Ansprechpartner: R. M. Bergsträßer / E. Biehl Tel.: 205-2965 Version 25.03.2010

Auftrags- Protokoll — MS-TOF-Messung GCT Waters

Eingangsdatum: May 2024

Name / Auftraggeber: Po-Chung Chien Arbeitskreis: Manolikakes

Tel.: 0151 58871443 E-mail.: pc.chien@chem.rptu.de

GC- HR-MS: ☐ **HR- MS-Feststoff**: ☒

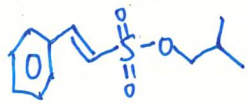
Auswertung: ☒ Exakte Masse (≤ 2mDa, ≤ 10 ppm) ☐ Fragmentierung zur Strukturaufklärung

Probenbezeichnung: PCC-219 Lösungsmittel: Acetone or CH_2Cl_2

Gewünschte Ionisierungs- Methode: EI^+ ☒ Cl^- ☐ Cl^+ ☐ (CI: Methan)

Mögliche Verbindungen (Strukturformel u. Molmasse)/ Bemerkungen:

Summenformel: $C_{12}H_{16}O_3S$ Exakte Masse: 240.0820



Zu internen Verwaltungszwecken:

Int. Auftragsnummer: 240603 Messdatum: 06062024 Operator: RS

Ionisations- Methode: : EI^+ ☒ Cl^+ ☐ Cl^- ☐

Speicherort: Feststoff-Daten-EI, Kalib.- Datum: 05062024

Bemerkungen: Range 2 / 70eV

$[M+]$

Ausgangsdatum: 10.06.24

FB Organische Chemie / Prof. Hartung Abteilung: Analytik

Elemental Composition Report

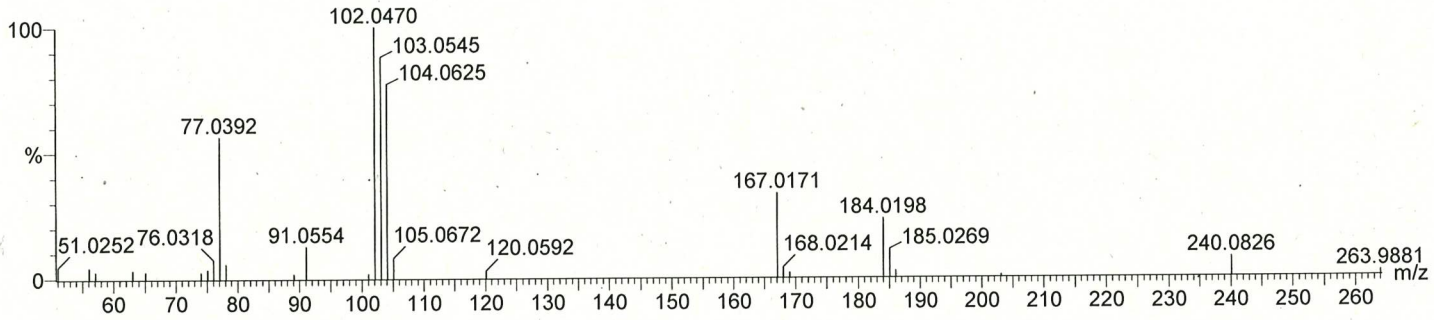
Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

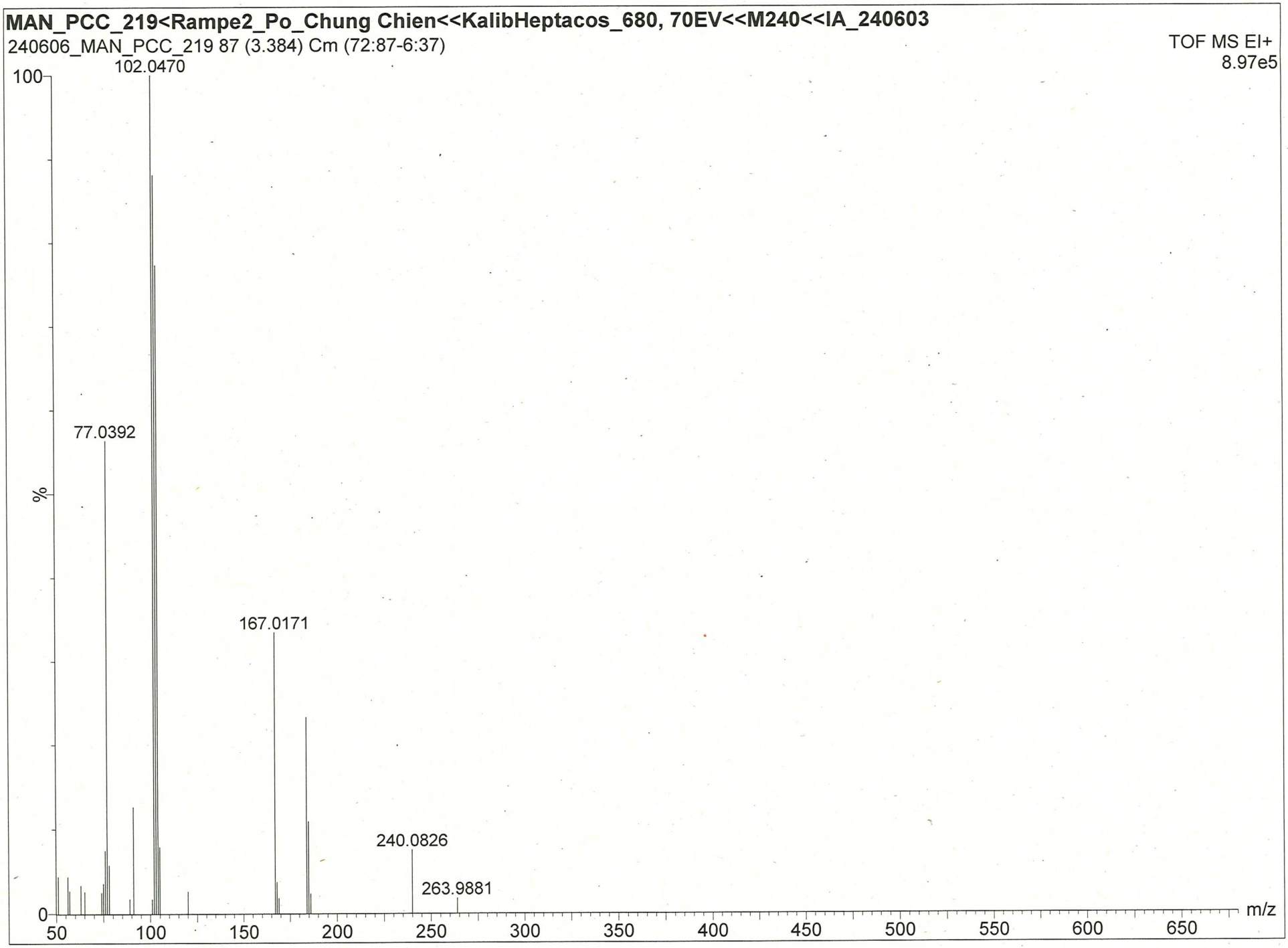
Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-12 H: 0-18 O: 0-3 S: 0-1

