ELECTRONIC SUPPLEMENTARY DATA

Synthesis, Antibacterial Activity and Mode of Action of Novel Linoleic acid-di-peptide-Spermidine Conjugates

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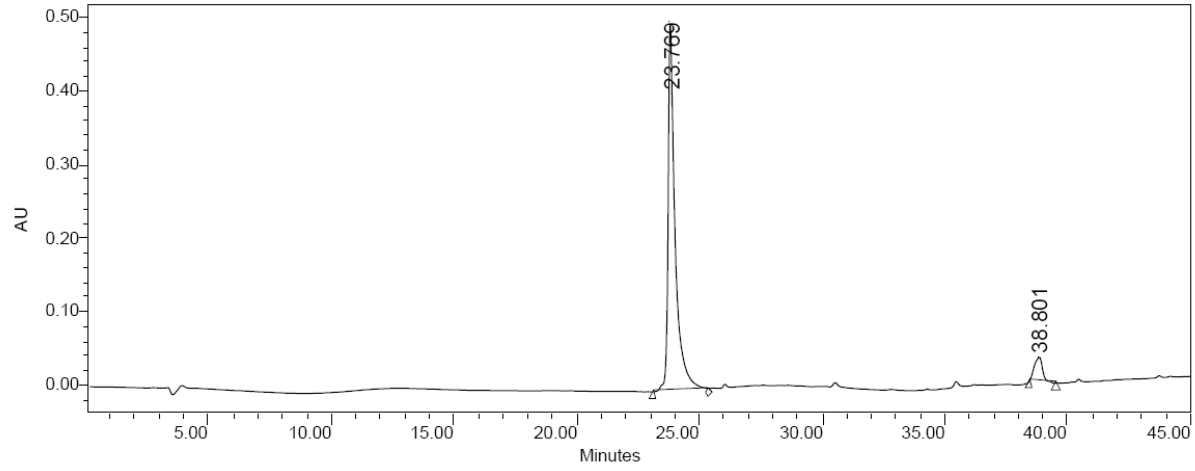
A) RP-HPLC profiles of sequences **12**-**19** (absorbance at 220 nm). For **12**, **13** and **16**, HPLC gradient of 10 to 90 % buffer 2 was run where, buffer 1 was water (0.05 % TFA) and buffer 2 was acetonitrile (0.05 % TFA) over 45 minutes. For sequences **14**-**19**, gradient of 30 to 100% buffer 2 was run over 45 minutes where, buffer 1 was water (0.1 % TFA) and buffer 2 was acetonitrile (0.1 % TFA).



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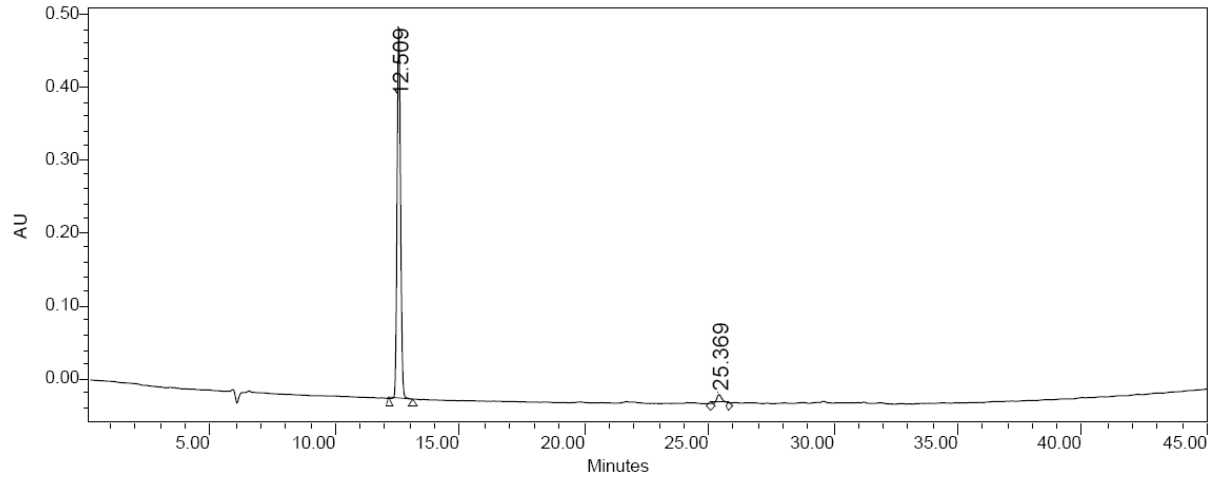

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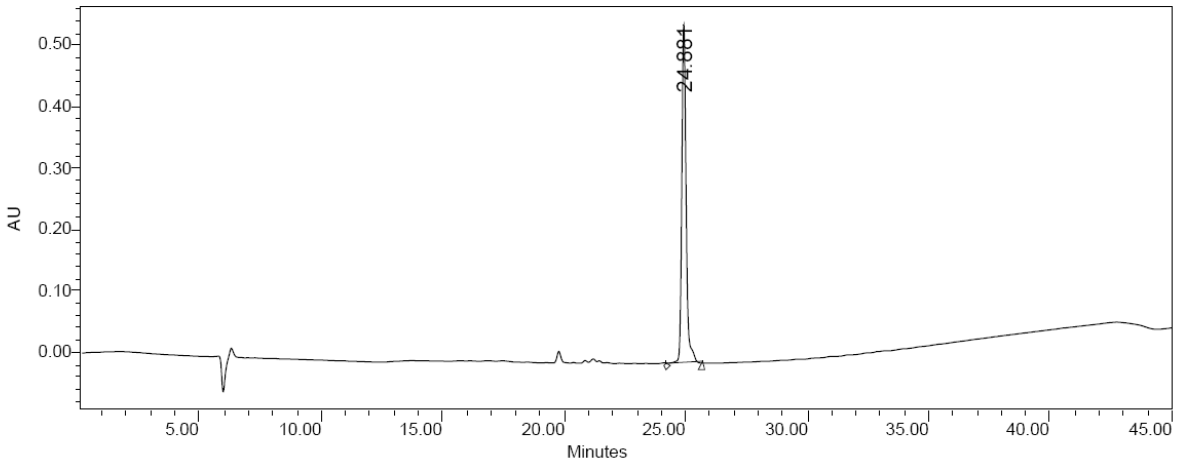

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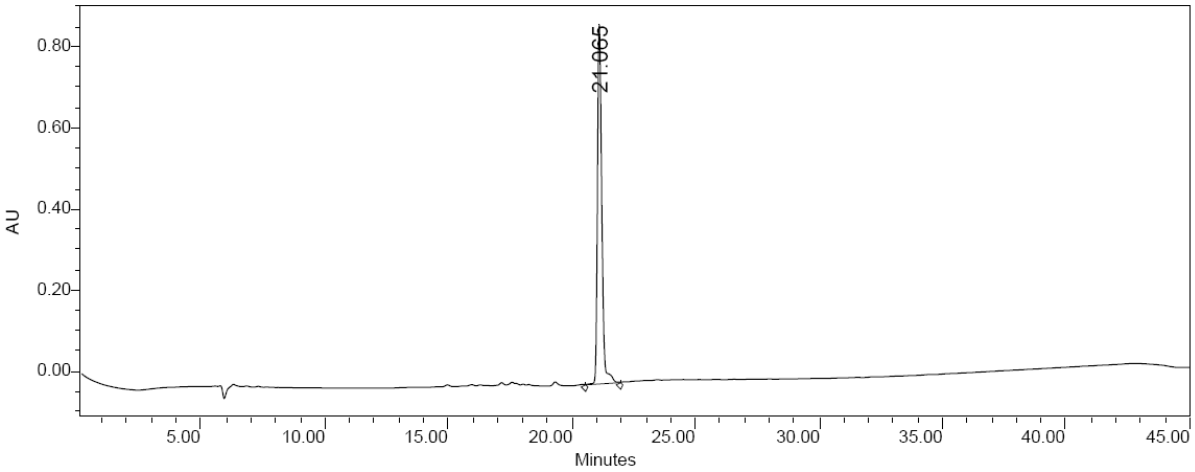

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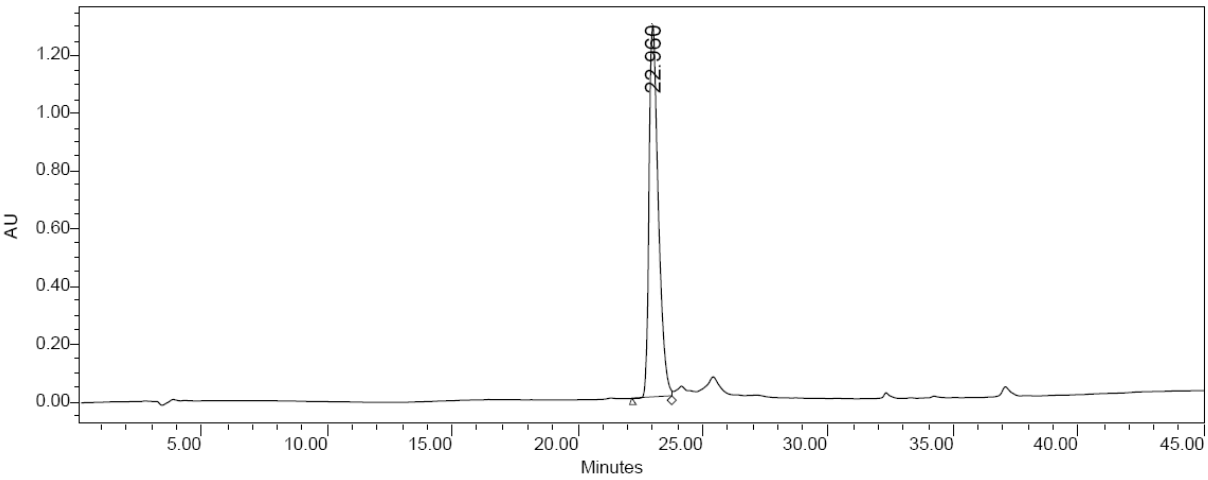

