

Supporting Information

Limonoids with diverse frameworks from stem barks of *Entandrophragma angolense* and their bioactivities

Wen-Yan Zhang, Fa-Liang An, Miao-Miao Zhou, Meng-Han Chen, Kai-Li Jian, Olga Quasie, Ming-Hua Yang, Jun Luo* and Ling-Yi Kong*

*State Key Laboratory of Natural Medicines, Department of Natural Medicinal Chemistry, China
Pharmaceutical University, 24 Tong Jia Xiang, Nanjing 210009, People's Republic of China*

Corresponding authors

* Jun Luo:

E-mail: luojun1981ly@163.com

Tel/Fax: +86-25-8327-1405

* Ling-Yi Kong:

E-mail: cpu_lykong@126.com

Tel/Fax: +86-25-8327-1405

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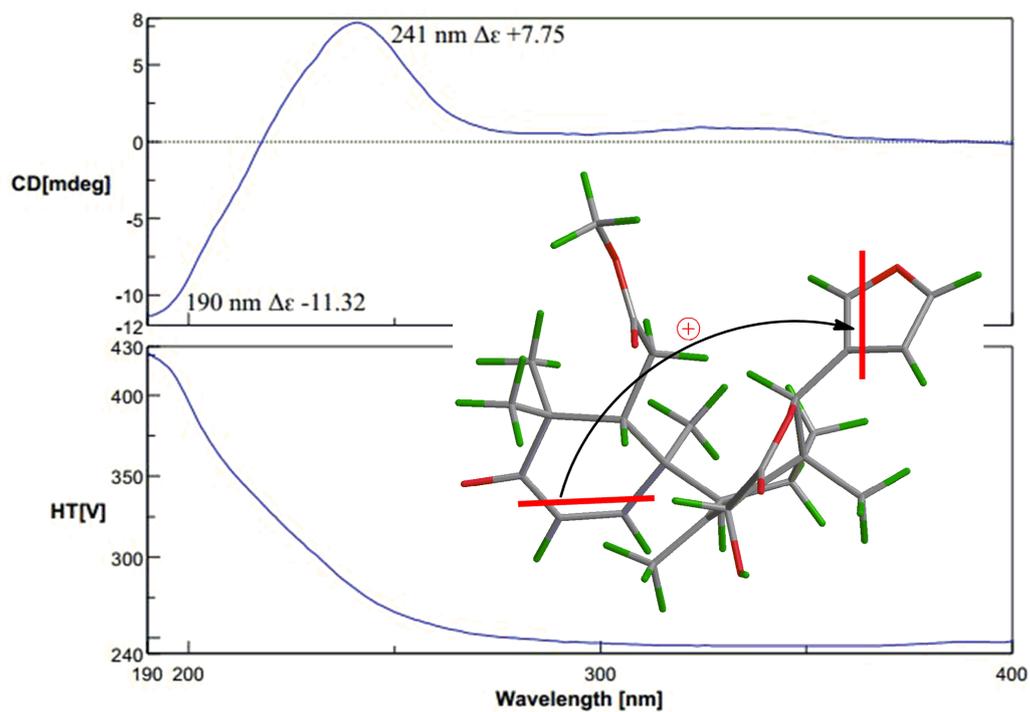


Figure S1. ECD and UV spectra of **2** (in MeCN).

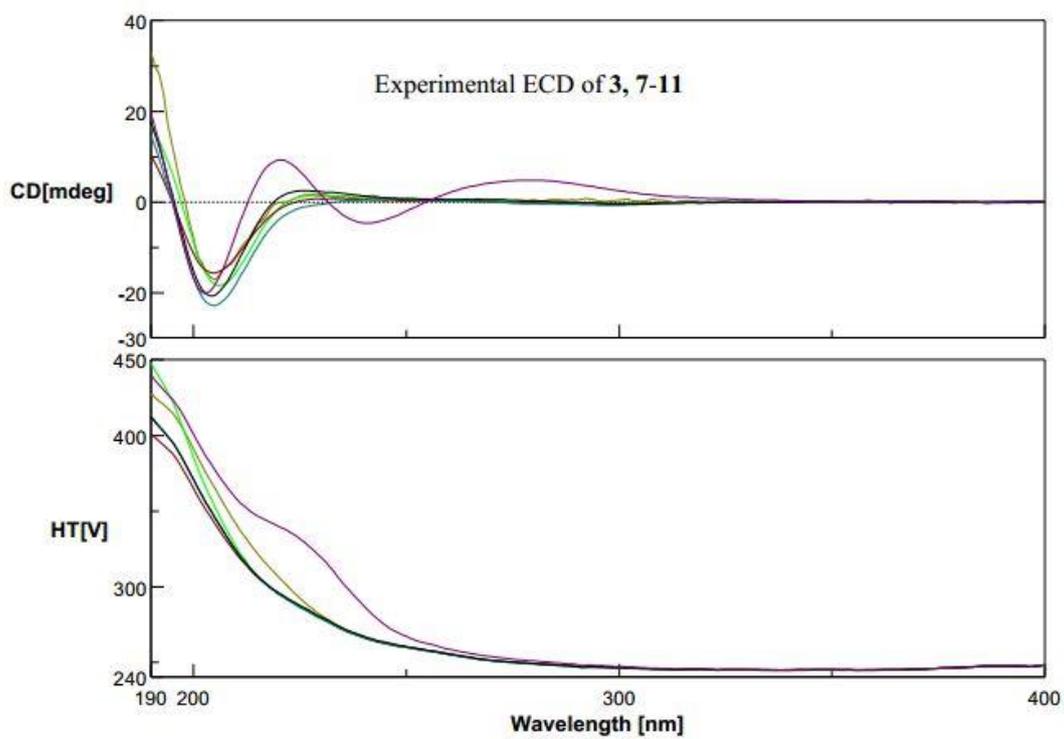


Figure S2. Experimental ECD of **3**, **7-11** (in MeCN).

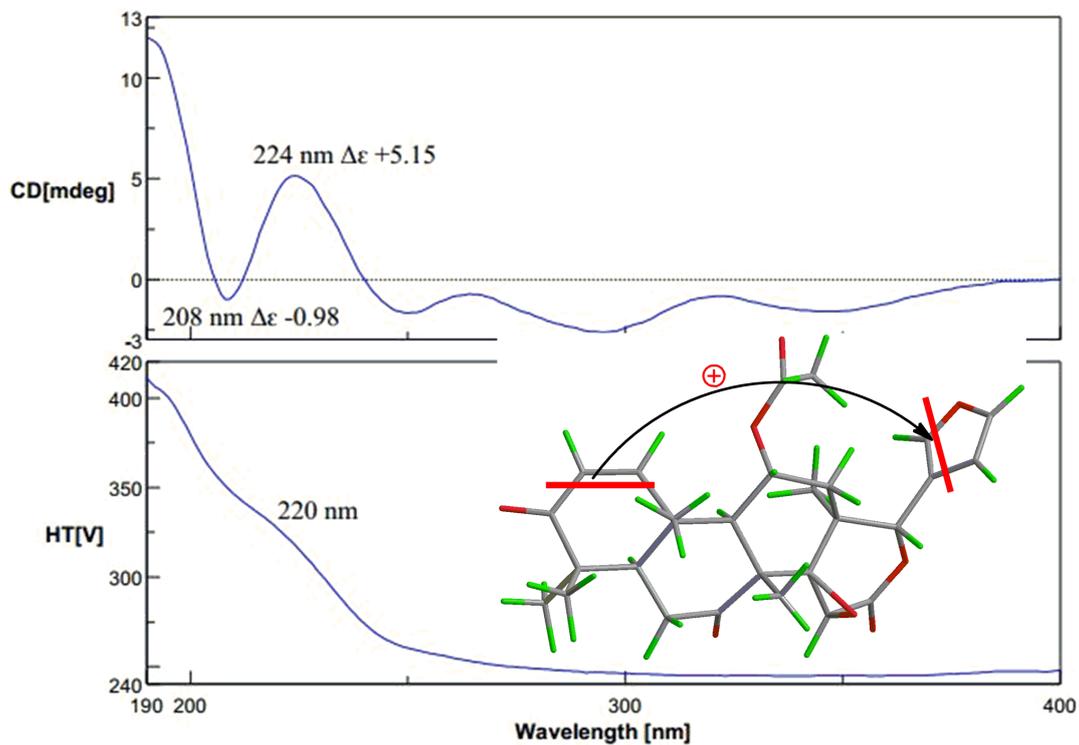


Figure S3. ECD and UV spectra of **12** (in MeCN).

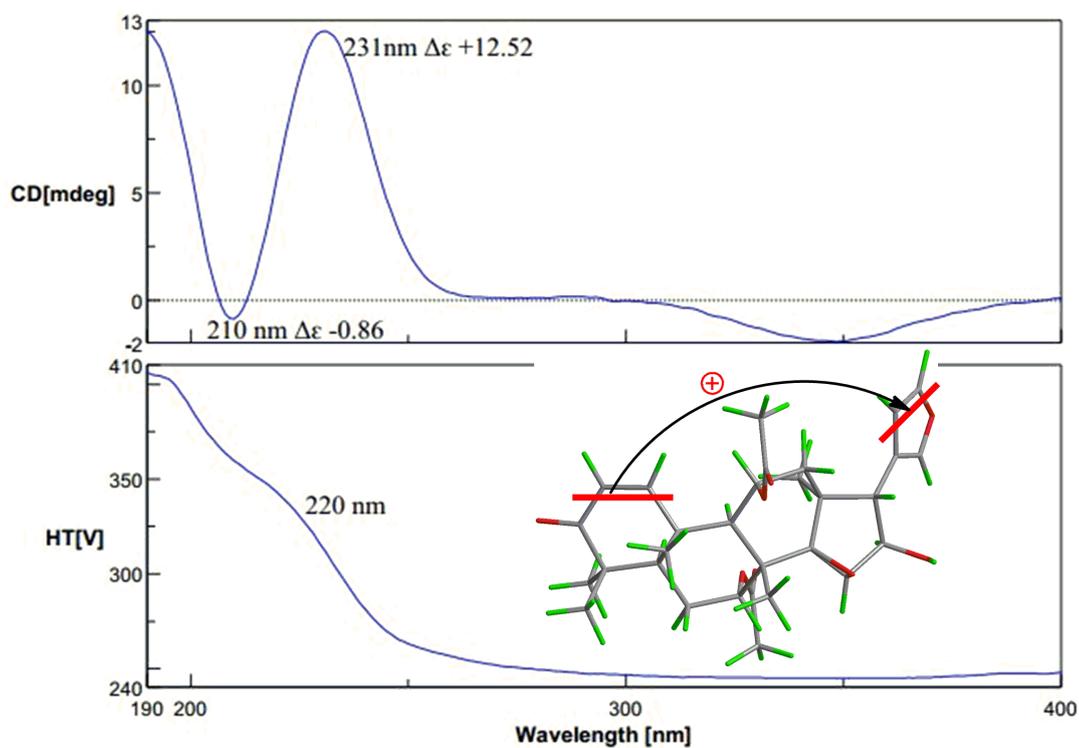
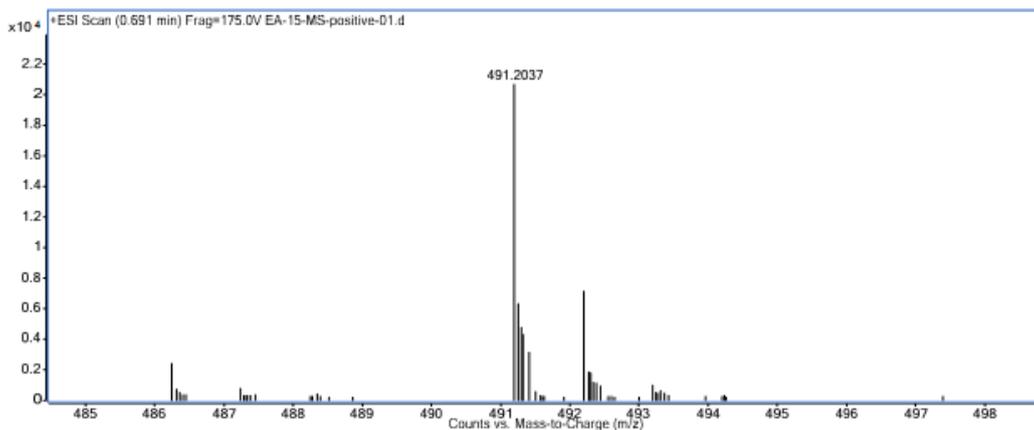


Figure S4. ECD and UV spectra of **15** (in MeCN).



Elemental Composition Calculator

Target m/z:	491.2037	Result type:	Positive ions	Species:	[M+Na] ⁺
Elements:	C (0-80); H (0-120); O (0-30); Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₇ H ₃₂ NaO ₇	491.2040		0.65		

Figure S5. HRESIMS spectrum of **1**.

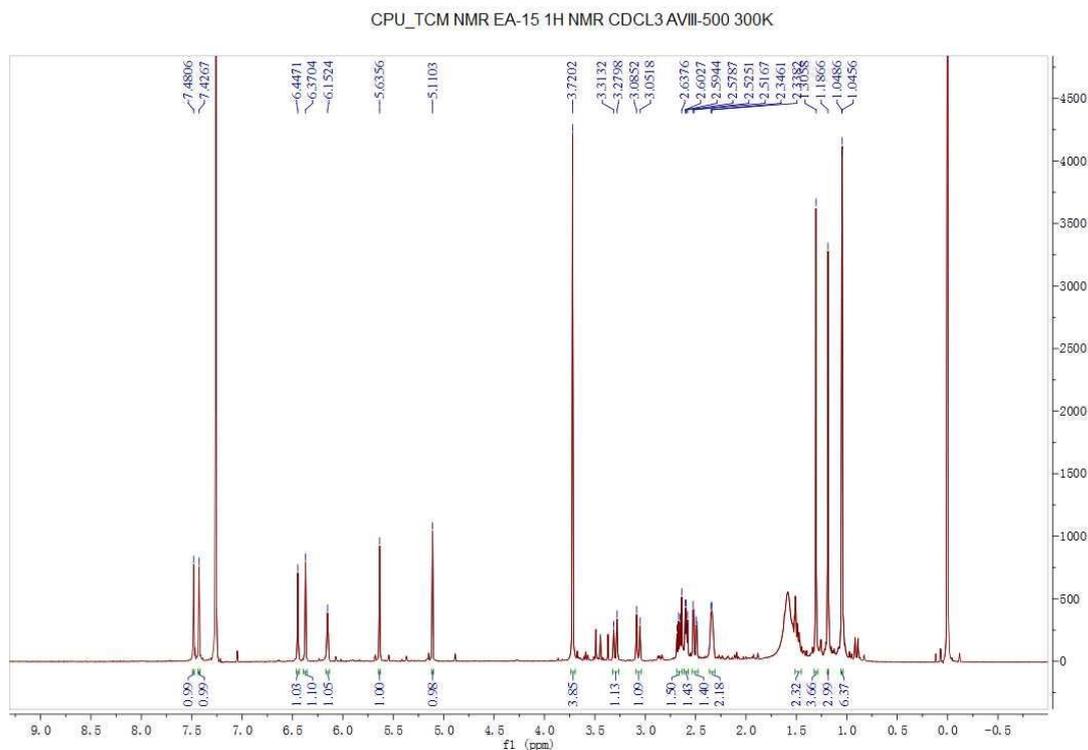


Figure S6. ¹H NMR spectrum of **1** in CDCl₃.

CPU_TCM NMR EA-15 13C NMR CDCL3 AVIII-500 300K

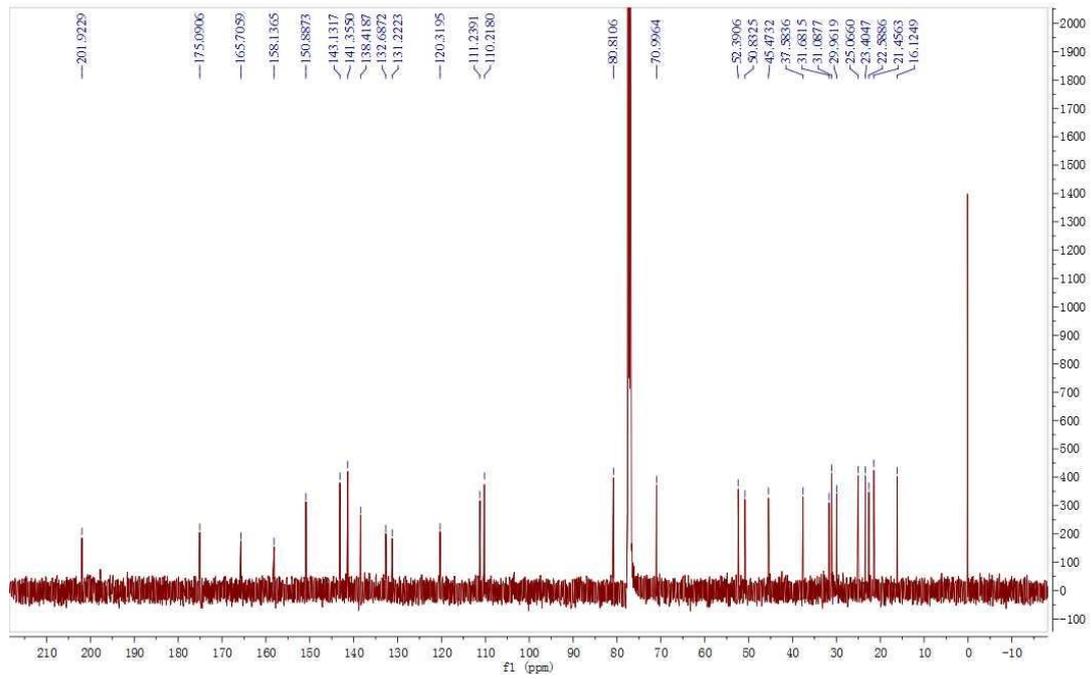


Figure S7. ^{13}C NMR spectrum of **1** in CDCl_3 .

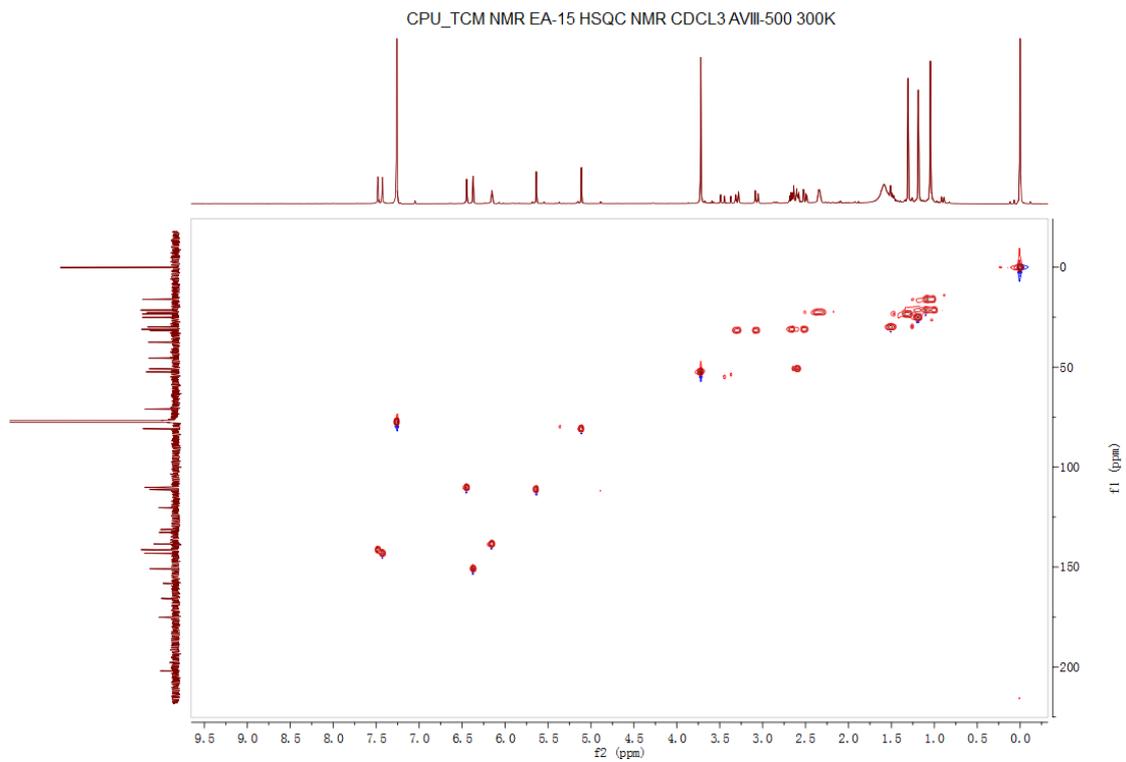
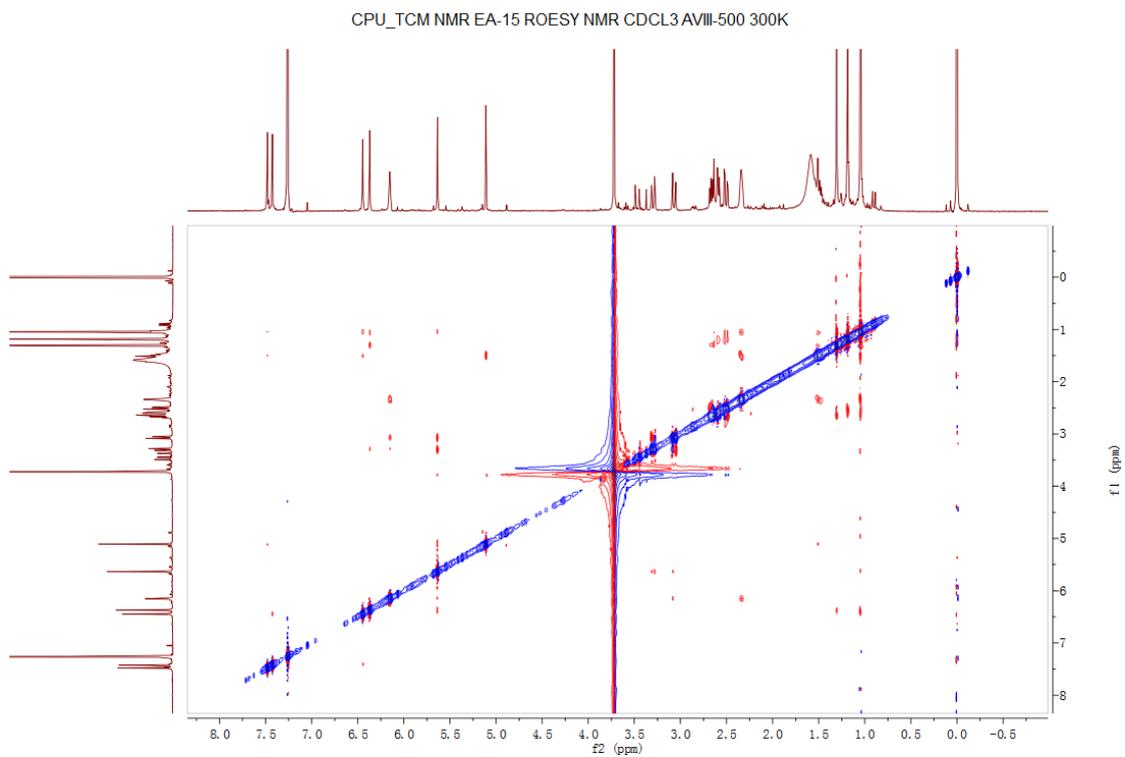
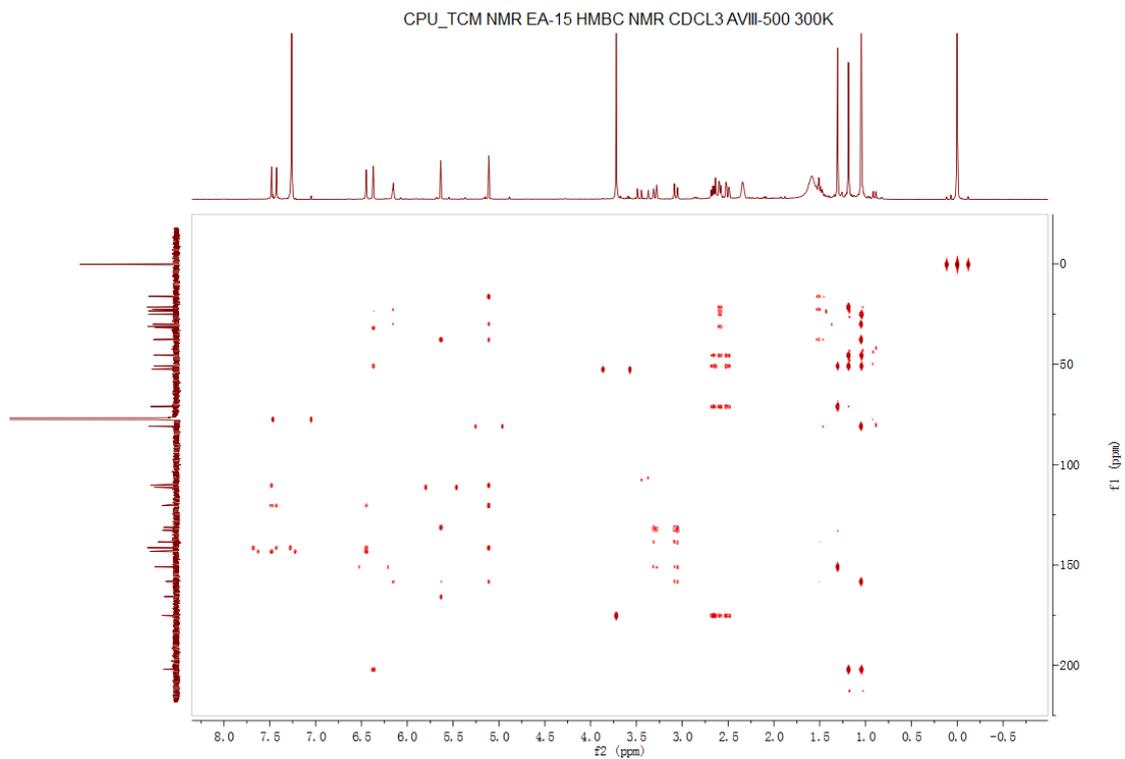
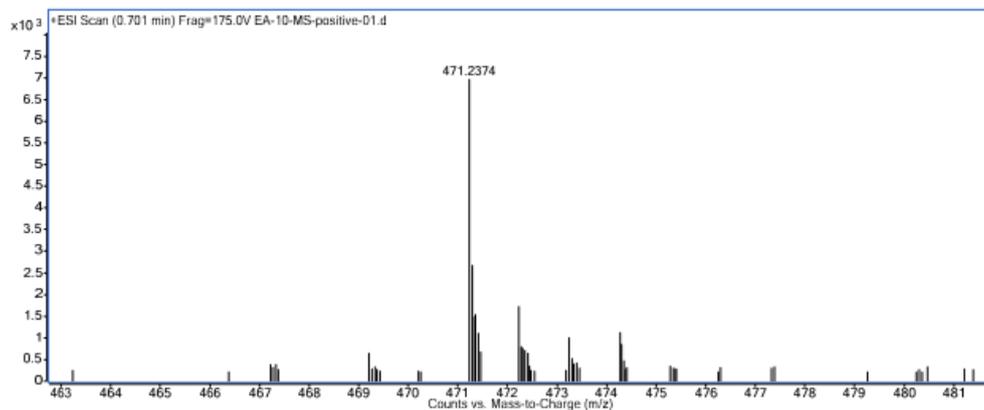


Figure S8. HSQC spectrum of **1** in CDCl_3 .





Elemental Composition Calculator

Target m/z:	471.2374	Result type:	Positive ions	Species:	[M+H] ⁺
Elements:	C (0-80); H (0-120); O (0-30)				
Ion Formula	Calculated m/z	PPM Error			
C ₂₇ H ₃₅ O ₇	471.2377	0.7			

Figure S11. HRESIMS spectrum of **2**.

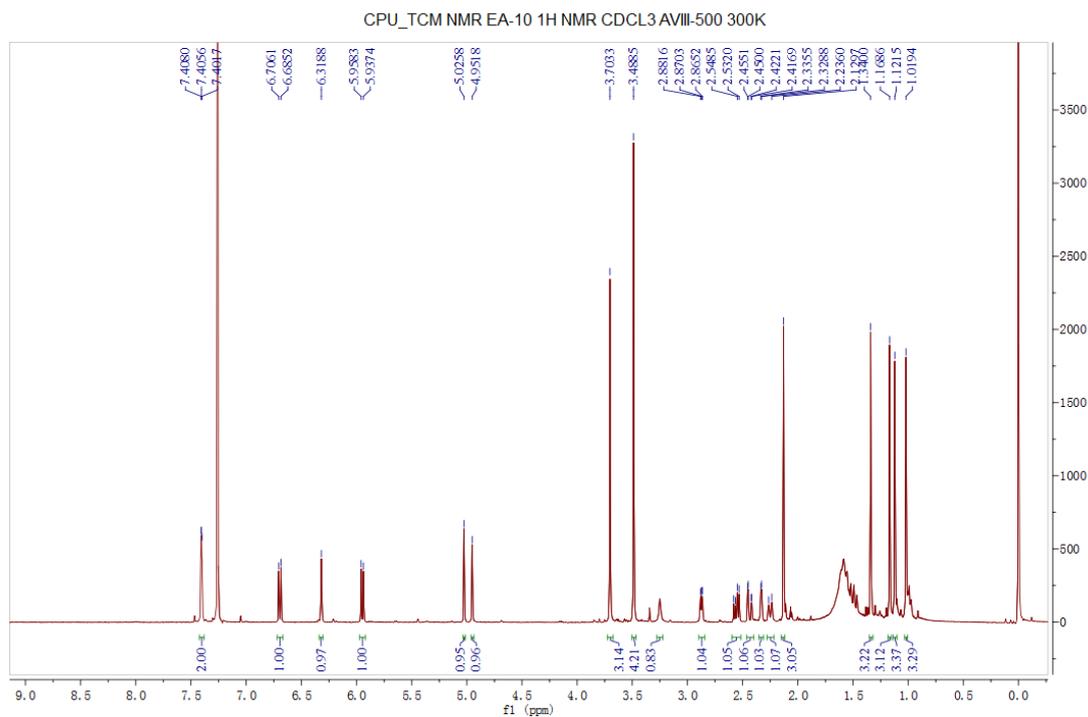


Figure S12. ¹H NMR spectrum of **2** in CDCl₃.

