Common Background Contamination Ions in Mass Spectrometry

Common background contamination ions encountered in mass spectrometers are polyethylene glycol, polypropylene glycol, phthalates, organic solvent clusters, solvent modifiers, fatty acids, metal ions, tritons, tweens and siloxanes. Metal ions form adducts with varying numbers of substrates to give characteristic ESI$^+$ ions. In this poster, the accurate mass of elements, organic solvents and all potential contaminant ions observed in mass spectrometry are listed in the tables below to help troubleshoot potential contamination in LC-MS systems.

Table 1. Accurate Mass of Organic Solvents

Solvents	Formula	Accurate Mass
Acetic acid	$C_2H_4O_2$	60.0211
Acetone	C_3H_6O	58.0419
Acetonitrile	C_2H_3N	41.0265
Benzene	C_6H_6	78.0470
Butanone (2-)	C_4H_8O	72.0575
Carbon disulfide	CS_2	75.9441
Chloroform	$CHCl_3$	117.9144
Dichloromethane	CH_2Cl_2	83.9534
Diethyl ether	$C_4H_{10}O$	74.0732
Diisopropyl ether	$C_6H_{14}O$	102.1045
Dimethylformamide	C_3H_7NO	73.0528
Dimethyl sulfoxide	C_2H_6OS	78.0139
Ethanol	C_2H_6O	46.0419
Ethyl acetate	$C_4H_8O_2$	88.0524
Formic acid	CH_2O_2	46.0055
Glycerol	$C_3H_8O_3$	92.0473
Hexane	C_6H_{14}	86.1096
Isopropanol	C_3H_8O	60.0575
Methanol	CH_4O	32.0262
Propanol	C_3H_8O	60.0575
Pyridine	C_5H_5N	79.0422
Tetrachlorocarbon	CCl_4	151.8754
Tetrachloroethylene	C_2Cl_4	163.8754
Tetrahydrofuran	C_4H_8O	72.0575
Toluene	C_7H_8	92.0626
Trichloroethylene	C_2HCl_3	129.9144
Trifluoroacetic acid	$C_2F_3O_2H$	113.9929
Triethylamine	$C_6H_{15}N$	101.1204
Tripropylamine	$C_9H_{21}N$	143.1674
Xylene	C_8H_{10}	106.0783
Water	H_2O	18.0106

Table 2. Accurate Mass of Proton, Electron and Selected Elements

Element	Abbreviation	Atomic Masses
Electron	e-	0.000549
Proton	H^+	1.007276
Carbon-12	C-12	12.000000
Carbon-13	C-13	13.003355
Hydrogen	H	1.007825
Deuterium	D	2.014101
Oxygen	O	15.994915
Oxygen-18	O-18	17.999160
Nitrogen-14	N-14	14.003074
Nitrogen-15	N-15	15.000109
Sulfur-32	S-32	31.972071
Sulfur-34	S-34	33.967867
Phosphorus	P	30.973762
Silicon	Si	27.976927
Sodium	Na	22.989769
Potassium	K	38.963706
Chlorine-35	Cl-35	34.968853
Chlorine-37	Cl-37	36.965903
Bromine-79	Br-79	78.918337
Bromine-81	Br-81	80.916291
Iodine	I	126.904473
Fluorine	F	18.998403
Iron-54	Fe-54	53.939611
Iron-56	Fe-56	55.934938
Lithium-6	Li-6	6.015123
Lithium-7	Li-7	7.016005
Boron-10	B-10	10.012937
Boron-11	B-11	11.009305
Copper-63	Cu-63	62.929601
Copper-65	Cu-65	64.927794
Silver-107	Ag-107	106.905094
Silver-109	Ag-109	108.904756
Tin-120	Sn-120	119.902199
Cesium	Cs-133	132.905450

Table 3. Common Adduct Ions in ESI Positive Mode

Solvents	Accurate Mass
$(M+H)^+$	M+1.007276
$(M+NH_4)^+$	M+18.03383
$M+Na)^+$	M+22.98977
$(M+K)^+$	M+38.96371
$(M+CH_3OH+H)^+$	M+33.03349
$(M+ACN+H)^+$	M+42.03383
$(M+ACN+Na)^+$	M+64.01632
$(M+DMSO+H)^+$	M+79.02118
$(M+2ACN+H)^+$	M+83.06037

