**RSC/RSB Joint Mass Spectrometry Facility Analysis Report**

**Analyst:** Joe Boileau

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| Job Details |
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| Job ID: | 64617 |
| Submitted by: | Benjamin Frogley |
| Group: | Hill |
| Title: |  |
| Area: | RSC |
| Building: | 137 |
| Room: | 2.28 |
| Telephone: | +61401207210 |
| Date submitted: | 09.09.2019 14:31:20 |
| Charging code: | S-46010-80 |
| Molecular weight: | 1458.1126 |
| Formula: | C79H62Cl2O3P4Ru2 |
| Special handling required: | none |
| Ionisation mode: | positive |
| Low resolution mode: | ESI |
| High resolution mode: | ESI |
| Sample: | solid |
| Solution type: | none |
| Suitable solvent: | MeCN |
| Purity: | good |
| Toxicity: | safe |
| Volatility: | low |
| Sample code: | BF-C17 |
| Keep sample: | No |
| Request text: |  |

**Instrument:** Orbitrap Elite, +ve mode ESI at 240k resolution

**Analysis Date:** 2019-09-11

**Detection status:** [M-Cl+CH3CN]+ ion: 8.79E5 counts

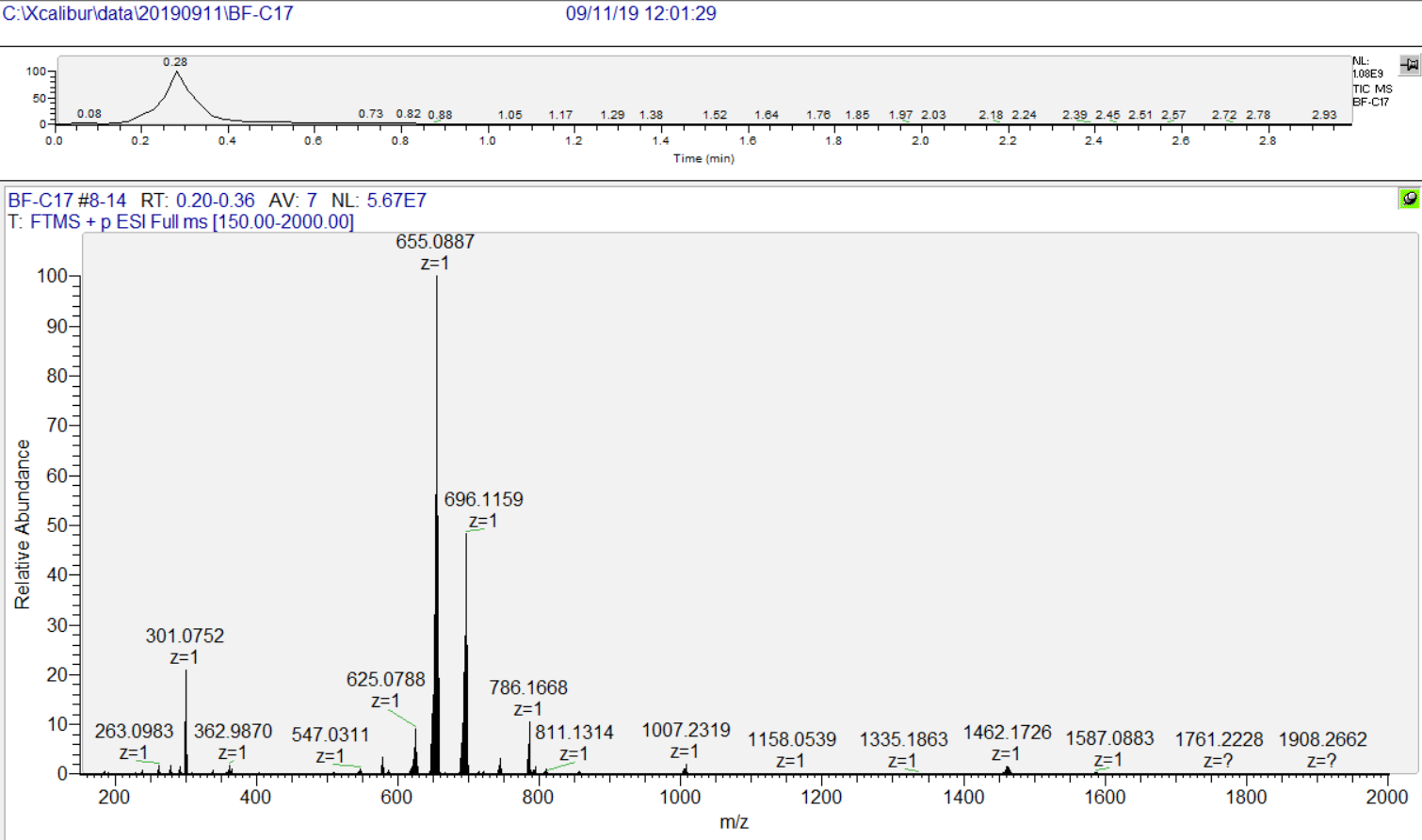
**Charge state:** z = +1

**Theoretical m/z (of most abundant isotopologue):** [M-Cl+CH3CN]+ ion: 1462.1716

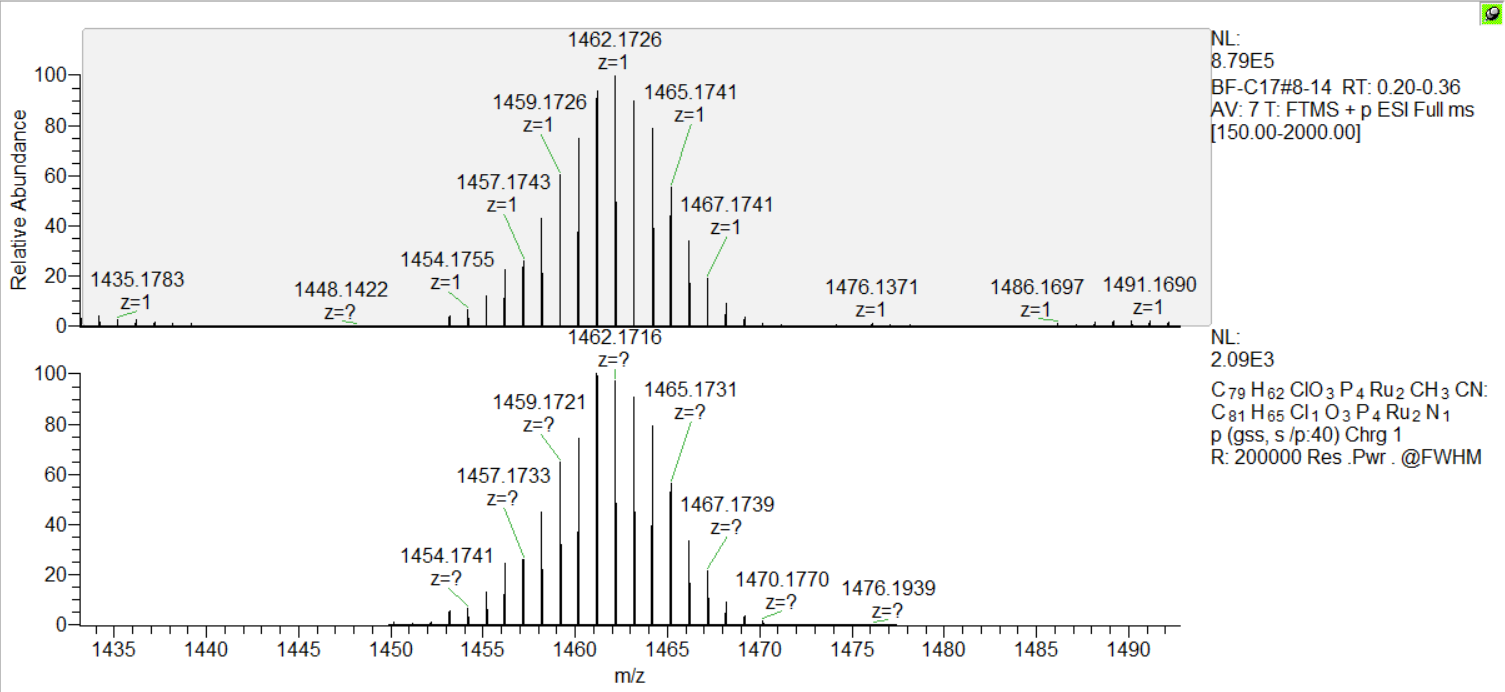
**Observed m/z (of most abundant isotopologue):** [M-Cl+CH3CN]+ ion: 1462.1726

