341	1.697	2.266	0.349
0.332	0.38	1.824	1.852	0.322
0.153	0.375	1.411	1.229	0.207
0.374	0.486	1.859	1.85	0.322
0.387	0.606	1.78	1.69	0.298
0.616	0.668	1.57	2.086	0.573
0.214	0.399	1.646	2.429	0.337
0.506	0.626	2.206	1.268	0.684
0.524	0.794	1.061	1.624	0.215
0.538	0.633	2.082	1.536	0.722
0.212	0.491	1.805	1.626	0.271
0.275	0.515	1.79	1.975	0.411
0.531	0.286	2.631	1.701	0.555
0.172	0.492	1.793	1.595	0.254
0.083	0.347	1.8	1.047	0.156
0.112	0.329	1.63	1.289	0.254
0.449	0.582	1.954	2.351	0.669
0.697	0.835	1.483	2.082	0.237
0.45	0.675	2.016	1.687	0.612
0.273	0.507	1.695	1.738	0.284
0.187	0.522	1.553	1.757	0.316
0.173	0.261	1.564	1.317	0.26
0.16	0.259	1.306	1.385	0.254
0.112	0.533	1.817	1.499	0.43

0.086	0.285	1.711	1.435	0.347
0.261	0.219	1.589	1.663	0.208
0.474	0.323	1.937	1.953	0.417
0.129	0.283	1.372	0.856	0.326
0.26	0.569	1.78	1.799	0.331
0.32	0.802	1.041	1.742	0.223
0.288	0.401	1.741	1.707	0.29
0.11	0.55	1.743	1.371	0.35
0.655	0.373	1.621	1.575	0.209
0.719	0.236	0.659	1.941	0.443
0.241	0.421	1.611	2.11	0.342
0.352	0.569	1.741	1.688	0.291
0.206	0.475	1.728	1.95	0.284
0.231	0.395	1.603	1.353	0.349
0.137	0.572	1.673	1.175	0.522
0.308	0.415	2.023	2.003	0.324
0.463	0.401	0.745	1.919	0.436
0.534	0.414	2.239	1.547	0.736
0.524	0.387	2.061	1.695	0.595
0.545	0.415	1.993	1.818	0.616
0.475	0.384	1.96	2.13	0.566
0.61	0.656	1.787	1.765	0.32
0.1	0.33	1.564	1.258	0.363
0.104	0.218	1.782	0.967	0.141
0.068	0.254	1.547	0.989	0.351
0.236	0.366	0.979	1.707	0.119
0.221	0.318	0.975	1.588	0.134
0.169	0.234	1.338	1.264	0.182
0.019	0.216	1.38	0.906	0.288
0.164	0.275	1.808	1.354	0.239
0.109	0.35	1.814	1.11	0.225
0.163	0.436	1.358	1.109	0.284
0.355	0.794	1.274	1.829	0.245
0.261	0.329	0.95	1.605	0.194
0.074	0.298	1.68	0.999	0.173
0.105	0.514	1.67	0.922	0.376
0.551	0.307	2.293	1.269	0.589
0.101	0.306	1.84	1.559	0.244
0.424	0.625	1.511	2.018	0.293
0.183	0.525	1.877	1.64	0.279
0.174	0.497	1.774	1.938	0.309

0.237	0.463	1.765	1.907	0.592
0.246	0.24	1.269	1.17	0.176
0.212	0.491	1.713	1.845	0.333
0.275	0.515	1.834	1.906	0.331
0.496	0.437	2.319	1.614	0.667
0.619	0.505	2.603	2.01	0.653
0.585	0.481	2.428	2.186	0.629
0.511	0.574	1.367	2.205	0.648
0.502	0.783	1.191	2.034	0.422
0.212	0.491	1.789	1.737	0.292
0.635	0.692	1.766	1.778	0.328
0.59	0.761	1.459	1.712	0.189
0.524	0.794	1.061	1.624	0.215
0.08	0.547	1.661	1.228	0.474
0.461	0.66	2.069	1.532	0.752
0.129	0.315	1.552	1.597	0.24
0.541	0.501	2.453	1.479	0.696
0.578	0.451	2.5	1.347	0.665
0.53	0.495	2.494	1.461	0.75
0.571	0.446	2.581	1.411	0.707
0.282	0.349	1.542	1.258	0.454
0.65	0.568	1.751	1.641	0.311
0.099	0.766	1.323	1.682	0.18
0.402	0.46	1.594	1.883	0.217
0.462	0.633	1.772	1.735	0.32
0.275	0.515	1.772	2.012	0.408
0.231	0.541	1.845	1.967	0.328
0.153	0.471	1.691	1.515	0.253
0.24	0.44	1.62	1.441	0.225
0.609	0.368	2.407	1.633	0.784
0.516	0.335	1.907	1.906	0.61
0.637	0.429	1.771	1.628	0.29
0.523	0.227	1.282	1.922	0.267
0.74	0.585	1.469	1.77	0.217
0.338	0.686	1.706	1.768	0.292
0.872	0.544	0.643	1.876	0.164
0.081	0.422	1.551	1.582	0.248
0.084	0.388	1.586	1.297	0.335
0.433	0.919	1.232	2.908	0.316
0.093	0.304	1.851	1.008	0.171
0.141	0.433	1.529	1.599	0.285

0.12	0.519	1.367	1.123	0.251
0.343	0.629	1.442	2.021	0.318
0.378	0.595	1.774	1.602	0.321
0.361	0.139	0.2	2.045	0.371
0.441	0.439	2.017	1.712	0.627
0.463	0.424	1.779	2.16	0.424
0.709	0.672	2.039	2.02	0.782
0.611	0.466	1.698	2.21	0.58
0.731	0.567	2.042	2.128	0.761
0.586	0.627	2.179	2.071	0.814
0.393	0.428	1.58	1.885	0.54
0.724	0.707	1.78	2.153	0.609
0.356	0.354	1.994	2.08	0.359
0.142	0.584	1.668	1.216	0.576
0.388	0.586	1.833	1.874	0.311
0.319	0.336	0.898	1.706	0.224
0.345	0.454	1.993	2.025	0.331
0.454	0.558	1.983	1.498	0.656
0.126	0.587	1.763	1.171	0.619
0.623	0.405	1.753	1.54	0.249
0.077	0.432	1.708	1.563	0.438
0.326	0.522	1.748	1.693	0.293
0.596	0.334	1.852	1.716	0.319
0.531	0.31	2.347	1.749	0.468
0.977	0.717	1.701	2.159	0.26
0.386	0.72	1.313	2.235	0.315
0.606	0.205	1.775	1.554	0.244
0.263	0.579	1.872	1.735	0.485
0.307	0.537	1.715	1.984	0.41
0.471	0.713	1.904	2.113	0.561
0.336	0.535	1.783	1.787	0.471
0.236	0.551	1.88	1.645	0.299
0.275	0.515	1.755	1.995	0.402
0.487	0.869	1.096	1.959	0.193
0.275	0.515	1.772	1.989	0.339
0.359	0.371	1.865	1.849	0.334
0.157	0.204	1.695	1.587	0.31
0.299	0.406	1.507	1.308	0.412
0.515	0.625	1.138	2.064	0.389

