

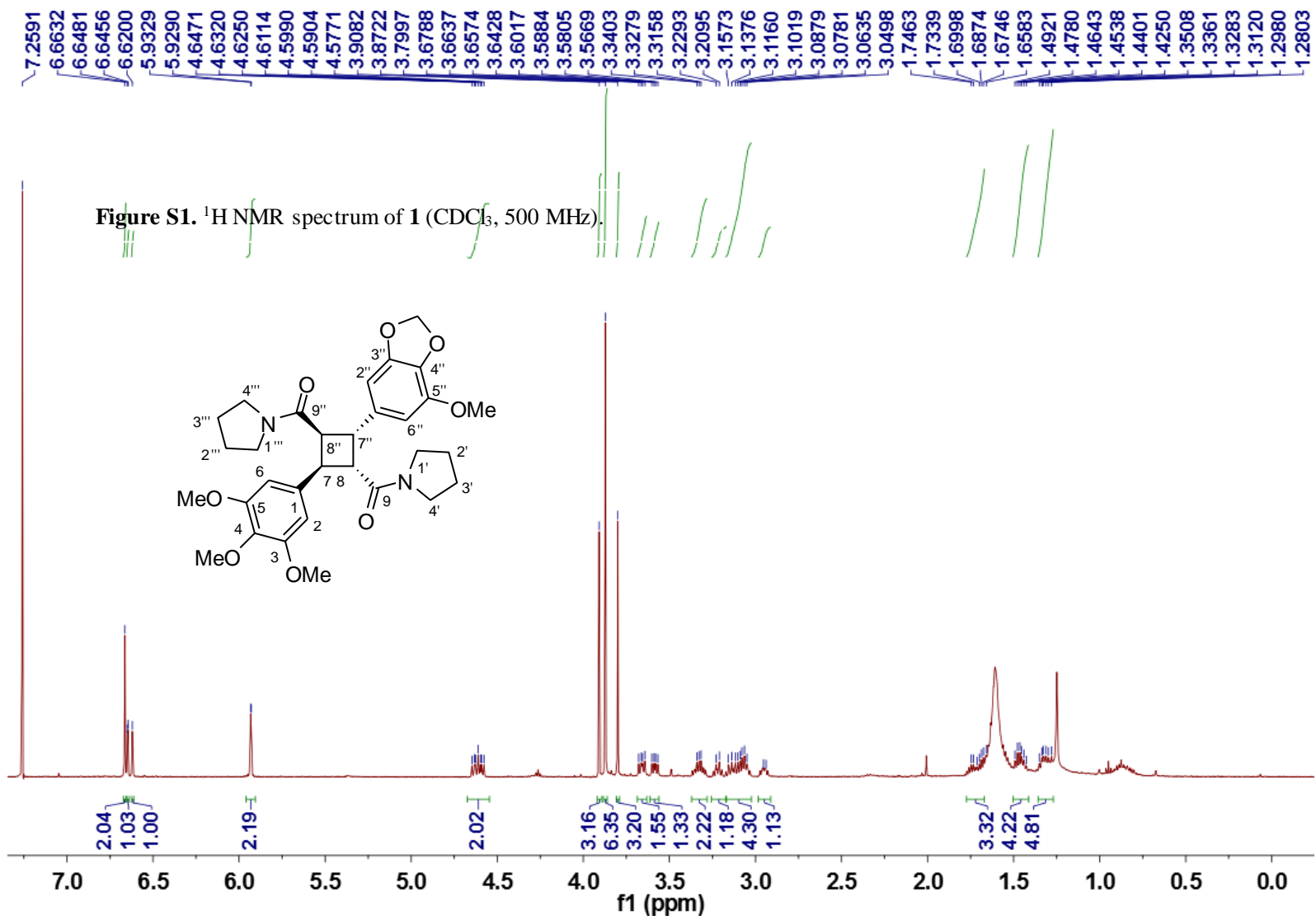
# 支持信息

## 蒟子的化学成分研究

### 目录

<b>Figure S1.</b> $^1\text{H}$ NMR spectrum of <b>1</b> ( $\text{CDCl}_3$ , 500 MHz).
<b>Figure S2.</b> $^{13}\text{C}$ NMR spectrum of <b>1</b> ( $\text{CDCl}_3$ , 126 MHz).
<b>Figure S3.</b> HSQC spectrum of <b>1</b> .
<b>Figure S4.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of <b>1</b> .
<b>Figure S5.</b> HMBC spectrum of <b>1</b> .
<b>Figure S6.</b> ROESY spectrum of <b>1</b> .
<b>Figure S7.</b> EI-MS spectrum of <b>1</b> .
<b>Figure S8.</b> HR-EI-MS spectrum of <b>1</b> .
<b>Figure S9.</b> $^1\text{H}$ NMR spectrum of <b>2</b> ( $\text{CDCl}_3$ , 500 MHz).
<b>Figure S10.</b> $^{13}\text{C}$ NMR spectrum of <b>2</b> ( $\text{CDCl}_3$ , 126 MHz).
<b>Figure S11.</b> HSQC spectrum of <b>2</b> .
<b>Figure S12.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of <b>2</b> .
<b>Figure S13.</b> HMBC spectrum of <b>2</b> .
<b>Figure S14.</b> ROESY spectrum of <b>2</b> .
<b>Figure S15.</b> EI-MS spectrum of <b>2</b> .
<b>Figure S16.</b> HR-EI-MS spectrum of <b>2</b> .
<b>Figure S17.</b> $^1\text{H}$ NMR spectrum of <b>3</b> ( $\text{CDCl}_3$ , 500 MHz).
<b>Figure S18.</b> $^{13}\text{C}$ NMR spectrum of <b>3</b> ( $\text{CDCl}_3$ , 126 MHz).
<b>Figure S19.</b> HSQC spectrum of <b>3</b> .
<b>Figure S20.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of <b>3</b> .
<b>Figure S21.</b> HMBC spectrum of <b>3</b> .
<b>Figure S22.</b> ROESY spectrum of <b>3</b> .
<b>Figure S23.</b> EI-MS spectrum of <b>3</b> .
<b>Figure S24.</b> HR-EI-MS spectrum of <b>3</b> .
<b>Figure S25.</b> $^1\text{H}$ NMR spectrum of <b>4</b> ( $\text{CDCl}_3$ , 500 MHz).
<b>Figure S26.</b> $^{13}\text{C}$ NMR spectrum of <b>4</b> ( $\text{CDCl}_3$ , 126 MHz).

<b>Figure S27.</b> HSQC spectrum of <b>4</b> .
<b>Figure S28.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of <b>4</b> .
<b>Figure S29.</b> HMBC spectrum of <b>4</b> .
<b>Figure S30.</b> ROESY spectrum of <b>4</b> .
<b>Figure S31.</b> EI-MS spectrum of <b>4</b> .
<b>Figure S32.</b> HR-EI-MS spectrum of <b>4</b> .



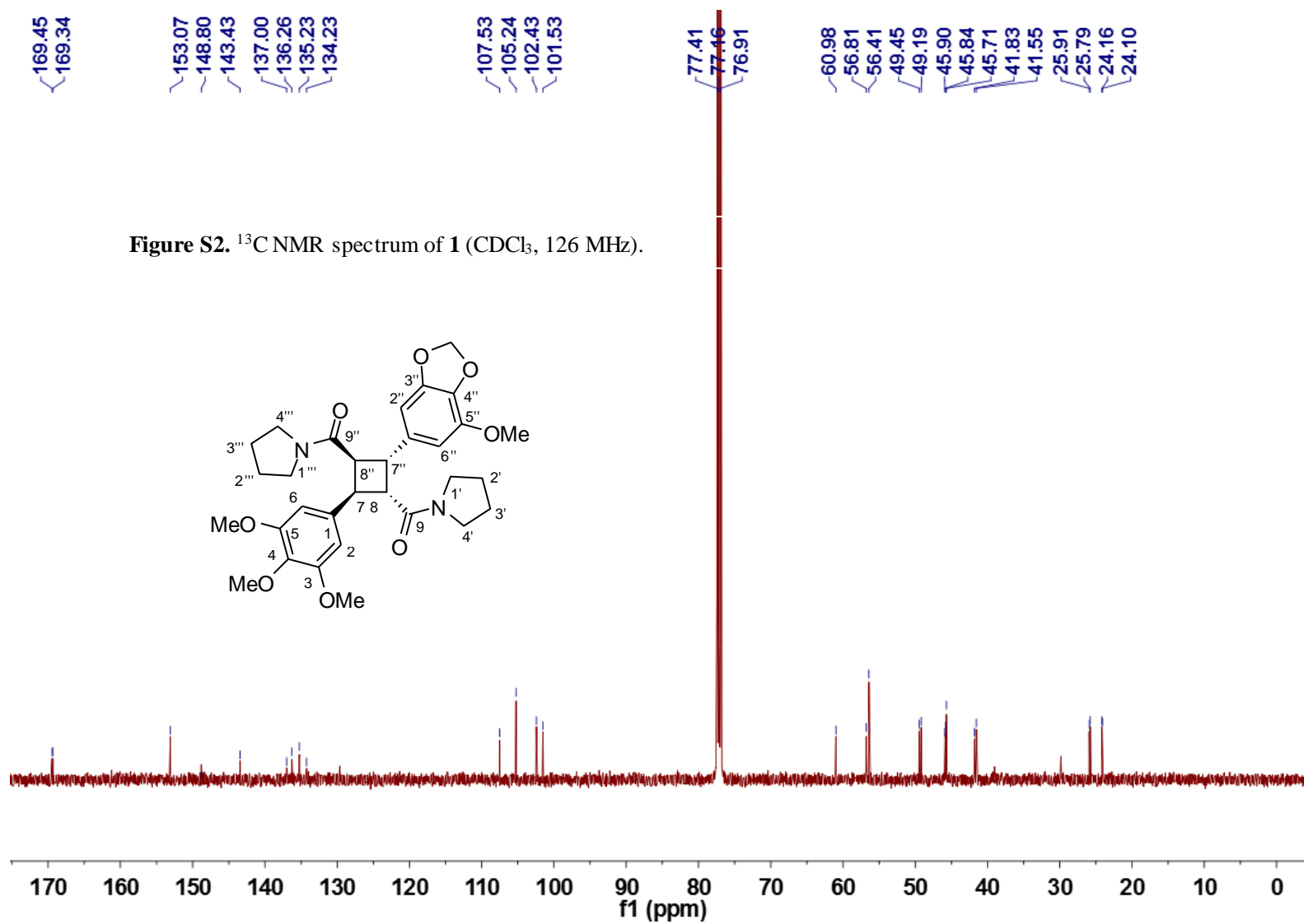


Figure S3. HSQC spectrum of 1.

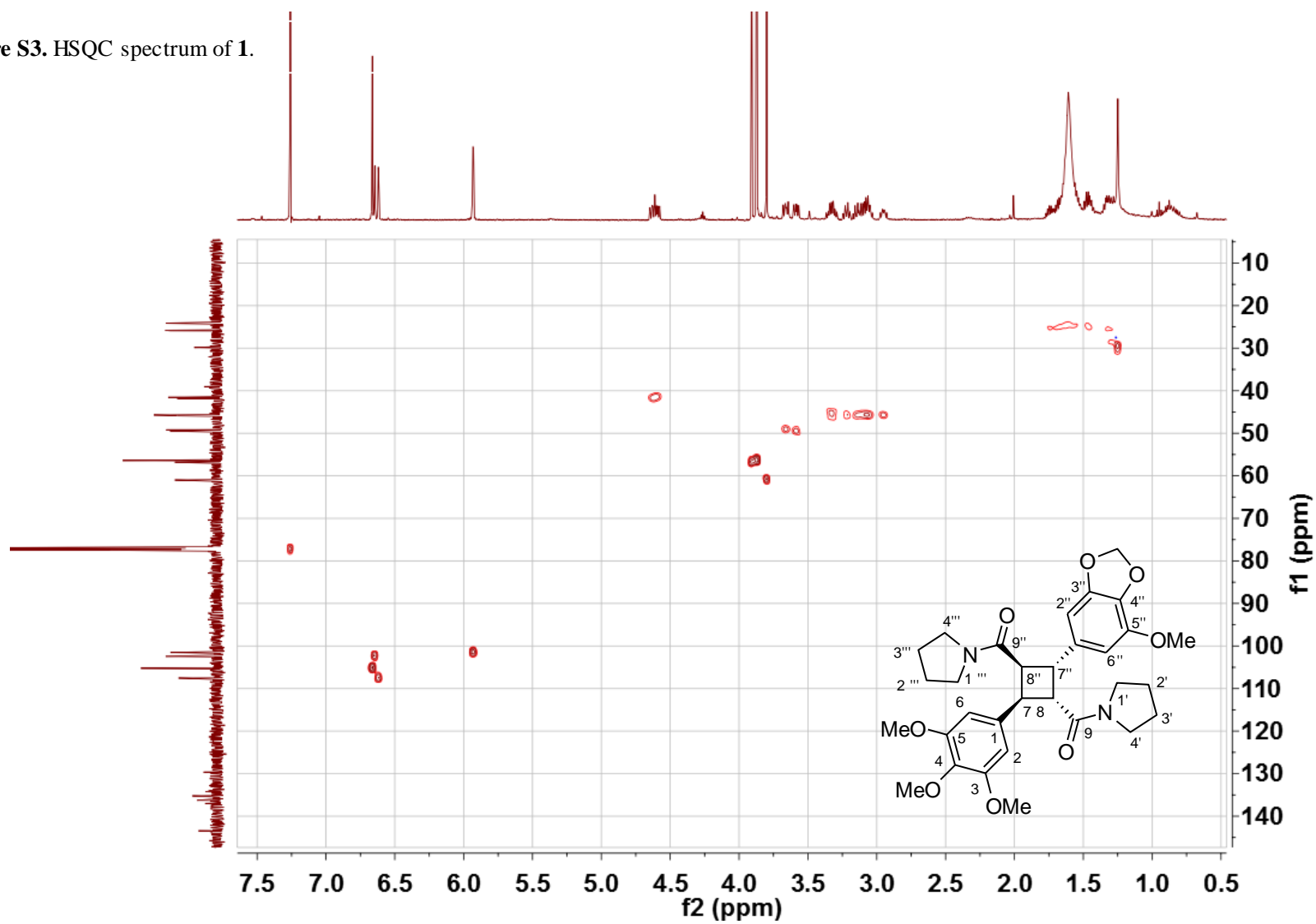


Figure S4.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1**.

