

## Supporting Information

### Antimalarial Oxoprotoberberine Alkaloids from the Leaves of *Milium cuneata*

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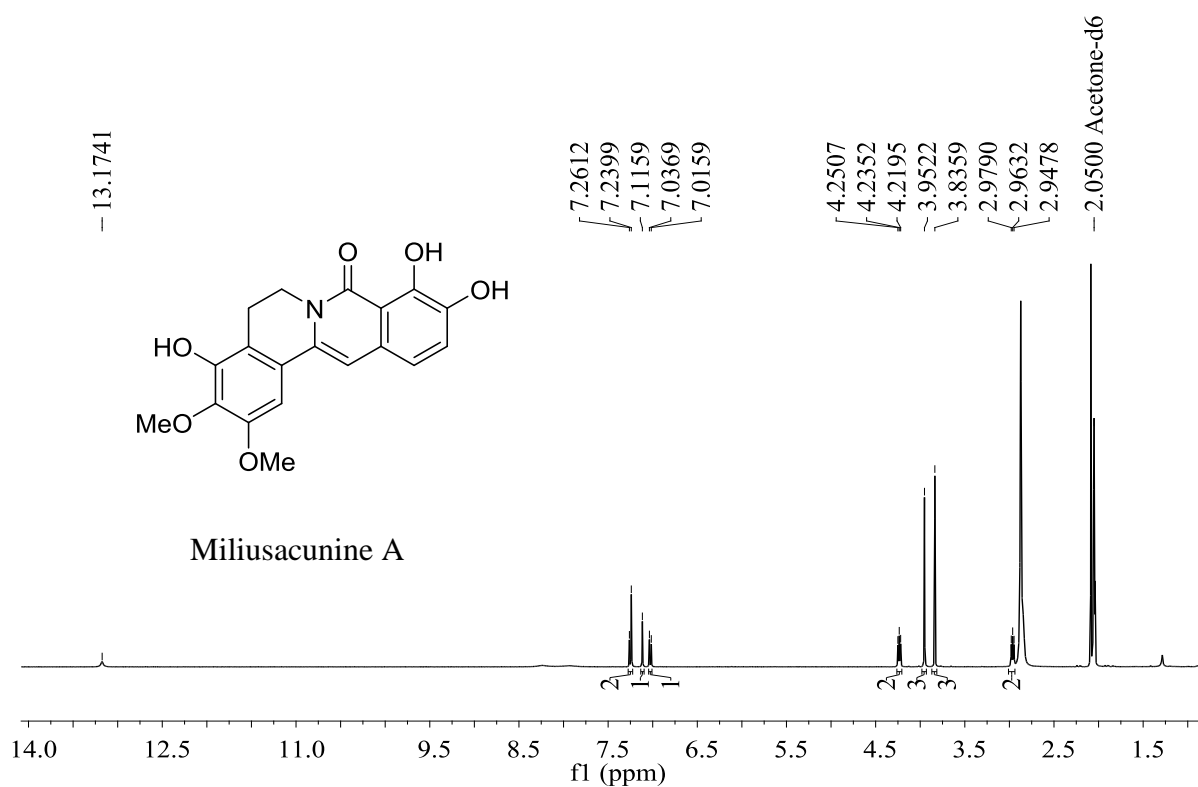
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<sup>||</sup>School of Chemistry, University of Wollongong, Wollongong, New South Wales 2522, Australia

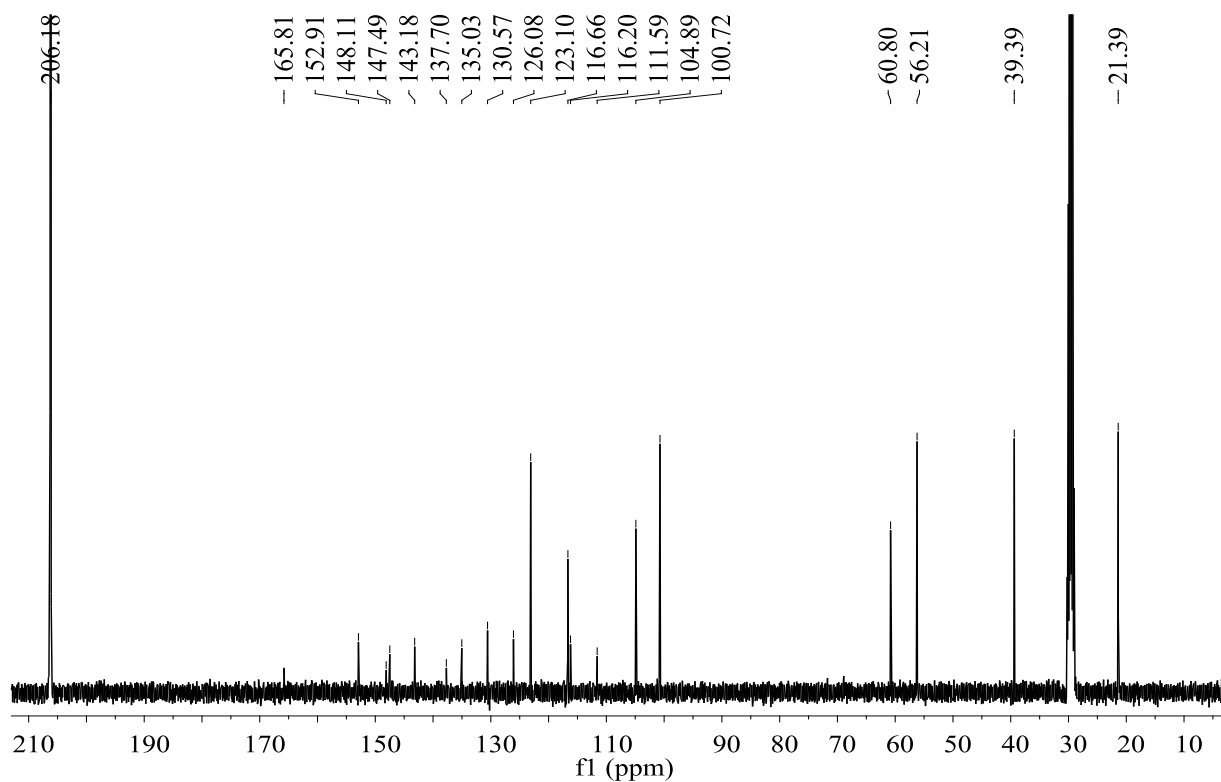
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*E-mail address:* thunwadee.r@cmu.ac.th, othunwadee@gmail.com.

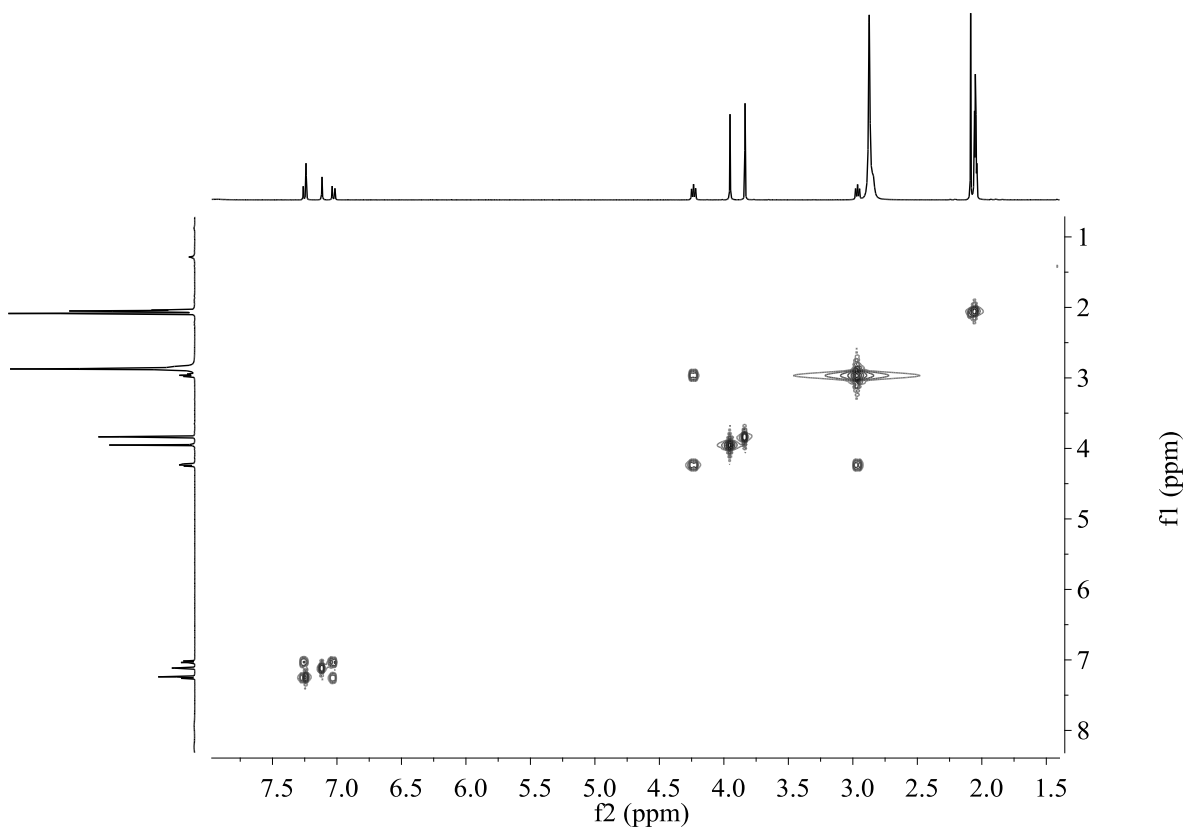
|      |  |    |
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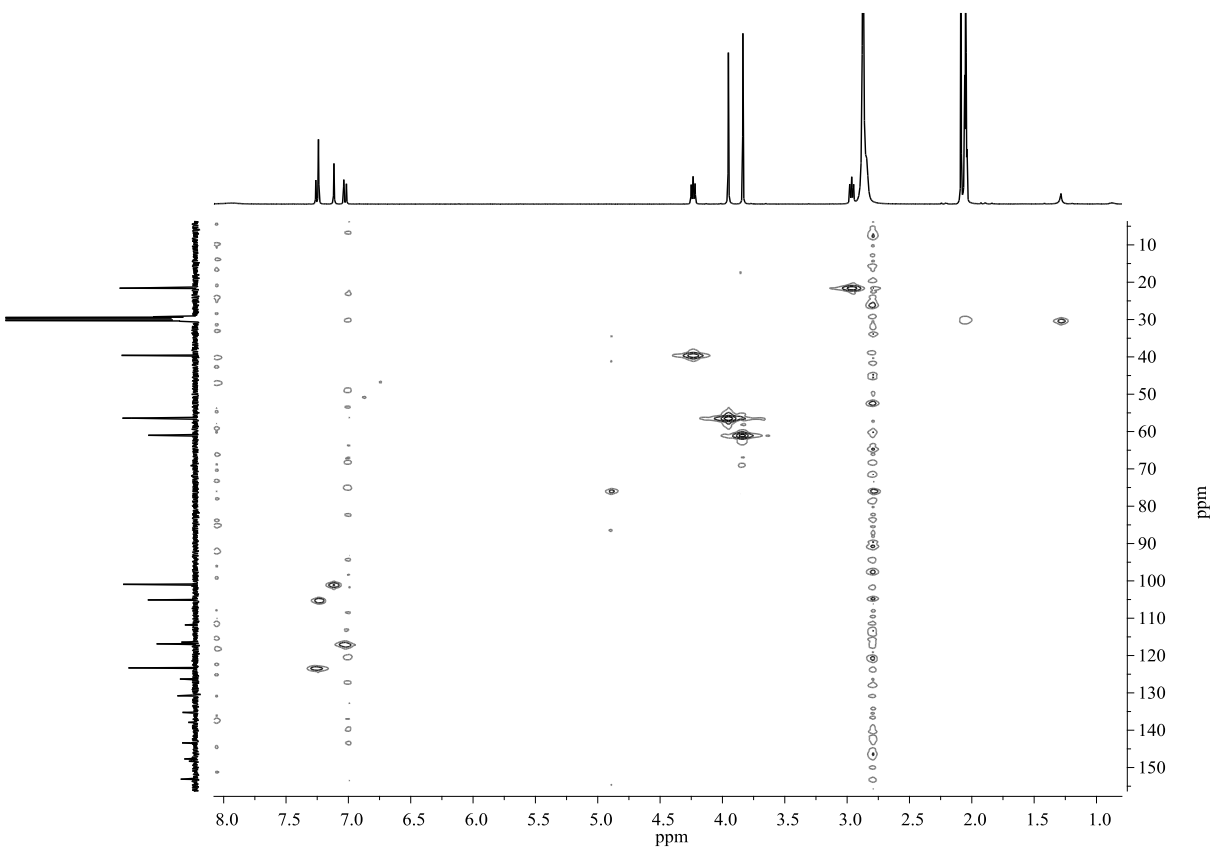
S1.  $^1\text{H}$  NMR spectrum of compound **1** in acetone- $d_6$  (400 MHz)



