

Supplementary Information

Anti-pulmonary fibrosis activities triterpenoids from the *Oenothera biennis*

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Abstract:

Five new triterpenoids, oenotheralanosterols C-G (1–5), with seven known triterpenoid compounds, namely 2 α ,3 α ,19 α -trihydroxy-24-norurs4,12-dien-28-oic acid (6), 3 β ,23-dihydroxy-1-oxo-olean-12-en-28-oic acid (7), reimagine C (8), knoxivalic acid A (9), termichebulolide (10), rosasecotriterpene A (11), rosanortriterpene C (12), were extracted and separated from the dichloromethane part of *Oenothera biennis* L. The anti-pulmonary fibrosis activities of all the compounds against TGF- β 1 induced damage on normal human lung epithelial (BEAS-2B) cells were investigated in vitro. The results showed that compounds 1–2, 6, 8, and 11 exhibited significant anti-pulmonary fibrosis activities, with EC₅₀ values ranging from 4.7 μ M to 9.9 μ M.

Keywords: *Oenothera biennis* L.; Triterpenoids; Anti-pulmonary fibrosis activities; BEAS-2B cells; RTCA

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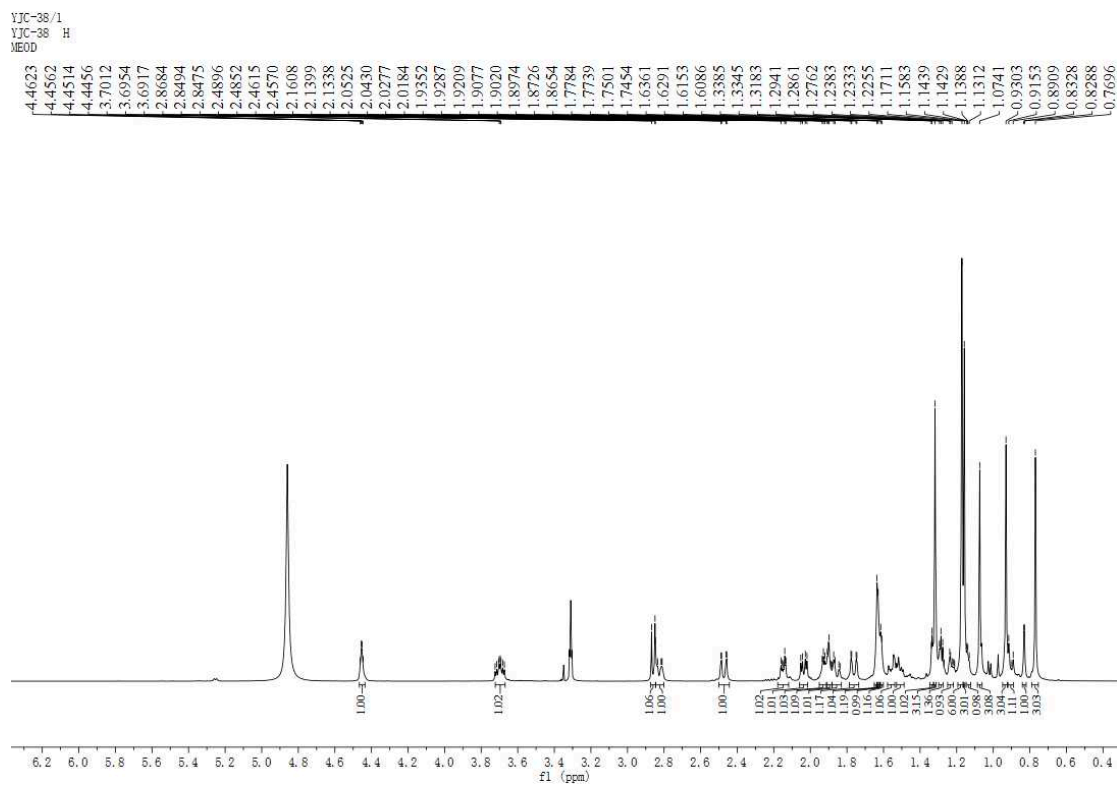


Figure S1. ^1H NMR spectrum (500 MHz, CD_3OD) of **1**

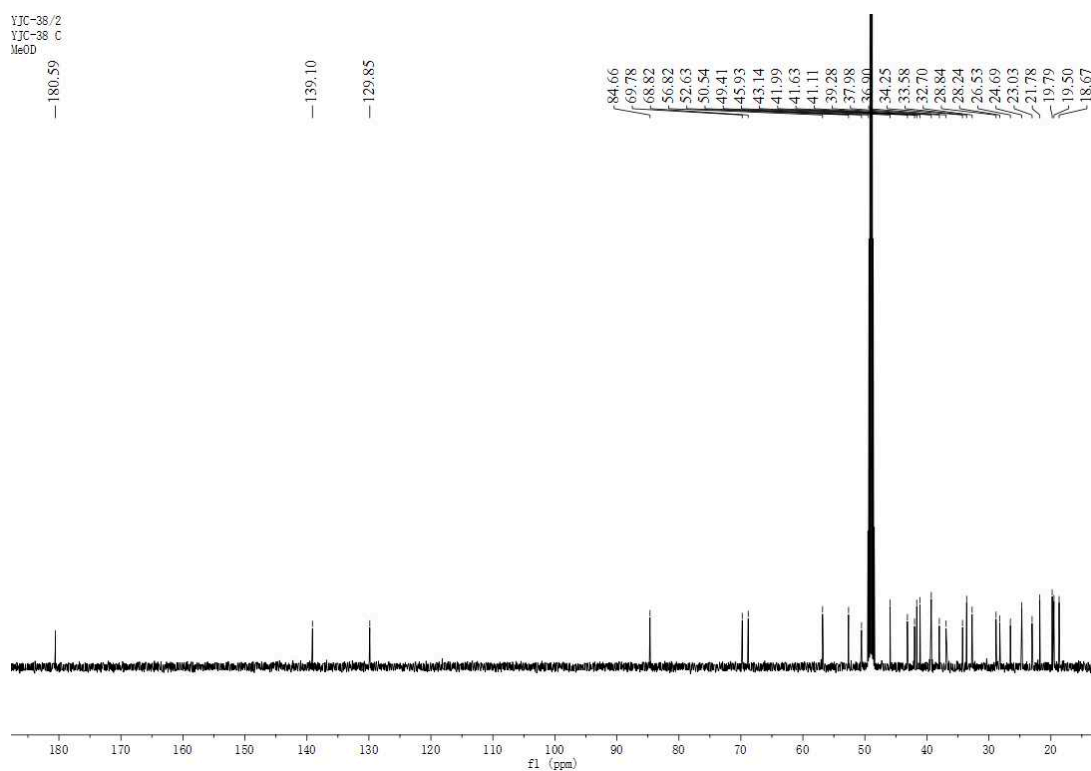


Figure S2. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **1**

YJC-38.3.fid
YJC-38 DEPT135
MEOD

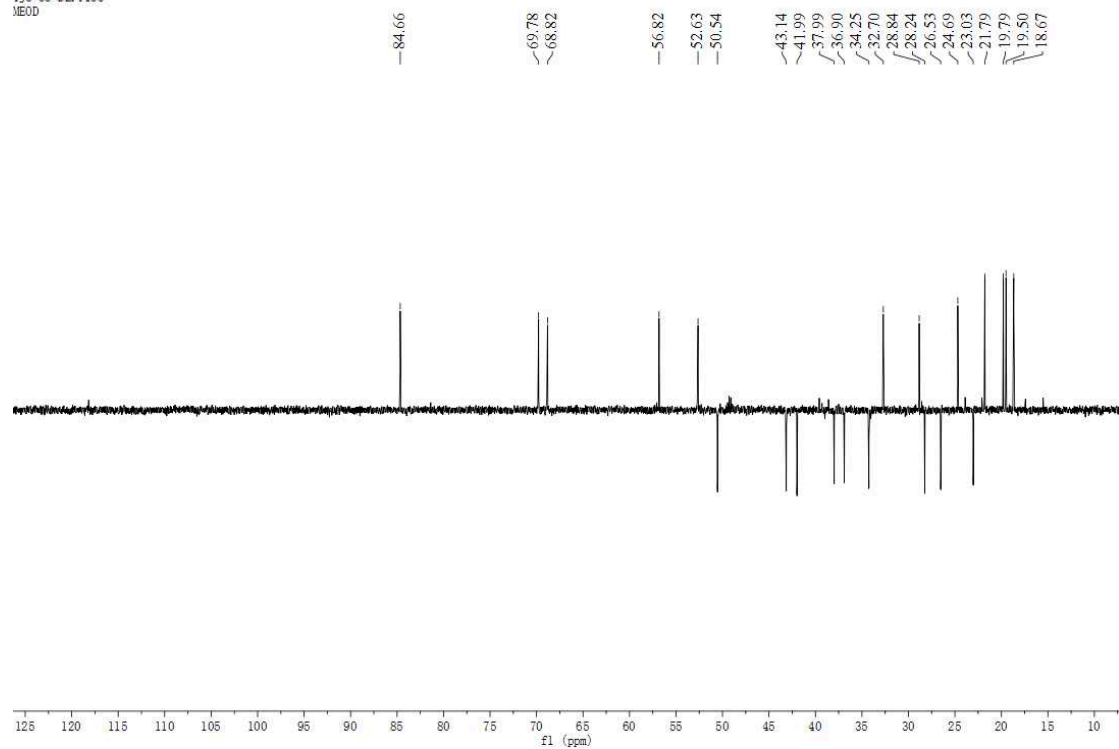


Figure S3. DEPT 135 spectrum (125 MHz, CD₃OD) of **1**

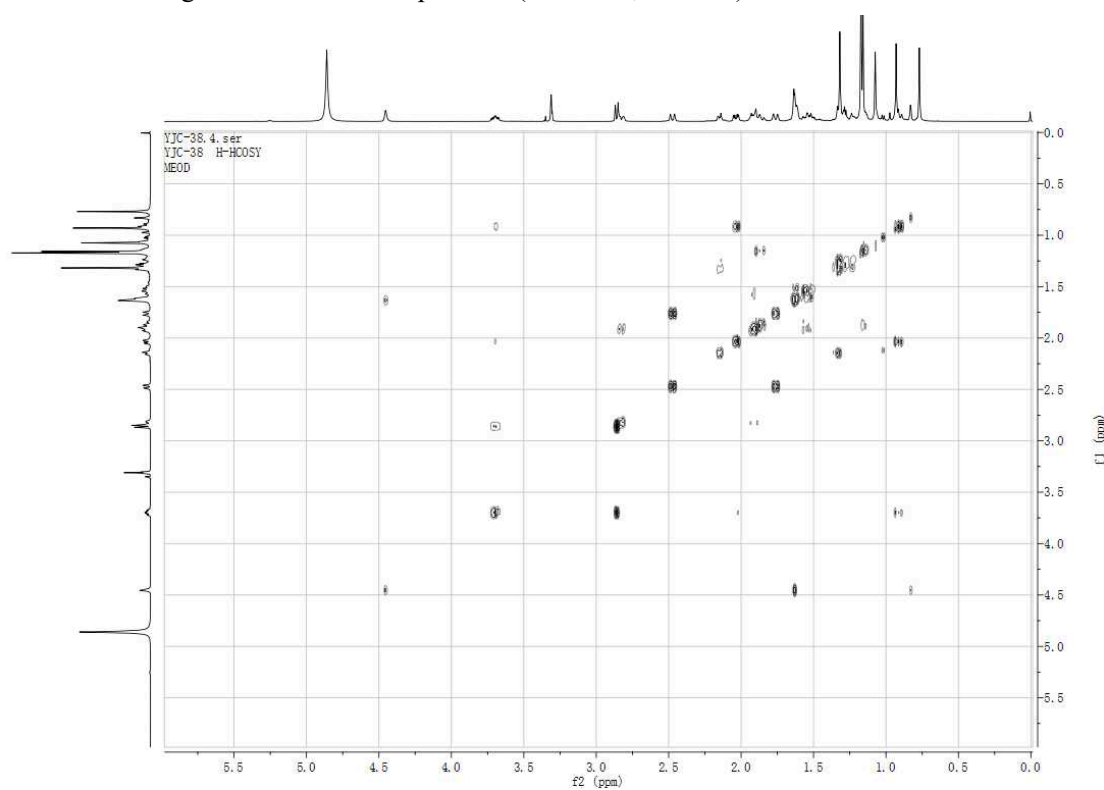


Figure S4. ¹H-¹H COSY spectrum of **1**

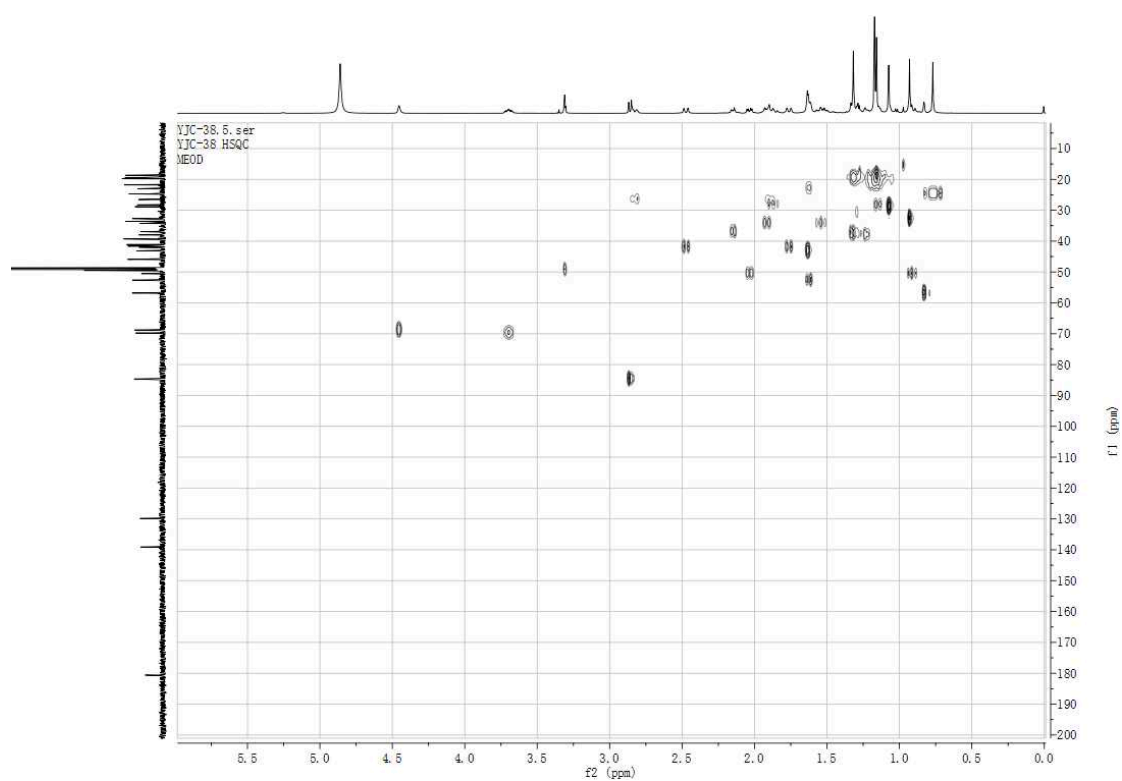


Figure S5. HSQC spectrum of **1**

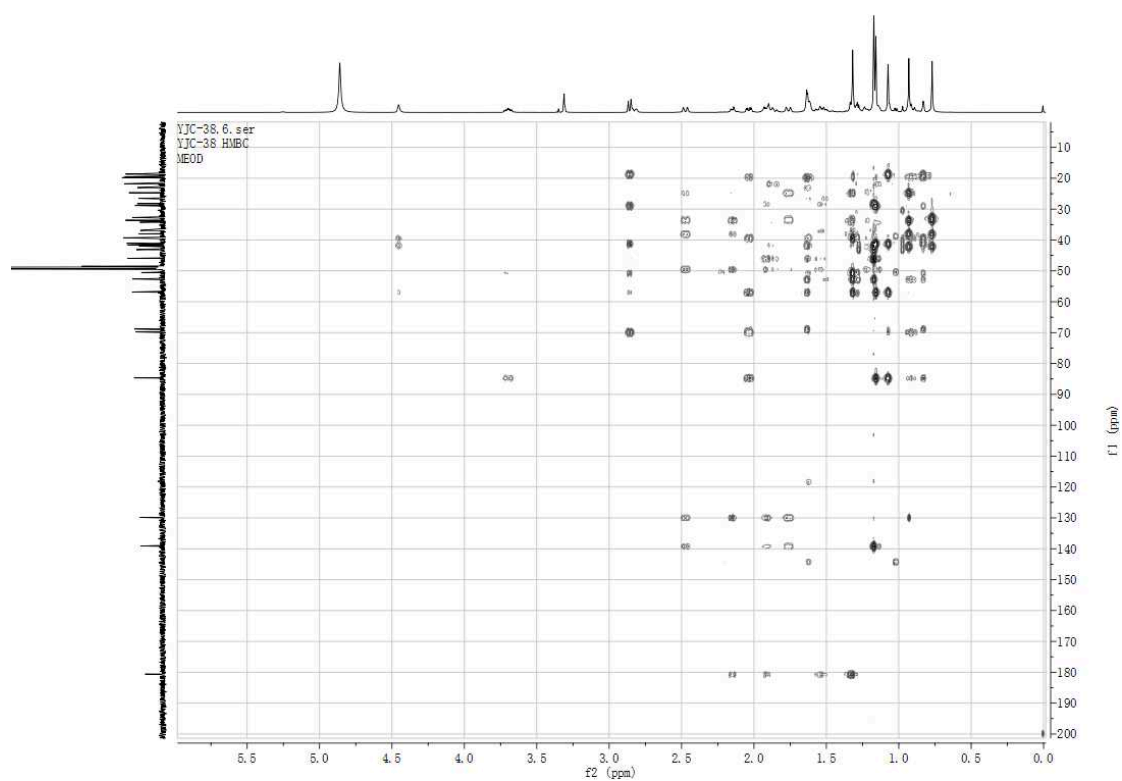


Figure S6. HMBC spectrum of **1**

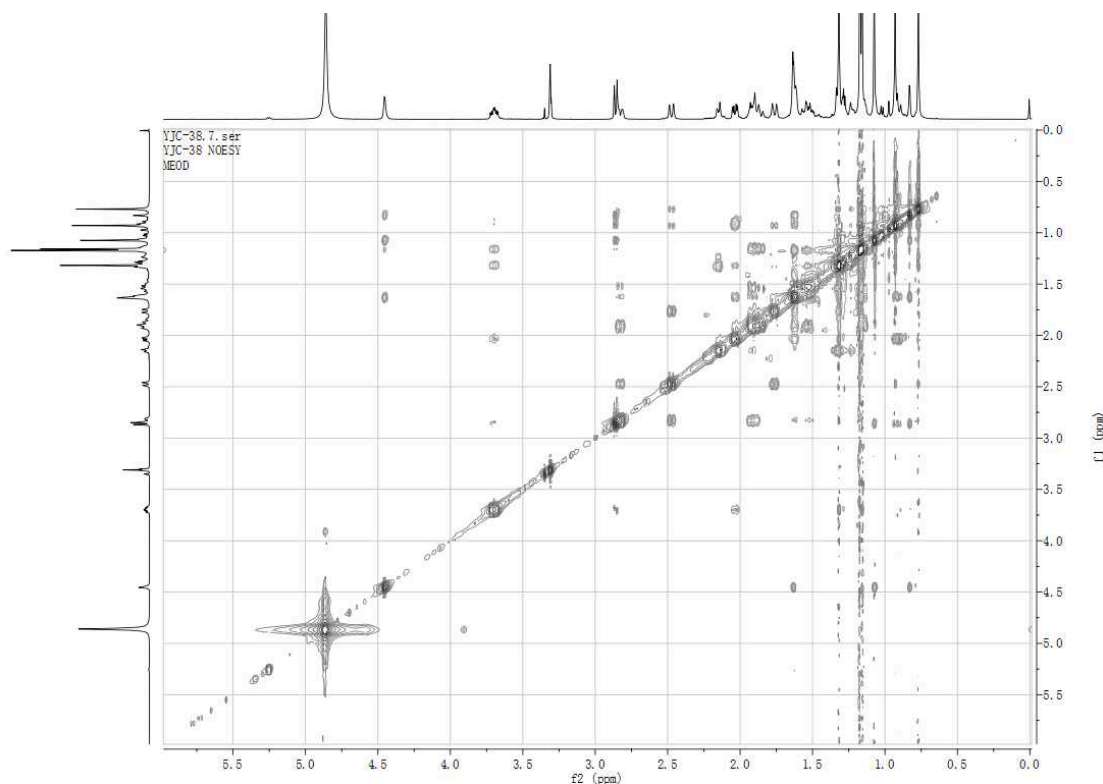


Figure S7. NOESY spectrum of **1**

Display Report

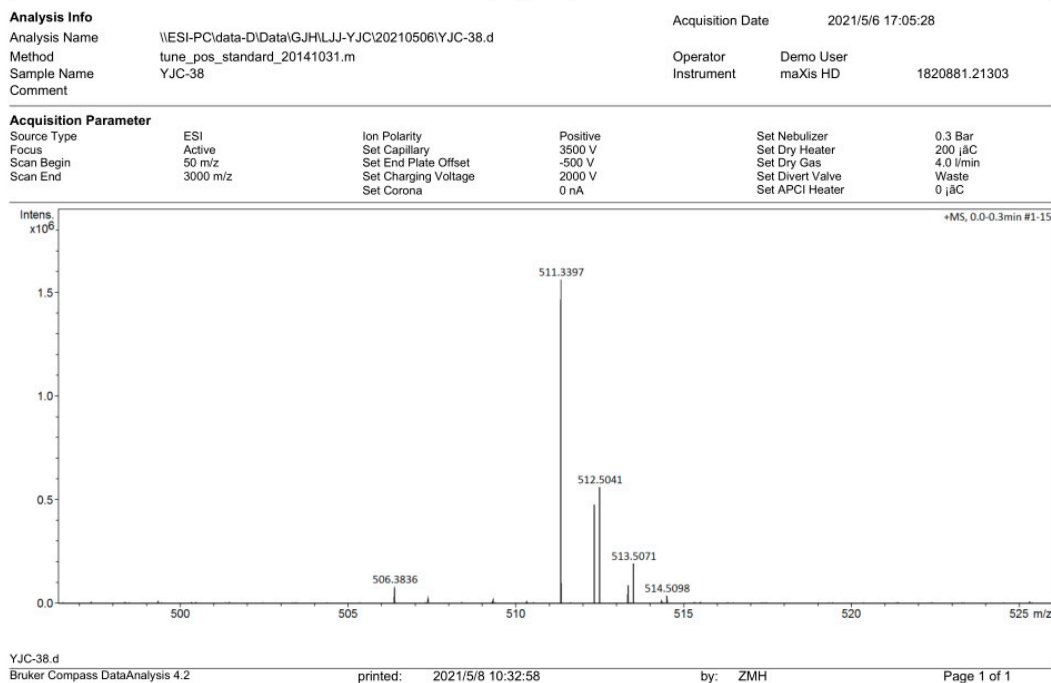
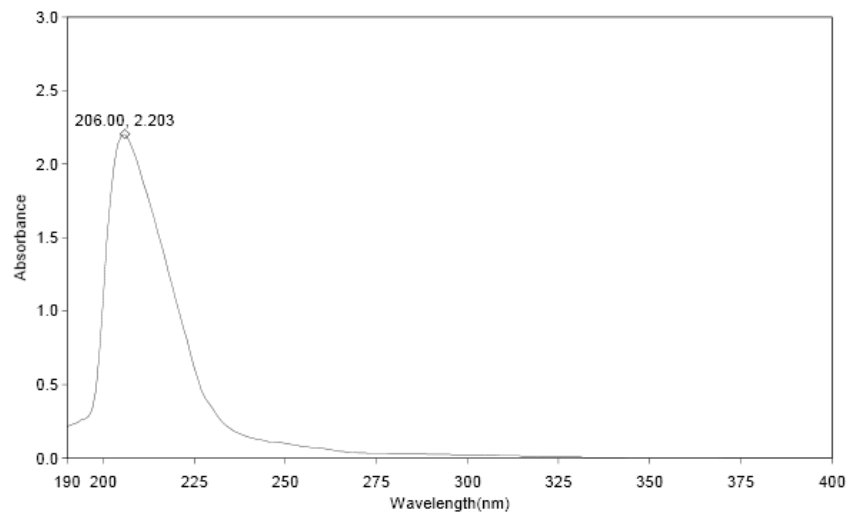


Figure S8. HR-ESI-MS Spectrum of **1**

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Department	(None Entered)	Time of Report	22:07:01下午
Organization	(None Entered)		
Information	(None Entered)		

Scan Graph



Results Table - scan021,YJC-38,Cycle01

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		Stop Wavelength 400.00 nm
		Sort By Wavelength

