

Supplementary material

NMR-guided isolation of anti-inflammatory carabranolides from
the fruits of *Carpesium abrotanoides* L.

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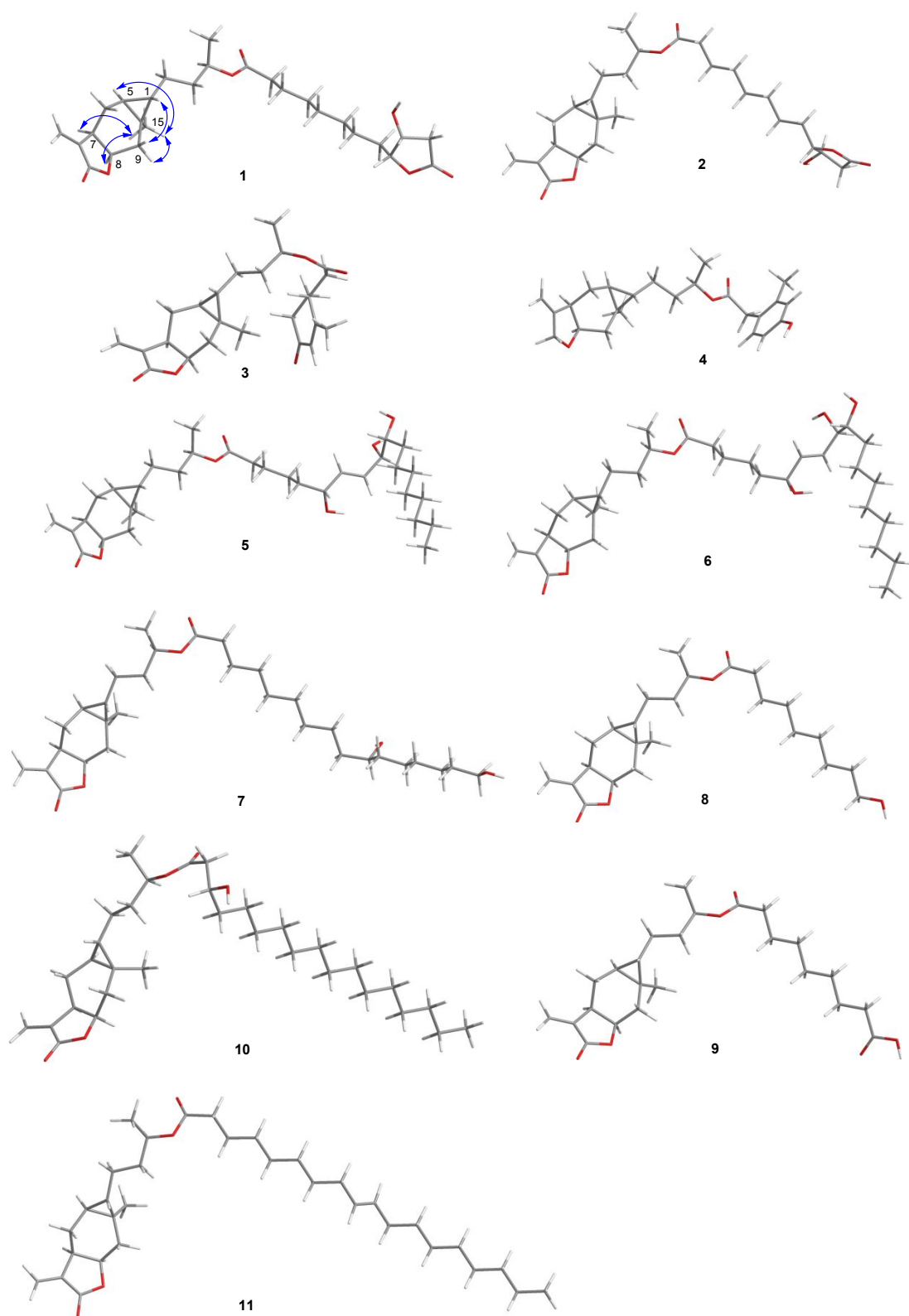


Figure S1. Key NOESY correlations of 1-11.

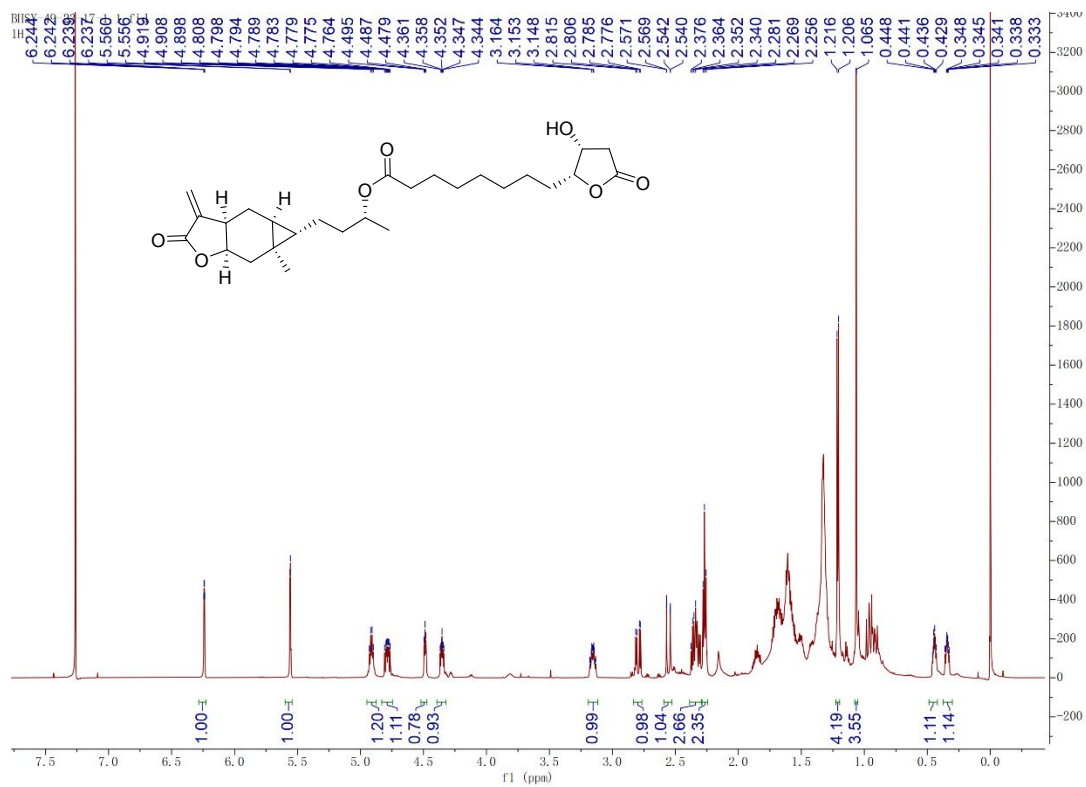


Figure S2. ^1H NMR spectrum (600 MHz) of carabrolate A (**1**) in CDCl_3

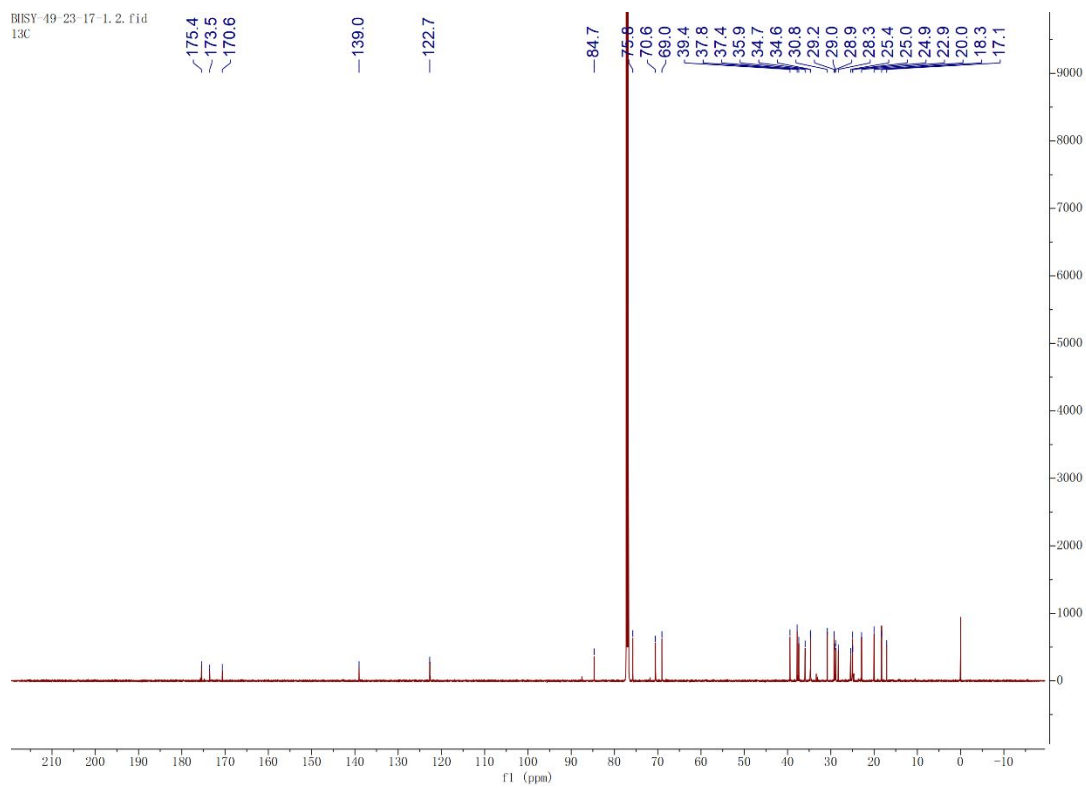


Figure S3. ^{13}C NMR spectrum (150 MHz) of carabrolate (**1**) in CDCl_3

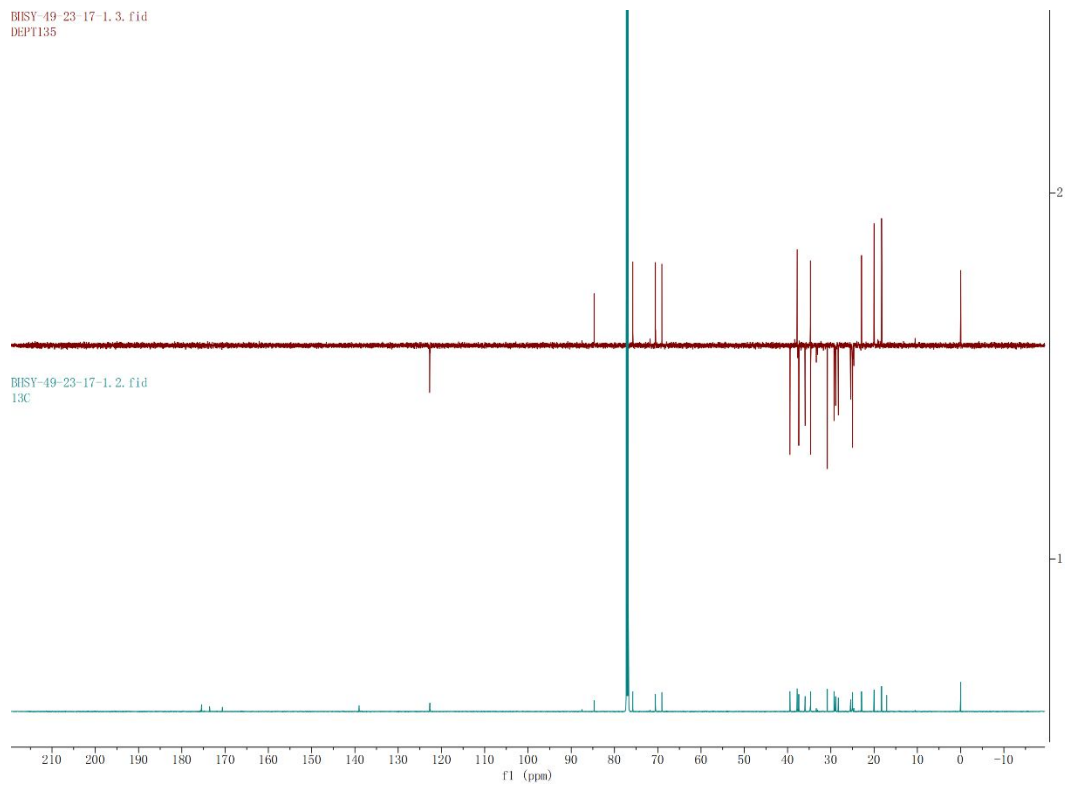


Figure S4. DEPT 135 spectrum (150 MHz) of carabrolate A (**1**) in CDCl_3

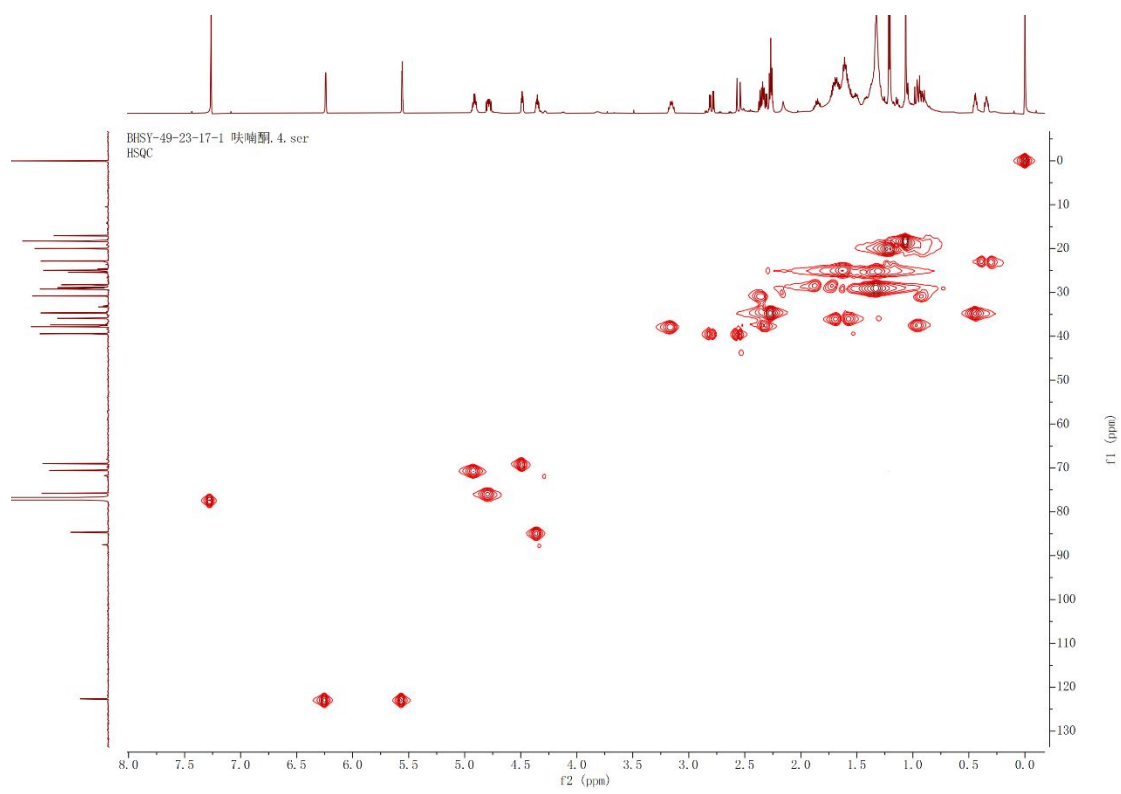


Figure S5. HSQC spectrum (600 MHz) of carabrolate A (**1**) in CDCl_3

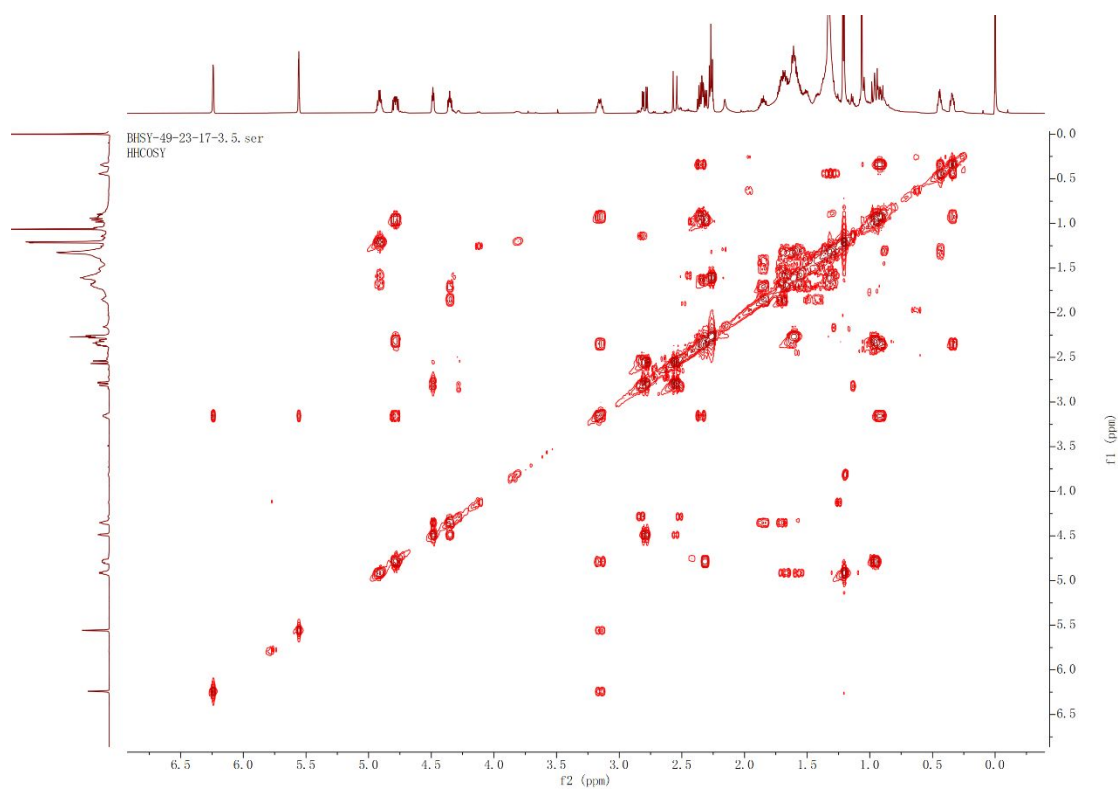


Figure S6. ^1H - ^1H COSY spectrum (600 MHz) of carabrolate A (**1**) in CDCl_3

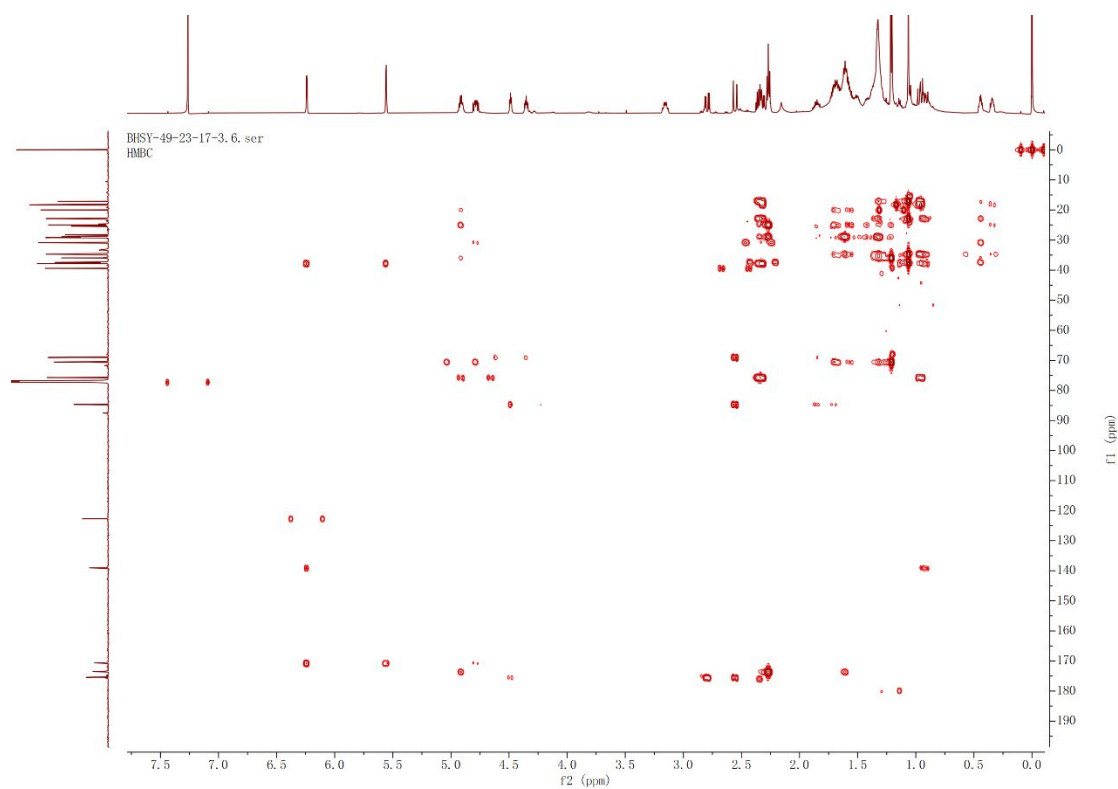


Figure S7. HMBC spectrum (600 MHz) of carabrolate A (**1**) in CDCl_3

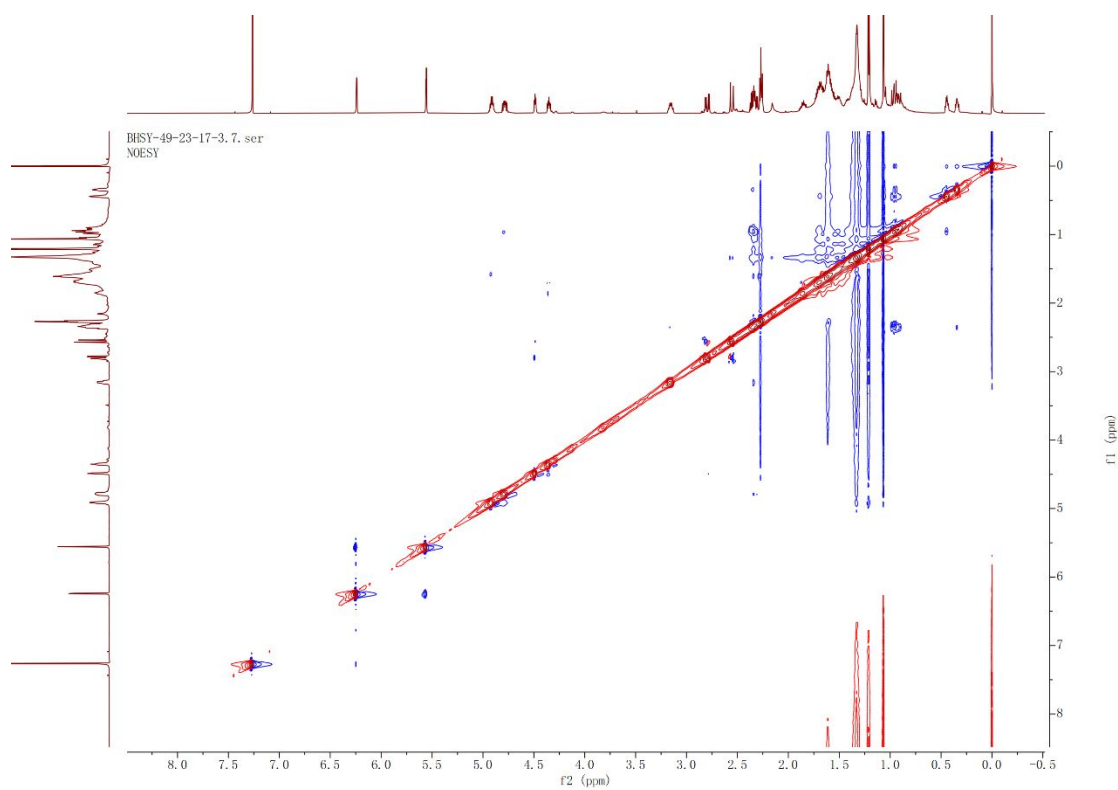


Figure S8. NOESY spectrum (600 MHz) of carabrolate A (**1**) in CDCl_3

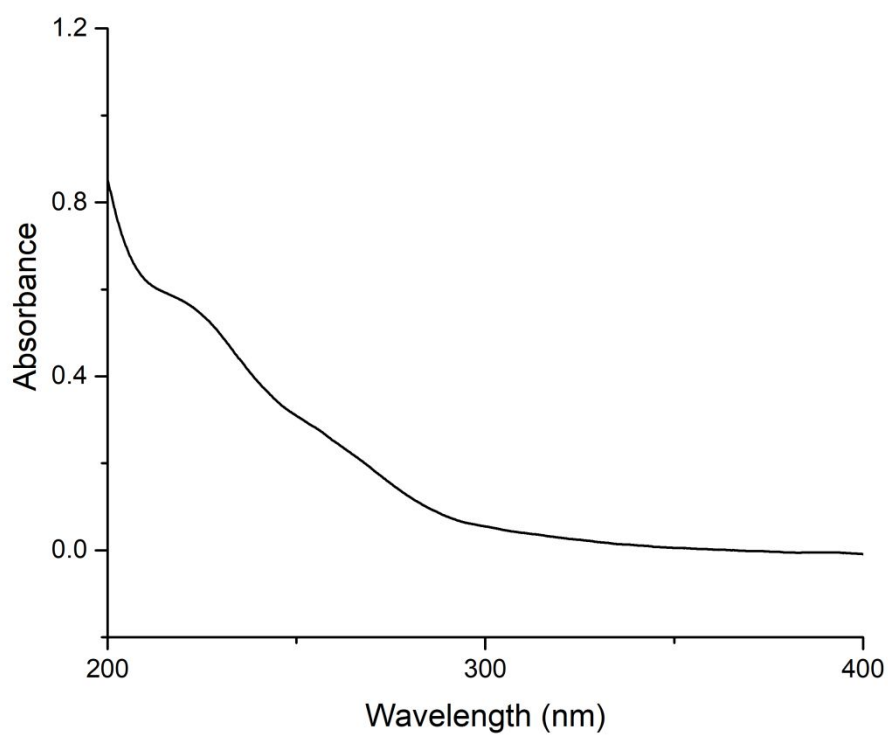


Figure S9. UV spectrum of carabrolate A (**1**) in MeOH

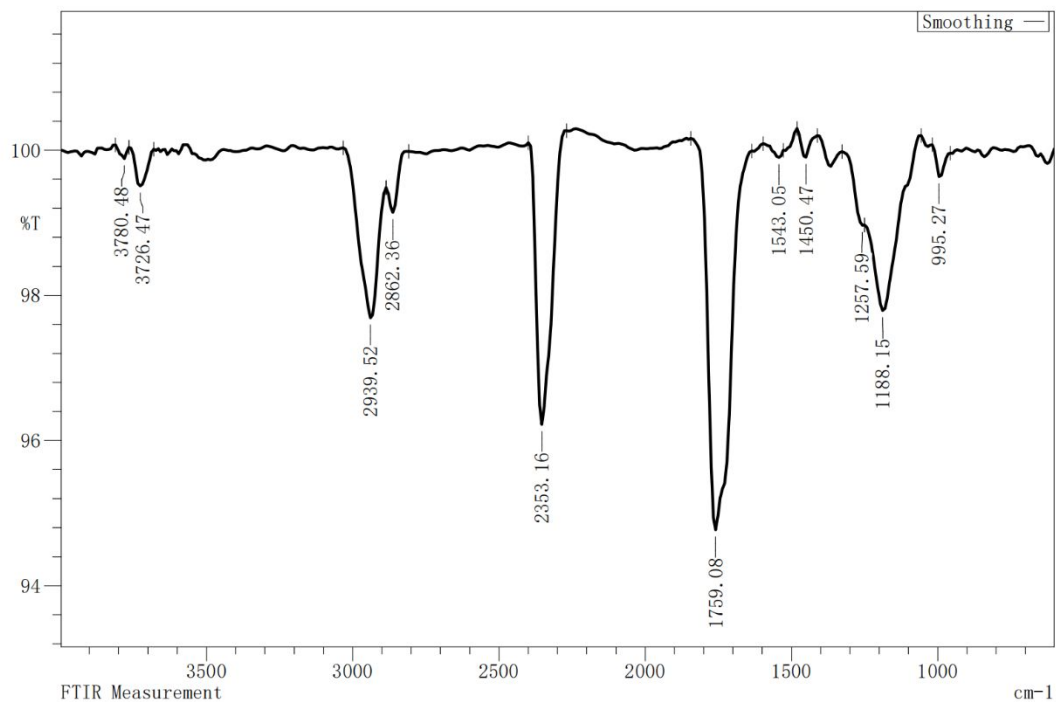
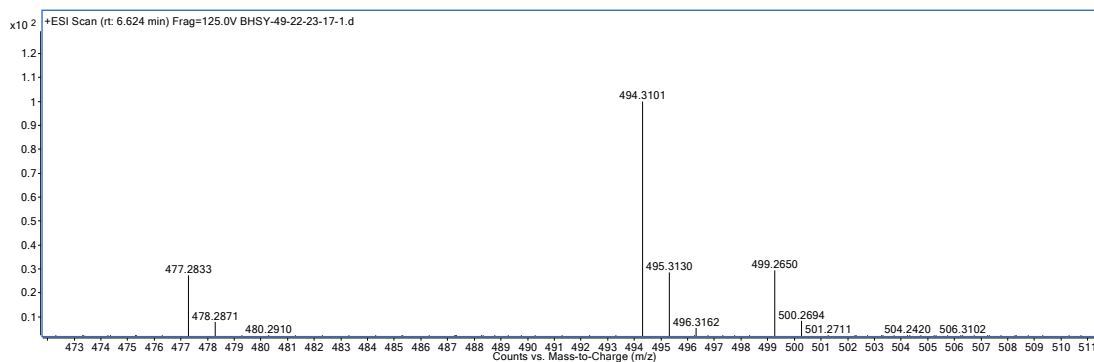