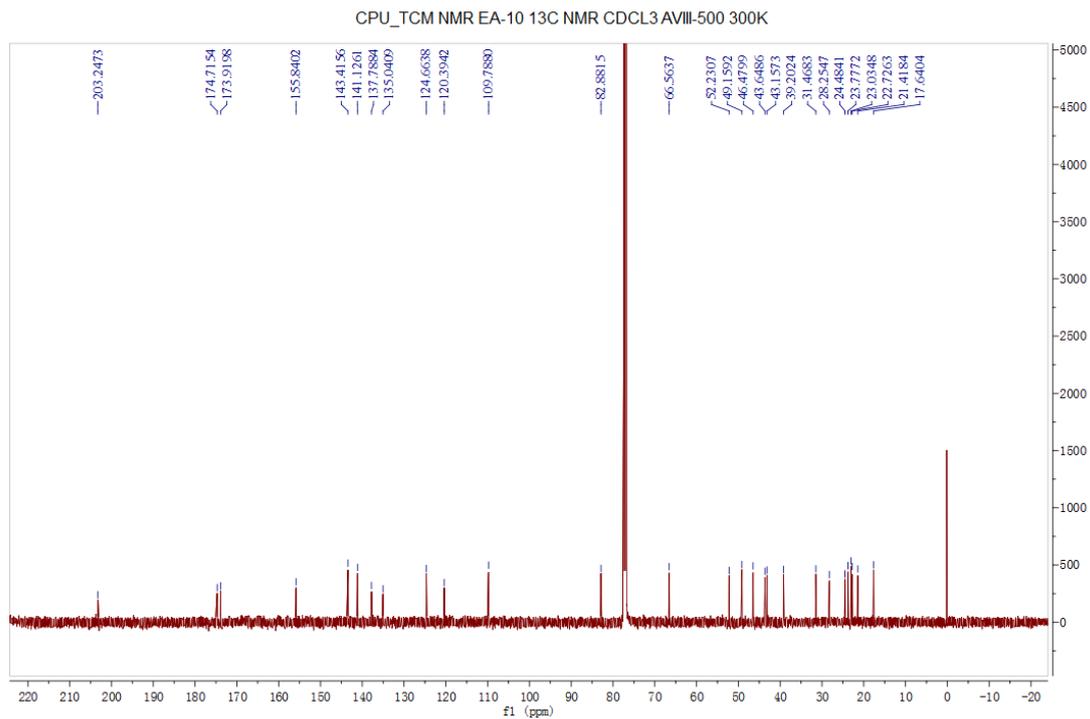


Figure S13. ^{13}C NMR spectrum of **2** in CDCl_3 .

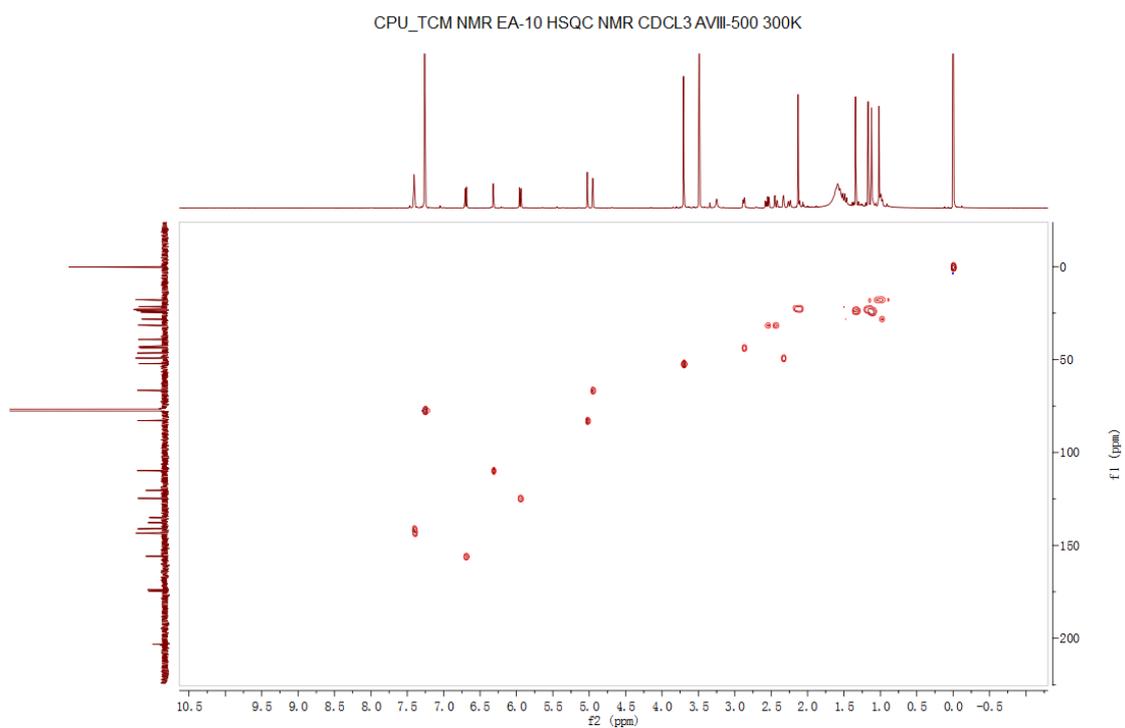


Figure S14. HSQC spectrum of **2** in CDCl_3 .

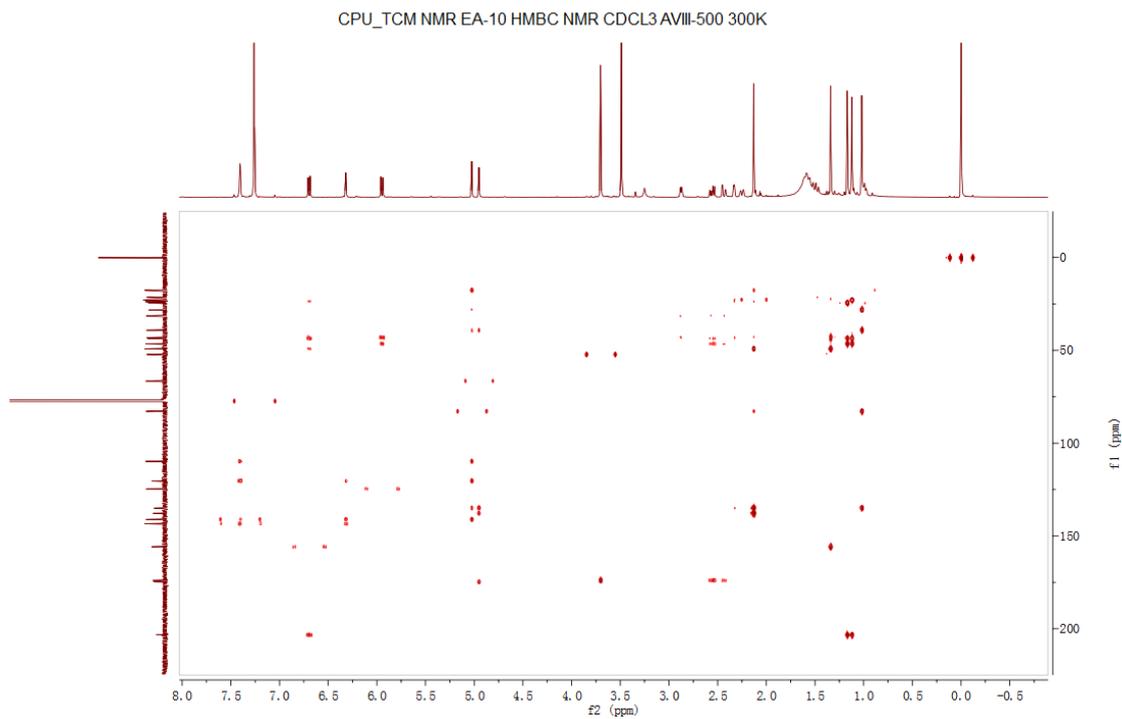


Figure S15. HMBC spectrum of **2** in CDCl₃.

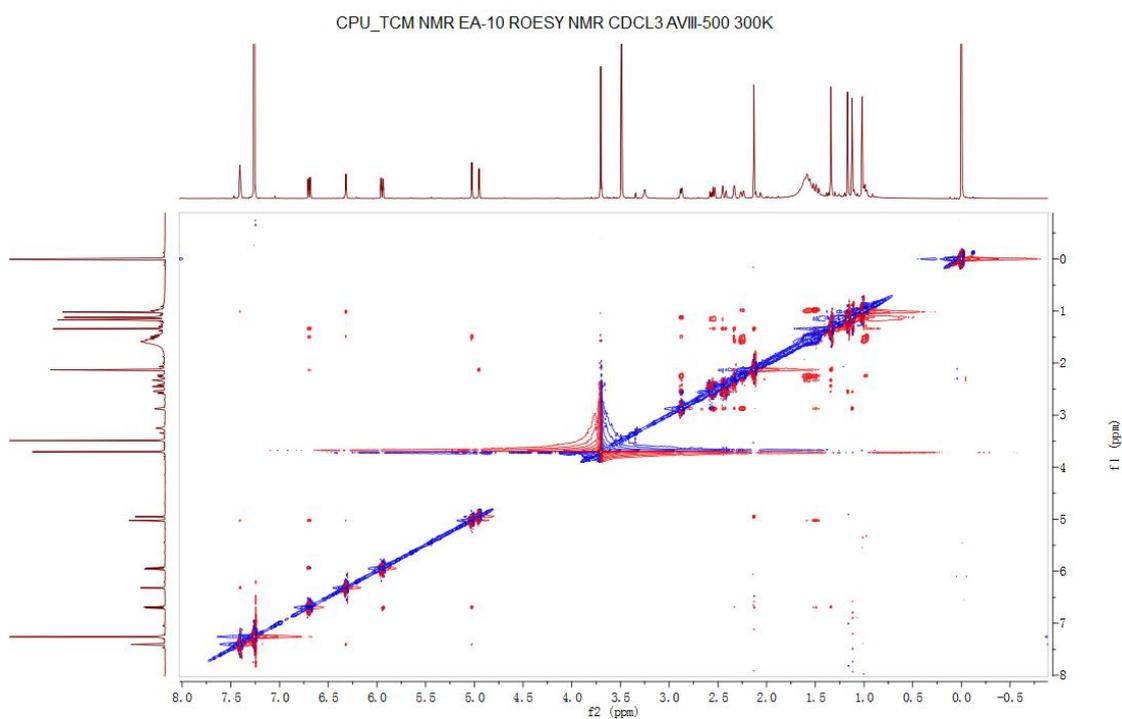
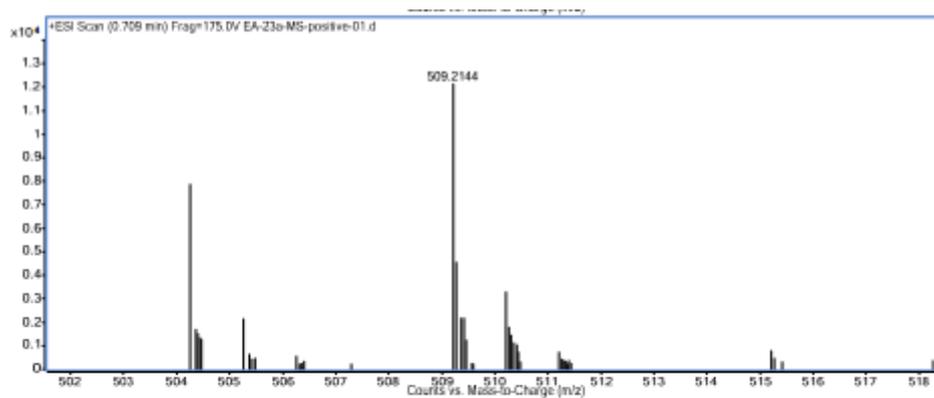


Figure S16. ROESY spectrum of **2** in CDCl₃.



Elemental Composition Calculator

Target m/z:	509.2144	Result type:	Positive ions	Species:	[M+Na] ⁺
Elements:	C (0-80); H (0-120); O (0-30); Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₇ H ₃₄ NaO ₈	509.2146		0.29		

Figure S17. HRESIMS spectrum of **3**.

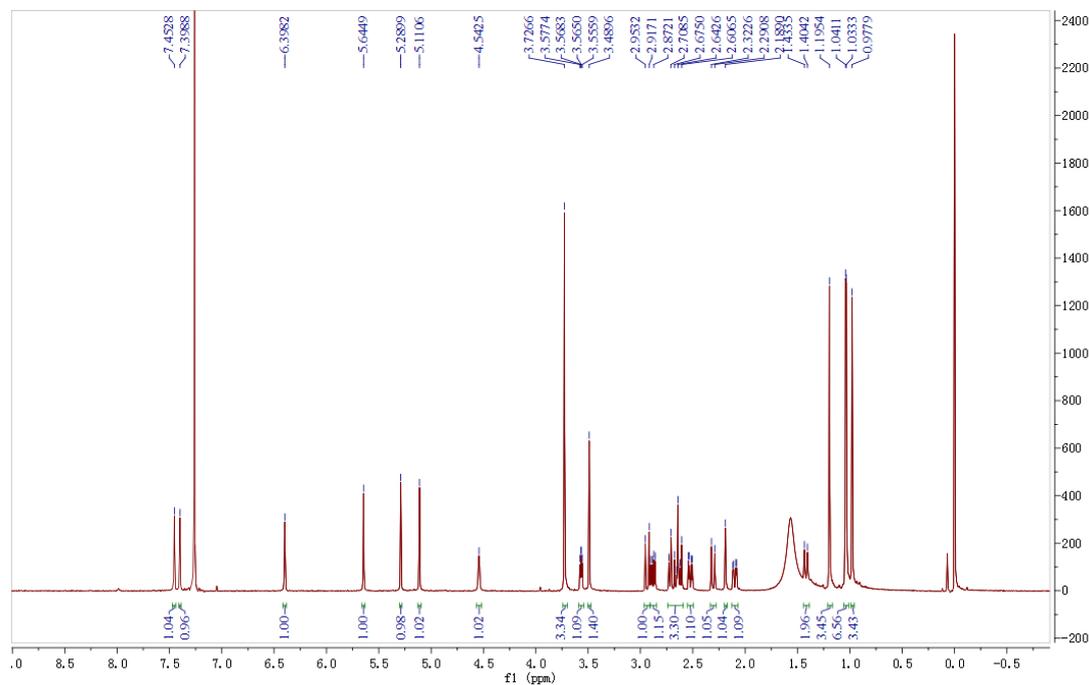


Figure S18. ¹H NMR spectrum of **3** in CDCl₃.

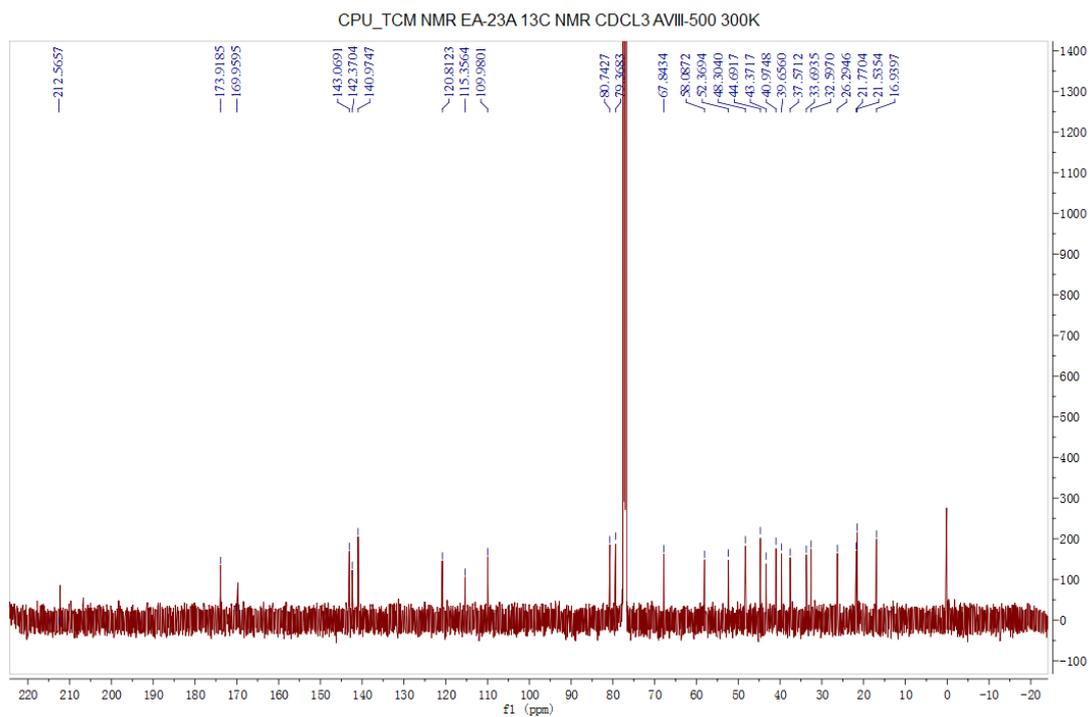


Figure S19. ^{13}C NMR spectrum of **3** in CDCl_3 .

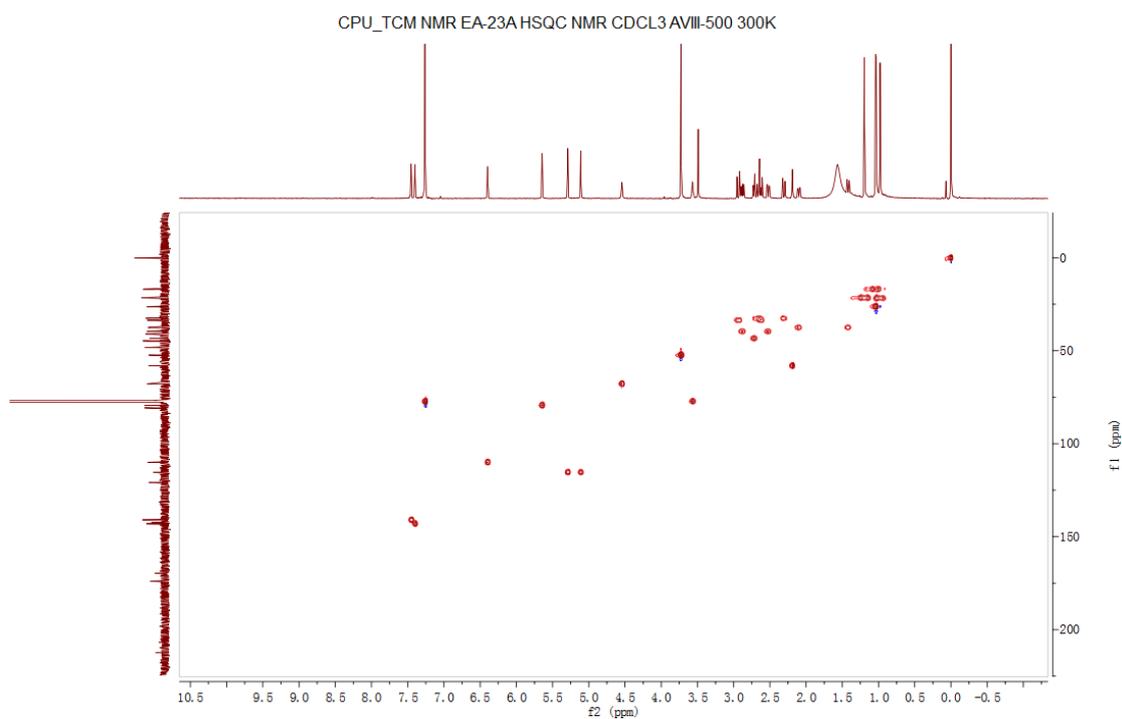


Figure S20. HSQC spectrum of **3** in CDCl_3 .

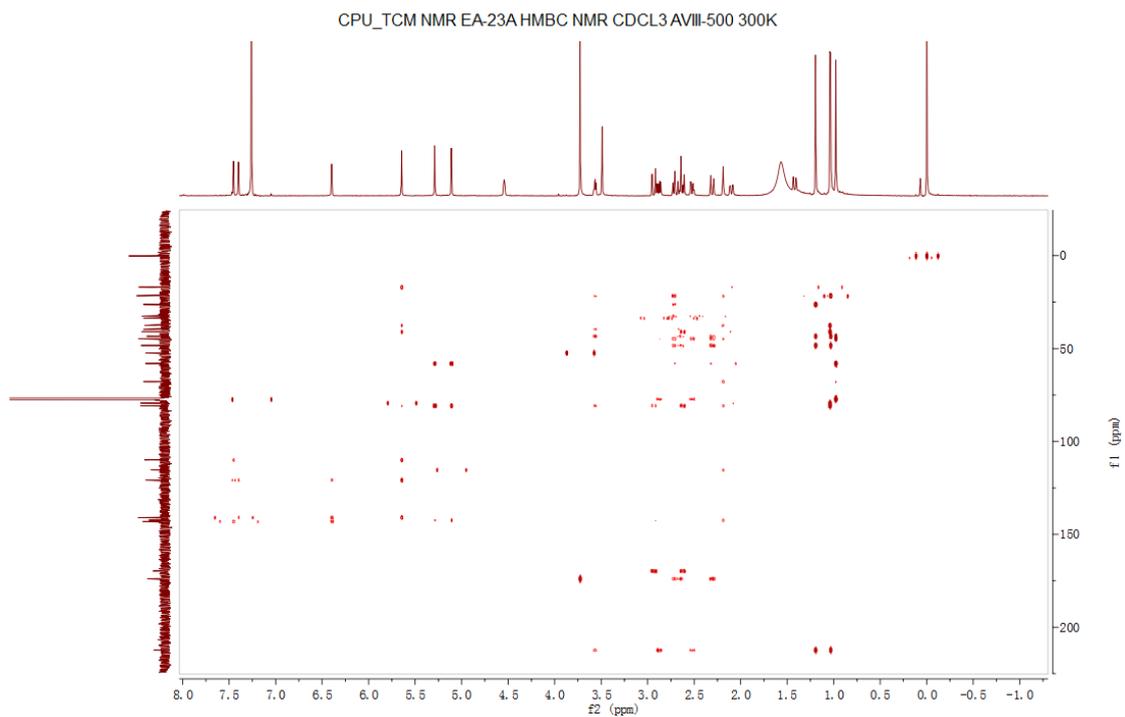


Figure S21. HMBC spectrum of **3** in CDCl₃.

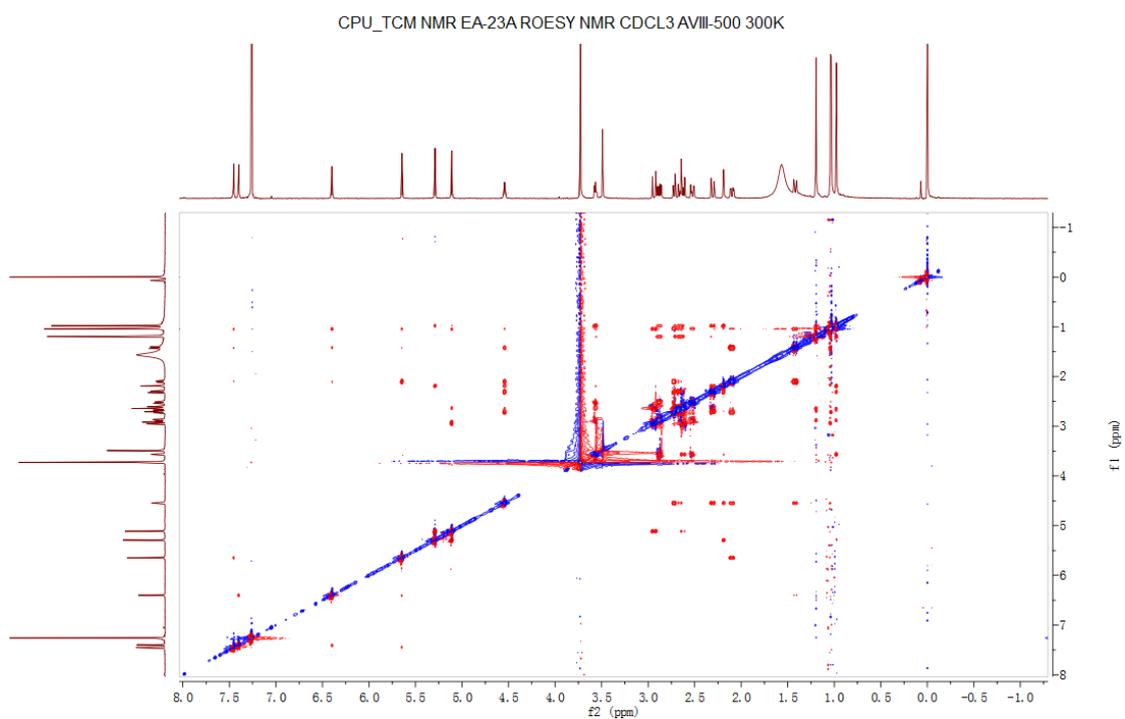
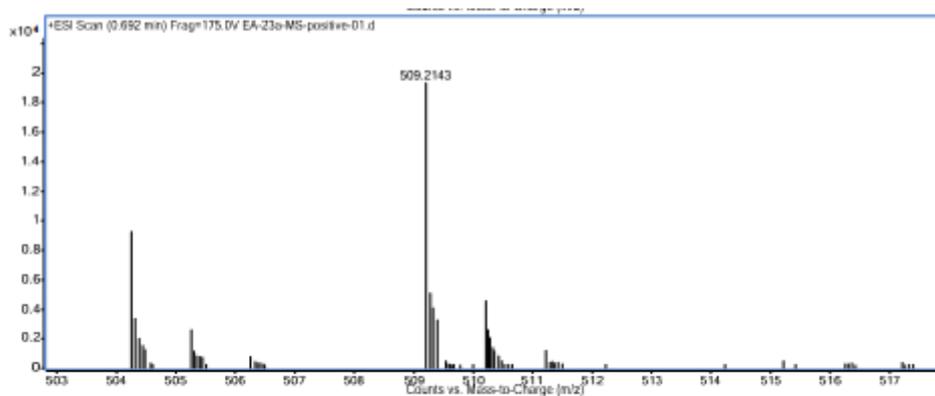


Figure S22. ROESY spectrum of **3** in CDCl₃.



Elemental Composition Calculator

Target m/z:	509.2143	Result type:	Positive ions	Species:	[M+Na] ⁺
Elements:	C (0-80); H (0-120); O (0-30); Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₇ H ₃₄ NaO ₈	509.2146		0.57		

Figure S23. HRESIMS spectrum of **4**.

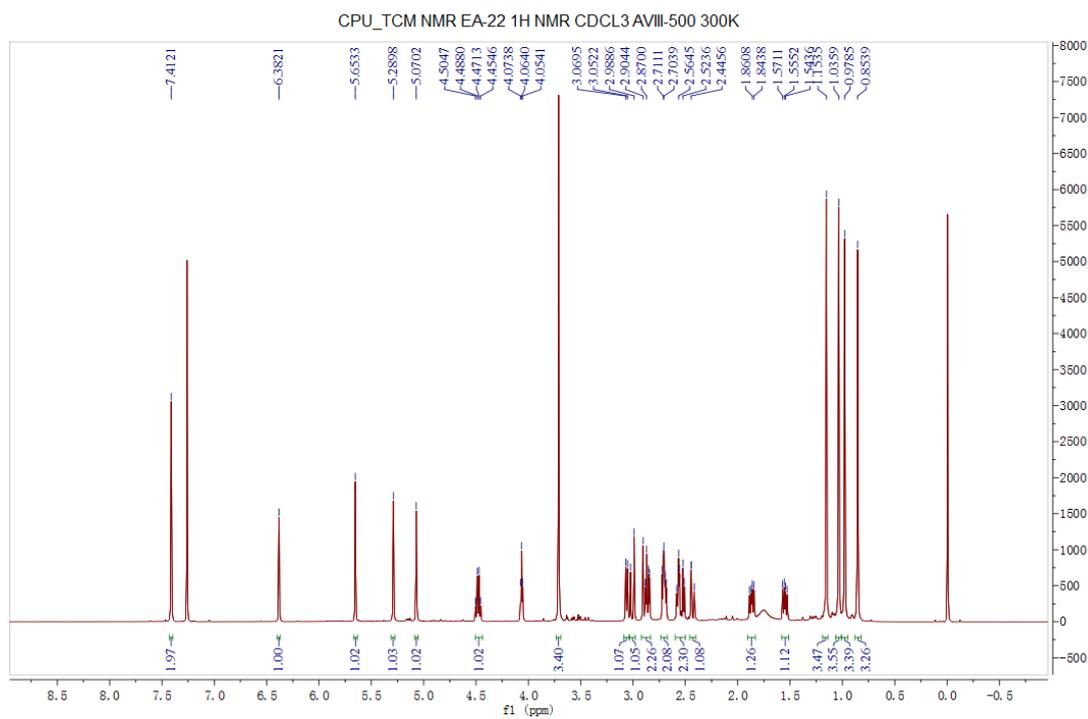


Figure S24. ¹H NMR spectrum of **4** in CDCl₃.

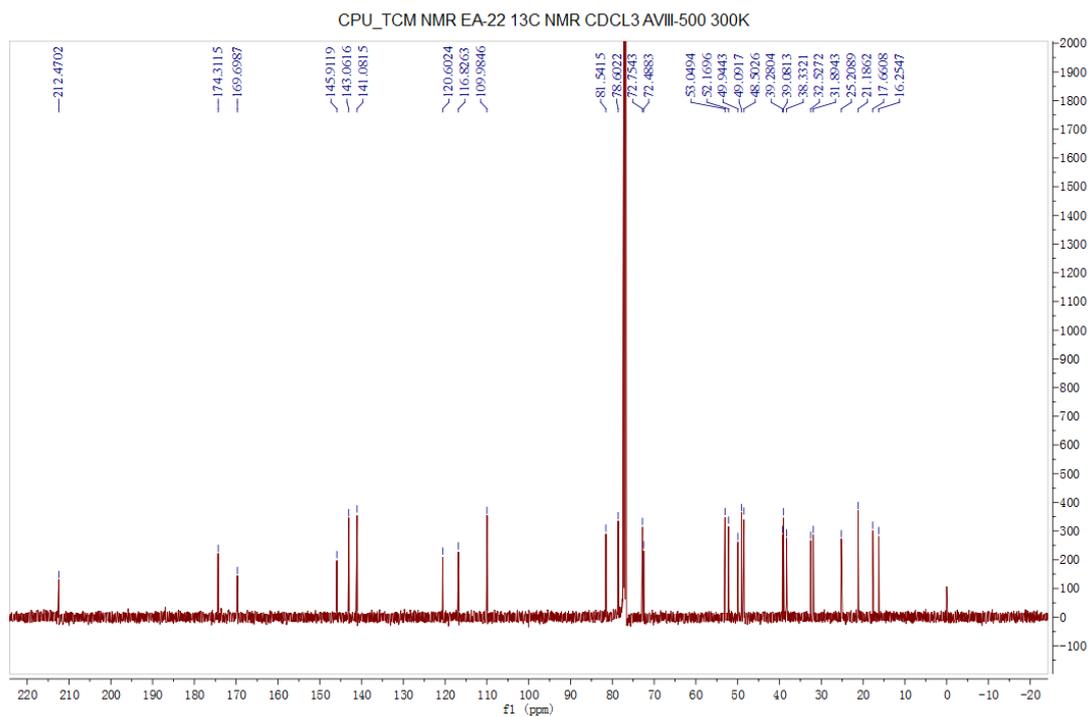


Figure S25. ^{13}C NMR spectrum of **4** in CDCl_3 .