Table 4. Common Observed and Predicted Background Ions in ESI Positive Mode

Compounds or Species	Formula	$[M+H]^+$	$[M+NH_4]^+$	$[M+Na]^+$	$[M+K]^+$
Methanol clusters	CH_3OH	33.0335	50.0600	55.0154	70.9894
	$(CH_3OH)_2$	65.0597	82.0863	87.0417	103.0156
	$(CH_3OH)_3$	97.0859	114.1125	119.0679	135.0418
Acetonitrile clusters	CH_3CN	42.0338	59.0604	64.0158	79.9897
	$(CH_3CN)_2$	83.0604	100.0869	105.0423	121.0163
	$(CH_3CN)_3$	124.0869	141.1135	146.0689	162.0428
MeOH + H_2O clusters	$(CH_3OH)(H_2O)$	51.0446	68.0712	73.0265	89.0005
	$(CH_3OH)_2(H_2O)_2$	101.0808	118.1074	123.0628	139.0367
	$(CH_3OH)_3(H_2O)_2$	133.1071	150.1336	155.0890	171.0629
Acetonitrile + Methanol clusters	$(CH_3CN)(CH_3OH)$	74.0600	91.0866	96.0420	112.0159
	$(CH_3CN)_2(CH_3OH)_2$	147.1128	164.1394	169.0947	185.0687
Dimethylformamide	C_3H_7NO	74.0600	91.0866	96.0420	112.0159
DMSO	C_2H_6OS	79.0212	96.0478	101.0032	116.9771
	$(C_2H_6OS)_2$	157.0351	174.0617	179.0171	194.9910
	$(C_2H_6OS)_3$	235.0491	252.0756	257.0310	273.0050
Acetonitrile/Formic acid	$(CH_3CN)(HCOOH)$	88.0393	105.0659	110.0212	125.9952
Acetonitrile/Acetic acid	$(CH_3CN)(CH_3COOH)$	102.0550	119.0815	124.0369	140.0108
Acetonitrile/Dimethylformamide	$(CH_3CN)(C_3H_7NO)$	115.0866	132.1131	137.0685	153.0425
DMSO+MeCN clusters	$[C_2H_6OS+CH_3CN]$	120.0478	137.0743	142.0297	158.0036
Sodium formate	CH_2O_2Na			90.9766	
Sodium acetate	$C_2H_3O_2Na$			104.9923	
(N-Methyl-2-pyrrolidone)	$C_5H_{10}NO$	100.0757	117.1022	122.0576	138.0316
Triethylamine (TEA)	$C_6H_{15}N$	102.1277	119.1543	124.1097	140.0836
TRIS	$C_4H_{11}NO_3$	122.0812	139.1077	144.0631	160.0371
Dimethylaminopyridine	$C_7H_{10}N_2$	123.0917	140.1182	145.0736	161.0476
Diisopropylethylamine	$C_8H_{19}N$	130.1590	147.1856	152.1410	168.1149
Tripropylamine	$C_9H_{21}N$	144.1747	161.2012	166.1566	182.1306
Phthalic anhydride	$C_8H_4O_3$	149.0233	166.0499	171.0053	186.9792
Phenyldiethylamine	$C_{10}H_{15}N$	150.1277	167.1543	172.1097	188.0836
1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU)	$C_9H_{16}N_2$	153.1386	170.1652	175.1206	191.0945
NaTFA	$C_2F_3O_2Na$			158.9640	
Diethylene glycol monobutyl ether	$C_8H_{18}O_3$	163.1329	180.1594	185.1148	201.0888
	$(C_8H_{18}O_3)_2$	325.2585	342.2850	347.2404	363.2143
α-Cyano-4-hydroxycinnamic acid (4-HCCA)-H_2O	$C_8H_5NO_3$	172.0393	189.0659	194.0212	209.9952
α-Cyano-4-hydroxycinnamic acid (4-HCCA)	$C_{10}H_7NO_3$	190.0499	207.0764	212.0318	228.0058
	$(C_{10}H_7NO_3)_2$	379.0925	396.1190	401.0744	417.0483
	$(C_{10}H_7NO_3)_3$	568.1351	585.1616	590.1170	606.0909
Butylated hydroxyanisole	$C_{11}H_{16}O_2$	181.1223	198.1489	203.1043	219.0782
Diphenyl ketone	$C_{13}H_{10}O$	183.0804	200.1070	205.0624	221.0363
Glycol ether	$C_8H_{18}O_3$	185.1148	202.1414	207.0968	223.0707
Tributylamine	$C_{12}H_{27}N$	186.2216	203.2482	208.2036	224.1775
n-Butyl benzenesulfonamide	$C_{10}H_{15}NO_2S$	214.0896	231.1162	236.0716	252.0455
Butylated hydroxytoluene	$C_{15}H_{24}O$	221.1900	238.2165	243.1719	259.1459
N,N'-Dicyclohexylurea	$C_{13}H_{24}N_2O$	225.1961	242.2227	247.1781	263.1520
	$(C_{13}H_{24}N_2O)_2$	449.3850	466.4116	471.3669	487.3409
TEA.HCl[35]	$C_6H_{15}N.HCl$	239.2249	256.2514	261.2068	277.1807
TEA.HCl[37]	$C_6H_{15}N.HCl$	241.2219	258.2485	263.2038	279.1778
Tetrabutylammonium	$C_{16}H_{36}N$	242.2842			
Tributylphosphate	$C_{12}H_{27}O_4P$	267.1720	284.1985	289.1539	305.1279
Monomethoxytrityl cation	$C_{20}H_{17}O$	273.1274			
Triphenylphosphine oxide	$C_{18}H_{15}OP$	279.0933	296.1199	301.0753	317.0492
Oleamide	$C_{18}H_{35}NO$	282.2791	299.3057	304.2611	320.2350
Stearamide	$C_{18}H_{37}NO$	284.2948	301.3213	306.2767	322.2507
n,n-bis(2-hydroxyethyl) dodecanamide	$C_{16}H_{33}NO_3$	288.2533	305.2799	310.2353	326.2092
Oleamide	$C_{18}H_{35}NO$	304.2611	321.2876	326.2430	342.2170
Dibutyl sebacate	$C_{18}H_{34}O_4$	315.2530	332.2795	337.2349	353.2089
Diethylene glycol monobutyl ether	$C_8H_{18}O_3$	325.2585	342.2850	347.2404	363.2143
Triphenyl phosphate	$C_{18}H_{15}O_4P$	327.0781	344.1046	349.0600	365.0340
Tributyl tin formate	$C_{13}H_{28}O_2Sn$	337.1184	354.1450	359.1003	375.0743
Erucamide	$C_{22}H_{43}NO$	338.3417	355.3683	360.3237	376.2976
Palmitamidopropyl-trimonium chloride	$C_{22}H_{47}N_2OCl$	355.3683	372.3948	377.3502	393.3242
Behentrimonium chloride (BTAC-228)	$C_{25}H_{54}NCl$	368.4251			
Bis(2-ethylhexyl) adipate	$C_{22}H_{42}O_4$	371.3156	388.3421	393.2975	409.2715
Dioctyl adipate	$C_{22}H_{42}O_4$	371.3156	388.3421	393.2975	409.2715
Dipalmityldimethylammonium chloride	$C_{34}H_{72}NCl$	494.5659			
Didodecyl 3,3′-thiodipropionate	$C_{30}H_{58}O_4S$	515.4129	532.4394	537.3948	553.3687
Stearyl-palmityldimethylammonium chloride	$C_{36}H_{76}NCl$	522.5972			
Didodecyl 3,3′-thiodipropionate oxidized to sulfoxide	$C_{30}H_{58}O_5S$	531.4078	548.4343	553.3897	569.3637
Irganox	$C_{35}H_{62}O_3$	531.4772	548.5037	553.4591	569.4331
Acetic acid-Fe-O- complex	$[C_2H_4O_2)_6$-6H+3Fe+O]	537.8790	554.9056	559.8610	575.8349
Didodecyl 3,3′-thiodipropionate oxidized to sulfone	$C_{30}H_{58}O_6S$	547.4027	564.4292	569.3846	585.3586
Distearyldimethylammonium chloride	$C_{38}H_{80}NCl$	550.6285			
Acetic acid-Fe-O- complex	$[(C_2H_4O2)_6$-6H+H_2O+3Fe+O]	555.8896			
Acetic acid-Fe-O- complex	$[(C_2H_4O2)_7$-6H+3Fe+O]	597.9001			
3-[(3-Cholamidopropyl)dimethylammonio] -1-propanesulfonate	$C_{32}H_{58}N_2O_7S$	615.4038	632.4303	637.3857	653.3596
Propionic acid Fe-O complex	$[(C_3H_6O_2)_6$-6H+3Fe+O]	621.9729			
Nylon	$C_{24}H_{44}N_4O_4$	453.3435	470.3701	475.3255	491.2994
	$C_{36}H_{66}N_6O_6$	679.5117	696.5382	701.4936	717.4675
	$C_{48}H_{88}N_8O_8$	905.6798	922.7063	927.6617	943.6357

