

Supplementary Material: PicROTOXANE Sesquiterpene Glycosides and Coumarin Derivative from *Coriaria nepalensis* and Their Neurotrophic Activity

Yuan-Yuan Wang, Jun-Mian Tian, Cheng-Chen Zhang, Bo Luo, and Jin-Ming Gao *

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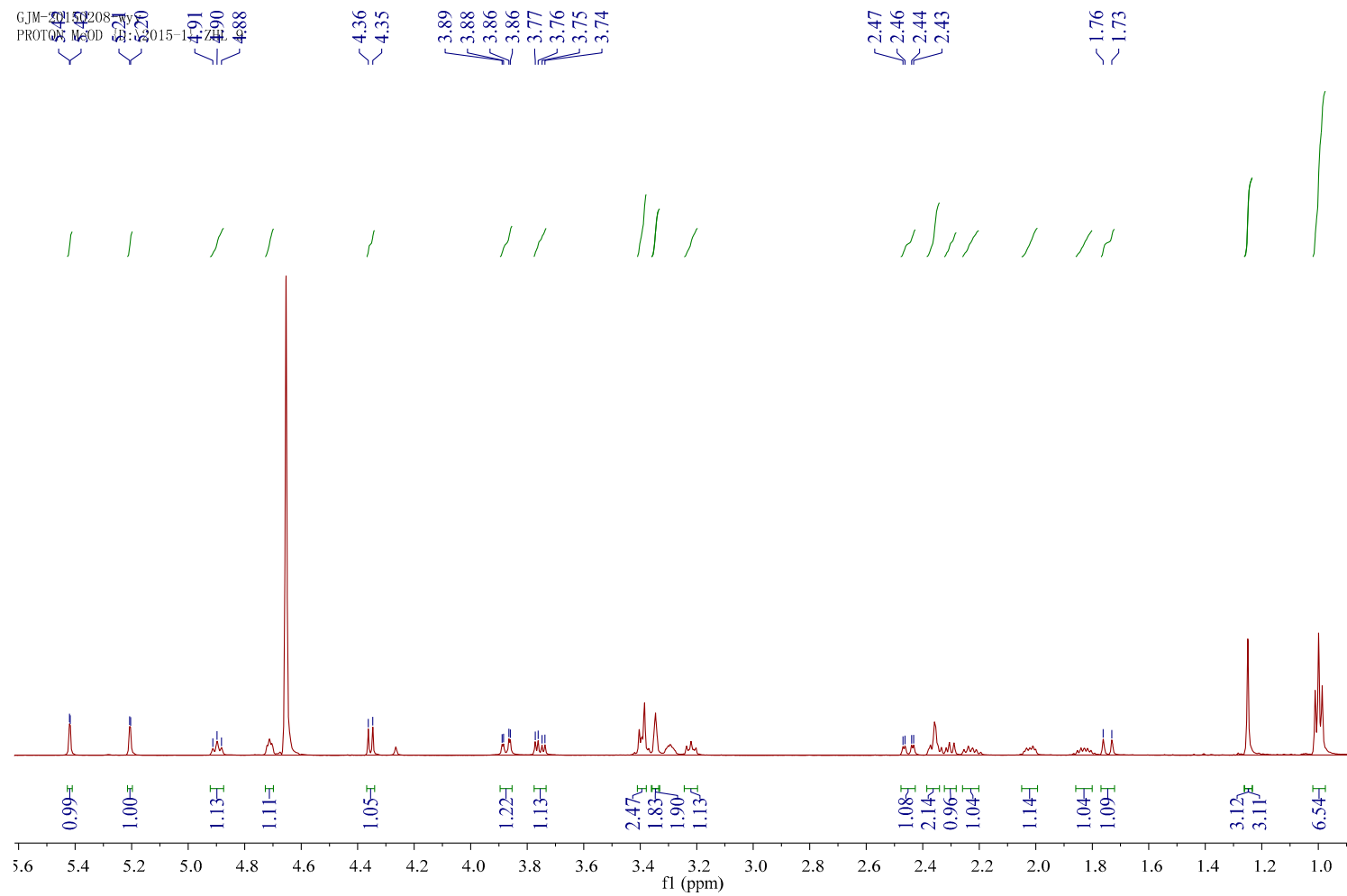


Figure S1. $^1\text{H-NMR}$ spectra of compound **1** in CD_3OD .

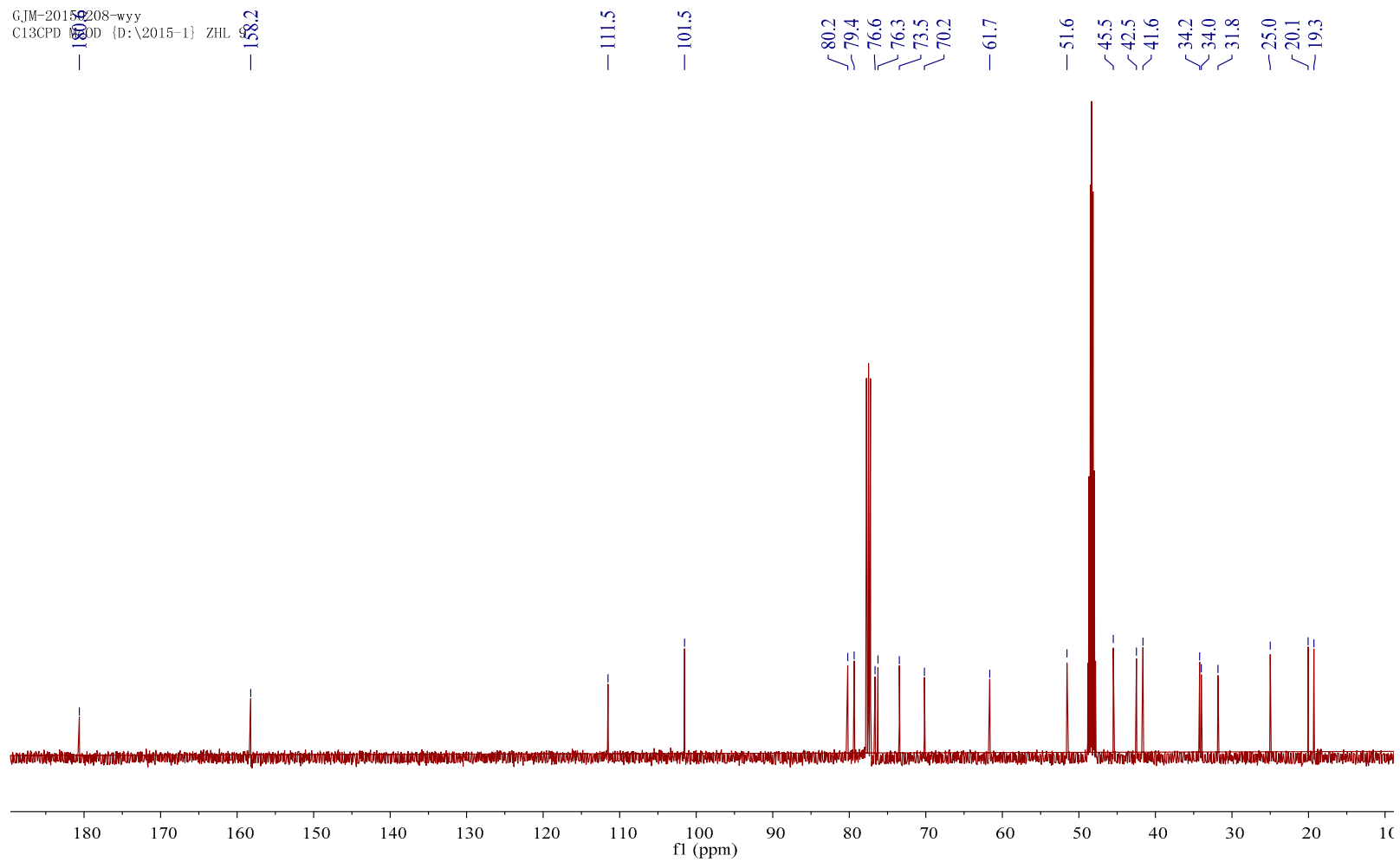


Figure S2. ^{13}C -NMR spectra of compound **1** in CD_3OD .

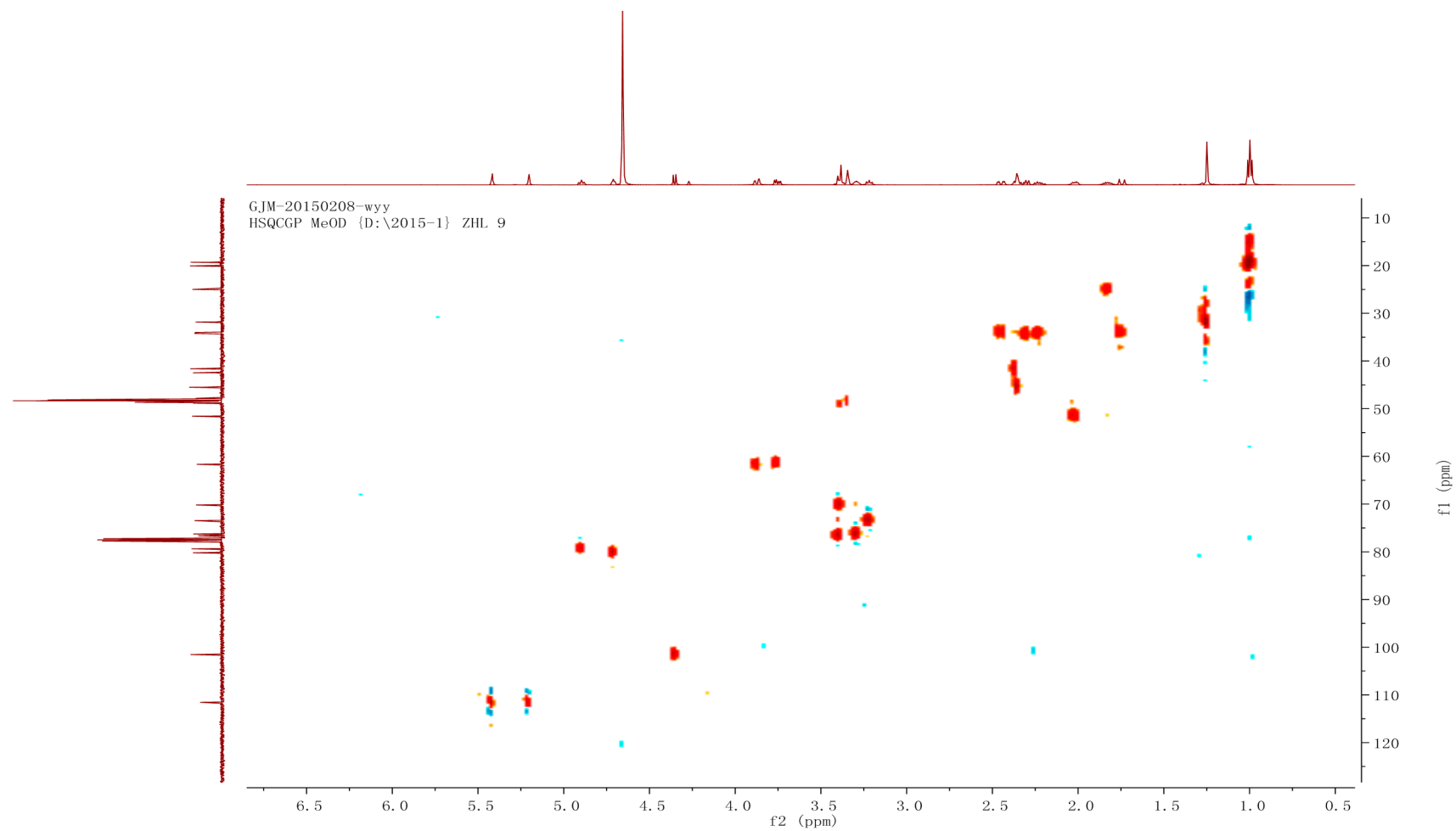


Figure S3. HSQC spectra of compound **1** in CD₃OD.

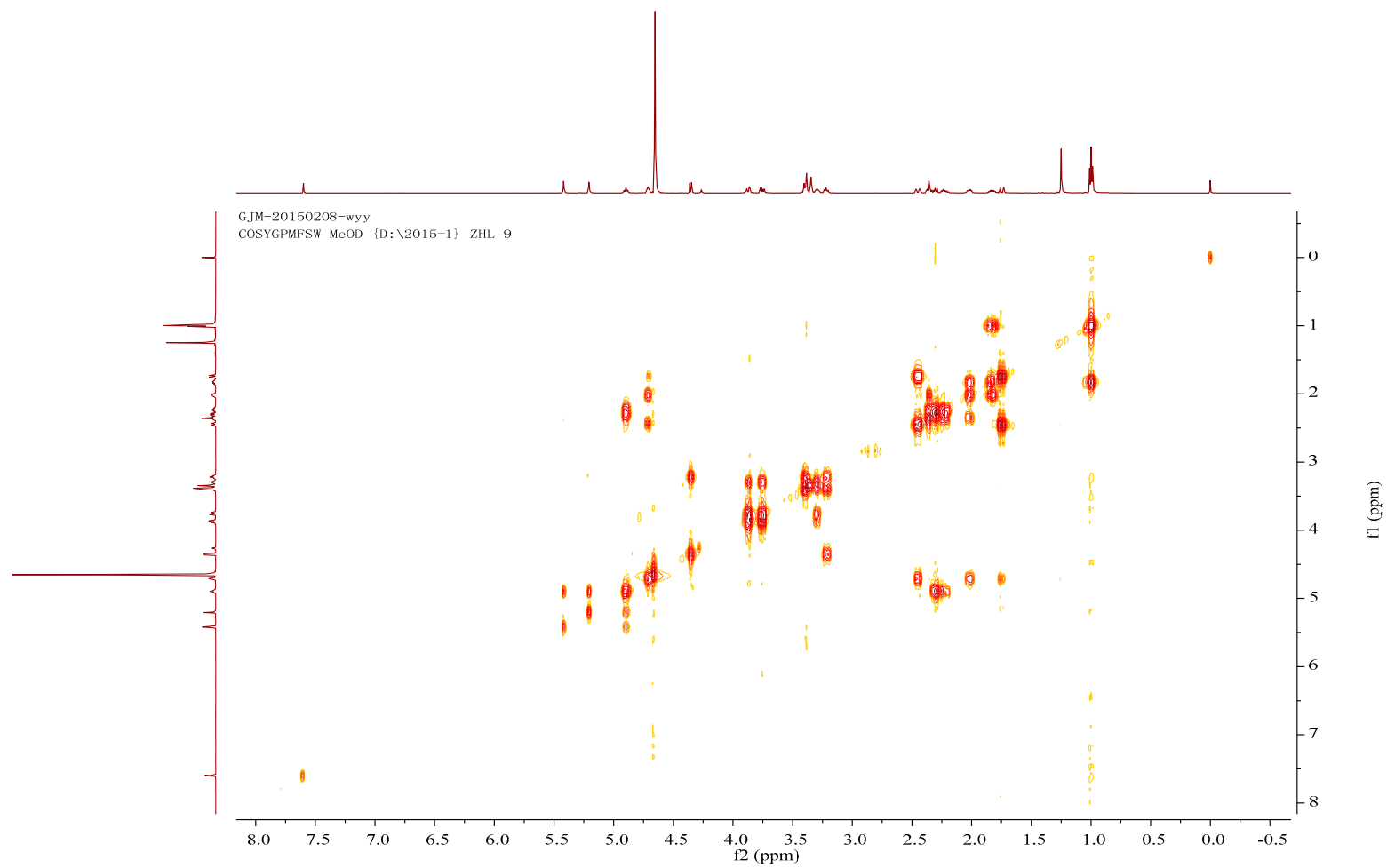


Figure S4. ^1H - ^1H COSY spectra of compound 1 in CD_3OD .

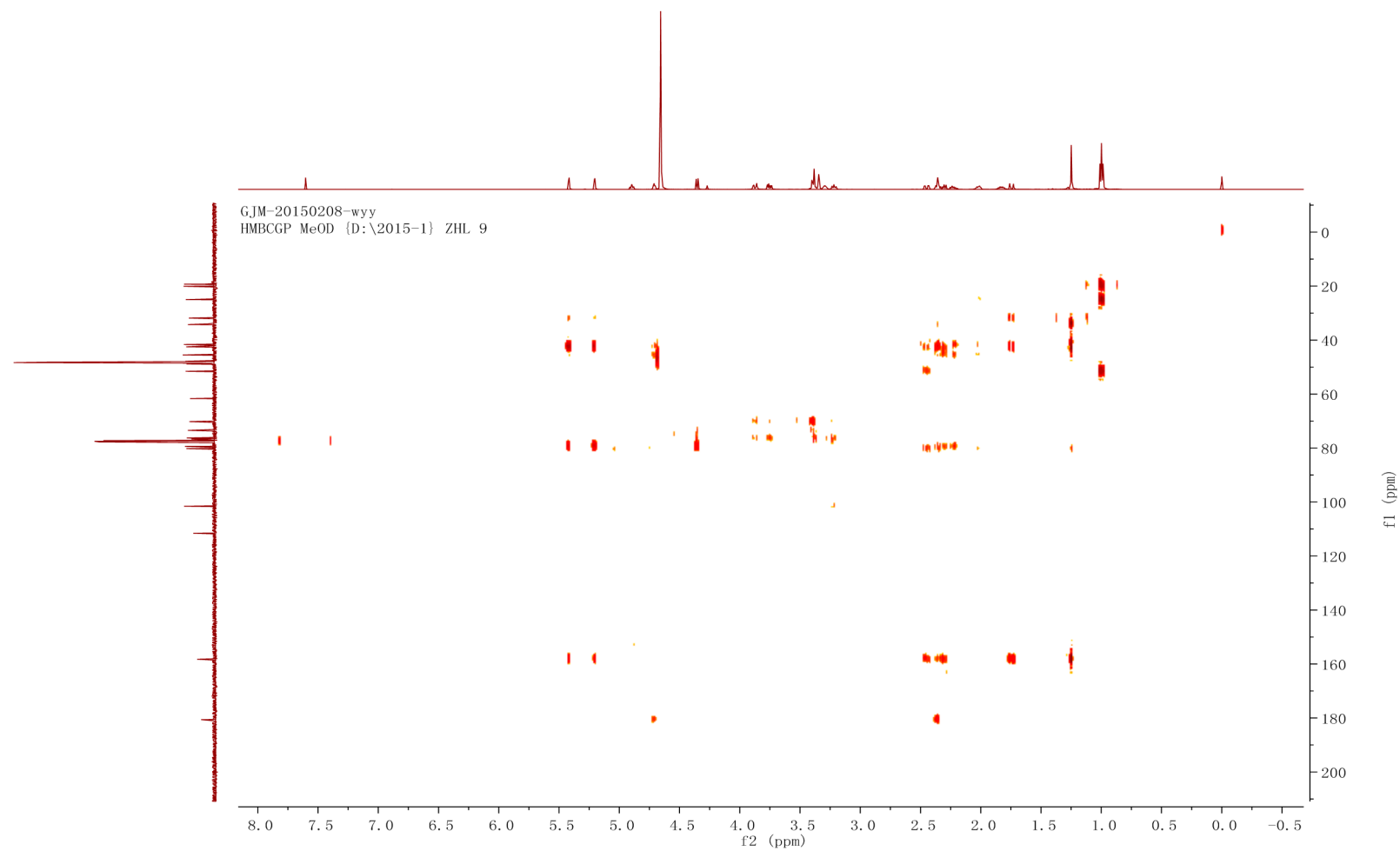


Figure S5. HMBC spectra of compound **1** in CD₃OD.