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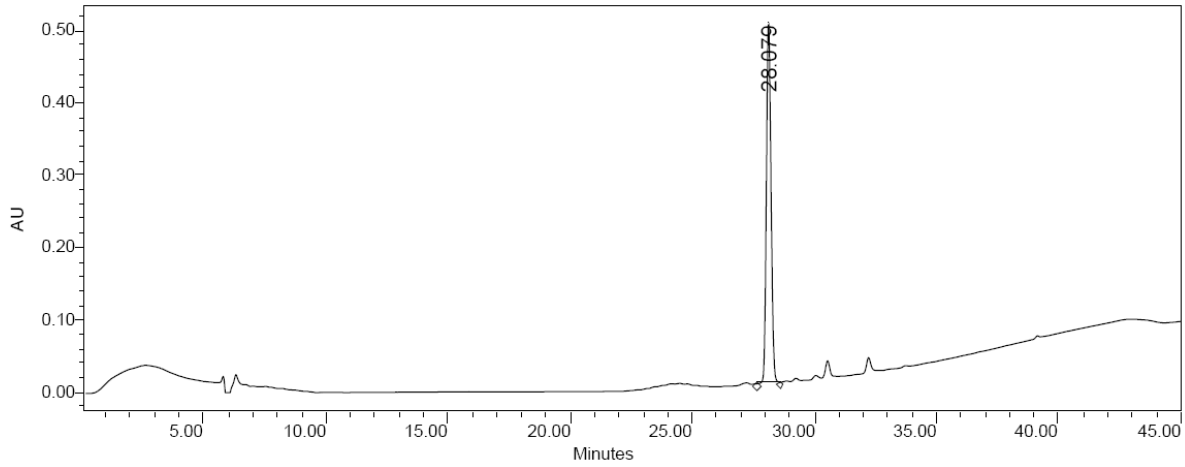

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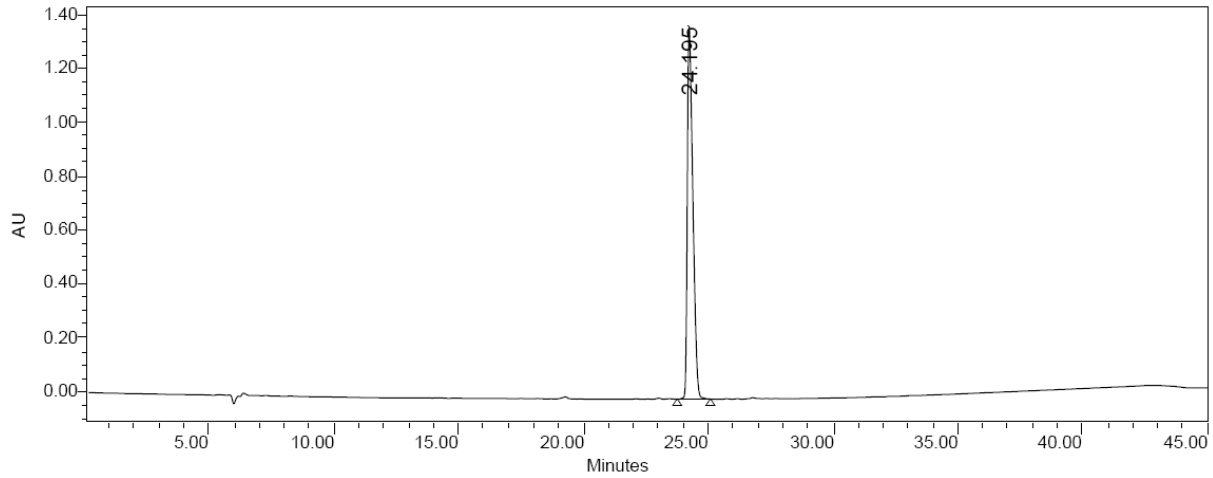

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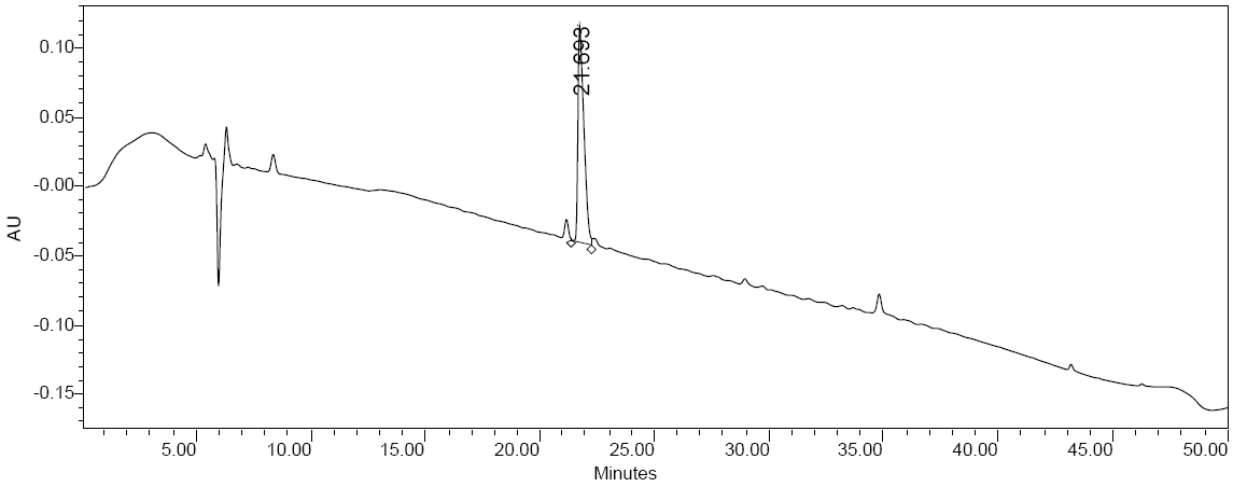
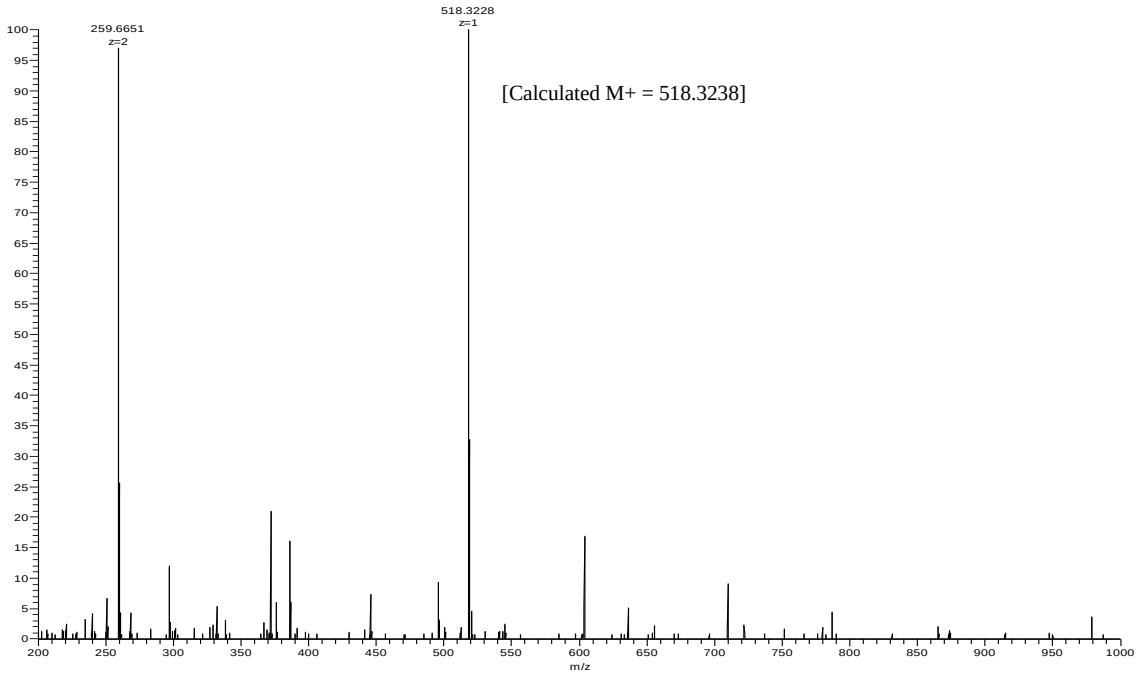


19

B) ESI-HRMS spectra of sequences **1**-**5**, **7, 8** and **10**-**19** using LC-ESI-HRMS on UHPLC (Dionex, Germany) and LTQ Orbitrap XL (Thermo Fisher Scientific, USA). The MS data was acquired in positive ion mode at a resolution of 60,000.



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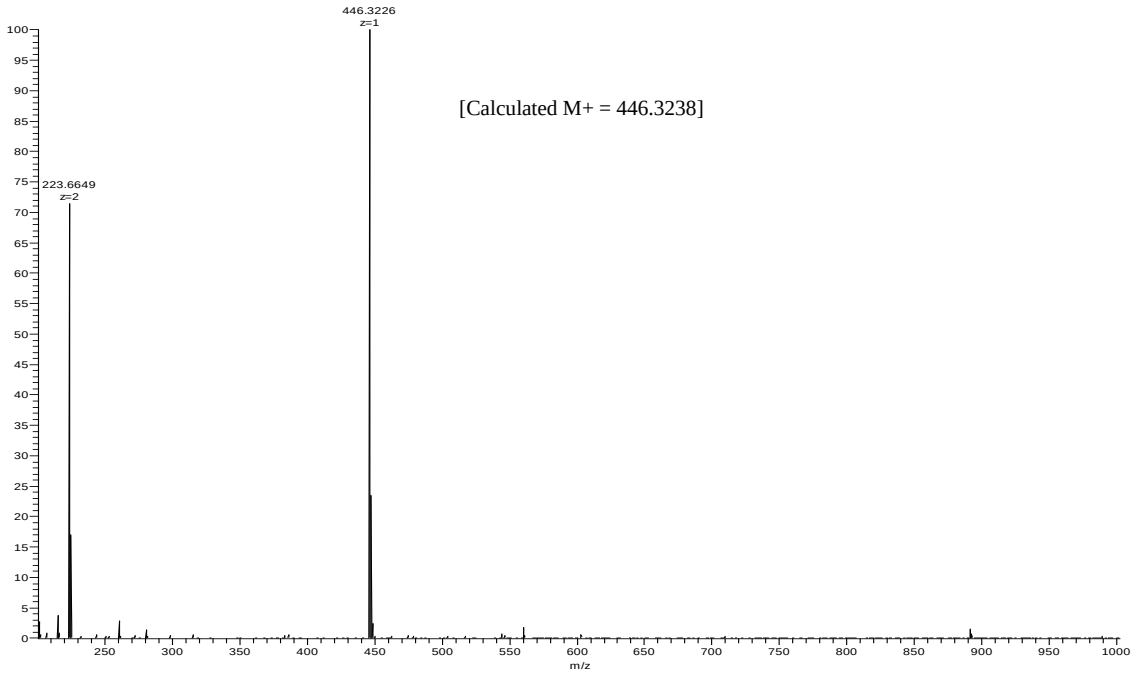

