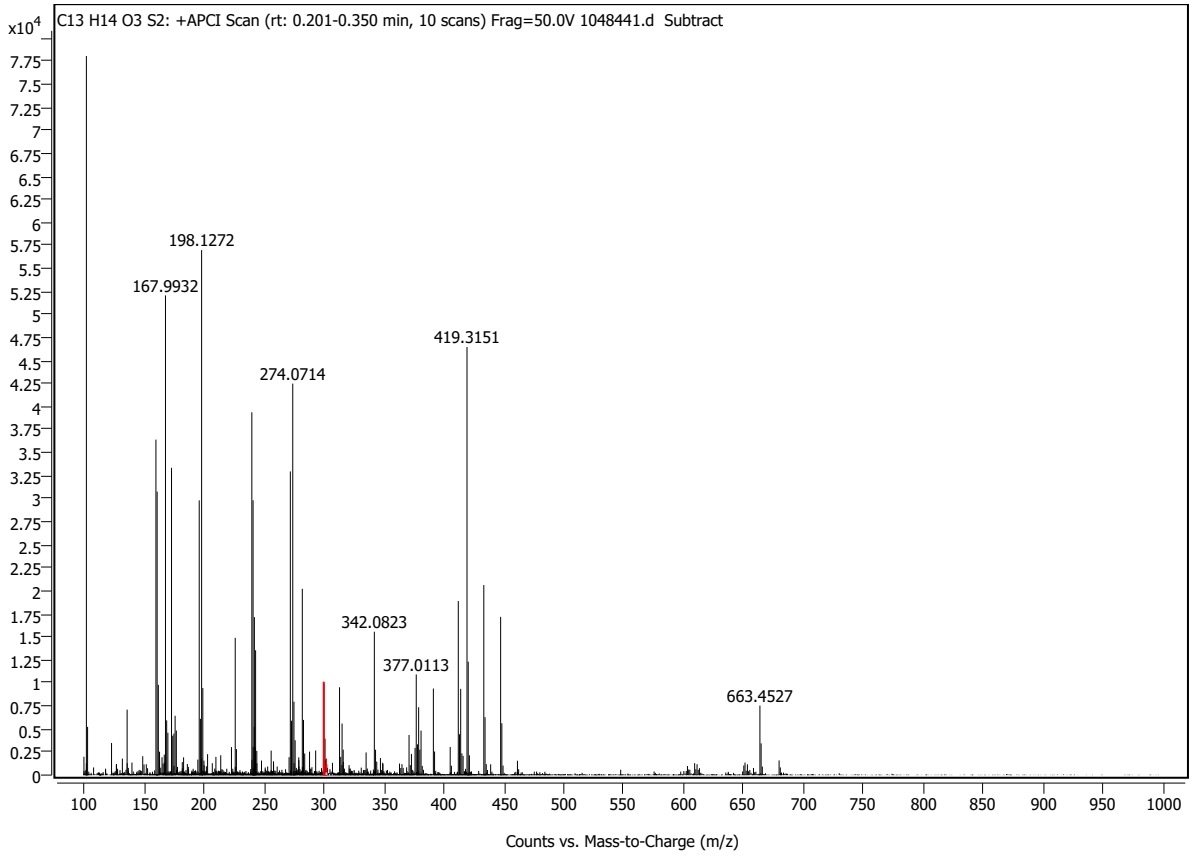
Sample Information

Sample_Name	PCC-463	Data File	1048441.d
Sample_ID		Acq. Time	24/09/2025 15:49:55 (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: 0.201-0.350 min) Sub



