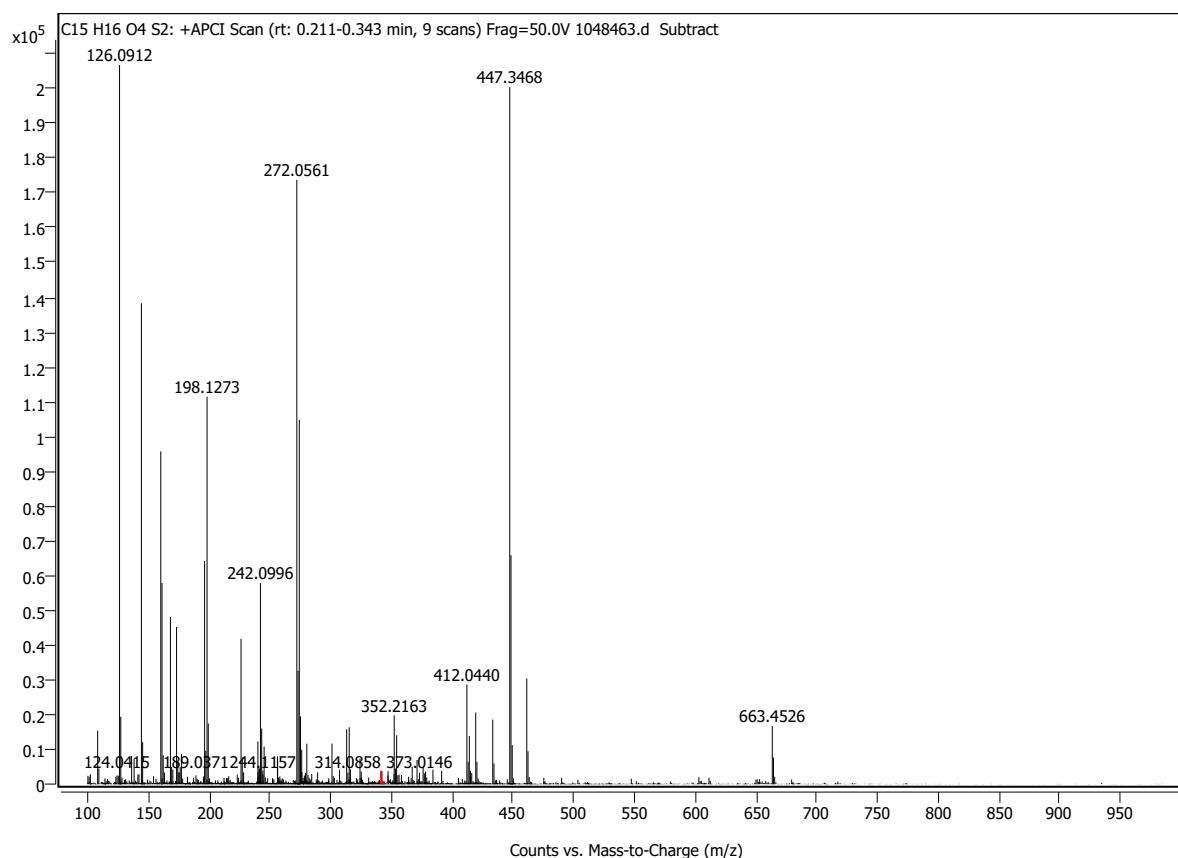


Sample Information

Sample_Name	PCC-474	Data File	1048463.d
Sample_ID		Acq. Time	25/09/2025 13:50:23 (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: 0.211-0.343 min) Sub