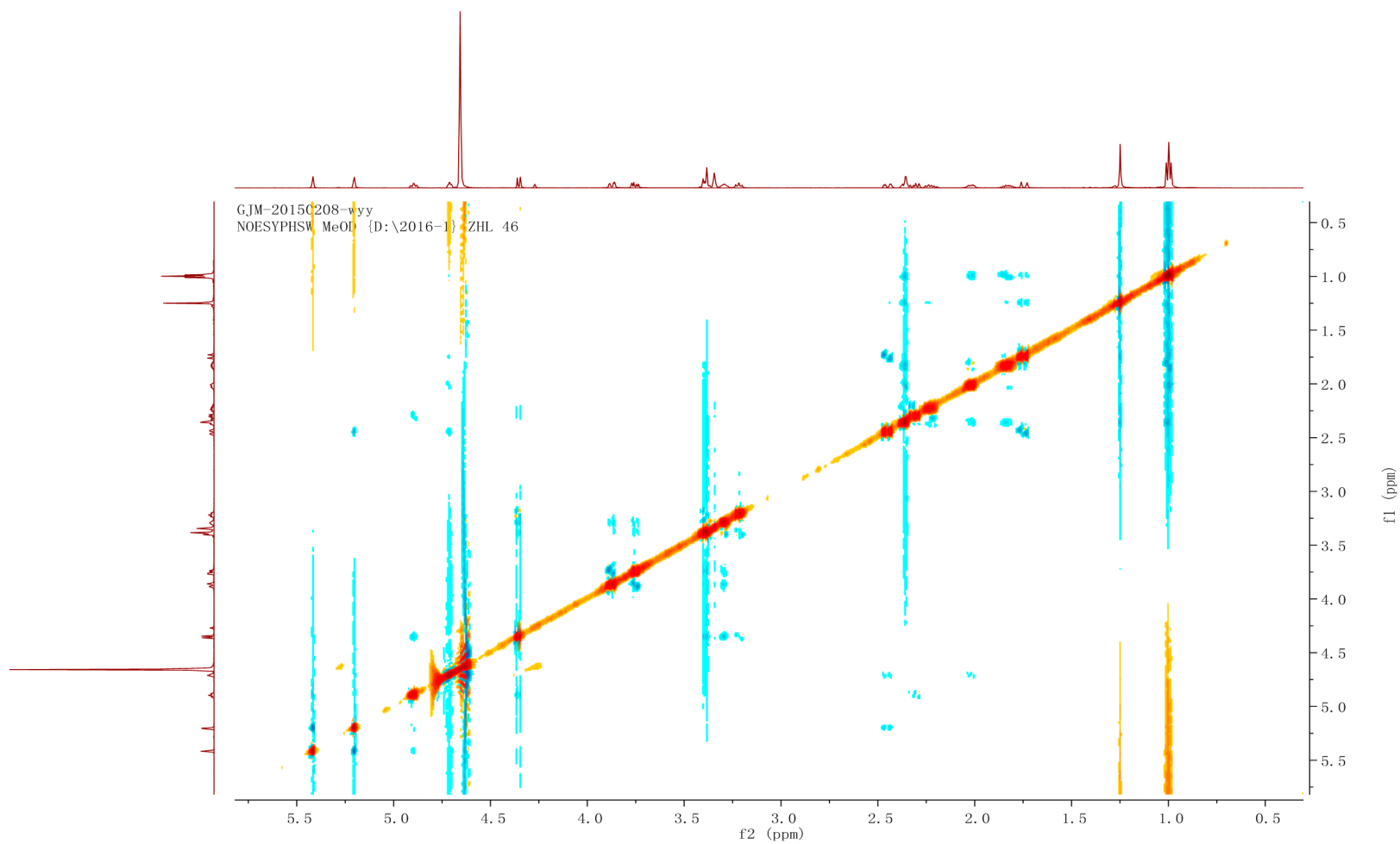


Figure S6. NOESY spectra of compound **1** in CD₃OD.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 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

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

Elements Used:

C: 5-80 H: 2-120 O: 0-20 Na: 0-1

wyy-1

LCT PXE KE324

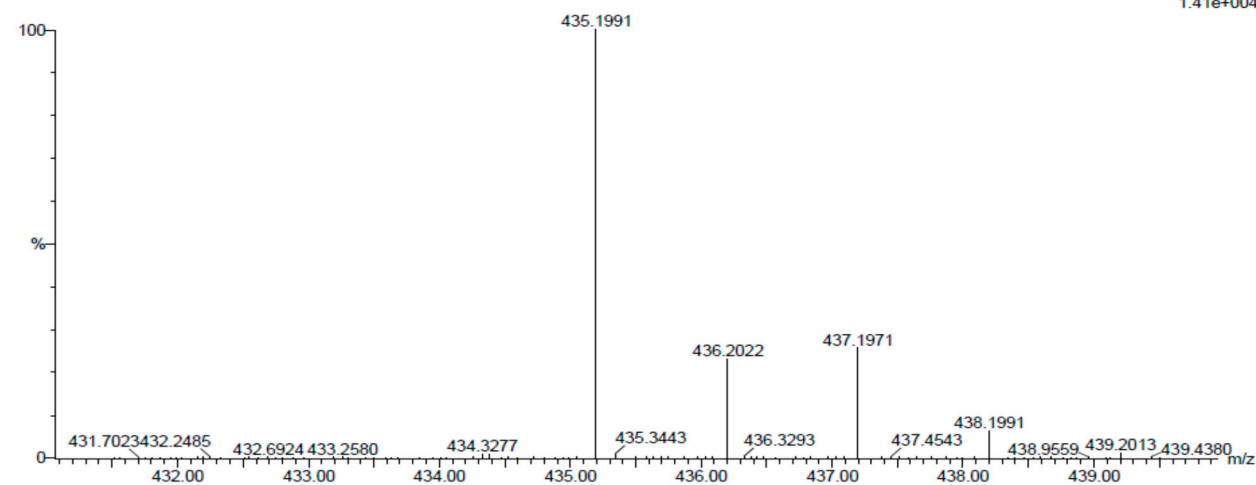
14-Oct-2015

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1: TOF MS ES+

1.41e+004

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Figure S7. HRESIMS spectrum of compound 1.

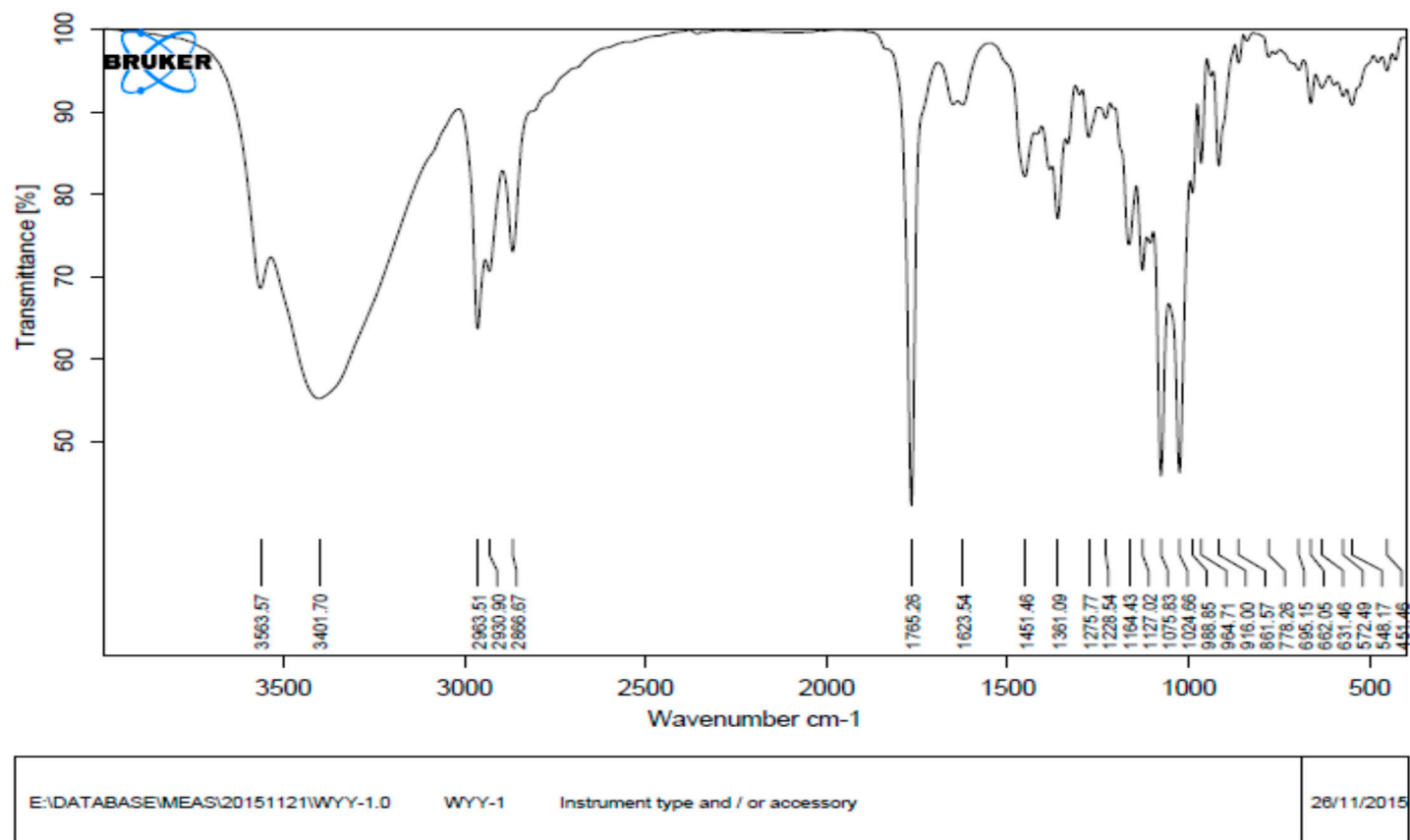


Figure S8. IR spectra of compound 1.

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Department (None Entered)
Organization (None Entered)
Information (None Entered)

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Time of Report 22:33:37下午

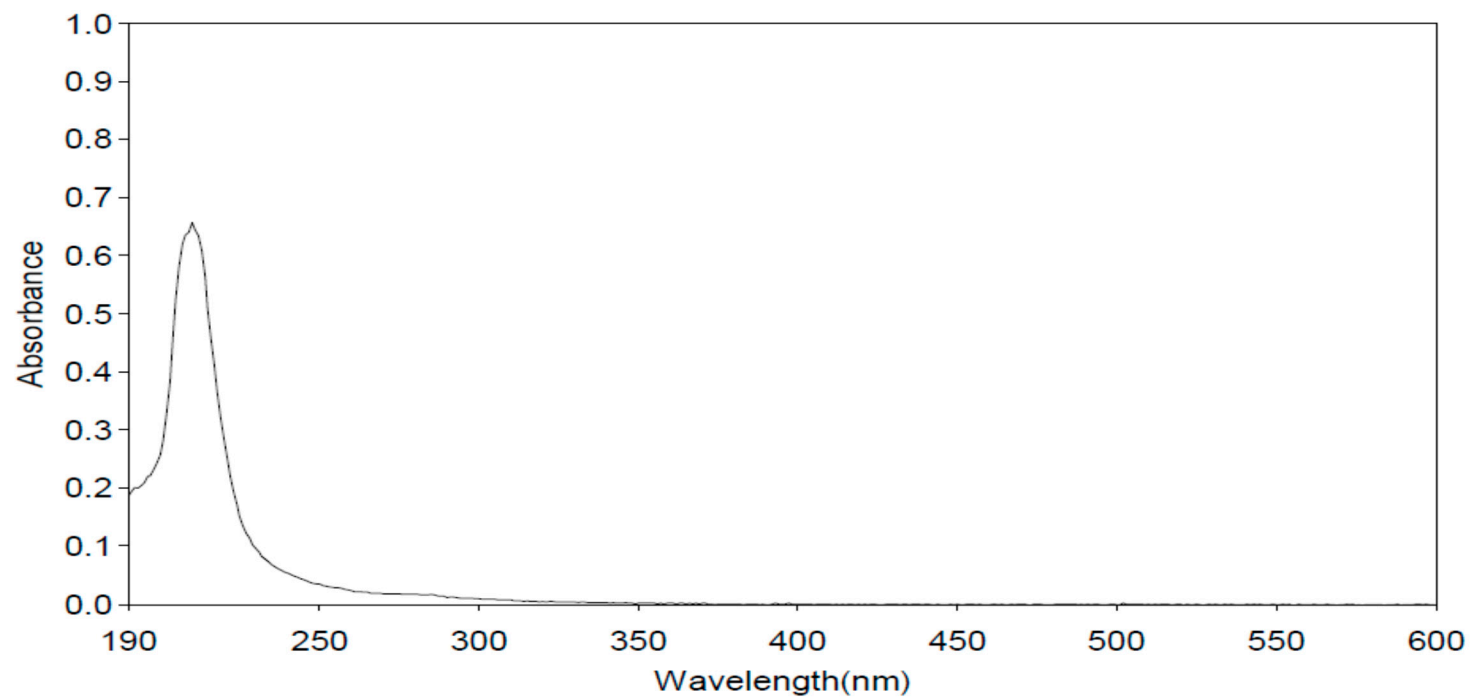
Scan Graph

Figure S9. UV spectra of compound 1.

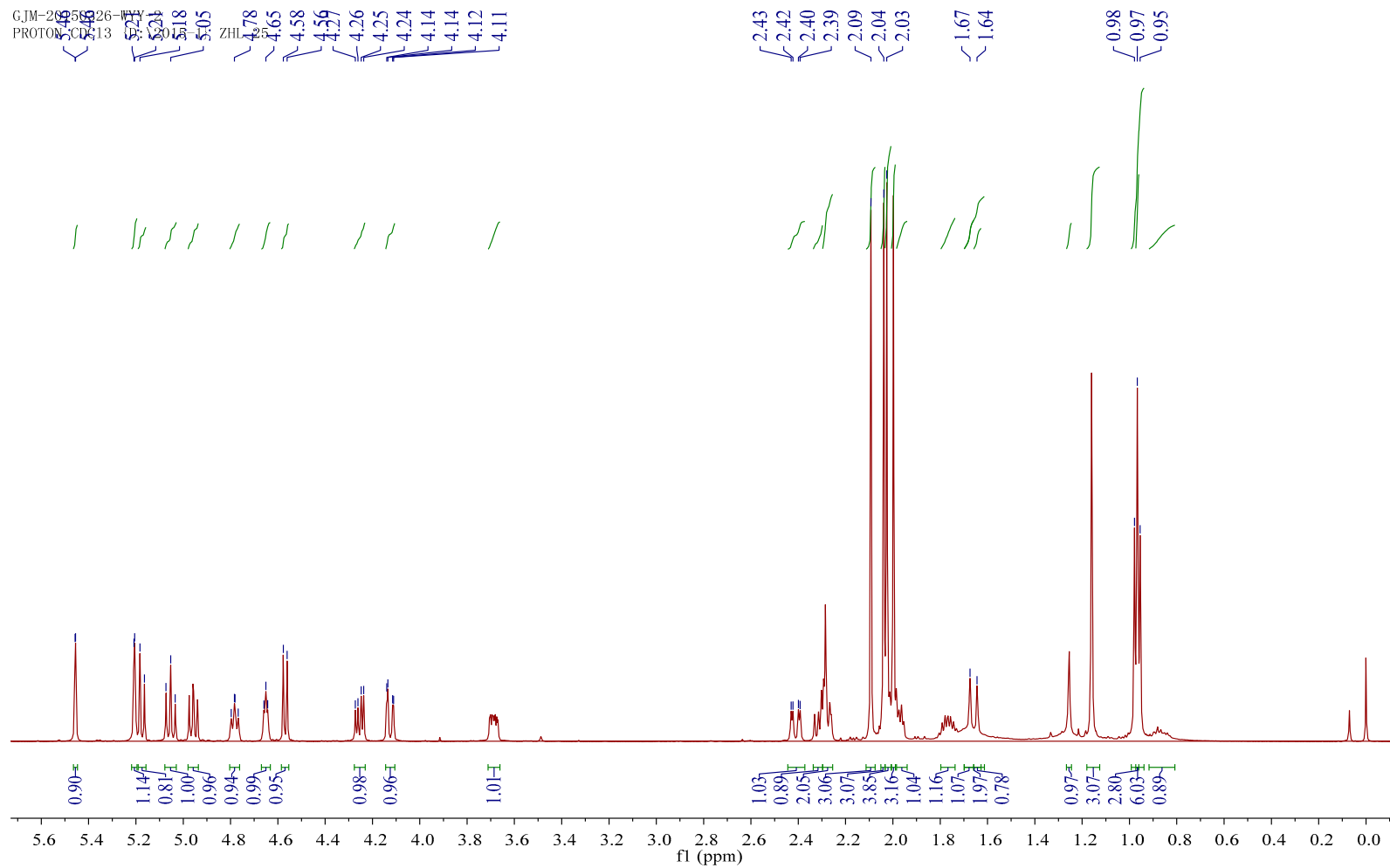


Figure S10. ¹H-NMR spectra of compound **1a** in CDCl₃.

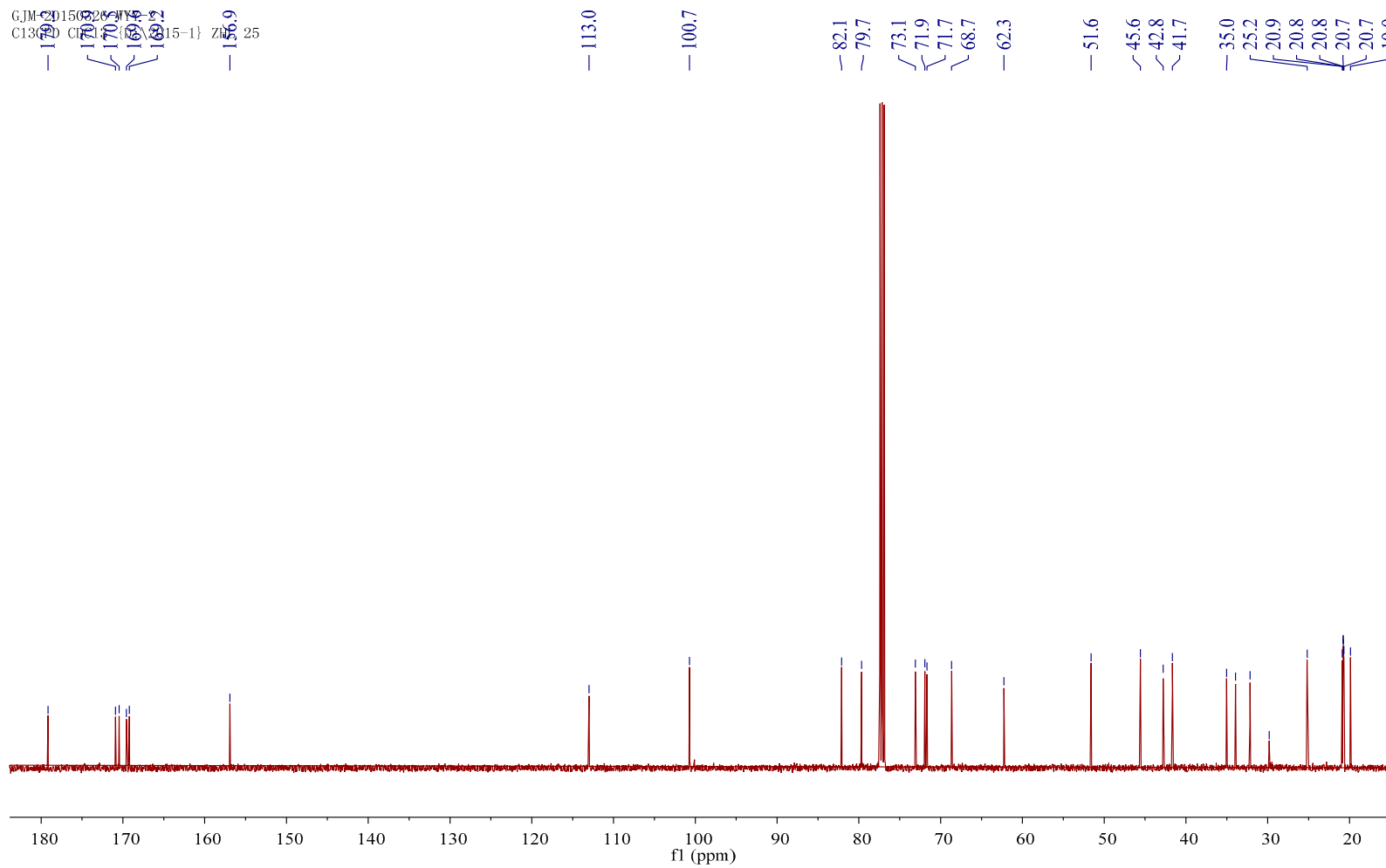


Figure S11. ¹³C-NMR spectra of compound **1a** in CDCl₃.

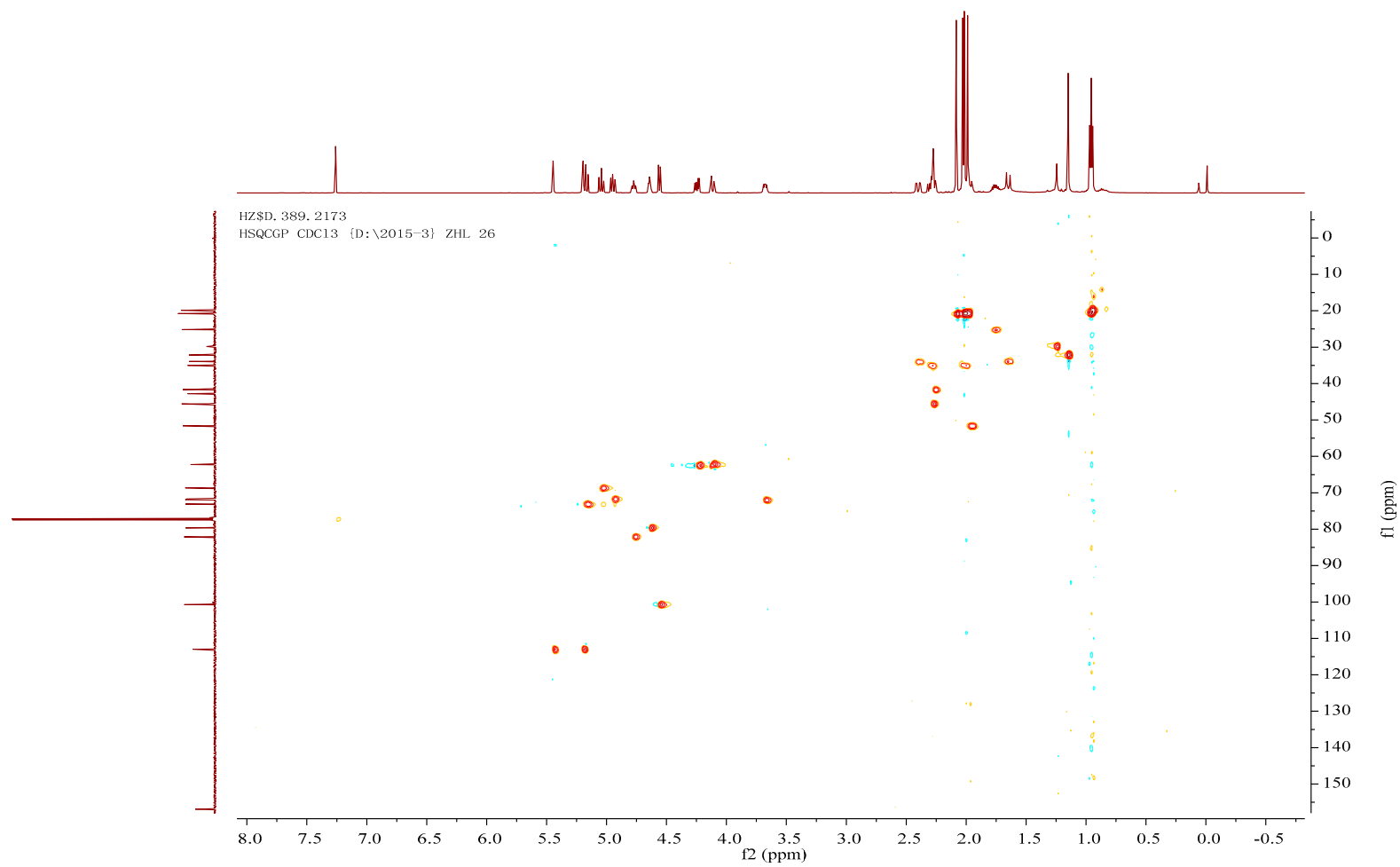


Figure S12. HSQC spectra of compound **1a** in CDCl₃.