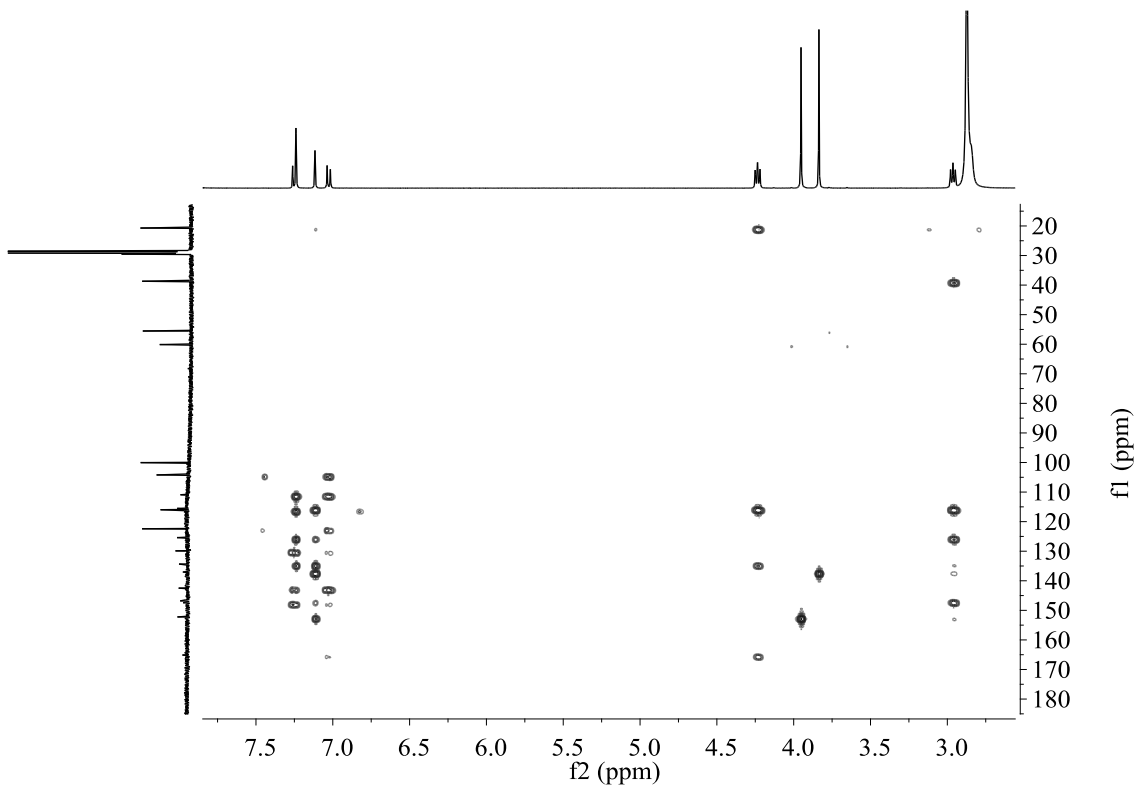
S2.  $^{13}\text{C}$  NMR spectrum of compound **1** in acetone- $d_6$  (100 MHz)



S3. COSY spectrum of compound **1** in acetone- $d_6$  (400 MHz)



S4. HMQC spectrum of compound **1** in acetone- $d_6$  (400 MHz)



S5. HMBC spectrum of compound **1** in acetone- $d_6$  (400 MHz)

Elemental Composition Report

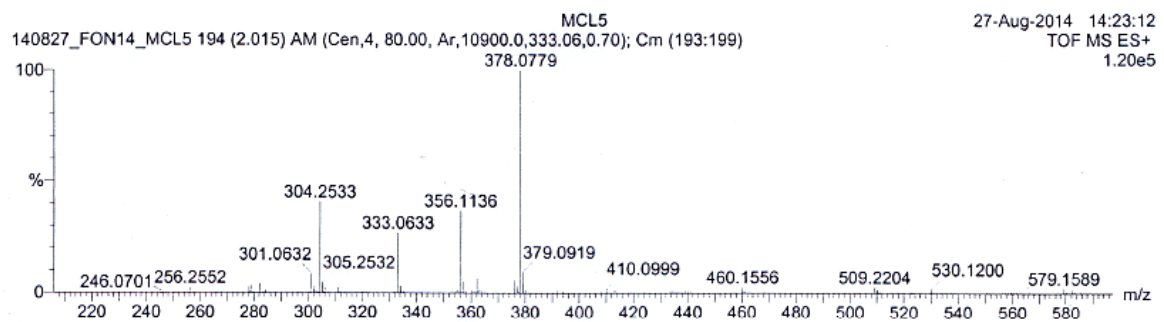
Single Mass Analysis

Tolerance = 5000.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

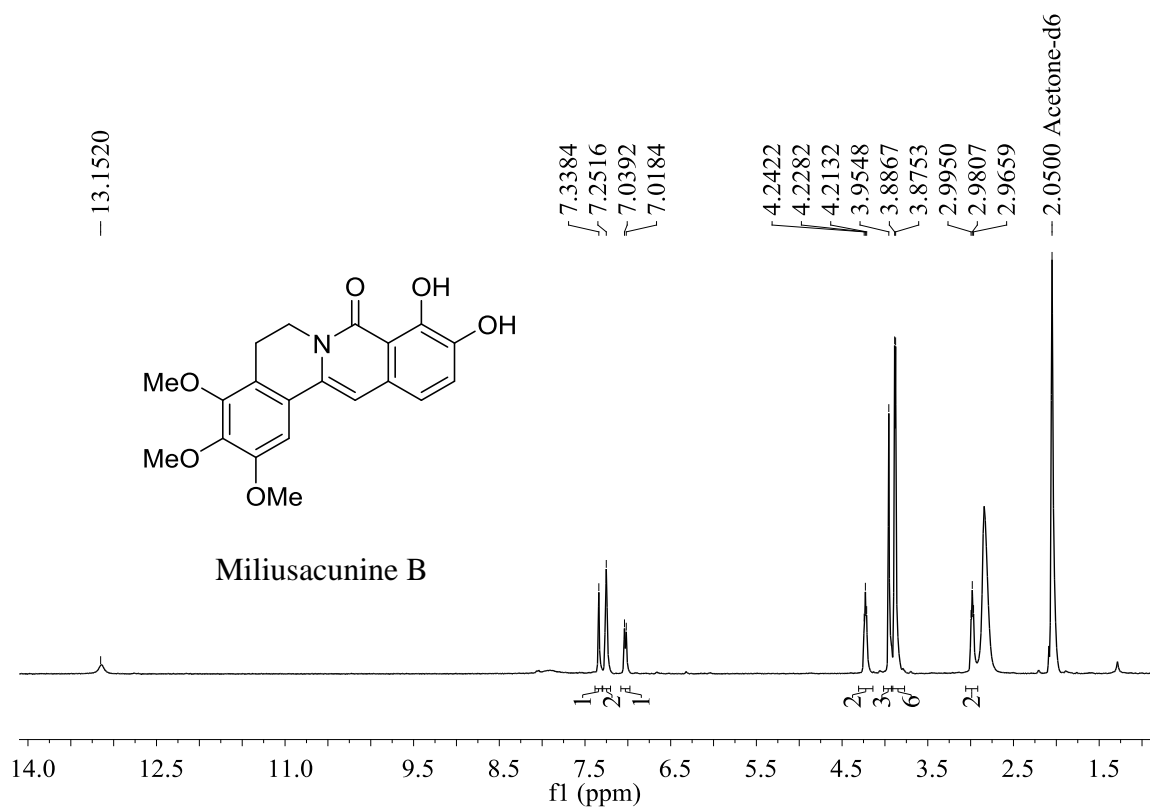
Monoisotopic Mass, Odd and Even Electron Ions

