

Supplementary Material III. 557 candidate non-carcinogenic chemicals, their betweenness and p-values of randomization test

Chemical ID	Chemical name	Betweenness	P-value of randomization test
CID000000312	chloride	19719	<0.001
CID000000671	d Na	981	<0.001
CID000001745	1H-imidazole-5-methanol	1	<0.001
CID000002341	benzphetamine	2	<0.001
CID000004595	ondansetron	389	<0.001
CID000005405	terfenadine	496	<0.001
CID000005796	sesamex	7	<0.001
CID000006029	uridine	1377	<0.001
CID000007289	1,3-DCP	6	<0.001
CID000007403	TBBA	1	<0.001
CID000007670	N-ethylaniline	1	<0.001
CID000008420	2-naphthalenesulfonate	3	<0.001
CID000008814	4-tert-octylphenol	7	<0.001
CID000011975	2,4-diaminoanisole	16	<0.001
CID000012329	dimethyl adipate	1	<0.001
CID000014888	arsenic trioxide	7	<0.001
CID000022094	chloropropylate	2	<0.001

CID000024482	ammate	3	<0.001
CID000025811	NSAR	3	<0.001
CID005280497	thromboxane A2	1490	<0.001
CID005282439	OKY-046	2	<0.001
CID005360001	4HAQO	2	<0.001
CID023690938	piroxicam	5	<0.001
CID000000801	auxin	2419	0.001
CID000000943	nitrate	4264	0.001
CID000001119	sulfur dioxide	4	0.001
CID000002997	nordiazepam	7	0.001
CID000005859	famphur	7	0.001
CID000005920	triiodothyronine	501	0.001
CID000006812	naphthalenesulfonate	2	0.001
CID000007293	dimethylurea	4	0.001
CID000010943	1,3-dichlorobenzene	2	0.001
CID000013711	deoxycytidine	998	0.001
CID000020226	Kelevan	1	0.001
CID000024529	nitrite	3426	0.001
CID000024924	lead nitrate	1	0.001
CID000025473	rose bengal	495	0.001
CID000062244	MeA alpha C	2	0.001

CID000071988	lamtidine	1	0.001
CID000086472	alpha-tocopheryl acetate	501	0.001
CID000098533	3-(methylnitrosamino)propionaldehyde	1	0.001
CID000000756	glycolaldehyde	975	0.002
CID000000923	sodium	10357	0.002
CID000000978	p-aminobenzoic acid	2831	0.002
CID000003562	halothane	1970	0.002
CID000006175	cytidine	1077	0.002
CID000006348	carbon disulfide	1	0.002
CID000009695	7-OH-2-AAF	2	0.002
CID000010518	heptabarbital	2	0.002
CID000016116	siduron	4	0.002
CID000024971	4-nitrosobiphenyl	1	0.002
CID000439516	agaritine	4	0.002
CID005289598	pentosan	1	0.002
CID005371560	dicrotophos	5	0.002
CID000000980	4-nitrophenol	3501	0.003
CID000002447	bromvalerylurea	3	0.003
CID000003869	labetalol	1	0.003
CID000004121	methyclothiazide	2	0.003
CID000004473	nicardipine	3	0.003

CID000004744	perazine	1	0.003
CID000005359	suprofen	1	0.003
CID000005625	delavirdine	1	0.003
CID000007047	quinoline	1967	0.003
CID000007112	4,4'-biphenol	2	0.003
CID000007725	p-tolualdehyde	988	0.003
CID000012541	thiometon	2	0.003
CID000012774	5-nitro-2-furaldehyde	2	0.003
CID000023611	phenylethylmalonamide	1	0.003
CID000023994	zinc	22385	0.003
CID005280754	Cyclosporin A	500	0.003
CID000000242	benzoate	991	0.004
CID000000259	bromide	1429	0.004
CID000002973	deferoxamine	1	0.004
CID000009298	ronnel	30	0.004
CID000022880	NMDA	1376	0.004
CID000213031	Decree	1	0.004
CID005281228	capsanthin	2	0.004
CID000000276	carbamate	2795	0.005
CID000000544	arsenite	990	0.005
CID000002331	Benzamide	496	0.005

