

Supplementary Information for

Acid-catalyzed transformation of cassane diterpenoids from *Ceasalpinia bonduc* to aromatic derivatives

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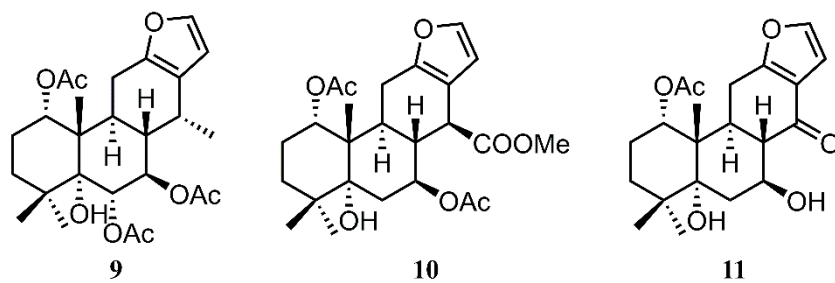


Figure S1. Structures of compounds 9-11.

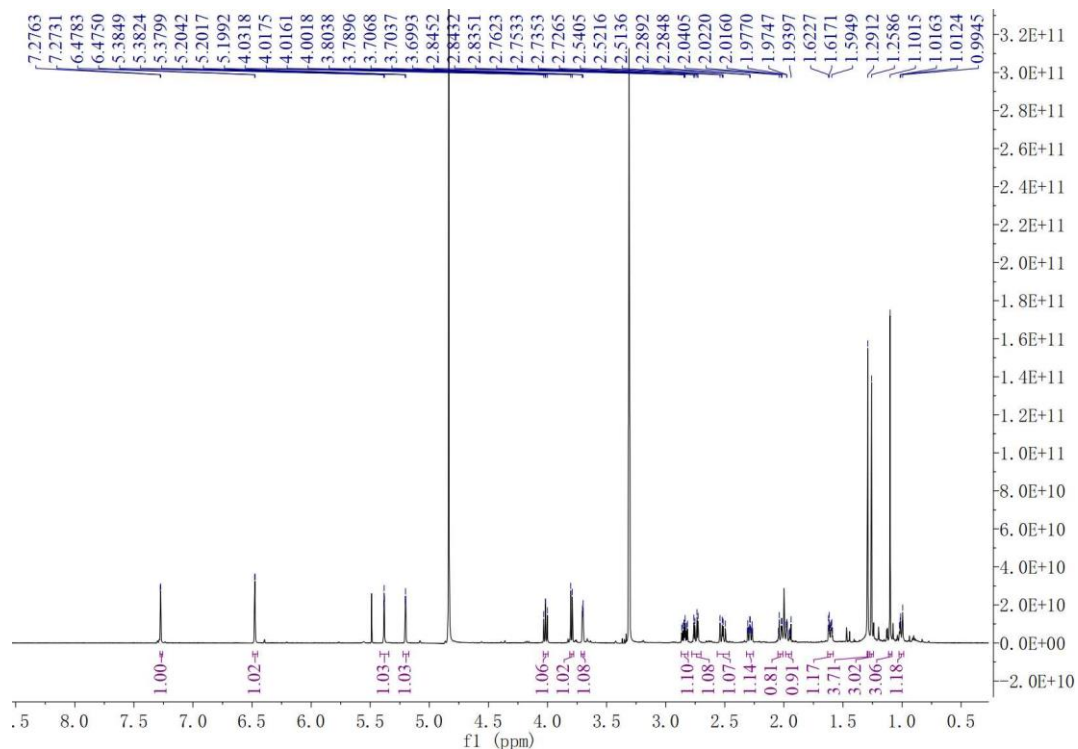


Figure S2. ^1H NMR (600 MHz, CD_3OD) spectrum of compound 1

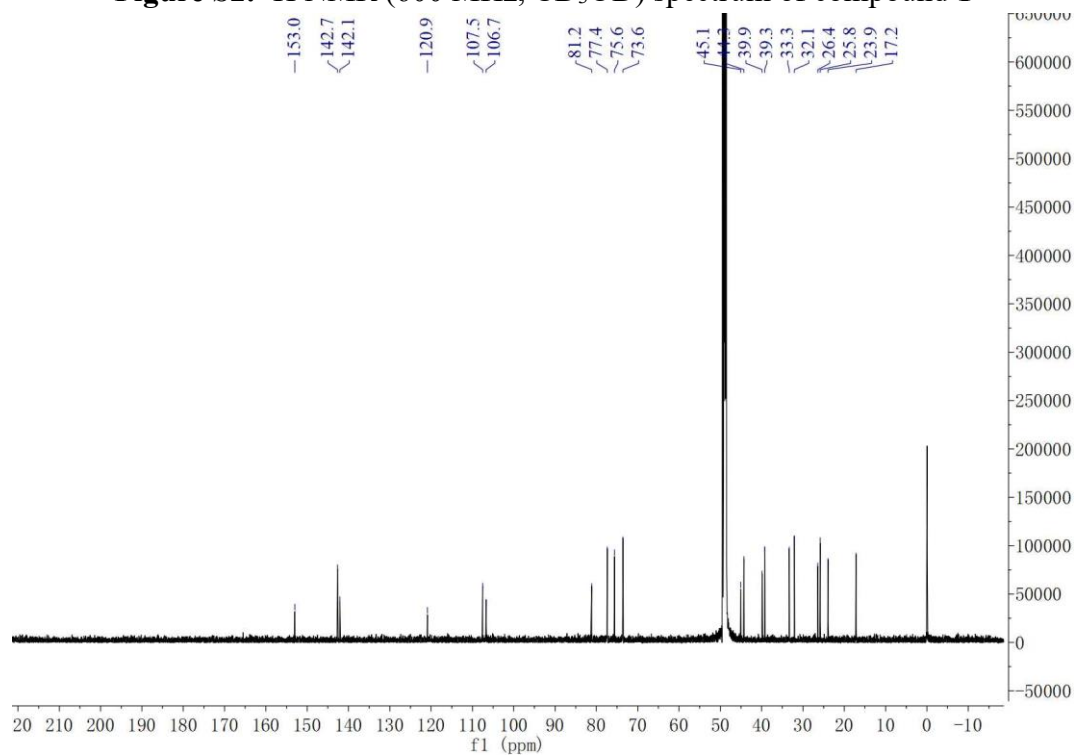


Figure S3. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 1

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	220 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

