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## Increasing the mass accuracy of high-resolution LC-MS data using background ions - a case study on the LTQ-Orbitrap

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# PROTEOMICS

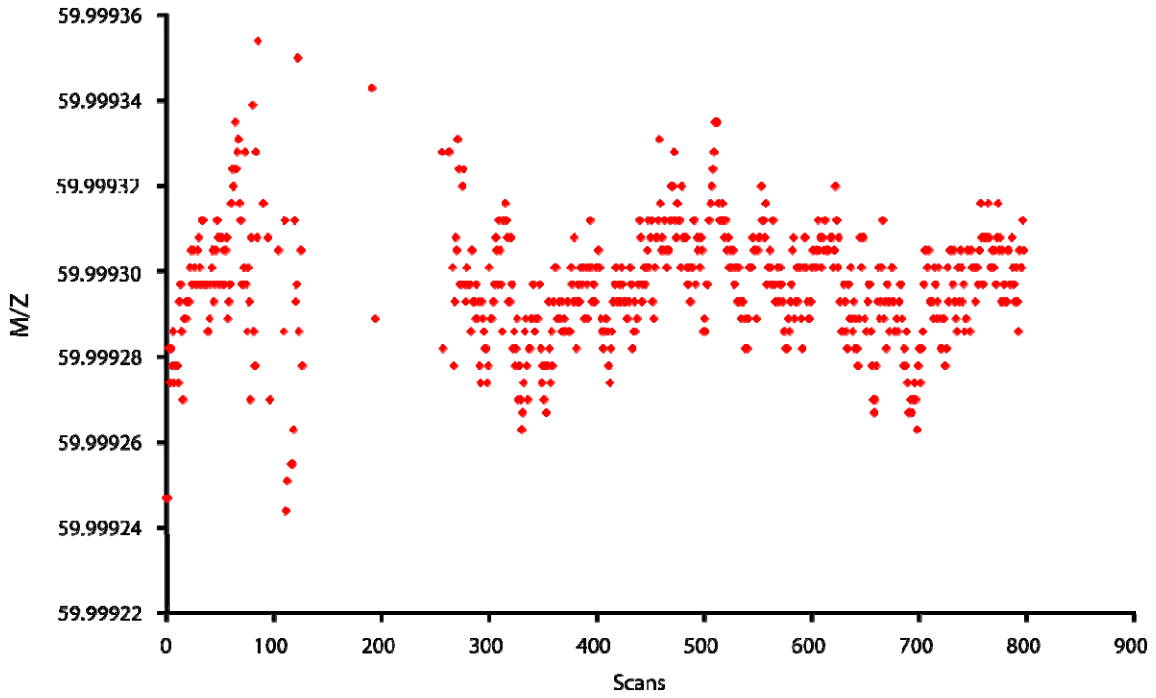
## Supporting Information for Proteomics

