

Supplementary Material II. 579 candidate carcinogenic chemicals, their betweenness and p-values of randomization test

Chemical ID	Chemical name	Betweenness	P-value of randomization test
CID000000004	aminopropanol	1805	<0.001
CID000000215	aminoacetone	14	<0.001
CID000000280	carbon dioxide	9609	<0.001
CID000000312	chloride	35389	<0.001
CID000000880	methylglyoxal	2997	<0.001
CID000000977	oxygen	77338	<0.001
CID000001673	3-methyladenine	1841	<0.001
CID000002236	aristolochic acid	5	<0.001
CID000002578	BCNU	14	<0.001
CID000002969	decanoate	1645	<0.001
CID000003031	dichlobenil	29	<0.001
CID000003657	hydroxyurea	2437	<0.001
CID000005799	triethylenemelamine	4	<0.001
CID000005993	chlordane	13	<0.001
CID000006113	ethyl methanesulfonate	31	<0.001
CID000006163	ethyl sulfate	1	<0.001
CID000006234	D-cycloserine	406	<0.001
CID000006782	DiBP	7	<0.001

CID000006913	mesidine	12	<0.001
CID000007000	o-anisidine	26	<0.001
CID000007242	o-toluidine	5	<0.001
CID000007251	Fast Red TR	3	<0.001
CID000007252	p-toluenediamine	19	<0.001
CID000007281	dibromopropanol	52	<0.001
CID000007411	chlorobenzal	17	<0.001
CID000007570	pMDI	6	<0.001
CID000007577	DAPM	105	<0.001
CID000007636	2-ethylhexyl acrylate	1	<0.001
CID000007697	p-chlorophenyl	7	<0.001
CID000008266	chlorendic acid	180	<0.001
CID000008299	acetol	3060	<0.001
CID000008413	o-tolidine	45	<0.001
CID000009718	benzenediazonium	14	<0.001
CID000009731	4-fluoroaniline	16	<0.001
CID000010317	chrysoidine	11	<0.001
CID000010686	trimethylbenzene	3	<0.001
CID000011137	3-nitrophenol	9	<0.001
CID000011369	2,6-diethylaniline	3	<0.001
CID000011473	nitrosobenzene	1	<0.001

CID000011767	9-nitroanthracene	26	<0.001
CID000011865	nitrofurran	40	<0.001
CID000011942	N,N'-diacetylbenzidine	3	<0.001
CID000011975	2,4-diaminoanisole	141	<0.001
CID000012254	polyurethane	53	<0.001
CID000012433	dibromoacetic acid	28	<0.001
CID000015032	pregnenolone-16 alpha-carbonitrile	17	<0.001
CID000015374	SDEH	13	<0.001
CID000020527	N-hydroxy-AABP	9	<0.001
CID000023741	1,2-epoxyhexadecane	3	<0.001
CID000024472	chloroethylene oxide	231	<0.001
CID000025811	NSAR	5	<0.001
CID000026541	dibenzo-18-crown-6	2	<0.001
CID000030086	7-nitrobenz(a)anthracene	1	<0.001
CID000031072	carbimazole	2	<0.001
CID000031170	indium phosphide	24	<0.001
CID000039184	1,6-dinitropyrene	24	<0.001
CID000042128	PeCDF	20	<0.001
CID000053230	1,3-dinitropyrene	4	<0.001
CID000061503	D-lactate	2983	<0.001
CID000062244	MeA alpha C	14	<0.001

CID000074128	2-NA	1	<0.001
CID000108009	2-hydroxyethylmercapturic acid	1	<0.001
CID000108081	methylnitrosamine	5	<0.001
CID000135538	4-hydroxymethylphenylhydrazine	38	<0.001
CID000255968	benzarone	1	<0.001
CID000439516	agaritine	9	<0.001
CID000441093	gamma-pentachlorocyclohexene	29	<0.001
CID000638186	trans-1,2-dichloroethylene	7	<0.001
CID003034368	mancozeb	32	<0.001
CID003344847	acid orange 3	4	<0.001
CID003392731	GW7647	5	<0.001
CID005284370	clivorine	2	<0.001
CID005360001	4HAQO	3	<0.001
CID006003770	Dipentum	1	<0.001
CID006433211	3-(5-nitro-2-furyl)acrylamide	39	<0.001
CID000000602	alanine	608	0.001
CID000005215	sulfadiazine	1	0.001
CID000006194	uracil mustard	5	0.001
CID000007250	2,4-dimethylaniline	13	0.001
CID000007293	dimethylurea	5	0.001
CID000007515	N-methylaniline	2	0.001

