

Compound #2

File : C:\Xcalibur\data\asf-i-7a-180124-c11.RAW
 Full ms [49.500 - 550.500] - Range: 63.000 - 220.000
 Scan No. 1 of 1

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
63.0251	2.1	63.0235	26.1	1.6	4.5	C ₅ H ₃
64.0323	0.4	64.0313	15.4	1.0	4.0	C ₅ H ₄
65.0407	1.1	65.0391	24.8	1.6	3.5	C ₅ H ₅
67.0540	0.4	67.0548	-10.9	-0.7	2.5	C ₅ H ₇
69.0694	0.5	69.0704	-15.4	-1.1	1.5	C ₅ H ₉
71.0852	0.3	71.0861	-11.9	-0.8	0.5	C ₅ H ₁₁
74.0153	0.5	74.0157	-4.5	-0.3	6.0	C ₆ H ₂
75.0231	0.6	75.0235	-4.5	-0.3	5.5	C ₆ H ₃
76.0280	0.4	76.0313	-43.3	-3.3	5.0	C ₆ H ₄
77.0390	1.3	77.0391	-1.4	-0.1	4.5	C ₆ H ₅
78.0481	0.5	78.0470	14.7	1.1	4.0	C ₆ H ₆
79.0567	0.3	79.0548	24.4	1.9	3.5	C ₆ H ₇
81.0726	0.3	81.0704	26.7	2.2	2.5	C ₆ H ₉
83.0850	0.3	83.0861	-12.7	-1.1	1.5	C ₆ H ₁₁
86.0244	0.5					
87.0230	0.5	87.0235	-5.4	-0.5	6.5	C ₇ H ₃
88.0331	0.8	88.0313	20.9	1.8	6.0	C ₇ H ₄
89.0403	1.9	89.0391	12.7	1.1	5.5	C ₇ H ₅
91.0551	0.8	91.0548	3.1	0.3	4.5	C ₇ H ₇
102.0490	0.5	102.0470	20.1	2.0	6.0	C ₈ H ₆
103.0542	0.9	103.0548	-5.2	-0.5	5.5	C ₈ H ₇
113.0362	0.7	113.0391	-25.5	-2.9	7.5	C ₉ H ₅
114.0434	1.7	114.0470	-31.2	-3.6	7.0	C ₉ H ₆
115.0516	10.0	115.0548	-28.0	-3.2	6.5	C ₉ H ₇
116.0570	2.6	116.0626	-48.5	-5.6	6.0	C ₉ H ₈
117.0665	0.7	117.0704	-33.3	-3.9	5.5	C ₉ H ₉
121.0268	0.5	121.0290	-17.8	-2.1	5.5	C ₇ H ₅ O ₂
127.0571	0.4	127.0548	17.9	2.3	7.5	C ₁₀ H ₇
131.0550	0.9	131.0497	40.3	5.3	6.5	C ₉ H ₇ O ₁
135.0450	0.3	135.0446	2.9	0.4	5.5	C ₈ H ₇ O ₂
143.0498	4.2	143.0497	0.9	0.1	7.5	C ₁₀ H ₇ O ₁
144.0569	1.1	144.0575	-4.4	-0.6	7.0	C ₁₀ H ₈ O ₁
145.0682	0.4	145.0653	19.5	2.8	6.5	C ₁₀ H ₉ O ₁
146.0400	0.4	146.0368	22.3	3.3	7.0	C ₉ H ₆ O ₂
147.0529	0.4					
148.0577	0.4	148.0524	35.3	5.2	6.0	C ₉ H ₈ O ₂
149.0292	0.4	149.0239	36.0	5.4	6.5	C ₈ H ₅ O ₃
159.0522	0.4	159.0446	47.5	7.6	7.5	C ₁₀ H ₇ O ₂
160.0536	0.3	160.0524	7.4	1.2	7.0	C ₁₀ H ₈ O ₂
171.0405	1.6	171.0446	-23.8	-4.1	8.5	C ₁₁ H ₇ O ₂
172.0537	2.6	172.0524	7.2	1.2	8.0	C ₁₁ H ₈ O ₂
173.0547	8.9	173.0603	-31.8	-5.5	7.5	C ₁₁ H ₉ O ₂
174.0657	1.6	174.0681	-13.8	-2.4	7.0	C ₁₁ H ₁₀ O ₂
200.0521	0.3	200.0473	24.0	4.8	9.0	C ₁₂ H ₈ O ₃
202.0629	0.3	202.0630	-0.4	-0.1	8.0	C ₁₂ H ₁₀ O ₃
218.0587	4.5	218.0579	3.5	0.8	8.0	C ₁₂ H ₁₀ O ₄
219.0641	0.6	219.0657	-7.6	-1.7	7.5	C ₁₂ H ₁₁ O ₄

Compound #3

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
174.0625	2.3	174.0681	-32.3	-5.6	7.0	C ₁₁ H ₁₀ O ₂
		174.0555	39.9	7.0	7.5	C ₁₀ H ₈ O ₂ N ₁
175.0635	0.5	175.0633	1.0	0.2	7.0	C ₁₀ H ₉ O ₂ N ₁
		175.0606	16.3	2.8	2.5	C ₇ H ₁₁ O ₅
179.0857	0.5	179.0861	-2.1	-0.4	9.5	C ₁₄ H ₁₁
		179.0919	-34.9	-6.3	0.5	C ₇ H ₁₅ O ₅
		179.0794	35.3	6.3	1.0	C ₆ H ₁₃ O ₅ N ₁
183.2138	0.6	183.2113	13.7	2.5	0.5	C ₁₃ H ₂₇
187.0562	0.8	187.0548	7.5	1.4	12.5	C ₁₅ H ₇
		187.0606	-23.9	-4.5	3.5	C ₈ H ₁₁ O ₅
		187.0633	-38.2	-7.1	8.0	C ₁₁ H ₉ O ₂ N ₁
188.0612	0.6	188.0626	-7.7	-1.4	12.0	C ₁₅ H ₈
		188.0559	28.0	5.3	3.5	C ₇ H ₁₀ O ₅ N ₁
		188.0685	-38.9	-7.3	3.0	C ₈ H ₁₂ O ₅
189.0658	0.6	189.0637	11.1	2.1	3.0	C ₇ H ₁₁ O ₅ N ₁
		189.0704	-24.3	-4.6	11.5	C ₁₅ H ₉
194.0975	0.8	194.0970	2.8	0.5	9.5	C ₁₄ H ₁₂ N ₁
		194.0943	16.6	3.2	5.0	C ₁₁ H ₁₄ O ₃
		194.1028	-27.5	-5.3	0.5	C ₇ H ₁₆ O ₅ N ₁
199.0554	1.2	199.0548	3.1	0.6	13.5	C ₁₆ H ₇
		199.0606	-26.4	-5.3	4.5	C ₉ H ₁₁ O ₅
		199.0481	36.8	7.3	5.0	C ₈ H ₉ O ₅ N ₁
		199.0633	-39.9	-7.9	9.0	C ₁₂ H ₉ O ₂ N ₁
201.0588	2.8	201.0578	4.8	1.0	13.0	C ₁₅ H ₇ N ₁
		201.0552	18.1	3.6	8.5	C ₁₂ H ₉ O ₃
		201.0637	-24.5	-4.9	4.0	C ₈ H ₁₁ O ₅ N ₁
202.0673	1.0	202.0657	8.3	1.7	12.5	C ₁₅ H ₈ N ₁
		202.0715	-20.8	-4.2	3.5	C ₈ H ₁₂ O ₅ N ₁
		202.0630	21.5	4.4	8.0	C ₁₂ H ₁₀ O ₃
205.0864	0.6	205.0865	-0.2	-0.0	6.5	C ₁₂ H ₁₃ O ₃
		205.0891	-13.2	-2.7	11.0	C ₁₅ H ₁₁ N ₁
207.0405	1.8	207.0446	-19.9	-4.1	11.5	C ₁₄ H ₇ O ₂
240.9788	0.5					
257.0699	5.6	257.0688	4.2	1.1	10.0	C ₁₄ H ₁₁ O ₄ N ₁
		257.0603	37.5	9.6	14.5	C ₁₈ H ₉ O ₂
258.0693	1.1	258.0681	4.8	1.2	14.0	C ₁₈ H ₁₀ O ₂
		258.0766	-28.4	-7.3	9.5	C ₁₄ H ₁₂ O ₄ N ₁

Compound # 4

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
178.0118	1.2	178.0055	35.7	6.3	12.0	C ₁₂ H ₂ O ₂
		178.0266	-83.0	-14.8	7.0	C ₉ H ₆ O ₄
181.9232	1.1					
185.0015	1.1	185.0027	-6.5	-1.2	14.5	C ₁₄ H ₁ O ₁
		185.0086	-38.2	-7.1	5.5	C ₇ H ₅ O ₆
		184.9875	76.0	14.1	10.5	C ₁₀ H ₁ O ₄
185.9455	2.4					
188.0230	9.1	188.0262	-17.3	-3.2	13.0	C ₁₄ H ₄ O ₁
		188.0321	-48.5	-9.1	4.0	C ₇ H ₈ O ₆
		188.0110	63.9	12.0	9.0	C ₁₀ H ₄ O ₄
189.0394	2.3	189.0399	-2.6	-0.5	3.5	C ₇ H ₉ O ₆
		189.0340	28.5	5.4	12.5	C ₁₄ H ₅ O ₁
		189.0552	-83.3	-15.7	7.5	C ₁₁ H ₉ O ₃
190.0441	1.4	190.0419	11.6	2.2	12.0	C ₁₄ H ₆ O ₁
		190.0477	-19.4	-3.7	3.0	C ₇ H ₁₀ O ₆
		190.0266	91.8	17.5	8.0	C ₁₀ H ₆ O ₄
192.0356	1.3	192.0423	-34.7	-6.7	7.0	C ₁₀ H ₈ O ₄
		192.0211	75.3	14.5	12.0	C ₁₃ H ₄ O ₂
199.0532	2.1	199.0548	-7.8	-1.6	13.5	C ₁₆ H ₇
		199.0606	-37.3	-7.4	4.5	C ₉ H ₁₁ O ₅
		199.0395	68.8	13.7	9.5	C ₁₂ H ₇ O ₃
200.0608	1.4	200.0626	-9.2	-1.8	13.0	C ₁₆ H ₈
		200.0685	-38.6	-7.7	4.0	C ₉ H ₁₂ O ₅
		200.0473	67.1	13.4	9.0	C ₁₂ H ₈ O ₃
201.0594	10.7	201.0552	21.2	4.3	8.5	C ₁₂ H ₉ O ₃
		201.0704	-54.7	-11.0	12.5	C ₁₆ H ₉
		201.0763	-83.9	-16.9	3.5	C ₉ H ₁₃ O ₅
202.0657	3.3	202.0630	13.6	2.8	8.0	C ₁₂ H ₁₀ O ₃
		202.0783	-61.9	-12.5	12.0	C ₁₆ H ₁₀
		202.0477	89.1	18.0	4.0	C ₈ H ₁₀ O ₆
207.0182	1.3	207.0235	-25.5	-5.3	16.5	C ₁₇ H ₃
		207.0082	48.2	10.0	12.5	C ₁₃ H ₃ O ₃
		207.0293	-53.9	-11.2	7.5	C ₁₀ H ₇ O ₅
211.9446	1.6					
212.9698	1.2	212.9824	-59.4	-12.6	11.5	C ₁₁ H ₁ O ₅
216.9739	3.6	216.9773	-15.5	-3.4	10.5	C ₁₀ H ₁ O ₆
		216.9926	-85.8	-18.6	14.5	C ₁₄ H ₁ O ₃
218.9018	10.0					
223.8808	1.1					
230.8755	12.9					
235.9193	1.2					
288.1358	9.5	288.1362	-1.1	-0.3	8.0	C ₁₇ H ₂₀ O ₄
		288.1514	-54.1	-15.6	12.0	C ₂₁ H ₂₀ O ₁
		288.1150	72.2	20.8	13.0	C ₂₀ H ₁₆ O ₂
289.1352	1.2	289.1440	-30.3	-8.8	7.5	C ₁₇ H ₂₁ O ₄
		289.1229	42.8	12.4	12.5	C ₂₀ H ₁₇ O ₂
		289.1592	-83.1	-24.0	11.5	C ₂₁ H ₂₁ O ₁