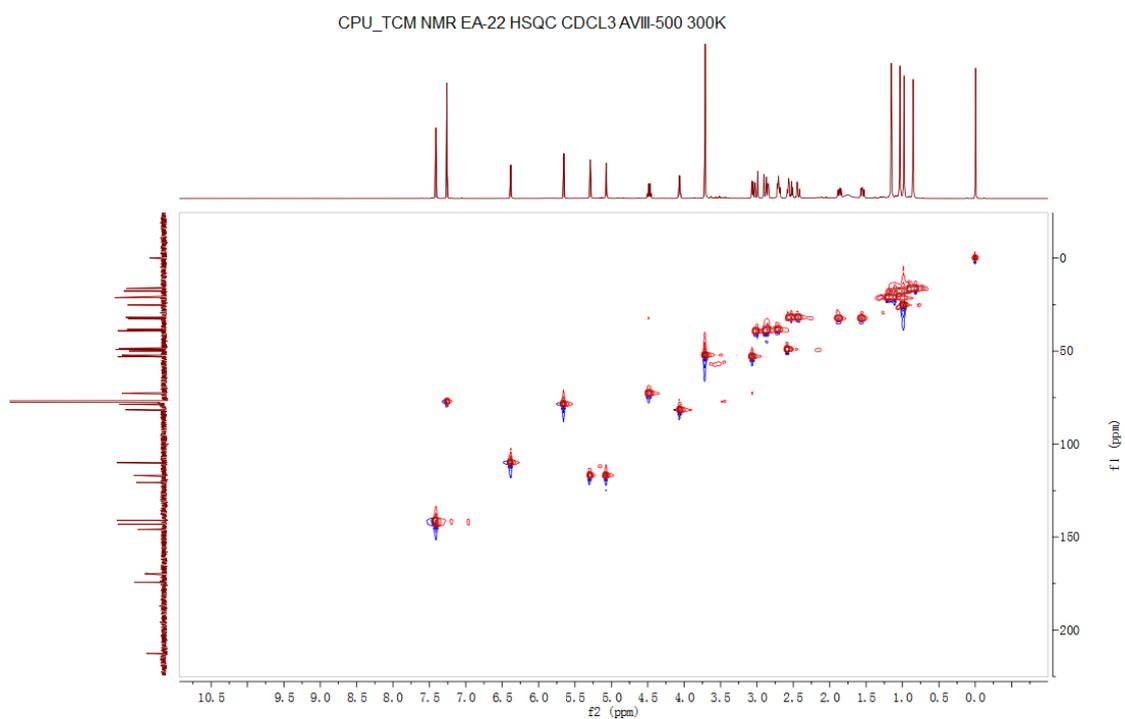
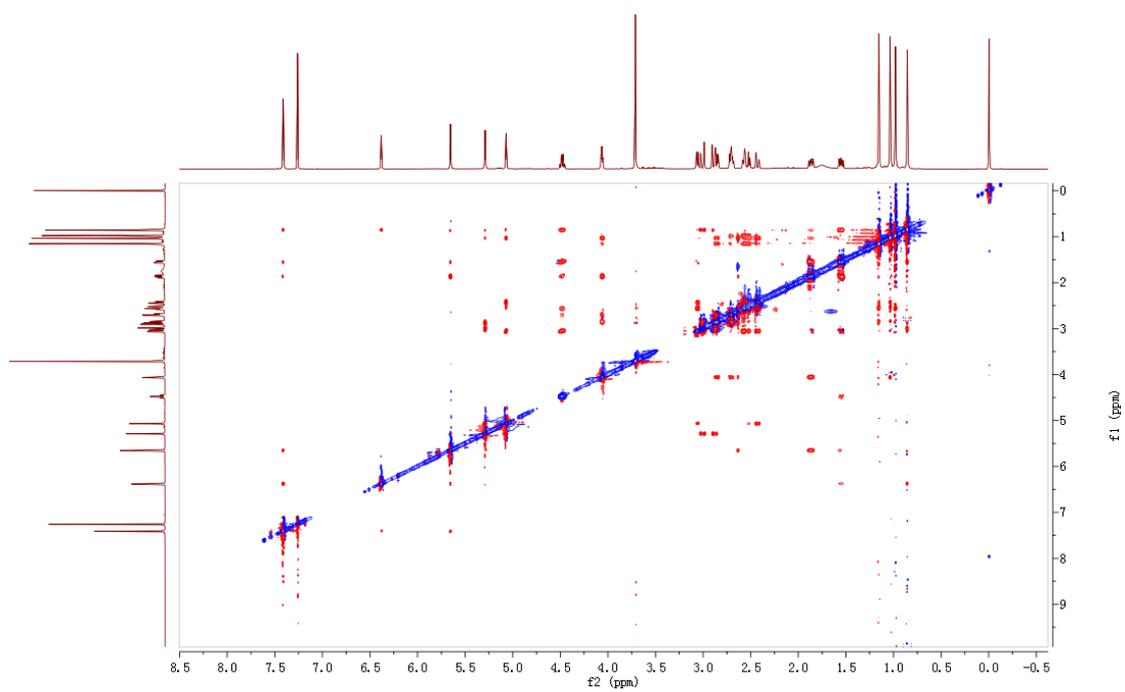
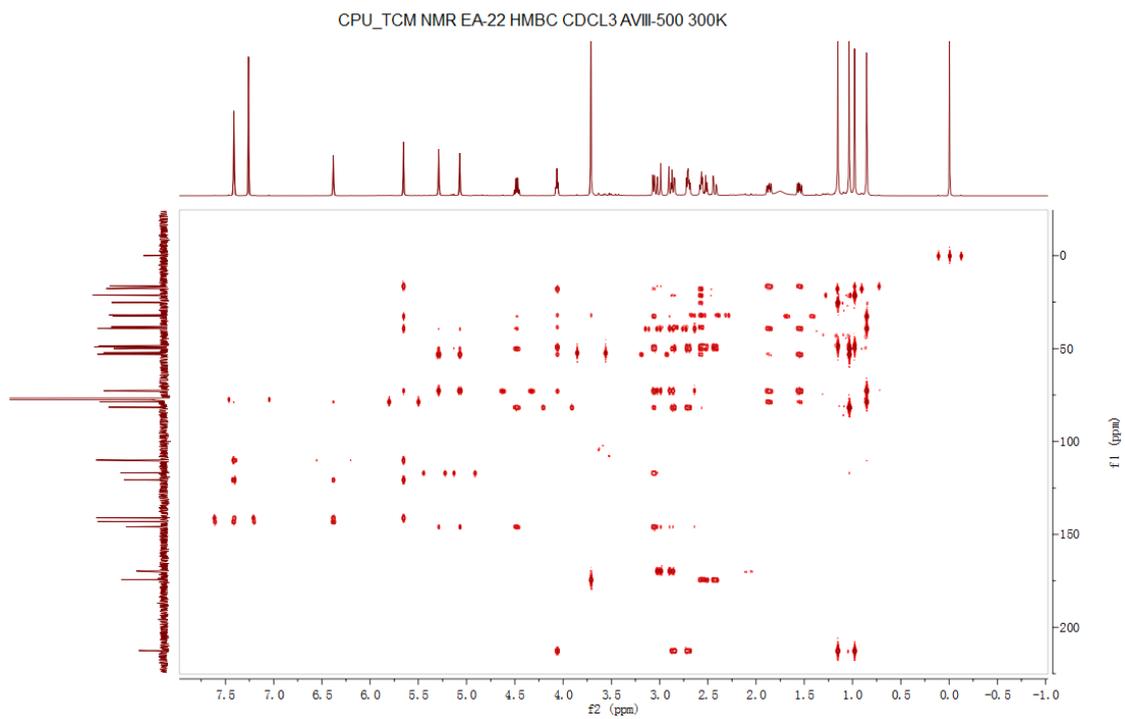
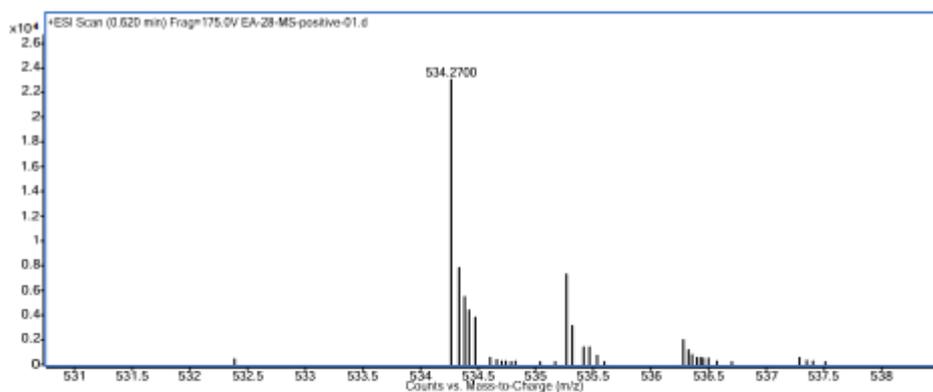


Figure S26. HSQC spectrum of **4** in CDCl_3 .





Elemental Composition Calculator

Target m/z:	534.2700	Result type:	Positive ions	Species:	[M+NH4] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₈ H ₄₀ N ₉ O ₉	534.2698		-0.46		

Figure S29. HRESIMS spectrum of **5**.

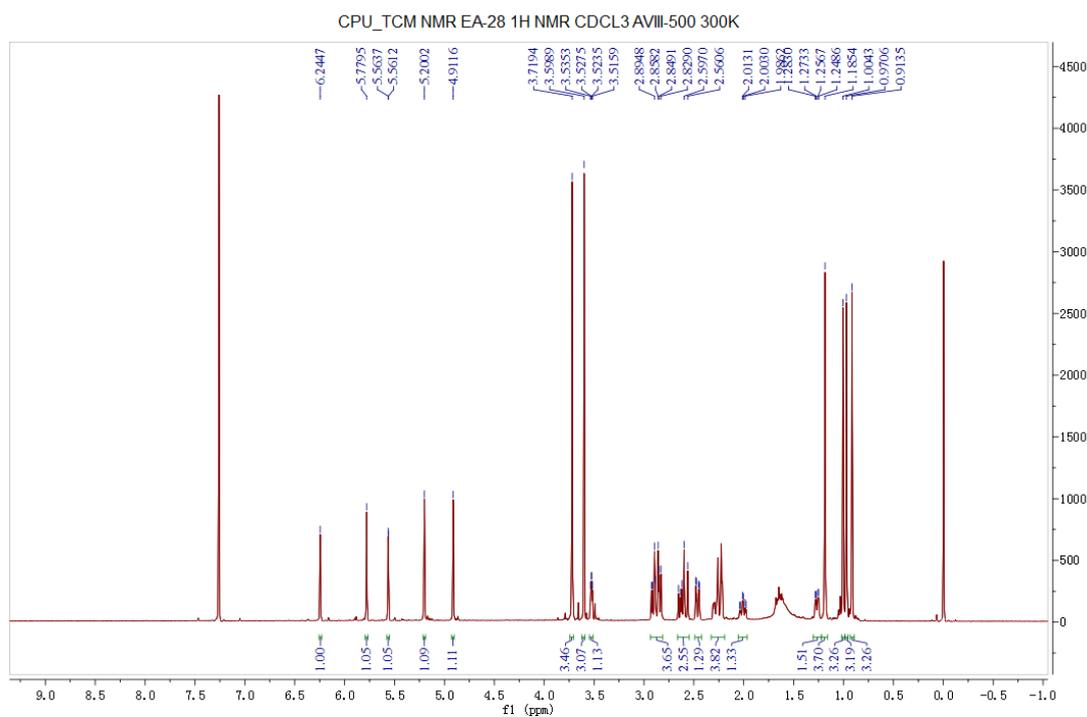


Figure S30. ¹H NMR spectrum of **5** in CDCl₃.

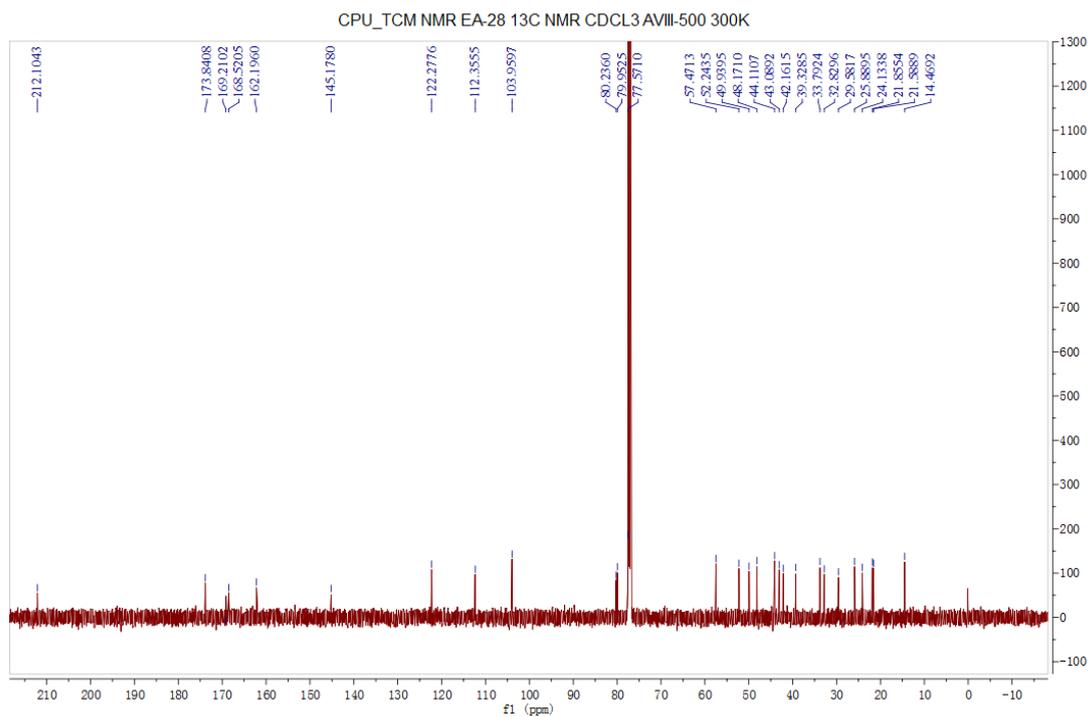


Figure S31. ^{13}C NMR spectrum of **5** in CDCl_3 .

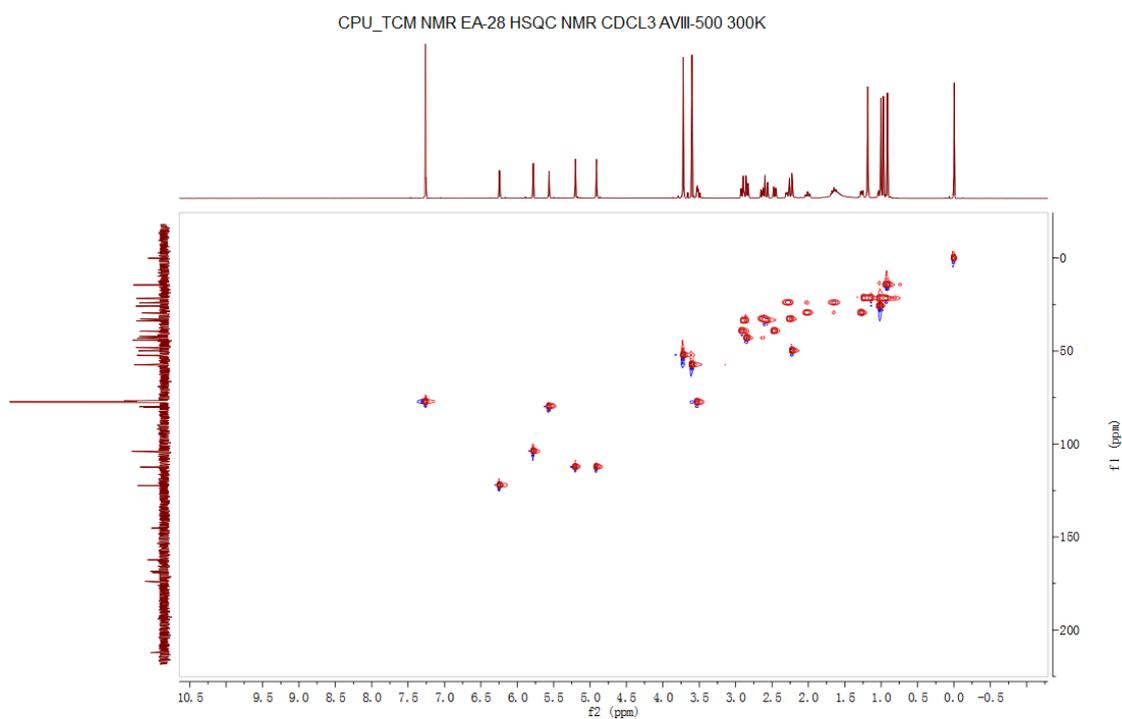


Figure S32. HSQC spectrum of **5** in CDCl_3 .

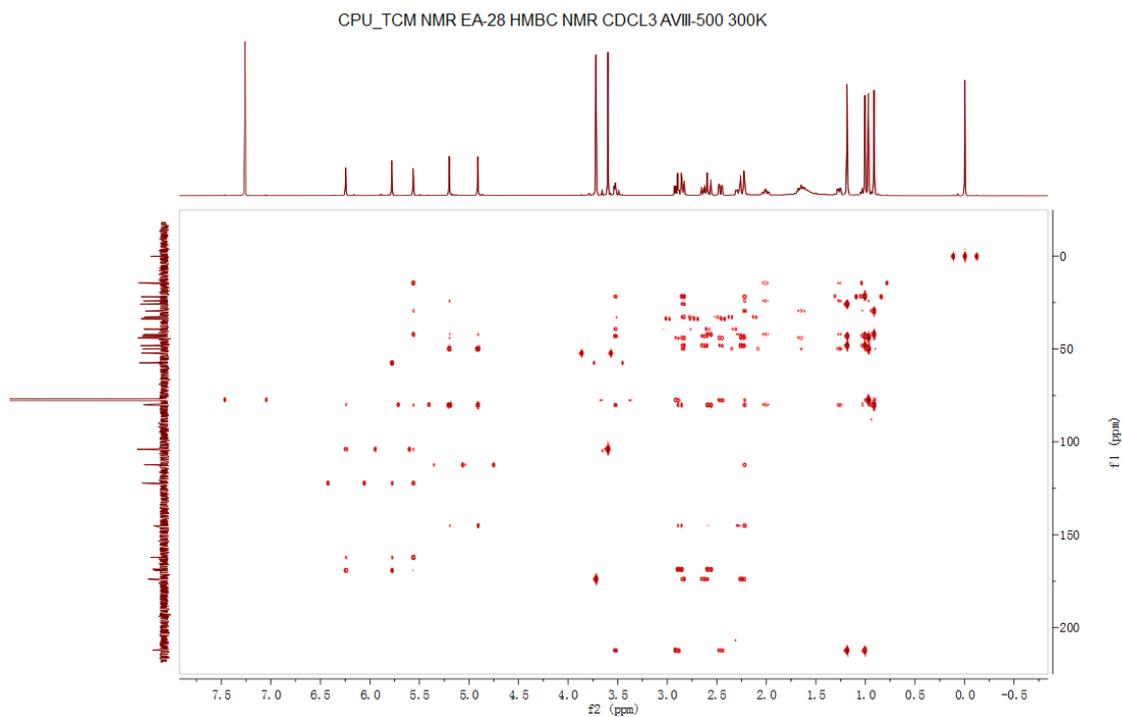


Figure S33. HMBC spectrum of **5** in CDCl₃.

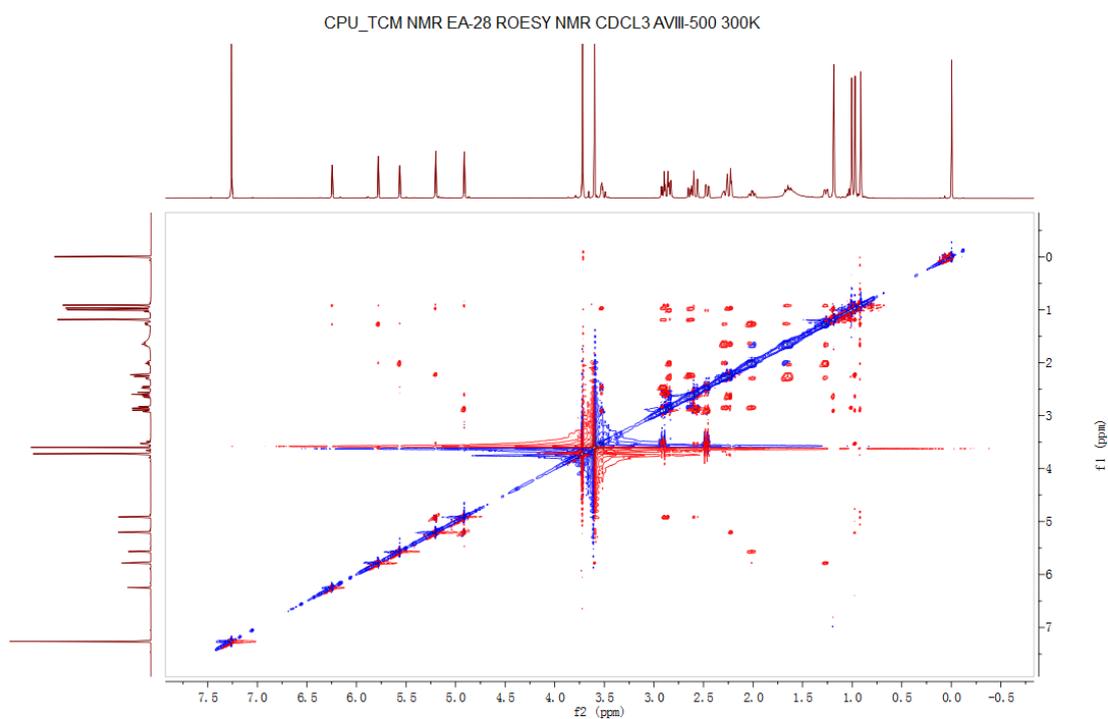
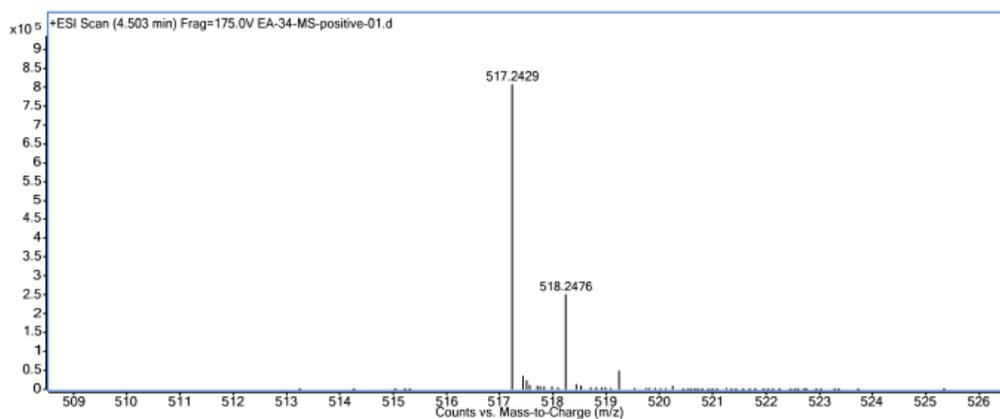


Figure S34. ROESY spectrum of **5** in CDCl₃.



Elemental Composition Calculator

Target m/z:	517.2429	Result type:	Positive ions	Species:	[M+H] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10)				
Ion Formula	Calculated m/z		PPM Error		
C28H37O9	517.2432		0.69		

Figure S35. HRESIMS spectrum of **6**.

