

School of Chemistry Mass Spectrometry Service

SampleID 142-Fe
Sample Description
Analysis Name D:\Data\malcolmhalcrow\cmic\142-Fe_223213_GB2_01_39730.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact

Source Type ESI **Ion Polarity** Positive

Submitter

Izar Capel

Supervisor

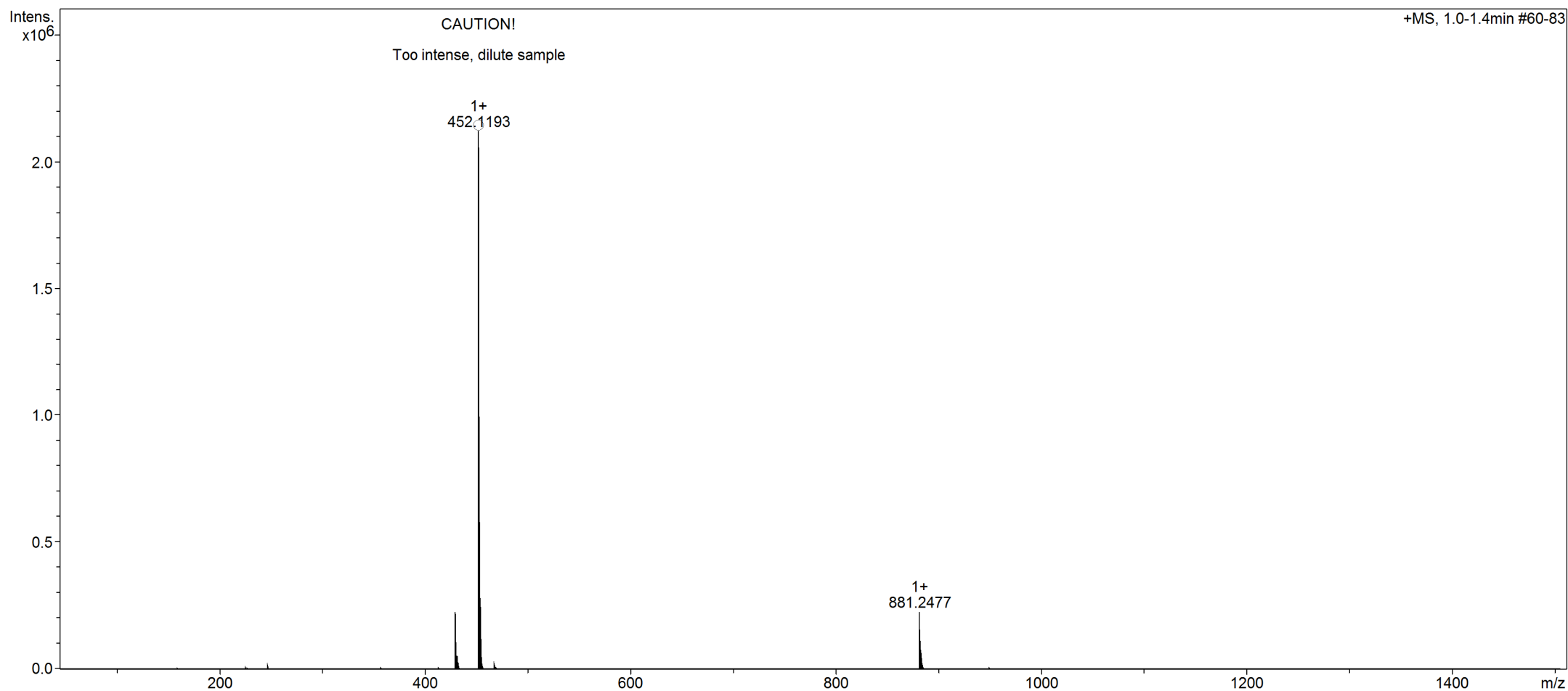
Malcolm Halcrow

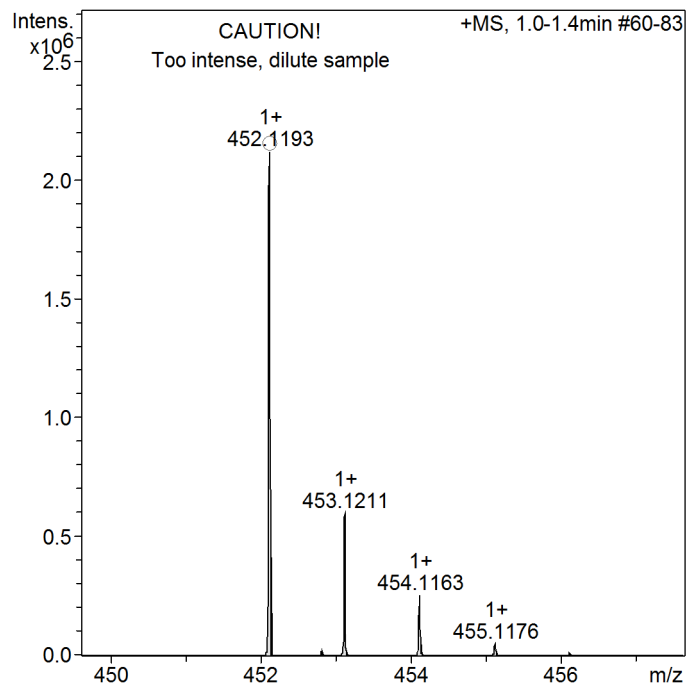
Acquisition Date

13/12/2017 16:37:00

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

Concentration too high. Dilute sample!

| Meas. m/z | Ion Formula | z | m/z | err [mDa] | err [ppm] | mSigma | Score | Sum Formula | Adduct |
|------------|-------------|----|------------|-----------|-----------|--------|--------|-------------|--------|
| 452.119284 | C18H15KN13 | 1+ | 452.120496 | 1.2 | 2.7 | 21.5 | 73.49 | C18H15N13 | M+K |
| | C17H19KN9O4 | 1+ | 452.119158 | -0.1 | -0.3 | 32.1 | 100.00 | C17H19N9O4 | M+K |

| Smart Formula Parameter | Value |
|-------------------------|--|
| Expected Formula | |
| Adducts Considered | M+H M+NH4 M+Na M+K M+Na2-H 2M+H 2M+Na |

Smart Formula Search Parameters
CHNO and adducts considered
implicitly

Formula Search Minimum
Formula Search Maximum

| | |
|----------------------------------|-------------------|
| 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 |