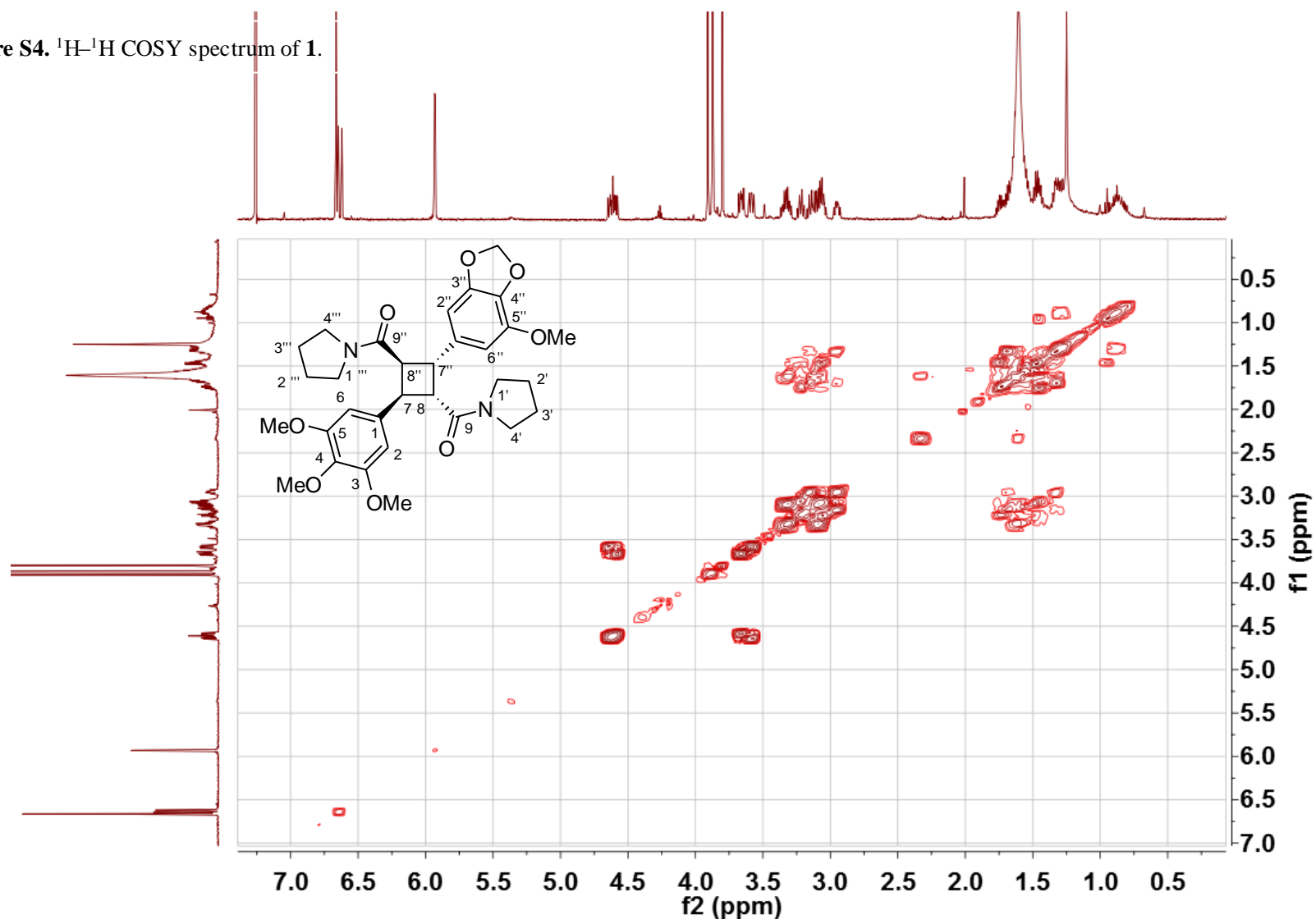


Figure S5. HMBC spectrum of **1**.

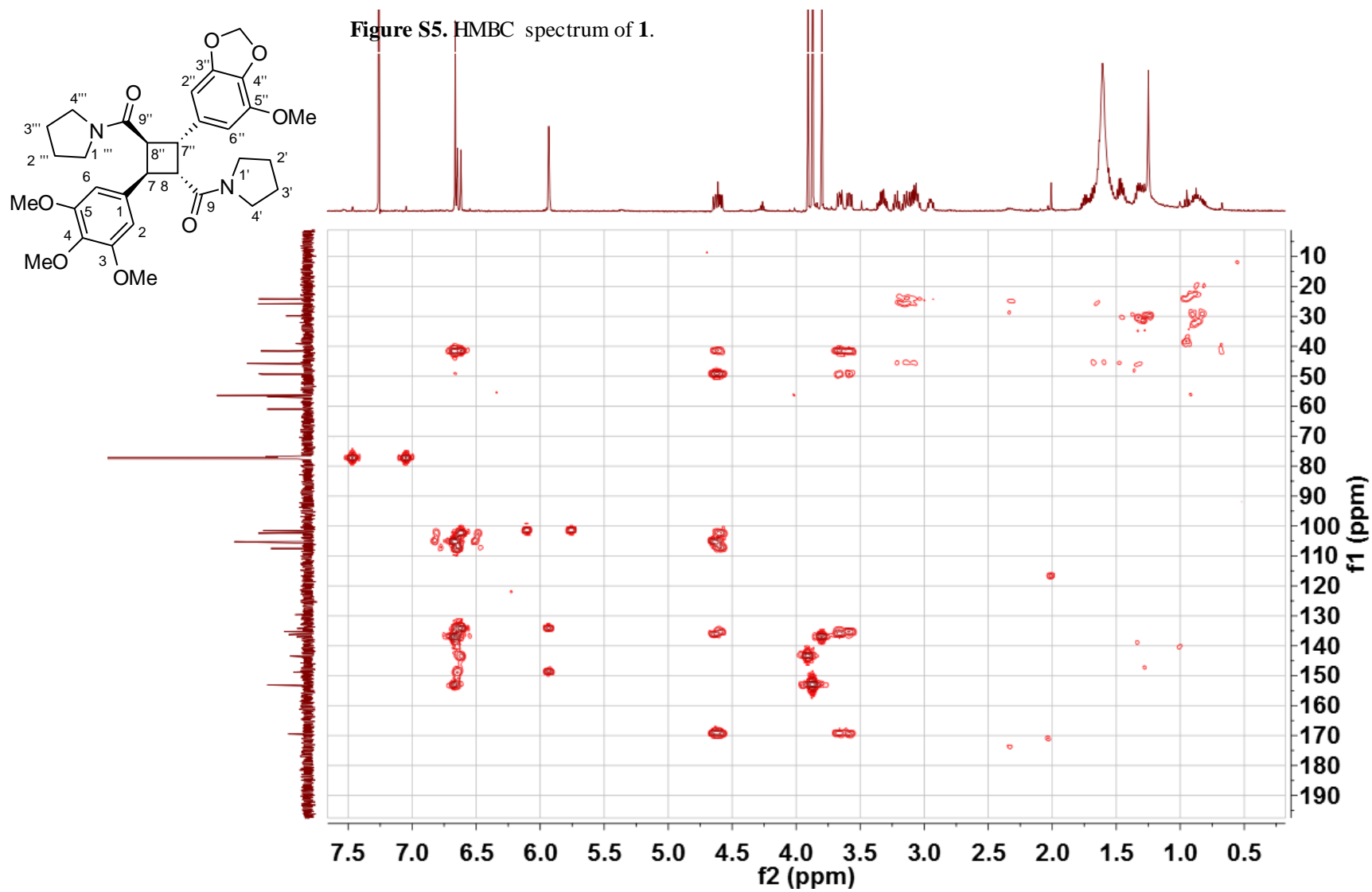
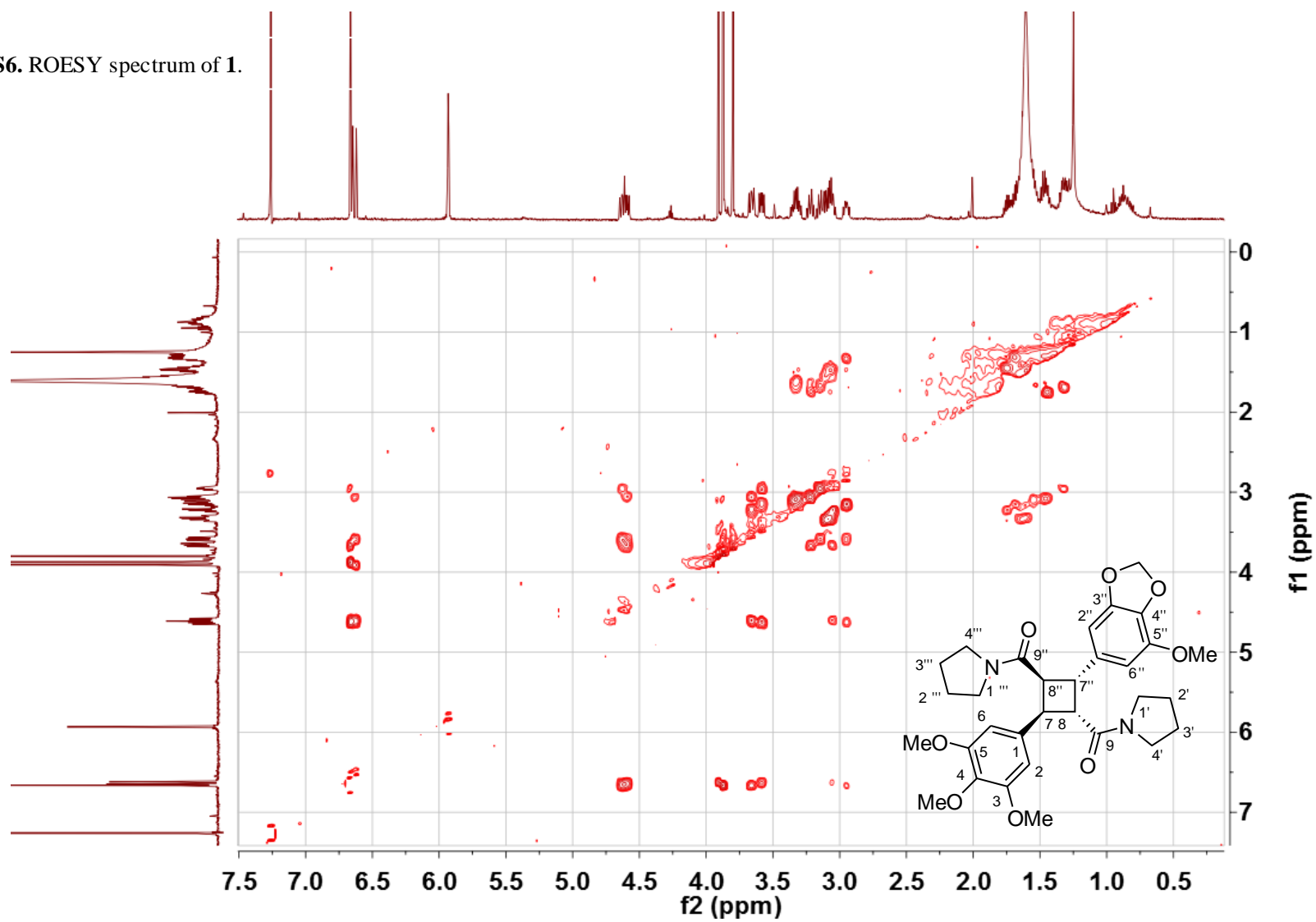


Figure S6. ROESY spectrum of 1.





pcp26

13:49:43 04-May-2015

M150504E-09 15 (1.103) Cn (Top,2, Ht); Cm (15-4:14)

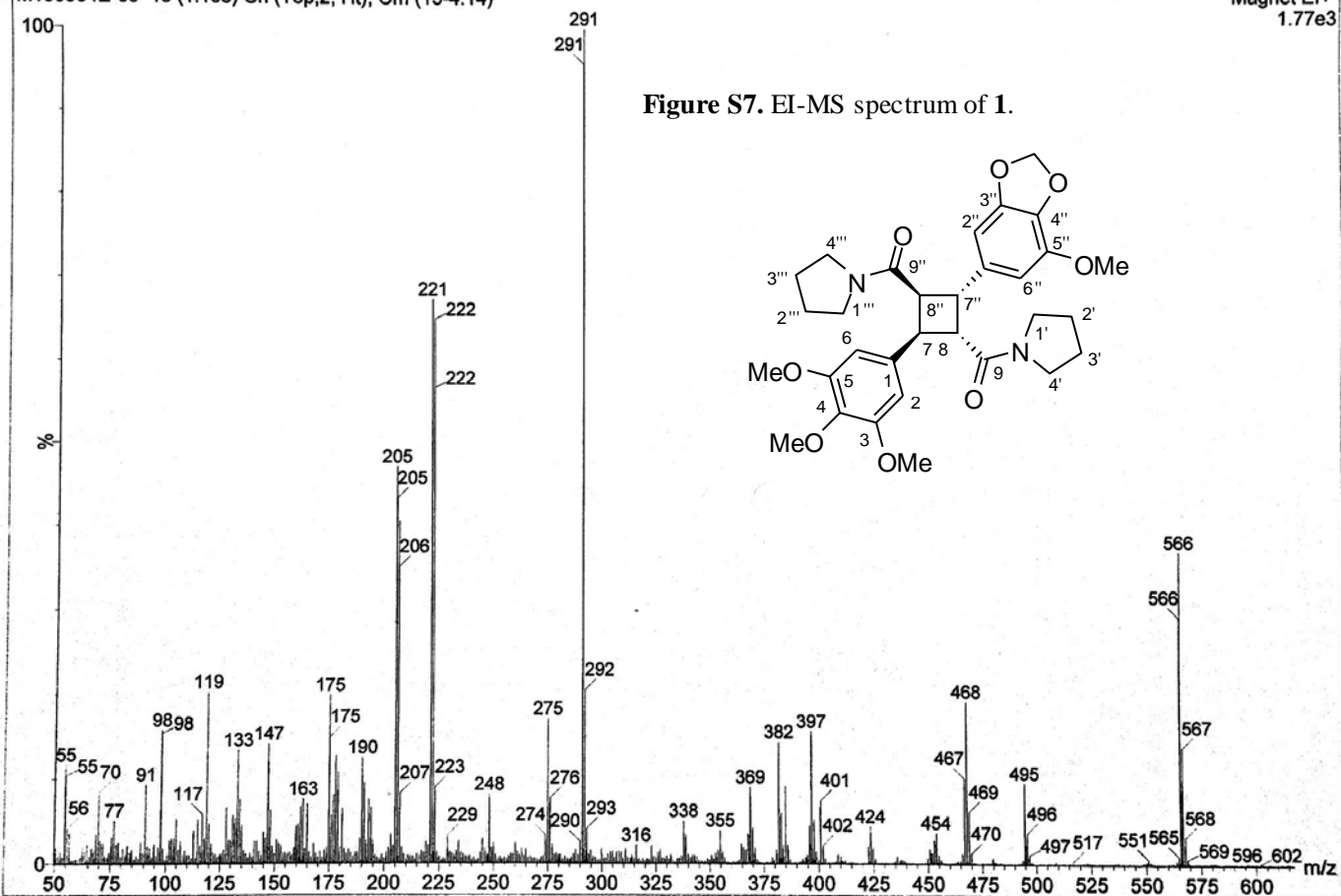
KIB

Autospec Premier

P776

Magnet EI+

1.77e3



## Elemental Composition Report

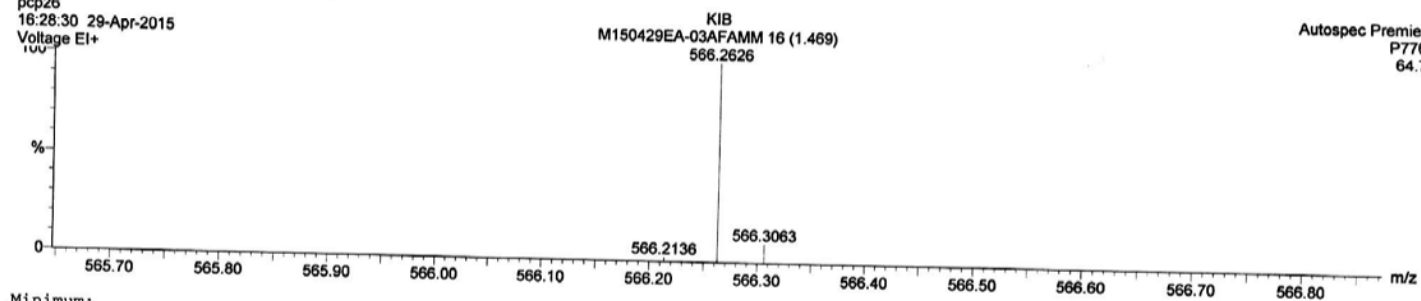
### Single Mass Analysis

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21 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)  
Elements Used:

