

Sample Information

 Sample Name
 shell_1

 Sample ID
 Instrument
 QTOF

 MS Type
 QTOF
 Inj Vol (ul)
 5

 Sample Position
 P3-C1

Data File Path Acq Time (Local) Acq Method Path Acq SW Version IRM Status

DA Method Path

Result Summary

Target Source Path

 $\label{lem:limit} $$D:\mathbb G_{0.0}$ D:\mathcal G_{0.00}$ D:\mathcal G_{0$

6200 series TOF/6500 series Q-TOF 10.1 (48.0)

Success

D:\MassHunter\Data\Users\Hunter\IHytse\70425_shell1.d\AcqData\seashell_c18_06302025_ms

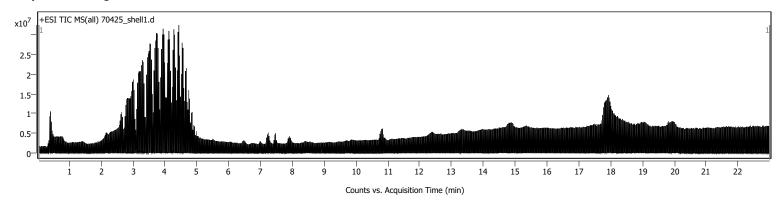
ms.m

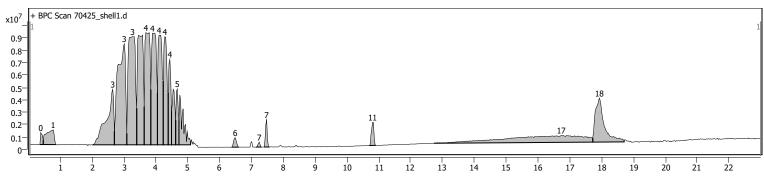
D:\MassHunter\PCDL\default.csv 7758 qualified (34080 targets)

Sample Chromatograms

Plate Position

Acq Operator

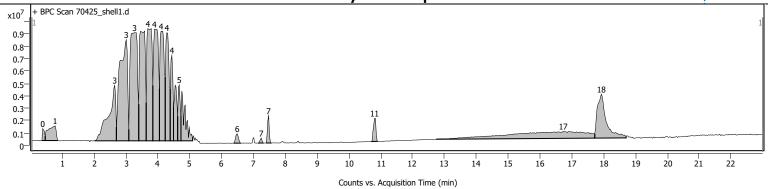




Counts vs. Acquisition Time (min)

Chromatog	gram Peaks						
Peak	Start	RT	End	Height	Area	Area %	SNR
1	0.357	0.383	0.461	966956	3497639	2.54	
2	0.461	0.773	0.850	1186809	20426048	14.82	
3	2.019	2.643	2.695	4479602	70324855	51.03	
4	2.695	3.007	3.085	8155244	135352463	98.21	
5	3.085	3.267	3.397	8741437	137818488	100.00	
6	3.397	3.579	3.631	8860201	111100588	80.61	
7	3.631	3.683	3.839	9068415	101832261	73.89	
8	3.839	3.891	4.047	9017489	98265146	71.30	
9	4.047	4.099	4.229	8857146	83277318	60.43	
10	4.229	4.281	4.385	8732868	65500642	47.53	
11	4.385	4.437	4.489	6894655	34988729	25.39	
12	4.489	4.541	4.619	4488337	27697614	20.10	
13	4.619	4.671	4.724	4512959	21727273	15.77	
14	4.724	4.750	5.088	4024607	34765323	25.23	
15	6.387	6.491	6.595	758811	4820751	3.50	
16	7.142	7.244	7.318	404359	1655591	1.20	
17	7.400	7.478	7.556	2200961	7884266	5.72	
18	10.703	10.805	10.906	1872734	10346726	7.51	
19	12.732	16.732	17.719	562409	94955583	68.90	
20	17.719	17.927	18.706	3554556	69640019	50.53	





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19	12.732	16.732	17.719	562409	94955583	68.90	

3554556

69640019

50.53

Sample Spectra

20

17.719

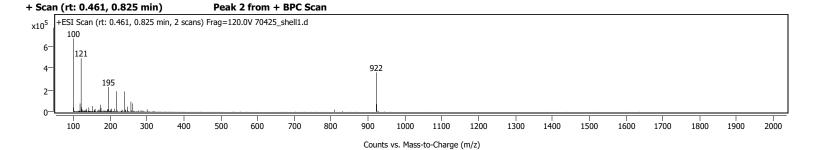
17.927

+ Scan (rt: 0.461 min) Peak 1 from + BPC Scan +ESI Scan (rt: 0.461 min) Frag=120.0V 70425_shell1.d x10⁵ 500 600 700 800 1200 1500 1600 1700 100 200 300 400 900 1000 1100 1300 1400 1800 1900 2000

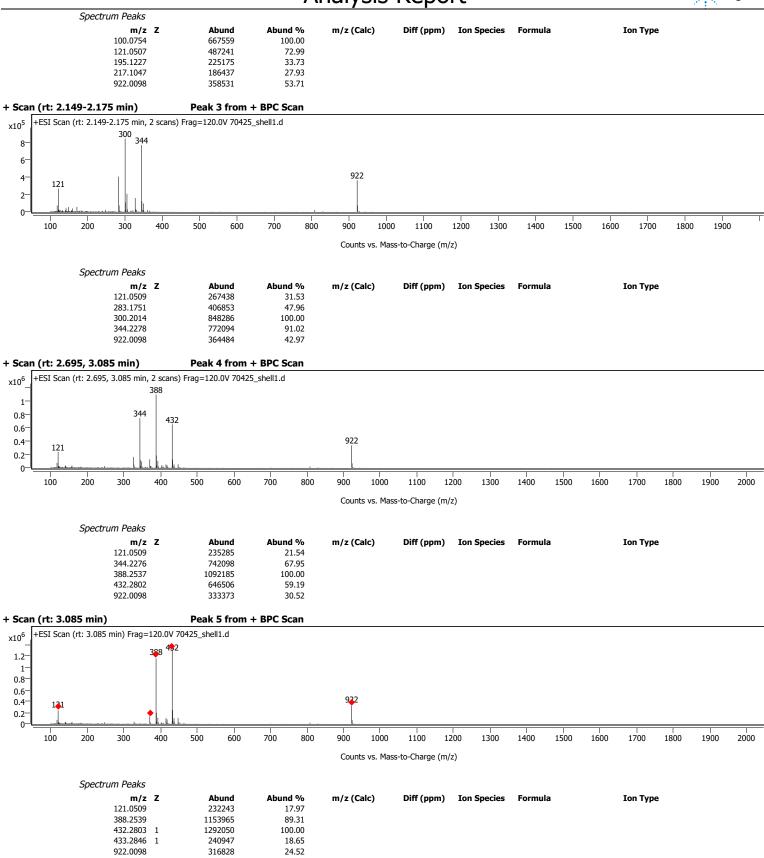
Counts vs. Mass-to-Charge (m/z)

18.706

Spectrum Peaks **m/z Z** 100.0757 Abund % **Abund** m/z (Calc) Diff (ppm) Ion Species Formula Ion Type 611261 81.44 121.0509 750548 100.00 195.1231 331548 44.17 239.1494 295776 39.41 922.0098 335213 44.66



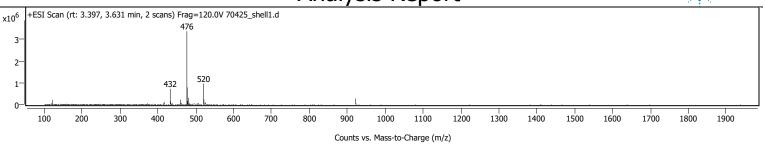




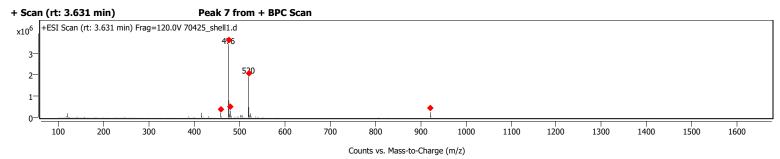
Peak 6 from + BPC Scan

+ Scan (rt: 3.397, 3.631 min)

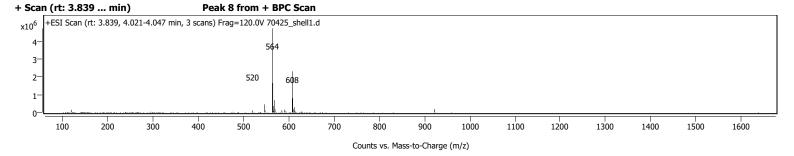




Spectrum Peaks								
m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
432.2800		718452	21.17					
476.3074	1	3393073	100.00					
477.3096	1	786249	23.17					
481.2620		299265	8.82					
520.3330		963935	28.41					

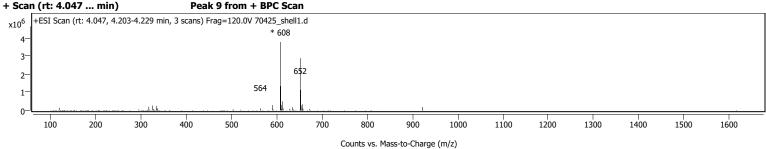


Spectrum Peaks								
m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
476.3072	1	3462725	100.00					
477.3094	1	799129	23.08					
481.2619		311047	8.98					
520.3327	1	1924868	55.59					
521.3358	1	481023	13.89					

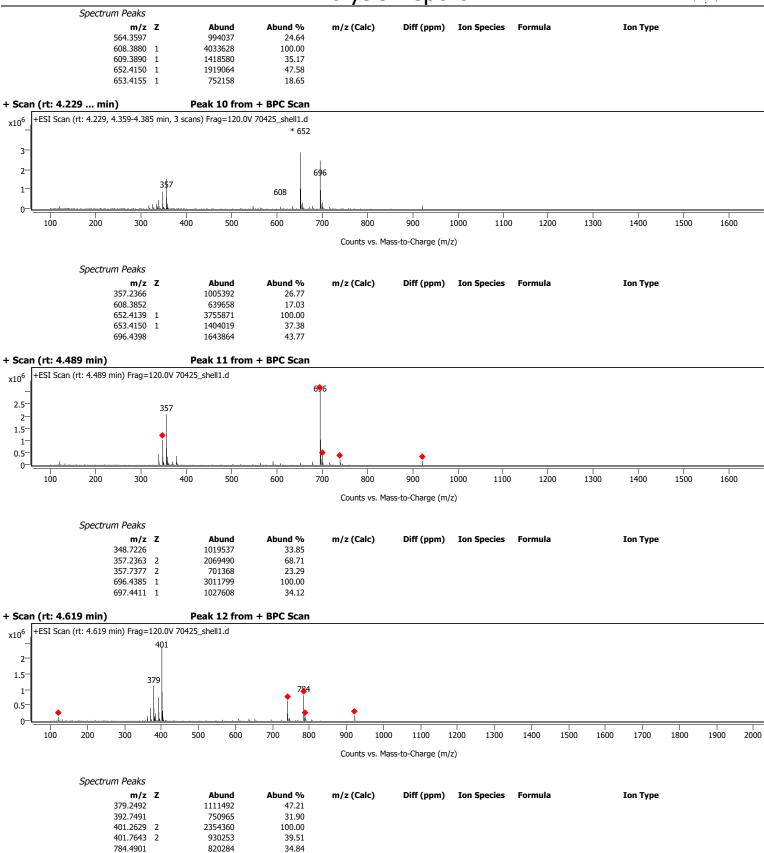


	m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
	520.3348		1683824	48.70					
	564.3621	1	3457709	100.00					
	565.3628	1	1180089	34.13					
	608.3872	1	1547850	44.77					
	609.3885	1	535004	15.47					
can (rt: 4 047	min)		Peak 0 from	I BBC Coom					

Spectrum Peaks



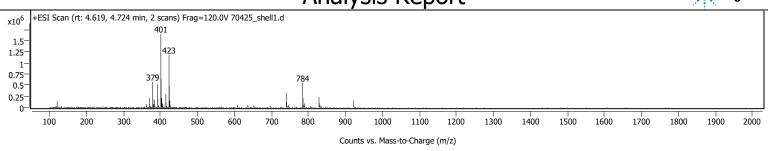




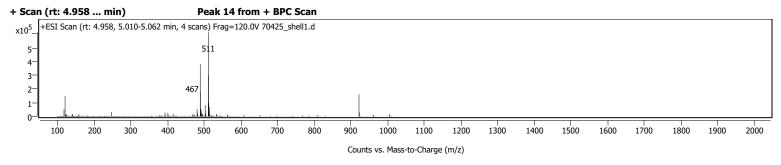
Peak 13 from + BPC Scan

+ Scan (rt: 4.619, 4.724 min)

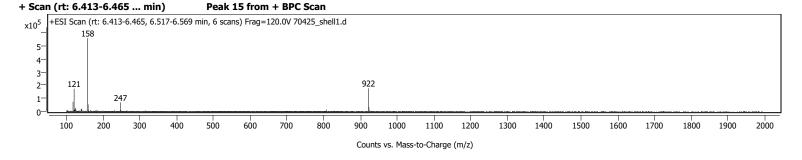




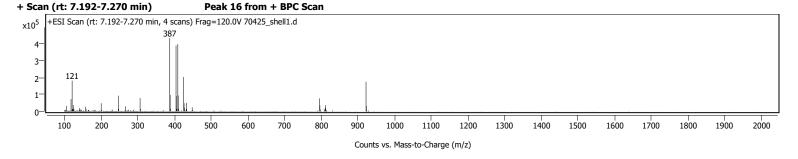
Spectrum Peaks								
m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Typ
379.2492		56910 4	34.57					
401.2627	2	1646133	100.00					
401.7642	2	640298	38.90					
423.2758		1175036	71.38					
784.4900		550125	33.42					



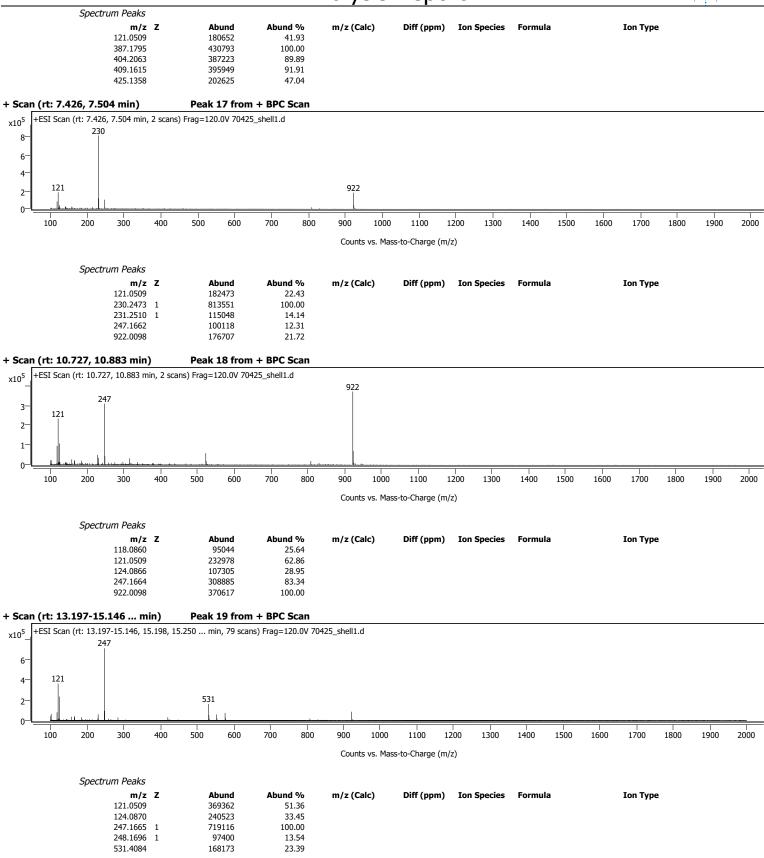
Spectrum Peaks								
m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
467.3014		165462	35.93					
489.3146	2	421434	91.51					
489.8167	2	192784	41.86					
511.3275	2	460535	100.00					
511.8294	2	225231	48.91					



Spectrum Peaks								
m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
118.0860		73521	13.07					
121.0509		173796	30.90					
158.1535		562364	100.00					
247.1665		68735	12.22					
922.0098		176951	31.47					



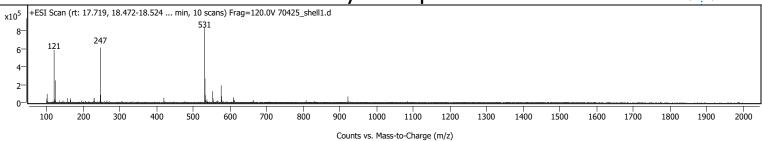




Peak 20 from + BPC Scan

+ Scan (rt: 17.719 ... min)





Diff (ppm) Ion Species

Formula

Ion Type

Spectrum Peaks

m/z	Z	Abund	Abund %	m/z (Calc)
121.0509		579496	70.98	
124.0873		254492	31.17	
247.1668		640870	78.49	
531.4086	1	816452	100.00	
532.4139	1	262068	32.10	

Cpd Name	Formula	RT	Mass	CAS ID	Source Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
1	C22 H20 N2 O7	7.244	424.1283	FBF	80.84				FBF
2	C16 H18 N2	6.621	238.1489	FBF	59.55				FBF
3	C21 H23 N O5	7.790	369.1593	FBF	85.46				FBF
4	C10 H15 N O	4.411	165.1141	FBF	62.69				FBF
5	C21 H24 N2 O2	4.437	336.1859	FBF	63.83				FBF
6	C18 H20 N2	4.281	264.1609	FBF	61.60				FBF
7	C15 H22 N2 O2	3.943	262.1680	FBF	59.15				FBF
8	C14 H8 N2 O	2.305	220.0624	FBF	60.43				FBF
9	C18 H35 N O2	6.491	297.2665	FBF	96.14				FBF
10	C8 H17 N	0.409	127.1362	FBF	86.17				FBF
11	C23 H30 N2 O4	10.883	398.2224	FBF	69.28				FBF
12	C32 H38 N2 O8	3.943	578.2618	FBF	75.75				FBF
13	C29 H40 N2 O4	4.984	480.2961	FBF	64.64				FBF
14	C18 H22 N2 O2	1.889	298.1693	FBF	90.86				FBF
15	C21 H35 N3	18.992	329.2840	FBF	55.23				FBF
16	C8 H15 N O	3.397	141.1146	FBF	84.16				FBF
17	C9 H17 N O	0.383	155.1316	FBF	87.16				FBF
18	C5 H13 N O	0.383	103.0999	FBF	99.77				FBF
19	C11 H17 N2	9.506	177.1388	FBF	75.92				FBF
20	C20 H33 N3	11.533	315.2664	FBF	80.48				FBF
21	C18 H35 N O3	9.116	313.2590	FBF	58.86				FBF
22	C18 H23 N O5	2.643	333.1557	FBF	81.74				FBF
23	C23 H25 N O4	13.353	379.1815	FBF	60.67				FBF
24	C19 H22 F N3 O4	2.591	375.1582	FBF	72.75				FBF
25	C19 H22 F N3 O3	8.960	359.1621	FBF	58.02				FBF
26	C11 H14 N4 O4	0.409	266.1002	FBF	78.94				FBF
27	C11 H16 N4 O5	9.896	284.1110	FBF	54.85				FBF
28	C25 H20 N4 O2	7.244	408.1546	FBF	67.85				FBF
29	C17 H20 N4 S	9.818	312.1381	FBF	69.38				FBF
30	C37 H50 N2 O	19.356	538.3907	FBF	55.81				FBF
31	C10 H9 N	0.409	143.0731	FBF	62.99				FBF
32	C9 H7 N	13.223	129.0578	FBF	87.09				FBF
33	C30 H49 N3 O	14.809	467.3869	FBF	63.79				FBF
34	C13 H21 N O	13.093	207.1606	FBF	63.32				FBF
35	C30 H49 N3 O2	15.328	483.3825	FBF	65.57				FBF
36	C4 H6 N4 O	3.813	126.0552	FBF	76.13				FBF
37	C15 H15 N3 O	8.310	253.1224	FBF	64.63				FBF
38	C5 H6 N2 O2	4.411	126.0425	FBF	76.67				FBF
39	C6 H7 N2 O2	2.253	139.0503	FBF	91.91		,	,	FBF
40	C14 H16 N4	4.906	240.1362	FBF	79.07				FBF
41	C6 H8 N2 O	12.391	124.0628	FBF	72.86				FBF
42	C19 H21 N3 O	9.376	307.1662	FBF	68.08		,	,	FBF
43	C6 H12 N2 O2	17.745	144.0889	FBF	64.38				FBF
43	C6 H12 N C O2	0.409	147.0893	FBF	71.55				FBF
45	C8 H17 N O5	5.919	207.1124	FBF	61.28				FBF
46	C7 H15 N O4	5.503	177.1002	FBF	69.27		-		FBF
40 47	C9 H17 N	0.357		FBF	76.92				FBF
48		4.307	139.1354 311.1541	FBF	63.27			-	FBF
	C19 H21 N O3								
49	C16 H26 N2 O2	21.642	278.1973	FBF					FBF
50 51	C30 H42 N2 O2 S	5.477	494.2966	FBF					FBF FBF
	C7 H16 N4 O	0.435	172.1337	FBF	89.04				
52	C4 H12 N2 S2	0.435	152.0451	FBF	55.70				FBF
53	C25 H31 N3 O4	3.293	437.2318	FBF		,			FBF
4	C14 H30 N4 O2	4.671	286.2342	FBF					FBF
55	C11 H23 N3 O2	4.567	229.1785	FBF					FBF
56	C9 H18 N2 O2	0.695	186.1368	FBF					FBF
57	C9 H18 N2 O3	1.838	202.1322	FBF					FBF
58	C7 H19 N3	0.357	145.1578	FBF					FBF
59	C6 H11 N O	1.396	113.0838	FBF		,			FBF
60	C8 H17 N O	5.763	143.1305	FBF					FBF
61	C8 H17 N O	5.062	143.1303	FBF					FBF
62	C5 H9 N O	0.773	99.0681	FBF					FBF
63	C4 H8 N2 O	16.706	100.0637	FBF					FBF
64	C16 H27 N O6	7.478	329.1849	FBF	73.02				FBF



Cpd Name	nary Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB	S) Score (MFG) Algorithm
65	C15 H25 N O6	10.909	315.1713	FBF	60.82		FBF
66	C15 H27 N O5	0.409	301.1889	FBF	95.72		FBF
67	C17 H32 Br N O2	10.571	361.1615	FBF	59.98		FBF
<u>68</u> 69	C7 H13 N O5 C9 H15 N O3	2.695 2.695	191.0807 185.1051	<u>FBF</u> FBF	69.86 85.44		FBF FBF
70	C7 H13 N O	2.591	127.0992	FBF	85.50		FBF
71	C13 H23 N O3	21.278	241.1683	FBF	52.20		FBF
72	C11 H16 N2 O5	18.836	256.1039	FBF	66.41		FBF
73	C7 H9 N2 O	7.764	137.0721	FBF	77.48		FBF
74	C8 H11 N	0.409	121.0887	FBF	81.02		FBF
75	C7 H9 N	0.409	107.0733	FBF	86.55		FBF
76 77	C6 H4 N2 C6 H5 N O	6.777 0.383	104.0371 107.0363	FBF FBF	56.33 86.07		FBF FBF
78	C7 H7 N O2	0.383	137.0473	FBF	74.12		FBF
79	C8 H7 N O3	2.643	165.0439	FBF	65.65		FBF
80	C6 H3 Cl2 N O2	0.331	190.9556	FBF	62.07		FBF
81	C24 H40 N5 O8	3.735	526.2874	FBF	79.69		FBF
82	C21 H29 N3 O	4.541	339.2335	FBF	61.38		FBF
83	C15 H17 F N4 O3	6.023	320.1263	FBF	58.97		FBF
84 85	C9 H6 F3 N3 O C10 H9 N O2	0.435 0.409	229.0472 175.0624	<u>FBF</u> FBF	76.67 67.69		FBF FBF
86	C9 H15 N O2	0.695	169.1102	FBF	92.62		FBF
87	C26 H37 N O6	7.920	459.2616	FBF	99.16		FBF
88	C15 H14 N4 O	7.244	266.1149	FBF	77.66		FBF
89	C8 H9 N3 O4	0.383	211.0611	FBF	60.19		FBF
90	C6 H8 N	0.669	94.0650	FBF	83.93		FBF
91	C9 H11 N3 O	0.435	177.0891	FBF	88.13		FBF
92 93	C12 H14 Cl2 N2 C16 H20 N2	7.140 8.102	256.0537 240.1620	<u>FBF</u> FBF	51.16 72.14		FBF FBF
94	C13 H21 N5 O	20.941	263.1743	FBF	65.27		FBF
95	C8 H13 N2 O5 P	1.448	248.0572	FBF	71.20		FBF
96	C8 H12 N O6 P	9.609	249.0388	FBF	72.73		FBF
97	C25 H22 N4 O8	9.870	506.1407	FBF	55.09		FBF
98	C12 H13 N O2	0.409	203.0945	FBF	74.67		FBF
99	C43 H48 N4 O6	4.437	716.3591	FBF	74.37		FBF
100 101	C21 H24 N2 O4 C24 H26 N2 O5	8.700 6.387	368.1741 422.1855	FBF FBF	71.30 53.42		FBF FBF
102	C24 H26 N2 O4	9.142	406.1855	FBF	66.74		FBF
103	C13 H9 N O2	5.451	211.0651	FBF	67.94		FBF
104	C29 H37 N3 O2	4.359	459.2883	FBF	58.87		FBF
105	C21 H23 N2 O3	5.477	351.1736	FBF	52.62		FBF
106	C12 H12 N2 O2	17.303	216.0897	FBF	86.99		FBF
107	C29 H34 N4	4.932	438.2792	FBF	70.70		FBF
108	C30 H20 N4 O6	6.257	532.1364	FBF	55.40		FBF
109 110	C20 H24 N2 O3 C19 H22 N2 O2	13.535 2.643	340.1788 310.1705	FBF FBF	59.75 71.99		FBF FBF
111	C26 H37 N5 O2	10.597	451.2949	FBF	56.44		FBF
112	C30 H37 N5 O5	5.140	547.2779	FBF	50.88		FBF
113	C21 H27 N3 O2	8.570	353.2069	FBF	63.87		FBF
114	C16 H21 N O6	7.998	323.1345	FBF	82.24		FBF
115	C19 H20 N2 O3	2.747	324.1445	FBF	73.65		FBF
116	C8 H7 N O	3.085	133.0525	FBF	86.70		FBF
117 118	C17 H18 N4 O C32 H40 N4	7.426 5.062	294.1475 480.3273	<u>FBF</u> FBF	74.59 56.91		FBF FBF
119	C16 H22 N4 O3	6.205	318.1706	FBF	78.22		FBF
120	C24 H30 N4	10.337	374.2436	FBF	51.84		FBF
121	C20 H16 N2 O4	13.015	348.1113	FBF	64.53		FBF
122	C23 H23 N3 O5	7.920	421.1668	FBF	61.36		FBF
123	C17 H18 N2 O	2.149	266.1419	FBF	88.83		FBF
124	C16 H19 N O7	12.027	337.1148	FBF	79.17		FBF
125 126	C16 H23 N5 O C40 H48 N4 O2	0.409 5.971	301.1889 616.3808	<u>FBF</u> FBF	88.86 62.70		FBF FBF
127	C40 H44 N4 O	5.322	596.3503	FBF	55.54		FBF
128	C40 H48 N4 O3	4.828	632.3726	FBF	66.25		FBF
129	C18 H22 N2 O8	7.244	394.1385	FBF	50.13		FBF
130	C12 H14 N2 O	0.409	202.1108	FBF	58.45		FBF
131	C11 H13 N3 O	4.671	203.1048	FBF	81.50		FBF
132	C18 H11 N O4	1.344	305.0674	FBF	57.41		FBF
133 134	C41 H48 N2 O8 C20 H15 N O5	12.651 8.934	696.3372 349.0978	FBF FBF	61.58 66.78		FBF FBF
135	C21 H17 N O5	8.960	363.1115	FBF	87.76		FBF
136	C20 H15 N O4	9.402	333.1021	FBF	87.19		FBF
137	C18 H18 N2 O8	9.896	390.1029	FBF	51.75		FBF
138	C14 H16 N4 O4	1.967	304.1150	FBF	76.80		FBF
139	C20 H19 N O6	9.870	369.1183	FBF	52.61		FBF
140	C38 H44 N2 O6	8.206	624.3230	FBF	54.70		FBF
141 142	C29 H38 N2 O4	5.244	478.2829	FBF	69.96		FBF
	C13 H17 N O3 C39 H40 N2 O6	5.867 14.938	235.1211 632.2847	FBF FBF	60.67 50.64		FBF FBF
	C19 H24 N2 O2	6.439	312.1863	FBF	50.64 55.45		FBF
143		U.TJ2	712,1007	ו טו			ו טו
143 144		6.179	259.0534	FBF	51.69		FRF
143 144 145	C19 H24 N2 O2 C10 H13 N O5 S C16 H17 N O3	6.179 8.908	259.0534 271.1219	FBF FBF	51.69 67.73		FBF FBF
143 144 145 146 147	C10 H13 N O5 S						
143 144 145 146	C10 H13 N O5 S C16 H17 N O3	8.908	271.1219	FBF	67.73		FBF



Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib)	Score (DB)	Score (MFG) Algorithm
151	C21 H27 N O5	2.695	373.1922	FBF	52.22			FBF
152 153	C19 H25 N O C14 H10 N2 O2	21.720 18.784	283.1941 238.0721	FBF FBF	74.04 82.83			FBF FBF
154	C14 H10 N2 O2 C10 H15 N O2	0.747	181.1100	FBF	98.97			FBF
155	C11 H18 N O	6.569	180.1384	FBF	79.98			FBF
156	C8 H11 N O2	0.383	153.0779	FBF	73.06			FBF
157	C9 H13 N	0.409	135.1040	FBF	72.45			FBF
158 159	C10 H15 N5 C8 H11 N O4 S	0.409 1.448	205.1314 217.0407	FBF FBF	72.16 64.86			FBF FBF
160	C22 H24 N O4	4.567	366.1721	FBF	55.70			FBF
161	C21 H25 N O4	4.541	355.1807	FBF	62.47			FBF
162	C22 H25 N O6	4.567	399.1682	FBF	79.12			FBF
163 164	C21 H32 N6 O3 C12 H13 N O2 S	3.293 6.751	416.2521 235.0664	<u>FBF</u> FBF	76.67 96.10			FBF FBF
165	C12 H15 N O2 S	0.669	220.1226	FBF	68.80			FBF
166	C6 H5 Cl2 N	6.751	160.9787	FBF	52.61			FBF
167	C6 H7 N O	0.383	109.0526	FBF	64.72			FBF
168	C14 H15 N3	1.084	225.1258	FBF	54.34			FBF
169 170	C8 H12 N2 C8 H8 O2	1.136 0.383	136.0988 136.0527	<u>FBF</u> FBF	68.26 66.80			FBF FBF
171	C15 H22 O2	9.116	234.1612	FBF	69.91			FBF
172	C12 H17 N O	6.283	191.1308	FBF	85.19			FBF
173	C15 H24 N2 O4 S	9.402	328.1470	FBF	85.98			FBF
174	C20 H22 N8 O5	3.007	454.1724	FBF	63.53			FBF
175 176	C20 H22 N2 O8 C9 H12 N2 O3	5.036 0.461	418.1362 196.0856	<u>FBF</u> FBF	78.17 74.72			FBF FBF
177	C21 H30 N4 O4	10.987	402.2258	FBF	91.16			FBF
178	C24 H34 N4 O5 S	11.325	490.2288	FBF	55.64			FBF
179	C18 H30 O3 S	3.293	326.1933	FBF	80.13			FBF
180	C17 H28 O3 S	2.409	312.1775	FBF	81.12			FBF
181 182	C15 H20 N2 O4 S	10.831	324.1153	<u>FBF</u> FBF	62.95			FBF FBF
183	C6 H8 Cl N3 O4 S2 C13 H19 N O4 S	6.751 2.383	284.9650 285.1056	FBF	70.51 63.42			FBF
184	C14 H12 N4 O2 S	6.725	300.0679	FBF	55.42			FBF
185	C7 H9 N O2 S	0.435	171.0370	FBF	60.91			FBF
186	C15 H22 O3	13.275	250.1547	FBF	56.25			FBF
187	C14 H21 N O2	0.409	235.1562	FBF	77.16			FBF
188 189	C11 H16 N O4 P S C16 H26 N2 O3	0.409 10.883	289.0556 294.1963	FBF FBF	57.30 69.70			FBF FBF
190	C24 H38 O4	15.042	390.2776	FBF	93.10			FBF
191	C7 H5 Cl O2	13.327	155.9974	FBF	78.05			FBF
192	C7 H7 N O4	2.097	169.0371	FBF	77.35			FBF
193	C15 H22 N4 O3	2.175	306.1674	FBF	74.43			FBF
194 195	C23 H29 CI F N3 O4 C16 H21 N O5	3.397 5.451	465.1841 307.1404	FBF FBF	67.09 70.05			FBF FBF
196	C22 H34 O3	10.493	346.2490	FBF	72.20			FBF
197	C18 H19 Cl N2 O2	0.435	330.1120	FBF	52.02			FBF
198	C27 H29 N3 O9	3.735	539.1907	FBF	84.69			FBF
199	C13 H18 N4 O3	3.943	278.1397	FBF	62.50			FBF
<u>200</u> 201	C20 H16 O4 C22 H18 N6	2.253 4.437	320.1074 366.1616	FBF FBF	60.69 50.29			FBF FBF
202	C14 H12 O4	7.088	244.0714	FBF	73.78			FBF
203	C13 H10 O	7.634	182.0736	FBF	76.17			FBF
204	C20 H21 Cl O4	9.896	360.1101	FBF	50.41			FBF
205	C16 H14 O3	9.922	254.0964	FBF	52.27			FBF
<u>206</u> 207	C22 H28 N2 O3 C17 H19 N5	7.088 3.995	368.2125 293.1616	FBF FBF	70.41 62.34			FBF FBF
208	C18 H15 CI N2 O	3.995 8.466	310.0868	FBF	71.50			FBF
209	C17 H22 N2 O	8.050	270.1724	FBF	72.36			FBF
210	C18 H15 Cl4 N3 O4	5.451	476.9821	FBF	61.11			FBF
211	C12 H14 O3	0.383	206.0946	FBF	84.41			FBF
<u>212</u> 213	C12 H16 O3	5.244	208.1112	FBF	50.95			FBF FBF
214	C9 H12 O2 C7 H4 Cl2 O4	9.116 1.084	152.0828 221.9482	FBF FBF	68.40 61.53			FBF
215	C15 H16 O4	6.179	260.1032	FBF	70.70			FBF
216	C32 H42 O8	3.943	554.2897	FBF	56.40			FBF
217	C20 H25 N O2	22.083	311.1873	FBF	50.21			FBF
218	C19 H14 O3	1.344	290.0964	FBF	62.49			FBF
<u>219</u> 220	C24 H26 O2 C28 H33 CI N2	8.622 7.218	346.1917 432.2341	FBF FBF	67.65 63.48			FBF FBF
221	C26 H28 N2	15.562	368.2224	FBF	50.59			FBF
222	C18 H22 N2	9.350	266.1782	FBF	61.28			FBF
223	C26 H26 F2 N2	7.244	404.2025	FBF	51.67			FBF
224	C16 H13 F2 N3 O	2.097	301.1033	FBF	83.15			FBF
<u>225</u> 226	C21 H27 CI N2 O2 C21 H24 O8	10.337 7.244	374.1755 404.1475	FBF FBF	71.69 94.95			FBF FBF
227	C25 H27 CI N2	6.257	390.1893	FBF	<u>94.95</u> 58.84			FBF
228	C24 H27 N O2	19.174	361.2025	FBF	54.04			FBF
229	C28 H29 F2 N3 O	3.371	461.2284	FBF	66.97			FBF
230	C23 H29 N O3	15.640	367.2118	FBF	61.69			FBF
231	C32 H41 N O2	5.062	471.3112	FBF	56.06			FBF
<u>232</u> 233	C25 H30 N O3 C9 H10 O3	7.920 0.409	392.2225 166.0636	FBF FBF	98.91 83.88			FBF FBF
234	C9 H10 O3	0.409	182.0578	FBF	78.07			FBF
235	C7 H8 O2	1.786	124.0535	FBF	68.13			FBF
236	C23 H38 O3	10.129	362.2815	FBF	71.62			FBF



Cpd Name	Formula	RT	Mass		Source Scor		Score (DB)	Score (MFG) Algorithm
237 238	C7 H8 O	5.581 9.818	108.0572	FBI FBI				FBF FBF
239	C19 H20 O4 C11 H14 O3	7.946	312.1378 194.0931	FBI				FBF
240	C12 H14 O4	7.062	222.0892	FBI				FBF
241	C16 H22 O4	9.870	278.1520	FBI				FBF
242	C12 H16 O5	5.893	240.0978	FBI				FBF
<u>243 </u>	C13 H16 O10 C7 H8 O3	6.828 0.981	332.0733 140.0478	FBI FBI				FBF FBF
245	C10 H14 O4	2.721	198.0876	FBI				FBF
246	C15 H18 O10	0.383	358.0917	FBI	61.0)		FBF
247	C10 H12 O4	0.409	196.0741	FBI			-	FBF
248	C14 H18 O4	8.492	250.1201	FBI				FBF
<u>249 </u>	C12 H16 O6 C7 H12 O6	3.527 1.552	256.0952 192.0643	FBI FBI				FBF FBF
251	C8 H6 O5	0.435	182.0209	FBI			-	FBF
252	C22 H23 N O6	4.567	397.1548	FBI				FBF
253	C9 H12 N2 O	1.396	164.0948	FBI				FBF
254	C16 H8 Cl2 F6 N2 O3	5.477	459.9798	FBI				FBF
255	C19 H20 N6 O	10.181	348.1703	FBI				FBF
<u>256</u> 257	C9 H11 Cl N2 O C12 H16 Cl2 N2 O	6.777 1.604	198.0567 274.0663	FBI FBI				FBF FBF
258	C12 H16 CI2 N2 O	0.435	313.9757	FBI				FBF
259	C16 H10 O	0.825	218.0746	FBI				FBF
260	C7 H4 Cl2 O3	12.963	205.9540	FBI				FBF
261	C11 H8	5.763	140.0628	FB	82.1			FBF
262	C17 H27 N3 O4 S	8.674	369.1741	FBI			-	FBF
263	C19 H23 N3	10.883	293.1886	FBI				FBF
264	C11 H9 Cl2 N O2	5.322	256.9991	FBI FBI				FBF FBF
2 <u>65</u> 266	C24 H34 N2 O C20 H18 O2	3.631 1.838	366.2674 290.1336	FBI				FBF
267	C12 H17 N O3	0.383	223.1216	FBI				FBF
268	C9 H5 Cl N4	0.409	204.0209	FBI				FBF
269	C17 H27 N O3	4.125	293.1965	FBI				FBF
270	C30 H32 N2 O2	4.906	452.2475	FBI				FBF
271	C11 H14 N2 O4	7.868	238.0952	FBI			-	FBF
272 273	C13 H17 Cl N2 O2 C13 H13 N3	21.226 0.721	268.0972 211.1126	FBI				FBF FBF
274	C16 H16 N2 O4	1.344	300.1120	FBI				FBF
275	C10 H9 Cl4 O4 P	0.409	363.8998	FBI				FBF
276	C12 H19 N2 O2	8.102	223.1442	FBI	80.6	3		FBF
277	C26 H36 N2 O3	4.854	424.2723	FBI				FBF
278	C23 H30 N2	12.781	334.2404	FBI				FBF
279	C27 H38 N2 O4	7.920	454.2818	FBI			-	FBF
280 281	C11 H15 N3 O2 C12 H18 N2 O2	0.435 20.759	221.1154 222.1365	FBI FBI				FBF FBF
282	C12 H10 N2 O2	8.986	206.1652	FBI				FBF
283	C14 H22 O2	6.984	222.1598	FBI				FBF
284	C15 H24 O	10.311	220.1814	FBI				FBF
285	C11 H16 O2	5.140	180.1138	FBI				FBF
286	C9 H12 O	0.409	136.0889	FBI				FBF
287	C22 H34 O4	5.010 4.671	362.2452	FBI FBI				FBF FBF
2 <u>88</u> 289	C20 H30 O6 C20 H26 O4	7.478	366.2020 330.1859	FBI				FBF
290	C20 H30 O4	4.255	334.2156	FBI				FBF
291	C26 H42 O4	15.042	418.3109	FBI				FBF
292	C30 H50 O4	19.148	474.3748	FBI	51.5	•		FBF
293	C18 H26 O4	13.379	306.1815	FBI				FBF
294	C16 H20 O6	5.192	308.1271	FBI				FBF
295	C16 H22 O5 C16 H20 O5	7.426	294.1459 292.1294	FBI FBI				FBF FBF
<u>296 </u>	C16 H20 O3 C15 H20 O4	8.310 6.179	264.1343	FBI				FBF
298	C18 H24 O6	5.062	336.1554	FBI				FBF
299	C17 H24 O4	5.607	292.1652	FBI				FBF
300	C17 H22 O5	6.777	306.1461	FBI				FBF
301	C13 H16 O4	6.413	236.1044	FBI			-	FBF
302	C15 H18 N4	5.685	254.1508	FBI				FBF
303 304	C24 H26 N6 O3 C18 H18 O3	5.555 2.279	446.2056 282.1268	FBI FBI				FBF FBF
305	C18 H16 O3 C12 H3 Cl7	14.393	391.8026	FBI				FBF
306	C20 H21 N	8.284	275.1672	FBI				FBF
307	C19 H21 N	7.010	263.1677	FBI				FBF
808	C6 H4 Cl2 O	0.669	161.9650	FBI				FBF
309	C10 H10 Cl2 O3	5.348	248.0017	FBI				FBF
310	C13 H15 Cl2 N O	1.889	271.0546	FBI			-	FBF
311	C13 H16 Cl N O	1.941 0.357	237.0931	FBI				FBF FBF
312 313	C6 H Cl5 C21 H24 Cl2 O4	0.35/ 7.244	247.8525 410.1050	FBI				FBF FBF
314	C9 H10	0.383	118.0788	FBI				FBF
315	C15 H10 O2	7.270	222.0679	FBI				FBF
316	C20 H28 O7	13.353	380.1838	FBI				FBF
317	C15 H20 O3	6.231	248.1407	FBI				FBF
318	C14 H18 O2	0.409	218.1305	FBI				FBF
319	C19 H14 O5	7.998	322.0815	FBI				FBF
320	C11 H8 O3 C10 H10 O2	0.409 9.480	188.0456 162.0671	FBI FBI				FBF FBF
321	C10 H10 O2 C11 H10 O	9.480 0.409	158.0716	FBI			-	FBF



Compound Summary							
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorith
323	C19 H21 N O7 S	7.244	407.1022	FBF	92.00		FBF
324	C34 H42 N2 O4	6.101	542.3126	FBF	60.30		FBF
325 326	C21 H25 N C10 H8 O3	8.908 7.088	291.1984 176.0470	FBF FBF	63.73 85.09		FBF FBF
327	C10 H8 O3	1.422	180.0697	FBF	88.32		FBF
328	C16 H22 N2	4.541	242.1782	FBF	72.72		FBF
329	C12 H16 O4	3.631	224.1035	FBF	68.74		FBF
330	C11 H14 O4	4.802	210.0891	FBF	86.57		FBF
331	C9 H12 O3	7.218	168.0794	FBF	85.13		FBF
332	C15 H22 N2 O4	21.304	294.1596	FBF	50.73		FBF
333 334	C6 H5 Cl O3 C6 H4 Cl2 O2	12.885 12.053	159.9939 177.9590	<u>FBF</u> FBF	52.76 63.05		FBF FBF
335	C8 H10 O5 S	1.448	218.0240	FBF	71.86		FBF
336	C6 H2 Cl4 O	10.519	229.8847	FBF	52.81		FBF
337	C6 H CI5 O	12.989	263.8453	FBF	58.32		FBF
338	C6 H4 Br2 O	12.287	249.8625	FBF	52.43		FBF
339	C16 H24 O8	4.281	344.1489	FBF	78.70		FBF
340	C14 H20 O9	2.149	332.1102	FBF	57.73		FBF
341	C9 H12 O4	16.784	184.0737	FBF	76.57		FBF
342 343	C17 H26 O3 C6 H4 N2 O5	6.647	278.1870	<u>FBF</u> FBF	58.89 57.25		FBF FBF
344	C18 H30 O	0.409 11.455	184.0136 262.2284	FBF	68.23		FBF
345	C14 H18 O7	5.607	298.1032	FBF	69.63		FBF
346	C13 H20 O2	8.024	208.1460	FBF	85.45		FBF
347	C17 H12 O5	7.348	296.0683	FBF	85.25		FBF
348	C17 H26 O4	13.587	294.1843	FBF	72.12		FBF
349	C14 H22 N2 O3	8.908	266.1656	FBF	75.53		FBF
350	C22 H30 N2 O3	8.570	370.2243	FBF	67.04		FBF
351	C13 H19 N O3 S	6.906	269.1097	FBF	53.62		FBF
352 353	C19 H24 N4 O2 C14 H18 CI N3 O2	6.802 10.207	340.1873 295.1088	FBF FBF	53.56 50.75		FBF FBF
354	C17 H24 O3	7.452	276.1714	FBF	70.84		FBF
355	C17 H24 O3 C18 H27 N O2	22.239	289.2033	FBF	52.46		FBF
356	C11 H14 N2 O2	13.353	206.1056	FBF	77.78		FBF
357	C17 H27 N O2	6.984	277.2021	FBF	68.66		FBF
58	C12 H21 N O17 S2	5.555	515.0230	FBF	50.12		FBF
359	C12 H23 N O10	8.960	341.1318	FBF	74.68		FBF
860	C12 H22 O11	0.409	342.1164	FBF	94.42		FBF
361	C12 H20 O10	0.409	324.1051	FBF	76.77		FBF
362	C11 H17 N O7	8.310	275.1025	FBF	70.90		FBF
363 364	C11 H19 N O6 C10 H17 N O6	5.893 6.828	261.1231 247.1047	<u>FBF</u> FBF	70.35 67.29		FBF FBF
365	C16 H27 N O11	7.244	409.1578	FBF	96.83		FBF
366	C16 H25 N O10	3.007	391.1498	FBF	74.22		FBF
367	C14 H20 O7	4.125	300.1219	FBF	72.22		FBF
368	C12 H16 O7	3.085	272.0870	FBF	60.49		FBF
369	C8 H16 N2 O7	2.617	252.0967	FBF	70.80		FBF
370	C10 H15 N O7	5.010	261.0834	FBF	69.24		FBF
371	C11 H18 O9	5.503	294.0956	FBF	83.75		FBF
372 373	C9 H18 O8 C10 H18 N2 O5	1.760 6.802	254.0982 246.1217	<u>FBF</u> FBF	73.21 71.29		FBF FBF
374	C6 H13 N O5	1.448	179.0783	FBF	76.81		FBF
375	C23 H43 N5 O14	4.125	613.2823	FBF	91.85		FBF
376	C6 H13 N O6	4.359	195.0759	FBF	72.32		FBF
377	C8 H15 N O7	5.114	237.0858	FBF	78.16		FBF
378	C9 H17 N O7	3.371	251.1013	FBF	72.83		FBF
379	C8 H15 N O6	5.374	221.0895	FBF	75.77		FBF
380	C8 H13 N O7	2.617	235.0701	FBF	70.80		FBF
81	C8 H17 N O6	6.439 5.400	223.1077 293.1112	<u>FBF</u> FBF	60.28 85.71	<u> </u>	FBF FBF
82	C11 H19 N O8 C11 H20 N O11 P	5.400 9.844	373.0770	FBF	50.88		FBF
84	C7 H14 O5	1.032	178.0852	FBF	86.77		FBF
85	C6 H12 O5	7.218	164.0682	FBF	66.38		FBF
86	C6 H12 O4	0.409	148.0737	FBF	86.89		FBF
887	C8 H16 O6	0.435	208.0947	FBF	86.76		FBF
388	C7 H14 O6	0.643	194.0774	FBF	76.19		FBF
889	C8 H14 O7	0.799	222.0729	FBF	79.25		FBF
90	C10 H13 N5 O4	5.062	267.0979 192.0990	<u>FBF</u> FBF	71.90 84.50	<u> </u>	FBF FBF
91	C8 H16 O5 C19 H37 N5 O7	1.110 3.085	192.0990 447.2676	FBF	91.46		FBF
93	C16 H20 N2 O8	10.467	368.1219	FBF	78.35		FBF
94	C14 H24 O8	9.012	320.1450	FBF	55.26		FBF
95	C5 H11 N O4	16.498	149.0681	FBF	79.09		FBF
96	C5 H8 O5	11.507	148.0364	FBF	71.50		FBF
397	C5 H10 O6	9.844	166.0466	FBF	73.17		FBF
398	C11 H17 N O8	5.685	291.0961	FBF	83.37		FBF
399	C13 H21 N O15 S	5.737	463.0629	FBF	74.25		FBF
00	C4 H8 O5	19.746	136.0375	FBF	81.07		FBF
01 02	C6 H12 O7 C12 H22 O12	6.751	196.0579 358 1110	<u>FBF</u> FBF	71.80 82.31		FBF FBF
03	C12 H22 O12 C14 H23 N O11	10.259 10.337	358.1110 381.1262	FBF	77.06		FBF
·04	C14 H23 N O11 C11 H19 N O9	5.633	309.1056	FBF	59.53		FBF
105	C9 H17 N O8	5.062	267.0978	FBF	51.73		FBF
106	C11 H19 N O10	9.012	325.1005	FBF	64.10		FBF
07	C5 H12 O4	1.396	136.0737	FBF	65.20		FBF
108	C4 H10 O3	7.244	106.0639	FBF	68.56		FBF



Cpd Name	mary Formula	RT	Mass	CAS ID Source	Score	Score (Lib)	Score (DB)	Score (MFG) Algorithm
409	C7 H16 O7	0.409	212.0890	FBF	58.02			FBF
<u>410</u> 411	C22 H32 O5 C17 H22 O4	13.249 6.387	376.2233 290.1506	FBF FBF	68.91 57.27			FBF FBF
412	C25 H34 O7	3.085	446.2336	FBF	61.36			FBF
413	C20 H32 O4	12.703	336.2271	FBF	67.75			FBF
414	C20 H30 O3	15.744	318.2167	FBF	57.10			FBF
415	C20 H28 O5	5.711	348.1953	FBF	64.53			FBF
<u>416</u> 417	C20 H30 O5 C20 H34 O4	8.986 13.665	350.2108 338.2464	FBF FBF	69.50 75.53			FBF FBF
418	C17 H28 O3	18.628	280.2016	FBF	71.34			FBF
419	C20 H34 O2	7.244	306.2578	FBF	70.79			FBF
420	C21 H34 O8	3.007	414.2272	FBF	51.96			FBF
<u>421</u> 422	C20 H40 C23 H37 N O6 S	9.012 7.920	280.3126 455.2339	<u>FBF</u> FBF	98.38 58.92			FBF FBF
423	C22 H37 N O4	2.851	379.2750	FBF	56.07			FBF
424	C25 H40 N2 O7 S	6.075	512.2573	FBF	57.64			FBF
425	C20 H36 O3	10.909	324.2655	FBF	65.50			FBF
426	C20 H34 O8	10.935	402.2257	FBF	90.91			FBF
<u>427</u> 428	C22 H36 O4 C20 H36 O4	11.793 13.717	364.2592 340.2583	<u>FBF</u> FBF	71.88 52.86			FBF FBF
429	C16 H26 O5	2.435	298.1764	FBF	90.91			FBF
430	C16 H28 O5	7.036	300.1934	FBF	79.53			FBF
431	C20 H38 O5	7.946	358.2706	FBF	62.30			FBF
432	C20 H28 O3	0.435	316.2056 382.2733	FBF	68.53			FBF
<u>433</u> 434	C22 H38 O5 C22 H28 O5	17.355 2.591	382.2733	<u>FBF</u> FBF	68.31 52.10			FBF FBF
435	C24 H38 O8	4.984	454.2543	FBF	63.82			FBF
436	C20 H34 O6	8.570	370.2333	FBF	81.64			FBF
437	C18 H30 O6	18.239	342.2054	FBF	55.84			FBF
438	C21 H34 O4	12.963	350.2424	FBF	68.32			FBF
<u>439</u> 440	C20 H32 F2 O5 C23 H40 O5	4.724 10.337	390.2216 396.2873	<u>FBF</u> FBF	59.49 76.32			FBF FBF
441	C20 H38 O2	12.911	310.2847	FBF	64.93			FBF
442	C18 H28 O6	6.802	340.1868	FBF	68.83			FBF
443	C19 H34 O5	8.492	342.2383	FBF	73.03			FBF
444	C11 H23 N O2	0.383	201.1728	FBF	99.86			FBF
<u>445</u> 446	C8 H17 N O2	0.383	159.1273 243.2194	<u>FBF</u> FBF	80.42			FBF FBF
447	C14 H29 N O2 C16 H33 N O2	8.128 7.192	271.2500	FBF	82.78 77.13	,		FBF
448	C13 H27 N O2	6.517	229.2048	FBF	70.44			FBF
449	C4 H9 N O2	0.409	103.0638	FBF	82.18			FBF
450	C9 H19 N O2	0.409	173.1416	FBF	86.87			FBF
451	C5 H11 N O2	0.357	117.0790	FBF	87.95			FBF
<u>452</u> 453	C6 H13 N O2 C12 H25 N O2	0.383 0.409	131.0947 215.1877	FBF FBF	83.07 65.58			FBF FBF
454	C9 H17 N O3	2.903	187.1207	FBF	69.00			FBF
455	C9 H17 N O3	2.357	187.1200	FBF	72.26			FBF
456	C18 H36 O2	7.868	284.2715	FBF	99.09			FBF
457	C17 H34 O2	7.426	270.2542	FBF	71.74			FBF
<u>458</u> 459	C17 H32 O2 C16 H32 O2	9.636 7.010	268.2379 256.2400	FBF FBF	65.24 98.97			FBF FBF
460	C16 H30 O2	7.374	254.2236	FBF	79.82			FBF
461	C6 H12 O2	0.383	116.0838	FBF	87.17			FBF
462	C10 H18 O2	12.391	170.1308	FBF	96.94			FBF
463	C20 H40 O2	8.804	312.3021	FBF	95.73			FBF
<u>464</u> 465	C6 H10 O2 C7 H14 O2	22.031 2.929	114.0681 130.1004	FBF FBF	83.63 81.86			FBF FBF
466	C8 H16 O2	7.244	144.1139	FBF	81.33			FBF
467	C19 H38 O2	8.154	298.2855	FBF	59.57			FBF
468	C8 H14 O2	2.877	142.0987	FBF	81.34			FBF
469	C14 H28 O2	6.075	228.2087	FBF	97.60			FBF
<u>470</u> 471	C14 H26 O2 C9 H18 O2	7.868 17.044	226.1922 158.1318	FBF FBF	78.96 74.54			FBF FBF
471 472	C5 H8 O2	10.519	100.0522	FBF	99.57			FBF
473	C22 H44 O2	9.922	340.3334	FBF	77.85			FBF
474	C26 H52 O2	7.868	396.3932	FBF	51.24			FBF
475	C12 H24 O2	4.802	200.1772	FBF	85.83			FBF
<u>476</u> 477	C28 H56 O2 C15 H30 O2	18.187 6.543	424.4278 242.2232	FBF FBF	59.83 57.98			FBF FBF
477 478	C13 H30 O2 C11 H22 O2	9.012	186.1634	FBF	73.29			FBF
479	C5 H8 O3	0.669	116.0469	FBF	86.29			FBF
480	C6 H8 O2	8.310	112.0521	FBF	86.41			FBF
481	C18 H32 O2	10.961	280.2399	FBF	74.46			FBF
482 483	C19 H36 O2 C16 H28 O2	11.403 17.096	296.2690 252.2071	FBF FBF	66.40 56.70			FBF FBF
484	C16 H28 O2 C19 H34 O2	8.440	252.2071 294.2563	FBF	88.01			FBF
485	C19 H30 O2	7.686	290.2236	FBF	63.83			FBF
486	C16 H30 O4	7.738	286.2151	FBF	68.84			FBF
487	C6 H10 O4	2.149	146.0569	FBF	65.35			FBF
488	C10 H18 O5	5.893	218.1153	FBF	81.93			FBF
489	C14 H26 O4	6.647	258.1820	FBF	80.64			FBF
<u>490</u> 491	<u>C8 H12 O4</u> C8 H14 O4	2.331 0.435	172.0722 174.0892	<u>FBF</u> FBF	77.56 87.04			FBF FBF
492	C9 H14 O5	1.838	202.0822	FBF	74.53			FBF
493	C6 H10 O4 S	13.301	178.0292	FBF	85.46			FBF
494	C12 H22 O5	5.296	246.1464	FBF	78.88			FBF



Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib)	Score (DB)	Score (MFG) Algorith
495 406	C8 H14 O5	3.007	190.0853	FBF	75.54			FBF
196 1 97	C14 H26 O5 C9 H16 O4	7.010 2.565	274.1779 188.1049	FBF FBF	73.26 85.40			FBF FBF
198	C15 H28 O4	5.841	272.1982	FBF	76.99			FBF
199	C10 H16 O4	9.844	200.1047	FBF	80.01			FBF
500 501	C17 H30 O4 C5 H7 N O5	18.966 1.552	298.2120 161.0340	FBF FBF	55.54 75.18			FBF FBF
502	C9 H14 O4	2.721	186.0886	FBF	82.85			FBF
503	C30 H58 O4 S	20.317	514.4061	FBF	98.25			FBF
504 505	C22 H42 O4 C12 H22 O4	15.042 5.529	370.3086 230.1524	FBF FBF	89.87 69.07			FBF FBF
506	C20 H38 O4	11.819	342.2770	FBF	82.60			FBF
507	C21 H40 O4	8.284	356.2899	FBF	55.10			FBF
i08 i09	C17 H32 O4 C7 H10 O4	9.090 1.032	300.2287 158.0580	FBF FBF	62.44 79.69			FBF FBF
510	C26 H50 O4	17.459	426.3715	FBF	97.81			FBF
511	C5 H9 N O4	0.409	147.0530	FBF	56.54			FBF
512	C4 H4 O4	0.435	116.0104	FBF	62.71			FBF
5 <u>13</u> 514	C18 H34 O4 C18 H32 O4	12.365 9.194	314.2460 312.2275	FBF FBF	82.65 77.78			FBF FBF
515	C10 H18 O4	6.621	202.1198	FBF	84.07			FBF
516	C24 H46 O4	15.042	398.3420	FBF	86.49			FBF
17 18	C12 H20 O4 C23 H44 O4	6.101 9.298	228.1357 384.3224	FBF FBF	81.65 86.88			FBF FBF
19	C13 H24 O4	6.465	244.1667	FBF	83.50			FBF
20	C11 H20 O4	7.426	216.1350	FBF	84.67			FBF
22	C16 H30 O5 C13 H18 O4	6.127 6.179	302.2088 238.1209	FBF FBF	81.38 81.26			FBF FBF
523	C15 H28 O2	8.622	240.2096	FBF	63.56			FBF
524	C7 H12 O2	3.371	128.0835	FBF	86.35			FBF
5 <u>25</u> 526	C22 H42 O2 C6 H4 Cl2 O5	9.246 8.102	338.3168 225.9434	<u>FBF</u> FBF	76.66 54.63			FBF FBF
527	C18 H30 O3	9.506	294.2193	FBF	71.54			FBF
528	C14 H20 O5	5.296	268.1286	FBF	58.27			FBF
29	C15 H14 O4	6.413	258.0869	FBF FBF	50.14		-	FBF
30 31	C12 H22 O3 C10 H20 O3	7.504 10.831	214.1555 188.1406	FBF	71.32 90.91			FBF FBF
32	C16 H32 O3	7.114	272.2349	FBF	99.32			FBF
33	C12 H24 O3	8.544	216.1722	FBF	68.19			FBF
5 <u>34</u> 535	C17 H30 O3 C14 H26 O3	8.674 19.304	282.2188 242.1882	<u>FBF</u> FBF	74.26 86.97			FBF FBF
536	C15 H30 O3	18.369	258.2186	FBF	63.72			FBF
37	C21 H42 O3	11.663	342.3104	FBF	50.02			FBF
538 539	C6 H12 O3 C20 H40 O3	4.541 7.894	132.0784 328.2962	FBF FBF	99.40 69.89			FBF FBF
540	C7 H14 O3	1.708	146.0950	FBF	79.40			FBF
541	C16 H30 O3	8.024	270.2174	FBF	75.60			FBF
542 543	C14 H28 O3 C8 H16 O3	6.205 1.344	244.2026	FBF FBF	81.63 74.87			FBF FBF
544	C18 H34 O3	8.102	160.1093 298.2487	FBF	68.31	-		FBF
545	C5 H6 O3	2.279	114.0312	FBF	84.89			FBF
546	C18 H36 O3	7.972	300.2660	FBF	83.34			FBF
547 548	C7 H12 O5 C6 H10 O3	2.305 0.409	176.0674 130.0624	FBF FBF	82.14 70.48			FBF FBF
49	C16 H32 O4	7.244	288.2291	FBF	95.56			FBF
550	C9 H18 O3	0.383	174.1254	FBF	99.47			FBF
551 552	C8 H16 O4 C9 H16 O3	4.437 0.383	176.1050 172.1100	FBF FBF	84.49 87.32			FBF FBF
553	C10 H16 O3	3.397	184.1088	FBF	81.67			FBF
554	C10 H18 O3	6.828	186.1253	FBF	82.20			FBF
5 <u>55</u> 556	C22 H40 O3 C22 H42 O3	11.871 9.740	352.2978 354.3120	FBF FBF	90.95 80.89			FBF FBF
57	C12 H20 O3	5.529	212.1393	FBF	73.65			FBF
58	C12 H18 O3	5.166	210.1254	FBF	76.79			FBF
59 60	C32 H50 O3 C32 H54 O3	13.613 17.173	482.3759 486.4062	FBF FBF	70.73 59.94			FBF FBF
61	C32 H62 O3	14.133	494.4683	FBF	87.66			FBF
62	C20 H38 O3	9.168	326.2800	FBF	69.93			FBF
63	C21 H38 O3	12.287	338.2797	FBF	79.03			FBF
<u>64</u> 65	C21 H32 O3 C21 H34 O3	12.287 12.781	332.2338 334.2494	FBF FBF	92.09 79.26			FBF FBF
66	C21 H40 O3	12.833	340.2967	FBF	61.42			FBF
67	C31 H58 O3	18.213	478.4353	FBF	51.58			FBF
<u>68</u> 69	C31 H62 O3 C31 H56 O3	17.225 17.589	482.4696 476.4255	FBF FBF	59.38 58.70			FBF FBF
70	C27 H50 O3	9.948	422.3753	FBF	97.29			FBF
71	C27 H40 O3	3.319	412.2996	FBF	51.09			FBF
<u>72</u>	C27 H44 O3 C17 H34 O3	12.339	416.3309	FBF FBF	59.45 50.04			FBF FBF
573 574	C17 H34 O3 C17 H32 O3	7.556 10.285	286.2519 284.2340	FBF FBF	59.94 75.83			FBF
75	C26 H48 O3	12.209	408.3605	FBF	55.98			FBF
76	C26 H44 O3	13.899	404.3271	FBF	67.22			FBF
77 78	C16 H28 O3 C16 H24 O3	6.231 0.383	268.2043 264.1705	FBF FBF	74.47 72.63			FBF FBF
76 79	C29 H54 O3	11.117	450.4056	FBF	84.67			FBF
580	C29 H46 O3	12.781	442.3456	FBF	75.51		· · · · · · · · · · · · · · · · · · ·	FBF



Compound Summary	F			CAC TO C		Constitution Constitution (PR) C. (MRC)
Cpd Name	Formula C29 H58 O3	RT	Mass 454.4390	CAS ID Source FBF	Score 67.86	Score (Lib) Score (DB) Score (MFG) Algo
581 582	C19 H34 O3	18.498 12.183	310.2507	FBF	96.22	
583	C19 H28 O3	8.804	304.2022	FBF	51.43	FBF
584	C19 H32 O3	10.337	308.2339	FBF	53.14	FBF
585	C19 H36 O3	12.781	312.2667	FBF	64.19	FBF
586	C28 H44 O3	14.886	428.3291	FBF	54.43	FBF
587	C28 H56 O3	13.275	440.4203	FBF	59.04	FBF
<u>588</u> 589	C18 H32 O3 C18 H26 O3	10.051 14.419	296.2339 290.1884	FBF FBF	78.77 80.27	FBF_FBF
590	C25 H46 O3	14.185	394.3451	FBF	77.44	FBF
591	C25 H36 O3	0.383	384.2664	FBF	64.61	FBF
592	C25 H44 O3	16.966	392.3293	FBF	56.07	FBF
593	C25 H48 O3	13.379	396.3618	FBF	52.11	FBF
594	C15 H26 O3	7.452	254.1875	FBF	72.82	FBF
595	C15 H24 O3	8.232	252.1750	FBF	69.90	FBF
<u>596</u> 597	C24 H44 O3 C24 H36 O3	12.391 8.440	380.3277 372.2685	<u>FBF</u> FBF	58.27 65.36	
598	C24 H40 O3	7.998	376.2955	FBF	51.86	FBF
599	C24 H42 O3	8.544	378.3167	FBF	57.59	FBF
500	C14 H24 O3	6.958	240.1725	FBF	75.34	FBF
501	C34 H66 O3	13.327	522.4994	FBF	87.33	FBF
502	C30 H56 O3	16.810	464.4208	FBF	70.18	FBF
503 504	C30 H46 O3 C30 H60 O3	15.354 14.783	454.3444 468.4543	FBF FBF	61.18 71.66	FBF_FBF
505	C30 H50 O3	17.667	458.3784	FBF	64.58	FBF
506	C23 H36 O3	7.608	360.2683	FBF	60.35	FBF
507	C23 H40 O3	12.443	364.2976	FBF	75.80	FBF
508	C13 H22 O3	6.231	226.1568	FBF	91.06	FBF
509	C13 H26 O3	6.387	230.1879	FBF	73.93	FBF
510	C13 H20 O3	5.919	224.1392	FBF	76.71	FBF
511 512	C13 H24 O3 C33 H62 O3	6.101 14.938	228.1723 506.4707	<u>FBF</u> FBF	73.15 58.87	
513	C33 H52 O3	19.356	496.3962	FBF	68.67	FBF
514	C33 H60 O3	18.654	504.4561	FBF	66.63	FBF
515	C11 H18 O3	12.989	198.1245	FBF	77.29	FBF
516	C11 H16 O3	0.383	196.1082	FBF	74.39	FBF
517	C11 H20 O3	6.673	200.1392	FBF	70.96	FBF
518	C11 H22 O3	5.919	202.1570	FBF	82.69	FBF
519 520	C10 H23 N3 O3	6.854	233.1735 344.2547	FBF FBF	63.82	FBF_FBF
621	C19 H36 O5 C19 H34 O4	10.571 11.377	326.2453	FBF	53.23 77.80	FBF
522	C10 H17 N O4	11.221	215.1176	FBF	64.16	FBF
523	C8 H14 O3	1.318	158.0941	FBF	86.18	FBF
624	C7 H12 O3	5.867	144.0777	FBF	74.20	FBF
625	C4 H6 O3	0.435	102.0315	FBF	79.17	FBF
626	C6 H11 N O3	6.179	145.0741	FBF	70.89	FBF
527 528	C27 H54 O2 C30 H60 O2	15.094	410.4140 452.4572	FBF FBF	55.94 69.50	FBF_FBF
629	C30 H60 O2	18.602 17.771	494.5073	FBF	64.79	FBF
530	C13 H26 O2	7.530	214.1923	FBF	69.32	FBF
531	C9 H19 N O2 S2	5.114	237.0858	FBF	67.43	FBF
532	C11 H20 O2	0.383	184.1462	FBF	99.86	FBF
533	C20 H36 O2	9.194	308.2726	FBF	83.64	FBF
534	C13 H22 O2	6.802	210.1615	FBF	82.85	FBF_
535	C22 H40 O2	10.831	336.3038	FBF ERE	63.80	FBF
536 537	C18 H34 O2 C24 H46 O2	13.613 14.860	282.2550 366.3469	FBF FBF	66.88 67.90	FBF_FBF
538	C8 H4 O2	1.032	132.0207	FBF	76.30	FBF
539	C10 H16 O2	5.010	168.1143	FBF	78.73	FBF
540	C9 H14 O2	1.967	154.0984	FBF	71.97	FBF
541	C12 H20 O2	8.440	196.1451	FBF	80.84	FBF
542	C20 H30 O2	9.688	302.2217	FBF	62.43	FBF
543	C8 H12 O2	9.168	140.0836	FBF	74.94	FBF
544 545	C12 H22 O2 C24 H36 O2	6.802 10.467	198.1607 356.2698	FBF FBF	77.72 54.66	
546	C7 H10 O2	2.409	126.0676	FBF	81.68	FBF
547	C11 H18 O2	6.984	182.1302	FBF	63.71	FBF
548	C14 H24 O2	22.057	224.1775	FBF	98.59	FBF
49	C10 H14 O3	3.085	182.0936	FBF	81.40	FBF
550	C5 H6 O2	0.409	98.0363	FBF	83.16	FBF
51	C4 H6 O2	0.383	86.0372	FBF	77.44 75.10	FBF
<u>52</u> 53	C23 H42 O2 C32 H60 O2	11.377 16.628	350.3172 476.4577	FBF FBF	75.10 54.55	FBF_FBF
53	C32 H56 O2	12.495	476.4577	FBF	55.27	FBF
555	C32 H62 O2	17.173	478.4725	FBF	74.22	FBF
556	C30 H44 O2	9.922	436.3374	FBF	69.97	FBF
557	C33 H64 O2	19.174	492.4875	FBF	62.90	FBF
58	C36 H52 O2	20.369	516.4014	FBF	64.01	FBF
559	C36 H68 O2	18.031	532.5245	FBF	57.49	FBF
560	C38 H72 O2	17.719	560.5537	FBF	57.31	FBF
61	C40 H68 O2	17.927	580.5216	FBF	55.29	FBF
662 663	C40 H66 O2 C42 H64 O2	21.252 11.325	578.5095 600.4928	FBF FBF	51.54 55.68	
64	C42 H60 O2	17.147	596.4602	FBF	72.56	FBF
65	C42 H70 O2	17.771	606.5379	FBF	53.59	FBF
566	C44 H74 O2	18.628	634.5713	FBF	52.23	FBF



Cpd Name	Formula	RT	Mass	CAS ID Source	e Score	Score (Lib)	Score (DB)	Score (MFG) Algorithr
667	C21 H38 O2	19.538	322.2891	FBF	75.10			FBF
568	C21 H40 O2	15.042	324.3003	FBF	58.85			FBF
569 570	C31 H56 O2 C27 H40 O2	18.602 14.315	460.4257 396.3049	FBF FBF	51.42 78.82			FBF FBF
571	C27 H40 O2 C27 H42 O2	5.503	398.3179	FBF	96.53			FBF
572	C27 H52 O2	13.093	408.3941	FBF	74.38			FBF
673	C17 H30 O2	7.868	266.2219	FBF	53.10			FBF
674	C26 H38 O2	13.379	382.2889	FBF	50.24	,		FBF
575	C26 H46 O2	20.525	390.3470	FBF	57.26			FBF
576	C26 H50 O2	15.042	394.3820	FBF	56.09			FBF
577 578	C16 H24 O2 C36 H60 O2	13.665 17.329	248.1775 524.4616	FBF FBF	59.93 62.54			FBF FBF
679	C36 H62 O2	14.990	526.4736	FBF	60.30			FBF
580	C29 H50 O2	16.940	430.3799	FBF	61.86			FBF
581	C29 H52 O2	14.445	432.3961	FBF	57.67			FBF
582	C9 H16 O2	8.622	156.1147	FBF	98.33			FBF
583	C28 H52 O2	16.160	420.3949	FBF	51.73			FBF
584	C28 H46 O2	13.275	414.3487	FBF	67.20			FBF
585	C28 H48 O2	11.871	416.3633	FBF	66.09			FBF
586 587	C25 H36 O2 C25 H38 O2	3.007 10.363	368.2727 370.2875	FBF FBF	57.17 59.16			FBF FBF
88	C24 H44 O2	14.860	364.3338	FBF	61.82			FBF
589	C30 H56 O2	21.019	448.4259	FBF	60.58			FBF
590	C30 H48 O2	14.003	440.3630	FBF	53.89	,		FBF
591	C30 H52 O2	10.753	444.3945	FBF	54.38			FBF
592	C23 H34 O2	7.608	342.2559	FBF	70.87			FBF
593	C23 H36 O2	11.247	344.2702	FBF	59.49			FBF
594	C13 H24 O2	9.116	212.1776	FBF	71.24			FBF
95	C33 H62 O2	19.746	490.4725	FBF	54.15			FBF
<u>96</u> 97	C25 H50 O7	18.758	462.3569	FBF FBF	50.66			FBF FBF
98	C14 H28 O6 C11 H19 CI O	5.192 0.409	292.1868 202.1125	FBF	60.65 64.19			FBF
99	C8 H18 O3	3.839	162.1253	FBF	86.07			FBF
00	C17 H32 O	12.703	252.2447	FBF	93.91			FBF
01	C16 H34 O	12.313	242.2604	FBF	83.64			FBF
02	C14 H26 O7	4.125	306.1662	FBF	63.73			FBF
03	C9 H20 O	5.945	144.1524	FBF	65.21			FBF
04	C11 H24 O	9.558	172.1830	FBF	77.95			FBF
05	C8 H16 O	13.821	128.1198	FBF	95.11			FBF
06 07	C5 H10 O C12 H20 O	0.383	86.0733	<u>FBF</u> FBF	99.77			FBF FBF
08	C18 H34 O	7.790 13.561	180.1509 266.2615	FBF	83.71 96.82			FBF
709	C20 H38 O	15.354	294.2925	FBF	98.16			FBF
10	C12 H24 O	6.075	184.1819	FBF	82.43			FBF
711	C16 H32 O	15.718	240.2454	FBF	99.93			FBF
'12	C15 H30 O	7.166	226.2280	FBF	67.85			FBF
13	C16 H30 O	11.871	238.2297	FBF	86.30			FBF
' <u>14</u>	C37 H66 O7	15.328	622.4811	FBF	63.79			FBF
7 <u>15 </u>	C22 H34 O5 C12 H26 O	4.958 7.634	378.2414 186.1981	<u>FBF</u> FBF	75.82 72.49			FBF FBF
'17	C8 H18 O2	13.821	146.1306	FBF	99.13	,		FBF
18	C41 H66 O13	5.010	766.4536	FBF	87.13			FBF
19	C14 H30 O	13.119	214.2308	FBF	64.16			FBF
'20	C11 H20 O	7.712	168.1506	FBF	61.04			FBF
21	C12 H14 O	6.283	174.1044	FBF	81.41			FBF
22	C13 H16 O	8.882	188.1213	FBF	80.87			FBF
23	C9 H14 O	0.409	138.1046	FBF	87.16			FBF
24	C6 H10 O	1.993	98.0730	FBF	77.74			FBF
25 26	C10 H18 O C15 H22 O	14.341 5.815	154.1356 218.1670	FBF FBF	82.50 99.91			FBF FBF
27	C18 H32 O	12.391	264.2454	FBF	99.32			FBF
28	C6 H12 O	0.383	100.0881	FBF	82.10			FBF
29	C8 H12 O	2.851	124.0879	FBF	66.63			FBF
30	C7 H14 O	19.538	114.1050	FBF	81.39			FBF
31	C14 H28 O	16.342	212.2142	FBF	99.83			FBF
32	C6 H8 O	1.370	96.0573	FBF	98.73			FBF
33	C18 H36 O	8.908	268.2759	FBF	98.20			FBF
'34 '35	C11 H19 N O3 C16 H29 N O5	0.383 12.287	213.1351 315.2067	FBF FBF	77.15 81.21			FBF FBF
36	C24 H41 N O	7.790	359.3201	FBF	65.54			FBF
37	C19 H35 N O5	18.343	357.2537	FBF	54.82			FBF
38	C22 H41 N O5	16.290	399.2969	FBF	70.45			FBF
39	C23 H43 N O5	10.337	413.3134	FBF	73.74			FBF
40	C23 H41 N O5	3.293	411.2966	FBF	71.07			FBF
41	C24 H45 N O5	13.457	427.3274	FBF	81.03			FBF
42	C24 H41 N O5	3.839	423.2979	FBF	69.92			FBF
43	C24 H39 N O5	17.018	421.2804	FBF	79.60			FBF
44	C24 H37 N O5	13.171	419.2667	FBF	69.36			FBF
² 45	C26 H41 N O5	17.485	447.2987	FBF	77.34			FBF
46 47	C26 H39 N O5 C29 H55 N O5	4.854 13.301	445.2845 497.4062	FBF FBF	53.21 57.95			FBF FBF
48	C30 H57 N O5	14.809	511.4240	FBF	86.93			FBF
49	C12 H21 N O5	5.893	259.1408	FBF	60.17			FBF
'50	C14 H25 N O5	8.310	287.1730	FBF	69.03			FBF
51	C13 H25 N O3	6.231	243.1833	FBF	97.48			FBF
752	C14 H27 N O3	10.285	257.1971	FBF	83.50			FBF



Cpd Name	nary Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (D	B) Score (MFG) Algorithm
753	C19 H37 N O3	8.648	327.2752	FBF	72.74		FBF
<u>754 </u>	C19 H35 N O3 C20 H39 N O3	7.192 19.070	325.2611 341.2906	FBF FBF	71.01 50.58	.	FBF FBF
756	C20 H39 N O3	16.056	339.2740	FBF	73.23		FBF
757	C21 H41 N O3	12.183	355.3074	FBF	80.51		FBF
758	C21 H39 N O3	8.206	353.2921	FBF	70.57		FBF
759	C22 H43 N O3	11.871	369.3216	FBF	51.58		FBF
760	C23 H45 N O3	13.509	383.3378	FBF	74.37		FBF
761	C23 H43 N O3	16.134	381.3206	FBF	51.87		FBF
7 <u>62</u> 763	C23 H37 N O3 C25 H49 N O3	7.010 18.550	375.2791 411.3715	FBF FBF	64.52 74.57		FBF FBF
764	C27 H53 N O3	9.948	439.4020	FBF	97.29		FBF
765	C28 H55 N O3	16.394	453.4157	FBF	56.18		FBF
766	C29 H57 N O3	11.117	467.4323	FBF	88.43		FBF
767	C10 H19 N O3	1.656	201.1363	FBF	80.93		FBF
768	C11 H21 N O3	0.383	215.1505	FBF	52.12		FBF
769	C12 H23 N O3	5.503	229.1661	FBF	68.81		FBF
770 771	C15 H31 N O C16 H33 N O	10.909	241.2414 255.2563	FBF FBF	98.28 86.30		FBF FBF
772	C17 H35 N O	11.871 12.625	269.2723	FBF	97.04		FBF
773	C18 H37 N O	13.561	283.2880	FBF	96.82		FBF
774	C19 H39 N O	14.886	297.3023	FBF	94.98		FBF
775	C20 H41 N O	15.380	311.3191	FBF	98.16		FBF
776	C20 H39 N O	13.743	309.3024	FBF	73.95		FBF
777	C21 H41 N O	17.173	323.3163	FBF	51.34		FBF
778	C22 H45 N O	15.952	339.3498	FBF	83.31		FBF
779 780	C22 H43 N O	15.302 8.232	337.3346	FBF FBF	99.02		FBF FBF
780 781	C23 H43 N O C23 H39 N O	8.232 7.842	349.3375 345.3035	FBF	60.19 61.33		FBF
782	C24 H47 N O	16.316	365.3627	FBF	59.32		FBF
783	C25 H51 N O	18.680	381.3965	FBF	78.97		FBF
784	C25 H47 N O	9.246	377.3638	FBF	68.35		FBF
785	C25 H43 N O	15.926	373.3373	FBF	75.92		FBF
786	C26 H53 N O	19.304	395.4112	FBF	89.82		FBF
787	C27 H45 N O	12.391	399.3489	FBF	64.25		FBF
788 789	C29 H59 N O C30 H61 N O	20.577 22.083	437.4572 451.4722	FBF FBF	68.51 61.77		FBF FBF
790	C9 H19 N O	6.491	157.1463	FBF	99.06		FBF
791	C10 H21 N O	6.958	171.1617	FBF	63.25		FBF
792	C11 H23 N O	7.738	185.1779	FBF	76.43		FBF
793	C12 H25 N O	8.622	199.1924	FBF	78.74		FBF
794	C14 H29 N O	10.805	227.2248	FBF	87.27		FBF
795	C17 H34 N4 O3	10.831	342.2637	FBF	74.21		FBF
796	C21 H40 N4 O3	13.847	396.3099	FBF	59.34		FBF
797 798	C26 H52 N4 O3 C26 H50 N4 O3	14.886	468.4072 466.3907	FBF FBF	60.39 54.66		FBF FBF
799 799	C26 H48 N4 O3	15.380 11.247	464.3701	FBF	83.74		FBF
800	C26 H42 N4 O3	14.471	458.3265	FBF	60.08		FBF
801	C27 H54 N4 O3	10.831	482.4171	FBF	75.63		FBF
802	C28 H56 N4 O3	17.147	496.4349	FBF	53.40		FBF
803	C28 H54 N4 O3	18.317	494.4203	FBF	59.40		FBF
804	C28 H52 N4 O3	13.379	492.4009	FBF	51.38		FBF
805	C28 H48 N4 O3	10.857	488.3724	FBF	77.64		FBF
806	C28 H46 N4 O3	14.367	486.3577	FBF	64.22		FBF
807 808	C28 H44 N4 O3 C10 H20 N4 O3	10.259 2.435	484.3403 244.1543	FBF FBF	86.58 94.61		FBF FBF
309	C13 H26 N4 O3	3.293	286.2007	FBF	95.32		FBF
810	C18 H32 N2 O4	4.541	340.2369	FBF	58.42		FBF
311	C21 H38 N2 O4	11.923	382.2799	FBF	53.50		FBF
312	C22 H42 N2 O4	5.503	398.3180	FBF	68.36		FBF
813	C22 H36 N2 O4	3.293	392.2645	FBF	73.79		FBF
314	C24 H46 N2 O4	9.870	426.3460	FBF	72.64		FBF
315	C24 H38 N2 O4	14.289	418.2870	FBF	51.04		FBF
816	C24 H36 N2 O4	4.854	416.2649	FBF ERE	63.67		FBF
317 318	C25 H48 N2 O4 C26 H40 N2 O4	14.055 12.313	440.3631 444.2991	FBF FBF	66.20 67.07		FBF FBF
319	C27 H52 N2 O4	14.055	468.3942	FBF	59.46		FBF
320	C9 H16 N2 O4	9.090	216.1098	FBF	51.12		FBF
821	C10 H18 N2 O4	12.001	230.1276	FBF	52.55		FBF
322	C21 H35 N O5	4.671	381.2535	FBF	60.83		FBF
323	C24 H35 N O5	5.348	417.2499	FBF	52.17		FBF
324	C18 H35 N3 O4	4.541	357.2633	FBF	58.11		FBF
325	C24 H47 N3 O4	14.315	441.3579	FBF	61.78		FBF
826 827	C24 H45 N3 O4	18.628	439.3432	FBF ERE	62.71 55.54		FBF FBF
827 828	C24 H43 N3 O4 C24 H39 N3 O4	3.267 12.261	437.3214 433.2968	FBF FBF	55.54 54.64		FBF
829	C26 H41 N3 O4	5.477	459.3074	FBF	61.44		FBF
830	C32 H63 N3 O4	17.927	553.4772	FBF	67.64		FBF
	C10 H19 N3 O4	7.218	245.1377	FBF	58.79		FBF
831	C14 H27 N3 O4	2.149	301.1985	FBF	69.69		FBF
832 833	C15 H29 N3 O4	4.255	315.2133	FBF	53.71		FBF
831 832 833 834	C15 H29 N3 O4 C13 H25 N O3 S	5.192	275.1574	FBF	61.42		FBF
832 833 834 835	C15 H29 N3 O4 C13 H25 N O3 S C14 H27 N O3 S	5.192 6.543	275.1574 289.1703	FBF FBF	61.42 66.92		FBF FBF
832 833 834	C15 H29 N3 O4 C13 H25 N O3 S	5.192	275.1574	FBF	61.42		FBF