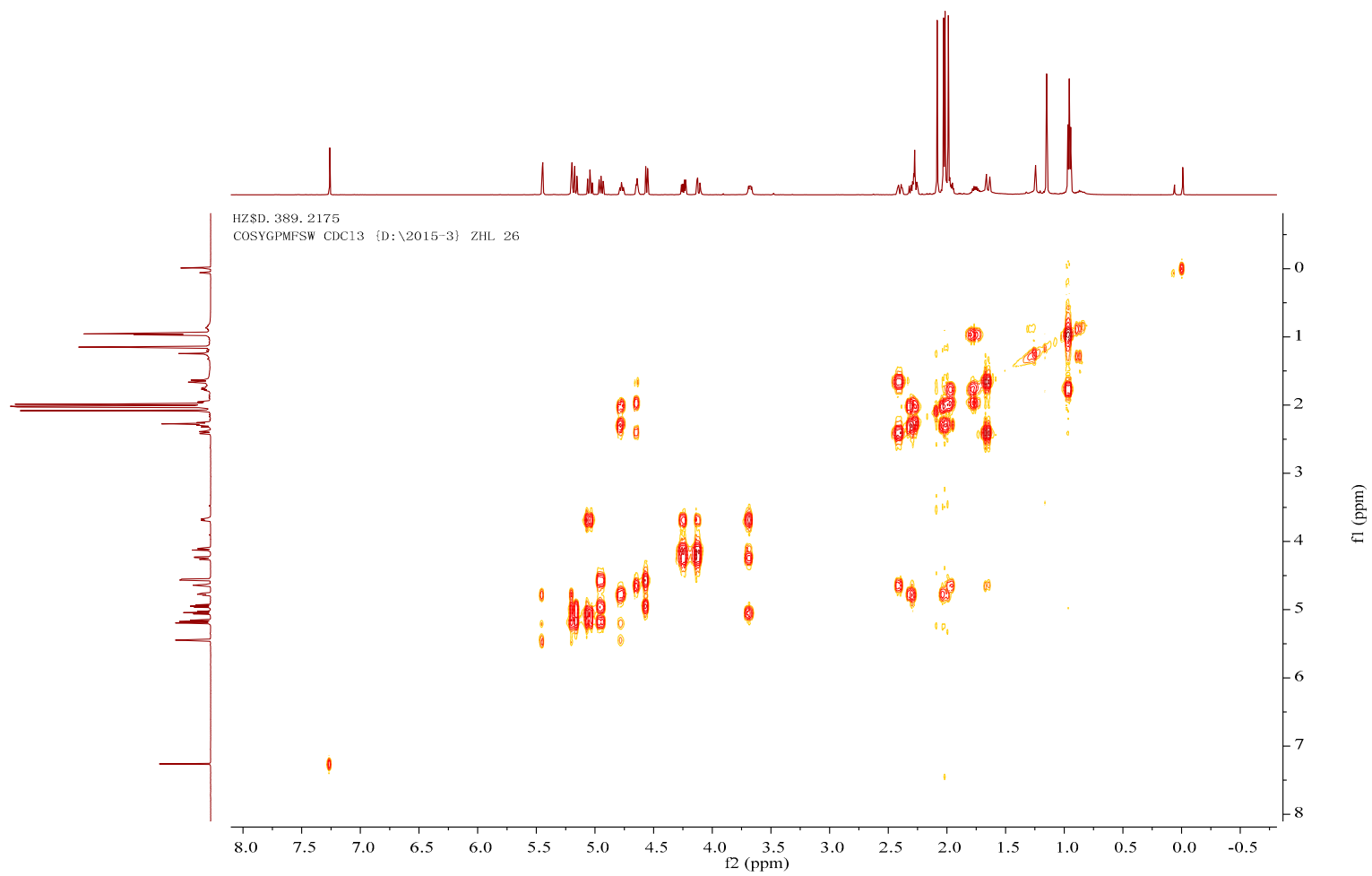


Figure S13. ^1H - ^1H COSY spectra of compound **1a** in CDCl_3 .

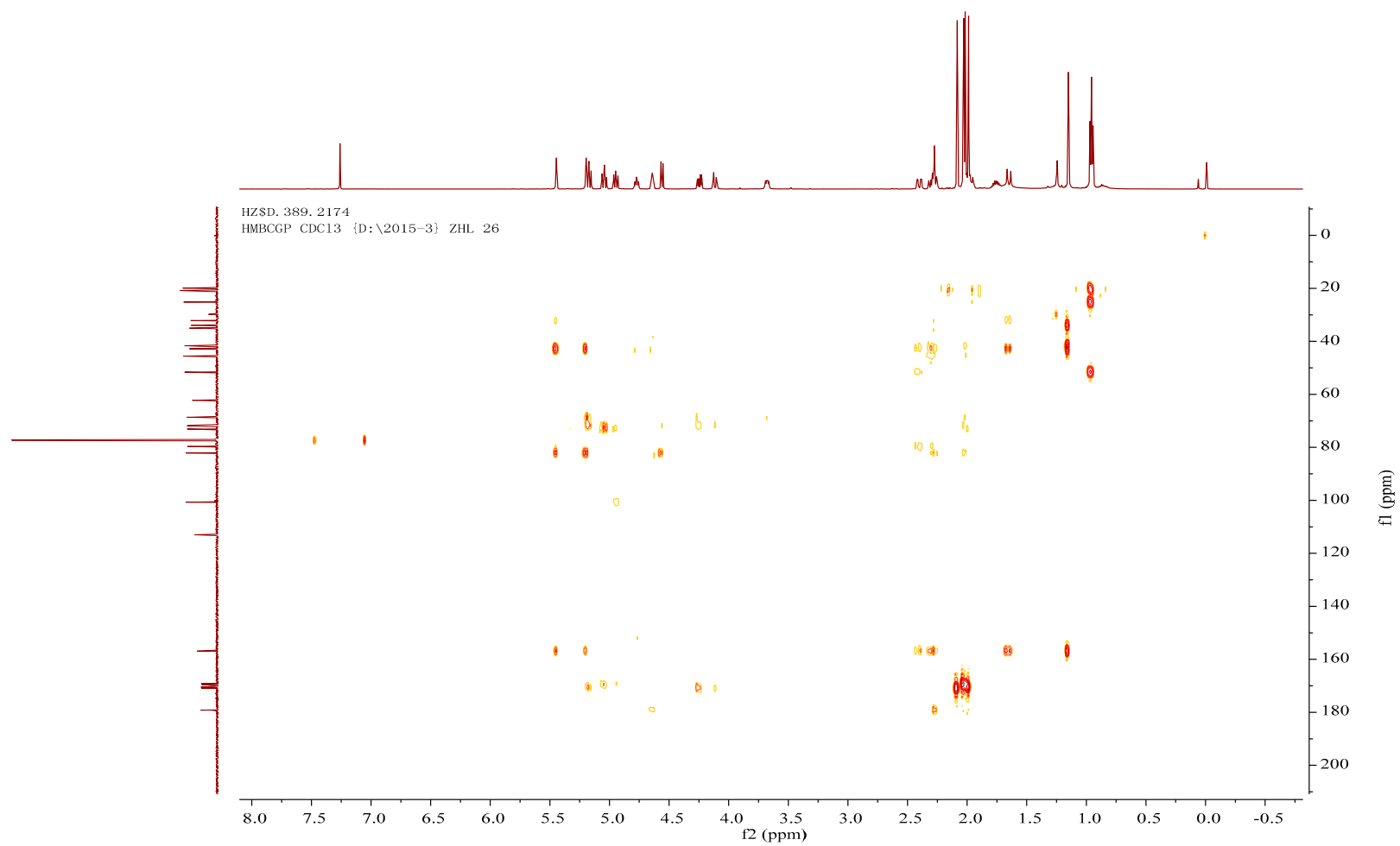


Figure S14. HMBC spectra of compound **1a** in CDCl₃.

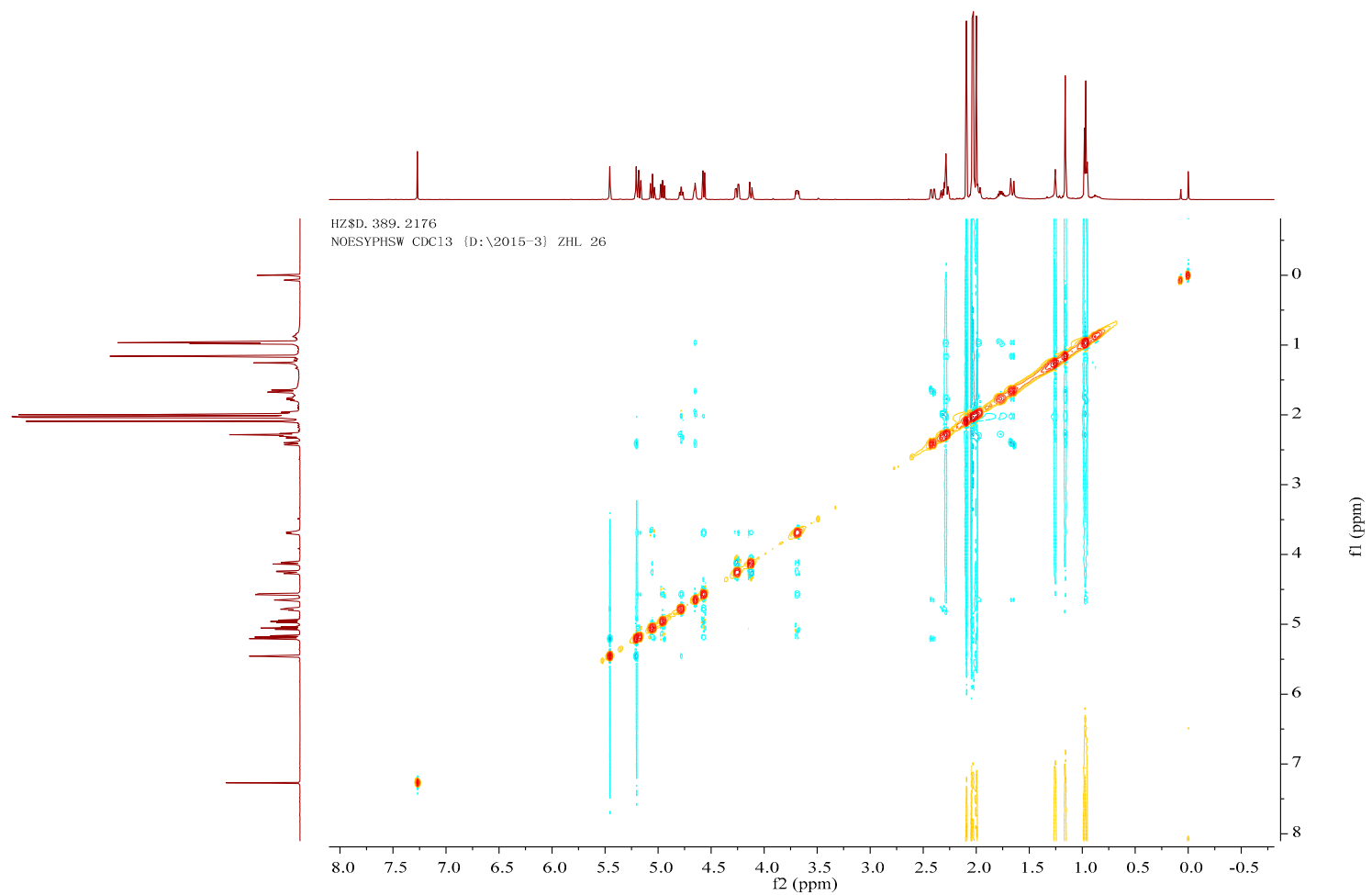


Figure S15. NOESY spectra of compound **1a** in CDCl₃.

Elemental Composition Report

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Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 5-80 H: 2-120 O: 0-20 Na: 0-1

wy-2

LCT PXE KE324

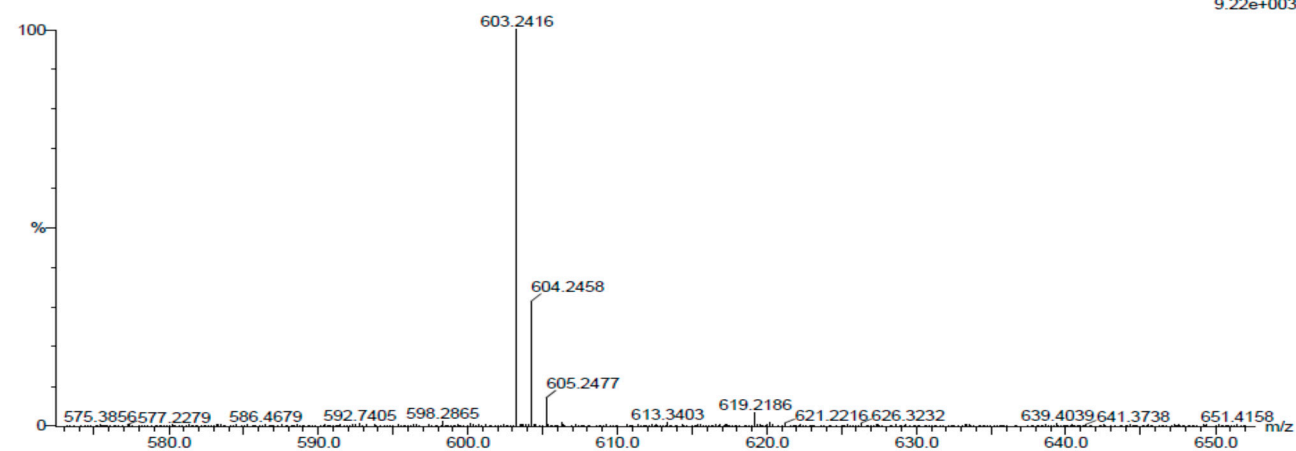
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9.22e+003

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Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
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Figure S16. HRESIMS spectrum of compound 1a.

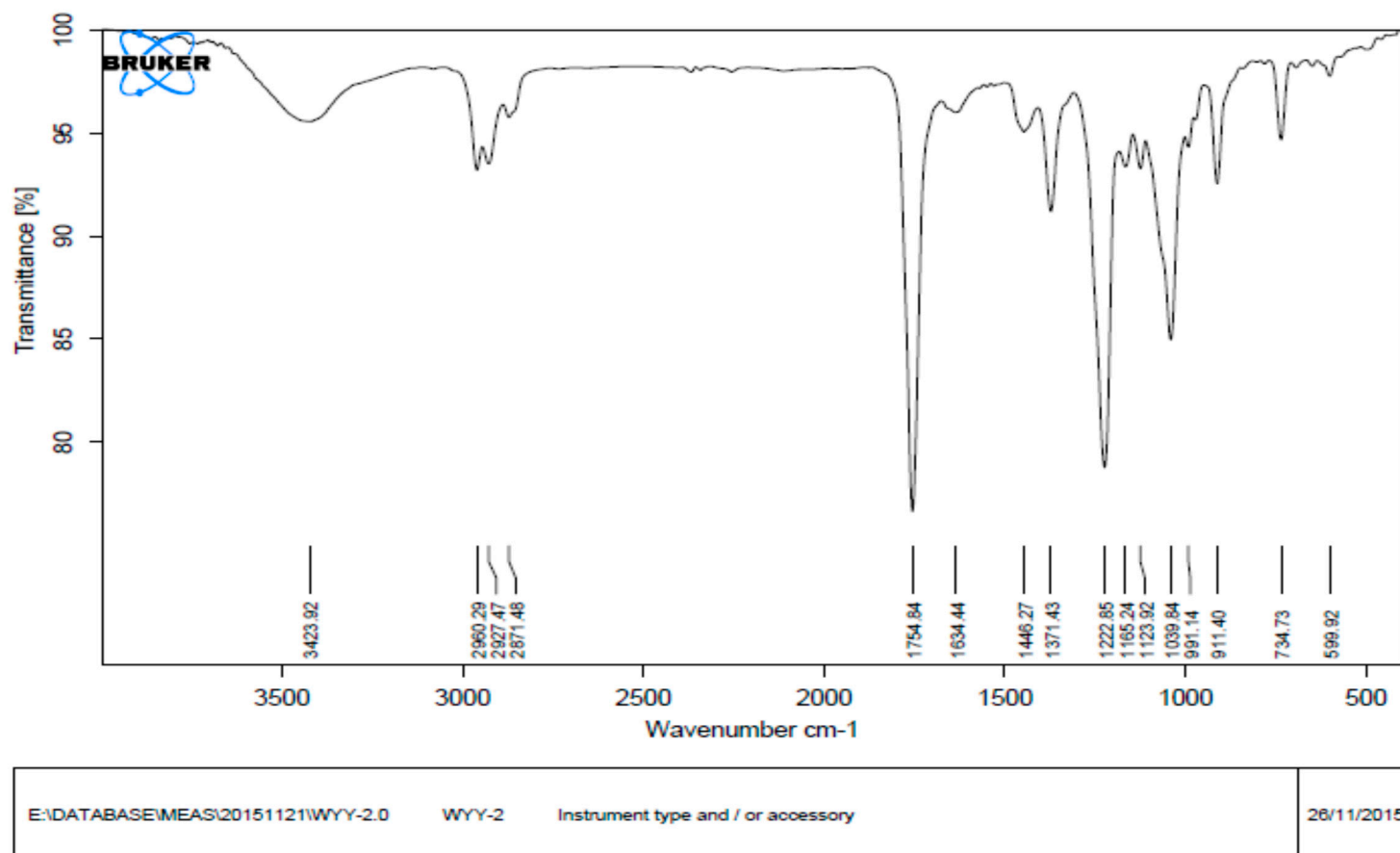


Figure S17. IR spectra of compound 1a.

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Department (None Entered)
Organization (None Entered)
Information (None Entered)

Date of Report 2015-9-16
Time of Report 22:39:59下午

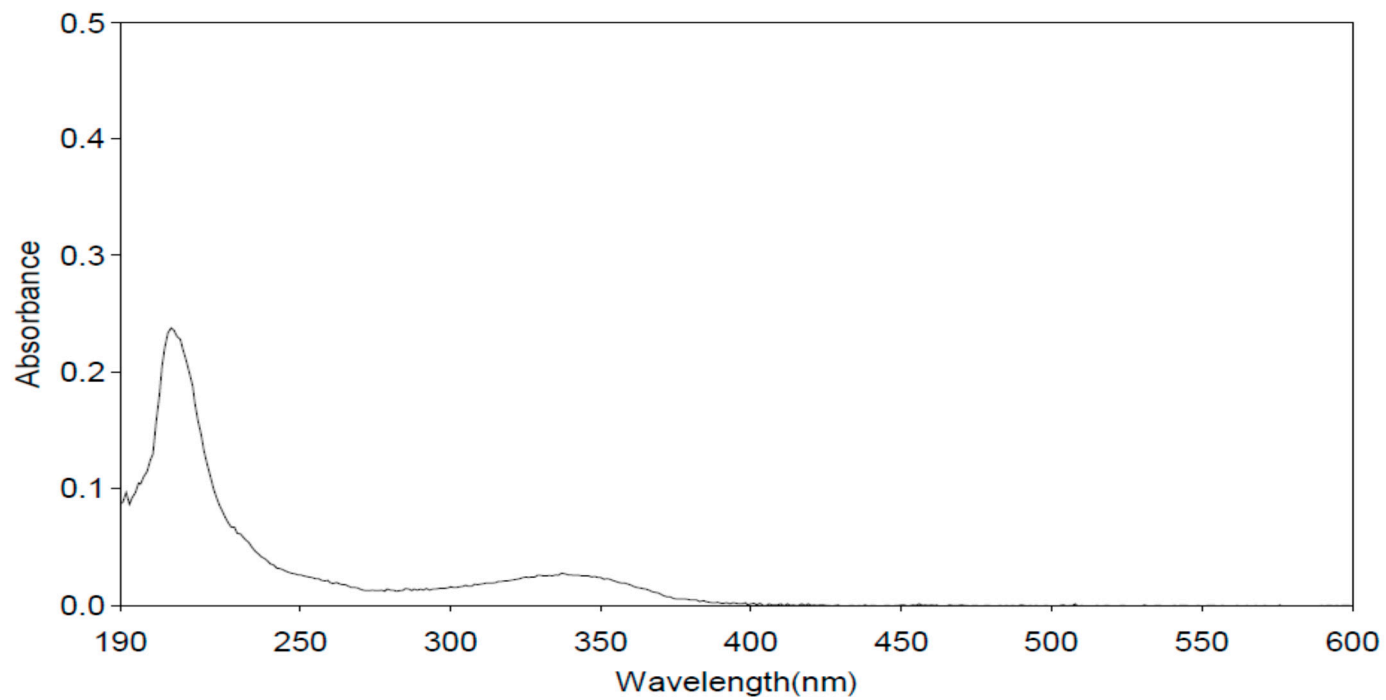
Scan Graph

Figure S18. UV spectra of compound **1a**.

