

Compounds.ID	Name	Tags	Formula	RT_min	Calc_MW
c1498			C25 H48 O3 P2 S	5.384	490.27986
c4653	Bis(methylbenzylidene)sorbitol		C22 H26 O6	12.298	386.17389
c2964			C23 H54 N8 O18	6.398	730.35368
c4659				3.423	1133.57992
c4594			C29 H59 N9 O15 S	6.588	805.3871
c93	Teprotide		C53 H76 N14 O12	7.571	1100.57197
c2364			C58 H82 N2 O2 P2 S3	5.05	996.50108
c1202	Not named		C25 H38 N4 O6	5.744	490.28055
c2608			C19 H35 N5 O5 S	1.234	445.23487
c801	4-(3-Pyridyl)-2-[(1,3,5-trimethyl-1H-pyrazol-4-yl)thio]pyrimidine		C15 H15 N5 S	3.281	297.10803
c971				5.033	460.2314
c1204			C32 H46 N5 O5 P S	7.169	643.29638
c359			C15 H34 N7 O4 P	4.836	407.24121
c3742			C31 H52 N7 O5 P3 S	5.146	727.29575
c817				8.123	1524.79932
c2605			C76 H93 N5 O8 P2 S	3.517	1297.6208
c2350	Gombapyrone A		C26 H30 O4	4.734	406.21395
c4892			C18 H43 N8 O8 P	7.531	530.29216
c4776			C24 H52 N8 O14	5.369	676.35857
c129			C69 H106 N8 O15 P2 S	4.751	1380.69627
c2499			C39 H64 N3 O6 P3	5.14	763.40064
c3446	Spliceostatin G		C21 H31 N O6	5.727	393.21543
c2081				5.257	1512.73662
c3780				3.489	1298.62375
c608	Methyl (2S,2aS,3a'R,4a'R,5aR,12bR,12b'R,12c'R,15aR,15a'S,17a'S)-12c'-hydroxy-10'-methoxy-2',3',4,4a',5,6,8,12c',13,13',14,14',17',17a'-tetradecahydro-4'H,5'H,16'H-spiro[furo[2',3':7,8]indolizino[8,1-c;d]carbazole-2,6'-furo[2',3':7,8]indolizino[8,1-cd]pyrido[1,2,3-lm]carbazole]-7-carboxylate		C43 H50 N4 O6	4.653	718.37089
c3425				6.731	550.79423
c1035				6.734	1080.60837
c4256				6.923	2170.07253
c842				6.719	1080.60825
c4034				7.217	1012.51261
c4731			C64 H106 N10 O17 P2 S	5.484	1380.69321
c2751			C12 H34 N10 O3 S	5.003	398.25198
c398				7.527	1101.57447
c766				7.098	1262.66322
c527			C31 H46 N2 O6 S	6.177	574.30805
c2192			C35 H64 N8 O8 P2	5.623	786.43238
c701			C18 H42 N5 O4 P S2	4.651	487.24261
c4161				5.92	540.3358
c1314	6a-Naltrexol		C20 H25 N O4	2.329	1029.51877
c603				7.299	993.46343
c2668				5.499	651.32014
c4670			C43 H47 N O6 S	6.778	705.31294
c2262			C33 H57 N6 O6 P3 S	1.225	758.32619
c3275			C42 H69 N8 O4 P3	9.601	842.46587
c684			C38 H66 N7 O8 P3 S	1.22	873.38906
c4426			C25 H35 N5 S2	4.589	469.23195
c3022	N-([(1S,4S,6S)-6-Isopropyl-3-methyl-4-[(5-(4-pyridinyl)-1,3,4-oxadiazol-2-yl)methyl]-2-cyclohexen-1-yl)methyl]-2-pyrazinecarboxamide		C24 H28 N6 O2	3.458	864.46762
c3164			C36 H65 N7 O6 P2	8.159	753.44545
c4749			C23 H51 N10 O11 P	5.932	674.3461
c866				8.264	1526.78255
c4735	7-Hydroxy-8,14-dimethyl-9-hexadecenoic A		C18 H34 O3	15.616	298.24996
c4305				0.779	886.47062
c2212				9.987	2185.22192
c1850			C47 H82 N10 O16 S2	7.734	1106.53556
c1760				7.083	2184.0653
c2818			C76 H120 N7 O13 P3 S3	5.729	1527.73224
c2106			C28 H63 N4 O8 P3 S	8.276	708.35875
c2902				5.069	1528.7333
c165			C37 H63 N5 O14	0.799	801.43604
c233			C27 H63 N6 O16 P	7.175	758.40332
c2570			C68 H116 O14	17.258	1156.83628
c3740	Stevioside		C38 H60 O18	5.899	826.36524
c484			C15 H27 N O5	0.825	301.18797
c1307				5.592	1244.6429
c3364				9.534	2123.09238
c712			C29 H47 N3 O10	5.603	597.3241
c2975	Biotin		C10 H16 N2 O3 S	0.998	244.08759
c2887				5.404	674.34497
c3827			C22 H41 N O2	16.334	351.31261
c3997	N1-(4,4-dimethyl-5-methylidene-1,3-thiazolan-2-yliden)-3-chloro-2-methylaniline		C13 H15 Cl N2 S	0.87	266.06921
c2928			C33 H59 N7 O7 P2	6.256	727.39316
c3072			C30 H64 N3 O10 P3	5.331	719.38376
c2647			C24 H41 N6 O2 P3	3.003	538.25035
c1199	(2R,3R,4S,5S,6R)-2-([(2E)-4-ethenyl-2,5-dimethylhexa-2,5-dien-1-yl]oxy)-6-(hydroxymethyl)oxane-3,4,5-triol		C16 H26 O6	10.654	296.16103
c3579			C19 H29 N6 O8 P	0.861	500.18063
c1947	Leucocin B-TA33a		C56 H77 N15 O12	3.737	1151.58941
c365				9.559	2086.15533
c378			C24 H49 N10 O4 P3	0.802	634.31291
c2032				8.372	1864.8718
c2618				9.929	2223.16051
c3539				4.814	997.50608
c1013			C30 H60 N7 O5 P3	6.683	691.38937
c3012			C31 H29 N7 O	0.801	515.2412
c4355				7.557	1783.87991

c4472			C83 H123 N4 O14 P3	7.541	1492.82468
c695			C27 H48 N4 O5 S	0.798	540.33667
c3919			C38 H61 N6 O10 P S2	1.219	856.36327
c3564			C12 H22 N4 O3	0.801	270.16832
c1795				9.603	842.80009
c1492			C23 H34 N4 O6	5.103	462.24652
c3980			C17 H34 N3 O6 P	4.389	407.2181
c4633				0.809	1263.61162
c622				5.6	864.47335
c2306				9.619	2548.31721
c1395			C19 H38 N5 O3 P S	0.785	447.24435
c2739				7.081	2037.02882
c2349	Octyl decyl phthalate		C26 H42 O4	16.921	418.30734
c1746	Oximoaspergillimide		C11 H20 N2 O3	5.449	228.14659
c2195				3.465	730.41112
c1751	Norpicacetin		C24 H33 N5 O7	0.796	503.23673
c1909			C25 H62 N9 O10 P3	6.162	741.38621
c1805			C55 H89 N8 O13 P3 S	0.768	1194.54806
c3765	Citreohybridone L		C31 H42 O10	5.156	574.27637
c4292			C37 H66 N4 O11 S2	5.677	806.41647
c3112			C24 H55 N7 O10 P2 S	4.101	695.32262
c4146				10.051	2186.21297
c2224			C54 H70 N3 O2 P3	0.803	885.46796
c4787			C19 H36 O13	5.212	472.21364
c465			C49 H77 N9 O10 P2	0.81	1013.52678
c4781			C33 H64 N10 O15	0.779	840.4553
c4272				7.587	593.8026
c1430	Maniwamycin F		C11 H21 N3 O3	2.148	243.15785
c2296				9.924	2222.15917
c1653			C79 H116 N7 O12 P3 S2	5.488	1511.734
c4614			C39 H70 N9 O10 P S	5.812	887.47147
c4089			C70 H106 N7 O9 P3	5.466	1281.72647
c526	SSR161421		C25 H20 N4 O2	12.553	408.15347
c4679				9.658	2087.14412
c4570			C75 H86 N9 O8 P S	0.777	1303.60581
c4496			C3 H3 N2 O6 P S	19.695	225.94454
c3806				5.338	718.36704
c1705			C18 H41 N3 O4 S2	0.794	427.25386
c4199				7.701	1107.53685
c391				3.606	1282.63021
c1151				6.462	1101.58606
c4590	Tirandamycin G		C22 H31 N O7	5.419	421.21129
c2736			C59 H103 N6 O8 P3 S3	6.974	1212.6201
c3104			C47 H88 N10 O14 S2	6.84	1080.59191
c1650			C39 H74 N3 O16 P S	6.894	903.45229
c2175			C65 H109 N9 O15 P2 S2	5.172	1381.69534
c4891				7.037	1575.79001
c3597	Stevioside		C38 H60 O18	6.105	826.36503
c3730	NNK		C14 H26 N6 O6	1.21	748.39481
c329			C29 H47 N3 O10	5.379	597.3237
c3340	(2R)-1-[(7Z,10Z,13Z,16Z)-7,10,13,16-Docosatetraenoyloxy]-3-(phosphonooxy)-2-propanyl (4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-docosahexaenoate		C47 H73 O8 P	4.798	796.50548
c1845			C23 H30 N4 O8	0.865	490.2042
c2734			C62 H91 N5 O9 P2	5.134	1111.62856
c2682			C60 H110 N4 O13 S4	8.654	1222.69516
c2267			C48 H74 N10 O12 S	4.594	1014.52325
c3482	NNK		C14 H26 N6 O6	1.25	374.19753
c1944				7.079	2168.07198
c1696			C58 H105 N6 O15 P3 S2	4.186	1282.62928
c1471			C28 H33 N5 O S	0.813	487.2418
c3478			C20 H47 N7 O6 P2 S	3.761	575.27631
c2704			C46 H63 N3 O7 S	3.216	801.43706
c4588			C82 H95 N8 O8 P	7.919	1350.70078
c2813			C59 H105 N8 O7 P	17.334	1068.78403
c2153			C55 H88 N8 O15 P2	0.798	1162.58438
c2423			C16 H37 N7 O8	0.792	455.27334
c4006				9.615	2530.40697
c346			C43 H31 Cl N P	17.591	627.18656
c3698				6.816	540.30235
c3266			C37 H72 N5 O10 P3 S	2.677	871.42077
c1391			C32 H63 N4 O9 P3	6.208	740.38062
c3440			C29 H63 N8 O4 P3	4.494	680.42049
c654				5.633	1380.7028
c987			C21 H53 N9 O14	0.804	655.37064
c2127			C10 H26 N8 O7	5.925	370.19267
c4306			C26 H50 N4 O10 P2	0.802	640.29829
c4370			C19 H44 N9 O5 P	5.807	509.32097
c2652			C13 H27 N8 O4 P	3.032	390.18873
c408			C27 H59 N7 O9 P2 S	0.798	719.35794
c81	Norpicacetin		C24 H33 N5 O7	4.082	503.23663
c4520			C28 H23 Cl N6 O3 S	16.902	558.12319
c2878				16.898	556.16549
c3152			C12 H23 N3 O2	0.826	241.17817
c1078				6.701	2184.06519
c900			C38 H61 N8 O6 P S	0.8	788.41568
c768			C20 H43 N6 O11 P	3.398	574.2737

c2829	Aurantimycin C	C38 H60 N8 O14	4.332	852.42307
c4592	Diprotin B	C16 H29 N3 O4	4.474	327.21515
c274		C23 H51 N10 O11 P	4.049	674.34497
c3906		C18 H43 N7 O3 S2	5.588	469.28925
c1971			4.349	426.21094
c1684		C21 H42 N2 O3	13.341	370.31867
c1296		C22 H41 N5 O5	3.207	455.30987
c294			4.891	748.36406
c3046		C20 H28 N O3 P	7.107	361.1811
c4029			4.182	1282.62905
c1775		C39 H53 N10 O8 P	4.394	820.37771
c4851			4.141	896.39078
c2843		C29 H61 N9 O13 P2	6.202	805.38558
c1286			5.645	1312.62571
c4330		C20 H33 N6 O5 P	0.889	468.22277
c1031		C16 H27 N3 O4	3.635	325.19942
c1855		C60 H56 S	5.412	808.41025
c2421	NP-022373	C23 H25 N O2	0.796	329.18053
c4595	Turgichelin	C24 H44 N8 O11	4.622	620.31558
c4408			0.798	1363.69579
c4296		C25 H61 N9 O6 P2 S	5.639	677.39273
c989	Barnesin A	C25 H37 N5 O5	0.802	487.27811
c2180		C33 H78 N9 O18 P	0.796	919.52119
c4847			7.346	1188.62107
c2156		C14 H26 N4 O4	1.187	314.19453
c260		C60 H90 N2 O16 P2	7.524	1156.57497
c306		C20 H31 N5 O5	5.353	421.23123
c2181			0.796	1678.92114
c2701		C29 H66 N9 O16 P3	0.8	889.38361
c1001		C14 H30 N7 O4 P	4.598	391.20992
c2897	Thiamine	C12 H16 N4 O S	0.931	264.10359
c1094		C69 H106 N8 O15 P2 S	5.738	1380.69796
c3733		C67 H112 N7 O17 P3 S2	0.782	1443.67663
c2584	Methyl (2S,2aS,3a'R,4a'R,5aR,12bR,12b'R,12c'R,15aR,15a'S,17a'S)-12c'-hydroxy-10'-methoxy-2',3',4,4a',5,6,8,12c',13,13',14,14',17',17a'-tetradecahydro-4'H,5'H,16'H-spiro[furo[2',3':7,8]indolizino[8,1-c;d]carbazole-2,6'-furo[2',3':7,8]indolizino[8,1-cd]pyrido[1,2,3-lm]carbazole]-7-carboxylate	C43 H50 N4 O6	5.327	718.36967
c2752			5.562	459.72268
c1822			9.702	2087.14794
c193		C60 H92 N8 O18	8.246	1212.653
c1154		C23 H43 N10 O6 P S	4.879	618.28328
c1039		C62 H102 N10 O18 P2	0.802	1336.68474
c3032		C39 H42 Cl N S3	17.593	655.21782
c2133		C16 H40 N10 O12	5.436	564.28293
c171			19.592	609.17629
c4338			9.905	2648.38418
c4434		C28 H57 N O2	18.111	439.4383
c375			16.897	553.16769
c572	Erucamide	C22 H43 N O	18.987	337.33408
c1268			9.967	2628.47066
c4858			0.784	1264.61966
c4160		C38 H53 N6 O6 P	3.394	720.3768
c570			18.261	701.20523
c4142		C26 H42 N8 O7 P2	4.541	640.2643
c4466			0.803	720.36056
c3222		C37 H78 N10 O17 P2	5.43	996.50157
c302		C36 H60 N4 O14 S	5.122	804.38252
c935	Virescenoside Z15	C27 H40 O10	4.21	524.26187
c2622		C19 H25 N3 O4	5.34	359.18384
c1482	Leucocin B-TA33a	C56 H77 N15 O12	3.36	1151.58938
c2425		C37 H62 N4 O15 S	4.78	834.39348
c1172			9.617	2532.35062
c4753			6.096	1304.6526
c4335		C18 H32 N4 O5 S	4.528	416.20837
c2729			9.716	2512.38477
c4133		C35 H39 N10 O P S	3.288	678.27692
c4630			0.786	1680.90761
c913		C27 H47 N4 O8 P S	4.434	618.28235
c218		C39 H63 N6 O4 P3 S	6.382	804.3833
c2300	Palmitic Acid	C16 H32 O2	12.325	273.26729
c1198		C69 H106 N8 O15 P2 S	5.708	1380.69826
c1043		C18 H38 N9 O2 P S2	3.575	507.23261
c3457		C26 H54 N3 O16 P S	4.844	727.29639
c1833		C9 H23 N8 P S3	16.897	370.09325
c4056		C55 H102 N9 O17 P S4	0.772	1319.60105
c3638		C45 H80 N10 O10 P2 S	4.588	1014.52642
c624		C18 H39 N9 O7	0.787	493.29975
c2882		C26 H57 N3 O17	6.353	683.36374
c195	N1-(2-cyclohex-1-enylethyl)-2-methylhydrazine-1-carbothioamide	C10 H19 N3 S	0.785	213.13348
c3419		C29 H54 N7 O6 P3 S	0.806	721.30829
c4224			9.624	2555.33411
c616		C29 H51 N3 O12	0.798	633.34662
c3210	Fusariumin D	C22 H45 N O2	16.231	355.34409
c4742			0.801	241.65756
c3345	Jamaicamide B	C27 H37 Cl N2 O4	4.42	488.24529
c4665		C23 H47 N2 O13 P	0.806	590.28
c3396			4.587	1014.53081
c3688		C18 H38 O9	5.66	398.25246

c2173			C26 H56 N7 O11 P	5.237	673.37568
c4366				5.898	763.36925
c1285			C80 H117 N10 O16 P	9.202	1504.83698
c325			C67 H93 N7 O14 P2	0.796	1281.62532
c2197			C62 H100 N5 O18 P S2	4.001	1297.62242
c1875				4.04	1014.53098
c4726			C30 H48 N9 O P S2	0.808	645.31437
c4574				0.839	1188.53225
c4274				5.022	393.23694
c4486			C25 H44 N3 O2 P S2	5.665	513.25908
c3421			C83 H123 N4 O17 P S2	8.197	1542.80839
c2719				4.84	814.42826
c2419			C24 H56 N5 O8 P3	5.702	635.33596
c2029			C36 H36 Cl N S2	16.897	581.1988
c176			C14 H36 N9 O5 P	0.81	441.25739
c916		1794967	C16 H31 N O3	8.953	285.23008
c3416			C50 H70 O12 S	6.107	894.45874
c366			C11 H33 N8 O2 P3	5.354	402.19145
c4818			C44 H57 N9 O3 S	5.484	791.42826
c3702			C52 H98 N10 O15 P2 S2	7.097	1228.61367
c3225				7.204	2170.07253
c3949				5.48	1528.73379
c1351			C43 H42 Cl N5 O S3	19.126	775.22398
c2901			C33 H50 N10 O11	6.096	762.36554
c3448			C20 H38 N4 O5	5.791	414.28371
c3053				5.39	1953.95587
c4354			C22 H46 N4 O16	4.994	622.28801
c3081			C21 H44 N6 O3 S	18.34	460.32185
c1626			C31 H18 N6 O13 P2 S3	0.793	839.95659
c3066			C29 H44 N8 O6 S	4.168	632.31109
c1104			C35 H64 N9 O5 P S	7.924	753.44761
c3682			C20 H33 N O8	4.958	415.21978
c2996			C11 H17 N10 O11 P3 S2	5.493	621.97359
c2875				6.184	2073.006
c4147			C59 H72 N O12 P	5.783	1017.48003
c4675				8.033	1525.79373
c2505			C44 H53 N8 O6 P	5.364	820.38213
c521				0.814	1280.61214
c2898			C27 H64 N8 O16 S	4.369	788.41604
c4495	Maniwamycin F		C11 H21 N3 O3	3.303	243.15784
c907				7.904	376.72134
c4385			C10 H24 Cl N9 O	0.785	321.17891
c157	[D-Asp3,Dha7]MC-FR		C50 H68 N10 O12	7.193	1000.50092
c3231			C34 H71 N5 O12 P2 S	4.776	835.42939
c4410				5.495	1867.92567
c3508				5.896	1524.73252
c4225			C16 H33 N O2	14.867	271.25057
c4429			C24 H47 N10 O3 P3 S	1.227	648.27841
c4832			C32 H28 N2 O2	4.509	472.21338
c1873			C22 H38 N4 O5	6.856	438.28391
c714	(2R)-1-[[[Hydroxy{[(1S,5R)-2,3,4,6-tetrahydroxy-5-(phosphonooxy)cyclohexyl]oxy}phosphoryl]oxy]-3-(palmitoyloxy)-2-propanyl (11Z)-11-octadecenoate		C43 H82 O16 P2	5.745	916.50726
c2860				5.048	1963.96985
c4546			C13 H25 N5 O3 S	2.571	331.16716
c2714	N-lauroylglycine		C14 H27 N O3	6.078	257.1987
c4642			C38 H67 N2 O9 P3 S	5.585	820.37705
c4890			C7 H22 N10 P2	0.755	308.15145
c2098			C27 H66 N10 O12 P2	5.735	784.4324
c1978				6.752	2052.02307
c1730				6.458	1148.61776
c4448	L-Arginyl-L-arginyl-L-arginine		C18 H38 N12 O4	3.294	486.31504
c4894				5.915	2085.97664
c1329				6.69	2183.06217
c3174				6.396	1998.967
c3677			C79 H121 N6 O18 P S	7.441	1504.82155
c3427			C55 H97 N5 O15 P2 S	6.693	1161.6171
c3258			C15 H27 N3 O7	4.85	361.18379
c1282				16.043	462.1223
c1064			C40 H66 N6 O12 P2	5.028	884.41902
c1912			C13 H26 N7 O3 P	5.346	359.1839
c3476				6.641	1101.58624
c3276			C29 H26 O2	0.79	406.19464
c1985				9.966	2629.47332
c1593			C39 H59 N2 O9 P S	5.909	762.36662
c4169				3.985	698.39413
c3229			C30 H44 N3 O3 P S	8.04	557.28318
c3138			C27 H55 N3 O13 P2	5.417	691.31999
c4043	Streptolydigin		C32 H44 N2 O9	6.768	600.30297
c4718			C16 H41 N10 O2 P S2	0.801	500.25821
c4328	lys-his		C12 H21 N5 O3	0.7	283.16408
c524	Diprotin A		C17 H31 N3 O4	5.36	341.23074
c3132				0.807	963.48801
c1514				0.781	1013.51546
c4898			C14 H23 N9 O2	6.182	349.19881
c3956			C17 H41 N7 O6 P2	5.393	501.25781
c825			C50 H61 N7 O9	7.271	903.453

c219			C50 H78 N8 O8 P2 S	0.796	1012.51373
c4025	Bis(2-ethylhexyl) terephthalate		C24 H38 O4	9.957	390.2758
c2664			C88 H141 N10 O14 P3 S4	7.312	1782.87361
c3940			C22 H47 N7 O8	7.074	537.35019
c4616				10.065	2188.21963
c4508				0.808	1484.72219
c3824			C77 H125 N8 O16 P3 S2	7.033	1574.78731
c4454			C5 H13 N8 O5 P	16.04	296.07488
c855	Ethyl (3-cyano-1H-1,5-benzodiazepin-4-yl)carbamate		C13 H12 N4 O2	0.878	256.09271
c2149	Petrobactin		C34 H50 N6 O11	5.301	718.35156
c4831				4.697	1336.6892
c3135			C78 H128 N3 O17 P3	7.656	1471.84327
c4488			C77 H125 N8 O16 P3 S2	7.051	1574.78659
c4713				3.474	666.33585
c4402				2.495	270.18801
c4373			C34 H60 N2 O12 S	7.454	720.38486
c1901			C29 H57 N3 O11 S	4.987	655.3704
c732			C62 H83 N10 O7 P3	0.774	1172.56621
c4870			C50 H84 O16 P2 S	3.315	1034.49546
c1231				5.182	952.5261
c2022			C19 H34 N4 O5	4.823	398.25242
c1717			C28 H60 N7 O10 P3	5.387	747.36111
c3074			C60 H89 N2 O16 P S2	0.779	1188.53816
c3288			C41 H74 N6 O10 S2	4.112	874.48961
c4235				5.065	1529.73385
c4230			C16 H29 N O2 S	10.363	299.19171
c4022	Blastmycetin C		C17 H23 N3 O4	3.553	333.16805
c2066				6.162	737.3948
c2750			C18 H42 N9 O10 P	4.315	575.27677
c1581			C15 H38 N6 O6 P2	5.727	460.23309
c689			C65 H96 N5 O17 P S	4.277	1281.62632
c2762				6.829	870.42338
c3903			C16 H38 N9 O P S2	0.808	467.23735
c4877	(S)-Malic acid-1-O-beta-D-glucopyranoside		C10 H16 O10	15.051	296.0743
c576			C53 H89 N10 O12 P3	3.428	1150.58717
c4485				0.812	1342.55393
c1162				6.173	1997.96553
c826				9.966	2631.41738
c4131				5.545	2085.99882
c1344				7.629	1123.55567
c1470				5.405	460.23438
c1099				6.63	1800.90332
c3422				9.594	2549.31862
c755				6.167	1850.92882
c3790			C80 H96 N9 O7 P S	6.727	1357.68894
c2791				5.342	358.6757
c2157			C16 H37 N10 O4 P	0.8	464.27365
c3899			C27 H41 N3 O6 S2	7.156	567.24612
c1962			C38 H57 N3 O7 P2	5.743	729.36935
c3270			C43 H84 N O8 P3 S2	5.554	899.48387
c4542			C40 H80 N5 O15 P	5.936	901.53905
c4097	NP-002336		C23 H36 O5	0.795	430.20473
c3829				6.747	2200.06346
c3101			C20 H44 N4 O4 P2 S	0.798	498.25745
c4071			C76 H111 N10 O17 P3	5.735	1528.73446
c3654			C19 H48 N10 O7 P2	0.789	590.31606
c4608			C20 H41 N O4	16.659	359.30259
c3580			C9 H23 N8 P S3	16.043	370.09326
c4379			C65 H124 N5 O18 P3 S3	4.274	1451.73173
c3241			C64 H106 N10 O18 P2 S	0.8	1396.68868
c243				6.672	2069.00195
c4761			C30 H64 N9 O14 P	4.316	805.43094
c4500				7.322	995.4672
c1791			C35 H71 N10 O17 P	0.799	934.47427
c1337			C31 H71 N8 O13 P3	5.006	856.43424
c4641	Bis(2-ethylhexyl) terephthalate		C24 H38 O4	9.122	390.27618
c34			C14 H29 N O2	8.751	243.21977
c1608			C15 H38 N6 O6 P2	5.738	460.23307
c4628			C26 H40 N10 O3	4.964	540.32945
c1851			C89 H118 N9 O10 P3 S	5.529	1597.79295
c396			C62 H120 N3 O18 P3 S	9.247	1319.75085
c3394				7.296	1521.85768
c1066			C27 H64 N7 O16 P S	5.574	805.38596
c1489				9.537	2107.12634
c513			C32 H47 N7 O9	5.894	673.3428
c4072			C23 H35 N5 O6	0.806	477.25626
c3558			C8 H17 N7 O4	1.277	275.13492
c2174				7.055	1737.90173
c3735			C19 H46 N8 O6 P2	0.801	544.30241
c1258			C19 H47 N6 O4 P S2	0.804	518.28345
c2233			C12 H33 N8 O4 P	5.015	384.23613
c1242				6.09	752.43884
c2609			C50 H99 N5 O17 P2 S	6.213	1135.62253
c627				0.804	574.27333
c418			C36 H60 N4 O14 S	5.607	804.3823

c846				5.468	1350.71335
c666			C66 H104 N4 O17 P2	7.091	1286.68853
c4282			C50 H94 N7 O16 P3 S	0.821	1173.56882
c728				6.674	2037.0312
c845			C16 H25 N5 O4	0.782	351.18966
c3692			C19 H49 N9 O9 P2	5.424	609.31188
c1469			C18 H41 N4 O5 P S2	5.538	488.22635
c4212				0.799	1174.56441
c829	(1S,16R)-7,11-Dihydroxy-8,8,10,16-tetramethyl-12-methylene-3-[(1E)-1-(2-methyl-1,3-thiazol-4-yl)-1-propen-2-yl]-17-oxa-4-azabicyclo[14.1.0]heptadecane-5,9-dione		C27 H40 N2 O5 S	2.936	504.26613
c4204	Virescenoside Z8		C26 H38 O9	6.881	494.2506
c1495				7.275	451.72704
c4181				5.639	1997.96425
c2997			C32 H67 N10 O11 P	6.944	798.47389
c4481			C42 H49 N5	0.79	623.39811
c3944	Palmitelaidic acid methyl ester		C17 H32 O2	15.172	268.23914
c4243				5.357	359.18514
c931				6.171	1996.96153
c1583			C36 H66 O13 P2	5.563	768.40002
c1923			C11 H29 N8 O5 P	5.565	384.20023
c2440	Dibutyl sebacate		C18 H34 O4	16.657	314.24484
c3904			C20 H51 N9 O10 S	5.414	609.34572
c4646				7.058	1738.90671
c3631			C34 H80 N7 O11 P3 S	4.894	887.48521
c1376			C40 H78 N5 O15 P3 S	7.497	993.44314
c4431			C71 H103 N6 O9 P3 S	7.083	1308.67168
c783				0.797	872.38913
c3873				7.089	1287.69052
c2733			C24 H50 N2 O6 S2	5.016	526.30946
c4104				7.135	851.51047
c2943	2-[[[(3S)-1-(Cyclohexylmethyl)-3-pyrrolidinyl]-5-(1-methyl-1H-imidazol-5-yl)-1,3,4-oxadiazole		C17 H25 N5 O	3.253	315.20406
c4568			C65 H111 N5 O15 P2	5.27	1263.75509
c1508	N-[[[(1S,4S,6S)-6-Isopropyl-3-methyl-4-[[5-(4-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl]-2-cyclohexen-1-yl]methyl]-2-pyrazinecarboxamide		C24 H28 N6 O2	3.377	432.2339
c4636				4.092	1336.687
c4031				7.626	1695.83941
c62				5.829	377.19291
c2583			C24 H43 N7 O8	7.568	557.31995
c2945				6.892	1340.61167
c1868			C62 H126 N2 O14 P2	18.361	1184.86863
c4073			C54 H95 N10 O18 P S2	3.063	1266.6004
c2205			C70 H105 N9 O18 P2	8.333	1421.70581
c3038				4.316	406.21835
c512				6.311	1980.96718
c3043			C30 H46 N4 O13	6.883	670.30563
c970				9.962	2627.46838
c4352			C24 H51 N10 O6 P	5.358	606.37267
c2760				9.601	2088.15364
c497			C23 H36 N6 O4	5.011	460.27847
c807			C20 H28 N4 O7	0.8	436.19441
c2614	Erucamide		C22 H43 N O	16.639	337.33352
c3864			C38 H74 N5 O15 P3	8.389	933.43967
c2931	Palmitic Acid		C16 H32 O2	12.327	273.2678
c1880	WF-14865A		C17 H27 N5 O4	1.254	365.20535
c923				5.382	1952.95238
c2054			C87 H122 N6 O13 P2	7.201	1520.85425
c2676			C55 H97 N8 O11 P3	6.963	1138.64832
c710				6.182	1953.95554
c1157			C14 H36 N9 O3 P S	5.331	441.24029
c3268			C22 H44 N5 O4 P S	5.056	505.28685
c369			C15 H29 N O4 S	8.831	319.18201
c2086			C55 H108 N3 O18 P3	7.545	1191.68434
c4627			C69 H101 N6 O16 P S	8.355	1332.67295
c3909			C51 H103 N2 O18 P3 S2	7.542	1188.58594
c3732				0.808	339.18996
c2840	12,14-Nonacosanedione		C29 H56 O2	19.237	436.42777
c1421			C29 H43 N5 O6	7.079	557.3214
c3892			C31 H66 O11 P2	4.148	676.411
c3652			C53 H89 N8 O10 P3 S	6.438	1122.56366
c4117			C46 H98 N3 O15 P3 S3	7.619	1121.53711
c3000			C32 H52 N4 O6 S2	5.205	652.33174
c3169			C35 H79 N7 O9 S5	7.086	901.45257
c4217			C47 H103 N10 O5 P3	17.416	980.7327
c2058	VLK		C17 H34 N4 O4	3.153	340.24656
c4009			C70 H87 N5 O17 P2 S	0.776	1363.52935
c1776			C77 H111 N9 O17 P2 S	5.381	1527.73022
c2446	Leptazoline B		C16 H21 Cl N2 O7	15.048	388.10352
c856			C24 H36 N4 O6	5.12	476.26256
c421			C33 H59 N8 O5 P3	5.954	740.38466
c2683				5.548	336.67076
c4341			C19 H45 N10 O9 P S	5.373	620.28417
c3324				9.999	2611.4512
c1116			C14 H34 N9 O5 P	3.46	439.24215
c2060			C62 H120 N3 O16 P3 S3	7.568	1351.70399
c3695			C20 H44 N10 O5 S2	0.776	568.29558
c2640			C24 H49 N10 O3 P3	5.165	618.31867
c4464	Koreenceine C		C14 H27 N O	5.544	225.20876

c885	Serpulanine C	C14 H18 N2 O3	3.768	262.13115
c861			3.788	654.43047
c412		C27 H39 N5 O6	6.426	529.28977
c379			6.555	1937.9617
c32		C19 H40 N6 O10	7.584	512.27933
c4269		C61 H65 N P2 S	5.471	905.43106
c4321		C36 H67 N9 O15 P2	8.335	927.42343
c3696		C70 H104 N10 O15 P2	8.294	1386.71518
c3625		C29 H49 N3 O5 P2 S	5.477	613.28831
c3553		C29 H59 N O2	19.242	453.45435
c3117			5.397	2100.98999
c1251	Bis(methylbenzylidene)sorbitol	C22 H26 O6	12.474	386.17414
c1628		C87 H154 N9 O18 P3 S5	6.292	1865.92139
c2766			5.405	1224.60569
c3166		C68 H103 N6 O17 P3	3.584	1368.65874
c4593		C31 H62 N6 O14	3.411	742.43174
c1343		C29 H56 N7 O5 P3	5.695	675.35627
c2459		C13 H35 N8 O4 P	5.434	398.25212
c4108		C36 H74 N9 O6 P3	7.026	821.49919
c4790		C33 H67 N6 O9 P S	4.412	754.44114
c2636		C43 H81 N10 O8 P3	4.335	958.5448
c3617		C49 H93 N3 O16 P2 S2	7.516	1105.54729
c3196		C53 H87 N10 O11 P3	3.935	1132.57729
c2537			7.924	1100.56206
c2080			0.797	1679.91635
c3860		C61 H102 N8 O15 P2 S2	0.797	1312.63718
c1691		C13 H28 N8 O5	6.119	376.21956
c2572	beloxamide	C18 H21 N O2	0.796	283.15607
c3399			5.974	2052.02377
c3168		C88 H134 N10 O14 P2 S3	7.249	1712.87041
c873	(2Ĥ±,3Ĥ±,5Ĥ±)-26-(Ĥ²-D-Glucopyranosyloxy)-2-hydroxy-22-methoxyfurost-25(27)-en-3-yl O-Ĥ²-D-glucopyranosyl-(1â†³3)-O-Ĥ²-D-glucopyranosyl-(1â†²2)-O-[Ĥ²-D-glucopyranosyl-(1â†³3)]-O-Ĥ²-D-glucopyranosyl-(1â†²4)-Ĥ²-D-galactopyranoside	C64 H106 O35	5.308	1434.65834
c1686		C31 H50 N8 O9	7.487	678.37063
c4371		C25 H58 N6 O14 P2	5.435	728.34781
c1948			9.934	2228.17471
c2812		C49 H63 N5 O8	0.794	849.46829
c2485		C18 H43 N8 O9 P	4.706	546.28819
c2694		C63 H95 N4 O11 P	5.466	1114.67195
c493		C16 H41 N10 O5 P S	0.794	516.27123
c864			9.541	2087.15647
c4202			6.35	1074.24997
c4632		C62 H104 N4 O15 P2	5.329	1206.69557
c4451	Meleagrin B	C43 H53 N5 O6	8.011	735.4016
c3792			7.62	2001.00685
c4060			6.688	1162.61842
c3248		C25 H46 N3 O4 P S2	4.298	547.26662
c1397			3.149	227.65498
c2236			5.508	1865.91986
c3623		C47 H84 N9 O15 P3	7.717	1107.53123
c2339		C90 H134 N6 O18 P2 S2	6.735	1712.86843
c1743	NP-012766	C31 H46 N4 O7	3.746	1248.57339
c4167			7.254	2067.99972
c3974		C16 H41 N6 O7 P	6.405	460.27932
c2064			5.74	1381.69943
c1603		C25 H38 N4 O7	7.563	506.27405
c3232		C21 H55 N9 O8 P2	5.588	623.36267
c4564			0.797	1049.53723
c1571		C61 H78 N8 O17	3.01	1194.54901
c1618	7,9-Hexacosanedione	C26 H50 O2	18.118	394.38066
c4471			7.044	1263.67002
c1319		C22 H41 N5 O5	3.144	455.30969
c3197			7.401	1505.82521
c4413			5.54	671.3599
c1022		C23 H54 N7 O8 P3	6.85	649.3264
c3437			9.603	2528.40311
c1177			7.349	994.46566
c3951		C19 H41 N8 O4 P	7.128	476.29981
c1238			6.047	1286.66418
c1788		C17 H46 N10 O13	5.463	598.32771
c3052	IPH	C17 H27 N5 O4	3.271	730.41088
c4336			6.349	1074.58457
c683	Cyclo(Pro-Leu-Pro-Ile)	C22 H36 N4 O4	5.326	420.27293
c2939		C40 H57 O8 P3	0.795	758.32547
c1883		C57 H83 N8 O8 P3	7.939	1100.55679
c840		C36 H70 N7 O18 P	6.808	919.45239
c544		C31 H46 N8 O4 P2	5.239	656.31283
c1107		C71 H96 N7 O13 P	8.046	1285.68193
c2687		C22 H50 N10 O2 P2 S2	5.398	612.30329
c1846	[D-Leu1]MC-RR	C52 H81 N13 O12	6.789	1079.60887
c4801		C10 H24 N10 O3 S	5.448	364.1741
c2333	D-(+)-Maltose	C12 H22 O11	0.757	364.09745
c3905			6.291	2013.95899
c4411			0.807	273.14043
c765		C73 H112 N7 O18 P3	4.023	1467.72736
c2488			5.743	460.23327
c1520			6.819	1998.96402