CID000016824	tricamba	1	0.005
CID005359467	Orange I	4	0.005
CID000002943	dacthal	2	0.006
CID000006753	musk ambrette	2	0.006
CID000008143	n-octylamine	4	0.006
CID000026173	3,5-dichlorocatechol	4	0.006
CID000441314	miglitol	500	0.006
CID005280970	cis-DCP	1	0.006
CID006433211	3-(5-nitro-2-furyl)acrylamide	5	0.006
CID000008413	o-tolidine	4	0.007
CID000014855	4-chloro-2-methylphenol	966	0.007
CID000065309	Neu5Ac2en	952	0.007
CID000156391	naproxen	935	0.007
CID000003284	ethinamate	1	0.008
CID000003291	ethosuximide	3	0.008
CID000006805	Fenac	1	0.008
CID000010317	chrysoidine	4	0.008
CID000013081	carbophenothion	5	0.008
CID000111178	L-threo-3-phenylserine	498	0.008
CID000005825	d-amphetamine	498	0.009
CID000006497	dimethyl sulfate	3	0.009

CID000006824	yellow AB	2	0.009
CID000007252	p-toluenediamine	5	0.009
CID000008280	paramethadione	3	0.009
CID000034192	thiobencarb	2	0.009
CID000083887	D-aspartate	498	0.009
CID000001099	sulfite	1485	0.01
CID000001245	vanillylmandelic acid	497	0.01
CID000003118	disulfoton	6	0.01
CID000004946	propranolol	991	0.01
CID000007153	mecoprop	5	0.01
CID000014777	calcium hydroxide	1	0.01
CID000024453	chlorite	499	0.01
CID000037125	sulprofos	4	0.01
CID005283731	25-hydroxyvitamin D	499	0.01
CID000000034	2-chloroethanol	1417	0.011
CID000009731	4-fluoroaniline	4	0.011
CID000010214	3'-phosphoadenosine 5'-phosphosulfate	2842	0.011
CID000104810	barium	500	0.011
CID005281404	harmane	1	0.011
CID005363234	decyl oleate	1	0.011
CID000001117	sulfate	1528	0.012

CID000004929	prometryn	7	0.012
CID000007809	p-xylene	985	0.012
CID000441093	gamma-pentachlorocyclohexene	5	0.012
CID000000119	gamma-aminobutyric acid	2870	0.013
CID000005587	tripelennamine	2	0.013
CID000006363	2-aminopropane	5	0.013
CID000007489	terephthalate	498	0.013
CID000008594	N-1-naphthylphthalamic acid	1	0.013
CID000010112	calcium carbonate	1	0.013
CID000024261	silica	997	0.013
CID000068152	3-OH	499	0.013
CID000091692	pencycuron	1	0.013
CID000105143	bismuth	2	0.013
CID000067296	nonylphenol	3	0.014
CID000012254	polyurethane	5	0.015
CID000001188	xanthine	1519	0.016
CID000004169	metolachlor	7	0.016
CID000004932	propafenone	1	0.016
CID000002912	cypermethrin	11	0.017
CID000004992	mepyramine	1	0.017
CID000012968	EPTC	6	0.017

CID000015730	4-octylphenol	3	0.017
CID000023931	mercury	996	0.017
CID000007966	cyclohexanol	1467	0.018
CID016048618	galactosylglycerol	495	0.018
CID000000977	oxygen	45186	0.019
CID000006503	tris	2850	0.019
CID003032296	zineb	3	0.019
CID000005962	lysine	5493	0.021
CID000023327	D-glutamate	997	0.021
CID000075049	reuterin	1	0.021
CID000736186	isoferulic acid	498	0.021
CID000008749	NDMA	4	0.022
CID000073668	cut less	1	0.022
CID000452967	steviol	1	0.023
CID005385314	penicillic acid	2	0.023
CID000020848	nitralin	4	0.024
CID000107649	Beryllium	498	0.024
CID000004612	oxamniquine	2	0.025
CID000006626	bisphenol S	1	0.027
CID000007577	DAPM	9	0.027
CID000006777	dicyclohexyl phthalate	1	0.028