Table 5. Common Background Ions in ESI Negative Mode

Compounds and Species	Ions	Mass of ions
Fragment from acetonitrile	CN^-	26.0036
Formic acid	$HCOO^-$	44.9982
Acetic acid	$CH_3SO_3^-$	59.0139
Phosphoric acid, and oligonucleotides or phosphopeptides	PO_3^-	78.9591
Sulfuric acid and other sulfated materials	SO_3^-	79.9574
Methanesulfuric acid	$CH_3SO_3^-$	94.9808
Sulfuric acid	HSO_4^-	96.9601
Phosphoric acid, and oligonucleotides or phosphopeptides	$H_2PO_4^-$	96.9696
Trifluoroacetic acid, TFA	CF_3COO^-	112.9856
Formic acid dimer sodiated anion	$[(HCOOH)_2$+Na-2H$]^-$	112.9856
Iodine anion (Iodide)	I^-	126.9050
Pentafluoropropionic acid	$CF_3CF_2COO^-$	162.9824
n-Butyl benzenesulfonamide	$C_{10}H_{14}NO_2S^-$	212.0751
Trifluoroacetic acid dimer	$CF_3COOHCF_3COO^-$	226.9785
Trifluoroacetic acid dimer sodiated anion	$[(CF_3COOH)_2$+Na-2H$]^-$	248.9604

