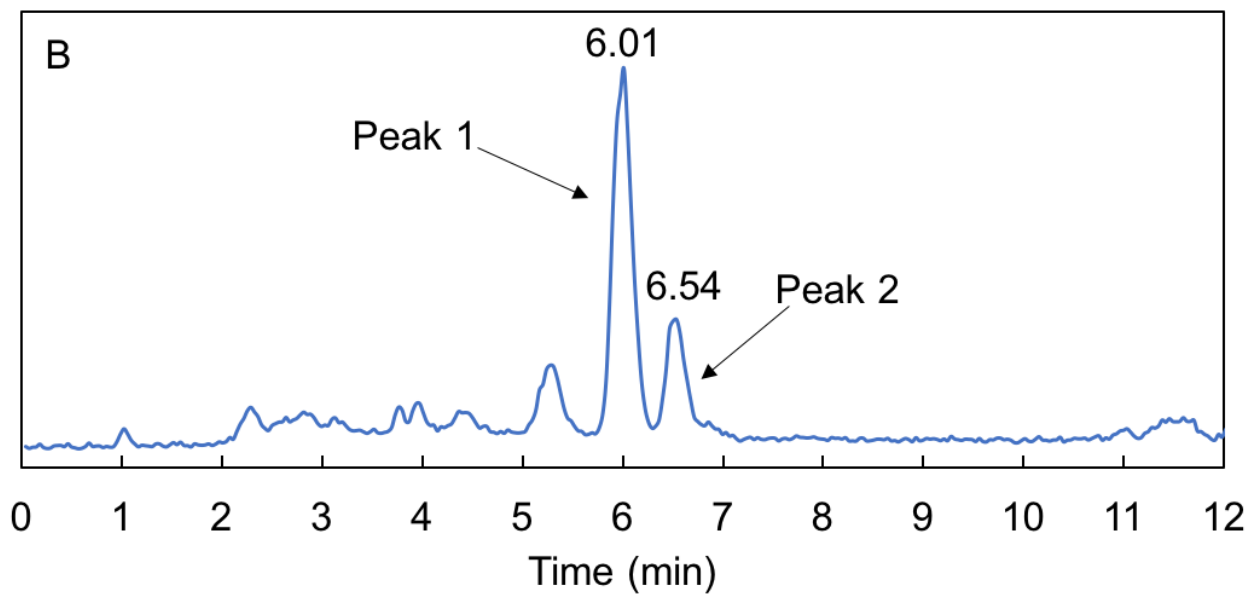
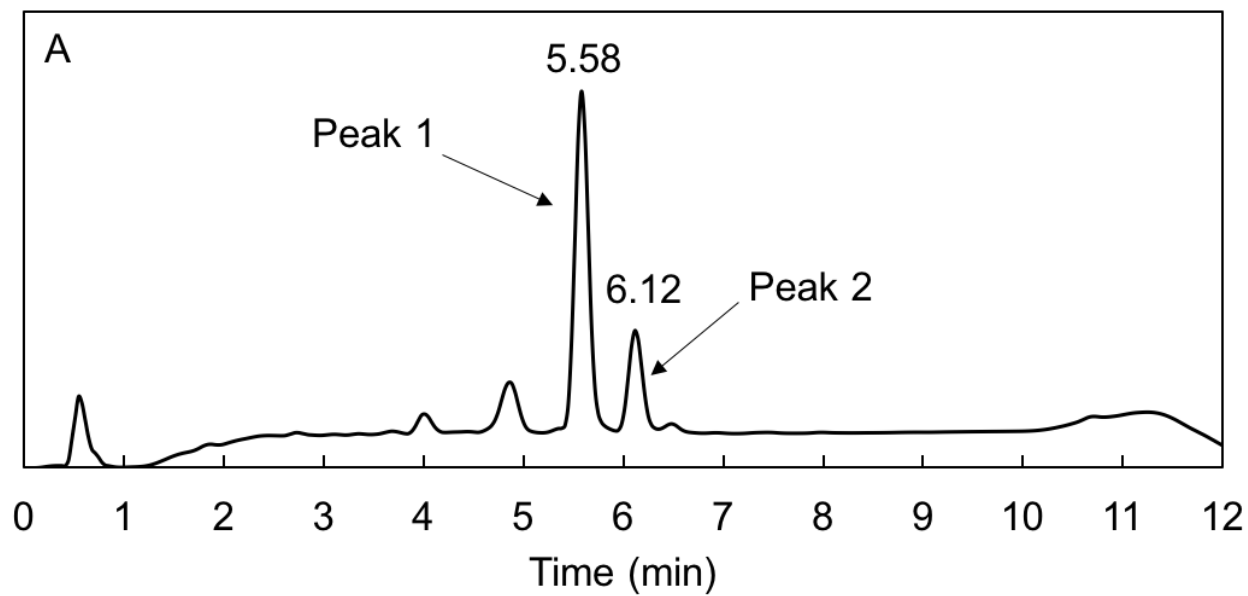


Supporting Information for:
Chlorophyll-Inspired Red-Region Fluorophores:
Building Block Synthesis and Studies in Aqueous Media

Rui Liu, Mengran Liu, Don Hood, Chih-Yuan Chen, Christopher J. MacNevin,
Dewey Holten and Jonathan S. Lindsey

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Topic	Pages
Cyclization data for H₂C10-PEG₆-NHS	S2, S3
Spectral data for new compounds	S4–S70



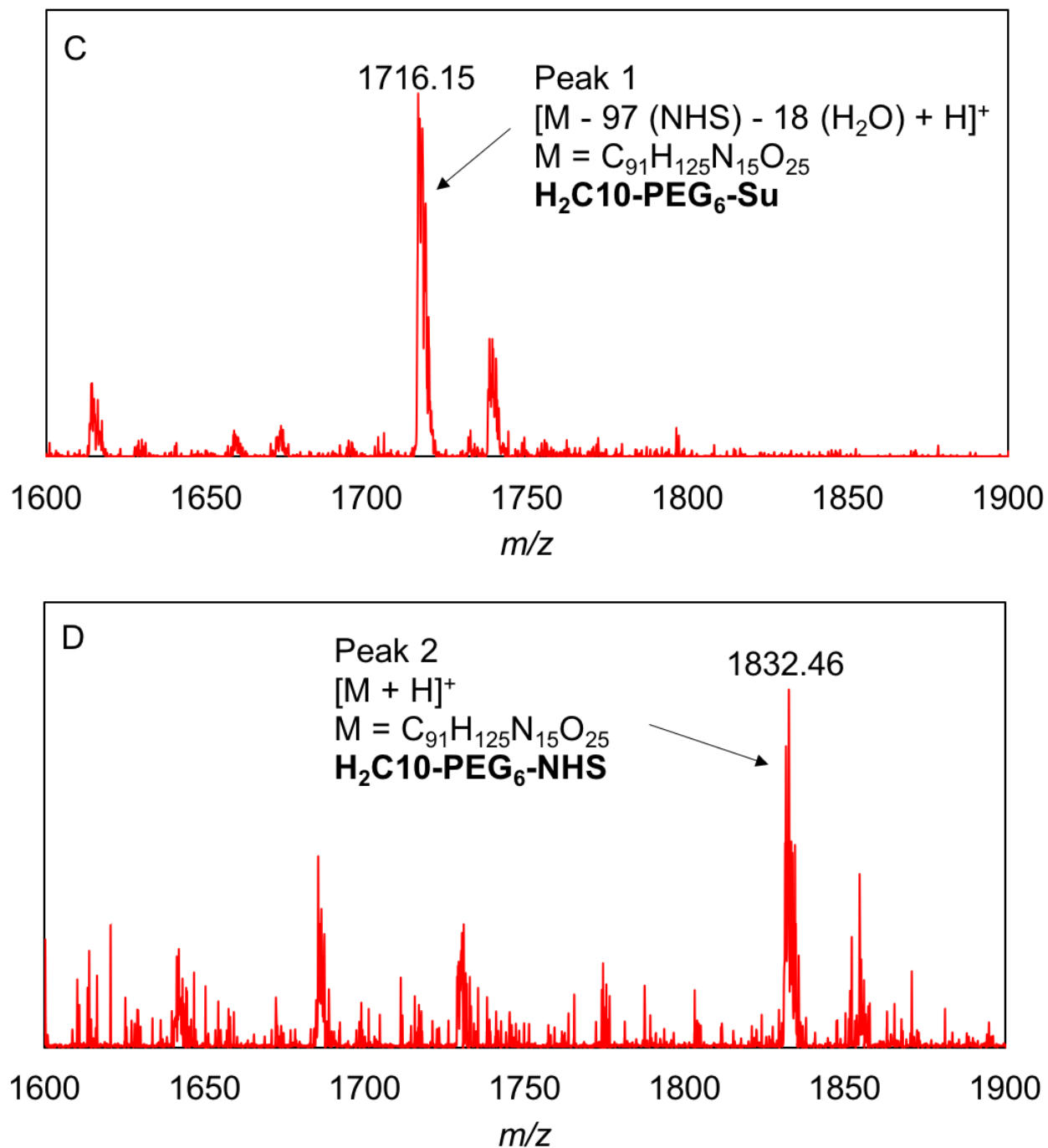
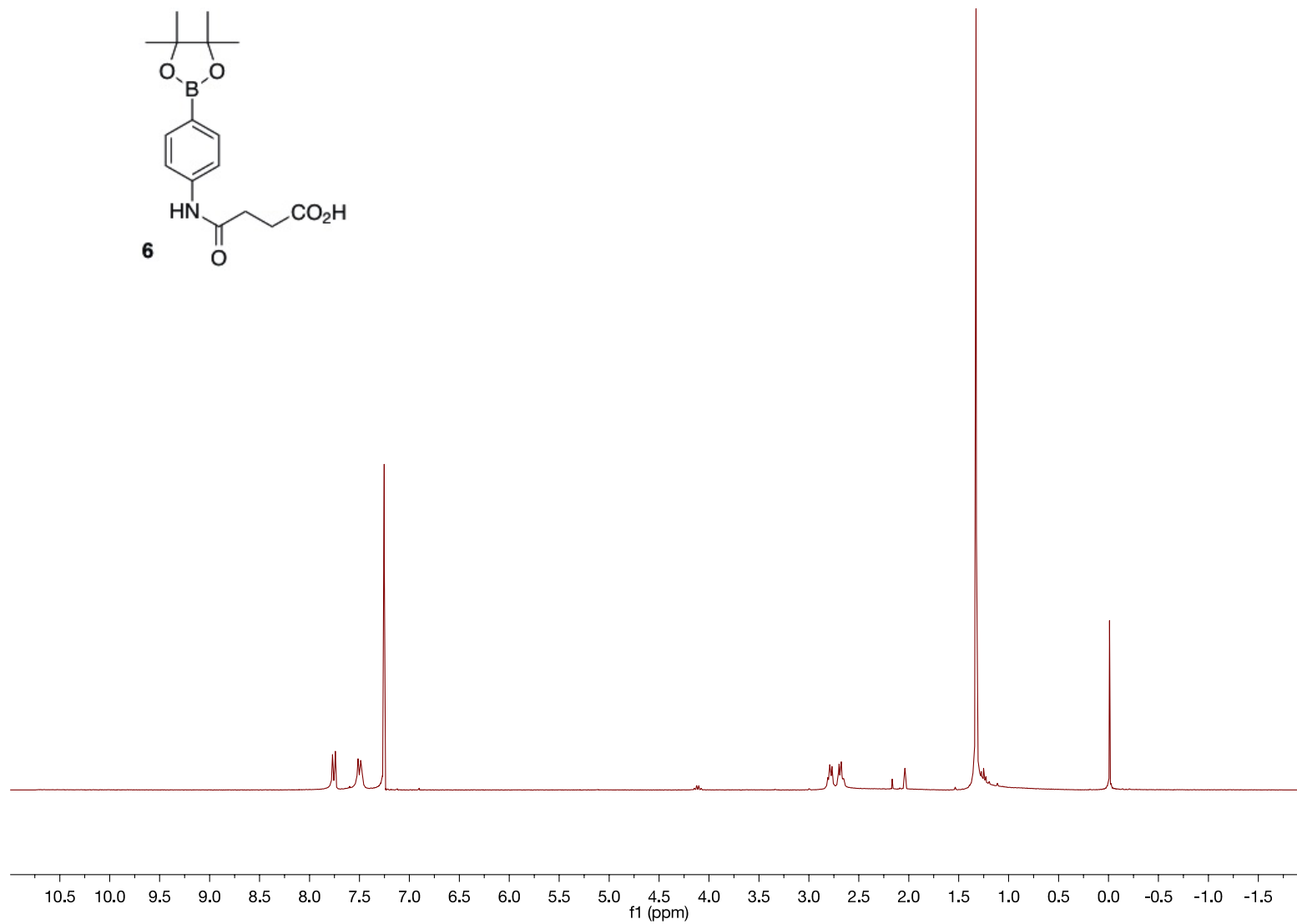
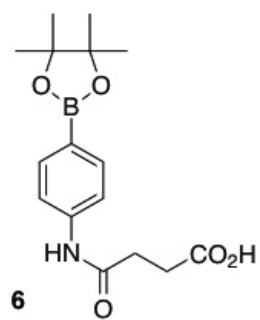
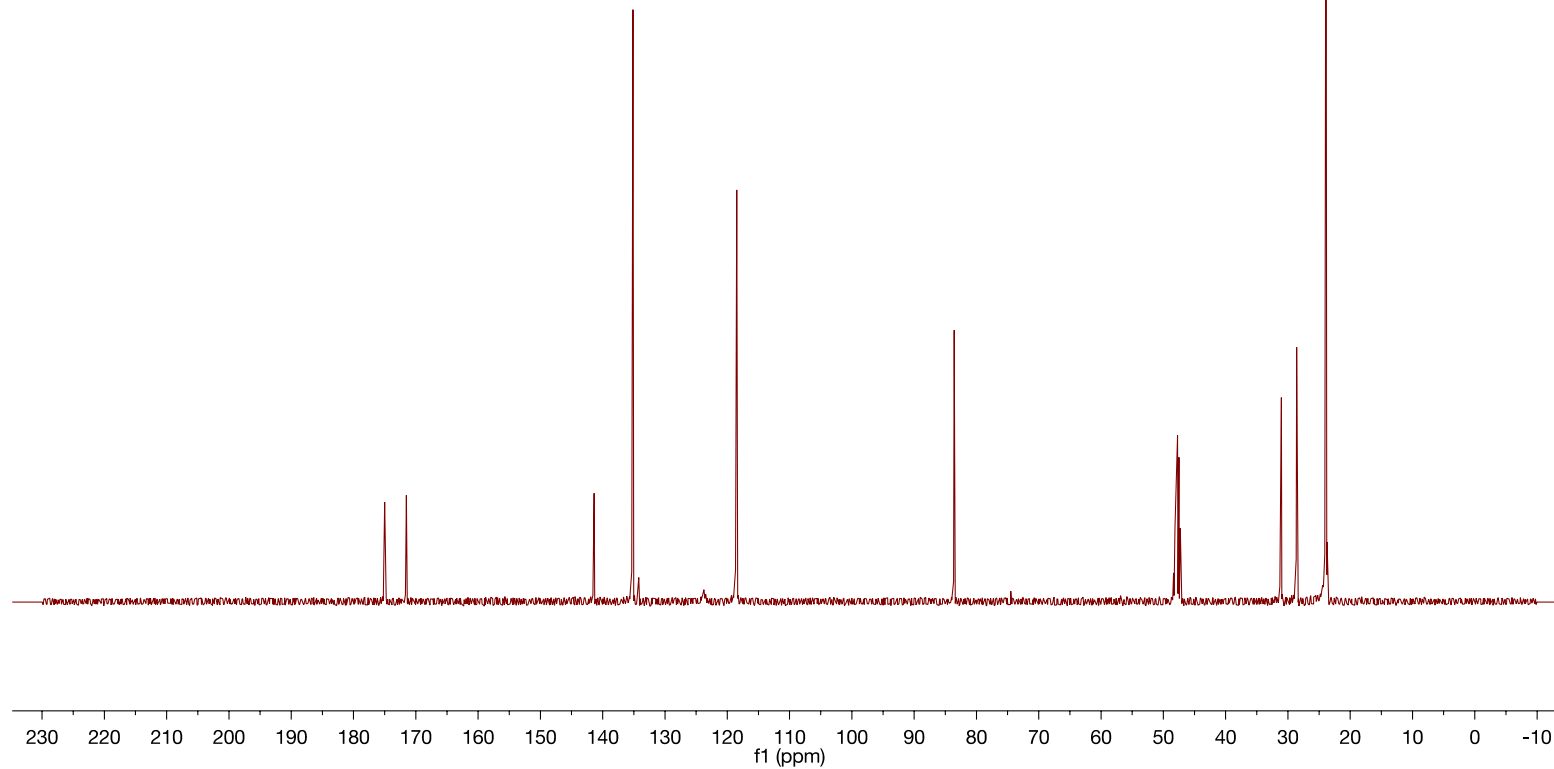
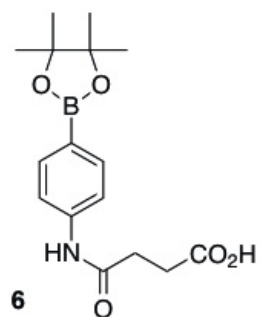
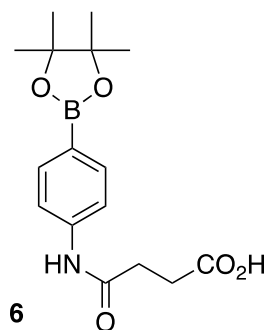
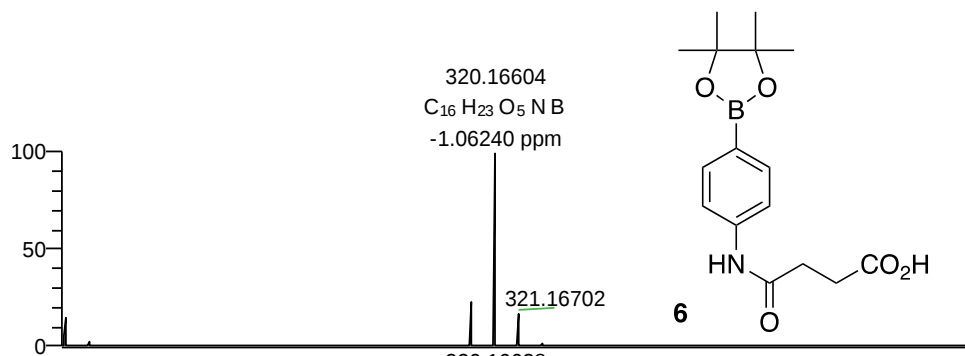
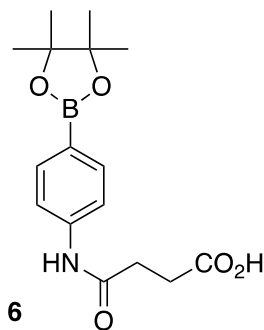
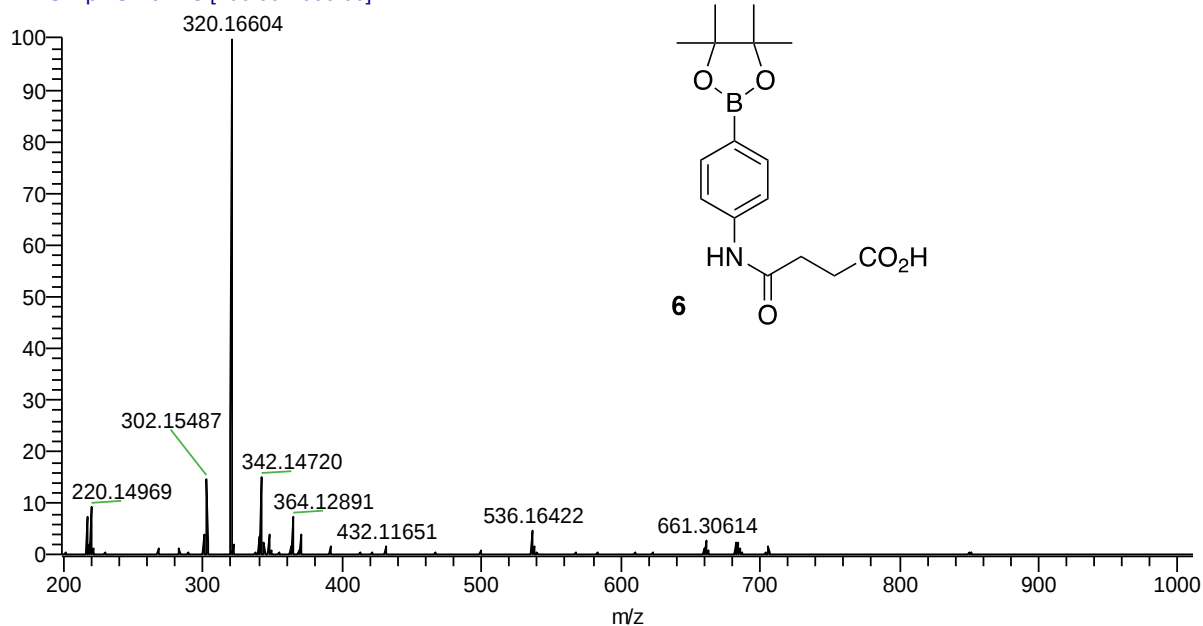


Figure S1. Chromatogram of **$\text{H}_2\text{C10-PEG}_6\text{-NHS}$** with detection by absorption spectroscopy (200 – 800 nm) (panel A) followed by ESI-MS with total ion current (panel B). ESI-MS data of peak 1 is shown in panel C, whereas peak 2 (panel D) is consistent with **$\text{H}_2\text{C10-PEG}_6\text{-NHS}$** .

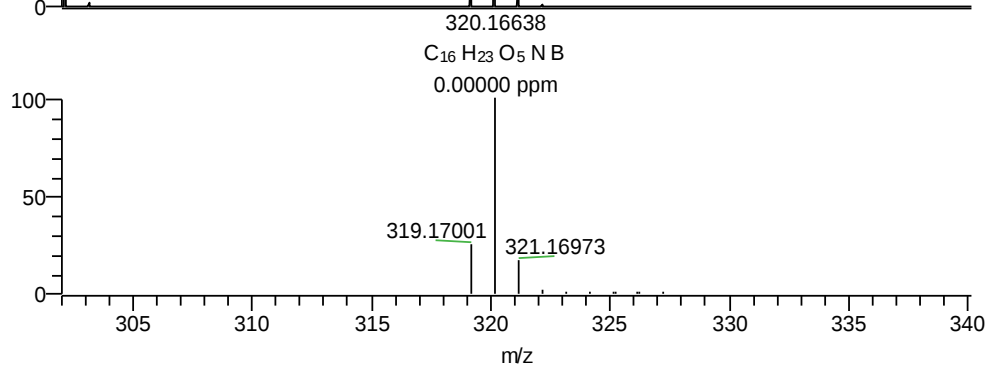




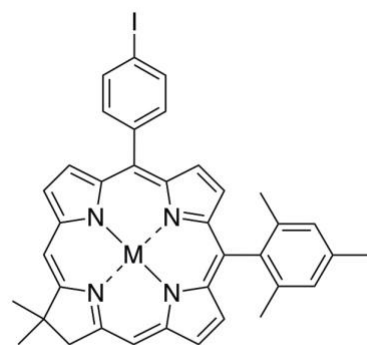
171915_BPin-amide #74-80 RT: 0.53-0.57 NL: 2.70E7
T: FTMS + p ESI Full ms [200.00-1000.00]



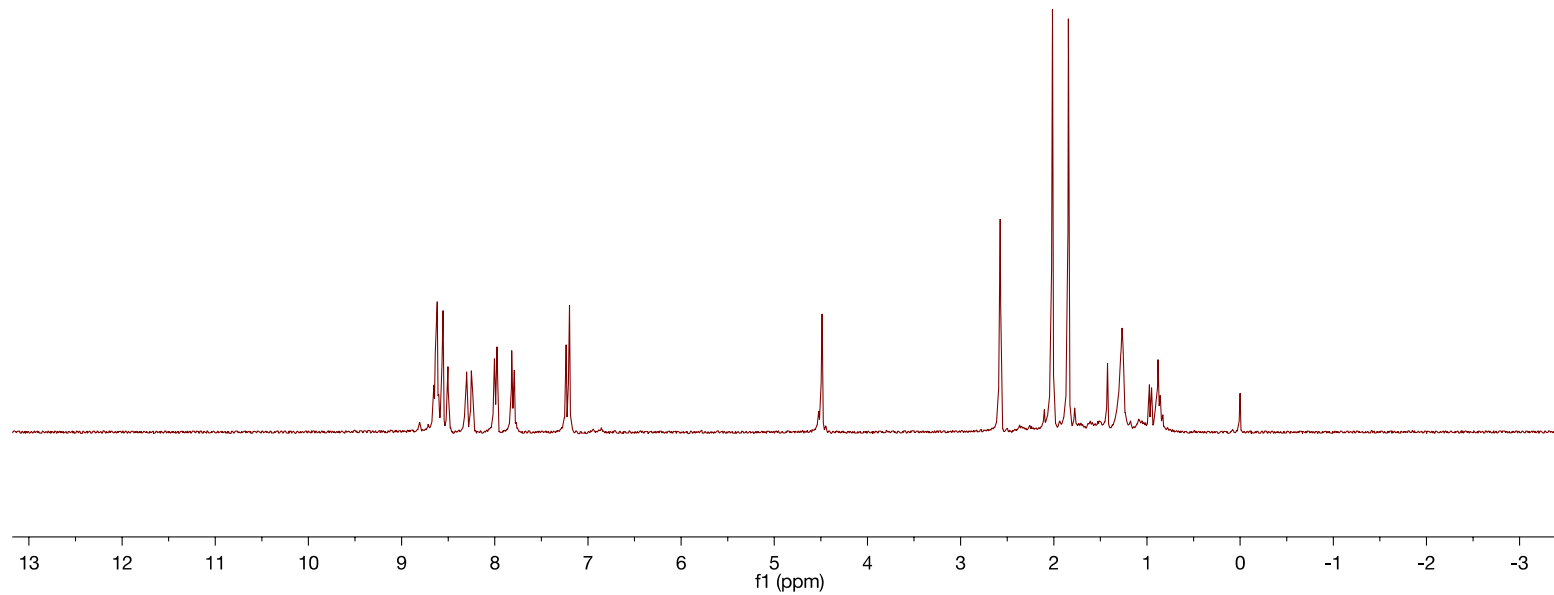
NL:
2.70E7
171915_BPin-
amide#74-80 RT:
0.53-0.57 AV: 7 T:
FTMS + p ESI Full ms
[200.00-1000.00]

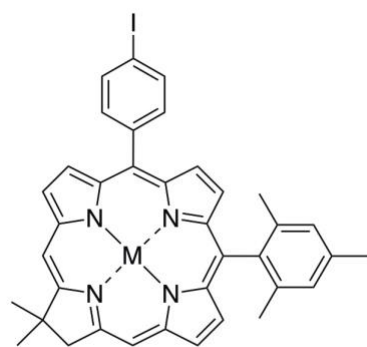


NL:
6.62E5
C₁₆ H₂₂ BNO₅ +H:
C₁₆ H₂₃ B₁N₁O₅
pa Chrg 1

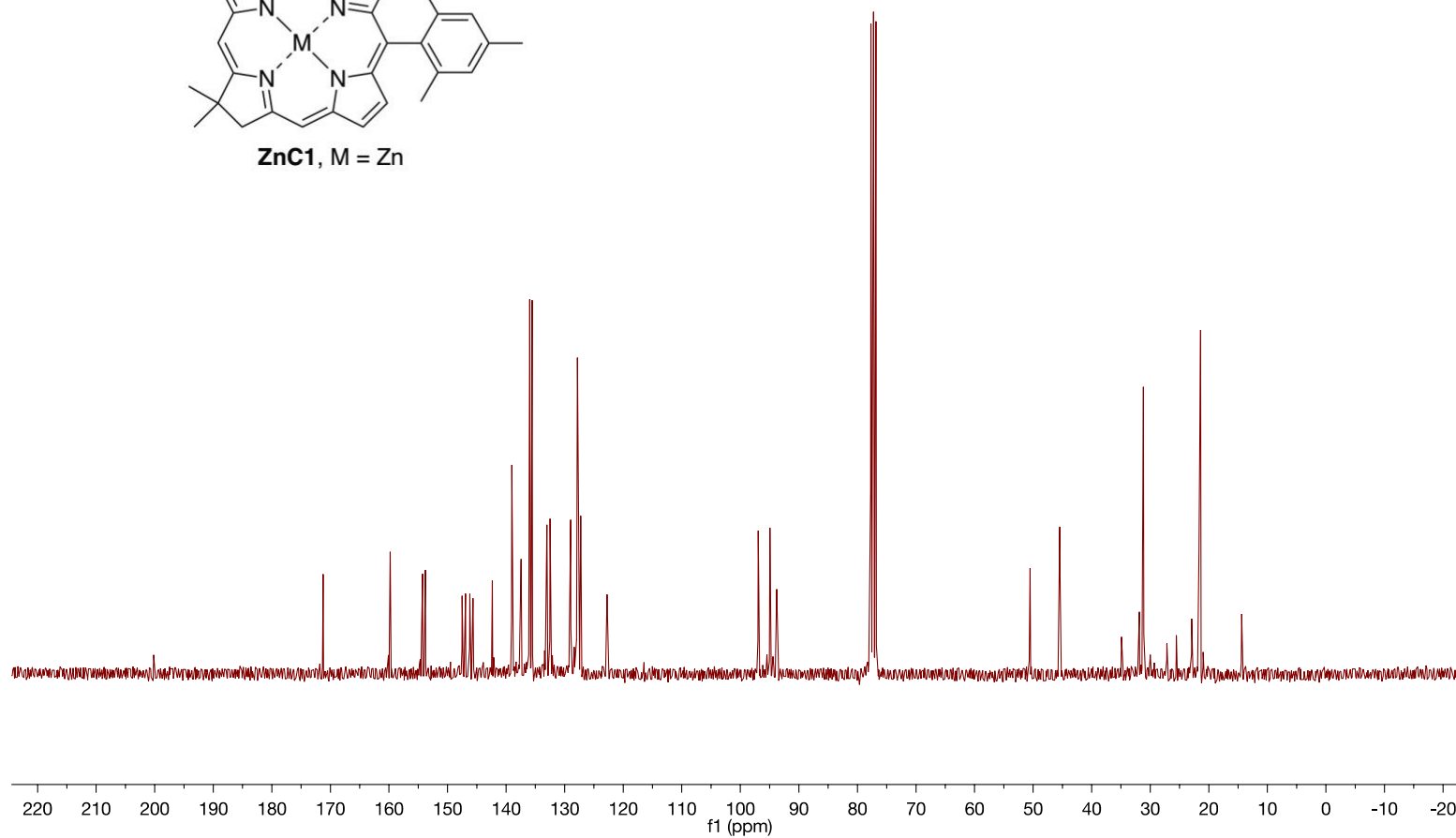


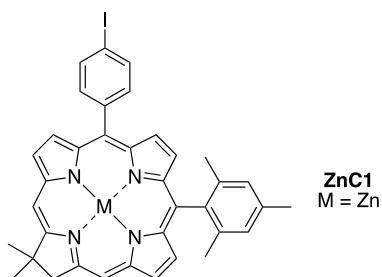
ZnC1, M = Zn



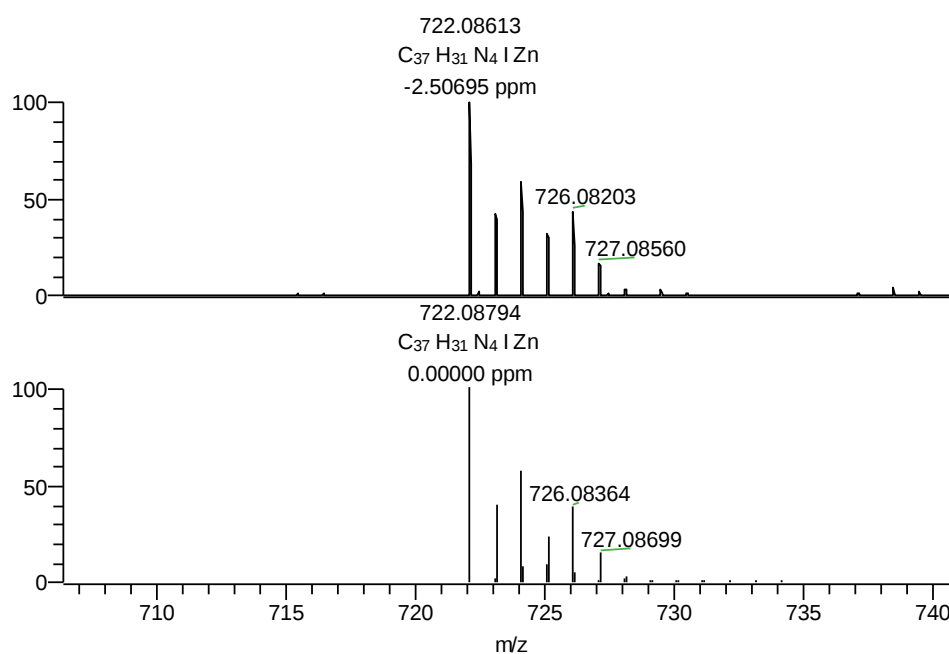
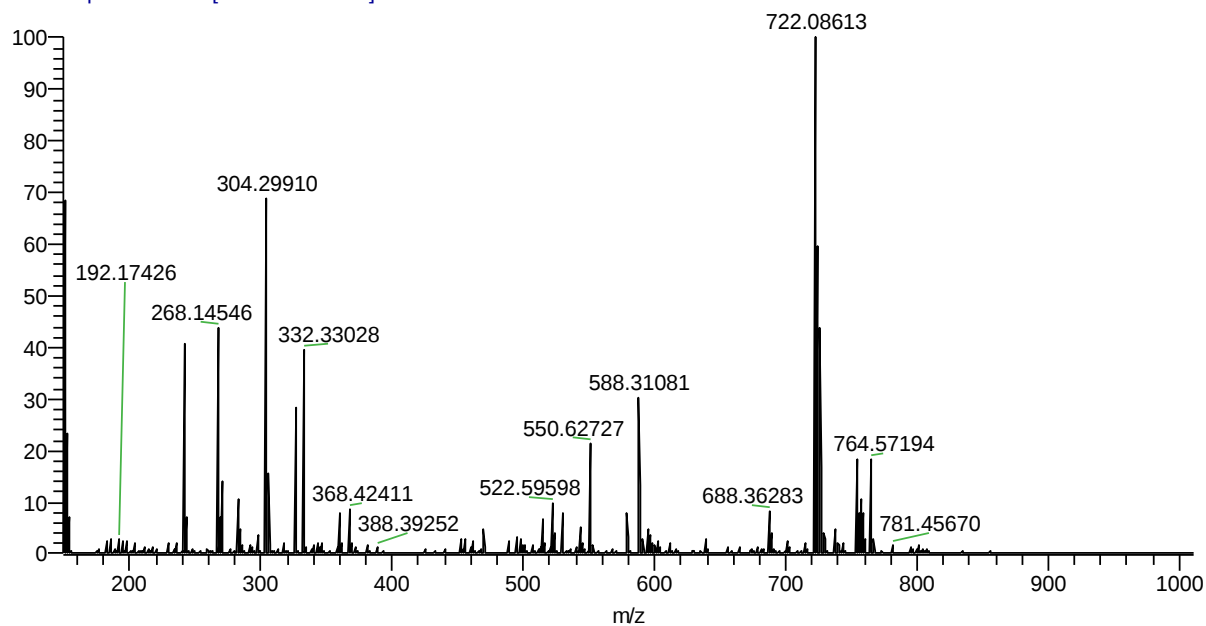