Cpd Name	mary Formula	DT	M	CAS ID Sames	E	Score (I :L)	Score (DB)	Score (MEC) Alasairian
839	Formula C20 H37 N O3 S	RT 2.643	Mass 371.2502	CAS ID Source FBF	72.23	Score (Lib)	Score (DB)	Score (MFG) Algorithm FBF
840	C21 H39 N O3 S	4.724	385.2662	FBF	68.88			FBF
841	C21 H37 N O3 S	11.455	383.2490	FBF	66.78			FBF
842	C21 H35 N O3 S	22.031	381.2362	FBF	57.29			FBF
843 844	C21 H33 N O3 S C23 H37 N O3 S	11.247 4.750	379.2198 407.2469	FBF FBF	70.94 59.68			FBF FBF
845	C25 H47 N O3 S	5.841	441.3289	FBF	65.85			FBF
846	C25 H39 N O3 S	4.854	433.2645	FBF	61.53			FBF
847	C9 H17 N O3 S	10.051	219.0942	FBF	64.26			FBF
848 849	C12 H23 N O3 S C27 H43 N O5	<u>17.537</u> 5.374	261.1401 461.3159	FBF FBF	64.62 64.40			FBF FBF
850	C27 H41 N O5	4.359	459.2980	FBF	86.58			FBF
851	C29 H45 N O5	15.354	487.3312	FBF	63.44			FBF
852	C29 H43 N O5	5.374	485.3125	FBF	59.64			FBF
853 854	C29 H39 N O5 C31 H45 N O5	15.276 3.839	481.2842 511.3287	FBF FBF	57.30 69.87			FBF FBF
855	C31 H43 N O5	4.359	509.3138	FBF	54.40			FBF
856	C32 H55 N O5	14.860	533.4063	FBF	80.36			FBF
857	C33 H57 N O5	17.615	547.4245	FBF	52.35			FBF
858 859	C34 H59 N O5 C35 H61 N O5	17.901 20.733	561.4421 575.4585	FBF FBF	67.55 78.25			FBF FBF
860	C15 H21 N O5	21.460	295.1444	FBF	64.06			FBF
861	C26 H37 N O3	5.348	411.2805	FBF	68.71			FBF
862	C28 H47 N O3	17.433	445.3530	FBF	52.70			FBF
863	C28 H39 N O3	3.553	437.2940	FBF	78.57			FBF
864 865	C23 H38 N2 O4 C23 H36 N2 O4	5.322 4.776	406.2847 404.2689	FBF FBF	77.46 54.58			FBF FBF
866	C25 H40 N2 O4	17.771	432.2992	FBF	56.52			FBF
867	C27 H42 N2 O4	4.984	458.3141	FBF	77.35			FBF
868	C25 H43 N O5	4.359	437.3160	FBF	83.36			FBF
869 870	C25 H37 N O5 C16 H29 N O3	5.374 11.663	431.2674 283.2137	FBF FBF	50.23 61.63			FBF FBF
871	C19 H33 N O3	2.643	323.2439	FBF	68.71			FBF
872	C24 H35 N O3	4.724	385.2648	FBF	71.30			FBF
873	C16 H27 N3 O3	1.993	309.2031	FBF	62.67			FBF
874	C20 H35 N3 O3	3.605	365.2644	FBF	68.03			FBF
875 876	C20 H33 N3 O3 C21 H35 N3 O3	4.619 12.937	363.2529 377.2686	FBF FBF	77.51 62.42			FBF FBF
877	C22 H39 N3 O3	3.007	393.2957	FBF	57.41			FBF
878	C22 H37 N3 O3	22.629	391.2847	FBF	71.26			FBF
879	C23 H39 N3 O3	14.912	405.2972	FBF	62.98			FBF
880 881	C24 H43 N3 O3 C24 H41 N3 O3	12.391 13.041	421.3324 419.3137	FBF FBF	70.51 52.74			FBF FBF
882	C24 H37 N3 O3	5.374	415.2821	FBF	65.40			FBF
883	C26 H47 N3 O3	17.459	449.3579	FBF	59.35			FBF
884	C26 H41 N3 O3	5.451	443.3174	FBF	62.16			FBF
885 886	C28 H49 N3 O3	19.070	475.3762	FBF FBF	66.13 77.98			FBF FBF
887	C28 H47 N3 O3 C29 H53 N3 O3	14.886 19.408	473.3609 491.4122	FBF	60.07			FBF
888	C31 H57 N3 O3	19.278	519.4364	FBF	55.31			FBF
889	C32 H59 N3 O3	17.329	533.4560	FBF	67.85			FBF
890	C11 H17 N3 O3	6.153	239.1287	FBF	52.40			FBF
891 892	C23 H43 N3 O C25 H43 N3 O	11.403 7.868	377.3424 401.3443	FBF FBF	73.86 60.25			FBF FBF
893	C25 H41 N3 O	13.379	399.3269	FBF	53.91		-	FBF
894	C27 H49 N3 O	12.027	431.3866	FBF	56.56		,	FBF
895	C29 H55 N3 O	15.744	461.4362	FBF	59.26			FBF
896 897	C30 H57 N3 O C31 H59 N3 O	20.733 14.601	475.4491 489.4683	FBF FBF	58.57 57.92			FBF FBF
898	C12 H21 N3 O	5.374	223.1701	FBF	68.80			FBF
899	C30 H59 N O3	17.667	481.4525	FBF	54.52			FBF
900	C31 H61 N O3	17.018	495.4633	FBF	54.85			FBF
901 902	C19 H38 N2 O3 C20 H38 N2 O3	7.192 15.042	342.2859 354.2873	FBF FBF	72.65 72.89			FBF FBF
903	C20 H38 N2 O3 C21 H42 N2 O3	8.206	354.2873 370.3170	FBF	60.28			FBF
904	C22 H42 N2 O3	15.900	382.3189	FBF	55.08			FBF
905	C23 H46 N2 O3	15.042	398.3490	FBF	65.53			FBF
906	C24 H46 N2 O3	17.459	410.3477	FBF	63.14			FBF
907 908	C24 H40 N2 O3 C26 H52 N2 O3	12.391 17.433	404.3052 440.3984	FBF FBF	68.46 75.73			FBF FBF
909	C26 H46 N2 O3	9.740	434.3490	FBF	58.16			FBF
910	C28 H48 N2 O3	14.938	460.3683	FBF	68.73			FBF
911	C28 H46 N2 O3	10.285	458.3492	FBF	72.38			FBF
912 913	C30 H60 N2 O3	17.667 3.553	496.4616 437.2944	FBF FRF	52.56 74.89			FBF FBF
914	C25 H43 N O3 S C27 H45 N O3 S	3.553 5.763	437.2944	FBF FBF	74.89 55.85			FBF
915	C19 H36 N2 O3	10.389	340.2733	FBF	50.89			FBF
916	C25 H46 N2 O3	16.680	422.3503	FBF	71.23			FBF
917	C25 H40 N2 O3	9.688	416.3049	FBF	54.28			FBF
918	C25 H35 N O3	7.010	397.2607	FBF	76.78			FBF
919 920	C27 H41 N O3 C27 H37 N O3	7.634 12.729	427.3056 423.2763	FBF FBF	60.98 52.40			FBF FBF
921	C27 H35 N O3	9.506	421.2614	FBF	74.55			FBF
922	C29 H49 N O3	16.394	459.3700	FBF	66.95			FBF
923	C29 H39 N O3	10.571	449.2914	FBF	76.57			FBF



Compound Summary							
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorith
925	C32 H55 N O3	17.641	501.4191	FBF	63.39		FBF
926	C14 H19 N O3	8.908	249.1383	FBF	75.53		FBF
927	C35 H61 N O3	18.836	543.4663	FBF	64.28		FBF
928	C18 H38 N2 O	8.518	298.2964	FBF	70.07		FBF
929 930	C20 H42 N2 O C22 H46 N2 O	12.495 7.738	326.3271 354.3598	FBF FBF	69.61 79.98		FBF FBF
931	C22 H44 N2 O	16.550	352.3472	FBF	59.78		FBF
932	C22 H38 N2 O	9.142	346.2984	FBF	57.88		FBF
933	C23 H48 N2 O	10.000	368.3757	FBF	80.00		FBF
934	C24 H50 N2 O	15.172	382.3899	FBF	72.41		FBF
935	C24 H48 N2 O	8.726	380.3746	FBF	61.41		FBF
936	C24 H42 N2 O	14.289	374.3326	FBF	54.42		FBF
937	C24 H40 N2 O	13.353	372.3151	FBF	73.73		FBF
938 939	C26 H50 N2 O C26 H46 N2 O	10.415 16.056	406.3929 402.3648	FBF FBF	54.41 73.07	.	FBF FBF
940	C13 H25 N O4	9.142	259.1770	FBF	60.12		FBF
941	C14 H27 N O4	4.125	273.1939	FBF	82.80		FBF
942	C16 H31 N O4	0.383	301.2246	FBF	74.91		FBF
943	C17 H33 N O4	9.376	315.2420	FBF	59.98		FBF
944	C17 H31 N O4	10.051	313.2260	FBF	71.57		FBF
945	C18 H35 N O4	12.963	329.2589	FBF	64.24		FBF
946	C19 H35 N O4	14.860	341.2545	FBF	68.13		FBF
947 948	C20 H37 N O4	13.665 15.952	355.2733 371.3050	FBF FBF	80.17 59.00		FBF FBF
949	C21 H41 N O4 C21 H39 N O4	10.363	369.2889	FBF	73.59		FBF
950	C21 H37 N O4	3.007	367.2704	FBF	71.52		FBF
951	C21 H33 N O4	10.337	363.2433	FBF	53.36		FBF
952	C22 H43 N O4	11.949	385.3210	FBF	52.69		FBF
953	C22 H41 N O4	11.819	383.3012	FBF	64.54		FBF
954	C24 H47 N O4	13.093	413.3482	FBF	77.57		FBF
955	C25 H49 N O4	18.784	427.3678	FBF	53.93		FBF
956	C25 H47 N O4	18.524	425.3523 423.3364	FBF FBF	59.95 66.27		FBF FBF
957 958	C25 H45 N O4 C25 H37 N O4	18.395 4.099	415.2760	FBF	63.33		FBF
959	C27 H53 N O4	13.353	455.3955	FBF	60.75		FBF
160	C29 H57 N O4	17.381	483.4284	FBF	69.62	· · · · · · · · · · · · · · · · · · ·	FBF
961	C9 H17 N O4	3.085	203.1156	FBF	77.95		FBF
962	C10 H19 N O4	7.608	217.1319	FBF	61.20		FBF
963	C12 H23 N O4	0.409	245.1624	FBF	68.06		FBF
964	C12 H25 N O4 S	4.125	279.1524	FBF	50.59		FBF
965	C14 H29 N O4 S	9.922	307.1830	FBF	51.88		FBF
966	C16 H31 N O4 S	5.867	333.1988	FBF	66.43		FBF
967 968	C17 H33 N O4 S	9.350 9.948	347.2134	<u>FBF</u> FBF	64.83 63.79		FBF FBF
969	C18 H35 N O4 S C19 H39 N O4 S	20.395	361.2297 377.2631	FBF	51.18		FBF
970	C19 H35 N O4 S	2.825	373.2296	FBF	81.86	-	FBF
971	C20 H37 N O4 S	3.007	387.2464	FBF	81.45		FBF
972	C20 H35 N O4 S	2.747	385.2306	FBF	65.89		FBF
973	C22 H41 N O4 S	4.099	415.2761	FBF	85.33		FBF
974	C24 H49 N O4 S	22.914	447.3382	FBF	52.98		FBF
975	C24 H41 N O4 S	5.218	439.2750	FBF	63.88		FBF
976	C25 H51 N O4 S	13.951	461.3556	FBF	57.98		FBF
977 978	C26 H53 N O4 S C6 H13 N O4 S	17.667 13.301	475.3696 195.0560	<u>FBF</u> FBF	59.83 71.45	.	FBF FBF
979	C7 H15 N O4 S	3.293	209.0703	FBF	78.13		FBF
980	C22 H35 N O4	13.223	377.2576	FBF	75.82		FBF
981	C24 H45 N O4	12.235	411.3347	FBF	58.95		FBF
982	C26 H39 N O4	4.906	429.2874	FBF	56.42		FBF
983	C22 H32 N2 O3	4.671	372.2385	FBF	53.55	<u> </u>	FBF
984	C24 H36 N2 O3	10.077	400.2723	FBF	68.85		FBF
985	C25 H38 N2 O3	4.854	414.2884	FBF	63.29		FBF
986	C26 H38 N2 O3	3.085 3.397	426.2886 440.3035	<u>FBF</u> FBF	82.73 77.81	.	FBF FBF
987 988	C27 H40 N2 O3 C28 H42 N2 O3	3.397	454.3197	FBF	80.90		FBF
989	C29 H42 N2 O3	5.503	466.3201	FBF	86.15		FBF
990	C29 H40 N2 O3	9.636	464.3046	FBF	58.61		FBF
991	C29 H38 N2 O3	3.423	462.2853	FBF	58.97		FBF
992	C30 H48 N2 O3	13.093	484.3699	FBF	50.13		FBF
993	C30 H46 N2 O3	4.515	482.3476	FBF	61.03		FBF
994	C31 H50 N2 O3	20.291	498.3813	FBF	60.72		FBF
95	C31 H40 N2 O3	5.477	488.3050	FBF	56.98 76.71		FBF
96	C33 H54 N2 O3	19.096	526.4128	FBF	76.71		FBF
97 98	C33 H50 N2 O3 C33 H46 N2 O3	11.845 6.075	522.3812 518.3525	<u>FBF</u> FBF	63.55 51.01		FBF FBF
999	C35 H58 N2 O3	19.148	516.3525	FBF	64.03		FBF
000	C36 H60 N2 O3	18.135	568.4629	FBF	59.31		FBF
.001	C16 H20 N2 O3	8.908	288.1485	FBF	67.73		FBF
002	C18 H24 N2 O3	10.883	316.1766	FBF	67.87		FBF
003	C20 H28 N2 O3	18.031	344.2072	FBF	62.80		FBF
.004	C20 H30 N2 O	17.433	314.2375	FBF	56.89		FBF
005	C25 H38 N2 O	13.379	382.3020	FBF	70.23		FBF
006	C26 H40 N2 O	13.457	396.3159	FBF	64.96		FBF
1007	C27 H44 N2 O	13.067	412.3446	FBF	56.62		FBF
008	C27 H40 N2 O	13.275	408.3135	FBF	60.98		FBF
009 010	C28 H38 N2 O C29 H48 N2 O	10.571 17.433	418.3007 440.3807	<u>FBF</u> FBF	69.40 52.86		FBF FBF
010	CES IT IO INC U	17.733	1 10.3007	וט ו	J2.00		FDF



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Cpd Name 1011	Formula C29 H46 N2 O	13.301	Mass 438.3635	CAS ID Source FBF	Score 59.75	Score (Lib) Score	e (DB) Score (MFG) Algorithn FBF
1012	C30 H48 N2 O	14.367	452.3790	FBF	61.18		FBF
013	C30 H46 N2 O	14.886	450.3609	FBF	62.75		FBF
014	C30 H40 N2 O	4.932	444.3122	FBF	65.89		FBF
015	C32 H54 N2 O	17.381	482.4262	FBF	59.34		FBF
016	C32 H52 N2 O	14.860	480.4049	FBF	56.29		FBF
017 018	C35 H60 N2 O C36 H62 N2 O	18.576 19.330	524.4736 538.4882	FBF FBF	72.66 74.29		<u>FBF</u> FBF
019	C27 H37 N O4	5.244	439.2749	FBF	54.02		FBF
020	C29 H49 N O4	17.667	475.3696	FBF	50.22		FBF
.021	C29 H39 N O4	4.177	465.2886	FBF	53.82		FBF
.022	C30 H51 N O4	13.353	489.3819	FBF	61.33		FBF
.023	C31 H49 N O4	6.335	499.3686	FBF	78.79		FBF
024	C32 H55 N O4	17.511	517.4130	FBF	69.46		FBF
025 026	C35 H61 N O4 C16 H23 N O4	19.356 3.995	559.4600 293.1615	<u>FBF</u> FBF	75.58 70.22		FBF FBF
027	C9 H19 N O4	0.409	205.1313	FBF	72.97		FBF
028	C19 H37 N O2	7.920	311.2824	FBF	89.89	,	FBF
029	C22 H43 N O2	11.117	353.3263	FBF	51.92		FBF
030	C22 H41 N O2	11.559	351.3144	FBF	55.93		FBF
031	C24 H47 N O2	16.966	381.3586	FBF	62.49		FBF
032	C28 H55 N O2	18.602	437.4242	FBF	57.12		FBF
033	C17 H33 N O2	7.062	283.2503	FBF FRE	59.40 59.72		FBF FRE
034 035	C21 H43 N O2 C21 H33 N O2	13.223 22.785	341.3280 331.2531	<u>FBF</u> FBF	68.90		FBF FBF
036	C21 H33 N O2	10.779	359.2858	FBF	56.13		FBF
037	C25 H49 N O2	14.964	395.3761	FBF	59.57		FBF
038	C27 H53 N O2	17.355	423.4078	FBF	80.31		FBF
039	C28 H57 N O2	17.173	439.4365	FBF	65.10		FBF
040	C28 H49 N O2	13.327	431.3755	FBF	76.60		FBF
041	C28 H45 N O2 C26 H51 N O2	16.108	427.3465	FBF	56.61		FBF
042 043	C20 H39 N O2	13.327 8.336	409.3910 325.2964	FBF FBF	51.90 88.47		FBF FBF
044	C18 H37 N O2	11.169	299.2810	FBF	70.61		FBF
045	C17 H35 N O2	9.662	285.2667	FBF	95.17		FBF
046	C20 H41 N O2	12.859	327.3120	FBF	76.29	-	FBF
047	C25 H51 N O2	15.536	397.3882	FBF	58.20		FBF
048	C8 H17 N O S2	4.880	207.0756	FBF	62.23		FBF
049	C18 H35 N O	12.417	281.2719	FBF	99.32		FBF
050 051	C18 H33 N O C8 H15 N O S2	11.455 9.844	279.2552 205.0606	FBF FBF	68.23 84.17		FBF FBF
052	C16 H31 N O	19.460	253.2413	FBF	55.35		FBF
053	C5 H11 N O	0.383	101.0838	FBF	86.24		FBF
054	C12 H23 N O2 S2	5.581	277.1183	FBF	59.60		FBF
055	C10 H19 N O2 S2	5.841	249.0872	FBF	58.39		FBF
056	C16 H35 N	8.284	241.2762	FBF	97.18		FBF
057	C6 H15 N	17.018	101.1206	FBF	99.82		FBF
058	C15 H33 N	8.154	227.2608	FBF	85.89		FBF FBF
.059 .060	C18 H39 N C8 H19 N	9.376 1.708	269.3077 129.1513	FBF FBF	89.40 83.52		FBF
061	C4 H12 N2	21.148	88.1007	FBF	83.17		FBF
062	C14 H31 N	7.348	213.2454	FBF	99.32		FBF
063	C13 H29 N	7.218	199.2290	FBF	95.08		FBF
064	C17 H33 N O5	9.350	331.2356	FBF	64.17		FBF
065	C18 H29 N O5	4.437	339.2025	FBF	67.67		FBF
066	C19 H31 N O4	4.437	337.2269	FBF	52.91		FBF
067	C21 H41 N O5	17.070	387.2948	FBF	63.00		FBF FBF
068 069	C23 H45 N O5 C24 H47 N O5	9.740 11.637	415.3275 429.3431	FBF FBF	52.85 51.77		FBF
070	C25 H49 N O5	13.639	443.3605	FBF	72.44		FBF
071	C26 H45 N O4	15.042	435.3371	FBF	64.90		FBF
072	C31 H54 N O4	10.831	504.4020	FBF	82.82		FBF
073	C28 H55 N O5	14.055	485.4087	FBF	62.67		FBF
074	C29 H57 N O5	16.498	499.4220	FBF	60.17		FBF
075	C29 H53 N O4	18.420	479.3976	FBF	54.76 52.01		FBF
076 077	C31 H61 N O4 C31 H55 N O4	16.706 9.142	511.4577 505.4171	<u>FBF</u> FBF	52.01 60.10		FBF FBF
077 078	C32 H63 N O4	16.628	525.4739	FBF	61.62		FBF
079	C33 H65 N O4	17.641	539.4918	FBF	70.22		FBF
080	C33 H63 N O4	19.278	537.4780	FBF	65.21		FBF
081	C33 H61 N O4	16.108	535.4611	FBF	63.62		FBF
082	C35 H57 N O4	10.337	555.4320	FBF	64.55		FBF
083	C12 H23 N O5	6.647	261.1578	FBF	75.92		FBF
084 085	C11 H21 N O5	0.383	247.1438	FBF FRE	75.47		FBF ERE
085 086	C11 H19 N O4 C12 H21 N O4	2.201 6.880	229.1319 243.1489	<u>FBF</u> FBF	95.39 64.56		FBF FBF
087	C12 H21 N 04 C13 H25 N 05	6.205	275.1720	FBF	56.60		FBF
088	C13 H23 N O4	4.958	257.1619	FBF	60.26		FBF
089	C14 H25 N O4	2.591	271.1762	FBF	84.26		FBF
090	C15 H29 N O5	9.246	303.2055	FBF	93.58		FBF
091	C15 H27 N O4	8.050	285.1940	FBF	79.80		FBF
092	C16 H31 N O5	4.437	317.2201	FBF	81.29		FBF
093	C17 H31 N O6	13.717	345.2152	FBF	64.13		FBF
<u>094</u> 095	C18 H29 N O6	3.007	355.1992	FBF	56.62		FBF
IIIIS	C19 H35 N O6	10.727	373.2449	FBF	70.93		FBF



Compound Summary							
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorithm
1097	C19 H29 N O6	7.218	367.1998	FBF	64.55		FBF
1098 1099	C20 H33 N O6 C20 H31 N O6	5.036 9.480	383.2286 381.2165	<u>FBF</u> FBF	58.50 91.85		FBF FBF
1100	C21 H33 N O6	15.068	395.2332	FBF	79.09		FBF
1101	C22 H41 N O6	16.654	415.2946	FBF	55.73		FBF
1102	C22 H39 N O6	12.521	413.2755	FBF	77.15		FBF
1103	C22 H35 N O6	7.244	409.2486	FBF	89.00		FBF
1104	C23 H43 N O6	5.140	429.3076	FBF	67.98		FBF
1105	C23 H39 N O6	4.854	425.2795	FBF	54.11		FBF
1106 1107	C23 H37 N O6 C24 H45 N O6	5.348 16.056	423.2618 443.3218	<u>FBF</u> FBF	50.46 65.01		FBF FBF
1108	C24 H43 N O6	5.659	441.3071	FBF	64.54		FBF
1109	C24 H41 N O6	7.894	439.2927	FBF	52.48	-	FBF
1110	C24 H39 N O6	7.920	437.2796	FBF	91.20		FBF
1111	C25 H47 N O6	10.285	457.3395	FBF	89.73		FBF
1112	C25 H45 N O6	3.553	455.3230	FBF	71.41		FBF
1113	C25 H41 N O6	10.597	451.2929	FBF	50.59		FBF
1114 1115	C26 H45 N O6 C27 H47 N O6	0.383 4.515	467.3240 481.3422	FBF FBF	97.67 74.65		FBF FBF
1116	C27 H47 N O6	3.449	475.2970	FBF	71.50		FBF
1117	C29 H51 N O6	10.857	509.3750	FBF	50.68		FBF
1118	C29 H47 N O6	5.426	505.3395	FBF	55.24		FBF
1119	C29 H45 N O6	4.515	503.3241	FBF	77.20		FBF
1120	C11 H17 N O6	5.607	259.1051	FBF	83.67		FBF
1121	C12 H21 N O6	8.050	275.1372	FBF	65.18		FBF
1122 1123	C13 H23 N O6 C13 H21 N O6	8.674 6.854	289.1523 287.1382	<u>FBF</u> FBF	83.91 52.64		FBF FBF
1124	C14 H23 N O6	7.972	301.1526	FBF	96.67		FBF
1125	C16 H29 N O6	11.325	331.2016	FBF	67.79		FBF
1126	C29 H48 N7 O17 P3 S	13.925	891.2027	FBF	65.71		FBF
1127	C26 H44 N7 O18 P3 S	13.197	867.1702	FBF	55.73		FBF
1128	C26 H44 N7 O17 P3 S	13.899	851.1683	FBF	57.51		FBF
1129	C25 H43 N8 O17 P3 S	13.509	852.1646	FBF	69.19		FBF
1130	C27 H46 N7 O18 P3 S	13.873	881.1869	FBF	51.50		FBF
l 131 l 132	C36 H64 N7 O18 P3 S C33 H56 N7 O18 P3 S	19.824 21.538	1007.3248 963.2645	<u>FBF</u> FBF	94.26 72.26	.	FBF FBF
133	C37 H64 N7 O18 P3 S	19.824	1019.3206	FBF	63.80		FBF
134	C31 H50 N7 O18 P3 S	18.265	933.2192	FBF	62.41		FBF
1135	C24 H41 N8 O17 P3 S	13.769	838.1550	FBF	78.26		FBF
1136	C25 H42 N7 O17 P3 S	14.393	837.1617	FBF	58.24		FBF
L137	C30 H42 N7 O19 P3 S	15.146	929.1433	FBF	50.06		FBF
1138	C33 H54 N7 O17 P3 S	19.850	945.2521	FBF	84.49		FBF
1139 1140	C24 H40 N7 O17 P3 S	13.899	823.1478 1013.2814	<u>FBF</u> FBF	50.02 83.42		FBF FBF
1141	C37 H58 N7 O18 P3 S C39 H62 N7 O18 P3 S	19.798 19.824	1041.3025	FBF	53.13		FBF
1142	C31 H44 N7 O19 P3 S	13.847	943.1699	FBF	53.07		FBF
1143	C28 H54 O4	17.459	454.4026	FBF	99.02		FBF
1144	C25 H48 O4	10.415	412.3529	FBF	74.24		FBF
1145	C19 H36 O4	12.963	328.2611	FBF	84.94		FBF
1146	C21 H36 O4	10.337	352.2624	FBF	76.59		FBF
1147	C22 H40 O4	15.042	368.2953	FBF	63.37		FBF
<u>1148 </u>	C23 H42 O4 C23 H40 O4	13.301 13.977	382.3073 380.2920	FBF FBF	62.68 51.96		FBF FBF
1150	C23 H36 O4	15.068	376.2639	FBF	95.15		FBF
1151	C24 H44 O4	15.952	396.3216	FBF	68.10		FBF
1152	C24 H42 O4	13.275	394.3088	FBF	54.95		FBF
1153	C24 H40 O4	15.068	392.2904	FBF	84.35		FBF
1154	C25 H46 O4	13.327	410.3382	FBF	63.92		FBF
155	C25 H44 O4	20.863	408.3219	FBF	74.19	· · · · · · · · · · · · · · · · · · ·	FBF
.156 .157	C25 H42 O4 C25 H40 O4	17.459 12.391	406.3076 404.2919	FBF FBF	83.65 51.90		FBF FBF
.158	C25 H30 O4	7.400	404.2919	FBF	66.27		FBF
159	C27 H50 O4	14.497	438.3709	FBF	59.62		FBF
160	C27 H44 O4	9.844	432.3235	FBF	58.98		FBF
161	C28 H50 O4	9.740	450.3743	FBF	57.93		FBF
.162	C28 H48 O4	17.459	448.3539	FBF	95.30		FBF
163	C29 H50 O4	0.383	462.3685	FBF	87.98		FBF
164 165	C29 H46 O4 C30 H56 O4	10.311 19.044	458.3414 480.4169	<u>FBF</u> FBF	72.80 70.79		FBF FBF
166	C30 H56 O4 C31 H52 O4	14.990	488.3853	FBF	61.83		FBF
167	C31 H46 O4	6.335	482.3410	FBF	77.13		FBF
168	C32 H58 O4	16.576	506.4349	FBF	51.03		FBF
.169	C33 H62 O4	18.213	522.4628	FBF	56.50		FBF
.170	C33 H58 O4	10.285	518.4361	FBF	53.26		FBF
171	C33 H54 O4	19.226	514.4057	FBF	74.03		FBF
1172	C33 H50 O4	9.168	510.3745	FBF	68.60		FBF
.173 .174	C34 H62 O4 C35 H66 O4	17.251 17.615	534.4628 550.4947	FBF FBF	55.18 53.65		FBF FBF
175	C35 H58 O4	17.615	542.4328	FBF	71.28		FBF
176	C35 H54 O4	10.311	538.4071	FBF	70.95		FBF
177	C36 H66 O4	19.174	562.4946	FBF	56.96		FBF
178	C36 H56 O4	11.143	552.4215	FBF	61.36		FBF
179	C18 H30 O4	8.102	310.2129	FBF	67.02		FBF
.180	C19 H32 O4	8.700	324.2296	FBF	68.78		FBF
.181	C23 H34 O4	10.337	374.2436	FBF	63.83		FBF
1182	C25 H36 O4	14.886	400.2635	FBF	72.66		FBF



Compound Sumr							
Cpd Name	Formula C20 H40 O4	RT	Mass 440 2044	CAS ID Source	Score	Score (Lib) Score	. ,
183 184	C28 H40 O4 C30 H44 O4	9.948 0.383	440.2944 468.3258	FBF FBF	62.19 55.68		FBF FBF
185	C31 H44 O4	5.322	480.3232	FBF	65.80		FBF
.186	C35 H52 O4	19.408	536.3877	FBF	90.29		FBF
187	C18 H28 O4	8.700	308.1993	FBF	69.46		FBF
.188	C19 H28 O4	8.856	320.1966	FBF	51.57		FBF
189	C21 H30 O4	7.972	346.2112	FBF	51.46		FBF
1190	C23 H32 O4	13.353	372.2313	FBF	79.50	.	FBF FBF
191 192	C25 H34 O4 C26 H36 O4	9.480 15.042	398.2435 412.2595	FBF FBF	88.48 87.66		FBF
193	C28 H38 O4	4.932	438.2791	FBF	64.73		FBF
1194	C31 H42 O4	3.553	478.3084	FBF	58.50		FBF
195	C34 H48 O4	5.477	520.3589	FBF	54.39		FBF
.196	C36 H52 O4	18.135	548.3908	FBF	78.48		FBF
.197	C24 H32 O4	4.671	384.2319	FBF	64.19		FBF
198 199	C28 H36 O4	5.374	436.2644	FBF	58.03		FBF
1200	C29 H38 O4 C37 H70 O4	7.920 19.226	450.2781 578.5279	FBF FBF	60.50 64.21	.	FBF FBF
201	C37 H58 O4	10.207	566.4301	FBF	63.17		FBF
.202	C37 H56 O4	7.218	564.4209	FBF	61.26		FBF
203	C38 H60 O4	13.249	580.4531	FBF	56.20		FBF
204	C38 H58 O4	13.327	578.4364	FBF	53.44		FBF
.205	C38 H56 O4	11.039	576.4212	FBF	52.45		FBF
1206	C24 H30 O4	17.147	382.2179	FBF	50.75		FBF
. <u>207</u> .208	C27 H34 O4 C33 H42 O4	14.886 5.062	422.2453 502.3064	FBF FBF	80.30 63.46		FBF FBF
.209	C38 H52 O4	10.207	572.3911	FBF	67.45		FBF
.210	C21 H26 O4	4.437	342.1823	FBF	56.98		FBF
211	C39 H74 O4	19.226	606.5576	FBF	53.73		FBF
212	C39 H66 O4	16.810	598.4976	FBF	50.34		FBF
.213	C39 H54 O4	4.125	586.3989	FBF	58.10		FBF
<u>214</u> 215	C40 H66 O4	17.615 13.275	610.4974	FBF FBF	50.10 57.77	.	FBF FBF
216	C40 H62 O4 C41 H80 O4	18.732	606.4602 636.6048	FBF	52.43		FBF
217	C41 H68 O4	16.212	624.5125	FBF	51.20		FBF
218	C38 H50 O4	4.125	570.3759	FBF	63.53		FBF
219	C40 H54 O4	5.555	598.4038	FBF	71.45		FBF
220	C42 H70 O4	17.277	638.5274	FBF	58.56		FBF
221	C42 H64 O4	13.353	632.4844	FBF	51.20		FBF
.222	C42 H62 O4	17.901	630.4700	FBF	58.44		FBF
<u>223</u> 224	C43 H78 O4 C43 H76 O4	19.824 6.257	658.5943 656.5763	FBF FBF	56.01 56.33		FBF FBF
.225	C43 H74 O4	21.200	654.5567	FBF	53.49		FBF
1226	C43 H72 O4	20.239	652.5445	FBF	59.93		FBF
.227	C43 H70 O4	13.275	650.5269	FBF	54.70		FBF
1228	C43 H68 O4	13.301	648.5168	FBF	68.89		FBF
1229	C43 H64 O4	16.056	644.4813	FBF	55.59		FBF
.230	C43 H62 O4	10.259	642.4643	FBF	77.42		FBF
. <u>231</u> .232	C44 H78 O4 C44 H74 O4	20.993 17.433	670.5904 666.5599	FBF FBF	57.22 58.24		FBF FBF
.233	C44 H72 O4	13.301	664.5414	FBF	50.55		FBF
234	C44 H66 O4	17.745	658,4949	FBF	72.42		FBF
.235	C45 H86 O4	20.369	690.6507	FBF	54.69		FBF
236	C45 H80 O4	18.680	684.6067	FBF	76.44		FBF
237	C45 H78 O4	19.538	682.5897	FBF	56.50		FBF
238	C45 H76 O4	14.964	680.5727	FBF	55.55		FBF
<u>239</u> 240	C45 H74 O4 C45 H72 O4	18.265 14.860	678.5557 676.5489	FBF FBF	53.28 82.32		FBF FBF
241	C46 H86 O4	17.147	702.6534	FBF	50.27		FBF
242	C46 H78 O4	17.563	694.5882	FBF	54.94		FBF
243	C46 H70 O4	17.693	686.5259	FBF	71.32		FBF
244	C46 H68 O4	19.070	684.5104	FBF	57.35		FBF
245	C46 H64 O4	17.745	680.4767	FBF	60.87		FBF
246	C47 H78 O4	16.966	706.5894	FBF ERE	51.71 57.10		FBF FRF
<u>247</u> 248	C47 H70 O4 C47 H66 O4	19.018 11.637	698.5239 694.4935	FBF FBF	57.10 62.05		FBF FBF
249	C43 H56 O4	5.400	636.4195	FBF	53.58		FBF
250	C44 H58 O4	6.257	650.4328	FBF	52.17		FBF
251	C45 H60 O4	19.070	664.4532	FBF	53.34	· · · · · · · · · · · · · · · · · · ·	FBF
252	C46 H62 O4	10.077	678.4697	FBF	58.15		FBF
253	C48 H94 O4	19.200	734.7142	FBF	51.73		FBF
254	C48 H90 O4	6.153	730.6857	FBF ERE	53.58		FBF FBF
<u>255</u> 256	C48 H82 O4 C48 H74 O4	18.654 19.954	722.6161 714.5553	FBF FBF	60.99 69.73		FBF
257	C48 H68 O4	18.420	714.5555	FBF	61.59		FBF
258	C48 H66 O4	19.980	706.4926	FBF	55.22		FBF
259	C49 H90 O4	20.941	742.6851	FBF	54.69		FBF
260	C49 H86 O4	18.498	738.6521	FBF	59.07	· · · · · · · · · · · · · · · · · · ·	FBF
261	C49 H76 O4	20.006	728.5742	FBF	73.74		FBF
262	C49 H74 O4	15.900	726.5579	FBF	53.94		FBF
263	C49 H68 O4	17.667	720.5089	FBF	74.67		FBF
264 265	C50 H96 O4	20.006	760.7287	FBF ERE	55.74 52.50		FBF FRF
<u>265</u> 266	C50 H92 O4 C50 H82 O4	17.329 17.589	756.7049 746.6227	FBF FBF	52.50 52.90		FBF FBF
267	C50 H78 O4	19.954	740.0227	FBF	61.90		FBF
<u></u>	C50 H72 O4	19.980	736.5382	FBF	52.99		FBF



Cpd Name	nary Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (D	B) Score (MFG) Algorithi
1269	C51 H100 O4	22.161	776.7573	FBF	57.34		FBF
270	C51 H96 O4	21.564	772.7296	FBF	54.43		FBF
271	C51 H86 O4	22.499	762.6539	FBF	58.53		FBF
<u>272 </u>	C51 H84 O4 C51 H80 O4	20.837 14.912	760.6375 756.5999	<u>FBF</u> FBF	73.40 57.95		FBF FBF
274	C51 H74 O4	20.006	750.5561	FBF	66.35		FBF
275	C52 H96 O4	18.109	784.7314	FBF	55.37		FBF
276	C52 H94 O4	18.940	782.7128	FBF	51.22		FBF
277	C52 H88 O4	22.629	776.6676	FBF	56.28		FBF
278	C52 H86 O4	19.044	774.6517	FBF	52.45		FBF
279	C52 H84 O4	17.329	772.6357	FBF	52.89		FBF
280 281	C53 H104 O4	14.549	804.7949 792.6985	FBF FBF	54.27		FBF FBF
282	C53 H92 O4 C53 H88 O4	21.798 17.901	788.6630	FBF	51.77 52.73		FBF
283	C53 H86 O4	20.577	786.6517	FBF	51.21		FBF
284	C54 H92 O4	21.019	804.6969	FBF	51.55		FBF
285	C54 H90 O4	13.431	802.6841	FBF	59.37		FBF
286	C55 H108 O4	14.029	832.8329	FBF	58.94		FBF
287	C55 H86 O4	14.809	810.6520	FBF	52.84		FBF
288	C55 H90 O4	19.460	814.6833	FBF	51.46		FBF
289 290	C56 H88 O4 C56 H102 O4	13.509 17.615	824.6665 838.7763	FBF FBF	60.17 50.65		FBF FBF
290 <u> </u>	C56 H98 O4	16.758	834.7443	FBF	50.52		FBF
292	C57 H92 O4	14.523	840.6954	FBF	54.64		FBF
293	C57 H110 O4	22.265	858.8387	FBF	50.30		FBF
294	C57 H108 O4	20.006	856.8317	FBF	61.76	· · · · · · · · · · · · · · · · · · ·	FBF
295	C57 H100 O4	15.770	848.7631	FBF	54.34		FBF
296	C58 H94 O4	14.055	854.7151	FBF	54.69		FBF
297	C58 H110 O4	13.977	870.8391	FBF	52.90		FBF
<u>298</u> 299	C58 H100 O4	21.174	860.7570	FBF FBF	50.61		FBF FBF
300	C59 H96 O4 C59 H94 O4	12.495 14.211	868.7309 866.7142	FBF	65.38 51.00		FBF
301	C59 H110 O4	12.079	882.8460	FBF	52.64		FBF
302	C59 H106 O4	18.524	878.8048	FBF	63.32		FBF
303	C60 H96 O4	12.001	880.7241	FBF	51.65		FBF
304	C60 H114 O4	21.097	898.8739	FBF	61.30		FBF
305	C60 H102 O4	18.524	886.7768	FBF	50.23		FBF
806	C60 H100 O4	16.914	884.7615	FBF	50.56		FBF
307	C61 H100 O4	14.107	896.7674	FBF	52.71		FBF
308 309	C61 H116 O4 C61 H110 O4	14.627 17.018	912.8900 906.8367	<u>FBF</u> FBF	55.80 50.03		FBF FBF
310	C61 H104 O4	22.447	900.7937	FBF	57.80		FBF
311	C62 H122 O4	14.471	930.9399	FBF	50.01		FBF
312	C62 H100 O4	18.966	908.7624	FBF	60.72		FBF
313	C62 H116 O4	19.772	924.8852	FBF	53.96		FBF
314	C62 H114 O4	20.110	922.8716	FBF	50.43		FBF
315	C62 H106 O4	20.213	914.8159	FBF	57.71		FBF
316 317	C62 H104 O4 C63 H116 O4	17.693 18.836	912.7999 936.8852	FBF FBF	51.41 51.57		FBF FBF
318	C63 H112 O4	21.148	932.8583	FBF	58.49		FBF
319	C63 H108 O4	19.330	928.8208	FBF	56.19		FBF
320	C64 H126 O4	9.402	958.9597	FBF	50.22		FBF
321	C64 H104 O4	22.629	936.7948	FBF	58.14		FBF
322	C64 H124 O4	14.263	956.9522	FBF	51.62		FBF
323	C64 H122 O4	18.862	954.9423	FBF	55.19		FBF
324	C64 H114 O4	18.524	946.8659	FBF	50.31		FBF
325 326	C65 H106 O4 C65 H116 O4	22.031 18.602	950.8091 960.8889	FBF FBF	51.52 57.31		FBF FBF
327	C66 H120 O4	21.382	976.9160	FBF	56.81		FBF
328	C66 H118 O4	18.420	974.8995	FBF	78.57		FBF
329	C67 H132 O4	10.961	1001.0156	FBF	82.92		FBF
330	C67 H116 O4	21.876	984.8875	FBF	57.04		FBF
331	C68 H114 O4	17.459	994.8748	FBF	56.92		FBF
332	C68 H120 O4	21.278	1000.9138	FBF	51.75		FBF
333	C16 H28 O4	8.570	284.1974	FBF	84.22		FBF
334 335	C16 H26 O4 C17 H28 O4	7.400 7.972	282.1811 296.1974	FBF FBF	65.51		FBF FBF
336	C17 H28 O4 C16 H24 O4	18.836	280.1661	FBF	77.50 73.44		FBF
337	C18 H22 O4	14.886	302.1493	FBF	54.91		FBF
338	C27 H44 N O2	10.909	414.3363	FBF	60.45		FBF
339	C40 H74 O2	18.083	586.5697	FBF	52.90		FBF
340	C43 H76 O2	20.603	624.5851	FBF	52.56		FBF
341	C47 H74 O2	20.993	670.5717	FBF	51.09		FBF
342	C50 H96 O2	19.408	728.7383	FBF	69.75		FBF
343	C53 H102 O2	18.239	770.7838	FBF	50.46		FBF
344 345	C54 H102 O2 C55 H110 O2	13.015 13.301	782.7831 802.8524	<u>FBF</u> FBF	53.01 58.69		FBF FBF
345 346	C56 H110 O2	12.703	814.8522	FBF	53.12		FBF
347	C32 H64	16.836	448.5001	FBF	94.24		FBF
348	C34 H68	21.902	476.5317	FBF	98.75		FBF
349	C8 H14	2.617	110.1092	FBF	97.46		FBF
350	C8 H16	19.408	112.1253	FBF	87.14		FBF
330		0.000	492.5600	FBF	52.12		FBF
351	C35 H72	8.388					
	C35 H72 C12 H24 C18 H36	7.088 9.350	168.1874 252.2821	FBF FBF	76.15 89.40		FBF FBF



Compound Summary							
Cpd Name	Formula C13 H26	7.218	Mass 182.2024	CAS ID Source FBF	Score 95.08	Score (Lib) Score (DB)	Score (MFG) Algorithm FBF
1355 1356	C13 H6	2.825	162.2024	FBF	60.68		FBF
1357	C36 H72	18.550	504.5625	FBF	94.82		FBF
1358	C6 H12	14.601	84.0938	FBF	99.88		FBF
1359	C21 H42	10.675	294.3274	FBF	79.94		FBF
1360 1361	C7 H14 C9 H20	19.460 7.842	98.1095 128.1577	FBF FBF	87.61 67.04		FBF FBF
1362	C14 H26 O	10.805	210.1982	FBF	87.23		FBF
1363	C13 H26 O	7.010	198.1970	FBF	54.79		FBF
1364	C11 H22 O	7.270	170.1658	FBF	72.55		FBF
1365	C8 H14 O	9.922	126.1037	<u>FBF</u> FBF	75.56 76.73		FBF FBF
1366 1367	C21 H38 O C9 H16 O	15.796 17.589	306.2936 140.1202	FBF	99.90		FBF
1368	C5 H8 O	0.383	84.0573	FBF	86.24		FBF
1369	C18 H36 O4	12.833	316.2630	FBF	66.37		FBF
1370	C18 H32 O5	8.440	328.2222	FBF	62.34		FBF
1371	C12 H18 O4	5.841	226.1189	FBF	74.38		FBF
1372 1373	C11 H16 O C18 H36 O6	7.140 8.570	164.1212 348.2511	FBF FBF	76.94 93.94		FBF FBF
1374	C18 H34 O5	8.570	330.2419	FBF	55.11		FBF
1375	C10 H21 N O2	0.383	187.1571	FBF	76.20		FBF
1376	C35 H68 O5	6.283	568.5093	FBF	82.46		FBF
1377	C35 H58 O5	16.914	558.4321	FBF	76.76		FBF
1378	C36 H68 O5	19.642	580.5104	FBF	75.94		FBF
1379 1380	C37 H68 O5 C38 H72 O5	15.458 21.356	592.5060 608.5374	<u>FBF</u> FBF	52.49 57.02		FBF FBF
1381	C39 H66 O5	17.953	614.4908	FBF	79.78		FBF
1382	C41 H80 O5	20.759	652.6028	FBF	50.86		FBF
1383	C41 H78 O5	19.616	650.5810	FBF	61.88		FBF
1384	C43 H84 O5	20.655	680.6317	FBF	59.92		FBF
1385	C43 H80 O5	20.785	676.5989	FBF	50.22		FBF
1386 1387	C43 H70 O5 C27 H52 O5	14.289 13.249	666.5265 456.3808	<u>FBF</u> FBF	58.95 61.22		FBF FBF
1388	C15 H28 O5	7.478	288.1916	FBF	78.85		FBF
1389	C23 H44 O5	9.818	400.3171	FBF	62.60		FBF
1390	C24 H46 O5	13.847	414.3334	FBF	68.65		FBF
1391	C26 H50 O5	14.341	442.3677	FBF	51.04		FBF
1392	C28 H54 O5	15.692	470.3964	FBF	60.79		FBF
1393 1394	C28 H52 O5 C29 H54 O5	14.029 11.247	468.3856 482.3981	FBF FBF	64.86 62.33		FBF FBF
1395	C30 H58 O5	19.824	498.4284	FBF	55.12		FBF
1396	C30 H56 O5	14.938	496.4139	FBF	56.74		FBF
1397	C31 H58 O5	13.379	510.4258	FBF	50.65		FBF
1398	C33 H54 O5	20.136	530.4004	FBF	77.05		FBF
1399	C44 H86 O5	19.824	694.6442	FBF	52.34		FBF
1400 1401	C46 H90 O5 C49 H96 O5	21.304 20.187	722.6787 764.7205	<u>FBF</u> FBF	50.88 52.41		FBF FBF
1402	C50 H98 O5	21.148	778.7435	FBF	50.13		FBF
1403	C51 H100 O5	20.395	792.7561	FBF	50.39		FBF
1404	C32 H58 O5	10.857	522.4314	FBF	57.90		FBF
1405	C32 H56 O5	19.642	520.4106	FBF	59.81		FBF
1406 1407	C32 H54 O5 C34 H56 O5	13.977 19.148	518.3993 544.4124	<u>FBF</u> FBF	58.95 66.73		FBF FBF
1408	C53 H104 O5	22.161	820.7880	FBF	68.26		FBF
1409	C28 H50 O5	10.753	466.3641	FBF	61.20		FBF
1410	C37 H62 O5	17.927	586.4623	FBF	61.32		FBF
1411	C37 H58 O5	10.571	582.4306	FBF	70.31		FBF
1412	C41 H66 O5	13.951	638.4926	FBF	55.62		FBF
1413 1414	C42 H80 O5 C42 H78 O5	18.810 22.291	664.6004 662.5851	<u>FBF</u> FBF	65.32 51.69		FBF FBF
1415	C55 H108 O5	13.301	848.8263	FBF	64.83		FBF
1416	C39 H62 O5	11.949	610.4628	FBF	65.45		FBF
1417	C48 H92 O5	18.369	748.7018	FBF	54.31		FBF
1418	C49 H94 O5	21.434	762.7091	FBF	57.44		FBF
1419 1420	C50 H96 O5 C52 H100 O5	19.616 21.122	776.7269 804.7538	<u>FBF</u> FBF	51.33 50.33		FBF FBF
1421	C52 H100 O5 C54 H104 O5	13.639	832.7883	FBF	50.33		FBF
1422	C44 H82 O5	19.668	690.6171	FBF	52.72		FBF
1423	C40 H64 O5	13.223	624.4763	FBF	64.21		FBF
1424	C18 H26 O5	7.036	322.1752	FBF	64.98		FBF
1425	C45 H84 O5	17.199	704.6318	FBF	53.26		FBF
<u>1426 </u>	C47 H76 O5 C19 H32 O5	14.523 17.355	720.5719 340.2244	FBF FBF	72.56 73.28		FBF FBF
1428	C42 H68 O5	14.835	652.5085	FBF	59.50		FBF
1429	C44 H76 O5	17.251	684.5712	FBF	51.00		FBF
1430	C46 H84 O5	21.122	716.6299	FBF	55.96		FBF
1431	C44 H74 O5	22.031	682.5539	FBF	50.75		FBF
1432	C46 H82 O5	18.395	714.6138	FBF	62.56		FBF
1433	C59 H108 O5	18.654	896.8204	FBF ERE	50.85		FBF FBF
<u>1434</u> 1435	C61 H108 O5 C23 H42 O5	21.278 9.688	920.8176 398.3008	<u>FBF</u> FBF	50.02 59.21		FBF
1436	C45 H76 O5	21.434	696.5702	FBF	50.38		FBF
1437	C47 H86 O5	21.564	730.6492	FBF	62.60		FBF
1438	C59 H106 O5	17.693	894.8046	FBF	59.75		FBF
1439	C41 H64 O5	17.329	636.4751	FBF	53.62		FBF
1440	C47 H82 O5	12.833	726.6145	FBF	58.87		FBF



Compound Summary						-	
Cpd Name	Formula C60 H112 O5	RT	Mass 012.9404	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorithn
<u>1441</u> 1442	C25 H46 O5	18.654 13.353	912.8494 426.3322	<u>FBF</u> FBF	51.28 58.54		FBF FBF
1443	C23 H38 O5	3.293	394.2702	FBF	52.24		FBF
1444	C49 H84 O5	16.966	752.6315	FBF	55.68		FBF
1445	C49 H74 O5	16.628	742.5537	FBF	55.48		FBF
1446	C60 H108 O5	22.083	908.8232	FBF	55.49		FBF
1447	C24 H38 O5	5.166	406.2721	<u>FBF</u> FBF	55.49 51.07		FBF FBF
1448 1449	C25 H42 O5 C51 H88 O5	4.854 18.732	422.2995 780.6645	FBF	51.97 58.60		FBF
1450	C47 H70 O5	19.226	714.5248	FBF	50.35		FBF
1451	C55 H96 O5	21.200	836.7203	FBF	51.57		FBF
1452	C56 H98 O5	20.785	850.7335	FBF	52.34		FBF
1453	C58 H102 O5	21.045	878.7730	FBF	59.38		FBF
1454	C65 H128 O5	14.731	988.9771	FBF	54.28		FBF
1455	C26 H46 O5	15.068 15.016	438.3343	FBF FBF	53.45 69.82		FBF
<u>1456 </u>	C27 H46 O5 C65 H120 O5	20.863	450.3316 980.9112	FBF	54.70		FBF FBF
1458	C67 H132 O5	14.237	1017.0016	FBF	56.45		FBF
1459	C28 H46 O5	12.339	462.3343	FBF	58.21		FBF
1460	C68 H132 O5	11.039	1029.0073	FBF	50.29		FBF
1461	C29 H52 O5	10.285	480.3855	FBF	53.39		FBF
1462	C67 H128 O5	10.961	1012.9741	FBF	56.29		FBF
1463 1464	C31 H50 O5	10.285 20.239	502.3662 552.3823	FBF FBF	69.93 90.29		FBF FBF
1465	C35 H52 O5 C34 H54 O5	19.044	542.3928	FBF	53.23		FBF
1466	C37 H56 O5	19.304	580.4134	FBF	70.64		FBF
1467	C41 H58 O5	4.281	630.4252	FBF	59.54		FBF
1468	C53 H86 O5	12.911	802.6471	FBF	50.31		FBF
1469	C54 H90 O5	13.379	818.6801	FBF	50.18		FBF
1470	C55 H86 O5	14.964	826.6490	FBF	50.17		FBF
<u>1471 </u>	C55 H84 O5 C55 H94 O5	14.341 18.862	824.6290 834.7105	<u>FBF</u> FBF	53.56 50.31		FBF FBF
1473	C55 H92 O5	18.446	832.6980	FBF	54.70		FBF
1474	C43 H88 O3	18.940	652.6707	FBF	67.04		FBF
1475	C30 H60 O4	14.289	484.4475	FBF	57.81		FBF
476	C31 H62 O4	15.224	498.4652	FBF	59.97		FBF
477	C34 H68 O4	15.588	540.5135	FBF	69.88		FBF
1478	C36 H72 O4	6.153	568.5432	FBF	64.62		FBF
1479	C52 H104 O4	13.821	792.7971	FBF	65.43		FBF
<u>1480</u> 1481	C53 H106 O4 C56 H112 O4	21.980 12.105	806.8079 848.8495	<u>FBF</u> FBF	53.29 53.58		FBF FBF
1482	C19 H38 O4	9.818	330.2754	FBF	66.48		FBF
1483	C39 H70 O15	14.263	778.4740	FBF	51.11		FBF
1484	C40 H72 O15	13.587	792.4852	FBF	50.33		FBF
1485	C42 H74 O15	5.607	818.5011	FBF	80.55		FBF
1486	C43 H80 O15	10.000	836.5467	FBF	79.53		FBF
1487	C43 H76 O15	4.854	832.5250	FBF	62.02		FBF
1488 1489	C45 H84 O15 C45 H76 O15	16.654 4.854	864.5853 856.5130	FBF FBF	59.08 56.43		FBF FBF
1490	C45 H74 O15	5.166	854.5050	FBF	84.29		FBF
1491	C47 H76 O15	13.327	880.5208	FBF	59.10		FBF
1492	C49 H90 O15	15.900	918.6370	FBF	57.97		FBF
1493	C49 H84 O15	14.237	912.5814	FBF	54.08		FBF
L494	C50 H94 O15	16.160	934.6621	FBF	51.11		FBF
1495	C51 H94 O15	18.472	946.6590	FBF	86.44		FBF
1496	C59 H112 O15	17.927	1060.8006	FBF	87.33		FBF
497	C48 H88 O15 C52 H96 O15	16.264	904.6124	FBF	51.34		FBF
L498 L499	C51 H86 O15	21.226 14.912	960.6776 938.5996	<u>FBF</u> FBF	53.40 62.54	<u> </u>	FBF FBF
1500	C53 H92 O15	13.613	968.6463	FBF	59.49	· · · · · · · · · · · · · · · · · · ·	FBF
501	C55 H102 O15	14.835	1002.7201	FBF	52.23		FBF
.502	C68 H130 O15	18.576	1186.9442	FBF	51.60		FBF
.503	C51 H90 O15	17.511	942.6243	FBF	52.57		FBF
504	C58 H108 O15	14.835	1044.7719	FBF	81.69		FBF
.505 .506	C60 H112 O15 C65 H122 O15	20.317 18.213	1072.7916 1142.8784	<u>FBF</u> FBF	53.96 50.37		FBF FBF
.507	C66 H124 O15	18.213	1142.8784	FBF	56.59		FBF
.508	C50 H88 O15	19.980	928.6121	FBF	54.37		FBF
509	C52 H86 O15	14.886	950.5993	FBF	55.43		FBF
510	C52 H84 O15	14.912	948.5859	FBF	61.21		FBF
511	C53 H88 O15	13.171	964.6124	FBF	53.48		FBF
512	C70 H134 O15	19.044	1214.9715	FBF	54.10		FBF
. <u>513</u> .514	C53 H94 O15 C71 H136 O15	15.796 17.745	970.6586 1228.9948	FBF FBF	60.40 56.26		FBF FBF
1514	C58 H104 O15	16.342	1040.7443	FBF	50.26		FBF
1516	C68 H126 O15	17.797	1182.9136	FBF	54.82		FBF
1517	C55 H90 O15	14.393	990.6255	FBF	61.87		FBF
1518	C57 H98 O15	14.912	1022.6883	FBF	50.10		FBF
519	C53 H84 O15	14.159	960.5719	FBF	51.85		FBF
.520	C55 H86 O15	13.847	986.5971	FBF	54.95		FBF
521	C61 H110 O15	17.927	1082.7826	FBF	89.52		FBF
522	C63 H114 O15	17.745	1110.8177	FBF	58.32		FBF
<u>523</u> 524	C55 H84 O15 C60 H106 O15	13.379 14.809	984.5787 1066.7549	<u>FBF</u> FBF	50.97 74.48		FBF FBF
525	C63 H112 O15	14.860	1108.7898	FBF	50.10		FBF
1526	C33 H58 O15	4.437	694.3772	FBF	87.71		FBF



	nary Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorithm
527	C57 H88 O15	14.393	1012.6114	FBF	53.27		FBF
<u>528</u> 529	C61 H104 O15 C62 H108 O15	14.886 21.071	1076.7386 1092.7653	FBF FBF	58.65 54.19		FBF FBF
530	C73 H130 O15	18.654	1246.9384	FBF	58.02		FBF
531	C74 H132 O15	20.110	1260.9679	FBF	53.03		FBF
532	C76 H144 O15	11.897	1297.0446	FBF	50.06		FBF
533	C61 H96 O15	13.509	1068.6811	FBF	51.34		FBF
534	C62 H106 O15	22.005	1090.7497	FBF	50.54		FBF
535	C77 H140 O15	11.923	1305.0197	FBF	55.57		FBF
<u>536</u> 537	C78 H146 O15 C44 H72 O15	20.759 4.828	1323.0585 840.4894	FBF FBF	50.64 82.19		FBF FBF
538	C46 H60 O15	7.920	852.3958	FBF	58.04		FBF
539	C47 H72 O15	4.854	876.4893	FBF	89.41		FBF
540	C54 H84 O15	14.393	972.5761	FBF	50.38		FBF
541	C29 H54 O10	19.044	562.3731	FBF	80.47		FBF
542	C30 H56 O10	5.503	576.3896	FBF	69.67		FBF
543	C31 H58 O10	19.044	590.4034	FBF	84.62		FBF
544	C33 H60 O10	10.155	616.4174	FBF	87.56		FBF
<u>545 </u>	C37 H70 O10	13.353	674.4956	FBF FBF	67.02 F7.10		FBF FBF
547	C37 H68 O10 C37 H66 O10	21.486 14.393	672.4795 670.4678	FBF	57.10 52.87		FBF
548	C39 H74 O10	19.876	702.5293	FBF	58.10		FBF
549	C39 H72 O10	10.103	700.5168	FBF	64.31		FBF
550	C40 H76 O10	18.680	716.5474	FBF	54.13		FBF
551	C41 H74 O10	18.498	726.5324	FBF	75.51		FBF
552	C41 H70 O10	10.103	722.4984	FBF	79.82		FBF
553	C41 H68 O10	4.541	720.4831	FBF	53.84		FBF
554	C41 H66 O10	14.886	718.4644	FBF	58.24		FBF
555	C43 H82 O10	13.223	758.5912	FBF	50.82		FBF
556	C43 H80 O10 C45 H82 O10	14.886	756.5816	FBF	54.49		FBF
557 558	C45 H82 O10 C46 H88 O10	15.042 14.835	782.5877 800.6383	FBF FBF	54.03 52.90		FBF FBF
559	C51 H98 O10	19.070	870.7192	FBF	53.95		FBF
560	C52 H100 O10	18.291	884.7299	FBF	53.58		FBF
561	C53 H102 O10	14.886	898.7451	FBF	64.51		FBF
562	C55 H106 O10	17.225	926.7721	FBF	89.31		FBF
563	C56 H108 O10	14.809	940.7927	FBF	60.08		FBF
564	C40 H66 O10	5.867	706.4648	FBF	58.75		FBF
565	C42 H70 O10	15.042	734.4908	FBF	51.80		FBF
566	C44 H76 O10	19.954	764.5479	FBF	51.67		FBF
567	C59 H114 O10	21.850	982.8394	FBF	51.25		FBF
568	C47 H88 O10	14.938	812.6388	FBF FBF	50.62		FBF FBF
569 570	C22 H40 O10 C44 H72 O10	5.477 19.070	464.2625 760.5106	FBF	71.94 72.76		FBF
571	C45 H76 O10	19.954	776.5452	FBF	61.03		FBF
572	C45 H74 O10	16.680	774.5276	FBF	56.22		FBF
573	C45 H80 O10	19.928	780.5743	FBF	52.18		FBF
574	C47 H80 O10	17.823	804.5736	FBF	53.49		FBF
575	C50 H94 O10	12.209	854.6838	FBF	55.98		FBF
576	C52 H98 O10	22.135	882.7161	FBF	77.66		FBF
577	C55 H104 O10	14.575	924.7593	FBF	51.55		FBF
578	C59 H112 O10	22.551	980.8197	FBF	61.54		FBF
579	C46 H74 O10 C65 H124 O10	19.902	786.5300	FBF FBF	62.92		FBF
580 581	C48 H76 O10	17.797 14.886	1064.9190 812.5455	FBF	50.20 57.46		FBF FBF
582	C50 H84 O10	15.120	844.6022	FBF	53.16		FBF
583	C56 H104 O10	12.287	936.7621	FBF	50.69		FBF
584	C57 H106 O10	14.003	950.7740	FBF	59.34		FBF
585	C59 H110 O10	13.665	978.8027	FBF	51.00		FBF
586	C64 H120 O10	20.395	1048.8883	FBF	50.49		FBF
587	C65 H122 O10	19.564	1062.9063	FBF	72.25		FBF
588	C53 H96 O10	13.327	892.7089	FBF	54.43		FBF
589	C49 H76 O10	18.524	824.5405	FBF	60.92		FBF
590 591	C55 H100 O10 C56 H102 O10	18.758 14.133	920.7318 934.7423	FBF FBF	62.41 50.07		FBF FBF
592	C47 H72 O10	5.815	796.5150	FBF	68.61		FBF
593	C51 H82 O10	14.809	854.5896	FBF	54.78		FBF
594	C58 H104 O10	14.029	960.7673	FBF	58.70		FBF
595	C64 H116 O10	17.667	1044.8494	FBF	53.53		FBF
596	C67 H128 O10	19.278	1092.9505	FBF	50.42		FBF
597	C33 H50 O10	3.865	606.3447	FBF	61.68		FBF
598	C68 H128 O10	19.252	1104.9552	FBF	50.72		FBF
i99	C53 H88 O10	13.977	884.6422	FBF	53.51		FBF
500	C55 H96 O10	19.382	916.6978	FBF	51.72		FBF
	C51 H78 O10 C55 H94 O10	4.854 19.824	850.5559 914.6836	FBF FBF	60.26 76.40		FBF FBF
501	C55 H94 O10 C57 H100 O10	19.824 18.628	914.6836	FBF	76.40 51.27		FBF
501 502			986.7844	FBF	65.18		FBF
501 502 503		14 573	2001/011				
501 502 503 504	C60 H106 O10	14.523 5.503		FBF	67.96		FRF
501 502 503 504 505		14.523 5.503 20.239	544.2329 588.3905	FBF FBF	67.96 68.98		FBF FBF
501 502 503 504 505 506	C60 H106 O10 C29 H36 O10	5.503	544.2329				
601 602 603 604 605 606 606 607	C60 H106 O10 C29 H36 O10 C31 H56 O10	5.503 20.239	544.2329 588.3905	FBF	68.98		FBF
501 502 503 504 505 506 507	C60 H106 O10 C29 H36 O10 C31 H56 O10 C69 H132 O10	5.503 20.239 10.935	544.2329 588.3905 1120.9779	FBF FBF	68.98 50.38		FBF FBF
501 502 503 504 505 506 507 508	C60 H106 O10 C29 H36 O10 C31 H56 O10 C69 H132 O10 C64 H112 O10	5.503 20.239 10.935 17.927	544.2329 588.3905 1120.9779 1040.8207	FBF FBF FBF	68.98 50.38 54.23		FBF FBF FBF



Compound Sumn	.							
Cpd Name 1613	Formula C33 H58 O10	RT 4.281	Mass 614.4017	CAS ID Source FBF	Score 95.87	Score (Lib)	Score (DB)	Score (MFG) Algorithm FBF
1614	C34 H52 O10	4.229	620.3594	FBF	62.88			FBF
1615	C43 H66 O10	4.541	742.4650	FBF	57.23			FBF
1616	C44 H62 O10	4.671	750.4310	FBF	59.57			FBF
1617	C48 H72 O10	22.135	808.5096	FBF	52.19			FBF
<u>1618</u> 1619	C54 H68 O10 C56 H84 O10	4.854 18.187	876.4893 916.6076	FBF FBF	50.82 56.88			FBF FBF
1620	C35 H66 O15	6.153	726.4436	FBF	54.13			FBF
1621	C35 H56 O15	4.437	716.3591	FBF	77.75			FBF
1622	C36 H68 O15	4.541	740.4600	FBF	61.33			FBF
1623 1624	C36 H64 O15 C36 H58 O14	5.036 12.599	736.4229 714.3820	FBF FBF	51.74 61.81			FBF FBF
1625	C37 H66 O15	5.555	750.4406	FBF	63.26			FBF
1626	C37 H64 O15	5.529	748.4209	FBF	52.50			FBF
1627	C38 H72 O14	5.529	752.4942	FBF	81.39			FBF
1 <u>628</u> 1629	C38 H70 O14 C38 H62 O14	17.070 6.257	750.4777 742.4109	FBF FBF	60.39 59.03			FBF FBF
1630	C39 H74 O15	19.928	782.4966	FBF	53.55		-	FBF
1631	C39 H68 O15	13.587	776.4555	FBF	57.14			FBF
1632	C39 H66 O15	19.304	774.4441	FBF	52.59			FBF
1633	C40 H76 O15	5.607	796.5193	FBF	81.63			FBF
<u>1634</u> 1635	C40 H70 O14 C41 H76 O14	5.529 10.000	774.4761 792.5218	FBF FBF	84.50 92.06			FBF FBF
1636	C41 H72 O14	4.750	788.4984	FBF	67.23			FBF
1637	C41 H70 O14	19.876	786.4745	FBF	53.80			FBF
1638	C42 H70 O14	5.971	798.4752	FBF	58.28			FBF
1639	C42 H68 O14 C42 H66 O14	4.724	796.4621	FBF FBF	84.15			FBF FBF
1640 1641	C42 H82 O14	5.088 16.368	794.4484 822.5722	FBF	78.73 53.95			FBF
1642	C43 H72 O14	4.750	812.4872	FBF	51.13			FBF
1643	C43 H70 O14	4.750	810.4820	FBF	78.93			FBF
1644	C43 H68 O15	7.946	824.4502	FBF	65.23			FBF
1645 1646	C44 H70 O14 C44 H70 O15	5.633 5.166	822.4737 838.4746	FBF FBF	51.53 75.37			FBF FBF
1647	C45 H84 O14	18.966	848.5837	FBF	68.14			FBF
1648	C45 H78 O14	13.275	842.5423	FBF	64.88			FBF
1649	C46 H84 O14	11.637	860.5903	FBF	51.74			FBF
1650	C46 H78 O14	18.836	854.5438	FBF	51.37			FBF
1651 1652	C46 H76 O14 C47 H90 O14	15.822 15.510	852.5248 878.6336	FBF FBF	56.19 50.15			FBF FBF
1653	C47 H86 O14	14.886	874.6057	FBF	53.00			FBF
1654	C47 H82 O14	18.576	870.5666	FBF	50.85			FBF
1655	C47 H80 O14	13.613	868.5587	FBF	63.36			FBF
<u>1656</u> 1657	C47 H78 O14 C47 H74 O15	13.665 14.912	866.5399 878.5014	FBF FBF	51.14 50.98			FBF FBF
1658	C47 H72 O14	13.483	860.4940	FBF	51.25			FBF
1659	C48 H92 O14	16.576	892.6525	FBF	52.52			FBF
1660	C48 H84 O14	14.912	884.5841	FBF	62.41			FBF
1661	C48 H76 O14	13.431	876.5315	FBF	53.62			FBF
1662 1663	C48 H74 O15 C49 H86 O14	13.457 9.948	890.5041 898.5947	FBF FBF	54.15 53.66			FBF FBF
1664	C49 H84 O14	4.932	896.5848	FBF	52.40			FBF
1665	C49 H78 O14	13.327	890.5392	FBF	70.14			FBF
1666	C49 H76 O14	13.405	888.5233	FBF	62.58			FBF
1667	C50 H94 O14	14.523	918.6597	FBF	53.09			FBF
1668 1669	C50 H92 O14 C50 H82 O14	18.213 14.912	916.6501 906.5689	FBF FBF	52.50 66.32			FBF FBF
1670	C52 H92 O14	16.498	940.6512	FBF	66.38			FBF
1671	C53 H102 O14	21.122	962.7265	FBF	77.04			FBF
1672	C53 H82 O14	14.107	942.5712	FBF	50.18			FBF
<u>1673 </u>	C53 H96 O14 C53 H86 O14	18.966 14.367	956.6715 946.6017	FBF FBF	60.45 53.85			FBF FBF
1675	C54 H82 O14	14.367	954.5727	FBF	53.85			FBF
1676	C54 H96 O14	16.446	968.6857	FBF	51.79			FBF
1677	C54 H94 O14	14.860	966.6704	FBF	57.09			FBF
1678	C54 H90 O14	16.498	962.6323	FBF	71.93		-	FBF
<u>1679</u> 1680	C55 H106 O15 C55 H84 O14	20.941 13.847	1006.7573 968.5841	FBF FBF	51.85 51.71			FBF FBF
1681	C55 H102 O14	19.980	986.7263	FBF	52.94			FBF
1682	C55 H98 O14	21.019	982.6968	FBF	50.92			FBF
1683	C55 H96 O14	13.353	980.6788	FBF	53.37			FBF
1 <u>684</u> 1685	C55 H90 O14 C56 H108 O14	13.249 17.745	974.6234 1004.7696	FBF FBF	50.11 55.37			FBF FBF
1686	C56 H94 O14	16.498	990.6669	FBF	64.60			FBF
1687	C56 H90 O14	13.483	986.6335	FBF	58.89			FBF
1688	C57 H96 O14	20.239	1004.6748	FBF	51.35			FBF
1689	C58 H106 O14	14.809	1026.7557	FBF	50.50			FBF
1690 1691	C59 H112 O14 C59 H94 O14	20.161 5.114	1044.8088 1026.6590	FBF FBF	51.80 53.50			FBF FBF
1692	C59 H100 O14	14.912	1026.6590	FBF	55.00			FBF
1693	C60 H114 O14	19.044	1058.8177	FBF	51.84			FBF
1694	C60 H96 O14	15.718	1040.6767	FBF	58.17			FBF
1695	C60 H106 O14	14.912	1050.7680	FBF	50.15			FBF
1696 1697	C61 H110 O14 C63 H102 O15	20.239 21.122	1066.7922 1098.7203	FBF FBF	61.13 63.22			FBF FBF
1031	C63 H118 O14	21.122	1098.8555	FBF	62.59			FBF



Compound Summ							
Cpd Name 1699	Formula C64 H104 O15	RT 18.862	Mass 1112.7335	CAS ID Source FBF	Score 50.21	Score (Lib) Score (DB)	Score (MFG) Algorith FBF
1700	C64 H108 O15	18.109	1116.7729	FBF	64.98		FBF
1701	C65 H126 O15	18.680	1146.9071	FBF	55.88		FBF
1702	C65 H122 O14	18.498	1126.8803	FBF	52.83		FBF
1703	C65 H118 O14	18.836	1122.8524	FBF	51.38		FBF
1704	C66 H106 O15	17.537	1138.7539	FBF	82.49		FBF
1705	C66 H110 O15	14.964	1142.7894	FBF	68.74		FBF FBF
1706 1707	C67 H130 O14 C67 H118 O14	17.719 18.550	1158.9479 1146.8487	FBF FBF	53.89 59.17		FBF
1708	C67 H114 O14	22.265	1142.8211	FBF	50.57		FBF
1709	C68 H132 O14	18.213	1172.9659	FBF	74.12		FBF
1710	C68 H112 O14	18.680	1152.8049	FBF	63.85		FBF
1711	C68 H120 O14	22.655	1160.8673	FBF	58.14		FBF
1712	C69 H134 O15	17.797	1202.9653	FBF	51.00		FBF
1713	C69 H132 O14	19.902	1184.9627	FBF	56.01		FBF
1714 1715	C69 H114 O15	20.161 20.006	1182.8098 1182.9460	<u>FBF</u> FBF	60.90 71.19		FBF FBF
716	C69 H130 O14 C69 H120 O14	17.875	1172.8694	FBF	71.19		FBF
717	C69 H118 O14	17.823	1170.8623	FBF	59.43		FBF
.718	C70 H136 O14	19.200	1201.0026	FBF	56.00		FBF
719	C70 H114 O14	17.875	1178.8260	FBF	52.91		FBF
720	C70 H112 O14	18.836	1176.8007	FBF	85.22		FBF
721	C71 H118 O14	19.954	1194.8545	FBF	72.57		FBF
722	C71 H116 O14	17.875	1192.8445	FBF	69.79		FBF
723	C71 H116 O15	20.006	1208.8353	FBF	71.94		FBF
724 725	C71 H134 O14	11.715	1210.9758	FBF FBF	57.57 53.02		FBF FBF
725 726	C71 H130 O14 C72 H138 O14	17.485 18.862	1206.9496 1226.9993	FBF	53.02		FBF
727	C72 H118 O15	17.277	1222.8499	FBF	76.49		FBF
728	C72 H124 O15	18.602	1228.8953	FBF	50.17		FBF
729	C73 H140 O14	11.897	1241.0247	FBF	50.27		FBF
730	C73 H118 O15	18.550	1234.8435	FBF	50.16		FBF
731	C73 H138 O14	19.876	1239.0071	FBF	51.58		FBF
732	C74 H130 O14	19.824	1242.9434	FBF	52.31		FBF
733	C75 H124 O14	18.161	1248.9076	FBF	53.02		FBF
734	C76 H128 O14	18.836	1264.9329	FBF	54.67		FBF
735	C76 H132 O14	18.966	1268.9706	FBF	53.42 67.22		FBF FBF
736 737	C76 H130 O14 C77 H138 O15	17.771 19.850	1266.9587 1303.0051	FBF FBF	55.91		FBF
738	C78 H128 O15	19.928	1304.9226	FBF	57.49		FBF
739	C78 H140 O14	11.897	1301.0164	FBF	54.74		FBF
740	C78 H136 O14	21.122	1296.9933	FBF	57.50		FBF
741	C79 H154 O14	21.824	1327.1228	FBF	57.35		FBF
.742	C79 H134 O14	11.871	1306.9710	FBF	50.47		FBF
1743	C79 H134 O15	19.070	1322.9597	FBF	52.38		FBF
1744	C79 H144 O14	18.914	1317.0517	FBF	56.80		FBF
745 746	C79 H140 O14	11.897 19.876	1313.0233	FBF FBF	52.02 54.31		FBF FBF
.747	C80 H150 O14 C80 H144 O14	21.304	1335.1117 1329.0546	FBF	56.88		FBF
.748	C80 H142 O15	20.187	1343.0335	FBF	55.82		FBF
.749	C80 H138 O14	18.472	1323.0094	FBF	58.53		FBF
750	C81 H136 O14	18.888	1332.9977	FBF	52.49		FBF
751	C81 H136 O15	19.096	1348.9908	FBF	58.67		FBF
752	C81 H154 O15	20.161	1367.1303	FBF	56.64		FBF
753	C81 H152 O14	19.434	1349.1055	FBF	50.09		FBF
754	C81 H150 O15	20.889	1363.0855	FBF	55.81		FBF
755	C81 H148 O15	19.642	1361.0728	FBF	52.07		FBF
<u>756</u> 757	C81 H144 O14 C82 H140 O15	19.330 19.252	1341.0518 1365.0158	FBF FBF	51.17 57.70		FBF FBF
758	C82 H148 O14	21.045	1357.0782	FBF	50.48		FBF
759	C83 H138 O14	18.550	1359.0100	FBF	51.89		FBF
760	C83 H146 O15	19.044	1383.0681	FBF	50.21		FBF
761	C29 H48 O9	4.984	540.3307	FBF	82.13		FBF
762	C30 H58 O10	5.503	578.4000	FBF	79.52		FBF
763	C30 H52 O10	5.919	572.3551	FBF	55.49		FBF
764	C30 H50 O9	5.451	554.3462	FBF	77.69		FBF
765 766	C30 H50 O10 C30 H46 O9	6.257	570.3426 550.3160	FBF FBF	56.06 53.67		FBF FBF
766 767	C30 H46 O9 C31 H56 O9	5.218 10.207	550.3169 572.3914	FBF	53.67 97.41		FBF
768	C31 H54 O9	4.125	570.3759	FBF	97.78		FBF
769	C31 H52 O10	19.044	584.3541	FBF	75.21		FBF
770	C32 H56 O10	4.203	600.3873	FBF	59.31		FBF
771	C32 H50 O9	5.685	578.3448	FBF	63.85		FBF
772	C33 H60 O9	15.380	600.4253	FBF	56.72		FBF
773	C33 H58 O9	5.296	598.4039	FBF	62.14		FBF
774	C33 H56 O9	18.914	596.3944	FBF	65.67		FBF
775	C33 H52 O9	4.125	592.3573	FBF	54.68		FBF
776	C33 H52 O10	5.711	608.3589	FBF	63.37		FBF
777 778	C34 H66 O10 C34 H54 O10	13.353 5.737	634.4672 622.3695	<u>FBF</u> FBF	69.97 64.34		FBF FBF
778 779	C34 H52 O9	5.737	604.3621	FBF	55.97		FBF
780	C35 H66 O9	17.901	630.4697	FBF	50.25		FBF
781	C35 H62 O10	5.374	642.4299	FBF	62.37		FBF
782	C35 H58 O9	14.860	622.4065	FBF	57.49		FBF
783	C35 H56 O10	4.281	636.3837	FBF	57.54		FBF
784	C35 H54 O9	4.932	618.3802	FBF	74.81		FBF



Compound Summ							
Cpd Name	Formula C35 U54 O10	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorithm
1785 1786	C35 H54 O10 C36 H66 O9	5.348 19.070	634.3742 642.4712	<u>FBF</u> FBF	79.84 73.12		FBF FBF
1787	C36 H58 O9	5.607	634.4125	FBF	69.16		FBF
1788	C36 H56 O9	4.854	632.3918	FBF	59.02		FBF
1789	C36 H56 O10	5.374	648.3878	FBF	58.69		FBF
1790	C37 H72 O10	16.160	676.5126	FBF	58.13		FBF
1791	C37 H68 O9	10.077	656.4901	FBF	71.77		FBF
1792 1793	C37 H58 O10 C38 H72 O9	5.036 19.954	662.4048 672.5165	FBF FBF	64.49 58.48		FBF FBF
1794	C38 H64 O9	17.667	664.4541	FBF	71.70		FBF
1795	C38 H62 O10	5.685	678.4387	FBF	54.79		FBF
1796	C39 H76 O9	19.980	688.5513	FBF	51.95		FBF
1797	C39 H76 O10	20.265	704.5474	FBF	58.13		FBF
1798	C39 H66 O9	10.077	678.4712	FBF	76.34		FBF
1799	C39 H64 O9	4.437	676.4573	FBF	51.65		FBF
1800 1801	C40 H78 O9 C40 H72 O9	18.498 13.431	702.5670 696.5233	<u>FBF</u> FBF	57.46 53.37		FBF FBF
1802	C40 H70 O9	17.901	694.5054	FBF	51.09		FBF
1803	C40 H68 O9	17.719	692.4855	FBF	71.57		FBF
1804	C40 H62 O10	6.647	702.4344	FBF	81.19		FBF
1805	C41 H68 O9	19.980	704.4826	FBF	73.37		FBF
1806	C41 H64 O9	5.711	700.4527	FBF	77.02		FBF
1807	C41 H62 O9	4.437	698.4392	FBF	57.76		FBF
1808 1809	C42 H80 O9 C42 H70 O9	19.044 19.954	728.5798 718.5089	FBF FBF	60.83 58.22		FBF FBF
1810	C43 H84 O9	18.031	744.6143	FBF	52.48		FBF
1811	C43 H74 O9	19.954	734.5327	FBF	52.28		FBF
1812	C43 H66 O9	14.211	726.4650	FBF	58.05		FBF
1813	C44 H80 O9	14.835	752.5783	FBF	50.73		FBF
1814	C44 H78 O9	19.044	750.5615	FBF	50.57		FBF
1815	C44 H76 O9	19.044	748.5459	FBF	51.59		FBF
1816 1817	C44 H74 O9 C45 H88 O9	19.980 18.732	746.5365 772.6428	FBF FBF	79.91 50.36		FBF FBF
1818	C45 H88 O10	13.509	788.6396	FBF	50.12		FBF
1819	C45 H84 O9	19.928	768.6083	FBF	52.67		FBF
1820	C45 H82 O9	13.353	766.5954	FBF	50.60		FBF
1821	C46 H90 O10	13.119	802.6526	FBF	56.56	<u> </u>	FBF
1822	C46 H70 O10	19.070	782.4940	FBF	69.13		FBF
1823	C46 H76 O9	17.096	772.5459	FBF	74.25		FBF
1824 1825	C47 H90 O9 C47 H72 O9	20.499 15.302	798.6602 780.5172	<u>FBF</u> FBF	50.57 54.91		FBF FBF
1826	C47 H82 O9	13.327	790.5975	FBF	60.04		FBF
1827	C48 H94 O9	14.185	814.6938	FBF	58.03		FBF
1828	C48 H92 O9	13.327	812.6723	FBF	51.47		FBF
1829	C48 H74 O9	17.044	794.5283	FBF	61.64		FBF
1830	C48 H74 O10	13.353	810.5255	FBF	62.75		FBF
1831	C48 H72 O9	10.000	792.5216	FBF	74.73		FBF
1832 1833	C48 H84 O9 C48 H76 O9	12.131 17.277	804.6085 796.5485	FBF FBF	54.31 59.13		FBF FBF
1834	C49 H96 O10	14.783	844.7052	FBF	51.71		FBF
1835	C49 H74 O9	4.750	806.5299	FBF	61.43		FBF
1836	C49 H92 O9	21.200	824.6793	FBF	50.90		FBF
1837	C49 H88 O9	17.018	820.6430	FBF	50.88		FBF
1838	C49 H84 O9	13.353	816.6124	FBF	54.49		FBF
1839	C49 H78 O9	18.992	810.5591	FBF	58.44		FBF
1840	C50 H96 O9	13.275	840.7023	FBF FBF	54.91 85.55		FBF FBF
1841	C50 H76 O10	10.000	836.5455 844.6436				
1842 1843	C51 H88 O9 C51 H86 O9	18.992 15.354	842.6277	FBF FBF	56.17 54.95		FBF FBF
1844	C52 H80 O10	14.860	864.5754	FBF	62.57		FBF
1845	C52 H78 O10	5.685	862.5592	FBF	62.33		FBF
1846	C53 H104 O10	18.914	900.7608	FBF	54.41		FBF
1847	C53 H88 O9	12.729	868.6476	FBF	56.80		FBF
1848	C53 H86 O9	14.393	866.6274	FBF	62.00		FBF
<u>1849</u> 1850	C54 H106 O10 C54 H84 O9	14.886 13.379	914.7763 876.6113	FBF FBF	52.89 50.66		FBF FBF
1851	C54 H102 O9	18.810	894.7516	FBF	62.43		FBF
1852	C55 H108 O10	14.679	928.7948	FBF	51.22		FBF
1853	C55 H86 O9	13.353	890.6226	FBF	54.22		FBF
1854	C55 H100 O9	18.836	904.7373	FBF	52.17		FBF
1855	C55 H90 O9	17.797	894.6632	FBF	51.25		FBF
1856	C56 H102 O9	15.666	918.7535	FBF	53.31		FBF
1857 1858	C56 H94 O9 C57 H92 O10	15.588 18.109	910.6890 936.6699	FBF FBF	52.05 68.86		FBF FBF
1859	C57 H92 O10 C57 H88 O9	18.109	936.6699	FBF	52.52		FBF
1860	C57 H88 O10	19.954	932.6324	FBF	51.39		FBF
1861	C57 H100 O10	19.824	928.7369	FBF	51.00		FBF
1862	C57 H94 O9	13.353	922.6959	FBF	53.06		FBF
1863	C58 H114 O9	13.847	954.8443	FBF	50.74		FBF
1864	C58 H92 O9	22.395	932.6723	FBF	56.86		FBF
1865	C58 H90 O9	22.135	930.6550	FBF	55.80		FBF
1866	C58 H90 O10	18.472	946.6589	FBF	62.45		FBF
1867 1868	C58 H106 O9	21.512 20.837	946.7825 944.7691	FBF FBF	51.25 50.62	.	FBF FBF
1869	C58 H104 O9 C58 H102 O9	20.837 14.886	944.7691	FBF	50.62 51.65		FBF
1870	C58 H102 O9	21.356	938.7180	FBF	51.66		FBF
20.0	030 1130 03	21.330	JJ0./ 100	, DI	31.00		1 01



