

Table S1. The metabolome Database of *Moringa oleifera* L. Cultivated with Vermicompost under Different Soil Types

Soil type	Native soil	Native soil	Agricultural soil	Agricultural soil
Fertilizacion	Vermicomposta	Control	Vermicomposta	Control
1:675.6499@22.8 (AC1L9I4L)	2529911.778	6813001.363	430172.0311	178695.826
2:679.7472@8.2 (Ammonium, (5-bromo-2-furfuryl)dimethyl(5-(2,4,6-tribromophenoxy)pentyl)-, bromide)	177762.8158	97364.04277	256009.46	345038.4112
3:677.3182@23.3 (Atropine)	126077.689		562.9794133	
4:622.6172@22.9 (Saginal)	144270.1996	9102.634917	68902.7389	
5:663.8078@24.8 (BRN 2909894)	61057.51118	53528.20363	90671.974	89552.47812
6:595.3104@5.3 (AC1L1BB5)	127832.0756	62915.5518	96098.19183	105506.9323
7:107.4392@0.5	91911.52378	16462.54636	10387.1042	16822.93421
8:166.7449@1.4	232160.3877	143758.4423	55358.39403	96057.77451
9:623.6534@22.5 (n,n'-[ethane-1,2-diylbis(iminoethane-2,1-diyl)]dihexadecanamide)	57683.17795	410603.1014	419526.5849	309392.6847
10:120.5232@1.4	147446.9185	208228.2564	80918.88223	83553.70509
11:679.7281@8.0 (Ammonium, (5-bromo-2-furfuryl)dimethyl(5-(2,4,6-tribromophenoxy)pentyl)-, bromide)	84605.72444	214633.398	63229.88485	167577.8298
12:636.7479@23.2 (3,3',5-triiodothyropropionic acid)	31493.93469	12642.33438	12018.39948	7907.696609
13:205.8961@2.8 (Carbonic acid, ammonium copper salt)	70073.79572	49613.32101	12265.76612	7586.61217
14:535.4002@8.0 (1,4-DIDODECYL SULFOSUCCINATE)	32215.81835	43414.99558	157857.0243	61301.22827
15:763.8226@25.5 (potassium hydrogen[(bis(2-bis(phosphonomethyl)amino)ethyl)amino)methylphosphonate(5:5:1)])	52986.46225	231945.6749	134605.0812	179547.3707
16:675.6009@22.7 (AC1L9I4L)	5940.057628	6547939.101	439806.8548	124170.5628
17:621.8614@22.5 (AC1ME2EK)	666929.2984	4663515.736	5352487.41	3407730.66
18:871.7282@24.8 (Triacylglycerol 17:1-18:1-18:1; LC-ESI-QTOF; MS; mouse WAT)	4889.626553	1245831.938	386581.2638	22015.92546
19:593.8939@21.6 (5-iodocytosine deoxyribonucleoside triphosphate)	315915.0017	2428474.216	1133079.217	2149410.547
20:619.7199@21.8 (n-tetradetracontane)	33866.76799	64558.46631	3935.236914	2373.771142
21:622.7225@22.6 (3,3',5-triiodothyroacetic acid)	1342.024016	43575.50835	257131.4343	293563.6476
22:871.7561@26.2 (Triacylglycerol 17:1-18:1-18:1; LC-ESI-QTOF; MS; mouse WAT)	5514.519142	40350.91045	34551.86697	17905.3634
23:677.3919@22.7 (Ammonium, (p-benzoquinon-2,5-ylenebis(iminotrimethylene))bis(diethyl(o-methoxybenzyl)-, dichloride)	44280.73512	365282.0873	51368.30105	25658.2744
24:637.6328@22.0 (7709-17-3)	137286.9081	2150759.987	821420.2986	89348.47636