Compound # 5

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
		218.0732	-64.7	-14.1	12.0	C ₁₆ H ₁₀ O ₁
		218.0790	-91.6	-20.0	3.0	C ₉ H ₁₄ O ₆
219.0637	1.6	219.0657	-9.1	-2.0	7.5	C ₁₂ H ₁₁ O ₄
		219.0810	-78.7	-17.2	11.5	C ₁₆ H ₁₁ O ₁
		219.0446	87.4	19.1	12.5	C ₁₅ H ₇ O ₂
224.0199	1.2	224.0262	-28.3	-6.3	16.0	C ₁₇ H ₄ O ₁
		224.0110	39.8	8.9	12.0	C ₁₃ H ₄ O ₄
		224.0321	-54.6	-12.2	7.0	C ₁₀ H ₈ O ₆
225.0181	1.6	225.0188	-2.8	-0.6	11.5	C ₁₃ H ₅ O ₄
		225.0340	-70.6	-15.9	15.5	C ₁₇ H ₅ O ₁
		224.9977	91.1	20.5	16.5	C ₁₆ H ₁ O ₂
226.0192	1.5	226.0266	-32.9	-7.4	11.0	C ₁₃ H ₆ O ₄
		226.0055	60.5	13.7	16.0	C ₁₆ H ₂ O ₂
230.8972	3.8					
242.0517	1.2	242.0579	-25.6	-6.2	10.0	C ₁₄ H ₁₀ O ₄
		242.0368	61.7	14.9	15.0	C ₁₇ H ₆ O ₂
		242.0732	-88.6	-21.5	14.0	C ₁₈ H ₁₀ O ₁
268.0740	1.4	268.0736	1.6	0.4	11.0	C ₁₆ H ₁₂ O ₄
		268.0888	-55.3	-14.8	15.0	C ₂₀ H ₁₂ O ₁
		268.0947	-77.2	-20.7	6.0	C ₁₃ H ₁₆ O ₆
271.1041	1.1	271.0970	26.0	7.1	9.5	C ₁₆ H ₁₅ O ₄
		271.1123	-30.2	-8.2	13.5	C ₂₀ H ₁₅ O ₁
		271.1182	-51.9	-14.1	4.5	C ₁₃ H ₁₉ O ₆
272.1042	21.9	272.1049	-2.4	-0.7	9.0	C ₁₆ H ₁₆ O ₄
		272.1201	-58.5	-15.9	13.0	C ₂₀ H ₁₆ O ₁
		272.0837	75.2	20.5	14.0	C ₁₉ H ₁₂ O ₂
273.1080	4.0	273.1127	-17.0	-4.6	8.5	C ₁₆ H ₁₇ O ₄
		273.0916	60.4	16.5	13.5	C ₁₉ H ₁₃ O ₂
		273.1279	-72.8	-19.9	12.5	C ₂₀ H ₁₇ O ₁

Compound # 6

File : C:\Xcalibur\data\asf-i-103a-180324-c2.RAW
 Full ms [49.500 - 600.500] - Range: 63.000 - 600.500
 Scan No. 1 of 1

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
63.0245	1.4	63.0235	16.5	1.0	4.5	C ₅ H ₃
64.0335	0.3	64.0313	33.7	2.2	4.0	C ₅ H ₄
65.0386	0.8	65.0391	-8.2	-0.5	3.5	C ₅ H ₅
69.0683	0.5	69.0704	-30.8	-2.1	1.5	C ₅ H ₉
71.0845	0.5	71.0861	-21.6	-1.5	0.5	C ₅ H ₁₁
73.0074	0.5	73.0078	-6.1	-0.4	6.5	C ₆ H ₁
73.0457	0.4					
74.0134	1.7	74.0157	-30.5	-2.3	6.0	C ₆ H ₂
75.0240	2.0	75.0235	7.0	0.5	5.5	C ₆ H ₃
76.0283	1.6	76.0313	-39.4	-3.0	5.0	C ₆ H ₄
77.0369	2.6	77.0391	-28.7	-2.2	4.5	C ₆ H ₅
78.0450	0.8	78.0470	-25.5	-2.0	4.0	C ₆ H ₆
79.0548	0.9	79.0548	0.5	0.0	3.5	C ₆ H ₇
83.0857	0.3	83.0861	-4.5	-0.4	1.5	C ₆ H ₁₁
85.1036	0.4	85.1017	21.7	1.8	0.5	C ₆ H ₁₃
88.0318	0.4	88.0313	6.1	0.5	6.0	C ₇ H ₄
89.0409	2.4	89.0391	20.4	1.8	5.5	C ₇ H ₅
90.0466	2.3	90.0470	-4.4	-0.4	5.0	C ₇ H ₆
91.0542	1.6	91.0548	-6.6	-0.6	4.5	C ₇ H ₇
102.0430	0.6	102.0470	-38.7	-3.9	6.0	C ₈ H ₆
103.0532	0.6	103.0548	-15.5	-1.6	5.5	C ₈ H ₇
107.0501	0.4	107.0497	3.9	0.4	4.5	C ₇ H ₇ O ₁
114.0451	0.6	114.0470	-16.2	-1.8	7.0	C ₉ H ₆
115.0526	3.5	115.0548	-18.6	-2.1	6.5	C ₉ H ₇
116.0571	0.7					
131.0519	1.0	131.0497	16.7	2.2	6.5	C ₉ H ₇ O ₁
135.0445	1.9	135.0446	-0.7	-0.1	5.5	C ₈ H ₇ O ₂
143.0507	1.0	143.0497	7.0	1.0	7.5	C ₁₀ H ₇ O ₁
144.0566	0.3	144.0575	-6.4	-0.9	7.0	C ₁₀ H ₈ O ₁
149.0294	0.4	149.0239	37.2	5.5	6.5	C ₈ H ₅ O ₃
154.9481	1.5	154.9496	-9.9	-1.5	4.5	C ₆ H ₄ Br ₁
156.9476	1.6					
159.0455	0.9	159.0446	5.7	0.9	7.5	C ₁₀ H ₇ O ₂
169.9809	1.0					
171.0438	0.7	171.0446	-4.7	-0.8	8.5	C ₁₁ H ₇ O ₂
171.9719	0.6					
172.0558	0.7	172.0524	19.3	3.3	8.0	C ₁₁ H ₈ O ₂
173.0598	2.0	173.0603	-2.7	-0.5	7.5	C ₁₁ H ₉ O ₂
174.0670	0.4	174.0681	-5.9	-1.0	7.0	C ₁₁ H ₁₀ O ₂
175.0410	0.5	175.0395	8.3	1.5	7.5	C ₁₀ H ₇ O ₃
182.9489	2.8	182.9446	23.9	4.4	5.5	C ₇ H ₄ O ₁ Br ₁
183.9523	2.0	183.9524	-0.2	-0.0	5.0	C ₇ H ₅ O ₁ Br ₁
184.9471	3.1	184.9449	11.8	2.2	0.5	C ₃ H ₆ O ₄ Br ₁
185.9564	2.1	185.9528	19.5	3.6	0.0	C ₃ H ₇ O ₄ Br ₁
187.0435	1.9	187.0395	21.4	4.0	8.5	C ₁₁ H ₇ O ₃
188.0485	0.3	188.0473	5.9	1.1	8.0	C ₁₁ H ₈ O ₃
189.0579	0.8	189.0552	14.3	2.7	7.5	C ₁₁ H ₉ O ₃
199.0474	0.5	199.0548	-37.2	-7.4	13.5	C ₁₆ H ₇
		199.0395	39.4	7.9	9.5	C ₁₂ H ₇ O ₃
201.0563	0.5	201.0552	5.7	1.1	8.5	C ₁₂ H ₉ O ₃
207.0383	0.4	207.0385	-1.0	-0.2	0.5	C ₈ H ₁₆ O ₁ Br ₁
		207.0446	-30.7	-6.3	11.5	C ₁₄ H ₇ O ₂
217.0460	6.2	217.0501	-18.7	-4.1	8.5	C ₁₂ H ₉ O ₄
218.0490	1.0					
328.9926	0.4	328.9966	-12.3	-4.0	15.5	C ₂₀ H ₁₀ Br ₁
		328.9875	15.4	5.1	22.5	C ₂₂ H ₁ O ₄
		329.0027	-31.0	-10.2	26.5	C ₂₆ H ₁ O ₁
386.0147	1.4	386.0154	-1.6	-0.6	12.0	C ₁₉ H ₁₅ O ₄ Br ₁
		386.0157	-2.4	-0.9	32.0	C ₃₂ H ₂
		386.0004	37.2	14.3	28.0	C ₂₈ H ₂ O ₃
387.0195	0.3	387.0232	-9.4	-3.6	11.5	C ₁₉ H ₁₆ O ₄ Br ₁
		387.0235	-10.1	-3.9	31.5	C ₃₂ H ₃
		387.0082	29.3	11.3	27.5	C ₂₈ H ₃ O ₃
388.0160	1.4	388.0160	-0.1	-0.0	27.0	C ₂₈ H ₄ O ₃
		388.0099	15.8	6.1	16.0	C ₂₂ H ₁₃ O ₂ Br ₁
		388.0310	-38.7	-15.0	11.0	C ₁₉ H ₁₇ O ₄ Br ₁

Compound # 7

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
		175.0122	19.7	3.5	1.5	C ₇ H ₁₂ Br ₁
		175.0031	71.7	12.6	8.5	C ₉ H ₃ O ₄
187.0407	3.1	187.0395	6.5	1.2	8.5	C ₁₁ H ₇ O ₃
		187.0548	-75.1	-14.0	12.5	C ₁₅ H ₇
188.0485	0.7	188.0473	5.9	1.1	8.0	C ₁₁ H ₈ O ₃
		188.0626	-75.2	-14.1	12.0	C ₁₅ H ₈
189.0585	1.6	189.0552	17.6	3.3	7.5	C ₁₁ H ₉ O ₃
		189.0704	-63.0	-11.9	11.5	C ₁₅ H ₉
199.0416	1.4	199.0395	10.5	2.1	9.5	C ₁₂ H ₇ O ₃
		199.0548	-66.2	-13.2	13.5	C ₁₆ H ₇
201.0569	1.7	201.0552	8.5	1.7	8.5	C ₁₂ H ₉ O ₃
		201.0704	-67.4	-13.5	12.5	C ₁₆ H ₉
202.0681	0.7	202.0630	25.3	5.1	8.0	C ₁₂ H ₁₀ O ₃
		202.0783	-50.2	-10.1	12.0	C ₁₆ H ₁₀
203.0805	0.5	203.0861	-27.7	-5.6	11.5	C ₁₆ H ₁₁
		203.0708	47.5	9.6	7.5	C ₁₂ H ₁₁ O ₃
216.9774	10.0	216.9864	-41.5	-9.0	3.5	C ₈ H ₁₀ O ₂ Br ₁
		216.9653	55.9	12.1	8.5	C ₁₁ H ₆ Br ₁
		216.9926	-69.8	-15.1	14.5	C ₁₄ H ₁ O ₃
217.9792	1.6	217.9731	27.7	6.0	8.0	C ₁₁ H ₇ Br ₁
		217.9942	-69.2	-15.1	3.0	C ₈ H ₁₁ O ₂ Br ₁
		218.0004	-97.4	-21.2	14.0	C ₁₄ H ₂ O ₃
		217.9579	97.7	21.3	4.0	C ₇ H ₇ O ₃ Br ₁
279.1575	6.6	279.1596	-7.7	-2.2	5.5	C ₁₆ H ₂₃ O ₄
		279.1749	-62.4	-17.4	9.5	C ₂₀ H ₂₃ O ₁
		279.1385	68.0	19.0	10.5	C ₁₉ H ₁₉ O ₂
280.1617	1.3	280.1675	-20.4	-5.7	5.0	C ₁₆ H ₂₄ O ₄
		280.1463	55.0	15.4	10.0	C ₁₉ H ₂₀ O ₂
		280.1827	-74.9	-21.0	9.0	C ₂₀ H ₂₄ O ₁
386.0143	1.9	386.0154	-2.9	-1.1	12.0	C ₁₉ H ₁₅ O ₄ Br ₁
		386.0157	-3.6	-1.4	32.0	C ₃₂ H ₂
		386.0004	35.9	13.9	28.0	C ₂₈ H ₂ O ₃
		386.0306	-42.4	-16.4	16.0	C ₂₃ H ₁₅ O ₁ Br ₁
388.0135	2.0	388.0160	-6.6	-2.5	27.0	C ₂₈ H ₄ O ₃
		388.0099	9.3	3.6	16.0	C ₂₂ H ₁₃ O ₂ Br ₁
		388.0310	-45.2	-17.5	11.0	C ₁₉ H ₁₇ O ₄ Br ₁
		388.0313	-45.9	-17.8	31.0	C ₃₂ H ₄

Compound # 8

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
226.0646	1.1	226.0630	6.9	1.6	10.0	C ₁₄ H ₁₀ O ₃
		226.0549	42.6	9.6	10.0	C ₁₅ H ₁₁ Cl ₁
		226.0761	-50.8	-11.5	5.0	C ₁₂ H ₁₅ O ₂ Cl ₁
259.0476	1.4	259.0526	-19.4	-5.0	9.5	C ₁₅ H ₁₂ O ₂ Cl ₁
		259.0548	-27.8	-7.2	18.5	C ₂₁ H ₇
		259.0395	31.0	8.0	14.5	C ₁₇ H ₇ O ₃
342.0668	3.5	342.0659	2.6	0.9	12.0	C ₁₉ H ₁₅ O ₄ Cl ₁
		342.0681	-3.8	-1.3	21.0	C ₂₅ H ₁₀ O ₂
		342.0811	-42.0	-14.4	16.0	C ₂₃ H ₁₅ O ₁ Cl ₁
344.0710	2.2	344.0626	24.4	8.4	25.0	C ₂₈ H ₈
		344.0815	-30.6	-10.5	11.0	C ₁₉ H ₁₇ O ₄ Cl ₁
		344.0604	30.8	10.6	16.0	C ₂₂ H ₁₃ O ₂ Cl ₁

