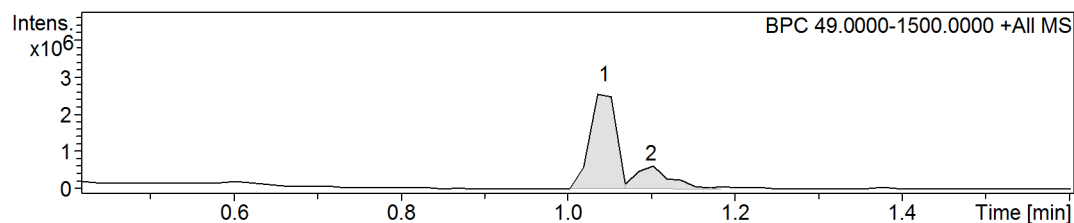


School of Chemistry Mass Spectrometry Service

SampleID bppCOOEOLA
Sample Description
Analysis Name D:\Data\malcolmhalcrow\cmic\bppCOOEOLA_239828_GE4_01_47123.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact **Source Type** ESI **Ion Polarity** Positive

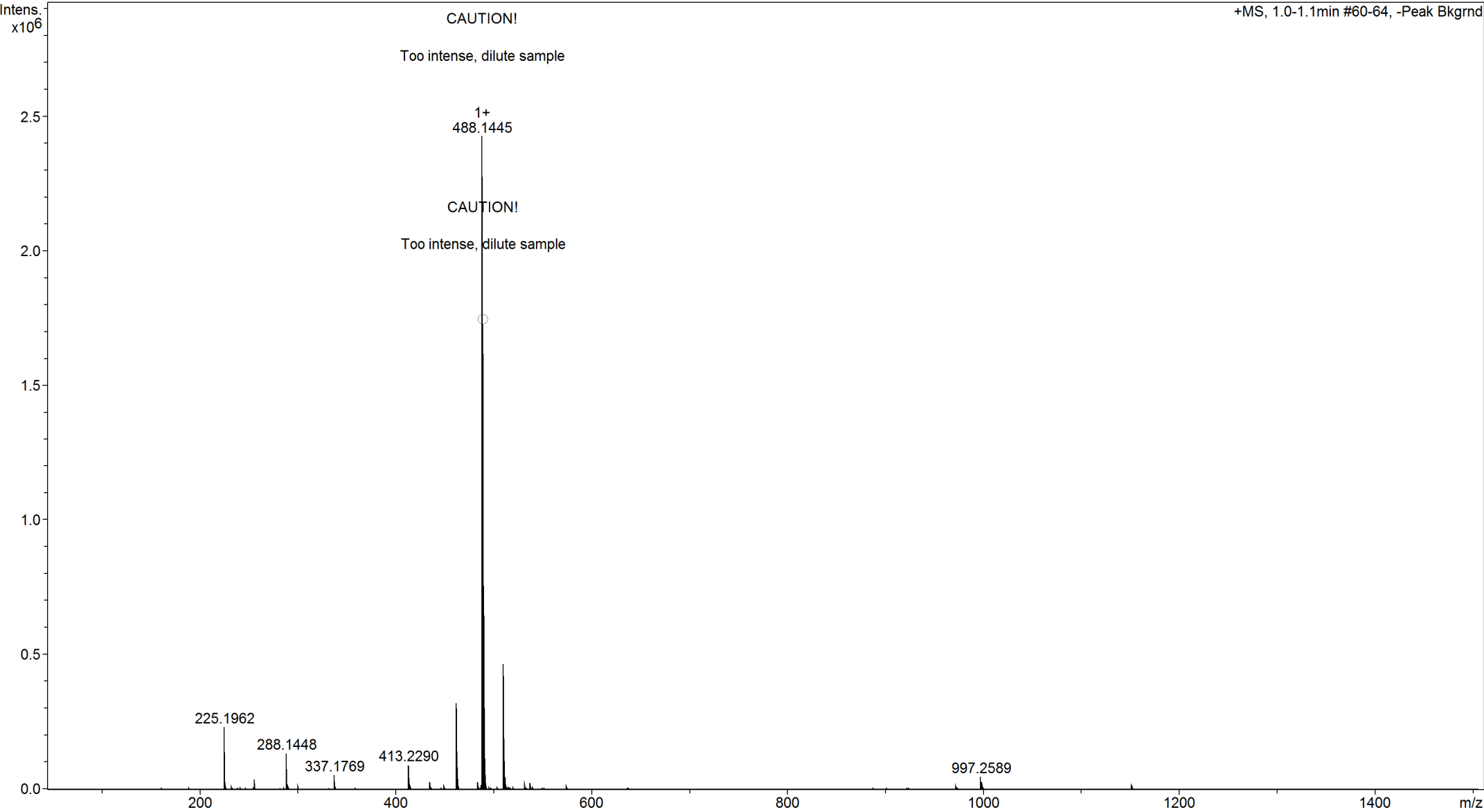
Submitter Izar Capel
Supervisor Malcolm Halcrow
Acquisition Date 12/06/2018 17:43:39
Scan Begin 50 m/z **Scan End** 1500 m/z