25:594.6963@21.8 (AI-942/13331563)	4392.397655	8795.097085		
26:885.7467@26.7 (Triolein)	19344.86146	97275.54937	179981.6746	104835.7643
27:873.6402@25.0 (NSC634595)	3768.522211	358353.9718	33390.20056	13150.54841
28:166.4141@1.4	50019.77523	58724.52313		

29:886.6297@26.7 (Tetracesium 4,4'-carbonyldipthalate)	17515.30093	50529.15955	100823.4708	57886.1266
30:533.8328@16.9 (Bis(4-iodophenyl)iodanium)	9279.495723	33580.90744	30546.70196	21942.43969
31:620.5238@18.2 (methyl 1,4,5,6,7,7-hexabromobicyclo[2.2.1]hept-5-ene-2-carboxylate)	9206.507089	167677.2201	244913.7704	182447.4022
32:609.7473@20.7 (NSC266232)	17941.19597	468395.2676	273311.2545	279353.9646
33:887.7525@26.7 (AC1L315G)	45357.78016	359083.3631	43410.45477	444086.2352
34:432.3389@1.0 ((1S*,4S*)-4-(2-(TERT-BUTYLDIMETHYLSILOXY)ETHYL)-3-OXO-4,8,12-TRIMETHYLCYCLOTETRADECA-7(E),11(E)-DIENYL CYANIDE; EI-B; MS)	23069.82307	21348.83233	2636.145087	64156.9252
35:596.5225@17.5 (Naphthalene, hexabromo-)	5074.08966	29073.49571	7963.681356	6556.159065
36:636.6877@21.6 (hexabromocyclododecane)	15195.43248	19535.63178	4521.551368	3972.522986
37:888.5870@23.5 (Phytic Acid)	216.9828424	25316.08506	8305.357041	818.6071326
38:763.8401@25.5 (potassium hydrogen[(bis(2-[bis(phosphonomethyl)amino]ethyl)amino)methyl]phosphonate(5:5:1))	23135.59592	136763.459	82589.05579	110752.2379
39:885.7074@26.4 (NCI60_005293)	4026.604196	134165.7246	191918.2166	107921.4901
40:625.7353@22.5 (trimethyl(octadecyl)azanium)	3962.175025	16869.64428	9696.198688	9563.640381
41:764.8101@25.6 (Disodium 2',2'-trithiobis(4,4'-dichloro-2-biphenylsulfinate))	21058.18732	38738.18254	64434.90453	94538.84176
42:643.6341@22.6 (1,1'-Ethylenebis(4,5-dihydro-2-heptadecyl-1H-imidazole))	7986.050046	30892.15732	16430.03709	25811.69963
43:679.7146@7.1 (Ammonium, (5-bromo-2-furfuryl)dimethyl(5-(2,4,6-tribromophenoxy)pentyl)-, bromide)	50424.60631	137641.8823	102352.0182	105870.6319
44:675.6358@23.0 (AC1L9I4L)	1965724.563	162668.7004	4752.600256	4186.940068
45:638.6694@21.8 (1,1,4,7,10,10-hexabromododecane)	44949.27057	544730.8351	240152.6652	174388.9365
46:623.5143@22.5 (Octadecyloctaglycol)	7440.671755	662641.0085	336008.3306	229768.1824
47:257.2740@20.1 (palmitate)	62.71790158	237107.9104	136.5708424	85.68130507
48:871.7021@25.4 (ALUMINUM OLEATE)	4390.281283	686002.2435	64166.50461	7601.980503
49:679.7482@8.3 (Ammonium, (5-bromo-2-furfuryl)dimethyl(5-(2,4,6-tribromophenoxy)pentyl)-, bromide)	243269.2499	310516.7799	299462.6925	304772.8898
50:653.6596@22.0 (CHOLESTERYL STEARATE; EI-B; MS)	4471.30377	189144.3446	113308.7749	115216.5223
51:622.8572@22.7 (quercetin 3, 3', 4', 7-tetrasulfate)	85211.50686	283106.9889	444944.0205	362721.4604