Figure S10. IR spectrum (film on KBr plate) of carabrolate A (1)



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	Ion Formula	m/z
C ₂₇ H ₄₀ O ₇	96.5	476.276	476.2774	477.2847	2.9	C ₂₇ H ₄₁ O ₇	477.2833
C ₂₇ H ₄₀ O ₇	97.62	476.2763	476.2774	494.3112	2.37	C ₂₇ H ₄₄ NO ₇	494.3101

Figure S11. HRESIMS spectrum of carabrolate A (1)

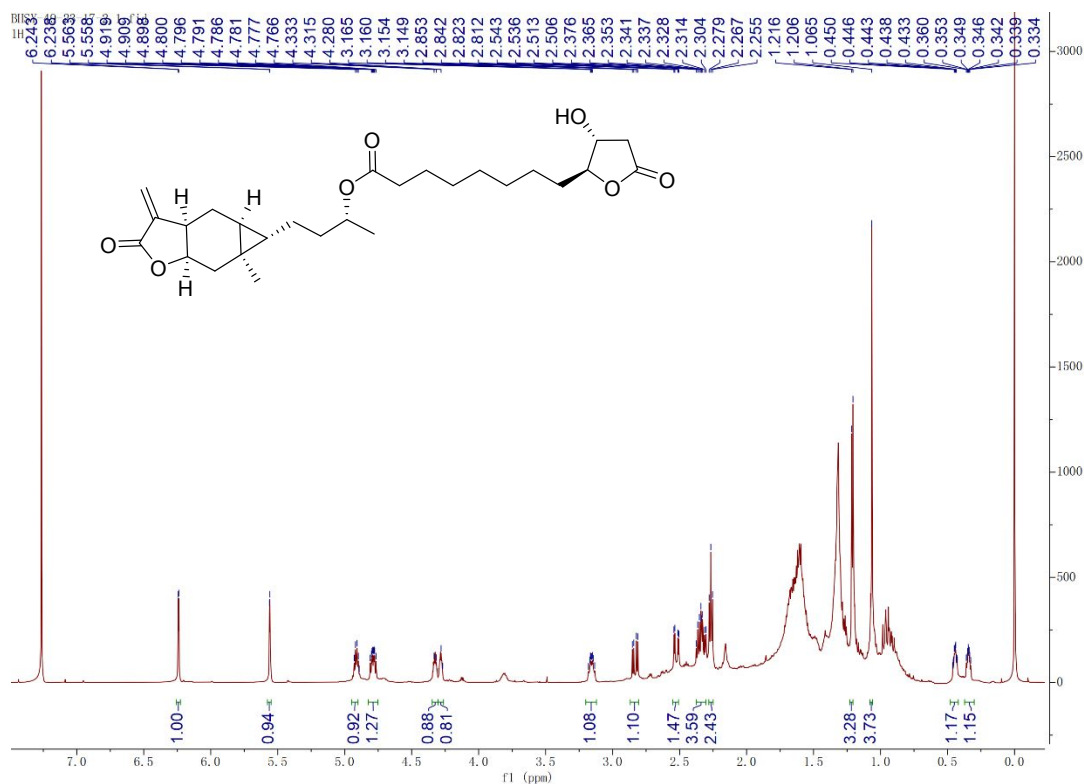


Figure S12. ^1H NMR spectrum (600 MHz) of carabrolate B (**2**) in CDCl_3

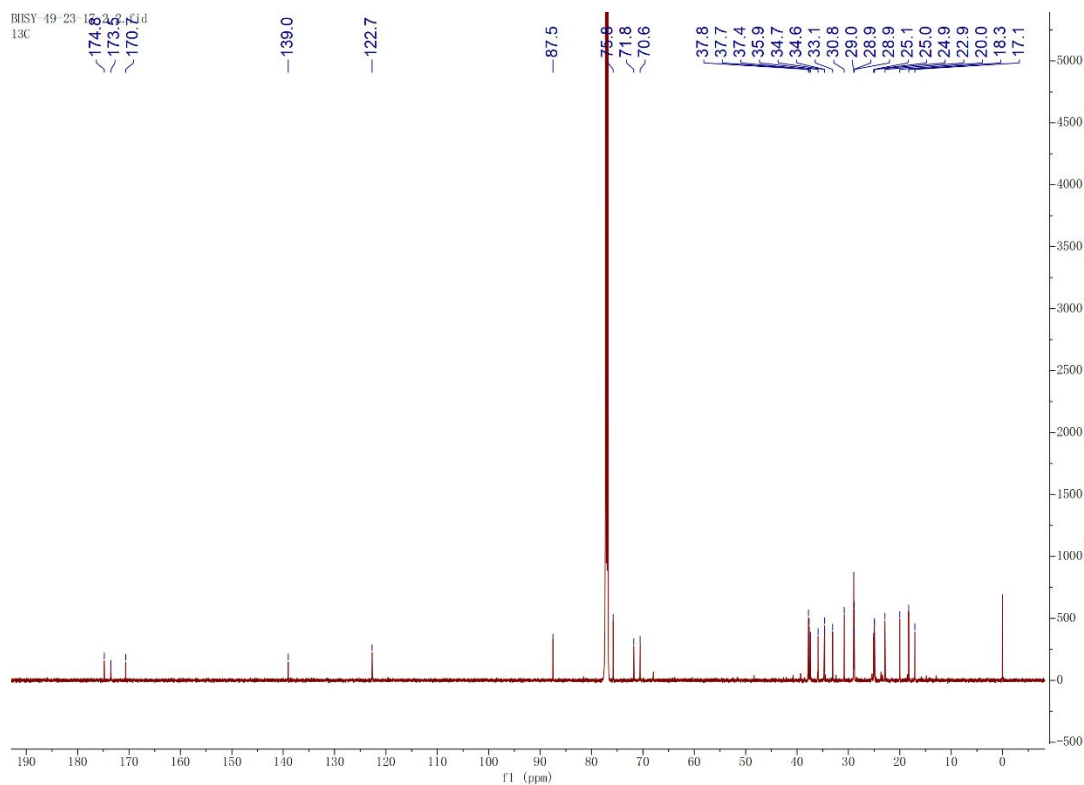


Figure S13. ^{13}C NMR spectrum (150 MHz) of carabrolate B (**2**) in CDCl_3

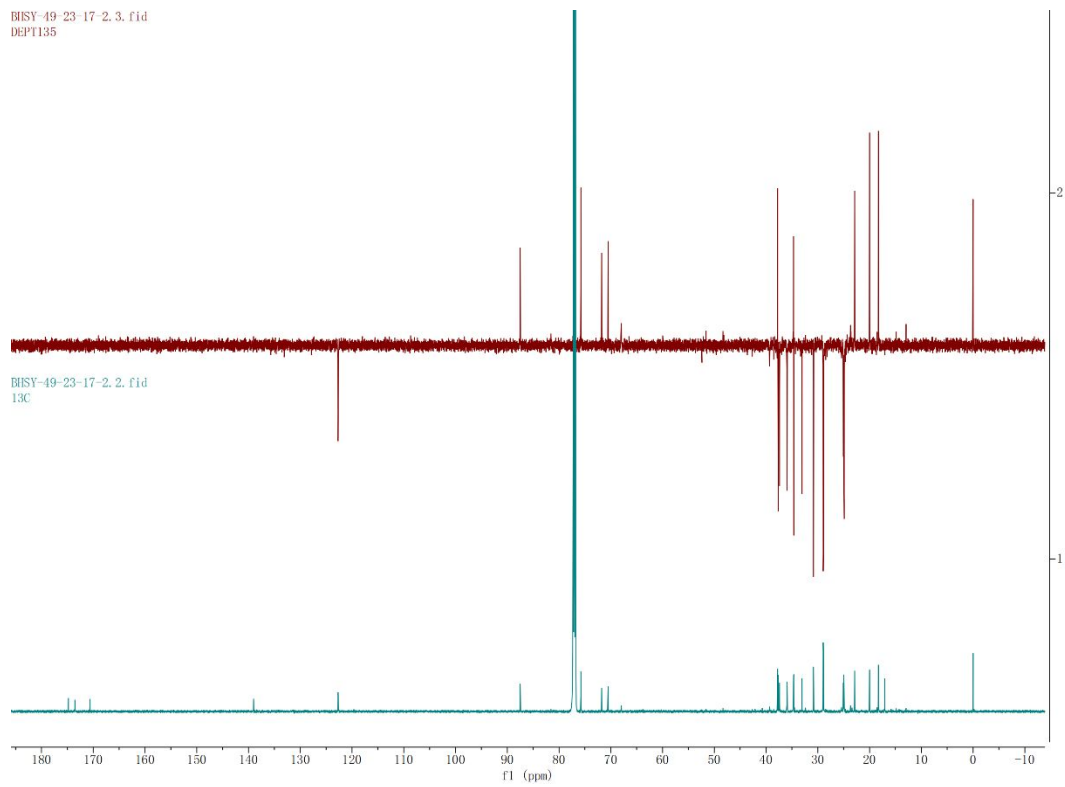


Figure S14. DEPT 135 spectrum (150 MHz) of carabrolate B (**2**) in CDCl_3

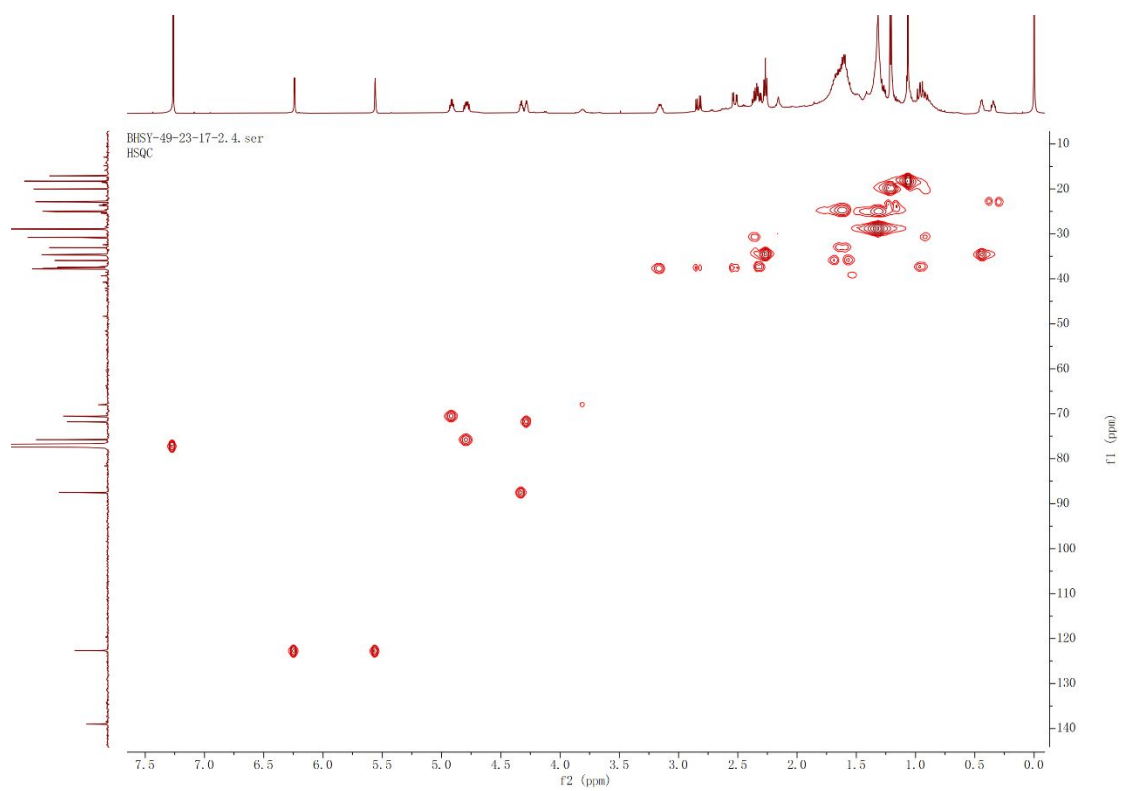


Figure S15. HSQC spectrum (600 MHz) of carabrolate B (**2**) in CDCl_3

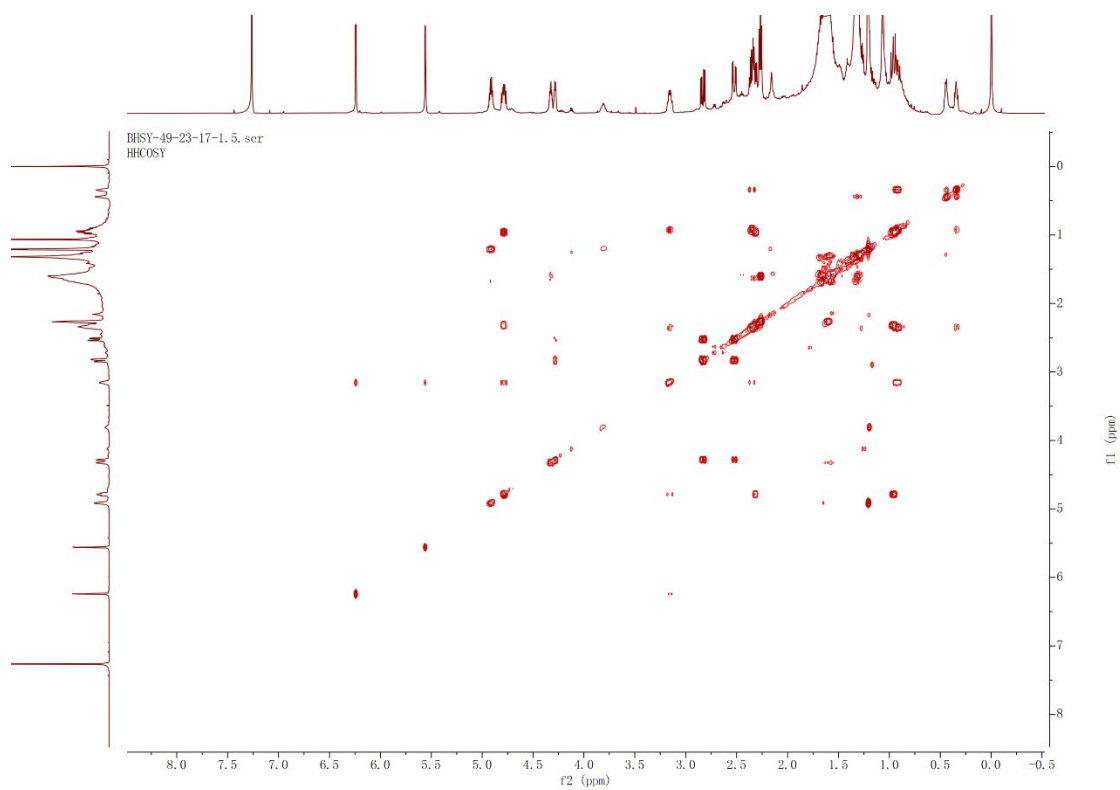


Figure S16. ^1H - ^1H COSY spectrum (600 MHz) of carabrolate B (**2**) in CDCl_3

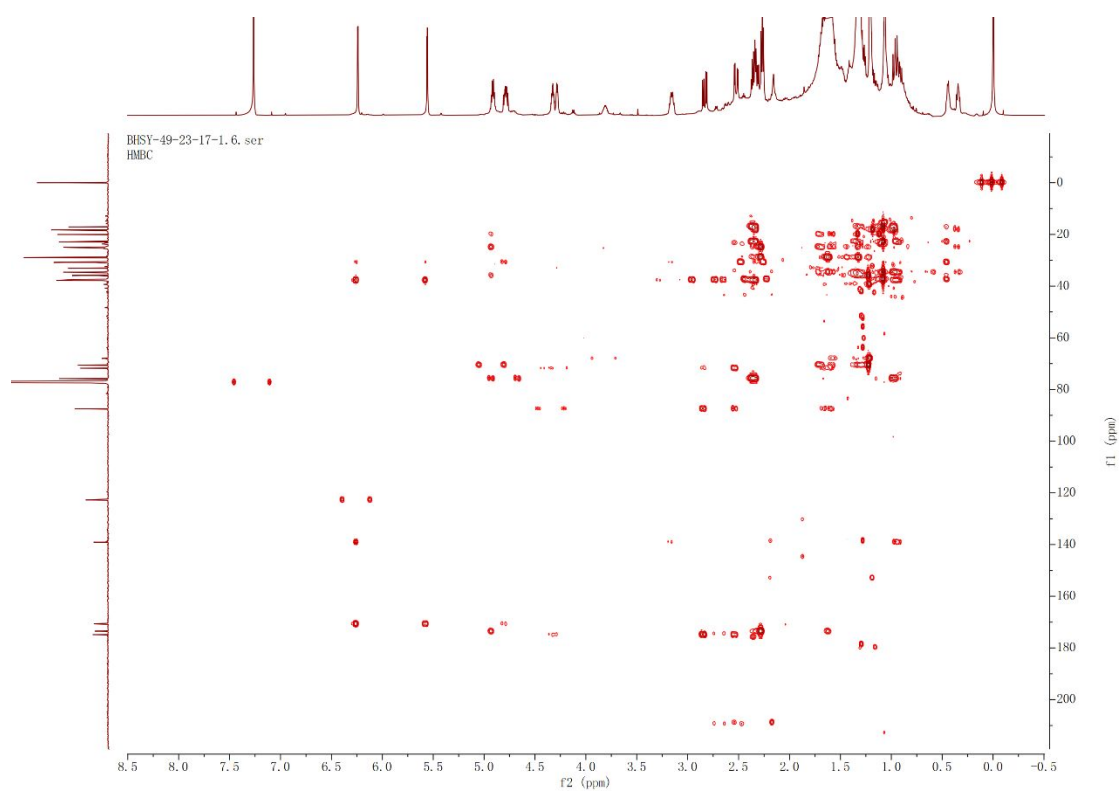


Figure S17. HMBC spectrum (600 MHz) of carabrolate B (**2**) in CDCl_3

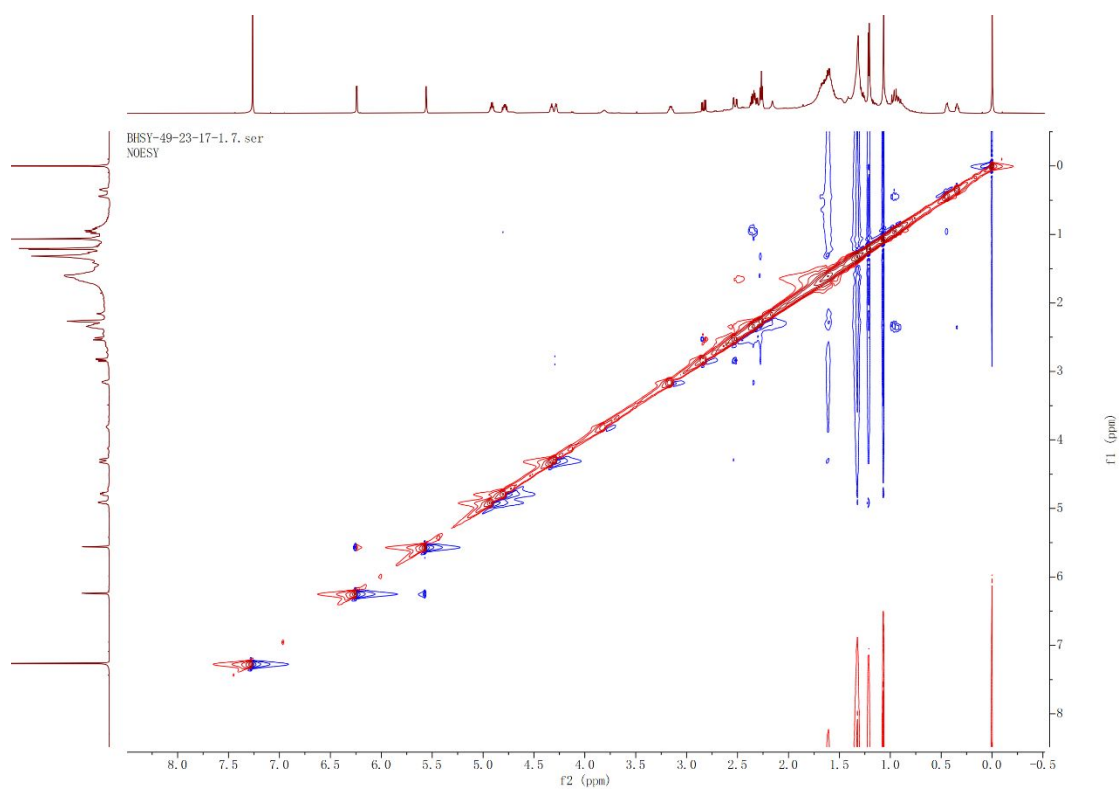


Figure S18. NOESY spectrum (600 MHz) of carabrolate B (**2**) in CDCl_3

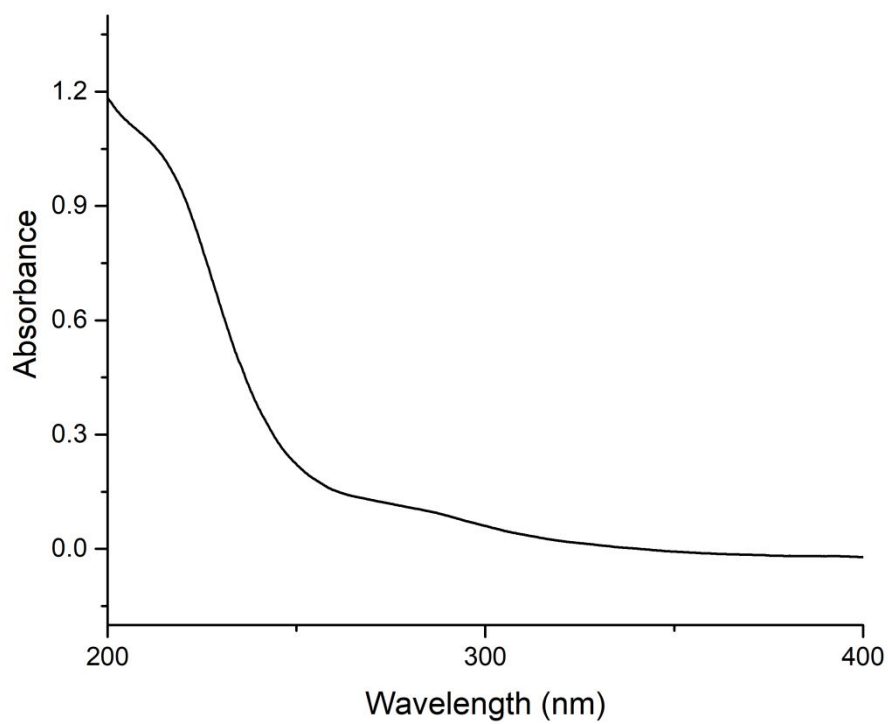


Figure S19. UV spectrum of carabrolate B (**2**) in MeOH

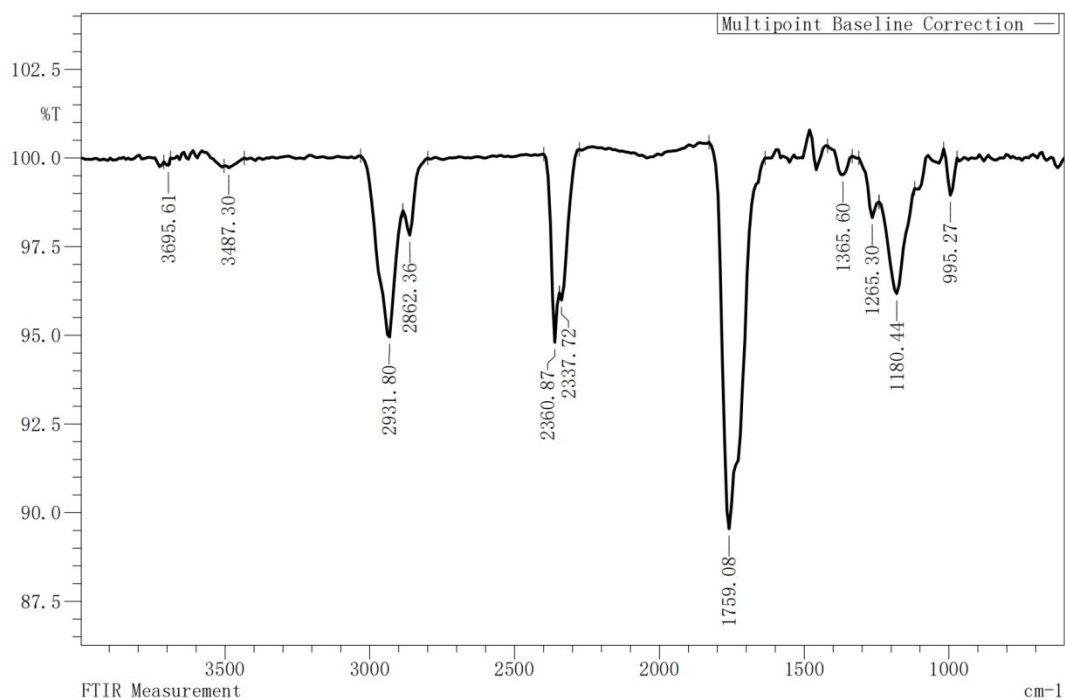
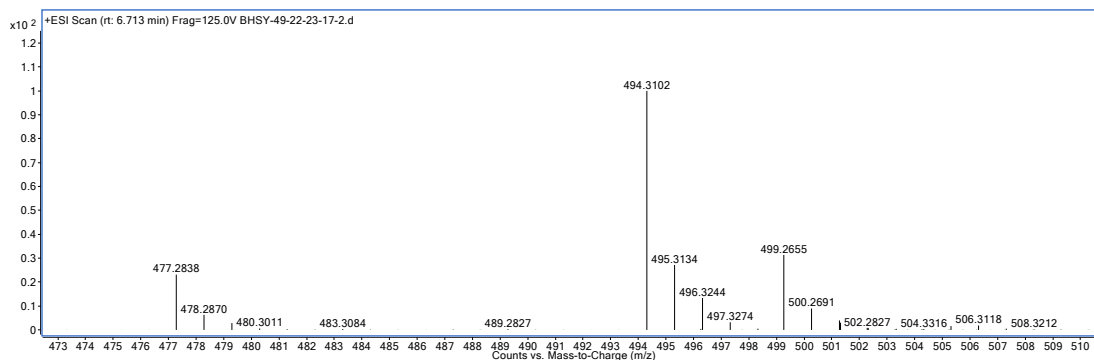


Figure S20. IR spectrum (film on KBr plate) of carabrolate B (2)



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	Ion Formula	m/z
C ₂₇ H ₄₀ O ₇	98.54	476.2765	476.2774	477.2847	1.85	C ₂₇ H ₄₁ O ₇	477.2838
C ₂₇ H ₄₀ O ₇	98.01	476.2764	476.2774	494.3112	2.16	C ₂₇ H ₄₄ NO ₇	494.3102

Figure S21. HRESIMS spectrum of carabrolate B (2).