Spectrum Peaks

m/z	m/z (Calc)	Diff (ppm)	Ion Species	Z	Formula	Abund	Abund %
100.0382						1987	2.55
102.0909				1		78056	100.00
103.0942				1		5234	6.71
123.0562						3480	4.46
132.0808						1790	2.29
136.0212						7106	9.10
149.0238	149.0233	3.02		1		2047	2.62
160.0337	160.0341	-2.40				36416	46.65
161.0414	161.0419	-3.59				30776	39.43
162.0400	162.0406	-3.44		1		9797	12.55
163.0418	163.0423	-3.55				2539	3.25
163.0718						1708	2.19
165.1233						1936	2.48
166.9976	166.9984	-4.76				2218	2.84
167.9932				1		52070	66.71
168.9955				1		5939	7.61
169.9890				1		4593	5.88
173.0415	173.0419	-2.40		1		33356	42.73
174.0466	174.0451	8.80		1		4280	5.48
175.0221	175.0222	-0.29				4507	5.77
176.0287	176.0290	-1.89				6438	8.25
177.0366	177.0369	-1.38		1		4835	6.19
183.0828	183.0838	-5.60		1		1926	2.47
194.9930	194.9933	-1.42		1		1679	2.15
196.1116	196.1121	-2.26		1		29823	38.21
197.1145	197.1153	-4.20		1		6107	7.82
198.0367						1510	1.93
198.1272	198.1277	-2.44		1		56991	73.01
198.1834						1813	2.32
199.1307	199.1310	-1.11		1		9448	12.10
200.0524	200.0528	-2.32				1568	2.01
203.0883						2268	2.91
210.0399	210.0406	-2.98		1		1974	2.53
214.0682	214.0685	-1.25				2151	2.76
222.9880	222.9882	-1.10		1		3034	3.89
226.1221	226.1226	-2.37		1		14895	19.08
227.1246	227.1259	-5.81		1		2826	3.62
239.9906	239.9909	-1.46				39383	50.45
240.0819						1669	2.14
240.9980	240.9964	6.74		1		29832	38.22
241.0970						3068	3.93
241.9964	241.9992	-11.30		1		5230	6.70
242.0995						17145	21.97
242.2836						1824	2.34
242.9948	242.9932	6.88		1		2965	3.80
243.1162	243.1168	-2.69		1		13549	17.36
244.1178	244.1202	-10.05		1		2629	3.37
248.0309	248.0300	3.74		1		1575	2.02
256.0784	256.0791	-2.62		1		2661	3.41
271.0246	271.0246	-0.04		1		1941	2.49
272.0560	272.0562	-0.76		1		32963	42.23
273.0594	273.0591	0.82		1		5899	7.56
274.0714	274.0719	-1.73		1		42496	54.44
275.0745	275.0748	-0.87		1		7963	10.20
276.0690	276.0692	-0.74		1		3778	4.84
279.0960						1930	2.47
279.1607						1628	2.09
282.0377				1		20221	25.91
283.0430				1		5989	7.67
284.0384				1		2338	3.00
288.0873	288.0875	-0.86		1		2547	3.26
293.1756						2673	3.42
300.0724	300.0723	0.33	(M+NH4)+	1	C13 H14 O3 S2	9900	12.68
300.9905						3958	5.07
301.0752	301.0751	0.37	(M+NH4)+	1	C13 H14 O3 S2	1726	2.21
313.0820				1		9531	12.21
314.0852				1		1975	2.53
315.1852	315.1863	-3.27		1		5597	7.17
316.1184	316.1188	-1.40		1		2760	3.54
335.2211						2458	3.15
342.0823	342.0805	5.27		1		15564	19.94
343.0847	343.0839	2.17		1		2752	3.53
347.1567	347.1583	-4.71		1		1848	2.37
371.0178						4350	5.57
373.0135						2297	2.94
376.0118	376.0131	-3.51				2947	3.77
377.0113				1		10929	14.00
378.0121				1		3340	4.28
379.0087				1		7367	9.44
380.0102				1		2769	3.55
381.0071				1		4827	6.18
391.2841				1		9395	12.04
392.2871				1		2560	3.28

Spectrum Peaks

m/z	m/z (Calc)	Diff (ppm)	Ion Species	Z	Formula	Abund	Abund %
405.2994						3052	3.91
412.0440				1		18894	24.21
413.0469				1		4430	5.68
414.0400				1		9358	11.99
415.0421				1		2354	3.02
416.0389				1		2085	2.67
419.3151				1		46467	59.53
420.3186				1		12309	15.77
421.3217				1		2147	2.75
433.3305				1		20630	26.43
434.3351				1		6283	8.05
447.3465				1		17177	22.01
448.3495				1		5624	7.20
461.3624						1554	1.99
663.4527	663.4536	-1.42		1		7544	9.66
664.4564	664.4570	-0.88		1		3441	4.41
679.4299	679.4308	-1.34		1		1593	2.04