Sensitivity Auto

Figure S9. UV spectrum of **1**

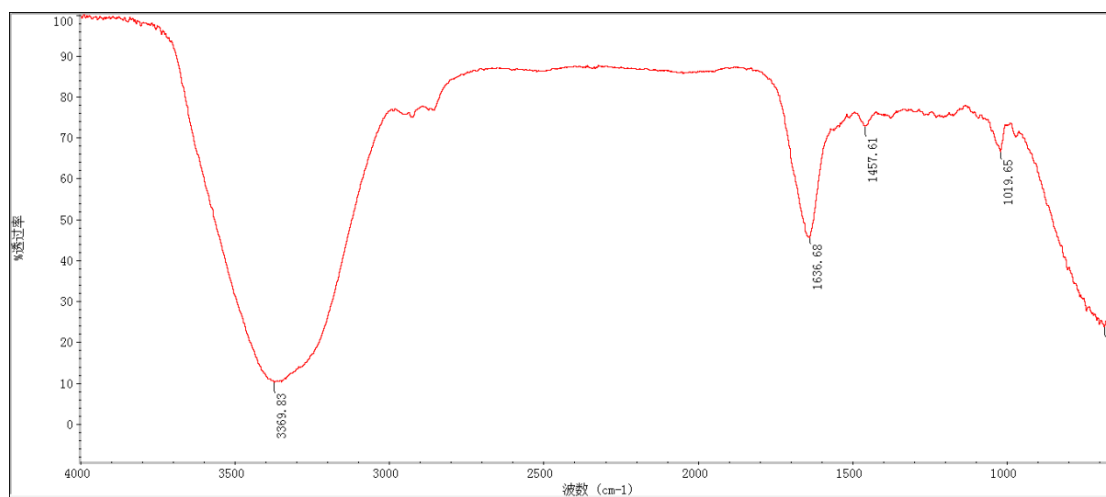


Figure S10. IR spectrum of **1**

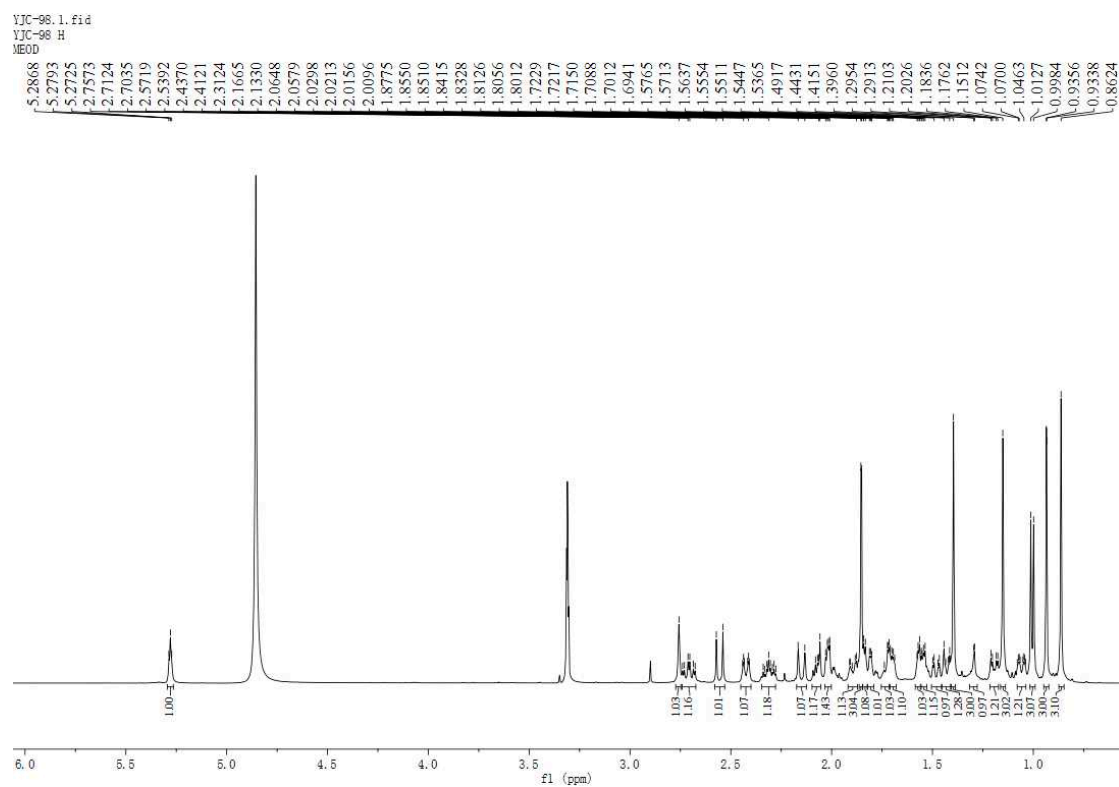


Figure S11. ^1H NMR spectrum (500 MHz, CD_3OD) of **2**

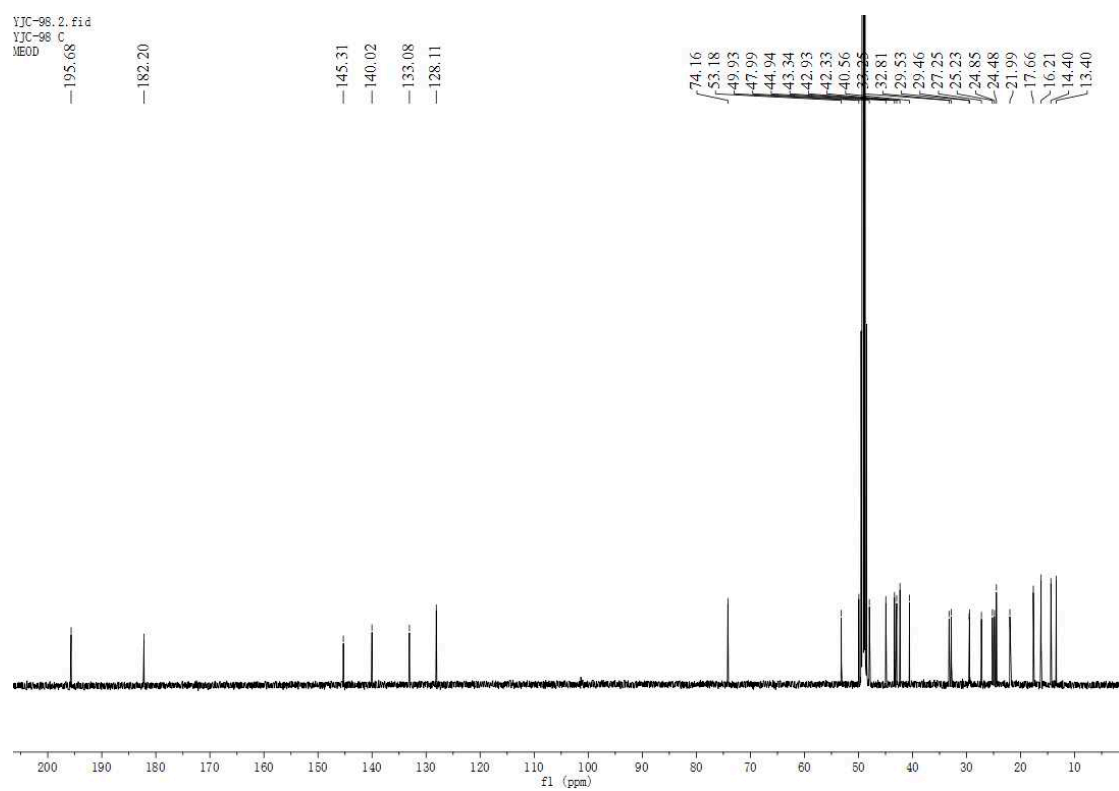


Figure S12. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **2**

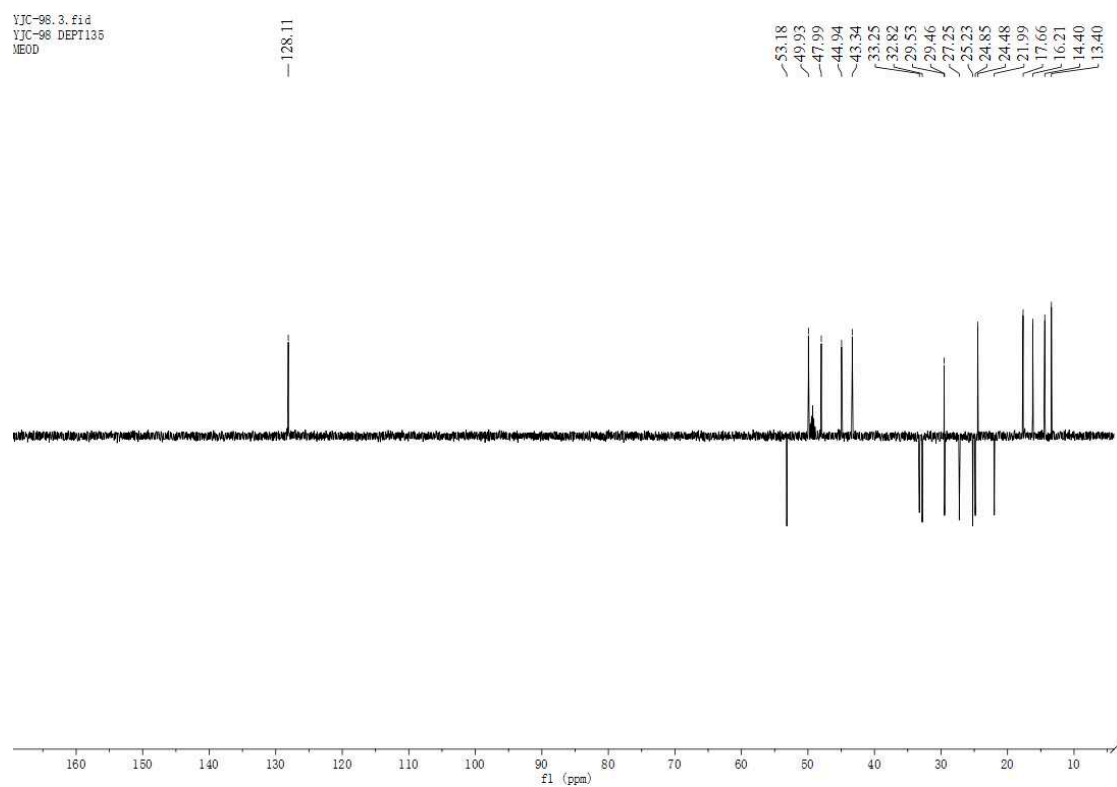


Figure S13. DEPT 135 spectrum (125 MHz, CD₃OD) of **2**

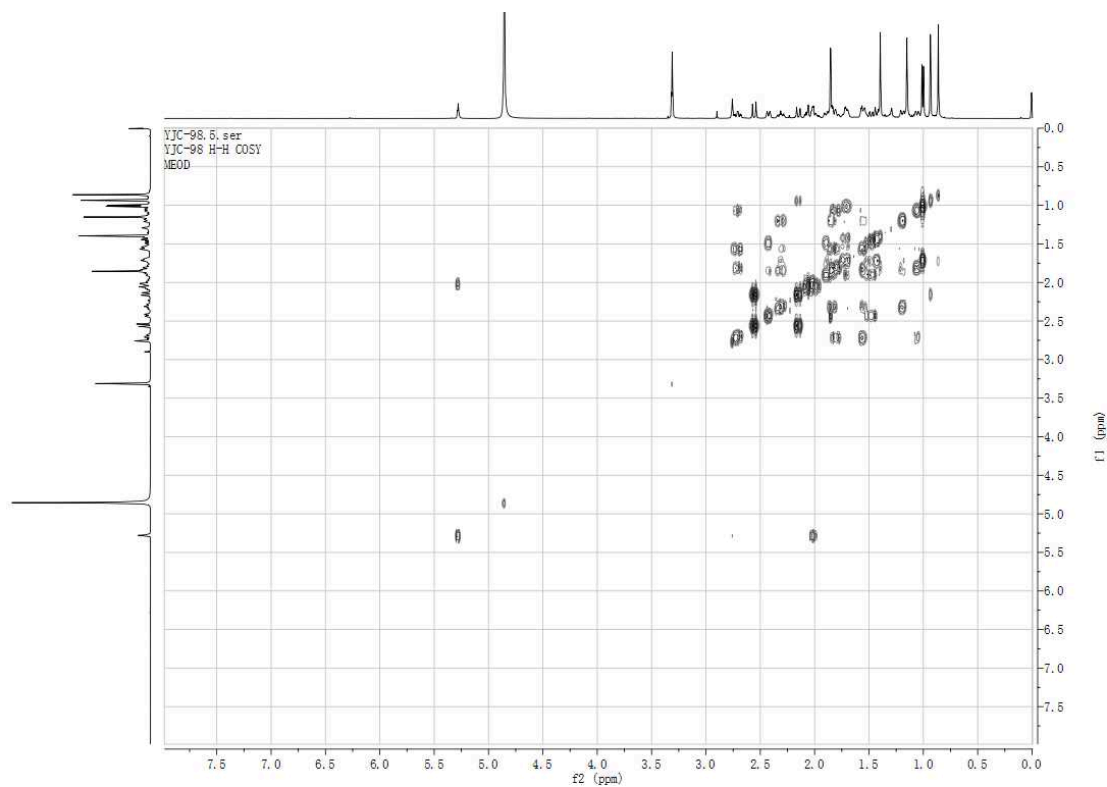


Figure S14. ¹H-¹H COSY spectrum of **2**

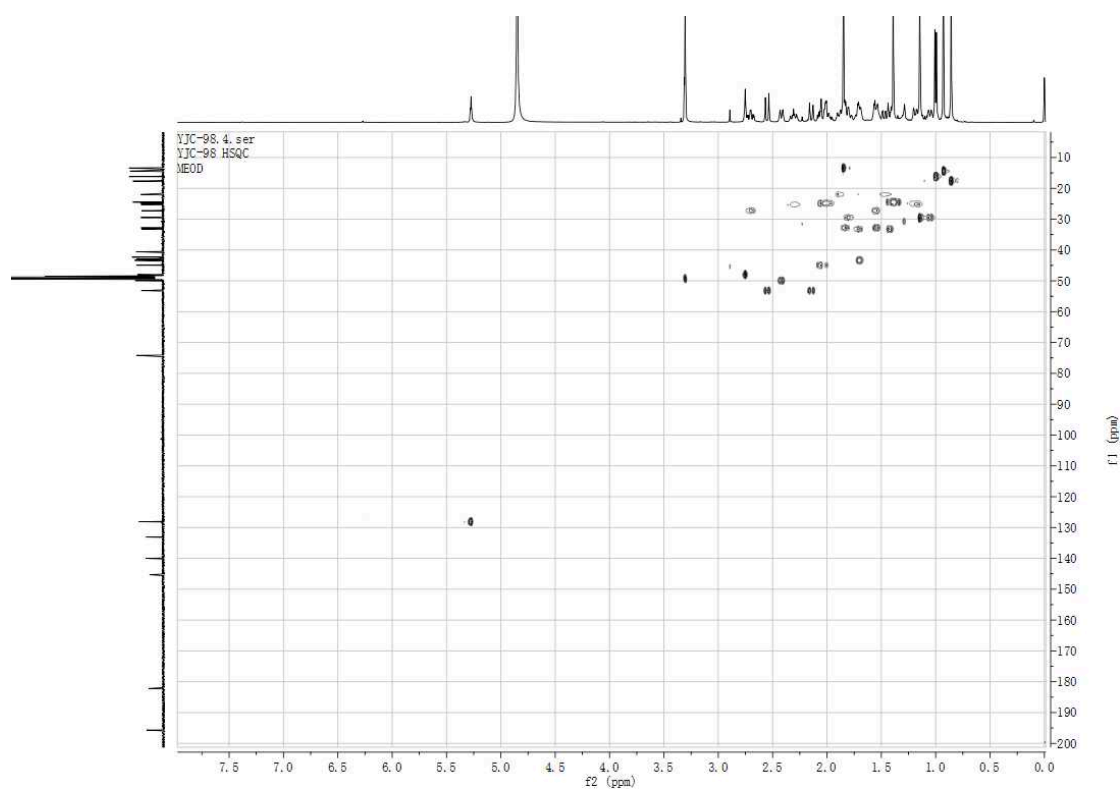


Figure S15. HSQC spectrum of **2**

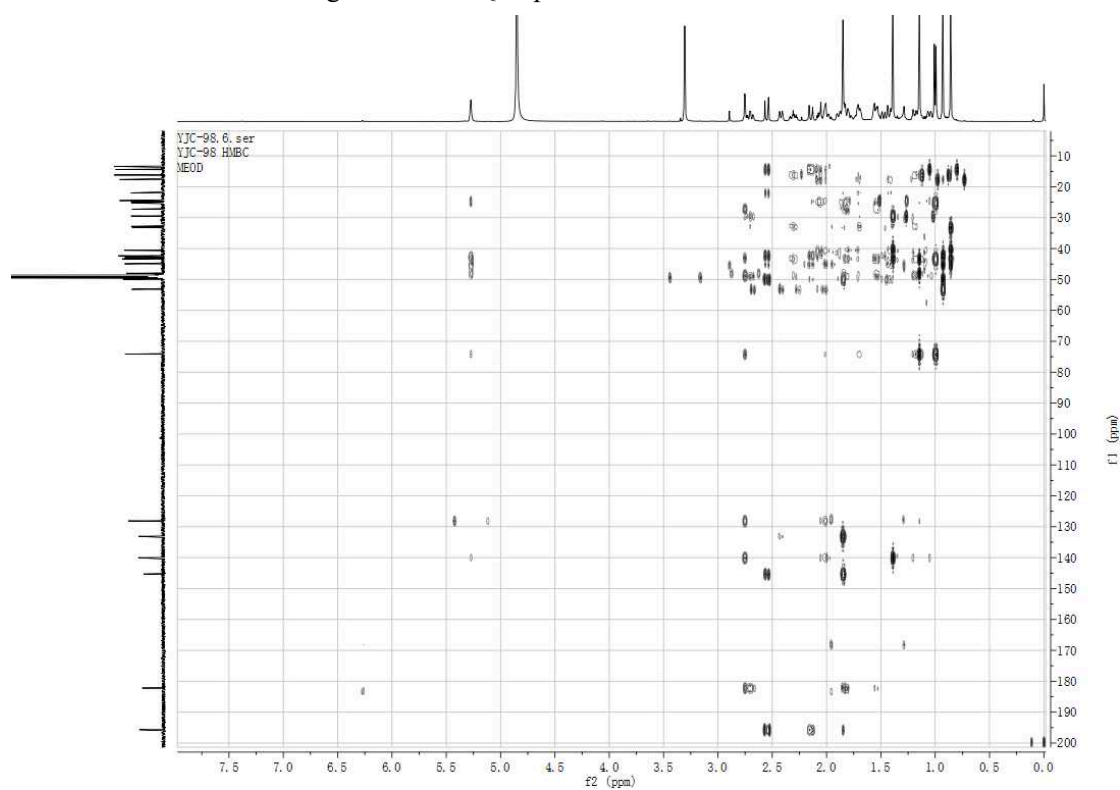


Figure S16. HMBC spectrum of **2**

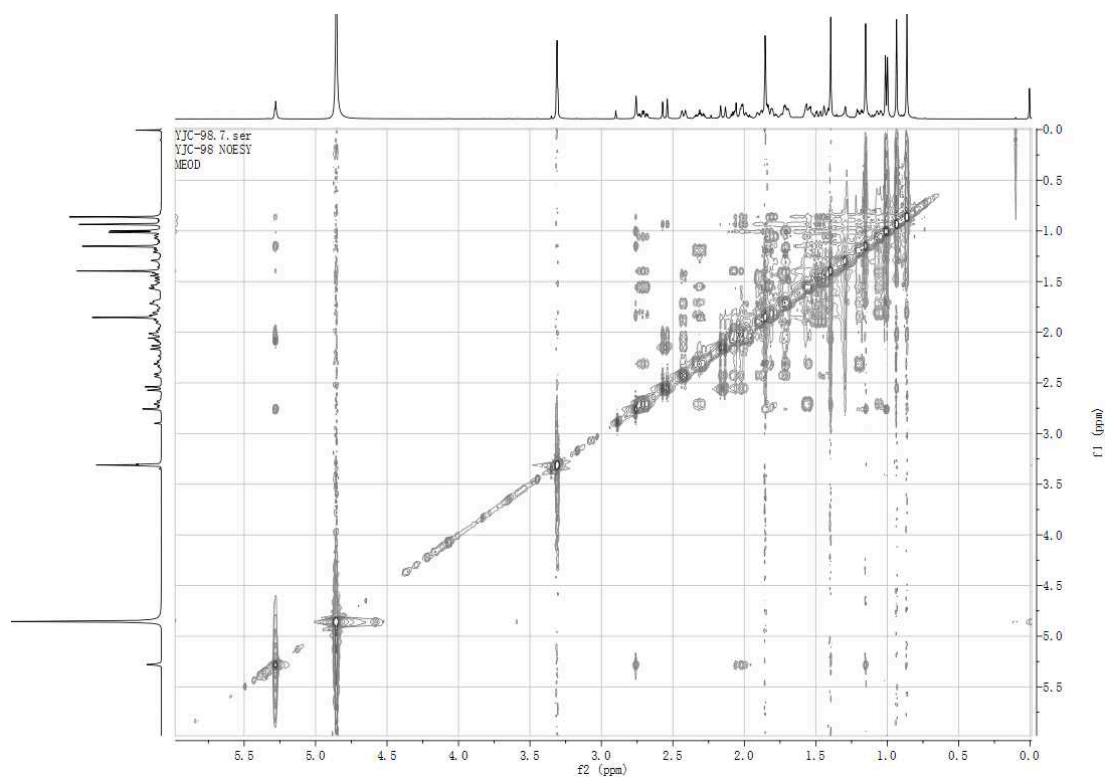


Figure S17. NOESY spectrum of **2**

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Analysis Info

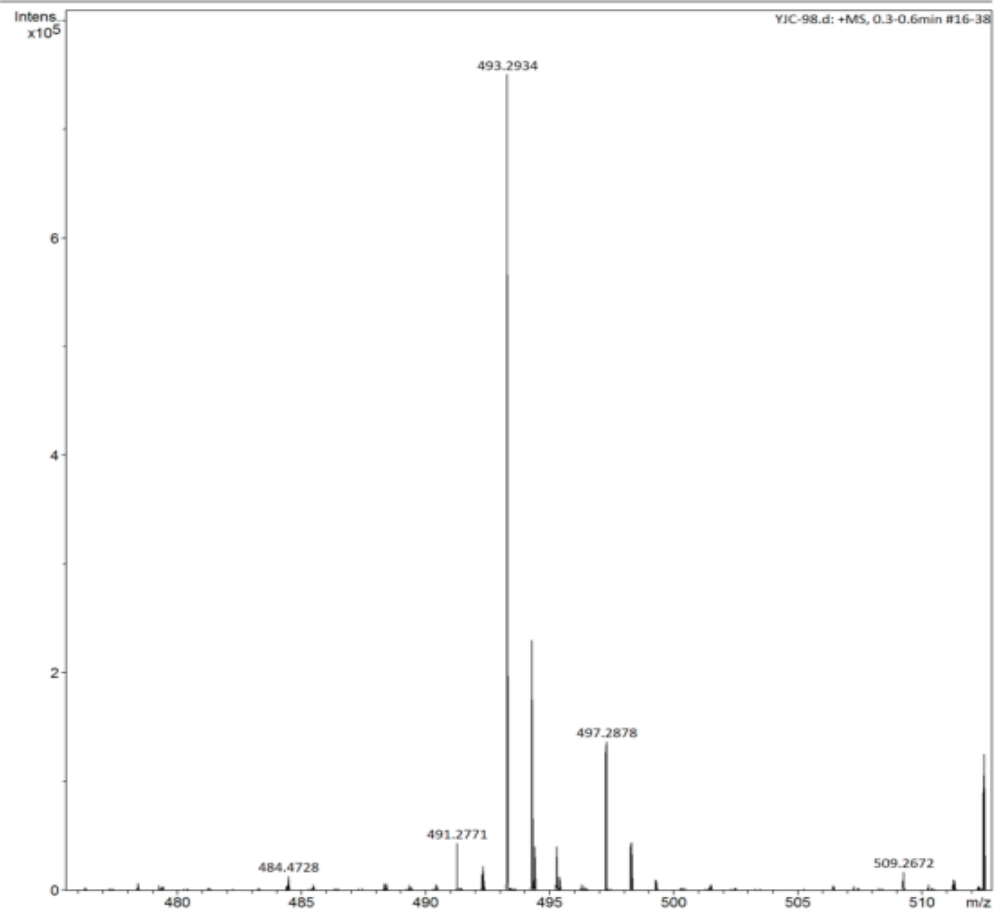
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Method tune_pos_standard_20141031.m
Sample Name YJC-98
Comment

Acquisition Date 2021/10/17 10:15:50

Operator Demo User
Instrument maXis HD 1820881.21303

Acquisition Parameter

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Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 μ C
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Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 μ C