Table 6. Potential Contaminant Ions from Polyethylene Glycol, $H(OCH_2CH_2)_nOH$ and Polypropylene Glycol, $H(OCH_2CH_2CH_2)_nOH$ in ESI Positive Mode

	Polyethylene Glycol			Polypropylene Glycol		
Repeating Units	$[M+H]^+$	$[M+Na]^+$	$[M+K]^+$	$[M+H]^+$	$[M+Na]^+$	$[M+K]^+$
1	63.0441	85.026	100.9999	77.0597	99.0417	115.0156
2	107.0703	129.0522	145.0261	135.1016	157.0835	173.0575
3	151.0965	173.0784	189.0523	193.1434	215.1254	231.0993
4	195.1227	217.1046	233.0785	251.1853	273.1672	289.1412
5	239.1490	261.1309	277.1048	309.2272	331.2091	347.1830
6	283.1752	305.1571	321.1310	367.2690	389.2510	405.2249
7	327.2014	349.1833	365.1572	425.3109	447.2928	463.2668
8	371.2276	393.2095	409.1834	483.3528	505.3347	521.3086
9	415.2538	437.2357	453.2096	541.3946	563.3766	579.3505
10	459.2800	481.2619	497.2358	599.4365	621.4184	637.3924
11	503.3062	525.2881	541.2620	657.4784	679.4603	695.4342
12	547.3325	569.3144	585.2883	715.5202	737.5022	753.4761
13	591.3587	613.3406	629.3145	773.5621	795.5440	811.5180
14	635.3849	657.3668	673.3407	831.6039	853.5859	869.5598
15	679.4111	701.3930	717.3669	889.6458	911.6278	927.6017
16	723.4373	745.4192	761.3931	947.6877	969.6696	985.6436
17	767.4635	789.4454	805.4193	1005.7295	1027.7115	1043.6854
18	811.4897	833.4716	849.4455	1063.7714	1085.7534	1101.7273
19	855.5160	877.4979	893.4718	1121.8133	1143.7952	1159.7692
20	899.5422	921.5241	937.4980	1179.8551	1201.8371	1217.8110

Table 7. Potential Contaminant Ions from Phthalates in ESI Positive Mode, Some Phthalates Form Dimer Ions.

Compounds and Species	Formula	$[M+H]^+$	$[M+NH_4]^+$	$[M+Na]^+$	$[M+K]^+$
Dimethyl phthalate (DMP)	$C_{10}H_{10}O_4$	195.0652	212.0917	217.0471	233.0211
Diethyl phthalate (DEP)	$C_{12}H_{14}O_4$	223.0965	240.1230	245.0784	261.0524
Diallyl phthalate (DAP)	$C_{14}H_{14}O_4$	247.0965	264.1230	269.0784	285.0524
Di-n-propyl phthalate (DPP)	$C_{14}H_{18}O_4$	251.1278	268.1543	273.1097	289.0837
Di-n-butyl phthalate (DBP)	$C_{16}H_{22}O_4$	279.1591	296.1856	301.1410	317.1150
Diisobutyl phthalate (DIBP)	$C_{16}H_{22}O_4$	279.1591	296.1856	301.1410	317.1150
Butyl cyclohexyl phthalate (BCP)	$C_{18}H_{24}O_4$	305.1747	322.2012	327.1566	343.1306
Di-n-pentyl phthalate (DNPP)	$C_{18}H_{26}O_4$	307.1904	324.2169	329.1723	345.1463
Dicyclohexyl phthalate (DCP)	$C_{20}H_{26}O_4$	331.1904	348.2169	353.1723	369.1463
Butyl benzyl phthalate (BBP)	$C_{19}H_{20}O_4$	313.1434	330.1699	335.1253	351.0993
Di-n-hexyl phthalate (DNHP)	$C_{20}H_{30}O_4$	335.2217	352.2482	357.2036	373.1776
Diisohexyl phthalate (DIHxP)	$C_{20}H_{30}O_4$	335.2217	352.2482	357.2036	373.1776
Diisoheptyl phthalate (DIHpP)	$C_{22}H_{34}O_4$	363.2530	380.2795	385.2349	401.2089
Butyl decyl phthalate (BDP)	$C_{22}H_{34}O_4$	363.2530	380.2795	385.2349	401.2089
Di(2-ethylhexyl) phthalate (DEHP)	$C_{24}H_{38}O_4$	391.2843	408.3108	413.2662	429.2402
Di(n-octyl) phthalate (DNOP)	$C_{24}H_{38}O_4$	391.2843	408.3108	413.2662	429.2402
Diisooctyl phthalate (DIOP)	$C_{24}H_{38}O_4$	391.2843	408.3108	413.2662	429.2402
n-Octyl n-decyl phthalate (ODP)	$C_{26}H_{42}O_4$	419.3156	436.3421	441.2975	457.2715
Diisononyl phthalate (DINP)	$C_{26}H_{42}O_4$	419.3156	436.3421	441.2975	457.2715
Diisodecyl phthalate (DIDP)	$C_{28}H_{46}O_4$	447.3469	464.3734	469.3288	485.3028
Diundecyl phthalate (DUP)	$C_{30}H_{50}O_4$	475.3782	492.4047	497.3601	513.3341
Diisoundecyl phthalate(DIUP)	$C_{30}H_{50}O_4$	475.3782	492.4047	497.3601	513.3341
Ditridecyl phthalate (DTDP)	$C_{34}H_{58}O_4$	531.4408	548.4673	553.4227	569.3967
Diisotridecyl phthalate (DITP)	$C_{34}H_{58}O_4$	531.4408	548.4673	553.4227	569.3967