MAN_PCC_219<Rampe2_Po_Chung Chien<<KalibHeptacos_680, 70EV<<M240<<IA_240603
240606_MAN_PCC_219 87 (3.384) Cm (72:87-6:37)

TOF MS EI+
8.97e+005



Minimum:				-1.5		
Maximum:		100.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
240.0826	240.0820	0.6	2.5	5.0	5579307.5	C12 H16 O3 S


MAN_PCC_219<Rampe2_Po_Chung Chien<<KalibHeptacos_680, 70EV<<M240<<IA_240603
240606_MAN_PCC_219 87 (3.384) Cm (72:87-6:37)
TOF MS EI+
8.97e5
100
%
0
102.0470
77.0392
167.0171
240.0826
263.9881
50
100
150
200
250
300
350
400
450
500
550
600
650
m/z

MAN_PCC_219<Rampe2_Po_Chung Chien<<KalibHeptacos_680, 70EV<<M240<<IA_240603

TOF MS EI+

240606_MAN_PCC_219 87 (3.384) Cm (72:87-6:37)

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%
1:	51.0252	3.88e4	4.32	0.82															
2:	52.0325	7.47e3	0.83	0.16															
3:	55.0565	4.58e3	0.51	0.10															
4:	56.0640	3.85e4	4.30	0.82															
5:	57.0717	2.35e4	2.62	0.50															
6:	62.0170	7.00e3	0.78	0.15															
7:	63.0247	2.95e4	3.29	0.62															
8:	64.0310	4.56e3	0.51	0.10															
9:	65.0401	2.26e4	2.52	0.48															
10:	74.0170	2.17e4	2.42	0.46															
11:	75.0246	3.13e4	3.49	0.66															
12:	76.0318	6.62e4	7.39	1.40															
13:	77.0392	5.05e5	56.33	10.70															
14:	78.0445	5.06e4	5.64	1.07															
15:	79.0540	8.41e3	0.94	0.18															
16:	89.0407	1.51e4	1.68	0.32															
17:	90.0479	1.14e4	1.27	0.24															
18:	91.0554	1.13e5	12.62	2.40															
19:	92.0605	1.13e4	1.25	0.24															
20:	101.0407	1.48e4	1.65	0.31															
21:	102.0470	8.97e5	100.00	19.00															
22:	103.0545	7.90e5	88.09	16.73															
23:	103.1488	4.99e3	0.56	0.11															
24:	104.0625	6.93e5	77.32	14.69															
25:	105.0324	6.29e3	0.70	0.13															
26:	105.0672	7.01e4	7.82	1.48															
27:	117.0726	7.21e3	0.80	0.15															
28:	118.0441	9.33e3	1.04	0.20															
29:	119.0512	1.19e4	1.33	0.25															
30:	120.0592	2.28e4	2.54	0.48															
31:	121.0663	1.25e4	1.39	0.26															
32:	123.0286	4.64e3	0.52	0.10															
33:	134.0209	6.26e3	0.70	0.13															
34:	143.0880	7.74e3	0.86	0.16															
35:	158.1109	9.15e3	1.02	0.19															
36:	167.0171	3.00e5	33.43	6.35															
37:	168.0214	3.26e4	3.64	0.69															
38:	169.0088	1.56e4	1.74	0.33															
39:	184.0198	2.08e5	23.25	4.42															
40:	185.0269	9.72e4	10.84	2.06															
41:	186.0227	2.03e4	2.26	0.43															
42:	187.0247	5.36e3	0.60	0.11															
43:	240.0826	6.66e4	7.43	1.41															
44:	241.0871	9.31e3	1.04	0.20															
45:	263.9881	1.52e4	1.69	0.32															
46:	413.9798	5.78e3	0.64	0.12															
47:	501.9740	9.70e3	1.08	0.21															