CID000011392	2-nitronaphthalene	7	0.001
CID000013597	N-methylpyridinium	4	0.001
CID000018209	T 90	1	0.001
CID000062369	degranol	2	0.001
CID000094989	9-OHNF	1	0.001
CID000107795	miserotoxin	1	0.001
CID000114881	queuine	607	0.001
CID000259329	estramustine phosphate	1	0.001
CID005359467	Orange I	5	0.001
CID023724599	myxocoxanthin	1171	0.001
CID000000950	N,N-dimethylaniline-N-oxide	2	0.002
CID000008182	dodecane	1	0.002
CID000010198	retronecine	15	0.002
CID000010701	2-nitroimidazole	1	0.002
CID000044374	6-nitrobenzo(a)pyrene	4	0.002
CID003032571	propineb	10	0.002
CID000000998	phenylacetaldehyde	9	0.003
CID000001017	phthalic acid	3332	0.003
CID000008507	patent blue	7	0.003
CID000008749	NDMA	10	0.003
CID000024971	4-nitrosobiphenyl	1	0.003

CID000091687	anilofos	8	0.003
CID005281754	symphytine	14	0.003
CID000000597	cytosine	3364	0.004
CID000005819	thyroxine	2192	0.004
CID000006093	niridazole	10	0.004
CID000006947	nitrophenol	1	0.004
CID000007289	1,3-DCP	3	0.004
CID000105079	N-hydroxy-IQ	2	0.004
CID005280970	cis-DCP	2	0.004
CID005372015	D Yellow 3	607	0.004
CID005473513	Ponceau 3R	608	0.004
CID000014814	V2O5	1	0.005
CID000440399	toluene cis-dihydrodiol	1046	0.005
CID001549007	terbinafine	3	0.005
CID005281407	olivacine	1	0.005
CID000000674	dimethylamine	953	0.006
CID000006348	carbon disulfide	1	0.006
CID000007237	o-xylene	1	0.006
CID023724459	UDP-D-xylose	821	0.006
CID000000943	nitrate	4658	0.007
CID000003162	doxylamine	3	0.007

CID000004649	APAs	5	0.007
CID000007259	2,5-xylidine	1098	0.007
CID000008330	TCNB	2	0.007
CID000029393	oryzalin	4	0.007
CID000047650	pCB123	1	0.007
CID000000034	2-chloroethanol	1703	0.008
CID000007947	mesitylene	3	0.008
CID000023977	cobalt	2180	0.008
CID000024529	nitrite	4234	0.008
CID000071616	voriconazole	1	0.008
CID000002997	nordiazepam	5	0.009
CID000031186	3,9-dinitrofluoranthene	1	0.009
CID011375554	zymosan	1502	0.009
CID000006824	yellow AB	2	0.01
CID005353562	dacarbazine	607	0.01
CID006433205	methylazoxymethanol	1632	0.01
CID000004139	methylene blue	1042	0.011
CID000005789	thymidine	841	0.011
CID000007810	p-chlorotoluene	2	0.011
CID000011719	methylurea	5	0.011
CID000007339	phosphoribosylpyrophosphate	3906	0.012

CID000039185	1,8-dinitropyrene	2	0.012
CID016683012	sodium stibogluconate	1	0.012
CID000006805	Fenac	1	0.013
CID000006503	tris	3965	0.014
CID000008289	triphenyl phosphate	11	0.014
CID005381226	rifampicin	607	0.014
CID000005196	semicarbazide	1184	0.015
CID000007522	2-cyanopyridine	1	0.015
CID000007799	ethyl octanoate	1	0.015
CID003032296	zineb	4	0.015
CID000000713	formamide	1153	0.016
CID000007412	benzoyl chloride	1	0.016
CID000004539	norfloxacin	1	0.017
CID000006134	lactose	985	0.017
CID000010461	sulfur mustard	1	0.017
CID000439520	bile salt	1	0.017
CID000010214	3'-phosphoadenosine 5'-phosphosulfate	3378	0.018
CID000064139	efavirenz	1	0.018
CID000013711	deoxycytidine	608	0.019
CID000016553	hydroxyatrazine	610	0.019
CID000011828	N-hydroxy-1-naphthylamine	3	0.02