CID000006613	pantothenic acid	969	0.029
CID000091683	nuarimol	1	0.029
CID000104781	TBPS	1	0.029
CID000188324	D-A5P	486	0.029
CID000002162	amlodipine	497	0.03
CID000003606	hexestrol	1	0.031
CID000031170	indium phosphide	2	0.031
CID000443447	GA51-catabolite	491	0.031
CID000452191	artemisinin	498	0.032
CID005377791	chlorfenvinphos	5	0.032
CID000015032	pregnenolone-16 alpha-carbonitrile	2	0.033
CID000041867	epirubicin	481	0.033
CID000023976	chromium	498	0.034
CID000023978	copper	1744	0.034
CID000031099	formetanate	3	0.034
CID000134490	L-2,4-diaminobutyric acid	499	0.034
CID000439220	dGDP	122	0.034
CID005359596	arsenic	507	0.034
CID000002118	alprazolam	1	0.035
CID000009864	carbodiimide	3	0.035
CID000004767	phenothrin	3	0.036

CID000003032	diclofenac	543	0.037
CID000004931	propachlor	2	0.037
CID000006325	ethylene	978	0.037
CID000007472	DMPD	464	0.037
CID000066603	tetrachlorohydroquinone	497	0.037
CID000073766	fluoroacetaldehyde	491	0.037
CID000150855	dCDP	483	0.037
CID000073949	2-oxazolidinone	1	0.038
CID000000654	diethyl phosphate	1	0.039
CID000011719	methylurea	2	0.039
CID000017531	azinphos-ethyl	2	0.039
CID000091687	anilofos	2	0.039
CID000444865	equilenin	945	0.039
CID005281955	Tween 80	492	0.039
CID000004737	pentobarbital	5	0.04
CID000067678	L-cystine	12	0.04
CID000000220	aminoparathion	6	0.041
CID000001738	homovanillic acid	480	0.041
CID000003728	iodoquinol	1	0.041
CID000107807	perindopril	2	0.041
CID000000778	homocysteine	500	0.042

CID005280971	beta- chloroacrolein	1	0.042
CID005473513	Ponceau 3R	7	0.042
CID000004826	pinacidil	492	0.043
CID000135538	4-hydroxymethylphenylhydrazine	2	0.043
CID005284566	granisetron	100	0.043
CID011966160	3H-9	487	0.043
CID000003162	doxylamine	1	0.044
CID000006051	4-aminoazobenzene	479	0.044
CID000023930	manganese	1570	0.044
CID000087310	alliin	494	0.044
CID000007250	2,4-dimethylaniline	3	0.045
CID000062302	tartrazine	7	0.045
CID000637566	geraniol	497	0.045
CID000003652	hydroxychloroquine	1	0.046
CID000000655	DETP	478	0.048
CID000007533	cyclamate	4	0.048
CID000008554	dimethyl phthalate	2	0.048
CID000010805	MHPG	12	0.048
CID000011937	2-aminoanthracene	11	0.048
CID005281767	curcumin	994	0.048
CID000000170	dihydropteroate	28	0.049