1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

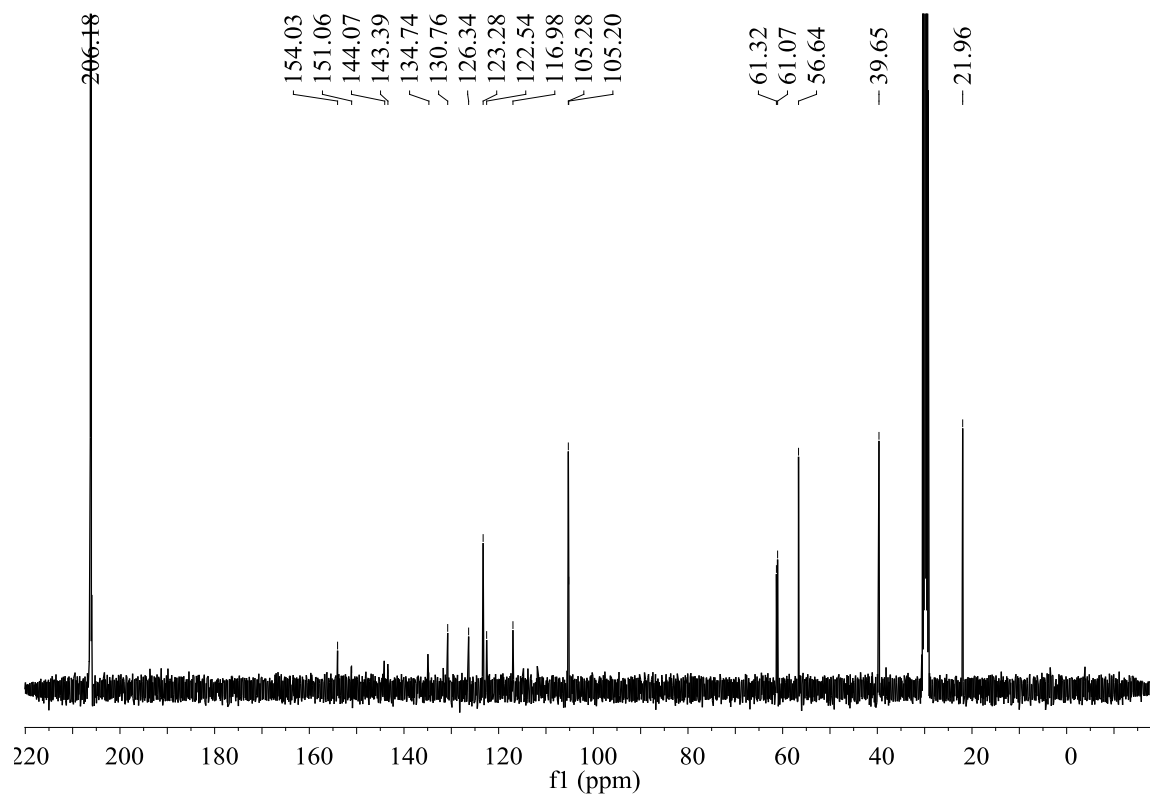


| Mass     | Calc. Mass | mDa | PPM | DBE  | Score | Formula      |
|----------|------------|-----|-----|------|-------|--------------|
| 356.1136 | 356.1134   | 0.2 | 0.5 | 11.5 | 1     | C19 H18 N O6 |

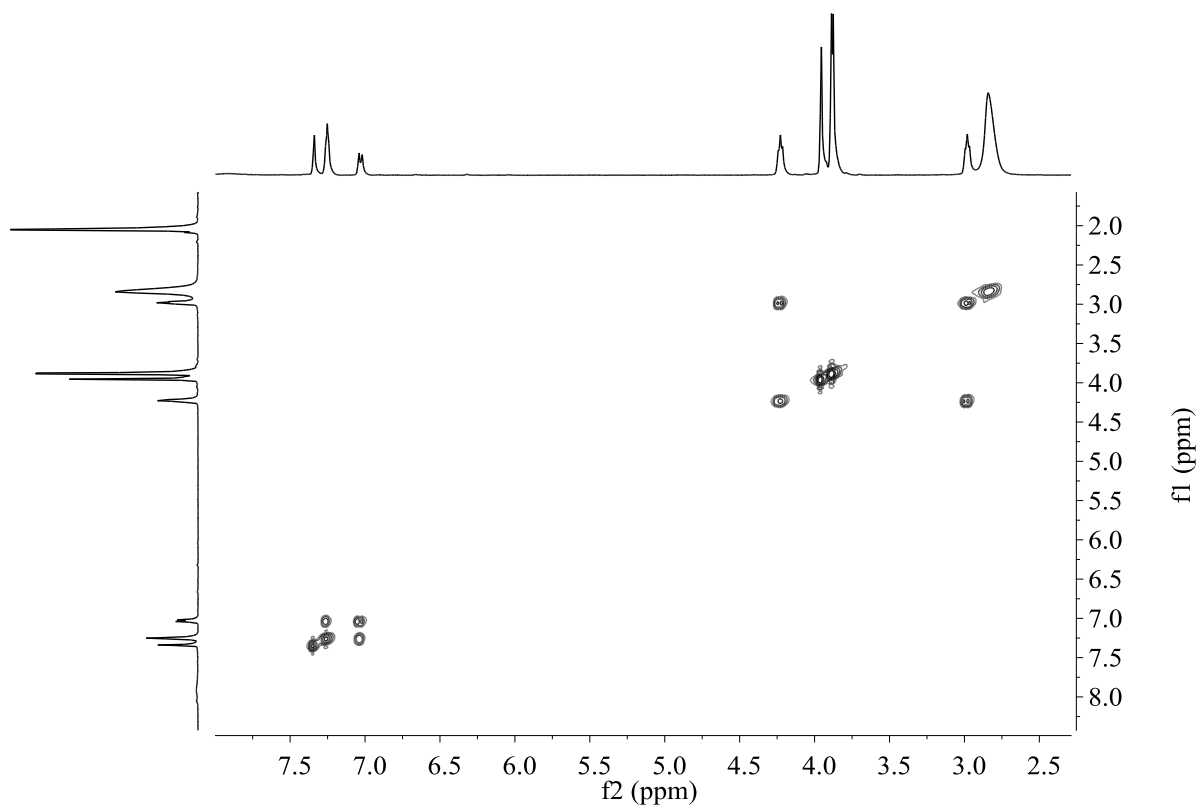
S6. HRESI-MS spectrum of compound **1**



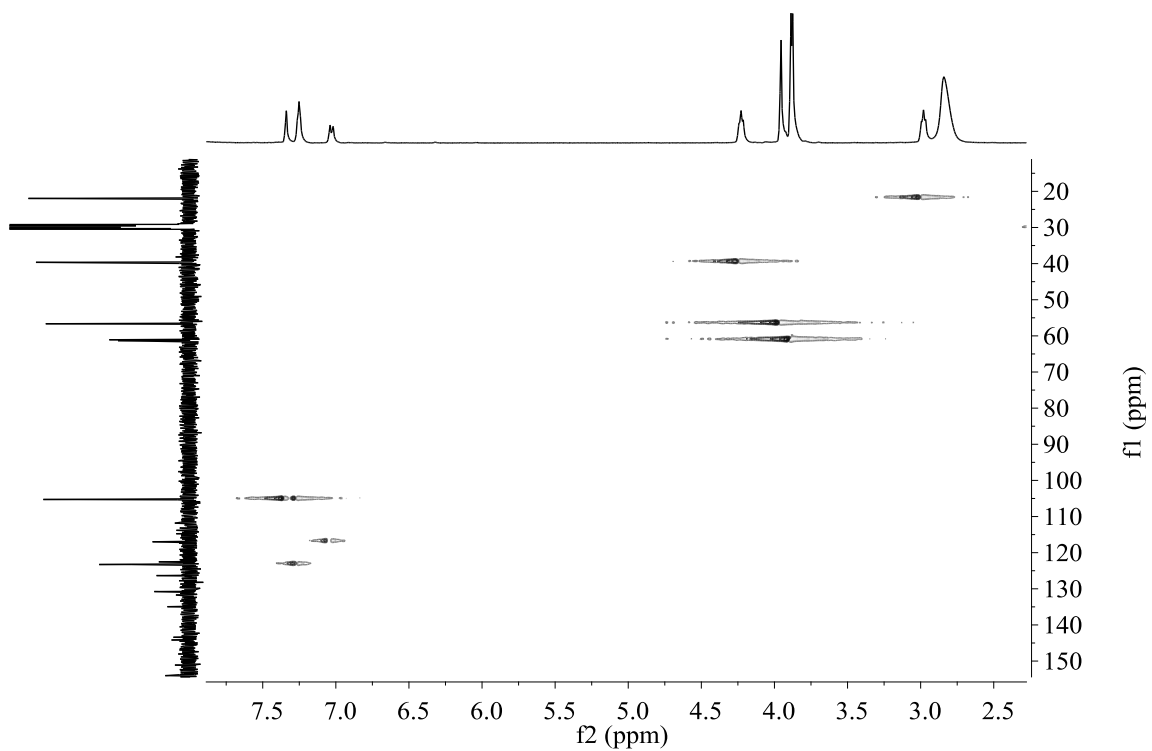
S7.  $^1\text{H}$  NMR spectrum of compound **2** in acetone- $d_6$  (400 MHz)



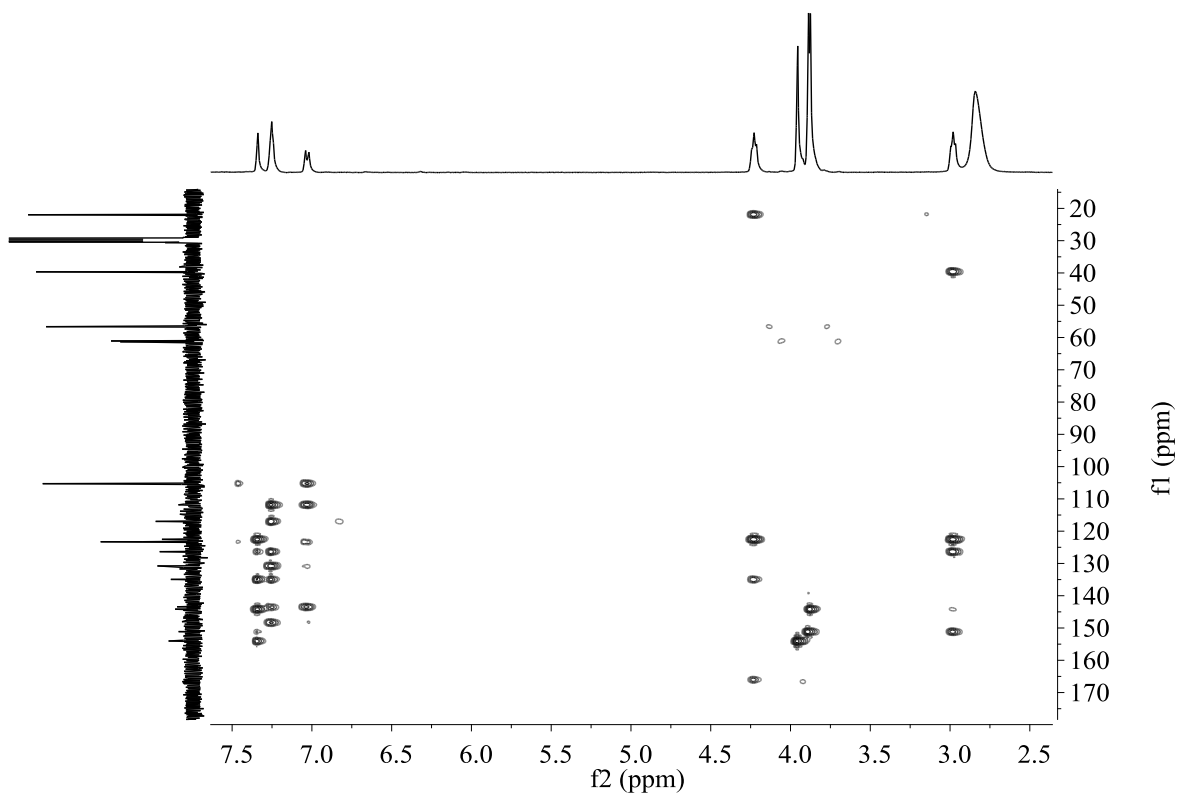
S8.  $^{13}\text{C}$  NMR spectrum of compound **2** in acetone- $d_6$  (100 MHz)



