

Table A Commonly Observed Background Ions in ESI

Compound Name	Compound Formula	Exact Mass (u)	
		if H <sup>+</sup> ionisation	if Na <sup>+</sup> Cationisation
MeOH + H <sub>2</sub> O Clusters	(CH <sub>3</sub> OH) <sub>n</sub> (H <sub>2</sub> O) <sub>m</sub>	101.080835	123.062778
		133.107050	155.088993
		183.143830	205.125772
MeCN + MeOH Clusters	(CH <sub>3</sub> CN) <sub>n</sub> (CH <sub>3</sub> OH) <sub>m</sub>	74.060040	96.041983
		147.112804	169.094747
MeCN + Acetic Acid	C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub>	102.054955	124.036898
Sodium Acetate	C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> Na	—	104.992291
Phthalic <sup>b</sup> anhydride	C <sub>8</sub> H <sub>4</sub> O <sub>3</sub>	149.023320	171.005263
Butylated Hydroxyanisole	C <sub>11</sub> H <sub>16</sub> O <sub>2</sub>	181.122306	203.104249
Butylated Hydroxytoluene	C <sub>15</sub> H <sub>24</sub> O	221.189992	243.171935
Dibutyl Phthalate	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	279.159086	301.141028
Triton <sup>a</sup>	see Table B		317.208714
			361.234929
Dioctyl Phthalate <sup>b</sup>	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>	391.284286	413.266229
3 Iron + 6 Acetic Acid + Oxygen	C <sub>12</sub> H <sub>18</sub> O <sub>12</sub> Fe <sub>3</sub> O	537.878952 (precharged)	

<sup>a</sup>distribution of peaks separated by 44.026215

<sup>b</sup>Ubiquitous plasticiser

NOTE:

Mass of H atom: 1.007825 u  
 Mass of Proton: 1.007276 u  
 Mass of Electron: 0.000549 u

Mass Na atom: 22.989768 u  
 Mass Na ion: 22.989219 u

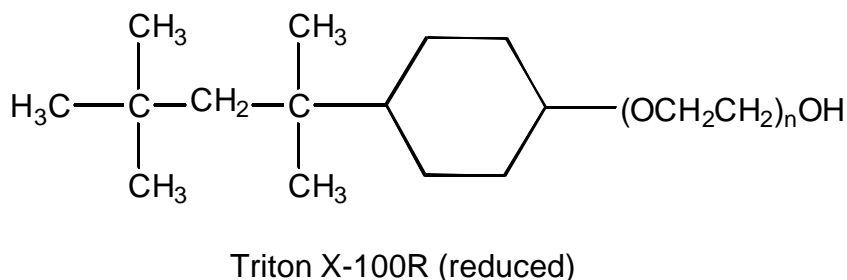
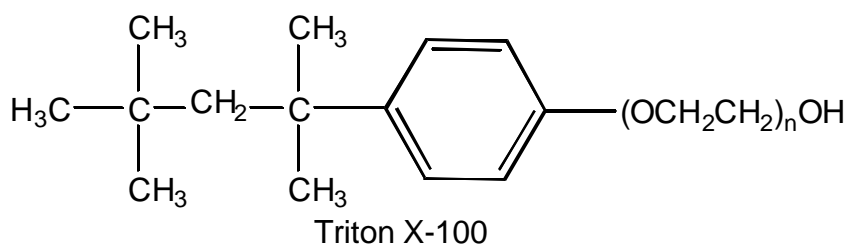


Table B Peaks that may be Observed in ESI Spectra if Triton X-100, X-114, X-405, or X-45 are Present

# of repeat units (n)	Exact Mass (u)		
	H <sup>+</sup>	Na <sup>+</sup>	Reduced Form Na <sup>+</sup>
1	251.2006	273.1825	279.2294
2	295.2268	317.2087	323.2557
3	339.2530	361.2349	367.2819
4	383.2792	405.2611	411.3081
5	427.3054	449.2874	455.3343
6	471.3316	493.3136	499.3605
7	515.3578	537.3398	543.3867
8	559.3841	581.3660	587.4130
9	603.4103	625.3922	631.4392
10	647.4365	669.4184	675.4654
11	691.4627	713.4446	719.4916
12	735.4889	757.4709	763.5178
13	779.5151	801.4971	807.5440
14	823.5414	845.5233	851.5702
15	867.5676	889.5495	895.5965
16	911.5938	933.5757	939.6227
17	955.6200	977.6019	983.6489
18	999.6462	1021.6282	1027.6751
19	1043.6724	1065.6544	1071.7013
20	1087.6986	1109.6806	1115.7275
— etc. —			