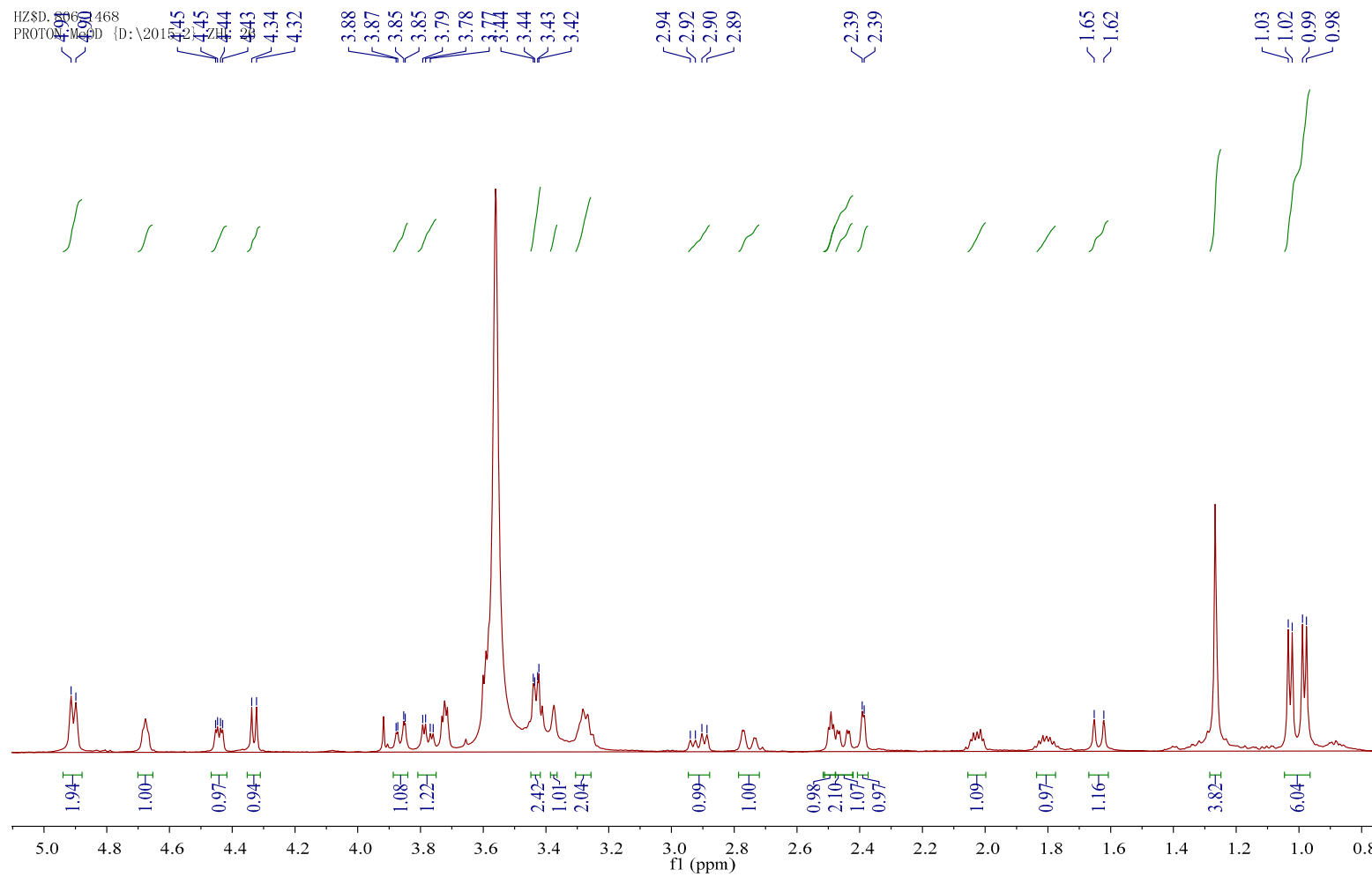


Figure S19. ^1H -NMR spectra of compound 2 in CD_3OD .

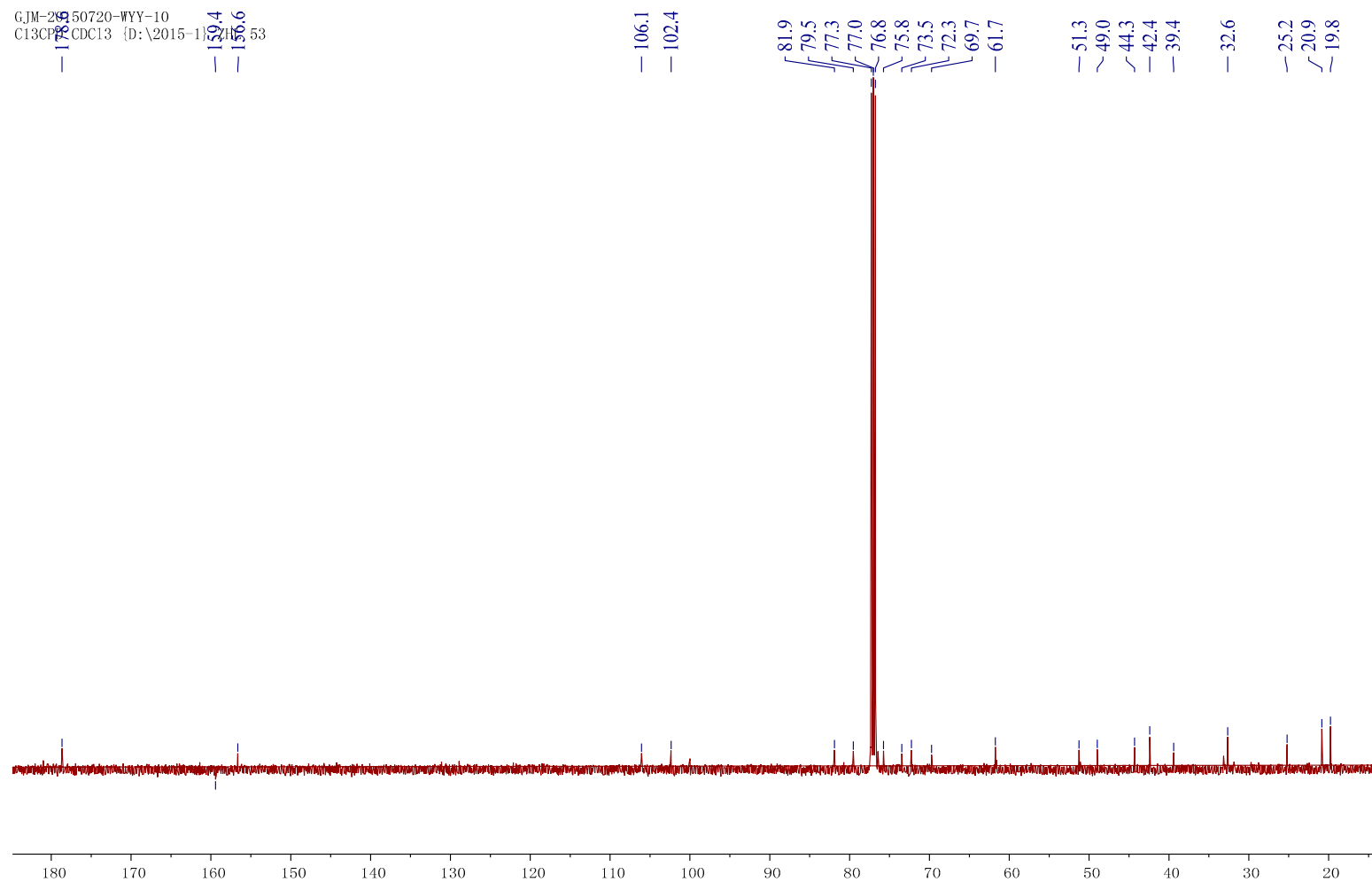
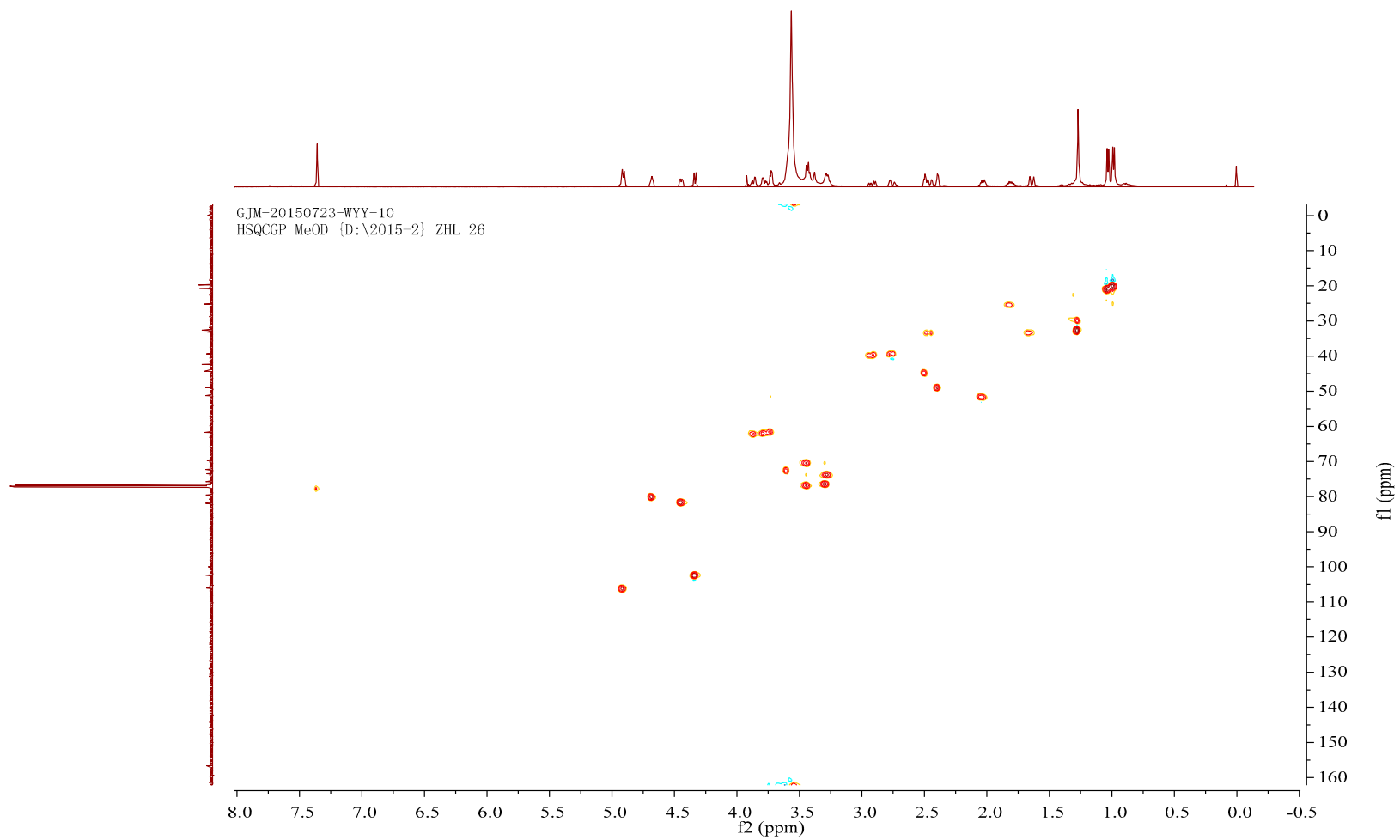
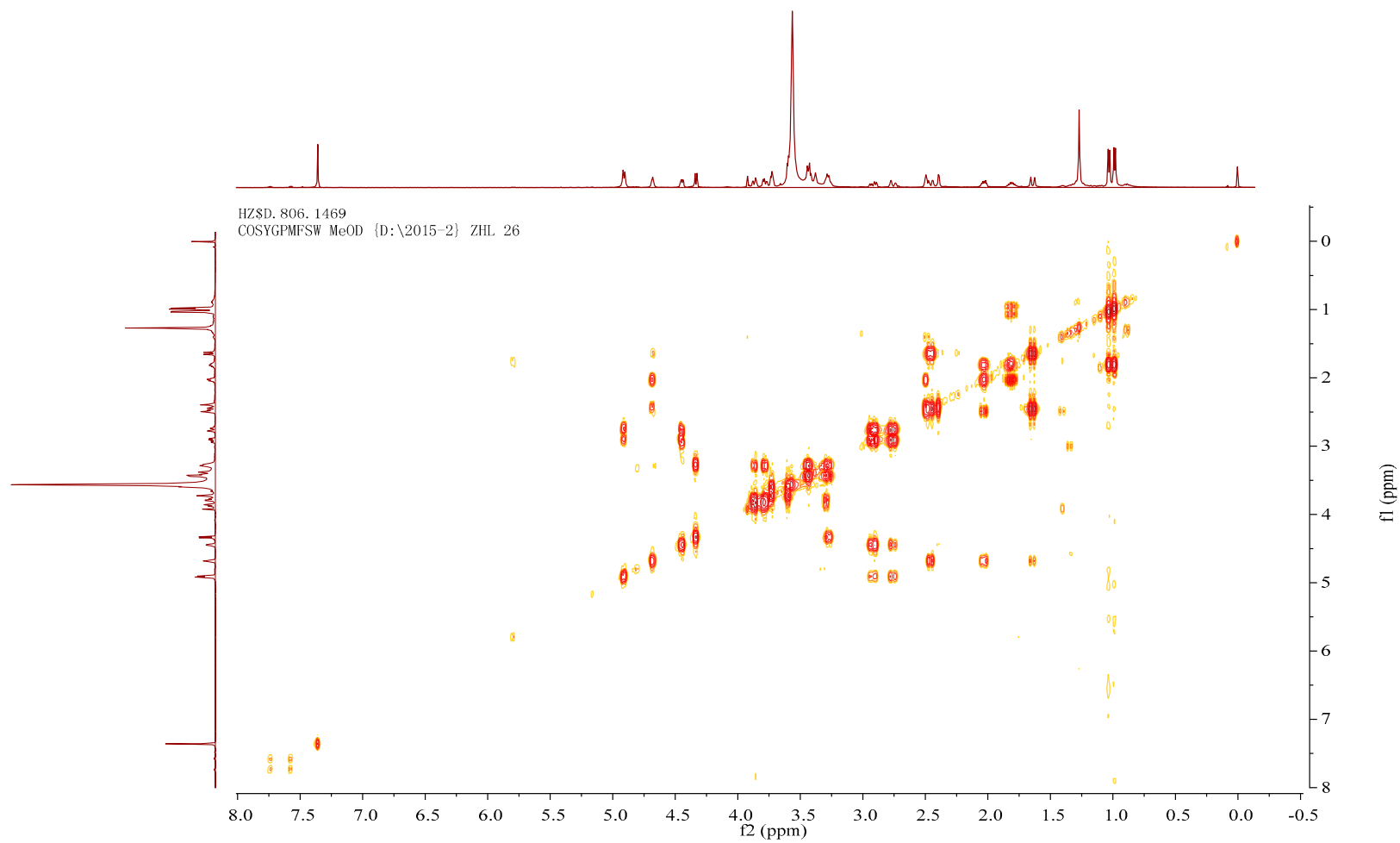


Figure S20. ^{13}C -NMR spectra of compound 2 in CD_3OD .



Finger S21. HSQC spectra of compound **2** in CD₃OD.



Finger S22. ^1H - ^1H COSY spectra of compound **2** in CD_3OD .

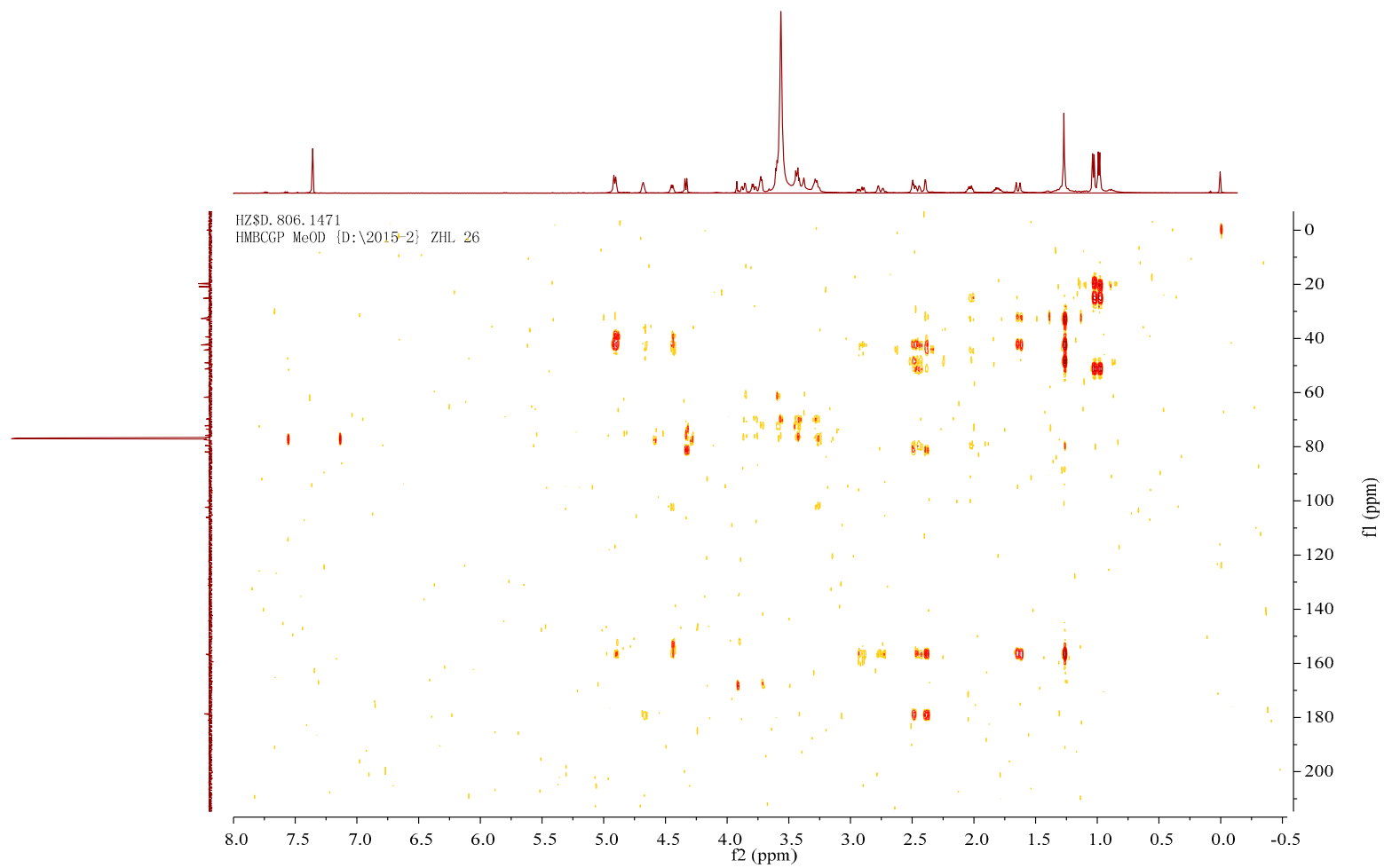


Figure S23. HMBC spectra of compound 2 in CD₃OD.

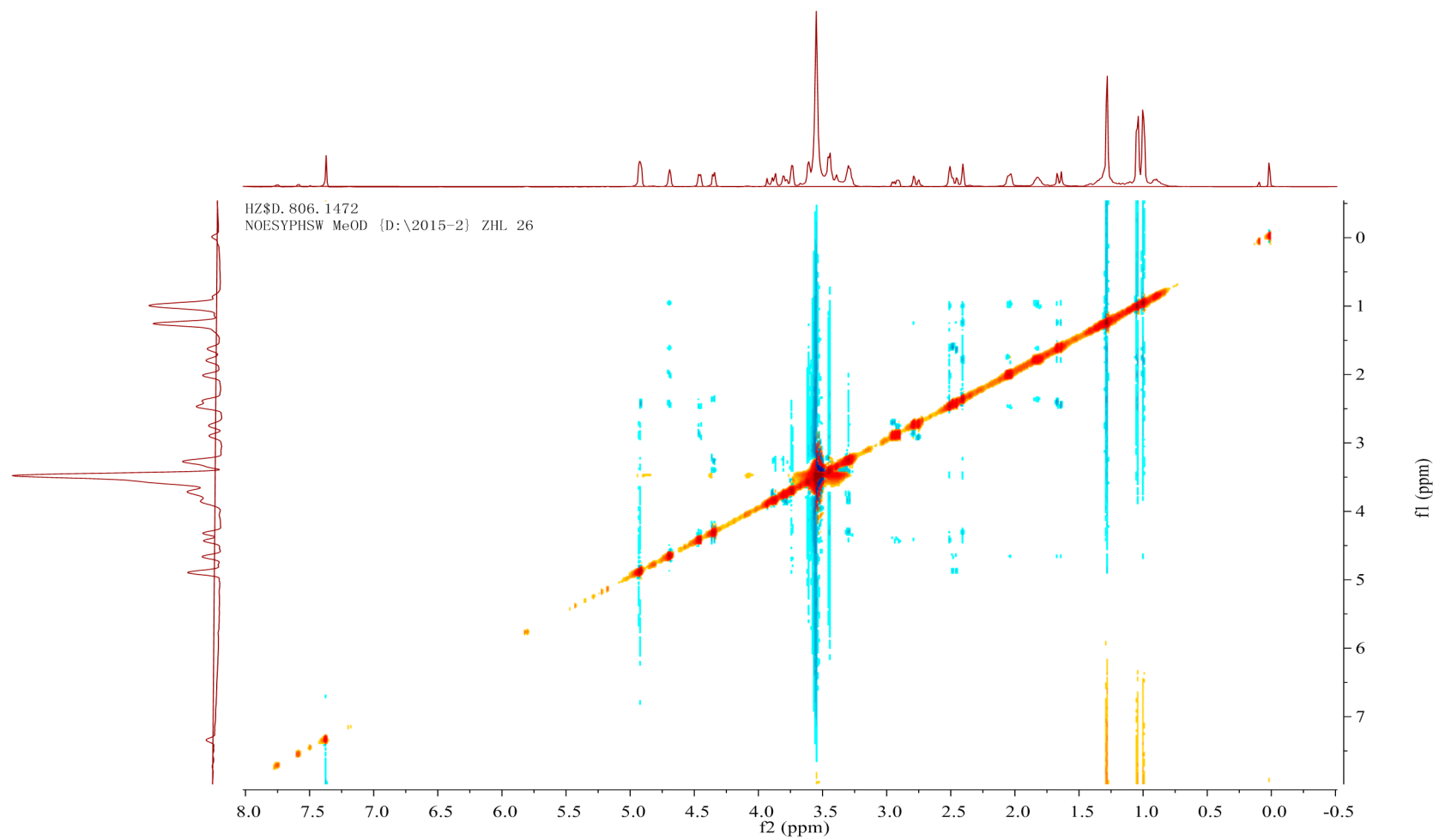


Figure S24. NOESY spectra of compound 2 in CD₃OD.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 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

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

Elements Used:

