

MLO180 MW=772??

ASAP (SOLID)

C₄₀H₄₁BO₁₅

BATJAM-LVFHJ-WR-A 415 (3.850) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Sm (SG, 15x3.00); Cm (403:423-298:319x5.000)

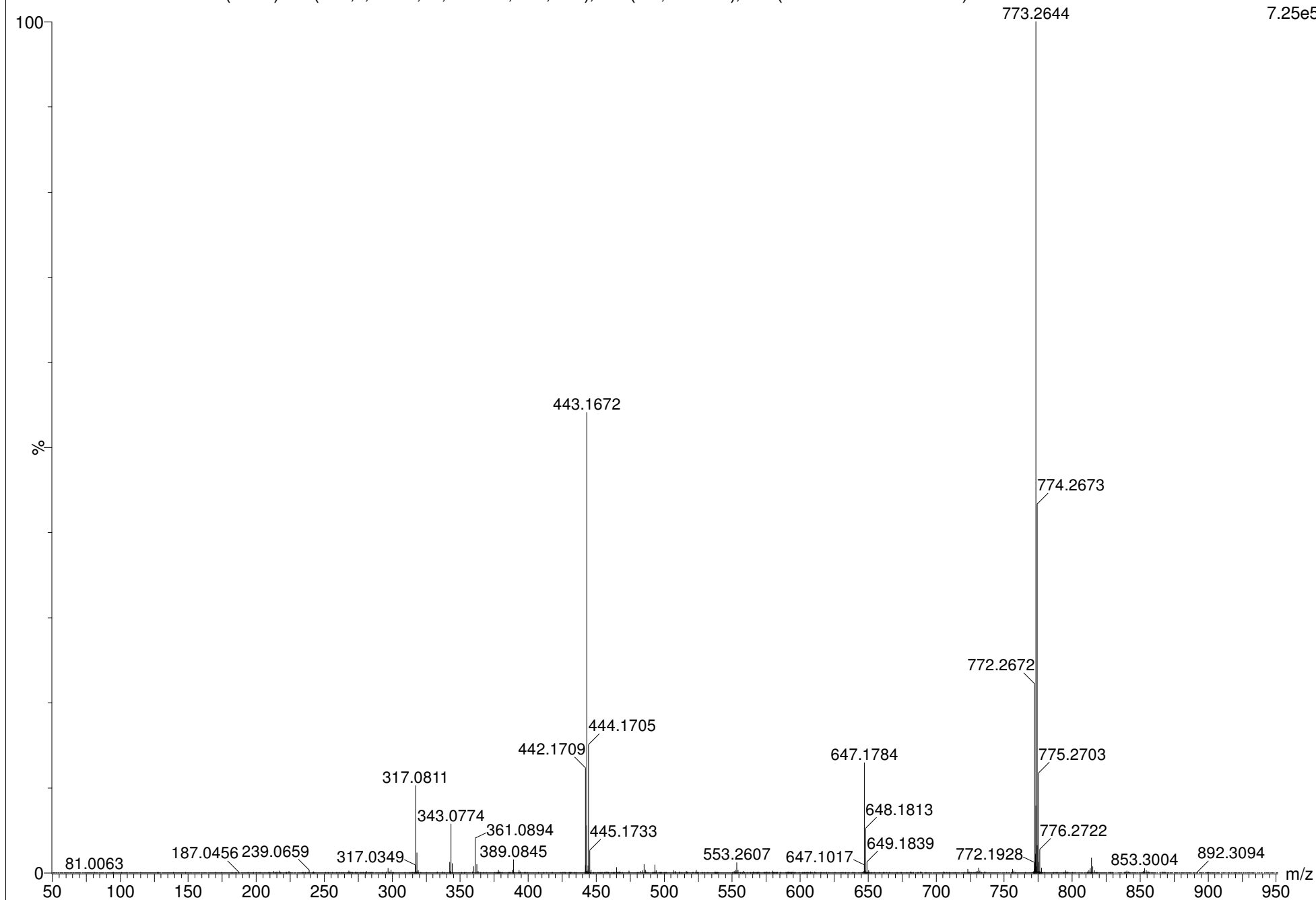
National Mass Spectrometry Facility, Swansea

Xevo G2-S

Maria Odyniec

12-Oct-2017

1: TOF MS ASAP+
7.25e5



MLO180 MW=772??