Common Background Contamination Ions in Mass Spectrometry

Table 8. Potential Contaminant Ions from X-100, Triton X-114, Triton X-405, Triton X-45 $C_{14}H_{22}O(C_2H_4O)_n$ and Their Reduced Forms $C_{14}H_{28}O(C_2H_4O)_n$ in ESI Positive Mode

	Triton			Reduced Form of Triton		
Repeating Units	$[M+H]^+$	$[M+Na]^+$	$[M+K]^+$	$[M+H]^+$	$[M+Na]^+$	$[M+K]^+$
1	251.2006	273.1825	289.1565	257.2476	279.2295	295.2034
2	295.2268	317.2087	333.1827	301.2738	323.2557	339.2296
3	339.2530	361.2349	377.2089	345.3000	367.2819	383.2558
4	383.2792	405.2611	421.2351	389.3262	411.3081	427.2820
5	427.3054	449.2873	465.2613	433.3524	455.3343	471.3082
6	471.3316	493.3135	509.2875	477.3786	499.3605	515.3344
7	515.3578	537.3397	553.3137	521.4048	543.3867	559.3606
8	559.3840	581.3659	597.3399	565.4310	587.4129	603.3868
9	603.4102	625.3921	641.3661	609.4572	631.4391	647.4130
10	647.4364	669.4183	685.3923	653.4834	675.4653	691.4392
11	691.4626	713.4445	729.4185	697.5096	719.4915	735.4654
12	735.4888	757.4707	773.4447	741.5358	763.5177	779.4916
13	779.5150	801.4969	817.4709	785.5620	807.5439	823.5178
14	823.5412	845.5231	861.4971	829.5882	851.5701	867.5440
15	867.5674	889.5493	905.5233	873.6144	895.5963	911.5702
16	911.5936	933.5755	949.5495	917.6406	939.6225	955.5964
17	955.6198	977.6017	993.5757	961.6668	983.6487	999.6226
18	999.6460	1021.6279	1037.6019	1005.6930	1027.6749	1043.6488
19	1043.6722	1065.6541	1081.6281	1049.7192	1071.7011	1087.6750
20	1087.6984	1109.6803	1125.6543	1093.7454	1115.7273	1131.7012

Table 9. Potential Contaminant Ions from Triton X-101, $C_{15}H_{24}O(C_2H_4O)_n$ and Triton X-101R, $C_{15}H_{30}O(C_2H_4O)_n$ in ESI Positive Mode

	Triton			Reduced Form of Triton		
Repeating Units	$[M+H]^+$	$[M+Na]^+$	$[M+K]^+$	$[M+H]^+$	$[M+Na]^+$	$[M+K]^+$
1	265.2163	287.1982	303.1721	271.2632	293.2451	309.2191
2	309.2425	331.2244	347.1983	315.2894	337.2713	353.2453
3	353.2687	375.2506	391.2245	359.3156	381.2975	397.2715
4	397.2949	419.2768	435.2507	403.3418	425.3237	441.2977
5	441.3211	463.3030	479.2769	447.3680	469.3499	485.3239
6	485.3473	507.3292	523.3031	491.3942	513.3761	529.3501
7	529.3735	551.3554	567.3293	535.4204	557.4023	573.3763
8	573.3997	595.3816	611.3555	579.4466	601.4285	617.4025
9	617.4259	639.4078	655.3817	623.4728	645.4547	661.4287
10	661.4521	683.4340	699.4079	667.4990	689.4809	705.4549
11	705.4783	727.4602	743.4341	711.5252	733.5071	749.4811
12	749.5045	771.4864	787.4603	755.5514	777.5333	793.5073
13	793.5307	815.5126	831.4865	799.5776	821.5595	837.5335
14	837.5569	859.5388	875.5127	843.6038	865.5857	881.5597
15	881.5831	903.5650	919.5389	887.6300	909.6119	925.5859
16	925.6093	947.5912	963.5651	931.6562	953.6381	969.6121
17	969.6355	991.6174	1007.5913	975.6824	997.6643	1013.6383
18	1013.6617	1035.6436	1051.6175	1019.7086	1041.6905	1057.6645
19	1057.6879	1079.6698	1095.6437	1063.7348	1085.7167	1101.6907
20	1101.7141	1123.6960	1139.6699	1107.7610	1129.7429	1145.7169