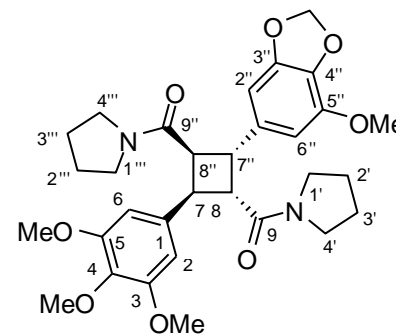
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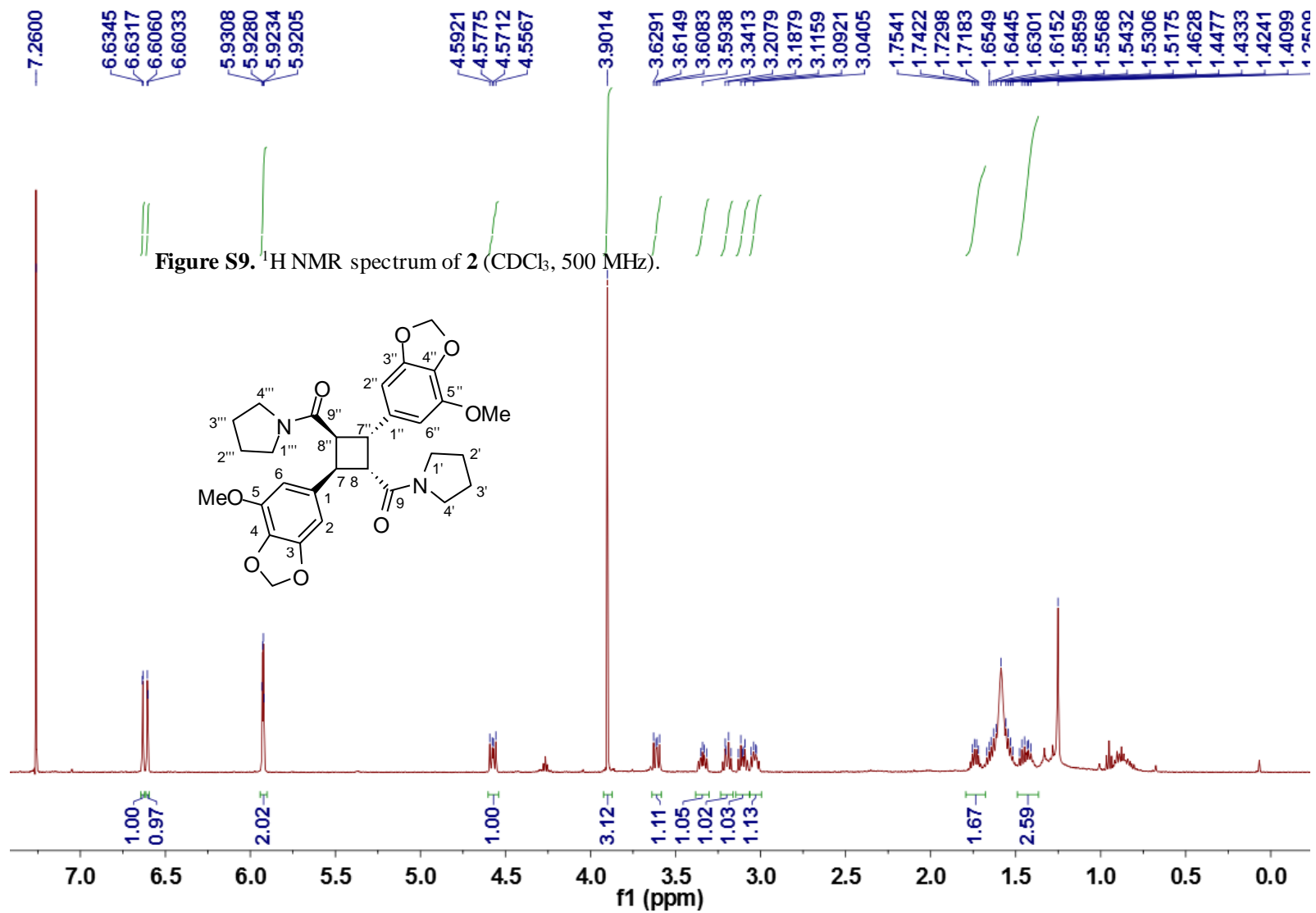
pcp26  
16:28:30 29-Apr-2015  
Voltage EI+



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Figure S8. HR-EI-MS spectrum of **1**.





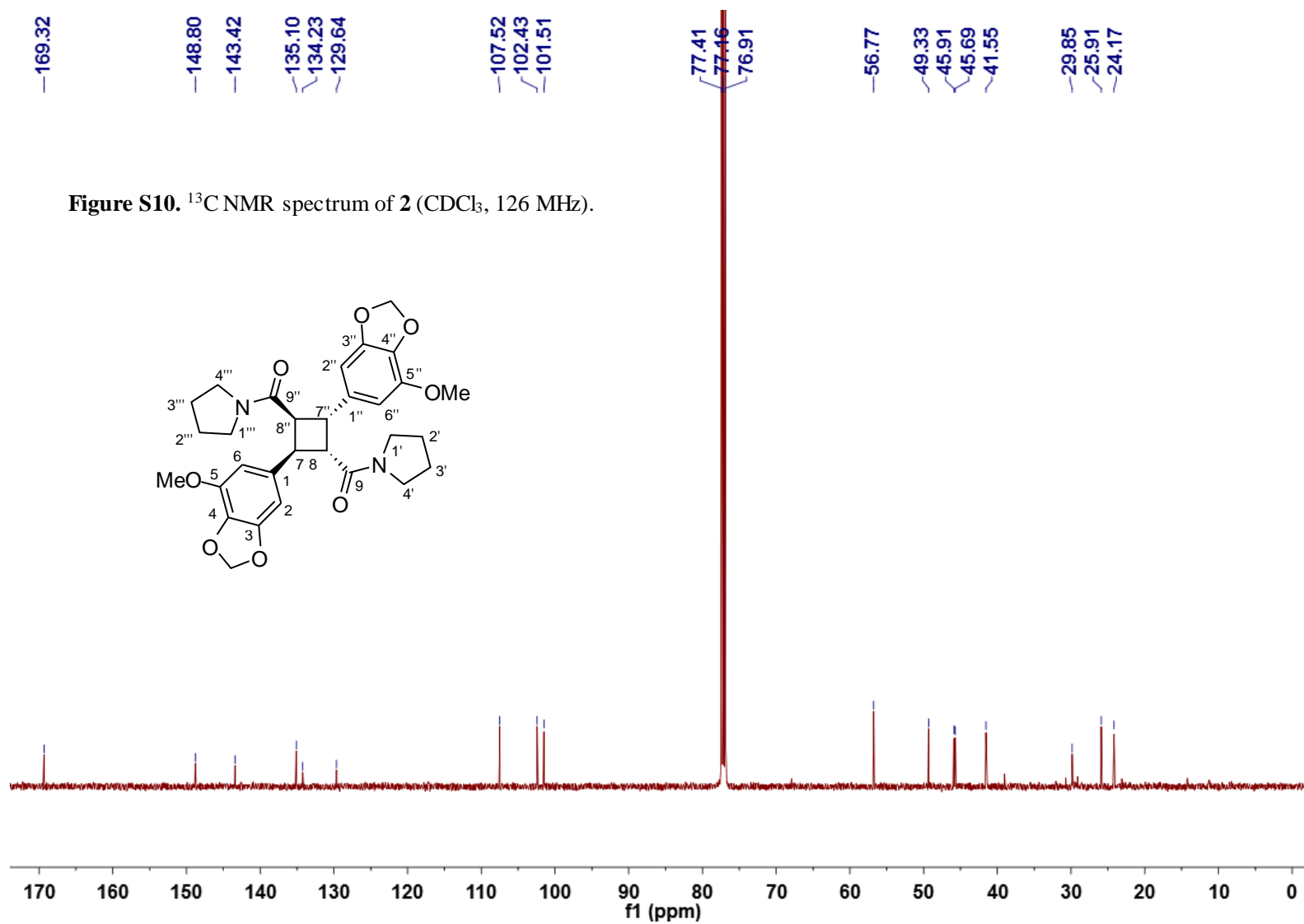


Figure S11. HSQC spectrum of **2**.

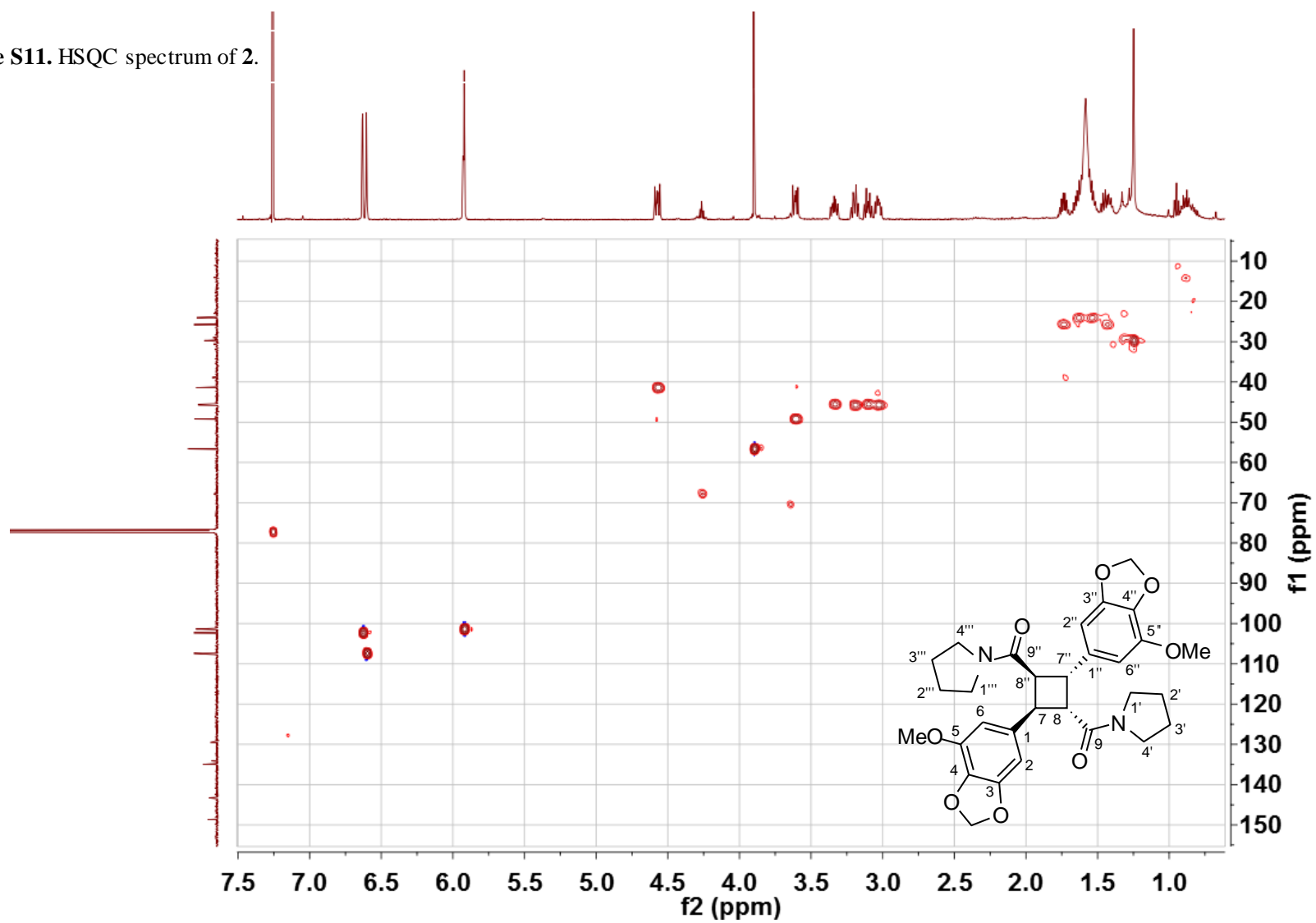
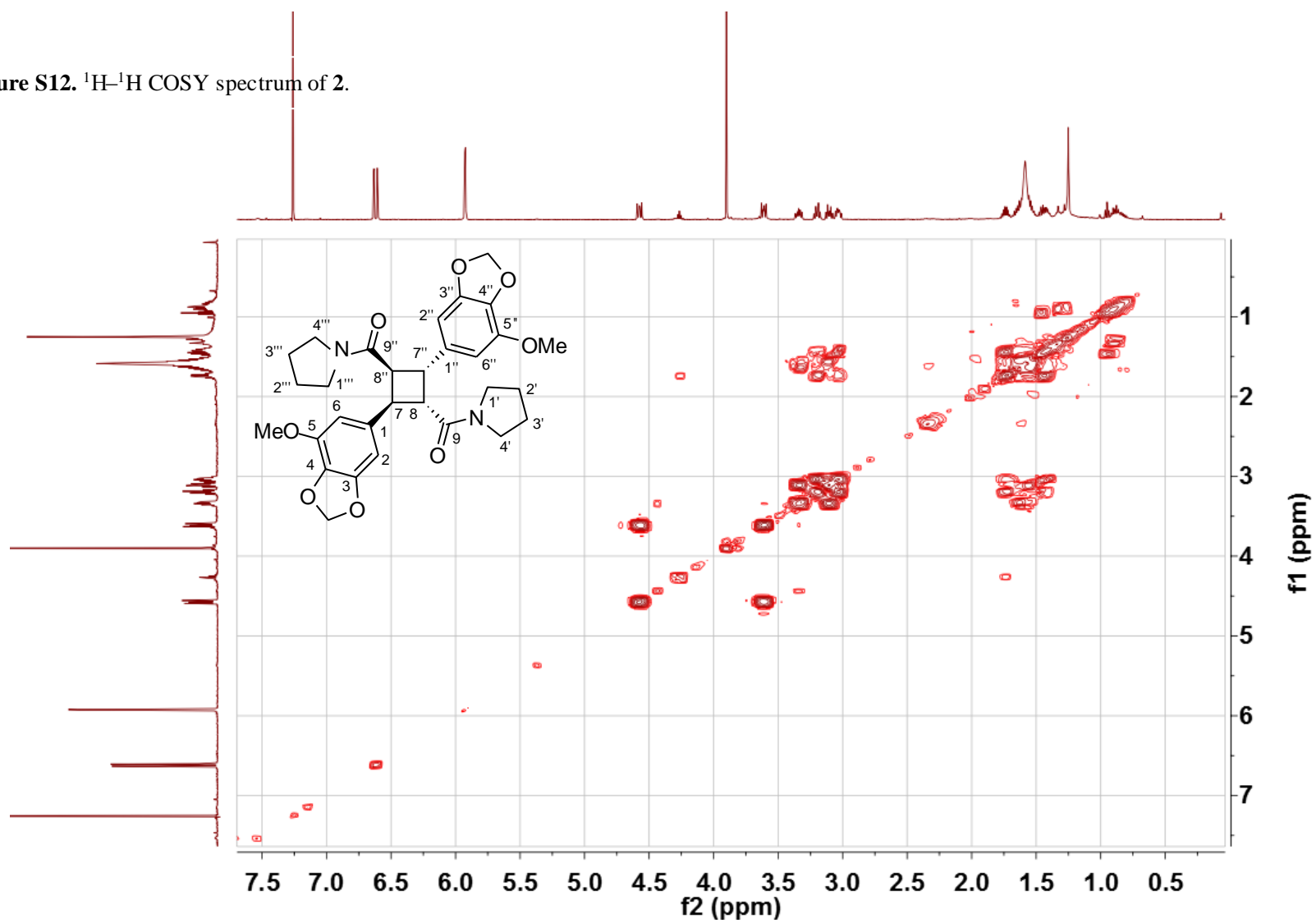