Spectrum Peaks

m/z	m/z (Calc)	Diff (ppm)	Ion Species	Z	Formula	Abund	Abund %
102.0905						2824	1.37
108.0801						15401	7.45
109.0819						4447	2.15
124.0415						2470	1.19
126.0912	126.0913	-0.99		1		206790	100.00
127.0931	127.0945	-10.53		1		19363	9.36
136.0212						8093	3.91
138.0658						7187	3.48
141.1635	141.1638	-2.26		1		2729	1.32
142.0887						2843	1.37
144.1016	144.1019	-2.05		1		138267	66.86
145.1047	145.1050	-2.17		1		12032	5.82
160.0338						95677	46.27
161.0412				1		57806	27.95
162.0421				1		8290	4.01
163.0379				1		3332	1.61
167.9931				1		48050	23.24
168.9960				1		4927	2.38
169.9893				1		4155	2.01
173.0415	173.0419	-2.59		1		45180	21.85
174.0470	174.0451	11.22		1		6624	3.20
175.0207						3444	1.67
175.0370	175.0392	-12.99		1		3300	1.60
176.0293						4884	2.36
177.0364	177.0369	-2.65		1		8701	4.21
189.0371						2490	1.20
196.1116	196.1121	-2.48		1		64193	31.04
197.1137	197.1153	-8.42		1		9554	4.62
198.1273	198.1277	-2.17		1		111398	53.87
199.1306	199.1310	-1.61		1		17418	8.42
222.9878	222.9882	-1.98		1		2735	1.32
226.1222	226.1226	-2.10		1		41796	20.21
227.1254	227.1259	-2.36		1		7696	3.72
228.2316	228.2322	-2.57		1		3397	1.64
239.9902						12257	5.93
240.0820						3497	1.69
240.9971						4524	2.19
241.0996						4467	2.16
242.0996				1		57755	27.93
243.1130				1		15980	7.73
244.0959				1		3830	1.85
244.1157						2861	1.38
245.0993	245.0995	-0.87		1		10788	5.22
256.0786						7969	3.85
256.2626	256.2635	-3.39		1		6833	3.30
272.0561				1		173759	84.03
273.0589				1		32581	15.76
274.0710	274.0719	-3.03		1		104719	50.64
275.0741	275.0748	-2.58		1		19452	9.41
276.0688	276.0692	-1.20		1		9897	4.79
276.2320	276.2322	-0.55		1		3408	1.65
278.2466						2426	1.17
279.0971						2886	1.40
279.1589	279.1591	-0.69		1		3240	1.57
280.2629	280.2635	-2.26		1		11606	5.61
281.2662	281.2668	-2.21		1		2631	1.27
284.2940	284.2948	-2.88		1		2901	1.40
289.1792						3376	1.63
300.9916						11639	5.63
307.1899	307.1904	-1.64		1		4079	1.97
313.0822				1		15759	7.62
314.0858				1		3306	1.60
315.1854	315.1863	-2.86		1		16316	7.89
316.1893	316.1894	-0.34		1		4236	2.05
324.0483						7277	3.52
325.0540	325.0529	3.22		1		3591	1.74
342.0822	342.0828	-1.72	(M+NH4)+	1	C15 H16 O4 S2	3656	1.77
347.0556						2464	1.19
347.1565	347.1583	-5.42		1		3706	1.79
352.0937	352.0928	2.81		1		2853	1.38
352.2163				1		19773	9.56
353.2195				1		4477	2.17
354.2137				1		14050	6.79
355.2165				1		2521	1.22
356.2113				1		2750	1.33
358.1293	358.1294	-0.26		1		2627	1.27
367.0280						4965	2.40
371.0181						6958	3.36
373.0146						3331	1.61
376.0120						4806	2.32
377.0131						3087	1.49
378.0106						3614	1.75
384.0933						4153	2.01

Spectrum Peaks

m/z	m/z (Calc)	Diff (ppm)	Ion Species	Z	Formula	Abund	Abund %
391.2836	391.2843	-1.71		1		3791	1.83
412.0440				1		28605	13.83
413.0474				1		6415	3.10
414.0404				1		13829	6.69
415.0424				1		3794	1.83
416.0378				1		3180	1.54
419.3152	419.3156	-0.80		1		20572	9.95
420.3184	420.3190	-1.53		1		6382	3.09
433.3307	433.3312	-1.33		1		18543	8.97
434.3343	434.3346	-0.70		1		5927	2.87
447.3468	447.3469	-0.26		1		200416	96.92
448.3498	448.3503	-1.19		1		65815	31.83
449.3526	449.3533	-1.69		1		11239	5.44
461.3618	461.3625	-1.61		1		30369	14.69
462.3650	462.3659	-2.14		1		9442	4.57
663.4526	663.4536	-1.50		1		16707	8.08
664.4559	664.4570	-1.67		1		7627	3.69

