

peak_n1	name	formula	calc_mw	m_z	day	height	location	mean	std	n	se
1509	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07435	263.08161	1	bottom	half	2680179.844	135079.5668	2	95515.6777
1509	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07435	263.08161	1	middle	half	1064649.468	22567.26252	2	15957.46436
1510	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	1	bottom	half	1000572.728	93324.00098	2	65990.03394
1510	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	1	bottom	quarter	1723174.313	10479.96167	2	7410.451965
1510	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	1	middle	half	387931.7657	12780.22232	2	9036.981864
1510	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	1	top	quarter	323393.8597	1787.44065	2	1263.911404
1510	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	29	middle	half	649162.8633	6594.065178	2	4662.708203
1512	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	1	bottom	quarter	723129.94	97011.44114	2	68597.44788
1512	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	1	middle	quarter	488100.0893	22746.53576	2	16084.22969
1512	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	1	top	half	840348.0313	40369.84687	2	28545.79247
1512	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	1	top	quarter	534006.5592	1399.81853	2	989.8211748
1512	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	4	bottom	half	770471.8473	19574.50528	2	13841.26543
1512	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	8	bottom	half	621287.6042	5740.837152	2	4059.38488
1512	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	15	bottom	half	731796.7679	128689.8539	2	90997.46839
1512	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	18	bottom	half	565111.0726	97818.13686	2	69167.86789
1512	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	25	bottom	half	646976.6809	92227.47204	2	65214.67089
1512	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	29	bottom	quarter	628483.6773	49505.43911	2	35005.6317
1512	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	29	middle	half	556786.7351	126238.0092	2	89263.75236
1512	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07434	263.08162	29	top	half	559479.1658	20867.7616	2	14755.73574
1514	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07431	263.08159	1	middle	half	199811.4251	1604.1523	2	1134.306969
1514	3e 3 3 oxo 1 3 dihydro 2h indol 2 ylidene 1 3 dihydro	C16 H10 N2 O2	262.07431	263.08159	8	bottom	half	179074.8281	23436.30579	2	16571.97075
3859	1 deoxymannojirimycin	C6 H13 N O4	163.08448	164.09175	1	top	half	181922.9337	35219.17716	2	24903.719
3859	1 deoxymannojirimycin	C6 H13 N O4	163.08448	164.09175	4	bottom	half	156837.7475	27617.05484	2	19528.20676
3859	1 deoxymannojirimycin	C6 H13 N O4	163.08448	164.09175	11	bottom	half	254278.9248	63166.24338	2	44665.27903
3859	1 deoxymannojirimycin	C6 H13 N O4	163.08448	164.09175	22	bottom	half	1009715.159	37676.12591	2	26641.04412
3859	1 deoxymannojirimycin	C6 H13 N O4	163.08448	164.09175	29	bottom	quarter	295569.6326	16848.5686	2	11913.73711
3859	1 deoxymannojirimycin	C6 H13 N O4	163.08448	164.09175	29	middle	half	1059180.732	227894.5745	2	161145.799
3859	1 deoxymannojirimycin	C6 H13 N O4	163.08448	164.09175	29	top	quarter	308686.569	41428.19497	2	29294.15759
6528	2 4 6 2 4 diamino 6 oxo 1 3 diazinan 5 yl 1 1 1 tr	C22 H30 F3 N5 O8	549.207	550.21431	18	bottom	half	128054.6305	1713.783933	2	1211.82824
6528	2 4 6 2 4 diamino 6 oxo 1 3 diazinan 5 yl 1 1 1 tr	C22 H30 F3 N5 O8	549.207	550.21431	22	bottom	half	240296.1213	22065.92492	2	15602.96514
6528	2 4 6 2 4 diamino 6 oxo 1 3 diazinan 5 yl 1 1 1 tr	C22 H30 F3 N5 O8	549.207	550.21431	29	bottom	half	367023.1405	22419.46591	2	15852.95637
6528	2 4 6 2 4 diamino 6 oxo 1 3 diazinan 5 yl 1 1 1 tr	C22 H30 F3 N5 O8	549.207	550.21431	29	middle	half	830997.0501	10914.95883	2	7718.041408
6528	2 4 6 2 4 diamino 6 oxo 1 3 diazinan 5 yl 1 1 1 tr	C22 H30 F3 N5 O8	549.207	550.21431	29	top	half	916094.2086	41119.46262	2	29075.85086
6528	2 4 6 2 4 diamino 6 oxo 1 3 diazinan 5 yl 1 1 1 tr	C22 H30 F3 N5 O8	549.207	550.21431	29	top	quarter	957762.8007	49890.29204	2	35277.76382
9239	3 4 methoxy 2 methylphenyl 2 5 dimethyl n 1 3 r	C22 H26 N6 O2	406.21206	407.21934	1	middle	half	2266001.766	118725.0597	2	83951.29478
9239	3 4 methoxy 2 methylphenyl 2 5 dimethyl n 1 3 r	C22 H26 N6 O2	406.21206	407.21934	4	bottom	half	2277812.299	207506.9953	2	146729.6035
9239	3 4 methoxy 2 methylphenyl 2 5 dimethyl n 1 3 r	C22 H26 N6 O2	406.21206	407.21934	15	bottom	half	3286547.258	17889.80163	2	12650.00005
9239	3 4 methoxy 2 methylphenyl 2 5 dimethyl n 1 3 r	C22 H26 N6 O2	406.21206	407.21934	29	bottom	half	2280837.211	192001.7498	2	135765.7393
11762	4 methoxy 4 oxobutan 2 yl 3 3 hydroxybutanoyl c	C13 H22 O7	290.13678	291.14405	4	bottom	half	182058.6212	7200.211571	2	5091.318428
11762	4 methoxy 4 oxobutan 2 yl 3 3 hydroxybutanoyl c	C13 H22 O7	290.13678	291.14405	11	bottom	half	138665.5401	12640.7226	2	8938.340673
13151	5 hydroxy 4 2r 6 hydroxy 5 3e 4 methyl 6 2 6 6 tr	C25 H36 O5	416.25607	434.29006	18	bottom	half	459606.0282	101159.651	2	71530.67519
13153	5 hydroxy 4 2r 6 hydroxy 5 3e 4 methyl 6 2 6 6 tr	C25 H36 O5	416.25626	417.26353	29	bottom	quarter	316280.0571	31920.02341	2	22570.86501
13578	6 7 dimethoxy 4 3 naphthalen 2 yloxy pyrrolidin c	C24 H23 N3 O3	401.1733	402.18058	11	bottom	half	246041.4903	18316.08204	2	12951.42582
13578	6 7 dimethoxy 4 3 naphthalen 2 yloxy pyrrolidin c	C24 H23 N3 O3	401.1733	402.18058	29	middle	quarter	879186.8114	96143.18993	2	67983.50156

14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	1 bottom	half	53859647.19	1565239.945	2	1106791.779
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	1 bottom	quarter	44956036.51	694779.8796	2	491283.5643
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	1 middle	half	43842176.35	976789.0978	2	690694.1949
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	1 middle	quarter	84533838.26	1309870.431	2	926218.2645
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	1 top	half	60096826.87	992057.7278	2	701490.7467
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	1 top	quarter	49611869.46	1315176.302	2	929970.0816
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	4 bottom	half	34219567.04	340688.1638	2	240902.9109
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	8 bottom	half	26647772.38	1189347.805	2	840995.8981
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	11 bottom	half	35750258.95	377125.3163	2	266667.8685
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	15 bottom	half	26723820.19	714421.7624	2	505172.4728
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	18 bottom	half	34349608.22	198669.8541	2	140480.801
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	22 bottom	half	15251590.7	129010.6188	2	91224.28341
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	25 bottom	half	66411213.38	561998.2515	2	397392.7746
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	29 bottom	half	43686938	778870.4432	2	550744.572
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	29 bottom	quarter	29870478.96	143513.5999	2	101479.4396
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	29 middle	half	42202243.21	170488.8361	2	120553.8122
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	29 middle	quarter	23996364.2	444422.0094	2	314253.8165
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	29 top	half	31390071.64	12045.45545	2	8517.423228
14603	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	29 top	quarter	53081299.8	1025260.571	2	724968.7022
