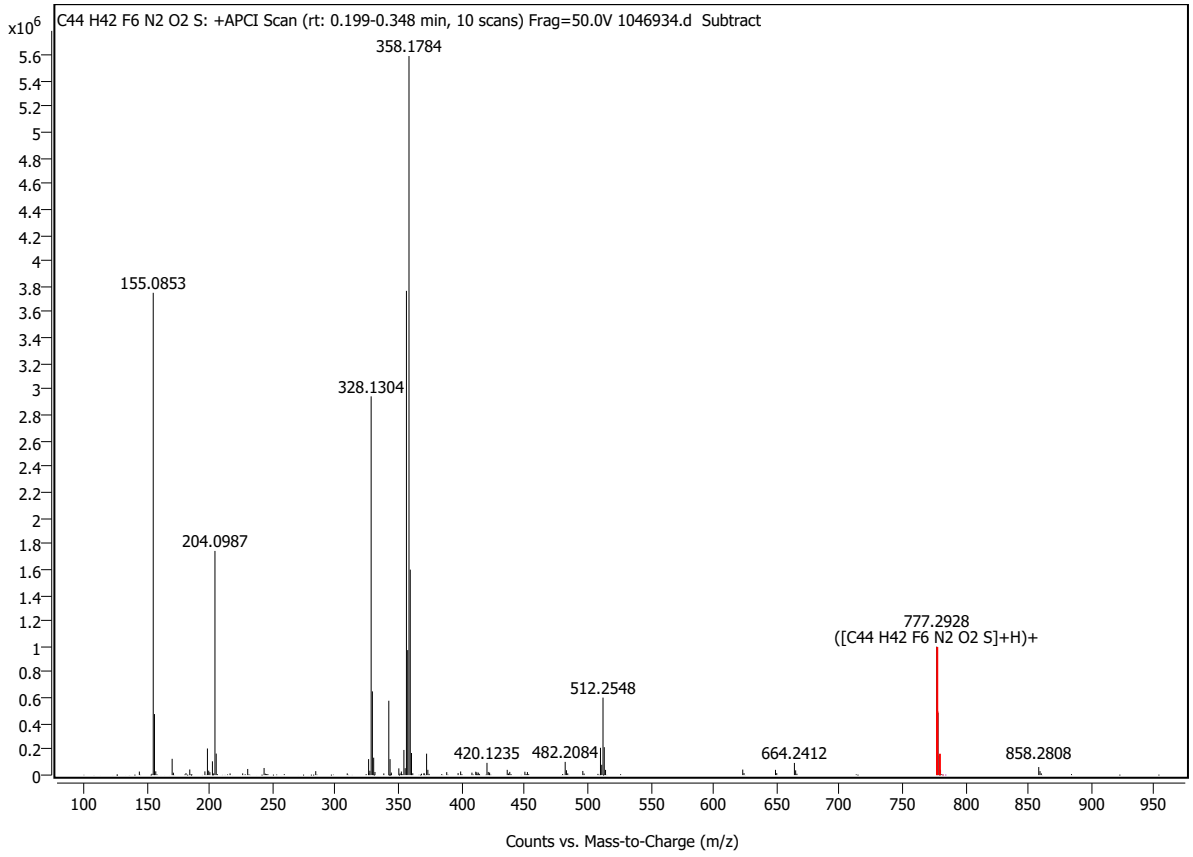
Sample Information

Sample_Name	PCC-557-1	Data File	1046934.d
Sample_ID		Acq. Time	17/06/2025 15:27:01 (UTC+02:00)
Client_Name	Chien, Opatz	Acq. Method	APCI_pos_ACN_below1000_CD.m
		Ver. Acq. SW	6200 series TOF/6500 series Q-TOF (11.0.221.1)
Inj. Vol. (ul)	0.2	Ver. Anal. SW	10.0