Compound # 9

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
		186.0003	47.3	8.8	5.0	C ₉ H ₈ Cl ₂
		186.0214	-66.3	-12.3	0.0	C ₆ H ₁₂ O ₂ Cl ₂
187.0608	8.7	187.0548	32.5	6.1	12.5	C ₁₅ H ₇
		187.0526	44.2	8.3	3.5	C ₉ H ₁₂ O ₂ Cl ₁
		187.0759	-80.5	-15.1	7.5	C ₁₂ H ₁₁ O ₂
188.0688	1.5	188.0626	33.0	6.2	12.0	C ₁₅ H ₈
		188.0604	44.7	8.4	3.0	C ₉ H ₁₃ O ₂ Cl ₁
		188.0837	-79.3	-14.9	7.0	C ₁₂ H ₁₂ O ₂
189.0810	3.6	189.0704	55.8	10.5	11.5	C ₁₅ H ₉
		189.0916	-56.0	-10.6	6.5	C ₁₂ H ₁₃ O ₂
		189.0682	67.4	12.7	2.5	C ₉ H ₁₄ O ₂ Cl ₁
199.0585	10.7	199.0548	18.9	3.8	13.5	C ₁₆ H ₇
		199.0526	29.9	6.0	4.5	C ₁₀ H ₁₂ O ₂ Cl ₁
		199.0759	-87.2	-17.4	8.5	C ₁₃ H ₁₁ O ₂
		199.0395	95.5	19.0	9.5	C ₁₂ H ₇ O ₃
200.0620	2.2	200.0626	-3.0	-0.6	13.0	C ₁₆ H ₈
		200.0604	7.9	1.6	4.0	C ₁₀ H ₁₃ O ₂ Cl ₁
		200.0473	73.2	14.6	9.0	C ₁₂ H ₈ O ₃
201.0678	7.7	201.0682	-2.2	-0.4	3.5	C ₁₀ H ₁₄ O ₂ Cl ₁
		201.0704	-13.1	-2.6	12.5	C ₁₆ H ₉
		201.0552	62.7	12.6	8.5	C ₁₂ H ₉ O ₃
202.0746	2.5	202.0761	-7.0	-1.4	3.0	C ₁₀ H ₁₅ O ₂ Cl ₁
		202.0783	-17.9	-3.6	12.0	C ₁₆ H ₁₀
		202.0630	57.6	11.6	8.0	C ₁₂ H ₁₀ O ₃
		202.0549	97.5	19.7	8.0	C ₁₃ H ₁₁ Cl ₁
203.0840	0.9	203.0839	0.4	0.1	2.5	C ₁₀ H ₁₆ O ₂ Cl ₁
		203.0861	-10.4	-2.1	11.5	C ₁₆ H ₁₁
		203.0708	64.8	13.2	7.5	C ₁₂ H ₁₁ O ₃
216.0393	0.9	216.0423	-13.5	-2.9	9.0	C ₁₂ H ₈ O ₄
		216.0342	23.8	5.1	9.0	C ₁₃ H ₉ O ₁ Cl ₁
		216.0320	34.0	7.3	0.0	C ₇ H ₄ O ₃ Cl ₂
		216.0473	-36.6	-7.9	4.0	C ₁₁ H ₁₄ Cl ₂
217.0496	55.5	217.0501	-2.3	-0.5	8.5	C ₁₂ H ₉ O ₄
		217.0551	-25.3	-5.5	3.5	C ₁₁ H ₁₅ Cl ₂
		217.0420	34.9	7.6	8.5	C ₁₃ H ₁₀ O ₁ Cl ₁
		217.0631	-62.4	-13.6	3.5	C ₁₀ H ₁₄ O ₃ Cl ₁
218.0542	7.3	218.0579	-17.0	-3.7	8.0	C ₁₂ H ₁₀ O ₄
		218.0498	19.9	4.3	8.0	C ₁₃ H ₁₁ O ₁ Cl ₁
		218.0629	-40.0	-8.7	3.0	C ₁₁ H ₁₆ Cl ₂
		218.0710	-77.0	-16.8	3.0	C ₁₀ H ₁₅ O ₃ Cl ₁
312.9658	0.7	312.9692	-11.0	-3.5	18.5	C ₁₉ H ₂ O ₃ Cl ₁
		312.9612	14.7	4.6	18.5	C ₂₀ H ₃ Cl ₂
		312.9823	-52.8	-16.5	13.5	C ₁₇ H ₇ O ₂ Cl ₂
		312.9845	-59.8	-18.7	22.5	C ₂₃ H ₂ Cl ₁
314.9608	0.7	314.9616	-2.5	-0.8	13.5	C ₁₆ H ₅ O ₃ Cl ₂
		314.9638	-9.5	-3.0	22.5	C ₂₂ O ₁ Cl ₁
		314.9485	39.0	12.3	18.5	C ₁₈ O ₄ Cl ₁
		314.9768	-50.9	-16.0	17.5	C ₂₀ H ₅ Cl ₂
347.9392	0.8	347.9381	3.2	1.1	18.0	C ₁₉ H ₂ O ₃ Cl ₂
		347.9534	-40.6	-14.1	22.0	C ₂₃ H ₂ Cl ₂
		347.9614	-63.8	-22.2	22.0	C ₂₂ H ₁ O ₃ Cl ₁
349.9209	0.7	349.9174	10.1	3.5	18.0	C ₁₈ O ₄ Cl ₂
		349.9326	-33.5	-11.7	22.0	C ₂₂ O ₁ Cl ₂
		349.9537	-93.8	-32.8	17.0	C ₁₉ H ₄ O ₃ Cl ₂
376.0257	9.1	376.0269	-3.1	-1.2	12.0	C ₁₉ H ₁₄ O ₄ Cl ₂
		376.0291	-8.9	-3.4	21.0	C ₂₅ H ₉ O ₂ Cl ₁
		376.0313	-14.8	-5.6	30.0	C ₃₁ H ₄
		376.0160	25.8	9.7	26.0	C ₂₇ H ₄ O ₃
377.0280	2.1	377.0239	10.9	4.1	25.5	C ₂₇ H ₅ O ₃
		377.0347	-18.0	-6.8	11.5	C ₁₉ H ₁₅ O ₄ Cl ₂
		377.0369	-23.8	-9.0	20.5	C ₂₅ H ₁₀ O ₂ Cl ₁
		377.0391	-29.6	-11.2	29.5	C ₃₁ H ₅

Compound # 10

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
		201.0188	17.3	3.5	9.5	C ₁₁ H ₅ O ₄
		201.0318	-47.7	-9.6	4.5	C ₉ H ₁₀ O ₃ Cl ₁
202.0456	1.5	202.0419	18.3	3.7	13.0	C ₁₅ H ₆ O ₁
		202.0397	29.1	5.9	4.0	C ₉ H ₁₁ O ₃ Cl ₁
		202.0549	-46.4	-9.4	8.0	C ₁₃ H ₁₁ Cl ₁
217.0583	35.1	217.0551	14.9	3.2	3.5	C ₁₁ H ₁₅ Cl ₂
		217.0631	-22.3	-4.8	3.5	C ₁₀ H ₁₄ O ₃ Cl ₁
		217.0653	-32.4	-7.0	12.5	C ₁₆ H ₉ O ₁
218.0592	5.7	218.0579	5.9	1.3	8.0	C ₁₂ H ₁₀ O ₄
		218.0629	-17.0	-3.7	3.0	C ₁₁ H ₁₆ Cl ₂
		218.0498	42.9	9.3	8.0	C ₁₃ H ₁₁ O ₁ Cl ₁
219.0602	1.2	219.0577	11.5	2.5	7.5	C ₁₃ H ₁₂ O ₁ Cl ₁
		219.0657	-25.3	-5.5	7.5	C ₁₂ H ₁₁ O ₄
		219.0707	-48.1	-10.5	2.5	C ₁₁ H ₁₇ Cl ₂
230.8980	6.6					
376.0273	7.1	376.0269	1.1	0.4	12.0	C ₁₉ H ₁₄ O ₄ Cl ₂
		376.0291	-4.7	-1.8	21.0	C ₂₅ H ₉ O ₂ Cl ₁
		376.0313	-10.6	-4.0	30.0	C ₃₁ H ₄
377.0252	1.8	377.0239	3.6	1.4	25.5	C ₂₇ H ₅ O ₃
		377.0217	9.5	3.6	16.5	C ₂₁ H ₁₀ O ₅ Cl ₁
		377.0158	25.0	9.4	25.5	C ₂₈ H ₆ Cl ₁
378.0265	4.7	378.0236	7.7	2.9	25.0	C ₂₈ H ₇ Cl ₁
		378.0295	-7.8	-3.0	16.0	C ₂₁ H ₁₁ O ₅ Cl ₁
		378.0214	13.5	5.1	16.0	C ₂₂ H ₁₂ O ₂ Cl ₂
379.0199	1.1	379.0184	4.1	1.6	29.5	C ₃₀ H ₃ O ₁
		379.0162	9.9	3.7	20.5	C ₂₄ H ₈ O ₃ Cl ₁
		379.0140	15.7	5.9	11.5	C ₁₈ H ₁₃ O ₅ Cl ₂
380.0234	1.1	380.0240	-1.6	-0.6	20.0	C ₂₄ H ₉ O ₃ Cl ₁
		380.0218	4.1	1.6	11.0	C ₁₈ H ₁₄ O ₅ Cl ₂
		380.0262	-7.4	-2.8	29.0	C ₃₀ H ₄ O ₁

