

## Elemental Composition Report

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### Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

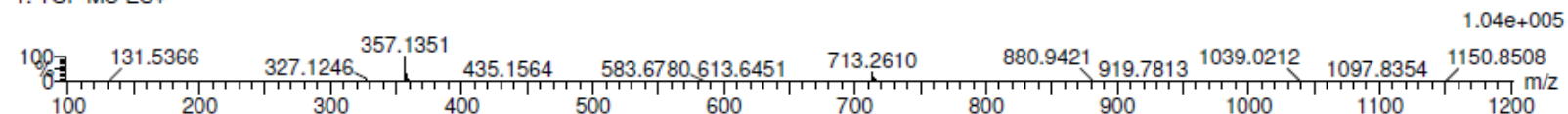
71 formula(e) evaluated with 10 results within limits (up to 100 closest results for each mass)

Elements Used:

C: 0-100 H: 0-100 O: 0-50

sauchinone 265 (4.551)

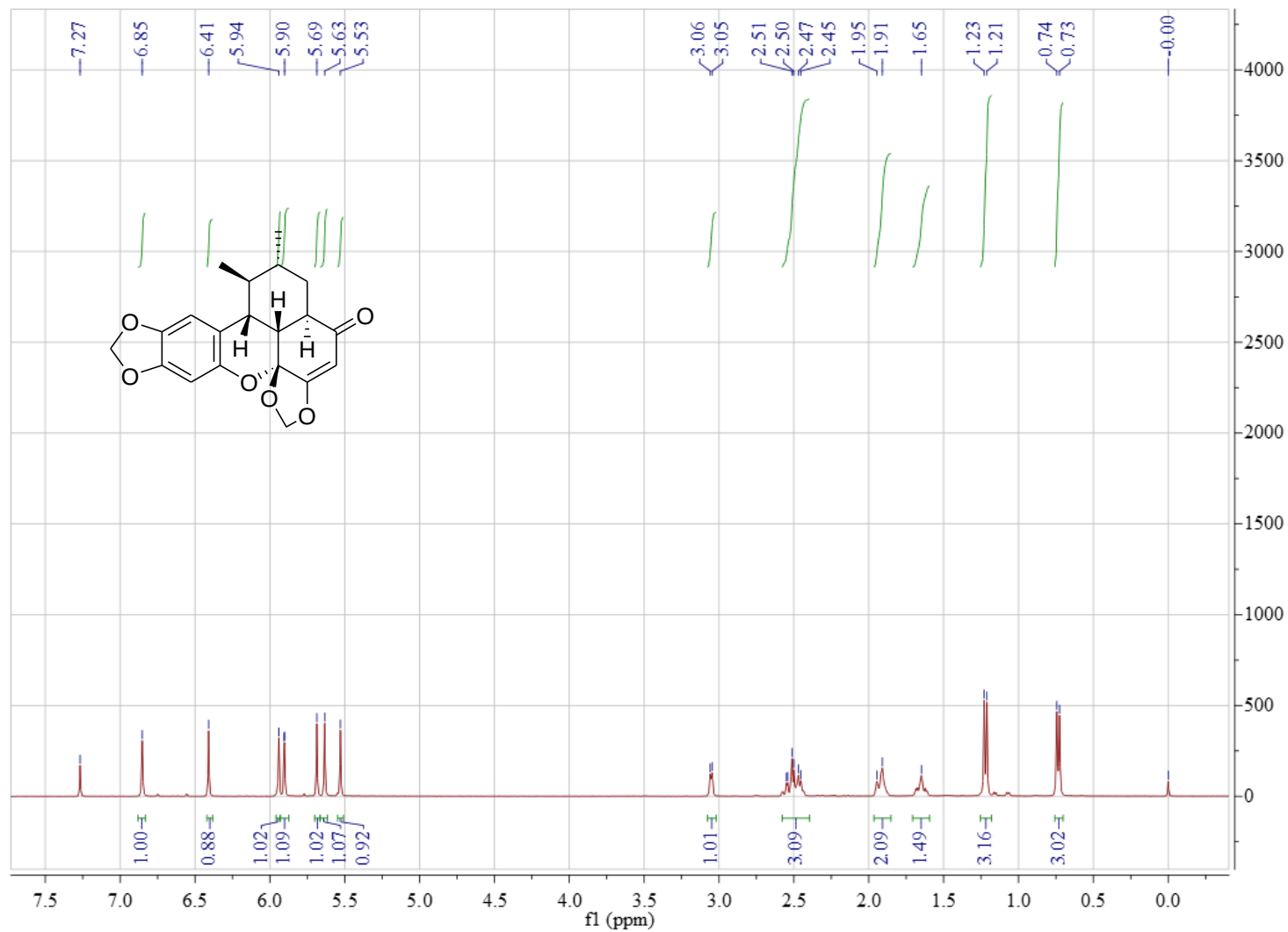
1: TOF MS ES+



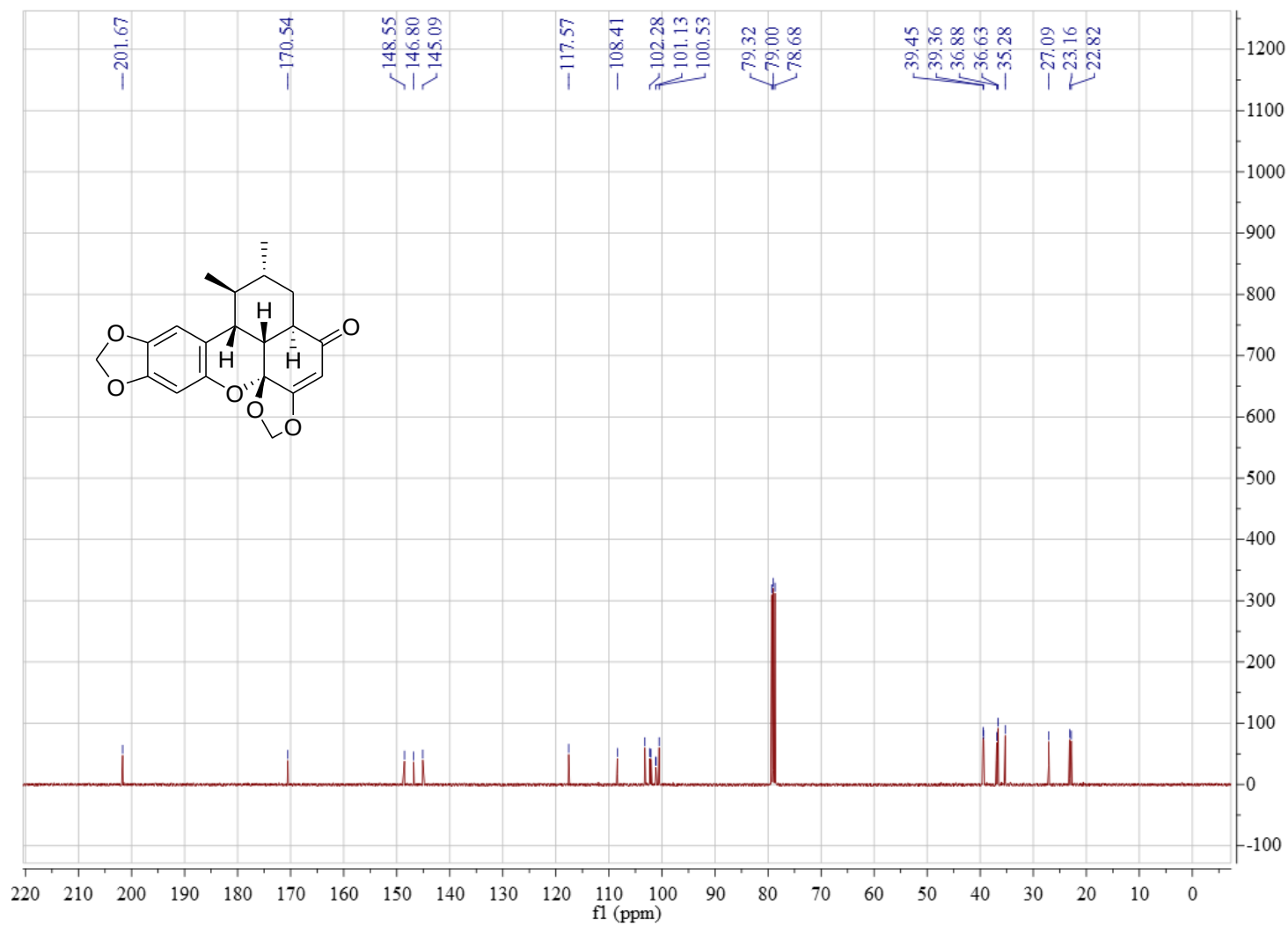
Minimum: -1.5  
Maximum: 5.0 100.0 50.0