C20H28O5, M+nNa, 371.1829

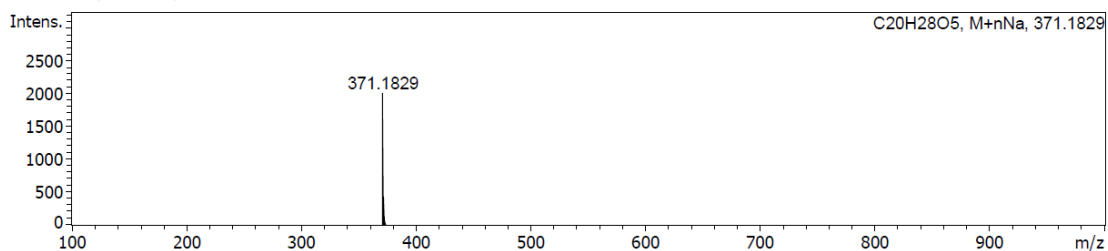


Figure S4. HRESIMS spectrum of compound 1

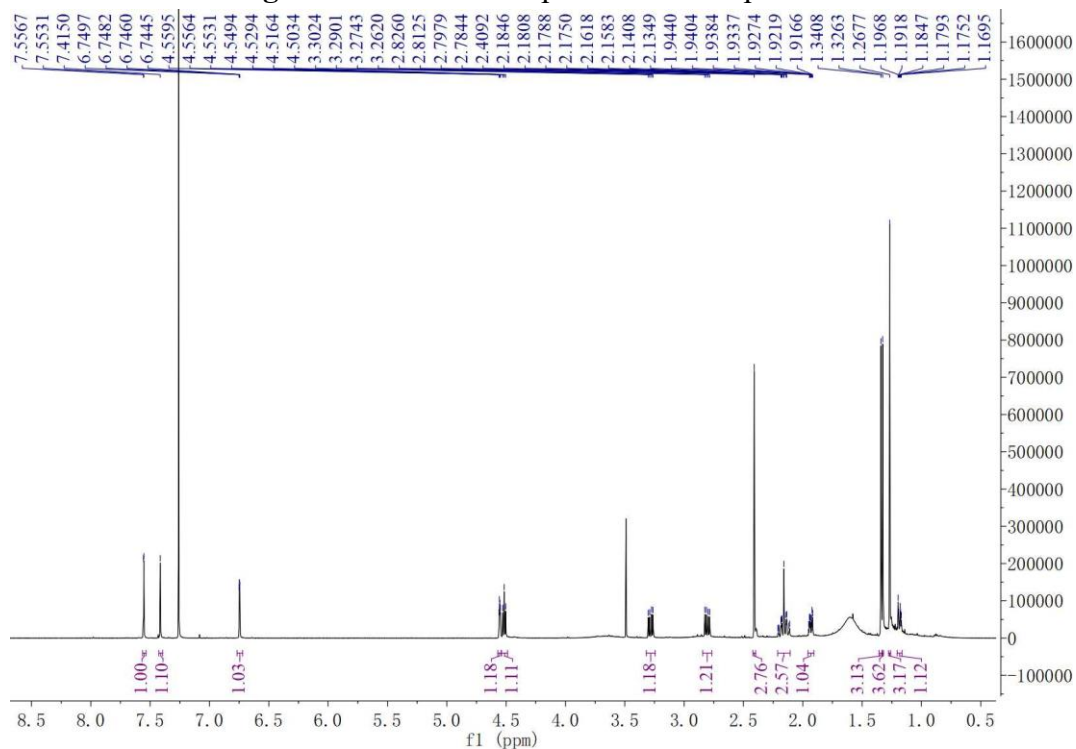


Figure S5. ¹H NMR (600 MHz, CDCl₃) spectrum of compound 1a

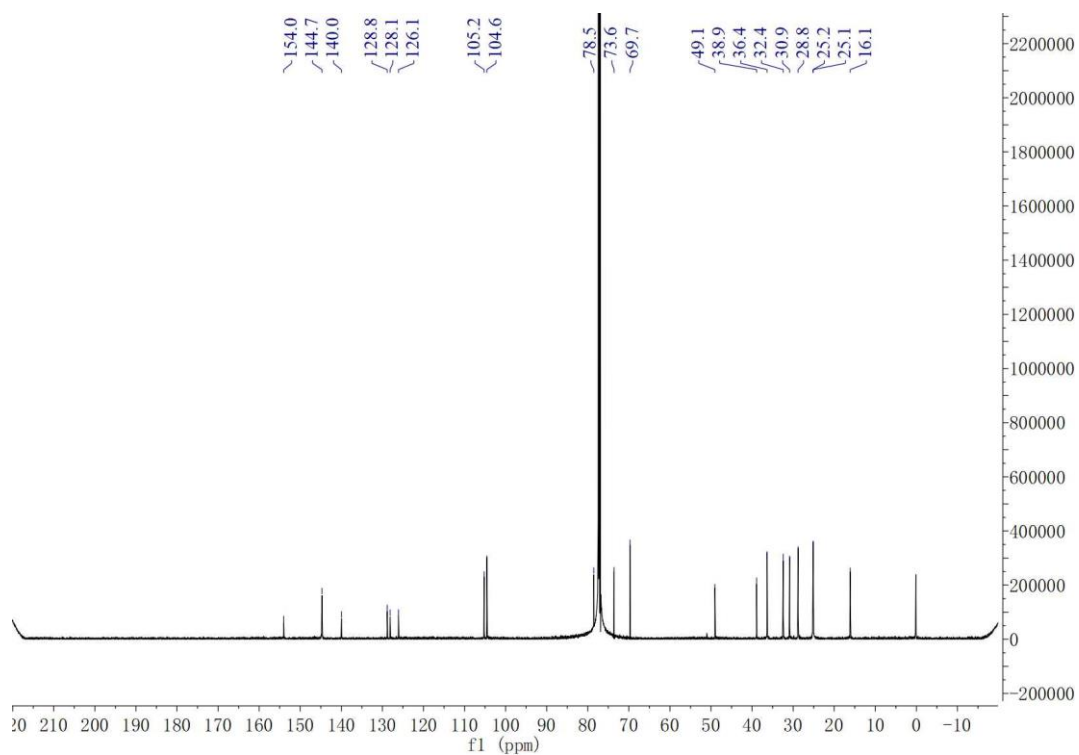


Figure S6. ^{13}C NMR (150 MHz, CDCl_3) spectrum of compound **1a**

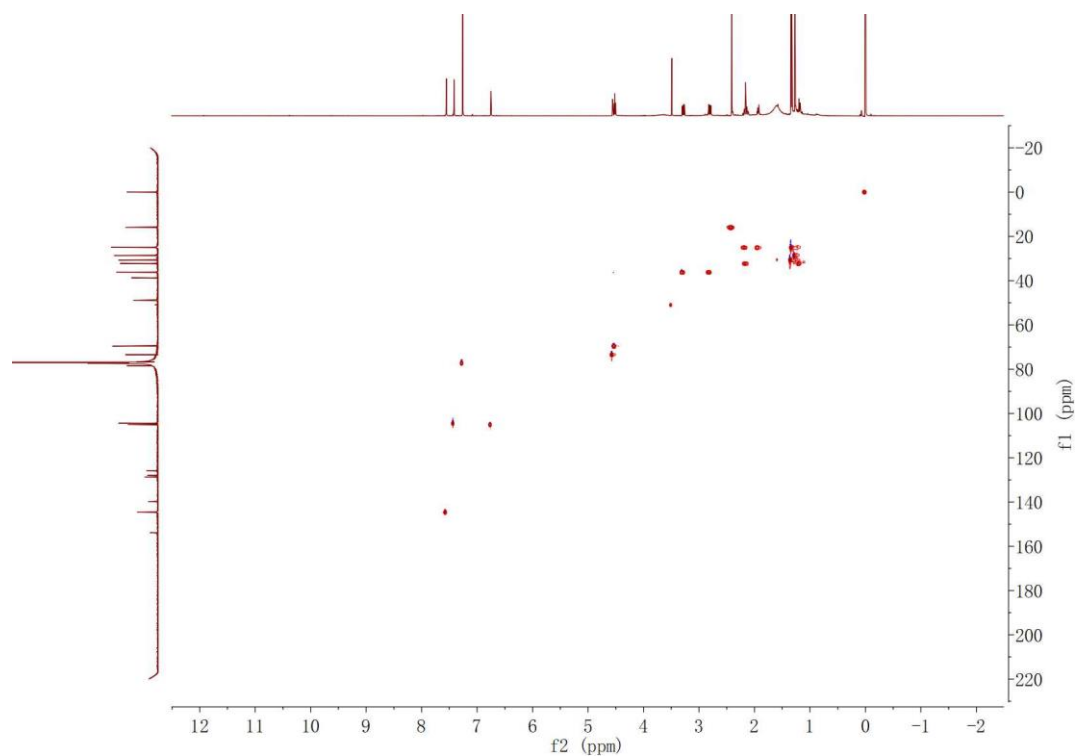


Figure S7. HSQC (600 MHz, CDCl_3) spectrum of compound **1a**

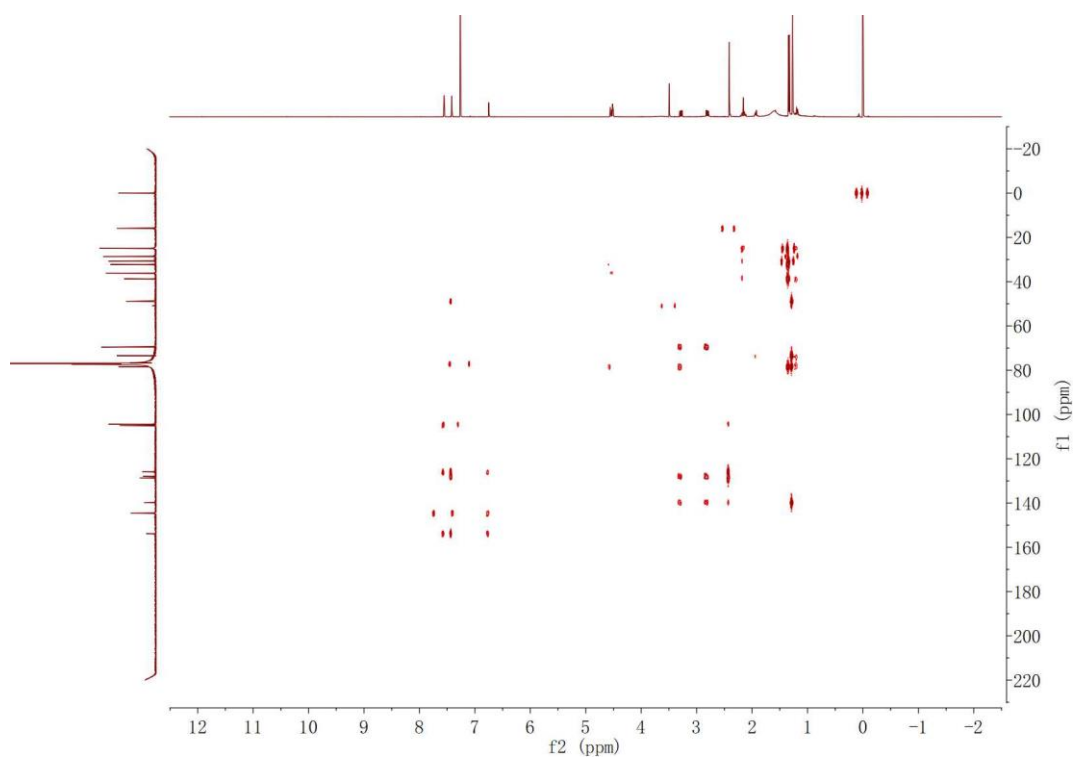


Figure S8. HMBC (600 MHz, CDCl₃) spectrum of compound **1a**

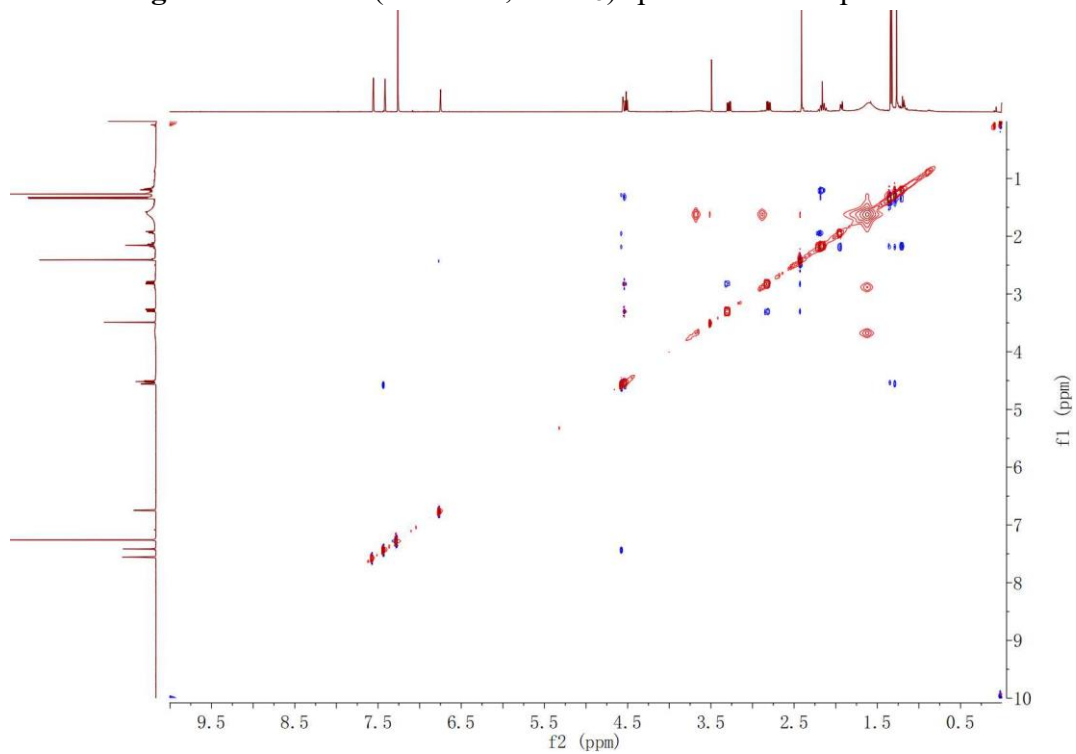
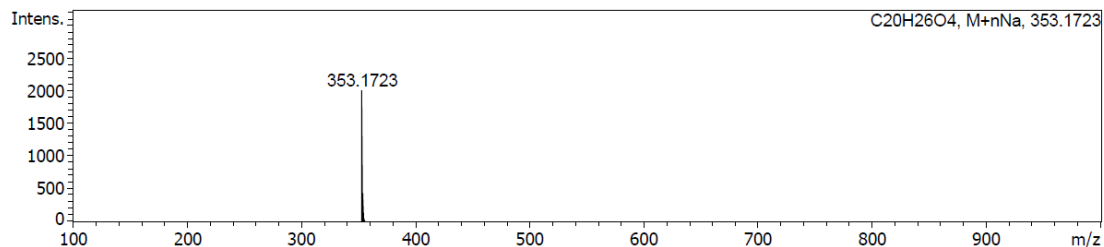
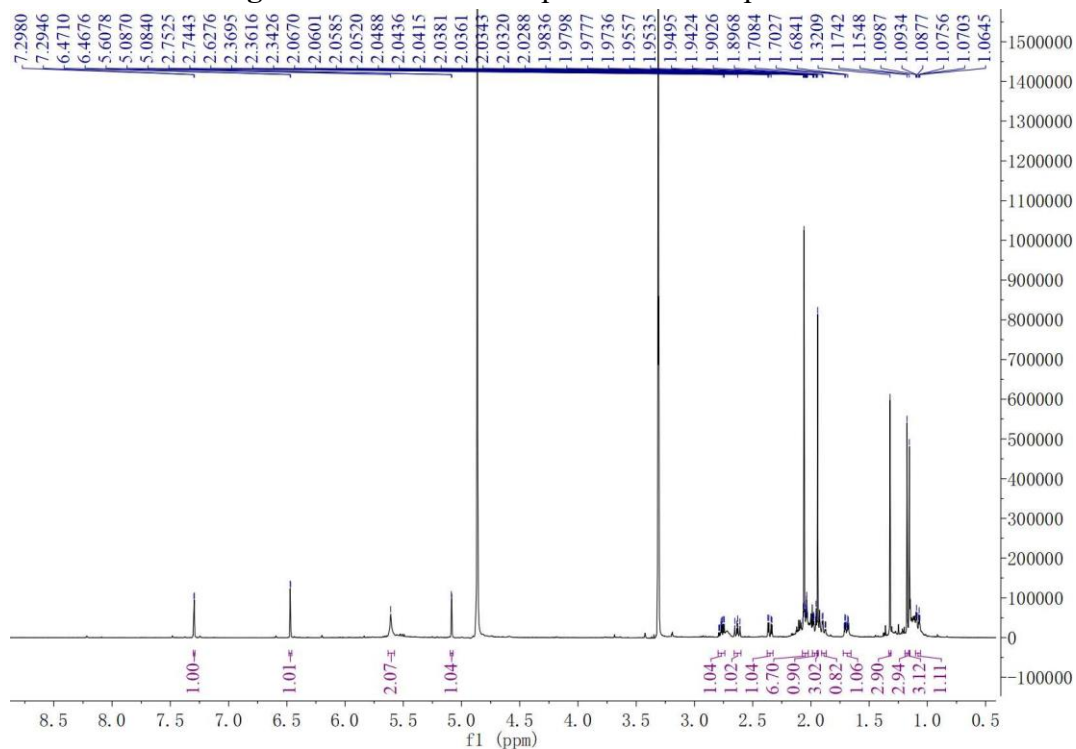


Figure S9. NOESY (600 MHz, CDCl₃) spectrum of compound **1a**

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	220 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

C20H26O4, M+nNa, 353.1723**Figure S10. HRESIMS spectrum of compound 1a****Figure S11. ¹H NMR (600 MHz, CD₃OD) spectrum of compound 2**

