

Article title: Glycan side-reaction may compromise ETD-based glycopeptide identification

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Tris-modified monosialo-glycoforms of **VLGFKPKPPKN*ESLETYPLMMK, [183-204] of sodium/potassium-transporting ATPase subunit beta-1 (Uniprot ID: P14094)**

m/z	z	MH exp	glycan	cal MH	ppm
1015.8666	5	5075.3017	HexNAc5Hex6FucSA+TRIS	5075.3018	0
1045.0820	5	5221.3787	HexNAc5Hex6Fuc2SA+TRIS	5221.3597	-4
1056.4827	5	5278.3822	HexNAc6Hex6FucSA+TRIS	5278.3812	0
1074.2936	5	5367.4367	HexNAc5Hex6Fuc3SA+TRIS	5367.4176	-4
1085.6981	5	5424.4592	HexNAc6Hex6Fuc2SA+TRIS	5424.4391	-4
1088.8980	5	5440.4587	HexNAc6Hex7FucSA+TRIS	5440.4340	-5
1097.1031	5	5481.4842	HexNAc7Hex6FucSA+TRIS	5481.4606	-4
1114.9091	5	5570.5142	HexNAc6Hex6Fuc3SA+TRIS	5570.4970	-3
1118.1090	5	5586.5137	HexNAc6Hex7Fuc2SA+TRIS	5586.4919	-4
1126.3125	5	5627.5312	HexNAc7Hex6Fuc2SA+TRIS	5627.5185	-2
1147.3201	5	5732.5692	HexNAc6Hex7Fuc3SA+TRIS	5732.5498	-3

All these glycoforms were also detected without the glycan modification

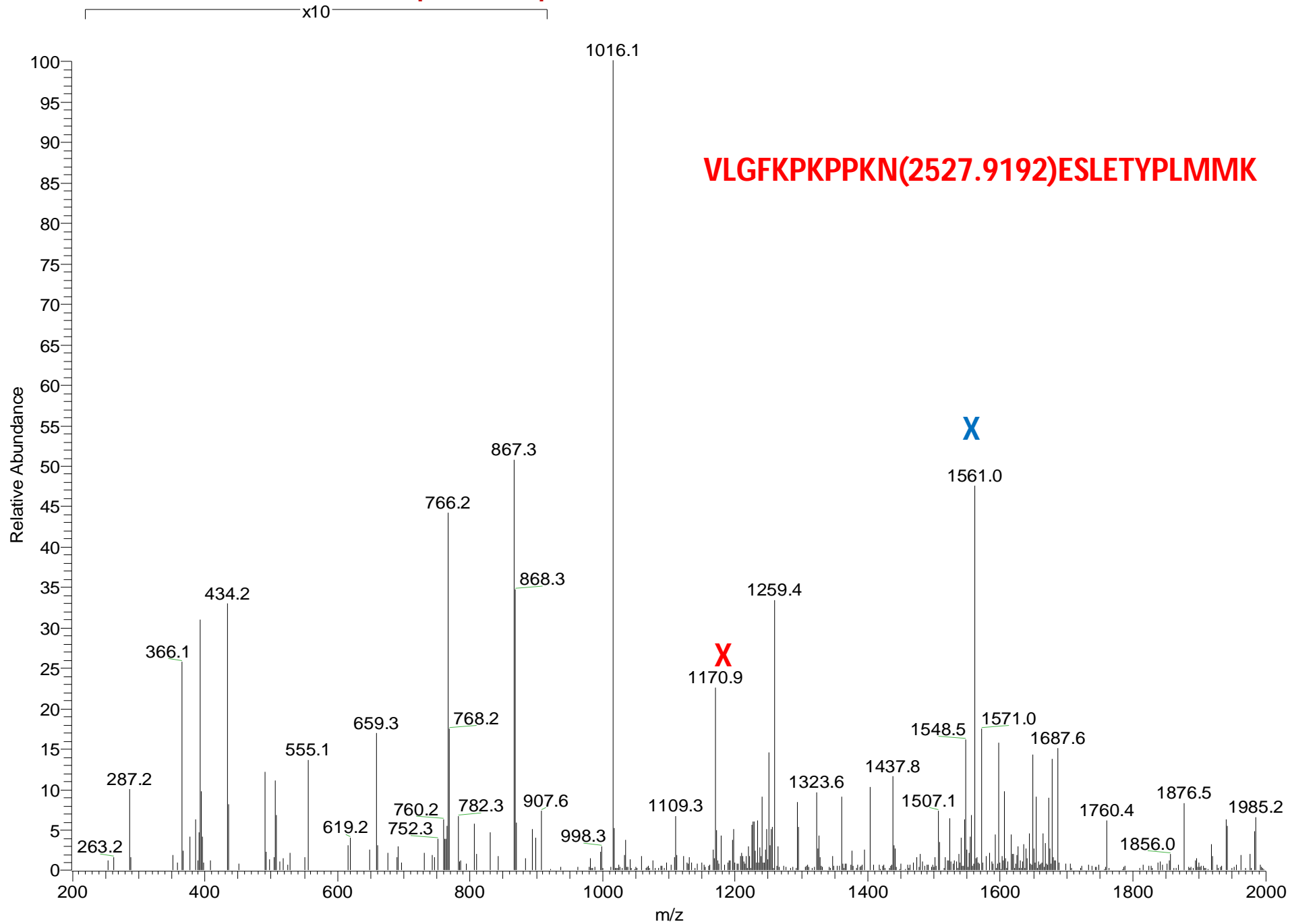
Peak assignment is only given for the first spectrum

In all spectra

4+ ions representing the modified SA loss are labeled with **X**;