ZnC1, M = Zn



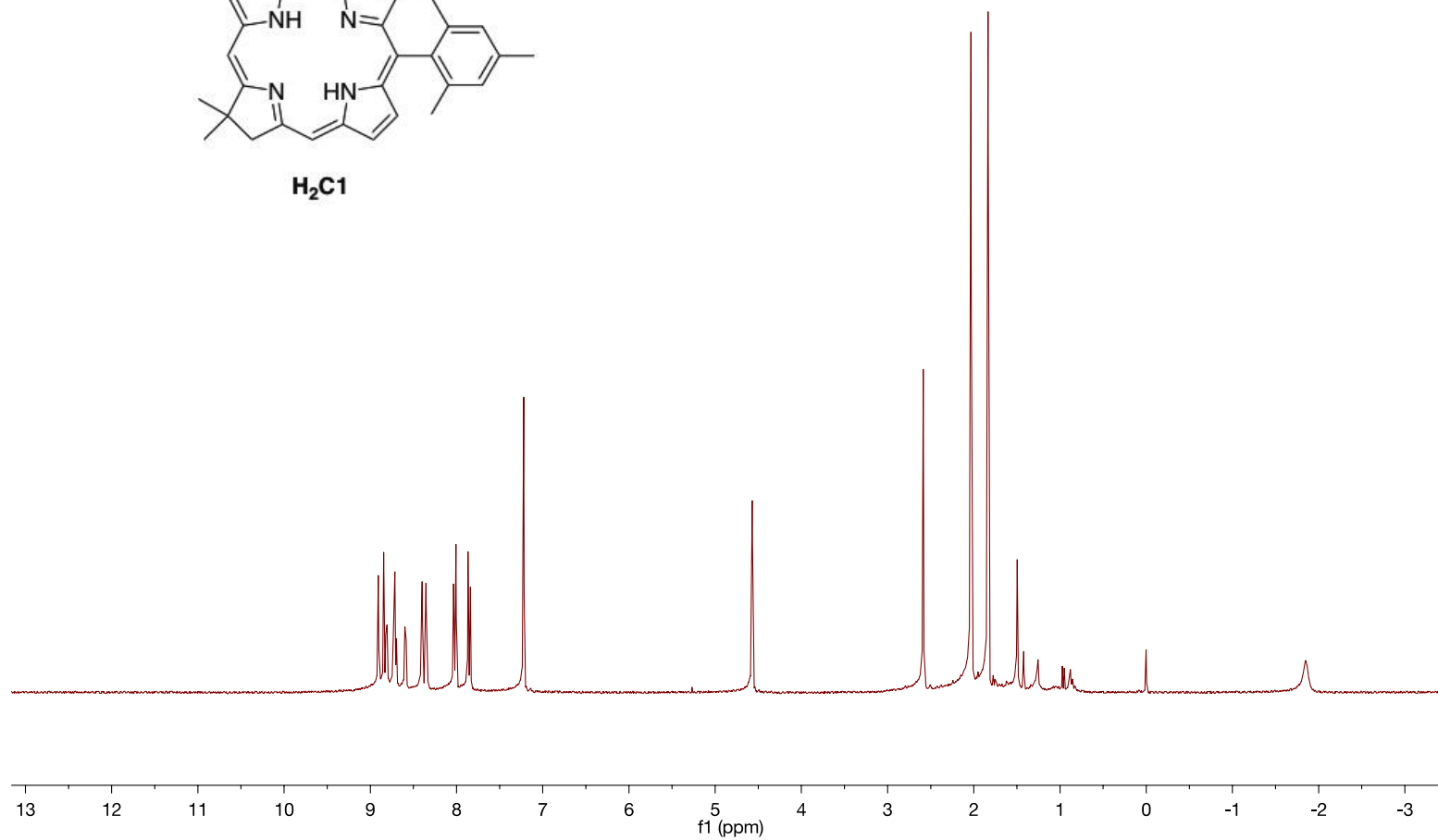
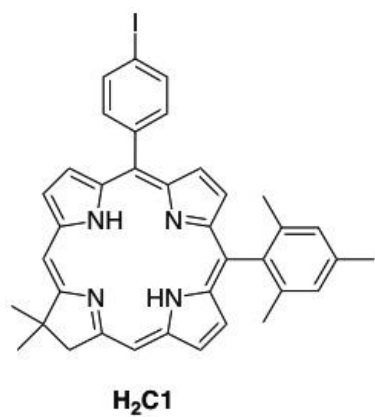


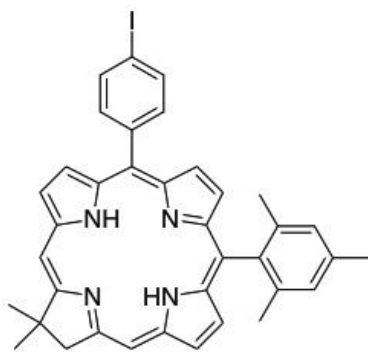
170821_ZnChlorin-Iodo #61-88 RT: 0.27-0.39 AV: 28 NL: 4.79E5
T: FTMS + p ESI Full ms [150.00-1000.00]



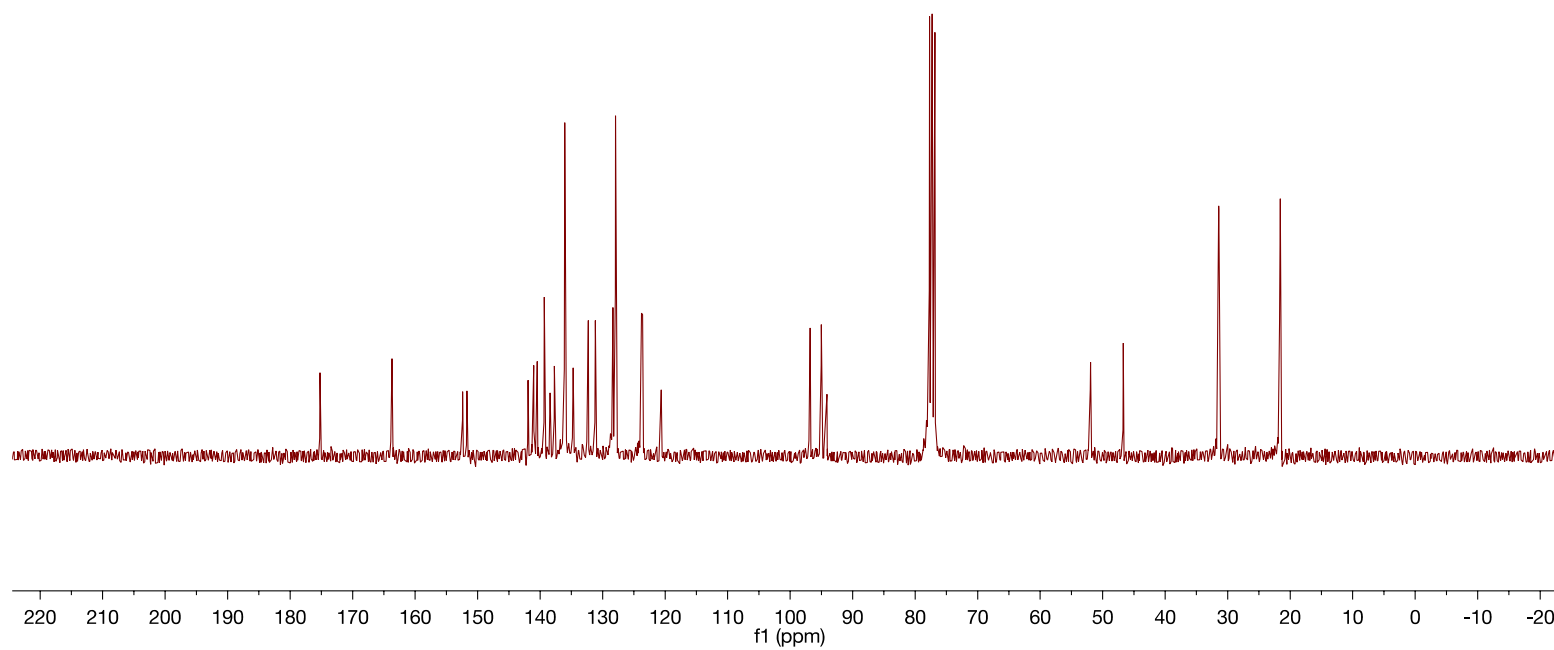
NL:
4.79E5
170821_ZnChlorin-Iodo#61-88 RT:
0.27-0.39 AV: 28 T:
FTMS + p ESI Full ms
[150.00-1000.00]

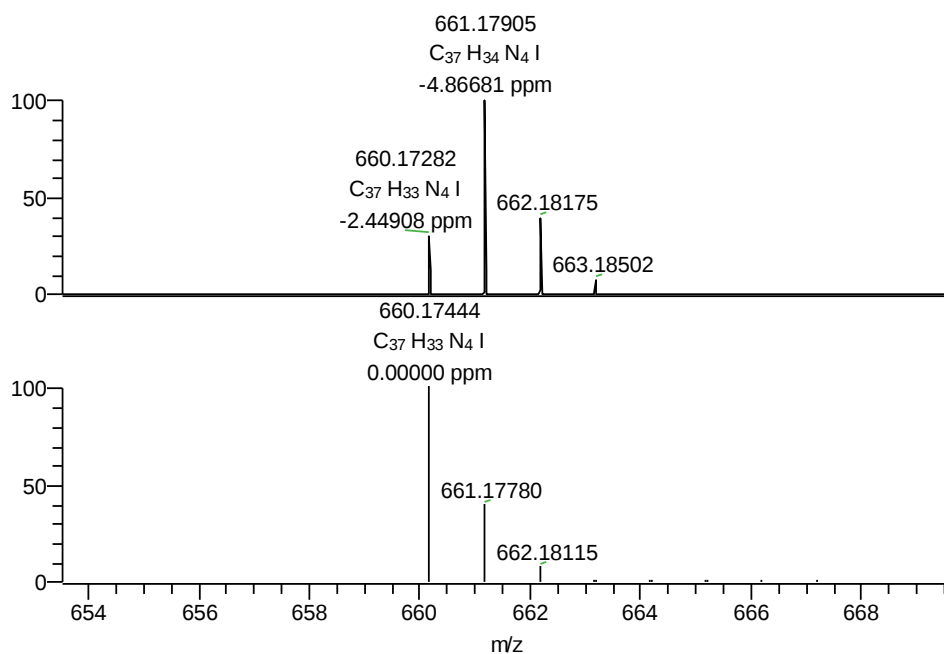
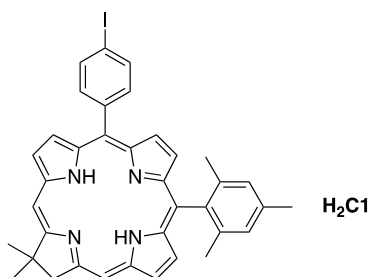
NL:
3.21E5
 $C_{37}H_{31}N_4 Zn$:
 $C_{37}H_{31}I N_4 Zn_1$
pa Chrg 1





H₂C1

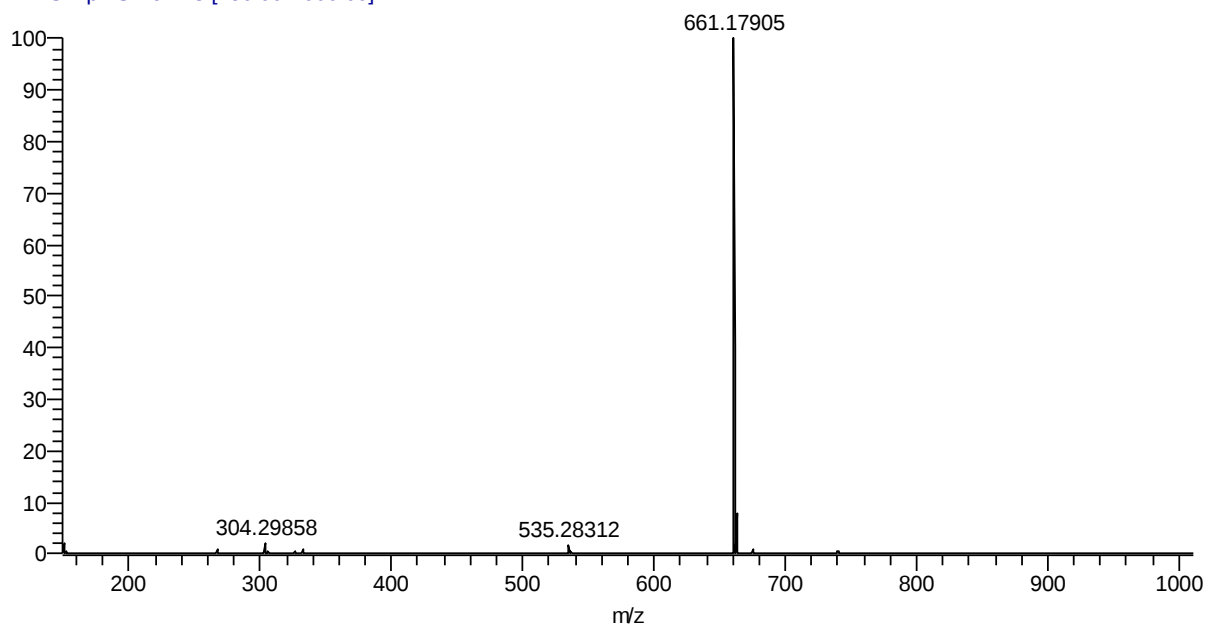


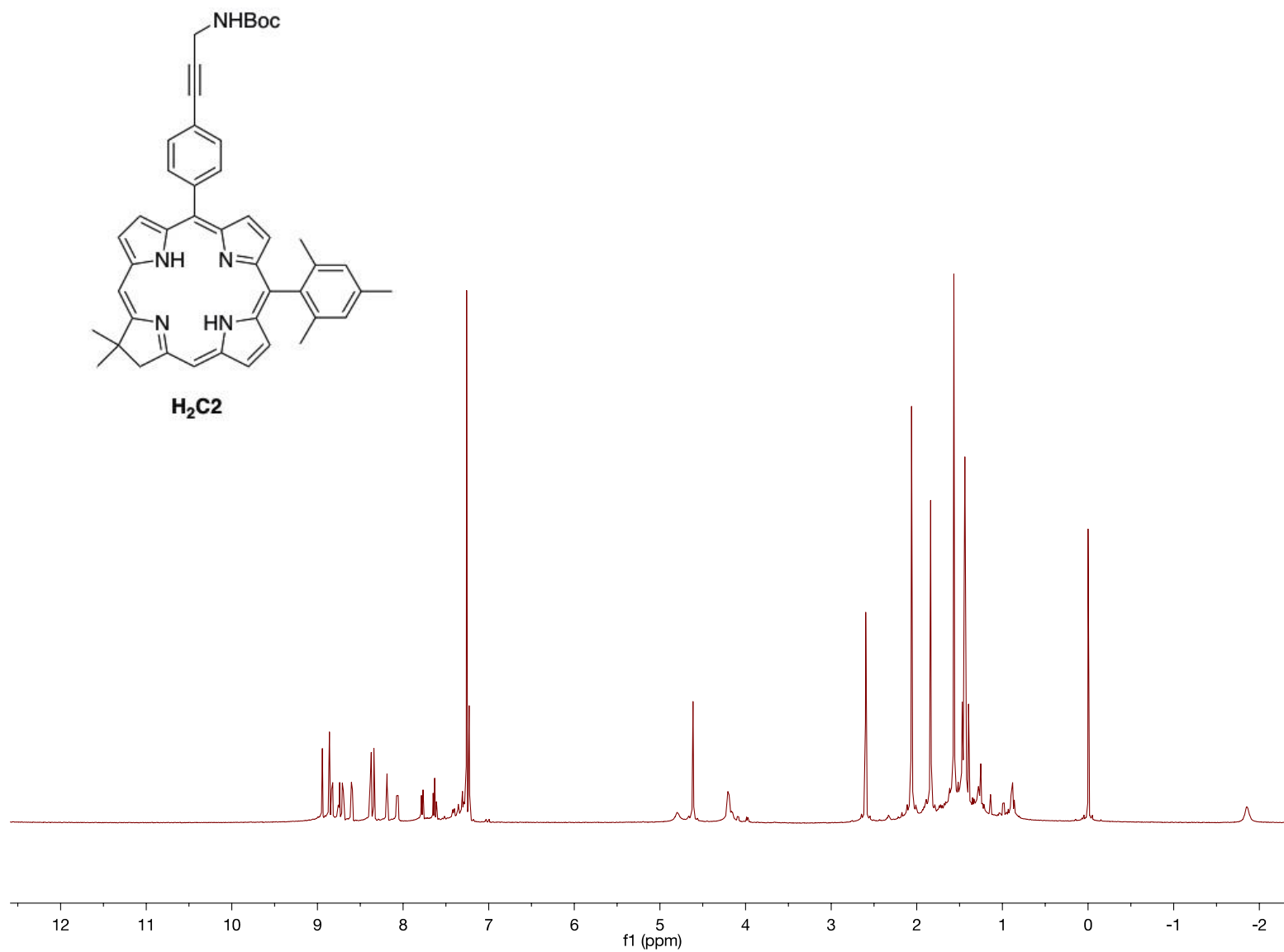


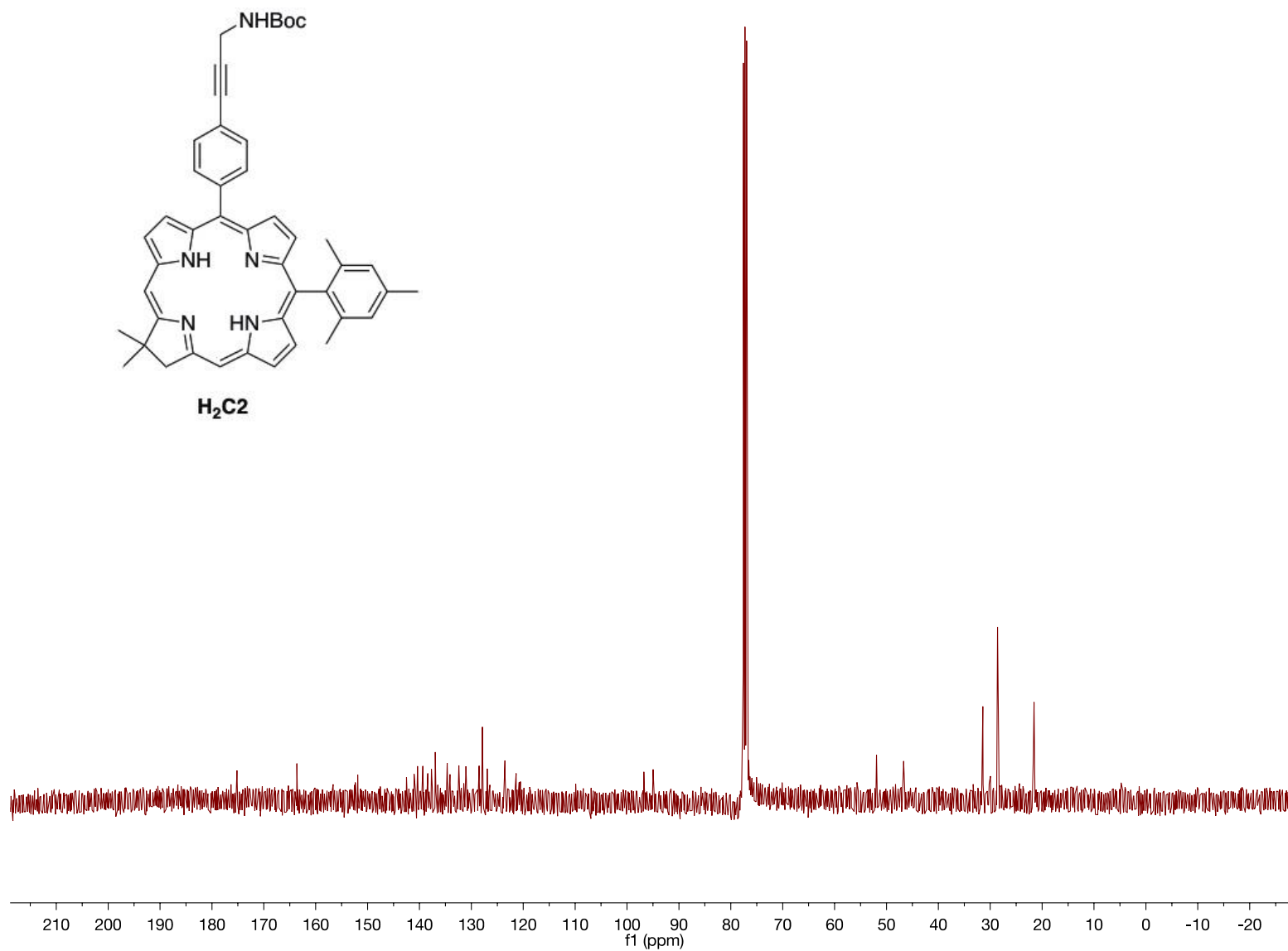
NL:
4.80E6
170822_FbChlorin-
Iodo#125-300 RT:
0.56-1.34 AV: 176 T:
FTMS + p ESI Full ms
[150.00-1000.00]

NL:
6.59E5
C₃₇ H₃₃ I N₄:
C₃₇ H₃₃ I₁ N₄
pa Chrg 1

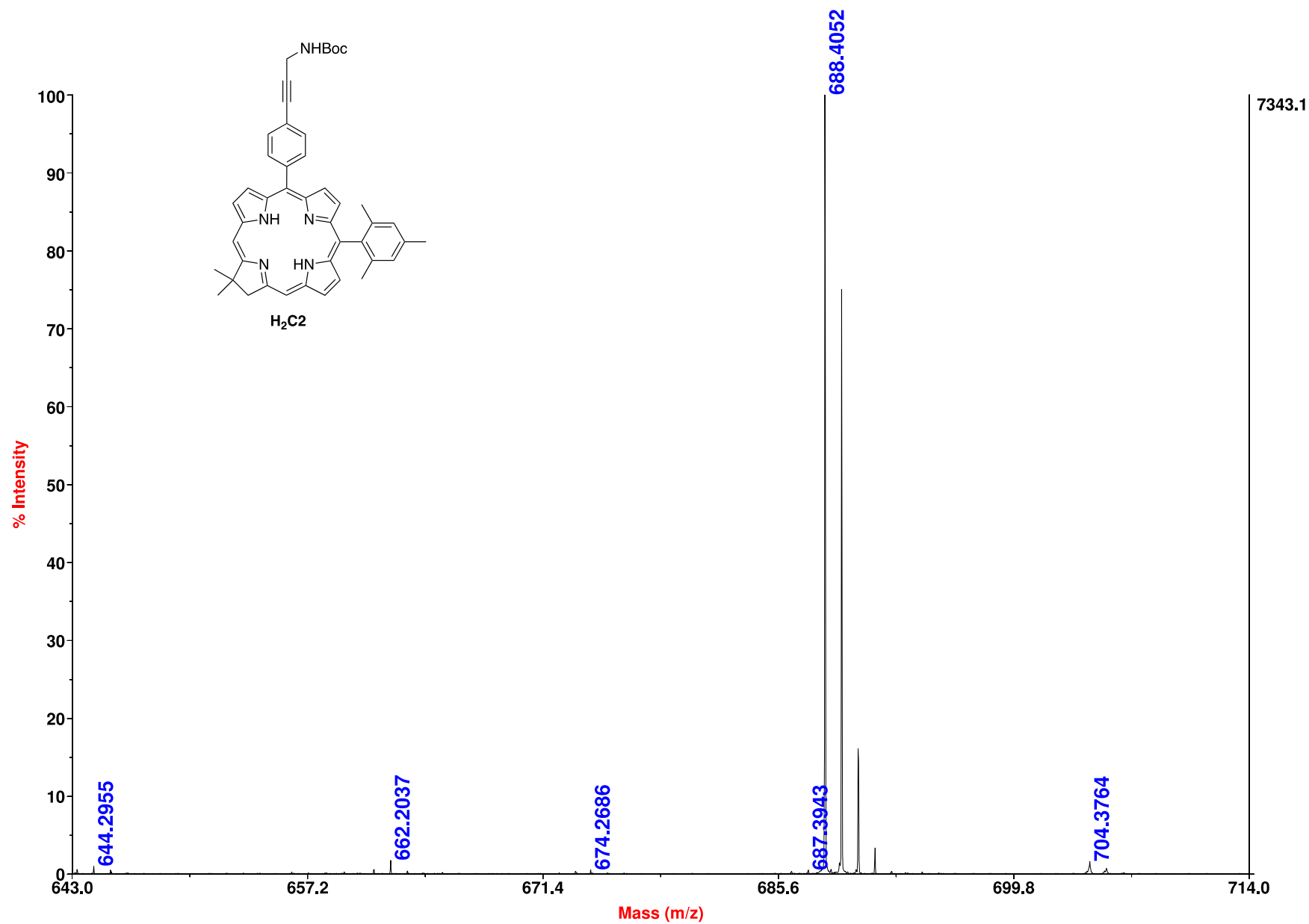
170822_FbChlorin-Iodo #125-300 RT: 0.56-1.34 AV: 176 NL: 4.80E6
T: FTMS + p ESI Full ms [150.00-1000.00]

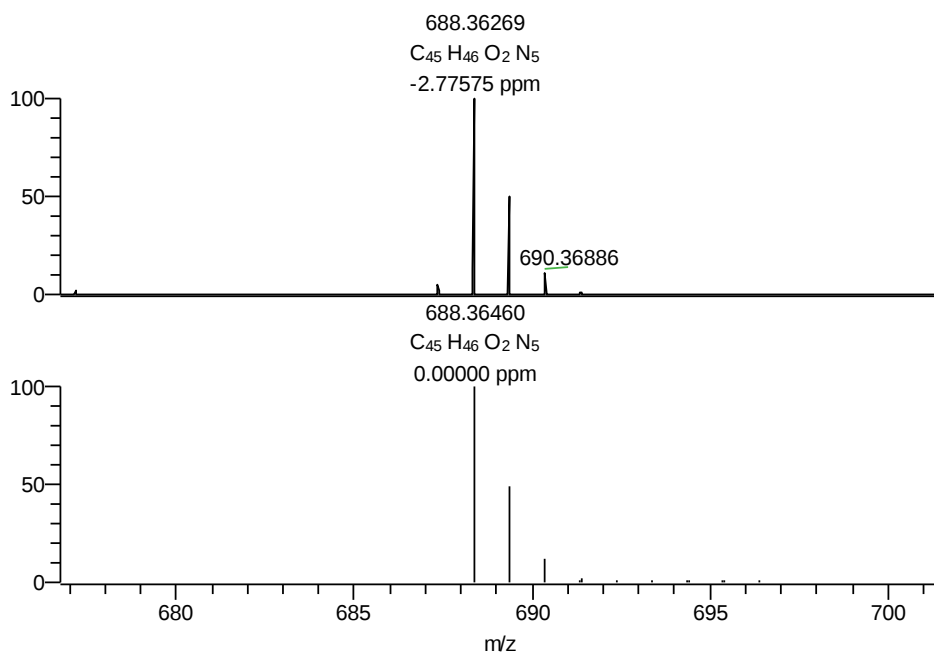
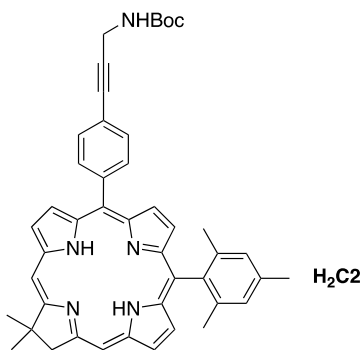






TOF/TOF™ Reflector Spec #1[BP = 535.1, 11119]

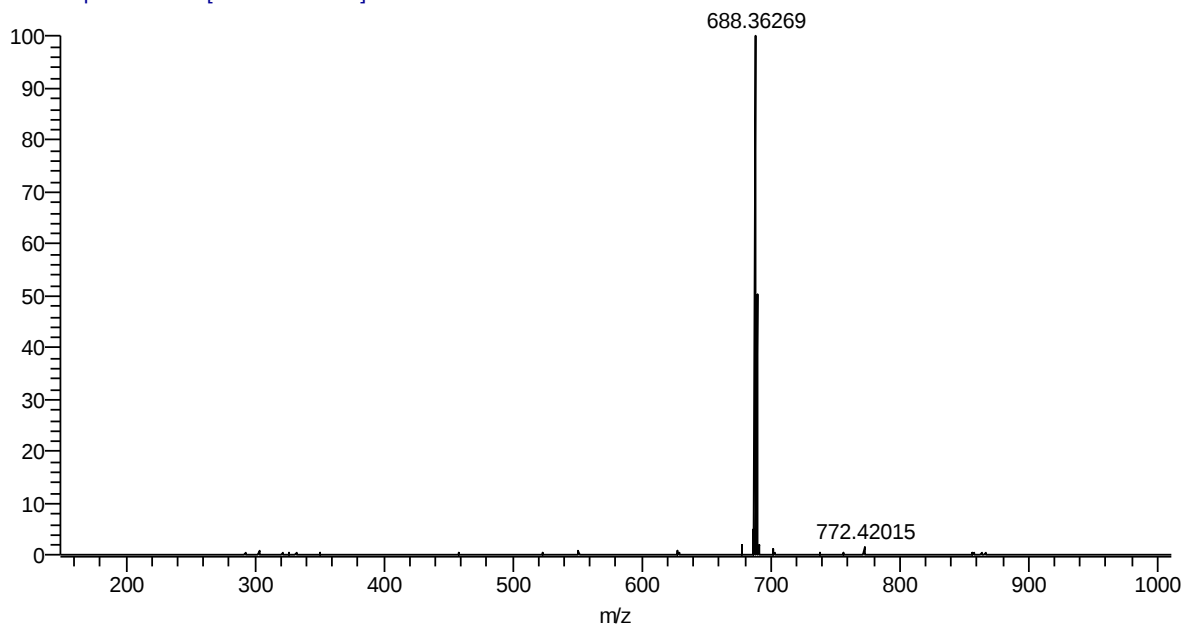


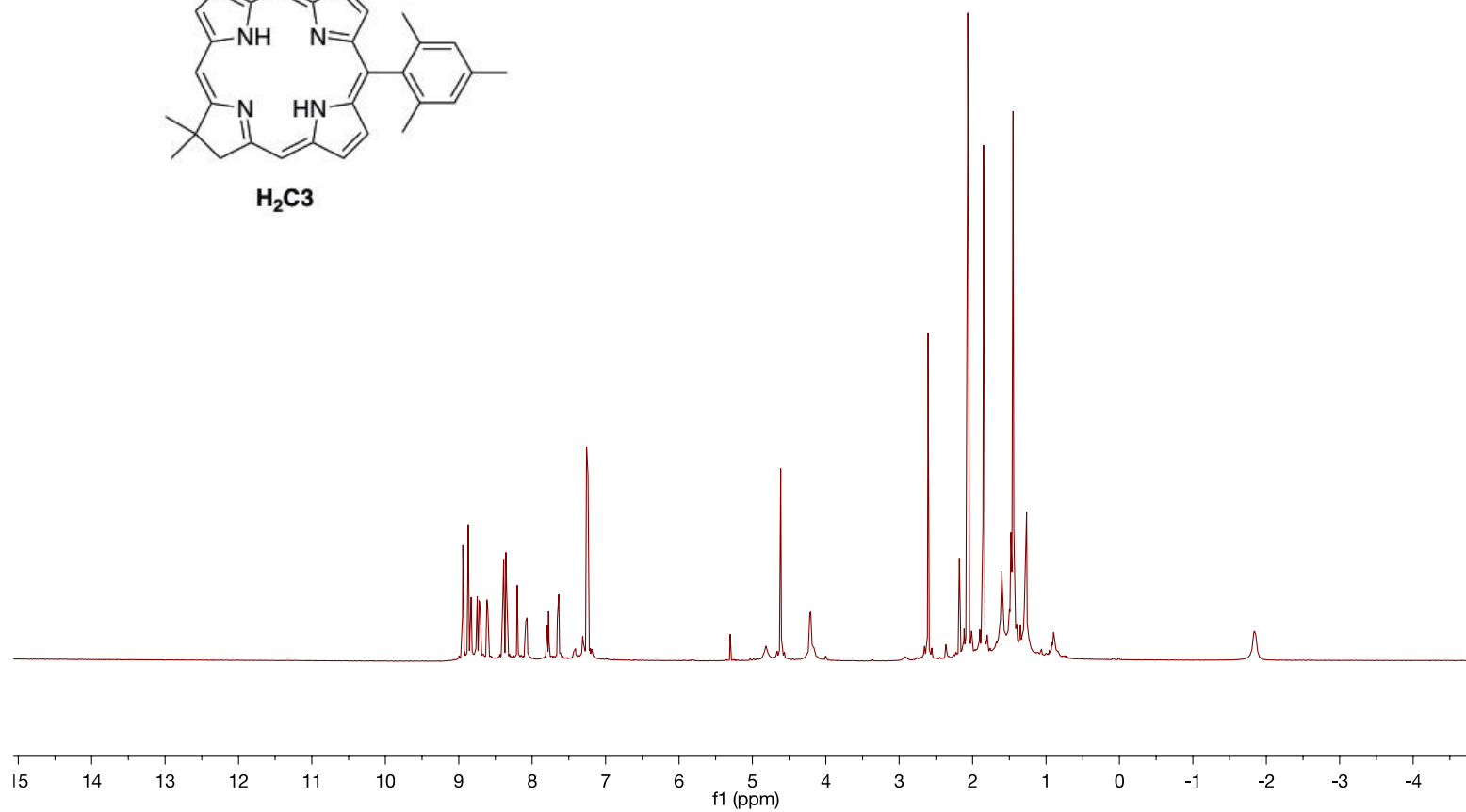
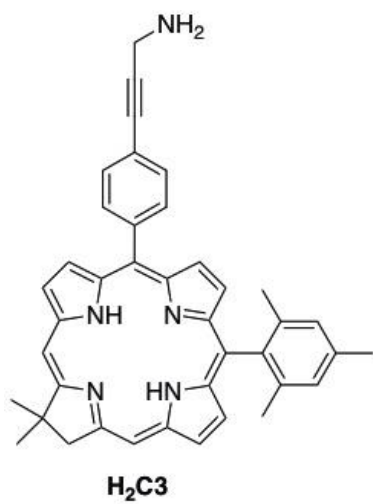


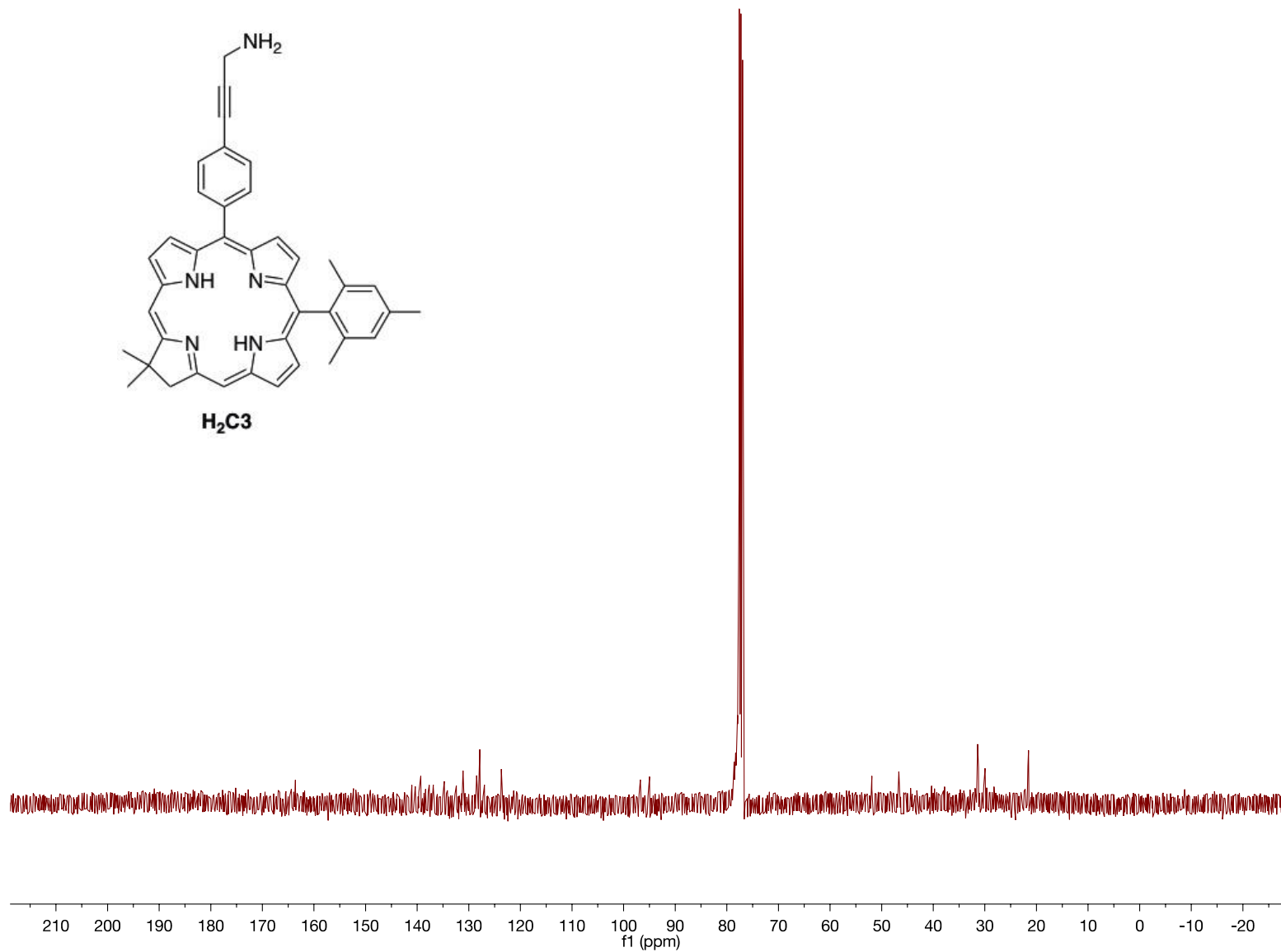
NL:
8.94E5
170819_FbChlorin-
Boc#302-307 RT:
1.37-1.39 AV: 6 T:
FTMS + p ESI Full ms
[150.00-1000.00]