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	1 bottom	half	1298275.931	46468.36201	2	32858.09389
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	1 bottom	quarter	2032844.479	146739.3327	2	103760.3772
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	1 middle	half	1234995.658	99529.79178	2	70378.1907
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	1 middle	quarter	1293117.003	8233.941937	2	5822.27618
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	1 top	half	817639.5543	117971.2955	2	83418.30301
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	1 top	quarter	986336.1197	50991.12679	2	36056.17153
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	4 bottom	half	1096599.263	211439.2258	2	149510.1104
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	8 bottom	half	638792.8361	70646.4328	2	49954.5717
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	11 bottom	half	639811.2161	9675.055751	2	6841.29753
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	15 bottom	half	711171.819	139288.6199	2	98491.92766
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	18 bottom	half	781288.0434	17934.51522	2	12681.61733
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	22 bottom	half	281762.145	37424.2292	2	26462.92625
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	25 bottom	half	600328.8716	9080.893808	2	6421.161591
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	29 bottom	half	636032.9623	20285.37709	2	14343.9277
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	29 middle	half	4107744.784	54766.0344	2	38725.4343
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	29 top	half	424426.9107	11834.48634	2	8368.245544
14604	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	29 top	quarter	585084.2487	36694.71181	2	25947.07955
14606	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	1 bottom	quarter	920222.0126	227642.4042	2	160967.4877
14606	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	1 middle	half	714866.0493	664.2112599	2	469.668286
14606	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	1 middle	quarter	618964.2804	85116.17938	2	60186.22763
14606	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	1 top	half	781548.1676	19829.73054	2	14021.73693
14606	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	1 top	quarter	888685.5862	137288.9229	2	97077.92834
14606	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	4 bottom	half	2120862.857	8334.654862	2	5893.490971
14606	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	25 bottom	half	674456.3797	98663.59935	2	69765.70016
14606	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	29 bottom	half	492127.7265	108885.739	2	76993.8444
14606	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	29 middle	half	722796.7	100767.2016	2	71253.17155

14606	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	29 top	half	2851412.069	147278.0985	2	104141.3422
14606	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	29 top	quarter	681457.7586	96136.48528	2	67978.76066
14607	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	1 top	half	1568571.839	49618.46037	2	35085.5498
14607	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	1 top	quarter	1137922.434	69035.79243	2	48815.67697
14607	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	29 bottom	half	1092730.598	83199.30564	2	58830.79321
14607	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	29 middle	half	876855.0801	57329.20778	2	40537.87158
14607	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	29 middle	quarter	1194784.095	83942.81884	2	59356.53644
14607	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	29 top	half	1101853.766	16202.17414	2	11456.66721
14607	8 hydroxyquinoline	C9 H7 N O	145.05282	146.0601	29 top	quarter	910692.8095	80970.86303	2	57255.04633
14608	8 hydroxyquinoline	C9 H7 N O	145.05282	146.06009	29 top	quarter	2275356.296	502631.6018	2	355414.2141
14609	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	1 bottom	quarter	630708.8037	189939.1285	2	134307.2458
14609	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	4 bottom	half	980653.1555	218502.0023	2	154504.2475
14609	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	8 bottom	half	491914.1533	91026.06279	2	64365.14626
14609	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	29 middle	half	1030328.655	82081.56133	2	58040.42863
14609	8 hydroxyquinoline	C9 H7 N O	145.05283	146.06011	29 top	half	953651.7482	106811.2033	2	75526.92619
14610	8 hydroxyquinoline	C9 H7 N O	145.05284	146.06012	1 bottom	quarter	647271.3917	123057.0292	2	87014.45984
14610	8 hydroxyquinoline	C9 H7 N O	145.05284	146.06012	1 middle	quarter	564168.0721	1945.975177	2	1376.012244
14610	8 hydroxyquinoline	C9 H7 N O	145.05284	146.06012	11 bottom	half	347661.3329	22415.76863	2	15850.342
14610	8 hydroxyquinoline	C9 H7 N O	145.05284	146.06012	18 bottom	half	408901.7228	17270.87171	2	12212.3505
14610	8 hydroxyquinoline	C9 H7 N O	145.05284	146.06012	29 bottom	half	453352.0117	13190.27778	2	9326.934861
14610	8 hydroxyquinoline	C9 H7 N O	145.05284	146.06012	29 middle	half	382921.1585	5192.52153	2	3671.667186
14610	8 hydroxyquinoline	C9 H7 N O	145.05284	146.06012	29 top	quarter	333481.805	2288.432114	2	1618.165866
15274	acycloguanosine aciclovir	C8 H11 N5 O3	225.08727	226.09454	29 bottom	quarter	731493.9424	63819.73749	2	45127.36915
15443	agroclavine	C16 H18 N2	238.14707	239.15434	29 middle	quarter	187252.0827	10080.21412	2	7127.787763
15501	alafosfalin	C5 H13 N2 O4 P	196.06128	197.06856	1 bottom	quarter	798410.473	17128.69768	2	12111.81829
15501	alafosfalin	C5 H13 N2 O4 P	196.06128	197.06856	1 middle	half	627860.0417	12707.54754	2	8985.593039
15501	alafosfalin	C5 H13 N2 O4 P	196.06128	197.06856	1 top	half	765182.6503	18142.23105	2	12828.4946
15501	alafosfalin	C5 H13 N2 O4 P	196.06128	197.06856	1 top	quarter	866549.2223	73166.86567	2	51736.78687
15501	alafosfalin	C5 H13 N2 O4 P	196.06128	197.06856	8 bottom	half	400091.0101	17101.4835	2	12092.57495
15501	alafosfalin	C5 H13 N2 O4 P	196.06128	197.06856	11 bottom	half	619996.587	30514.87517	2	21577.27516
15501	alafosfalin	C5 H13 N2 O4 P	196.06128	197.06856	15 bottom	half	422183.5583	23232.26708	2	16427.69359
15501	alafosfalin	C5 H13 N2 O4 P	196.06128	197.06856	18 bottom	half	472471.7711	13652.72659	2	9653.935553
15501	alafosfalin	C5 H13 N2 O4 P	196.06128	197.06856	29 bottom	half	492809.9488	13624.30715	2	9633.839977
15501	alafosfalin	C5 H13 N2 O4 P	196.06128	197.06856	29 top	half	437050.6433	15569.25355	2	11009.12476
15810	amastatin	C21 H38 N4 O8	474.26743	492.30124	29 middle	quarter	7481146.872	676311.5963	2	478224.516
15891	amicycline	C21 H23 N3 O7	429.15228	430.15956	29 top	half	164155.1061	32845.35724	2	23225.17483
16267	anisomycin	C14 H19 N O4	265.13151	266.13879	29 middle	half	160880.6648	39096.52334	2	27645.41678
16268	anisomycin	C14 H19 N O4	265.13151	266.13878	29 top	half	156904.6766	17429.16727	2	12324.28237
16306	aphidicolin	C20 H34 O4	338.24577	361.23502	8 bottom	half	1680681.587	1057.702627	2	747.9086999
16401	arbekacin	C22 H44 N6 O10	552.31458	553.32185	1 bottom	quarter	200492.6548	14981.17082	2	10593.28748
16401	arbekacin	C22 H44 N6 O10	552.31458	553.32185	8 bottom	half	250242.4674	5820.39987	2	4115.644217
16401	arbekacin	C22 H44 N6 O10	552.31458	553.32185	11 bottom	half	154305.5603	6691.765061	2	4731.792453
16401	arbekacin	C22 H44 N6 O10	552.31458	553.32185	18 bottom	half	152436.5503	8695.998744	2	6148.999681
16401	arbekacin	C22 H44 N6 O10	552.31458	553.32185	29 bottom	half	253124.0077	5909.051947	2	4178.330702
16541	astromicin	C17 H35 N5 O6	405.26031	406.26759	25 bottom	half	129316.9253	3906.249281	2	2762.135355

