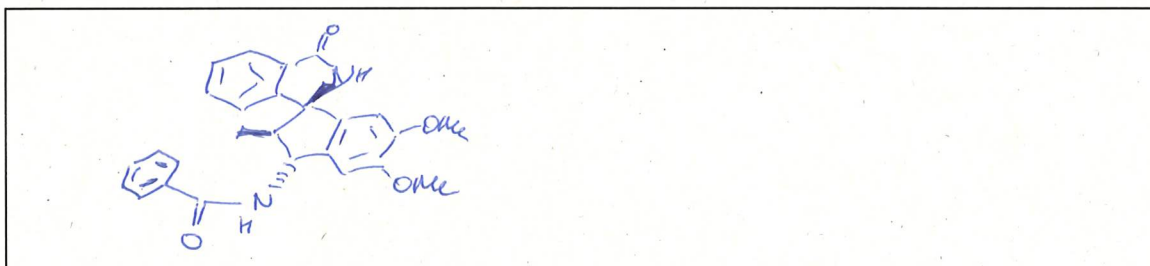


Auftrags- Protokoll – MS-TOF-Messung GCT Waters

Eingangsdatum: _____

Name / Auftraggeber: Miro Halaczkiwicz Arbeitskreis: ManolikakesTel.: 2527 E-mail.: halaczki@rhrk.uni-kl.deGC- HR-MS: ☐HR- MS-Feststoff: ☒Auswertung: ☒ Exakte Masse ($\leq 2\text{mDa}$, $\leq 10\text{ ppm}$) ☐ Fragmentierung zur StrukturaufklärungProbenbezeichnung: MHA-R112 Lösungsmittel: Aceton, DM, MeOHGewünschte Ionisierungs- Methode: EI^+ ☒ CI^- ☐ CI^+ ☐ (CI: Methan)

Mögliche Verbindungen (Strukturformel u. Molmasse)/ Bemerkungen:

Summenformel: $\text{C}_{26}\text{H}_{24}\text{N}_2\text{O}_4$ Exakte Masse: 428,1736**Zu internen Verwaltungszwecken:**Int. Auftragsnummer: 23-11-12Messdatum: 8.11.23 Operator: RSIonisations- Methode: : EI^+ ☒ CI^+ ☐ CI^- ☐Speicherort: Feststoff-Daten Kalib.- Datum: 8.11.23Bemerkungen: Reinpe 2, 70eV(M+)⁺Ausgangsdatum: 29.11.2023

Single Mass Analysis

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

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

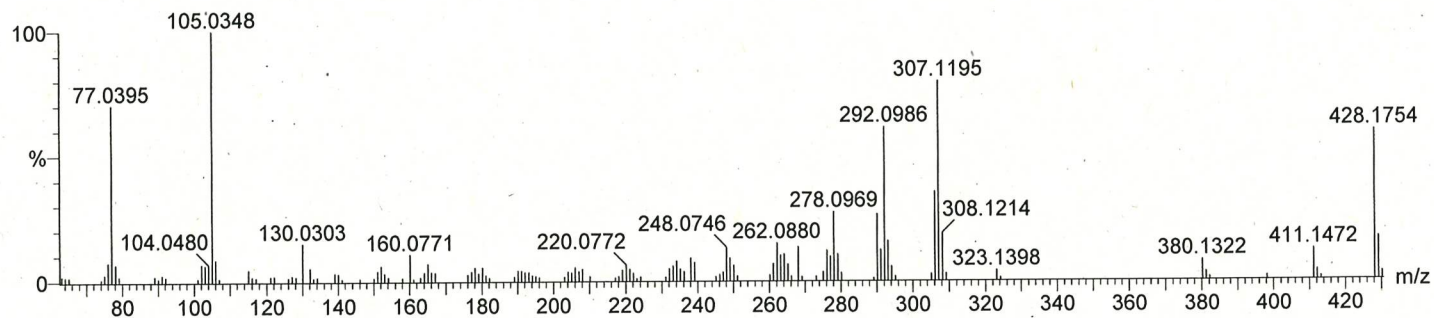
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-26 H: 0-28 N: 0-2 O: 0-5

