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

# Auftrags- Protokoll – MS-TOF-Messung GCT Waters

Eingangsdatum: _____

Name / Auftraggeber: Miro Halaczkiewicz Arbeitskreis: Manolikakes

Tel.: 2527 E-mail.: halaczki@rhrk.uni-kl.de

**GC- HR-MS**: ☐ **HR- MS-Feststoff**: ☒

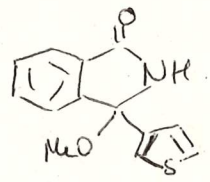
**Auswertung:** ☒ Exakte Masse ( ≤ 2mDa, ≤ 10 ppm) ☐ Fragmentierung zur Strukturaufklärung

Probenbezeichnung: MHA-R64 Lösungsmittel: DCM, Aceton

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

Mögliche Verbindungen (Strukturformel u. Molmasse)/ Bemerkungen:

Summenformel: $C_{13}H_{11}NO_2S$ Exakte Masse: 245,0510




**Zu internen Verwaltungszwecken:**

Int. Auftragsnummer: 230913 Messdatum: 210923 Operator: RB

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

Speicherort: Feststoff-EI, Rempe 2, 70eV Kalib.- Datum: 210923

Bemerkungen:

[M+]·

Ausgangsdatum: 210923

FB Organische Chemie / Prof. Hartung Abteilung: Analytik