16541 astromicin	C17 H35 N5 O6	405.26031	406.26759	29 bottom	quarter	146172.1689	24845.13664	2	17568.1646
16541 astromicin	C17 H35 N5 O6	405.26031	406.26759	29 top	quarter	234054.3867	96026.51153	2	67900.99748
16671 aurantiogliocladin	C10 H12 O4	196.07357	197.08084	4 bottom	half	210620.9596	18409.94331	2	13017.79576
16671 aurantiogliocladin	C10 H12 O4	196.07357	197.08084	8 bottom	half	788945.0658	171419.0714	2	121211.5878
16671 aurantiogliocladin	C10 H12 O4	196.07357	197.08084	29 bottom	half	1779005.903	56459.57948	2	39922.95151
16671 aurantiogliocladin	C10 H12 O4	196.07357	197.08084	29 middle	half	1494769.911	442631.4088	2	312987.6707
16672 aurantiogliocladin	C10 H12 O4	196.07357	197.08085	29 top	quarter	1476791.632	442385.004	2	312813.4362
16673 aurantiogliocladin	C10 H12 O4	196.07359	197.08086	1 middle	quarter	1194202.593	157666.9796	2	111487.3904
16673 aurantiogliocladin	C10 H12 O4	196.07359	197.08086	8 bottom	half	731626.6108	231483.5785	2	163683.6081
16673 aurantiogliocladin	C10 H12 O4	196.07359	197.08086	15 bottom	half	339800.2028	26982.25085	2	19079.33254
16673 aurantiogliocladin	C10 H12 O4	196.07359	197.08086	25 bottom	half	658496.4775	11605.18188	2	8206.102804
16673 aurantiogliocladin	C10 H12 O4	196.07359	197.08086	29 bottom	half	1471967.437	142652.6639	2	100870.666
16673 aurantiogliocladin	C10 H12 O4	196.07359	197.08086	29 middle	half	1167282.382	203034.6215	2	143567.1577
16673 aurantiogliocladin	C10 H12 O4	196.07359	197.08086	29 middle	quarter	1274043.569	63832.27473	2	45136.23432
16673 aurantiogliocladin	C10 H12 O4	196.07359	197.08086	29 top	quarter	1474398.206	220615.0054	2	155998.3663
16674 aurantiogliocladin	C10 H12 O4	196.07357	197.08084	25 bottom	half	629036.1429	604853.5452	2	427696.0434
16677 aurantiogliocladin	C10 H12 O4	196.07359	197.08087	29 middle	half	471597.8975	161686.297	2	114329.477
16678 aurantiogliocladin	C10 H12 O4	196.07359	197.08086	25 bottom	half	897780.5335	96102.80244	2	67954.9433
16685 aurantiogliocladin	C10 H12 O4	196.0736	197.08087	4 bottom	half	252724.5053	16149.86179	2	11419.67679
16685 aurantiogliocladin	C10 H12 O4	196.0736	197.08087	29 middle	half	366760.5845	36910.94294	2	26099.97805
16685 aurantiogliocladin	C10 H12 O4	196.0736	197.08087	29 top	half	313563.9398	49991.59887	2	35349.39856
16686 aurantiogliocladin	C10 H12 O4	196.07356	197.08084	29 bottom	quarter	369556.6653	269566.7351	2	190612.4664
16687 aurantiogliocladin	C10 H12 O4	196.07361	197.08088	1 middle	quarter	281391.4883	25153.2218	2	17786.0137
16778 bacimethrin	C6 H9 N3 O2	155.06951	156.07679	4 bottom	half	199329.0623	30530.92654	2	21588.62519
16778 bacimethrin	C6 H9 N3 O2	155.06951	156.07679	29 top	quarter	225269.1902	25188.68309	2	17811.08862
17136 bestatin ubenimex	C16 H24 N2 O4	308.1738	309.18105	4 bottom	half	342096.6901	67508.78197	2	47735.91752
17137 bestatin ubenimex	C16 H24 N2 O4	308.1738	309.181	29 middle	half	120217.6821	25039.34732	2	17705.49229
17138 bestatin ubenimex	C16 H24 N2 O4	308.17378	309.18106	1 bottom	quarter	298350.6283	34483.21976	2	24383.31853
17138 bestatin ubenimex	C16 H24 N2 O4	308.17378	309.18106	1 top	quarter	196580.4893	25566.09939	2	18077.96225
17138 bestatin ubenimex	C16 H24 N2 O4	308.17378	309.18106	15 bottom	half	303667.373	10820.18325	2	7651.024948
17138 bestatin ubenimex	C16 H24 N2 O4	308.17378	309.18106	18 bottom	half	246720.2375	34678.40296	2	24521.3339
17138 bestatin ubenimex	C16 H24 N2 O4	308.17378	309.18106	29 bottom	half	303764.9361	11339.68081	2	8018.365197
17435 brefeldin a	C16 H24 O4	280.16761	281.17489	1 middle	half	1446480.047	137881.6172	2	97497.02649
17435 brefeldin a	C16 H24 O4	280.16761	281.17489	1 middle	quarter	1664806.705	192650.0478	2	136224.1552
17435 brefeldin a	C16 H24 O4	280.16761	281.17489	25 bottom	half	849452.7959	151571.4403	2	107177.1933
17435 brefeldin a	C16 H24 O4	280.16761	281.17489	29 bottom	half	391614.7958	35219.81812	2	24904.17222
17436 brefeldin a	C16 H24 O4	280.16747	281.17475	1 middle	quarter	739450.5612	85929.21942	2	60761.13375
17437 brefeldin a	C16 H24 O4	280.16759	281.17487	25 bottom	half	354851.949	76768.35969	2	54283.42772
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	1 bottom	half	1002933.97	40358.5502	2	28537.80453
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	1 bottom	quarter	773020.5417	52904.41749	2	37409.07236
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	1 middle	half	2287174.867	232135.0064	2	164144.2371
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	1 middle	quarter	1032707.456	209758.3757	2	148321.5699
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	1 top	half	2745432.143	233286.5406	2	164958.4948
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	1 top	quarter	1635186.324	216798.6098	2	153299.7672
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	4 bottom	half	258359.1212	51624.84851	2	36504.28046

17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	8 bottom	half	182750.2348	48430.41582	2	34245.47544
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	11 bottom	half	493297.5103	686.2484923	2	485.2509625
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	15 bottom	half	304657.4695	56263.2763	2	39784.1442
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	18 bottom	half	270012.0856	23613.7212	2	16697.42239
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	25 bottom	half	801038.8696	23616.68401	2	16699.51742
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	29 bottom	half	1134179.33	71688.36361	2	50691.32804
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	29 bottom	quarter	594700.7817	16338.31176	2	11552.93104
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	29 middle	half	1770758.279	223993.3049	2	158387.1848
17611 caerulomycin a	C12 H11 N3 O2	229.08522	230.0925	29 middle	quarter	218889.5363	21768.89906	2	15392.93614
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	1 bottom	quarter	322099.6292	4042.294886	2	2858.334125
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	1 middle	half	403038.1092	44287.65622	2	31316.10204
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	1 middle	quarter	177393.7052	3566.300508	2	2521.755273
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	1 top	half	490455.8914	14020.57266	2	9914.042007
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	1 top	quarter	210352.2533	20216.99674	2	14295.57549
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	4 bottom	half	476252.4955	34518.13788	2	24408.00937
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	8 bottom	half	276663.7203	29036.78458	2	20532.10728
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	11 bottom	half	354465.1538	58996.81677	2	41717.0492
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	15 bottom	half	348268.9545	5641.478386	2	3989.127622
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	18 bottom	half	339686.5105	33263.20898	2	23520.64064
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	22 bottom	half	113524.1499	9305.370425	2	6579.890529
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	29 bottom	half	129161.4034	6414.408572	2	4535.671798
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	29 bottom	quarter	195671.4146	9744.67732	2	6890.527413
17612 caerulomycin a	C12 H11 N3 O2	229.08523	230.0925	29 middle	quarter	165116.6212	9450.648842	2	6682.617883
17613 caerulomycin a	C12 H11 N3 O2	229.08524	230.09252	29 middle	half	178892.1961	100.6441603	2	71.1661682
17613 caerulomycin a	C12 H11 N3 O2	229.08524	230.09252	29 middle	quarter	202841.1176	5534.070911	2	3913.179069
18358 clofoctol	C21 H26 Cl2 O	364.13744	365.14472	4 bottom	half	206365.8736	34586.73685	2	24456.51617