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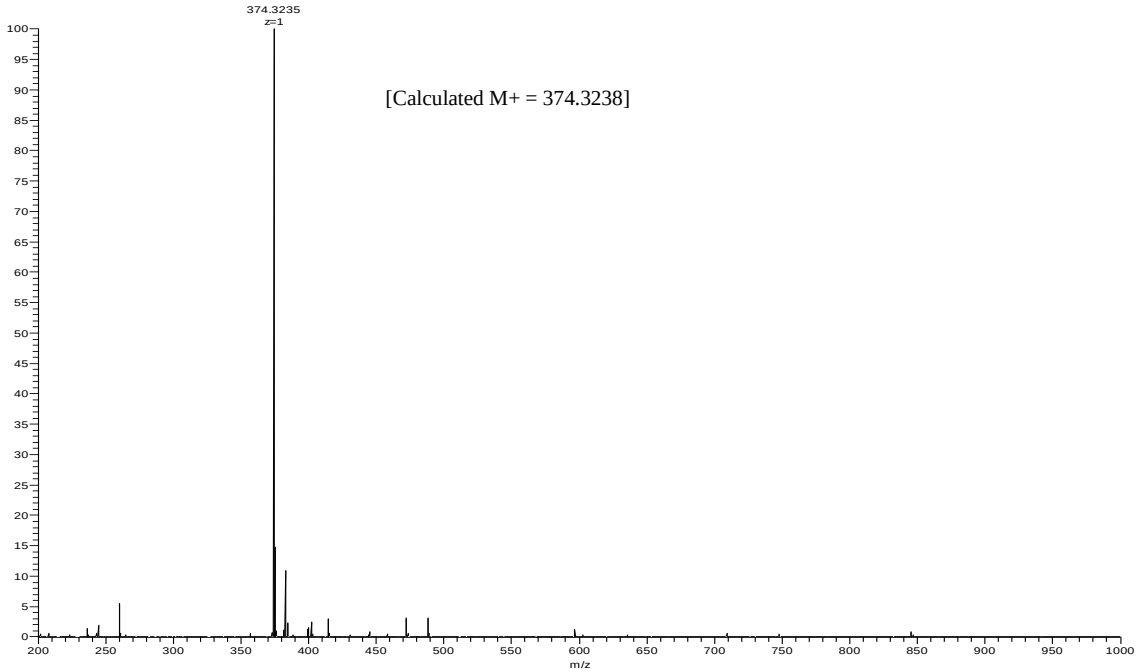

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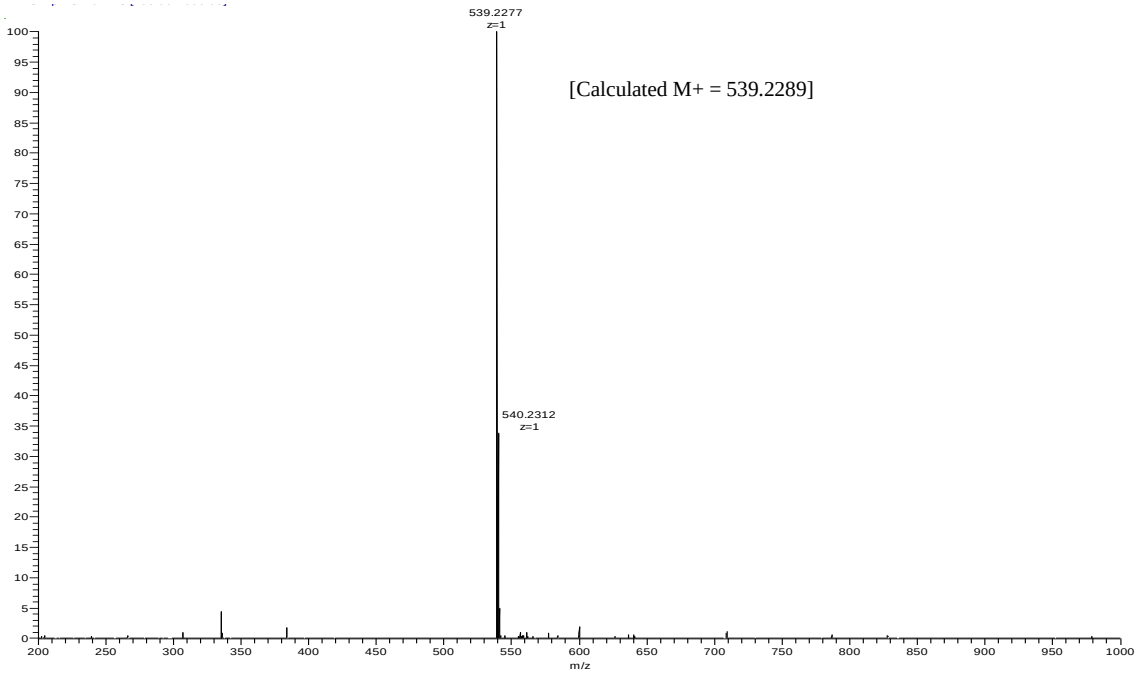

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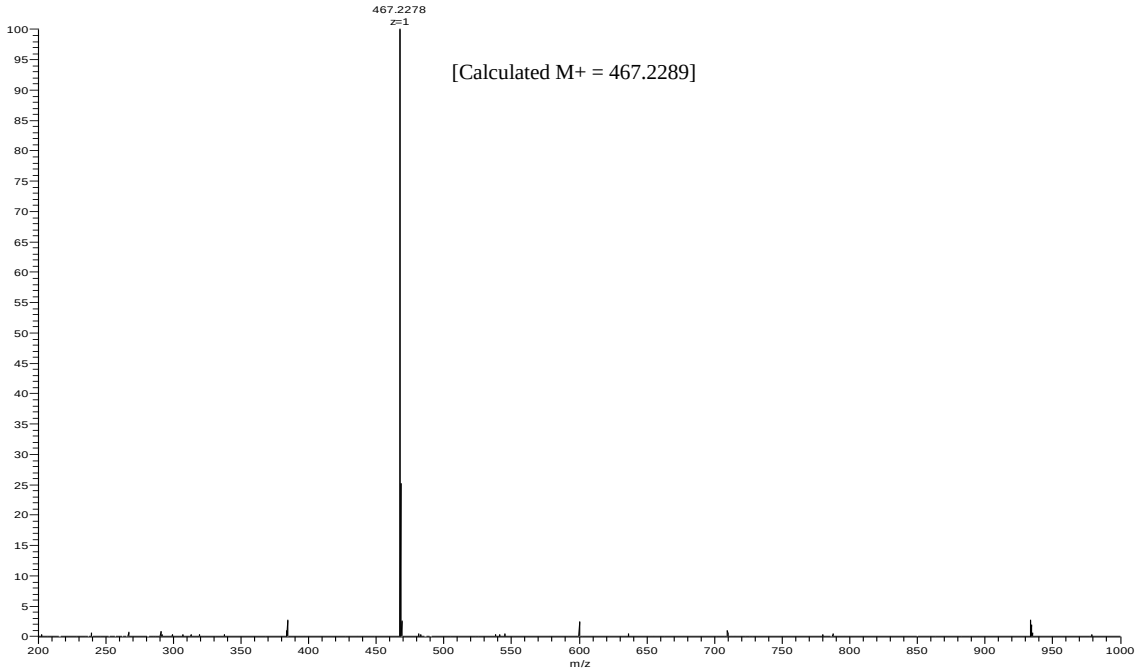

[Calculated M+ = 467.2289]

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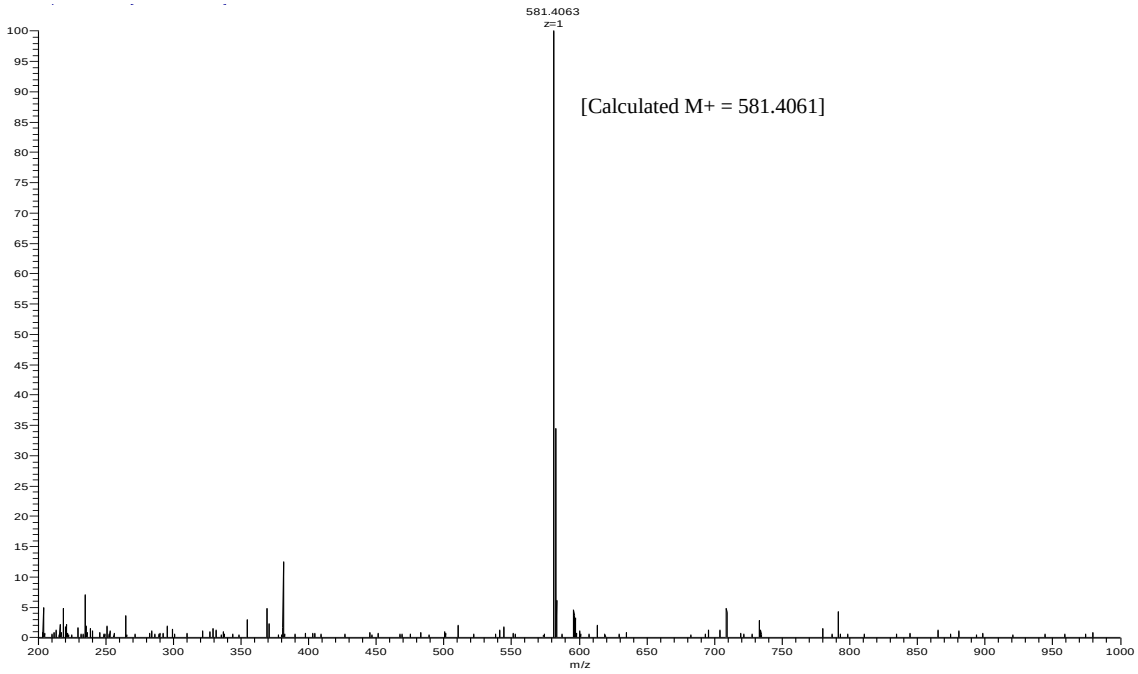