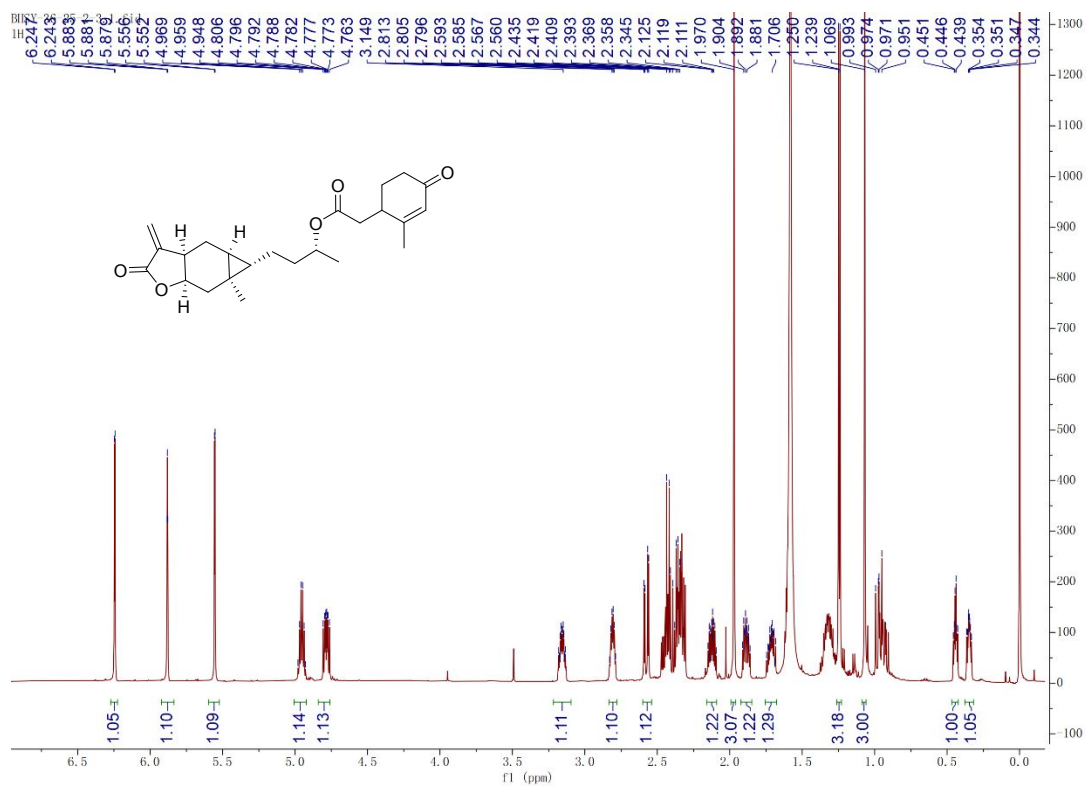


Figure S22. ^1H NMR spectrum (600 MHz) of carabrolate C (**3**) in CDCl_3

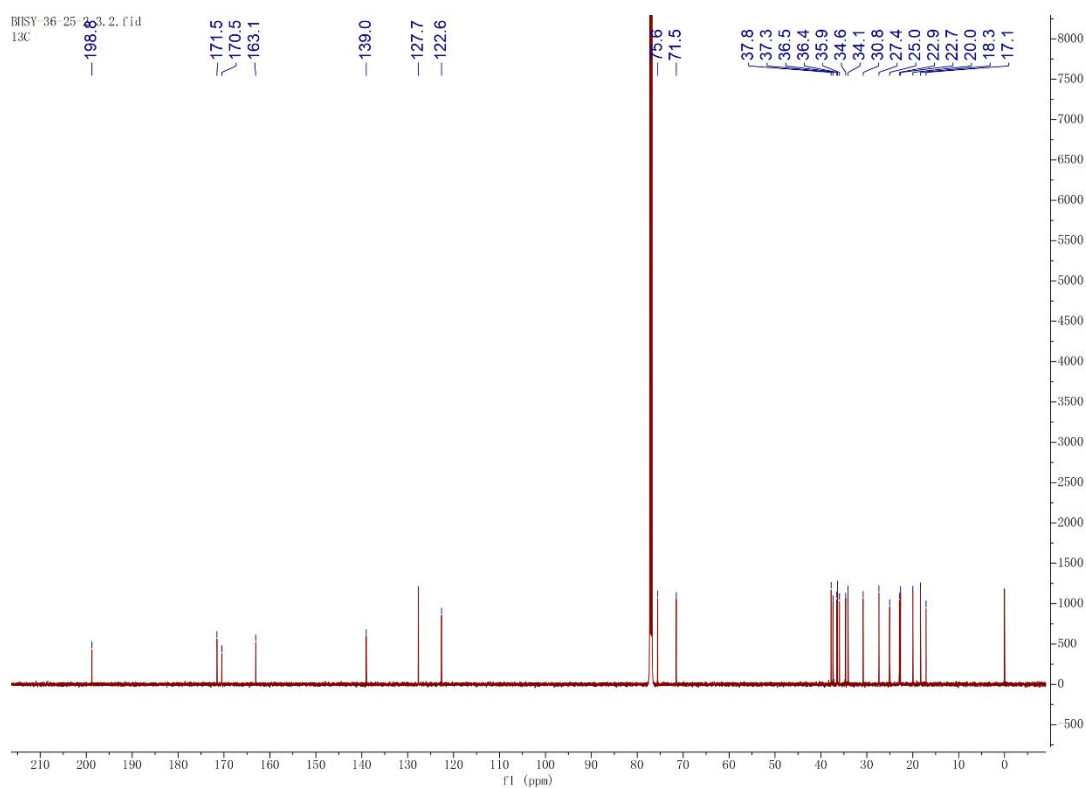


Figure S23. ^{13}C NMR spectrum (150 MHz) of carabrolate C (**3**) in CDCl_3

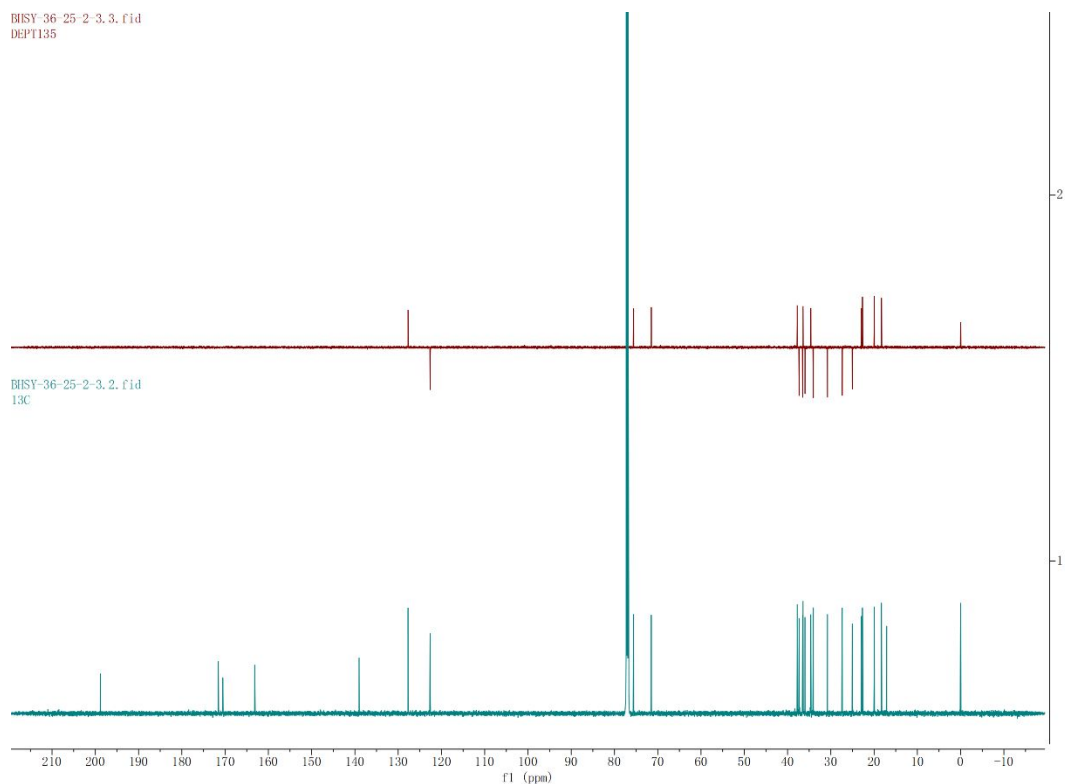


Figure S24. DEPT 135 spectrum (150 MHz) of carabrolate C (**3**) in CDCl_3

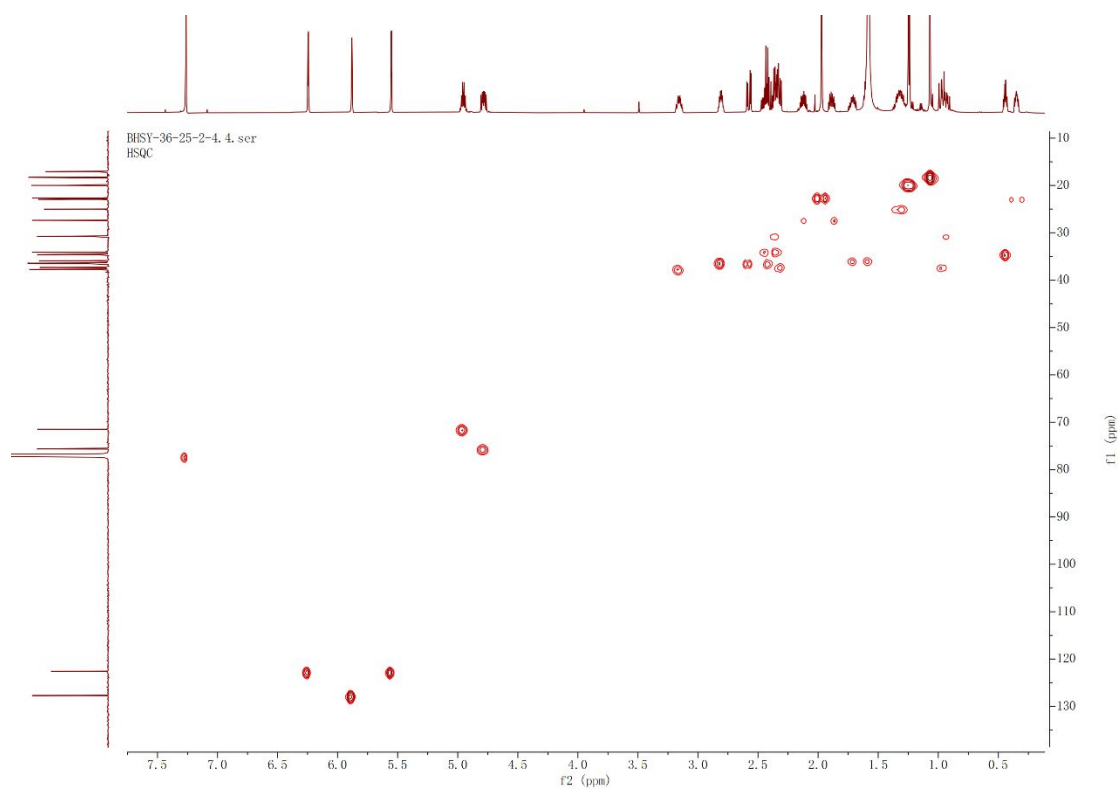


Figure S25. HSQC spectrum (600 MHz) of carabrolate C (**3**) in CDCl_3

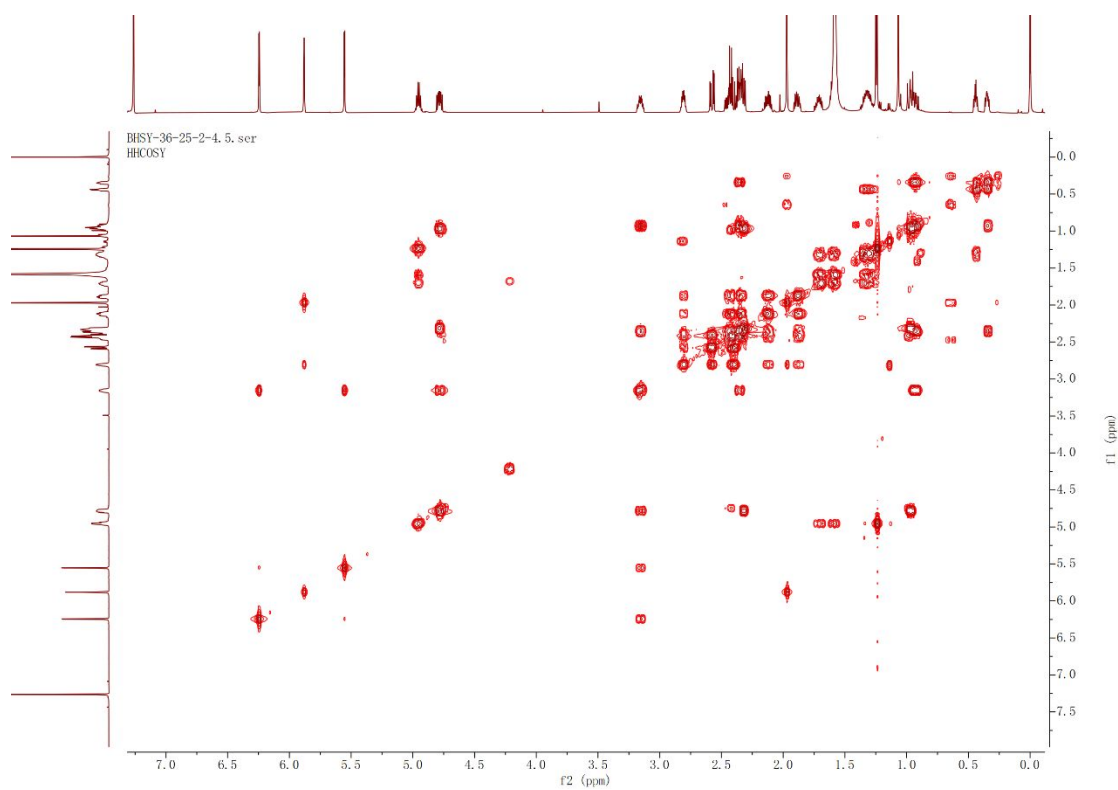


Figure S26. ^1H - ^1H COSY spectrum (600 MHz) of carabrolate C (**3**) in CDCl_3

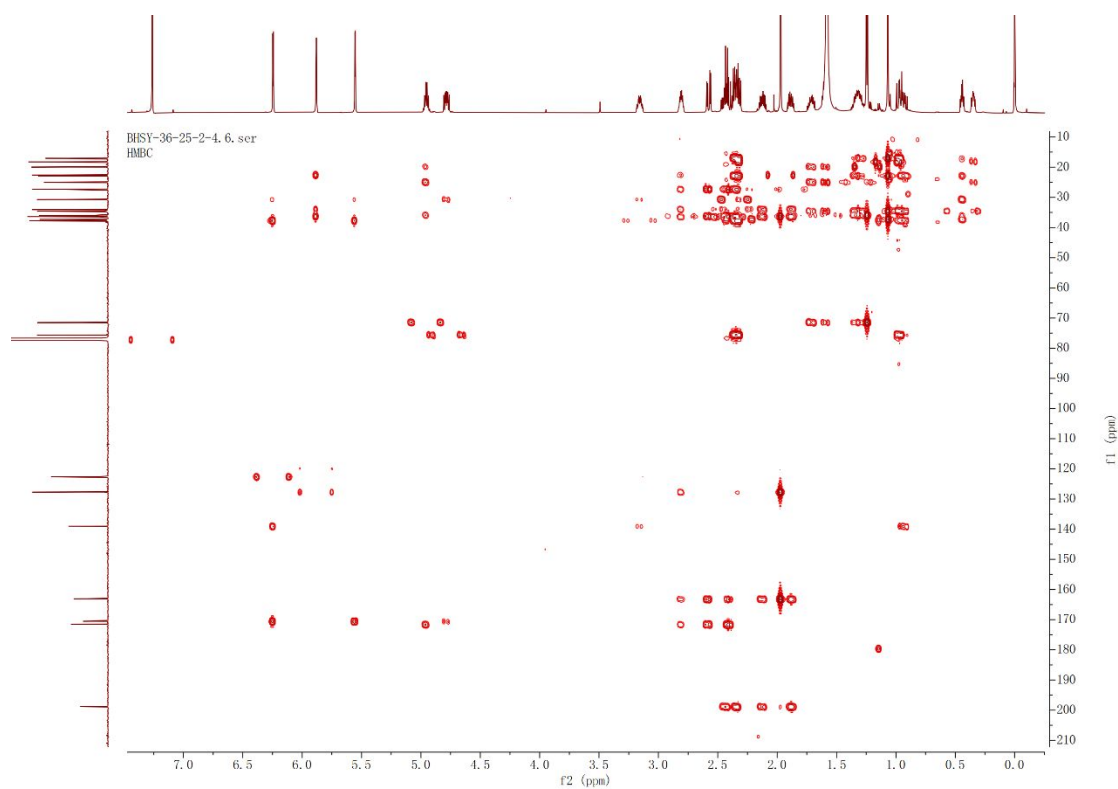


Figure S27. HMBC spectrum (600 MHz) of carabrolate C (**3**) in CDCl_3

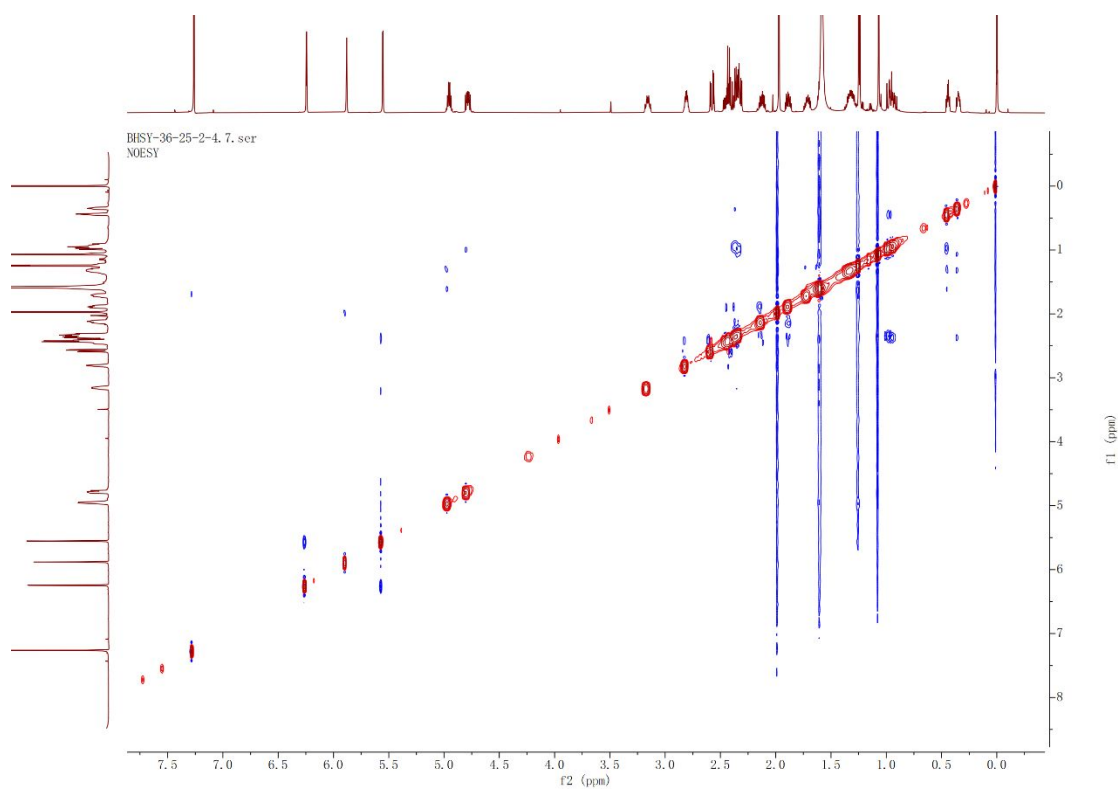


Figure S28. NOESY spectrum (600 MHz) of carabrolate C (**3**) in CDCl_3

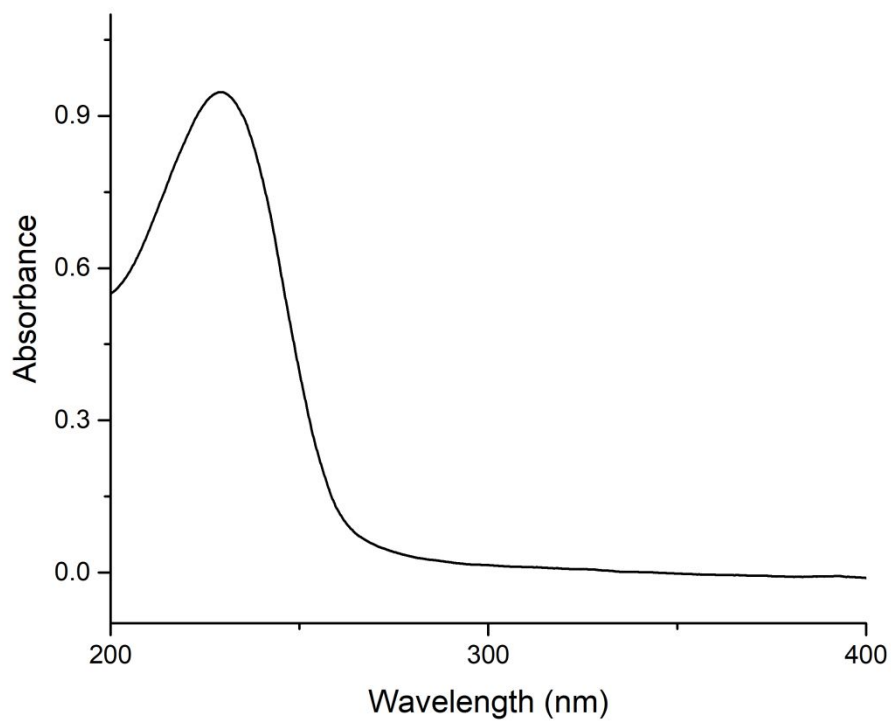


Figure S29. UV spectrum of carabrolate C (**3**) in MeOH

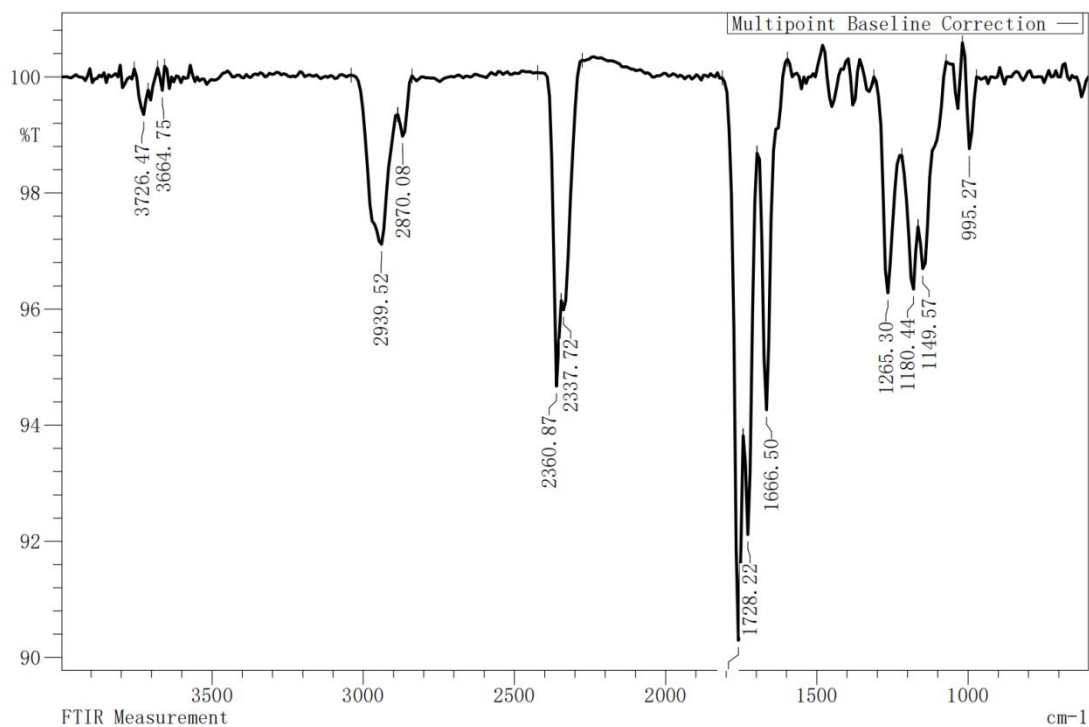
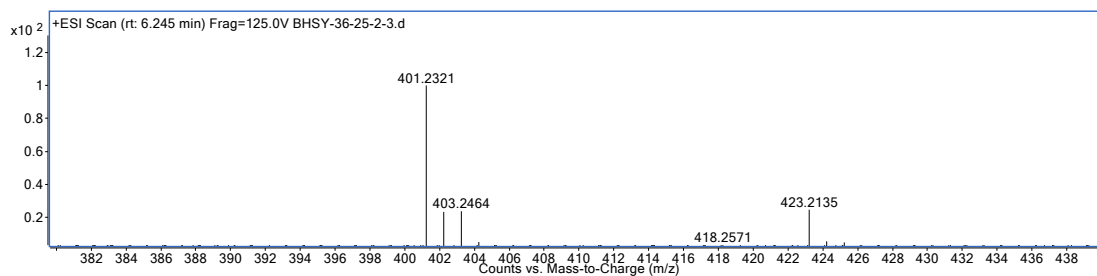


Figure S30. IR spectrum (film on KBr plate) of carabrolate C (**3**)



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	Ion Formula	m/z
C ₂₇ H ₄₀ O ₇	98.54	476.2765	476.2774	477.2847	1.85	C ₂₇ H ₄₁ O ₇	477.2838
C ₂₇ H ₄₀ O ₇	98.01	476.2764	476.2774	494.3112	2.16	C ₂₇ H ₄₄ NO ₇	494.3102

Figure S31. HRESIMS spectrum of carabrolate C (**3**)