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ompound Sumi	mary Formula	RT	Mass	CAS ID Source	Score	Score (Lib)	Score (DB)	Score (MFG) Algorithm
1871	C59 H96 O9	16.966	948.7045	FBF	50.94		` `	FBF
1872	C59 H94 O9	16.446	946.6931	FBF	52.06			FBF
1873 1874	C59 H108 O9 C59 H100 O10	12.963 19.200	960.8002 968.7297	FBF FBF	56.86 56.91			FBF FBF
.875	C60 H116 O9	19.304	980.8630	FBF	51.56			FBF
1876	C60 H114 O9	14.679	978.8468	FBF	55.15			FBF
.877	C60 H110 O9	14.886	974.8177	FBF	50.28			FBF
878	C60 H106 O9	19.148	970.7840	FBF	51.65	-		FBF
879	C60 H100 O10	17.329	980.7262	FBF FBF	50.92			FBF FBF
880 881	C61 H118 O9 C61 H106 O9	17.303 14.886	994.8815 982.7868	FBF	67.97 50.38			FBF
882	C62 H122 O10	18.940	1026.9046	FBF	70.82			FBF
883	C62 H98 O10	13.977	1002.7161	FBF	58.90			FBF
884	C63 H124 O9	21.642	1024.9238	FBF	51.18			FBF
885	C63 H120 O9	17.537	1020.8911	FBF	67.61			FBF
886 887	C63 H118 O9 C63 H112 O9	22.655 13.795	1018.8822 1012.8300	<u>FBF</u> FBF	50.29 50.80			FBF FBF
888	C63 H108 O10	18.758	1012.8300	FBF	55.61			FBF
889	C64 H106 O10	20.317	1034.7745	FBF	71.30			FBF
890	C64 H104 O10	20.343	1032.7592	FBF	50.42			FBF
891	C64 H102 O10	20.915	1030.7406	FBF	62.35			FBF
892	C64 H120 O9	18.758	1032.8882	FBF	51.84			FBF
393 394	C64 H110 O10 C65 H126 O9	17.927 22.499	1038.8176 1050.9357	<u>FBF</u> FBF	61.43 66.40			FBF FBF
39 4 395	C65 H126 O9	22.499 17.927	1050.9357	FBF	70.58			FBF
396	C65 H104 O10	14.835	1044.7684	FBF	58.04			FBF
397	C65 H112 O10	22.343	1052.8267	FBF	58.36			FBF
398	C66 H110 O9	17.901	1046.8055	FBF	50.61			FBF
399	C66 H108 O10	17.927	1060.8003	FBF	73.64			FBF
900	C66 H126 O9	19.174	1062.9450	FBF	50.38			FBF
901	C66 H122 O9 C66 H112 O9	19.148	1058.9042 1048.8279	<u>FBF</u> FBF	68.37			FBF FBF
903	C67 H108 O10	20.395 20.317	1072.7916	FBF	51.65 53.82			FBF
904	C68 H130 O9	11.091	1090.9741	FBF	54.97			FBF
905	C68 H126 O9	20.343	1086.9372	FBF	59.26			FBF
906	C68 H122 O9	21.902	1082.9082	FBF	53.81			FBF
907	C69 H136 O10	19.460	1125.0099	FBF	58.42			FBF
908	C69 H116 O9	19.356	1088.8575	FBF	50.13			FBF
909 910	C70 H130 O9 C71 H118 O9	20.006 18.213	1114.9787 1114.8762	FBF FBF	65.88 56.49			FBF FBF
911	C71 H118 O9	22.161	1130.8764	FBF	53.05			FBF
912	C71 H136 O9	20.395	1133.0181	FBF	58.82			FBF
913	C72 H120 O10	19.538	1144.8857	FBF	57.10			FBF
914	C72 H134 O10	19.356	1158.9905	FBF	52.32			FBF
915	C72 H132 O9	20.733	1140.9927	FBF	50.02			FBF
916	C73 H124 O9	11.039	1144.9244	FBF	50.08			FBF
9 <u>17</u> 918	C73 H120 O10 C74 H126 O9	14.912 20.733	1156.8813 1158.9419	<u>FBF</u> FBF	55.37 57.50			FBF FBF
919	C74 H132 O9	20.058	1164.9912	FBF	50.17			FBF
920	C74 H128 O10	19.096	1176.9505	FBF	61.68			FBF
921	C75 H126 O10	18.576	1186.9430	FBF	50.36			FBF
922	C76 H130 O10	17.823	1202.9653	FBF	55.27			FBF
923	C76 H128 O9	14.912	1184.9531	FBF	54.39			FBF
925	C76 H126 O10 C76 H144 O9	17.589 22.603	1198.9411 1201.0781	FBF FBF	52.81 67.35			FBF FBF
926	C76 H140 O9	19.668	1197.0499	FBF	64.24			FBF
927	C77 H130 O9	19.980	1198.9740	FBF	55.66			FBF
928	C77 H144 O10	11.845	1229.0781	FBF	63.53			FBF
929	C77 H142 O10	20.655	1227.0614	FBF	56.44			FBF
930	C77 H134 O9	20.655	1203.0044	FBF	56.95			FBF
931 932	C29 H56 O12 S C29 H52 O12 S	5.348 8 206	628.3506	<u>FBF</u> FBF	55.48 56.99			FBF FBF
932	C30 H54 O13 S	8.206 13.353	624.3194 654.3321	FBF	56.99 88.66			FBF
934	C30 H52 O13 S	13.977	652.3100	FBF	52.63			FBF
935	C30 H48 O12 S	14.938	632.2870	FBF	55.31			FBF
936	C30 H46 O12 S	3.943	630.2768	FBF	57.80			FBF
937	C31 H60 O12 S	5.374	656.3741	FBF	56.45			FBF
938	C31 H60 O13 S	5.400	672.3749	FBF	60.91			FBF
939	C31 H56 O12 S	4.281	652.3532	FBF	64.52	-		FBF
940 941	C31 H52 O12 S C32 H60 O13 S	7.998 19.954	648.3194 684.3779	<u>FBF</u> FBF	56.14 51.20			FBF FBF
942	C32 H58 O13 S	12.651	682.3589	FBF	79.91			FBF
943	C32 H56 O12 S	4.724	664.3536	FBF	55.40			FBF
944	C32 H56 O13 S	13.951	680.3481	FBF	51.70			FBF
945	C32 H52 O12 S	16.030	660.3240	FBF	51.74	•		FBF

FBF

61.67

64.81

53.25

76.77

82.07

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1950 1951

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C32 H50 O13 S

C33 H60 O13 S

C33 H56 O12 S

C33 H54 O12 S

C34 H62 O12 S

C34 H62 O13 S

C34 H60 O12 S

C34 H60 O13 S

C34 H58 O12 S

C34 H56 O12 S C35 H64 O12 S

4.125

4.437

4.880

4.281

4.229

4.489

4.489

4.828

8.986

14.860 4.515

674.3027

696.3795

676.3513

674.3352

694.3975

710.3962

692.3838

708.3796

690.3630 688.3482 708.4085



ompound Summary						
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB) Score (MFG) Algorit
<u>.957</u> .958	C35 H62 O12 S C35 H58 O13 S	4.906 4.437	706.3970 718.3614	<u>FBF</u> FBF	92.36 76.32	FBF FBF
959	C36 H70 O13 S	6.179	742.4588	FBF	52.09	FBF
960	C36 H66 O12 S	4.906	722.4282	FBF	92.96	FBF
961	C36 H64 O12 S	5.010	720.4132	FBF	57.35	FBF
962	C36 H64 O13 S	4.619	736.4126	FBF	52.88	FBF
963	C36 H62 O12 S	5.477	718.3971	FBF	52.38	FBF
964	C36 H62 O13 S	18.576	734.3963	FBF	59.12	FBF
965	C37 H68 O12 S	5.166	736.4443	FBF	60.34	FBF
9 <u>66</u> 967	C37 H68 O13 S C37 H66 O13 S	4.619 5.010	752.4360 750.4225	<u>FBF</u> FBF	54.65 95.13	FBF FBF
968	C37 H62 O12 S	4.541	730.3920	FBF	60.17	FBF
969	C37 H60 O12 S	4.906	728.3804	FBF	64.11	FBF
970	C37 H56 O12 S	4.281	724.3473	FBF	51.76	FBF
971	C37 H56 O13 S	3.371	740.3456	FBF	59.01	FBF
972	C38 H72 O12 S	18.810	752.4809	FBF	52.38	FBF
973	C38 H72 O13 S	17.745	768.4697	FBF	50.21	FBF
974	C38 H70 O12 S	21.382	750.4617	FBF	50.38	FBF
975	C38 H70 O13 S	5.010	766.4539	FBF	94.64	FBF
976 977	C38 H64 O12 S C38 H62 O13 S	4.541 4.619	744.4124 758.3922	<u>FBF</u> FBF	89.79 62.84	FBF FBF
978	C38 H58 O12 S	15.380	738.3631	FBF	52.77	FBF
979	C39 H76 O12 S	17.745	768.5027	FBF	66.22	FBF
980	C39 H74 O13 S	6.205	782.4812	FBF	56.94	FBF
981	C39 H70 O13 S	13.639	778.4572	FBF	58.68	FBF
982	C39 H64 O13 S	4.984	772.4028	FBF	59.89	FBF
983	C39 H60 O12 S	14.912	752.3815	FBF	52.64	FBF
984	C39 H60 O13 S	4.437	768.3728	FBF	58.37	FBF
985	C40 H76 O12 S	13.847	780.5082	FBF	86.43	FBF
986 987	C40 H74 O12 S C40 H68 O13 S	11.715 4.671	778.4946 788.4383	FBF FBF	55.51 91.68	FBF FBF
988	C41 H78 O13 S	20.006	810.5210	FBF	70.36	FBF
989	C41 H76 O12 S	4.750	792.5059	FBF	52.01	FBF
990	C41 H74 O12 S	5.088	790.4907	FBF	50.11	FBF
991	C41 H72 O12 S	5.815	788.4822	FBF	59.98	FBF
992	C41 H66 O12 S	4.671	782.4297	FBF	89.06	FBF
993	C41 H64 O13 S	21.356	796.4116	FBF	56.00	FBF
994	C42 H80 O13 S	13.691	824.5320	FBF	71.18	FBF
995	C42 H76 O12 S	18.109	804.5085	FBF	50.88	FBF
996 997	C42 H74 O12 S C42 H68 O12 S	14.055 18.810	802.4889	<u>FBF</u> FBF	80.24	FBF FBF
998	C43 H80 O13 S	15.276	796.4422 836.5266	FBF	79.76 68.75	FBF
999	C43 H78 O12 S	12.885	818.5242	FBF	65.15	FBF
000	C43 H78 O13 S	19.902	834.5103	FBF	58.06	FBF
001	C43 H74 O12 S	13.665	814.4858	FBF	53.14	FBF
002	C43 H74 O13 S	11.715	830.4850	FBF	60.37	FBF
003	C43 H70 O13 S	4.750	826.4550	FBF	92.72	FBF
004	C44 H84 O13 S	4.854	852.5600	FBF	50.63	FBF
005 006	C44 H80 O12 S C44 H78 O13 S	13.665 13.223	832.5378 846.5153	<u>FBF</u> FBF	66.25 67.32	FBF FBF
007	C45 H88 O12 S	18.914	852.6011	FBF	50.92	FBF
008	C45 H68 O13 S	4.750	848.4368	FBF	91.15	FBF
009	C46 H84 O13 S	14.445	876.5662	FBF	57.43	FBF
010	C46 H80 O13 S	5.166	872.5352	FBF	52.02	FBF
011	C46 H78 O12 S	13.509	854.5199	FBF	63.99	FBF
012	C46 H76 O12 S	13.171	852.5034	FBF	57.42	FBF
013	C46 H76 O13 S	13.119	868.5003	FBF	50.20	FBF
014	C46 H72 O12 S C47 H84 O12 S	13.353	848.4686	FBF	54.51	FBF
)15)16	C47 H84 O12 S	17.355 5.685	872.5677 884.5706	<u>FBF</u> FBF	52.09 59.93	FBF FBF
017	C48 H82 O13 S	13.353	898.5429	FBF	62.33	FBF
018	C48 H78 O13 S	11.663	894.5178	FBF	55.38	FBF
)19	C49 H96 O13 S	13.535	924.6553	FBF	54.80	FBF
)20	C49 H94 O12 S	16.238	906.6534	FBF	55.43	FBF
21	C49 H88 O13 S	15.328	916.5914	FBF	51.60	FBF
)22	C49 H86 O13 S	14.601	914.5773	FBF	73.75	FBF
)23	C49 H84 O12 S	20.317	896.5672	FBF	50.02	FBF
) <u>24 </u>	C49 H82 O13 S C50 H92 O12 S	13.899 18.187	910.5388 916.6319	<u>FBF</u> FBF	54.43 53.34	FBF FBF
026	C50 H92 O12 S	5.711	916.6319	FBF	67.78	FBF
27	C50 H80 O13 S	13.405	920.5310	FBF	61.70	FBF
)28	C51 H86 O12 S	19.044	922.5880	FBF	51.67	FBF
29	C51 H84 O13 S	14.601	936.5616	FBF	77.05	FBF
)30	C51 H82 O13 S	14.860	934.5472	FBF	50.32	FBF
031	C52 H102 O12 S	21.434	950.7033	FBF	50.83	FBF
032	C52 H80 O12 S	4.984	928.5403	FBF	52.28	FBF
133	C52 H78 O12 S	5.270	926.5269	FBF	71.29	FBF
034	C52 H86 O13 S	5.763	950.5837	FBF	61.71	FBF
035 036	C53 H104 O12 S C53 H104 O13 S	13.041 16.784	964.7293 980.7221	<u>FBF</u> FBF	58.59 58.46	FBF FBF
037	C53 H104 O13 S	4.984	944.5649	FBF	58.46 57.28	FBF
038	C53 H84 O13 S	14.159	960.5691	FBF	59.72	FBF
)39	C53 H82 O12 S	14.107	942.5602	FBF	76.43	FBF
)40	C53 H82 O13 S	15.172	958.5449	FBF	57.10	FBF
41	C53 H94 O13 S	13.223	970.6444	FBF	50.19	FBF
042	C53 H88 O12 S	18.992	948.5978	FBF	51.67	FBF



Compound Sumn								
Cpd Name 2043	Formula C54 H106 O12 S	RT 17.563	Mass 978.7415	CAS ID Source FBF	Score 57.91	Score (Lib)	Score (DB)	Score (MFG) Algorithm FBF
2044	C54 H82 O13 S	5.348	970.5496	FBF	77.13			FBF
2045	C54 H100 O13 S	15.328	988.6815	FBF	65.42			FBF
2046	C54 H92 O12 S	18.966	964.6260	FBF	51.76			FBF
2047	C55 H88 O13 S	5.062	988.5912	FBF	58.38			FBF
2048	C55 H86 O13 S	5.062	986.5843	FBF	72.07			FBF
2 <u>049</u> 2050	C55 H104 O12 S C55 H104 O13 S	20.577 20.993	988.7244 1004.7199	FBF FBF	50.94 59.15			FBF FBF
2051	C55 H102 O13 S	20.110	1004.7199	FBF	51.33			FBF
2052	C55 H102 O13 S	14.835	984.7004	FBF	50.49		-	FBF
2053	C55 H96 O13 S	13.275	996.6562	FBF	70.70			FBF
2054	C56 H104 O12 S	14.835	1000.7212	FBF	56.79			FBF
2055	C56 H102 O13 S	17.719	1014.7052	FBF	56.79			FBF
2056	C56 H92 O13 S	14.860	1004.6287	FBF	52.81			FBF
<u>2057</u> 2058	C57 H110 O13 S C57 H104 O12 S	20.343 19.434	1034.7741 1012.7288	FBF FBF	51.46 55.38			FBF FBF
2059	C57 H94 O13 S	13.535	1012.7288	FBF	62.19			FBF
2060	C58 H114 O13 S	20.317	1050.7902	FBF	63.91		,	FBF
2061	C58 H110 O12 S	14.783	1030.7685	FBF	55.05			FBF
2062	C58 H104 O12 S	20.785	1024.7299	FBF	51.35			FBF
2063	C58 H96 O13 S	13.327	1032.6614	FBF	57.18			FBF
2064	C59 H116 O12 S	19.122	1048.8171	FBF	57.47			FBF
<u>2065</u> 2066	C59 H114 O12 S C59 H96 O12 S	16.212 16.966	1046.7958 1028.6591	FBF FBF	50.02 50.46			FBF FBF
2067	C59 H114 O13 S	17.927	1062.8033	FBF	56.65			FBF
2068	C60 H98 O12 S	21.460	1042.6729	FBF	50.71			FBF
2069	C60 H110 O13 S	17.927	1070.7683	FBF	52.30			FBF
2070	C60 H108 O13 S	14.886	1068.7511	FBF	74.10			FBF
2071	C61 H96 O12 S	14.757	1052.6660	FBF	51.37			FBF
2072	C61 H112 O13 S	17.927	1084.7851	FBF	62.54			FBF
<u>2073</u> 2074	C61 H106 O12 S	21.019	1062.7391 1082.6753	FBF	53.99			FBF FBF
2075	C62 H98 O13 S C62 H118 O12 S	21.512 18.758	1082.6753	FBF FBF	55.03 50.36			FBF
2076	C62 H116 O13 S	19.564	1100.8138	FBF	52.74		-	FBF
2077	C62 H110 O13 S	21.226	1094.7622	FBF	57.74			FBF
2078	C62 H106 O13 S	14.886	1090.7381	FBF	72.29			FBF
2079	C63 H122 O12 S	18.940	1102.8630	FBF	50.28			FBF
2080	C63 H100 O13 S	19.070	1096.6949	FBF	56.28			FBF
2081	C63 H116 O12 S	18.602	1096.8123	FBF	51.21			FBF
<u>2082</u> 2083	C63 H112 O12 S C63 H108 O12 S	18.109 17.381	1092.7869 1088.7545	FBF FBF	57.67 55.71			FBF FBF
2084	C63 H108 O13 S	19.096	1104.7564	FBF	55.61			FBF
2085	C64 H106 O12 S	18.992	1098.7370	FBF	67.67			FBF
2086	C64 H120 O13 S	19.564	1128.8507	FBF	57.96			FBF
2087	C64 H118 O12 S	14.860	1110.8364	FBF	57.30			FBF
2088	C64 H110 O13 S	18.187	1118.7695	FBF	52.50			FBF
2089	C65 H128 O12 S	22.135	1132.9195	FBF FBF	51.03		,	FBF FBF
<u>2090</u> 2091	C65 H128 O13 S C65 H108 O13 S	18.343 22.966	1148.8979 1128.7485	FBF	51.19 55.22			FBF
2092	C65 H126 O13 S	21.278	1146.8935	FBF	50.08			FBF
2093	C65 H116 O12 S	20.967	1120.8141	FBF	58.49		,	FBF
2094	C65 H110 O12 S	18.109	1114.7699	FBF	77.19			FBF
2095	C66 H106 O12 S	17.459	1122.7332	FBF	50.59			FBF
2096	C66 H126 O12 S	19.824	1142.8956	FBF	51.27			FBF
2097	C66 H126 O13 S	21.174	1158.8924	FBF	52.31			FBF
<u>2098</u> 2099	C66 H124 O12 S C66 H120 O13 S	20.811 18.109	1140.8919 1152.8412	FBF FBF	50.29 50.11			FBF FBF
2100	C68 H112 O13 S	18.031	1168.7857	FBF	61.30			FBF
2101	C68 H122 O13 S	19.876	1178.8590	FBF	77.91			FBF
2102	C68 H120 O13 S	20.032	1176.8405	FBF	53.22			FBF
2103	C68 H116 O12 S	20.006	1156.8130	FBF	56.75			FBF
2104	C69 H120 O12 S	18.836	1172.8485	FBF	74.55			FBF
2105	C69 H120 O13 S	22.655	1188.8456	FBF	54.20			FBF
<u>2106</u> 2107	C70 H138 O12 S C70 H118 O13 S	20.525 19.980	1202.9938 1198.8275	FBF FBF	54.94 63.55			FBF FBF
2107	C70 H118 O13 S	18.836	1178.8011	FBF	62.47			FBF
2109	C70 H124 O12 S	18.654	1188.8783	FBF	53.05			FBF
2110	C70 H120 O13 S	20.058	1200.8431	FBF	75.00			FBF
2111	C71 H140 O12 S	22.083	1217.0103	FBF	59.41			FBF
2112	C71 H120 O12 S	17.849	1196.8554	FBF	50.20			FBF
2113	C71 H118 O12 S	18.836	1194.8311	FBF	65.96			FBF
<u>2114 </u>	C71 H116 O13 S C71 H136 O13 S	18.187 19.616	1208.8239 1228.9625	FBF FBF	52.22 53.07			FBF FBF
2116	C71 H134 O12 S	18.732	1210.9598	FBF	63.52			FBF
2117	C71 H124 O12 S	17.277	1200.8753	FBF	55.88			FBF
2118	C72 H140 O12 S	17.745	1229.0016	FBF	61.97			FBF
2119	C72 H138 O12 S	17.745	1226.9879	FBF	53.95			FBF
2120	C72 H138 O13 S	18.888	1242.9856	FBF	50.16			FBF
2121	C72 H128 O13 S	18.161	1232.9142	FBF	50.93			FBF
2122	C72 H124 O13 S	18.472	1228.8721	FBF	51.45			FBF
2123	C73 H144 O12 S	11.897	1245.0437	FBF	50.47			FBF
2124	C73 H122 O13 S C73 H140 O12 S	18.472 20.447	1238.8497 1241.0020	FBF FBF	51.84 66.68			FBF FBF
<u>2125</u> 2126	C73 H140 O12 S C73 H140 O13 S	20. 44 7 18.602	1241.0020	FBF	55.84			FBF
2127	C73 H138 O12 S	19.876	1238.9936	FBF	51.07			FBF
	C73 H136 O13 S	17.771	1252.9673	FBF	54.20			FBF



Compound Summary	-						
Cpd Name	Formula	RT 17.771	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorithm
<u>2129</u> 2130	C73 H134 O13 S C73 H130 O13 S	17.771 19.512	1250.9502 1246.9261	<u>FBF</u> FBF	52.64 52.28		FBF FBF
2131	C74 H126 O12 S	14.886	1238.8969	FBF	50.12		FBF
2132	C74 H142 O12 S	19.200	1255.0257	FBF	53.00		FBF
2133	C74 H138 O12 S	19.668	1250.9884	FBF	57.90		FBF
2134	C74 H136 O13 S	19.122	1264.9702	FBF	59.45		FBF
2135	C75 H146 O12 S	19.798	1271.0409	FBF	56.63		FBF
<u>2136</u> 2137	C75 H136 O12 S C77 H150 O12 S	17.771 20.136	1260.9790 1299.0767	FBF FBF	54.82 52.05		FBF FBF
2138	C77 H130 O12 S	18.784	1278.9358	FBF	50.16		FBF
2139	C77 H128 O13 S	11.065	1292.9089	FBF	58.88		FBF
2140	C77 H148 O13 S	19.798	1313.0624	FBF	51.37		FBF
2141	C77 H144 O12 S	20.447	1293.0380	FBF	51.21		FBF
2142	C77 H142 O12 S	17.745	1291.0184	FBF	51.30		FBF
2143	C77 H136 O13 S	18.161	1300.9689	FBF	50.29		FBF
2144	C34 H50 O12 S	3.917	682.2989	FBF	64.95		FBF
<u>2145</u> 2146	C35 H52 O13 S C38 H56 O13 S	1.448 13.743	712.3163 752.3402	FBF FBF	74.29 51.85		FBF FBF
2147	C39 H58 O12 S	14.912	750.3614	FBF	51.76		FBF
2148	C43 H64 O12 S	4.671	804.4116	FBF	92.26		FBF
2149	C44 H64 O13 S	4.750	832.4122	FBF	66.78		FBF
2150	C52 H76 O13 S	22.499	940.4934	FBF	60.31		FBF
2151	C59 H90 O12 S	13.691	1022.6072	FBF	50.46		FBF
2152	C66 H104 O12 S	17.537	1120.7251	FBF	73.33		FBF
2153	C72 H116 O12 S	18.810	1204.8222	FBF	69.55		FBF
2154	C75 H122 O12 S	21.200	1246.8626	FBF	65.88		FBF
2155	C25 H46 O14	5.737	570.2943 582.2884	FBF ERF	67.28		FBF FBF
<u>2156</u> 2157	C26 H46 O14 C26 H44 O14	4.047 4.515	582.2884 580.2766	FBF FBF	65.48 76.99		FBF
2158	C26 H42 O14	3.943	578.2618	FBF	63.41		FBF
2159	C27 H50 O14	4.099	598.3152	FBF	71.04		FBF
2160	C27 H48 O14	4.489	596.3051	FBF	79.00		FBF
2161	C28 H52 O14	4.125	612.3334	FBF	90.05		FBF
2162	C29 H52 O14	21.876	624.3382	FBF	60.02		FBF
2163	C29 H48 O14	12.807	620.3039	FBF	71.93		FBF
2164	C30 H56 O14	5.633	640.3686	FBF	56.97		FBF
2165	C31 H56 O14	5.322	652.3655	FBF	70.22		FBF
2166 2167	C31 H54 O14 C32 H60 O14	4.281 20.006	650.3516 668.4049	FBF FBF	86.85 58.76		FBF FBF
2168	C32 H56 O14	4.724	664.3634	FBF	71.36		FBF
2169	C33 H62 O14	4.411	682.4118	FBF	55.45		FBF
2170	C33 H54 O14	12.625	674.3534	FBF	52.81		FBF
2171	C33 H52 O14	4.281	672.3336	FBF	79.66		FBF
2172	C34 H64 O14	4.437	696.4329	FBF	68.91		FBF
2173	C34 H60 O14	4.932	692.3962	FBF	53.84		FBF
2174	C34 H56 O14	17.511	688.3710	FBF	55.46		FBF
2175	C19 H34 O9	7.244 7.244	406.2194 404.2025	FBF FBF	69.82 82.03		FBF FBF
<u>2176</u> 2177	C19 H32 O9 C20 H36 O9	5.374	420.2374	FBF	71.11		FBF
2178	C20 H34 O9	7.192	418.2195	FBF	54.53		FBF
2179	C20 H32 O9	4.776	416.2065	FBF	63.73		FBF
2180	C21 H40 O9	5.140	436.2662	FBF	82.88		FBF
2181	C21 H36 O9	7.920	432.2343	FBF	87.30		FBF
2182	C21 H34 O9	3.293	430.2201	FBF	81.29		FBF
2183	C22 H40 O9	3.085	448.2703	FBF	70.55		FBF
2184	C22 H36 O9	4.906	444.2358	FBF	91.57		FBF
2185	C23 H42 O9	3.527	462.2852	FBF	74.40		FBF
2186	C23 H40 O9	7.920	460.2653	FBF	65.96		FBF FBF
2187 2188	C24 H44 O9 C25 H42 O9	3.839 4.489	476.3016 486.2816	FBF FBF	71.35 72.36		FBF
2189	C26 H50 O9	5.841	506.3477	FBF	53.77		FBF
2190	C26 H48 O9	4.515	504.3295	FBF	85.06		FBF
2191	C27 H52 O9	20.317	520.3636	FBF	76.08		FBF
2192	C28 H52 O9	5.166	532.3649	FBF	63.03		FBF
2193	C35 H48 O9	4.359	612.3321	FBF	81.17		FBF
2194	C19 H36 O11 S	11.325	472.1973	FBF	90.42		FBF
2195	C19 H32 O11 S	3.293	468.1653	FBF	54.26		FBF
2196 2197	C23 H42 O11 S C25 H48 O11 S	3.735 9.870	526.2446 556.2913	FBF FBF	60.48 51.99		FBF FBF
2198	C26 H46 O11 S	3.631	566.2785	FBF	53.14		FBF
2199	C27 H50 O11 S	18.836	582.3070	FBF	50.01		FBF
2200	C29 H52 O11 S	4.125	608.3269	FBF	67.23		FBF
2201	C30 H54 O11 S	4.047	622.3415	FBF	68.21		FBF
2202	C30 H52 O11 S	4.593	620.3281	FBF	72.07		FBF
2203	C31 H60 O11 S	4.802	640.3883	FBF	61.38		FBF
2204	C31 H50 O11 S	4.125	630.3088	FBF	79.79		FBF
2205	C32 H62 O11 S	6.049 E 700	654.4030	FBF	57.05		FBF EDE
2206 2207	C32 H60 O11 S	5.789	652.3868	FBF FBF	76.46 57.40		FBF FBF
2208	C32 H58 O11 S C32 H56 O11 S	4.281 4.359	650.3710 648.3575	FBF	57.40 57.31		FBF
2209	C32 H54 O11 S	8.154	646.3373	FBF	50.03		FBF
2210	C32 H50 O11 S	4.593	642.3113	FBF	53.42		FBF
2211	C33 H60 O11 S	4.359	664.3842	FBF	82.53		FBF
2212	C33 H58 O11 S	4.802	662.3719	FBF	92.44		FBF
213	C33 H54 O11 S	4.099	658.3368	FBF	60.95		FBF
2214	C34 H62 O11 S	4.776	678.4022	FBF	93.10		FBF



Compound Summary							
Cpd Name	Formula	RT	Mass	CAS ID Source		core (Lib) Score (DB	
<u>215</u> 216	C34 H60 O11 S C34 H56 O11 S	4.802 4.047	676.3848 672.3534	<u>FBF</u> FBF	59.65 56.84		FBF FBF
217	C34 H54 O11 S	4.359	670.3374	FBF	56.34		FBF
218	C35 H64 O11 S	4.802	692.4152	FBF	59.59		FBF
219	C35 H62 O11 S	13.951	690.4014	FBF	54.27		FBF
220	C35 H58 O11 S	4.437	686.3659	FBF	53.68		FBF
221	C35 H56 O11 S	4.776	684.3542	FBF	64.16		FBF
222	C36 H66 O11 S C36 H62 O11 S	5.114 20.084	706.4287 702.4044	<u>FBF</u> FBF	75.60 57.61		FBF FBF
2224	C36 H60 O11 S	4.437	702.4044	FBF	89.19		FBF
2225	C36 H56 O11 S	10.285	696.3542	FBF	60.67		FBF
2226	C37 H70 O11 S	5.763	722.4663	FBF	74.67		FBF
227	C39 H74 O11 S	0.383	750.4998	FBF	72.14		FBF
228	C39 H70 O11 S	5.010	746.4631	FBF	61.33		FBF
229	C39 H68 O11 S	5.737	744.4476	FBF	78.10		FBF
230	C39 H62 O11 S C40 H78 O11 S	4.541 10.026	738.4037 766.5252	<u>FBF</u> FBF	85.57 71.30	-	FBF FBF
232	C40 H64 O11 S	4.932	752.4149	FBF	55.91		FBF
233	C41 H78 O11 S	17.096	778.5241	FBF	59.66		FBF
234	C41 H68 O11 S	14.860	768.4429	FBF	59.35		FBF
235	C42 H82 O11 S	14.912	794.5532	FBF	55.12		FBF
236	C42 H80 O11 S	14.731	792.5457	FBF	51.08		FBF
237	C42 H76 O11 S	13.587	788.5109	FBF	61.15		FBF
238 239	C42 H74 O11 S	16.758	786.4987	FBF FBF	59.04 51.45		FBF FBF
239 240	C43 H82 O11 S C43 H70 O11 S	16.342 4.750	806.5616 794.4637	FBF	51.45 61.66		FBF
241	C14 H28 O4	7.426	260.1978	FBF	60.02		FBF
242	C20 H40 O4	11.741	344.2910	FBF	73.00		FBF
243	C7 H14 O4	1.604	162.0884	FBF	69.89		FBF
244	C10 H20 O4	5.841	204.1365	FBF	81.56		FBF
245	C11 H22 O4	6.465	218.1523 288.2663	FBF	76.50		FBF
<u>246</u> 247	C17 H36 O3 C21 H44 O3	12.131 21.772	344.3321	<u>FBF</u> FBF	66.09 54.48		FBF FBF
248	C30 H57 N O10	5.322	591.3946	FBF	52.33		FBF
249	C30 H55 N O9	5.893	573.3844	FBF	71.57		FBF
250	C30 H53 N O8	3.969	555.3759	FBF	74.59		FBF
251	C30 H49 N O8	14.860	551.3442	FBF	77.73		FBF
252	C30 H47 N O8	3.943	549.3345	FBF	58.19		FBF FBF
253	C31 H59 N O9	10.207	589.4181	FBF	97.41		FBF
<u>254</u> 255	C31 H57 N O9 C31 H57 N O10	4.125 18.732	587.4019 603.3965	<u>FBF</u> FBF	71.42 62.61		FBF FBF
256	C31 H55 N O8	4.828	569.3977	FBF	63.75		FBF
257	C31 H55 N O10	5.296	601.3832	FBF	56.86		FBF
258	C31 H51 N O8	3.943	565.3576	FBF	53.80		FBF
259	C31 H51 N O9	0.409	581.3519	FBF	63.23		FBF
2260	C31 H49 N O8	4.489	563.3513	FBF	61.13		FBF
2261 2262	C31 H49 N O9 C31 H49 N O10	3.839 3.839	579.3452 595.3399	<u>FBF</u> FBF	63.08 62.96		FBF FBF
2263	C32 H59 N O10	5.737	617.4145	FBF	70.73		FBF
264	C32 H57 N O8	4.750	583.4072	FBF	73.16		FBF
265	C32 H57 N O9	4.593	599.4011	FBF	67.70		FBF
266	C32 H53 N O9	5.685	595.3715	FBF	64.34		FBF
267	C32 H53 N O10	6.205	611.3655	FBF	52.34		FBF
268	C32 H51 N O8	5.218	577.3631	FBF	52.96		FBF
269	C32 H51 N O9	4.125	593.3608	FBF	57.54		FBF
<u>270</u> 271	C32 H51 N O10 C33 H63 N O8	5.711 14.029	609.3486 601.4535	<u>FBF</u> FBF	66.91 51.08		FBF FBF
272	C33 H63 N O10	10.155	633.4436	FBF	88.89		FBF
273	C33 H61 N O10	4.281	631.4284	FBF	72.11		FBF
274	C33 H59 N O10	6.361	629.4182	FBF	54.31		FBF
275	C33 H57 N O10	4.828	627.4028	FBF	51.14		FBF
276	C33 H55 N O9	4.125	609.3839	FBF	54.68		FBF
277	C33 H55 N O10	5.711	625.3855	FBF ERE	52.39		FBF FRE
<u>278 </u>	C33 H53 N O8 C33 H53 N O9	4.802 4.359	591.3795 607.3772	<u>FBF</u> FBF	80.99 62.75		FBF FBF
280	C33 H53 N O10	4.021	623.3718	FBF	59.69		FBF
281	C33 H51 N O9	4.697	605.3601	FBF	54.51		FBF
282	C34 H65 N O8	15.822	615.4691	FBF	51.79		FBF
283	C34 H65 N O9	17.901	631.4713	FBF	61.23		FBF
284	C34 H61 N O9	4.854	627.4352	FBF	69.71		FBF
285 286	C34 H59 N O8	6.569 5.737	609.4292	<u>FBF</u> FBF	54.91 64.34		FBF FBF
286 287	C34 H57 N O10 C34 H55 N O9	5.737	639.3965 621.3886	FBF	55.97		FBF
288	C34 H55 N O10	4.281	637.3872	FBF	65.44		FBF
289	C35 H67 N O8	18.524	629.4839	FBF	51.08		FBF
290	C35 H65 N O8	22.343	627.4687	FBF	61.82		FBF
291	C35 H63 N O10	5.036	657.4498	FBF	50.53		FBF
292	C35 H61 N O9	16.862	639.4392	FBF	51.45		FBF
293	C35 H59 N O10	4.281	653.4103	FBF	57.48		FBF
294	C35 H57 N O8	5.607	619.4076	FBF	51.77		FBF
295	C35 H57 N O9	4.932	635.4066	FBF ERE	80.71		FBF ERE
<u>296</u> 297	C35 H57 N O10 C35 H55 N O9	4.776 16.134	651.4030 633.3880	<u>FBF</u> FBF	69.39 54.08		FBF FBF
298	C35 H55 N O10	4.828	649.3843	FBF	78.44		FBF
299	C35 H53 N O8	4.593	615.3813	FBF	51.67		FBF
	C36 H69 N O9	19.070	659.4993	FBF	71.15		FBF



Compound Sumn								
Cpd Name 2301	Formula C36 H69 N O10	RT 17.979	Mass 675.4912	CAS ID Source FBF	Score 57.32	Score (Lib)	Score (DB)	Score (MFG) Algorithm FBF
2301 2302	C36 H69 N O10 C36 H67 N O10	21.382	673.4825	FBF	57.32 51.67			FBF
2303	C36 H63 N O9	6.621	653.4550	FBF	55.21			FBF
2304	C36 H61 N O9	16.628	651.4323	FBF	67.46			FBF
2305	C36 H59 N O9	4.854	649.4171	FBF	64.64			FBF
2306	C36 H59 N O10	4.724	665.4139	FBF	67.81			FBF
<u>2307</u> 2308	C36 H57 N O8 C36 H55 N O10	6.569 5.659	631.4130 661.3812	FBF FBF	74.41 89.95			FBF FBF
2309	C37 H71 N O8	17.329	657.5170	FBF	62.76			FBF
2310	C37 H67 N O8	17.875	653.4822	FBF	64.73		-	FBF
2311	C37 H59 N O8	19.070	645.4209	FBF	86.16			FBF
2312	C37 H57 N O8	4.776	643.4064	FBF	62.08			FBF
2313	C37 H57 N O9	4.724	659.4067	FBF	68.95			FBF
2314	C38 H73 N O9	19.980	687.5293	FBF	69.22			FBF
<u>2315</u> 2316	C38 H69 N O9 C38 H69 N O10	14.912 10.103	683.5030 699.4900	FBF FBF	55.79 56.61			FBF FBF
2317	C38 H67 N O8	13.041	665.4865	FBF	50.43			FBF
2318	C38 H67 N O9	17.797	681.4813	FBF	61.52	,	,	FBF
2319	C38 H67 N O10	6.647	697.4793	FBF	68.32			FBF
2320	C38 H61 N O8	6.283	659.4370	FBF	54.42			FBF
2321	C38 H59 N O8	4.437	657.4250	FBF	71.78			FBF
2322	C38 H57 N O10	12.651	687.3973	FBF	61.56			FBF
<u>2323</u> 2324	C39 H75 N O10 C39 H73 N O9	17.018 19.980	717.5327 699.5267	FBF FBF	56.42 86.37			FBF FBF
2325	C39 H65 N O10	13.587	707.4626	FBF	80.06			FBF
2326	C39 H61 N O8	5.841	671.4417	FBF	62.14			FBF
2327	C39 H61 N O9	4.880	687.4325	FBF	77.95			FBF
2328	C39 H61 N O10	4.828	703.4281	FBF	75.42			FBF
2329	C39 H59 N O10	17.693	701.4142	FBF	59.08			FBF
2330	C40 H77 N O8 C40 H77 N O9	15.796	699.5672	FBF FBF	72.20 63.48			FBF FBF
<u>2331</u> 2332	C40 H77 N O9	19.954 17.693	715.5584 709.5121	FBF	71.57			FBF
2333	C40 H69 N O9	17.693	707.5043	FBF	61.33			FBF
2334	C40 H67 N O9	19.070	705.4837	FBF	57.60			FBF
2335	C40 H65 N O10	6.647	719.4609	FBF	75.42			FBF
2336	C40 H63 N O9	4.541	701.4508	FBF	74.25			FBF
2337	C40 H63 N O10	17.147	717.4454	FBF	51.15			FBF
2338	C41 H75 N O8	10.181	709.5553	FBF	59.72			FBF
2339 2340	C41 H71 N O9 C41 H67 N O9	19.980 4.541	721.5101 717.4744	FBF FBF	66.67 54.75			FBF FBF
2341	C41 H65 N O9	5.010	715.4635	FBF	56.36			FBF
2342	C41 H65 N O10	4.619	731.4618	FBF	72.90			FBF
2343	C41 H63 N O10	13.587	729.4468	FBF	89.65			FBF
2344	C42 H81 N O9	19.954	743.5919	FBF	60.12			FBF
2345	C42 H81 N O10	19.096	759.5877	FBF	54.49			FBF
2346	C42 H79 N O9	19.980	741.5812 723.5693	FBF	62.17			FBF
2347 2348	C42 H77 N O8 C42 H75 N O8	10.935 18.187	723.5693	FBF FBF	68.41 67.77			FBF FBF
2349	C42 H75 N O9	19.980	737.5405	FBF	50.62			FBF
2350	C42 H73 N O9	19.954	735.5354	FBF	58.44			FBF
2351	C42 H67 N O10	4.671	745.4757	FBF	69.99			FBF
2352	C43 H77 N O9	14.783	751.5580	FBF	58.96			FBF
2353	C43 H75 N O8	18.992	733.5497	FBF	50.39			FBF
2354	C43 H75 N O9 C43 H73 N O8	11.611 10.181	749.5476 731.5370	FBF FBF	68.81 75.06			FBF FBF
<u>2355</u> 2356	C43 H71 N O8	13.379	729.5159	FBF	51.20			FBF
2357	C43 H71 N O10	4.671	761.5010	FBF	58.28			FBF
2358	C43 H65 N O8	5.529	723.4701	FBF	75.16			FBF
2359	C44 H85 N O9	17.667	771.6205	FBF	51.46			FBF
2360	C44 H83 N O9	14.860	769.6102	FBF	59.25			FBF
2361	C44 H83 N O10	12.911	785.5994	FBF	57.37			FBF
2362 2363	C44 H79 N O9 C44 H77 N O9	19.954 19.980	765.5718 763.5587	FBF FBF	53.58 79.41			FBF FBF
2364	C44 H77 N O9	10.935	745.5509	FBF	79.41 83.11			FBF
2365	C44 H73 N O8	10.955	743.5402	FBF	64.27			FBF
2366	C44 H67 N O9	22.525	753.4795	FBF	50.13			FBF
2367	C44 H67 N O10	20.006	769.4791	FBF	55.66			FBF
2368	C45 H67 N O8	5.919	749.4900	FBF	51.65			FBF
2369	C45 H67 N O10	19.018	781.4808	FBF	50.08			FBF
<u>2370</u> 2371	C45 H85 N O10 C45 H83 N O10	14.835 13.327	799.6189 797.5999	FBF FBF	62.18 55.96			FBF FBF
2372	C45 H79 N O8	13.275	761.5849	FBF	62.28			FBF
2373	C45 H79 N O9	19.850	777.5782	FBF	53.41			FBF
2374	C45 H77 N O8	19.122	759.5675	FBF	61.27			FBF
2375	C45 H77 N O10	16.680	791.5526	FBF	56.22			FBF
2376	C45 H75 N O9	16.992	773.5439	FBF	51.36			FBF
2377	C45 H73 N O9	13.431	771.5253	FBF	60.50			FBF
2378	C45 H69 N O8	0.383	751.5032	FBF	65.69			FBF
<u>2379</u> 2380	C45 H69 N O9 C46 H69 N O8	5.555 15.354	767.4989 763.5074	FBF FBF	61.77 57.94			FBF FBF
2381	C46 H87 N O9	15.354	797.6371	FBF	57.9 4 53.59			FBF
2382	C46 H87 N O10	18.862	813.6313	FBF	58.34			FBF
2383	C46 H79 N O9	10.909	789.5797	FBF	69.10			FBF
2384	C46 H79 N O10	18.940	805.5715	FBF	63.18			FBF
2385	C46 H77 N O9	10.026	787.5662	FBF	62.38			FBF
2386	C46 H73 N O8	0.383	767.5260	FBF	55.71			FBF



Compound Sum	•							
Cpd Name 2387	Formula C46 H71 N O8	10.0F1	Mass 765.5221	CAS ID Source FBF	Score 78.46	Score (Lib)	Score (DB)	Score (MFG) Algorith
.388	C46 H71 N O9	10.051 19.018	781.5088	FBF	56.96			FBF
389	C47 H89 N O9	19.460	811.6541	FBF	58.24			FBF
390	C47 H83 N O8	14.912	789.6122	FBF	63.25			FBF
391	C47 H79 N O10	15.224	817.5692	FBF	50.20			FBF
392	C47 H77 N O8	13.301	783.5673	FBF	50.67			FBF
393	C47 H75 N O10	20.032	813.5420	FBF	52.60		-	FBF
394 395	C48 H93 N O9 C48 H73 N O9	17.615 4.750	827.6870 807.5319	FBF FBF	52.34 59.72			FBF FBF
396	C48 H89 N O10	13.379	839.6468	FBF	51.46			FBF
2397	C48 H85 N O8	13.353	803.6280	FBF	52.90			FBF
2398	C48 H85 N O10	17.225	835.6203	FBF	55.51			FBF
399	C48 H83 N O9	22.603	817.6110	FBF	53.62			FBF
2400	C48 H81 N O10	9.948	831.5895	FBF	71.83			FBF
2401 2402	C48 H77 N O9	17.849 18.992	811.5554	FBF FBF	50.40 51.73			FBF FBF
2403	C48 H77 N O10 C48 H75 N O9	10.000	827.5535 809.5485	FBF	75.15			FBF
1404	C49 H95 N O9	21.382	841.7030	FBF	64.45			FBF
1405	C49 H93 N O9	18.992	839.6825	FBF	54.37			FBF
406	C49 H83 N O10	12.885	845.6010	FBF	50.92			FBF
407	C50 H97 N O9	14.886	855.7146	FBF	53.01			FBF
408	C50 H77 N O10	4.854	851.5574	FBF	64.56		-	FBF
409	C50 H87 N O9	14.860	845.6370	FBF	57.72			FBF
410	C50 H83 N O8	14.860	825.6119	FBF	56.79			FBF
<u>411</u> 412	C50 H79 N O10 C51 H77 N O8	9.974 13.431	853.5734 831.5652	<u>FBF</u> FBF	84.95 71.08			FBF FBF
413	C51 H95 N O8	18.966	849.7094	FBF	50.62			FBF
414	C51 H87 N O9	20.006	857.6395	FBF	55.09			FBF
415	C51 H85 N O10	21.668	871.6167	FBF	51.34			FBF
416	C51 H81 N O8	21.045	835.5937	FBF	56.74			FBF
417	C52 H101 N O8	20.265	867.7500	FBF	51.06			FBF
418	C52 H99 N O8	18.758	865.7373	FBF	54.27			FBF
419 420	C52 H91 N O8 C52 H87 N O9	15.510 14.886	857.6706 869.6384	FBF FBF	52.30 51.75			FBF FBF
421	C53 H83 N O8	15.510	861.6084	FBF	65.10			FBF
422	C53 H81 N O10	19.096	891.5785	FBF	66.59			FBF
423	C53 H79 N O9	22.057	873.5739	FBF	55.87			FBF
424	C53 H99 N O10	18.992	909.7263	FBF	50.17			FBF
425	C53 H93 N O9	18.940	887.6851	FBF	51.32			FBF
426	C53 H91 N O9	16.966	885.6756	FBF	59.00			FBF
427	C53 H89 N O8 C53 H87 N O10	12.781 14.938	867.6640 897.6292	FBF FBF	52.52 51.12			FBF FBF
1429	C54 H105 N O9	13.847	911.7796	FBF	54.42			FBF
2430	C54 H103 N O8	12.833	893.7668	FBF	57.27			FBF
2431	C54 H85 N O10	17.771	907.6144	FBF	50.49			FBF
2432	C54 H83 N O9	20.499	889.6010	FBF	58.25			FBF
.433	C54 H97 N O8	21.304	887.7235	FBF	54.54			FBF
434	C54 H97 N O10	21.720	919.7142	FBF	53.65			FBF
435	C54 H95 N O10	19.928	917.6952	FBF	62.34			FBF
. <u>436</u> .437	C54 H89 N O9	13.301	895.6524 911.6472	FBF FBF	53.62 51.72			FBF FBF
1438	C54 H89 N O10 C54 H87 N O9	16.082 17.173	893.6341	FBF	50.71		-	FBF
439	C54 H87 N O9	17.745	887.6266	FBF	77.41			FBF
440	C55 H83 N O10	14.912	917.6015	FBF	65.91			FBF
441	C55 H105 N O10	21.694	939.7711	FBF	54.84			FBF
442	C56 H83 N O9	14.860	913.6060	FBF	50.62			FBF
443	C56 H107 N O9	13.977	937.7966	FBF	52.33			FBF
444	C56 H101 N O9	14.783	931.7395	FBF	52.41			FBF
445	C56 H99 N O10	20.421	945.7241	FBF	51.37			FBF
446 447	C56 H97 N O8 C56 H95 N O9	18.784 16.914	911.7206 925.7017	FBF FBF	58.05 56.11			FBF FBF
44 7	C57 H111 N O10	19.746	969.8189	FBF	53.74			FBF
449	C57 H111 N O10	14.886	915.6513	FBF	60.43			FBF
450	C57 H89 N O10	15.016	947.6473	FBF	56.91			FBF
451	C57 H85 N O8	19.928	911.6203	FBF	58.24			FBF
452	C57 H105 N O9	16.654	947.7784	FBF	76.59			FBF
453	C57 H103 N 09	13.847	945.7646	FBF	50.75			FBF
454 455	C57 H103 N O10	18.836 13.847	961.7580 927.7527	FBF FBF	59.84 61.02			FBF FBF
455 456	C57 H101 N O8 C57 H101 N O9	13.847	943.7478	FBF	52.65			FBF
450 457	C57 H99 N O9	20.058	941.7308	FBF	55.09			FBF
458	C57 H93 N O10	18.213	951.6796	FBF	55.84			FBF
459	C58 H91 N O10	18.810	961.6630	FBF	68.82			FBF
460	C58 H89 N O9	14.912	943.6508	FBF	50.60			FBF
461	C58 H87 N O8	15.068	925.6462	FBF	50.87			FBF
462	C58 H111 N O10	14.185	981.8216	FBF	52.32			FBF
463	C58 H109 N 09	14.731	963.8080	FBF	55.66			FBF
464	C58 H107 N O8	14.601	945.8023	FBF	51.48		-	FBF
<u>465</u> 466	C58 H107 N O10	22.083 13.977	977.7841 959.7789	<u>FBF</u> FBF	59.33 50.96			FBF FBF
467	C58 H105 N O9 C58 H97 N O9	21.798	959.7789	FBF	50.96 67.83			FBF
468	C58 H95 N O8	19.902	933.7063	FBF	50.72			FBF
469	C59 H95 N O8	13.327	945.7020	FBF	68.22			FBF
1470	C59 H93 N O10	17.719	975.6804	FBF	56.33			FBF
471	C59 H91 N O9	22.655	957.6679	FBF	50.15			FBF
	C59 H87 N O8	13.405	937.6428	FBF	85.18			FBF



Compound Summary							
Cpd Name 2473	Formula C59 H87 N O10	13.613	Mass 969.6421	CAS ID Source FBF	Score 58.14	Score (Lib) Score (DB)	Score (MFG) Algorith
2474 2474	C59 H109 N O8	14.159	959.6421	FBF	59.02		FBF
2475	C59 H107 N O8	21.019	957.8019	FBF	55.63		FBF
2476	C59 H107 N O9	19.330	973.7933	FBF	58.48		FBF
2477	C59 H101 N O8	12.313	951.7550	FBF	64.32		FBF
<u>2478 </u>	C59 H99 N O10	13.379 17.667	981.7324	FBF	50.10 55.65		FBF FBF
2480	C60 H117 N O10 C61 H119 N O9	20.941	1011.8656 1009.8905	<u>FBF</u> FBF	58.06		FBF
2481	C61 H97 N O9	20.473	987.7213	FBF	51.23		FBF
2482	C61 H97 N O10	18.291	1003.7040	FBF	50.05		FBF
2483	C61 H93 N O10	14.549	999.6865	FBF	50.04		FBF
2484	C61 H109 N O9	21.746	999.8117	FBF	50.48		FBF
2485	C61 H105 N O8	20.655	979.7845	FBF	50.27		FBF
<u>2486</u> 2487	C62 H99 N O10 C62 H95 N O8	20.369 21.564	981.7033	<u>FBF</u> FBF	51.49 51.07		FBF FBF
2488	C62 H93 N O9	13.275	995.6835	FBF	50.71		FBF
2489	C62 H117 N O9	19.434	1019.8641	FBF	57.81		FBF
2490	C62 H115 N O9	21.019	1017.8580	FBF	58.42		FBF
2491	C62 H111 N O10	20.317	1029.8214	FBF	71.86		FBF
2492	C62 H103 N O9	21.097	1005.7618	FBF	70.29		FBF
2493	C63 H123 N O10	20.369	1053.9206	FBF	51.70		FBF
<u>2494 </u>	C63 H97 N O9 C63 H95 N O10	14.860 14.886	1011.7193 1025.6967	<u>FBF</u> FBF	51.07 58.77		FBF FBF
2496	C63 H121 N O10	18.135	1051.9029	FBF	68.80		FBF
2497	C63 H119 N O10	18.680	1049.8846	FBF	73.74		FBF
2498	C63 H117 N O10	20.136	1047.8717	FBF	53.76		FBF
2499	C63 H115 N O9	19.642	1029.8576	FBF	50.68		FBF
2500	C63 H113 N O9	20.317	1027.8439	FBF	55.77		FBF
2501	C63 H111 N O8	13.925	1009.8243	FBF	53.00		FBF
2502 2503	C63 H111 N O10 C63 H105 N O9	17.927 20.759	1041.8232 1019.7868	FBF FBF	64.88 50.05		FBF FBF
2504	C64 H125 N O10	21.538	1067.9256	FBF	71.74		FBF
2505	C64 H103 N O9	22.083	1029.7651	FBF	50.59		FBF
2506	C64 H101 N O8	19.850	1011.7521	FBF	75.38		FBF
507	C64 H101 N O10	17.927	1043.7453	FBF	54.06		FBF
1508	C64 H99 N O9	20.239	1025.7278	FBF	55.27		FBF
509	C64 H99 N O10	18.265	1041.7192	FBF	50.81		FBF
2510 2511	C64 H97 N O10 C64 H121 N O10	21.564 16.758	1039.7038 1063.8974	<u>FBF</u> FBF	54.27 51.46		FBF FBF
2512	C64 H115 N O10	19.824	1057.8450	FBF	50.29		FBF
2513	C64 H109 N O10	20.317	1051.8028	FBF	71.02		FBF
2514	C65 H105 N O9	17.927	1043.7732	FBF	71.28		FBF
2515	C65 H103 N O8	16.654	1025.7621	FBF	50.33		FBF
2516	C65 H103 N O10	22.603	1057.7648	FBF	51.97		FBF
2517	C65 H99 N O9 C65 H121 N O9	21.876	1037.7227	FBF	70.46		FBF FBF
<u>2518</u> 2519	C65 H121 N O9	19.616 20.187	1059.9008 1073.8926	<u>FBF</u> FBF	50.67 54.78		FBF
2520	C65 H115 N O8	16.784	1037.8558	FBF	52.28		FBF
2521	C65 H109 N O10	17.927	1063.8044	FBF	70.02		FBF
2522	C66 H129 N O10	17.901	1095.9572	FBF	63.23		FBF
2523	C66 H127 N O8	21.876	1061.9535	FBF	50.05		FBF
2524	C66 H103 N O8	14.809	1037.7706	FBF	58.58		FBF
2525 2526	C66 H103 N O9	22.213 17.927	1053.7734	<u>FBF</u> FBF	54.02 57.49		FBF FBF
.526 .527	C66 H103 N O10 C66 H127 N O9	19.330	1069.7617 1077.9524	FBF	64.08		FBF
2528	C66 H123 N O8	21.148	1057.9204	FBF	50.55		FBF
2529	C67 H131 N O8	20.032	1077.9963	FBF	59.03		FBF
2530	C67 H131 N O10	21.278	1109.9776	FBF	70.64		FBF
2531	C67 H109 N O10	21.928	1087.8069	FBF	54.40		FBF
2532	C67 H107 N O10	17.927	1085.7864	FBF	60.84		FBF
<u>533</u> 534	C67 H105 N O9 C67 H103 N O8	14.783 18.187	1067.7699 1049.7703	FBF FBF	50.45 71.83		FBF FBF
535	C67 H103 N O9	17.927	1049.7703	FBF	65.22		FBF
536	C67 H103 N O10	17.927	1081.7488	FBF	52.23		FBF
537	C67 H119 N O8	19.902	1065.8893	FBF	61.45		FBF
538	C68 H113 N O10	21.928	1103.8393	FBF	57.22		FBF
539	C68 H111 N O8	20.551	1069.8350	FBF	50.62		FBF
540	C68 H105 N 09	18.109	1079.7881	FBF	53.00		FBF
541 542	C68 H131 N O10 C68 H123 N O8	21.876 18.161	1121.9714 1081.9235	FBF FBF	63.45 65.92		FBF FBF
543	C68 H119 N O10	17.745	1109.8761	FBF	53.61		FBF
5 45 544	C68 H115 N O8	19.252	1073.8630	FBF	63.32		FBF
545	C68 H115 N O10	14.783	1105.8505	FBF	55.18		FBF
546	C69 H109 N O9	22.031	1095.8066	FBF	50.28		FBF
547	C69 H107 N O8	18.109	1077.7979	FBF	80.30		FBF
2548	C69 H107 N O9	18.109	1093.7900	FBF	73.92		FBF
2549	C69 H127 N O10	20.343	1129.9453	FBF	64.51		FBF
2550	C70 H115 N O8	11.585	1120.0375	FBF	52.29		FBF
<u>1551</u> 1552	C70 H115 N O8 C70 H113 N O8	18.213 19.018	1097.8652 1095.8502	FBF FBF	58.40 55.93		FBF FBF
553	C70 H113 N O8	14.938	1093.8324	FBF	55.93		FBF
554	C70 H109 N O9	18.992	1107.8128	FBF	50.80		FBF
555	C70 H135 N O9	22.213	1134.0128	FBF	55.51		FBF
556	C70 H133 N O8	18.836	1116.0002	FBF	50.02		FBF
557	C70 H131 N O8	21.304	1113.9900	FBF	65.89		FBF
2558	C70 H127 N O8	22.655	1109.9582	FBF	50.23		FBF



Compound Summary							
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorith
<u>2559</u> 2560	C70 H127 N O9 C70 H127 N O10	22.551 19.356	1125.9500 1141.9462	<u>FBF</u> FBF	50.71 50.58		FBF FBF
2561	C71 H139 N O8	20.032	1134.0600	FBF	51.69		FBF
2562	C71 H113 N O9	18.940	1123.8400	FBF	51.44		FBF
2563	C71 H113 N O10	17.719	1139.8335	FBF	51.43		FBF
2564	C71 H135 N O9	20.733	1146.0137	FBF	50.93		FBF
2565	C71 H131 N O10	17.693	1157.9711	FBF	71.44		FBF
2566	C71 H129 N O10	20.681	1155.9626	FBF	58.46		FBF
2567	C71 H127 N O8	18.732	1121.9491	FBF	78.79		FBF
<u>2568</u> 2569	C71 H125 N O9 C72 H115 N O8	18.550 21.045	1135.9306 1121.8622	<u>FBF</u> FBF	53.32 50.10		FBF FBF
2570	C72 H137 N O9	20.084	1160.0343	FBF	56.77		FBF
2571	C72 H131 N O8	18.836	1137.9874	FBF	50.10		FBF
2572	C72 H127 N O9	18.784	1149.9485	FBF	61.04		FBF
2573	C72 H125 N O10	19.356	1163.9316	FBF	56.44		FBF
2574	C73 H143 N O9	21.460	1178.0691	FBF	62.75		FBF
2575	C73 H117 N O8	19.304	1135.8783	FBF	51.14		FBF
2576	C73 H117 N O9	17.407	1151.8766	FBF	54.85		FBF
<u>2577</u> 2578	C73 H141 N O9 C73 H135 N O10	22.577 19.434	1176.0611 1186.0091	<u>FBF</u> FBF	53.25 54.00		FBF FBF
2579	C73 H127 N O10	19.174	1177.9550	FBF	50.37		FBF
2580	C74 H125 N O9	19.226	1171.9306	FBF	56.57		FBF
2581	C74 H119 N O10	18.550	1181.8821	FBF	57.33		FBF
1582	C74 H139 N O10	20.421	1202.0389	FBF	58.00		FBF
583	C74 H131 N O9	21.278	1177.9922	FBF	53.79		FBF
2584	C74 H127 N O8	11.065	1157.9534	FBF	59.20		FBF
1585	C74 H127 N O10	18.836	1189.9571	FBF	52.97		FBF
2586	C75 H127 N O8	20.032	1169.9594	FBF	51.96		FBF
<u>1587</u> 1588	C75 H125 N O9 C75 H121 N O9	17.667 19.174	1183.9297 1179.8945	<u>FBF</u> FBF	50.19 53.77		FBF FBF
1589	C75 H143 N O8	11.897	1186.0799	FBF	62.51		FBF
590	C75 H139 N O10	18.940	1214.0348	FBF	58.13		FBF
591	C76 H129 N O9	19.928	1199.9743	FBF	51.51		FBF
592	C76 H143 N O9	21.382	1214.0760	FBF	52.43		FBF
593	C76 H141 N O10	11.897	1228.0542	FBF	58.40		FBF
594	C76 H139 N O8	20.915	1194.0598	FBF	57.71		FBF
595	C76 H133 N O9	19.018	1203.9979	FBF	52.73		FBF
596	C76 H133 N O10	13.093	1219.9928	FBF	51.21		FBF
<u>597</u> 598	C77 H129 N O8 C77 H129 N O9	18.628 22.057	1195.9735 1211.9644	FBF FBF	51.14 51.08		FBF FBF
599	C77 H123 N O8	17.667	1189.9190	FBF	52.98		FBF
2600	C77 H141 N O8	22.395	1208.0759	FBF	58.78		FBF
2601	C77 H139 N O10	11.923	1238.0384	FBF	57.63		FBF
2602	C77 H137 N O9	20.941	1220.0315	FBF	57.54		FBF
2603	C77 H133 N O10	18.836	1232.0007	FBF	50.15		FBF
2604	C78 H133 N O9	11.715	1228.0083	FBF	54.07		FBF
605	C78 H125 N O10	17.719	1235.9314	FBF	52.91		FBF
2606 2607	C78 H147 N O8	19.668 13.093	1226.1175	FBF FBF	58.47 60.87		FBF FBF
2608	C78 H137 N O8 C29 H52 O11	5.945	1216.0348 576.3529	FBF	58.27		FBF
609	C29 H52 O12	4.489	592.3499	FBF	70.91		FBF
610	C29 H50 O11	5.270	574.3368	FBF	74.73		FBF
2611	C29 H48 O11	5.244	572.3240	FBF	60.12		FBF
612	C29 H44 O12	3.943	584.2807	FBF	73.90		FBF
613	C30 H50 O11	5.296	586.3324	FBF	58.12		FBF
614	C31 H54 O12	5.348	618.3619	FBF	63.32		FBF
2615	C31 H52 O11	17.381	600.3509	FBF	68.10		FBF
616 617	C32 H58 O11	20.187	618.3997	<u>FBF</u> FBF	67.20		FBF FBF
617 618	C32 H56 O11 C32 H54 O12	5.971 5.374	616.3817 630.3599	FBF	62.17 56.82		FBF
619	C32 H52 O11	6.179	612.3541	FBF	76.93		FBF
620	C32 H48 O11	5.893	608.3192	FBF	64.97		FBF
621	C32 H48 O12	8.206	624.3194	FBF	54.41		FBF
622	C33 H58 O12	6.231	646.3984	FBF	55.26		FBF
623	C33 H56 O11	5.192	628.3815	FBF	72.67		FBF
624	C33 H54 O12	5.685	642.3630	FBF	51.08		FBF
625	C33 H50 O11	4.047	622.3414	FBF	54.94		FBF
<u>626</u> 627	C33 H50 O12 C34 H62 O11	13.223 17.719	638.3275 646.4239	<u>FBF</u> FBF	50.55 56.05		FBF FBF
628	C34 H62 O11	17.719	644.4098	FBF	53.53		FBF
629	C34 H60 O12	4.724	660.4082	FBF	59.44		FBF
630	C34 H58 O11	5.348	642.3995	FBF	79.18		FBF
631	C34 H56 O11	20.187	640.3788	FBF	57.79		FBF
632	C34 H56 O12	5.374	656.3722	FBF	61.25		FBF
633	C35 H64 O11	10.103	660.4432	FBF	92.16		FBF
1634	C35 H62 O11	4.437	658.4266	FBF	74.53		FBF
635	C35 H60 O12	5.270	672.4088	FBF	66.13		FBF
1636	C35 H58 O12	19.304	670.3880	FBF	50.92		FBF
637	C35 H56 O12	7.218	668.3814	FBF	51.50		FBF
.638 .639	C36 H62 O12	5.400 5.815	686.4251	FBF ERE	86.90		FBF
640	C36 H58 O11 C36 H56 O11	5.815 4.359	666.3958 664.3840	FBF FBF	63.79 73.62		FBF FBF
641	C36 H54 O11	4.802	662.3716	FBF	67.13		FBF
642	C37 H68 O12	10.103	704.4688	FBF	92.98		FBF
643	C37 H66 O11	5.451	686.4558	FBF	66.67		FBF
2644	C37 H60 O11	4.437	680.4095	FBF	56.11		FBF



Compound Sumn	.							
Cpd Name	Formula C27 HEQ O11	RT	Mass 679,4030	CAS ID Source	Score	Score (Lib)	Score (DB)	Score (MFG) Algorithm
<u>2645</u> 2646	C37 H58 O11 C37 H58 O12	4.776 5.451	678.4020 694.3915	FBF FBF	85.87 64.95			FBF FBF
.0 10 .647	C37 H56 O11	4.802	676.3851	FBF	56.77			FBF
2648	C37 H56 O12	4.489	692.3838	FBF	54.35			FBF
2649	C37 H52 O11	4.047	672.3534	FBF	50.38			FBF
2650	C37 H52 O12	14.860	688.3407	FBF	62.10			FBF
2651	C38 H62 O12	5.867	710.4219	FBF	65.86			FBF
<u>2652</u> 2653	C38 H60 O11	4.802 4.515	692.4152 708.4082	FBF FBF	61.54 76.17	.		FBF FBF
2654	C38 H60 O12 C38 H58 O12	4.906	706.3969	FBF	68.56			FBF
2655	C38 H54 O11	4.437	686.3658	FBF	69.82			FBF
2656	C39 H70 O12	5.503	730.4818	FBF	66.76			FBF
2657	C39 H64 O12	4.541	724.4360	FBF	58.36			FBF
2658	C39 H62 O11	5.114	706.4284	FBF	87.45			FBF
2659	C39 H62 O12	4.906	722.4279	FBF	79.62			FBF
2660	C39 H60 O12	5.140	720.4072	FBF	60.60			FBF
<u>.661</u> .662	C39 H58 O12 C39 H56 O11	20.707 4.437	718.3971 700.3857	FBF FBF	50.92 74.87			FBF FBF
2663	C40 H66 O11	5.763	722.4657	FBF	58.78			FBF
664	C40 H64 O12	5.763	736.4398	FBF	57.95			FBF
665	C40 H58 O12	4.541	730.3919	FBF	69.38			FBF
666	C41 H76 O11	10.026	744.5411	FBF	65.23			FBF
667	C41 H74 O11	18.187	742.5295	FBF	54.05			FBF
1668	C41 H72 O11	19.070	740.5045	FBF	56.52			FBF
.669 .670	C41 H70 O11 C41 H68 O12	18.057 18.810	738.4914 752.4786	FBF FBF	50.90 62.40			FBF FBF
.671	C41 H60 O12	4.541	744.4122	FBF	75.82			FBF
672	C42 H72 O12	17.719	768.5015	FBF	80.20			FBF
673	C42 H66 O11	5.010	746.4627	FBF	58.22			FBF
1674	C42 H64 O11	5.737	744.4470	FBF	74.27			FBF
2675	C43 H80 O11	17.096	772.5717	FBF	69.12			FBF
676 677	C43 H78 O12	10.026	786.5417	FBF FBF	51.75	.		FBF FBF
678	C43 H74 O11 C43 H72 O11	10.026 13.327	766.5247 764.5042	FBF	72.91 56.37			FBF
679	C43 H66 O12	18.213	774.4553	FBF	51.39			FBF
680	C44 H80 O11	13.301	784.5701	FBF	52.45			FBF
681	C44 H62 O12	4.671	782.4293	FBF	61.59			FBF
682	C44 H76 O12	17.277	796.5394	FBF	50.80			FBF
683	C44 H70 O12	15.510	790.4804	FBF	53.38			FBF
684	C44 H68 O11	13.769	772.4768	FBF	56.68			FBF
685 686	C44 H66 O11 C44 H64 O11	4.671 5.010	770.4612 768.4461	FBF FBF	54.23 61.93			FBF FBF
687	C45 H78 O12	10.000	810.5519	FBF	64.29			FBF
688	C45 H76 O12	4.750	808.5338	FBF	57.25			FBF
689	C45 H72 O11	13.951	788.5109	FBF	50.98			FBF
690	C45 H70 O11	4.671	786.4902	FBF	53.65			FBF
691	C45 H70 O12	14.497	802.4862	FBF	52.26			FBF
692	C45 H68 O12	13.769	800.4732	FBF	51.72			FBF
<u>1693</u> 1694	C46 H66 O11 C46 H74 O11	4.750 13.379	794.4637 802.5202	FBF FBF	53.17 68.12			FBF FBF
695	C46 H72 O11	11.793	800.5062	FBF	54.80			FBF
696	C47 H68 O11	13.743	808.4760	FBF	54.46			FBF
697	C47 H84 O12	17.329	840.6026	FBF	54.32			FBF
698	C47 H78 O11	13.717	818.5534	FBF	51.24			FBF
699	C47 H76 O12	13.249	832.5379	FBF	50.76			FBF
700	C47 H74 O12	4.750	830.5158	FBF	51.89			FBF
701	C47 H70 O11	13.587	810.4924	FBF	59.32			FBF
702	C48 H70 O12 C48 H88 O12	13.873 13.327	838.4843 856.6275	FBF FBF	55.92 54.58			FBF FBF
704	C48 H78 O12	14.289	846.5450	FBF	59.87			FBF
705	C48 H72 O11	15.406	824.5054	FBF	52.49			FBF
706	C49 H72 O12	13.717	852.5013	FBF	60.09			FBF
707	C49 H86 O11	17.355	850.6126	FBF	53.75			FBF
708	C49 H80 O11	22.317	844.5673	FBF	62.05			FBF
709 710	C49 H76 O11 C49 H74 O12	14.886 5.893	840.5404 854.5187	FBF FBF	56.14 53.72			FBF FBF
711	C50 H92 O11	13.223	868.6612	FBF	53.72			FBF
712	C50 H74 O11	0.409	850.5181	FBF	51.04			FBF
713	C50 H90 O12	14.860	882.6393	FBF	62.27			FBF
714	C50 H88 O11	13.405	864.6290	FBF	58.62			FBF
715	C50 H86 O12	13.275	878.6132	FBF	52.97			FBF
716	C50 H82 O12	19.954	874.5817	FBF	55.53			FBF
717 718	C50 H78 O11 C51 H96 O11	15.068 14.809	854.5532 884.7004	FBF FBF	69.54 70.89			FBF FBF
718	C51 H76 O12	13.379	880.5301	FBF	50.97			FBF
720	C51 H74 O11	5.659	862.5253	FBF	66.00			FBF
721	C51 H74 O12	17.693	878.5177	FBF	61.73			FBF
722	C51 H72 O12	11.455	876.5024	FBF	54.79			FBF
723	C51 H82 O12	20.265	886.5851	FBF	51.69			FBF
724	C51 H80 O12	13.275	884.5663	FBF	72.56			FBF
725	C51 H78 O11	19.330	866.5570	FBF	53.81			FBF
726	C52 H98 O12	19.824	914.7028	FBF	51.66			FBF
727 728	C52 H78 O11	5.218	878.5514	FBF FRE	53.34			FBF FBF
728 729	C52 H88 O11 C52 H86 O11	20.006 19.980	888.6306 886.6224	FBF FBF	64.32 78.02			FBF
, _ ,	C52 H80 O11	9.896	880.5697	FBF	87.50			FBF



Compound Summary							
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorith
<u>2731</u> 2732	C53 H100 O12 C53 H78 O12	<u>17.537</u> 5.685	928.7209 906.5520	<u>FBF</u> FBF	59.52 60.89		FBF FBF
2733	C53 H76 O11	14.886	888.5357	FBF	80.83		FBF
2734	C53 H96 O12	18.758	924.6909	FBF	50.76		FBF
2735	C53 H92 O12	14.938	920.6579	FBF	52.92		FBF
2736	C53 H86 O11	17.667	898.6167	FBF	65.84		FBF
2737	C53 H82 O11	4.906	894.5807	FBF	53.88		FBF
<u>2738</u> 2739	C54 H82 O11 C54 H78 O11	5.685 18.732	906.5832 902.5492	FBF FBF	57.05 76.54		FBF FBF
2740	C54 H100 O12	21.148	940.7221	FBF	51.78		FBF
2741	C54 H94 O12	18.966	934.6771	FBF	53.86		FBF
2742	C54 H86 O11	20.006	910.6121	FBF	52.45		FBF
2743	C54 H84 O11	19.980	908.6044	FBF	91.83		FBF
2744	C54 H84 O12	13.535	924.5883	FBF	52.68		FBF
<u>2745 </u>	C55 H104 O11	14.523	940.7571	FBF	52.76		FBF FBF
27 40	C55 H104 O12 C55 H102 O11	17.537 21.382	956.7533 938.7444	<u>FBF</u> FBF	59.18 53.15		FBF
2748	C55 H84 O11	17.381	920.5930	FBF	52.48		FBF
2749	C55 H80 O11	18.862	916.5659	FBF	68.52		FBF
2750	C55 H100 O12	14.912	952.7135	FBF	55.71		FBF
2751	C55 H92 O12	14.445	944.6602	FBF	64.77		FBF
2752	C55 H90 O12	14.783	942.6431	FBF	52.49		FBF
2753 2754	C55 H86 O11 C55 H86 O12	19.200 4.984	922.6165 938.6069	FBF FBF	50.80 55.84		FBF FBF
2755	C56 H106 O11	18.862	954.7747	FBF	58.44		FBF
2756	C56 H86 O12	14.315	950.6099	FBF	57.20		FBF
2757	C56 H82 O11	22.473	930.5898	FBF	64.81		FBF
2758	C56 H102 O12	20.889	966.7363	FBF	57.42		FBF
2759	C56 H100 O11	16.056	948.7265	FBF	52.18		FBF
2760	C57 H108 O11	14.783	968.7870	FBF	50.75		FBF
<u>2761</u> 2762	C57 H84 O11 C58 H106 O11	16.498 13.665	944.6008 978.7766	<u>FBF</u> FBF	92.97 59.28		FBF FBF
2763	C58 H98 O12	17.355	986.6991	FBF	53.71		FBF
2764	C59 H90 O11	16.550	974.6479	FBF	54.20		FBF
2765	C59 H88 O11	16.472	972.6346	FBF	70.73		FBF
766	C59 H104 O11	21.980	988.7630	FBF	70.63		FBF
767	C59 H98 O12	18.810	998.7043	FBF	55.74		FBF
768	C59 H94 O11	14.003	978.6801	FBF	53.03		FBF
2769 2770	C60 H112 O12 C60 H108 O11	13.925 13.899	1024.8119 1004.7907	FBF FBF	50.52 55.46		FBF FBF
2771	C60 H98 O11	18.862	994.7107	FBF	52.41		FBF
2772	C61 H116 O11	19.044	1024.8527	FBF	51.47		FBF
2773	C61 H96 O11	18.239	1004.6998	FBF	51.84		FBF
2774	C61 H110 O11	22.421	1018.8136	FBF	52.35		FBF
2775	C61 H108 O11	18.265	1016.7910	FBF	57.12		FBF
2776	C62 H116 O12	18.680	1052.8390	FBF	51.48		FBF
2777 2778	C62 H104 O11 C62 H104 O12	22.395 20.967	1024.7593 1040.7552	FBF FBF	51.99 50.85		FBF FBF
2779	C62 H107 O12	20.032	1022.7402	FBF	61.08		FBF
2780	C62 H102 O12	21.642	1038.7395	FBF	54.72		FBF
2781	C63 H118 O11	19.824	1050.8697	FBF	51.15		FBF
2782	C63 H100 O11	16.836	1032.7257	FBF	50.25		FBF
2783	C63 H112 O11	19.382	1044.8104	FBF	50.72		FBF
2784	C63 H110 O11	17.927	1042.8021 1052.7563	FBF	51.41		FBF
2785 2786	C63 H104 O12 C64 H122 O11	18.161 19.902	1066.8993	FBF FBF	52.16 54.13		FBF FBF
.787	C64 H122 O12	17.615	1082.8916	FBF	53.71		FBF
2788	C64 H120 O12	19.330	1080.8836	FBF	54.06		FBF
789	C64 H112 O12	14.912	1072.8159	FBF	50.56		FBF
790	C64 H106 O11	20.317	1050.7726	FBF	82.01		FBF
791	C64 H106 O12	20.291	1066.7588	FBF	53.71		FBF
792 793	C65 H102 O11 C65 H102 O12	14.886 18.239	1058.7365 1074.7443	FBF FBF	56.70 58.97		FBF FBF
793 794	C65 H102 O12 C65 H100 O11	18.239	1074.7443	FBF	72.38		FBF
795	C65 H116 O11	21.954	1072.8548	FBF	53.41		FBF
796	C65 H114 O12	15.406	1086.8295	FBF	54.68		FBF
797	C66 H124 O11	19.226	1092.9194	FBF	50.15		FBF
798	C66 H122 O11	19.252	1090.8990	FBF	50.09		FBF
799	C66 H118 O12	18.940	1102.8624	FBF	53.54		FBF
800 801	C66 H116 O11 C66 H114 O12	21.824 18.758	1084.8507 1098.8321	FBF FBF	50.46 53.47		FBF FBF
802	C66 H114 O12	16.758	1098.8321	FBF	56.68		FBF
803	C66 H110 O11	18.109	1078.7997	FBF	62.21		FBF
804	C66 H108 O11	14.809	1076.7926	FBF	67.69		FBF
805	C66 H108 O12	18.109	1092.7902	FBF	50.27		FBF
2806	C67 H108 O12	18.109	1104.7825	FBF	57.81		FBF
2807	C67 H104 O11	17.927	1084.7598	FBF	56.45		FBF
808	C67 H116 O12	17.122	1112.8442	FBF	58.13		FBF
2809	C67 H110 O11	22.369	1090.8080	FBF	52.87 E1.21		FBF
810 811	C68 H108 O11 C68 H106 O11	18.135 18.109	1100.7831 1098.7769	FBF FBF	51.31 82.71		FBF FBF
812	C68 H106 O11	18.109	1114.7696	FBF	78.35		FBF FBF
813	C68 H126 O11	19.616	1118.9336	FBF	52.45		FBF
814	C69 H132 O11	10.909	1136.9773	FBF	50.36		FBF
815	C69 H110 O11	14.860	1114.8052	FBF	55.07		FBF
816	C70 H112 O11	14.809	1128.8192	FBF	58.98	·	FBF