MS Spectra

+ Scan (rt: 0.199-0.348 min) Sub



Spectrum Peaks

m/z	m/z (Calc)	Diff (ppm)	Ion Species	Z	Formula	Abund	Abund %
155.0853	155.0855	-1.29		1		3750037	67.07
156.0881	156.0889	-5.04		1		474425	8.49
170.0959	170.0964	-3.01		1		126512	2.26
198.1274	198.1277	-1.66		1		206891	3.70
202.0834	202.0838	-1.89		1		106939	1.91
204.0987	204.0995	-3.51		1		1742935	31.17
205.1024	205.1027	-1.04		1		167210	2.99
326.1147	326.1151	-1.30		1		124250	2.22
328.1304	328.1308	-1.18		1		2944804	52.67
329.1333	329.1341	-2.25		1		650780	11.64
330.1435	330.1370	19.64		1		135258	2.42
342.1457	342.1464	-2.05		1		577969	10.34
343.1494	343.1497	-0.92		1		124097	2.22
354.1462	354.1464	-0.47		1		195471	3.50
356.1620	356.1621	-0.22		1		3765115	67.34
357.1646	357.1653	-2.07		1		972014	17.39
358.1784	358.1778	1.93		1		5590977	100.00
359.1803	359.1810	-2.02		1		1597438	28.57
360.1842	360.1840	0.49		1		171796	3.07
372.1567	372.1570	-0.69		1		166499	2.98
420.1235	420.1240	-1.03		1		95006	1.70
482.2084	482.2086	-0.23		1		102671	1.84
510.2395	510.2403	-1.50		1		212157	3.79
511.2430	511.2436	-1.22		1		80060	1.43
512.2548	512.2560	-2.25		1		602309	10.77
513.2589	513.2593	-0.77		1		216910	3.88
664.2412	664.2416	-0.47		1		94489	1.69
777.2928	777.2944	-2.03	(M+H)+	1	C44 H42 F6 N2 O2 S	998843	17.87
778.2963	778.2976	-1.76	(M+H)+	1	C44 H42 F6 N2 O2 S	485591	8.69
779.2977	779.2980	-0.38	(M+H)+	1	C44 H42 F6 N2 O2 S	152574	2.73
858.2808	858.2811	-0.34		1		62448	1.12