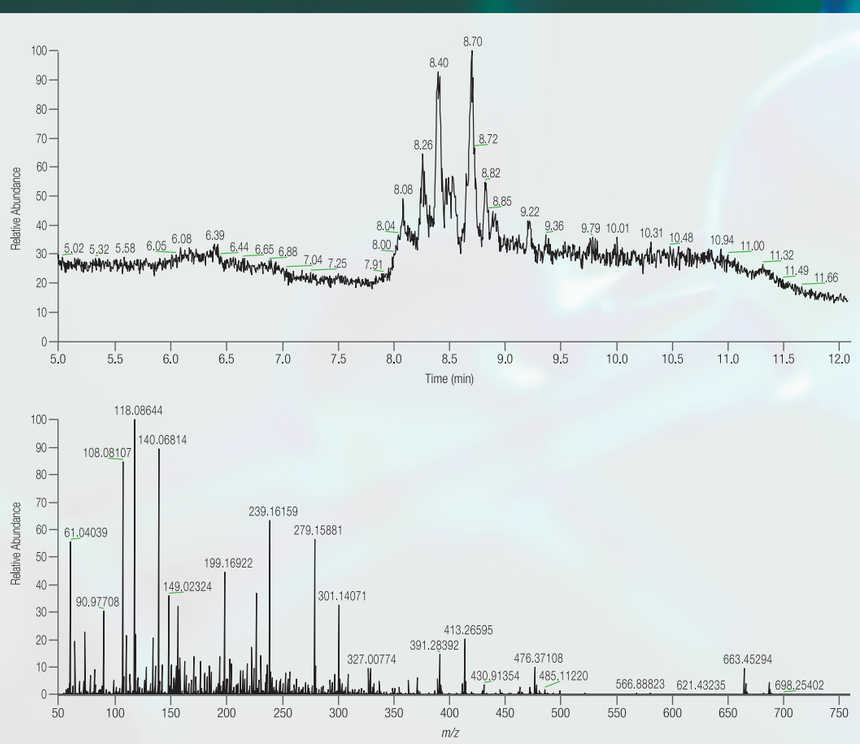

Figure 1. Typical Chromatogram and Spectrum Profile of Blank Sample With Water and Methanol Gradient Acquired by Q Exactive Focus Orbitrap MS in ESI Positive Mode

Table 10. Potential Contaminant Ions from Polysiloxane, $(C_2H_6SiO)_n$

Repeating Units	$[M+H-CH_4]^+$	$[M+H]^+$	$[M+NH_4]^+$
1	58.9947	75.0260	92.0526
2	133.0135	149.0448	166.0714
3	207.0323	223.0636	240.0902
4	281.0511	297.0824	314.1090
5	355.0699	371.1012	388.1278
6	429.0887	445.1200	462.1466
7	503.1075	519.1388	536.1654
8	577.1263	593.1576	610.1842
9	651.1451	667.1764	684.2030
10	725.1639	741.1952	758.2217
11	799.1827	815.2140	832.2405
12	873.2015	889.2328	906.2593
13	947.2203	963.2516	980.2781
14	1021.2391	1037.2704	1054.2969
15	1095.2579	1111.2892	1128.3157
16	1169.2766	1185.3079	1202.3345
17	1243.2954	1259.3267	1276.3533
18	1317.3142	1333.3455	1350.3721
19	1391.3330	1407.3643	1424.3909
20	1465.3518	1481.3831	1498.4097

Table 11. Potential Sodium Ions of Tween 20 $[C_{18}H_{34}O_6][C_2H_4O]_n$ Tween 40 $[C_{22}H_{42}O_6][C_2H_4O]_n$ Tween 60 $[C_{24}H_{46}O_6][C_2H_4O]_n$ and Tween 80 $[C_{24}H_{44}O_6][C_2H_4O]_n$ in ESI Positive Mode.

	Tween 20	Tween 40	Tween 60	Tween 80
Repeating Units	$[M+Na]^+$	$[M+Na]^+$	$[M+Na]^+$	$[M+Na]^+$
10	809.4869	865.5495	893.5808	891.5652
11	853.5131	909.5757	937.6070	935.5914
12	897.5393	953.6019	981.6332	979.6176
13	941.5656	997.6282	1025.6595	1023.6438
14	985.5918	1041.6544	1069.6857	1067.6700
15	1029.6180	1085.6806	1113.7119	1111.6962
16	1073.6442	1129.7068	1157.7381	1155.7225
17	1117.6704	1173.7330	1201.7643	1199.7487
18	1161.6966	1217.7592	1245.7905	1243.7749
19	1205.7228	1261.7854	1289.8167	1287.8011
20	1249.7491	1305.8117	1333.8430	1331.8273
21	1293.7753	1349.8379	1377.8692	1375.8535
22	1337.8015	1393.8641	1421.8954	1419.8797
23	1381.8277	1437.8903	1465.9216	1463.9060
24	1425.8539	1481.9165	1509.9478	1507.9322
25	1469.8801	1525.9427	1553.9740	1551.9584
26	1513.9064	1569.9690	1598.0003	1595.9846
27	1557.9326	1613.9952	1642.0265	1640.0108
28	1601.9588	1658.0214	1686.0527	1684.0370
29	1645.9850	1702.0476	1730.0789	1728.0632
30	1690.0112	1746.0738	1774.1051	1772.0895
31	1734.0374	1790.1000	1818.1313	1816.1157
32	1778.0636	1834.1262	1862.1575	1860.1419