CID000637090	crotonate	480	0.049
CID000003114	disopyramide	4	0.05
CID000005345	sulfobromophthalein	492	0.05
CID000010442	1,3-propanediol	499	0.05
CID000002769	cisapride	2	0.051
CID000008419	veratraldehyde	493	0.051
CID000050516	fluvalinate	3	0.051
CID000000763	guanidinoacetate	500	0.052
CID000002541	candesartan	2	0.052
CID000008411	o-dianisidine	12	0.052
CID005939523	Z-phenylacetaldoxime	1	0.052
CID000023990	vanadium	495	0.053
CID000643833	dichloroethene	9	0.053
CID000024502	potassium dichromate	1	0.054
CID000036187	PCB 77	6	0.054
CID001548952	clomiphene	2	0.054
CID005371562	monocrotophos	2	0.054
CID000002720	thiazide	2	0.055
CID000002726	chlorpromazine	990	0.055
CID000005839	aldosterone	1470	0.055
CID000021157	buthionine sulfoximine	495	0.055

CID000440918	6-oxohexanoate	2	0.055
CID000007259	2,5-xylidine	493	0.056
CID000007271	2,4,5-trichlorophenol	1	0.056
CID000017109	oxythioquinox	1	0.056
CID000081261	N-hydroxy-4-aminobiphenyl	49	0.056
CID000114790	aluminum hydroxide	1	0.056
CID000447320	angiotensin I	2	0.056
CID000008266	chlorendic acid	2	0.057
CID000446220	cocaine	985	0.057
CID005483506	Ponceau 4R	4	0.058
CID000006853	fluorene	14	0.059
CID000104806	peroxynitrite	495	0.059
CID000183009	NNAL-Gluc	1	0.059
CID005364545	cyhexatin	2	0.059
CID000004784	phenylmethylsulfonyl fluoride	2	0.06
CID000055245	mifepristone	497	0.06
CID000003110	dipyrrone	2	0.062
CID000003608	hexobarbital	2	0.062
CID000005815	epinephrine	975	0.063
CID000004768	phenoxybenzamine	2	0.064
CID000006093	niridazole	2	0.064

CID000157350	hydroxyl radical	497	0.064
CID000091590	Irgarol 1051	1	0.065
CID000010787	1,2,4-benzenetriol	5	0.066
CID000013945	dCMP	310	0.067
CID000008434	ethylparaben	498	0.068
CID009570290	phoxim	2	0.068
CID015942880	Kd 0	486	0.068
CID000000278	carbamoyl phosphate	498	0.069
CID000006559	isobutyronitrile	493	0.07
CID000172197	angiotensin II	988	0.07
CID005280541	hexadecenal	480	0.07
CID000007961	bromobenzene	1	0.071
CID000011392	2-nitronaphthalene	1	0.071
CID000000180	acetone	3	0.072
CID000000215	aminoacetone	1	0.073
CID000001110	succinate	503	0.076
CID000005819	thyroxine	988	0.077
CID005280954	rescinamine	1	0.078
CID000013109	levonorgestrel	497	0.079
CID000004893	prazosin	495	0.08
CID005462328	heroin	494	0.08

CID000000540	cyanate	7	0.083
CID000000611	glutamate	1376	0.083
CID000004585	olanzapine	1	0.084
CID000012540	triphenyltin chloride	1	0.085
CID000023932	molybdenum	541	0.085
CID000000934	nickel	496	0.086
CID000004098	histidyl	487	0.086
CID000004944	propoxur	23	0.087
CID000000896	melatonin	499	0.089
CID000003289	ethoprop	1	0.089
CID000000547	DOPAC	478	0.09
CID000006230	norethisterone	2	0.09
CID000019829	3MGA	2	0.09
CID000003637	hydralazine	1	0.091
CID000060749	gemcitabine	460	0.091
CID000006113	ethyl methanesulfonate	1	0.092
CID000014210	omethoate	2	0.093
CID000004171	metoprolol	4	0.094
CID000439963	5-oxopentanoic acid	486	0.095
CID000443231	K-PC	478	0.095
CID000000767	bicarbonate	2929	0.096