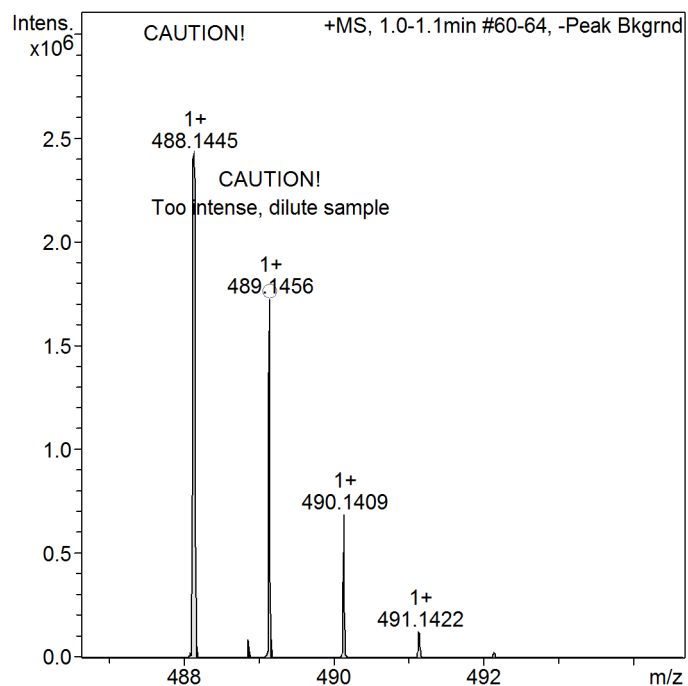


Summary of Results

| Name | RT | BPC Area(%) | UV Area(%) | Confirm Formula Results |
|-----------------|------|-------------|------------|-------------------------|
| Cmpd 1, 1.0 min | 1.04 | 76.7 | no uv | |
| Cmpd 2, 1.1 min | 1.10 | 23.3 | no uv | |

Cmpd 1, 1.0 min





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

Cmpd 1, 1.0 min

| Meas. m/z | Ion Formula | z | m/z | err [mDa] | err [ppm] | mSigma | Score | Sum Formula | Adduct |
|------------|-------------|----|------------|-----------|-----------|--------|--------|-------------|---------|
| 489.145575 | C31H17N6O | 1+ | 489.145836 | 0.3 | 0.5 | 20.4 | 100.00 | C31H16N6O | M+H |
| | C30H21N2O5 | 1+ | 489.144498 | -1.1 | -2.2 | 32.0 | 50.36 | C30H20N2O5 | M+H |
| | C31H17N6O | 1+ | 489.145836 | 0.3 | 0.5 | 20.4 | 100.00 | C31H13N5O | M+NH4 |
| | C30H21N2O5 | 1+ | 489.144498 | -1.1 | -2.2 | 32.0 | 50.36 | C30H17NO5 | M+NH4 |
| | C33H22NaO3 | 1+ | 489.146115 | 0.5 | 1.1 | 19.8 | 100.00 | C33H22O3 | M+Na |
| | C31H23Na2O3 | 1+ | 489.143710 | -1.9 | -3.8 | 30.6 | 100.00 | C31H24O3 | M+Na2-H |