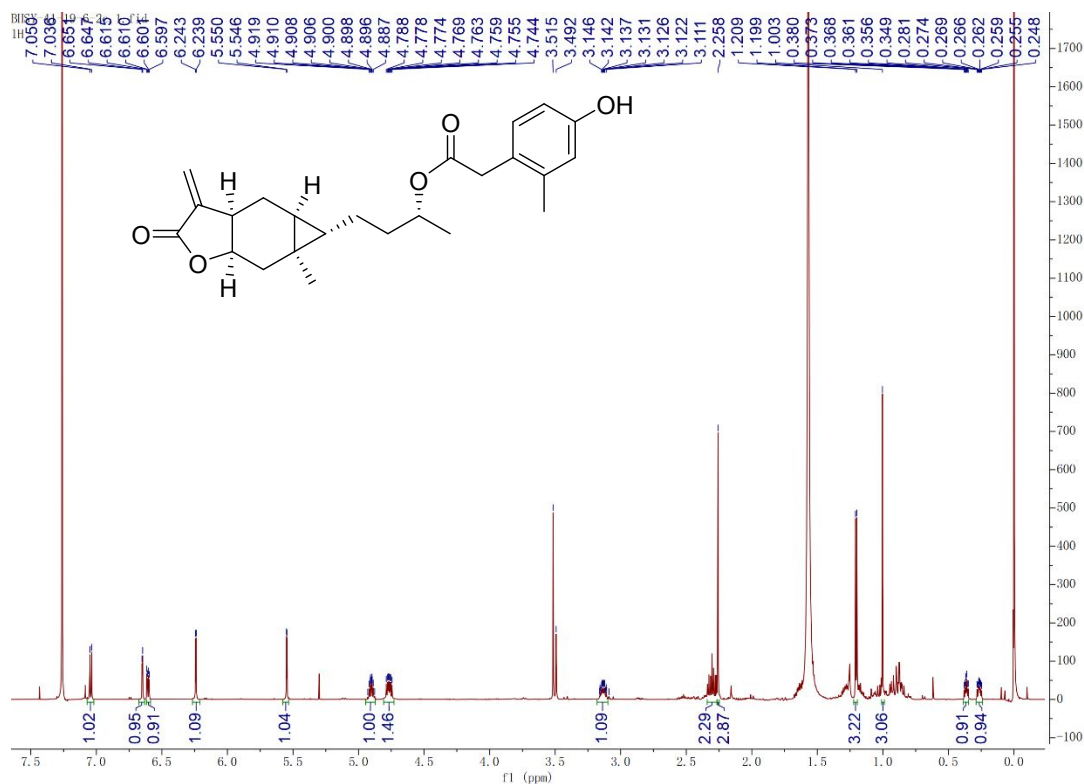


Figure S32. ^1H NMR spectrum (600 MHz) of carabrolate D (**4**) in CDCl_3

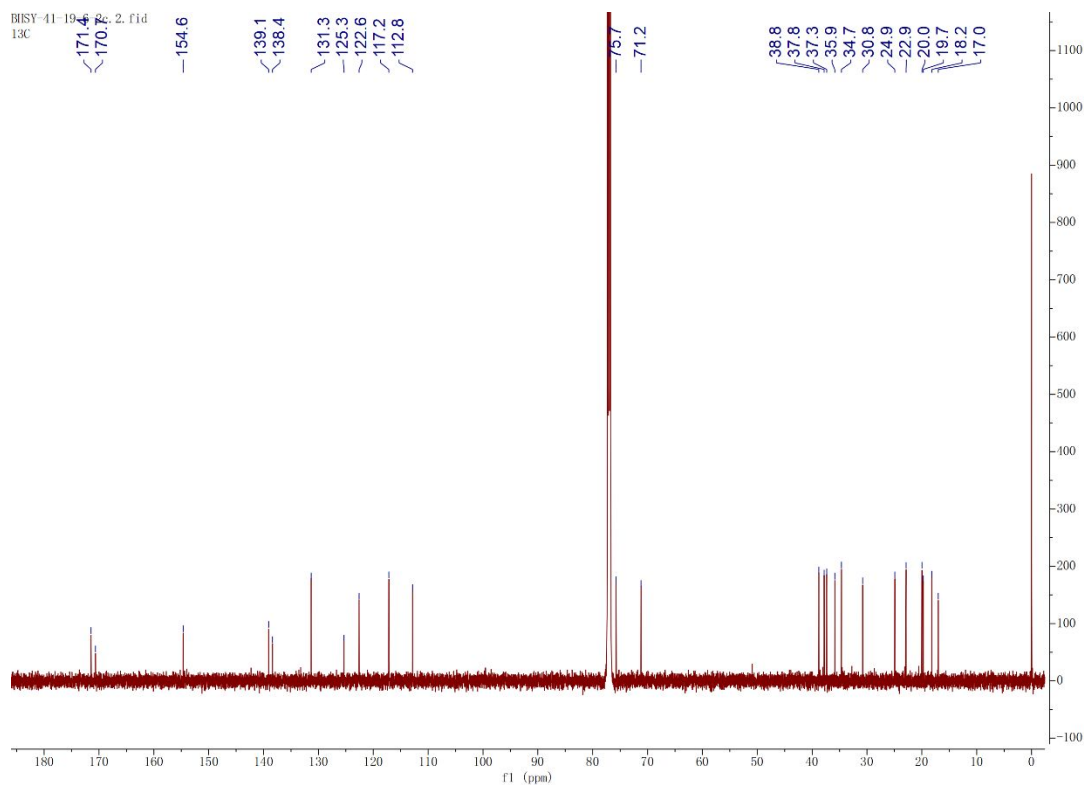


Figure S33. ^{13}C NMR spectrum (150 MHz) of carabrolate D (**4**) in CDCl_3

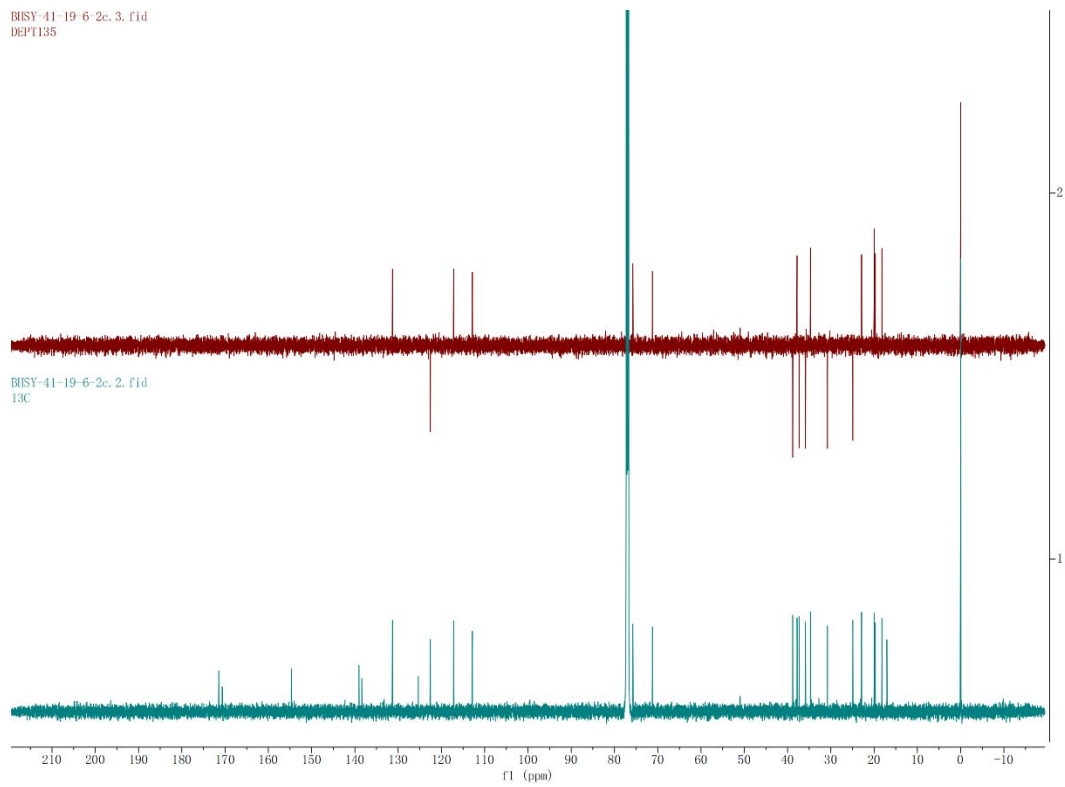


Figure S34. DEPT 135 spectrum (150 MHz) of carabrolate D (**4**) in CDCl_3

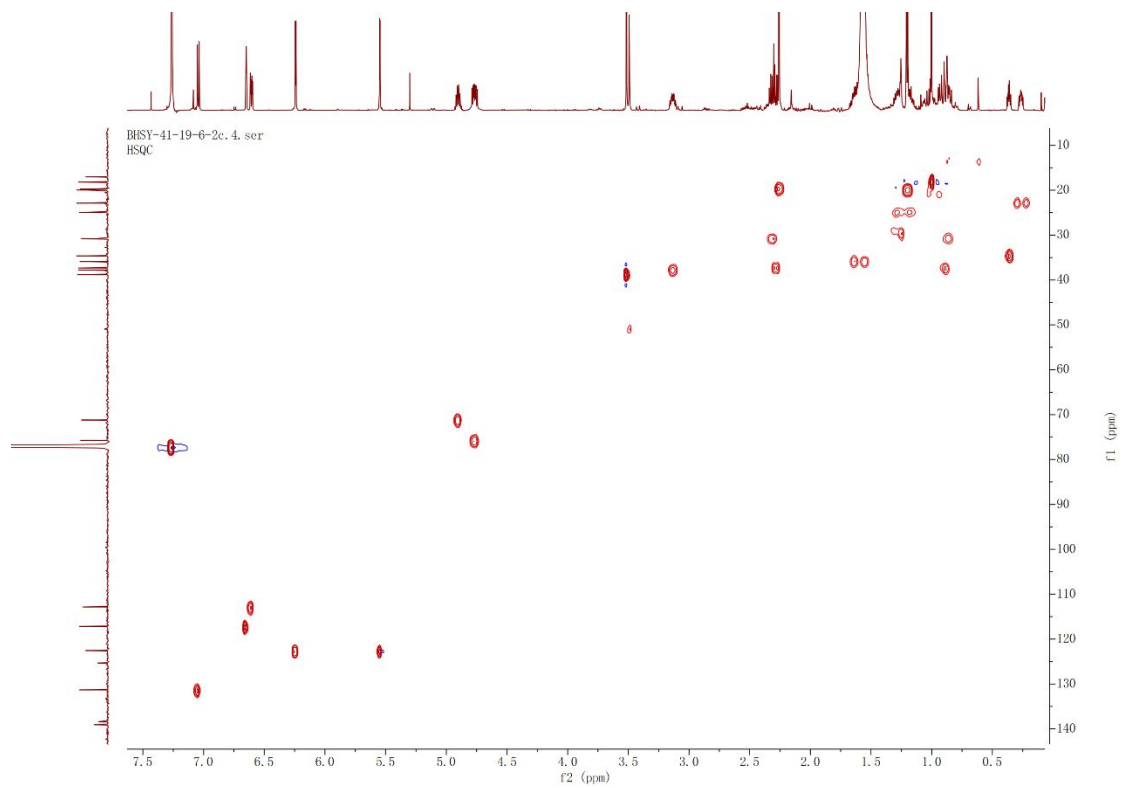


Figure S35. HSQC spectrum (600 MHz) of carabrolate D (**4**) in CDCl_3

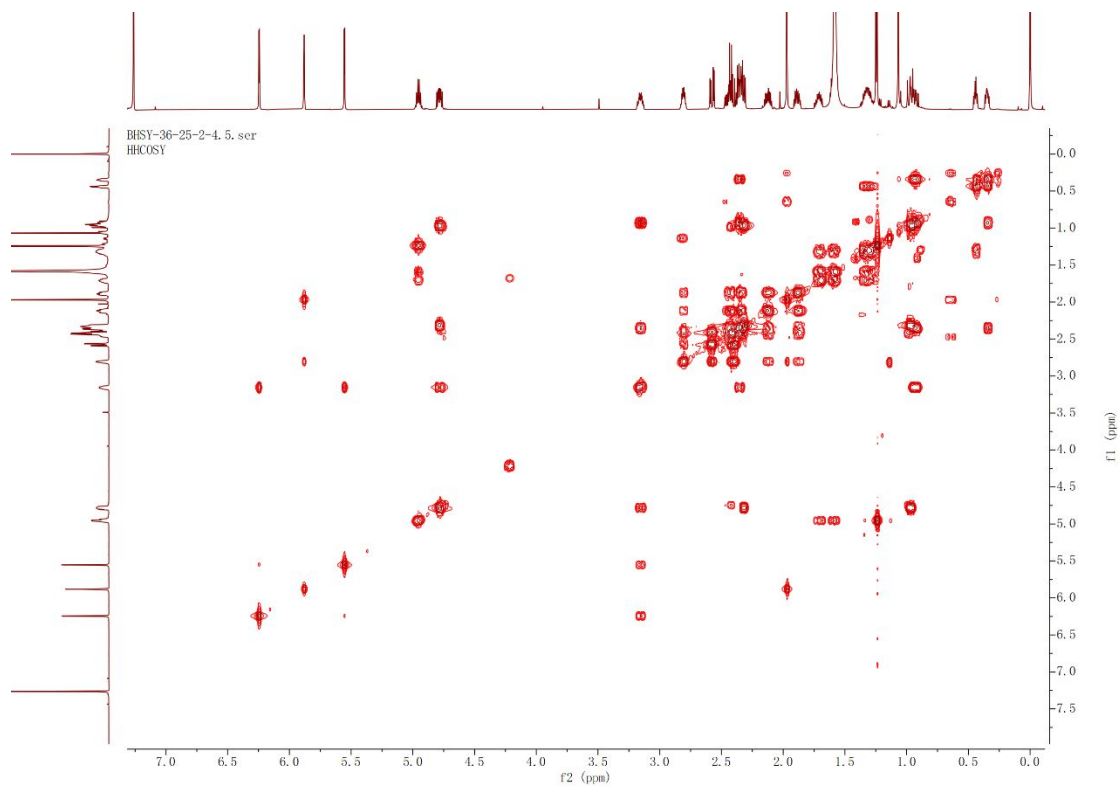


Figure S36. ^1H - ^1H COSY spectrum (600 MHz) of carabrolate D (**4**) in CDCl_3

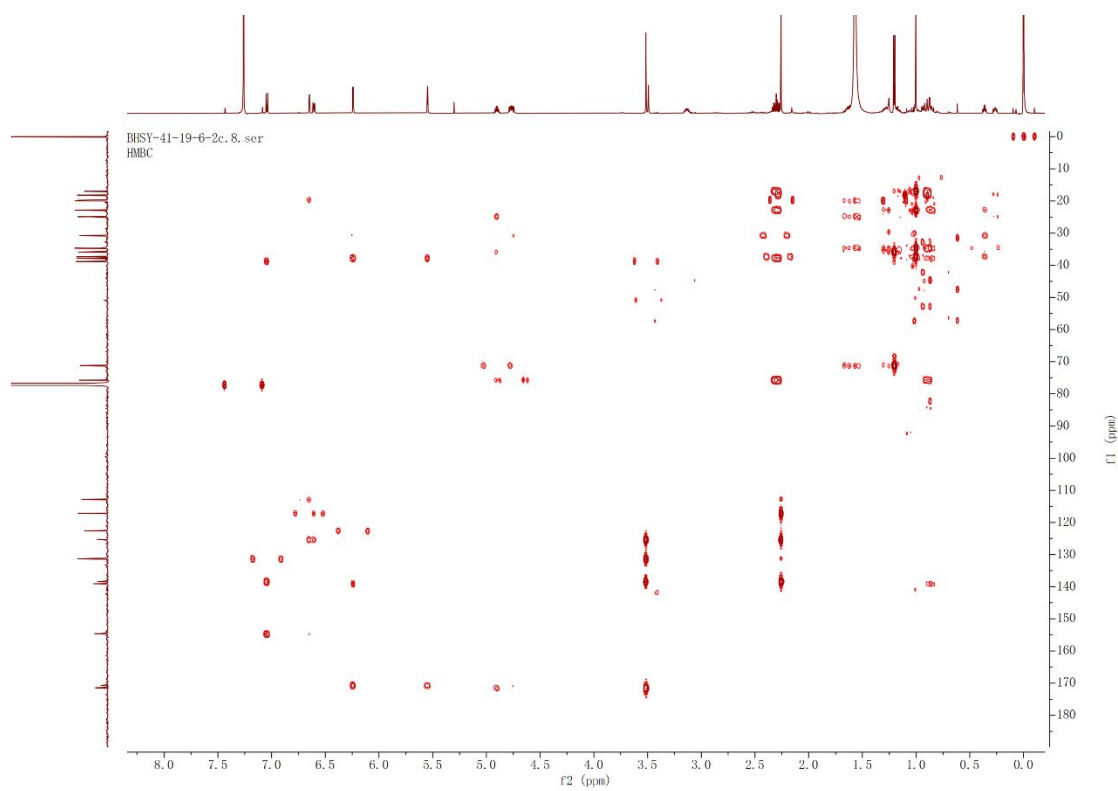


Figure S37. HMBC spectrum (600 MHz) of carabrolate D (**4**) in CDCl_3

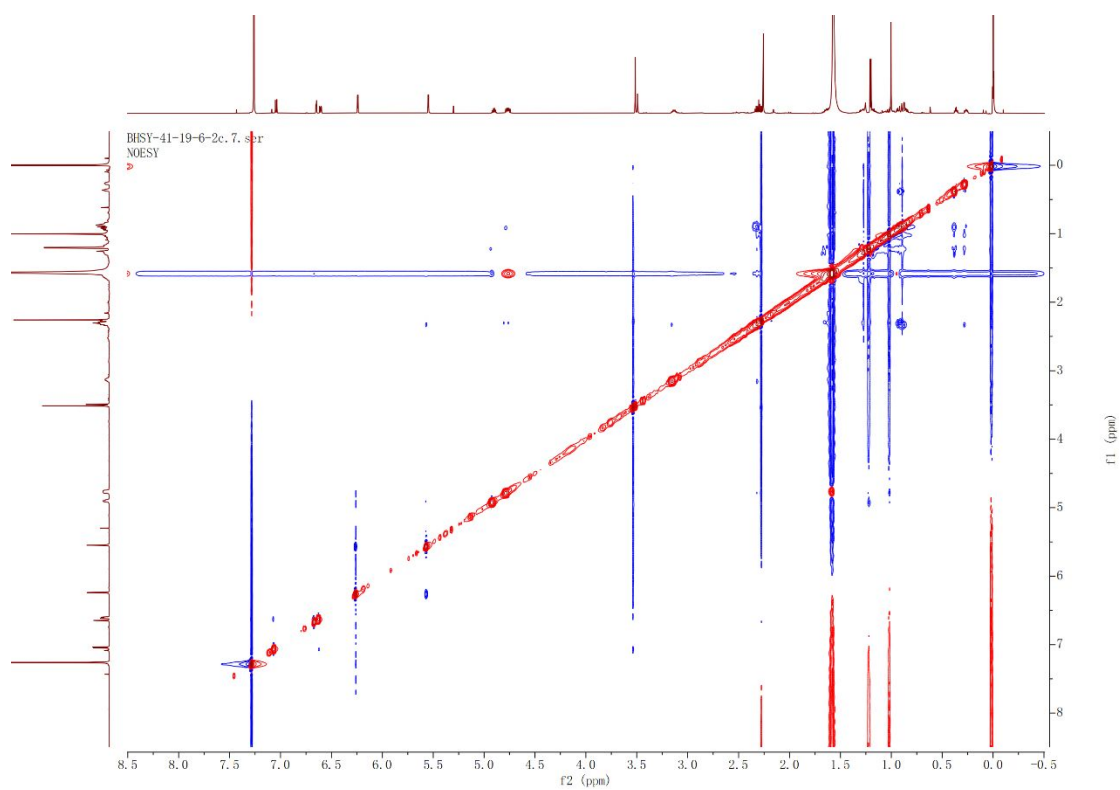


Figure S38. NOESY spectrum (600 MHz) of carabrolate D (**4**) in CDCl_3

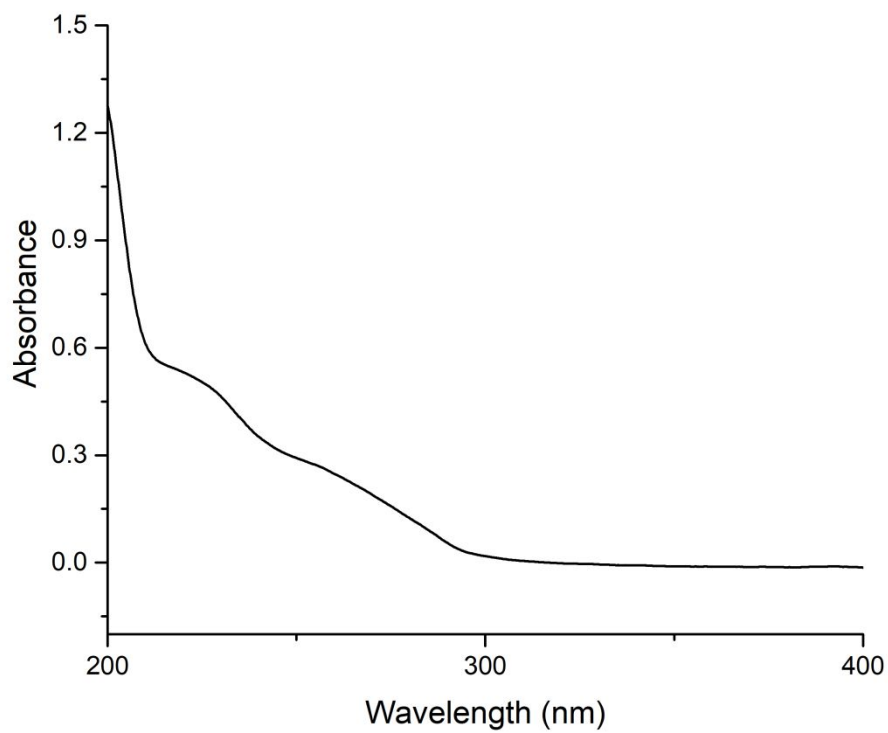


Figure S39. UV spectrum of carabrolate D (**4**) in MeOH

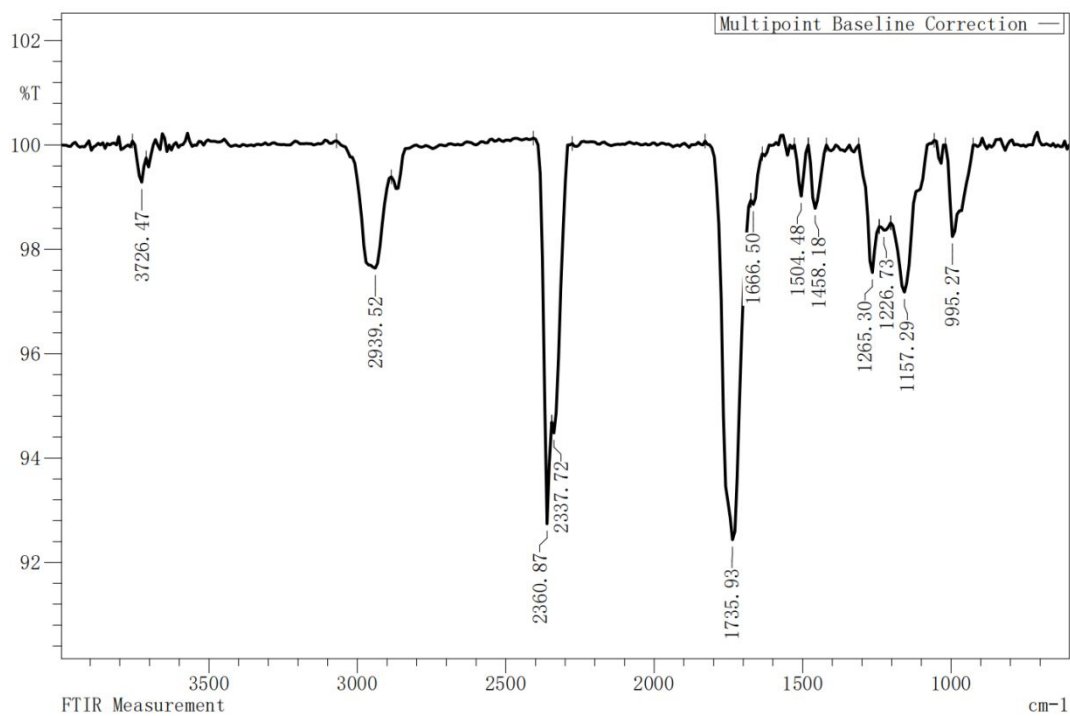
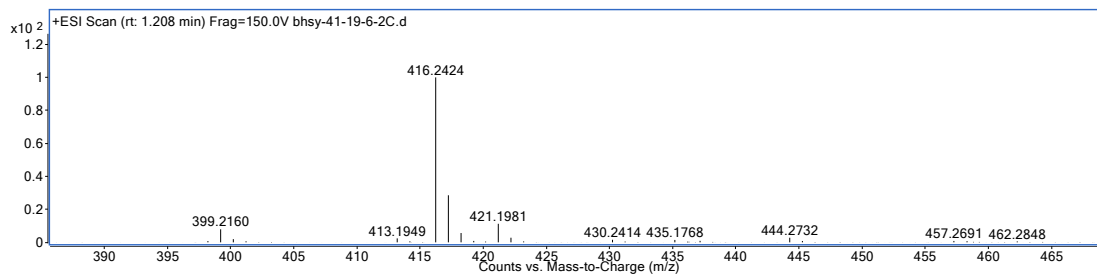


Figure S40. IR spectrum (film on KBr plate) of carabrolate D (4)



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	Ion Formula	m/z
C ₂₄ H ₃₀ O ₅	99.09	398.2087	398.2093	399.2166	1.51	C ₂₄ H ₃₁ O ₅	399.216
C ₂₄ H ₃₀ O ₅	98.59	398.2086	398.2093	416.2431	1.88	C ₂₄ H ₃₄ NO ₅	416.2424

Figure S41. HRESIMS spectrum of carabrolate D (4)