3+ ions representing the modified SA loss are labeled with **X**

V20100910-12 #5797 RT: 45.39 AV: 1 NL: 3.72E3
F: ITMS + c NSI d w sa Full ms2 1015.87@etd40.00 [50.00-2000.00]

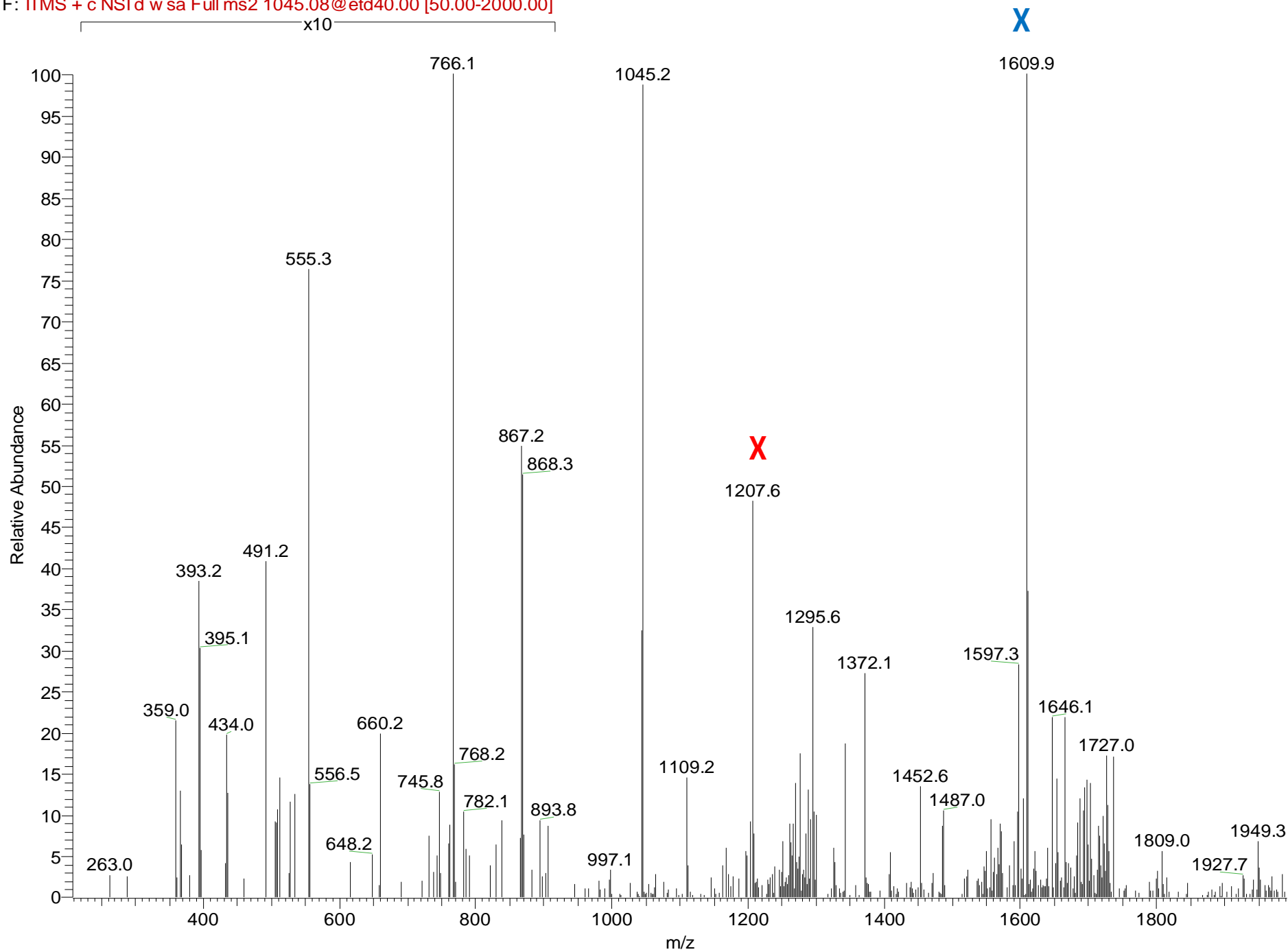


c10 ↓ ↓ c11
VLGFKPKPPKN(2527.9410)ESLETYPLMMK⁺⁵

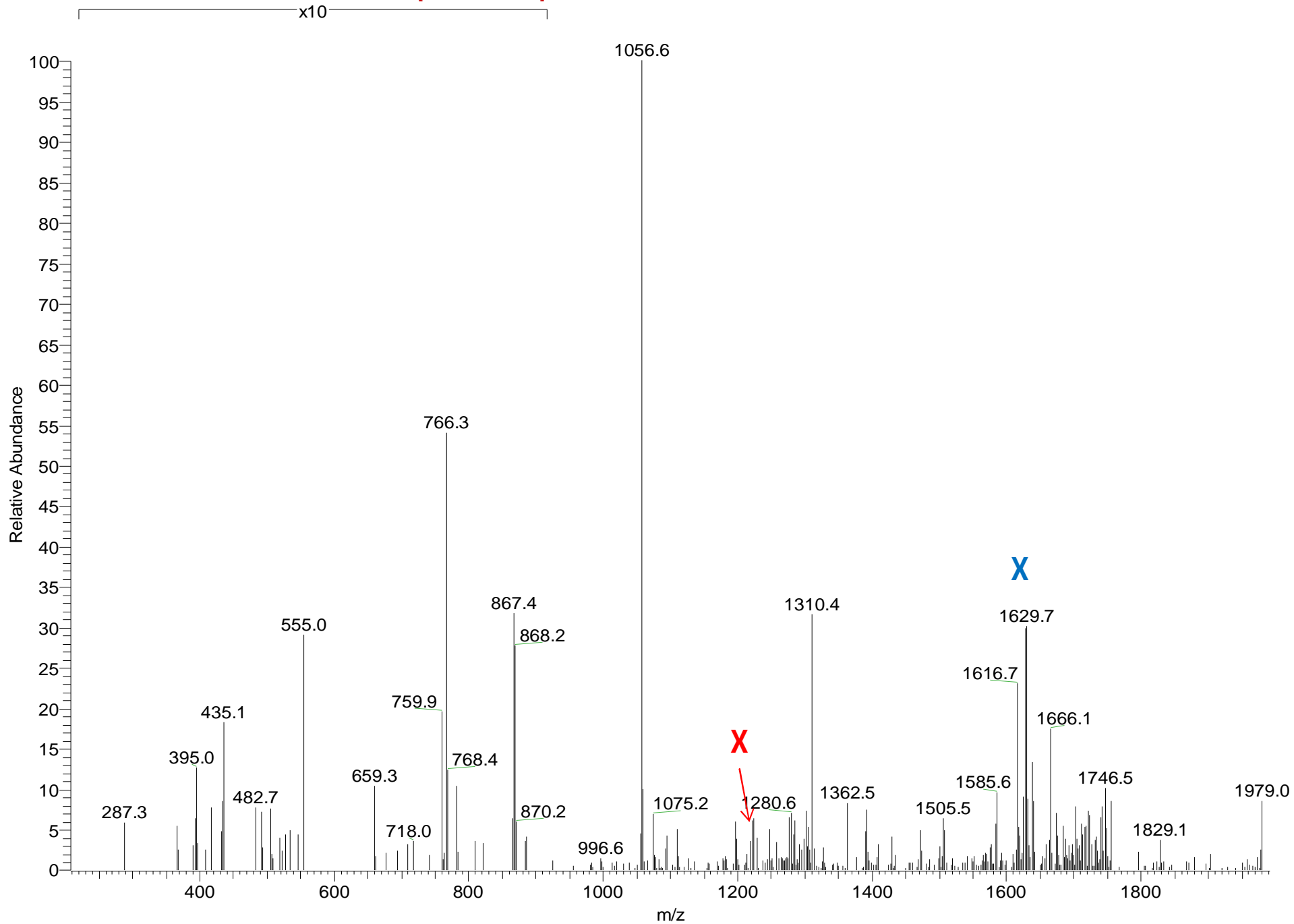
[-] Peak Matches

287.2030	366.1230	377.1940	385.8090	393.2120	434.2190	491.2680	506.1300	555.1240	615.2900
c ₃ ^{-0.0048}			b ₇ ⁺² (0.059)	z ₃ (0.037) z+1 ₃ ^{-0.97}	c ₄ ^{-0.057} b ₈ ⁺² ^{-0.057} c-1 ₄ (0.95)	c ₉ ⁺² ^{-0.048} c-1 ₉ ⁺² (0.46)	z ₄ ^{-0.13}	c ₁₀ ⁺² ^{-0.24} c-1 ₁₀ ⁺² (0.26)	
619.2140	659.3210	752.3220	760.2360	763.0550	766.1680	782.3380	806.5890	831.2010	867.2870
y ₅ ^{-0.12}	c ₆ ^{-0.10} c-1 ₆ (0.90)				z ₆ ^{-0.21}	y ₆ ^{-0.056}			z ₇ ^{-0.14} b ₈ ^{-0.26}