NL:
5.99E5
C₄₅ H₄₅ O₂ N₅ +H:
C₄₅ H₄₆ O₂ N₅
pa Chrg 1

170819_FbChlorin-Boc #302-307 RT: 1.37-1.39 AV: 6 NL: 8.94E5
T: FTMS + p ESI Full ms [150.00-1000.00]

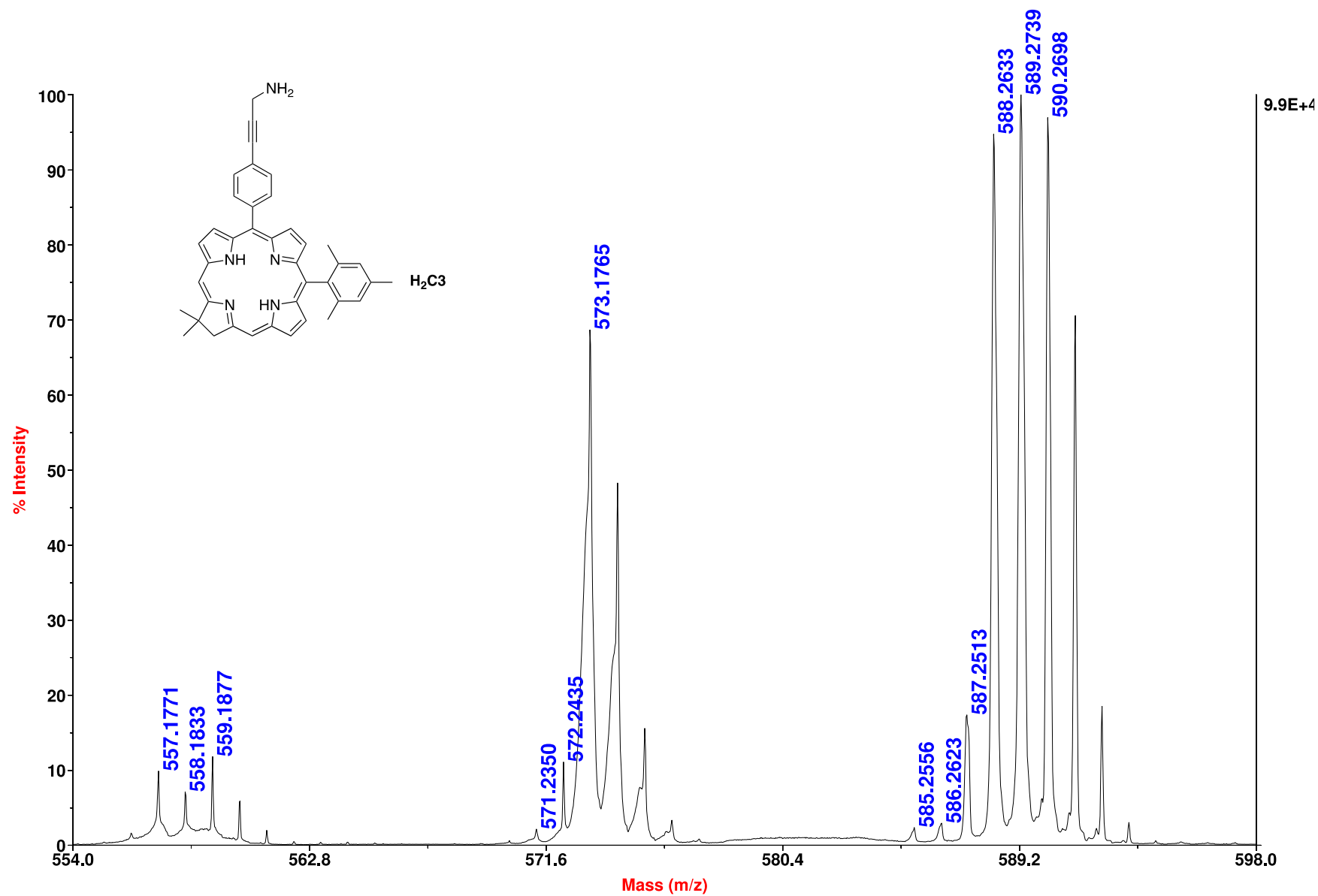


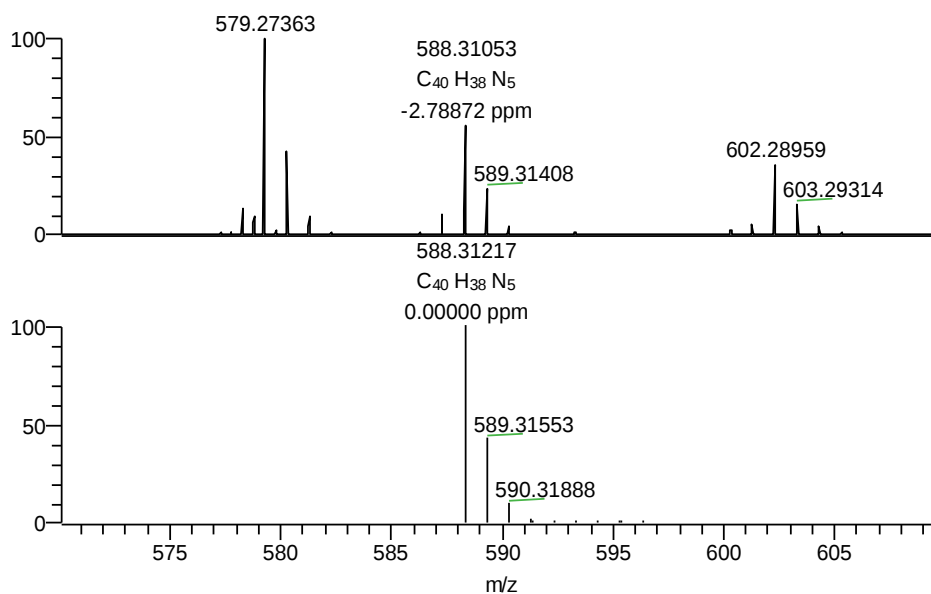
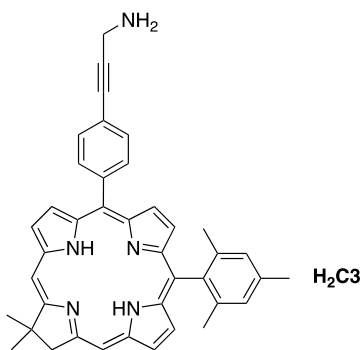




AB Sciex TOF/TOF™ Series Explorer™ 72098

TOF/TOF™ Reflector Spec #1[BP = 589.3, 99008]

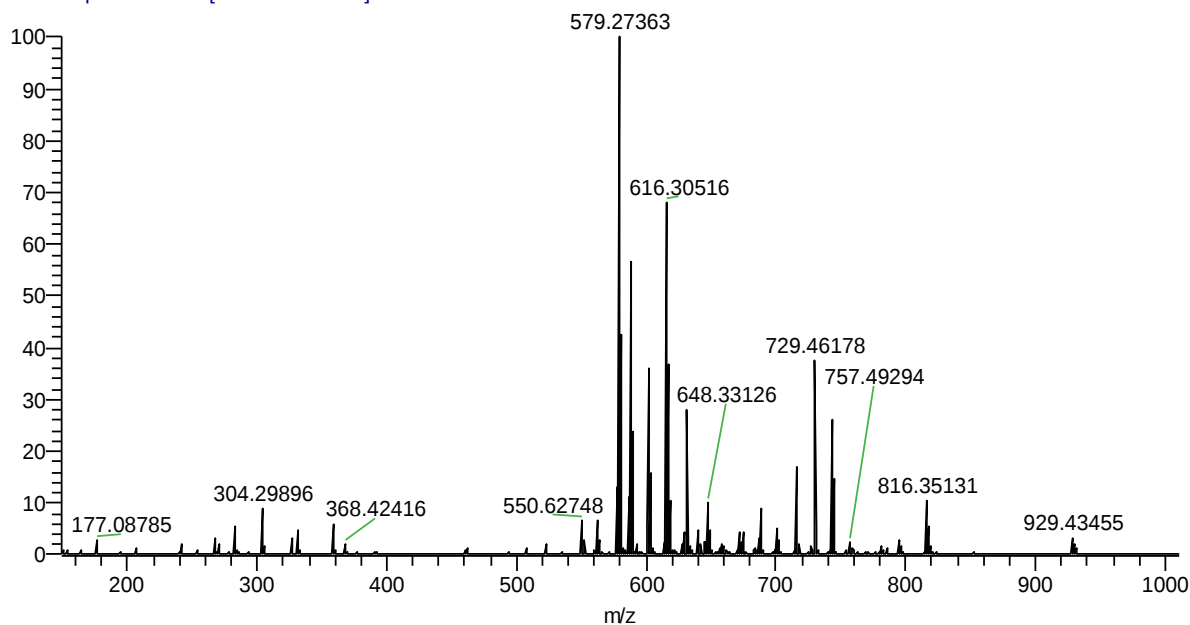


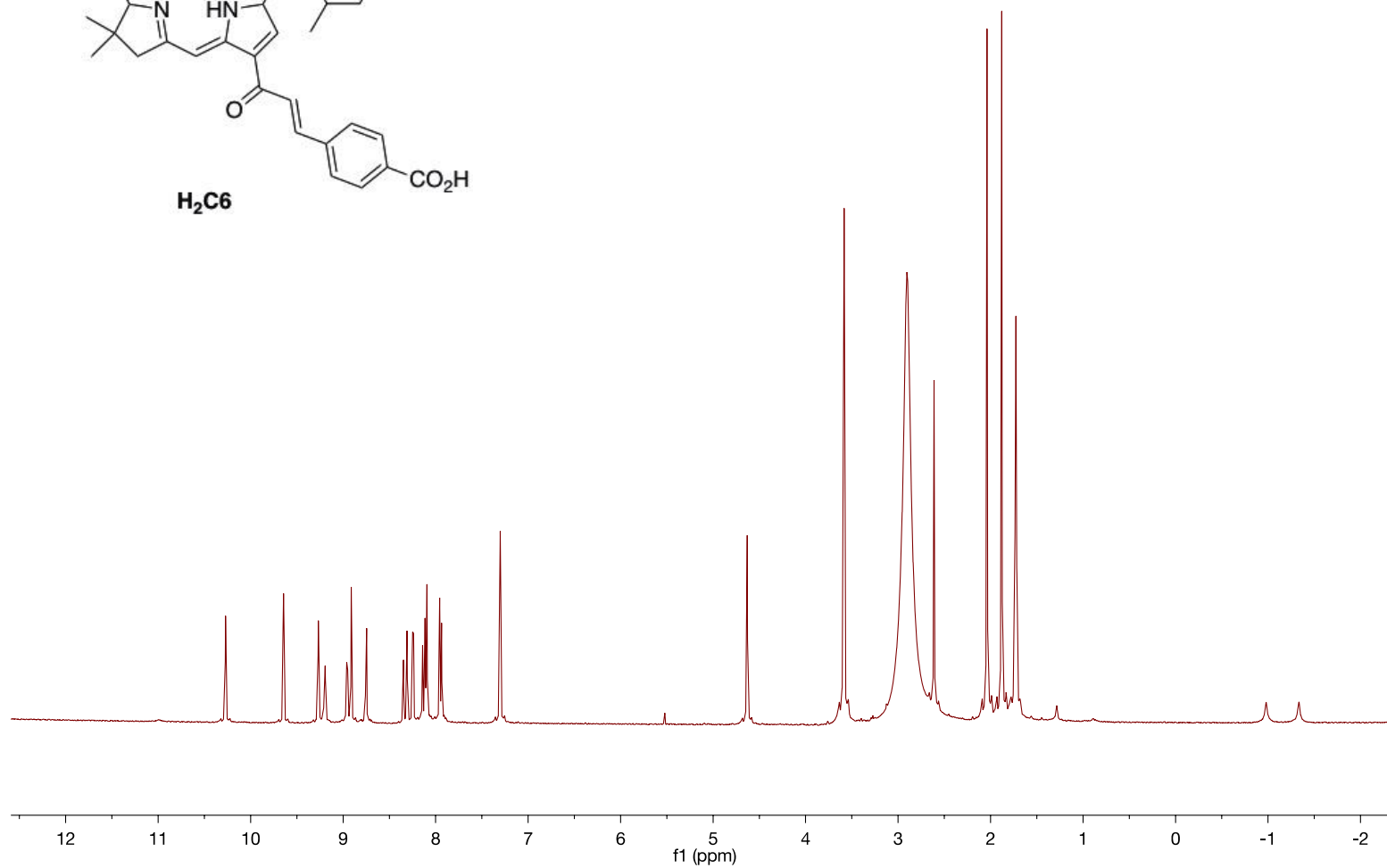
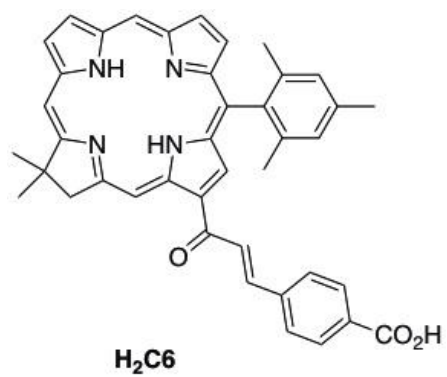


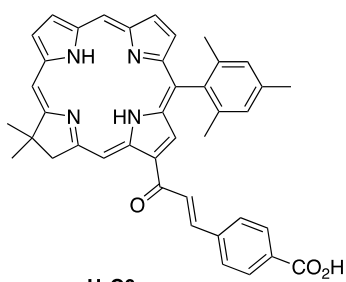
NL:
2.25E5
170820_FbChlorin-
NH2#216-334 RT:
0.96-1.49 AV: 119 T:
FTMS + p ESI Full ms
[150.00-1000.00]

NL:
6.36E5
C₄₀ H₃₇ N₅ +H:
C₄₀ H₃₈ N₅
pa Chrg 1

170820_FbChlorin-NH2 #216-334 RT: 0.96-1.49 AV: 119 NL: 2.25E5
T: FTMS + p ESI Full ms [150.00-1000.00]

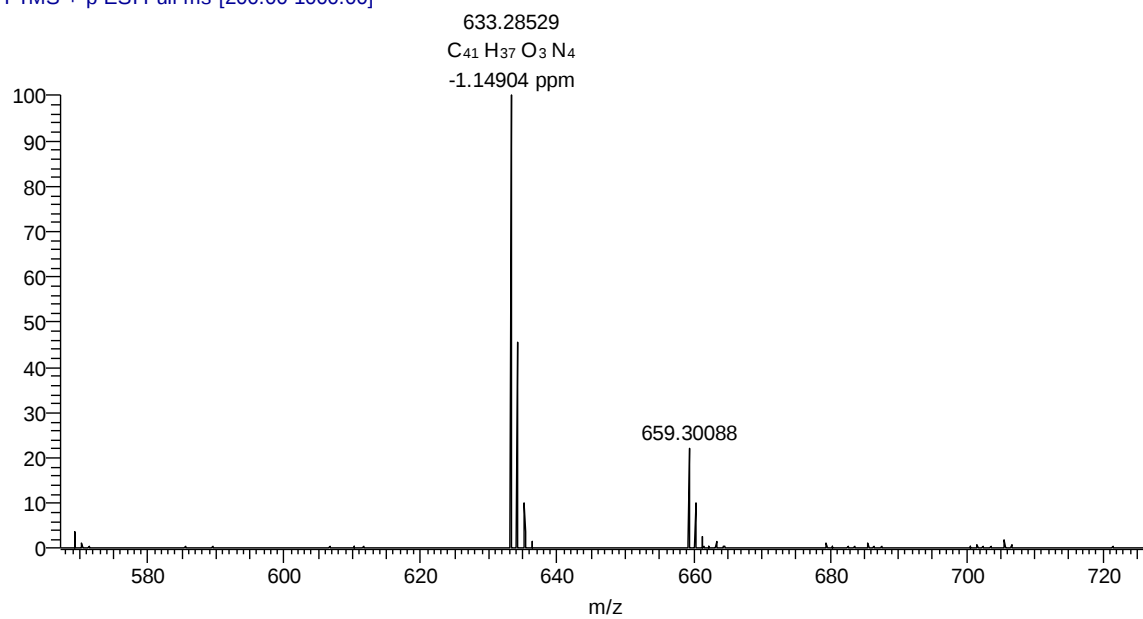


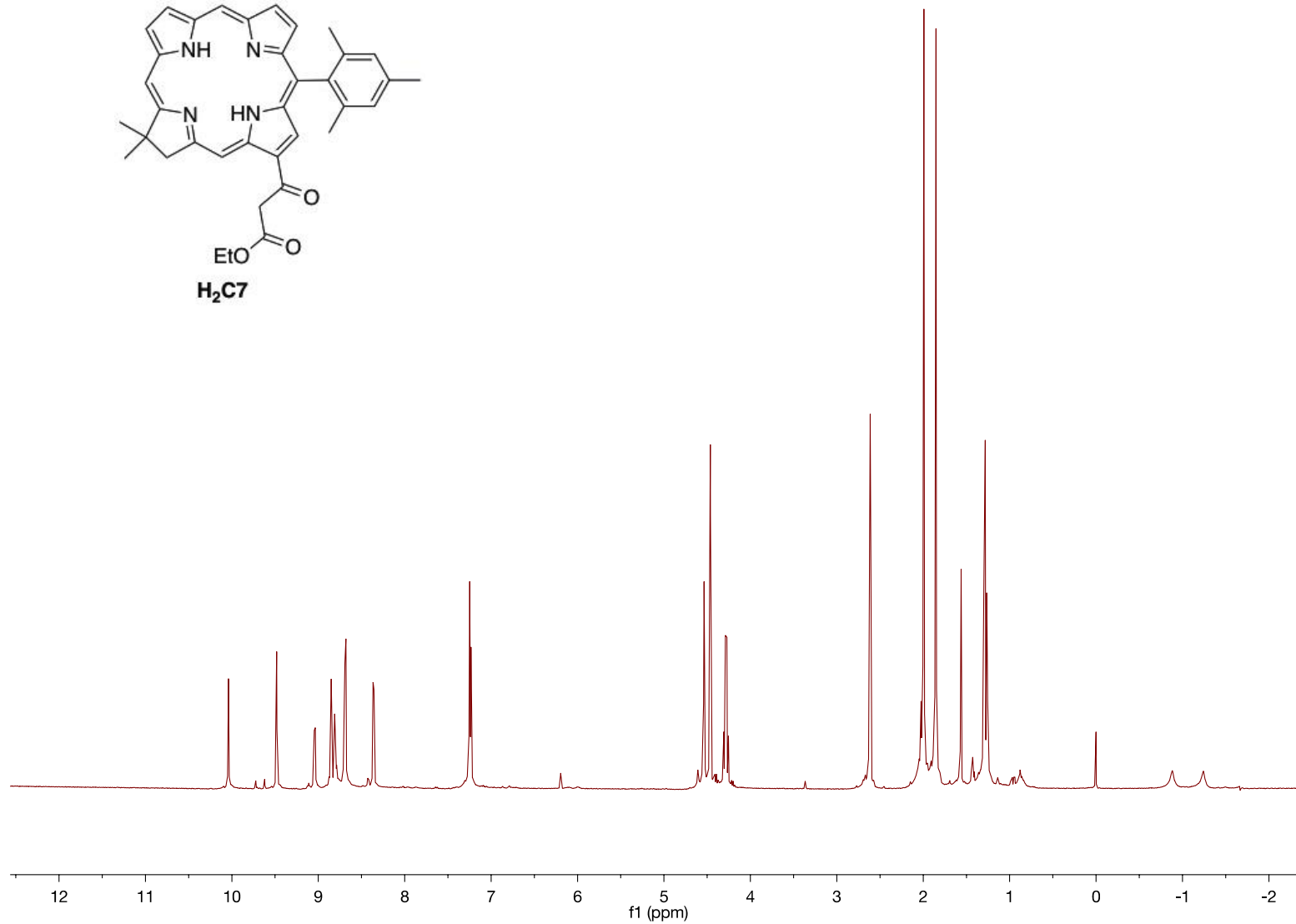
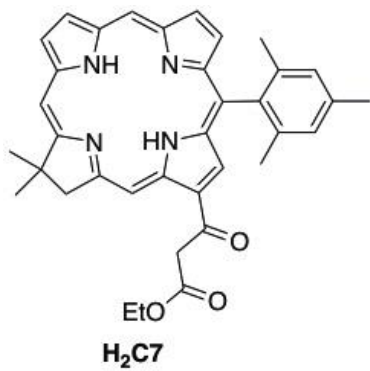


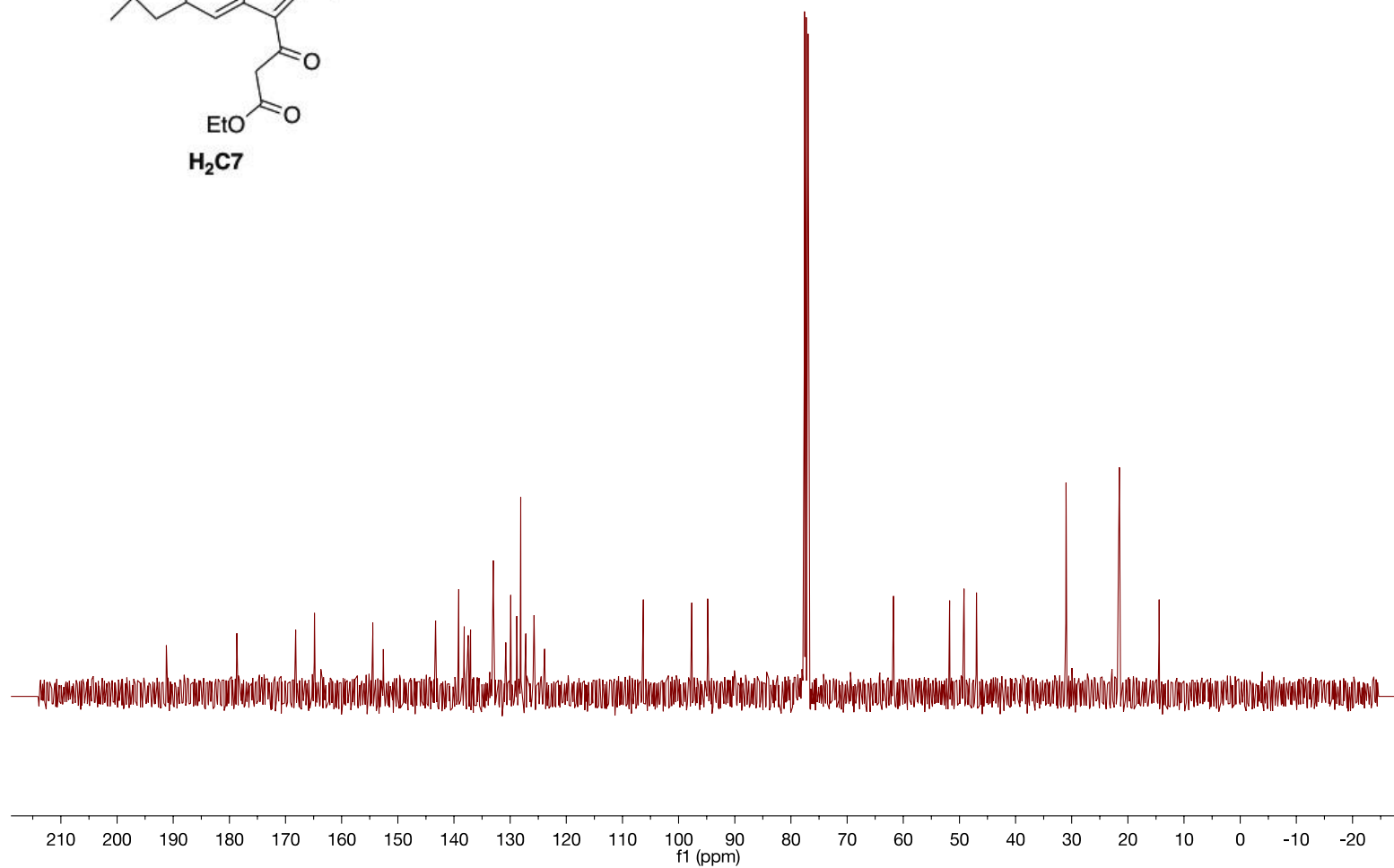
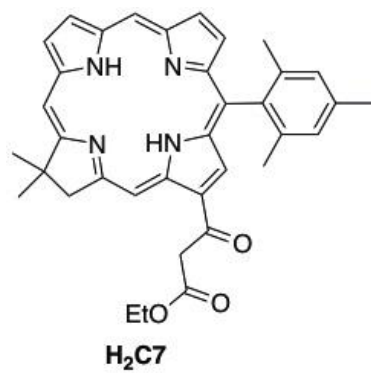


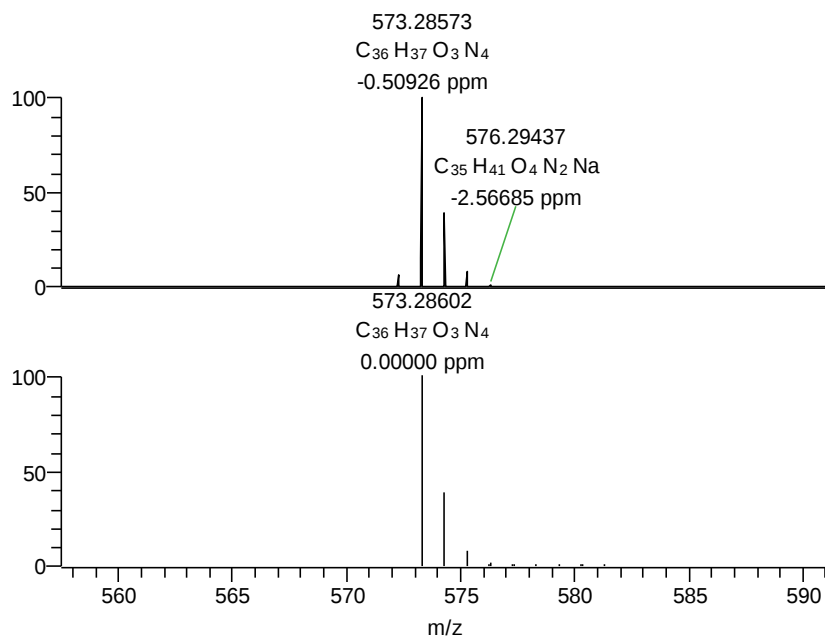
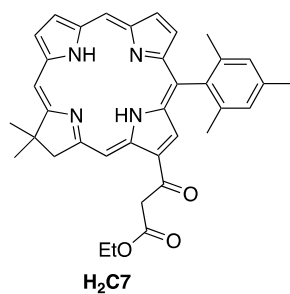
H₂C6

141760_Chalcone #459-501 RT: 2.75-3.01 Av. 4.5 nL: 3.22E6
T: FTMS + p ESI Full ms [200.00-1000.00]





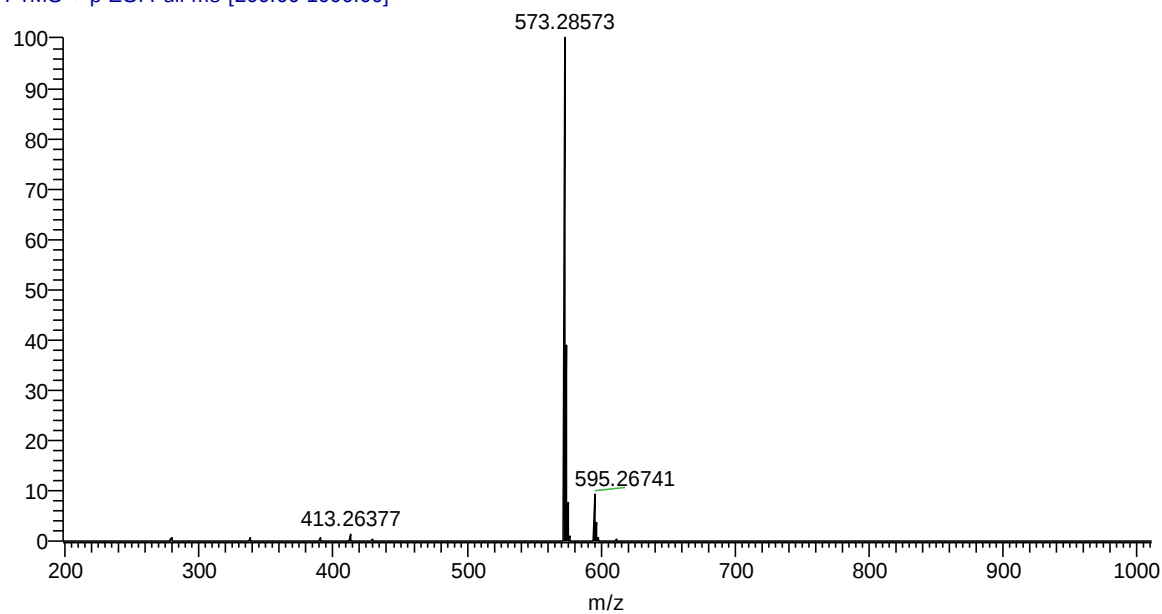


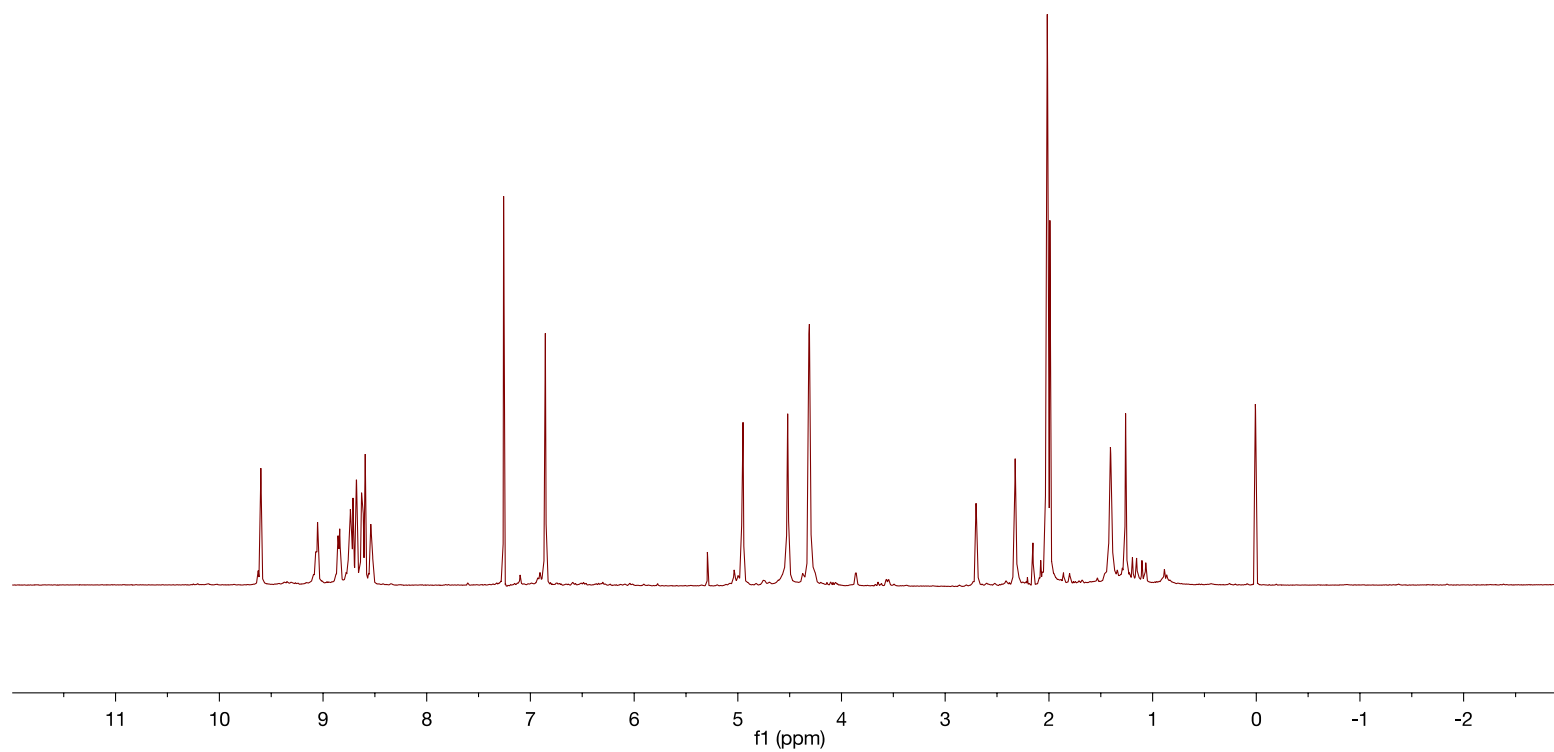
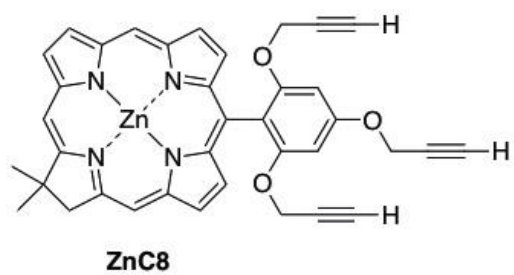