**Mass error (ppm; <5 ppm is OK):** [M-Cl+CH3CN]+ ion: 2.821 ppm

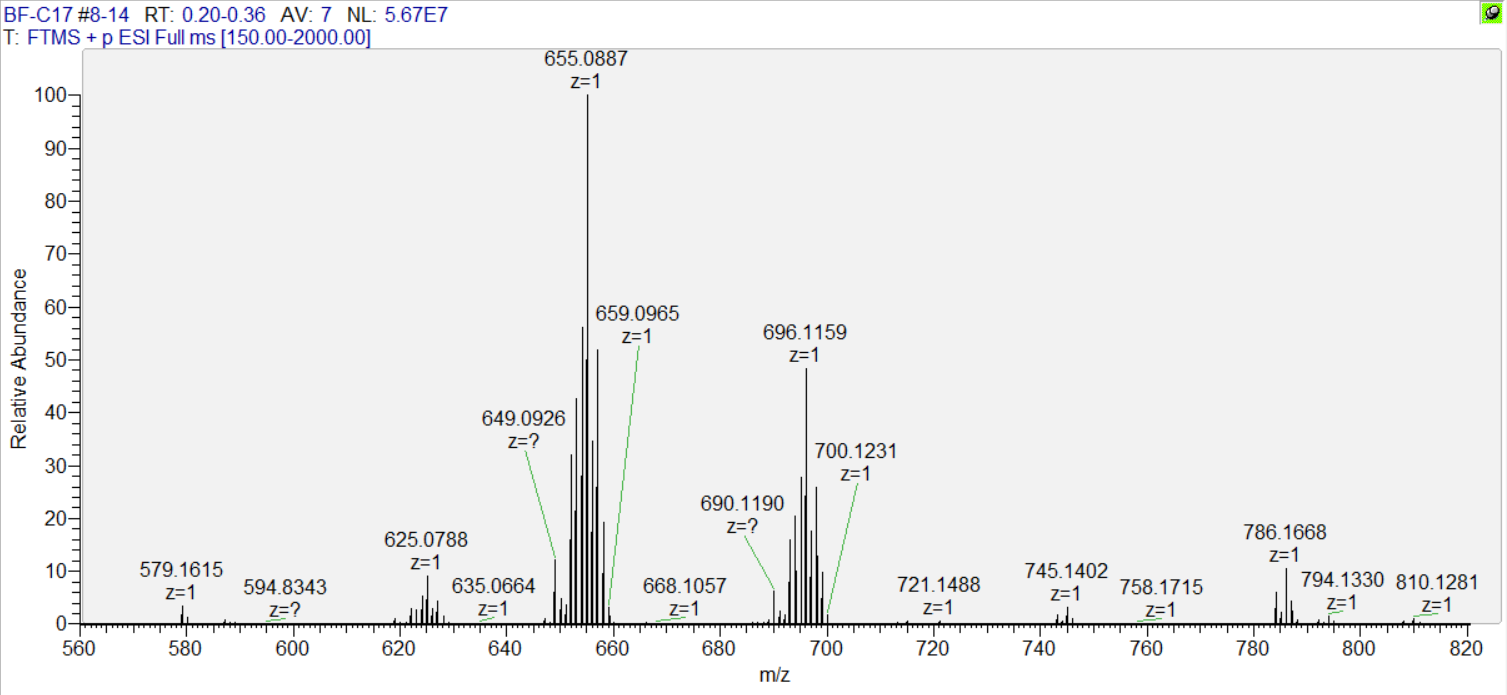
**Raw Total Ion Chromatogram (TIC) and full m/z spectrum**



**Observed versus simulated spectrum for detected target formulas [M-Cl+CH3CN]+ ion**



**Zoom-in:**



**Elemental Composition [M-Cl+CH3CN]+ ion:**

