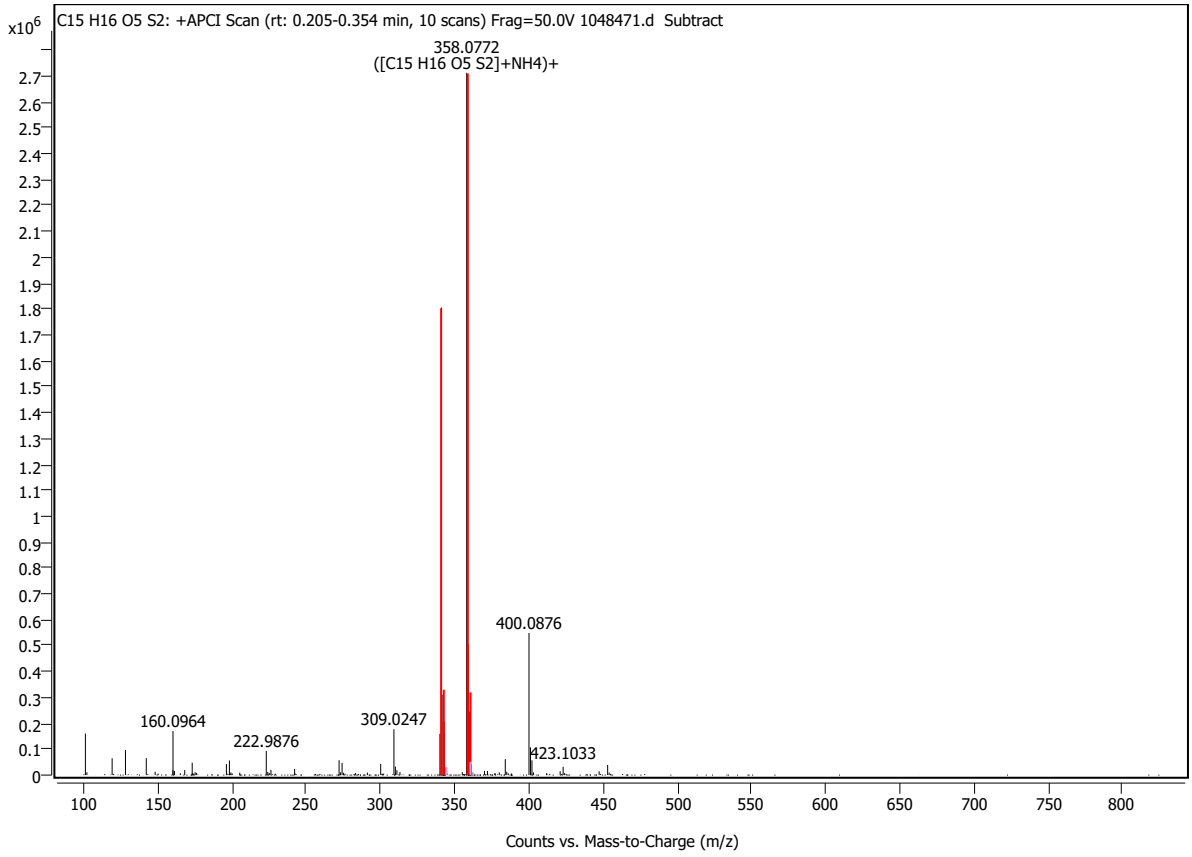
Sample Information

Sample_Name	PCC-622	Data File	1048471.d
Sample_ID		Acq. Time	25/09/2025 14:33:11 (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)	2	Ver. Anal. SW	10.0