Compound # 11

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition		
188.0453	1.3	188.0473	-10.7	-2.0	8.0	C ₁₁ H ₈ O ₃		
		188.0393	32.2	6.1	8.0	C ₁₂ H ₉ Cl ₁		
		188.0604	-80.2	-15.1	3.0	C ₉ H ₁₃ O ₂ Cl ₁		
		188.0626	-91.8	-17.3	12.0	C ₁₅ H ₈		
189.0600	2.2	189.0552	25.8	4.9	7.5	C ₁₁ H ₉ O ₃		
		189.0682	-43.3	-8.2	2.5	C ₉ H ₁₄ O ₂ Cl ₁		
		189.0704	-54.9	-10.4	11.5	C ₁₅ H ₉		
		189.0471	68.4	12.9	7.5	C ₁₂ H ₁₀ Cl ₁		
		199.0394	2.6	199.0395	-0.7	-0.1	9.5	C ₁₂ H ₇ O ₃
199.0394	2.6	199.0315	39.9	7.9	9.5	C ₁₃ H ₈ Cl ₁		
		199.0293	50.9	10.1	0.5	C ₇ H ₁₃ O ₂ Cl ₂		
		199.0526	-66.3	-13.2	4.5	C ₁₀ H ₁₂ O ₂ Cl ₁		
		200.0464	0.8	200.0473	-4.8	-1.0	9.0	C ₁₂ H ₈ O ₃
		200.0393	35.5	7.1	9.0	C ₁₃ H ₉ Cl ₁		
200.0464	0.8	200.0371	46.5	9.3	0.0	C ₇ H ₁₄ O ₂ Cl ₂		
		200.0604	-70.1	-14.0	4.0	C ₁₀ H ₁₃ O ₂ Cl ₁		
		201.0532	2.9	201.0552	-9.7	-2.0	8.5	C ₁₂ H ₉ O ₃
		201.0471	30.4	6.1	8.5	C ₁₃ H ₁₀ Cl ₁		
		201.0682	-74.7	-15.0	3.5	C ₁₀ H ₁₄ O ₂ Cl ₁		
201.0532	2.9	201.0704	-85.6	-17.2	12.5	C ₁₆ H ₉		
		202.0667	1.0	202.0630	18.3	3.7	8.0	C ₁₂ H ₁₀ O ₃
		202.0761	-46.3	-9.4	3.0	C ₁₀ H ₁₅ O ₂ Cl ₁		
		202.0783	-57.2	-11.6	12.0	C ₁₆ H ₁₀		
		202.0549	58.3	11.8	8.0	C ₁₃ H ₁₁ Cl ₁		
216.0475	0.6	216.0473	1.0	0.2	4.0	C ₁₁ H ₁₄ Cl ₂		
		216.0423	24.1	5.2	9.0	C ₁₂ H ₈ O ₄		
		216.0553	-36.4	-7.9	4.0	C ₁₀ H ₁₃ O ₃ Cl ₁		
		216.0575	-46.5	-10.0	13.0	C ₁₆ H ₈ O ₁		
		217.0498	14.2	217.0501	-1.5	-0.3	8.5	C ₁₂ H ₉ O ₄
217.0498	14.2	217.0551	-24.5	-5.3	3.5	C ₁₁ H ₁₅ Cl ₂		
		217.0420	35.7	7.7	8.5	C ₁₃ H ₁₀ O ₁ Cl ₁		
		217.0631	-61.7	-13.4	3.5	C ₁₀ H ₁₄ O ₃ Cl ₁		
		218.0567	2.5	218.0579	-5.4	-1.2	8.0	C ₁₂ H ₁₀ O ₄
		218.0629	-28.3	-6.2	3.0	C ₁₁ H ₁₆ Cl ₂		
218.0567	2.5	218.0498	31.6	6.9	8.0	C ₁₃ H ₁₁ O ₁ Cl ₁		
		218.0710	-65.3	-14.2	3.0	C ₁₀ H ₁₅ O ₃ Cl ₁		
		273.1272	1.2	273.1279	-2.6	-0.7	12.5	C ₂₀ H ₁₇ O ₁
		273.1257	5.4	1.5	3.5	C ₁₄ H ₂₂ O ₃ Cl ₁		
		273.1177	34.9	9.5	3.5	C ₁₅ H ₂₃ Cl ₂		
273.1272	1.2	273.1410	-50.5	-13.8	7.5	C ₁₈ H ₂₂ Cl ₁		
		274.1351	0.9	274.1358	-2.3	-0.6	12.0	C ₂₀ H ₁₈ O ₁
		274.1336	5.7	1.6	3.0	C ₁₄ H ₂₃ O ₃ Cl ₁		
		274.1255	35.1	9.6	3.0	C ₁₅ H ₂₄ Cl ₂		
		274.1488	-49.9	-13.7	7.0	C ₁₈ H ₂₃ Cl ₁		
331.9937	0.5	331.9898	11.6	3.8	26.0	C ₂₅ O ₂		
		331.9876	18.2	6.0	17.0	C ₁₉ H ₅ O ₄ Cl ₁		
		332.0007	-21.2	-7.0	12.0	C ₁₇ H ₁₀ O ₃ Cl ₂		
		332.0029	-27.8	-9.2	21.0	C ₂₃ H ₅ O ₁ Cl ₁		
		376.0276	4.7	376.0269	1.7	0.6	12.0	C ₁₉ H ₁₄ O ₄ Cl ₂
376.0276	4.7	376.0291	-4.1	-1.6	21.0	C ₂₅ H ₉ O ₂ Cl ₁		
		376.0313	-10.0	-3.7	30.0	C ₃₁ H ₄		
		376.0160	30.6	11.5	26.0	C ₂₇ H ₈ O ₃		
		377.0286	1.1	377.0239	12.4	4.7	25.5	C ₂₇ H ₅ O ₃
		377.0347	-16.4	-6.2	11.5	C ₁₉ H ₁₅ O ₄ Cl ₂		
377.0286	1.1	377.0369	-22.2	-8.4	20.5	C ₂₅ H ₁₀ O ₂ Cl ₁		
		377.0391	-28.0	-10.6	29.5	C ₃₁ H ₅		
		378.0259	3.1	378.0236	6.0	2.3	25.0	C ₂₈ H ₇ Cl ₁
		378.0214	11.8	4.5	16.0	C ₂₂ H ₁₂ O ₂ Cl ₂		
		378.0317	-15.3	-5.8	25.0	C ₂₇ H ₆ O ₃		
378.0106	40.6	40.6	15.3	30.0	C ₃₀ H ₂ O ₁			

Compound # 12

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
		201.0563	-5.0	-1.0	4.5	C ₉ H ₁₀ O ₄ F ₁
		201.0482	35.1	7.1	4.5	C ₁₀ H ₁₁ O ₁ Cl ₁ F ₁
202.0603	2.2	202.0630	-13.3	-2.7	8.0	C ₁₂ H ₁₀ O ₃
		202.0641	-19.0	-3.8	4.0	C ₉ H ₁₁ O ₄ F ₁
		202.0561	20.9	4.2	4.0	C ₁₀ H ₁₂ O ₁ Cl ₁ F ₁
207.0572	0.6	207.0577	-2.3	-0.5	6.5	C ₁₂ H ₁₂ O ₁ Cl ₁
		207.0588	-7.8	-1.6	2.5	C ₉ H ₁₃ O ₂ Cl ₁ F ₁
		207.0610	-18.4	-3.8	11.5	C ₁₅ H ₈ F ₁
216.0431	1.5	216.0434	-1.2	-0.3	5.0	C ₉ H ₉ O ₅ F ₁
		216.0423	4.1	0.9	9.0	C ₁₂ H ₈ O ₄
		216.0401	14.3	3.1	0.0	C ₆ H ₁₃ O ₆ Cl ₁
217.0490	95.7	217.0501	-4.8	-1.0	8.5	C ₁₂ H ₉ O ₄
		217.0512	-10.0	-2.2	4.5	C ₉ H ₁₀ O ₅ F ₁
		217.0454	17.0	3.7	13.5	C ₁₆ H ₆ F ₁
218.0521	13.7	218.0532	-4.9	-1.1	13.0	C ₁₆ H ₇ F ₁
		218.0510	5.2	1.1	4.0	C ₁₀ H ₁₂ O ₂ Cl ₁ F ₁
		218.0498	10.4	2.3	8.0	C ₁₃ H ₁₁ O ₁ Cl ₁
219.0522	2.3	219.0505	7.7	1.7	3.5	C ₈ H ₁₁ O ₇
		219.0577	-25.2	-5.5	7.5	C ₁₃ H ₁₂ O ₁ Cl ₁
		219.0457	29.2	6.4	8.5	C ₁₂ H ₈ O ₃ F ₁
220.0667	1.2	220.0666	0.4	0.1	3.0	C ₁₀ H ₁₄ O ₂ Cl ₁ F ₁
		220.0655	5.6	1.2	7.0	C ₁₃ H ₁₃ O ₁ Cl ₁
		220.0688	-9.6	-2.1	12.0	C ₁₆ H ₉ F ₁
221.0754	1.2	221.0745	4.3	0.9	2.5	C ₁₀ H ₁₅ O ₂ Cl ₁ F ₁
		221.0767	-5.7	-1.3	11.5	C ₁₆ H ₁₀ F ₁
		221.0733	9.4	2.1	6.5	C ₁₃ H ₁₄ O ₁ Cl ₁
222.0823	0.7	222.0823	0.1	0.0	2.0	C ₁₀ H ₁₆ O ₂ Cl ₁ F ₁
		222.0811	5.2	1.2	6.0	C ₁₃ H ₁₅ O ₁ Cl ₁
		222.0845	-9.8	-2.2	11.0	C ₁₆ H ₁₁ F ₁
247.0363	0.5	247.0373	-4.3	-1.1	4.5	C ₁₀ H ₁₂ O ₅ Cl ₁
		247.0385	-8.9	-2.2	0.5	C ₇ H ₁₃ O ₆ Cl ₁ F ₁
		247.0395	-13.2	-3.3	13.5	C ₁₆ H ₇ O ₃
249.0646	0.7	249.0682	-14.5	-3.6	7.5	C ₁₄ H ₁₄ O ₂ Cl ₁
		249.0694	-19.1	-4.8	3.5	C ₁₁ H ₁₅ O ₃ Cl ₁ F ₁
		249.0704	-23.3	-5.8	16.5	C ₂₀ H ₉
277.0415	4.4	277.0420	-1.8	-0.5	13.5	C ₁₈ H ₁₀ O ₁ Cl ₁
		277.0432	-5.9	-1.6	9.5	C ₁₅ H ₁₁ O ₂ Cl ₁ F ₁
		277.0454	-13.8	-3.8	18.5	C ₂₁ H ₆ F ₁
278.0469	0.8	278.0498	-10.5	-2.9	13.0	C ₁₈ H ₁₁ O ₁ Cl ₁
		278.0510	-14.6	-4.1	9.0	C ₁₅ H ₁₂ O ₂ Cl ₁ F ₁
		278.0427	15.4	4.3	9.0	C ₁₃ H ₁₀ O ₇
279.0412	1.8	279.0424	-4.5	-1.3	8.5	C ₁₄ H ₁₂ O ₄ Cl ₁
		279.0436	-8.6	-2.4	4.5	C ₁₁ H ₁₃ O ₅ Cl ₁ F ₁
		279.0446	-12.3	-3.4	17.5	C ₂₀ H ₇ O ₂
280.0709	0.5	280.0714	-1.6	-0.5	3.0	C ₁₁ H ₁₇ O ₆ Cl ₁
		280.0688	7.4	2.1	17.0	C ₂₁ H ₉ F ₁
		280.0736	-9.4	-2.6	12.0	C ₁₇ H ₁₂ O ₄
360.0565	23.9	360.0565	0.1	0.0	12.0	C ₁₉ H ₁₄ O ₄ Cl ₁ F ₁
		360.0575	-2.8	-1.0	25.0	C ₂₈ H ₈ O ₁
		360.0553	3.3	1.2	16.0	C ₂₂ H ₁₃ O ₃ Cl ₁
361.0603	4.8	361.0631	-8.0	-2.9	15.5	C ₂₂ H ₁₄ O ₃ Cl ₁
		361.0643	-11.2	-4.0	11.5	C ₁₉ H ₁₅ O ₄ Cl ₁ F ₁
		361.0653	-14.1	-5.1	24.5	C ₂₈ H ₉ O ₁
362.0580	8.3	362.0579	0.3	0.1	20.0	C ₂₄ H ₁₀ O ₄
		362.0591	-2.8	-1.0	16.0	C ₂₁ H ₁₁ O ₅ F ₁
		362.0569	3.2	1.2	7.0	C ₁₅ H ₁₆ O ₇ Cl ₁ F ₁