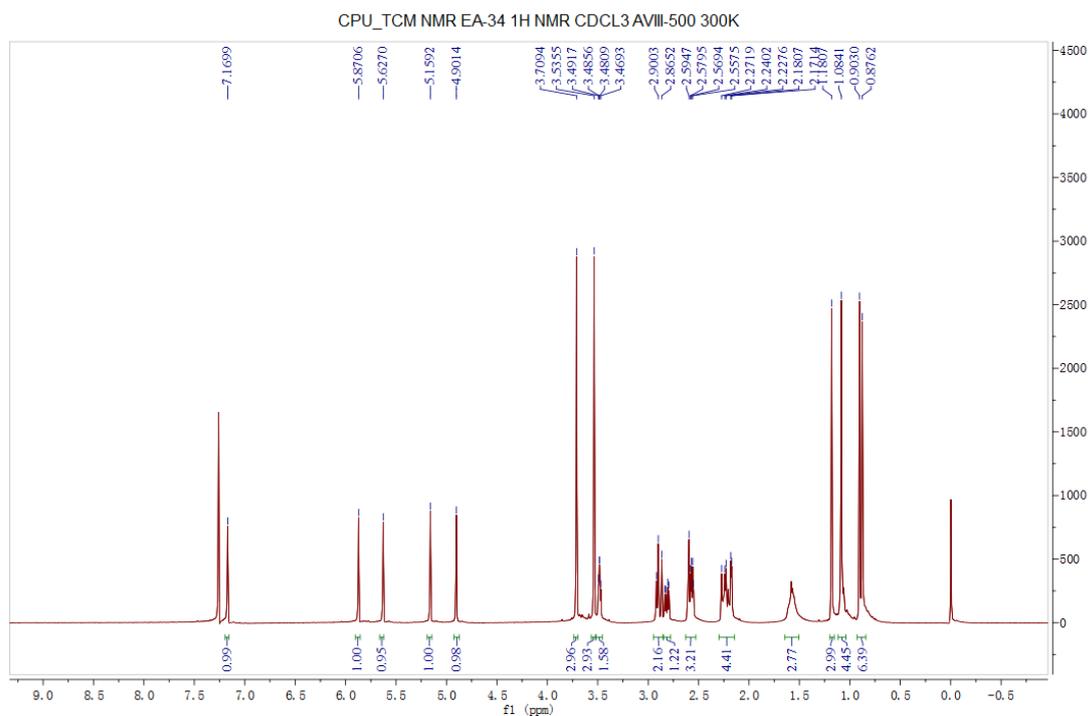
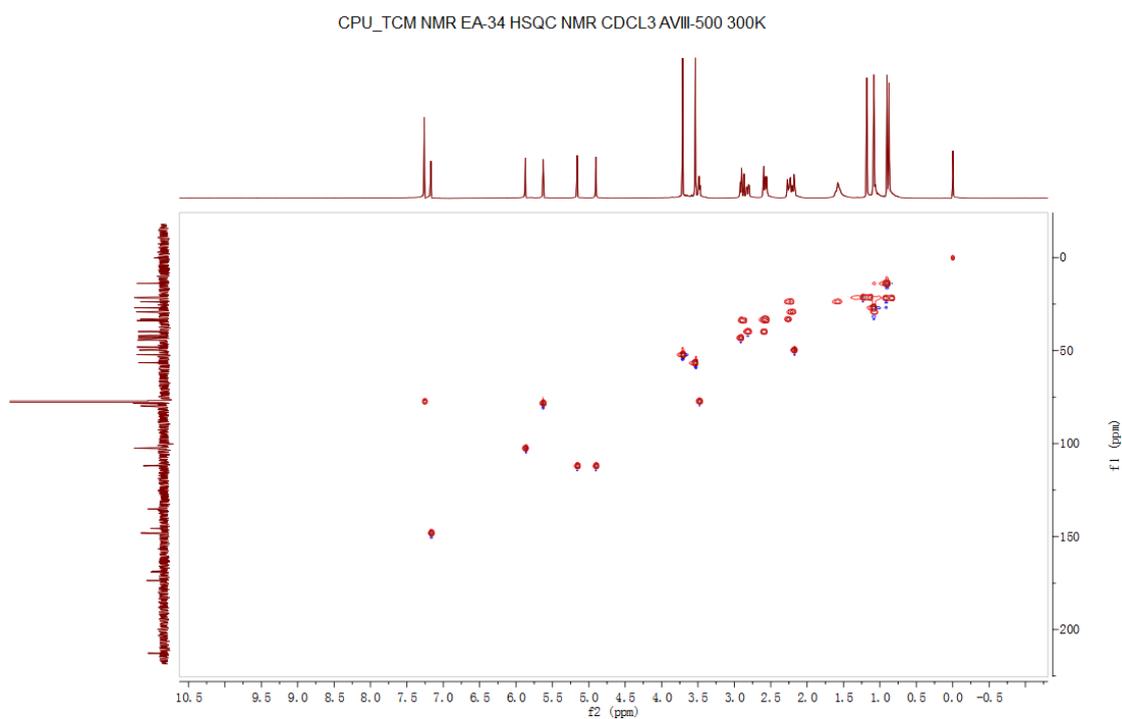
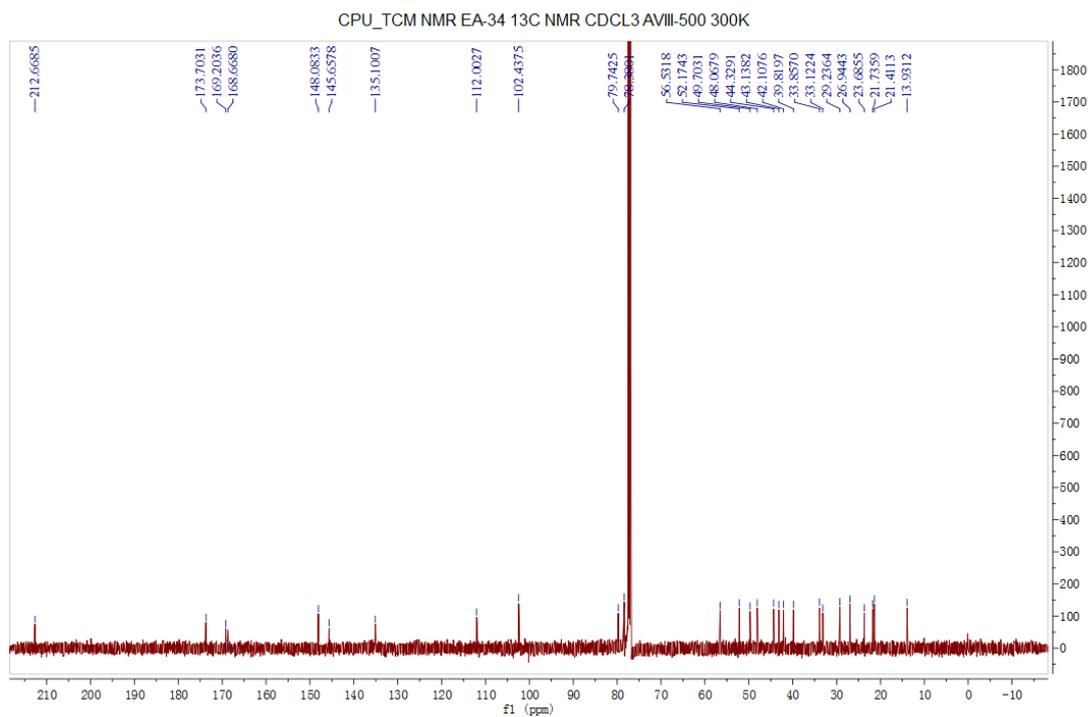
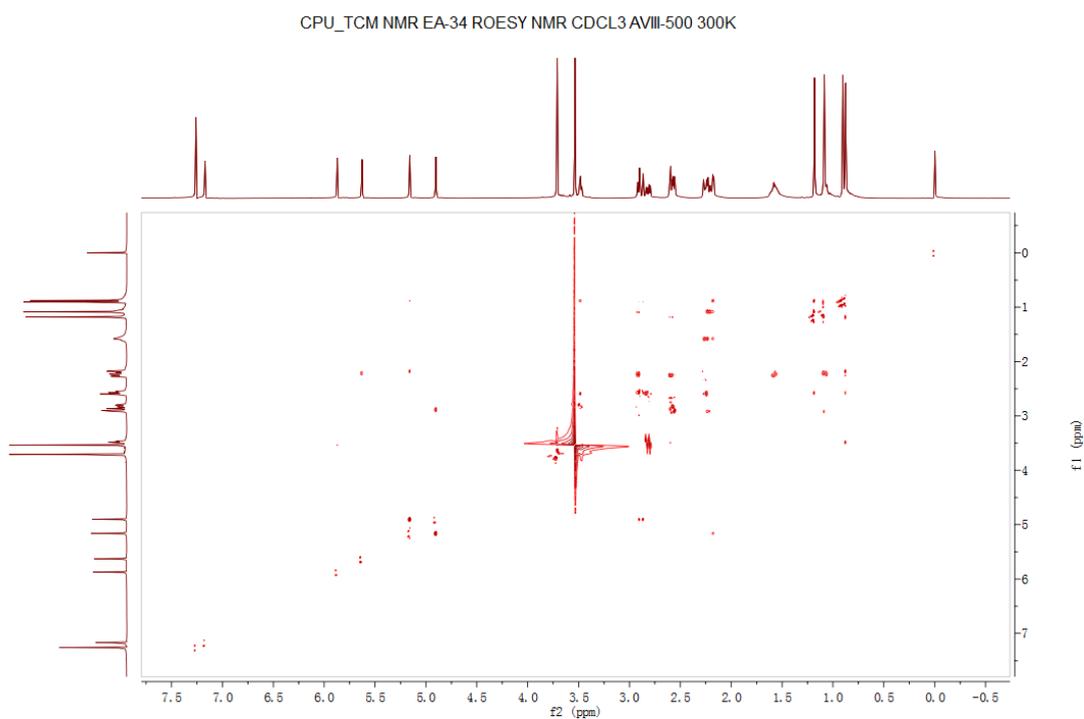
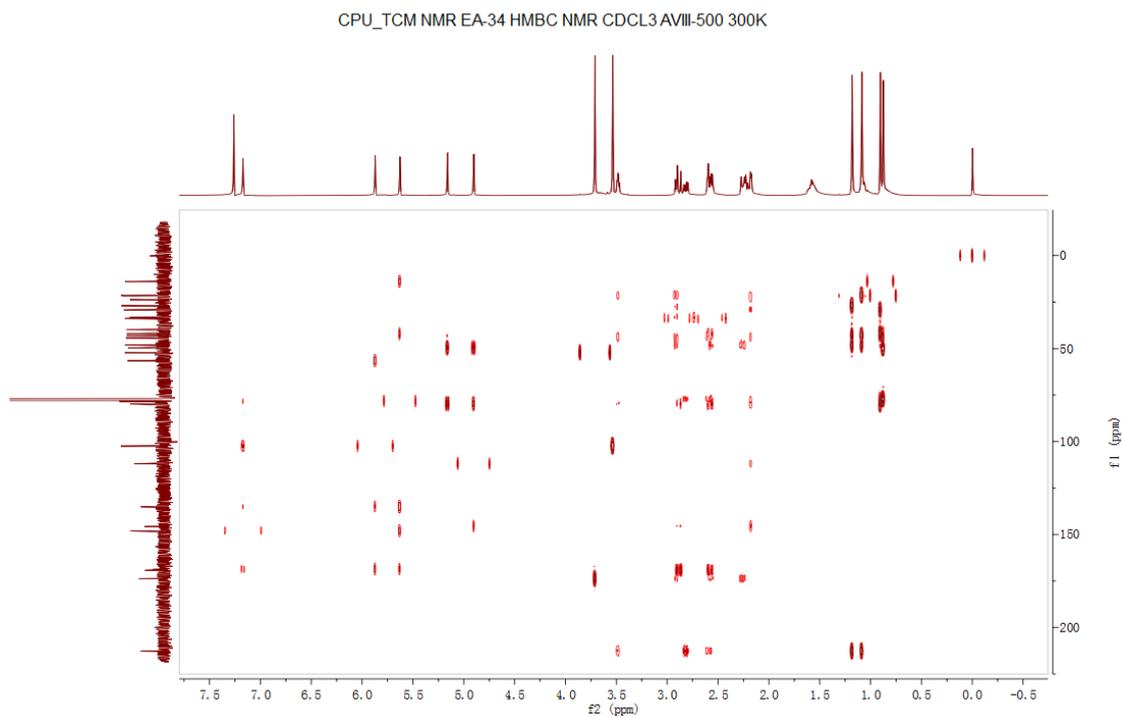
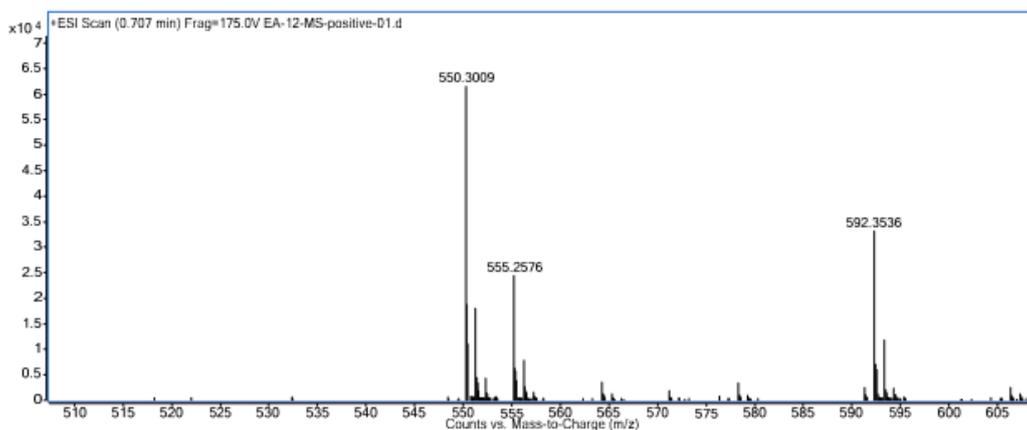


Figure S36. ¹H NMR spectrum of **6** in CDCl₃.







Elemental Composition Calculator

Target m/z:	550.3009	Result type:	Positive ions	Species:	[M+NH ₄] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₉ H ₄₄ NO ₉	550.3011		0.34		

Figure S41. HRESIMS spectrum of **7**.

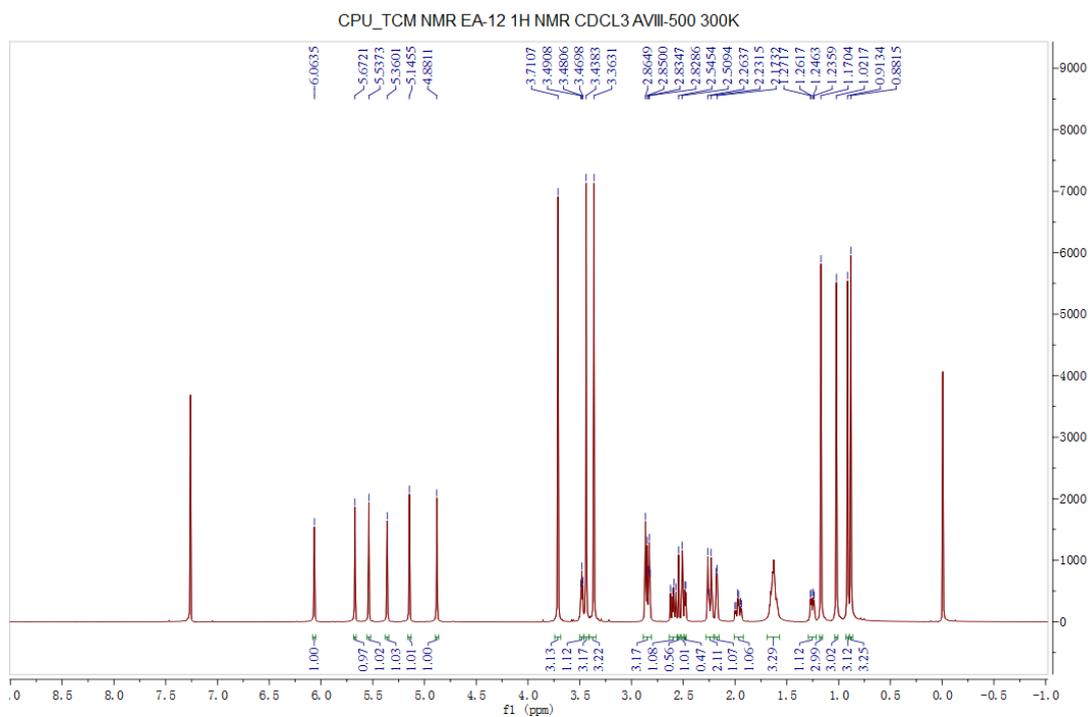


Figure S42. ¹H NMR spectrum of **7** in CDCl₃.

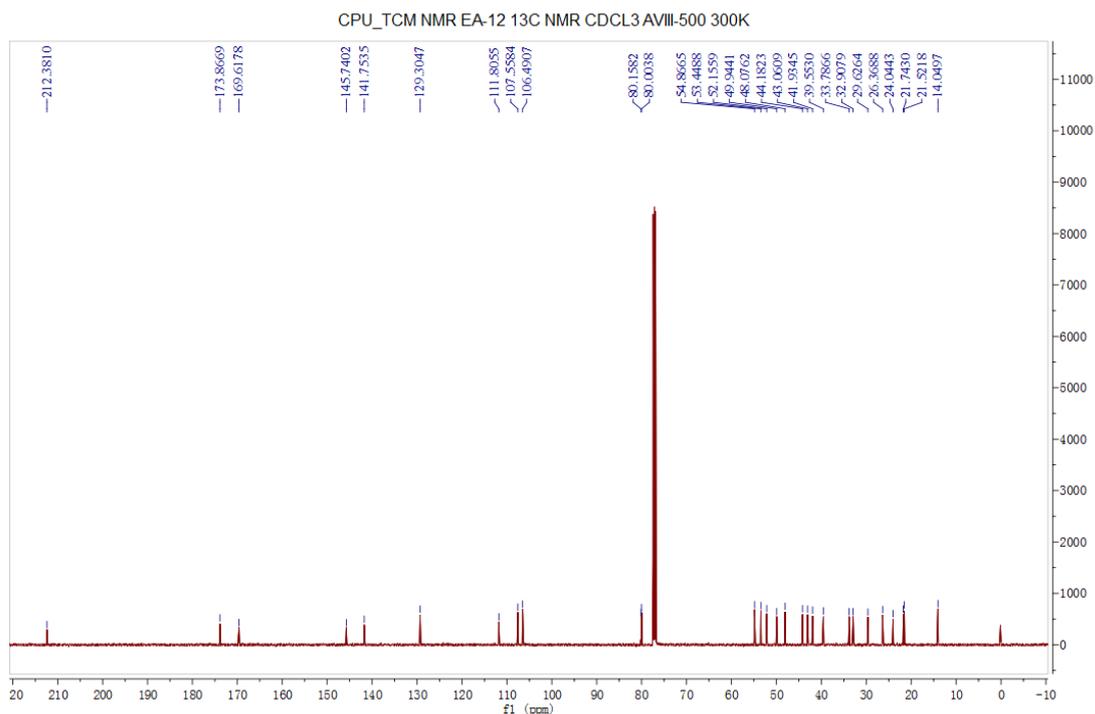


Figure S43. ¹³C NMR spectrum of **7** in CDCl₃

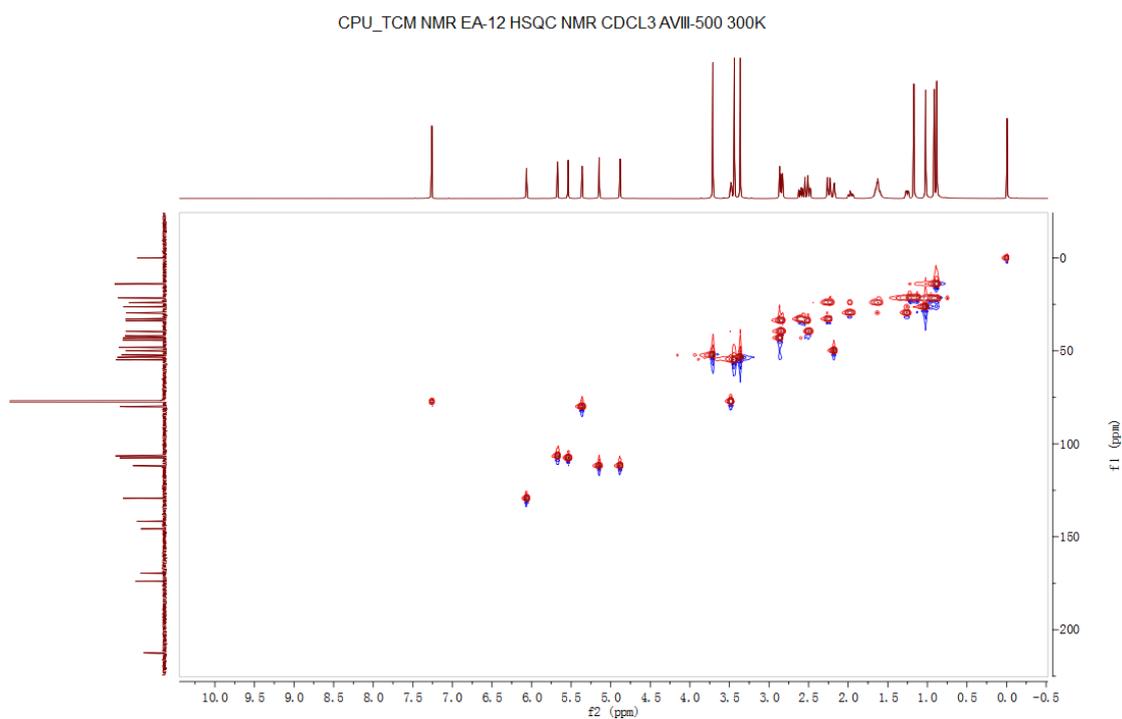


Figure S44. HSQC spectrum of **7** in CDCl₃.

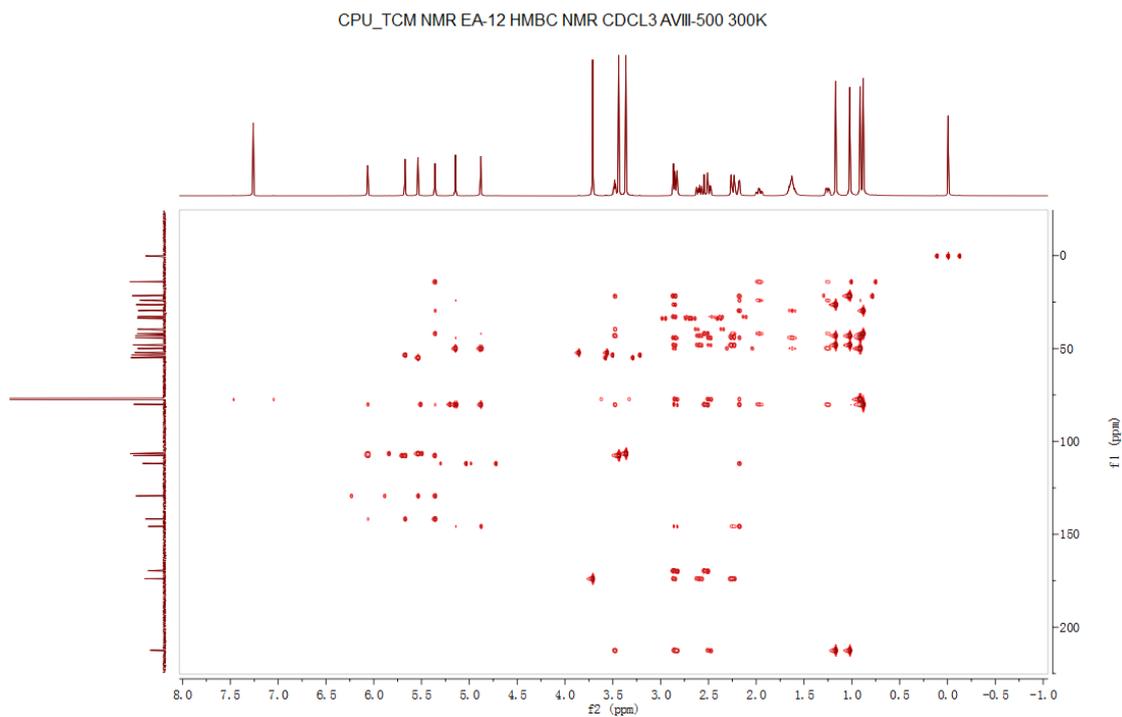


Figure S45. HMBC spectrum of **7** in CDCl₃.

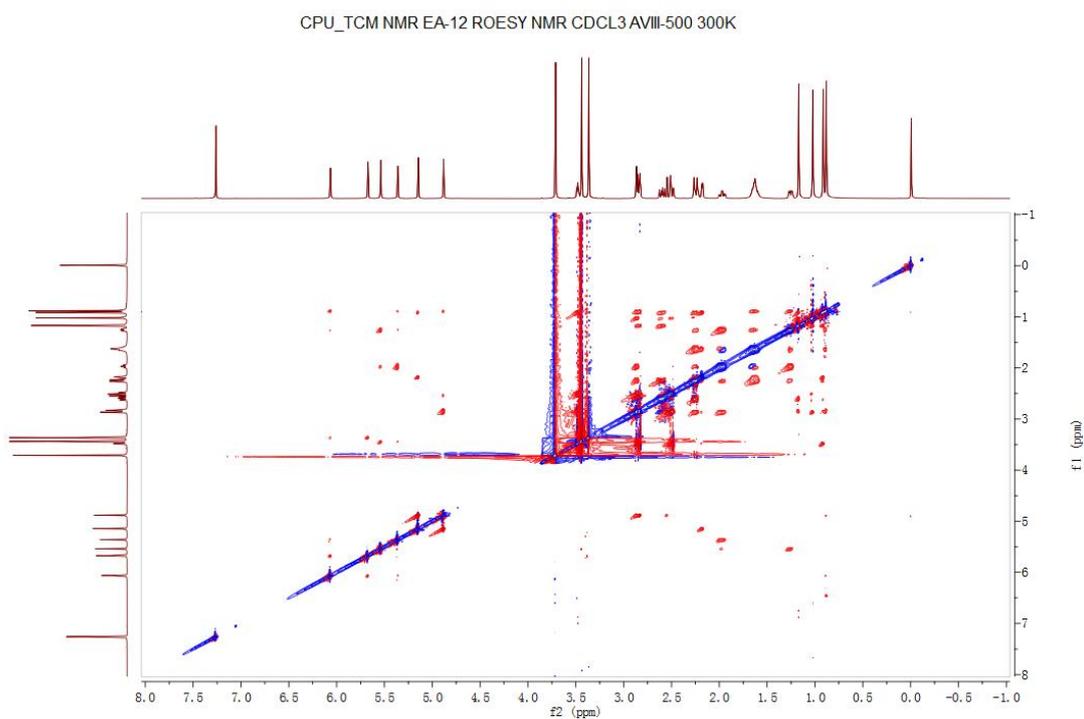
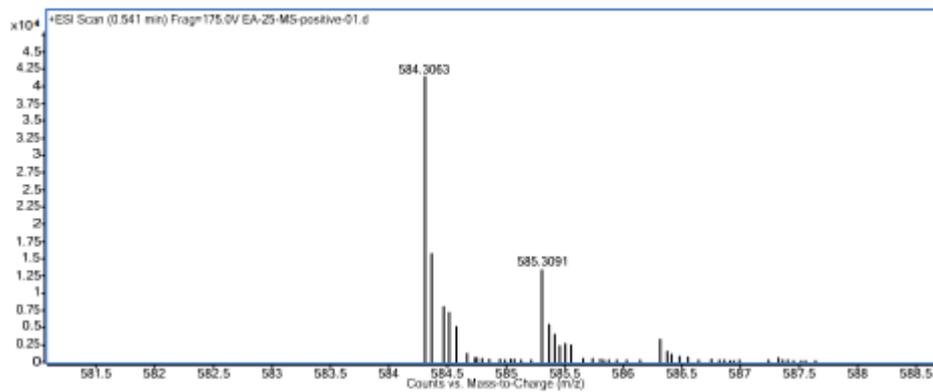


Figure S46. ROESY spectrum of **7** in CDCl₃.



Elemental Composition Calculator

Target m/z:	584.3063	Result type:	Positive ions	Species:	[M+NH4] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₉ H ₄₆ N ₁ O ₁₁	584.3065		0.33		

Figure S47. HRESIMS spectrum of **8**.

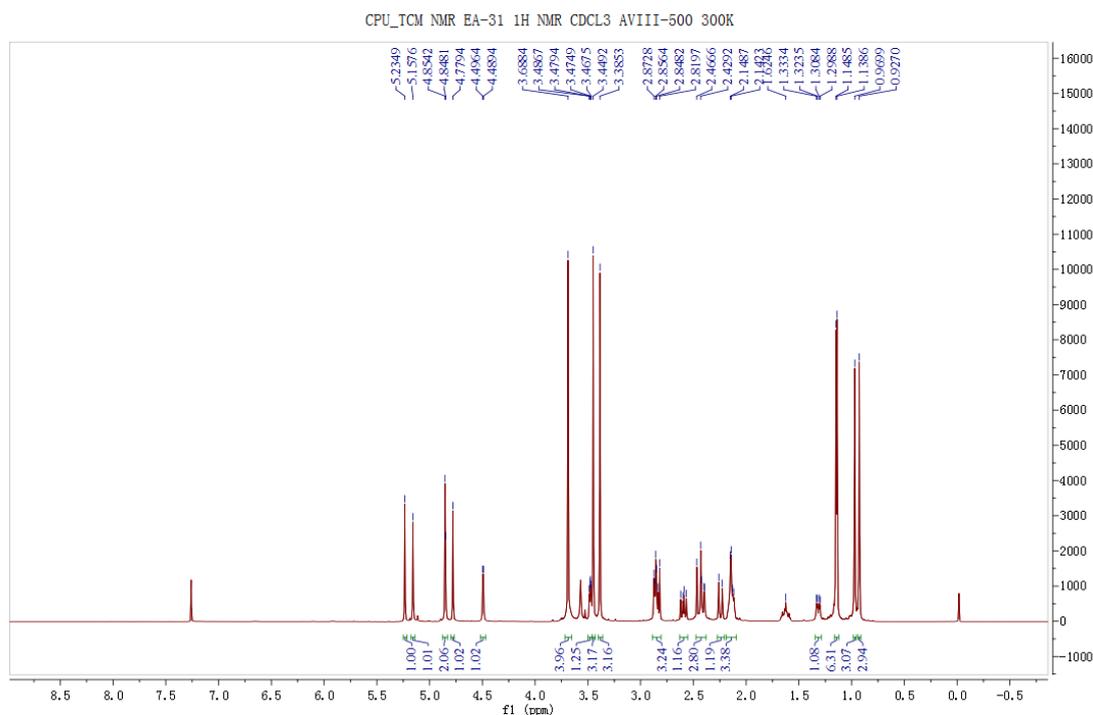


Figure S48. ¹H NMR spectrum of **8** in CDCl₃

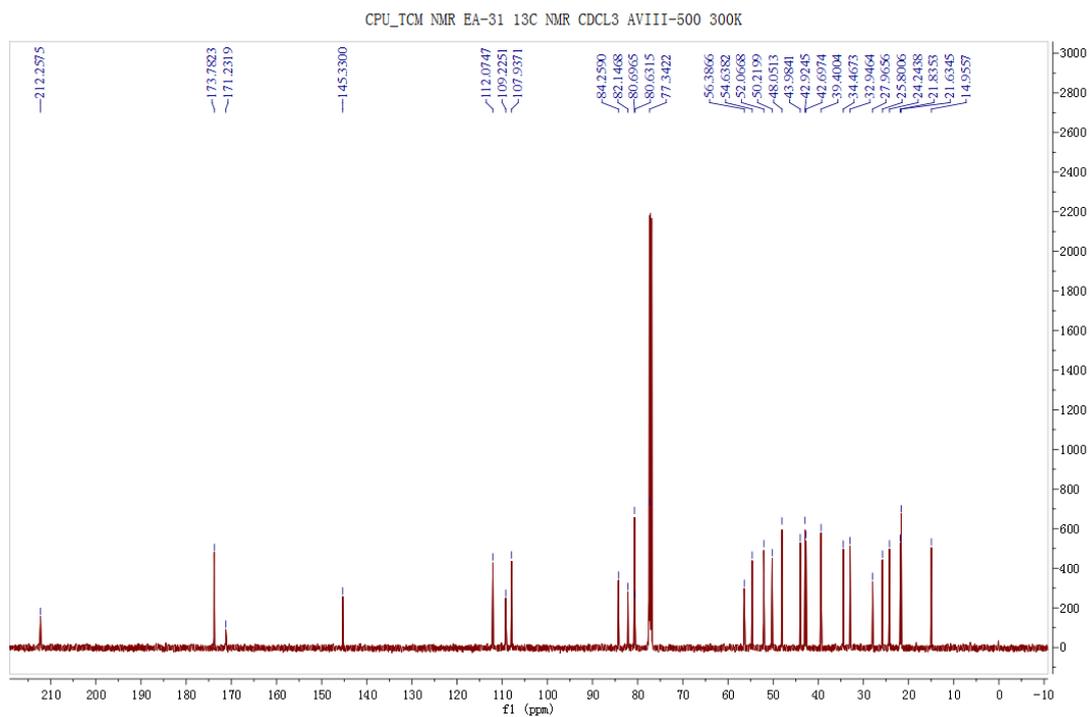


Figure S49. ^{13}C NMR spectrum of **8** in CDCl_3

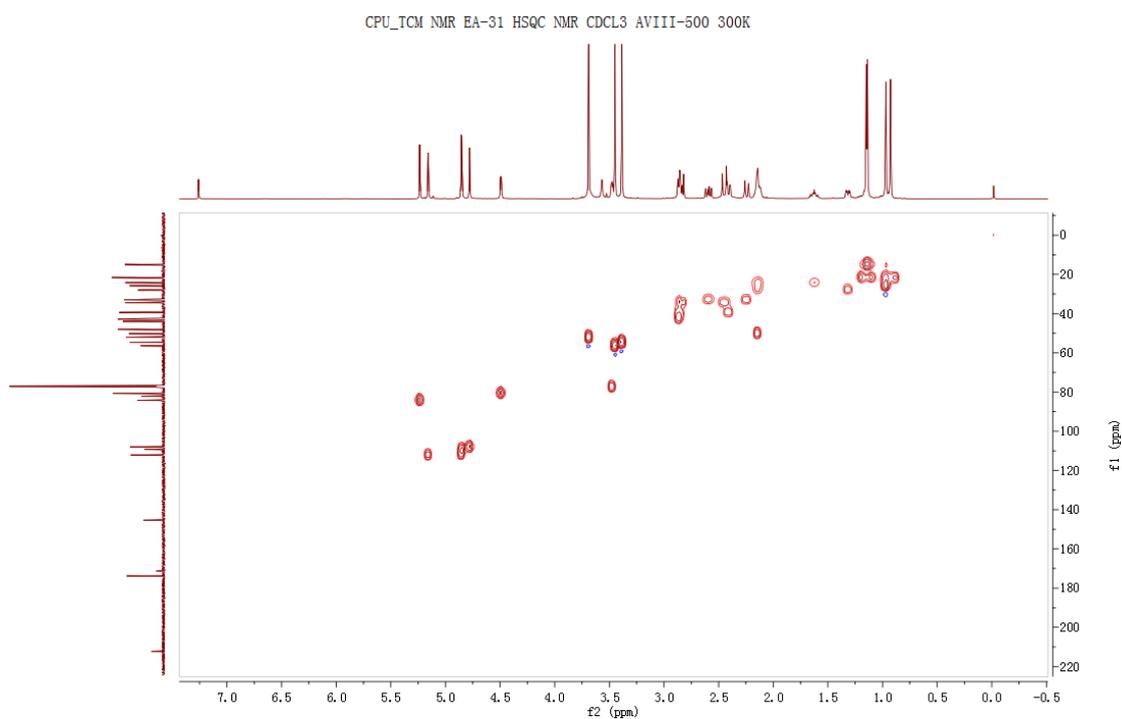


Figure S50. HSQC spectrum of **8** in CDCl_3

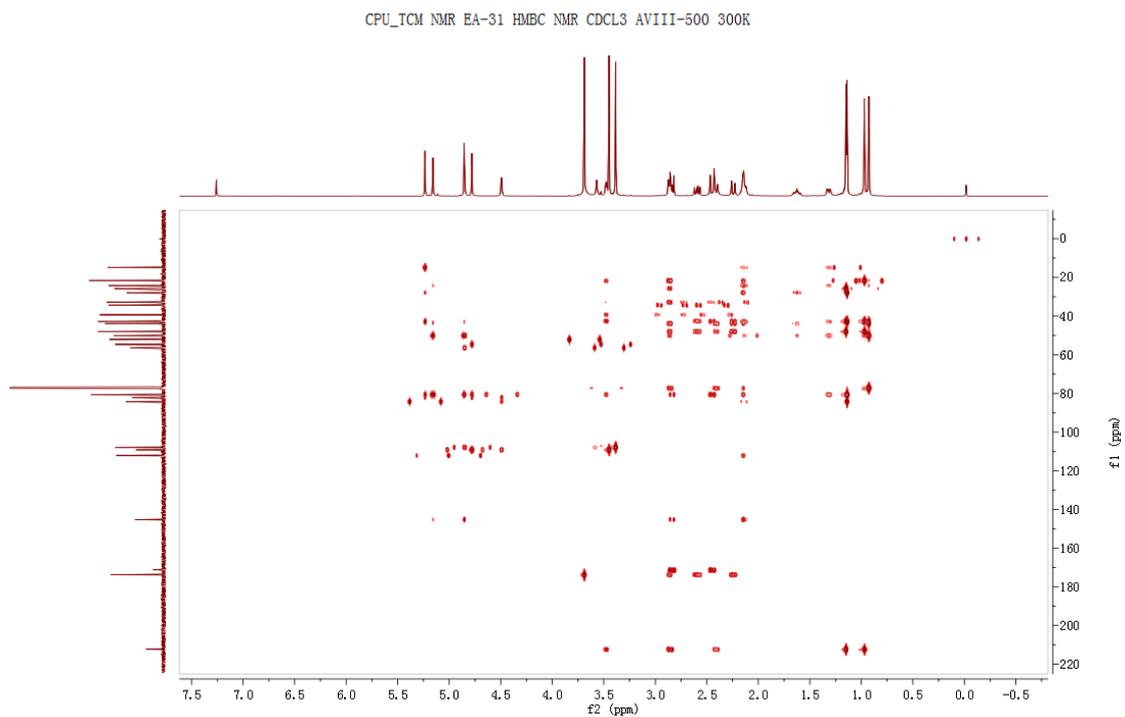


Figure S51. HMBC spectrum of **8** in CDCl₃.