	Metabolites after MDS using CDK (165) (used for MDS using ADMET)			
D6-In	D6-Subs	T1/2	CL	hERG
0.178	0.273	1.304	1.327	0.256
0.542	0.37	2.276	1.557	0.636
0.492	0.386	1.799	1.375	0.617
0.502	0.317	1.994	2.054	0.477
0.548	0.401	1.96	1.82	0.626
0.142	0.409	1.428	1.608	0.236
0.518	0.704	1.632	1.897	0.518
0.455	0.402	1.927	1.788	0.605
0.446	0.491	1.802	1.713	0.58
0.459	0.602	1.807	1.88	0.533
0.4	0.373	1.7	1.434	0.574
0.562	0.601	1.961	2.146	0.599
0.487	0.351	1.612	1.964	0.42
0.53	0.313	1.867	1.606	0.497
0.552	0.358	2.746	1.363	0.656
0.472	0.428	2.065	1.654	0.653
0.526	0.412	2.277	2.029	0.571
0.322	0.672	1.942	1.986	0.592
0.466	0.34	1.992	1.922	0.486
0.492	0.305	2.46	1.738	0.566
0.452	0.32	2.317	1.616	0.626
0.558	0.356	2.291	1.592	0.524
0.531	0.31	2.347	1.749	0.468
0.474	0.297	2.356	1.741	0.59
0.541	0.37	1.937	1.614	0.445
0.458	0.376	2.124	1.87	0.439
0.519	0.365	2.106	1.864	0.453
0.461	0.254	2.27	1.49	0.606
0.492	0.558	1.993	1.602	0.669
0.446	0.491	1.802	1.713	0.58
0.474	0.696	1.801	2.441	0.428
0.328	0.441	1.563	2.152	0.317
0.142	0.584	1.728	1.203	0.608
0.295	0.339	1.618	1.426	0.2

0.483	0.599	1.864	1.821	0.598
0.523	0.85	1.525	1.65	0.242
0.458	0.487	2.138	1.752	0.607
0.378	0.571	1.872	2.017	0.552
0.502	0.557	1.962	1.868	0.717
0.474	0.696	1.801	2.441	0.428
0.399	0.366	1.643	2.143	0.517
0.491	0.395	1.921	1.891	0.562
0.501	0.371	1.971	2.013	0.408
0.433	0.276	1.75	2.01	0.483
0.462	0.431	2.267	1.676	0.67
0.475	0.386	2.353	1.685	0.708
0.445	0.374	1.87	2.133	0.523
0.447	0.374	2.23	1.919	0.731
0.427	0.326	1.737	2.18	0.548
0.561	0.35	2.452	1.705	0.508
0.471	0.34	2.178	1.867	0.682
0.536	0.368	2.47	1.984	0.447
0.503	0.4	1.929	1.967	0.354
0.517	0.376	2.256	2.23	0.469
0.511	0.423	2.391	1.483	0.66
0.512	0.58	2.525	1.468	0.762
0.384	0.456	1.984	1.936	0.546
0.483	0.416	2.217	1.737	0.646
0.507	0.392	1.664	1.944	0.371
0.511	0.388	2.068	1.705	0.57
0.618	0.583	2.718	1.999	0.687
0.461	0.66	2.069	1.532	0.752
0.368	0.393	1.823	1.075	0.578
0.416	0.529	1.894	1.786	0.702
0.533	0.375	1.984	2.031	0.444
0.451	0.559	1.983	1.563	0.669
0.539	0.563	2.42	1.73	0.694
0.5	0.568	2.208	1.965	0.662
0.644	0.565	2.672	1.842	0.814
0.627	0.483	2.736	1.852	0.647
0.585	0.481	2.428	2.186	0.629
0.619	0.505	2.603	2.01	0.653
0.476	0.513	2.333	2.081	0.554
0.402	0.419	1.885	1.94	0.607
0.4	0.396	2.276	2.077	0.484

0.389	0.447	2.036	2.475	0.382
0.32	0.364	1.578	2.107	0.318
0.686	0.545	2.503	1.902	0.755
0.294	0.605	1.795	2.039	0.331
0.533	0.406	1.865	1.737	0.621
0.602	0.494	2.451	2.169	0.638
0.406	0.57	0.874	1.881	0.241
0.236	0.215	1.725	1.365	0.347
0.436	0.582	2.108	1.938	0.755
0.194	0.466	1.67	2.286	0.345
0.212	0.41	1.553	1.292	0.346
0.202	0.382	1.68	1.255	0.348
0.469	0.354	1.677	2.069	0.408
0.429	0.3	1.704	1.729	0.411
0.462	0.431	2.267	1.676	0.67
0.407	0.403	2.158	1.519	0.697
0.312	0.407	1.524	1.534	0.215
0.32	0.297	1.824	2.195	0.428
0.577	0.772	2.102	1.876	0.822
0.545	0.728	2.082	1.539	0.78
0.577	0.586	2.573	1.853	0.653
0.504	0.359	2.375	1.91	0.625
0.526	0.359	2.792	1.509	0.667
0.537	0.36	2.898	1.456	0.657
0.476	0.313	2.097	1.98	0.467
0.509	0.225	2.613	1.865	0.635
0.482	0.361	2.006	1.938	0.457
0.528	0.335	2.754	1.455	0.645
0.524	0.204	2.775	1.674	0.655
0.383	0.331	2.222	2.007	0.509
0.476	0.313	2.097	1.98	0.467
0.441	0.331	2.143	1.956	0.441
0.466	0.305	2.029	1.968	0.471
0.576	0.662	1.947	1.956	0.706
0.324	0.359	1.147	1.764	0.617
0.082	0.25	1.075	1.751	0.209
0.389	0.284	1.411	1.287	0.242
0.914	0.674	1.802	1.892	0.873
0.695	0.92	1.449	1.703	0.244
0.559	0.943	1.041	1.766	0.216
0.361	0.769	0.87	1.838	0.263

0.156	0.252	1.761	1.877	0.35
0.419	0.434	1.857	1.783	0.436
0.472	0.43	1.852	1.918	0.425
0.391	0.476	2.196	1.73	0.576
0.616	0.668	1.57	2.086	0.573
0.538	0.633	2.082	1.536	0.722
0.531	0.286	2.631	1.701	0.555
0.112	0.329	1.63	1.289	0.254
0.697	0.835	1.483	2.082	0.237
0.45	0.675	2.016	1.687	0.612
0.261	0.219	1.589	1.663	0.208
0.474	0.323	1.937	1.953	0.417
0.32	0.802	1.041	1.742	0.223
0.241	0.421	1.611	2.11	0.342
0.231	0.395	1.603	1.353	0.349
0.137	0.572	1.673	1.175	0.522
0.534	0.414	2.239	1.547	0.736
0.524	0.387	2.061	1.695	0.595
0.545	0.415	1.993	1.818	0.616
0.475	0.384	1.96	2.13	0.566
0.355	0.794	1.274	1.829	0.245
0.424	0.625	1.511	2.018	0.293
0.496	0.437	2.319	1.614	0.667
0.619	0.505	2.603	2.01	0.653
0.585	0.481	2.428	2.186	0.629
0.511	0.574	1.367	2.205	0.648
0.502	0.783	1.191	2.034	0.422
0.08	0.547	1.661	1.228	0.474
0.461	0.66	2.069	1.532	0.752
0.541	0.501	2.453	1.479	0.696
0.53	0.495	2.494	1.461	0.75
0.099	0.766	1.323	1.682	0.18
0.24	0.44	1.62	1.441	0.225
0.609	0.368	2.407	1.633	0.784
0.516	0.335	1.907	1.906	0.61
0.433	0.919	1.232	2.908	0.316
0.441	0.439	2.017	1.712	0.627
0.463	0.424	1.779	2.16	0.424
0.709	0.672	2.039	2.02	0.782
0.611	0.466	1.698	2.21	0.58
0.731	0.567	2.042	2.128	0.761