# Elemental Composition Report

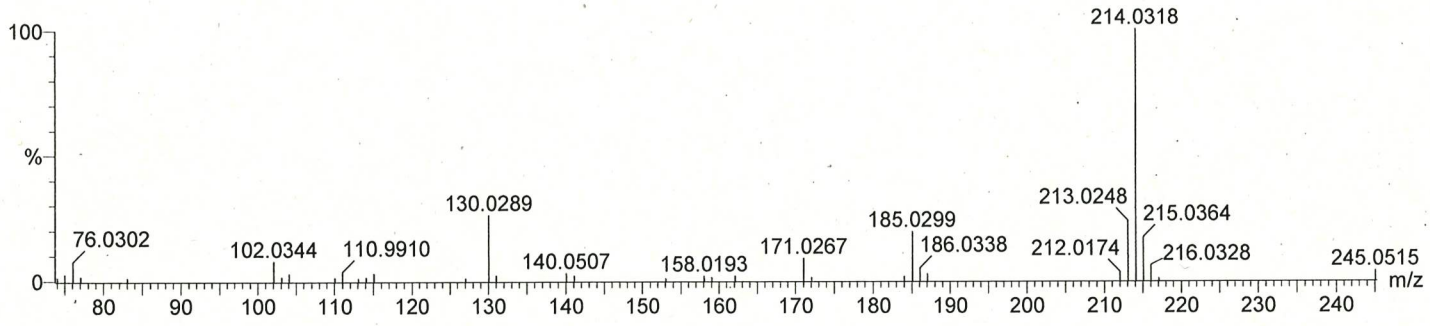
## Single Mass Analysis

Tolerance = 25.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

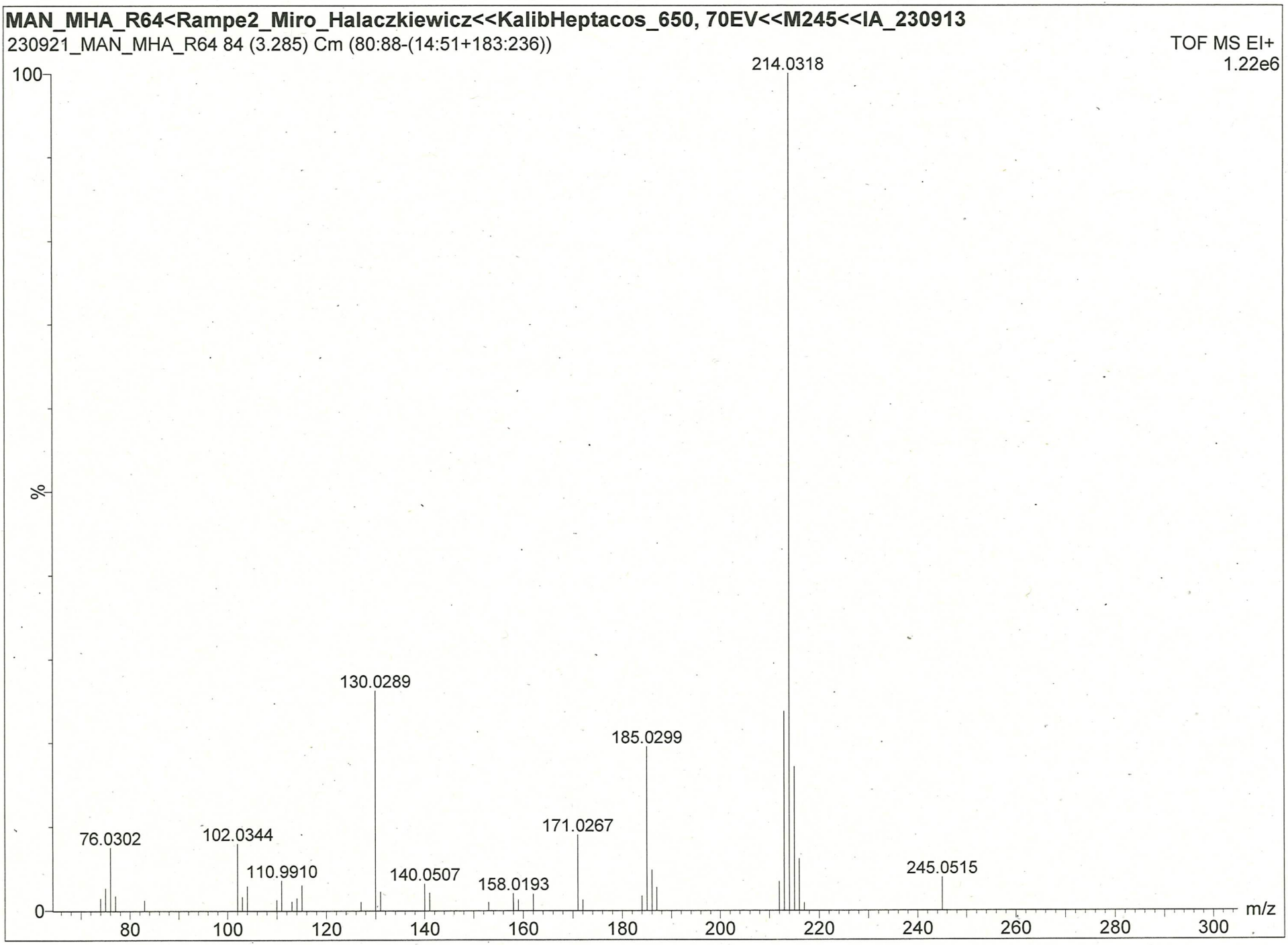
Monoisotopic Mass, Odd and Even Electron Ions
21 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-13 H: 0-12 N: 0-2 O: 0-2 S: 0-2

MAN_MHA_R64<Rampe2_Miro_Halaczkiewicz<<KalibHeptacos_650, 70EV<<M245<<IA_230913
230921_MAN_MHA_R64 84 (3.285) Cm (80:88-(14:51+183:236))

TOF MS EI+
1.22e+006




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 100.0 | 25.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 245.0515 | 245.0511 | 0.4 | 1.6 | 9.0 | 5569775.5 | C13 H11 N O2 S |


MAN_MHA_R64<Rampe2_Miro_Halaczkiewicz<<KalibHeptacos_650, 70EV<<M245<<IA_230913
230921_MAN_MHA_R64 84 (3.285) Cm (80:88-(14:51+183:236))
TOF MS EI+
1.22e6
100
%
0
214.0318
130.0289
185.0299
171.0267
76.0302
102.0344
110.9910
140.0507
158.0193
245.0515
m/z
80
100
120
140
160
180
200
220
240
260
280
300