c4081				7.217	1898.96988
c4626				4.45	1863.9576
c2654			C23 H38 N2 O11	3.384	518.24626
c271	APK		C14 H26 N4 O4	0.789	314.19441
c3606				5.36	1674.88012
c1084				7.777	1025.56413
c3182			C55 H102 N7 O14 P3	7.048	1177.66946
c1074				7.106	2036.02709
c3388				6.087	2183.06208
c1121			C14 H31 N5 O9	6.13	413.21061
c3755			C66 H102 N2 O15 P2	8.6	1224.67526
c4717			C20 H42 N9 P S2	6.164	503.27401
c1928				5.1	333.69415
c1991			C46 H86 N3 O15 P3	3.993	1013.52728
c3316				6.091	2184.06333
c146			C73 H98 N5 O14 P	8.411	1299.6846
c3333			C62 H106 N9 O17 P S	8.362	1311.7173
c4597			C15 H34 N6 O12	5.379	490.22396
c2284			C29 H65 N9 O13 P2	5.491	809.41675
c4092			C22 H47 N O11	7.076	501.31552
c1426	FPK		C20 H30 N4 O4	2.145	390.22604
c1550	Leucyl-leucyl-norleucine		C18 H35 N3 O4	6.094	357.2623
c3240			C22 H39 N5 O5	1.084	453.29404
c2699				0.785	934.43323
c3035			C58 H100 N8 O15 P2	5.377	1210.67976
c4706				8.379	1252.68406
c4582			C21 H46 N5 O6 P	4.066	495.31661
c528			C29 H56 N7 O5 P3	5.455	675.35724
c4423	Lokisin-2(CH2)	A;B	C62 H107 N11 O20	14.399	1325.76623
c3998			C25 H60 N10 O8 P2 S	4.826	722.37885
c2190			C22 H55 N7 O3 P2 S2	5.052	591.32578
c1876			C53 H115 N10 O7 P3	18.434	1096.8165
c4365			C35 H51 N9 O3 P2 S	6.52	739.33238
c4724			C50 H92 N2 O13 P2	6.147	990.60765
c3389			C18 H32 N2 O3 S	8.936	356.2131
c3335			C85 H111 N10 O17 P	6.519	1574.78797
c1665			C78 H115 N9 O12 P2 S3	5.072	1527.7298
c650			C25 H47 N3 O12	0.798	581.31529
c4113			C25 H59 N10 O13 P	5.441	738.39837
c1183			C29 H53 N3 O12	5.421	635.36272
c2147			C22 H44 N8 O4	2.724	484.35056
c3413			C56 H99 N8 O13 P3	7.82	1184.65398
c2802				9.965	2654.40086
c3129			C63 H100 N8 O11 P2	6.383	1206.6982
c471	Lokisin isomer M+H+NH4 adduct	B	C74 H116 N8 O12 P2	14.919	1370.82026
c2625			C23 H56 N8 O14	5.041	668.39098
c895				4.154	352.65664
c2514			C19 H29 N3 O4	5.431	363.21461
c2911				5.655	1996.96193
c204			C33 H57 N3 O6 P2	6.026	653.37398
c2565			C35 H48 N2 O9 S	6.607	672.31056
c478			C27 H52 N O6 P3	6.592	579.3021
c1350			C20 H49 N9 O4 P2	5.335	541.33687
c1839	Micropeptin SD1002		C51 H70 N8 O13	7.287	1002.50855
c1218				7.088	1800.90168
c3512				4.312	1094.53441
c1023				6.615	1799.9003
c4859			C74 H97 O11 P	6.122	1192.67661
c4050			C41 H66 N5 O10 P3	6.344	881.40035
c1287			C26 H45 N O4	18.015	435.33411
c645			C23 H56 N7 O16 P	5.35	717.35142
c3293				7.101	2185.06765
c3778			C25 H40 N9 O9 P	5.091	641.26873
c4613			C14 H27 N5 O3	2.672	313.2105
c591			C29 H48 N2 O13	4.643	632.31584
c4829			C21 H49 N7 O7 S3	6.319	607.28546
c2526			C67 H113 N4 O17 P3 S2	4.742	1402.67631
c4149				0.786	342.18972
c3881			C16 H41 N7 O6 P2	5.015	489.25718
c2748			C16 H40 N9 O4 P S2	0.79	517.23782
c4791			C26 H60 N3 O3 P3 S2	0.809	619.32993
c1814			C17 H46 N9 O8 P	5.415	535.31887
c4177	(2S,3R,4E)-3-Hydroxy-2-(tetradecanoylamino)-4-octadecen-1-yl 5-acetamido-6-[(1S,2R)-2-({5-acetamido-3,5-dideoxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]-beta-L-threo-hex-2-ulopyranonosyl}oxy)-1,3-dihydroxypropyl]-3,5-dideoxy-beta-L-threo-hex-2-ulopyranonosyl-[2->3]-[5-acetamido-3,5-dideoxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]-3,5-dideoxy-beta-L-threo-hex-2-ulopyranonosyl]oxy)-1,3-dihydroxypropyl]-3,5-dideoxy-beta-L-threo-hex-2-ulopyranonosyl		C92 H158 N4 O47	6.441	2071.00459
c4425			C40 H69 N3 O10 P2	6.662	813.44779
c3064			C44 H87 N10 O10 P S2	5.021	1010.57915
c1165	NP-012766		C31 H46 N4 O7	3.815	1248.58965
c4288				5.359	1116.5864
c2980			C49 H107 N10 O5 P3	18.51	1008.76389
c3757	Cyclobenzaprime		C20 H21 N	2.843	275.16275
c3847			C28 H51 P3 S	4.193	512.29472
c2821	(2R,8S)-5,8,11,11-Tetrahydroxy-2-[(5Z,8Z,11Z)-5,8,11-icosatrienoyloxy]-5,11-dioxido-4,6,10-trioxa-5lambda~5~,11lambda~5~-diphosphaundec-1-yl (4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-docosahexaenoate		C48 H78 O13 P2	5.145	924.49302
c3322			C26 H46 N7 O13 P S	4.091	727.26059
c3832			C32 H74 N7 O12 P S	4.508	811.4831
c2861				3.002	839.96163
c4443			C27 H58 N9 O10 P	4.432	699.40616

c1368			C19 H45 N7 O8 P2	6.171	561.27942
c411	Leualacin C		C30 H45 N3 O7	6.513	559.32598
c748				6.783	2168.0713
c4263	N1-cyclohexyl-4-(4-fluorobenzyl)-1,4-diazepane-1-carbothioamide		C19 H28 F N3 S	3.504	349.19698
c4754	Novonestmycin B		C68 H110 O26	5.546	1342.72446
c1380				6.761	1947.97751
c1335	Palmitelaidic acid methyl ester		C17 H32 O2	15.016	268.23943
c117			C34 H52 N6 O7	7.399	656.38993
c4309			C56 H56 N9 O P	5.416	901.43486
c4559			C54 H61 N4 O5 P	7.079	876.4367
c726				6.795	1980.96783
c1220			C14 H29 N5 O6	4.937	363.21304
c4663			C53 H49 N O3 S2	7.006	811.31668
c3085			C25 H51 N O2	17.251	397.39123
c1747			C70 H105 N6 O18 P S	4.392	1380.69466
c3308				6.289	2012.95531
c3587	Oxichaetoglobosin I		C31 H38 N2 O7	0.779	550.26993
c2597			C32 H59 N9 O4 P2 S	6.273	727.38977
c4492				4.972	540.32707
c824				6.139	1938.96393
c3630				4.185	632.32449
c1869			C18 H32 N4 O5	4.7	384.23689
c3720			C40 H34 Cl N5 S2	19.58	683.19466
c2689			C33 H63 N9 O4 P2	4.25	711.45086
c3901			C57 H89 N3 O10 P2	6.671	1037.60211
c2842			C23 H41 N O S5	16.042	507.18027
c984	Ethyl oleate		C20 H38 O2	16.233	310.28635
c4567				4.895	663.31456
c4440			C35 H34 N4 O	6.297	526.27562
c149				9.969	2610.44893
c594				8.278	890.47905
c3489			C15 H40 N10 O5 P2	0.81	502.26508
c3207			C25 H53 N2 O11 P	4.899	588.33644
c2021				5.986	786.37945
c3228			C36 H72 N7 O12 P	5.584	825.49507
c2219			C42 H82 N4 O16 P2 S	4.137	992.49109
c1605			C20 H31 N3 O4	5.85	377.23007
c2344			C20 H32 N4 O5	5.006	408.23647
c3841	(1S,3S,4S,5R,6R,7R)-1-(4-Acetamido-5-methyl-3-methylene-6-phenylhexyl)-4,7-dihydroxy-3-[(3-hydroxy-4,6-dimethyloctanoyl)oxy]-2,8-dioxabicyclo[3.2.1]octane-3,4,5-tricarboxylic acid (non-preferred name)		C35 H49 N O14	5.114	707.31853
c2755			C12 H15 N5	19.711	229.13287
c2709			C34 H72 N10 O15 P2	6.092	922.46536
c4391			C25 H55 N10 O10 P	0.792	686.38331
c2207			C38 H57 N3 O7 P2	5.847	729.36912
c3598			C16 H43 N8 O4 P	6.156	442.31501
c326			C19 H25 N3 O4	4.58	359.18404
c1750	pro-gln		C10 H17 N3 O4	2.584	243.12137
c1950				2.586	486.24284
c209				9.614	2511.38157
c3317			C31 H66 N9 O13 P	7.641	803.45284
c991				9.941	2207.19778
c250				9.934	2184.21823
c1374			C70 H102 N5 O13 P	7.072	1251.72033
c2410			C71 H110 N10 O15 P2	6.727	1404.76055
c3003			C90 H159 N7 O16 P2 S3	5.536	1752.04746
c4273				5.551	1753.04957
c2466	Namalide E		C28 H43 N5 O6	7.037	545.32051
c961			C59 H97 N7 O13 P2	5.545	1173.66212
c1102			C55 H104 N5 O14 P3	5.553	1151.6804
c785			C52 H98 N8 O11 P2 S2	5.446	1136.62487
c4678			C25 H58 N5 O13 P	5.604	667.37883
c3432			C69 H104 N8 O18 S2	4.091	1396.69002
c1160			C16 H35 N O3	12.474	289.26125
c1420			C24 H53 N9 O9 P2	5.361	673.34206
c84	Prolylleucine		C11 H20 N2 O3	5.142	228.14705
c965			C35 H50 N2 O6 P2	5.873	656.31501
c4334	Alternarizine A		C24 H28 N2 O3	17.197	392.21158
c2000			C34 H73 N10 O16 P	4.258	908.49418
c2661				6.236	1939.96596
c3802			C37 H47 N4 O3 P3	5.217	688.28784
c3255			C19 H45 N4 O8 P	7.593	488.2992
c3793			C66 H99 N8 O18 P3	4.091	1384.62974
c1849				6.402	966.56435
c1676			C24 H34 N4 O6 S	4.965	506.21927
c4479				7.586	637.82317
c4311			C68 H114 N10 O14 P2	7.581	1356.79899
c1619	Tanzawaic acid C		C18 H26 O3	14.142	290.18761
c535	Stenothricin D		C49 H85 N11 O17 S	3.277	1131.5833
c1666			C18 H43 N2 O6 P3	2.251	476.2349
c2757			C82 H132 N7 O17 P3 S	5.603	1611.86334
c3863				3.549	1152.5924
c1101			C41 H51 N4 O7 P	0.783	742.34903
c3739			C37 H56 N2 O10 S	0.78	720.36846
c4078			C47 H83 N3 O16 P2 S	6.511	1039.49705
c2830			C28 H67 N10 O15 P	5.015	814.45157
c4268				4.053	443.23695

c2274				7.2	2168.07125
c2095		C35 H50 N6 O10 S		7.169	746.32954
c2665				6.013	1302.63279
c2264		C70 H94 N7 O15 P		6.01	1303.65509
c3789		C65 H102 N3 O15 P3		5.572	1257.65283
c2580				6.747	1713.86976
c4150				9.523	2124.09556
c3897		C61 H114 N3 O18 P3 S2		8.497	1333.67481
c3544		C17 H43 N10 O P S		18.451	466.3088
c3830	Erucamide	C22 H43 N O		18.191	337.33389
c3747		C68 H114 N9 O17 P3 S		7.219	1453.72641
c2890		C16 H43 N10 O7 P S		7.945	550.27886
c1305		C28 H60 N7 O6 P3		5.814	683.38466
c1385		C45 H62 N10 O4 P2 S		3.582	900.41473
c2310				3.093	275.1418
c2265		C27 H41 N5 O7		5.349	547.29872
c687		C21 H38 N4 O5		5.391	426.2834
c2433				6.007	651.82776
c1245				6.674	1997.96572
c3809				5.429	462.24724
c1259		C39 H70 N3 O8 P3		3.679	801.43731
c3960				6.562	816.47721
c3819		C25 H52 O7 P2 S		5.356	558.29338
c4155				6.239	1940.96572
c4231	Nodulisporic acid D	C38 H49 N O4		0.797	583.36692
c4030		C57 H90 N6 O11 P2		5.647	1096.61509
c1725		C20 H45 N4 O12 P		5.44	564.27945
c2673		C70 H117 N7 O14 P2 S3		7.695	1437.73089
c4052				7.622	2000.00321
c2834		C18 H31 N5 O7		1.261	429.22107
c2904		C29 H63 N10 O13 P		5.147	790.43292
c4788		C29 H59 N O2		17.644	453.45342
c2977		C50 H79 N O9 P2		6.089	899.52148
c3872		C47 H65 N4 O12 P		4.487	908.43347
c4751				9.618	2554.3304
c4457		C31 H40 O3 P2		7.051	522.24657
c3027	PPK	C16 H28 N4 O4		2.145	340.21041
c707		C30 H52 N5 O10 P		4.643	673.34263
c2004		C52 H81 N10 O14 P3		5.925	1162.5147
c1302		C14 H24 N4 O7		0.79	360.16344
c2462		C24 H57 N9 O8 S2		5.537	663.37681
c3572				3.656	1338.69304
c3247		C18 H43 N4 O8 P		6.56	474.28417
c2012		C19 H42 N6 O11		6.451	530.29387
c2260		C26 H40 N6 O10		4.374	596.27852
c1224		C60 H90 N9 O4 P3 S		7.513	1125.60579
c4685		C23 H55 N10 O8 P S2		0.796	694.33804
c4455		C17 H36 N6 O4 P2 S		0.795	482.20142
c1742	N-((1S,2S,8S,8aS)-8-Hydroxy-1,4a-dimethyl-7-[(2S)-1-oxo-1-(1-piperidinyl)-2-propanyl]decahydro-2-naphthalenyl)methanesulfonamide	C21 H38 N2 O4 S		4.954	904.41272
c3635		C45 H66 N3 O3 P S2		3.311	791.42761
c634		C59 H84 N4 O9		4.998	992.62418
c1276		C39 H62 N5 O4 P3		7.302	757.40038
c2258		C78 H115 N8 O10 P3		7.035	1416.79595
c4325				0.786	1053.56945
c2593		C56 H115 N10 O18 P3 S		5.026	1340.73173
c3320		C51 H111 N10 O15 P3 S		5.468	1228.71719
c2347	GERI-155	C35 H58 O14		0.786	702.3797
c836		C24 H51 N3 O7 P2 S		6.996	587.29468
c4699		C35 H79 N10 O5 P3 S		7.53	844.51569
c3507		C73 H88 N7 O12 P3		3.5	1347.57095
c1054		C28 H64 N9 O14 P		5.129	781.43183
c4388		C8 H24 N7 O4 P		0.799	313.16301
c231	F1839-B	C24 H33 N O6		12.467	431.22977
c1726				0.79	839.46044
c3377		C83 H129 N6 O18 P3		6.806	1590.85907
c3882		C41 H78 N10 O16 P2		3.331	1028.50747
c1799	VM55597	C28 H33 N3 O6		3.576	507.23567
c776		C35 H65 N5 O16 P2		0.792	873.38871
c2679	Muraymycin B2	C48 H81 N11 O18		7.946	1099.57199
c2895		C45 H73 N3 O6 P2		6.167	813.49773
c4866		C19 H32 N4 O10		2.216	476.21095
c1503		C25 H50 N5 O3 P3		5.526	561.31315
c1073	Radiosumin	C22 H32 N4 O5		5.54	432.23637
c1147		C29 H62 N10 O10 P2 S		6.349	804.3837
c2819		C55 H94 N5 O11 P3 S		8.194	1125.58843
c955				7.197	2167.06905
c601				6.778	2167.06826
c2863		C39 H74 N6 O6 P2 S		5.96	816.48587
c4744		C13 H32 N6 O4 P2		6.283	398.1949
c4383		C23 H47 N O11		6.17	513.31539
c4226		C84 H149 N6 O18 P3 S5		7.765	1782.87531
c491				3.631	1336.68733
c2528		C31 H61 N6 O5 P3 S		7.113	722.36225
c1293	4-Benzoylbiphenyl	C19 H14 O		3.819	258.1076
c1221		C45 H54 N5 O5 P		7.048	775.38845

c3874	Erucamide		C22 H43 N O	17.459	337.33391
c659			C23 H56 N9 O8 P3	0.802	679.3466
c2077			C43 H80 N4 O14	5.794	876.5677
c2552			C32 H48 N4 O3 P2	4.913	598.32181
c2366	Unknown Lok MF	B	C64 H132 N6 O18 P2 S2	15.115	1398.85123
c754			C65 H85 N9 O18 P2	0.792	1341.54862
c3945				6.181	368.69744
c4386				7.123	2125.94214
c4604				3.325	1679.90702
c2467			C61 H75 N8 O4 P S	6.131	1046.53795
c4023			C20 H46 N8 O9 S	0.791	574.31238
c3582			C50 H96 N7 O13 P3	6.744	1095.62847
c1396			C46 H77 N4 O10 P3	6.359	938.48563
c889			C25 H44 N6 O6	3.296	524.33088
c3972			C44 H67 N O9 P2	4.127	815.42826
c2534			C27 H46 N2 O10	0.805	558.31839
c4398				16.211	349.31841
c2427	WF-14865A		C17 H27 N5 O4	3.47	365.20544
c3510			C13 H30 N9 O4 P	4.383	407.2162
c519			C71 H111 N9 O14 P2	14.919	1375.77405
c3021	pro-gln		C10 H17 N3 O4	0.797	243.12126
c854			C35 H53 N3 O7 P2 S	4.832	721.30933
c2307				5.746	379.69011
c4283			C78 H117 N8 O18 P S	8.623	1516.79442
c399	Spumigin 640		C32 H44 N6 O8	6.998	640.3207
c4680			C42 H77 N4 O9 P3	7.567	874.49039
c3173			C47 H101 N10 O18 P3	5.396	1186.65525
c213			C84 H111 N3 O18 P2	5.053	1511.73433
c1217			C87 H148 N7 O18 P3 S4	7.087	1799.89918
c3435			C30 H54 N6 O8 S	6.912	658.3705
c2110			C54 H90 N6 O11 P2	5.196	1060.61469
c3675			C50 H97 N6 O9 P3 S2	5.198	1082.59677
c1113				7.427	994.4476
c3876			C6 H21 N7 O6	0.797	287.15669
c1535			C29 H59 N3 O5 P2 S	6.049	623.36372
c3568			C38 H60 N3 O9 P3	7.03	795.35555
c3959			C59 H86 N6 O17 S	3.941	1182.57812
c1852			C23 H40 N4 O5	7.144	452.299
c3145			C13 H30 Cl N5 O3 S	0.784	371.17421
c1191				5.559	2084.99357
c3856				7.251	1713.87197
c2695				8.26	1374.72616
c4621			C8 H21 N4 O5 P	5.515	284.12535
c4758				4.384	385.7426
c1958			C28 H63 N5 O14 S	7.557	725.40894
c4805			C39 H68 N O9 P S	4.589	757.43779
c2847			C23 H49 N9 O10	0.792	611.36178
c3264	Janthinocin C		C57 H82 N12 O15	6.917	1174.59641
c4144				7.084	1802.90489
c4643			C77 H123 N10 O14 P3 S	8.423	1536.8141
c1636			C44 H92 N5 O15 P3 S	7.295	1055.55106
c2417				9.988	2187.22202
c4447			C42 H92 N8 O17 S4	5.203	1108.54607
c3454				0.799	305.68165
c2871			C22 H51 N7 O5 P2 S2	4.314	619.28563
c4182			C10 H22 N7 O2 P S	4.963	335.1303
c3883			C42 H79 N8 O14 P3 S	7.235	1044.46456
c1689			C55 H85 N3 O16 P2	7.513	1105.54167
c3996			C37 H69 N4 O8 P3	4.346	790.43195
c3114			C42 H77 N2 O6 P3	7.075	798.49915
c187	Aderbasib		C21 H28 N4 O5	5.199	416.20599
c256			C27 H40 N10 O3	6.633	552.32704
c871				6.795	1981.97061
c4878			C43 H77 O13 P3	5.392	894.4581
c1442				3.572	1521.70339
c328			C20 H36 N4 O6	4.845	428.26271
c2137				6.168	1118.60517
c353			C56 H92 N9 O7 P3	9.195	1095.63331
c1460			C27 H37 N5 O5	6.315	511.27873
c2187			C29 H59 N8 O14 P	4.393	774.38949
c4458			C34 H52 N5 O6 P S2	3.098	721.30873
c2658			C21 H36 N3 O6 P S	0.792	489.20558
c1735			C27 H52 N7 O3 P3	3.804	615.33701
c605	FPK		C20 H30 N4 O4	0.795	390.22542
c2965			C60 H86 N4 O14 P2	5.91	1148.56127
c3216			C25 H43 N O12	7.067	549.27904
c4874			C89 H136 N3 O18 P S3	9.215	1661.87229
c4893	(2S)-8-[(1E)-3-hydroxy-3-methylbut-1-en-1-yl]-5,7-dimethoxy-2-phenyl-3,4-dihydro-2H-1-benzopyran-4-one		C22 H24 O5	0.791	390.13716
c3498	Nostocyclophane D		C36 H54 Cl2 O6	6.02	652.3277
c3525			C41 H76 N4 O7 P2	6.519	798.52026
c2509			C44 H80 N5 O8 P3	5.88	899.52194
c1283			C31 H55 N4 O8 P	8.592	642.37428
c959			C30 H48 N6 O9	7.482	636.34847
c1308			C78 H100 N8 O15 S	8.309	1420.70259
c1313			C27 H48 N3 O P	18.45	461.35329

c3183			C36 H57 O6 P3	5.642	678.33751
c1765				6.313	1981.96935
c4876				7.635	1031.58292
c1284			C89 H161 N10 O18 P3 S4	7.101	1879.00915
c2084			C76 H120 N7 O12 P3 S3	5.9	1511.73702
c2922			C73 H78 N7 P S	5.373	1115.57672
c3862				7.109	1880.01264
c3103			C25 H42 N3 O6 P	6.748	511.27919
c4698			C31 H61 N4 O14 P	6.044	744.39206
c4216				6.067	2185.06618
c3323				0.794	455.30949
c4374			C19 H26 N4 O5	3.827	390.18923
c3835				5.849	1815.89555
c2894			C40 H47 N2 O6 P	5.579	682.31805
c2796			C58 H90 N5 O13 P	6.456	1095.627
c909			C23 H43 N7 O9	5.256	561.31414
c4250			C29 H57 N O18	3.093	707.35965
c2121			C22 H41 N O6	12.699	415.29282
c4450	Maniwamycin F		C11 H21 N3 O3	1.212	243.1578
c1938			C41 H48 N4 O7	8.245	708.35066
c1358			C28 H56 Cl P3	0.795	520.32661
c3992				4.05	886.47372
c2071			C85 H115 N9 O14 P2	4.041	1547.80284
c3295			C33 H50 N6 O7	8.478	642.37411
c112			C15 H29 N O2	8.854	255.21986
c2958			C54 H100 N7 O15 P3	6.436	1179.64848
c2143	Adenosine 3'5'-cyclic monophosphate		C10 H12 N5 O6 P	0.797	329.05151
c4762			C59 H94 N9 O18 P	7.897	1247.64389
c2744				7.77	511.27998
c2586			C67 H81 N8 O6 P S	7.659	1156.57396
c2506			C15 H26 N4 O5	2.742	342.18973
c3937			C31 H50 N6 O9	9.694	650.36492
c1515			C85 H113 N3 O17 P2	4.979	1509.75563
c2519			C23 H53 N7 O14	5.228	651.36733
c109			C15 H29 N O	10.655	239.22446
c4331	Desertomycin B		C61 H106 O22	5.042	1190.7227
c4477			C34 H58 N2 O11	9.071	670.40526
c4580			C81 H140 N10 O16 P2 S2	9.207	1634.93667
c4405			C46 H85 N8 O12 P3	3.593	1034.54953
c1863				9.974	2647.38301
c1267			C50 H67 N5 O17	5.132	1009.45262
c4266				7.585	1275.64711
c3569			C34 H72 N2 O10 P2 S	4.313	762.4392
c2313			C18 H45 N7 O3	16.7	407.36016
c383				9.531	2085.15262
c4848				4.09	862.41874
c1144			C30 H50 N6 O7	5.012	606.37254
c2577			C87 H118 N5 O15 P3	7.056	1565.78417
c200			C30 H57 N4 O7 P3	0.795	678.34306
c2615				4.745	619.28545
c2328			C22 H36 N3 O P S	6.026	421.23212
c2553			C26 H51 N10 O7 P	4.331	646.36749
c4856			C26 H56 N7 O4 P3	6.053	623.36339
c3157			C17 H40 N9 O9 P S	4.535	577.24163
c1149			C22 H40 N4 O5 S	6.317	472.27122
c1100			C30 H58 N5 O P3	0.796	597.38328
c2994	Octyl decyl phthalate		C26 H42 O4	18.745	440.29005
c4449	val-arg		C11 H23 N5 O3	0.803	273.17919
c2967				6.526	358.67536
c1859			C24 H52 N8 O12 P2	4.188	706.31708
c3734	Aderbasib		C21 H28 N4 O5	4.646	416.20569
c611			C41 H71 N5 O13 P2	6.335	903.45129
c4617			C30 H63 N5 O15	4.241	733.43376
c1441			C34 H77 N9 O15 P2	5.504	913.50093
c2072			C23 H49 N9 O9	0.802	595.36698
c2763				0.806	297.6837
c2272			C62 H107 N8 O18 P S	5.927	1314.71463
c4369				15.11	1296.70964
c3761			C28 H52 N8 O8	9.48	628.39183
c641			C10 H27 N7 O2 P2	0.795	339.17135
c1173				6.381	1997.96545
c3391			C36 H77 N10 O16 P	5.443	936.52557
c713			C82 H121 N8 O10 P3	7.561	1470.84169
c210			C42 H59 N9 O10	6.79	849.43725
c3769	Piptamine		C23 H41 N	14.928	331.32251
c1232			C80 H106 N O16 P3	7.476	1429.67246
c4555				7.464	1158.61313
c2888				0.787	257.13649
c3895				0.779	514.27298
c4852			C48 H42 N10 O5	4.273	838.33359
c245			C69 H118 N10 O15 P2 S	9.184	1420.79723
c4124				0.793	314.17693
c3105			C32 H72 N10 O14 P2	6.148	882.46946
c2732				6.028	842.46404
c4070			C50 H77 N3 O7 P2	7.488	893.52314

c4493		C7 H18 N10 O2	1.21	274.16221
c4156		C43 H63 N6 P3 S2	6.246	820.37776
c2626		C35 H63 N6 O10 P3	5.359	820.3825
c4822		C66 H101 N9 O17 S	7.103	1323.70391
c3561		C20 H49 N8 O8 P3	3.316	622.28811
c2482		C38 H82 N8 P2 S5	0.795	872.47675
c2503		C56 H83 N5 O16 P2	7.584	1143.53113
c1356		C34 H38 O2	3.472	478.28936
c2068			7.537	1104.55857
c4198		C55 H110 Cl N6 O15 P3	8.711	1222.69297
c2817	(2R,3R,4S,5S,6R)-3-(acetyloxy)-2-[(acetyloxy)methyl]-5-(hexanoyloxy)-6-[[2S,3R)-2,3,4-trihydroxybutoxy]oxan-4-yl tetradecanoate	C34 H60 O13	8.238	1428.73479
c3745	Versipelostatin F	C61 H94 O18	7.583	1114.6407
c2589		C12 H28 N7 O3 P	4.247	349.19909
c4407			5.85	1816.89833
c3430		C30 H62 N6 O12	4.892	698.44297
c4540		C20 H48 N9 O5 P S	6.382	557.3239
c3077		C74 H87 N9 O10 S	4.1	1293.62718
c703		C49 H69 N9 O5 P2	6.963	925.48941
c1400			7.052	621.8167
c3641		C22 H42 N5 O9 P	6.429	551.27165
c1249			1.089	799.46577
c1225		C44 H71 N4 O8 P3	9.008	876.44902
c2477		C17 H27 N5 O3 S	0.746	381.18315
c3566		C17 H26 N4 O6	6.504	382.18488
c4605		C57 H94 N3 O8 P3 S	7.627	1073.59876
c3589		C29 H46 N6 O P2	6.146	556.32154
c2450		C29 H42 N6 O4 P2	5.218	600.27187
c4896			5.34	836.44327
c3106		C66 H92 N O11 P3	8.298	1167.58822
c2020		C38 H66 N4 O8 P2	5.209	768.4367
c4897		C23 H44 N2 O4 S2	5.033	476.27458
c4416		C39 H83 N9 O12 S4	5.024	997.5047
c4286		C7 H21 N7 S	0.797	235.15788
c4864		C26 H51 N9 O7 P2 S	4.073	695.31027
c434		C35 H57 N O8 P2	16.559	681.3537
c3771		C24 H49 N10 O4 P3	4.514	634.31275
c4872		C21 H50 N9 O5 P	6.809	539.36839
c3397		C29 H57 N O3	17.528	467.43322
c881		C35 H68 N3 O18 P S	4.733	881.39469
c2502		C90 H119 N2 O13 P3	8.183	1528.79182
c2575		C68 H106 N2 O14 P2	9.24	1236.71142
c1208		C18 H34 N9 O5 P	3.575	487.24349
c3750	(2R,3R,4S,5S,6R)-3-(acetyloxy)-2-[(acetyloxy)methyl]-5-(hexanoyloxy)-6-[[2S,3R)-2,3,4-trihydroxybutoxy]oxan-4-yl tetradecanoate	C34 H60 O13	8.231	714.36784
c4403	Caprazamycin E	C51 H83 N5 O22	6.442	1117.551
c3464		C43 H84 N O12 P3	6.284	899.52103
c1980		C66 H85 N8 O16 P3 S	0.795	1370.5019
c2765		C34 H77 N8 O11 P3	5.642	866.49261
c1591		C20 H31 N3 O4	5.85	377.23004
c4640		C23 H40 N6 O7	3.21	512.29485
c4326		C23 H44 N2 O3 S2	6.695	460.27929
c1082		C25 H46 N3 O7 P	6.955	531.30514
c490		C40 H67 N5 O11 P2	5.046	855.43112
c2607		C54 H97 N4 O18 P3	5.054	1182.60101
c1630			5.911	754.42202
c92	Radiosumin	C22 H32 N4 O5	5.232	432.23638
c2856		C43 H70 N10 O S4	4.193	870.46251
c3203			9.544	2129.10887
c1853		C37 H67 N7 O15	3.074	849.46857
c3651		C20 H38 N4 O5	6.022	414.28398
c3968	Cyclo-(Leu-Ile)	C12 H22 N2 O2	2.932	226.16778
c3567		C87 H119 N6 O14 P3	6.965	1564.79736
c921		C22 H31 N9 O6	0.688	517.23905
c4591			4.395	1188.57676
c1496		C33 H66 N4 O18	0.794	806.43746
c3092			7.174	1086.53655
c577		C68 H105 N9 O15 P2	7.095	1349.72095
c581		C82 H121 N5 O14 P2 S2	8.184	1525.78333
c4277		C17 H38 N8 O5 P2	4.146	496.24556
c3844			8.289	583.79433
c2193		C19 H41 N5 O5	18.737	419.31112
c4689			7.053	1566.78536
c4109			5.977	2053.02793
c1881		C23 H47 N6 O13 P	5.572	646.29518
c4417		C48 H85 N3 O11 P2 S2	5.657	1005.51177
c3060		C27 H64 N9 O4 P3 S	4.717	703.40179
c3040		C38 H74 N3 O15 P3	6.553	905.43102
c1611	SMTP-11L	C28 H39 N O6	12.471	485.27632
c4869			7.116	2126.941
c4855		C28 H59 N9 O4 P2 S	7.057	679.38878
c4453		C56 H101 N2 O17 P S	5.359	1136.65497
c4347		C34 H44 N6 O3 S	3.818	616.32175
c1188		C37 H67 N4 O6 P3	5.894	756.42743
c2114	Methyl (2S,2aS,3a'R,4a'R,5aR,12bR,12b'R,12c'R,15aR,15a'S,17a'S)-12c'-hydroxy-10'-methoxy-2',3',4,4a',5,6,8,12c',13,13',14,14',17',17a'-tetradecahydro-4'H,5'H,16'H-spiro[furo[2',3':7,8]indolizino[8,1-c;d]carbazole-2,6'-furo[2',3':7,8]indolizino[8,1-cd]pyrido[1,2,3-lm]carbazole]-7-carboxylate	C43 H50 N4 O6	4.398	718.37383
c2983		C24 H52 N9 O10 P	5.928	657.35694
c2761			5.158	390.71592

c894			C28 H62 N O6 P3 S	3.802	633.34765
c738				9.339	2043.14246
c444			C36 H68 N5 O10 P3	3.353	823.41764
c3706				0.757	243.13252
c3583			C29 H61 N3 O11 P2	4.503	689.37669
c2458			C68 H91 N8 O9 P	8.6	1194.66528
c4360			C22 H36 N6 O5	3.397	464.2735
c372				6.097	1937.96299
c3520			C19 H43 N7 O4 P2 S	0.798	527.25743
c4257				0.793	263.62883
c4285			C34 H54 N4 O P2 S	0.794	628.35314
c1667			C46 H59 N7 O6 S	0.8	837.42219
c4528			C24 H49 N O4	18.029	415.36526
c4424			C47 H91 N10 O2 P3 S3	4.557	1016.57091
c2633			C23 H40 O10	5.287	476.26304
c4118			C25 H52 N9 O3 P3	8.064	619.33719
c1992			C40 H51 N7 O10	12.457	789.36919
c2141			C75 H115 N6 O15 P3	9.332	1432.7633
c911			C15 H36 N5 O8 P	2.838	445.23147
c943	PPK		C16 H28 N4 O4	3.283	340.21005
c4516				6.455	1079.10283
c4377			C21 H35 O6 P	4.098	414.2175
c2092	Moriniafungin G		C38 H56 O13	4.603	720.37443
c3848			C37 H59 N6 O5 P3	4.364	760.37506
c3683			C39 H85 N4 O16 P3	4.539	958.51744
c1318			C35 H68 N5 O14 P	4.911	813.44894
c3452				7.693	1368.71675
c2784			C20 H32 N6 O5	0.803	436.24226
c2102	Hexadecanedioic acid mono-L-carnitine ester		C23 H43 N O6	13.075	429.30771
c4904			C33 H65 N O3	19.544	523.49632
c1119			C25 H48 O4 S	18.45	444.32693
c2865			C19 H43 N7 O7 P2	7.175	543.26818
c3159	Erythrochelin		C24 H41 N7 O11	5.575	603.28915
c2955			C16 H41 N8 O4 P S	6.097	472.2716
c3486			C68 H96 N4 O16	8.595	1224.67876
c2230				7.525	332.70473
c2646			C32 H69 N4 O18 P	4.105	828.4351
c880			C21 H42 N3 O7 P	4.903	479.27557
c4314			C88 H109 N9 O12 S2	8.179	1547.76397
c2198			C28 H49 N O4	18.77	463.36573
c3134				8.976	1352.71516
c1584			C45 H102 N9 O17 P3 S	6.299	1165.63247
c3783	Zolpidem		C19 H21 N3 O	0.8	307.16318
c3711			C29 H66 N7 O5 P3	5.812	685.43661
c974				3.488	1148.54758
c3890			C49 H86 N9 O13 P3	7.93	1101.55571
c3212			C18 H42 N8 O5 P2	4.536	512.27355
c4176			C52 H75 N O11 P2	5.79	951.48075
c3523			C28 H61 N4 O8 P3	6.545	674.36652
c4688			C19 H29 N3 O5	4.468	379.20967
c1892			C67 H111 N6 O16 P3 S	5.728	1380.69855
c4106			C49 H60 N2 O6 P2	4.947	834.39313
c4107				2.919	588.31511
c303			C44 H95 N8 O17 P3 S	0.795	1132.57436
c4295			C26 H50 N7 O6 P3	4.669	649.30266
c3609			C38 H84 N10 O17 P2	6.407	1014.55029
c1205			C83 H126 N6 O13 P2 S	7.073	1508.85752
c2118			C16 H30 N4 O6	2.831	374.21565
c716			C87 H154 N9 O17 P3 S5	6.685	1849.92783
c2495			C25 H62 N9 O4 P	16.541	583.46426
c3431			C23 H48 N5 O P3	5.504	503.30934
c2329	PLK		C17 H32 N4 O4	0.792	356.24117
c3501			C79 H100 N6 O13 P2 S	5.036	1434.65595
c3534				8.455	856.48342
c1895			C21 H41 N7 O4 S2	5.586	519.26811
c810				5.441	563.28475
c4026	Gln-Leu-Val-Pro		C21 H37 N5 O6	3.917	455.27385
c2370			C59 H105 N5 O16 P2 S	5.518	1233.673
c3386				0.784	1305.6639
c4654			C16 H41 N7 O3	15.607	379.3291
c4710			C87 H111 N4 O14 P3	4.072	1528.73113
c2907			C46 H65 N5 O11 S	3.602	895.43822
c2116			C57 H104 N7 O16 P S	5.408	1205.69931
c2496				0.798	614.32676
c3194			C33 H42 N10 O5	5.954	658.33278
c3989				0.8	486.24229
c3472			C14 H37 N8 O5 P S	5.733	460.2339
c3958	Cyclotryprostatin F		C23 H27 N3 O6	4.973	441.18889
c2511				6.745	2053.0273
c3083				7.116	1588.87269
c4740			C9 H24 N7 O2 P	0.799	293.17302
c3871			C35 H69 N3 O15 P2	13.162	833.42164
c3220			C16 H39 N10 O5 P S	0.782	514.25463
c3916			C27 H42 N10 O4	10.662	570.33797
c3407			C12 H29 Cl N3 O P	0.793	297.17347

c1186			C47 H70 N2 O13 P2	8.399	932.43614
c3410			C19 H52 N10 O7 P2	0.792	594.3472
c2804			C26 H60 N8 O4 P2 S2	6.421	674.36608
c1951			C48 H90 N6 O15 P2 S	6.623	1084.56614
c639			C26 H57 N9 O8 P2 S	6.528	717.351
c1633			C30 H60 N7 O13 P	6.127	757.39946
c1106			C33 H63 N8 O10 P S	7.077	794.41503
c3187				4.679	1298.60674
c4127				5.232	1563.71987
c438			C18 H35 N8 O4 P	5.778	458.25346
c315			C43 H76 N10 O12	6.508	924.56369
c1741	unknown Lok MF isotope misassignment	B	C24 H6 N3 O15 P3	15.149	668.90073
c2403			C85 H107 N7 O5 S	15.146	1337.80179
c3143	(3S)-3-((Z)-[[(3S)-3-((Z)-[(3R)-3-Amino-1-hydroxy-4-methylpentylidene]amino)-1-hydroxybutylidene]amino)-5-methylhexanoic acid		C17 H33 N3 O4	5.201	343.24644
c1417			C52 H96 N7 O17 P S	0.793	1153.63202
c2379			C26 H58 N9 O11 P	5.519	703.39977
c4838			C53 H88 N O16 P3	6.985	1087.53208
c3543			C51 H109 N8 O12 P3 S3	5.437	1214.65328
c2489			C38 H58 N8 O10	5.688	786.42702
c2161			C20 H47 N10 O6 P	5.796	554.34278
c4163	N-Pentadecanoylglycine		C17 H33 N O3	9.486	299.24628
c4460			C70 H114 N10 O13 P2	9.256	1364.80393
c3473	1-[[[(3-Methoxypropyl)imino](methylthio)methyl]amino]-2,4,5-trimethylbenzene		C15 H24 N2 O S	11.163	280.16494
c3086			C24 H44 N3 O8 P	5.275	533.28418
c638			C22 H44 N8 O4	0.798	484.34958
c2314			C76 H108 N3 O18 P3	7.58	1443.68429
c4261				0.783	218.12126
c1264				6.35	2085.99683
c199				9.613	2510.38322
c1964			C23 H39 N5 O6	3.244	481.28914
c2769			C30 H57 N6 O4 P3	6.059	658.36795
c3684			C25 H58 N10 O13 S	5.783	738.39083
c4037			C41 H71 N9 O12 P2	4.824	943.46899
c4800	PNH		C15 H22 N6 O5	3.686	732.32936
c4553			C38 H48 Cl N O5 S3	18.256	729.23723
c4677				6.995	810.30936
c2667			C22 H47 N7 O	16.669	425.3858
c1137			C18 H33 N3 O9	0.796	435.22154
c4264			C33 H72 N9 O14 P S	6.983	881.46568
c1994			C45 H78 N8 O16 S	6.285	1018.52534
c4652			C32 H61 N5 O5 P2 S	3.453	689.38449
c3788			C27 H47 N4 O11 P	3.778	634.29599
c2642			C67 H100 N8 O17 S	3.917	1320.69323
c4738				8.307	1581.86126
c3459			C22 H35 N5 O4 P2	11.898	495.21429
c3814			C28 H65 N7 O8	16.488	627.49061
c3042			C59 H91 N10 O12 P3 S	5.404	1256.57563
c4868				5.82	807.2952
c2982			C45 H89 N8 O14 P3	4.601	1058.57084
c3353			C17 H32 O16	0.79	492.16884
c4116			C66 H68 N2 O S	7.539	936.50521
c2402			C17 H40 N9 O7 P	5.044	513.27873
c2707			C41 H58 N2 O4 S2	6.866	706.3832
c3346			C26 H51 N3 O13	5.301	613.3423
c3149			C39 H71 N8 O4 P3	4.702	808.48031
c1815			C14 H27 N3 O4	5.043	301.19916
c162	3-Hydroxytetradecanedioic acid		C14 H26 O5	10.673	274.17738
c3344			C56 H65 N4 O5 P	8.654	904.47084
c4623			C24 H49 N10 P3 S	4.104	602.30528
c3006			C13 H20 N4 O9	0.782	376.12157
c2632			C40 H88 N9 O15 P	5.197	965.61372
c3797	(2R)-1-[(7Z,10Z,13Z,16Z)-7,10,13,16-Docosatetraenoyloxy]-3-(phosphonooxy)-2-propanyl (4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-docosahexaenoate		C47 H73 O8 P	5.434	796.5037
c3694			C34 H62 N4 O15	6.534	766.42163
c4173			C30 H45 N O4 P2	3.697	545.28111
c4625	Maniwamycin F		C11 H21 N3 O3	3.853	243.15788
c3671			C14 H31 N O4	2.792	277.22443
c2960			C48 H46 N2 O8 S	12.458	810.29814
c336			C60 H101 N9 O12 P2 S3	0.794	1297.62021
c1518			C28 H45 N7 O6	5.86	575.34254
c2285				5.625	393.21787
c3137	Desthiobiotin		C10 H18 N2 O3	2.19	214.13142
c1784			C20 H49 N7 O4	16.675	451.3863
c1389			C80 H108 N5 O17 P	7.065	1441.74652
c1862			C14 H29 O P	1.627	244.19535
c2229			C41 H75 N2 O9 P3 S	7.395	864.44125
c3599	MDPBP		C15 H19 N O3	14.831	261.13594
c3672				6.672	1816.89837
c2185				5.551	1174.66534
c2529	12-benzyl-5,8,21-trimethyl-3-(2-methylpropyl)-6,9-bis(propan-2-yl)-icosahydropyrrolo[1,2-q]1-oxa-4,7,10,13,17-pentaazacyclononadecane-1,4,7,10,13,17-hexone		C36 H55 N5 O7	7.755	707.37528
c2046			C24 H57 N7 O6	16.591	539.43826
c4778			C30 H36 N2 O3	6.49	472.27144
c4024			C23 H43 O4 P3	4.048	476.23718
c331				6.079	2083.99501
c4128			C64 H116 N10 O18 P2 S2	7.274	1438.73825
c3557			C38 H57 N3 O6 P2	6.531	713.37322

