

Acq. Data Name: PetterThorsen_030521_seq 1-6_ESI+_DI

Internal Sample Id:

Ionization Mode: ESI+

MS Calibration Name: PEG_ESI+_2000

Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%]];Average(MS[1] 10.796..10.896)-1.0*Average(MS[1] 10.398..10.524);Correct Base[5.0%]

Experiment Date/Time: 5/3/2021 13:07:25

Orifice1 Volt Sweep: 23V

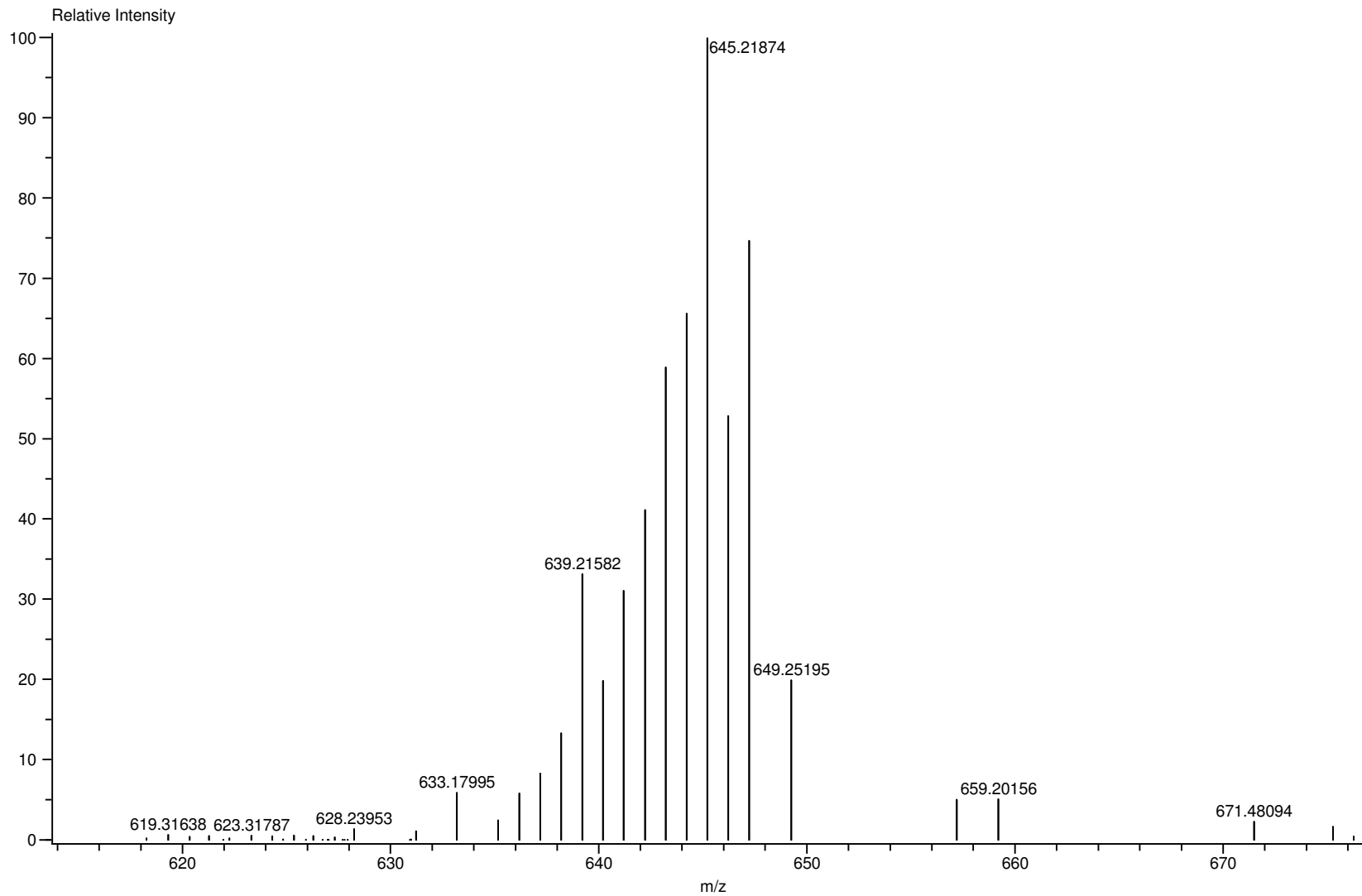
Acquired m/z Range: 30.0..2000.0

Spec. Record Interval: 0.6[s]

Ring Lens Volt: 11[V]

Time of Maximum: 10.842[min]

Operator Name: Accutof



Data:PetterThorsen_030521_seq 1-6_ESI+_DI

Sample Name:

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%]];Average(MS[1] 10.796..10.896)-1.0*Av...

Acquired:5/3/2021 13:07:25

Operator:Accutof

Mass Calibration data:PEG_ESI+_2000

Created:11/22/2021 9:36:51

Created by:Accutof

Charge number:1

Tolerance:5.00(mmu)

Unsaturation Number:-1.5 .. 40.0 (Fraction:Both)

Element:¹²C:35 .. 35, ¹H:0 .. 200, ³⁵Cl:0 .. 1, ³⁷Cl:0 .. 1, ¹⁴N:0 .. 2, ¹⁶O:0 .. 2, ⁹⁶Ru:0 .. 1, ⁹⁸Ru:0 .. 1, ⁹⁹Ru:0 .. 1, ¹⁰⁰Ru:0 .. 1, ¹⁰¹Ru:0 .. 1, ¹⁰²Ru:0 .. 1, ¹⁰⁴Ru:0 .. 1

| Mass | Intensity | Calc. Mass | Mass Difference (ppm) | Possible Formula | ¹² C | ¹ H | ³⁵ Cl | ³⁷ Cl | ¹⁴ N | ¹⁶ O | ⁹⁶ Ru | ⁹⁸ Ru | ⁹⁹ Ru |
|-----------|-----------|------------|-----------------------|---|-----------------|----------------|------------------|------------------|-----------------|-----------------|------------------|------------------|------------------|
| 645.21874 | 97149.65 | 645.21856 | 0.27 | ¹² C ₃₅ ¹ H ₄₄ ³⁵ Cl ₁ ¹⁴ N ₂ ¹⁶ O ₁ ¹⁰² Ru ₁ | 35 | 44 | 1 | | 2 | 1 | | | |
| | | 645.21982 | -1.68 | ¹² C ₃₅ ¹ H ₄₅ ³⁵ Cl ₁ ¹⁴ N ₁ ¹⁶ O ₂ ⁹⁹ Ru ₁ | 35 | 45 | 1 | | 1 | 2 | | | 1 |
| | | 645.21548 | 5.04 | ¹² C ₃₅ ¹ H ₄₄ ³⁷ Cl ₁ ¹⁴ N ₂ ¹⁶ O ₁ ¹⁰⁰ Ru ₁ | 35 | 44 | | 1 | 2 | 1 | | | |
| | | 645.22361 | -7.55 | ¹² C ₃₅ ¹ H ₄₉ ³⁵ Cl ₁ ³⁷ Cl ₁ ¹⁰⁴ Ru ₁ | 35 | 49 | 1 | 1 | | | | | |

| ^{100}Ru | ^{101}Ru | ^{102}Ru | ^{104}Ru | Unsaturation Number |
|-------------------|-------------------|-------------------|-------------------|---------------------|
| | | 1 | | 15.0 |
| | | | | 14.0 |
| 1 | | | | 15.0 |
| | | | 1 | 11.0 |