Figure S12.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2**.



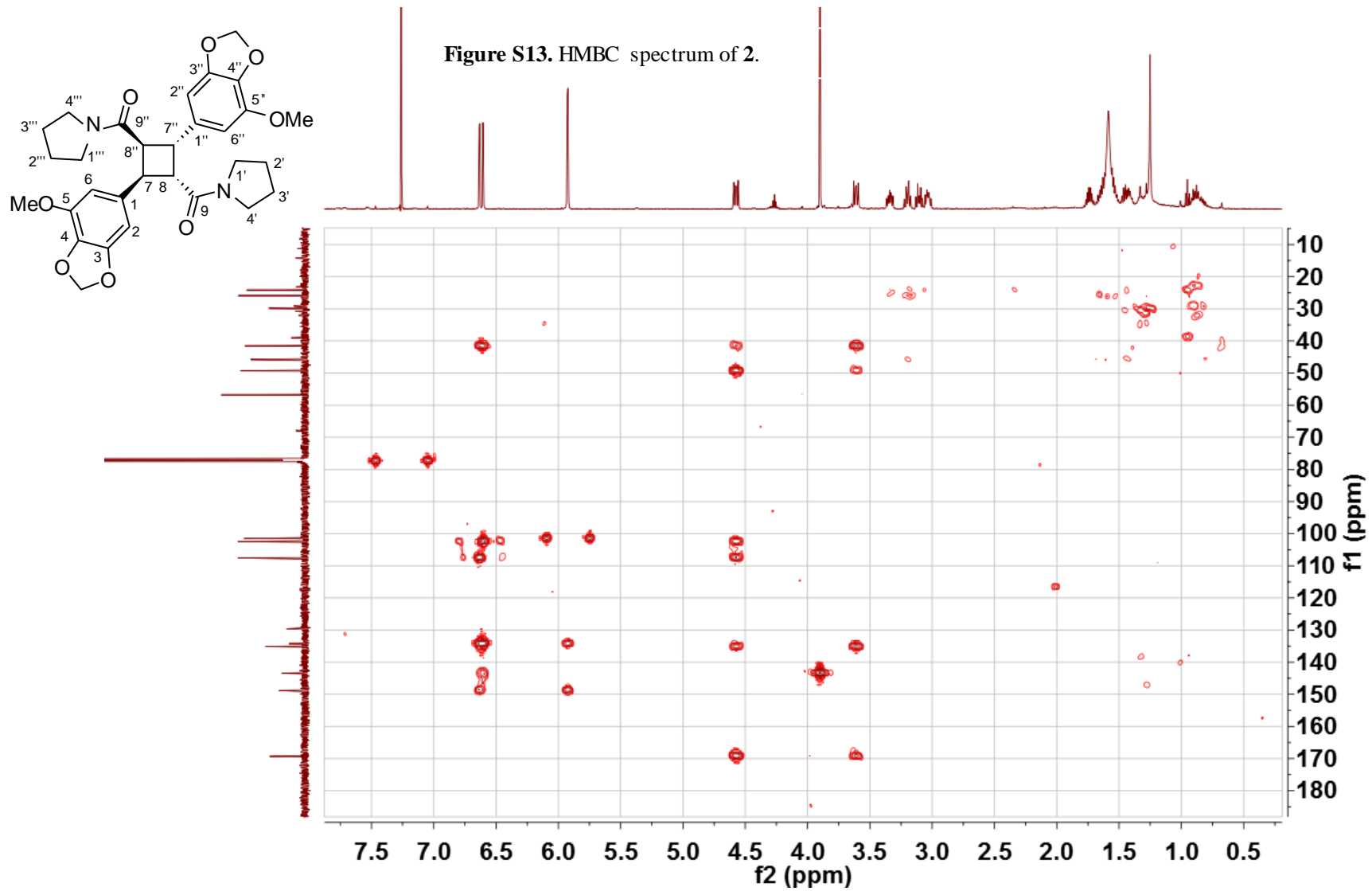
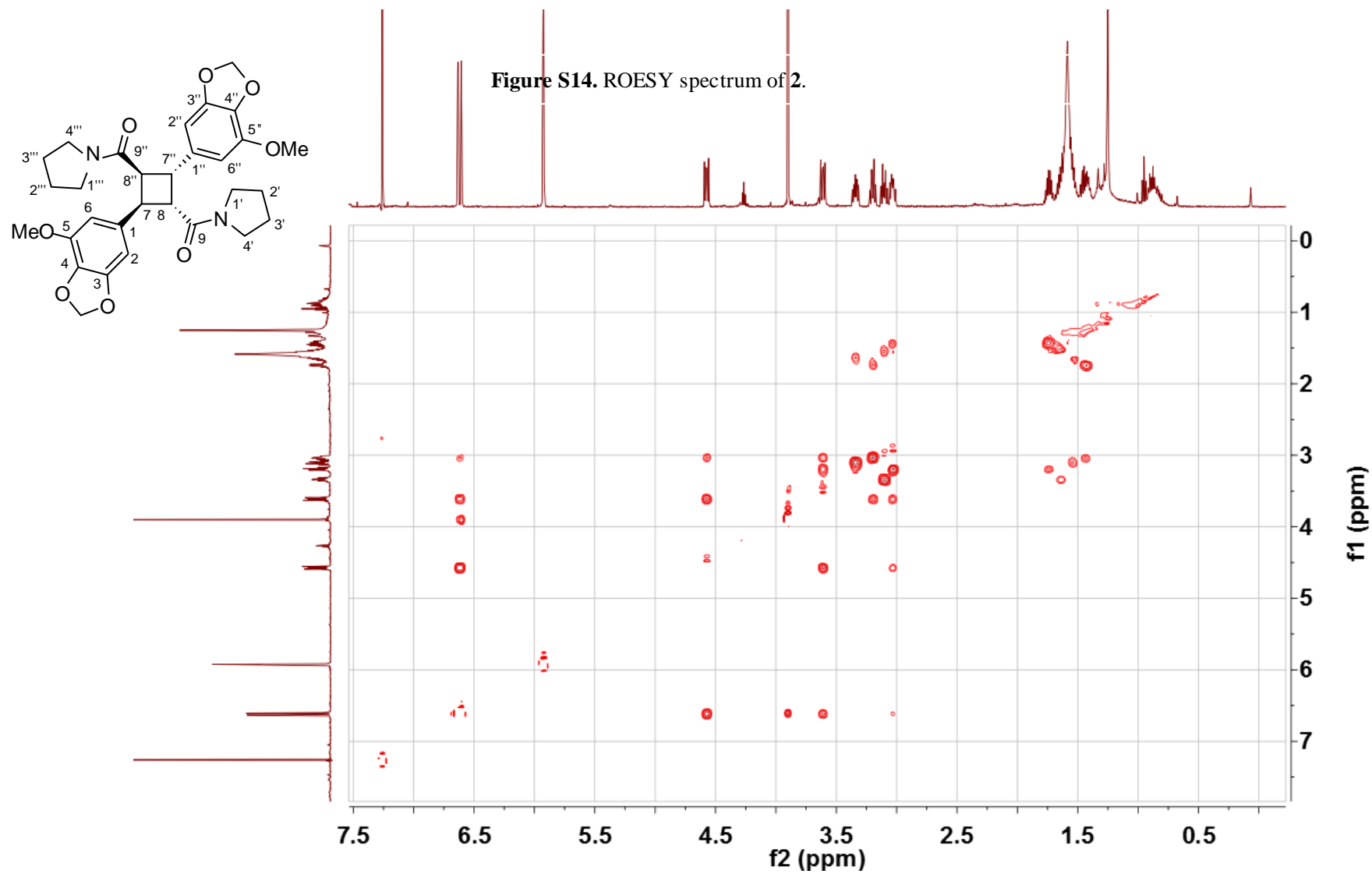


Figure S14. ROESY spectrum of 2.

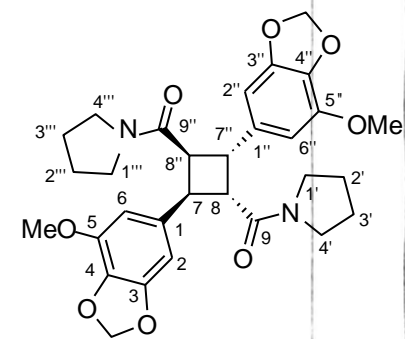
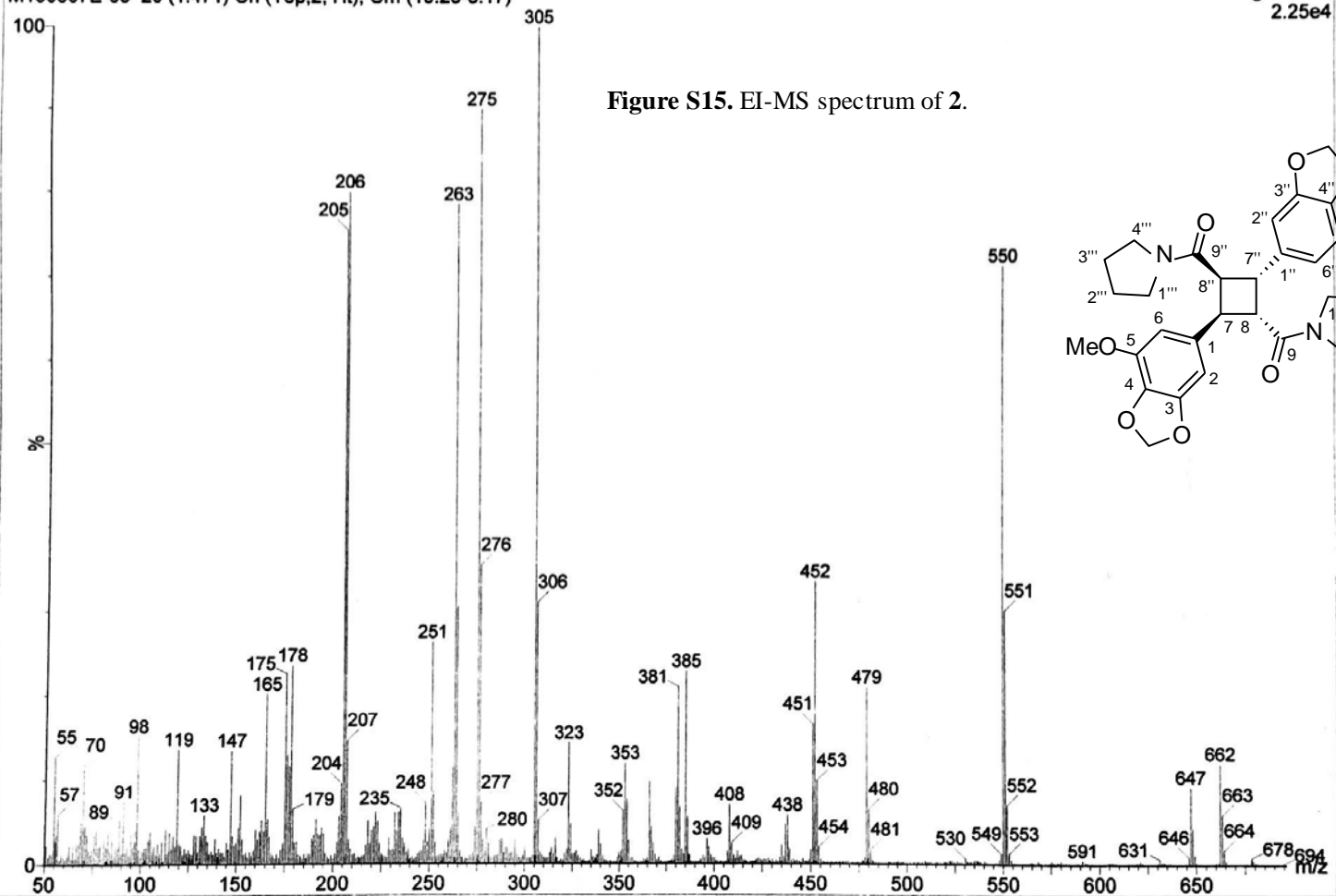




pcp27  
11:00:10 07-May-2015  
M150507E-03 20 (1.471) Cn (Top,2, Ht); Cm (19:23-3:17)

KIB

Autospec Premier  
P776  
Magnet EI+  
2.25e4



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

21 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

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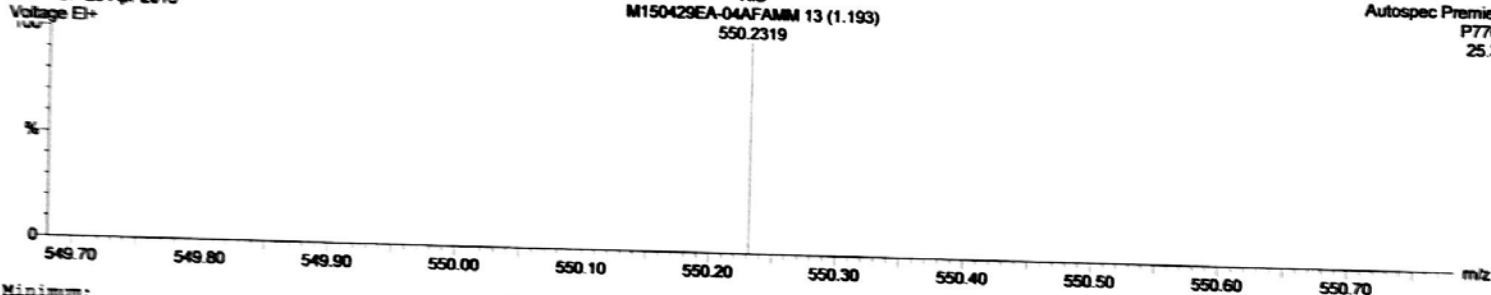
pcp27

16:32:27 29-Apr-2015

Voltage EI+

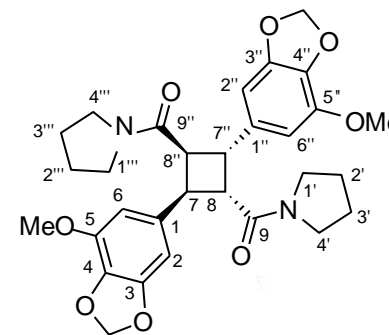
K18  
M150429EA-04AFAMM 13 (1.193)  
550.2319

Autospec Premier  
P776  
25.3



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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Figure S16. HR-EI-MS spectrum of 2.