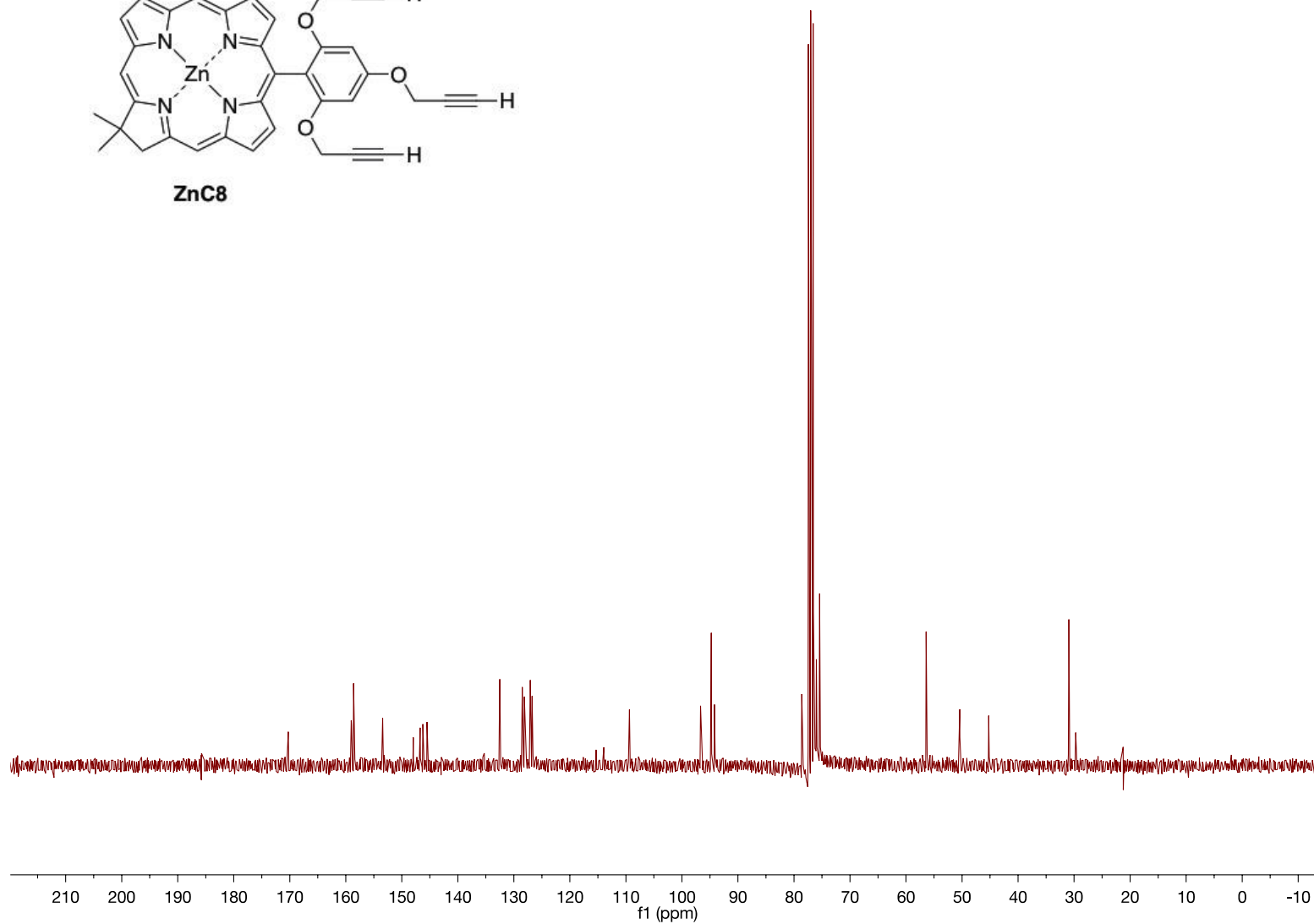
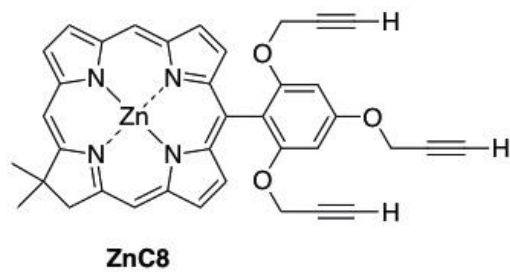
NL:
9.18E6
161981_ketoester#201-214 RT:
1.57-1.66 AV: 14 SB: 51
0.04-0.29 , 1.86-2.01 T: FTMS
+ p ESI Full ms
[200.00-1000.00]

NL:
6.61E5
C₃₆H₃₆O₃N₄ + H:
C₃₆H₃₇O₃N₄
pa Chrg 1

161981_ketoester #201-214 RT: 1.57-1.66 AV: 14 SB: 36 0.06-0.24 , 1.88-1.98 NL: 9.18E6
T: FTMS + p ESI Full ms [200.00-1000.00]

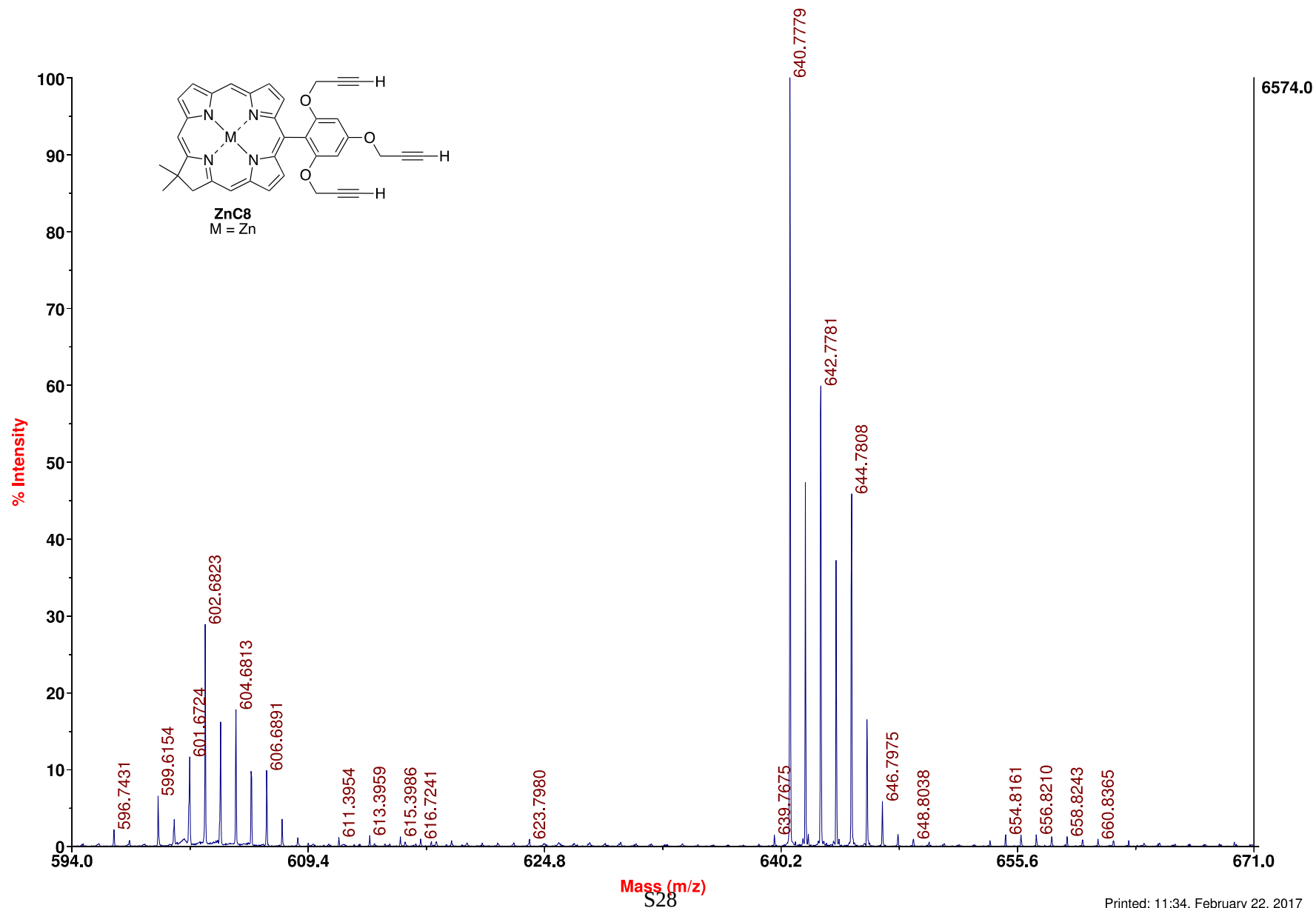


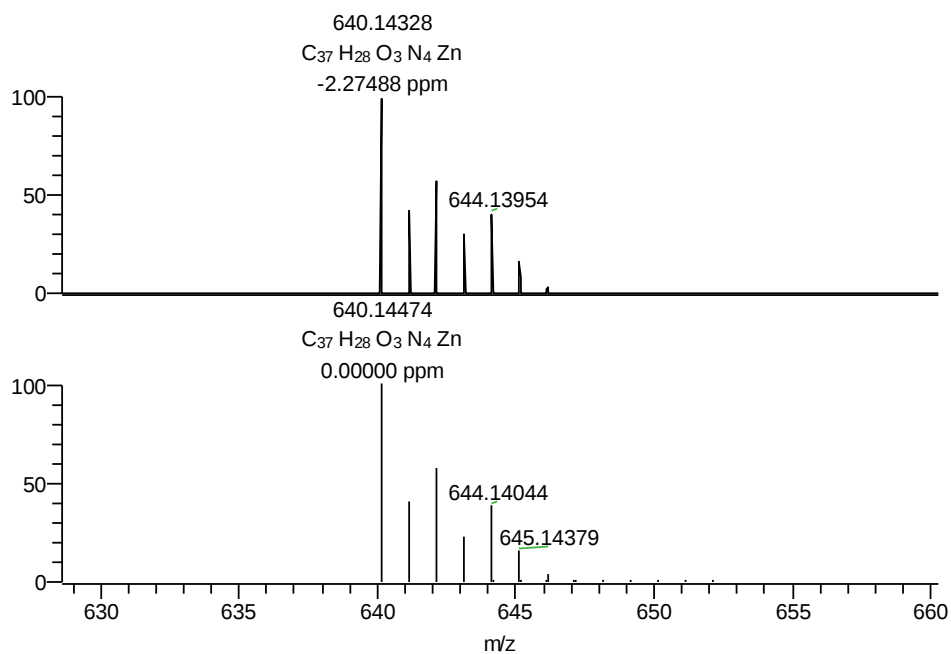
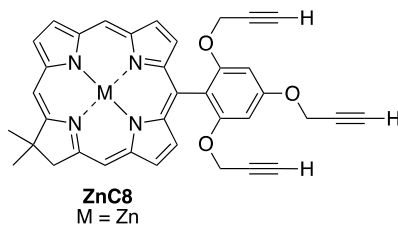




AB Sciex TOF/TOF™ Series Explorer™ 20981201

TOF/TOF™ Reflector Spec #1[BP = 640.8, 6574]

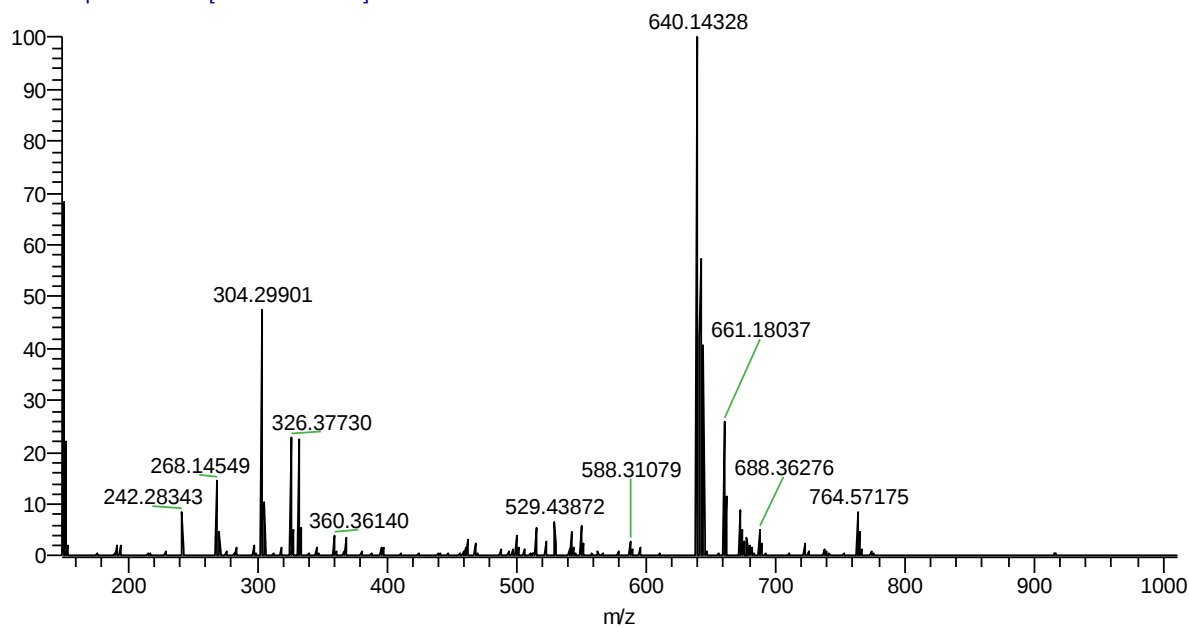


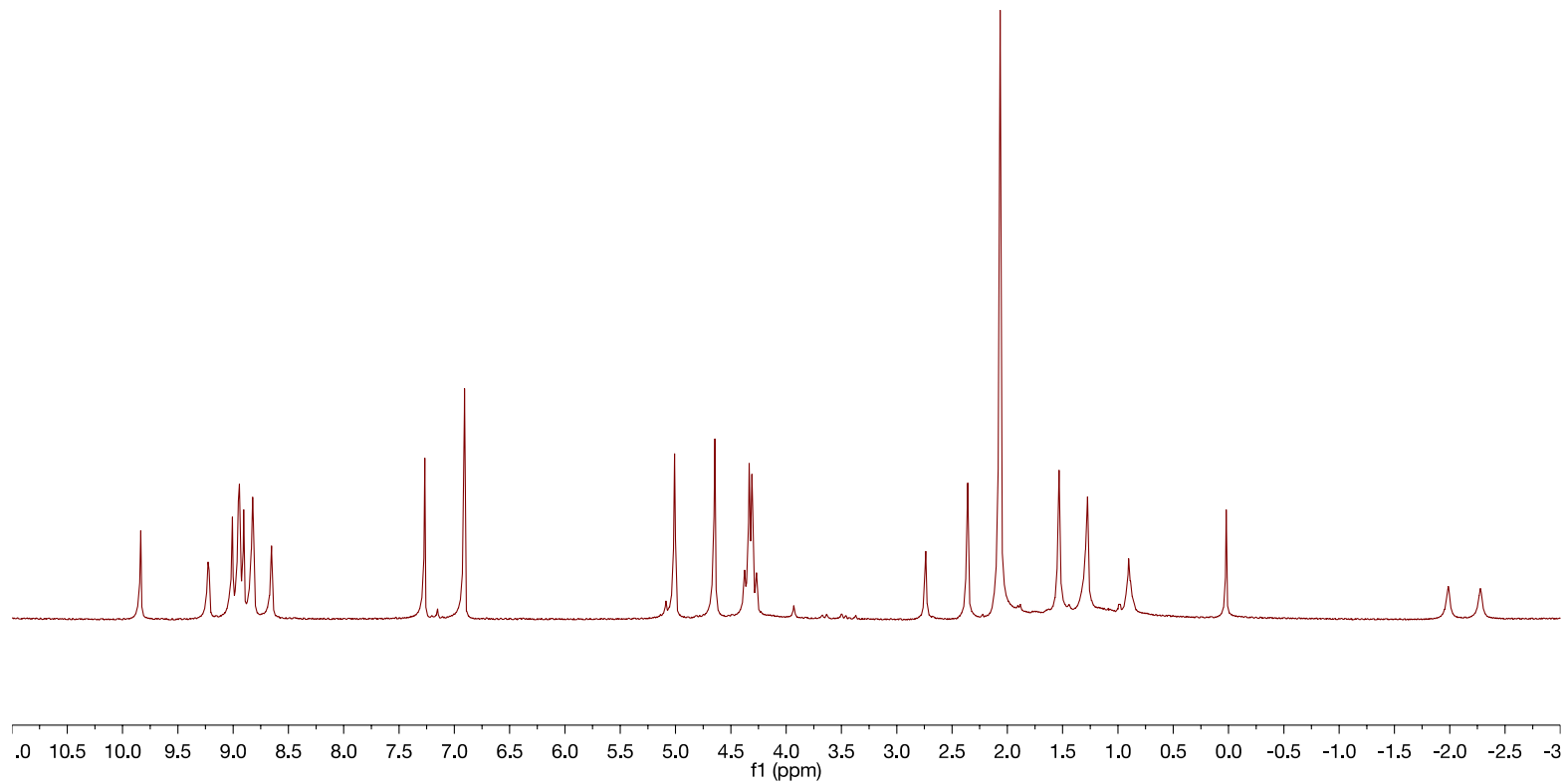
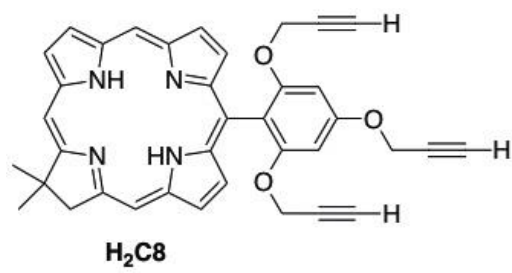


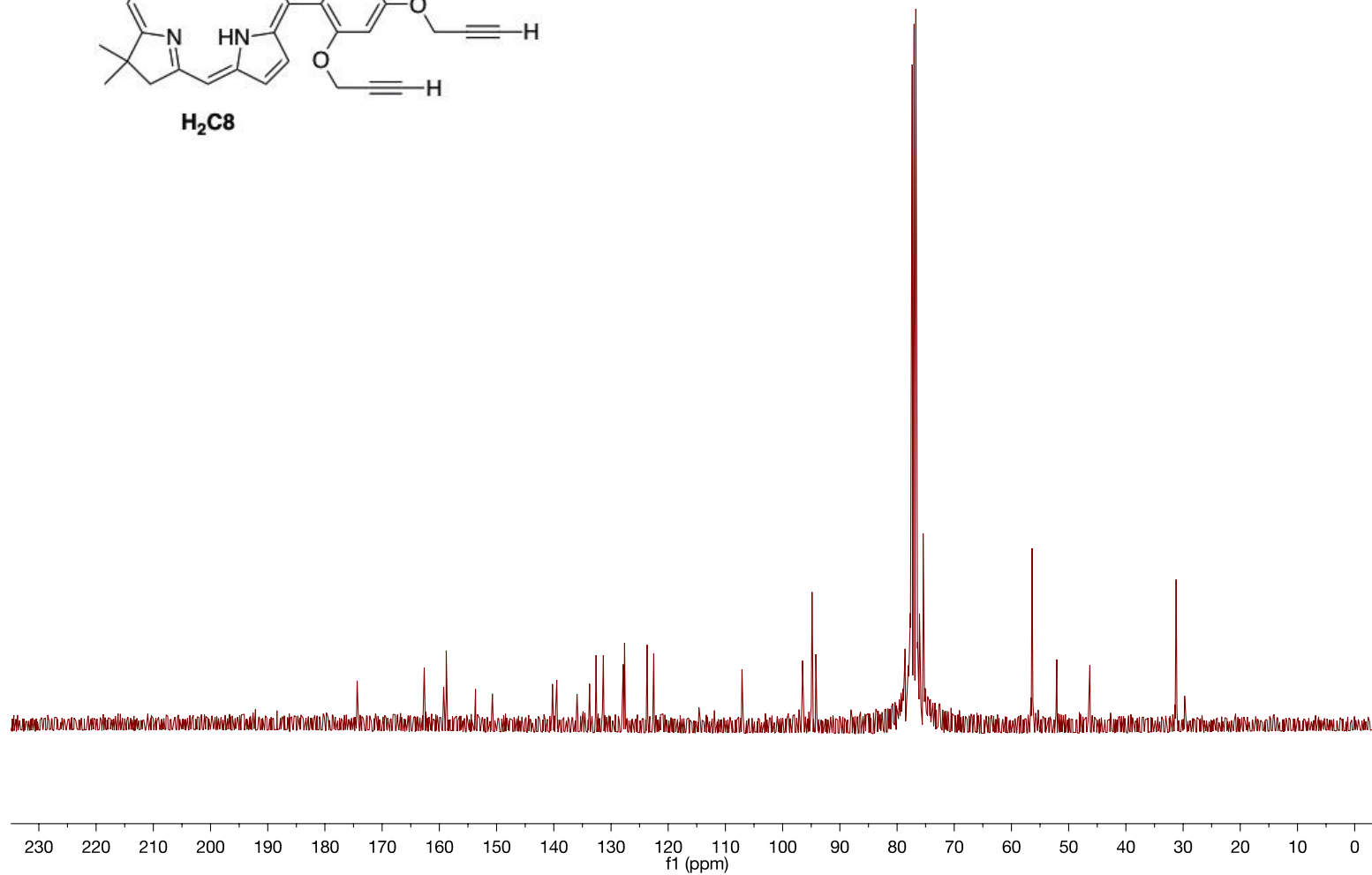
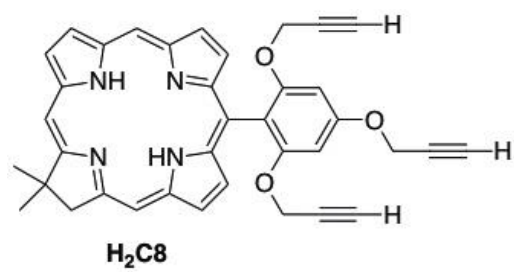
NL:
4.68E5
170823_ZnChlorin-
ethyne#5-185 RT:
0.02-0.82 AV: 181 T:
FTMS + p ESI Full ms
[150.00-1000.00]

NL:
3.18E5
 $C_{37}H_{28}N_4O_3Zn$:
 $C_{37}H_{28}N_4O_3Zn_1$
pa Chrg 1

170823_ZnChlorin-ethyne #5-185 RT: 0.02-0.82 AV: 181 NL: 4.68E5
T: FTMS + p ESI Full ms [150.00-1000.00]

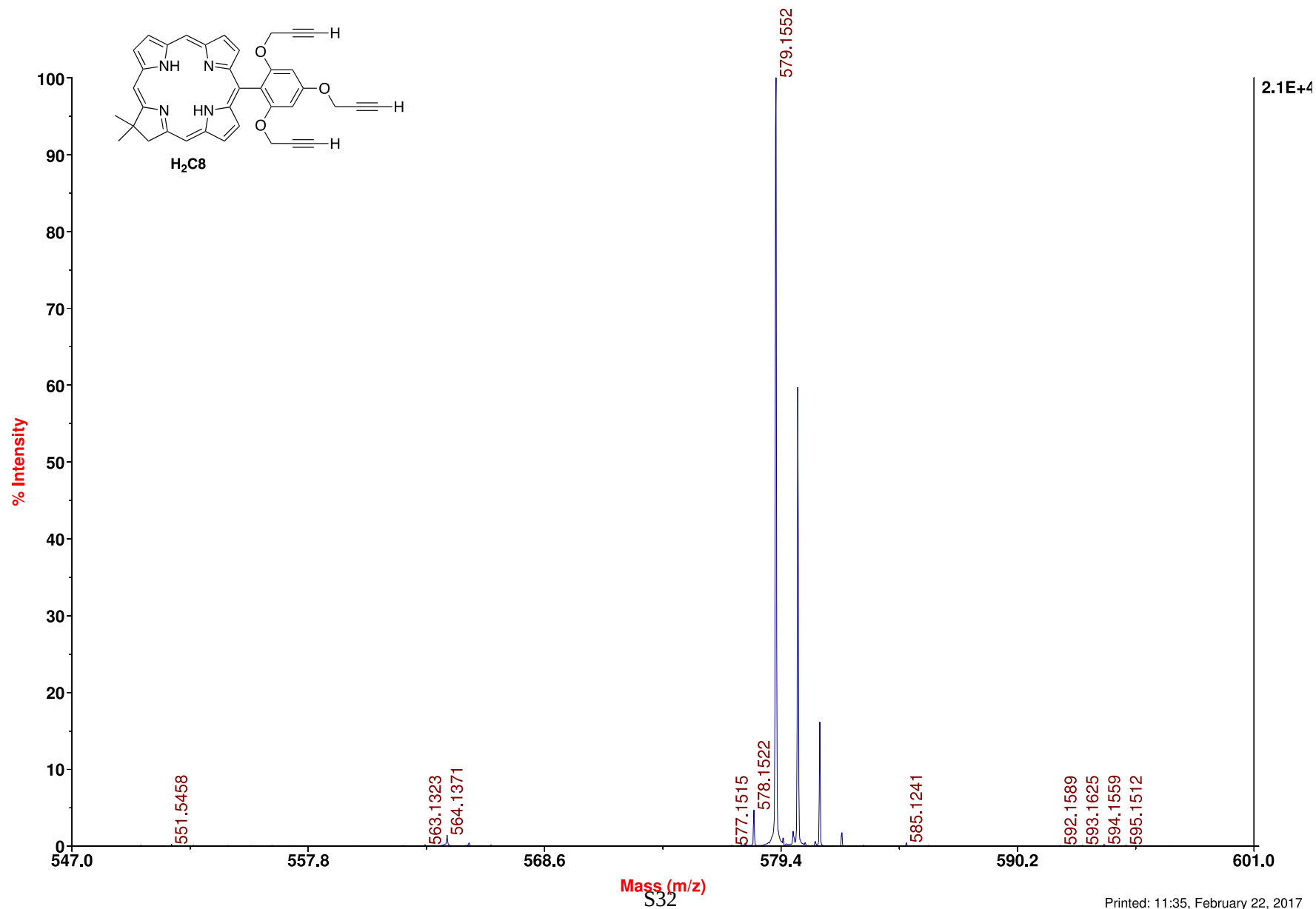


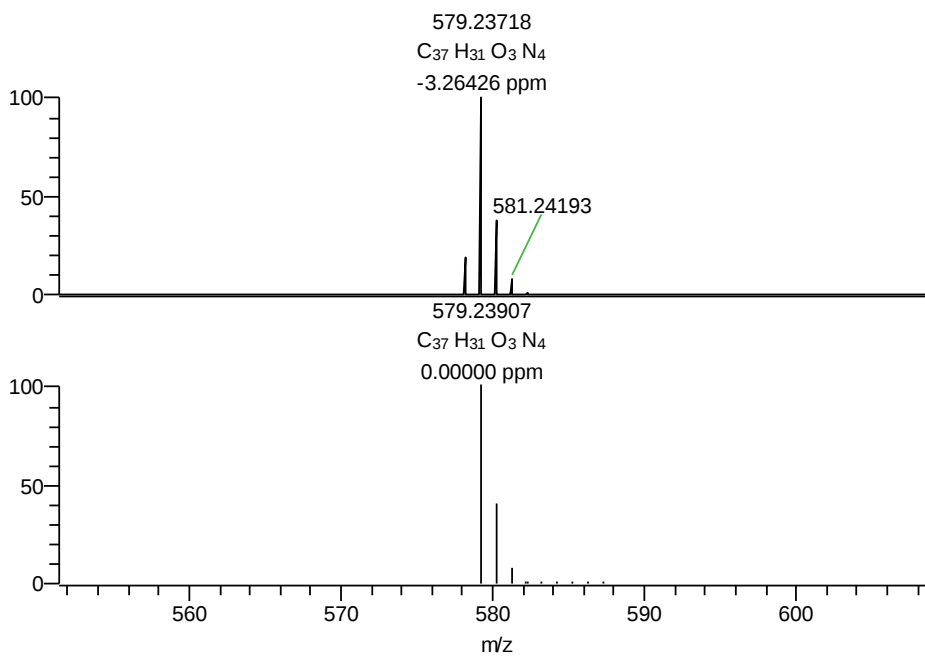
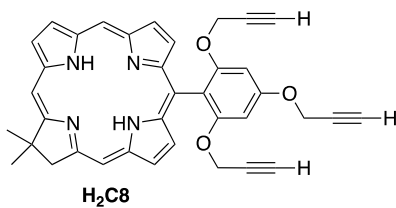




AB Sciex TOF/TOF™ Series Explorer™ 20981201

TOF/TOF™ Reflector Spec #1[BP = 579.2, 21493]

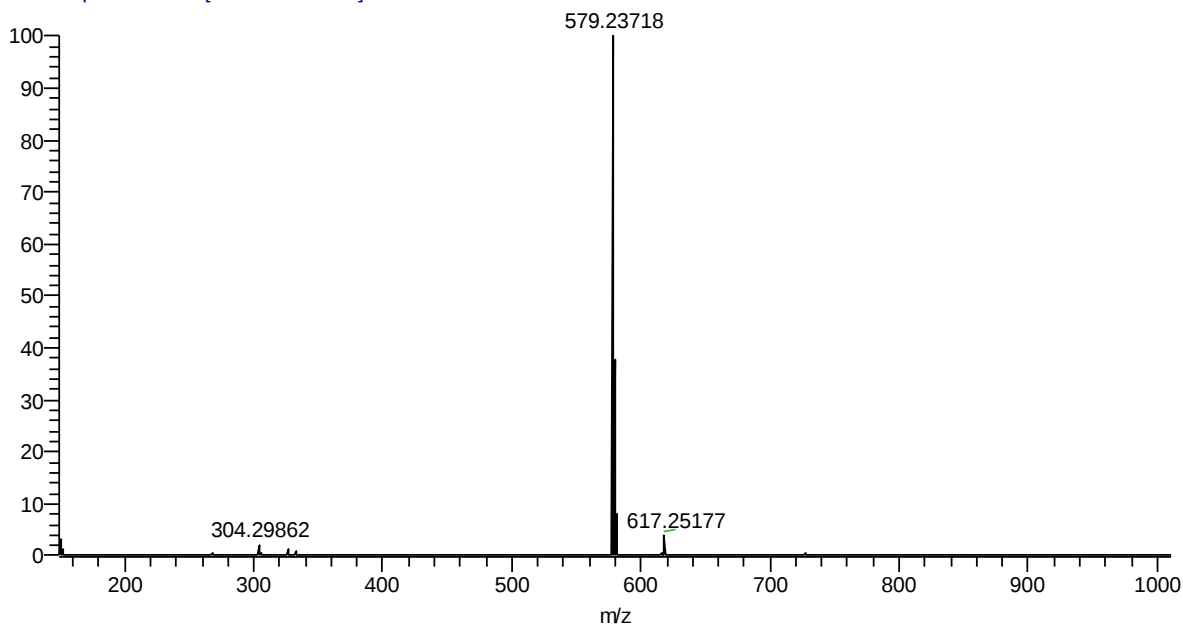


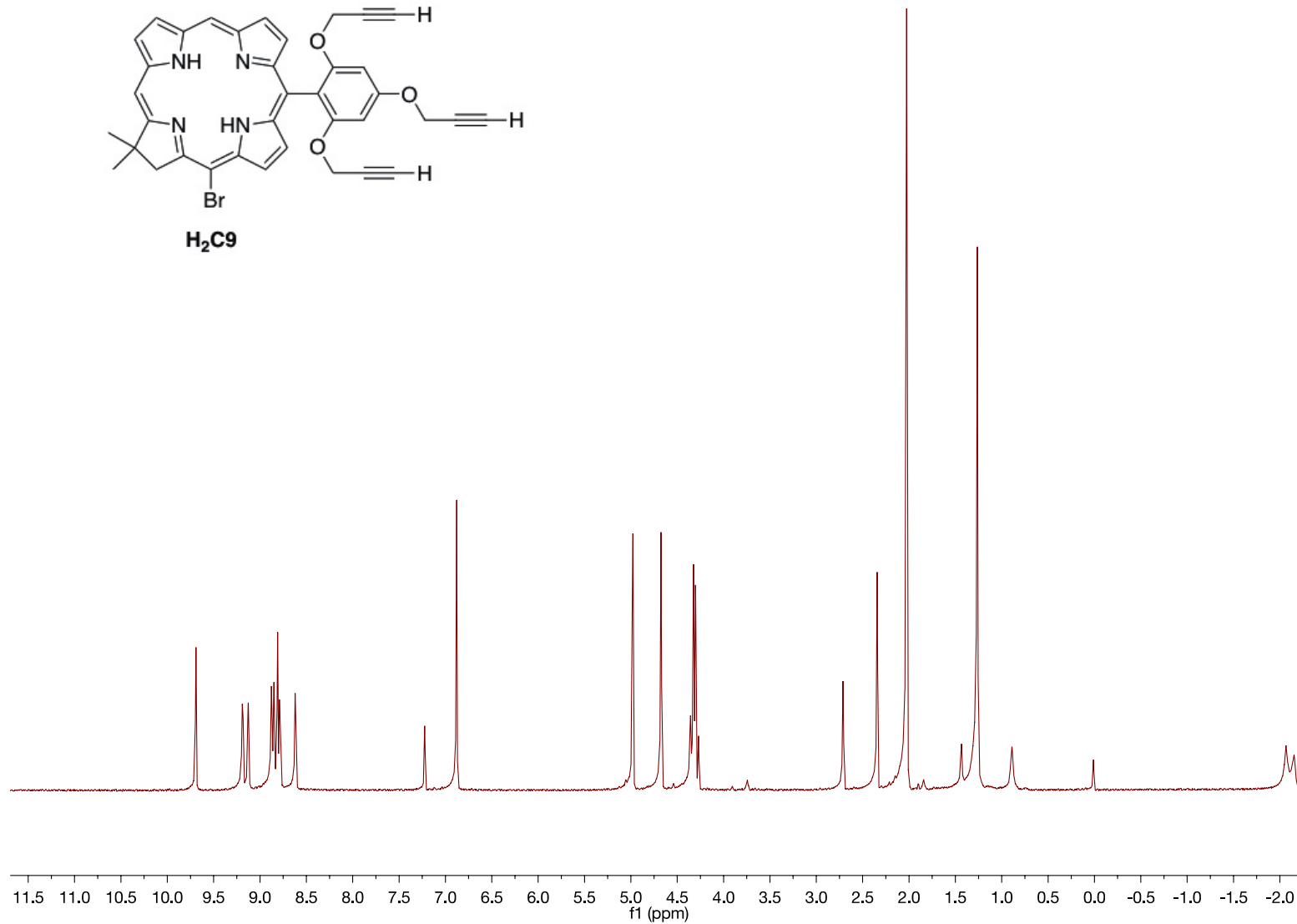
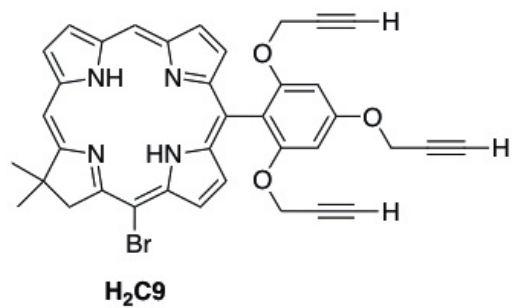


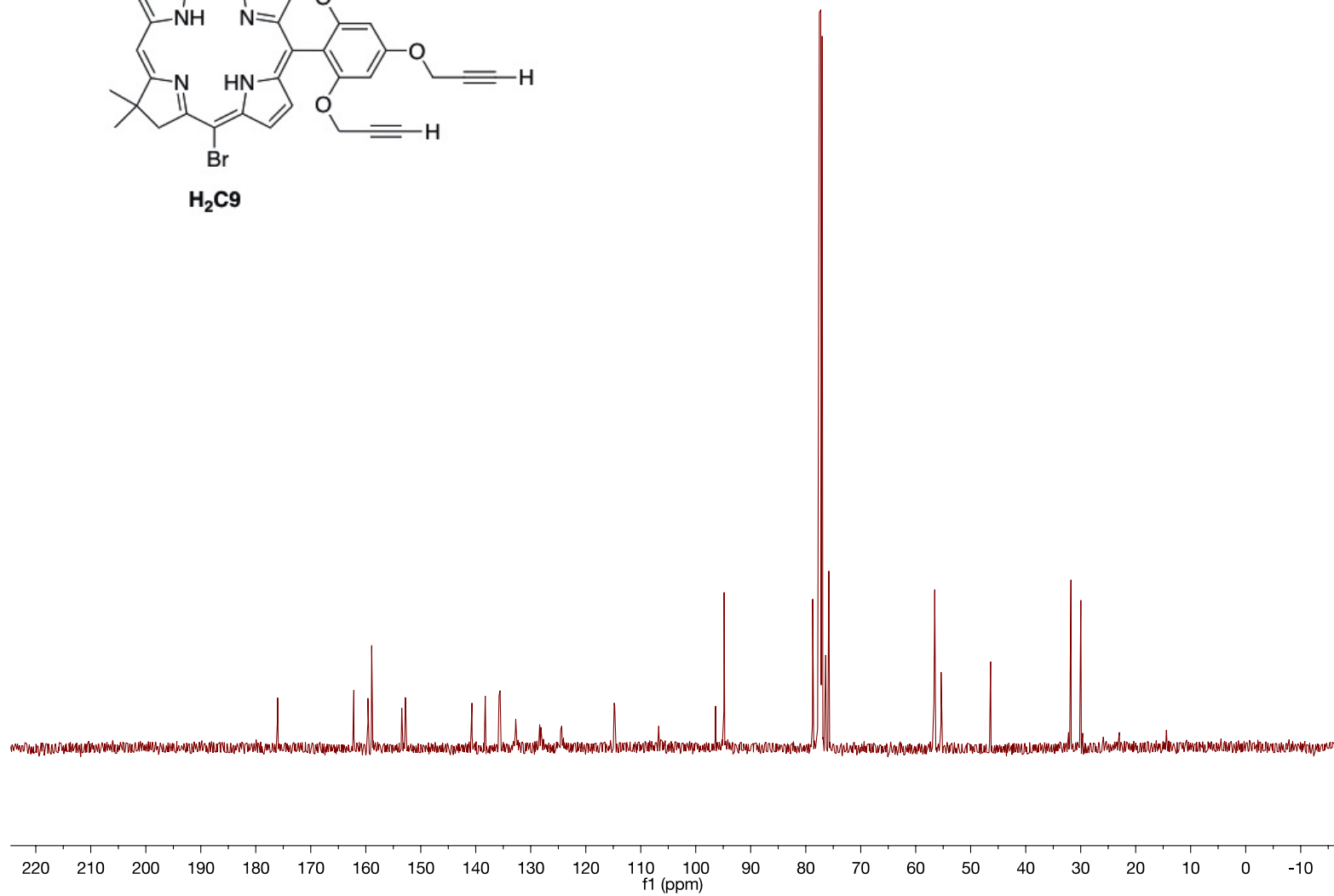
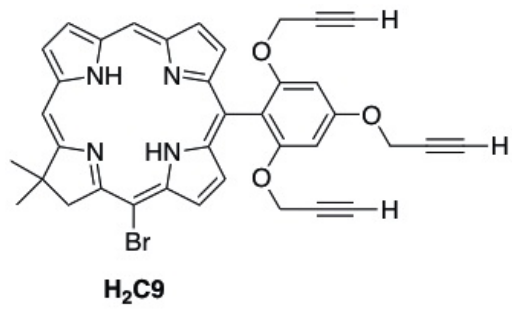
NL:
 8.77E6
 170824_FbChlorin-
 ethyne#37-115 RT:
 0.16-0.51 AV: 79 T:
 FTMS + p ESI Full ms
 [150.00-1000.00]