CID000007956	cyanuric acid	6	0.021
CID000011123	2,4-DCA	1	0.021
CID000644109	palmitoyl-CoA	1444	0.024
CID000005543	triallate	1	0.025
CID000443040	imide	2	0.025
CID023690938	piroxicam	1	0.025
CID027885548	tetracycline	1675	0.025
CID000041381	ethalfluralin	1	0.026
CID005743740	orange G	1	0.026
CID000004944	propoxur	609	0.027
CID000008663	2-naphthol	757	0.027
CID005283731	25-hydroxyvitamin D	605	0.027
CID000007262	2,5-DCA	3	0.031
CID000006753	musk ambrette	1	0.032
CID000011768	Acid Brown	2	0.032
CID000066587	2-dibenzofuranol	2	0.032
CID002723601	6-thioguanine	605	0.034
CID005284648	3'-hydroxydaidzein	604	0.034
CID000081261	N-hydroxy-4-aminobiphenyl	113	0.036
CID000104940	O-methylsterigmatocystin	606	0.036
CID005323714	furazolidone	1	0.036

CID005371578	SImax	1	0.036
CID000000764	guanine	1180	0.037
CID000023994	zinc	29022	0.037
CID000002541	candesartan	588	0.039
CID000006971	N-acetylanthranilate	1	0.039
CID000006844	1H-n	957	0.04
CID000441336	mometasone furoate	1176	0.04
CID000004506	nitrazepam	1	0.041
CID000013195	4-methylimidazole	587	0.041
CID000006377	propylene imine	1	0.042
CID000004908	primaquine	2	0.043
CID000006325	ethylene	651	0.043
CID000024841	iodide	2147	0.043
CID000193305	glutamyl group	572	0.044
CID000009115	coronene	9	0.045
CID000007518	phenylhydroxylamine	1062	0.046
CID000008578	yellow OB	4	0.046
CID000115287	methyldiazonium ion	4	0.046
CID000000013	1,2,4-trichlorobenzene	1146	0.047
CID000003110	dipyrrone	524	0.047
CID000008076	EGEE	601	0.047

CID000091532	AMP-PCP	602	0.047
CID000165331	C-S-S	488	0.047
CID000160647	DAHP	586	0.048
CID006328134	fosetyl	2	0.048
CID000000190	adenine	6435	0.049
CID000003675	phenelzine	8	0.049
CID000006884	2,4,6-trichloroanisole	573	0.049
CID000000180	acetone	47	0.05
CID000005955	4NQO	30	0.05
CID000007485	p-nitroanisole	1	0.05
CID000643833	dichloroethene	150	0.05
CID054675779	oxytetracycline	520	0.05
CID000006051	4-aminoazobenzene	4	0.051
CID000011937	2-aminoanthracene	86	0.051
CID000017514	OOEt	575	0.051
CID000002901	cycloleucine	496	0.052
CID000062302	tartrazine	4	0.052
CID000000038	ketopantoate	42	0.053
CID000001322	1,2-dimethylhydrazine	531	0.053
CID000002770	cDDP	546	0.053
CID000000670	dihydroxyacetone	535	0.054