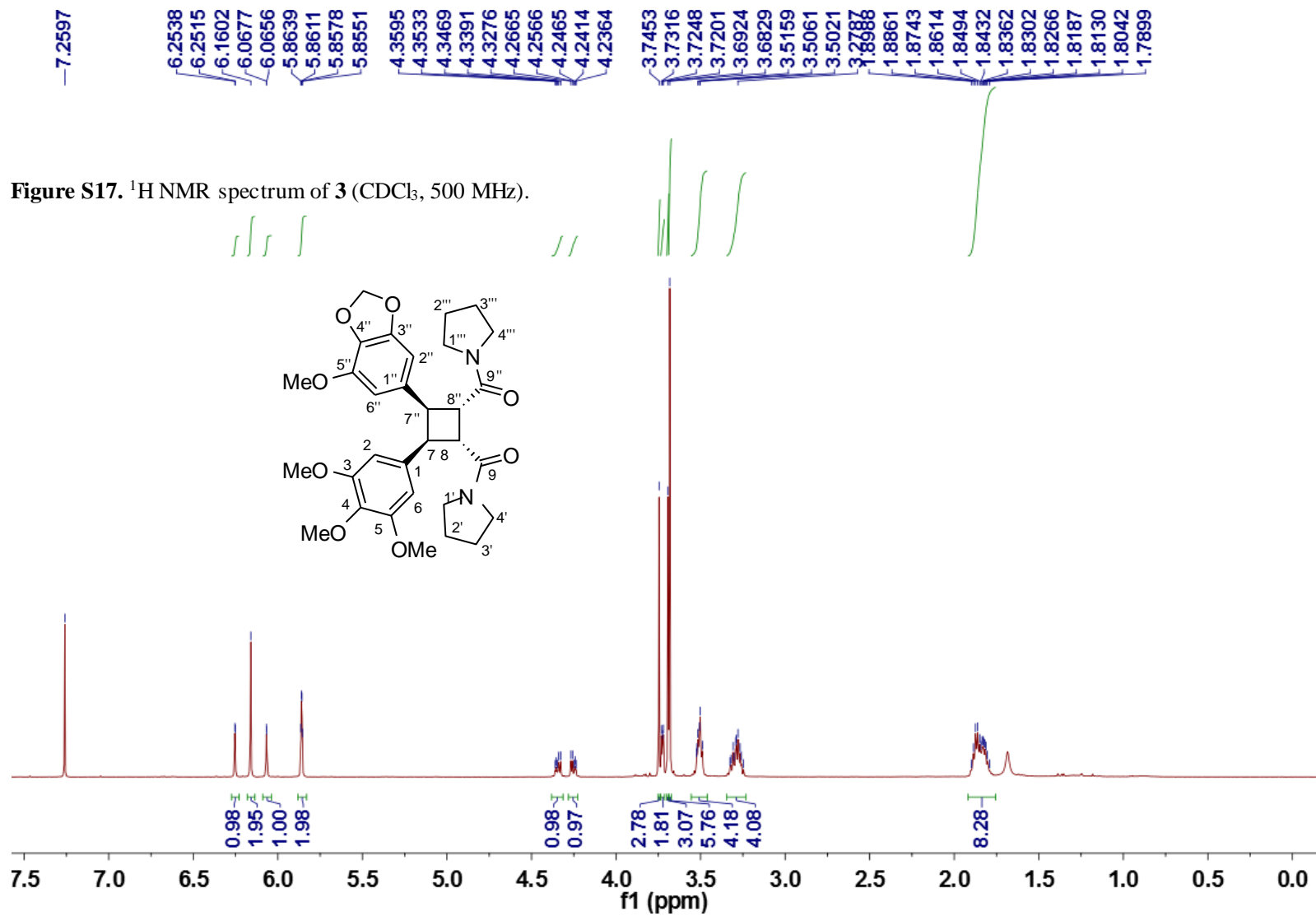




Figure S18.  $^{13}\text{C}$  NMR spectrum of **3** ( $\text{CDCl}_3$ , 126 MHz).

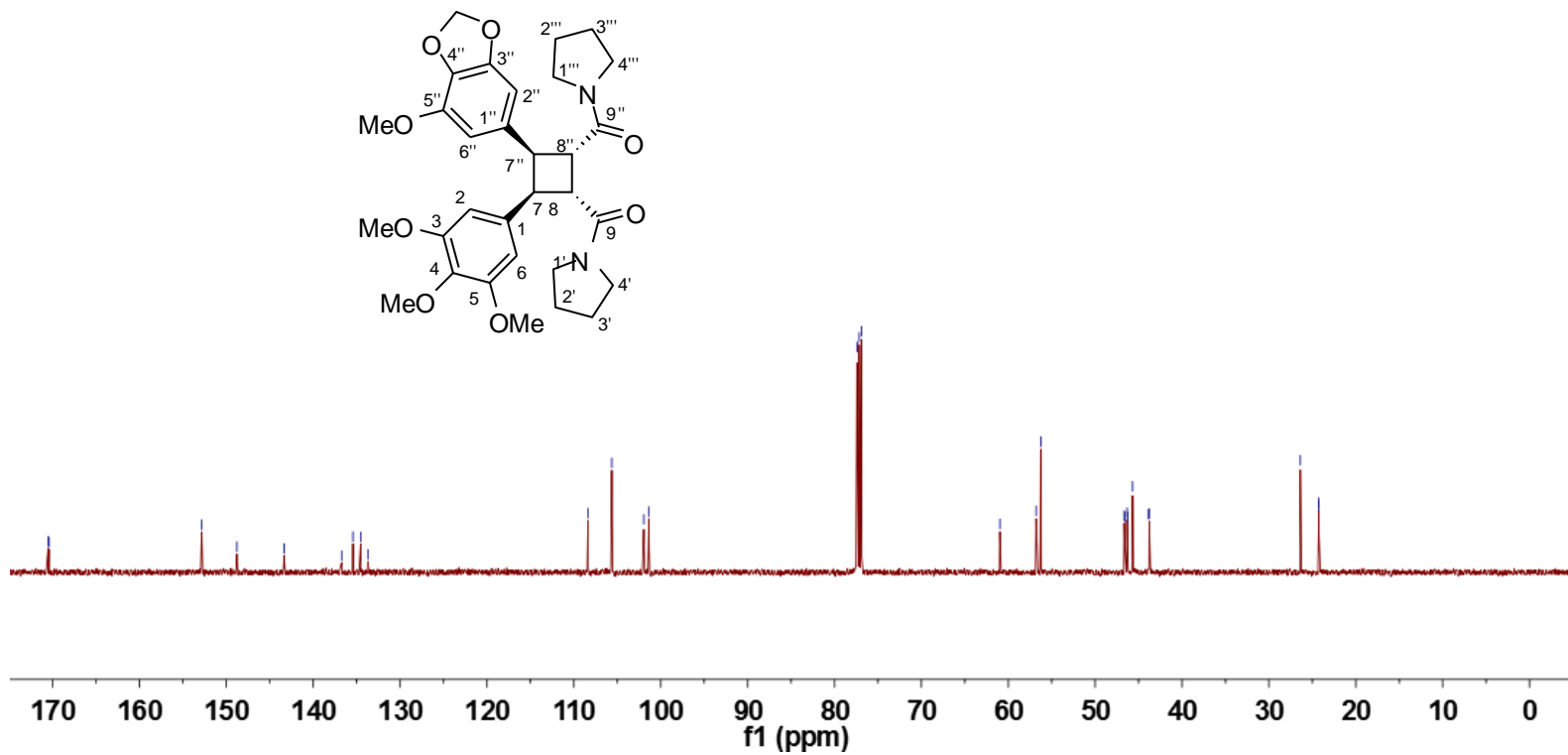


Figure S19. HSQC spectrum of 3.

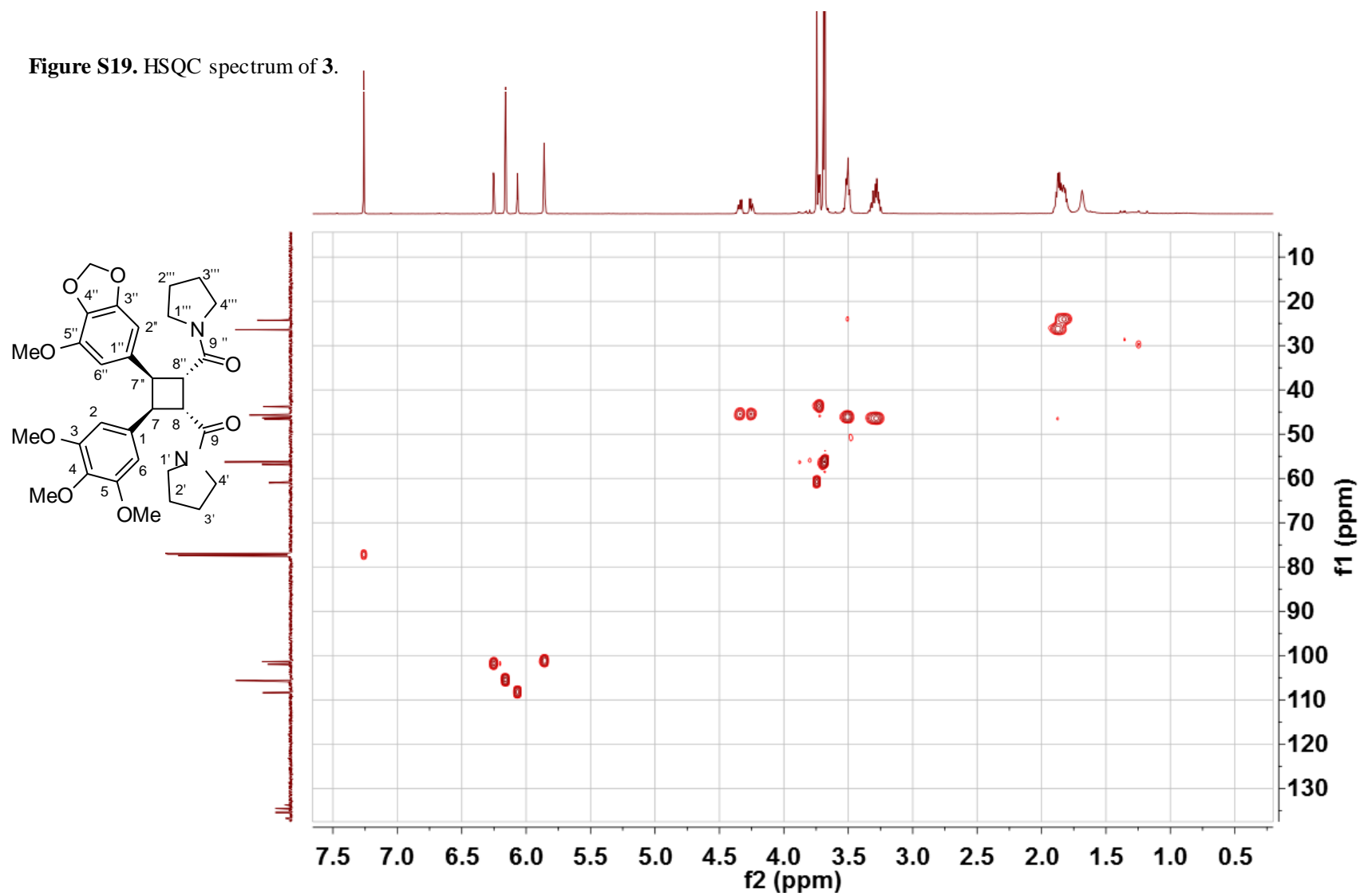


Figure S20.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **3**.