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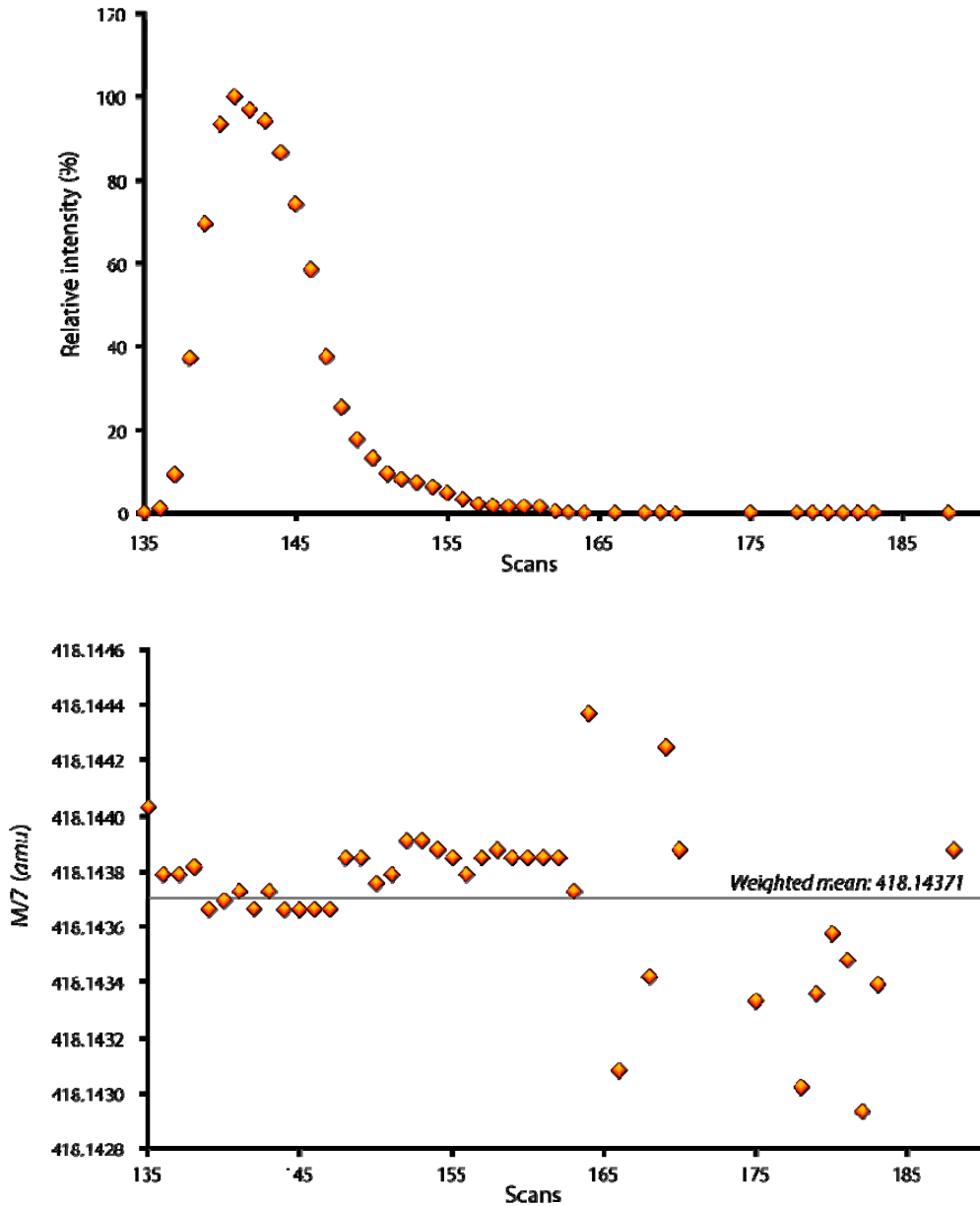
**Increasing the mass accuracy of high-resolution  
LC-MS data using background ions – a case study  
on the LTQ-Orbitrap**

## Supporting Information Figure 1



**Figure 1** | Detected background ion. The graph shows all peaks (mass-over-charge value against scan number) assigning to a single background ion from an Orbitrap LTQ measurement. A window size of 2 ppm and a threshold of 18% were used for the collection of the peaks. The discrete distance between groups of mass-values can be attributed to the discrete Fourier Transform that is used for deconvoluting the signal into mass values.

## Supporting Information Figure 2



**Figure 2** | Use of weighted mean for mass estimation. For the mass estimation a weighted mean is calculated, which exploits the fact that the accuracy of the mass measurement decreases for less intense peaks. The top graph shows a typical mass chromatogram from the Orbitrap LTQ data, which has a retention time of 141 (most intense peak). The bottom graph shows the associated mass values. It can clearly be seen that the highly intense peaks have a mass close to the mean and show little variation. The less intense peaks in the tail of the elution profile scatter far more around the mean.

## Supporting Information Table 1

**Table 1** | Commonly occurring background ions for positive-mode electrospray ionization, including various adduct forms of solvents and plasticizers.