ASAP (SOLID)

C₄₀H₄₁BO₁₅

BATJAM-LVFHJ-WR-A 415 (3.850) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Sm (SG, 15x3.00); Cm (403:423-298:319x5.000)

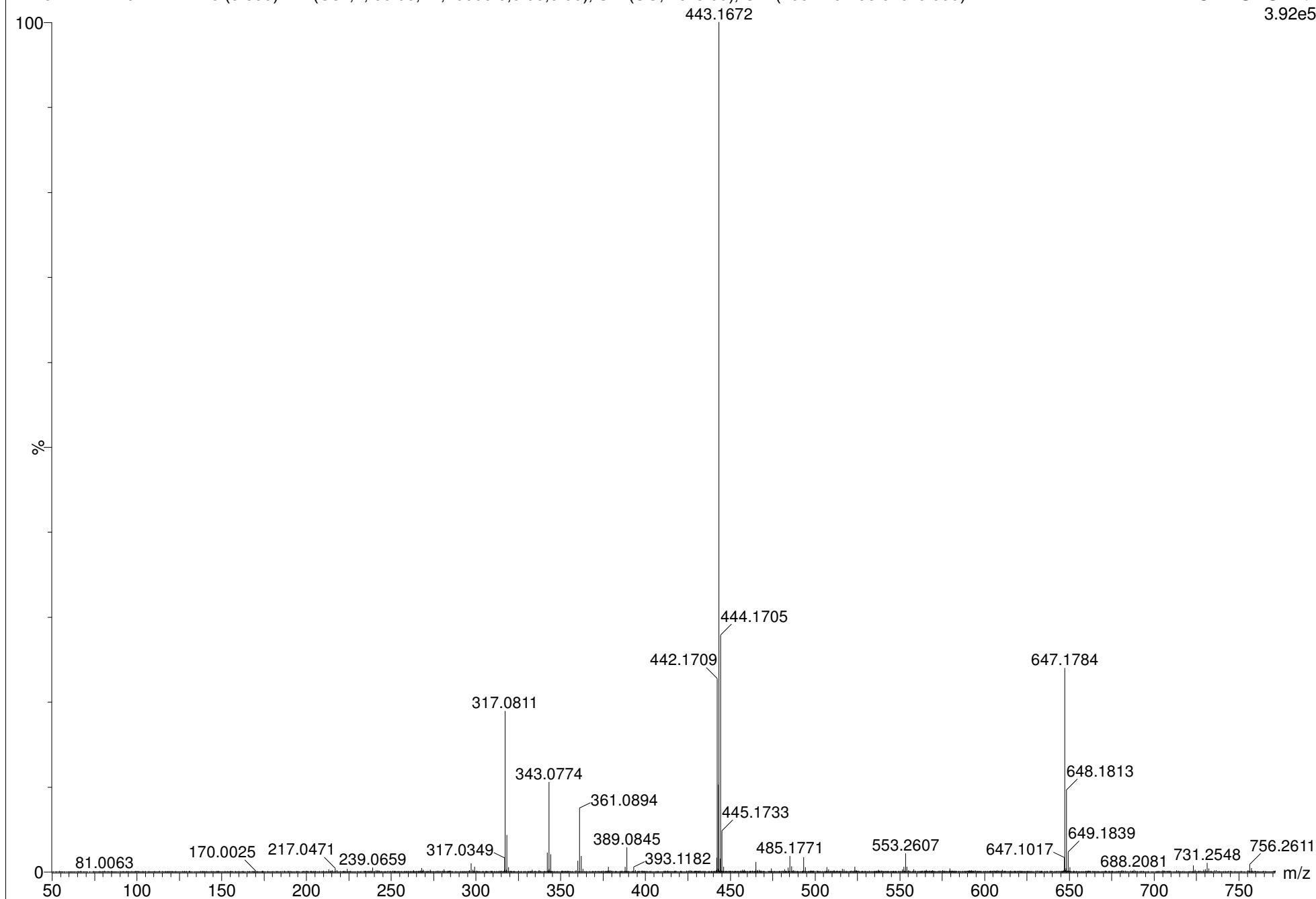
National Mass Spectrometry Facility, Swansea

Xevo G2-S

Maria Odyniec

12-Oct-2017

1: TOF MS ASAP+
3.92e5



MLO180 MW=772??