c292			C14 H27 N O2	7.636	241.20353
c1234			C22 H53 N9 O9 P2 S	5.56	681.31627
c4824			C16 H36 N6 O6 S	7.699	440.24172
c3875	L-Glutathione (reduced)		C10 H17 N3 O6 S	1.022	307.08276
c4473	Oleamide		C18 H35 N O	16.787	281.27114
c4404			C46 H74 O14 S	5.712	882.47987
c2862				5.309	997.48611
c4702				8.212	1529.79697
c2023				5.396	2099.98721
c4041			C35 H48 O2 P2 S	4.4	594.28758
c4820			C33 H47 N O2 S3	4.973	585.27928
c119			C30 H49 N7 O9	3.804	651.35798
c254				6.669	2067.99931
c63			C60 H87 N4 O16 P	0.794	1150.58524
c4193			C35 H57 N8 O5 P	3.053	700.42198
c1906			C87 H114 N7 O11 P3	8.383	1525.77857
c283	Diprotin B		C16 H29 N3 O4	3.53	327.215
c904			C18 H46 N9 O5 P3	5.644	561.28272
c4376				4.369	1180.56267
c3076			C28 H46 N7 O4 P	6.002	575.33246
c2452			C19 H45 N10 O5 P	2.824	524.33106
c2411			C21 H39 N O8 P2	11.396	495.21417
c4271	Bis(2-ethylhexyl) terephthalate		C24 H38 O4	4.078	390.27635
c3363			C14 H37 N5 P2 S2	7.047	401.19766
c3926			C29 H55 N4 O12 P	9.172	682.35346
c2891			C30 H47 N2 O6 P	5.226	562.31666
c3964			C40 H83 N8 O17 P3	4.115	1040.50832
c2217				6.676	1815.89561
c3840			C22 H42 N2 O4 P2 S	4.685	492.23338
c4436			C35 H80 N10 O17 P2	5.383	974.5174
c1493			C46 H89 N6 O18 P3	7.704	1106.54292
c1920			C42 H72 N8 O17	4.974	960.50093
c1816	Prolylleucine		C11 H20 N2 O3	5.549	228.14609
c1804			C61 H112 N5 O17 P3	7.188	1279.7281
c3547			C28 H61 N9 O17	7.067	795.41771
c4303				7.66	1184.64537
c4170			C30 H66 N9 O12 P	7.104	775.45703
c2879			C57 H91 N10 O17 P S	3.907	1250.60319
c2780			C75 H108 N5 O15 P3 S	3.547	1443.67885
c2463	Arg-pro		C11 H21 N5 O3	0.794	271.16344
c382	(2E,4E)-N-(2-methylpropyl)deca-2,4-dienamide		C14 H25 N O	8.548	223.19339
c330				15.079	1371.82405
c2942			C37 H68 N7 O3 P3	9.013	751.46235
c4047	Granisetron		C18 H24 N4 O	11.824	312.19166
c1946			C30 H70 N9 O14 P	4.502	811.4792
c3097			C26 H59 N6 O6 P3	7.415	644.37399
c4815				7.856	1247.65635
c586			C45 H68 N4 O15	8.291	904.46727
c805			C47 H82 N6 O9 P2	4.333	936.5622
c2044			C13 H29 N9 O2 S	5.357	375.21526
c3453			C23 H51 N7 O2 S	18.451	489.38453
c1952			C21 H44 N3 O9 P	4.304	513.27912
c148			C29 H41 N5 O5	8.254	539.30992
c3879	Marimastat		C15 H29 N3 O5	4.932	331.21009
c226				6.214	2067.99817
c685			C38 H71 N3 O13 P2 S	6.792	871.41971
c3005			C8 H20 N2 O3 S2	4.134	256.09136
c3479			C30 H50 N3 O2 P3	5.856	577.31017
c3090			C23 H50 N5 O9 P	9.015	571.33577
c3922			C34 H59 N2 O5 P3	5.811	668.36113
c3417			C28 H59 N9 O9 P2 S	5.644	759.36083
c3061			C34 H73 N3 O12 P2 S	4.455	809.43827
c3753			C34 H55 N10 O2 P S2	5.028	730.36758
c1027	NP-008993		C18 H34 O4	13.069	336.22658
c345			C16 H30 N6 O4	0.777	370.23172
c2716			C22 H39 N2 O6 P	6.546	458.25266
c3907				5.523	392.2049
c2501			C34 H49 N4 O2 P S	6.725	608.33173
c3838			C26 H53 O5 P3	5.438	538.31024
c1233	N-(((1S,4S,6S)-6-Isopropyl-3-methyl-4-[2-oxo-2-(1-pyrrolidinyl)ethyl]-2-cyclohexen-1-yl)methyl)-4-methoxybenzenesulfonamide		C24 H36 N2 O4 S	4.01	470.21365
c3665			C21 H52 N7 O9 P	4.379	577.35771
c133	Lokisin M+H+NH4 adduct	B	C66 H120 N10 O14 P2 S	15.115	1370.81857
c2858			C31 H56 N4 O17	3.803	756.36403
c4884				9.111	1594.90744
c562	(2R,3R,4S,5S,6R)-2-(((2E)-4-ethenyl-2,5-dimethylhexa-2,5-dien-1-yl)oxy)-6-(hydroxymethyl)oxane-3,4,5-triol		C16 H26 O6	10.665	296.15948
c3028			C35 H57 N7 O2 P2 S2	5.965	733.34702
c3163			C28 H60 N7 O11 P3 S	12.459	795.32803
c1973			C46 H80 N8 O16	6.816	1000.56995
c1622			C34 H59 N3 O5 P2	6.911	651.39493
c3600				7.494	2019.0269
c2179			C14 H37 N8 O5 P	5.536	428.26291
c3069			C56 H98 N5 O15 P S	5.546	1143.65175
c3524			C68 H79 N5 O11	8.286	1141.57778
c3646				5.435	1123.56731
c3243				6.17	456.7503

c3503			C43 H42 N2 O	6.746	602.3322
c1456			C51 H69 N6 O7 P	6.106	908.49664
c546			C23 H36 N8 O3	5.985	472.28983
c3088			C17 H32 N2 O8	2.353	392.215
c3185			C36 H72 N9 O9 P3	7.131	867.46799
c4888			C30 H33 N2 P	0.798	452.23793
c4237				4.972	273.65007
c4737			C12 H34 N6 O3 P2 S	1.041	404.18926
c1488	Leucyltryptophan		C17 H23 N3 O3	5.324	317.17352
c4886			C18 H42 N9 O5 P	5.281	495.3048
c3291			C50 H94 N3 O17 P3	6.232	1101.57948
c229			C49 H74 N8 O10 P2	4.556	996.501
c976			C6 H15 N8 P S	0.799	262.08797
c4806				7.65	457.54955
c76			C32 H46 N6 O7	6.841	626.34225
c3804			C25 H48 N5 O3 P3	7.426	559.29872
c1737			C22 H53 N7 O5	16.638	495.41237
c1090			C19 H43 N10 O3 P3	7.188	552.27446
c952	Juvenimicin C		C29 H48 O10	5.17	556.32248
c3338			C22 H57 N10 O5 P S2	5.463	636.36658
c4239			C19 H30 N6 O4	3.921	406.23114
c1635	Reserpine		C33 H40 N2 O9	3.005	1216.53048
c715			C28 H46 N5 O9 P	2.972	627.30338
c1911			C24 H46 N3 O10 P	6.152	567.2897
c3595			C15 H39 N7 O10 S	0.801	509.24658
c4122			C87 H131 N4 O14 P3 S	8.309	1580.85942
c4087				5.205	1050.53657
c3917			C57 H91 N3 O13 P2	5.263	1087.60157
c1771			C40 H69 N6 O12 P	7.469	856.46974
c4780			C24 H46 N9 P3 S	4.459	585.27872
c1197				6.18	2099.98679
c3751	2-furyl[4-(1H-indol-4-yl)piperazino]methanone		C17 H17 N3 O2	6.029	590.2737
c4298	Methionylleucine		C11 H22 N2 O3 S	3.079	262.1346
c339	Santacruzamate A		C15 H22 N2 O3	5.262	278.16268
c3191			C13 H28 N6 O14	1.029	492.16805
c206			C35 H53 N3 O6 P2 S	5.216	705.31418
c2720			C13 H26 N7 O3 P	7.061	359.18378
c2132			C25 H54 N5 O8 P	3.391	583.36782
c4210			C74 H104 N9 O15 P3	4.523	1451.68667
c1728	Dibutyl phthalate		C16 H22 O4	15.176	278.15078
c224			C34 H42 N10 O3	7.492	638.34276
c3836			C11 H13 N7	4.09	243.12242
c1576				5.32	634.34647
c4175			C25 H34 N4 O5	6.98	470.2553
c3517	JWH-302		C22 H25 N O2	4.683	670.36401
c3500			C12 H18 N6	19.699	246.15939
c4507				7.124	1659.83181
c3465			C37 H50 N5 O6 P3	6.618	753.29871
c1028			C45 H102 N8 O18 P2 S	6.349	1136.65019
c3224			C32 H64 N5 O13 P3 S	13.16	851.34278
c4879			C39 H68 N2 O12	4.024	756.47409
c1976			C21 H53 N9 O15	0.793	671.36567
c2321			C20 H43 N10 O5 P	6.121	534.31642
c2033			C42 H80 N7 O15 P3	2.698	1015.49222
c1885			C58 H88 N6 O12 P2	5.31	1122.59373
c420				9.09	1649.90061
c4389				9.191	1466.85373
c1109			C47 H82 N4 O7 P2	6.198	876.56633
c3605			C51 H84 N10 O14 P2	6.442	1122.56325
c3514				4.347	486.24266
c582			C19 H47 N6 O8 P S	6.471	550.29064
c4038			C53 H86 N5 O6 P3 S	4.266	1013.55215
c2428			C14 H25 N O3 S	7.846	287.15521
c3121			C27 H58 N8 O6 P2	7.545	652.39356
c1393				6.245	974.55721
c4586			C25 H51 O13 P	5.488	590.30479
c1114	Not named		C25 H38 N4 O6	6.598	490.27846
c4577			C16 H40 N9 O6 P	3.618	485.28398
c841			C26 H42 N6 O6	5.085	534.31572
c2785			C42 H74 N9 O15 P	8.271	975.50468
c4812			C35 H52 O2 S	5.069	536.36736
c3655	Kojistatin A		C17 H32 N4 O5	4.661	372.23683
c2886			C30 H64 N4 O6 P2 S	3.52	670.39975
c4603	N-{4-[(3R,4R,6R,7S,8R,9E,11E,13E,15R)-16-Carboxy-3,7,15-trihydroxy-4,6,8-trimethyl-9,11,13-hexadecatrienoyl]phenyl}-beta-D-glucopyranosylamine		C32 H47 N O11	6.739	621.31803
c4275			C60 H72 O S3	0.791	904.47507
c1438			C54 H86 N8 O12 P2	6.735	1100.58374
c4190			C30 H36 N2 O3	6.497	472.27068
c4353			C66 H86 N6 O18	8.248	1250.59944
c792			C32 H70 N9 O15 P	5.085	851.4735
c3868			C44 H68 N9 O16 P	5.268	1009.45264
c4658			C58 H91 N7 O11 P2	9.109	1123.62497
c3366			C65 H106 N7 O15 P3	8.822	1317.69899
c1668	Streptocidin Q		C66 H92 N14 O12	7.485	1272.69919
c2563				0.789	646.35212
c3991			C13 H26 N4 O3	2.945	286.19978

c665		C32 H58 N4 O11	6.544	674.41063
c1158			7.084	2300.06564
c2740		C40 H68 N3 O10 P3	8.246	843.4113
c626		C87 H154 N9 O17 P3 S5	6.169	1849.92673
c2075		C46 H65 N3 O3	19.381	707.50327
c3460		C16 H33 N O5	10.676	319.23495
c4662		C28 H50 N8 O4 P2 S	5.84	656.31438
c3977			3.655	854.48378
c4795		C25 H62 N9 O12 P S	5.21	743.3997
c2770		C13 H36 N9 O4 P	0.791	413.26253
c1443	WF-14865A	C17 H27 N5 O4	1.543	365.20567
c311	Bis(2-ethylhexyl) phthalate	C24 H38 O4	18.015	390.27635
c4042		C35 H59 N3 O10 S2	5.703	745.36408
c2567		C16 H35 N O4	10.398	305.25625
c3691	Hexadecanamide	C16 H33 N O	16.648	255.25542
c404		C50 H87 N8 O18 P3	13.164	1180.53582
c3350		C56 H111 N2 O17 P3 S2	6.637	1240.65357
c1055			9.116	1593.81608
c2281		C33 H65 N8 O11 P	8.289	780.45108
c3041		C79 H87 N5 O7 P2	3.138	1279.6101
c1965		C16 H40 N9 O5 P S	4.287	501.26086
c4696		C12 H18 N3 O P S	0.805	283.09093
c4362			7.558	1444.68613
c2573			4.614	2236.12429
c2767		C30 H57 N4 O4 P3	1.025	630.35839
c2203		C50 H98 N10 O13 P2 S	8.292	1140.65081
c430		C45 H78 N8 O16 S	5.23	1018.52527
c4001		C19 H33 N5 O6	3.662	427.2419
c2923			5.195	1094.59912
c2559		C14 H34 N9 O7 P	8.288	471.23209
c4244			8.287	942.46317
c2011		C82 H109 N3 O15 P2	7.223	1437.73321
c514	Leuhistin	C11 H19 N3 O3	2.947	241.14209
c3604		C38 H71 N4 O9 P3	3.739	820.44344
c4792		C38 H82 N10 O11 P2 S	3.846	948.53604
c4547		C29 H60 N4 O14 P2	3.849	750.35761
c2730	SMTP-11L	C28 H39 N O6	11.958	485.27618
c1913			5.551	228.14593
c3186		C17 H43 N7 O10 P2 S	5.436	599.22826
c1432		C25 H37 N5 O6	5.659	503.27384
c3010		C45 H80 N3 O14 P S	5.203	949.51059
c4174		C20 H46 N10 O7 S	8.301	570.32524
c3679		C25 H49 N O10	5.588	523.33633
c436	(2S,8R)-8-hydroxy-2-([(1S)-1-hydroxyheptyl]-3,4,5,6,7,8-hexahydro-2H-1-benzopyran-5-one	C16 H26 O4	10.396	282.18064
c2492		C39 H65 N4 O10 P S	5.249	812.41722
c3055		C15 H27 N8 O3 P	7.299	398.19561
c2050		C56 H87 N7 O9 P2	5.333	1063.60445
c3707		C17 H40 N9 O5 P	4.421	481.28891
c4119	Cyclocarbamide B	C15 H22 N2 O4	3.138	294.15727
c2408		C51 H95 N7 O16 P2	9.071	1123.62795
c2781	2,19-dihydroxy-13,20-dimethoxy-4,7,17,22,22-pentamethyl-5,10,21,23-tetraoxahexacyclo[18.2.1.0Aa,Âaâ-.0â´,Âaâ¶.0â¶¶,Âaâ´.0â„,ÂaÂ?]tricoso-6(14),7,12-trien-11-one	C26 H34 O9	6.466	512.20683
c3921		C23 H42 N3 O4 P3	1.035	517.23815
c433			6.303	2083.9931
c4101		C49 H81 N O12 P2	4.655	937.52304
c344			6.732	1079.60444
c3261		C15 H38 N7 O8 P	3.429	475.25354
c1987		C27 H50 N3 O3 P S2	6.236	559.30305
c4497			5.673	892.50426
c1130			5.086	425.73689
c2926		C78 H114 N8 O17 P2 S	6.83	1528.74961
c946		C34 H45 N7 O S2	4.844	631.31452
c4363		C58 H109 N2 O17 P3	5.009	1198.69382
c2124		C16 H30 N4 O5	4.93	358.22118
c248			6.082	1936.96071
c4349		C22 H47 N7 O	17.246	425.38607
c806		C49 H67 N6 O7 P	5.276	882.47943
c2320			4.183	392.20428
c3369		C63 H103 N6 O3 P3 S4	7.589	1212.6199
c104			4.175	314.65811
c2472		C22 H52 N10 O P2 S	3.353	566.35246
c4579		C10 H28 N5 O5 P	5.156	329.18321
c4320		C15 H3 N4 O18 P3 S	5.941	651.83745
c4382	Benzyl 2-({[4-(carbamimidamidomethyl)cyclohexyl]carbonyl}oxy)benzoate	C23 H27 N3 O4	5.336	409.19939
c2257		C89 H141 N7 O17 P2 S3	7.053	1737.90086
c4661		C8 H24 N7 O4 P	5.211	313.16317
c2684		C47 H60 N10 O3 P2	5.572	874.43063
c402			6.305	2084.99601
c2131			3.011	2389.0986
c978		C49 H77 N9 O5 P2	5.697	933.55196
c4396			5.942	1303.67307
c4817			6.686	1978.94692
c1436		C59 H95 N9 O15 P2 S	3.515	1263.61521
c2295			5.558	1598.7936
c1404	Rhizomide B	C35 H53 N7 O11	5.847	747.38003
c4297		C9 H22 N7 O2 P	0.801	291.15741

c2036		C20 H30 N4 O4	6.242	390.22616
c1252		C19 H41 N O6 S2	2.985	443.23686
c2989		C47 H85 N4 O18 P	8.111	1024.56085
c1652		C47 H71 N6 O3 P3	10.674	860.47935
c214		C78 H134 N7 O17 P3 S	9.115	1565.87777
c563		C37 H73 N3 O10 P2 S	4.769	813.44798
c1332		C24 H38 N8 O7	3.102	550.28438
c3639		C28 H66 N10 O5 P2 S	3.75	716.44188
c1510		C66 H119 N6 O18 P3	8.249	1376.77957
c3402	(Z)-N-((2R)-1-Hydroxy-2-((Z)-((2S)-1-hydroxy-2-((Z)-(hydroxy[(2R)-1-(D-tyrosyl)-2-pyrrolidinyl)methylene]amino)-3-phenylpropylidene)amino)-3-methylbutylidene)-L-alpha-glutamyl-L-proline	C38 H50 N6 O10	3.573	750.35829
c4290		C25 H51 N4 O12 P	0.798	630.32239
c3821		C25 H36 N6 O5	4.196	500.27379
c3438		C26 H59 N9 O2 P2 S2	4.934	655.37284
c3302			7.08	1509.86252
c1616		C50 H84 N10 O18	4.64	1112.59749
c1637			7.945	1896.07427
c1572		C23 H47 N9 O11 S	6.959	657.31313
c3861		C53 H112 N8 O17 P2 S	5.017	1226.73491
c583		C18 H34 N4 O5 S	5.207	418.22457
c4184		C45 H67 N10 O16 P	4.556	1034.44689
c2378		C26 H59 N10 O9 P	5.509	686.42068
c509		C71 H82 N4 O10	7.095	1150.60364
c3309		C25 H59 N9 O6 P2	7.584	643.40447
c2612		C75 H98 N9 P3	7.107	1217.71536
c722		C27 H49 N O6 P2 S	3.621	577.27706
c2968		C71 H114 N6 O17 P2	8.241	1384.77133
c4392		C29 H46 N2 O10	0.793	582.31485
c2674		C52 H81 N5 O15 S	6.529	1047.54475
c2711		C59 H90 N8 O14	10.677	1134.65691
c1586		C47 H74 N9 O7 P3	7.41	969.49339
c3627		C79 H103 N3 O13 P2	3.528	1363.6967
c2165		C15 H29 N O4 S	8.139	319.18149
c2424		C33 H63 N6 O10 P	4.455	734.43136
c71		C16 H29 N3 O4 S	4.627	359.187
c960		C23 H40 N3 O7 P	4.908	501.25797
c905			5.048	1949.95787
c872	(2E,4E)-N-(2-methylpropyl)deca-2,4-dienamide	C14 H25 N O	8.846	223.19394
c2159		C58 H100 N7 O11 P3 S2	6.325	1227.61319
c2400		C32 H72 N8 O14 P2	6.297	854.46341
c4716		C12 H33 N8 O4 P	3.793	384.23638
c814		C42 H63 N6 O7 P S	6.126	826.42129
c4505		C8 H21 N6 O2 P	5.533	264.14656
c2985	Indole-3-acetyl-epsilon-L-lysine	C16 H21 N3 O3	4.504	303.15787
c1831		C54 H88 N3 O17 P3	7.697	1143.5324
c3013		C26 H64 N10 O12 P2	5.428	770.4159
c2525	(4aS,9aR)-7-Benzyl-2-[[4-methoxyphenyl]acetyl]decahydro-6H-pyrido[3,4-d]azepin-6-one	C25 H30 N2 O3	3.525	812.437
c592			6.185	1952.95331
c656		C18 H43 Cl N8 O2	0.788	438.32115
c1485			5.137	504.72624
c3621		C37 H81 N6 O13 P3 S	8.348	942.48023
c3016		C27 H48 N3 O8 P	6.879	573.31953
c1475		C16 H31 N8 O4 P	6.345	430.2227
c3536	unknown Lok MF	C74 H113 N5 O16 P2	15.632	1389.76383
c3178	B	C60 H98 N10 O6 P2 S2	6.705	1180.65844
c3522			0.792	467.21773
c2893		C19 H24 N4 O6	4.226	404.16887
c1692		C31 H53 N6 O9 P	7.587	684.35845
c2617		C43 H94 N9 O15 P3 S	6.232	1101.57967
c3529		C33 H62 N6 O6 P2	4.942	700.41842
c4021		C26 H58 N8 O15	5	722.3995
c1694			4.172	632.3197
c3575		C23 H53 N5 O9	10.388	543.38266
c4446		C24 H52 N8 O9	7.086	596.38744
c3474	2'-O-Methyladenosine	C11 H15 N5 O4	1.59	281.11178
c429			5.576	1380.70462
c3170		C45 H92 N3 O16 P3	4.372	1023.5698
c1254		C19 H39 N8 O4 P	7.137	474.28389
c445		C56 H81 N10 O11 P	6.447	1100.58239
c4192		C8 H28 N7 P3	0.808	315.16124
c2585		C28 H47 Cl N10 O5	7.219	638.34252
c884	6,8-Tricosanedione	C23 H44 O2	17.251	352.33344
c3645		C24 H55 N4 O7 P	10.386	542.37981
c3537		C13 H27 N8 O4 P	3.814	390.1898
c2941		C36 H50 N8 O7	5.441	706.38204
c2413		C42 H70 N7 O3 P S3	6.496	847.44328
c4525	glycyclamide	C14 H20 N2 O3 S	4.617	296.11918
c1167			6.178	2100.98959
c3024		C22 H32 N4 O6	3.333	448.23092
c852		C28 H54 N5 O10 P	4.884	651.35868
c838			6.67	2036.02826
c4151	(20Z)-20-Nonacosene-2,4-dione	C29 H54 O2	18	434.41183
c3816		C72 H86 N4 O4 P2	7.236	1132.61361
c2418		C64 H99 N8 O14 P3 S	7.597	1328.62272
c3336		C20 H47 N7 O9 S	6.118	561.31474
c3680		C32 H51 N7 O10	4.86	693.36909

c1346	NP-004917		C15 H26 O3	14.83	276.17187
c3791				5.258	504.72638
c756			C42 H64 N3 O11 P	13.165	817.42641
c4687				7.557	592.32115
c1693	unknown Lok MF	B		15.117	2762.50803
c3100				3.816	870.49479
c3250			C19 H35 N3 O9	3.717	449.23653
c2756				7.489	1962.00602
c454			C25 H41 N5 O7	3.691	523.2997
c3381			C32 H63 O9 P3	5.871	684.36589
c3772			C52 H84 N9 O10 P3	6.076	1087.55549
c2441			C24 H43 N5 O6	5.566	497.32004
c1411				9.536	2102.17362
c3831				5.035	842.46155
c4765			C24 H58 N10 O10 P2	5.82	708.37966
c3842			C54 H105 N2 O18 P3 S2	5.602	1226.6012
c3803			C18 H39 N8 O5 P3	3.366	540.22716
c468			C62 H94 N7 O8 P3	6.128	1157.63797
c1339			C48 H91 N6 O15 P3 S	6.451	1116.54861
c3442				8.355	888.97394
c1370			C55 H93 N7 O14 P2	5.442	1137.6269
c4445			C43 H60 N9 O5 P	5.523	813.44746
c3913			C13 H31 N9 P2	4.959	375.2181
c1437			C55 H92 N8 O18	6.595	1152.65328
c44			C20 H36 N4 O6 S	5.148	460.23482
c4343			C32 H53 N5 O6 P2 S	5.109	697.31589
c3019			C31 H65 N8 O11 P3	5.339	818.39884
c4218	Nodulisporic acid A1		C43 H53 N O7	6.269	695.38048
c95			C81 H120 N9 O12 P3	7.194	1503.82786
c4036			C69 H97 N2 O16 P S	3.332	1272.62954
c2957				9.621	2527.40062
c3794			C38 H75 N2 O15 P3	3.031	892.43788
c3131	(2E,4E)-N-(2-methylpropyl)deca-2,4-dienamide		C14 H25 N O	7.609	223.1932
c3096	Cyclocarbamide B		C15 H22 N2 O4	3.301	294.1572
c2993			C57 H88 N7 O4 P S2	5.547	1029.60772
c4601			C23 H44 O2 P2 S	6.717	446.25206
c3935	(6Z,9Z,21R,27S)-24,27,30,30-Tetrahydroxy-24,30-dioxido-18-oxo-19,23,25,29-tetraoxa-24lambda~5~,30lambda~5~-diphosphatriaconta-6,9-dien-21-yl (4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-docosahexaenoate		C46 H76 O13 P2	3.714	898.47342
c4576				6.715	1959.84507
c4209			C22 H57 N9 O16 P2	4.263	765.34154
c819			C30 H42 N6 O10	5.474	646.29485
c2453			C19 H29 N3 O5	5.651	379.21027
c2742			C44 H77 N8 O13 P3	4.558	1018.48326
c3494			C50 H104 N5 O14 P3 S2	5.43	1155.62418
c1132			C47 H62 N5 O8 P	5.518	855.43193
c1222			C16 H41 N10 O5 P S	1.164	516.27134
c2199	Maniwamycin F		C11 H21 N3 O3	4.904	243.15787
c3954			C42 H58 N7 O5 P3	7.92	833.36986
c2201			C27 H50 O3	17.528	422.37537
c2438			C35 H49 N7 O4 S2	4.103	695.32591
c3946			C22 H51 N6 O3 P3	4.044	540.32551
c833			C29 H46 N10 O6	0.691	630.35918
c1861			C24 H51 N9 O10	0.796	625.37783
c4656			C74 H124 N6 O17 P2	7.929	1430.84983
c2015				5.359	948.42676
c4013			C60 H77 N6 O7 P	8.391	1024.55852
c1585			C40 H70 N5 O7 P3	5.364	825.44866
c101	Bis(methylbenzylidene)sorbitol		C22 H26 O6	12.47	386.17209
c3172			C80 H93 N6 O9 P	6.589	1312.67537
c2801			C25 H41 N5 O5	9.013	491.30982
c4491			C60 H99 N6 O16 P3	4.645	1252.63349
c3596			C33 H45 N8 O P S	5.193	632.31852
c2877			C38 H75 N6 O16 P	5.134	902.49684
c234			C66 H95 N5 O14 P2	5.412	1243.63519
c2042				5.453	531.27269
c387			C43 H67 N8 O4 P3 S	4.712	884.4214
c2166			C45 H43 Cl2 N3 O S2	17.68	775.22331
c1908				6.433	2086.99765
c897			C22 H48 N3 O7 P	6.401	497.32099
c3301			C20 H41 N O8	4.336	423.2838
c3215			C57 H93 N9 O11 P2 S4	6.487	1269.53579
c3056			C49 H93 N9 O14 P2 S2	7.658	1157.57493
c646	Benzyl butyl phthalate		C19 H20 O4	15.03	312.13514
c3950			C29 H42 N3 O3 P S	8.602	543.26906
c10	Lokisin	A,B	C64 H111 N11 O20	15.114	1353.79464
c1764			C14 H37 N8 O4 P	5.911	412.26853
c3378			C73 H83 N3 O2 P2	7.916	1095.59698
c982			C20 H30 N4 O4	4.509	390.22576
c3719			C24 H55 N10 O3 P3 S	6.588	656.33772
c2880			C47 H99 N9 O13 P2 S	5.404	1091.65648
c1298			C27 H54 N5 O9 P	7.854	623.36385
c3374			C57 H100 N7 O16 P3	4.762	1231.64407
c4720			C79 H101 N4 O16 P	4.973	1392.69521
c4348			C64 H95 N7 O12 P2	6.5	1215.65195
c1422	DAMGO		C26 H35 N5 O6	5.082	513.25804
c830			C11 H21 N5 O2	0.789	255.16898

c4543				5.901	532.20542
c4551			C44 H94 N7 O14 P3 S	4.923	1069.57895
c620			C31 H49 N9 O4 P2 S	4.155	705.31353
c3725			C18 H22 N4 O6	4.019	390.15332
c4452				5.948	1302.67539
c277	Santacruzamate A		C15 H22 N2 O3	5.156	278.16197
c4191				8.483	1270.66401
c360				6.084	2084.99733
c1675	Zeatin-7-N-glucoside		C16 H23 N5 O6	4.846	381.16907
c3219			C29 H53 O8 P S	10.676	592.31884
c1379			C27 H39 N5 O6	5.896	529.28984
c2167	Lobophorin B		C61 H90 N2 O21	7.602	1186.59803
c1981			C15 H25 N3 O6	8.291	343.1735
c2178			C9 H26 N9 O P	0.79	307.19844
c2238	Leucyl-leucyl-norleucine		C18 H35 N3 O4	6.377	357.26246
c1075	1-[(2R,4S,5R)-5-(3-Cyclohexyl-1-methyl-1H-pyrazol-5-yl)-1-azabicyclo[2.2.2]oct-2-yl]-N-(4-methoxybenzyl)methanamine		C26 H38 N4 O	5.87	460.26545
c2692			C30 H53 N4 O8 P	6.311	628.35734
c4560			C22 H44 N2 O12	4.554	528.2896
c3538	Ceramide (d18:1/12:0)		C30 H59 N O3	18.359	481.44914
c3570			C30 H56 O3	18.351	464.42284
c1963			C72 H110 N7 O16 P S	15.12	1391.74734
c3721				7.142	361.69679
c2299			C30 H42 N7 O5 P	7.413	611.29613
c3426			C22 H53 N7 O7 P2	6.647	589.3465
c1415			C58 H77 N3 O P2 S2	4.898	957.4983
c2286				9.953	2626.46646
c3718			C23 H50 N O6 P S2	5.149	531.27982
c2690	Nostopeptolide A2		C52 H78 N10 O14	5.266	1066.5677
c3331			C26 H35 N9 O2	3.646	505.28913
c4045	7'-Methoxy NABUTIE		C25 H25 N O2	5.677	742.36795
c585			C49 H97 N6 O16 P3 S	3.933	1150.58843
c3130	Banegasine		C11 H12 N2 O2	3.371	204.08946
c837			C37 H64 N4 O7 P2	4.832	738.42639
c920			C40 H68 N4 O14 S	6.341	860.44568
c3094			C22 H41 N5 O5	3.475	455.30969
c4188			C56 H97 N3 O14 P2	6.012	1097.64476
c4232			C26 H39 N10 O4 P S	4.201	618.26315
c4581			C42 H64 N3 O7 P	8.15	753.44811
c2372			C43 H94 N9 O15 P3 S	6.231	1101.58016
c197	leu-his		C12 H20 N4 O3	0.802	268.15279
c198	Desmethylmianserin		C17 H18 N2	0.803	250.14229
c811	PPK		C16 H28 N4 O4	3.297	680.42054
c4826			C34 H68 N7 O11 P3 S	6.286	875.39043
c3768			C51 H95 N6 O15 P3	5.546	1124.60795
c2789	Natalenamide A		C19 H25 N3 O5	3.569	375.17895
c3626			C35 H71 N8 O13 P	5.195	842.48814
c520			C43 H77 N7 O18	6.17	979.53249
c4644			C20 H44 N5 O7 P	4.483	497.29534
c3987			C26 H48 N6 O2 S2	6.22	540.32605
c456			C17 H43 N10 O10 P	7.521	578.28706
c2542	7'-Methoxy NABUTIE		C25 H25 N O2	5.674	371.1842
c225				6.214	2069.00076
c2688				4.461	1862.9559
c3483			C18 H36 O5 S2	5.11	396.20014
c3450			C63 H115 N6 O18 P S5	4.86	1434.66027
c1091			C13 H29 N9 O3 S	4.153	391.20972
c2934			C15 H29 N3 O4	4.963	315.21539
c3115	1-[[[(3-Methoxypropyl)imino](methylthio)methyl]amino]-2,4,5-trimethylbenzene		C15 H24 N2 O S	10.716	280.16472
c3624			C44 H55 N6 O6 P	4.493	794.39051
c1433			C10 H22 N4 O5	5.036	278.16046
c3786				4.249	391.20989
c2355	2-[5-[(2S)-1-(1H-Imidazol-2-ylmethyl)-2-pyrrolidinyl]-1,2,4-oxadiazol-3-yl]-4-(2-methoxyethoxy)pyridine		C18 H22 N6 O3	8.967	784.30996
c1921			C48 H84 N10 O15 P2 S	6.173	1134.5307
c708				9.931	2201.24014
c2590			C20 H29 N3 O5	4.25	391.20931
c3744	(-)-Erythromycin		C37 H67 N O13	5.342	771.41156
c4344			C18 H43 N9 O P2 S	4.045	495.2794
c4208			C20 H38 O4 S2	17.701	406.22033
c1372	Celestolide		C17 H24 O	3.448	244.17822
c440			C24 H34 N4 O7	5.718	490.24272
c1745			C16 H30 N6 O4	2.989	370.23206
c588			C54 H99 N9 O10 P2 S	5.417	1127.66997
c2777			C23 H55 N5 O12 P2 S	5.217	687.30391
c3607			C75 H124 N3 O18 P3 S3	3.763	1543.72519
c4062			C33 H76 N8 O16 P2	3.617	902.48455
c1644			C35 H56 N10 O2 P2	7.051	710.40755
c3213			C19 H49 N10 O3 P3	3.905	558.31941
c2696			C48 H94 N7 O13 P3 S	6.73	1101.58718
c4090			C41 H85 N9 O17 P2 S	6.538	1069.52593
c3825			C29 H48 N3 O P3	5.158	547.29924
c922			C37 H56 N8 O11 S	5.792	820.37804
c3433			C28 H53 N O4 P2 S	6.123	561.31501
c3521			C76 H126 N9 O11 P3 S	9.186	1465.85157
c579			C75 H95 N3 O14 P2	4.121	1323.62767
c3728			C26 H48 O2	17.108	392.36473

c4406			C24 H50 N7 O4 P3	5.093	593.31589
c4510				5.096	296.6581
c1993			C46 H100 N8 O12 P2 S3	5.426	1114.61019
c3018			C12 H31 N5 O11	4.27	421.20351
c2803			C28 H46 N5 O5 P3	5.107	625.27379
c2469			C67 H107 N9 O7 P2 S2	6.274	1275.72026
c4302			C14 H36 N9 O5 P	5.545	441.25792
c4557			C15 H24 O8 P2	11.398	394.0941
c266	WF-14865A		C17 H27 N5 O4	0.789	365.20525
c3644			C28 H41 N7 O2 P2	4.961	569.28227
c3398			C26 H40 O2 P2	5.691	446.25236
c3716	N1-acetyl-N7-o-hydroxyphenylacetyl cadaverine		C15 H22 N2 O3	8.254	278.16233
c3140			C17 H32 N4 O3	4.494	340.24661
c4064			C30 H48 N5 O3 P S	5.934	589.32263
c2213	Methionylphenylalanine		C14 H20 N2 O3 S	4.067	296.11859
c2442				6.389	786.379
c1540				0.793	1042.51644
c1478			C65 H96 N5 O17 P	4.033	1249.65433
c1945	Chaiyaphumine A		C40 H44 N6 O7	0.794	720.32676
c2523			C59 H80 N7 O8 P3	3.557	1107.52872
c140			C45 H84 N5 O12 P3	5.799	979.53285
c2645			C45 H65 N9 O5 P2	8.239	873.4583
c41			C26 H41 N5 O7	4.343	535.29965
c2815			C15 H25 N3 O8	2.637	375.16353
c61			C40 H63 N7 O8	9.013	769.47265
c356			C28 H45 N7 O6	5.011	575.3416
c3180			C75 H86 N5 O13 P3	0.791	1357.54328
c1554			C18 H45 N7 O7 P2	5.677	533.28449
c2112	Microviridin N1		C88 H116 N18 O24	6.143	1808.84166
c3146			C22 H50 N6 O6 P2 S	6.991	588.29799
c3743	Methyl (2R,4S,6S,12bR)-4-(4-fluorophenyl)-2-[[3-{1H-imidazol-1-yl}propyl]amino]-1,2,3,4,6,7,12,12b-octahydroindolo[2,3-a]quinolizine-6-carboxylate		C29 H32 F N5 O2	4.483	501.25769
c3602	Ethyl oleate		C20 H38 O2	16.363	310.28638
c1917			C63 H123 N4 O5 P3 S	18.398	1140.8425
c3023			C36 H71 N4 O12 P3	7.092	844.43107
c2435			C22 H42 N4 O3 P2	5.599	472.2712
c3615				8.14	601.32738
c3031			C36 H48 N6 O7	8.978	676.35766
c3490				5.148	1148.55374
c4427			C23 H53 N10 O6 P	7.557	596.38848
c24			C23 H36 N6 O4	5.453	460.27882
c4895			C36 H42 Cl N O4 S3	18.395	683.1956
c4889			C23 H34 N4 O7	3.457	478.24187
c1549			C36 H60 N4 O15 S	6.082	820.37806
c3859			C34 H63 N2 O13 P	6.75	738.40594
c3852			C21 H24 N4 O6	4.424	428.16912
c2079			C72 H110 N7 O9 P3 S	6.294	1341.73118
c3588			C37 H67 N2 O16 P	7.542	826.42146
c2151				5.824	2263.1548
c4565				5.827	2264.15561
c4259			C10 H28 N7 O3 P	6.036	325.19984
c1678			C39 H80 N2 O17 P2 S	4.874	942.46446
c1464			C13 H33 N9 O6	4.851	411.25561
c4509			C50 H59 N3 O8 S	4.586	861.40366
c4096			C25 H52 N10 O10 S	7.836	684.3588
c2507				6.361	2295.02577
c1939				6.345	1137.6449
c1559			C62 H94 N3 O18 P	4.166	1199.62751
c223	Nostosin D		C21 H33 N5 O5	4.27	435.24698
c2808			C26 H57 N10 O6 P	7.711	636.42076
c2018	unknown Lok MF	B		15.117	2763.50763
c2913	N6-Dimethyladenosine		C12 H17 N5 O4	2.769	295.1276
c4138				6.034	650.39951
c2117			C23 H34 N10 O3	3.631	498.27951
c3254			C21 H53 N10 O11 P	4.868	652.36064
c4631			C18 H45 N10 O6 P	2.581	528.32639
c2962				3.64	1329.63699
c3530			C45 H73 N9 O18	4.367	1027.50715
c853			C62 H83 N9 O8 S	5.428	1113.60651
c962				5.426	556.80352
c3574			C28 H54 N9 O14 P	5.507	771.35305
c3068			C50 H64 N8 O3 P2	8.045	886.45927
c1697			C32 H34 N10 O5 S	5.078	670.24375
c3120			C25 H55 N7 O2	18.011	485.44382
c4566	Syringolin E		C25 H43 N5 O6	5.29	509.32182
c173			C36 H60 N8 O13	4.832	812.42672
c1927			C53 H82 N8 O17 P2 S	13.163	1196.50055
c2415				6.342	567.82945
c3988			C25 H44 N9 O6 P3	7.056	659.26191
c4599			C85 H103 N7 O16 P2 S	6.237	1571.66572
c2368				15.127	2783.4979
c4359			C19 H42 N2 O11 S	7.661	506.25259
c4811			C32 H65 N9 O11 P2	6.303	813.42654
c2234			C88 H136 N7 O12 P3 S2	9.205	1639.89141
c2644			C38 H66 N7 O10 P	4.474	811.45888
c423			C20 H45 N10 O6 P	5.026	552.32543