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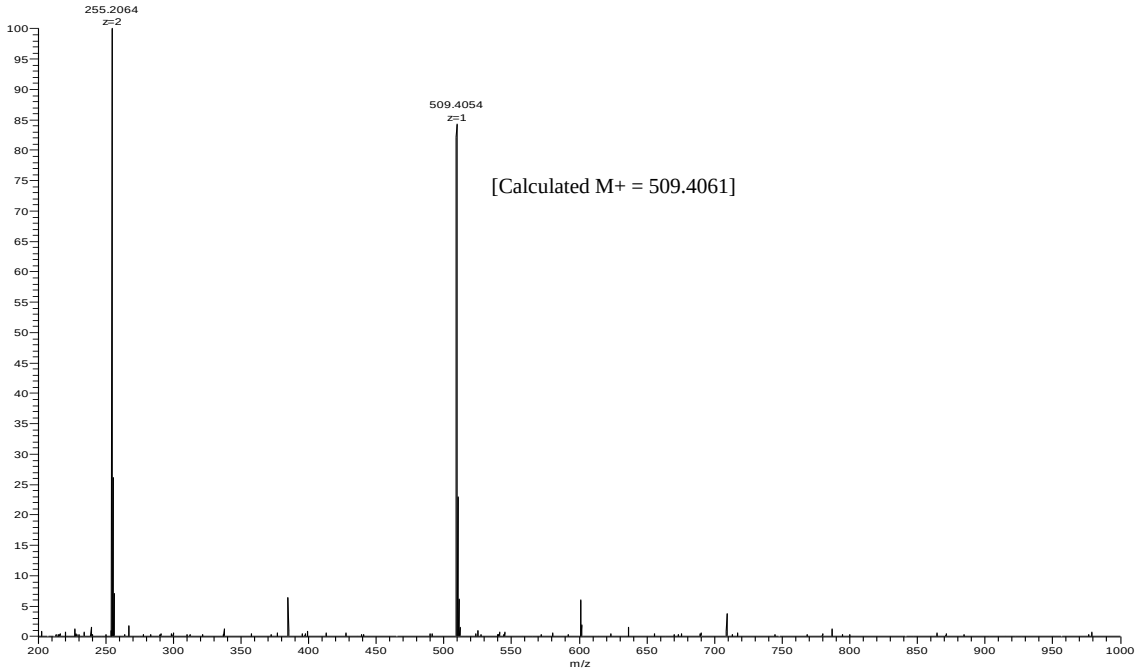

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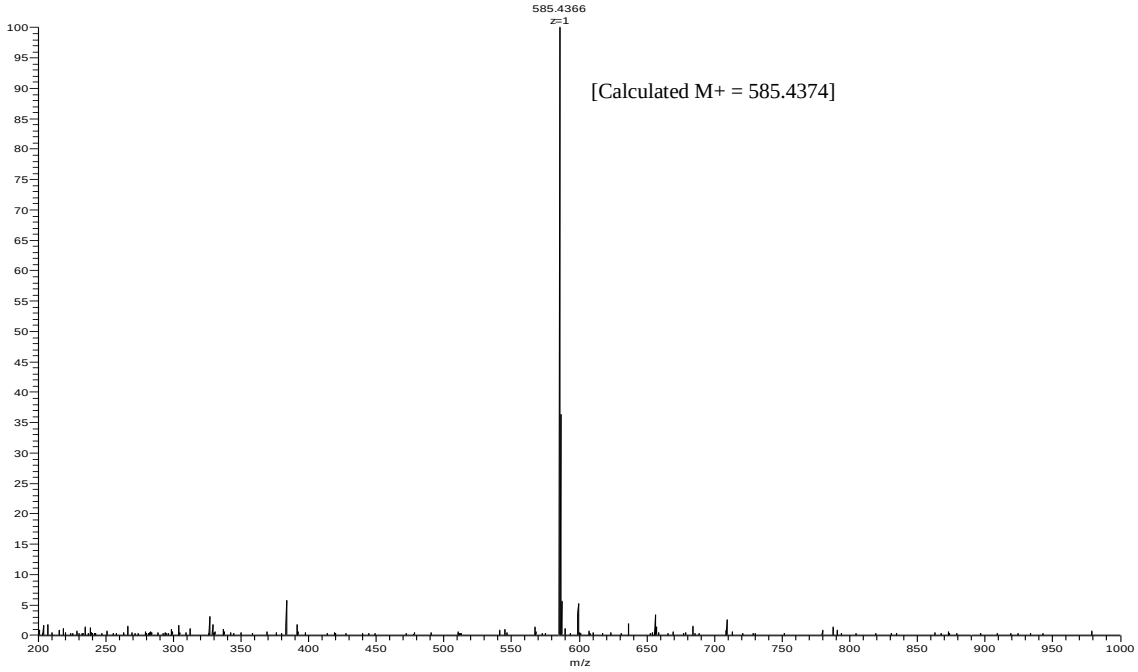

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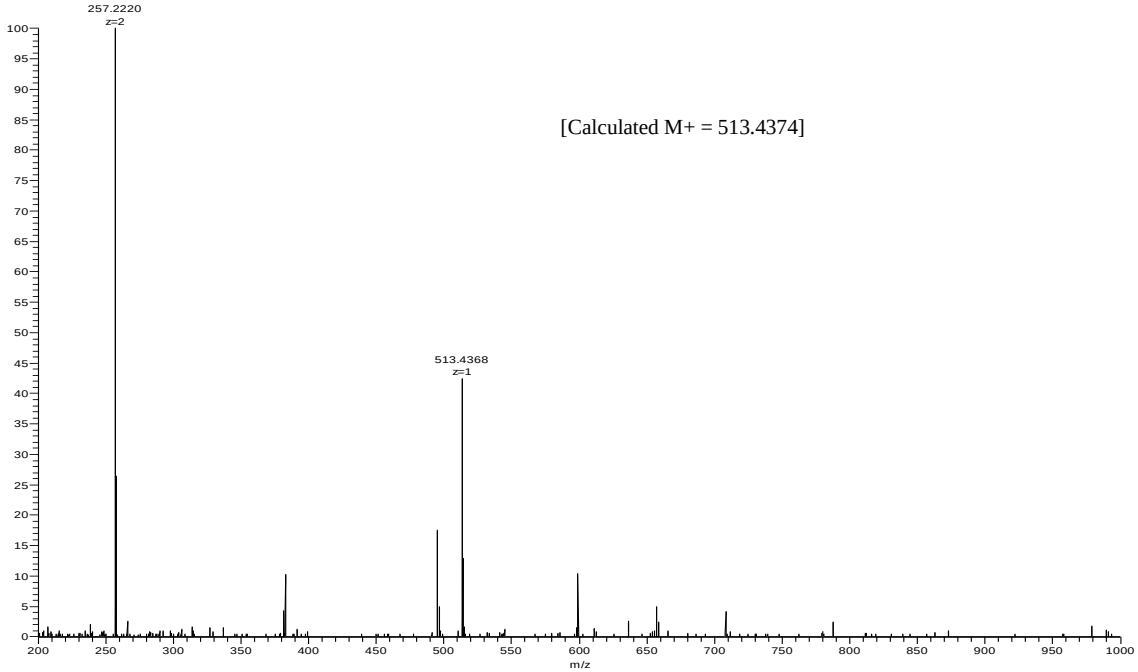

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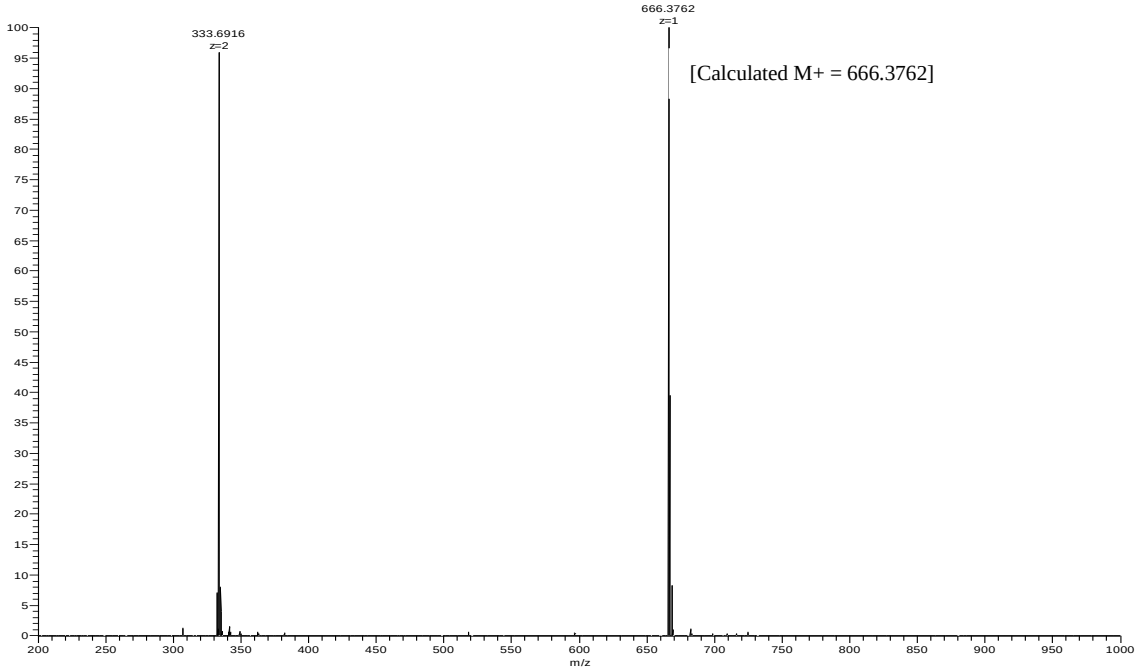