C: 5-80 H: 2-120 O: 0-20 Na: 0-1

wyy-10

LCT PXE KE324

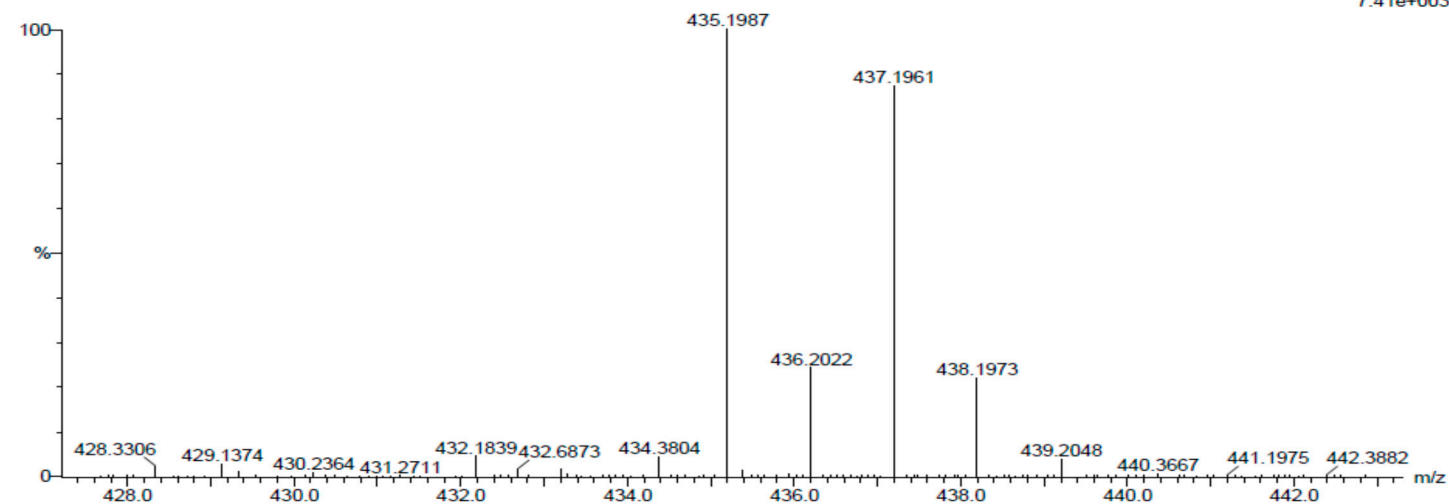
14-Oct-2015

14:02:31

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7.41e+003

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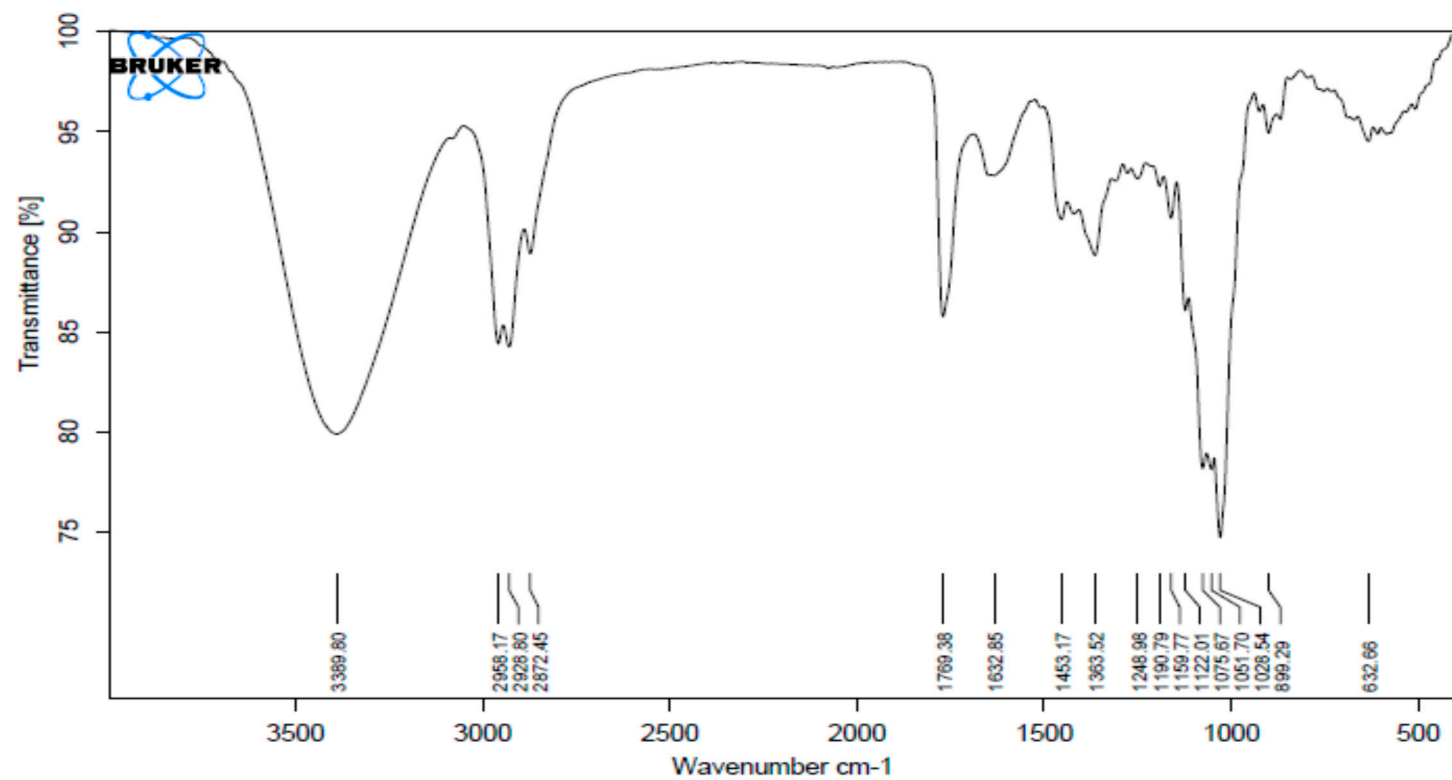
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Maximum: 5.0 5.0 -1.5

5.0 50.0

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435.1987	435.1995	-0.8	-1.8	5.5	141.0	0.0	C21 H32 O8 Na

Figure S25. HRESIMS spectrum of compound 2.



E:\DATABASE\MEAS\20151121\WYY-10.0	WYY-10	Instrument type and / or accessory	26/11/2015
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Figure S26. IR spectra of compound 2.

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Department (None Entered)
Organization (None Entered)
Information (None Entered)

Date of Report 2015-9-16
Time of Report 23:11:36下午

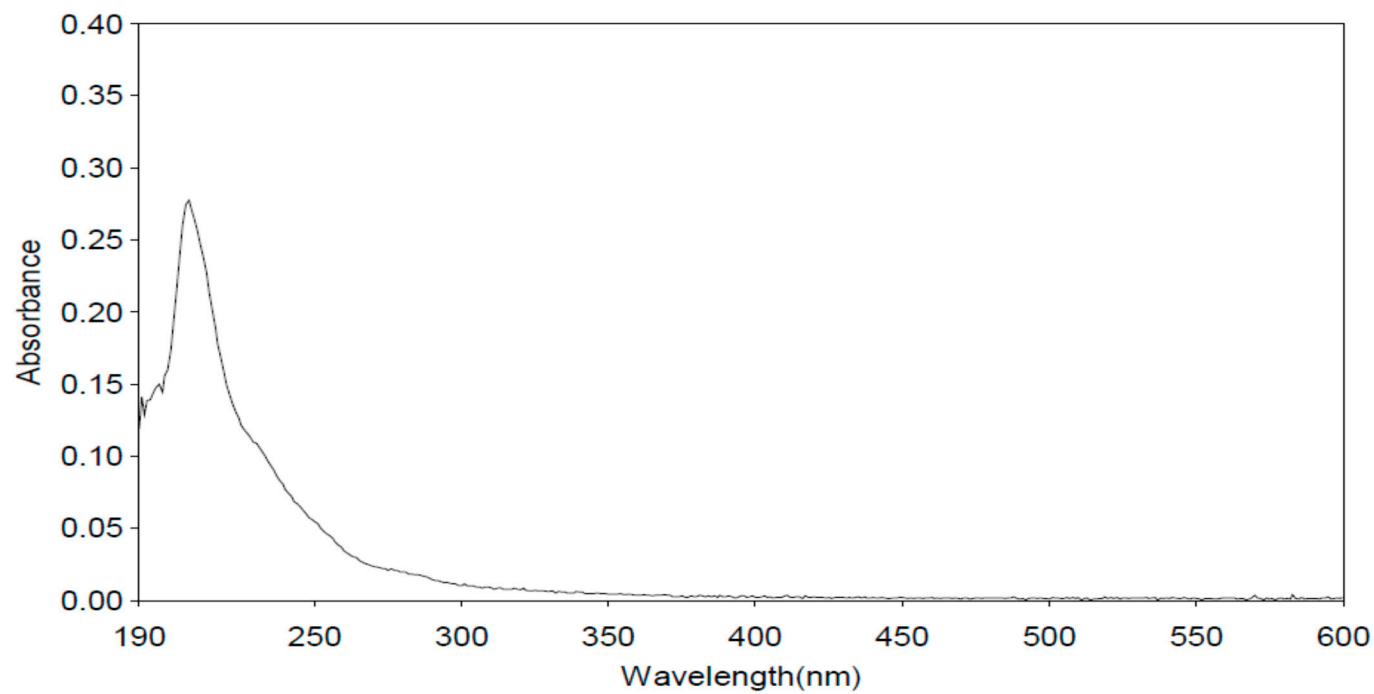
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Figure S27. UV spectra of compound 2.

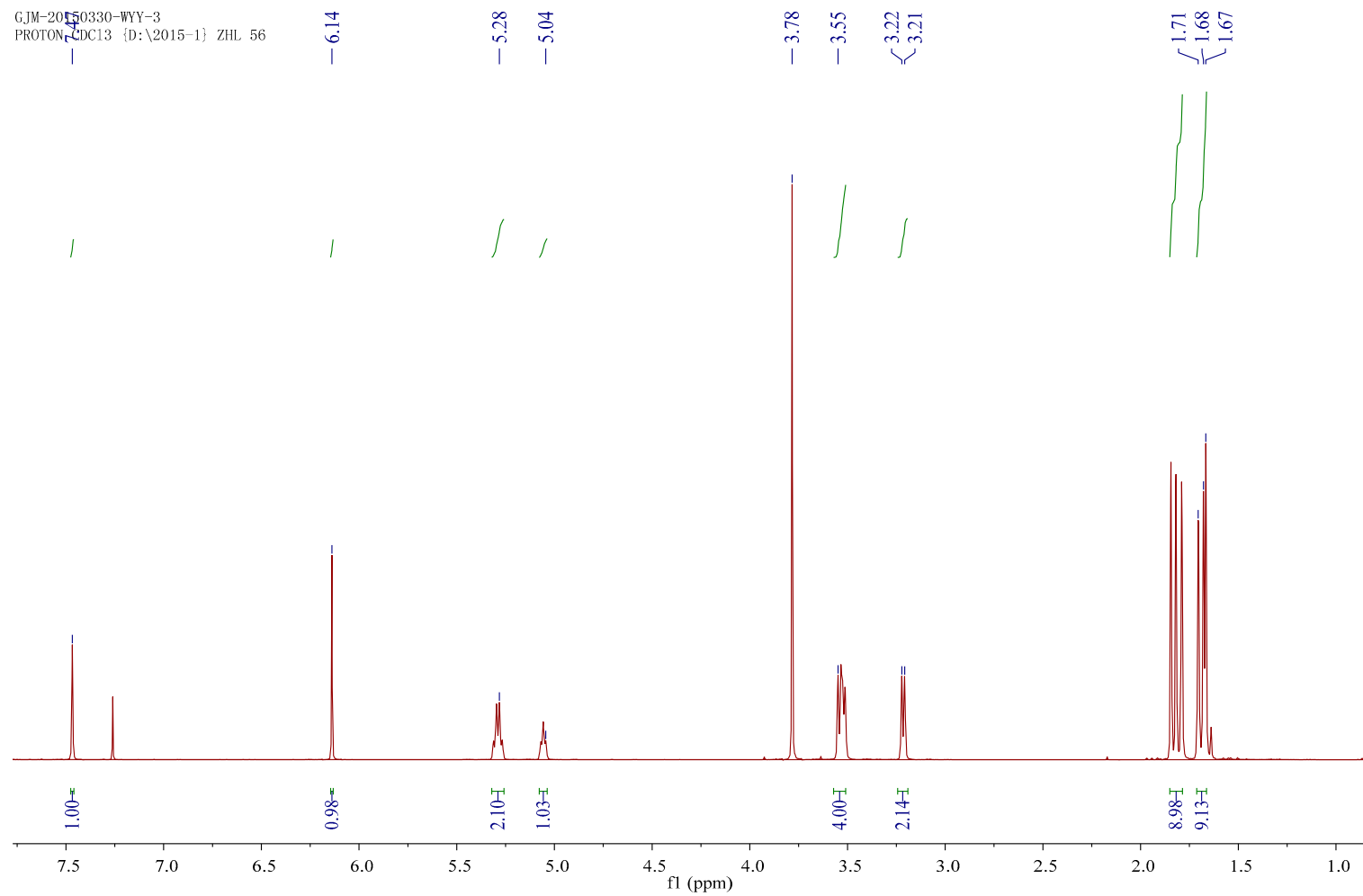


Figure S28. $^1\text{H-NMR}$ spectra of compound **3** in CDCl_3 .

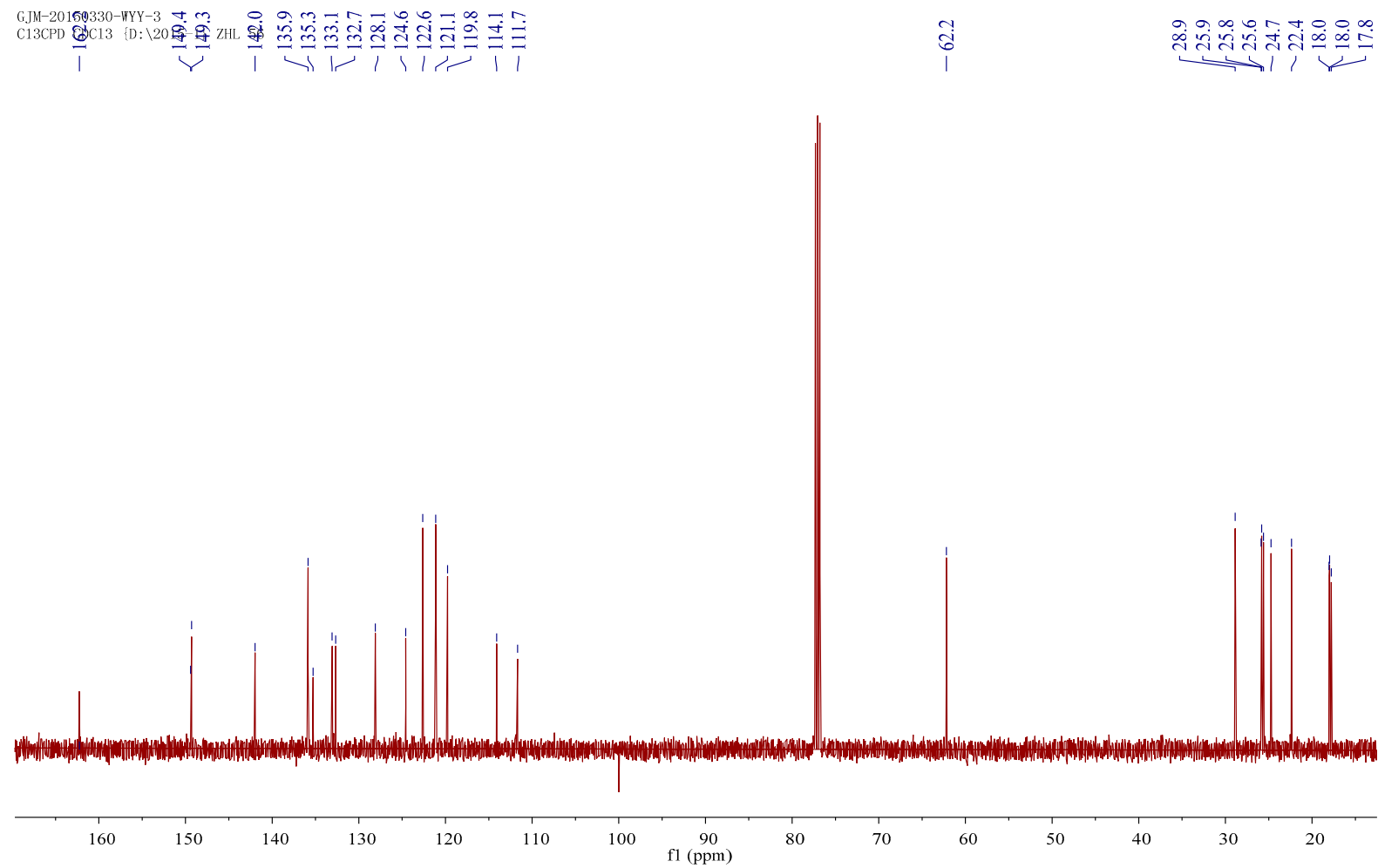
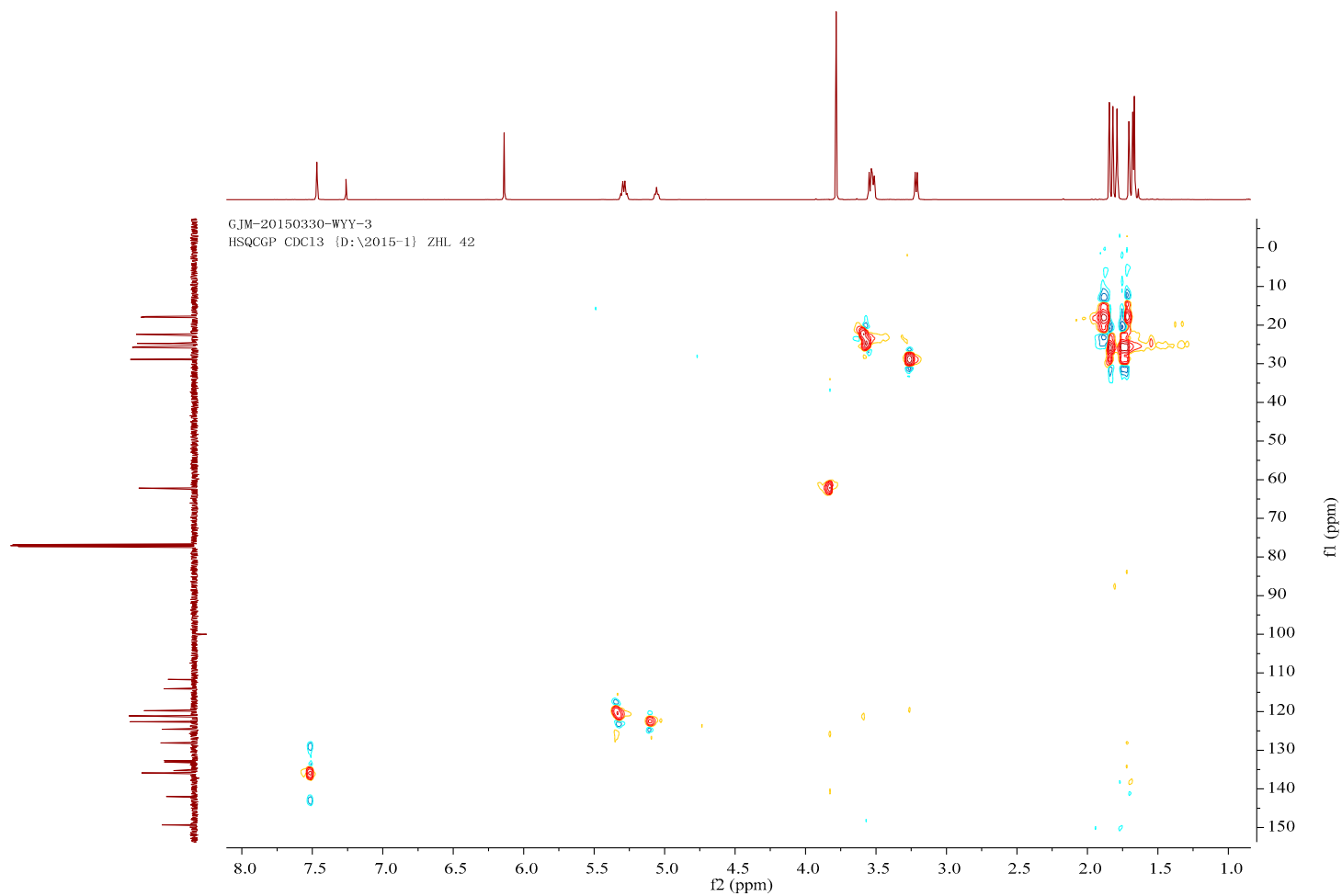
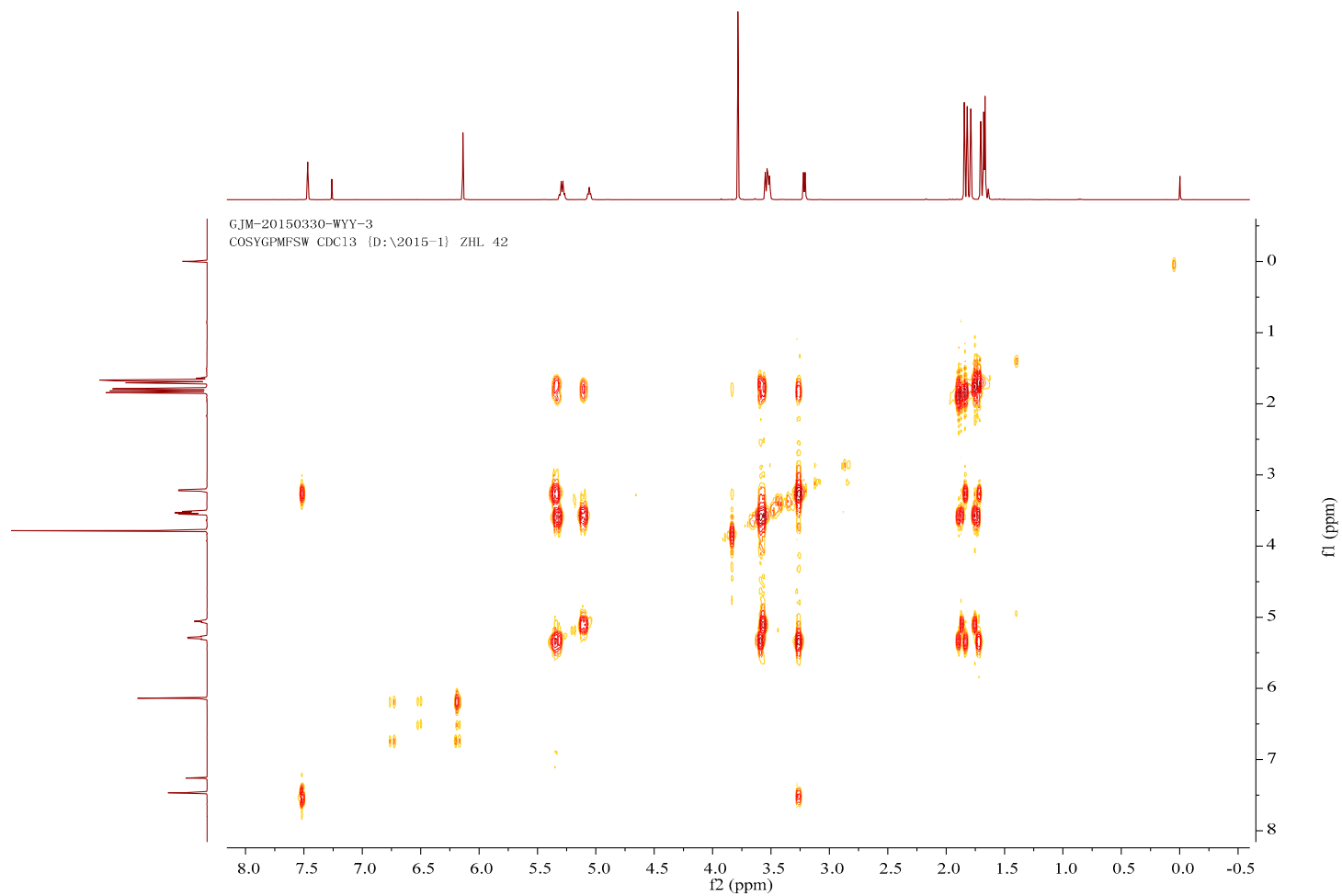