NL:
 6.55E5
 C₃₇ H₃₀ N₄ O₃ +H:
 C₃₇ H₃₁ N₄ O₃
 pa Chrg 1

170824_FbChlorin-ethyne #37-115 RT: 0.16 AV: 79 NL: 8.77E6
 T: FTMS + p ESI Full ms [150.00-1000.00]

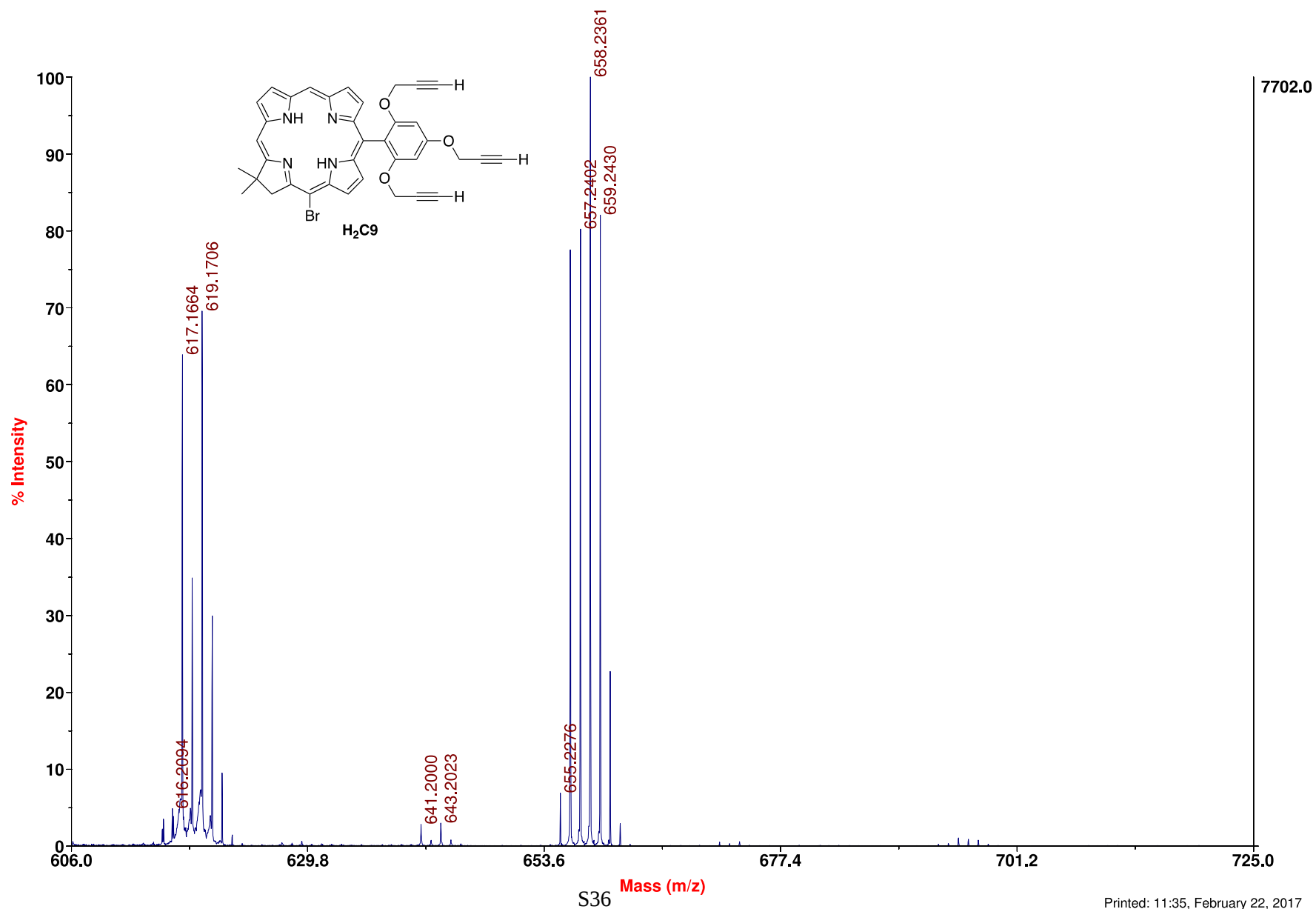


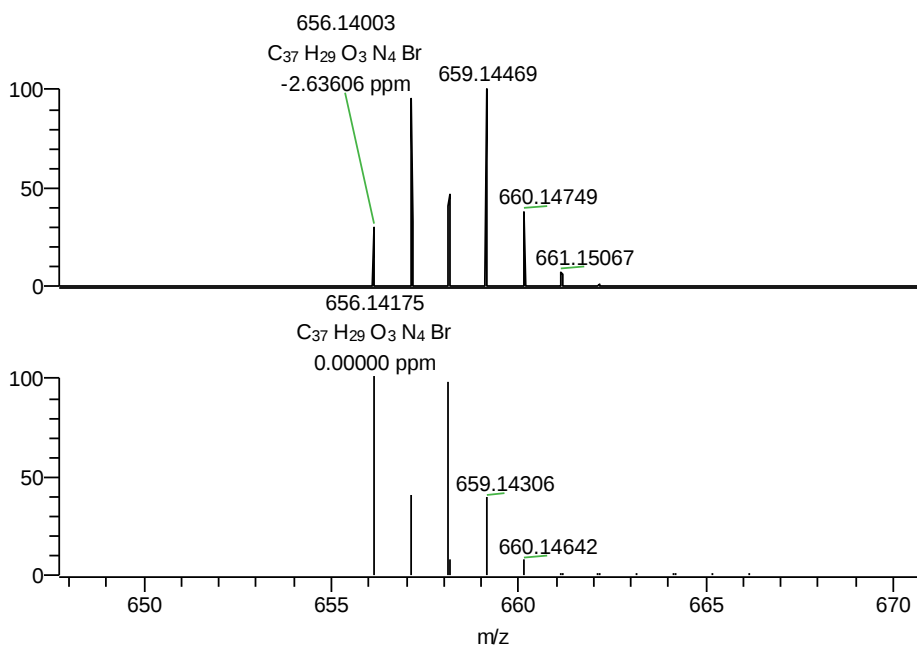
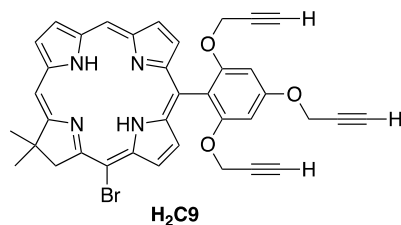




AB Sciex TOF/TOF™ Series Explorer™ 20981201

TOF/TOF™ Reflector Spec #1[BP = 658.2, 7702]

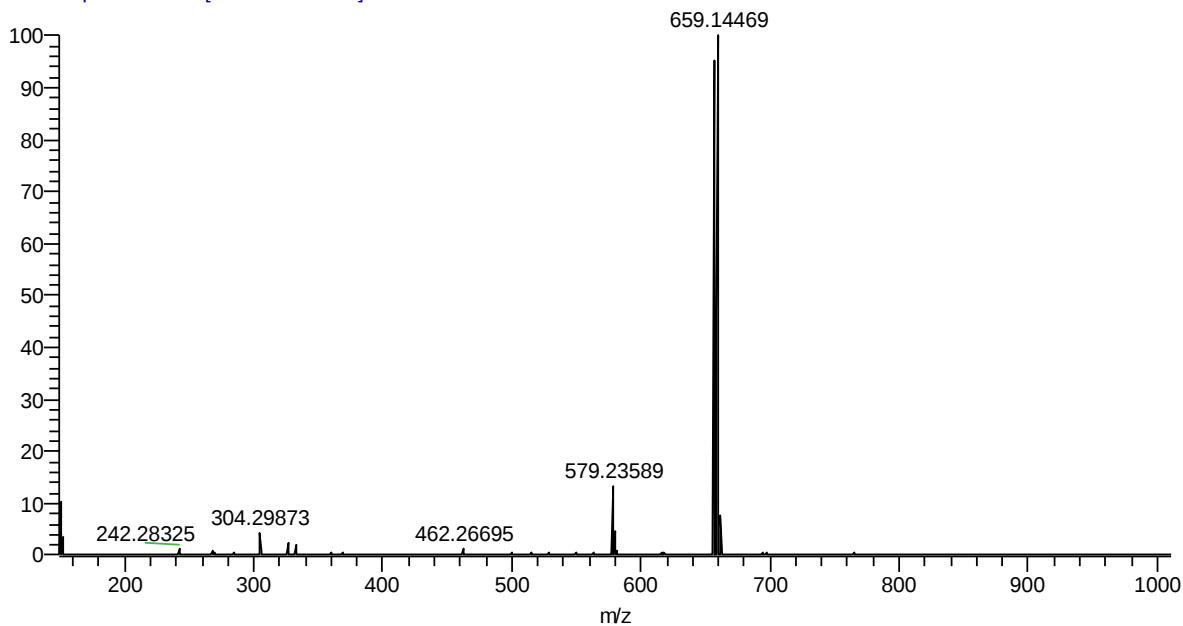


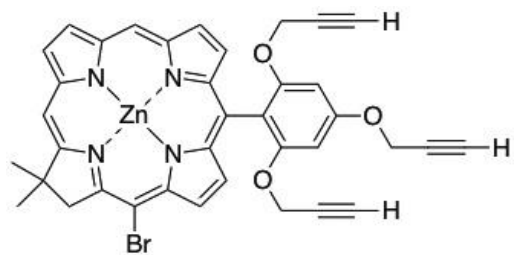


NL:
4.53E6
170825_FbChlorin-
ethyne-Br#92-137 RT:
0.41-0.61 AV: 46 T:
FTMS + p ESI Full ms
[150.00-1000.00]

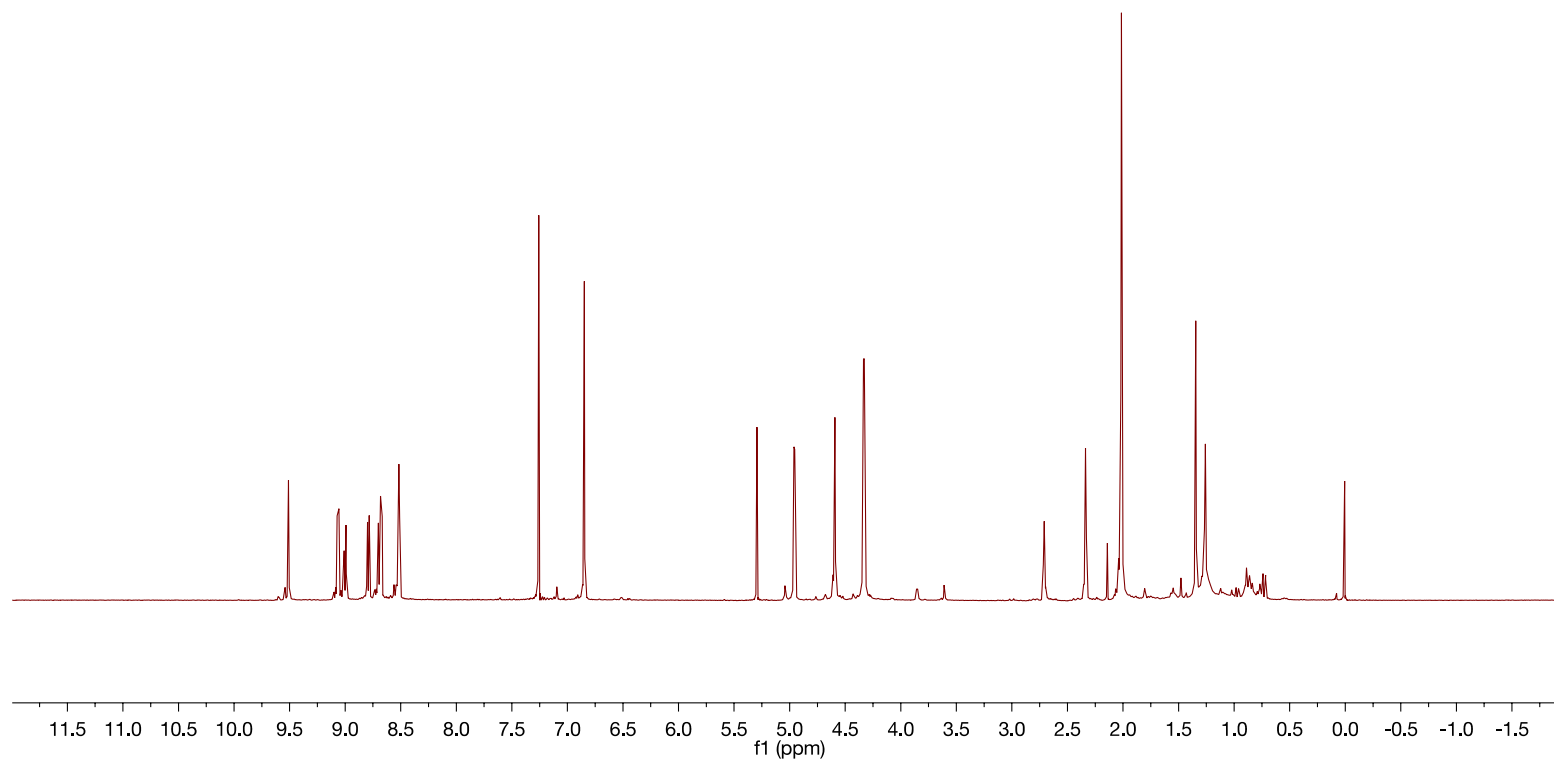
NL:
3.32E5
C₃₇ H₂₉ N₄ O₃ Br:
C₃₇ H₂₉ N₄ O₃ Br₁
pa Chrg 1

170825_FbChlorin-ethyne-Br #92-137 RT: 0.41-0.61 AV: 46 NL: 4.53E6
T: FTMS + p ESI Full ms [150.00-1000.00]

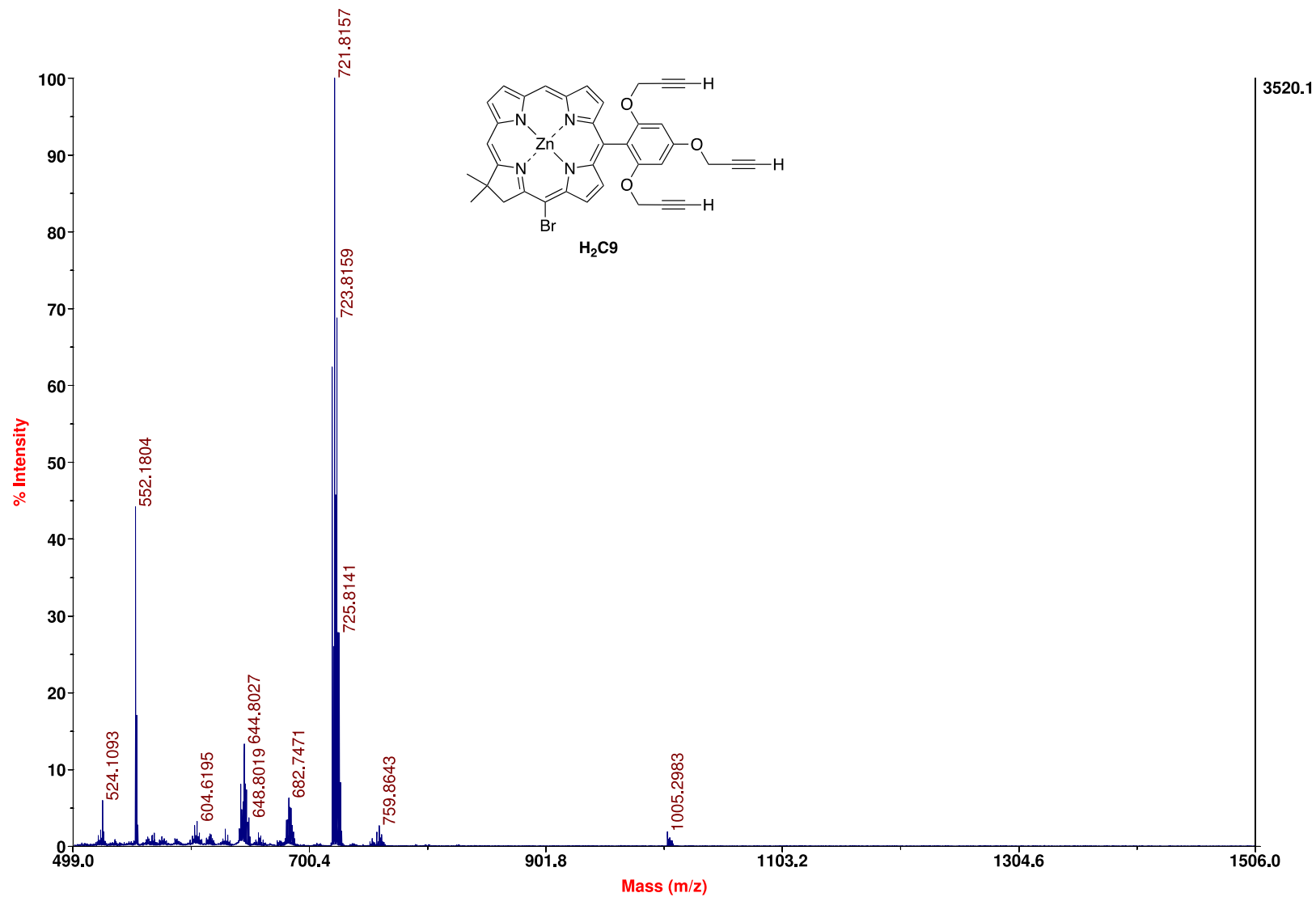


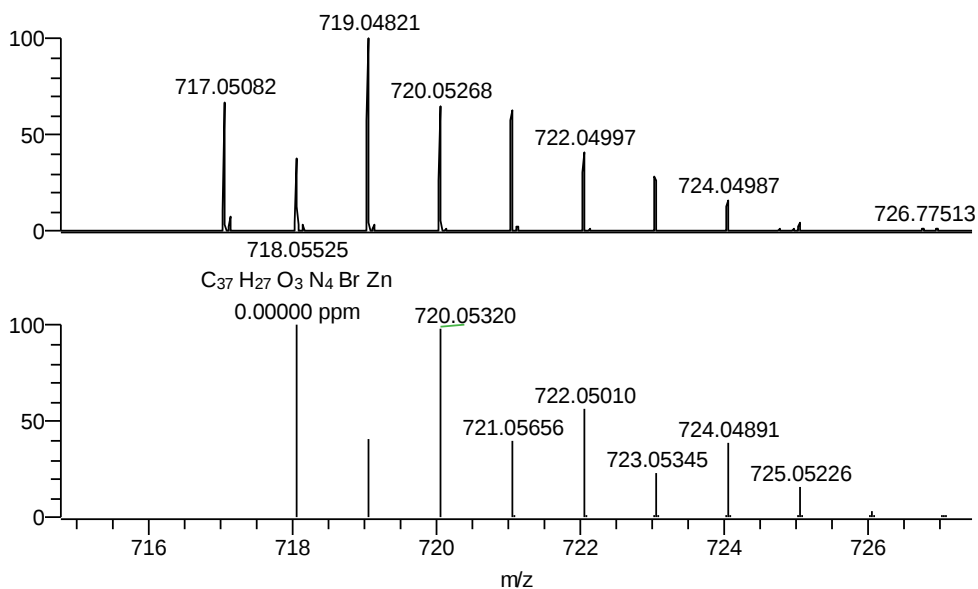
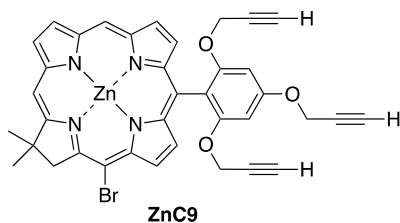


ZnC9





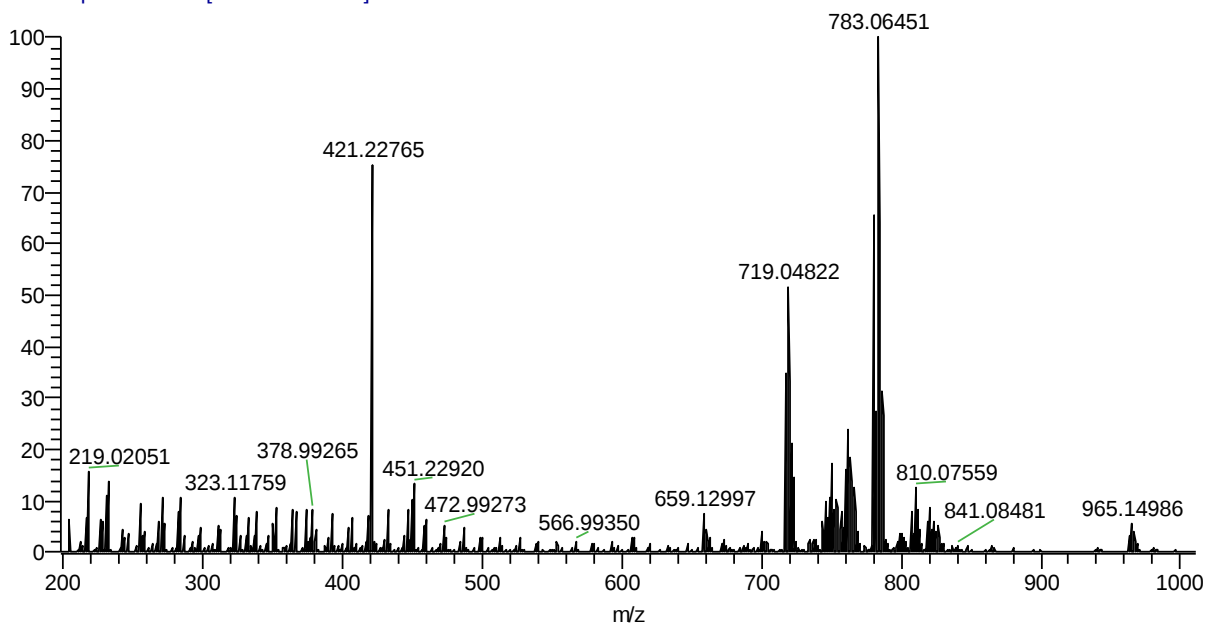


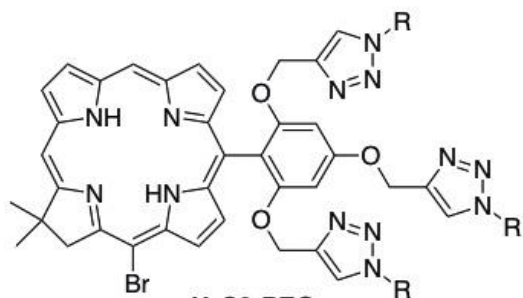


NL:
1.64E7
171154_ZnC-Br#525-
570 RT: 2.34-2.54
AV: 46 T: FTMS - p
ESI Full ms
[200.00-1000.00]

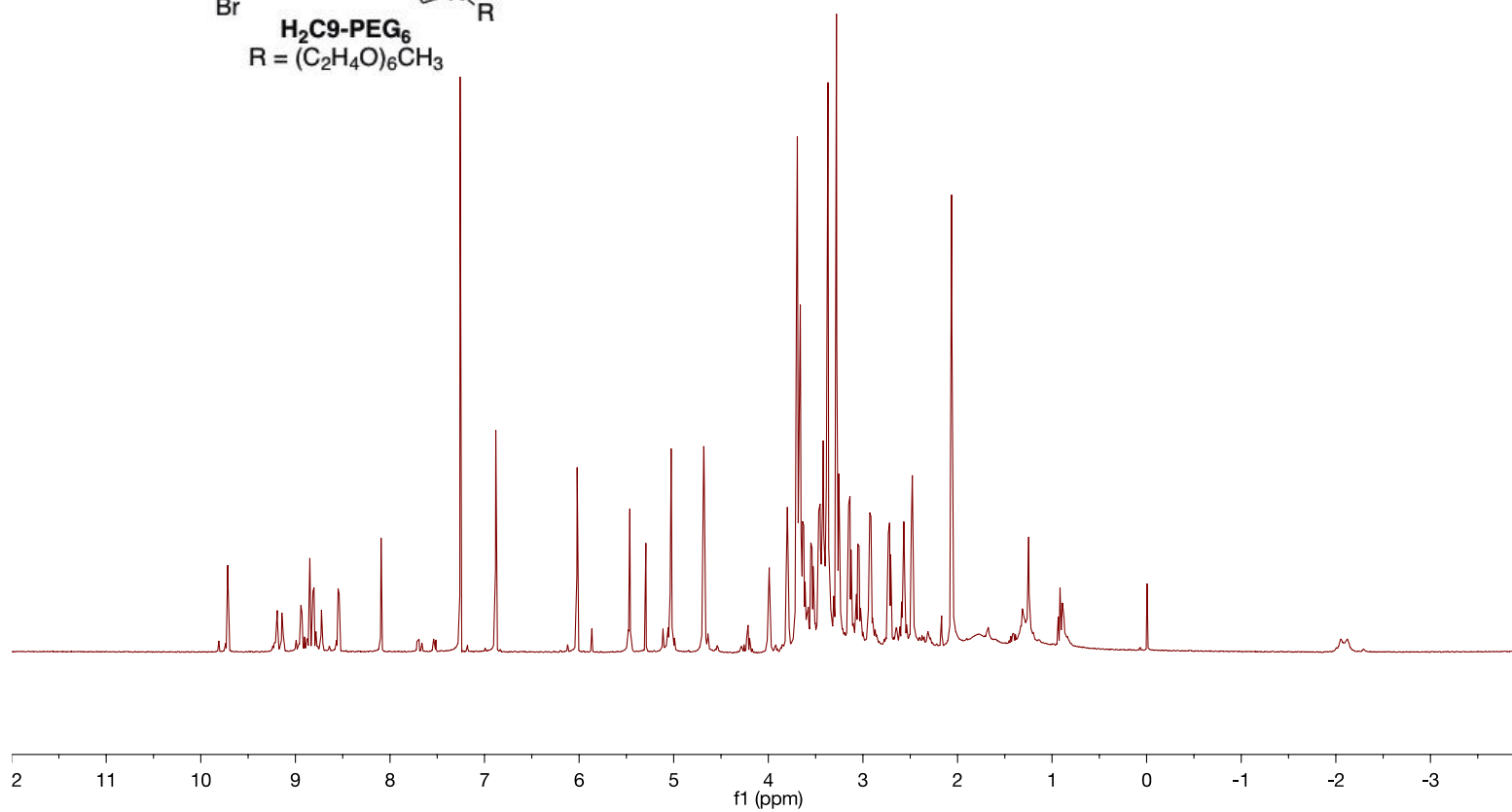
NL:
1.61E5
C₃₇H₂₇O₃N₄BrZn:
C₃₇H₂₇O₃N₄Br₁Zn₁
pa Chrg 1

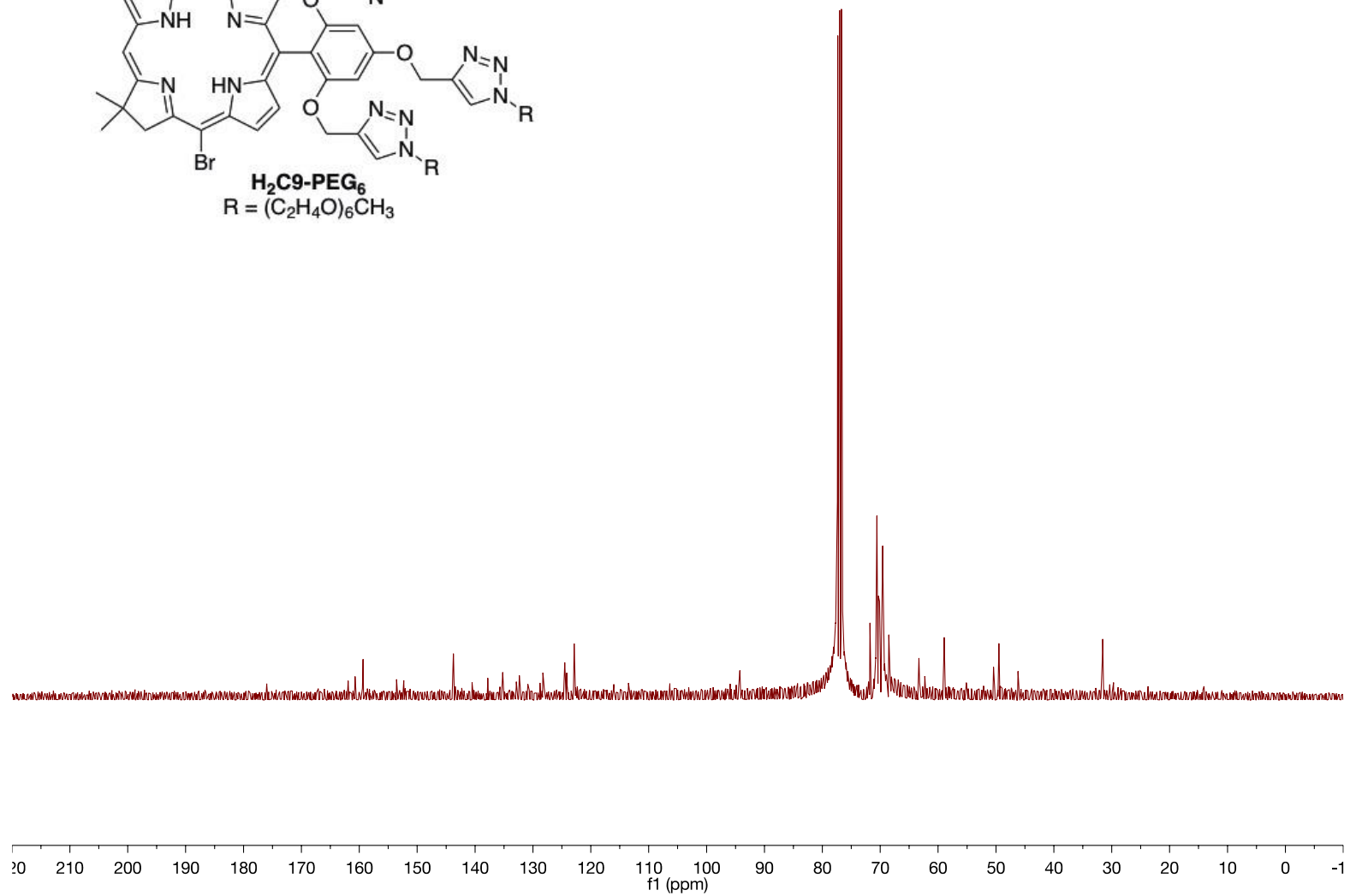
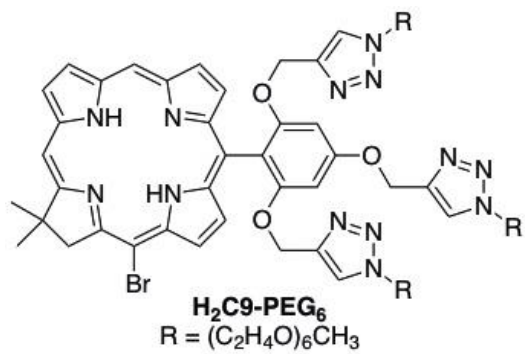
171154_ZnC-Br #524-569 RT: 2.34-2.54 NL: 3.19E7
T: FTMS - p ESI Full ms [200.00-1000.00]

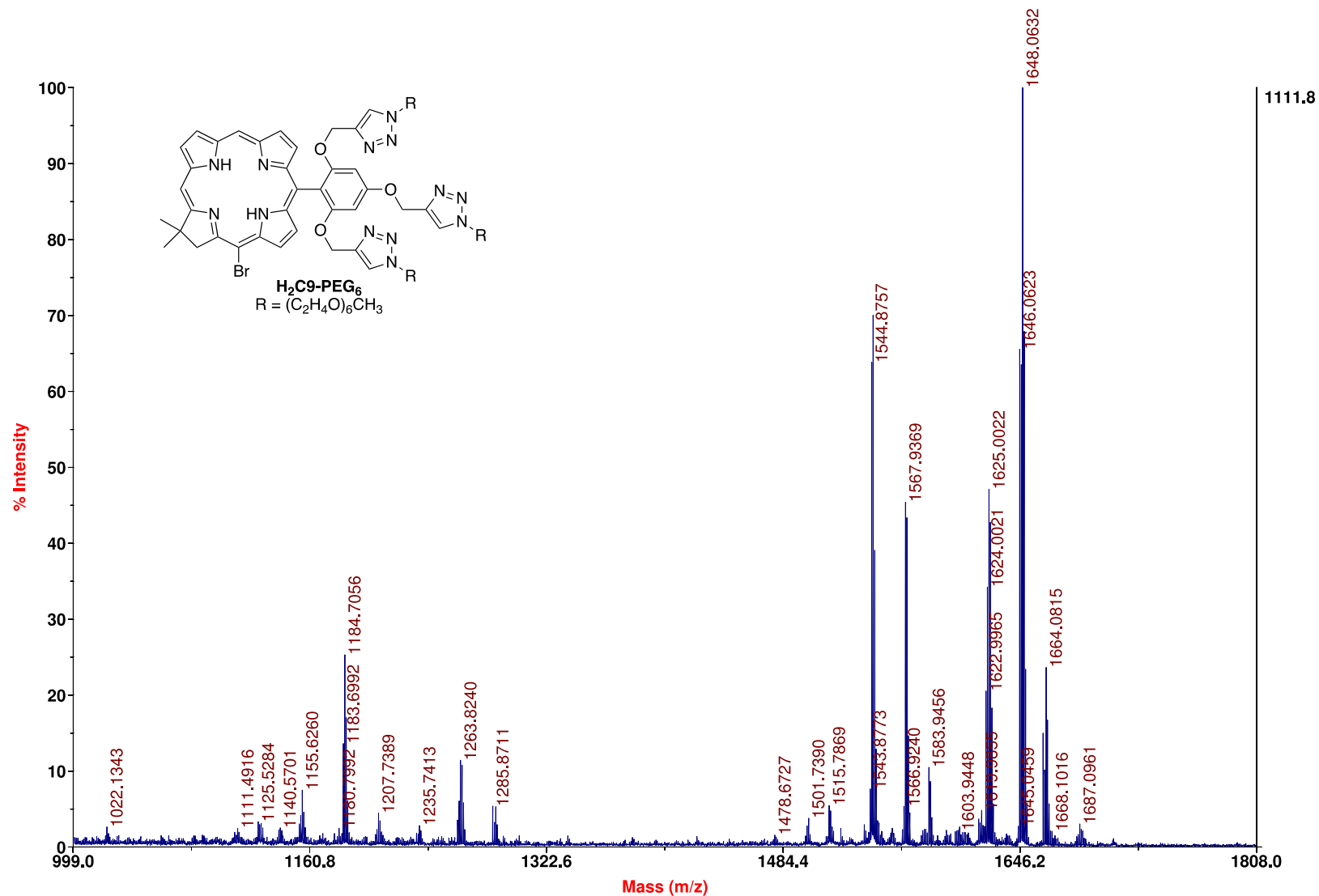


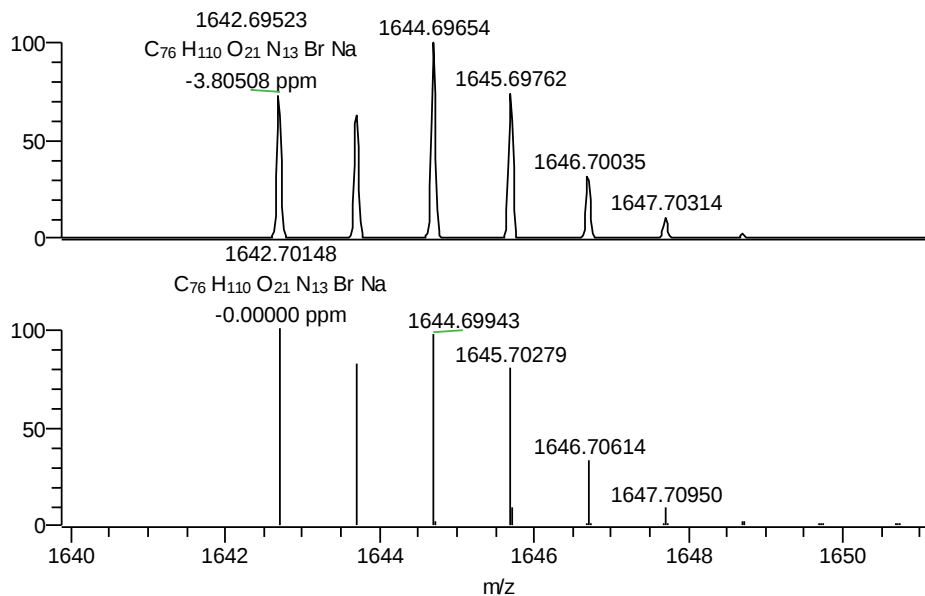
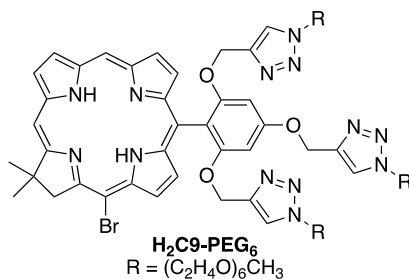