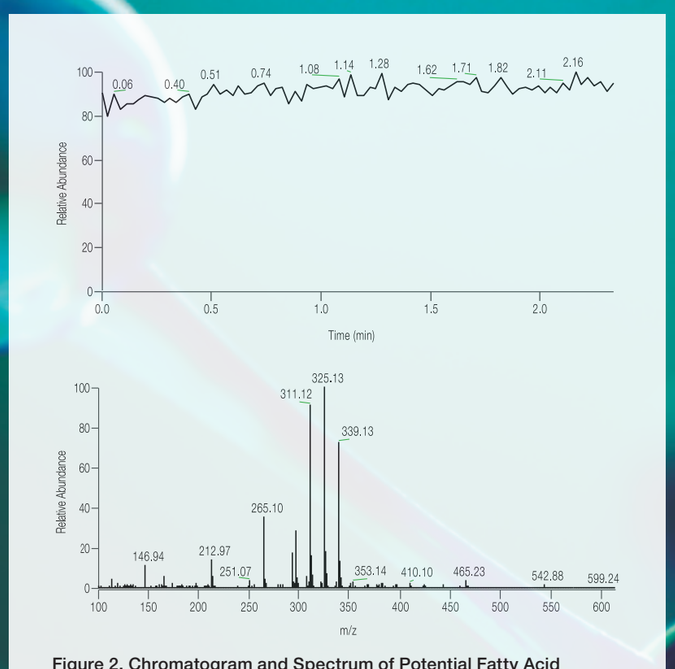

Figure 2. Chromatogram and Spectrum of Potential Fatty Acid Contamination in Blank Methanol Acquired in ESI Negative Mode Using Triple Quadruple Mass Spectrometry

Table 12. Potential Contaminant Ions from Fatty Acids in ESI Negative Mode

Compounds and Species	Structural Formula	Lipid Numbers	$(M-H)^-$
Decanoic acid	$C_{10}H_{20}O_2$	C10:0	171.1391
Undecanoic acid	$C_{11}H_{22}O_2$	C11:0	185.1547
Dodecanoic acid	$C_{12}H_{24}O_2$	C12:0	199.1704
Tridecanoic acid	$C_{13}H_{26}O_2$	C13:0	213.1860
Tetradecanoic acid	$C_{14}H_{28}O_2$	C14:0	227.2017
Pentadecanoic acid	$C_{15}H_{30}O_2$	C15:0	241.2173
Tetradecanoic acid	$C_{16}H_{32}O_2$	C16:0	255.2330
Heptadecanoic acid	$C_{17}H_{34}O_2$	C17:0	269.2486
Octadecanoic acid	$C_{18}H_{36}O_2$	C18:0	283.2643
Nonadecanoic acid	$C_{19}H_{38}O_2$	C19:0	297.2799
Eicosanoic acid	$C_{20}H_{40}O_2$	C20:0	311.2956
Heneicosanoic acid	$C_{21}H_{42}O_2$	C21:0	325.3112
Docosanoic acid	$C_{22}H_{44}O_2$	C22:0	339.3269
Tricosanoic acid	$C_{23}H_{46}O_2$	C23:0	353.3425
Tetracosanoic acid	$C_{24}H_{48}O_2$	C24:0	367.3582
Caproleic acid	$C_{10}H_{18}O_2$	C10:1	169.1234
Lauroleic acid	$C_{12}H_{22}O_2$	C12:1	197.1547
Myristoleic acid	$C_{14}H_{26}O_2$	C14:1	225.1860
Palmitoleic acid	$C_{16}H_{30}O_2$	C16:1	253.2173
Oleic acid	$C_{18}H_{34}O_2$	C18:1	281.2486
Gadoleic acid	$C_{20}H_{38}O_2$	C20:1	309.2799
Erucic acid	$C_{22}H_{42}O_2$	C22:1	337.3112
Nervonic acid	$C_{24}H_{46}O_2$	C24:1	365.3425
Linoleic acid (LA)	$C_{18}H_{32}O_2$	C18:2	279.2330
Linolenic acid (ALA)	$C_{18}H_{30}O_2$	C18:3	277.2173
Stearidonic acid	$C_{18}H_{28}O_2$	C18:4	275.2017
Mead acid	$C_{20}H_{34}O_2$	C20:3	305.2486
Arachidonic acid	$C_{20}H_{32}O_2$	C20:4	303.2330
Eicosapentaenoic acid (EPA)	$C_{20}H_{30}O_2$	C20:5	301.2173
Docosapentaenoic acid (DPA)	$C_{22}H_{34}O_2$	C22:5	329.2486
Docosahexaenoic acid (DHA)	$C_{22}H_{32}O_2$	C22:6	327.2330