S9. COSY spectrum of compound **2** in acetone- $d_6$  (400 MHz)



S10. HMQC spectrum of compound **2** in acetone- $d_6$  (500 MHz)



S11. HMBC spectrum of compound **2** in acetone- $d_6$  (400 MHz)

Elemental Composition Report

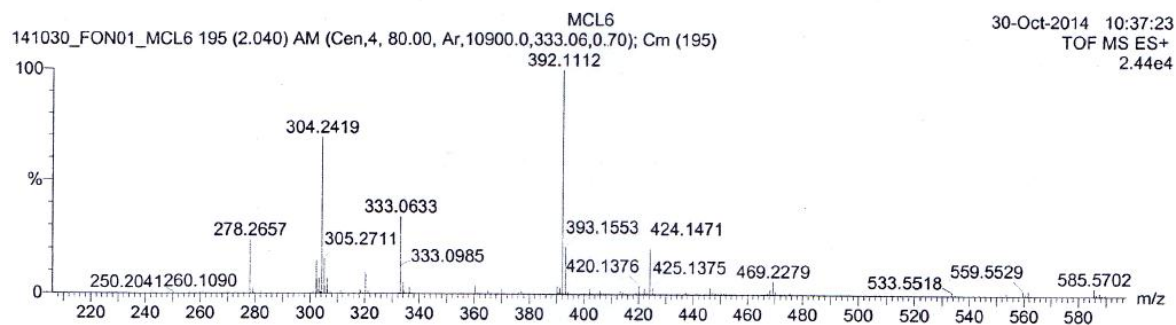
Single Mass Analysis

Tolerance = 5000.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

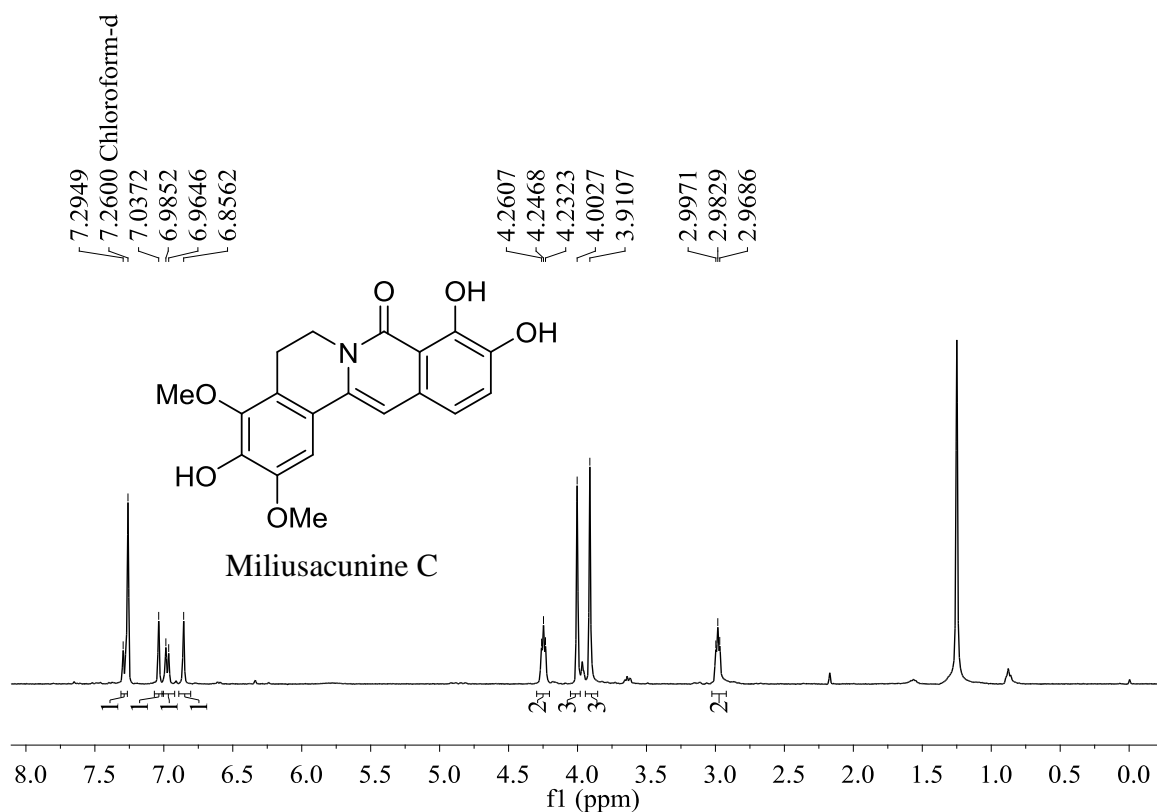
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)



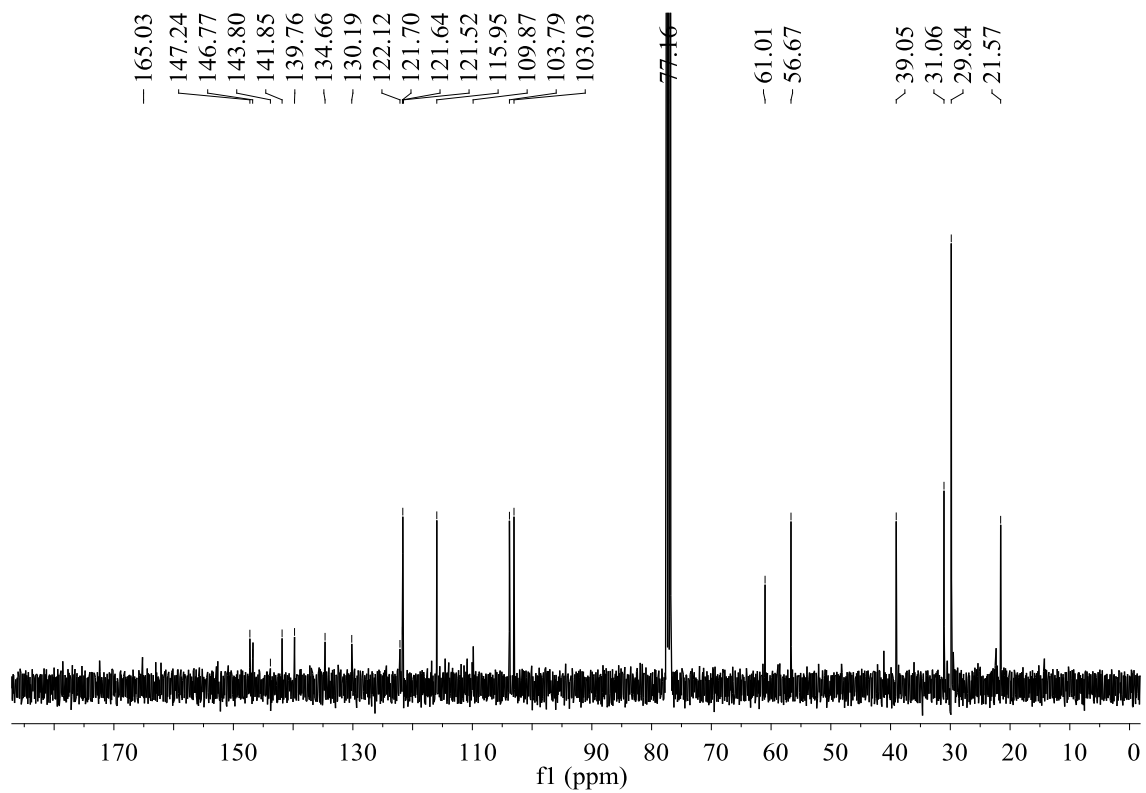
| Mass     | Calc. Mass | mDa | PPM | DBE  | Score | Formula         |
|----------|------------|-----|-----|------|-------|-----------------|
| 392.1112 | 392.1110   | 0.2 | 0.5 | 11.5 | 1     | C20 H19 N O6 Na |