ASAP (SOLID)

C40H41BO15

BATJAM-LVFHJ-WR-A (0.037) Is (1.00,0.01) C40H41BO15H

National Mass Spectrometry Facility, Swansea

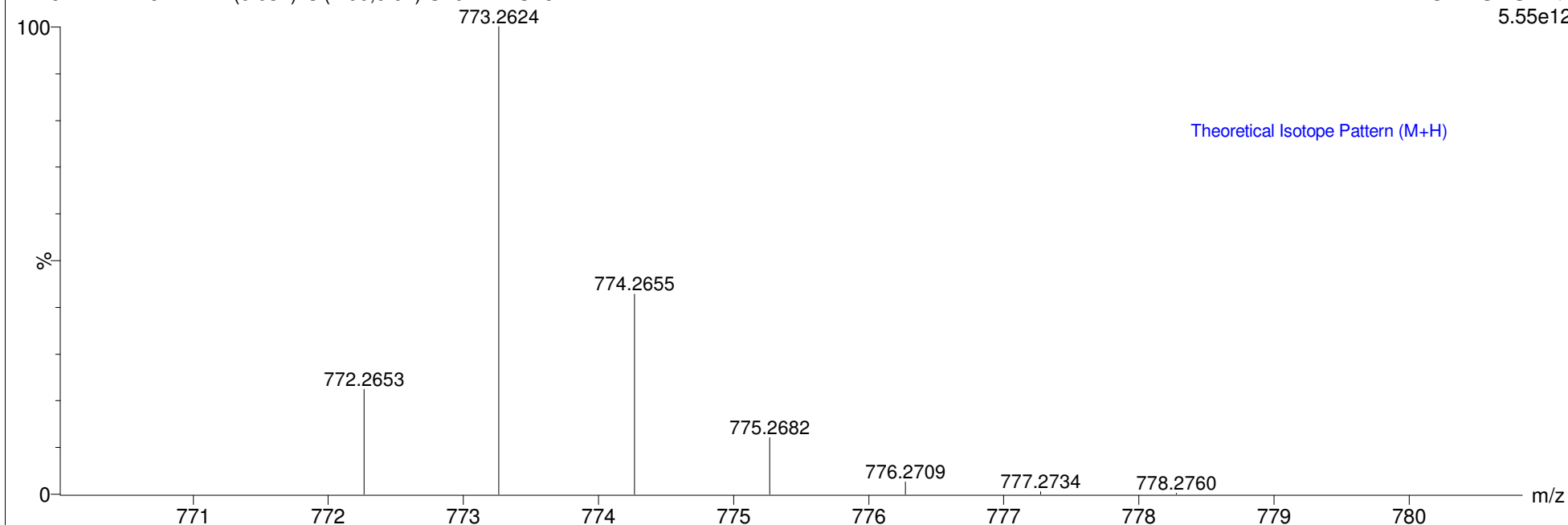
Xevo G2-S

Maria Odyniec

12-Oct-2017

1: TOF MS ASAP+

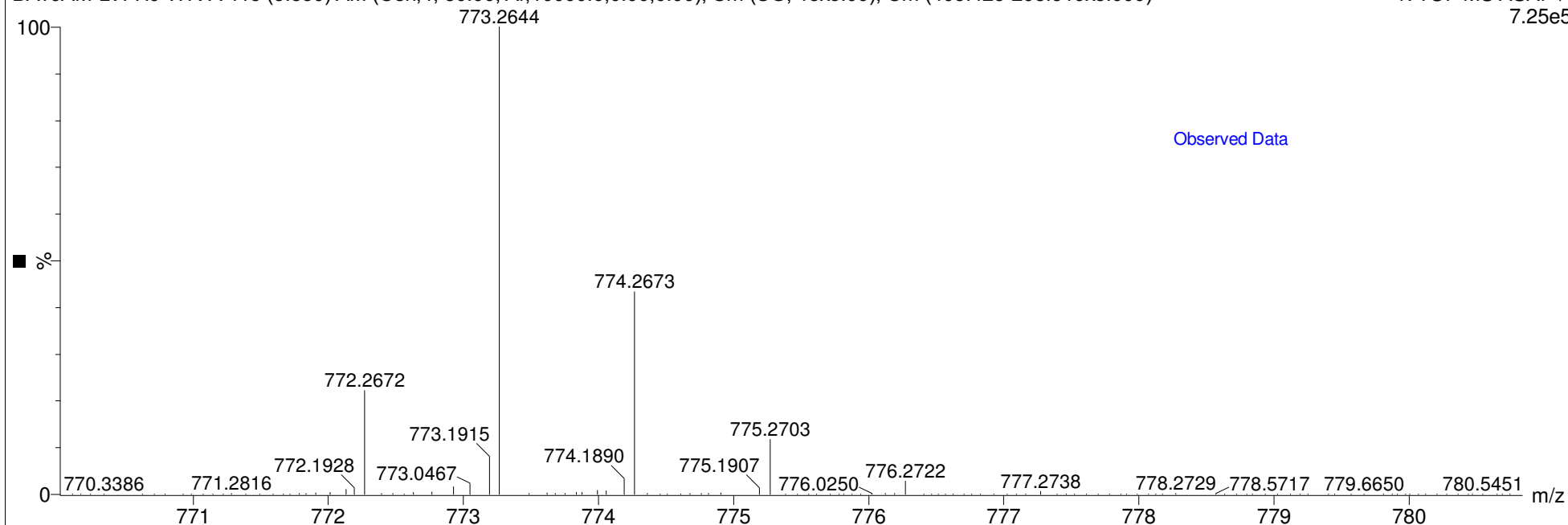
5.55e12



BATJAM-LVFHJ-WR-A 415 (3.850) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Sm (SG, 15x3.00); Cm (403:423-298:319x5.000)

1: TOF MS ASAP+

7.25e5



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -150.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