0.393	0.428	1.58	1.885	0.54
0.724	0.707	1.78	2.153	0.609
0.126	0.587	1.763	1.171	0.619
0.531	0.31	2.347	1.749	0.468
0.977	0.717	1.701	2.159	0.26
0.386	0.72	1.313	2.235	0.315
0.471	0.713	1.904	2.113	0.561
0.157	0.204	1.695	1.587	0.31
	468 Metabolites and positive & negative controls			
H-HT	AMES	Skinsen	LD50	DILI
0.664	0.29	0.286	130	0.08
0.436	0.158	0.494	624	0.148
0.25	0.29	0.38	320	0.124
0.574	0.158	0.392	426	0.076
0.386	0.142	0.469	782	0.094
0.788	0.316	0.34	221	0.514
0.768	0.328	0.433	454	0.124
0.856	0.292	0.363	327	0.39
0.87	0.836	0.534	1018	0.666
0.858	0.232	0.304	820	0.246
0.798	0.144	0.436	410	0.008
0.48	0.396	0.388	191	0.456
0.132	0.236	0.53	619	0.014
0.784	0.242	0.44	377	0.24
0.748	0.31	0.614	1084	0.174
0.54	0.322	0.537	754	0.636
0.58	0.162	0.436	324	0.096
0.626	0.16	0.432	3122	0.162
0.608	0.3	0.522	738	0.646
0.926	0.858	0.459	1143	0.616
0.67	0.238	0.337	167	0.056
0.86	0.3	0.436	397	0.114
0.26	0.286	0.334	256	0.168
0.836	0.216	0.386	495	0.012
0.91	0.208	0.427	581	0.006
0.842	0.126	0.542	407	0.318
0.738	0.148	0.5	962	0.046
0.784	0.242	0.44	377	0.24

0.136	0.158	0.544	1031	0.04
0.896	0.138	0.482	425	0.01
0.312	0.196	0.501	538	0.182
0.86	0.264	0.329	263	0.014
0.886	0.274	0.393	292	0.02
0.744	0.268	0.484	1330	0.492
0.954	0.17	0.464	433	0.32
0.732	0.176	0.575	858	0.226
0.386	0.142	0.469	782	0.094
0.202	0.142	0.469	892	0.094
0.898	0.152	0.489	494	0.292
0.872	0.238	0.515	372	0.076
0.662	0.256	0.54	1708	0.088
0.728	0.322	0.419	447	0.09
0.502	0.366	0.464	480	0.15
0.812	0.166	0.313	299	0.084
0.67	0.308	0.373	313	0.168
0.836	0.24	0.331	464	0.282
0.408	0.146	0.552	773	0.112
0.268	0.166	0.488	1031	0.088
0.092	0.228	0.459	528	0.022
0.494	0.136	0.366	849	0.052
0.95	0.262	0.395	580	0.384
0.324	0.266	0.407	802	0.408
0.624	0.218	0.387	295	0.106
0.256	0.194	0.491	439	0.112
0.692	0.326	0.408	905	0.396
0.478	0.232	0.498	729	0.36
0.418	0.172	0.393	611	0.128
0.654	0.152	0.584	841	0.328
0.416	0.332	0.582	712	0.146
0.32	0.568	0.26	818	0.274
0.838	0.3	0.422	821	0.32
0.914	0.578	0.251	285	0.922
0.176	0.37	0.426	657	0.114
0.198	0.066	0.633	3664	0.044
0.154	0.126	0.558	8358	0.12
0.144	0.066	0.633	3940	0.044
0.138	0.066	0.633	4537	0.044
0.102	0.158	0.544	5368	0.096
0.484	0.266	0.475	1400	0.04

0.304	0.266	0.475	1682	0.04
0.18	0.026	0.684	2688	0.212
0.274	0.102	0.712	3664	0.09
0.804	0.186	0.516	836	0.202
0.132	0.016	0.685	1310	0.286
0.318	0.088	0.408	871	0.204
0.04	0.032	0.58	1169	0.048
0.696	0.228	0.307	10981	0.064
0.114	0.078	0.246	2088	0.15
0.278	0.22	0.364	1305	0.528
0.072	0.198	0.372	1757	0.098
0.166	0.03	0.247	1018	0.264
0.124	0.148	0.38	2217	0.088
0.198	0.498	0.543	2957	0.008
0.118	0.12	0.433	1096	0.098
0.142	0.196	0.377	1507	0.058
0.044	0.256	0.478	732	0.308
0.6	0.266	0.238	1314	0.584
0.322	0.086	0.433	780	0.212
0.32	0.076	0.352	766	0.62
0.25	0.188	0.296	1343	0.016
0.05	0.19	0.353	1674	0.084
0.848	0.09	0.535	679	0.246
0.624	0.824	0.47	143	0.178
0.114	0.652	0.654	5846	0.06
0.3	0.11	0.526	3783	0.128
0.498	0.088	0.565	1468	0.61
0.674	0.002	0.213	642	0.096
0.32	0.02	0.536	4119	0.138
0.444	0.086	0.163	1094	0.216
0.31	0.114	0.591	3375	0.152
0.284	0	0.416	1214	0.178
0.128	0	0.416	3822	0.178
0.178	0.086	0.518	5070	0.112
0.208	0.044	0.431	4600	0.032
0.418	0.114	0.767	917	0.046
0.356	0.004	0.666	1814	0.04
0.502	0.2	0.6	541	0.426
0.352	0.65	0.676	859	0.492
0.134	0.052	0.676	897	0.316
0.306	0.002	0.513	890	0.17

0.604	0.912	0.511	1660	0.26
0.618	0.134	0.671	2788	0.212
0.238	0.078	0.519	2647	0.172
0.25	0.002	0.539	3378	0.166
0.328	0.096	0.573	4235	0.11
0.718	0.116	0.406	498	0.36
0.512	0.218	0.509	2173	0.192
0.172	0.046	0.717	1980	0.29
0.594	0.152	0.558	959	0.162
0.534	0.124	0.634	434	0.404
0.582	0.73	0.565	145	0.33
0.358	1	0.673	1640	0.706
0.558	0.064	0.494	528	0.594
0.13	0.108	0.451	158	0.01
0.246	0.022	0.355	4049	0.162
0.692	0.872	0.643	641	0.28
0.3	0.1	0.525	1378	0.208
0.422	0.438	0.249	316	0.246
0.596	0.246	0.237	2065	0.344
0.586	0.208	0.413	536	0.172
0.43	0.114	0.767	1117	0.046
0.346	0.106	0.405	4573	0.15
0.348	0.06	0.509	4507	0.146
0.208	0.212	0.539	4254	0.122
0.6	0.208	0.441	800	0.342
0.51	0.024	0.636	1733	0.296
0.584	0.102	0.648	1624	0.232
0.186	0.002	0.523	6135	0.154
0.478	0.122	0.712	579	0.422
0.26	0.046	0.416	3471	0.13
0.438	0.438	0.249	64	0.246
0.478	0.32	0.365	2029	0.182
0.664	0.552	0.309	523	0.728
0.866	0.802	0.352	663	0.792
0.884	0.252	0.326	736	0.298
0.654	0.14	0.472	1036	0.228
0.234	0.212	0.549	3701	0.164
0.388	0.15	0.297	2132	0.306
0.628	0.532	0.299	512	0.75
0.488	0.47	0.181	3111	0.956
0.12	0.002	0.523	7980	0.154