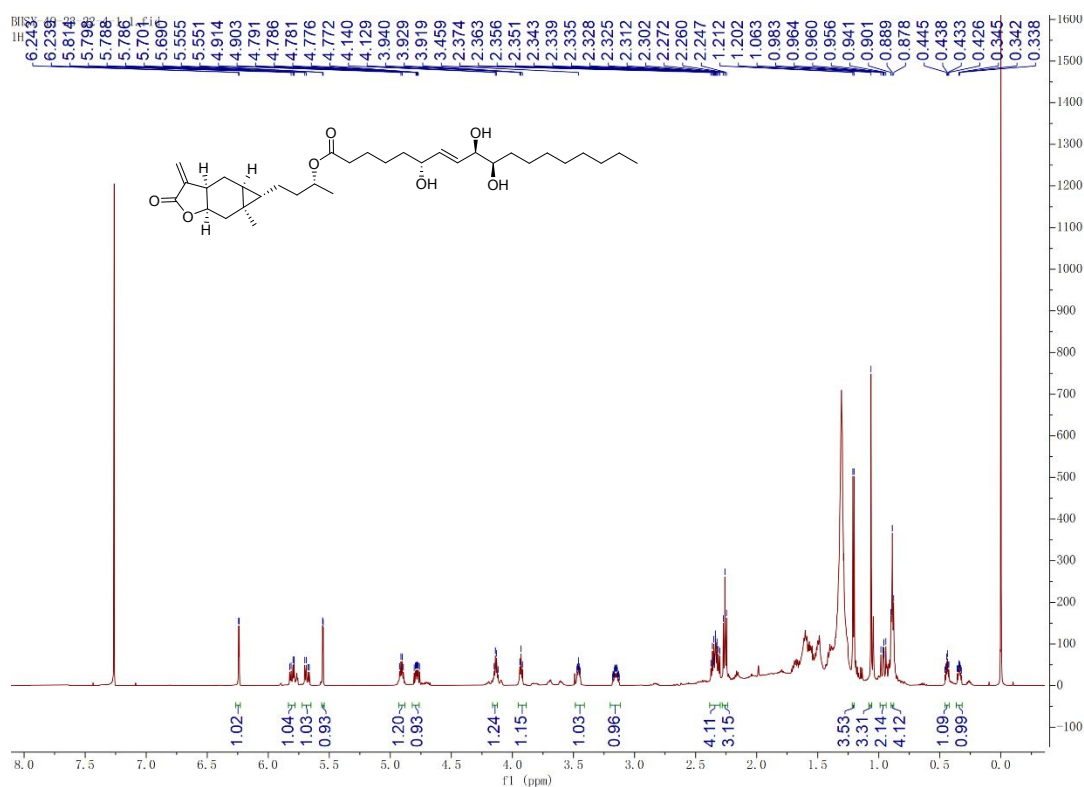


Figure S42. ^1H NMR spectrum (600 MHz) of carabrolate E (**5**) in CDCl_3

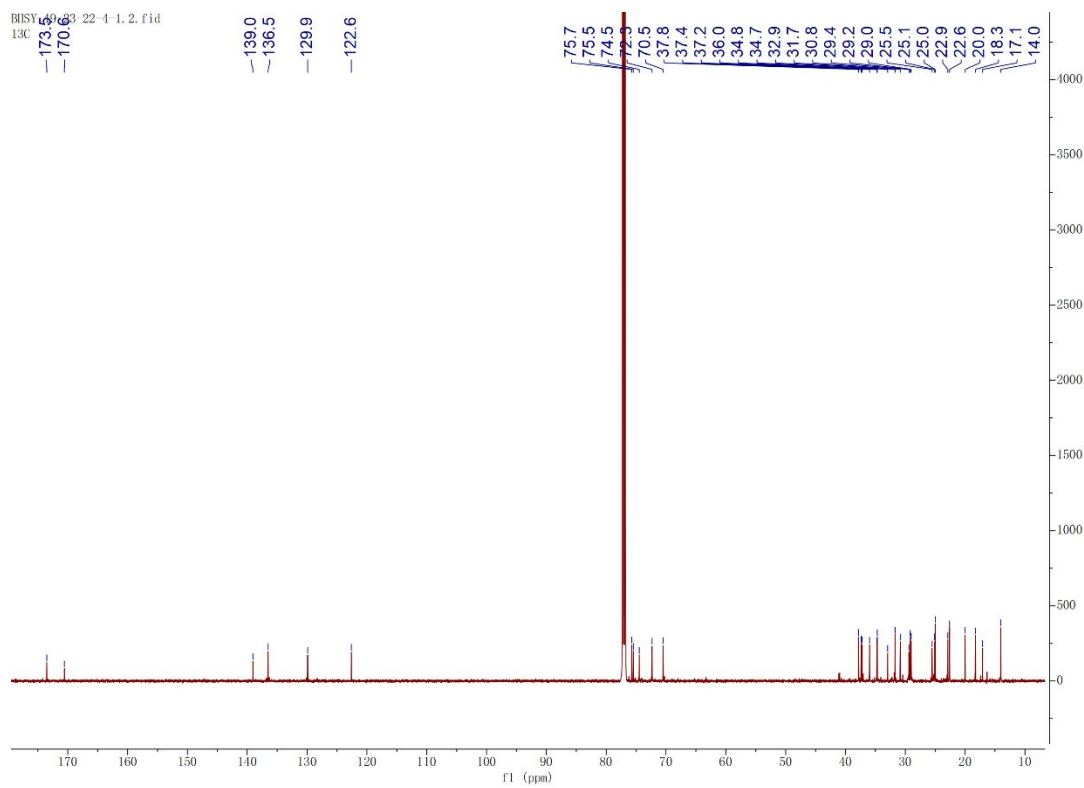


Figure S43. ^{13}C NMR spectrum (150 MHz) of carabrolate E (**5**) in CDCl_3



Figure S44. DEPT 135 spectrum (150 MHz) of carabrolate E (**5**) in CDCl_3

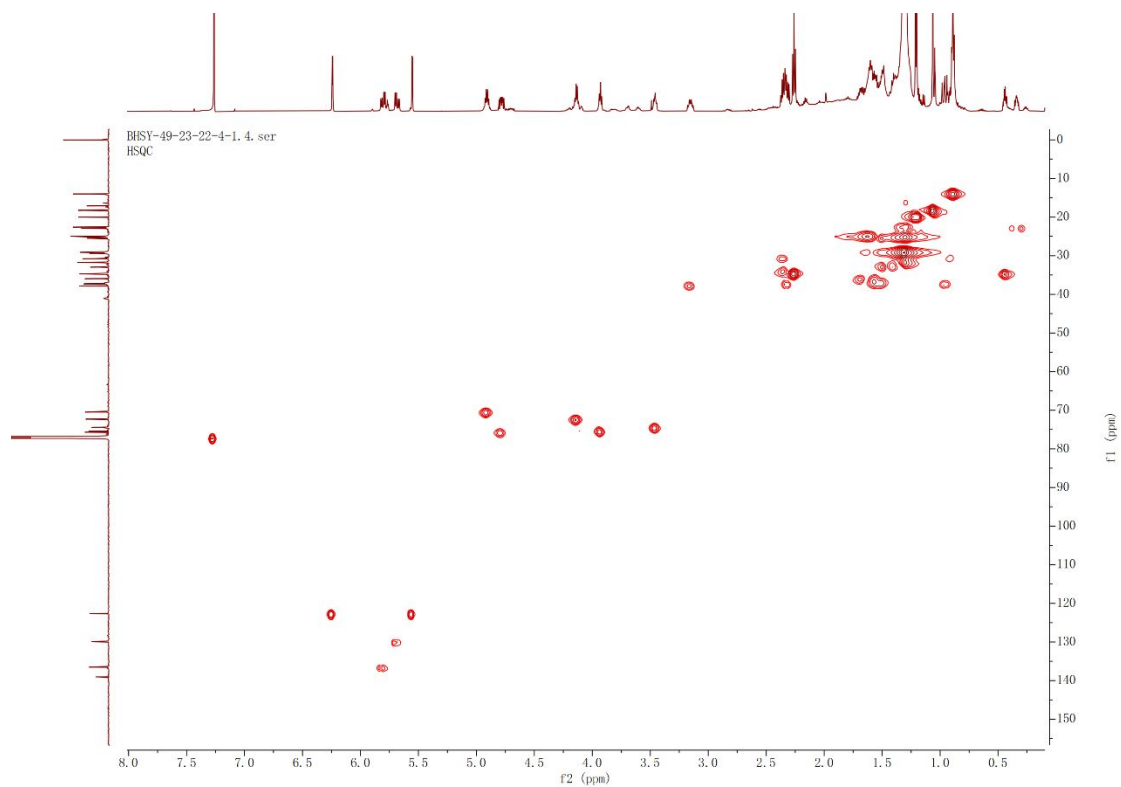


Figure S45. HSQC spectrum (600 MHz) of carabrolate E (**5**) in CDCl_3

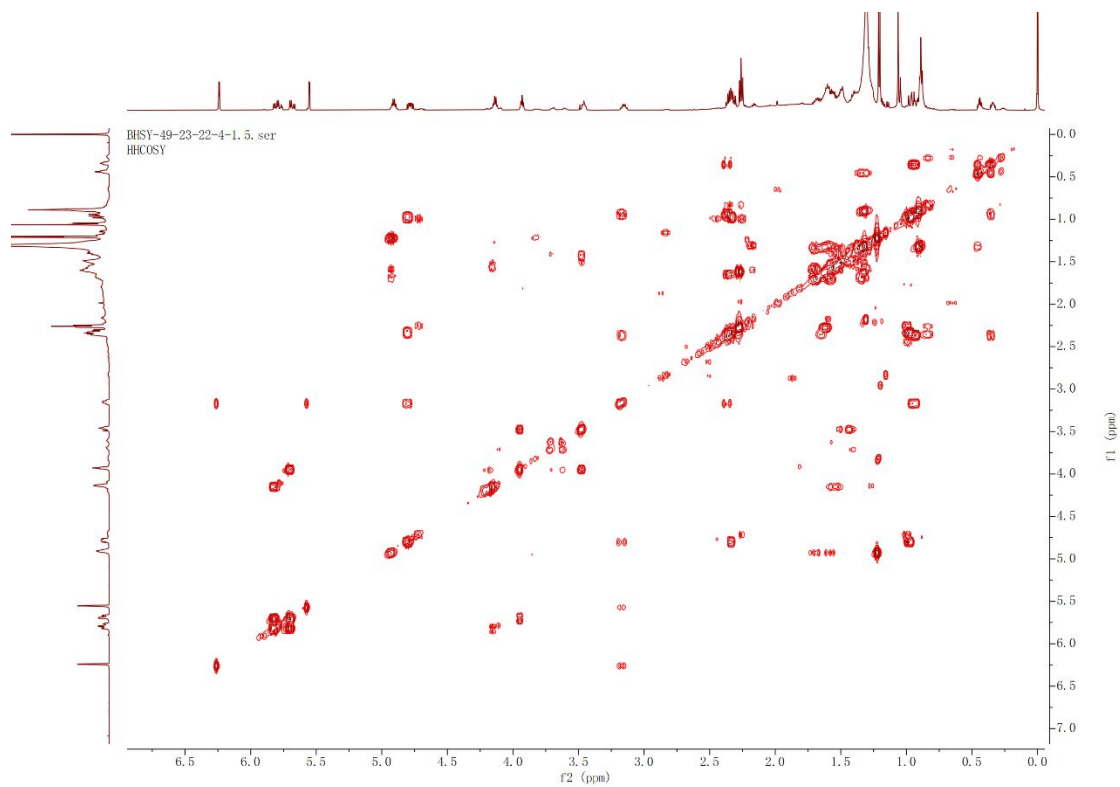


Figure S46. ^1H - ^1H COSY spectrum (600 MHz) of carabrolate E (**5**) in CDCl_3

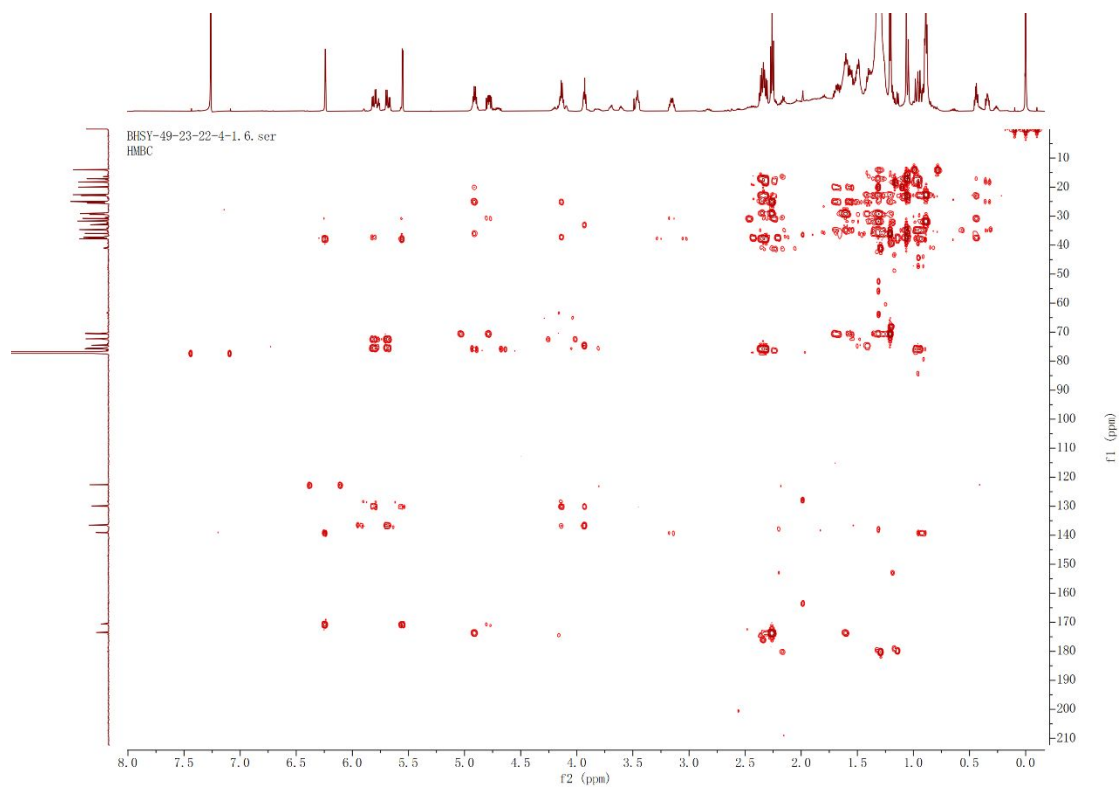


Figure S47. HMBC spectrum (600 MHz) of carabrolate E (**5**) in CDCl_3

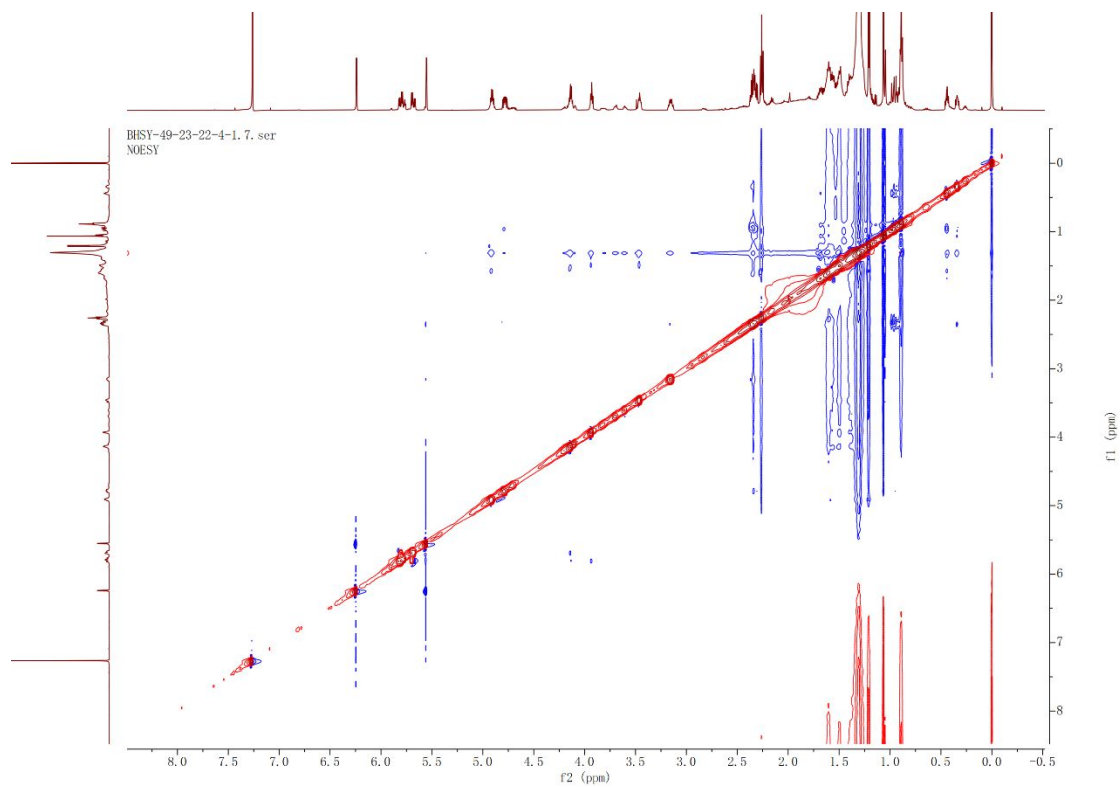


Figure S48. NOESY spectrum (600 MHz) of carabrolate E (**5**) in CDCl_3

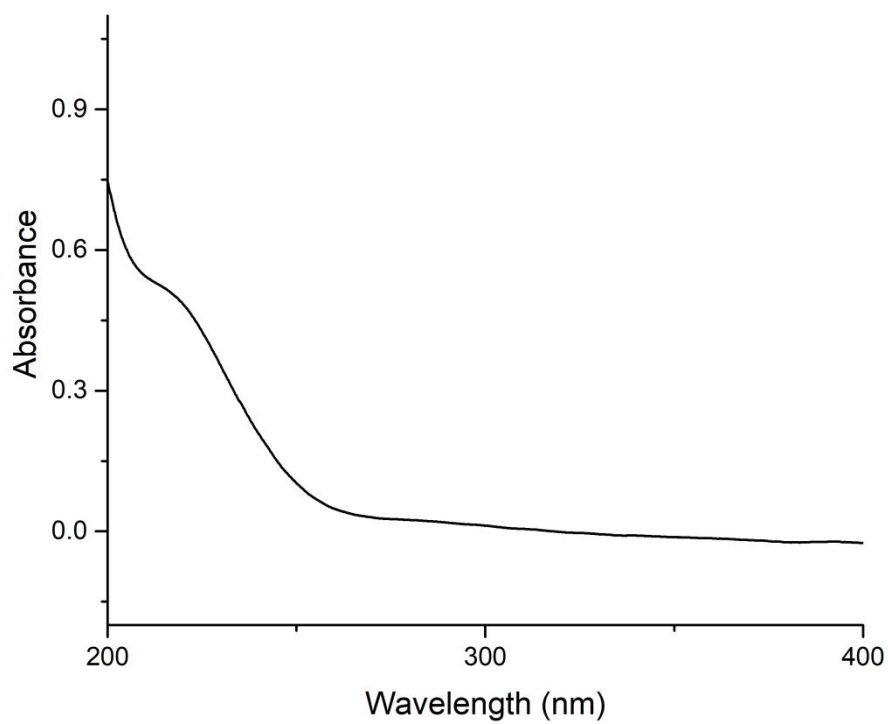


Figure S49. UV spectrum of carabrolate E (**5**) in MeOH

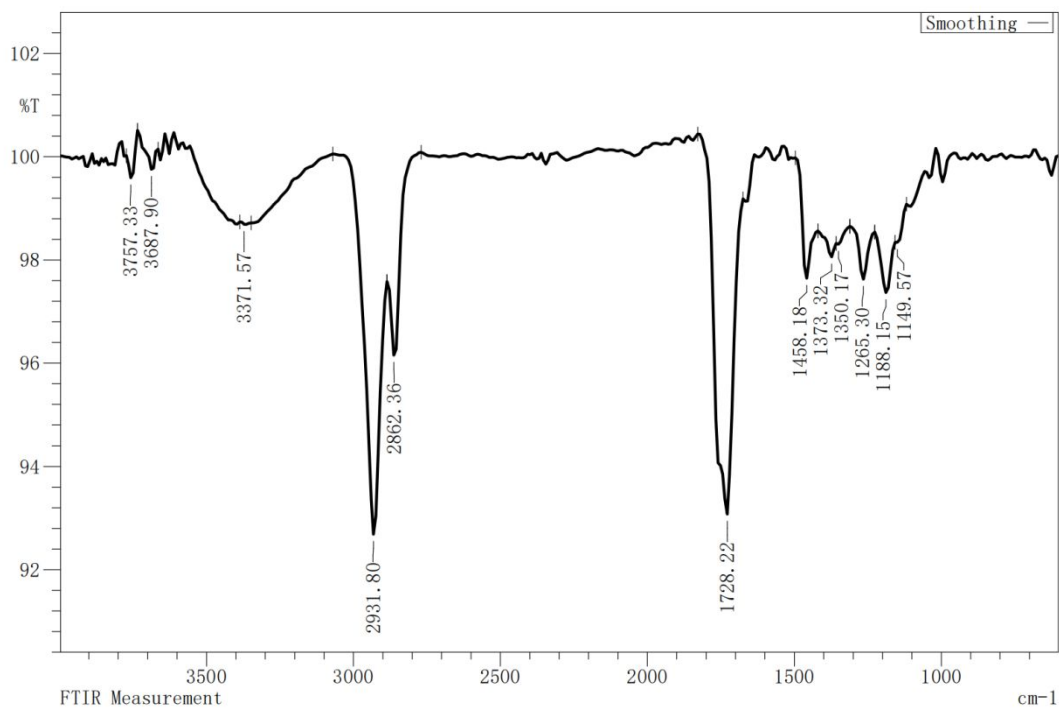
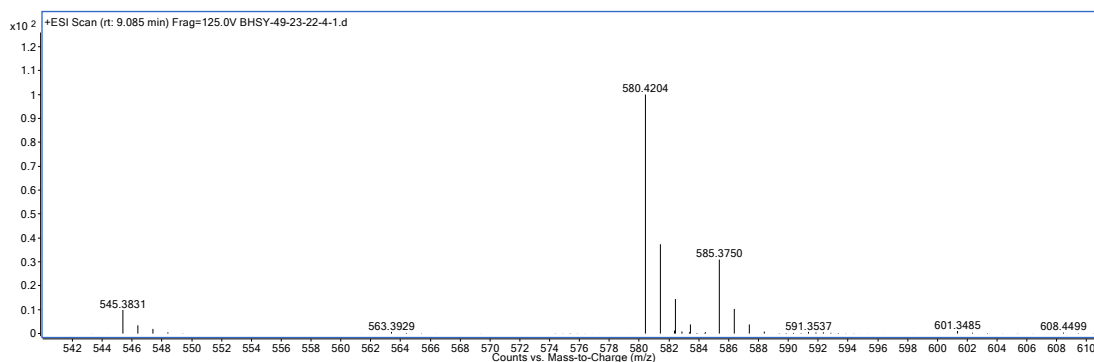


Figure S50. IR spectrum (film on KBr plate) of carabrolate E (5)



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	Ion Formula	m/z
C ₃₃ H ₅₄ O ₇	99.77	562.3866	562.387	580.4208	0.68	C ₃₀ H ₅₈ NO ₇	580.4204
C ₃₃ H ₅₄ O ₇	97.86	562.3858	562.387	585.3762	2.09	C ₃₀ H ₅₄ NaO ₇	585.375

Figure S51. HRESIMS spectrum of carabrolate E (5)