c448			C26 H41 N5 O7	5.024	535.29897
c2003			C41 H67 N4 O12 P S	6.328	870.42201
c1749	Madurastatin A2		C27 H41 N7 O10	0.681	623.29237
c3674			C53 H57 N3 O6	3.925	831.42308
c3057			C24 H45 N10 O10 P	3.79	664.30505
c2678			C42 H49 N O3 S	6.371	647.34294
c3272				3.006	1195.55223
c1169				7.171	1102.54209
c4839			C50 H78 N6 O11 P2	6.457	1000.52005
c2538	(5E)-2,10-Diamino-5-[[[(5-amino-5-carboxypentyl)amino]methyl]-5-undecenedioic acid (non-preferred name)		C18 H34 N4 O6	4.073	402.24673
c1524				5.353	750.43035
c2341				8.519	622.33308
c1891			C19 H36 N4 O5	5.853	400.26807
c2680			C42 H78 N10 O15 P2	4.113	1024.5128
c1967			C29 H55 N5 O15 S	4.057	745.34049
c3468			C19 H25 N3 O7	2.45	407.1682
c4775			C67 H128 N10 O18 P2 S3	6.683	1518.80316
c4722				0.781	326.67388
c3462			C49 H82 N9 O8 P3	6.66	1017.54801
c4701			C17 H43 N8 O P S3	5.916	502.24628
c2588	Pezizolide D		C14 H18 O5	12.47	266.11442
c1709				9.998	876.15724
c4607				5.072	1026.51596
c2706			C49 H85 N4 O9 P3	7.659	966.55303
c2754			C25 H56 N3 O14 P	0.795	653.34787
c1052			C79 H99 N10 O12 P	9.083	1410.71804
c3118			C51 H81 N9 O3 S3	6.16	963.56311
c2892			C22 H51 N7 O3 S2	6.288	525.35177
c4748	SSR161421		C25 H20 N4 O2	13.037	408.15376
c2746			C40 H90 N9 O17 P3 S	4.532	1093.53842
c4704			C60 H88 N6 O13 P2	3.681	1162.58835
c3230			C75 H105 N9 O13	14.81	1339.78173
c3632			C38 H62 N9 O6 P	8.564	771.45338
c2592	4,4-dimethyl-1-(3-nitrophenyl)-2-(1H-1,2,4-triazol-1-yl)pent-1-en-3-one		C15 H16 N4 O3	0.796	300.12134
c2867	PPK		C16 H28 N4 O4	1.057	340.21014
c4637				9.964	2655.40366
c323			C21 H51 N8 O2 P3	5.353	540.33398
c1164			C16 H27 N7 O5	7.075	397.20766
c3299			C38 H68 N10 O12	4.764	856.50177
c1961			C90 H113 N8 O11 P3 S	4.049	1606.74499
c4249				4.837	722.36666
c3371			C18 H30 N4 O5	4.237	382.22124
c3957			C45 H68 O9 S	6.743	784.45869
c1857	Emericelloxide		C21 H26 O3	5.381	326.18848
c1753			C15 H28 N5 O3 P	15.031	357.19289
c555				5.576	1380.70534
c1802			C12 H23 N3 O2	2.501	241.17852
c2582			C32 H70 N7 O16 P	3.004	839.45999
c154			C69 H106 N8 O15 P2 S	4.768	1380.69636
c4865	Microphycin AL828		C40 H60 N8 O11	6.865	828.43802
c779			C23 H48 N8 O11 S	5.97	644.32012
c3636			C16 H27 N3 O4	4.911	325.19982
c688			C54 H85 N3 O16 P2	4.333	1093.53893
c2113	Diprotin A		C17 H31 N3 O4	5.864	341.23087
c2666			C28 H43 N9 O4	6.49	569.34171
c1526				4.604	561.28231
c1858	WF-14865A		C17 H27 N5 O4	2.133	365.20564
c4219			C24 H59 N10 O10 P	6.598	678.41347
c4506			C37 H7 N4 O5 P S	5.037	649.98723
c3375			C29 H59 N5 O14 P2	4.913	763.35501
c1428	Prolylleucine		C11 H20 N2 O3	5.549	228.14635
c2171			C36 H53 N7 O11	5.745	759.37971
c4756			C19 H42 N8 O4 S2	4.453	510.27901
c3265			C45 H83 O9 P3 S2	6.098	924.46896
c1349			C52 H100 N7 O14 P3 S2	6.739	1203.59869
c1793			C25 H57 N8 O10 P S	5.702	692.36374
c1887			C56 H97 N10 O16 P	9.16	1196.68101
c351			C20 H36 N4 O6	4.708	428.26339
c560				4.09	673.8432
c2794			C24 H52 N8 O3 P2 S2	7.142	626.30854
c1425			C59 H76 N4 O10	4.102	1000.55618
c4841				6.238	733.35283
c3283			C34 H63 N8 O14 P	6.61	838.42058
c917			C71 H107 N6 O17 P S	7.028	1378.71534
c2738			C19 H44 N3 O8 P	3.495	473.28396
c635			C21 H35 N5 O8	3.852	485.24755
c3902			C23 H53 N3 O6 P2 S	6.119	561.31505
c2972			C55 H88 N8 O16 P2	3.739	1178.58055
c1168			C22 H41 N5 O5 P2	4.64	517.25647
c2999			C47 H63 N3 O2 S2	5.753	765.43791
c1561			C17 H43 N8 O4 P	7.113	454.31496
c2635			C54 H98 N3 O13 P3 S2	4.214	1153.57413
c2591	(2S,3S,4S,5R,6S)-6-(Hydroxymethyl)-5-[[[(2R,3S,4S,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)-5-[[[(2R,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl]oxy]tetrahydro-2H-pyran-2-yl];oxy]tetrahydro-2H-pyran-2,3,4,5-tetrol		C18 H32 O18	19.655	536.15843
c1338			C35 H59 N6 O8 P	7.692	722.41102
c4234			C24 H30 N4 O8	7.058	502.20563

c1998			C34 H76 N6 O15 P2	8.298	870.48405
c1184	unknown Lok MF	B		15.116	2746.53464
c2332			C22 H55 N6 O3 P3 S	3.115	576.32556
c2240				7.638	1373.15011
c2966			C31 H72 N7 O16 P S	6.345	861.44876
c2443			C48 H69 N8 O10 P3 S	5.881	1042.4085
c1504			C23 H54 N5 O3 P3 S	7.018	573.31863
c2944				4.218	629.81501
c3612			C24 H44 N9 O P3 S	3.616	599.25897
c3591				8.233	1527.78415
c3614				9.96	2653.39713
c3656			C14 H30 N10 O5	4.244	418.24172
c4055				4.238	836.48331
c4537				4.609	239.14473
c2346			C64 H130 N2 O15 P2	18.328	1228.89426
c2643	Fijimycin C		C44 H62 N8 O12	3.598	894.44561
c258			C23 H28 N8 O2	4.004	448.23155
c973				9.931	2206.192
c3930				5.556	759.37904
c1032			C20 H30 N4 O8	4.331	454.20535
c4863			C72 H79 N2 O4 P S2	3.753	1130.52207
c3527			C17 H25 N3 O4	4.776	335.18413
c51			C41 H59 N9 O10	6.296	837.43722
c3710			C20 H33 N2 O5 P	6.483	412.21057
c1253	Roseothricin (H-277)		C18 H37 N7 O6	15.776	447.28204
c2846			C33 H53 N O3 P2	8.074	573.35249
c2896			C12 H33 N9 O7 S	3.585	447.22228
c2522	NP-006862		C20 H32 O4	15.188	318.21602
c458				7.142	2033.11563
c3931			C24 H38 N9 O P3	6.762	561.24299
c3001			C80 H115 N O14 P2	15.065	1375.7791
c4294			C25 H41 N2 O6 P3	3.042	558.21886
c2315	Syringolin C		C25 H41 N5 O6	5.587	507.30493
c3400			C41 H71 N2 O10 P S3	6.494	878.40146
c4883	Octyl decyl phthalate		C26 H42 O4	16.253	418.30675
c796			C23 H40 N6 O9	2.658	544.2849
c1926			C32 H76 N8 O18 P2	5.355	922.47573
c2620				5.401	461.23831
c1552			C51 H91 N4 O15 P S2	5.154	1094.56582
c1835			C23 H27 N9 O4 S	3.987	525.18883
c3237			C40 H81 N2 O13 P3	2.568	890.49552
c175			C51 H89 N10 O9 P3	6.736	1078.60214
c1271			C28 H58 N7 O13 P	6.136	731.38457
c2401			C56 H88 N8 O14 P2 S	4.024	1190.56203
c4529			C61 H106 N2 O18 P2 S2	7.585	1280.63547
c3362			C50 H89 N7 O16 P2 S	3.705	1137.55518
c2465	Semagacestat		C19 H27 N3 O4	5.136	361.19955
c3318				7.249	1548.79471
c2085	Elaiomycin H		C12 H25 N3 O3	0.801	259.18869
c1641			C13 H32 N10 O2 S	8.256	392.24138
c1597	5S-hydroxynorvaline-S-Ile		C11 H20 N2 O3	4.566	228.14701
c4518	Brasilicardin B		C44 H66 N2 O15	4.106	862.44736
c4332			C35 H57 N3 O8 P2	7.046	709.36352
c1413			C35 H53 N3 O7 P2	5.88	689.33635
c3555				4.888	836.4485
c2266			C28 H43 N8 O4 P S	4.654	618.28678
c1272			C29 H51 N9 O9	4.363	669.37977
c1798			C18 H36 N4 O S2	3.179	388.23115
c4433			C8 H15 N9 O3	2.615	285.13008
c2547	MDMB-CHMICA		C23 H32 N2 O3	4.158	1218.65383
c1953				5.231	372.68173
c2065			C26 H59 N3 O6 P2 S	7.692	603.36231
c1758			C20 H36 N4 O6	3.476	428.26244
c4098			C25 H44 N6 O6	2.151	524.33111
c3560			C20 H45 N6 O3 P S2	4.097	512.27308
c4785			C81 H110 N3 O17 P	7.788	1427.75734
c3205			C18 H45 N6 O4 P	3.268	440.32406
c3236			C57 H101 N5 O16 P2 S	6.821	1205.64457
c4079				6.121	1348.6347
c2335	Leucyl-leucyl-norleucine		C18 H35 N3 O4	6.498	357.26226
c4252			C65 H85 N8 O9 P	7.312	1152.61822
c3717			C73 H112 N3 O13 P3 S	6.296	1363.71379
c1621			C21 H50 N9 O5 P	7.205	539.36746
c619	(+/-)-pantetheine		C11 H22 N2 O4 S	3.309	278.12919
c667	N-[4-[(2R,3R)-3-(Hydroxymethyl)-4-methyl-5-oxo-2-morpholinyl]phenyl]acetamide		C14 H18 N2 O4	3.31	300.11133
c3062			C18 H33 N3 S2	5.544	355.20979
c749			C21 H55 N10 O11 P	5.997	654.37838
c795				6.687	1850.93037
c4587			C53 H74 N9 O11 P	3.941	1043.52488
c1462			C26 H53 N4 O8 P	5.916	580.35825
c2749			C80 H117 N2 O17 P3 S2	7.597	1534.70072
c1587			C13 H32 N5 O5 P	5.804	369.21344
c4583				5.524	1234.67961
c2150			C23 H55 N8 O15 P S	4.199	746.32475
c1558			C8 H7 N2 O17 P S2	0.719	497.89258

c4779			C85 H129 N9 O16 P2	9.116	1593.90366
c1685			C72 H118 N3 O17 P3 S	5.855	1421.73763
c186			C29 H36 N10 O7	4.825	636.27448
c850			C11 H25 N4 O4 P	6.289	308.16049
c2576	Febarbamate		C20 H27 N3 O6	5.373	405.18935
c2244			C21 H55 N10 O4 P3 S	5.19	636.33678
c2280				4.2	1302.59552
c2885				3.742	546.30074
c4456			C11 H15 N5 O4 S	1.075	313.0833
c3634			C36 H70 N3 O9 P3	5.651	781.43218
c1842				9.913	2229.17679
c4901			C55 H104 N8 O12 P2 S2	8.223	1194.66916
c461	(3S,9aS)-3-benzyl-octahydro-1H-pyrido[1,2-a]pyrazin-1-one		C15 H20 N2 O	0.799	266.13703
c2909			C34 H70 N3 O14 P	7.297	775.45892
c3337			C22 H38 N5 O5 P	6.723	483.25912
c2515			C31 H51 N6 O10 P	3.615	698.34195
c4598				5.608	914.48624
c2650			C30 H51 N3 O8 P2 S	6.502	675.28498
c668	methyl 2-cyano-3-[1-[3-(1H-imidazol-1-yl)propyl]-1H-pyrrol-2-yl]acrylate		C15 H16 N4 O2	2.635	284.12681
c1501			C8 H23 N4 O3 P	0.794	254.15007
c2007				6.426	1148.61761
c2188			C60 H96 N O18 P	6.421	1149.63699
c2279			C56 H67 N9 O3 S4	6.251	1041.42455
c409			C19 H33 O7 P	9.771	404.19704
c2601			C23 H48 N3 O7 P	4.64	509.32101
c4375			C45 H60 N2 O3 S2	6.222	740.40641
c1449			C34 H72 N9 O5 P3	4.068	779.48851
c4428			C45 H92 N8 O5 P2 S5	7.54	1046.52733
c1269			C36 H70 N3 O17 P	6.082	847.44333
c2357			C64 H94 N5 O10 P	6.179	1123.67349
c671			C18 H45 N7 O2 P2 S	4.04	485.28398
c566				3.585	1338.65586
c2524			C21 H40 N8 O3 P2 S	4.555	546.24289
c3887			C48 H88 N O15 P3	9.3	1011.5374
c3436			C67 H111 N7 O14 P2 S2	14.51	1363.7109
c1390			C15 H39 N9 O9 S	0.805	521.25818
c3800	Arphamenine A		C16 H24 N4 O3	3.066	320.18388
c4498	Kribelloside A		C30 H56 O14	3.062	640.36777
c500	Valorphin		C44 H60 N8 O12	3.578	892.43726
c2030			C71 H120 N9 O15 P3 S3	4.066	1527.72918
c3260			C16 H37 Cl N4 O10	4.067	480.22102
c1112			C23 H47 N4 O10 P	3.639	570.30081
c1079	Leucyltryptophan		C17 H23 N3 O3	6.066	317.17344
c516			C15 H30 N10 O4 S	3.59	446.21885
c893	N-Pentadecanoylglycine		C17 H33 N O3	10.759	299.24587
c4201			C32 H50 N3 O8 P	8.49	635.3318
c2282			C28 H55 N3 O10 S2	4.971	657.33203
c2252			C32 H60 N5 O7 P3	6.348	719.37336
c1331				5.437	430.18762
c2455				7.23	625.86146
c1255			C17 H34 N3 O10 P	4.828	471.19609
c2809			C25 H41 N5 O5	7.401	491.31121
c1733			C29 H55 N9 O4 S2	5.042	657.38201
c23	Cl-4		C11 H19 N5 O2	0.794	253.15302
c3759			C68 H95 N10 O14 P	3.764	1306.67687
c4304				4.472	1002.51462
c2028	LQH		C17 H28 N6 O5	0.793	396.21111
c1403			C36 H52 N8 O10	8.064	756.38157
c4059				8.263	1213.65642
c1579			C11 H21 N3 O2	0.797	227.16277
c4180				5.173	338.6924
c4860			C39 H64 N7 O14 P	6.577	885.42575
c4310			C28 H59 N7 O	18.36	509.48041
c2848				3.983	774.35768
c2369			C24 H51 N9 O10 S	6.181	657.347
c1574			C23 H40 N4 O3	12.93	420.3088
c2103			C39 H66 N4 O14	6.335	814.45831
c4480			C42 H61 N O5 P2	5.361	721.39933
c3663			C20 H38 N4 O6	3.999	430.27865
c4714			C31 H56 N O7 P3 S	4.911	679.29843
c2398			C37 H67 N5 O16	4.481	837.45744
c3594			C12 H23 N3 O2 S	3.737	273.15041
c2481			C61 H120 N8 O17 P2 S4	7.616	1426.71407
c3428			C24 H51 N6 O5 P3	4.833	596.31616
c725				9.936	2202.24422
c4900				6.306	1880.88003
c4247	Cyclizidine		C17 H25 N O3	13.056	291.18263
c2541			C23 H56 N7 O3 P S2	7.074	573.36253
c2604			C26 H41 N2 O3 P S	5.805	492.25837
c718			C34 H50 N6 O6	9.013	638.37808
c3471			C63 H101 N4 O13 P	4.29	1152.70923
c3256				7.61	1100.06952
c3808			C21 H49 N10 P3 S	5.181	566.30565
c3628			C15 H38 N6 O6 P2	4.172	460.23437
c4727				6.858	2170.07515

c3354			C52 H87 N9 O16 P2	3.556	1155.57476
c1563			C50 H86 N9 O12 P3	5.288	1097.55883
c4345				5.508	385.67686
c2841			C22 H46 N8 O11	5.604	598.32831
c3049			C43 H86 N3 O15 P3	3.438	977.52773
c4711	1,3-Dipropylxanthine		C11 H16 N4 O2	1.196	236.12656
c230			C19 H32 O8 P2	11.398	450.15689
c30	1,3-Dipropylxanthine		C11 H16 N4 O2	0.795	236.12649
c2557	5,5'-epoxy-MKN-349A		C22 H34 N4 O5	6.516	434.25253
c2182			C31 H66 N3 O8 P3	3.426	701.40535
c4690			C38 H35 N3 O	4.164	549.27933
c3511				4.329	619.28531
c1700			C39 H65 N3 O13 P2	3.372	845.39964
c1352	Bis(2-ethylhexyl)adipate		C22 H42 O4	18.028	370.30787
c2595			C42 H65 N7 O16	5.401	923.44799
c4033	NP-018248		C31 H56 O16	2.583	722.30681
c1613			C88 H112 N9 O10 P3 S	4.602	1579.74599
c460	Lokisin+CH2	A;B	C65 H113 N11 O20	15.39	1367.81269
c4549			C15 H26 P2	0.786	268.15215
c1680			C87 H141 N6 O17 P3 S	9.092	1666.9263
c208			C70 H115 N5 O18 P2	15.115	1375.77271
c969			C19 H43 N10 O4 P	5.408	506.32043
c930				7.398	1356.74307
c4016	(2S)-4-Methyl-2-((((3S,4S,5R)-2,3,4-trihydroxy-5-(hydroxymethyl)tetrahydro-2-furanyl)methyl)amino)pentanoic acid (non-preferred name)		C12 H23 N O7	1.123	293.14635
c45	Diprotin A		C17 H31 N3 O4	4.946	341.23109
c4313				4.932	393.22572
c4100			C35 H57 N3 O2 P2	4.635	613.3909
c3845			C19 H35 N2 O6 P	4.892	418.22427
c1527			C27 H32 N6 O2	14.05	472.25826
c1142			C39 H79 N10 O11 P3 S	7.136	988.48477
c2362			C23 H42 N10 O6 S	10.674	586.30178
c3981				7.627	1375.65649
c1544			C28 H62 N5 O15 P	6.553	739.40106
c2172			C23 H41 N2 O6 P	8.512	472.26888
c2399	Fenspiride		C15 H20 N2 O2	8.05	260.15262
c4809			C27 H43 O6 P3	4.211	556.22795
c455			C31 H40 N10 O7	3.996	664.30571
c740			C34 H22 Cl N5	19.646	535.15776
c3343				0.783	568.31764
c2089	NP-018430		C38 H68 O18	4.834	834.40764
c4115				5.171	256.63976
c1506				6.56	2113.96591
c2600				4.202	1052.50896
c3434				6.64	1227.66371
c1336			C24 H43 N5 O5 P2	4.299	543.27155
c1878			C61 H93 N8 O14 P	3.859	1192.65385
c1045			C29 H57 N9 O11	5.27	707.42043
c1879	5S-hydroxynorvaline-S-Ile		C11 H20 N2 O3	5.87	228.14709
c3767				3.55	2114.98198
c3708			C20 H51 N8 O9 P	5.518	578.35084
c2062			C20 H48 N10 O7	7.483	540.37179
c1406			C48 H87 N7 O9 P2	4.28	967.60398
c3758			C39 H60 N5 O4 P3	4.625	755.38732
c1359				7.027	1379.71778
c127			C75 H95 N3 O14 P2	4.478	1323.62821
c1025			C66 H115 N7 O17 P2	15.042	1339.78099
c4615			C22 H47 N10 O3 P3	4.212	592.30312
c3712			C75 H86 N9 O8 P S	3.511	1303.60664
c1690			C74 H80 N8 O3 P2	3.68	1190.58174
c1954			C17 H46 N10 O15	4.401	630.31528
c50			C14 H27 N O4 S	7.615	305.16537
c3629			C71 H114 N4 O17 P2 S2	8.638	1420.70743
c2317			C73 H120 N3 O18 P3 S2	3.704	1483.72228
c3833			C22 H36 N6 O12	1.096	576.23744
c3036			C31 H49 N5 O7	7.35	603.36359
c4318			C38 H56 N5 O11 P	5.822	789.3724
c4844				4.083	497.28258
c1687			C17 H40 N9 O7 P S	4.378	545.25119
c2868			C56 H93 N7 O17 S	6.236	1167.63463
c4093			C24 H44 N6 O6	3.688	512.33149
c2473			C16 H29 N3 O4 S	4.1	359.18667
c3754				0.788	284.15895
c3966				0.78	852.47634
c1723			C31 H65 N8 O11 P3	5.071	818.39808
c4639			C48 H57 N3 O S3	4.246	787.36649
c3158			C32 H68 N10 O10 P2 S2	6.046	878.40278
c3519			C21 H20 N8 O2	3.647	416.16916
c1392			C36 H61 N10 O2 P3	0.683	758.41774
c2735			C25 H54 N9 O9 P	6.059	655.3803
c1949	N1-(2-[2-[2-(acetylamino)phenoxy]ethoxy]phenyl)acetamide		C18 H20 N2 O4	4.493	328.14148
c2949			C48 H49 Cl2 N3 O S3	19.152	849.24205
c3267			C14 H39 N7 O P2 S	4.072	415.24199
c181				9.973	2609.44718
c1373			C20 H45 N2 O6 P	6.068	440.29999
c633			C16 H27 N3 O3	4.336	309.20451

c1265			C52 H103 N6 O14 P3	5.413	1128.67491
c1086			C86 H144 N9 O18 P3 S2	4.061	1747.9282
c2935			C14 H34 N9 O5 P	7.451	439.24178
c4515				3.738	1179.5845
c3098			C8 H26 N7 O4 P	1.025	315.179
c3221	NP-020706		C14 H22 O7	0.795	638.32697
c3799			C20 H33 N5 O8	2.757	471.23202
c4552			C48 H85 N10 O16 P	8.255	1088.58811
c2596			C41 H58 N3 O7 P	16.56	735.40045
c22			C26 H42 N6 O6	5.431	534.31563
c1213				8.982	1536.69114
c769	Not named		C31 H52 N6 O9	5.417	652.37688
c4017			C40 H80 N O14 P3	4.307	891.47955
c3002	[Ser7]MC-HtyR		C52 H74 N10 O14	4.874	1062.54314
c804	APK		C14 H26 N4 O4	1.03	314.19443
c1824			C40 H79 N7 O15 P2	8.301	959.50976
c1595	Matlystatin A		C22 H40 N4 O5	5.948	440.30054
c670			C15 H27 N3 O4	4.08	313.19933
c2820			C29 H61 N5 O11 P2	3.702	717.38319
c903			C64 H83 N5 O9	5.544	1065.61965
c3963			C43 H85 N7 O18	5.202	987.59589
c899			C88 H107 N9 O15	7.153	1529.78847
c2587	1,3-Diphenylacetone		C15 H14 O	2.707	454.2537
c2019			C23 H46 N8 O9 S	4.286	610.3101
c1856			C62 H104 N7 O10 P3 S2	7.493	1263.65041
c2228			C44 H81 N10 O9 P3	6.382	986.54036
c2845			C63 H109 N2 O12 P3 S2	8.648	1242.66349
c2915	2-[(1S,4S,5S)-5-Isopropyl-2-methyl-4-[[[phenylsulfonyl]amino]methyl]-2-cyclohexen-1-yl]-N-[2-(4-morpholinyl)ethyl]acetamide		C25 H39 N3 O4 S	5.908	998.51576
c2365				6.287	1454.77767
c3384			C23 H47 N9 O10	4.387	609.34667
c4602			C26 H55 N7 O2	17.751	497.44382
c4141			C32 H74 N6 O15 P2 S	4.598	876.44006
c998			C29 H62 N7 O4 P3	7.57	665.41007
c2539	MC-NfkA		C51 H66 N8 O14	5.907	1014.46495
c4882	Tetrocarcin P		C61 H88 N2 O20	8.307	1168.59092
c2995	Stevioside		C38 H60 O18	6.368	826.3642
c3585	Flocculosin		C40 H72 O18	4.887	840.47169
c2311				8.01	2246.15714
c4186				8.01	2247.16056
c57			C30 H49 N7 O10	5.869	667.35319
c1484			C14 H27 N5 O3	3.574	313.21075
c2677				3.602	1296.63456
c2671	Not named		C56 H86 N10 O14	5.137	1122.62729
c4105			C28 H60 N7 O6 P3	4.967	683.38398
c1843			C35 H59 N9 O10	4.6	765.43723
c4676	Kojistatin A		C17 H32 N4 O5	2.624	372.23674
c4068	Not named		C59 H77 N7 O14	7.653	1107.54844
c4152			C27 H37 N5 O5	6.64	511.27905
c4409			C20 H29 N7 O4	12.593	431.22978
c1646			C36 H75 N8 O5 P S4	7.146	858.44686
c1080	Destruxin-A4 chlorohydrin		C30 H50 Cl N5 O8	6.042	643.3324
c4300			C49 H91 N3 O15 P2 S2	9.011	1087.53538
c4739			C65 H89 N2 O6 P S	5.692	1056.61773
c4619			C74 H102 N2 O17 P2 S2	7.632	1416.60943
c3738			C41 H63 N3 O7 P2	7.91	771.41653
c4569			C20 H51 N10 O4 P3	3.035	588.32877
c1932			C28 H47 N5 O13	3.333	661.31676
c908			C28 H53 N3 O12	5.313	623.36302
c475			C46 H77 N8 O8 P3 S2	5.215	1026.45021
c4044			C53 H67 O8 P S	6.814	894.42995
c3218			C55 H107 N7 O17 P2 S2	7.044	1263.66712
c4139			C15 H12 N9 O8 P3 S2	6.137	602.94695
c2783			C61 H129 N10 O13 P S	18.296	1272.92002
c487			C54 H105 N8 O10 P3 S	7.864	1150.68702
c4242	Pimprinol A		C13 H12 N2 O2	4.306	228.08933
c1328	Lokisin+CH2+NH4 adduct	B	C65 H116 N12 O20	15.393	1384.83854
c3723	Stanozolol		C21 H32 N2 O	9.888	328.24668
c927			C32 H51 N9 O8	4.129	689.38371
c4834			C25 H53 N9 O13	6.953	687.37688
c1047			C14 H37 N8 O5 P S	3.878	460.23476
c4421			C20 H46 N8 O4 S2	6.32	526.31005
c2298			C18 H27 N P2	0.793	319.16345
c3279			C58 H104 N7 O17 P3	3.607	1263.67072
c797	4-oxododecanedioic acid		C12 H20 O5	2.953	244.12802
c2969			C17 H42 N6 O5 P2	7.805	472.26891
c2691			C19 H34 N4 O5	5.293	398.25245
c1036	Dehydroradiosumin		C22 H30 N4 O5	4.096	430.22058
c3034			C33 H54 N5 O3 P S	4.304	631.36808
c4584				7.629	2044.91883
c2239				6.13	378.70003
c2461			C27 H63 N9 O11 S2	6.127	753.40896
c876				6.285	1879.8776
c3423				7.4	1526.77903
c2747			C21 H50 N9 O5 P	7.312	539.36829
c647			C38 H60 N10 O8	6.615	784.45927

c3160				7.089	2301.06696
c143	3-(2-methylpropyl)-octahydropyrrolo[1,2-a]pyrazine-1,4-dione		C11 H18 N2 O2	4.89	210.13652
c1011			C30 H49 N7 O10	6.061	667.35333
c3029			C21 H49 N10 O4 P	4.423	536.36787
c2866			C64 H98 N8 O15 P2	6.707	1280.66024
c2056			C56 H114 N2 O11 P2	18.467	1052.79001
c2444				7.211	991.47588
c2140			C53 H106 N O16 P3 S	8.88	1137.64614
c332			C20 H34 N4 O5	4.847	410.25228
c4145			C4 H6 N3 O4 P S	19.699	222.98102
c1407			C20 H48 N8 O6 P2	3.893	558.31648
c1905			C25 H54 N9 O10 P	5.4	671.37405
c3285			C50 H109 N10 O13 P3 S3	7.851	1246.65587
c457			C49 H90 N2 O14 P2 S	7.83	1024.55942
c1486				8.015	2189.13528
c2603			C25 H49 N3 O13 S	3.876	631.29876
c652			C20 H46 N4 O7 P2	9.124	516.28429
c4265			C30 H55 N O14	3.804	653.36303
c105			C57 H102 N7 O17 P3 S	3.516	1281.6267
c1773	NP-020706		C14 H22 O7	0.795	319.16347
c2289			C64 H89 N5 O17	9.893	1199.62428
c4323				9.033	1628.87741
c319			C12 H30 N10 O4 S	7.068	410.21593
c1525			C18 H33 N8 O4 P	3.721	456.23632
c1727			C15 H36 N8 O10	5.735	488.25414
c2037			C11 H31 N5 O4 P2	4.387	359.18703
c2294			C41 H94 N10 O18 P2	7.269	1076.62325
c4082			C42 H67 N6 O6 P S2	6.412	846.42983
c4077			C21 H36 N5 O12 P	2.708	581.20842
c3175			C15 H32 N9 O6 P	3.46	465.22072
c1266			C50 H79 N2 O10 P	6.151	898.54857
c1040			C35 H51 N7 O8 S	6.408	729.35107
c4412			C23 H46 N9 O P S2	5.856	559.3014
c1270	Bac-Lokisin-Metabolite	A;B	C64 H113 N11 O20	14.572	1355.81226
c1575			C65 H92 N2 O13 P2	7.788	1170.60799
c2275			C62 H117 N4 O16 P3 S3	6.227	1362.68454
c459			C32 H48 N6 O7	7.759	628.35874
c1274			C20 H45 N2 O6 P	6.418	440.29999
c2445			C34 H71 N8 O4 P3 S	7.545	780.45172
c1580			C12 H30 N6 O6 S	4.196	386.19443
c2259			C59 H78 N2 O8	6.283	942.576
c3014			C31 H50 N3 O4 P S	6.083	591.3261
c3109			C84 H107 N8 O17 P S	5.233	1562.72122
c2222	nummularine F		C23 H32 N4 O4	9.088	428.24199
c2493	Arginyltyrosine		C15 H23 N5 O4	0.804	337.17391
c551			C27 H43 N7 O8	4.063	593.31579
c862				7.634	1374.65376
c4808			C29 H63 N10 O4 P3	3.555	708.42746
c362			C18 H32 N4 O5	3.536	384.23619
c1522				5.947	378.66994
c2864			C23 H46 N3 O8 P	4.796	523.29999
c1256	Cyclo-(L-Ala-L-Tyr)		C12 H14 N2 O3	2.957	234.09996
c3865			C24 H49 N8 O6 P S2	1.223	640.29863
c1600			C27 H58 N8 O6 P2	8.257	652.39374
c2810	NP-004713		C15 H24 O2	4.059	258.15719
c4051			C15 H28 N4 O4	3.607	328.21049
c4322			C18 H38 N10 O3 S2	7.414	506.25603
c4465			C38 H55 N10 P3 S	5.825	776.35321
c2471	Maniwamycin F		C11 H21 N3 O3	2.785	243.15779
c111			C38 H60 N8 O12	7.069	820.43116
c2186			C32 H63 N9 O17	5.47	845.43628
c1682				4.524	987.58245
c2061			C23 H55 N9 O2 P2 S2	6.494	615.33713
c4035			C64 H71 N3 O7 S	4.88	1025.50158
c19			C32 H47 N7 O9	4.09	673.3417
c2422	2-Methoxy-N-(((2R,4S,5R)-5-[3-(4-methoxyphenyl)-1-methyl-1H-pyrazol-5-yl]-1-azabicyclo[2.2.2]oct-2-yl)methyl)acetamide		C22 H30 N4 O3	2.735	398.22728
c4187	XLR11 N-(4-pentenyl) analog		C21 H27 N O	1.05	331.19586
c4075			C26 H44 N4 O S2	6.293	492.29443
c3929	NP-018248		C31 H56 O16	2.58	1444.61336
c4490			C41 H85 N8 O17 P3	4.21	1054.5251
c4380			C31 H50 N3 O4 P3	7.936	621.30035
c1836			C16 H30 N10 O4	5.403	426.24707
c174	mebhydrolin		C19 H20 N2	4.341	276.16315
c4484			C52 H68 N8 O3 P2	8.998	914.48906
c3193				9.831	2843.52488
c1405			C73 H105 N10 O13 P S	6.979	1392.73092
c2091			C36 H54 N6 O4 P2	6.975	696.36563
c3973			C36 H64 N5 O9 P	8.939	741.44254
c3724				9.003	1752.89634
c128			C45 H75 N9 O17	3.563	1013.52819
c4561			C23 H39 N7 O8	3.149	541.28478
c4499			C45 H72 N7 O2 P3 S2	5.339	899.4412
c1897			C57 H107 O18 P3	5.479	1172.6668
c4783				5.439	1138.62883
c2713			C17 H25 N6 O P S2	12.476	424.12776

c3188	N1-(2-cyclohex-1-enylethyl)-2-methylhydrazine-1-carbothioamide		C10 H19 N3 S	1.029	639.40082
c4085			C8 H3 N2 O14 P S2	8.413	445.87663
c3933			C36 H60 N10 O P2 S	5.896	742.41747
c4649			C20 H46 N9 O2 P S	5.414	507.32428
c2793				8.51	986.52938
c3540			C66 H95 N5 O7 P2 S2	5.428	1195.61328
c4442			C17 H42 N9 O5 P	6.188	483.30503
c296			C27 H38 N6 O8	4.559	574.27406
c533			C21 H45 N4 O8 P	4.832	512.29511
c288				6.566	1936.9595
c679	Pinolenic acid		C18 H30 O2	13.064	278.22363
c2073			C33 H70 N10 O10 P2 S	7.203	860.44649
c607			C21 H38 N3 O3 P S	2.611	443.23728
c631	Lok isomer NH4 isotope misassignment	B	C27 H62 N9 O5 P3	14.923	685.40978
c2517				9.83	2844.52701
c4664	Subtulene A		C49 H74 N12 O14	4.104	1054.54673
c4121	Sclerotiotide F		C21 H32 N4 O5	8.465	420.23668
c2225	Muraymycin A2		C48 H82 N14 O19	4.198	1158.58369
c2276			C46 H59 N10 O8 P	6.048	910.42549
c1299				8.136	1200.64953
c3900			C40 H75 N4 O12 P S	4.64	866.48175
c4063			C14 H27 N5 O3	3.353	313.21038
c251			C29 H47 N8 O P3 S	0.788	648.27829
c4821				4.608	2249.13241
c996			C21 H53 N10 O11 P	3.861	652.36103
c3063			C43 H74 N5 O18 P3	5.349	1041.42427
c4585			C37 H60 N8 O5 P2	1.028	758.41558
c642			C12 H33 N8 O4 P S	4.068	416.20811
c3443			C33 H73 N7 O17 P2	7.634	901.4536
c1924			C26 H57 N10 O2 P3 S	5.544	666.35728
c2792			C23 H45 N O12 S	5.497	559.26336
c1334			C27 H37 N5 O6	4.096	527.27321
c4238			C21 H42 N2 O4 P2 S	5.863	480.23478
c3782	Actinozine A		C11 H18 N2 O4	3.997	242.1262
c821			C32 H65 N8 O14 P S	5.117	848.40927
c2138			C25 H42 N3 O3 P S	6.301	495.26874
c1457	Stenothricin D		C49 H85 N11 O17 S	3.514	1131.58337
c1237			C29 H64 N9 O17 P	5.41	841.41634
c1087	N1-(2-cyclohex-1-enylethyl)-2-methylhydrazine-1-carbothioamide		C10 H19 N3 S	1.029	426.26697
c3983			C19 H32 N8	4.739	372.27361
c4789			C26 H49 N10 P3 S4	4.061	722.2246
c3592	Gunnilactam B		C20 H28 N4 O5	3.326	404.20488
c3099			C65 H117 N4 O13 P3 S3	7.388	1350.70032
c2144			C20 H51 N9 O6 P2	4.112	575.34164
c2772			C21 H46 N3 O7 P S	5.846	515.27719
c2540	Indole-3-acetyl-epsilon-L-lysine		C16 H21 N3 O3	4.354	303.15749
c1163				3.615	1154.55409
c2381				7.223	1265.65468
c510			C30 H70 N7 O12 P3	4.841	813.42733
c1577			C22 H44 N9 O6 P	5.137	561.31288
c4301			C24 H50 N2 O7 S2	2.983	542.30516
c762			C20 H46 N4 O7 P2	9.122	578.76725
c1180			C20 H39 N9 O3 S	13.168	485.28914
c1989			C27 H54 N5 O10 P	5.148	639.35799
c205			C78 H111 N5 O10 P2	14.936	1339.78094
c709			C26 H45 N10 O5 P	6.299	608.33127
c3206			C42 H63 N3 O9	8.179	753.45512
c1511				9.531	2108.1301
c3475	Biotin		C10 H16 N2 O3 S	4.05	266.06933
c4681	Confluenine A		C11 H22 N2 O3	2.565	230.16265
c2416			C31 H60 N5 O13 P	4.714	741.39003
c1657			C22 H55 N10 O18 P S	13.163	810.31588
c3749			C18 H49 N9 O9 P2	3.964	597.31176
c1444				5.887	1464.72497
c1698			C14 H32 N7 O3 P	6.524	377.23098
c2561	Desmethylestruxin B2		C27 H45 N5 O7	5.548	551.33116
c2546	Diprotin A		C17 H31 N3 O4	6.914	341.23131
c3516			C17 H34 N10 O3 S2	5.85	490.22711
c432	Maniwamycin F		C11 H21 N3 O3	0.793	243.15752
c4229	Juvenimicin C		C29 H48 O10	4.86	556.32523
c2396			C57 H117 N10 O17 P3 S	8.614	1338.75468
c4291			C24 H57 N10 O6 P3	7.419	674.36745
c1292	Eurotiumin A		C19 H23 N3 O3	8.257	341.17292
c4671			C26 H49 N4 O7 P S	3.281	592.30347
c739			C34 H47 N9 O11	5.942	757.33927
c2518			C80 H114 N5 O13 P3 S2	6.734	1509.70693
c2120	N1-cyclohexyl-4-(4-fluorobenzyl)-1,4-diazepane-1-carbothioamide		C19 H28 F N3 S	3.721	349.1971
c657			C38 H66 N4 O7 P2	5.219	752.44193
c4692			C14 H36 N10 O5 S	5.158	456.25791
c2109			C46 H75 N2 O12 P S2	5.144	942.45082
c3477				1.047	235.14159
c1412			C6 H19 N8 O P	5.448	250.14237
c1250			C22 H52 N5 O6 P3	4.35	575.31109
c3071			C15 H37 N8 O3 P	6.005	408.27341
c4794				7.25	1138.60215