H₂C₉-PEG₆
 R = (C₂H₄O)₆CH₃





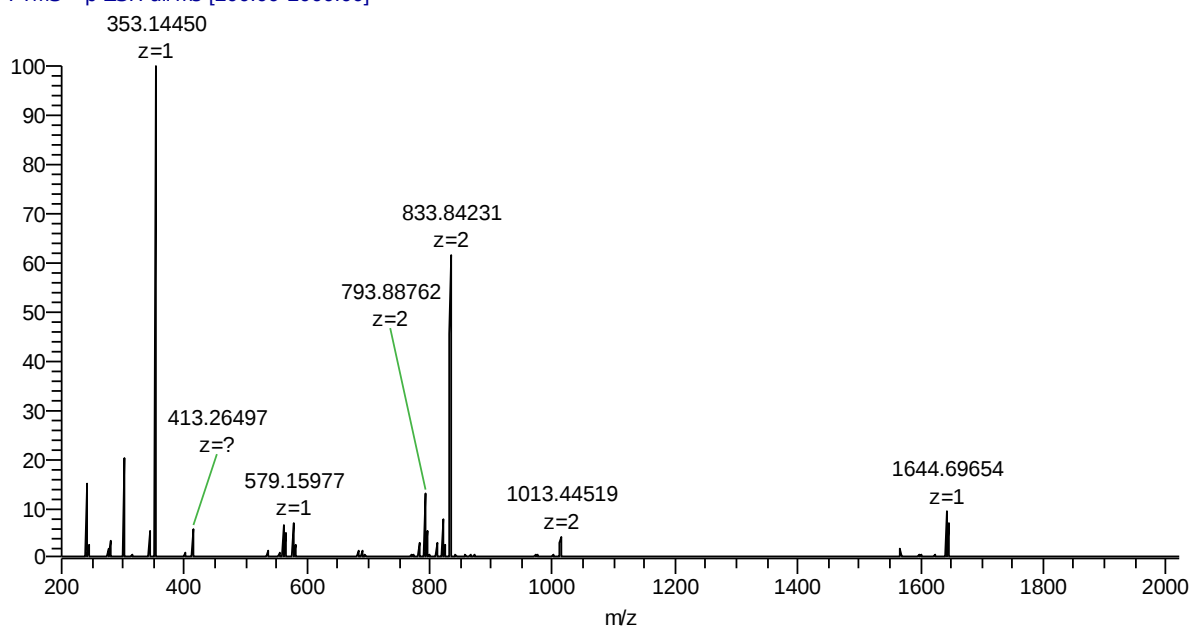


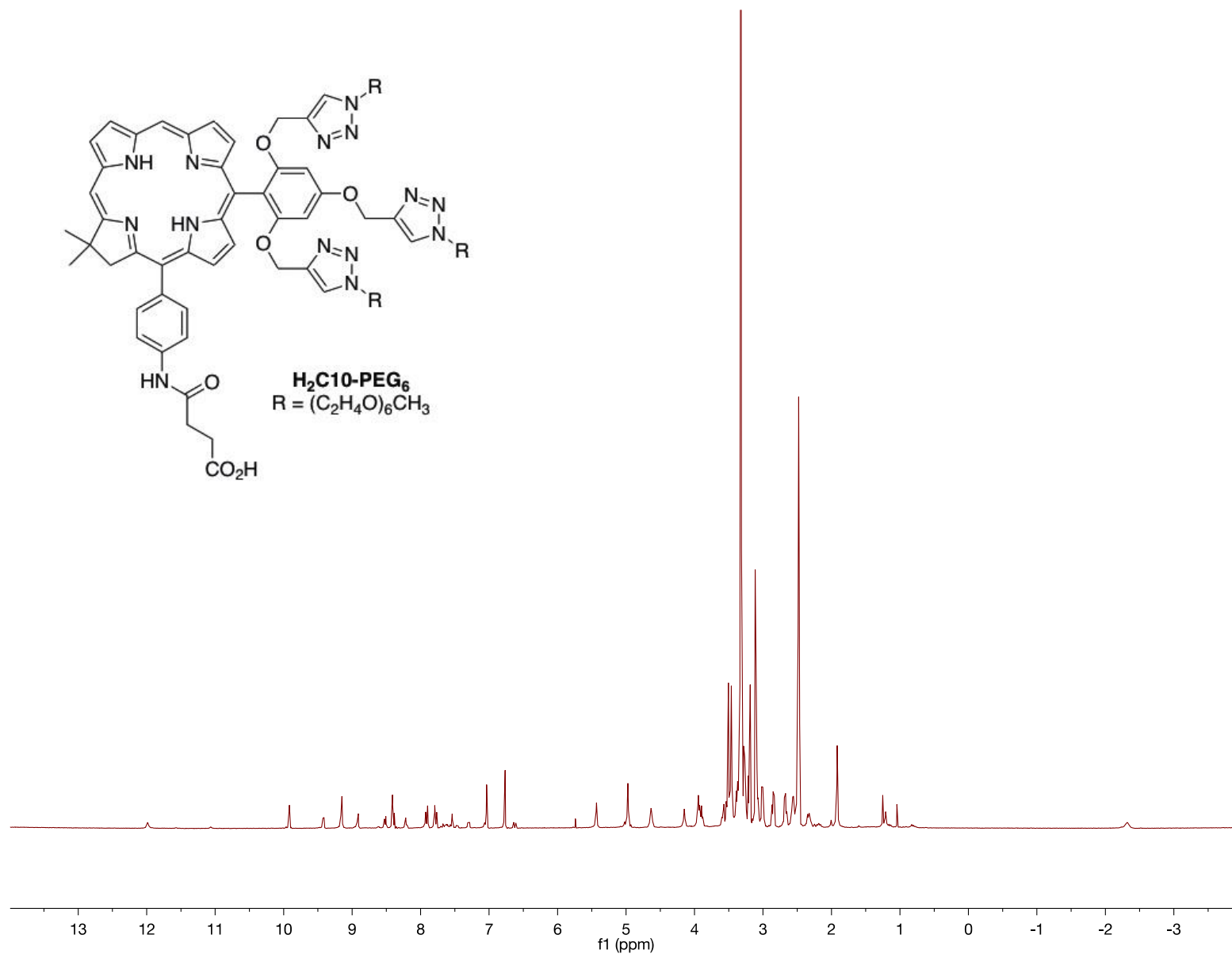


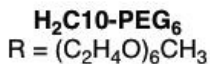
NL:
 6.25E7
 171155_Fb-PEG-C-
 Br#285-335 RT:
 1.27-1.49 AV: 51 T:
 FTMS + p ESI Full ms
 [200.00-2000.00]

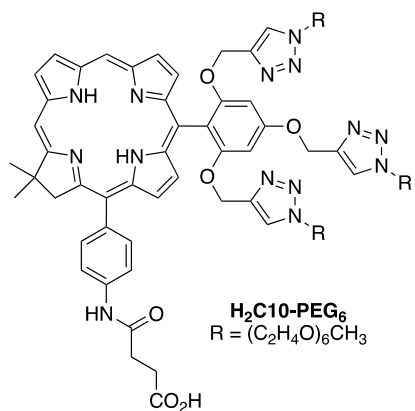
NL:
 2.00E5
 C₇₆ H₁₁₀ O₂₁ N₁₃ Br +Na:
 C₇₆ H₁₁₀ O₂₁ N₁₃ Br₁ Na₁
 pa Chrg 1

171155_Fb-PEG-C-Br #285-335 RT: 1.27-1.49 ... 51 NL: 6.71E8
 T: FTMS + p ESI Full ms [200.00-2000.00]

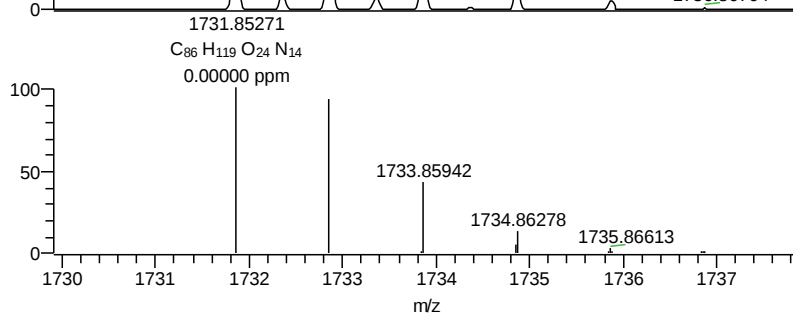
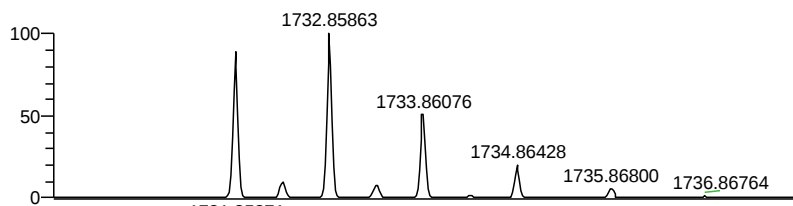
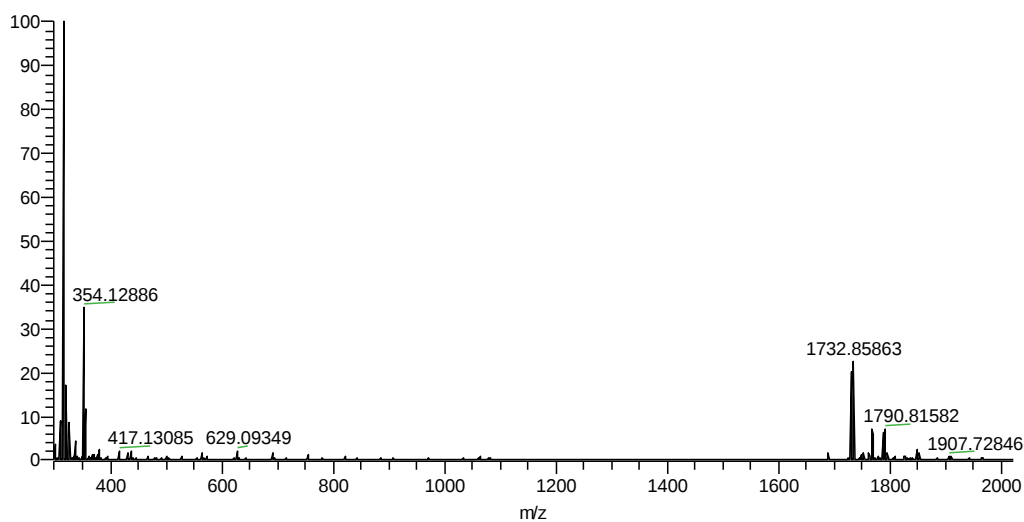






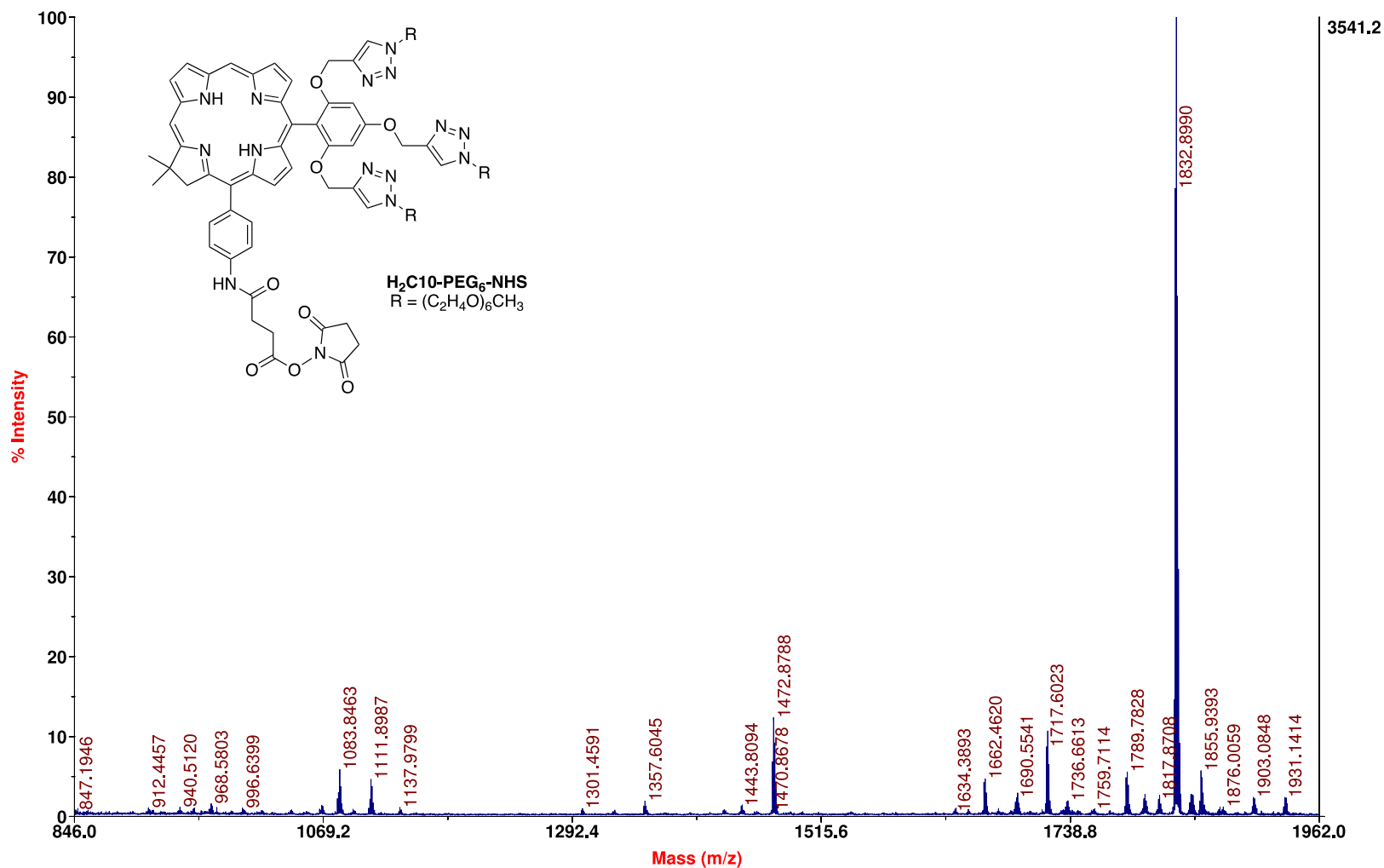


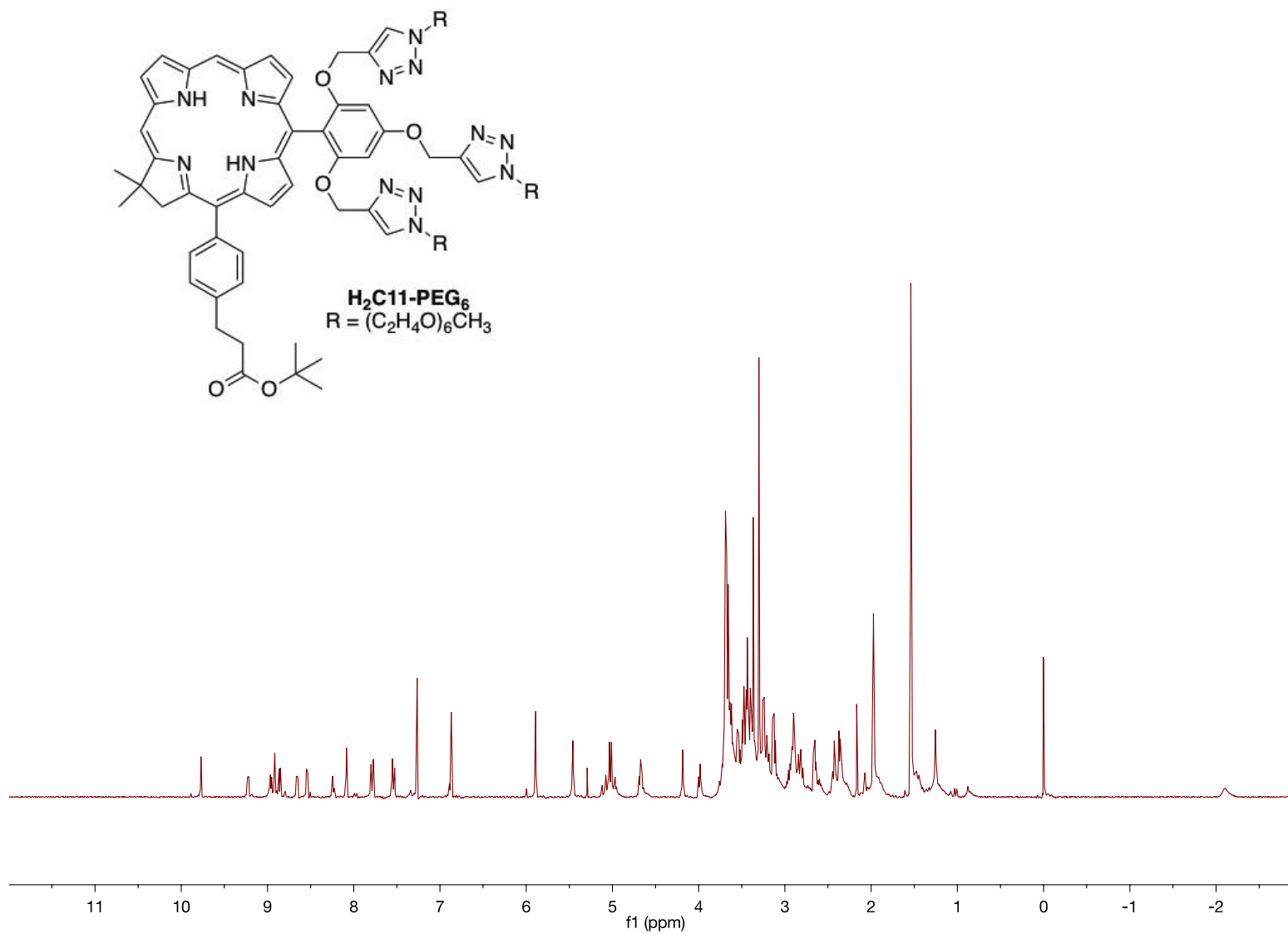
171271_Fb-PEG-C-CO2H_NEG #116-218 F... 0.97 AV: 103 NL: 2.07E7
 T: FTMS - p ESI Full ms [300.00-2000.00]

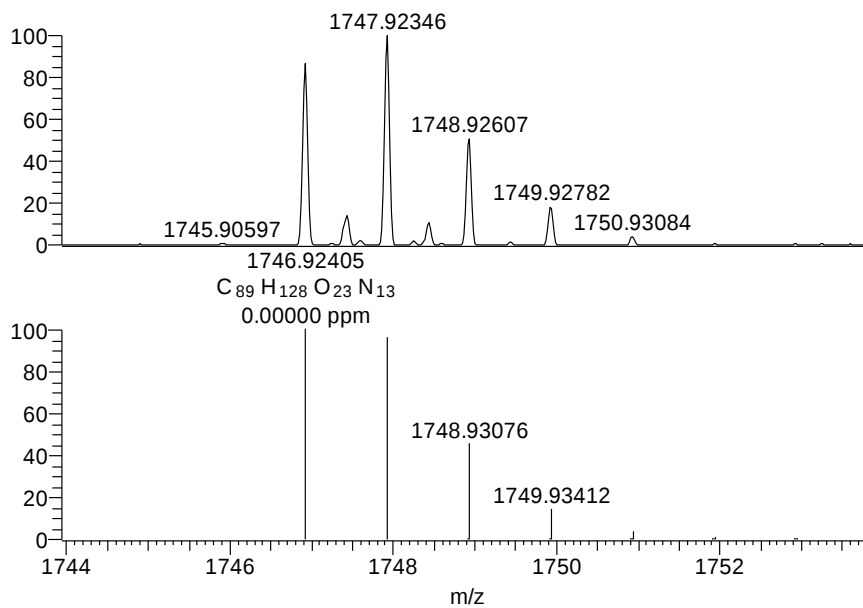
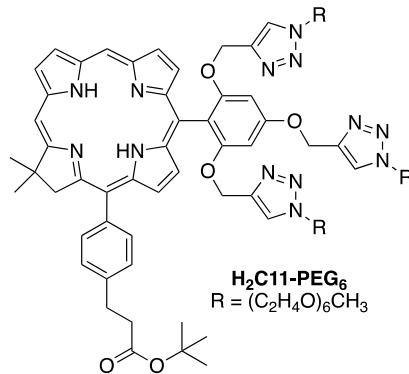


NL:
 4.69E6
 171271_Fb-PEG-C-
 CO2H_NEG#116-218 RT:
 0.52-0.97 AV: 103 T:
 FTMS - p ESI Full ms
 [300.00-2000.00]

NL:
 3.50E5
 C₈₆ H₁₂₀ N₁₄ O₂₄ +H:
 C₈₆ H₁₁₉ N₁₄ O₂₄
 pa Chrg -1





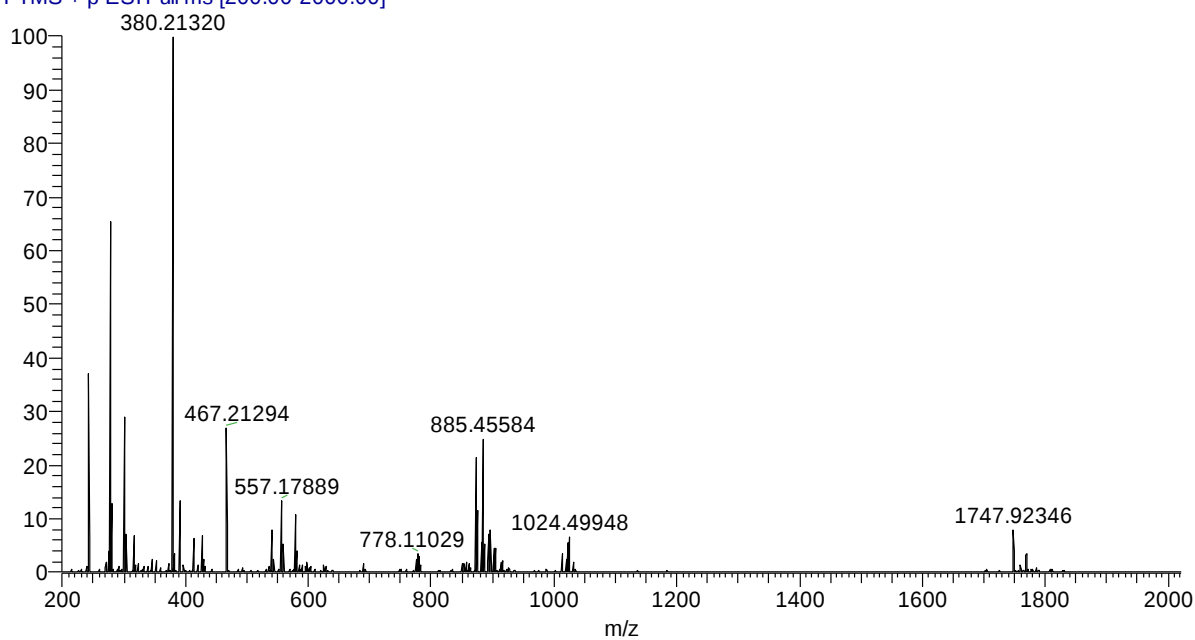


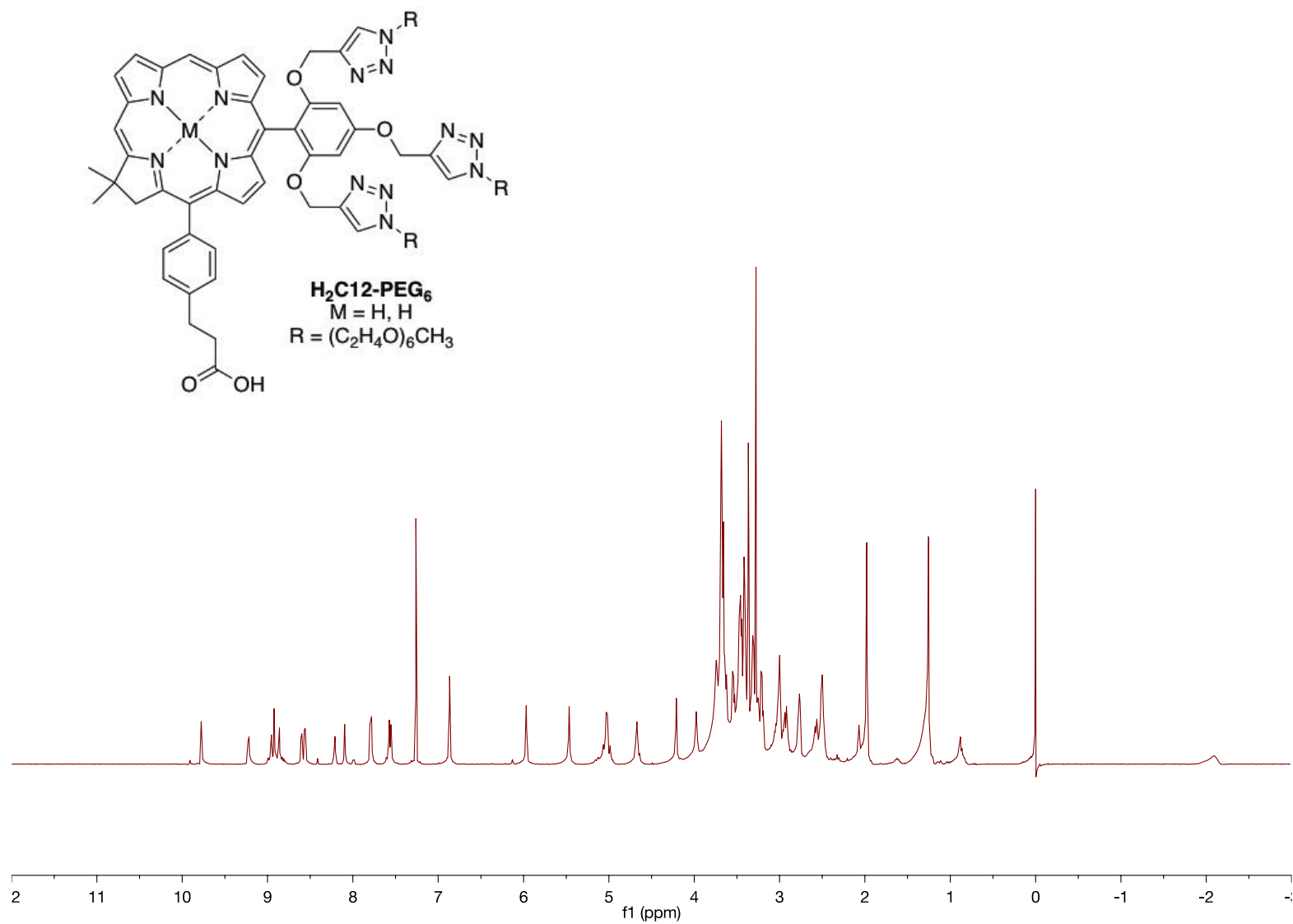
NL:
 2.29E6
 173791_FbC-10TriPEG-
 15COOtBu#311-421 RT:
 1.39-1.88 AV: 111 SB: 71
 0.99-1.31 T: FTMS + p ESI Full
 ms [200.00-2000.00]

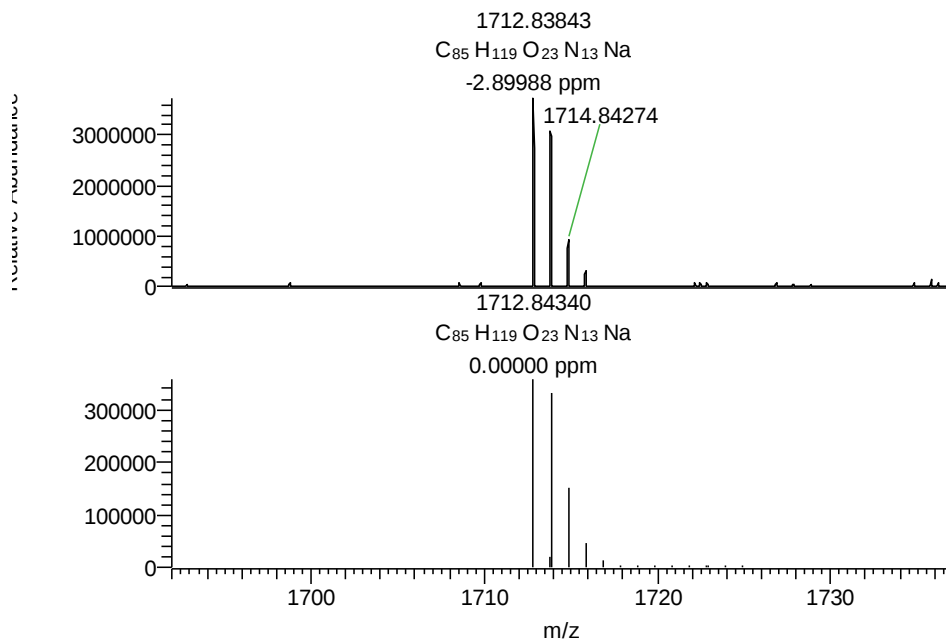
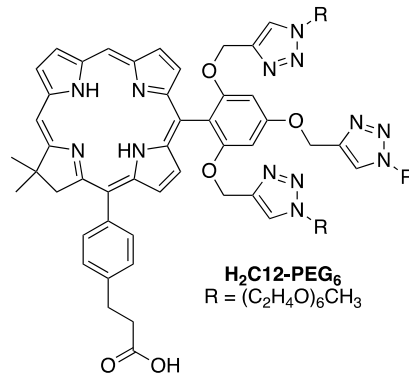
NL:
 3.41E5
 C₈₉ H₁₂₇ N₁₃ O₂₃ +H:
 C₈₉ H₁₂₈ N₁₃ O₂₃
 pa Chrg 1

173791_FbC-10TriPEG-15COOtBu #311-4
 T: FTMS + p ESI Full ms [200.00-2000.00]