0.65	0.176	0.715	534	0.534
0.386	0.084	0.78	862	0.072
0.47	0.32	0.531	488	0.082
0.438	0.516	0.639	261	0.642
0.43	0.206	0.341	269	0.238
0.524	0.284	0.309	329	0.552
0.536	0.152	0.518	2918	0.238
0.714	0.154	0.46	1053	0.228
0.636	0.02	0.755	611	0.492
0.57	0.134	0.455	759	0.24
0.584	0.12	0.323	1482	0.538
0.122	0.274	0.551	3142	0.266
0.37	0.128	0.625	5080	0.378
0.708	0.246	0.52	531	0.258
0.708	0.246	0.52	531	0.258
0.626	0.2	0.378	364	0.384
0.758	0.216	0.308	388	0.296
0.374	0.336	0.269	201	0.656
0.67	0.316	0.323	330	0.674
0.51	0.202	0.345	502	0.244
0.698	0.088	0.538	674	0.25
0.754	0.2	0.422	648	0.218
0.698	0.24	0.35	473	0.52
0.546	0.344	0.275	814	0.406
0.834	0.31	0.282	281	0.69
0.696	0.232	0.399	412	0.238
0.672	0.366	0.287	326	0.578
0.66	0.228	0.32	493	0.508
0.774	0.188	0.421	439	0.276
0.72	0.154	0.406	493	0.308
0.6	0.29	0.492	934	0.282
0.742	0.31	0.416	733	0.494
0.65	0.304	0.448	875	0.254
0.702	0.15	0.403	384	0.298
0.632	0.204	0.338	441	0.178
0.704	0.248	0.381	312	0.27
0.608	0.324	0.311	446	0.282
0.724	0.126	0.416	485	0.296
0.892	0.302	0.304	281	0.31
0.89	0.302	0.304	283	0.31
0.41	0.112	0.618	2006	0.158

0.268	0.214	0.705	551	0.192
0.564	0.066	0.521	3651	0.22
0.066	0.194	0.562	511	0.302
0.066	0.036	0.517	2618	0.194
0.654	0.14	0.472	1036	0.228
0.536	0.152	0.518	2918	0.238
0.642	0.974	0.714	64	0.33
0.572	0.108	0.69	943	0.23
0.158	0.156	0.485	2597	0.25
0.4	0.136	0.735	3460	0.15
0.24	0.216	0.472	4077	0.348
0.252	0.436	0.538	3930	0.266
0.334	0.206	0.341	181	0.238
0.448	0.398	0.321	634	0.198
0.164	0.174	0.551	2651	0.22
0.234	0.072	0.623	4913	0.232
0.154	0.074	0.563	2814	0.3
0.154	0.234	0.555	2597	0.28
0.404	0.08	0.621	1734	0.23
0.172	0.216	0.472	4031	0.348
0.144	0.222	0.582	2241	0.258
0.226	0.172	0.577	4824	0.18
0.432	0.234	0.676	3308	0.156
0.098	0.108	0.734	8866	0.336
0.182	0.1	0.563	2860	0.302
0.478	0.148	0.799	2055	0.358
0.4	0.122	0.735	5050	0.162
0.224	0.012	0.656	3778	0.268
0.236	0.108	0.518	4059	0.324
0.476	0.188	0.348	282	0.234
0.38	0.152	0.615	4368	0.198
0.416	0.086	0.681	2240	0.172
0.232	0.186	0.561	3029	0.176
0.234	0.072	0.623	4913	0.232
0.154	0.074	0.563	2814	0.3
0.866	0.218	0.36	641	0.588
0.7	0.128	0.395	618	0.56
0.736	0.23	0.334	634	0.59
0.684	0.148	0.366	479	0.566
0.374	0.046	0.746	2147	0.142
0.604	0.206	0.523	512	0.43

0.44	0.288	0.443	1505	0.194
0.856	0.362	0.393	539	0.338
0.5	0.368	0.354	424	0.416
0.6	0.212	0.264	859	0.906
0.748	0.168	0.392	2387	0.6
0.83	0.126	0.524	2186	0.572
0.71	0.23	0.352	1489	0.436
0.81	0.23	0.352	1344	0.436
0.192	0.256	0.52	2847	0.28
0.158	0.156	0.485	2597	0.25
0.478	0.078	0.341	790	0.256
0.48	0.016	0.542	611	0.068
0.174	0.008	0.536	2242	0.688
0.834	0.24	0.556	1012	0.05
0.442	0.112	0.687	2469	0.388
0.196	0.018	0.598	1071	0.172
0.308	0.176	0.703	1528	0.422
0.566	0.022	0.588	472	0.082
0.448	0.398	0.321	634	0.198
0.366	0.052	0.648	1423	0.316
0.236	0.016	0.484	4481	0.274
0.172	0.116	0.453	2645	0.254
0.268	0.214	0.38	4543	0.234
0.436	0.06	0.572	1754	0.216
0.394	0.054	0.552	2620	0.132
0.388	0.242	0.32	284	0.314
0.82	0.202	0.52	449	0.296
0.304	0.126	0.752	3010	0.312
0.438	0.076	0.56	4616	0.256
0.318	0.014	0.324	4259	0.336
0.284	0.088	0.5	4040	0.36
0.012	0.3	0.25	314	0.18
0.162	0.42	0.485	405	0.456
0.712	0.292	0.356	337	0.42
0.752	0.318	0.364	158	0.406
0.71	0.258	0.438	419	0.372
0.62	0.306	0.385	323	0.282
0.288	0.014	0.564	2548	0.13
0.362	0.172	0.349	158	0.236
0.318	0.05	0.339	1872	0.172
0.192	0.086	0.691	4151	0.368