52:563.9034@23.5 (ferric-adenosine triphosphate complex)	543.5124346	130808.0705	82145.52884	50828.2931
53:639.5956@21.7 (2-octaprenylphenol)	9527.98229	163831.9886	59569.71001	58921.74512
54:636.7542@22.8 (3,3',5-triiodothyropropionic acid)	22328.29083	149306.6523	200452.3627	131594.4146
55:636.6551@21.3 (hexabromocyclododecane)	8809.967358	229648.8466	155489.4965	138100.3051
56:671.5713@22.1 (Diocadecyl phthalate)	2064.789551	71672.11763	6711.606632	4236.012216
57:620.5723@18.2 (AC1L1SJC)	2539.874215	166369.8091	234142.1555	180188.8526
58:903.6381@27.0 (64346-20-9)	1462.229055	106382.9277	94202.8677	44853.87353
59:565.4674@20.5 (2-Ethylhexyl titanate)	448.0015755	152804.3512	4982.323411	1507.286718

60:813.8707@26.6 (AC1L2IAV)	7169.113717	127439.418	52105.99293	5265.524202
61:625.6852@20.9 (2-methyloxirane; 1-octadecoxyoctadecane; oxirane)	3976.702973	79402.2646	48141.5579	33225.91505
62:655.0140@25.9 (EOSIN TOLUIDINE BLUE)	1468.360778	53029.35677	29608.79383	10791.89576
63:889.6010@27.0 (Phosphatidylinositol 18:0-20:3; LC-ESI-ITFT; MS2; [M-H] ⁻ ; RT: 23.31; Exp: 1)				
	3998.036069	92315.62087	89300.51829	66790.09761
64:747.9729@26.7 (AC1L4XFZ)	5720.88355	69578.17496	34341.51765	45930.92636
65:651.5600@20.5 (cholesteryl oleate)	743.869135	61784.9814	20033.95348	16333.01192
66:120.5236@1.4	152304.1906	204549.0473	60026.25246	96185.70634
67:166.7520@1.4	185415.7596	188893.5703	71005.35256	83574.09992
68:745.9112@25.2 (AC1Q4PGR)	31590.4135	108922.3487	69818.02557	108074.5859
69:623.9246@22.9 (copper(2+) hydrogen 3-[(e)-[3-methyl-5-oxido-1-(4-[[2-(sulfonatooxy)ethyl]sulfonyl]phenyl)-1h-pyrazol-4-yl]diazanyl]-4-oxidobenzenesulfonate(1:2:1))	14354.02538	57405.33371	46759.45318	24731.67272
70:607.7361@20.2 (pentacobaltic dodecacyanide)	3836.631098	129910.5793	104237.4099	81208.6643
71:697.0368@25.2 (14569-54-1)	567.1552154	33012.54991	6937.213796	2541.730297
72:609.7955@20.6 (NSC266232)	10765.62312	49522.69324	259135.2622	310265.7692
73:681.6229@21.2 (Cholesteryl oleyl carbonate)	4091.995452	92634.72533	90423.49357	64684.07565
74:886.6378@25.2 (Tetracesium 4,4'-carbonyldiphthalate)	802.1233566	54258.10253	2967.673962	1431.857474
75:759.7042@23.9 (Bis[17-(1,5-dimethylhexyl)-4,13-dimethyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl]diazene)	4378.20887	33854.97422	9682.715578	12322.79126
76:625.5510@22.5 (ETHYLENEBIS-12-HYDROXYSTEARAMIDE)	89.24579239	29954.74121	8076.49354	5208.902753
77:653.5911@20.4 (CHOLESTERYL STEARATE; EI-B; MS)	1521.882855	27439.77832	13781.04912	11817.15288
78:132.6454@0.6	38613.17209	53597.27183	18228.45706	18117.31183