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Cpd Name	Formula	RT	Mass	CAS ID Source		e (Lib) Score (DB) Score (MFG) Algorithm
2817	C70 H126 O11	11.065	1142.9307	FBF	52.08	FBF
2818	C70 H122 O12	20.967	1154.8948	FBF	55.02	FBF
2819	C71 H136 O11	21.876	1164.9994	FBF	51.13	FBF
2820	C71 H116 O11	17.589	1144.8492	FBF	52.56	FBF
2821	C71 H128 O11	21.408	1156.9437	FBF	57.21	FBF
822	C71 H126 O12	20.941	1170.9250	FBF	50.01	FBF
823	C72 H116 O12	18.836	1172.8484	FBF	68.56	FBF
824	C72 H132 O11	19.642	1172.9792	FBF	53.78	FBF
825	C72 H132 O12	17.693	1188.9741	FBF	67.01	FBF
826	C73 H120 O12	17.771	1188.8873	FBF	50.01	FBF
827	C73 H118 O11	17.823	1170.8624	FBF	83.16	FBF
828	C73 H136 O12	19.746	1205.0031	FBF	50.82	FBF
829	C73 H130 O11	19.954	1182.9511	FBF	50.01	FBF
330	C73 H130 O12	17.745	1198.9609	FBF	64.75	FBF
331	C73 H128 O12	19.746	1196.9385	FBF	50.40	FBF
332	C74 H120 O12	17.381	1200.8751	FBF	59.31	FBF
333	C74 H136 O12	22.135	1217.0071	FBF	52.99	FBF
334	C74 H132 O11	19.382	1196.9822	FBF	54.25	FBF
335	C75 H122 O12	21.460	1214.8887	FBF	50.41	FBF
336	C75 H120 O12	18.498	1212.8759	FBF	68.98	FBF
337	C75 H140 O12	11.897	1233.0338	FBF	68.52	FBF
338	C75 H136 O12	17.745	1228.9961	FBF	56.61	FBF
339	C76 H136 O12	19.148	1240.9936	FBF	52.19	FBF
40	C76 H134 O11	19.304	1222.9927	FBF	50.41	FBF
341	C77 H146 O11	20.759	1247.0774	FBF	50.29	FBF
42	C77 H128 O11	17.745	1228.9496	FBF	67.74	FBF
43	C77 H124 O11	18.161	1224.9182	FBF	50.49	FBF
44	C77 H142 O11	22.057	1243.0592	FBF	55.33	FBF
45	C77 H138 O11	13.093	1239.0211	FBF	51.07	FBF
46	C77 H138 O12	20.006	1255.0288	FBF	52.10	FBF
47	C77 H132 O12	18.836	1248.9749	FBF	54.71	FBF
348	C77 H130 O11	22.265	1230.9602	FBF	53.77	FBF
349	C28 H53 N O7	17.251	515.3802	FBF	83.97	FBF
50	C28 H51 N O8	5.607	529.3643	FBF	52.42	FBF
51	C28 H49 N O7	4.255	511.3536	FBF	51.53	FBF
52	C28 H49 N O8	4.359	527.3436	FBF	63.57	FBF
53	C28 H47 N O9	6.101	541.3289	FBF	55.63	FBF
54	C28 H45 N O7	5.503	507.3195	FBF	59.37	FBF
55	C28 H43 N O7	3.735	505.3083	FBF	58.50	FBF
56	C28 H43 N O8	5.555	521.2954	FBF	53.13	FBF
57	C28 H43 N O9	5.114	537.2937	FBF	71.50	FBF
58	C29 H55 N O8	10.233	545.3917	FBF	90.06	FBF
859	C29 H53 N O8	3.943	543.3757	FBF	71.87	FBF
360	C29 H51 N O7	4.671	525.3710	FBF	70.55	FBF
861	C29 H51 N O9	5.218	557.3575	FBF	57.98	FBF
362		3.735	521.3315	FBF	53.45	FBF
863	C29 H47 N O7	5.789	537.3276	FBF	53.74	FBF
	C29 H47 N O8	3.683	519.3203	FBF	75.65	FBF
864	C29 H45 N O7					
65	C29 H45 N O8	3.631	535.3194	FBF	63.74	FBF
66	C29 H45 N O9	3.631	551.3148	FBF	52.28	FBF
67	C30 H49 N O7	20.239	535.3559	FBF	64.18	FBF
68	C30 H47 N O7	5.114	533.3371	FBF	51.86	FBF
69	C31 H57 N O7	5.503	555.4147	FBF	96.81	FBF
70	C31 H51 N O7	5.555	549.3648	FBF	60.10	FBF
71	C31 H49 N O7	4.671	547.3534	FBF	83.69	FBF
72	C32 H57 N O7	20.239	567.4122	FBF	58.03	FBF
73	C32 H53 N O7	6.283	563.3793	FBF	50.78	FBF
74	C32 H51 N O7	5.659	561.3679	FBF	65.73	FBF
75	C33 H55 N O7	5.503	577.3964	FBF	96.55	FBF
76	C33 H51 N O7	20.239	573.3654	FBF	61.90	FBF
77	C34 H59 N O7	11.741	593.4259	FBF	61.20	FBF
78	C35 H67 N O7	17.953	613.4886	FBF	53.52	FBF
79	C35 H53 N O7	4.619	599.3822	FBF	93.92	FBF
80	C36 H57 N O7	6.205	615.4132	FBF	53.74	FBF
81	C36 H55 N O7	4.281	613.3992	FBF	75.57	FBF
82	C37 H69 N O7	15.328	639.5093	FBF	50.94	FBF
83	C37 H57 N O7	5.815	627.4139	FBF	67.86	FBF
84	C38 H67 N O7	7.920	649.4939	FBF	59.49	FBF
85	C38 H65 N O7	13.249	647.4752	FBF	50.69	FBF
86	C38 H59 N O7	16.602	641.4318	FBF	67.57	FBF
87	C39 H71 N O7	10.207	665.5281	FBF	61.33	FBF
88	C40 H73 N O7	10.987	679.5453	FBF	59.19	FBF
89	C40 H69 N O7	17.277	675.5107	FBF	52.57	FBF
90	C40 H65 N O7	7.920	671.4765	FBF	70.90	FBF
91	C40 H63 N O7	16.602	669.4632	FBF	56.73	FBF
92	C41 H69 N O7	10.207	687.5100	FBF	79.27	FBF
193	C42 H71 N O7	10.285	701.5248	FBF	84.58	FBF
394	C42 H69 N O7	10.103	699.5134	FBF	64.42	FBF
	C42 H67 N O7	18.446	697.4932	FBF	63.43	FBF
395 396	C42 H63 N O7	9.870	697.4932	FBF	56.55	FBF
		16.810	721.5840	FBF	53.21	FBF
	C43 H79 N O7					
397	CAALIDE N. CT					
897 898	C44 H85 N O7	17.797	739.6349	FBF	61.25	FBF
997 998 999	C44 H71 N O7	18.498	725.5278	FBF	60.79	FBF
990 998 999 900 901						



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Cpd Name 2903	Formula C45 H79 N O7	RT 15.068	Mass 745.5882	CAS ID Source FBF	Score 54.29	Score (Lib) Score (Di	B) Score (MFG) Algorithn FBF
2904	C45 H77 N O7	14.912	743.5707	FBF	58.82		FBF
905	C46 H89 N O7	19.018	767.6644	FBF	60.13		FBF
906	C46 H79 N O7	19.980	757.5865	FBF	83.96		FBF
907	C47 H89 N O7	17.329	779.6626	FBF	52.44		FBF
908	C47 H71 N O7	19.980	761.5229	FBF	57.00		FBF
909	C47 H85 N O7	22.473	775.6328	FBF	59.31		FBF
<u>1910 </u>	C48 H93 N O7 C48 H91 N O7	19.330 18.732	795.6903 793.6793	FBF FBF	60.57 52.44		FBF FBF
912	C48 H89 N O7	18.576	791.6645	FBF	54.83		FBF
2913	C48 H81 N O7	14.886	783.6001	FBF	53.95		FBF
2914	C48 H77 N O7	19.928	779.5699	FBF	86.22		FBF
2915	C48 H75 N O7	13.379	777.5522	FBF	58.76		FBF
2916	C49 H73 N O7	19.980	787.5391	FBF	57.78		FBF
2917	C49 H83 N O7	19.070	797.6156	FBF	82.95		FBF
<u>2918</u> 2919	C50 H95 N O7 C50 H75 N O7	21.174 19.928	821.7121 801.5593	FBF FBF	50.02 51.90		FBF FBF
2920	C50 H93 N O7	19.148	819.6930	FBF	52.58		FBF
921	C51 H79 N O7	21.226	817.5857	FBF	55.09		FBF
922	C51 H89 N O7	20.136	827.6653	FBF	54.23		FBF
923	C51 H87 N O7	17.537	825.6512	FBF	51.87		FBF
.924	C51 H81 N O7	16.602	819.6023	FBF	53.37		FBF
925	C52 H83 N O7	21.019	833.6208	FBF	53.77		FBF
926	C53 H93 N O7	17.641 15.276	855.7001 877.7701	FBF	50.95		FBF FBF
927	C54 H103 N O7 C54 H95 N O7	15.276 20.006	877.7791 869.7077	FBF FBF	54.40 71.69		FBF
2929	C55 H107 N O7	18.446	893.8059	FBF	64.53		FBF
1930	C55 H105 N O7	21.071	891.7894	FBF	59.75		FBF
931	C55 H93 N O7	21.356	879.6953	FBF	50.13		FBF
932	C55 H89 N O7	20.006	875.6636	FBF	58.33		FBF
.933	C56 H99 N O7	19.824	897.7418	FBF	52.65		FBF
934	C56 H97 N O7	18.940 19.044	895.7231	FBF	50.03		FBF
935 936	C56 H95 N O7 C56 H93 N O7	19.044	893.7123 891.6906	FBF FBF	55.52 62.16		FBF FBF
937	C57 H89 N O7	16.446	899.6656	FBF	57.11		FBF
938	C57 H87 N O7	14.860	897.6470	FBF	56.99		FBF
939	C58 H91 N O7	20.889	913.6834	FBF	57.87		FBF
940	C58 H97 N O7	19.928	919.7257	FBF	52.53		FBF
941	C58 H95 N O7	14.912	917.7095	FBF	56.77		FBF
942	C59 H89 N O7	21.668	923.6697	FBF	50.81		FBF
943	C59 H99 N O7 C60 H117 N O7	13.847	933.7502	FBF	67.13		FBF FBF
945	C61 H119 N O7	17.433 21.434	963.8831 977.9017	FBF FBF	61.12 53.23		FBF
.9 1 5 !946	C61 H97 N O7	14.809	955.7239	FBF	57.45		FBF
1947	C61 H93 N O7	19.382	951.6900	FBF	55.66		FBF
948	C62 H121 N O7	20.110	991.9168	FBF	54.62		FBF
949	C62 H119 N O7	21.200	989.8999	FBF	50.26		FBF
950	C62 H95 N O7	19.408	965.7098	FBF	55.05		FBF
951	C62 H93 N O7	17.641	963.6952	FBF	57.45		FBF
952 953	C62 H113 N O7 C63 H97 N O7	21.382 21.824	983.8429 979.7213	FBF FBF	55.28 52.65		FBF FBF
954	C63 H117 N O7	17.251	999.8865	FBF	50.01		FBF
955	C63 H105 N O7	13.977	987.7860	FBF	56.30		FBF
956	C65 H105 N O7	21.876	1011.7888	FBF	52.08		FBF
957	C65 H121 N O7	18.888	1027.9164	FBF	56.52		FBF
958	C66 H123 N O7	21.902	1041.9226	FBF	51.47		FBF
959	C66 H121 N 07	22.499	1039.9130	FBF	53.56		FBF
960	C66 H117 N O7 C67 H109 N O7	19.252 17.927	1035.8872 1039.8200	FBF FBF	57.91 74.75		FBF FBF
962	C67 H109 N O7	20.317	1039.8200	FBF			FBF
963	C67 H119 N O7	17.979	1049.8969	FBF	67.40		FBF
964	C67 H115 N O7	22.343	1045.8705	FBF	51.50		FBF
965	C68 H133 N O7	10.961	1076.0061	FBF	52.75		FBF
966	C68 H113 N O7	18.836	1055.8481	FBF	54.36		FBF
967	C68 H109 N O7	22.395	1051.8156	FBF	56.24		FBF
968	C68 H127 N O7 C68 H121 N O7	19.408	1069.9665	FBF	56.61		FBF FBF
969 970	C69 H121 N O7	17.251 20.136	1063.9159 1069.8718	FBF FBF	50.28 51.21		FBF
971	C69 H107 N O7	17.927	1061.8026	FBF	70.64		FBF
972	C69 H123 N O7	18.213	1077.9281	FBF	56.96		FBF
973	C69 H117 N O7	19.928	1071.8779	FBF	72.23		FBF
974	C71 H119 N O7	18.498	1097.8992	FBF	59.06		FBF
975	C71 H117 N O7	17.693	1095.8771	FBF	55.19		FBF
976	C71 H115 N O7	18.680	1093.8750	FBF	55.94 50.17		FBF
977	C73 H141 N O7	11.897	1144.0658	FBF	59.17		FBF
978 979	C73 H117 N O7 C73 H115 N O7	19.044 21.278	1119.8936 1117.8651	FBF FBF	59.02 58.13		FBF FBF
980	C73 H115 N O7	21.278	1117.8651	FBF	53.19		FBF
981	C73 H129 N O7	17.433	1131.9722	FBF	52.19		FBF
982	C73 H127 N O7	22.083	1129.9587	FBF	51.39		FBF
983	C75 H139 N O7	11.897	1166.0504	FBF	67.39		FBF
984	C75 H131 N O7	20.369	1157.9866	FBF	56.67		FBF
1985	C76 H123 N O7	19.902	1161.9223	FBF	51.37		FBF
986	C77 H135 N O7	21.382	1186.0206	FBF	56.53		FBF
987	C20 H39 N O7	4.854	405.2729	FBF	77.10		FBF



Cpd Name	mary Formula	RT	Mass	CAS ID Source	Score	Score (Lib)	Score (DB)	Score (MFG) Algorith
2989	C21 H37 N O7	5.088	415.2546	FBF	55.24	Score (LID)	Jene (DB)	FBF
2990	C22 H37 N O7	4.854	427.2548	FBF	69.25			FBF
2991	C23 H43 N O7	5.451	445.3024	FBF	66.54			FBF
<u>1992</u> 1993	C24 H41 N O7 C24 H39 N O7	15.016 7.920	455.2874 453.2757	<u>FBF</u> FBF	78.97 57.90			FBF FBF
2994	C25 H43 N O7	4.984	469.3049	FBF	68.44			FBF
2995	C26 H47 N O7	5.503	485.3375	FBF	51.56			FBF
2996	C27 H51 N O7	10.259	501.3658	FBF	90.72			FBF
2997	C27 H49 N O7	3.735	499.3496	FBF	72.54			FBF
1998	C30 H59 N O7	18.654 18.369	545.4298	<u>FBF</u> FBF	58.65 E2.96			FBF FBF
<u>2999</u> 3000	C36 H71 N O7 C19 H34 O10	3.137	629.5222 422.2110	FBF	53.86 58.21			FBF
3001	C19 H32 O10	3.631	420.1963	FBF	63.23	-		FBF
3002	C20 H36 O10	3.293	436.2282	FBF	82.23			FBF
3003	C21 H36 O10	7.244	448.2303	FBF	70.49			FBF
3004	C22 H38 O10	6.880	462.2474	FBF	67.66			FBF
8005	C22 H36 O10	4.906	460.2318	FBF	69.42			FBF FBF
006 007	C23 H40 O10 C23 H38 O10	5.036 3.527	476.2621 474.2463	FBF FBF	75.28 83.31			FBF
008	C24 H44 O10	3.371	492.2962	FBF	71.73			FBF
009	C25 H46 O10	3.683	506.3110	FBF	61.32			FBF
010	C25 H42 O10	3.605	502.2786	FBF	56.02			FBF
011	C26 H48 O10	4.021	520.3278	FBF	74.52			FBF
012	C26 H42 O10	5.529	514.2795	FBF	62.82			FBF
013 014	C27 H46 O10	5.192	530.3104	<u>FBF</u> FBF	80.73			FBF FBF
015	C28 H52 O10 C28 H46 O10	4.671 5.218	548.3569 542.3063	FBF	74.70 62.46			FBF
016	C28 H42 O10	13.379	538.2752	FBF	66.34			FBF
017	C30 H44 O10	7.946	564.2931	FBF	58.76			FBF
018	C31 H46 O10	3.839	578.3134	FBF	62.96			FBF
019	C34 H50 O10	4.671	618.3457	FBF	66.93			FBF
020	C35 H52 O10	4.828	632.3581	FBF	67.56			FBF
021 022	C36 H54 O10	5.997	646.3731 403.2941	FBF FBF	58.37 69.73			FBF FBF
023	C21 H41 N O6 C22 H43 N O6	10.909 12.235	417.3066	FBF	51.25			FBF
024	C23 H45 N O6	17.459	431.3274	FBF	83.31			FBF
025	C25 H49 N O6	13.977	459.3544	FBF	72.02			FBF
026	C30 H49 N O6	20.317	519.3610	FBF	62.18			FBF
027	C31 H61 N O6	15.380	543.4497	FBF	56.43			FBF
028	C31 H59 N O6	13.353	541.4357	FBF	58.71			FBF
029 030	C31 H57 N O6 C32 H53 N O6	10.311 10.233	539.4153 547.3918	FBF FBF	72.69 67.11	-		FBF FBF
031	C32 H55 N O6	18.161	571.4810	FBF	65.96			FBF
032	C33 H63 N O6	18.135	569.4683	FBF	52.58			FBF
033	C33 H61 N O6	11.429	567.4465	FBF	68.77			FBF
034	C33 H57 N O6	18.135	563.4220	FBF	71.97			FBF
035	C33 H55 N O6	13.379	561.4049	FBF	57.11			FBF
036	C35 H69 N O6	21.512	599.5099	FBF	75.10			FBF
3037 3038	C35 H63 N O6 C35 H61 N O6	7.192 14.809	593.4707 591.4539	<u>FBF</u> FBF	56.48 70.68			FBF FBF
039	C35 H55 N O6	7.218	585.3997	FBF	66.56			FBF
040	C36 H71 N O6	16.524	613.5275	FBF	50.59			FBF
041	C36 H69 N O6	16.108	611.5073	FBF	70.05			FBF
042	C36 H63 N O6	15.666	605.4670	FBF	74.42			FBF
043	C36 H61 N O6	14.964	603.4479	FBF	56.30			FBF
044	C37 H73 N O6	21.071	627.5448	FBF	50.63	-		FBF
045 046	C37 H71 N O6 C37 H67 N O6	15.198 10.207	625.5300 621.5028	FBF FBF	52.74 54.45			FBF FBF
047	C37 H67 N O6	7.192	615.4515	FBF	74.18			FBF
048	C38 H67 N O6	22.629	633.4968	FBF	57.67			FBF
049	C38 H65 N O6	17.901	631.4855	FBF	50.91			FBF
050	C38 H61 N O6	11.351	627.4480	FBF	57.63			FBF
051	C39 H65 N O6	10.259	643.4832	FBF	70.36			FBF
052	C39 H63 N O6	17.719	641.4683	FBF	67.62			FBF
<u>053 </u>	C40 H79 N O6 C40 H69 N O6	22.135 14.912	669.5858 659.5169	FBF FBF	50.88 58.60			FBF FBF
055	C40 H67 N O6	19.980	657.4920	FBF	71.70			FBF
056	C40 H65 N O6	10.103	655.4873	FBF	61.70	-		FBF
057	C41 H81 N O6	20.889	683.6051	FBF	62.14			FBF
058	C41 H71 N O6	20.421	673.5290	FBF	54.65			FBF
059	C41 H69 N O6	19.980	671.5174	FBF	76.40			FBF
060	C42 H81 N O6	18.732	695.6073	FBF	56.58 FF 04			FBF
061 062	C42 H79 N O6 C42 H71 N O6	18.784 19.980	693.5892 685.5230	<u>FBF</u> FBF	55.94 74.78			<u>FBF</u> FBF
063	C42 H/1 N O6 C42 H69 N O6	19.980	683.5131	FBF	74.78 59.01			FBF
064	C43 H79 N O6	16.420	705.5916	FBF	52.78			FBF
065	C43 H75 N O6	17.122	701.5583	FBF	58.77			FBF
066	C44 H85 N O6	18.810	723.6378	FBF	57.04			FBF
067	C44 H75 N O6	19.954	713.5535	FBF	65.53			FBF
068	C63 H100 O5	13.847	936.7560	FBF	52.02			FBF
069	C40 H58 O5	21.122	618.4275	FBF	58.12			FBF
8070	C58 H96 O5	22.551	872.7223	FBF	52.12			FBF
071 072	C33 H62 O6 C33 H54 O6	14.341 10.259	554.4534 546.3905	FBF FBF	64.82 81.70			FBF FBF
073	C35 H66 O6	21.460	582.4830	FBF	76.24			FBF
	222 1100 00	21,100	610.5149	FBF	50.71			FBF



Compound Summary							
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorith
3075 3076	C37 H68 O6	15.900	608.5027	<u>FBF</u> FBF	65.55 67.19		FBF FBF
3077	C39 H74 O6 C40 H74 O6	18.784 14.783	638.5483 650.5493	FBF	54.99		FBF
3078	C41 H74 O6	20.577	662.5511	FBF	50.03	-	FBF
3079	C43 H80 O6	18.135	692.5970	FBF	62.67		FBF
3080	C43 H78 O6	15.874	690.5817	FBF	56.01		FBF
3081	C43 H76 O6	14.809	688.5622	FBF	51.40		FBF
3082	C44 H84 O6	20.473	708.6253	FBF	58.04		FBF
3083 3084	C45 H86 O6 C45 H78 O6	19.902 22.265	722.6412 714.5793	FBF FBF	56.07 53.93		FBF FBF
3085	C47 H82 O6	17.875	742.6116	FBF	77.96		FBF
3086	C48 H92 O6	18.940	764.6940	FBF	53.37	· · · · · · · · · · · · · · · · · · ·	FBF
3087	C58 H112 O6	22.447	904.8531	FBF	52.78		FBF
3088	C42 H78 O6	18.420	678.5799	FBF	53.81		FBF
3089	C42 H76 O6	22.083	676.5613	FBF	50.09		FBF
3090	C42 H74 O6	16.888	674.5487	FBF	58.87		FBF
8091	C46 H84 O6	21.642	732.6266	FBF	61.89		FBF
3092	C35 H58 O6	18.135	574.4286	FBF	68.05		FBF
3093 3094	C36 H62 O6 C47 H84 O6	22.966 20.525	590.4575 744.6247	<u>FBF</u> FBF	53.44 52.04		FBF FBF
095	C56 H106 O6	18.966	874.7995	FBF	50.07		FBF
8096	C59 H112 O6	18.057	916.8389	FBF	51.97		FBF
097	C61 H116 O6	19.460	944.8725	FBF	50.43		FBF
098	C63 H120 O6	19.226	972.9114	FBF	56.30		FBF
099	C64 H122 O6	20.707	986.9258	FBF	56.84		FBF
100	C50 H84 O6	17.277	780.6259	FBF	50.51		FBF
101	C50 H82 O6	12.885	778.6185	FBF	57.94		FBF
3102 3103	C55 H102 O6	20.136	858.7601	<u>FBF</u> FBF	57.30		FBF FBF
104	C68 H130 O6 C54 H92 O6	21.824 18.628	1042.9877 836.6926	FBF	53.56 67.05		FBF
105	C61 H114 O6	18.420	942.8599	FBF	63.57		FBF
106	C53 H90 O6	17.667	822.6740	FBF	50.12		FBF
107	C53 H86 O6	13.327	818.6409	FBF	50.91		FBF
108	C70 H132 O6	10.961	1069.0009	FBF	55.76		FBF
109	C51 H82 O6	14.886	790.6103	FBF	50.79		FBF
110	C61 H112 O6	21.694	940.8464	FBF	59.76		FBF
111	C64 H118 O6	17.615	982.8955	FBF	50.78		FBF
112	C59 H106 O6	17.044	910.7968	FBF	58.55	· · · · · · · · · · · · · · · · · · ·	FBF
3113 3114	C61 H110 O6 C64 H116 O6	17.303 20.525	938.8333 980.8790	FBF FBF	51.45 55.66		FBF FBF
3115	C66 H120 O6	22.005	1008.9031	FBF	58.39		FBF
3116	C67 H122 O6	16.836	1022.9238	FBF	50.07		FBF
3117	C69 H126 O6	18.758	1050.9596	FBF	52.50		FBF
3118	C71 H136 O6	20.421	1085.0290	FBF	52.57		FBF
3119	C71 H134 O6	21.590	1083.0127	FBF	50.42		FBF
3120	C71 H132 O6	21.356	1080.9996	FBF	51.69		FBF
3121	C72 H134 O6	21.772	1095.0223	FBF	57.77		FBF
122	C57 H92 O6	21.122	872.6962	FBF FBF	53.78		FBF
3123 3124	C63 H112 O6 C73 H142 O6	21.148 11.611	964.8397 1115.0821	FBF	50.03 56.81		FBF FBF
125	C61 H102 O6	14.705	930.7614	FBF	51.59	-	FBF
126	C90 H176 O6	17.719	1353.3487	FBF	50.44		FBF
3127	C40 H64 O6	19.070	640.4654	FBF	75.14		FBF
128	C39 H62 O6	10.597	626.4573	FBF	77.61		FBF
129	C41 H58 O6	17.719	646.4238	FBF	75.79		FBF
130	C41 H64 O6	13.119	652.4764	FBF	50.25		FBF
131	C58 H98 O6	14.912	890.7364	FBF	50.10		FBF
132	C37 H58 O6	7.192	598.4261	FBF	74.18		FBF
133	C53 H80 O6 C41 H54 O6	16.862 5.607	812.5973 642.3960	<u>FBF</u> FBF	56.94 50.61		FBF FBF
135	C42 H60 O6	10.103	660.4432	FBF	76.02		FBF
136	C43 H70 O6	14.912	682.5201	FBF	53.80		FBF
137	C35 H60 O6	14.783	576.4410	FBF	51.60		FBF
138	C54 H88 O6	16.680	832.6565	FBF	57.80		FBF
139	C56 H90 O6	18.940	858.6691	FBF	61.39		FBF
140	C56 H88 O6	15.510	856.6544	FBF	55.76		FBF
141	C58 H96 O6	19.746	888.7209	FBF	51.38		FBF
<u>142 </u>	C60 H100 O6 C62 H106 O6	22.031 18.369	916.7533 946.7974	<u>FBF</u> FBF	51.77 51.29		FBF FBF
144	C39 H68 O6	20.889	632.5023	FBF	52.56		FBF
145	C15 H22 O6	10.909	298.1440	FBF	62.75		FBF
146	C77 H138 O6	20.655	1159.0519	FBF	55.44		FBF
147	C16 H24 O6	6.127	312.1583	FBF	68.79		FBF
148	C63 H104 O6	22.317	956.7787	FBF	50.43		FBF
149	C63 H102 O6	13.951	954.7680	FBF	50.97		FBF
3150	C63 H100 O6	18.810	952.7553	FBF	51.06		FBF
151	C73 H128 O6	18.966	1100.9797	FBF	64.09		FBF
152	C95 H184 O6	6.673	1421.4109	FBF	66.93		FBF
153	C64 H104 O6	14.783	968.7810	FBF	50.11		FBF
154 155	C62 H94 O6 C66 H110 O6	16.914 18.732	934.7011 998.8255	<u>FBF</u> FBF	50.38 51.41		FBF FBF
156	C48 H74 O6	0.383	746.5478	FBF	64.75		FBF
157	C65 H102 O6	14.185	978.7732	FBF	52.93		FBF
3158	C67 H112 O6	19.954	1012.8377	FBF	54.33		FBF
159	C19 H30 O6	8.024	354.2035	FBF	51.56		FBF
	C63 H94 O6	17.615	946.7050	FBF	55.78		FBF



Compound Sumn								
Cpd Name 3161	Formula C66 H106 O6	RT 14.029	Mass 994.7998	CAS ID Source FBF	Score 55.76	Score (Lib)	Score (DB)	Score (MFG) Algorithm FBF
3162	C76 H132 O6	21.304	1140.9999	FBF	50.98			FBF
3163	C81 H142 O6	13.067	1211.0786	FBF	58.38			FBF
3164	C65 H96 O6	16.316	972.7209	FBF	58.49			FBF
3165	C71 H120 O6	20.187	1068.9184	FBF	51.00			FBF
3 <u>166</u> 3167	C74 H126 O6 C76 H130 O6	22.057 22.213	1110.9469 1138.9854	FBF FBF	50.01 55.45			FBF FBF
3168	C63 H92 O6	14.809	944.6827	FBF	52.35			FBF
3169	C78 H132 O6	22.161	1165.0054	FBF	54.57			FBF
3170	C97 H182 O6	6.075	1443.3929	FBF	67.85			FBF
3171 3172	C22 H40 O6 C25 H44 O6	4.750 10.285	400.2863 440.3132	FBF FBF	52.18 89.82			FBF FBF
3173	C33 H58 O6	11.429	550.4214	FBF	68.56			FBF
3174	C23 H38 O6	12.417	410.2646	FBF	62.52			FBF
3175	C69 H106 O6	21.019	1030.8074	FBF	59.43			FBF
3176 3177	C69 H102 O6 C85 H150 O6	22.525 13.431	1026.7645 1267.1424	<u>FBF</u> FBF	58.02 52.53			<u>FBF</u> FBF
3178	C43 H56 O6	19.070	668.4061	FBF	70.57			FBF
3179	C65 H92 O6	16.446	968.6859	FBF	62.48			FBF
3180	C68 H110 O6	14.731	1022.8204	FBF	50.27			FBF
3181	C75 H124 O6	21.356	1120.9375	FBF	53.80			FBF
3182 3183	C77 H128 O6 C83 H140 O6	17.745 13.093	1148.9743 1233.0606	<u>FBF</u> FBF	51.91 50.36			FBF FBF
3184	C24 H44 O6	10.077	428.3139	FBF	72.31			FBF
3185	C24 H42 O6	3.085	426.2986	FBF	66.68			FBF
3186	C24 H40 O6	12.391	424.2806	FBF	90.92			FBF
3187	C24 H38 O6	5.114	422.2679	FBF	76.41			FBF
3188 3189	C71 H108 O6 C71 H104 O6	19.590 17.251	1056.8185 1052.7786	<u>FBF</u> FBF	53.09 50.85			FBF FBF
3190	C73 H116 O6	14.964	1088.8846	FBF	57.96			FBF
3191	C71 H106 O6	14.809	1054.7993	FBF	55.65			FBF
3192	C73 H106 O6	18.109	1078.7987	FBF	53.31		-	FBF
3193 3194	C74 H120 O6 C76 H124 O6	19.434 22.083	1104.9034 1132.9390	FBF FBF	50.73 50.14			FBF FBF
3195	C78 H128 O6	21.278	1160.9791	FBF	64.58			FBF
3196	C82 H136 O6	13.093	1217.0339	FBF	58.68			FBF
3197	C86 H144 O6	13.457	1273.0990	FBF	62.18			FBF
3198	C26 H46 O6	9.662	454.3266	FBF	74.79			FBF
3199 3200	C26 H38 O6 C27 H40 O6	5.400 3.527	446.2667 460.2784	FBF FBF	70.54 53.04			FBF FBF
3201	C27 H38 O6	3.449	458.2698	FBF	71.50			FBF
3202	C28 H40 O6	4.047	472.2832	FBF	64.30			FBF
3203	C29 H54 O6	13.951	498.3934	FBF	54.35			FBF
3204	C29 H42 O6	4.515	486.2979	FBF	77.20			FBF
3205 3206	C30 H56 O6 C31 H58 O6	18.057 11.247	512.4085 526.4231	FBF FBF	54.82 63.44			FBF FBF
3207	C31 H56 O6	10.285	524.4091	FBF	71.32			FBF
3208	C31 H54 O6	10.259	522.3923	FBF	67.30			FBF
3209	C32 H44 O6	5.374	524.3161	FBF	56.48			FBF
3210	C41 H66 O6	18.005	654.4853	FBF FBF	51.11			FBF FBF
3211 3212	C33 H56 O6 C34 H62 O6	17.122 17.797	548.4053 566.4514	FBF	64.70 55.19			FBF
3213	C35 H50 O6	3.943	566.3612	FBF	57.50			FBF
3214	C36 H66 O6	12.053	594.4882	FBF	66.62			FBF
3215	C36 H60 O6	15.692	588.4389	FBF	59.36			FBF
3216	C37 H66 O6 C41 H62 O6	15.562	606.4818	FBF	50.56			FBF
3217 3218	C41 H62 O6	22.525 13.119	650.4513 668.5014	FBF FBF	56.35 58.01			FBF FBF
3219	C42 H62 O6	4.437	674.4510	FBF	57.18			FBF
3220	C27 H36 O6	10.597	456.2518	FBF	58.75			FBF
3221	C47 H72 O6	19.044	732.5294	FBF	57.17			FBF
3222 3223	C15 H26 O6 C44 H64 O6	5.659 19.070	302.1719 688.4685	FBF FBF	81.74 55.39			FBF FBF
3224	C44 H62 O6	5.451	686.4558	FBF	78.73			FBF
3225	C46 H70 O6	17.849	718.5173	FBF	59.00			FBF
3226	C49 H64 O6	13.249	748.4721	FBF	56.38			FBF
3227	C51 H68 O6	13.353	776.4997	FBF	52.80			FBF
3228 3229	C52 H76 O6 C56 H84 O6	14.964 16.732	796.5645 852.6273	FBF FBF	54.68 51.04		-	FBF FBF
3230	C59 H84 O6	20.006	888.6306	FBF	58.19			FBF
3231	C60 H90 O6	16.966	906.6776	FBF	50.66			FBF
3232	C60 H88 O6	17.225	904.6586	FBF	53.72			FBF
3233	C60 H86 O6	14.575	902.6455	FBF	50.24			FBF
3 <u>234</u> 3235	C61 H86 O6 C27 H46 O6	16.394 4.984	914.6385 466.3253	FBF FBF	51.99 50.81			FBF FBF
3236	C28 H52 O6	17.745	484.3764	FBF	80.08			FBF
3237	C21 H38 O6	5.296	386.2660	FBF	51.56			FBF
3238	C66 H96 O6	19.226	984.7232	FBF	50.18			FBF
3239	C68 H102 O6	21.019	1014.7631	FBF	59.57			FBF
3240 3241	C72 H106 O6 C73 H108 O6	17.901 17.122	1066.7996 1080.8162	FBF FBF	69.31 60.84			FBF FBF
3242	C74 H114 O6	18.758	1098.8607	FBF	54.70			FBF
3243	C74 H110 O6	18.135	1094.8363	FBF	61.81			FBF
3244	C78 H124 O6	21.382	1156.9394	FBF	50.28			FBF
3245	C79 H120 O6	22.005	1164.9118	FBF	50.05			FBF



Compound Summary							
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB) Score (MI	G) Algorithm
3247	C81 H122 O6	19.200	1190.9247	FBF	56.11		FBF
3248 3249	C82 H128 O6 C83 H134 O6	17.745 11.897	1208.9726 1227.0152	FBF FBF	55.93 52.11		FBF FBF
3250	C84 H134 O6	13.093	1239.0211	FBF	50.28		FBF
3251	C66 H120 O17 P2	18.940	1246.7918	FBF	51.34		FBF
3252	C74 H142 O17 P2	19.252	1364.9749	FBF	50.84		FBF
3253	C81 H154 O17 P2	19.148	1461.0687	FBF	52.11		FBF
3254	C87 H148 O17 P2	9.792	1527.0207	FBF	50.80		FBF
3255	C81 H156 O17 P2	13.561	1463.0796	FBF	56.46		FBF
3256	C82 H150 O17 P2	18.810	1469.0423	FBF	56.72		FBF
3257 3258	C88 H162 O17 P2 C77 H150 O17 P2	18.732 19.148	1553.1286 1409.0435	<u>FBF</u> FBF	58.49 61.27		FBF FBF
3259	C93 H168 O17 P2	13.119	1619.1706	FBF	50.45		FBF
3260	C94 H162 O17 P2	13.119	1625.1300	FBF	89.76		FBF
3261	C21 H39 O7 P	4.906	434.2450	FBF	73.44		FBF
3262	C13 H27 O7 P	2.721	326.1494	FBF	73.75		FBF
3263	C17 H33 O7 P	13.353	380.1934	FBF	66.70	<u> </u>	FBF
3264	C18 H35 O7 P	13.353	394.2133	FBF	74.84		FBF
3265	C19 H37 O7 P	6.880	408.2268	FBF	67.35		FBF
3266 3267	C19 H35 O7 P C20 H39 O7 P	7.244 14.912	406.2127 422.2453	FBF FBF	54.18 70.50		FBF FBF
3268	C20 H37 O7 P	9.454	420.2263	FBF	77.79		FBF
3269	C20 H35 O8 P	8.882	434.2055	FBF	62.20		FBF
3270	C23 H43 O8 P	5.036	478.2710	FBF	56.50		FBF
3271	C23 H41 O7 P	4.932	460.2611	FBF	73.55		FBF
3272	C24 H49 O7 P	3.761	480.3174	FBF	73.45		FBF
3273	C25 H43 O7 P	4.437	486.2759	FBF	88.37		FBF
3274	C25 H39 O7 P	4.984	482.2437	FBF	52.29		FBF
<u>3275 </u>	C27 H47 O7 P C27 H45 O7 P	6.049 21.019	514.3039 512.2874	<u>FBF</u> FBF	50.37 53.46		FBF FBF
3277	C28 H57 O7 P	20.317	536.3875	FBF	74.23		FBF
3278	C29 H57 O7 P	18.135	548.3843	FBF	92.56		FBF
3279	C30 H61 O7 P	6.543	564.4128	FBF	54.27		FBF
3280	C31 H63 O7 P	11.637	578.4324	FBF	59.63		FBF
3281	C31 H59 O7 P	10.207	574.4022	FBF	64.61		FBF
3282	C34 H69 O7 P	14.003	620.4771	FBF	55.64		FBF
3283	C38 H77 O7 P	18.265	676.5395	FBF	50.97		FBF
3284	C39 H79 O7 P	21.122	690.5566	FBF	57.05		FBF
3285	C42 H85 O7 P	15.926	732.6073	FBF	50.86		FBF
3286 3287	C17 H35 O6 P C19 H39 O6 P	14.081 4.750	366.2182 394.2508	<u>FBF</u> FBF	75.34 73.25		FBF FBF
3288	C23 H45 O6 P	4.906	448.2934	FBF	53.35		FBF
3289	C25 H53 O6 P	7.686	480.3612	FBF	64.34		FBF
3290	C25 H51 O6 P	12.677	478.3405	FBF	60.86		FBF
3291	C25 H49 O6 P	15.354	476.3266	FBF	69.72		FBF
3292	C31 H61 O7 P	11.039	576.4168	FBF	66.80		FBF
3293	C34 H67 O7 P	16.290	618.4647	FBF	65.26		FBF
3294	C37 H71 O7 P	19.070	658.4945	FBF	79.63		FBF
3295 3296	C39 H75 O7 P C39 H69 O7 P	17.693 17.745	686.5259 680.4767	<u>FBF</u> FBF	79.20 77.93		FBF FBF
3297	C43 H83 O7 P	19.954	742.5880	FBF	77.93		FBF
3298	C44 H89 O7 P	20.837	760.6375	FBF	63.42		FBF
3299	C46 H93 O7 P	15.848	788.6729	FBF	56.00		FBF
3300	C47 H95 O7 P	14.029	802.6845	FBF	54.66		FBF
3301	C53 H107 O7 P	18.057	886.7787	FBF	51.19		FBF
3302	C54 H109 O7 P	17.563	900.7882	FBF	73.28		FBF
3303	C34 H63 O7 P	4.932	614.4286	FBF	51.12		FBF
3304	C35 H61 O7 P	6.231	624.4149	FBF	67.03		FBF
3305 3306	C37 H63 O7 P C39 H73 O7 P	6.257 19.070	650.4328 684.5102	FBF FBF	50.45 71.81		FBF FBF
3307	C41 H79 O7 P	19.070	714.5565	FBF	83.75		FBF
3308	C41 H73 O7 P	18.420	708.5076	FBF	75.45		FBF
3309	C43 H81 O7 P	14.938	740.5719	FBF	59.14		FBF
3310	C45 H89 O7 P	16.056	772.6330	FBF	51.54		FBF
3311	C46 H91 O7 P	15.848	786.6517	FBF	51.01		FBF
3312	C51 H101 O7 P	19.330	856.7275	FBF	53.04		FBF
3313	C31 H59 O10 P	19.772	622.3869	FBF	55.54		FBF
3314	C37 H71 O8 P	19.772	674.4888	FBF	53.68	<u> </u>	FBF
3315 3316	C37 H71 O9 P C39 H73 O11 P	19.980 10.051	690.4784 748.4953	FBF FBF	71.55 62.46		FBF FBF
3317	C39 H73 O11 P	5.503	730.4817	FBF	78.56		FBF
3318	C39 H67 O9 P	22.031	710.4522	FBF	66.95		FBF
3319	C41 H75 O8 P	13.301	726.5240	FBF	57.11		FBF
3320	C41 H71 O7 P	19.980	706.4937	FBF	65.83		FBF
3321	C41 H71 O8 P	17.615	722.4889	FBF	54.58		FBF
3322	C24 H47 O9 P	5.503	510.2949	FBF	63.34		FBF
3323	C26 H47 O8 P	5.815	518.3006	FBF	53.72		FBF
3324	C27 H53 O8 P	6.075	536.3483	FBF	60.73		FBF
3325	C27 H53 O9 P	18.135	552.3421	FBF	65.18		FBF
3326	C28 H49 O9 P	4.047	560.3087 704.4826	FBF ERE	70.93		FBF
3327	C41 H69 O7 P C43 H77 O7 P	19.980	704.4826	FBF ERE	68.42 73.99		FBF FBF
3328 3329	C38 H73 O7 P	19.980 16.680	736.5383 672.5091	FBF FBF	75.99		FBF
3330	C42 H81 O7 P	20.006	728.5742	FBF	78.04		FBF
3331	C50 H97 O7 P	19.928	840.6916	FBF	50.02		FBF
3332	C51 H99 O7 P	13.509	854.7124	FBF	50.15		FBF



compound Sumi	marv					
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB) Score (MFG) Algorithm
333	C52 H101 O7 P	14.601	868.7269	FBF	50.72	FBF
334	C55 H107 O7 P	14.783	910.7768	FBF	53.39	FBF
335	C58 H113 O7 P	17.018	952.8163	FBF	50.17	FBF
336 337	C32 H59 O10 P C33 H61 O8 P	5.581 6.205	634.3804 616.4078	<u>FBF</u> FBF	86.87 56.48	FBFFBF
338	C34 H63 O8 P	4.281	630.4248	FBF	77.93	FBF
339	C34 H63 O9 P	17.719	646.4239	FBF	73.24	FBF
340	C39 H75 O9 P	19.070	718.5108	FBF	61.45	FBF
341	C41 H77 O11 P	13.275	776.5195	FBF	63.97	FBF
342 343	C41 H73 O10 P C43 H77 O9 P	13.327 0.383	756.4944 768.5289	<u>FBF</u> FBF	63.83 67.44	FBFFBF
344	C43 H73 O8 P	16.160	748.5053	FBF	58.33	FBF
345	C28 H51 O8 P	5.426	546.3288	FBF	74.37	FBF
346	C29 H57 O8 P	19.044	564.3749	FBF	63.14	FBF
347	C30 H59 O8 P	5.503	578.4000	FBF	55.39	FBF
348 349	C30 H53 O9 P C43 H73 O7 P	5.711 13.431	588.3422 732.5095	<u>FBF</u> FBF	69.21 55.70	FBF FBF
350	C45 H81 O7 P	19.954	764.5686	FBF	65.51	FBF
351	C43 H69 O7 P	13.015	728.4761	FBF	66.55	FBF
352	C40 H75 O7 P	19.018	698.5239	FBF	57.53	FBF
353	C42 H73 O7 P	19.070	720.5056	FBF	68.46	FBF
854	C35 H67 O9 P	19.070	662.4472	FBF	71.50	FBF
355 356	C35 H65 O9 P C36 H67 O9 P	10.103 4.437	660.4432 674.4510	FBF FBF	62.67 76.81	FBF FBF
357	C43 H77 O10 P	17.823	784.5195	FBF	54.15	FBF
358	C45 H83 O8 P	16.498	782.5794	FBF	53.52	FBF
359	C45 H81 O8 P	19.148	780.5642	FBF	50.36	FBF
360	C45 H79 O8 P	14.367	778.5520	FBF	59.43	FBF
861	C62 H125 O7 P	17.537	1012.9188	FBF	50.16	FBF
362 363	C30 H55 O9 P C31 H61 O8 P	5.503 17.563	590.3546 592.4062	FBF FBF	74.58 61.52	FBF FBF
364	C47 H85 O7 P	12.547	792.6034	FBF	60.05	FBF
365	C49 H93 O7 P	12.911	824.6662	FBF	72.64	FBF
366	C49 H91 O7 P	13.457	822.6498	FBF	50.06	FBF
367	C61 H119 O7 P	20.993	994.8699	FBF	50.23	FBF
168	C45 H73 O7 P	16.082	756.5116	FBF	50.93	FBF
369 370	C24 H45 O9 P C46 H75 O7 P	4.541 17.693	508.2808 770.5241	<u>FBF</u> FBF	52.03 54.84	FBF FBF
371	C24 H41 O7 P	3.631	472.2554	FBF	63.22	FBF
372	C64 H129 O7 P	20.551	1040.9549	FBF	56.46	FBF
373	C47 H81 O7 P	10.000	788.5716	FBF	67.13	FBF
374	C63 H123 O7 P	20.239	1022.8932	FBF	58.95	FBF
375	C25 H43 O9 P	4.203	518.2624	FBF	63.16	FBF
376 377	C45 H67 O7 P C26 H49 O8 P	4.567 5.555	750.4602 520.3169	FBF FBF	59.66 53.37	FBF FBF
378	C26 H45 O8 P	3.839	516.2831	FBF	74.43	FBF
379	C26 H45 O9 P	4.229	532.2752	FBF	56.74	FBF
380	C26 H43 O8 P	4.880	514.2694	FBF	66.81	FBF
881	C27 H47 O8 P	3.943	530.3021	FBF	79.21	FBF
882	C46 H85 O7 P	13.873	780.6007	FBF	58.90	FBF
383 384	C28 H49 O10 P C28 H47 O9 P	5.503 4.489	576.3091 558.2946	FBF FBF	50.51 57.77	FBF FBF
85	C49 H79 O7 P	10.000	810.5522	FBF	62.43	FBF
386	C50 H75 O7 P	5.607	818.5318	FBF	52.77	FBF
87	C52 H89 O7 P	17.225	856.6370	FBF	51.03	FBF
888	C29 H51 O8 P	6.127	558.3301	FBF	55.72	FBF
189	C29 H51 O9 P	4.125	574.3282	FBF	81.75	FBF
90 91	C30 H53 O8 P C30 H53 O10 P	20.084 4.203	572.3514 604.3354	<u>FBF</u> FBF	52.34 70.53	FBF FBF
192	C30 H51 O9 P	22.473	586.3261	FBF	68.71	FBF
393	C30 H51 O10 P	4.645	602.3211	FBF	63.55	FBF
194	C31 H55 O8 P	5.555	586.3608	FBF	63.50	FBF
95	C31 H55 O9 P	6.179	602.3638	FBF	60.71	FBF
96 97	C31 H55 O10 P	4.281	618.3546	<u>FBF</u> FBF	82.28 50.37	FBF FBF
397 398	C31 H53 O9 P C46 H77 O7 P	18.836 18.057	600.3463 772.5409	FBF	70.33	FBF
199	C32 H57 O10 P	6.023	632.3714	FBF	53.46	FBF
100	C33 H59 O8 P	4.645	614.3922	FBF	76.60	FBF
01	C33 H57 O9 P	22.629	628.3736	FBF	69.07	FBF
02	C34 H57 O9 P	5.400	640.3743	FBF	62.36	FBF
03 04	C34 H55 O9 P C35 H63 O8 P	4.593 5.633	638.3587 642.4275	FBF FBF	56.53 81.45	FBF FBF
105	C35 H63 O8 P	4.802	658.4189	FBF	77.98	FBF FBF
06	C35 H61 O10 P	6.101	672.4003	FBF	59.65	FBF
107	C36 H63 O8 P	6.205	654.4276	FBF	50.61	FBF
108	C36 H61 O9 P	20.006	668.4049	FBF	87.86	FBF
109	C37 H67 O9 P	5.451	686.4558	FBF	75.28	FBF
110	C39 H69 O11 P	17.771	744.4516	FBF	50.36	FBF
111 112	C39 H67 O8 P	6.309	694.4546	<u>FBF</u> FBF	50.33	FBF ERE
+12 +13	C39 H67 O10 P C39 H65 O9 P	6.127 5.451	726.4457 708.4377	FBF	65.28 84.90	FBF FBF
114	C39 H65 O10 P	4.541	724.4359	FBF	80.98	FBF
15	C41 H75 O11 P	5.555	774.5066	FBF	77.06	FBF
116	C41 H69 O10 P	5.503	752.4637	FBF	86.86	FBF
17	C41 H67 O10 P	19.928	750.4502	FBF	50.71	FBF
ł18	C43 H69 O8 P	4.671	744.4732	FBF	93.16	FBF



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Compound Sumi	mary								
Cpd Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG) Algorithm
3419	C43 H69 O9 P	13.327	760.4680		FBF	54.78			FBF
3420	C46 H73 O7 P	17.745	768.5020		FBF	52.88			FBF
3421	C53 H81 O7 P	13.665	860.5715		FBF	50.47			FBF
3422	C46 H81 O7 P	16.108	776.5675		FBF	65.30			FBF
3423	C50 H93 O7 P	13.249	836.6683		FBF	56.62			FBF
3424	C24 H47 O7 P	6.725	478.3049		FBF	75.85			FBF
3425	C26 H43 O7 P	5.114	498.2768		FBF	52.85			FBF
3426	C15 H27 O9 P	4.567	382.1409		FBF	60.11			FBF
3427	C15 H27 O10 P	8.050	398.1345		FBF	80.79			FBF
3428	C15 H25 O8 P	4.906	364.1315		FBF	60.06			FBF
3429	C16 H27 O9 P	7.244	394.1385		FBF	57.58			FBF
3430	C21 H39 O9 P	3.527	466.2370		FBF	51.07			FBF
3431	C23 H37 O9 P	11.325	488.2202		FBF	69.63			FBF
3432	C25 H41 O9 P	18.343	516.2480		FBF	50.48			FBF
3433	C12 H23 O9 P	6.023	342.1084		FBF	61.79			FBF
3434	C29 H53 O11 P	4.125	608.3267		FBF	57.03			FBF
3435	C37 H63 O10 P	6.101	698.4188		FBF	54.38			FBF
3436	C37 H61 O10 P	5.477	696.3966		FBF	50.81			FBF
3437	C22 H41 O9 P	3.839	480.2530		FBF	54.21			FBF
3438	C24 H43 O10 P	3.605	522.2558		FBF	69.79			FBF
3439	C24 H41 O10 P	3.501	520.2425		FBF	94.34			FBF
3440	C24 H41 O11 P	7.920	536.2390		FBF	66.60			FBF
3441	C25 H47 O10 P	9.402	538.2935		FBF	54.83			FBF
3442	C25 H45 O11 P	4.359	552.2736		FBF	58.24			FBF
3443	C28 H47 O11 P	9.870	590.2867		FBF	68.52			FBF
3444	C30 H49 O10 P	22.603	600.3095		FBF	63.25			FBF
3445	C37 H61 O9 P	4.437	680.4095		FBF	75.14			FBF
3446	C39 H63 O10 P	5.893	722.4228		FBF	64.45			FBF
3447	C21 H37 O9 P	3.839	464.2216		FBF	52.31			FBF
3448	C24 H39 O9 P	3.527	502.2368		FBF	55.13			FBF
3449	C25 H41 O11 P	3.553	548.2412		FBF	52.38			FBF
3450	C30 H53 O11 P	4.593	620.3372		FBF	59.37			FBF
3451	C31 H55 O11 P	12.651	634.3492		FBF	69.15			FBF
3452	C37 H71 O10 P	17.693	706.4823		FBF	55.45			FBF
3453	C37 H69 O10 P	10.103	704.4689		FBF	65.45			FBF
3454	C39 H67 O11 P	18.706	742.4471		FBF	57.67			FBF
3455	C24 H45 O10 P	22.421	524.2765		FBF	75.10			FBF
3456	C26 H47 O11 P	3.917	566.2860		FBF	70.07			FBF
3457	C26 H45 O11 P	3.761	564.2688		FBF	95.63			FBF
3458	C27 H47 O11 P	9.896	578.2864		FBF	68.46			FBF
3459	C32 H57 O11 P	4.359	648.3602		FBF	57.40			FBF
3460	C33 H59 O11 P	4.437	662.3804		FBF	77.24			FBF
3461	C32 H55 O11 P	5.218	646.3464		FBF	71.47			FBF
3462	C41 H69 O11 P	4.671	768.4620		FBF	62.73			FBF
3463	C32 H53 O11 P	18.836	644.3383		FBF	58.28			FBF
3464	C43 H67 O9 P	5.529	758.4518		FBF	57.23			FBF
3465	C32 H51 O11 P	4.593	642.3180		FBF	55.70			FBF
3466	C33 H53 O10 P	4.281	640.3367		FBF	81.64			FBF
3467	C33 H53 O11 P	12.651	656.3319		FBF	64.31			FBF
3468	C41 H65 O11 P	19.278	764.4315		FBF	56.11			FBF
3469	C41 H63 O10 P	4.541	746.4173		FBF	69.68			FBF
3470	C28 H43 O11 P	3.761	586.2509		FBF	78.60			FBF
3471	C29 H45 O10 P	4.802	584.2785		FBF	59.86			FBF
3472	C34 H53 O9 P	5.322	636.3413		FBF	76.36			FBF
3473	C41 H67 O12 P	5,555	782.4360		FRF	61.82			FRF

5.555

4.619

5.036

19.980

5.633

9.662

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4.125

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4.776

4.671

4.515

4.489

4.125

12.651

C34 H53 O9 P C41 H67 O12 P

C43 H63 O9 P

C26 H41 O9 P

C41 H79 O10 P

C43 H79 O12 P

C34 H59 O11 P

C36 H61 O10 P

C43 H77 O12 P

C43 H73 O11 P

C45 H73 O9 P

C43 H71 O11 P

C31 H51 O10 P

C35 H57 O11 P

C35 H57 O9 P

C36 H59 O9 P

C43 H73 O12 P

C45 H69 O9 P

C30 H47 O11 P

C31 H49 O9 P

C31 H49 O11 P

C34 H53 O11 P

C43 H67 O11 P

C30 H45 O11 P

C32 H47 O10 P

C35 H53 O11 P

C30 H45 O9 P

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782.4360

754.4204

528.2480

762.5424

818.5315

674.3732

684.3994

816.5159

796.4886

788.4984

794.4781

614.3241

652.3759

684.3625

666.3941

812.4872

784.4698

614.2833

596.3104

628.3071

668.3279

790.4429

580.2766

612.2748

622.2866

680.3320

FBF

61.82

55.73

50.26

79.91

86.63

61.21

58.17

54.84

77.91

90.12

62.65

64.58

58.34

78.83

50.37

64.47

55.25

59.50

82.79

52.31

58.37

71.81

72.38

66.15

50.90

52.73



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ompound Sum						
Cpd Name	Formula C45 H83 O11 P	RT 19.278	Mass 830.5674	CAS ID Source FBF	Score Score 50.71	re (Lib) Score (DB) Score (MFG) Algorith FBF
3505 3506	C45 H81 O10 P	14.886	812.5537	FBF	54.63	FBF
3507	C45 H81 O11 P	20.006	828.5484	FBF	53.93	FBF
3508	C47 H83 O10 P	13.301	838.5727	FBF	59.74	FBF
3509	C47 H79 O9 P	22.239	818.5441	FBF	53.73	FBF
8510	C36 H63 O11 P	9.064	702.4051	FBF	53.33	FBF
8511	C38 H65 O10 P	5.867	712.4329	FBF FBF	58.88	FBF FBF
3512 3513	C47 H77 O9 P C38 H65 O9 P	17.823 4.437	816.5254 696.4329	FBF	54.58 61.12	FBF
3514	C38 H63 O10 P	5.867	710.4200	FBF	60.15	FBF
8515	C47 H77 O10 P	4.854	832.5287	FBF	55.62	FBF
3516	C36 H57 O11 P	9.896	696.3605	FBF	66.76	FBF
517	C37 H59 O9 P	18.810	678.3867	FBF	62.49	FBF
518	C47 H71 O9 P	4.750	810.4821	FBF	88.18	FBF
519	C37 H57 O11 P	7.270	708.3666	FBF	69.78	FBF
520 521	C33 H49 O10 P	13.977 12.625	636.3004	FBF FBF	68.92	FBF FBF
522	C37 H55 O9 P C37 H55 O11 P	20.421	674.3550 706.3469	FBF	61.00 60.23	FBF
523	C38 H57 O9 P	17.096	688.3703	FBF	57.72	FBF
524	C45 H71 O12 P	4.750	834.4687	FBF	71.49	FBF
525	C47 H69 O10 P	14.159	824.4637	FBF	64.75	FBF
526	C15 H29 O8 P	7.244	368.1626	FBF	74.63	FBF
527	C35 H57 O8 P	4.645	636.3800	FBF	70.29	FBF
528	C46 H91 O8 P	17.433	802.6528	FBF	56.52	FBF
529	C51 H101 O8 P	21.356	872.7223	FBF	60.37	FBF
530 531	C17 H33 O8 P C36 H61 O8 P	9.609 4.281	396.1934 652.4071	FBF FBF	53.00 63.44	FBF FBF
532	C40 H75 O8 P	14.912	714.5199	FBF	53.07	FBF FBF
533	C53 H105 O8 P	21.512	900.7536	FBF	51.27	FBF
534	C32 H53 O8 P	5.322	596.3504	FBF	63.26	FBF
535	C37 H61 O8 P	5.374	664.4118	FBF	78.37	FBF
536	C19 H35 O8 P	3.137	422.2109	FBF	60.18	FBF
537	C42 H79 O8 P	11.793	742.5464	FBF	65.87	FBF
538	C20 H39 O8 P	3.293	438.2342	FBF	58.87	FBF
539 540	C20 H37 O8 P	4.776 19.954	436.2198 870.7135	FBF FBF	56.73 56.78	FBF FBF
541	C51 H99 O8 P C55 H107 O8 P	13.327	926.7703	FBF	53.86	FBF
542	C56 H109 O8 P	13.795	940.7907	FBF	56.43	FBF
543	C40 H69 O8 P	13.587	708.4738	FBF	63.96	FBF
544	C44 H83 O8 P	14.860	770.5817	FBF	54.86	FBF
545	C22 H43 O8 P	5.400	466.2713	FBF	64.67	FBF
546	C42 H73 O8 P	12.443	736.5045	FBF	50.11	FBF
547	C44 H81 O8 P	14.705	768.5651	FBF	55.43	FBF
548 549	C47 H85 O8 P C58 H115 O8 P	14.835 19.252	808.5982 970.8295	FBF FBF	50.71 59.06	FBF FBF
550	C42 H71 O8 P	13.353	734.4892	FBF	60.31	FBF
551	C46 H87 O8 P	14.886	798.6137	FBF	63.16	FBF
552	C46 H71 O8 P	19.070	782.4899	FBF	54.55	FBF
553	C37 H55 O8 P	4.281	658.3659	FBF	64.57	FBF
554	C59 H115 O8 P	19.330	982.8352	FBF	50.04	FBF
555	C48 H91 O8 P	17.251	826.6485	FBF	57.65	FBF
556	C51 H97 O8 P	13.327	868.6912	FBF	58.87	FBF
557	C54 H103 O8 P	14.912 19.096	910.7335	FBF FBF	52.03 53.73	FBF FBF
558 559	C55 H105 O8 P C57 H109 O8 P	16.524	924.7521 952.7803	FBF	55.05	FBF
560	C48 H89 O8 P	13.509	824.6297	FBF	58.65	FBF
561	C48 H85 O8 P	19.850	820.5987	FBF	54.92	FBF
562	C48 H81 O8 P	10.883	816.5725	FBF	50.17	FBF
563	C47 H81 O8 P	17.745	804.5706	FBF	55.95	FBF
564	C48 H75 O8 P	20.006	810.5210	FBF	85.39	FBF
565	C60 H115 O8 P	13.951	994.8328	FBF	51.28	FBF
566	C48 H73 O8 P	14.549	808.4968	FBF	50.38	FBF
567 568	C49 H91 O8 P C56 H105 O8 P	13.301 14.549	838.6426 936.7591	FBF FBF	69.09 54.68	FBF FBF
569	C56 H105 O8 P	14.549	950.7732	FBF	54.68	FBF
570	C58 H109 O8 P	20.110	964.7858	FBF	51.61	FBF
571	C41 H63 O8 P	5.477	714.4272	FBF	54.72	FBF
572	C43 H65 O8 P	5.919	740.4432	FBF	60.30	FBF
573	C53 H97 O8 P	17.771	892.6905	FBF	71.75	FBF
574	C55 H101 O8 P	14.809	920.7206	FBF	52.55	FBF
575	C50 H85 O8 P	12.885	844.5958	FBF	55.39 E4.40	FBF
576 577	C47 H79 O8 P C47 H73 O8 P	14.263 18.706	802.5569 796.5062	FBF FBF	54.40 53.12	FBF FBF
578	C49 H87 O8 P	13.067	834.6074	FBF	53.12	FBF
579	C50 H83 O8 P	16.654	842.5812	FBF	54.18	FBF
580	C50 H77 O8 P	11.767	836.5321	FBF	68.51	FBF
581	C61 H115 O8 P	19.824	1006.8354	FBF	54.35	FBF
582	C45 H67 O8 P	4.671	766.4563	FBF	92.53	FBF
583	C63 H125 O8 P	18.992	1040.9123	FBF	57.60	FBF
584	C51 H89 O8 P	16.654	860.6305	FBF	51.15	FBF
585	C64 H119 O8 P	22.525	1046.8604	FBF	56.01	FBF
586	C51 H87 O8 P	13.353 17.641	858.6070 1030.8296	FBF FBF	50.61 52.79	FBF FBF
		17.041	1030.0230	FDF	32./9	FRE
587	C63 H115 O8 P C29 H45 O8 P			FRF	84.90	
	C03 H113 O6 P C29 H45 O8 P C49 H77 O8 P	3.943 13.665	552.2842 824.5320	FBF FBF	84.90 51.38	FBF FBF



Compound Sumn	.							
Cpd Name 3591	Formula C51 H85 O8 P	RT 15.692	Mass 856.5969	CAS ID Source FBF	Score 54.41	Score (Lib)	Score (DB)	Score (MFG) Algorithm FBF
3592	C52 H75 O8 P	14.055	858.5150	FBF	70.15			FBF
3593	C56 H99 O8 P	20.889	930.7100	FBF	65.59			FBF
3594	C59 H105 O8 P	18.836	972.7571	FBF	55.89			FBF
3595	C60 H107 O8 P	18.576	986.7770	FBF	54.70			FBF
3596	C63 H113 O8 P	20.291	1028.8104	FBF	52.97			FBF
3597	C65 H127 O8 P	14.990	1066.9202	FBF	57.22			FBF
<u>3598</u> 3599	C68 H133 O8 P C66 H127 O8 P	17.693 17.901	1108.9650 1078.9256	FBF FBF	52.73 52.60			FBF FBF
3600	C72 H143 O8 P	11.923	1167.0504	FBF	70.86			FBF
3601	C26 H41 O8 P	6.075	512.2573	FBF	56.94			FBF
3602	C33 H51 O8 P	4.359	606.3266	FBF	51.26			FBF
3603	C34 H55 O8 P	6.023	622.3641	FBF	62.93			FBF
3604	C35 H53 O8 P	12.651	632.3454	FBF	71.45			FBF
3605	C51 H79 O8 P	5.166	850.5532	FBF	58.47			FBF
3606 3607	C53 H81 O8 P C22 H46 N O7 P	13.483 3.631	876.5630 467.3004	FBF FBF	65.89 80.10			FBF FBF
3608	C23 H48 N O7 P	4.177	481.3142	FBF	69.26			FBF
3609	C24 H50 N O7 P	4.359	495.3280	FBF	50.11			FBF
3610	C25 H52 N O7 P	5.789	509.3439	FBF	56.66			FBF
3611	C25 H50 N O7 P	9.844	507.3291	FBF	61.79			FBF
3612	C28 H52 N O7 P	19.044	545.3470	FBF	77.19			FBF
3613	C30 H54 N O7 P	20.239	571.3640	FBF	81.95			FBF
3614	C30 H52 N O7 P	5.218	569.3499	FBF	61.79		-	FBF
3615 3616	C30 H50 N O7 P	5.218 5.322	567.3299 411.2401	FBF FRF	58.57 77.03			FBF FBF
3 <u>616</u> 3617	C18 H38 N O7 P C18 H36 N O7 P	5.322 4.776	411.2401	FBF FBF	77.03 54.52			FBF
3618	C22 H42 N O7 P	4.984	463.2695	FBF	70.90			FBF
3619	C24 H46 N O8 P	5.789	507.2944	FBF	66.09			FBF
3620	C24 H44 N O7 P	3.631	489.2836	FBF	80.87			FBF
3621	C25 H46 N O7 P	3.735	503.3029	FBF	96.81			FBF
3622	C26 H50 N O8 P	5.867	535.3268	FBF	52.13			FBF
3623	C26 H48 N O8 P	3.839	533.3086	FBF	62.20		-	FBF
3624 3625	C26 H46 N O8 P C27 H50 N O7 P	4.359 6.075	531.2970 531.3307	FBF FBF	88.54 55.35			FBF FBF
3626	C27 H48 N O7 P	4.567	529.3186	FBF	85.20			FBF
3627	C27 H44 N O7 P	3.735	525.2843	FBF	85.06			FBF
3628	C29 H56 N O7 P	5.919	561.3789	FBF	52.66			FBF
3629	C29 H54 N O7 P	5.244	559.3612	FBF	65.79			FBF
3630	C29 H50 N O7 P	5.919	555.3334	FBF	62.21			FBF
3631	C31 H52 N O7 P	5.244	581.3462	FBF	77.41			FBF
3632	C32 H62 N O7 P	17.667	603.4256	FBF	70.05			FBF
3633	C32 H58 N O7 P	4.593	599.4003	FBF	65.51			FBF
3634 3635	C32 H54 N O7 P C34 H62 N O7 P	5.971 4.828	595.3617 627.4247	FBF FBF	62.06 66.30			FBF FBF
3636	C34 H60 N O7 P	16.602	625.4093	FBF	51.84			FBF
3637	C34 H58 N O7 P	5.348	623.3949	FBF	54.06			FBF
3638	C34 H56 N O7 P	4.593	621.3823	FBF	81.61			FBF
3639	C36 H72 N O7 P	14.860	661.5070	FBF	62.25			FBF
3640	C36 H64 N O7 P	11.065	653.4405	FBF	55.79			FBF
3641	C36 H60 N O7 P	4.828	649.4067	FBF	50.33			FBF
3642	C39 H78 N O7 P	18.420	703.5459	FBF	54.12			FBF
3643	C41 H82 N O7 P	20.707	731.5865	FBF	54.21			FBF
3644 3645	C44 H80 N O7 P C48 H84 N O7 P	13.275 17.303	765.5644 817.6009	FBF FBF	52.45 50.15			FBF FBF
3646	C50 H90 N O7 P	19.850	847.6507	FBF	51.42			FBF
3647	C17 H36 N O7 P	3.293	397.2199	FBF	80.64			FBF
3648	C18 H40 N O6 P	7.010	397.2607	FBF	58.71			FBF
3649	C20 H42 N O6 P	3.397	423.2744	FBF	73.06			FBF
3650	C22 H46 N O6 P	4.984	451.3027	FBF	51.67			FBF
3651	C23 H48 N O6 P	5.477	465.3212	FBF	67.61			FBF
3652	C25 H54 N O6 P	16.680	495.3685	FBF	65.20			FBF
3653	C25 H50 N O6 P	10.857	491.3411	FBF	64.09			FBF
<u>3654</u> 3655	C26 H50 N O6 P C28 H52 N O6 P	15.328 10.259	503.3355 529.3558	FBF FBF	69.26 62.90			FBF FBF
3656	C28 H50 N O6 P	4.359	527.3377	FBF	68.81			FBF
3657	C38 H76 N O6 P	20.421	673.5391	FBF	62.80			FBF
3658	C38 H74 N O6 P	20.006	671.5289	FBF	65.78			FBF
3659	C13 H30 N O6 P	17.927	327.1806	FBF	50.80			FBF
3660	C41 H80 N O7 P	19.902	729.5745	FBF	51.85			FBF
3661	C36 H70 N O7 P	13.249	659.4908	FBF	53.90			FBF
3662 3663	C40 H68 N O7 P C21 H42 N O7 P	10.103	705.4719 451.2715	FBF FBF	78.78 73.44			FBF FBF
3664	C21 H42 N O7 P	4.906 12.833	825.6623	FBF	61.06			FBF
3665	C38 H72 N O7 P	11.013	685.5041	FBF	64.51			FBF
3666	C42 H76 N O7 P	19.044	737.5366	FBF	68.57			FBF
3667	C37 H72 N O7 P	14.860	673.5020	FBF	54.00			FBF
3668	C41 H72 N O7 P	19.980	721.5099	FBF	71.60			FBF
3669	C43 H84 N O7 P	18.109	757.5976	FBF	56.37			FBF
3670	C40 H78 N O7 P	19.018	715.5552	FBF	56.55			FBF
3671	C44 H78 N O7 P	17.745	763.5512	FBF	61.16			FBF
3672	C48 H98 N O7 P	21.746	831.7060	FBF	60.80			FBF
3673	C50 H102 N O7 P	17.251	859.7334	FBF	63.05			FBF
3674	C52 H106 N O7 P	22.109	887.7717	FBF	50.37			FBF
3675	C53 H108 N O7 P	19.876 17.433	901.7883 1013.9133	FBF FBF	57.98 56.23			FBF FBF



Compound Summary							
Cpd Name	Formula	RT 10.103	Mass	CAS ID Source	Score	Score (Lib) Score (DB) Scor	e (MFG) Algorithr
3677 3678	C39 H74 N O7 P C60 H120 N O7 P	10.103 21.512	699.5138 997.8857	<u>FBF</u> FBF	64.33 54.51		FBF FBF
679	C43 H82 N O7 P	22.940	755.5817	FBF	58.03		FBF
680	C45 H88 N O7 P	17.122	785.6271	FBF	56.08		FBF
681	C45 H78 N O7 P	20.213	775.5466	FBF	55.03		FBF
682	C41 H76 N O7 P	13.093	725.5361	FBF	60.74		FBF
583	C35 H66 N O10 P	5.477	691.4379	FBF	53.93		FBF
684	C36 H70 N O9 P	17.693	691.4813	FBF	75.31		FBF
685 686	C36 H68 N O10 P	13.951 19.096	705.4547 703.4774	FBF FBF	54.56 60.87		FBF FBF
687	C37 H70 N O9 P C42 H86 N O8 P	14.705	763.6078	FBF	54.48		FBF
588	C44 H84 N O8 P	14.705	785.5893	FBF	55.74		FBF
689	C44 H84 N O10 P	14.938	817.5884	FBF	51.24		FBF
690	C44 H84 N O11 P	21.538	833.5801	FBF	52.96		FBF
691	C44 H80 N O10 P	14.964	813.5519	FBF	61.89		FBF
692	C46 H84 N O8 P	15.952	809.6008	FBF	50.22		FBF
693	C46 H80 N O8 P	20.006	805.5639	FBF	78.91		FBF
694	C50 H98 N O7 P	13.691	855.7093	FBF	50.87		FBF
695	C62 H126 N O7 P	17.641	1027.9294	FBF	58.12		FBF
<u>696</u> 697	C63 H128 N O7 P	18.862 6.205	1041.9469 637.3926	FBF FBF	50.30 51.22		FBF FBF
598	C31 H60 N O10 P C31 H58 N O8 P	5.322	603.3873	FBF	66.60		FBF
599	C31 H58 N O9 P	6.205	619.3846	FBF	60.71		FBF
700	C31 H58 N O10 P	4.645	635.3749	FBF	88.15		FBF
701	C32 H62 N O9 P	5.400	635.4195	FBF	66.00		FBF
702	C32 H60 N O8 P	6.023	617.4074	FBF	61.16		FBF
703	C32 H60 N O10 P	4.828	649.3992	FBF	54.34		FBF
'04	C33 H66 N O8 P	13.769	635.4561	FBF	60.29		FBF
705	C47 H82 N O7 P	14.912	803.5844	FBF	56.45		FBF
706	C50 H96 N O7 P	20.006	853.6916	FBF	54.51		FBF
707	C49 H96 N O7 P C56 H110 N O7 P	17.277	841.6918	FBF ERE	51.99 52.37		FBF ERE
<u>708</u> 709	C56 H110 N O7 P	19.720 18.109	939.8013 953.8188	FBF FBF	52.37 56.09		FBF FBF
'10	C38 H74 N O9 P	19.980	719.5119	FBF	83.61		FBF
11	C38 H72 N O10 P	16.628	733.4869	FBF	52.94		FBF
12	C46 H90 N O8 P	14.886	815.6406	FBF	62.68		FBF
13	C46 H88 N O8 P	21.252	813.6270	FBF	54.28		FBF
14	C46 H88 N O11 P	17.901	861.6093	FBF	55.51		FBF
15	C48 H88 N O8 P	14.757	837.6222	FBF	58.01		FBF
'16	C48 H86 N O8 P	17.225	835.6153	FBF	54.93		FBF
'17	C48 H84 N O8 P	14.886	833.5927	FBF	52.74		FBF
'18	C33 H64 N O9 P	6.049	649.4305	FBF	61.37		FBF
7 <u>19</u> 720	C34 H66 N O9 P	19.980 5.477	663.4506 679.4447	<u>FBF</u> FBF	86.21 73.76		FBF FBF
721	C34 H66 N O10 P C35 H70 N O9 P	19.980	679.4734	FBF	67.95		FBF
722	C48 H84 N O9 P	13.847	849.5809	FBF	53.43		FBF
723	C48 H84 N O10 P	18.680	865.5806	FBF	51.86		FBF
724	C52 H100 N O7 P	17.251	881.7183	FBF	52.13		FBF
725	C49 H94 N O7 P	13.717	839.6769	FBF	54.03		FBF
726	C64 H126 N O7 P	20.161	1051.9254	FBF	58.14		FBF
727	C40 H78 N O9 P	20.006	747.5423	FBF	81.34		FBF
728	C40 H76 N O8 P	16.264	729.5338	FBF	60.08		FBF
729	C40 H76 N O10 P	19.070	761.5166	FBF	60.35		FBF FBF
<u>730 </u>	C41 H78 N O8 P C48 H94 N O8 P	10.051 13.379	743.5403 843.6653	FBF FBF	63.94 54.78		FBF
732	C48 H92 N O11 P	19.044	889.6433	FBF	51.32		FBF
733	C50 H90 N O9 P	15.510	879.6409	FBF	54.51		FBF
34	C35 H68 N O9 P	10.103	677.4696	FBF	62.67		FBF
35	C36 H72 N O9 P	19.980	693.4901	FBF	70.75		FBF
36	C37 H74 N O9 P	19.980	707.5050	FBF	71.55		FBF
37	C28 H52 N O9 P	4.047	577.3358	FBF	70.12		FBF
38	C50 H78 N O7 P	17.381	835.5523	FBF	60.48		FBF
39	C29 H54 N O8 P	6.127	575.3571	FBF	57.07		FBF
40	C29 H54 N O9 P	4.515	591.3495	FBF	87.58		FBF
<u>41</u> 42	C58 H110 N O7 P C30 H56 N O9 P	<u>17.745</u> 5.711	963.8040 605.3717	FBF FBF	56.09 59.65		FBF FBF
42 43	C58 H96 N O7 P	17.563	949.6903	FBF	60.25		FBF
44	C30 H54 N O8 P	5.244	587.3597	FBF	62.68		FBF
45	C30 H54 N O9 P	5.555	603.3590	FBF	57.22		FBF
46	C31 H54 N O10 P	12.651	631.3426	FBF	67.17		FBF
47	C54 H94 N O7 P	14.860	899.6810	FBF	52.07		FBF
48	C51 H98 N O7 P	19.824	867.7083	FBF	50.39		FBF
49	C32 H58 N O9 P	6.023	631.3858	FBF	62.50		FBF
50	C32 H58 N O10 P	5.374	647.3853	FBF	58.49		FBF
<u>'51</u>	C32 H56 N O8 P	5.322	613.3758	FBF	83.47		FBF
752 753	C32 H56 N O9 P	6.231	629.3743	FBF ERE	65.04		FBF ERE
<u>753 </u>	C33 H58 N O10 P	12.651 5.348	659.3737 625.3728	FBF FBF	66.98 81.32		FBF FBF
754 755	C33 H56 N O8 P C33 H56 N O10 P	5.348 4.281	625.3728	FBF	81.32		FBF
756	C56 H98 N O7 P	18.628	927.7079	FBF	56.52		FBF
757	C34 H62 N O8 P	4.724	643.4198	FBF	66.11		FBF
'58	C34 H60 N O9 P	5.400	657.4001	FBF	76.92		FBF
759	C34 H58 N O8 P	6.023	639.3887	FBF	60.87		FBF
760	C34 H58 N O9 P	5.374	655.3802	FBF	57.42		FBF
61	C35 H62 N O10 P	6.101	687.4131	FBF	53.82		FBF
762	C35 H60 N O9 P	5.400	669.3986	FBF	84.53		FBF



Compound Sum	.						
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB) Score (MFG) A	
3763 3764	C36 H66 N O8 P C36 H64 N O9 P	4.958 20.006	671.4520 685.4314	<u>FBF</u> FBF	68.43 87.03		BF BF
3765	C36 H64 N O10 P	5.477	701.4267	FBF	77.85		BF
766	C37 H66 N O10 P	6.101	715.4395	FBF	51.88		BF
767	C37 H64 N O7 P	15.484	665.4440	FBF	59.88		BF
768	C37 H64 N O9 P	4.437	697.4362	FBF	52.96		BF
769	C37 H64 N O10 P	5.477	713.4248	FBF	75.26		BF
770	C38 H66 N O10 P	5.867	727.4456	FBF	56.25		BF
771	C39 H72 N O10 P	17.667	745.4863	FBF	57.41	F	BF
772	C39 H68 N O8 P	12.053	709.4628	FBF	61.64	F	BF
773	C39 H66 N O9 P	16.108	723.4493	FBF	55.41	F	BF
774	C40 H72 N O10 P	14.886	757.4919	FBF	54.87		BF
775	C40 H70 N O7 P	19.980	707.4869	FBF	61.65		BF
776	C40 H66 N O7 P	4.515	703.4538	FBF	63.51		BF
777	C40 H64 N O7 P	4.906	701.4416	FBF	83.74		BF
778	C41 H72 N O9 P	5.529	753.4960	FBF	55.37		BF
779	C41 H66 N O7 P	5.010	715.4577	FBF	65.76		BF
780	C42 H78 N O8 P	15.354	755.5438	FBF	57.78		BF
781 782	C44 H86 N O10 P	19.018	819.5973 829.5440	FBF	83.63 55.08		BF BF
783	C44 H80 N O11 P	14.107 10.000	793.5261	<u>FBF</u> FBF	80.91		BF
784	C44 H76 N O9 P C44 H74 N O9 P	4.750	793.5201	FBF	75.75		BF
785	C45 H72 N O7 P	19.902	769.5036	FBF	67.95		BF
786	C46 H74 N O7 P	13.301	783.5210	FBF	60.82		BF
787	C46 H80 N O10 P	10.000	837.5498	FBF	59.60		BF
788	C46 H78 N O10 P	4.828	835.5340	FBF	87.96		BF
789	C46 H76 N O9 P	11.507	817.5216	FBF	79.83		BF
790	C48 H78 N O8 P	19.980	827.5469	FBF	85.34		BF
791	C48 H90 N O11 P	17.745	887.6271	FBF	81.54		BF
792	C50 H76 N O7 P	4.854	833.5384	FBF	56.01		BF
793	C51 H78 N O7 P	14.783	847.5501	FBF	56.99		BF
794	C51 H94 N O7 P	17.277	863.6767	FBF	51.31		BF
795	C51 H90 N O7 P	17.641	859.6472	FBF	63.83		BF
796	C54 H90 N O7 P	19.772	895.6532	FBF	51.20		BF
797	C55 H88 N O7 P	22.005	905.6282	FBF	60.49		BF
798	C56 H104 N O7 P	13.847	933.7522	FBF	50.83		BF
799	C41 H68 N O7 P	4.958	717.4729	FBF	97.12		BF
800	C46 H72 N O7 P	13.613	781.5034	FBF	51.74		BF
801	C19 H34 N O10 P	4.776	467.1947	FBF	52.09		BF
802	C20 H36 N O10 P	3.527	481.2029	FBF	66.97		BF BF
803 804	C26 H52 N O9 P C26 H50 N O9 P	17.953 5.477	553.3397 551.3175	<u>FBF</u> FBF	88.51 53.57		BF
805	C28 H52 N O11 P	4.099	609.3281	FBF	72.92		BF
8806	C28 H50 N O9 P	4.489	575.3227	FBF	90.29		BF
807	C30 H50 N O9 P	17.485	599.3189	FBF	59.54		BF
808	C13 H26 N O8 P	4.281	355.1396	FBF	61.58		BF
809	C15 H26 N O8 P	5.296	379.1366	FBF	62.48		BF
810	C16 H32 N O9 P	6.777	413.1819	FBF	59.37		BF
8811	C16 H30 N O9 P	7.192	411.1644	FBF	56.84		BF
812	C34 H64 N O11 P	6.101	693.4252	FBF	51.36		BF
813	C34 H62 N O11 P	5.451	691.4108	FBF	66.58	F	BF
814	C24 H48 N O8 P	4.880	509.3138	FBF	56.53	F	BF
815	C42 H78 N O10 P	19.928	787.5391	FBF	55.25	F	BF
816	C42 H76 N O9 P	19.902	769.5262	FBF	60.98	F	BF
817	C42 H76 N O10 P	19.954	785.5259	FBF	60.64	F	BF
818	C42 H74 N O10 P	19.928	783.5052	FBF	59.56		BF
819	C29 H54 N O11 P	4.047	623.3424	FBF	54.49		BF
820	C30 H56 N O10 P	4.619	621.3641	FBF	97.70		BF
821	C30 H56 N O11 P	4.593	637.3626	FBF	65.45		BF
822	C30 H54 N O10 P	4.645	619.3476	FBF	86.60		BF
823	C42 H70 N O10 P	14.990	779.4721	FBF	58.15 96.22		BF
324 325	C44 H72 N O9 P C26 H48 N O10 P	5.088 3.943	789.4932 565.3024	<u>FBF</u> FBF	86.23 71.23		BF BF
825 826	C27 H50 N O10 P	3.943	579.3156	FBF	71.23 54.64		BF
827	C30 H52 N O11 P	5.322	633.3270	FBF	56.61		BF
828	C36 H66 N O11 P	4.385	719.4394	FBF	54.07		BF
829	C28 H54 N O10 P	5.555	595.3437	FBF	68.59		BF
830	C32 H60 N O11 P	6.075	665.3912	FBF	61.18		BF
831	C32 H58 N O11 P	4.802	663.3741	FBF	87.25		BF
832	C33 H62 N O11 P	4.802	679.3999	FBF	85.20	F	BF
833	C38 H68 N O11 P	5.529	745.4519	FBF	79.63		BF
834	C39 H68 N O10 P	4.541	741.4627	FBF	51.53		BF
835	C46 H84 N O12 P	22.057	873.5739	FBF	60.49		BF
836	C46 H82 N O12 P	13.431	871.5604	FBF	55.57		BF
837	C46 H78 N O11 P	13.977	851.5317	FBF	56.29		BF
838	C46 H76 N O10 P	5.140	833.5190	FBF	79.43		BF
839	C48 H80 N O10 P	12.833	861.5532	FBF	61.71		BF
840	C48 H78 N O9 P	22.759	843.5398	FBF	51.94		BF
841	C34 H56 N O9 P	5.348	653.3686	FBF	55.80		BF
842	C34 H56 N O10 P	17.355	669.3652	FBF	54.03		BF
843	C34 H56 N O11 P	4.776	685.3536	FBF	58.37		BF
844	C38 H62 N O9 P	5.451	707.4157	FBF	50.93		BF
845	C38 H62 N O11 P	4.541	739.4050	FBF	89.50		BF
846	C46 H72 N O10 P C48 H76 N O10 P	14.341 4.854	829.4874 857.5156	FBF FBF	66.28 73.42		BF BF
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Compound Sumi	ompound Summary												
Cpd Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm			
3849	C30 H50 N O10 P	12.651	615.3198		FBF	80.41				FBF			
3850	C31 H52 N O9 P	4.125	613.3369		FBF	82.79				FBF			
3851	C34 H54 N O9 P	4.281	651.3531		FBF	82.88				FBF			
3852	C40 H74 N O11 P	13.353	775.5061		FBF	66.86				FBF			
3853	C37 H72 N O10 P	10.103	721.4956		FBF	65.76				FBF			
3854	C39 H70 N O11 P	13.327	759.4680		FBF	50.84				FBF			
3855	C39 H68 N O11 P	5.529	757.4504		FBF	74.62				FBF			
3856	C40 H70 N O11 P	5.919	771.4719		FBF	53.54				FBF			
3857	C41 H70 N O10 P	19.070	767.4742		FBF	61.14				FBF			
3858	C48 H82 N O11 P	4.906	879.5619		FBF	68.61				FBF			
3859	C35 H60 N O11 P	4.437	701.3890		FBF	78.83				FBF			
3860	C36 H62 N O9 P	5.815	683.4204		FBF	50.37				FBF			
3861	C48 H80 N O11 P	5.218	877.5477		FBF	93.38				FBF			
3862	C50 H80 N O9 P	14.211	869.5572		FBF	62.63				FBF			
3863	C36 H60 N O9 P	5.841	681.4039		FBF	60.56	,			FBF			
3864	C36 H60 N O11 P	20.369	713.3908		FBF	50.04				FBF			
3865	C37 H60 N O10 P	10.701	709.3967		FBF	53.69				FBF			
3866	C41 H68 N O9 P	4.567	749.4642		FBF	60.86				FBF			
3867	C50 H78 N O9 P	0.409	867.5447		FBF	60.55				FBF			
3868	C36 H58 N O10 P	4.411	695.3786		FBF	88.16				FBF			
3869	C40 H64 N O10 P	4.671	749.4286		FBF	92.03				FBF			
3870	C41 H66 N O9 P	14.211	747.4443		FBF	55.06				FBF			
3871	C48 H74 N O10 P	5.166	855.5025		FBF	66.90				FBF			
3872	C50 H78 N O10 P	13.561	883.5362		FBF	50.05				FBF			
3873	C48 H94 N O9 P	17.485	859.6652		FBF	50.97				FBF			
3874	C50 H96 N O9 P	15.432	885.6836		FBF	57.16				FBF			
3875	C50 H94 N O10 P	16.446	899.6656		FBF	62.27				FBF			
3876	C50 H94 N O11 P	14.886	915.6513		FBF	54.99				FBF			
3877	C50 H92 N O10 P	17.018	897.6435		FBF	53.31				FBF			
3878	C50 H90 N O11 P	19.928	911.6203		FBF	50.48				FBF			
					FBF	69.93				FBF			
3879	C39 H76 N O9 P C43 H78 N O9 P	20.006	733.5292 783.5423		FBF	52.08				FBF			
3880		16.186											
3881	C50 H88 N O11 P	17.797	909.6087		FBF	82.27				FBF			
3882	C52 H90 N O10 P	20.343	919.6295		FBF	57.78				FBF			
3883	C41 H72 N O11 P	4.671	785.4888		FBF	52.11				FBF			
3884	C43 H72 N O9 P	4.489	777.4942		FBF	57.93				FBF			
3885	C50 H86 N O12 P	4.984	923.5849		FBF	52.11				FBF			
3886	C50 H84 N O11 P	13.457	905.5765		FBF	58.17				FBF			
3887	C52 H84 N O9 P	9.948	897.5957		FBF	53.37				FBF			
3888	C42 H68 N O11 P	4.750	793.4538		FBF	92.99				FBF			
3889	C43 H70 N O9 P	4.724	775.4808		FBF	69.92				FBF			
3890	C50 H84 N O12 P	5.270	921.5712		FBF	92.04				FBF			
3891	C50 H80 N O11 P	4.932	901.5417		FBF	55.61				FBF			
3892	C38 H60 N O9 P	4.541	705.4036		FBF	83.52	-		-	FBF			
3893	C50 H82 N O12 P	14.627	919.5590		FBF	52.77				FBF			
3894	C50 H78 N O11 P	5.218	899.5302		FBF	92.60				FBF			
3895	C50 H76 N O10 P	18.940	881.5192		FBF	54.12				FBF			
3896	C52 H78 N O9 P	13.327	891.5435		FBF	72.35				FBF			
3897	C37 H56 N O9 P	4.906	689.3694		FBF	57.54				FBF			
3898	C37 H56 N O11 P	19.642	721.3524		FBF	51.32				FBF			
3899	C18 H36 N O8 P	3.891	425.2147		FBF	80.55				FBF			
3900	C38 H76 N O8 P	21.408	705.5289		FBF	50.37				FBF			
2001	044 1100 11 00 0	20.400	745 5630			F2 00							