	Name	Mass	Formula
41	acetonitrile	41.0265491	(M+H)+; M='C2H3N'
58	acetonitrile	58.0530982	(M+NH4)+; M='C2H3N'
63	acetonitrile	63.00849335	(M+Na)+; M='C2H3N'
103	acetonitrile	102.948323	(M+Cu)+; M='C2H3N'
105	acetonitrile	104.9465156	(M+Cu)+ (isotope); M='C2H3N'
104	acetonitrile	104.0350425	(2M+Na)+; M='C2H3N'
144	acetonitrile	143.9748721	(2M+Cu)+; M='C2H3N'
147	acetonitrile	146.9808919	(2M+Cu)+ (isotope); M='C2H3N'
145	acetonitrile	145.0615916	(3M+Na)+; M='C2H3N'
78	dimethyl sulfoxide	78.0139355	(M+H)+; M='C2H6OS'
84	d6-dimethyl sulfoxide	84.0516	(M+H)+; M='C2H6OS'
100	dimethyl sulfoxide	99.99587975	(M+Na)+; M='C2H6OS'
156	dimethyl sulfoxide	156.027871	(2M+H)+; M='C2H6OS'
168	d6-dimethyl sulfoxide	168.1032	(2M+H)+; M='C2H6OS'
178	dimethyl sulfoxide	178.0098153	(2M+Na)+; M='C2H6OS'
256	dimethyl sulfoxide	256.0237508	(3M+Na)+; M='C2H6OS'
101	triethylamine	101.1204495	(M+H)+; M='C6H15N'
121	tris(hydroxymethyl)aminomethane	121.0738932	(M+H)+; M='C4H11NO3'
122	dimethylaminopyridine	122.0843983	(M+H)+; M='C7H10N2'
129	diisopropylethylamine	129.1517496	(M+H)+; M='C8H19N'
143	tripropylamine	143.1673997	(M+H)+; M='C9H21N'
152	1,8-diazabicyclo[5.4.0]undec-7-ene	152.1313485	(M+H)+; M='C9H16N2'
213	N-butyl benzenesulfonamide	213.0823494	(M+H)+; M='C10H15NO2S'
235	N-butyl benzenesulfonamide	235.0642937	(M+Na)+; M='C10H15NO2S'
224	dicyclohexyl urea	224.1888634	(M+H)+; M='C13H24N2O'
448	dicyclohexyl urea	448.3777268	(2M+H)+; M='C13H24N2O'
241	tetrabutylammonium	241.2769501	M+; M='C16H36N'
337	erucamide	337.334465	(M+H)+; M='C22H43NO'
359	erucamide	359.3164093	(M+Na)+; M='C22H43NO'
390	diisooctyl phthalate	390.2770097	(M+H)+; M='C24H38O4'
412	diisooctyl phthalate	412.258954	(M+Na)+; M='C24H38O4'
428	diisooctyl phthalate	428.2328914	(M+K)+; M='C24H38O4'
453	diisooctyl phthalate	453.2855031	(M+NaC2H3N)+; M='C24H38O4'
798	diisooctyl phthalate	797.5805685	(2M+NH4)+; M='C24H38O4'
803	diisooctyl phthalate	802.5359637	(2M+Na)+; M='C24H38O4'
819	diisooctyl phthalate	818.5099011	(2M+K)+; M='C24H38O4'
390	dioctyl phthalate	390.2770097	(M+H)+; M=''
412	dioctyl phthalate	412.258954	(M+Na)+; M=''
238	triethylamine (TEA)	238.2175767	((M.HCl)2-Cl)+; M='NC6H15'
240	triethylamine (TEA)	240.2146266	((M.HCl)2-Cl)+; M='NC6H15'
242	trityl cation	242.1095504	M+ (triphenylmethane-H); M='C19H16'
149	phenyldiethylamine	149.1204495	(M+H)+; M='C10H15N'
158	sodium trifluoroacetate	157.9567524	(M+Na)+; M='C2F3Na2O2'
294	sodium trifluoroacetate	293.9315605	(M+Na)+ + M; M='C2F3Na2O2'
430	sodium trifluoroacetate	429.9063687	(M+Na)+ + 2M; M='C2F3Na2O2'
566	sodium trifluoroacetate	565.8811768	(M+Na)+ + 3M; M='C2F3Na2O2'
185	tributylamine	185.2143499	(M+H)+; M='C12H27N'
266	tributyl phosphate	266.1646959	(M+H)+; M='C12H27O4P'
278	dibutyl phthalate	278.1518092	(M+H)+; M='C16H22O4'
300	dibutyl phthalate	300.1337534	(M+Na)+; M='C16H22O4'
316	dibutyl phthalate	316.1076908	(M+K)+; M='C16H22O4'
76	polypropylene glycol	76.0524295	(M+H)+; M='H[OCH(CH3)CH2]nOH'
134	polypropylene glycol	134.0942943	(M+H)+; M='H[OCH(CH3)CH2]nOH'
192	polypropylene glycol	192.1361591	(M+H)+; M='H[OCH(CH3)CH2]nOH'
250	polypropylene glycol	250.1780239	(M+H)+; M='H[OCH(CH3)CH2]nOH'
308	polypropylene glycol	308.2198888	(M+H)+; M='H[OCH(CH3)CH2]nOH'
366	polypropylene glycol	366.2617536	(M+H)+; M='H[OCH(CH3)CH2]nOH'
424	polypropylene glycol	424.3036184	(M+H)+; M='H[OCH(CH3)CH2]nOH'