YJC-98.d

Bruker Compass DataAnalysis 4.2

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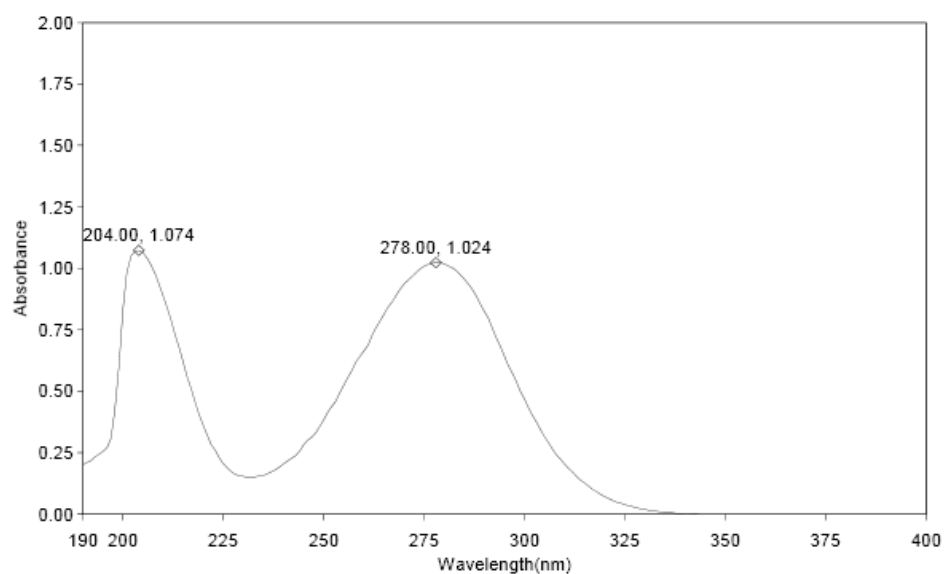
Figure S18. HR-ESI-MS Spectrum of **2**

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 Organization (None Entered)
 Information (None Entered)

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 Time of Report 22:11:18下午

Scan Graph



Results Table - scan022,YJC-98,Cycle01

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		Stop Wavelength400.00 nm
		Sort By Wavelength

Sensitivity Auto

Figure S19. UV spectrum of **2**

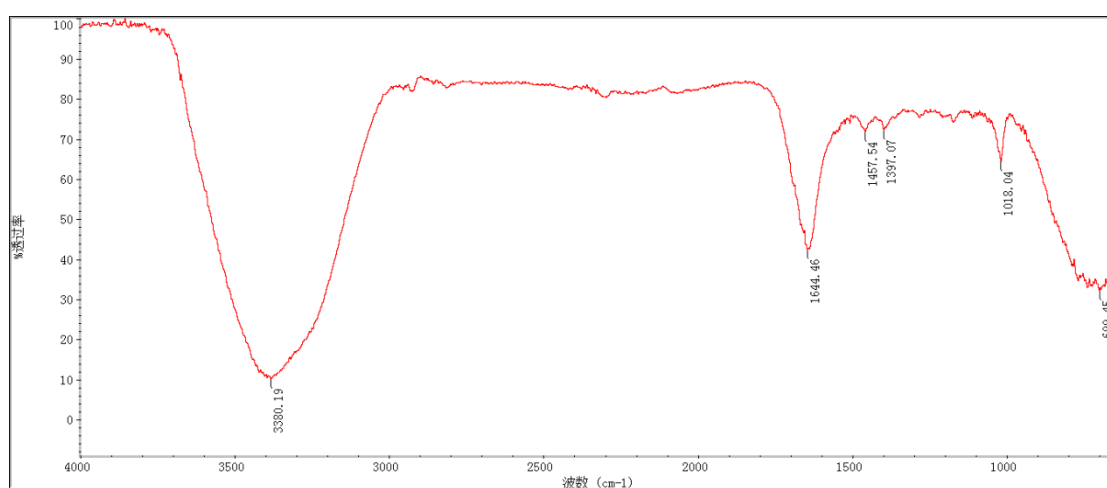


Figure S20. IR spectrum of **2**

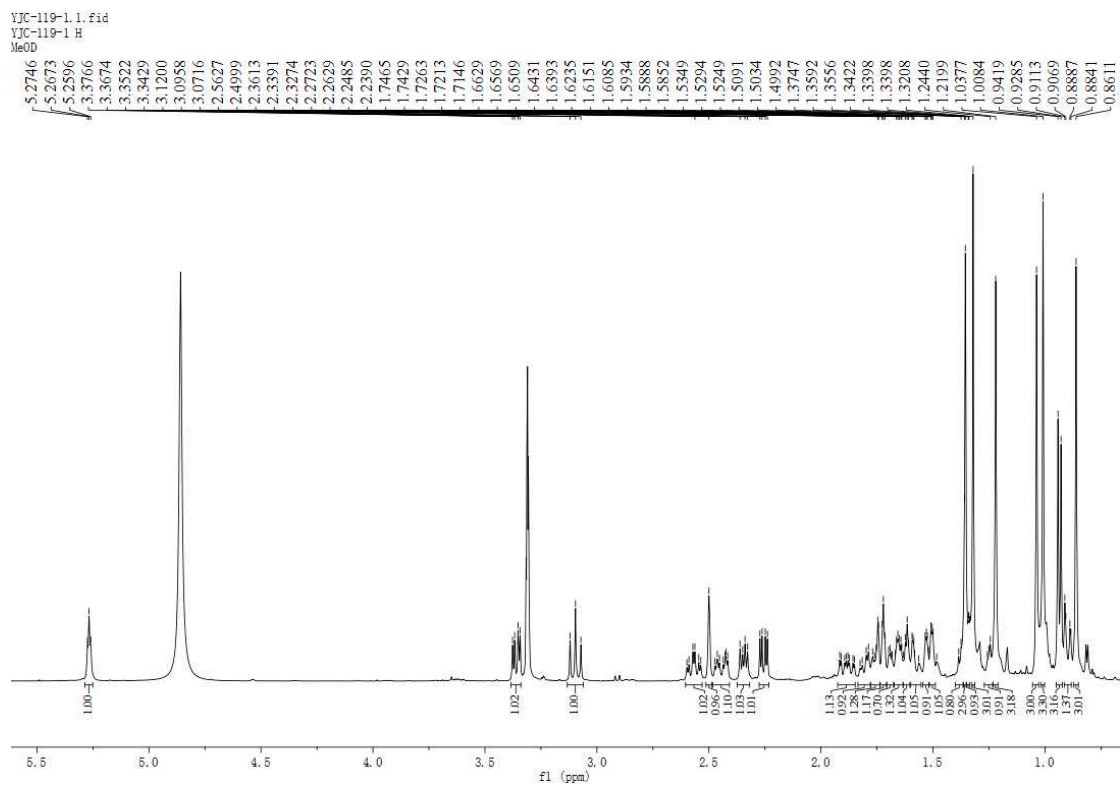


Figure S21. ^1H NMR spectrum (500 MHz, CD_3OD) of **3**

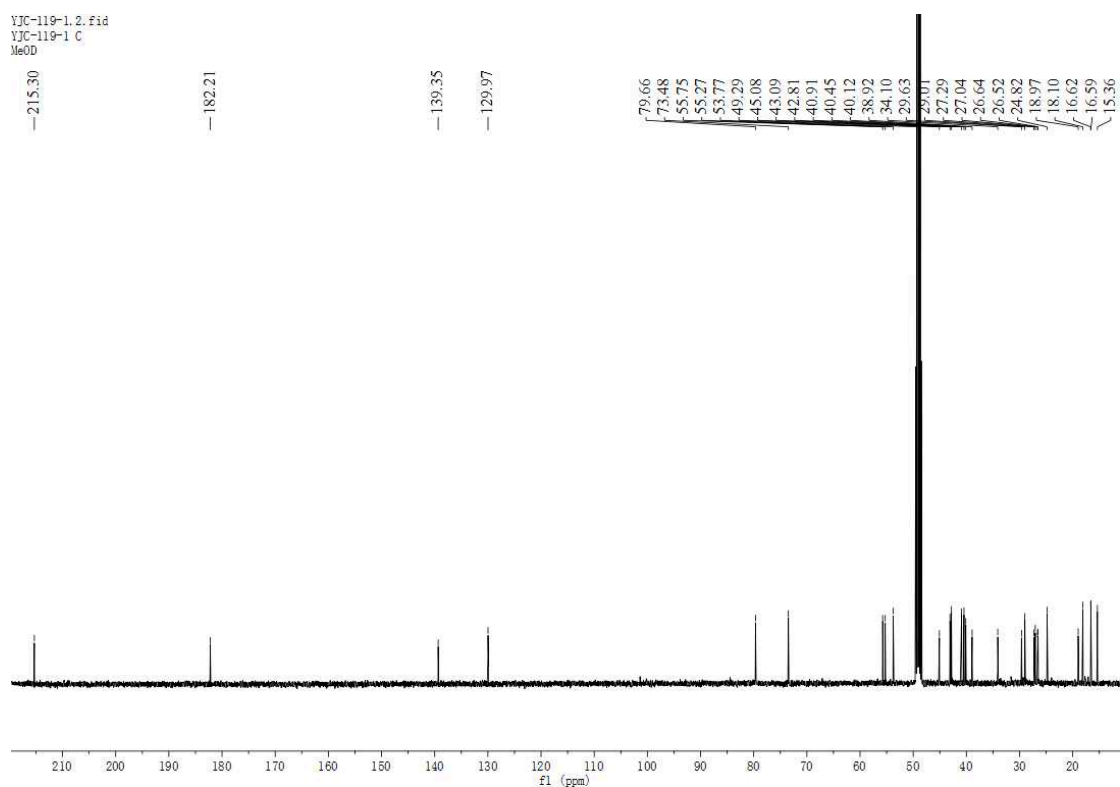


Figure S22. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **3**

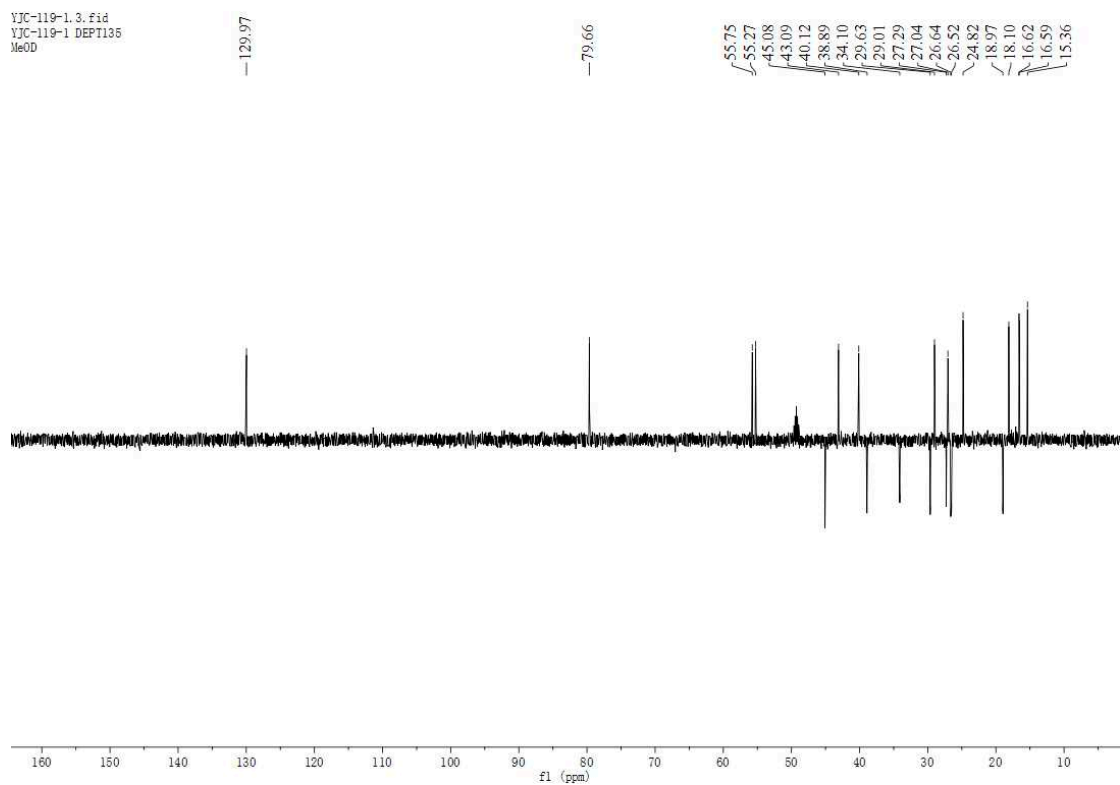


Figure S23. DEPT 135 spectrum (125 MHz, CD₃OD) of **3**

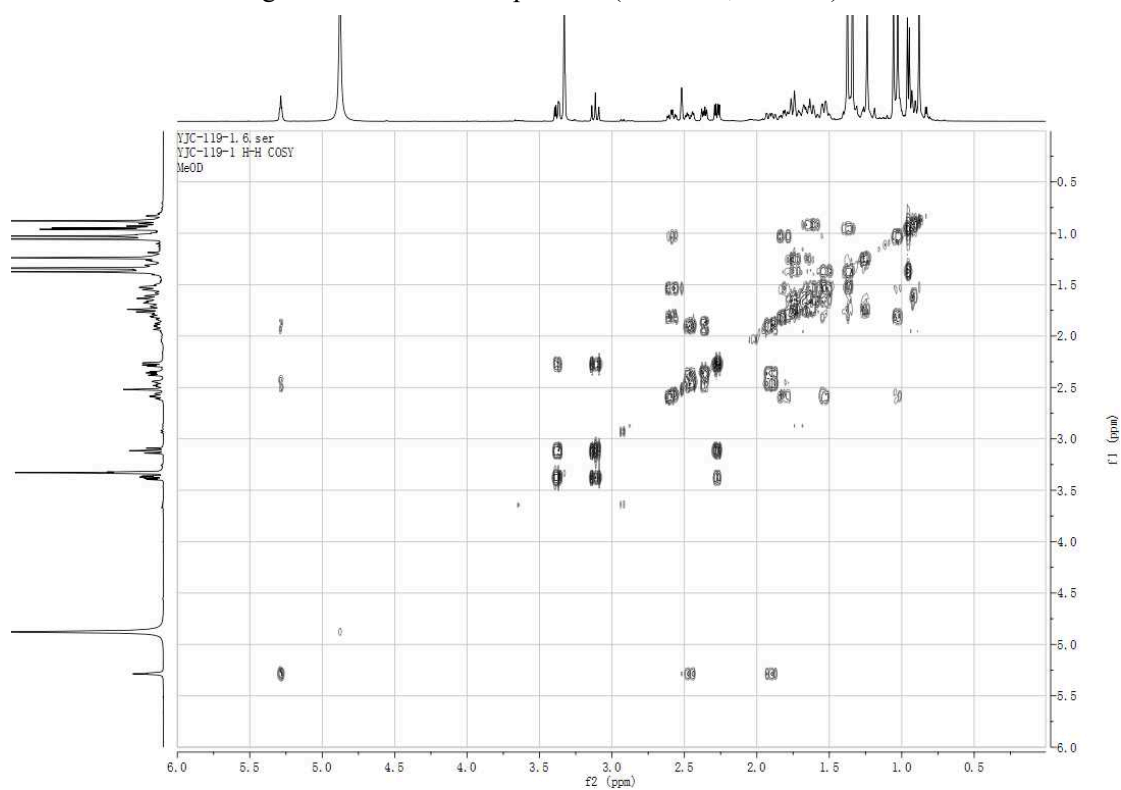


Figure S24. ¹H-¹H COSY spectrum of **3**

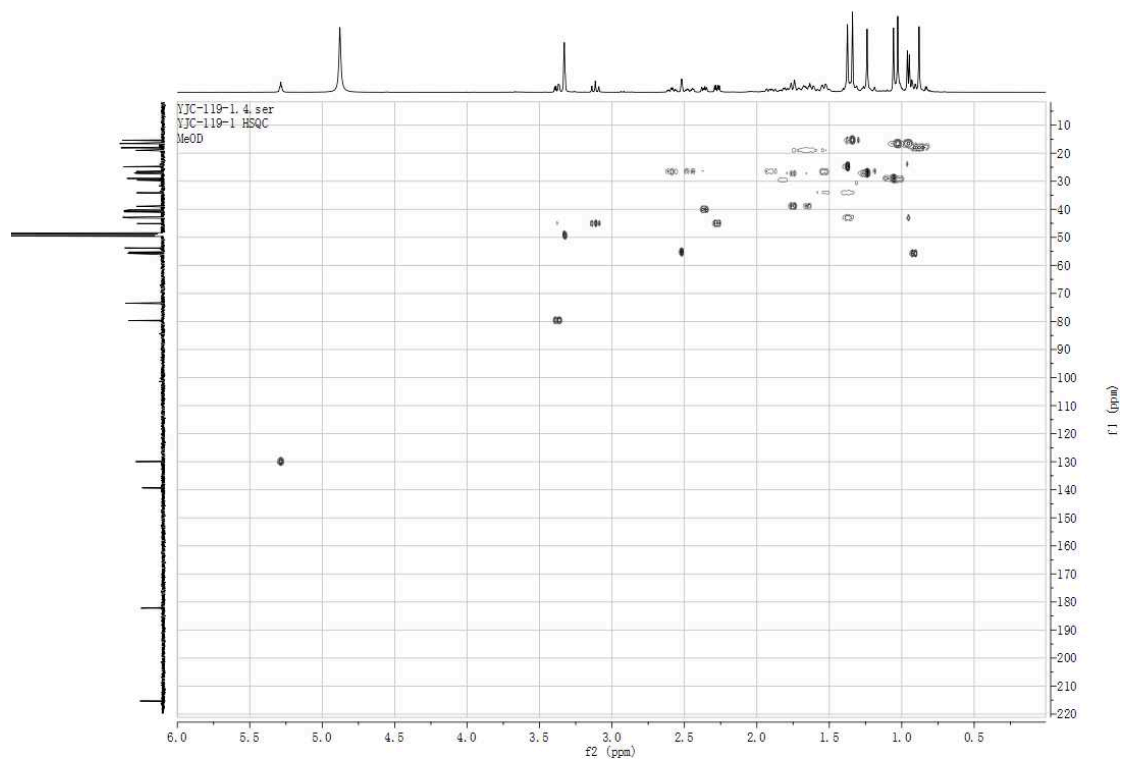


Figure S25. HSQC spectrum of **3**

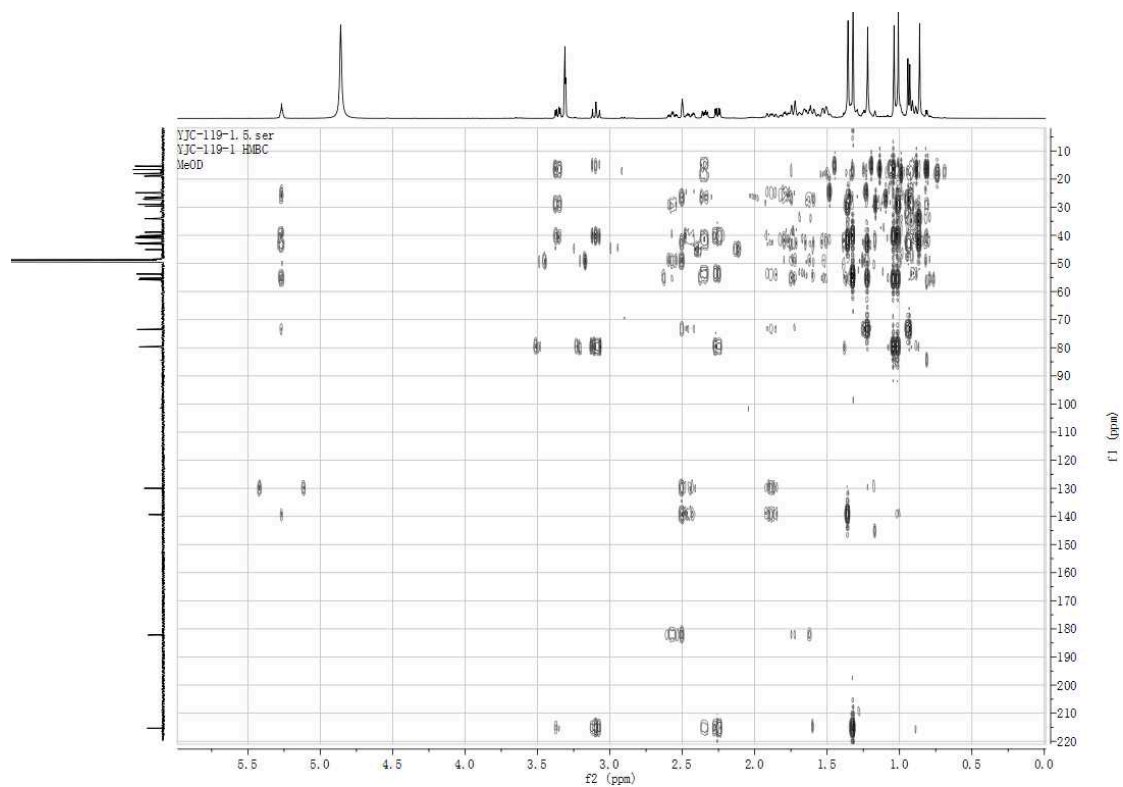


Figure S26. HMBC spectrum of **3**

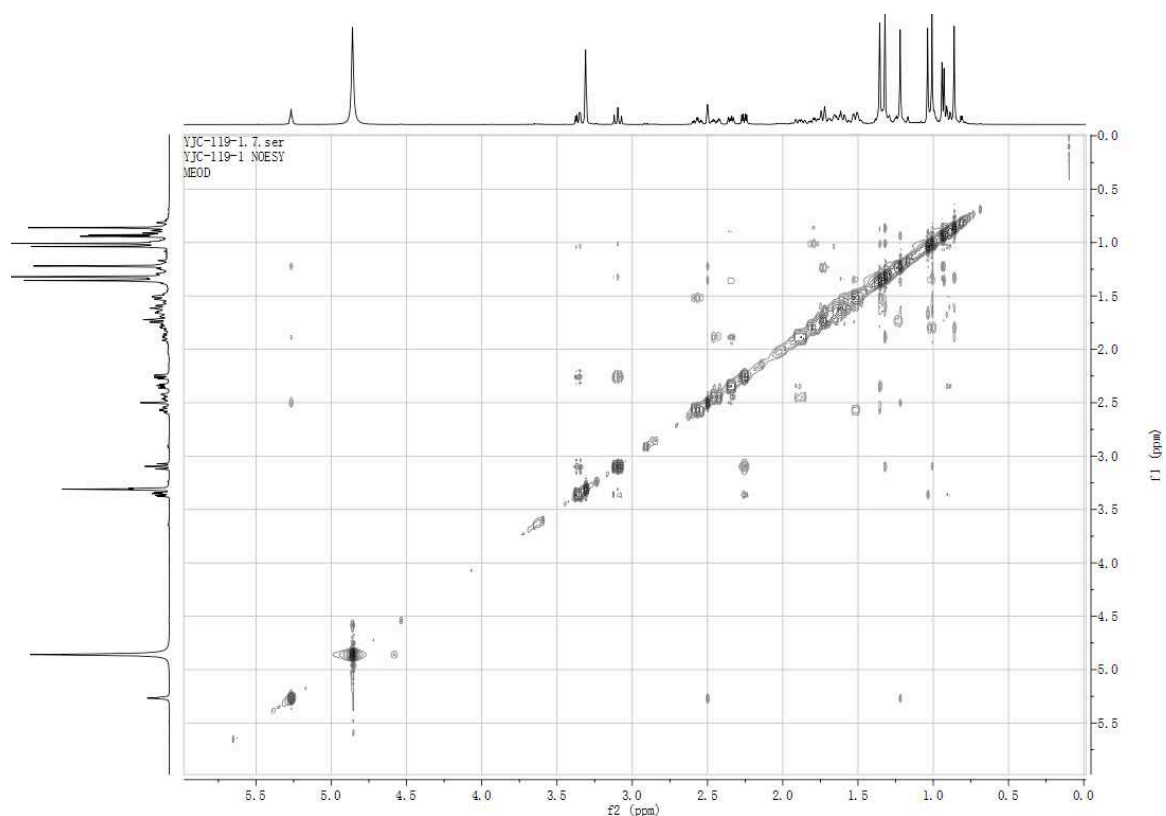


Figure S27. NOESY spectrum of **3**

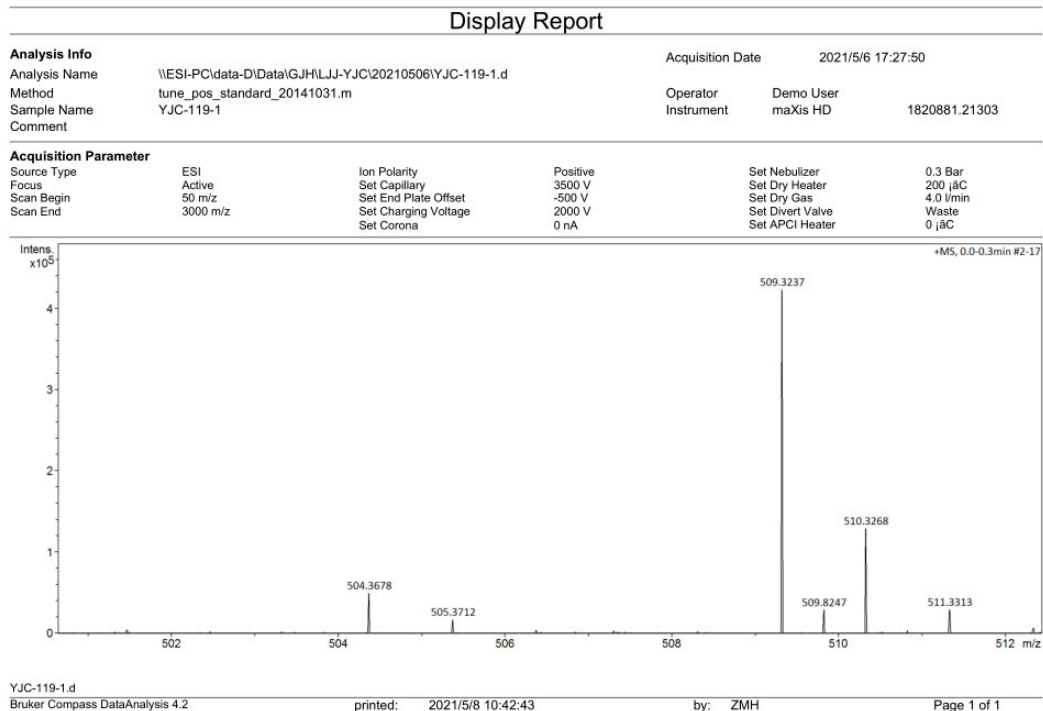
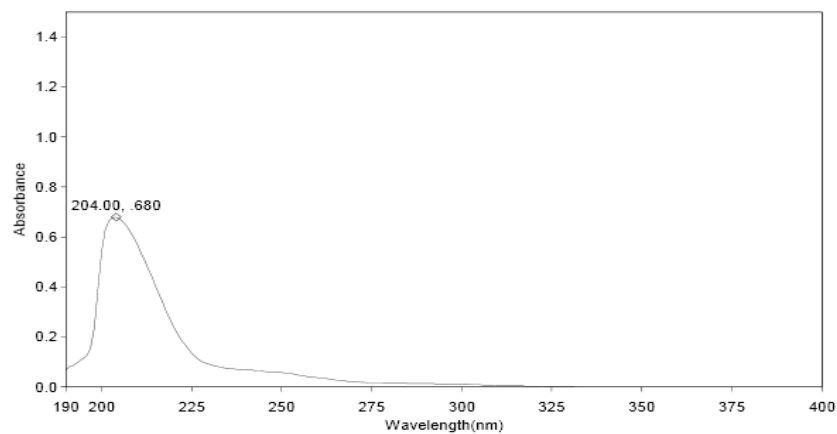