S12. HRESI-MS spectrum of compound **2**

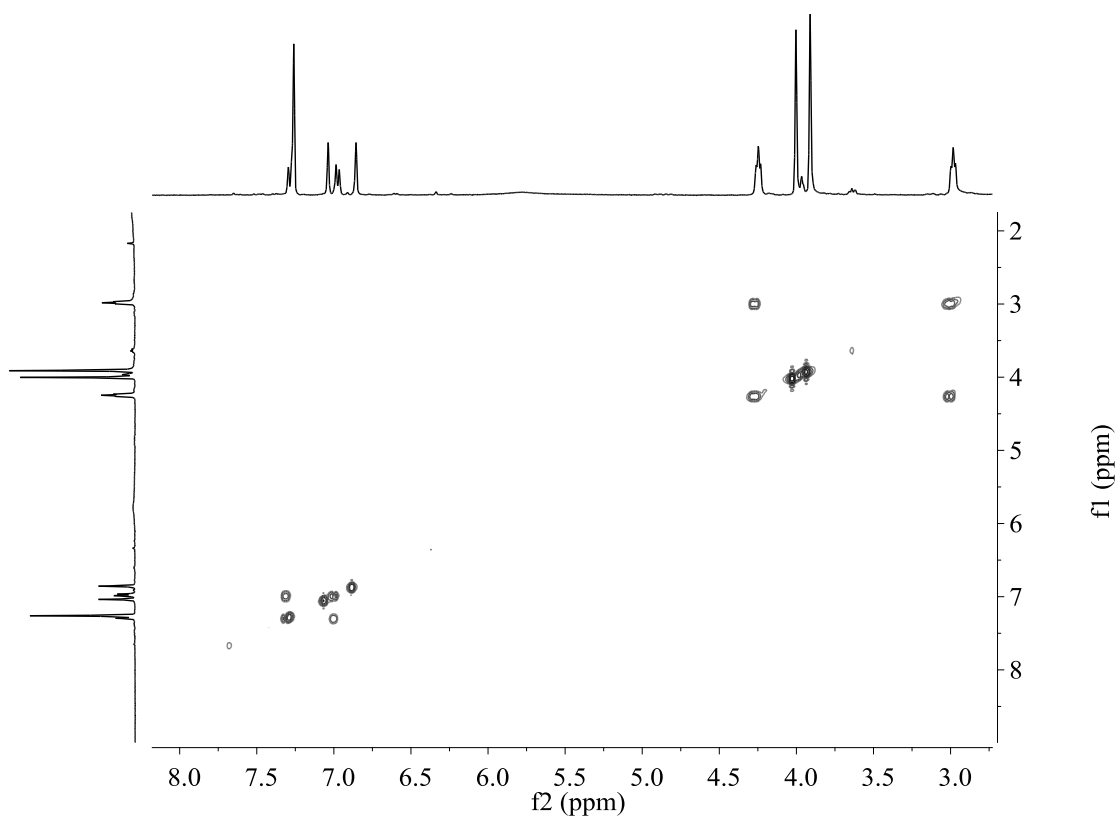




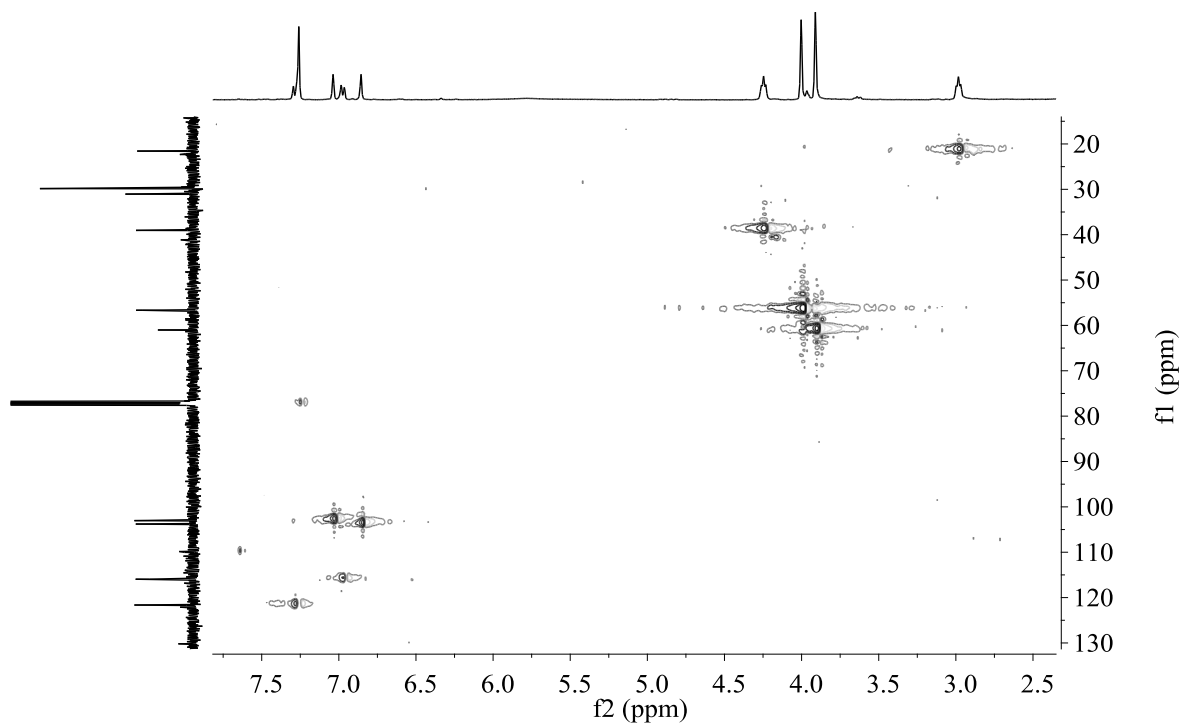
S13.  $^1\text{H}$  NMR spectrum of compound **3** in  $\text{CDCl}_3$  (400 MHz)



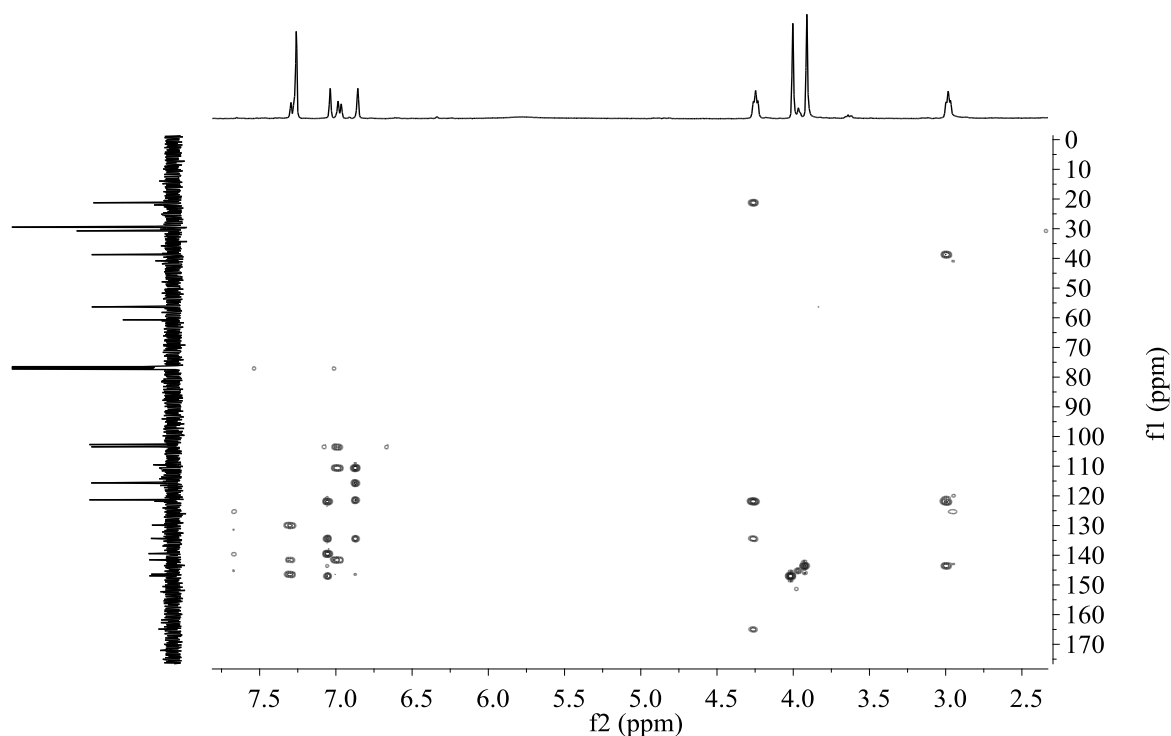
S14.  $^{13}\text{C}$  NMR spectrum of compound **3** in  $\text{CDCl}_3$  (100 MHz)



S15. COSY spectrum of compound **3** in  $\text{CDCl}_3$  (400 MHz)



S16. HMQC spectrum of compound **3** in  $\text{CDCl}_3$  (500 MHz)



S17. HMBC spectrum of compound **3** in CDCl<sub>3</sub> (400 MHz)

Elemental Composition Report

Single Mass Analysis

Tolerance = 8.0 PPM / DBE: min = -1.5, max = 120.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1004 formula(e) evaluated with 6 results within limits (up to 20 closest results for each mass)

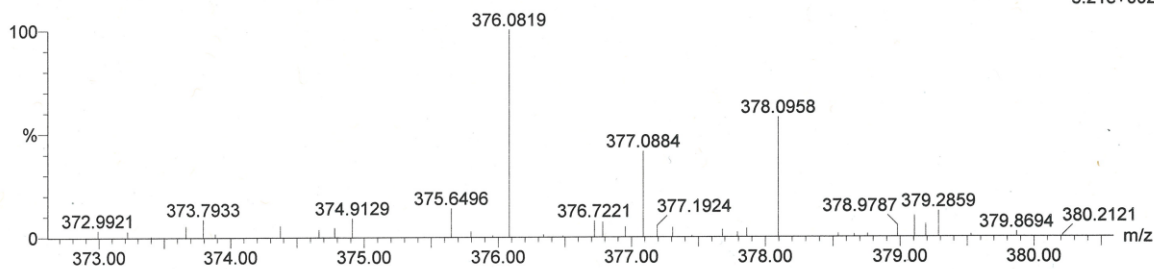
Elements Used:

C: 8-40 H: 0-70 N: 0-10 O: 0-12 Na: 0-1

MC 3

SP Thanaphat MC 3 73 (1.754) AM2 (Ar,8000.0,0.00,0.57); ABS; Cm (71:73)