0.35	0.156	0.372	242	0.24
0.192	0.256	0.52	2907	0.28
0.242	0.008	0.433	4049	0.278
0.634	0.204	0.31	474	0.298
0.38	0.18	0.474	837	0.354
0.596	0.122	0.534	1385	0.244
0.774	0.278	0.383	457	0.294
0.604	0.164	0.524	1384	0.28
0.808	0.346	0.369	466	0.324
0.352	0.174	0.557	1223	0.222
0.706	0.264	0.343	1010	0.622
0.564	0.172	0.484	1332	0.268
0.54	0.3	0.345	335	0.31
0.46	0.208	0.469	1109	0.308
0.546	0.078	0.537	758	0.282
0.718	0.096	0.418	348	0.374
0.584	0.11	0.56	704	0.316
0.47	0.122	0.57	838	0.368
0.488	0.108	0.541	731	0.308
0.786	0.132	0.402	363	0.398
0.714	0.27	0.364	173	0.372
0.698	0.276	0.363	195	0.344
0.762	0.218	0.441	352	0.34
0.83	0.268	0.291	341	0.7
0.822	0.302	0.409	776	0.566
0.464	0.112	0.618	2195	0.158
0.57	0.134	0.455	759	0.24
0.56	0.112	0.484	873	0.23
0.494	0.158	0.627	1964	0.172
0.418	0.09	0.647	2658	0.25
0.512	0.112	0.618	2143	0.158
0.61	0.112	0.484	946	0.23
0.744	0.254	0.398	493	0.294
0.662	0.206	0.41	376	0.36
0.464	0.112	0.618	2195	0.158
0.56	0.112	0.484	873	0.23
0.648	0.078	0.476	861	0.56
0.62	0.126	0.474	990	0.644
0.724	0.256	0.378	817	0.55
0.81	0.206	0.399	746	0.52
0.73	0.34	0.341	941	0.63

0.75	0.3	0.369	861	0.598
0.81	0.366	0.287	322	0.578
0.668	0.388	0.366	996	0.678
0.57	0.214	0.552	1319	0.29
0.844	0.362	0.393	529	0.338
0.242	0.168	0.546	1507	0.258
0.428	0.23	0.501	773	0.352
0.534	0.368	0.354	422	0.416
0.768	0.322	0.477	908	0.624
0.716	0.28	0.351	408	0.186
0.518	0.304	0.389	886	0.174
0.39	0.396	0.306	402	0.378
0.438	0.362	0.357	479	0.408
0.472	0.34	0.259	521	0.388
0.522	0.312	0.252	587	0.356
0.528	0.37	0.228	720	0.374
0.652	0.232	0.399	432	0.238
0.656	0.21	0.42	514	0.262
0.712	0.296	0.372	845	0.606
0.826	0.22	0.331	397	0.546
0.83	0.268	0.291	341	0.7
0.844	0.22	0.331	413	0.546
0.726	0.12	0.251	36	0.526
0.556	0.208	0.506	1171	0.166
0.362	0.01	0.691	866	0.042
0.466	0.012	0.675	2036	0.46
0.358	0.274	0.322	299	0.606
0.21	0.13	0.568	1956	0.384
0.044	0	0.416	1536	0.178
0.862	0.49	0.32	2495	0.634
0.878	0.25	0.381	790	0.418
0.682	0.044	0.186	678	0.904
0.434	0.046	0.57	2029	0.182
0.208	0.014	0.494	4671	0.204
0.252	0.078	0.549	5005	0.156
0.318	0.112	0.495	3064	0.216
0.138	0.152	0.533	3879	0.158
0.362	0.006	0.84	6270	0.31
0.358	0.006	0.84	6449	0.31
0.626	0.268	0.311	331	0.264
0.704	0.216	0.308	356	0.296

0.38	0.18	0.474	837	0.354
0.668	0.148	0.563	1330	0.178
0.358	0.006	0.55	3597	0.1
0.594	0.024	0.636	1678	0.296
0.732	0.224	0.415	445	0.248
0.684	0.312	0.394	260	0.428
0.294	0.032	0.878	3971	0.286
0.678	0.172	0.499	1905	0.484
0.642	0.17	0.499	1258	0.44
0.796	0.286	0.471	826	0.668
0.208	0.252	0.62	4308	0.186
0.618	0.13	0.526	710	0.236
0.754	0.13	0.526	714	0.236
0.842	0.09	0.535	679	0.246
0.65	0.25	0.386	208	0.288
0.674	0.14	0.525	759	0.282
0.72	0.374	0.362	213	0.398
0.694	0.178	0.468	685	0.322
0.746	0.14	0.525	746	0.282
0.608	0.194	0.563	593	0.334
0.65	0.25	0.386	208	0.288
0.69	0.244	0.387	212	0.31
0.662	0.322	0.37	194	0.316
0.314	0.324	0.499	3805	0.298
0.73	0.22	0.354	616	0.602
0.64	0.148	0.488	1883	0.494
0.58	0.152	0.433	1075	0.272
0.488	0.358	0.339	310	0.546
0.412	0.242	0.324	360	0.492
0.236	0.328	0.31	147	0.61
0.404	0.3	0.329	149	0.588
0.508	0.054	0.579	2109	0.334
0.402	0.064	0.322	6104	0.444
0.388	0.05	0.215	2522	0.434
0.432	0.108	0.635	3482	0.426
0.11	0.156	0.594	621	0.346
0.294	0.118	0.487	1813	0.146
0.068	0	0.484	12598	0.154
0.904	0.19	0.507	725	0.684
0.118	0.652	0.654	6149	0.06
0.15	0.186	0.46	1930	0.1

0.342	0.22	0.322	141	0.256
0.338	0.022	0.792	2084	0.264
0.138	0.102	0.703	4721	0.326
0.124	0.664	0.815	267	0.148
0.08	0.956	0.635	142	0.224
0.622	0.79	0.62	119	0.302
0.452	0.12	0.33	223	0.26
0.164	0.03	0.791	1855	0.246
0.604	0.386	0.518	2520	0.454
0.29	0.004	0.586	3536	0.292
0.394	0.054	0.552	2620	0.132
0.6	0.21	0.452	328	0.262
0.58	0.228	0.425	439	0.232
0.784	0.106	0.441	511	0.254
0.034	0.234	0.542	167	0.294
0.378	0.818	0.501	133	0.418
0.352	0.3	0.47	747	0.194
0.258	0.078	0.549	5400	0.156
0.366	0.074	0.622	1858	0.258
0.258	0.216	0.472	4059	0.348
0.374	0.082	0.675	4350	0.328
0.256	0.268	0.388	4059	0.296
0.416	0.05	0.615	3893	0.178
0.56	0.23	0.408	1570	0.568
0.3	0.176	0.578	1510	0.148
0.67	0.376	0.194	590	0.522
0.124	0.04	0.696	616	0.07
0.618	0.142	0.497	1749	0.426
0.23	0.032	0.878	3017	0.286
0.022	0	0.484	13995	0.154
0.678	0.112	0.505	784	0.14
0.312	0.026	0.759	2671	0.3
0.302	0.038	0.738	5815	0.374
0.218	0	0.807	10054	0.324
0.656	0.122	0.522	1336	0.576
0.326	0.238	0.606	1600	0.108
0.6	0.15	0.418	1288	0.442
0.42	0.138	0.465	2252	0.268
0.412	0.046	0.319	1649	0.228
0.3	0.072	0.565	5727	0.36
0.45	0.07	0.539	835	0.338