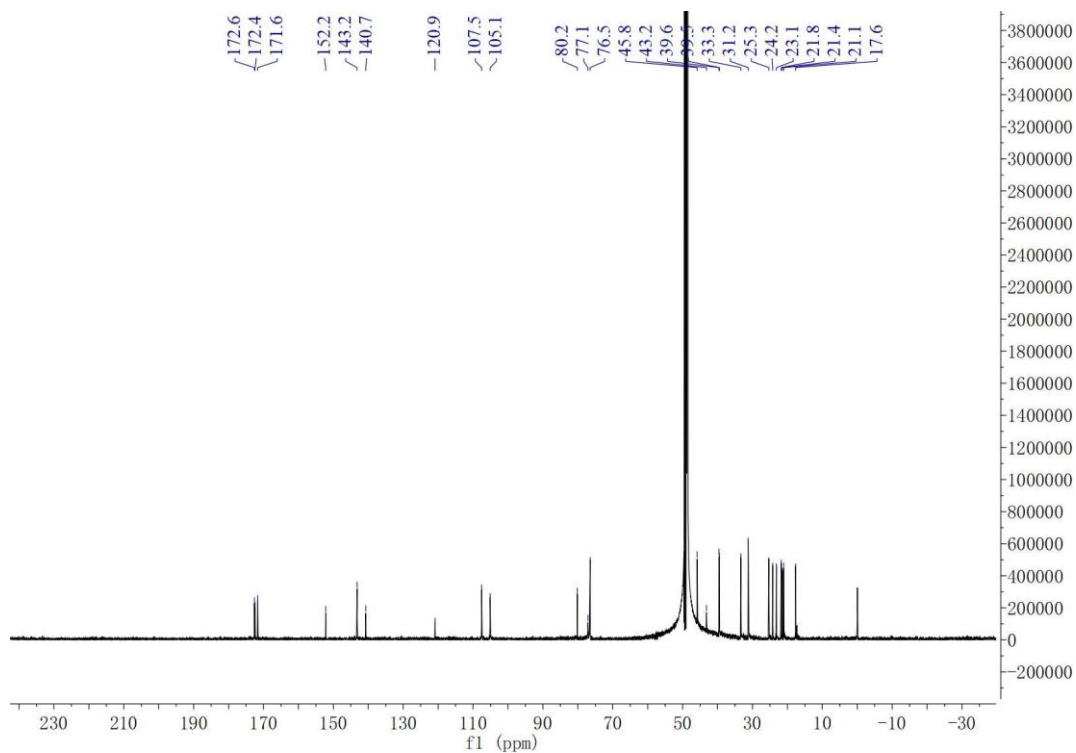


Figure S12. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **2**

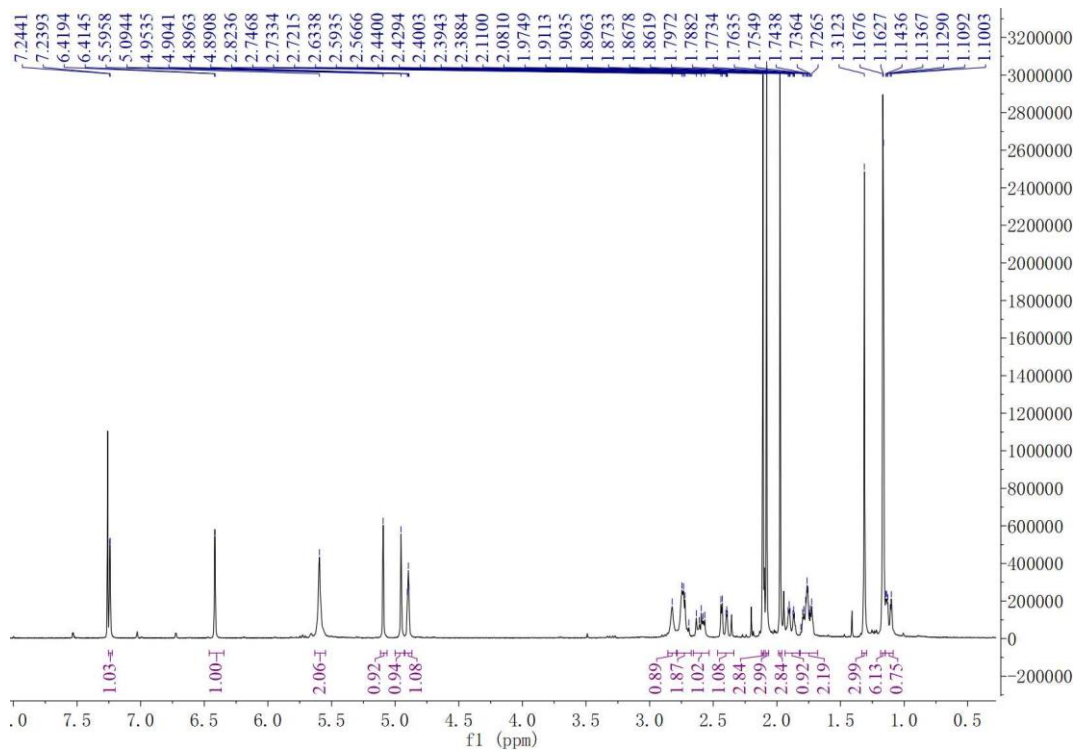


Figure S13. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2**

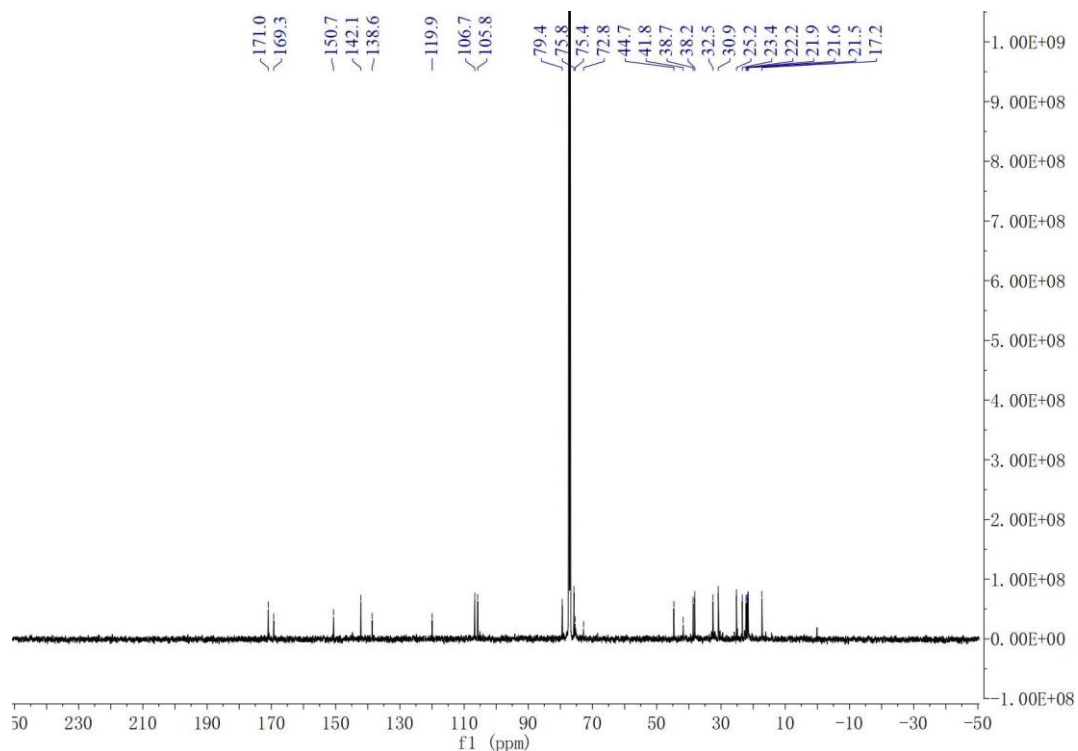


Figure S14. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **2**

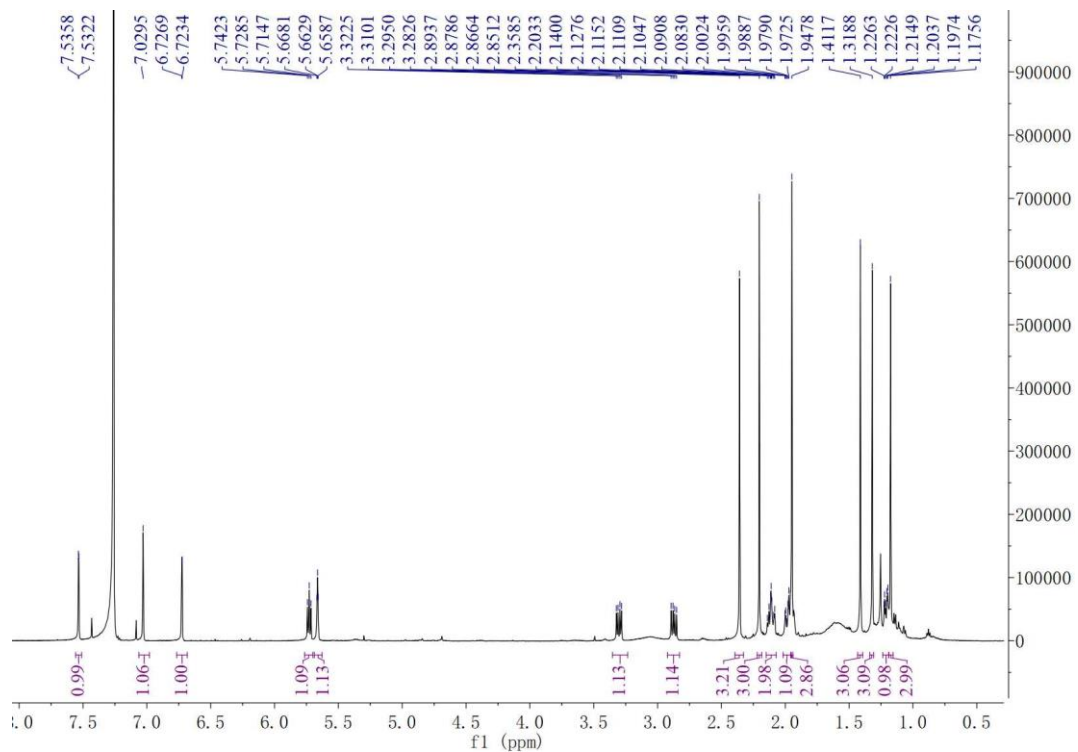


Figure S15. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **2a**

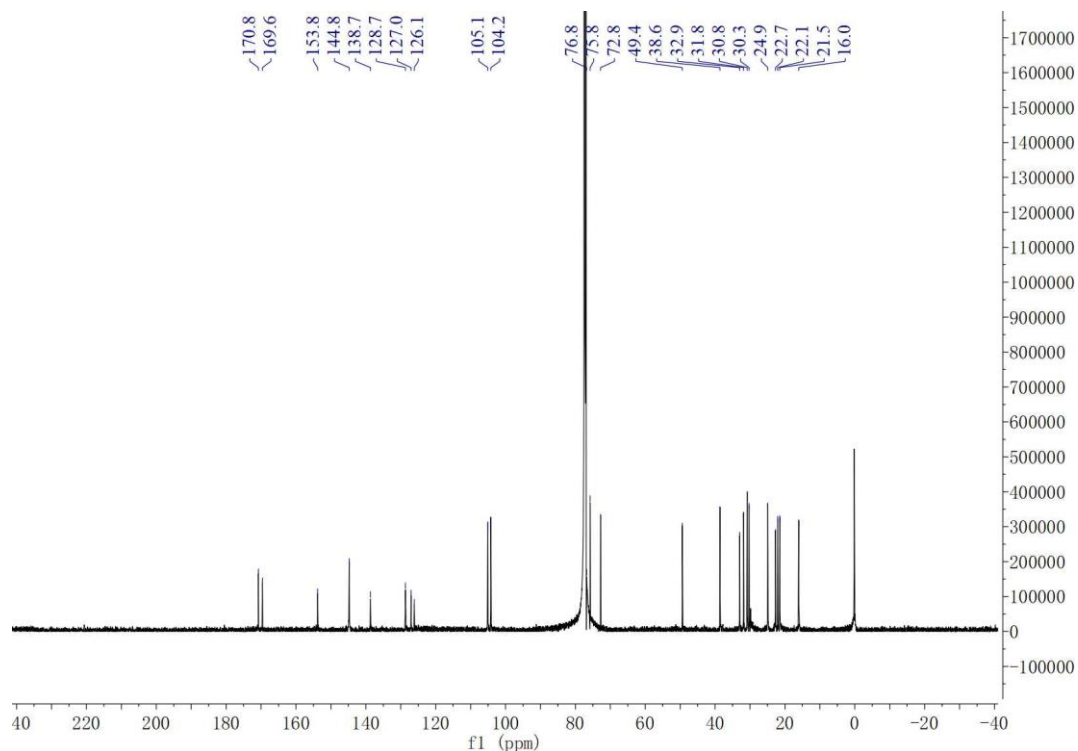


Figure S16. ^{13}C NMR (150 MHz, CDCl_3) spectrum of compound **2a**

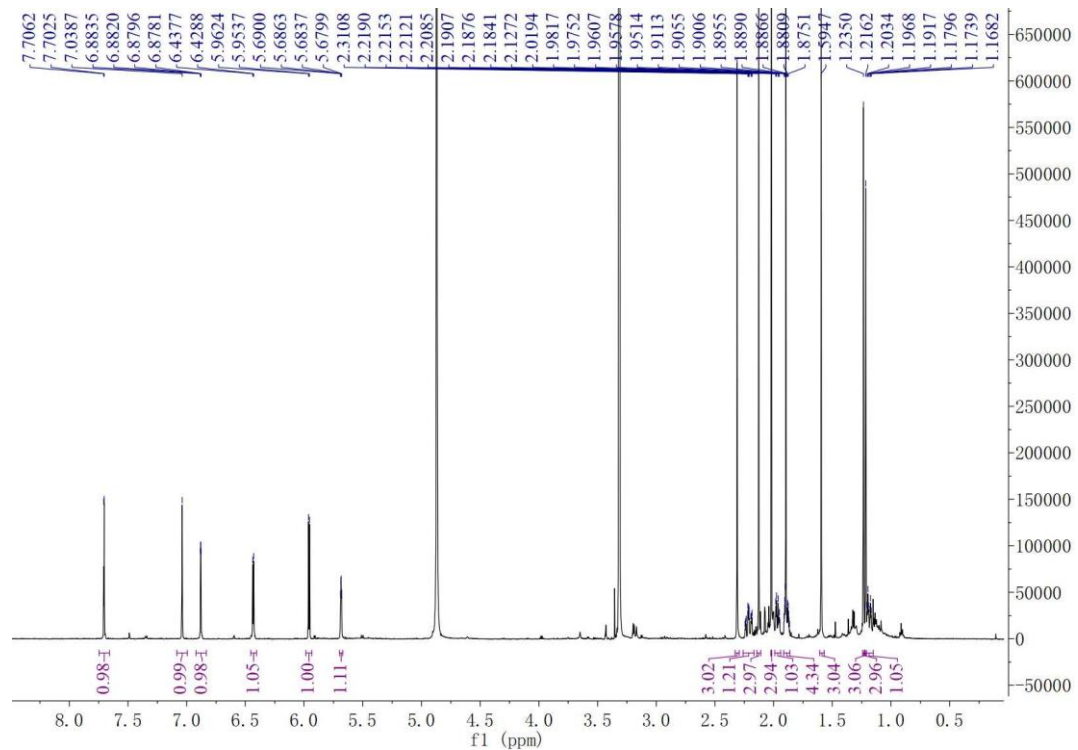


Figure S17. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **2b**

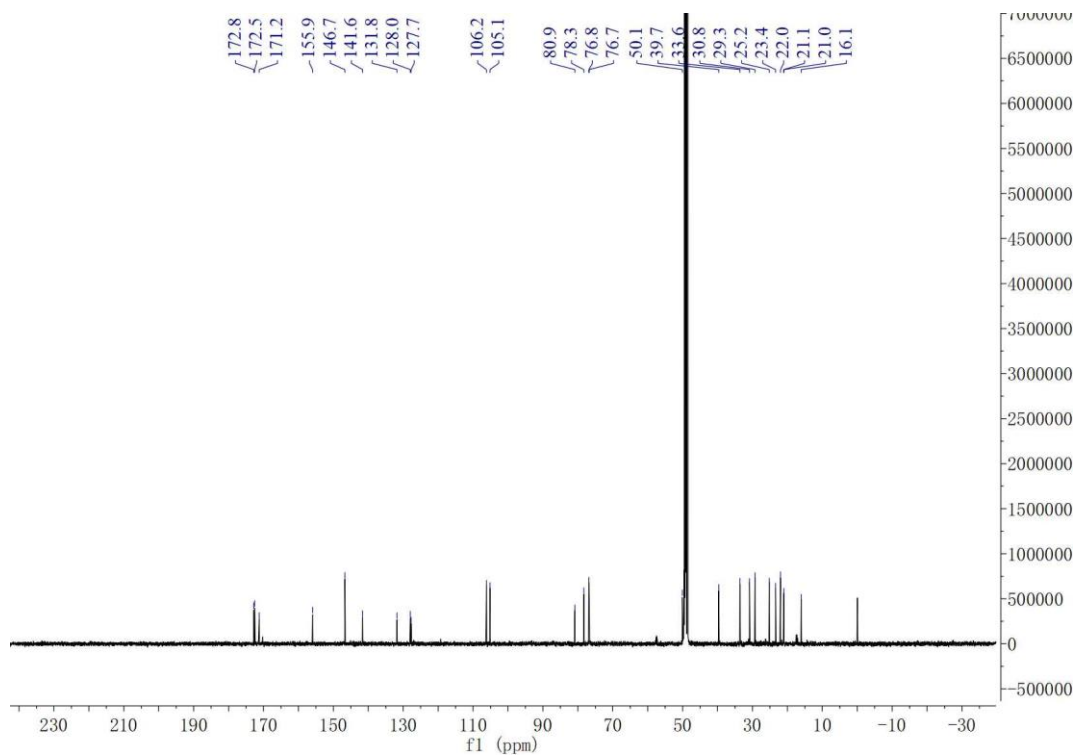


Figure S18. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **2b**

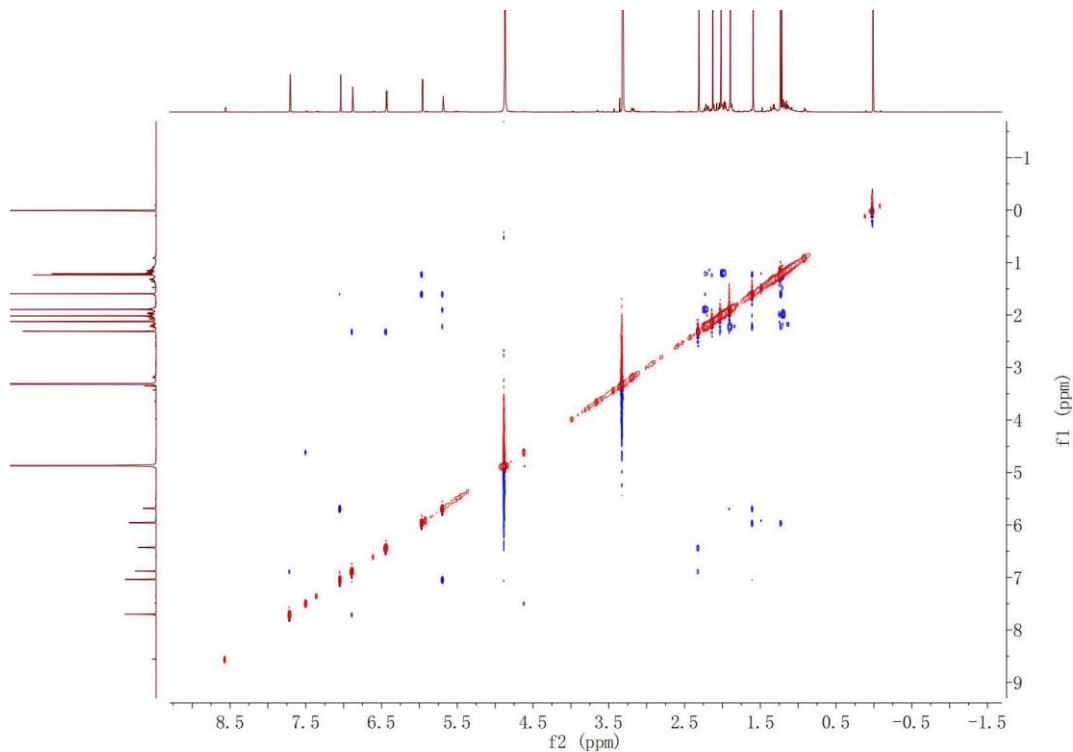
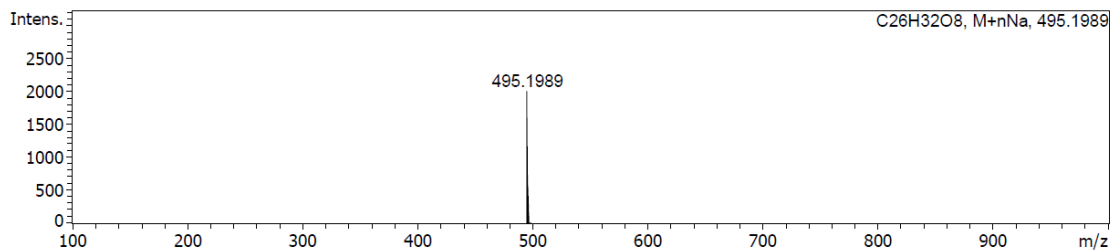
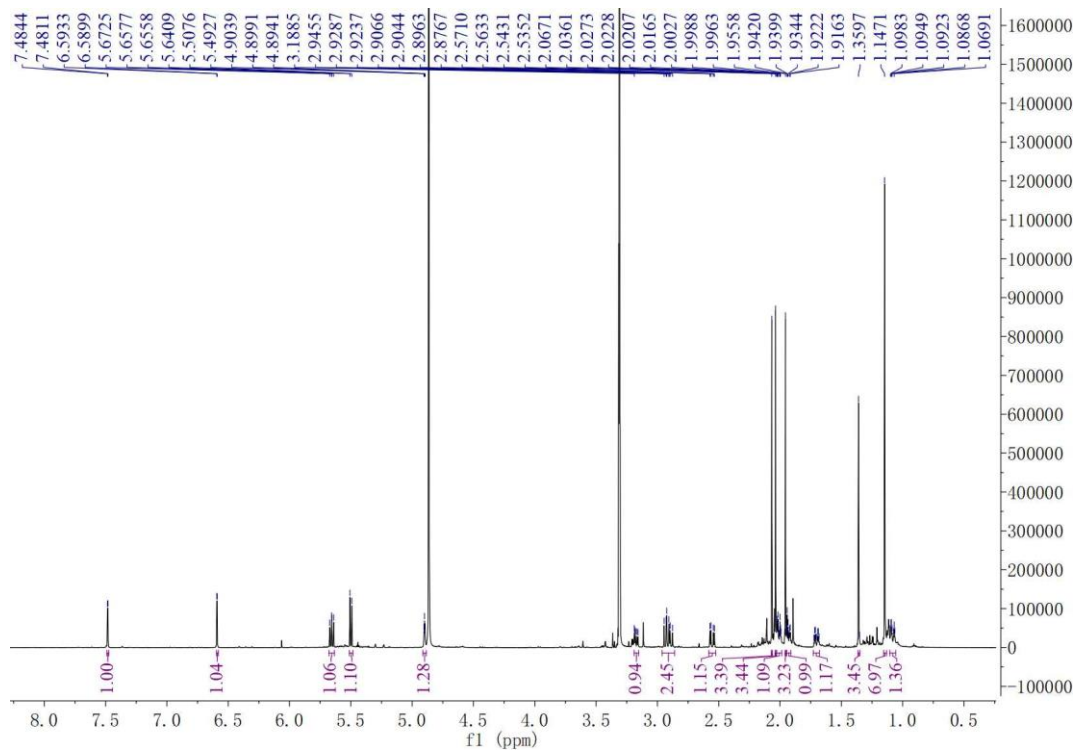


Figure S19. NOESY (600 MHz, CD_3OD) spectrum of compound **2b**

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	220 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

C26H32O8, M+nNa, 495.1989**Figure S20. HRESIMS spectrum of compound 2b****Figure S21. ¹H NMR (600 MHz, CD₃OD) spectrum of compound 2c**