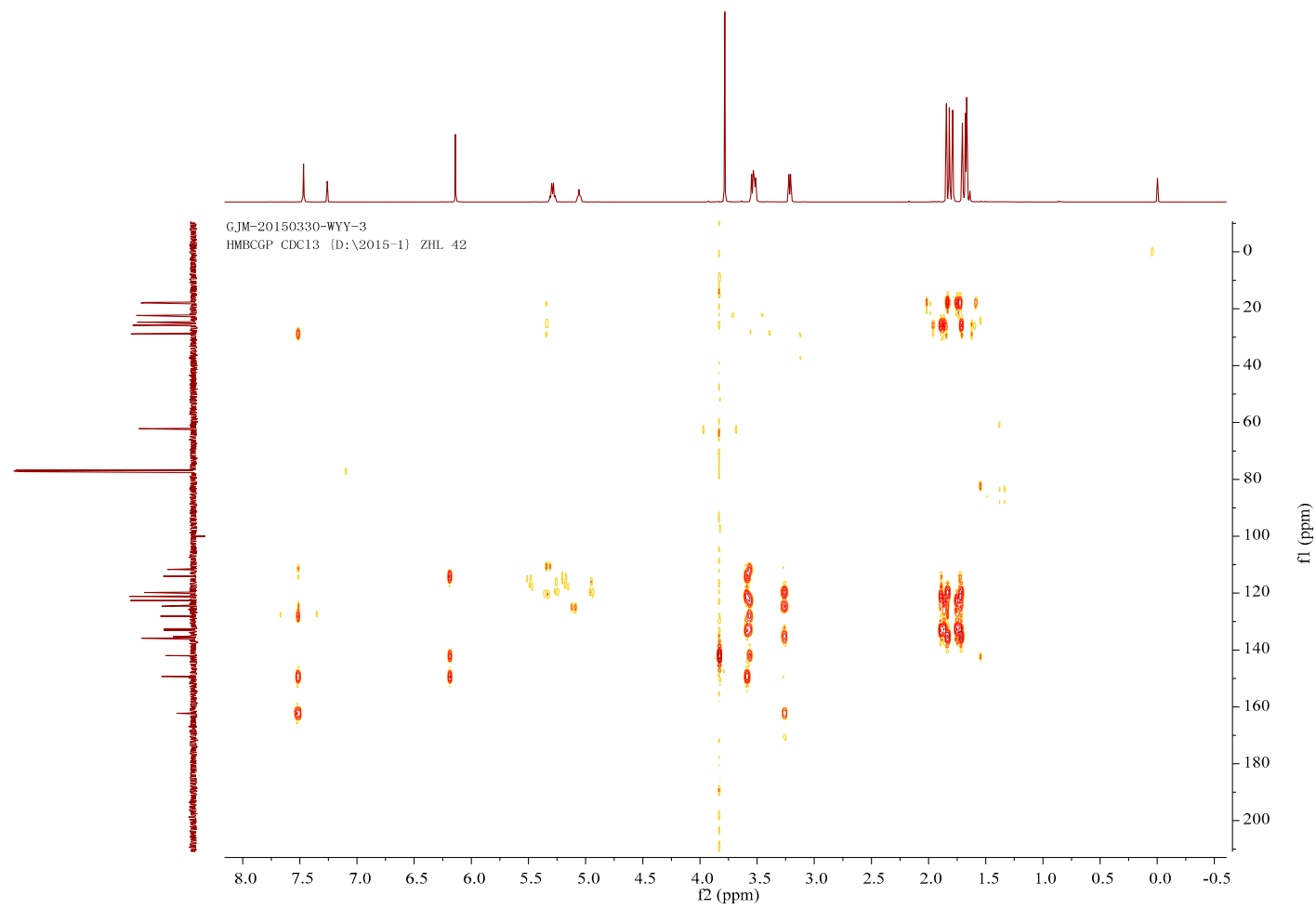
Figure S29. ^{13}C -NMR spectra of compound 3 in CDCl_3 .



Finger S30. HSQC spectra of compound **3** in CDCl_3 .



Finger S31. ^1H - ^1H COSY spectra of compound **3** in CDCl_3 .



Finger S32. HMBC spectra of compound **3** in CDCl₃.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 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

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

Elements Used:

C: 5-80 H: 2-120 O: 0-20 Na: 0-1

wyy-3n

LCT PXE KE324

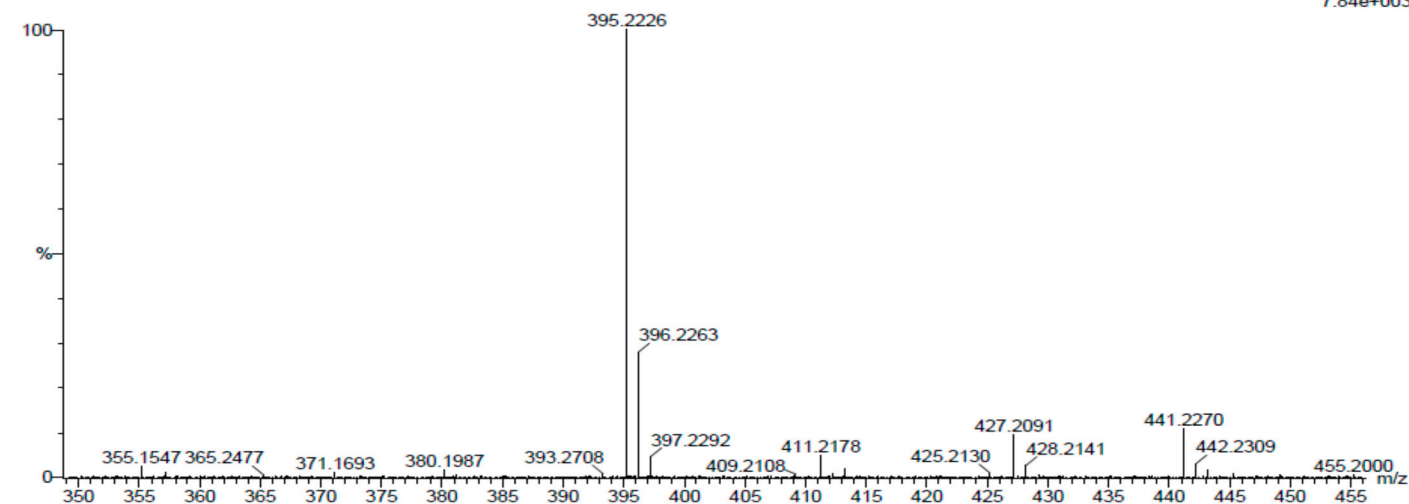
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7.84e+003

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Minimum:

Maximum: 5.0 5.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
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Figure S33. HRESTM of compound 3 in CD₃OD.

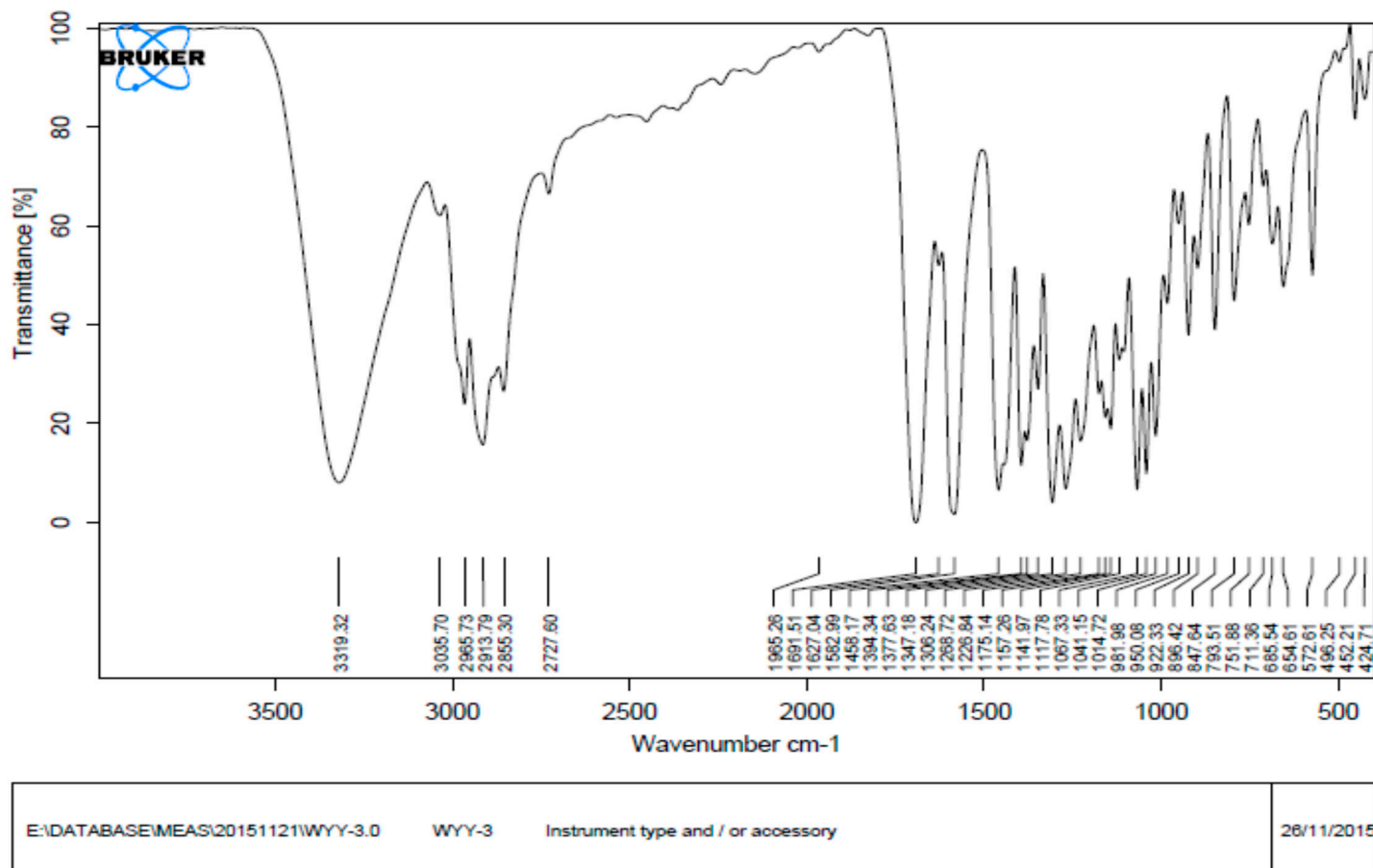


Figure S34. IR spectra of compound 3.

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Department (None Entered)
Organization (None Entered)
Information (None Entered)

Date of Report 2015-9-23
Time of Report 12:36:01下午

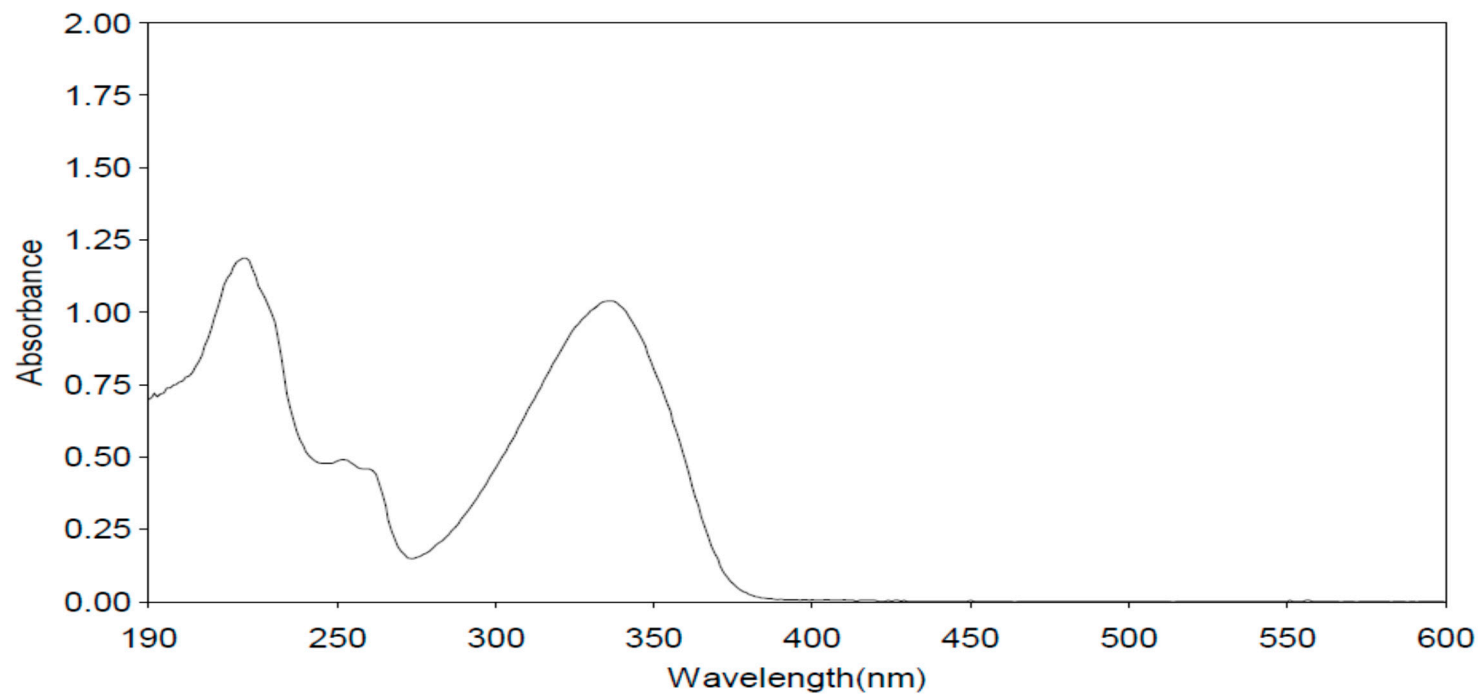
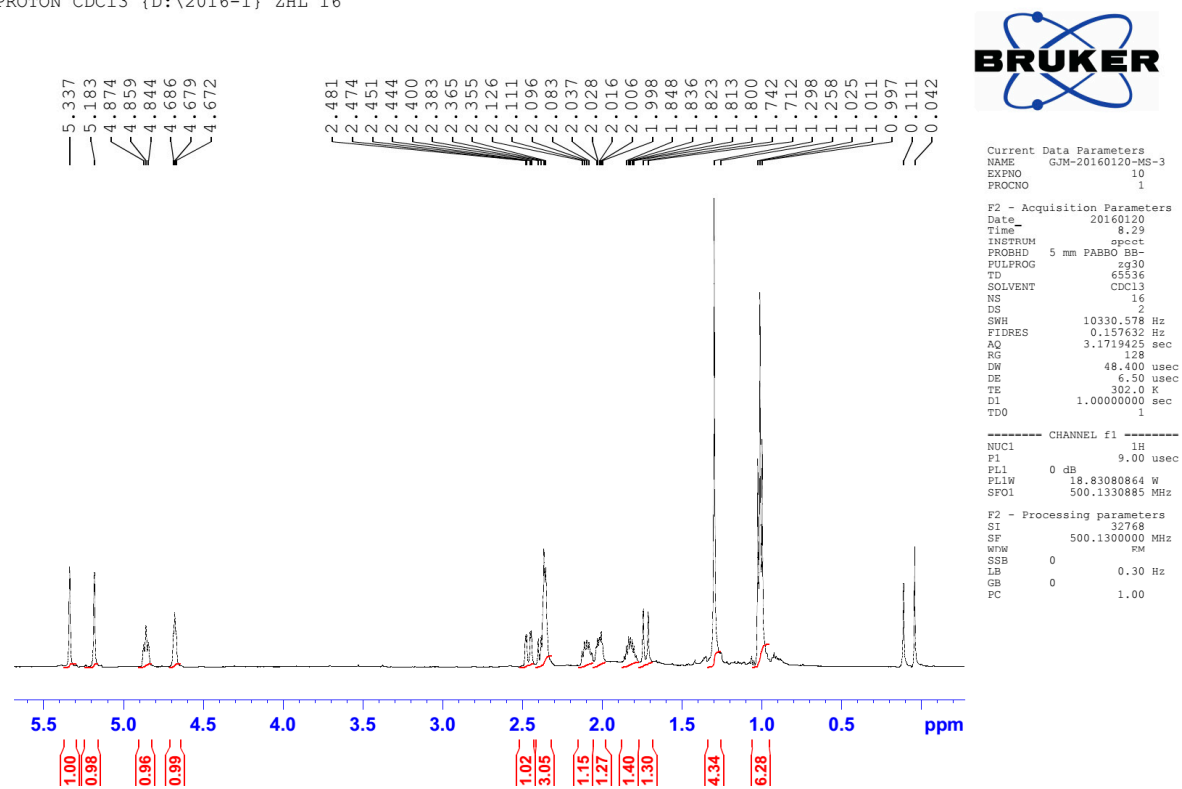
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Figure S35. UV spectra of compound 3.

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Figure S36. ¹H-NMR spectra of compound **1b** in CDCl₃.

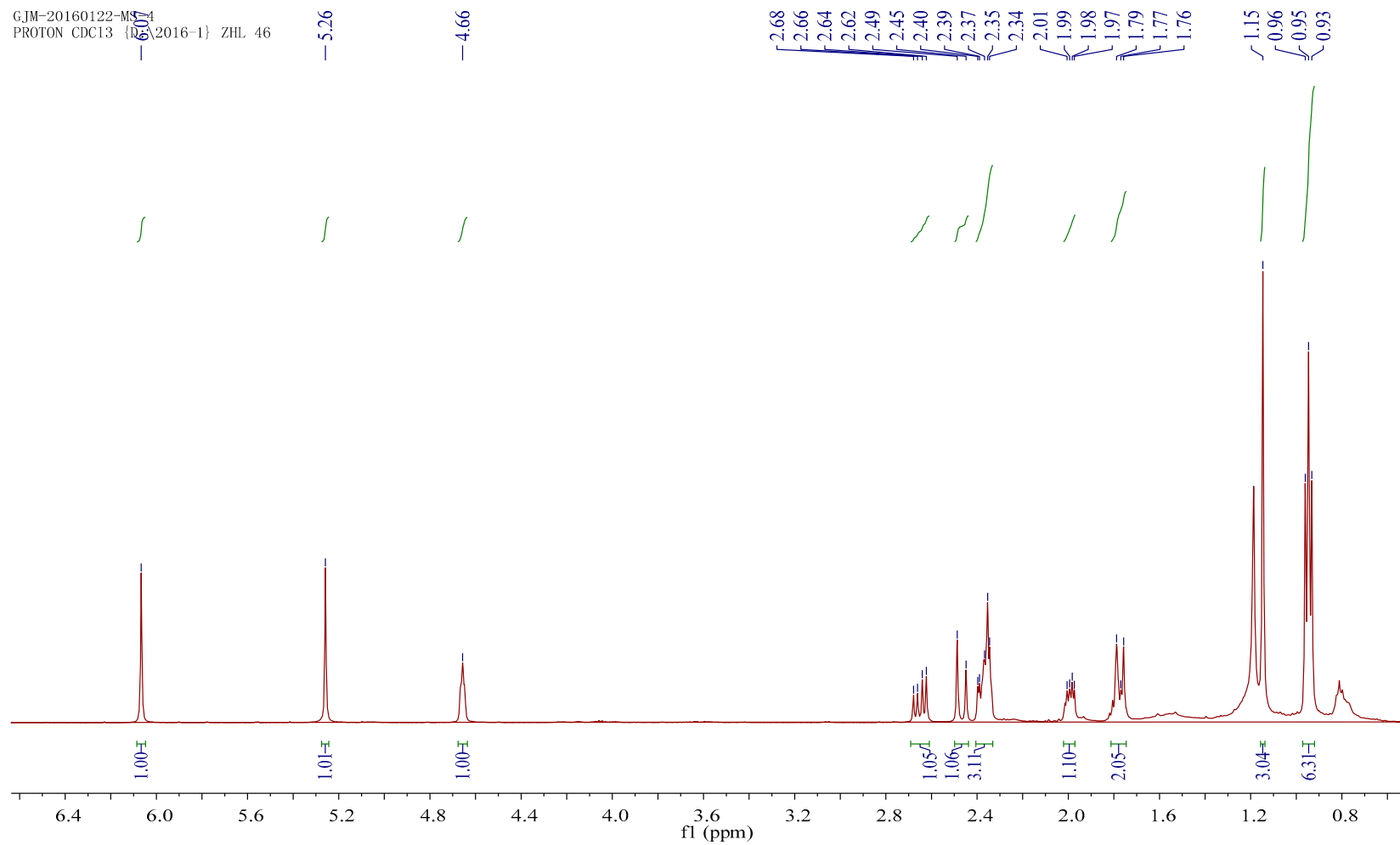


Figure S37. ^1H -NMR spectra of compound **1c** in CDCl_3 .