1109.3350	1170.9150	1240.9500	1251.5210	1294.1600	1323.6360	1360.8740	1404.4800	1437.7870	1507.1300
z ₉ ^{-0.21} c ₁₀ ^{-0.38} c-1 ₁₀ (0.62)	c-1 ₁₉ ⁺⁴ ^{-0.63} c ₁₉ ⁺⁴ ^{-0.88}	z+1 ₂₁ ⁺⁴ ^{-0.11} z ₂₁ ⁺⁴ (0.14)	c ₁₁ ⁺³ (0.28) c-1 ₁₁ ⁺³ (0.62)	c ₁₂ ⁺³ ^{-0.093} c-1 ₁₂ ⁺³ (0.24)	c ₁₃ ⁺³ (0.37) c-1 ₁₃ ⁺³ (0.71)	c ₁₄ ⁺³ ^{-0.085} c-1 ₁₄ ⁺³ (0.25)	c ₁₅ ⁺³ (0.51) c-1 ₁₅ ⁺³ (0.84)	c ₁₆ ⁺³ (0.13) c-1 ₁₆ ⁺³ (0.47)	
1548.5120	1556.5170	1561.0290	1570.9830	1598.1310	1606.0590	1649.7070	1654.9930	1876.5470	1985.2280
z ₁₈ ⁺³ (0.16) z+1 ₁₈ ⁺³ ^{-0.18}	b ₁₉ ⁺³ (0.14)	c-1 ₁₉ ⁺³ ^{-0.69}		z+1 ₁₉ ⁺³ (0.42) z ₁₉ ⁺³ (0.75)	c ₂₀ ⁺³ (0.32) c-1 ₂₀ ⁺³ (0.66)	c ₂₁ ⁺³ (0.29) c-1 ₂₁ ⁺³ (0.63)	z+1 ₂₁ ⁺³ (0.58) z ₂₁ ⁺³ (0.91)	c ₁₁ ⁺² (0.19) c-1 ₁₁ ⁺² (0.70)	c ₁₃ ⁺² (0.84)