18376 cloranolol	C13 H19 Cl2 N O2	291.07918	292.08646	1 bottom	half	252975.3266	16208.4973	2	11461.13835
18376 cloranolol	C13 H19 Cl2 N O2	291.07918	292.08646	1 bottom	quarter	196624.1414	6127.088234	2	4332.505639
18376 cloranolol	C13 H19 Cl2 N O2	291.07918	292.08646	1 middle	quarter	236813.0922	381.517637	2	269.7737083
18376 cloranolol	C13 H19 Cl2 N O2	291.07918	292.08646	1 top	half	233013.4088	53412.52693	2	37768.35999
18376 cloranolol	C13 H19 Cl2 N O2	291.07918	292.08646	1 top	quarter	190108.4784	31256.67601	2	22101.80757
18376 cloranolol	C13 H19 Cl2 N O2	291.07918	292.08646	4 bottom	half	184281.6147	10052.35694	2	7108.089762
18376 cloranolol	C13 H19 Cl2 N O2	291.07918	292.08646	8 bottom	half	126237.8963	24010.90973	2	16978.27709
18376 cloranolol	C13 H19 Cl2 N O2	291.07918	292.08646	11 bottom	half	133749.4859	9029.541169	2	6384.849792
18376 cloranolol	C13 H19 Cl2 N O2	291.07918	292.08646	15 bottom	half	175866.9944	8485.379241	2	6000.069202
18376 cloranolol	C13 H19 Cl2 N O2	291.07918	292.08646	18 bottom	half	108998.5521	6551.035588	2	4632.281688
18507 cordycepin	C10 H13 N5 O3	251.10228	269.13606	1 bottom	half	2695060.674	14668.10828	2	10371.91883
18507 cordycepin	C10 H13 N5 O3	251.10228	269.13606	1 bottom	quarter	3619575.859	134648.7388	2	95211.03628
18507 cordycepin	C10 H13 N5 O3	251.10228	269.13606	1 middle	half	3326926.632	121625.0699	2	86001.91166
18507 cordycepin	C10 H13 N5 O3	251.10228	269.13606	1 middle	quarter	3362431.545	676662.7049	2	478472.7872
18507 cordycepin	C10 H13 N5 O3	251.10228	269.13606	1 top	quarter	3338538.803	7647.700938	2	5407.741194
18507 cordycepin	C10 H13 N5 O3	251.10228	269.13606	4 bottom	half	2901216.902	68863.88083	2	48694.11711
18507 cordycepin	C10 H13 N5 O3	251.10228	269.13606	8 bottom	half	2727293.214	245253.0104	2	173420.0667
18507 cordycepin	C10 H13 N5 O3	251.10228	269.13606	15 bottom	half	3336347.436	687761.6067	2	486320.896
18508 cordycepin	C10 H13 N5 O3	251.10196	252.10919	1 middle	quarter	384650.5422	119298.5037	2	84356.78095

18508 cordycepin	C10 H13 N5 O3	251.10196	252.10919	18 bottom	half	340857.081	61968.71332	2	43818.49741
18508 cordycepin	C10 H13 N5 O3	251.10196	252.10919	29 middle	quarter	564166.0981	47895.90838	2	33867.52161
18508 cordycepin	C10 H13 N5 O3	251.10196	252.10919	29 top	half	404840.7103	88852.05517	2	62827.89073
18509 cordycepin	C10 H13 N5 O3	251.10193	252.10921	4 bottom	half	648479.2327	80929.68575	2	57225.92959
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	1 bottom	half	6793652.79	2431487.887	2	1719321.573
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	1 bottom	quarter	9289440.43	1884083.203	2	1332248.009
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	1 middle	half	8874811.071	535912.0901	2	378947.073
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	1 middle	quarter	4414266.267	363645.6558	2	257136.3092
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	1 top	half	12695860.74	2564516.781	2	1813387.206
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	1 top	quarter	8799480.215	329788.5924	2	233195.75
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	4 bottom	half	2481446.8	815340.8404	2	576533.0372
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	8 bottom	half	11921061	1609947.545	2	1138404.826
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	11 bottom	half	8922592.415	964626.4791	2	682093.9247
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	15 bottom	half	7103144.288	1473467.854	2	1041899.111
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	18 bottom	half	6409528.406	781370.7857	2	552512.5812
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	25 bottom	half	6610594.813	4575.603027	2	3235.439928
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	29 bottom	half	9933327.355	496605.3902	2	351153.039
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	29 middle	half	13265612.54	358120.1772	2	253229.2058
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	29 top	half	2467151.118	72036.28778	2	50937.34758
18647 cryptotanshinone	C19 H20 O3	296.14143	297.14871	29 top	quarter	8733689.706	5284487.457	2	3736696.916
18648 cryptotanshinone	C19 H20 O3	296.14142	297.14869	22 bottom	half	5089695.42	1129931.827	2	798982.4573
18648 cryptotanshinone	C19 H20 O3	296.14142	297.14869	29 middle	quarter	8063886.882	1553386.617	2	1098410.211
18649 cryptotanshinone	C19 H20 O3	296.14143	297.14871	29 bottom	quarter	5419368.582	196167.6912	2	138711.5047
18771 cycloheximide	C15 H23 N O4	281.16309	282.17036	29 top	quarter	236178.5874	30639.01331	2	21665.05408
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	1 bottom	half	12408293.75	471267.4463	2	333236.407
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	1 bottom	quarter	14835522.34	1206688.497	2	853257.6193
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	1 middle	half	9996967.165	175213.0372	2	123894.3268
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	1 middle	quarter	13973087.18	3827877.455	2	2706718.106
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	1 top	half	10507105.06	581711.7231	2	411332.3041
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	1 top	quarter	12083702.69	837097.5177	2	591917.3312
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	4 bottom	half	18205100.12	1397229.986	2	987990.7982
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	8 bottom	half	20603870.48	2072863.532	2	1465735.86
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	11 bottom	half	13795006.28	16942.49377	2	11980.15224
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	15 bottom	half	17042696.1	405970.0718	2	287064.1907
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	18 bottom	half	9696076.294	583742.6453	2	412768.383
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	22 bottom	half	3064692.612	154566.1243	2	109294.7547
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	25 bottom	half	9544785.203	172834.9223	2	122212.7456
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	29 bottom	half	12522570.02	332594.7307	2	235179.9895
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	29 bottom	quarter	8051011.647	293575.1712	2	207588.9944
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	29 middle	half	11432088.49	321316.5723	2	227205.1271
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	29 middle	quarter	17440133.74	697379.8226	2	493122.0016
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	29 top	half	11244598.06	130651.3448	2	92384.45188
19037 dacarbazine	C6 H10 N6 O	182.09194	183.09921	29 top	quarter	11855854.15	969635.7102	2	685635.986
19049 daidzin	C21 H20 O9	416.11068	439.09989	1 bottom	half	17768984.3	536818.3672	2	379587.9077
19049 daidzin	C21 H20 O9	416.11068	439.09989	1 bottom	quarter	29262691.9	515637.3101	2	364610.6386

19049 daidzin	C21 H20 O9	416.11068	439.09989	1 middle	half	44050916.97	664632.3765	2	469966.0604
19049 daidzin	C21 H20 O9	416.11068	439.09989	1 middle	quarter	105204193.3	6347955.862	2	4488682.637
19049 daidzin	C21 H20 O9	416.11068	439.09989	1 top	half	38638595.31	2859919.093	2	2022268.184
19049 daidzin	C21 H20 O9	416.11068	439.09989	1 top	quarter	38736351.63	2332456.664	2	1649295.924
19049 daidzin	C21 H20 O9	416.11068	439.09989	4 bottom	half	26056395.73	337126.4375	2	238384.3901
19049 daidzin	C21 H20 O9	416.11068	439.09989	8 bottom	half	22289121.96	1800131.951	2	1272885.51
19049 daidzin	C21 H20 O9	416.11068	439.09989	11 bottom	half	39523546.89	1324143.973	2	936311.1828
19049 daidzin	C21 H20 O9	416.11068	439.09989	15 bottom	half	23489416.3	833620.8482	2	589458.9547
19049 daidzin	C21 H20 O9	416.11068	439.09989	18 bottom	half	19118456.8	1743988.143	2	1233185.842