c4418			C37 H64 N8 O6 S2	7.251	780.43872
c2142	3-[18-(3-Methoxy-3-oxopropyl)-3,7,12,17-tetramethyl-8,13-divinyl-2-porphyrinyl]propanoic acid		C35 H36 N4 O4	3.593	576.27179
c3502	Norplicacetin		C24 H33 N5 O7	3.722	503.23693
c2850			C30 H61 N8 O4 P3	8.441	690.40527
c4381				5.179	780.43625
c4245				5.724	2244.92373
c4526				5.736	2243.92067
c1115			C13 H32 N5 O5 P	4.829	369.21306
c4833				3.74	1006.47477
c2031	Cordycedipeptide A		C10 H17 N3 O3	2.708	227.12667
c2290			C25 H42 N3 O6 P	7.124	511.27836
c757			C27 H34 N4 O6	9.425	510.24916
c2053			C78 H103 N6 O17 P	7.845	1426.71288
c1135	1-[4-[[3-[[5-(2-Hydroxy-2-propanyl)-1,2-oxazol-3-yl]methyl]-3-oxetanyl]amino]-1-piperidinyl]ethanone		C17 H27 N3 O4	7.856	359.18416
c4207			C67 H95 N4 O11 P	9.133	1162.67366
c2959	Not named		C22 H25 N3 O6	6.952	427.17375
c130	Adenosine		C10 H13 N5 O4	0.796	267.09578
c1361			C85 H101 N7 O12 P2	7.39	1473.69915
c1744			C20 H37 N10 O5 P	6.044	528.26939
c1865	3-[[[2,6-Dimethylheptanoyl]oxy]-4-(trimethylammonio)butanoate		C16 H31 N O4	12.605	301.22529
c2569			C35 H55 N3 O4 P2 S	4.545	675.33989
c291			C44 H70 N7 O7 P3	6.902	901.4541
c2215			C44 H89 N9 O14 P2 S3	5.875	1125.51825
c3676			C31 H41 N8 O6 P	4.607	652.28791
c1564			C18 H43 N7 O4 P2	7.121	483.28364
c3552				7.551	2091.16971
c3801			C20 H45 N7 O9 P2	7.521	589.27775
c2008	1-Octen-3-yl 6-O-beta-D-xylopyranosyl-beta-D-glucopyranoside		C19 H34 O10	5.022	422.2151
c3858			C41 H69 N7 O8 P2	2.877	849.46955
c1656			C31 H51 N3 O13	4.327	673.34175
c3355				9.117	1691.8582
c4539				8.901	1220.6843
c3850				7.554	2092.17384
c4278			C18 H38 N10 O4 S2	5.574	522.24953
c3065			C14 H29 N5 O4	2.803	331.22101
c574	2-[[[(4,5-dimethoxy-2-nitrophenethyl)imino]methyl]phenol		C17 H18 N2 O5	13.164	330.12212
c3545			C21 H48 N8 O13	6.788	620.33137
c89	(5R)-2-{3,4-Dihydroxyphenyl}-N-{3-[[3-[[Z)-[[2,3-dihydroxyphenyl](hydroxy)methylene]amino]propyl]amino]propyl}-5-methyl-4,5-dihydro-1,3-oxazole-4-carboximidic acid		C24 H30 N4 O7	4.096	486.21016
c919	TMC-52A		C20 H30 N4 O6	4.342	422.21556
c1002			C14 H34 N9 O5 P	4.343	439.24224
c763	Leu-Leu		C12 H24 N2 O3	3.936	244.17862
c2302			C44 H60 N4 O8 S	4.754	804.4126
c2987			C17 H42 N9 O6 P S	4.875	531.27166
c692			C35 H70 N4 O7 P2 S	5.223	752.44175
c3306	Clavamycin F		C15 H24 N4 O7	7.545	372.16383
c610			C17 H30 N10 O2	4.344	406.25691
c1896			C25 H48 N5 O7 P	5.776	561.3289
c3039			C20 H46 N9 O5 P	5.005	523.33577
c3894			C28 H59 N8 O11 P3	6.011	776.35234
c3934				6.077	1179.61228
c3603	ile-his		C12 H20 N4 O3	1.034	268.15257
c1381	Maniwamycin F		C11 H21 N3 O3	6.242	243.15782
c3849			C26 H36 N6 O5	3.558	512.27365
c2375			C17 H37 N6 O4 P S	8.291	452.23363
c1330			C26 H34 N6 O4 S	5.829	526.23827
c2439			C16 H41 N10 O6 P S	4.292	532.26695
c1722			C72 H102 N8 O16 P2	3.706	1396.69018
c568			C81 H121 N4 O14 P3	8.57	1466.81036
c767			C14 H36 N9 O5 P	4.001	441.25823
c2405			C23 H41 N4 O10 P	3.628	564.25365
c1229			C37 H61 N9 O4 P2	7.508	757.4363
c2235			C71 H98 N5 O6 P3	5.444	1209.6721
c1325			C81 H108 N O17 P3	7.311	1459.682
c132	Barnesin A		C25 H37 N5 O5	4.508	487.2785
c1239			C29 H50 N2 O7 S3	4.972	634.27766
c2797			C56 H86 N6 O16	6.833	1098.60969
c3176			C61 H90 N2 O13 P2	6.837	1120.59207
c2013			C19 H34 N4 O5 S	4.475	430.2242
c1451			C36 H64 N6 O15	3.467	820.443
c799	(4aR,7aS)-6-(Cyclopropylcarbonyl)-4-(3-pyridinylmethyl)hexahydropyrrolo[3,4-b][1,4]oxazin-3(2H)-one		C16 H19 N3 O3	4.116	301.14188
c2724			C53 H90 N9 O15 P	8.772	1123.6298
c4885			C38 H53 N O2 P2	4.071	617.35294
c486			C89 H133 N7 O14 P2 S	9.194	1617.91078
c4459	Serinolamide A		C23 H45 N O3	17.458	383.33926
c48			C26 H44 N6 O7	4.341	552.32605
c625	Bis(3,5,5-trimethylhexyl) phthalate		C26 H42 O4	18.785	418.3079
c1281			C38 H60 N8 O3 P2	5.806	738.42691
c3550			C15 H32 N2 O3	10.434	288.2408
c1487			C44 H75 N9 O8 P2	2.599	919.52181
c1990			C26 H46 N6 O7	4.97	554.34204
c3813			C28 H66 N10 O13 S	6.994	782.45192
c3701			C23 H43 N3 O4 S2	4.057	489.26738
c4651			C58 H92 N8 O18 P2 S	5.986	1282.57285
c3923			C38 H78 N5 O10 P S	3.255	827.52105
c3347			C31 H44 N3 O11 P	6.522	665.26879

c1500			C22 H35 N4 O9 P	4.344	530.21174
c1041			C24 H48 N3 O8 P	7.428	537.31685
c1026			C29 H58 N5 O9 P	6.49	651.39478
c2930			C37 H68 N9 O7 P3	4.17	843.44727
c3664				0.794	380.70204
c4736	Flocculosin		C40 H72 O18	8.462	840.47391
c4228			C47 H77 N7 O16 P2	3.555	1057.49074
c2927			C19 H45 N7 O7 P2	5.345	545.28459
c2189			C39 H55 N3 O5 S	5.184	677.38497
c1860				9.03	1626.87125
c1505			C18 H33 N8 O4 P	3.483	456.23635
c1499	5S-hydroxynorvaline-S-Ile		C11 H20 N2 O3	4.567	228.14702
c2500				15.116	2761.50086
c839			C25 H60 N10 O17	5.082	772.41276
c693	B-factor		C14 H22 N5 O7 P	3.529	403.12479
c1341			C31 H51 N3 O13	4.933	673.34202
c2134				4.909	336.67118
c4854	LNH		C16 H26 N6 O5	3.181	764.38138
c3727				6.705	1076.62274
c963			C24 H52 N3 O7 P	6.57	525.35242
c2726			C55 H94 N O14 P3	10.632	1085.59119
c664			C33 H65 N6 O11 P	5.219	752.44176
c4315				5.039	1341.73471
c3424			C28 H62 N9 O13 P	5.831	763.42113
c3812				6.788	391.2462
c1447			C12 H19 N6 O2 P	6.167	310.13113
c1069	Aspartocin E		C56 H87 N13 O20	7.327	1261.62348
c368			C31 H45 N7 O13	4.2	723.30566
c4522			C22 H44 N4 O4 P2 S	6.08	522.25845
c4810			C16 H34 N10 S2	4.551	430.24239
c3080			C20 H47 N10 O6 P	4.566	554.34211
c997			C21 H40 N9 O5 P	5.895	529.28976
c1609			C20 H26 N10 O3 S	4.905	486.19302
c3200				7.293	796.39121
c717				4.827	730.38956
c1706			C48 H78 N5 O16 P S	3.889	1043.49126
c660			C36 H64 N6 O13	4.056	788.45251
c3896			C21 H40 O2 P2	4.608	386.25244
c4088				5.466	337.67884
c3313			C68 H94 N6 O18 S	7.942	1314.63325
c2725			C19 H37 N8 O4 P	8.519	472.26904
c1536			C21 H30 N8 O3 S	5.359	474.21336
c691			C21 H36 N9 O6 P	6.485	541.2531
c136			C51 H74 N10 O7 P2	6.658	1000.52221
c473			C46 H73 N7 O12 P2 S2	5.546	1041.42354
c107	Lokisin Isomer	A;B	C64 H111 N11 O20	14.919	1353.79566
c2242			C30 H57 N7 O7 P2	3.527	689.37659
c4533			C27 H63 N8 O5 P3 S	5.786	704.38515
c1808				4.624	2234.11438
c1729			C15 H27 N3 O5	4.528	329.19415
c1941			C29 H63 N10 O4 P3	4.218	708.42657
c3969			C15 H25 N9 P2	5.86	393.17176
c1713				4.765	1383.69896
c1048			C73 H89 N3 O15 P2 S	1.072	1341.5496
c1872			C37 H43 N5 O10	5.766	717.30063
c270			C64 H109 N9 O14 P2 S	8.615	1321.73
c3226			C57 H74 N3 O11 P	8.546	1007.50731
c750				0.792	226.64688
c3947	Cyclo-[isoleucyl-prolyl-leucyl-alanyl]		C20 H34 N4 O4	7.393	394.25845
c534			C30 H57 N6 O9 P	5.783	676.39052
c2209			C27 H56 N5 O11 P	4.879	657.36836
c1606	Arg-Trp		C17 H24 N6 O3	4.841	360.191
c470			C22 H39 N5 O5	0.793	453.29382
c1557			C42 H67 N10 O8 P	7.973	870.4863
c2122				6.767	750.87325
c2040			C46 H89 N4 O17 P3	3.58	1062.54392
c1402	Halymecin G		C38 H68 O16	4.528	780.45263
c940			C7 H19 N9 O4	6.645	293.15525
c2126	NP-004917		C15 H26 O3	12.528	276.1726
c1386	Cyclo(D-Tyr- L-Leu)		C15 H20 N2 O3	4.531	276.14689
c2544			C14 H33 N5 O8	7.777	399.23216
c3030			C55 H97 N10 O5 P3 S4	5.771	1198.57338
c3156			C14 H25 N3 O4	4.111	299.18413
c3924			C25 H53 O12 P3	5.587	638.27235
c4734				4.118	602.28409
c1241	3-(6-aminopurin-9-yl)nonan-2-ol		C14 H23 N5 O	4.492	277.18897
c675	(3S)-3-[(Z)-[(3S)-3-[(Z)-[(3R)-3-Amino-1-hydroxy-4-methylpentylidene]amino]-1-hydroxybutylidene]amino]-5-methylhexanoic acid		C17 H33 N3 O4	5.587	343.24623
c3787				4.231	808.33768
c844			C15 H25 N9 O2	5.578	363.21485
c2051			C19 H34 N4 O5	4.066	398.25194
c672			C58 H69 N7 O5 S	5.737	975.50654
c116	NP-020534		C27 H31 N5 O2	6.178	457.24283
c2543			C22 H47 N4 O10 P S	4.345	590.27268
c649			C25 H54 N3 O7 P	7.485	539.36857
c3877			C60 H107 N8 O18 P3 S	3.588	1352.66312

c1062			1.063	532.27441
c2297		C26 H60 N9 O5 P3	14.515	671.39585
c2490		C23 H43 N4 O2 P S	1.046	470.2829
c595		C23 H35 N9 O3 S	5.241	517.25635
c1095	Matlystatin A	C22 H40 N4 O5	6.631	440.29963
c3244		C24 H39 N5 O13	3.633	605.25317
c1007	N1-cyclohexyl-4-(4-fluorobenzyl)-1,4-diazepane-1-carbothioamide	C19 H28 F N3 S	4.09	349.19654
c724	1-Tetrahydro-1H-pyrrol-1-yl-3-[3-(trifluoromethyl)-1H-pyrazol-1-yl]propan-2-ol	C11 H16 F3 N3 O	2.938	526.24812
c2097	Tolycaine	C15 H22 N2 O3	4.848	556.32566
c1523	3,9-bis(acetyloxy)-2,6,6,13-tetramethyl-12-oxotetracyclo[11.2.1.0			

c1159		C45 H83 N4 O17 P	7.303	982.55004
c4195		C32 H59 N8 O6 P3	4.609	744.37929
c1732		C22 H48 N6 O4 P2 S	6.178	554.2956
c2648		C25 H50 N8 O8 P2	6.395	652.31999
c4578		C32 H44 S3	4.898	524.25829
c1288	5S-hydroxynorvaline-S-Ile	C11 H20 N2 O3	4.171	228.14689
c4478			7.931	1897.0753
c3451			6.793	1240.66262
c1889		C39 H66 N4 O14	6.609	814.45789
c3199		C36 H66 N9 O13 P	6.754	863.45349
c2376			4.614	2235.11971
c553	Natalenamide A	C19 H25 N3 O5	3.031	375.17872
c699		C31 H53 N7 O8	6.142	651.39439
c1070		C28 H55 N2 O6 P3 S	4.515	640.30016
c355		C20 H34 N4 O5	4.846	410.25236
c1008		C53 H83 N5 O17	8.048	1061.57769
c2305		C40 H76 N3 O9 P3	6.167	835.47998
c1943	(3S)-3-[(Z)-[(3S)-3-{(Z)-[(3R)-3-Amino-1-hydroxy-4-methylpentylidene]amino}-1-hydroxybutylidene]amino]-5-methylhexanoic acid	C17 H33 N3 O4	4.959	343.24657
c1721		C81 H92 N6 O9 P2	8.059	1354.64183
c3144		C31 H71 N9 O10 P2 S	4.873	823.45357
c1778			7.086	2183.06192
c4721			7.269	1146.63888
c1414	Cyclocarbamide B	C15 H22 N2 O4	3.735	294.15756
c517	Barnesin A	C25 H37 N5 O5	4.905	487.27872
c3559			9.029	1546.80575
c1631		C31 H56 N O5 P3 S	3.747	647.30901
c4203		C24 H49 O3 P3	4.097	478.28923
c4857		C25 H57 N6 O10 P	5.177	632.38828
c3093		C13 H35 N8 O4 P	5.441	398.25255
c4634		C68 H112 N9 O12 P3 S	5.964	1371.73578
c2325		C26 H50 N8 O9	3.489	618.37256
c280		C75 H116 N7 O18 P3 S	4.801	1527.73143
c363		C25 H40 N6 O8	5.049	552.28983
c3154		C22 H53 N9 O9 P2	5.867	649.34271
c467	Santacruzamate A	C15 H22 N2 O3	4.855	278.16264
c1465		C43 H68 N4 O6 P2	7.783	798.46411
c4040		C63 H100 N10 O17 P2 S2	7.636	1394.61809
c3693		C22 H49 N7 O5 S3	6.765	587.29575
c1734		C14 H30 N7 O4 P	4.149	391.21016
c2034		C13 H29 N9 O3 S	4.153	391.20973
c2394			4.633	1006.47428
c1638			7.428	2445.28667
c1904			8.248	494.76064
c1766		C24 H43 N5 O6	5.885	497.32069
c1977		C83 H135 N9 O18 P2 S2	9.091	1671.88026
c3506		C32 H59 N10 O3 P3	5.822	724.39805
c4703		C61 H92 N6 O18	5.546	1196.64641
c3286	NP-012836	C38 H61 N O8	6.844	697.40049
c2354		C54 H84 N5 O12 P3	8.716	1087.53536
c1942			8.291	479.75473
c1560		C19 H25 N3 O4	3.723	359.18366
c142		C37 H60 N5 O4 P3 S	3.531	763.35614
c40	3-[[[4-(hydroxyphenyl)methyl]-octahydropyrrolo[1,2-a]pyrazine-1,4-dione	C14 H16 N2 O3	3.495	260.11553
c1312	2-[14-hydroxy-10,14-dimethyl-10-(4-methylpent-3-en-1-yl)-5-oxo-9,18-dioxo-4-azapentacyclo[13.2.1.0A?,â¶.0â„,,Ãaâ‚.0ÃaÃa,Ãaâ¶]octadeca-1(17),2(6),7-trien-4-yl]]pentanedioic acid	C28 H35 N O8	3.301	513.23592
c4575		C27 H62 N10 O7 P2	7.44	700.42742
c780		C26 H38 N4 O5	8.666	486.28513
c822			4.069	832.41612
c747		C66 H126 Br Cl2 N6 O8 P S3	15.118	1406.70898
c623		C34 H67 N6 O10 P	6.176	750.462
c1260		C28 H62 N8 O11 P2 S	4.419	780.37157
c3870		C45 H91 N6 O11 P3 S	6.554	1016.5685
c3939		C17 H28 N7 O4 P	5.81	425.19482
c3822		C89 H117 N9 O16	8.557	1567.85971
c3341		C66 H125 N4 O15 P	17.178	1244.88791
c744		C15 H27 N8 O3 P	6.826	398.19508
c286		C32 H64 N3 O15 P	0.795	761.40498
c2870		C26 H53 N O4	17.174	443.39675
c1003		C41 H76 N8 O18	4.24	968.52817
c2353		C26 H44 N6 O7	5.194	552.32605
c1529		C33 H51 N3 O5 P2 S	6.604	663.30392
c334		C52 H64 N5 O7 P	6.907	909.15794
c381		C33 H58 N O7 P3	3.845	673.33965
c2852			7.521	552.27878
c2940	Hydrolyzed Lokisin	C77 H120 N3 O12 P3	14.016	1371.80831
c384		C46 H61 N7 O3 P2	8.253	821.43046
c314	NP-008993	C18 H34 O4	13.069	296.23429
c4840		C23 H48 O13	6.948	532.30919
c3070		C38 H60 N8 O8 P2 S	4.829	850.37432
c36	Koreenceine C	C14 H27 N O	8.733	225.20925
c4164		C5 H5 Cl N4 O6 P2	19.712	313.93604
c1848	Jiangrine B	C18 H20 N2 O4	3.902	328.14216
c169		C27 H39 N5 O7	4.832	545.28423
c556		C53 H85 N8 O14 P	9.132	1088.58994
c2041		C18 H45 N4 O P3 S2	5.85	490.22674
c156		C22 H36 N6 O7	3.388	496.26334

c469			C5 H17 N8 O2 P	0.8	252.1214
c2611				3.86	1262.59775
c4813	Maristachone C		C18 H28 O4	14.52	308.19795
c447			C67 H118 N5 O13 P3 S	14.52	1325.76623
c4159			C7 H22 N7 O2 P	8.284	267.15753
c3352			C23 H38 N6 O5	4.113	478.28908
c2183	Norplicacetin		C24 H33 N5 O7	3.696	503.23676
c2052			C41 H81 N7 O16 P2	7.748	989.52272
c4083				7.13	1054.56577
c859			C34 H51 N7 O4 S	5.088	653.37334
c2512				4.503	243.63932
c1143			C20 H49 N10 O6 P3	4.971	618.30401
c4842				7.227	1980.97353
c1979			C30 H63 N9 O10 P2	6.574	771.41561
c358			C23 H44 N3 O P3	3.785	471.26866
c2814			C35 H62 N4 O4 S4	4.124	730.36301
c3777			C66 H101 N10 O9 P3	9.507	1270.69543
c3271			C55 H104 N O11 P S5	8.291	1145.59481
c4002				5.738	412.71126
c337				6.901	450.7269
c1375			C20 H42 N5 O8 P	5.549	511.2784
c1176			C21 H36 N6 O5	3.851	452.27382
c1701			C66 H125 N2 O17 P3 S	14.514	1342.79202
c1702			C54 H74 N5 O17 P	4.263	1095.48127
c3025			C50 H73 N9 O6 S2	8.026	959.51331
c3348	Darapladib		C36 H38 F4 N4 O2 S	4.621	666.26411
c809	(3S,9aS)-3-benzyl-octahydro-1H-pyrido[1,2-a]pyrazin-1-one		C15 H20 N2 O	1.063	266.13708
c758	Gln-Leu-Val-Pro		C21 H37 N5 O6	4.205	455.2734
c4135				6.261	455.23696
c3484				7.432	2446.28904
c3703			C24 H53 N7 O7 P2 S	5.974	645.32311
c35	MR-387-B		C25 H36 N4 O6	5.32	488.26282
c4544			C68 H71 N3 O6	6.631	1025.53415
c3280	Antimycin A15		C29 H42 N2 O9	5.635	562.28679
c168				8.247	606.3265
c3238			C38 H76 N5 O7 P3	4.624	807.49563
c1716			C47 H87 N4 O15 P3	3.748	1040.53741
c552	(3S,9aS)-3-benzyl-octahydro-1H-pyrido[1,2-a]pyrazin-1-one		C15 H20 N2 O	0.795	532.27418
c1806			C36 H50 N8 O4 P2 S	6.066	752.31515
c4589			C19 H27 N O9	3.32	413.16896
c4005			C17 H41 N8 O4 P	7.985	452.30023
c1185			C20 H32 N4 O5	4.649	408.23682
c428			C7 H N5 O17 P2 S2	5.406	552.82764
c305				7.633	2745.29629
c1010			C28 H46 N5 O10 P	5.42	643.29494
c3925			C17 H38 N10 O5 S	5.419	494.27343
c4028				6.572	2114.96786
c3722				6.755	385.70809
c547			C22 H48 N3 O7 P	6.049	497.32107
c2610			C38 H65 N2 O13 P3	4.831	850.37167
c2170			C72 H95 N O10 P2	5.547	1195.64334
c3748	Barnesin A		C25 H37 N5 O5	3.64	487.27877
c3685			C31 H57 N3 O12	6.578	663.39482
c1024	R-Chloroquine		C18 H26 Cl N3	8.486	319.18163
c2991			C42 H81 N3 O10 P2 S	6.783	881.51177
c1228			C18 H32 N4 O7 S	3.279	448.19812
c4018			C61 H80 N4 O11 P2	7.819	1106.52904
c2420	Serinolamides C		C21 H41 N O3	15.497	355.30745
c56	D-Isoleucyl-L-prolyl-L-tyrosyl-D-isoleucine		C26 H40 N4 O6	6.29	504.294
c2330			C30 H51 N3 O14	5.49	677.3365
c2771				3.59	765.36205
c2088			C28 H67 N9 O13 P2	5.379	799.43298
c2283	Leu-Leu		C12 H24 N2 O3	3.771	244.17842
c380			C27 H37 N5 O8	4.831	559.26333
c1801			C19 H32 N4 O5	4.579	396.23653
c2168			C28 H56 N9 O10 P	6.251	709.39007
c2309			C12 H24 N4 O3	4.009	272.18434
c1867				5.48	1452.77976
c4846			C27 H57 N4 O8 P	6.901	596.38954
c2470			C21 H43 N9 O4 P2	4.416	547.29241
c3445			C65 H100 N6 O17	9.459	1236.71459
c682			C17 H31 N5 O6	2.727	401.22686
c507			C55 H94 N6 O16 P2	5.424	1156.62063
c3277			C35 H69 N4 O14 P	5.739	800.45414
c3368			C21 H48 N10 O7	8.068	552.37219
c2148			C20 H35 N5 O6	4.64	441.25818
c761				14.504	662.88402
c828			C32 H70 N9 O15 P S	6.108	883.44529
c124	Diprotin B		C16 H29 N3 O4	4.111	327.21502
c674			C38 H68 N7 O6 P3	4.599	811.4424
c2621			C82 H118 N3 O14 P3	6.683	1461.78064
c3051			C27 H64 N7 O4 P3	4.438	643.42542
c737			C25 H52 N5 O7 P	3.854	565.35776
c1623			C16 H31 N3 O4 S	4.356	361.20278
c1476			C38 H65 N7 O17	4.675	891.44436

c52		C57 H88 N6 O10 P2	6.45	1078.60204
c589		C58 H86 N5 O8 P3 S	7.675	1105.54193
c1578			5.531	976.4524
c1053		C18 H30 N4 O5	3.699	382.22091
c216		C44 H61 N3 O6 P2	7.869	789.40544
c1289	N-Benzyl-2-[(3R,4S)-3-[[5-(4-fluorophenyl)-1,2-oxazol-3-yl]methyl]-4-piperidinyl]acetamide	C24 H26 F N3 O2	7.068	858.3786
c196			6.689	503.78235
c972		C51 H98 N7 O15 P3 S	6.132	1173.60491
c604			9.97	2610.45794
c3962		C32 H44 N3 O2 P3	6.337	595.26684
c3165		C21 H36 O9	5.869	432.23692
c3461		C20 H37 N2 O6 P	5.872	432.23703
c4378		C25 H36 N4 O5	9.022	472.26759
c1521	Spumigin C	C30 H40 N6 O8	4.203	612.2896
c4750		C68 H92 N3 O13 P S	4.476	1221.60918
c3089			3.726	979.51448
c3943			3.724	653.01023
c3214		C23 H57 N10 O2 P3 S2	4.89	662.32959
c1179	Cyclo-(L-Pro-L-Tyr-L-Pro-Val-)	C24 H32 N4 O5	3.341	456.23612
c2919		C24 H55 N9 O11 P2	5.028	707.35132
c593		C27 H55 N4 O10 P	4.014	626.36269
c1290		C77 H129 N6 O18 P3 S	8.559	1550.82932
c4046		C75 H112 N8 O15 P2 S	9.182	1458.74339
c385		C42 H74 N7 O5 P3 S	6.024	881.46717
c1818		C23 H48 N3 O9 P S	5.835	573.28266
c2351			3.703	288.18737
c3843		C43 H72 N5 O2 P3	9.63	783.49011
c1434	Cyclo(D-Tyr- L-Leu)	C15 H20 N2 O3	5.116	276.147
c2578		C32 H64 N10 O5 P2 S	6.817	762.42637
c938		C28 H47 N5 O13	3.619	661.31714
c2835		C10 H17 N5 O4	4.172	271.1274
c869		C21 H36 N6 O5	4.05	452.27376
c238		C67 H104 N2 O14 P2	8.952	1222.6963
c1955	[D-Met1,D-Asp3]MC-LR	C50 H76 N10 O12 S	6.976	1040.53598
c249			9.011	384.73644
c1704	1,3-Diphenylacetone	C15 H14 O	2.543	227.12664
c1681		C31 H47 N4 O2 P S	4.51	570.31548
c1038		C17 H25 N3 O4	4.053	335.18364
c4039		C61 H90 N3 O8 P3	10.629	1085.59434
c66		C90 H116 N8 O15	9.116	1548.85574
c462		C24 H34 N4 O7	5.309	490.2418
c1602			3.846	874.4636
c4830		C26 H44 N3 O7 P	7.393	541.29003
c3217		C22 H58 N9 O11 P3	3.421	717.34676
c3851			3.751	556.25185
c4019	(S)-methyl-2-acetamido-4-(2-(methylamino)phenyl)-4-oxobutanoate	C14 H18 N2 O4	3.731	278.12595
c1136		C20 H44 N8 O10	5.163	556.32081
c1929		C56 H89 N7 O12 P2	7.198	1113.60582
c1111		C49 H80 N4 O15 P2	7.853	1026.51104
c1599		C16 H31 N3 O4	4.7	329.23133
c2954			8.03	1114.56651
c979	N-(2-Methoxyethyl)-3-{5-[(2S)-1-methyl-2-pyrrolidiny]-1,2,4-oxadiazol-3-yl}-2-pyridinamine	C15 H21 N5 O2	2.632	303.16892
c8		C27 H40 N10 O3	5.408	552.3262
c548		C20 H30 N4 O8	3.612	454.20542
c3204		C30 H47 N5 O15	4.062	717.30522
c1710		C20 H34 N4 O7	4.852	442.24208
c1398		C17 H29 N3 O5	7.037	355.21019
c1187			8.42	1148.62003
c1416		C89 H113 N10 O15 P	9.111	1592.81314
c1545		C16 H27 N3 O3	5.027	309.20444
c4610	Dapoxetine	C21 H23 N O	3.325	305.17308
c3613		C16 H31 N O2	10.848	269.23526
c1984	glu-pro	C10 H16 N2 O5	5.554	244.10543
c2269			6.403	1956.95761
c3387		C21 H36 N7 O2 P S	1.094	481.24032
c941		C22 H46 N3 O9 P	4.421	527.29477
c1907		C37 H71 N2 O15 P S	5.721	846.43083
c1065		C52 H72 N O9 P	6.071	885.49539
c227		C21 H38 N O6 P	13.168	431.24226
c2825		C16 H29 N3 O4 S	4.1	359.18665
c1813			6.964	363.7003
c135		C19 H32 O8 P2	11.9	450.15684
c203	N-(5-acetamidopentyl)acetamide	C9 H18 N2 O2	0.794	208.12056
c1899	Daidzein	C15 H10 O4	8.239	254.05739
c4752		C21 H54 N8 O8 P2	4.01	608.3522
c1139		C42 H71 N5 O15	5.375	885.49472
c4162		C55 H69 O10 P	7.622	920.46264
c3315			6.53	754.46225
c2910		C35 H60 N9 O6 P3	4.311	795.38877
c700	2-(2-amino-3-methylbutanamido)-3-phenylpropanoic acid	C14 H20 N2 O3	3.799	264.14708
c4126		C12 H36 N10 O3 S	5.2	400.26806
c1327			6.239	1502.66372
c4319	(7Z,19R,25S)-22,25,28,28-Tetrahydroxy-22,28-dioxido-16-oxo-17,21,23,27-tetraoxa-22lambda~5~-28lambda~5~-diphosphaoctacos-7-en-19-yl (5Z,8Z,11Z,14Z)-5,8,11,14-icosatetraenoate	C42 H74 O13 P2	5.292	848.46256
c2447			4.176	316.15987
c1812		C30 H61 N2 O16 P	5.826	736.37522

c1677			C20 H36 N4 O5	4.38	412.26789
c1291			C58 H95 N2 O18 P S	7.62	1170.60479
c4414				6.357	2296.02908
c860			C32 H61 N10 O4 P3	5.902	742.41272
c4728				7.756	1214.6063
c1834				4.096	442.27828
c2533				4.098	486.24254
c820	Chrysopiperazine A		C20 H27 N3 O5	7.764	389.19535
c202			C28 H34 N4 O6	6.44	522.2478
c1200			C8 H18 N3 O3 P	0.791	235.10821
c2484			C27 H58 N10 O10 P2	4.42	744.37957
c406			C22 H33 N2 O2 P S	4.266	420.19964
c2111			C33 H58 N4 O14 S2	3.826	798.33889
c4054			C78 H92 N4 O4 S2	8.07	1212.65566
c1847				4.183	966.49576
c915			C20 H36 N4 O6	3.759	428.26274
c3007			C35 H65 N5 O14	4.748	779.45385
c3573			C20 H39 N O9	4.283	437.2632
c2497			C30 H60 N5 O9 P	6.903	665.4106
c770	Not named		C11 H20 N2 O2	6.162	212.15211
c1792			C28 H68 N10 O9 P2 S	6.792	782.43522
c1148			C36 H64 N5 O2 P3 S	5.826	723.39516
c58			C28 H43 N5 O6 S	4.515	577.2918
c2057			C55 H70 N10 O S2	4.86	950.51786
c2059			C31 H57 N3 O14	6.275	695.3828
c2200				0.791	708.37825
c4276	(2R)-1-[[Hydroxy[[[(1S,5R)-2,3,4,6-tetrahydroxy-5-(phosphonooxy)cyclohexyl]oxy]phosphoryl]oxy]-3-(palmitoyloxy)-2-propanyl (9Z)-9-octadecenoate		C43 H82 O16 P2	6.556	916.50437
c3189			C23 H43 N2 O6 P S	6.901	506.25627
c1388			C28 H53 N3 O13	5.862	639.35859
c259			C38 H57 N3 O6 P2 S	4.553	745.34525
c2094				9.615	1971.10761
c2936			C50 H87 N7 O11 P2 S2	8.716	1087.53865
c3714				5.877	864.47501
c1914			C23 H60 N9 O7 P3	6.178	667.37991
c812			C13 H29 N8 O4 P	5.682	392.20553
c2374			C68 H110 N7 O12 P3 S	5.542	1341.71514
c891			C55 H88 N9 O9 P3	7.365	1111.59209
c888	Not named		C25 H38 N4 O6	5.086	490.27823
c1966	Eprosartan		C23 H24 N2 O4 S	13.205	424.14079
c2795			C18 H36 N6 O4	3.32	400.2789
c4280				5.977	2654.19945
c1408				6.999	686.34739
c4845	PA-46101 B		C61 H86 O22	3.717	1170.55686
c480			C28 H43 N5 O8	5.763	577.31081
c3867				5.653	758.42063
c518				8.979	500.77935
c1588				8.262	410.71568
c2799			C27 H59 N4 O10 P3	6.981	692.34515
c3828			C25 H55 N7 O13 P2	5.412	723.33426
c300			C20 H28 N10 O5	4.477	488.22625
c3171			C17 H25 N3 O4	4.51	335.18377
c1821	Cladosporiumin H		C14 H23 N O5	4.508	285.15771
c3444				9.595	1972.11181
c1759	1,3-Diphenylacetone		C15 H14 O	2.547	454.25317
c123			C19 H34 N4 O5	4.564	398.25216
c1935			C25 H53 N3 O7 P2 S	7.534	601.31007
c3011				7.544	1202.61972
c1589	8,9-dihydrolactimidomycin		C26 H37 N O6	13.331	459.26079
c392			C22 H38 N4 O6	5.542	454.27825
c21			C24 H43 N5 O8 S	5.439	561.28204
c1280			C30 H58 N5 O P3	2.606	597.38406
c4057			C43 H81 N4 O6 P S4	6.054	908.478
c2550			C20 H38 N9 O5 P S	6.489	547.2462
c1604			C87 H132 N9 O6 P3 S3	7.123	1587.86714
c3392			C40 H81 O16 P3	6.255	910.47406
c4517				8.598	1086.53892
c530			C18 H33 N3 O4	6.984	355.24645
c435			C20 H33 N5 O6	5.866	439.24255
c636	Trans-6-hydroxymethyl-3-methyl-7-oxo-undecan-4-olide		C14 H24 O4	10.664	256.16714
c3456			C31 H70 N9 O8 P3	4.642	789.45715
c617			C45 H92 N5 O18 P	6.793	1021.61667
c3327	Stenothricin D		C49 H85 N11 O17 S	3.796	1131.58413
c1108				4.332	1168.63146
c310			C18 H31 N5 O6	2.838	413.22646
c540				4.689	626.39985
c4674			C24 H44 N6 O2	17.17	448.35244
c3292			C19 H37 N4 O9 P	4.651	496.22799
c4205			C14 H28 N6 O5 P2	5.595	422.16155
c1546			C25 H45 N	16.617	359.35428
c4873				5.537	727.39366
c118			C23 H36 N6 O8	4.214	524.2588
c1915			C29 H50 N2 O14	5.869	650.32701
c2107				4.215	991.50687
c4519			C29 H50 N2 O4 P2	4.559	552.3264
c2412				4.261	832.41672

c472	Boydine B		C31 H38 N2 O7 S2	6.908	614.21086
c1654			C52 H74 N2 O8 S	5.173	886.51739
c2832			C39 H83 N4 O11 P3 S	5.178	908.49922
c335			C40 H66 N3 O8 P3	3.616	809.40599
c4435	val-arg		C11 H23 N5 O3	2.979	273.17914
c1925			C35 H44 N6 O8	6.459	676.32029
c640	Bis(methylbenzylidene)sorbitol		C22 H26 O6	12.606	386.17277
c2822			C26 H62 N9 O6 P3	3.414	689.40493
c426			C25 H36 N4 O5	8.256	472.26775
c59	Koreenceine A	C	C14 H25 N	10.523	207.19853
c400			C26 H54 N3 O7 P	8.067	551.36891
c479			C15 H24 N4 O4	5.408	324.17893
c137			C31 H40 N10 O4	6.288	616.32098
c3941				4.167	868.43259
c2857			C35 H51 N7 O8 S	5.194	729.35102
c4076			C48 H87 N7 O16	7.646	1017.62094
c937			C59 H102 N10 O14 P2	6.225	1236.70564
c1674			C28 H57 N5 O11	3.62	639.40557
c2731			C33 H60 N5 O3 P S	3.621	637.41524
c2555			C30 H71 N7 O16 P2	6.545	847.4432
c1134	Barnesin A		C25 H37 N5 O5	6.241	487.27859
c4504				9.611	1972.11637
c2263			C71 H86 N6 O11	7.807	1198.63582
c932	Didecyldimethylammonium		C22 H47 N	15.893	325.37021
c4	[Similar to: 2-hydroxy-6-[4-hydroxy-2-methoxy-6-(methoxycarbonyl)phenoxy]-4-methylbenzoic acid; ?Mass: 38.1001 Da]		C19 H31 O6 P	13.164	386.1846
c1150			C36 H57 N3 O13	6.997	739.38986
c1894				4.173	632.32034
c4563			C25 H45 N O3 P2	5.911	469.28974
c545				4.48	976.45238
c942				5.247	1034.51206
c317			C38 H63 N8 O3 P3	5.594	772.42182
c389			C44 H80 N8 O12 S2	5.908	976.53355
c3551			C31 H59 N9 O5 P2 S	4	731.38468
c1811			C30 H69 N8 O14 P	7.232	796.46914
c452			C21 H36 N4 O5	5.285	424.26796
c2657			C41 H86 O18 P2 S	3.719	960.5011
c1756			C29 H51 N4 O3 P S	4.277	566.34161
c194			C30 H53 N9 O8 P2	4.905	729.35174
c466			C32 H59 N3 O14	6.093	709.40036
c3948			C70 H98 N8 O13	5.53	1258.72605
c1671			C36 H51 N7 O6	8.869	677.39149
c1275			C47 H62 N10 O13	7.724	974.4498
c1531			C38 H57 N3 O6 P2	6.079	713.37391
c439				9.519	2086.15196
c1278	Santacruzamate A		C15 H22 N2 O3	4.56	278.16257
c2826			C36 H45 N3 O13	4.192	727.29528
c2220			C25 H54 N7 O12 P	6.063	675.35609
c2937	IPH		C17 H27 N5 O4	3.097	365.20523
c4189				4.948	750.3649
c1695			C49 H77 N7 O11 P2	5.796	1001.51414
c3593			C30 H62 N10 O12 S	6.604	786.42707
c3975				3.173	636.31847
c2464				5.869	864.47405
c4767				6.47	1352.6406
c2917				5.512	685.41441
c1933			C22 H4 N10 O16 P2 S	6.996	757.90092
c228			C39 H50 N6 O9	8.969	746.3632
c2520			C25 H45 N5 O7	4.549	527.33096
c2594			C44 H62 N8 O10 S	7.368	894.43164
c4432			C6 H17 N9 O4	4.396	279.14128
c3590	N-[2-(4-hydroxyphenyl)-2-oxoethyl]-3-methylbutanamide		C13 H17 N O3	8.037	235.12083
c7			C54 H89 N7 O18	8.292	1123.62659
c993			C25 H55 N4 O7 P	4.496	554.37804
c2336			C16 H17 N8 O4 P	5.23	416.11045
c139				6.557	278.6604
c3658			C22 H57 N10 O10 P	6.154	652.39757
c3764			C29 H42 N9 O6 P	5.919	643.29665
c1363	Santacruzamate A		C15 H22 N2 O3	4.553	278.1625
c2287			C33 H57 N6 O12 P	3.976	760.37495
c2431	3-Piperidino-4H-chromen-4-one		C14 H15 N O2	6.298	229.10591
c4835			C26 H56 N10 O2 P2 S	4.714	634.38007
c1223			C23 H38 N6 O5	3.092	478.28914
c4137			C17 H38 Cl N9 S2	4.37	467.23747
c2304			C31 H57 N3 O13	5.247	679.38898
c834			C20 H30 N4 O4	2.795	390.22583
c4240			C14 H35 N10 O5 P S	2.343	486.22544
c1311			C18 H28 N10 O3	4.687	432.23632
c3704			C24 H51 N3 O8 P2 S	8.017	603.29058
c2271			C14 H25 N O4	4.078	271.17755
c3262			C38 H76 N5 O9 P3	4.689	839.48619
c1138			C40 H63 N9 O5 P2	5.784	811.44344
c42			C33 H54 N8 O12	5.834	754.38521
c416				6.556	2083.99354
c60			C14 H27 N O3 S	8.133	289.17109
c702			C14 H29 N O4 S	7.757	307.18169