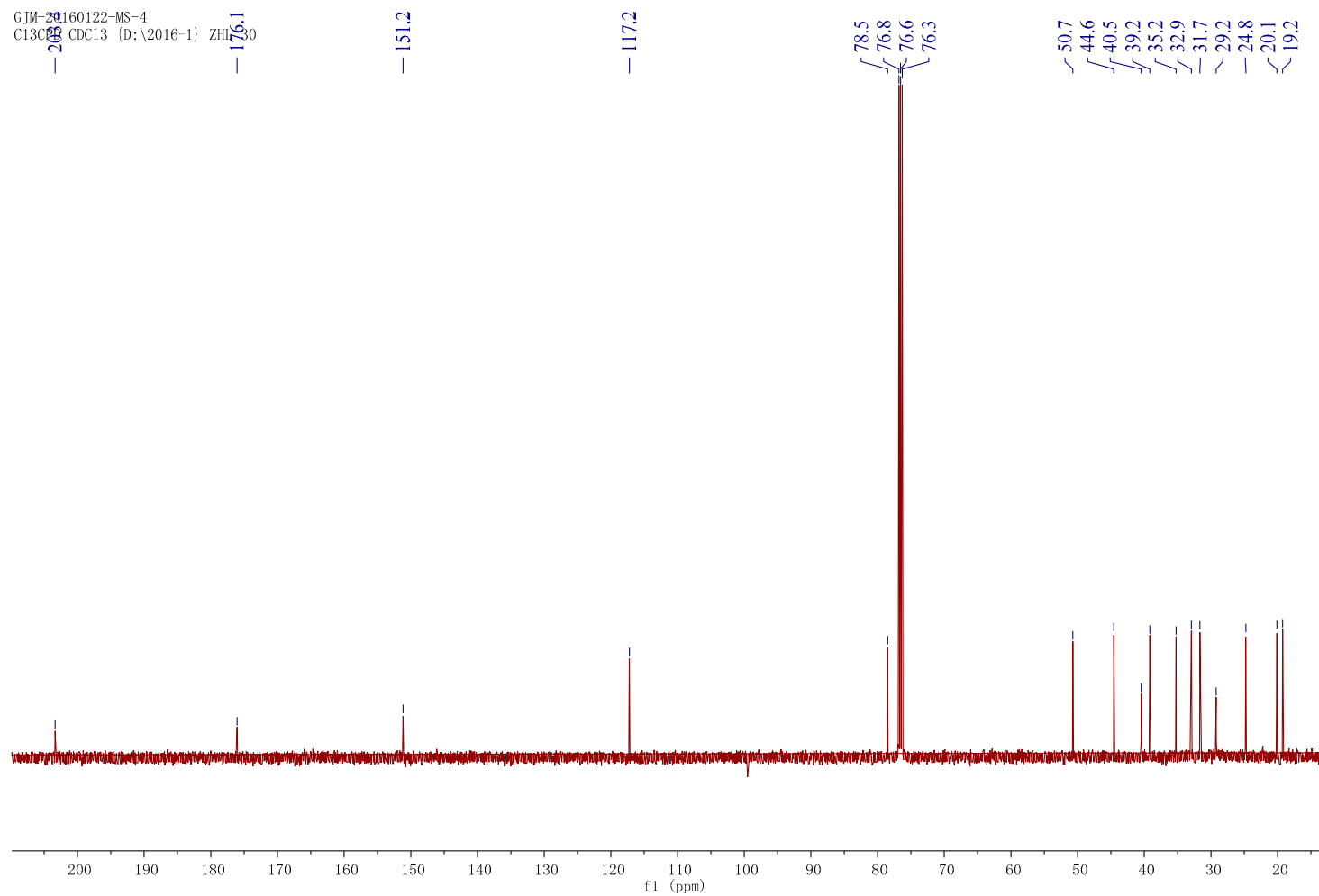
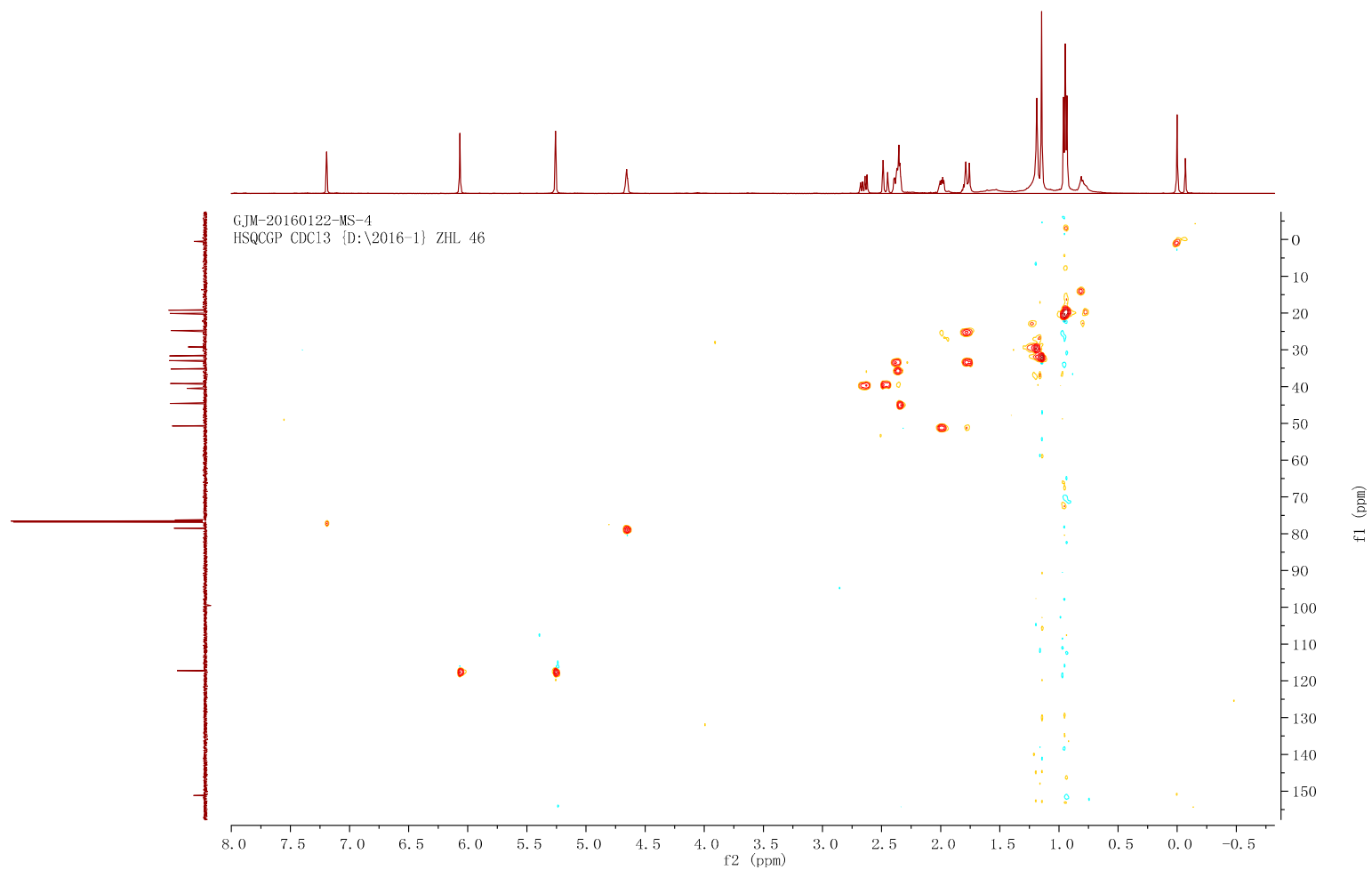
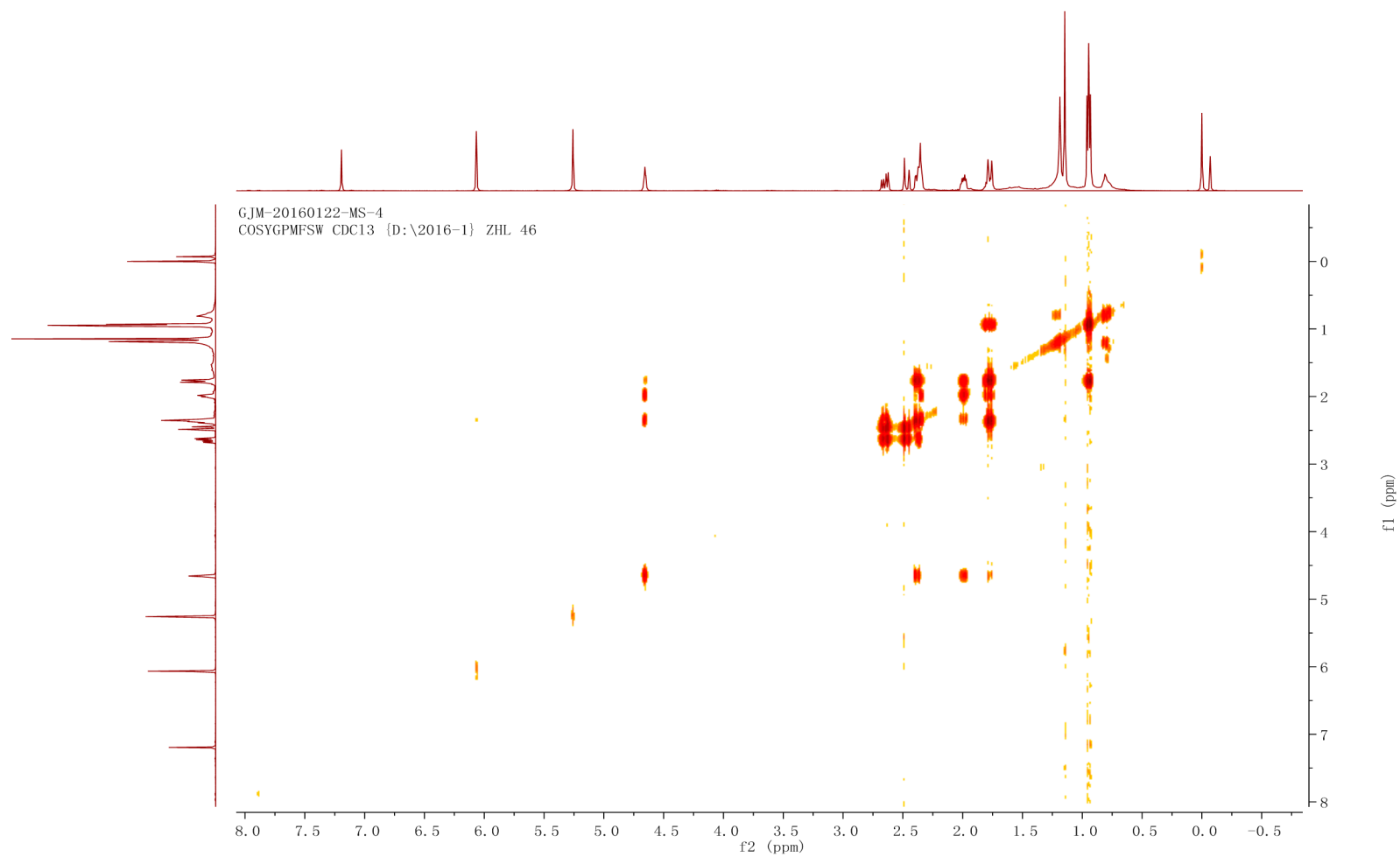


Figure S38. ^{13}C -NMR spectra of compound **1c** in CDCl_3 .



Finger S39. HSQC spectra of compound **1c** in CDCl₃.



Finger S40. ^1H - ^1H COSY spectra of compound **1c** in CDCl_3 .

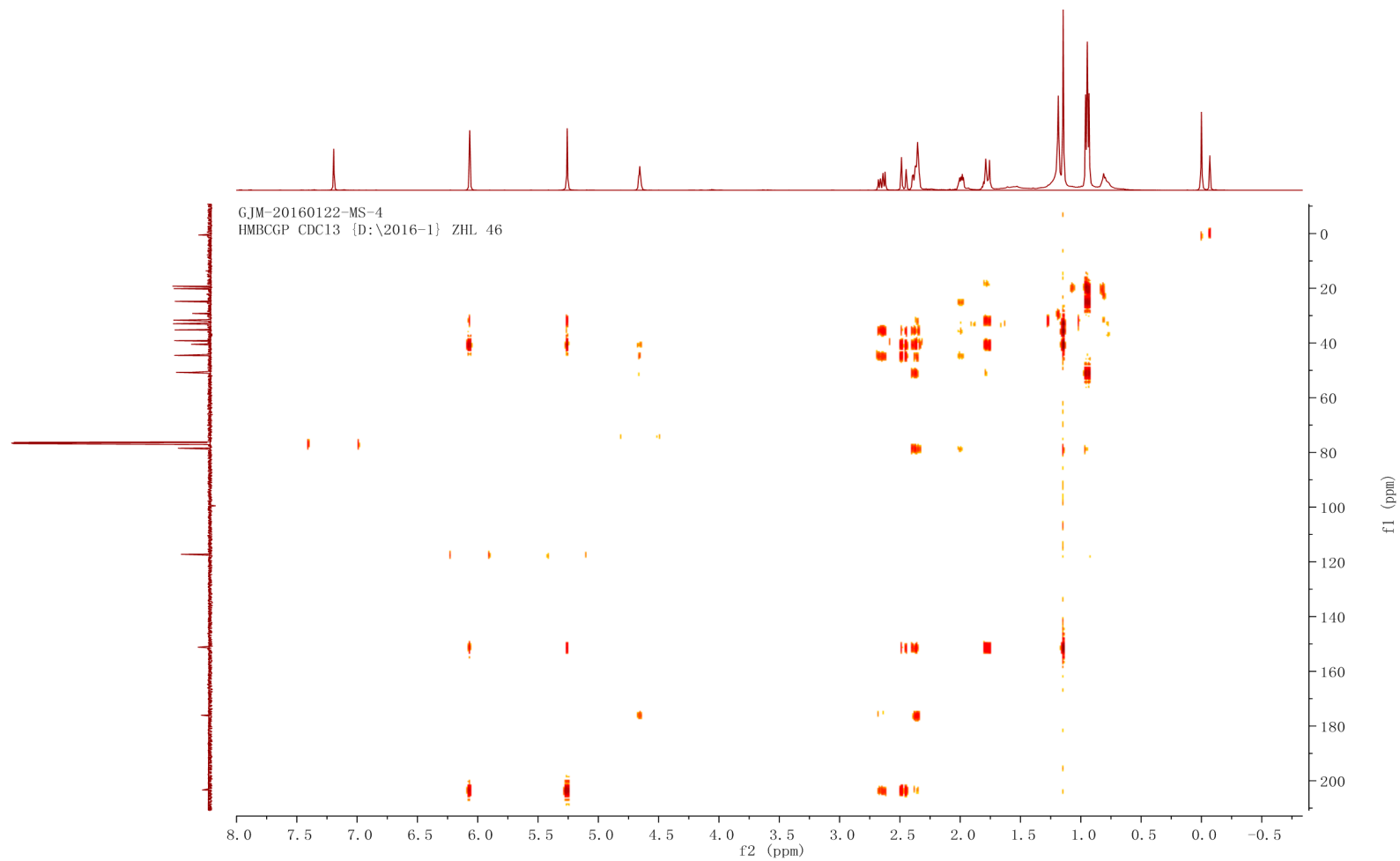


Figure S41. HMBC spectra of compound **1c** in CDCl_3 .

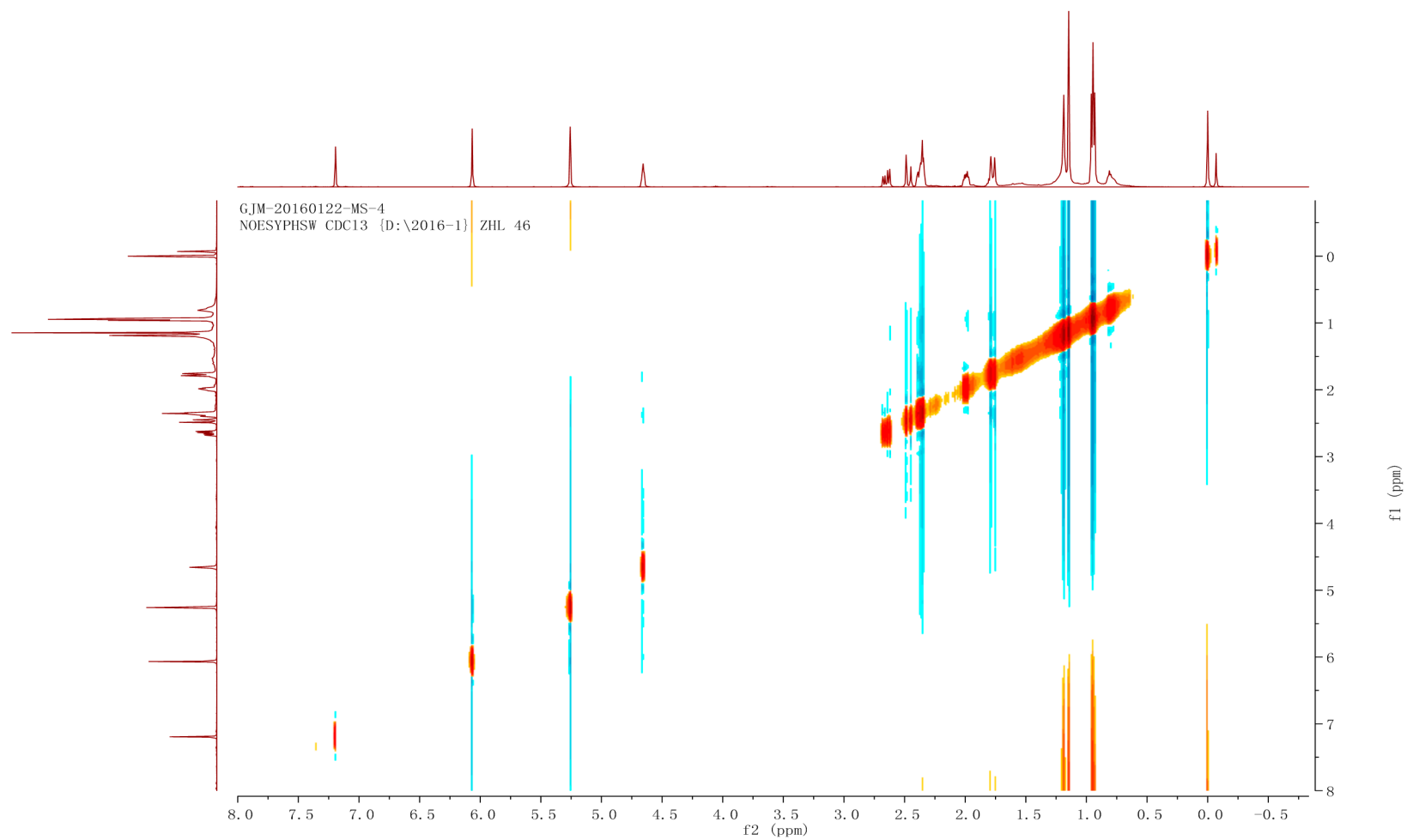


Figure S42. NOESY spectra of compound **1c** in CDCl₃.

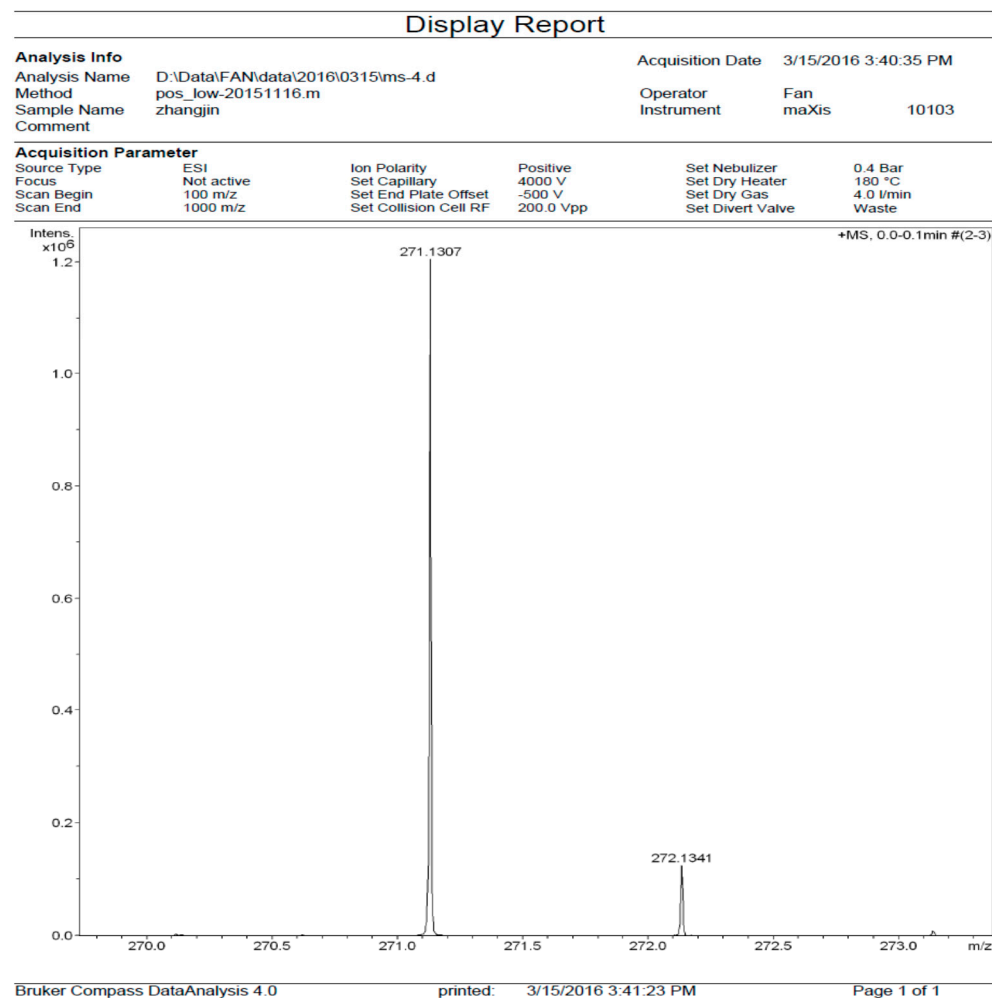


Figure S43. HRESIMS spectrum of compound **1c**.

