

# School of Chemistry Mass Spectrometry Service

**SampleID** ICB-18-f4  
**Sample Description**  
**Analysis Name** ICB-18-f4\_156927\_BD8\_01\_19326.d  
**Method** 3a\_AccMass\_Loop\_Positive.m  
**Instrument** maXis impact

**Source Type** ESI **Ion Polarity** Positive

**Submitter**

Izar Capel

**Supervisor**

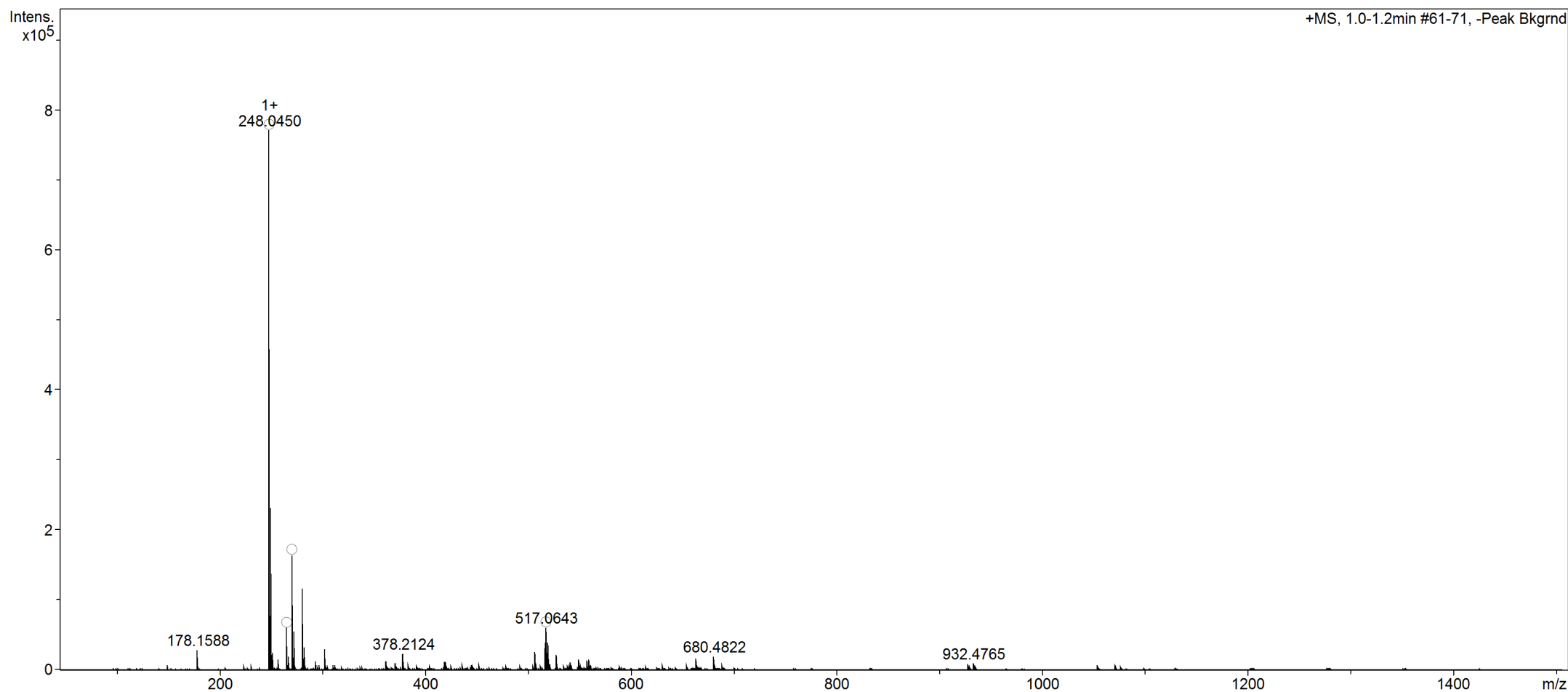
Malcolm Halcrow

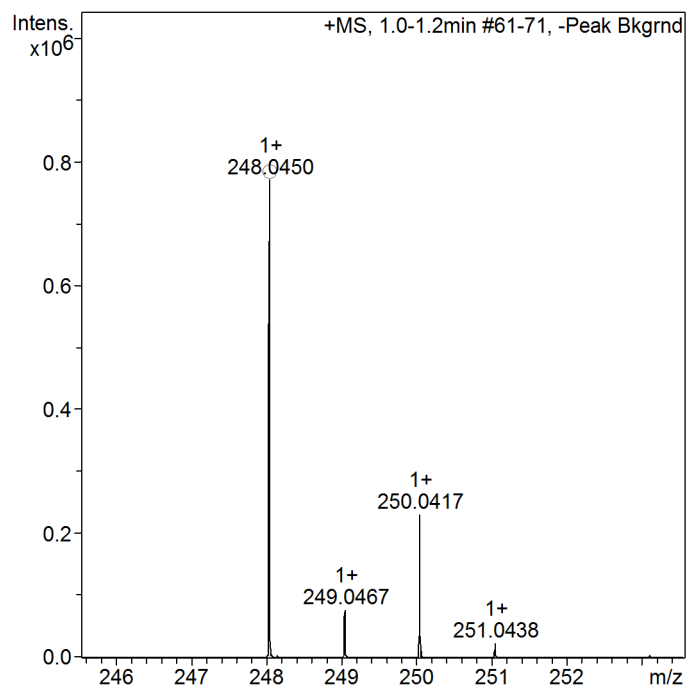
**Acquisition Date**

18/02/2016 09:27:57

**Scan Begin** 50 m/z

**Scan End** 1500 m/z





## Confirm/Find Formula Results

The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
248.044974	C <sub>9</sub> H <sub>7</sub> ClN <sub>7</sub>	1+	248.044597	-0.4	-1.5	18.3	100.00	C <sub>9</sub> H <sub>6</sub> ClN <sub>7</sub>	M+H
265.070857	C <sub>9</sub> H <sub>10</sub> ClN <sub>8</sub>	1+	265.071146	0.3	1.1	14.4	100.00		M+NH <sub>4</sub>
270.026548	C <sub>9</sub> H <sub>6</sub> ClN <sub>7</sub> Na	1+	270.026542	-0.0	-0.0	10.1	100.00	C <sub>9</sub> H <sub>6</sub> ClN <sub>7</sub>	M+Na
517.064268	C <sub>18</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>14</sub> Na	1+	517.063863	-0.4	-0.8	18.1	100.00		2M+Na

Smart Formula Parameter	Value
Expected Formula	C <sub>9</sub> H <sub>6</sub> N <sub>7</sub> Cl
Adducts Considered	;M+H;;M+NH <sub>4</sub> ;;M+Na;;M+K;;M+Na 2-H;;2M+H;;2M+Na;

Smart Formula Search Parameters  
CHNO and adducts considered  
implicitly

Formula Search Minimum	
Formula Search Maximum	Cl 2

Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	even
Estimate No of Carbons	yes
Filter by H/C Ratio	0 < H/C < 3
Number of Double Bonds & Rings	0 < rings&DB < 80