Molecular Formula Generation Results

Best	m/z	Diff (ppm)	Species	Formula	Score (MFG)
No	155.0853	-1.75	(M+H)+	C12 H10	98.74
No	155.0853	0.21	(M+NH4)+	C7 H6 F N2	95.34
No	155.0853	-1.74	M+	C12 H11	98.74
No	170.0959	-3.54	(M+H)+	C12 H11 N	84.55
No	170.0959	4.59	(M+Na)+	C7 H14 F N O	73.98
No	170.0959	-3.93	(M+NH4)+	C12 H8	84.55
No	170.0959	-3.52	M+	C12 H12 N	84.55
No	198.1274	-1.77	(M+H)+	C14 H15 N	98.61
No	198.1274	-1.94	(M+NH4)+	C14 H12	98.61
No	198.1274	2.49	(M+NH4)+	C6 H16 N2 O2 S	78.11
No	198.1274	-1.76	M+	C14 H16 N	98.61
No	202.0834	-1.77	(M+H)+	C10 H10 F3 N	86.91
No	202.0834	0.55	(M+H)+	C7 H15 F2 O2 S	75.36
No	202.0834	-2.21	(M+Na)+	C10 H13 N O2	86.55
No	202.0834	-1.93	(M+NH4)+	C10 H7 F3	86.91
No	202.0834	-1.76	M+	C10 H11 F3 N	86.91
No	204.0987	-3.30	(M+H)+	C10 H12 F3 N	96.44
No	204.0987	4.73	(M+H)+	C10 H16 F O S	86.79
No	204.0987	-3.91	(M+Na)+	C10 H15 N O2	96.04
No	204.0987	-3.61	(M+NH4)+	C10 H9 F3	96.44
No	204.0987	-3.29	M+	C10 H13 F3 N	96.44
No	204.0987	4.70	M+	C10 H17 F O S	86.79
No	326.1147	-0.85	(M+H)+	C20 H14 F3 N	80.12
No	326.1147	-1.04	(M+Na)+	C20 H17 N O2	79.54
No	326.1147	-0.89	(M+NH4)+	C20 H11 F3	80.12
No	326.1147	-0.84	M+	C20 H15 F3 N	80.12
No	328.1304	-0.52	(M+H)+	C20 H16 F3 N	94.11
No	328.1304	-3.98	(M+H)+	C17 H17 F4 N O	86.90
No	328.1304	1.70	(M+H)+	C17 H21 F2 O2 S	86.46
No	328.1304	0.65	(M+K)+	C15 H25 F2 N S	72.29
No	328.1304	-0.66	(M+Na)+	C20 H19 N O2	94.27
No	328.1304	3.63	(M+Na)+	C15 H19 F4 N O	84.67
No	328.1304	-2.64	(M+Na)+	C15 H22 F3 N S	83.28
No	328.1304	-0.05	(M+Na)+	C12 H20 F5 N O2	81.20
No	328.1304	-0.55	(M+NH4)+	C20 H13 F3	94.11
No	328.1304	-4.20	(M+NH4)+	C17 H14 F4 O	86.90
No	328.1304	2.83	(M+NH4)+	C12 H17 F3 N2 O2 S	77.66
No	328.1304	-0.52	M+	C20 H17 F3 N	94.11
No	328.1304	-3.97	M+	C17 H18 F4 N O	86.90
No	328.1304	1.69	M+	C17 H22 F2 O2 S	86.46
No	342.1457	-1.70	(M+H)+	C21 H18 F3 N	97.48
No	342.1457	0.21	(M+H)+	C18 H23 F2 O2 S	91.33
No	342.1457	3.51	(M+H)+	C21 H22 F O S	87.22
No	342.1457	4.15	(M+H)+	C13 H23 F6 O S	78.05
No	342.1457	2.40	(M+K)+	C13 H25 F4 N O2	77.83
No	342.1457	-1.00	(M+K)+	C16 H27 F2 N S	74.84
No	342.1457	-1.92	(M+Na)+	C21 H21 N O2	97.45
No	342.1457	2.17	(M+Na)+	C16 H21 F4 N O	94.87
No	342.1457	-1.37	(M+Na)+	C13 H22 F5 N O2	89.30
No	342.1457	-4.08	(M+Na)+	C16 H24 F3 N S	85.10
No	342.1457	-1.79	(M+NH4)+	C21 H15 F3	97.48
No	342.1457	1.17	(M+NH4)+	C13 H19 F3 N2 O2 S	84.73
No	342.1457	4.60	(M+NH4)+	C16 H18 F2 N2 O S	83.72
No	342.1457	-1.70	M+	C21 H19 F3 N	97.48
No	342.1457	0.21	M+	C18 H24 F2 O2 S	91.33
No	342.1457	3.50	M+	C21 H23 F O S	87.22
No	354.1462	-0.50	(M+H)+	C22 H18 F3 N	83.01
No	354.1462	-3.73	(M+H)+	C19 H19 F4 N O	73.52
No	354.1462	0.80	(M+H)+	C19 H23 F2 O2 S	70.42
No	354.1462	-0.66	(M+Na)+	C22 H21 N O2	82.30
No	354.1462	3.29	(M+Na)+	C17 H21 F4 N O	71.00
No	354.1462	-0.53	(M+NH4)+	C22 H15 F3	83.01
No	354.1462	-3.92	(M+NH4)+	C19 H16 F4 O	73.52
No	354.1462	-0.50	M+	C22 H19 F3 N	83.01
No	354.1462	-3.72	M+	C19 H20 F4 N O	73.52
No	354.1462	0.80	M+	C19 H24 F2 O2 S	70.42
No	356.1620	-0.60	(M+H)+	C22 H20 F3 N	84.18
No	356.1620	-3.81	(M+H)+	C19 H21 F4 N O	75.79
No	356.1620	0.69	(M+H)+	C19 H25 F2 O2 S	71.94
No	356.1620	-0.76	(M+Na)+	C22 H23 N O2	83.41
No	356.1620	3.16	(M+Na)+	C17 H23 F4 N O	74.07
No	356.1620	-0.27	(M+Na)+	C14 H24 F5 N O2	70.55
No	356.1620	-0.63	(M+NH4)+	C22 H17 F3	84.18
No	356.1620	-4.01	(M+NH4)+	C19 H18 F4 O	75.79
No	356.1620	-0.60	M+	C22 H21 F3 N	84.18
No	356.1620	-3.80	M+	C19 H22 F4 N O	75.79
No	356.1620	0.69	M+	C19 H26 F2 O2 S	71.94
No	358.1784	1.13	(M+H)+	C22 H22 F3 N	94.34
No	358.1784	-2.05	(M+H)+	C19 H23 F4 N O	87.57
No	358.1784	2.91	(M+H)+	C19 H27 F2 O2 S	79.87
No	358.1784	2.09	(M+K)+	C17 H31 F2 N S	70.04
No	358.1784	1.10	(M+Na)+	C22 H25 N O2	94.35