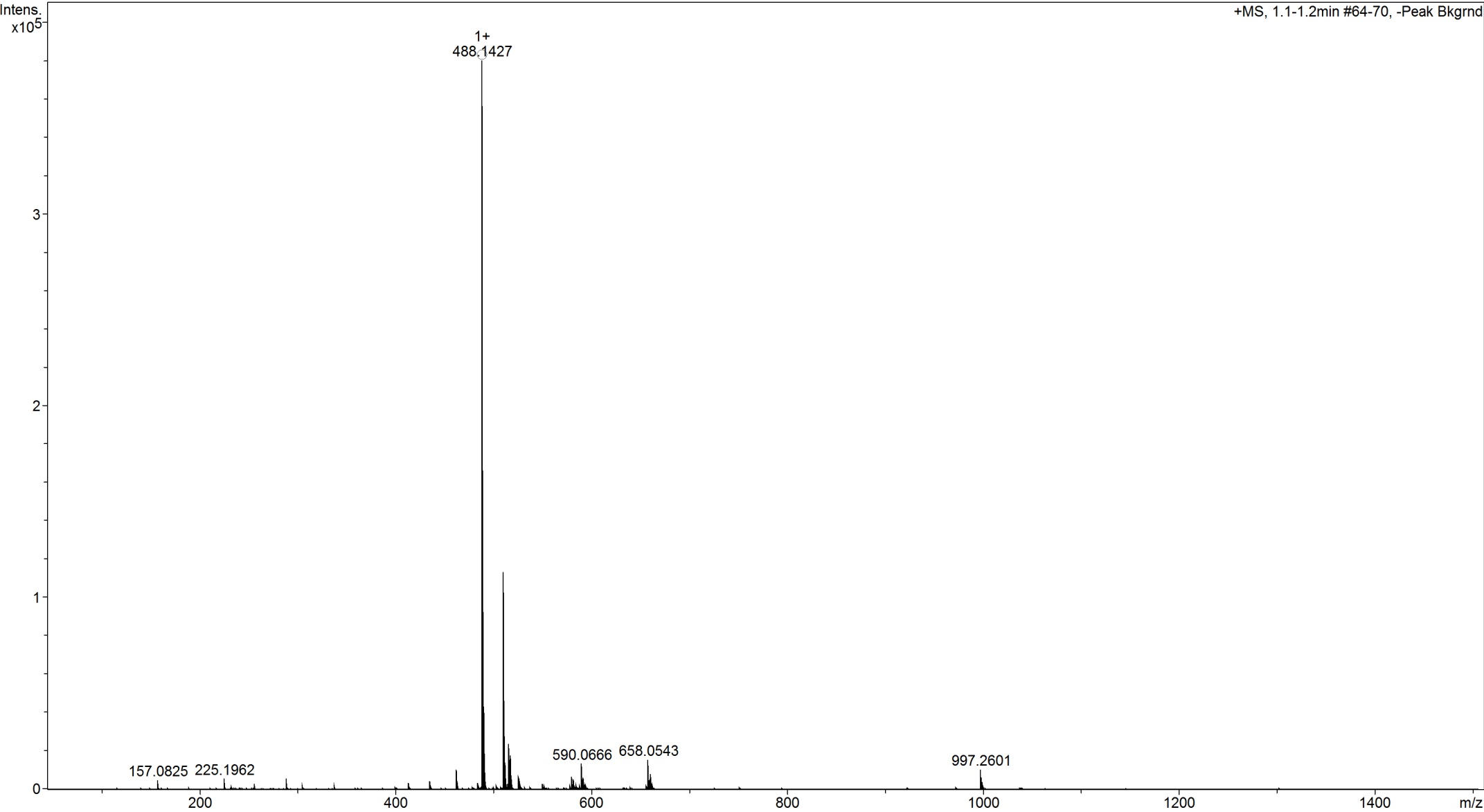
| Smart Formula Parameter | Value |
|-------------------------|--|
| Expected Formula | |
| Adducts Considered | M+H M+NH4 M+Na M+K M+Na2-H 2M+H 2M+Na |