Compound # 13

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
147.0449	1.0	145.0665	-18.2	-2.6	2.5	C ₇ H ₁₀ O ₂ F ₁
		147.0446	2.3	0.3	6.5	C ₉ H ₇ O ₂
		147.0457	-5.5	-0.8	2.5	C ₆ H ₈ O ₃ F ₁
149.0237	10.7	149.0239	-1.0	-0.1	6.5	C ₈ H ₅ O ₃
		149.0250	-8.7	-1.3	2.5	C ₅ H ₆ O ₄ F ₁
150.0240	1.3					
159.0397	7.3	159.0446	-30.9	-4.9	7.5	C ₁₀ H ₇ O ₂
		159.0457	-38.1	-6.1	3.5	C ₇ H ₈ O ₃ F ₁
160.0461	1.0	160.0524	-39.5	-6.3	7.0	C ₁₀ H ₈ O ₂
		160.0536	-46.7	-7.5	3.0	C ₇ H ₉ O ₃ F ₁
161.0622	1.4	161.0614	5.1	0.8	2.5	C ₇ H ₁₀ O ₃ F ₁
		161.0603	12.2	2.0	6.5	C ₁₀ H ₉ O ₂
167.0320	2.7	167.0297	13.6	2.3	10.5	C ₁₂ H ₄ F ₁
		167.0344	-14.7	-2.5	5.5	C ₈ H ₇ O ₄
		167.0356	-21.6	-3.6	1.5	C ₅ H ₈ O ₅ F ₁
171.0510	4.5	171.0457	30.7	5.3	4.5	C ₈ H ₈ O ₃ F ₁
		171.0446	37.4	6.4	8.5	C ₁₁ H ₇ O ₂
172.0495	4.5	172.0524	-16.9	-2.9	8.0	C ₁₁ H ₈ O ₂
		172.0536	-23.6	-4.1	4.0	C ₈ H ₉ O ₃ F ₁
173.0624	17.6	173.0614	6.0	1.0	3.5	C ₉ H ₁₀ O ₃ F ₁
		173.0603	12.6	2.2	7.5	C ₁₁ H ₉ O ₂
174.0670	4.0	174.0681	-6.0	-1.0	7.0	C ₁₁ H ₁₀ O ₂
		174.0692	-12.6	-2.2	3.0	C ₈ H ₁₁ O ₃ F ₁
175.0425	3.4	175.0407	10.3	1.8	3.5	C ₇ H ₈ O ₄ F ₁
		175.0395	16.8	2.9	7.5	C ₁₀ H ₇ O ₃
185.0714	0.5	185.0767	-28.3	-5.2	8.5	C ₁₃ H ₁₀ F ₁
187.0358	9.7	187.0395	-19.6	-3.7	8.5	C ₁₁ H ₇ O ₃
		187.0407	-25.7	-4.8	4.5	C ₈ H ₈ O ₄ F ₁
188.0470	1.8	188.0473	-1.9	-0.4	8.0	C ₁₁ H ₈ O ₃
		188.0485	-8.0	-1.5	4.0	C ₈ H ₉ O ₄ F ₁
189.0564	3.7	189.0563	0.7	0.1	3.5	C ₈ H ₁₀ O ₄ F ₁
		189.0552	6.7	1.3	7.5	C ₁₁ H ₉ O ₃
190.0584	0.6	190.0630	-24.3	-4.6	7.0	C ₁₁ H ₁₀ O ₃
		190.0641	-30.3	-5.8	3.0	C ₈ H ₁₁ O ₄ F ₁
199.0393	4.5	199.0395	-1.1	-0.2	9.5	C ₁₂ H ₇ O ₃
		199.0407	-6.8	-1.4	5.5	C ₉ H ₈ O ₄ F ₁
200.0488	1.2	200.0485	1.4	0.3	5.0	C ₉ H ₉ O ₄ F ₁
		200.0473	7.1	1.4	9.0	C ₁₂ H ₈ O ₃
201.0533	4.8	201.0552	-9.5	-1.9	8.5	C ₁₂ H ₉ O ₃
		201.0563	-15.2	-3.1	4.5	C ₉ H ₁₀ O ₄ F ₁
202.0618	1.4	202.0630	-5.9	-1.2	8.0	C ₁₂ H ₁₀ O ₃
		202.0641	-11.6	-2.3	4.0	C ₉ H ₁₁ O ₄ F ₁
216.0350	0.7	216.0375	-11.7	-2.5	14.0	C ₁₆ H ₅ F ₁
		216.0423	-33.6	-7.3	9.0	C ₁₂ H ₈ O ₄
		216.0434	-38.9	-8.4	5.0	C ₉ H ₉ O ₅ F ₁
217.0478	26.0	217.0501	-10.3	-2.2	8.5	C ₁₂ H ₉ O ₄
		217.0454	11.5	2.5	13.5	C ₁₆ H ₆ F ₁
		217.0512	-15.6	-3.4	4.5	C ₉ H ₁₀ O ₅ F ₁
218.0483	3.8	218.0532	-22.5	-4.9	13.0	C ₁₆ H ₇ F ₁
		218.0579	-44.2	-9.6	8.0	C ₁₂ H ₁₀ O ₄
		218.0379	47.5	10.4	9.0	C ₁₂ H ₇ O ₃ F ₁
219.0587	0.8	219.0610	-10.5	-2.3	12.5	C ₁₆ H ₈ F ₁
		219.0657	-32.1	-7.0	7.5	C ₁₂ H ₁₁ O ₄
		219.0669	-37.3	-8.2	3.5	C ₉ H ₁₂ O ₅ F ₁
243.0795	1.8	243.0810	-6.2	-1.5	13.5	C ₁₈ H ₁₁ O ₁
		243.0821	-10.9	-2.6	9.5	C ₁₅ H ₁₂ O ₂ F ₁
279.1564	0.7	279.1549	5.3	1.5	10.5	C ₂₀ H ₂₀ F ₁
		279.1596	-11.6	-3.2	5.5	C ₁₆ H ₂₃ O ₄
		279.1608	-15.7	-4.4	1.5	C ₁₃ H ₂₄ O ₅ F ₁
285.1333	0.7	285.1291	14.9	4.2	9.5	C ₁₈ H ₁₈ O ₂ F ₁
		285.1279	18.9	5.4	13.5	C ₂₁ H ₁₇ O ₁
326.0962	14.3	326.0954	2.4	0.8	12.0	C ₁₉ H ₁₅ O ₄ F ₁
		326.0943	5.9	1.9	16.0	C ₂₂ H ₁₄ O ₃
		326.1096	-40.9	-13.3	20.0	C ₂₆ H ₁₄
327.1074	3.0	327.1033	12.6	4.1	11.5	C ₁₉ H ₁₆ O ₄ F ₁
		327.1021	16.1	5.3	15.5	C ₂₂ H ₁₅ O ₃
		327.1174	-30.5	-10.0	19.5	C ₂₆ H ₁₅
328.1088	0.5	328.1099	-3.4	-1.1	15.0	C ₂₂ H ₁₆ O ₃
		328.1111	-6.9	-2.3	11.0	C ₁₉ H ₁₇ O ₄ F ₁
		328.1252	-49.9	-16.4	19.0	C ₂₆ H ₁₆

Compound # 14

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
218.0570	2.4	218.0579	-4.1	-0.9	8.0	C ₁₂ H ₁₀ O ₄
		218.0555	7.1	1.6	5.0	C ₁₀ H ₉ O ₂ F ₃
		218.0591	-9.3	-2.0	4.0	C ₉ H ₁₁ O ₅ F ₁
		218.0543	12.4	2.7	9.0	C ₁₃ H ₈ O ₁ F ₂
230.8785	10.3					
235.9138	1.2					
301.1058	1.8	301.1052	2.2	0.7	6.5	C ₁₅ H ₁₆ O ₃ F ₃
		301.1076	-6.0	-1.8	9.5	C ₁₇ H ₁₇ O ₅
		301.1040	6.0	1.8	10.5	C ₁₈ H ₁₅ O ₂ F ₂
		301.1029	9.8	2.9	14.5	C ₂₁ H ₁₄ O ₁ F ₁
357.0867	1.3	357.0891	-6.8	-2.4	17.5	C ₂₄ H ₁₂ F ₃
		357.0916	-13.6	-4.9	20.5	C ₂₆ H ₁₃ O ₂
		357.0927	-16.8	-6.0	16.5	C ₂₃ H ₁₄ O ₃ F ₁
		357.0938	-20.0	-7.1	12.5	C ₂₀ H ₁₅ O ₄ F ₂
		376.0911	-0.3	-0.1	16.0	C ₂₃ H ₁₄ O ₃ F ₂
		376.0900	2.7	1.0	20.0	C ₂₆ H ₁₃ O ₂ F ₁
		376.0922	-3.3	-1.3	12.0	C ₂₀ H ₁₅ O ₄ F ₃
		376.0888	5.8	2.2	24.0	C ₂₉ H ₁₂ O ₁
377.0939	1.5	377.0966	-7.3	-2.7	23.5	C ₂₉ H ₁₃ O ₁
		377.0978	-10.3	-3.9	19.5	C ₂₆ H ₁₄ O ₂ F ₁
		377.0989	-13.4	-5.0	15.5	C ₂₃ H ₁₅ O ₃ F ₂
		377.1001	-16.4	-6.2	11.5	C ₂₀ H ₁₆ O ₄ F ₃

Compound # 15

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
149.0268	100.0	149.0250	12.0	1.8	2.5	C ₅ H ₆ O ₄ F ₁
		149.0239	19.7	2.9	6.5	C ₈ H ₅ O ₃
150.0306	10.8	150.0317	-7.3	-1.1	6.0	C ₈ H ₆ O ₃
		150.0292	9.0	1.3	3.0	C ₆ H ₅ O ₁ F ₃
		150.0328	-14.9	-2.2	2.0	C ₅ H ₇ O ₄ F ₁
		150.0281	16.6	2.5	7.0	C ₉ H ₄ F ₂
151.0344	1.7	151.0359	-10.3	-1.6	6.5	C ₉ H ₅ F ₂
		151.0371	-17.9	-2.7	2.5	C ₆ H ₆ O ₁ F ₃
155.0755	1.1					
159.0430	8.3	159.0422	5.3	0.8	4.5	C ₈ H ₆ F ₃
		159.0446	-10.0	-1.6	7.5	C ₁₀ H ₇ O ₂
		159.0457	-17.2	-2.7	3.5	C ₇ H ₈ O ₃ F ₁
160.0493	1.7	160.0500	-4.6	-0.7	4.0	C ₈ H ₇ F ₃
		160.0524	-19.8	-3.2	7.0	C ₁₀ H ₈ O ₂
167.0347	30.7	167.0344	1.4	0.2	5.5	C ₈ H ₇ O ₄
		167.0356	-5.4	-0.9	1.5	C ₅ H ₈ O ₅ F ₁
		167.0320	16.1	2.7	2.5	C ₆ H ₆ O ₂ F ₃
168.0379	2.9	168.0375	2.5	0.4	10.0	C ₁₂ H ₅ F ₁
		168.0387	-4.3	-0.7	6.0	C ₉ H ₆ O ₁ F ₂
		168.0398	-11.1	-1.9	2.0	C ₆ H ₇ O ₂ F ₃
171.0454	2.2	171.0457	-1.9	-0.3	4.5	C ₈ H ₈ O ₃ F ₁
		171.0446	4.8	0.8	8.5	C ₁₁ H ₇ O ₂
		171.0469	-8.6	-1.5	0.5	C ₅ H ₉ O ₄ F ₂
		171.0422	19.1	3.3	5.5	C ₉ H ₆ F ₃
172.0529	2.7	172.0524	2.5	0.4	8.0	C ₁₁ H ₈ O ₂
		172.0536	-4.1	-0.7	4.0	C ₈ H ₉ O ₃ F ₁
		172.0547	-10.8	-1.9	0.0	C ₅ H ₁₀ O ₄ F ₂
		172.0500	16.7	2.9	5.0	C ₉ H ₇ F ₃
173.0608	11.6	173.0603	3.0	0.5	7.5	C ₁₁ H ₉ O ₂
		173.0614	-3.6	-0.6	3.5	C ₈ H ₁₀ O ₃ F ₁
		173.0578	17.1	3.0	4.5	C ₉ H ₈ F ₃
174.0638	2.7	174.0656	-10.8	-1.9	4.0	C ₉ H ₉ F ₃
175.0433	1.5	175.0407	15.1	2.6	3.5	C ₇ H ₈ O ₄ F ₁
187.0403	3.0	187.0407	-2.0	-0.4	4.5	C ₈ H ₈ O ₄ F ₁
		187.0395	4.1	0.8	8.5	C ₁₁ H ₇ O ₃
		187.0418	-8.2	-1.5	0.5	C ₅ H ₉ O ₅ F ₂
		187.0371	17.1	3.2	5.5	C ₉ H ₆ O ₁ F ₃
189.0599	1.3	189.0563	19.1	3.6	3.5	C ₈ H ₁₀ O ₄ F ₁
199.0384	2.0	199.0395	-5.6	-1.1	9.5	C ₁₂ H ₉ O ₃
		199.0371	6.6	1.3	6.5	C ₁₀ H ₆ O ₁ F ₃
		199.0407	-11.4	-2.3	5.5	C ₉ H ₈ O ₄ F ₁
		199.0359	12.4	2.5	10.5	C ₁₃ H ₅ F ₂
201.0532	1.7	201.0527	2.3	0.5	5.5	C ₁₀ H ₈ O ₁ F ₃
		201.0516	8.0	1.6	9.5	C ₁₃ H ₇ F ₂
		201.0552	-9.9	-2.0	8.5	C ₁₂ H ₉ O ₃
		201.0563	-15.5	-3.1	4.5	C ₉ H ₁₀ O ₄ F ₁
217.0478	5.2	217.0476	0.8	0.2	5.5	C ₁₀ H ₈ O ₂ F ₃
		217.0465	6.1	1.3	9.5	C ₁₃ H ₇ O ₁ F ₂
		217.0501	-10.5	-2.3	8.5	C ₁₂ H ₉ O ₄
		217.0454	11.3	2.5	13.5	C ₁₆ H ₆ F ₁
218.0596	1.0	218.0591	2.5	0.5	4.0	C ₉ H ₁₁ O ₅ F ₁
		218.0579	7.7	1.7	8.0	C ₁₂ H ₁₀ O ₄
		218.0555	18.9	4.1	5.0	C ₁₀ H ₉ O ₂ F ₃
279.1589	6.4	279.1596	-2.5	-0.7	5.5	C ₁₆ H ₂₃ O ₄
		279.1572	6.2	1.7	2.5	C ₁₄ H ₂₂ O ₂ F ₃
		279.1608	-6.6	-1.8	1.5	C ₁₃ H ₂₄ O ₅ F ₁
		279.1560	10.3	2.9	6.5	C ₁₇ H ₂₁ O ₁ F ₂
280.1631	1.4	280.1627	1.2	0.3	10.0	C ₂₀ H ₂₁ F ₁
		280.1639	-2.9	-0.8	6.0	C ₁₇ H ₂₂ O ₁ F ₂
		280.1650	-7.0	-2.0	2.0	C ₁₄ H ₂₃ O ₂ F ₃
		280.1675	-15.7	-4.4	5.0	C ₁₆ H ₂₄ O ₄
376.0931	5.2	376.0922	2.4	0.9	12.0	C ₂₀ H ₁₅ O ₄ F ₃
		376.0911	5.4	2.0	16.0	C ₂₃ H ₁₄ O ₃ F ₂
		376.0900	8.5	3.2	20.0	C ₂₆ H ₁₃ O ₂ F ₁
		376.0888	11.5	4.3	24.0	C ₂₉ H ₁₂ O ₁
377.0953	1.2	377.0966	-3.6	-1.3	23.5	C ₂₉ H ₁₃ O ₁
		377.0978	-6.6	-2.5	19.5	C ₂₆ H ₁₄ O ₂ F ₁
		377.0989	-9.6	-3.6	15.5	C ₂₃ H ₁₅ O ₃ F ₂
		377.1001	-12.7	-4.8	11.5	C ₂₀ H ₁₆ O ₄ F ₃