Molecular Formula Generation Results

Best	m/z	Diff (ppm)	Species	Formula	Score (MFG)
No	358.1784	-0.98	(M+Na)+	C17 H28 F3 N S	80.32
No	358.1784	1.63	(M+Na)+	C14 H26 F5 N O2	77.10
No	358.1784	5.00	(M+Na)+	C17 H25 F4 N O	76.87
No	358.1784	1.18	(M+NH4)+	C22 H19 F3	94.34
No	358.1784	-2.15	(M+NH4)+	C19 H20 F4 O	87.57
No	358.1784	3.99	(M+NH4)+	C14 H23 F3 N2 O2 S	71.59
No	358.1784	1.12	M+	C22 H23 F3 N	94.34
No	358.1784	-2.05	M+	C19 H24 F4 N O	87.57
No	358.1784	2.90	M+	C19 H28 F2 O2 S	79.87
No	372.1567	-0.73	(M+H)+	C22 H20 F3 N O	97.78
No	372.1567	2.32	(M+H)+	C25 H19 F2 N	94.63
No	372.1567	-3.78	(M+H)+	C19 H21 F4 N O2	90.52
No	372.1567	4.29	(M+H)+	C22 H24 F O2 S	86.28
No	372.1567	4.95	(M+H)+	C14 H25 F6 O2 S	71.61
No	372.1567	-4.59	(M+K)+	C17 H25 F4 N2	78.07
No	372.1567	0.37	(M+K)+	C17 H29 F2 N O S	75.28
No	372.1567	3.75	(M+K)+	C20 H28 F N S	73.66
No	372.1567	0.65	(M+Na)+	C20 H25 F2 N S	92.14
No	372.1567	2.88	(M+Na)+	C17 H23 F4 N O2	89.55
No	372.1567	-2.54	(M+Na)+	C17 H26 F3 N O S	85.73
No	372.1567	-0.77	(M+NH4)+	C22 H17 F3 O	97.78
No	372.1567	2.43	(M+NH4)+	C25 H16 F2	94.63
No	372.1567	-3.97	(M+NH4)+	C19 H18 F4 O2	90.52
No	372.1567	-0.73	M+	C22 H21 F3 N O	97.78
No	372.1567	2.32	M+	C25 H20 F2 N	94.63
No	372.1567	-3.77	M+	C19 H22 F4 N O2	90.52
No	372.1567	4.28	M+	C22 H25 F O2 S	86.28
No	420.1235	-1.05	(M+H)+	C22 H20 F3 N O2 S	97.67
No	420.1235	1.61	(M+H)+	C25 H19 F2 N O S	96.45
No	420.1235	-2.82	(M+H)+	C25 H15 F4 N2	90.01
No	420.1235	4.87	(M+H)+	C20 H19 F6 N S	87.57
No	420.1235	4.28	(M+H)+	C28 H18 F N S	86.96
No	420.1235	0.04	(M+K)+	C25 H21 N2 O2	93.26
No	420.1235	3.57	(M+K)+	C20 H21 F4 N2 O	88.06
No	420.1235	0.62	(M+K)+	C17 H22 F5 N2 O2	87.81
No	420.1235	-2.04	(M+K)+	C20 H24 F3 N2 S	82.28
No	420.1235	-4.98	(M+K)+	C17 H25 F4 N2 O S	72.67
No	420.1235	0.25	(M+Na)+	C20 H18 F5 N2 O	92.30
No	420.1235	-0.20	(M+Na)+	C28 H17 N2 O	90.70
No	420.1235	-3.05	(M+Na)+	C25 H18 F N2 O2	90.54