482	polypropylene glycol	482.3454832	(M+H)+; M='H[OCH(CH3)CH2]nOH'
540	polypropylene glycol	540.387348	(M+H)+; M='H[OCH(CH3)CH2]nOH'
598	polypropylene glycol	598.4292128	(M+H)+; M='H[OCH(CH3)CH2]nOH'
656	polypropylene glycol	656.4710777	(M+H)+; M='H[OCH(CH3)CH2]nOH'
715	polypropylene glycol	714.5129425	(M+H)+; M='H[OCH(CH3)CH2]nOH'
773	polypropylene glycol	772.5548073	(M+H)+; M='H[OCH(CH3)CH2]nOH'
831	polypropylene glycol	830.5966721	(M+H)+; M='H[OCH(CH3)CH2]nOH'
889	polypropylene glycol	888.6385369	(M+H)+; M='H[OCH(CH3)CH2]nOH'
947	polypropylene glycol	946.6804017	(M+H)+; M='H[OCH(CH3)CH2]nOH'
1005	polypropylene glycol	1004.722267	(M+H)+; M='H[OCH(CH3)CH2]nOH'
1063	polypropylene glycol	1062.764131	(M+H)+; M='H[OCH(CH3)CH2]nOH'
1121	polypropylene glycol	1120.805996	(M+H)+; M='H[OCH(CH3)CH2]nOH'
1179	polypropylene glycol	1178.847861	(M+H)+; M='H[OCH(CH3)CH2]nOH'
1237	polypropylene glycol	1236.889726	(M+H)+; M='H[OCH(CH3)CH2]nOH'
1295	polypropylene glycol	1294.931591	(M+H)+; M='H[OCH(CH3)CH2]nOH'
1353	polypropylene glycol	1352.973455	(M+H)+; M='H[OCH(CH3)CH2]nOH'
1411	polypropylene glycol	1411.01532	(M+H)+; M='H[OCH(CH3)CH2]nOH'
1469	polypropylene glycol	1469.057185	(M+H)+; M='H[OCH(CH3)CH2]nOH'
1527	polypropylene glycol	1527.09905	(M+H)+; M='H[OCH(CH3)CH2]nOH'
1585	polypropylene glycol	1585.140915	(M+H)+; M='H[OCH(CH3)CH2]nOH'
1643	polypropylene glycol	1643.18278	(M+H)+; M='H[OCH(CH3)CH2]nOH'
1701	polypropylene glycol	1701.224644	(M+H)+; M='H[OCH(CH3)CH2]nOH'
62	polyethylene glycol	62.03677944	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
106	polyethylene glycol	106.0629942	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
150	polyethylene glycol	150.0892089	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
194	polyethylene glycol	194.1154237	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
238	polyethylene glycol	238.1416384	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
282	polyethylene glycol	282.1678532	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
326	polyethylene glycol	326.1940679	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
370	polyethylene glycol	370.2202827	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
414	polyethylene glycol	414.2464974	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
458	polyethylene glycol	458.2727122	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
502	polyethylene glycol	502.2989269	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
546	polyethylene glycol	546.3251417	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
590	polyethylene glycol	590.3513564	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
634	polyethylene glycol	634.3775712	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
678	polyethylene glycol	678.4037859	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
722	polyethylene glycol	722.4300007	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
766	polyethylene glycol	766.4562154	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
810	polyethylene glycol	810.4824302	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
855	polyethylene glycol	854.5086449	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
899	polyethylene glycol	898.5348597	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
943	polyethylene glycol	942.5610745	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
987	polyethylene glycol	986.5872892	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1031	polyethylene glycol	1030.613504	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1075	polyethylene glycol	1074.639719	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1119	polyethylene glycol	1118.665933	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1163	polyethylene glycol	1162.692148	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1207	polyethylene glycol	1206.718363	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1251	polyethylene glycol	1250.744578	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1295	polyethylene glycol	1294.770792	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1339	polyethylene glycol	1338.797007	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1383	polyethylene glycol	1382.823222	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1427	polyethylene glycol	1426.849437	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1471	polyethylene glycol	1470.875651	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1515	polyethylene glycol	1514.901866	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1559	polyethylene glycol	1558.928081	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1603	polyethylene glycol	1602.954296	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1647	polyethylene glycol	1646.98051	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1691	polyethylene glycol	1691.006725	(M+H)+; M='C(2n)H(4n+2)O(n+1)'
1735	polyethylene glycol	1735.03294	(M+H)+; M='C(2n)H(4n+2)O(n+1)'