CID000060946	tirofiban	465	0.097
CID000119405	DHICA	1	0.097
CID000024341	HOCl	497	0.098
CID000001982	acephate	2	0.099
CID000004534	NDGA	488	0.099
CID005371769	indole-3-acetaldoxime	495	0.099
CID000007257	3,4-dichloroaniline	1	0.101
CID000024841	iodide	1252	0.101
CID011020241	ascorbate	500	0.102
CID000008794	phenylacetonitrile	493	0.103
CID000010413	hydroxybutyrate	500	0.104
CID000024621	molybdate	429	0.104
CID000061021	metaldehyde	1	0.104
CID000000597	cytosine	1350	0.105
CID000009126	dibenzo(a,e)pyrene	1	0.105
CID000638015	11-cis-retinal	5	0.108
CID005283157	20-HETE	494	0.108
CID000002719	chloroquine	497	0.109
CID000010401	epsilon-caprolactone	5	0.111
CID000015993	dATP	317	0.112
CID005280453	1,25(OH)2D3	496	0.112

CID000005862	cystein	6	0.113
CID011953960	dialdehyde	1	0.117
CID000065063	dUMP	995	0.119
CID000520535	superoxide	987	0.119
CID000018290	metobromuron	2	0.12
CID005280421	2'-carboxybenzalpyruvate	480	0.122
CID000006076	cyclic AMP	498	0.123
CID000006134	lactose	482	0.125
CID000447903	8-oxo-dGMP	456	0.125
CID000093072	ureidosuccinate	3	0.126
CID000115205	BzATP	499	0.126
CID000000904	acetanilide	474	0.13
CID000188966	dADP	47	0.13
CID000005333	sulfonamide	15	0.131
CID005357402	triphenyltin	1	0.131
CID000014917	fluoride	419	0.133
CID000006238	17-hydroxyprogesterone	763	0.135
CID000036462	etoposide	2	0.136
CID000115224	thiacloprid	1	0.136
CID000000568	dibenzofurans	498	0.138
CID000005753	corticosterone	1470	0.138

CID000005884	NADPH2	2955	0.138
CID000034468	Cobex	1	0.139
CID000159296	A3P5P	1639	0.139
CID000000254	2,3-dihydroxybiphenyl	6	0.14
CID011271640	chlorantraniliprole	2	0.144
CID000000402	sulfur	2365	0.145
CID000004687	paraxanthine	2	0.145
CID003032571	propineb	1	0.145
CID000000787	hydroxylamine	487	0.15
CID000031261	acetylacetone	8	0.151
CID000442514	hematoxylin	5	0.152
CID000104727	aluminum	494	0.155
CID000000760	glyoxylate	906	0.156
CID000001673	3-methyladenine	491	0.156
CID000003372	fluphenazine	1	0.156
CID000008376	2,4,6-trinitrotoluene	1	0.157
CID000025429	carbendazim	2	0.159
CID000065103	deoxyguanosine triphosphate	457	0.161
CID000000247	betaine	445	0.162
CID000187790	deoxyguanosine	483	0.162
CID000014985	vitamin E	484	0.163

CID000005789	thymidine	24	0.164
CID000002156	amiodarone	3	0.165
CID000039676	vinclozolin	2	0.179
CID000091528	DOPEG	9	0.182
CID000000674	dimethylamine	3	0.183
CID000439155	AdoHcy	6066	0.185
CID000000967	orotic acid	5	0.187
CID000010789	tropolone	491	0.187
CID000013730	deoxyadenosine	481	0.187
CID000008289	triphenyl phosphate	1	0.191
CID000011145	neburon	1	0.192
CID000445354	retinol	6	0.193
CID000441276	paclitaxel	2	0.194
CID005281232	crocetin	497	0.195
CID000016553	hydroxyatrazine	5	0.197
CID000036324	amitraz	2	0.197
CID000000004	aminopropanol	477	0.198
CID000034755	S-adenosylmethionine	1443	0.201
CID000000527	propionaldehyde	4	0.202
CID000000757	glycolic acid	67	0.206
CID000493570	riboflavin	430	0.207