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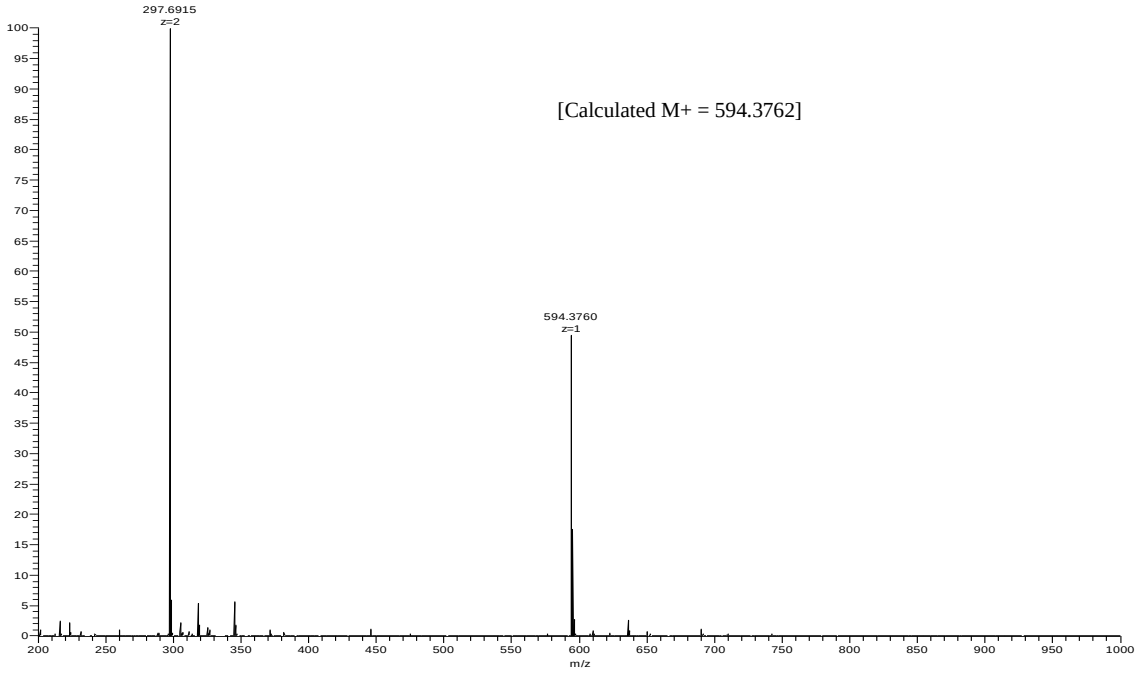

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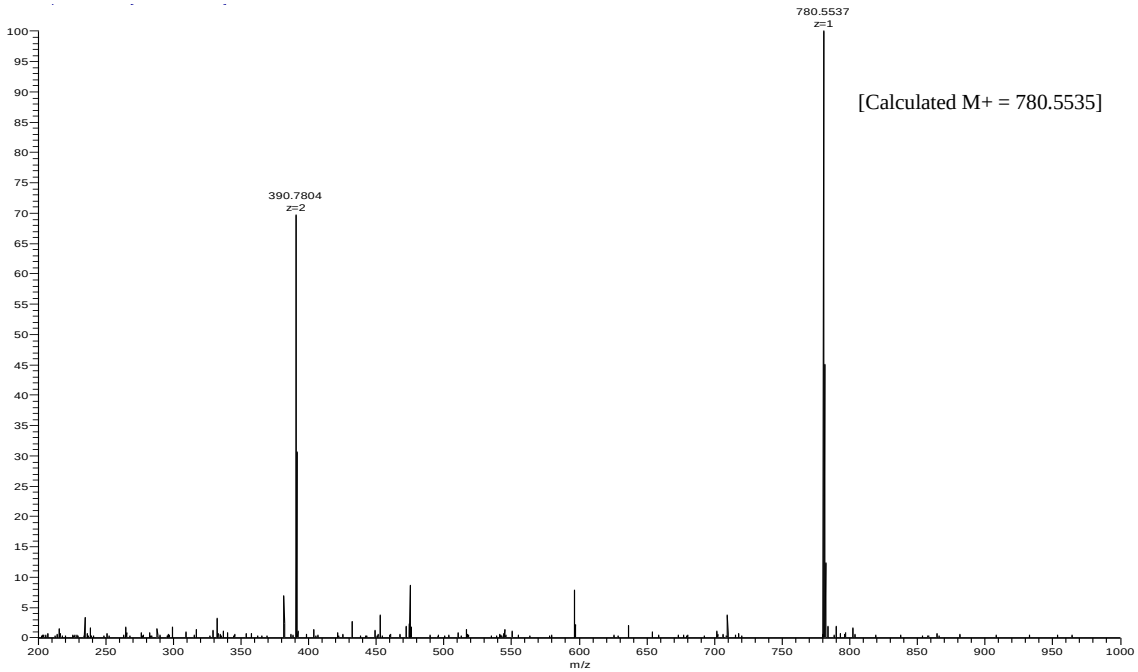

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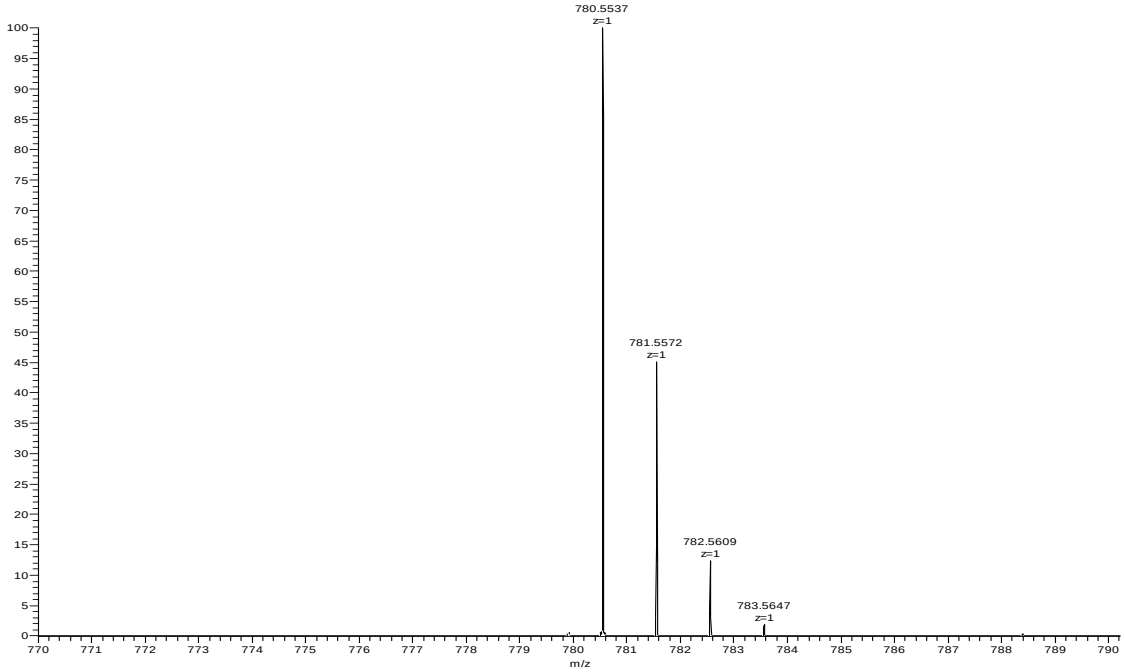
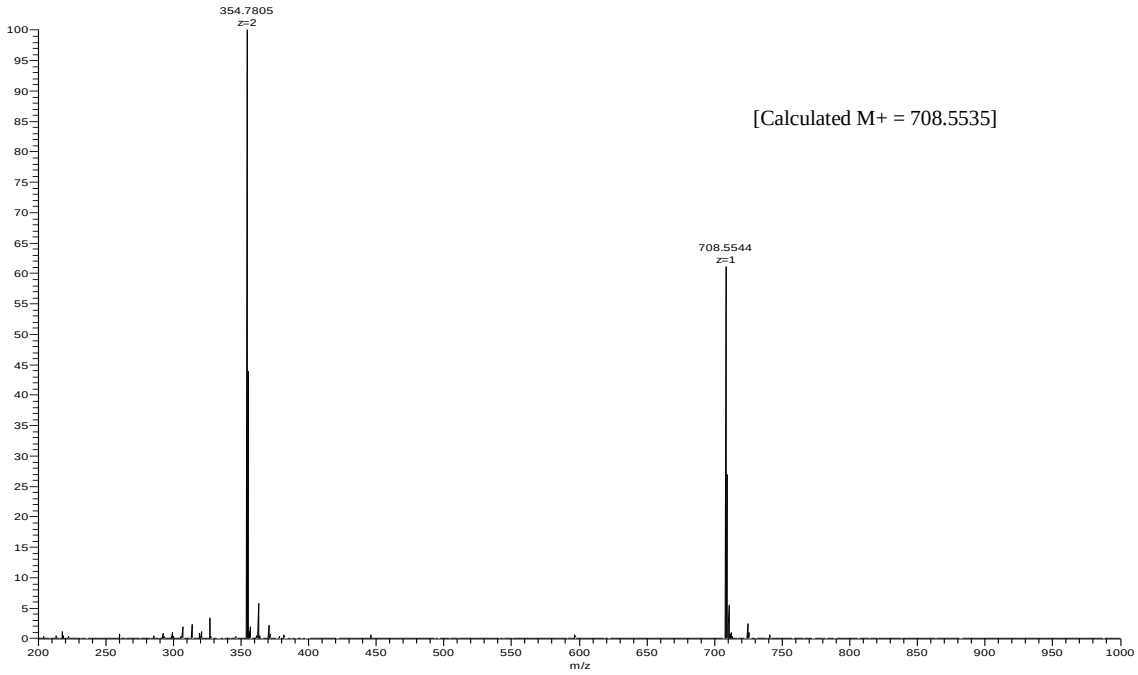
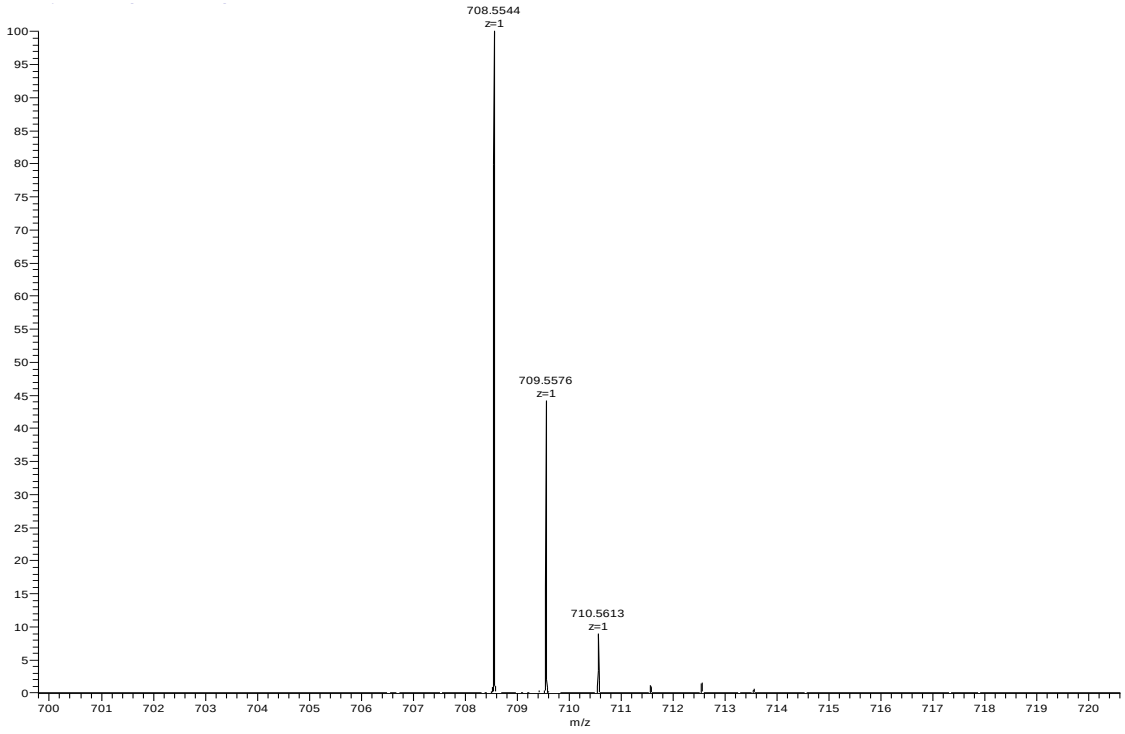