Molecular Formula Generation Results

Best	m/z	Diff (ppm)	Species	Formula	Score (MFG)
No	149.0238	1.45	M+	C8 H5 O3	67.50
No	160.0337	-2.41	(M+H)+	C10 H7 S	46.79
No	160.0337 161.0414	-2.40	M+ (M+H)+	C10 H8 S	46.79
No	161.0414	-3.59	M+	C10 H9 S	45.77
No	162.0400	-4.39	(M+NH4)+	C6 H8 S2	79.08
No	163.0418	-3.57	(M+H)+	C6 H10 O3 S	45.78
No	163.0418	-3.55	M+	C6 H11 O3 S	45.78
No	166.9976	-4.79	(M+H)+	C8 H6 S2	44.25
No	166.9976	-4.76	M+	C8 H7 S2	44.25
No	173.0415	-0.98	(M+H)+	C11 H8 S	86.70
No	173.0415	-0.97	M+	C11 H9 S	86.70
No	175.0221	-0.33	(M+Na)+	C5 H12 O S2	47.61
No	176.0287	-1.90	(M+H)+	C10 H7 O S	47.03
No	176.0287 177.0366	-3.95	M+ (M+H)+	C10 H8 O S	76.47
No	177.0366	-3.93	M+	C10 H9 O S	76.47
No	183.0828	-4.95	(M+H)+	C10 H14 O S	70.12
No	183.0828	-4.92	M+	C10 H15 O S	70.12
No	194.9930	-1.65	(M+H)+	C9 H6 O S2	82.45
No	194.9930	-1.64	M+	C9 H7 O S2	82.45
No	196.1116	-2.85	(M+NH4)+	C14 H10	80.32
No	198.1272	-2.54	(M+NH4)+	C14 H12	98.55
No	200.0524	-2.55	(M+NH4)+	C12 H6 S	46.57
No	210.0399	-4.17	(M+NH4)+	C10 H8 S2	60.49
No	214.0682	-4.50	(M+H)+	C7 H17 O3 S2	43.53
No	214.0682	-1.36	(M+NH4)+	C13 H8 S	47.29
No	222.9880	-2.35	(M+H)+	C10 H6 O2 S2	95.50
No	222.9880	-2.34	M+	C10 H7 O2 S2	95.50
No	226.1221	-3.28	(M+NH4)+	C15 H12 O	95.49
No	239.9906	-1.47	(M+H)+	C10 H7 O3 S2	47.10
No	239.9906	-1.46	M+	C10 H8 O3 S2	47.10
No	240.9980	4.72	(M+Na)+	C8 H10 O3 S2	75.52
No	243.1162	-4.00	(M+H)+	C19 H14	91.26
No	243.1162	-3.98	M+	C19 H15	91.26
No	248.0309	3.23	(M+K)+	C8 H17 O2 S2	85.39
No	248.0309	3.83	(M+Na)+	C11 H13 O S2	87.84
No	256.0784	-1.93	(M+NH4)+	C15 H10 O S	74.04
No	271.0246	-1.86	(M+H)+	C15 H10 O S2	71.94
No	271.0246	-1.86	M+	C15 H11 O S2	71.94
No	272.0560	-0.56	(M+NH4)+	C15 H10 S2	67.73
No	274.0714	-1.65	(M+NH4)+	C15 H12 S2	97.61
No	288.0873	2.49	(M+NH4)+	C16 H14 S2	73.70
Yes	300.0724	-0.04	(M+NH4)+	C13 H14 O3 S2	97.86
No	315.1852	-3.20	(M+NH4)+	C16 H25 O3 S	82.33
No	316.1184	-3.25	(M+NH4)+	C18 H18 S2	82.46
No	342.0823	4.70	(M+K)+	C24 H15	78.16
No	347.1567	-3.91	(M+NH4)+	C16 H25 O3 S2	76.25
No	376.0118	-3.74	(M+Na)+	C25 H5 O3	42.94
No	663.4527	-1.28	(M+K)+	C44 H64 O2	89.50
No	663.4527	4.61	(M+NH4)+	C42 H61 O S2	74.23
No	663.4527 679.4299	-1.44	(M+Na)+ (M+K)+	C47 H60 O	95.99
No	679.4299	-0.15	(M+H)+	C52 H54	92.35
No	679.4299	-4.49	(M+H)+	C49 H58 S	86.70
No	679.4299	-0.84	(M+K)+	C44 H64 O S	89.10
No	679.4299	-0.95	(M+Na)+	C47 H60 S	97.97
No	679.4299	3.50	(M+Na)+	C50 H56	85.77
No	679.4299	-0.15	M+	C52 H55	92.35
No	679.4299	-4.49	M+	C49 H59 S	86.70

MassHunter Qual 10.0
(End of Report)