MS Spectra

+ Scan (rt: 0.205-0.354 min) Sub



Spectrum Peaks

m/z	m/z (Calc)	Diff (ppm)	Ion Species	Z	Formula	Abund	Abund %
101.0611						160329	5.91
119.0720						65008	2.40
128.0702	128.0706	-2.98		1		96700	3.57
142.0860	142.0863	-1.74		1		65342	2.41
160.0964	160.0968	-2.77		1		170026	6.27
173.0412	173.0419	-4.05		1		47615	1.76
196.1113						42377	1.56
198.1268						56490	2.08
222.9876	222.9882	-2.52		1		93644	3.45
272.0557	272.0553	1.38		1		57417	2.12
274.0707	274.0719	-4.33		1		46837	1.73
300.1105						42643	1.57
309.0247	309.0250	-0.80		1		177135	6.53
310.0275	310.0280	-1.65		1		32719	1.21
340.0428						159541	5.88
341.0504	341.0512	-2.18	(M+H)+	1	C15 H16 O5 S2	1805633	66.57
342.0538	342.0542	-1.38	(M+H)+	1	C15 H16 O5 S2	309710	11.42
343.0492	343.0491	0.14	(M+H)+	1	C15 H16 O5 S2	163657	6.03
344.0513						29049	1.07
358.0772	358.0777	-1.48	(M+NH4)+	1	C15 H16 O5 S2	2712465	100.00
359.0801	359.0807	-1.70	(M+NH4)+	1	C15 H16 O5 S2	472694	17.43
360.0757	360.0757	-0.02	(M+NH4)+	1	C15 H16 O5 S2	245028	9.03
361.0775						41853	1.54
384.0927	384.0934	-1.77		1		61516	2.27
400.0876	400.0894	-4.39		1		548845	20.23
401.0909	401.0926	-4.36		1		107163	3.95
402.0865	402.0888	-5.67		1		57099	2.11
423.1033	423.1027	1.38		1		32056	1.18
453.1141	453.1133	1.77		1		38976	1.44

Molecular Formula Generation Results

Best	m/z	Diff (ppm)	Species	Formula	Score (MFG)
No	128.0702	-4.24	(M+NH4)+	C6 H6 O2	74.83
No	142.0860	-3.45	(M+NH4)+	C7 H8 O2	78.89
No	160.0964	-3.67	(M+NH4)+	C7 H10 O3	84.03
No	173.0412	-3.17	(M+H)+	C11 H8 S	74.48
No	173.0412	-4.51	(M+Na)+	C5 H10 O5	71.05
No	173.0412	-3.15	M+	C11 H9 S	74.48
No	222.9876	-2.41	(M+H)+	C10 H6 O2 S2	98.08
No	222.9876	-2.40	M+	C10 H7 O2 S2	98.08
No	272.0557	1.38	(M+NH4)+	C14 H6 O5	83.78
No	274.0707	-4.02	(M+NH4)+	C15 H12 S2	93.42
No	274.0707	-3.43	(M+NH4)+	C14 H8 O5	73.01
No	309.0247	-0.99	(M+H)+	C14 H12 O4 S2	98.65
No	309.0247	-0.98	M+	C14 H13 O4 S2	98.65
No	341.0504	-0.38	(M+NH4)+	C21 H7 O2 S	89.46
No	341.0504	-1.90	M+	C15 H17 O5 S2	96.13
Yes	341.0504 358.0772	-1.48	(M+H)+ (M+NH4)+	C15 H16 O5 S2	96.79
No	358.0772	4.76	(M+K)+	C24 H15 O	79.79
No	358.0772	-4.94	(M+Na)+	C24 H15 S	76.59
No	384.0927	3.94	(M+K)+	C26 H17 O	84.47
No	384.0927	-1.72	(M+NH4)+	C17 H18 O5 S2	97.12
No	400.0876	-4.97	(M+K)+	C23 H21 O2 S	83.22
No	400.0876	3.90	(M+K)+	C26 H17 O2	81.65
No	400.0876	-4.71	(M+Na)+	C26 H17 O S	76.17
No	423.1033	-4.53	(M+H)+	C27 H18 O3 S	77.94
No	423.1033	1.38	(M+K)+	C22 H24 O4 S	95.50
No	423.1033	1.32	(M+Na)+	C25 H20 O3 S	88.17
No	423.1033	-4.52	M+	C27 H19 O3 S	77.94
No	453.1141	-4.01	(M+H)+	C28 H20 O4 S	79.74
No	453.1141	1.50	(M+K)+	C23 H26 O5 S	93.45
No	453.1141	1.45	(M+Na)+	C26 H22 O4 S	88.72
No	453.1141	-4.00	M+	C28 H21 O4 S	79.74

MassHunter Qual 10.0
(End of Report)