Note: X-100 has on average 9 to 10 repeat units (also reduced form)  
 X-114 has on average 7 to 8 repeat units (also reduced form)  
 X-405 has on average 40 repeat units (also reduced form)  
 X-45 has on average 2 repeat units (only reduced form)  
 Na<sup>+</sup> cationised form is observed most intensely, H<sup>+</sup> weakly (if at all)  
 K<sup>+</sup> cationised form also possible  
 a by-product of Triton production is polyethylene glycol

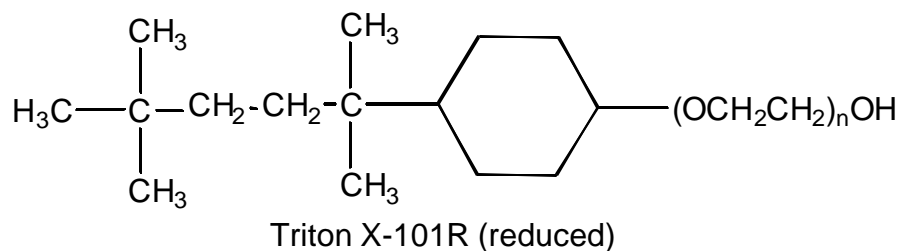
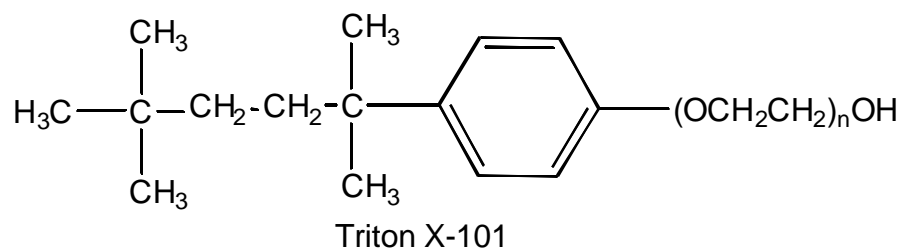


Table C Peaks that may be Observed in ESI Spectra if Triton X-101 or X-101 Reduced are Present

# of repeat units (n)	Exact Mass (u)		
	H <sup>+</sup>	Na <sup>+</sup>	Reduced Form Na <sup>+</sup>
1	265.2162	287.1981	293.2451
2	309.2424	331.2244	337.2713
3	353.2686	375.2506	381.2975
4	397.2949	419.2768	425.3237
5	441.3211	463.3030	469.3500
6	485.3473	507.3292	513.3762
7	529.3735	551.3554	557.4024
8	573.3997	595.3817	601.4286
9	617.4259	639.4079	645.4548
10	661.4521	683.4341	689.4810
11	705.4784	727.4603	733.5072
12	749.5046	771.4865	777.5335
13	793.5308	815.5127	821.5597
14	837.5570	859.5389	865.5859
15	881.5832	903.5652	909.6121
16	925.6094	947.5914	953.6383
17	969.6356	991.6176	997.6645
18	1013.6619	1035.6438	1041.6908
19	1057.6881	1079.6700	1085.7170
20	1101.7143	1123.6962	1129.7432
— etc. —			

Note: X-101 has on average 9 to 10 repeat units (also reduced form)  
 Na<sup>+</sup> cationised form is observed most intensely, H<sup>+</sup> weakly (if at all)  
 K<sup>+</sup> cationised form also possible  
 a by-product of Triton production is polyethylene glycol

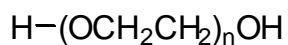


Table D Peaks that may be Observed in ESI Spectra if Polyethylene Glycol is Present