19049 daidzin	C21 H20 O9	416.11068	439.09989	22 bottom	half	17315694.29	1296407.295	2	916698.3892
19049 daidzin	C21 H20 O9	416.11068	439.09989	25 bottom	half	120470294.1	7428958.961	2	5253067.259
19049 daidzin	C21 H20 O9	416.11068	439.09989	29 bottom	half	75876209.85	631196.0419	2	446323.0015
19049 daidzin	C21 H20 O9	416.11068	439.09989	29 bottom	quarter	464807255.9	24681945.57	2	17452771.09
19049 daidzin	C21 H20 O9	416.11068	439.09989	29 middle	half	47206267.03	281333.3174	2	198932.6965
19049 daidzin	C21 H20 O9	416.11068	439.09989	29 middle	quarter	38254824.55	538215.7338	2	380575.9951
19049 daidzin	C21 H20 O9	416.11068	439.09989	29 top	half	16105897.72	380808.8353	2	269272.5098
19049 daidzin	C21 H20 O9	416.11068	439.09989	29 top	quarter	49556617.39	4546791.883	2	3215067.373
19050 daidzin	C21 H20 O9	416.11066	417.11797	29 middle	quarter	157653.1169	1604.056432	2	1134.23918
20949 ethacridine	C15 H15 N3 O	253.12159	254.12887	22 bottom	half	501252.515	37348.96235	2	26409.70455
20949 ethacridine	C15 H15 N3 O	253.12159	254.12887	29 bottom	half	1064109.206	55572.55032	2	39295.72718
20949 ethacridine	C15 H15 N3 O	253.12159	254.12887	29 middle	half	1255098.392	78073.6316	2	55206.39433
20949 ethacridine	C15 H15 N3 O	253.12159	254.12887	29 middle	quarter	707084.6499	64449.51434	2	45572.68863
20949 ethacridine	C15 H15 N3 O	253.12159	254.12887	29 top	quarter	868241.4077	25930.35373	2	18335.52896
20950 ethacridine	C15 H15 N3 O	253.12162	254.1289	18 bottom	half	115050.5	2410.79897	2	1704.6923
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	1 bottom	half	1079840.324	62062.50011	2	43884.81468
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	1 bottom	quarter	1037994.718	3028.443716	2	2141.433088
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	1 middle	half	1199249.649	63521.31496	2	44916.35256
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	1 top	half	1854159.274	28066.72595	2	19846.17224
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	1 top	quarter	907842.7405	12135.75363	2	8581.273687
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	4 bottom	half	1159734.945	100232.8203	2	70875.30694
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	8 bottom	half	1993983.62	190439.2493	2	134660.8846
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	11 bottom	half	2290208.21	47836.63932	2	33825.61205
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	15 bottom	half	2397343.676	88161.15277	2	62339.34896
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	18 bottom	half	1529578.347	32625.11715	2	23069.44157
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	22 bottom	half	1228338.792	78134.78184	2	55249.63408
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	29 bottom	half	1776488.535	81463.06068	2	57603.08262
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	29 middle	half	1722335.936	10617.33923	2	7507.592567
21015 ethyl 1 2 chlorophenyl 3 5 dimethyl 1h pyrazole + C14 H15 Cl N2 O2		278.08239	279.08967	29 top	half	6800461.527	106675.0845	2	75430.67565
21500 feroxacin	C17 H18 F3 N3 O3	369.12999	370.13727	1 top	half	155864.2002	30470.64235	2	21545.99783
21544 flumethasone	C22 H28 F2 O5	410.19174	411.19902	1 top	quarter	508043.4542	319444.2634	2	225881.2049
21702 fomecin a	C8 H8 O5	184.03722	185.0445	1 middle	quarter	156784.7159	24404.92885	2	17256.89068
21746 fortimicin b	C15 H32 N4 O5	348.23881	349.24628	1 bottom	half	291472.0181	57226.86091	2	40465.50141
21777 fusaric acid	C10 H13 N O2	179.09466	180.10194	15 bottom	half	1169339.867	40050.59645	2	28320.04834
21777 fusaric acid	C10 H13 N O2	179.09466	180.10194	29 middle	quarter	878941.7991	83103.62545	2	58763.13709
21779 fusaric acid	C10 H13 N O2	179.09466	180.10194	1 bottom	half	123116.3609	10987.62209	2	7769.422087

21779 fusaric acid	C10 H13 N O2	179.09466	180.10194	1 middle	half	149107.1587	17215.16007	2	12172.95643
21782 fusaric acid	C10 H13 N O2	179.09465	180.10193	29 top	half	224521.6832	26108.96887	2	18461.82894
21782 fusaric acid	C10 H13 N O2	179.09465	180.10193	29 top	quarter	193779.1255	1914.214917	2	1353.554349
21965 gliorosein	C10 H14 O4	198.08923	199.0965	4 bottom	half	404842.1616	8930.760305	2	6315.001173
21965 gliorosein	C10 H14 O4	198.08923	199.0965	29 top	half	323866.5391	86266.2632	2	60999.4597
21971 gliorosein	C10 H14 O4	198.08927	199.09653	1 top	half	193124.2743	13678.75848	2	9672.342879
22101 guamecycline	C29 H38 N8 O8	626.28168	644.31551	1 bottom	quarter	318768.9375	36435.04731	2	25763.46903
22101 guamecycline	C29 H38 N8 O8	626.28168	644.31551	1 middle	half	248747.5822	12657.47442	2	8950.185992
22101 guamecycline	C29 H38 N8 O8	626.28168	644.31551	1 middle	quarter	272412.8868	36681.14136	2	25937.4838
22101 guamecycline	C29 H38 N8 O8	626.28168	644.31551	1 top	quarter	246801.08	43221.48246	2	30562.20334
22101 guamecycline	C29 H38 N8 O8	626.28168	644.31551	4 bottom	half	643761.7272	46376.832	2	32793.3724
22101 guamecycline	C29 H38 N8 O8	626.28168	644.31551	15 bottom	half	434903.6654	74861.93097	2	52935.37904
22101 guamecycline	C29 H38 N8 O8	626.28168	644.31551	18 bottom	half	289613.7644	18861.1645	2	13336.85732
22101 guamecycline	C29 H38 N8 O8	626.28168	644.31551	29 bottom	half	337930.8897	41668.57552	2	29464.13231
22101 guamecycline	C29 H38 N8 O8	626.28168	644.31551	29 middle	quarter	371429.8238	31446.80206	2	22236.24699
22350 honokiol	C18 H18 O2	266.13084	267.13813	29 middle	quarter	1974950.531	300152.6283	2	212239.9589
23081 k 252a	C27 H21 N3 O5	467.14949	468.15677	1 bottom	quarter	719693.4806	19884.09838	2	14060.1808
23094 kalamycin	C16 H12 O6	300.06348	301.07076	1 middle	quarter	183946.5159	15288.71142	2	10810.75152
23094 kalamycin	C16 H12 O6	300.06348	301.07076	29 top	quarter	324123.826	28677.14871	2	20277.80632
23095 kalamycin	C16 H12 O6	300.0636	301.07088	4 bottom	half	141921.7944	4109.443815	2	2905.815588
23095 kalamycin	C16 H12 O6	300.0636	301.07088	29 bottom	half	179139.8081	2460.584145	2	1739.895735
23095 kalamycin	C16 H12 O6	300.0636	301.07088	29 middle	quarter	204391.3693	28262.97011	2	19984.93782
23095 kalamycin	C16 H12 O6	300.0636	301.07088	29 top	half	178256.9876	33262.98617	2	23520.48309
23095 kalamycin	C16 H12 O6	300.0636	301.07088	29 top	quarter	304067.7461	2969.57454	2	2099.806294
23314 leucomycin a1	C40 H67 N O14	785.45563	786.46291	29 bottom	half	1131559.846	52780.13295	2	37321.18992
23314 leucomycin a1	C40 H67 N O14	785.45563	786.46291	29 top	half	4362167.935	179235.3169	2	126738.508
24553 mevastatin	C23 H34 O5	390.24048	391.24761	1 top	quarter	635247.3895	17717.3523	2	12528.05995
24553 mevastatin	C23 H34 O5	390.24048	391.24761	15 bottom	half	720752.8967	283022.5392	2	200127.1567
24627 milbemycin a3	C31 H44 O7	528.30639	529.31366	1 middle	half	686863.4246	55994.47362	2	39594.07201
24892 mucidin	C16 H18 O3	258.12572	259.133	25 bottom	half	321636.3571	17413.44294	2	12313.16358
25306 n 3 chloro 2 methylphenyl 1 cyclohexyl 5 oxopyrri	C18 H23 Cl N2 O2	334.14566	335.15294	15 bottom	half	305355.33	42370.18623	2	29960.24601
25306 n 3 chloro 2 methylphenyl 1 cyclohexyl 5 oxopyrri	C18 H23 Cl N2 O2	334.14566	335.15294	29 bottom	half	397399.819	8279.428675	2	5854.44016
25310 n 3 chloro 2 methylphenyl 1 cyclohexyl 5 oxopyrri	C18 H23 Cl N2 O2	334.14481	335.15209	29 middle	half	135248.3378	19860.00203	2	14043.14211
25926 n allyl 6 diazo 5 oxonorleucyl 6 diazo 5 oxonorlei	C15 H20 N6 O5	364.14935	365.15663	1 bottom	quarter	263117.6244	16108.23527	2	11390.24239
25926 n allyl 6 diazo 5 oxonorleucyl 6 diazo 5 oxonorlei	C15 H20 N6 O5	364.14935	365.15663	1 middle	half	242023.9187	19045.78244	2	13467.40192