CID005280795	vitamin D3	2	0.214
CID005353758	methomyl	5	0.214
CID000002082	albendazole	495	0.215
CID000000713	formamide	1	0.216
CID000003030	dicamba	1	0.217
CID000033042	ribostamycin	1	0.219
CID000004913	procainamide	493	0.224
CID000004933	propanil	1	0.224
CID000006844	1H-n	479	0.226
CID000031200	fenitrothion	4	0.226
CID000002818	clozapine	2	0.227
CID000000781	thiocyanate	797	0.23
CID000000271	calcium	26218	0.231
CID000006132	cytidine diphosphate	4	0.231
CID005280346	ubiquinone	987	0.234
CID000063090	PCB 126	1	0.235
CID000003488	glibenclamide	492	0.242
CID000003961	losartan	2	0.243
CID000000961	hydroxyl radicals	18149	0.244
CID000006804	5'-GMP	16	0.244
CID000001015	phosphoethanolamine	480	0.246

CID000007099	proflavine	480	0.246
CID023724459	UDP-D-xylose	1	0.246
CID000000264	butyrate	478	0.249
CID000003559	haloperidol	2	0.253
CID000000187	acetylcholine	988	0.254
CID000002520	verapamil	2	0.254
CID000006176	cytidine triphosphate	1	0.258
CID003034368	mancozeb	2	0.259
CID000004095	methadone	4	0.26
CID000005768	quinidine	1	0.263
CID000006167	colchicine	946	0.265
CID000121991	nicotinate mononucleotide	489	0.265
CID000008299	acetol	479	0.266
CID000010238	adenosine 5'-phosphosulfate	25	0.266
CID000005800	2-AF	2	0.268
CID000001045	putrescine	492	0.27
CID000031242	4-ethylphenol	483	0.27
CID000002328	bentazone	1	0.271
CID000003657	hydroxyurea	457	0.272
CID000007518	phenylhydroxylamine	466	0.272
CID000000013	1,2,4-trichlorobenzene	7	0.273

CID000000190	adenine	3504	0.274
CID000221493	cholic acid	2227	0.275
CID000001130	thiamine	492	0.284
CID000001993	methacholine	3	0.284
CID000001054	pyridoxine	58	0.286
CID000124886	Glutathione	975	0.287
CID000028486	lithium	491	0.289
CID005280450	linoleic acid	499	0.297
CID000005810	hydroxyproline	22	0.309
CID000003893	lauric acid	1	0.31
CID000000222	ammonia	2231	0.312
CID000004943	propofol	1	0.314
CID000008947	monomethylarsonic acid	494	0.314
CID005280389	sterigmatocystin	496	0.314
CID000000280	carbon dioxide	3817	0.318
CID000000880	methylglyoxal	475	0.324
CID000006274	histidine	486	0.325
CID000000049	alpha-ketoisovalerate	202	0.326
CID000000305	choline	519	0.326
CID000006047	levodopa	1446	0.33
CID000011318	1,2-dihydroxynaphthalene	2	0.333

CID005281969	anandamide	498	0.336
CID000036679	isoproturon	1	0.34
CID005281166	jasmonic acid	473	0.341
CID000092753	propionyl-CoA	280	0.344
CID000000903	N-acetylserotonin	76	0.347
CID000040326	permethrin	29	0.366
CID000031070	fenamiphos	1	0.367
CID000009395	paraoxon	482	0.37
CID000016248	methiocarb	2	0.373
CID000000887	methanol	1311	0.374
CID000030323	anthracycline	972	0.379
CID000061503	D-lactate	473	0.389
CID000001112	succinic semialdehyde	508	0.393
CID000009154	fluoranthene	7	0.398
CID000036242	procymidone	1	0.399
CID000006083	adenosine monophosphate	2829	0.402
CID000001175	uric acid	163	0.406
CID000000867	malonate	486	0.41
CID000005994	progesterone	529	0.412
CID000037034	PCB 153	1	0.415
CID000006030	uridyate	597	0.42