# of repeat units (n)	Exact Mass (u)		
	H <sup>+</sup>	Na <sup>+</sup>	K <sup>+</sup>
1	63.0441	85.0260	100.9999
2	107.0703	129.0522	145.0262
3	151.0965	173.0784	189.0524
4	195.1227	217.1046	233.0786
5	239.1489	261.1309	277.1048
6	283.1751	305.1571	321.1310
7	327.2013	349.1833	365.1572
8	371.2276	393.2095	409.1834
9	415.2538	437.2357	453.2097
10	459.2800	481.2619	497.2359
11	503.3062	525.2881	541.2621
12	547.3324	569.3144	585.2883
13	591.3586	613.3406	629.3145
14	635.3849	657.3668	673.3407
15	679.4111	701.3930	717.3669
16	723.4373	745.4192	761.3932
17	767.4635	789.4454	805.4194
18	811.4897	833.4717	849.4456
19	855.5159	877.4979	893.4718
20	899.5421	921.5241	937.4980
— etc. —			

Note: Na<sup>+</sup> cationised form is observed most intensely, H<sup>+</sup> weakly (if at all)

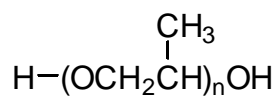


Table E Peaks that may be Observed in ESI Spectra if Polypropylene Glycol is Present

# of repeat units (n)	Exact Mass (u)		
	H <sup>+</sup>	Na <sup>+</sup>	K <sup>+</sup>
1	77.0597	99.0416	115.0156
2	135.1016	157.0835	173.0575
3	193.1434	215.1254	231.0993
4	251.1853	273.1672	289.1412
5	309.2272	331.2091	347.1830
6	367.2690	389.2510	405.2249
7	425.3109	447.2928	463.2668
8	483.3528	505.3347	521.3086
9	541.3946	563.3766	579.3505
10	599.4365	621.4184	637.3924
11	657.4784	679.4603	695.4342
12	715.5202	737.5022	753.4761
13	773.5621	795.5440	811.5180
14	831.6040	853.5859	869.5598
15	889.6458	911.6278	927.6017
16	947.6877	969.6696	985.6436
17	1005.7295	1027.7115	1043.6854
18	1063.7714	1085.7534	1101.7273
19	1121.8133	1143.7952	1159.7692
20	1179.8551	1201.8371	1217.8110
— etc. —			

Note: Na<sup>+</sup> cationised form is observed most intensely, H<sup>+</sup> weakly (if at all)

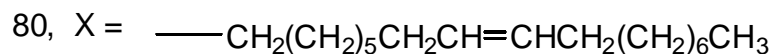
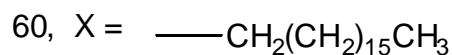
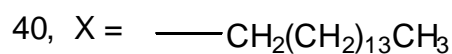
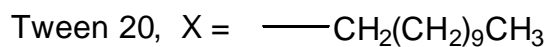
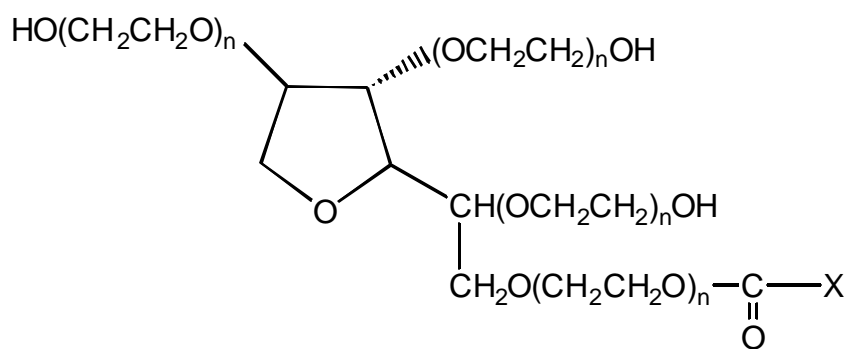


Table F Peaks that may be Observed in ESI Spectra if Tween is Present

# of repeat units (n)	Exact Mass (u)			
	Tween 20	Tween 40	Tween 60	Tween 80
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	1155.7224
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	1513.9063	1569.9689	1598.0002	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
— etc. —				

Note: masses assuming Na<sup>+</sup> cationisation