## Supporting Information Table 2

**Table 2 |** Commonly occurring background ions for negative-mode electrospray ionization.

	<b>Name</b>	<b>Mass</b>	<b>Formula</b>
44	ethoxylate	44.02621475	(M)-; M='C2OH4'
58	propoxylate	58.04186481	(M)-; M='C3OH6'
74	dimethylsiloxane	74.01879135	(M)-; M='SiOC2H6'
36	chloride	35.97667774	M-; M='Cl'
38	chloride37	37.97372763	M-; M='Cl'
80	bromide	79.92616263	M-; M='Br'
82	bromide81	81.92411603	M-; M='Br'
46	formic acid	46.00547931	(M-H)-; M='CH2O2'
60	ethanoic acid	60.02112937	(M-H)-; M='C2H4O2'
97	phosphoric acid	96.96907006	(M-H)-; M='H3O4P'
98	sulfuric acid	97.96737924	(M-H)-; M='H2O4S'
98	phosphate	97.9768951	M-; M='H3O4P'
213	N-butyl benzenesulfonamide	213.0823494	(M-H)-; M='C10H15NO2S'
114	trifluoroacetic acid	113.9928639	(M-H)-; M='C2HF3O2'
228	trifluoroacetic acid	227.9857278	(M-H)- + M
342	trifluoroacetic acid	341.9785917	(M-H)- + 2M
456	trifluoroacetic acid	455.9714556	(M-H)- + 3M
228	trifluoroacetic acid dimer	227.9857278	(2M-H)-; M='C2HF3O2'
342	trifluoroacetic acid dimer	341.9785917	(2M-H)- + M
456	trifluoroacetic acid dimer	455.9714556	(2M-H)- + 2M
570	trifluoroacetic acid dimer	569.9643195	(2M-H)- + 3M
114	sodium formate	113.9929029	(2M-Na)-; M='CHNaO2'
182	sodium formate	181.9803264	(2M-Na)- + M; M='CHNaO2'
250	sodium formate	249.96775	(2M-Na)- + 2M; M='CHNaO2'
318	sodium formate	317.9551735	(2M-Na)- + 3M; M='CHNaO2'
250	sodium trifluoroacetate	249.967672	(2M-Na)-; M='C2F3NaO2'
386	sodium trifluoroacetate	385.9424802	(2M-Na)- + M; M='C2F3NaO2'
522	sodium trifluoroacetate	521.9172883	(2M-Na)- + 2M; M='C2F3NaO2'
658	sodium trifluoroacetate	657.8920964	(2M-Na)- + 3M; M='C2F3NaO2'