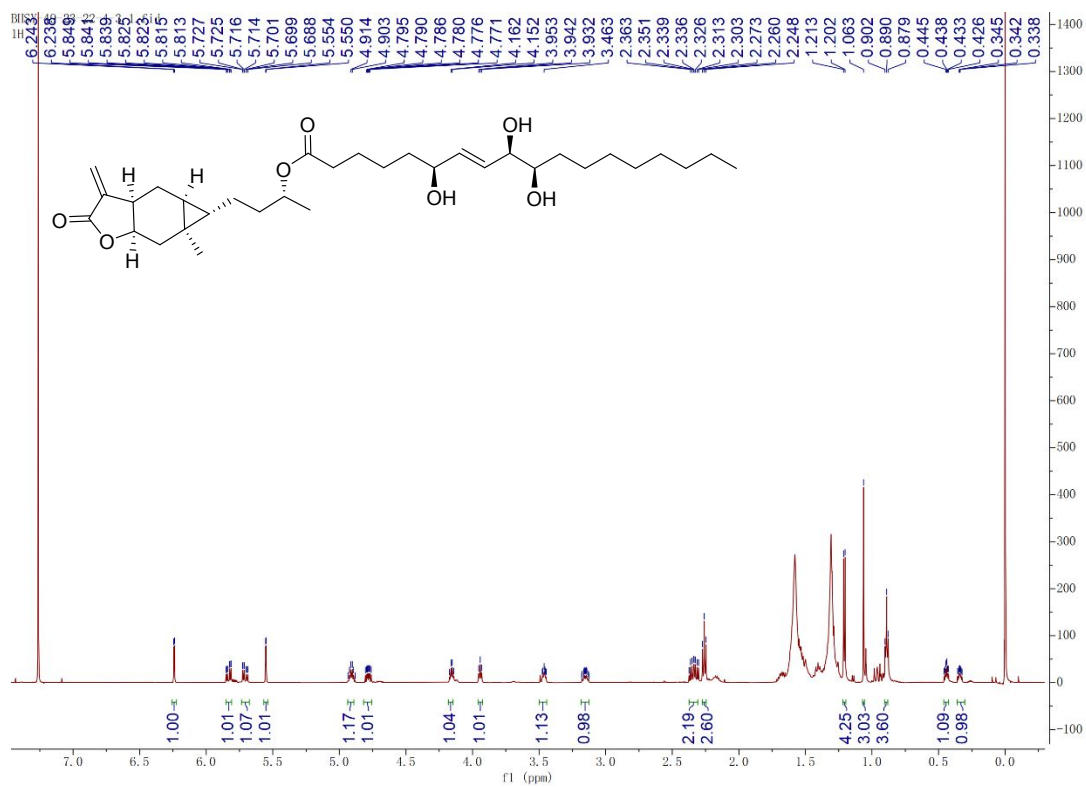


Figure S52. ^1H NMR spectrum (600 MHz) of carabrolate F (6) in CDCl_3

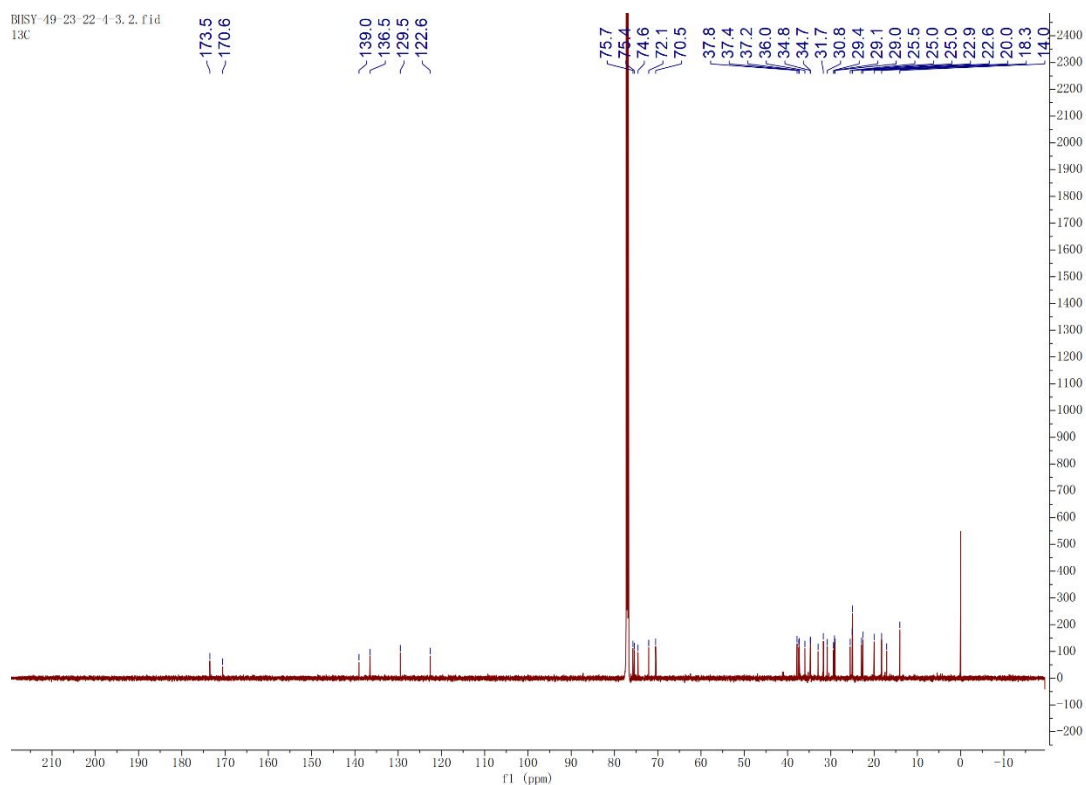


Figure S53. ^{13}C NMR spectrum (150 MHz) of carabrolate F (6) in CDCl_3

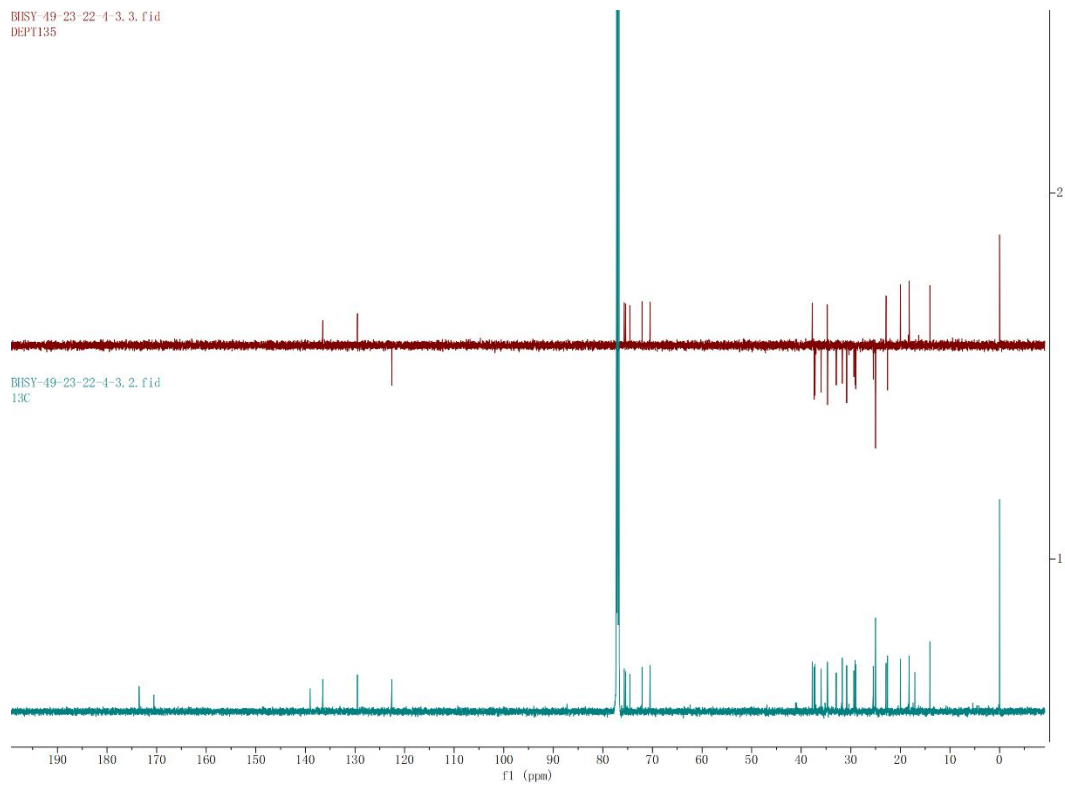


Figure S54. DEPT 135 spectrum (150 MHz) of carabrolate F (**6**) in CDCl_3

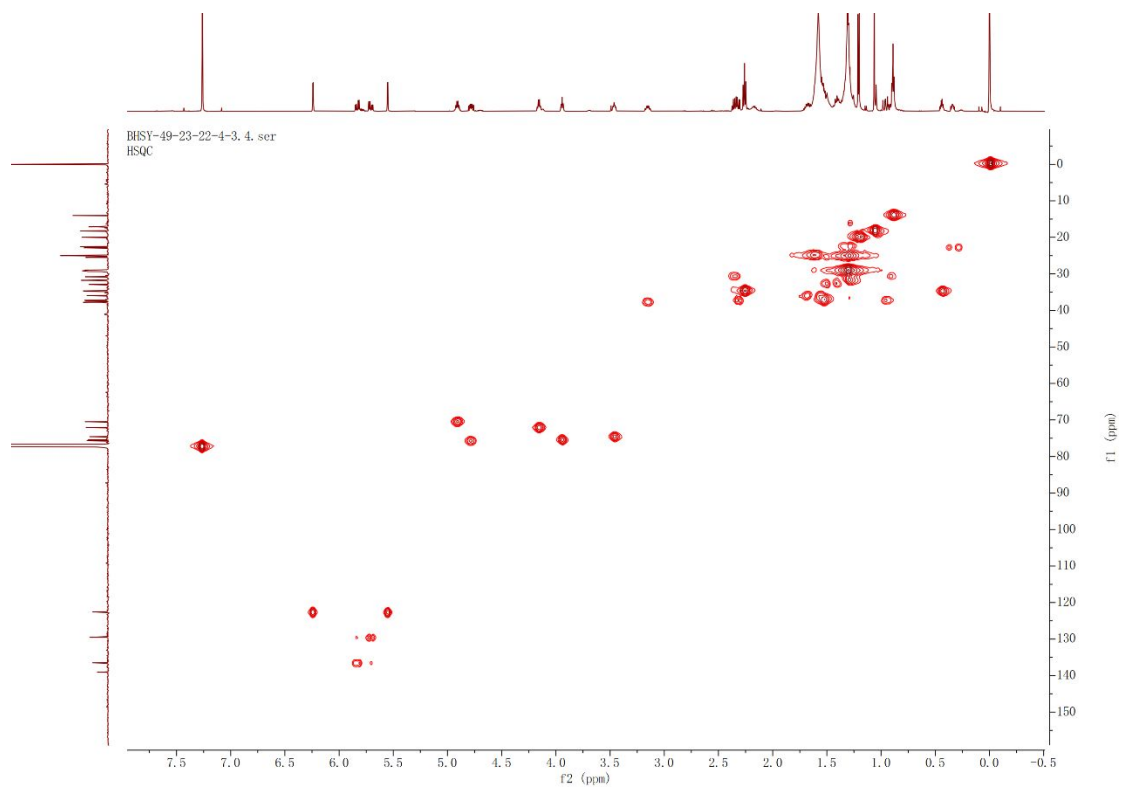


Figure S55. HSQC spectrum (600 MHz) of carabrolate F (**6**) in CDCl_3

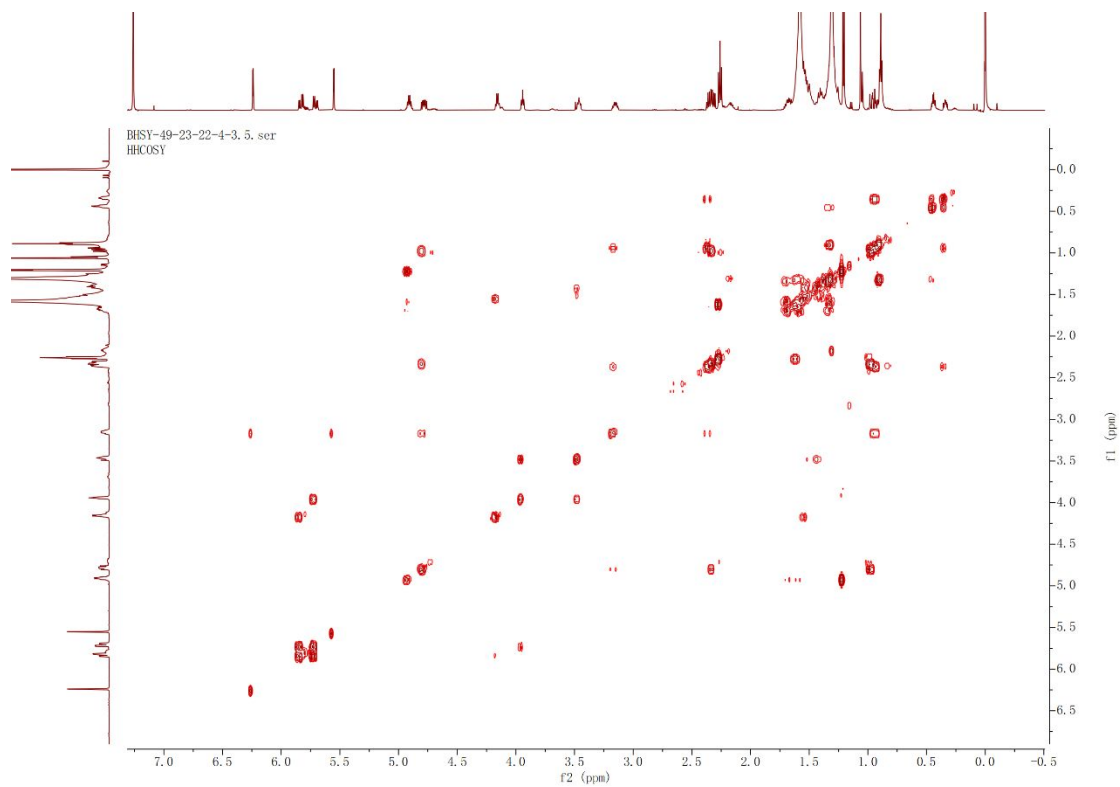


Figure S56. ^1H - ^1H COSY spectrum (600 MHz) of carabrolate F (**6**) in CDCl_3

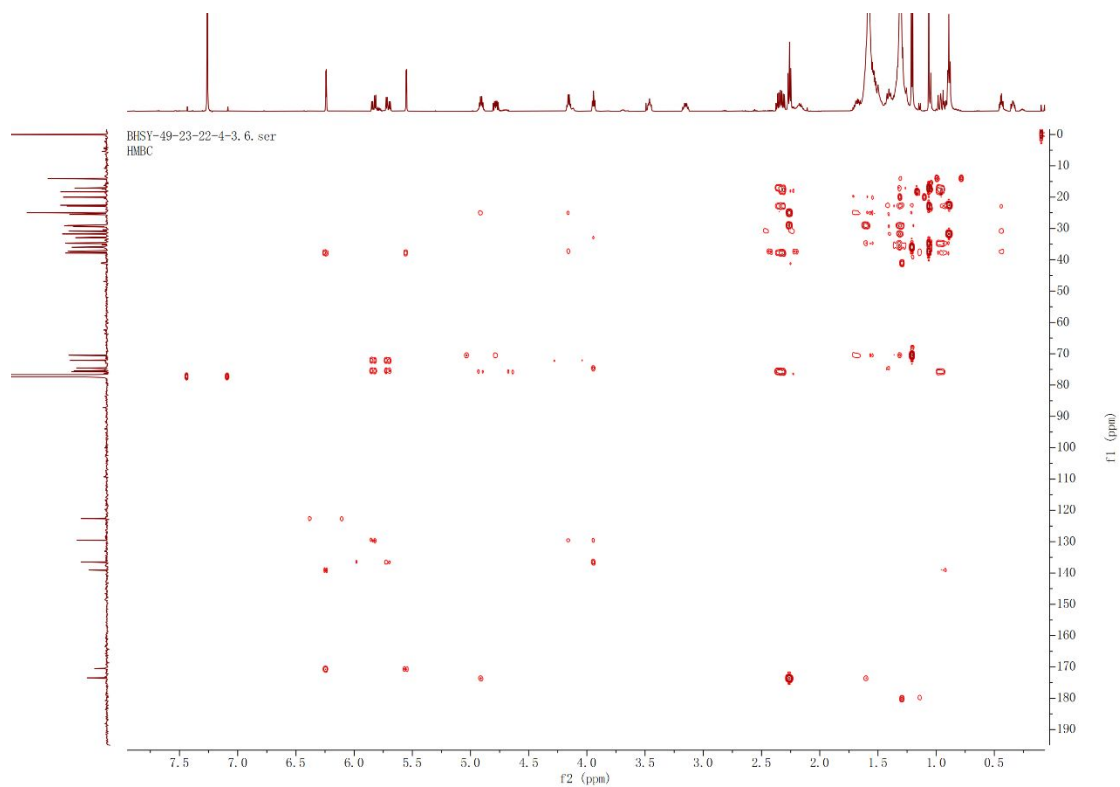


Figure S57. HMBC spectrum (600 MHz) of carabrolate F (**6**) in CDCl_3

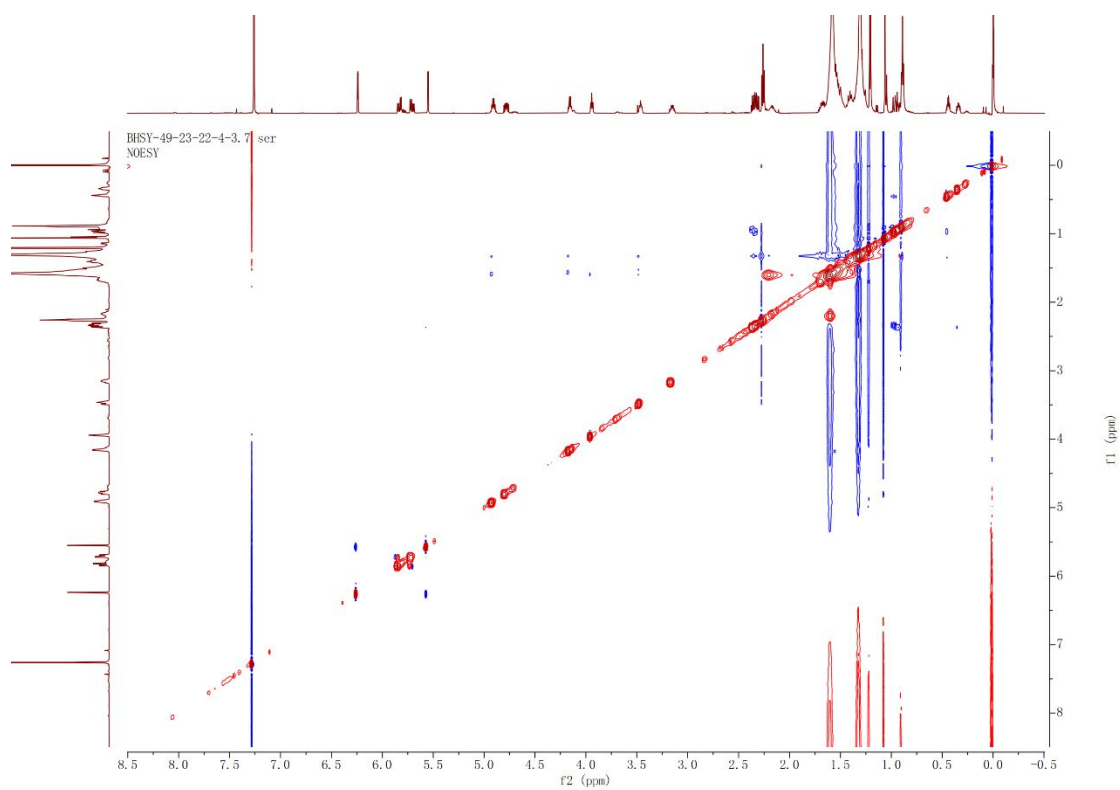


Figure S58. NOESY spectrum (600 MHz) of carabrolate F (**6**) in CDCl_3

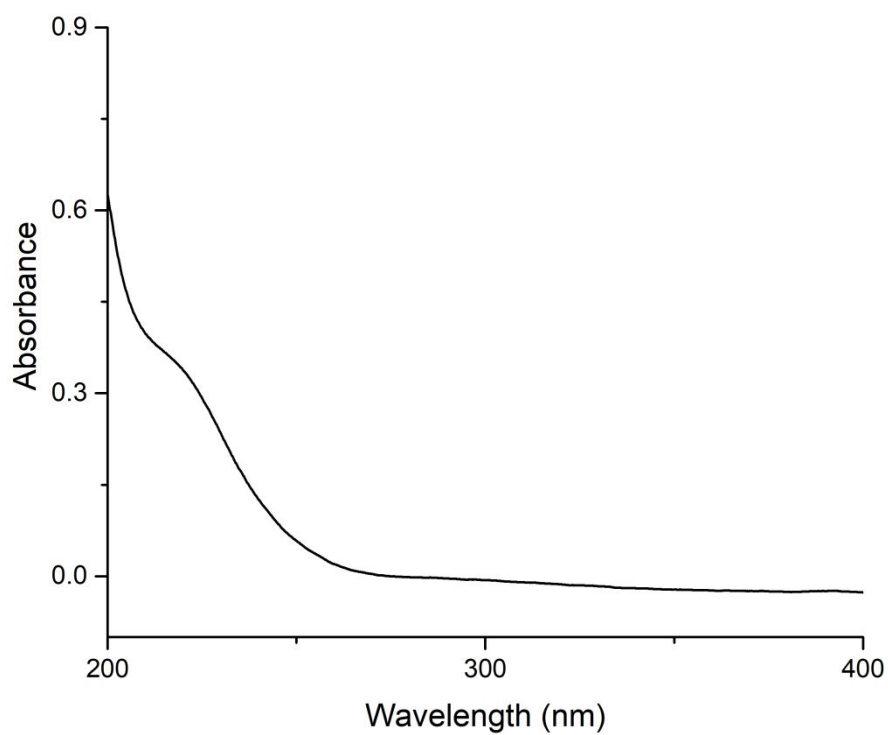


Figure S59. UV spectrum of carabrolate F (**6**) in MeOH

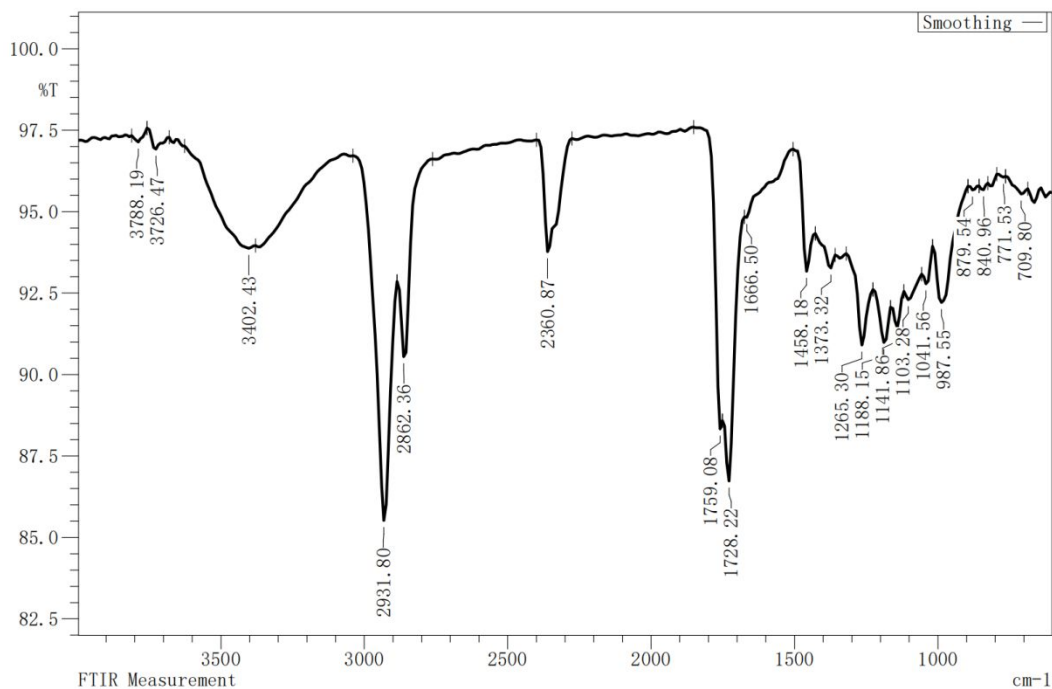
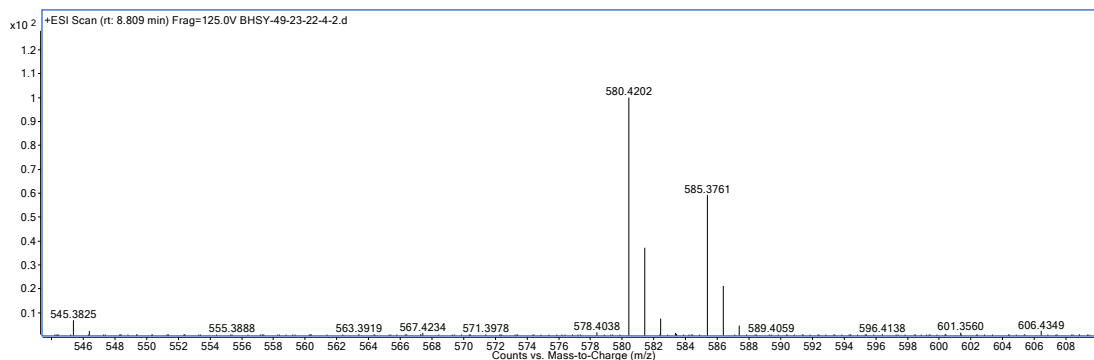
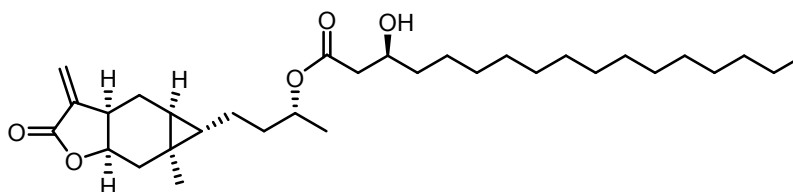


Figure S60. IR spectrum (film on KBr plate) of carabrolate F (6)



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	Ion Formula	m/z
C ₃₃ H ₅₄ O ₇	99.47	562.3864	562.387	580.4208	1.03	C ₃₀ H ₅₈ NO ₇	580.4202
C ₃₃ H ₅₄ O ₇	99.99	562.3869	562.387	585.3762	0.13	C ₃₀ H ₅₄ NaO ₇	585.3761

Figure S61. HRESIMS spectrum of carabrolate F (6)