No	420.1235	3.09	(M+Na)+	C23 H17 F4 N2	90.22
No	420.1235	-4.54	(M+Na)+	C20 H21 F4 N2 S	89.86
No	420.1235	-2.59	(M+Na)+	C17 H19 F6 N2 O2	85.22
No	420.1235	-1.09	(M+NH4)+	C22 H17 F3 O2 S	97.67
No	420.1235	1.68	(M+NH4)+	C25 H16 F2 O S	96.45
No	420.1235	-2.94	(M+NH4)+	C25 H12 F4 N	90.01
No	420.1235	4.46	(M+NH4)+	C28 H15 F S	86.96
No	420.1235	-1.05	M+	C22 H21 F3 N O2 S	97.67
No	420.1235	1.61	M+	C25 H20 F2 N O S	96.45
No	420.1235	-2.81	M+	C25 H16 F4 N2	90.01
No	420.1235	4.86	M+	C20 H20 F6 N S	87.57
No	420.1235	4.27	M+	C28 H19 F N S	86.96
No	482.2084	1.79	(M+H)+	C29 H31 F2 O2 S	85.56
No	482.2084	-0.20	(M+H)+	C32 H26 F3 N	84.23
No	482.2084	4.08	(M+H)+	C32 H30 F O S	81.53
No	482.2084	-2.55	(M+H)+	C29 H27 F4 N O	79.19
No	482.2084	1.41	(M+K)+	C27 H35 F2 N S	79.86
No	482.2084	-1.10	(M+K)+	C24 H36 F3 N O S	76.15
No	482.2084	3.54	(M+K)+	C24 H33 F4 N O2	74.01
No	482.2084	-5.00	(M+K)+	C24 H32 F5 N2	70.18
No	482.2084	-0.26	(M+Na)+	C32 H29 N O2	85.00
No	482.2084	-1.06	(M+Na)+	C27 H32 F3 N S	84.20
No	482.2084	2.57	(M+Na)+	C27 H29 F4 N O	77.10
No	482.2084	0.12	(M+Na)+	C24 H30 F5 N O2	76.11
No	482.2084	-3.44	(M+Na)+	C24 H33 F4 N O S	74.89
No	482.2084	-0.20	(M+NH4)+	C32 H23 F3	84.23
No	482.2084	-2.64	(M+NH4)+	C29 H24 F4 O	79.19
No	482.2084	2.61	(M+NH4)+	C24 H27 F3 N2 O2 S	78.28
No	482.2084	4.96	(M+NH4)+	C27 H26 F2 N2 O S	75.64
No	482.2084	1.78	M+	C29 H32 F2 O2 S	85.56
No	482.2084	-0.20	M+	C32 H27 F3 N	84.23
No	482.2084	4.07	M+	C32 H31 F O S	81.53
No	482.2084	-2.54	M+	C29 H28 F4 N O	79.19
No	510.2395	-1.42	(M+H)+	C34 H30 F3 N	76.97
No	510.2395	-3.67	(M+H)+	C31 H31 F4 N O	70.85
No	510.2395	-1.57	(M+Na)+	C34 H33 N O2	75.92
No	510.2395	1.10	(M+Na)+	C29 H33 F4 N O	75.60
No	510.2395	3.45	(M+Na)+	C32 H32 F3 N	72.74
No	510.2395	-1.24	(M+Na)+	C26 H34 F5 N O2	71.95
No	510.2395	-1.47	(M+NH4)+	C34 H27 F3	76.97
No	510.2395	-3.79	(M+NH4)+	C31 H28 F4 O	70.85
No	510.2395	-1.42	M+	C34 H31 F3 N	76.97