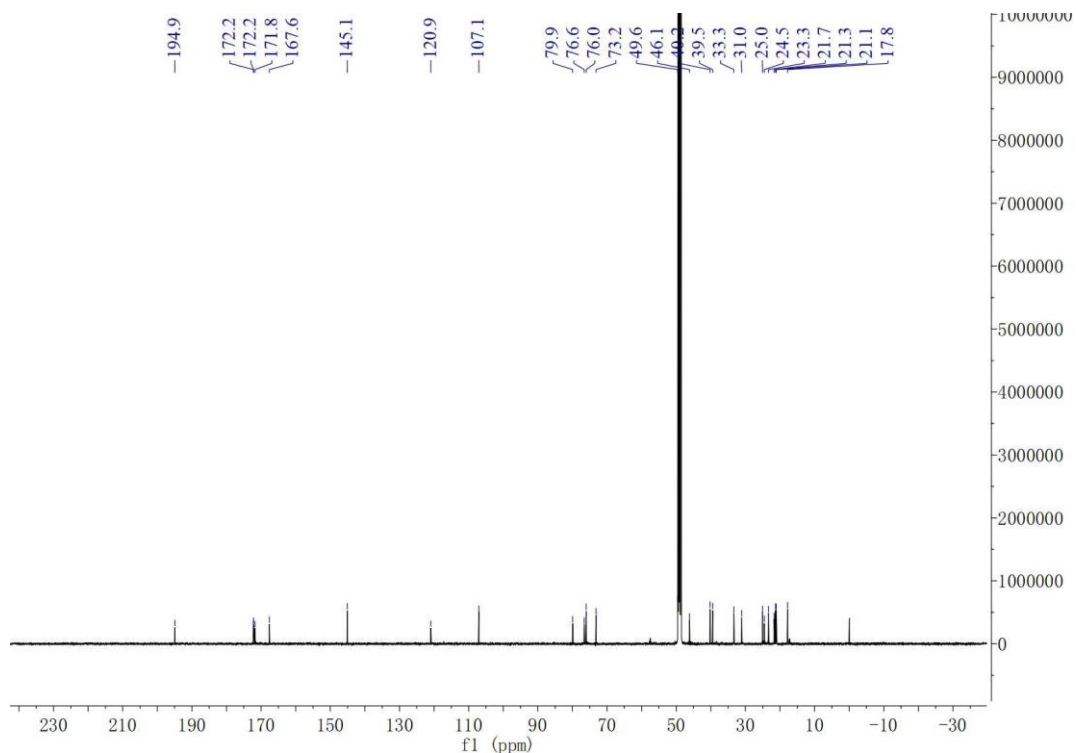


Figure S22. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **2c**

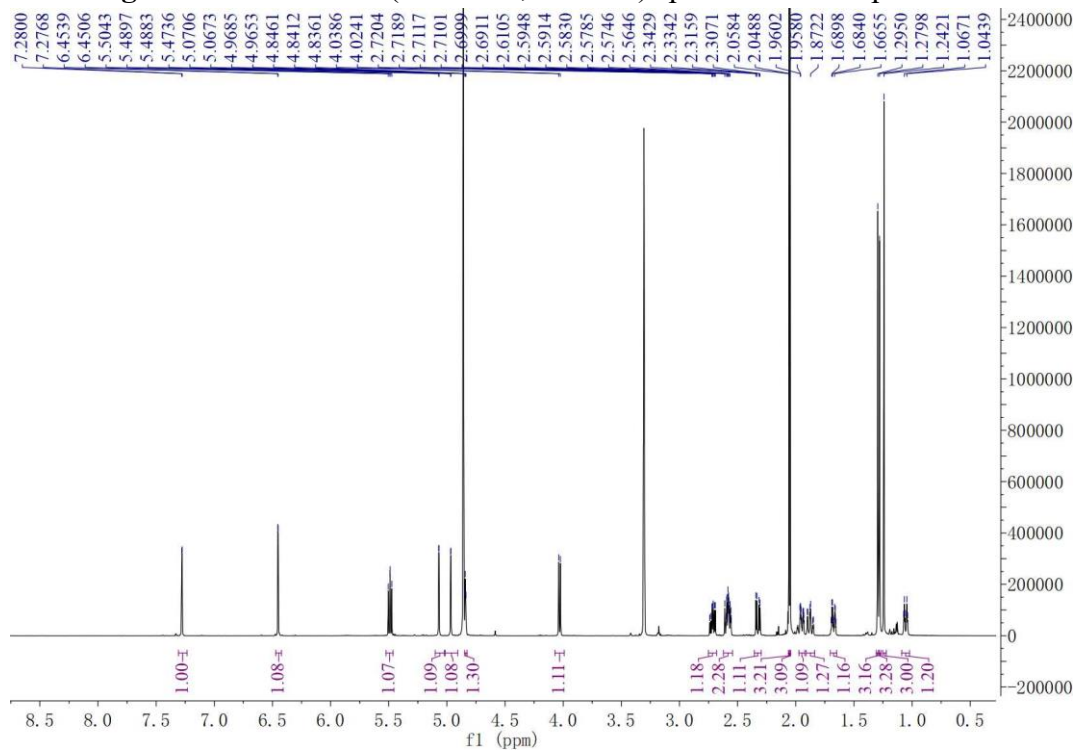


Figure S23. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **3**

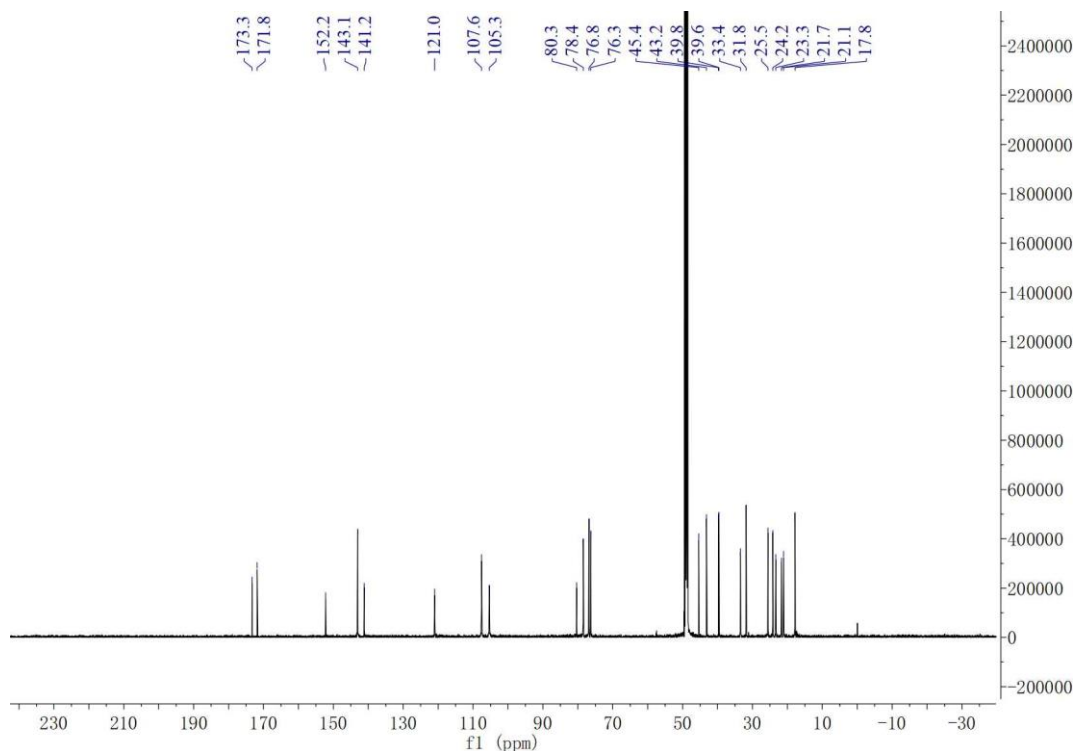


Figure S24. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **3**

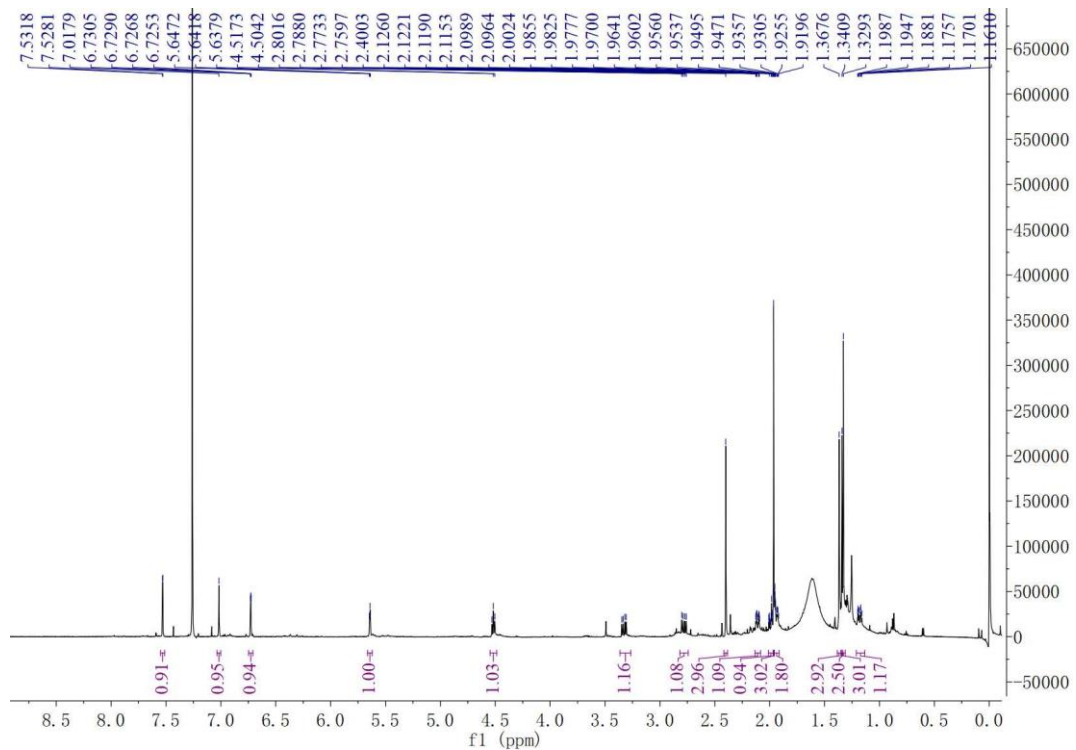


Figure S25. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **3a**

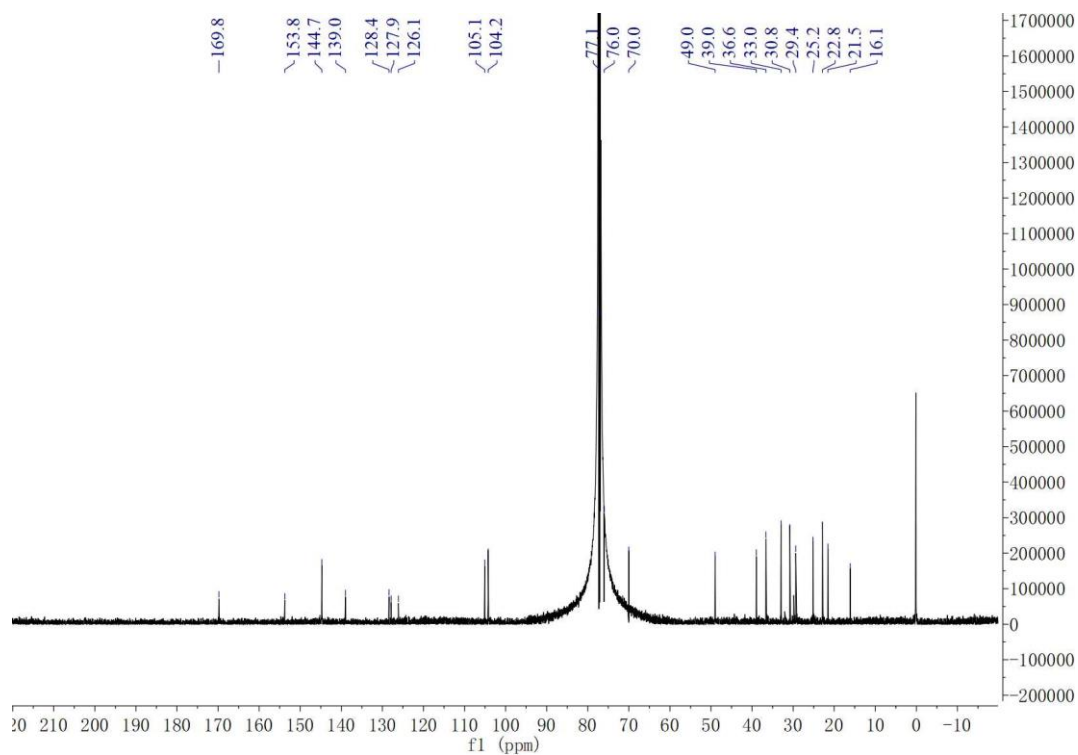


Figure S26. ^{13}C NMR (150 MHz, CDCl_3) spectrum of compound **3a**

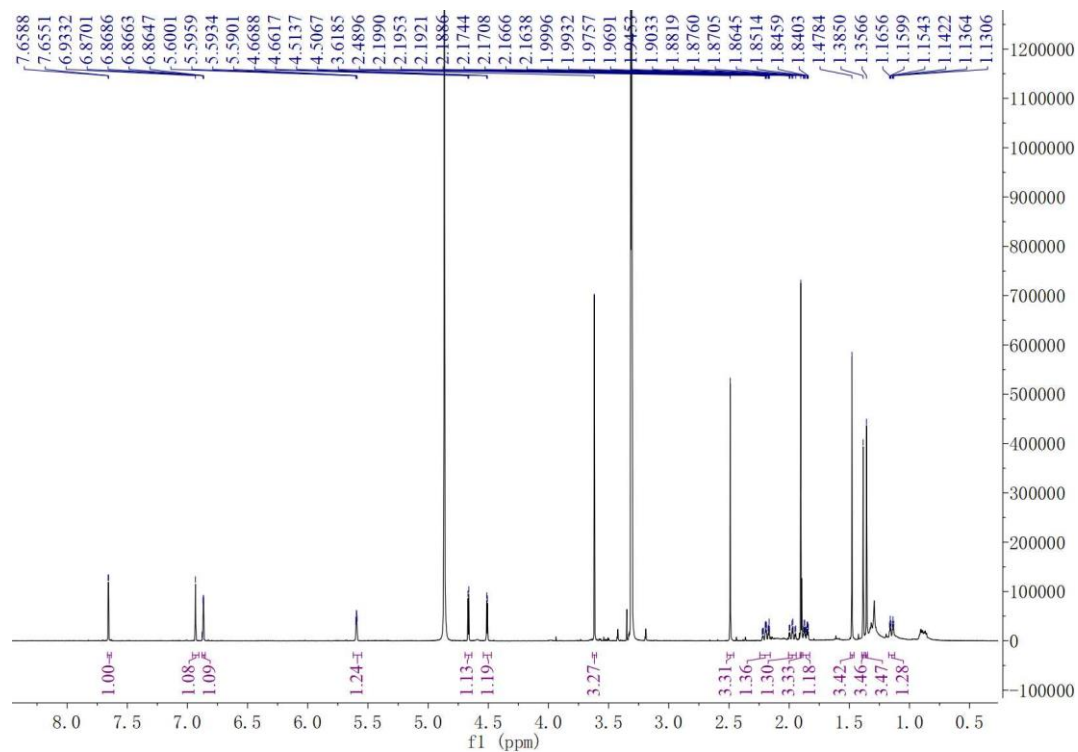


Figure S27. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **3b**

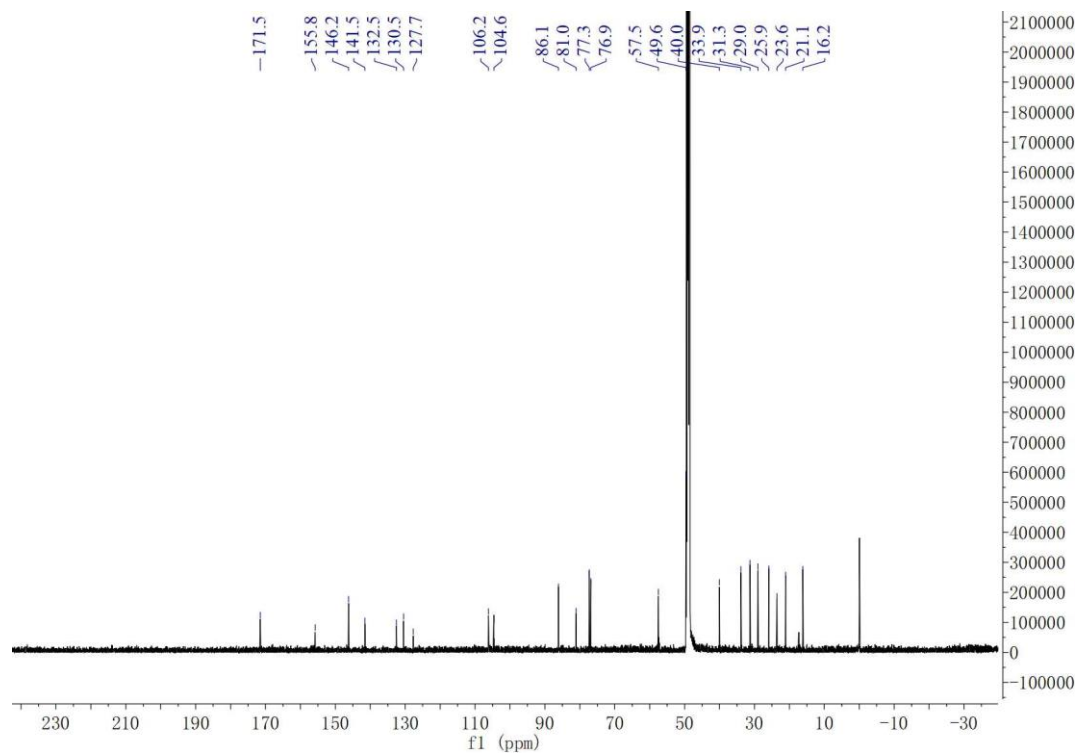


Figure S28. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **3b**

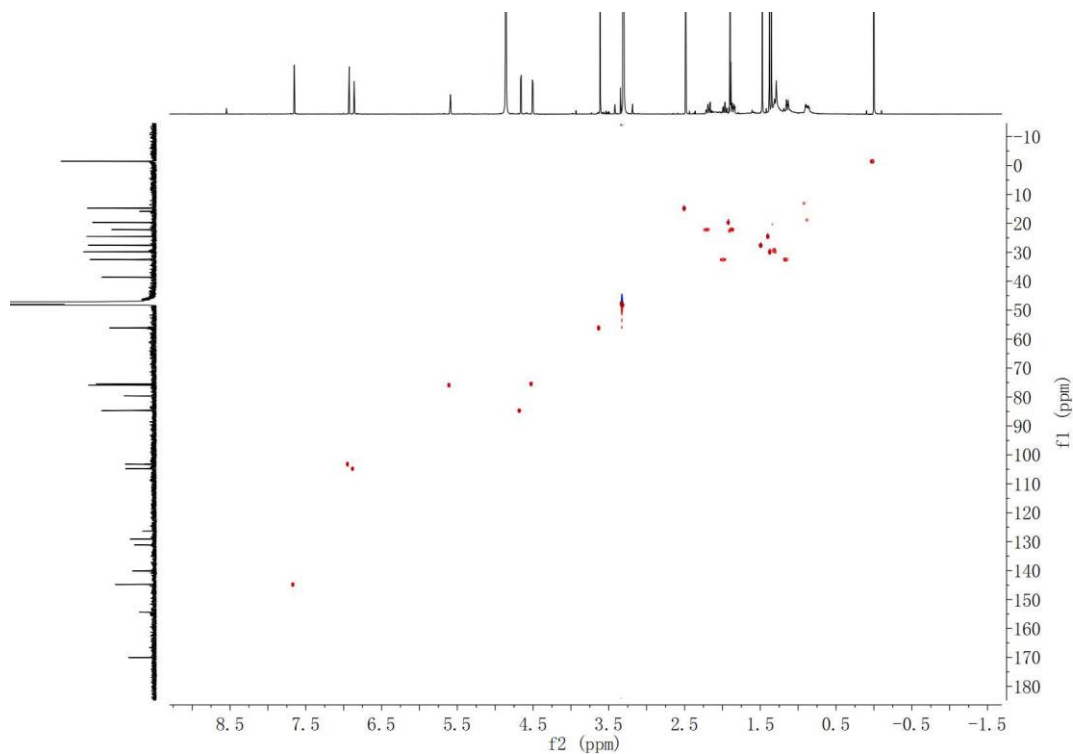


Figure S29. HSQC (600 MHz, CD_3OD) spectrum of compound **3b**

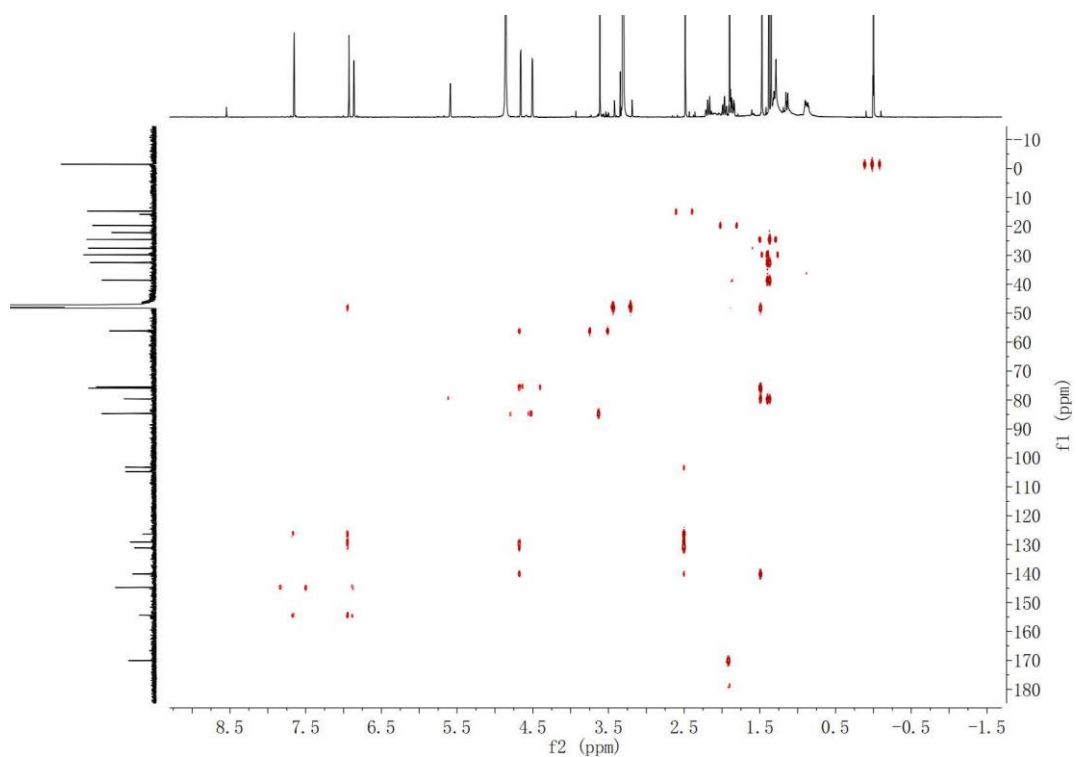


Figure S30. HMBC (600 MHz, CD₃OD) spectrum of compound **3b**

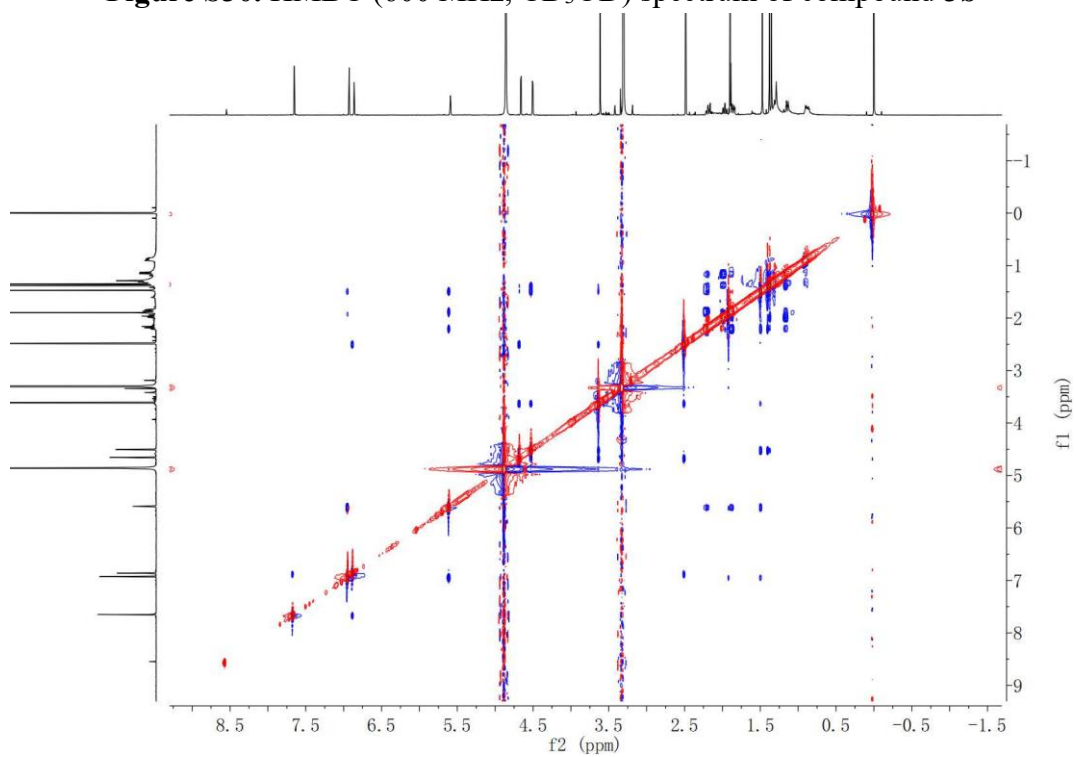
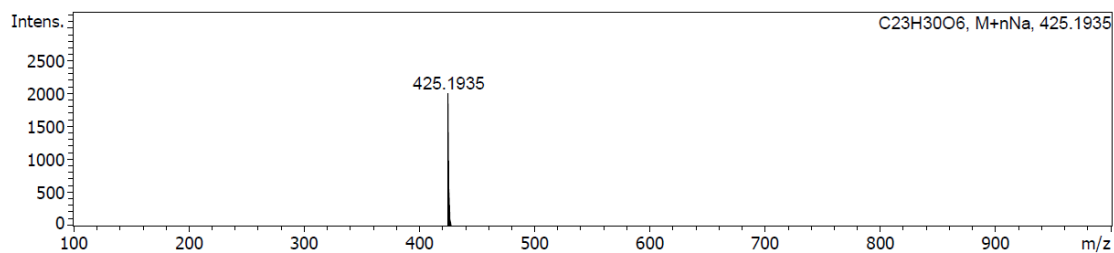
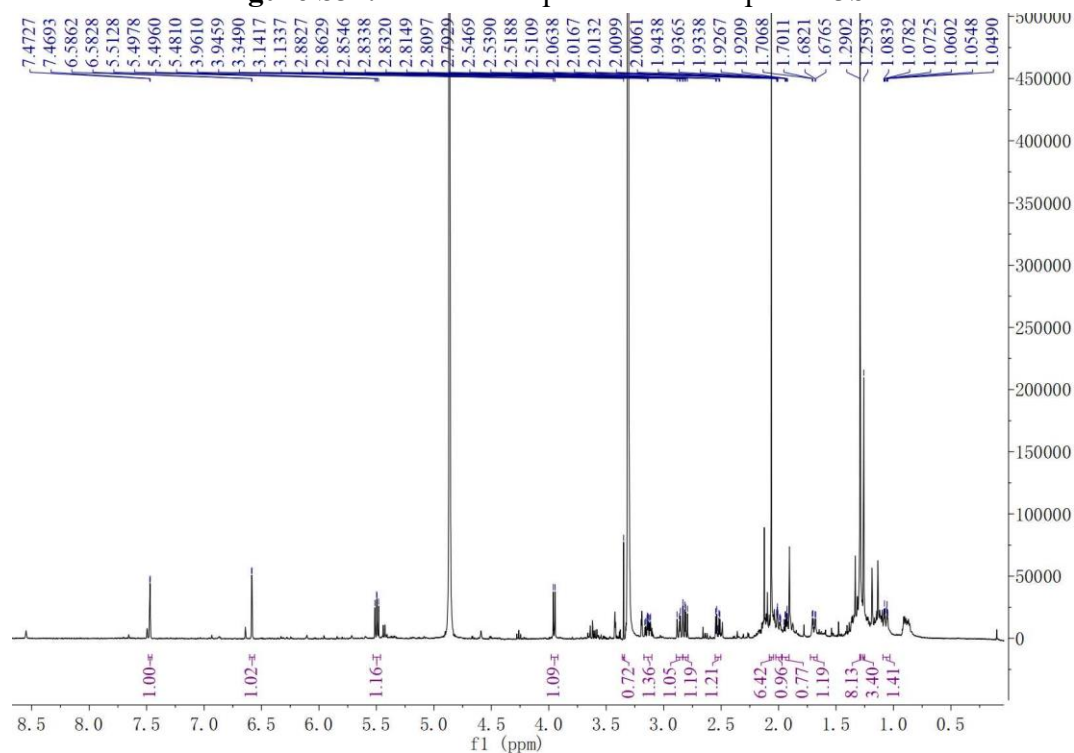


Figure S31. NOESY (600 MHz, CD₃OD) spectrum of compound **3b**

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	220 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

