

LC-MS Auswertung

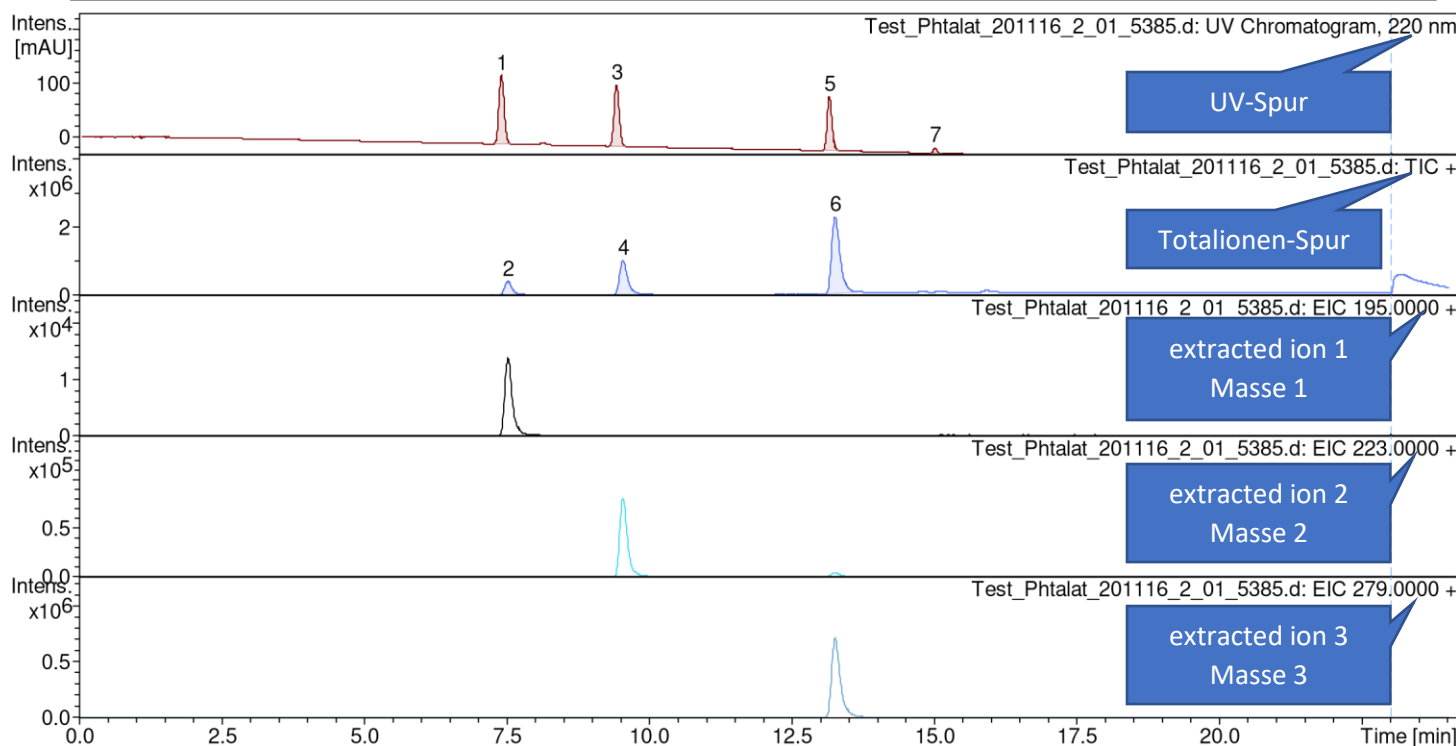


**BERGISCHE
UNIVERSITÄT
WUPPERTAL**

Analysis Name D:\Data\201116\Test_Phtalat_201116_2_01_5385.d
 Method ms_low_110_bis_1000_24min_pos_Standard.m Operator MASSE AK Kirsch
 Comment ESI: Gradient 90% Wasser/ 10% ACN WL 220nm Time 24 min 168

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	110 m/z	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste
Sample Name	Test_Phtalat_201116		Instrument / Ser#	micrOTOF	213750.00