Molecular Formula Generation Results

Best	m/z	Diff (ppm)	Species	Formula	Score (MFG)
No	510.2395	-3.66	M+	C31 H32 F4 N O	70.85
No	512.2548	-1.84	(M+H)+	C34 H32 F3 N	97.48
No	512.2548	-4.07	(M+H)+	C31 H33 F4 N O	91.02
No	512.2548	-0.50	(M+H)+	C31 H37 F2 O2 S	90.73
No	512.2548	1.70	(M+H)+	C34 H36 F O S	89.87
No	512.2548	2.14	(M+H)+	C26 H37 F6 O S	83.61
No	512.2548	3.90	(M+H)+	C37 H35 S	82.74
No	512.2548	4.33	(M+H)+	C29 H36 F5 S	81.16
No	512.2548	0.92	(M+K)+	C26 H39 F4 N O2	80.59
No	512.2548	3.29	(M+K)+	C29 H38 F3 N O	79.68
No	512.2548	-1.21	(M+K)+	C29 H41 F2 N S	74.33
No	512.2548	-1.99	(M+Na)+	C34 H35 N O2	97.28
No	512.2548	0.67	(M+Na)+	C29 H35 F4 N O	97.11
No	512.2548	2.99	(M+Na)+	C32 H34 F3 N	95.19
No	512.2548	-1.65	(M+Na)+	C26 H36 F5 N O2	91.64
No	512.2548	-3.33	(M+Na)+	C29 H38 F3 N S	85.16
No	512.2548	4.43	(M+Na)+	C29 H39 F2 O2 S	80.99
No	512.2548	-1.90	(M+NH4)+	C34 H29 F3	97.48
No	512.2548	-4.21	(M+NH4)+	C31 H30 F4 O	91.02
No	512.2548	2.35	(M+NH4)+	C29 H32 F2 N2 O S	87.44
No	512.2548	0.10	(M+NH4)+	C26 H33 F3 N2 O2 S	86.70
No	512.2548	4.61	(M+NH4)+	C32 H31 F N2 S	81.98
No	512.2548	-1.84	M+	C34 H33 F3 N	97.48
No	512.2548	-4.06	M+	C31 H34 F4 N O	91.02
No	512.2548	-0.50	M+	C31 H38 F2 O2 S	90.73
No	512.2548	1.69	M+	C34 H37 F O S	89.87
No	512.2548	2.14	M+	C26 H38 F6 O S	83.61
No	512.2548	3.89	M+	C37 H36 S	82.74
No	512.2548	4.32	M+	C29 H37 F5 S	81.16
No	664.2412	-0.85	(M+H)+	C42 H35 F4 O S	93.62
No	664.2412	-2.54	(M+H)+	C39 H36 F5 O2 S	92.66
No	664.2412	0.84	(M+H)+	C45 H34 F3 S	90.33
No	664.2412	2.12	(M+H)+	C42 H32 F5 O2	89.26
No	664.2412	-3.62	(M+H)+	C42 H31 F6 N	83.84
No	664.2412	-2.87	(M+H)+	C47 H35 O2 S	82.92
No	664.2412	3.84	(M+H)+	C45 H31 F4 O	80.39
No	664.2412	0.24	(M+K)+	C37 H37 F6 N O	94.47
No	664.2412	2.03	(M+K)+	C40 H36 F5 N	91.03
No	664.2412	-1.91	(M+K)+	C42 H37 F2 N O2	88.96
No	664.2412	-0.11	(M+K)+	C45 H36 F N O	88.30
No	664.2412	1.69	(M+K)+	C48 H35 N	83.74
No	664.2412	-3.11	(M+K)+	C37 H40 F5 N S	80.80
No	664.2412	2.97	(M+K)+	C37 H41 F4 O2 S	80.63
No	664.2412	-3.48	(M+K)+	C45 H39 N S	75.72
No	664.2412	-4.90	(M+K)+	C34 H41 F6 N O S	73.74
No	664.2412	4.76	(M+K)+	C40 H40 F3 O S	73.59
No	664.2412	1.16	(M+Na)+	C37 H38 F5 O2 S	96.89
No	664.2412	0.01	(M+Na)+	C40 H33 F6 N	92.98
No	664.2412	2.90	(M+Na)+	C40 H37 F4 O S	91.25
No	664.2412	0.81	(M+Na)+	C45 H37 O2 S	89.96
No	664.2412	-2.02	(M+Na)+	C45 H33 F2 N O	86.34
No	664.2412	-4.77	(M+Na)+	C37 H37 F6 N S	86.09
No	664.2412	-0.24	(M+Na)+	C48 H32 F N	85.21
No	664.2412	-3.79	(M+Na)+	C42 H34 F3 N O2	84.00
No	664.2412	4.65	(M+Na)+	C43 H36 F3 S	81.85
No	664.2412	-0.42	(M+NH4)+	C37 H31 F5 N2 O S	97.33
No	664.2412	-2.14	(M+NH4)+	C34 H32 F6 N2 O2 S	95.23
No	664.2412	1.31	(M+NH4)+	C40 H30 F4 N2 S	94.32
No	664.2412	2.59	(M+NH4)+	C37 H28 F6 N2 O2	90.86
No	664.2412	-2.51	(M+NH4)+	C42 H31 F N2 O2 S	89.13
No	664.2412	-0.77	(M+NH4)+	C45 H30 N2 O S	89.06
No	664.2412	2.33	(M+NH4)+	C45 H27 F N2 O2	85.16
No	664.2412	-3.71	(M+NH4)+	C42 H28 F6	83.84
No	664.2412	4.35	(M+NH4)+	C40 H27 F5 N2 O	82.84
No	664.2412	4.09	(M+NH4)+	C48 H26 N2 O	75.67
No	664.2412	-0.85	M+	C42 H36 F4 O S	93.62
No	664.2412	-2.53	M+	C39 H37 F5 O2 S	92.66
No	664.2412	0.84	M+	C45 H35 F3 S	90.33
No	664.2412	2.12	M+	C42 H33 F5 O2	89.26
No	664.2412	-3.61	M+	C42 H32 F6 N	83.84
No	664.2412	-2.86	M+	C47 H36 O2 S	82.92
No	664.2412	3.84	M+	C45 H32 F4 O	80.39
Yes	777.2928	-1.78	(M+H)+	C44 H42 F6 N2 O2 S	97.08
No	777.2928	-0.35	(M+H)+	C47 H41 F5 N2 O S	98.24
No	777.2928	1.09	(M+H)+	C50 H40 F4 N2 S	95.55
No	777.2928	2.00	(M+H)+	C47 H38 F6 N2 O2	93.90
No	777.2928	-2.10	(M+H)+	C52 H41 F N2 O2 S	91.35
No	777.2928	-0.66	(M+H)+	C55 H40 N2 O S	91.30
No	777.2928	1.78	(M+H)+	C55 H37 F N2 O2	89.13
No	777.2928	3.46	(M+H)+	C50 H37 F5 N2 O	87.21
No	777.2928	-3.26	(M+H)+	C52 H38 F6	86.80
No	777.2928	3.25	(M+H)+	C58 H36 N2 O	81.59