1.39-1.88 AV: 111 SB: 71 0.99-1.31 NL: 2.87E7



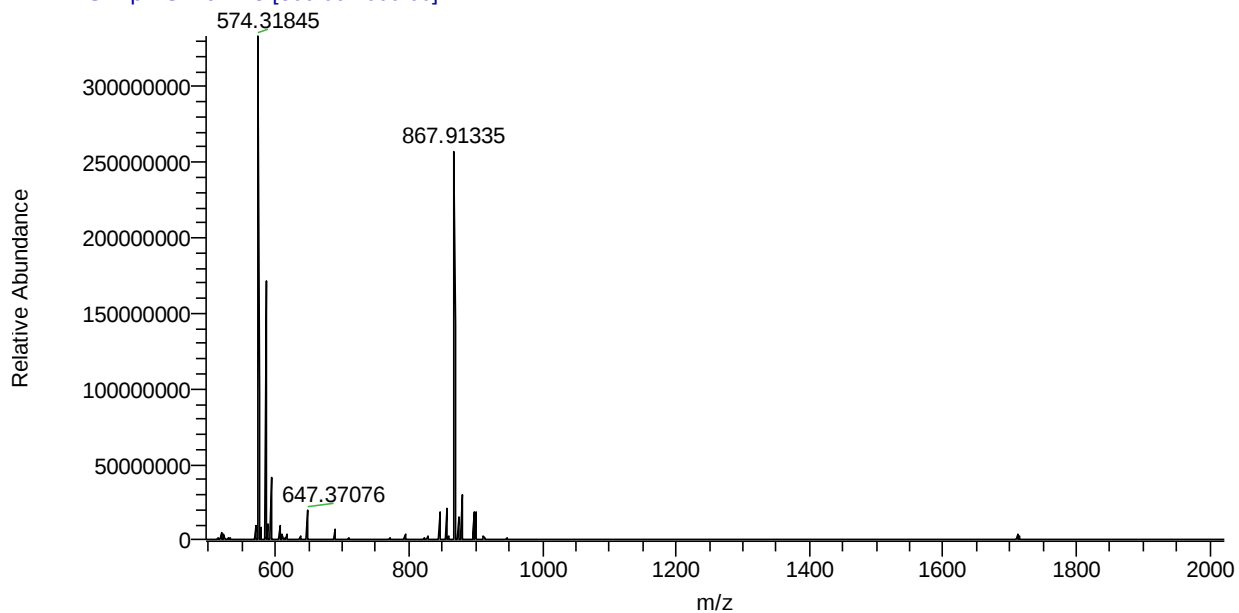


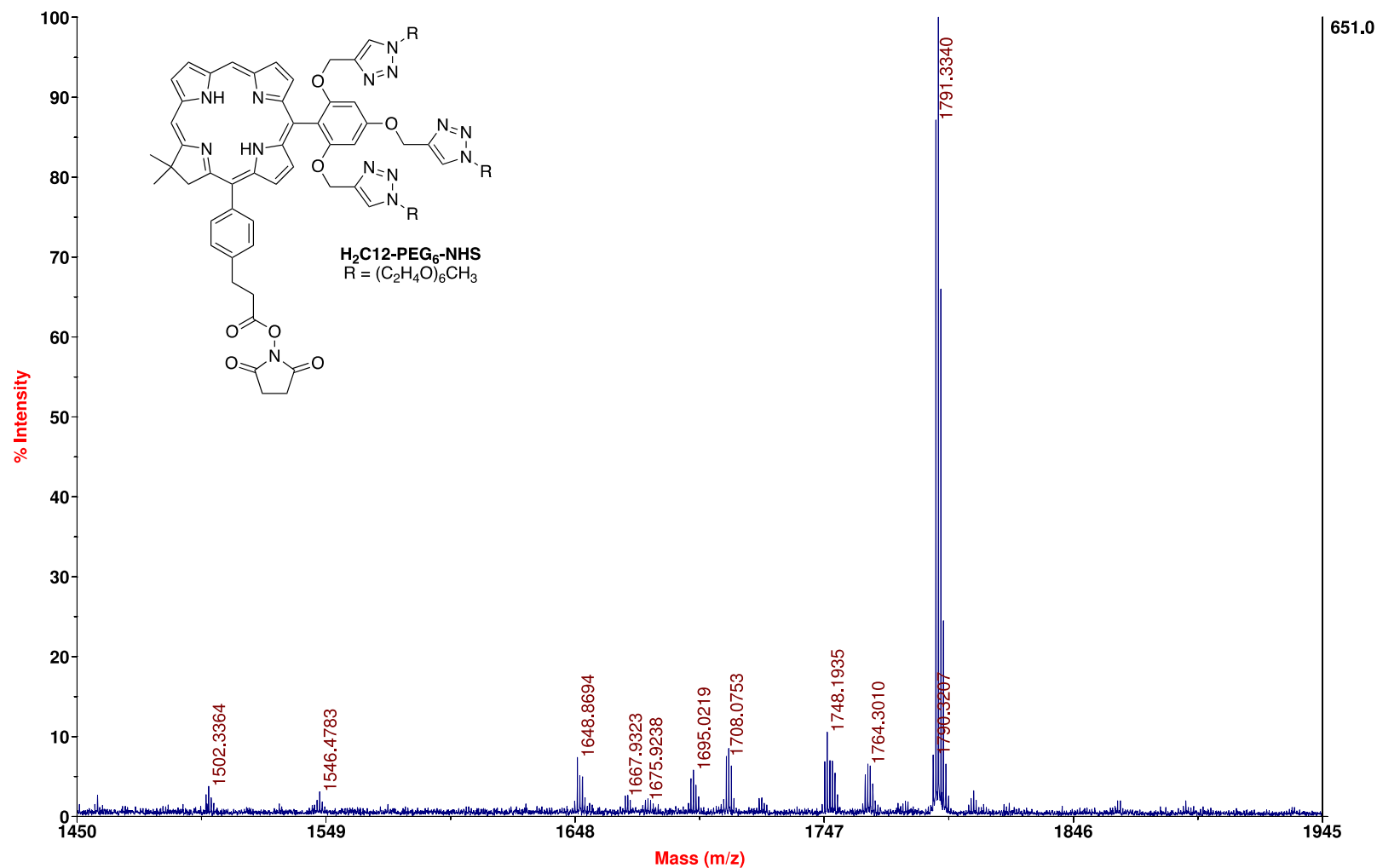


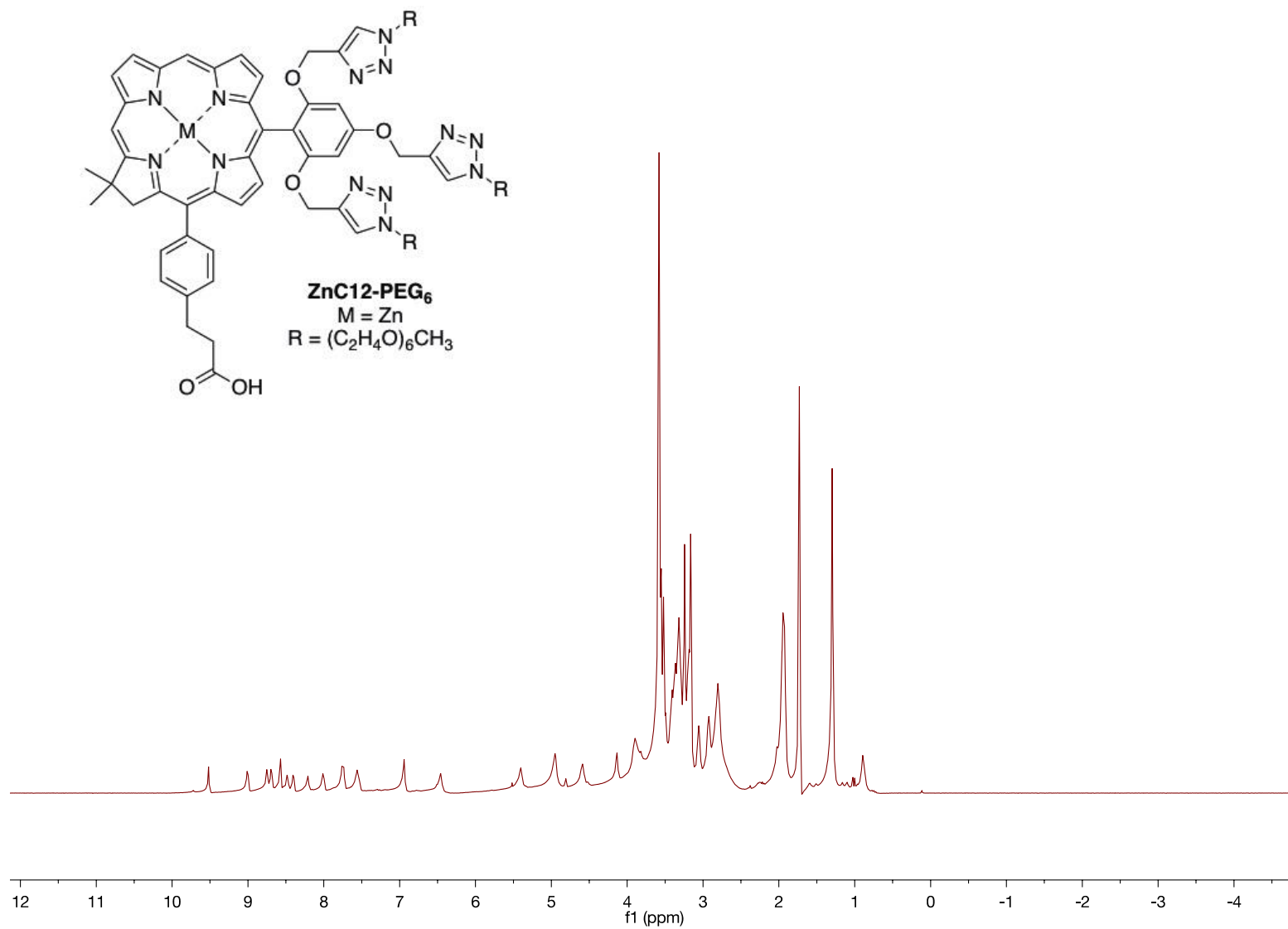
NL:
3.71E6
174605_FbC-10TiPEG-
15COOH#117-134 RT:
0.52-0.60 AV: 18 T:
FTMS + p ESI Full ms
[500.00-2000.00]

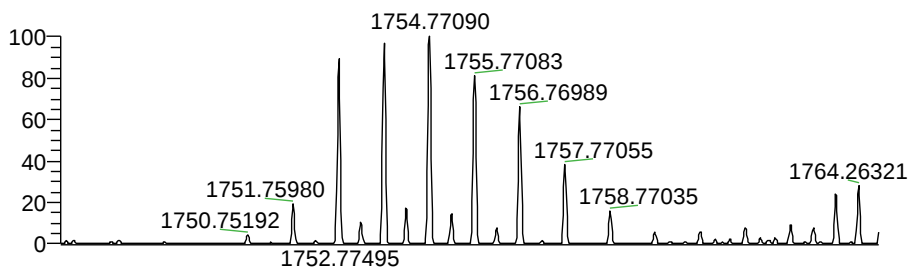
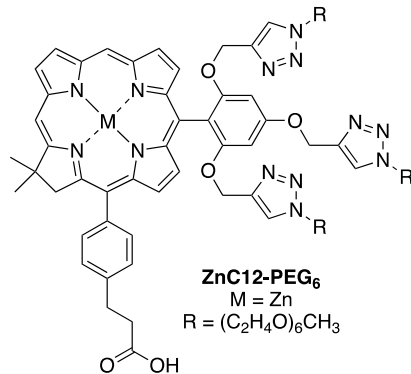
NL:
3.56E5
C₈₅ H₁₁₉ N₁₃ O₂₃ +Na:
C₈₅ H₁₁₉ N₁₃ O₂₃ Na₁
pa Chrg 1

174605_FbC-10TiPEG-15COOH #117-135 RT: 0.52-0.60 AV: 19 NL: 3.33E8
T: FTMS + p ESI Full ms [500.00-2000.00]

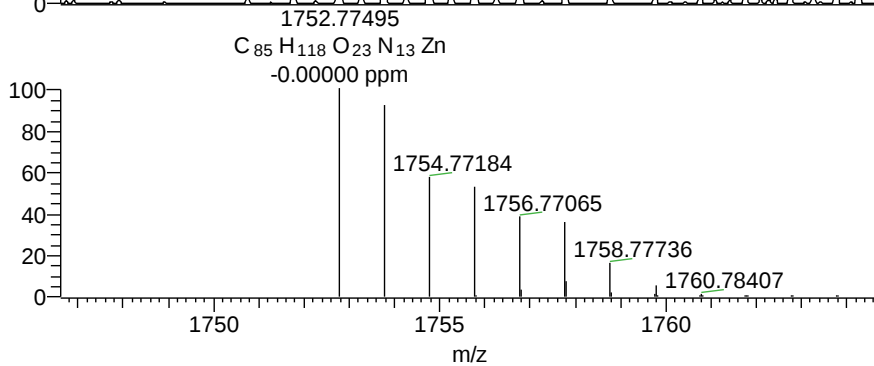






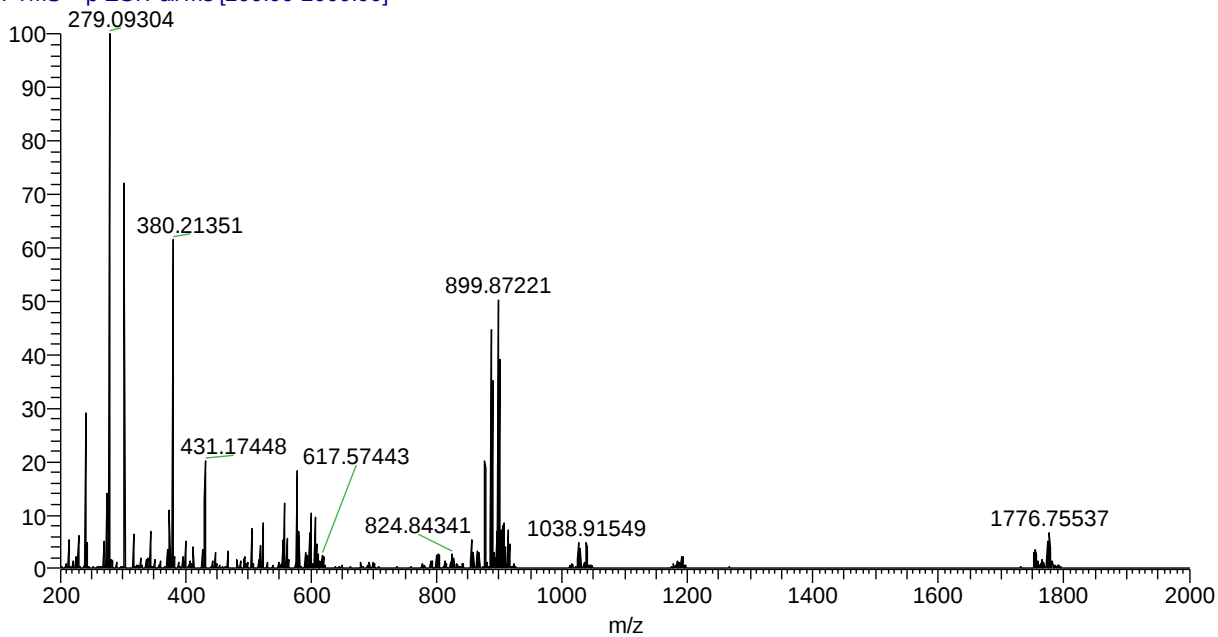


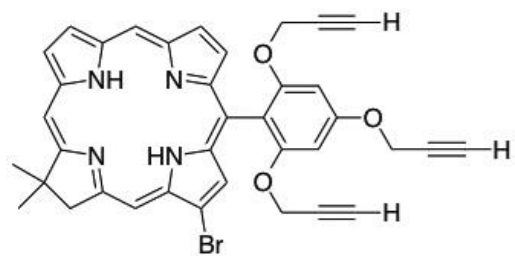
NL:
3.05E5
173792_ZnC-10TriPEG-
15COOH#427-778 RT:
1.90-3.47 AV: 352 SB: 137
0.39-1.00 T: FTMS + p ESI Full
ms [200.00-2000.00]



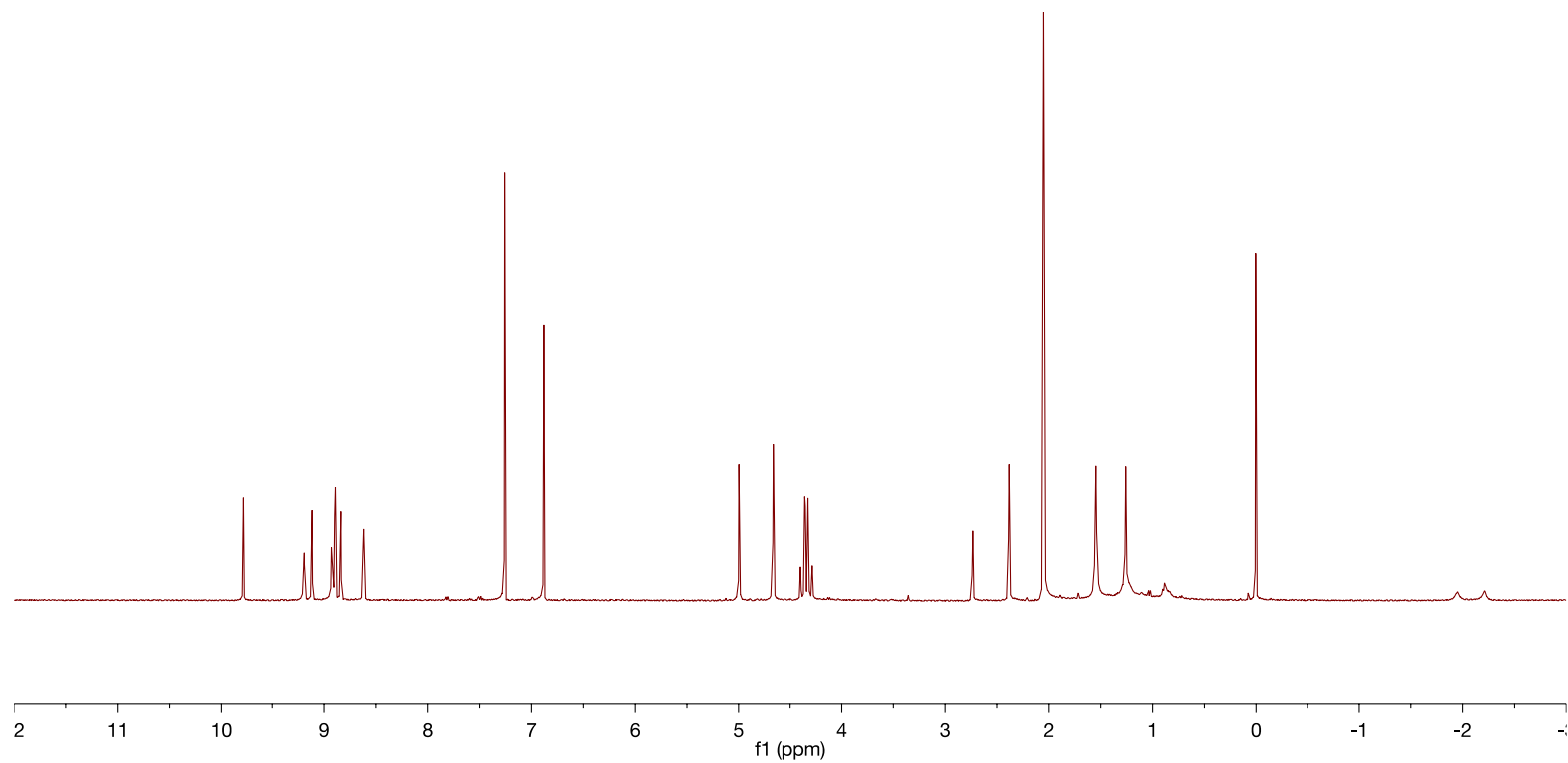
NL:
1.73E5
C₈₅ H₁₁₇ N₁₃ O₂₃ Zn +H:
C₈₅ H₁₁₈ N₁₃ O₂₃ Zn₁
pa Chrg 1

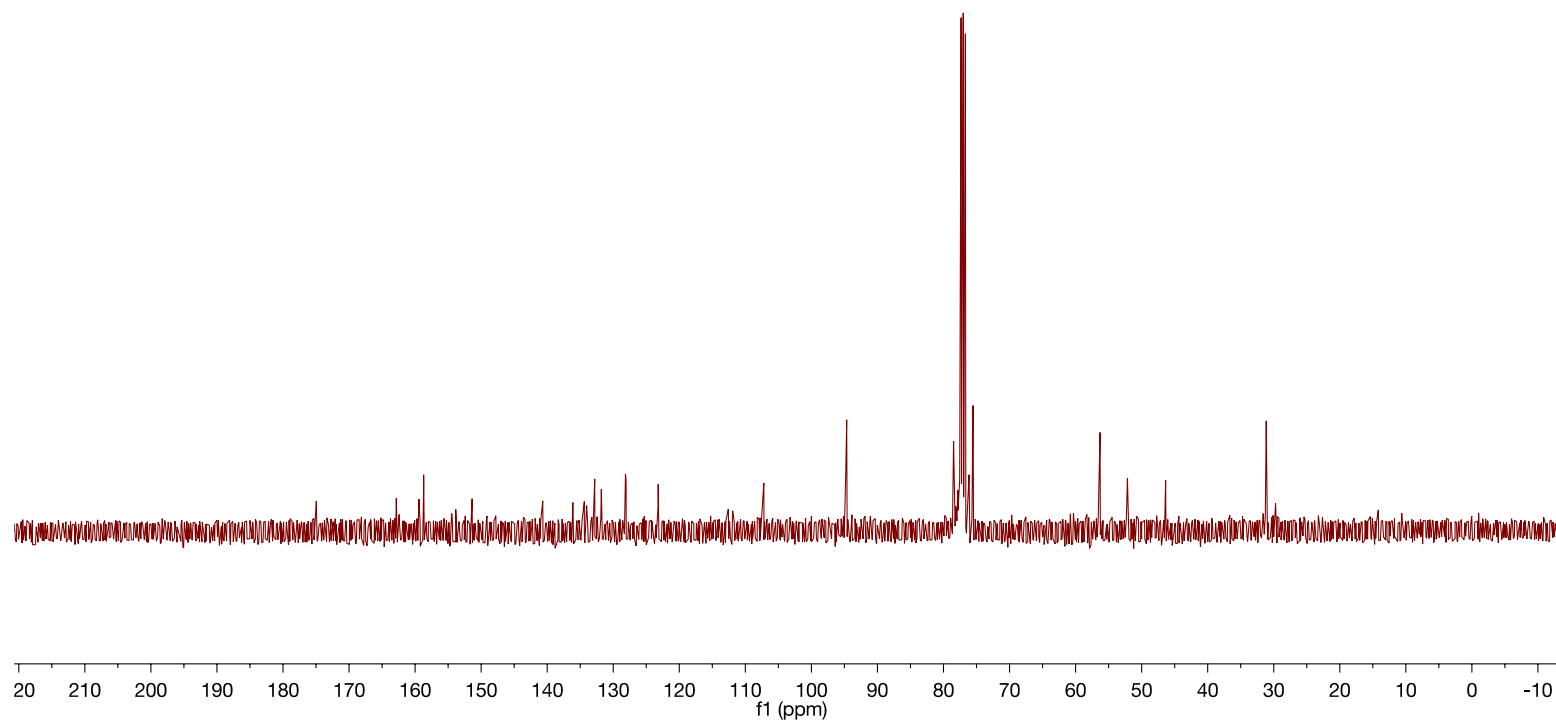
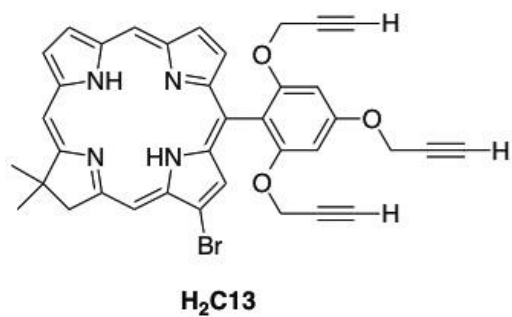
173792_ZnC-10TriPEG-15COOH #427-778 RT: 1.90-3.47 AV: 352 SB: 137 0.39-1.00 NL: 8.89E6
T: FTMS + p ESI Full ms [200.00-2000.00]

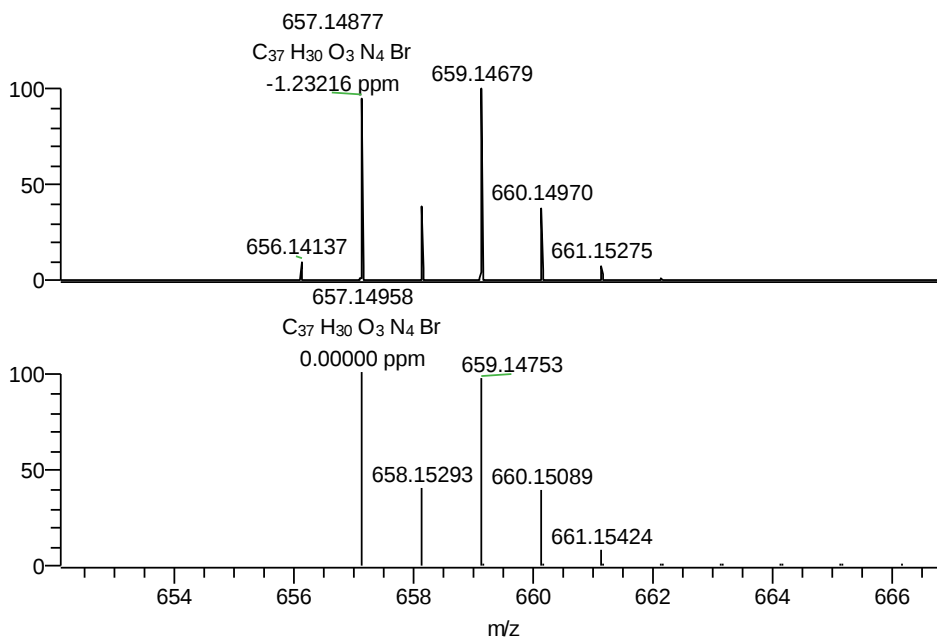
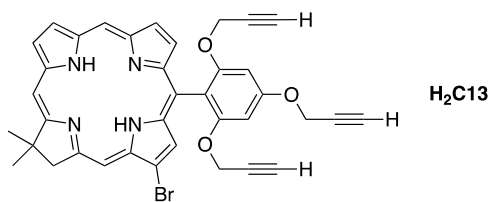




H₂C13



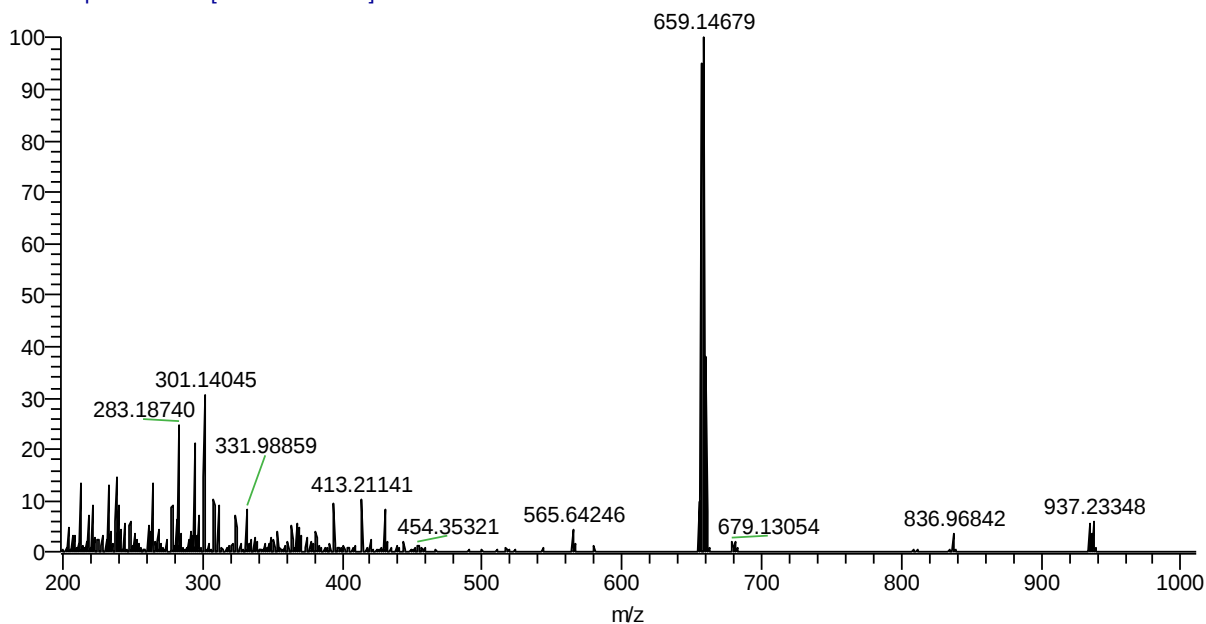


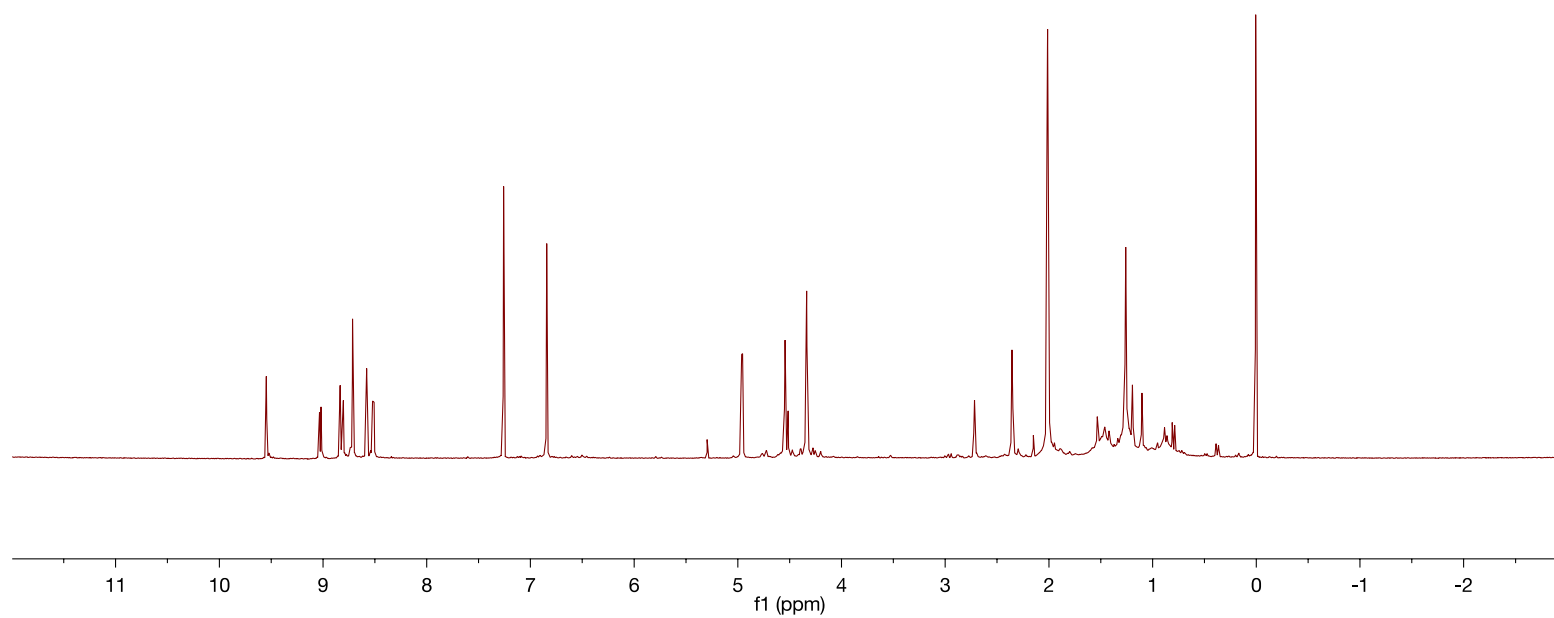
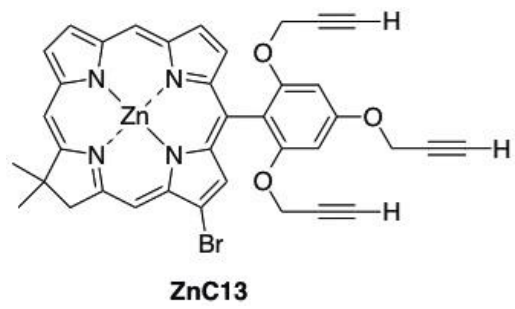


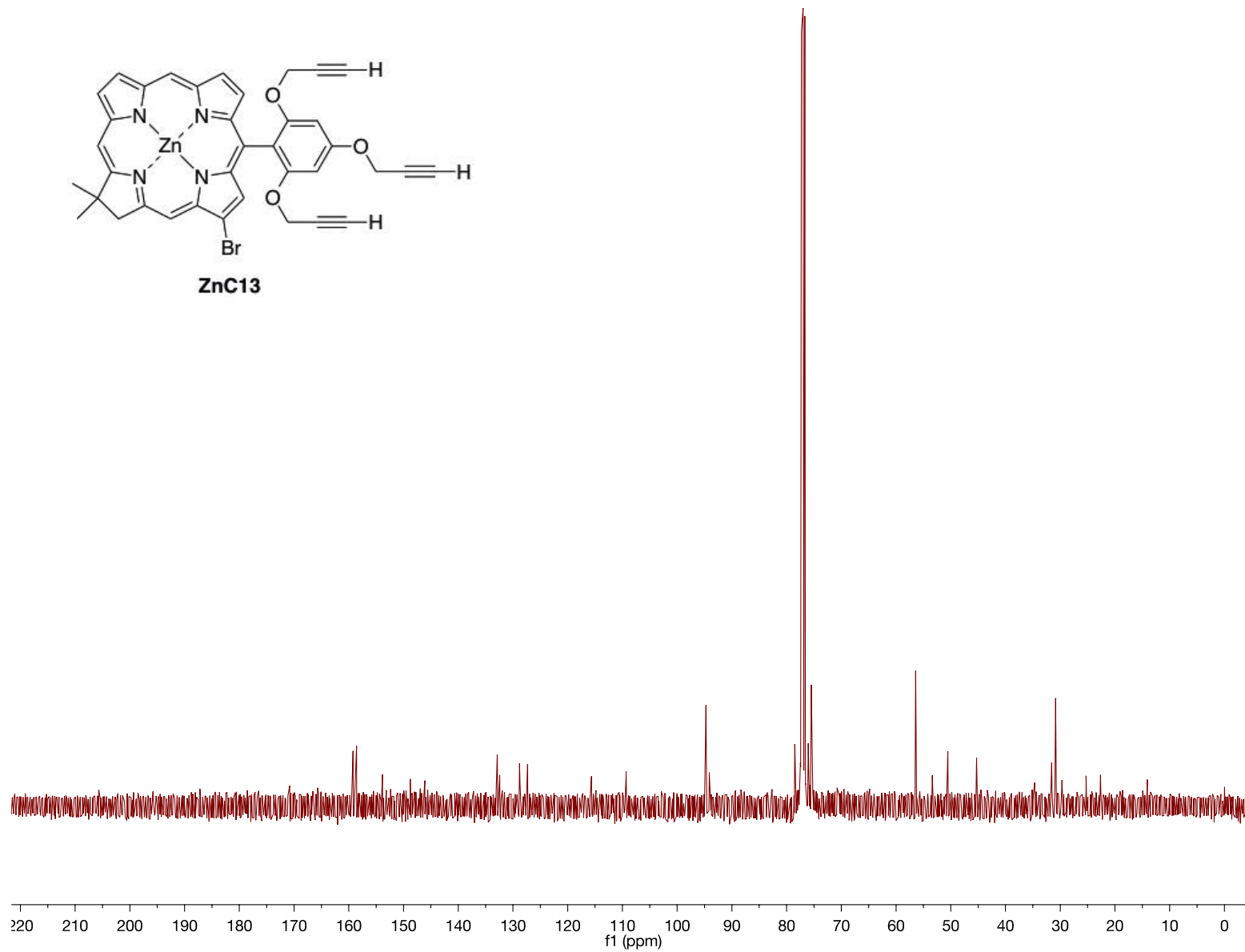
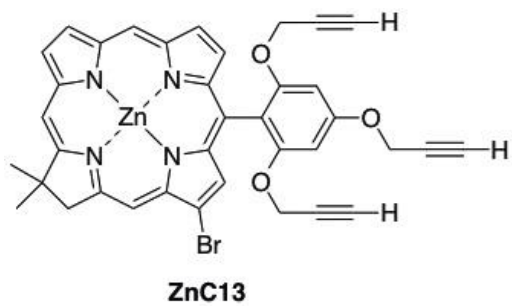
NL:
7.31E6
172265_FbC-10TriE-
13Br#385-455 RT:
1.72-2.03 AV: 71 T:
FTMS + p ESI Full ms
[200.00-1000.00]

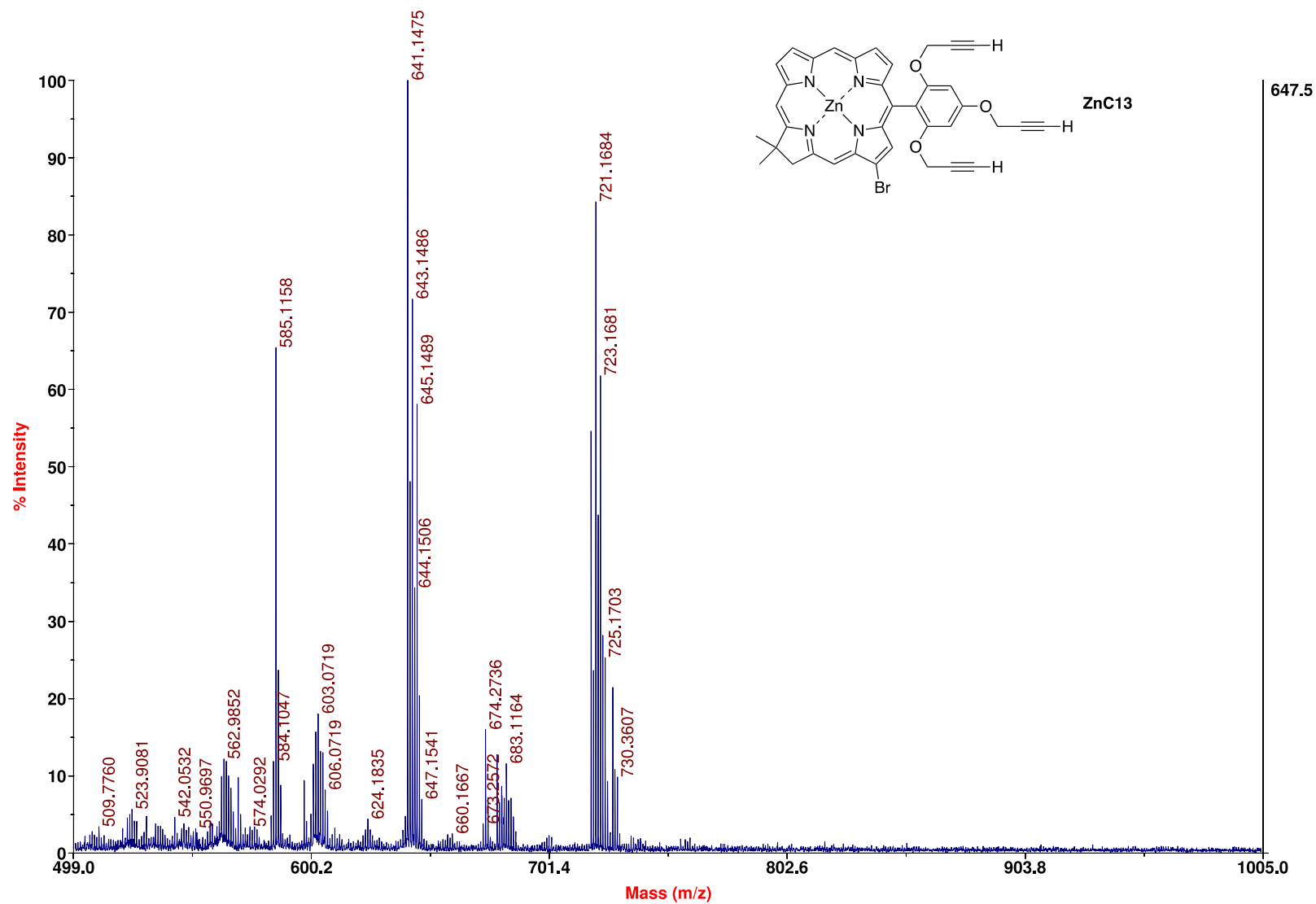
NL:
3.32E5
C₃₇ H₂₉ BrN₄ O₃ +H:
C₃₇ H₃₀ Br₁ N₄ O₃
pa Chrg 1