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C41 H80 N O8 P

C56 H112 N O8 P

C57 H114 N O8 P

C47 H90 N O8 P

C21 H42 N O8 P

C43 H80 N O8 P

C45 H88 N O8 P

C45 H86 N O8 P

C58 H116 N O8 P

C23 H46 N O8 P

C42 H72 N O8 P

C43 H72 N O8 P

C47 H80 N O8 P

C59 H118 N O8 P

C49 H96 N O8 P

C47 H92 N O8 P

C47 H78 N O8 P

C47 H82 N O8 P

C58 H114 N O8 P

C59 H116 N O8 P

C22 H40 N O8 P

C45 H80 N O8 P

C47 H84 N O8 P

C49 H86 N O8 P

C27 H50 N O8 P

C42 H82 N O11 P

C51 H98 N O8 P

C50 H82 N O8 P

C52 H86 N O8 P

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5.036

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19.044

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21.148

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16.368

17.381

3.943

20.993

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745.5638

957.8077

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801.6244

799.6092

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761.4986

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999.8517

857.6928

829.6516

815.5447

819.5788

983.8289

997.8422

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Comp	ound	Summary

Compound Sumn Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorithm
3935	C62 H120 N O8 P	17.797	1037.8853	FBF	51.32	Score (EIB) Score (EB)	FBF
3936	C58 H110 N O8 P	17.225	979.7964	FBF	50.94		FBF
3937	C50 H78 N O8 P	12.755	851.5443	FBF	55.41		FBF
3938	C61 H116 N O8 P	18.654	1021.8445	FBF	51.71		FBF
939	C64 H122 N O8 P	16.758	1063.8902	FBF	57.76		FBF
3940	C65 H124 N O8 P	16.888	1077.9103	FBF	62.24		FBF
3941 3942	C48 H76 N O8 P C59 H110 N O8 P	14.393 14.912	825.5288 991.8060	<u>FBF</u> FBF	50.34 52.61		FBF FBF
3943	C56 H98 N O8 P	17.693	943.7065	FBF	58.12		FBF
3944	C66 H130 N O8 P	17.901	1095.9549	FBF	51.59		FBF
3945	C32 H54 N O8 P	6.205	611.3600	FBF	61.64		FBF
3946	C32 H52 N O8 P	5.244	609.3422	FBF	61.45		FBF
3947	C52 H80 N O8 P	20.032	877.5636	FBF	53.21		FBF
3948	C62 H114 N O8 P	20.239	1031.8353	FBF	54.55		FBF
3949 3950	C66 H124 N O8 P C55 H100 N O8 P	19.694 21.928	1089.9082 933.7215	FBF FBF	66.81 51.98		FBF FBF
3951	C56 H100 N O8 P	20.421	933.7215	FBF	59.25		FBF
3952	C58 H104 N O8 P	21.019	973.7547	FBF	52.09	-	FBF
3953	C60 H108 N O8 P	14.860	1001.7871	FBF	65.65		FBF
3954	C68 H134 N O8 P	17.719	1123.9779	FBF	50.22		FBF
3955	C69 H136 N O8 P	21.408	1137.9895	FBF	63.13		FBF
956	C68 H128 N O8 P	19.382	1117.9302	FBF	50.41		FBF
957	C69 H130 N O8 P	18.836	1131.9551	FBF	59.61		FBF
958	C62 H112 N O8 P	20.317	1029.8181 637.3797	FBF	62.63		FBF
3959 3960	C34 H56 N O8 P C57 H102 N O8 P	5.763 17.407	959.7326	<u>FBF</u> FBF	62.87 55.30		FBF FBF
1961	C71 H142 N O8 P	11.897	1168.0513	FBF	69.07		FBF
1962	C36 H62 N O8 P	5.400	667.4205	FBF	71.03		FBF
3963	C32 H50 N O8 P	4.125	607.3270	FBF	75.82		FBF
3964	C73 H146 N O8 P	21.486	1196.0839	FBF	59.04		FBF
3965	C36 H60 N O8 P	4.724	665.4027	FBF	52.31		FBF
3966	C36 H56 N O8 P	4.437	661.3772	FBF	82.14		FBF
3967 3968	C38 H64 N O8 P C38 H60 N O8 P	4.958 5.867	693.4342 689.4033	FBF FBF	53.29 59.30		FBF FBF
3969	C40 H62 N O8 P	5.477	715.4213	FBF	65.68		FBF
3970	C41 H68 N O8 P	4.359	733.4682	FBF	56.21	-	FBF
971	C41 H66 N O8 P	4.984	731.4521	FBF	61.27		FBF
972	C42 H68 N O8 P	5.010	745.4669	FBF	84.36		FBF
973	C46 H72 N O8 P	21.538	797.4936	FBF	52.22		FBF
1974	C46 H70 N O8 P	14.445	795.4840	FBF	62.25		FBF
3975	C53 H82 N O8 P	19.980	891.5778	FBF	99.49		FBF
3976 3977	C54 H82 N O8 P C64 H110 N O8 P	15.588 20.317	903.5848 1051.8011	FBF FBF	55.14 70.58		FBF FBF
3978	C24 H40 N O8 P	4.984	501.2491	FBF	50.37		FBF
3979	C94 H162 N O8 P	22.031	1464.2015	FBF	52.54	-	FBF
3980	C96 H154 N O8 P	20.239	1480.1348	FBF	72.76		FBF
3981	C25 H50 N O9 P	5.166	539.3221	FBF	56.61		FBF
3982	C25 H46 N O8 P	3.631	519.2949	FBF	77.02		FBF
3983	C25 H46 N O9 P	3.631	535.2893	FBF	56.33		FBF
3984	C25 H44 N O9 P	4.229	533.2775	FBF	62.78		FBF
3985 3986	C26 H44 N O9 P C26 H42 N O9 P	5.114 3.735	545.2738	FBF FBF	50.04 67.05		FBF FBF
3987	C28 H44 N O8 P	4.359	543.2582 553.2781	FBF	68.93		FBF
3988	C29 H48 N O8 P	3.943	569.3107	FBF	84.90		FBF
3989	C29 H48 N O9 P	14.860	585.3070	FBF	62.62		FBF
3990	C30 H48 N O9 P	4.489	597.3074	FBF	67.48		FBF
3991	C33 H52 N O8 P	5.374	621.3418	FBF	65.17		FBF
3992	C35 H54 N O8 P	5.348	647.3526	FBF	56.89		FBF
3993	C39 H78 N O9 P	19.954	735.5355	FBF	59.99		FBF
3994	C39 H64 N O8 P	4.411 19.954	705.4402	FBF ERE	57.21 61.90		FBF FBF
<u>3995</u> 3996	C40 H80 N O9 P C40 H60 N O8 P	19.954 19.070	749.5519 713.4101	<u>FBF</u> FBF	66.75		FBF
3997	C41 H62 N O8 P	5.737	713.4101	FBF	84.65		FBF
3998	C43 H66 N O9 P	5.919	771.4458	FBF	66.22		FBF
3999	C43 H82 N O9 P	10.026	787.5666	FBF	67.50		FBF
1000	C44 H68 N O9 P	13.405	785.4655	FBF	59.59		FBF
1001	C44 H66 N O8 P	5.010	767.4507	FBF	54.62		FBF
1002	C45 H70 N O8 P	4.671	783.4830	FBF	86.85		FBF
1003 1004	C45 H70 N O9 P	4.489 4.724	799.4762 797.4627	FBF ERE	50.09 69.53		FBF FBF
1004 1005	C45 H68 N O9 P C45 H76 N O9 P	4.724 4.750	805.5269	<u>FBF</u> FBF	91.19		FBF
1006	C46 H72 N O9 P	4.750	813.4894	FBF	73.41		FBF
1007	C46 H70 N O9 P	5.088	811.4769	FBF	74.22		FBF
1008	C47 H74 N O9 P	4.750	827.5088	FBF	88.18		FBF
1009	C47 H72 N O8 P	20.006	809.4964	FBF	66.63		FBF
4010	C47 H72 N O9 P	11.403	825.4875	FBF	78.85		FBF
4011	C47 H92 N O9 P	14.315	845.6519	FBF	56.13		FBF
1012	C47 H90 N O9 P	19.980	843.6272	FBF	56.29		FBF
1013	C47 H84 N O9 P	20.006	837.5846	FBF	54.52		FBF
1014 1 015	C48 H96 N O9 P C48 H72 N O9 P	17.589 12.131	861.6799 837.4937	<u>FBF</u> FBF	50.86 56.29		FBF FBF
1016	C48 H72 N 09 P	13.301	863.6040	FBF	64.11		FBF
1017	C49 H84 N O9 P	13.405	861.5864	FBF	50.82		FBF
4018	C49 H82 N O9 P	0.409	859.5747	FBF	76.43		FBF
1019	C51 H82 N O9 P	13.353	883.5699	FBF	71.10		FBF
4020	C51 H78 N O8 P	14.835	863.5471	FBF	53.21		FBF



Compound Summary										
•	nmary Formula	RT	Mass C	AS ID Source	Saara Sa	ore (Lib) Scare (DP) Scare (MEG) Algorithm				
Cpd Name 4021	C53 H106 N O9 P	13.327	Mass C 931.7559	AS ID Source FBF	Score Score 52.20	ore (Lib) Score (DB) Score (MFG) Algorithm FBF				
4022	C53 H86 N O9 P	18.888	911.6053	FBF	53.53	FBF				
4023	C53 H104 N O9 P	13.587	929.7424	FBF	52.10	FBF				
4024	C53 H98 N O9 P	19.954	923.6972	FBF	50.17	FBF				
1025	C53 H90 N O9 P	16.654	915.6400	FBF	50.65	FBF				
1026	C54 H106 N O9 P	22.395	943.7697	FBF	54.54	FBF				
1027	C54 H102 N O9 P	17.693	939.7339	FBF	53.48	FBF				
1028	C54 H92 N O9 P	15.640	929.6528	FBF	54.51	FBF				
1029	C55 H90 N O9 P	15.146	939.6316	FBF	53.52	FBF				
1030	C55 H100 N O9 P	18.187	949.7101	FBF	73.22	FBF				
4031	C55 H96 N O9 P	14.860	945.6850	FBF	56.82	FBF				
1032	C55 H92 N O9 P	16.524	941.6492	FBF	58.69	FBF				
1033	C56 H112 N O9 P	17.303	973.8053	FBF	54.68	FBF				
1034	C56 H108 N O9 P	13.769	969.7726	FBF	57.39	FBF				
1035	C56 H100 N O9 P	14.757	961.7194	FBF	58.09	FBF				
1036	C57 H90 N O8 P	16.888	947.6336	FBF	51.34	FBF				
1037	C57 H90 N O9 P	16.498	963.6373	FBF	57.03	FBF				
1038	C57 H108 N O9 P	18.550	981.7786	FBF	56.61	FBF				
1039	C59 H96 N O8 P	16.316	977.6896	FBF	58.79	FBF				
040	C59 H102 N O8 P	14.393	983.7273	FBF	60.51	FBF				
041	C61 H110 N O9 P	14.341	1031.7984	FBF	50.02	FBF				
042	C61 H108 N O8 P	17.745	1013.7807	FBF	50.75	FBF				
043	C61 H108 N O9 P	17.719	1029.7843	FBF	52.28	FBF				
044	C62 H112 N O9 P	20.239	1045.8041	FBF	53.43	FBF				
045	C62 H110 N O9 P	20.317	1043.7856	FBF	51.90	FBF				
046	C63 H122 N O9 P	19.330	1067.8847	FBF	52.39	FBF				
047	C64 H128 N O9 P	20.343	1085.9320	FBF	50.64	FBF				
1048	C64 H106 N O9 P	18.395	1063.7576	FBF	50.46	FBF				
1049	C64 H126 N O9 P	21.798	1083.9184	FBF	51.77	FBF				
050	C64 H116 N O9 P	19.694	1073.8414	FBF	56.57	FBF				
051	C64 H112 N O9 P	17.979	1069.8065	FBF	56.77	FBF				
052	C64 H110 N O9 P	17.927	1067.7912	FBF	51.10	FBF				
053	C65 H110 N O8 P	14.860	1063.7972	FBF	52.46	FBF				
054	C65 H110 N O9 P	14.860	1079.7841	FBF	57.02	FBF				
055	C65 H112 N O8 P	13.951	1065.8170	FBF	59.20	FBF				
056	C66 H110 N O9 P	14.886	1091.7833	FBF	55.75	FBF				
057	C66 H114 N O9 P	19.564	1095.8260	FBF	52.46	FBF				
058	C67 H132 N O9 P	20.551	1125.9620	FBF	70.16	FBF				
059	C67 H122 N O9 P	20.032	1115.8843	FBF	51.01	FBF				
060	C67 H116 N O8 P	21.694	1093.8468	FBF	53.09	FBF				
061	C69 H114 N O9 P	14.886	1131.8214	FBF	50.66	FBF				
062	C71 H136 N O9 P	19.902	1177.9924	FBF	84.21	FBF				
1063	C71 H128 N O9 P	20.032	1169.9345	FBF	51.13	FBF				
1064	C72 H120 N O9 P	17.875	1173.8722	FBF	64.42	FBF				
065	C73 H126 N O8 P	18.317	1175.9289	FBF	54.50	FBF				
066	C73 H126 N O9 P	17.251	1191.9165	FBF	53.76	FBF				
067	C73 H144 N O9 P	22.057	1210.0532	FBF	64.76	FBF				
1068	C73 H134 N O9 P	19.928	1199.9763	FBF	78.91	FBF				
069	C73 H130 N O8 P	19.616	1179.9498	FBF	50.12	FBF				
070	C19 H38 N O7 P	4.411	423.2350	FBF	55.70	FBF				
071	C23 H42 N O7 P	3.371	475.2697	FBF	86.65	FBF				
072	C25 H42 N O7 P	4.984	499.2704	FBF	52.10	FBF				
073	C17 H34 N O7 P	3.007	395.2106	FBF	53.99	FBF				
074	C19 H36 N O7 P	4.854	421.2204	FBF	71.08	FBF				
075	C21 H38 N O7 P	3.085	447.2371	FBF	70.55	FBF				
076	C24 H42 N O7 P	4.177	487.2701	FBF	56.44	FBF				
077	C26 H42 N O7 P	3.683	511.2693	FBF	53.43	FBF				
078	C19 H40 N O6 P	12.365	409.2609	FBF	72.77	FBF				
079	C19 H38 N O6 P	4.750	407.2469	FBF	62.30	FBF				
080	C21 H44 N O6 P	3.553	437.2940	FBF	71.62	FBF				
081	C25 H46 N O6 P	4.515	487.3033	FBF	68.64	FBF				
082	C31 H52 N O6 P	4.203	565.3541	FBF	50.47	FBF				
083	C33 H64 N O7 P	13.353	617.4385	FBF	55.97	FBF				
084	C41 H82 N O10 P	19.928	779.5699	FBF	74.90	FBF				
085	C45 H80 N O10 P	10.935	825.5521	FBF	58.94	FBF				
086	C51 H82 N O7 P	18.369	851.5775	FBF	53.15	FBF				
087	C45 H86 N O10 P	17.719	831.5967	FBF	57.37	FBF				
088	C61 H112 N O7 P	13.431	1001.8156	FBF	60.08	FBF				
089	C39 H64 N O7 P	4.229	689.4404	FBF	74.79	FBF				
090	C39 H62 N O7 P	4.880	687.4274	FBF	65.94	FBF				
091	C41 H64 N O7 P	5.477	713.4420	FBF	60.74	FBF				
092	C45 H70 N O7 P	4.567	767.4867	FBF	61.32	FBF				
093	C45 H68 N O7 P	18.992	765.4675	FBF	52.63	FBF				
094	C47 H70 N O7 P	13.847	791.4889	FBF	50.51	FBF				
095	C55 H102 N O7 P	18.680	919.7393	FBF	53.42	FBF				
096	C50 H72 N O7 P	13.847	829.5031	FBF	50.07	FBF				
097	C18 H32 N O8 P	6.205	421.1892	FBF	51.32	FBF				
098	C18 H30 N O9 P	6.699	435.1635	FBF	53.56	FBF				
099	C23 H42 N O8 P	3.397	491.2640	FBF	77.97	FBF				
100	C25 H46 N O10 P	3.943	551.2809	FBF	70.42	FBF				
101	C25 H44 N O10 P	6.984	549.2651	FBF	53.20	FBF				
	C9 H20 N O7 P	3.943	285.0955	FBF	63.14	FBF				
102 103	C12 H20 N O10 P	4.906	369.0820	FBF	73.70	FBF				
	C12 H20 N O10 P C13 H24 N O9 P C14 H22 N O9 P	4.906 9.870 9.064	369.0820 369.1183 379.1045	FBF FBF FBF	73.70 59.78 68.20	FBF FBF FBF				



Cpd Name	nary Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB) Score (MFG) Algorithm
4107	C27 H50 N O11 P	4.125	595.3069	FBF	69.17	Score (LID) Score (DB	FBF
4108	C27 H48 N O10 P	5.555	577.3020	FBF	51.06		FBF
4109	C27 H48 N O11 P	19.486	593.2933	FBF	58.73		FBF
1110 1 111	C24 H44 N O9 P C24 H44 N O10 P	3.735 7.504	521.2763 537.2667	<u>FBF</u> FBF	72.42 62.51		FBF FBF
1112	C28 H46 N O10 P	7.920	587.2809	FBF	67.21	······································	FBF
1113	C41 H74 N O12 P	12.703	803.5026	FBF	53.06		FBF
4114	C43 H80 N O12 P	4.854	833.5384	FBF	53.11		FBF
4115	C43 H76 N O12 P	4.750	829.5139	FBF	60.45		FBF
4116	C43 H72 N O11 P	18.654	809.4881	FBF	54.11		FBF
4117 4118	C45 H74 N O10 P C30 H50 N O11 P	4.802 4.099	819.5076 631.3102	<u>FBF</u> FBF	61.71 62.69		FBF FBF
4119	C43 H74 N O12 P	12.911	827.4966	FBF	51.80		FBF
4120	C43 H70 N O11 P	13.379	807.4740	FBF	56.94		FBF
4121	C45 H72 N O10 P	11.689	817.4929	FBF	55.42		FBF
4122	C45 H70 N O10 P	5.867	815.4725	FBF	55.13		FBF
4123 4124	C30 H46 N O10 P	4.359	611.2806	FBF	63.49		FBF
1125	C32 H48 N O10 P C45 H84 N O12 P	12.651 20.058	637.3010 861.5786	FBF FBF	91.00 56.38		FBF FBF
4126	C45 H82 N O12 P	15.744	859.5554	FBF	52.27		FBF
1127	C47 H80 N O10 P	4.854	849.5527	FBF	93.73		FBF
1128	C45 H78 N O12 P	13.691	855.5195	FBF	53.08		FBF
1129	C47 H74 N O10 P	4.593	843.5062	FBF	53.60		FBF
4130	C32 H50 N O11 P	4.281	655.3070	FBF	59.36		FBF
1131 1132	C34 H52 N O10 P C45 H74 N O12 P	12.651 14.081	665.3319 851.4987	<u>FBF</u> FBF	79.05 60.70		FBF FBF
+132 +133	C47 H72 N O10 P	4.828	851.4987 841.4902	FBF	67.99		FBF
1134	C45 H88 N O10 P	22.369	833.6198	FBF	54.38		FBF
4135	C47 H88 N O10 P	18.836	857.6142	FBF	55.99		FBF
4136	C47 H88 N O11 P	20.655	873.6029	FBF	53.93		FBF
4137	C49 H86 N O10 P	18.836	879.6062	FBF	75.94		FBF
4138 4139	C47 H78 N O11 P C49 H80 N O10 P	5.685 14.964	863.5296 873.5536	<u>FBF</u> FBF	50.39 59.90		FBF FBF
4140	C49 H78 N O10 P	4.854	871.5347	FBF	89.48		FBF
4141	C34 H52 N O11 P	13.275	681.3258	FBF	54.42		FBF
1142	C47 H76 N O12 P	12.573	877.5190	FBF	50.48		FBF
4143	C47 H70 N O10 P	15.432	839.4739	FBF	50.25		FBF
1144	C49 H74 N O10 P	13.353	867.5088	FBF	54.98		FBF
4145	C49 H72 N O9 P	18.550	849.4941	FBF	57.76		FBF FBF
4 <u>146 </u>	C34 H50 N O11 P C35 H52 N O11 P	12.651 17.096	679.3105 693.3255	<u>FBF</u> FBF	69.21 53.48		FBF
4148	C41 H80 N O11 P	13.301	793.5490	FBF	60.36		FBF
4149	C23 H40 N O8 P	4.047	489.2518	FBF	66.03		FBF
4150	C19 H38 N O8 P	5.166	439.2334	FBF	59.83		FBF
4151	C27 H40 N O8 P	7.868	537.2443	FBF	50.65		FBF
4152	C27 H38 N O8 P	3.735	535.2368	FBF	55.12		FBF
<u>4153</u> 4154	C31 H46 N O8 P C35 H52 N O8 P	4.489 4.802	591.2947 645.3439	<u>FBF</u> FBF	69.33 57.94		FBF FBF
4155	C43 H64 N O8 P	4.984	753.4328	FBF	54.45		FBF
4156	C43 H62 N O8 P	5.400	751.4213	FBF	55.27		FBF
4157	C89 H130 N O8 P	20.006	1371.9592	FBF	57.79		FBF
4158	C49 H72 N O8 P	14.757	833.5012	FBF	65.62		FBF
4159	C51 H72 N O8 P	18.758	857.4921	FBF	51.00		FBF
4160	C38 H75 O10 P	19.928	722.5122	FBF	53.80		FBF
4161 4162	C40 H75 O10 P C42 H75 O10 P	17.719 19.928	746.5093 770.5113	FBF FBF	61.17 55.25		FBF FBF
4163	C42 H73 O10 P	19.954	768.4995	FBF	61.25		FBF
4164	C44 H83 O10 P	19.018	802.5710	FBF	83.80		FBF
4165	C38 H71 O10 P	4.541	718.4781	FBF	76.74		FBF
4166	C42 H71 O10 P	19.928	766.4779	FBF	58.38		FBF
4167	C46 H89 O10 P	14.938	832.6137	FBF	50.90		FBF
1168 1 169	C46 H77 O10 P C48 H89 O10 P	22.083 14.549	820.5247 856.6196	FBF FBF	53.04 50.81		FBF FBF
1170	C48 H81 O10 P	11.169	848.5566	FBF	58.08		FBF
1170 1 171	C48 H79 O10 P	13.353	846.5464	FBF	62.00		FBF
1172	C48 H77 O10 P	14.185	844.5283	FBF	51.04		FBF
4173	C46 H71 O10 P	10.779	814.4768	FBF	53.55		FBF
1174	C50 H93 O10 P	12.469	884.6544	FBF	51.37		FBF
4175	C50 H83 O10 P	19.954	874.5642	FBF	60.75		FBF
<u>4176 </u>	C50 H77 O10 P C50 H75 O10 P	13.795 13.665	868.5261 866.5103	FBF FBF	75.49 63.55		FBF FBF
+1// +178	C40 H69 O10 P	4.541	740.4600	FBF	66.02	<u>, </u>	FBF
1179	C47 H85 O10 P	17.329	840.5950	FBF	50.11		FBF
4180	C48 H71 O10 P	14.133	838.4773	FBF	53.13		FBF
1181	C49 H95 O10 P	19.044	874.6643	FBF	70.53		FBF
4182	C49 H75 O10 P	4.854	854.5080	FBF	89.48		FBF
4183	C49 H73 O10 P	12.417	852.4970	FBF	62.56	· · · · · · · · · · · · · · · · · · ·	FBF
4184 4185	C49 H79 O10 P	18.940	858.5424 880.5273	FBF FBF	53.48		FBF FBF
4186 4186	C51 H77 O10 P C51 H91 O10 P	13.379 16.732	880.5273 894.6354	FBF	90.67 59.65		FBF
4187	C51 H83 O10 P	19.356	886.5679	FBF	78.56		FBF
4188	C52 H103 O10 P	18.862	918.7273	FBF	51.61		FBF
	C52 H99 O10 P	18.109	914.6931	FBF	52.81		FBF
4189							
1190 1191	C52 H89 O10 P C53 H105 O10 P	21.200 18.498	904.6199 932.7467	FBF FBF	52.47 54.86		FBF FBF



Cpd Name	Formula	RT	Mass	CAS ID	Source Sco	e Score (Lib)	Score (DB)	Score (MFG) Algorithm
4193	C54 H83 O10 P	5.270	922.5732	CAS ID			Score (DB)	FBF
4194	C55 H109 O10 P	14.601	960.7677	FB				FBF
1195	C55 H89 O10 P	14.263	940.6199	FB				FBF
1196	C55 H87 O10 P	4.984	938.6067	FB				FBF
1197 1198	C55 H103 O10 P	14.809	954.7375	FB				FBF
+198 +199	C56 H109 O10 P C56 H87 O10 P	18.602 20.603	972.7716 950.5950	FB FB				FBF FBF
4200	C56 H103 O10 P	19.408	966.7295	FB				FBF
4201	C59 H117 O10 P	12.963	1016.8409	FB			,	FBF
4202	C59 H113 O10 P	19.200	1012.8047	FB				FBF
4203	C60 H95 O10 P	14.912	1006.6617	FB	F 59.4	4		FBF
4204	C60 H111 O10 P	13.483	1022.7989	FB				FBF
4205	C60 H107 O10 P	14.133	1018.7600	FB				FBF
4206	C61 H121 O10 P	17.667	1044.8672	FB				FBF
4207 4208	C61 H115 O10 P C62 H103 O10 P	17.927 19.616	1038.8180 1038.7191	FB FB			-	FBF FBF
4209	C62 H101 O10 P	19.928	1036.7047	FB				FBF
1209 1 210	C62 H109 O10 P	17.927	1044.7754	FB				FBF
1211	C62 H105 O10 P	20.291	1040.7458	FB				FBF
1212	C63 H101 O10 P	13.353	1048.7203	FB	F 55.8	8		FBF
1213	C63 H119 O10 P	17.147	1066.8540	FB	F 54.1	8		FBF
1214	C63 H113 O10 P	17.927	1060.8004	FB				FBF
1215	C64 H107 O10 P	20.291	1066.7588	FB				FBF
1216	C64 H117 O10 P	14.860	1076.8384	FB				FBF
1217	C64 H115 O10 P	18.680	1074.8190	FB ED				FBF
1218 1 219	C65 H129 O10 P C65 H109 O10 P	20.265 14.860	1100.9290 1080.7812	FB FB				FBF FBF
1 219	C65 H109 O10 P	22.213	1080.7812	FB				FBF
1 221	C65 H111 O10 P	17.927	1082.7829	FB				FBF
1222	C66 H111 O10 P	18.109	1094.7868	FB				FBF
1223	C66 H109 O10 P	19.070	1092.7771	FB				FBF
1224	C68 H113 O10 P	19.824	1120.8140	FB	F 58.4	5		FBF
1225	C68 H127 O10 P	18.966	1134.9163	FB				FBF
1226	C69 H131 O10 P	11.065	1150.9477	FB				FBF
1227	C70 H131 O10 P	17.667	1162.9447	FB				FBF
1228	C70 H121 O10 P	17.771	1152.8745	FB				FBF
1229 1230	C71 H135 O10 P C71 H133 O10 P	19.902 22.057	1178.9858 1176.9612	FB FB				FBF FBF
1231	C72 H135 O10 P	21.928	1190.9712	FB			,	FBF
1232	C73 H141 O10 P	19.044	1209.0326	FB			-	FBF
1233	C73 H139 O10 P	14.185	1207.0112	FB				FBF
1234	C73 H137 O10 P	19.018	1204.9976	FB				FBF
1235	C74 H145 O10 P	21.382	1225.0657	FB	F 55.8	3		FBF
4236	C74 H137 O10 P	22.135	1216.9933	FB				FBF
1237	C36 H67 O12 P	5.711	722.4340	FB				FBF
4238	C36 H65 O12 P	6.101	720.4225	FB				FBF
4239 4240	C36 H59 O12 P C36 H57 O12 P	12.599 13.249	714.3797 712.3582	FB FB				FBF FBF
4241	C36 H55 O12 P	17.199	712.3362	FB				FBF
1242	C37 H61 O12 P	4.541	728.3891	FB				FBF
4243	C38 H69 O12 P	5.763	748.4498	FB				FBF
1244	C38 H65 O11 P	5.529	728.4250	FB				FBF
1245	C38 H63 O11 P	4.828	726.4106	FB	F 68.2	3		FBF
1246	C38 H61 O11 P	14.081	724.3911	FB				FBF
1247	C38 H59 O11 P	7.244	722.3795	FB				FBF
1248	C39 H75 O11 P	0.383	750.4994	FB				FBF
1249	C39 H61 O12 P	14.912	752.3848	FB				FBF
1250 1251	C40 H75 O11 P C40 H69 O12 P	4.671 18.732	762.5040 772.4530	FB FB				FBF FBF
1252	C40 H67 O12 P	4.906	772.4530	FB				FBF
1253	C40 H63 O12 P	18.317	766.4090	FB				FBF
1254	C41 H77 O12 P	10.000	792.5216	FB				FBF
255	C42 H81 O11 P	14.731	792.5466	FB	F 50.7	4		FBF
256	C42 H79 O12 P	4.750	806.5299	FB				FBF
257	C42 H75 O11 P	16.758	786.5021	FB				FBF
1258	C42 H73 O11 P	4.671	784.4859	FB				FBF
259	C43 H83 O11 P	20.006	806.5652	FB ED				FBF
1260 1261	C44 H77 O12 P C45 H77 O12 P	4.750 5.633	828.5118 840.5147	FB FB				FBF FBF
1262	C46 H89 O11 P	16.030	848.6112	FB				FBF
1263	C46 H87 O12 P	14.159	862.5955	FB				FBF
1264	C46 H81 O11 P	14.367	840.5515	FB				FBF
265	C46 H75 O12 P	21.304	850.5038	FB				FBF
1266	C47 H85 O11 P	13.067	856.5870	FB				FBF
1267	C48 H89 O11 P	16.524	872.6165	FB				FBF
1268	C48 H81 O11 P	12.443	864.5535	FB				FBF
1269	C48 H81 O12 P	13.327	880.5441	FB				FBF
270	C49 H91 O11 P	19.096	886.6231	FB				FBF
1271	C49 H87 O12 P	9.948	898.5921	FB FB				FBF FBF
1272 1273	C50 H89 O11 P C50 H85 O11 P	13.405 19.096	896.6181 892.5819	FB FB				FBF
1274	C50 H65 O11 P	22.395	932.6723	FB				FBF
1275	C51 H95 O11 P	14.938	914.6668	FB				FBF
1276	C51 H93 O11 P	16.602	912.6484	FB				FBF
277	C51 H89 O11 P	19.096	908.6052	FB				FBF
	C51 H89 O12 P	13.353	924.6071	FB				FBF



Compound Sumn	.						
Cpd Name	Formula C12 P	RT	Mass	CAS ID Source	Score	Score (Lib) Score	e (DB) Score (MFG) Algorithm
<u>4279</u> 4280	C52 H101 O12 P C52 H97 O12 P	19.564 18.810	948.6947 944.6646	<u>FBF</u> FBF	51.74 50.51		FBF FBF
4281	C52 H87 O11 P	14.809	918.5964	FBF	50.29		FBF
4282	C53 H103 O12 P	19.226	962.7240	FBF	51.48		FBF
4283	C53 H97 O12 P	14.912	956.6738	FBF	51.11		FBF
4284	C53 H89 O11 P	14.912	932.6122	FBF	55.07		FBF
4285	C54 H99 O11 P	17.173	954.6923	FBF	59.20		FBF
<u>4286</u> 4287	C54 H99 O12 P	18.758 19.980	970.6877	FBF FBF	55.98		FBF FBF
4287 4288	C55 H103 O12 P C55 H99 O11 P	21.850	986.7100 966.7003	FBF	59.36 53.15		FBF
4289	C56 H107 O11 P	20.759	986.7515	FBF	50.63		FBF
4290	C56 H103 O11 P	18.161	982.7240	FBF	53.80		FBF
4291	C57 H105 O12 P	19.434	1012.7246	FBF	54.21		FBF
4292	C57 H101 O11 P	14.783	992.7075	FBF	51.71		FBF
4293	C58 H113 O11 P	18.836	1016.8076	FBF	51.53		FBF
4294	C58 H109 O11 P	17.745	1012.7772	FBF	57.03 F0.49		FBF
4295 4296	C58 H107 O11 P C58 H103 O11 P	16.342 20.577	1010.7566 1006.7216	FBF FBF	50.48 56.17		FBF FBF
4297	C59 H115 O11 P	14.705	1030.8113	FBF	52.78		FBF
4298	C59 H113 O11 P	22.161	1028.8078	FBF	51.91		FBF
4299	C59 H109 O11 P	22.759	1024.7728	FBF	50.62		FBF
4300	C59 H105 O12 P	22.213	1036.7410	FBF	68.21		FBF
4301	C60 H105 O12 P	14.912	1048.7408	FBF	50.19		FBF
4302	C61 H117 O11 P	14.445	1056.8343	FBF	58.03		FBF
4303 4304	C61 H109 O11 P C62 H121 O12 P	17.147 19.278	1048.7769 1088.8559	FBF FBF	72.35 55.78		FBF FBF
4305	C62 H121 O12 P	17.953	1066.8215	FBF	55.78		FBF
4306	C62 H113 O11 P	17.927	1064.8059	FBF	55.46		FBF
4307	C62 H107 O12 P	17.044	1074.7478	FBF	51.30		FBF
4308	C63 H119 O12 P	17.667	1098.8445	FBF	51.23		FBF
4309	C63 H117 O12 P	21.538	1096.8270	FBF	50.16		FBF
4310	C63 H115 O12 P	21.694	1094.8151	FBF	58.34		FBF
4311 4312	C63 H113 O11 P	15.900	1076.8041	FBF	74.26		FBF FBF
4312 4313	C64 H125 O11 P C64 H123 O12 P	18.369 18.213	1100.8976 1114.8690	FBF FBF	56.29 53.99		FBF
4314	C64 H119 O12 P	21.694	1110.8451	FBF	50.11		FBF
4315	C64 H117 O11 P	22.005	1092.8240	FBF	51.01		FBF
4316	C64 H115 O11 P	22.940	1090.8201	FBF	51.11		FBF
4317	C64 H111 O11 P	17.927	1086.7886	FBF	61.88		FBF
4318	C65 H125 O11 P	19.278	1112.9041	FBF	50.44		FBF
4319	C65 H123 O11 P	19.798	1110.8845	FBF	57.70		FBF
4320	C65 H113 O11 P	16.940	1100.8054	FBF	50.55		FBF
<u>4321</u> 4322	C66 H127 O12 P C67 H131 O12 P	19.824 20.707	1142.9036 1158.9441	FBF FBF	50.28 56.63		FBF FBF
4323	C67 H131 O12 P	11.091	1140.9257	FBF	56.54		FBF
4324	C67 H123 O11 P	19.278	1134.8822	FBF	54.33		FBF
4325	C67 H119 O12 P	16.628	1146.8448	FBF	64.09		FBF
4326	C68 H131 O11 P	22.135	1154.9386	FBF	55.63		FBF
4327	C68 H129 O11 P	18.810	1152.9275	FBF	51.47		FBF
4328	C68 H125 O12 P	17.771	1164.8973	FBF	50.22		FBF
4329	C69 H133 O12 P	14.912	1184.9522	FBF	57.79		FBF
4330 4331	C69 H127 O12 P C69 H123 O12 P	19.174 17.849	1178.9096 1174.8744	FBF FBF	51.77 58.55		FBF FBF
4332	C69 H121 O11 P	14.912	1156.8746	FBF	59.52		FBF
4333	C70 H135 O12 P	18.940	1198.9658	FBF	50.59		FBF
4334	C70 H127 O11 P	19.148	1174.9119	FBF	53.82		FBF
4335	C71 H135 O12 P	17.693	1210.9764	FBF	58.62		FBF
4336	C72 H135 O12 P	19.200	1222.9699	FBF	53.46		FBF
4337	C73 H139 O11 P	20.421	1223.0075	FBF	57.45		FBF
4338	C73 H129 O12 P	22.239	1228.9242	FBF	57.43		FBF
4339 4340	C74 H143 O11 P C74 H143 O12 P	11.897 19.980	1239.0397 1255.0288	FBF FBF	50.40 50.56		FBF FBF
4340 4341	C74 H143 O12 P	19.512	1226.9440	FBF	50.56		FBF
1342	C75 H143 O11 P	11.897	1251.0475	FBF	50.23		FBF
4343	C75 H137 O11 P	11.897	1244.9905	FBF	50.03		FBF
1344	C76 H145 O11 P	19.720	1265.0519	FBF	50.59		FBF
1345	C77 H137 O11 P	18.940	1268.9932	FBF	53.90		FBF
1346	C78 H153 O12 P	21.122	1313.1140	FBF	54.53		FBF
4347	C78 H149 O11 P	20.136	1293.0837	FBF	57.34		FBF
1348	C78 H147 O11 P	19.018	1291.0699	FBF FRE	50.94 58.40		FBF ERF
1349 1 350	C78 H141 O11 P C78 H141 O12 P	18.992 11.897	1285.0175 1301.0164	FBF FBF	58.40 76.08		FBF FBF
1 351	C78 H139 O12 P	20.058	1298.9985	FBF	59.04		FBF
1352	C80 H155 O12 P	20.603	1339.1231	FBF	52.13		FBF
4353	C80 H143 O12 P	20.291	1327.0358	FBF	54.39		FBF
4354	C81 H147 O11 P	21.512	1327.0695	FBF	58.77		FBF
4355	C82 H149 O12 P	20.603	1357.0664	FBF	50.53		FBF
4356	C83 H151 O12 P	21.071	1371.0999	FBF	67.59		FBF
4357	C85 H159 O11 P	12.599	1387.1557	FBF	58.37		FBF
4358 4350	C86 H157 O11 P	19.954	1397.1470	FBF	53.47		FBF
1359 1360	C17 H35 O9 P	7.244	414.2038	FBF	82.54		FBF
1360	C19 H39 O9 P	7.920	442.2350 456.2510	FBF FRE	83.23		FBF FRE
4361 4362	C20 H41 O9 P C22 H43 O9 P	10.597 3.527	456.2510 482.2609	FBF FBF	50.55 63.52		FBF FBF
4363	C25 H51 O9 P	5.633	526.3258	FBF	55.05		FBF
	C28 H57 O9 P	4.125	568.3696	FBF	73.73		FBF



Cpd Name	nary Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB) Score (MFG) Algorithi
4365	C43 H87 O9 P	13.275	778.6143	FBF	54.80		FBF
366	C44 H89 O9 P	15.822	792.6283	FBF	58.75		FBF
367	C15 H31 O9 P	7.244	386.1725	FBF	84.40		FBF
368 369	C20 H40 O12 P2 C23 H48 O12 P2	6.257 3.943	534.1986 578.2618	<u>FBF</u> FBF	76.44 85.98		FBF FBF
370	C26 H54 O12 P2	19.460	620.3112	FBF	58.11		FBF
371	C27 H56 O12 P2	8.960	634.3236	FBF	63.52		FBF
1372	C30 H60 O12 P2	12.625	674.3534	FBF	50.21		FBF
1373	C32 H64 O12 P2	4.437	702.3909	FBF	60.44		FBF
374	C33 H68 O12 P2	14.938	718.4211	FBF	59.59		FBF
375	C36 H74 O12 P2	13.327	760.4661	FBF	59.26		FBF
1376 1 377	C37 H76 O12 P2 C38 H78 O12 P2	5.555 4.750	774.4761 788.4984	FBF FBF	64.58 95.17		FBF FBF
378	C44 H90 O12 P2	13.249	872.5915	FBF	51.83		FBF
379	C45 H92 O12 P2	14.912	886.6112	FBF	52.49		FBF
380	C19 H41 O8 P	3.839	428.2535	FBF	75.52		FBF
381	C20 H43 O8 P	4.359	442.2715	FBF	90.12		FBF
382	C20 H41 O8 P	12.391	440.2554	FBF	62.25		FBF
383	C21 H43 O8 P	7.920	454.2659	FBF	56.41		FBF
384 385	C26 H53 O8 P C28 H57 O8 P	5.426 22.940	524.3498 552.3823	FBF FBF	80.69 77.34		FBF FBF
386	C30 H63 O8 P	10.571	582.4300	FBF	54.25		FBF
387	C26 H56 O11 P2	4.125	606.3254	FBF	62.76		FBF
388	C28 H58 O11 P2	12.651	632.3454	FBF	90.21		FBF
389	C40 H73 O9 P	10.207	728.5004	FBF	51.65		FBF
390	C44 H81 O9 P	14.705	784.5633	FBF	53.61		FBF
391	C44 H79 O9 P	13.847	782.5477	FBF	55.51		FBF
392	C40 H77 O9 P	19.954	732.5257	FBF	61.90		FBF
393 394	C42 H75 O9 P C42 H73 O9 P	14.705 5.529	754.5177 752.4942	FBF FBF	53.83 62.99		FBF FBF
395	C46 H89 O9 P	13.353	816.6241	FBF	53.76		FBF
396	C49 H99 O9 P	20.265	862.7008	FBF	64.13		FBF
397	C52 H105 O9 P	19.824	904.7518	FBF	52.34		FBF
398	C24 H49 O9 P	5.555	512.3129	FBF	51.27		FBF
399	C36 H69 O9 P	19.980	676.4653	FBF	78.17		FBF
400	C42 H71 O9 P	14.886	750.4881	FBF	55.97		FBF
401	C54 H107 O9 P	14.705	930.7642	FBF	53.53		FBF
402 403	C59 H117 O9 P	19.720	1000.8450	FBF FBF	57.26		FBF FBF
403 404	C47 H87 O9 P C34 H65 O12 P	14.860 18.317	826.6088 696.4211	FBF	53.73 60.18		FBF
405	C34 H63 O11 P	5.659	678.4054	FBF	82.55		FBF
406	C48 H91 O9 P	13.301	842.6334	FBF	51.78		FBF
407	C26 H51 O11 P	3.943	570.3138	FBF	65.46		FBF
408	C29 H53 O12 P	8.206	624.3283	FBF	63.44		FBF
409	C47 H91 O9 P	20.733	830.6401	FBF	58.32		FBF
410	C49 H95 O9 P	19.070	858.6697	FBF	56.01		FBF
<u>411</u> 412	C44 H83 O13 P C29 H57 O11 P	4.854 5.555	850.5559 612.3689	FBF FBF	74.33 61.32		FBF FBF
413	C31 H57 O12 P	4.281	652.3531	FBF	57.58		FBF
414	C32 H63 O11 P	13.899	654.4091	FBF	65.67		FBF
415	C33 H65 O10 P	16.602	652.4361	FBF	62.66		FBF
416	C50 H79 O9 P	18.836	854.5448	FBF	51.49		FBF
417	C51 H97 O9 P	17.459	884.6882	FBF	53.12		FBF
418	C51 H89 O9 P	14.783	876.6233	FBF	52.16		FBF
419	C33 H63 O12 P	4.411	682.4110	FBF	56.99		FBF
420	C64 H127 O9 P	19.694	1070.9221	FBF	55.75		FBF
<u>421</u> 422	C52 H97 O9 P C49 H81 O9 P	17.615 20.032	896.6871 844.5584	FBF FBF	53.07 56.37		FBF FBF
423	C54 H103 O9 P	15.900	926.7335	FBF	58.97		FBF
424	C66 H133 O9 P	18.966	1100.9796	FBF	53.53		FBF
425	C50 H87 O9 P	21.200	862.6107	FBF	67.11		FBF
126	C52 H95 O9 P	14.783	894.6736	FBF	50.16		FBF
127	C52 H93 O9 P	15.588	892.6519	FBF	60.13		FBF
428	C54 H87 O9 P	20.006	910.6119	FBF	59.67		FBF
129	C51 H81 O9 P	12.755	868.5611	FBF	75.12		FBF
430	C29 H51 O12 P	20.317	622.3094	FBF	65.55		FBF
431 432	C56 H105 O9 P C52 H79 O9 P	13.379 14.211	952.7502 878.5408	<u>FBF</u> FBF	51.30 53.15		FBF FBF
133	C31 H55 O12 P	4.593	650.3470	FBF	61.88		FBF
434	C31 H53 O12 P	20.006	648.3275	FBF	52.98		FBF
135	C52 H81 O9 P	14.419	880.5583	FBF	60.83		FBF
136	C55 H99 O9 P	16.914	934.7039	FBF	51.74		FBF
137	C32 H57 O12 P	4.724	664.3614	FBF	76.12		FBF
138	C32 H53 O12 P	16.030	660.3244	FBF	93.57		FBF
139	C56 H107 O9 P	12.183	954.7640	FBF	51.37		FBF
44 0	C50 H83 O9 P	13.925	858.5736	FBF	50.34		FBF
	C56 H99 O9 P	17.615	946.6988	FBF FBF	50.65 54.66		FBF FBF
141	C56 H101 O9 P	16.108 5.296	948.7183 690.3742	FBF	54.66 57.72		FBF
141 142		3.230			78.52		
141 142 143	C34 H59 O12 P C35 H63 O12 P	4,541	706.4062	FBF			FDF
441 442 443 444	C34 H59 O12 P C35 H63 O12 P C42 H75 O13 P	4.541 13.691	706.4062 818.4928	FBF FBF	52.95		FBF FBF
441 442 443 444 445 446	C35 H63 O12 P						
441 442 443 444 445	C35 H63 O12 P C42 H75 O13 P	13.691	818.4928	FBF	52.95		FBF
141 142 143 144 145 146	C35 H63 O12 P C42 H75 O13 P C44 H77 O13 P	13.691 13.223	818.4928 844.5130	FBF FBF	52.95 52.67		FBF FBF



Compound Sumr	.							
Cpd Name 4451	Formula C24 H47 O10 P	RT 3.735	Mass 526.2873	CAS ID Source FBF	Score 64.07	Score (Lib)	Score (DB)	Score (MFG) Algorithm FBF
4452	C24 H47 O11 P	14.886	542.2810	FBF	56.22			FBF
4453	C31 H55 O13 P	12.651	666.3365	FBF	58.45			FBF
4454	C40 H73 O13 P	6.205	792.4793	FBF	75.77			FBF
4455	C25 H47 O12 P	3.735	570.2852	FBF	52.49			FBF
<u>4456 </u>	C27 H49 O12 P C28 H53 O12 P	4.489 4.359	596.3013 612.3321	FBF FBF	62.71 71.25			FBF FBF
4458	C28 H51 O12 P	8.830	610.3168	FBF	59.05			FBF
4459	C31 H53 O13 P	12.651	664.3290	FBF	64.92			FBF
4460	C27 H45 O12 P	3.735	592.2672	FBF	67.80			FBF
<u>4461</u> 4462	C34 H63 O13 P C34 H61 O13 P	4.489 4.828	710.4015 708.3834	FBF FBF	52.85 80.40			FBF FBF
4463	C42 H73 O13 P	14.107	816.4770	FBF	50.63			FBF
4464	C27 H51 O12 P	4.099	598.3152	FBF	74.61			FBF
4465	C29 H53 O13 P	4.645	640.3252	FBF	64.54			FBF
<u>4466</u> 4467	C29 H51 O13 P C30 H53 O13 P	12.651 4.125	638.3041 652.3205	<u>FBF</u> FBF	68.82 90.03			FBF FBF
4468	C29 H49 O13 P	3.943	636.2930	FBF	68.00			FBF
4469	C36 H65 O13 P	4.619	736.4127	FBF	66.26			FBF
4470	C44 H79 O14 P	5.659	862.5253	FBF	60.21			FBF
4471	C44 H75 O13 P	13.665	842.4932	FBF	63.39			FBF
4472	C44 H77 O14 P C33 H53 O12 P	13.899 4.281	860.5108 672.3335	<u>FBF</u> FBF	71.17 53.17			FBF FBF
<u>4473</u> 4474	C35 H57 O13 P	4.437	716.3591	FBF	59.99		,	FBF
4475	C31 H49 O13 P	12.651	660.2858	FBF	56.16			FBF
4476	C32 H51 O12 P	4.281	658.3091	FBF	54.58			FBF
4477	C32 H51 O13 P	4.125	674.3025	FBF	72.60			FBF
<u>4478</u> 4479	C46 H69 O11 P	4.750	828.4561 642.2798	FBF FRF	71.69			FBF FBF
4480	C31 H47 O12 P C31 H47 O13 P	12.651 12.651	658.2787	FBF FBF	55.56 84.63			FBF
4481	C32 H49 O12 P	9.376	656.2964	FBF	58.95			FBF
4482	C37 H67 O13 P	4.671	750.4311	FBF	70.55		,	FBF
4483	C38 H71 O13 P	5.763	766.4609	FBF	79.37			FBF
<u>4484</u> 4485	C46 H81 O13 P	4.854	872.5379	FBF	62.73			FBF FBF
4486	C33 H61 O13 P C46 H81 O14 P	4.437 14.886	696.3793 888.5357	FBF FBF	55.76 87.77		,	FBF
4487	C34 H55 O13 P	4.437	702.3370	FBF	80.44			FBF
4488	C35 H55 O12 P	6.725	698.3455	FBF	61.23		,	FBF
4489	C37 H57 O13 P	18.057	740.3506	FBF	53.30			FBF
4490	C38 H59 O13 P	13.353	754.3714	FBF	55.74			FBF FBF
4491 4492	C48 H73 O12 P C30 H47 O12 P	4.854 3.943	872.4828 630.2766	FBF FBF	60.85 74.82		,	FBF
4493	C33 H49 O13 P	4.724	684.2883	FBF	79.31			FBF
4494	C48 H89 O14 P	17.381	920.5898	FBF	53.24		,	FBF
4495	C48 H87 O13 P	13.483	902.5864	FBF	60.50			FBF
4496	C48 H85 O14 P	4.906	916.5626	FBF	55.51			FBF
4497 4498	C50 H77 O11 P C39 H61 O13 P	4.906 14.860	884.5156 768.3853	FBF FBF	63.37 71.65		,	FBF FBF
4499	C50 H75 O11 P	5.218	882.5026	FBF	92.60			FBF
4500	C35 H53 O13 P	10.857	712.3172	FBF	54.85		,	FBF
4501	C40 H61 O11 P	14.912	748.3924	FBF	54.99			FBF
4502	C37 H73 O10 P	19.980 18.758	708.4936 864.4948	<u>FBF</u> FBF	64.05			FBF FBF
<u>4503</u> 4504	C50 H73 O10 P C52 H75 O10 P	12.599	890.5089	FBF	53.44 51.90			FBF
4505	C44 H65 O10 P	4.671	784.4317	FBF	72.91			FBF
4506	C42 H80 O13 P2	4.854	854.5080	FBF	98.39		,	FBF
4507	C41 H78 O15 P2	4.854	872.4829	FBF	64.22			FBF
4508	C45 H86 O15 P2	4.984	928.5417	FBF	61.65			FBF
<u>4509</u> 4510	C45 H84 O15 P2 C43 H76 O15 P2	5.270 4.854	926.5266 894.4665	FBF FBF	93.22 68.20			FBF FBF
4511	C47 H82 O15 P2	4.984	948.5140	FBF	72.41			FBF
4512	C49 H90 O15 P2	11.325	980.5785	FBF	53.23			FBF
4513	C39 H64 O15 P2	7.920	834.3656	FBF	59.35			FBF
<u>4514</u> 4515	C42 H84 O15 P2 C44 H88 O15 P2	18.446 16.784	890.5360 918.5643	<u>FBF</u> FBF	52.27 59.29			FBF FBF
4515 4516	C44 H72 O15 P2	4.671	918.5643	FBF	60.33			FBF
4517	C46 H88 O15 P2	4.984	942.5589	FBF	97.95			FBF
4518	C48 H86 O15 P2	4.984	964.5400	FBF	80.00			FBF
4519 4520	C51 H88 O15 P2	5.062	1002.5615	FBF	58.44			FBF
<u>4520</u> 4521	C52 H100 O15 P2 C53 H106 O15 P2	5.114 16.628	1026.6585 1044.7074	<u>FBF</u> FBF	60.34 52.01			FBF FBF
4522	C53 H86 O15 P2	5.062	1024.5439	FBF	56.43			FBF
4523	C61 H112 O16 P2	14.860	1162.7385	FBF	51.29			FBF
4524	C63 H124 O16 P2	19.980	1198.8280	FBF	79.04			FBF
4525	C65 H108 O16 P2	5.296	1206.7126	FBF	92.07			FBF
4526 4527	C54 H104 O16 P2	5.166	1070.6846	FBF	61.50			FBF
<u>4527</u> 4528	C54 H100 O16 P2 C54 H96 O16 P2	14.835 15.640	1066.6430 1062.6139	FBF FBF	51.96 51.26			FBF FBF
4529	C54 H96 O16 P2	5.166	1062.6139	FBF	69.27			FBF
4530	C56 H94 O16 P2	13.301	1084.6001	FBF	50.21			FBF
4531	C56 H92 O16 P2	14.860	1082.5868	FBF	71.25	<u></u>		FBF
4532	C60 H110 O16 P2	17.719	1148.7218	FBF	53.02			FBF
4533	C62 H120 O16 P2	20.161	1182.8128	FBF	53.47			FBF
<u>4534</u> 4535	C70 H114 O16 P2 C71 H138 O16 P2	14.886 17.667	1272.7636 1308.9475	FBF FBF	51.47 50.73			FBF FBF
4536	C72 H138 O16 P2	19.070	1320.9430	FBF	65.12			FBF



Compound Sum							
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB) S	core (MFG) Algorith
<u>4537</u> 4538	C73 H142 O16 P2	19.902	1336.9708	<u>FBF</u> FBF	55.44		FBF FBF
4539	C73 H136 O16 P2 C73 H132 O16 P2	18.992 19.980	1330.9368 1326.8985	FBF	52.50 64.26		FBF
4540	C73 H130 O16 P2	19.980	1324.8906	FBF	77.59		FBF
1541	C74 H146 O16 P2	19.382	1353.0131	FBF	53.80		FBF
1542	C74 H142 O16 P2	19.980	1348.9755	FBF	59.43		FBF
4543	C74 H136 O16 P2	17.823	1342.9304	FBF	57.96		FBF
1544 4545	C75 H128 O16 P2	20.006	1346.8739	FBF	73.42		FBF
4545 4546	C75 H136 O16 P2 C75 H134 O16 P2	20.006 19.980	1354.9331 1352.9233	FBF FBF	60.48 54.28		FBF FBF
4547	C75 H134 O16 F2	19.954	1348.8816	FBF	54.14		FBF
4548	C35 H69 O18 P3	13.899	870.3705	FBF	84.03		FBF
1549	C27 H49 O19 P3	14.367	770.2010	FBF	58.74		FBF
1550	C36 H71 O19 P3	12.105	900.3753	FBF	51.99	<u> </u>	FBF
1551	C39 H77 O19 P3	13.691	942.4268	FBF	60.48		FBF
1552 1553	C41 H79 O19 P3 C45 H75 O19 P3	4.750 14.263	968.4362 1012.4095	FBF FBF	63.24 54.15		FBF FBF
1554	C49 H97 O19 P3	14.860	1082.5868	FBF	76.92		FBF
1555	C58 H113 O19 P3	5.296	1206.7126	FBF	82.68		FBF
1556	C31 H57 O17 P	13.275	732.3368	FBF	50.15		FBF
557	C31 H53 O17 P	4.828	728.2996	FBF	64.31		FBF
1558	C32 H57 O17 P	14.783	744.3348	FBF	52.49		FBF
559	C33 H63 O17 P	4.541	762.3878	FBF	53.87		FBF
560	C33 H57 O17 P	12.703	756.3398	FBF	58.36		FBF
561 562	C34 H59 O17 P	4.307 13.405	770.3508 766.3234	<u>FBF</u> FBF	83.42 63.16		FBF FBF
563	C34 H55 O17 P C35 H65 O22 P	7.920	766.3234 868.3675	FBF	77.31		FBF FBF
564	C35 H63 O22 P	13.431	866.3518	FBF	58.73		FBF
565	C36 H61 O22 P	14.029	876.3386	FBF	54.09		FBF
566	C38 H67 O22 P	14.809	906.3829	FBF	55.26		FBF
567	C41 H69 O22 P	13.743	944.3946	FBF	50.04		FBF
568	C43 H79 O18 P	4.906	914.5053	FBF	58.62		FBF
569	C44 H75 O18 P	21.382	922.4647	FBF	64.47		FBF
570	C45 H77 O18 P	4.906	936.4872	<u>FBF</u> FBF	70.84 53.21		<u>FBF</u> FBF
571 572	C45 H73 O18 P C46 H75 O18 P	13.561 13.275	932.4521 946.4602	FBF	51.99		FBF
573	C47 H87 O18 P	13.977	970.5676	FBF	55.76		FBF
574	C47 H81 O18 P	14.549	964.5200	FBF	55.82		FBF
575	C48 H91 O18 P	13.847	986.5875	FBF	51.29		FBF
576	C49 H93 O18 P	14.731	1000.6165	FBF	54.33		FBF
577	C49 H89 O18 P	13.795	996.5811	FBF	51.86		FBF
578	C49 H85 O18 P	5.036	992.5437	FBF	60.48		FBF
1579	C50 H93 O18 P	14.393	1012.6114	FBF	55.26		FBF
580 581	C50 H77 O18 P C51 H91 O18 P	22.862 13.691	996.4820 1022.6038	FBF FBF	73.72 61.99		FBF FBF
582	C52 H93 O18 P	13.873	1036.6128	FBF	60.23		FBF
1583	C53 H95 O18 P	13.743	1050.6170	FBF	50.35		FBF
584	C54 H103 O18 P	5.166	1070.6846	FBF	65.81		FBF
585	C55 H95 O18 P	5.166	1074.6355	FBF	53.63		FBF
586	C49 H83 O23 P	20.915	1070.5016	FBF	66.68		FBF
587	C23 H46 O15 P2	6.231	624.2267	FBF	65.83		FBF
588	C23 H44 O15 P2 C27 H52 O15 P2	6.361	622.2175	FBF	59.44		FBF
1589 1590	C27 H32 O13 P2 C29 H50 O15 P2	9.402 13.353	678.2762 700.2630	<u>FBF</u> FBF	51.95 64.14		FBF FBF
591	C31 H54 O15 P2	15.016	728.2953	FBF	72.77		FBF
592	C32 H64 O15 P2	14.912	750.3672	FBF	52.03		FBF
593	C33 H58 O15 P2	12.755	756.3321	FBF	53.19		FBF
594	C35 H66 O15 P2	4.671	788.3865	FBF	85.16		FBF
595	C38 H76 O15 P2	4.750	834.4687	FBF	66.12		FBF
596 507	C25 H52 O14 P2	10.311	638.2852	FBF	52.06		FBF
597 598	C27 H56 O14 P2 C31 H64 O14 P2	4.281 7.244	666.3147 722.3764	<u>FBF</u> FBF	53.02 58.18		<u>FBF</u> FBF
598 599	C31 H64 O14 P2	15.406	822.3438	FBF	59.70		FBF
600	C37 H56 O16 P2	11.221	818.3059	FBF	50.34		FBF
601	C43 H82 O16 P2	4.932	916.5078	FBF	55.52		FBF
602	C45 H80 O16 P2	4.932	938.4902	FBF	52.61		FBF
603	C47 H88 O16 P2	5.348	970.5494	FBF	59.76		FBF
604	C47 H80 O16 P2	13.223	962.4872	FBF	51.71		FBF
605	C49 H86 O16 P2	5.036	992.5437	FBF	56.13		FBF
606 607	C28 H55 O12 P C31 H61 O12 P	4.125 5.607	614.3397 656.3931	<u>FBF</u> FBF	62.59 64.56		<u>FBF</u> FBF
608	C31 H61 G12 P	19.980	684.4279	FBF	54.79		FBF
609	C34 H67 O12 P	4.437	698.4392	FBF	52.62		FBF
610	C44 H87 O12 P	15.458	838.6010	FBF	52.48		FBF
611	C26 H57 O12 P	4.125	592.3573	FBF	76.68		FBF
612	C28 H61 O12 P	5.555	620.3860	FBF	70.28		FBF
613	C50 H99 O12 P	13.353	922.6958	FBF	51.71		FBF
614	C39 H79 O12 P	16.472	770.5308	FBF	59.53		FBF
615	C37 H69 O14 P	5.945	768.4385	FBF	53.33		FBF
616	C37 H69 O15 P	4.671	784.4317	FBF	54.17		FBF
617 618	C37 H67 O15 P	4.671	782.4294 854.5530	FBF ERF	52.07 56.95		FBF FBF
618 619	C43 H83 O14 P C43 H81 O13 P	12.781 10.000	854.5530 836.5456	<u>FBF</u> FBF	68.16		FBF
620	C45 H85 O13 P	18.680	864.5756	FBF	51.98		FBF
621	C45 H83 O13 P	5.685	862.5592	FBF	61.19		FBF
	C45 H83 O14 P	5.218	878.5514	FBF	63.86		FBF



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Compound Sum						
Cpd Name	Formula C4E H91 O14 D	RT 14.938	Mass 976 5247	CAS ID Source FBF		Score (Lib) Score (DB) Score (MFG) Algorithm
4623 4624	C45 H81 O14 P C45 H79 O14 P	14.938	876.5347 874.5176	FBF	58.35 51.06	FBF FBF
4625	C47 H83 O13 P	18.109	886.5575	FBF	54.27	FBF
4626	C47 H81 O13 P	5.685	884.5411	FBF	63.80	FBF
4627	C47 H81 O14 P	4.932	900.5381	FBF	68.32	FBF
4628	C63 H125 O12 P	17.615	1104.8907	FBF	50.85	FBF
4629	C29 H55 O13 P	4.281	642.3413	FBF	53.18 59.04	FBF
4630 4631	C29 H55 O14 P C30 H57 O13 P	4.099 4.281	658.3364 656.3598	FBF FBF	65.61	FBF FBF
4632	C32 H59 O15 P	4.489	714.3630	FBF	55.70	FBF
4633	C32 H57 O14 P	4.307	696.3492	FBF	90.53	FBF
4634	C33 H63 O14 P	16.836	714.3973	FBF	57.86	FBF
4635	C34 H65 O13 P	13.613	712.4194	FBF	72.64	FBF
4636	C45 H85 O14 P	9.896	880.5698	FBF	90.19	FBF
4637 4638	C47 H87 O14 P C49 H85 O13 P	5.711 20.369	906.5832 912.5731	FBF FBF	64.33 55.60	FBF FBF
4639	C49 H85 O14 P	5.737	928.5652	FBF	58.21	FBF
4640	C65 H129 O12 P	19.538	1132.9275	FBF	56.80	FBF
4641	C31 H59 O14 P	4.437	686.3658	FBF	71.70	FBF
4642	C32 H61 O14 P	4.437	700.3857	FBF	68.38	FBF
4643	C34 H61 O14 P	7.894	724.3843	FBF	51.26	FBF
4644	C35 H65 O14 P	4.541	740.4058	FBF	62.47	FBF
4645	C40 H73 O15 P	12.963	824.4709 824.5001	FBF ERF	53.77 51.01	FBF
4646 4647	C41 H77 O14 P C41 H75 O15 P	14.055 13.873	824.5001 838.4842	FBF FBF	51.01 55.02	FBF FBF
4648	C41 H/3 O13 P	13.275	826.5950	FBF	57.12	FBF
4649	C47 H91 O14 P	17.797	910.6142	FBF	76.51	FBF
4650	C47 H89 O14 P	19.980	908.6042	FBF	74.81	FBF
4651	C49 H89 O15 P	14.081	948.5849	FBF	57.89	FBF
4652	C51 H89 O14 P	19.408	956.5944	FBF	67.99	FBF
4653	C67 H133 O12 P	22.499	1160.9530	FBF	50.27	FBF
4654 4655	C36 H65 O14 P	4.932 17.070	752.4136	FBF FBF	78.69 51.83	FBF FBF
4656	C37 H71 O14 P C31 H53 O14 P	4.099	770.4605 680.3188	FBF	70.23	FBF
4657	C29 H61 O12 P	4.854	632.3918	FBF	67.87	FBF
4658	C32 H55 O14 P	13.353	694.3332	FBF	75.03	FBF
4659	C56 H113 O12 P	20.551	1008.7981	FBF	56.53	FBF
4660	C57 H119 O12 P	14.081	1026.8370	FBF	51.21	FBF
4661	C34 H55 O14 P	4.307	718.3318	FBF	70.26	FBF
4662	C35 H61 O15 P	13.353	752.3791	FBF	56.02	FBF
4663 4664	C36 H59 O14 P C38 H63 O15 P	4.567 4.671	746.3633 790.3875	FBF FBF	72.43 54.51	FBF FBF
4665	C39 H67 O14 P	9.844	790.4238	FBF	51.44	FBF
4666	C39 H65 O13 P	4.671	772.4144	FBF	75.03	FBF
4667	C39 H65 O15 P	4.671	804.4114	FBF	64.65	FBF
4668	C43 H79 O14 P	0.409	850.5182	FBF	63.36	FBF
4669	C43 H77 O13 P	13.353	832.5079	FBF	50.94	FBF
4670	C43 H75 O13 P	22.213	830.4950	FBF	52.32	FBF
4671 4672	C45 H77 O13 P C47 H85 O16 P	4.854 15.146	856.5130 936.5593	<u>FBF</u> FBF	65.09 52.04	FBF FBF
4673	C47 H75 O13 P	4.854	878.4957	FBF	71.74	FBF
4674	C49 H85 O15 P	4.984	944.5648	FBF	59.41	FBF
4675	C51 H85 O13 P	14.341	936.5757	FBF	50.19	FBF
4676	C24 H51 O12 P	5.218	562.3124	FBF	61.84	FBF
4677	C22 H35 O14 P	6.127	554.1778	FBF	54.54	FBF
4678 4679	C27 H51 O13 P C35 H61 O16 P	3.943 4.437	614.3111 768.3721	FBF FBF	54.24 66.02	FBF FBF
4680	C43 H73 O15 P	4.854	860.4657	FBF	69.49	FBF
4681	C28 H51 O14 P	21.616	642.2987	FBF	53.60	FBF
4682	C30 H51 O15 P	3.917	682.2988	FBF	83.10	FBF
4683	C45 H77 O16 P	4.906	904.4912	FBF	67.56	FBF
4684	C32 H55 O16 P	4.099	726.3244	FBF	65.30	FBF
4685	C39 H71 O16 P	4.750	826.4547	FBF	58.08	FBF
4686	C47 H85 O17 P	13.665	952.5539	FBF ERF	55.59 65.38	FBF ERE
<u>4687</u> 4688	C34 H53 O16 P C38 H59 O16 P	4.099 13.509	748.3063 802.3539	FBF FBF	65.38 50.79	FBF FBF
4689	C47 H73 O16 P	22.733	924.4659	FBF	50.49	FBF
4690	C35 H53 O16 P	12.235	760.3068	FBF	59.74	FBF
4691	C36 H53 O15 P	13.743	756.3124	FBF	63.23	FBF
4692	C42 H73 O15 P	13.353	848.4684	FBF	51.20	FBF
4693	C49 H89 O17 P	14.419	980.5829	FBF	53.44	FBF
4694	C38 H71 O15 P	4.697	798.4568	FBF	56.79	FBF
<u>4695</u> 4696	C41 H69 O14 P C41 H69 O16 P	4.750 4.750	816.4401 848.4366	<u>FBF</u> FBF	71.89 71.90	FBF FBF
4697	C41 H69 O16 P C37 H61 O14 P	4.750	760.3853	FBF	61.77	FBF
4698	C41 H67 O15 P	7.920	830.4148	FBF	72.63	FBF
4699	C51 H81 O15 P	4.984	964.5400	FBF	56.43	FBF
4700	C41 H65 O15 P	7.920	828.4068	FBF	94.20	FBF
4701	C33 H53 O15 P	7.920	720.3159	FBF	62.56	FBF
4702	C37 H57 O14 P	13.275	756.3482	FBF	62.49	FBF
4703	C37 H57 O15 P	7.244	772.3449	FBF	94.47	FBF
4704	C43 H79 O16 P	5.218	882.5026	FBF	58.72	FBF
4705 4706	C44 H79 O15 P C51 H89 O16 P	17.693 5.062	878.5177 988.5906	FBF FBF	60.91 69.50	FBF FBF
4707	C51 H89 O16 P	12.443	1000.6209	FBF	76.75	FBF
4708	C40 H75 O14 P	4.750	810.4821	FBF	64.73	FBF
			P			Generated at 2:10 PM on 7/5/20



Cpd Name	Formula	RT	Mass	CAS I	D Source	Score	Score (Lib)	Score (DB)	Score (MFG) Algorithm
4709	C40 H75 O15 P	13.327	826.4879		BF	50.21	Score (LID)	JUNE (DD)	FBF
4710	C53 H89 O15 P	13.925	996.5959	F	BF	56.02			FBF
1711	C53 H87 O14 P	14.575	978.5795		BF	57.08			FBF
1712	C44 H71 O15 P	13.327	870.4538		BF	60.59			FBF
4713 4714	C40 H59 O15 P	13.795	810.3590		BF	61.27			FBF
4714 4715	C42 H63 O16 P C39 H57 O15 P	12.157 13.691	854.3858 796.3467		BF BF	54.21 54.86			FBF FBF
4716	C40 H57 O15 P	12.859	808.3463		BF	59.08			FBF
4717	C39 H75 O13 P	19.070	782.4940		BF	72.25	,	,	FBF
4718	C41 H79 O13 P	13.353	810.5261	F	BF	70.56			FBF
4719	C46 H89 O13 P	13.353	880.6049	F	BF	52.74	,	,	FBF
4720	C50 H97 O13 P	18.109	936.6699		BF	59.85			FBF
4721	C57 H111 O13 P	20.343	1034.7717		BF	77.12			FBF
4722	C42 H69 O13 P	13.795	812.4511		BF	54.51			FBF
<u>4723</u> 4724	C59 H115 O13 P C55 H105 O13 P	17.927 17.537	1062.8032 1004.7272		BF BF	57.85 52.19			FBF FBF
4725	C58 H111 O13 P	17.927	1046.7780		BF	71.36			FBF
4726	C59 H113 O13 P	14.809	1060.7974		BF	59.29			FBF
4727	C62 H119 O13 P	22.499	1102.8372		BF	58.37			FBF
4728	C50 H89 O13 P	5.763	928.6038	F	BF	67.66			FBF
4729	C55 H103 O13 P	13.977	1002.7161		BF	60.64			FBF
1730	C57 H107 O13 P	20.915	1030.7406		BF	56.21			FBF
4731	C60 H113 O13 P	21.226	1072.7821		BF	57.78			FBF
4732	C64 H121 O13 P	18.057	1128.8548		BF	53.40			FBF
4733 173 <i>4</i>	C66 H125 O13 P	14.912	1156.8813		BF	56.35 50.21			FBF
4734 4735	C55 H99 O13 P C60 H109 O13 P	14.835 17.927	998.6775 1068.7605		BF BF	50.21 66.96			FBF FBF
1 736	C61 H111 O13 P	14.809	1082.7789		BF	72.43			FBF
4737	C50 H83 O13 P	21.876	922.5495		BF	59.60			FBF
4738	C51 H79 O13 P	13.379	930.5224		BF	53.54			FBF
4739	C68 H127 O13 P	17.797	1182.8998		BF	54.56			FBF
4740	C68 H125 O13 P	21.460	1180.8877		BF	70.22			FBF
4741	C62 H111 O13 P	20.213	1094.7851		BF	53.79			FBF
4742	C20 H37 O13 P	8.492	516.2008		BF	73.71			FBF
4743	C69 H135 O13 P	20.136	1202.9541		BF	50.24			FBF
4744	C52 H87 O13 P	14.003	950.5908		BF	52.49			FBF
4745 4746	C70 H137 O13 P C70 H133 O13 P	19.668 17.355	1216.9846 1212.9384		BF BF	50.99 50.01			FBF FBF
4747	C57 H99 O13 P	14.912	1022.6856		BF	52.11	,		FBF
4748	C70 H129 O13 P	17.719	1208.9227		BF	55.66			FBF
4749	C55 H87 O13 P	5.062	986.5841		BF	84.21			FBF
4750	C56 H97 O13 P	18.966	1008.6715		BF	50.45			FBF
4751	C57 H95 O13 P	14.419	1018.6512	F	BF	52.98			FBF
4752	C57 H85 O13 P	5.062	1008.5673		BF	76.40			FBF
4753	C60 H105 O13 P	13.379	1064.7342		BF	54.70			FBF
4754	C63 H111 O13 P	18.395	1106.7847		BF	56.61			FBF
4755	C67 H119 O13 P	22.810 20.032	1162.8431		BF BF	50.10		,	FBF FBF
<u>4756 </u>	C68 H121 O13 P C77 H151 O13 P	20.032	1176.8432 1315.0870		BF	79.28 50.22			FBF
4758	C41 H59 O13 P	7.192	790.3735		BF	52.35			FBF
4759	C45 H67 O13 P	7.920	846.4328		BF	74.54			FBF
4760	C59 H91 O13 P	16.030	1038.6216		BF	56.38			FBF
4761	C59 H101 O13 P	17.303	1048.6890	F	BF	54.26			FBF
4762	C59 H99 O13 P	14.964	1046.6854	F	BF	50.23			FBF
4763	C61 H99 O13 P	5.166	1070.6846		BF	65.39			FBF
4764	C24 H50 O21 P4	15.380	798.1751		BF	58.66		,	FBF
4765	C25 H52 O21 P4	13.665	812.1969		BF	64.35			FBF
4766 4767	C26 H50 O21 P4	14.601	822.1877		BF	63.66			FBF
4767 4768	C29 H54 O21 P4 C31 H52 O21 P4	14.653 13.197	862.2144 884.1975		BF BF	67.96 55.84			FBF FBF
4769	C27 H54 O22 P4	15.197	854.2087		BF	55.71			FBF
1 770	C37 H60 O22 P4	17.329	980.2556		BF	57.83			FBF
4771	C26 H42 N O11 P	5.945	575.2473		BF	58.64			FBF
1772	C27 H52 N O11 P	10.623	597.3252		BF	51.92			FBF
1773	C28 H46 N O11 P	20.291	603.2833	F	BF	64.12			FBF
1774	C30 H58 N O11 P	5.607	639.3695		BF	64.81			FBF
4775	C32 H62 N O11 P	19.070	667.4025		BF	67.41			FBF
1776	C33 H64 N O11 P	6.283	681.4211		BF	62.73			FBF
4777 4770	C36 H70 N O11 P	5.529	723.4701		BF	80.26			FBF
<u>4778 </u>	C37 H72 N O11 P C38 H74 N O11 P	13.379 0.383	737.4827 751.5032		BF BF	57.18 59.21	-		FBF FBF
4780	C38 H56 N O10 P	4.411	717.3606		BF	76.40		,	FBF
1781	C39 H76 N O11 P	10.051	765.5219		BF	62.46			FBF
4782	C40 H60 N O11 P	4.541	761.3869		BF	78.47			FBF
4783	C42 H62 N O10 P	4.671	771.4115		BF	91.57			FBF
4784	C42 H64 N O10 P	18.654	773.4268	F	BF	57.73			FBF
4785	C44 H86 N O11 P	21.045	835.5937		BF	60.35			FBF
4786	C44 H66 N O11 P	4.750	815.4375		BF	94.48			FBF
1787	C45 H88 N O11 P	16.082	849.6094		BF	54.94			FBF
4788	C45 H68 N O11 P	4.776	829.4572		BF	54.37			FBF
4789	C46 H70 N O11 P	16.212	843.4725		BF	57.13			FBF
4790 4701	C47 H92 N O10 P	13.691	861.6421		BF	55.17			FBF
4791 4702	C49 H76 N O11 P	11.793	885.5181		BF	56.80		,	FBF
1792 1 793	C49 H92 N O11 P C49 H90 N O11 P	14.835 18.187	901.6381 899.6235		BF BF	57.51 52.47			FBF FBF
		וא ואו	044 D/35						



ompound Sumn Opd Name	Formula	RT	Mass	CAS ID Source	ce Score	Score (Lib)	Score (DB)	Score (MFG) Algorith
795	C49 H82 N O11 P	14.835	891.5648	FBF	54.12	Score (LID)	(DD)	FBF
796	C51 H100 N O10 P	14.990	917.7095	FBF	57.96			FBF
797	C51 H78 N O11 P	14.938	911.5309	FBF	62.62			FBF
798	C51 H84 N O11 P	19.902	917.5744	FBF	54.52			FBF
799	C51 H82 N O11 P	4.906	915.5602	FBF	86.22			FBF
800 801	C52 H78 N O10 P C52 H100 N O11 P	10.675 13.327	907.5367 945.7020	FBF FBF	59.14 70.76			FBF FBF
802	C52 H92 N O11 P	13.405	937.6428	FBF	82.17			FBF
803	C53 H84 N O10 P	14.445	925.5821	FBF	59.77			FBF
804	C53 H80 N O11 P	14.315	937.5499	FBF	50.85			FBF
805	C53 H98 N O11 P	14.809	955.6887	FBF	50.41			FBF
806	C53 H88 N O11 P	16.498	945.6046	FBF	62.03			FBF
807	C54 H86 N O10 P	14.912	939.5963	FBF	52.68			FBF
808	C54 H90 N O10 P	21.694	943.6270	FBF	51.70			FBF
809	C55 H108 N O11 P	19.798	989.7596	FBF	50.54			FBF
810 811	C55 H106 N O10 P C55 H88 N O11 P	19.798 15.250	971.7558 969.6115	FBF FBF	54.26 50.41			FBF FBF
812	C55 H104 N O11 P	18.395	985.7335	FBF	60.30			FBF
813	C55 H100 N O10 P	19.408	965.7134	FBF	68.86			FBF
814	C55 H96 N O11 P	22.681	977.6700	FBF	60.27			FBF
315	C55 H92 N O10 P	17.173	957.6519	FBF	52.53			FBF
816	C55 H92 N O11 P	16.446	973.6390	FBF	64.22			FBF
317	C56 H110 N O10 P	13.977	987.7831	FBF	55.15			FBF
818	C56 H98 N O10 P	21.460	975.6980	FBF	50.42			FBF
319	C56 H98 N O11 P	18.472	991.6873	FBF	51.88			FBF
320	C57 H110 N O11 P	19.642	1015.7811	FBF	52.82			FBF
321	C57 H108 N O10 P	14.159	997.7746	FBF	57.36			FBF
822	C58 H90 N O10 P	18.940	991.6361	FBF	51.47			FBF
823 824	C58 H110 N O10 P C58 H100 N O10 P	19.876 18.966	1011.7924 1001.7038	FBF FBF	54.86 67.19			FBF FBF
824 825	C58 H100 N O10 P	18.966	1001.7038	FBF FBF	52.16			FBF
826	C58 H98 N O11 P	20.811	1015.6879	FBF	50.88			FBF
827	C58 H96 N O11 P	19.928	1013.6770	FBF	53.65			FBF
828	C59 H116 N O11 P	19.226	1045.8267	FBF	54.27			FBF
829	C59 H96 N O10 P	16.108	1009.6808	FBF	51.76			FBF
830	C59 H92 N O10 P	14.653	1005.6524	FBF	50.13			FBF
831	C59 H112 N O10 P	19.564	1025.8091	FBF	57.35			FBF
332	C60 H114 N O10 P	17.927	1039.8198	FBF	78.35			FBF
333	C60 H112 N O11 P	18.472	1053.8009	FBF	52.16			FBF
834	C60 H108 N O10 P	20.317	1033.7679	FBF	68.54			FBF
835	C60 H108 N O11 P	20.317	1049.7646	FBF	59.80			FBF
836 837	C60 H102 N O10 P C61 H120 N O11 P	22.395 19.252	1027.7238 1073.8630	FBF FBF	61.04 58.62			FBF FBF
838	C61 H120 N O11 P	15.744	1053.7038	FBF	51.10			FBF
839	C61 H108 N O10 P	17.927	1045.7763	FBF	53.88			FBF
840	C62 H122 N O10 P	21.928	1071.8795	FBF	74.16			FBF
841	C62 H102 N O10 P	21.850	1051.7272	FBF	67.53			FBF
842	C62 H116 N O10 P	14.497	1065.8332	FBF	51.11			FBF
843	C62 H116 N O11 P	20.967	1081.8229	FBF	54.17			FBF
844	C62 H112 N O10 P	17.927	1061.8024	FBF	78.67			FBF
845	C62 H112 N O11 P	18.135	1077.7978	FBF	84.70			FBF
846	C63 H124 N O11 P	21.772	1101.8913	FBF	52.59			FBF
847 848	C63 H102 N O10 P	13.379	1063.7250 1097.8568	FBF FBF	51.59			FBF FBF
849	C63 H120 N O11 P C63 H118 N O10 P	21.019 19.330	1079.8590	FBF	52.65 53.96			FBF
850	C63 H110 N O10 P	22.343	1071.7913	FBF	58.05			FBF
851	C63 H106 N O10 P	17.927	1067.7587	FBF	59.73			FBF
852	C63 H106 N O11 P	17.927	1083.7563	FBF	51.10			FBF
853	C64 H120 N O10 P	18.680	1093.8737	FBF	50.37			FBF
854	C64 H110 N O10 P	17.927	1083.7849	FBF	74.15			FBF
355	C64 H110 N O11 P	18.135	1099.7797	FBF	80.16			FBF
356	C65 H120 N O11 P	18.836	1121.8564	FBF	51.47			FBF
357	C65 H116 N O10 P	16.654	1101.8397	FBF	51.41			FBF
358	C66 H108 N O10 P	14.860	1105.7742	FBF	53.37			FBF
859	C66 H106 N O11 P	14.886	1119.7564	FBF	56.19			FBF
860 861	C66 H118 N O10 P C66 H116 N O11 P	18.706	1115.8446	FBF FBF	50.25			FBF FBF
862	C67 H132 N O11 P	18.706 11.065	1129.8193 1157.9534	FBF	53.30 56.84			FBF
363	C67 H112 N O10 P	17.745	1121.8078	FBF	59.54			FBF
364	C67 H124 N O10 P	19.070	1133.8951	FBF	58.47			FBF
365	C67 H122 N O11 P	18.758	1147.8758	FBF	51.12			FBF
866	C67 H120 N O11 P	18.940	1145.8630	FBF	57.43			FBF
367	C68 H114 N O11 P	22.239	1151.8108	FBF	53.55			FBF
868	C68 H124 N O11 P	18.758	1161.8884	FBF	54.83			FBF
869	C68 H122 N O10 P	19.148	1143.8796	FBF	50.38			FBF
870	C69 H124 N O10 P	16.862	1157.8881	FBF	55.97			FBF
871	C69 H122 N O11 P	19.824	1171.8717	FBF	65.88			FBF
372	C69 H120 N O10 P	17.771	1153.8656	FBF	55.54			FBF
873	C69 H120 N O11 P	17.823	1169.8611	FBF	51.73			FBF
874 075	C69 H118 N O11 P	20.863	1167.8442	FBF	50.69			FBF
875 876	C70 H116 N O11 P	17.875	1177.8241	FBF	60.62			FBF
	C70 H114 N O11 P C70 H136 N O11 P	17.875 17.771	1175.8178 1197.9849	FBF FBF	82.78 50.73			<u>FBF</u> FBF
877 878	C71 H136 N O11 P	20.110	1197.9849	FBF	50.73			FBF
								FBF
879 880	C71 H120 N O11 P C71 H136 N O11 P	19.980 20.187	1193.8511 1209.9852	FBF FBF	50.44 50.08			
	C/1 H136 N O11 P	20.18/	1209.9852	FBF	50.08			FBF