0.368	0.044	0.431	1590	0.032
0.556	0.026	0.565	923	0.22
0.418	0.058	0.614	1741	0.262
0.69	0.232	0.389	534	0.266
0.094	0.044	0.657	111	0.22
0.12	0.652	0.654	5405	0.06
0.336	0.094	0.885	1872	0.126
0.466	0.118	0.57	3920	0.284
0.44	0.19	0.481	996	0.238
0.224	1	0.664	582	0.816
0.674	0.686	0.258	645	0.916
0.274	0.282	0.647	3953	0.292
0.424	0.012	0.379	4790	0.274
0.444	0.014	0.687	2507	0.186
0.414	0.028	0.802	8849	0.398
0.068	0.016	0.645	10089	0.338
0.194	0.14	0.402	2440	0.244
0.592	0.74	0.278	737	0.9
0.772	0.12	0.479	846	0.596
0.79	0.124	0.409	518	0.612
0.788	0.24	0.391	367	0.622
0.662	0.42	0.316	471	0.55
0.306	0.03	0.568	3068	0.086
0.588	0.798	0.561	133	0.386
0.478	0.192	0.547	1710	0.452
0.104	0.054	0.602	1806	0.286
0.714	0.236	0.282	1850	0.188
0.59	0.108	0.299	2549	0.526
0.302	0.01	0.621	1259	0.374
0.098	0.116	0.392	1141	0.204
0.328	0.076	0.47	2183	0.268
0.194	0.01	0.81	6457	0.34
0.358	0.848	0.587	70	0.148
0.36	0.736	0.882	2438	0.146
0.792	0.68	0.029	1130	0.164
0.366	0.074	0.729	6593	0.38
0.628	0.864	0.444	1151	0.088
0.18	0.284	0.375	269	0.47
0.274	0.022	0.835	2931	0.28
0.474	0.012	0.613	1261	0.07
0.316	0.054	0.543	3383	0.228

0.372	0.028	0.709	3157	0.158
0.314	0.05	0.707	4625	0.148
0.256	0.192	0.777	434	0.588
0.28	0.032	0.878	3918	0.286
0.122	0	0.484	11043	0.154
0.53	0.108	0.541	703	0.308
0.75	0.3	0.369	861	0.598
0.73	0.34	0.341	941	0.63
0.784	0.352	0.368	1413	0.236
0.856	0.368	0.273	1603	0.254
0.24	0.032	0.878	3531	0.286
0.296	0.36	0.624	2629	0.07
0.288	0.308	0.763	1838	0.096
0.124	0.04	0.696	616	0.07
0.046	0.016	0.645	12161	0.338
0.494	0.158	0.627	1964	0.172
0.544	0.192	0.681	1621	0.208
0.58	0.118	0.472	986	0.34
0.478	0.172	0.453	599	0.306
0.62	0.118	0.472	755	0.34
0.478	0.172	0.453	525	0.306
0.312	0.644	0.269	323	0.656
0.308	0.142	0.65	3724	0.06
0.154	0.102	0.267	1862	0.262
0.57	0.672	0.656	353	0.28
0.308	0.03	0.568	4082	0.086
0.032	0	0.484	14832	0.154
0.1	0.652	0.654	4305	0.06
0.472	0.098	0.732	3390	0.314
0.548	0.038	0.646	2156	0.422
0.802	0.262	0.456	634	0.558
0.788	0.426	0.331	309	0.59
0.344	0.02	0.536	4415	0.138
0.238	0.022	0.758	370	0.084
0.514	0.038	0.511	1472	0.23
0.47	0.174	0.623	347	0.48
0.494	0.08	0.465	2170	0.552
0.496	0.102	0.648	1621	0.232
0.458	0.158	0.776	653	0.284
0.678	0.01	0.691	815	0.042
0.486	0.16	0.549	2633	0.344

0.504	0.118	0.457	174	0.124
0.154	0.072	0.153	2034	0.122
0.412	0.012	0.613	2017	0.07
0.31	0.006	0.584	3963	0.076
0.558	0.74	0.278	699	0.9
0.556	0.284	0.546	1235	0.222
0.714	0.308	0.504	347	0.262
0.706	0.348	0.478	1287	0.524
0.622	0.318	0.361	545	0.574
0.64	0.386	0.422	717	0.522
0.846	0.74	0.427	1044	0.664
0.912	0.538	0.336	468	0.696
0.748	0.344	0.382	1318	0.516
0.546	0.266	0.415	256	0.312
0.176	0.108	0.734	7221	0.336
0.322	0.092	0.286	3526	0.264
0.508	0.076	0.607	687	0.166
0.166	0.132	0.417	2579	0.288
0.486	0.112	0.618	1330	0.158
0.102	0.108	0.734	7271	0.336
0.772	0.634	0.654	2464	0.22
0.086	0.048	0.364	1089	0.048
0.32	0.082	0.461	4269	0.182
0.33	0.038	0.59	2923	0.068
0.65	0.304	0.448	875	0.254
0.256	0.202	0.503	443	0.438
0.19	0.01	0.691	889	0.042
0.162	0.006	0.613	819	0.072
0.194	0.014	0.494	4471	0.204
0.684	0.242	0.422	1636	0.632
0.596	0.17	0.39	2182	0.518
0.252	0.078	0.549	5005	0.156
0.318	0.112	0.495	3064	0.216
0.066	0	0.484	14213	0.154
0.2	0.316	0.716	1661	0.028
0.088	0	0.484	12359	0.154
0.252	0.094	0.42	4240	0.348
0.538	0.068	0.657	1544	0.418
0.356	0.644	0.269	391	0.656
0.752	0.37	0.378	1420	0.284

	Metabolites after MDS using CDK (165) (used for MDS using ADMET)			
H-HT	AMES	Skinsen	LD50	DILI
0.604	0.912	0.511	1660	0.26
0.718	0.116	0.406	498	0.36
0.512	0.218	0.509	2173	0.192
0.586	0.208	0.413	536	0.172
0.6	0.208	0.441	800	0.342
0.584	0.102	0.648	1624	0.232
0.664	0.552	0.309	523	0.728
0.884	0.252	0.326	736	0.298
0.654	0.14	0.472	1036	0.228
0.628	0.532	0.299	512	0.75
0.536	0.152	0.518	2918	0.238
0.584	0.12	0.323	1482	0.538
0.626	0.2	0.378	364	0.384
0.51	0.202	0.345	502	0.244
0.698	0.088	0.538	674	0.25
0.754	0.2	0.422	648	0.218
0.698	0.24	0.35	473	0.52
0.546	0.344	0.275	814	0.406
0.834	0.31	0.282	281	0.69
0.774	0.188	0.421	439	0.276
0.72	0.154	0.406	493	0.308
0.6	0.29	0.492	934	0.282
0.65	0.304	0.448	875	0.254
0.702	0.15	0.403	384	0.298
0.632	0.204	0.338	441	0.178
0.704	0.248	0.381	312	0.27
0.608	0.324	0.311	446	0.282
0.724	0.126	0.416	485	0.296
0.41	0.112	0.618	2006	0.158
0.654	0.14	0.472	1036	0.228
0.448	0.398	0.321	634	0.198
0.432	0.234	0.676	3308	0.156
0.098	0.108	0.734	8866	0.336