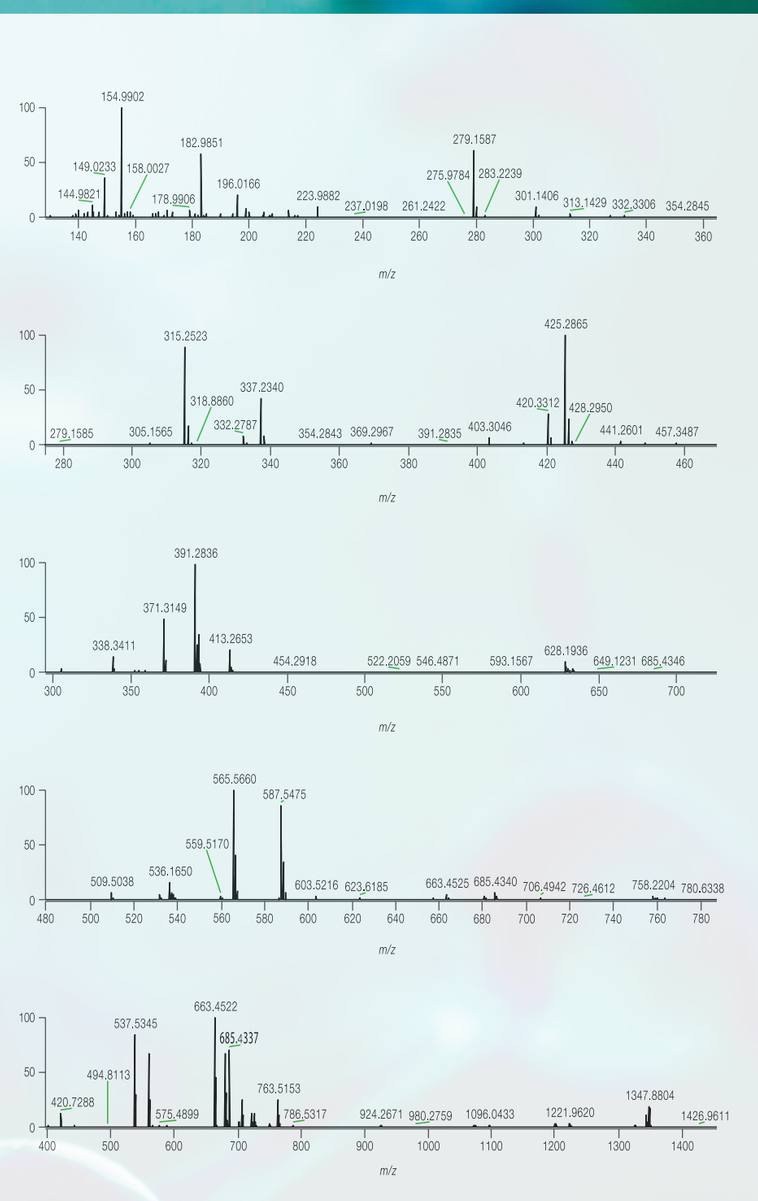

Figure 3. Potential Contaminant Ions in Organic Solvents Detected by Q Exactive Plus Orbitrap Mass Spectrometer in ESI Positive Mode

References

1. Keller, B. O.; Sui, J; Young A. B.; Whittal, R. M. Interferences and contaminants encountered in modern mass spectrometry. Analytica Chimica Acta 627 (2008) 71-81
2. Tong, H.; Bell, D.; Tabei, K.; Siegel, M.M. Automated Data Massaging, Interpretation, and E-Mailing Modules for High Throughput Open Access Mass Spectrometry. J. Am. Soc. Mass Spectrom. 10 (1999) 1174
3. http://www.newobjective.com/downloads/technotes/PV-3.pdf
4. https://www.fishersci.com/us/en/products.html
5. Mahn, B. Thermo Fisher Scientific technical support
6. Guo, X.; Bruins, A. P.; Covey, T. R. Characterization of typical chemical background interferences in atmospheric pressure ionization liquid chromatography-mass spectrometry. Rapid Commun. Mass Spectrom. 20 (2006) 3145–3150
7. http://www.proteomicsresource.washington.edu/protocols05/esi_background_ions_repeat_units.php
8. http://www.waters.com/webassets/cms/support/docs/bkgrnd_ion_mstr_list.pdf
9. John C.; Tran J. C.; Doucette A. A. Cyclic Polyamide Oligomers Extracted from Nylon 66 Membrane Filter Disks as a Source of Contamination in Liquid Chromatography/Mass Spectrometry. J Am Soc. Mass Spectrom. 17 (2006), 652– 656

BN040317CH30