Figure S28. HR-ESI-MS Spectrum of **3**

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Department	(None Entered)	Time of Report	22:15:57下午
Organization	(None Entered)		
Information	(None Entered)		

Scan Graph



Results Table - scan023,YJC-119-1,Cycle01

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		Stop Wavelength 400.00 nm
		Sort By Wavelength

Sensitivity Auto

Figure S29. UV spectrum of **3**

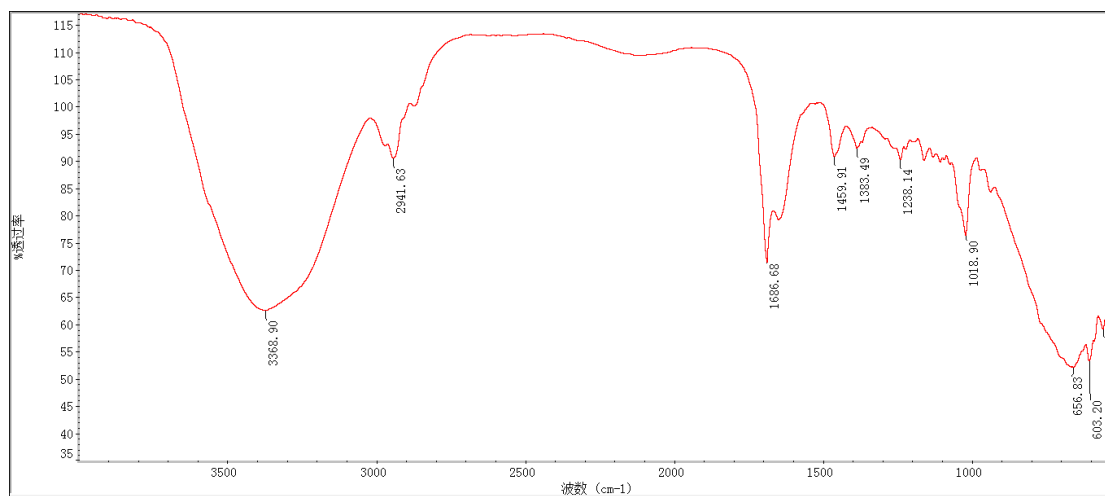


Figure S30. IR spectrum of **3**

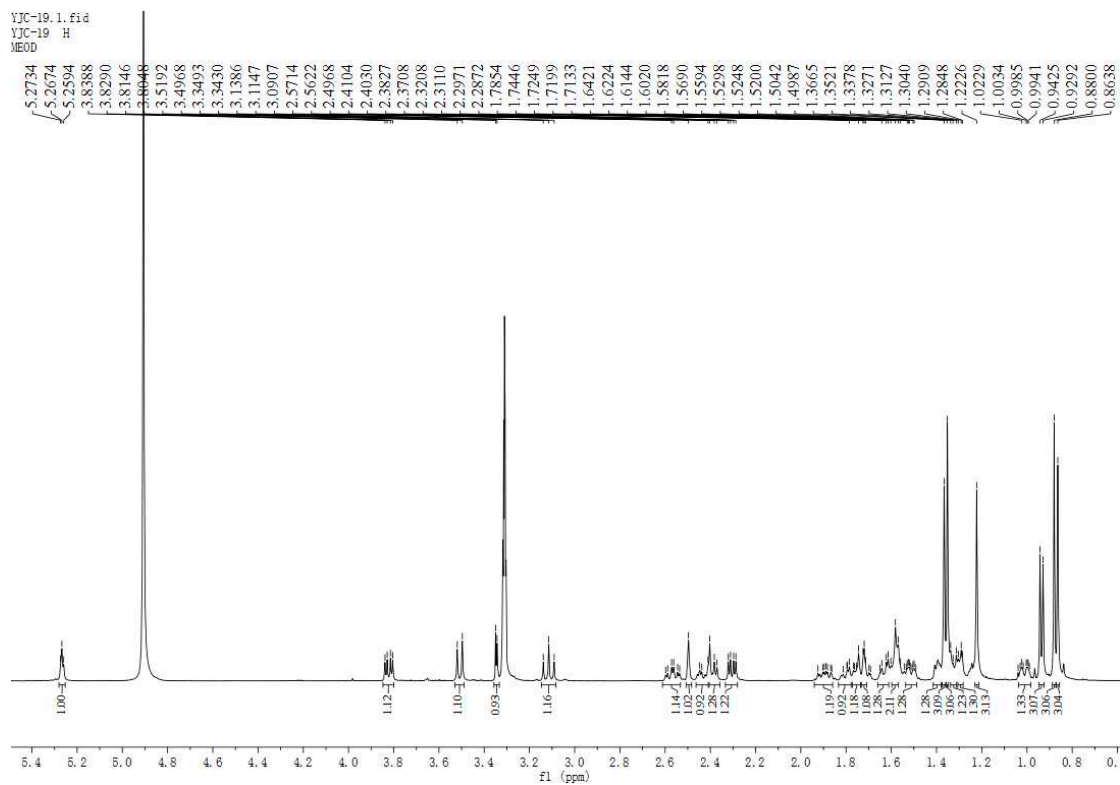


Figure S31. ^1H NMR spectrum (500 MHz, CD_3OD) of **4**

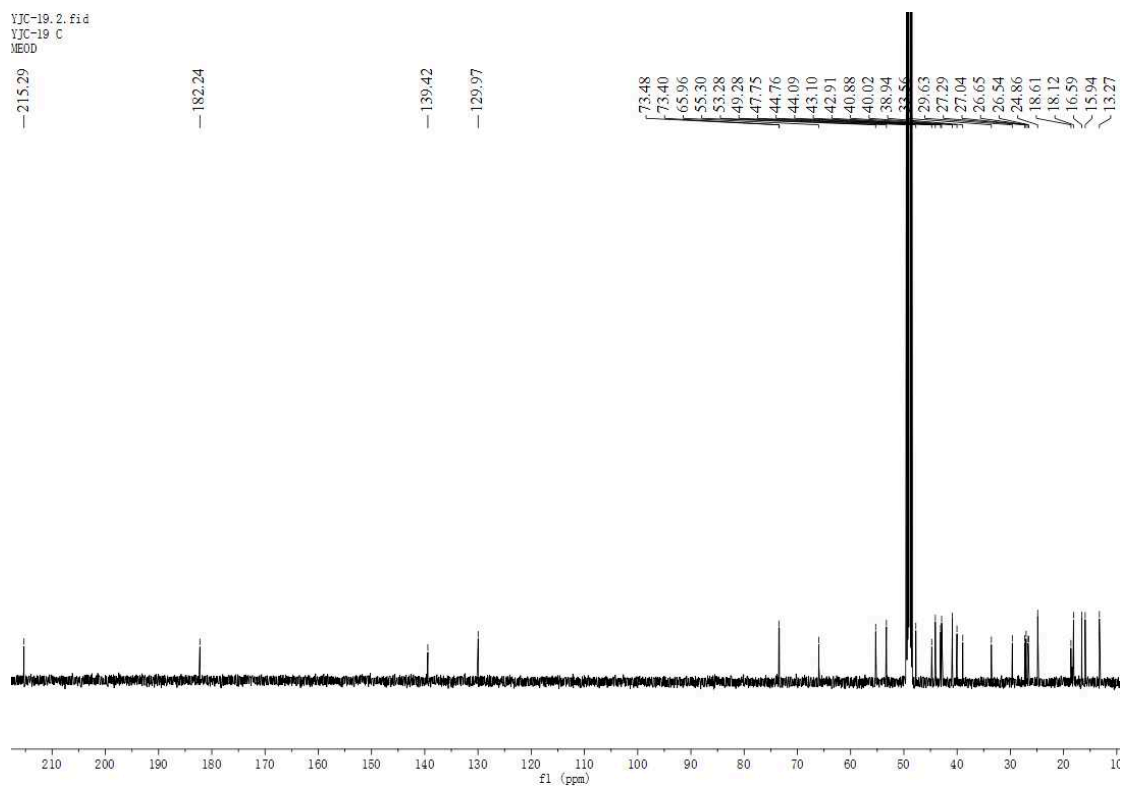


Figure S32. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **4**

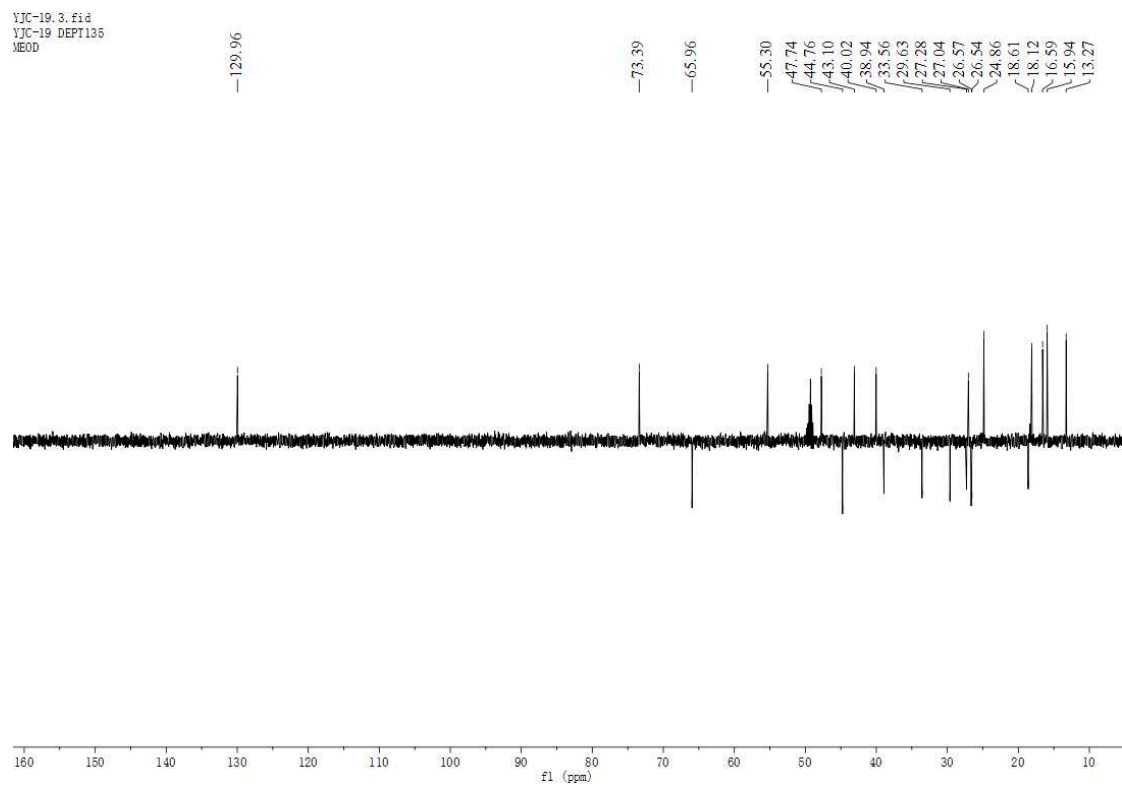


Figure S33. DEPT 135 spectrum (125 MHz, CD₃OD) of **4**

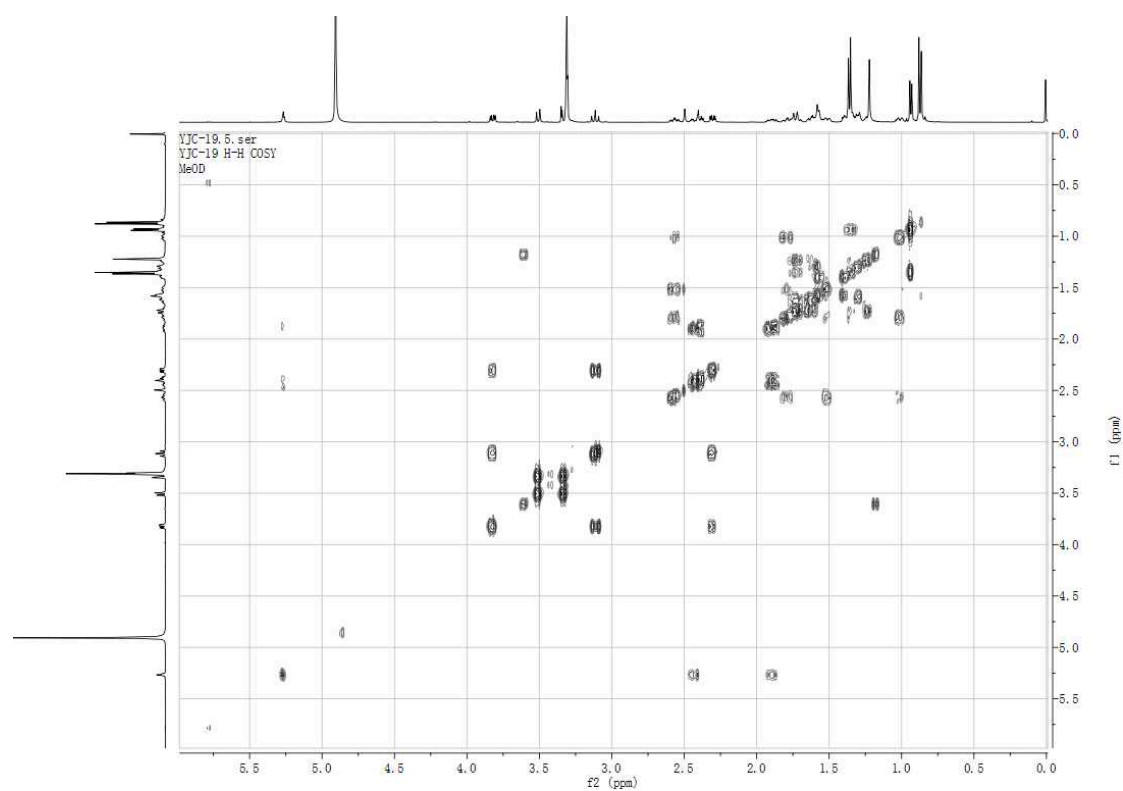


Figure S34. ¹H-¹H COSY spectrum of **4**

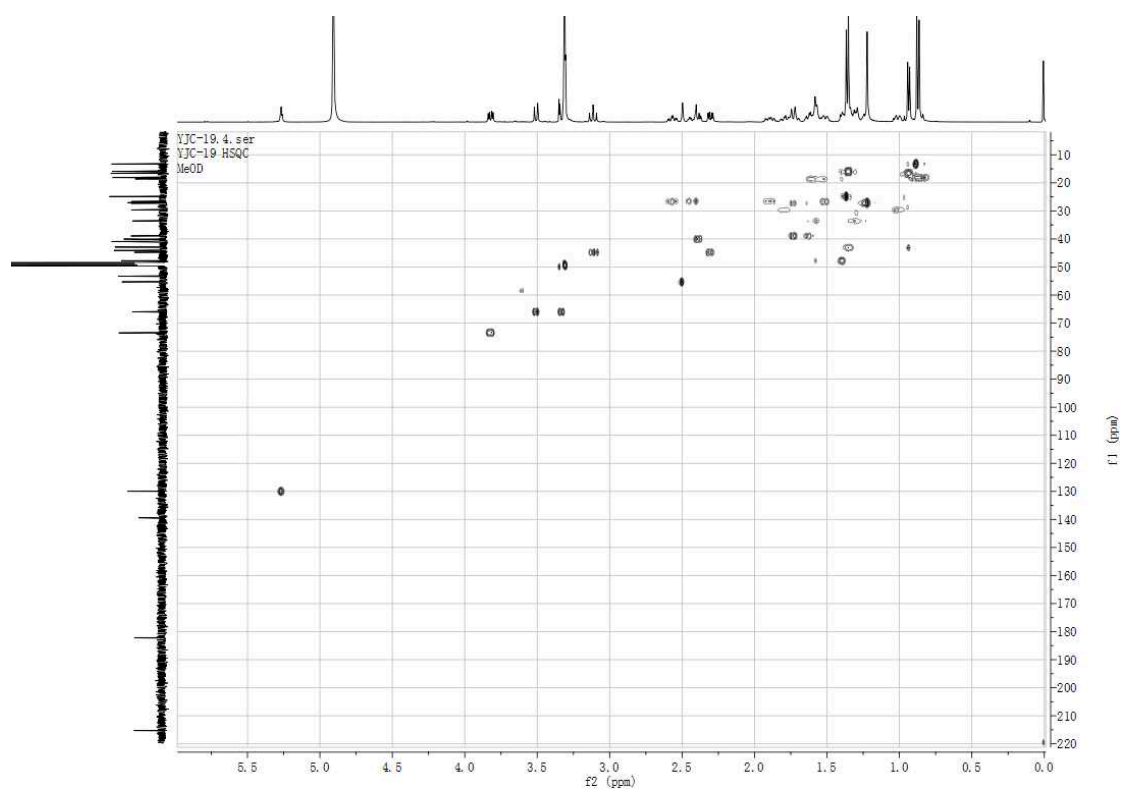


Figure S35. HSQC spectrum of **4**

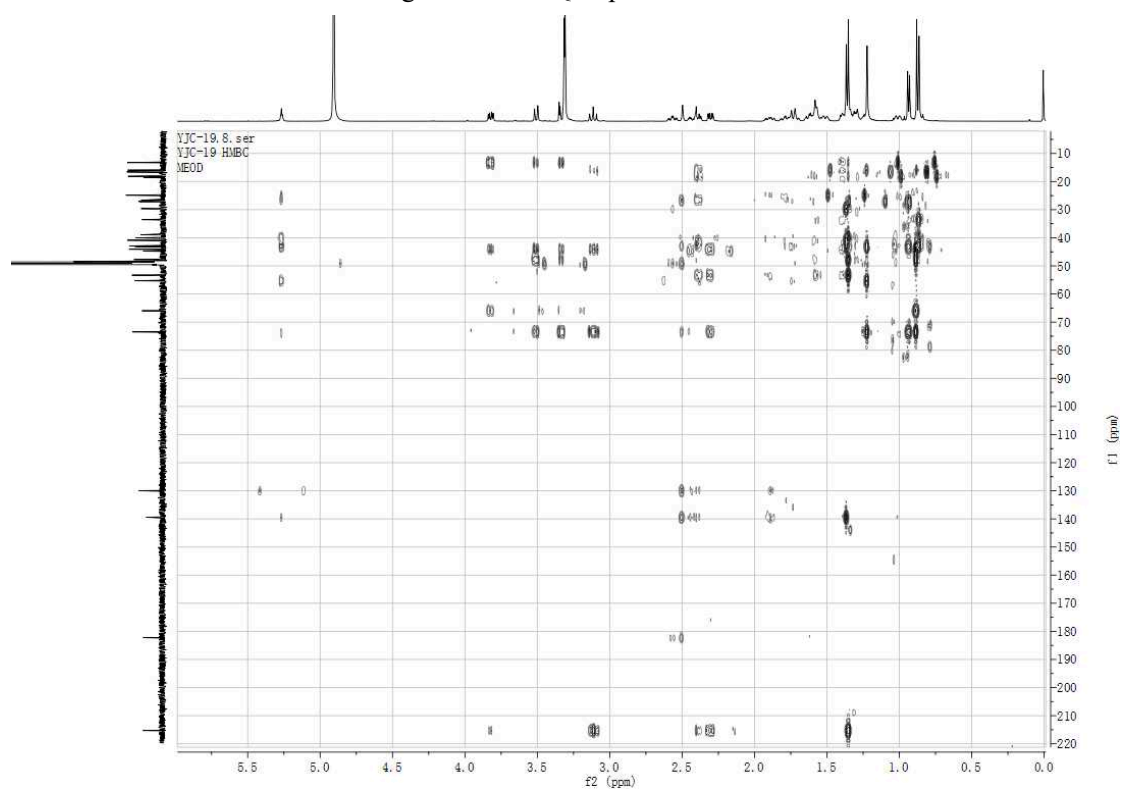


Figure S36. HMBC spectrum of **4**

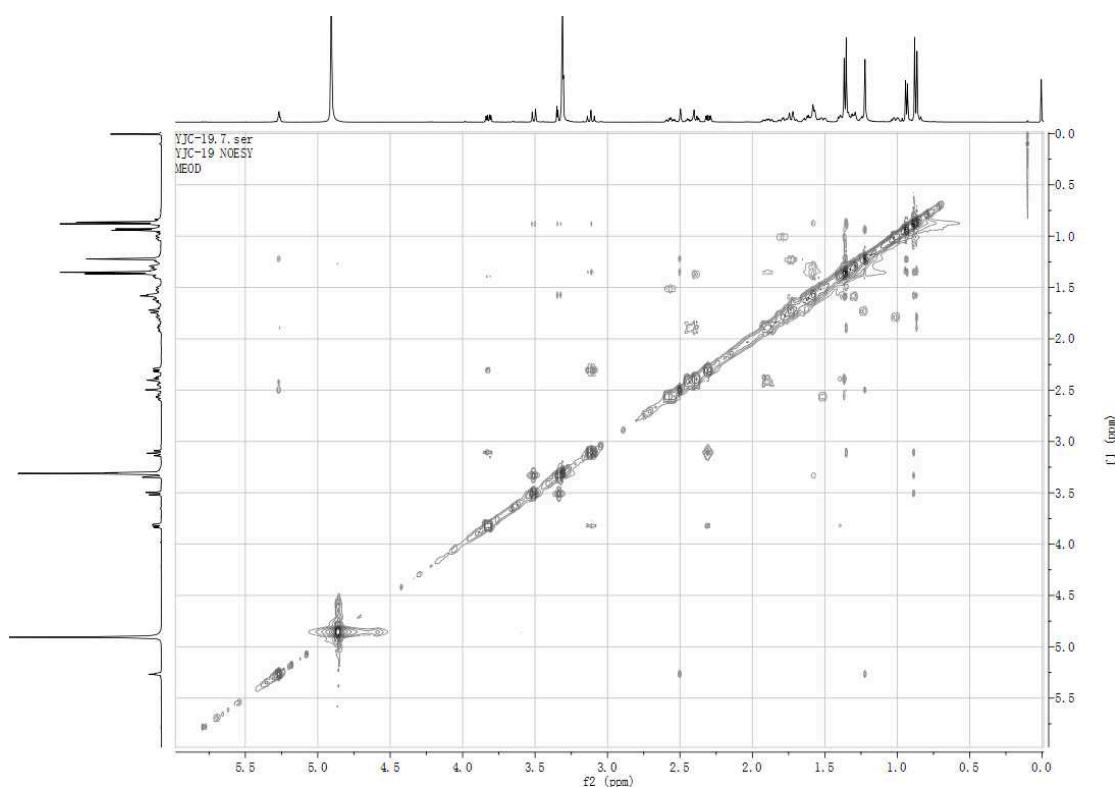


Figure S37. NOESY spectrum of **4**

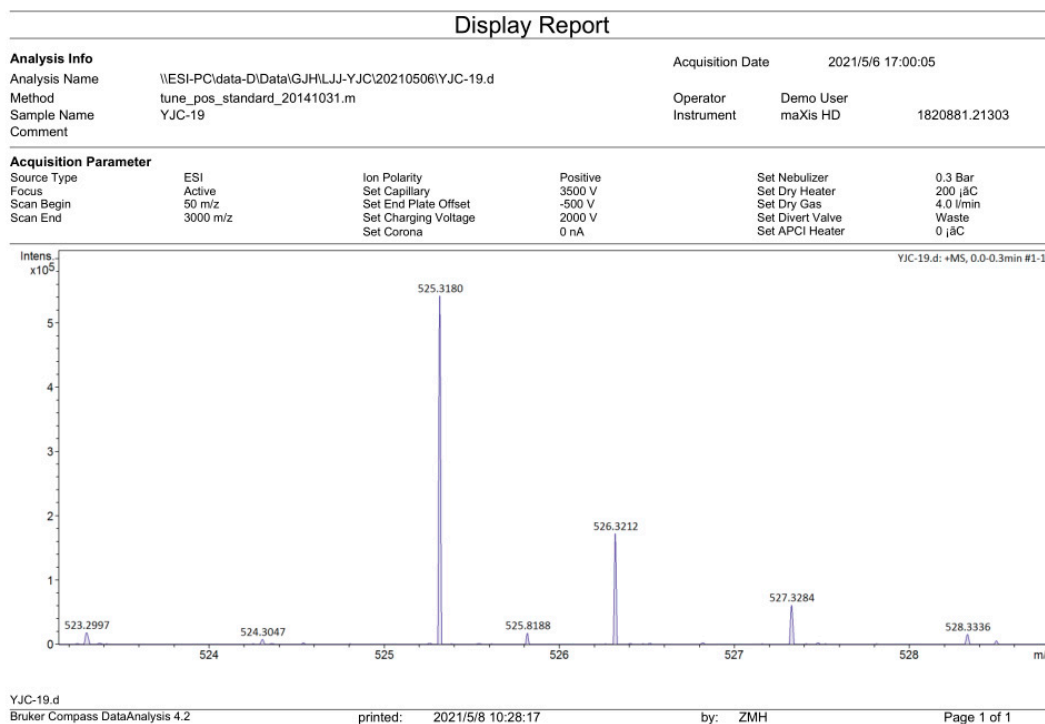


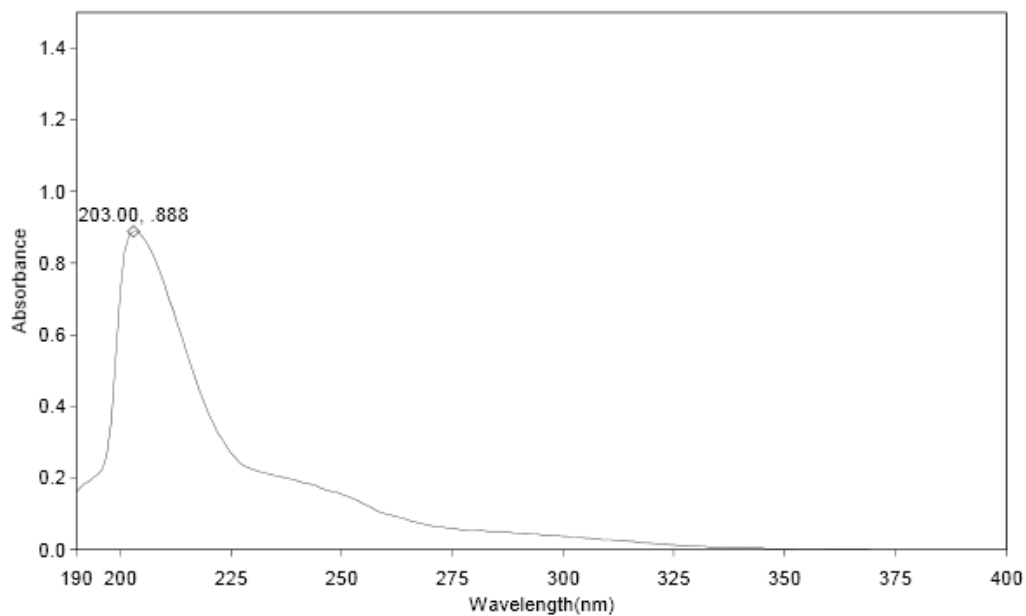
Figure S38. HR-ESI-MS Spectrum of **4**

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

Date of Report 2021/10/9
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Scan Graph



Results Table - scan020,YJC-19,Cycle01

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Start Wavelength190.00 nm		
Stop Wavelength400.00 nm		
Sort By Wavelength		