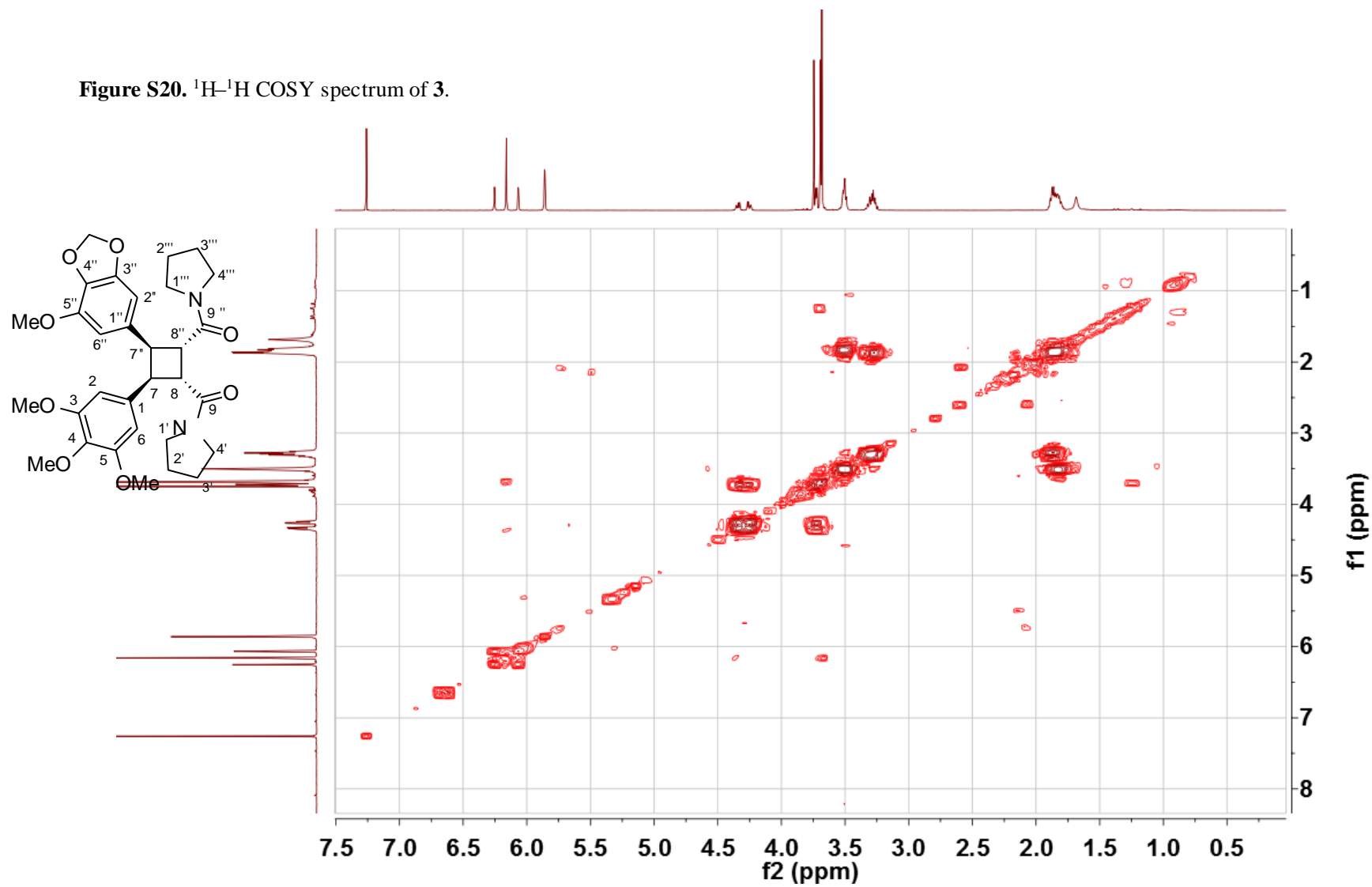


Figure S21. HMBC spectrum of 3.

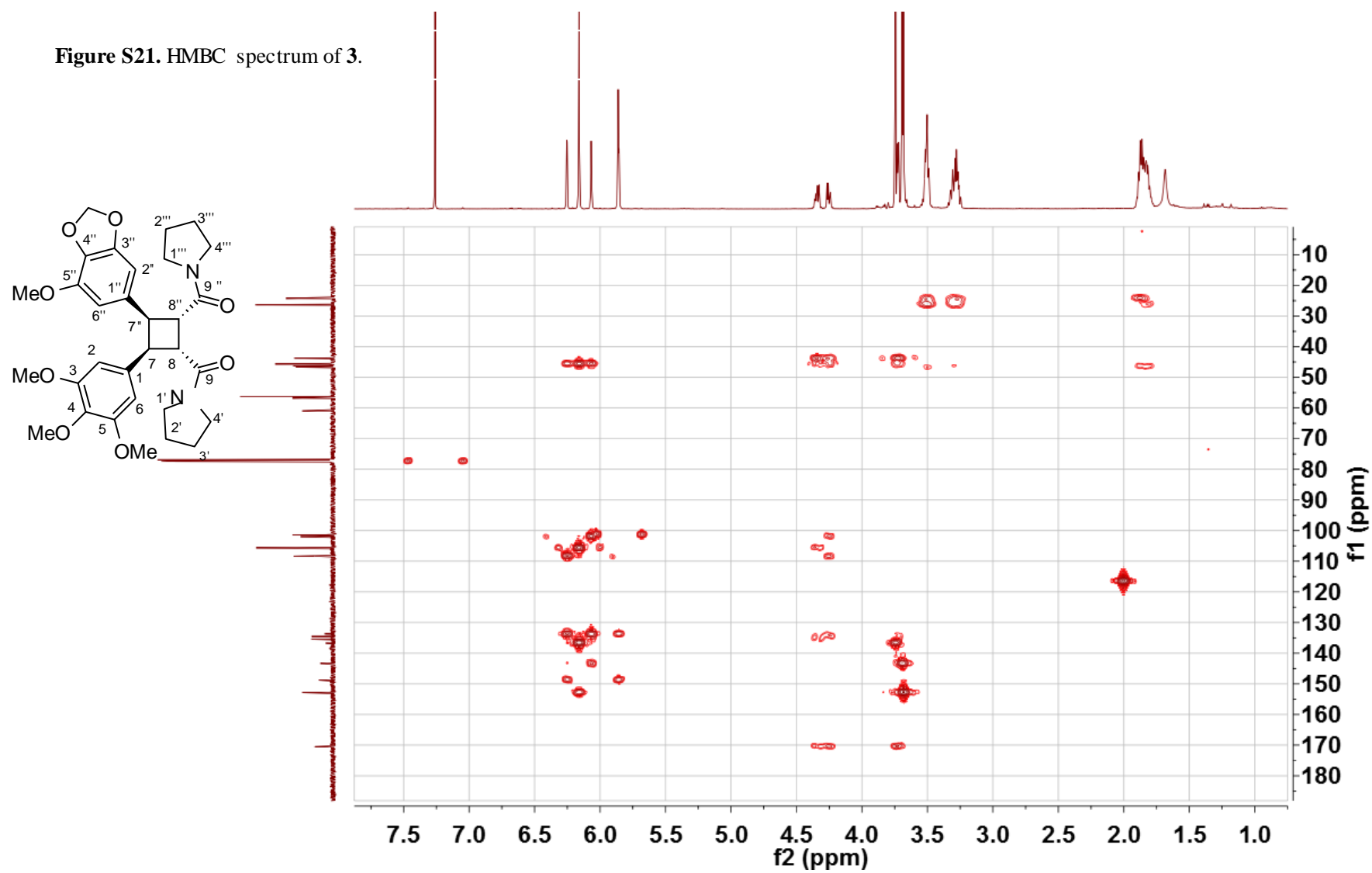


Figure S22. ROESY spectrum of **3**.

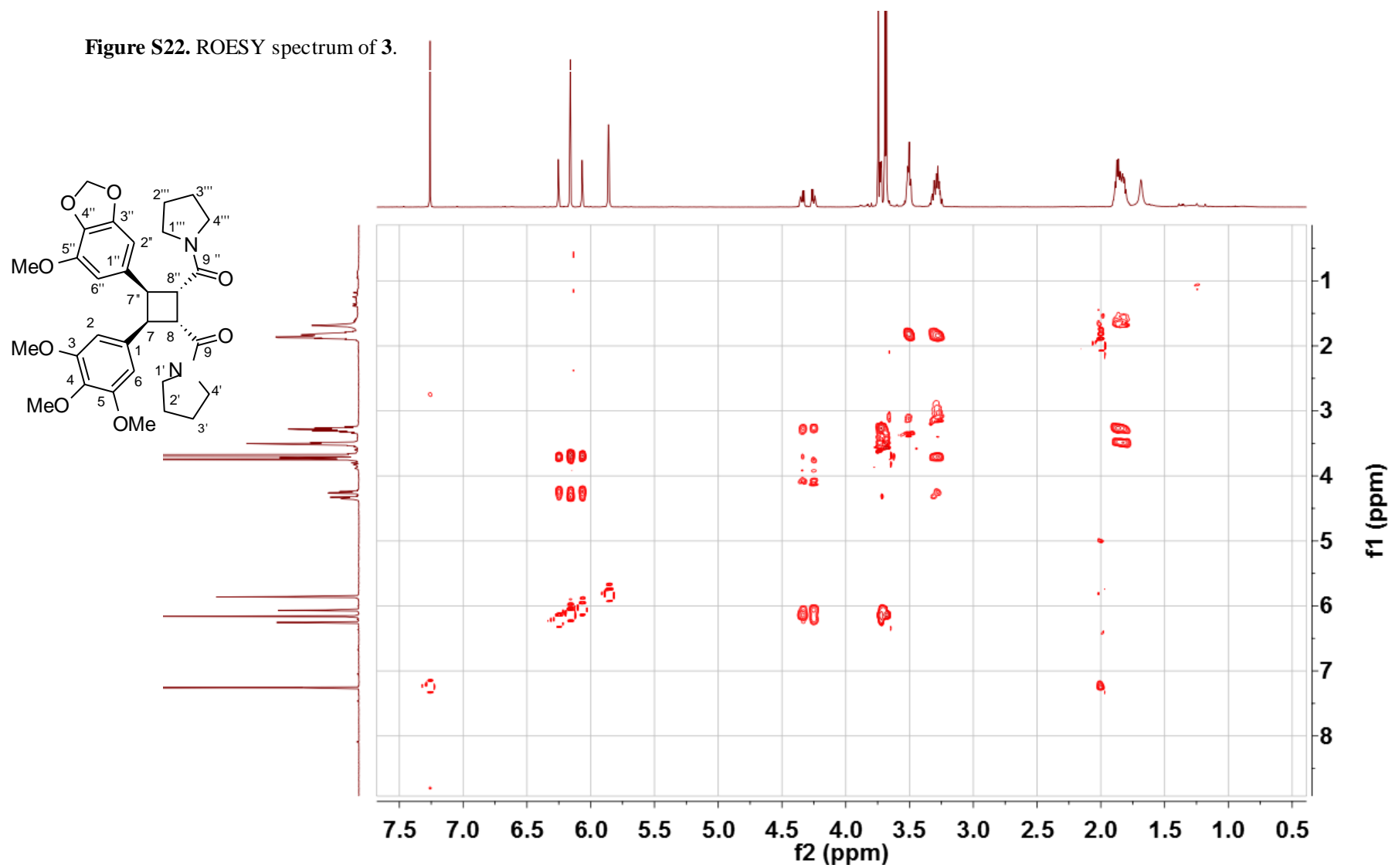
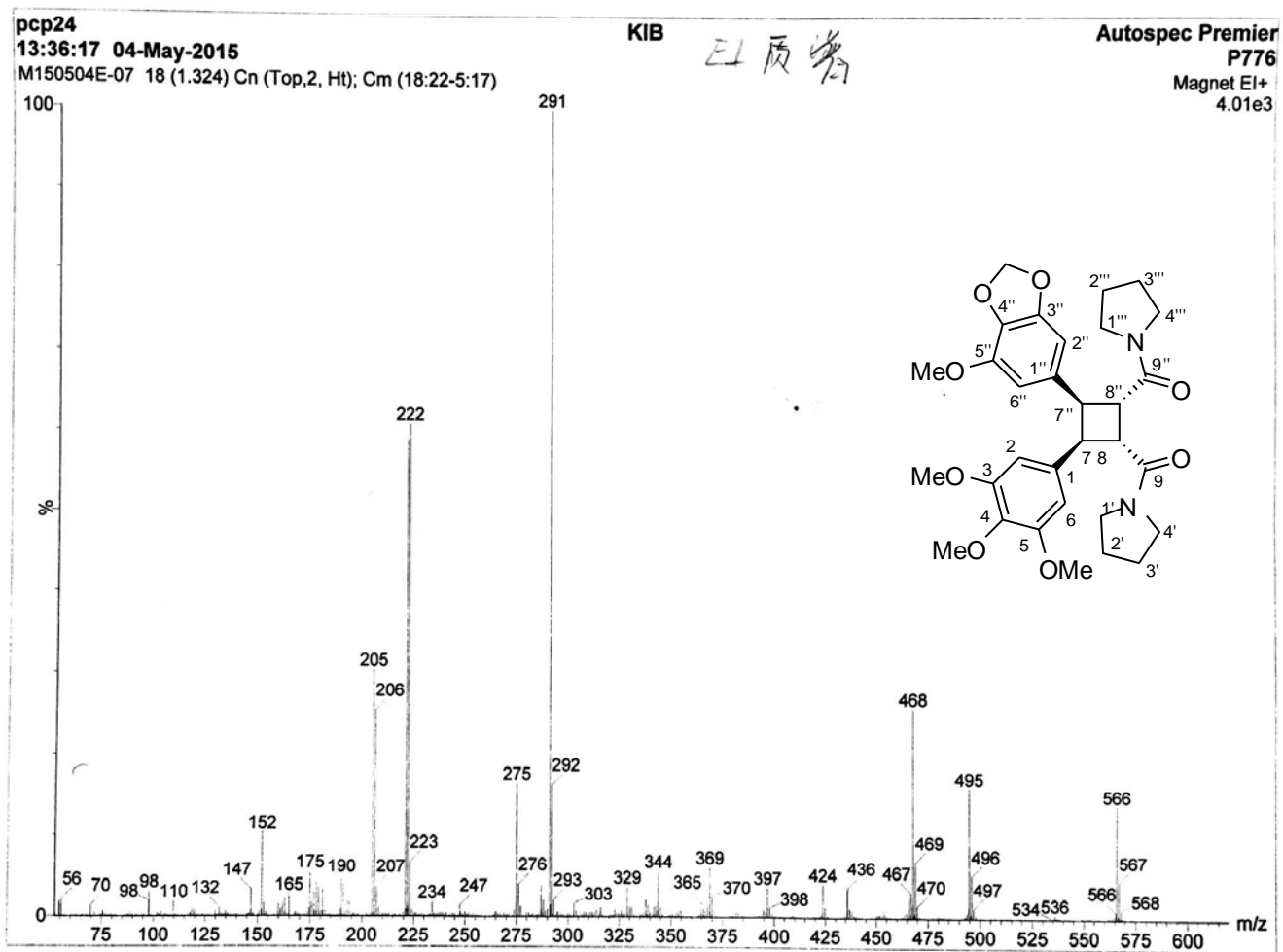




Figure S23. EI-MS spectrum of 3.