Molecular Formula Generation Results

Best	m/z	Diff (ppm)	Species	Formula	Score (MFG)
No	777.2928	4.92	(M+H)+	C53 H36 F4 N2	78.24
No	777.2928	-4.93	(M+H)+	C57 H38 F2 O	75.41
No	777.2928	0.20	(M+K)+	C47 H44 F6 O	96.56
No	777.2928	1.72	(M+K)+	C50 H43 F5	93.36
No	777.2928	-1.62	(M+K)+	C52 H44 F2 O2	91.53
No	777.2928	-0.10	(M+K)+	C55 H43 F O	90.85
No	777.2928	1.42	(M+K)+	C58 H42	87.03
No	777.2928	-2.55	(M+K)+	C47 H47 F5 S	84.59
No	777.2928	3.01	(M+K)+	C42 H47 F5 N2 O2 S	82.61
No	777.2928	2.67	(M+K)+	C50 H46 N2 O2 S	81.97
No	777.2928	-2.88	(M+K)+	C55 H46 S	79.52
No	777.2928	-4.05	(M+K)+	C44 H48 F6 O S	79.19
No	777.2928	4.52	(M+K)+	C45 H46 F4 N2 O S	76.95
No	777.2928	-4.39	(M+K)+	C52 H47 F O S	75.15
No	777.2928	1.39	(M+Na)+	C42 H44 F6 N2 O2 S	97.97
No	777.2928	1.06	(M+Na)+	C50 H43 F N2 O2 S	95.38
No	777.2928	-0.17	(M+Na)+	C50 H40 F6	94.99
No	777.2928	2.86	(M+Na)+	C45 H43 F5 N2 O S	93.97
No	777.2928	2.54	(M+Na)+	C53 H42 N2 O S	89.43
No	777.2928	-1.89	(M+Na)+	C55 H40 F2 O	89.32
No	777.2928	-4.06	(M+Na)+	C47 H44 F6 S	88.93
No	777.2928	-0.38	(M+Na)+	C58 H39 F	88.80
No	777.2928	-3.40	(M+Na)+	C52 H41 F3 O2	87.06
No	777.2928	4.33	(M+Na)+	C48 H42 F4 N2 S	86.75
No	777.2928	-4.38	(M+Na)+	C55 H43 F S	81.15
No	777.2928	-0.36	(M+NH4)+	C47 H38 F5 N O S	98.24
No	777.2928	-1.82	(M+NH4)+	C44 H39 F6 N O2 S	97.08
No	777.2928	1.11	(M+NH4)+	C50 H37 F4 N S	95.55
No	777.2928	2.04	(M+NH4)+	C47 H35 F6 N O2	93.90
No	777.2928	-2.14	(M+NH4)+	C52 H38 F N O2 S	91.35
No	777.2928	-0.67	(M+NH4)+	C55 H37 N O S	91.30
No	777.2928	1.82	(M+NH4)+	C55 H34 F N O2	89.13
No	777.2928	3.54	(M+NH4)+	C50 H34 F5 N O	87.21
No	777.2928	-3.20	(M+NH4)+	C55 H33 F2 N2	84.34
No	777.2928	-4.69	(M+NH4)+	C52 H34 F3 N2 O	80.59
No	777.2928	-0.35	M+	C47 H42 F5 N2 O S	98.24
No	777.2928	-1.78	M+	C44 H43 F6 N2 O2 S	97.08
No	777.2928	1.08	M+	C50 H41 F4 N2 S	95.55
No	777.2928	2.00	M+	C47 H39 F6 N2 O2	93.90
No	777.2928	-2.09	M+	C52 H42 F N2 O2 S	91.35
No	777.2928	-0.65	M+	C55 H41 N2 O S	91.30
No	777.2928	1.78	M+	C55 H38 F N2 O2	89.13