Molecular Formula Generation Results

Best	m/z	Diff (ppm)	Species	Formula	Score (MFG)
No	126.0912	-2.16	(M+NH ₄) ⁺	C7 H8 O	96.11
No	141.1635	-2.79	(M+H) ⁺	C10 H20	85.35
No	141.1635	-2.77	M ⁺	C10 H21	85.35
No	144.1016	-2.41	(M+NH ₄) ⁺	C7 H10 O2	99.28
No	173.0415	-1.57	(M+H) ⁺	C11 H8 S	88.92
No	173.0415	-1.56	M ⁺	C11 H9 S	88.92
No	177.0364	-2.26	(M+H) ⁺	C10 H8 O S	83.56
No	177.0364	-2.25	M ⁺	C10 H9 O S	83.56
No	196.1116	-3.59	(M+NH ₄) ⁺	C14 H10	83.11
No	198.1273	-2.32	(M+NH ₄) ⁺	C14 H12	99.08
No	222.9878	-1.44	(M+H) ⁺	C10 H6 O2 S2	88.35
No	222.9878	-1.43	M ⁺	C10 H7 O2 S2	88.35
No	226.1222	-4.74	(M+H) ⁺	C9 H21 O4 S	78.28
No	226.1222	-2.59	(M+NH ₄) ⁺	C15 H12 O	97.67
No	228.2316	-1.99	(M+NH ₄) ⁺	C14 H26 O	82.54
No	245.0993	-0.72	(M+H) ⁺	C15 H16 O S	98.07
No	245.0993	-4.54	(M+Na) ⁺	C10 H22 O S2	82.02
No	245.0993	-0.71	M ⁺	C15 H17 O S	98.07
No	256.2626	-3.77	(M+NH ₄) ⁺	C16 H30 O	93.76
No	274.0710	-3.03	(M+NH ₄) ⁺	C15 H12 S2	96.45
No	276.2320	-2.45	(M+NH ₄) ⁺	C18 H26 O	76.56
No	279.1589	-0.18	(M+H) ⁺	C16 H22 O4	78.80
No	279.1589	-0.18	M ⁺	C16 H23 O4	78.80
No	280.2629	-2.41	(M+NH ₄) ⁺	C18 H30 O	83.37
No	284.2940	-3.49	(M+NH ₄) ⁺	C18 H34 O	95.76
No	307.1899	-0.38	(M+H) ⁺	C18 H26 O4	90.64
No	307.1899	-0.38	M ⁺	C18 H27 O4	90.64
No	315.1854	-2.00	(M+NH ₄) ⁺	C16 H25 O3 S	83.91
No	325.0540	1.40	(M+H) ⁺	C18 H12 O4 S	76.03
No	325.0540	1.40	M ⁺	C18 H13 O4 S	76.03
No	342.0822	3.11	(M+K) ⁺	C24 H15	84.55
Yes	342.0822	-3.04	(M+NH ₄) ⁺	C15 H16 O4 S2	83.55
No	347.1565	-2.45	(M+NH ₄) ⁺	C16 H25 O3 S2	77.92
No	352.0937	0.68	(M+K) ⁺	C16 H25 O2 S2	90.09
No	352.0937	1.02	(M+Na) ⁺	C19 H21 O S2	81.35
No	358.1293	-1.70	(M+NH ₄) ⁺	C20 H20 O S2	80.75
No	391.2836	-1.81	(M+H) ⁺	C24 H38 O4	95.20
No	391.2836	4.61	(M+Na) ⁺	C22 H40 O4	91.23
No	391.2836	-1.80	M ⁺	C24 H39 O4	95.20
No	419.3152	0.35	(M+H) ⁺	C26 H42 O4	88.49
No	419.3152	0.35	M ⁺	C26 H43 O4	88.49
No	433.3307	-1.18	(M+H) ⁺	C27 H44 O4	98.37
No	433.3307	4.62	(M+Na) ⁺	C25 H46 O4	88.95
No	433.3307	-1.17	M ⁺	C27 H45 O4	98.37
No	447.3468	-0.56	(M+H) ⁺	C28 H46 O4	99.13
No	447.3468	-0.56	M ⁺	C28 H47 O4	99.13
No	461.3618	-1.74	(M+H) ⁺	C29 H48 O4	97.99
No	461.3618	3.66	(M+Na) ⁺	C27 H50 O4	93.68
No	461.3618	-1.74	M ⁺	C29 H49 O4	97.99
No	663.4526	-1.51	(M+K) ⁺	C44 H64 O2	91.81
No	663.4526	-1.79	(M+Na) ⁺	C47 H60 O	94.78
No	663.4526	4.43	(M+NH ₄) ⁺	C42 H61 O S2	77.94