# Elemental Composition Report

## Single Mass Analysis

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Selected filters: None

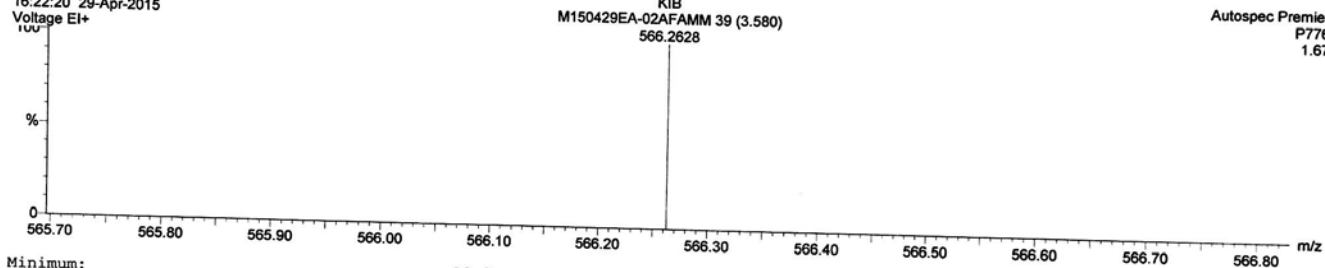
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pcp24  
16:22:20 29-Apr-2015  
Voltage E1+

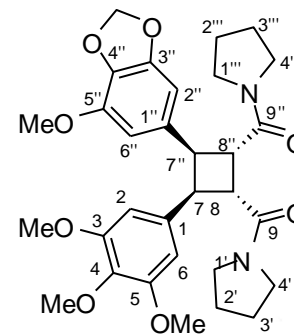
KIB  
M150429EA-02AFAMM 39 (3.580)  
566.2628

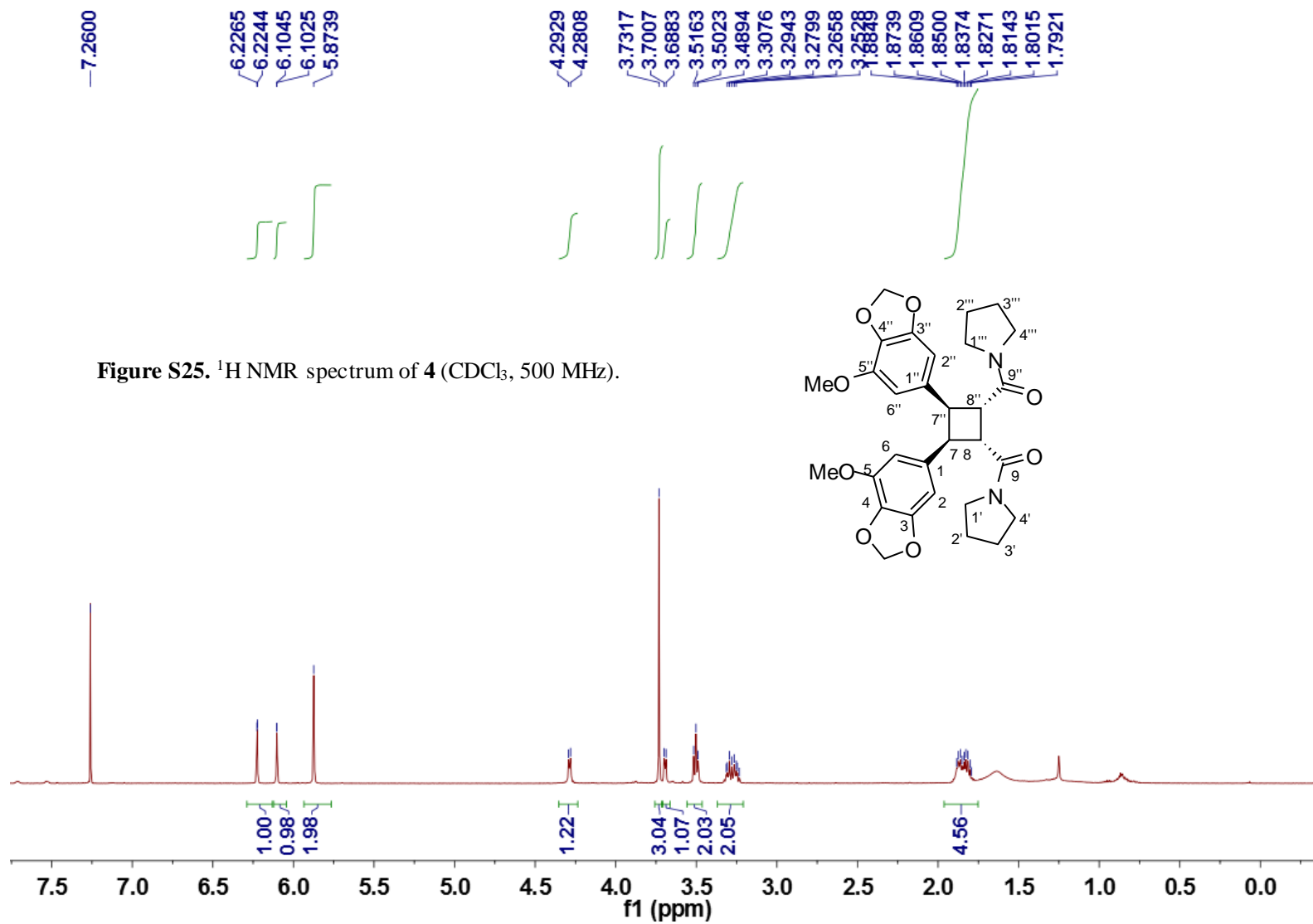
Autospec Premier  
P776  
1.67



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
566.2628	566.2628	0.0	0.0	14.0	5546025.5	C31 H38 N2 O8

Figure S24. HR-EI-MS spectrum of 3.





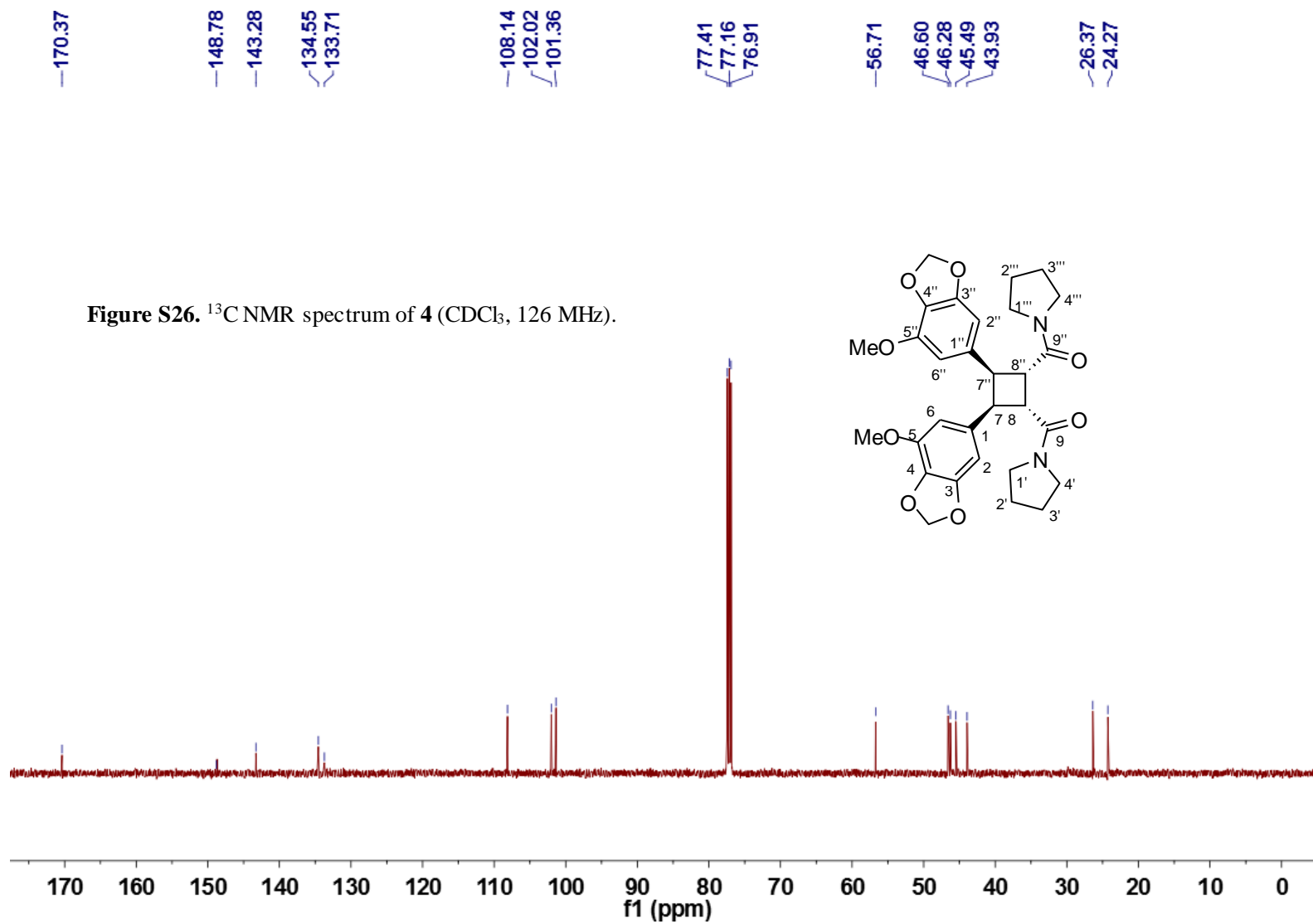


Figure S27. HSQC spectrum of 4.

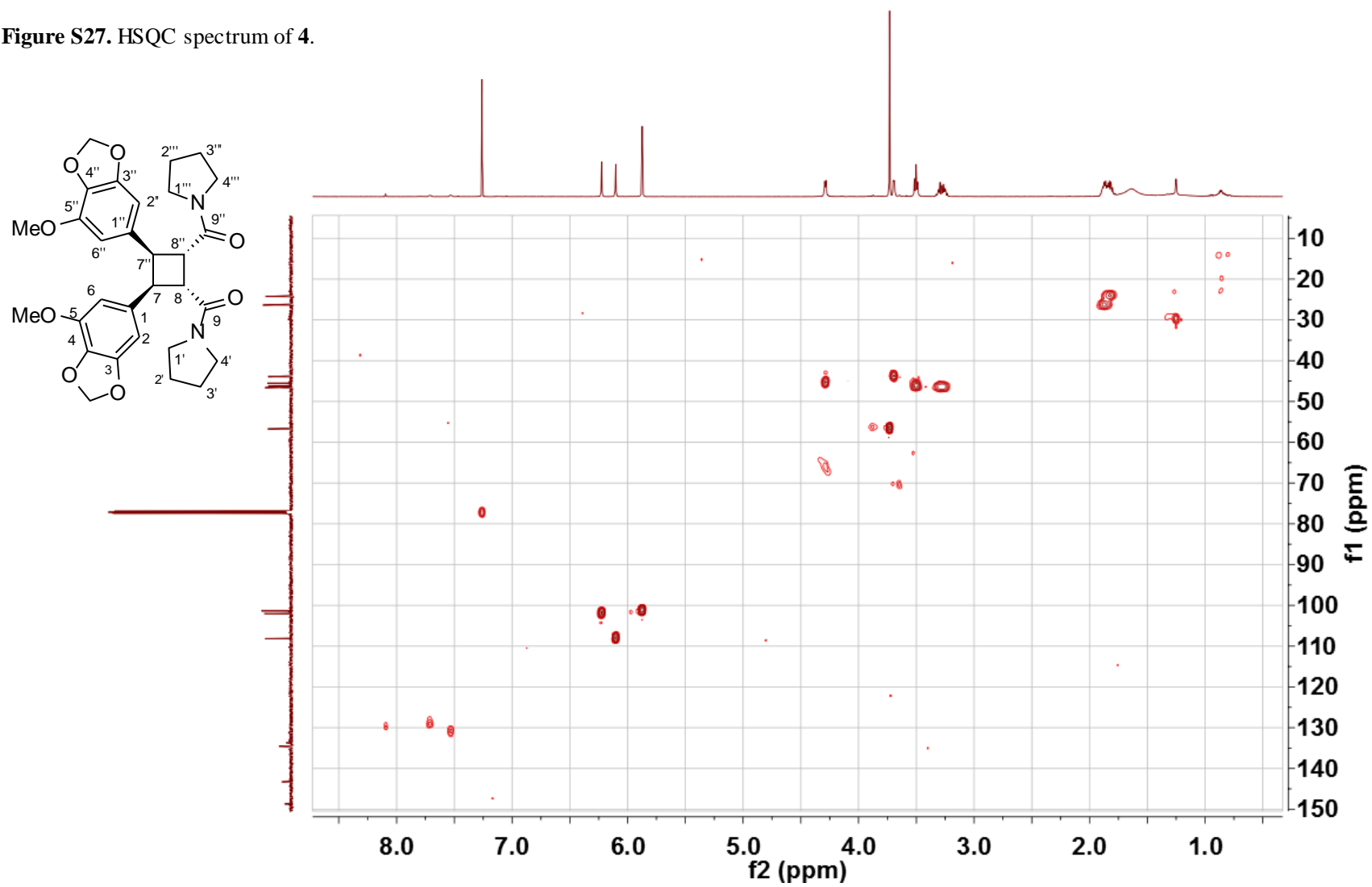


Figure S28.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **4**.

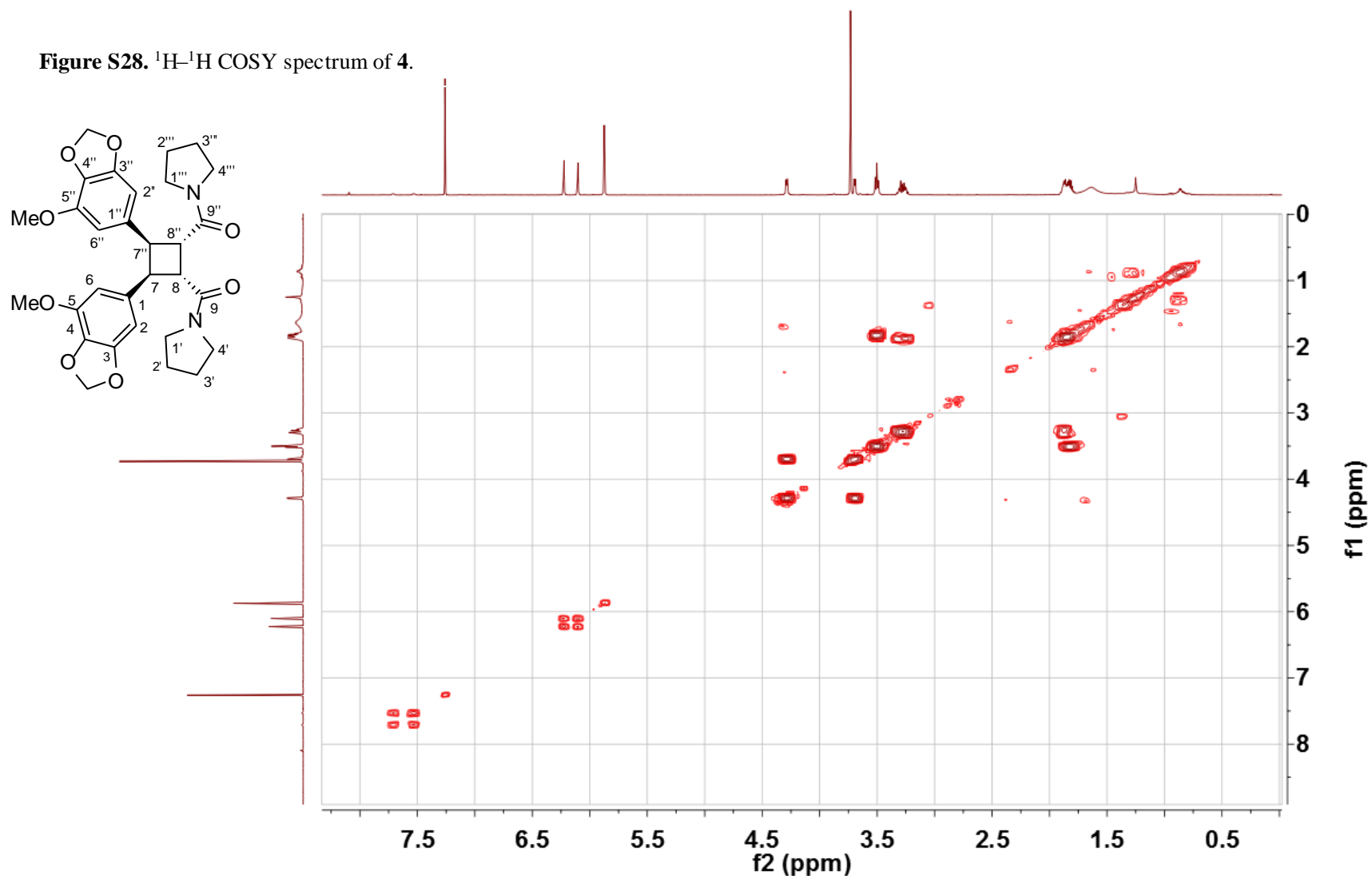


Figure S29. HMBC spectrum of 4.