Sensitivity Auto

Figure S39. UV spectrum of 4

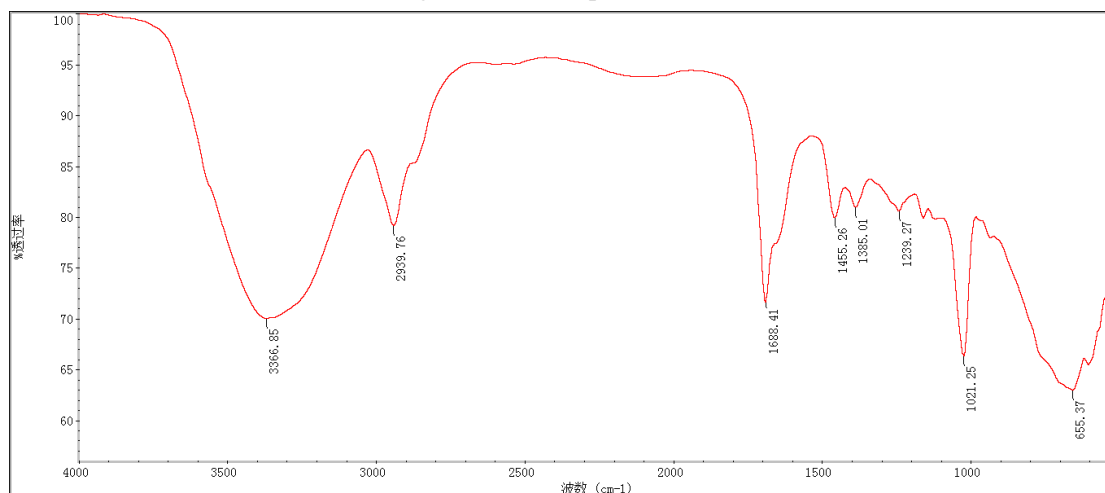


Figure S40. IR spectrum of 4

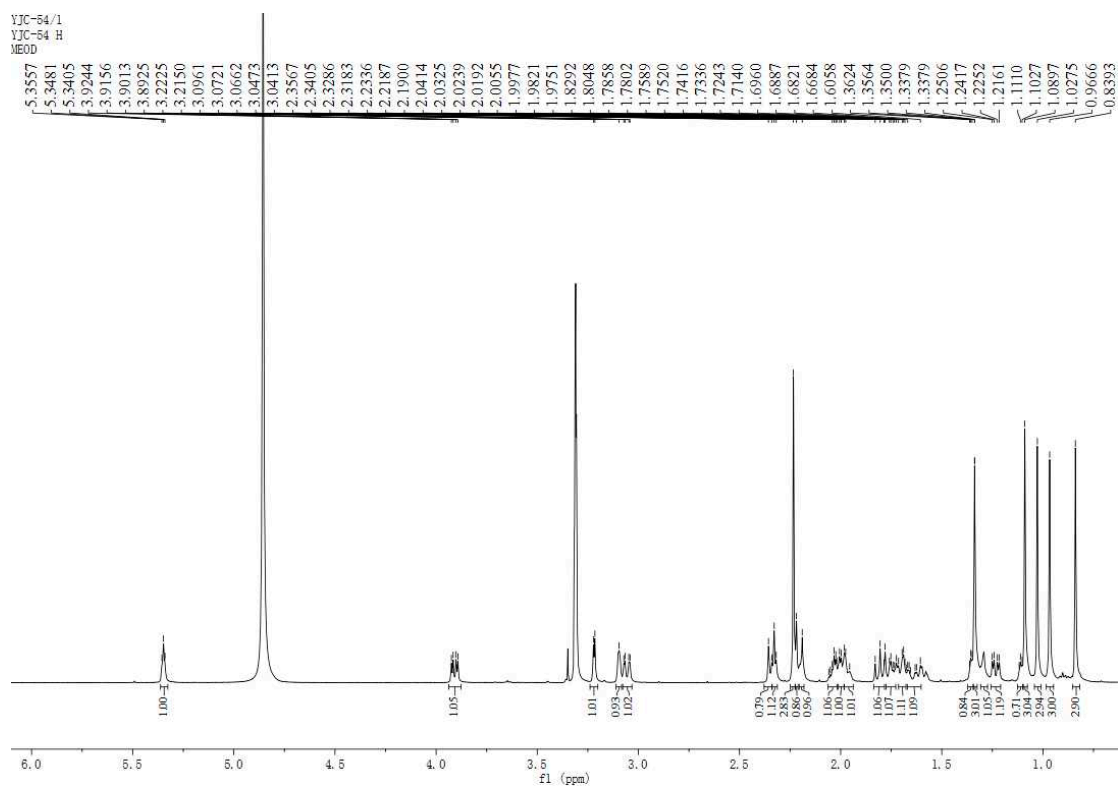


Figure S41. ^1H NMR spectrum (500 MHz, CD_3OD) of **5**

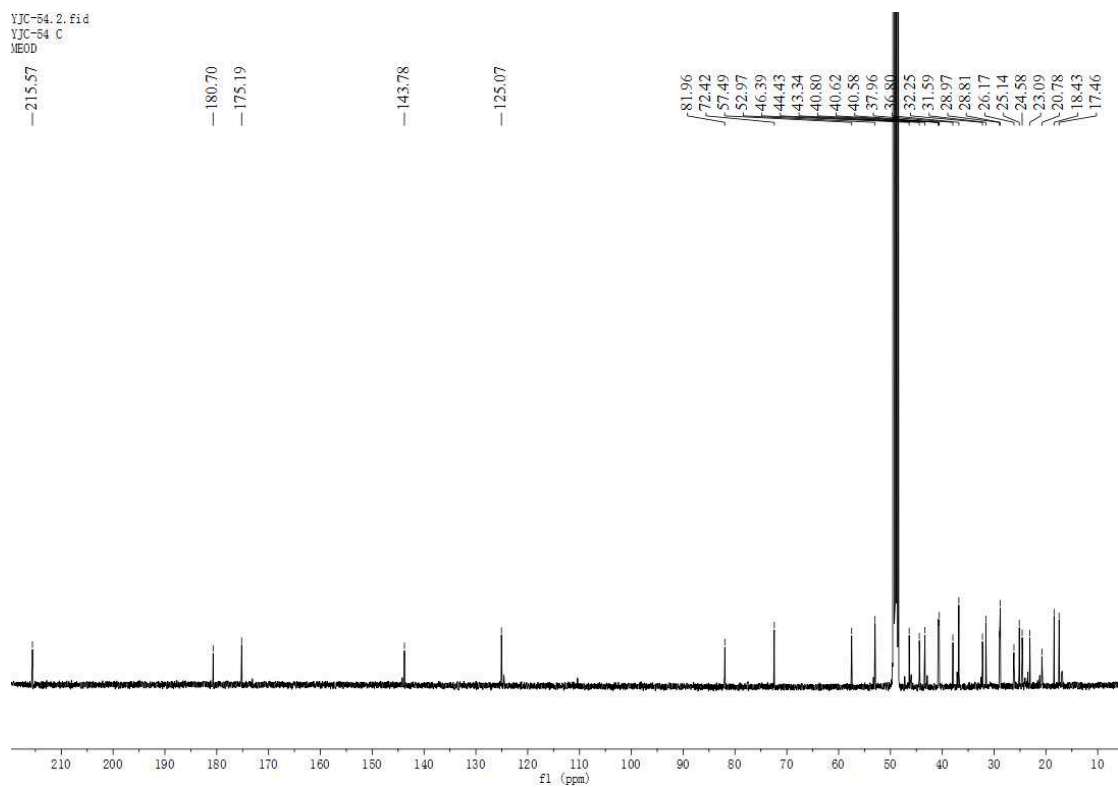


Figure S42. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **5**

YJC-54.3.fid
YJC-59 DEPT135
MEOD

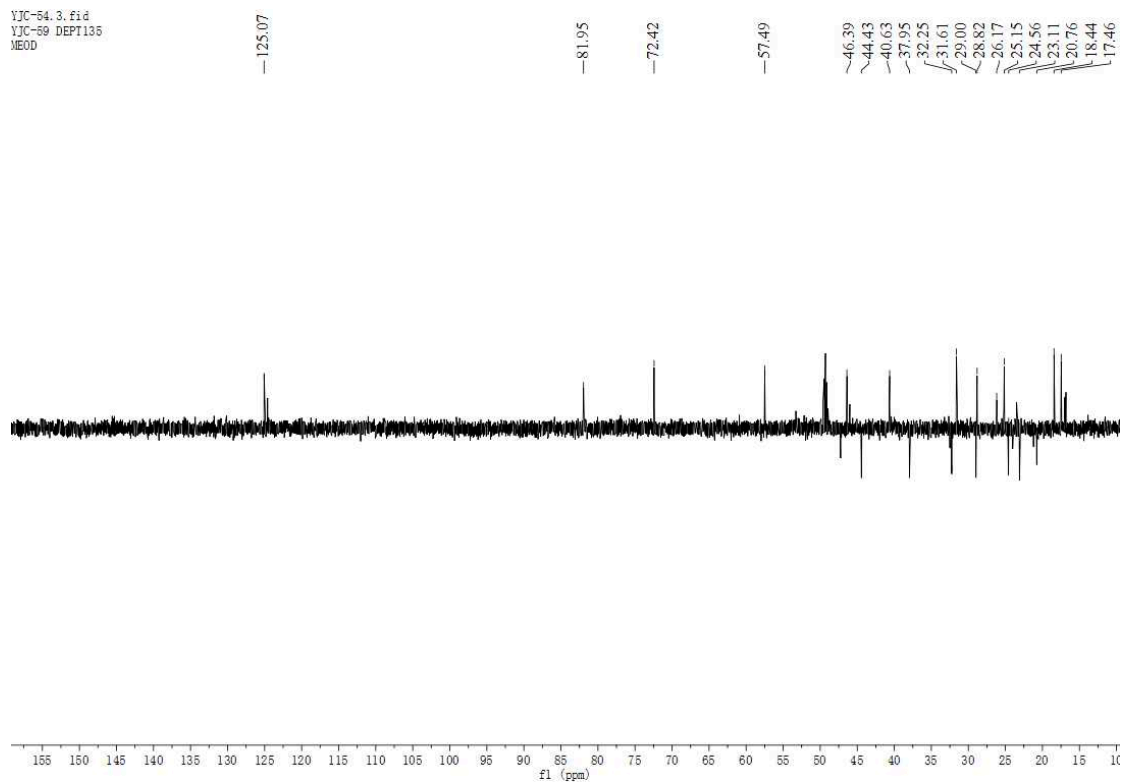


Figure S43. DEPT 135 spectrum (125 MHz, CD₃OD) of **5**

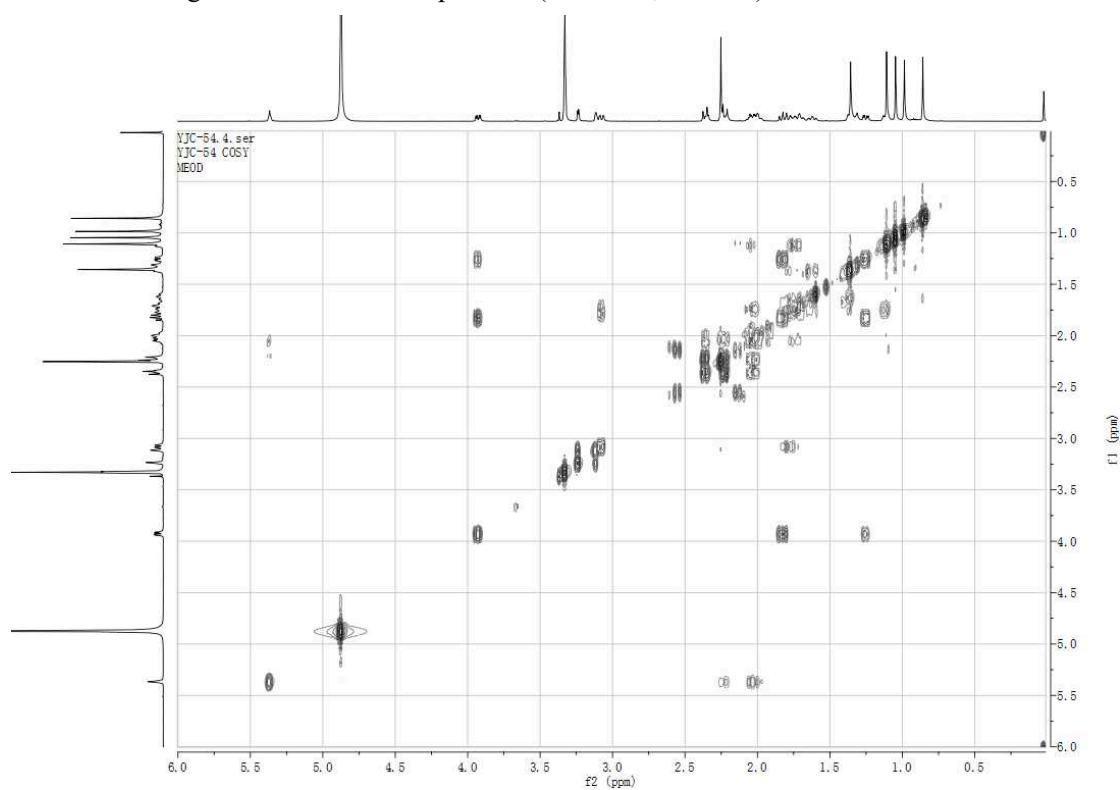


Figure S44. ¹H-¹H COSY spectrum of **5**

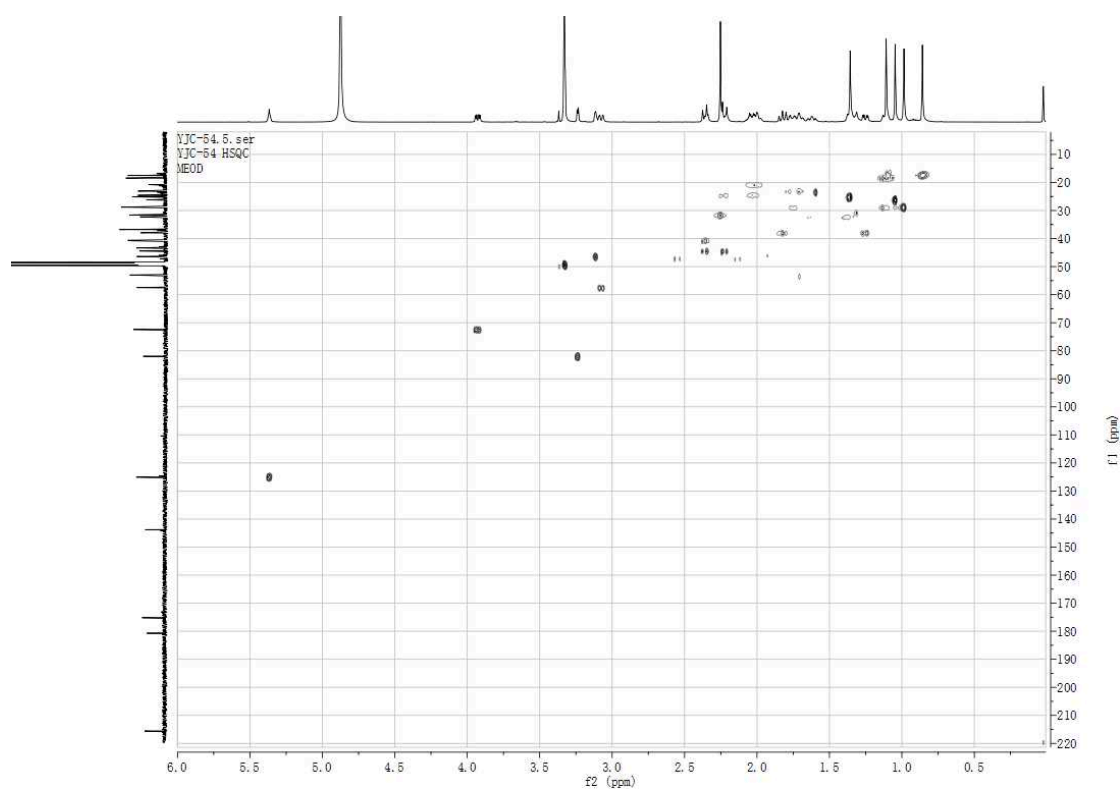


Figure S45. HSQC spectrum of **5**

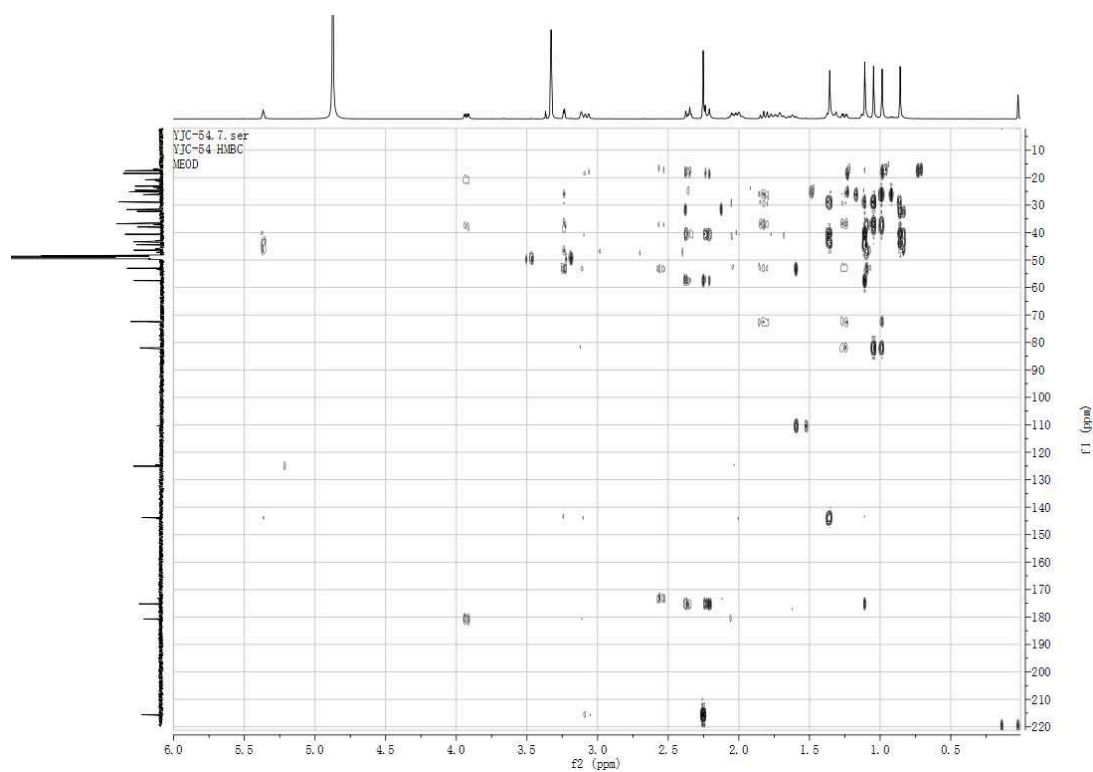


Figure S46. HMBC spectrum of **5**

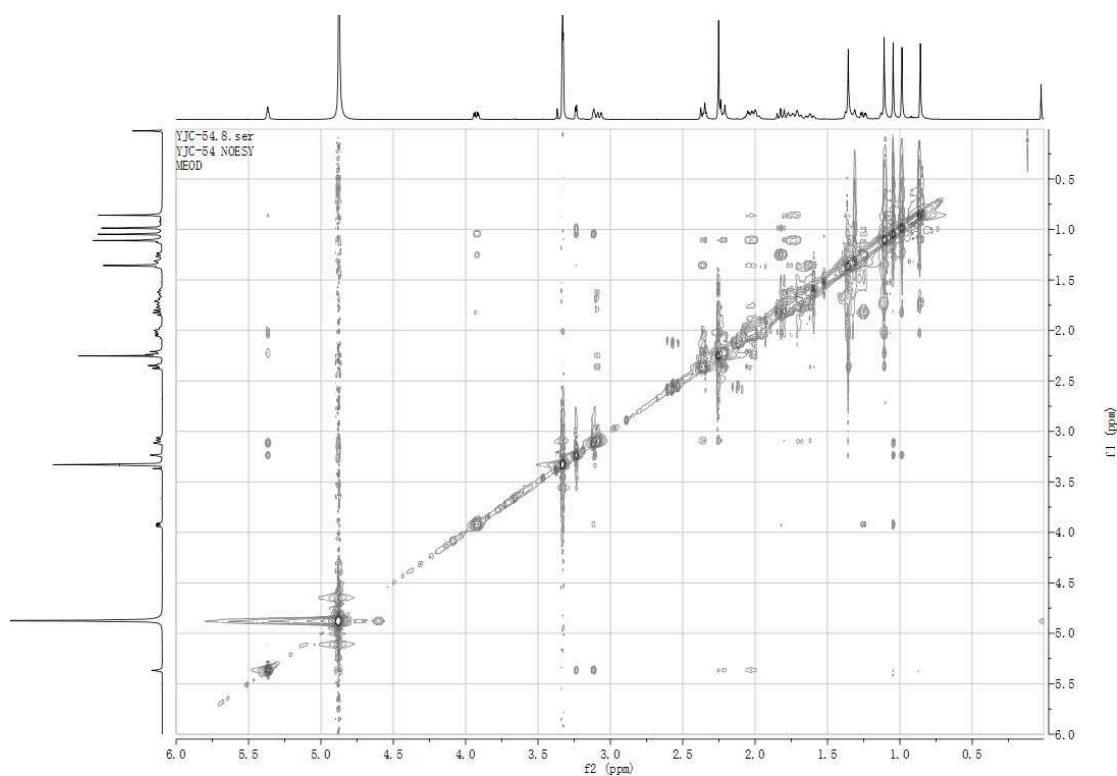


Figure S47. NOESY spectrum of **5**

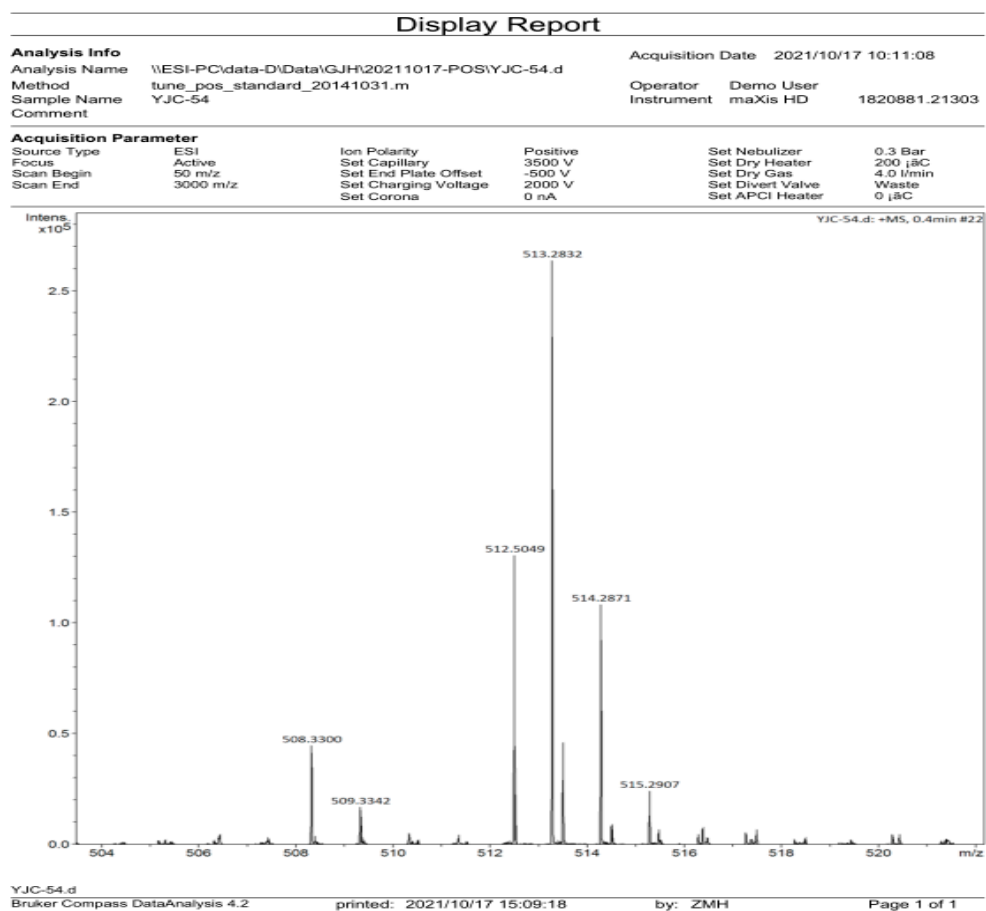


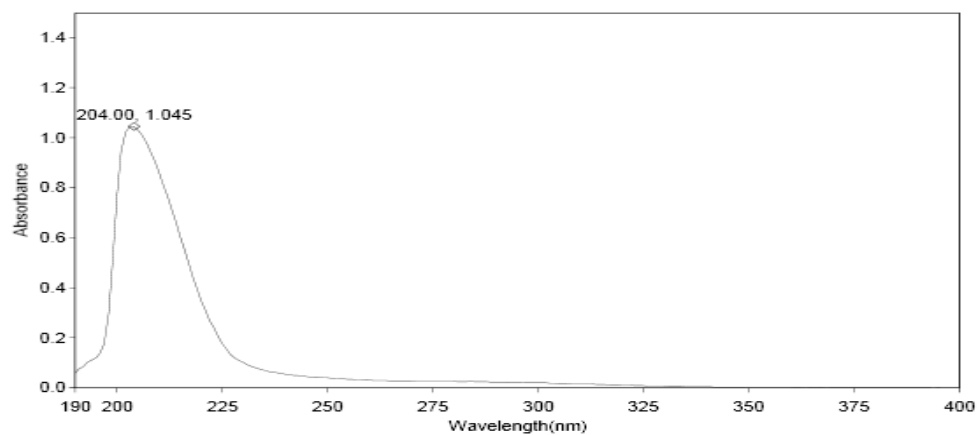
Figure S48. HR-ESI-MS Spectrum of **5**

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Operator Name (None Entered)
 Department (None Entered)
 Organization (None Entered)
 Information (None Entered)

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 Time of Report 22:45:59下午

Scan Graph



Results Table - scan030,YJC-54,Cycle01

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Start Wavelength 190.00 nm		
Stop Wavelength 400.00 nm		
Sort By Wavelength		