MAN_MHA_R112<Rampe2_Miro Halaczkiwicz<<KalibHeptacos_650, 70EV<<M428<<IA_231112

231108_MAN_MHA_R112 168 (6.084) Cm (131:175-7:76)

TOF MS EI+
5.84e+004

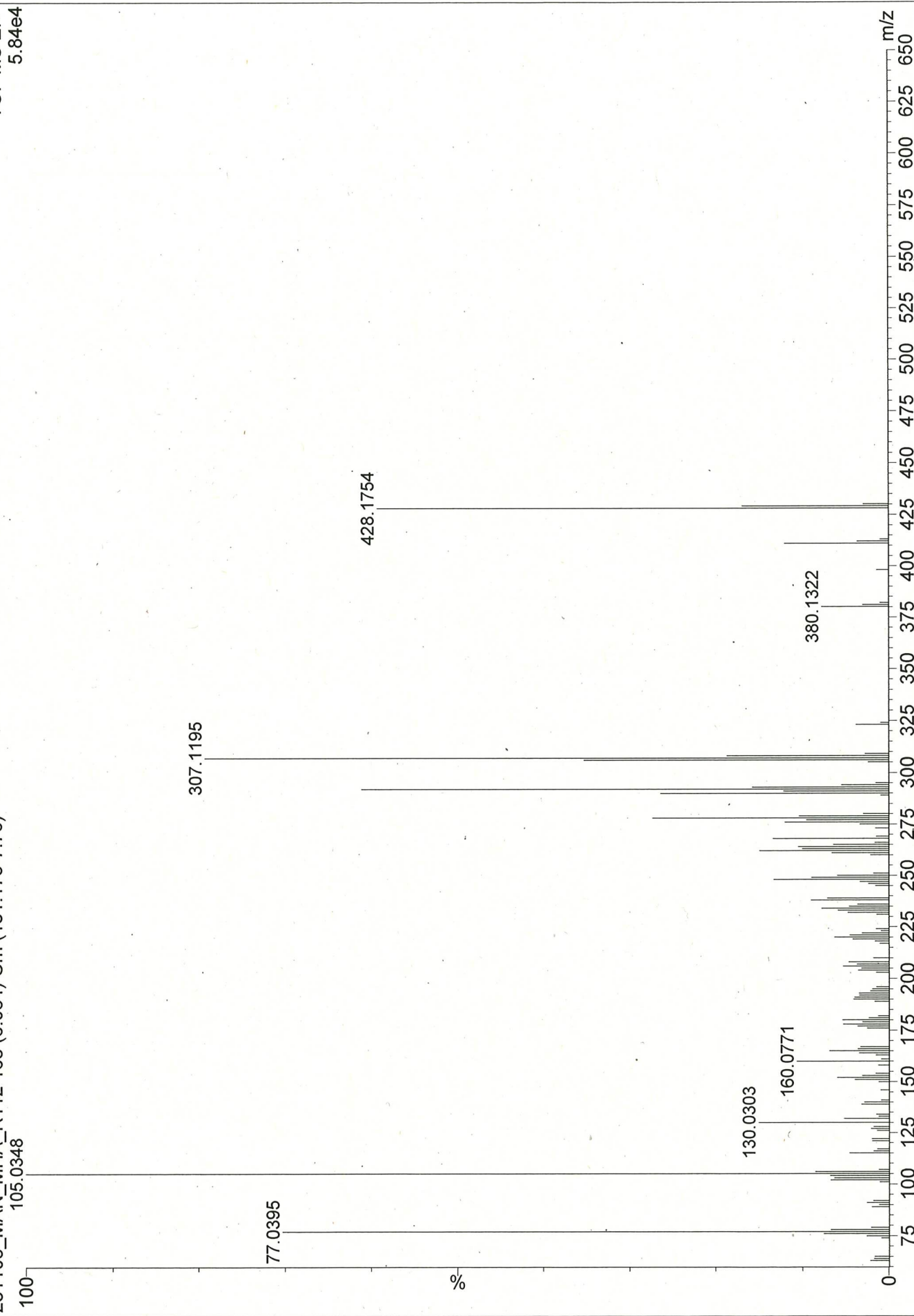
Minimum: -1.5
Maximum: 100.0 25.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
428.1754	428.1736	1.8	4.2	16.0	21.0	C26 H24 N2 O4