79:659.6326@22.1 (1-amino-n-(2-[[2-[(2-aminoethyl)amino]ethyl]amino)ethyl]amino)ethyl)-13-(1-hydroxynonyl)-3,6,9,12-tetraazahenicosan-21-amide)	8738.951	24131.22469	14580.41659	15971.84092
80:781.7518@25.8 (Pentaerythritol dibehenate)	13967.01681	63977.90958	31372.76609	41541.08193
81:765.7792@25.3 (AC1LBKDL)	9597.210961	23803.75948	19449.52672	47829.97816
82:874.6099@24.7 (AC1MHVM3)	265.6377058	35891.72572	2748.13762	670.7748299
83:625.7433@23.6 (trimethyl(octadecyl)azanium)	4068.471331	20867.99644	16549.68072	18967.23382
84:815.7785@25.1 (AC1N7TCR)	449.6768001	18317.26842	42608.77197	4755.84223
85:746.9758@25.4 ((2,4,5-Trichlorophenoxy)acetic acid 1,4-piperazinediyl-di-3,1-propanediyl ester 2HCl)	4566.837613	26527.05316	16933.64759	20311.05155
86:635.8218@22.6 (BRN 0575813)	126077.1326	593490.6427	28233.63105	939794.5582
87:621.8651@22.7 (AC1ME2EK)	602321.5501	931538.0137	1068526.384	329328.2451
88:651.7410@22.1 (METRIZOATE MAGNESIUM)	2708.57798	56387.58545	84558.2127	73987.67338

89:690.4404@21.5 (3,7,12,17-Tetramethyl-21H,23H-porphine-2,18-dipropionic acid dihydrochloride)	150.1905117	13264.90391	1306.468605	697.4722516
90:742.6915@24.7 (93803-15-7)	1173.117921	28821.04835	18740.66746	7330.946102
91:676.5589@23.0 (1,2-dimyristoylamido-1,2-deoxyphosphatidylcholine)	1251.402089	38724.45948	1584.680223	994.1112331
92:667.5920@22.2 (2,3-bis(octanoyloxy)propyl docosanoate)	2673.629213	13926.24196	24495.11955	9525.155859
93:770.6070@25.3 (Phosphatidylcholine 17:1-18:2; LC-ESI-ITFT; MS2; [M+CH3COO] ⁻ ; RT: 16.00; Exp: 1)	1374.354467	44408.15959	57509.37538	22203.8728
94:595.3025@5.3 (AC1L1BB5)	54755.43277	57710.02144	87716.47621	101067.4943
95:654.6260@22.0 (tetrachlororhenium(1-))	2034.61417	74031.9433	37515.78507	20391.48913
96:681.5758@22.1 (Cholesteryl oleyl carbonate)	2523.99342	29022.36664	10393.68646	6437.043054
97:901.5952@26.1 (Phosphatidylinositol 19:0-20:4; LC-ESI-ITFT; MS2; [M-H] ⁻ ; RT: 24.37; Exp: 1)	4340.53675	35645.84239	48483.63522	27018.93203
98:635.6624@21.6 (2,3-bis(octadec-9-enoxy)propyl-trimethylazanium)	17865.1446	31481.36615	8995.504039	6920.648695
99:635.7665@21.2 (BRN 0575813)	952.7627114	446555.0282	311115.4469	191688.1886
100:631.0820@25.3 (AC1L2VDW)	1194.589981	26538.89783	7792.024475	9755.12217
101:609.7167@20.6 (AC1L98SZ)	6826.500293	178355.4852	212988.8778	275154.4649
102:432.6118@0.5 (AC1NRVRU)	62681.62637	44968.83593	23988.48291	119197.8493
103:773.5139@22.1 (Phosphatidylglyceride 18:1-18:2; LC-ESI-ITFT; MS2; [M-H] ⁻ ; RT: 10.90; Exp: 1)	3473.081368	30385.77629	56433.30697	29179.31689
104:903.6351@26.0 (64346-20-9)	12615.91904	33905.3847	41471.37209	38074.45687