25926 n allyl 6 diazo 5 oxonorleucyl 6 diazo 5 oxonorlei	C15 H20 N6 O5	364.14935	365.15663	1 top	half	282298.4478	25609.9131	2	18108.94322
25926 n allyl 6 diazo 5 oxonorleucyl 6 diazo 5 oxonorlei	C15 H20 N6 O5	364.14935	365.15663	4 bottom	half	241326.1389	18546.38677	2	13114.27585
25926 n allyl 6 diazo 5 oxonorleucyl 6 diazo 5 oxonorlei	C15 H20 N6 O5	364.14935	365.15663	8 bottom	half	189827.3366	50406.16867	2	35642.54368
25926 n allyl 6 diazo 5 oxonorleucyl 6 diazo 5 oxonorlei	C15 H20 N6 O5	364.14935	365.15663	11 bottom	half	157439.1313	23483.9756	2	16605.6784
25926 n allyl 6 diazo 5 oxonorleucyl 6 diazo 5 oxonorlei	C15 H20 N6 O5	364.14935	365.15663	15 bottom	half	221643.6812	13917.34066	2	9841.045957
25926 n allyl 6 diazo 5 oxonorleucyl 6 diazo 5 oxonorlei	C15 H20 N6 O5	364.14935	365.15663	18 bottom	half	162845.2375	14224.9269	2	10058.54228
25926 n allyl 6 diazo 5 oxonorleucyl 6 diazo 5 oxonorlei	C15 H20 N6 O5	364.14935	365.15663	29 bottom	half	256437.6817	4433.148413	2	3134.709305
25926 n allyl 6 diazo 5 oxonorleucyl 6 diazo 5 oxonorlei	C15 H20 N6 O5	364.14935	365.15663	29 middle	half	285216.2562	14910.23768	2	10543.13017
25926 n allyl 6 diazo 5 oxonorleucyl 6 diazo 5 oxonorlei	C15 H20 N6 O5	364.14935	365.15663	29 middle	quarter	270194.3762	54837.88055	2	38776.2372
25926 n allyl 6 diazo 5 oxonorleucyl 6 diazo 5 oxonorlei	C15 H20 N6 O5	364.14935	365.15663	29 top	quarter	244997.5613	85724.91725	2	60616.6703

26311 n methyl 1 deoxynojirimycin	C7 H15 N O4	177.10012	178.1074	4 bottom	half	174840.312	26884.28421	2	19010.05967
27317 n2 4s 4as 6s 12as 4 dimethylamino 3 6 10 12 12 C29 H38 N4 O10		602.25741	620.29129	1 bottom	half	1758159.509	321170.0676	2	227101.5327
27317 n2 4s 4as 6s 12as 4 dimethylamino 3 6 10 12 12 C29 H38 N4 O10		602.25741	620.29129	1 bottom	quarter	1273159.606	145602.8368	2	102956.7533
27317 n2 4s 4as 6s 12as 4 dimethylamino 3 6 10 12 12 C29 H38 N4 O10		602.25741	620.29129	1 top	half	1131483.443	249433.0165	2	176375.7774
27317 n2 4s 4as 6s 12as 4 dimethylamino 3 6 10 12 12 C29 H38 N4 O10		602.25741	620.29129	4 bottom	half	2559548.984	276623.9508	2	195602.6714
27317 n2 4s 4as 6s 12as 4 dimethylamino 3 6 10 12 12 C29 H38 N4 O10		602.25741	620.29129	8 bottom	half	2377220.098	489531.8123	2	346151.2641
27317 n2 4s 4as 6s 12as 4 dimethylamino 3 6 10 12 12 C29 H38 N4 O10		602.25741	620.29129	11 bottom	half	1007274.941	347297.4391	2	245576.3743
27317 n2 4s 4as 6s 12as 4 dimethylamino 3 6 10 12 12 C29 H38 N4 O10		602.25741	620.29129	15 bottom	half	2076632.086	217480.3422	2	153781.8247
27317 n2 4s 4as 6s 12as 4 dimethylamino 3 6 10 12 12 C29 H38 N4 O10		602.25741	620.29129	18 bottom	half	1944416.11	222769.3804	2	157521.7395
27317 n2 4s 4as 6s 12as 4 dimethylamino 3 6 10 12 12 C29 H38 N4 O10		602.25741	620.29129	29 top	half	2454186.007	318002.879	2	224861.9922
27633 nanafrocin	C16 H14 O6	302.07925	303.08653	25 bottom	half	127382.9553	27591.2895	2	19509.98791
27633 nanafrocin	C16 H14 O6	302.07925	303.08653	29 bottom	half	1962912.435	829366.415	2	586450.6161
27634 nanafrocin	C16 H14 O6	302.07923	303.08651	4 bottom	half	340357.6282	3750.124154	2	2651.73822
27634 nanafrocin	C16 H14 O6	302.07923	303.08651	15 bottom	half	278057.0463	90677.40223	2	64118.60602
27789 nicarbazin	C19 H18 N6 O6	426.12926	427.13653	11 bottom	half	600562.9727	31447.31399	2	22236.60897
27789 nicarbazin	C19 H18 N6 O6	426.12926	427.13653	15 bottom	half	674775.743	89694.77371	2	63423.78273
27790 nicarbazin	C19 H18 N6 O6	426.12905	427.13633	1 bottom	half	336804.2737	46861.23627	2	33135.89794
27790 nicarbazin	C19 H18 N6 O6	426.12905	427.13633	1 bottom	quarter	274147.5735	7680.308106	2	5430.797943
27790 nicarbazin	C19 H18 N6 O6	426.12905	427.13633	1 middle	half	285105.6809	14298.17657	2	10110.33761
27790 nicarbazin	C19 H18 N6 O6	426.12905	427.13633	1 top	half	304151.95	30248.47166	2	21388.89943
27790 nicarbazin	C19 H18 N6 O6	426.12905	427.13633	1 top	quarter	213136.9846	7481.284893	2	5290.06728
27790 nicarbazin	C19 H18 N6 O6	426.12905	427.13633	11 bottom	half	314451.082	3681.960764	2	2603.539424
27790 nicarbazin	C19 H18 N6 O6	426.12905	427.13633	15 bottom	half	379375.8084	50516.96064	2	35720.88543
27791 nicarbazin	C19 H18 N6 O6	426.1291	427.13638	1 top	half	172819.2991	12085.08853	2	8545.448049
27791 nicarbazin	C19 H18 N6 O6	426.1291	427.13638	4 bottom	half	145356.1262	17724.33758	2	12532.9993
27792 nicarbazin	C19 H18 N6 O6	426.12906	427.13634	15 bottom	half	138230.224	3774.290705	2	2668.826552
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	1 bottom	half	1352754.941	323178.4422	2	228521.668
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	1 bottom	quarter	995039.0688	95048.58443	2	67209.49859
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	1 middle	half	1142739.075	79382.96777	2	56132.23482
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	1 middle	quarter	1172737.692	654560.8026	2	462844.3822
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	1 top	half	1416321.334	43304.21935	2	30620.70715
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	1 top	quarter	1332236.797	358704.9128	2	253642.6763
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	8 bottom	half	1727097.058	117207.6737	2	82878.34088
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	11 bottom	half	1076167.203	302908.3404	2	214188.5416
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	15 bottom	half	995303.5489	187047.689	2	132262.6893
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	18 bottom	half	1165764.057	144270.6306	2	102014.7412
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	22 bottom	half	1053960.924	124687.2418	2	88167.19422
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	25 bottom	half	1293163.749	225195.9142	2	159237.558
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	29 bottom	half	1856512.399	456736.638	2	322961.574
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	29 bottom	quarter	2867122.984	29318.6294	2	20731.40166
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	29 middle	half	1251831.824	141944.3227	2	100369.7931
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	29 middle	quarter	1115556.135	24100.98285	2	17041.96841
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	29 top	half	720779.7986	27753.82142	2	19624.91533
31431 pirlimycin	C17 H31 Cl N2 O5	410.16472	411.172	29 top	quarter	2955470.427	1121320.365	2	792893.2338
31432 pirlimycin	C17 H31 Cl N2 O5	410.16474	411.17202	1 middle	half	1001185.78	74720.48509	2	52835.3617

31432 pirlimycin	C17 H31 Cl N2 O5	410.16474	411.17202	1 middle	quarter	800502.641	5005.909593	2	3539.712619
31432 pirlimycin	C17 H31 Cl N2 O5	410.16474	411.17202	1 top	half	948619.4545	265210.3034	2	187532.0039
31432 pirlimycin	C17 H31 Cl N2 O5	410.16474	411.17202	1 top	quarter	971948.2016	95926.5481	2	67830.31265
31432 pirlimycin	C17 H31 Cl N2 O5	410.16474	411.17202	18 bottom	half	805318.9374	91583.54393	2	64759.34496
31432 pirlimycin	C17 H31 Cl N2 O5	410.16474	411.17202	22 bottom	half	846387.8028	83200.12855	2	58831.3751
31432 pirlimycin	C17 H31 Cl N2 O5	410.16474	411.17202	29 bottom	half	1548162.655	260330.1188	2	184081.1924
31432 pirlimycin	C17 H31 Cl N2 O5	410.16474	411.17202	29 bottom	quarter	2437429.248	256026.7091	2	181038.2222
31432 pirlimycin	C17 H31 Cl N2 O5	410.16474	411.17202	29 middle	half	1315488.007	40513.62905	2	28647.46183
31432 pirlimycin	C17 H31 Cl N2 O5	410.16474	411.17202	29 top	quarter	1983788.285	98816.05446	2	69873.5022
31433 pirlimycin	C17 H31 Cl N2 O5	410.16475	411.17203	1 bottom	quarter	762376.6603	51880.93936	2	36685.36403
31433 pirlimycin	C17 H31 Cl N2 O5	410.16475	411.17203	1 middle	quarter	607622.7916	225.2099183	2	159.2474605