0.478	0.148	0.799	2055	0.358
0.684	0.148	0.366	479	0.566
0.374	0.046	0.746	2147	0.142
0.604	0.206	0.523	512	0.43
0.748	0.168	0.392	2387	0.6
0.83	0.126	0.524	2186	0.572
0.448	0.398	0.321	634	0.198
0.712	0.292	0.356	337	0.42
0.71	0.258	0.438	419	0.372
0.62	0.306	0.385	323	0.282
0.634	0.204	0.31	474	0.298
0.38	0.18	0.474	837	0.354
0.596	0.122	0.534	1385	0.244
0.774	0.278	0.383	457	0.294
0.604	0.164	0.524	1384	0.28
0.808	0.346	0.369	466	0.324
0.352	0.174	0.557	1223	0.222
0.706	0.264	0.343	1010	0.622
0.564	0.172	0.484	1332	0.268
0.54	0.3	0.345	335	0.31
0.46	0.208	0.469	1109	0.308
0.546	0.078	0.537	758	0.282
0.584	0.11	0.56	704	0.316
0.47	0.122	0.57	838	0.368
0.488	0.108	0.541	731	0.308
0.698	0.276	0.363	195	0.344
0.762	0.218	0.441	352	0.34
0.822	0.302	0.409	776	0.566
0.494	0.158	0.627	1964	0.172
0.418	0.09	0.647	2658	0.25
0.512	0.112	0.618	2143	0.158
0.744	0.254	0.398	493	0.294
0.464	0.112	0.618	2195	0.158
0.648	0.078	0.476	861	0.56
0.62	0.126	0.474	990	0.644
0.724	0.256	0.378	817	0.55
0.81	0.206	0.399	746	0.52
0.73	0.34	0.341	941	0.63
0.75	0.3	0.369	861	0.598
0.668	0.388	0.366	996	0.678
0.57	0.214	0.552	1319	0.29

0.242	0.168	0.546	1507	0.258
0.428	0.23	0.501	773	0.352
0.534	0.368	0.354	422	0.416
0.768	0.322	0.477	908	0.624
0.528	0.37	0.228	720	0.374
0.656	0.21	0.42	514	0.262
0.712	0.296	0.372	845	0.606
0.726	0.12	0.251	36	0.526
0.21	0.13	0.568	1956	0.384
0.862	0.49	0.32	2495	0.634
0.434	0.046	0.57	2029	0.182
0.362	0.006	0.84	6270	0.31
0.358	0.006	0.84	6449	0.31
0.626	0.268	0.311	331	0.264
0.704	0.216	0.308	356	0.296
0.38	0.18	0.474	837	0.354
0.668	0.148	0.563	1330	0.178
0.594	0.024	0.636	1678	0.296
0.684	0.312	0.394	260	0.428
0.678	0.172	0.499	1905	0.484
0.642	0.17	0.499	1258	0.44
0.796	0.286	0.471	826	0.668
0.618	0.13	0.526	710	0.236
0.754	0.13	0.526	714	0.236
0.842	0.09	0.535	679	0.246
0.65	0.25	0.386	208	0.288
0.674	0.14	0.525	759	0.282
0.72	0.374	0.362	213	0.398
0.694	0.178	0.468	685	0.322
0.746	0.14	0.525	746	0.282
0.608	0.194	0.563	593	0.334
0.65	0.25	0.386	208	0.288
0.69	0.244	0.387	212	0.31
0.662	0.322	0.37	194	0.316
0.64	0.148	0.488	1883	0.494
0.402	0.064	0.322	6104	0.444
0.388	0.05	0.215	2522	0.434
0.432	0.108	0.635	3482	0.426
0.15	0.186	0.46	1930	0.1
0.338	0.022	0.792	2084	0.264
0.164	0.03	0.791	1855	0.246

0.604	0.386	0.518	2520	0.454
0.29	0.004	0.586	3536	0.292
0.6	0.21	0.452	328	0.262
0.58	0.228	0.425	439	0.232
0.784	0.106	0.441	511	0.254
0.56	0.23	0.408	1570	0.568
0.618	0.142	0.497	1749	0.426
0.678	0.112	0.505	784	0.14
0.218	0	0.807	10054	0.324
0.326	0.238	0.606	1600	0.108
0.6	0.15	0.418	1288	0.442
0.418	0.058	0.614	1741	0.262
0.69	0.232	0.389	534	0.266
0.336	0.094	0.885	1872	0.126
0.274	0.282	0.647	3953	0.292
0.414	0.028	0.802	8849	0.398
0.068	0.016	0.645	10089	0.338
0.772	0.12	0.479	846	0.596
0.79	0.124	0.409	518	0.612
0.788	0.24	0.391	367	0.622
0.662	0.42	0.316	471	0.55
0.36	0.736	0.882	2438	0.146
0.474	0.012	0.613	1261	0.07
0.53	0.108	0.541	703	0.308
0.75	0.3	0.369	861	0.598
0.73	0.34	0.341	941	0.63
0.784	0.352	0.368	1413	0.236
0.856	0.368	0.273	1603	0.254
0.046	0.016	0.645	12161	0.338
0.494	0.158	0.627	1964	0.172
0.58	0.118	0.472	986	0.34
0.62	0.118	0.472	755	0.34
0.154	0.102	0.267	1862	0.262
0.548	0.038	0.646	2156	0.422
0.802	0.262	0.456	634	0.558
0.788	0.426	0.331	309	0.59
0.678	0.01	0.691	815	0.042
0.556	0.284	0.546	1235	0.222
0.714	0.308	0.504	347	0.262
0.706	0.348	0.478	1287	0.524
0.622	0.318	0.361	545	0.574

0.64	0.386	0.422	717	0.522
0.912	0.538	0.336	468	0.696
0.748	0.344	0.382	1318	0.516
0.102	0.108	0.734	7271	0.336
0.65	0.304	0.448	875	0.254
0.256	0.202	0.503	443	0.438
0.19	0.01	0.691	889	0.042
0.596	0.17	0.39	2182	0.518
0.538	0.068	0.657	1544	0.418
	468 Metabolites and positive & negative controls			
FDAMDD				
0.202				
0.26				
0.522				
0.536				
0.248				
0.19				
0.16				
0.248				
0.494				
0.28				
0.21				
0.2				
0.102				
0.146				
0.424				
0.676				
0.074				
1				
0.612				
0.44				
0.148				
0.092				
0.276				
0.076				
0.038				
0.434				
0.414				

0.146				
0.822				
0.158				
0.218				
0.11				
0.052				
0.268				
0.444				
0.528				
0.248				
0.148				
0.414				
0.328				
0.276				
0.21				
0.156				
0.464				
0.478				
0.138				
0.192				
0.582				
0.134				
0.576				
0.246				
0.102				
0.254				
0.282				
0.22				
0.47				
0.344				
0.478				
0.324				
0.036				
0.636				
0.5				
0.61				
0.728				
0.752				
0.708				
0.708				
0.754				

0.548				
0.56				
0.84				
0.714				
0.444				
0.984				
0.28				
0.966				
1				
0.844				
0.864				
0.96				
0.978				
0.978				
0.978				
0.856				
0.954				
0.944				
0.224				
0.7				
0.804				
0.974				
0.92				
0.248				
0.918				
0.884				
0.926				
0.968				
0.852				
0.924				
0.98				
0.75				
0.894				
0.894				
0.862				
0.934				
0.76				
0.43				
0.74				
0.846				
0.908				

0.736				
0.742				
0.826				
0.928				
0.906				
0.902				
0.334				
0.602				
0.89				
0.912				
0.768				
0.902				
0.73				
0.738				
0.928				
0.944				
0.824				
0.87				
0.66				
0.688				
0.272				
0.78				
0.884				
0.718				
0.842				
0.48				
0.71				
0.802				
0.932				
0.71				
0.962				
0.704				
0.952				
0.366				
0.486				
0.478				
0.542				
0.554				
0.624				
0.338				
0.454				