Sensitivity Auto

Figure S49. UV spectrum of **5**

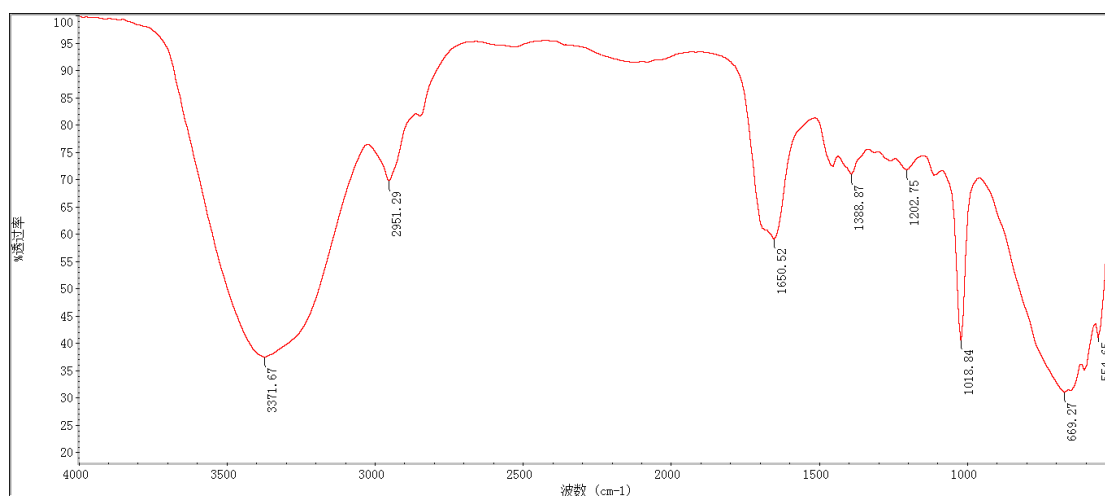


Figure S50. IR spectrum of **5**

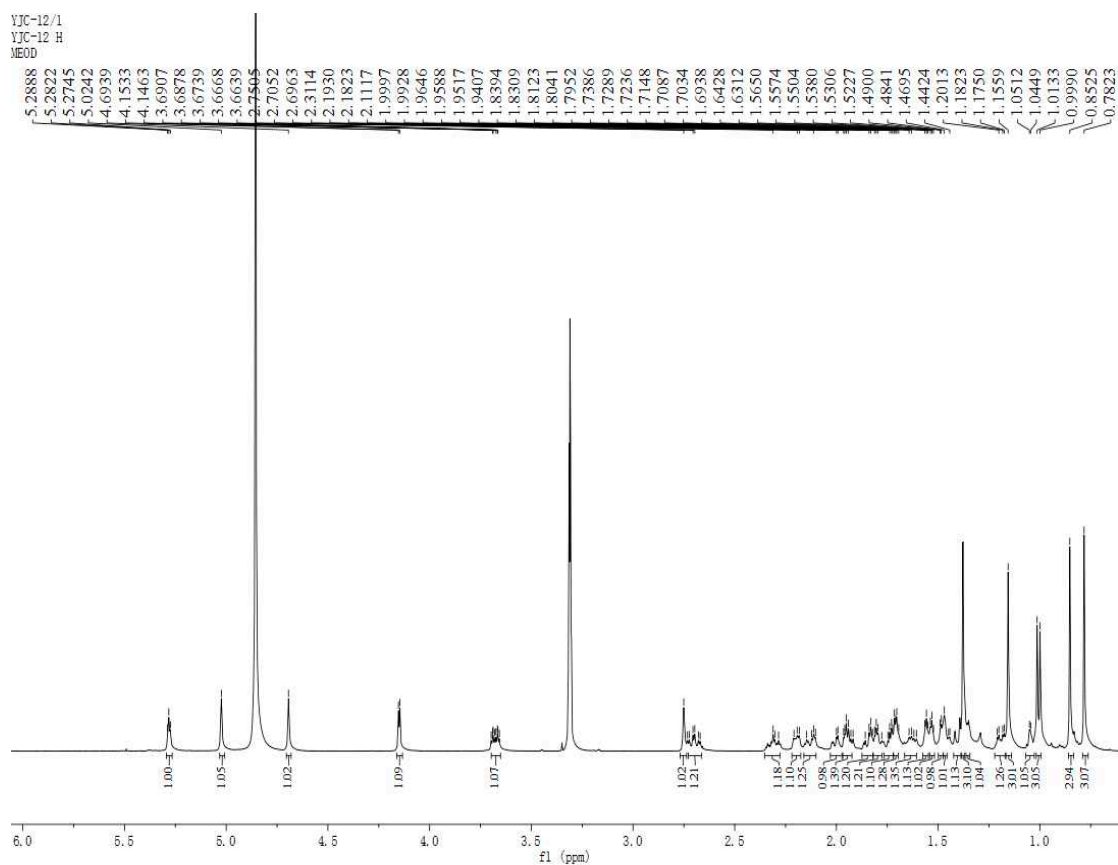


Figure S51. ^1H NMR spectrum (500 MHz, CD_3OD) of **6**

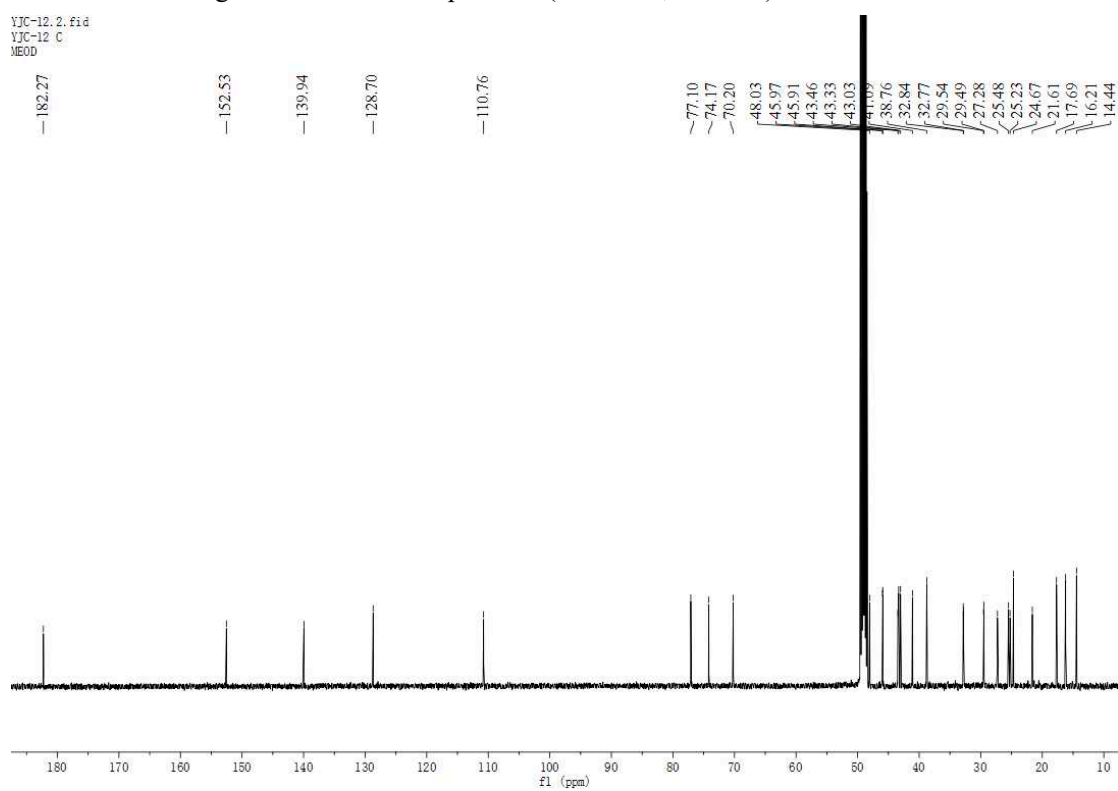


Figure S52. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **6**

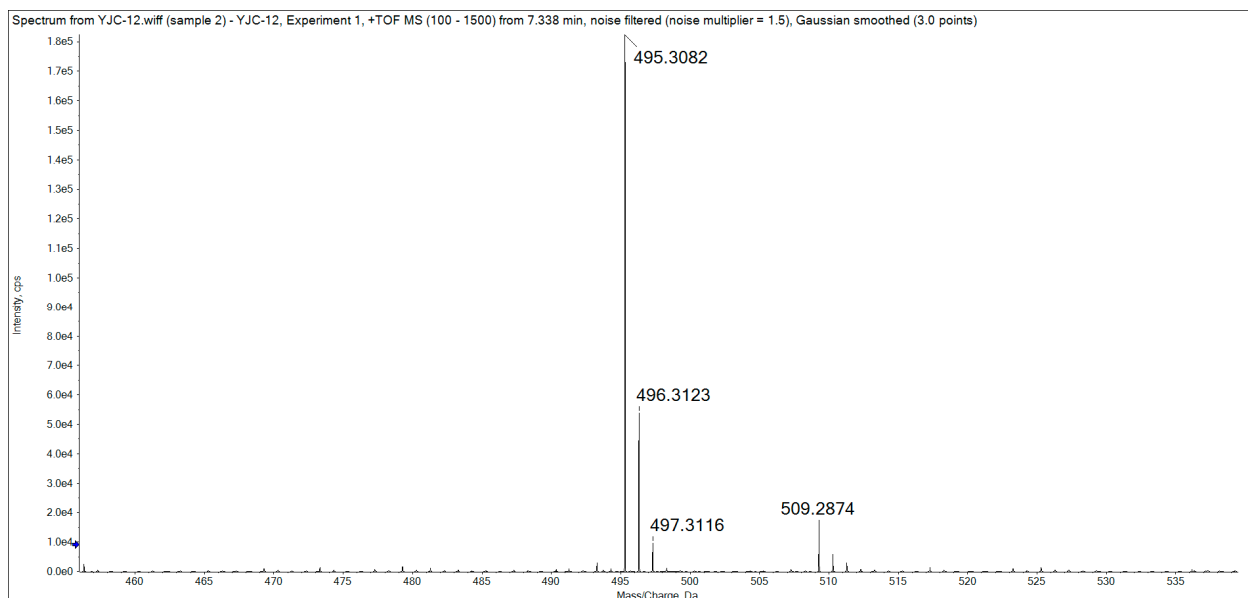


Figure S53. HR-ESI-MS Spectrum of **6**

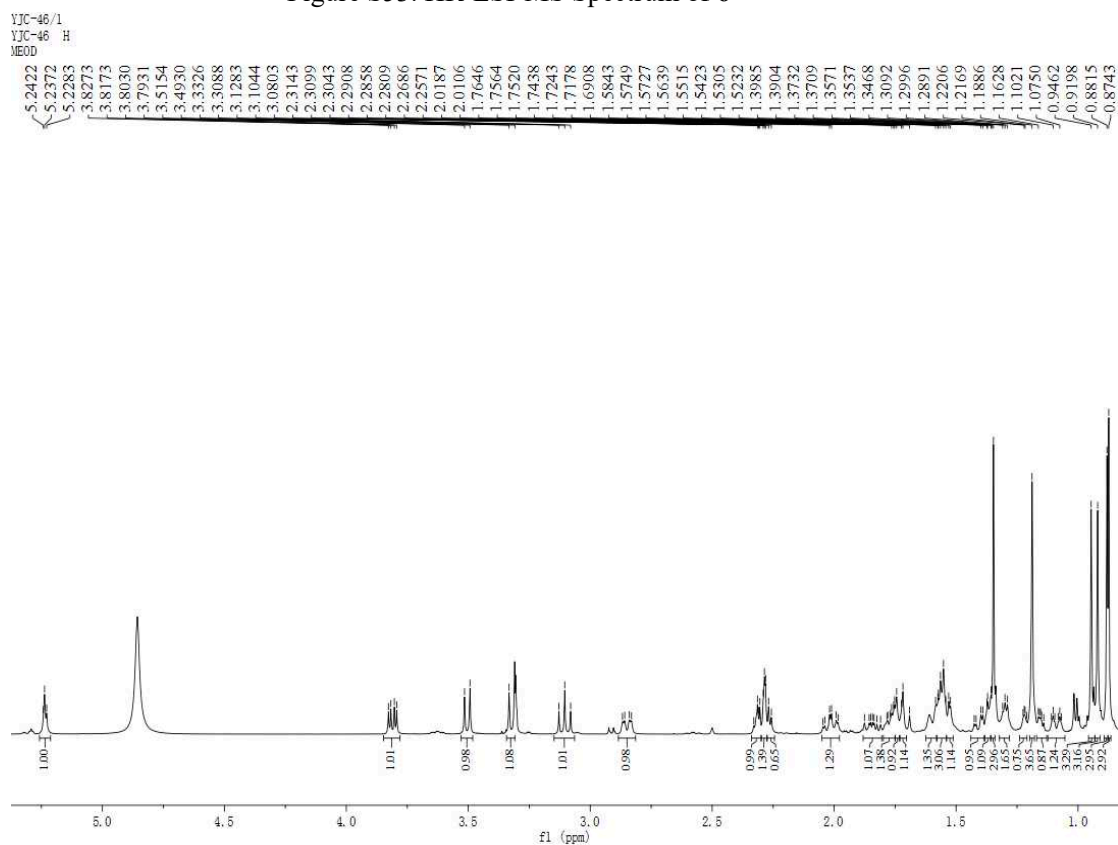


Figure S54. ^1H NMR spectrum (500 MHz, CD_3OD) of **7**

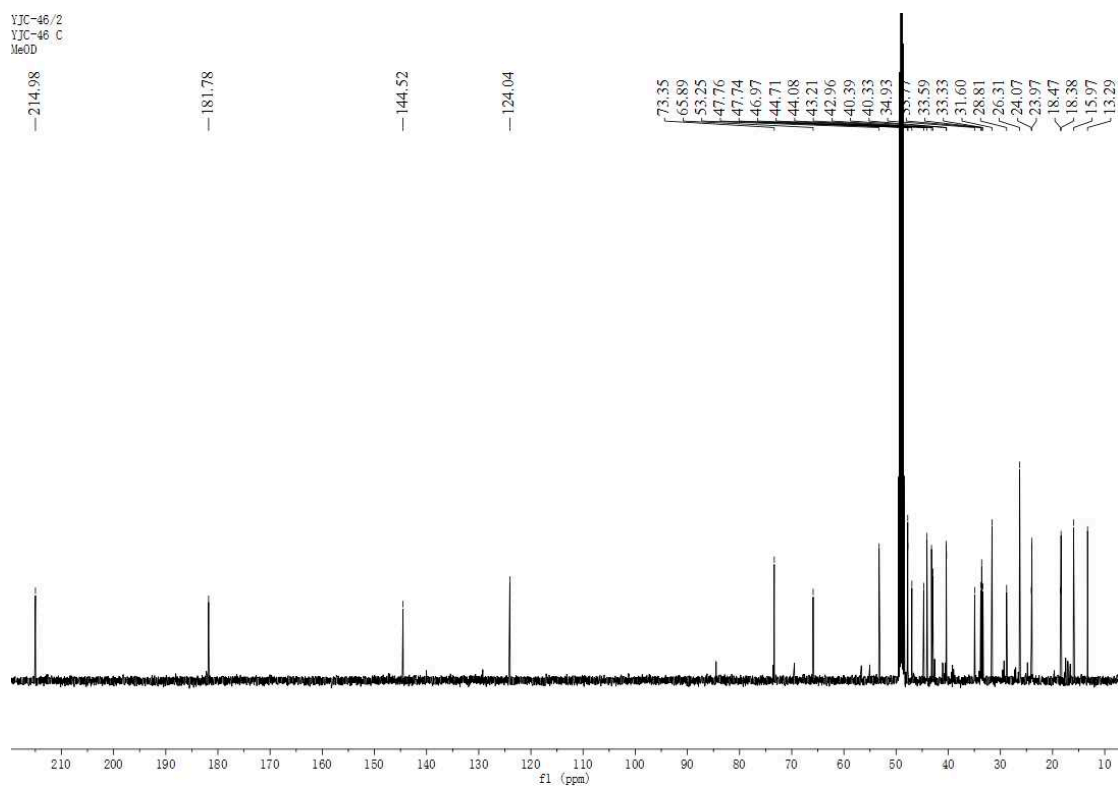


Figure S55. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **7**

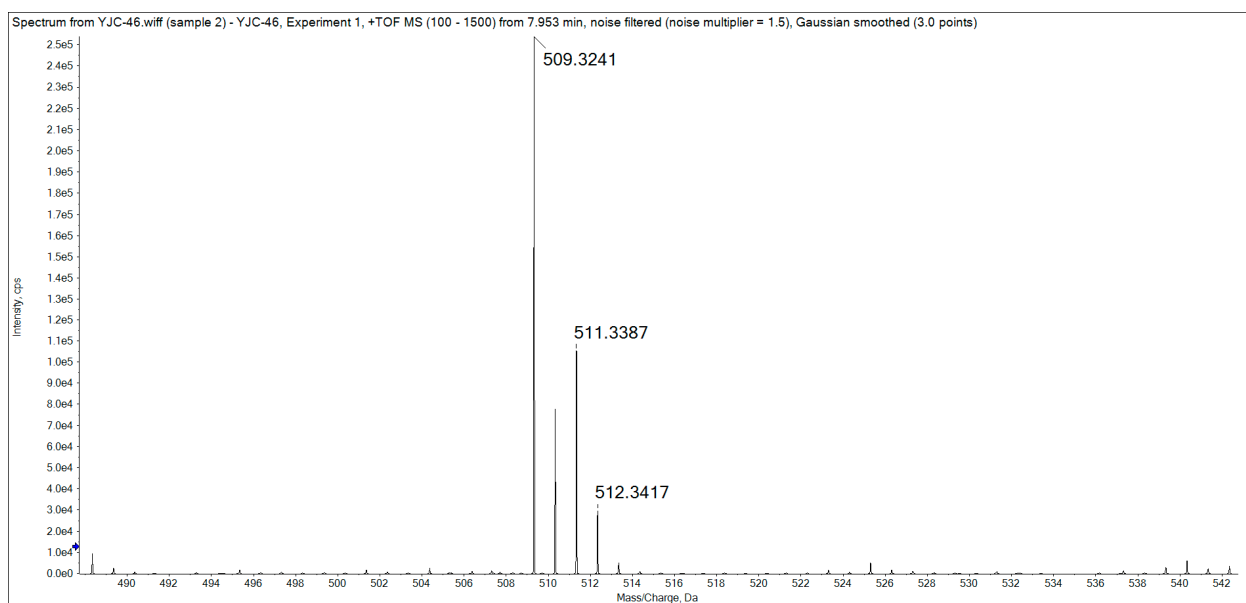


Figure S56. HR-ESI-MS Spectrum of **7**

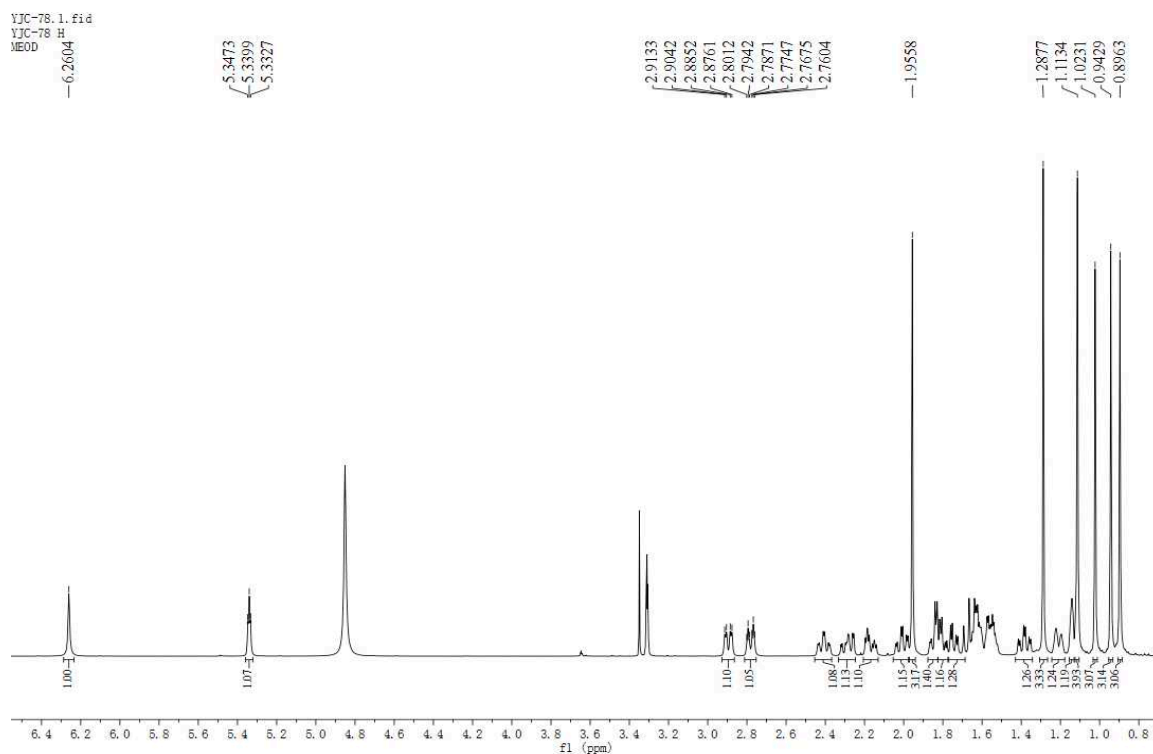


Figure S57. ^1H NMR spectrum (500 MHz, CD_3OD) of **8**

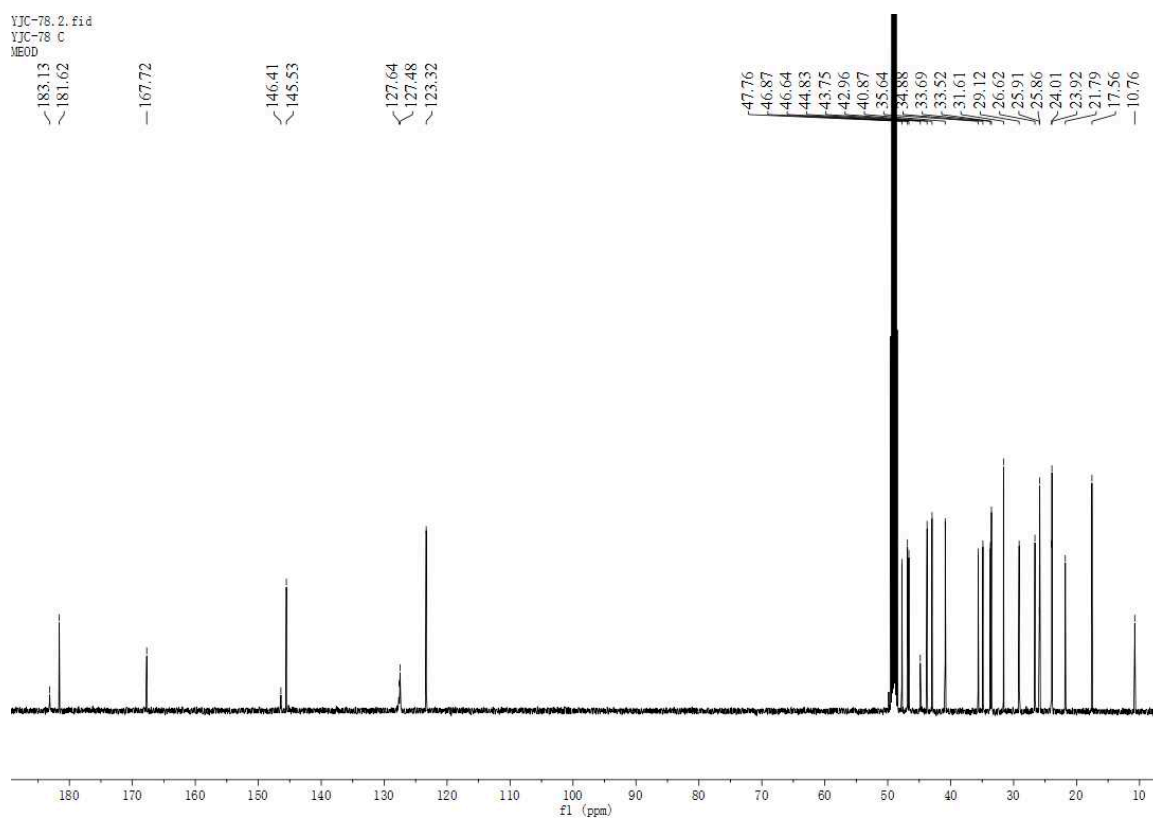


Figure S58. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **8**

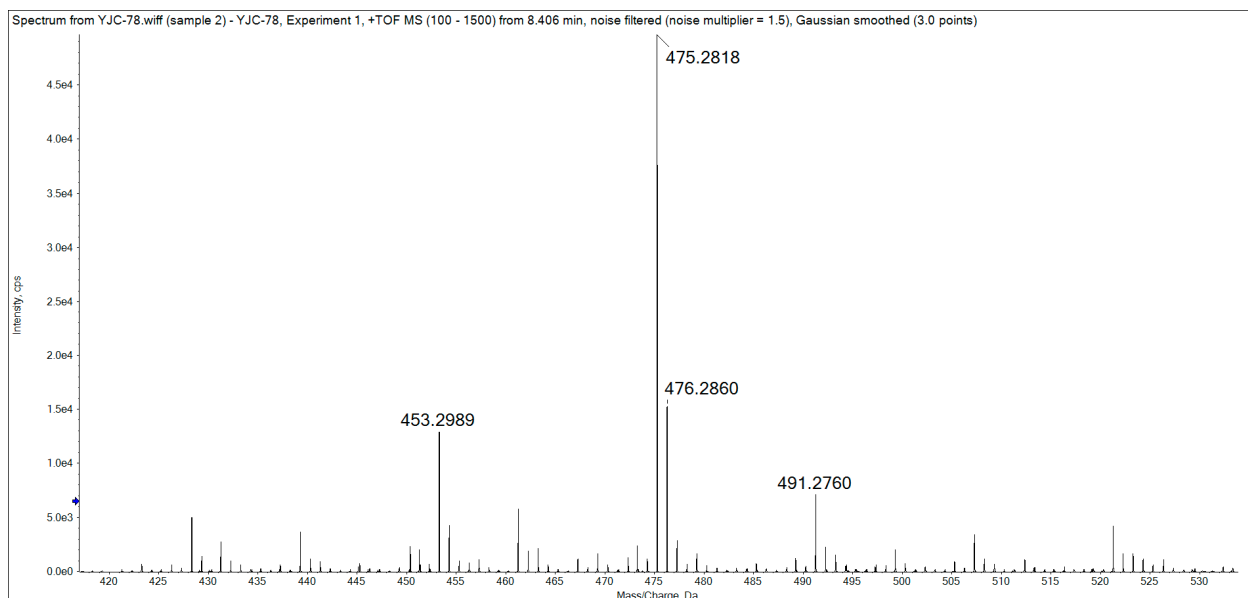


Figure S59. HR-ESI-MS Spectrum of **8**