105:624.9524@21.2 (perfluorophenanthrene)	2168.456645	6363.473913	8663.852014	4828.75051
106:762.9229@25.5 (NSC718384)	21297.44388	79168.9453	57764.26349	75721.39462
107:659.6807@22.2 (1-amino-n-(2-([2-([2-(2-aminoethyl)amino]ethyl)amino]ethyl)amino]ethyl)-13-(1-hydroxynonyl)-3,6,9,12-tetraazahenicosan-21-amide)	5559.972206	24751.8911	6503.717453	5884.989033
108:773.4615@22.4 (AC1L1B5J)	10394.31588	10999.18318	10226.70116	4641.20146
109:931.6710@26.3 (piperazine-1,4-diyl diethane-2,1-diyl dioctadecanoate- methyl hydrogen sulfate(1:2))	786.6463632	14908.51452	33447.12195	14528.38074
110:735.0153@25.3 (AC1L1X9E)	2125.55213	44525.23842	13023.88782	37741.69976
111:737.0443@25.7 (adenosine tetraphosphopyridoxal)	1336.917125	37128.6875	10859.44365	79892.15196
112:813.8235@25.9 (AC1L2IAV)		12814.41649	8968.906265	7467.021249
113:762.7354@24.1 (ST50986961)	3671.898019	40416.83911	27260.50423	34405.75782
114:739.0619@26.0 (Disufene)	632.8263625	22735.76804	4653.879015	18130.52016
115:777.6725@24.0 (Triacylglycerol 12:0-16:0-18:1; LC-ESI-QTOF; MS; mouse WAT)	4602.249725	16833.67855	10036.85564	12259.15277
116:675.4602@22.7 (1-18:1-2-16:0-phosphatidate)	1830.389351	11640.45777	46088.9202	172916.6486
117:637.6866@21.8 (2,4,6-tritridecyl-1,3,5-trioxane)	105772.4694	2105823.161	732231.7496	671373.8162

118:622.7689@22.8 (3,3',5-triiodothyroacetic acid)	129801.8355	202653.3747	492153.6769	227815.1963
119:694.4269@18.0 (Dehydag Wax E)	20552.29898	219512.2844	477240.5081	394352.5295
120:636.7246@22.8 (17086-13-4)	18979.8503	112551.0466	246384.3267	169231.0917
121:887.6776@26.7 (AC1L315G)	16934.00689	43017.8784	65740.82827	63431.04909
122:694.3914@18.0 (germerine)	34269.3425	128922.6355	283011.327	98091.60583
123:903.6399@27.0 (64346-20-9)	2449.570934	106957.9849	101227.9671	86909.79868
124:595.6419@21.6 ((3R,7R,11S,15S,18S,22S,26R,30R)-3,7,11,15,18,22,26,30-Octamethyldotriacontane-1,32-diol; FAB-B; MS)	2069.363448	151610.9796	185911.0812	130768.2623
125:613.9537@23.8 (diiodoplatinum(2+);piperidin-1-ide;2H-pyridin-1-ide)	17304.86711	29951.31977	56950.0302	26713.02539
126:901.6038@26.1 (Phosphatidylinositol 19:0-20:4; LC-ESI-ITFT; MS2; [M-H] ⁻ ; RT: 24.37; Exp: 1)	3242.175969	19676.1069	46596.49894	26535.91598
127:607.8383@20.2 (AC1L4HXI)	4680.724289	63928.26745	159231.1264	78510.33586
128:570.0368@23.6 (rebeccamycin)	6391.774222	21011.90476	40058.48683	32405.85284
129:622.5629@19.0 (UNII-VYP38H02CO)	1060.953581	18147.29171	34931.41289	25791.44428
130:813.8709@26.6 (AC1L2IAV)	3575.299225	91308.75469	42743.99351	2281.270955