C23H30O6, M+nNa, 425.1935

**Figure S32. HRESIMS spectrum of compound 3b****Figure S33. ¹H NMR (600 MHz, CD₃OD) spectrum of compound 3c**

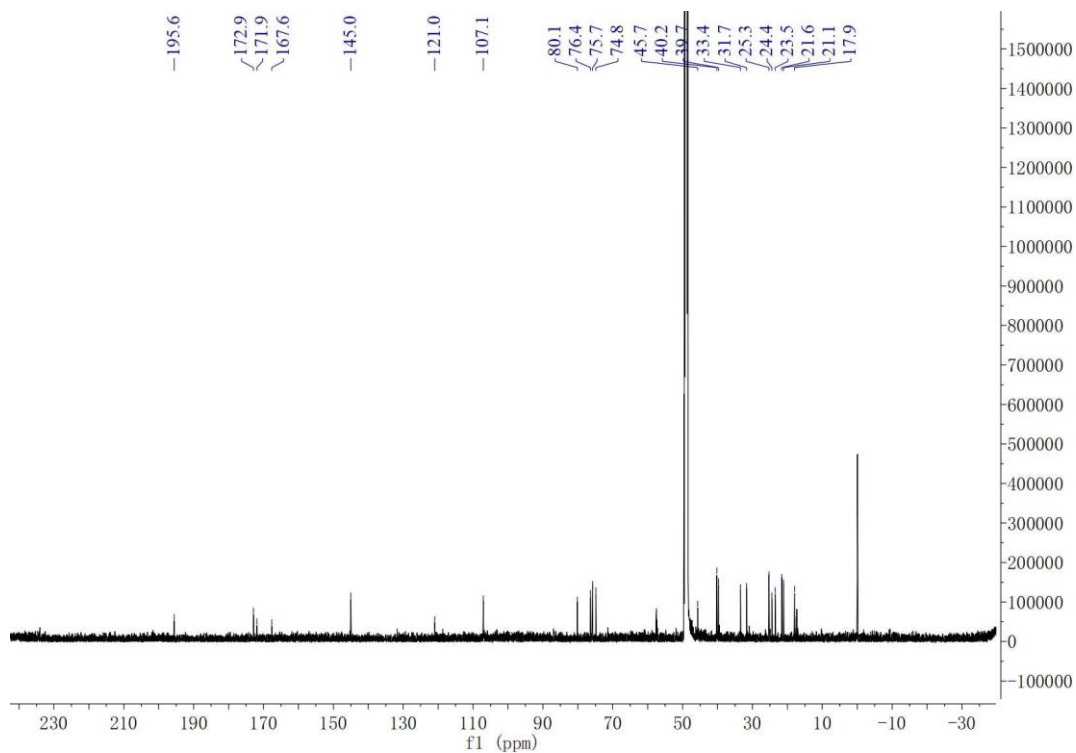


Figure S34. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **3c**

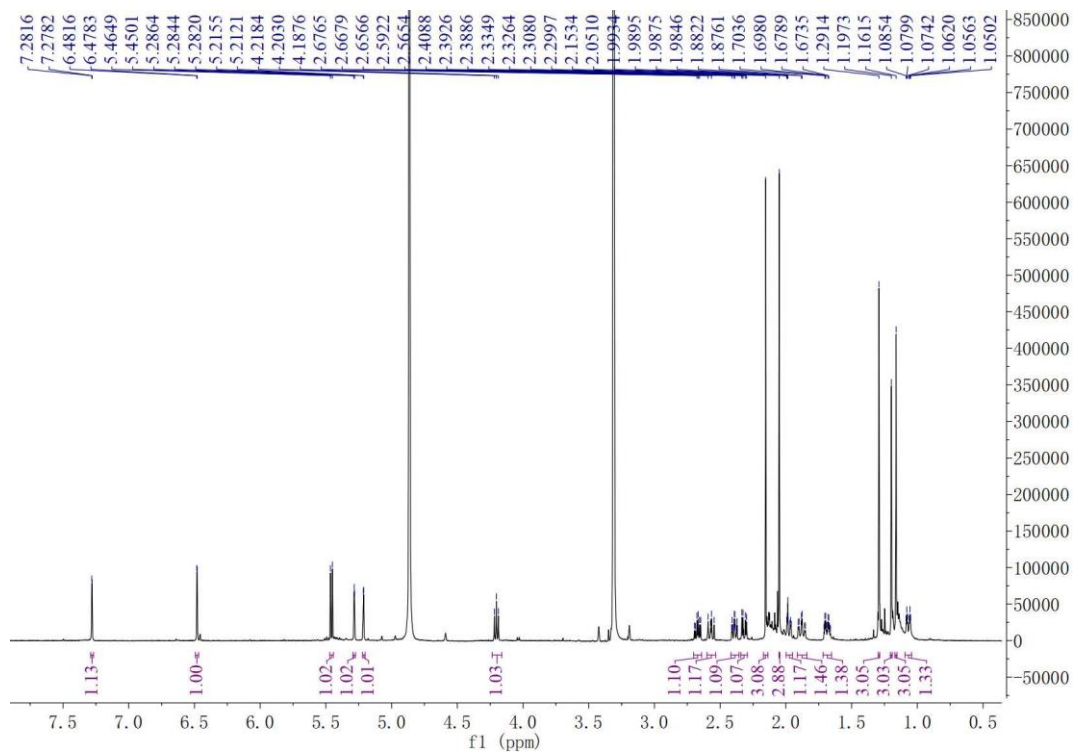


Figure S35. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **4**

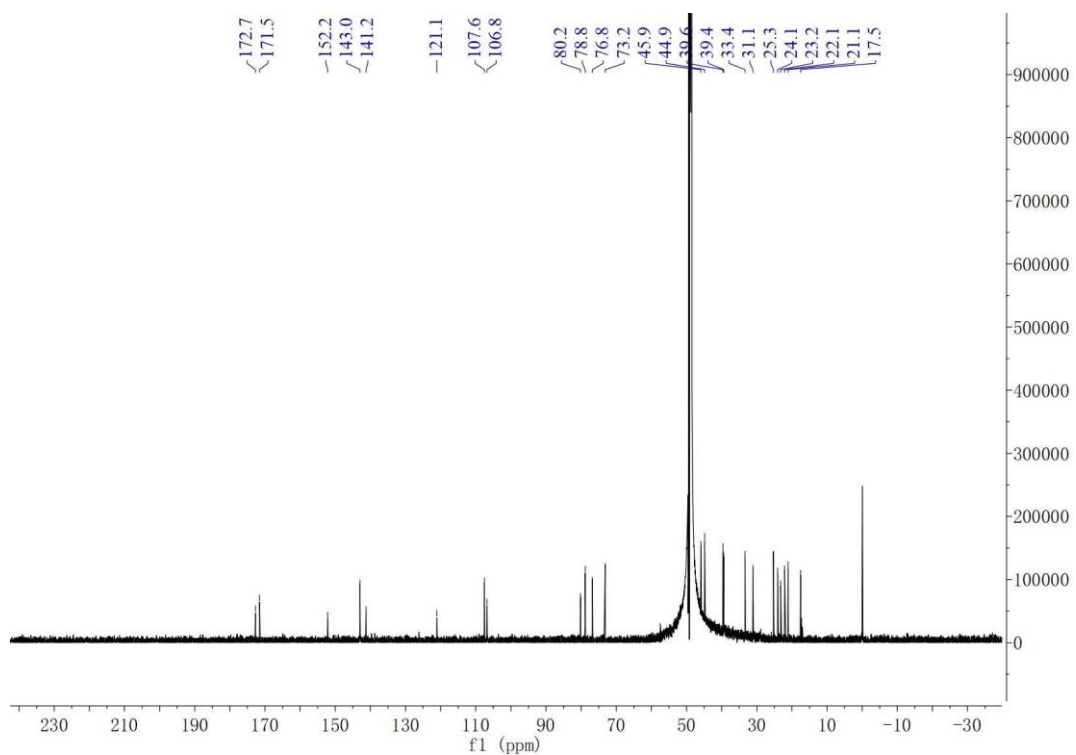


Figure S36. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 4

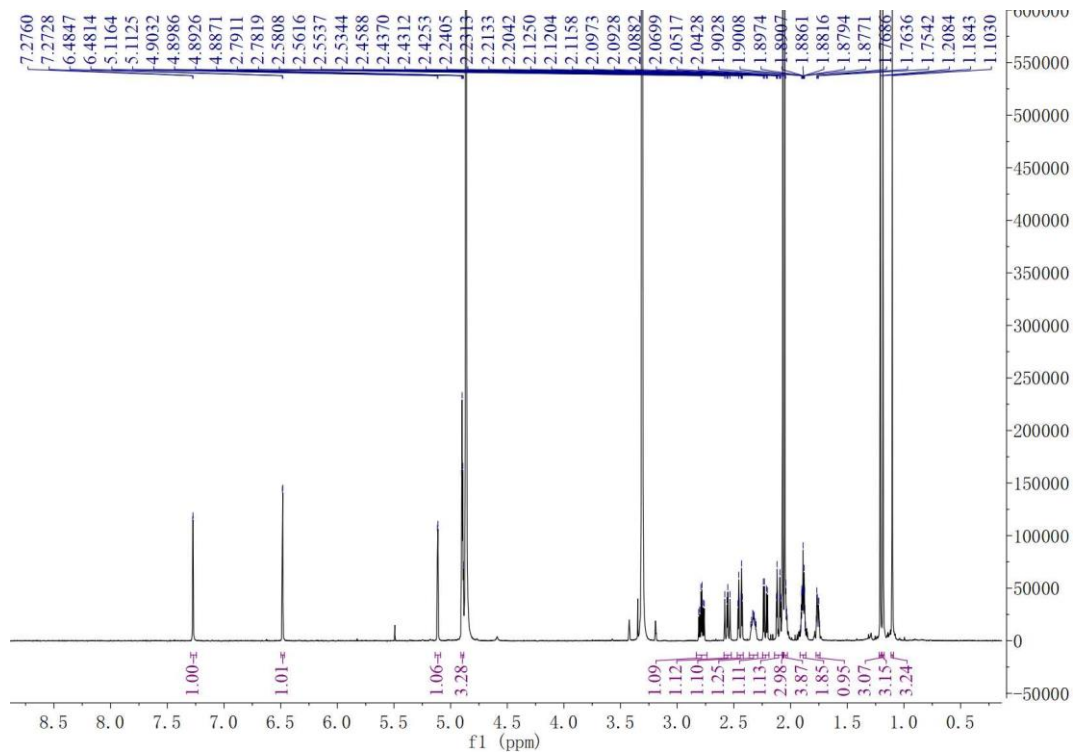


Figure S37. ^1H NMR (600 MHz, CD_3OD) spectrum of compound 5

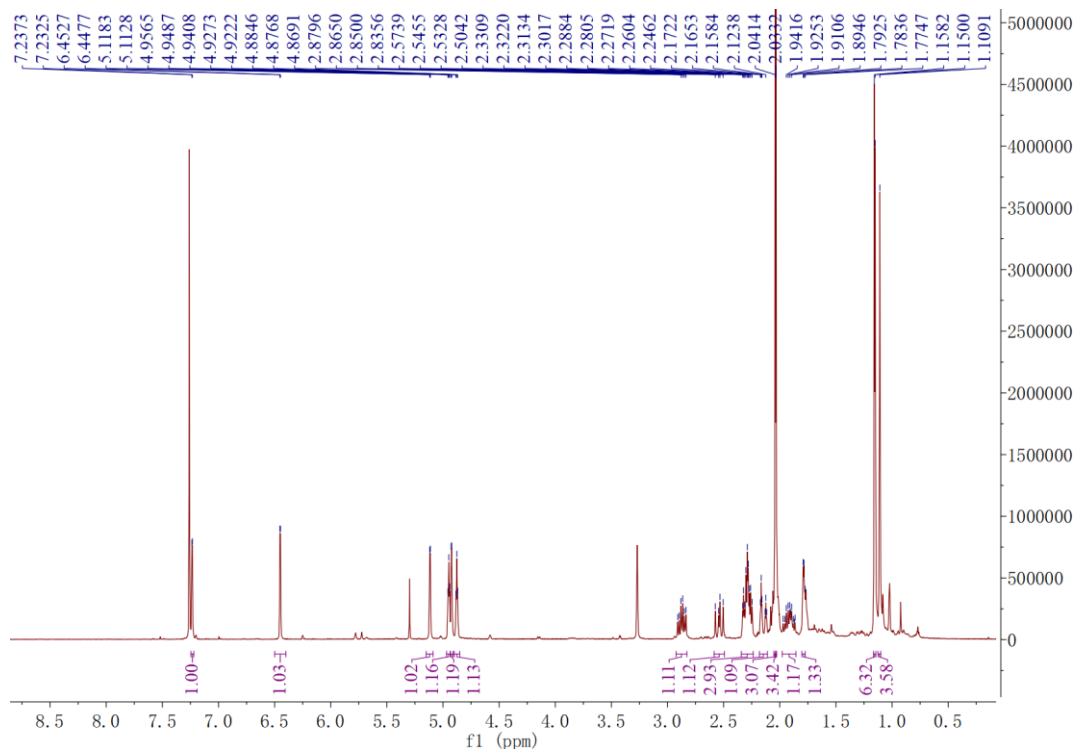


Figure S38. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **5**

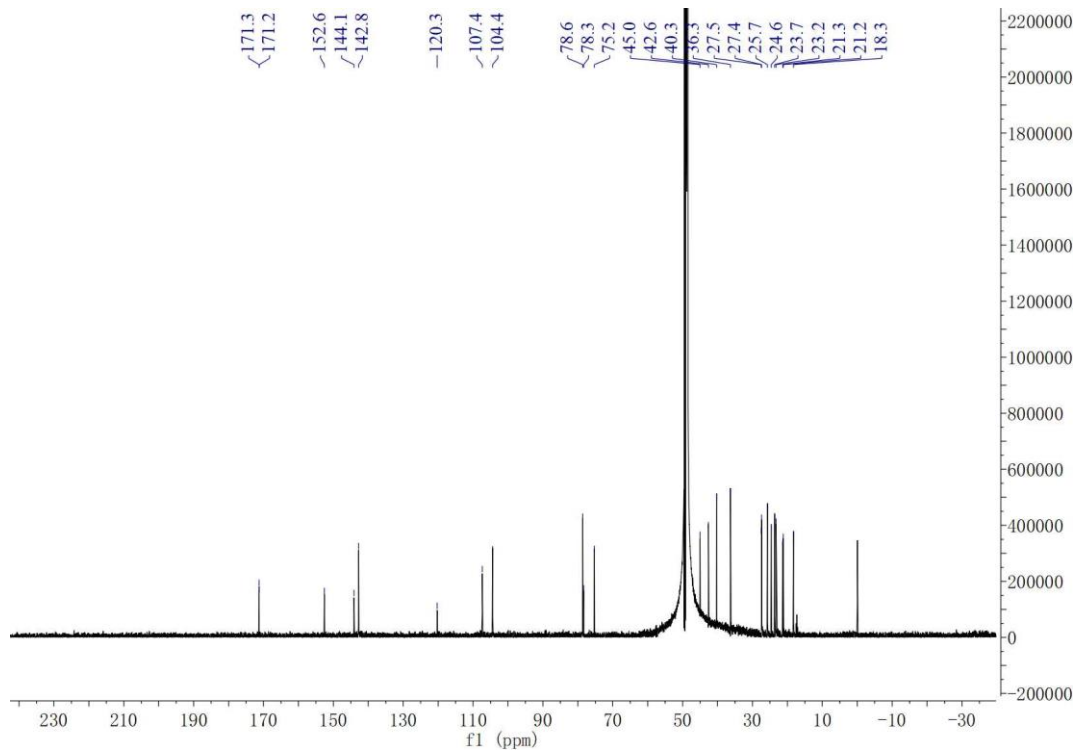


Figure S39. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **5**

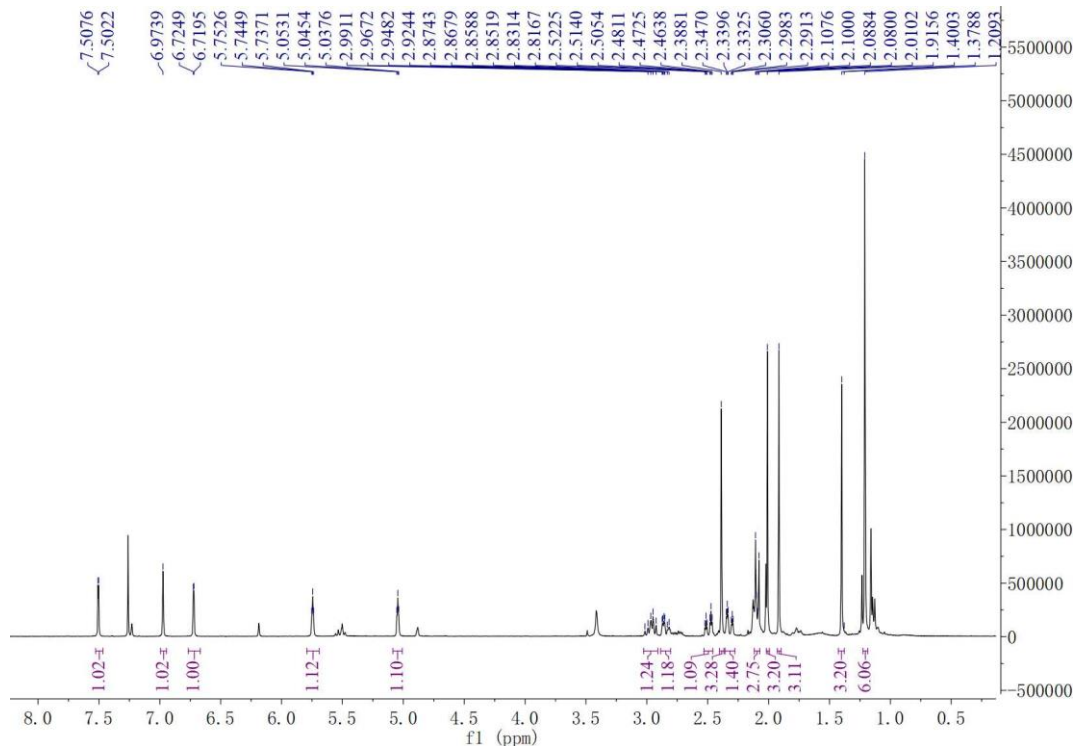


Figure S40. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **5a**

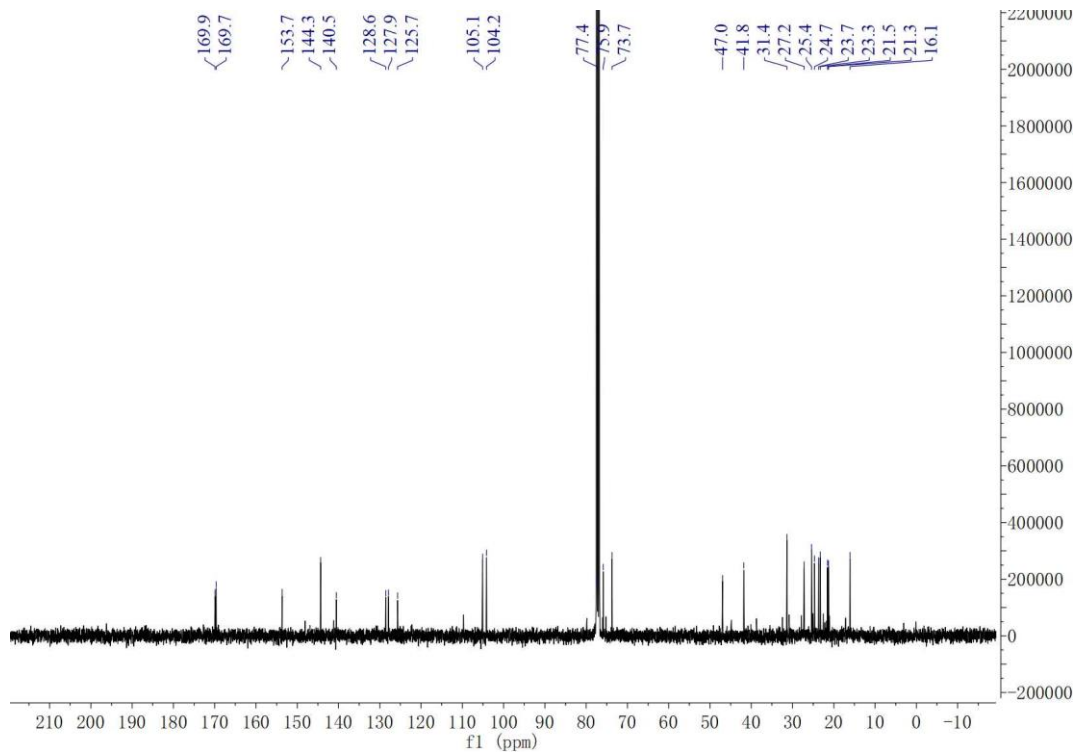


Figure S41. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **5a**

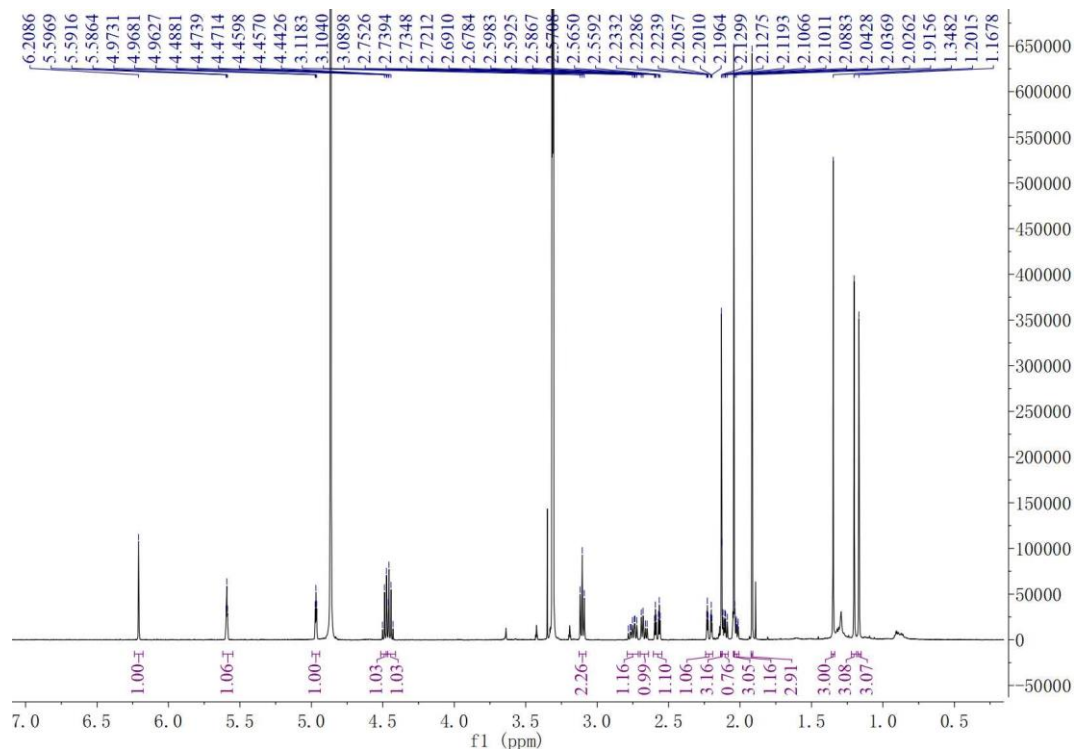


Figure S42. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **5b**

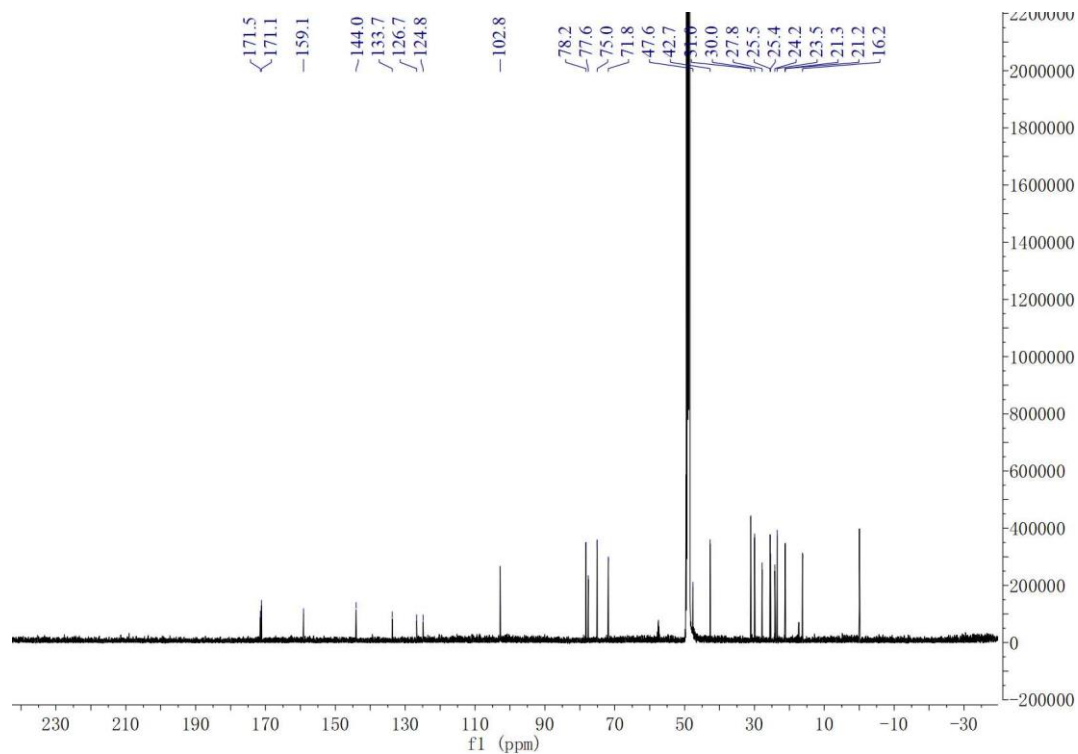