Compound # 16

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
217.0925	0.9	215.0497	-97.1	-20.9	13.5	C ₁₆ H ₇ O ₁
		217.0865	27.9	6.1	7.5	C ₁₃ H ₁₃ O ₃
		217.1017	-42.4	-9.2	11.5	C ₁₇ H ₁₃
		218.0004	-83.6	-18.2	14.0	C ₁₄ H ₂ O ₃
217.9822	3.8					
218.9070	1.6					
230.8678	2.1					
242.8927	1.3					
263.0661	1.0	263.0708	-17.8	-4.7	12.5	C ₁₇ H ₁₁ O ₃
		263.0497	62.5	16.4	17.5	C ₂₀ H ₇ O ₁
		263.0861	-75.8	-19.9	16.5	C ₂₁ H ₁₁
		267.0082	12.5	3.3	17.5	C ₁₈ H ₃ O ₃
267.0115	6.1	267.0235	-44.7	-11.9	21.5	C ₂₂ H ₃
		268.0160	-21.6	-5.8	17.0	C ₁₈ H ₄ O ₃
268.0103	1.4	267.9949	57.3	15.4	22.0	C ₂₁ O ₁
		268.0313	-78.5	-21.0	21.0	C ₂₂ H ₄
268.8420	0.6					
279.1399	6.1	279.1385	4.8	1.4	10.5	C ₁₉ H ₁₉ O ₂
		279.1596	-70.8	-19.8	5.5	C ₁₆ H ₂₃ O ₄
		279.1174	80.5	22.5	15.5	C ₂₂ H ₁₅
		280.1675	-36.3	-10.2	5.0	C ₁₆ H ₂₄ O ₄
280.1573	1.2	280.1463	39.2	11.0	10.0	C ₁₉ H ₂₀ O ₂
		280.1827	-90.7	-25.4	9.0	C ₂₀ H ₂₄ O ₁
350.1520	2.5	350.1518	0.5	0.2	12.0	C ₂₂ H ₂₂ O ₄
		350.1671	-43.1	-15.1	16.0	C ₂₆ H ₂₂ O ₁
		350.1307	60.8	21.3	17.0	C ₂₅ H ₁₈ O ₂
		351.1596	-1.8	-0.6	11.5	C ₂₂ H ₂₃ O ₄
351.1590	0.7	351.1749	-45.2	-15.9	15.5	C ₂₆ H ₂₃ O ₁
		351.1385	58.4	20.5	16.5	C ₂₅ H ₁₉ O ₂

Compound # 17

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
203.0712	1.3	203.0708	1.8	0.4	7.5	C ₁₂ H ₁₁ O ₃
		203.0861	-73.3	-14.9	11.5	C ₁₆ H ₁₁
		203.0556	77.0	15.6	3.5	C ₈ H ₁₁ O ₆
216.0432	3.9	216.0423	4.4	1.0	9.0	C ₁₂ H ₈ O ₄
		216.0575	-66.2	-14.3	13.0	C ₁₆ H ₈ O ₁
		216.0270	75.0	16.2	5.0	C ₈ H ₈ O ₇
217.0494	89.1	217.0501	-3.3	-0.7	8.5	C ₁₂ H ₉ O ₄
		217.0348	67.0	14.5	4.5	C ₈ H ₉ O ₇
		217.0653	-73.6	-16.0	12.5	C ₁₆ H ₉ O ₁
218.0525	11.7	218.0579	-24.9	-5.4	8.0	C ₁₂ H ₁₀ O ₄
		218.0427	45.1	9.8	4.0	C ₈ H ₁₀ O ₇
		218.0368	72.0	15.7	13.0	C ₁₅ H ₆ O ₂
219.0606	2.5	219.0657	-23.3	-5.1	7.5	C ₁₂ H ₁₁ O ₄
		219.0505	46.3	10.2	3.5	C ₈ H ₁₁ O ₇
		219.0446	73.2	16.0	12.5	C ₁₅ H ₇ O ₂
225.0895	1.6	225.0916	-9.1	-2.0	9.5	C ₁₅ H ₁₃ O ₂
		225.0974	-35.2	-7.9	0.5	C ₈ H ₁₇ O ₇
		225.0763	58.7	13.2	5.5	C ₁₁ H ₁₃ O ₅
255.1011	27.3	255.1021	-3.8	-1.0	9.5	C ₁₆ H ₁₅ O ₃
		255.0869	56.0	14.3	5.5	C ₁₂ H ₁₅ O ₆
		255.1174	-63.6	-16.2	13.5	C ₂₀ H ₁₅
256.1072	4.5	256.1099	-10.8	-2.8	9.0	C ₁₆ H ₁₆ O ₃
		256.0947	48.7	12.5	5.0	C ₁₂ H ₁₆ O ₆
		256.1252	-70.4	-18.0	13.0	C ₂₀ H ₁₆
338.1148	37.3	338.1154	-1.9	-0.6	12.0	C ₂₀ H ₁₈ O ₅
		338.1096	15.5	5.2	21.0	C ₂₇ H ₁₄
		338.1307	-47.0	-15.9	16.0	C ₂₄ H ₁₈ O ₂
339.1203	7.6	339.1174	8.6	2.9	20.5	C ₂₇ H ₁₅
		339.1232	-8.7	-3.0	11.5	C ₂₀ H ₁₉ O ₅
		339.1021	53.6	18.2	16.5	C ₂₃ H ₁₅ O ₃
340.1221	1.5	340.1252	-9.2	-3.1	20.0	C ₂₇ H ₁₆
		340.1311	-26.5	-9.0	11.0	C ₂₀ H ₂₀ O ₅
		340.1099	35.7	12.1	16.0	C ₂₃ H ₁₆ O ₃

Compound # 18

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
151.0661	2.7	151.0606	36.2	5.5	0.5	C ₅ H ₁₁ O ₅
		151.0759	-64.8	-9.8	4.5	C ₉ H ₁₁ O ₂
		151.0548	75.1	11.3	9.5	C ₁₂ H ₇
152.0469	19.3	152.0473	-3.2	-0.5	5.0	C ₈ H ₈ O ₃
		152.0321	97.1	14.8	1.0	C ₄ H ₈ O ₆
153.0506	1.9	153.0552	-29.8	-4.6	4.5	C ₆ H ₉ O ₃
		153.0399	69.8	10.7	0.5	C ₄ H ₉ O ₆
159.0455	4.2	159.0446	5.5	0.9	7.5	C ₁₀ H ₇ O ₂
160.0518	1.1	160.0524	-3.8	-0.6	7.0	C ₁₀ H ₈ O ₂
		160.0372	91.6	14.7	3.0	C ₆ H ₈ O ₅
164.0487	1.1	164.0473	8.2	1.3	6.0	C ₉ H ₈ O ₃
		164.0626	-84.8	-13.9	10.0	C ₁₃ H ₈
171.0453	17.7	171.0446	4.1	0.7	8.5	C ₁₁ H ₇ O ₂
		171.0293	93.3	16.0	4.5	C ₇ H ₇ O ₅
172.0525	54.3	172.0524	0.2	0.0	8.0	C ₁₁ H ₈ O ₂
		172.0372	88.8	15.3	4.0	C ₇ H ₈ O ₅
173.0601	29.7	173.0603	-0.7	-0.1	7.5	C ₁₁ H ₉ O ₂
		173.0450	87.5	15.1	3.5	C ₇ H ₉ O ₅
174.0658	5.2	174.0681	-12.9	-2.3	7.0	C ₁₁ H ₁₀ O ₂
		174.0528	74.7	13.0	3.0	C ₇ H ₁₀ O ₅
185.0596	1.2	185.0603	-3.7	-0.7	8.5	C ₁₂ H ₉ O ₂
		185.0450	78.8	14.6	4.5	C ₈ H ₉ O ₅
187.0644	1.1	187.0606	19.9	3.7	3.5	C ₈ H ₁₁ O ₅
		187.0548	51.3	9.6	12.5	C ₁₅ H ₇
		187.0759	-61.6	-11.5	7.5	C ₁₂ H ₁₁ O ₂
189.0703	1.1	189.0704	-0.6	-0.1	11.5	C ₁₅ H ₉
		189.0763	-31.6	-6.0	2.5	C ₈ H ₁₃ O ₅
		189.0552	80.1	15.1	7.5	C ₁₁ H ₉ O ₃
199.0427	1.8	199.0395	15.8	3.2	9.5	C ₁₂ H ₇ O ₃
		199.0548	-60.8	-12.1	13.5	C ₁₆ H ₇
		199.0606	-90.3	-18.0	4.5	C ₉ H ₁₁ O ₅
200.0477	9.8	200.0473	1.8	0.4	9.0	C ₁₂ H ₈ O ₃
		200.0626	-74.5	-14.9	13.0	C ₁₆ H ₈
		200.0321	78.1	15.6	5.0	C ₈ H ₈ O ₆
201.0538	66.5	201.0552	-6.8	-1.4	8.5	C ₁₂ H ₉ O ₃
		201.0399	69.1	13.9	4.5	C ₈ H ₉ O ₆
		201.0704	-82.7	-16.6	12.5	C ₁₆ H ₉
202.0594	9.5	202.0630	-17.6	-3.5	8.0	C ₁₂ H ₁₀ O ₃
		202.0477	57.9	11.7	4.0	C ₈ H ₁₀ O ₆
		202.0419	87.0	17.6	13.0	C ₁₅ H ₆ O ₁
203.0651	1.4	203.0708	-28.0	-5.7	7.5	C ₁₂ H ₁₁ O ₃
		203.0556	47.1	9.6	3.5	C ₈ H ₁₁ O ₆
		203.0497	76.0	15.4	12.5	C ₁₅ H ₇ O ₁
213.0549	1.2	213.0552	-1.0	-0.2	9.5	C ₁₃ H ₉ O ₃
		213.0399	70.6	15.0	5.5	C ₉ H ₉ O ₆
		213.0704	-72.6	-15.5	13.5	C ₁₇ H ₉
214.0633	2.7	214.0630	1.7	0.4	9.0	C ₁₃ H ₁₀ O ₃
		214.0783	-69.6	-14.9	13.0	C ₁₇ H ₁₀
		214.0477	72.9	15.6	5.0	C ₉ H ₁₀ O ₆
216.0653	2.1	216.0634	8.9	1.9	4.0	C ₉ H ₁₂ O ₆
		216.0575	36.1	7.8	13.0	C ₁₆ H ₈ O ₁
		216.0786	-61.7	-13.3	8.0	C ₁₃ H ₁₂ O ₃
217.0506	1.3	217.0501	2.4	0.5	8.5	C ₁₂ H ₉ O ₄
		217.0653	-67.8	-14.7	12.5	C ₁₆ H ₉ O ₁
		217.0348	72.7	15.8	4.5	C ₈ H ₉ O ₇
218.0592	3.0	218.0579	5.9	1.3	8.0	C ₁₂ H ₁₀ O ₄
		218.0732	-64.1	-14.0	12.0	C ₁₆ H ₁₀ O ₁
		218.0427	75.8	16.5	4.0	C ₈ H ₁₀ O ₇
285.1367	1.5	285.1338	10.0	2.9	4.5	C ₁₄ H ₂₁ O ₆
		285.1279	30.6	8.7	13.5	C ₂₁ H ₁₇ O ₁
		285.1491	-43.5	-12.4	8.5	C ₁₈ H ₂₁ O ₃
320.1062	2.6	320.1049	4.3	1.4	13.0	C ₂₀ H ₁₆ O ₄
		320.1201	-43.4	-13.9	17.0	C ₂₄ H ₁₆ O ₁
		320.0896	52.0	16.6	9.0	C ₁₆ H ₁₆ O ₇
366.1093	21.4	366.1103	-2.8	-1.0	13.0	C ₂₁ H ₁₈ O ₆
		366.1045	13.3	4.9	22.0	C ₂₈ H ₁₄ O ₁
		366.1256	-44.5	-16.3	17.0	C ₂₅ H ₁₈ O ₃
367.1133	4.8	367.1123	2.7	1.0	21.5	C ₂₈ H ₁₅ O ₁
		367.1182	-13.3	-4.9	12.5	C ₂₁ H ₁₉ O ₆
		367.0970	44.3	16.2	17.5	C ₂₄ H ₁₅ O ₄