Isotopic peaks for molecular ion peak of **14**

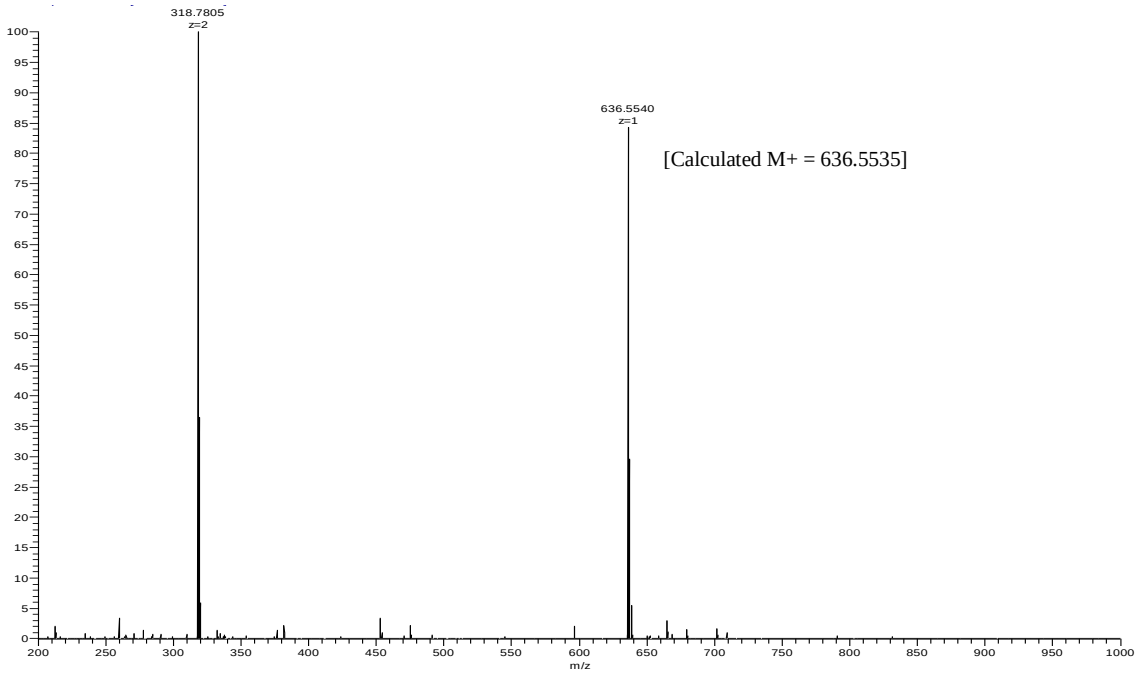


[Calculated M+ = 708.5535]

15



Isotopic peaks for molecular ion peak of **15**



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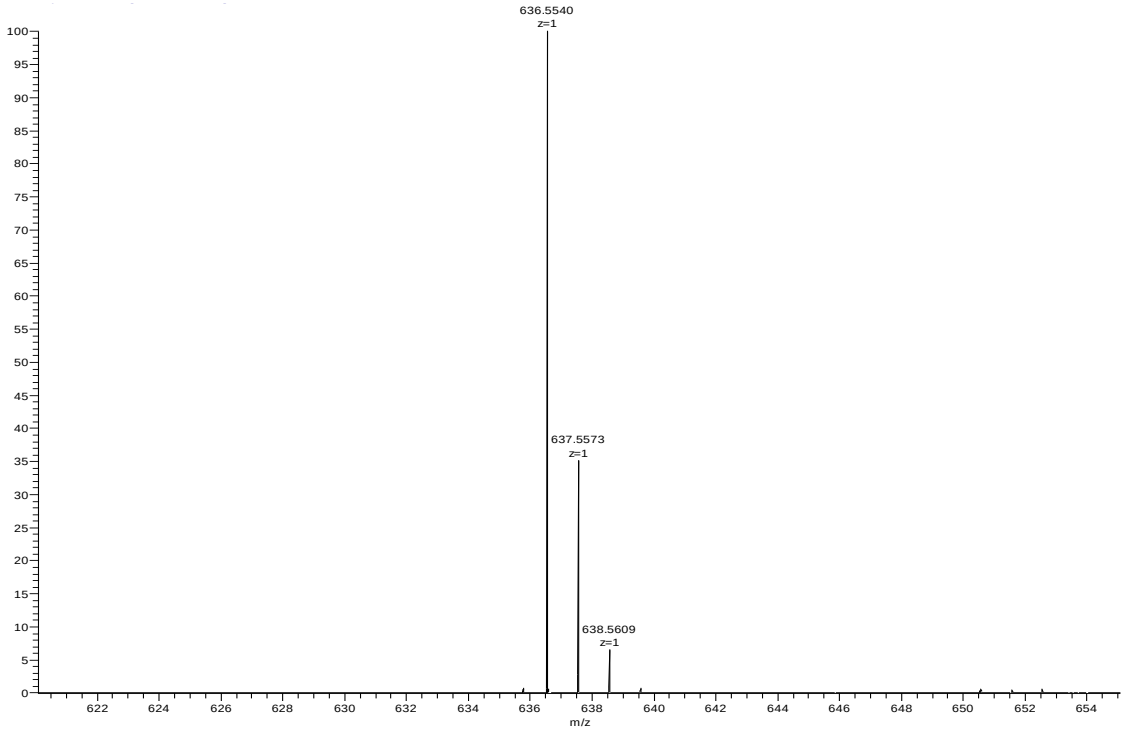
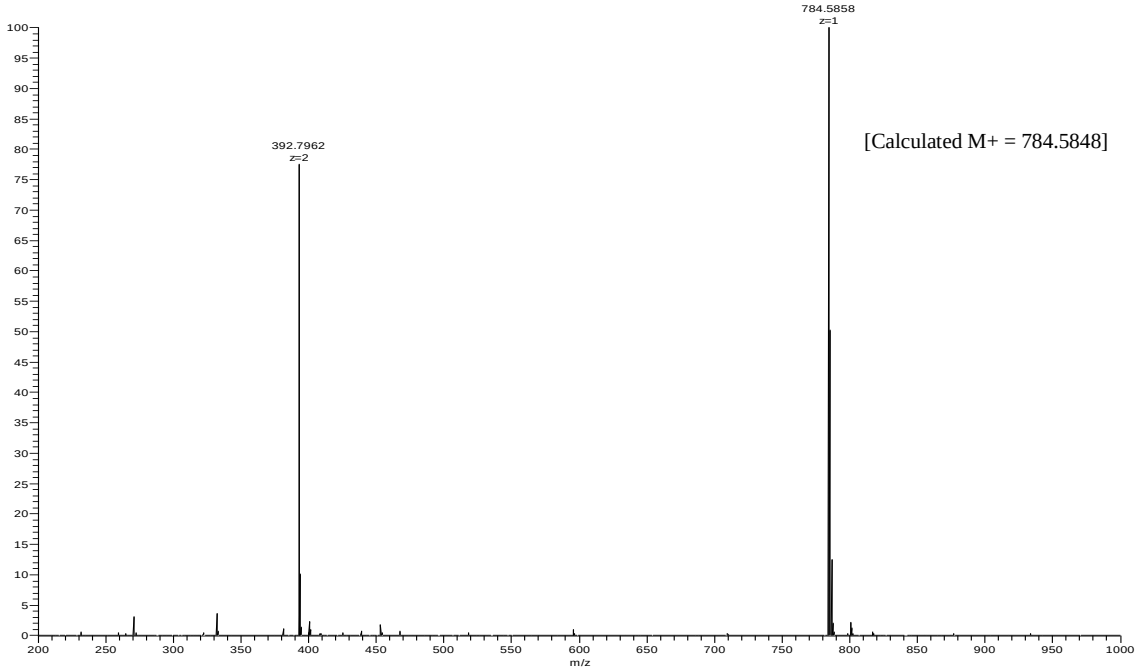