#	RT [min]	Area	Area Frac. %	S/N	Chromatogram	Int. %	Compound Label
1	7.4	820.483	37.5048	2646.1	UV Chromatogram, 220 nm	0.00	Cmpd 1, 7.4 min 2 7.5
		4085047.500	10.5902	330.9	TIC +	17.70	Cmpd 2, 7.5 min
3	9.4	724.929	33.1369	2373.3	UV Chromatogram, 220 nm	0.00	
		10935217.000	28.3489	841.6	TIC +	44.50	Cmpd 4, 9.5 min

Massen können in der ESI auftreten als:

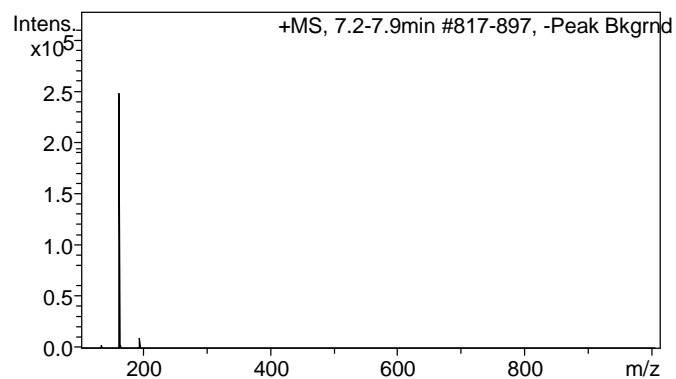
- M - H⁺ (ESI-negativ)
- M + H⁺ (ESI-positiv)
- M + NH₄⁺ (ESI-positiv)
- M + Na⁺ (ESI-positiv)



5 13.2 593.564 27.1321 2097.2 UV Chromatogram, 220 nm 0.00 Cmpd 5, 13.2 min
 6 13.3 23553474.000 61.0609 1868.6 TIC + 100.00 Cmpd 6, 13.3 min 7 15.0 48.701 2.2262 221.1 UV
 Chromatogram, 220 nm Cmpd 7, 15.0 min

Cmpd 1, 7.4 min

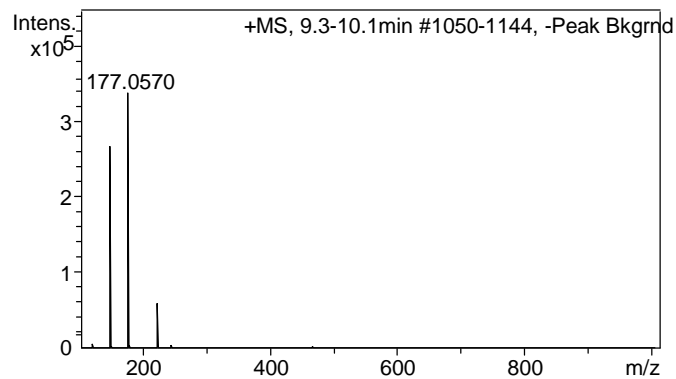
Cmpd 2, 7.5 min



#	m/z	Res.	S/N	I	I%	FWHM
1	133.0274	3513	25.0	690	0.3	0.0379
2	135.0438	3340	104.0	2872	1.2	0.0404
3	163.0397	3409	8697.2	247562	100.0	0.0478
4	163.2322	1253	16.8	477	0.2	0.1303
5	163.3134	2005	15.3	436	0.2	0.0814
6	164.0426	3471	833.6	23710	9.6	0.0473
7	165.0449	3477	87.4	2486	1.0	0.0475
8	195.0667	3606	444.4	10232	4.1	0.0541
9	196.0702	3713	50.6	1140	0.5	0.0528
10	500.3824	3846	56.2	558	0.2	0.1301