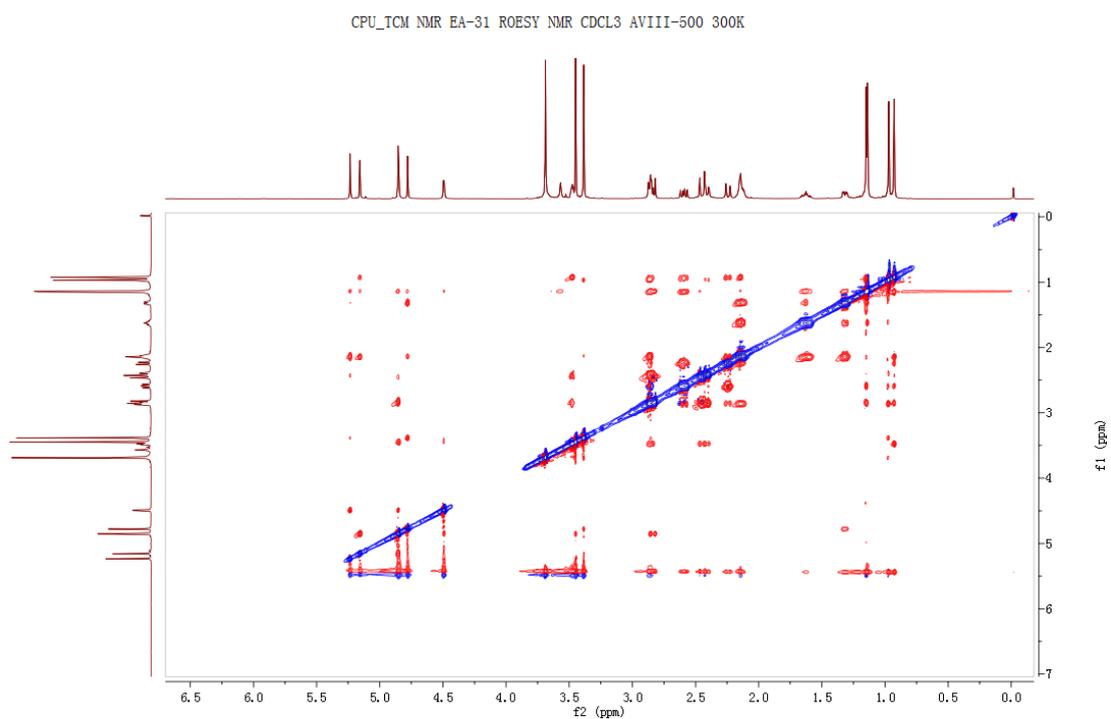
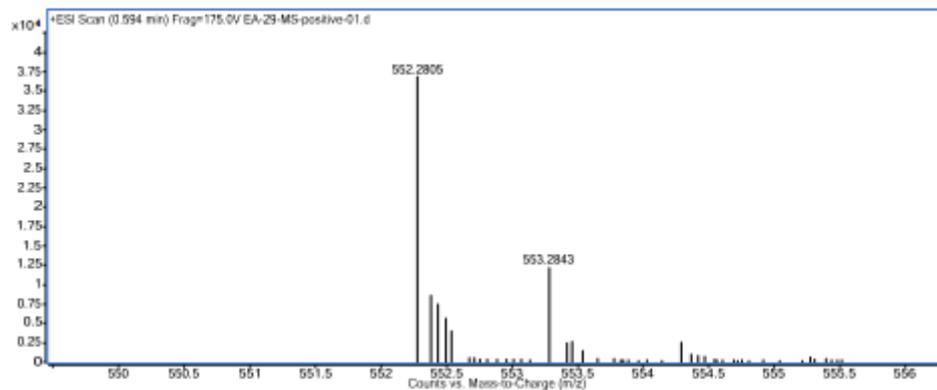


Figure S52. ROESY spectrum of **8** in CDCl₃.



Elemental Composition Calculator

Target m/z:	552.2805	Result type:	Positive ions	Species:	[M+NH4] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10)				
Ion Formula	Calculated m/z		PPM Error		
C28H42NO10	552.2803		-0.34		

Figure S53. HRESIMS spectrum of **9**

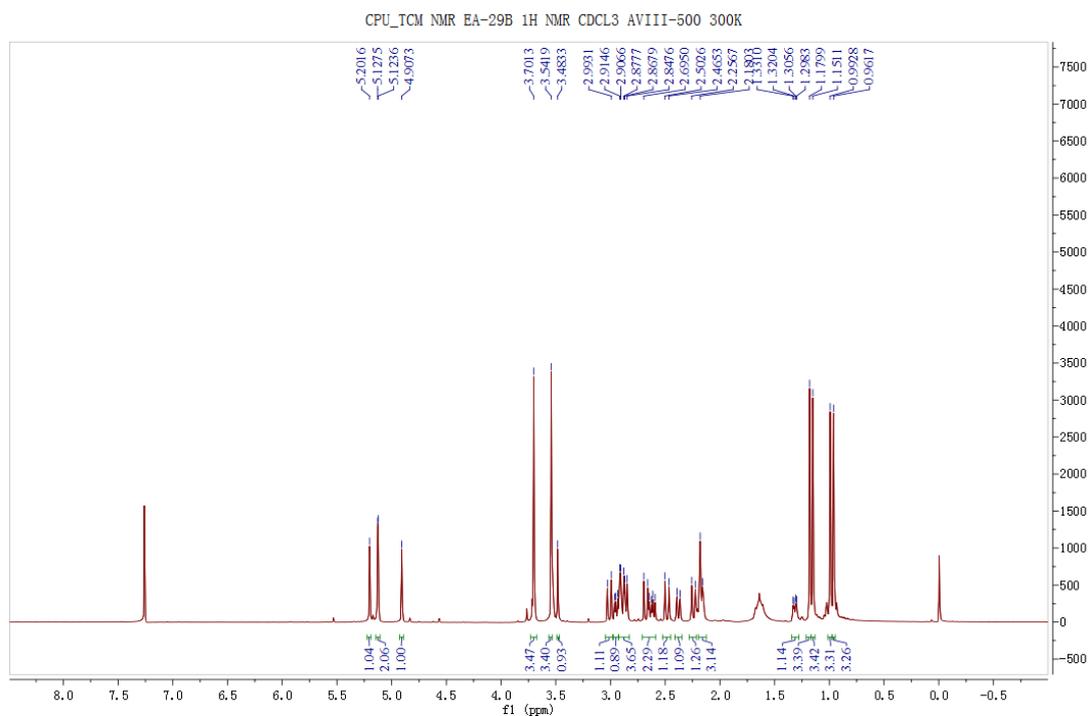
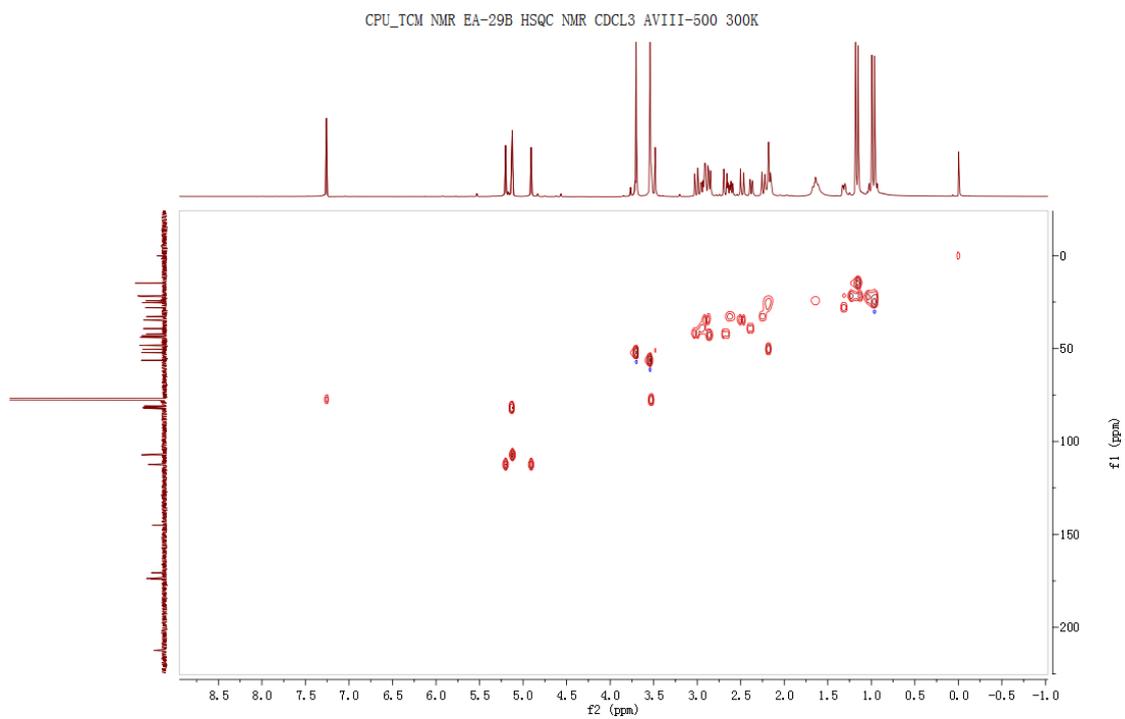
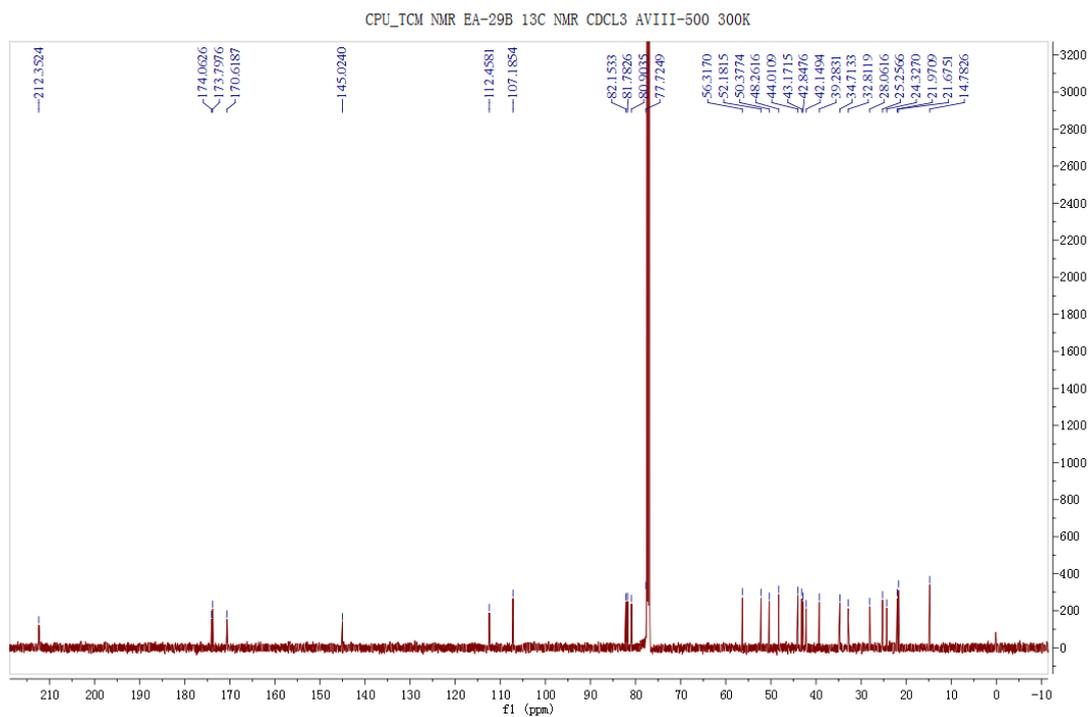


Figure S54. ¹H NMR spectrum of **9** in CDCl₃



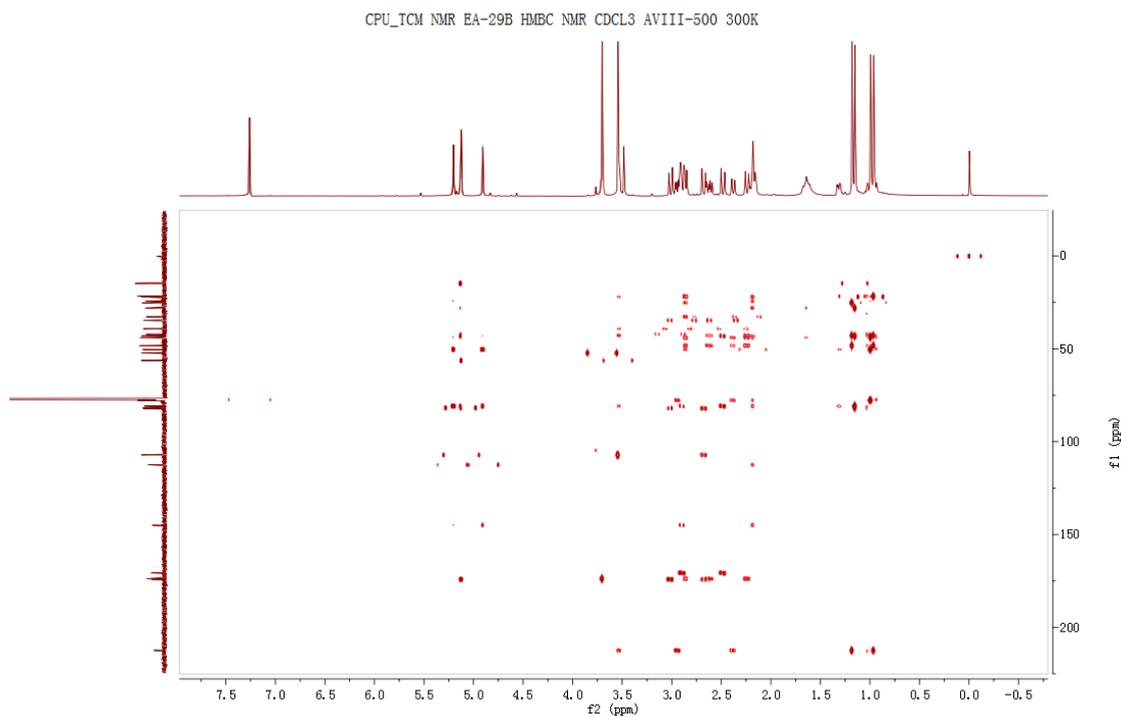


Figure S57. HMBC spectrum of **9** in CDCl₃.

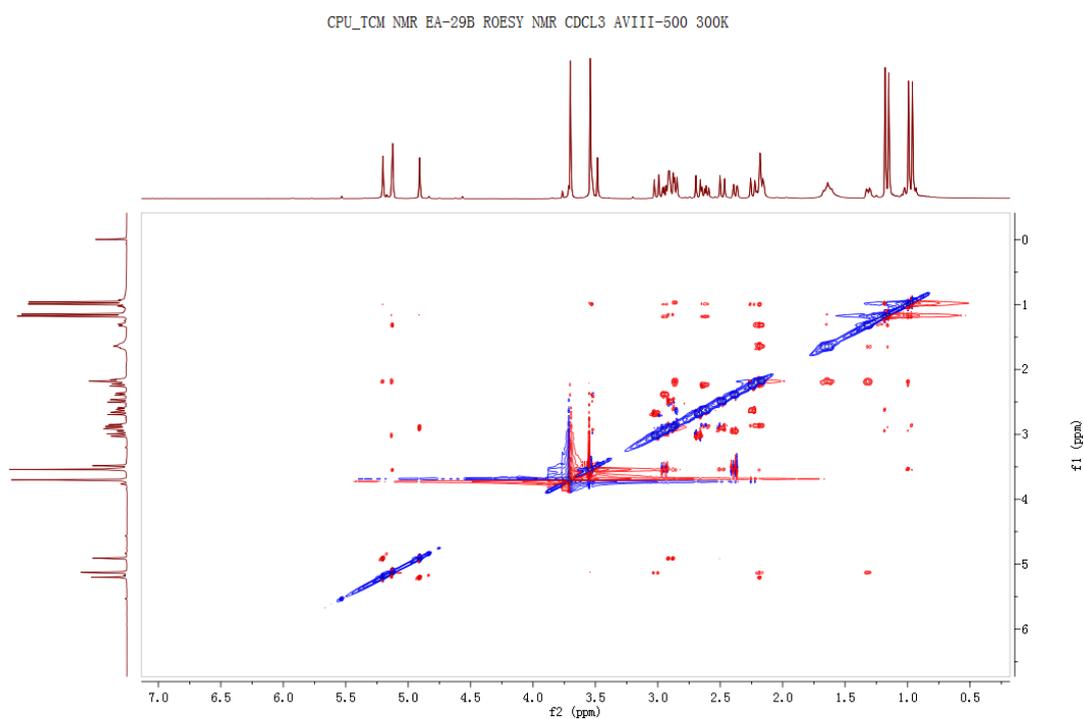
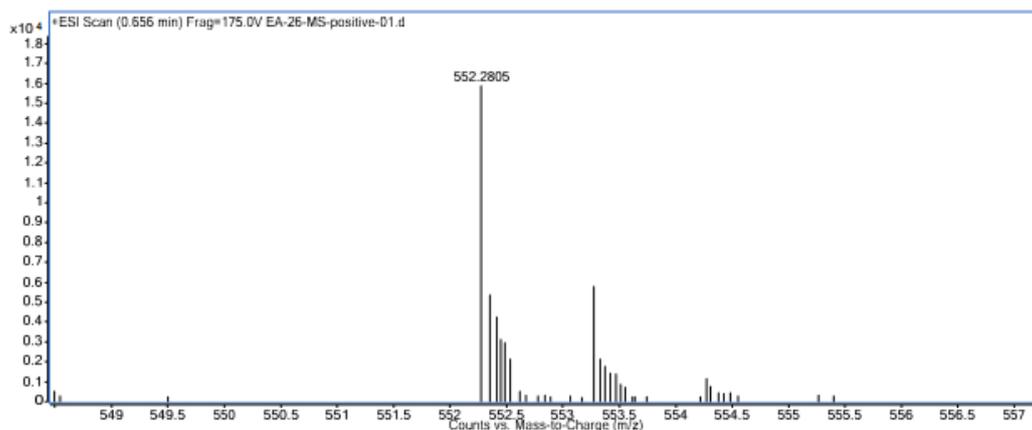


Figure S58. ROESY spectrum of **9** in CDCl₃.



Elemental Composition Calculator

Target m/z:	552.2805	Result type:	Positive ions	Species:	[M+NH ₄] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₈ H ₄₂ N ₁₀ O	552.2803		-0.26		

Figure S59. HRESIMS spectrum of **10**.