Compound Sur	mmary Formula	RT	Mass	CAS ID Source	£	Score (Lib) Score (DB)	Score (MFG) Algorith
4881	C72 H140 N O10 P	19.798	1210.0237	FBF	Score 56.78	Score (LIB) Score (DB)	Score (MFG) Algoriti
1882	C73 H144 N O10 P	20.655	1226.0586	FBF	54.63		FBF
4883	C73 H144 N O11 P	22.057	1242.0520	FBF	58.11		FBF
1884	C73 H122 N O10 P	19.044	1203.8846	FBF	50.31		FBF
4885 4006	C73 H120 N O10 P	17.745	1201.8578	FBF	67.02		FBF
1886 1887	C73 H142 N O11 P C73 H140 N O10 P	13.951 19.616	1240.0233 1222.0300	FBF FBF	55.99 50.98		FBF FBF
1888	C73 H140 N O10 P	13.093	1238.0192	FBF	54.61		FBF
1889	C74 H144 N O11 P	21.902	1254.0482	FBF	52.54		FBF
4890	C74 H142 N O11 P	19.486	1252.0283	FBF	50.48		FBF
4891	C74 H138 N O11 P	18.135	1248.0051	FBF	58.34		FBF
4892	C74 H136 N O10 P	20.421	1229.9806	FBF	51.43		FBF
4893	C18 H34 N O9 P	7.920	439.1970	FBF	58.60		FBF
1894 1895	C20 H40 N O9 P C23 H40 N O10 P	4.151 10.077	469.2408 521.2441	FBF FBF	79.99 66.89		FBF FBF
1 896	C24 H42 N O9 P	7.894	519.2579	FBF	50.32		FBF
1897	C20 H42 N O8 P	5.451	455.2651	FBF	50.55		FBF
1898	C22 H46 N O8 P	4.047	483.2921	FBF	73.29		FBF
1899	C24 H50 N O8 P	3.839	511.3271	FBF	78.45		FBF
1900	C26 H54 N O8 P	4.541	539.3565	FBF	68.78		FBF
901	C34 H64 N O12 P	4.880	709.4144	FBF	83.30		FBF
902	C34 H62 N O12 P	5.296	707.4017	FBF	58.98		FBF
1903	C42 H78 N O13 P	19.824	835.5177	FBF	62.37		FBF
904	C29 H54 N O12 P	4.281	639.3333	FBF	72.37		FBF
905 906	C30 H56 N O12 P C36 H68 N O12 P	4.281 5.010	653.3549 737.4437	FBF FBF	65.19 57.92		FBF FBF
907	C36 H66 N O12 P	5.503	735.4369	FBF	68.57		FBF
1908	C31 H56 N O12 P	15.146	665.3568	FBF	71.34		FBF
1909	C32 H60 N O12 P	4.724	681.3895	FBF	76.12		FBF
910	C46 H86 N O13 P	19.096	891.5786	FBF	75.76		FBF
911	C33 H62 N O12 P	18.109	695.4058	FBF	69.46		FBF
912	C56 H86 N O9 P	14.809	947.6039	FBF	52.07		FBF
913	C32 H54 N O12 P	13.249	675.3383	FBF	68.56		FBF
914	C36 H64 N O12 P	15.198	733.4142	FBF	66.07		FBF
915	C37 H64 N O12 P	4.541 13.379	745.4156 761.4520	FBF FBF	77.23 52.10		FBF FBF
916 917	C38 H68 N O12 P C44 H72 N O12 P	4.854	837.4818	FBF	70.29		FBF
918	C19 H32 N O11 P	3.293	481.1717	FBF	93.59		FBF
919	C24 H44 N O11 P	7.920	553.2655	FBF	66.60		FBF
920	C31 H54 N O13 P	12.677	679.3321	FBF	60.65		FBF
1921	C40 H72 N O12 P	5.581	789.4810	FBF	64.66		FBF
1922	C40 H66 N O12 P	4.671	783.4311	FBF	88.07		FBF
1923	C24 H44 N O12 P	3.917	569.2559	FBF	71.75		FBF
1924	C27 H48 N O13 P	4.593	625.2900	FBF	55.75		FBF
1925	C27 H46 N O13 P	2.201	623.2695	FBF	51.88		FBF
1926	C28 H50 N O13 P	12.651	639.3055	FBF	62.50		FBF
1927	C32 H46 N O13 P	13.301 12.651	691.3324 619.2712	FBF FBF	55.27 71.92		FBF FBF
1928 1929	C28 H46 N O12 P C30 H52 N O13 P	21.460	665.3205	FBF	64.06		FBF
1930	C34 H58 N O13 P	4.437	719.3635	FBF	80.44		FBF
931	C42 H70 N O13 P	4.750	827.4565	FBF	85.12		FBF
1932	C35 H62 N O13 P	17.173	735.3938	FBF	84.65		FBF
1933	C42 H80 N O12 P	10.831	821.5367	FBF	52.78		FBF
1934	C44 H80 N O14 P	12.859	877.5276	FBF	60.50		FBF
935	C31 H56 N O13 P	12.651	681.3556	FBF	64.92		FBF
936	C35 H56 N O13 P	21.330	729.3476	FBF	78.25		FBF
1937	C36 H58 N O13 P	4.541	743.3588	FBF	59.80		FBF
938	C44 H74 N O14 P	4.854	871.4827	FBF	86.78		FBF
939 940	C36 H56 N O13 P C44 H68 N O13 P	22.239 4.750	741.3488 849.4384	FBF FBF	68.32 72.44		FBF FBF
941	C44 H68 N O13 P C46 H70 N O12 P	4.750	859.4628	FBF	93.98		FBF
942	C32 H48 N O13 P	10.181	685.2835	FBF	52.69		FBF
943	C37 H66 N O13 P	15.744	763.4297	FBF	86.76	· · · · · · · · · · · · · · · · · · ·	FBF
944	C38 H70 N O13 P	5.555	779.4609	FBF	71.28		FBF
945	C46 H84 N O14 P	14.886	905.5679	FBF	79.51		FBF
946	C33 H60 N O13 P	4.828	709.3839	FBF	56.23		FBF
947	C35 H66 N O12 P	4.906	723.4261	FBF	81.37		FBF
948	C38 H64 N O12 P	22.291	757.4218	FBF	55.67		FBF
949	C38 H64 N O13 P	4.671	773.4164	FBF	53.60		FBF
950 951	C35 H56 N O12 P C37 H60 N O13 P	4.489 4.619	713.3540 757.3825	<u>FBF</u> FBF	59.25 83.70		FBF FBF
952	C34 H54 N O12 P	4.437	699.3326	FBF	57.90		FBF
953	C34 H52 N O13 P	13.379	713.3228	FBF	52.19		FBF
954	C38 H58 N O12 P	17.225	751.3711	FBF	58.07		FBF
955	C33 H48 N O11 P	16.030	665.2926	FBF	56.54		FBF
956	C34 H50 N O12 P	18.420	695.3076	FBF	85.01		FBF
1957	C39 H70 N O13 P	19.304	791.4557	FBF	67.10		FBF
958	C41 H72 N O12 P	5.607	801.4750	FBF	66.44		FBF
1959	C48 H88 N O13 P	14.912	917.6015	FBF	56.80		FBF
960	C39 H68 N O13 P	4.671	789.4410	FBF	75.03		FBF
961	C41 H70 N O12 P	5.555	799.4624	FBF	50.40		FBF
962	C41 H66 N O12 P	17.563	795.4309	FBF	50.30		FBF
1963 1964	C48 H74 N O13 P	4.906 14.497	903.4879 723.3396	FBF FBF	78.59 63.85	· · · · · · · · · · · · · · · · · · ·	FBF FBF
96 4 965	C36 H54 N O12 P C36 H54 N O13 P	14.497	723.3396	FBF	57.46		FBF
	CAD FIRMULA P	13 3/9		FDF			



Compound Summary							
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorithm
4967	C19 H36 N O10 P	7.244 14.575	469.2089 847.3471	<u>FBF</u> FBF	75.14 58.92		FBF FBF
<u>4968</u> 4969	C49 H54 N O10 P C53 H78 N O10 P	14.601	919.5308	FBF	58.02		FBF
4970	C37 H68 O11 P2	5.010	750.4223	FBF	87.29	-	FBF
4971	C37 H58 O11 P2	3.371	740.3456	FBF	65.69		FBF
4972	C39 H74 O11 P2	14.938	780.4701	FBF	52.71		FBF
4973	C39 H66 O11 P2	4.984	772.4026	FBF	56.96		FBF
<u>4974</u> 4975	C39 H62 O11 P2 C43 H84 O11 P2	13.275 14.185	768.3795 838.5495	FBF FBF	53.91 56.22	· · · · · · · · · · · · · · · · · · ·	FBF FBF
4976	C43 H76 O11 P2	11.715	830.4866	FBF	57.41		FBF
4977	C45 H70 O11 P2	4.750	848.4366	FBF	77.89	-	FBF
4978	C45 H84 O11 P2	15.068	862.5481	FBF	56.72		FBF
4979	C18 H33 O7 P	4.567	392.1993	FBF	54.19		FBF
4980	C22 H39 O7 P	5.815	446.2414	FBF	58.14		FBF
4981	C22 H37 O7 P	3.839	444.2295	FBF	58.42		FBF
<u>4982</u> 4983	C24 H39 O7 P C26 H45 O7 P	17.537 5.114	470.2450 500.2932	<u>FBF</u> FBF	70.70 62.96		FBF FBF
4984	C30 H49 O7 P	5.218	552.3232	FBF	61.79		FBF
4985	C31 H55 O7 P	4.489	570.3675	FBF	82.42		FBF
4986	C32 H59 O7 P	4.125	586.3989	FBF	79.43		FBF
4987	C32 H51 O7 P	5.919	578.3387	FBF	66.48		FBF
4988	C33 H59 O7 P	18.836	598.3986	FBF	66.34		FBF
4989	C33 H53 O7 P	4.359	592.3542	FBF	57.09		FBF
4990	C34 H57 O7 P C35 H57 O7 P	4.125 5.296	608.3808 620.3858	FBF FBF	62.69 76.48		FBF
<u>4991</u> 4992	C38 H67 O7 P	19.954	666.4603	FBF	54.37		FBF FBF
4993	C38 H65 O7 P	5.400	664.4433	FBF	71.01		FBF
4994	C15 H25 O7 P	2.643	348.1325	FBF	55.02		FBF
4995	C18 H29 O7 P	2.617	388.1636	FBF	51.78		FBF
4996	C22 H35 O7 P	22.836	442.2140	FBF	62.03		FBF
4997	C26 H39 O9 P	3.735	526.2320	FBF	66.48		FBF
<u>4998</u> 4999	C32 H49 O8 P C34 H51 O9 P	5.244 8.960	592.3160 634.3236	<u>FBF</u> FBF	65.90 63.14		FBF FBF
5000	C37 H57 O8 P	12.651	660.3765	FBF	68.35		FBF
5001	C38 H61 O8 P	4.958	676.4078	FBF	56.35		FBF
5002	C39 H59 O8 P	19.304	686.3978	FBF	66.93		FBF
5003	C39 H59 O9 P	4.437	702.3910	FBF	68.52		FBF
5004	C40 H61 O8 P	20.006	700.4061	FBF	53.03		FBF
5005	C42 H65 O8 P	5.867	728.4365	FBF	51.43		FBF
<u>5006</u> 5007	C46 H69 O8 P C46 H75 O9 P	10.441 11.299	780.4762 802.5152	<u>FBF</u> FBF	53.85 73.07		FBF FBF
5008	C48 H73 O9 P	12.287	824.5010	FBF	89.07		FBF
5009	C48 H71 O9 P	14.419	822.4839	FBF	59.74	-	FBF
5010	C49 H93 O9 P	19.434	856.6535	FBF	54.81		FBF
5011	C49 H91 O9 P	13.925	854.6462	FBF	59.48		FBF
5012	C49 H79 O9 P	19.928	842.5453	FBF	64.07		FBF
5013	C50 H75 O9 P	0.409	850.5181	FBF	60.55		FBF
5014 5015	C51 H83 O9 P C52 H83 O8 P	12.625 20.213	870.5771 866.5834	FBF FBF	56.70 52.56		FBF FBF
5016	C52 H79 O8 P	13.977	862.5512	FBF	64.26	-	FBF
5017	C53 H83 O9 P	4.906	894.5806	FBF	64.27		FBF
5018	C55 H85 O9 P	17.407	920.5898	FBF	53.92		FBF
5019	C56 H89 O8 P	22.005	920.6361	FBF	60.69		FBF
5020	C56 H93 O9 P	16.498	940.6512	FBF	53.97		FBF
5021	C57 H89 O9 P	20.499	948.6181	FBF	<u>59.56</u>		FBF
5022 5023	C57 H109 O9 P C57 H97 O8 P	14.783 18.732	968.7843 940.6923	FBF FBF	55.28 50.66		FBF FBF
5024	C57 H95 O8 P	14.809	938.6812	FBF	52.54		FBF
5025	C58 H99 O9 P	19.954	970.6953	FBF	50.58		FBF
5026	C58 H97 O9 P	16.446	968.6886	FBF	70.91		FBF
5027	C59 H111 O9 P	14.003	994.7998	FBF	51.64		FBF
5028	C59 H109 O9 P	14.860	992.7895	FBF	63.44		FBF
5029	C59 H103 O8 P	21.045	970.7396	FBF	55.12 56.27		FBF
5030 5031	C60 H99 O9 P C60 H95 O9 P	14.912 16.472	994.7100 990.6669	<u>FBF</u> FBF	56.27 58.20		FBF FBF
5032	C61 H99 O9 P	18.135	1006.7037	FBF	57.40		FBF
5033	C61 H105 O8 P	18.213	996.7557	FBF	56.29		FBF
5034	C62 H103 O9 P	20.032	1022.7382	FBF	54.91		FBF
5035	C62 H101 O8 P	20.993	1004.7207	FBF	56.58		FBF
5036	C62 H99 O8 P	17.122	1002.7066	FBF	55.81	.	FBF
5037 5038	C62 H119 O9 P C62 H107 O9 P	21.097 22.525	1038.8545 1026.7712	<u>FBF</u> FBF	57.60 65.77		FBF FBF
5039	C62 H107 O9 P C63 H113 O9 P	22.525 17.901	1026.7712	FBF	53.17		FBF FBF
5040	C64 H107 O8 P	20.343	1034.7738	FBF	74.02		FBF
5041	C64 H123 O9 P	21.824	1066.8871	FBF	51.37		FBF
5042	C64 H113 O8 P	17.927	1040.8207	FBF	60.88		FBF
5043	C64 H113 O9 P	19.590	1056.8169	FBF	53.28		FBF
5044	C64 H111 O9 P	14.809	1054.7897	FBF	50.42		FBF
5045	C65 H115 O8 P	18.862	1054.8340	FBF	57.89		FBF
5046	C65 H111 O9 P	14.990	1070.8187	FBF	57.23		FBF
5047 5048	C66 H111 O8 P	17.927	1062.8031	FBF ERF	67.94		FBF
5048 5049	C66 H111 O9 P C66 H121 O8 P	18.109 21.512	1078.7989 1072.8875	<u>FBF</u> FBF	62.77 70.09		FBF FBF
5050	C67 H117 O8 P	18.576	1080.8449	FBF	50.55		FBF
051	C68 H111 O8 P	21.928	1086.7984	FBF	57.39		FBF
5052	C68 H123 O8 P	18.550	1098.8991	FBF	50.61		FBF



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Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB) Score (MFG) Algor
5053	C68 H119 O9 P	20.655	1110.8668	FBF	58.05	FBF
5054 5055	C69 H135 O9 P C69 H131 O9 P	18.836 11.065	1138.9815 1134.9436	FBF FBF	56.58 50.85	FBF FBF
5056	C69 H123 O9 P	19.824	1126.8912	FBF	52.74	FBF
5057	C69 H119 O9 P	18.680	1122.8602	FBF	51.52	FBF
058	C70 H117 O9 P	21.304	1132.8402	FBF	50.34	FBF
5059	C70 H133 O8 P	20.915	1132.9780	FBF	52.52	FBF
5060	C71 H137 O9 P	22.161	1164.9983	FBF	53.02	FBF
5061	C71 H129 O9 P	21.382	1156.9374	FBF	52.89	FBF
5062	C72 H123 O8 P	21.278	1146.8969	FBF	58.24	FBF
5063 5064	C72 H121 O8 P C72 H137 O9 P	18.161 19.980	1144.8828 1176.9912	FBF FBF	71.19 51.82	FBF FBF
5065	C72 H137 O9 P	22.005	1164.9086	FBF	53.16	FBF
5066	C73 H145 O9 P	19.356	1197.0595	FBF	50.17	FBF
5067	C73 H123 O8 P	19.512	1158.8955	FBF	50.24	FBF
5068	C73 H121 O8 P	21.928	1156.8753	FBF	50.55	FBF
069	C73 H121 O9 P	17.875	1172.8700	FBF	56.00	FBF
5070	C73 H131 O8 P	18.914	1166.9520	FBF	57.93	FBF
071	C73 H131 O9 P	20.006	1182.9485	FBF	76.74	
072	C46 H67 O8 P	13.769	778.4593	FBF	60.03	FBF
073	C46 H67 O9 P	5.088	794.4487	FBF	74.22	FBF
074 075	C21 H18 O7 C24 H30 O6	11.351 7.920	382.1071 414.2045	<u>FBF</u> FBF	61.43 99.60	FBF FBF
076	C20 H26 O7	5.607	378.1699	FBF	55.98	FBF
077	C22 H24 O7	6.153	400.1547	FBF	64.78	FBF
078	C22 H26 O6	7.244	386.1725	FBF	99.42	FBF
079	C22 H29 N10 O8 P	18.472	592.1909	FBF	76.00	FBF
080	C21 H29 N8 O9 P	6.153	568.1767	FBF	75.05	FBF
081	C21 H28 N7 O10 P	6.283	569.1682	FBF	55.12	FBF
082	C21 H28 N7 O11 P	6.153	585.1598	FBF	55.90	FBF
083	C8 H14 N3 O7 P	4.984	295.0563	FBF	93.92	FBF
084	C10 H14 N2 O6	6.413	258.0865	FBF	54.14	FBF FBF
085 086	C9 H14 N4 O6 C7 H9 N5	9.844 17.044	274.0917 163.0869	FBF FBF	64.83 62.52	FBF FBF
087	C12 H11 N5	9.194	225.1002	FBF	61.91	FBF
)88	C10 H9 N5 O	6.777	215.0810	FBF	73.62	FBF
89	C10 H13 N5	3.085	203.1156	FBF	62.40	FBF
90	C10 H13 N5 O	8.284	219.1108	FBF	71.53	FBF
91	C5 H5 N5	22.473	135.0545	FBF	99.20	FBF
092	C9 H14 N5 O4 P	2.279	287.0801	FBF	75.96	FBF
)93	C6 H7 N5 O	10.571	165.0656	FBF	74.34	FBF
094	C6 H7 N5 O2	2.721	181.0602	FBF	83.28	FBF
095	C5 H5 N5 O2	2.201	167.0450	FBF	74.60	FBF
)96)97	C5 H4 N4 O C10 H15 N5 O	19.746 6.647	136.0376 221.1263	FBF FBF	84.72 63.80	FBF FBF
098	C16 H25 N5 O6	13.327	383.1794	FBF	80.33	FBF
099	C12 H13 N5 O3	8.310	275.1027	FBF	82.42	FBF
100	C13 H18 N6 O3	6.777	306.1433	FBF	80.96	FBF
101	C13 H17 N5 O4	5.815	307.1276	FBF	82.86	FBF
102	C5 H4 N4	1.318	120.0436	FBF	98.88	FBF
103	C8 H12 N4 O5	6.179	244.0813	FBF	54.13	FBF
104	C15 H23 N6 O5 S	11.377	399.1416	FBF	52.43	FBF
105	C10 H13 N5 O2	5.529	235.1067	FBF	69.27	FBF
106	C10 H13 N5 O3	5.296	251.1022	FBF	79.68	FBF
107 108	C10 H12 N4 O3	1.422 5.763	236.0887 265.1168	<u>FBF</u> FBF	67.05	FBF FBF
109	C11 H15 N5 O3 C11 H16 N4 O4	1.889	268.1155	FBF	58.49 76.88	FBF
110	C10 H16 N5 O12 P3	5.426	491.0006	FBF	73.11	FBF
111	C12 H17 N5 O5	9.402	311.1206	FBF	65.73	FBF
.12	C11 H15 N5 O4	5.477	281.1097	FBF	52.51	FBF
113	C11 H15 N5 O5	8.986	297.1066	FBF	70.37	FBF
14	C10 H14 N6 O4	6.854	282.1099	FBF	76.96	FBF
.15	C10 H11 N5 O4	6.854	265.0832	FBF	76.96	FBF
16	C11 H15 N5 O3 S	8.258	297.0886	FBF FBF	89.35	FBF
117	C11 H15 N4 O6	7.426	299.1015	FBF	70.91	FBF FBF
l 18 l 19	C15 H21 N5 O5 C15 H24 N5 O17 P3	8.700 5.763	351.1520	FBF FBF	71.58 55.15	FBF FBF
120	C15 H24 N5 O17 P3 C10 H17 N5 O16 P4	5.763 6.153	639.0387 586.9610	FBF	55.15 59.89	FBF
121	C10 H17 N5 O10 P4	6.179	602.9581	FBF	50.04	FBF
122	C7 H8 N4 O3	6.751	196.0580	FBF	68.50	FBF
123	C6 H6 N4 O2	7.686	166.0499	FBF	59.98	FBF
24	C12 H12 N4 O3	1.474	260.0922	FBF	68.70	FBF
.25	C9 H12 N4 O3	3.553	224.0901	FBF	74.88	FBF
.26	C6 H9 N5 O2	1.967	183.0755	FBF	81.95	FBF
127	C13 H16 N4 O2	6.854	260.1289	FBF	81.24	FBF
128	C5 H7 N5 O	2.071	153.0654	FBF	94.85	FBF FBF
129	C9 H14 N2 O3	8.076	198.1008	FBF	77.17	FBF
130	C6 H10 N2 O2	0.409	142.0732	FBF	64.56	FBF
131 132	C12 H15 N2 O4 C7 H5 N5 O	5.919 2.357	251.1024 175.0502	<u>FBF</u> FBF	81.33 76.57	FBF FBF
133	C14 H13 N3	4.906	223.1087	FBF	69.77	FBF
134	C23 H27 F N4 O3	4.515	426.2105	FBF	54.55	FBF
135	C12 H13 N3	7.426	199.1092	FBF	74.85	FBF
136	C12 H13 Cl N4	0.409	248.0823	FBF	52.68	FBF
.37	C9 H13 N3 O4	17.251	227.0900	FBF	74.52	FBF
38	C18 H31 N3 O13 P2	6.127	559.1314	FBF	58.11	FBF



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Compound Sun		DT	N	CAS ID C	C C	(Lib) Come (DD) Come (MEC) Alexaithment
Cpd Name 5139	Formula C16 H24 N2 O17 P2	RT 6.309	Mass 578.0571	CAS ID Source FBF	Score Sco 52.02	ore (Lib) Score (DB) Score (MFG) Algorithm FBF
5140	C16 H26 N2 O16 P2	5.919	564.0767	FBF	56.91	FBF
5141	C11 H15 N3 O6	3.943	285.0955	FBF	77.84	FBF
5142	C9 H12 N2 O6	7.088	244.0713	FBF	68.64	FBF
5143	C14 H25 N3 O15 P2	5.867	537.0722	FBF	61.10	FBF
5144	C17 H25 N3 O18 P2	5.997	621.0582	FBF	50.36	FBF FBF
5145 5146	C9 H16 N3 O14 P3 C12 H18 N2 O3	5.555 6.854	482.9819 238.1295	FBF FBF	52.01 52.28	FBF
5147	C14 H30 O3	9.194	246.2183	FBF	86.26	FBF
5148	C15 H22 O4	6.257	266.1503	FBF	80.01	FBF
5149	C20 H30 N2 O4	4.541	362.2187	FBF	51.54	FBF
5150	C12 H18 N2 O4	0.435	254.1279	FBF	71.88	FBF
5151	C4 H7 N O2	0.435	101.0480	FBF	69.54	FBF
5152 5153	C5 H11 N O3 C6 H11 N O5	11.065 1.915	133.0728 177.0646	FBF FBF	54.16 81.36	FBF FBF
5154	C6 H9 N3 O2	2.305	155.0680	FBF	69.52	FBF
5155	C5 H9 N O5	1.318	163.0495	FBF	70.73	FBF
5156	C9 H21 N2 O3	0.435	205.1556	FBF	70.28	FBF
5157	C7 H11 N O3	10.155	157.0736	FBF	75.51	FBF
5158	C5 H11 N2 O7 P	0.383	242.0308	FBF	51.20	FBF
5159	C9 H16 N2 O5	6.647	232.1065	FBF	83.07	FBF
5160 5161	C4 H9 N O4 C12 H12 N2 O4	22.473 0.409	135.0544 248.0820	FBF FBF	86.80 66.08	FBF FBF
5162	C23 H27 N O6	17.199	413.1836	FBF	52.16	FBF
5163	C7 H14 N2 O4 S	7.270	222.0679	FBF	62.24	FBF
5164	C7 H10 N2 O4	2.097	186.0639	FBF	80.82	FBF
5165	C10 H18 N4 O6	2.539	290.1232	FBF	76.59	FBF
5166	C31 H53 N11 O5	4.776	659.4200	FBF	67.66	FBF
5167	C46 H65 N15 O12 S2	16.134	1083.4357	FBF	55.84	FBF
5168	C4 H7 N O4	6.049	133.0370	FBF	69.97	FBF
5169 5170	C6 H10 N2 O5 C16 H26 N2 O5 S	2.201 10.051	190.0591 358.1570	FBF FBF	61.45 79.97	FBF FBF
5171	C62 H111 N11 O12	20.084	1201.8414	FBF	50.32	FBF
5172	C7 H9 N O4 S	0.409	203.0262	FBF	64.19	FBF
5173	C6 H12 N2 O4 S2	6.777	240.0220	FBF	63.96	FBF
5174	C6 H10 N6 O	1.344	182.0915	FBF	72.10	FBF
5175	C18 H28 N4 O7	6.802	412.1989	FBF	54.45	FBF
5176	C9 H18 N2 O4	7.088	218.1279	FBF	77.76	FBF
5177	C15 H27 N5 O5	2.721	357.2031	FBF	80.75 70.46	FBF FBF
5178 5179	C5 H11 N O3 S C30 H46 N O7 P	7.634 3.943	165.0466 563.3006	FBF FBF	69.34	FBF
5180	C12 H24 N2 O7	5.607	308.1587	FBF	82.08	FBF
5181	C18 H24 N2 O5	10.181	348.1702	FBF	63.08	FBF
5182	C6 H9 N O6	2.669	191.0434	FBF	83.34	FBF
5183	C11 H17 N O6 S	8.336	291.0778	FBF	64.15	FBF
5184	C21 H32 N4 O6	3.293	436.2282	FBF	66.27	FBF
5185 5186	C9 H16 N3 O2 C11 H23 N O2 S	0.435 14.964	198.1247 233.1457	FBF FBF	69.02 64.56	FBF FBF
5187	C4 H9 N O5 S	6.751	183.0210	FBF	64.35	FBF
5188	C10 H11 N O4	3.293	209.0704	FBF	65.66	FBF
5189	C27 H47 N7 O6	3.943	565.3577	FBF	73.47	FBF
5190	C6 H12 N2 O4 S	0.409	208.0508	FBF	55.90	FBF
5191	C14 H22 N2 O	6.777	234.1724	FBF	74.93	FBF
5192	C9 H16 N3 O3	0.409	214.1189	FBF	85.32	FBF
5193 5194	C29 H38 N4 O4 C28 H36 N4 O4	5.114 7.868	506.2887 492.2740	FBF FBF	52.74 60.70	FBF FBF
5195	C12 H23 N O7	5.400	293.1465	FBF	57.19	FBF
5196	C10 H19 N O8	5.555	281.1096	FBF	68.68	FBF
5197	C11 H21 N O7	9.922	279.1306	FBF	52.38	FBF
5198	C10 H17 N3 O6	3.943	275.1101	FBF	68.32	FBF
5199	C9 H13 N O7	15.952	247.0705	FBF	82.36	FBF
5200	C7 H14 N2 O3	10.155	174.1013	FBF	75.51	FBF
5201	C8 H18 N2 O2	5.919	174.1370	FBF	76.22	FBF
5 <u>202</u> 5203	C8 H13 N O4 S C12 H14 N2 O4	0.409 7.244	219.0570 250.0933	FBF FBF	61.10 61.57	FBF FBF
5204	C8 H13 N O6	5.296	219.0761	FBF	67.65	FBF
5205	C7 H13 N O4 S	9.636	207.0582	FBF	56.81	FBF
5206	C8 H14 N2 O4 S	1.448	234.0688	FBF	64.85	FBF
5207	C7 H12 N2 O4 S	0.409	220.0525	FBF	65.93	FBF
5208	C23 H36 N4 O5	3.085	448.2704	FBF	79.07	FBF
5209 5210	C10 H18 N2 O8 C14 H16 N2 O4	7.946 0.435	294.1086 276.1098	FBF FBF	59.16 71.04	FBF FBF
5210	C8 H13 N3 O2	9.948	183.0995	FBF	71.04	FBF
5212	C10 H18 N2 O6	4.932	262.1182	FBF	73.89	FBF
5213	C9 H15 N O5	19.382	217.0934	FBF	59.34	FBF
5214	C9 H18 N4 O3	16.758	230.1357	FBF	80.80	FBF
5215	C7 H11 N O5	3.397	189.0646	FBF	81.04	FBF
5216	C9 H17 N3 O4	4.411	231.1231	FBF	74.20	FBF
5217	C12 H15 N O5	3.761	253.0967	FBF	66.63	FBF
5218 5219	C12 H15 N O3 C6 H11 N O4	0.383 7.192	221.1067 161.0702	FBF FBF	65.65 63.47	FBF FBF
5219	C6 H11 N 04 C11 H18 N2 O7	12.157	290.1089	FBF	57.41	FBF
5220 5221	C11 H18 N2 O7 C16 H28 N2 O4	4.151	312.2026	FBF	52.01	FBF
5222	C17 H26 N6 O4	11.429	378.2032	FBF	75.06	FBF
5223	C4 H10 N3 O5 P	1.967	211.0348	FBF	82.35	FBF
5224						



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Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB) Score	e (MFG) Algorith
<u>5225</u> 5226	C11 H20 N2 O6 C14 H21 N3 O9 S	6.880 7.244	276.1334 407.1023	<u>FBF</u> FBF	72.33 78.32		FBF FBF
5227	C14 H21 N3 O9 S C9 H13 N O5	6.777	215.0810	FBF	70.89		FBF
228	C3 H5 N5 O2	2.227	143.0456	FBF	55.19		FBF
229	C8 H19 N4 O6 P	5.607	298.1030	FBF	73.32		FBF
230	C8 H17 N O2 S	22.395	191.0980	FBF	61.51		FBF
231	C14 H17 N3 O7	7.972	339.1080	FBF	74.62		FBF
232	C9 H17 N5 O2	0.435	227.1371	FBF	66.31		FBF
233	C9 H12 N4 O2	0.435	208.0948	FBF	77.00		FBF
234	C12 H24 N8 O2	4.151	312.2027	FBF	70.02		FBF
235	C10 H17 N5 O4	3.111	271.1302	FBF	63.29		FBF
236	C9 H17 N5 O2 S	21.200	259.1112	FBF	66.14		FBF
237	C11 H20 N6 O3	6.802	284.1608	FBF	72.40		FBF
238	C11 H19 N5 O4	3.943	285.1449	FBF	61.51		FBF
239	C12 H23 N5 O2	2.461	269.1858	FBF	61.71		FBF
240	C12 H24 N6 O2	13.041	284.1965	FBF	78.38		FBF
241	C15 H21 N5 O2	10.026	303.1700	FBF	55.09		FBF
242	C11 H19 N5 O2	17.485	253.1536	FBF	61.14		FBF
243	C10 H19 N5 O3	6.699	257.1500	FBF	69.08		FBF
244	C17 H22 N6 O2	4.437	342.1824	FBF	51.25		FBF
245	C15 H21 N5 O3	5.763	319.1641	FBF	73.42		FBF
246	C11 H21 N5 O2	0.435	255.1682	FBF	90.23		FBF
247 248	C8 H12 N4 O4	21.798 0.461	228.0874 245.0810	<u>FBF</u> FBF	77.41 50.27		FBF FBF
248 249	C9 H15 N3 O3 S C7 H11 N3 O4	0.461 11.429	245.0810	FBF	68.68		FBF
2 49 250	C15 H16 N4 O3	3.943	300.1220	FBF	76.74		FBF
251	C15 H15 N3 O4	2.097	301.1033	FBF	60.38		FBF
252	C13 H14 N2 O5	7.972	278.0905	FBF	51.94		FBF
253	C9 H14 N2 O4	18.628	214.0954	FBF	72.86		FBF
254	C6 H10 N2 O3 S	0.409	190.0430	FBF	61.14		FBF
255	C14 H15 N3 O2 S	0.435	289.0889	FBF	62.33		FBF
256	C10 H16 N4 O4	4.906	256.1172	FBF	74.48		FBF
257	C11 H18 N2 O4	9.194	242.1271	FBF	78.79		FBF
258	C10 H16 N2 O4 S	1.266	260.0830	FBF	65.43		FBF
259	C10 H14 N2 O4	3.293	226.0970	FBF	65.66		FBF
260	C16 H17 N3 O4	8.258	315.1195	FBF	64.40		FBF
261	C7 H12 N2 O2 S	0.435	188.0635	FBF	60.91		FBF
262	C12 H18 N4 O2	2.877	250.1412	FBF	69.47		FBF
263	C15 H16 N4 O2	7.972	284.1261	FBF	84.09		FBF
264	C11 H14 N4 O2	16.212	234.1113	FBF	80.82		FBF
265	C11 H16 N4 O2	0.409	236.1267	FBF	75.65	<u> </u>	FBF
266	C11 H18 N2 O2	22.213	210.1389	FBF	65.44		FBF
267	C12 H24 N4 O2	0.409	256.1904	FBF	64.75		FBF
268	C11 H19 N3 O2	2.071	225.1485	FBF	83.82		FBF
269	C15 H21 N3 O3	4.411	291.1569	FBF	77.94		FBF
270	C11 H21 N3 O2	13.275	227.1646	FBF	51.34		FBF
271	C10 H18 N2 O2 S2	7.244	262.0831	FBF	54.03		FBF
272	C14 H18 N2 O2 S	3.735	278.1095	FBF	84.98		FBF
273	C8 H14 N2 O3 S	0.825	218.0745	FBF	69.74		FBF
274	C9 H16 N2 O3 S	0.435	232.0865	FBF	52.76		FBF
275	C8 H14 N2 O3	7.140	186.1018	FBF	56.55		FBF
276	C20 H19 N3 O2	2.903	333.1472	FBF	60.53		FBF
277	C10 H18 N2 O2	0.747	198.1367 665.3569	<u>FBF</u> FBF	98.97 78.32		FBF FBF
278	C39 H47 N5 O5	15.120					
279	C34 H38 N4 O5	4.047	582.2884	FBF	51.08		FBF
<u>280 </u>	C22 H30 N4 O4 C9 H19 N5 O3	3.007 3.059	414.2272 245.1499	<u>FBF</u> FBF	57.15 58.91		FBF FBF
282	C9 H19 N5 O3	0.435	245.1499	FBF	58.91		FBF
282 283	C10 H16 N2 O6	6.179	260.1080	FBF	65.75		FBF
284	C10 H20 N6 O4	6.075	288.1544	FBF	77.95		FBF
285	C10 H19 N5 O5	2.149	289.1392	FBF	80.56		FBF
286	C9 H19 N5 O3 S	1.266	277.1221	FBF	65.25		FBF
287	C11 H22 N6 O4	5.659	302.1720	FBF	75.95		FBF
288	C11 H21 N5 O5	7.998	303.1554	FBF	67.45		FBF
289	C12 H26 N6 O3	6.127	302.2089	FBF	68.19		FBF
290	C11 H23 N5 O3 S	2.149	305.1534	FBF	71.64		FBF
291	C15 H23 N5 O3	6.023	321.1792	FBF	52.10		FBF
292	C11 H21 N5 O3	0.409	271.1633	FBF	77.65		FBF
293	C10 H21 N5 O4	5.192	275.1583	FBF	72.05		FBF
294	C15 H18 N4 O4	2.097	318.1297	FBF	60.95		FBF
295	C7 H12 N2 O5 S	6.725	236.0477	FBF	54.90		FBF
296	C10 H19 N3 O5	22.395	261.1307	FBF	75.91		FBF
297	C22 H27 Cl N4 O3	7.920	430.1784	FBF	64.61		FBF
298	C10 H18 N4 O6 S2	9.896	354.0665	FBF	53.13		FBF
299	C5 H11 N3 O2	4.437	145.0865	FBF	74.97		FBF
300	C10 H18 N2 O5 S	7.972	278.0938	FBF	68.20		FBF
301	C9 H16 N2 O6	5.010	248.1011	FBF	67.49		FBF
302	C11 H22 N4 O4	2.227	274.1641	FBF	54.66		FBF
303	C14 H19 N3 O4	2.955	293.1357	FBF	70.25		FBF
304	C12 H16 N6 O3	8.310	292.1295	FBF	83.18		FBF
305	C12 H20 N4 O3	1.812	268.1517	FBF	85.84		FBF
306	C12 H21 N5 O3	2.435	283.1629	FBF	87.55		FBF
307	C15 H18 N4 O3	21.590	302.1373	FBF	64.72		FBF
308	C11 H16 N4 O3	0.435	252.1215	FBF	75.78 77.65		FBF
809	C11 H18 N4 O3	0.461	254.1367	FBF			FBF



	nary						
Cpd Name	Formula C11 H22 N2 O3 S	RT 3.735	Mass 262.1342	CAS ID Source FBF	Score	Score (Lib) Score (DB)	Score (MFG) Algorithm FBF
5311 5312	C11 H22 N2 O3 S C9 H19 N3 O4	12.183	233.1373	FBF	58.53 75.92		FBF
5313	C15 H23 N3 O4	2.643	309.1673	FBF	90.19		FBF
5314	C10 H18 N2 O3 S	3.761	246.1042	FBF	63.90		FBF
5315	C11 H16 N2 O8	9.038	304.0891	FBF	86.11		FBF
316	C23 H32 N2 O5	4.750	416.2327	FBF	70.57		FBF
5317	C11 H22 N5 O6 P	9.402	351.1314	FBF	82.00		FBF
5318 5319	C7 H14 N2 O5 C22 H22 N4 O3	3.397 2.331	206.0920 390.1719	FBF FBF	81.04 52.41		FBF FBF
5320	C18 H20 N2 O5	9.376	344.1342	FBF	73.24		FBF
5321	C14 H20 N2 O4	3.943	280.1401	FBF	61.03		FBF
5322	C21 H38 N4 O8	3.371	474.2671	FBF	92.27		FBF
5323	C40 H53 N7 O5 S2	7.244	775.3564	FBF	70.65		FBF
5324	C35 H56 N6 O6	5.659	656.4257	FBF	95.37		FBF
5325	C37 H48 N4 O5	22.603	628.3661	FBF	57.10		FBF
5326 5327	C44 H69 N5 O10 C33 H61 N5 O9	5.114 4.958	827.5070 671.4467	FBF FBF	78.38 68.66		FBF FBF
5328	C16 H22 N6 O4	11.429	362.1690	FBF	89.26		FBF
5329	C12 H24 N6 O4	5.114	316.1862	FBF	69.68		FBF
5330	C11 H19 N3 O6	1.292	289.1253	FBF	63.14		FBF
5331	C12 H19 N5 O4	10.883	297.1409	FBF	62.36		FBF
5332	C12 H24 N4 O4	2.955	288.1803	FBF	83.19		FBF
5333	C17 H22 N4 O4	6.880	346.1643	FBF	70.77		FBF
5334	C15 H21 N3 O5	2.721	323.1456	FBF	57.68		FBF
5 <u>335</u> 5336	C13 H25 N7 O5 C13 H24 N6 O6	8.024 9.636	359.1930 360.1757	FBF FBF	63.33 71.50		FBF FBF
5337	C12 H24 N6 O4 S	10.207	348.1553	FBF	52.88		FBF
5338	C14 H27 N7 O5	9.376	373.2077	FBF	76.19		FBF
339	C15 H31 N7 O4	4.671	373.2427	FBF	50.30		FBF
5340	C12 H24 N6 O5	6.049	332.1829	FBF	74.01		FBF
341	C13 H26 N6 O5	7.348	346.1976	FBF	71.62		FBF
342	C20 H29 N7 O4	7.244	431.2305	FBF	86.31		FBF
i343 i344	C11 H19 N5 O6 C12 H21 N5 O6	2.383 2.643	317.1328 331.1495	FBF FBF	59.14 98.50		FBF FBF
i345	C12 H21 N3 00 C13 H20 N6 O5	5.010	340.1483	FBF	66.67		FBF
346	C13 H24 N4 O5	10.051	316.1717	FBF	62.92		FBF
347	C13 H25 N5 O5	1.993	331.1854	FBF	83.16		FBF
348	C16 H22 N4 O6	9.558	366.1553	FBF	55.13		FBF
5349	C12 H22 N4 O5	7.972	302.1571	FBF	64.60		FBF
350	C10 H17 N3 O6 S	5.503	307.0813	FBF	50.21		FBF
351	C13 H19 N5 O6	8.960	341.1319 317.1578	FBF	71.10		FBF
5352 5353	C13 H23 N3 O6 C18 H22 N4 O6	4.125 9.844	390.1535	FBF FBF	69.25 78.44		FBF FBF
5354	C9 H17 N3 O5 S	0.591	279.0864	FBF	59.27		FBF
5355	C13 H22 N4 O5	1.993	314.1576	FBF	91.64		FBF
356	C14 H26 N4 O6	7.244	346.1823	FBF	69.61		FBF
5357	C13 H23 N3 O6 S	5.841	349.1315	FBF	64.37		FBF
358	C19 H24 N4 O6	3.631	404.1723	FBF	56.64		FBF
359	C18 H23 N5 O4	12.651	373.1737	FBF	59.66		FBF
5360 5361	C14 H21 N5 O4 C13 H21 N5 O5	6.802 9.870	323.1591 327.1517	FBF FBF	82.47 60.68		FBF FBF
5362	C13 H21 N3 O3 C14 H23 N5 O4	4.281	325.1743	FBF	69.58		FBF
5363	C15 H30 N4 O4	4.437	330.2275	FBF	95.32		FBF
364	C14 H25 N3 O4	6.958	299.1841	FBF	76.09		FBF
365	C18 H27 N3 O5	7.244	365.1940	FBF	92.60		FBF
366	C18 H28 N4 O4	22.161	364.2112	FBF	72.95		FBF
367	C13 H26 N4 O5	2.721	318.1903	FBF	91.43		FBF
368	C20 H29 N5 O4	7.790	403.2207	FBF	60.84		FBF
369 370	C17 H23 N3 O4 C16 H23 N3 O5	4.437 3.345	333.1671 337.1623	FBF FBF	58.94 92.19		FBF FBF
371	C17 H25 N3 O4	4.437	335.1830	FBF	90.50		FBF
372	C11 H19 N3 O5	3.709	273.1320	FBF	61.69		FBF
373	C19 H24 N4 O4	2.461	372.1788	FBF	62.49		FBF
374	C17 H23 N3 O5	19.824	349.1665	FBF	67.86		FBF
375	C18 H24 N4 O5	5.841	376.1774	FBF	55.98		FBF
376	C25 H27 N5 O4	10.545	461.2095	FBF	60.51		FBF
377 378	C23 H26 N4 O5 C19 H26 N4 O4	7.920 21.148	438.1935 374.1933	FBF FBF	61.36 74.47		FBF FBF
379	C21 H25 N3 O6	12.235	415.1757	FBF	77.15	.	FBF
380	C17 H25 N3 O5	10.259	351.1777	FBF	74.82		FBF
381	C16 H32 N10 O5	3.397	444.2561	FBF	94.47		FBF
382	C15 H31 N9 O4 S	3.319	433.2236	FBF	65.30		FBF
383	C17 H34 N10 O5	4.437	458.2725	FBF	96.59		FBF
384	C14 H29 N9 O4	11.923	387.2363	FBF	62.45		FBF
385	C18 H37 N9 O4	5.400	443.2979	FBF	65.09		FBF
386	C18 H38 N10 O4	5.270	458.3099 461.3540	FBF FRF	72.16		FBF
387 388	C17 H35 N9 O4 S C15 H31 N9 O5	3.839 5.607	461.2549 417.2435	FBF FBF	58.35 69.46		FBF FBF
389	C23 H36 N10 O4	4.359	516.2890	FBF	58.13		FBF
i390	C15 H28 N8 O6	7.920	416.2114	FBF	83.60		FBF
391	C15 H27 N7 O7	7.478	417.1961	FBF	72.34		FBF
392	C16 H27 N9 O5	3.891	425.2149	FBF	95.36		FBF
393	C16 H32 N8 O5	3.293	416.2521	FBF	74.01		FBF
	0.0	0.702	375.1839	FBF	62.57		FBF
394 395	C13 H25 N7 O6 C21 H30 N8 O5	9.792 3.839	474.2345	FBF	53.51		FBF



Compound Summar								
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib)	Score (DB)	Score (MFG) Algorith
5397	C12 H22 N6 O6	2.409	346.1591	FBF	66.69			FBF
<u>5398</u> 5399	C16 H30 N6 O6 C16 H31 N7 O6	10.935 4.750	402.2258 417.2343	FBF FBF	68.93 70.29			FBF FBF
5400	C15 H26 N6 O6	10.909	386.1946	FBF	63.35			FBF
5401	C13 H24 N6 O7	3.371	376.1709	FBF	94.85			FBF
5402	C19 H28 N6 O7	3.293	452.2022	FBF	81.12			FBF
5403	C15 H28 N6 O6	11.429	388.2036	FBF	62.38			FBF
5404	C11 H22 N6 O4 S	9.090	334.1417	FBF	66.34			FBF
5405	C15 H26 N8 O4 S	4.567	414.1815	FBF	56.74			FBF
3406	C15 H30 N6 O4 S	14.990	390.2083	FBF	51.25			FBF
5407 5408	C14 H26 N6 O4 S C12 H24 N6 O5 S	13.613 2.643	374.1761 364.1525	FBF FBF	63.94 94.16			FBF FBF
409	C17 H33 N7 O5	5.088	415.2520	FBF	73.51			FBF
410	C20 H31 N7 O5	4.854	449.2376	FBF	69.38			FBF
411	C15 H29 N7 O6	10.000	403.2167	FBF	68.03	,		FBF
412	C22 H32 N8 O5	4.047	488.2476	FBF	84.92			FBF
413	C20 H31 N7 O6	3.527	465.2345	FBF	82.58			FBF
414	C17 H33 N7 O6	8.206	431.2518	FBF	59.59			FBF
415	C16 H28 N6 O6	13.301	400.2050	FBF	78.93			FBF
<u>416</u> 417	C15 H28 N6 O7 C13 H26 N6 O4	7.244 11.195	404.2026 330.2007	FBF FBF	95.95 61.33			FBF FBF
418	C18 H28 N10 O4	7.244	448.2304	FBF	68.31			FBF
419	C18 H32 N8 O4	0.409	424.2570	FBF	54.39			FBF
420	C17 H28 N8 O4	4.750	408.2219	FBF	69.29			FBF
421	C17 H34 N6 O4 S	21.330	418.2351	FBF	60.08			FBF
422	C15 H30 N6 O5	13.353	374.2270	FBF	68.81			FBF
423	C16 H32 N6 O5	5.244	388.2410	FBF	61.54			FBF
424	C17 H34 N6 O4	5.296	386.2642	FBF	59.41			FBF
425	C18 H38 N8 O4	11.715	430.3009	FBF	70.35			FBF
426	C15 H31 N7 O5	4.645	389.2367	FBF	66.97			FBF
<u>427</u> 428	C23 H36 N8 O4 C21 H35 N7 O5	3.631 14.653	488.2820 465.2711	FBF FBF	66.18 69.33			FBF FBF
429	C20 H32 N6 O4 S	3.085	452.2202	FBF	85.74			FBF
430	C16 H30 N6 O4 S	2.903	402.2081	FBF	63.61			FBF
431	C22 H33 N7 O4 S	7.244	491.2318	FBF	55.40			FBF
132	C16 H32 N6 O4 S	6.049	404.2181	FBF	54.02			FBF
433	C20 H30 N6 O4	12.755	418.2304	FBF	72.58			FBF
134	C24 H32 N6 O5	8.960	484.2412	FBF	52.96			FBF
435	C16 H30 N6 O4	8.570	370.2328	FBF	89.85			FBF
436	C12 H24 N6 O6	2.643	348.1761	FBF	98.50			FBF
437 438	C20 H29 N7 O5 C18 H28 N6 O6	7.244 10.909	447.2253 424.2083	FBF FBF	61.95 73.50			FBF FBF
439	C19 H30 N6 O6	4.854	438.2198	FBF	59.51			FBF
440	C26 H33 N7 O5	7.088	523.2556	FBF	50.47			FBF
441	C22 H33 N7 O4	7.920	459.2618	FBF	87.42			FBF
442	C12 H20 N6 O7	9.012	360.1364	FBF	57.01			FBF
443	C12 H19 N5 O8	2.461	361.1229	FBF	75.48			FBF
444	C13 H22 N6 O7	9.064	374.1538	FBF	52.96			FBF
445	C10 H17 N5 O6	2.253	303.1156	FBF	71.02			FBF
446	C14 H25 N5 O6	2.721	359.1794	FBF	71.02			FBF
447	C13 H23 N5 O6 S	2.461	377.1344	FBF	50.47			FBF
448	C13 H21 N5 O6	9.584	343.1503	FBF	78.93			FBF
149 450	C11 H19 N5 O7 C19 H24 N6 O6	4.099 7.920	432.1791	FBF	73.78			FBF FBF
451	C17 H23 N5 O7	7.244	409.1578	FBF	86.90			FBF
1 52	C12 H18 N4 O9	9.844	362.1066	FBF	70.46			FBF
153	C11 H18 N4 O7 S	9.844	350.0917	FBF	76.69			FBF
454	C14 H24 N4 O7	2.669	360.1656	FBF	60.56			FBF
455	C14 H25 N5 O7	3.007	375.1757	FBF	97.80			FBF
156	C12 H20 N4 O8	2.643	348.1289	FBF	51.08			FBF
157	C12 H22 N4 O5 S2	9.402	366.1046	FBF	79.46			FBF
158	C10 H18 N4 O6 S	1.396	322.0941	FBF	66.25			FBF
159 160	C14 H23 N5 O8 C15 H27 N5 O6	3.085 2.461	389.1530 373.1943	FBF FBF	67.29 69.73			FBF FBF
161	C14 H25 N5 O6 S	3.007	391.1504	FBF	87.14			FBF
162	C18 H25 N5 O6	10.909	407.1816	FBF	85.64			FBF
163	C13 H23 N5 O7	2.799	361.1592	FBF	96.70			FBF
164	C20 H26 N6 O6	6.777	446.1912	FBF	65.97			FBF
165	C18 H25 N5 O7	13.353	423.1750	FBF	57.17			FBF
166	C15 H22 N6 O7	12.001	398.1539	FBF	72.43			FBF
167	C15 H26 N4 O7	12.859	374.1791	FBF	67.86	,		FBF
168	C18 H24 N4 O7	7.790	408.1658	FBF	68.73			FBF
469 470	C12 H18 N6 O5	5.997	326.1357	FBF	73.67			FBF
470 471	C11 H18 N4 O5 C15 H20 N4 O6	20.785 7.270	286.1295 352.1391	FBF FBF	52.49 74.64			FBF FBF
4 71 472	C15 H20 N4 O6 C16 H26 N6 O5	7.270 9.896	352.1391	FBF	80.64			FBF
1 72 473	C16 H26 N6 O5 C16 H27 N7 O5	13.353	397.2091	FBF	50.92			FBF
1 73	C15 H24 N6 O5 S	6.335	400.1547	FBF	52.71			FBF
175	C13 H20 N6 O6	8.492	356.1423	FBF	63.84			FBF
476	C15 H24 N6 O5	8.700	368.1783	FBF	71.58			FBF
477	C16 H31 N5 O5	2.825	373.2296	FBF	87.69			FBF
478	C15 H28 N4 O5 S	3.007	376.1793	FBF	87.82			FBF
479	C19 H28 N4 O5	3.007	392.2022	FBF	65.66			FBF
480	C15 H26 N4 O5	2.331	342.1884	FBF	88.98 50.20			FBF FBF
181	C15 H28 N4 O5	11.767	344.2034	FBF				



Compound Summary									
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorith		
5483	C19 H29 N5 O5	14.860	407.2135	FBF	60.77	Score (LIB) Score (DB)	FBF		
484	C19 H29 N5 O6	3.163	423.2124	FBF	69.24		FBF		
485	C15 H29 N5 O5	2.331	359.2149	FBF	88.83		FBF		
186	C18 H26 N4 O5 S	7.244	410.1611	FBF	58.26		FBF		
87	C14 H24 N4 O5 S	3.345	360.1479	FBF	60.45		FBF		
188	C12 H22 N4 O6 S	9.402	350.1292	FBF	64.64		FBF		
489 490	C18 H26 N4 O6 S	13.327 2.747	426.1539 362.1617	<u>FBF</u> FBF	53.02		FBF FBF		
490 491	C14 H26 N4 O5 S C12 H20 N4 O6	2.747	316.1389	FBF	60.56 64.06		FBF		
492	C18 H24 N4 O6	4.437	392.1703	FBF	65.62		FBF		
493	C11 H20 N4 O7	0.435	320.1327	FBF	74.98		FBF		
494	C13 H21 N3 O8 S	9.064	379.1069	FBF	59.31		FBF		
495	C11 H17 N3 O9	9.480	335.0959	FBF	74.72		FBF		
496	C12 H19 N3 O8 S	9.012	365.0914	FBF	51.79		FBF		
497	C12 H19 N3 O6 S	9.402	333.1024	FBF	64.64		FBF		
498	C18 H22 N4 O6 S	11.481	422.1295	FBF	50.80		FBF		
499	C15 H21 N5 O8	10.285	399.1394	FBF	66.09		FBF		
500	C15 H26 N4 O8	2.331	390.1719	FBF	74.71		FBF		
501	C14 H23 N3 O8 S	2.617	393.1191	FBF	51.97		FBF		
502	C15 H23 N5 O6 S	6.335	401.1369	FBF	70.90		FBF		
503	C16 H29 N3 O6	10.909	359.2029	FBF	51.82		FBF		
<u>504 </u>	C16 H30 N4 O6 C13 H23 N3 O7	7.894 2.643	374.2152 333.1556	<u>FBF</u> FBF	51.09 79.17		FBF FBF		
506	C14 H25 N3 O7	5.763	347.1700	FBF	71.34		FBF		
507	C21 H28 N4 O6	12.261	432.2017	FBF	75.87		FBF		
508	C15 H27 N3 O6	4.906	345.1904	FBF	65.91		FBF		
509	C15 H28 N4 O6 S	4.437	392.1703	FBF	52.26		FBF		
510	C15 H26 N4 O6	2.513	358.1826	FBF	77.23		FBF		
511	C14 H26 N4 O7	13.639	362.1804	FBF	52.25		FBF		
512	C13 H23 N3 O7 S	6.699	365.1277	FBF	56.28		FBF		
513	C24 H26 N4 O6	3.371	466.1839	FBF	58.73		FBF		
514	C18 H25 N3 O6	14.081	379.1744	FBF	58.77		FBF		
515	C18 H23 N3 O7	2.981	393.1502	FBF	57.01		FBF		
516	C18 H22 N4 O7	13.327	406.1469	FBF	51.24		FBF		
517 518	C19 H24 N4 O7 C20 H26 N4 O6	7.920 4.750	420.1630 418.1867	FBF FBF	85.80 53.37		FBF FBF		
519	C22 H25 N3 O8	11.481	459.1661	FBF	58.41		FBF		
520	C12 H23 N3 O4 S2	12.053	337.1150	FBF	82.15		FBF		
521	C12 H24 N4 O4 S2	9.454	352.1222	FBF	54.48		FBF		
522	C11 H21 N3 O4 S3	13.041	355.0669	FBF	53.71		FBF		
523	C15 H21 N3 O4 S2	12.989	371.0970	FBF	58.14		FBF		
524	C17 H22 N4 O4 S2	7.244	410.1051	FBF	53.52		FBF		
525	C14 H27 N5 O5 S	3.345	377.1742	FBF	60.45		FBF		
526	C17 H24 N4 O5 S	15.094	396.1468	FBF	52.08		FBF		
527	C10 H17 N3 O4 S	11.481	275.0946	FBF	62.00		FBF		
528	C16 H20 N4 O4 S	8.986	364.1203	FBF	63.50		FBF		
529	C15 H26 N6 O4 S	7.244	386.1729	FBF	88.97		FBF		
530	C18 H23 N5 O4 S	7.218	405.1495	FBF	61.00		FBF		
531 532	C20 H24 N6 O4 S C15 H30 N4 O4 S	7.140 6.205	444.1586 362.1991	<u>FBF</u> FBF	62.98 51.51		FBF FBF		
533	C18 H28 N4 O4 S	6.335	396.1810	FBF	63.26		FBF		
534	C13 H26 N4 O5 S	4.463	350.1634	FBF	58.27		FBF		
535	C20 H29 N5 O4 S	3.085	435.1934	FBF	83.85		FBF		
536	C13 H23 N3 O4 S2	11.403	349.1118	FBF	54.31		FBF		
537	C25 H27 N5 O4 S	11.299	493.1758	FBF	64.31		FBF		
538	C15 H26 N6 O7	18.498	402.1850	FBF	73.31		FBF		
539	C15 H25 N5 O8	3.631	403.1697	FBF	87.85		FBF		
540	C19 H27 N5 O6	3.631	421.1988	FBF	56.64		FBF		
541	C19 H27 N5 O7	7.920	437.1896	FBF	85.80		FBF		
542	C15 H24 N4 O9	4.645	404.1535	FBF	60.46		FBF		
543 E44	C16 H24 N6 O7	7.244	412.1723	FBF	51.40		FBF		
544 545	C16 H28 N4 O7	3.007	388.1948	FBF FBF	93.81 53.74		FBF FBF		
546	C17 H28 N6 O5 C20 H26 N6 O5	13.353 7.244	396.2090 430.1991	FBF	75.89		FBF		
547	C15 H24 N6 O6	6.205	384.1775	FBF	57.99		FBF		
548	C22 H27 N7 O5	7.244	469.2090	FBF	70.41		FBF		
549	C17 H32 N4 O5	4.671	372.2382	FBF	70.38		FBF		
550	C17 H33 N5 O5	3.605	387.2463	FBF	88.05		FBF		
551	C16 H30 N4 O5 S	6.257	390.1948	FBF	60.74		FBF		
552	C20 H30 N4 O5	7.452	406.2206	FBF	59.70		FBF		
553	C16 H28 N4 O5	2.825	356.2040	FBF	88.83	<u> </u>	FBF		
554	C22 H31 N5 O5	7.920	445.2290	FBF	76.68		FBF		
555	C17 H34 N6 O5	14.860	402.2581	FBF	79.49		FBF		
556	C16 H31 N5 O5 S	7.244	405.2053	FBF	64.48		FBF		
557	C20 H31 N5 O5	12.495	421.2353	FBF	64.79		FBF		
558	C16 H29 N5 O5	3.371	371.2158	FBF	92.47		FBF		
559 560	C15 H29 N5 O6	5.010	375.2134	FBF	84.80		FBF		
560 E61	C20 H31 N5 O6	8.466	437.2275	FBF	55.76 52.07		FBF		
<u>561</u> 562	C15 H26 N4 O5 S C23 H28 N4 O5	4.437 4.854	374.1650 440.2071	<u>FBF</u> FBF	52.07 62.39		FBF FBF		
563	C19 H26 N4 O5	7.244	390.1897	FBF	62.39		FBF		
564	C15 H24 N4 O5	2.721	340.1731	FBF	81.11		FBF		
565	C14 H24 N4 O6	2.643	344.1681	FBF	76.34		FBF		
566	C19 H26 N4 O6	3.085	406.1815	FBF	57.31		FBF		
567	C20 H27 N5 O6	6.361	433.1928	FBF	53.39		FBF		
	C18 H26 N4 O7	2.981	410.1767	FBF	70.12		FBF		



Compound Sun	nmarv		-	•		
Cpd Name	Formula	RT	Mass	CAS ID Source	Score Sco	ore (Lib) Score (DB) Score (MFG) Algorithm
5569	C23 H28 N4 O7	11.325	472.1972	FBF	92.07	FBF
5570	C15 H23 N3 O10	3.059	405.1392	FBF	68.19	FBF
5571	C17 H23 N7 O6	7.920	421.1668	FBF	59.29	FBF
5572	C20 H25 N5 O6	7.920	431.1807	FBF	50.80	FBF
5573 5574	C16 H29 N3 O6 S C15 H27 N3 O7	22.447 4.411	391.1764 361.1846	FBF FBF	60.58 77.81	FBF FBF
5575	C20 H29 N3 O7	7.868	423.1971	FBF	59.69	FBF
5576	C17 H33 N5 O6	2.721	403.2414	FBF	91.89	FBF
5577	C16 H30 N4 O6 S	9.142	406.1848	FBF	53.42	FBF
5578	C15 H28 N4 O7	5.815	376.1973	FBF	66.17	FBF
5579	C22 H31 N5 O6	3.371	461.2285	FBF	57.81	FBF
5580 5581	C15 H25 N3 O6 S C19 H25 N3 O6	4.437 12.391	375.1438 391.1758	FBF FBF	52.26 63.74	FBF FBF
5582	C19 H25 N3 O8	7.192	411.1644	FBF	54.93	FBF
5583	C13 H21 N5 O4 S	9.012	343.1311	FBF	50.40	FBF
5584	C17 H21 N5 O4	8.960	359.1608	FBF	73.41	FBF
5585	C13 H19 N5 O4	6.335	309.1462	FBF	61.70	FBF
5586	C11 H17 N5 O5	2.253	299.1255	FBF	61.97	FBF
5587	C17 H26 N4 O4	6.828	350.1972	FBF	66.96	FBF
5588 5589	C11 H22 N4 O5 C19 H27 N5 O4	9.818 5.088	290.1563 389.2064	FBF FBF	57.89 50.15	FBF FBF
5590	C18 H24 N4 O4 S	2.981	392.1530	FBF	56.47	FBF
5591	C22 H24 N4 O4	3.007	408.1768	FBF	57.67	FBF
5592	C16 H23 N3 O4	4.307	321.1693	FBF	52.52	FBF
5593	C18 H24 N4 O4	8.050	360.1788	FBF	80.73	FBF
5594	C18 H27 N7 O4	4.645	405.2116	FBF	66.79	FBF
5595	C18 H28 N8 O4	9.454	420.2264	FBF	66.57	FBF
<u>5596</u> 5597	C17 H25 N7 O4 S	13.353 7.920	423.1697 439.1970	FBF FBF	63.57 59.12	FBF FBF
5598	C21 H25 N7 O4 C17 H23 N7 O4	7.920	389.1827	FBF	83.50	FBF
5599	C15 H21 N7 O5	4.567	379.1584	FBF	54.05	FBF
5600	C17 H29 N5 O4 S	13.353	399.1959	FBF	62.47	FBF
5601	C17 H27 N5 O4	7.244	365.2059	FBF	61.30	FBF
5602	C18 H33 N7 O4	7.920	411.2568	FBF	57.94	FBF
5603	C17 H30 N6 O4 S	7.920	414.2049	FBF	89.74	FBF
5604	C21 H30 N6 O4	4.854	430.2349	FBF	52.02	FBF
5605	C23 H31 N7 O4	4.151	469.2409	FBF	80.77	FBF
5606 5607	C17 H30 N6 O4 C20 H27 N5 O4 S	7.244 7.946	382.2320 433.1799	FBF FBF	71.16 56.94	FBF FBF
5608	C20 H27 N3 O4 3	13.353	399.1904	FBF	68.09	FBF
5609	C26 H28 N6 O4	11.325	488.2204	FBF	74.38	FBF
5610	C14 H21 N5 O5	5.140	339.1527	FBF	75.13	FBF
5611	C14 H23 N5 O5	3.085	341.1694	FBF	68.14	FBF
5612	C16 H27 N5 O4	8.570	353.2070	FBF	89.77	FBF
5613	C18 H36 N4 O4	8.258	372.2718	FBF	63.39	FBF
5614	C17 H33 N3 O4 S	11.689	375.2206	FBF	52.39	FBF
5615 5616	C15 H29 N3 O5 C16 H31 N3 O5	13.041 2.643	331.2082 345.2258	FBF FBF	57.44 85.82	FBF FBF
5617	C17 H32 N4 O4	18.369	356.2421	FBF	53.57	FBF
5618	C15 H30 N4 O5	10.337	346.2239	FBF	62.17	FBF
5619	C17 H34 N4 O4	10.701	358.2602	FBF	73.20	FBF
5620	C14 H27 N3 O5 S	9.090	349.1664	FBF	54.13	FBF
5621	C16 H31 N3 O4 S	18.395	361.2053	FBF	63.80	FBF
5622	C20 H29 N3 O4	4.671	375.2171	FBF	57.25	FBF
5623	C19 H29 N3 O5	4.541	379.2085	FBF	73.16	FBF
5624 5625	C20 H31 N3 O4 C14 H25 N3 O5	10.909 4.125	377.2343 315.1784	FBF FBF	51.63 73.94	FBF FBF
5626	C20 H28 N4 O5	7.244	404.2025	FBF	66.10	FBF
5627	C18 H27 N3 O6	3.631	381.1881	FBF	89.02	FBF
5628	C21 H30 N4 O5	7.192	418.2218	FBF	64.50	FBF
5629	C28 H33 N5 O4	7.244	503.2528	FBF	80.07	FBF
5630	C22 H32 N4 O4	3.631	416.2447	FBF	77.48	FBF
5631	C20 H31 N3 O5	7.920	393.2257	FBF	92.73	FBF
5632 5633	C18 H38 N6 O4 C17 H35 N5 O4 S	12.391 4.750	402.2988 405.2418	FBF FBF	77.52 78.92	FBF FBF
5634	C21 H35 N5 O4 S	16.992	421.2660	FBF	69.61	FBF
5635	C17 H33 N5 O4	3.839	371.2518	FBF	91.67	FBF
5636	C15 H31 N5 O5	17.485	361.2347	FBF	79.68	FBF
5637	C23 H36 N6 O4	3.527	460.2785	FBF	76.70	FBF
5638	C21 H35 N5 O5	5.374	437.2649	FBF	63.70	FBF
5639	C17 H35 N5 O4	13.197	373.2655	FBF	53.89	FBF
5640	C14 H32 N4 OF S	10.909	408.1874	FBF	64.50	FBF
5641 5642	C14 H28 N4 O5 S C22 H33 N5 O4 S	7.244 3.839	364.1808 463.2266	FBF FBF	54.45 66.38	FBF FBF
5643	C22 H33 N5 O4 S C20 H32 N4 O5 S	4.828	440.2072	FBF	54.99	FBF
5644	C16 H32 N4 O4 S	12.755	376.2177	FBF	52.12	FBF
5645	C20 H30 N4 O4	5.010	390.2249	FBF	69.60	FBF
5646	C19 H30 N4 O5	4.671	394.2205	FBF	70.87	FBF
5647	C20 H32 N4 O4	4.671	392.2437	FBF	57.25	FBF
5648	C22 H31 N5 O4	5.400	429.2389	FBF	66.67	FBF
5649	C12 H24 N4 O6	9.558	320.1678	FBF	73.88	FBF
5650	C21 H31 N5 O5	4.776	433.2332	FBF	67.10	FBF
		4.203	518.2625	FBF	60.94	FBF
5651	C26 H34 N6 O4			FDF	F0 27	
	C26 H33 N5 O5 C16 H32 N4 O4	3.085 17.018	495.2507 344.2403	FBF FBF	50.27 53.03	FBF FBF



Compo	und S	ummary
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Compound Su							
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorithm
5655	C14 H27 N3 O5 S2	5.841	381.1394	FBF	59.22		FBF
5656	C15 H29 N3 O4 S2	4.541	379.1584	FBF	50.43		FBF
5657	C23 H29 N3 O4 S	7.504	443.1874	FBF	72.54		FBF
5658	C21 H28 N4 O4 S	7.920	432.1792	FBF	60.12		FBF
5659	C13 H25 N3 O6 S	8.674	351.1474	FBF	54.10		FBF
5660	C20 H28 N4 O5 S	3.293	436.1792	FBF	56.70		FBF
5661	C29 H30 N4 O4	3.657	498.2294	FBF	67.41		FBF
5662	C23 H29 N3 O4	4.828	411.2189	FBF	52.17		FBF
5663	C19 H25 N3 O4	2.539	359.1834	FBF	69.21		FBF
5664	C17 H25 N3 O6	9.766	367.1723	FBF	64.07		FBF
5665	C24 H28 N4 O5	3.293	452.2026	FBF	54.92		FBF
5666	C13 H21 N3 O5	10.883	299.1506	FBF	59.13		FBF
5667	C15 H25 N3 O4	0.409	311.1866	FBF	57.20		FBF
5668	C21 H28 N4 O4	3.397	400.2119	FBF	69.82		FBF
5669	C19 H27 N3 O5	4.671	377.1940	FBF	70.87		FBF
5670	C15 H21 N3 O7	4.281	355.1396	FBF	51.08		FBF
5671	C12 H19 N3 O7 S	2.149	349.0938	FBF	68.31		FBF
5672	C18 H22 N6 O7 S	11.507	466.1239	FBF	53.22		FBF
5673	C17 H25 N3 O7	7.816	383.1728	FBF	80.42		FBF
5674	C33 H32 N6 O4	8.076	576.2491	FBF	60.96		FBF
5675	C25 H32 O12	6.257	524.1898	FBF	72.66		FBF
5676	C5 H8 N6 O	6.049	168.0774	FBF	82.17		FBF
5677	C38 H40 N2 O11	13.353	700.2630	FBF	62.90		FBF
5678	C12 H18 O5 S2	8.466	306.0570	FBF	54.55		FBF
5679	C10 H16 N2 O8	5.633	292.0918	FBF	69.63		FBF
5680	C9 H16 O5	2.409	204.0994	FBF	84.45		FBF
5681	C8 H14 O5 S	9.896	222.0562	FBF	74.65		FBF
5682	C3 H7 O4 P	0.383	138.0082	FBF	85.02		FBF
5683	C2 H5 O5 P	13.015	139.9875	FBF	87.03		FBF
5684	C5 H15 N4 O3 P	4.802	210.0892	FBF	76.44		FBF
5685	C3 H10 N O4 P	0.383	155.0347	FBF	85.02		FBF
5686	C3 H7 O5 P	7.374	154.0024	FBF	82.31		FBF
5687	C6 H15 O4 P	2.643	182.0704	FBF	80.37		FBF
5688	C18 H15 O4 P	9.038	326.0706	FBF	95.65		FBF
5689	C6 H12 N3 P S	0.409	189.0495	FBF	65.44		FBF
5690	C10 H13 N O4 S	1.240	243.0564	FBF	65.43		FBF
5691	C14 H16 O5	13.509	264.0974	FBF	55.72		FBF
5692	C12 H10 O4	3.267	218.0567	FBF	71.58		FBF
5693	C25 H26 O14	5.893	550.1315	FBF	64.02		FBF
5694	C19 H18 O11 S	5.919	454.0567	FBF	59.31		FBF
5695	C16 H13 N O5	9.896	299.0797	FBF	69.54		FBF
5696	C14 H20 N O4	2.149	266.1417	FBF	74.63		FBF
5697	C11 H12 O2	7.478	176.0835	FBF	62.30		FBF
5698	C9 H8 O2	8.284	148.0520	FBF	81.62		FBF
5699	C9 H8 O3	0.383	164.0466	FBF	74.65		FBF
5700	C10 H12 O5	3.007	212.0684	FBF	81.06		FBF
5701	C9 H8 O5	0.383	196.0362	FBF	73.44		FBF
5702	C17 H19 N O5	7.998	317.1261	FBF	79.75		FBF
5703	C16 H24 N O5	2.929	310.1627	FBF	71.73		FBF
5704	C8 H8	7.244	104.0617	FBF	82.54		FBF
5705	C14 H12 O3 S	2.981	260.0532	FBF	55.59		FBF
5706	C14 H12 O3 3	8.908	266.1656	FBF	86.77		FBF
5707	C12 H11 O4 P	12.599	250.0396	FBF	94.07		FBF
5708	C4 H9 O6 P	9.194	184.0129	FBF	56.18		FBF
	C7 H17 O7 P	7.088	244.0712	FBF	68.07		FBF
5709							
5710	C6 H9 N2 O5 P	1.396	220.0241	FBF FBF	64.68		FBF
5711	C4 H12 N O4 P	1.396	169.0504	FBF	59.30		FBF
5712	C18 H39 O7 P	9.480	398.2434	FBF	97.60		FBF
5713	C16 H35 N O2	7.010	273.2665	FBF	98.97		FBF
5714	C21 H36 N O	10.857	318.2784	FBF	68.81		FBF
5715	C10 H17 N3 S	0.721	211.1131	FBF	71.41		FBF
5716	C24 H40 N8 O4	4.047	504.3146	FBF	53.66		FBF
5717	C11 H18 N4 O2	0.435	238.1418	FBF	92.55		FBF
5718	C12 H27 N	19.460	185.2139	FBF	71.20		FBF
5719	C14 H31 N O	16.082	229.2407	FBF	99.91		FBF
5720	C13 H28 N O2	6.075	230.2134	FBF	56.05		FBF
5721	C14 H30 N2 O4	4.151	290.2207	FBF	70.85		FBF
5722	C6 H13 N O3 S	8.310	179.0618	FBF	53.70		FBF
5723	C6 H13 N	15.146	99.1049	FBF	77.28		FBF
5724	C12 H23 N	3.631	181.1832	FBF	68.63		FBF
5725	C6 H11 N2 O	5.503	172.1426	FBF	81.09		FBF
5726	C5 H11 N3 O	13.847	129.0891	FBF	77.22		FBF
5727	C7 H15 N3 O5	5.919	221.1009	FBF	69.80		FBF
5728	C3 H5 N5 O3	0.799	197.0185	FBF	74.71		FBF
5729	C2 H5 N5 O3	6.751	147.0380	FBF	77.81		FBF
5730	C15 H13 N3 O2	5.062	267.0988	FBF	56.28		FBF
5731	C7 H13 Cl2 N2 O3 P	0.435	274.0035	FBF	56.64		FBF
5732	C15 H14 N4 O2	6.854	282.1102	FBF	80.13		FBF
5733	C7 H14 N2 O2 S	7.218	190.0778	FBF	83.92		FBF
5734	C9 H23 N O3 P S	7.972	256.1131	FBF	67.43		FBF
5735	C5 H12 N6 O3	2.513	204.0971	FBF	58.09		FBF
5736	C9 H16 Cl N3 O2	3.267	233.0922	FBF	50.22		FBF
5737	C8 H18 N6 O4	2.409	262.1411	FBF	68.00		FBF
5738	C21 H43 N5 O7	4.671	477.3151	FBF	78.32		FBF
F720	C20 H41 N5 O7	9.922	463.3006	FBF	68.29		FBF
5739 5740	C21 H41 N5 O7	3.839	475.2989	FBF	94.04		FBF