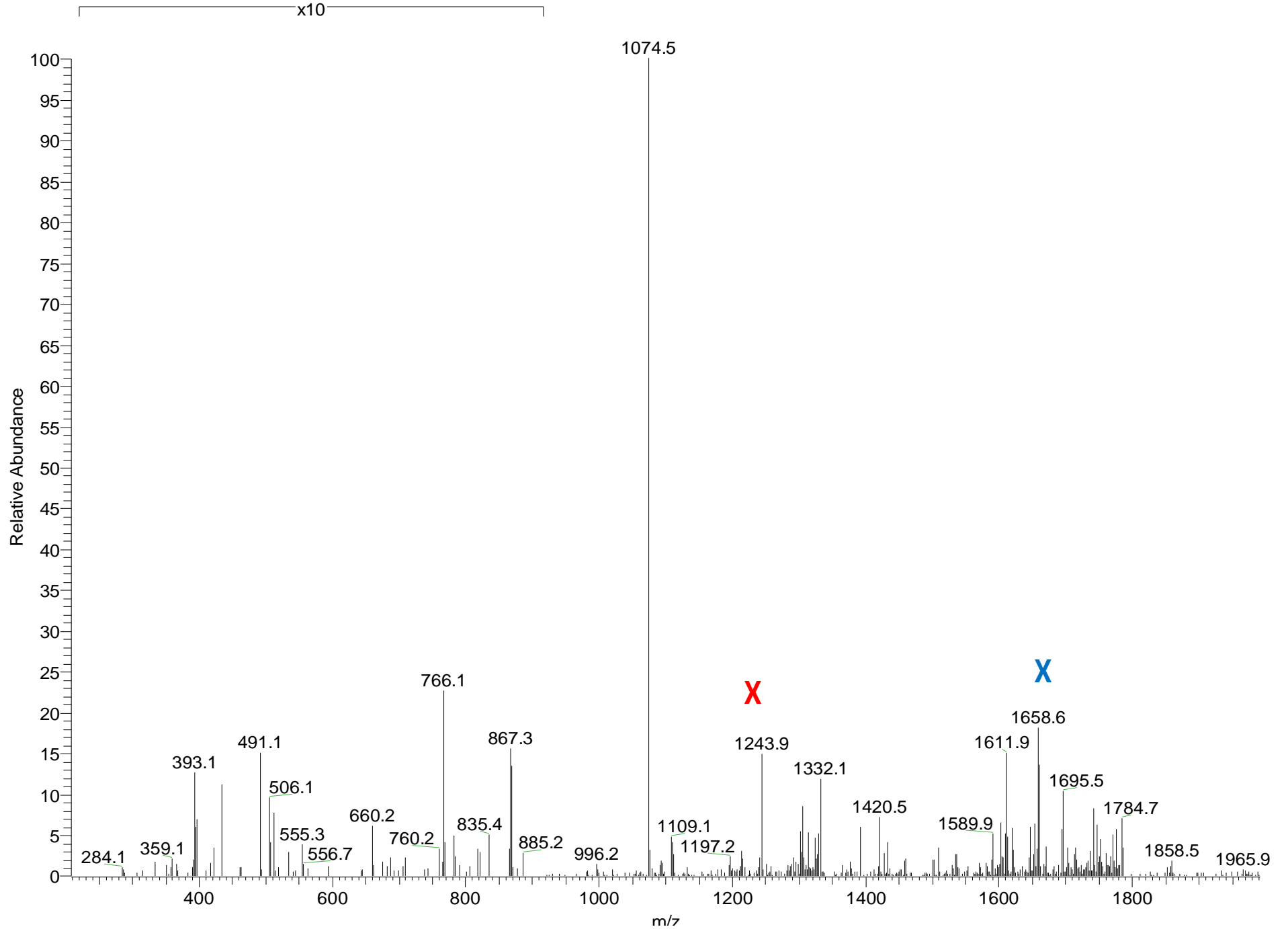
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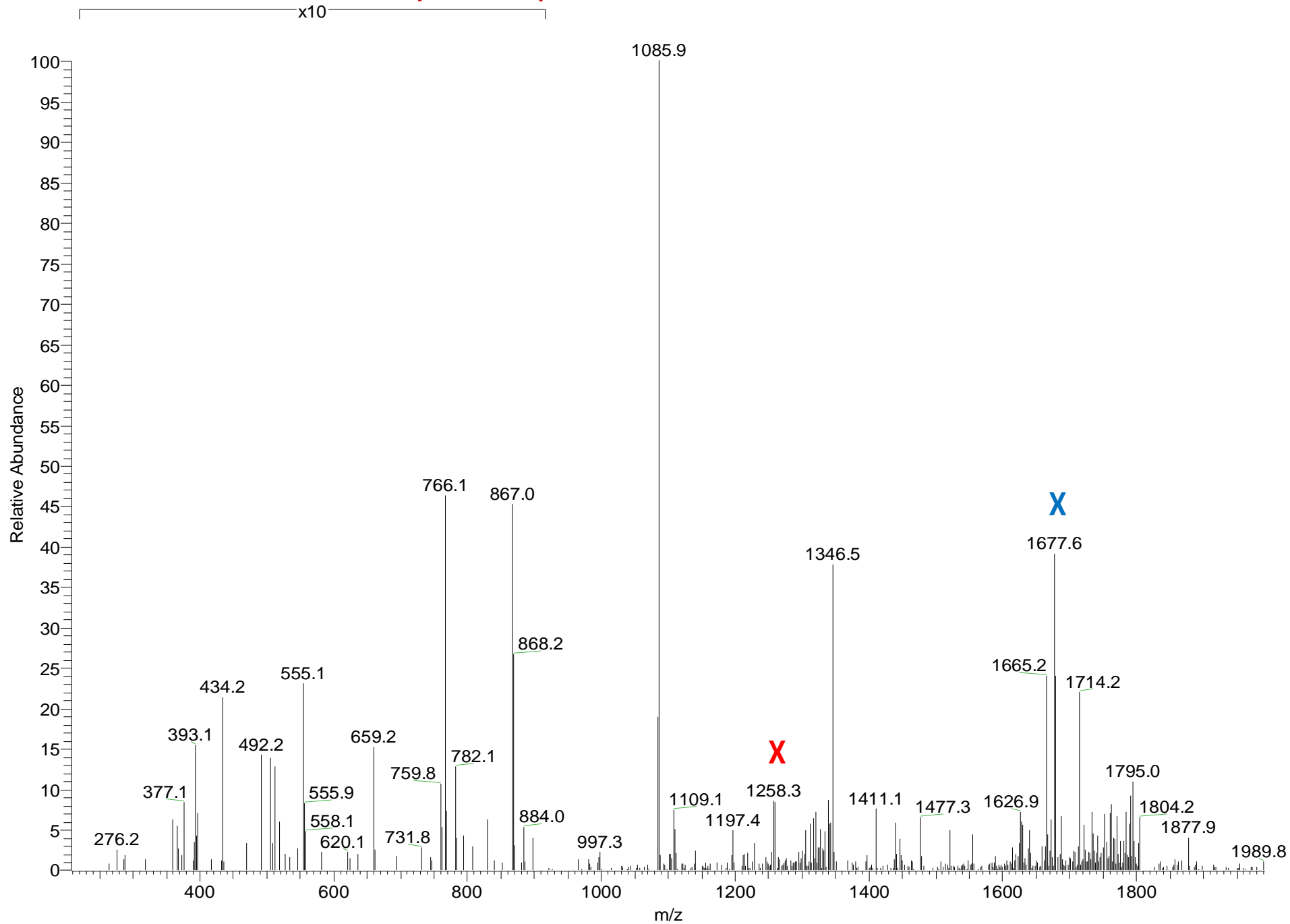
/20100910-12 #5790 RT: 45.33 AV: 1 NL: 1.44E3
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