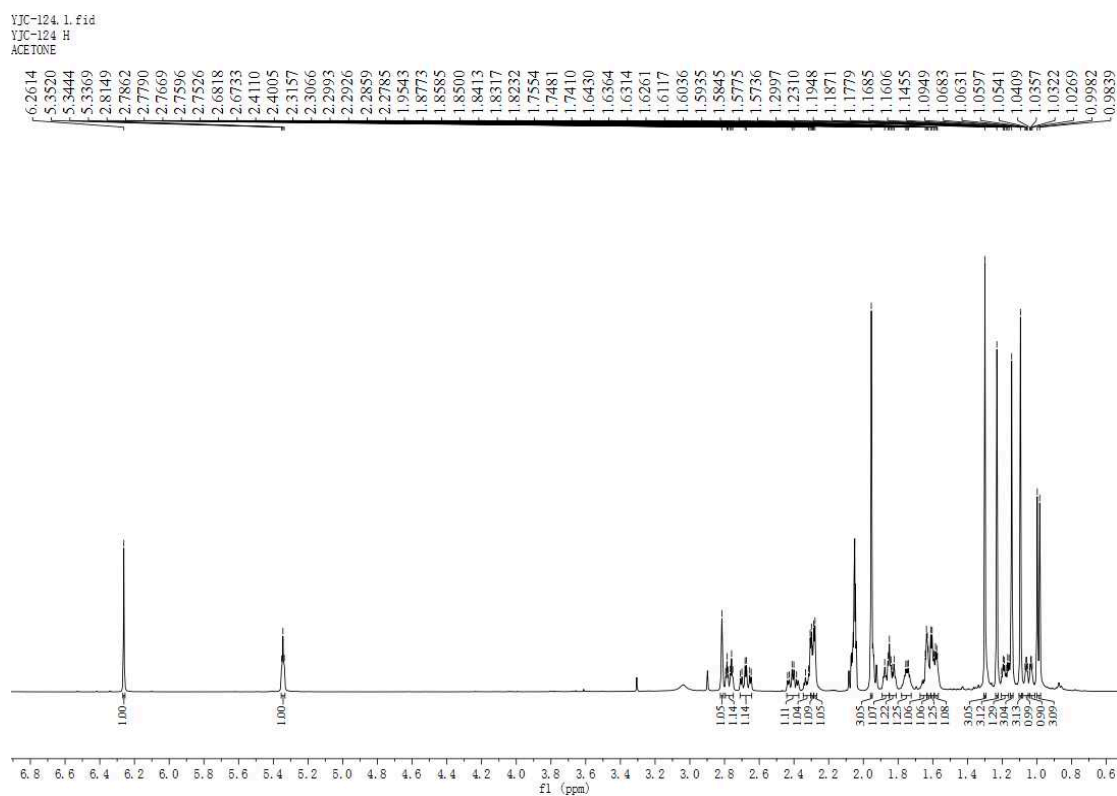


Figure S60. ^1H NMR spectrum (500 MHz, Acetone- d_6) of **9**

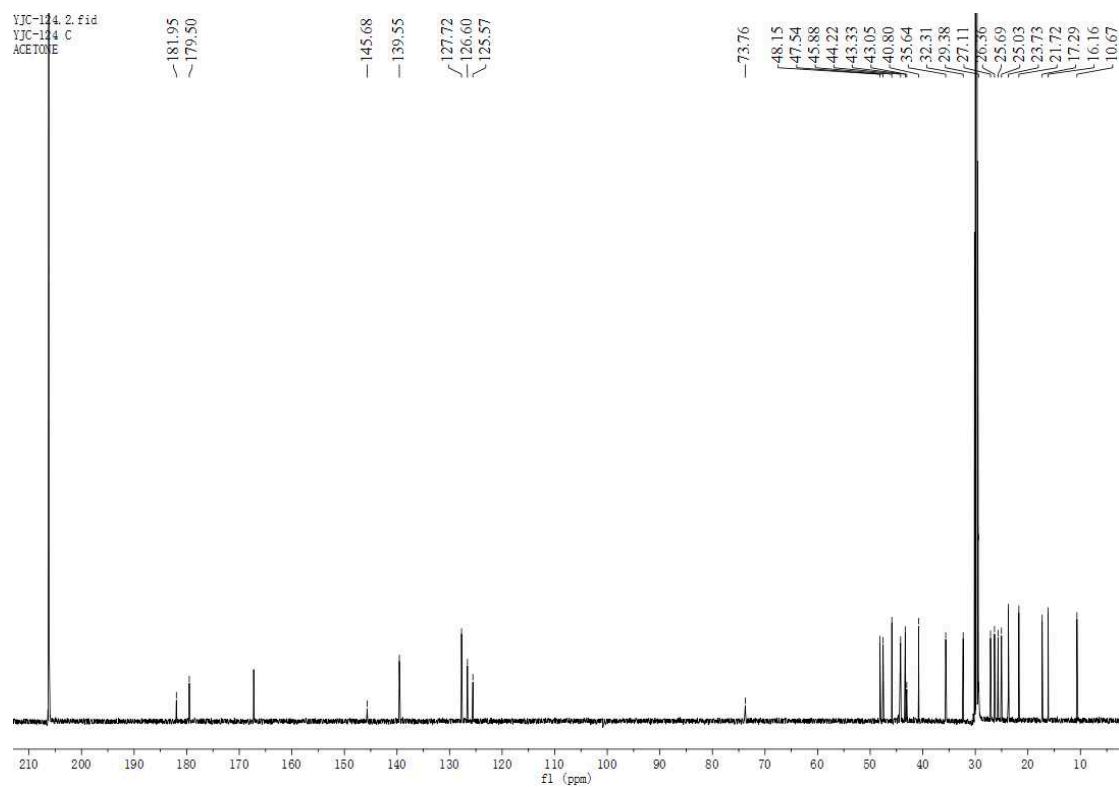


Figure S61. ^{13}C NMR spectrum (125 MHz, Acetone- d_6) of **9**

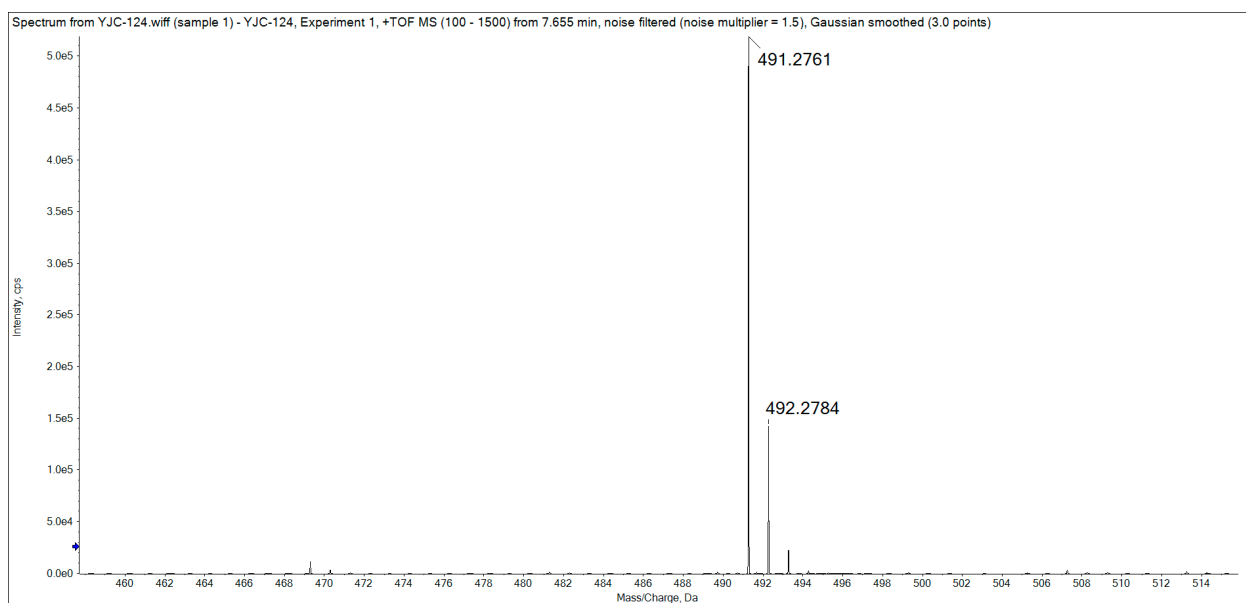


Figure S62. HR-ESI-MS Spectrum of **9**

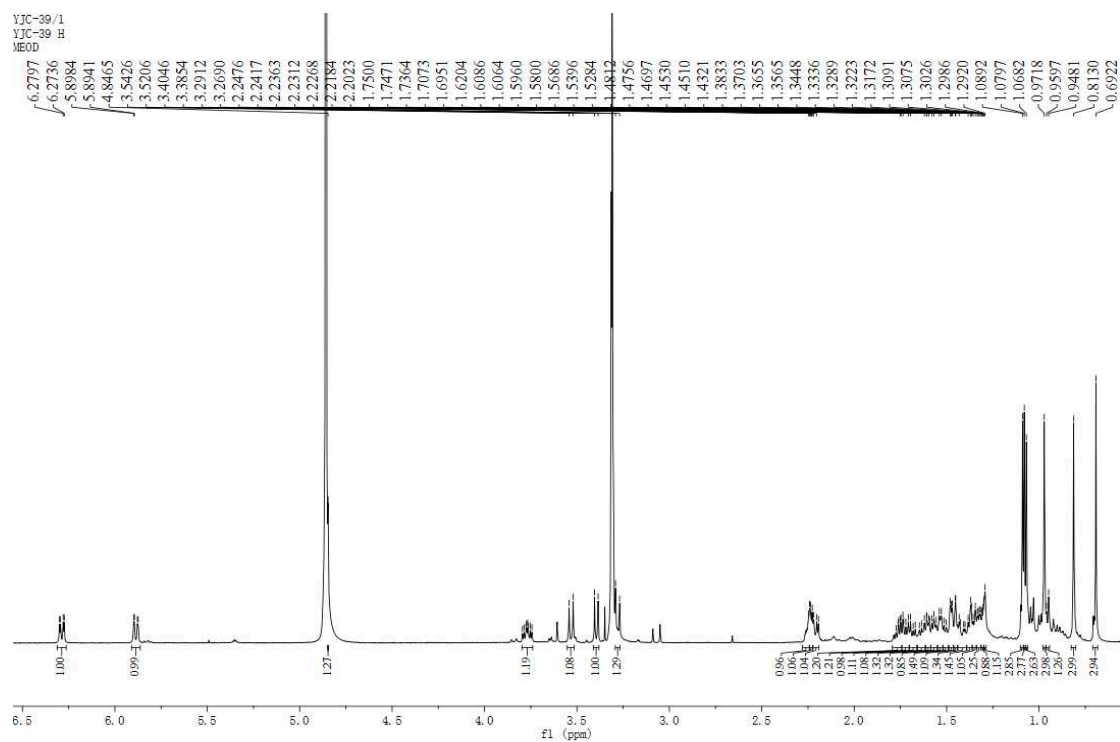


Figure S63. ^1H NMR spectrum (500 MHz, CD_3OD) of **10**

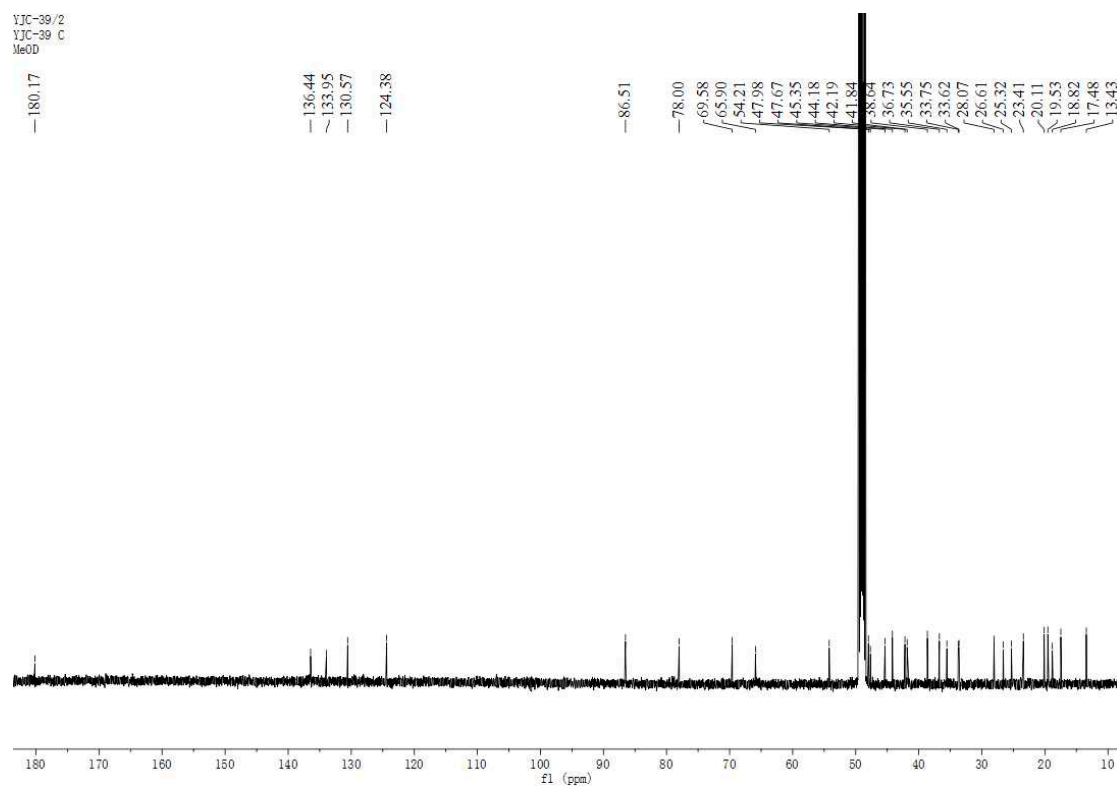


Figure S64. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **10**

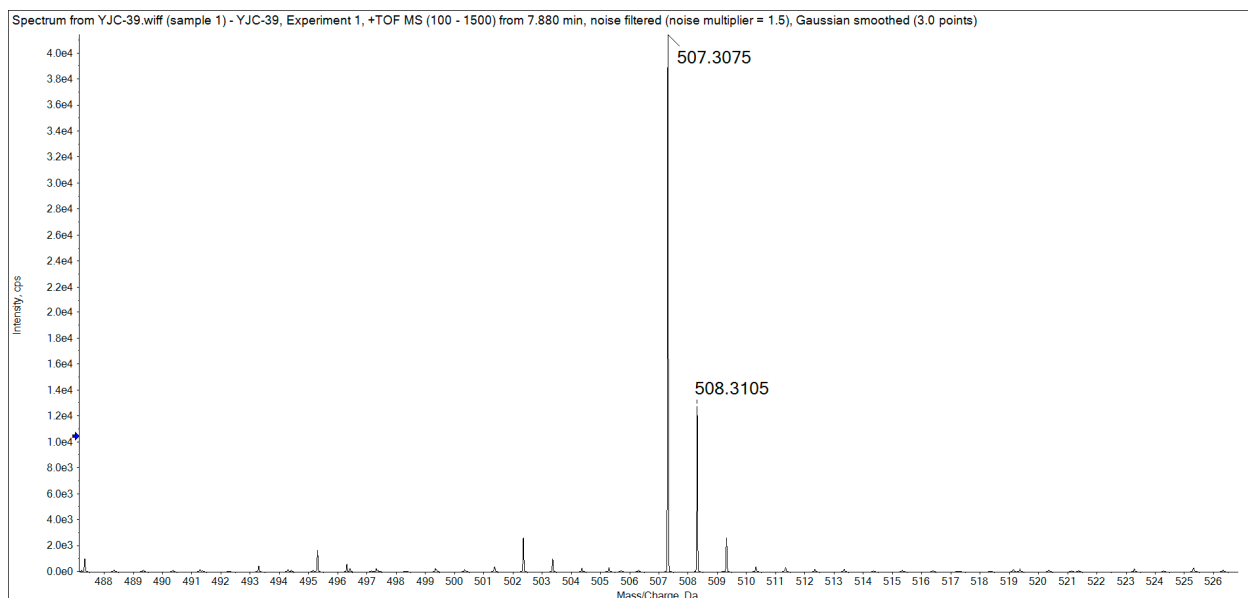


Figure S65. HR-ESI-MS Spectrum of **10**

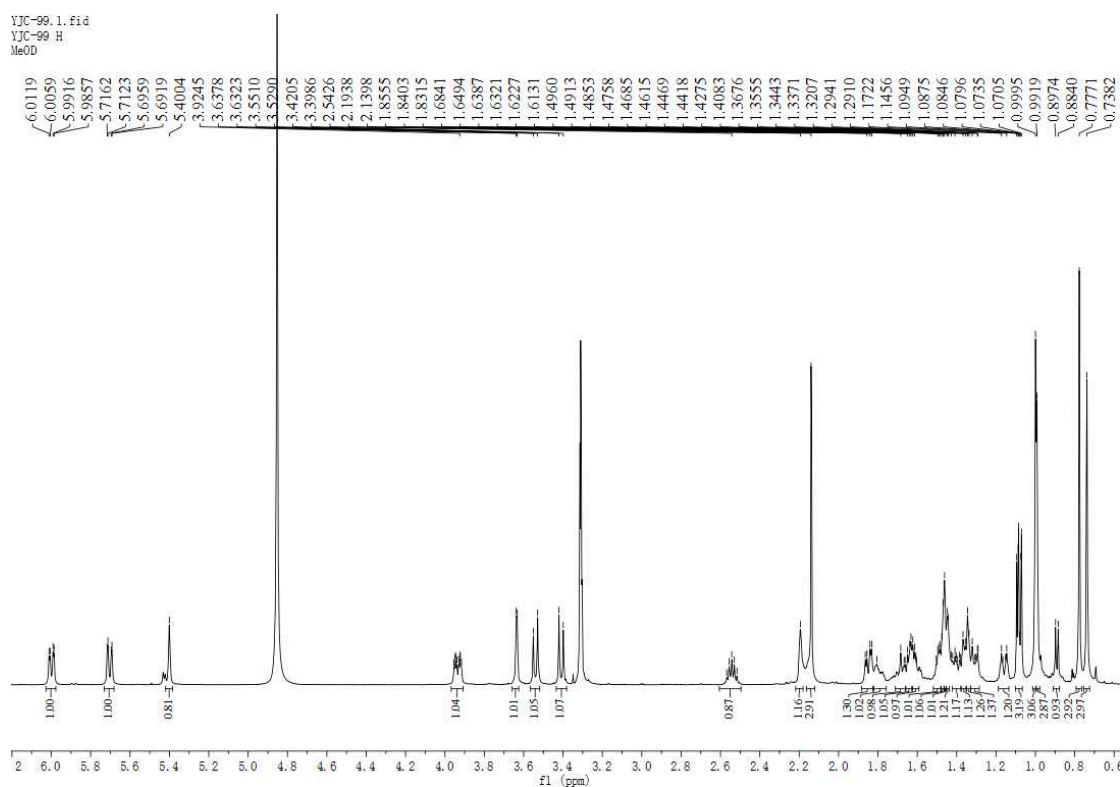


Figure S66. ^1H NMR spectrum (500 MHz, CD_3OD) of **11**

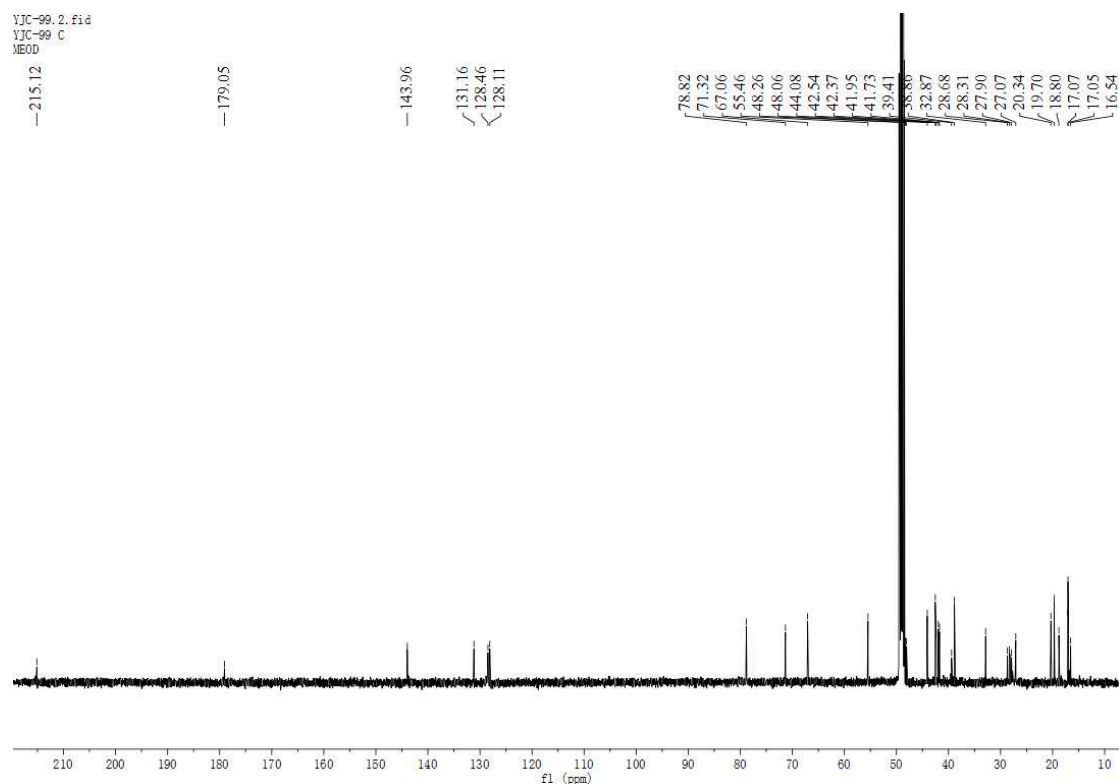


Figure S67. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **11**

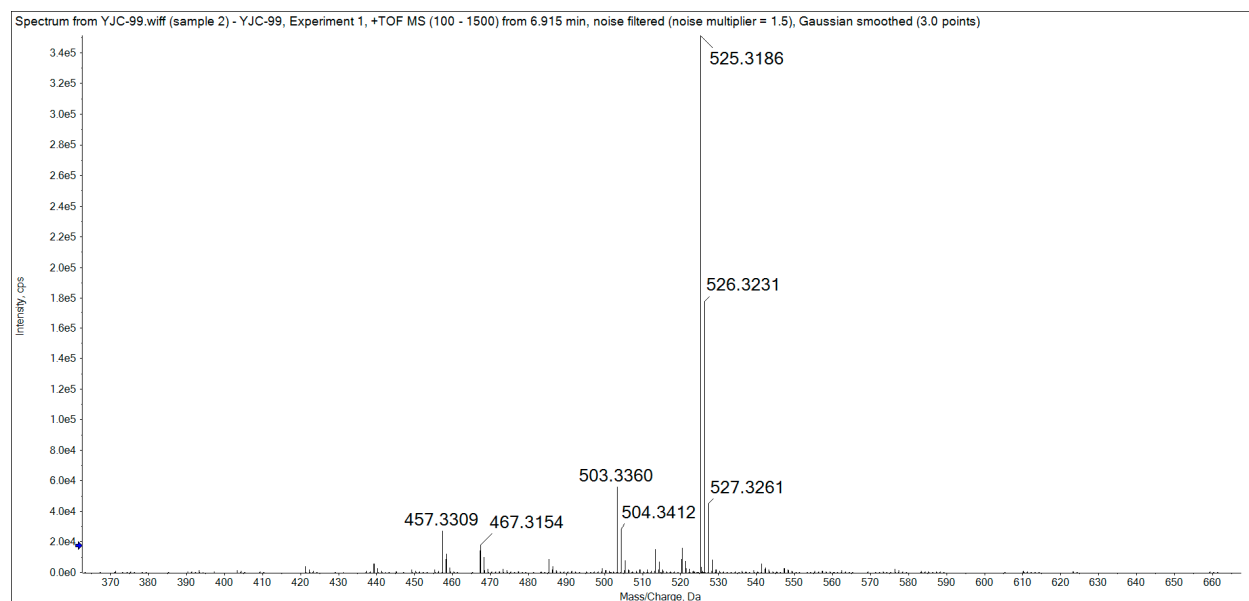


Figure S68. HR-ESI-MS Spectrum of **11**

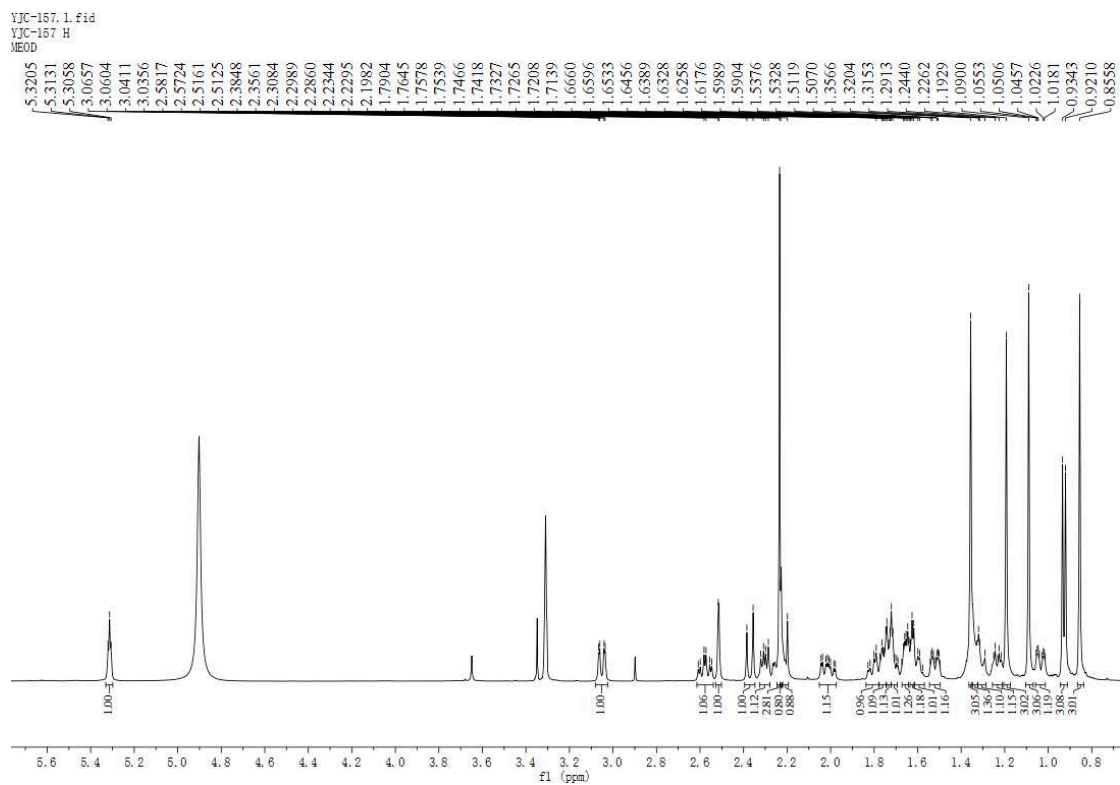


Figure S69. ^1H NMR spectrum (500 MHz, CD_3OD) of **12**

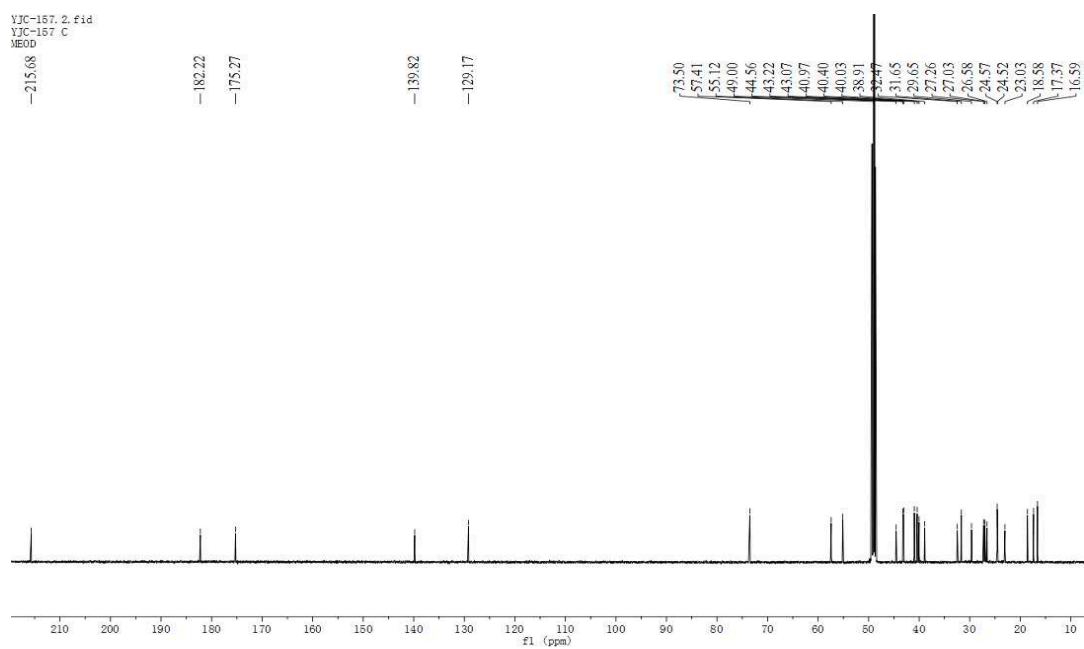