31433 pirlimycin	C17 H31 Cl N2 O5	410.16475	411.17203	1 top	quarter	737371.867	12049.10904	2	8520.006707
31433 pirlimycin	C17 H31 Cl N2 O5	410.16475	411.17203	8 bottom	half	1133625.701	122022.4504	2	86282.90217
31433 pirlimycin	C17 H31 Cl N2 O5	410.16475	411.17203	11 bottom	half	839878.0248	27510.93061	2	19453.16559
31433 pirlimycin	C17 H31 Cl N2 O5	410.16475	411.17203	15 bottom	half	820033.9241	161500.7738	2	114198.2923
31433 pirlimycin	C17 H31 Cl N2 O5	410.16475	411.17203	22 bottom	half	621855.0991	45805.18184	2	32389.1547
31433 pirlimycin	C17 H31 Cl N2 O5	410.16475	411.17203	29 bottom	half	1074284.095	21233.42431	2	15014.29832
31433 pirlimycin	C17 H31 Cl N2 O5	410.16475	411.17203	29 bottom	quarter	2322937.496	11823.89895	2	8360.759128
31433 pirlimycin	C17 H31 Cl N2 O5	410.16475	411.17203	29 top	quarter	1774978.962	278607.1361	2	197004.9953
31434 pirlimycin	C17 H31 Cl N2 O5	410.16482	411.1721	29 bottom	quarter	703787.7806	66020.43735	2	46683.49895
31435 pirlimycin	C17 H31 Cl N2 O5	410.16409	411.17134	29 top	quarter	192470.0346	6358.533556	2	4496.162196
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	1 bottom	half	564617.3971	13900.33395	2	9829.020394
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	1 bottom	quarter	535152.3792	59948.66577	2	42390.10809
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	1 middle	half	680229.1507	102868.5009	2	72739.01459
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	1 top	half	1346713.859	75609.5051	2	53463.99378
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	1 top	quarter	394543.7456	1684.807041	2	1191.338483
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	4 bottom	half	1027670.345	159324.125	2	112659.1692
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	8 bottom	half	996779.0329	70556.75889	2	49891.16267
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	11 bottom	half	935978.7521	89920.05959	2	63583.0839
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	15 bottom	half	797929.3958	26494.02368	2	18734.10381
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	18 bottom	half	800722.0811	65570.47189	2	46365.32532
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	22 bottom	half	388666.4752	21449.87447	2	15167.3517
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	29 middle	quarter	744276.906	338.0032145	2	239.004365
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	29 top	half	660395.5031	3608.405347	2	2551.52789
31473 piromidic acid	C14 H16 N4 O3	288.1224	289.12969	29 top	quarter	589725.8228	23645.46906	2	16719.87152
31502 pleuromutilin	C22 H34 O5	378.2415	379.24878	29 top	half	177468.1596	60852.64264	2	43029.31627
32141 quinoxin	C8 H6 N2 O2	162.04299	163.05024	29 top	half	714590.8944	70188.74278	2	49630.93598
32141 quinoxin	C8 H6 N2 O2	162.04299	163.05024	29 top	quarter	499499.7788	19037.66793	2	13461.66409
32142 quinoxin	C8 H6 N2 O2	162.04296	163.05023	29 top	half	383107.8454	67340.35797	2	47616.82377
32142 quinoxin	C8 H6 N2 O2	162.04296	163.05023	29 top	quarter	714472.1927	35721.41244	2	25258.85297
32143 quinoxin	C8 H6 N2 O2	162.04296	163.05024	1 bottom	quarter	623278.2938	44929.04354	2	31769.63136
32143 quinoxin	C8 H6 N2 O2	162.04296	163.05024	1 top	quarter	516373.5806	29665.9392	2	20976.98678
32143 quinoxin	C8 H6 N2 O2	162.04296	163.05024	4 bottom	half	889928.057	155927.0642	2	110257.0845
32143 quinoxin	C8 H6 N2 O2	162.04296	163.05024	29 top	half	806782.0575	38414.03612	2	27162.82543
32202 r flecainide	C17 H20 F6 N2 O3	414.13787	415.14514	8 bottom	half	2589401.211	225041.9225	2	159128.6694

32202 r flecainide	C17 H20 F6 N2 O3	414.13787	415.14514	11 bottom	half	2372277.611	53588.80648	2	37893.00846
32202 r flecainide	C17 H20 F6 N2 O3	414.13787	415.14514	15 bottom	half	2877084.804	148064.1696	2	104697.1784
32202 r flecainide	C17 H20 F6 N2 O3	414.13787	415.14514	18 bottom	half	1896354.411	143819.4376	2	101695.6996
32202 r flecainide	C17 H20 F6 N2 O3	414.13787	415.14514	22 bottom	half	1115535.732	163197.3017	2	115397.9187
32202 r flecainide	C17 H20 F6 N2 O3	414.13787	415.14514	29 bottom	half	2031322.87	86080.1254	2	60867.84039
32202 r flecainide	C17 H20 F6 N2 O3	414.13787	415.14514	29 middle	quarter	2317661.049	4681.13199	2	3310.060173
32202 r flecainide	C17 H20 F6 N2 O3	414.13787	415.14514	29 top	half	2302579.089	198193.4264	2	140143.9158
32202 r flecainide	C17 H20 F6 N2 O3	414.13787	415.14514	29 top	quarter	2473143.811	170567.8087	2	120609.6542
32340 resorcinomycin b	C13 H18 N4 O5	310.12654	333.11574	18 bottom	half	458426.978	9138.507229	2	6461.900432
32497 rimonabant	C22 H21 Cl3 N4 O	462.07979	463.08707	1 middle	quarter	1141723.901	74928.61061	2	52982.52866
32497 rimonabant	C22 H21 Cl3 N4 O	462.07979	463.08707	22 bottom	half	188338.387	3503.094835	2	2477.062113
32497 rimonabant	C22 H21 Cl3 N4 O	462.07979	463.08707	29 bottom	half	613397.2704	12270.07846	2	8676.255682
32565 roridin a	C29 H40 O9	532.26516	533.27243	29 middle	half	555695.2908	89558.95561	2	63327.74483
32566 roridin a	C29 H40 O9	532.26469	533.27197	29 middle	half	375367.2574	22264.12114	2	15743.11103
32570 rosoxacin	C17 H14 N2 O3	294.10063	295.10791	1 bottom	half	167711.8043	20292.03793	2	14348.63763
32570 rosoxacin	C17 H14 N2 O3	294.10063	295.10791	18 bottom	half	141846.7617	1608.243733	2	1137.20005
32582 rpr128515	C27 H30 N4 O3	458.23154	459.23882	25 bottom	half	305434.3911	232315.1153	2	164271.5934
32898 sisomicin sisomycin	C19 H37 N5 O7	447.26771	448.27498	29 middle	half	6003007.87	516048.0113	2	364901.0482
32898 sisomicin sisomycin	C19 H37 N5 O7	447.26771	448.27498	29 middle	quarter	8649458.96	1510651.91	2	1068192.209
32924 sordarin	C27 H40 O8	492.27357	493.28079	1 bottom	half	403388.0879	10763.81211	2	7611.164536
32924 sordarin	C27 H40 O8	492.27357	493.28079	1 bottom	quarter	749060.0832	4865.35504	2	3440.325542
32924 sordarin	C27 H40 O8	492.27357	493.28079	1 middle	half	776778.296	126928.0732	2	89751.70129
32924 sordarin	C27 H40 O8	492.27357	493.28079	1 middle	quarter	675009.2736	53892.25104	2	38107.57616
32924 sordarin	C27 H40 O8	492.27357	493.28079	1 top	half	841266.2479	30035.31554	2	21238.17529
32924 sordarin	C27 H40 O8	492.27357	493.28079	1 top	quarter	808208.4365	64237.36705	2	45422.67784
32924 sordarin	C27 H40 O8	492.27357	493.28079	4 bottom	half	1084253.019	381433.9881	2	269714.5596
32924 sordarin	C27 H40 O8	492.27357	493.28079	8 bottom	half	819157.9366	487743.5124	2	344886.7451
32924 sordarin	C27 H40 O8	492.27357	493.28079	11 bottom	half	792203.5435	430685.8554	2	304540.8889
32924 sordarin	C27 H40 O8	492.27357	493.28079	15 bottom	half	445343.3832	381251.3984	2	269585.4492
32924 sordarin	C27 H40 O8	492.27357	493.28079	18 bottom	half	748946.7568	54374.99791	2	38448.92975
32924 sordarin	C27 H40 O8	492.27357	493.28079	22 bottom	half	330504.6369	137462.705	2	97200.81084
32924 sordarin	C27 H40 O8	492.27357	493.28079	25 bottom	half	955831.3972	250489.5613	2	177122.8674
32924 sordarin	C27 H40 O8	492.27357	493.28079	29 bottom	half	602205.6474	11781.8112	2	8330.998591
32924 sordarin	C27 H40 O8	492.27357	493.28079	29 middle	quarter	698245.0038	44857.79222	2	31719.24907
32924 sordarin	C27 H40 O8	492.27357	493.28079	29 top	half	1033729.411	179204.9456	2	126717.0323
32924 sordarin	C27 H40 O8	492.27357	493.28079	29 top	quarter	366343.3704	107504.6347	2	76017.25619
32926 sordarin	C27 H40 O8	492.27346	515.26266	29 bottom	quarter	1219367.574	23158.24838	2	16375.35447
32943 sphingofungin c	C22 H41 N O7	431.28823	432.29551	29 middle	quarter	450653.4583	52544.77424	2	37154.76618
33334 tazobactam	C10 H12 N4 O5 S	300.05235	301.05963	4 bottom	half	1583525.627	60069.5596	2	42475.59294
33334 tazobactam	C10 H12 N4 O5 S	300.05235	301.05963	25 bottom	half	140861.1529	4163.757773	2	2944.221357