131:626.7040@20.8 (2,2'-oxybis[5,5-bis(bromomethyl)-1,3,2-dioxaphosphinane] 2,2'-dioxide)	1296.278009	22944.6816	32298.95478	34626.91137
132:627.8252@23.9 (BRN 3038217)	3941.309999	98210.32513	38777.55467	55381.32607
133:749.8475@25.1 (AC1MR3SH)	1197.657953	6419.388759	22864.58742	13380.26621
134:621.8934@22.4 (8-((4-bromo-2,3-dioxobutyl)thio)adenosine 5'diphosphate)	4136.017217	3984408.344	5076695.431	4001610.126
135:676.4283@22.6 (NSC720385)	1300.399521	5583.315325	95318.58459	149995.4728
136:607.8898@21.9 (AC1L2NSX)	7734.027198	143764.4051	210284.5947	221502.549
137:610.8076@20.8 (tetrasodium pyrene-1,3,6,8-tetrasulfonate)	10727.65088	96988.82855	119361.3542	125170.7325
138:888.6278@27.0 (AC1N12U6)	12593.64772	133775.7146	80705.43536	138015.3574
139:596.5136@17.3 (Naphthalene, hexabromo-)	1296.658889	33751.6473	58678.89347	95001.15458
140:767.2388@8.4 (28043-31-4)	6353.768241	11885.51076	10491.47082	64067.30336
141:637.8304@21.9 (G 1026)	1426.241153	204374.9711	89802.46811	84532.8607
142:602.5644@20.2 (tetrasilver(1+) diphosphate)	284.3051758	305.1602261	1955.962446	64169.81786
143:637.7492@21.1 (NSC407180)	3603.49602	70547.72411	79760.0035	91660.52107
144:621.7727@23.2 (Potassium hexathiocyanatoplatinate(IV))	82731.54297	61964.62036	60812.68873	37329.03837
145:575.6412@18.7 (AC1L2ATR)	764.6167061	3480.343019	6270.860599	70844.27236
146:800.1313@22.8 (coenzyme A persulfide)	131.6693818	35376.56261	22132.83389	25459.53283
147:764.7908@25.5 (Disodium 2',2'-trithiobis(4,4'-dichloro-2-biphenylsulfinate))	17303.13196	100349.975	72552.53382	96503.48286
148:679.7171@6.4 (Ammonium, (5-bromo-2-furfuryl)dimethyl(5-(2,4,6-tribromophenoxy)pentyl)-. bromide)	4949.684367	34657.23574	43192.31115	57060.43826

149:779.6987@25.1 (Triacylglycerol 14:0-16:0-16:0; LC-ESI-QTOF; MS; mouse WAT)	14999.3872	50228.46989	32912.83676	42184.88854
150:760.9891@25.2 (bis(dipropoxyphosphinothioylsulfanyl)stibanylsulfanyl-dipropoxy-sulfanylidene- P^{5} -phosphane)	725.8085703	5572.356196	2761.244721	15556.1687
151:675.4434@22.7 (AC1L1ELZ)	2799.053879	583717.7987	283987.0592	174684.1394
152:694.6335@17.9 (Tetrarubidium 4,4'-carbonyldipthalate)		61048.27442	227175.0879	126393.2829
153:563.8990@23.4 (ferric-adenosine triphosphate complex)	479.9114032	107155.9479	181414.1521	220006.8826
154:887.7874@27.0 (Triacylglycerol 18:0-18:1-18:1; LC-ESI-QTOF; MS; mouse WAT)	9433.857026	215422.7699	120011.106	139272.258
155:638.6735@21.8 (1,1,4,7,10,10-hexabromododecane)	37496.22891	312800.0458	244084.4247	184829.2464
156:533.8178@17.0 (Bis(4-iodophenyl)iodanium)	27584.70926	38737.93057	38007.10984	28839.19148
157:637.6131@22.8 (7709-17-3)	6828.275649	10540.84629	78453.04169	77009.56345