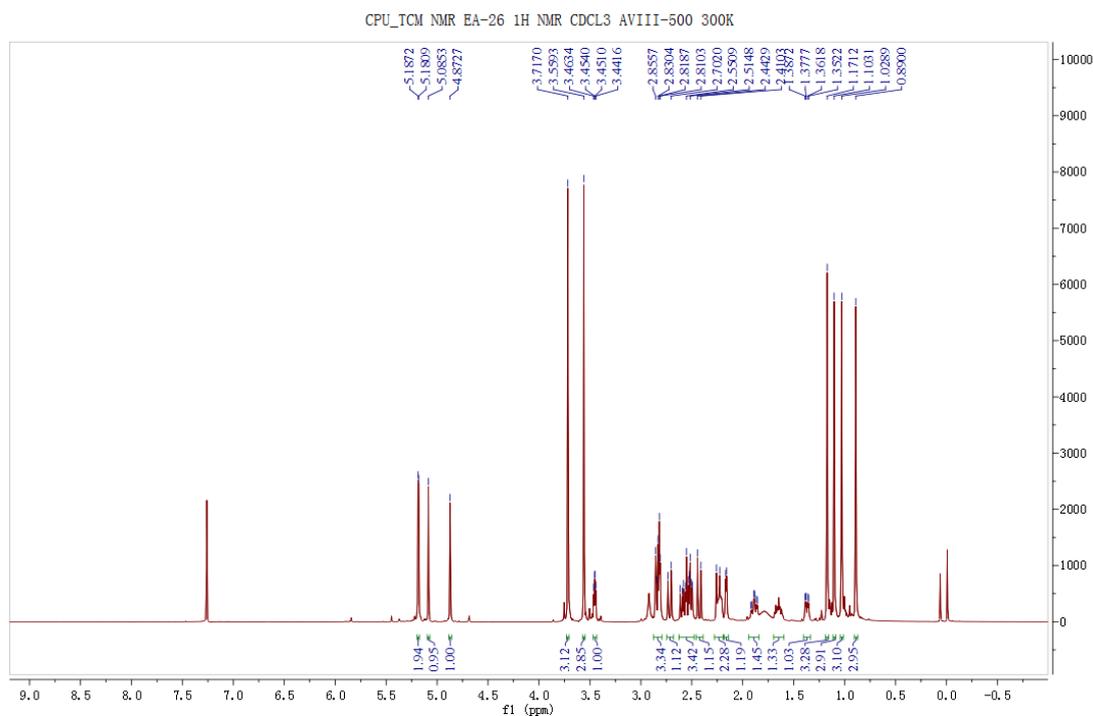


Figure S60. ¹H NMR spectrum of **10** in CDCl₃

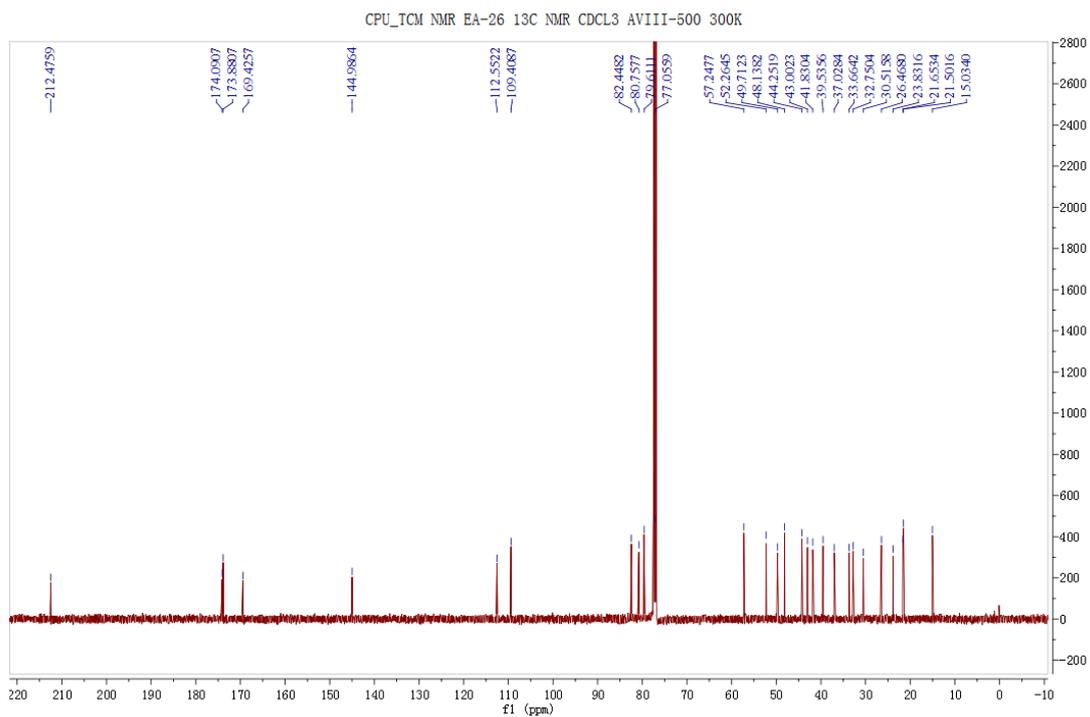


Figure S61. ^{13}C NMR spectrum of **10** in CDCl_3

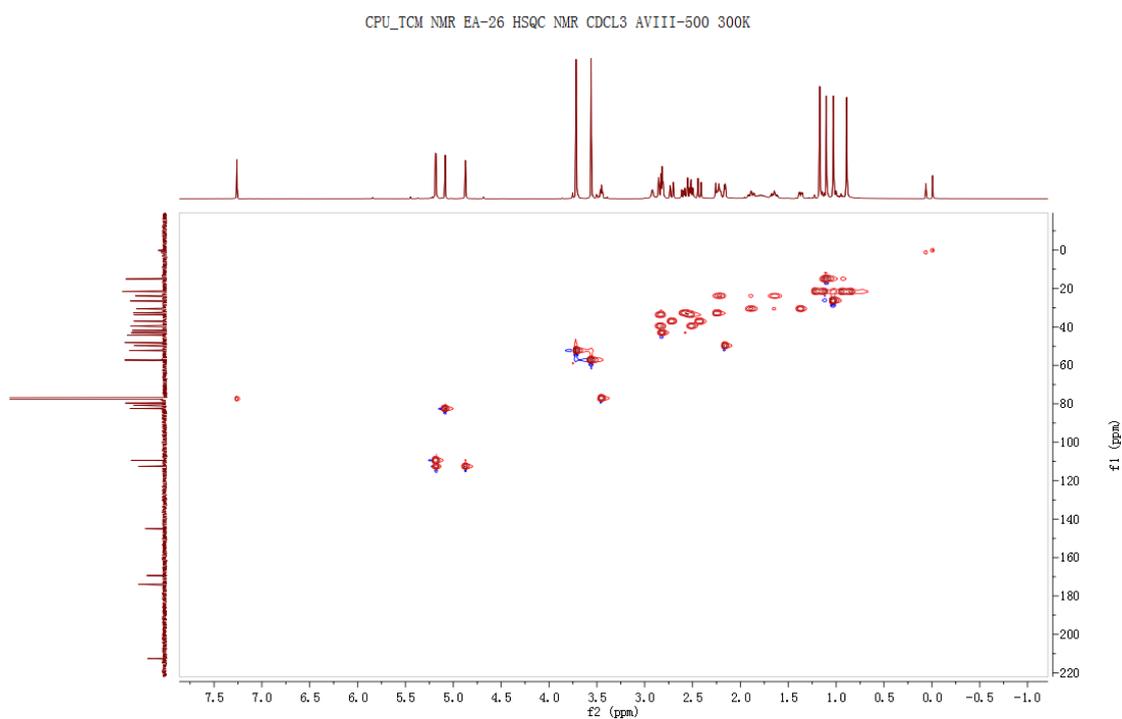


Figure S62. HSQC spectrum of **10** in CDCl_3

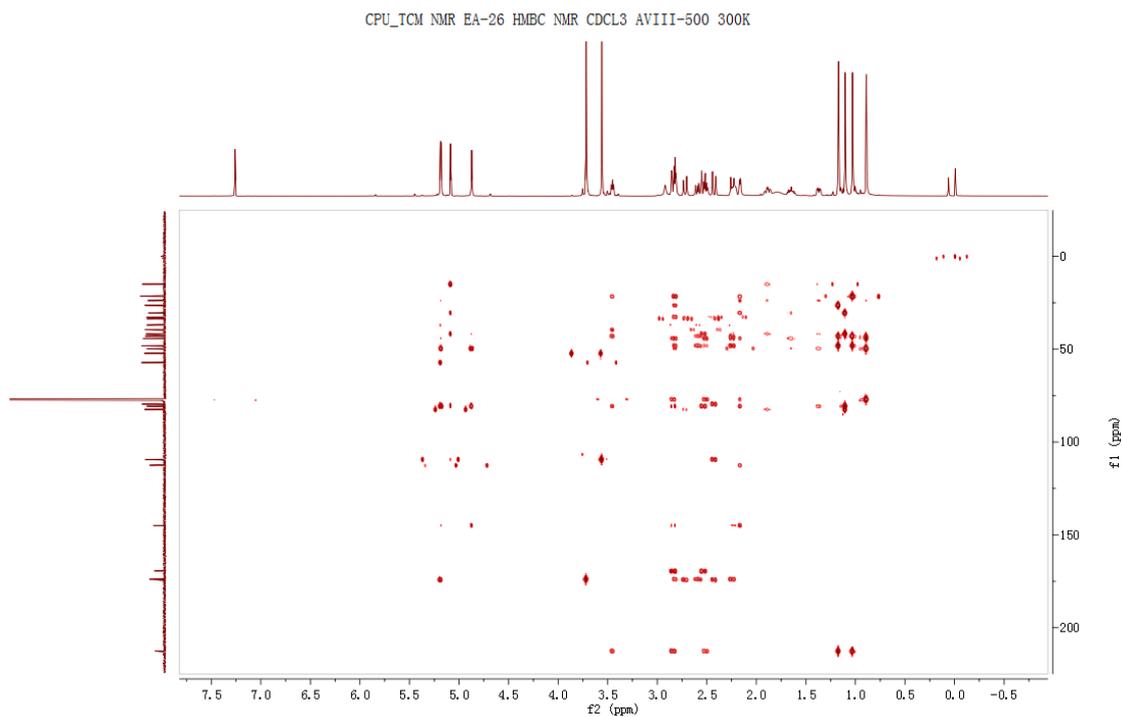


Figure S63. HMBC spectrum of **10** in CDCl₃

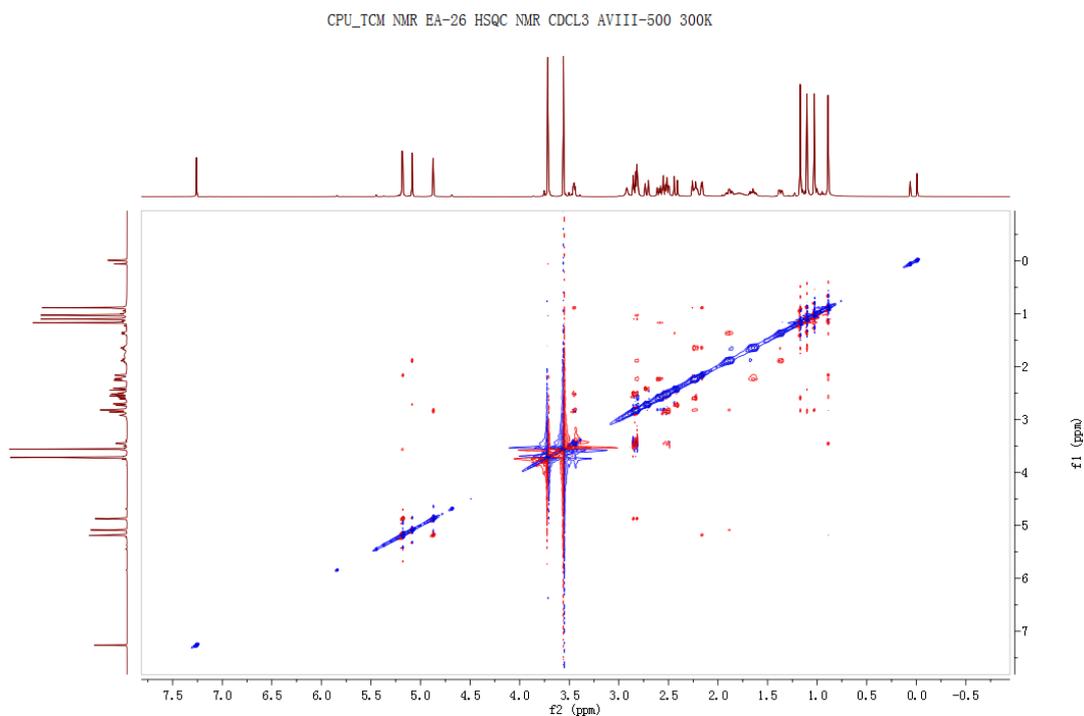
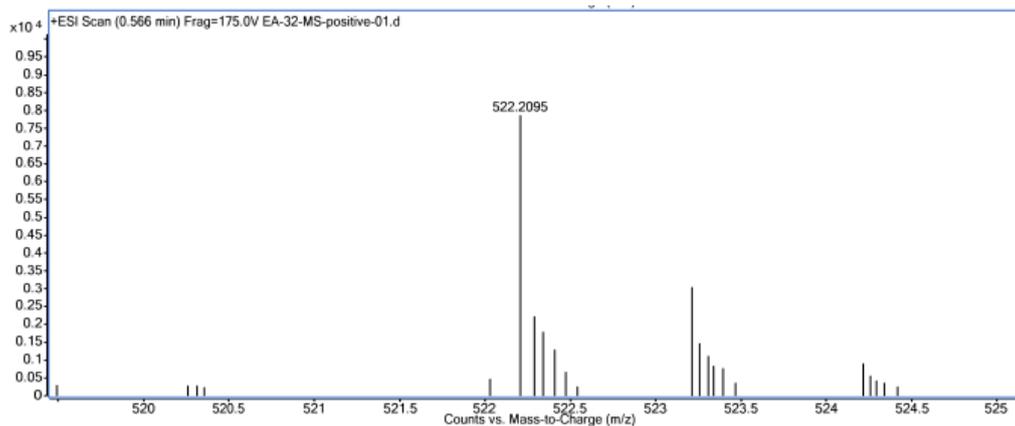


Figure S64. ROESY spectrum of **10** in CDCl₃



Elemental Composition Calculator

Target m/z:	522.2095	Result type:	Positive ions	Species:	[M+Na] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N (0-10)Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₇ H ₃₃ NNaO ₈	522.2098		0.70		

Figure S65. HRESIMS spectrum of **11**.

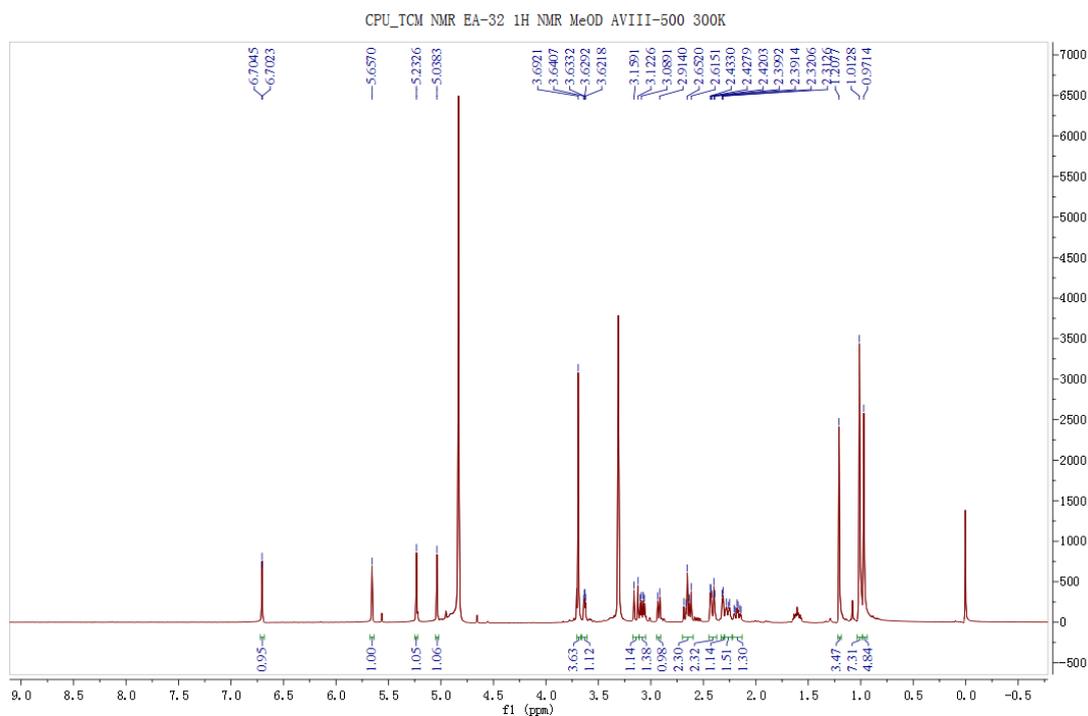


Figure S66. ¹H NMR spectrum of **11** in CD₃OD

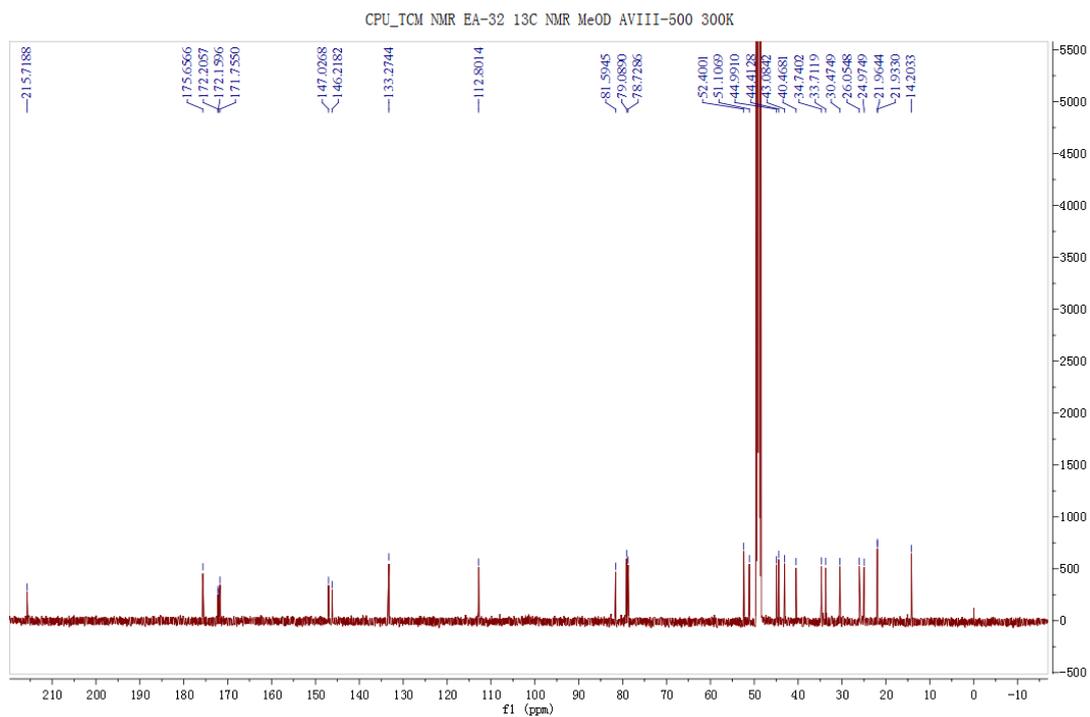


Figure S67. ^{13}C NMR spectrum of **11** in CD_3OD

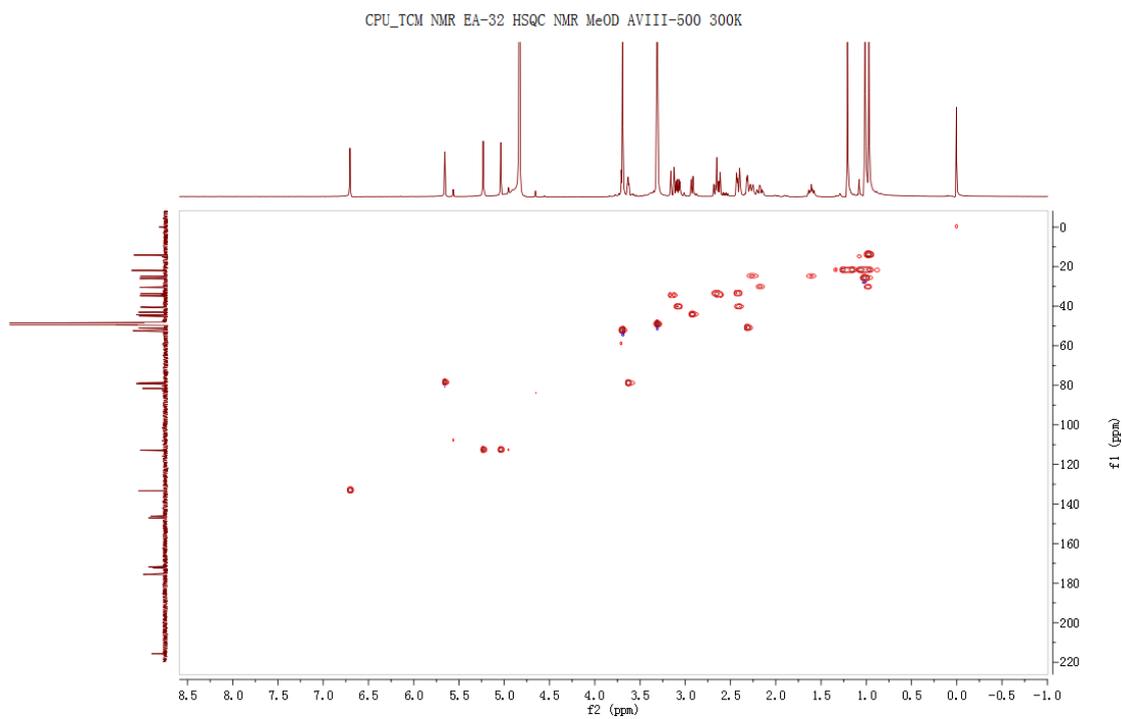


Figure S68. HSQC spectrum of **11** in CD_3OD

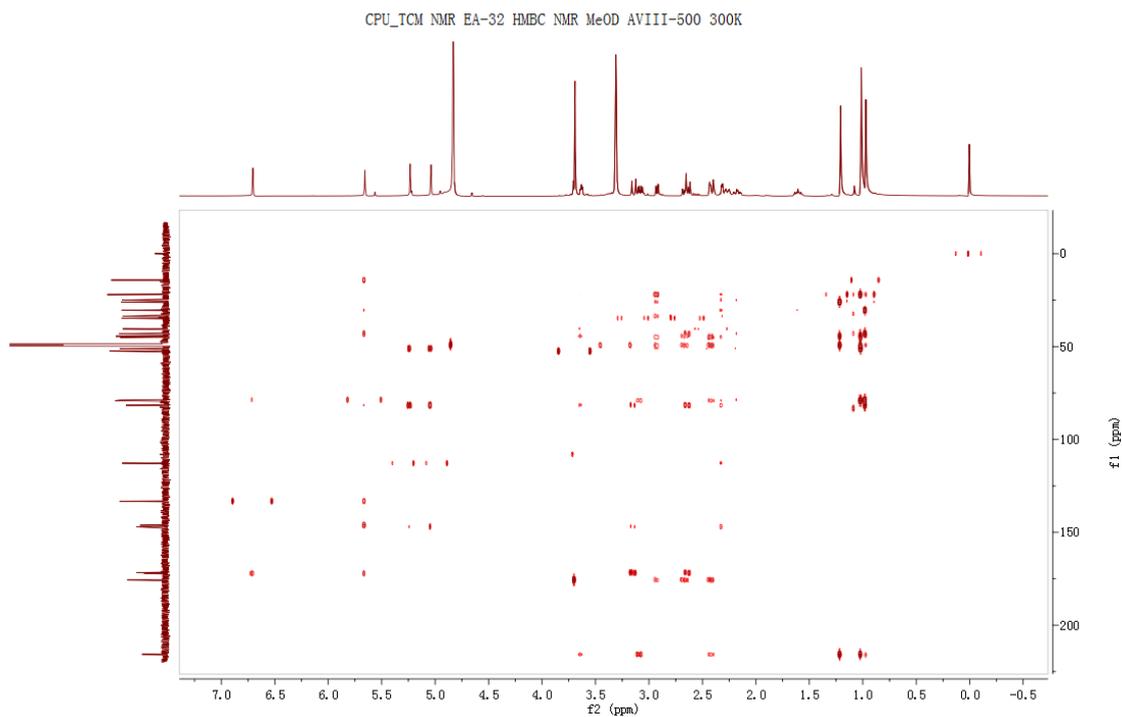


Figure S69. HMBC spectrum of **11** in CD₃OD

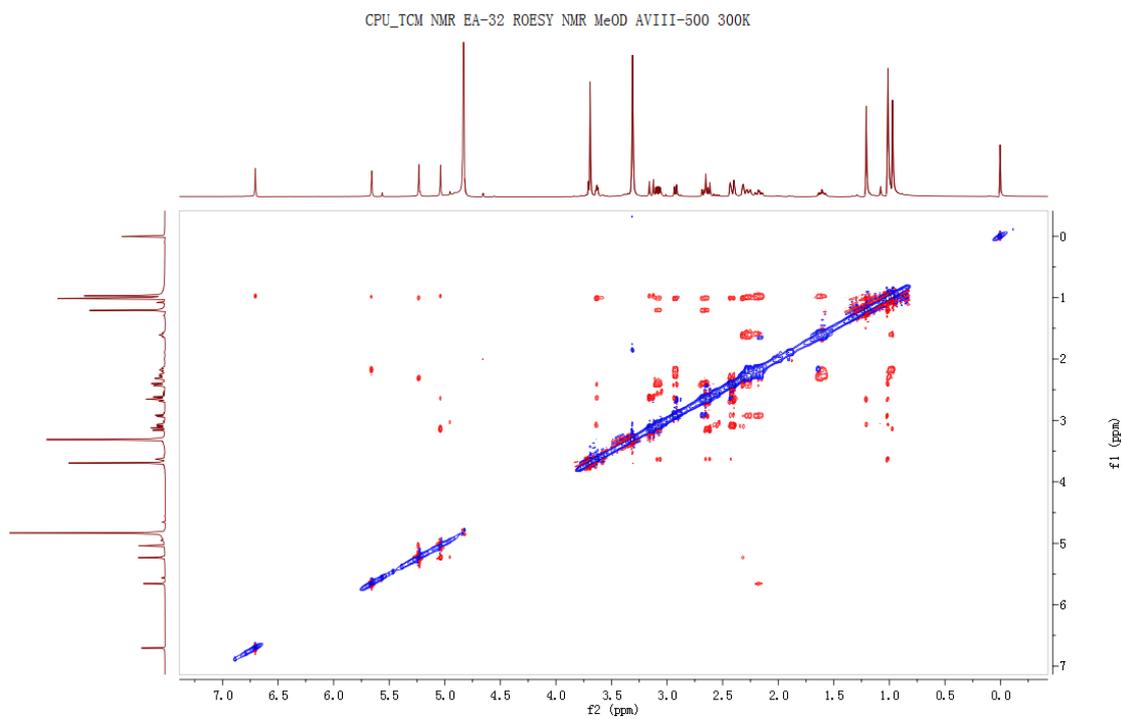
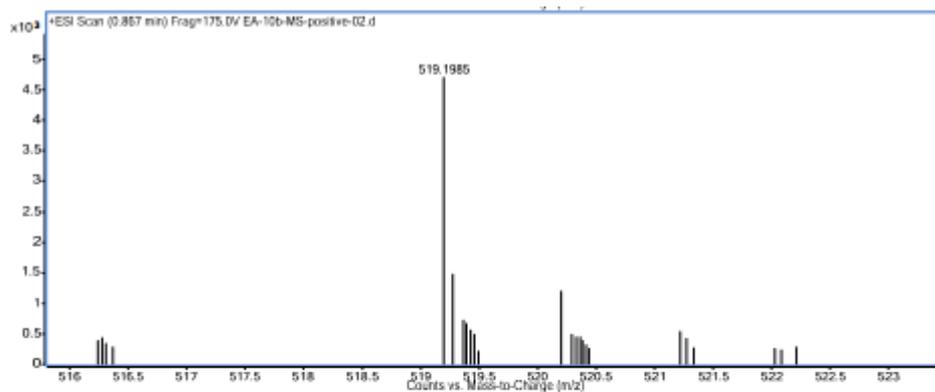


Figure S70. ROESY spectrum of **11** in CD₃OD



Elemental Composition Calculator

Target m/z:	519.1985	Result type:	Positive ions	Species:	[M+Na] ⁺
Elements:	C (0-80); H (0-120); O (0-30); Na (0-5)				
Ion Formula	Calculated m/z	PPM Error			
C ₂₈ H ₃₂ NaO ₈	519.1989	0.85			

Figure S71. HRESIMS spectrum of **12**

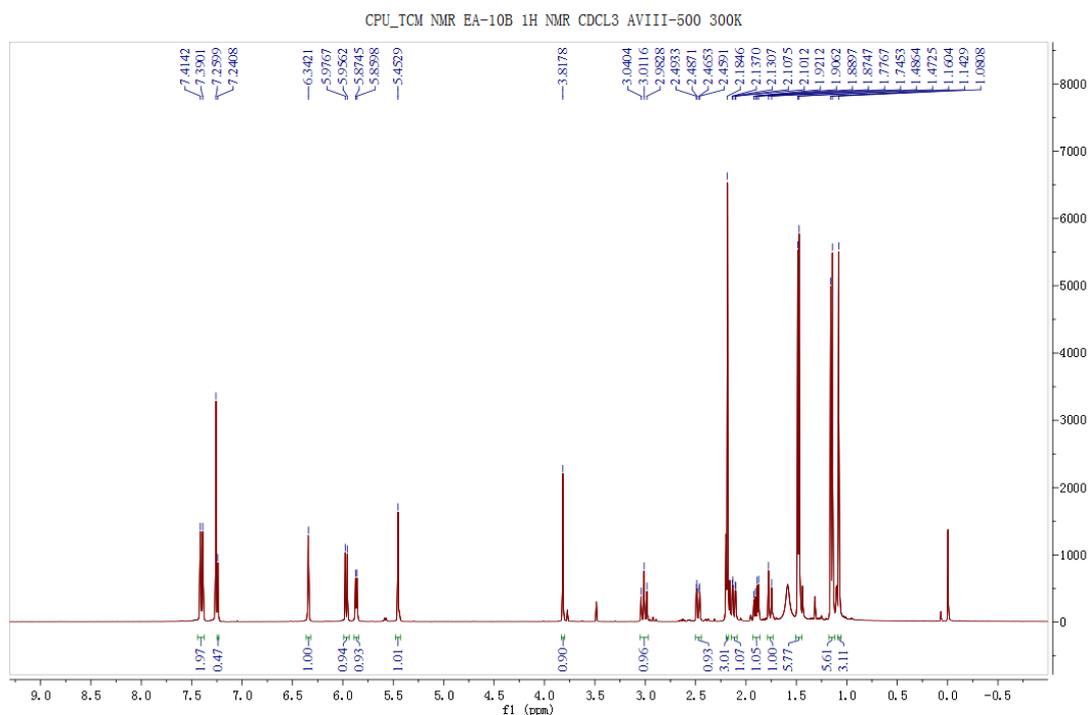


Figure S72. ¹H NMR spectrum of **12** in CDCl₃

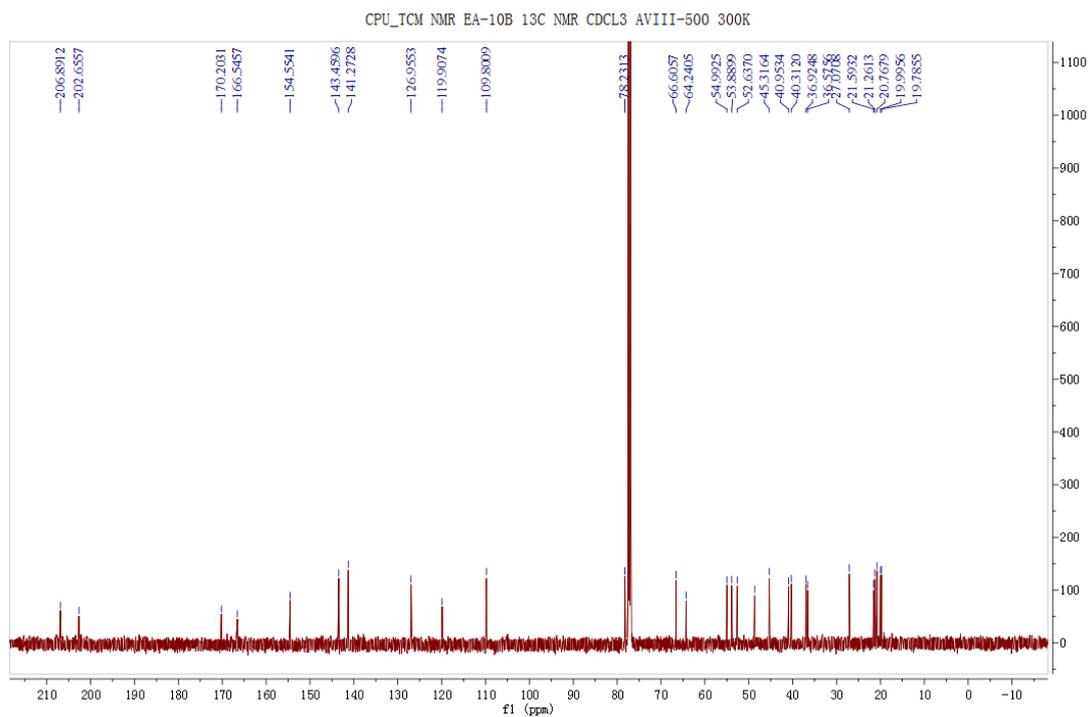


Figure S73. ^{13}C NMR spectrum of **12** in CDCl_3

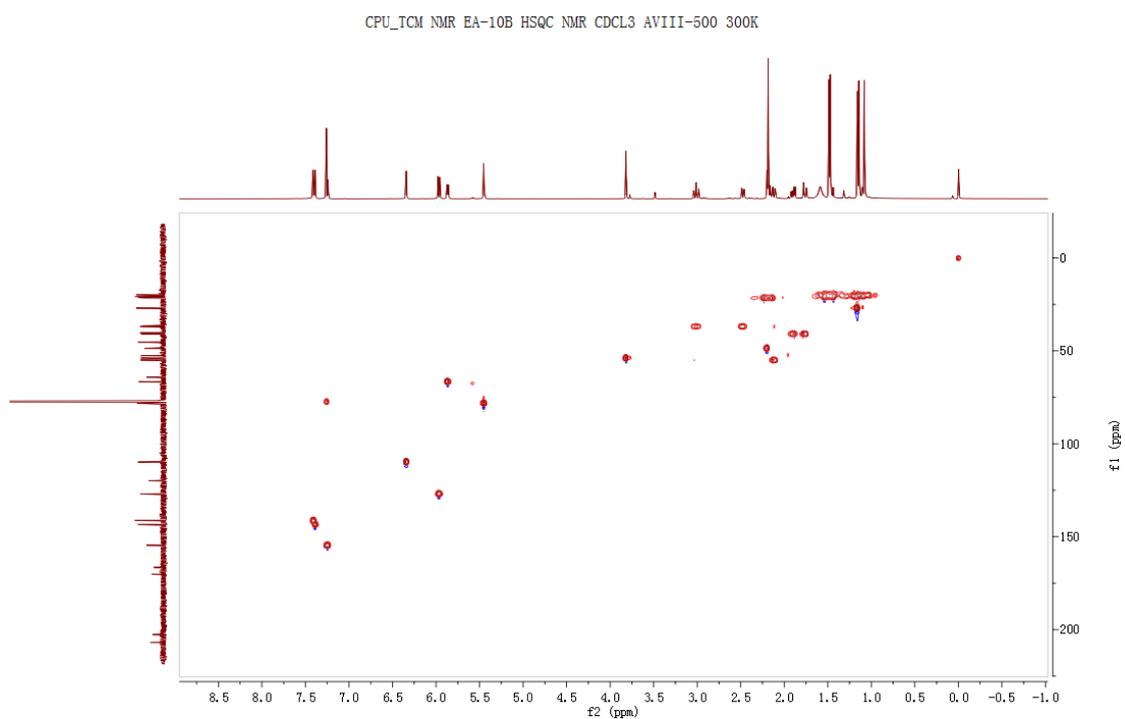


Figure S74. HSQC spectrum of **12** in CDCl_3

CPU_TCM NMR EA-10B HMBC NMR CDCL3 AVIII-500 300K

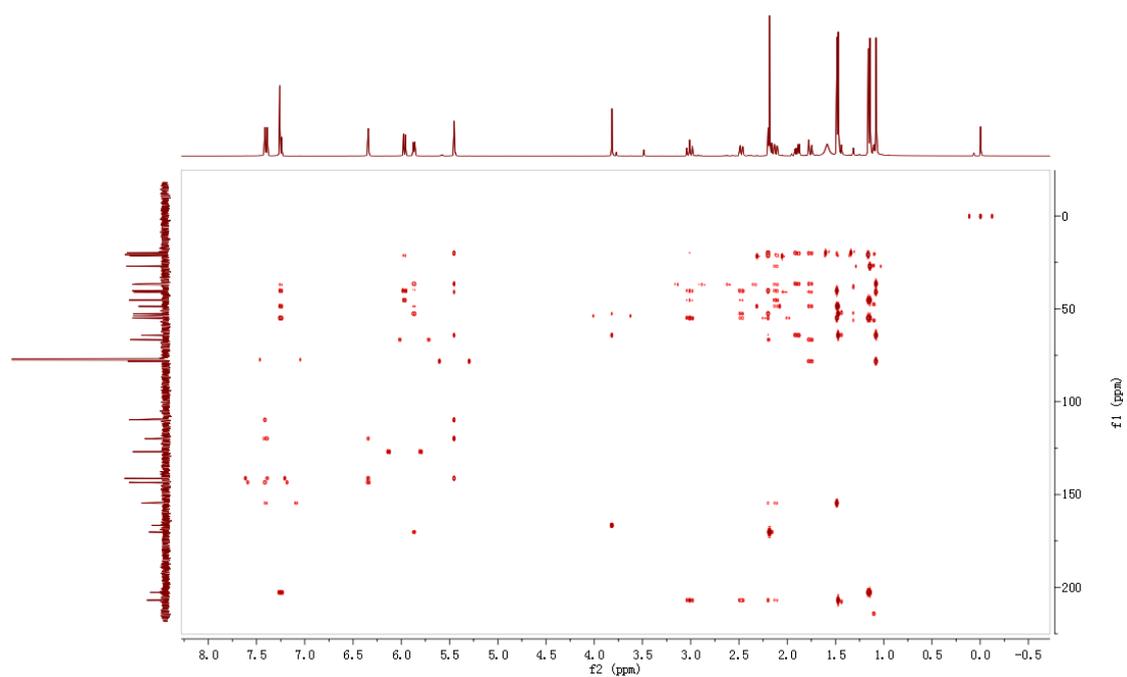


Figure S75. HMBC spectrum of **12** in CDCl₃.