3157 formula(e) evaluated with 37 results within limits (up to 500 closest results for each mass)

Elements Used:

C: 0-60 H: 0-80 10B: 0-1 N: 0-10 O: 5-25

MLO180 MW=772??

National Mass Spectrometry Facility, Swansea

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ASAP (SOLID)

Xevo G2-S

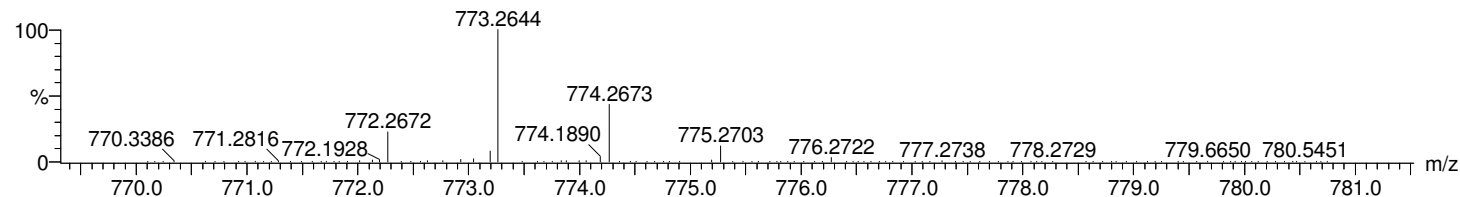
12-Oct-2017

C40H41BO15

BATJAM-LVFHJ-WR-A 415 (3.850) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Sm (SG, 15x3.00); Cm (403:423-298:319x5.000)