c2933			C27 H53 N9 O11	4.422	679.38943
c269			C20 H33 N5 O6	5.408	439.24212
c1261			C22 H51 N6 O4 P3	5.005	556.32064
c1458			C22 H41 N4 O9 P	5.867	536.25895
c1366			C20 H43 N8 O10 P	3.024	586.28349
c3952			C70 H99 N10 O17 P S	7.938	1414.6629
c150			C29 H42 N6 O8	3.724	602.30526
c1541			C28 H55 N9 O10	6.594	677.41016
c2383			C9 H17 N5 O2	0.786	227.13765
c395			C15 H27 N3 O4	4.69	313.19986
c3541			C39 H72 N3 O12 P3	4.885	867.43248
c504			C45 H67 N9 O12	7.175	925.48983
c3650				4.053	1607.74801
c1089	Desthiobiotin		C10 H18 N2 O3	5.192	214.13124
c506			C25 H42 N7 O4 P	8.033	535.30132
c163			C27 H40 N8 O6	4.398	572.30612
c1651			C19 H29 N3 O5	4.209	379.20993
c790			C65 H103 N6 O15 P3 S	6.927	1332.64109
c1810			C21 H31 N3 O4	8.727	389.23198
c1322			C23 H44 N4 O5	7.195	456.33089
c308			C25 H43 N5 O7	4.975	525.31595
c669			C18 H27 N3 O5	4.824	365.19453
c2449	(3S)-3-{(Z)-[(3S)-3-{(Z)-[(3R)-3-Amino-1-hydroxy-4-methylpentylidene]amino}-1-hydroxybutylidene]amino}-5-methylhexanoic acid		C17 H33 N3 O4	5.901	343.24677
c2093			C12 H33 N8 O4 P S	4.261	416.20827
c3891			C53 H96 N3 O17 P3	9.195	1139.59561
c1532			C13 H30 N9 O6 P	5.869	439.20665
c643			C18 H39 N9 O7	1.034	493.29943
c2873			C17 H46 N9 O4 P	5.193	471.34142
c4254				5.92	1929.89311
c2474			C27 H66 N9 O15 P	5.648	787.44089
c4463			C71 H101 N10 O11 P	8.12	1300.73886
c1466			C17 H42 N9 O5 P	5.417	483.30462
c2340			C18 H46 N9 P S2	5.417	483.30447
c3533			C27 H49 N3 O9	6.523	559.34672
c2874			C32 H53 N4 O9 P	7.502	668.35273
c1236			C62 H104 N4 O16 P2	6.056	1222.69146
c4786			C32 H63 N10 O5 P3	4.715	760.42239
c3513	Malyngamide I		C26 H42 Cl N O5	7.665	483.27623
c1030			C24 H45 N10 O P3 S	3.116	614.27176
c1762			C44 H61 N3 O3	19.368	679.47189
c580			C12 H31 N7 O2 P2	8.062	367.20058
c2700			C15 H29 N O2	9.149	255.21947
c3192	Imazapyr		C13 H15 N3 O3	3.158	261.11075
c373				7.632	1373.65145
c2135			C38 H69 N2 O7 P S	3.997	728.45355
c1156			C18 H28 N10 O3	4.849	432.235
c4693	4'-methyl Acetyl fentanyl-d5		C22 H23 [2]H5 N2 O	8.709	341.25768
c3700			C42 H73 N4 O12 P S	3.287	888.46866
c4513				4.646	484.30865
c1005			C21 H46 N3 O7 P	4.674	483.3052
c1324			C60 H110 N9 O14 P S3	6.403	1307.70682
c653			C79 H125 N8 O17 P3	8.555	1550.83363
c2163			C35 H71 N10 O17 P	3.014	934.47505
c1519				6.983	1376.63355
c590			C21 H32 N8 O2 S	5.587	460.23532
c2672				8.199	750.43151
c851			C43 H85 N2 O16 P3	3.722	978.51148
c1321				4.673	864.47293
c2139			C24 H36 N3 O3 P S	3.134	477.22109
c3073	N-(4-hydroxyphenethyl)-2-(1H-indol-3-yl)acetamide		C18 H18 N2 O2	8.615	294.13677
c4351			C80 H120 N O18 P3	6.348	1475.77181
c1724			C31 H48 N5 P3	5.428	583.30947
c3246	N-(1,3-benzodioxol-5-ylmethyl)-N'-[4-(benzyloxy)phenyl]urea		C22 H20 N2 O4	4.522	376.13731
c340			C15 H30 N10 O3 S	4.961	430.22436
c16				8.289	561.81354
c727	3-hydroxy-6-[(4E)-3-hydroxy-2,4-dimethylhept-4-enamido]-2,4-dimethyl-5-oxohexanoic acid		C17 H29 N O6	9.482	325.18705
c3601	Curvularide A		C18 H35 N O5	10.383	345.25132
c3548			C41 H73 N5 O6 P2	4.573	793.50506
c1562			C32 H59 N3 O13	6.688	693.40546
c485			C27 H59 N6 O4 P3 S	5.573	656.35545
c867				4.692	864.47218
c2388			C57 H88 N5 O13 P	4.571	1081.61192
c2254			C9 H22 N9 O2 P	0.806	319.16374
c2291				0.789	454.2754
c3297			C49 H60 N5 O5 P	6.085	829.43294
c1215			C15 H25 N3 O6	6.996	343.17377
c606			C74 H108 N9 O11 P3	15.116	1391.73849
c3622			C17 H34 N3 O4 P S2	6.756	439.17391
c3914				4.055	1748.93056
c2456			C13 H35 N8 O5 P	3.1	414.24656
c3515			C78 H114 N3 O15 P S2	9.082	1427.74405
c55			C10 H25 N9 O4	8.252	335.20228
c2096			C49 H75 N2 O9 P	4.605	866.52161
c2554			C16 H41 N8 O4 P S	6.083	472.2716
c1601			C12 H23 N5 O2	2.789	269.18446

c847	MFCD00020424		C18 H20 N2 O3	5.752	312.14725
c3136	Terretrione D		C16 H20 N2 O3	6.151	288.14686
c4461			C32 H33 P	4.618	448.2307
c1940			C36 H61 N3 O12	7.613	727.42523
c3496	KS-502		C34 H48 O12	4.643	648.31433
c1362			C23 H41 N5 O6	5.373	483.30457
c1207	Not named		C9 H15 N3 O4	5.542	229.10575
c397			C24 H43 N5 O8 S	5.306	561.28231
c4899			C30 H58 N O6 P3	5.869	621.34671
c4390			C16 H31 N3 O4 S	4.194	361.20253
c73	Cyclo-(L-Pro-L-Met)		C10 H16 N2 O2 S	4.062	228.09268
c3253			C22 H39 N5 O4	4.497	437.29941
c1922			C20 H45 N2 O7 P S	5.908	488.26675
c4650			C35 H77 N8 O10 P	8.352	800.551
c285	Glulisine A		C11 H19 N3 O2	0.79	225.14703
c178			C45 H81 N7 O18	6.685	1007.56416
c211				6.788	424.71876
c1624			C17 H34 N3 O8 P	7.405	439.20915
c1612			C24 H39 N5 O7	7.545	509.28536
c4853			C12 H28 N7 O4 P	3.491	365.19411
c1056			C16 H31 N3 O4	4.383	329.23082
c4444			C29 H63 N7 O14 P2	4.758	795.39243
c37			C35 H51 N7 O8 S	6.242	729.35068
c4129			C25 H51 O13 P	6.369	590.30546
c1937				5.796	489.76703
c4562			C40 H35 N5 O2	5.889	617.27999
c966			C7 H23 N7 O7	5.217	317.16568
c80			C33 H49 N3 O5 P2	4.2	629.31613
c1866			C20 H30 N6 S	8.746	386.2236
c2970			C10 H24 N10 O6	3.976	380.18761
c4573			C16 H30 N4 O5	2.453	358.22089
c4620			C19 H49 N9 O8 P2	5.614	593.31635
c2564	Gln-Leu-Val-Pro		C21 H37 N5 O6	3.757	455.27357
c386			C18 H35 N8 O5 P	4.465	474.24694
c2035				6.935	1333.64468
c1294				5.873	1504.73923
c4609	Leucylproline		C11 H20 N2 O3	2.712	456.29386
c4712	Leucylproline		C11 H20 N2 O3	2.7	228.14696
c705	Streptcytosine M		C16 H23 N3 O4	3.226	321.16818
c2581			C25 H32 N6 O8	3.346	544.22691
c4004			C31 H68 N9 O12 P	6.519	789.47404
c4849				7.518	1514.80344
c246			C28 H37 N9 O3	4.973	547.29972
c614			C19 H33 N5 O6	2.681	427.24256
c3329			C14 H25 N3 O5	1.823	315.17876
c1424				7.295	527.77608
c342				9.125	831.70345
c5			C51 H103 N5 O16 P2 S	6.131	1135.6593
c1898				5.363	816.47264
c2786			C7 H23 N9 O5	4.024	313.18181
c144	(Z)-N-((2R)-1-Hydroxy-2-[(Z)-((2S)-1-hydroxy-2-[(Z)-{hydroxy[(2R)-1-(D-tyrosyl)-2-pyrrolidinyl]methylene}amino]-3-phenylpropylidene)amino]-3-methylbutylidene)-L-alpha-glutamyl-L-proline		C38 H50 N6 O10	6.793	750.35781
c18			C37 H60 N5 O3 P3 S	4.905	747.36192
c2717	N-(2-Methoxyethyl)-3-[5-[(2S)-1-methyl-2-pyrrolidinyl]-1,2,4-oxadiazol-3-yl]-2-pyridinamine		C15 H21 N5 O2	2.645	909.50713
c450			C31 H58 N4 O15	5.453	726.38924
c4527			C43 H58 N5 O6 P	7.726	771.41567
c874			C9 H30 N10 O3 S	3.292	358.22061
c3661			C45 H100 N7 O14 P3 S	7.213	1087.62623
c2278			C82 H134 N5 O18 P3 S2	9.07	1633.83811
c282			C28 H46 N2 O11 S	5.375	618.28221
c3314			C23 H48 Br N3 O S	6.301	493.27038
c1124			C26 H50 N7 O4 P3	8.244	617.31662
c1140			C43 H58 N8 O12	7.407	878.41758
c1105			C61 H72 N5 O5 P	8.496	985.52696
c1452			C19 H34 N4 O5	3.866	398.25229
c1490			C19 H36 N4 O6	3.859	416.26246
c4462				4.038	662.4202
c2836			C26 H44 N3 O8 P	8.367	557.28457
c3586			C27 H37 N5 O2 S	6.291	495.26879
c1497			C35 H58 N5 O6 P3	5.83	737.35882
c2479				7.315	438.71663
c1131			C30 H48 N2 O7 P2	6.391	610.29582
c4437				6.785	990.49619
c3150			C17 H33 N7 O7	1.036	447.24463
c25				4.904	373.68096
c2883				6.903	1996.23043
c106	N-[(5aR,6aS,7S,9Z,10aS)-9-[Amino(hydroxy)methylene]-4,7-bis(dimethylamino)-1,10a,12-trihydroxy-8,10,11-trioxo-5,5a,6,6a,7,8,9,10,10a,11-decahydrotetracen-2-yl]-N~2~-tert-butylglycinamide		C29 H39 N5 O8	3.723	585.27852
c496			C78 H102 N7 O8 P3 S	7.637	1389.67351
c508			C49 H77 N9 O11	9.295	967.57538
c3372			C18 H37 N2 O7 P	5.289	424.23147
c1435			C17 H26 N7 O4 P	8.319	423.17861
c1828				10.022	2070.17608
c1209			C23 H57 N9 O7 P2	5.027	633.38411
c600			C19 H37 N10 O6 P	5.456	532.26362
c4123	Anabaenopeptin C		C41 H60 N8 O9	9.476	808.44969
c2324			C24 H50 N8 O8 P2	5.554	640.32083

c499			C21 H43 N4 O6 P	4.62	478.28987
c1019			C18 H31 N8 O4 P S	6.241	486.19285
c2741				3.276	1134.59376
c2128			C46 H76 N2 O12 P2	4.76	910.48702
c151			C23 H41 N5 O6	4.981	483.30454
c1226				3.537	426.21129
c3379				5.312	311.68141
c1230	Plusbacin A4		C50 H83 N11 O20	7.512	1157.57712
c483			C21 H39 N5 O5	3.609	441.29441
c1315				5.458	1151.69004
c4902			C66 H123 Cl N O15 P3 S3	14.942	1393.6959
c719			C53 H92 N5 O12 P3	7.853	1083.59661
c731			C25 H55 N9 O7 P2	3.266	655.37135
c1326				6.675	1996.96259
c1538			C5 H4 N2 O13 P2	0.719	361.9179
c612			C34 H58 N8 O9	5.764	722.43217
c3380			C39 H88 N10 O15 P2	6.417	998.59083
c2277			C22 H46 N3 O9 P	3.913	527.29501
c4084				6.16	576.29392
c2241				10.019	2071.1812
c3620				6.984	1850.9802
c721			C29 H46 N4 O6 P2	0.796	608.28975
c1474			C24 H43 N5 O7	4.287	513.31515
c261			C43 H66 N8 O10	7.896	854.48963
c2087			C19 H46 N7 O9 P	5.529	547.31139
c4732			C70 H102 N O18 P3	8.414	1337.63063
c333			C53 H86 N3 O9 P3	8.983	1001.55762
c12			C35 H54 N6 O7	8.257	670.40403
c777			C36 H69 N7 O13	4.147	807.49486
c2208			C10 H29 N6 O6 P	4.551	360.18718
c3817			C48 H77 N5 O8 P2 S	7.876	945.49612
c3562			C50 H78 N7 O6 P3	8.808	965.52315
c1012	Blastmycetin C		C17 H23 N3 O4	4.202	333.168
c3349	NAc		C17 H18 N2 O2	6.227	282.13628
c1969				4.851	884.48388
c690			C71 H93 N10 O16 P	7.461	1372.65138
c33	(Z)-N-((2S)-1-Hydroxy-2-[(Z)-[hydroxy[(2R)-1-(D-tyrosyl)-2-pyrrolidinyl]methylene]amino]-3-methylbutylidene)-D-alpha-glutamyl-D-proline		C29 H41 N5 O9	4.482	603.28928
c2776			C32 H54 N6 O12	5.361	714.37844
c3563			C18 H34 N P3	5.353	357.18909
c4871			C40 H64 N O8 P S2	5.815	781.38187
c2119			C58 H93 N3 O14 P2	9.195	1117.61363
c3332			C69 H97 N4 O14 P	7.203	1236.67386
c4279			C31 H65 N2 O16 P S	4.81	784.37756
c367			C89 H116 N7 O7 P3	9.204	1487.81374
c2571				6.327	1030.54673
c1769			C18 H33 N3 O9	3.099	435.22175
c4112				8.015	2190.13958
c1688			C34 H62 N7 O5 P3	3.571	741.40119
c4534				5.866	878.41312
c788	Carbazoquinocin F		C22 H27 N O2	6.558	337.20516
c2136			C45 H66 N7 O5 P3	7.314	877.43338
c322			C15 H27 N8 O3 P	7.122	398.19473
c4430			C71 H115 N5 O18 P2	8.008	1387.77173
c975				4.844	864.47007
c1864				4.278	678.35739
c1203			C20 H36 N4 O7 S	3.374	476.22929
c957			C15 H35 N4 O7 P	6.998	414.22593
c1542			C25 H58 N10 O12 P2	5.87	752.3697
c1273			C17 H31 N5 O5	0.791	385.23114
c3785	2,3,4,9-Tetrahydro-1H-β-carboline-3-carboxylic acid		C12 H12 N2 O2	3.759	216.08952
c628	NP-000510		C21 H25 N O3	4.282	339.17862
c2169			C10 H21 N6 O2 P	5.962	288.14728
c3990			C18 H19 N3 O3	13.562	325.14179
c495			C66 H103 N4 O11 P3	8.646	1220.68284
c1193	Carnosifloside VI		C48 H80 O18	7.393	944.53768
c2510				8.479	492.76415
c2221				4.656	313.66091
c3690			C34 H58 N2 O11	8.068	670.40579
c2389			C16 H28 N10 O3	5.396	408.23637
c2164	4-Amino-1-[(2xi)-5-O-[hydroxy{(hydroxy[(2R)-2-[(5Z,8Z,11Z,14Z)-5,8,11,14-icosatetraenoyloxy]-3-(stearoyloxy)propoxy)phosphoryl}oxy)phosphoryl]-beta-D-threo-pentofuranosyl]-2(1H)-pyrimidinone		C50 H85 N3 O15 P2	6.686	1029.54625
c3026	Malpinin D		C42 H58 N10 O8	4.342	830.44168
c4683			C85 H103 N9 O14 P2	7.908	1535.71053
c4759			C10 H23 N6 O2 P	7.045	290.16234
c4770			C74 H136 N5 O18 P3 S3	9.111	1571.82546
c800			C31 H62 N9 O5 P3	8.564	733.40533
c3985			C34 H61 N8 O13 P	6.84	820.4111
c2005			C27 H54 N4 O8 P2 S	5.496	656.3131
c390				6.56	2084.99595
c896			C78 H110 Cl N5 O10 S3	15.118	1407.71094
c113	D-(+)-Tryptophan		C11 H12 N2 O2	2.82	204.08947
c2598			C38 H57 N3 O5 P2	6.536	697.37746
c3846			C23 H56 N8 O6 P2 S	3.084	634.34917
c3102				4.099	347.66287
c4027				4.875	433.71678
c2457				7.157	1530.79087

c1837			C16 H42 N6 O P2 S	3.345	428.26245
c415	NP-001346		C11 H15 N5 O3 S	2.846	297.08891
c677				5.142	658.38852
c451			C33 H65 N6 O11 P	5.733	752.44261
c2006			C57 H88 N4 O18 P2	7.518	1178.55625
c2900			C19 H36 N4 O5	4.998	400.26759
c1882			C14 H37 N8 O4 P	4.547	412.26787
c1353			C11 H26 N7 P S	7.485	319.1715
c1648	N-(2-Methoxyethyl)-3-[5-[(2S)-1-methyl-2-pyrrolidinyl]-1,2,4-oxadiazol-3-yl]-2-pyridinamine		C15 H21 N5 O2	2.638	606.3385
c734	Selodenoson		C17 H24 N6 O4	5.873	376.18474
c1664			C35 H65 N8 O10 P	4.645	788.45401
c2014	Leucocin B-TA33a		C56 H77 N15 O12	3.979	1151.59079
c3578			C64 H103 N9 O15 P2	6.978	1299.70574
c673			C29 H38 N8 O10	4.288	658.26955
c2536			C28 H52 N5 O7 P	5.862	601.3579
c2531			C15 H39 N8 O4 P	6.841	426.2839
c4262	2-methylamino-3H-phenoxazin-3-one		C13 H10 N2 O2	4.831	226.07386
c2432			C35 H74 N8 O15 P2	6.592	908.47471
c663			C18 H33 N3 O4	6.751	355.24676
c2017			C28 H52 N5 O7 P	6.702	601.3581
c103			C20 H44 N8 O8	0.793	524.33053
c565			C19 H36 N10 O3	6.612	452.29949
c3535				8.122	972.49722
c1736				5.721	459.25626
c977			C29 H41 N5 O8	5.828	587.29503
c3078	IPH		C17 H27 N5 O4	3.101	730.41103
c3911			C61 H96 N4 O5	18.539	964.73819
c4763	B-5354a		C19 H29 N O3	14.196	319.21376
c1988			C50 H100 N7 O17 P S2	5.984	1165.63375
c1715			C25 H53 N3 O11 S	7.113	603.33762
c3351	4-Hydroxypropylproline		C10 H16 N2 O4	2.668	228.1107
c2912				3.88	730.38965
c4255			C18 H46 N9 O7 P	6.33	531.32585
c477			C23 H36 N6 O4	7.076	460.279
c1755			C19 H34 N4 O5	3.161	398.25199
c1133			C38 H66 N8 O17	4.264	906.45368
c781			C14 H30 N7 O3 P	8.249	375.21518
c316			C25 H45 N4 O9 P	4.558	576.28984
c787	Aeruginosin TR642		C32 H46 N6 O8	3.223	642.33601
c3504			C27 H62 N7 O4 P3	4.663	641.41063
c2827			C16 H32 N2 O3	9.618	300.24091
c4200				5.886	757.43049
c1262			C23 H27 N9 O4 S2	3.85	557.16071
c1995			C51 H72 N10 O6 P2	7.72	982.51299
c1371	(7Z,21R,27S)-24,27,30,30-Tetrahydroxy-24,30-dioxido-18-oxo-19,23,25,29-tetraoxa-24lambda~5~,30lambda~5~-diphosphatriacont-7-en-21-yl (9Z,12Z)-9,12-octadecadienoate		C42 H78 O13 P2	5.057	852.49448
c549			C29 H43 N5 O6 P2	6.755	619.26702
c951	Marimastat		C15 H29 N3 O5	4.033	331.21005
c532	(3S)-3-[(Z)-[(3S)-3-[(Z)-[(3R)-3-Amino-1-hydroxy-4-methylpentylidene]amino)-1-hydroxybutylidene]amino]-5-methylhexanoic acid		C17 H33 N3 O4	5.373	343.24638
c1018			C14 H29 N O5	10.664	291.20426
c2002				5.791	500.75679
c1884			C37 H56 N9 O4 P S	6.38	753.38993
c1629			C7 H23 N10 O3 P	3.725	326.17057
c4682			C52 H60 N2 O8	4.427	840.43661
c4067			C83 H107 N7 O11 P2 S	8.058	1471.72117
c2853			C65 H102 N5 O14 P3	7.904	1269.66252
c4804	(6Z,9Z,12Z,21R,27S)-24,27,30,30-Tetrahydroxy-24,30-dioxido-18-oxo-19,23,25,29-tetraoxa-24lambda~5~,30lambda~5~-diphosphatriaconta-6,9,12-trien-21-yl (4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-docosahexae;noate		C46 H74 O13 P2	3.334	896.46097
c3305			C14 H23 N	8.414	205.18282
c11	5,6-diphenyl-2,3-dihydropyrazine		C16 H14 N2	0.793	234.111
c453			C18 H39 N2 O7 P	4.899	426.24712
c2619			C15 H27 N O5 S	8.613	333.16062
c3984				9.344	2109.0836
c4782				9.349	2110.08872
c1782			C20 H31 N3 O4	6.792	377.23091
c207			C26 H39 N2 O9 P	4.495	554.23654
c431			C27 H40 N10 O5	4.336	584.31565
c1077	vellosimine		C19 H20 N2 O	4.33	292.15781
c352			C26 H52 N5 O11 P	4.9	641.33739
c557			C46 H57 N10 O3 P	4.331	828.43609
c3770			C31 H60 N6 O6 P2 S	3.899	706.37569
c3467	3-[3-(1,3-dimethyl-1H-pyrazol-4-yl)-1H-1,2,4-triazol-1-yl]-5-methylisoxazole		C11 H12 N6 O	7.546	244.1055
c4757			C25 H63 N8 O14 P3	4.154	792.3682
c161	(3R,4R)-N-(3-Cyanophenyl)-4-hydroxy-3-({4-[2-(4-morpholinyl)ethoxy]benzoyl}amino)-1-azepanecarboxamide		C27 H33 N5 O5	3.455	507.24318
c4227			C24 H42 N6 O7	4.235	526.30989
c2979			C43 H49 N3 O4 S	5.611	703.34645
c2409			C15 H38 N7 O9 P	5.743	491.24611
c3736			C75 H86 N5 O13 P3	1.048	1357.54424
c2009				5.648	432.74516
c813			C26 H47 N2 O6 P S	4.39	546.28937
c2574	?-L-glutamyl-L-leucine		C11 H20 N2 O5	1.206	260.13622
c4708			C27 H35 N5 O S	4.21	477.2549
c926			C23 H41 N2 O6 P	7.402	472.26899
c4287	Tolperisone		C16 H23 N O	0.79	245.17902
c2475				9.494	2744.45203
c2782				9.475	2745.45572
c347			C10 H30 N5 P3	6.834	313.17156

c835			C35 H62 N4 O13	5.668	746.43199
c1634			C34 H60 N7 O10 P	6.626	757.41168
c240			C32 H46 N6 O7	7.311	626.34293
c2406				6.252	243.63957
c3328			C46 H85 N4 O17 P	7.439	996.56542
c1607				4.171	456.29384
c4007			C44 H80 N9 O13 P3	3.571	1035.5095
c2800				4.928	319.67952
c3649			C69 H122 Cl N4 O11 P S5	14.917	1408.71396
c1383			C14 H23 N	10.457	205.183
c4372			C29 H43 N7 O8	2.825	617.3156
c2359				0.718	633.86666
c1797	1-Methyl-1,2,3,4-tetrahydro- β -carboline-3-carboxylic acid		C13 H14 N2 O2	3.073	230.10493
c1910			C17 H38 N9 O6 P S	5.659	527.24097
c870			C27 H44 N3 O8 P S	7.928	601.25727
c925				5.544	2083.9898
c1731			C59 H78 N6 O10	7.629	1030.5793
c2823	Incarnatapeptin A		C35 H58 N8 O12	4.682	782.42073
c4875			C21 H47 N2 O6 P	6.904	454.31536
c3715			C58 H100 N O5 P3 S4	8.103	1111.57031
c1507			C36 H75 N4 O18 P	4.676	882.48113
c578			C12 H23 N3 O2	2.127	241.17862
c4166				4.68	3075.30007
c4415				3.844	1677.8547
c2363			C35 H68 N9 O6 P3	6.189	803.45284
c3095			C35 H78 N9 O13 P	7.152	863.54652
c4236			C36 H68 N3 O15 P	3.917	813.4376
c349			C20 H32 N4 O4	6.557	392.24182
c3406			C17 H32 N8 O	12.152	364.27062
c2659	Leuhistin		C11 H19 N3 O3	3.142	241.142
c1551			C33 H76 N9 O12 P3	5.383	883.48374
c1377			C26 H48 N3 O9 P	4.646	577.3107
c2460	Cereusitin A		C25 H34 N4 O6	8.124	486.24822
c3361			C19 H45 N10 O7 P	4.527	556.32101
c1401			C29 H59 N8 O7 P3	5.645	724.3746
c1219			C31 H70 N6 O15 P2	7.142	828.43616
c160			C23 H51 N6 O10 P S	3.171	634.31362
c3385			C37 H60 N9 O5 P	8.58	741.44262
c1548			C33 H68 N9 O6 P3	5.567	779.45197
c2651	Vazabotide A		C12 H21 N3 O4	4.287	271.15259
c27			C32 H55 N5 O11	6.177	685.3903
c3610			C19 H34 N4 O5	6.019	398.2527
c3893				5.731	1377.76882
c377			C23 H51 N4 O13 P	6.997	622.3181
c759			C20 H34 N4 O6	5.06	426.24707
c1446			C34 H66 N4 O4 P2 S	6.706	688.42672
c131			C33 H50 O8 P2	16.558	636.29632
c1323			C35 H48 N3 O7 P	16.559	653.32278
c2634	LPH		C17 H27 N5 O4	3.269	365.20544
c2253				4.293	542.30512
c4091			C64 H64 O2 S	4.623	896.4622
c2805			C58 H106 N5 O18 P3 S	6.233	1285.64673
c2476			C26 H45 N9 O9	3.574	627.33679
c953			C60 H88 N6 O14 S	5.552	1148.6088
c1566			C14 H27 N O3 S	8.976	289.17086
c4183				5.632	1448.75071
c20			C21 H38 N4 O5	5.191	426.28361
c1996			C16 H34 N5 O5 P	6.6	407.22928
c3303				4.504	572.3259
c1125			C16 H34 N2 O3 S	8.135	334.22874
c98			C49 H85 N4 O10 P3	7.854	982.54848
c4837			C20 H29 N3 O4	8.72	375.2156
c1110			C38 H69 N6 O3 P3 S	6.628	782.43525
c2024	Cyclic-(Tyr-Ala-Leu-Ser)		C21 H30 N4 O6	4.157	434.21584
c3633			C41 H66 N4 O9 P2	5.813	820.43158
c2426			C35 H66 N9 O3 P3	8.127	753.45308
c74			C77 H113 N9 O14 P2	8.57	1449.78843
c3045			C18 H36 N2 O2 S	5.371	344.24988
c1983			C26 H56 N7 O11 P3 S	6.241	767.29736
c3284	Gln-Leu-Val-Pro		C21 H37 N5 O6	4.687	455.2741
c559			C18 H43 N10 O6 P S	4.406	558.28257
c655	Penicimutanin B		C51 H66 N4 O9	5.87	878.485
c82			C35 H52 N2 O6 P2	6.485	658.33159
c75			C26 H44 N6 O7	6.033	552.32687
c3669			C35 H47 N2 O8 P	15.379	654.30663
c309			C62 H107 N8 O17 P S	6.81	1298.72136
c3370	JS-3		C14 H16 N2 O4	4.004	276.1106
c3884				3.939	1044.02625
c3837			C26 H37 N2 O3 P S	6.545	488.22677
c318				0.79	890.46866
c327	Methyl (2S,4S,6S,12bR)-2-(4-morpholinyl)-4-phenyl-1,2,3,4,6,7,12,12b-octahydroindolo[2,3-a]quinolizine-6-carboxylate		C27 H31 N3 O3	0.788	1335.70348
c4387			C20 H38 N9 O4 P	3.933	499.2791
c2293			C27 H64 N7 O6 P3	6.485	675.4144
c31			C33 H43 N5 O7	7.063	621.3152
c3439				6.645	796.39004

c4111			C34 H65 N2 O5 P3	4.872	674.41033
c1957			C89 H124 N9 O14 P3 S2	7.63	1699.79255
c1569	Asperphenalenone B		C35 H44 O10	5.746	624.29461
c1502			C55 H88 N9 O8 P3	7.652	1095.59632
c2628	Drechslerine C		C14 H24 O2	10.402	224.17753
c3497				8.554	1572.81457
c2177			C18 H42 N9 O7 P	3.919	527.2951
c410			C78 H116 N5 O16 P3	8.57	1471.76414
c2816			C51 H72 N2 O6 P2	7.822	870.48578
c2715			C73 H107 N7 O11 P2	9.481	1319.75085
c3662			C33 H72 N9 O11 P	8.37	801.50997
c542			C51 H64 N9 O2 P	5.677	865.49013
c4468				3.882	1380.70574
c38			C54 H81 N7 O17	7.619	1099.56839
c474			C19 H35 N5 O5 S	1.031	445.23481
c882			C34 H53 N3 O17	5.475	775.33656
c3123			C36 H72 N3 O15 P	6.62	817.46913
c1348	unknown Lok MF	B		15.115	1373.26598
c2210			C23 H42 N4 O5	6.768	454.31512
c3142	NP-003319		C11 H14 N4 O4 S	3.163	298.07288
c2043			C14 H36 N9 O5 P	3.787	441.2581
c1480	Maniwamycin F		C11 H21 N3 O3	1.032	243.15749
c1409			C16 H28 N4 O5	4.281	356.20514
c1683			C69 H84 N9 O8 P3	6.466	1259.566
c1067	Natalenamide A		C19 H25 N3 O5	6.42	375.17927
c1364	Cyclo-(Leu-Ile)		C12 H22 N2 O2	7.439	226.16825
c886			C35 H67 N5 O10 P2 S	5.616	811.40599
c28			C31 H53 N7 O10	5.543	683.38359
c2486			C16 H39 N7 O7 P2	3.383	503.23655
c803	1,3-Diphenylacetone		C15 H14 O	2.257	454.25307
c742	1-[4-[[3-[[5-(2-Hydroxy-2-propanyl)-1,2-oxazol-3-yl]methyl]-3-oxetanyl]amino]-1-piperidiny]ethanone		C17 H27 N3 O4	6.562	359.18389
c279			C38 H58 N2 O12	8.063	734.40061
c1175			C36 H65 N9 O14 P2	4.824	909.41449
c2855			C14 H26 Cl N7 O2	7.058	359.1836
c1295	Prolylleucine		C11 H20 N2 O3	7.106	228.14676
c2001			C37 H63 N5 O4 P2	4.268	703.43671
c4760			C37 H72 N3 O18 P3	6.902	939.40165
c4220				3.13	482.28373
c1886	(2R)-1-[[7Z,10Z,13Z,16Z]-7,10,13,16-Docosatetraenoxy]-3-(phosphonoxy)-2-propanyl (4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-docosahexaenoate		C47 H73 O8 P	3.158	796.50402
c3195			C21 H31 N3 O4	9.572	389.23297
c2145	R-1 Methanandamide phosphate		C23 H40 N O5 P	2.425	463.23927
c6	Not named		C25 H38 N4 O6	5.551	490.27818
c159			C18 H37 N8 O2 P3	6.484	490.22463
c2976			C89 H121 N3 O17	9.305	1503.87032
c1679			C24 H46 N5 O6 P	5.768	531.31678
c370			C29 H52 N5 O4 P3	4.647	627.32192
c745			C25 H37 N9 O4	3.139	527.29432
c662			C25 H38 N8 O6	4.39	546.28947
c2889				7.608	363.71273
c110			C34 H53 N3 O17	5.653	775.3376
c637			C27 H50 N5 O7 P	5.737	587.34278
c2798				0.804	607.28678
c1916			C22 H46 N3 O9 P	3.902	527.29498
c3037	Namalide E		C28 H43 N5 O6	6.789	545.32094
c1785			C55 H77 N10 O5 P3	7.977	1050.52972
c4531			C26 H47 N4 O4 P S	3.903	542.30582
c293			C13 H25 N3 O4	3.703	287.18393
c1820			C21 H31 N3 O4	9.574	389.23189
c1614			C24 H42 N3 O7 P	6.319	515.27375
c1257				5.355	682.46161
c2038				3.876	920.47036
c3177			C9 H5 N10 O13 P3 S3	0.719	649.84105
c4358				0.721	1299.68113
c1461			C41 H81 N7 O16 P2	8.246	989.52076
c2214			C30 H63 Cl N4 O14	6.157	738.40574
c2566			C16 H31 N O5 S	8.6	349.19193
c1357			C36 H76 N5 O16 P	4.685	865.50189
c3365				3.923	1054.59079
c615				4.766	406.72394
c3008			C16 H40 N6 O9 S	6.642	492.2581
c1516			C38 H59 N6 O2 P	19.382	662.44561
c2162				5.178	384.21857
c802	NNK		C14 H26 N6 O6	0.792	374.19762
c4441				6.713	1960.84788
c4148			C46 H95 N8 O18 P S3	3.519	1174.56585
c3823				9.342	2065.11953
c4015	Streptoprenylindole C		C15 H21 N O3	11.071	263.15205
c1817			C23 H45 N5 O5	5.114	471.34138
c753	1,3-Diphenylacetone		C15 H14 O	2.251	227.12659
c100	PPK		C16 H28 N4 O4	0.792	340.21001
c1021			C39 H59 N6 O5 P	5.532	722.43044
c1570			C87 H113 N7 O12 P2	9.203	1509.7924
c1590			C35 H50 N2 O6 P2	4.095	656.31553
c2082				4.278	712.40997
c818			C26 H47 N4 O8 P	5.8	574.31114

c2916	Natalenamide B		C20 H27 N3 O5	7.449	389.19527
c492			C32 H55 N3 O12	3.892	673.3789
c798	(3aR,8aS)-1-acetyl-1,2,3,3a,8,8ahexahydropyrrolo[2,3-b]indol-3a-ol		C12 H14 N2 O2	4.414	218.10518
c79			C50 H66 N8 O3 P2	8.354	888.47291
c3737			C27 H60 N10 O18	5.609	812.4094
c4099			C26 H54 N3 O16 P S	4.442	727.29557
c597			C41 H72 N9 O15 P	8.414	961.48925
c4102			C29 H42 N6 O6	3.171	570.31522
c2905				8.598	698.384
c145			C37 H65 N9 O9	4.428	779.48913
c1161			C71 H97 N O16 P2	3.278	1281.62658
c164	Kempopeptin B		C46 H73 Br N8 O11	7.344	992.46126
c1825			C40 H77 N8 O6 P3	5.208	858.51933
c3128			C41 H79 N4 O10 P3	5.21	880.50099
c488			C31 H41 N9 O2	7.68	571.33619
c3485			C19 H31 N7	6.774	357.26234
c720	Fenspiride		C15 H20 N2 O2	7.912	260.1524
c4312			C22 H56 N7 O14 P3	0.795	735.31058
c4686			C15 H36 N5 O7 P	3.135	429.23658
c1473			C19 H2 N4 O18 P2 S	5.87	667.85468
c1669			C74 H93 O7 P3	7.325	1186.61296
c1645				4.639	1034.51345
c981			C49 H75 N8 O16 P	7.545	1062.5036
c1568	2-methyl-3-(2-thienyl)-3,3a,4,5-tetrahydro-2H-benzo[g]indazole		C16 H16 N2 S	0.795	268.09841
c3687				14.932	1362.7623
c2947			C10 H23 Br N2 O	0.786	266.10039
c4299	(3S)-3-({(Z)-[(3S)-3-({(Z)-[(3R)-3-Amino-1-hydroxy-4-methylpentylidene]amino)-1-hydroxybutylidene]amino)-5-methylhexanoic acid		C17 H33 N3 O4	5.812	343.24679
c102	Syringolin G		C26 H45 N5 O6	6.003	523.33703
c878			C31 H55 N6 O9 P	7.004	686.37376
c1658			C13 H26 N7 O2 P	6.998	343.18739
c1058			C12 H23 N3 O3 S	1.728	289.14525
c2653			C16 H31 N3 O5	3.316	345.22543
c343	Versicotide C		C28 H34 N6 O6	3.094	550.25229
c2906	Methoxyacetyl norfentanyl		C14 H20 N2 O2	5.909	248.15191
c4715			C29 H67 N4 O15 P3	4.907	804.38211
c848			C38 H74 N3 O15 P S	3.839	875.45642
c1068			C38 H65 N5 O16	6.086	847.44348
c4798				2.133	242.18166
c122				5.026	651.8952
c569	Leu-Leu		C12 H24 N2 O3	4.277	244.17814
c4165			C40 H70 N7 O3 P3	7.278	789.47529
c1740	(Z)-N-({(2R)-1-Hydroxy-2-[(Z)-{(2S)-1-hydroxy-2-[(Z)-{hydroxy[(2R)-1-(D-tyrosyl)-2-pyrrolidinyl]methylene}amino)-3-phenylpropylidene]amino)-3-methylbutylidene)-L-alpha-glutamyl-L-proline		C38 H50 N6 O10	6.416	750.35825
c4881			C48 H90 N4 O17 P2 S	5.237	1088.54936
c2160				6.685	514.77281
c2395			C29 H60 N10 O7 P2 S	5.43	754.3839
c3499				5.862	1317.62139
c3151			C44 H89 N4 O16 P	7.778	960.60177
c138	Methyl (2S,2aS,3a'R,4a'R,5aR,12b'R,12b'R,12c'R,15aR,15a'S,17a'S)-12c'-hydroxy-10'-methoxy-2',3',4,4a',5,6,8,12c',13,13',14,14',17',17a'-tetradecahydro-4'H,5'H,16'H-spiro[furo[2',3':7,8]indolizino[8,1-c;d]carbazole-2,6'-furo[2',3':7,8]indolizino[8,1-cd]pyrido[1,2,3-lm]carbazole]-7-carboxylate		C43 H50 N4 O6	4.832	718.37411
c4136			C31 H61 N8 O6 P3	3.433	734.39521
c267			C31 H40 N10 O3	6.748	600.32649
c906			C87 H116 N10 O12 P2 S	9.117	1586.79898
c1093			C16 H31 N3 O4	4.131	329.23062
c2216	Androsterone		C19 H30 O2	6.881	272.20974
c2343				6.302	990.53751
c1448				5.405	682.38864
c232			C15 H26 N6 O5 S	4.172	402.16765
c2273			C17 H32 N7 O4 P	7.144	429.22359
c463	Prolylleucine		C11 H20 N2 O3	6.178	228.14702
c39	Cyclo(phenylalanyl-prolyl)		C14 H16 N2 O2	5.878	244.12092
c2876				5.992	1298.71665
c2025	5-(tert-butyl)-2-methyl-N-(5-methyl-3-isoxazolyl)-3-furamide		C14 H18 N2 O3	5.229	262.13125
c1211				4.833	272.64201
c4130	Tetranor-12(S)-HETE		C16 H26 O3	14.588	248.17695
c1774			C28 H62 N9 O11 P	5.167	731.43182
c681			C28 H35 N5 O9	3.864	585.24249
c1789			C12 H30 N9 O3 P	4.181	379.22109
c2764	12-Carbamoylstreptothricin D		C31 H58 N12 O10	4.19	758.44126
c1247			C26 H49 N10 O7 P	5.816	644.35293
c4157			C22 H39 N5 O6	3.74	469.28937
c1763				4.105	670.36736
c1974			C43 H70 N3 O8 P3	6.543	849.43714
c1212			C23 H41 N5 O6	4.649	483.30503
c262	F1839-B		C24 H33 N O6	11.958	431.23009
c651			C68 H95 N3 O14 P2 S	7.65	1271.60117
c2226			C9 H24 N4 O9	4	332.1532
c1046				3.76	938.57854
c1248	Cyclo(S-Phe-S-Gln)		C14 H17 N3 O3	3.509	275.12622
c764			C49 H91 N8 O18 P3	3.015	1172.56628
c304	Bohemamine		C14 H18 N2 O3	4.347	262.13119
c954			C45 H64 N4 O4 P2	5.642	786.4383
c3776			C27 H55 N3 O3 P2 S	4.661	563.34255
c3184			C15 H35 N9 O5	5.301	421.2765
c2656				4.178	314.17017
c3401			C31 H68 N7 O11 P3	9.015	807.41896
c2308			C9 H21 N6 P S	3.069	276.12938