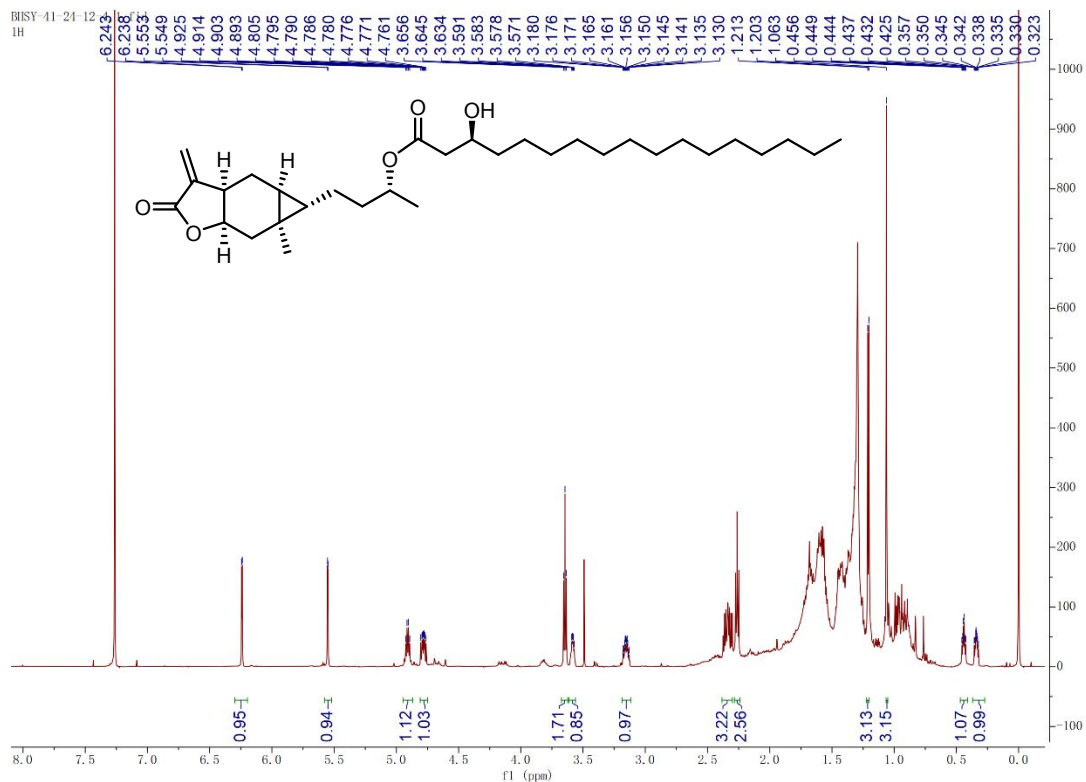


Figure S62. ^1H NMR spectrum (600 MHz) of carabrolate G (**7**) in CDCl_3

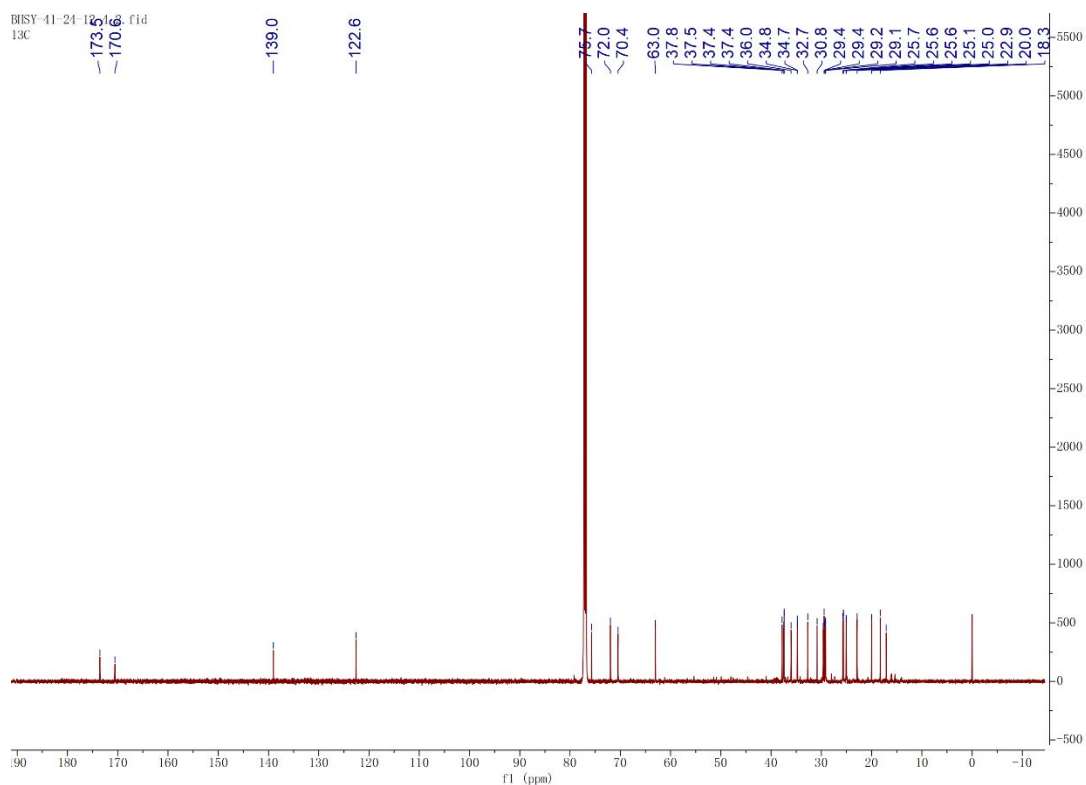


Figure S63. ^{13}C NMR spectrum (150 MHz) of carabrolate G (**7**) in CDCl_3

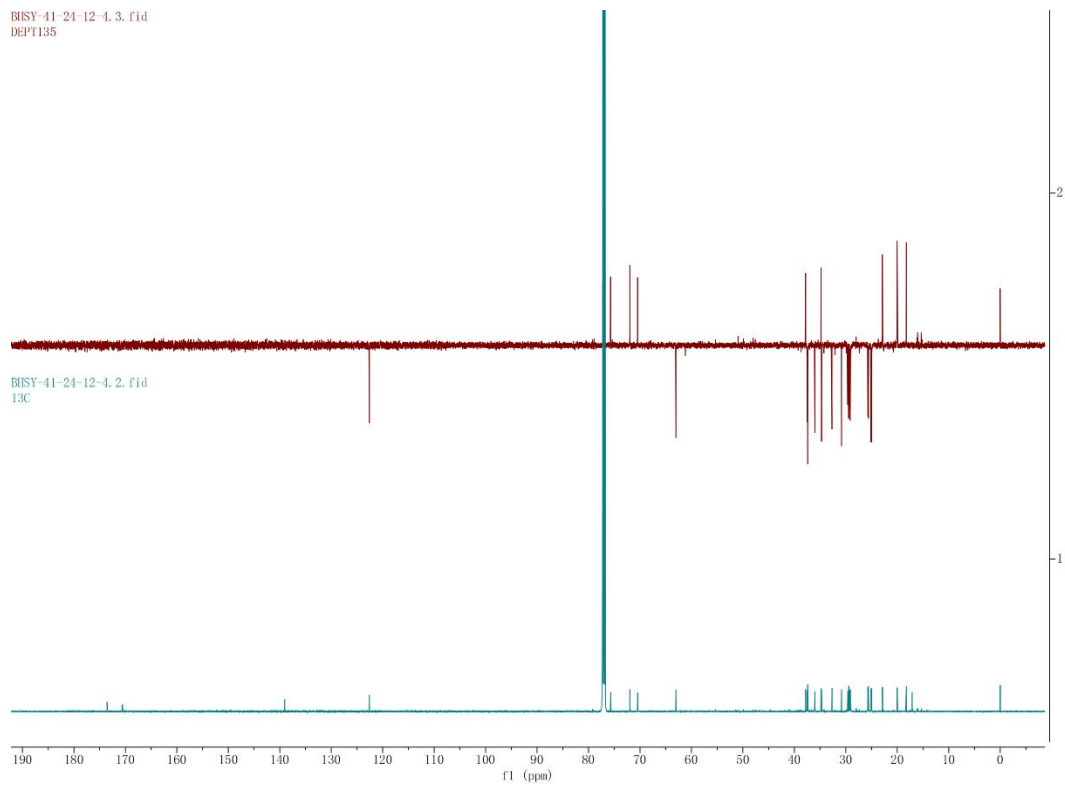


Figure S64. DEPT 135 spectrum (150 MHz) of carabrolate G (7) in CDCl_3

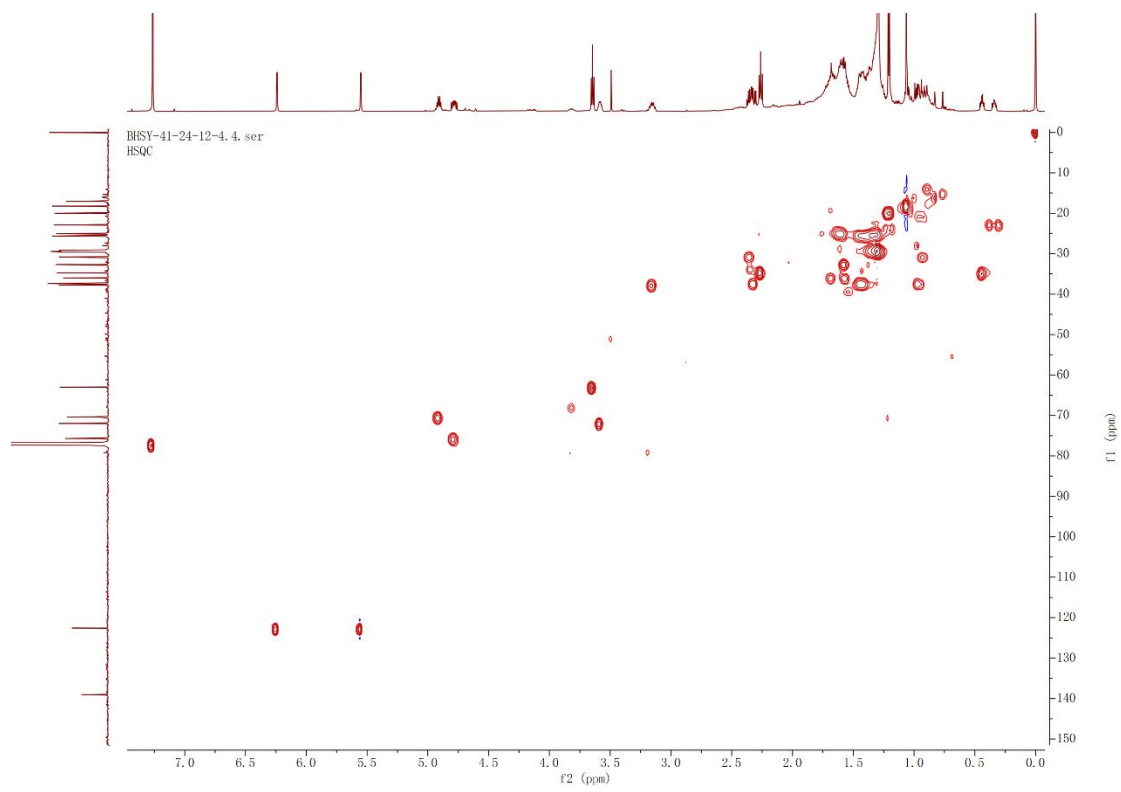


Figure S65. HSQC spectrum (600 MHz) of carabrolate G (7) in CDCl_3

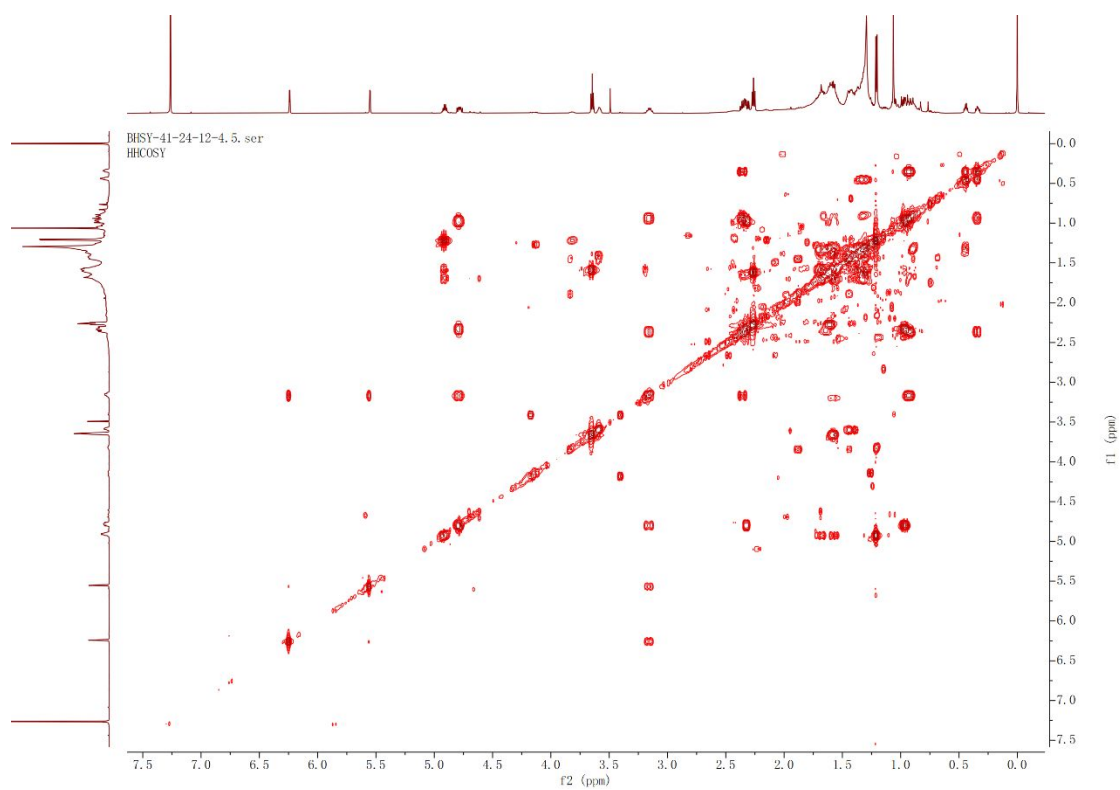


Figure S66. ^1H - ^1H COSY spectrum (600 MHz) of carabrolate G (**7**) in CDCl_3

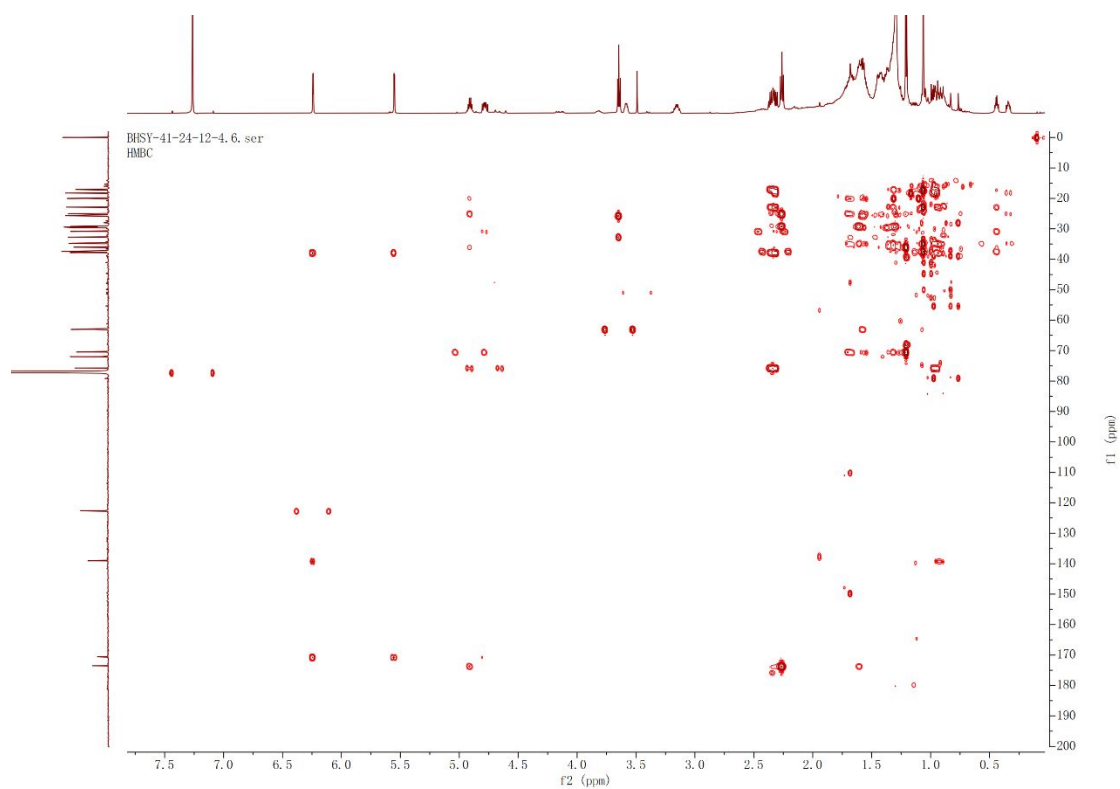


Figure S67. HMBC spectrum (600 MHz) of carabrolate G (**7**) in CDCl_3

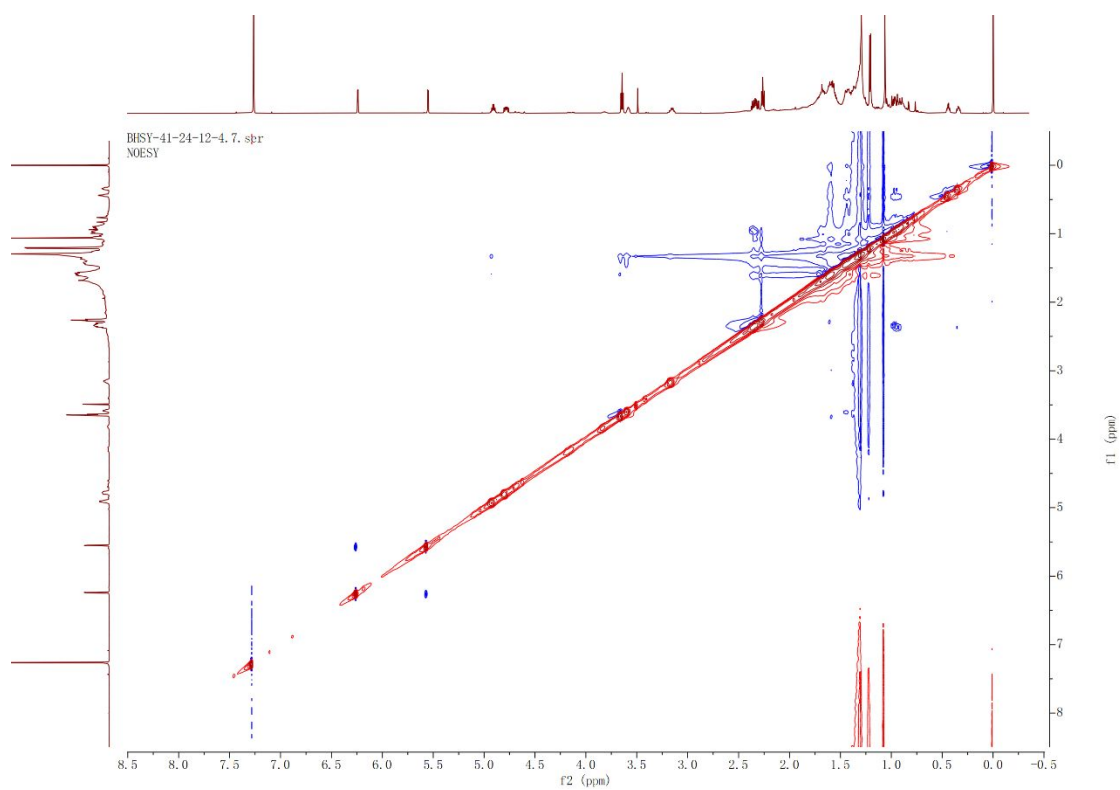


Figure S68. NOESY spectrum (600 MHz) of carabrolate G (7) in CDCl_3

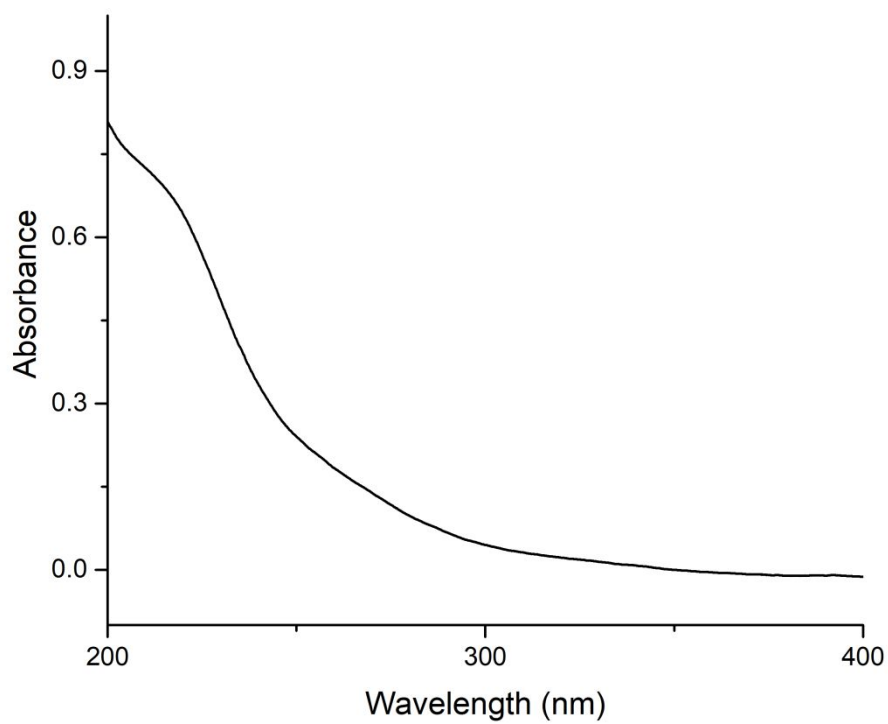


Figure S69. UV spectrum of carabrolate G (7) in MeOH

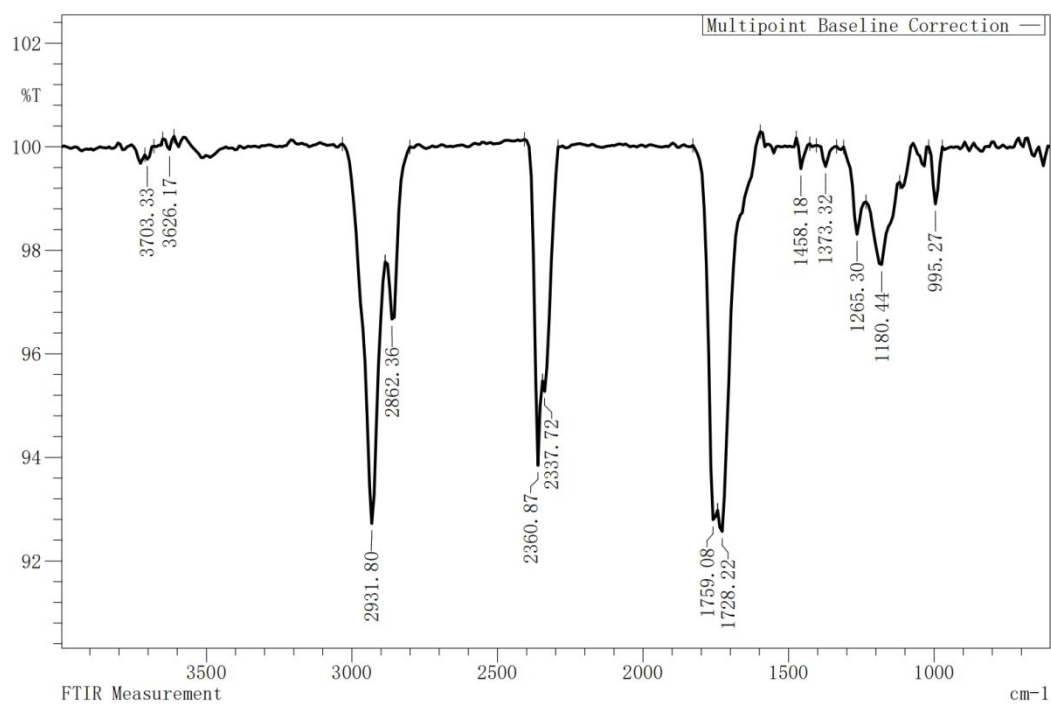
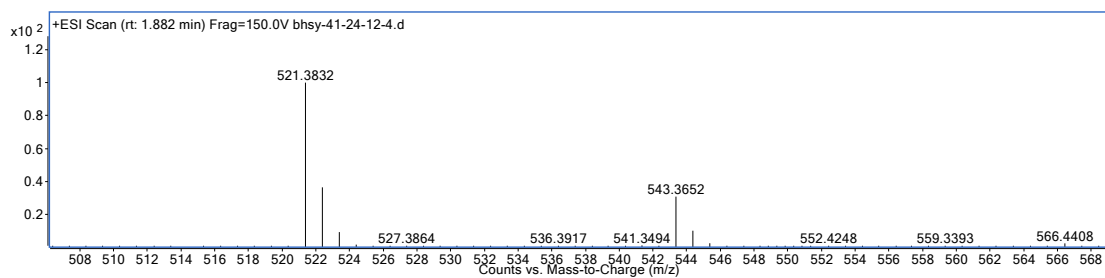


Figure S70. IR spectrum (film on KBr plate) of carabrolate G (7)



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	Ion Formula	m/z
C ₃₁ H ₅₂ O ₆	99.59	520.3759	520.3764	521.3837	0.9	C ₃₁ H ₅₃ O ₆	521.383
C ₃₁ H ₅₂ O ₆	99.68	520.376	520.3764	543.3656	0.79	C ₃₁ H ₅₂ NaO ₆	543.3652

Figure S71. HRESIMS spectrum of carabrolate G (7)