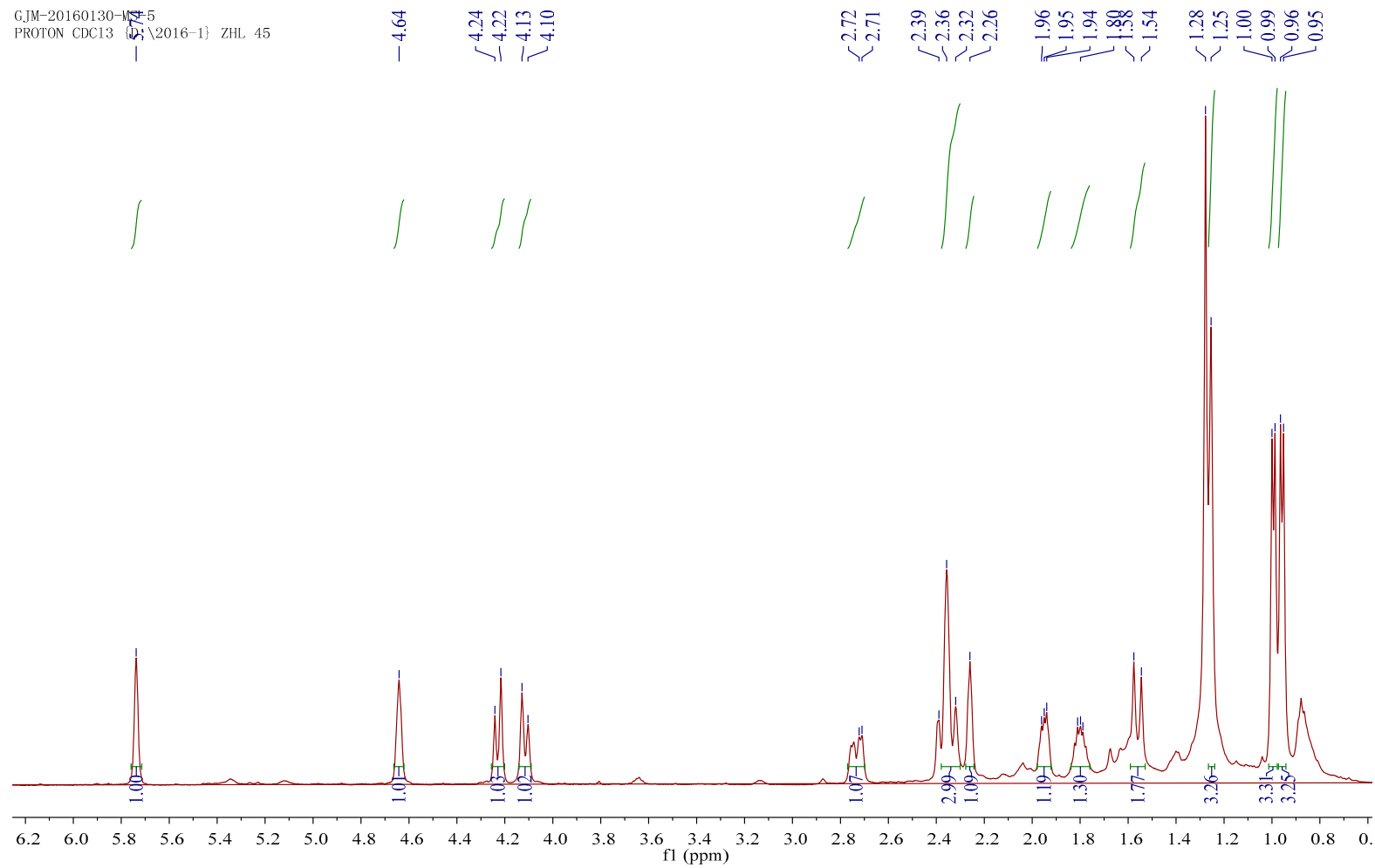


Figure S44. $^1\text{H-NMR}$ spectra of compound **1d** in CDCl_3 .

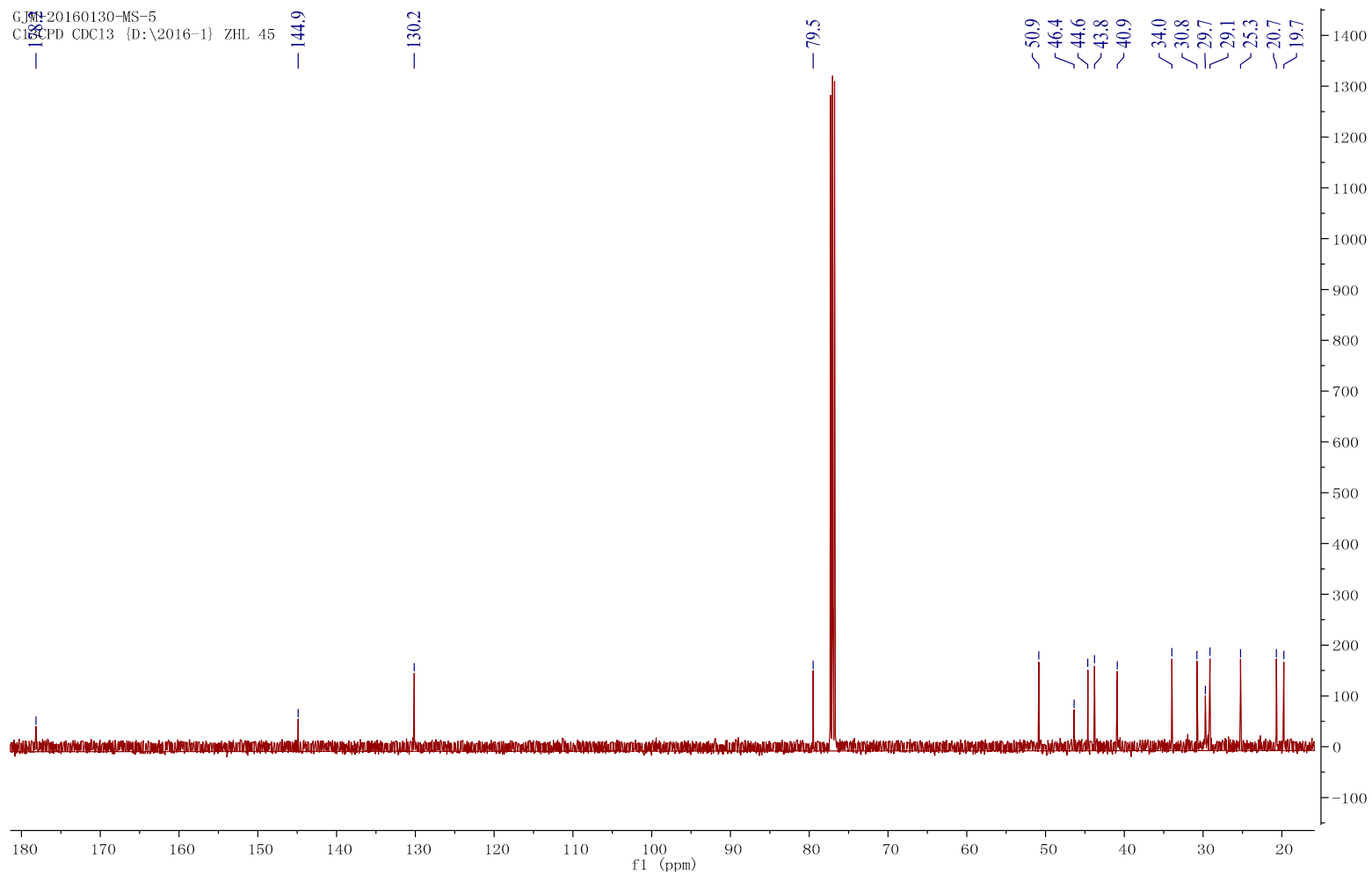


Figure S45. ¹³C-NMR spectra of compound **1d** in CDCl₃.

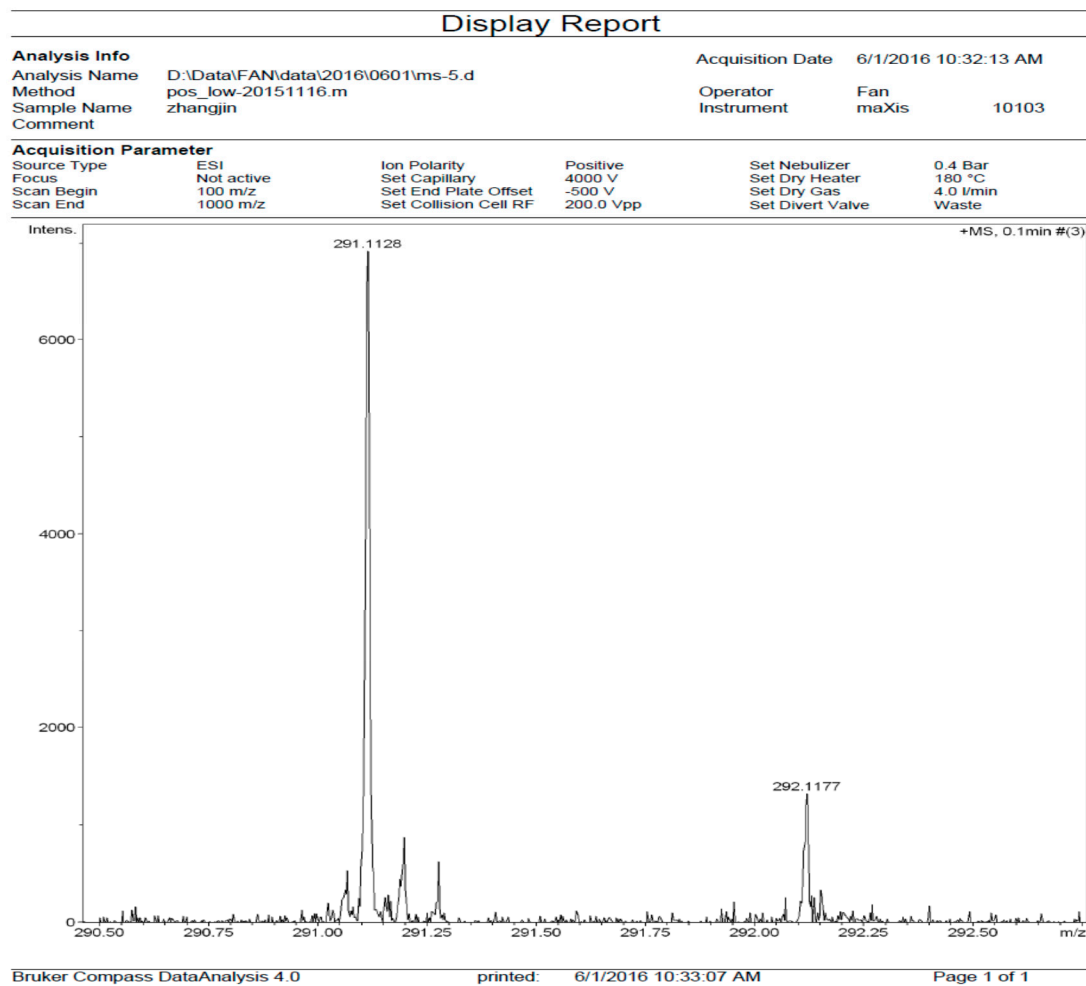


Figure S46. HRESIMS spectrum of compound **1d**.

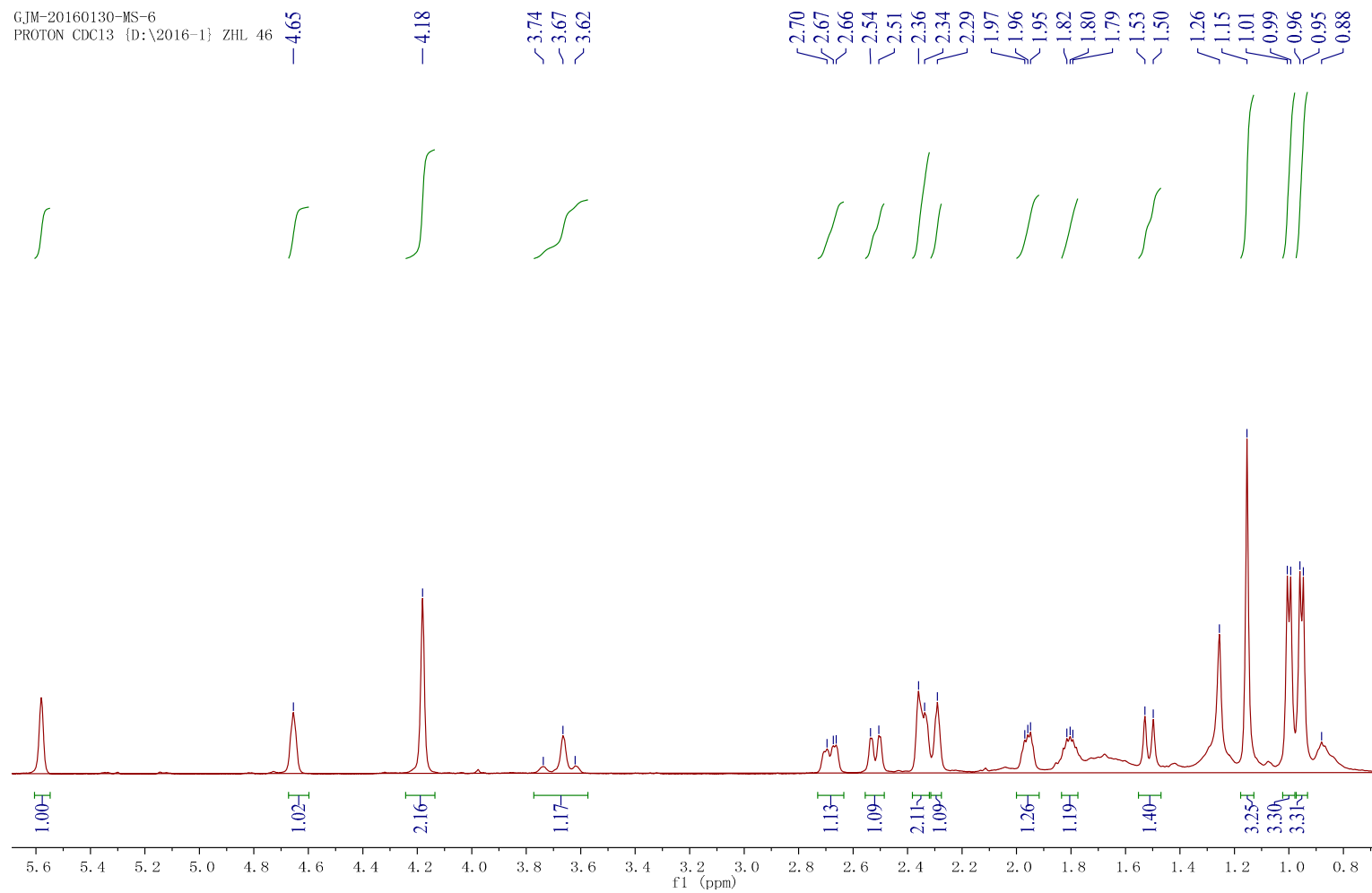


Figure S47. ^1H -NMR spectra of compound **1e** in CDCl_3 .

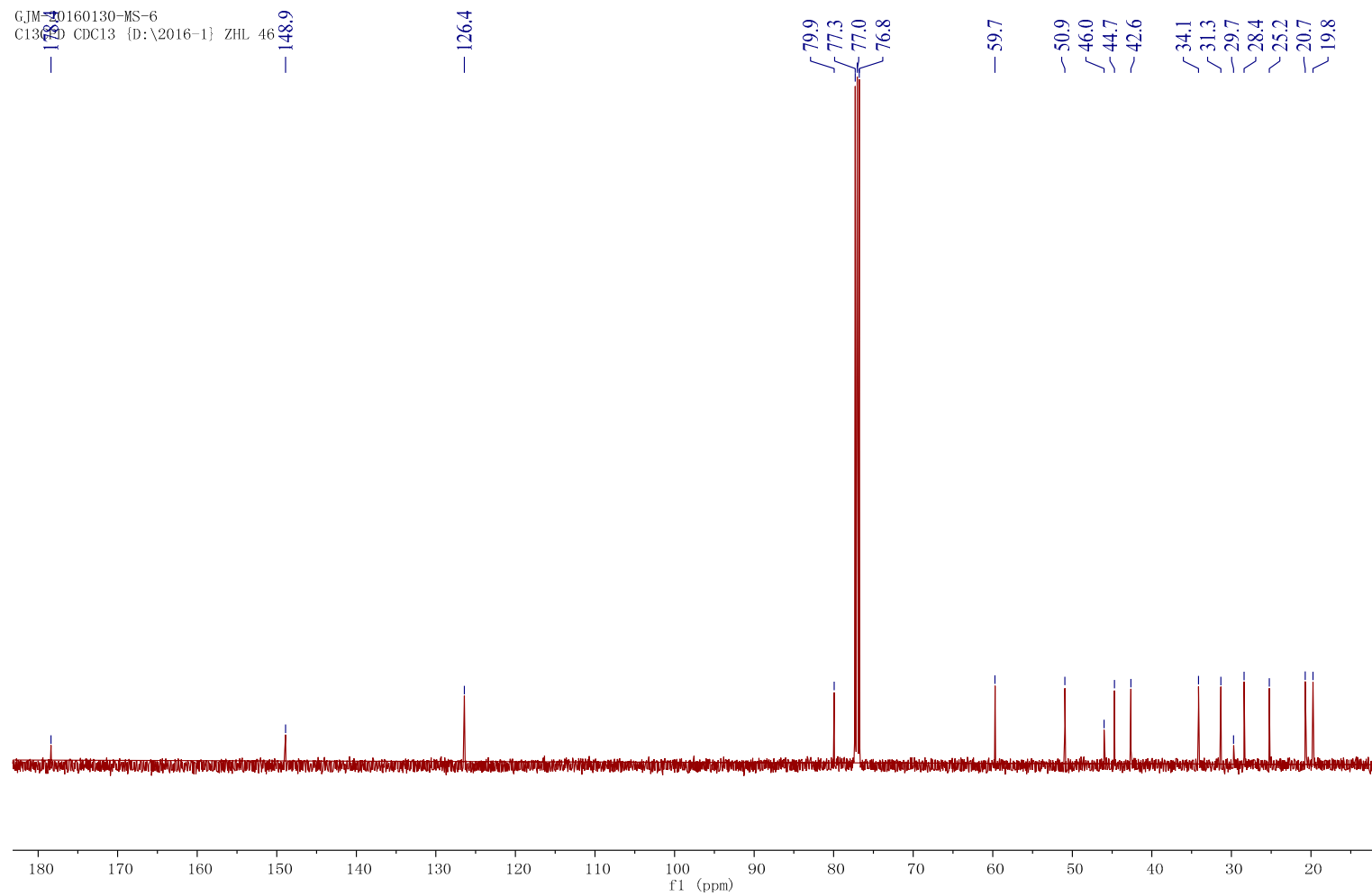


Figure S48. ^{13}C -NMR spectra of compound **1e** in CDCl_3 .

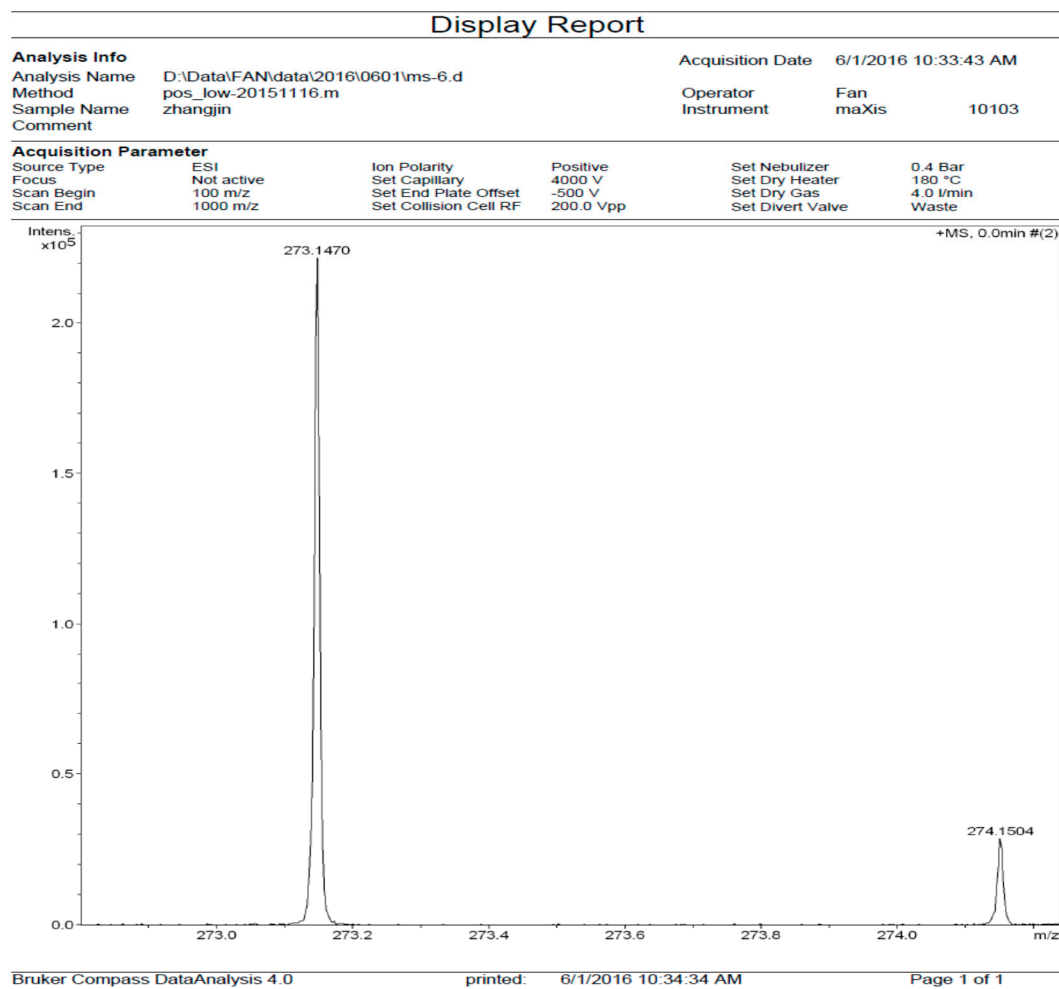


Figure S49. HRESIMS spectrum of compound **1e**.