CID000005323	sulfadimethoxine	3	0.054
CID000006230	norethisterone	50	0.054
CID000007533	cyclamate	496	0.054
CID000011914	R)-mandelate	601	0.054
CID000014798	NaOH	8	0.054
CID000005198	methyl-CCNU	498	0.055
CID000013804	CDP-choline	581	0.055
CID005281857	geroquinol	1	0.055
CID000033500	profluralin	1	0.056
CID000020393	MEHP	168	0.057
CID000440980	6-CHQ	1	0.057
CID000009128	B(e)P	2	0.058
CID000011294	malachite green	590	0.058
CID000021700	beclomethasone dipropionate	582	0.058
CID000442651	nitramine	1	0.058
CID005280971	beta- chloroacrolein	1	0.058
CID005360531	Reactive Black 5	16	0.058
CID000088366	dich	2	0.059
CID005283204	11,12-EET	603	0.059
CID000003289	ethoprop	2	0.06
CID000061898	dodemorph	1	0.061

CID000024121	6-nitrochrysene	2	0.062
CID000041867	epirubicin	32	0.062
CID000007114	4-nitrobiphenyl	7	0.063
CID000011638	CH3F	602	0.063
CID000024502	potassium dichromate	1	0.063
CID000034526	pirimiphos-methyl	3	0.063
CID000000254	2,3-dihydroxybiphenyl	18	0.064
CID000018617	dibromoacetonitrile	1	0.064
CID000002078	alachlor	5	0.066
CID000037786	BP-4,5-oxide	3	0.066
CID000444865	equilenin	1054	0.066
CID000009750	citrulline	953	0.067
CID000008227	MGK-264	1	0.068
CID000031423	pyrene	1066	0.068
CID000121991	nicotinate mononucleotide	1098	0.069
CID000068161	piperidine	1	0.07
CID000036159	PBDE	2	0.073
CID005354198	Cl-930	1	0.073
CID003084169	phosphonic acid	168	0.074
CID000003030	dicamba	4	0.077
CID000000239	beta-alanine	912	0.078

CID000001489	2,4-DB	1	0.079
CID000010039	carbonyl sulfide	603	0.081
CID000013462	3-nitrofluoranthene	3	0.081
CID000000402	sulfur	3825	0.083
CID000006213	methyl sulfone	1	0.083
CID000440104	DH-R	457	0.083
CID005280389	sterigmatocystin	1496	0.083
CID000638124	trans-3-chloroacrylic acid	1	0.085
CID000003102	benzophenone	3	0.087
CID000076292	3-methylguanine	467	0.087
CID000638015	11-cis-retinal	13	0.087
CID000007047	quinoline	1733	0.089
CID000001986	acetazolamide	506	0.093
CID000005798	benzimidazole	585	0.093
CID000124886	Glutathione	2280	0.093
CID000000170	dihydropteroate	24	0.094
CID000000438	4-hydroxy-4-(3-pyridyl)butyric acid	586	0.094
CID000009727	N-methyltyramine	517	0.094
CID000036980	PCB 9	1	0.094
CID000000340	3-methylcatechol	4	0.096
CID054671203	doxycycline	518	0.096

CID005281168	E)-2-hexenal	574	0.097
CID000439616	S)-mandelate	10	0.099
CID000007871	MF I	575	0.1
CID000006050	tributylin	562	0.101
CID000012463	tetrachlorobenzene	1	0.102
CID005483506	Ponceau 4R	2	0.103
CID000000611	glutamate	1618	0.104
CID000351795	indole-3-acetonitrile	9	0.104
CID000003469	2,5-dihydroxybenzoic acid	494	0.105
CID000008987	diethyldithiocarbamate	542	0.105
CID000104996	GTX5	1	0.106
CID000441401	linezolid	1	0.106
CID000004212	mitoxantrone	6	0.109
CID000066603	tetrachlorohydroquinone	2	0.111
CID000008418	anthracene	363	0.112
CID000039230	bifenox	1	0.112
CID000007040	toluene diisocyanate	35	0.113
CID000092851	D-cysteine	485	0.113
CID000005920	triiodothyronine	7	0.114
CID000006032	kanamycin	1	0.114
CID000020848	nitralin	1	0.116