Isotopic peaks for molecular ion peak of **16**



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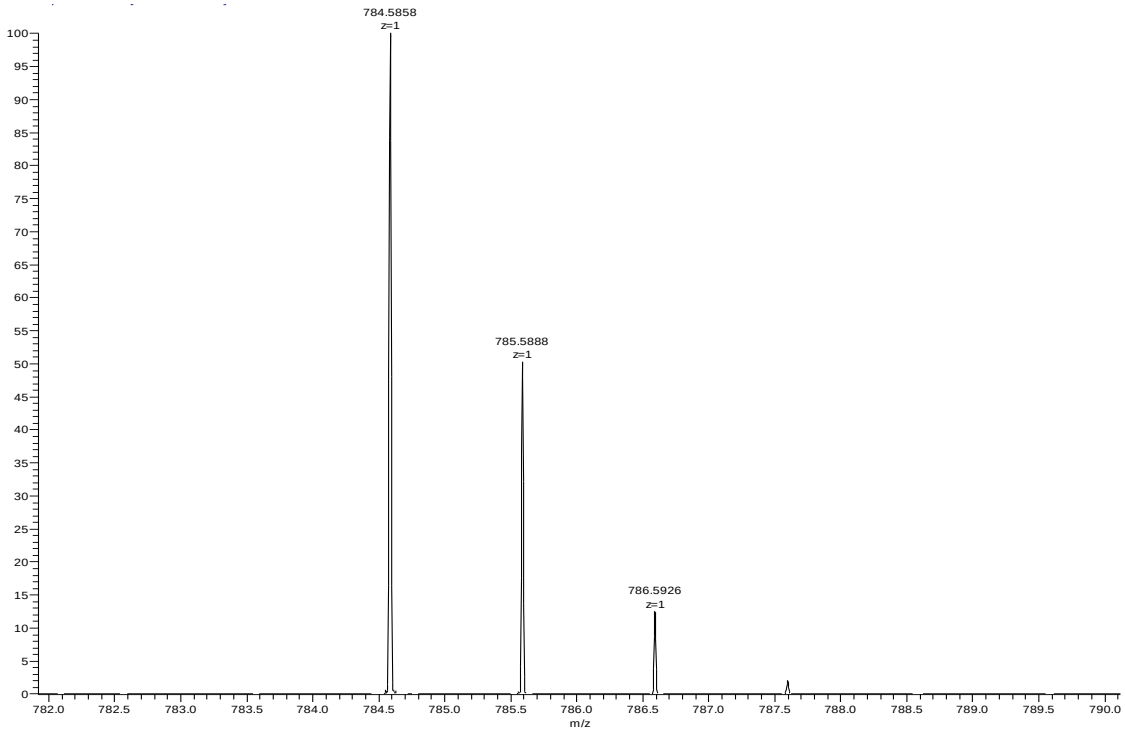
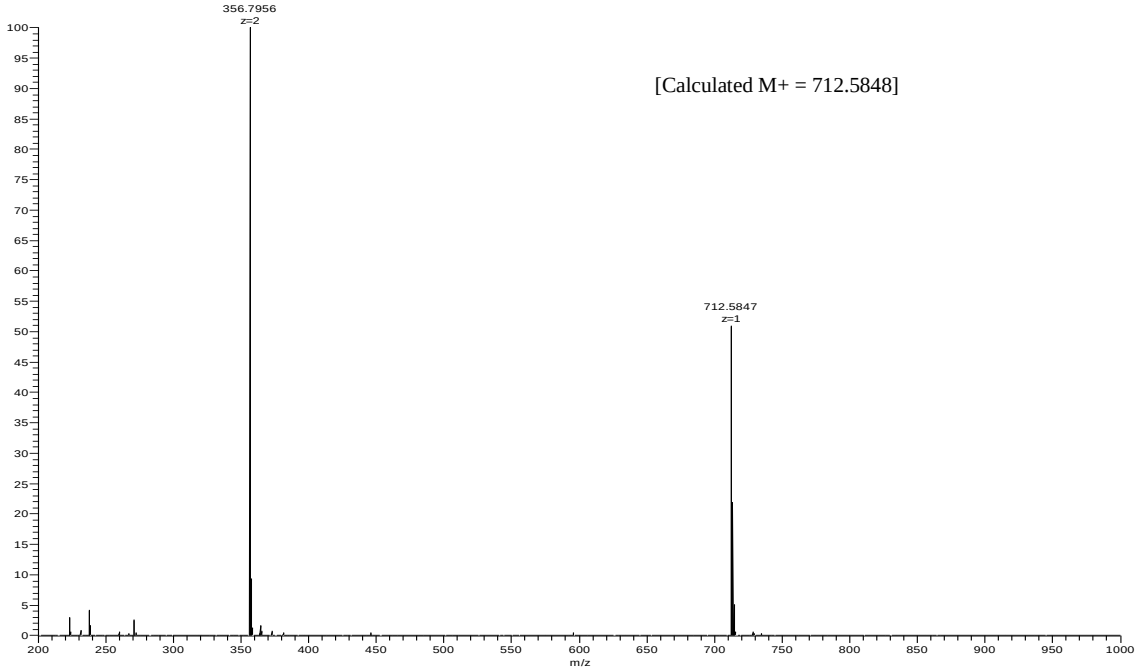


Isotopic peaks for molecular ion peak of **17**



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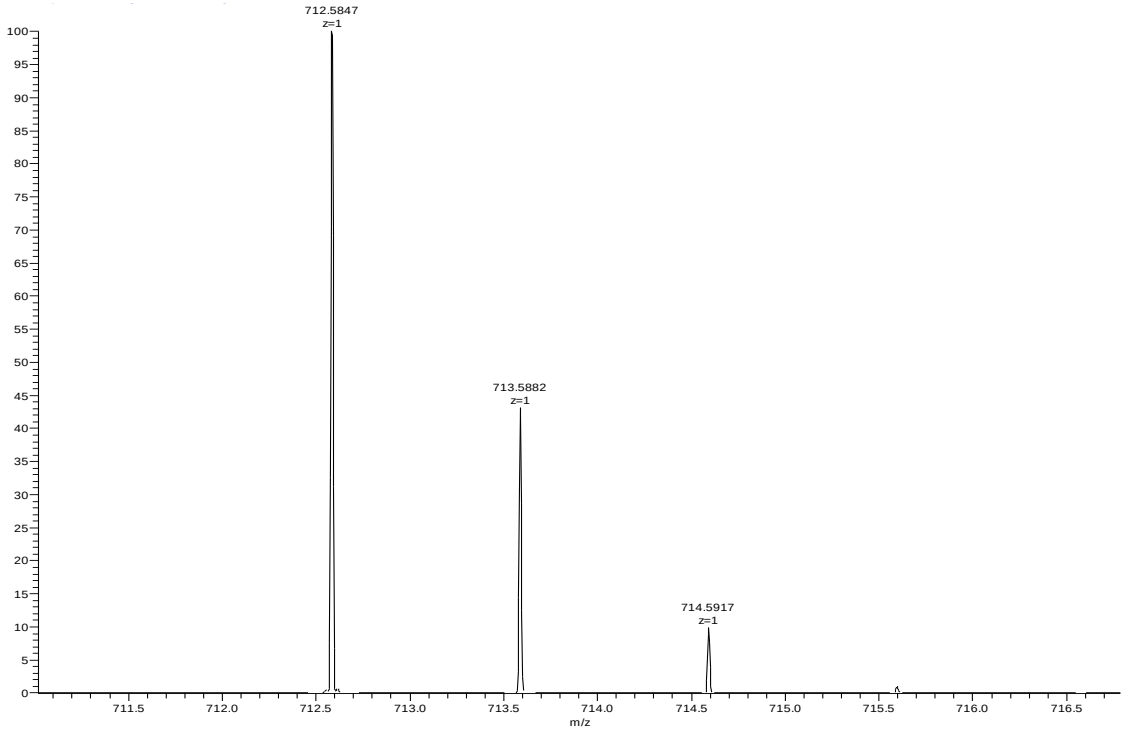
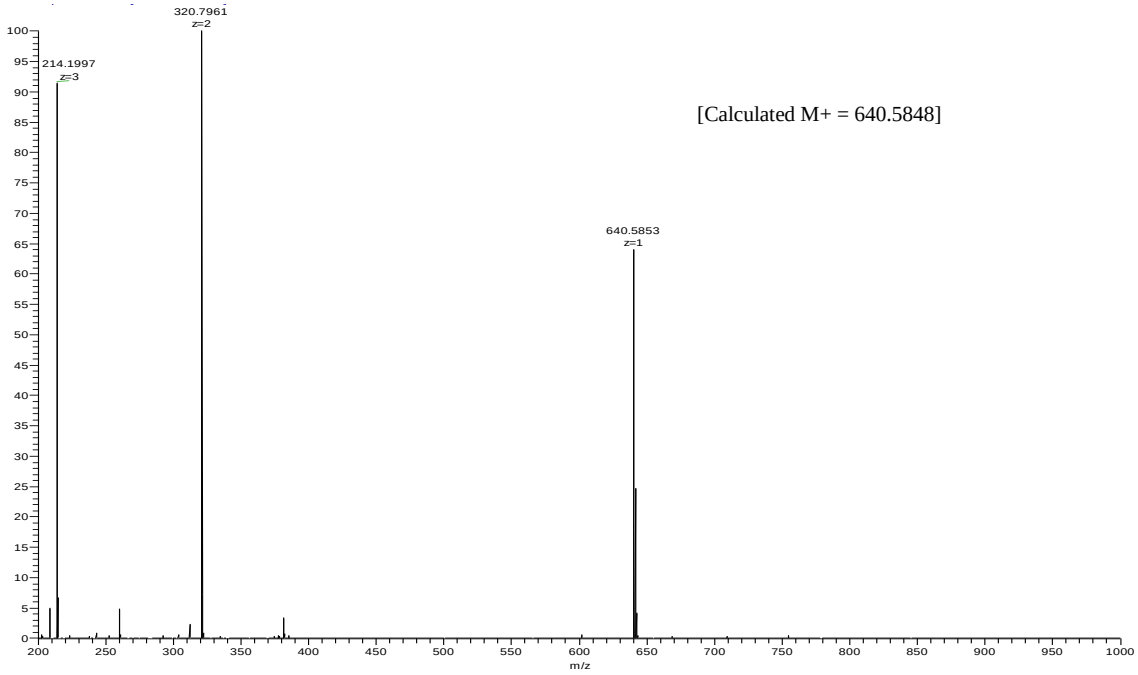
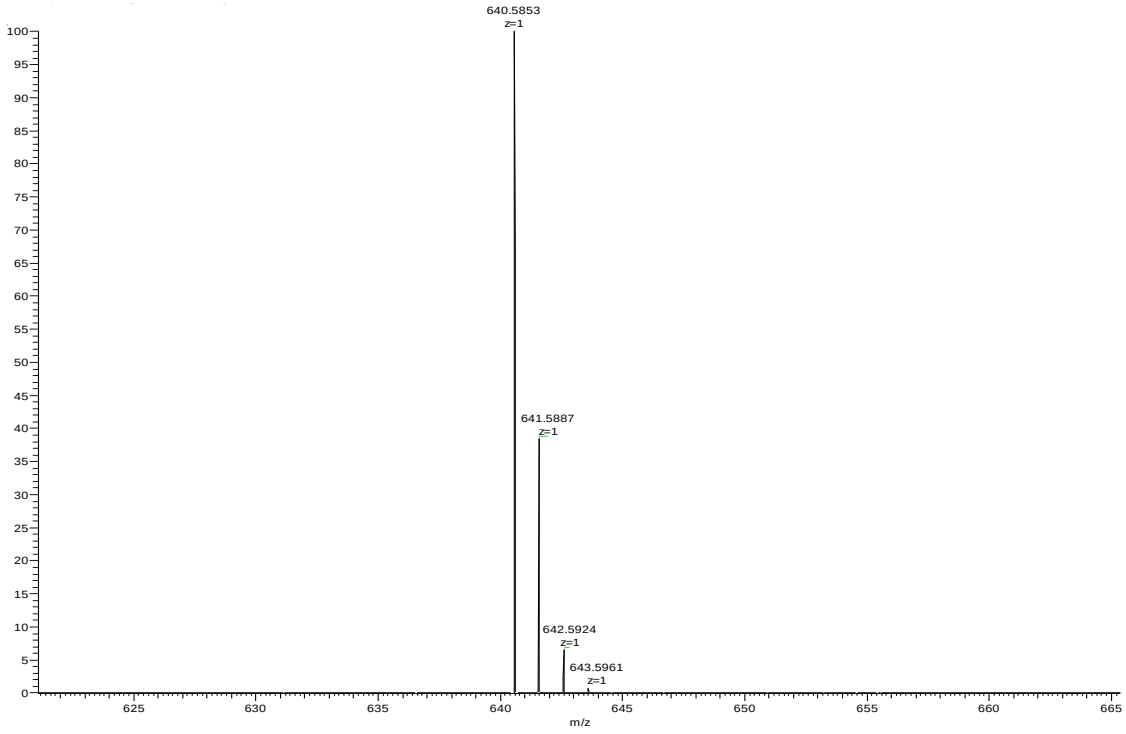