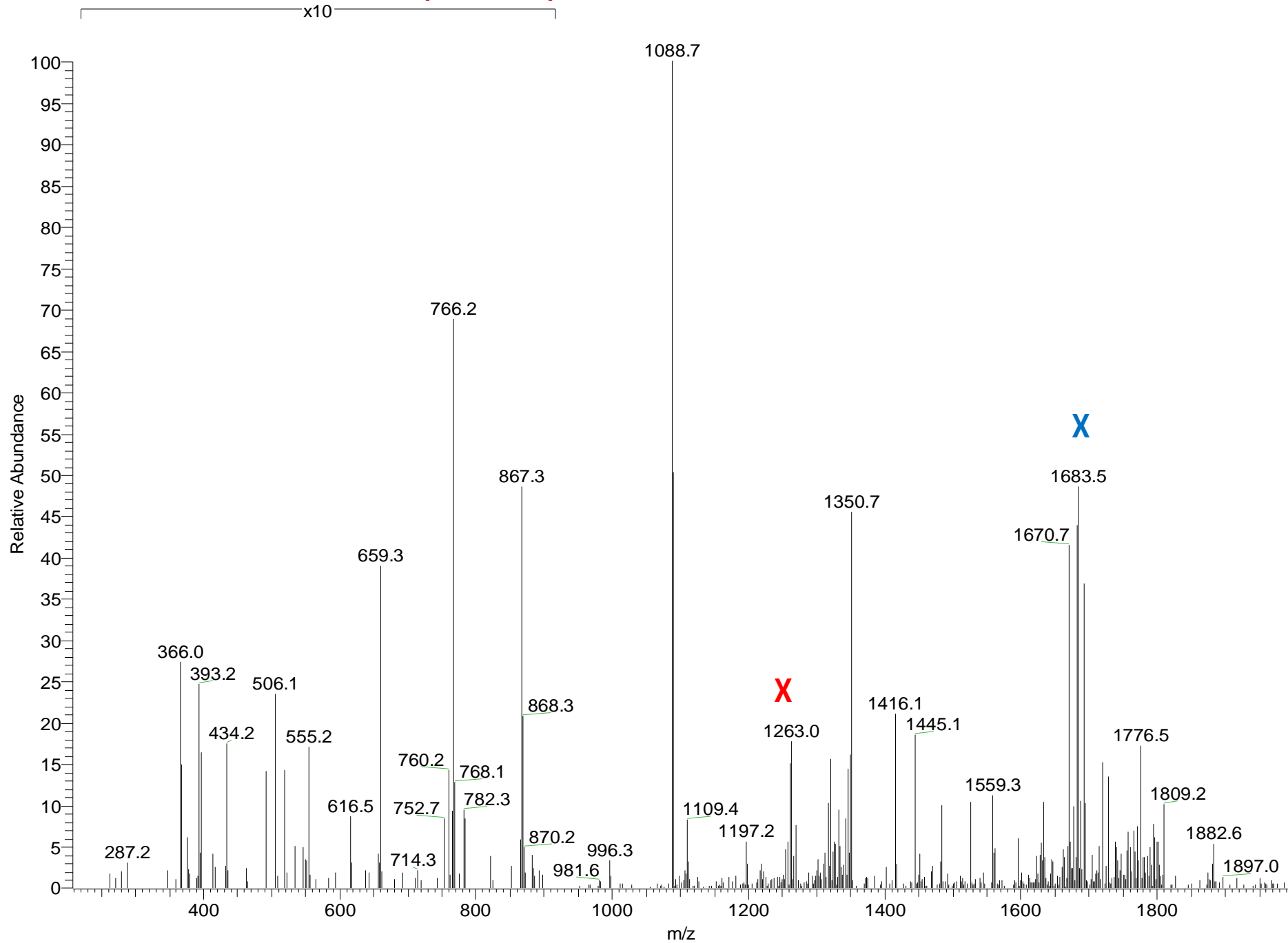
V20100910-12 #5794 RT: 45.36 AV: 1 NL: 4.78E3
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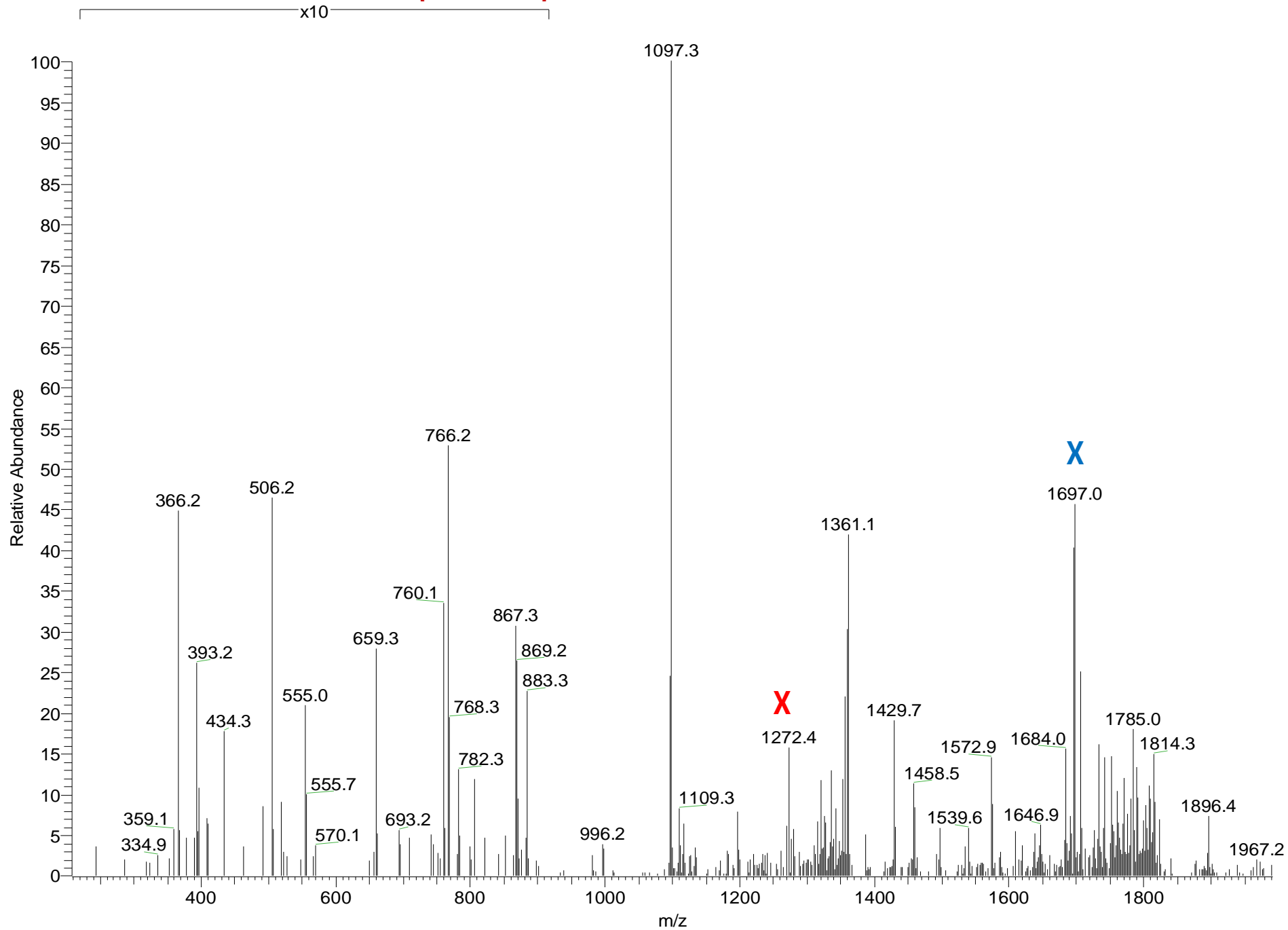
V20100910-12 #5766 RT: 45.15 AV: 1 NL: 4.09E3