1: TOF MS ES+  
5.21e+002

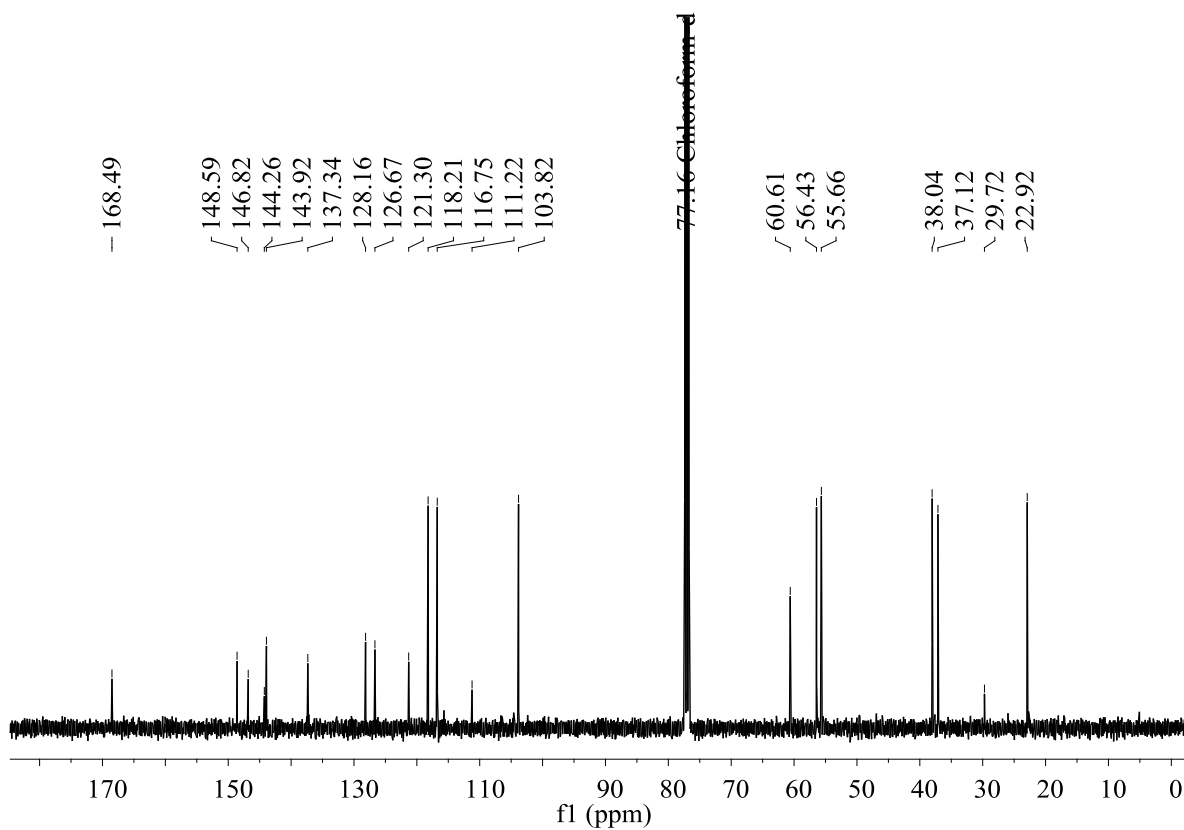
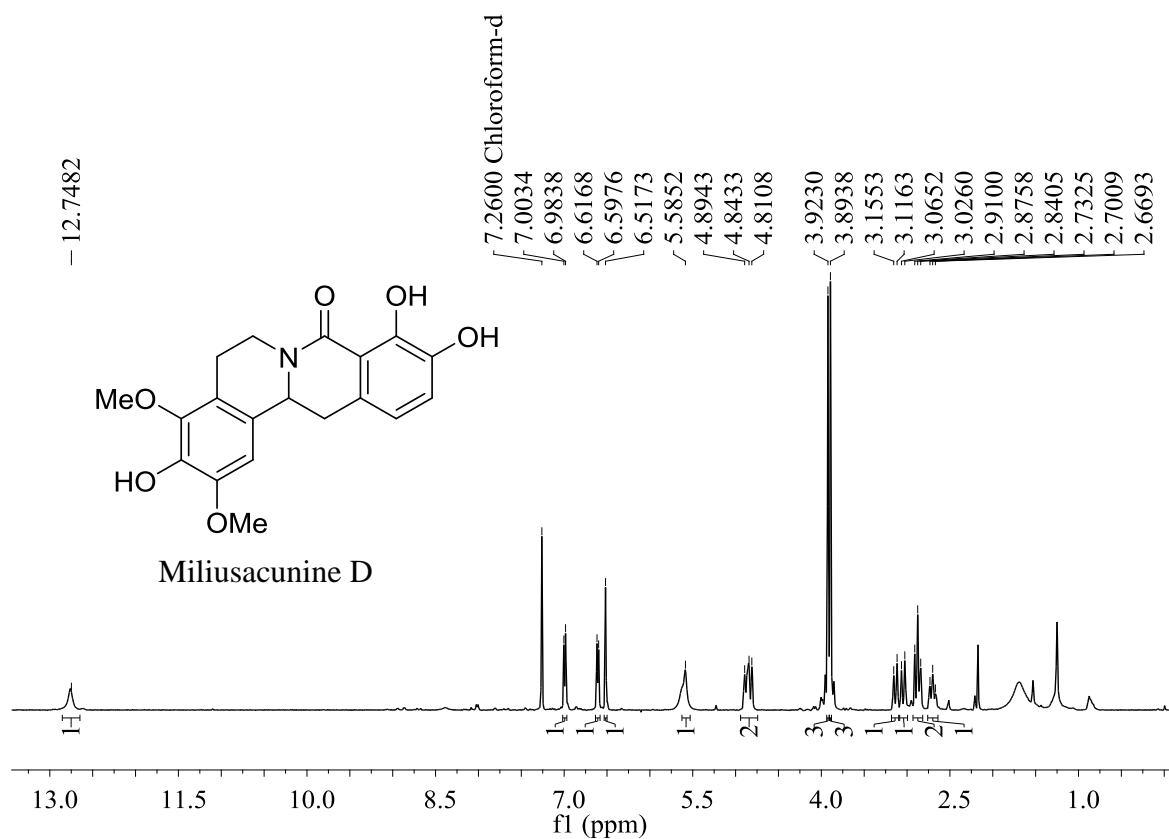


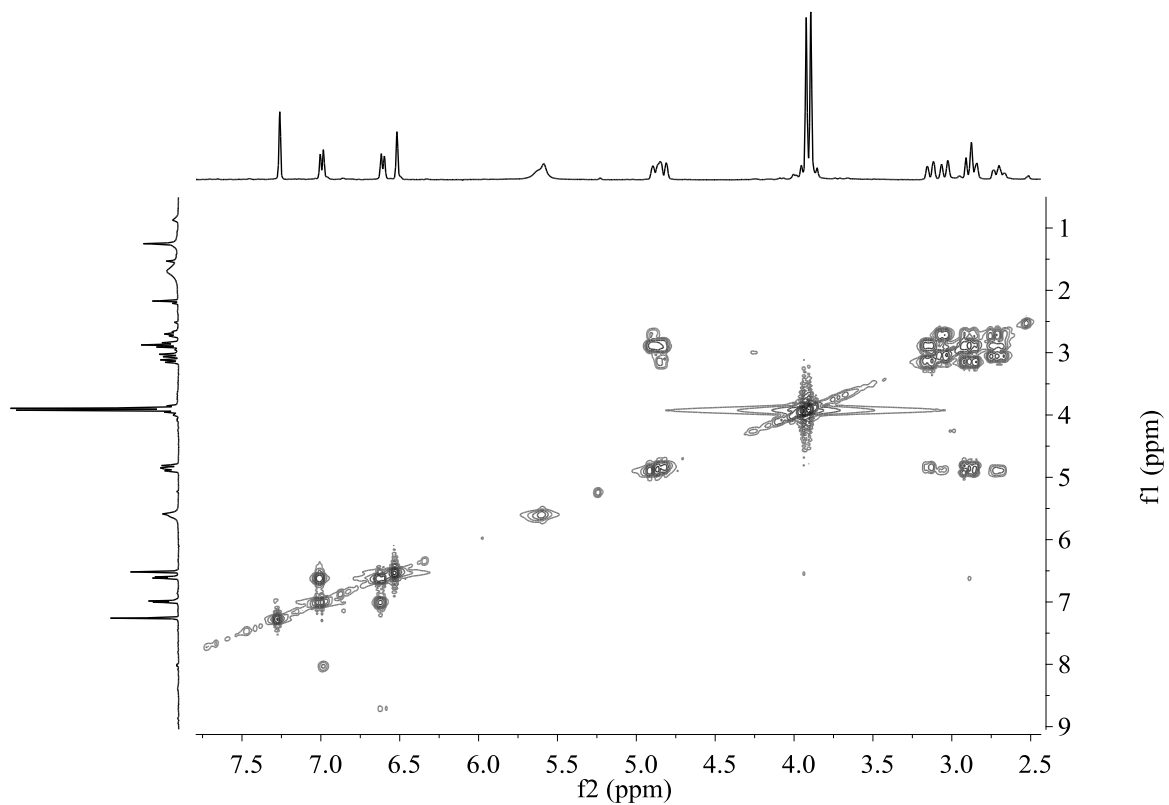
Minimum:

Maximum: 5.0 8.0 -1.5 120.0

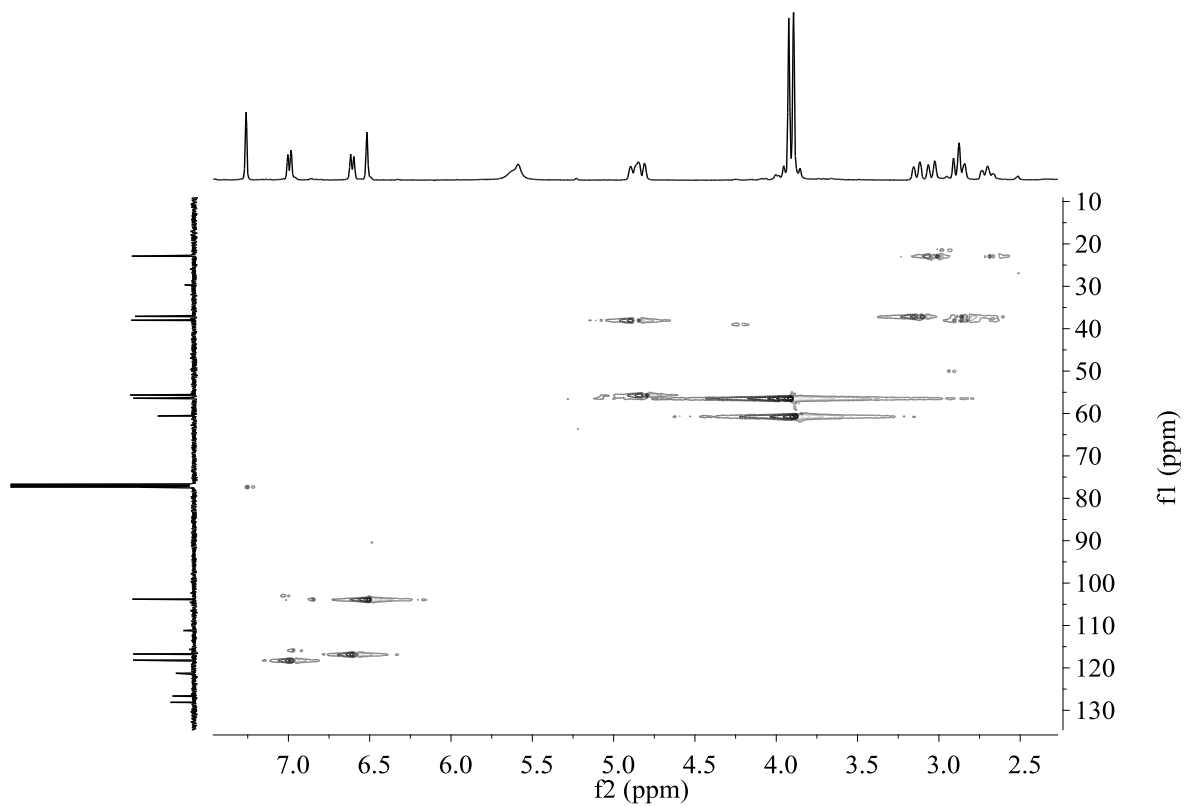
| Mass     | Calc. Mass | mDa | PPM | DBE  | i-FIT | i-FIT (Norm) | Formula  |
|----------|------------|-----|-----|------|-------|--------------|--|
| 378.0958 | 378.0954   | 0.4 | 1.1 | 11.5 | 59.8  | 1.9          | C <sub>19</sub> H <sub>17</sub> N O <sub>6</sub><br>Na |