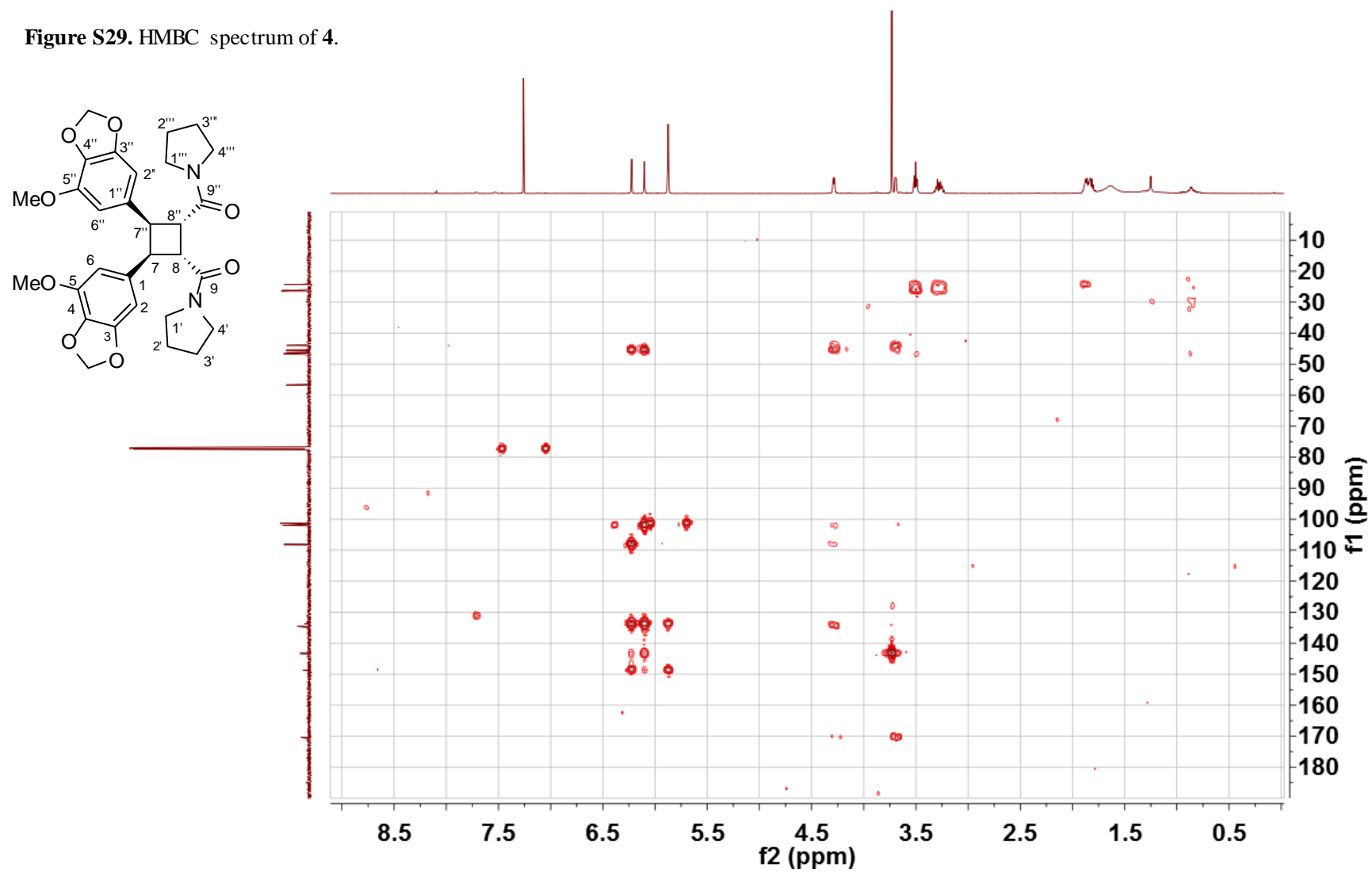
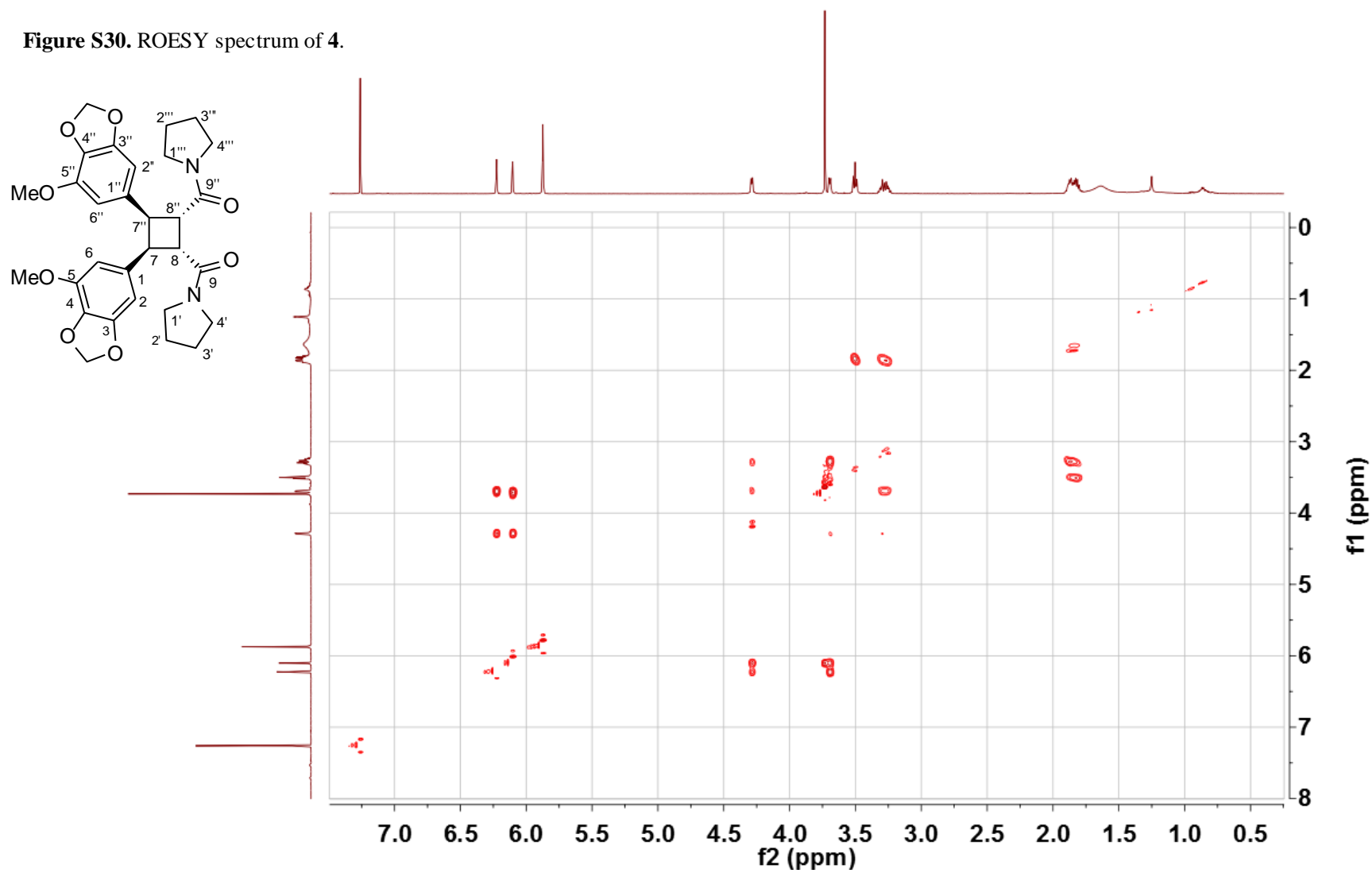


Figure S30. ROESY spectrum of 4.





pcp25

13:42:42 04-May-2015

M150504E-08 15 (1.103) Cn (Top,2, Ht); Cm (15-3:12)

KIB

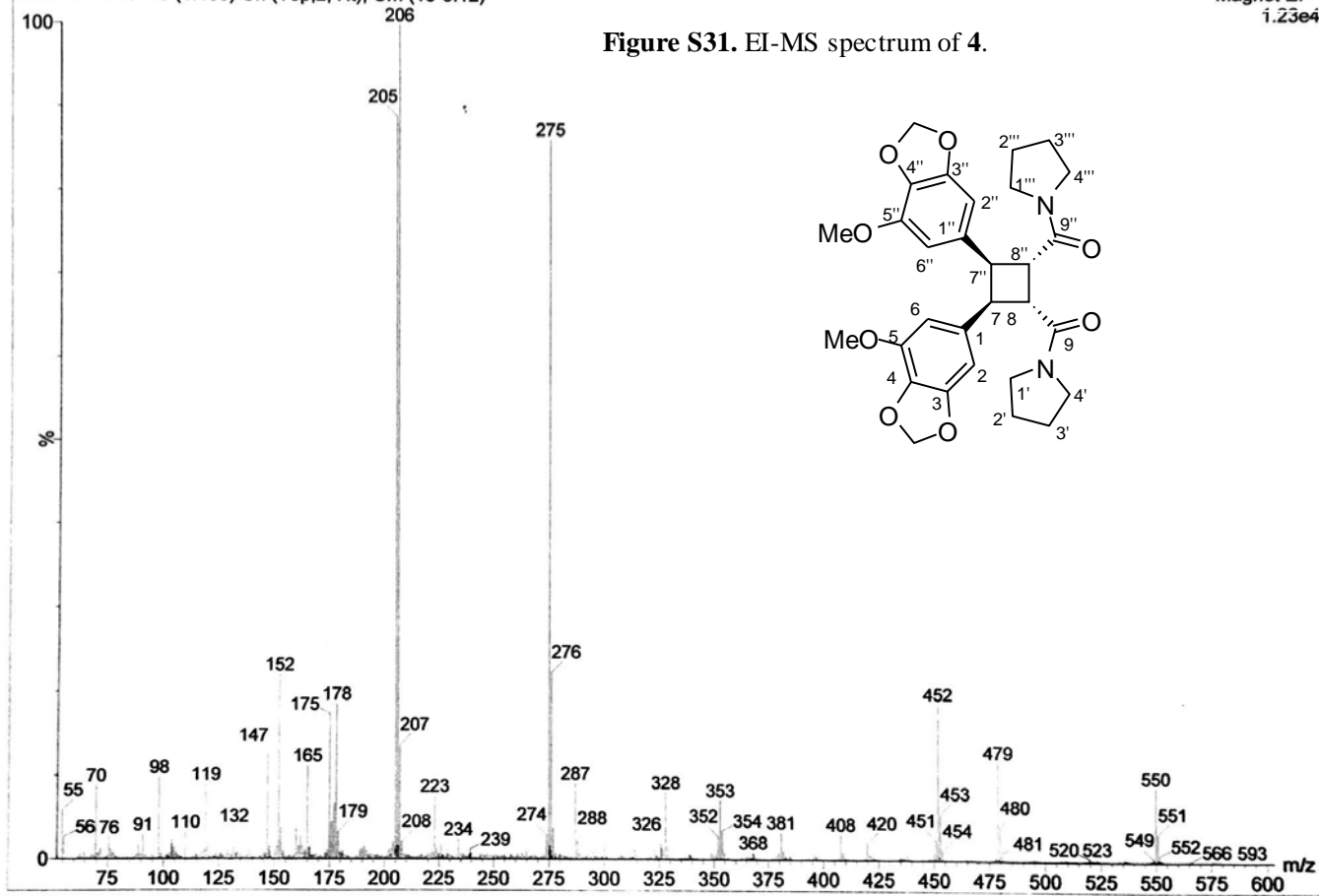
Autospec Premier

P776

Magnet EI+

i.23e4

Figure S31. EI-MS spectrum of 4.



## Elemental Composition Report

Page 1

### Single Mass Analysis

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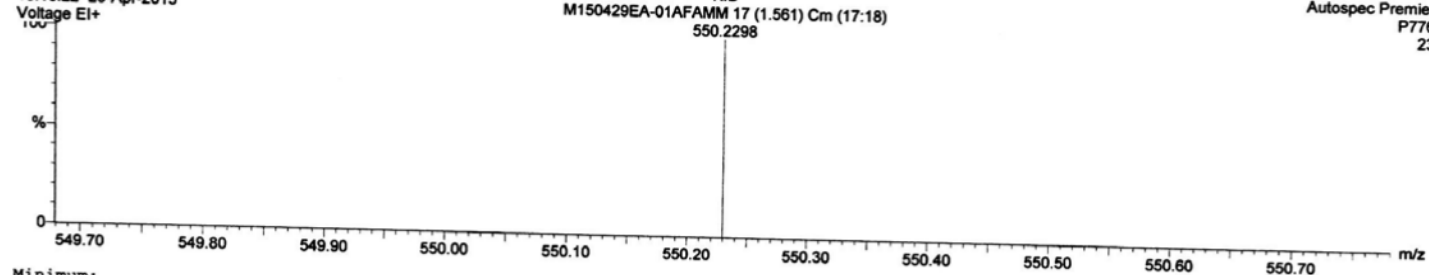
Monoisotopic Mass, Odd and Even Electron Ions  
21 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)  
Elements Used:

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pcp25  
16:16:22 29-Apr-2015  
Voltage EI+

KIB  
M150429EA-01AFAMM 17 (1.561) Cm (17:18)  
550.2298

Autospec Premier  
P776  
23



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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Figure S32. HR-EI-MS spectrum of 4.