Figure S43. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **5b**

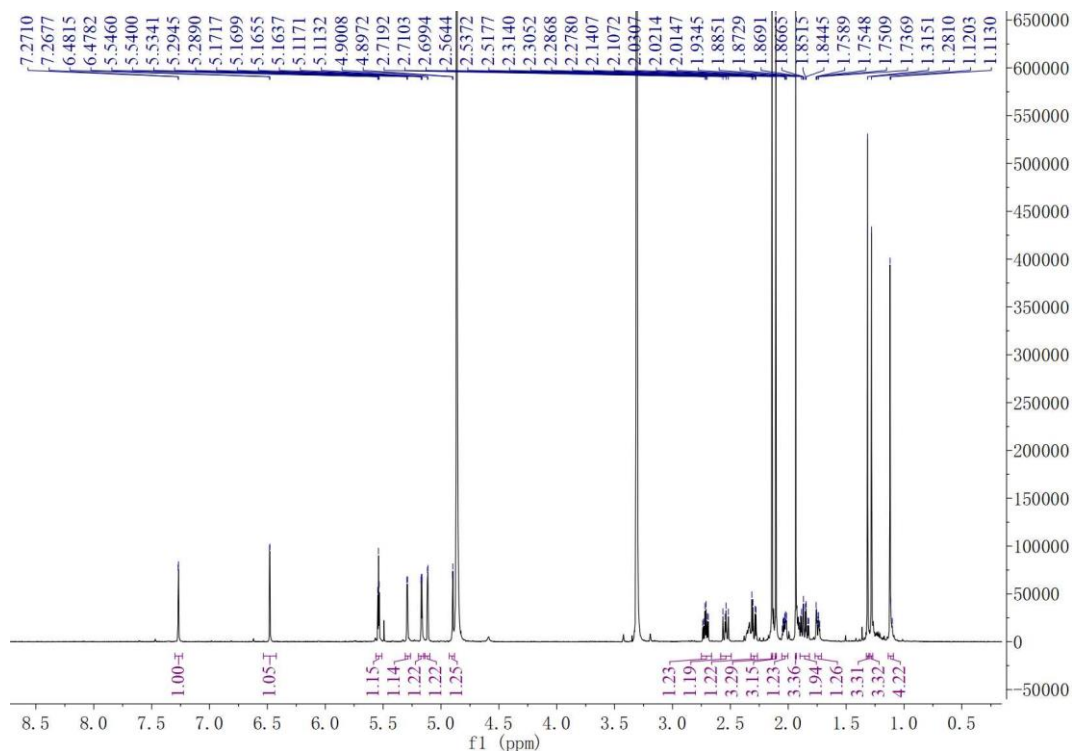


Figure S44. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **6**

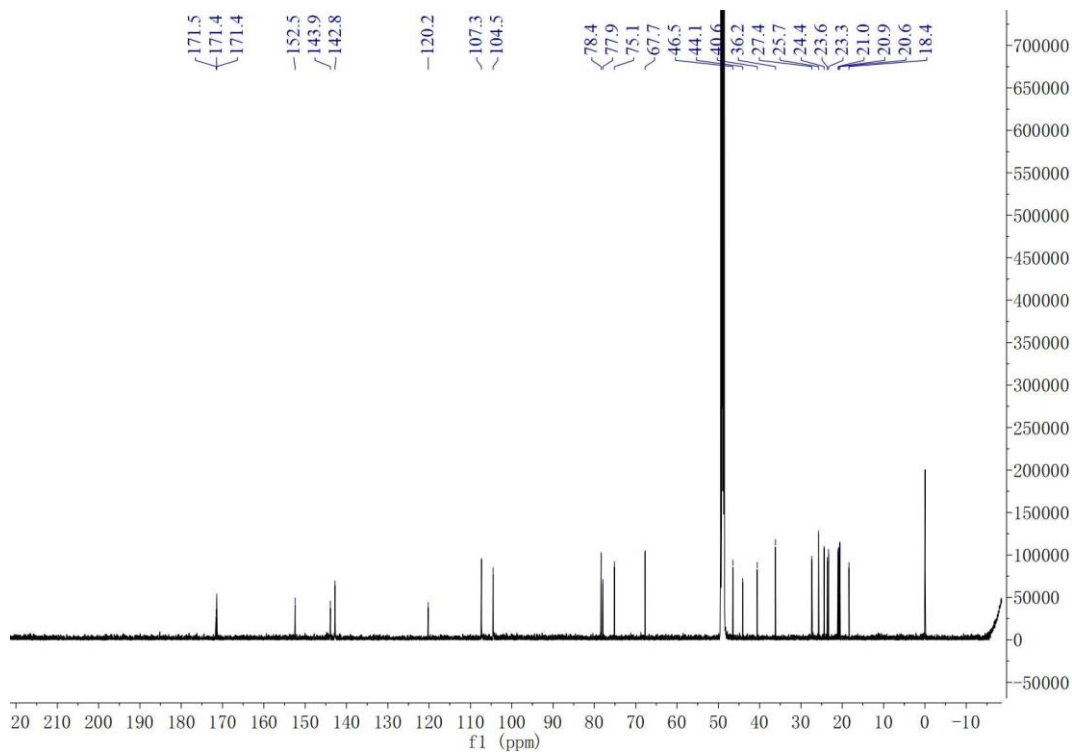


Figure S45. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **6**

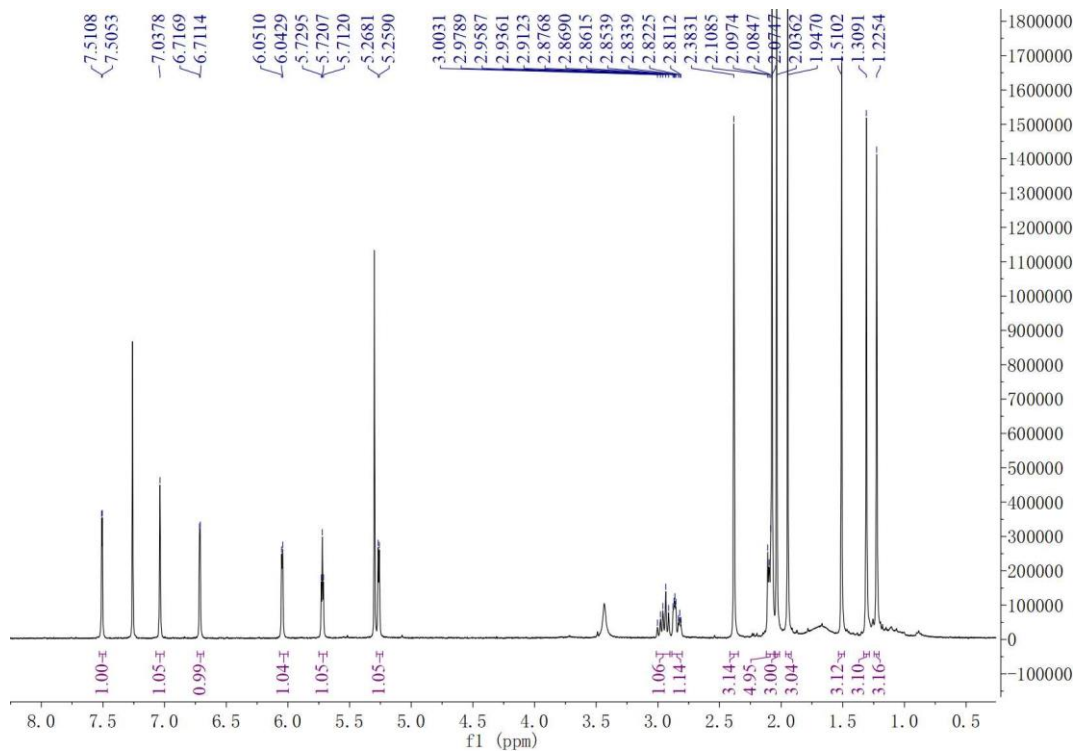


Figure S46. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **6a**

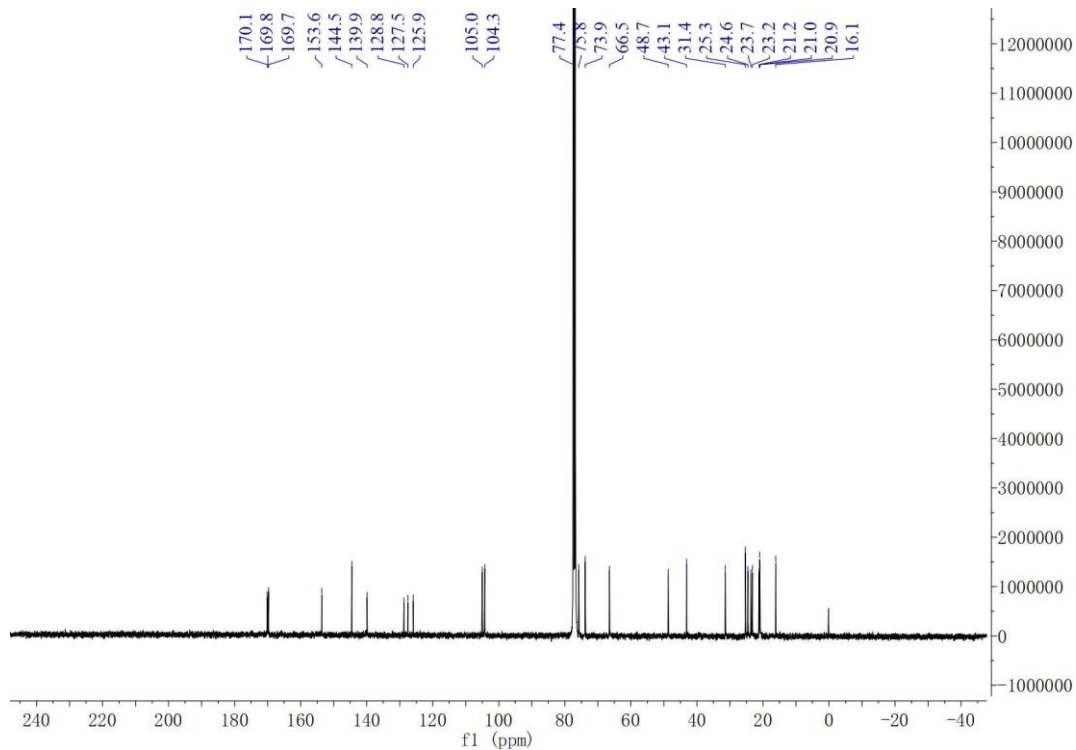


Figure S47. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **6a**

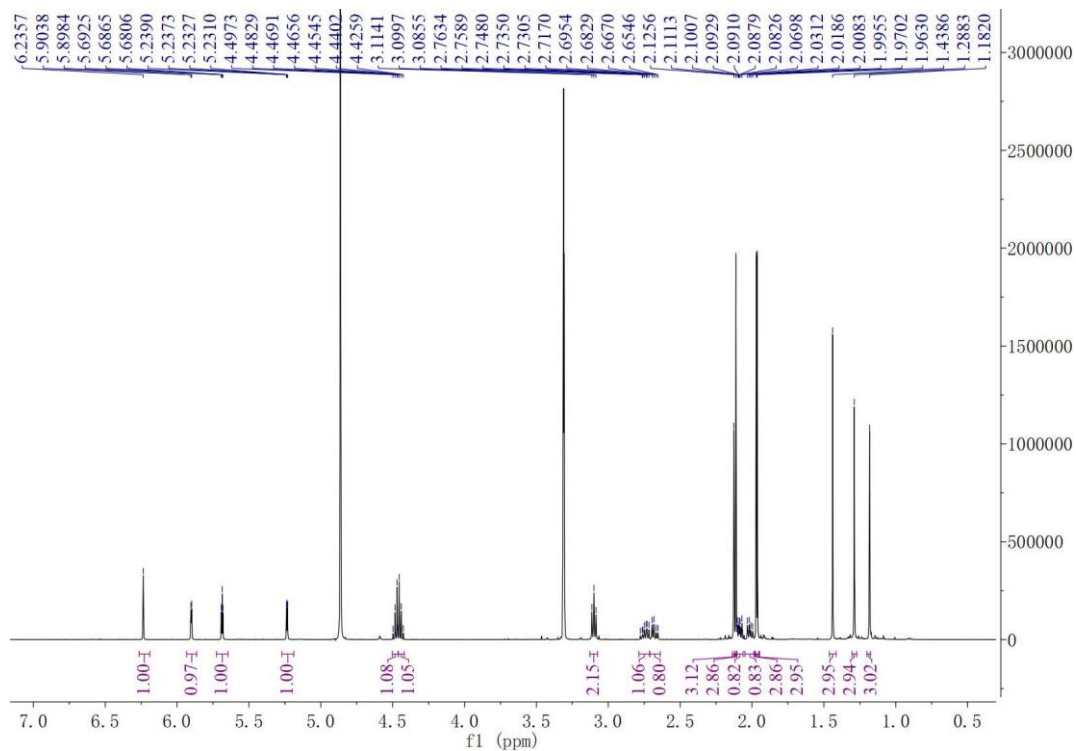


Figure S48. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **6b**

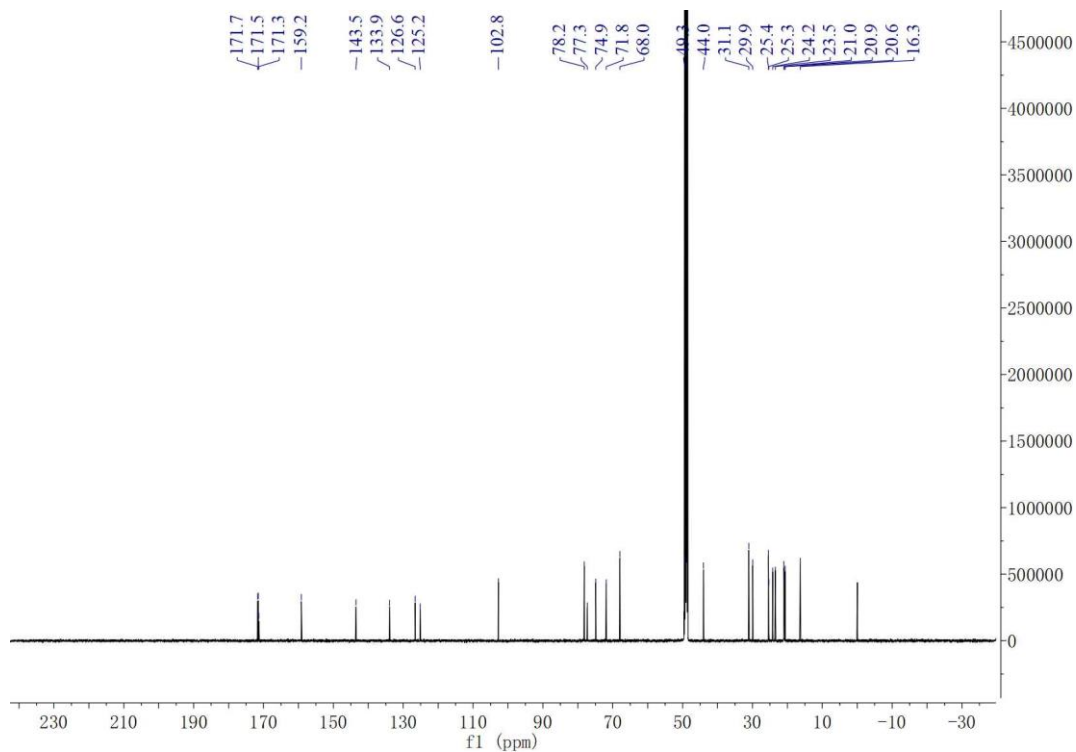


Figure S49. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **6b**

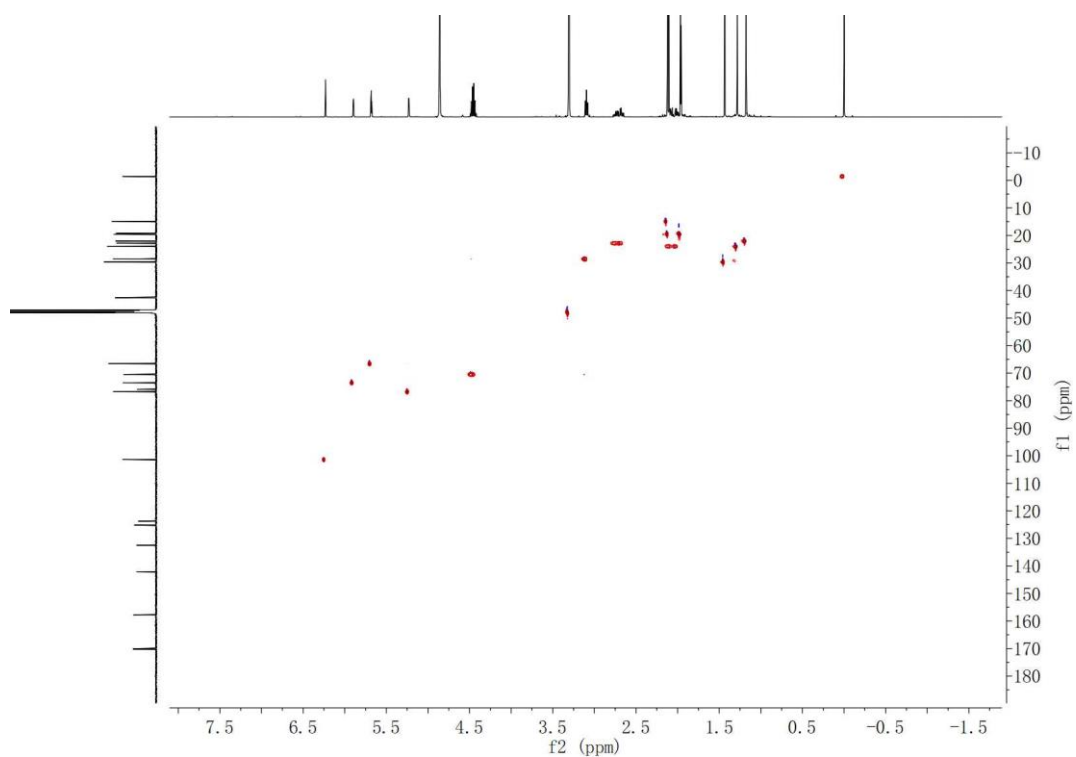


Figure S50. HSQC (600 MHz, CD₃OD) spectrum of compound **6b**

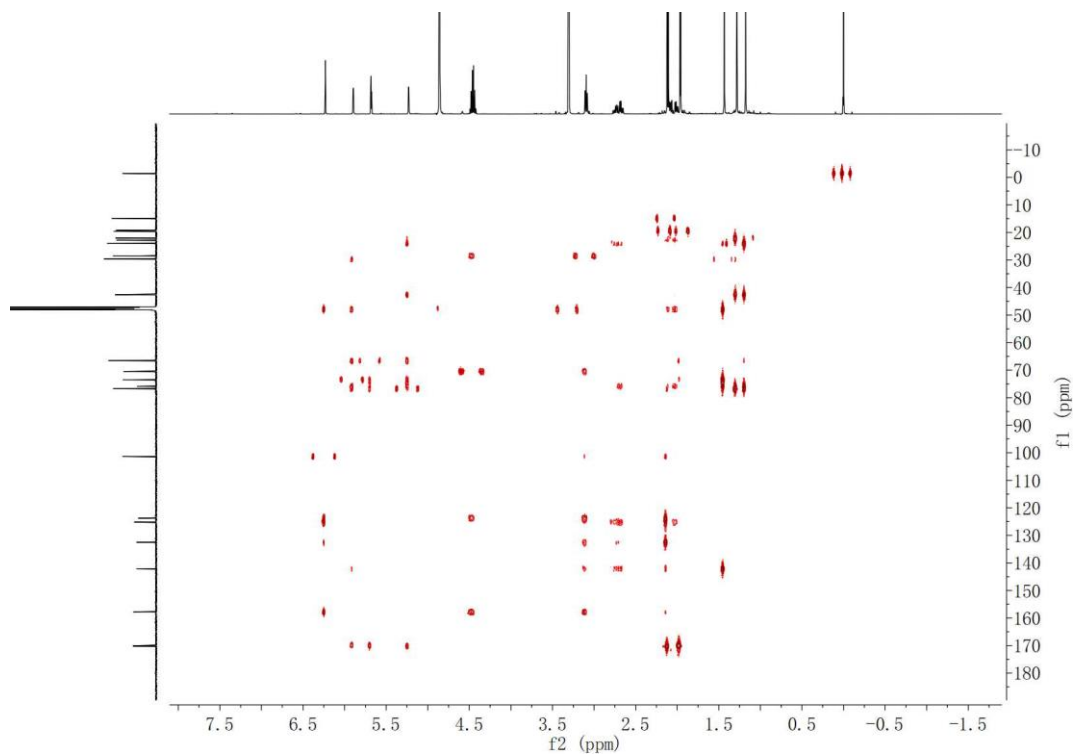


Figure S51. HMBC (600 MHz, CD₃OD) spectrum of compound **6b**

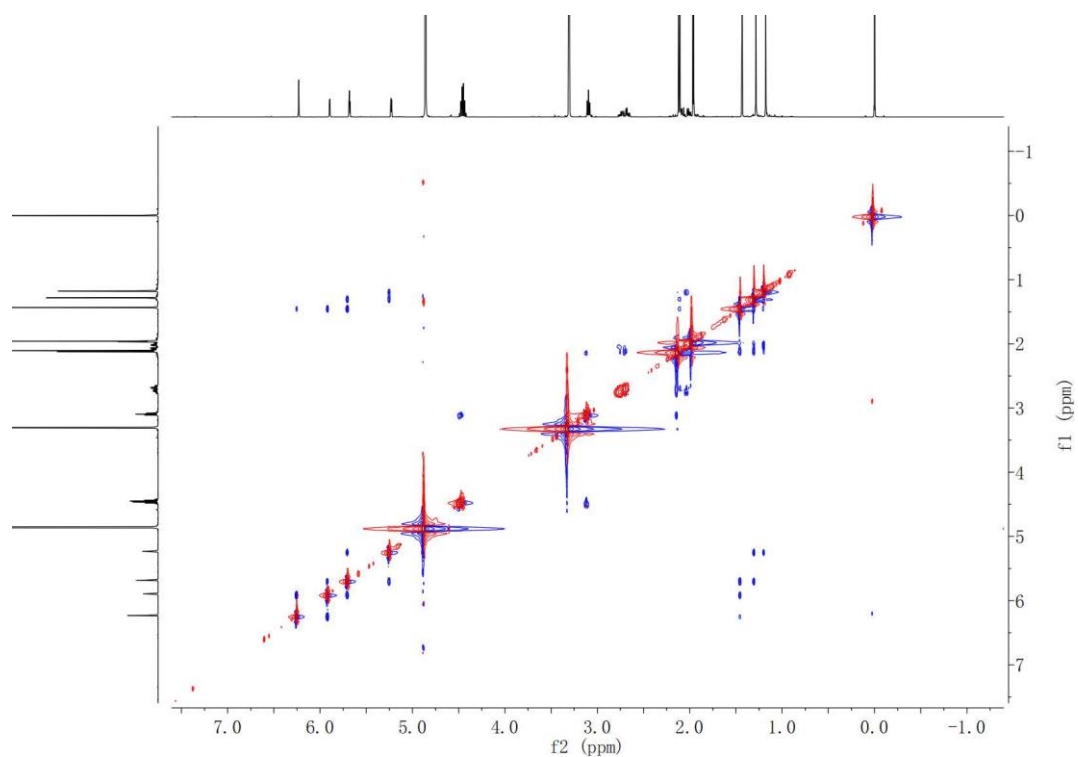


Figure S52. NOESY (600 MHz, CD₃OD) spectrum of compound **6b**

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	220 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