MAN_MHA_R112<Rampe2_Miro Halaczekiewicz<<KaibHeptacos_650, 70EV<<M428<<IA_231112

231108_MAN_MHA_R112 168 (6.084) Cm (131:175-7:76)

TOF MS EI+
5.84e4



1000

TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	
1:	63.0241	1.22e3	2.10	0.20	50:	176.0623	1.43e3	2.46	0.23	99:	264.1021	6.09e3	10.43	0.99						
2:	64.0305	9.50e2	1.63	0.15	51:	177.0641	2.08e3	3.57	0.34	100:	265.1091	3.70e3	6.34	0.60						
3:	65.0390	9.22e2	1.58	0.15	52:	178.0727	3.07e3	5.26	0.50	101:	266.1192	8.74e2	1.50	0.14						
4:	74.0155	4.81e2	0.82	0.08	53:	179.0743	1.75e3	2.99	0.28	102:	268.0995	7.76e3	13.29	1.26						
5:	75.0232	1.48e3	2.53	0.24	54:	180.0800	3.12e3	5.33	0.50	103:	269.1090	7.90e2	1.35	0.13						
6:	76.0312	4.38e3	7.50	0.71	55:	181.0698	1.31e3	2.25	0.21	104:	273.1060	8.41e2	1.44	0.14						
7:	77.0395	4.10e4	70.27	6.65	56:	182.0645	6.77e2	1.16	0.11	105:	275.0946	1.91e3	3.26	0.31						
8:	78.0442	3.90e3	6.67	0.63	57:	189.0672	9.14e2	1.56	0.15	106:	276.0823	6.97e3	11.93	1.13						
9:	79.0532	1.16e3	1.98	0.19	58:	190.0678	2.37e3	4.06	0.38	107:	277.0891	5.53e3	9.47	0.90						
10:	89.0382	1.12e3	1.91	0.18	59:	191.0752	2.29e3	3.92	0.37	108:	278.0969	1.59e4	27.25	2.58						
11:	90.0426	6.18e2	1.06	0.10	60:	192.0793	1.97e3	3.37	0.32	109:	279.0969	6.02e3	10.30	0.97						
12:	91.0514	1.45e3	2.49	0.24	61:	193.0753	1.98e3	3.39	0.32	110:	280.1016	1.67e3	2.86	0.27						
13:	92.0288	1.01e3	1.73	0.16	62:	194.0721	1.21e3	2.06	0.20	111:	289.1021	4.86e2	0.83	0.08						
14:	101.0387	5.77e2	0.99	0.09	63:	195.0694	1.07e3	1.84	0.17	112:	290.0908	1.54e4	26.30	2.49						
15:	102.0372	3.90e3	6.68	0.63	64:	196.0751	7.81e2	1.34	0.13	113:	291.0936	7.06e3	12.08	1.14						
16:	103.0457	3.66e3	6.27	0.59	65:	203.0733	8.02e2	1.37	0.13	114:	292.0986	3.56e4	61.02	5.77						
17:	104.0480	3.95e3	6.75	0.64	66:	204.0808	2.04e3	3.49	0.33	115:	293.1026	9.13e3	15.62	1.48						
18:	105.0348	5.84e4	100.00	9.46	67:	205.0803	1.82e3	3.11	0.29	116:	294.1049	3.16e3	5.41	0.51						
19:	106.0385	4.97e3	8.52	0.81	68:	206.0684	3.06e3	5.24	0.50	117:	295.1106	8.18e2	1.40	0.13						
20:	107.0459	6.37e2	1.09	0.10	69:	207.0636	2.12e3	3.62	0.34	118:	305.1110	1.34e3	2.30	0.22						
21:	115.0549	2.64e3	4.52	0.43	70:	208.0743	2.68e3	4.58	0.43	119:	306.1141	2.06e4	35.22	3.33						
22:	116.0536	9.96e2	1.70	0.16	71:	210.0938	9.97e2	1.71	0.16	120:	307.1195	4.63e4	79.19	7.49						