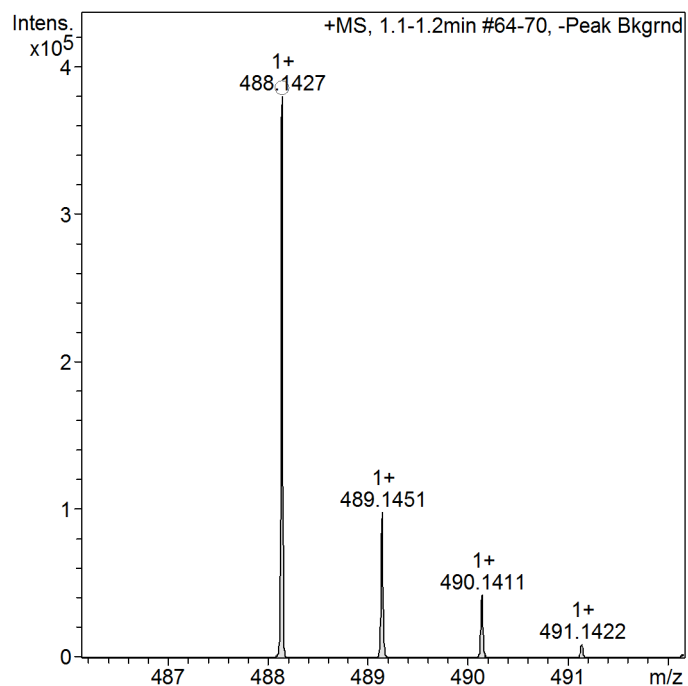
Smart Formula Search Parameters
CHNO and adducts considered
implicitly

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 |

Cmpd 2, 1.1 min





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

Cmpd 2, 1.1 min

| Meas. m/z | Ion Formula | z | m/z | err [mDa] | err [ppm] | mSigma | Score | Sum Formula | Adduct |
|------------|--------------|----|------------|-----------|-----------|--------|--------|-------------|---------|
| 488.142655 | C21H22N5O9 | 1+ | 488.141204 | -1.5 | -3.0 | 33.0 | 75.74 | C21H21N5O9 | M+H |
| | C22H18N9O5 | 1+ | 488.142541 | -0.1 | -0.2 | 38.7 | 100.00 | C22H17N9O5 | M+H |
| | C21H22N5O9 | 1+ | 488.141204 | -1.5 | -3.0 | 33.0 | 75.74 | C21H18N4O9 | M+NH4 |
| | C22H18N9O5 | 1+ | 488.142541 | -0.1 | -0.2 | 38.7 | 100.00 | C22H14N8O5 | M+NH4 |
| | C24H23N3NaO7 | 1+ | 488.142821 | 0.2 | 0.3 | 32.7 | 100.00 | C24H23N3O7 | M+Na |
| | C22H23KN7O4 | 1+ | 488.144310 | 1.7 | 3.4 | 4.2 | 50.04 | C22H23N7O4 | M+K |
| | C21H27KN3O8 | 1+ | 488.142973 | 0.3 | 0.7 | 8.2 | 100.00 | C21H27N3O8 | M+K |
| | C18H19KN13O2 | 1+ | 488.141625 | -1.0 | -2.1 | 8.2 | 69.34 | C18H19N13O2 | M+K |
| | C27H24NNa2O5 | 1+ | 488.144438 | 1.8 | 3.7 | 36.5 | 86.07 | C27H25NO5 | M+Na2-H |

| 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 |