Cmpd 3, 9.4 min

Cmpd 4, 9.5 min

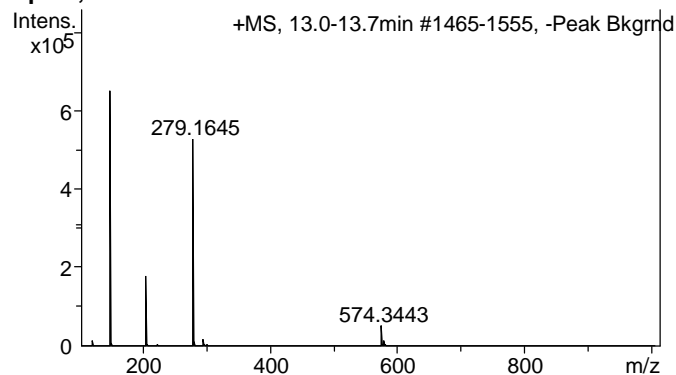


#	m/z	Res.	S/N	I	I%	FWHM
1	121.0330	3149	99.7	5966	1.8	0.0384
2	149.0248	3352	4425.8	266914	79.0	0.0445
3	150.0277	3508	381.5	23021	6.8	0.0428
4	151.0292	3598	42.5	2539	0.8	0.0420
5	177.0570	3385	5892.8	337749	100.0	0.0523
6	178.0598	3595	642.2	36824	10.9	0.0495
7	179.0613	3546	67.1	3824	1.1	0.0505
8	223.0994	3551	1217.2	59551	17.6	0.0628
9	224.1029	3672	165.1	7981	2.4	0.0610
10	245.0812	3763	78.6	3453	1.0	0.0651



Cmpd 5, 13.2 min

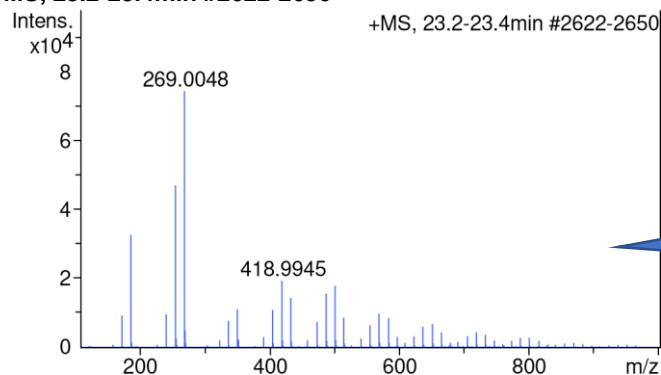
Cmpd 6, 13.3 min



#	m/z	Res.	S/N	I	I%	FWHM
1	149.0258	3330	10969.2	651098	100.0	0.0447
2	150.0285	3569	947.7	56355	8.7	0.0420
3	205.0898	3503	3106.8	177806	27.3	0.0586
4	206.0928	3535	396.5	22730	3.5	0.0583
5	279.1645	3510	8785.8	526829	80.9	0.0795
6	280.1676	3632	1514.9	90770	13.9	0.0771
7	296.1896	3844	336.1	17853	2.7	0.0771
8	574.3443	3801	1391.5	52070	8.0	0.1511
9	575.3457	3892	494.1	18484	2.8	0.1478
10	579.2987	3878	376.8	14260	2.2	0.1494

Cmpd 7, 15.0 min

+MS, 23.2-23.4min #2622-2650



Tunemix

wird nach 22min zugeführt
siehe Totalionen-Spur
(dient der internen Kalibrierung)

#	m/z	Res.	S/N	I	I%	FWHM
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1	186.9993	3625	117910.6	32527	43.8	0.0516
2	254.9884	3735	169934.8	46879	63.2	0.0683
3	269.0048	3700	268978.9	74201	100.0	0.0727
4	351.0069	3766	39722.4	10958	14.8	0.0932
5	404.9787	3812	39623.9	10931	14.7	0.1062
6	418.9945	3678	70209.0	19368	26.1	0.1139
7	433.0097	3828	51891.8	14315	19.3	0.1131
8	486.9825	3752	56789.8	15666	21.1	0.1298
9	500.9972	3833	64937.0	17914	24.1	0.1307
10	568.9882	3821	35480.3	9788	13.2	0.1489