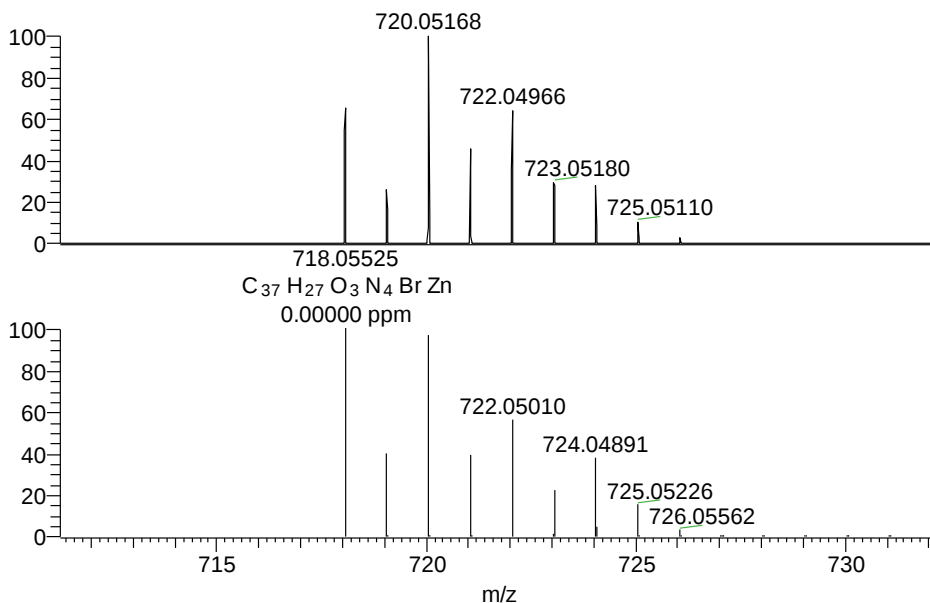
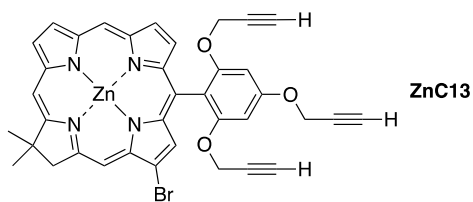
172265_FbC-10TriE-13Br #385-455 RT: 1.72-2.03 AV: 71 NL: 7.31E6
T: FTMS + p ESI Full ms [200.00-1000.00]



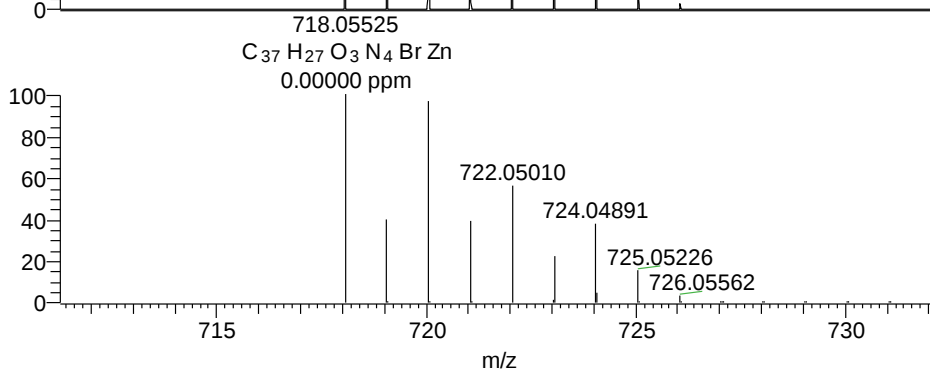






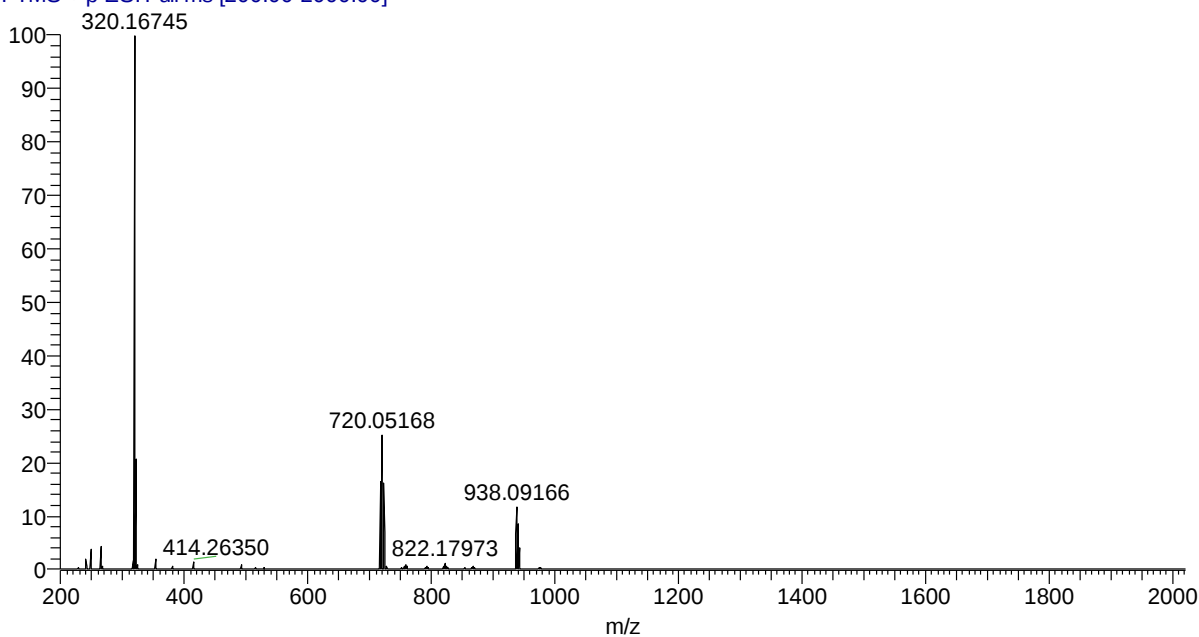


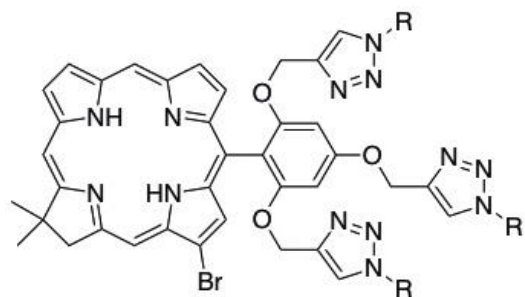
NL:
2.43E6
173796_ZnC-10TriE-
13Br#400-481 RT:
1.78-2.14 AV: 82 T:
FTMS + p ESI Full ms
[200.00-2000.00]



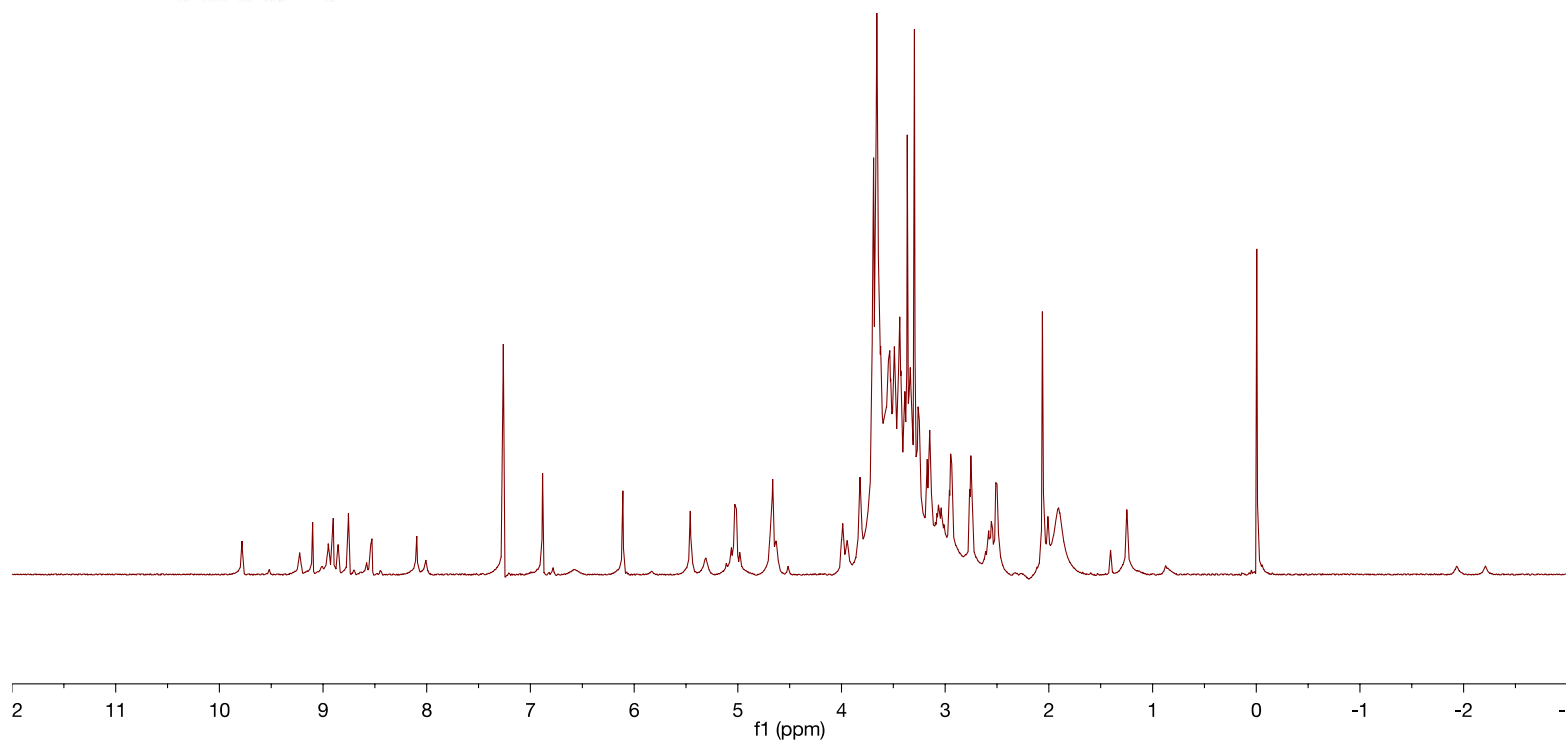
NL:
1.61E5
C₃₇ H₂₇ O₃ N₄ Br Zn:
C₃₇ H₂₇ Br₁ N₄ O₃ Zn:
pa Chrg 1

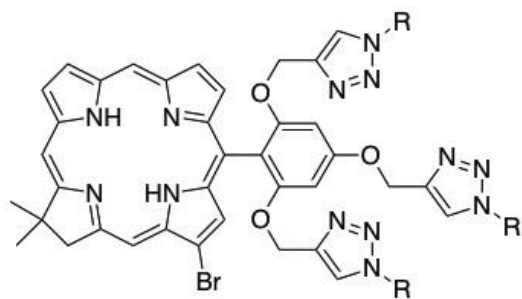
173796_ZnC-10TriE-13Br #400-481 RT: 1
T: FTMS + p ESI Full ms [200.00-2000.00]



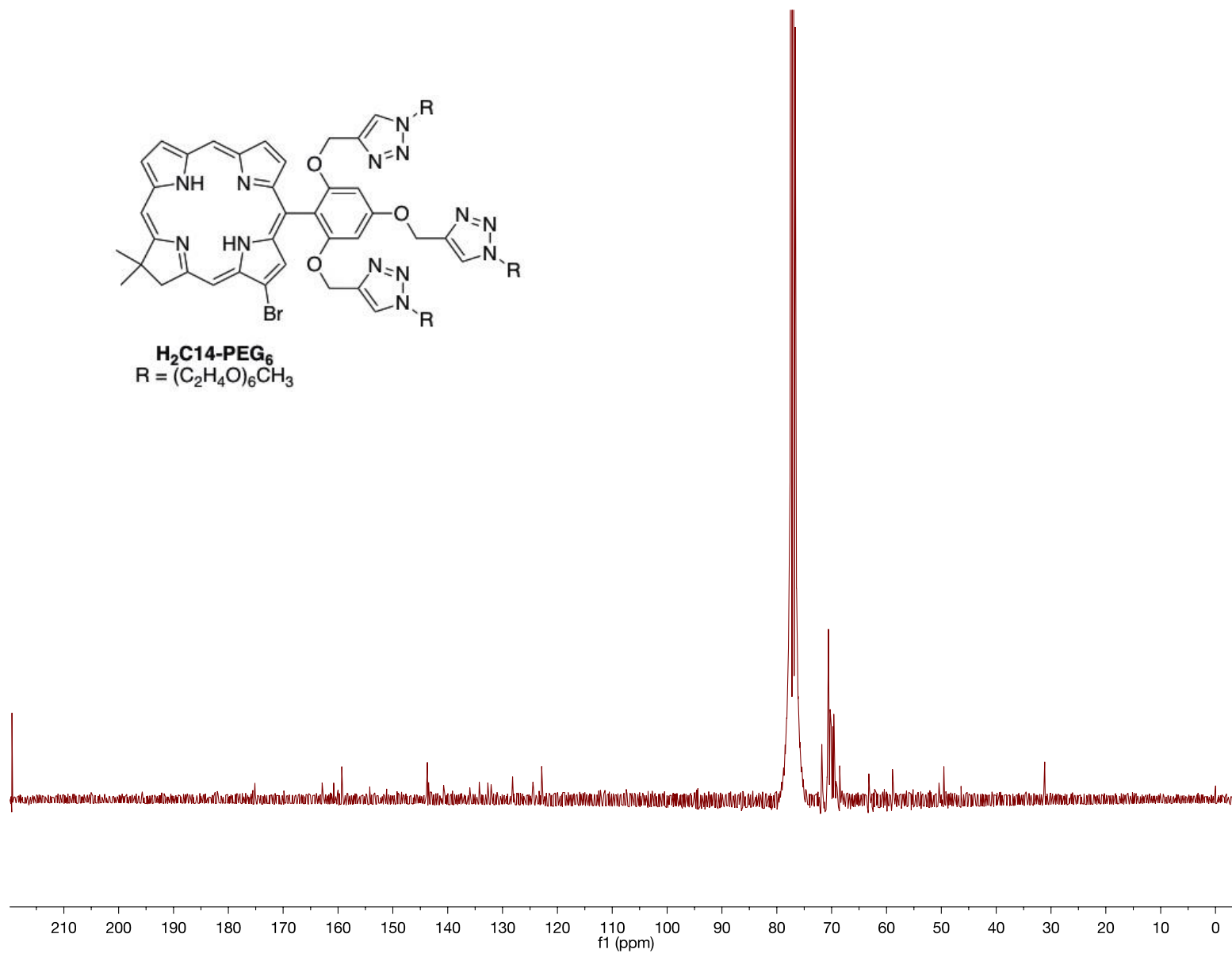


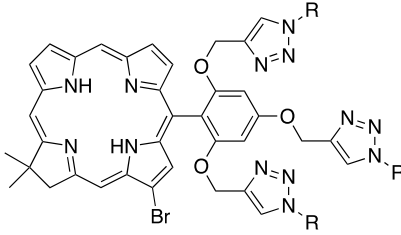
H₂C14-PEG₆
 R = (C₂H₄O)₆CH₃





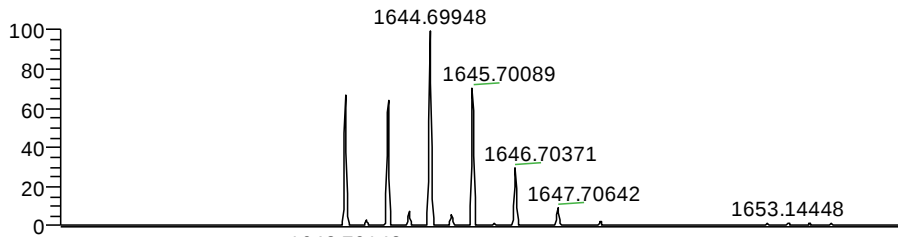
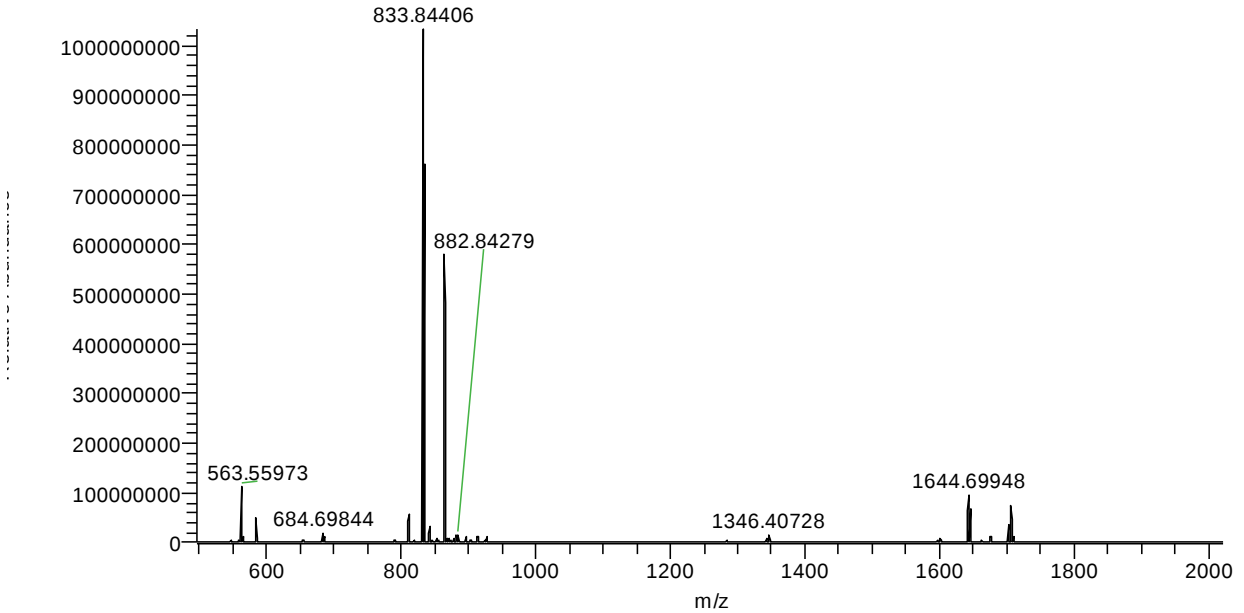
H₂C14-PEG₆
 R = (C₂H₄O)₆CH₃



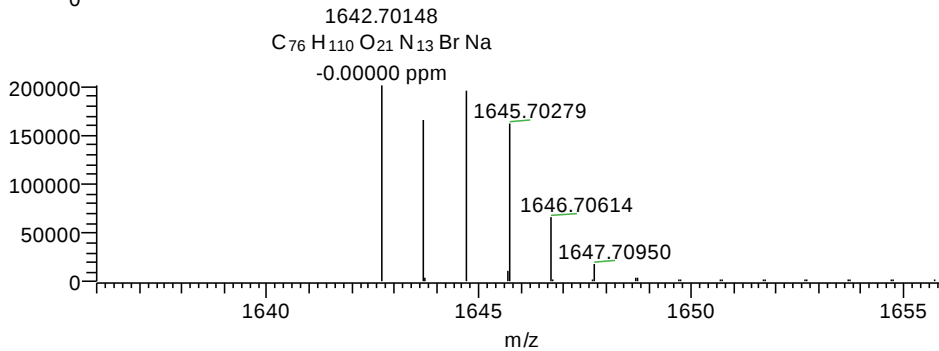


H₂C14-PEG₆
 R = (C₂H₄O)₆CH₃

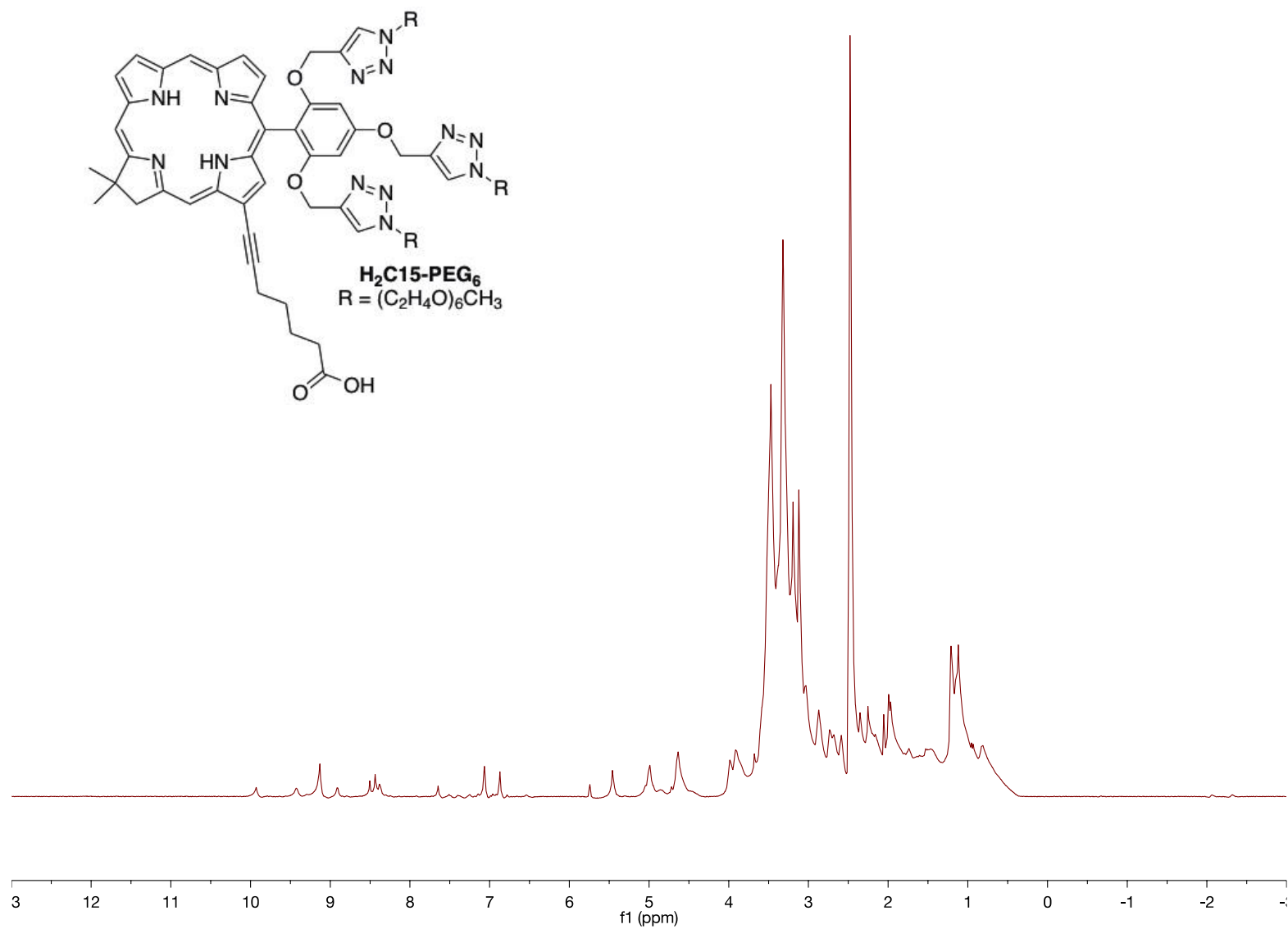
174606_FbC-10TiPEG-13Br #218-615 RT: 0.97-2.74 AV: 398 NL: 1.03E9
 T: FTMS + p ESI Full ms [500.00-2000.00]

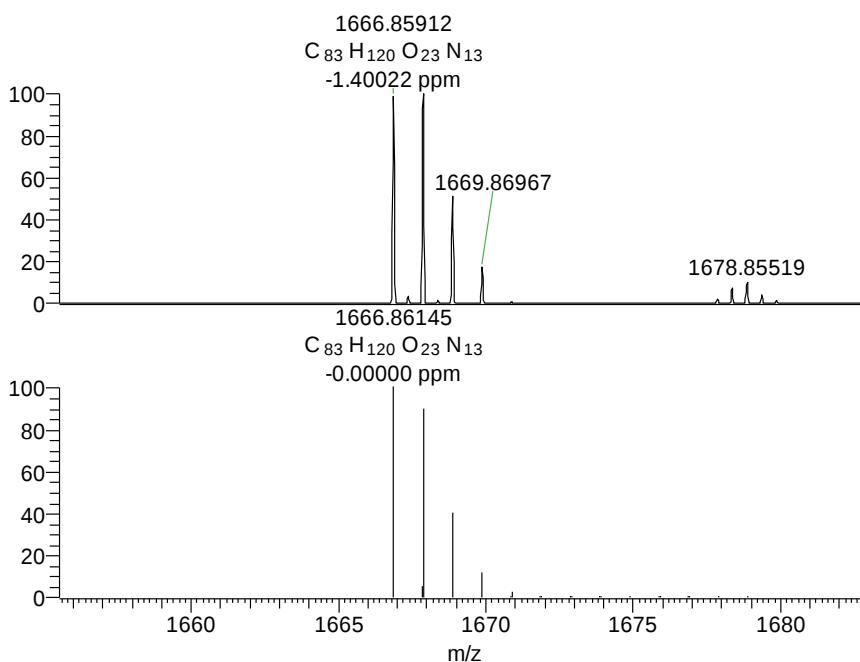
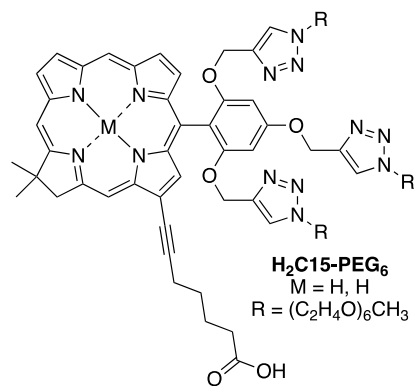


NL:
 9.65E7
 174606_FbC-10TiPEG-
 13Br#218-615 RT:
 0.97-2.74 AV: 398 T:
 FTMS + p ESI Full ms
 [500.00-2000.00]



NL:
 2.00E5
 C₇₆ H₁₁₀ BrN₁₃ O₂₁+Na:
 C₇₆ H₁₁₀ Br₁N₁₃ O₂₁Na₁
 pa Chrg 1

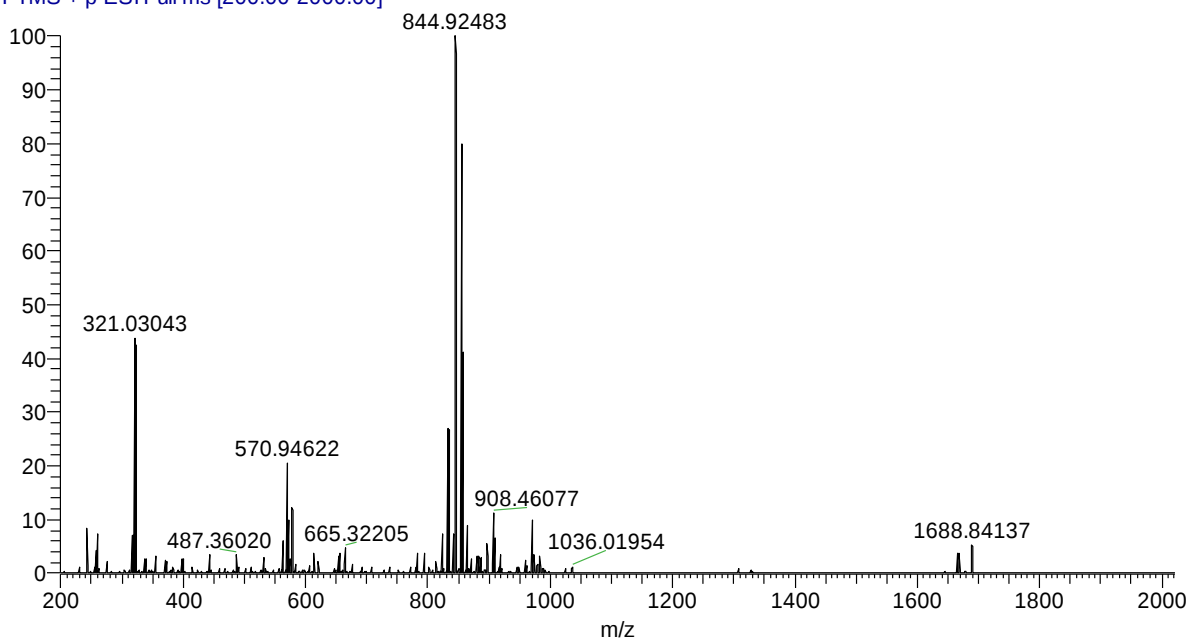


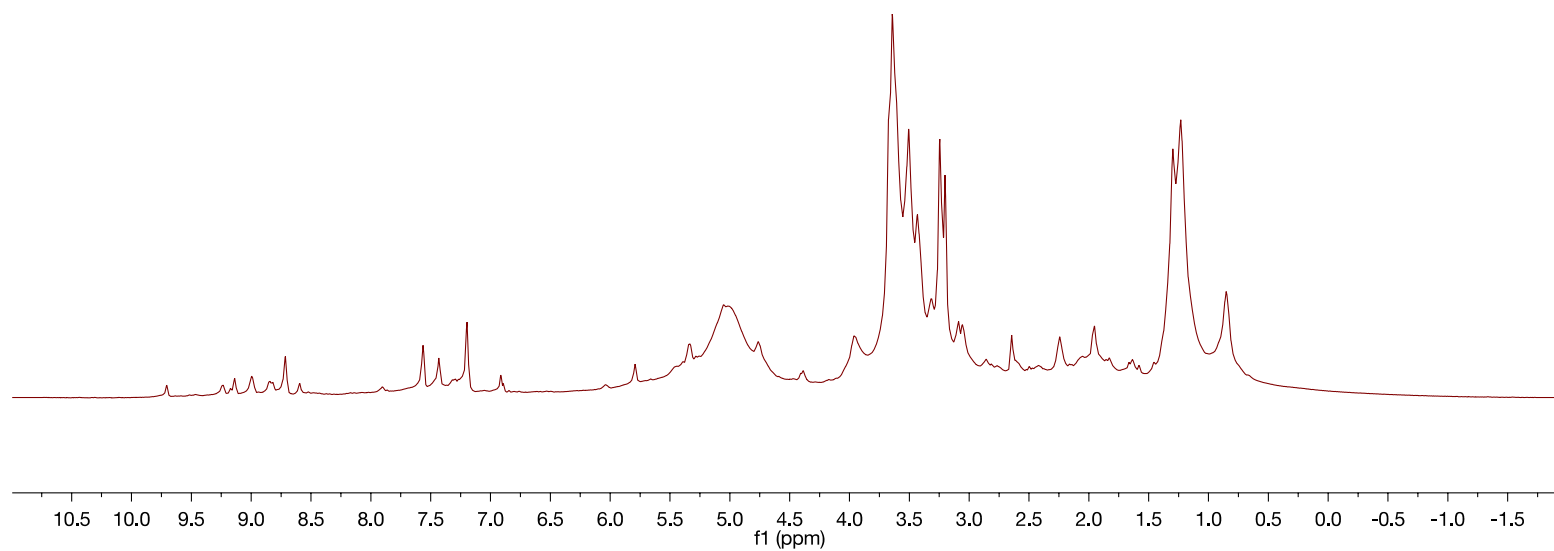
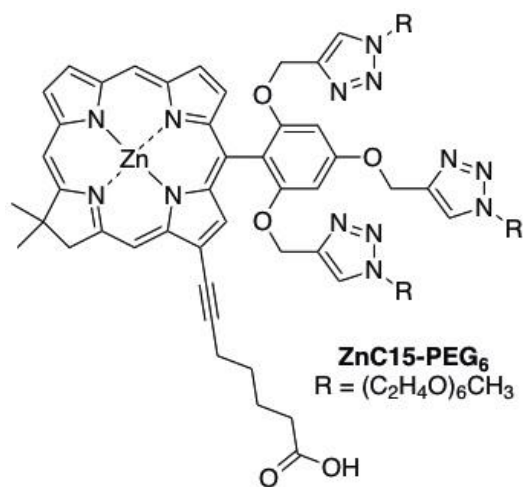


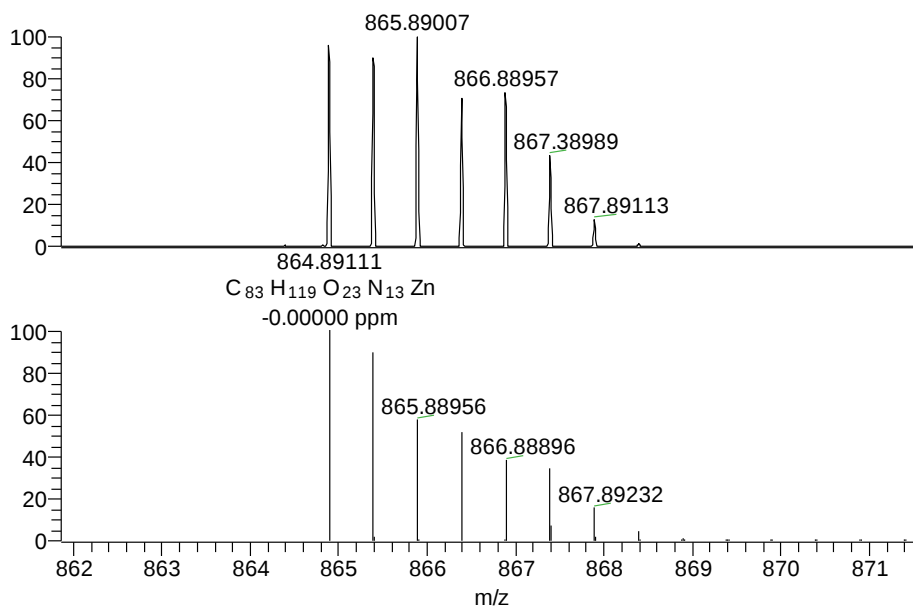
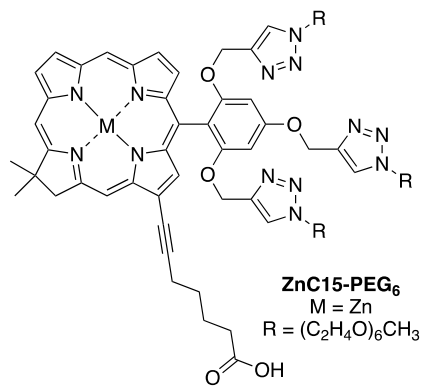
NL:
2.49E6
173793_FbC-10TriPEG-
13COOH#423-531 RT:
1.89-2.37 AV: 109 SB: 137
0.40-1.01 T: FTMS + p ESI Full
ms [200.00-2000.00]

NL:
3.64E5
C₈₃ H₁₁₉ N₁₃ O₂₃ +H:
C₈₃ H₁₂₀ N₁₃ O₂₃
pa Chrg 1

173793_FbC-10TriPEG-13COOH #423-531 .89-2.37 AV: 109 SB: 137 0.40-1.01 NL: 6.55E7
T: FTMS + p ESI Full ms [200.00-2000.00]







NL:
1.94E6
173794_ZnC-10TriPEG-
13COOH#117-194 RT:
0.52-0.86 AV: 78 T:
FTMS + p ESI Full ms
[200.00-2000.00]

NL:
1.77E5
C₈₃ H₁₁₇ N₁₃ O₂₃ Zn +H:
C₈₃ H₁₁₉ N₁₃ O₂₃ Zn₁
pa Chrg 2

173794_ZnC-10TriPEG-13COOH #117-194
T: FTMS + p ESI Full ms [200.00-2000.00]