c912	N-Undecanoylglycine	C13 H25 N O3	10.436	243.1835
c2206		C29 H36 N7 O8 P	4.476	641.23553
c3756		C17 H38 N6 O3 S2	6.958	438.24237
c3148		C50 H102 N3 O13 P3 S	8.095	1077.63548
c3084		C20 H38 N4 O6	5.858	430.27866
c1594		C40 H61 O9 P3 S	13.165	810.32506
c1930		C29 H51 N10 O10 P S	5.237	762.32411
c3075		C49 H87 N6 O14 P3 S2	6.314	1140.49293
c357		C32 H43 N O3 P2	7.184	551.27063
c3307			6.375	376.69461
c134		C30 H46 N6 O9	5.215	634.33141
c1360	L-Tyrosylglycylglycyl-D-phenylalanylleucyl-D-arginyl-D-arginyl-L-isoleucine	C46 H72 N14 O10	6.598	980.55726
c1844	Syringolin F	C26 H43 N5 O6	5.31	521.32036
c3774		C49 H86 N9 O16 P	7.456	1087.59206
c2513		C40 H62 N3 O8 P S	3.924	775.39695
c550		C39 H65 N9 O11	5.346	835.47862
c3763			6.378	864.47425
c4308		C18 H38 N6 P2 S	6.382	432.23685
c4333			9.128	1615.7966
c602		C34 H46 N8 O2 P2	7.489	660.32441
c1970			4.909	320.66854
c257		C24 H44 N8 O6	2.99	540.33696
c242	Tamsulosin	C20 H28 N2 O5 S	13.169	408.16625
c2387		C37 H53 N3 O4 P2	10.174	665.35473
c182		C21 H44 N3 O9 P	5.159	513.27895
c2527		C36 H39 N3 S	5.339	545.28444
c4606	10-Hydroxy-trans-paspalic acid Amide	C16 H17 N3 O2	5.853	283.13154
c1565		C19 H45 N10 O6 P	5.999	540.32707
c158		C19 H35 N5 O5 S	0.79	445.23467
c3067		C13 H25 N3 O4 S	2.824	319.15576
c272		C20 H47 N8 O8 P	6.463	558.32326
c515		C37 H72 N9 O11 P3	8.322	911.45743
c613		C19 H34 N4 O5 S	4.291	430.22395
c1060		C16 H28 N4 O3	4.278	324.21538
c808		C18 H29 N3 O6	8.547	383.20552
c4755	Vinorelbine	C45 H54 N4 O8	7.439	778.39084
c114		C20 H29 N3 O4	6.167	375.21527
c1752		C73 H111 N3 O16 P2	14.514	1347.74576
c1639		C17 H39 N10 O4 P	3.275	478.28941
c255	NP-020534	C27 H31 N5 O2	4.396	457.24293
c183		C20 H34 N4 O5	3.126	410.25192
c64	Adenosine	C10 H13 N5 O4	1.106	267.09598
c2768		C21 H9 O18 P3 S	14.514	673.87257
c696			7.648	635.80028
c299	Cyclo(S-Phe-S-Gln)	C14 H17 N3 O3	3.072	275.12627
c1553		C9 H26 N5 O5 P	6.394	315.16869
c2787		C36 H71 N5 O8 P2 S	4.799	795.44882
c1643		C32 H58 N4 O11 S	6.382	706.38321
c3412		C25 H57 N9 O11 P2	2.969	721.36344
c723			9.905	2612.45037
c599		C16 H40 N10 O3 S	6.946	452.29928
c3961		C33 H60 N O14 P	6.701	725.3735
c2176		C28 H45 N7 O8	6.563	607.33209
c1431		C29 H61 N8 O6 P S	4.112	680.41948
c1017		C37 H58 N5 O10 P	7.399	763.39051
c220		C24 H53 N4 O8 P	3.61	556.35755
c1196			6.4	1996.96285
c4020	Imatinib	C29 H31 N7 O	3.785	986.5009
c2708		C16 H28 N10 O2	3.436	392.24111
c910		C39 H50 N3 O3 P	4.934	639.3582
c49		C32 H46 N6 O9	5.55	658.33105
c1893		C11 H11 N4 O6 P	0.719	326.04313
c53	Cotteslosin A	C34 H45 N5 O7	6.968	635.33081
c1004		C14 H29 N5 O4 S	5.446	363.19491
c4342			5.858	2177.12607
c1748		C17 H36 N10 O4	4.529	444.29393
c3565			6.594	1214.66446
c676			4.199	361.65312
c3766			6.786	1937.96132
c2938		C33 H62 N9 O5 P3	6.833	757.41165
c87		C23 H41 N2 O6 P	6.831	472.26833
c4861	N-{4-[(2R,3R)-3-(Hydroxymethyl)-4-isopropyl-5-oxo-2-morpholinyl]phenyl}-2-methoxyacetamide	C17 H24 N2 O5	2.577	716.29026
c537		C31 H72 N9 O14 P	6.154	825.49478
c1534		C40 H63 N3 O10	6.67	745.44813
c786	Pyridindolol	C14 H14 N2 O3	3.09	258.09966
c1827	Leucyltryptophan	C17 H23 N3 O3	5.649	317.17356
c571	Leucyl-3-epi-deoxynegamycin	C15 H31 N5 O4	3.35	345.23641
c1772			4.67	445.72222
c890		C26 H44 N3 O6 P	8.419	525.29446
c401		C45 H67 N9 O5 P2	5.229	875.47338
c222			6.159	750.43019
c4880			6.324	473.27455
c2454	Marimastat	C15 H29 N3 O5	2.355	331.20994
c1020		C40 H79 N7 O16 P2	7.59	975.50509
c704	(3S)-3-({(Z)-[(3S)-3-({(Z)-[(3R)-3-Amino-1-hydroxy-4-methylpentylidene]amino}-1-hydroxybutylidene)amino}-5-methylhexanoic acid	C17 H33 N3 O4	5.49	343.24625

c1320			C20 H36 N4 O3	5.026	380.27758
c2108				9.571	2514.3843
c2599			C61 H97 N3 O18 P2	6.782	1221.62352
c2326			C47 H81 N7 O18	7.773	1031.56487
c185			C29 H42 N6 O7	6.643	586.31057
c4511	D-Isoleucyl-L-prolyl-L-tyrosyl-D-isoleucine		C26 H40 N4 O6	7.243	504.29472
c4772			C27 H55 N9 O5 P2 S	3.948	679.35324
c2831			C10 H23 N O6	3.82	253.15226
c2521			C17 H35 N7 O6	9.393	433.26414
c2710			C28 H63 N5 O5 P2 S	7.826	643.40563
c26			C22 H38 N4 O5	6.189	438.28361
c1076			C41 H77 N9 O17	4.119	967.54317
c1903			C22 H51 N10 O5 P3	4.738	628.32524
c3373			C30 H65 N5 O11 P2 S	7.154	765.38751
c3269			C44 H78 N9 O14 P	8.512	987.5417
c2494			C12 H22 N4 O4	4.508	286.16335
c522				6.382	965.56097
c1796			C7 H3 N8 O17 P S2	0.721	565.87975
c498			C16 H29 N5 O5	0.789	371.21572
c525	EPK		C16 H28 N4 O6	0.787	354.18921
c2903				8.441	1668.90495
c751				5.46	1596.79056
c529			C15 H37 N9 O6	5.743	439.28723
c3			C18 H32 N4 O5	4.29	384.23656
c3469			C33 H57 N3 O3 P2	5.029	605.38817
c621			C19 H43 N6 O4 P S	6.367	482.27913
c4270			C23 H56 N10 O7 P2	3.691	646.37956
c72			C27 H49 N7 O7	4.278	583.36798
c3798	Atenolol		C14 H22 N2 O3	3.435	266.16225
c427			C35 H53 N9 O7	6.721	711.40597
c403	Marimastat		C15 H29 N3 O5	4.691	331.21052
c4215	Grifolinone B		C44 H54 O7	5.458	694.38883
c1999			C16 H29 N3 O4 S	4.1	359.18666
c2292	2-(Cyclohexylmethylidene)-1,2,3,4-tetrahydronaphthalen-1-one		C17 H20 O	3.247	262.13124
c15			C29 H43 N5 O6	6.559	557.3208
c936				8.443	1667.90129
c1317			C18 H36 N10 O3 S	6.317	472.27102
c298			C32 H52 N8 O9	8.26	692.38539
c877			C26 H36 N4 O5	7.66	484.26773
c2371	Lobophorin B		C61 H90 N2 O21	7.6	1186.5982
c2045			C40 H70 N7 O7 P3	6.462	853.45386
c177			C18 H28 N4 O6	4.617	396.20027
c4400	N-Tridecanoylglycine		C15 H29 N O3	8.571	271.21433
c1057			C22 H41 N4 O5 P	5.738	472.27959
c244			C15 H34 N10 O9	4.552	498.25087
c188				4.277	291.68405
c4635	Paecilopeptin		C13 H24 N2 O3	4.152	256.17806
c1097			C32 H62 N3 O13 P	6.797	727.4011
c3326			C28 H63 N9 O7 P2 S	6.957	731.40344
c9			C35 H60 N5 O11 P	6.997	757.39981
c2451	5-(tert-butyl)-2-methyl-N-(5-methyl-3-isoxazolyl)-3-furamide		C14 H18 N2 O3	3.245	524.2626
c1936				1.167	1370.50291
c1972			C15 H29 N3 O4	3.471	315.21506
c1655			C36 H66 N9 O14 P	6.801	879.44827
c773				7.066	310.65755
c538				4.617	792.40195
c321			C42 H82 N10 O11 P2 S2	0.792	1028.50811
c3705			C29 H61 N10 O16 P	3.424	836.40062
c354			C20 H34 N4 O5	4.71	410.25289
c4611			C64 H98 N9 O18 P S	8.417	1343.64733
c1243			C67 H104 N5 O18 P	6.008	1297.7121
c1477			C18 H45 N10 O6 P3	5.406	590.27228
c3047	Norpicacetin		C24 H33 N5 O7	3.381	503.23638
c3239			C38 H73 N10 O7 P S2	6.963	876.48493
c2			C28 H35 N9 O2	7.12	529.28949
c1871				4.171	942.50929
c892	3-[6-(tert-butyl)-1,1-dimethyl-2,3-dihydro-1H-inden-4-yl]-5-(trifluoromethyl)-4,5-dihydro-1H-pyrazol-5-ol		C19 H25 F3 N2 O	1.028	354.18914
c1122	QPK		C16 H29 N5 O5	1.031	371.21577
c1037				5.587	522.31359
c4467			C22 H38 O11 P2	3.478	540.1885
c784				6.972	345.67069
c827			C30 H56 N5 O7 P3	6.974	691.34141
c1959			C51 H80 N9 O7 P3	8.983	1023.53914
c992			C42 H65 N6 O5 P	6.712	764.47876
c4474			C27 H37 N5 O5	10.986	511.27949
c247	NP-005457		C48 H82 N2 O16	6.387	964.55853
c2675				7.629	2746.3001
c4329			C43 H84 N5 O12 P3	3.66	955.53303
c1029			C29 H43 N9 O10	3.001	677.31157
c501	3-Hydroxy-3-[(3-methylbutanoyl)oxy]-4-(trimethylammonio)butanoate		C12 H23 N O5	5.581	261.157
c1152			C18 H38 N7 O8 P	6.656	511.25181
c3760			C22 H51 N10 O13 P	2.343	694.33879
c1369	Pestalolide B		C14 H22 O4	11.747	254.15184
c4645				8.608	1344.71311
c374			C20 H34 N4 O5	4.707	410.25331

c539			C24 H30 N10 O3	7.053	506.25242
c849				4.649	1254.64374
c1081			C22 H48 N3 O8 P	6.038	513.31627
c3936			C33 H55 N6 O4 P3	7.505	692.3529
c4600			C57 H86 N9 O6 P3	10.289	1085.59267
c2047			C26 H38 N3 O3 P S	4.639	503.23732
c1306			C39 H66 N4 O13	7.511	798.46282
c863				8.241	1124.62976
c736			C30 H63 N8 O5 P3	5.036	708.41447
c1533			C27 H37 N5 O5	7.001	511.27876
c4638			C32 H62 N9 O8 P	3.884	731.44275
c1190			C31 H48 N2 O4 P2	5.793	574.31118
c3358			C23 H25 N3 O6	6.422	439.17416
c217			C32 H55 N7 O10	4.423	697.39962
c2323			C22 H49 N7 O3 P2 S	6.42	553.31017
c939				9.065	1550.86188
c3976			C51 H85 N O15 P2 S	6.687	1045.51098
c1826			C72 H128 N9 O18 P3 S	9.888	1531.8301
c3660			C13 H4 N8 O18 P2 S3	0.718	717.82829
c3235			C30 H43 N O3 S	3.875	497.29572
c407			C47 H77 N10 O4 P3	6.827	938.53393
c1819				5.317	1530.73384
c1355				4.776	719.36672
c2250				7.433	2502.30804
c3678	Questionomycin C		C13 H10 N2 O3 S	9.399	274.04163
c14			C28 H45 N7 O6	5.454	575.34182
c153			C21 H30 N8 O3 S	5.199	474.21394
c3181				0.792	236.11757
c3912				14.509	1348.74875
c2483				6.402	1953.9587
c4796			C30 H66 N9 O12 P	6.415	775.45917
c1598				4.778	359.68301
c1547			C13 H35 N7 O4	13.56	353.27692
c3390			C43 H73 N5 O9 P2 S	4.521	897.46144
c928			C82 H118 N7 O9 P3	9.184	1437.82176
c4178			C20 H47 N8 O2 P3	0.725	524.30563
c287			C26 H40 N6 O7	0.792	548.29387
c2638	Lobophorin B		C61 H90 N2 O21	7.602	1186.59833
c68			C22 H38 N4 O5	5.716	438.28398
c3657			C20 H32 N8 O	5.714	400.26849
c1530	N-{4-[(2R,3R)-3-(Hydroxymethyl)-4-methyl-5-oxo-2-morpholinyl]phenyl}acetamide		C14 H18 N2 O4	2.279	278.12606
c147			C23 H43 N4 O2 P3	6.658	500.26139
c180			C43 H66 N7 O4 P3	6.727	837.43745
c1061	Adenosine 3'5'-cyclic monophosphate		C10 H12 N5 O6 P	1.03	329.05144
c78	Iso-isariin D		C26 H45 N5 O7	5.331	539.33099
c3325			C14 H15 N3 O3	3.737	273.11074
c3015			C25 H44 N2 O12	2.33	564.28958
c441			C24 H55 N6 O11 P	5.026	634.36803
c2859			C57 H96 N10 O14 P2	6.362	1206.65895
c2807			C36 H73 N8 O13 P	4.641	856.50111
c284			C85 H120 N8 O16 P2	9.116	1570.83082
c1718			C48 H87 N2 O13 P3 S	3.528	1024.51426
c301			C35 H69 N6 O10 P	6.933	764.47825
c2992	2-[(Allylcarbamoyl)amino]-1,4:3,6-dianhydro-2,5-dideoxy-5-{[4-(3-fluorophenyl)-2-pyrimidinyl]amino}-L-iditol		C20 H22 F N5 O3	3.295	399.17615
c4548	Streptcytosine M		C16 H23 N3 O4	4.763	321.1689
c1170			C12 H21 N7 O2 S	7.619	327.14757
c618			C44 H89 N3 O14 P2 S	7.198	977.55416
c2270			C16 H37 N10 O2 P	5.455	432.28395
c4618			C70 H99 N4 O14 P3	3.205	1312.63806
c3726			C20 H32 N4 O7	2.732	440.2264
c967	1-{4-[(3-{[5-(2-Hydroxy-2-propanyl)-1,2-oxazol-3-yl]methyl}-3-oxetanyl)amino]-1-piperidiny]ethanone		C17 H27 N3 O4	6.56	718.3678
c4171			C42 H70 N3 O4 P3 S	5.907	805.43099
c482			C29 H47 N8 O P3 S	1.03	648.27843
c644	NP-012766		C31 H46 N4 O7	3.718	624.28667
c980	NP-008521		C14 H18 N2 O2	6.895	246.13664
c697			C29 H55 N6 O8 P	5.771	646.38019
c4535			C33 H64 N9 O13 P3	6.802	887.38409
c2984			C30 H64 N10 O10 P2	4.728	786.42743
c394			C35 H55 N7 O7 P2	5.194	747.36146
c414				5.422	326.68691
c2745			C81 H107 N6 O9 P3	8.402	1400.73108
c2076			C75 H126 N5 O18 P3 S2	7.199	1541.77498
c933			C47 H77 N10 O4 P3	6.359	938.53326
c4773			C22 H58 N10 O12 P2	5.676	716.37328
c543	Gln-Leu-Val-Pro		C21 H37 N5 O6	4.881	455.27366
c1044			C25 H45 N4 O6 P S	4.665	560.27773
c4709	NP-008993		C18 H34 O4	14.416	296.2346
c4545	Phthoxazolin		C16 H22 N2 O3	6.765	290.1624
c3855			C56 H79 N5 O8 P2	8.012	1011.54112
c774	Cyclo-(Leu-Ile)		C12 H22 N2 O2	7.675	226.16775
c1155			C8 H19 N7 O6	4.596	309.14139
c2243			C30 H41 N8 O8 P	5.226	672.27841
c3481			C29 H40 N O8 P	4.178	561.24604
c1042	2-(2-amino-3-methylbutanamido)-3-phenylpropanoic acid		C14 H20 N2 O3	3.315	264.1465
c986				6.015	440.73366

c1617			C32 H51 N5 O8 P2	3.808	695.32152
c1472			C16 H27 N3 O5	5.404	341.1942
c1494			C16 H29 N3 O6	5.404	359.20482
c1279	Scalusamide C		C16 H29 N O3	10.945	283.21462
c1660			C13 H17 N5 O5	3.028	323.12209
c3124	[(3R,4S)-1-[(4-Methoxyphenyl)acetyl]-3-{2-[4-(2-oxo-2,3-dihydro-1H-benzimidazol-1-yl)-1-piperidinyl]ethyl}-4-piperidinyl]acetic acid		C30 H38 N4 O5	4.832	534.27742
c1931			C16 H30 N6 O4	1.27	370.23183
c3643			C11 H21 N3 O2	4.275	227.16283
c1777				9.971	2632.42661
c2516				6.387	1304.63807
c2697			C17 H25 N5 O3	5.452	347.19485
c1342			C25 H55 N8 O12 P	6.155	690.36828
c4032			C32 H68 N9 O13 P	7.478	817.4701
c4422			C27 H50 N6 O6	3.141	554.37772
c2391			C19 H34 N4 O5	4.273	398.25158
c3050				4.498	860.44826
c2562			C69 H122 N O14 P3 S3	14.941	1377.72421
c3009				7.272	1002.55288
c1874			C16 H33 N5 O3 S	6.704	375.23201
c69				7.616	549.7852
c1387			C15 H27 N O5	3.104	301.18814
c632			C4 H4 O7 P2	0.722	225.94354
c598			C37 H64 N5 O9 P	7.906	753.44308
c65			C32 H56 N8 O10	3.852	712.41085
c1662			C32 H64 N9 O13 P3	6.302	875.38415
c2129			C28 H59 N3 O6 S2	3.998	597.3843
c4289			C43 H85 N2 O16 P3	3.396	978.51113
c2778			C45 H64 N10 O14 P2	7.346	1030.40774
c2115			C10 H29 N9 O3 S	6.718	355.21056
c2718	Diprotin A		C17 H31 N3 O4	5.656	341.23098
c1625	(4aR,5R,6R)-6-hydroxy-4a,5-dimethyl-3-(prop-1-en-2-yl)-2,4a,5,6,7,8-hexahydronaphthalen-2-one		C15 H20 O2	4.291	214.13142
c1347			C38 H67 N6 O5 P S	6.699	750.46305
c192			C22 H40 N6 O6	0.789	484.29946
c253			C11 H20 N10 O2	0.794	324.17869
c3161			C41 H72 N6 O10 P2	3.672	870.47984
c2914			C20 H31 N3 O5	4.243	393.22547
c4684	Cryptophycin D		C35 H44 N2 O7	1.228	604.31595
c2556			C11 H18 N4 O	5.456	222.14755
c4695				3.878	2086.07882
c2026			C44 H57 N7 O3 P2	9.113	793.40205
c730			C86 H112 N9 O14 P	7.224	1525.80867
c371				7.23	1504.83256
c2727				4.187	1176.61278
c3234	Koreenceine C		C14 H27 N O	11.129	225.20922
c3167			C19 H46 N8 O10 P2 S	4.107	640.25157
c1573			C43 H75 N6 O10 P	9.391	866.52834
c4502			C35 H53 N4 O14 P3	2.116	846.27793
c4132			C50 H79 N5 O17	5.139	1021.54704
c2480			C22 H43 N10 O5 P	3.378	558.31526
c1166	NP-022512		C13 H19 N O	10.702	205.1468
c4284			C19 H49 N6 P3 S	5.858	486.29469
c782			C29 H41 N5 O8	6.291	587.29471
c91			C30 H51 N7 O9	5.434	653.37305
c1365	N-{4-[(2R,3R)-3-(Hydroxymethyl)-4-methyl-5-oxo-2-morpholinyl]phenyl}acetamide		C14 H18 N2 O4	2.283	556.2525
c4777				9.343	2066.12449
c4367	Bis(2-ethylhexyl) terephthalate		C24 H38 O4	8.341	390.27627
c2981	16-O-(2'',3'',4'',6''-tetra-O-acetyl-β-cellobiosyl)-2-hydroxydecanoic acid		C36 H60 O18	3.488	780.37864
c2558			C25 H36 N6 O9	2.786	564.25301
c2099				0.786	323.17601
c4260			C63 H87 N4 O15 P	5.57	1170.59062
c2361			C26 H53 N9 O2 P2 S	6.45	617.35295
c1809			C40 H59 N3 O5 P2	7.137	723.39415
c661			C35 H50 N8 O3 S	5.522	662.37328
c2560			C79 H120 N7 O18 P3	7.254	1547.79054
c1450			C14 H24 N4 O7	1.029	360.16325
c3227	Spumigin 638		C32 H42 N6 O8	4.222	638.30405
c3666			C40 H56 N O5 P3	6.177	723.3365
c2247				5.155	304.67372
c2487			C40 H65 N5 O13 P2	4.104	885.40538
c3918	Mitragynine		C23 H30 N2 O4	2.509	398.22697
c949			C10 H28 N7 O3 P	3.742	325.19953
c4368			C47 H64 N O2 P S2	7.184	769.4116
c121	11-Aminoundecanoic acid		C11 H23 N O2	0.792	201.17232
c575			C31 H46 N5 O12 P	4.087	711.28821
c3854				6.344	1086.61173
c4774			C16 H42 N10 O6 P2	2.582	532.27403
c2083				7.584	1442.67902
c2101			C21 H35 N2 O8 P S	13.164	506.18408
c3233			C22 H41 N5 O5	4.708	455.31046
c1316				5.692	682.38925
c2392				14.92	1392.74414
c3004				9.068	1571.84018
c1096			C45 H79 N5 O7 P2 S	7.832	895.51679
c1127			C66 H115 N8 O14 P3	9.247	1336.7758
c4612	Cyclo-(L-Ala-L-Tyr)		C12 H14 N2 O3	2.176	234.09998

c1720	(2R)-1-[(Hydroxy[[(1S,5R)-2,3,4,6-tetrahydroxy-5-(phosphonooxy)cyclohexyl]oxy]phosphoryl]oxy]-3-[(9Z,12Z)-9,12-octadecadienoyloxy]-2-propanyl (11Z)-11-icosenoate	C47 H86 O16 P2	7.661	968.53641
c1794			8.571	1494.74943
c43		C20 H33 N5 O6	5.026	439.24188
c567	2-[2-[(19-acetamido-16,18-dihydroxy-5,9-dimethyl-6-oxoicosan-7-yl)oxy]-2-oxoethyl]butanedioic acid	C30 H53 N O10	5.162	609.34739
c2839	HPH	C17 H23 N7 O4	1.03	742.34916
c120	Cyclo-(L-Pro-L-Met)	C10 H16 N2 O2 S	3.735	228.09286
c289			3.506	427.209
c1934	3-amino-2-phenyl-2H-pyrazolo[4,3-c]pyridine-4,6-diol	C12 H10 N4 O2	6.793	242.08006
c252	Odioperazine D	C16 H17 N3 O4	5.647	315.12155
c3278		C49 H90 N8 O17 P2 S2	3.011	1188.5324
c3955		C20 H36 N8 O11	3.028	564.25288
c3281		C20 H46 N9 O5 P	5.833	523.33729
c2039		C12 H29 N8 O5 P	5.104	396.2003
c1440		C33 H58 N3 O13 P3	5.652	797.31879
c449			3.901	336.68948
c3393		C87 H132 N9 O14 P3 S2	9.205	1683.85476
c1009			0.721	241.91746
c4814	Bis(methylbenzylidene)sorbitol	C22 H26 O6	11.953	386.17296
c90	Cyclo(leucylpropyl)	C11 H18 N2 O2	4.779	210.13661
c2920		C58 H114 N10 O17 P2	8.15	1284.78428
c711		C37 H65 N9 O9	3.926	779.48977
c85	NP-011220	C11 H18 N2 O2	5.142	210.13647
c4074	Cyclo-(Ile-Ser)	C9 H16 N2 O3	2.04	200.11582
c947		C67 H117 N10 O18 P3	9.183	1442.77597
c1181		C34 H71 N8 O5 P3	7.578	764.47814
c1703		C50 H95 N8 O16 P S2	5.448	1158.60546
c1986		C16 H21 N3 O4	4.214	319.15229
c4125		C32 H75 N6 O16 P3	4.668	892.44602
c2606			7.114	793.93381
c1118		C9 H3 O18 P	0.719	429.90527
c1378			3.805	1390.64176
c2384		C35 H63 N5 O12	7.345	745.4492
c3869			10.676	1172.60295
c1227	Bis(4-ethylbenzylidene)sorbitol	C24 H30 O6	13.331	414.20308
c858	JS-3	C14 H16 N2 O4	5.138	276.11049
c2248		C35 H44 N6 O7	7.873	660.32997
c4867		C22 H42 N8 O8	1.241	546.31243
c3811		C35 H60 N O12 P	6.13	717.38719
c94		C32 H61 N6 O8 P	7.088	688.42602
c4048	gamma-Glutamyl-gamma-glutamyl-S-methylcysteine	C14 H23 N3 O8 S	1.21	393.1191
c4512		C28 H54 N5 O5 P S	7.562	603.3621
c2686		C14 H28 N4 O3	7.203	300.21583
c2204		C22 H53 N7 O3 S2	7.636	527.36731
c4194			9.339	2044.14777
c1649	Torrubiellone B	C22 H29 N O6	11.949	403.19841
c3668			5.172	602.30453
c2478		C30 H52 N2 O9	3.955	584.36673
c141		C16 H29 N3 O4 S	4.843	359.18714
c3458		C21 H37 N2 O5 P	8.464	428.24179
c1182	Confluenine A	C11 H22 N2 O3	2.263	230.16257
c1399	Cyclobenzaprine	C20 H21 N	2.255	275.16283
c313		C15 H27 N O	10.471	237.20918
c2074	LMA-P3	C14 H28 O5	10.239	276.1939
c2743		C34 H73 N8 O11 P3	6.563	862.46206
c3746			7.429	2503.31184
c771		C33 H46 N8 O7	5.13	666.34771
c816			18.316	609.17626
c2681		C46 H81 N9 O12 P2 S	8.982	1045.52056
c2055		C74 H113 N9 O17 P2 S	8.569	1493.74639
c13			4.507	618.31877
c1539		C22 H53 N6 O2 P3 S	2.575	558.31861
c4253			7.625	2763.32431
c3518		C62 H101 N6 O16 P3	7.329	1278.64995
c4747		C7 H16 N4 O11 P2	0.72	394.03044
c3282	Decarbamoyl-neosaxitoxin	C9 H16 N6 O4	1.337	272.12404
c86		C24 H33 N9 O3	5.698	495.26893
c443	1-(2-Furyl)-N-({[(2R,4S,5R)-5-[1-methyl-3-(2-naphthyl)-1H-pyrazol-5-yl]-1-azabicyclo[2.2.2]oct-2-yl)methyl]methanamine	C27 H30 N4 O	2.992	426.24675
c1767	Clozapine N-oxide	C18 H19 Cl N4 O	4.49	342.1217
c1830		C13 H24 N2 O5 S	4.497	320.13965
c4154		C27 H50 N3 O2 P S2	6.343	543.30593
c1968		C22 H36 N6 O5	2.664	464.27414
c3179		C18 H34 N6 O10 S2	3.505	558.17764
c2414	Hyapyrone A	C32 H42 O5	3.823	506.30448
c4065		C14 H27 N3 O4	3.377	301.19937
c789		C49 H101 N10 O15 P3 S2	6.329	1226.61057
c212	Bis(methylbenzylidene)sorbitol	C22 H26 O6	11.959	386.17232
c735		C42 H72 N5 O11 P S	3.453	885.46902
c4206		C16 H31 N3 O5	3.03	345.22529
c422		C38 H63 N8 O4 P3	3.218	788.41662
c2407		C44 H76 N6 O18 P2	6.66	1038.46891
c2318	N-(2-methyl-3-oxodecanoyl)pyrrolidine	C15 H27 N O2	10.221	253.20441
c2790		C41 H84 N7 O18 P	4.757	993.55956
c502	TKK	C16 H33 N5 O5	12.931	375.25114
c4214			5.894	1102.54221
c3971		C49 H81 N10 O9 P3	7.827	1046.54094

c1768				5.021	427.71575
c630			C64 H95 N6 O8 P3 S	7.576	1200.61545
c2261			C24 H43 N5 O6	4.879	497.32029
c265			C26 H43 N5 O5	5.026	505.32515
c263	Barnesin A		C25 H37 N5 O5	2.774	487.27858
c3556	1,3-Dipropylxanthine		C11 H16 N4 O2	1.041	236.12631
c167			C60 H92 N O18 P	8.294	1145.60547
c2844				0.72	581.85374
c4700	methyl 2-cyano-3-[1-[3-(1H-imidazol-1-yl)propyl]-1H-pyrrol-2-yl]acrylate		C15 H16 N4 O2	2.631	306.10848
c4114			C34 H40 N6 O5	4.169	612.30527
c929			C56 H79 N7 O14 P2	6.64	1135.51475
c3411	3-(tert-butyl)-1-methyl-N-(6-quinoxaliny)-1H-pyrazole-5-carboxamide		C17 H19 N5 O	3.714	618.33127
c4745			C29 H56 N2 O12	6.531	624.38378
c2973			C4 H N4 O7 P3	0.719	309.9046
c3403	2-[1-(2H-1,3-benzodioxol-5-yl)propan-2-yl]-6-methoxy-4-(prop-2-en-1-yl)phenol		C20 H22 O4	6.485	696.27862
c88	3-[(4-hydroxyphenyl)methyl]-octahydropyrrolo[1,2-a]pyrazine-1,4-dione		C14 H16 N2 O3	3.338	260.11549
c3491			C29 H67 N7 O9	15.902	657.50102
c446			C12 H23 N5 O2	2.519	269.18459
c2705			C42 H77 O14 P3	7.914	898.45278
c393				5.006	287.67071
c2641			C55 H102 N6 O18 P2	4.293	1196.67308
c2775			C50 H108 N6 O18 P2 S	4.288	1174.69151
c4629	NP-013663		C18 H34 O5	10.54	347.26663
c2337				9.612	2533.35897
c2155			C24 H44 O3	16.669	380.32817
c1015			C45 H89 N8 O18 P3	7.629	1122.55119
c3834	Brunnein A		C13 H12 N2 O3	3.035	244.08405
c3531			C28 H49 N7 O9 P2	3.774	689.30491
c901			C19 H39 N10 O5 P	2.731	518.28444
c67	Cyclo(phenylalanyl-prolyl)		C14 H16 N2 O2	5.476	244.12063
c1427			C38 H57 N7 O4 P2	5.462	737.3942
c561				7.272	1001.50492
c3995	Forpinic acid A		C40 H62 O9	3.847	686.44034
c2211	Bis(methylbenzylidene)sorbitol		C22 H26 O6	12.885	386.1719
c47			C80 H98 N2 O14 P2	7.637	1372.64908
c752	Not named		C11 H20 N2 O2	5.026	212.15193
c1340			C76 H120 N3 O16 P3 S2	8.57	1487.73229
c2191			C7 H2 O11 S	0.715	293.9307
c4669	Fusaricidin C		C45 H74 N10 O12	6.327	946.55075
c2925				0.72	701.85404
c1049	NP-008993		C18 H34 O4	15.18	296.23399
c99	Koreenceine B	C	C14 H27 N	11.093	209.21419
c3611	L-Prolylhydroxy-L-proline diketopiperazi		C10 H14 N2 O3	2.259	210.10002
c1453	pro-his		C11 H16 N4 O3	1.536	252.12184
c1829	Cyclo-(L-Ala-L-Tyr)		C12 H14 N2 O3	3.306	234.09993
c1244			C62 H108 N9 O17 P3	8.614	1343.70901
c2806	2-[1-(2H-1,3-benzodioxol-5-yl)propan-2-yl]-6-methoxy-4-(prop-2-en-1-yl)phenol		C20 H22 O4	5.565	696.27774
c3110			C32 H57 N2 O4 P S2	1.221	628.35251
c2288			C44 H48 N5 O4 P	3.311	741.3431
c2884				3.301	370.67156
c2616			C24 H37 N4 O2 P S	3.902	476.23803
c2698			C8 H25 N5 O3 P2	7.123	301.14203
c2918				7.328	1187.61408
c3455			C62 H94 N5 O12 P3	8.138	1193.61151
c3249			C32 H41 N5 O10	4.964	655.28404
c4538	SSR161421		C25 H20 N4 O2	11.727	408.15462
c1555			C63 H110 N9 O16 P3	9.248	1341.73026
c155			C28 H48 N6 O9	5.209	612.34921
c1627			C77 H113 N7 O12 P2	15.392	1389.79303
c3287			C26 H52 N10 O4 S2	5.535	632.36363
c3223			C12 H19 N5 O2	0.696	265.15307
c2990	Oximoaspergillimide		C11 H20 N2 O3	5.417	228.14687
c832	DesmethyImianserin		C17 H18 N2	2.136	250.14246
c2833			C11 H5 N2 O14 P3 S	0.717	513.86681
c868	NP-022076		C25 H34 O4	4.577	420.23413
c2837	Oximoaspergillimide		C11 H20 N2 O3	5.415	228.14692
c1670			C66 H97 N6 O15 P	8.952	1244.67641
c887			C54 H76 N9 O16 P	7.612	1137.51494
c1877			C54 H85 N4 O16 P3	7.631	1138.51774
c4053			C20 H37 N7 O3	3.105	423.2972
c865			C19 H33 N5 O7	2.273	443.23712
c4823			C15 H28 N2 O3 S	5.541	316.18172
c2693			C25 H59 N9 O9 P2	7.166	691.3894
c3058			C30 H49 N10 O7 P	7.204	692.35219
c1975			C9 H4 N2 O7 P2 S2	0.72	377.8919
c964			C14 H30 N7 O4 P	4.677	391.20985
c241			C30 H54 N7 O11 P	3.032	719.35854
c3141				19.727	329.90856
c97	(2Z)-N-(3-Aminopropyl)-N-{4-[(3-aminopropyl)amino]butyl}-3-(4-hydroxy-3,5-dimethoxyphenyl)acrylamide		C21 H36 N4 O4	5.026	408.27251
c1807	Piptamine		C23 H41 N	15.133	331.32249
c1429			C35 H44 N9 O12 P	5.652	813.2849
c678	(4aS,9aR)-7-(1,3-Benzodioxol-5-ylmethyl)-N-cyclohexyl-6-oxodecahydro-2H-pyrido[3,4-d]azepine-2-carboxamide		C24 H33 N3 O4	2.988	427.25314
c1592			C20 H48 N8 O4 P2 S2	5.026	590.27221
c1483			C37 H84 N5 O15 P3 S	3.324	963.4894
c2010			C17 H40 N6 O4 S2	5.011	456.25705

c680			C61 H98 N7 O17 P S	7.192	1263.64854
c2231	N-Tridecanoylglycine		C15 H29 N O3	8.058	271.21502
c2712			C25 H57 N9 O11 S	7.173	691.38957
c505	(2R,5R,6R)-3-[[1E,3E]-hepta-1,3-dien-1-yl]-5,6-dihydroxy-2-(hydroxymethyl)cyclohexan-1-one		C14 H22 O4	11.917	254.15167
c944			C63 H82 N10 O13	7.394	1186.60683
c2404			C26 H59 N8 O10 P	5.264	674.41046
c3466			C38 H72 N O14 P S	3.445	829.4426
c609				1.057	489.20571
c1790	Indoprofen		C17 H15 N O3	4.215	562.20526
c2194			C29 H61 N3 O13 S	7.162	691.38945
c348				3.025	359.67894
c3673			C73 H115 N10 O13 P3 S	9.185	1464.75707
c2356				6.668	1023.5073
c3762				6.557	590.37823
c4267			C9 H21 N9 P2	4.981	317.13872
c3155			C10 H21 N4 O13 P3 S	0.717	530.00497
c2956			C30 H50 N4 O6 P2 S	3.227	656.29503
c698			C64 H85 N5 O11 P2	8.293	1161.57222
c760			C32 H65 N5 O14 P2	7.156	805.39954
c3190			C41 H67 N9 O9 P2	2.727	891.4514
c4094			C22 H49 N2 O14 P	5.81	596.29283
c2624			C8 H3 N O2 P2 S2	19.732	270.9093
c1663	3-Hydroxycyclobenzaprine		C20 H21 N O	1.229	291.15733
c2301	NP-016455		C11 H18 N2 O4	4.407	242.12624
c489	2-[[3S]-1-(Cyclohexylmethyl)-3-pyrrolidinyl]-5-(1-methyl-1H-imidazol-5-yl)-1,3,4-oxadiazole		C17 H25 N5 O	3.848	315.20415
c3866			C9 H28 N9 O P	0.793	309.21415
c3107			C9 H17 N7 O4	0.698	287.13489
c2104			C16 H28 N4 O5	2.112	356.20528
c2386	[1-(2'-methylpropoxy)-2-hydroxy-2-methylpropoxy]butane		C12 H26 O3	12.95	218.18772
c4213			C20 H47 N6 O11 P3	3.721	640.25202
c1615	NP-001501		C16 H17 N3 O2	6.366	283.13177
c2630	Oxibendazole		C12 H15 N3 O3	2.544	249.10845
c1711			C36 H67 N9 O7 P2	1.223	799.46576
c990	unknown Lok MF	B	C77 H104 N9 O11 P	14.938	1361.7598
c1902			C30 H63 N6 O17 P	3.302	810.39964
c364			C22 H40 N6 O6	1.031	484.2992
c4746			C57 H95 N9 O18 P2 S2	3.491	1319.57151
c1543			C9 H N6 O8 P3 S	0.72	445.8792
c476	[Dha7]MC-FR		C51 H70 N10 O12	3.364	1014.5169
c1345				6.983	760.40732
c1			C31 H53 N7 O8	5.025	651.39402
c2932			C28 H56 N7 O3 P3	3.135	631.36833
c3044			C36 H62 N3 O17 P	3.37	839.38291
c531			C15 H27 N3 O5	5.147	329.19433
c2373			C17 H37 N9 O5 P2	4.554	509.24149
c1870				19.803	286.88159
c190	Cyclo(leucylprolyl)		C11 H18 N2 O2	4.631	210.13657
c1770	Not named		C11 H20 N2 O2	6.048	212.15229
c629			C21 H37 N	14.338	303.29184
c2974			C10 H20 N6 O	12.953	240.16958
c276				3.191	317.15682
c1661				6.705	1244.61613
c4707				9.609	2529.40683
c3532			C52 H72 N4 O10 P2	7.316	974.47242
c2549	7-Methyl-2-phenylquinoline-4-carboxylic acid		C17 H13 N O2	5.881	526.18842
c1194			C62 H100 N9 O18 P S	8.413	1321.66525
c1841			C53 H72 N4 O16	7.855	1020.49541
c1997	L-Arginyl-L-arginyl-L-arginine		C18 H38 N12 O4	1.026	486.31519
c3298			C13 H35 N8 O5 P S	13.167	446.21698
c1528				6.745	1866.92407
c1000			C26 H43 N2 O6 P3	3.088	572.23442
c189			C50 H85 N9 O15	7.624	1051.61638
c1098	Gln-Leu-Val-Pro		C21 H37 N5 O6	2.538	455.2735
c746	Tapentadol		C14 H23 N O	8.69	221.17839
c1235			C74 H108 N9 O11 P3	14.918	1391.73985
c1463			C21 H50 N9 O9 P S	3.066	635.31626
c1659	cGMP		C10 H12 N5 O7 P	1.034	345.04638
c4339			C24 H23 N2 P3	6.391	432.10525
c3576			C36 H51 N3 O6 S	1.216	653.34781
c3405			C18 H29 N10 O3 P S2	1.746	528.15783
c3807			C26 H57 N5 O4 P2 S	3.048	597.35821
c108	(4S,5S,8S,10R)-4,5,8-trihydroxy-10-methyl-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one		C10 H16 O5	5.575	216.0993
c523	Syringolin H		C25 H43 N5 O6	4.16	509.32028
c1781			C19 H30 O8 P2	11.981	448.14141
c3932			C15 H29 N5 O4	3.838	343.22013
c191	NP-003672		C15 H14 O2	5.025	226.0947
c4103	Methyl N-[[[(2S)-1-(cyclohexylcarbonyl)-4-(isopropylcarbamoyl)-2-piperazinyl]carbonyl]-3-(3-pyridinyl)-D-alaninate		C25 H37 N5 O5	2.776	509.26057
c273				7.639	525.80834
c4655			C69 H109 N8 O17 P3	6.972	1414.71233
c221	2-(4-Methoxybenzylidene)quinuclidin-3-one		C15 H17 N O2	5.028	243.12118
c1481	13-methoxy-1,6-diazatetracyclo[7.6.1.0âµ.0âµ]hexadeca-3,5,7,9(16),10,12,14-heptaen-2-one		C15 H10 N2 O2	3.725	500.14991
c54			C38 H59 N9 O10	3.38	801.43698
c2908			C55 H85 N6 O15 P S	9.131	1132.55273
c3908	2-[[[1-ethyl-1H-1,2,3,4-tetraazol-5-yl)sulfanyl]-1-(4-phenylpiperazino)-1-ethanone		C15 H20 N6 O S	6.845	664.28907
c1467			C58 H97 N3 O16 P2	2.31	1153.63371