| Mass     | Calc. Mass | mDa   | PPM   | DBE  | i-FIT | Norm   | Conf(%) | Formula     |
|----------|------------|-------|-------|------|-------|--------|---------|-------------|
| 357.1351 | 357.1338   | 1.3   | 3.6   | 10.5 | 321.5 | 2.882  | 5.60    | C20 H21 O6  |
|          | 357.1397   | -4.6  | -12.9 | 1.5  | 330.3 | 11.675 | 0.00    | C13 H25 O11 |
|          | 357.1279   | 7.2   | 20.2  | 19.5 | 323.0 | 4.320  | 1.33    | C27 H17 O   |
|          | 357.1491   | -14.0 | -39.2 | 14.5 | 320.8 | 2.164  | 11.48   | C24 H21 O3  |
|          | 357.1186   | 16.5  | 46.2  | 6.5  | 327.9 | 9.222  | 0.01    | C16 H21 O9  |
|          | 357.1549   | -19.8 | -55.4 | 5.5  | 327.1 | 8.516  | 0.02    | C17 H25 O8  |
|          | 357.1127   | 22.4  | 62.7  | 15.5 | 319.0 | 0.370  | 69.08   | C23 H17 O4  |
|          | 357.1643   | -29.2 | -81.8 | 18.5 | 326.0 | 7.360  | 0.06    | C28 H21     |
|          | 357.1033   | 31.8  | 89.0  | 2.5  | 331.3 | 12.681 | 0.00    | C12 H21 O12 |
|          | 357.1702   | -35.1 | -98.3 | 9.5  | 320.7 | 2.087  | 12.41   | C21 H25 O5  |