CPU_TCM NMR EA-10B ROESY NMR CDCL3 AVIII-500 300K

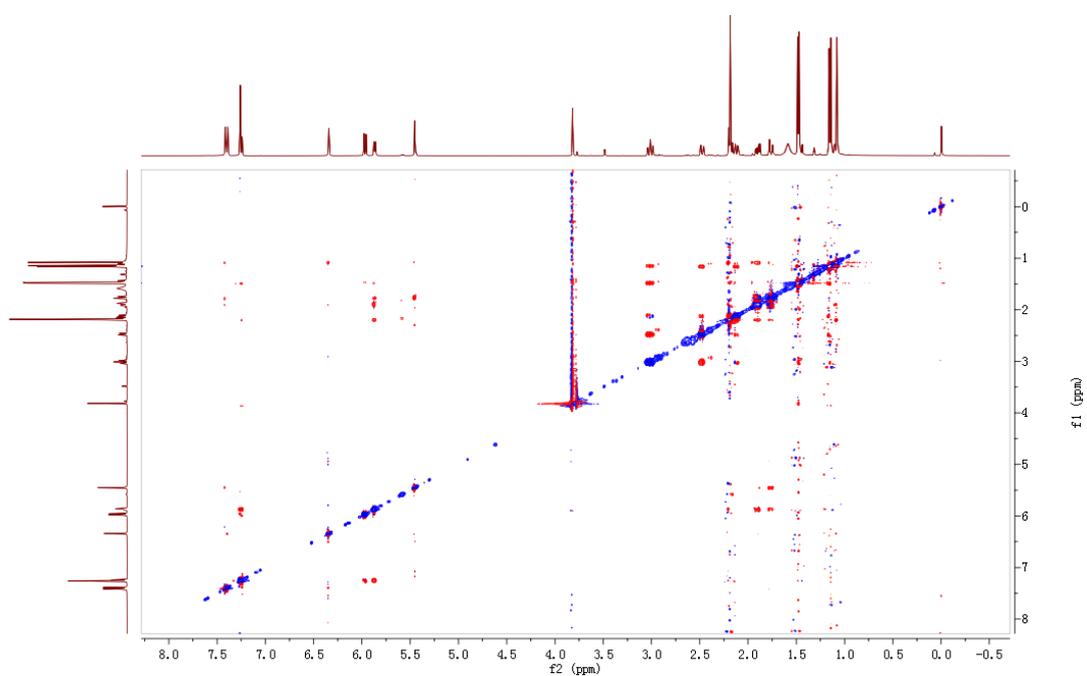
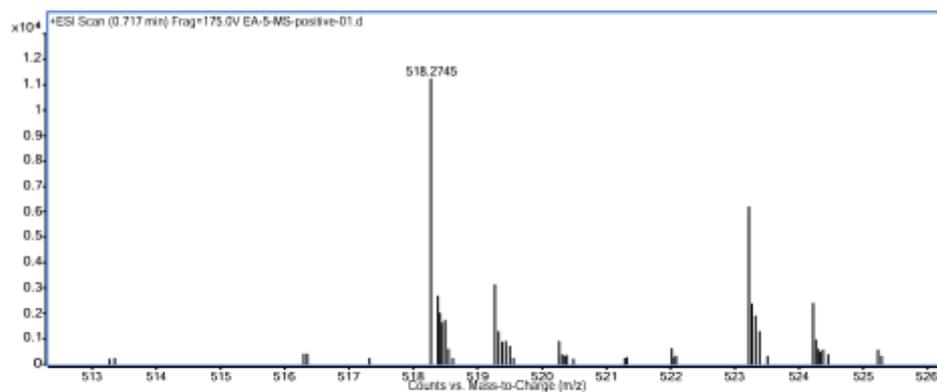


Figure S76. ROESY spectrum of **12** in CDCl₃.



Elemental Composition Calculator

Target m/z:	518.2745	Result type:	Positive ions	Species:	[M+NH4] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₈ H ₄₀ N ₀ O ₈	518.2748		0.73		

Figure S77. HRESIMS spectrum of **13**

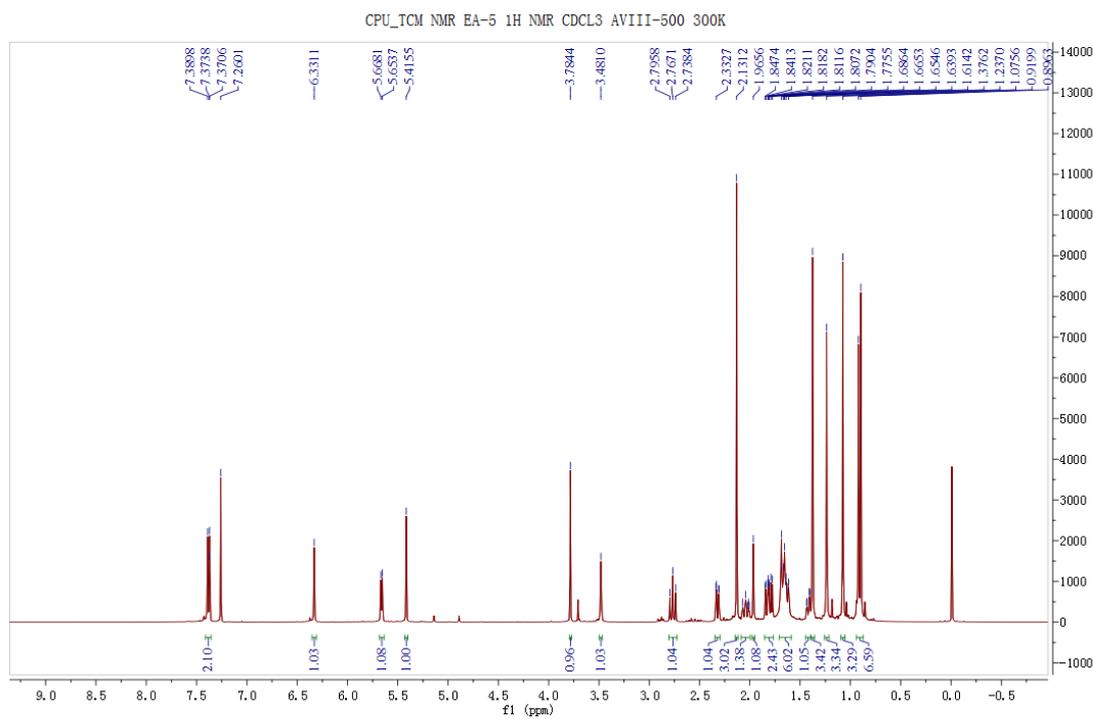


Figure S78. ¹H NMR spectrum of **13** in CDCl₃

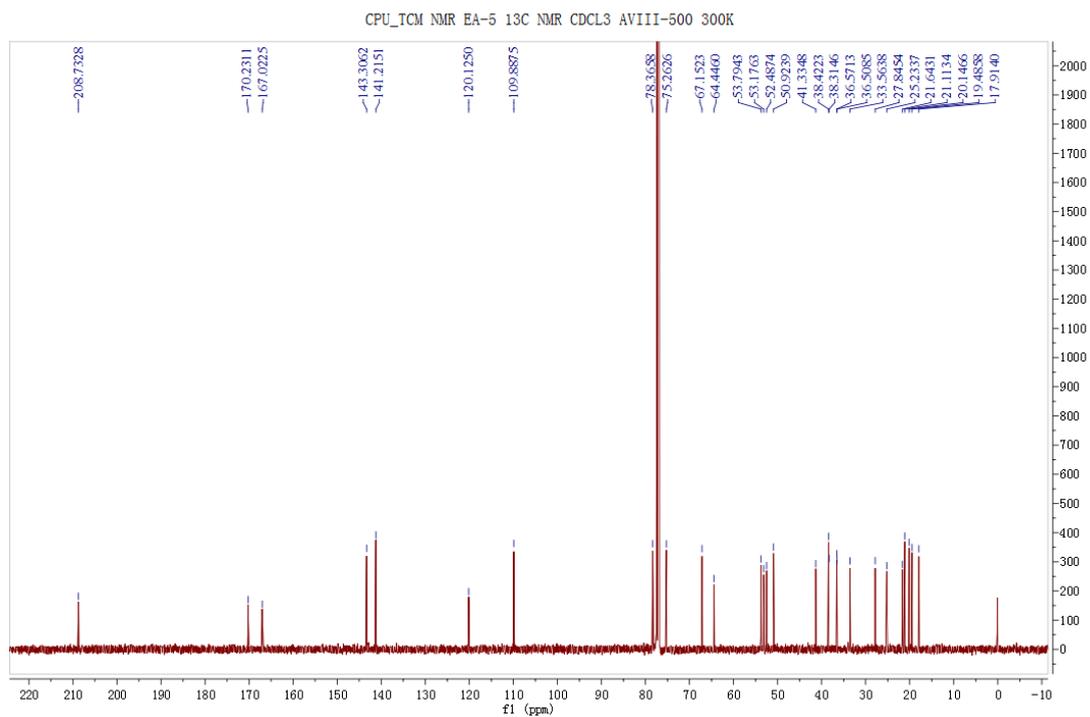


Figure S79. ^{13}C NMR spectrum of **13** in CDCl_3

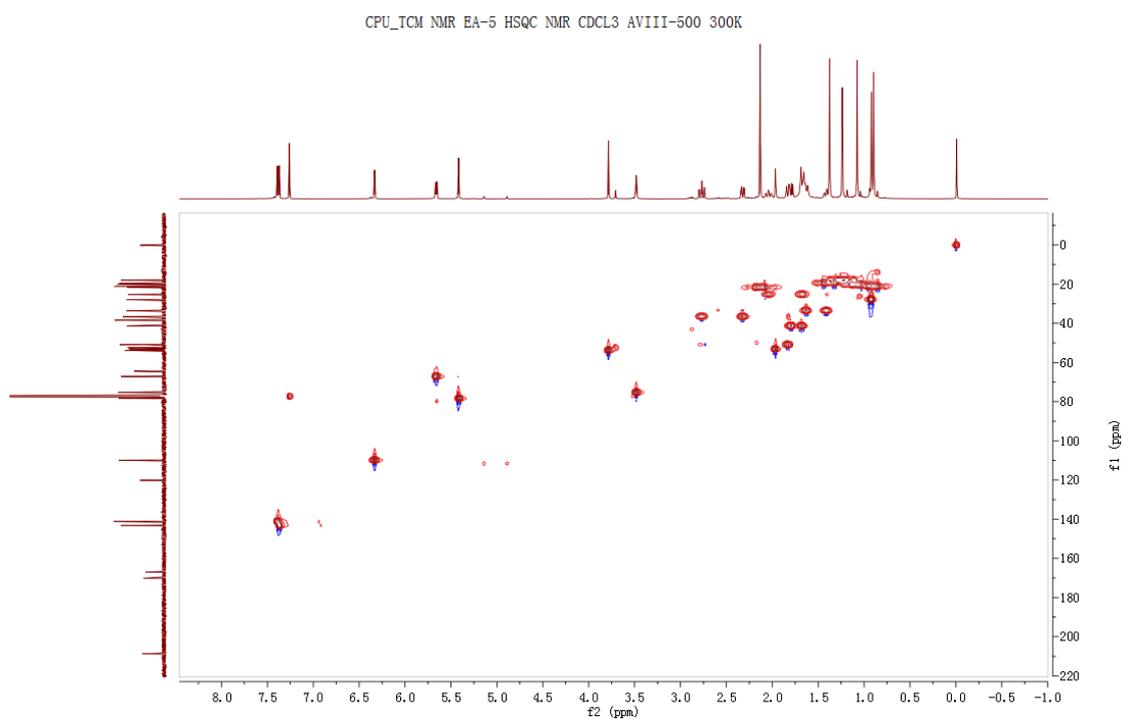


Figure S80. HSQC spectrum of **13** in CDCl_3

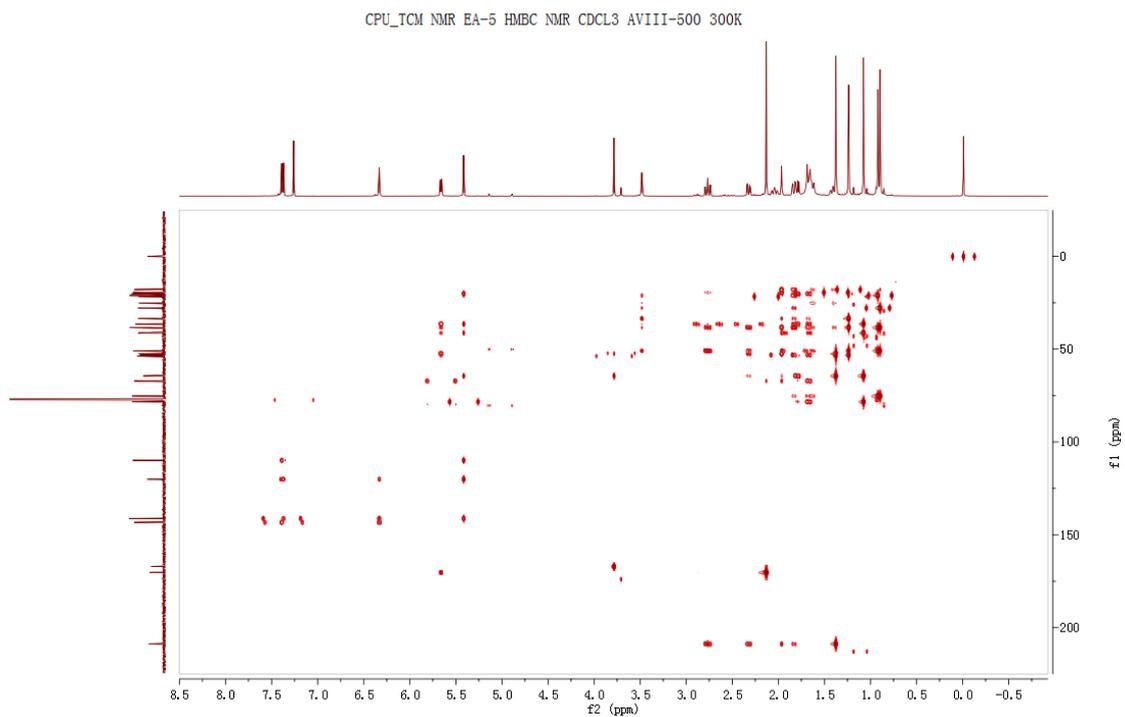


Figure S81. HMBC spectrum of **13** in CDCl₃

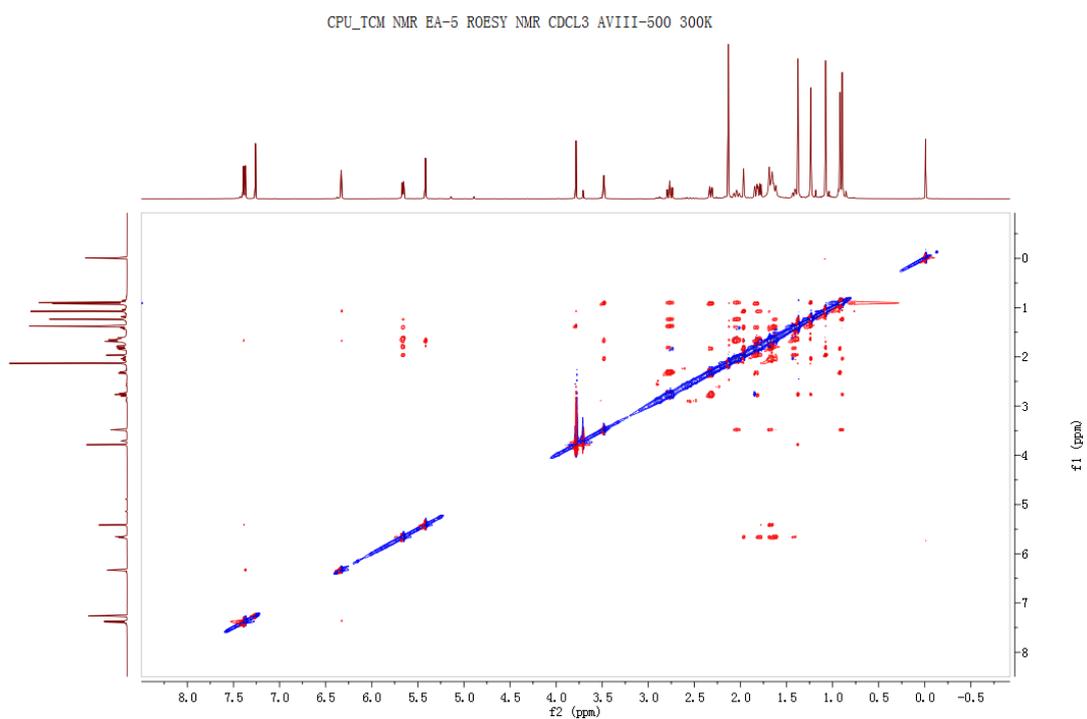
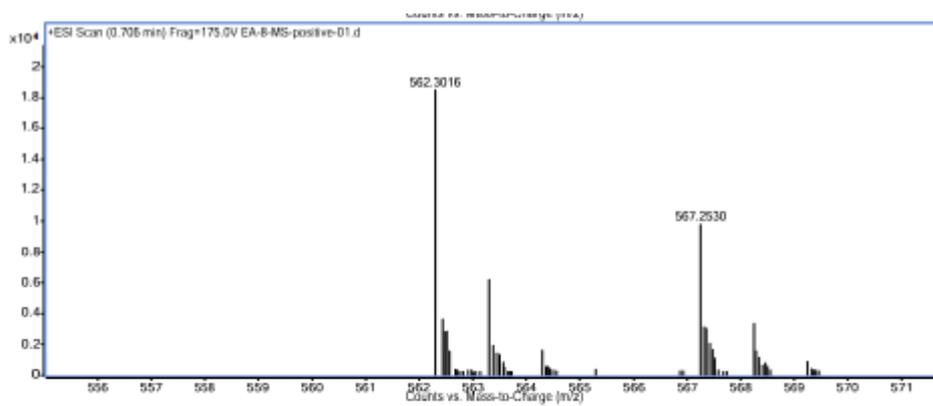


Figure S82. ROESY spectrum of **13** in CDCl₃



Elemental Composition Calculator

Target m/z:	562.3016	Result type:	Positive ions	Species:	[M+NH ₄] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10)				
Ion Formula	Calculated m/z		PPM Error		
C ₃₀ H ₄₄ N ₉ O	562.3011		-0.95		

Figure S83. HRESIMS spectrum of **14**

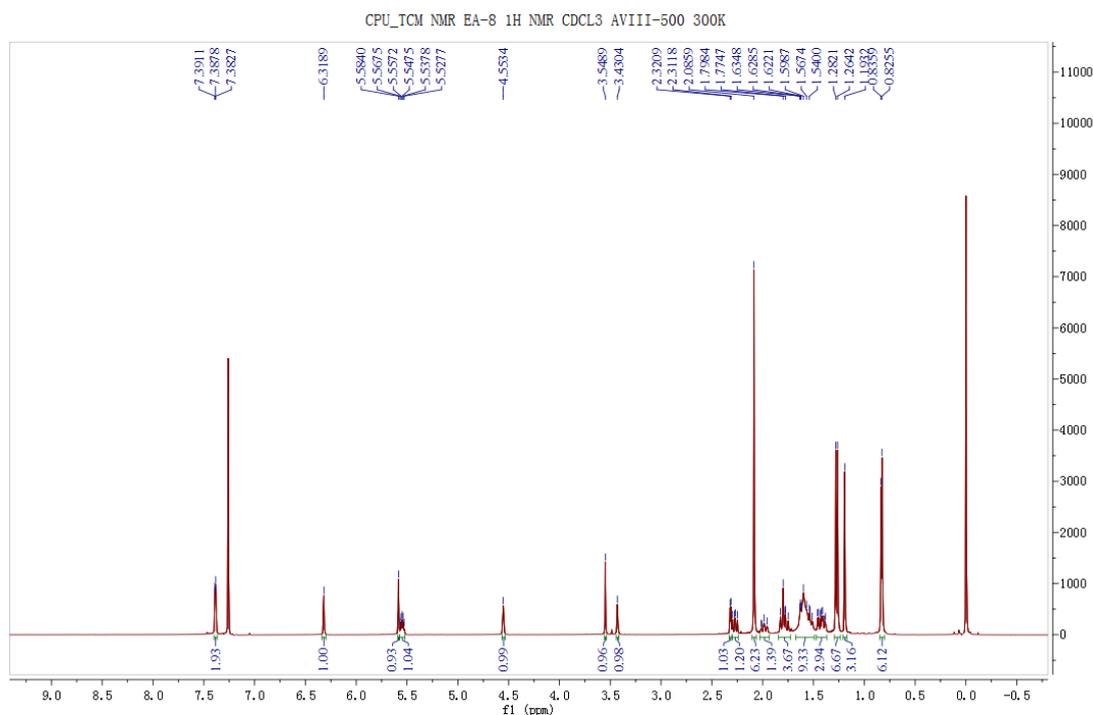


Figure S84. ¹H NMR spectrum of **14** in CDCl₃

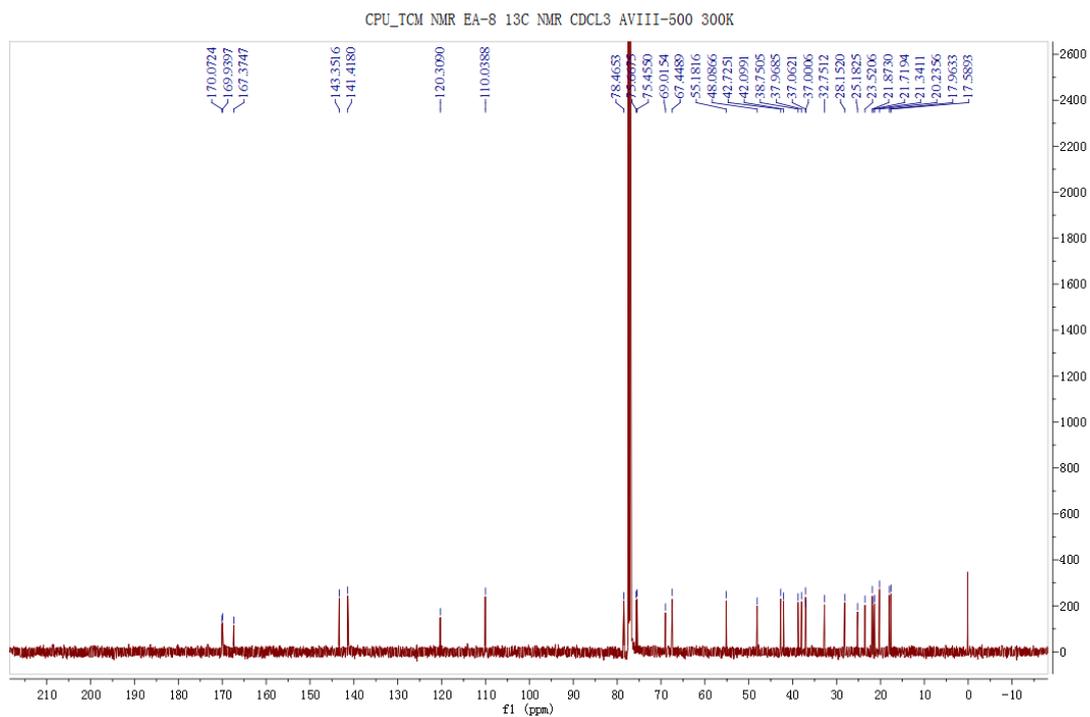


Figure S85. ^{13}C NMR spectrum of **14** in CDCl_3

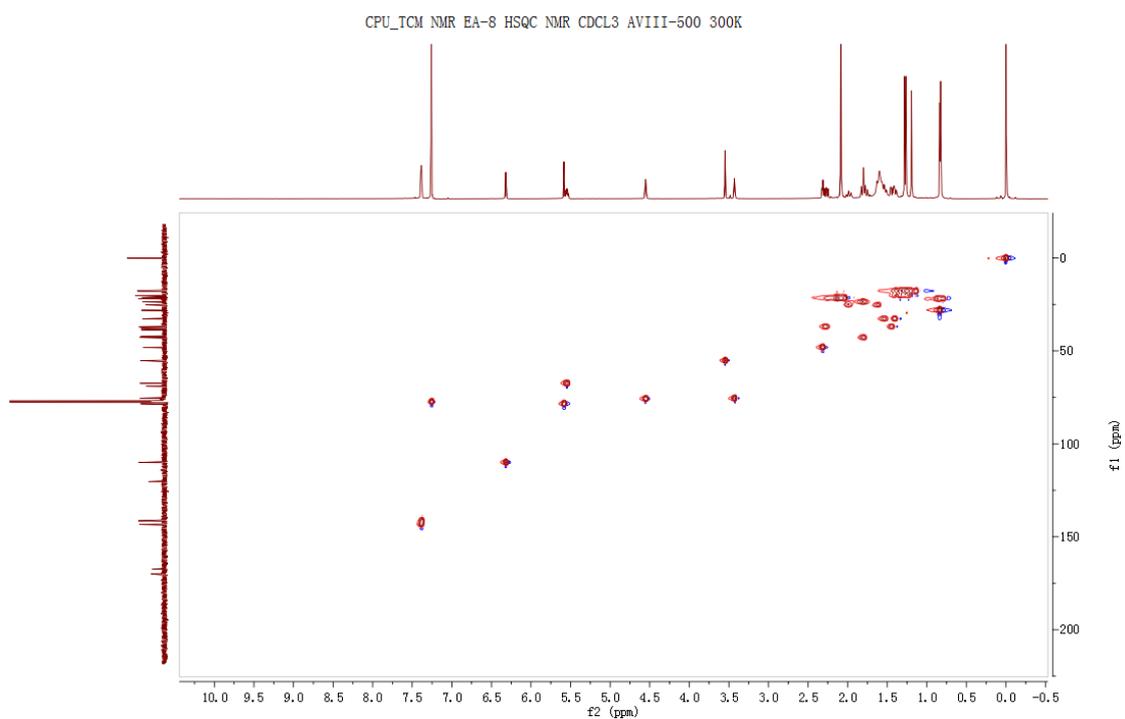


Figure S86. HSQC spectrum of **14** in CDCl_3

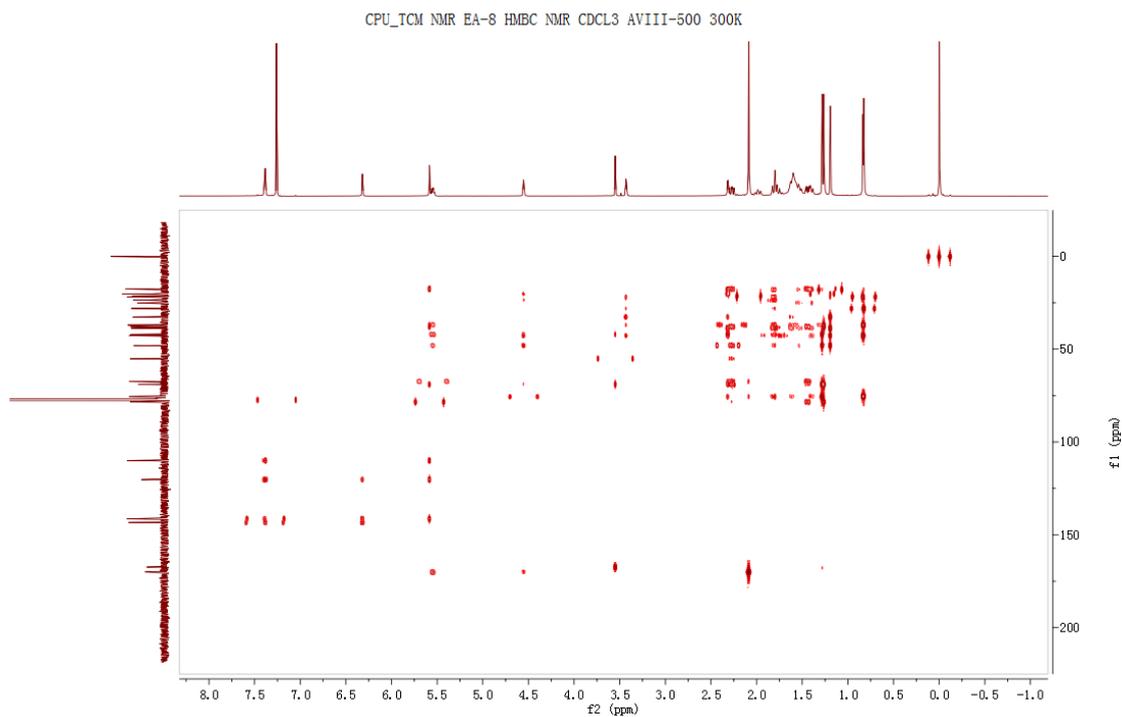


Figure S87. HMBC spectrum of **14** in CDCl₃.