CID000008419	veratraldehyde	1	0.117
CID000005800	2-AF	8	0.12
CID000443239	DL-THA	592	0.12
CID005355863	mevinphos	1	0.121
CID000006076	cyclic AMP	1180	0.122
CID000003339	fenofibrate	562	0.123
CID000019427	5-methylchrysene	1	0.124
CID009543161	2-chloromaleylacetate	1	0.124
CID000006327	methyl chloride	565	0.126
CID000006336	myclobutanil	1	0.128
CID005283205	14,15-EET	588	0.128
CID000005253	sotalol	1	0.129
CID000140765	furanone	1	0.13
CID000101399	N-formylanthranilate	582	0.135
CID000439788	N-formylkynurenine	6	0.135
CID000442514	hematoxylin	33	0.135
CID011150163	mefenoxam	1	0.139
CID000000276	carbamate	1754	0.14
CID000006618	tetrabromobisphenol A	1	0.14
CID000014017	aminophosphonates	364	0.14
CID000000890	phytate	529	0.141

CID000008629	UDP-glucose	904	0.143
CID005280878	LTD4	599	0.143
CID000439251	pantoate	42	0.144
CID000094140	stearoyl-CoA	604	0.146
CID000054687	pravastatin	5	0.148
CID000013930	heptachlor epoxide	2	0.15
CID000003634	hycanthone	1	0.152
CID000018177	dichloroacetonitrile	3	0.152
CID005280625	2-aminomuconic semialdehyde	1	0.152
CID000008947	monomethylarsonic acid	606	0.153
CID005315892	cinnamyl alcohol	450	0.154
CID000007809	p-xylene	599	0.155
CID000024316	cyclic GMP	594	0.155
CID000063090	PCB 126	3	0.156
CID000000700	monoethanolamine	459	0.157
CID000006029	uridine	328	0.161
CID000445354	retinol	18	0.162
CID000005870	estrone	1341	0.163
CID005280421	2'-carboxybenzalpyruvate	2	0.163
CID005460887	S-(2-hydroxyethyl)glutathione	496	0.164
CID000071077	D-serine	4	0.171

CID005280795	vitamin D3	5	0.172
CID000099456	2,5-dihydroxypyridine	2	0.174
CID000000175	acetate	624	0.176
CID000006175	cytidine	598	0.176
CID000440623	2-hydroxyestrone	216	0.178
CID000023931	mercury	608	0.179
CID000023736	DMSP	577	0.181
CID000000437	3-succinoylpyridine	372	0.184
CID000001175	uric acid	605	0.184
CID000439196	dithiothreitol	2	0.184
CID005280453	1,25(OH)2D3	600	0.184
CID000002764	ciprofloxacin	6	0.186
CID000012968	EPTC	2	0.186
CID000009477	agritox	1	0.187
CID000008871	pyridone	608	0.189
CID000055245	mifepristone	50	0.189
CID000439743	3-dehydroecdysone	606	0.19
CID000035823	PCB 118	2	0.191
CID000439155	AdoHcy	8675	0.191
CID000004687	paraxanthine	4	0.193
CID000007410	acetophenone	1196	0.196

CID000016559	lenacil	1	0.197
CID000073614	indicine	545	0.197
CID005364079	cymoxanil	1	0.197
CID000003562	halothane	1161	0.2
CID000021387	1-hydroxypyrene	6	0.2
CID000006031	uridine diphosphate	3535	0.201
CID000439236	ribose 1-phosphate	6	0.202
CID000002156	amiodarone	3	0.207
CID000002082	albendazole	603	0.21
CID000002165	amodiaquine	544	0.211
CID000029746	geosmin	571	0.211
CID000005951	L-serine	119	0.213
CID000000768	cyanide	993	0.219
CID000001068	dimethyl sulfide	1	0.219
CID000010168	rhein	2	0.219
CID000005997	cholesterol	2803	0.225
CID000159296	A3P5P	2117	0.226
CID000000527	propionaldehyde	397	0.227
CID000000138	delta-aminovaleric acid	1	0.228
CID000006049	EDTA	270	0.232
CID000006057	tyrosine	559	0.233