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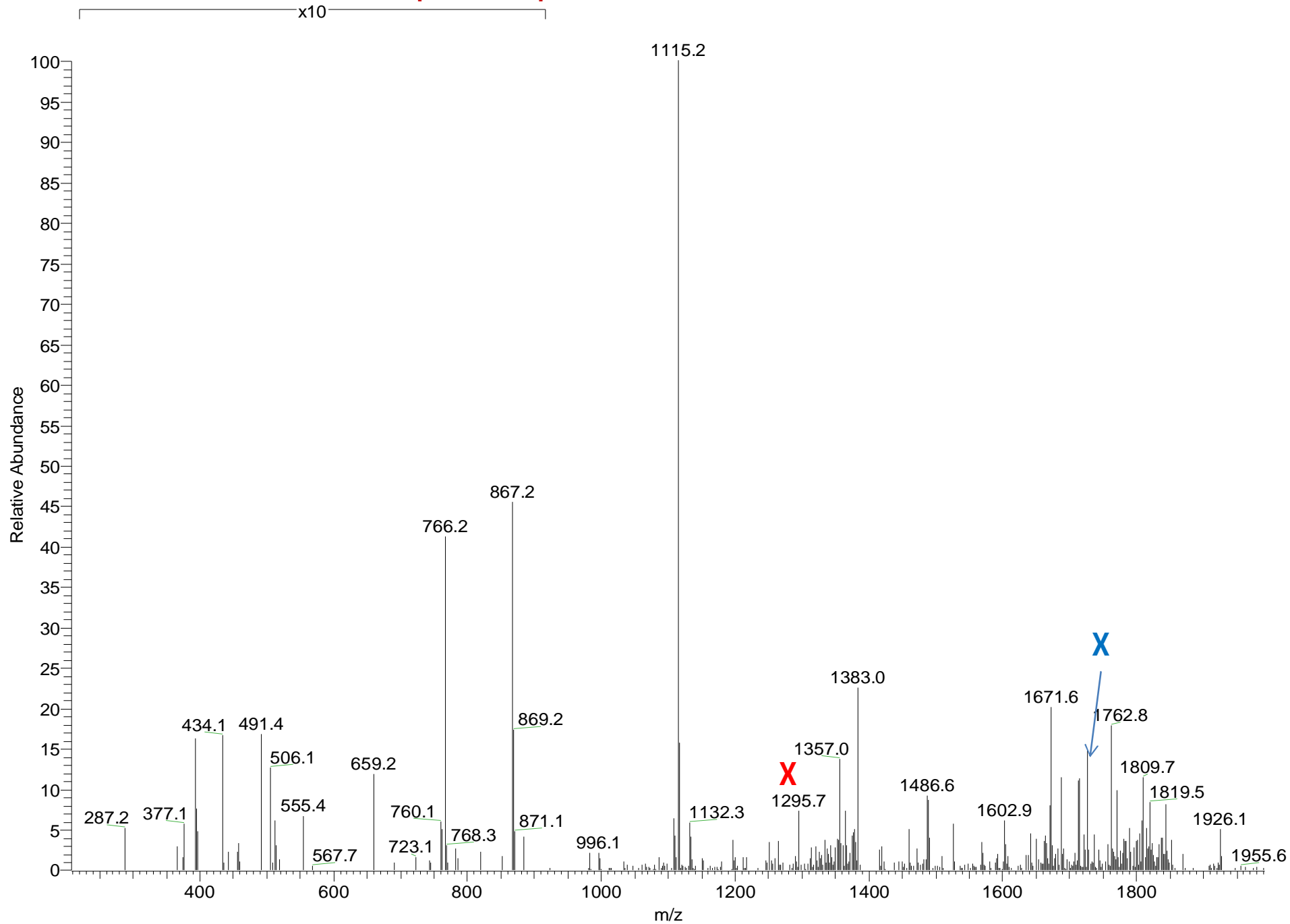
V20100910-12 #5734 RT: 44.91 AV: 1 NL: 2.27E3
F: ITMS + c NSI d w sa Full ms2 1088.90@etd40.00 [50.00-2000.00]