158:1184.7423@21.5 (AC1LAAM2)	33.24350225	35325.54504	53079.90484	23021.33691
159:625.7446@20.8 (trimethyl(octadecyl)azanium)	2480.186211	54780.66182	51999.94339	53472.42904
160:278.2439@16.6 (EHNA)	559.7160526	111401.3058	92284.32824	120573.3859
161:534.6741@16.8 (NSC39610)	689.7231747	10905.9554	5279.969644	4100.994283
162:749.9248@25.2 (AC1L5BTC)	2463.786851	11680.67608	33689.10064	18786.59679
163:873.6276@24.6 (AC1L2JBC)	240.5163911	107651.9176	25357.20839	971.2806241
164:608.8796@20.5 (copper(2+) hydrogen 7-amino-4-oxido-3-[(e)-(2-oxido-4-[[2-(sulfonatooxy)ethyl]sulfonyl]phenyl)diazeryl]naphthalene-2-sulfonate(1:2:1))	992.7681558	14197.0214	14287.18655	14847.01305
165:653.7434@19.9 (AC1LAX5N)	749.2433345	15298.99979	17983.69759	10259.1133
166:765.7531@25.0 (AC1LBKDL)	2123.418021	23412.08978	19077.08795	15531.77503
167:328.4758@1.5	27119.96077	30884.34239	16032.88103	105687.756
168:745.9251@25.2 (AC1Q4PGR)	21982.96058	115459.162	78858.24947	109133.4535
169:675.5621@22.7 (AC1L1T8U)	5959.481181	5624990.109	400730.6682	640636.6485
170:638.5282@21.7 (Hexabromodiphenyl oxide)	1145.628586	189864.164	215224.4523	201133.7327
171:622.9079@22.7 (quercetin 3, 3', 4', 7-tetrasulfate)	33644.14011	231569.6482	122952.7372	168204.9931
172:623.7985@22.5 (2-((2-Benzothiazolylsulfonyl)methyl)-6,8-dibromo-3-(2-chlorophenyl)-4(3H)-quinazolinone)	16733.73259	276811.2476	245031.8993	161360.6349
173:677.3493@22.7 (Atropine)	1900.56311	317390.1609	52429.94246	67404.33343
174:636.6580@21.3 (hexabromocyclododecane)	1495.376674	193396.7515	170698.9714	159418.2973
175:651.7677@22.0 (3,5,3'-triiodo-L-thyronine)	792.2958808	52102.68331	86130.23163	70705.70517
176:680.7176@8.3 (BRN 0066005)	38170.73009	89940.34155	75714.20702	81995.75004
177:654.6171@22.0 (SCHEMBL6253692)	1114.923913	46520.435	46603.05352	41608.11885
178:651.6301@20.4 (hexanedioic acid)	1267.5863	23331.74008	24174.91176	24705.10973
179:885.6624@25.0 (AC1L4CS8)	922.4128926	27250.62368	21448.65781	3320.249013
180:575.6921@18.8 (AC1L2ATR)	693.0572819	5608.266859	7278.628332	29482.53016

181:643.8606@23.9 (trisodium;8-[(3,5-dinitrobenzoyl)amino]naphthalene-1,3,5-trisulfonate)	11909.94696	28587.26983	11257.0672	14831.46123
182:626.8689@23.6 (bismuth titanate)	2846.565888	15468.02366	8823.984869	12350.70819
183:831.8249@26.3 (AC1N581S)	3083.491725	17228.80947	8401.72286	8660.759556
184:765.8247@25.5 (AC1N4QAW)	1559.036455	25058.39513	28378.30719	16731.61203
185:661.6792@23.4 (AC1L6HD5)	4172.512118	18149.0648	7109.663623	9708.378291
186:780.7258@25.3 (kartocid)	8636.627928	43110.714	29589.94738	37233.30204