Isotopic peaks for molecular ion peak of **18**



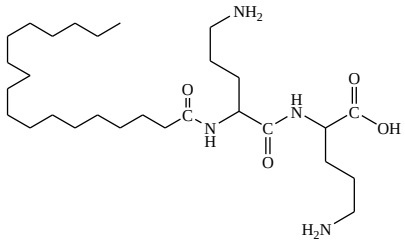
[Calculated M+ = 640.5848]

19

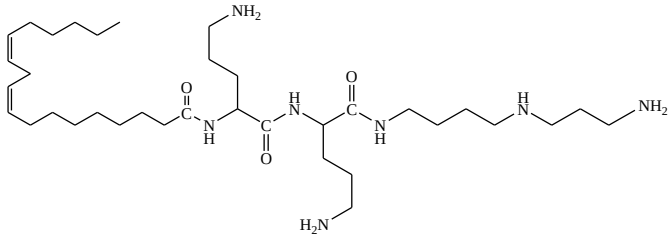


Isotopic peaks for molecular ion peak of **19**

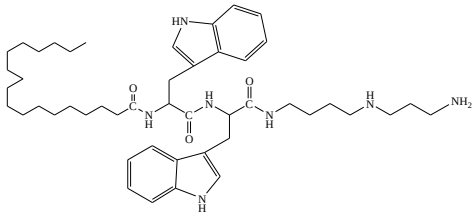
C) NMR based characterization



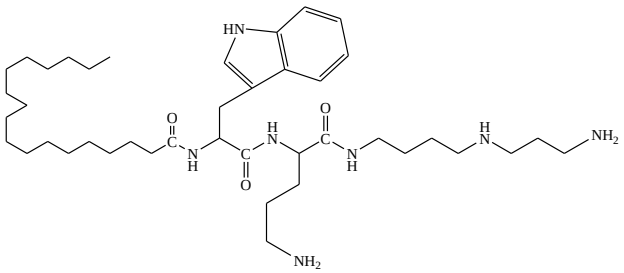
Sequence 11: $[C_{28}H_{56}N_4O_4].2CF_3COOH$; ^{1}H NMR (400 MHz, DMSO-d_6): 8.04 (d, J = 8 Hz, 1H), 7.96 (d, J = 8 Hz, 1H), 7.78 (brs, 4H), 4.27-4.29 (m, 1H), 4.04-4.05 (m, 1H), 2.75 (brs, 4H), 2.10-2.06 (m, 2H), 1.73-1.67 (m, 2H), 1.57-1.52(m, 6H), 1.46 (t, J = 6.6 Hz, 2H), 1.25-1.21 (brs, 30H), 0.83 (t, J = 6.5 Hz, 3H).



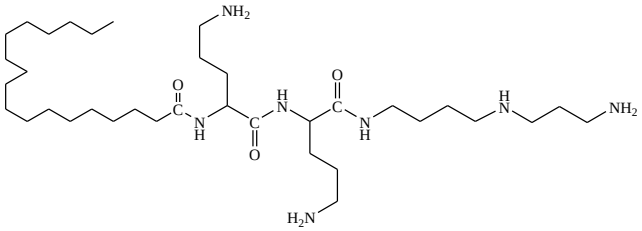
Sequence 16: $[C_{35}H_{69}N_7O_3].4CF_3COOH$; ^{1}H NMR (400 MHz, DMSO-d_6): 8.72 (brs, 2H), 8.04-8.01 (m, 3H), 7.84 (brs, 9H), 5.34-5.30 (m, 2H), 4.24-4.18 (m, 4H), 3.08-3.05 (m, 2H), 2.97-2.94 (m, 2H), 2.88-2.85 (m, 4H), 2.75-2.70 (brs, 4H), 2.11-2.09 (m, 2H), 2.02-1.97 (m, 2H), 1.91-1.86 (m, 2H), 1.66 (brs, 2H), 1.52-1.44 (m, 8H), 1.44-1.38 (m, 6H), 1.22 (brs, 16H), 0.83 (t, J = 6.5 Hz, 3H).



Sequence 17: $[C_{47}H_{73}N_7O_3].2CF_3COOH$; ^{1}H NMR (400 MHz, DMSO-d_6): 10.8 (brs, 2H), 7.91 (d, J = 8 Hz, 1H), 7.79 (d, J = 8 Hz, 1H), 7.72-7.69 (m, 1H), 7.49 (dd, J = 8 Hz, 2H), 7.29 (d, J = 8 Hz, 2H), 7.06 (d, J = 4Hz, 2H), 7.04-7.0 (m, 2H), 6.95-6.91 (m, 2H), 4.47-4.41 (m, 2H), 3.02-2.96 (m, 6H), 2.83-2.80 (m, 3H), 2.74 (t, J = 7.3 Hz, 2H), 2.61-2.59 (m, 2H), 1.96 (t, J = 7.3, 2H), 1.72 (pentet, J = 7.3 Hz, 2H), 1.33-1.29 (m, 2H), 1.27-1.21 (m, 4H), 1.12 (brs, 22H), 1.12-1.05 (m, 6H), 0.98 (d, 4H), 0.83 (t, J = 6.5 Hz, 3H).



Sequence 18: [$C_{41}H_{73}N_7O_3$].3CF_3COOH; ^{1}H NMR (400 MHz, DMSO-*d6*): 10.82 (s, 1H), 8.03 (d, *J* = 8Hz, 1H), 7.94 (d, *J* = 7.3 Hz, 1H), 7.76 (m, *J* = 5.3 Hz, 1H), 7.55 (d, *J* = 8 Hz, 1H), 7.29 (d, *J* = 8 Hz, 1H), 7.1 (s, 1H), 7.03 (t, *J* = 6.6 Hz, 1H), 6.96-6.92 (m, *J* = 7.3 Hz, 1H), 4.48 (m, 1H), 4.19 (m, 1H), 3.14-3.12 (m, 2H), 3.10-3.08 (m, 4H), 3.01-2.99 (m, 2H), 2.85-2.81 (m, 4H), 2.76-2.72 (m, 4H), 2.02 (t, *J* = 7.3 Hz, 2H), 1.79-1.75 (m, 2H), 1.74-1.68 (m, 2H), 1.54-1.44 (m, 4H), 1.39-1.36(m, 4H), 1.31 (brs, 22H), 1.25-1.21 (m, 6H), 1.14-1.07 (m, 4H), 0.83 (t, *J* = 6.9 Hz, 3H).



Sequence 19: [$C_{35}H_{73}N_7O_3$].4CF_3COOH; ^{1}H NMR (400 MHz, DMSO-d_6): 7.99-7.97 (m, 3H), 7.82 (brs, 9H), 4.23-4.17 (m, 2H), 3.2 (brs, 2H), 3.07-3.01 (m, 2H), 2.93 (t, *J* = 7.3 Hz, 2H), 2.87-2.83 (t, *J* = 8Hz, 4H), 2.74 (brs, 4H), 2.44 (brs, 2H), 2.11-2.08 (m, 2H), 1.85 (pentet, *J* = 8.0 Hz, 2H), 1.65 (brs, 2H), 1.51 (brs , 6H), 1.47-1.39 (m , 4H), 1.27-1.21 (brs, 28H), 0.83 (t, *J* = 6.5 Hz, 3H).