Compound # 19

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
218.0552	1.1	218.0532	9.4	2.1	13.0	C ₁₆ H ₇ F ₁
		218.0579	-12.2	-2.7	8.0	C ₁₂ H ₁₀ O ₄
		218.0591	-17.5	-3.8	4.0	C ₉ H ₁₁ O ₅ F ₁
		218.0427	57.7	12.6	4.0	C ₈ H ₁₀ O ₇
		338.0999	0.6	338.0954	13.3	4.5
384.1007	11.2	338.0943	16.7	5.7	17.0	C ₂₃ H ₁₄ O ₃
		338.1096	-28.4	-9.6	21.0	C ₂₇ H ₁₄
		338.1107	-31.8	-10.7	17.0	C ₂₄ H ₁₅ O ₁ F ₁
		384.1009	-0.7	-0.3	13.0	C ₂₁ H ₁₇ O ₆ F ₁
		384.0998	2.3	0.9	17.0	C ₂₄ H ₁₆ O ₅
		384.0950	14.6	5.6	22.0	C ₂₈ H ₁₃ O ₁ F ₁
		384.0939	17.6	6.8	26.0	C ₃₁ H ₁₂
		385.1029	3.9	1.5	21.5	C ₂₈ H ₁₄ O ₁ F ₁
		385.1017	6.8	2.6	25.5	C ₃₁ H ₁₃
		385.1076	-8.4	-3.2	16.5	C ₂₄ H ₁₇ O ₅
385.1044	2.5	385.1087	-11.4	-4.4	12.5	C ₂₁ H ₁₈ O ₆ F ₁

Compound # 20

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
201.0482	10.3	201.0552	-34.5	-6.9	8.5	C ₁₂ H ₉ O ₃
		201.0399	41.4	8.3	4.5	C ₈ H ₉ O ₆
		201.0340	70.6	14.2	13.5	C ₁₅ H ₅ O ₁
202.0558	1.7	202.0630	-35.6	-7.2	8.0	C ₁₂ H ₁₀ O ₃
		202.0477	39.9	8.1	4.0	C ₈ H ₁₀ O ₆
		202.0419	69.0	13.9	13.0	C ₁₅ H ₆ O ₁
350.1150	6.4	350.1154	-1.2	-0.4	13.0	C ₂₁ H ₁₈ O ₅
		350.1096	15.6	5.5	22.0	C ₂₈ H ₁₄
		350.1307	-44.7	-15.7	17.0	C ₂₅ H ₁₈ O ₂
351.1143	1.0	351.1174	-8.7	-3.1	21.5	C ₂₈ H ₁₅
		351.1232	-25.4	-8.9	12.5	C ₂₁ H ₁₉ O ₅
		351.1021	34.7	12.2	17.5	C ₂₄ H ₁₅ O ₃

Compound # 21

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition	
357.0522	1.2	357.0527	-1.5	-0.5	18.5	C ₂₃ H ₉ O ₁ F ₃	
		357.0516	1.7	0.6	22.5	C ₂₆ H ₇ F ₂	
		357.0552	-8.3	-3.0	21.5	C ₂₅ H ₉ O ₃	
		357.0563	-11.5	-4.1	17.5	C ₂₂ H ₁₀ O ₄ F ₁	
		357.0575	-14.7	-5.3	13.5	C ₁₉ H ₁₁ O ₅ F ₂	
359.0434	7.6	359.0497	-17.5	-6.3	25.5	C ₂₈ H ₇ O ₁	
		359.0508	-20.7	-7.4	21.5	C ₂₅ H ₈ O ₂ F ₁	
		359.0356	21.8	7.8	17.5	C ₂₁ H ₈ O ₅ F ₁	
		359.0520	-23.9	-8.6	17.5	C ₂₂ H ₉ O ₃ F ₂	
		359.0344	25.0	9.0	21.5	C ₂₄ H ₇ O ₄	
		360.0434	16.7	6.0	17.0	C ₂₁ H ₉ O ₅ F ₁	
		360.0423	19.8	7.1	21.0	C ₂₄ H ₈ O ₄	
360.0494	1.9	360.0575	-22.5	-8.1	25.0	C ₂₈ H ₈ O ₁	
		360.0587	-25.7	-9.3	21.0	C ₂₅ H ₉ O ₂ F ₁	
		360.0398	26.6	9.6	18.0	C ₂₂ H ₇ O ₂ F ₃	
		385.0816	1.1	-3.4	-1.3	22.5	C ₂₈ H ₁₁ F ₂
		385.0840	-6.4	-2.5	18.5	C ₂₅ H ₁₂ O ₁ F ₃	
		385.0865	-12.7	-4.9	21.5	C ₂₇ H ₁₃ O ₃	
		385.0876	-15.7	-6.0	17.5	C ₂₄ H ₁₄ O ₄ F ₁	
404.0866	6.7	385.0888	-18.7	-7.2	13.5	C ₂₁ H ₁₅ O ₅ F ₂	
		404.0872	-1.3	-0.5	13.0	C ₂₁ H ₁₅ O ₅ F ₃	
		404.0860	1.6	0.6	17.0	C ₂₄ H ₁₄ O ₄ F ₂	
		404.0849	4.4	1.8	21.0	C ₂₇ H ₁₃ O ₃ F ₁	
		404.0837	7.2	2.9	25.0	C ₃₀ H ₁₂ O ₂	
		404.0813	13.3	5.4	22.0	C ₂₈ H ₁₁ F ₃	
		405.0868	1.6	-5.6	-2.3	21.5	C ₂₈ H ₁₂ F ₃
405.0888	1.6	405.0891	-5.6	-2.3	21.5	C ₂₈ H ₁₂ F ₃	
		405.0916	-11.6	-4.7	24.5	C ₃₀ H ₁₃ O ₂	
		405.0927	-14.5	-5.9	20.5	C ₂₇ H ₁₄ O ₃ F ₁	
		405.0938	-17.3	-7.0	16.5	C ₂₄ H ₁₅ O ₄ F ₂	
		405.0950	-20.1	-8.1	12.5	C ₂₁ H ₁₆ O ₅ F ₃	

Compound #22

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
173.0601	13.0	173.0603	-1.0	-0.2	7.5	C ₁₁ H ₉ O ₂
		173.0733	-76.5	-13.2	2.5	C ₉ H ₁₄ O ₁ Cl ₁
		173.0450	87.2	15.1	3.5	C ₇ H ₉ O ₅
174.0658	1.8	174.0681	-12.8	-2.2	7.0	C ₁₁ H ₁₀ O ₂
		174.0528	74.8	13.0	3.0	C ₇ H ₁₀ O ₅
		174.0811	-87.9	-15.3	2.0	C ₉ H ₁₅ O ₁ Cl ₁
200.0518	3.0	200.0473	22.1	4.4	9.0	C ₁₂ H ₈ O ₃
		200.0452	33.1	6.6	0.0	C ₆ H ₁₃ O ₅ Cl ₁
		200.0604	-43.2	-8.6	4.0	C ₁₀ H ₁₃ O ₂ Cl ₁
201.0551	18.9	200.0626	-54.2	-10.8	13.0	C ₁₆ H ₈
		201.0552	-0.2	-0.0	8.5	C ₁₂ H ₉ O ₃
		201.0471	39.9	8.0	8.5	C ₁₃ H ₁₀ Cl ₁
202.0586	2.5	201.0682	-65.2	-13.1	3.5	C ₁₀ H ₁₄ O ₂ Cl ₁
		201.0399	75.6	15.2	4.5	C ₉ H ₉ O ₆
		202.0549	18.0	3.6	8.0	C ₁₃ H ₁₁ Cl ₁
216.0717	1.0	202.0630	-21.9	-4.4	8.0	C ₁₂ H ₁₀ O ₃
		202.0477	53.6	10.8	4.0	C ₉ H ₁₀ O ₆
		202.0419	82.7	16.7	13.0	C ₁₅ H ₆ O ₁
370.0596	6.3	216.0706	5.4	1.2	8.0	C ₁₄ H ₁₃ Cl ₁
		216.0786	-32.0	-6.9	8.0	C ₁₃ H ₁₂ O ₃
		216.0634	38.6	8.3	4.0	C ₉ H ₁₂ O ₆
371.0629	1.3	216.0575	65.8	14.2	13.0	C ₁₆ H ₉ O ₁
		370.0608	-3.2	-1.2	13.0	C ₂₀ H ₁₅ O ₅ Cl ₁
		370.0630	-9.1	-3.4	22.0	C ₂₆ H ₁₀ O ₃
371.0629	1.3	370.0549	12.7	4.7	22.0	C ₂₇ H ₁₁ Cl ₁
		370.0477	32.1	11.9	18.0	C ₂₂ H ₁₀ O ₆
		371.0628	0.3	0.1	21.5	C ₂₇ H ₁₂ Cl ₁
		371.0686	-15.5	-5.8	12.5	C ₂₀ H ₁₆ O ₅ Cl ₁
		371.0556	19.7	7.3	17.5	C ₂₂ H ₁₁ O ₆
		371.0708	-21.4	-8.0	21.5	C ₂₆ H ₁₁ O ₃

Compound # 23

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
		201.9629	-89.0	-18.0	4.0	C ₇ H ₇ O ₂ Br ₁
		201.9266	91.2	18.4	5.0	C ₆ H ₂ O ₃ Br ₁
202.0629	3.0	202.0630	-0.4	-0.1	8.0	C ₁₂ H ₁₀ O ₃
		202.0783	-75.9	-15.3	12.0	C ₁₆ H ₁₀
203.0791	1.0	203.0861	-34.2	-7.0	11.5	C ₁₆ H ₁₁
		203.0708	40.9	8.3	7.5	C ₁₂ H ₁₁ O ₃
		203.0919	-63.2	-12.8	2.5	C ₉ H ₁₅ O ₅
204.0801	0.5	204.0786	7.0	1.4	7.0	C ₁₂ H ₁₂ O ₃
		204.0939	-67.8	-13.8	11.0	C ₁₆ H ₁₂
		204.0998	-96.5	-19.7	2.0	C ₉ H ₁₆ O ₅
205.0846	0.8	205.0865	-9.4	-1.9	6.5	C ₁₂ H ₁₃ O ₃
		205.1017	-83.7	-17.2	10.5	C ₁₆ H ₁₃
		205.0653	93.7	19.2	11.5	C ₁₅ H ₉ O ₁
213.0673	0.6	213.0704	-14.8	-3.2	13.5	C ₁₇ H ₉
		213.0763	-42.4	-9.0	4.5	C ₁₀ H ₁₃ O ₅
		213.0552	56.8	12.1	9.5	C ₁₃ H ₉ O ₃
213.1820	0.6	213.1855	-16.3	-3.5	1.5	C ₁₃ H ₂₅ O ₂
		213.1643	82.8	17.6	6.5	C ₁₆ H ₂₁
214.0691	0.7	214.0630	28.4	6.1	9.0	C ₁₃ H ₁₀ O ₃
		214.0783	-42.8	-9.2	13.0	C ₁₇ H ₁₀
		214.0841	-70.3	-15.0	4.0	C ₁₀ H ₁₄ O ₅
215.0737	0.8	215.0708	13.6	2.9	8.5	C ₁₃ H ₁₁ O ₃
		215.0861	-57.4	-12.3	12.5	C ₁₇ H ₁₁
		215.0919	-84.7	-18.2	3.5	C ₁₀ H ₁₅ O ₅
216.0814	1.2	216.0786	12.8	2.8	8.0	C ₁₃ H ₁₂ O ₃
		216.0939	-57.8	-12.5	12.0	C ₁₇ H ₁₂
		216.0998	-85.0	-18.4	3.0	C ₁₀ H ₁₆ O ₅
217.1869	0.5	217.1804	29.9	6.5	0.5	C ₁₂ H ₂₅ O ₃
		217.1956	-40.3	-8.8	4.5	C ₁₆ H ₂₅
217.9743	0.6	217.9731	5.3	1.2	8.0	C ₁₁ H ₇ Br ₁
		217.9579	75.3	16.4	4.0	C ₇ H ₇ O ₃ Br ₁
		217.9942	-91.6	-20.0	3.0	C ₈ H ₁₁ O ₂ Br ₁
218.0560	3.8	218.0579	-8.6	-1.9	8.0	C ₁₂ H ₁₀ O ₄
		218.0670	-50.3	-11.0	1.0	C ₁₀ H ₁₉ Br ₁
		218.0732	-78.5	-17.1	12.0	C ₁₆ H ₁₀ O ₁
		218.0368	88.4	19.3	13.0	C ₁₅ H ₆ O ₂
220.0817	0.6	220.0827	-4.2	-0.9	0.0	C ₁₀ H ₂₁ Br ₁
		220.0888	-32.2	-7.1	11.0	C ₁₆ H ₁₂ O ₁
		220.0736	37.1	8.2	7.0	C ₁₂ H ₁₂ O ₄
263.1572	0.5	263.1647	-28.6	-7.5	5.5	C ₁₆ H ₂₃ O ₃
		263.1436	51.7	13.6	10.5	C ₁₉ H ₁₉ O ₁
		263.1800	-86.6	-22.8	9.5	C ₂₀ H ₂₃
279.1609	6.9	279.1596	4.5	1.2	5.5	C ₁₆ H ₂₃ O ₄
		279.1749	-50.2	-14.0	9.5	C ₂₀ H ₂₃ O ₁
		279.1385	80.2	22.4	10.5	C ₁₉ H ₁₉ O ₂
280.1626	1.4	280.1675	-17.2	-4.8	5.0	C ₁₆ H ₂₄ O ₄
		280.1463	58.2	16.3	10.0	C ₁₉ H ₂₀ O ₂
		280.1827	-71.7	-20.1	9.0	C ₂₀ H ₂₄ O ₁
281.2768	0.6	281.2844	-27.2	-7.6	1.5	C ₁₉ H ₃₇ O ₁
414.0087	2.0	414.0103	-3.9	-1.6	13.0	C ₂₀ H ₁₅ O ₅ Br ₁
		414.0106	-4.6	-1.9	33.0	C ₃₃ H ₂ O ₁
		414.0044	10.3	4.2	22.0	C ₂₇ H ₁₁ Br ₁
		413.9953	32.2	13.3	29.0	C ₂₉ H ₂ O ₄
		414.0255	-40.8	-16.9	17.0	C ₂₄ H ₁₅ O ₂ Br ₁
		413.9892	47.1	19.5	18.0	C ₂₃ H ₁₁ O ₃ Br ₁
414.9984	0.6	414.9970	3.4	1.4	17.5	C ₂₃ H ₁₂ O ₃ Br ₁
		415.0031	-11.4	-4.7	28.5	C ₂₉ H ₃ O ₄
		415.0122	-33.4	-13.8	21.5	C ₂₇ H ₁₂ Br ₁
		415.0181	-47.5	-19.7	12.5	C ₂₀ H ₁₆ O ₅ Br ₁
		415.0184	-48.2	-20.0	32.5	C ₃₃ H ₃ O ₁
		414.9759	54.3	22.5	22.5	C ₂₆ H ₉ O ₁ Br ₁
416.0040	2.0	416.0048	-1.9	-0.8	17.0	C ₂₃ H ₁₃ O ₃ Br ₁
		416.0110	-16.7	-7.0	28.0	C ₂₉ H ₄ O ₄
		415.9898	34.1	14.2	33.0	C ₃₂ O ₂
		416.0201	-38.6	-16.1	21.0	C ₂₇ H ₁₃ Br ₁
		415.9837	48.9	20.3	22.0	C ₂₆ H ₉ O ₁ Br ₁
		416.0259	-52.7	-21.9	12.0	C ₂₀ H ₁₇ O ₅ Br ₁