CID000091650	pyrimethanil	5	0.237
CID003001028	Oestrogen	523	0.238
CID000005578	trimethoprim	588	0.239
CID000001099	sulfite	1041	0.241
CID000003779	isoproterenol	580	0.244
CID000002879	p-cresol	577	0.249
CID000002912	cypermethrin	4	0.254
CID000000978	p-aminobenzoic acid	1598	0.255
CID000005610	tyramine	1093	0.26
CID006400657	nocardicin A	490	0.26
CID000439423	7-dehydrocholesterol	5	0.264
CID000000790	hypoxanthine	581	0.269
CID000005564	triclosan	571	0.273
CID000010442	1,3-propanediol	592	0.275
CID000000264	butyrate	562	0.277
CID003081439	arachidoyl-CoA	1	0.279
CID000006341	ethanamine	576	0.28
CID000441276	paclitaxel	1	0.28
CID000037034	PCB 153	6	0.282
CID000246983	lanosterol	608	0.282
CID000005954	1,2-benzanthracene	2	0.286

CID000024341	HOCl	576	0.288
CID000003954	loperamide	525	0.289
CID000006734	acenaphthene	1	0.294
CID000000781	thiocyanate	975	0.295
CID000066414	2-methoxyestradiol	390	0.298
CID016667385	germacradienol	2	0.299
CID000004933	propanil	1	0.3
CID000439162	alpha-glycerophosphate	336	0.304
CID000013109	levonorgestrel	556	0.305
CID000005665	vigabatrin	594	0.306
CID000006613	pantothenic acid	579	0.306
CID000000586	creatine	608	0.307
CID000002230	arecoline	1	0.307
CID000001567	2-mercaptoethanol	76	0.311
CID000006262	ornithine	572	0.312
CID000055717	disoxaril	1	0.314
CID000001188	xanthine	848	0.315
CID000000887	methanol	2094	0.316
CID000005281	stearic acid	603	0.319
CID005281969	anandamide	607	0.32
CID005359596	arsenic	1	0.325

CID000029216	methabenzthiazuron	1	0.326
CID000187790	deoxyguanosine	2	0.326
CID000001993	methacholine	13	0.33
CID000439551	gibberellin	575	0.33
CID000000338	salicylate	1097	0.331
CID000023930	manganese	1261	0.338
CID000091634	azocyclotin	1	0.339
CID000022880	NMDA	571	0.344
CID000005852	D-penicillamine	598	0.345
CID000023932	molybdenum	600	0.346
CID005281877	glucuronide	1	0.348
CID000002554	carbamazepine	6	0.351
CID000010467	arachidic acid	591	0.351
CID000025429	carbendazim	1	0.353
CID000006038	quinolone	599	0.354
CID000010207	aloe-emodin	5	0.354
CID005280493	LTC4	4	0.385
CID000003007	amphetamine	11	0.388
CID000039676	vinclozolin	1	0.393
CID000027375	chlorotoluron	1	0.396
CID000000980	4-nitrophenol	2205	0.398

CID000006853	fluorene	3	0.399
CID000006128	androstenedione	1172	0.408
CID000009171	chrysene	10	0.41
CID000000259	bromide	84	0.411
CID000124062	rubiadin	1	0.411
CID000005154	sanguinarine	489	0.414
CID000439357	Gal alpha	6	0.416
CID000000679	DMSO	1211	0.422
CID000392622	ritonavir	551	0.432
CID000040326	permethrin	32	0.433
CID000001028	prephenate	3	0.443
CID000003559	haloperidol	1	0.448
CID000072307	sesamin	2	0.45
CID000000813	potassium	593	0.465
CID005280360	PGE2	605	0.468
CID000024139	chitin	1478	0.478
CID000005815	epinephrine	22	0.481
CID000013945	dCMP	8	0.481
CID000028486	lithium	372	0.484
CID000000795	imidazole	602	0.5
CID000005793	glucose	1192	0.501

CID005459802	dopachrome	551	0.506
CID000006249	ampicillin	601	0.513
CID000000568	dibenzofurans	549	0.516
CID000122357	erythrose 4-phosphate	586	0.518
CID000638014	beta-ionone	553	0.528
CID000000846	kynurenine	6	0.53
CID000000995	phenanthrene	5	0.532
CID000004189	miconazole	559	0.537
CID000003496	glyphosate	192	0.538
CID000009395	paraoxon	572	0.538
CID000011442	pyrethrin	1	0.539
CID000029732	oxadiazon	1	0.544
CID000637542	p-coumaric acid	608	0.545
CID000010413	hydroxybutyrate	561	0.546
CID000005962	lysine	4215	0.547
CID002724385	digoxin	1	0.548
CID005353758	methomyl	2	0.561
CID000121947	shikimate 3-phosphate	192	0.565
CID000001001	phenylethylamine	20	0.573
CID000006199	psoralen	596	0.588
CID000065063	dUMP	597	0.588