Compound Summary							
Cpd Name 5741	Formula C23 H45 N5 O14	RT 14.809	Mass 615.3005	CAS ID Source FBF	Score 52.26	Score (Lib) Score (DB)	Score (MFG) Algorith
5742	C18 H37 N5 O9	4.411	467.2593	FBF	73.83		FBF
5743	C6 H11 O8 P	6.699	242.0187	FBF	62.62		FBF
5744	C22 H22 F N3 O2	7.894	379.1696	FBF	71.90		FBF
5745 5746	C6 H7 N O2 C10 H13 N3 O2	0.409 15.770	125.0466 207.1007	FBF FBF	64.94 73.47		FBF FBF
5747	C11 H18 O	18.576	166.1352	FBF	65.38		FBF
5748	C16 H28 O	21.512	236.2130	FBF	77.37		FBF
5749	C9 H14 O3	2.903	170.0940	FBF	81.67		FBF
5750 5751	C16 H24 O5 C6 H10 O3 S	7.010 9.480	296.1608 162.0350	<u>FBF</u> FBF	71.21 67.48		FBF FBF
5752	C3 H5 O7 P	12.885	183.9779	FBF	78.88		FBF
5753	C9 H11 N3 O4	0.435	225.0766	FBF	50.60		FBF
5754	C10 H22 O5	2.643	222.1454	FBF	73.03		FBF
5755 5756	C20 H42 O11 C14 H30 O8	4.437 2.643	458.2722 326.1941	FBF FBF	98.85 99.71		FBF FBF
5757	C14 H30 O6 C12 H26 O7	2.149	282.1677	FBF	99.69		FBF
5758	C18 H38 O10	3.631	414.2461	FBF	98.90		FBF
5759	C16 H34 O9	3.007	370.2195	FBF	97.50		FBF
5760	C10 H22 O6	0.435	238.1417	FBF	99.21		FBF
5761 5762	C8 H18 O5 C10 H16 O	0.435 5.893	194.1155 152.1195	FBF FBF	99.78 60.09		FBF FBF
5763	C7 H9 Cl O	0.461	144.0337	FBF	57.69		FBF
5764	C6 H14 O2	1.318	118.1004	FBF	56.54		FBF
765	C30 H62 O10	10.285	582.4334	FBF	69.55		FBF
766	C9 H12 N6 O4 C25 H43 N O18	11.351 6.361	268.0934	FBF FBF	84.29 52.48		FBF FBF
5767 5768	C38 H72 N2 O12	16.160	645.2452 748.5065	FBF	55.23		FBF
5769	C25 H30 F N3 O9	6.257	535.1973	FBF	77.69		FBF
5770	C22 H40 O8	3.293	432.2761	FBF	66.85		FBF
5771	C11 H16 O8	7.400	276.0835	FBF	66.73		FBF
5772 5773	C17 H34 N4 O10 C43 H65 N5 O10	4.932 5.088	454.2241 811.4770	FBF FBF	58.75 84.18	<u> </u>	FBF FBF
5774	C11 H18 O8	4.906	278.0991	FBF	69.42		FBF
5775	C6 H14 N2 O4	7.192	178.0966	FBF	63.28		FBF
776	C6 H6 Cl6	9.870	287.8618	FBF	55.78		FBF
777	C3 H F5 O2	0.357	163.9895	FBF	77.89		FBF
778 779	C14 H F27 O2 C8 H Cl F16 O4 S	5.503 6.361	713.9544 531.9007	FBF FBF	77.34 55.67		FBF FBF
5780	C3 H7 Cl O2	12.807	110.0125	FBF	53.52		FBF
5781	C9 H8 N2	5.270	144.0686	FBF	83.59		FBF
5782	C9 H7 CI N2	13.847	178.0288	FBF	55.16		FBF
5783 5784	C18 H26 CI N3 O C6 H10 CI N5	7.010 0.435	335.1788 187.0635	<u>FBF</u> FBF	61.96 57.46		FBF FBF
5785	C10 H19 N5 O	0.409	225.1586	FBF	52.74		FBF
5786	C9 H18 N6	13.275	210.1609	FBF	70.85		FBF
5787	C10 H19 N5 S	4.880	241.1382	FBF	64.26	<u> </u>	FBF
5788	C7 H12 CI N5	9.870	201.0770	FBF	50.23		FBF
5789 5790	C6 H10 N4 C12 H13 N5 O2 S	1.058 8.336	138.0915 291.0778	FBF FBF	76.70 57.72		FBF FBF
5791	C24 H27 N3 O4	3.631	421.1988	FBF	73.12		FBF
5792	C20 H26 N2 O4 S2	11.481	422.1296	FBF	50.95		FBF
5793	C3 H3 N O S2	0.539	132.9654	FBF	63.73		FBF
5794 5795	C22 H25 N2 O S C21 H20 N2 O7	9.948 5.296	365.1709 412.1282	FBF FBF	68.66 62.63		FBF FBF
i796	C19 H23 CI N2	1.993	314.1569	FBF	59.39		FBF
5797	C19 H24 N2	20.967	280.1947	FBF	58.34		FBF
5798	C17 H26 N4 O	6.127	302.2090	FBF	72.18		FBF
5799	C9 H9 N3 O2	0.435	191.0685 290.1765	FBF	77.84		FBF
5800 5801	C20 H22 N2 C22 H23 CI N2 O2	6.127 13.327	382.1467	FBF FBF	65.37 50.72		FBF FBF
802	C10 H6 N2 O S2	0.539	233.9930	FBF	85.66		FBF
5803	C19 H21 N5 O3 S	11.377	399.1362	FBF	64.70		FBF
804	C20 H16 O6	0.435	352.0930	FBF	52.00		FBF
5805 5806	C8 H6 O C18 H26 N2 O5 S	7.218 11.429	118.0411 382.1545	FBF FBF	80.66 55.03		FBF FBF
5807	C18 H20 O4	11.221	300.1370	FBF	73.00		FBF
808	C17 H17 Cl O6	8.258	352.0690	FBF	56.35		FBF
809	C18 H16 O3	3.709	280.1094	FBF	54.20		FBF
5810 5811	C22 H30 O10 C16 H22 O7 S	15.016	454.1819 358.1110	FBF	51.26 57.44		FBF FBF
5812	C46 H46 N2 O23	10.259 21.278	994.2528	FBF FBF	65.97	<u> </u>	FBF
813	C23 H30 O5	4.671	386.2089	FBF	69.65		FBF
814	C13 H14 O3	5.867	218.0936	FBF	60.70		FBF
815	C15 H18 O4	4.932	262.1185	FBF	66.14		FBF
5816 5817	C28 H31 N2 O3	4.932 8.986	443.2352 347.0825	FBF ERE	68.27 62.55		FBF FBF
5818	C20 H13 N O5 C21 H18 N O4	8.986 9.896	347.0825	FBF FBF	63.05		FBF
5819	C7 H5 N O S	6.751	151.0106	FBF	60.69		FBF
5820	C12 H10 O2 S	6.751	218.0399	FBF	99.34		FBF
5821	C16 H21 N5 O2	10.909	315.1713	FBF	73.83		FBF
822	C14 H9 N O3	21.876	239.0565	FBF	66.46		FBF
823 824	C15 H14 O6 C19 H29 N5 O2	10.155 8.674	290.0775 359.2300	FBF FBF	64.41 63.07		FBF FBF
825	C21 H27 N5 O9 S2	6.127	557.1225	FBF	71.44		FBF
5826	C18 H19 N3 O5 S	9.896	389.1049	FBF	55.82		FBF



Compound	Summary

Compound Sumn	Formula	RT	Mass	CAS ID Source	Scara	Score (Lib) Score (DR)	Score (MEG) Algorithm
Cpd Name 5827	C22 H20 N4 O8 S2	9.922	Mass 532.0765	CAS ID Source FBF	Score 59.32	Score (Lib) Score (DB)	Score (MFG) Algorithm FBF
5828	C16 H22 N4 O9 S	11.481	446.1110	FBF	61.87		FBF
5829	C16 H18 N2 O5 S	9.844	350.0924	FBF	68.23		FBF
5830	C24 H23 N3 O6 S	13.353	481.1324	FBF	70.19		FBF
5831	C33 H38 N4 O6	3.917	586.2824	FBF	63.50		FBF
5832	C33 H46 N4 O6	5.296	594.3404	FBF	70.96		FBF
5833 5834	C33 H48 N4 O6 C55 H74 N4 O5	4.645 19.434	596.3629 870.5622	FBF FBF	53.34 61.45		FBF FBF
5835	C44 H55 Co N4 O16	18.265	954.2891	FBF	56.46		FBF
5836	C45 H62 N6 O12	4.854	878.4423	FBF	52.17		FBF
5837	C17 H17 CI N6 O3	9.896	388.1040	FBF	69.73		FBF
5838	C24 H36 O5	12.651	404.2553	FBF	56.22		FBF
5839	C25 H38 O5	12.339	418.2730	FBF	65.85		FBF
5840	C21 H25 N3 O2 S	7.816	383.1683	FBF	64.31		FBF
5841	C19 H21 N S	5.426	295.1404	FBF	53.93		FBF
5842 5843	C21 H23 N O3 C18 H22 N O4	21.798 5.789	337.1673 316.1553	FBF FBF	66.28 59.61		FBF FBF
5844	C7 H10 O6 S	1.474	222.0203	FBF	51.78		FBF
5845	C4 H6 O2 S2	2.331	149.9816	FBF	63.78		FBF
5846	C5 H4 O3	0.383	112.0152	FBF	73.71		FBF
5847	C13 H12 O4	4.828	232.0714	FBF	78.02		FBF
5848	C26 H27 CI N2 O3 S2	14.860	514.1176	FBF	71.81		FBF
5849	C7 H10 O	2.591	110.0727	FBF	79.90		FBF
5850	C5 H6 O	0.773	82.0417	FBF	87.62		FBF
5851 5852	C10 H16 N2 O5 S C32 H45 N O4	1.760 5.763	<u>276.0802</u> 507.3370	FBF FBF	58.43 65.33		FBF FBF
5853	C32 H45 N O4 C7 H11 N O	2.097	125.0837	FBF	78.04		FBF
5854	C15 H21 N3 O	21.616	259.1674	FBF	76.03		FBF
5855	C15 H18 N2	19.824	226.1470	FBF	75.97		FBF
5856	C19 H26 N2 S	8.804	314.1827	FBF	76.69		FBF
5857	C17 H20 O6	6.023	320.1262	FBF	68.21		FBF
5858	C11 H18 O4	5.296	214.1203	FBF	85.80		FBF
5859	C15 H18 O6	7.894	294.1092 177.1153	FBF	73.65		FBF
5860 5861	C11 H15 N O C14 H20 O4	0.383 9.870	252.1371	<u>FBF</u> FBF	98.26 76.73		FBF FBF
5862	C27 H33 N O4	7.582	435.2415	FBF	53.31		FBF
5863	C14 H21 N3 O3	9.870	279.1567	FBF	55.36		FBF
5864	C7 H14 N4 O3	7.920	202.1065	FBF	63.31		FBF
5865	C32 H44 F3 N3 O2 S	3.631	591.3077	FBF	52.22		FBF
5866	C21 H26 CI N3 O S	7.244	403.1485	FBF	61.02		FBF
5867	C18 H22 N2 S	4.125	298.1519	FBF	57.11		FBF
5868	C18 H15 CI F N O3	0.409	347.0719	FBF	58.45		FBF
5869 5870	C19 H22 CI N5 O C8 H12 N4	7.244 3.111	371.1521 164.1052	<u>FBF</u> FBF	68.60 66.13		FBF FBF
5871	C8 H18 N2 O4 S	1.240	238.0996	FBF	62.06		FBF
5872	C26 H31 Cl2 N5 O3	7.998	531.1816	FBF	50.50		FBF
5873	C9 H15 N O	0.383	153.1151	FBF	83.15		FBF
5874	C20 H16 N4	9.818	312.1379	FBF	91.79		FBF
5875	C34 H40 N4 O4	3.943	568.3075	FBF	76.31		FBF
5876	C6 H8 N4	1.396	136.0738	FBF	67.14		FBF
5877	C9 H10 N4 O4	20.681	238.0718	FBF	84.42		FBF
<u>5878</u> 5879	C9 H15 N5 O4 C9 H11 N5 O3	2.279 3.085	257.1099 237.0859	FBF FBF	64.00 78.20		FBF FBF
5880	C9 H14 N5 O7 P	0.435	335.0659	FBF	51.35		FBF
5881	C9 H15 N5 O3	3.553	241.1166	FBF	74.88		FBF
5882	C7 H5 N5 O3	1.838	207.0377	FBF	70.82		FBF
5883	C9 H11 N5 O2	5.997	221.0927	FBF	71.48		FBF
5884	C6 H5 N5 O2	1.838	179.0445	FBF	81.86		FBF
5885	C6 H5 N5 O	1.318	163.0496	FBF	82.34		FBF
5886 5887	C20 H22 N7 O6	9.038	456.1614 377.2434	FBF FBF	67.26		FBF FBF
<u>5887</u> 5888	C24 H31 N3 O C5 H7 N O2	10.805 0.461	3//.2434 113.0480	FBF	53.38 54.32		FBF
5889	C15 H25 N O5	1.760	299.1743	FBF	76.52		FBF
5890	C12 H15 N5 O3	5.581	277.1184	FBF	81.60		FBF
5891	C14 H12 F N O3	3.735	261.0821	FBF	58.83		FBF
5892	C9 H7 N O5 S	6.751	241.0028	FBF	52.75		FBF
5893	C35 H32 Mg N4 O5	6.361	612.2282	FBF	51.82		FBF
5894	C35 H36 N4 O5	3.735	592.2671	FBF	61.73		FBF
5895 5896	C16 H23 N3 O S C14 H13 F4 N3 O2 S	2.149 10.259	305.1532	FBF FBF	66.34 75.12		FBF FBF
5896 5897	C14 H13 F4 N3 O2 S C10 H14 S	0.435	363.0665 166.0815	FBF	75.12		FBF
5898	C6 H12 N4	1.604	140.1064	FBF	76.92		FBF
5899	C11 H21 N5 O S	8.310	271.1486	FBF	55.96		FBF
5900	C8 H15 N5 S	21.148	213.1051	FBF	89.85		FBF
5901	C3 H3 N3 O3	13.275	129.0179	FBF	78.19		FBF
5902	C6 H10 N6	5.555	166.0976	FBF	71.20		FBF
5903	C12 H22 S2	5.529	230.1151	FBF	62.96		FBF
5904	C6 H12 S	0.383	116.0657	FBF	72.11		FBF
5905	C9 H20 S2	1.110	192.0993	FBF	60.16		FBF
5906	C6 H14 S	7.920	118.0807	FBF ERE	74.12		FBF FBF
5907 5908	C4 H7 N S2 C6 H11 N S2	0.357 1.552	133.0019 161.0340	FBF FBF	59.61 63.74		FBF
5908	C6 H11 N S2 C7 H14 S2	1.396	162.0525	FBF	80.74		FBF
5910	C5 H12 S2	19.746	136.0376	FBF	65.50		FBF
5911	C18 H18 O6	0.435	330.1102	FBF	62.74		FBF
5912	C18 H10 O2	1.422	258.0702	FBF	59.01		FBF



Compound Summary	Farmer I.			CAC		C (11h)	
Cpd Name	Formula C14 H10 O3	RT	Mass	CAS ID Source FBF	Score	Score (Lib) Score (DB) Score (MFG)	
5913 5914	C30 H18 O8	9.506 6.023	226.0645 506.0980	FBF	63.06 56.76		FBF FBF
915	C18 H12	2.877	228.0947	FBF	54.11		FBF
916	C22 H14	3.735	278.1100	FBF	79.22		FBF
917	C30 H19 N O9	5.893	537.1047	FBF	66.90		FBF
918	C30 H35 N O11	3.943	585.2185	FBF	52.05		FBF
919	C22 H19 Cl O3	9.402	366.1044	FBF	54.64		FBF
920	C29 H26 O10	6.257	534.1525	FBF	53.55		FBF
921	C15 H14 O2	0.409	226.1001	FBF	81.69		FBF
922	C10 H6 O2	0.435	158.0368	FBF	78.38		FBF
923	C26 H29 N O2	2.695	387.2177	FBF	65.05		FBF
924	C14 H12 O	0.461	196.0893	FBF	58.63		FBF
925	C16 H16 O3	7.972	256.1119	FBF	50.87		FBF
926	C26 H29 N O	3.007	371.2232	FBF	82.99		FBF
927	C26 H28 CI N O	3.085	405.1854	FBF	70.57		FBF
928	C24 H26 O6	2.981	410.1766	FBF	57.15		FBF
929	C38 H44 O8	4.125	628.3071	FBF	61.62		FBF
930	C13 H8 O5	6.725	244.0356	FBF	69.66		FBF
931 932	C19 H18 O10	6.699	406.0926	FBF	64.28		FBF
933	C29 H35 N O5 C21 H24 O5	3.527 2.695	477.2493 356.1653	<u>FBF</u> FBF	57.80 67.41		FBF FBF
934	C27 H31 O16	6.205	611.1633	FBF	50.11		FBF
935	C30 H27 O13	18.472	595.1473	FBF	67.76		FBF
936	C28 H33 O15	17.771	609.1792	FBF	55.02		FBF
937	C29 H35 O17	6.257	655.1868	FBF	61.42		FBF
938	C21 H19 O11	11.481	447.0949	FBF	54.22		FBF
939	C24 H25 O12	9.688	505.1389	FBF	61.64		FBF
940	C24 H25 O13	15.874	521.1286	FBF	65.18		FBF
941	C30 H22 O13	6.153	590.1100	FBF	57.17		FBF
942	C33 H24 O10	10.545	580.1398	FBF	53.94		FBF
943	C15 H12 O2	7.998	224.0841	FBF	63.54		FBF
944	C26 H32 O15	6.127	584.1750	FBF	54.01		FBF
945	C25 H28 O4	4.567	392.1994	FBF	70.58		FBF
946	C15 H12 O	9.428	208.0901	FBF	74.49		FBF
947	C18 H18 O5	8.284	314.1152	FBF	94.98		FBF
948	C26 H32 O7	13.275	456.2165	FBF	73.84		FBF
949	C35 H44 O5	5.036	544.3196	FBF	62.03		FBF
950 951	C19 H22 O3	2.019	298.1551	FBF	81.85		FBF FBF
952	C19 H16 O4 C20 H16 O5	8.336 8.284	308.1040 336.0971	FBF FBF	<u>56.84</u> 79.88		FBF
953	C20 H20 O4	7.972	324.1380	FBF	68.72		FBF
954	C22 H24 O10	13.327	448.1356	FBF	75.87		FBF
955	C28 H30 O17	6.023	638.1470	FBF	60.21		FBF
956	C25 H22 O9	11.507	466.1240	FBF	72.06		FBF
957	C30 H36 O4	4.932	460.2611	FBF	72.03		FBF
958	C17 H18 O7	9.402	334.1048	FBF	89.35		FBF
959	C16 H12 O6	0.435	300.0625	FBF	65.79		FBF
960	C19 H18 O6	6.023	342.1089	FBF	72.28		FBF
961	C29 H30 O17	6.023	650.1500	FBF	60.44		FBF
962	C30 H28 O7	14.886	500.1862	FBF	60.77		FBF
963	C27 H30 O15	6.153	594.1581	FBF	75.49		FBF
964	C29 H32 O16	6.283	636.1657	FBF	64.25		FBF
965	C20 H18 O12	10.441	450.0783	FBF	58.17		FBF
966	C24 H30 O7	7.244	430.1990	FBF	93.64		FBF
967	C13 H16 O5	5.529	252.0977	FBF	61.12		FBF
968	C14 H14 O6	6.751	278.0810	FBF	78.08		FBF
969	C27 H26 O16	5.971	606.1191	FBF	56.53		FBF
970	C20 H22 O5	16.264	342.1490	FBF	82.26		FBF
971 972	C21 H20 O4	1.993	336.1370	<u>FBF</u> FBF	69.71		FBF FBF
	C22 H22 O6 C23 H24 O6	<u>4.567</u> 5.296	382.1408 396.1593	FBF	79.14 71.70		FBF
973 974	C28 H38 N8 O4	4.229	550.3036	FBF	62.97		FBF
975	C30 H26 O11	13.977	562.1479	FBF	54.74		FBF
976	C21 H18 O4	9.818	334.1193	FBF	79.58		FBF
977	C22 H26 O5	9.532	370.1802	FBF	68.67		FBF
978	C19 H20 O5	6.075	328.1318	FBF	57.16		FBF
979	C22 H20 O7	10.026	396.1197	FBF	75.33		FBF
980	C22 H24 O5	7.244	368.1634	FBF	93.46		FBF
981	C27 H30 O12	6.257	546.1717	FBF	66.53		FBF
982	C25 H33 N O6	4.932	443.2350	FBF	62.44		FBF
983	C35 H45 N O10	12.651	639.3057	FBF	64.38		FBF
984	C35 H45 N O11	4.489	655.3026	FBF	55.20		FBF
985	C28 H50 N2 O4	10.311	478.3738	FBF	66.18		FBF
986	C38 H69 N O13	4.619	747.4795	FBF	68.49		FBF
987	C37 H67 N O12	4.958	717.4728	FBF	67.59		FBF
988	C36 H65 N O12	4.515	703.4538	FBF	74.30		FBF
989	C46 H82 N2 O16	16.784	918.5643	FBF	60.76		FBF
990	C48 H84 N2 O17	14.159	960.5715	FBF	52.46		FBF
991	C37 H61 N O11	4.854	695.4289	FBF	72.12		FBF
992	C35 H57 N O11	4.047	667.3973	FBF	67.03		FBF
993	C20 H34 O7	15.146	386.2310	FBF	59.12		FBF
994	C21 H22 N2 O3	4.463	350.1633	FBF	57.69		FBF
995	C35 H52 O9	4.671	616.3613	FBF	58.44		FBF
96	C33 H48 O9	4.515	588.3334	FBF	57.65		FBF
997	C34 H28 O22	15.718	788.1112	FBF	59.65		FBF
998	C27 H22 O18	5.763	634.0794	FBF	61.51		FBF



Com	pound	Summary
Cpd	Name	

Compound Sumn	nary								
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Scor	re (DB)	Score (MFG)	
<u>5999</u> 6000	C24 H14 O11 C39 H44 N2 O7	5.763 13.301	478.0505 652.3142	FBF FBF	55.93 56.52				FBF FBF
5001	C39 H44 N2 O7 C22 H22 N2 O8	13.301	442.1395	FBF	56.35				FBF
5002	C20 H15 N O6	9.012	365.0915	FBF	86.86				FBF
5003	C22 H23 CI N2 O8	11.481	478.1161	FBF	50.17				FBF
5004	C10 H16 S4	0.409	264.0131	FBF	73.06				FBF
5005	C25 H32 O14	6.257	556.1825	FBF	65.00				FBF
5006	C26 H21 F6 N O5	6.101	541.1277	FBF	61.22				FBF
5007	C10 H16	6.725	136.1243	FBF	77.60				FBF
5008 5009	C15 H22 O9 C24 H25 N O3	3.059 9.792	346.1254 375.1837	FBF FBF	71.32 66.40				FBF FBF
5010	C17 H26 O9	4.593	374.1601	FBF	55.21				FBF
6011	C22 H32 O8	10.909	424.2083	FBF	87.75				FBF
5012	C22 H23 N O3	9.090	349.1663	FBF	58.20				FBF
013	C38 H50 O6	6.179	602.3638	FBF	54.24				FBF
5014	C11 H14 O5	22.473	226.0857	FBF	79.32				FBF
5015	C13 H22 O	9.350	194.1664	FBF	81.84				FBF
016	C15 H20 O5	7.920	280.1310	FBF	92.85				FBF
5017 5018	C24 H34 O11 C18 H28 O11	3.657 7.920	498.2095 420.1629	FBF FBF	52.64 95.18				FBF FBF
5019	C17 H23 N O2	4.567	273.1716	FBF	53.41	,			FBF
020	C17 H26 O10	9.844	390.1515	FBF	75.12				FBF
021	C27 H36 O15	6.309	600.2068	FBF	66.65				FBF
022	C36 H52 O8	5.555	612.3689	FBF	78.89				FBF
023	C16 H30 O6	6.802	318.2031	FBF	79.19				FBF
024	C18 H20 F4 O3	9.012	360.1361	FBF	82.39				FBF
025	C26 H33 N O5	3.319	439.2371	FBF	55.64				FBF
026	C10 Cl12	5.919	539.6262	FBF	50.52				FBF
027 028	C18 H26 O C15 H20	17.667 20.161	258.1972 200.1577	FBF FBF	52.90 56.00				FBF FBF
028 029	C15 H20 C15 H18 O8	9.012	326.1015	FBF	55.00				FBF
030	C15 H18 O5	22.603	278.1134	FBF	53.60				FBF
031	C33 H50 O2	12.079	478.3845	FBF	55.12				FBF
032	C15 H24 O5	0.409	284.1622	FBF	95.72				FBF
033	C22 H26 O8	6.335	418.1633	FBF	73.21	· ·			FBF
034	C18 H31 N O2 S	4.021	325.2088	FBF	60.29				FBF
035	C12 H22 O	8.622	182.1659	FBF	86.99				FBF
036	C21 H28 O11	9.038	456.1613	FBF	66.01				FBF
)37)38	C15 H14 O C15 H20 O7	8.622	210.1049 312.1232	FBF FBF	84.28 65.37				FBF FBF
038	C15 H20 O7	9.376 7.504	296.1252	FBF	61.61				FBF
040	C43 H73 O6 P	15.406	716.5198	FBF	51.63				FBF
041	C19 H22 O4	6.958	314.1535	FBF	59.11				FBF
042	C31 H43 N O7	13.379	541.3010	FBF	66.20				FBF
043	C36 H51 N3 O10	4.776	685.3536	FBF	70.03				FBF
044	C25 H30 O4	13.353	394.2133	FBF	79.12				FBF
045	C33 H45 N O9	17.459	599.3089	FBF	73.05				FBF
<u>046</u> 047	C43 H53 N O14 C20 H28 O5 S	13.197 8.258	807.3514 380.1655	FBF FBF	59.98 56.58				FBF FBF
048	C20 H26 O5	7.244	346.1806	FBF	81.63				FBF
049	C19 H24 O7	2.643	364.1525	FBF	80.81				FBF
050	C37 H48 O10	4.125	652.3205	FBF	65.53	,			FBF
051	C22 H32 O6	7.920	392.2225	FBF	85.03				FBF
052	C20 H26 O3	8.778	314.1859	FBF	57.46				FBF
053	C36 H48 N2 O10	4.776	668.3279	FBF	70.03				FBF
054	C32 H48 O8	5.218	560.3366	FBF	52.96				FBF
055	C38 H50 N2 O11	17.199	710.3432	FBF	60.72				FBF
056	C20 H41 O4 P	17.667	376.2707	FBF	54.22				FBF
)57)58	C17 H22 O3	16.420	274.1564	FBF FBF	67.95				FBF FBF
0 <u>58</u> 059	C22 H27 N O3 C28 H47 N O4 S	4.906 5.114	353.2000 493.3239	FBF	60.30 64.11				FBF
060	C31 H52 N2 O5 S	18.446	564.3620	FBF	55.88				FBF
061	C20 H24 O7	8.050	376.1518	FBF	80.09				FBF
062	C42 H68 O13	10.441	780.4645	FBF	50.73				FBF
063	C40 H52 O16	7.244	788.3185	FBF	55.69				FBF
064	C32 H44 O8	9.870	556.3039	FBF	67.24				FBF
065	C30 H46 O8	5.607	534.3194	FBF	62.13				FBF
066	C30 H44 O8	3.839	532.3077	FBF	58.09				FBF
)67)68	C30 H44 O7	4.229	516.3090 386.3303	FBF	60.58				FBF
)68)69	C25 H42 N2 O C25 H36 O10	13.379 3.527	386.3303 496.2282	FBF FBF	66.85 68.89				FBF FBF
070	C25 H30 O10 C27 H32 O10	8.492	516.2017	FBF	74.98				FBF
)71	C22 H34 O7	4.854	410.2283	FBF	64.22				FBF
772	C26 H30 O7	3.423	454.2029	FBF	58.36				FBF
173	C30 H52 O7 P2	18.602	586.3201	FBF	58.34				FBF
074	C30 H44 O5	13.899	484.3230	FBF	55.15				FBF
075	C34 H44 O9	4.489	596.3043	FBF	74.42				FBF
076	C25 H28 O11	3.657	504.1632	FBF	53.44				FBF
077	C35 H46 O13	14.783	674.2965	FBF	50.95				FBF
078	C46 H66 O7	5.503	730.4818	FBF	82.03				FBF
<u>)79 </u>	C40 H56 O5	10.155	616.4170	FBF	73.36				FBF
)80)81	C40 H56 C30 H40 O	15.406 9.688	536.4357 416.3057	FBF FBF	60.31 50.72				FBF FBF
082	C40 H56 O	17.459	552.4305	FBF	61.40				FBF
083	C40 H54 O	13.379	550.4127	FBF	54.25				FBF
084	C40 H54 O2	20.239	566.4085	FBF	62.13				FBF
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FBF

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Compound Sumi	mary						
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorithi
5085	C42 H58 O6	4.437	658.4265	FBF	79.90		FBF
086 087	C35 H46 O2 C24 H28 O4	3.735 5.062	498.3466 380.1998	FBF FBF	57.57 56.50		FBF FBF
088	C72 H116 O4	18.420	1044.8863	FBF	50.42		FBF
089	C40 H62	17.745	542.4802	FBF	63.78		FBF
090	C41 H60 O2	11.975	584.4640	FBF	57.36		FBF
091	C40 H50 O2	6.127	562.3814	FBF	60.58		FBF
092	C41 H60 O	18.135	568.4674	FBF	53.04		FBF
)93	C13 H18 O	13.093	190.1347	FBF	60.71		FBF
094 095	C22 H32 O9 C40 H47 N O13	4.854 12.287	440.2070 749.3039	<u>FBF</u> FBF	56.21 55.45		FBF FBF
096	C31 H38 O11	6.335	586.2382	FBF	52.12		FBF
097	C41 H68 O13	4.671	768.4620	FBF	56.76		FBF
)98	C18 H20 O5	6.880	316.1291	FBF	70.48		FBF
099	C26 H38 O7	4.984	462.2623	FBF	68.02		FBF
100	C50 H82 O	21.122	698.6387	FBF	58.45		FBF
101 102	C46 H70 O	18.732 17.303	638.5438 244.1457	FBF FBF	61.22 74.65		FBF FBF
103	C16 H20 O2 C53 H80 O2	20.707	748.6148	FBF	59.16		FBF
104	C31 H46 O3	9.142	466.3469	FBF	62.91		FBF
105	C44 H89 N O2	22.187	663.6883	FBF	57.56		FBF
106	C36 H71 N O2	13.535	549.5447	FBF	55.02		FBF
107	C38 H75 N O2	22.005	577.5798	FBF	53.35		FBF
108	C36 H69 N O2	22.836	547.5328	FBF	98.77		FBF
109	C39 H77 N O2	6.179	591.5991	FBF	54.76		FBF
110	C41 H81 N O2	21.720 21.928	619.6276 575.5623	<u>FBF</u> FBF	50.15 67.80	.	FBF FBF
111 112	C38 H73 N O2 C30 H59 N O2	21.928 16.836	465.4528	FBF	57.74		FBF
113	C50 H97 N O4	16.446	775.7435	FBF	58.31		FBF
114	C44 H87 N O3	21.097	677.6714	FBF	67.57		FBF
115	C46 H81 N O3	17.901	695.6222	FBF	52.51		FBF
116	C52 H99 N O5	17.745	817.7524	FBF	52.49		FBF
117	C38 H65 N O3	18.135	583.5008	FBF	82.91		FBF
18	C30 H61 N O3	13.041	483.4615	FBF	56.58		FBF
.19	C35 H71 N O3	19.772	553.5438	FBF	58.10		FBF
.20	C24 H49 N O4	15.042	415.3652	FBF	75.92		FBF
.21	C33 H65 N O3 C34 H67 N O3	12.625 17.459	523.4972 537.5124	<u>FBF</u> FBF	87.47 58.60		FBF FBF
123	C34 H67 N O4	17.693	553.5036	FBF	53.45		FBF
124	C34 H65 N O4	17.251	551.4910	FBF	61.87		FBF
125	C35 H69 N O3	17.070	551.5280	FBF	62.79		FBF
126	C36 H71 N O3	17.122	565.5438	FBF	62.51		FBF
127	C36 H59 N O3	13.327	553.4526	FBF	57.31		FBF
128	C37 H73 N O3	22.213	579.5596	FBF	50.72		FBF
129	C38 H73 N O4	19.434	607.5565	FBF	57.30		FBF
130 131	C39 H77 N O3 C39 H77 N O4	21.122 19.434	607.5943 623.5843	<u>FBF</u> FBF	50.89 60.11		FBF FBF
132	C40 H79 N O3	16.784	621.6080	FBF	53.59		FBF
133	C46 H91 N O3	17.563	705.6977	FBF	54.37		FBF
134	C49 H97 N O3	21.538	747.7453	FBF	59.75		FBF
135	C53 H105 N O3	19.720	803.8100	FBF	50.01		FBF
136	C32 H53 N O3	15.276	499.4031	FBF	58.63	<u> </u>	FBF
137	C34 H55 N O3	10.545	525.4205	FBF	67.93		FBF
138	C35 H65 N O4	17.277	563.4896	FBF	56.19		FBF
<u>39</u>	C39 H75 N O4 C39 H73 N O4	16.654 18.940	621.5723	<u>FBF</u> FBF	64.37		FBF FBF
. <u>40</u> .41	C39 H/3 N O4 C52 H101 N O3	18.940 21.954	619.5549 787.7822	FBF	58.85 53.50		FBF FBF
.42	C53 H103 N O3	13.249	801.7940	FBF	53.78		FBF
.43	C42 H75 N O4	21.278	657.5712	FBF	58.94		FBF
44	C45 H83 N O4	18.966	701.6339	FBF	62.48		FBF
.45	C41 H77 N O3	17.589	631.5883	FBF	57.03		FBF
46	C35 H63 N O3	12.625	545.4790	FBF	83.36		FBF
.47	C54 H107 N O3	12.495	817.8248	FBF	59.44		FBF
. <u>48</u> .49	C55 H105 N O4	20.707 12.443	843.8049 530.4374	<u>FBF</u> FBF	59.47 57.17		FBF FBF
.50	C35 H57 N O3 C37 H67 N O3	12.443	539.4374 573.5092	FBF	55.03		FBF
.51	C37 H59 N O3	14.835	565.4482	FBF	52.41		FBF
.52	C41 H75 N O3	18.031	629.5744	FBF	55.56		FBF
.53	C45 H83 N O5	18.810	717.6320	FBF	52.42		FBF
54	C53 H97 N O4	21.980	811.7404	FBF	66.65		FBF
.55	C34 H69 N O3	15.510	539.5253	FBF	83.73		FBF
.56	C34 H65 N O2	21.798	519.5019	FBF	99.22		FBF
157	C58 H63 N O3	14.835	581.4803	FBF	61.44		FBF
. <u>58</u> .59	C55 H109 N O3 C58 H111 N O5	12.885 20.473	831.8356 901.8514	FBF FBF	54.26 52.41		FBF FBF
159	C38 H69 N O3	20.473 17.537	587.5264	FBF	55.07		FBF
161	C42 H77 N O3	18.732	643.5889	FBF	57.67		FBF
162	C55 H107 N O3	22.031	829.8219	FBF	56.56		FBF
163	C60 H93 N O3	13.743	875.7140	FBF	51.85		FBF
164	C38 H71 N O2	22.395	573.5435	FBF	56.73		FBF
165	C39 H73 N O2	16.030	587.5660	FBF	53.19		FBF
166	C51 H99 N O4	19.330	789.7527	FBF	53.33		FBF
167	C53 H91 N O3	18.732	789.7026	FBF	55.80		FBF
168	C39 H65 N O3	15.978	595.4979	FBF	59.59		FBF
169	C41 H73 N O3	18.446	627.5603	FBF	58.74		FBF

FBF

58.74 60.32

18.446 18.576

C41 H73 N O3 C43 H85 N O4

6170



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Compound Sun	nmary Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB) Score (MFG) Algorithm
6171	C41 H79 N O2	5.997	617.6123	FBF	64.55	Score (Lib) Score (DB) Score (MFG) Algorithm FBF
6172	C65 H125 N O3	19.304	967.9651	FBF	50.91	FBF
6173	C59 H113 N O5	18.135	915.8615	FBF	69.94	FBF
6174	C39 H71 N O3	16.784	601.5443	FBF	56.26	FBF
6175	C39 H63 N O3	12.053	593.4860	FBF	64.60	FBF
6176 6177	C41 H71 N O3 C41 H69 N O3	16.654 16.836	625.5455 623.5265	FBF FBF	58.49 59.11	FBF FBF
6178	C30 H61 N O5	19.824	515.4533	FBF	53.57	FBF
6179	C42 H85 N O5	19.252	683.6409	FBF	52.61	FBF
6180	C43 H87 N O5	21.071	697.6560	FBF	60.97	FBF
6181	C50 H99 N O4	20.655	777.7559	FBF	55.29	FBF
6182	C54 H105 N O4	12.547	831.8018	FBF	55.12	FBF
6183	C24 H49 N O3	12.963	399.3701 331.2709	FBF FBF	55.00 78.26	FBF FBF
6184 6185	C18 H37 N O4 C30 H59 N O5	7.868 14.938	513.4394	FBF	57.81	FBF
6186	C36 H69 N O5	22.499	595.5163	FBF	59.76	FBF
6187	C38 H73 N O5	18.291	623.5478	FBF	82.84	FBF
6188	C44 H87 N O4	17.096	693.6579	FBF	50.75	FBF
6189	C44 H85 N O4	17.511	691.6476	FBF	54.02	FBF
6190	C44 H77 N O3	22.265	667.5879	FBF	78.52	FBF
6191	C58 H111 N O3 C70 H131 N O5	20.577	869.8562 1065.9962	FBF	51.53	FBFFBF
6192 6193	C34 H67 N O5	21.330 16.888	569.5019	FBF FBF	54.15 54.03	FBF
6194	C34 H67 N O3 C41 H81 N O5	19.720	667.6109	FBF	64.27	FBF
6195	C34 H65 N O5	18.524	567.4871	FBF	61.06	FBF
6196	C36 H65 N O5	10.415	591.4914	FBF	54.76	FBF
6197	C32 H57 N O4	19.278	519.4318	FBF	58.88	FBF
6198	C19 H39 N O3	7.478	329.2919	FBF	75.45	FBF
6199	C43 H85 N O2	20.473	647.6581	FBF	57.07	FBF
6200	C43 H83 N O2 C44 H81 N O2	22.083	645.6375	FBF	58.79 55.32	FBF FBF
6201 6202	C45 H85 N O3	19.304 6.101	655.6291 687.6575	FBF FBF	55.75	FBF
6203	C45 H87 N O4	18.836	705.6611	FBF	54.22	FBF
6204	C45 H83 N O3	18.680	685.6366	FBF	51.05	FBF
6205	C59 H109 N O5	21.330	911.8292	FBF	57.64	FBF
6206	C44 H89 N O5	19.694	711.6711	FBF	51.13	FBF
6207	C20 H41 N O4	11.897	359.3029	FBF	76.37	FBF
6208	C21 H43 N O3	12.755	357.3240	FBF	71.33	FBF
6209	C49 H89 N O3	18.291	739.6787	FBF	50.06	FBF
6210 6211	C45 H85 N O2 C21 H43 N O4	19.720 8.284	671.6594 373.3182	FBF FBF	52.71 55.10	FBF FBF
6212	C45 H79 N O3	19.512	681.6064	FBF	51.32	FBF
6213	C47 H93 N O4	21.200	735.7062	FBF	52.75	FBF
6214	C43 H71 N O3	14.757	649.5405	FBF	51.69	FBF
6215	C45 H85 N O4	22.005	703.6488	FBF	52.20	FBF
6216	C22 H45 N O3	9.714	371.3382	FBF	73.66	FBF
6217 6218	C22 H45 N O4	11.793 21.798	387.3335 749.7273	FBF FBF	64.23 52.62	FBF FBF
6219	C48 H95 N O4 C66 H107 N O3	20.187	961.8220	FBF	51.62	FBF
6220	C41 H83 N O3	18.550	637.6366	FBF	83.57	FBF
6221	C25 H51 N O3	16.498	413.3839	FBF	70.19	FBF
6222	C45 H91 N O3	19.434	693.6934	FBF	50.36	FBF
6223	C50 H101 N O3	19.902	763.7805	FBF	61.27	FBF
6224	C29 H59 N O3	14.990	469.4472	FBF	51.16	FBF
6225	C73 H119 N O3	17.667	1057.9149	FBF	55.64	FBF
<u>6226</u> 6227	C30 H55 N O5 C34 H61 N O5	17.927 18.836	509.4070 563.4579	FBF FBF	60.79 64.16	FBF FBF
6228	C35 H69 N O2	6.257	535.5332	FBF	67.27	FBF
6229	C81 H135 N O3	20.603	1170.0434	FBF	50.02	FBF
6230	C38 H67 N O2	22.785	569.5157	FBF	76.82	FBF
6231	C38 H63 N O4	13.275	597.4784	FBF	55.40	FBF
6232	C39 H79 N O3	18.732	609.6071	FBF	91.95	FBF
6233	C40 H73 N O5	16.732	647.5452	FBF	56.94 E9 21	FBF
<u>6234</u> 6235	C41 H77 N O5 C44 H83 N O5	21.642 17.641	663.5798 705.6265	FBF FBF	58.21 52.83	FBF FBF
6236	C44 H83 N O5 C45 H85 N O5	17.745	705.6265	FBF	62.70	FBF
6237	C47 H87 N O5	19.642	745.6595	FBF	56.04	FBF
6238	C47 H83 N O3	16.472	709.6394	FBF	83.80	FBF
6239	C48 H83 N O4	14.575	737.6322	FBF	54.49	FBF
6240	C51 H103 N O3	19.928	777.7917	FBF	52.86	FBF
6241	C52 H91 N O3	22.655	777.6972	FBF	54.32	FBF
6242	C52 H91 N O5	17.199	809.6837	FBF	54.31	FBF
6243 6244	C52 H89 N O3 C53 H107 N O3	18.680 22.914	775.6829 805.8229	FBF FBF	53.59 63.65	FBF FBF
6244	C54 H97 N O5	13.587	839.7359	FBF	63.65	FBF
6246	C54 H95 N O5	18.784	837.7200	FBF	58.18	FBF
6247	C56 H97 N O3	18.810	831.7429	FBF	53.64	FBF
6248	C57 H115 N O3	13.301	861.8872	FBF	54.23	FBF
6249	C59 H113 N O3	11.533	883.8712	FBF	58.25	FBF
6250	C65 H131 N O3	13.951	974.0111	FBF	59.01	FBF
6251	C29 H58 N O6 P	18.109	547.3981	FBF	58.01	FBF
6252	C31 H62 N O6 P	14.783	575.4314	FBF	76.63	FBF
6253 6254	C31 H60 N O6 P C32 H58 N O6 P	18.836 4.724	573.4120 583.3962	FBF FBF	65.06 56.70	FBF FBF
<u></u>		18.836	617.4771	FBF	58.11	FBF
6255	C34 H68 N O6 P					



Compound Summary							
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorith
6257	C40 H82 N O6 P	15.484	703.5853	FBF	56.36		<u>FBF</u> FBF
<u>6258</u> 6259	C42 H86 N O6 P C51 H104 N O6 P	18.498 21.382	731.6181 857.7641	<u>FBF</u> FBF	62.18 73.23		FBF
5260	C34 H58 N O6 P	6.049	607.3987	FBF	68.74	-	FBF
5261	C36 H68 N O6 P	11.065	641.4760	FBF	72.27		FBF
5262	C40 H76 N O6 P	14.809	697.5420	FBF	52.75		FBF
5263	C43 H86 N O6 P	21.148	743.6187	FBF	61.98		FBF
5264	C49 H98 N O6 P	21.928	827.7125	FBF	50.35		FBF
5265	C31 H56 N O6 P	5.270 18.914	569.3819	FBF FBF	67.28 75.70		FBF
<u>6266</u> 6267	C32 H54 N O6 P C33 H64 N O6 P	17.018	579.3688 601.4461	FBF	69.39		<u>FBF</u> FBF
6268	C36 H58 N O6 P	5.763	631.3980	FBF	54.57	-	FBF
5269	C37 H72 N O6 P	19.980	657.5101	FBF	57.56		FBF
5270	C40 H74 N O6 P	21.460	695.5239	FBF	61.59		FBF
5271	C41 H80 N O6 P	19.096	713.5727	FBF	58.34		FBF
272	C42 H82 N O6 P	19.980	727.5881	FBF	52.97		FBF
5273 5274	C45 H88 N O6 P C48 H94 N O6 P	13.847 19.642	769.6300 811.6755	<u>FBF</u> FBF	56.67 56.17		FBF FBF
5275	C52 H102 N O6 P	19.042	867.7452	FBF	53.59		FBF
5276	C37 H68 N O6 P	17.927	653.4832	FBF	61.29		FBF
277	C33 H58 N O6 P	18.914	595.3945	FBF	51.30		FBF
278	C37 H70 N O6 P	13.379	655.4936	FBF	55.21		FBF
279	C37 H62 N O6 P	17.719	647.4275	FBF	55.74		FBF
280	C33 H56 N O6 P	5.555	593.3855	FBF	66.21		FBF
281	C35 H58 N O6 P	5.737	619.4037	FBF	52.02		FBF
282	C37 H60 N O6 P	4.047	645.4154	FBF ERE	84.35		FBF
283 284	C39 H68 N O6 P C38 H64 N O6 P	17.927 10.077	677.4787 661.4460	FBF FBF	63.23 59.11		FBF FBF
285	C40 H72 N O6 P	13.405	693.5116	FBF	58.87		FBF
286	C38 H62 N O6 P	4.385	659.4292	FBF	59.78		FBF
287	C56 H112 N O6 P	18.602	925.8236	FBF	59.29		FBF
288	C39 H64 N O6 P	4.854	673.4470	FBF	91.97		FBF
289	C41 H72 N O6 P	19.980	705.5098	FBF	50.20		FBF
290	C20 H40 N O6 P	9.896	421.2603	FBF	69.66		FBF
291	C57 H114 N O6 P	19.512	939.8358	FBF	57.09		FBF
292	C40 H66 N O6 P	4.828	687.4604	FBF	58.55		FBF
<u>293 </u>	C45 H86 N O6 P C41 H68 N O6 P	14.886 5.114	767.6201 701.4740	<u>FBF</u> FBF	50.10 68.57		<u>FBF</u> FBF
295	C43 H76 N O6 P	18.992	733.5385	FBF	57.51		FBF
296	C59 H116 N O6 P	22.421	965.8531	FBF	50.02		FBF
297	C47 H90 N O6 P	12.989	795.6495	FBF	58.96		FBF
298	C47 H88 N O6 P	15.848	793.6339	FBF	57.70		FBF
299	C60 H118 N O6 P	19.304	979.8740	FBF	58.70		FBF
3300	C44 H76 N O6 P	0.383	745.5440	FBF	82.52		FBF
301	C61 H120 N O6 P	18.888	993.8857	FBF	50.88		FBF
i302 i303	C54 H109 N O5 C57 H109 N O3	13.899 21.252	851.8337 855.8389	<u>FBF</u> FBF	55.89 57.33		<u>FBF</u> FBF
304	C55 H111 N O5	13.301	865.8442	FBF	65.48		FBF
5305	C25 H51 N O4	10.415	429.3795	FBF	73.28		FBF
306	C26 H53 N O4	17.459	443.3976	FBF	97.34		FBF
307	C28 H57 N O4	17.459	471.4291	FBF	99.02		FBF
308	C32 H65 N O3	14.133	511.4952	FBF	89.28		FBF
309	C32 H65 N O4	16.602	527.4871	FBF	60.08		FBF
310	C35 H71 N O4	22.785	569.5357	FBF	53.41		FBF
311	C56 H109 N O4	12.885	859.8350 867.8423	<u>FBF</u> FBF	56.37 59.32		<u>FBF</u> FBF
312 313	C58 H109 N O3 C53 H105 N O4	20.525 14.211	819.8093	FBF	51.66		FBF
314	C55 H109 N O4	21.045	847.8371	FBF	54.84		FBF
315	C55 H107 N O4	20.213	845.8214	FBF	51.91		FBF
316	C57 H111 N O4	20.863	873.8491	FBF	53.07		FBF
317	C57 H115 N O5	22.551	893.8791	FBF	57.10		FBF
318	C56 H113 N O3	13.197	847.8722	FBF	59.34		FBF
319	C59 H117 N O5	21.097	919.8894	FBF	50.44		FBF
320	C62 H105 N O3 C62 H113 N O3	20.395 18.213	911.8052 919.8709	<u>FBF</u> FBF	51.62 57.30		FBF FBF
321 322	C62 H113 N O3	18.213	919.8709	FBF	57.30 54.45		FBF
323	C65 H127 N O3	14.653	969.9845	FBF	57.87		FBF
324	C65 H117 N O3	18.524	959.9027	FBF	80.95		FBF
325	C66 H117 N O3	19.538	971.9051	FBF	54.90		FBF
326	C68 H121 N O3	17.693	999.9318	FBF	53.01		FBF
327	C70 H129 N O3	10.935	1031.9989	FBF	54.31		FBF
328	C69 H137 N O4	15.120	1044.0496	FBF	59.71		FBF
329	C69 H135 N O5	10.935	1058.0327	FBF	57.72 F0 F3		FBF
330	C75 H133 N O3	19.954 11.897	1096.0286	<u>FBF</u> FBF	50.53 56.55		FBF FBF
331 332	C81 H145 N O3 C48 H75 N O3	11.897	1180.1217 713.5733	FBF	56.55		FBF
333	C34 H69 N O5	13.327	571.5170	FBF	63.44		FBF
334	C35 H71 N O5	6.309	585.5332	FBF	69.73		FBF
335	C48 H97 N O5	21.304	767.7335	FBF	57.99		FBF
336	C48 H93 N O5	21.408	763.7077	FBF	53.04		FBF
337	C45 H71 N O3	20.421	673.5391	FBF	51.54		FBF
338	C51 H79 N O3	16.914	753.6069	FBF	50.32		FBF
339	C33 H63 N O5	16.992	553.4761	FBF	59.41	<u> </u>	FBF
340	C37 H71 N O5	17.927	609.5329	FBF	80.88		FBF
341	C43 H83 N O5	18.966	693.6292	FBF	63.44		FBF



Cpd Name	Formula	RT	Mass	CAS ID	Source Score	Score (Lib)	Score (DB)	Score (MFG) Algorith
5343	C53 H97 N O6	17.589	843.7320	FBI				FBF
344	C53 H95 N O5	14.055	825.7203	FBI				FBF
345	C54 H107 N O5	18.654	849.8142	FBI				FBF
<u>346</u> 347	C54 H101 N O6 C54 H95 N O6	19.226 15.276	859.7640 853.7180	FBI FBI				FBF FBF
348	C55 H107 N O6	16.758	877.8130	FBI				FBF
349	C55 H103 N O6	17.641	873.7782	FBI				FBF
350	C55 H99 N O6	19.564	869.7476	FBI				FBF
351	C56 H109 N O6	17.537	891.8303	FBI	81.67			FBF
352	C56 H107 N O6	22.135	889.8096	FBI				FBF
353	C56 H105 N O5	18.654	871.7950	FBI				FBF
354 355	C56 H99 N O6 C57 H111 N O5	19.200 22.785	881.7429 889.8487	FBI				FBF FBF
356	C57 H111 N O5	18.472	887.8304	FBI				FBF
357	C57 H107 N O6	19.018	901.8139	FBI				FBF
358	C58 H107 N O5	21.174	897.8144	FBI				FBF
359	C58 H105 N O5	18.654	895.7965	FBI				FBF
360	C58 H103 N O5	14.860	893.7833	FBI				FBF
361	C60 H113 N O5	20.941	927.8545	FBI				FBF
362	C60 H109 N O5	14.886	923.8299	FBI				FBF
363	C61 H117 N O6	21.019	959.8969	FBI				FBF
364	C61 H111 N O5	19.174	937.8446	FBI FBI				FBF FBF
365 366	C63 H121 N O6 C63 H115 N O5	17.693 18.732	987.9174 965.8729	FBI				FBF
367	C63 H113 N O5	19.148	963.8651	FBI				FBF
368	C64 H127 N O5	12.495	989.9735	FBI				FBF
369	C64 H119 N O5	18.446	981.9114	FBI				FBF
370	C64 H119 N O6	20.421	997.9025	FBI				FBF
371	C64 H117 N O5	18.654	979.8923	FBI				FBF
372	C64 H115 N O6	18.472	993.8788	FBI				FBF
373	C65 H121 N O6	17.719	1011.9171	FBI				FBF
374	C65 H117 N O5	18.732	991.8930	FBI				FBF
375	C65 H117 N O6	18.369	1007.8856	FBI				FBF FBF
376 377	C66 H127 N O5 C66 H123 N O5	10.961 20.525	1013.9730 1009.9393	FBI FBI				FBF
378	C66 H121 N O6	21.304	1023.9225	FBI		 		FBF
379	C66 H119 N O5	16.602	1005.9073	FBI				FBF
380	C67 H131 N O5	10.961	1029.9999	FBI				FBF
381	C67 H121 N O6	20.291	1035.9169	FBI				FBF
382	C68 H133 N O6	21.668	1060.0189	FBI	53.22			FBF
383	C68 H131 N O6	21.876	1057.9887	FBI				FBF
384	C68 H129 N O5	20.603	1039.9900	FBI				FBF
385	C68 H127 N O5	19.434	1037.9642	FBI				FBF
386	C70 H135 N O6	11.091	1086.0281	FBI				FBF
387 388	C70 H129 N O5 C71 H137 N O5	11.065 18.732	1063.9844 1084.0468	FBI				FBF FBF
389	C71 H137 N O5	20.032	1077.9966	FBI				FBF
390	C73 H135 N O5	22.239	1106.0275	FBI				FBF
391	C74 H135 N O6	21.460	1134.0337	FBI				FBF
392	C26 H53 N O5	17.615	459.3934	FBI	53.50			FBF
393	C27 H55 N O5	15.198	473.4071	FBI	63.39			FBF
394	C36 H63 N O4	15.744	573.4739	FBI				FBF
395	C33 H59 N O4	14.912	533.4444	FBI		 		FBF
396	C39 H71 N O4	20.265	617.5344	FBI				FBF
397	C38 H65 N O4	18.576	599.4896	FBI				FBF
398 399	C39 H67 N O4 C40 H71 N O4	16.160 18.888	613.5097 629.5406	FBI FBI				FBF FBF
1 00	C40 H69 N O4	17.745	627.5236	FBI				FBF
101	C41 H71 N O4	21.876	641.5360	FBI				FBF
402	C45 H91 N O5	21.746	725.6939	FBI				FBF
103	C58 H117 N O4	11.741	891.8999	FBI	50.69			FBF
104	C61 H123 N O4	13.951	933.9499	FB	55.32			FBF
105	C83 H143 N3 O27	11.741	1613.9884	FBI				FBF
106	C61 H110 N2 O21	13.405	1206.7544	FB				FBF
107	C64 H118 N2 O21	18.888	1250.8214	FBI				FBF
108	C68 H128 N2 O22	19.980	1324.8906	FBI				FBF
109 1 10	C55 H102 N2 O16 C39 H75 N O13	17.485 10.051	1046.7195 765.5219	FBI FBI				FBF FBF
1 11	C39 F73 N O13 C41 H79 N O14	10.000	809.5485	FBI				FBF
†12	C42 H81 N O14	13.405	823.5647	FBI				FBF
13	C43 H83 N O13	20.187	821.5851	FBI				FBF
114	C44 H83 N O13	14.886	833.5904	FBI				FBF
115	C44 H83 N O14	17.277	849.5845	FBI				FBF
416	C44 H79 N O13	19.824	829.5524	FBI				FBF
417	C44 H77 N O13	20.006	827.5461	FBI				FBF
118	C46 H87 N O14	20.837	877.6116	FBI				FBF
119	C46 H81 N O13	14.809	855.5702	FBI				FBF
20	C47 H91 N O13	17.953	877.6515	FBI				FBF
421	C47 H91 N O14	13.327	893.6448	FBI				FBF
122 123	C48 H93 N O14 C48 H89 N O13	17.329 17.745	907.6544 887.6270	FBI FBI				FBF FBF
1 23	C51 H99 N O14	17.745	949.7144	FBI				FBF
124 125	C65 H127 N O13	19.642	1129.9335	FBI				FBF
126	C37 H69 N O13	21.850	735.4830	FBI				FBF
127	C38 H71 N O13	5.919	749.4919	FBI				FBF
	C39 H73 N O13	4.671	763.5068	FBI				FBF



Compound Sum							
Cpd Name	Formula C20 H73 N O14	RT	Mass 770 F076	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorithi FBF
6429 6430	C39 H73 N O14 C40 H75 N O14	15.484 10.000	779.5076 793.5253	<u>FBF</u> FBF	58.79 52.46		FBF
6431	C40 H73 N O13	13.353	775.5087	FBF	53.77		FBF
6432	C41 H77 N O14	4.750	807.5319	FBF	65.25		FBF
6433	C45 H85 N O14	17.407	863.5939	FBF	56.41		FBF
6434	C46 H85 N O14	15.276	875.5970	FBF	57.15		FBF
6435	C46 H77 N O13	13.977	851.5409	FBF	56.74		FBF
6436 6437	C48 H79 N O13	5.218	877.5478 903.6681	<u>FBF</u> FBF	62.40 50.51		FBF FBF
6438	C49 H93 N O13 C49 H93 N O14	18.472 13.353	919.6552	FBF	53.63		FBF
6439	C52 H99 N O14	21.330	961.7135	FBF	56.02		FBF
6440	C36 H65 N O14	5.503	735.4372	FBF	78.41		FBF
6441	C39 H71 N O13	5.036	761.4982	FBF	68.92		FBF
6442	C40 H73 N O14	4.750	791.5073	FBF	68.42		FBF
6443	C41 H75 N O14	5.114	805.5254	FBF	59.10		FBF
6444	C42 H77 N O14	5.633	819.5340	FBF	50.69		FBF
6445	C43 H79 N O14	14.964	833.5444	FBF	66.87		FBF
6446	C50 H91 N O14	15.640	929.6500	FBF	55.26		FBF FBF
<u>6447 </u>	C60 H113 N O13 C64 H121 N O13	21.278 19.798	1055.8221 1111.8822	<u>FBF</u> FBF	50.31 51.93		FBF
6449	C49 H83 N O13	19.954	893.5845	FBF	69.14		FBF
6450	C51 H91 N O13	19.070	925.6521	FBF	50.57		FBF
6451	C27 H51 N O14	4.385	613.3356	FBF	66.90		FBF
6452	C45 H77 N O13	14.107	839.5422	FBF	58.42		FBF
6453	C49 H81 N O13	19.980	891.5779	FBF	67.68		FBF
6454	C45 H81 N O14	18.940	859.5592	FBF	55.04		FBF
6455	C54 H105 N O14	18.680	991.7597	FBF	58.21		FBF
5456	C67 H131 N O13	11.065	1157.9543	FBF	58.46		FBF
5457 5458	C50 H83 N O13 C53 H97 N O14	13.301 13.353	905.5802 971.6866	<u>FBF</u> FBF	51.41 53.85		FBF FBF
5459	C55 H99 N O13	19.434	981.7085	FBF	58.54		FBF
5460	C56 H109 N O14	20.317	1019.7871	FBF	60.32		FBF
5461	C31 H59 N O13	13.899	653.3957	FBF	50.91		FBF
5462	C70 H133 N O13	19.382	1195.9829	FBF	54.45		FBF
5463	C31 H55 N O14	4.724	665.3636	FBF	51.94		FBF
5464	C32 H57 N O13	4.437	663.3820	FBF	79.29		FBF
465	C71 H135 N O13	21.226	1209.9931	FBF	50.21		FBF
466	C72 H139 N O13	22.213	1226.0301	FBF	54.06		FBF
5467	C57 H99 N O13	22.810	1005.7043	FBF	62.79		FBF
5468 5469	C56 H95 N O13 C60 H113 N O14	17.459 20.759	989.6812 1071.8193	<u>FBF</u> FBF	51.03 58.04		FBF FBF
5470	C36 H67 N O15	13.509	753.4512	FBF	68.69		FBF
5471	C38 H69 N O15	5.555	779.4619	FBF	64.04		FBF
6472	C38 H67 N O13	5.010	745.4669	FBF	63.38		FBF
5473	C39 H63 N O13	10.051	753.4339	FBF	71.82		FBF
6474	C40 H71 N O14	5.088	789.4932	FBF	64.19		FBF
6475	C40 H69 N O13	5.919	771.4738	FBF	52.28		FBF
5476	C42 H79 N O15	10.000	837.5470	FBF	51.51		FBF
5477	C42 H77 N O15	4.828	835.5340	FBF	75.35		FBF
<u>6478</u> 6479	C42 H75 N O15 C43 H79 N O15	5.140 5.192	833.5191 849.5507	<u>FBF</u> FBF	61.18 71.56		FBF FBF
5480	C48 H93 N O12	19.954	875.6780	FBF	64.19		FBF
5481	C48 H89 N O12	17.147	871.6425	FBF	54.20		FBF
5482	C49 H85 N O14	14.860	911.5912	FBF	55.46		FBF
5483	C50 H93 N O15	13.405	947.6556	FBF	56.88		FBF
5484	C50 H89 N O15	16.108	943.6230	FBF	55.12		FBF
5485	C50 H85 N O14	13.301	923.5999	FBF	59.95		FBF
5486	C51 H87 N O14	4.984	937.6036	FBF	57.73		FBF
5487	C51 H85 N O14	19.850	935.5943	FBF	52.73		FBF
5488 5489	C52 H81 N O13	13.873	927.5661	FBF ERE	54.31 55.29		FBF FBF
489	C54 H91 N O12 C55 H97 N O14	18.083 14.860	945.6560 995.6980	<u>FBF</u> FBF	55.29 58.60		FBF
491	C56 H89 N O13	5.062	983.6349	FBF	67.65		FBF
492	C56 H97 N O14	13.275	1007.6903	FBF	58.08		FBF
493	C87 H149 N O13	12.599	1416.0953	FBF	50.31		FBF
494	C88 H149 N O13	18.862	1428.0992	FBF	52.26		FBF
495	C90 H147 N O13	22.005	1450.0884	FBF	53.51		FBF
496	C42 H77 N O20	4.932	915.5069	FBF	69.26		FBF
497	C42 H71 N O19	4.854	893.4652	FBF	85.61		FBF
498	C44 H75 N O20	4.932	937.4889	FBF ERE	78.13 67.91		FBF FBF
5499 5500	C44 H73 N O18 C46 H83 N O18	4.906 14.159	903.4877 937.5556	<u>FBF</u> FBF	51.08		FBF FBF
501	C47 H89 N O18	14.315	955.6091	FBF	60.80		FBF
502	C48 H85 N O19	13.483	979.5710	FBF	63.09		FBF
5503	C50 H91 N O19	12.339	1009.6147	FBF	51.29		FBF
5504	C50 H87 N O19	13.691	1005.5849	FBF	56.51		FBF
5505	C55 H97 N O20	5.166	1091.6628	FBF	89.76		FBF
5506	C56 H107 N O18	17.927	1081.7488	FBF	84.36		FBF
5507	C56 H107 N O19	18.109	1097.7421	FBF	57.59		FBF
508	C58 H111 N O18	18.888	1109.7818	FBF	52.65		FBF
509	C59 H107 N O17	14.783	1101.7619	FBF	50.27		FBF
510	C60 H109 N 017	18.109	1115.7741	FBF	68.51		FBF
F11		18.550	1165.8431	FBF	56.51		FBF
	C62 H119 N O18			EDE	72 07		
511 512 513	C62 H119 N O18 C62 H107 N O17 C74 H131 N O18	17.537 20.006	1137.7506 1321.9415	FBF FBF	73.97 51.39		FBF FBF



Compound	Summary

ompound Sun	•						
Cpd Name	Formula C02 H145 N C19	RT 20.041		CAS ID Source		Score (Lib) Score (DB) Score (MFG) Algorithm
5515 5516	C82 H145 N O18 C30 H59 N O9	20.941 10.103	1432.0460 577.4195	<u>FBF</u> FBF	53.55 59.92		FBF FBF
517	C34 H67 N O8	17.901	617.4866	FBF	59.45		FBF
518	C36 H71 N O9	19.538	661.5135	FBF	50.81		FBF
519	C37 H73 N O9	19.434	675.5288	FBF	56.78		FBF
520	C38 H75 N O8	22.395	673.5460	FBF	60.71		FBF
521	C39 H77 N O9	20.161	703.5617	FBF	54.61		FBF
522 523	C42 H83 N O9 C45 H89 N O8	19.382 20.785	745.6059 771.6630	FBF FBF	57.72 57.23		FBF FBF
524	C55 H109 N O8	15.588	911.8161	FBF	59.31		FBF
525	C56 H111 N O8	14.783	925.8360	FBF	54.14	-	FBF
526	C47 H93 N O9	16.758	815.6795	FBF	51.84		FBF
527	C60 H119 N O9	19.122	997.8945	FBF	53.60		FBF
528	C63 H125 N O9	17.381	1039.9372	FBF	50.61		FBF
529	C20 H35 N O8	4.750	417.2342	FBF	53.98		FBF
530	C22 H37 N O8	3.527	443.2523	FBF	97.41		FBF
531 532	C24 H41 N O8 C25 H49 N O9	4.984 5.841	471.2807 507.3391	FBF FBF	67.37 61.31		FBF FBF
533	C29 H57 N O9	19.122	563.4060	FBF	75.57	-	FBF
534	C74 H147 N O8	11.897	1178.1205	FBF	57.58		FBF
535	C35 H69 N O10	16.940	663.4897	FBF	57.64		FBF
536	C46 H91 N O10	13.379	817.6646	FBF	57.51		FBF
537	C22 H43 N O8	4.984	449.2990	FBF	77.36		FBF
538	C54 H107 N O10	14.341	929.7916	FBF	52.80		FBF
539	C56 H111 N O10	19.018	957.8187	FBF	59.28		FBF
540 541	C16 H29 N O8 C17 H31 N O8	6.880 8.232	363.1890 377.2043	FBF FBF	60.81 59.88		FBF FBF
542	C46 H89 N O11 S	17.511	863.6197	FBF	51.00		FBF
643	C48 H91 N O11 S	20.032	889.6346	FBF	52.29		FBF
544	C28 H51 N O12 S	4.229	625.3154	FBF	57.01		FBF
545	C30 H57 N O11 S	5.607	639.3676	FBF	76.15		FBF
546	C30 H57 N O12 S	5.296	655.3548	FBF	52.09		FBF
547	C30 H55 N O11 S	4.593	637.3548	FBF	60.24		FBF
548 549	C32 H61 N O11 S C32 H59 N O11 S	4.047 4.359	667.3974 665.3845	FBF FBF	82.29 62.80		FBF FBF
550	C32 H39 N O11 S	4.437	681.4121	FBF	87.06		FBF
551	C34 H65 N O11 S	4.854	695.4292	FBF	92.01		FBF
52	C34 H65 N O12 S	4.229	711.4225	FBF	78.15		FBF
53	C34 H65 N O13 S	5.737	727.4209	FBF	62.93		FBF
54	C34 H63 N O11 S	4.932	693.4134	FBF	54.49		FBF
555	C34 H63 N O12 S	4.489	709.4101	FBF	66.97		FBF
556	C34 H57 N O11 S	14.757 4.828	687.3589	FBF FBF	55.65 62.57		FBF FBF
557 558	C35 H67 N O11 S C35 H67 N O12 S	4.541	709.4423 725.4379	FBF	79.23		FBF
559	C35 H65 N O12 S	4.906	723.4261	FBF	60.51		FBF
560	C35 H63 N O11 S	5.711	705.4093	FBF	74.73		FBF
561	C35 H61 N O11 S	4.437	703.3925	FBF	54.87		FBF
562	C35 H57 N O12 S	7.946	715.3587	FBF	57.43		FBF
563	C36 H69 N O12 S	4.958	739.4551	FBF	93.34		FBF
564	C36 H67 N O12 S	5.010	737.4384	FBF	57.35		FBF
565 566	C36 H63 N O11 S	20.707 13.327	717.4173 755.4896	FBF FBF	55.25 50.81		FBF FBF
567	C37 H73 N O12 S C37 H65 N O12 S	4.541	747.4201	FBF	59.24		FBF
568	C38 H71 N O11 S	17.070	749.4795	FBF	52.99		FBF
569	C38 H71 N O12 S	18.992	765.4676	FBF	67.33		FBF
570	C38 H69 N O11 S	4.932	747.4575	FBF	74.63		FBF
571	C38 H69 N O12 S	13.873	763.4527	FBF	54.39		FBF
572	C38 H63 N O11 S	4.567	741.4081	FBF	55.02		FBF
573 :74	C39 H77 N O11 S	0.383	767.5264	FBF ERE	72.14 51.12		FBF ERE
574 575	C39 H73 N O11 S C40 H79 N O11 S	6.673 16.160	763.4908 781.5355	FBF FBF	51.12 52.43		FBF FBF
76	C40 H77 N O11 S	13.301	795.5112	FBF	65.86		FBF
77	C40 H75 N O11 S	19.512	777.5083	FBF	75.21		FBF
78	C40 H73 N O11 S	4.724	775.4876	FBF	50.18		FBF
579	C40 H69 N O11 S	13.951	771.4571	FBF	52.60		FBF
80	C40 H67 N O11 S	4.932	769.4412	FBF	53.63		FBF
81	C41 H77 N O11 S	18.135	791.5205	FBF	51.73		FBF
83	C41 H75 N O11 S C41 H73 N O12 S	4.750 13.795	789.5083 803.4872	FBF FBF	57.24 55.63		FBF FBF
84	C41 H73 N O12 S	5.841	801.4707	FBF	65.71		FBF
85	C42 H81 N O13 S	14.107	839.5417	FBF	67.67		FBF
86	C42 H75 N O12 S	14.419	817.4977	FBF	60.62		FBF
87	C42 H71 N O11 S	13.847	797.4803	FBF	52.39		FBF
88	C43 H79 N O12 S	11.845	833.5303	FBF	55.00		FBF
89	C43 H73 N O11 S	4.750	811.4853	FBF	53.73		FBF
90	C43 H73 N O12 S	13.223	827.4850	FBF	56.98		FBF
591	C44 H87 N O12 S	17.719	853.6009 847.5489	FBF ERE	51.89		FBF ERE
592 593	C44 H81 N O12 S C44 H77 N O11 S	14.783 13.431	847.5489 827.5220	FBF FBF	60.76 52.26		FBF FBF
594	C44 H77 N O11 S C44 H73 N O11 S	5.633	827.5220 823.4882	FBF	56.90		FBF
595	C45 H89 N O11 S	13.197	851.6113	FBF	50.31		FBF
596	C45 H87 N O11 S	13.327	849.5961	FBF	55.00		FBF
	C45 H77 N O12 S	4.854	855.5113	FBF	53.04		FBF
597							
597 598 599	C45 H75 N O11 S C46 H85 N O12 S	13.951 22.083	837.5027 875.5778	FBF FBF	51.42 51.85		FBF FBF



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Analysis Report											
Compound Summary											
Cpd Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG) Algorithm		
6601	C46 H79 N O12 S	18.940	869.5391		FBF	75.78			FBF		
6602	C46 H77 N O11 S	14.081	851.5202		FBF	56.09			FBF		
6603	C47 H89 N O11 S	9.870	875.6140		FBF	87.22			FBF		
6604	C47 H83 N O10 S	9.948	853.5736		FBF	85.57		-	FBF		
6605	C47 H83 N O11 S	13.327	869.5632		FBF	51.81		-	FBF		
6606	C48 H95 N O11 S	16.680	893.6681		FBF	57.99		-	FBF		
6607	C48 H85 N O11 S	14.835	883.5843		FBF	85.84			FBF		
6608	C48 H85 N O12 S	22.525	899.5731		FBF	50.01			FBF		
6609	C48 H83 N O11 S	14.886	881.5678		FBF	58.90			FBF		
6610	C48 H81 N O11 S	13.925	879.5554		FBF	79.30			FBF		
6611	C48 H79 N O12 S	14.860	893.5298		FBF	51.41			FBF		
6612	C49 H87 N O11 S	9.948	897.5954		FBF	74.78			FBF		
6613	C49 H85 N O11 S	4.932	895.5832		FBF	70.64			FBF		
6614	C49 H85 N O12 S	19.850	911.5783		FBF	56.67			FBF		
6615	C50 H95 N O12 S	17.225	933.6576		FBF	50.42			FBF		
6616	C50 H89 N O11 S	19.928	911.6166		FBF	68.65			FBF		
6617	C50 H85 N O11 S	5.711	907.5841		FBF	50.51			FBF		
6618	C50 H83 N O11 S	14.886	905.5693		FBF	82.14			FBF		
6619	C50 H83 N O12 S	5.270	921.5715		FBF	60.26			FBF		
6620	C51 H99 N O11 S	21.928	933.6928		FBF	57.64			FBF		
6621	C51 H99 N O12 S	19.408	949.6912		FBF	65.94			FBF		
6622	C51 H95 N O11 S	21.746	929.6655		FBF	50.83			FBF		
6623	C51 H89 N O12 S	4.984	939.6101		FBF	64.93			FBF		
6624	C51 H87 N O12 S	14.341	937.5972		FBF	73.54			FBF		
6625	C52 H99 N O12 S	14.757	961.6882		FBF	69.28			FBF		
6626	C52 H97 N O12 S	13.301	959.6725		FBF	56.27			FBF		
6627	C52 H93 N O11 S	16.498	939.6460		FBF	85.53			FBF		
6628	C52 H89 N O12 S	16.420	951.6190		FBF	53.33			FBF		
6629	C53 H105 N O12 S	19.980	979.7448		FBF	51.20			FBF		
6630	C53 H103 N O12 S	14.835	977.7141		FBF	57.39			FBF		
6631	C54 H103 N O11 S	21.538	973.7241		FBF	50.14			FBF		
6632	C54 H101 N O11 S	20.733	971.7122		FBF	52.93			FBF		
6633	C54 H97 N O11 S	16.498	967.6791		FBF	68.78			FBF		
6634	C54 H95 N O11 S	16.524	965.6657		FBF	51.02			FBF		
6635	C55 H105 N O12 S	21.694	1003.7364		FBF	50.76			FBF		
6636	C55 H103 N 012 S	14.912	983.7078		FBF	54.77			FBF		
6637	C55 H101 N O12 S	14.835	999.7031		FBF	52.49			FBF		
6638	C55 H97 N O11 S	21.720	979.7031		FBF	59.35			FBF		
0030	C33 H3/ N O11 3	21./20	3/3.0/1/		I DF	23.22			ГОГ		

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80.27

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C56 H111 N O11 S

C56 H95 N O11 S

C57 H109 N O11 S

C58 H111 N O12 S

C58 H109 N O12 S

C59 H115 N O11 S

C59 H109 N O11 S

C59 H99 N O11 S

C60 H115 N O11 S

C60 H109 N O12 S

C60 H107 N O12 S

C63 H125 N O11 S

C64 H125 N O11 S

C71 H141 N O11 S

C30 H57 N2 O6 P

C33 H69 N2 O7 P

C36 H67 N2 O6 P

C39 H79 N2 O7 P

C27 H53 N2 O7 P

C30 H53 N2 O6 P

C35 H67 N2 O6 P

C38 H73 N2 O7 P

C38 H65 N2 O6 P

C26 H49 N2 O7 P

C32 H59 N2 O7 P

C35 H65 N2 O6 P

C37 H69 N2 O6 P

C39 H67 N2 O6 P

C26 H55 N2 O6 P

C28 H59 N2 O6 P

C28 H59 N2 O7 P

C29 H61 N2 O6 P

C29 H61 N2 O7 P

C31 H65 N2 O6 P

C31 H65 N2 O7 P

C32 H67 N2 O6 P

C33 H69 N2 O6 P

C34 H69 N2 O6 P

C35 H73 N2 O6 P

C36 H75 N2 O6 P

C36 H71 N2 O6 P

C36 H69 N2 O6 P

C38 H79 N2 O6 P

C38 H77 N2 O7 P

14.783

16.472

18.109

17.927

17.927

20.239

17.199

16.966

17.563

20.239

17.927

19,434

18.940

18.446

10.207

13.301

10.103

17,459

4.671

18.109

17.667

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4.437

5.581

4.281

22.966

13.119

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11.845

13.379

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14.912

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19.408

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16.706

18,498

1005.7851

989.6596

1015.7745

1045.7774

1043.7736

1045.8164

1039.7715

1029.6895

1057.8219

1067.7660

1065.7564

1103.8939

1115.8983

1216.0237

572.3914

636.4827

654.4721

718.5631

548.3570

568.3671

642.4722

700.5168

676.4573

532.3291

614.4018

640.4641

668.4868

690.4779

522.3812

550.4094

566.4086

564.4279

580.4164

592.4590

608.4516

606.4754

620.4900

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662.5341

658.5024

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	nmary						
Cpd Name 6687	Formula	RT		CAS ID Source		Score (Lib) Score (DB) Score	e (MFG) Algorithm
6688	C42 H85 N2 O6 P C42 H83 N2 O7 P	22.239 20.032	744.6179 758.5942	<u>FBF</u> FBF	52.63 52.92		FBF FBF
689	C49 H101 N2 O6 P	18.550	844.7404	FBF	64.26		FBF
690	C26 H53 N2 O6 P	19.408	520.3639	FBF	87.77		FBF
691	C26 H53 N2 O7 P	17.927	536.3591	FBF	92.37		FBF
692	C27 H55 N2 O7 P	5.919	550.3737	FBF	53.33		FBF
693	C28 H57 N2 O6 P	18.135	548.3944	FBF	71.41		FBF
694	C30 H61 N2 O7 P	10.103	592.4209	FBF	62.90		FBF FBF
695 696	C30 H59 N2 O6 P C33 H67 N2 O7 P	18.498 13.353	574.4116 634.4672	FBF FBF	77.58 55.97		FBF
6697	C38 H75 N2 O7 P	11.013	702.5305	FBF	65.00		FBF
5698	C41 H83 N2 O7 P	18.706	746.5948	FBF	55.42		FBF
5699	C52 H105 N2 O6 P	15.016	884.7700	FBF	70.68		FBF
5700	C27 H53 N2 O6 P	5.166	532.3649	FBF	82.61		FBF
5701	C28 H55 N2 O7 P	17.589	562.3741	FBF	75.13		FBF
5702	C29 H57 N2 O6 P	22.057	560.3995	FBF	50.73		FBF
6703 6704	C29 H57 N2 O7 P C30 H59 N2 O7 P	5.244 17.589	576.3909 590.4050	FBF FBF	85.52 75.89		FBF FBF
5705	C36 H61 N2 O6 P	19.954	648.4297	FBF	58.81		FBF
6706	C42 H69 N2 O6 P	13.275	728.4948	FBF	54.89		FBF
5707	C49 H97 N2 O6 P	13.249	840.7052	FBF	53.21		FBF
5708	C53 H105 N2 O6 P	14.107	896.7783	FBF	52.80		FBF
5709	C28 H51 N2 O7 P	6.127	558.3432	FBF	52.14		FBF
5710	C34 H55 N2 O6 P	4.932	618.3803	FBF	92.15		FBF
5711 5712	C39 H73 N2 O6 P C39 H71 N2 O6 P	13.301 17.901	696.5246 694.5054	FBF FBF	57.89 63.45		FBF FBF
5713	C39 H69 N2 O6 P	20.785	692.4889	FBF	66.67		FBF
5714	C43 H89 N2 O7 P	14.835	776.6353	FBF	70.87		FBF
5715	C43 H87 N2 O7 P	18.836	774.6328	FBF	57.14		FBF
5716	C37 H65 N2 O6 P	17.667	664.4542	FBF	54.63		FBF
5717	C37 H63 N2 O6 P	19.980	662.4472	FBF	80.47		FBF
5718	C39 H75 N2 O7 P	10.181	714.5290	FBF	53.25		FBF
5719 5720	C43 H85 N2 O7 P	20.499 18.706	772.6069 956.8603	FBF FBF	51.45 54.03		FBF FBF
5721	C57 H117 N2 O6 P C40 H69 N2 O6 P	19.980	704.4826	FBF	55.32		FBF
5722	C44 H75 N2 O6 P	13.405	758.5327	FBF	55.12		FBF
5723	C42 H75 N2 O6 P	19.070	734.5367	FBF	57.72		FBF
5724	C44 H87 N2 O7 P	22.369	786.6244	FBF	53.50		FBF
5725	C45 H91 N2 O7 P	13.743	802.6550	FBF	52.82		FBF
5726	C41 H71 N2 O6 P	19.954	718.5089	FBF	75.89		FBF
5727	C58 H115 N2 O6 P	17.719	966.8520	FBF	60.18		FBF
5728 5729	C42 H73 N2 O6 P C47 H97 N2 O7 P	19.954 13.717	732.5255 832.7030	FBF FBF	66.69 55.67		FBF FBF
5730	C60 H123 N2 O6 P	19.642	998.9120	FBF	74.84		FBF
5731	C43 H75 N2 O6 P	19.980	746.5366	FBF	90.11		FBF
5732	C47 H91 N2 O6 P	15.796	810.6659	FBF	57.33		FBF
6733	C47 H91 N2 O7 P	17.589	826.6572	FBF	56.96		FBF
5734	C60 H119 N2 O6 P	17.303	994.8815	FBF	69.35		FBF
6735	C48 H89 N2 O6 P	13.873	820.6470	FBF	56.77		FBF
<u>6736</u> 6737	C44 H77 N2 O6 P C48 H95 N2 O7 P	19.928 17.303	760.5534 842.6894	FBF FBF	55.21 51.30		FBF FBF
6738	C49 H101 N2 O7 P	20.889	860.7315	FBF	57.11		FBF
5739	C45 H79 N2 O6 P	19.980	774.5683	FBF	50.69		FBF
5740	C49 H99 N2 O7 P	17.459	858.7105	FBF	55.06		FBF
6741	C45 H77 N2 O6 P	10.857	772.5526	FBF	88.85		FBF
6742	C50 H103 N2 O7 P	17.459	874.7561	FBF	53.74		FBF
5743	C50 H93 N2 O6 P	17.199	848.6760	FBF	51.86		FBF
5744	C50 H89 N2 O6 P	19.876	844.6488	FBF	58.82		FBF
5745 5746	C50 H99 N2 O7 P C50 H85 N2 O6 P	19.954 14.081	870.7138 840.6134	FBF FBF	54.51 53.66		FBF FBF
5747	C54 H109 N2 O7 P	19.720	928.8012	FBF	58.38		FBF
5748	C45 H90 N O12 P	14.029	867.6202	FBF	50.57		FBF
5749	C30 H60 N O11 P	4.802	641.3914	FBF	55.70		FBF
5750	C32 H64 N O11 P	5.400	669.4183	FBF	51.91		FBF
5751	C38 H74 N O12 P	5.581	767.4989	FBF	53.58		FBF
5752	C39 H78 N O11 P	0.383	767.5261	FBF	67.72		FBF
5753 5754	C56 H112 N O11 P C36 H70 N O12 P	18.602 4.541	1005.7999 739.4564	FBF FBF	51.51 60.88		FBF FBF
5755	C36 H70 N O12 P	13.379	781.5119	FBF	54.99		FBF
5756	C41 H80 N O12 P	10.000	809.5485	FBF	64.05		FBF
5757	C49 H88 N O12 P	14.860	913.6042	FBF	52.75		FBF
5758	C51 H102 N O12 P	21.798	951.7202	FBF	55.44		FBF
5759	C52 H100 N O12 P	21.330	961.6974	FBF	58.23		FBF
5760	C66 H132 N O11 P	10.961	1145.9450	FBF	51.66		FBF
5761	C54 H102 N O12 P	20.473	987.7185	FBF	53.83		FBF
5762 5763	C56 H102 N O12 P	13.327 16.212	1011.7055 960.7120	FBF FBF	55.31 57.26		FBF FBF
6764	C59 H97 N2 O6 P C59 H95 N2 O6 P	14.237	958.6981	FBF	51.02		FBF
6765	C60 H117 N2 O6 P	18.992	992.8594	FBF	50.08		FBF
5766	C22 H43 N2 O6 P	3.527	462.2853	FBF	86.29		FBF
6767	C23 H45 N2 O6 P	3.839	476.3017	FBF	90.02		FBF
5768	C25 H49 N2 O6 P	4.515	504.3296	FBF	68.64		FBF
	000 1144 110 04 0	2.005	460.2701	FBF	66.96		FBF
6769	C22 H41 N2 O6 P	3.865					
	C22 H41 N2 O6 P C24 H45 N2 O6 P C20 H43 N2 O6 P	5.503 7.920	488.3032 438.2833	FBF FBF	66.54 66.82		FBF FBF