1: TOF MS ASAP+

7.25e+005



Minimum: -150.0

Maximum: 5.0 5.0 100.0

| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula |
|----------|------------|------|------|------|-------|-------|----------|---------------------|
| 772.2672 | 772.2672 | 0.0 | 0.0 | 13.0 | 383.2 | 3.435 | 3.22 | C27 H40 10B N9 O17 |
| | 772.2672 | 0.0 | 0.0 | 7.5 | 383.5 | 3.775 | 2.29 | C28 H46 10B N2 O22 |
| | 772.2672 | 0.0 | 0.0 | 30.0 | 383.5 | 3.717 | 2.43 | C49 H40 O9 |
| | 772.2669 | 0.3 | 0.4 | 0.0 | 383.3 | 3.518 | 2.97 | C20 H48 N6 O25 |
| | 772.2677 | -0.5 | -0.6 | 17.5 | 383.5 | 3.701 | 2.47 | C35 H42 N5 O15 |
| | 772.2666 | 0.6 | 0.8 | 25.5 | 383.3 | 3.545 | 2.89 | C41 H38 10B N4 O11 |
| | 772.2680 | -0.8 | -1.0 | 25.0 | 383.6 | 3.827 | 2.18 | C43 H40 10B N O12 |
| | 772.2664 | 0.8 | 1.0 | 18.0 | 383.1 | 3.364 | 3.46 | C33 H40 N8 O14 |
| | 772.2680 | -0.8 | -1.0 | 30.5 | 383.3 | 3.578 | 2.79 | C42 H34 10B N8 O7 |
| | 772.2664 | 0.8 | 1.0 | 12.5 | 383.4 | 3.678 | 2.53 | C34 H46 N O19 |
| | 772.2682 | -1.0 | -1.3 | 5.0 | 383.3 | 3.543 | 2.89 | C21 H44 N10 O21 |
| | 772.2659 | 1.3 | 1.7 | 30.5 | 383.2 | 3.469 | 3.12 | C47 H38 N3 O8 |
| | 772.2685 | -1.3 | -1.7 | 12.5 | 383.5 | 3.789 | 2.26 | C29 H42 10B N6 O18 |
| | 772.2686 | -1.4 | -1.8 | 35.0 | 383.5 | 3.740 | 2.37 | C50 H36 N4 O5 |
| | 772.2658 | 1.4 | 1.8 | 8.0 | 383.2 | 3.459 | 3.15 | C26 H44 10B N5 O21 |
| | 772.2656 | 1.6 | 2.1 | 0.5 | 382.9 | 3.156 | 4.26 | C18 H46 N9 O24 |
| | 772.2691 | -1.9 | -2.5 | 22.5 | 383.5 | 3.759 | 2.33 | C36 H38 N9 O11 |
| | 772.2653 | 1.9 | 2.5 | 26.0 | 383.0 | 3.281 | 3.76 | C39 H36 10B N7 O10 |
| | 772.2691 | -1.9 | -2.5 | 17.0 | 383.8 | 4.039 | 1.76 | C37 H44 N2 O16 |
| | 772.2653 | 1.9 | 2.5 | 20.5 | 383.3 | 3.569 | 2.82 | C40 H42 10B O15 |
| | 772.2693 | -2.1 | -2.7 | 30.0 | 383.7 | 3.902 | 2.02 | C44 H36 10B N5 O8 |
| | 772.2651 | 2.1 | 2.7 | 13.0 | 383.2 | 3.427 | 3.25 | C32 H44 N4 O18 |
| | 772.2696 | -2.4 | -3.1 | 4.5 | 383.7 | 3.964 | 1.90 | C23 H46 N7 O22 |
| | 772.2698 | -2.6 | -3.4 | 17.5 | 383.6 | 3.879 | 2.07 | C30 H38 10B N10 O14 |
| | 772.2698 | -2.6 | -3.4 | 12.0 | 383.9 | 4.191 | 1.51 | C31 H44 10B N3 O19 |
| | 772.2645 | 2.7 | 3.5 | 31.0 | 383.0 | 3.249 | 3.88 | C45 H36 N6 O7 |
| | 772.2645 | 2.7 | 3.5 | 3.0 | 383.3 | 3.561 | 2.84 | C25 H48 10B N O25 |
| | 772.2645 | 2.7 | 3.5 | 8.5 | 382.9 | 3.183 | 4.15 | C24 H42 10B N8 O20 |
| | 772.2699 | -2.7 | -3.5 | 34.5 | 383.8 | 4.050 | 1.74 | C52 H38 N O6 |
| | 772.2703 | -3.1 | -4.0 | -0.5 | 383.8 | 4.069 | 1.71 | C17 H46 10B N8 O25 |
| | 772.2640 | 3.2 | 4.1 | 21.0 | 383.2 | 3.397 | 3.35 | C38 H40 10B N3 O14 |
| | 772.2704 | -3.2 | -4.1 | 22.0 | 383.9 | 4.130 | 1.61 | C38 H40 N6 O12 |
| | 772.2640 | 3.2 | 4.1 | 26.5 | 382.9 | 3.106 | 4.48 | C37 H34 10B N10 O9 |
| | 772.2637 | 3.5 | 4.5 | 13.5 | 383.0 | 3.220 | 3.99 | C30 H42 N7 O17 |
| | 772.2707 | -3.5 | -4.5 | 29.5 | 384.0 | 4.246 | 1.43 | C46 H38 10B N2 O9 |
| | 772.2637 | 3.5 | 4.5 | 8.0 | 383.3 | 3.554 | 2.86 | C31 H48 O22 |
| | 772.2709 | -3.7 | -4.8 | 4.0 | 384.1 | 4.376 | 1.26 | C25 H48 N4 O23 |