CID000009502	linuron	1	0.443
CID005280492	LTB4	1	0.445
CID027885548	tetracycline	1	0.448
CID000091650	pyrimethanil	1	0.451
CID000098792	dihydrofolate	381	0.454
CID000008530	naphthoquinone	1	0.457
CID000037517	iprodione	1	0.462
CID000005793	glucose	977	0.465
CID000023977	cobalt	455	0.468
CID005459802	dopachrome	466	0.47
CID000444539	cinnamic acid	4	0.488
CID000000774	histamine	1965	0.492
CID000060961	adenosine	481	0.505
CID000006049	EDTA	2	0.507
CID000439260	norepinephrine	1748	0.513
CID000444899	arachidonic acid	2476	0.516
CID000006288	L-threonine	280	0.518
CID000007339	phosphoribosylpyrophosphate	1009	0.528
CID000000681	dopamine	3244	0.543
CID000006249	ampicillin	490	0.556
CID000145742	L-proline	22	0.561

CID000001032	propionate	476	0.571
CID000001567	2-mercaptoethanol	30	0.572
CID000000768	cyanide	12	0.579
CID000001023	pyrophosphate	489	0.584
CID000001017	phthalic acid	487	0.597
CID000000070	alpha-ketoisocaproate	202	0.608
CID000006128	androstenedione	498	0.62
CID000171548	factor S	473	0.63
CID000012039	chorismate	6	0.663
CID000643976	flavin mononucleotide	66	0.663
CID000006830	guanosine triphosphate	1712	0.676
CID000011005	myristate	1	0.681
CID005288826	morphine	501	0.696
CID000001102	spermidine	491	0.707
CID000001060	pyruvic acid	480	0.71
CID000444972	fumarate	2	0.715
CID000445639	oleic acid	494	0.743
CID000009700	poly(dT	335	0.753
CID000000135	p-hydroxybenzoic acid	3	0.766
CID003034285	azoxystrobin	474	0.769
CID000006106	L-leucine	175	0.774

CID000001003	phosphate	2618	0.778
CID000445995	geranyl diphosphate	497	0.79
CID000008418	anthracene	2	0.799
CID000008955	pregnenolone	13	0.808
CID000444493	acetyl-CoA	1776	0.832
CID000006137	L-methionine	10	0.833
CID000000175	acetate	9	0.837
CID000000679	DMSO	155	0.843
CID000031423	pyrene	7	0.847
CID000005950	L-alanine	133	0.853
CID000006013	testosterone	1152	0.86
CID000000985	palmitate	985	0.869
CID000001051	pyridoxal 5'-phosphate	60	0.873
CID000001005	phosphoenolpyruvate	407	0.882
CID000023925	IRON	8119	0.892
CID000643975	flavin adenine dinucleotide	51	0.907
CID000005997	cholesterol	485	0.92
CID000001132	thiamine pyrophosphate	19	0.924
CID000439153	reduced nicotinamide adenine dinucleotide	109	0.926
CID000005957	adenosine triphosphate	28943	0.931
CID000005892	beta-NAD	4652	0.94

CID000000283	formate	1721	0.943
CID000000970	oxaloacetate	37	0.945
CID000005202	serotonin	558	0.959
CID000006140	phenylalanine	17	0.97
CID000008977	guanosine diphosphate	7	0.974
CID000000647	DMAPP	1	0.986
CID000001195	isopentenyl diphosphate	476	0.993
CID000000888	magnesium	7112	0.994
CID000024139	chitin	1	0.996
CID000000051	alpha-ketoglutarate	1436	0.997
CID000006022	adenosine diphosphate	1322	0.999
CID000000783	hydride	870	1
CID000005885	NADP	4553	1
CID000006322	arginine	12	1
CID000087642	coenzyme A	545	1