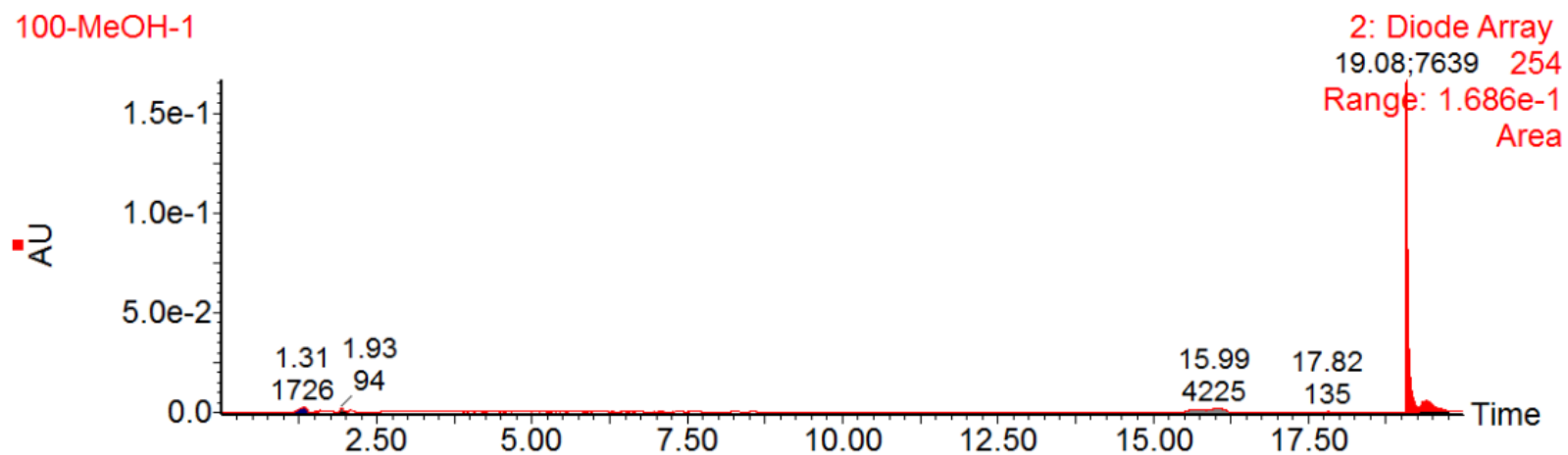
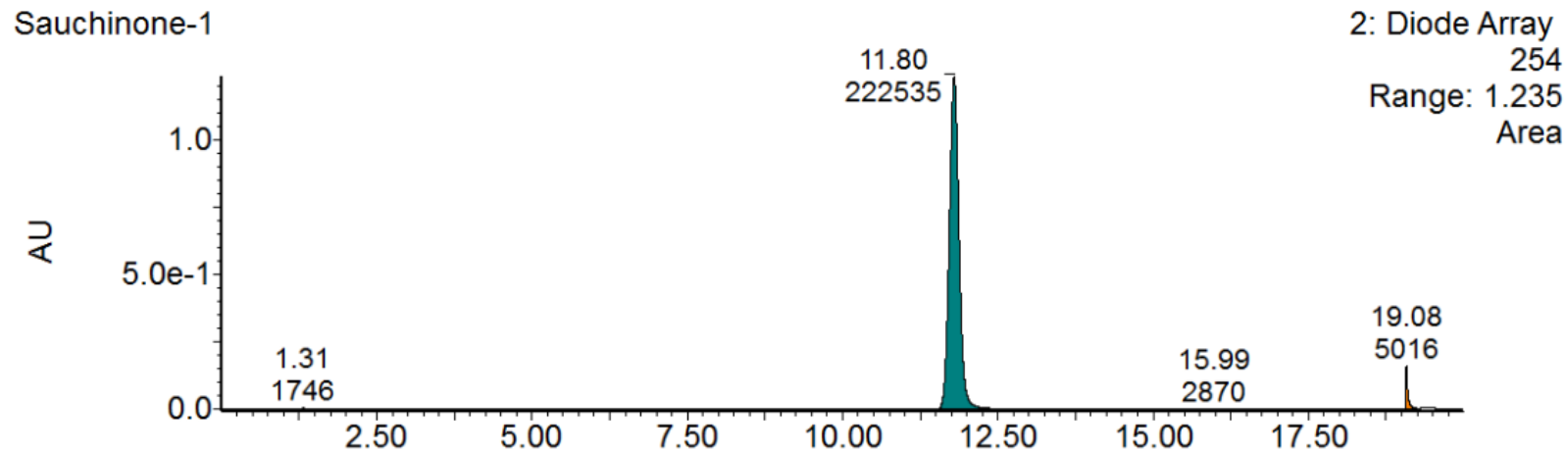
# $^1\text{H}$ NMR spectrum of Sauchinone in $\text{CDCl}_3$ (400MHz)



# $^{13}\text{C}$ NMR spectrum of Sauchinone in $\text{CDCl}_3$ (100MHz)



## Peak area value of Sauchinone and Blank



## Analytical Condition for Sauchinone

- UPLC: Waters Acquity™ Ultra Performance LC system (Waters Corp., Milford, MA)
- Column: ACQUITY UPLC®BEH C18 column (2.1 mm×150 mm, 1.7 µm)
- Mobile phase

A (0.1% formic acid in water)

B (0.1% formic acid in acetonitrile)

Injection volume: 2 µl (1 mg/ml in 100% MeOH)

### Gradient elution program of UPLC

| Time (min) | Flow rate (ml/min) | %A | %B  |
|------------|--------------------|----|-----|
| 0.0-14.0   | 0.3 ml/min         | 60 | 40  |
| 14.0-14.5  | 0.3 ml/min         | 0  | 100 |
| 14.5-17.0  | 0.3 ml/min         | 0  | 100 |
| 17.0-17.5  | 0.3 ml/min         | 60 | 40  |
| 17.5-20.0  | 0.3 ml/min         | 60 | 40  |