33334 tazobactam	C10 H12 N4 O5 S	300.05235	301.05963	29 middle	half	242655.2985	1241.506997	2	877.8780164
33334 tazobactam	C10 H12 N4 O5 S	300.05235	301.05963	29 top	half	1317207.551	8607.459021	2	6086.392642
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	1 bottom	half	5297618.682	262303.3318	2	185476.4646
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	1 bottom	quarter	6234244.627	160147.7366	2	113241.5506
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	1 middle	half	5840531.025	210311.9711	2	148713.0209

33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	1 middle	quarter	5289546.255	179953.0568	2	127246.0268
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	1 top	half	6384069.597	203730.6454	2	144059.3209
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	1 top	quarter	5780371.369	188661.298	2	133403.6832
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	4 bottom	half	5508381.552	150041.3615	2	106095.2642
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	8 bottom	half	5508606.102	491941.1136	2	347854.8974
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	11 bottom	half	5334605.597	54467.29843	2	38514.19607
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	15 bottom	half	5988453.272	301618.491	2	213276.4803
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	18 bottom	half	4231001.671	65474.24409	2	46297.28199
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	22 bottom	half	1900049.202	194942.321	2	137845.0372
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	25 bottom	half	5298641.223	151484.4262	2	107115.665
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	29 bottom	half	4839732.069	167427.3745	2	118389.0319
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	29 bottom	quarter	5277087.866	75286.2676	2	53235.43035
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	29 middle	half	4636057.854	17964.05193	2	12702.50294
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	29 middle	quarter	4537282.251	291095.637	2	205835.6989
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	29 top	half	4017598.102	19556.87929	2	13828.80197
33622 thiabendazole	C10 H7 N3 S	201.03608	202.04336	29 top	quarter	4535740.765	208743.5574	2	147603.985
33690 thymol	C10 H14 O	150.10452	168.13834	29 top	quarter	1088221.691	79099.38966	2	55931.71481
33691 thymol	C10 H14 O	150.10451	151.11179	1 bottom	quarter	1418725.787	349116.8146	2	246862.867
33691 thymol	C10 H14 O	150.10451	151.11179	1 middle	quarter	1037083.657	151699.3507	2	107267.6396
33691 thymol	C10 H14 O	150.10451	151.11179	1 top	half	1268544.606	321201.5819	2	227123.8167
33691 thymol	C10 H14 O	150.10451	151.11179	1 top	quarter	958725.2556	79112.94325	2	55941.29865
33691 thymol	C10 H14 O	150.10451	151.11179	8 bottom	half	1272416.866	309295.4658	2	218704.9212
33691 thymol	C10 H14 O	150.10451	151.11179	25 bottom	half	668250.9814	25507.27437	2	18036.36668
33693 thymol	C10 H14 O	150.10452	151.11179	1 bottom	quarter	969841.2129	6150.642174	2	4349.16079
33695 thymol	C10 H14 O	150.10452	151.11179	29 bottom	quarter	451996.1416	127183.7987	2	89932.52655
33697 thymol	C10 H14 O	150.10451	151.11179	29 bottom	quarter	519227.3837	19005.08784	2	13438.62649
33700 thymol	C10 H14 O	150.10451	151.11179	1 top	quarter	674954.992	32758.52605	2	23163.77591
33700 thymol	C10 H14 O	150.10451	151.11179	25 bottom	half	534944.2352	199364.5534	2	140972.0277
33936 toyocamycin	C12 H13 N5 O4	291.09692	314.08617	4 bottom	half	407155.8686	9168.370056	2	6483.016639
34310 trospectomycin	C17 H30 N2 O7	374.20714	375.21441	25 bottom	half	403142.9883	11224.75205	2	7937.098295
34314 trospectomycin	C17 H30 N2 O7	374.20696	375.21423	11 bottom	half	339617.6773	26648.82969	2	18843.56818
34314 trospectomycin	C17 H30 N2 O7	374.20696	375.21423	29 middle	quarter	308633.48	139025.6394	2	98305.97235
34329 tuberin	C10 H11 N O2	177.07902	178.08629	11 bottom	half	605629.0795	101019.5074	2	71431.57871
34329 tuberin	C10 H11 N O2	177.07902	178.08629	15 bottom	half	3877853.344	46393.76568	2	32805.34632
34331 tuberin	C10 H11 N O2	177.07901	178.08629	1 bottom	quarter	649933.8789	62221.4885	2	43997.23646
34331 tuberin	C10 H11 N O2	177.07901	178.08629	11 bottom	half	511103.0722	45037.335	2	31846.20499
34331 tuberin	C10 H11 N O2	177.07901	178.08629	18 bottom	half	715067.2081	464518.9139	2	328464.474
34335 tuberin	C10 H11 N O2	177.07901	178.08629	1 middle	quarter	1134577.52	25129.91777	2	17769.53527
34752 xenysalate	C19 H23 N O3	313.16799	314.17527	1 top	quarter	2685563.145	116440.7769	2	82336.06294
34752 xenysalate	C19 H23 N O3	313.16799	314.17527	25 bottom	half	190848.4876	44765.03719	2	31653.66136
34753 xenysalate	C19 H23 N O3	313.16786	314.17513	29 top	half	584505.0447	76470.49346	2	54072.80449
34754 xenysalate	C19 H23 N O3	313.1679	314.17519	8 bottom	half	155154.4664	14783.42476	2	10453.45989
34779 xibornol	C18 H26 O	258.19848	259.20576	1 bottom	half	7653296.314	724361.1206	2	512200.6604
34779 xibornol	C18 H26 O	258.19848	259.20576	1 bottom	quarter	15156299.63	1977419.519	2	1398246.751
34779 xibornol	C18 H26 O	258.19848	259.20576	1 middle	half	14452643.85	567084.9087	2	400989.5844

34779 xibornol	C18 H26 O	258.19848	259.20576	1 middle	quarter	11501214.02	1182579.763	2	836210.1697
34779 xibornol	C18 H26 O	258.19848	259.20576	1 top	half	14622420.86	751466.2731	2	531366.8975
34779 xibornol	C18 H26 O	258.19848	259.20576	1 top	quarter	14201596.56	1230962.308	2	870421.7956
34779 xibornol	C18 H26 O	258.19848	259.20576	4 bottom	half	5881959.053	474685.8079	2	335653.5537
34779 xibornol	C18 H26 O	258.19848	259.20576	8 bottom	half	12021818.49	1109808.618	2	784753.1993
34779 xibornol	C18 H26 O	258.19848	259.20576	11 bottom	half	12927393.11	414070.6076	2	292792.1345
34779 xibornol	C18 H26 O	258.19848	259.20576	15 bottom	half	8810365.844	2545755.732	2	1800121.141
34779 xibornol	C18 H26 O	258.19848	259.20576	18 bottom	half	8907236.124	1016897.132	2	719054.858
34779 xibornol	C18 H26 O	258.19848	259.20576	22 bottom	half	5679789.863	456062.9818	2	322485.2271
34779 xibornol	C18 H26 O	258.19848	259.20576	25 bottom	half	15531192.87	273947.0617	2	193709.825
34779 xibornol	C18 H26 O	258.19848	259.20576	29 bottom	half	9774538.174	193589.5661	2	136888.495
34779 xibornol	C18 H26 O	258.19848	259.20576	29 bottom	quarter	26262635.05	782051.4478	2	552993.8819
34779 xibornol	C18 H26 O	258.19848	259.20576	29 middle	half	10443519.58	547327.3226	2	387018.8613
34779 xibornol	C18 H26 O	258.19848	259.20576	29 middle	quarter	5997760.11	12869.83011	2	9100.344146
34779 xibornol	C18 H26 O	258.19848	259.20576	29 top	half	8503331.285	950050.8728	2	671787.4146
34779 xibornol	C18 H26 O	258.19848	259.20576	29 top	quarter	13812529.06	2296377.973	2	1623784.437
34780 xibornol	C18 H26 O	258.19846	259.20576	1 bottom	quarter	3452619.149	428302.0345	2	302855.273
34780 xibornol	C18 H26 O	258.19846	259.20576	1 middle	quarter	3093906.143	63593.54546	2	44967.42724
34780 xibornol	C18 H26 O	258.19846	259.20576	1 top	half	3813934.881	631273.5497	2	446377.8078
34780 xibornol	C18 H26 O	258.19846	259.20576	1 top	quarter	3617438.767	994142.6945	2	702965.0407
34780 xibornol	C18 H26 O	258.19846	259.20576	8 bottom	half	3488949.63	318300.8621	2	225072.6981
34780 xibornol	C18 H26 O	258.19846	259.20576	11 bottom	half	2925151.748	248412.1461	2	175653.913
34780 xibornol	C18 H26 O	258.19846	259.20576	29 bottom	half	3048371.466	407015.6016	2	287803.4919
34780 xibornol	C18 H26 O	258.19846	259.20576	29 bottom	quarter	7226050.915	277740.7935	2	196392.3985
34780 xibornol	C18 H26 O	258.19846	259.20576	29 top	quarter	3829704.848	591002.6876	2	417902.0081