S18. HRESI-MS spectrum of compound **3**

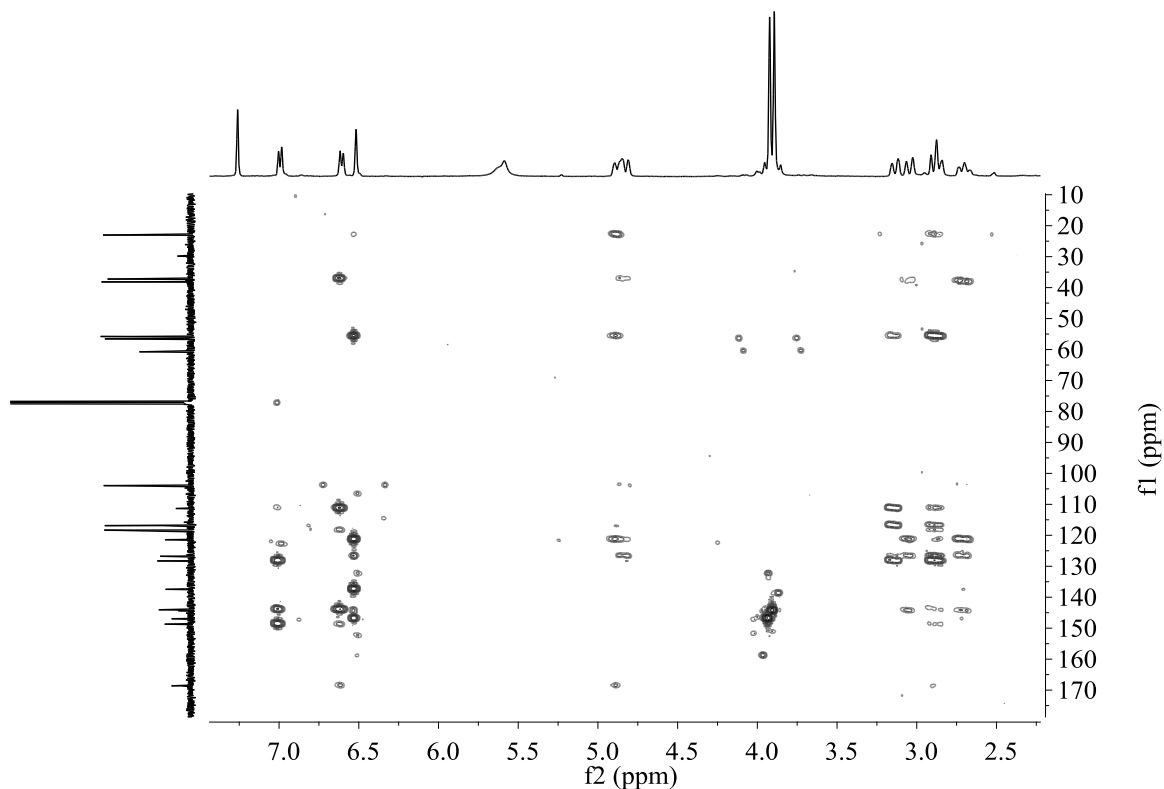




S21. COSY spectrum of compound **4** in  $\text{CDCl}_3$  (400 MHz)



S22. HMQC spectrum of compound **4** in  $\text{CDCl}_3$  (500 MHz)



S23. HMBC spectrum of compound **4** in CDCl<sub>3</sub> (400 MHz)

**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 8.0 PPM / DBE: min = -1.5, max = 120.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1013 formula(e) evaluated with 7 results within limits (up to 20 closest results for each mass)

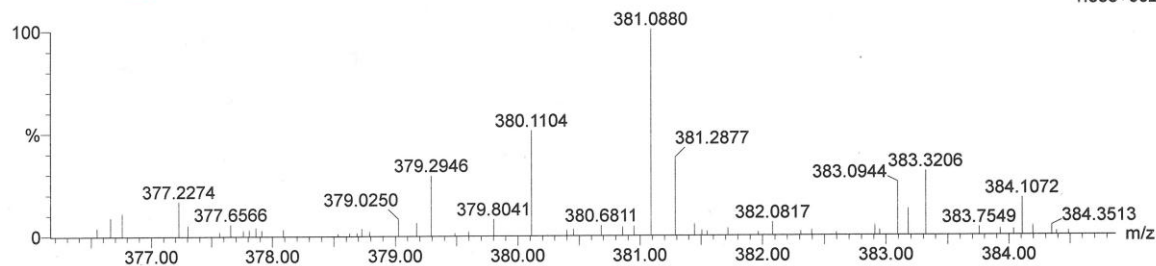
Elements Used:

C: 8-40 H: 0-70 N: 0-10 O: 0-12 Na: 0-1

MC 4

SP Thanaphat MC 4 37 (0.904) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (36:37)

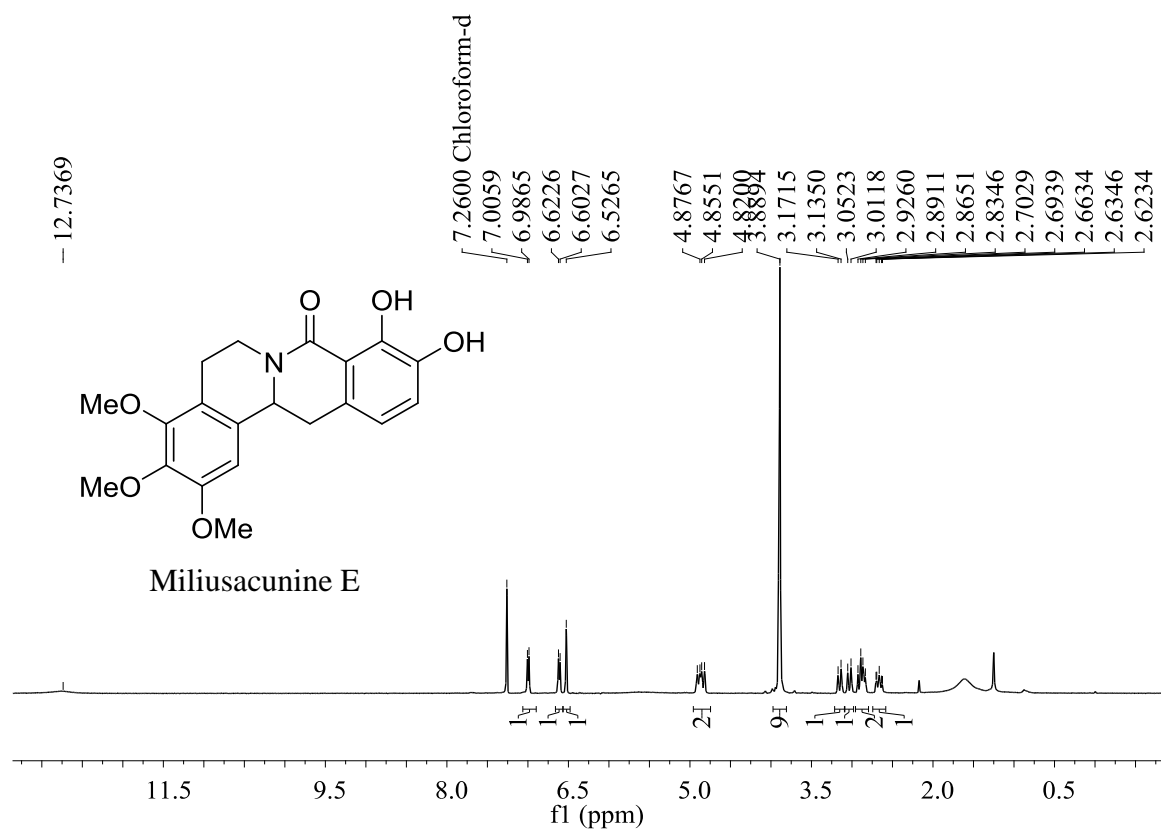
1: TOF MS ES+  
1.33e+002



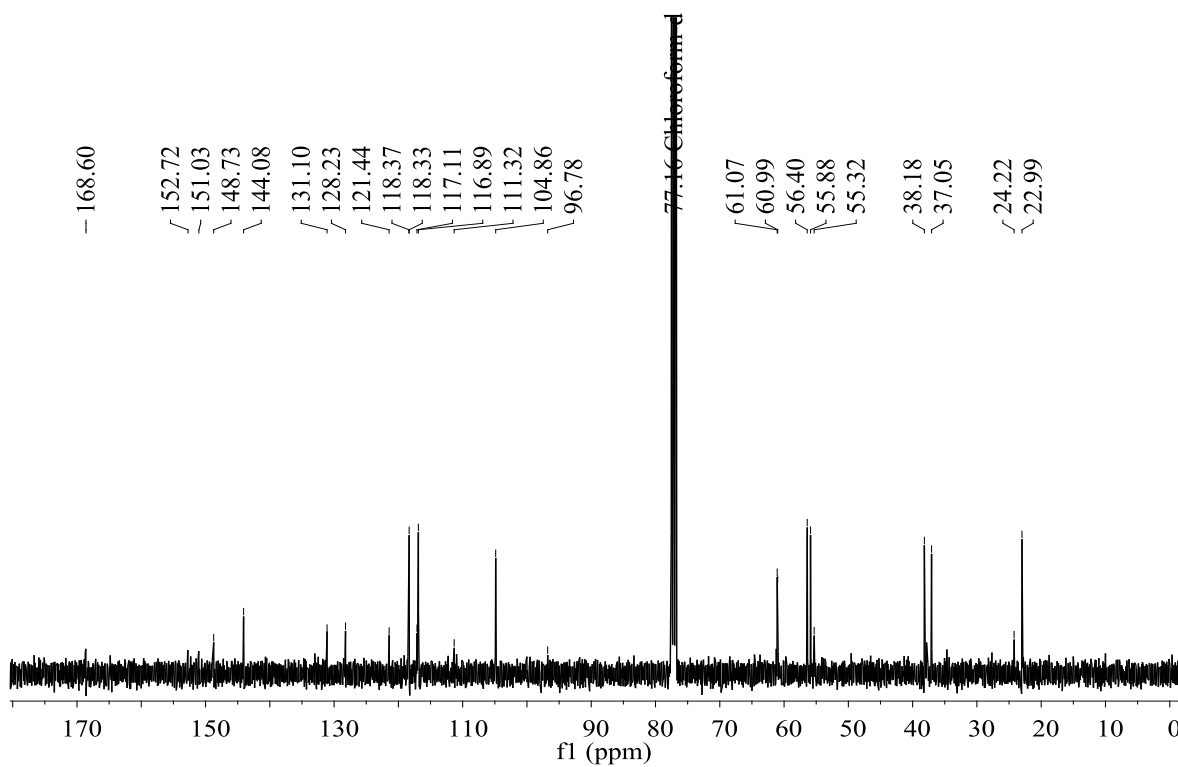
Minimum: -1.5  
 Maximum: 5.0 8.0 120.0

| Mass     | Calc. Mass | mDa  | PPM  | DBE  | i-FIT | i-FIT (Norm) | Formula       |
|----------|------------|------|------|------|-------|--------------|---------------|
| 380.1104 | 380.1107   | -0.3 | -0.8 | 14.5 | 68.8  | 2.1          | C17 H14 N7 O4 |
|          | 380.1110   | -0.6 | -1.6 | 10.5 | 68.9  | 2.2          | C19 H19 N O6  |
|          |            |      |      |      |       |              | Na            |