Figure S70. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **12**

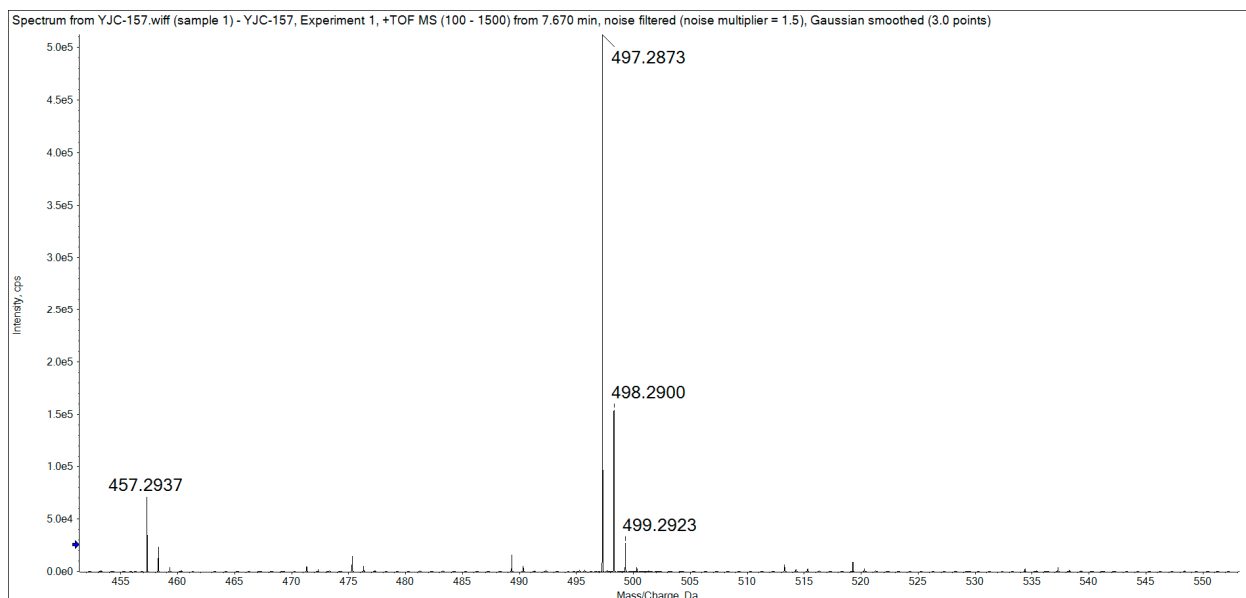


Figure S71. HR-ESI-MS Spectrum of **12**

Table 4 Melting points of compounds **6-12**

compound	mp (°C)	Group	mp (°C)
6	234	10	253
7	245	11	240
8	215	12	238
9	241		

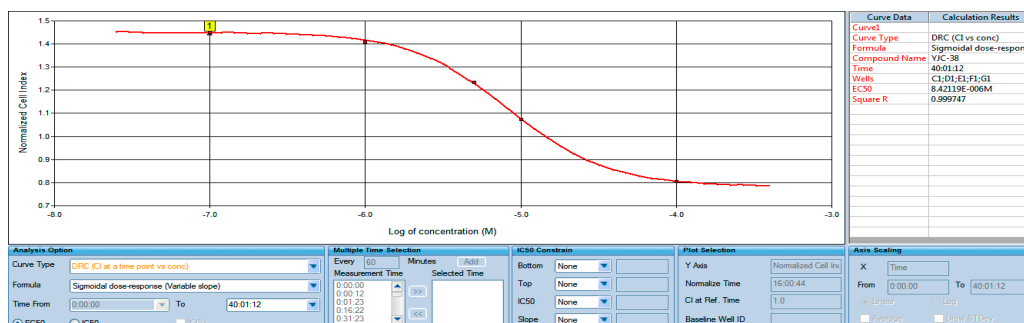


Figure S72. The curve obtained with compound **1**

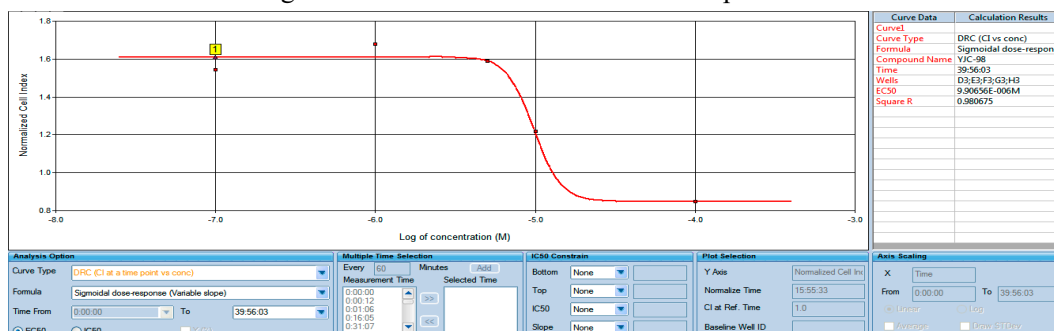


Figure S73. The curve obtained with compound **2**

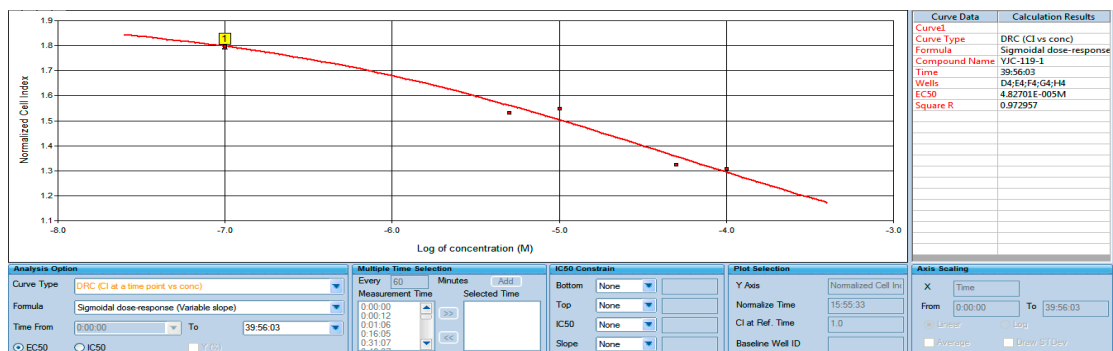


Figure S74. The curve obtained with compound 3

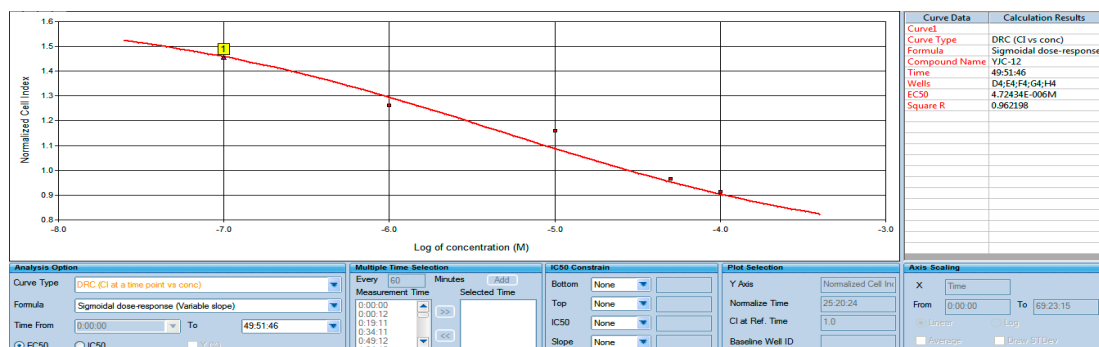


Figure S75. The curve obtained with compound 6

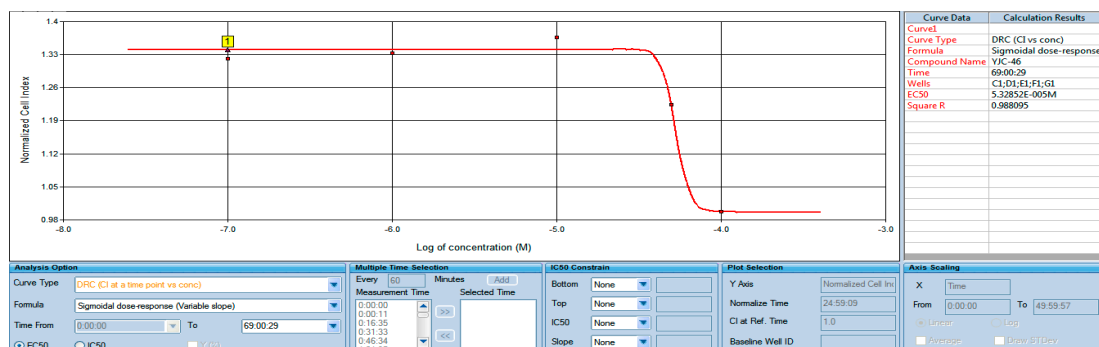


Figure S76. The curve obtained with compound 7

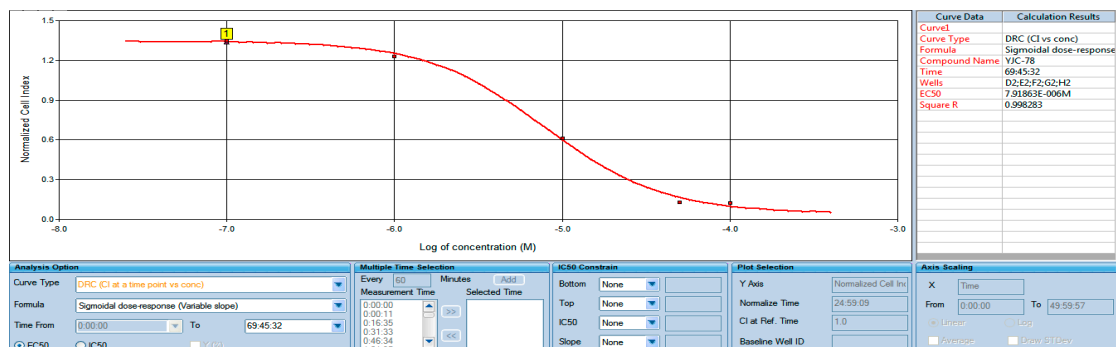


Figure S77. The curve obtained with compound 8

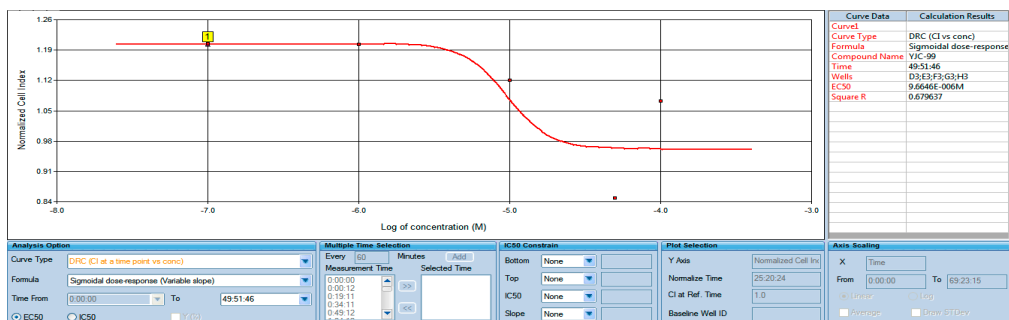


Figure S78. The curve obtained with compound 11

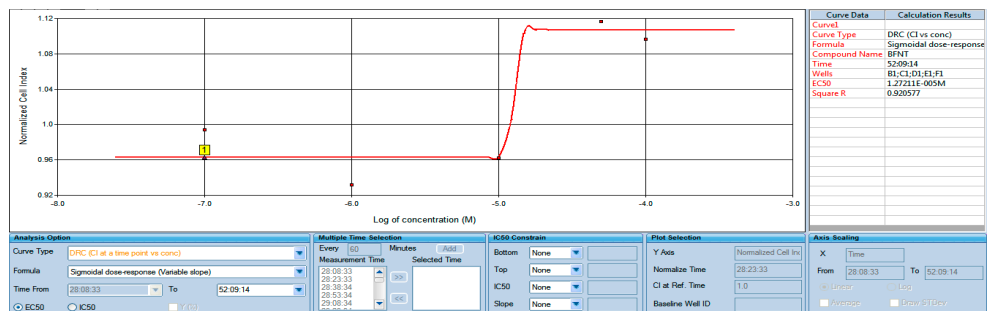


Figure S79. The curve obtained with positive control compound Pirfenidone