Compound Sumi	mary					
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB) Score (MFG) Algo
773	C52 H83 N2 O6 P	16.654	862.5946	FBF	53.25	FBF
774 775	C64 H101 N2 O6 P	17.667 6.049	1024.7384 508.3608	FBF FBF	50.32 66.72	FBF_
776	C25 H53 N2 O6 P C67 H115 N2 O6 P	18.550	1074.8504	FBF	53.34	FBF
777	C67 H131 N2 O6 P	11.091	1090.9737	FBF	57.96	FBF
778	C45 H79 N2 O7 P	16.628	790.5682	FBF	54.90	FBF
779	C24 H49 N2 O7 P	0.383	508.3268	FBF	75.46	FBF
780	C24 H47 N2 O6 P	11.117	490.3204	FBF	55.88	FBF
781	C25 H51 N2 O6 P	9.818	506.3472	FBF	69.65	FBF
782 783	C64 H127 N2 O6 P C25 H49 N2 O7 P	21.382 4.021	1050.9451 520.3278	<u>FBF</u> FBF	59.32 91.16	FBF_
784	C48 H85 N2 O6 P	17.433	816.6145	FBF	50.36	FBF
785	C53 H107 N2 O7 P	15.042	914.7781	FBF	73.08	FBF
786	C49 H85 N2 O6 P	14.549	828.6144	FBF	51.41	FBF
787	C73 H127 N2 O6 P	17.719	1158.9510	FBF	59.25	FBF
788	C29 H59 N2 O8 P	5.971	594.3994	FBF	57.75	FBF
789 790	C29 H57 N2 O8 P C31 H57 N2 O8 P	4.802 5.971	592.3833 616.3832	FBF FBF	70.64 59.98	FBF_
791	C32 H57 N2 O7 P	4.281	612.3962	FBF	61.57	FBF
792	C34 H69 N2 O5 P	17.901	616.4937	FBF	58.41	FBF
793	C35 H73 N2 O8 P	13.951	680.5138	FBF	52.73	FBF
794	C39 H81 N2 O8 P	14.497	736.5699	FBF	50.12	FBF
795	C39 H77 N2 O8 P	10.181	732.5419	FBF	65.11	FBF
796 797	C40 H71 N2 O7 P	10.103 16.576	722.4991 768.5403	FBF FBF	79.39 51.44	FBF_ FBF
797 798	C42 H77 N2 O8 P C43 H75 N2 O5 P	18.654	730.5421	FBF	54.16	FBF
799	C44 H73 N2 O6 P	13.327	756.5232	FBF	54.21	FBF
800	C45 H91 N2 O8 P	17.044	818.6499	FBF	57.98	FBF
801	C45 H75 N2 O6 P	16.498	770.5314	FBF	56.63	FBF
802	C45 H75 N2 O7 P	19.902	786.5300	FBF	67.34	FBF
803 804	C47 H95 N2 O8 P C47 H89 N2 O8 P	13.483 16.498	846.6808 840.6358	<u>FBF</u> FBF	56.27 57.39	FBF_
805	C48 H79 N2 O6 P	17.823	810.5663	FBF	51.33	FBF
806	C48 H93 N2 O5 P	18.654	808.6847	FBF	55.35	FBF
807	C49 H101 N2 O8 P	12.833	876.7319	FBF	63.86	FBF
808	C49 H99 N2 O8 P	17.485	874.7180	FBF	74.18	FBF
809	C50 H95 N2 O8 P	13.041	882.6795	FBF	54.47	FBF
810 811	C51 H91 N2 O7 P C51 H87 N2 O7 P	17.849 16.420	874.6609 870.6264	FBF FBF	62.48 51.41	FBF_
812	C53 H101 N2 O7 P	18.395	924.7310	FBF	55.54	FBF
813	C55 H107 N2 O6 P	18.550	922.7864	FBF	50.67	FBF
814	C57 H113 N2 O7 P	16.706	968.8237	FBF	51.41	FBF
815	C60 H113 N2 O7 P	18.732	1004.8295	FBF	57.60	FBF
816	C62 H123 N2 O7 P	17.537	1038.9045	FBF	58.56	FBF
817	C63 H113 N2 O6 P	17.719	1024.8321	FBF	50.94	FBF
818 819	C65 H103 N2 O7 P C65 H127 N2 O7 P	18.161 20.369	1054.7468 1078.9368	<u>FBF</u> FBF	51.18 63.38	FBF_
820	C65 H123 N2 O7 P	20.187	1074.9076	FBF	50.33	FBF
821	C57 H107 N2 O6 P	18.628	946.7873	FBF	57.26	FBF
822	C18 H39 N2 O6 P	7.920	410.2525	FBF	86.41	FBF
823	C24 H49 N2 O6 P	5.997	492.3303	FBF	53.32	FBF
824	C19 H41 N2 O5 P	12.131	408.2765 434.2949	FBF	81.58	FBF
<u>825 </u>	C21 H43 N2 O5 P C22 H47 N2 O5 P	11.637 10.597	450.3232	FBF FBF	60.20 75.04	FBF_
827	C23 H51 N2 O5 P	19.668	466.3570	FBF	62.64	FBF
828	C23 H51 N2 O6 P	4.515	482.3476	FBF	88.57	FBF
829	C25 H55 N2 O5 P	18.576	494.3844	FBF	71.23	FBF
830	C27 H59 N2 O5 P	18.628	522.4166	FBF	58.86	FBF
331 332	C18 H37 N O3 C18 H39 N O3	16.446 7.972	315.2758 317.2925	FBF FBF	68.93 83.34	FBF_
832	C18 H39 N O3 C16 H35 N O3	7.972	289.2615	FBF	99.32	FBF
834	C20 H43 N O2	8.804	329.3287	FBF	95.73	FBF
335	C19 H41 N O2	8.154	315.3116	FBF	57.29	FBF
836	C20 H43 N O	13.951	313.3327	FBF	54.92	FBF
337	C22 H47 N O2	9.896	357.3599	FBF	79.93	FBF
338	C16 H34 N OF D	7.868	301.2980	FBF	99.09	FBF
839 840	C16 H34 N O5 P C19 H40 N O5 P	3.111 4.437	351.2172 393.2672	<u>FBF</u> FBF	63.94 74.60	FBF_
841	C20 H42 N O5 P	4.828	407.2768	FBF	56.33	FBF
842	C18 H38 N O4 P	4.619	363.2528	FBF	80.36	FBF
843	C14 H27 N O2	7.244	241.2034	FBF	53.80	FBF
844	C28 H58 N2 O4	15.354	486.4381	FBF	67.02	FBF
845	C34 H59 N O13	5.400	689.4025	FBF	53.17	FBF
<u>846 </u>	C33 H57 N O15 C33 H57 N O13	4.828 4.932	707.3799 675.3818	FBF FBF	59.17 55.30	FBF_
848	C18 H39 N O	9.480	285.3025	FBF	98.24	FBF
849	C19 H36 N Na O8 S	10.597	461.2088	FBF	55.50	FBF
850	C17 H37 N O2	7.426	287.2809	FBF	71.74	FBF
851	C24 H32 O3	16.576	368.2359	FBF	57.13	FBF
852	C24 H32 O5	6.075	400.2234	FBF	60.90	FBF
353	C24 H40 O8 S	4.047	488.2473	FBF	54.13	FBF
354	C29 H52 N4 O4	14.419	520.3983	FBF	70.28	FBF
355 356	C29 H52 N4 O3 C30 H52 N4 O5	10.831 15.354	504.4021 548.3923	FBF FBF	93.87 51.36	FBF_
857	C28 H46 N2 O7	5.529	522.3296	FBF	51.45	FBF
	C29 H52 N2 O4	17.693	492.3968	FBF	50.22	FBF



Compound	l Summary

Compound Summary							
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB) S	core (MFG) Algorithm
<u>6859</u> 6860	C29 H52 N2 O3 C32 H58 N2 O7 S	20.161 4.645	476.3984 614.3923	<u>FBF</u> FBF	66.05 64.27		FBF FBF
6861	C24 H40 O7 S	3.631	472.2517	FBF	60.79		FBF
6862	C24 H40 O10 S2	6.283	552.2074	FBF	55.86		FBF
6863	C27 H45 N O6 S	11.325	511.2975	FBF	52.03		FBF
5864	C27 H45 N O5 S	5.036	495.3008	FBF	70.67		FBF
5865	C24 H34 O5	5.296	402.2401	FBF	55.19		FBF
5866	C33 H49 N O8	4.958	587.3489	FBF	55.44		FBF
5867 5868	C33 H53 N O12	5.348 7.582	655.3572 545.2646	FBF FBF	50.99 60.47		FBF FBF
5869	C26 H43 N O9 S C26 H42 N O7 S	7.582	545.2646	FBF	66.97		FBF
5870	C30 H47 N3 O6	19.044	545.3470	FBF	79.19		FBF
5871	C30 H47 N3 O5	10.259	529.3537	FBF	51.06		FBF
5872	C24 H40 O6 S	3.345	456.2538	FBF	58.18		FBF
5873	C30 H52 N2 O6	20.317	536.3875	FBF	62.18		FBF
5874	C31 H52 N2 O7	19.044	564.3750	FBF	76.83		FBF
6875	C31 H52 N2 O6	18.109	548.3843	FBF	84.31		FBF
5876 5877	C33 H49 N O6	4.047	555.3540	FBF	65.90		FBF
5878	C33 H49 N O5 C33 H59 N3 O5	4.541 12.053	539.3595 577.4444	<u>FBF</u> FBF	69.57 50.75		FBF FBF
5879	C34 H64 N4 O4	11.091	592.4943	FBF	61.68		FBF
5880	C26 H43 N O10 S2	6.361	593.2296	FBF	63.36		FBF
5881	C26 H45 N O10 S2	4.489	595.2488	FBF	86.23		FBF
5882	C35 H50 N2 O5	17.381	578.3685	FBF	58.50		FBF
883	C27 H48 O7	10.259	484.3402	FBF	90.72		FBF
884	C27 H44 O6	9.636	464.3125	FBF	55.06		FBF
885	C27 H48 O8 S	3.839	532.3079	FBF	81.53		FBF
5886 5887	C34 H52 O8 C27 H44 O	4.750 18.161	588.3625 384.3399	<u>FBF</u> FBF	56.83 55.25		FBF FBF
5888	C33 H52 O7	5.503	560.3701	FBF	96.55		FBF
5889	C20 H24 O2	4.125	296.1789	FBF	54.19		FBF
5890	C19 H26 O	0.409	270.1960	FBF	59.14		FBF
891	C18 H24 O3	17.563	288.1752	FBF	53.43		FBF
892	C19 H26 O3	9.350	302.1867	FBF	56.27		FBF
893	C25 H32 O2	10.857	364.2421	FBF	67.24		FBF
894	C18 H30 O7	2.565	358.2001	FBF	73.38		FBF
<u>895</u> 896	C18 H28 O C18 H28 O7	8.414 9.428	260.2129	<u>FBF</u> FBF	70.05 64.64		FBF FBF
897	C18 H28 O8	2.461	356.1814 372.1787	FBF	67.91		FBF
898	C18 H26 O7	5.685	354.1696	FBF	57.83		FBF
5899	C18 H24 O7	5.867	352.1512	FBF	53.07		FBF
5900	C18 H24 O8	6.854	368.1457	FBF	71.39		FBF
5901	C18 H22 O6	9.090	334.1415	FBF	78.65		FBF
5902	C18 H20 O7	9.896	348.1223	FBF	56.90		FBF
5903	C19 H28 O6 S	7.244	384.1634	FBF	61.63		FBF
5904 5905	C19 H28 O5 S C19 H32 O6	7.244 18.602	368.1649 356.2179	<u>FBF</u> FBF	92.21 63.32		FBF FBF
5906	C19 H32 O7	3.371	372.2175	FBF	68.83		FBF
5907	C19 H30 O7	2.435	370.2026	FBF	57.28		FBF
5908	C19 H30 O8	3.007	386.1948	FBF	80.50		FBF
5909	C19 H28 O7	11.715	368.1812	FBF	52.52		FBF
910	C19 H28 O8	6.205	384.1774	FBF	74.60		FBF
911	C19 H26 O5	6.828	334.1790	FBF	51.45		FBF
912	C19 H26 O8	7.790	382.1636	FBF	78.88		FBF
913	C19 H22 O	8.908	266.1659	FBF	82.85		FBF
914 915	C27 H40 O11 C21 H30 O6	3.735 11.429	540.2545 378.2038	FBF FBF	71.59 57.73		FBF FBF
916	C21 H30 O6 C21 H34 O5 S	3.631	378.2038	FBF	77.87		FBF
i917	C22 H29 F O5	3.007	392.2021	FBF	77.54		FBF
918	C25 H34 O6	4.854	430.2349	FBF	70.13		FBF
919	C23 H30 O6	2.903	402.2078	FBF	56.89		FBF
920	C27 H34 F2 O7	18.784	508.2310	FBF	68.13		FBF
921	C23 H31 F O6	3.137	422.2109	FBF	81.28		FBF
922	C22 H28 F2 O5	5.503	410.1908	FBF	52.59		FBF
923	C24 H31 F O6	3.059	434.2101 444.1585	FBF	55.47		FBF
924 925	C22 H27 F3 O4 S C28 H40 O7	7.140 3.631	488.2819	FBF FBF	60.77 57.63		FBF FBF
926	C21 H34 O	7.296	302.2582	FBF	51.47		FBF
927	C27 H44 O8	4.854	496.3042	FBF	72.81		FBF
928	C21 H32 O5 S	9.609	396.1941	FBF	53.72		FBF
929	C21 H36 O8	3.631	416.2446	FBF	68.06		FBF
930	C21 H28 O8	3.007	408.1767	FBF	71.84		FBF
931	C21 H26 O	13.327	294.2006	FBF	72.62		FBF
932	C21 H26 O6	10.233	374.1765	FBF	53.52		FBF
933	C21 H24 O	10.883 4.229	292.1853	FBF FBF	79.82 71.73		FBF FBF
9 <u>934</u> 935	C30 H41 F O7 C24 H38 O11	4.229 4.203	532.2848 502.2396	FBF	66.73		FBF
5936	C24 H38 O13	3.735	534.2352	FBF	64.54		FBF
5937	C24 H38 O7	12.547	438.2634	FBF	66.08		FBF
5938	C24 H36 O14	4.021	548.2088	FBF	51.51		FBF
5939	C24 H32 O12	3.553	512.1917	FBF	76.63		FBF
5940	C24 H28 O8	6.647	444.1827	FBF	65.83		FBF
5941	C24 H28 O13	6.205	524.1482	FBF	50.51		FBF
942	C24 H28 O14	15.796	540.1526	FBF	56.18		FBF
943	C25 H40 O7	4.724	452.2769	FBF	65.49		FBF
5944	C25 H36 O7	5.062	448.2459	FBF	64.07		FBF



Compound Sumn	.						
Cpd Name	Formula COE H24 O12	RT	Mass 542 1093	CAS ID Source	Score	Score (Lib) Score (
<u>5945</u> 5946	C25 H34 O13 C26 H42 O11	6.257 12.469	542.1983 530.2702	FBF FBF	73.20 50.32		FBF FBF
5947	C26 H42 O12	4.359	546.2666	FBF	55.50		FBF
5948	C26 H42 O13	9.948	562.2649	FBF	57.05		FBF
5949	C26 H42 O7	4.932	466.2941	FBF	73.92		FBF
5950	C26 H38 O11	7.192	526.2398	FBF	71.70		FBF
5951	C26 H36 O13	3.735	556.2172	FBF	82.18		FBF
5952	C26 H36 O14	6.335	572.2095	FBF FBF	53.29		FBF FBF
5953 5954	C26 H34 O7 C27 H38 O8	7.920 3.397	458.2312 490.2615	FBF	75.13 57.51		FBF
5955	C27 H38 O13	3.709	570.2294	FBF	63.56		FBF
5956	C27 H38 O14	6.335	586.2298	FBF	57.02		FBF
5957	C27 H38 O7	4.984	474.2603	FBF	66.34		FBF
5958	C27 H34 O12	6.283	550.2022	FBF	66.76		FBF
5959	C27 H32 O12	14.886	548.1917	FBF	57.73		FBF
5960 5961	C28 H46 O8	5.348	510.3204	FBF	78.94		FBF
5962	C28 H46 O13 C28 H42 O9	4.489 5.581	590.2930 522.2814	FBF FBF	93.61 65.46		FBF FBF
5963	C28 H42 O11	7.894	554.2743	FBF	51.38		FBF
964	C28 H42 O14	8.544	602.2600	FBF	62.19		FBF
965	C28 H42 O7	5.503	490.2929	FBF	76.41		FBF
966	C28 H40 O10	5.503	536.2623	FBF	67.41		FBF
967	C28 H40 O14	3.943	600.2437	FBF	78.62		FBF
968	C28 H38 O10	7.894	534.2481	FBF	61.58		FBF
969 970	C28 H36 O13 C28 H34 O8	6.335 3.657	580.2136 498.2294	FBF FBF	52.32 59.79		FBF FBF
5971	C28 H34 O8 C29 H44 O7	3.735	504.3049	FBF	53.01		FBF
5972	C29 H42 O8	5.114	518.2866	FBF	54.66		FBF
5973	C29 H42 O9	3.631	534.2878	FBF	62.89		FBF
5974	C29 H42 O10	4.203	550.2784	FBF	53.33		FBF
5975	C29 H42 O14	3.943	614.2576	FBF	68.52		FBF
976	C29 H42 O7	5.062	502.2968	FBF FBF	68.26		FBF FBF
977 978	C29 H40 O13 C29 H40 O7	4.489 4.203	596.2501 500.2814	FBF	58.67 52.75		FBF
979	C29 H36 O11	6.387	560.2256	FBF	53.67		FBF
980	C30 H44 O13	4.489	612.2748	FBF	78.64		FBF
981	C30 H40 O14	8.544	624.2409	FBF	64.91		FBF
982	C30 H38 O9	4.021	542.2560	FBF	58.16		FBF
983	C30 H38 O7	3.735	510.2634	FBF	57.00		FBF
984	C31 H52 O13	12.651	632.3454	FBF	61.72		FBF
985 986	C31 H52 O7 C31 H48 O8	20.317 3.943	536.3701 548.3312	FBF FBF	54.79 61.80		FBF FBF
987	C31 H48 O13	4.125	628.3072	FBF	77.73		FBF
5988	C31 H46 O8	4.203	546.3246	FBF	63.66		FBF
5989	C31 H46 O9	5.218	562.3124	FBF	54.57		FBF
5990	C31 H46 O7	4.671	530.3270	FBF	83.69		FBF
5991	C31 H44 O13	7.296	624.2771	FBF	63.03		FBF
5992	C31 H42 O10	3.631	574.2804	FBF	53.46		FBF
5993 5994	C31 H40 O7 C31 H38 O8	3.735 3.839	524.2807 538.2602	FBF FBF	68.49 56.02		FBF FBF
5995	C31 H38 O8	18.446	564.3639	FBF	55.14		FBF
996	C32 H48 O9	4.047	576.3339	FBF	66.17		FBF
5997	C32 H48 O14	4.281	656.3084	FBF	62.63		FBF
998	C32 H46 O10	17.693	590.3142	FBF	54.29		FBF
999	C32 H42 O9	3.735	570.2851	FBF	61.79		FBF
000	C32 H42 O10	3.917	586.2824	FBF	56.38	-	FBF
7001	C32 H42 O7	21.642	538.2898	FBF	61.30 77.10		FBF FBF
<u>'002</u> '003	C32 H40 O8 C33 H56 O13	4.359 12.651	552.2744 660.3765	FBF FBF	62.40		FBF
003	C33 H52 O13	4.047	656.3398	FBF	58.20		FBF
005	C33 H50 O8	4.828	574.3533	FBF	78.89		FBF
006	C33 H50 O9	5.244	590.3476	FBF	79.15		FBF
007	C33 H50 O13	12.651	654.3273	FBF	74.99		FBF
008	C33 H50 O14	17.979	670.3201	FBF	63.84		FBF
009	C33 H48 O8 C33 H48 O13	4.541	572.3372	FBF FRE	60.30	.	FBF FRF
010 011	C33 H48 O13 C33 H46 O8	13.977 4.958	652.3093 570.3226	FBF FBF	60.39 52.85		FBF FBF
012	C33 H46 O7	6.257	554.3261	FBF	69.01		FBF
013	C33 H44 O8	3.943	568.3074	FBF	70.06		FBF
014	C33 H42 O8	3.917	566.2860	FBF	60.23		FBF
015	C34 H56 O13	5.400	672.3749	FBF	58.14		FBF
016	C34 H48 O9	18.836	600.3280	FBF	70.79		FBF
017	C34 H48 O10	12.651	616.3230	FBF	63.74		FBF
018 019	C34 H48 O7 C34 H46 O9	5.477 4.099	568.3435 598.3152	FBF FBF	72.81 79.20		FBF FBF
019	C34 H46 O9 C34 H46 O10	3.943	614.3111	FBF	62.36		FBF
020	C34 H46 O11	4.125	630.3086	FBF	56.69		FBF
022	C34 H44 O8	5.296	580.3012	FBF	58.30		FBF
023	C35 H60 O8	19.044	608.4316	FBF	63.87		FBF
024	C35 H58 O7	10.207	590.4214	FBF	69.16		FBF
025	C35 H56 O13	19.954	684.3775	FBF	51.18		FBF
026	C35 H54 O13	12.651	682.3586	FBF	74.40		FBF
027	C35 H52 O14	12.651	696.3372	FBF	69.61		FBF
028 029	C35 H48 O10 C35 H48 O14	3.865	628.3211	FBF FRE	54.15 52.57		FBF FBF
U43	C23 H40 O14	17.797	692.3018	FBF FBF	52.57 64.29		FBF



Compound Sum	•						
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorithm
7031 7032	C20 H33 N O7 C20 H31 N O7	3.293 13.353	399.2256 397.2100	<u>FBF</u> FBF	58.87 60.65		FBF FBF
7033	C20 H29 N O4	7.608	347.2109	FBF	59.07		FBF
7034	C20 H29 N O7	9.506	395.1950	FBF	71.04		FBF
7035	C20 H27 N O4	4.541	345.1923	FBF	51.65		FBF
7036	C20 H27 N O6	2.981	377.1813	FBF	68.35		FBF
7037 7038	C20 H27 N O7 C20 H27 N O8	5.789 7.790	393.1798 409.1737	FBF FBF	62.58 65.84		FBF FBF
7039	C20 H25 N O5	2.539	359.1750	FBF	55.30		FBF
7040	C20 H25 N O8	2.695	407.1589	FBF	55.25		FBF
7041	C21 H35 N O8	5.400	429.2388	FBF	53.07		FBF
7042	C21 H35 N O9	7.894	445.2293	FBF	74.49		FBF
7043 7044	C21 H31 N O4 C21 H31 N O6	9.948	361.2237	FBF	61.05		FBF FBF
7045	C21 H31 N O7	3.007 13.561	393.2154 409.2129	FBF FBF	76.95 54.41		FBF
7046	C21 H31 N O9	7.868	441.2030	FBF	51.63		FBF
7047	C21 H29 N O4	0.435	359.2100	FBF	67.22		FBF
7048	C21 H27 N O6	7.218	389.1829	FBF	60.16		FBF
7049	C21 H27 N O8	13.301	421.1766	FBF	56.81		FBF
7050	C21 H25 N O8	7.920	419.1599	FBF	90.88		FBF
7051 7052	C22 H35 N O7 C22 H33 N O7	7.244 12.391	425.2436 423.2290	FBF FBF	81.24 56.98		FBF FBF
7053	C22 H31 N O5	4.750	389.2177	FBF	81.49		FBF
7054	C22 H31 N O6	14.886	405.2188	FBF	57.49		FBF
7055	C22 H31 N O7	3.293	421.2076	FBF	68.85		FBF
7056	C22 H29 N O6	7.244	403.1991	FBF	99.10		FBF
7057	C22 H27 N O7	8.882	417.1791	FBF	72.64		FBF
7058	C23 H39 N O9	5.503	473.2647	<u>FBF</u> FBF	71.65		FBF FBF
7059 7060	C23 H33 N O5 C23 H33 N O6	4.671 5.529	403.2354 419.2338	FBF	69.65 57.49		FBF
7061	C23 H31 N O6	7.920	417.2143	FBF	67.17		FBF
7062	C23 H29 N O5	4.750	399.2062	FBF	70.57		FBF
7063	C23 H27 N O4	10.883	381.1960	FBF	69.28		FBF
7064	C24 H41 N O9	3.761	487.2787	FBF	91.62		FBF
7065	C24 H35 N O4	2.851 3.527	401.2569 465.2344	FBF FBF	68.23 72.81		FBF FBF
7066 7067	C24 H35 N O8 C24 H33 N O6	7.920	431.2311	FBF	99.60		FBF
7068	C24 H33 N O7	7.244	447.2260	FBF	90.34		FBF
7069	C24 H33 N O8	6.828	463.2208	FBF	71.72		FBF
7070	C24 H31 N O5	9.609	413.2230	FBF	63.16		FBF
7071	C24 H31 N O7	4.776	445.2099	FBF	54.12		FBF
7072	C24 H29 N O4	3.007	395.2106	FBF	61.08		FBF
7073	C25 H39 N O8	13.275	481.2682	FBF	68.15		FBF
7074 7075	C25 H37 N O6 C25 H33 N O4	4.854 5.322	447.2614 411.2387	FBF FBF	70.13 69.09		FBF FBF
7076	C26 H45 N O9	5.114	515.3073	FBF	73.79		FBF
7077	C26 H41 N O6	5.400	463.2932	FBF	59.85		FBF
7078	C26 H41 N O9	5.114	511.2774	FBF	74.82		FBF
7079	C26 H39 N O6	5.451	461.2770	FBF	58.30		FBF
7080	C26 H39 N O7	5.477	477.2701	FBF	58.30		FBF
7081	C26 H39 N O8	4.984	493.2688	FBF	68.95		FBF
7082 7083	C26 H39 N O9 C26 H37 N O7	3.735 7.920	509.2607 475.2582	FBF FBF	72.39 73.44		FBF FBF
7084	C26 H35 N O5	5.218	441.2528	FBF	77.44		FBF
7085	C26 H35 N O9	3.631	505.2322	FBF	67.99		FBF
7086	C26 H33 N O6	7.920	455.2320	FBF	55.35		FBF
7087	C27 H47 N O8	5.114	513.3312	FBF	56.57		FBF
7088	C27 H41 N O7	4.984	491.2869	FBF	66.34		FBF
7089 7090	C27 H37 N O8 C28 H43 N O6	7.244 4.047	503.2527 489.3099	FBF FBF	76.94 65.59		FBF FBF
7090 7091	C28 H39 N O6	5.322	485.2786	FBF	68.50		FBF
7092	C28 H37 N O4	4.906	451.2715	FBF	77.01		FBF
7093	C28 H37 N O6	3.527	483.2635	FBF	57.62		FBF
7094	C28 H35 N O5	4.984	465.2529	FBF	64.62		FBF
7095	C29 H43 N O8	4.359	533.3000	FBF	57.80		FBF
7096	C29 H41 N O8	7.920	531.2831	FBF	74.36	-	FBF
7097 7098	C29 H37 N O4 C30 H47 N O4	4.984 0.383	463.2695 485.3531	FBF FBF	64.64 55.68		FBF FBF
7098 7099	C30 H47 N O4	4.437	485.3531	FBF	81.55	.	FBF
7100	C30 H43 N O7	5.426	529.3052	FBF	84.15		FBF
7101	C30 H41 N O5	5.036	495.3006	FBF	60.93		FBF
7102	C30 H41 N O7	3.735	527.2896	FBF	56.77		FBF
7103	C30 H39 N O4	4.984	477.2883	FBF	55.88		FBF
7104	C31 H47 N OF	12.443	521.4087	FBF	58.04		FBF
7105	C31 H47 N O5	5.867 5.374	513.3455	FBF FRE	56.68 58.32		FBF ERE
7106 7107	C31 H43 N O6 C24 H40 O7	5.374 10.519	525.3089 440.2773	FBF FBF	58.32 59.30		FBF FBF
7108	C24 H40 O11	7.244	504.2581	FBF	79.43		FBF
7109	C24 H40 O13	4.359	536.2508	FBF	54.58		FBF
7110	C24 H34 O6	21.330	418.2364	FBF	68.99		FBF
7111	C25 H42 O11	3.735	518.2725	FBF	84.44		FBF
7112	C25 H42 O6	3.527	438.2969	FBF	55.96		FBF
7113	C26 H44 O7	5.503	468.3087	FBF	79.82		FBF
7114	C26 H44 O12	3.631	548.2849 444.2504	FBF FBF	56.45 51.55		FBF
7115	C26 H36 O6	7.894					FBF



compound Sum							
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib) Score (DB) Sco	ore (MFG) Algorith
7 <u>117</u> 7118	C27 H46 O7 C27 H46 O8	3.761 15.406	482.3232 498.3223	<u>FBF</u> FBF	93.69 55.86		FBF FBF
7119	C27 H46 O12	3.943	562.2988	FBF	85.22		FBF
7120	C28 H48 O8	5.581	512.3329	FBF	62.49		FBF
121	C28 H48 O12	4.515	576.3148	FBF	73.87		FBF
7122	C28 H48 O13	3.839	592.3149	FBF	58.82		FBF
7123	C28 H36 O6	5.763	468.2535	FBF	63.09		FBF
7124	C29 H50 O7	5.114	510.3519	FBF	57.82		FBF
7 <u>125</u> 7126	C29 H50 O8 C29 H50 O13	3.943 4.125	526.3495 606.3252	FBF FBF	96.77 86.89		FBF FBF
7127	C30 H52 O13	4.593	620.3378	FBF	51.27		FBF
7128	C31 H54 O8	5.218	554.3778	FBF	60.36		FBF
7129	C31 H40 O6	5.555	508.2848	FBF	54.71		FBF
7130	C33 H58 O13	5.426	662.3846	FBF	56.20		FBF
7131	C34 H60 O13	4.932	676.4023	FBF	69.26		FBF
7 <u>132</u> 7133	C34 H48 O6 C35 H52 O6	18.135 5.503	552.3421 568.3755	FBF FBF	61.44 66.05		FBF FBF
7134	C27 H45 N O10	5.114	543.3066	FBF	50.75		FBF
135	C27 H43 N O10	5.192	541.2886	FBF	59.74		FBF
136	C27 H41 N O10	3.397	539.2744	FBF	59.02		FBF
137	C27 H41 N O13	3.709	587.2564	FBF	63.56		FBF
138	C27 H39 N O12	7.868	569.2463	FBF	63.15		FBF
139	C27 H35 N O12	6.465	565.2182	FBF	60.51		FBF
140	C28 H45 N O12	7.686	587.2976	FBF	62.49		FBF
141 142	C28 H43 N O10 C29 H47 N O11	3.943 13.951	553.2872 585.3138	FBF FBF	73.09 52.97		<u>FBF</u> FBF
143	C29 H43 N O11	4.047	581.2891	FBF	63.93		FBF
144	C29 H43 N O13	4.489	613.2766	FBF	58.67		FBF
145	C29 H39 N O10	9.870	561.2598	FBF	62.44		FBF
146	C29 H37 N O11	3.735	575.2407	FBF	52.18		FBF
147	C30 H49 N O12	12.651	615.3198	FBF	58.66		FBF
148	C30 H47 N O11	4.125	597.3132	FBF	70.70		FBF
149 150	C30 H47 N O13 C30 H45 N O12	4.125 3.865	629.3089 611.2918	FBF FBF	52.62 59.68		FBF FBF
151	C30 H45 N O12	4.125	627.2907	FBF	61.61		FBF
152	C31 H49 N O12	3.839	627.3249	FBF	58.18		FBF
153	C31 H45 N O10	3.631	591.3077	FBF	53.46		FBF
154	C31 H45 N O12	4.671	623.3000	FBF	58.52		FBF
155	C31 H43 N O12	12.651	621.2799	FBF	68.84		FBF
156	C31 H41 N O12	3.943	619.2665	FBF	54.09		FBF
157 158	C32 H55 N O11	6.231 4.281	629.3755 641.3394	<u>FBF</u> FBF	73.10 70.69		FBF FBF
159	C32 H51 N O12 C32 H51 N O13	7.270	657.3380	FBF	52.81		FBF
160	C32 H49 N O12	4.645	639.3308	FBF	69.66		FBF
161	C32 H47 N O8	5.503	573.3309	FBF	67.51		FBF
162	C32 H47 N O10	4.645	605.3246	FBF	71.12		FBF
163	C32 H45 N O8	3.943	571.3162	FBF	53.68		FBF
164	C32 H45 N O10	6.699	603.3059	FBF	66.61		FBF
165	C32 H43 N O8	5.218	569.2971	FBF	55.87		FBF
166 167	C33 H57 N O12 C33 H55 N O12	5.685 6.283	659.3912 657.3787	<u>FBF</u> FBF	58.74 63.77		FBF FBF
168	C33 H53 N O12	5.607	639.3678	FBF	58.50		FBF
169	C33 H51 N O6	5.945	557.3725	FBF	66.33		FBF
170	C33 H47 N O7	6.283	569.3381	FBF	56.17		FBF
171	C33 H47 N O6	17.953	553.3397	FBF	89.80		FBF
172	C33 H45 N O10	14.835	615.3043	FBF	53.10		FBF
173	C33 H45 N O13	4.099	663.2922	FBF	59.94		FBF
174	C33 H43 N O7	3.943	565.3024	FBF	59.18		FBF
<u>175 </u>	C34 H55 N O11 C34 H55 N O13	5.789 4.437	653.3743 685.3645	<u>FBF</u> FBF	56.60 63.34		FBF FBF
177	C34 H53 N O13	4.776	683.3551	FBF	76.99		FBF
178	C34 H51 N O9	5.581	617.3576	FBF	89.32		FBF
179	C34 H51 N O10	12.651	633.3483	FBF	57.98		FBF
180	C34 H51 N O6	4.125	569.3728	FBF	75.27		FBF
181	C34 H49 N O9	4.125	615.3417	FBF	56.41		FBF
182	C35 H59 N O11	20.006	669.4096	FBF	59.47		FBF
<u>183 </u>	C35 H53 N O6 C35 H51 N O8	5.711 5.555	583.3872 613.3664	<u>FBF</u> FBF	62.93 55.35		FBF FBF
185	C35 H51 N O9	19.304	629.3582	FBF	56.59		FBF
186	C35 H51 N O6	5.296	581.3739	FBF	50.63		FBF
187	C35 H49 N O13	13.301	691.3231	FBF	56.28		FBF
188	C35 H47 N O8	4.099	609.3281	FBF	58.47		FBF
189	C35 H47 N O6	5.945	577.3375	FBF	56.43		FBF
190	C36 H63 N O12	4.906	701.4416	FBF	53.83		FBF
191	C36 H61 N O11	5.815	683.4222	FBF	63.13		FBF
192 193	C36 H59 N O11	4.437 4.802	681.4121	<u>FBF</u> FBF	81.01 56.53		<u>FBF</u> FBF
193	C36 H57 N O11 C36 H55 N O13	4.802 14.886	679.3983 709.3665	FBF	<u>56.53</u> 50.38		FBF
195	C36 H55 N O6	6.179	597.4030	FBF	65.84		FBF
196	C36 H53 N O8	5.737	627.3777	FBF	58.95		FBF
197	C36 H53 N O10	4.281	659.3680	FBF	53.89		FBF
198	C36 H53 N O11	4.906	675.3640	FBF	56.17		FBF
199	C36 H51 N O7	5.322	609.3683	FBF	64.62		FBF
	C36 H49 N O10	13.353	655.3357	FBF	55.23		FBF
200 201	C36 H49 N O11	17.979	671.3253	FBF	55.69		FBF



Compound Sumn								
Cpd Name 7203	Formula C37 H65 N O12	RT 5.166	Mass 715.4525	CAS ID Source FBF	Score 61.96	Score (Lib)	Score (DB)	Score (MFG) Algorithm FBF
720 3 7204	C37 H63 N O12	4.437	697.4362	FBF	56.11			FBF
7205	C37 H61 N O12	4.229	711.4224	FBF	69.03			FBF
206	C37 H61 N O13	4.385	727.4204	FBF	51.17			FBF
7207	C37 H59 N O12	4.489	709.4100	FBF	53.44			FBF
7208	C37 H57 N O11	13.275	691.3887	FBF	60.99			FBF
7 <u>209</u> 7210	C37 H55 N O7 C37 H55 N O11	5.374 13.327	625.3992 689.3753	FBF FBF	61.31 68.01			FBF FBF
7211	C37 H53 N O11	14.757	687.3583	FBF	56.76			FBF
7212	C37 H53 N O12	14.990	703.3576	FBF	52.72		-	FBF
7213	C37 H51 N O7	4.619	621.3641	FBF	83.17			FBF
7214	C37 H51 N O8	4.593	637.3630	FBF	57.62			FBF
7215	C37 H51 N O9	4.281	653.3549	FBF	57.86			FBF
7216	C37 H51 N O6	5.971	605.3721	FBF	63.60			FBF
7 <u>217</u> 7218	C18 H30 O5 S C18 H30 O6 S	2.513 13.613	358.1825 374.1760	FBF FBF	84.97 66.15			FBF FBF
7219	C18 H30 O11 S	7.244	454.1537	FBF	60.77			FBF
7220	C18 H30 O4 S	2.331	342.1884	FBF	64.92		,	FBF
7221	C18 H28 O5 S	2.461	356.1666	FBF	64.50			FBF
7222	C18 H28 O8 S	7.244	404.1477	FBF	70.37		,	FBF
7223	C18 H28 O4 S	2.721	340.1729	FBF	73.06			FBF
7224	C18 H26 O5 S	2.461	354.1508	FBF	67.36			FBF
7 <u>225</u> 7226	C18 H26 O4 S C18 H24 O4 S	10.155 1.993	338.1543 336.1393	FBF FBF	62.25 65.77			FBF FBF
7227	C18 H22 O7 S	11.481	382.1088	FBF	59.71			FBF
7228	C18 H22 O4 S	2.721	334.1240	FBF	60.30			FBF
7229	C18 H20 O6 S	0.409	364.0984	FBF	72.38			FBF
7230	C18 H20 O7 S	10.363	380.0923	FBF	67.60			FBF
7231	C18 H20 O9 S	9.922	412.0852	FBF	64.84			FBF
7232	C19 H32 O6 S C19 H32 O9 S	3.007 17.693	388.1948 436.1774	FBF FBF	70.47 73.14			FBF FBF
7233 7234	C19 H32 O10 S	7.608	452.1703	FBF	73.14			FBF
7235	C19 H32 O4 S	2.825	356.2040	FBF	81.07			FBF
7236	C19 H30 O6 S	7.244	386.1727	FBF	69.10			FBF
7237	C19 H30 O7 S	6.517	402.1683	FBF	50.08			FBF
7238	C19 H30 O8 S	6.335	418.1650	FBF	61.76			FBF
7239	C19 H30 O4 S	3.371	354.1891	FBF	78.50			FBF
7240	C19 H28 O7 S	6.153	400.1575	FBF	67.50			FBF
7241 7242	C19 H28 O10 S C19 H26 O6 S	7.244 2.617	448.1421 382.1452	FBF FBF	61.89 50.90			FBF FBF
7243	C19 H24 O5 S	9.974	364.1356	FBF	58.01			FBF
7244	C19 H24 O10 S	11.481	444.1111	FBF	61.47			FBF
7245	C19 H22 O8 S	7.218	410.1050	FBF	70.88			FBF
7246	C19 H22 O4 S	3.059	346.1254	FBF	54.92			FBF
7247	C20 H34 O5 S	2.721	386.2149	FBF	80.09			FBF
<u>7248 </u>	C20 H34 O6 S	2.903	402.2078 370.2197	FBF FBF	87.29			FBF FBF
7250	C20 H34 O4 S C20 H32 O5 S	3.007 9.844	384.1981	FBF	81.62 66.64			FBF
7251	C20 H32 O8 S	7.920	432.1791	FBF	70.85			FBF
7252	C20 H32 O4 S	2.721	368.2037	FBF	65.89			FBF
7253	C20 H28 O6 S	5.296	396.1596	FBF	71.32			FBF
7254	C20 H28 O11 S	7.244	476.1362	FBF	65.63			FBF
7255	C20 H26 O5 S	2.461	378.1492	FBF	59.64			FBF
7256 7257	C20 H26 O4 S C20 H24 O6 S	2.747 7.244	362.1555 392.1312	FBF FBF	55.76 62.54			FBF FBF
7258	C20 H24 O4 S	9.012	360.1365	FBF	67.44			FBF
7259	C21 H36 O5 S	3.085	400.2301	FBF	81.09			FBF
7260	C21 H36 O7 S	3.293	432.2212	FBF	69.61			FBF
7261	C21 H36 O4 S	3.631	384.2326	FBF	84.59			FBF
7262	C21 H34 O6 S	7.920	414.2047	FBF	75.43			FBF
7263	C21 H34 O7 S	7.244	430.1993	FBF	60.13			FBF
<u>7264 </u>	C21 H34 O8 S C21 H34 O4 S	6.802 9.480	446.1962 382.2202	FBF FBF	58.32 59.69			FBF FBF
7266	C21 H32 O4 S	16.888	380.2020	FBF	53.76			FBF
7267	C21 H30 O6 S	3.007	410.1767	FBF	83.26			FBF
7268	C21 H30 O7 S	4.750	426.1732	FBF	50.40			FBF
7269	C21 H30 O4 S	2.799	378.1850	FBF	82.52			FBF
7270	C21 H28 O9 S	5.503	456.1470	FBF	78.55			FBF
7271	C21 H28 O4 S	3.371	376.1709	FBF	79.60			FBF
<u>7272</u> 7273	C21 H26 O5 S C21 H26 O6 S	3.397 13.327	390.1516 406.1435	FBF FBF	50.68 54.52			FBF FBF
7274	C21 H26 O8 S	7.946	438.1348	FBF	62.49			FBF
7275	C21 H26 O10 S	7.244	470.1243	FBF	68.83			FBF
7276	C21 H24 O4 S	8.700	372.1403	FBF	57.18			FBF
7277	C22 H38 O5 S	3.293	414.2457	FBF	83.76	·	· · · · · · · · · · · · · · · · · · ·	FBF
7278	C22 H38 O6 S	3.085	430.2411	FBF	82.25			FBF
7279	C22 H38 O7 S	3.085	446.2337	FBF	82.18			FBF
7280	C22 H38 O9 S	3.085	478.2245	FBF	52.71			FBF
7 <u>281</u> 7282	C22 H38 O4 S C22 H36 O5 S	4.099 3.631	398.2496 412.2285	FBF FBF	85.33 64.63			FBF FBF
7282 7283	C22 H36 O5 S C22 H36 O6 S	3.631	412.2285	FBF	57.45			FBF
7284	C22 H36 O4 S	4.750	396.2341	FBF	75.49			FBF
7285	C22 H34 O4 S	4.671	394.2201	FBF	59.51			FBF
7286	C22 H32 O4 S	3.007	392.2023	FBF	84.00	-		FBF
7287	C22 H30 O5 S	3.085	406.1834	FBF	62.42			FBF
7288	C22 H28 O6 S	7.920	420.1629	FBF	56.95			FBF



Cpd Name	Formula	RT	Mass	CAS ID Source	e Score	Score (Lib)	Score (DB)	Score (MFG) Algorith
7289	C22 H26 O5 S	7.244	402.1468	FBF	77.21			FBF
290	C22 H26 O8 S	3.319	450.1354	FBF	56.67			FBF
291	C22 H26 O11 S	7.244	498.1182	FBF	64.41			FBF
<u>292 </u>	C23 H40 O5 S C23 H40 O6 S	4.854 3.397	428.2579 444.2560	FBF FBF	52.95 82.33			FBF FBF
294 294	C23 H40 O8 S	3.527	476.2476	FBF	71.13			FBF
295	C23 H38 O5 S	5.633	426.2471	FBF	54.99			FBF
296	C23 H38 O6 S	3.865	442.2412	FBF	83.48			FBF
297	C23 H38 O7 S	7.920	458.2312	FBF	52.49			FBF
298	C23 H38 O4 S	7.218	410.2527	FBF	53.00			FBF
299	C23 H36 O6 S	5.451	440.2238	FBF	56.17			FBF
7 <u>300</u> 7301	C23 H34 O5 S C23 H34 O7 S	3.137 3.423	422.2110 454.2031	FBF FBF	81.13 82.46			FBF FBF
302	C23 H32 O4 S	7.244	404.2024	FBF	66.46			FBF
303	C23 H30 O7 S	10.181	450.1723	FBF	69.84			FBF
304	C23 H30 O10 S	7.920	498.1534	FBF	70.71			FBF
305	C24 H42 O5 S	3.241	442.2773	FBF	85.97			FBF
306	C24 H42 O6 S	4.437	458.2725	FBF	85.18			FBF
307	C24 H42 O7 S	3.397	474.2672	FBF	86.48			FBF
308 309	C24 H42 O8 S C24 H38 O5 S	3.397 3.657	490.2617 438.2459	FBF FBF	78.86 61.12			FBF FBF
310	C24 H36 O5 S	3.293	436.2283	FBF	84.92			FBF
311	C24 H36 O6 S	3.085	452.2204	FBF	52.60			FBF
312	C24 H36 O10 S	8.492	516.2019	FBF	60.33			FBF
313	C24 H34 O5 S	7.790	434.2119	FBF	52.07			FBF
314	C24 H34 O6 S	3.371	450.2073	FBF	62.88			FBF
315	C24 H34 O4 S	12.781	418.2159	FBF	58.57			FBF
316	C24 H32 O5 S	14.938	432.1935	FBF	59.61			FBF
317 318	C24 H30 O5 S C24 H30 O4 S	7.920 3.631	430.1781 414.1895	FBF FBF	78.46 50.11			FBF FBF
319	C25 H44 O6 S	4.047	472.2830	FBF	67.02			FBF
320	C25 H44 O7 S	3.631	488.2821	FBF	83.54			FBF
321	C25 H44 O9 S	3.735	520.2742	FBF	69.26			FBF
322	C25 H42 O7 S	4.177	486.2681	FBF	78.86			FBF
323	C25 H42 O10 S	7.894	534.2480	FBF	66.60			FBF
324	C25 H42 O4 S	4.932	438.2793	FBF	76.74			FBF
325	C25 H40 O9 S	6.517	516.2370	FBF	56.63			FBF
3 <u>26</u> 327	C25 H40 O4 S C25 H38 O6 S	5.166 11.325	436.2661 466.2396	FBF FBF	71.94 80.86			FBF FBF
328	C25 H38 O7 S	3.293	482.2334	FBF	56.72			FBF
329	C25 H38 O8 S	3.657	498.2295	FBF	83.88			FBF
330	C25 H36 O5 S	7.244	448.2302	FBF	52.84			FBF
331	C25 H36 O6 S	3.865	464.2227	FBF	72.11			FBF
332	C25 H36 O4 S	7.218	432.2339	FBF	66.81			FBF
333	C25 H34 O4 S	3.293	430.2205	FBF	73.31			FBF
334	C25 H32 O5 S	4.750	444.1979	FBF	52.11			FBF
335 336	C25 H30 O9 S C25 H30 O10 S	6.205 13.379	506.1564 522.1577	FBF FBF	59.63 51.76			FBF FBF
337	C25 H30 O10 S	15.874	538.1553	FBF	51.59			FBF
338	C25 H30 O4 S	7.270	426.1859	FBF	52.97			FBF
339	C26 H46 O5 S	12.287	470.3066	FBF	77.12			FBF
340	C26 H46 O6 S	4.515	486.3001	FBF	82.65			FBF
341	C26 H46 O7 S	3.735	502.2982	FBF	85.89			FBF
342	C26 H46 O8 S	3.735	518.2930	FBF	62.32			FBF
343	C26 H46 O9 S	3.631	534.2879	FBF	74.26			FBF FBF
344 345	C26 H44 O6 S C26 H44 O8 S	4.437 3.839	484.2874 516.2799	FBF FBF	56.12 58.80			FBF
346	C26 H44 O9 S	4.229	532.2735	FBF	52.97			FBF
347	C26 H42 O7 S	14.835	498.2686	FBF	60.69			FBF
348	C26 H42 O8 S	7.868	514.2611	FBF	59.10			FBF
349	C26 H42 O9 S	8.336	530.2551	FBF	63.30			FBF
350	C26 H40 O6 S	3.527	480.2551	FBF	86.84			FBF
351	C26 H40 O10 S	5.503	544.2329	FBF	65.48			FBF
352	C26 H38 O6 S C26 H38 O7 S	10.649 3.631	478.2361 494.2335	FBF FBF	50.78 66.59			FBF FBF
353 354	C26 H38 O11 S	6.335	558.2153	FBF	57.40			FBF
355	C26 H36 O5 S	3.397	460.2295	FBF	88.29			FBF
356	C26 H34 O5 S	22.914	458.2101	FBF	60.96			FBF
357	C27 H48 O5 S	13.899	484.3247	FBF	62.83			FBF
358	C27 H48 O7 S	5.114	516.3104	FBF	52.92			FBF
359	C27 H48 O10 S	3.917	564.3004	FBF	69.58			FBF
360	C27 H48 O4 S	0.383	468.3266	FBF	73.74			FBF
361	C27 H46 O6 S	10.415	498.3028	FBF	50.22			FBF ERE
362 363	C27 H46 O7 S C27 H46 O8 S	5.815 4.359	514.2991 530.2947	FBF FBF	54.92 86.09	·		FBF FBF
364	C27 H44 O5 S	5.270	480.2920	FBF	63.31			FBF
365	C27 H42 O7 S	3.735	510.2634	FBF	67.90			FBF
366	C27 H42 O8 S	3.553	526.2579	FBF	55.79			FBF
367	C27 H42 O9 S	3.735	542.2562	FBF	82.43			FBF
368	C27 H40 O5 S	5.062	476.2621	FBF	52.53			FBF
369	C27 H40 O7 S	4.203	508.2490	FBF	68.34			FBF
370	C27 H40 O4 S	7.920	460.2650	FBF	64.99			FBF
371	C27 H38 O5 S	3.527	474.2466	FBF	75.56			FBF
372 373	C27 H38 O7 S	8.960	506.2292	FBF	51.30			FBF FBF
	C27 H36 O6 S	11.325	488.2212	FBF	75.60			FKF



Compound Sun	mmarv					
Cpd Name	Formula	RT	Mass (CAS ID Source	Score S	core (Lib) Score (DB) Score (MFG) Algorithm
7375	C27 H34 O5 S	17.122	470.2118	FBF	59.97	FBF
7376	C27 H34 O10 S	6.309	550.1854	FBF	71.41	FBF
7377	C27 H34 O4 S	13.275	454.2196	FBF	53.17	FBF
7378	C28 H50 O7 S	4.671	530.3272	FBF	89.97	FBF
7379 7380	C28 H50 O8 S C28 H50 O9 S	3.943 3.943	546.3253 562.3195	<u>FBF</u> FBF	86.40 60.85	FBF FBF
7381	C28 H50 O10 S	3.839	578.3146	FBF	79.53	FBF
7382	C28 H50 O4 S	6.335	482.3419	FBF	72.36	FBF
7383	C28 H48 O7 S	4.541	528.3141	FBF	59.84	FBF
7384	C28 H48 O8 S	4.359	544.3084	FBF	57.46	FBF
7385	C28 H48 O9 S	4.047	560.3071	FBF	51.15	FBF
7386	C28 H48 O4 S	5.062	480.3273	FBF	59.61	FBF
7387 7388	C28 H46 O7 S C28 H46 O10 S	4.828 3.631	526.2975 574.2804	<u>FBF</u> FBF	81.94 61.20	FBF FBF
7389	C28 H44 O5 S	13.275	492.2925	FBF	59.82	FBF
7390	C28 H44 O7 S	3.735	524.2809	FBF	85.98	FBF
7391	C28 H44 O4 S	4.984	476.2984	FBF	51.67	FBF
7392	C28 H42 O8 S	3.839	538.2579	FBF	50.52	FBF
7393	C28 H42 O10 S	6.465	570.2502	FBF	53.42	FBF
7394	C28 H40 O6 S	3.397	504.2559	FBF	75.76	FBF
7395	C28 H38 O6 S	4.203	502.2396	FBF	60.88	FBF
7396	C28 H38 O7 S	5.737	518.2312	FBF	58.36	FBF
7397 7398	C28 H38 O9 S C28 H36 O9 S	3.319 4.021	550.2202 548.2088	<u>FBF</u> FBF	50.79 55.34	FBF FBF
7399	C29 H52 O8 S	5.218	560.3366	FBF	52.64	FBF
7400	C29 H52 O9 S	4.047	576.3341	FBF	86.84	FBF
7401	C29 H50 O8 S	5.867	558.3252	FBF	57.37	FBF
7402	C29 H48 O6 S	5.374	524.3175	FBF	65.25	FBF
7403	C29 H48 O8 S	9.896	556.3038	FBF	62.50	FBF
7404	C29 H46 O6 S	5.581	522.3018	FBF	58.22	FBF
7405	C29 H46 O8 S	3.943	554.2897	FBF	63.82	FBF
7406 7407	C29 H46 O9 S C29 H46 O10 S	3.735 3.917	570.2851 586.2825	<u>FBF</u> FBF	64.76 80.45	FBF FBF
7408	C29 H44 O5 S	5.062	504.2927	FBF	51.97	FBF
7409	C29 H44 O7 S	7.920	536.2828	FBF	58.64	FBF
7410	C29 H44 O8 S	4.359	552.2740	FBF	75.80	FBF
7411	C29 H42 O6 S	3.735	518.2729	FBF	76.95	FBF
7412	C29 H42 O4 S	4.437	486.2760	FBF	52.50	FBF
7413	C29 H40 O7 S	8.102	532.2506	FBF	56.96	FBF
7414	C29 H38 O4 S	4.984	482.2484	FBF	53.12	FBF
7415	C20 H35 N O8 S	3.397	449.2112	FBF	55.68	FBF
7416 7417	C20 H33 N O5 S C20 H33 N O8 S	4.750 3.839	399.2063 447.1954	FBF FBF	73.14 71.32	FBF FBF
7418	C20 H27 N O6 S	7.244	409.1577	FBF	62.54	FBF
7419	C21 H37 N O5 S	5.296	415.2405	FBF	53.26	FBF
7420	C21 H37 N O6 S	7.920	431.2313	FBF	75.43	FBF
7421	C21 H37 N O7 S	7.244	447.2261	FBF	60.13	FBF
7422	C21 H37 N O8 S	3.839	463.2266	FBF	57.93	FBF
7423	C21 H37 N O10 S	3.527	495.2131	FBF	61.73	FBF
7424	C21 H35 N O7 S	4.854	445.2142	FBF	69.03	FBF
7425 7426	C21 H35 N O8 S C21 H33 N O5 S	10.545 15.042	461.2093 411.2092	FBF FBF	64.84 56.30	FBF FBF
7 420 7427	C21 H33 N O3 S	4.750	443.1990	FBF	50.40	FBF
7428	C21 H29 N O5 S	7.790	407.1771	FBF	60.98	FBF
7429	C21 H29 N O6 S	13.353	423.1718	FBF	51.03	FBF
7430	C21 H29 N O8 S	9.038	455.1586	FBF	63.09	FBF
7431	C22 H39 N O5 S	3.059	429.2564	FBF	62.88	FBF
7432	C22 H37 N O6 S	4.932	443.2354	FBF	80.65	FBF
7433	C22 H35 N O5 S	12.313	425.2221	FBF	57.24	FBF
7434	C22 H33 N O8 S	11.325	471.1947	FBF	68.64	FBF
7435 7436	C22 H33 N O9 S C22 H31 N O6 S	3.293 7.920	487.1888 437.1895	<u>FBF</u> FBF	54.37 56.95	FBF FBF
7437	C22 H31 N O0 S	3.319	467.1620	FBF	56.60	FBF
7438	C23 H41 N O5 S	5.633	443.2736	FBF	54.99	FBF
7439	C23 H41 N O6 S	3.839	459.2687	FBF	83.48	FBF
7440	C23 H41 N O7 S	7.920	475.2582	FBF	51.76	FBF
7441	C23 H41 N O9 S	4.255	507.2534	FBF	53.99	FBF
7442	C23 H39 N O5 S	5.218	441.2528	FBF	72.52	FBF
7443	C23 H39 N O9 S	3.631	505.2322	FBF	54.69	FBF
'444 '445	C23 H39 N O10 S	3.839	521.2314	FBF	52.41	FBF
7445 7446	C23 H35 N O8 S C23 H35 N O10 S	3.553 8.492	485.2103 517.2032	<u>FBF</u> FBF	60.31 50.27	FBF FBF
7447	C23 H33 N O10 S	4.776	467.1954	FBF	60.11	FBF
7448	C23 H31 N O7 S	3.397	465.1839	FBF	86.05	FBF
7449	C23 H31 N O9 S	6.205	497.1740	FBF	53.88	FBF
7450	C24 H43 N O6 S	3.345	473.2826	FBF	59.75	FBF
7451	C24 H43 N O8 S	4.047	505.2739	FBF	54.13	FBF
7452	C24 H43 N O10 S	3.839	537.2636	FBF	56.30	FBF
7453	C24 H41 N O5 S	4.489	455.2729	FBF	54.61	FBF
7454	C24 H41 N O8 S	7.244	503.2526	FBF	52.51	FBF
7455	C24 H41 N O10 S	4.359	535.2483	FBF	77.22	FBF
7 <u>456</u> 7457	C24 H39 N O10 S C24 H37 N O5 S	6.075 6.569	533.2295 451.2421	<u>FBF</u> FBF	52.01 52.37	FBF FBF
7458	C24 H37 N O5 S C24 H37 N O10 S	3.553	531.2147	FBF	56.93	FBF
,				FBF	65.47	
7459	C24 H33 N O7 S	3.527	479.2021	FDF		FBF



Compound Summary	Eaumoule	F-	¥4.	CAS ID C	C	Seems (Lib.) Seems (DR.) S. (MES.)
Cpd Name	Formula C24 H31 N C0 C	RT 11.299	Mass 403 1757	CAS ID Source FBF	Score	Score (Lib) Score (DB) Score (MFG) Algori
7 <u>461</u> 7462	C24 H31 N O8 S C25 H45 N O6 S	5.711	493.1757 487.2997	FBF	70.75 56.03	FBFFBF
463	C25 H45 N O10 S	3.943	551.2811	FBF	65.91	FBF
464	C25 H43 N O6 S	5.322	485.2799	FBF	66.98	FBF
465	C25 H43 N O9 S	22.109	533.2644	FBF	54.56	FBF
466	C25 H43 N O10 S	6.932	549.2637	FBF	58.41	FBF
467	C25 H41 N O6 S	3.527	483.2635	FBF	54.37	FBF
468	C25 H41 N O7 S	10.077	499.2634	FBF	64.17	FBF
469	C25 H39 N O5 S	4.984	465.2530	FBF	54.75	FBF
470	C25 H39 N O9 S	3.761	529.2347	FBF	53.82	FBF
471	C25 H35 N O8 S	7.192	509.2103	FBF	61.37	FBF FDF
472	C25 H35 N O9 S	3.501	525.1980	FBF	55.84	FBF
473	C25 H33 N O5 S	6.439	459.2125	<u>FBF</u> FBF	53.02	
<u>474 </u>	C25 H33 N O8 S C25 H33 N O9 S	4.203 7.842	507.1951 523.1883	FBF	54.14 60.53	FBF
476	C26 H47 N O8 S	4.359	533.3000	FBF	52.34	FBF
477	C26 H47 N O9 S	4.229	549.2999	FBF	52.97	FBF
478	C26 H45 N O8 S	7.920	531.2835	FBF	53.38	FBF
479	C26 H43 N O5 S	15.276	481.2842	FBF	52.30	FBF
480	C26 H43 N O10 S	9.948	561.2601	FBF	66.60	FBF
481	C26 H41 N O5 S	5.503	479.2708	FBF	62.39	FBF
182	C26 H37 N O8 S	3.735	523.2284	FBF	67.49	FBF
183	C26 H35 N O7 S	7.244	505.2144	FBF	56.37	FBF
184	C26 H35 N O9 S	8.076	537.2039	FBF	58.88	FBF
185	C27 H49 N O7 S	5.789	531.3260	FBF	54.92	FBF
486	C27 H49 N O8 S	4.359	547.3233	FBF	69.45	FBF
187	C27 H47 N O7 S	5.426	529.3045	FBF	69.35	FBF
488	C27 H45 N O7 S	3.735	527.2896	FBF	53.01	FBF
489	C27 H43 N O10 S	3.943	573.2624	FBF	50.48	FBF
190	C27 H39 N O6 S	11.351	505.2480	FBF	60.99	FBF
191 1 92	C27 H39 N O7 S C27 H39 N O8 S	10.077 7.868	521.2445 537.2449	<u>FBF</u> FBF	63.20 51.82	
1 93	C27 H39 N O10 S	3.761	537.2449	FBF	51.82	FBF
194	C27 H35 N O7 S	6.075	517.2117	FBF	54.65	FBF
195	C27 H35 N O9 S	6.283	549.2006	FBF	52.70	FBF
196	C28 H49 N O5 S	4.333	511.3336	FBF	65.27	FBF
197	C28 H49 N O10 S	3.631	591.3077	FBF	61.20	FBF
198	C28 H47 N O6 S	5.555	525.3122	FBF	55.54	FBF
199	C28 H43 N O6 S	3.397	521.2805	FBF	75.61	FBF
500	C28 H41 N O7 S	17.096	535.2578	FBF	63.04	FBF
501	C28 H41 N O9 S	4.802	567.2523	FBF	70.21	FBF
502	C28 H39 N O7 S	7.894	533.2400	FBF	57.98	FBF
503	C28 H39 N O9 S	4.021	565.2353	FBF	55.34	FBF
504	C28 H37 N O5 S	13.275	499.2378	FBF	56.42	FBF
505	C29 H53 N O5 S	14.809	527.3644	FBF	52.66	FBF
506	C29 H53 N O8 S	5.867	575.3516	FBF	53.91	FBF
507	C29 H53 N O9 S	4.515	591.3489	FBF	74.46	FBF
508 509	C29 H51 N O5 S C29 H51 N O8 S	3.943 5.685	525.3472	FBF FBF	73.53 65.64	FBFFBF
510	C29 H49 N O8 S	3.943	573.3326 571.3162	FBF	54.30	FBF
511	C29 H43 N O5 S	5.607	517.2879	FBF	52.55	FBF
512	C29 H43 N O8 S	3.709	565.2730	FBF	58.69	FBF
513	C29 H41 N O10 S	4.489	595.2486	FBF	77.11	FBF
514	C29 H39 N O10 S	6.361	593.2291	FBF	76.36	FBF
515	C30 H55 N O9 S	4.697	605.3602	FBF	66.92	FBF
516	C30 H53 N O5 S	5.633	539.3645	FBF	56.67	FBF
517	C30 H53 N O6 S	4.489	555.3608	FBF	55.21	FBF
518	C30 H53 N O9 S	17.901	603.3463	FBF	54.46	FBF
519	C30 H51 N O5 S	5.218	537.3488	FBF	64.84	FBF
520	C30 H51 N O6 S	17.953	553.3402	FBF	76.44	FBF
521	C30 H49 N O7 S	19.044	567.3280	FBF	63.70	FBF
522	C30 H49 N O8 S	18.862	583.3209	FBF	72.89	FBF
523	C30 H47 N O7 S	3.631	565.3075	FBF	61.00	FBF
524	C30 H47 N O9 S	5.218	597.3006	FBF	64.62	FBF
25	C30 H45 N O5 S	3.943	531.3051	FBF	75.80	FBF
526 527	C30 H45 N O10 S	4.125	611.2810	FBF ERE	71.01	FBFFBF
528	C31 H57 N O7 S C31 H57 N O10 S	20.239 4.645	587.3826 635.3740	<u>FBF</u> FBF	63.21 77.80	FBF FBF
529	C31 H55 N O5 S	14.809	553.3854	FBF	50.49	FBF
530	C31 H55 N O6 S	4.125	569.3731	FBF	73.97	FBF
i31	C31 H55 N O9 S	5.581	617.3578	FBF	77.70	FBF
32	C31 H55 N O10 S	16.446	633.3555	FBF	51.45	FBF
33	C31 H53 N O7 S	5.244	583.3522	FBF	52.72	FBF
34	C31 H53 N O8 S	5.971	599.3528	FBF	51.37	FBF
535	C31 H53 N O10 S	12.651	631.3428	FBF	75.74	FBF
536	C31 H51 N O6 S	5.218	565.3476	FBF	56.22	FBF
537	C31 H49 N O5 S	3.943	547.3284	FBF	50.86	FBF
38	C31 H47 N O6 S	5.685	561.3118	FBF	58.32	FBF
539	C31 H47 N O8 S	18.135	593.3031	FBF	63.21	FBF
540	C31 H47 N O10 S	4.593	625.2915	FBF	56.84	FBF
541	C31 H45 N O6 S	21.616	559.2975	FBF	60.89	FBF
i42	C31 H45 N O10 S	13.249	623.2741	FBF	70.30	FBF
i43	C39 H68 O2	17.303	568.5219	FBF	55.53	FBF
14	C45 H72 O2	19.096	644.5551	FBF	54.71	FBF
45	C46 H80 O2	18.654	664.6161	FBF	59.21	FBF
546	C47 H84 O2	19.6 4 2	680.6467	FBF	57.13	FBF



Compound Summary								
Cpd Name	Formula	RT	Mass	CAS ID Source	Score	Score (Lib)	Score (DB)	Score (MFG) Algorith
<u>'547</u>	C48 H86 O2 C48 H84 O2	6.335	694.6618 692.6464	FBF FBF	59.24			FBF FBF
<u>'548</u> '549	C49 H88 O2	18.602 18.628	708.6780	FBF	59.30 66.30			FBF
550	C49 H84 O2	20.733	704.6462	FBF	53.03			FBF
551	C49 H80 O2	17.381	700.6160	FBF	58.45			FBF
552	C49 H78 O2	21.304	698.6002	FBF	90.85			FBF
553	C51 H88 O2	19.018	732.6782	FBF	57.19			FBF
554	C51 H82 O2	20.733	726.6313	FBF	65.90			FBF
555 556	C52 H90 O2 C53 H96 O2	18.395 21.071	746.6904 764.7405	FBF FBF	50.84 51.09			FBF FBF
557	C53 H94 O2	19.174	762.7271	FBF	56.34			FBF
558	C53 H92 O2	18.654	760.7115	FBF	51.96			FBF
559	C55 H100 O2	20.395	792.7705	FBF	50.56			FBF
560	C57 H104 O2	13.223	820.8077	FBF	59.35			FBF
561	C63 H114 O2	18.369	902.8736	FBF	54.26			FBF
<u>562</u> 563	C63 H108 O2 C63 H106 O2	21.356 18.862	896.8290 894.8170	FBF FBF	50.16 50.25			FBF FBF
564	C43 H74 O7	19.876	702.5500	FBF	51.74			FBF
565	C50 H76 O6	14.783	772.5716	FBF	55.31			FBF
566	C36 H56 O5	18.758	568.4129	FBF	81.57			FBF
567	C38 H60 O5	11.117	596.4468	FBF	71.69			FBF
568	C42 H64 O5	16.628	648.4762	FBF	52.71			FBF
569	C46 H70 O5	14.886	702.5228	FBF	51.71			FBF
570	C50 H82 O5	17.485	762.6170	FBF	55.44 51.79			FBF
571 572	C52 H86 O5 C53 H82 O5	17.771 14.886	790.6501 798.6137	FBF FBF	51.78 56.25	-		FBF FBF
573	C53 H84 O5	13.899	812.6312	FBF	53.70	-		FBF
574	C42 H65 N O6	18.446	679.4746	FBF	58.32			FBF
575	C44 H67 N O6	19.070	705.4950	FBF	55.39	· 	-	FBF
576	C45 H77 N O6	20.006	727.5721	FBF	69.20			FBF
577	C45 H69 N O6	19.980	719.5118	FBF	77.71			FBF
578 579	C46 H81 N O6 C46 H75 N O6	21.408 17.277	743.6044 737.5594	FBF FBF	68.05 53.23			FBF FBF
580	C46 H73 N O6	17.771	735.5444	FBF	59.87			FBF
581	C46 H71 N O6	20.006	733.5296	FBF	75.03			FBF
582	C47 H81 N O6	19.954	755.6033	FBF	54.50			FBF
583	C47 H75 N O6	19.044	749.5551	FBF	53.67			FBF
584	C47 H73 N O6	20.006	747.5423	FBF	73.06	-		FBF
585	C48 H73 N O6	11.845	759.5407	FBF	62.35			FBF
586	C49 H85 N O6	21.071	783.6369	FBF	52.45			FBF
587 588	C49 H83 N O6 C50 H87 N O6	21.304 17.122	781.6178 797.6485	FBF FBF	51.61 54.28			FBF FBF
589	C50 H85 N O6	15.328	795.6392	FBF	51.33			FBF
590	C50 H79 N O6	19.798	789.5986	FBF	52.49			FBF
591	C51 H87 N O6	15.796	809.6571	FBF	74.15			FBF
592	C51 H85 N O6	13.535	807.6401	FBF	59.30			FBF
593	C51 H81 N O6	20.032	803.6063	FBF	52.51			FBF
594	C52 H81 N O6	19.642	815.6055	FBF	52.77			FBF
<u>595</u> 596	C54 H91 N O6 C54 H87 N O6	20.187 14.886	849.6839 845.6487	FBF FBF	51.04 52.57			FBF FBF
597	C55 H95 N O6	15.640	865.7142	FBF	54.97			FBF
598	C55 H87 N O6	15.510	857.6559	FBF	51.79			FBF
599	C56 H95 N O6	20.058	877.7147	FBF	50.55			FBF
600	C56 H89 N O6	20.187	871.6709	FBF	52.61			FBF
501	C36 H61 N O5	14.835	587.4536	FBF	53.00			FBF
502	C37 H63 N O5	20.058	601.4699	FBF	50.78			FBF
503	C37 H61 N O5	10.285	599.4576	FBF	70.66			FBF
504 505	C38 H65 N O5 C38 H63 N O5	17.251 11.117	615.4828 613.4740	FBF FBF	55.09 72.12			FBF FBF
506	C38 H61 N O5	18.420	611.4538	FBF	56.92			FBF
507	C39 H65 N O5	11.923	627.4895	FBF	63.25			FBF
508	C40 H67 N O5	13.171	641.5001	FBF	54.94			FBF
09	C40 H61 N O5	17.225	635.4564	FBF	57.45			FBF
510	C41 H69 N O5	13.977	655.5194	FBF	55.08	-1		FBF
511 512	C44 H77 N O5 C45 H79 N O5	22.265 17.641	699.5807 713.5954	FBF FBF	55.16 56.71			FBF FBF
513	C45 H79 N O5 C45 H75 N O5	17.641	713.5954	FBF FBF	56.71	-		FBF
514	C46 H81 N O5	20.863	727.6157	FBF	61.53			FBF
515	C47 H79 N O5	14.523	737.6001	FBF	75.53			FBF
16	C47 H77 N O5	17.251	735.5836	FBF	50.43			FBF
517	C48 H79 N O5	13.327	749.5972	FBF	58.67			FBF
518	C48 H77 N O5	14.549	747.5827	FBF	52.06			FBF
519	C49 H85 N O5	21.564	767.6431	FBF	50.61			FBF
520 521	C49 H77 N O5 C51 H87 N O5	15.068 14.938	759.5817 793.6584	FBF FBF	51.80 62.93			FBF FBF
522	C51 H87 N O5 C52 H89 N O5	13.873	807.6731	FBF	52.93			FBF
623	C53 H91 N O5	17.147	821.6904	FBF	50.09			FBF
524	C53 H89 N O5	14.938	819.6772	FBF	53.00			FBF
525	C53 H85 N O5	14.886	815.6416	FBF	57.86			FBF
526	C53 H81 N O5	14.912	811.6071	FBF	57.75			FBF
527	C55 H93 N O5	13.327	847.7053	FBF	66.02			FBF
528	C56 H97 N O5	15.120	863.7310	FBF	56.44			FBF
629	C56 H95 N O5	12.677	861.7219	FBF	61.92	-		FBF
530 531	C56 H91 N O5	17.485	857.6952	FBF FRE	87.55 62.04			FBF
(JI	C36 H59 N O7 S	4.828	649.4011	FBF	62.04			FBF



Compound Summary							
Cpd Name	Formula	RT	Mass 702 4520	CAS ID Source	Score	Score (Lib) Score (DB)	Score (MFG) Algorithi FBF
7633 7634	C40 H65 N O7 S C41 H71 N O7 S	4.515 10.103	703.4538 721.4960	<u>FBF</u> FBF	53.66 95.83		FBF
7635	C41 H69 N O7 S	4.541	719.4809	FBF	69.36		FBF
7636	C42 H69 N O7 S	12.339	731.4829	FBF	52.63		FBF
7637	C44 H77 N O7 S	17.745	763.5495	FBF	56.72		FBF
7638	C45 H81 N O7 S	19.928	779.5725	FBF	69.22		FBF
7639 7640	C46 H75 N O7 S	19.954	785.5262	<u>FBF</u> FBF	84.06		FBF FBF
7641	C46 H73 N O7 S C47 H81 N O7 S	19.928 20.032	783.5052 803.5708	FBF	51.68 51.79		FBF
7642	C48 H85 N O7 S	16.784	819.6071	FBF	58.53		FBF
7643	C48 H83 N O7 S	16.888	817.5865	FBF	50.48		FBF
7644	C48 H75 N O7 S	19.902	809.5220	FBF	54.43		FBF
7645	C49 H87 N O7 S	20.473	833.6206	FBF	51.43		FBF
7646	C50 H91 N O7 S	18.291	849.6485	FBF	50.72		FBF
7647	C51 H79 N O7 S	4.854	849.5530	FBF	70.44		FBF
7648 7649	C52 H87 N O7 S C52 H83 N O7 S	15.692 19.434	869.6218 865.5853	<u>FBF</u> FBF	54.49 52.46		FBF FBF
7650	C54 H91 N O7 S	14.549	897.6580	FBF	53.28		FBF
7651	C56 H103 N O7 S	13.847	933.7501	FBF	59.83		FBF
7652	C36 H63 N O6 S	21.980	637.4334	FBF	56.15		FBF
7653	C36 H61 N O6 S	5.400	635.4196	FBF	63.75		FBF
7654	C37 H59 N O6 S	5.374	645.4076	FBF	55.68		FBF
7655	C38 H65 N O6 S	17.719	663.4507	FBF	72.68		FBF
7 <u>656</u> 7657	C38 H63 N O6 S	5.815 4.776	661.4389	FBF	70.91 63.74		FBF FBF
7658	C38 H61 N O6 S C39 H67 N O6 S	10.103	659.4191 677.4696	<u>FBF</u> FBF	97.16		FBF
7659	C39 H65 N O6 S	4.437	675.4544	FBF	70.59		FBF
7660	C40 H69 N O6 S	17.693	691.4816	FBF	63.79		FBF
7661	C41 H69 N O6 S	17.667	703.4835	FBF	72.08		FBF
7662	C42 H73 N O6 S	19.980	719.5120	FBF	63.85		FBF
7663	C43 H75 N O6 S	17.693	733.5328	FBF	78.94		FBF
⁷ 664 ⁷ 665	C44 H77 N O6 S	20.006 19.980	747.5425 767.5138	FBF FBF	55.51 55.26		FBF FBF
666	C46 H73 N O6 S C47 H83 N O6 S	19.798	789.5996	FBF	67.61		FBF
667	C48 H85 N O6 S	21.668	803.6099	FBF	74.70		FBF
668	C48 H83 N O6 S	15.042	801.6008	FBF	50.64		FBF
669	C48 H77 N O6 S	12.365	795.5501	FBF	54.71		FBF
670	C48 H75 N O6 S	21.798	793.5276	FBF	54.05		FBF
671	C49 H81 N O6 S	13.015	811.5705	FBF	70.63		FBF
<u>'672</u>	C50 H91 N O6 S	13.925	833.6636	FBF	50.96		FBF
7673	C51 H93 N O6 S	21.434	847.6721	FBF	67.06		FBF
<u>'674</u> '675	C51 H91 N O6 S C52 H95 N O6 S	12.469 13.873	845.6564 861.6881	FBF FBF	58.77 61.94		FBF FBF
7676	C52 H91 N O6 S	15.510	857.6562	FBF	65.08		FBF
7677	C52 H87 N O6 S	18.680	853.6246	FBF	53.38		FBF
7678	C53 H97 N O6 S	19.044	875.6980	FBF	50.12		FBF
7679	C53 H95 N O6 S	13.327	873.6815	FBF	51.39		FBF
7680	C53 H93 N O6 S	14.912	871.6654	FBF	54.63		FBF
7681	C53 H89 N O6 S	14.886	867.6410	FBF	55.56		FBF
7682 7683	C54 H95 N O6 S C54 H93 N O6 S	18.628 13.457	885.6867 883.6773	<u>FBF</u> FBF	51.80 51.72		FBF FBF
7684	C54 H89 N O6 S	15.510	879.6412	FBF	65.67		FBF
['] 685	C54 H87 N O6 S	15.510	877.6262	FBF	50.60		FBF
7686	C54 H85 N O6 S	18.031	875.6135	FBF	50.11		FBF
7687	C55 H99 N O6 S	14.393	901.7239	FBF	52.46		FBF
688	C55 H91 N O6 S	14.860	893.6635	FBF	50.11		FBF
'689	C55 H87 N O6 S	12.781	889.6280	FBF	66.88		FBF
'690 '601	C56 H103 N O6 S	14.938	917.7523 903.6457	FBF	50.60 50.78		FBF FBF
7 <u>691</u> 7692	C56 H89 N O6 S C41 H64 O13	13.925 19.096	764.4316	FBF FBF	50.78		FBF
693	C29 H48 O	12.521	412.3705	FBF	71.56		FBF
694	C49 H84 O7	20.395	784.6219	FBF	55.76		FBF
695	C49 H80 O7	13.249	780.5908	FBF	52.41		FBF
696	C51 H90 O7	12.547	814.6692	FBF	53.50		FBF
697	C51 H88 O7	19.512	812.6537	FBF	57.38		FBF
698 699	C55 H98 O7 C24 H42	22.681 8.830	870.7295 330.3311	FBF FBF	58.89 53.99		FBF FBF
700	C24 H42 C27 H46	8.830 11.741	370.3572	FBF	74.19		FBF
701	C37 H64 O13	5.348	716.4333	FBF	53.33		FBF
702	C28 H48 O5	13.951	464.3500	FBF	56.09		FBF
703	C50 H88 O7	18.992	800.6457	FBF	54.81		FBF
704	C52 H90 O7	17.589	826.6652	FBF	51.41		FBF
705	C56 H96 O7	18.706	880.7155	FBF	53.65		FBF
706 707	C27 H41 N O2	20.213	411.3128	FBF	54.38		FBF
707 708	C27 H43 N O2	14.315	413.3328 415.3445	FBF FBF	54.19 96.53		FBF FBF
708	C27 H45 N O2 C50 H83 N O21	5.503 5.503	1033.5425	FBF	96.53		FBF
710	C57 H94 O7	13.301	890.7031	FBF	61.47		FBF
711	C22 H30 O6	14.990	390.2060	FBF	52.59		FBF
712	C22 H26 O3	16.472	338.1905	FBF	56.62		FBF
713	C22 H26 O7	6.517	402.1683	FBF	66.79		FBF
714	C23 H38 O8	4.307	442.2595	FBF	59.23		FBF
715	C23 H36 O6	4.489	408.2521	FBF	63.55		FBF
716	C23 H28 O3	7.010	352.2058	FBF	68.97		FBF
7 <u>17</u> 718	C23 H28 O5 C23 H28 O8	8.466 7.920	384.1950 432.1789	<u>FBF</u> FBF	72.70 89.43		FBF FBF
, 10	CZJ 1120 00	7.720	134.1/07	וט ו	U7.73		FDF



Cpd Name	Formula	RT	Mass	CAS ID Source	e Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
7719	C25 H34 O3	7.608	382.2511	FBF	69.08				FBF
7720	C25 H32 O3	7.010	380.2351	FBF	75.10				FBF
7721	C25 H30 O3	17.511	378.2206	FBF	63.58	,			FBF
7722	C25 H30 O6	7.270	426.2031	FBF	53.95				FBF
7723	C26 H42 O5	11.637	434.2997	FBF	62.27				FBF
7724	C26 H36 O5	4.854	428.2579	FBF	58.05				FBF
7725	C26 H34 O3	4.750	394.2508	FBF	73.09				FBF
7726	C27 H38 O5	4.359	442.2715	FBF	86.58				FBF
7727	C27 H36 O5	4.932	440.2537	FBF	59.01	,			FBF
7728	C28 H36 O3	5.296	420.2663	FBF	50.43				FBF
7729	C29 H40 O3	5.218	436.2983	FBF	71.74				FBF
7730	C29 H38 O3	3.319	434.2816	FBF	57.33	,			FBF
7731	C29 H38 O5	5.400	466.2713	FBF	69.44				FBF
7732	C22 H38 O	10.441	318.2938	FBF	75.81				FBF
7733	C22 H34 O	19.668	314.2622	FBF	57.56				FBF
7734	C22 H28 O	4.724	308.2162	FBF	78.14				FBF
7735	C22 H26 O	4.307	306.1987	FBF	70.45				FBF
7736	C22 H26 O2	9.870	322.1960	FBF	62.89				FBF
7737	C23 H38 O	7.478	330.2914	FBF	61.79				FBF
7738	C23 H36 O	15.016	328.2754	FBF	72.18				FBF
7739	C23 H32 O	2.643	324.2463	FBF	60.41	,			FBF
7740	C23 H30 O	17.953	322.2269	FBF	55.96				FBF
7741	C23 H28 O2	22.395	336.2067	FBF	54.30				FBF
7742	C24 H38 O	10.363	342.2903	FBF	64.39				FBF
7743	C24 H36 O	10.389	340.2758	FBF	77.78				FBF
7744	C24 H34 O	11.975	338.2618	FBF	70.70				FBF
7745	C24 H30 O	17.251	334.2304	FBF	57.51				FBF
7746	C24 H30 O2	4.541	350.2253	FBF	71.09				FBF
7747	C25 H40 O	21.824	356.3070	FBF	74.45				FBF
7748	C25 H34 O2	5.348	366.2587	FBF	75.95				FBF
 7749	C25 H32 O	4.906	348.2446	FBF	58.60				FBF
7750	C25 H30 O	9.584	346.2306	FBF	71.38				FBF
7751	C26 H38 O	15.120	366.2919	FBF	70.57				FBF
7752	C26 H34 O2	10.337	378.2546	FBF	50.40				FBF
7753	C27 H38 O	15.926	378.2926	FBF	95.70				FBF
7754	C27 H34 O2	3.007	390.2546	FBF	55.31				FBF
7755	C28 H38 O2	5.322	406.2847	FBF	67.01				FBF
7756	C28 H36 O	13.717	388.2784	FBF	63.27				FBF
7757	C29 H52 O8	10.259	528.3658	FBF	90.00	,			FBF
//5/									

MassHunter Qual 12.0 (End of Report)