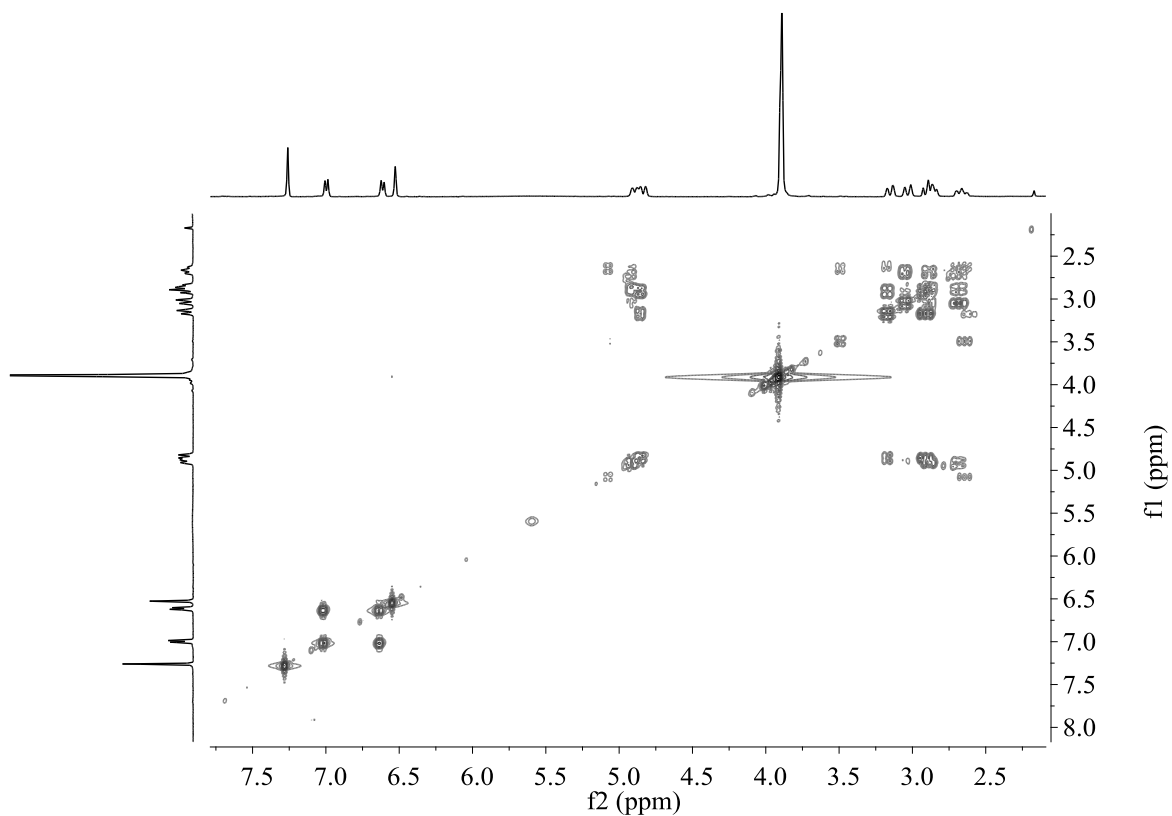
S24. HRESI-MS spectrum of compound **4**



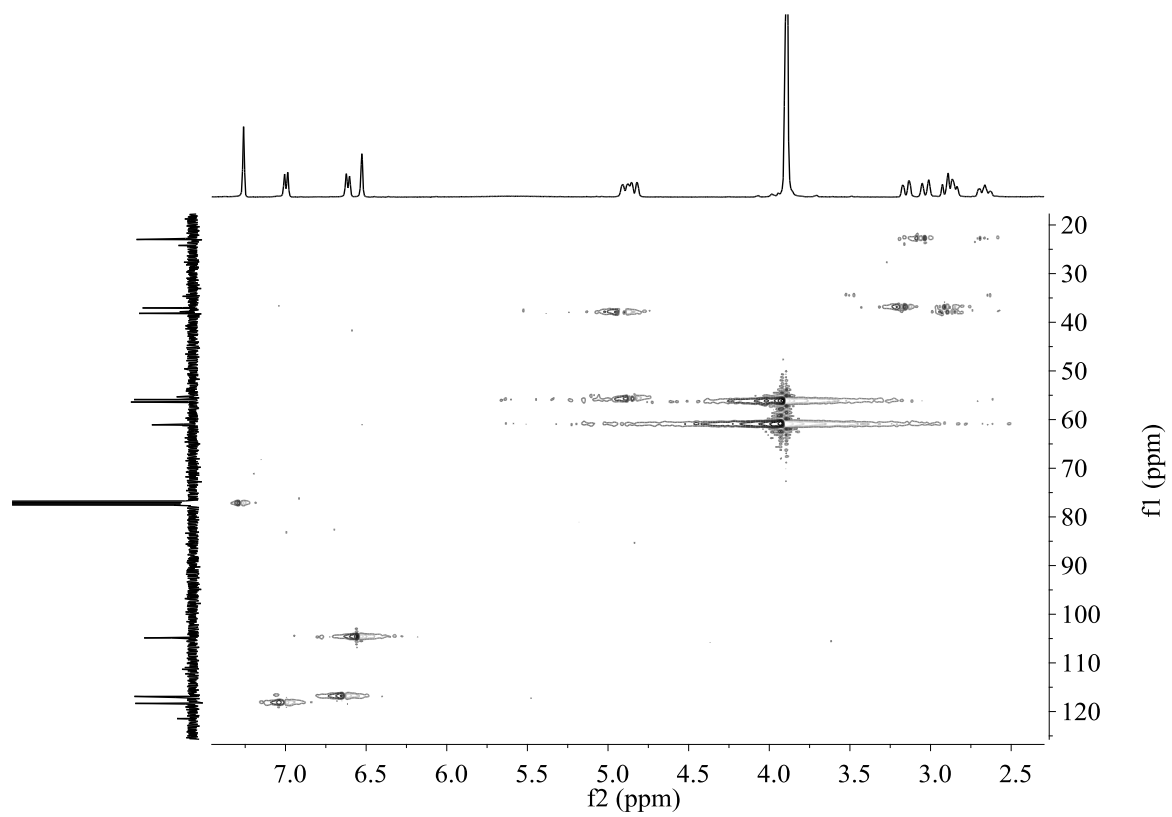
S25. <sup>1</sup>H NMR spectrum of compound **5** in CDCl<sub>3</sub> (400 MHz)



S26. <sup>13</sup>C NMR spectrum of compound **5** in CDCl<sub>3</sub> (100 MHz)

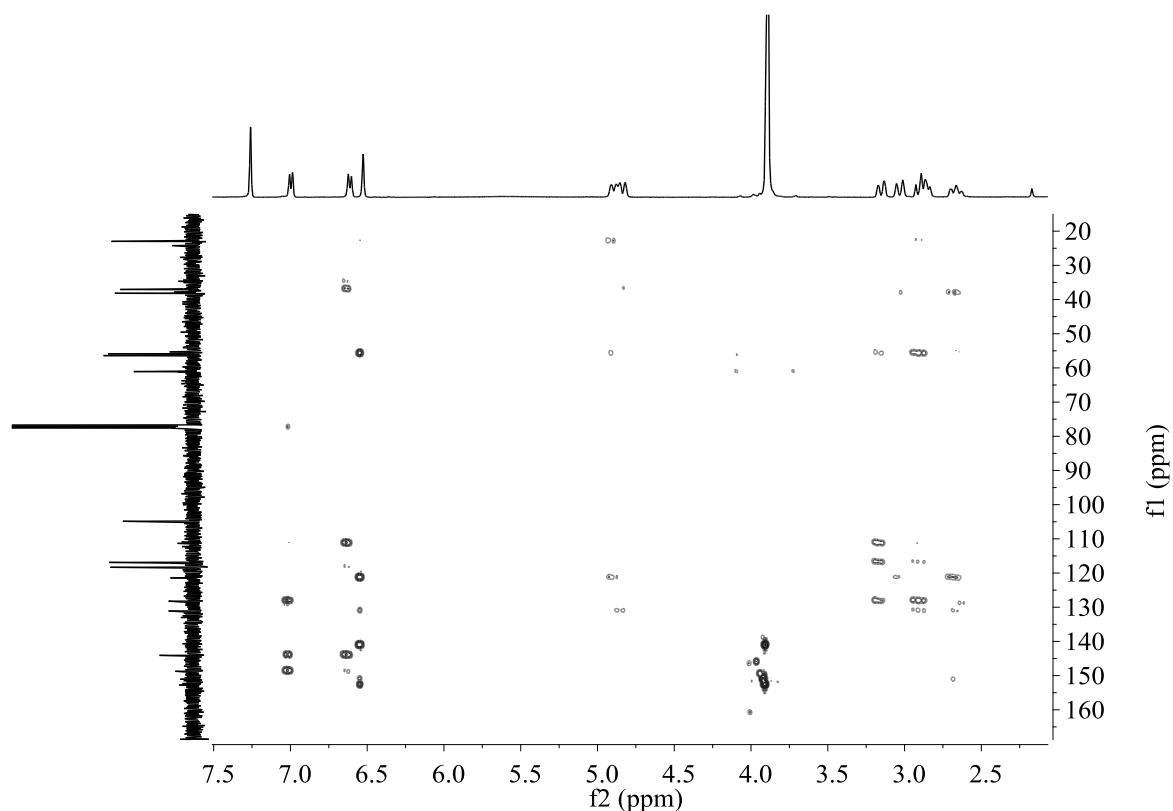


S27. COSY spectrum of compound **5** in  $\text{CDCl}_3$  (400 MHz)



S28. HMQC spectrum of compound **5** in  $\text{CDCl}_3$  (500 MHz)





S29. HMBC spectrum of compound **5** in CDCl<sub>3</sub> (400 MHz)

**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 8.0 PPM / DBE: min = -1.5, max = 120.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

979 formula(e) evaluated with 6 results within limits (up to 20 closest results for each mass)

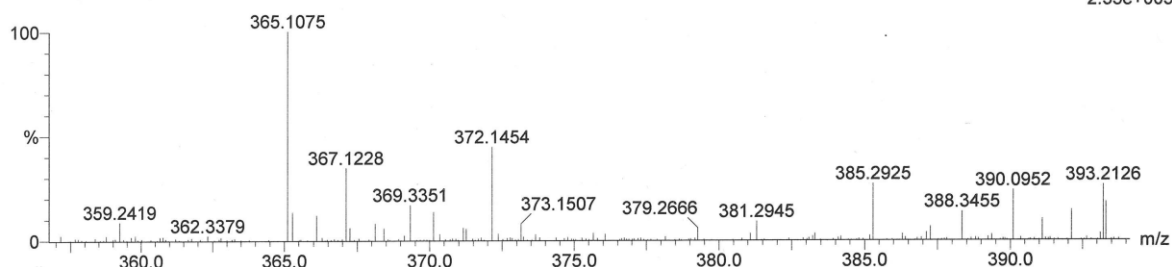
Elements Used:

C: 8-40 H: 0-70 N: 0-10 O: 0-12 Na: 0-1

MC 5

SP Thanaphat MC 5 54 (1.292) AM2 (Ar,8000.0,0.00,0.57); ABS; Cm (52:54)

1: TOF MS ES+  
2.35e+003



Minimum: -1.5  
Maximum: 5.0 8.0 120.0

| Mass     | Calc. Mass | mDa | PPM | DBE  | i-FIT | i-FIT (Norm) | Formula  |
|----------|------------|-----|-----|------|-------|--------------|--|
| 372.1454 | 372.1447   | 0.7 | 1.9 | 10.5 | 94.7  | 1.5          | C <sub>20</sub> H <sub>22</sub> N O <sub>6</sub> |

S30. HRESI-MS spectrum of compound **5**