Compound #24

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
161.0092	1.3	161.0027 161.0239	40.1 -91.1	6.5 -14.7	12.5 7.5	C ₁₂ H ₁₁ O ₁ C ₉ H ₅ O ₃
161.9483	1.4					
165.0451	1.8	165.0552 165.0340	-61.2 66.8	-10.1 11.0	5.5 10.5	C ₉ H ₉ O ₃ C ₁₂ H ₅ O ₁
171.0465	3.4	171.0446	11.3	1.9	8.5	C ₁₁ H ₇ O ₂
172.0540	3.6	172.0524 172.0372	8.9 97.6	1.5 16.8	8.0 4.0	C ₁₁ H ₈ O ₂ C ₇ H ₈ O ₅
173.0631	9.9	173.0603	16.5	2.9	7.5	C ₁₁ H ₉ O ₂
174.0686	2.8	174.0681 174.0528	3.1 90.7	0.5 15.8	7.0 3.0	C ₁₁ H ₁₀ O ₂ C ₇ H ₁₀ O ₅
175.0462	1.8	175.0395 175.0548 175.0606	38.4 -48.8 -82.3	6.7 -8.5 -14.4	7.5 11.5 2.5	C ₁₀ H ₇ O ₃ C ₁₄ H ₇ C ₇ H ₁₁ O ₅
178.0810	1.4	178.0783 178.0841	15.6 -17.4	2.8 -3.1	10.0 1.0	C ₁₄ H ₁₀ C ₇ H ₁₄ O ₅
187.0416	4.3	187.0395 187.0548	10.9 -70.7	2.0 -13.2	8.5 12.5	C ₁₁ H ₇ O ₃ C ₁₅ H ₇
188.0495	1.2	188.0473 188.0626	11.3 -69.8	2.1 -13.1	8.0 12.0	C ₁₁ H ₈ O ₃ C ₁₅ H ₈
189.0613	2.7	189.0552 189.0704 189.0763	32.2 -48.5 -79.6	6.1 -9.2 -15.0	7.5 11.5 2.5	C ₁₁ H ₉ O ₃ C ₁₅ H ₉ C ₈ H ₁₃ O ₅
199.0410	1.7	199.0395 199.0548 199.0606	7.5 -69.1 -98.6	1.5 -13.8 -19.6	9.5 13.5 4.5	C ₁₂ H ₇ O ₃ C ₁₆ H ₇ C ₉ H ₁₁ O ₅
201.0563	2.6	201.0552 201.0704 201.0763	5.9 -70.0 -99.2	1.2 -14.1 -20.0	8.5 12.5 3.5	C ₁₂ H ₉ O ₃ C ₁₆ H ₉ C ₉ H ₁₃ O ₅
202.0691	1.7	202.0630 202.0783 202.0841	30.2 -45.3 -74.4	6.1 -9.2 -15.0	8.0 12.0 3.0	C ₁₂ H ₁₀ O ₃ C ₁₆ H ₁₀ C ₉ H ₁₄ O ₅
203.0799	1.1	203.0861 203.0708 203.0919	-30.3 44.9 -59.2	-6.1 9.1 -12.0	11.5 7.5 2.5	C ₁₆ H ₁₁ C ₁₂ H ₁₁ O ₃ C ₉ H ₁₅ O ₅
216.9564	62.7	216.9514 216.9362	22.8 93.1	4.9 20.2	4.5 0.5	C ₇ H ₆ I ₁ C ₃ H ₆ O ₃ I ₁
217.0561	15.4	217.0501 217.0653	27.8 -42.5	6.0 -9.2	8.5 12.5	C ₁₂ H ₉ O ₄ C ₁₆ H ₉ O ₁
217.9635	14.8	217.9592 217.9440	19.4 89.4	4.2 19.5	4.0 0.0	C ₇ H ₇ I ₁ C ₃ H ₇ O ₃ I ₁
218.0637	3.4	218.0579 218.0732	26.7 -43.3	5.8 -9.4	8.0 12.0	C ₁₂ H ₁₀ O ₄ C ₁₆ H ₁₀ O ₁
219.0760	1.1	219.0810 219.0657	-22.6 47.0	-5.0 10.3	11.5 7.5	C ₁₆ H ₁₁ O ₁ C ₁₂ H ₁₁ O ₄
231.9443	1.4	231.9385 231.9596 231.9233	24.9 -66.2 90.7	5.8 -15.4 21.0	5.0 0.0 1.0	C ₇ H ₅ O ₁ I ₁ C ₄ H ₉ O ₃ I ₁ C ₃ H ₅ O ₄ I ₁
233.9552	2.1	233.9542 233.9389	4.4 69.6	1.0 16.3	4.0 0.0	C ₇ H ₇ O ₁ I ₁ C ₃ H ₇ O ₄ I ₁
251.9194	6.9	251.9283 251.9072 251.9436	-35.4 48.5 -95.9	-8.9 12.2 -24.2	4.0 9.0 8.0	C ₆ H ₅ O ₃ I ₁ C ₉ H ₁ O ₁ I ₁ C ₁₀ H ₅ I ₁
253.9156	2.3	253.9229 253.9076	-28.4 31.7	-7.2 8.0	8.0 4.0	C ₉ H ₃ O ₁ I ₁ C ₅ H ₃ O ₄ I ₁
274.0084	3.0	274.0066 274.0055 274.0218 273.9902	6.6 10.7 -49.1 66.3	1.8 2.9 -13.4 18.2	0.0 20.0 4.0 16.0	C ₇ H ₁₅ O ₃ I ₁ C ₂₀ H ₂ O ₂ C ₁₁ H ₁₅ I ₁ C ₁₆ H ₂ O ₅
343.8484	1.4					
434.0002	4.7	434.0004 434.0015 434.0157 434.0168	-0.5 -3.0 -35.6 -38.2	-0.2 -1.3 -15.5 -16.6	32.0 12.0 36.0 16.0	C ₃₂ H ₂ O ₃ C ₁₉ H ₁₅ O ₄ I ₁ C ₃₆ H ₂ C ₂₃ H ₁₅ O ₁ I ₁
435.0002	1.0	435.0082 435.0093 434.9882 435.0235	-18.5 -21.0 27.6 -53.5	-8.0 -9.1 12.0 -23.3	31.5 11.5 16.5 35.5	C ₃₂ H ₃ O ₃ C ₁₉ H ₁₆ O ₄ I ₁ C ₂₂ H ₁₂ O ₂ I ₁ C ₃₆ H ₃

Compound # 25

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
189.0642	1.0	188.0559	-24.6	-4.6	3.5	C ₇ H ₁₀ O ₅ N ₁
		189.0637	2.6	0.5	3.0	C ₇ H ₁₁ O ₅ N ₁
		189.0704	-32.9	-6.2	11.5	C ₁₅ H ₉
190.0650	1.1	189.0578	33.6	6.4	12.0	C ₁₄ H ₇ N ₁
		190.0657	-3.4	-0.6	11.5	C ₁₄ H ₈ N ₁
		190.0630	10.7	2.0	7.0	C ₁₁ H ₁₀ O ₃
199.0399	13.4	190.0715	-34.3	-6.5	2.5	C ₇ H ₁₂ O ₅ N ₁
		199.0395	1.8	0.4	9.5	C ₁₂ H ₇ O ₃
		199.0422	-11.6	-2.3	14.0	C ₁₅ H ₅ N ₁
200.0470	5.4	199.0454	-27.7	-5.5	0.5	C ₅ H ₁₁ O ₈
		200.0473	-1.9	-0.4	9.0	C ₁₂ H ₈ O ₃
		200.0500	-15.3	-3.1	13.5	C ₁₅ H ₆ N ₁
201.0537	22.7	200.0532	-31.3	-6.3	0.0	C ₅ H ₁₂ O ₈
		201.0552	-7.4	-1.5	8.5	C ₁₂ H ₈ O ₃
		201.0578	-20.7	-4.2	13.0	C ₁₅ H ₉ N ₁
202.0584	4.2	201.0485	25.9	5.2	0.0	C ₄ H ₁₁ O ₈ N ₁
		202.0630	-22.8	-4.6	8.0	C ₁₂ H ₁₀ O ₃
		202.0657	-36.1	-7.3	12.5	C ₁₅ H ₈ N ₁
216.0422	1.8	202.0504	39.4	8.0	8.5	C ₁₁ H ₈ O ₃ N ₁
		216.0423	-0.5	-0.1	9.0	C ₁₂ H ₈ O ₄
		216.0449	-12.9	-2.8	13.5	C ₁₅ H ₆ O ₁ N ₁
217.0489	2.0	216.0508	-40.1	-8.7	4.5	C ₈ H ₁₀ O ₆ N ₁
		217.0501	-5.2	-1.1	8.5	C ₁₂ H ₉ O ₄
		217.0528	-17.6	-3.8	13.0	C ₁₅ H ₇ O ₁ N ₁
218.0554	25.3	217.0586	-44.6	-9.7	4.0	C ₈ H ₁₁ O ₆ N ₁
		218.0579	-11.5	-2.5	8.0	C ₁₂ H ₁₀ O ₄
		218.0606	-23.7	-5.2	12.5	C ₁₅ H ₈ O ₁ N ₁
219.0603	3.8	218.0453	46.2	10.1	8.5	C ₁₁ H ₉ O ₄ N ₁
		219.0657	-24.6	-5.4	7.5	C ₁₂ H ₁₁ O ₄
		219.0532	32.8	7.2	8.0	C ₁₁ H ₉ O ₄ N ₁
220.0581	1.2	219.0684	-36.8	-8.1	12.0	C ₁₅ H ₉ O ₁ N ₁
		220.0583	-0.7	-0.2	3.0	C ₈ H ₁₂ O ₇
		220.0610	-12.9	-2.8	7.5	C ₁₁ H ₁₀ O ₄ N ₁
381.0857	10.5	220.0524	26.0	5.7	12.0	C ₁₅ H ₈ O ₂
		381.0849	2.2	0.9	14.0	C ₂₀ H ₁₅ O ₇ N ₁
		381.0916	-15.4	-5.9	22.5	C ₂₈ H ₁₃ O ₂
382.0880	2.6	381.0790	17.6	6.7	23.0	C ₂₇ H ₁₁ O ₂ N ₁
		382.0868	3.2	1.2	22.5	C ₂₇ H ₁₂ O ₂ N ₁
		382.0841	10.2	3.9	18.0	C ₂₄ H ₁₄ O ₅
		382.0927	-12.2	-4.6	13.5	C ₂₀ H ₁₆ O ₇ N ₁