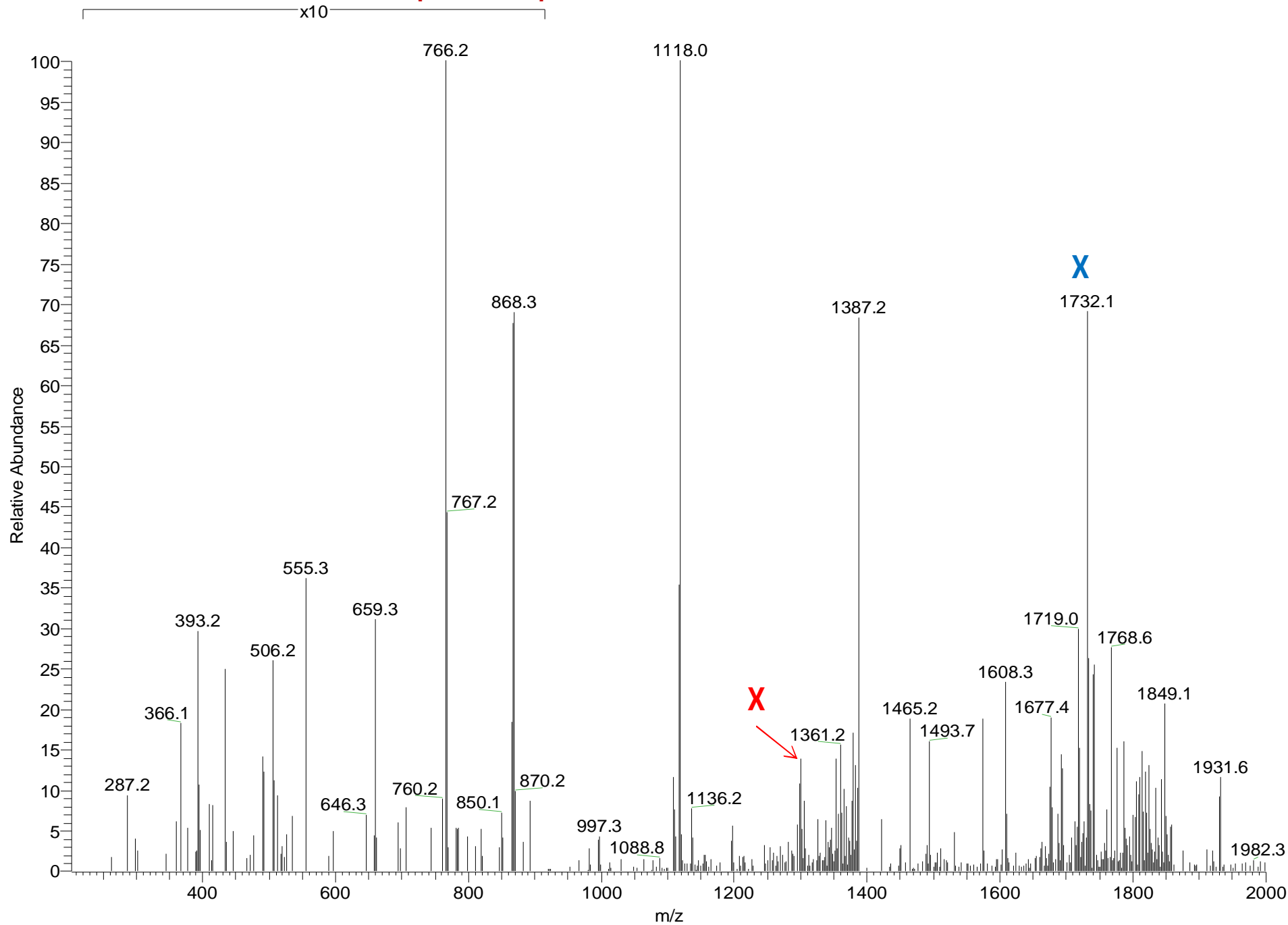
V20100910-12 #5795 RT: 45.37 AV: 1 NL: 1.75E3
F: ITMS + c NSI d w sa Full ms2 1097.50@etd40.00 [50.00-2000.00]