C26H34O8, M+nNa, 497.2146

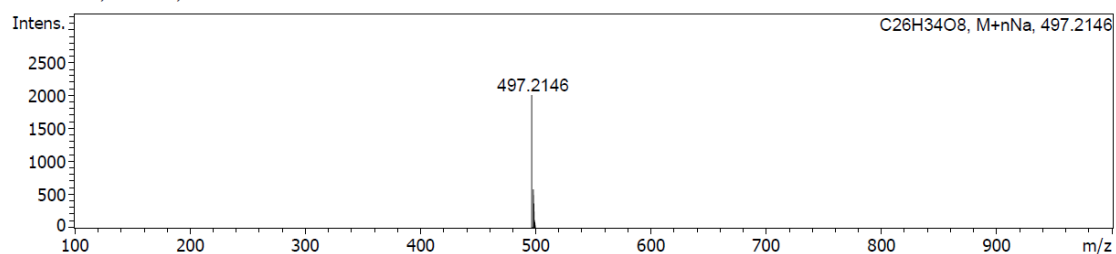


Figure S53. HRESIMS spectrum of compound **6b**

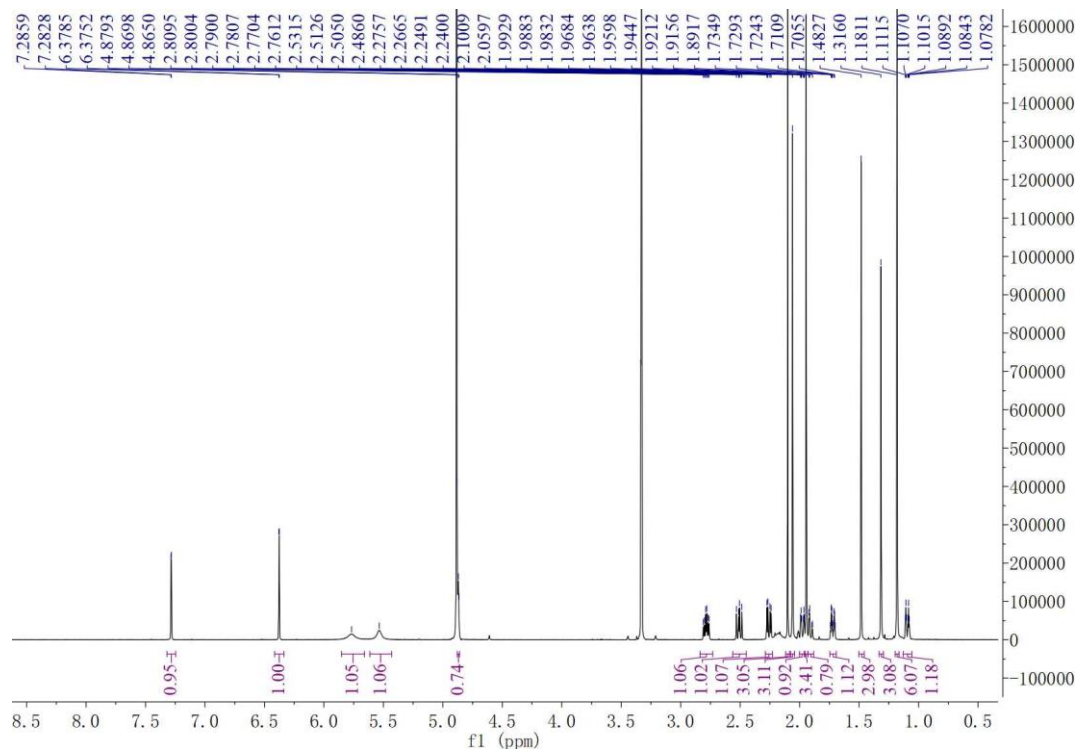


Figure S54. ^1H NMR (600 MHz, CD_3OD) spectrum of compound 7

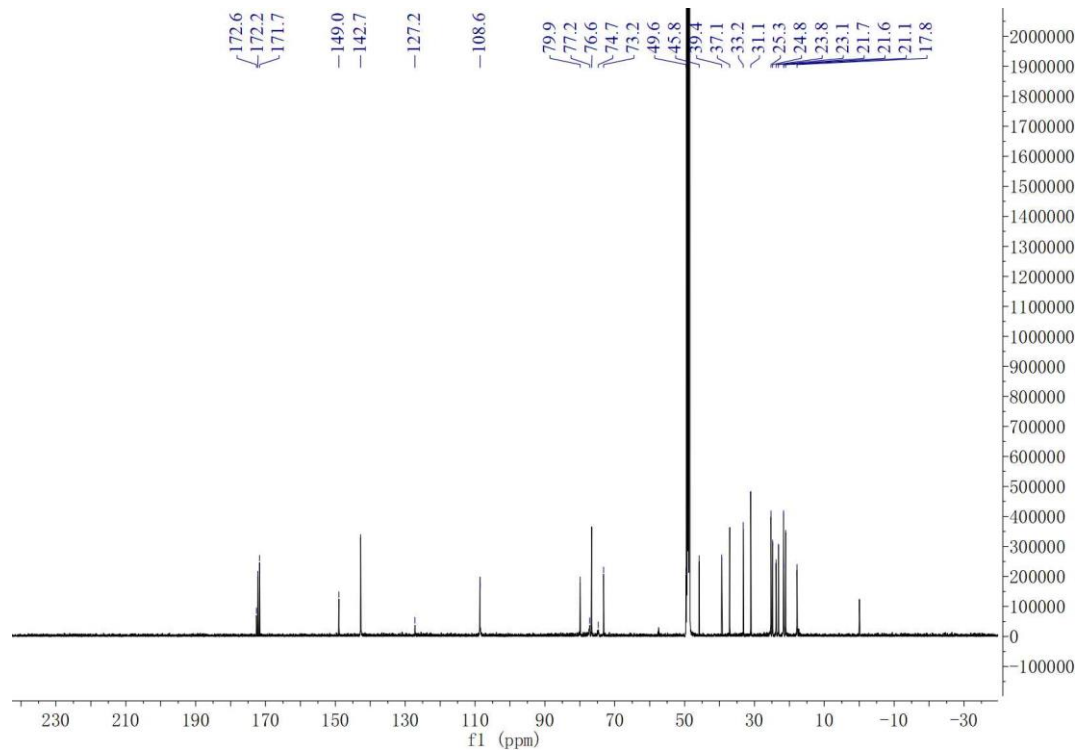


Figure S55. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 7

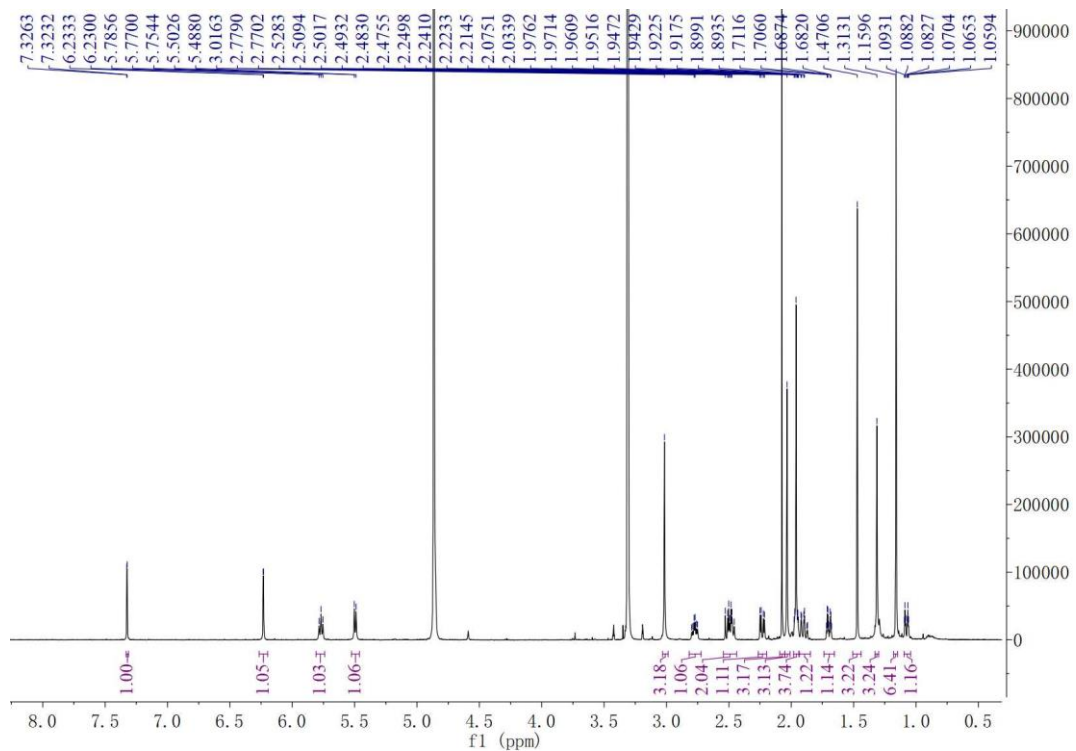


Figure S56. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **8**

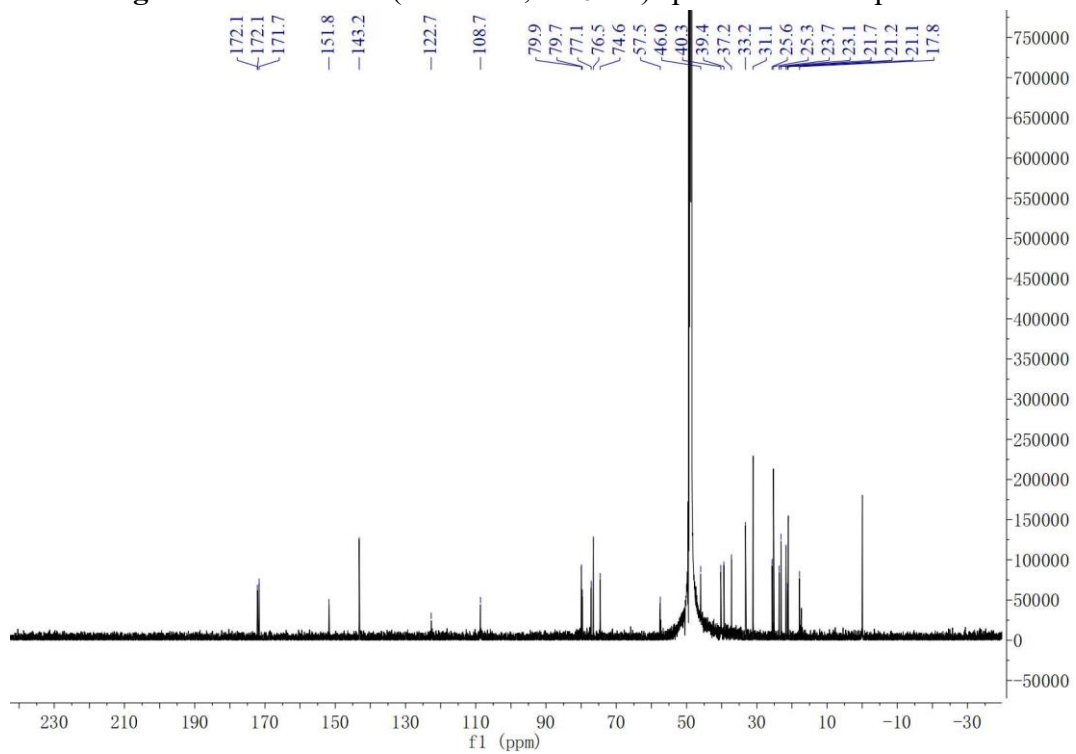


Figure S57. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **8**

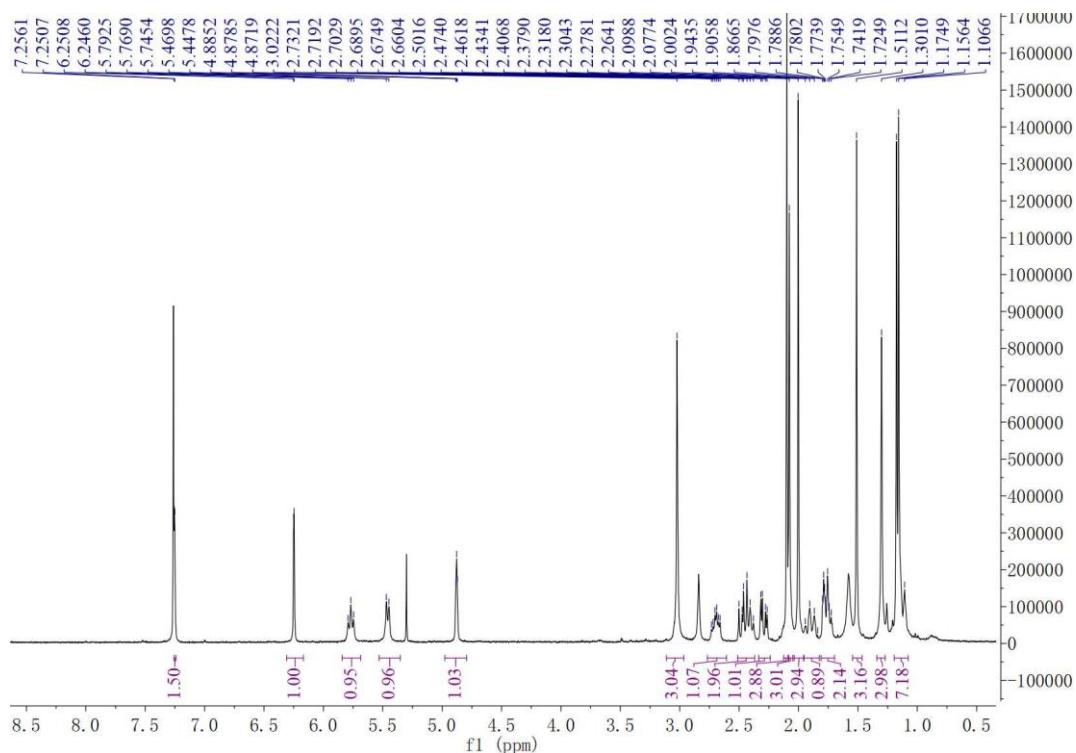


Figure S58. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **8**

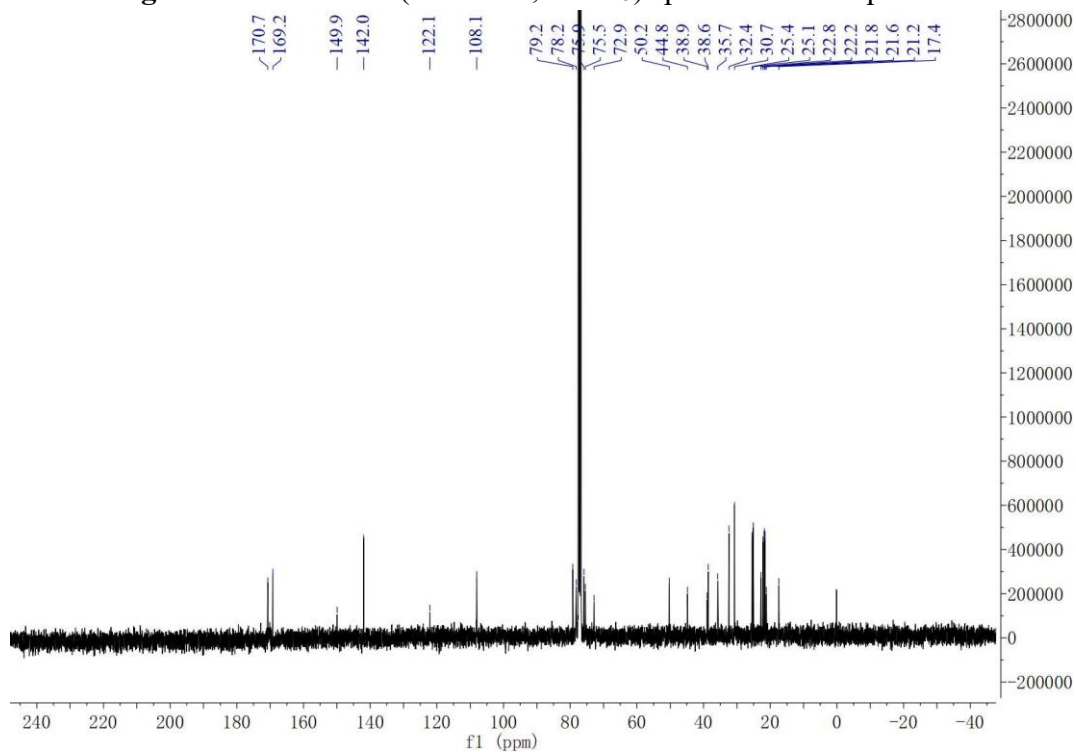