c236	N-(5-acetamidopentyl)acetamide		C9 H18 N2 O2	1.106	208.12058
c239	Glutisine A		C11 H19 N3 O2	1.112	225.14725
c201	2-(4-Methoxybenzylidene)quinuclidin-3-one		C15 H17 N O2	5.026	729.36369
c1840	Azithromycin		C38 H72 N2 O12	6.934	786.46004
c3681			C24 H53 N9 O16 P2	4.907	785.30725
c2662			C31 H55 N7 O8	3.108	653.40924
c648			C40 H58 N6 O9 P2	3.425	828.37475
c1632	8-hydroxy-deoxyguanosine		C10 H13 N5 O5	1.173	283.09088
c3713			C13 H23 P S	4.278	242.12607
c4489			C6 H19 Cl N6 O2	4.283	242.12596
c2952	N-[(1R,9S)-11-(4-Fluorobenzyl)-6-oxo-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-5-yl]isonicotinamide		C24 H23 F N4 O2	4.616	418.18256
c2627			C67 H115 Cl N5 O18 P S2	14.919	1407.71177
c295			C48 H85 N6 O13 P3	7.545	1046.53838
c587			C43 H62 N10 O12	8.359	910.45466
c3360	Taichunin C		C25 H36 O10	3.42	496.23131
c2728			C17 H40 N3 O6 P S	1.507	445.23532
c1888			C32 H67 N10 O8 P3	4.289	812.43586
c3826			C19 H30 O8 P2	11.984	448.14283
c237	11-Aminoundecanoic acid		C11 H23 N O2	1.032	201.17237
c1310			C27 H53 N3 O14 P2	5.872	705.29974
c3686			C14 H30 N7 O3 P	8.2	375.21646
c2256			C23 H51 N6 O12 P3	6.996	696.27833
c235			C30 H61 N O11 P2	5.027	673.37512
c2146			C57 H102 N7 O17 P3 S	3.721	1281.62686
c3017				7.126	1096.52503
c743	Citroflex A-4		C20 H34 O8	15.776	402.22434
c536	Biotin		C10 H16 N2 O3 S	1.721	244.08763
c2924	PEG Diethylhexanoate n5		C26 H50 O8	2.824	512.3311
c3079			C37 H56 N8 O8 P2	2.266	802.36904
c658			C19 H29 N7 O5	2.586	435.22215
c875				7.638	1410.59529
c1178			C46 H77 N10 O10 P3	6.66	1022.50357
c1673			C29 H67 N9 O16 P2	6.727	859.41998
c29	Cl-4		C11 H19 N5 O2	1.266	253.15321
c184			C15 H27 N O5	2.501	301.18829
c1216				6.134	701.73617
c4836			C15 H25 N5 O4	1.56	339.19008
c1479	3-(tert-Butyl)-N-[4-(2,3-dihydroimidazo[2,1-b][1,3]thiazol-6-yl)phenyl]-1-methyl-1H-pyrazole-5-carboxamide		C20 H23 N5 O S	4.634	381.16939
c1712	4,4-dimethyl-1-(3-nitrophenyl)-2-(1H-1,2,4-triazol-1-yl)pent-1-en-3-one		C15 H16 N4 O3	1.235	300.12128
c2027			C22 H51 N3 O5 P2 S	6.234	531.30516
c3616	Community Metabolite	A;B	C54 H97 N9 O16	14.868	1127.70285
c2048				5.037	1378.69724
c1900			C20 H37 N5 O7	2.237	459.26835
c350			C58 H90 N2 O16 P2	3.015	1132.57551
c2352			C36 H51 N5 O2 P2 S2	4.098	711.2965
c96			C20 H35 N5 O6	2.418	441.25798
c1419			C53 H93 N6 O16 P3	3.207	1162.58623
c2382			C10 H25 N7 O4	1.204	307.19844
c3116			C21 H35 N5 O8	2.215	485.24733
c307				5.017	336.68772
c4697			C10 H8 O9 P2 S4	0.721	461.85338
c2491				7	1590.70775
c1088	1-[(2R,4S,5R)-5-(3-Cyclohexyl-1-methyl-1H-pyrazol-5-yl)-1-azabicyclo[2.2.2]oct-2-yl]-N-(4-methoxybenzyl)methanamine		C26 H38 N4 O	6.199	920.52976
c4723			C8 H15 N6 O6 P S	0.73	354.04955
c1512			C15 H23 N5 O2 S2	6.069	369.12776
c3367				7.636	2473.22037
c83			C14 H25 N O3 S	8.41	287.15504
c2737				7.261	1526.81439
c3618			C59 H85 N6 O17 P	2.681	1180.57089
c2067			C16 H27 N3 O8	1.844	389.1792
c3383			C18 H44 N9 P S3	5.561	513.26238
c2430			C7 H3 N6 P3 S2	19.756	327.90855
c1854			C61 H69 N8 O P3	7.213	1022.48341
c857			C14 H29 N5 O4 S	2.479	363.19313
c46	5,6-diphenyl-2,3-dihydropyrazine		C16 H14 N2	1.033	234.11107
c879			C19 H38 N2 O3	12.161	342.28866
c2921	Abbeymycin		C13 H16 N2 O3	3.424	248.11562
c2448			C7 H15 N4 P S	0.722	218.07509
c4827	(1R,9S)-5-(1-Benzothiophen-2-yl)-11-(cyclohexylcarbonyl)-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one		C26 H28 N2 O2 S	13.153	470.13696
c1509	Cyclotine		C24 H33 N5 O7	2.435	503.23683
c3449			C25 H34 N6 O5	2.549	498.25797
c281			C40 H64 N9 O6 P3	6.303	859.41902
c172	Thiamine		C12 H16 N4 O S	0.722	264.10372
c995	Oxibendazole		C12 H15 N3 O3	2.246	249.10836
c4066	Paroxetine		C19 H20 F N O3	2.001	329.14603
c3970			C28 H37 N10 O6 P	4.222	640.26363
c3147				3.425	1015.51946
c3994	NP-022373		C23 H25 N O2	1.206	329.18058
c2070			C50 H76 N4 O14 P2	4.556	1018.48313
c1455			C34 H68 N3 O18 P	3.015	837.42226
c694			C46 H83 N6 O12 P3	7.855	1004.52926
c2100			C23 H32 N7 O6 P	5.701	533.21576
c1699				5.257	908.43619
c2130			C25 H48 N6 O4 P2	2.718	558.31929
c3127			C27 H45 Cl N6 O3 P2	4.562	598.27178

c1738		C37 H69 N8 O13 P3	8.358	926.41979
c1596	Hirsutellone C	C28 H31 N O5	5.029	461.22112
c3059		C22 H41 N7 O5	2.807	483.31591
c3898	4-[(Dimethylamino)methylidene]-1-phenyl-3-(trifluoromethyl)-4,5-dihydro-1H-pyrazol-5-one	C13 H12 F3 N3 O	3.016	283.09245
c1761		C22 H43 N5 O	16.174	393.34456
c1210		C67 H91 N6 O14 P	8.244	1234.63335
c115		C29 H46 N10 O9	2.581	678.34384
c3667	N-{4-[(2R,3R)-3-(Hydroxymethyl)-5-oxo-2-morpholinyl]phenyl}-3-methylbutanamide	C16 H22 N2 O4	2.313	288.14656
c4694		C13 H38 N9 O5 P	4.715	431.27284
c1050		C21 H41 N7 O10 S	5.451	583.26359
c2811		C15 H25 N3 O6	1.88	343.17397
c1956		C11 H21 N5 O2	1.45	255.16872
c1192		C24 H53 N9 O12 P2	5.544	721.3304
c2090	pro-his	C11 H16 N4 O3	1.544	252.12187
c70		C50 H78 N8 O8 P2 S	3.34	1012.51456
c297	Fluvirucin B6	C26 H48 N2 O6	3.104	484.35003
c361		C40 H87 N8 O12 P3 S2	2.22	1028.50976
c4475		C51 H105 N4 O18 P3 S2	5.151	1218.60776
c2202		C30 H69 N7 O14 P2	9.018	813.43692
c945		C23 H56 N9 O8 P3	2.513	679.34586
c2548		C41 H73 N10 O15 P3	7.203	1038.448
c3311	NP-002336	C23 H36 O5	1.32	430.20528
c3304		C25 H45 N	16.188	359.35426
c1246		C11 H21 N3 O2	1.213	227.16287
c1787		C32 H67 N6 O15 P	1.824	806.43906
c3252	Cathestatin B	C17 H23 N3 O6	2.003	365.15817
c584		C34 H54 N5 O4 P3	5.027	689.33996
c3319		C78 H125 N10 O16 P3 S2	9.119	1614.7941
c541		C27 H40 N3 O3 P S	5.7	517.25081
c843		C28 H60 N7 O13 P3	6.997	795.34624
c126		C30 H47 N7 O8	3.092	633.3471
c3296	TQH	C15 H24 N6 O6	8.461	384.16916
c1201			2.334	290.65811
c3528		C10 H16 N4 O13 P2	0.718	462.0177
c2721		C22 H32 N10 O4	2.096	500.2585
c2223		C32 H63 N5 O6	15.947	613.47485
c983	N-{[(2R,4S,5R)-5-(1-Methyl-3-phenyl-1H-pyrazol-5-yl)-1-azabicyclo[2.2.2]oct-2-yl]methyl}methanesulfonamide	C19 H26 N4 O2 S	5.834	792.33171
c4346	Avaroferrin	C17 H30 N4 O6	1.737	386.21553
c3697	L-Arginyl-L-arginyl-L-arginine	C18 H38 N12 O4	2.269	486.31515
c3888		C38 H73 N9 O12 S3	5.138	943.45323
c4120	2-[(2-chlorobenzyl)sulfanyl]-4,6-dimethylnicotinonitrile	C15 H13 Cl N2 S	12.862	326.00038
c2854		C13 H39 N9 O8 P2	7.217	511.24162
c494		C26 H43 N7 O8	2.329	581.31618
c1033	EKK	C17 H33 N5 O6	1.239	385.23137
c2358		C26 H43 O6 P3	4.194	544.22756
c312		C26 H40 N6 O7	1.239	548.29397
c3020	Zolpidem	C19 H21 N3 O	2.008	307.16403
c77		C61 H83 N8 O12 P	3.016	1150.58597
c170	PPK	C16 H28 N4 O4	1.223	340.21011
c4648		C78 H116 N7 O13 P3 S2	8.579	1515.72849
c2468			6.394	1174.59078
c686			7.646	560.77422
c3294		C28 H41 N7 O10 S	4.199	667.26265
c1301		C29 H46 N4 O6 P2	1.66	608.2904
c1146		C21 H51 N7 O5	16.085	481.39677
c3376		C13 H27 N9 O8	2.111	437.19854
c3321	MDMB-CHMICA	C23 H32 N2 O3	4.455	1218.65519
c464		C60 H84 N O17 P	7.624	1121.54862
c419		C71 H97 N8 O15 P3	7.639	1394.62788
c2629	4-Benzoylbiphenyl	C19 H14 O	2.852	258.1074
c264			3.087	316.67354
c1123	N'-Allyl-N-(2-cyanoethyl)-N-cyclohexylthiourea	C13 H21 N3 S	1.265	251.14579
c2828	Ilanefuranone	C21 H38 O3	15.649	338.2813
c902	[(3R,4S)-1-(4-Morpholinylcarbonyl)-3-(2-{4-[3-(trifluoromethyl)phenyl]-1-piperazinyl}ethyl)-4-piperidiny]acetic acid	C25 H35 F3 N4 O4	5.55	512.26015
c405		C22 H53 N9 O10 P2 S	7.628	697.31359
c215		C25 H44 N6 O6	1.222	524.33049
c413		C20 H28 N4 O7	2.172	436.19511
c324		C35 H55 N9 O10	2.189	761.40581
c1754	(R)-3-Hydroxy myristic acid	C14 H28 O3	13.405	226.19273
c1297		C17 H45 N10 O10 P	6.554	580.30532
c1423		C23 H35 N7 O7	1.296	521.25804
c3054	Oxibendazole	C12 H15 N3 O3	2.709	249.10858
c4095		C18 H37 N4 O6 P	2.135	436.24282
c275		C64 H97 N7 O15 P2 S	3.138	1297.62123
c918		C25 H39 N5 O6 P2	7.124	567.23576
c2971	Zolpidem	C19 H21 N3 O	1.998	614.3281
c2345		C14 H29 N O2	13.612	243.21928
c4394	Microcyclamide MZ568	C25 H40 N6 O7 S	4.772	568.27007
c481			1.227	274.14745
c3670	3-amino-2,6-diphenyl-4,7-dihydro-2H-pyrazolo[3,4-d]pyrimidin-4-one	C17 H13 N5 O	0.715	303.10867
c166	N-cyclohexyl-N'-(2-fluorobenzyl)urea	C14 H19 F N2 O	1.287	250.14267
c338		C36 H60 N7 O6 P3	6.965	779.38114
c1174		C19 H47 N7 O4	16.128	437.37067
c3119	Oxibendazole	C12 H15 N3 O3	2.708	498.21683
c417		C29 H44 N8 O11	5.615	680.31304

c2670		C18 H45 N7 O4	15.561	423.35505
c341		C33 H46 N8 O2 P2	6.943	648.32442
c1783			1.657	304.14501
c2773		C32 H63 N O2 P2	15.436	555.43321
c2380		C25 H49 N5 O3	15.521	467.38126
c4158	Decarbamoyl-neosaxitoxin	C9 H16 N6 O4	2.134	544.24896
c1153		C23 H55 N7 O6	16.04	525.42278
c1439	ethyl 2-[(4-methyl-2-oxo-2H-chromen-8-yl)oxy]acetate	C14 H14 O5	1.793	262.08851
c772	Piptamine	C23 H41 N	15.401	331.32298
c2331		C22 H53 N7 O6	15.479	511.40737
c1567	NP-020706	C14 H22 O7	1.321	319.16361
c3642	[Similar to: PEG n10; ?Mass: 141.1865 Da]	C26 H61 N7 O8	15.393	599.45921
c1919		C23 H51 N3 O18	5.316	657.31673
c320	N-cyclohexyl-N'-(2-fluorobenzyl)urea	C14 H19 F N2 O	1.336	250.14275
c1240			2.136	1029.51238
c1382		C33 H65 N O2 P2	15.993	569.44884
c125	Prolylleucine	C11 H20 N2 O3	5.245	228.14691
c179			3.265	1013.51703
c268		C19 H49 N10 O8 P	5.359	576.34485
c278		C25 H49 N10 O3 P3	4.26	630.31804
c376		C18 H32 N4 O5	4.469	384.23644
c388			8.255	889.47642
c425			6.941	759.40491
c442		C24 H53 N6 O7 P3	4.285	630.31753
c503			6.327	1135.65904
c511			7.659	1026.56508
c554	Koreenceine C	C14 H27 N O	8.945	225.20903
c564	terlakiren	C31 H48 N4 O7 S	4.585	620.32376
c573			5.511	920.47021
c706			5.523	574.30836
c729			5.377	1380.70431
c741		C22 H57 N10 O10 P	5.2	652.39714
c775		C33 H52 N2 O6 P2	5.744	634.33176
c794		C23 H50 N9 O11 P	5.681	659.33481
c831		C24 H49 N4 O8 P	5.564	552.32622
c883			7.35	1505.82991
c914		C18 H45 N5 O3 P2 S	6.775	473.27191
c924			5.446	563.28135
c948		C27 H39 N5 O6	7.524	529.28882
c950	1-Tetrahydro-1H-pyrrol-1-yl-3-[3-(trifluoromethyl)-1H-pyrazol-1-yl]propan-2-ol	C11 H16 F3 N3 O	2.859	263.12426
c956		C21 H48 N10 O16	4.032	696.32701
c958			6.46	1891.01381
c968		C32 H60 N7 O6 P3 S	0.81	763.35538
c985			4.336	1324.63174
c994		C45 H103 N8 O16 P3 S	6.346	1136.64368
c999		C21 H55 N10 O11 P	5.778	654.37873
c1006			5.395	427.71605
c1014	NP-022076	C25 H34 O4	4.67	840.4687
c1034			4.03	675.34745
c1063		C20 H31 N3 O4	6.117	377.23068
c1071	Furanodictine A	C13 H21 N O6	0.728	287.1358
c1083		C73 H93 N O17 P2	2.127	1317.59187
c1085		C40 H84 N7 O P3 S3	8.125	867.5118
c1092		C31 H67 N8 O16 P	6.507	838.44123
c1103			7.067	462.74498
c1120		C59 H96 N10 O9 P2	5.493	1150.68419
c1126			5.365	1380.70498
c1128		C19 H25 N3 O4	5.137	359.18422
c1129			7.364	994.45332
c1141	Incarnatapeptin A	C35 H58 N8 O12	4.342	782.42006
c1145			5.033	749.36797
c1171	Bacilosarcin A	C24 H33 N3 O8	6.599	491.22862
c1189		C19 H37 N8 O4 P	7.224	472.2691
c1195	XR586	C91 H138 N20 O23	7.071	1879.02636
c1206			4.572	974.48675
c1214		C19 H27 N3 O6	6.225	393.18992
c1263			5.771	976.48349
c1303		C59 H98 N7 O18 P3 S	0.793	1317.59047
c1309		C27 H62 N10 O10 P2 S	6.933	780.385
c1384			3.209	1152.59225
c1394		C24 H33 N5 O6	4.152	487.24198
c1418		C45 H68 N3 O6 P	1.074	777.48342
c1459		C43 H71 N9 O10 S2	7.62	937.47713
c1468		C34 H64 N6 O11 P2	7.092	794.4102
c1491		C21 H54 N7 O10 P3	5.168	657.31626
c1513		C13 H34 N10 O7	2.309	442.26097
c1517		C24 H55 N3 O4 P2 S2	6.13	575.30988
c1537	Destruxin A	C29 H47 N5 O7	5.309	577.34744
c1556		C39 H79 N5 O11 S3	8.134	889.49459
c1582		C45 H75 N9 O17	4.501	1013.52769
c1620	pro-his	C11 H16 N4 O3	1.523	252.12191
c1640			0.942	260.6289
c1647		C24 H42 N3 O7 P	5.66	515.27699
c1672			7.99	983.55364
c1707		C25 H44 N6 O7	5.698	540.3267

c1708	5,6-diphenyl-2,3-dihydropyrazine	C16 H14 N2	1.288	234.11112
c1714			5.028	651.0824
c1719			7.501	1105.54862
c1739		C11 H31 N9 O6	4.448	385.24012
c1757			7.547	1105.557
c1779			7.26	1264.6541
c1780		C18 H36 N10 O3 S	6.211	472.27114
c1786		C78 H132 N7 O18 P3 S	5.849	1579.85471
c1803		C23 H51 N7 O9 P2	4.267	631.32116
c1823		C14 H36 N9 O5 P	2.714	441.25808
c1838			4.43	718.36917
c1890		C18 H10 N7 O5 P3 S	7.127	528.96711
c1960		C22 H57 N10 O12 P	5.623	684.38742
c1982		C31 H51 N3 O13	4.455	673.34063
c2016			6.949	628.35054
c2063			5.035	651.70613
c2069			6.834	1079.59518
c2078			7.141	529.61214
c2105		C42 H89 N10 O18 P S2	6.503	1116.55536
c2123		C36 H50 N10 O3	8.696	670.40795
c2125		C54 H107 N2 O18 P S	5.034	1134.69773
c2152			4.949	864.46968
c2154		C38 H78 N9 O11 P3 S2	7.481	993.44955
c2158		C33 H55 N9 O5 P2	4.461	719.38127
c2218		C53 H105 N7 O4	19.616	903.82292
c2227			5.022	651.71154
c2232		C30 H72 N9 O15 P	5.022	829.48896
c2237		C21 H14 N3 O4 P3 S2	7.108	528.96337
c2245			8.314	1940.03206
c2246	NP-012766	C31 H46 N4 O7	3.82	1248.58234
c2249	VLK	C17 H34 N4 O4	3.2	340.24664
c2251	Dodecamethylcyclohexasiloxane	C12 H36 O6 Si6	19.411	444.11193
c2255		C18 H34 N9 O5 P	2.972	487.24185
c2268			5.618	864.47348
c2303			7.964	984.5553
c2312			4.537	814.43172
c2316		C40 H66 N5 O5 P	5.838	727.48373
c2319			7.332	2168.07297
c2322			7.632	2043.91323
c2327			5.729	392.21653
c2334			4.394	1325.63525
c2342		C37 H65 N9 O9	3.942	779.4896
c2367			4.789	720.37879
c2377		C18 H38 N5 O3 P S	8.135	435.24309
c2385			7.124	529.61808
c2390			5.033	651.83816
c2393		C40 H62 N6 O11 P2	7.059	864.39465
c2429		C21 H24 N8 O13	1.255	596.14736
c2436			13.16	1968.869
c2437		C64 H89 N4 O9 P3	1.04	1150.58553
c2498			7.072	2067.99862
c2504		C25 H7 N O11 S	7.127	528.97451
c2530			5.027	651.69974
c2532		C29 H58 N5 O9 P	5.722	651.3947
c2535		C30 H45 N O4 P2	5.342	545.28451
c2545			6.756	2068.00086
c2551		C12 H32 N7 O7 P	5.387	417.20907
c2579			6.605	1807.96621
c2602			8.658	1451.7927
c2613			8.662	1323.73532
c2623		C23 H52 N5 O4 P3 S	6.859	587.29703
c2631	3-[(4-hydroxyphenyl)methyl]-octahydropyrrolo[1,2-a]pyrazine-1,4-dione	C14 H16 N2 O3	4.092	260.11521
c2637			5.085	1382.70056
c2639			5.036	651.07761
c2649		C25 H44 N6 O7	5.1	540.32618
c2660		C35 H57 N7 O11	3.977	751.41072
c2663		C48 H90 N9 O12 P S2	6.857	1079.5896
c2669		C85 H137 N10 O9 P3 S5	7.631	1694.83984
c2685		C53 H99 N4 O13 P3 S	8.514	1124.61551
c2703		C43 H89 N4 O14 P3	7.332	978.56129
c2722		C42 H80 N6 O18	4.963	956.55277
c2723			15.116	1371.32082
c2753		C25 H28 N5 O8 P3 S	5.026	651.08925
c2758			6.337	1137.65097
c2774			8.658	1450.79221
c2824			5.468	1251.62636
c2838			15.123	2747.53112
c2849			7.111	529.60597
c2851		C39 H70 N10 O8 S3	6.989	902.45424
c2869		C29 H61 N7 O6 S4	6.321	731.35584
c2872	{2,3-Bis[(E)-2-(1,3-benzodioxol-5-yl)vinyl]-4-(1-piperidinylcarbonyl)cyclobutyl}(1-pyrrolidinyl)methanone	C33 H36 N2 O6	3.303	556.25931
c2881		C9 H16 Br2 Cl3 N2 O3 P3 S3	5.03	651.69666
c2899		C53 H113 N10 O10 P S	17.296	1112.81003
c2929	Kitacinnamycin H	C56 H80 N10 O12	7.798	1084.59999
c2946		C26 H46 N5 O10 P S	5.045	651.26997

c2948			C29 H48 N7 O4 P3	4.221	651.29743
c2950				0.768	1216.52961
c2951			C26 H62 N9 O3 P3	4.831	641.42137
c2953				4.286	384.43865
c2961			C20 H27 N7 O12 P2 S	5.02	651.09136
c2963			C25 H64 N10 O14 P2	7.782	790.4097
c2978			C45 H65 N10 O7 P	9.339	888.47696
c2986				4.627	310.16182
c2998			C20 H44 N5 O10 P	5.331	545.28472
c3033				4.293	768.87242
c3048			C31 H64 Br N5 O8 S	5.175	745.36388
c3082				6.854	1079.6021
c3087			C29 H42 N O7 P	5.253	547.26678
c3091				5.819	877.56822
c3108				5.024	651.82488
c3111				6.775	2299.08083
c3122				6.829	1080.60499
c3126			C44 H73 N7 O5	19.683	779.56658
c3133	(2S,3R,4E)-2-[(13Z)-13-Docosenoylamino]-3-hydroxy-4-octadecen-1-yl 5-acetamido-6-[(1S,2R)-2-({5-acetamido-6-[(1S,2R)-2-({5-acetamido-3,5-dideoxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]-beta-L-threo-hex-2-u;lopyranonosyl)oxy)-1,3-dihydroxypropyl]-3,5-dideoxy-beta-L-threo-hex-2-ulopyranonosyl)oxy)-1,3-dihydroxypropyl]-		C111 H189 N5 O55	7.632	2472.21481
c3139			C55 H94 N8 O11 P2	4.35	1104.6519
c3153			C15 H19 N2 O2 P3 S	4.292	384.03732
c3162				5.045	651.83074
c3198			C16 H12 N5 O10 P S2	7.103	528.97673
c3201			C26 H26 N3 O11 P S2	5.026	651.07403
c3202			C51 H82 N7 O16 P S	5.199	1111.52799
c3209			C49 H100 N4 O13 P2 S2	5.662	1078.62013
c3242			C19 H10 N5 O6 P3 S	7.116	528.95794
c3245			C22 H45 N4 O2 P3	5.388	490.27742
c3251			C88 H132 N3 O18 P S4	7.628	1677.81212
c3257			C21 H46 O7 P2	7.131	472.2697
c3259			C63 H95 N5 O10 P2 S	8.413	1175.62802
c3263				5.361	509.76416
c3274			C45 H88 N4 O14 P2	4.1	970.57839
c3289				5.651	682.38938
c3290			C29 H48 O11 S	4.636	604.293
c3300			C49 H90 N5 O18 P S	7.813	1099.57358
c3310				7.633	1700.79819
c3312				15.117	5468.26085
c3330			C69 H119 N8 O3 P3	17.219	1200.86216
c3334				6.949	2084.99666
c3339			C25 H40 N2 O2	0.786	400.30949
c3342				6.45	1136.6655
c3356			C55 H87 N10 O11 P3	7.449	1156.57604
c3357			C13 H27 N8 O4 P	3.66	390.18943
c3359				8.679	1322.73447
c3382	Bis(2-ethylhexyl) terephthalate		C24 H38 O4	15.224	390.27493
c3395	(2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-(2-phenylethoxy)oxane-3,4,5-triol		C14 H20 O6	5.016	306.10738
c3404	(2R)-2-[(9Z,12Z)-9,12-Hexadecadienoyloxy]-3-[(hydroxy{[(1S,5S)-2,3,6-trihydroxy-4,5-bis(phosphonooxy)cyclohexyl]oxy}phosphoryl)oxy]propyl stearate		C43 H81 O19 P3	7.302	994.46156
c3408			C55 H54 N10 O13 P2	8.28	1124.33511
c3409				7.621	1264.6229
c3414			C56 H59 N9 O4	5.501	921.46982
c3415	UR-144 N-Heptyl analog		C23 H33 N O	4.545	339.2517
c3418			C88 H119 N8 O12 P3	5.129	1572.81546
c3420			C22 H38 Cl2 N6 O2	5.907	488.24404
c3429			C16 H35 N5 O3 P2	4.375	407.219
c3441			C40 H72 N10 O9 P2 S	3.462	930.46668
c3447			C34 H73 N8 O12 P	5.88	816.50975
c3463			C6 H19 N4 O9 P3	4.286	384.03554
c3470	(1'S,2R,2'S,4a'S,5'S,6'S,6a'R,7a'S,9'R,10a'R,11a'S,12'S,13a'R,14a'S,15'Z,17a'R,18a'S,19a'R,20a'S,25a'R,26'R,26a'S,27a'R,29a'S,30a'R,32'E,34a'S,35a'R,36a'S,37a'R,38a'S,39a'R)-1',2',4,4a',5,5',6',6a',7a',8',9',10',10a',11a',12',13',13a',14a',17',17a',18a',19',19a',20a',21',24',25a',26',26a',27a',29a',30a',31		C57 H82 O16	6.515	1022.559
c3487			C15 H20 Br3 N4 O4 P S2	5.027	651.82133
c3488				7.115	529.60223
c3492			C26 H33 N O	16.42	375.25511
c3495			C28 H58 N10 O9 P2	6.457	740.38532
c3505			C68 H138 N2 O17 P2	18.261	1316.94675
c3509			C69 H89 N7 O16 P2	0.791	1333.58503
c3526			C21 H52 N9 O6 P3	4.638	619.32329
c3542				7.031	689.85881
c3546			C26 H54 N8 O17	4.846	750.36003
c3549			C35 H60 N6 O14	3.599	788.41629
c3554			C54 H104 N9 O17 P S	5.085	1213.7009
c3577				6.987	1248.65366
c3581				5.351	748.36563
c3584				5.026	651.71551
c3608			C24 H10 N3 O4 P3 S	7.129	528.96093
c3619				15.123	5469.2682
c3637			C28 H56 N2 O13 S	6.266	660.35085
c3640				0.792	1318.57935
c3647			C32 H67 N8 O11 P S	3.538	802.43948
c3653				0.796	234.01605
c3659			C58 H101 N5 O15 P2	4.674	1169.67616
c3689			C30 H70 N9 O2 P	7.05	619.53661
c3699				8.523	1125.61713
c3709	Janthinocin C		C57 H82 N12 O15	6.897	1174.59824
c3731			C77 H95 N10 O15 P	7.52	1430.6716
c3741			C58 H127 N9 O5 P2 S	8.306	1123.91673

c3752			C30 H70 N8 O13 P2 S	7.088	844.42536
c3773	Muraymycin B1		C49 H83 N11 O18	5.404	1113.59685
c3775			C37 H75 N10 O18 P	6.329	978.49979
c3781				6.969	2083.99264
c3784			C30 H63 N2 O17 P	5.988	754.38559
c3795			C21 H23 N9 O3 P2 S2	5.457	575.08327
c3796				5.023	651.84392
c3810			C30 H73 N10 O13 P	7.03	812.51032
c3818			C41 H90 N8 O3 P2 S5	4.955	964.52109
c3820				7.124	1610.85298
c3839	Amichalasine A		C57 H72 N2 O12	7.643	976.50741
c3853	MPK		C16 H30 N4 O4 S	5.021	748.40812
c3857			C38 H52 N6 O2 S	7.809	656.38915
c3878			C54 H110 N2 O11 P2	17.376	1024.75864
c3880				6.6	1808.9703
c3885				7.121	1857.81253
c3886			C31 H56 N9 O9 P S	0.804	761.36526
c3889			C66 H113 N10 O11 P3 S	5.023	1346.75237
c3910				5.538	1866.91952
c3915	Micropeptin T2		C52 H73 N9 O12	3.657	1015.53446
c3928	[Similar to: HPH; ?Mass: -154.9755 Da]		C10 H26 N4 O2	0.79	234.20569
c3938				0.79	419.21257
c3942			C29 H61 N5 O11 S	5.147	687.40628
c3953			C22 H41 N O11	5.855	495.26839
c3965			C11 H12 N8 O4 S2	4.286	384.04195
c3967				8.306	1941.03628
c3978			C36 H67 N2 O8 P S	4.517	718.43537
c3979			C39 H77 N O	5.431	575.60071
c3982			C26 H58 N10 O14 S	4.273	766.38353
c3986				5.617	864.47397
c3993			C35 H36 N2 O3	16.225	532.2722
c3999				7.101	2952.35607
c4003			C59 H104 N4 O12 S3	5.033	1156.6812
c4010	Leupyrrin C		C40 H56 N2 O10	7.087	724.39672
c4011	[Similar to: 2-hydroxy-6-[4-hydroxy-2-methoxy-6-(methoxycarbonyl)phenoxy]-4-methylbenzoic acid; ?Mass: 424.6869 Da]			13.168	772.7714
c4014			C32 H67 N7 O11 P2	5.649	787.43558
c4049			C16 H31 N3 O5	5.307	345.22565
c4058			C45 H78	4.501	618.60802
c4061			C59 H111 N8 O14 P3	7.113	1248.74279
c4069			C40 H69 N3 O10 P2	4.922	813.44438
c4080				4.289	384.43612
c4086				0.798	839.96183
c4110				13.158	1583.68723
c4134			C14 H27 N O2	8.02	241.20424
c4140			C27 H43 N7 O4 S	5.549	561.31249
c4153			C37 H74 N5 O17 P	8.286	891.48264
c4168				3.844	1283.63357
c4172				4.279	384.43201
c4179			C75 H78 N4 O3	5.079	1082.60758
c4185				7.528	1022.88219
c4196			C27 H8 N7 O8 P3	5.017	650.9644
c4197				0.799	1024.5141
c4211				13.167	1582.69533
c4221			C27 H32 N3 O6 P3 S2	5.023	651.09527
c4222	[Similar to: 2-hydroxy-6-[4-hydroxy-2-methoxy-6-(methoxycarbonyl)phenoxy]-4-methylbenzoic acid; ?Mass: 38.3047 Da]			13.175	386.38921
c4223			C57 H112 N3 O13 P3 S2	5.039	1203.68372
c4233				5.553	864.47391
c4241				8.37	1147.61728
c4246				5.424	575.59685
c4248				5.056	325.54644
c4251			C31 H67 N10 O10 P	9.106	770.47789
c4258	Bis(2-ethylhexyl) terephthalate		C24 H38 O4	19.952	390.27688
c4281			C37 H81 N8 O6 P3 S2	0.793	890.49413
c4293			C32 H66 N9 O16 P S2	4.087	927.38102
c4307				5.076	855.92319
c4316			C21 H40 N8 O2 S	0.775	468.29874
c4317				7.34	1263.63599
c4324				6.962	1565.80083
c4337			C28 H62 N6 O18 P2	5.582	832.35896
c4340			C38 H60 N3 O9 P3	6.948	795.35503
c4350				7.118	529.62238
c4356	[Similar to: HPH; ?Mass: -154.9749 Da]		C10 H26 N4 O2	0.786	234.20621
c4357			C25 H17 N8 O4 P3 S	4.511	618.03024
c4361				4.292	768.07358
c4364				15.117	2730.55332
c4384			C84 H120 N O18 P3	4.967	1523.77181
c4393				5.735	491.28292
c4395			C34 H38 N6 O6 S	4.822	658.25707
c4397			C23 H50 N9 O9 P	7.07	627.34404
c4399				7.143	2563.41059
c4401			C90 H111 N8 O7 P S5	7.584	1606.69175
c4419			C51 H66 N3 O10 P	4.849	911.44826
c4420				6.121	2271.31856
c4438				7.619	2045.91733
c4439			C53 H90 N2 O14 P2	5.393	1040.58708

c4469			C45 H73 N7 O5	19.682	791.56761
c4470			C11 H25 N5 O4	0.743	291.1902
c4476			C64 H94 N2 O13 P2 S	3.757	1192.59555
c4482				0.815	839.95198
c4483			C35 H52 O7 S2	5.478	648.31676
c4487			C72 H87 N O10 P2	7.534	1187.58017
c4494				5.057	1528.73379
c4501			C52 H62 N4 O18 P2 S	8.275	1124.32578
c4503			C26 H14 N6 O9 S2	4.503	618.02677
c4514			C25 H55 N3 O11 P2	7.15	635.33165
c4521			C41 H68 N8 O7	19.683	784.5219
c4523	Biotin		C10 H16 N2 O3 S	1.401	244.08791
c4524			C14 H24 N6 O3	10.88	324.19109
c4530			C61 H93 N8 O16 P S	8.24	1256.61676
c4532			C26 H62 N7 O8 P3	8.444	693.38933
c4536			C32 H58 N9 O6 P S	6.249	727.39983
c4541				6.711	2169.07064
c4550			C42 H69 N3 O7 P2 S	8.188	821.43497
c4554			C31 H74 N10 O2	4.529	618.60166
c4556			C13 H24 Br2 Cl N4 O4 P S4	5.021	651.84761
c4558			C21 H3 N10 O2 P S	5.549	489.99037
c4571				6.882	1851.93453
c4572			C41 H73 N10 O17 P S4	6.143	1136.37766
c4596			C16 H35 N9 O2 S2	4.054	449.23454
c4624			C41 H60 N7 O6 P S	0.805	809.40464
c4647				4.506	618.0344
c4657			C21 H44 N9 O P S2	5.053	533.28437
c4660				4.98	498.75212
c4666			C48 H73 N3 O4 S4	8.408	883.44744
c4667			C24 H28 N5 O2 P3 S2	5.443	575.09079
c4668				7.291	2037.03567
c4673			C21 H51 N7 O11 S	6.372	609.33537
c4691			C23 H52 N3 O9 P	5.746	545.34227
c4705				0.795	1029.51696
c4719			C33 H59 N4 O8 P	8.748	670.40813
c4725			C25 H18 N7 O6 P S	5.443	575.07798
c4729			C34 H80 N9 O16 P3 S	4.478	995.46452
c4730			C51 H73 N2 O4 P S2	1.267	872.47609
c4733			C49 H83 N6 O12 P3	4.476	1040.52769
c4741				6.936	1938.96493
c4743			C48 H59 N O3 S	5.153	729.42485
c4764	Bis(2-ethylhexyl) terephthalate		C24 H38 O4	5.36	390.27586
c4766			C39 H81 N8 O11 P S2	7.608	932.52098
c4768			C6 H6 N2 O8	0.799	234.01251
c4769				7.003	757.79087
c4771			C20 H41 N10 O10 P3	4.822	674.22192
c4784	Septentrionine		C38 H54 N2 O11	6.143	714.37554
c4793				4.303	768.86557
c4797			C26 H23 N7 O P2 S2	5.472	575.08695
c4799			C57 H108 N10 O13 P2 S	7.129	1234.7291
c4802				5.838	2176.12412
c4803			C50 H110 N5 O16 P3 S4	6.308	1257.60422
c4816				7.109	529.6245
c4819			C9 H N8 O16 P	4.988	507.92406
c4825				5.756	1581.71718
c4843			C61 H129 N10 O14 P S	17.138	1288.91465
c4850			C79 H125 N9 O16 P2 S3	4.993	1613.78811
c4862			C65 H137 N10 O15 P S	18.226	1360.97251
c4887			C29 H61 N5 O4 S	5.43	575.44541
c4903	F1839-B		C24 H33 N O6	12.44	431.23158