23:	117.0586	7.45e2	1.28	0.12	72:	217.0908	5.72e2	0.98	0.08	121:	308.1214	1.09e4	18.60	1.76						
24:	121.0511	1.08e3	1.85	0.18	73:	218.0932	8.75e2	1.50	0.14	122:	309.1232	1.54e3	2.64	0.25						
25:	122.0457	1.12e3	1.92	0.18	74:	219.0797	2.39e3	4.09	0.39	123:	323.1398	2.17e3	3.72	0.35						
26:	126.0460	7.57e2	1.30	0.12	75:	220.0772	3.63e3	6.22	0.59	124:	324.1417	4.87e2	0.83	0.08						
27:	127.0520	1.18e3	2.02	0.19	76:	221.0784	2.61e3	4.47	0.42	125:	380.1322	4.49e3	7.69	0.73						
28:	128.0549	9.92e2	1.70	0.16	77:	222.0730	1.77e3	3.03	0.29	126:	381.1354	1.71e3	2.92	0.28						
29:	130.0303	8.74e3	14.97	1.42	78:	223.0620	4.71e2	0.81	0.08	127:	382.1481	5.35e2	0.92	0.09						
30:	132.0461	3.02e3	5.17	0.49	79:	224.0711	8.23e2	1.41	0.13	128:	398.1643	7.58e2	1.30	0.12						
31:	133.0516	6.47e2	1.11	0.10	80:	231.0641	7.72e2	1.32	0.13	129:	411.1472	6.99e3	11.97	1.13						
32:	134.0604	8.24e2	1.41	0.13	81:	232.0764	2.72e3	4.66	0.44	130:	412.1509	2.08e3	3.56	0.34						
33:	139.0548	1.84e3	3.14	0.30	82:	233.0843	3.40e3	5.83	0.55	131:	413.1554	5.18e2	0.89	0.08						
34:	140.0528	1.63e3	2.79	0.26	83:	234.0813	4.51e3	7.72	0.73	132:	428.1754	3.46e4	59.18	5.60						
35:	141.0623	4.77e2	0.82	0.08	84:	235.0749	2.64e3	4.52	0.43	133:	429.1787	9.81e3	16.80	1.59						
36:	146.0585	5.14e2	0.88	0.08	85:	236.0752	2.06e3	3.53	0.33	134:	430.1813	1.65e3	2.83	0.27						
37:	150.0482	6.51e2	1.12	0.11	86:	238.0886	5.23e3	8.95	0.85											
38:	151.0545	2.27e3	3.89	0.37	87:	239.0971	4.11e3	7.04	0.67											
39:	152.0613	3.47e3	5.94	0.56	88:	245.0815	8.41e2	1.44	0.14											
40:	153.0629	1.77e3	3.03	0.29	89:	246.0857	1.32e3	2.26	0.21											
41:	154.0651	8.50e2	1.46	0.14	90:	247.0742	1.90e3	3.25	0.31											
42:	158.0598	6.82e2	1.17	0.11	91:	248.0746	7.71e3	13.21	1.25											
43:	160.0771	6.20e3	10.62	1.00	92:	249.0798	5.19e3	8.88	0.84											
44:	161.0829	4.73e2	0.81	0.08	93:	250.0851	3.44e3	5.89	0.56											
45:	163.0531	8.45e2	1.45	0.14	94:	251.0932	9.77e2	1.67	0.16											
46:	164.0603	1.97e3	3.38	0.32	95:	260.0754	1.17e3	2.01	0.19											
47:	165.0697	3.99e3	6.83	0.65	96:	261.0857	3.81e3	6.53	0.62											
48:	166.0688	2.07e3	3.54	0.33	97:	262.0880	8.65e3	14.81	1.40											
49:	167.0728	1.89e3	3.24	0.31	98:	263.0905	5.81e3	9.95	0.94											