**MAN_MHA_R64<Rampe2_Miro_Halaczkiewicz<<KalibHeptacos_650, 70EV<<M245<<IA_230913**

230921_MAN_MHA_R64 84 (3.285) Cm (80:88-(14:51+183:236)) TOF MS EI+

| No | Mass | Inten | %BPI | %TIC | No | Mass | Inten | %BPI | %TIC | No | Mass | Inten | %BPI | %TIC | No | Mass | Inten | %BPI | % |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1: | 74.0164 | 1.73e4 | 1.42 | 0.47 | | | | | | | | | | | | | | | |
| 2: | 75.0228 | 3.21e4 | 2.64 | 0.87 | | | | | | | | | | | | | | | |
| 3: | 76.0302 | 9.08e4 | 7.47 | 2.45 | | | | | | | | | | | | | | | |
| 4: | 77.0384 | 2.10e4 | 1.73 | 0.57 | | | | | | | | | | | | | | | |
| 5: | 82.9955 | 1.45e4 | 1.20 | 0.39 | | | | | | | | | | | | | | | |
| 6: | 102.0344 | 9.62e4 | 7.91 | 2.60 | | | | | | | | | | | | | | | |
| 7: | 103.0422 | 1.95e4 | 1.61 | 0.53 | | | | | | | | | | | | | | | |
| 8: | 104.0279 | 3.51e4 | 2.89 | 0.95 | | | | | | | | | | | | | | | |
| 9: | 110.0078 | 1.52e4 | 1.25 | 0.41 | | | | | | | | | | | | | | | |
| 10: | 110.9910 | 4.30e4 | 3.54 | 1.16 | | | | | | | | | | | | | | | |
| 11: | 113.0398 | 1.26e4 | 1.03 | 0.34 | | | | | | | | | | | | | | | |
| 12: | 114.0453 | 1.76e4 | 1.45 | 0.48 | | | | | | | | | | | | | | | |
| 13: | 115.0547 | 3.66e4 | 3.01 | 0.99 | | | | | | | | | | | | | | | |
| 14: | 127.0531 | 1.20e4 | 0.99 | 0.32 | | | | | | | | | | | | | | | |
| 15: | 130.0289 | 3.18e5 | 26.20 | 8.59 | | | | | | | | | | | | | | | |
| 16: | 131.0329 | 2.67e4 | 2.20 | 0.72 | | | | | | | | | | | | | | | |
| 17: | 140.0507 | 3.83e4 | 3.15 | 1.03 | | | | | | | | | | | | | | | |
| 18: | 141.0572 | 2.50e4 | 2.05 | 0.67 | | | | | | | | | | | | | | | |
| 19: | 153.0577 | 1.14e4 | 0.94 | 0.31 | | | | | | | | | | | | | | | |
| 20: | 158.0193 | 2.41e4 | 1.99 | 0.65 | | | | | | | | | | | | | | | |
| 21: | 158.0612 | 1.15e4 | 0.94 | 0.31 | | | | | | | | | | | | | | | |
| 22: | 159.0201 | 1.50e4 | 1.24 | 0.41 | | | | | | | | | | | | | | | |
| 23: | 162.0561 | 2.32e4 | 1.91 | 0.63 | | | | | | | | | | | | | | | |
| 24: | 171.0267 | 1.09e5 | 8.96 | 2.94 | | | | | | | | | | | | | | | |
| 25: | 172.0311 | 1.50e4 | 1.23 | 0.40 | | | | | | | | | | | | | | | |
| 26: | 184.0226 | 2.05e4 | 1.69 | 0.55 | | | | | | | | | | | | | | | |
| 27: | 185.0299 | 2.37e5 | 19.48 | 6.39 | | | | | | | | | | | | | | | |
| 28: | 186.0338 | 5.85e4 | 4.82 | 1.58 | | | | | | | | | | | | | | | |
| 29: | 187.0265 | 3.27e4 | 2.69 | 0.88 | | | | | | | | | | | | | | | |
| 30: | 212.0174 | 4.11e4 | 3.38 | 1.11 | | | | | | | | | | | | | | | |
| 31: | 213.0248 | 2.88e5 | 23.70 | 7.77 | | | | | | | | | | | | | | | |
| 32: | 214.0318 | 1.22e6 | 100.00 | 32.81 | | | | | | | | | | | | | | | |
| 33: | 215.0364 | 2.07e5 | 17.04 | 5.59 | | | | | | | | | | | | | | | |
| 34: | 216.0328 | 7.44e4 | 6.12 | 2.01 | | | | | | | | | | | | | | | |
| 35: | 217.0356 | 1.04e4 | 0.86 | 0.28 | | | | | | | | | | | | | | | |
| 36: | 245.0515 | 4.75e4 | 3.91 | 1.28 | | | | | | | | | | | | | | | |