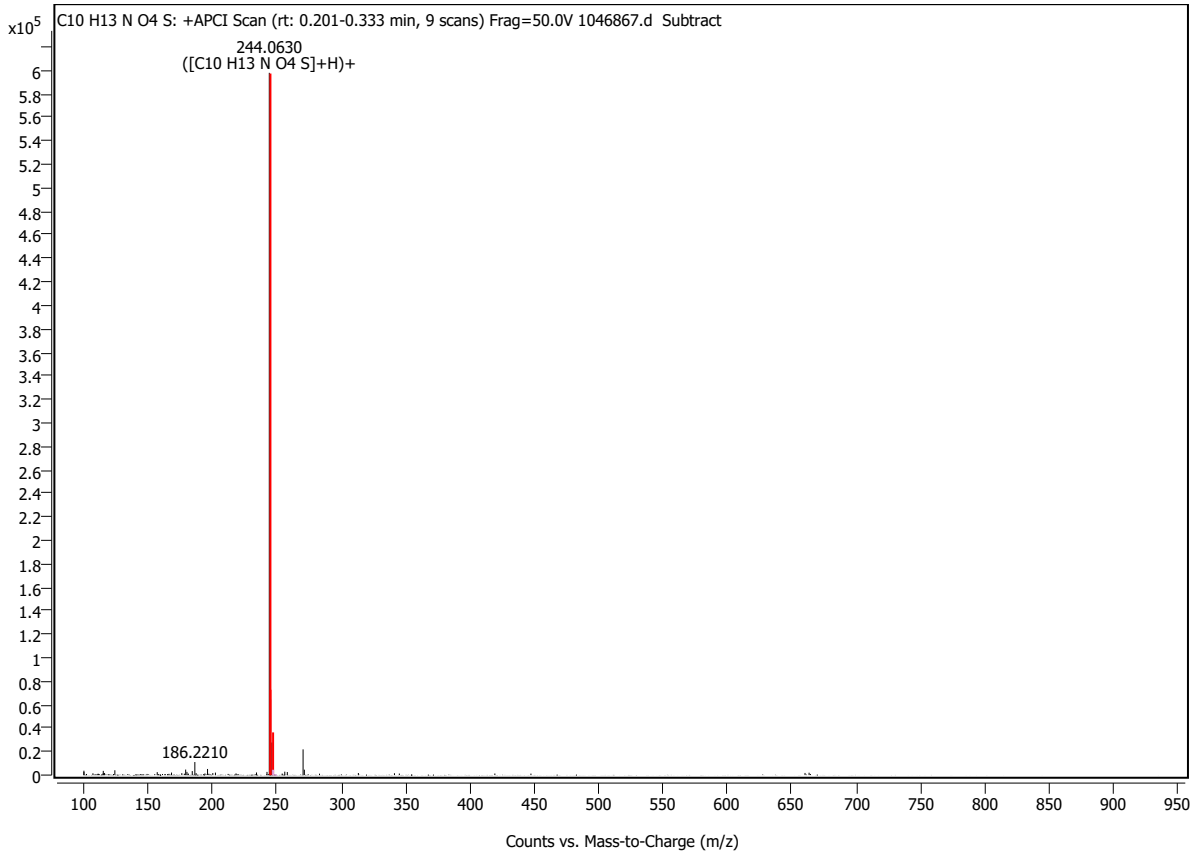
Sample Information

Sample_Name	PCC-371	Data File	1046867.d
Sample_ID		Acq. Time	16/06/2025 15:01:29 (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: 0.201-0.333 min) Sub



Spectrum Peaks

m/z	m/z (Calc)	Diff (ppm)	Ion Species	Z	Formula	Abund	Abund %
186.2210	186.2216	-3.35		1		11112	1.86
244.0630	244.0638	-3.15	(M+H)+	1	C10 H13 N O4 S	598041	100.00
245.0665	245.0668	-1.15	(M+H)+	1	C10 H13 N O4 S	64327	10.76
246.0619	246.0619	-0.30	(M+H)+	1	C10 H13 N O4 S	27717	4.63
270.3146	270.3155	-3.32		1		21903	3.66

Molecular Formula Generation Results

Best	m/z	Diff (ppm)	Species	Formula	Score (MFG)
No	186.2210	-3.39	(M+H)+	C12 H27 N	85.27
No	186.2210	-3.73	(M+NH4)+	C12 H24	85.27
No	186.2210	-3.37	M+	C12 H28 N	85.27
Yes	244.0630	-2.86	(M+H)+	C10 H13 N O4 S	96.37
No	244.0630	-3.08	(M+NH4)+	C10 H10 O4 S	96.37
No	244.0630	-2.85	M+	C10 H14 N O4 S	96.37
No	270.3146	-3.34	(M+H)+	C18 H39 N	96.02
No	270.3146	-3.56	(M+NH4)+	C18 H36	96.02
No	270.3146	-3.32	M+	C18 H40 N	96.02

MassHunter Qual 10.0
(End of Report)