Figure S59. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **8**

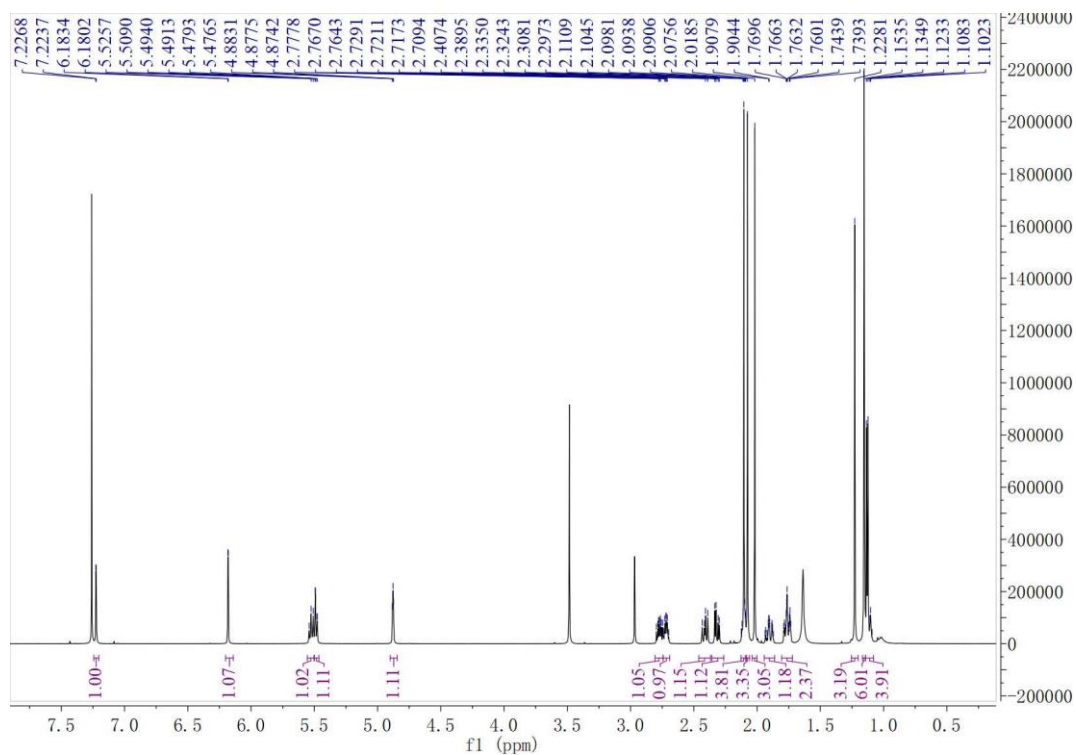


Figure S60. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **9**

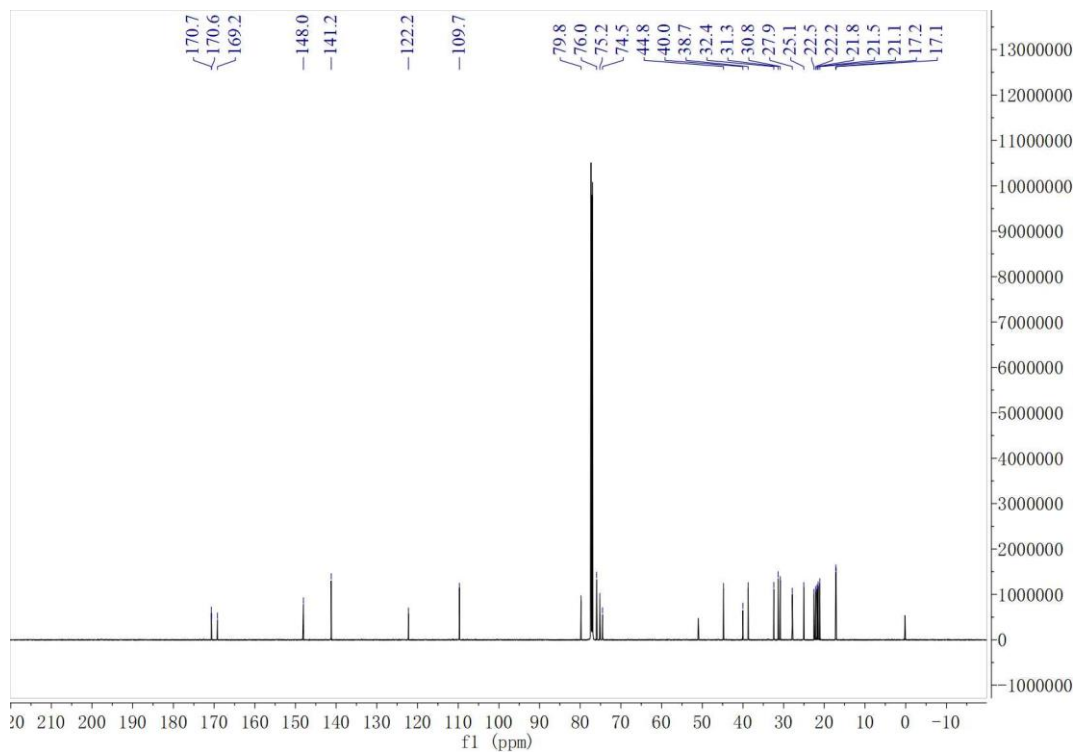


Figure S61. ^{13}C NMR (150 MHz, CDCl_3) spectrum of compound **9**

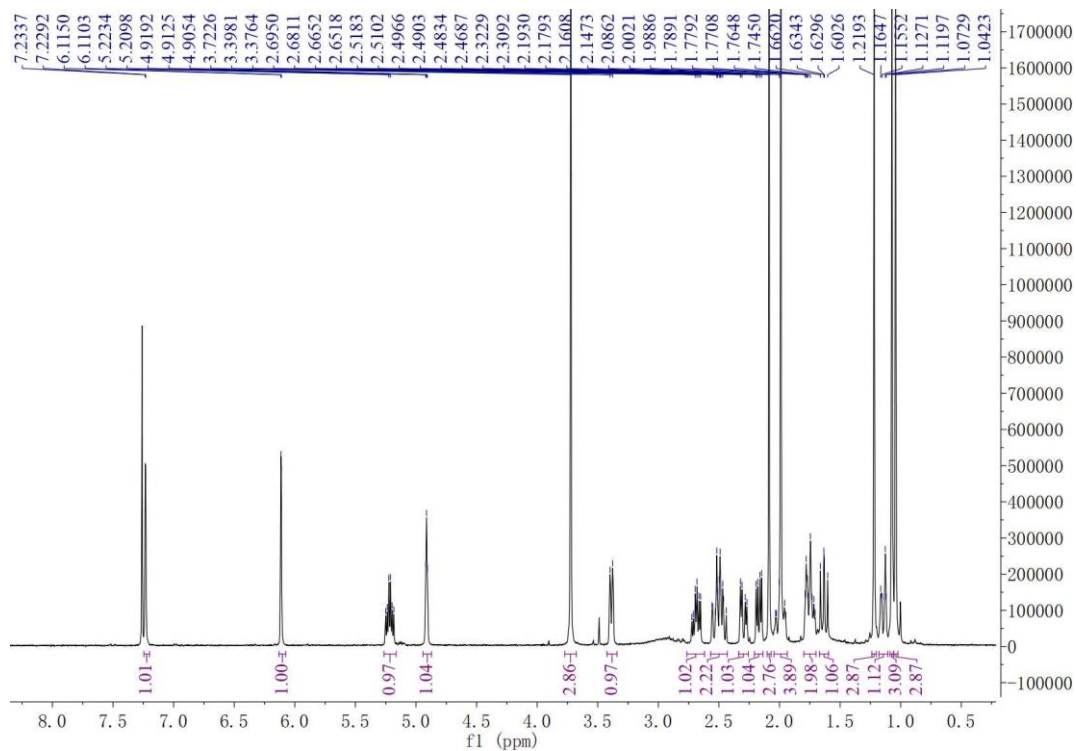


Figure S62. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **10**

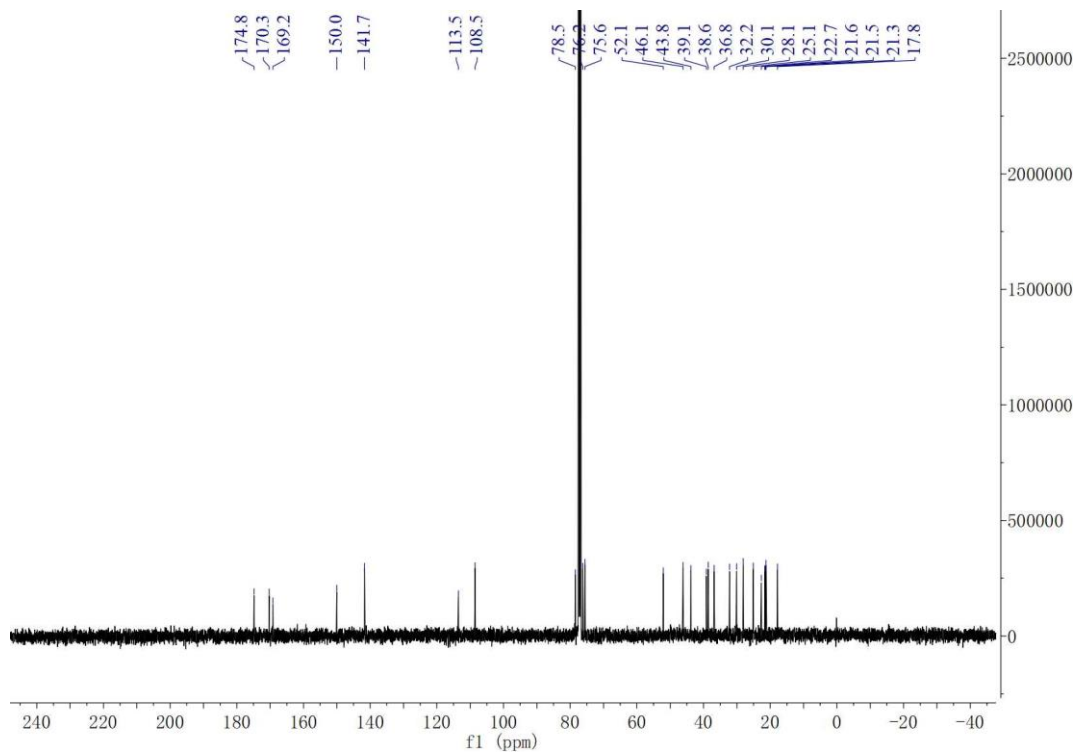


Figure S63. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **10**

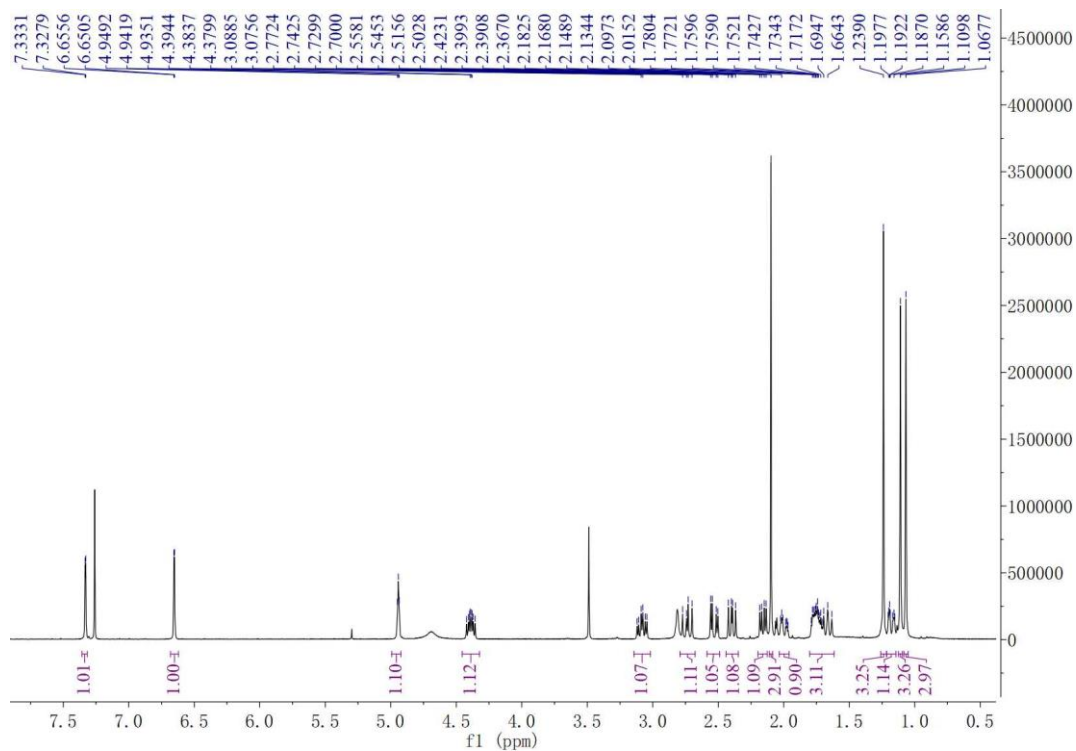


Figure S64. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **11**

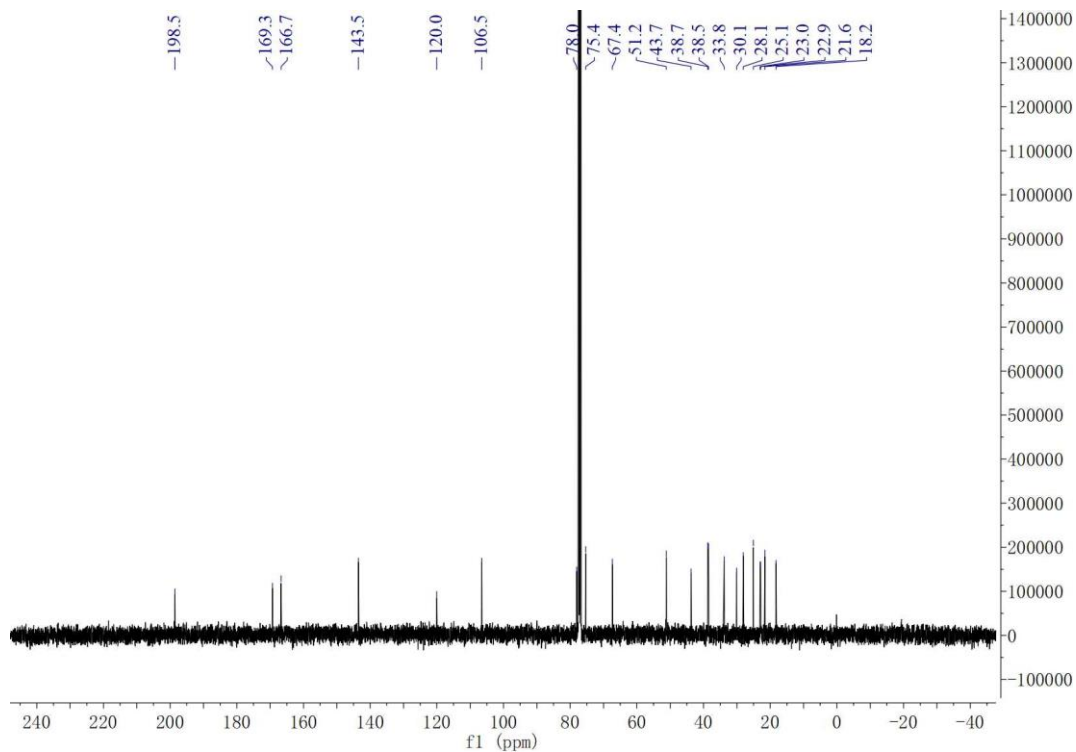


Figure S65. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **11**