CID000000767	bicarbonate	2454	0.591
CID000000126	p-hydroxybenzaldehyde	1	0.593
CID000031200	fenitrothion	1	0.622
CID000172197	angiotensin II	1	0.623
CID000005961	glutamine	402	0.628
CID000000801	auxin	546	0.632
CID000643976	flavin mononucleotide	199	0.634
CID000439353	galactose	501	0.642
CID000030323	anthracycline	601	0.66
CID000008955	pregnenolone	38	0.663
CID000001032	propionate	566	0.666
CID000010238	adenosine 5'-phosphosulfate	8	0.67
CID000005839	aldosterone	587	0.676
CID000441199	cefoxitin	6	0.679
CID000071080	D-alanine	405	0.681
CID000001117	sulfate	27	0.688
CID000001003	phosphate	4503	0.693
CID000006167	colchicine	554	0.714
CID000000305	choline	572	0.721
CID000005994	progesterone	166	0.722
CID000001112	succinic semialdehyde	561	0.726

CID000011005	myristate	3	0.746
CID000006274	histidine	29	0.758
CID000444539	cinnamic acid	1	0.76
CID000006083	adenosine monophosphate	3230	0.773
CID000221493	cholic acid	1852	0.778
CID000023978	copper	509	0.78
CID000005950	L-alanine	437	0.786
CID000008742	shikimic acid	2	0.803
CID000098792	dihydrofolate	242	0.804
CID000000923	sodium	7595	0.806
CID000446925	lycopene	4	0.807
CID000005753	corticosterone	587	0.809
CID000006030	uridylate	223	0.813
CID000000970	oxaloacetate	150	0.816
CID000001005	phosphoenolpyruvate	767	0.817
CID000000961	hydroxyl radicals	22074	0.819
CID000006022	adenosine diphosphate	4872	0.82
CID000000119	gamma-aminobutyric acid	603	0.824
CID000005884	NADPH2	1550	0.826
CID000001060	pyruvic acid	550	0.838
CID000034755	S-adenosylmethionine	602	0.857

CID000012039	chorismate	4	0.867
CID000000985	palmitate	1442	0.878
CID000444899	arachidonic acid	2100	0.896
CID000009700	poly(dT	304	0.897
CID000000222	ammonia	1495	0.901
CID000006804	5'-GMP	1	0.906
CID000006047	levodopa	551	0.914
CID000000774	histamine	1239	0.916
CID000638072	squalene	607	0.919
CID000005892	beta-NAD	7673	0.926
CID000439153	reduced nicotinamide adenine dinucleotide	394	0.926
CID000000271	calcium	31231	0.96
CID000001132	thiamine pyrophosphate	8	0.964
CID000006137	L-methionine	4	0.965
CID000643975	flavin adenine dinucleotide	50	0.968
CID000006013	testosterone	1164	0.975
CID000000681	dopamine	2216	0.98
CID000005202	serotonin	607	0.992
CID000006106	L-leucine	4	0.993
CID000006322	arginine	257	0.993
CID000006830	guanosine triphosphate	714	0.993

CID000006140	phenylalanine	9	0.995
CID000005885	NADP	12712	0.996
CID000008977	guanosine diphosphate	3	0.996
CID000000283	formate	1670	0.998
CID000439260	norepinephrine	171	0.998
CID000000888	magnesium	9756	0.999
CID000001195	isopentenyl diphosphate	758	0.999
CID000000051	alpha-ketoglutarate	463	1
CID000000783	hydride	1704	1
CID000005957	adenosine triphosphate	31408	1
CID000023925	IRON	6799	1
CID000064689	D-glucose	33	1
CID000087642	coenzyme A	700	1
CID000444493	acetyl-CoA	154	1
CID000445713	farnesyl pyrophosphate	608	1