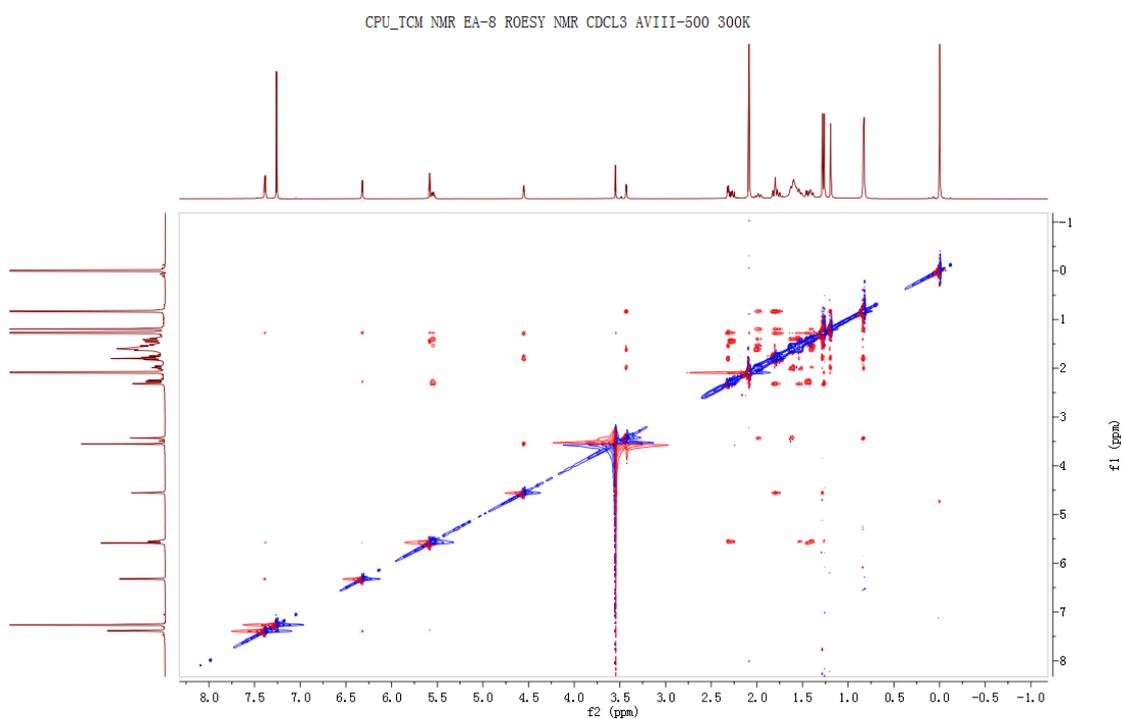
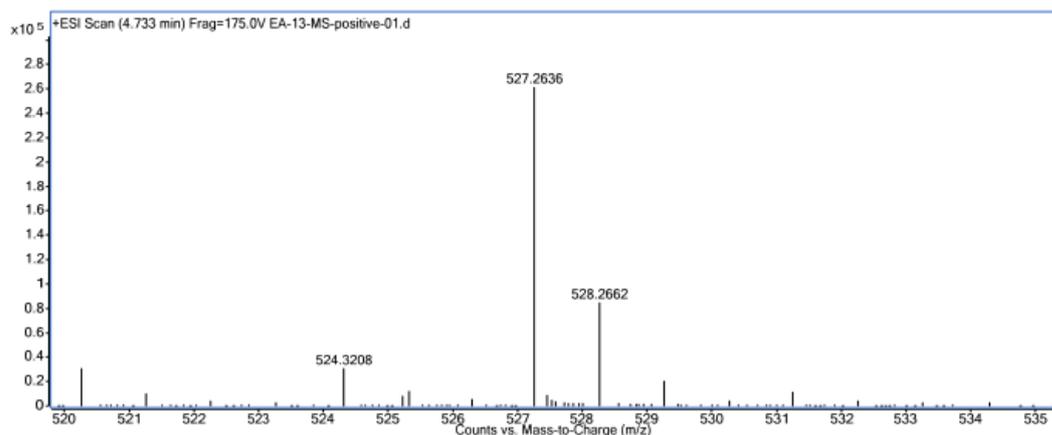


Figure S88. ROESY spectrum of **14** in CDCl₃



Elemental Composition Calculator

Target m/z:	527.2636	Result type:	Positive ions	Species:	[M+H] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10)				
Ion Formula	Calculated m/z		PPM Error		
C30H39O8	527.2639		0.63		

Figure S89. HRESIMS spectrum of **15**

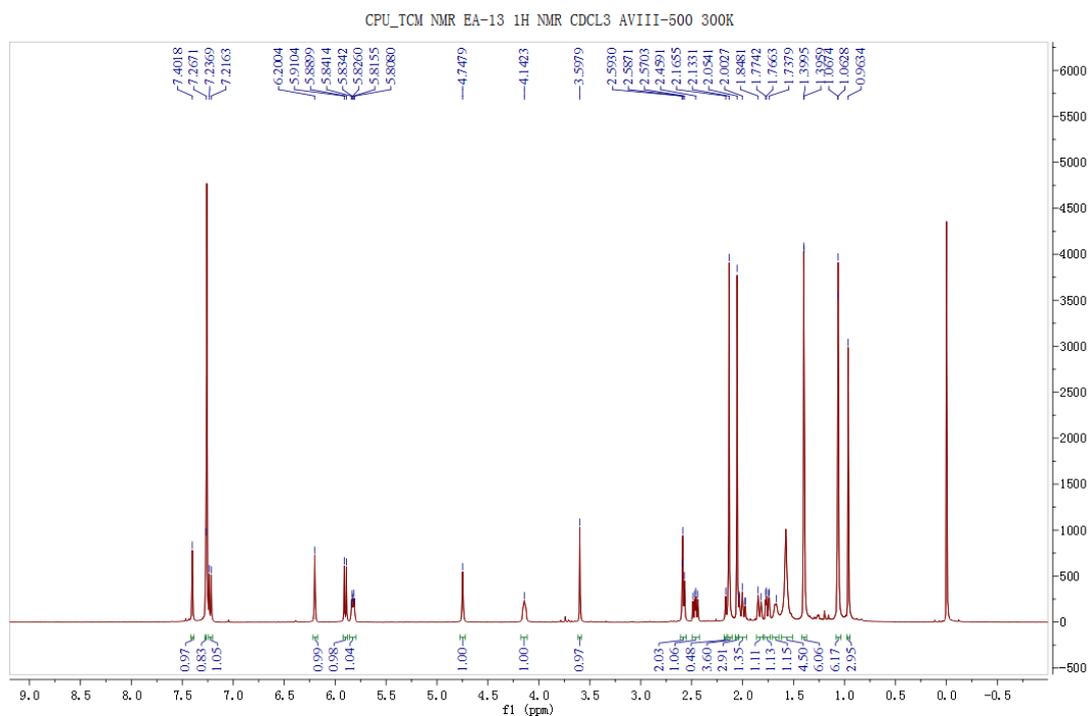


Figure S90. ¹H NMR spectrum of **15** in CDCl₃

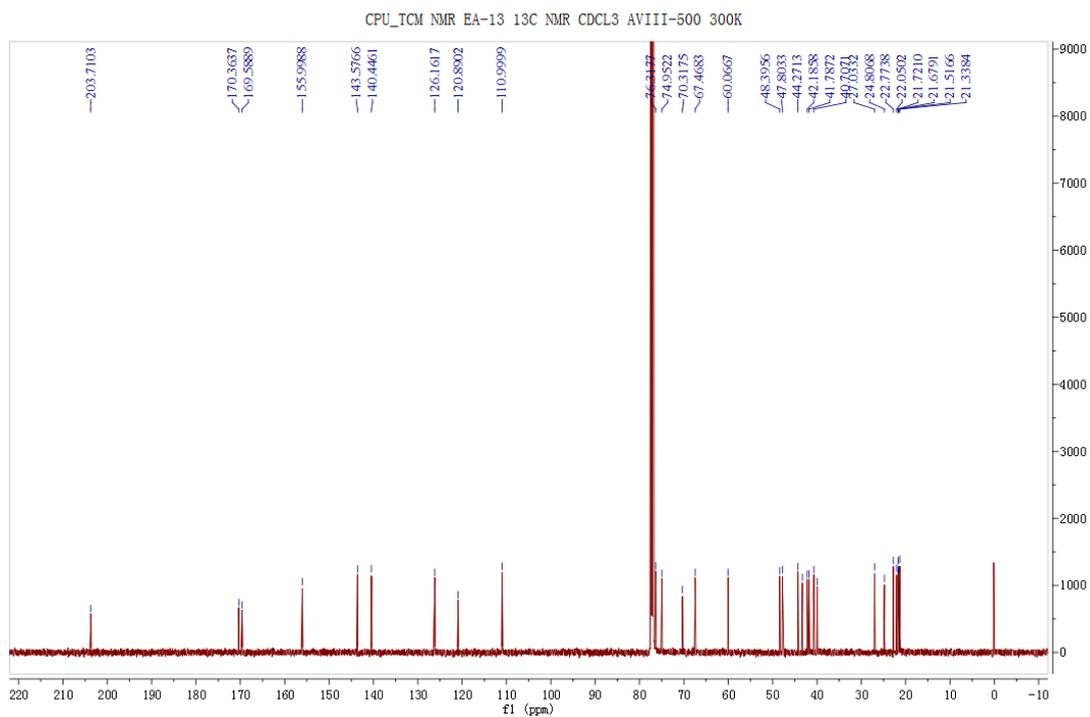


Figure S91. ^{13}C NMR spectrum of **15** in CDCl_3

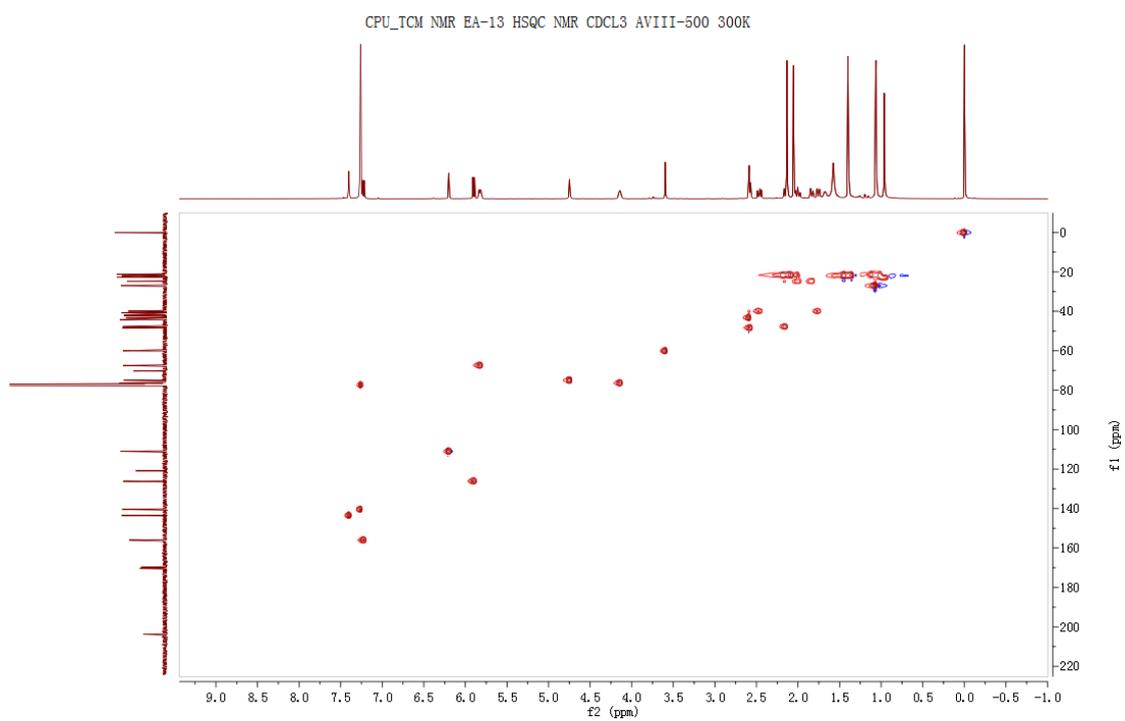
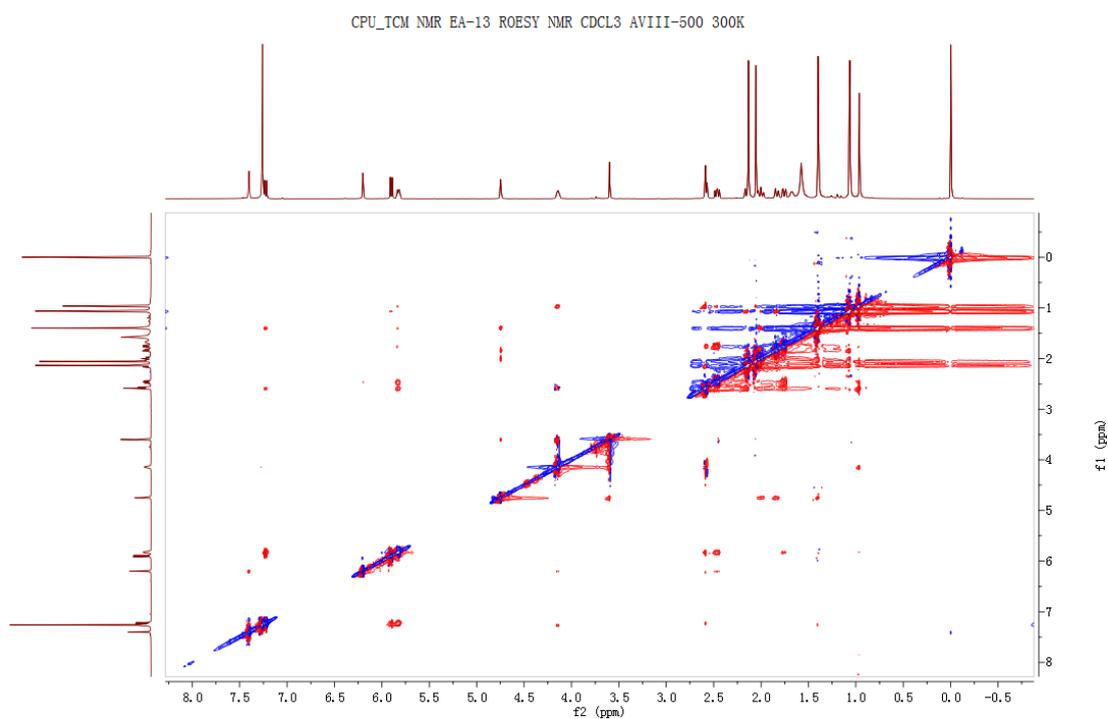
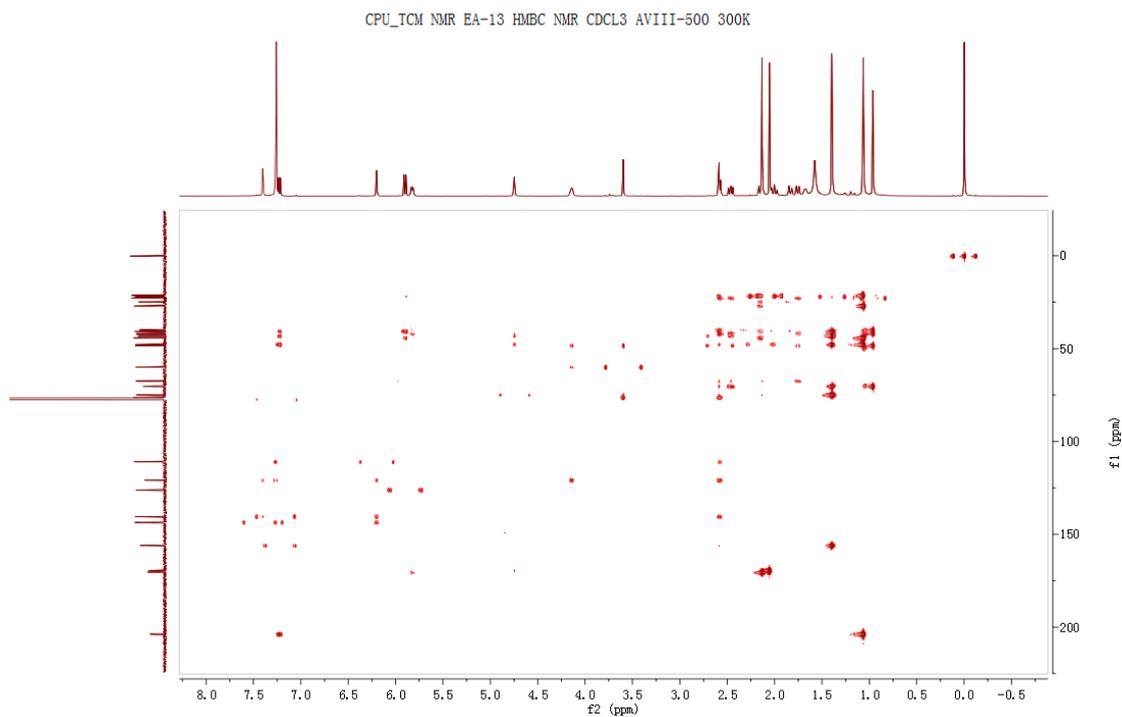
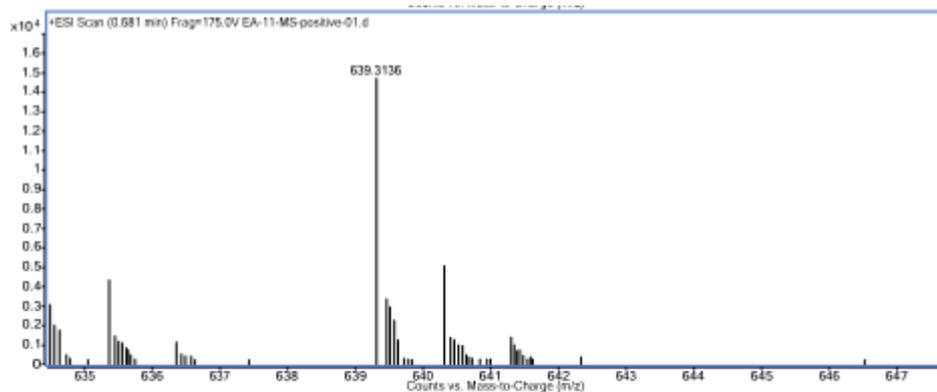


Figure S92. HSQC spectrum of **15** in CDCl_3





Elemental Composition Calculator

Target m/z:	639.3136	Result type:	Positive ions	Species:	[M+Na] ⁺
Elements:	C (0-80); H (0-120); O (0-30); Na (0-5)				
Ion Formula	Calculated m/z	PPM Error			
C ₃₄ H ₄₈ NaO ₁₀	639.3140	0.64			

Figure S95. HRESIMS spectrum of **16**

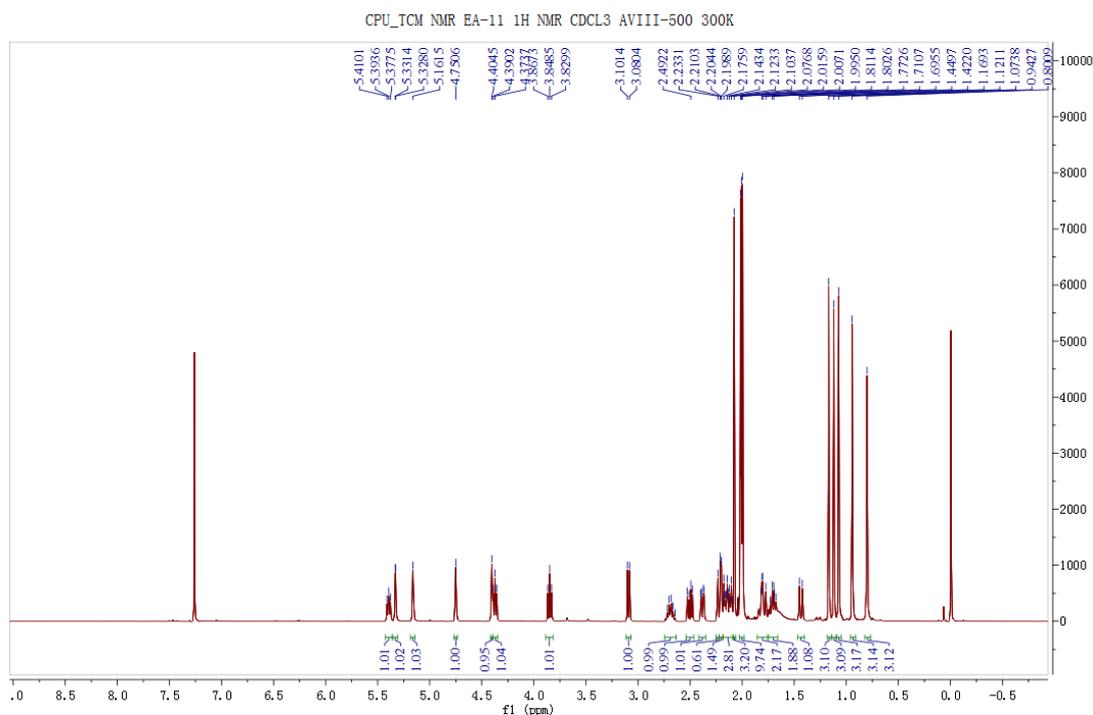


Figure S96. ¹H NMR spectrum of **16** in CDCl₃

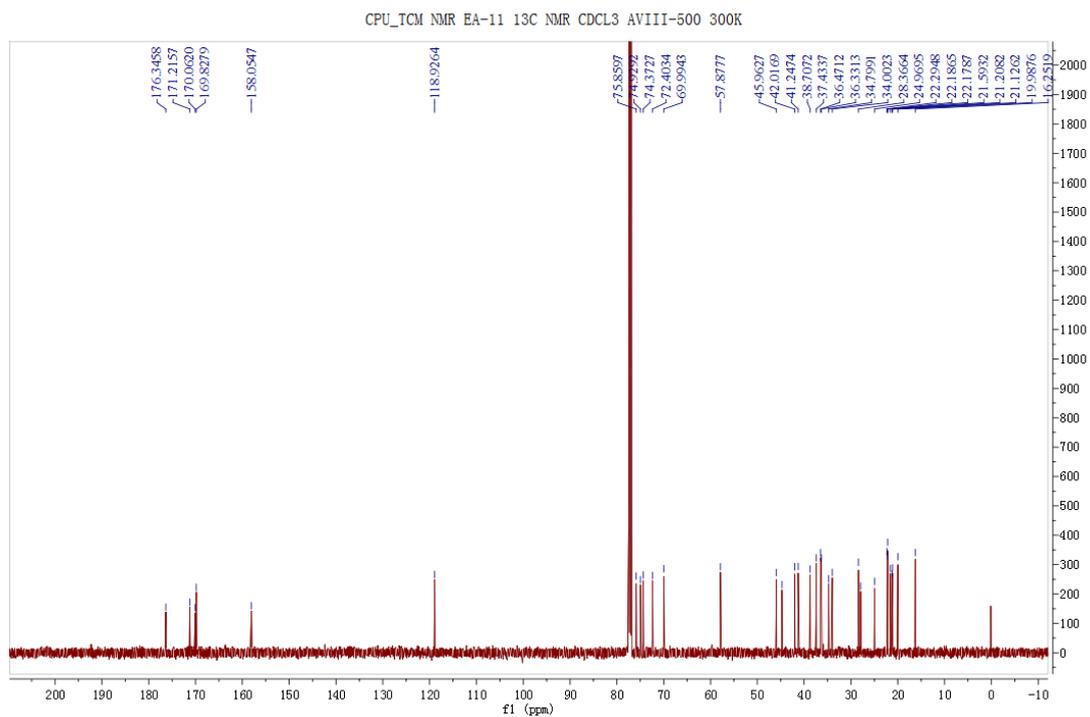


Figure S97. ^{13}C NMR spectrum of **16** in CDCl_3

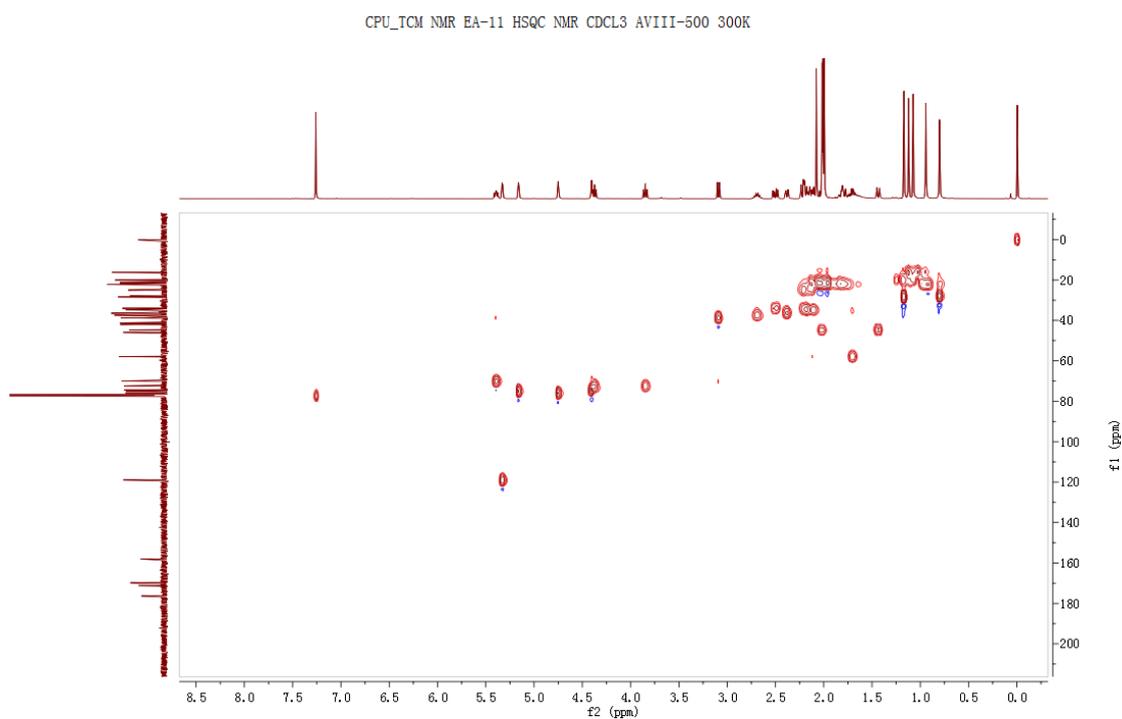


Figure S98. HSQC spectrum of **16** in CDCl_3

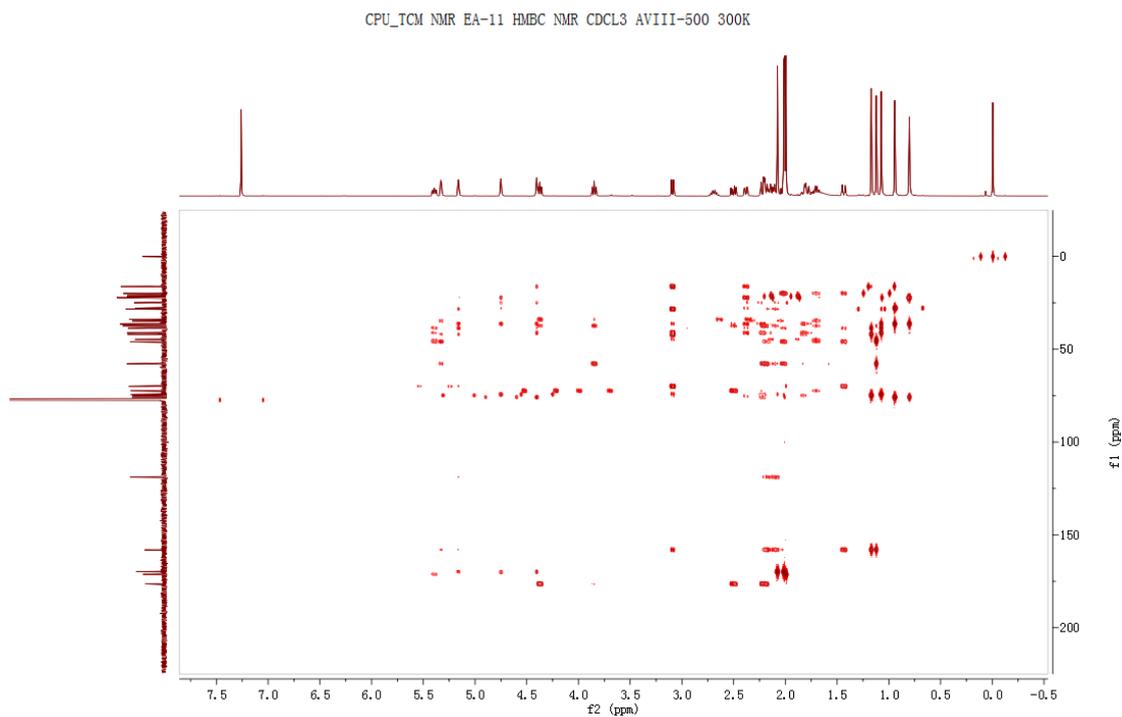


Figure S99. HMBC spectrum of **16** in CDCl₃

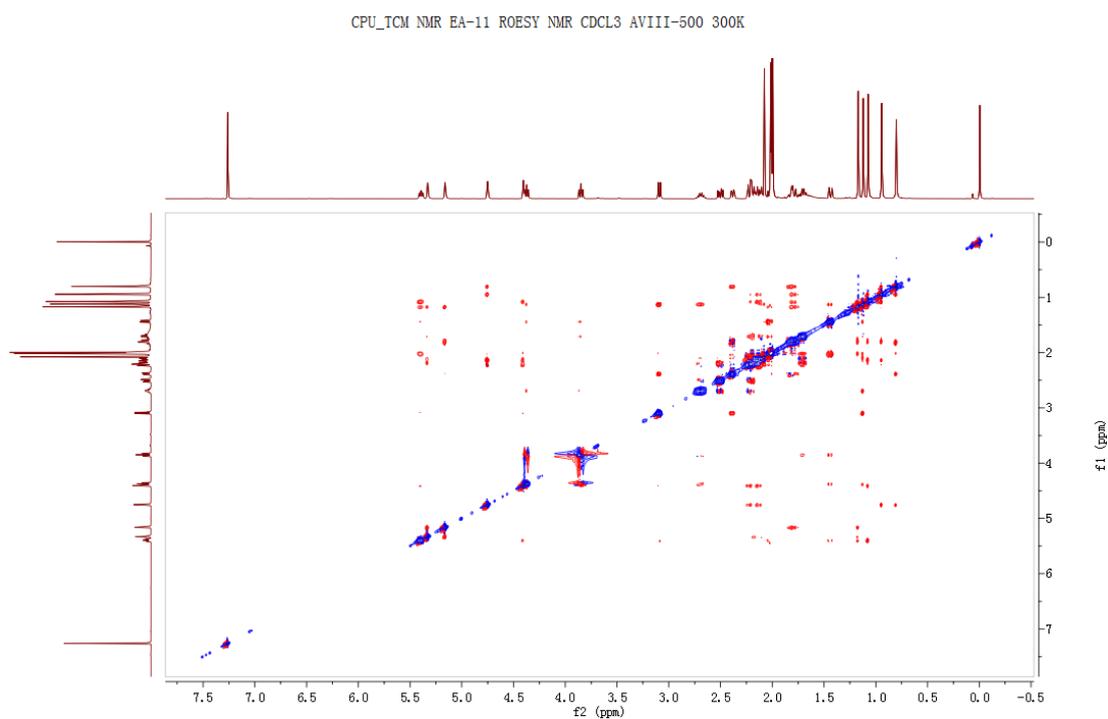


Figure S100. ROESY spectrum of **16** in CDCl₃