No	777.2928	3.45	M+	C50 H38 F5 N2 O	87.21
No	777.2928	-3.26	M+	C52 H39 F6	86.80
No	777.2928	3.24	M+	C58 H37 N2 O	81.59
No	777.2928	4.92	M+	C53 H37 F4 N2	78.24
No	777.2928	-4.93	M+	C57 H39 F2 O	75.41
No	858.2808	-0.93	(M+H)+	C58 H39 F4 N S	88.60
No	858.2808	-2.23	(M+H)+	C55 H40 F5 N O S	87.83
No	858.2808	-0.01	(M+H)+	C55 H37 F6 N O2	86.19
No	858.2808	-3.53	(M+H)+	C52 H41 F6 N O2 S	84.78
No	858.2808	1.32	(M+H)+	C58 H36 F5 N O	83.46
No	858.2808	3.51	(M+H)+	C58 H40 F3 O2 S	80.99
No	858.2808	-0.07	(M+K)+	C53 H41 F6 N2	93.20
No	858.2808	0.73	(M+K)+	C50 H46 F5 N O2 S	90.88
No	858.2808	-1.72	(M+K)+	C58 H41 F2 N2 O	87.32
No	858.2808	2.08	(M+K)+	C53 H45 F4 N O S	86.90
No	858.2808	0.43	(M+K)+	C58 H45 N O2 S	85.91
No	858.2808	-3.08	(M+K)+	C55 H42 F3 N2 O2	85.45
No	858.2808	-3.91	(M+K)+	C50 H45 F6 N2 S	82.13
No	858.2808	4.57	(M+K)+	C53 H42 F5 N O2	80.75
No	858.2808	3.44	(M+K)+	C56 H44 F3 N S	80.48
No	858.2808	-4.22	(M+K)+	C58 H44 F N2 S	75.44
No	858.2808	-0.72	(M+Na)+	C50 H43 F6 N O2 S	93.89
No	858.2808	0.61	(M+Na)+	C53 H42 F5 N O S	92.45
No	858.2808	-1.00	(M+Na)+	C58 H42 F N O2 S	88.53
No	858.2808	1.95	(M+Na)+	C56 H41 F4 N S	88.07
No	858.2808	2.87	(M+Na)+	C53 H39 F6 N O2	81.17
No	858.2808	-3.24	(M+Na)+	C58 H38 F3 N2 O	77.71
No	858.2808	4.24	(M+Na)+	C56 H38 F5 N O	74.27
No	858.2808	-4.61	(M+Na)+	C55 H39 F4 N2 O2	73.14
No	858.2808	-0.95	(M+NH4)+	C58 H36 F4 S	88.60
No	858.2808	-2.28	(M+NH4)+	C55 H37 F5 O S	87.83
No	858.2808	-0.01	(M+NH4)+	C55 H34 F6 O2	86.19
No	858.2808	-3.61	(M+NH4)+	C52 H38 F6 O2 S	84.78
No	858.2808	1.35	(M+NH4)+	C58 H33 F5 O	83.46
No	858.2808	3.93	(M+NH4)+	C53 H36 F4 N2 O2 S	82.48
No	858.2808	-0.93	M+	C58 H40 F4 N S	88.60
No	858.2808	-2.23	M+	C55 H41 F5 N O S	87.83
No	858.2808	-0.01	M+	C55 H38 F6 N O2	86.19
No	858.2808	-3.53	M+	C52 H42 F6 N O2 S	84.78
No	858.2808	1.32	M+	C58 H37 F5 N O	83.46

Molecular Formula Generation Results

Best	m/z	Diff (ppm)	Species	Formula	Score (MFG)
No	858.2808	3.51	M+	C58 H41 F3 O2 S	80.99

MassHunter Qual 10.0
(End of Report)