0.832				
0.84				
0.746				
0.752				
0.818				
0.276				
0.332				
0.642				
0.542				
0.712				
0.56				
0.536				
0.424				
0.562				
0.55				
0.55				
0.474				
0.506				
0.434				
0.608				
0.422				
0.46				
0.406				
0.514				
0.362				
0.532				
0.456				
0.502				
0.406				
0.338				
0.298				
0.372				
0.442				
0.236				
0.248				
0.404				
0.486				
0.2				
0.314				
0.408				
0.314				

0.594				
0.942				
0.966				
0.998				
0.994				
0.542				
0.642				
0.924				
0.916				
0.416				
0.482				
0.458				
0.418				
0.268				
0.264				
0.392				
0.554				
0.438				
0.434				
0.462				
0.48				
0.422				
0.67				
0.496				
0.734				
0.522				
0.726				
0.568				
0.646				
0.402				
0.326				
0.67				
0.478				
0.698				
0.554				
0.438				
0.484				
0.516				
0.546				
0.512				
0.588				

0.506				
0.478				
0.502				
0.304				
0.684				
0.57				
0.576				
0.508				
0.514				
0.338				
0.416				
0.854				
0.634				
0.924				
0.562				
0.846				
0.938				
0.768				
0.706				
0.264				
0.356				
0.414				
0.3				
0.536				
0.404				
0.548				
0.288				
0.538				
0.396				
0.37				
0.432				
0.362				
0.392				
0.732				
0.484				
0.338				
0.32				
0.236				
0.52				
0.31				
0.976				

0.794				
0.32				
0.308				
0.378				
0.506				
0.4				
0.48				
0.568				
0.476				
0.56				
0.256				
0.42				
0.226				
0.262				
0.218				
0.32				
0.382				
0.326				
0.352				
0.322				
0.366				
0.354				
0.34				
0.318				
0.548				
0.516				
0.572				
0.56				
0.606				
0.554				
0.688				
0.566				
0.6				
0.342				
0.492				
0.572				
0.606				
0.548				
0.534				
0.47				
0.456				

0.496				
0.462				
0.514				
0.5				
0.498				
0.586				
0.326				
0.258				
0.284				
0.326				
0.25				
0.474				
0.504				
0.456				
0.442				
0.494				
0.354				
0.424				
0.364				
0.444				
0.528				
0.548				
0.45				
0.598				
0.43				
0.536				
0.62				
0.382				
0.45				
0.894				
0.53				
0.614				
0.578				
0.532				
0.784				
0.634				
0.676				
0.546				
0.854				
0.76				
0.432				

0.48				
0.4				
0.488				
0.77				
0.714				
0.564				
0.334				
0.834				
0.536				
0.496				
0.56				
0.628				
0.274				
0.274				
0.38				
0.334				
0.25				
0.376				
0.31				
0.25				
0.278				
0.334				
0.298				
0.34				
0.396				
0.566				
0.558				
0.6				
0.378				
0.446				
0.262				
0.3				
0.906				
0.834				
0.83				
0.668				
0.874				
0.942				
0.876				
0.324				
0.806				

0.48				
0.296				
0.562				
0.984				
0.97				
0.926				
0.934				
0.314				
0.608				
0.626				
0.502				
0.548				
0.348				
0.314				
0.342				
0.962				
0.672				
0.5				
0.606				
0.374				
0.432				
0.534				
0.392				
0.718				
0.508				
0.458				
0.522				
0.926				
0.496				
0.834				
0.876				
0.274				
0.906				
0.9				
0.878				
0.726				
0.732				
0.52				
0.83				
0.924				
0.51				

0.504				
0.978				
0.926				
0.892				
0.358				
0.918				
0.758				
0.626				
0.548				
0.874				
0.842				
0.682				
0.548				
0.41				
0.82				
0.804				
0.73				
0.39				
0.576				
0.376				
0.326				
0.36				
0.396				
0.736				
0.884				
0.928				
0.948				
0.844				
0.822				
0.842				
0.976				
0.766				
0.84				
0.888				
0.664				
0.88				
0.902				
0.842				
0.304				
0.838				
0.692				

0.8				
0.774				
0.806				
0.748				
0.834				
0.876				
0.332				
0.462				
0.496				
0.712				
0.552				
0.834				
0.816				
0.93				
0.926				
0.808				
0.554				
0.906				
0.324				
0.368				
0.326				
0.372				
0.548				
0.894				
0.72				
0.924				
0.754				
0.876				
0.784				
0.918				
0.35				
0.25				
0.294				
0.896				
0.938				
0.754				
0.786				
0.664				
0.942				
0.922				
0.762				

0.94				
0.974				
0.966				
0.754				
0.932				
0.586				
0.378				
0.452				
0.426				
0.414				
0.398				
0.464				
0.438				
0.494				
0.344				
0.734				
0.586				
0.694				
0.362				
0.564				
0.78				
0.786				
0.95				
0.71				
0.636				
0.236				
0.284				
0.71				
0.864				
0.67				
0.532				
0.57				
0.634				
0.676				
0.876				
0.774				
0.876				
0.334				
0.648				
0.59				
0.594				

	Metabolites after MDS using CDK (165) (used for MDS using ADMET)			
FDAMDD				
0.742				
0.334				
0.602				
0.272				
0.48				
0.802				
0.366				
0.478				
0.542				
0.338				
0.642				
0.536				
0.474				
0.422				
0.46				
0.406				
0.514				
0.362				
0.532				
0.338				
0.298				
0.372				
0.236				
0.248				
0.404				
0.486				
0.2				
0.314				
0.594				
0.542				
0.264				
0.496				

0.734				
0.726				
0.512				
0.588				
0.506				
0.57				
0.576				
0.264				
0.484				
0.32				
0.236				
0.506				
0.4				
0.48				
0.568				
0.476				
0.56				
0.256				
0.42				
0.226				
0.262				
0.218				
0.32				
0.326				
0.352				
0.322				
0.34				
0.318				
0.516				
0.554				
0.688				
0.566				
0.342				
0.572				
0.548				
0.534				
0.47				
0.456				
0.496				
0.462				
0.5				

0.498				
0.326				
0.258				
0.284				
0.326				
0.354				
0.364				
0.444				
0.598				
0.45				
0.53				
0.532				
0.854				
0.76				
0.432				
0.48				
0.4				
0.488				
0.714				
0.334				
0.536				
0.496				
0.56				
0.274				
0.274				
0.38				
0.334				
0.25				
0.376				
0.31				
0.25				
0.278				
0.334				
0.298				
0.34				
0.558				
0.834				
0.83				
0.668				
0.48				
0.562				

0.608				
0.626				
0.502				
0.348				
0.314				
0.342				
0.508				
0.496				
0.274				
0.878				
0.732				
0.52				
0.892				
0.358				
0.626				
0.548				
0.804				
0.73				
0.376				
0.326				
0.36				
0.396				
0.664				
0.692				
0.332				
0.462				
0.496				
0.712				
0.552				
0.808				
0.554				
0.324				
0.326				
0.72				
0.35				
0.25				
0.294				
0.762				
0.378				
0.452				
0.426				

0.414				
0.398				
0.438				
0.494				
0.78				
0.236				
0.284				
0.71				
0.57				
0.648				