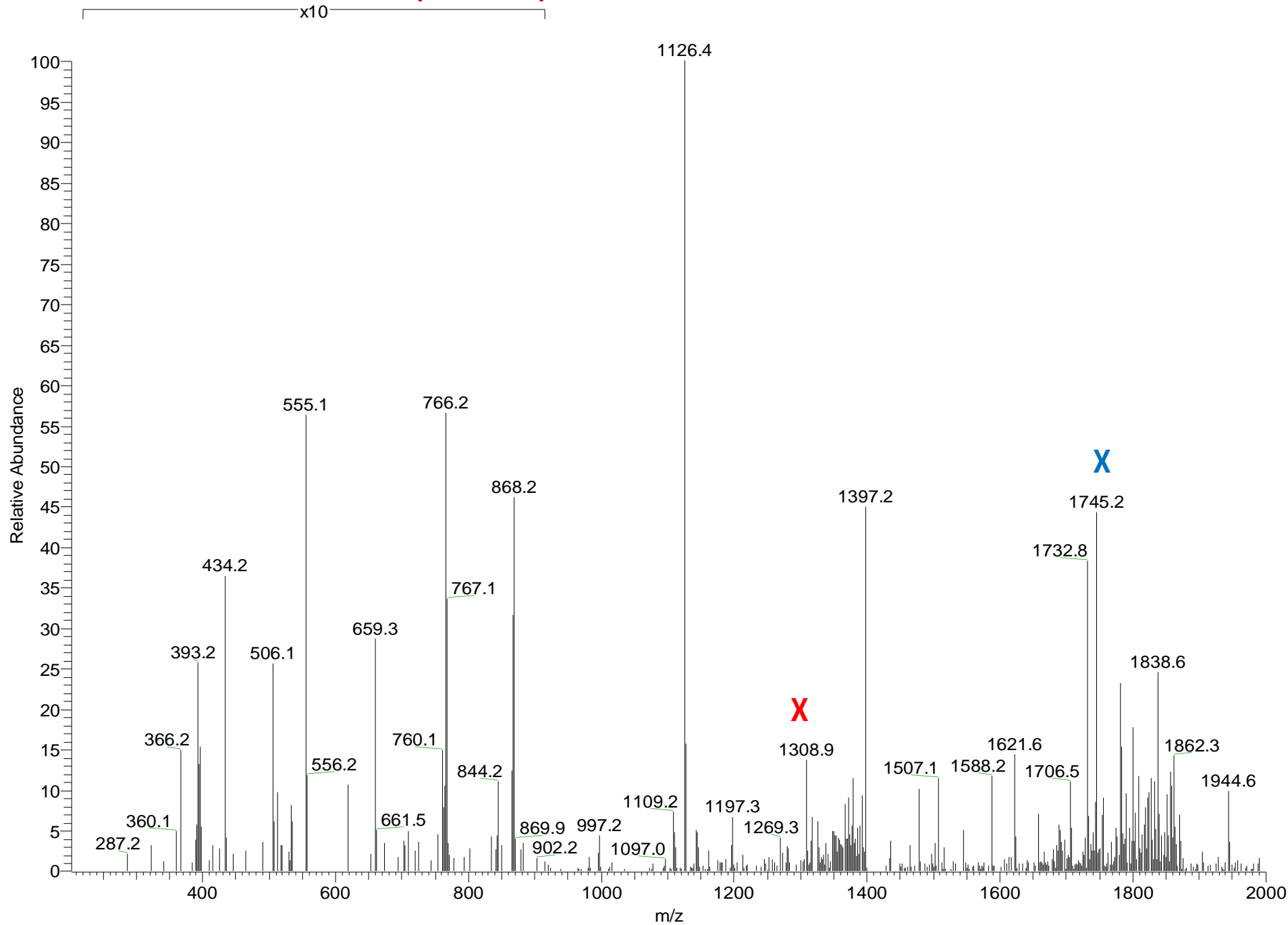
V20100910-12 #5742 RT: 44.97 AV: 1 NL: 2.40E3
F: ITMS + c NSI d w sa Full ms2 1115.10@etd40.00 [50.00-2000.00]



V20100910-12 #5712 RT: 44.73 AV: 1 NL: 1.31E3
F: ITMS + c NSI d w sa Full ms2 1118.11@etd40.00 [50.00-2000.00]



V20100910-12 #5740 RT: 44.96 AV: 1 NL: 3.27E3
F: ITMS + c NSI d w sa Full ms2 1126.31 @etd40.00 [50.00-2000.00]



V20100910-12 #5759 RT: 45.09 AV: 1 NL: 4.97E3
F: ITMS + c NSI d w sa Full ms2 1147.32@etd40.00 [50.00-2000.00]