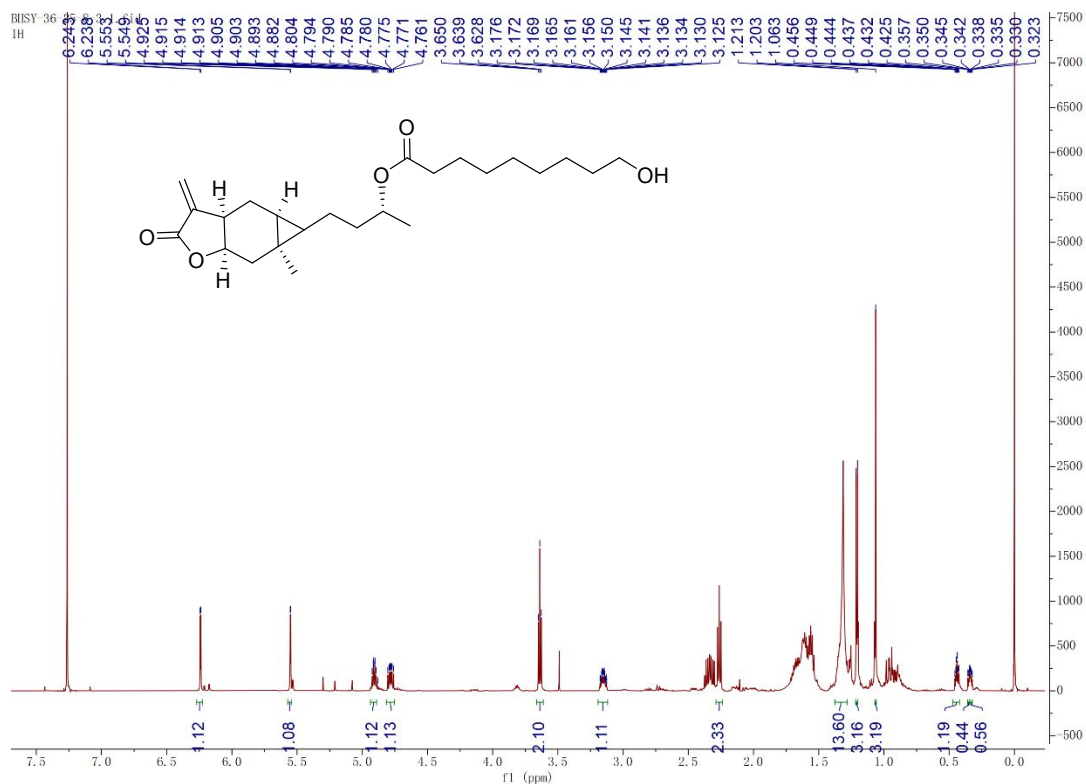


Figure S72. ^1H NMR spectrum (600 MHz) of carabrolate H (**8**) in CDCl_3

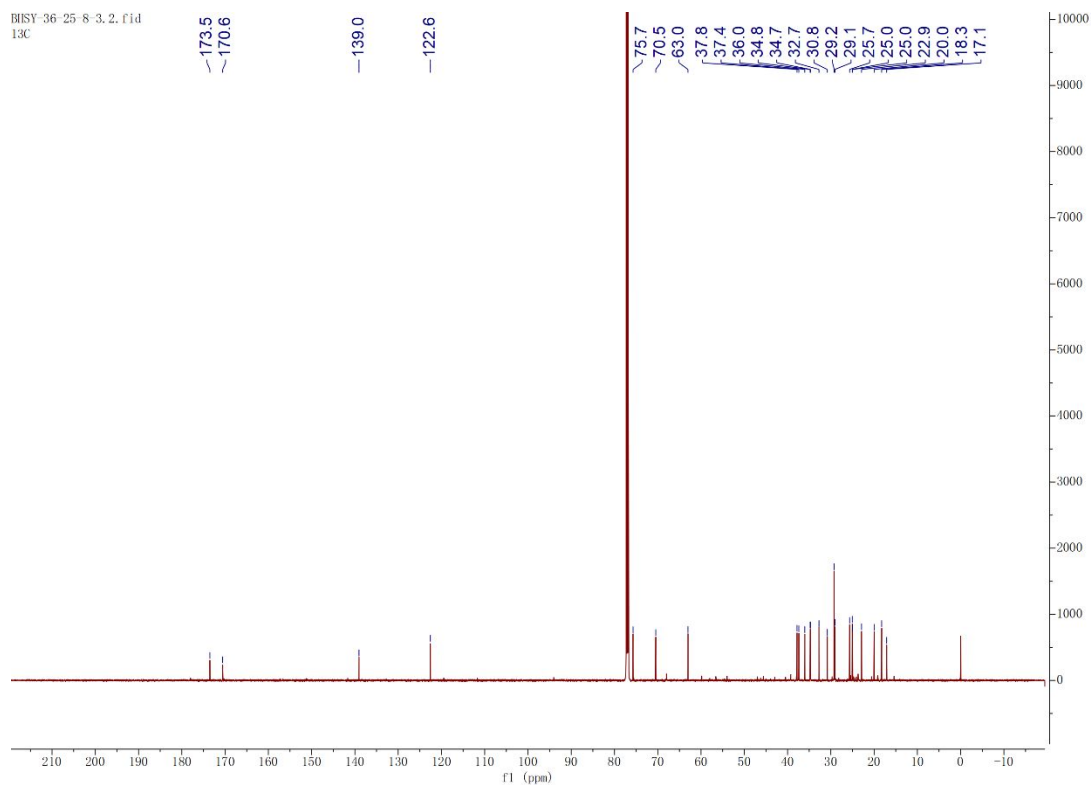


Figure S73. ^{13}C NMR spectrum (150 MHz) of carabrolate H (**8**) in CDCl_3

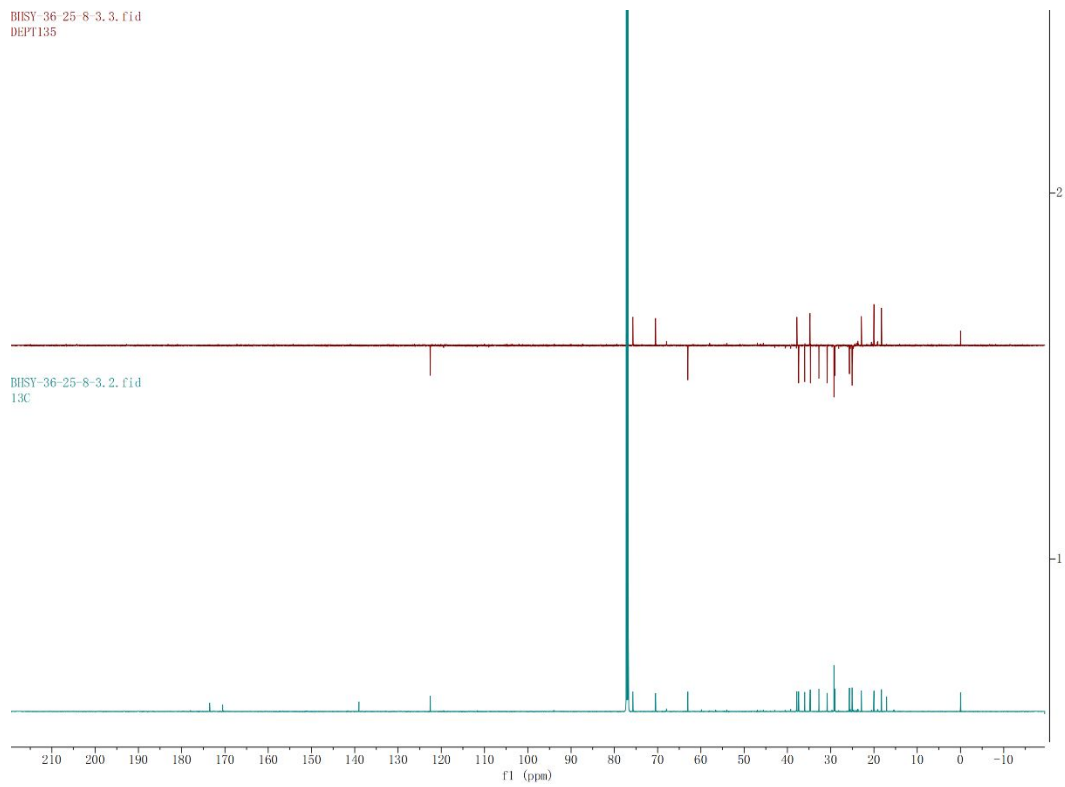


Figure S74. DEPT 135 spectrum (150 MHz) of carabrolate H (**8**) in CDCl_3

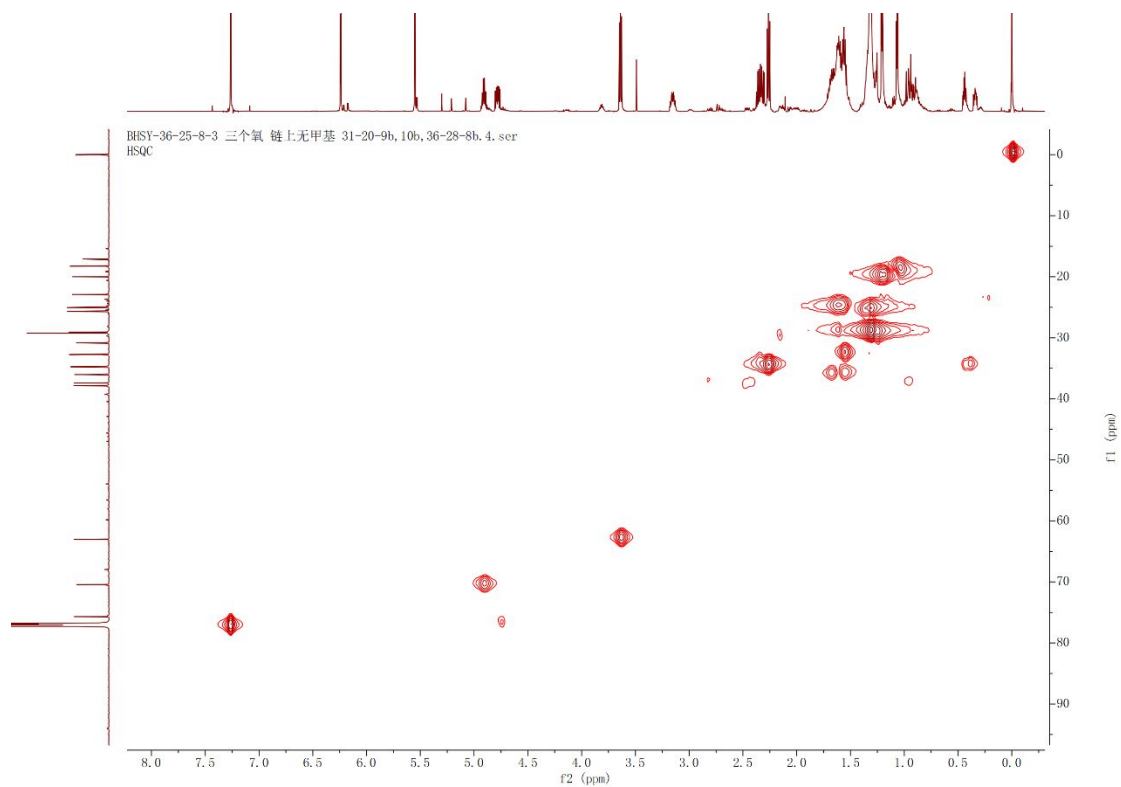


Figure S75. HSQC spectrum (600 MHz) of carabrolate H (**8**) in CDCl_3

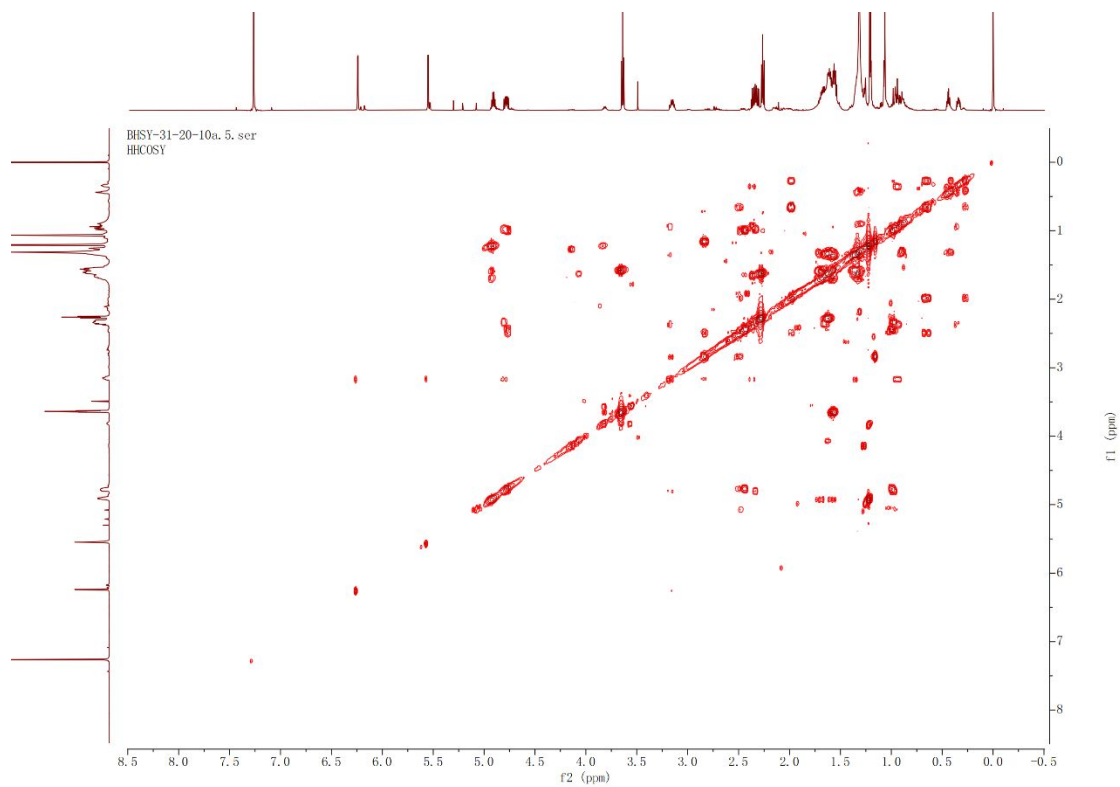


Figure S76. ^1H - ^1H COSY spectrum (600 MHz) of carabrolate H (**8**) in CDCl_3

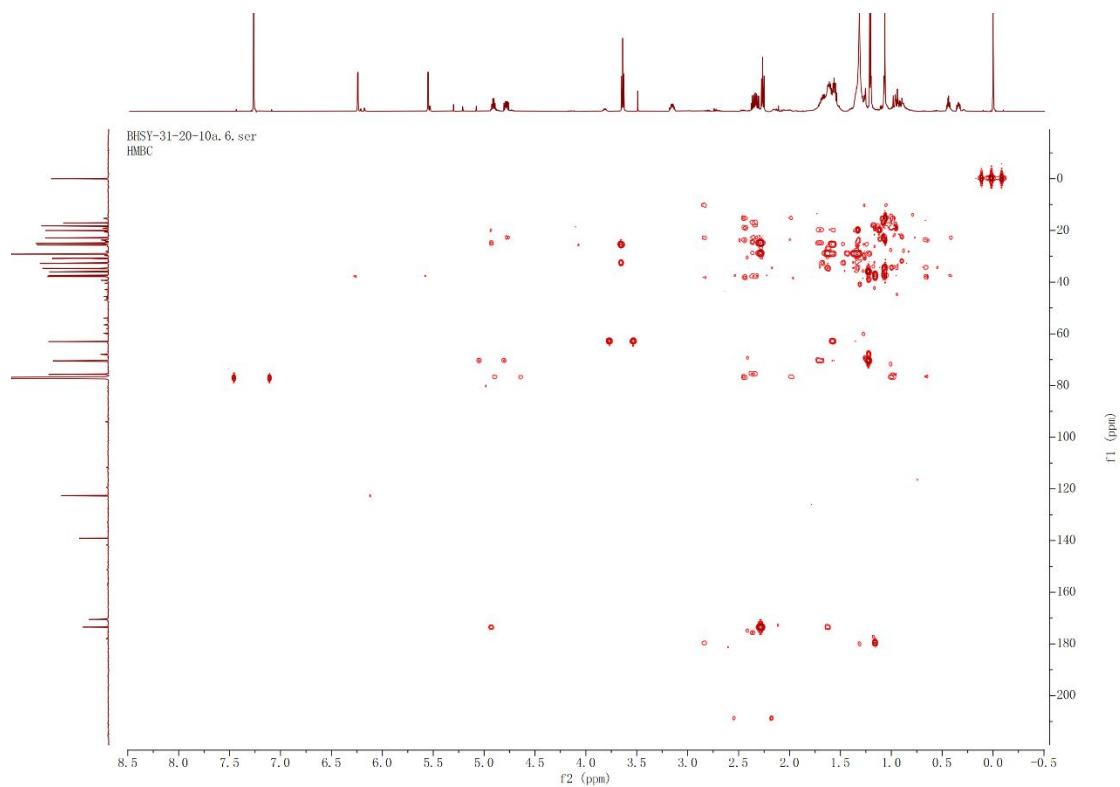


Figure S77. HMBC spectrum (600 MHz) of carabrolate H (**8**) in CDCl_3

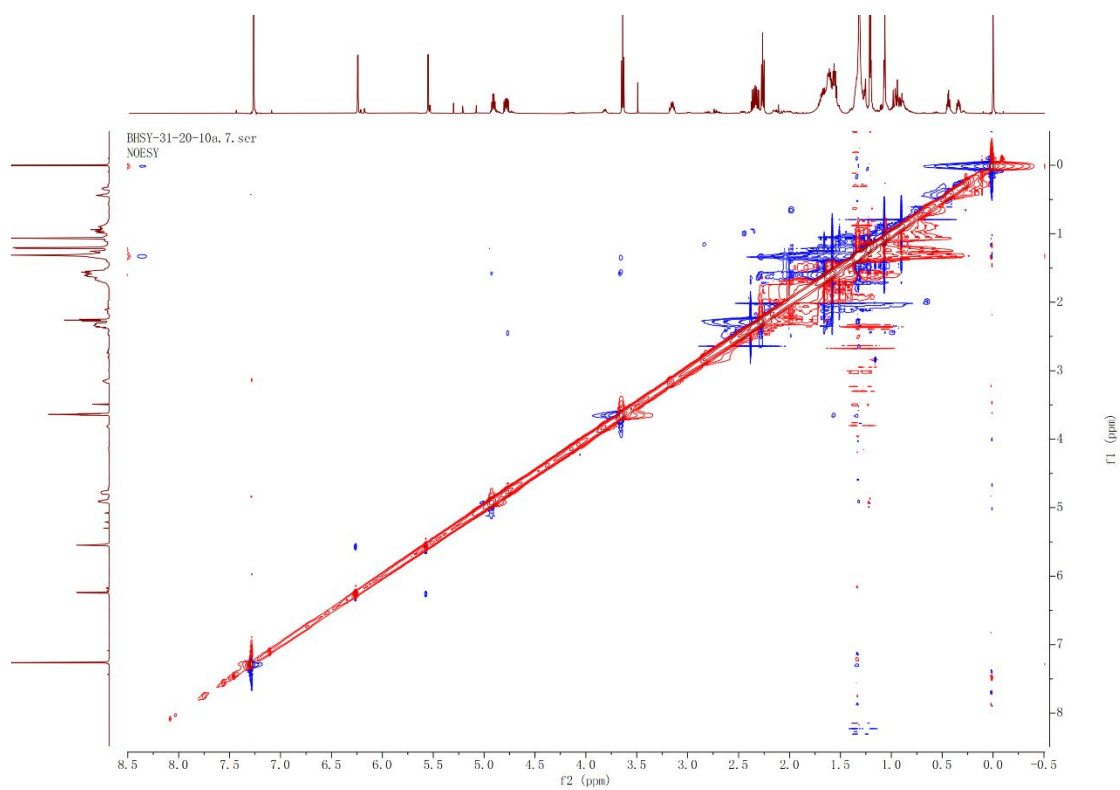


Figure S78. NOESY spectrum (600 MHz) of carabrolate H (**8**) in CDCl_3

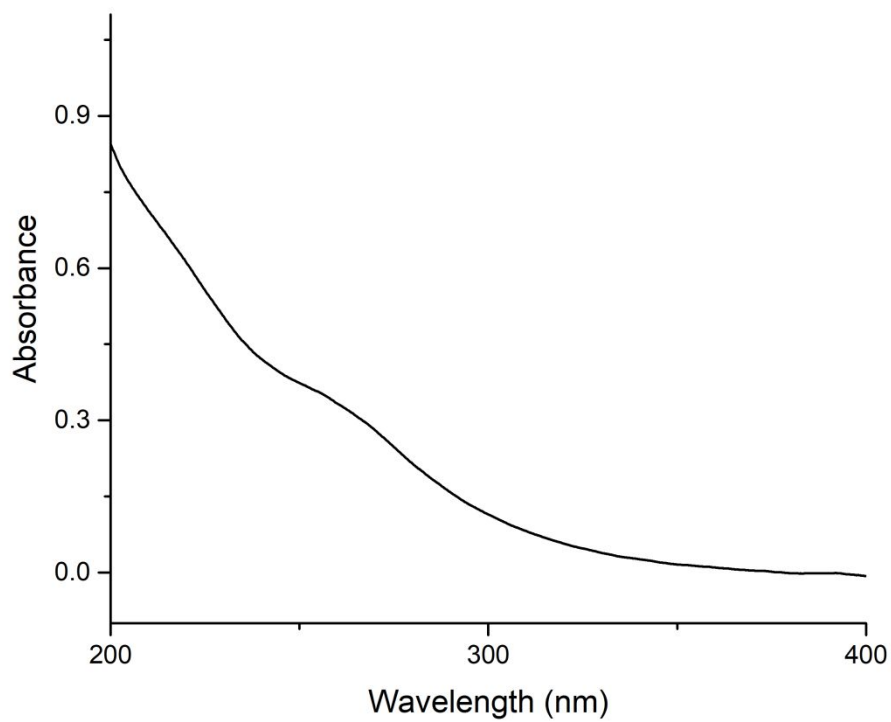


Figure S79. UV spectrum of carabrolate H (**8**) in MeOH

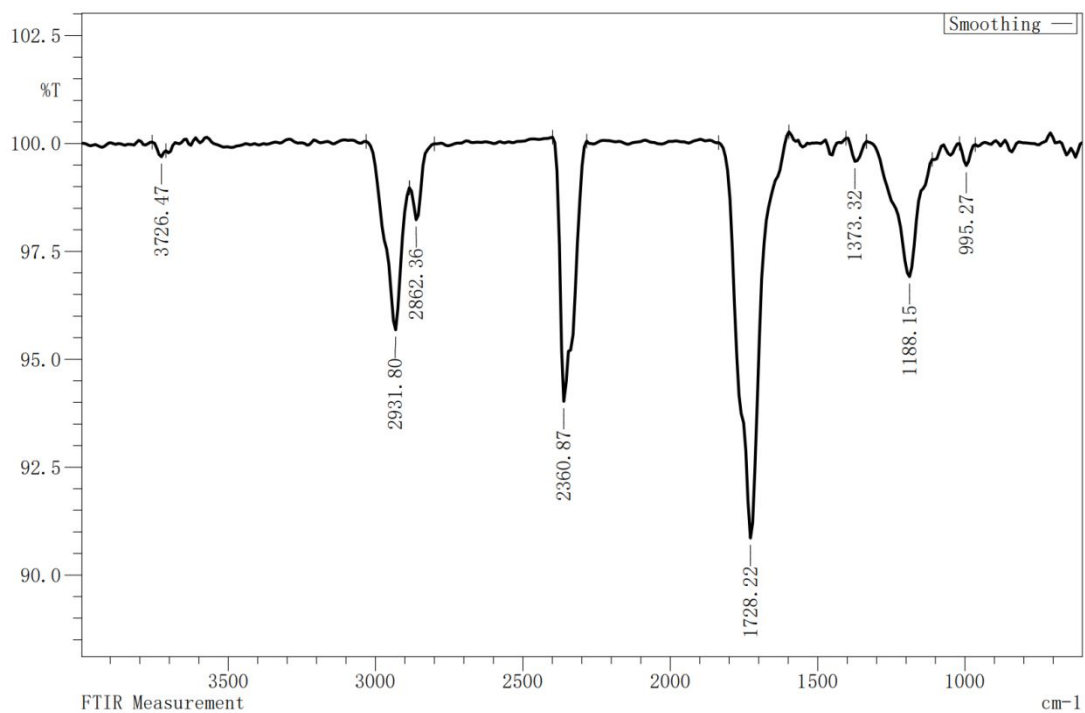
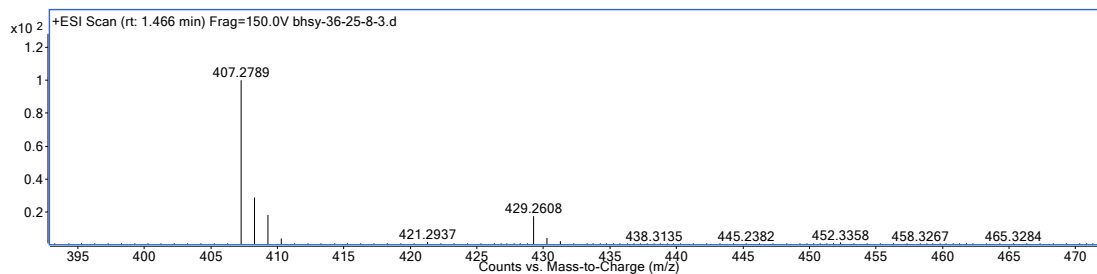


Figure S80. IR spectrum (film on KBr plate) of carabrolate H (8)



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	Ion Formula	m/z
C ₂₄ H ₃₈ O ₅	99.78	406.2716	406.2719	407.2792	0.74	C ₂₄ H ₃₉ O ₅	407.2789
C ₂₄ H ₃₈ O ₅	99.7	406.2716	406.2719	429.2611	0.85	C ₂₄ H ₃₈ NaO ₅	429.2608

Figure S81. HRESIMS spectrum of carabrolate H (8)

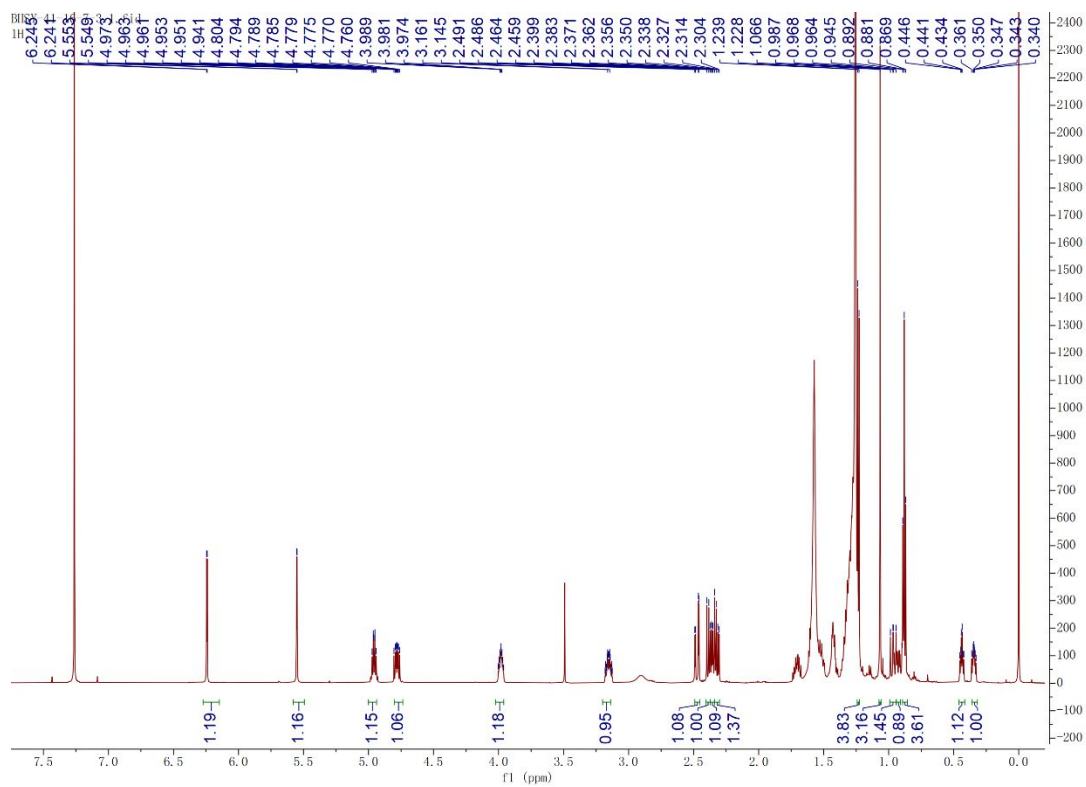


Figure S82. ^1H NMR spectrum (600 MHz) of carabrolate I (**9**) in CDCl_3

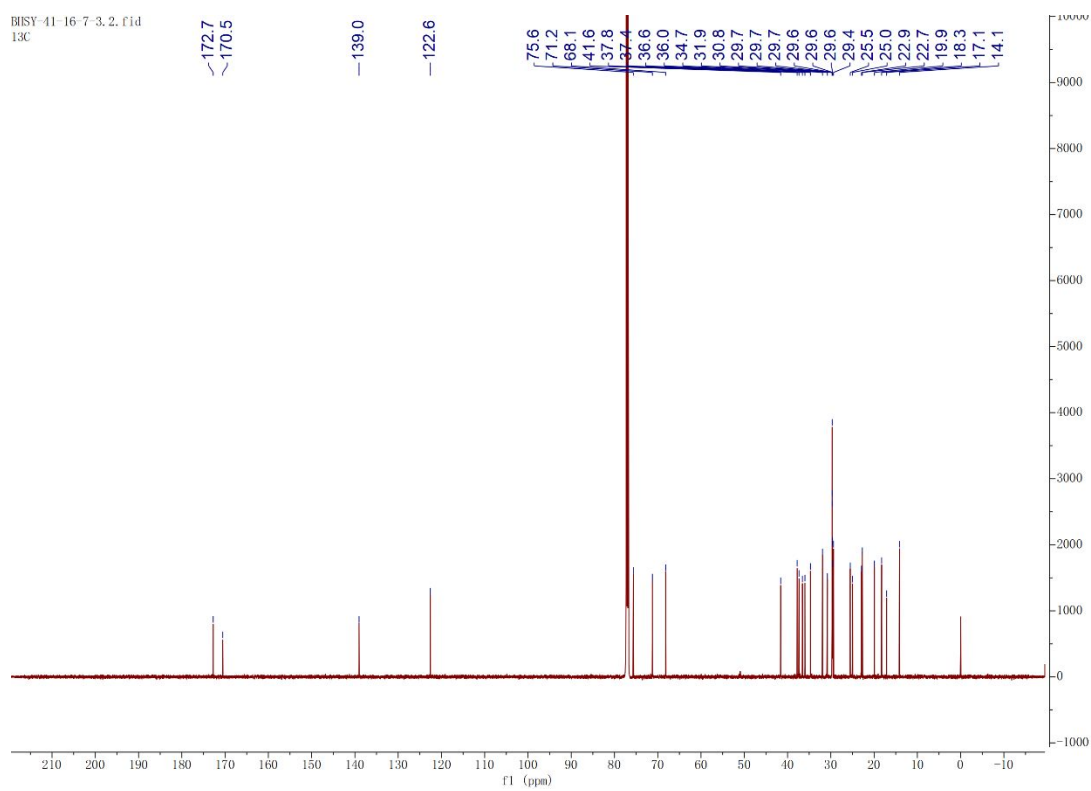


Figure S83. ^{13}C NMR spectrum (150 MHz) of carabrolate I (**9**) in CDCl_3

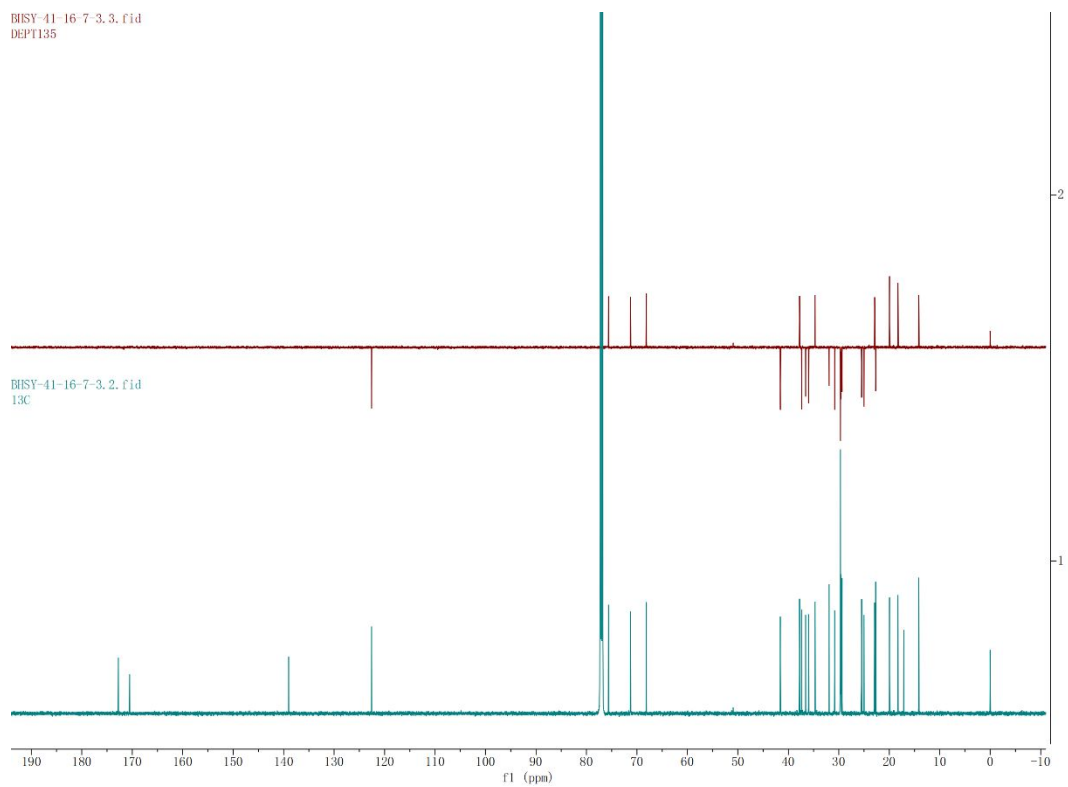


Figure S84. DEPT 135 spectrum (150 MHz) of carabrolate I (**9**) in CDCl_3

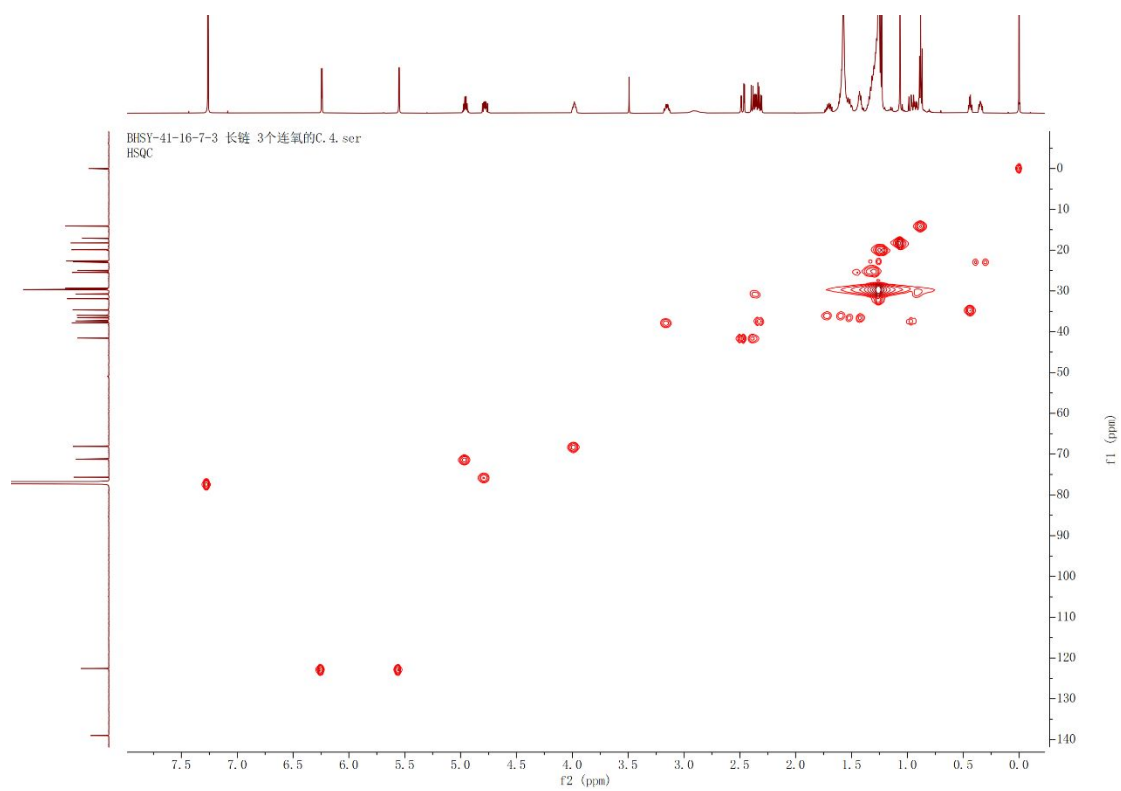


Figure S85. HSQC spectrum (600 MHz) of carabrolate I (**9**) in CDCl_3

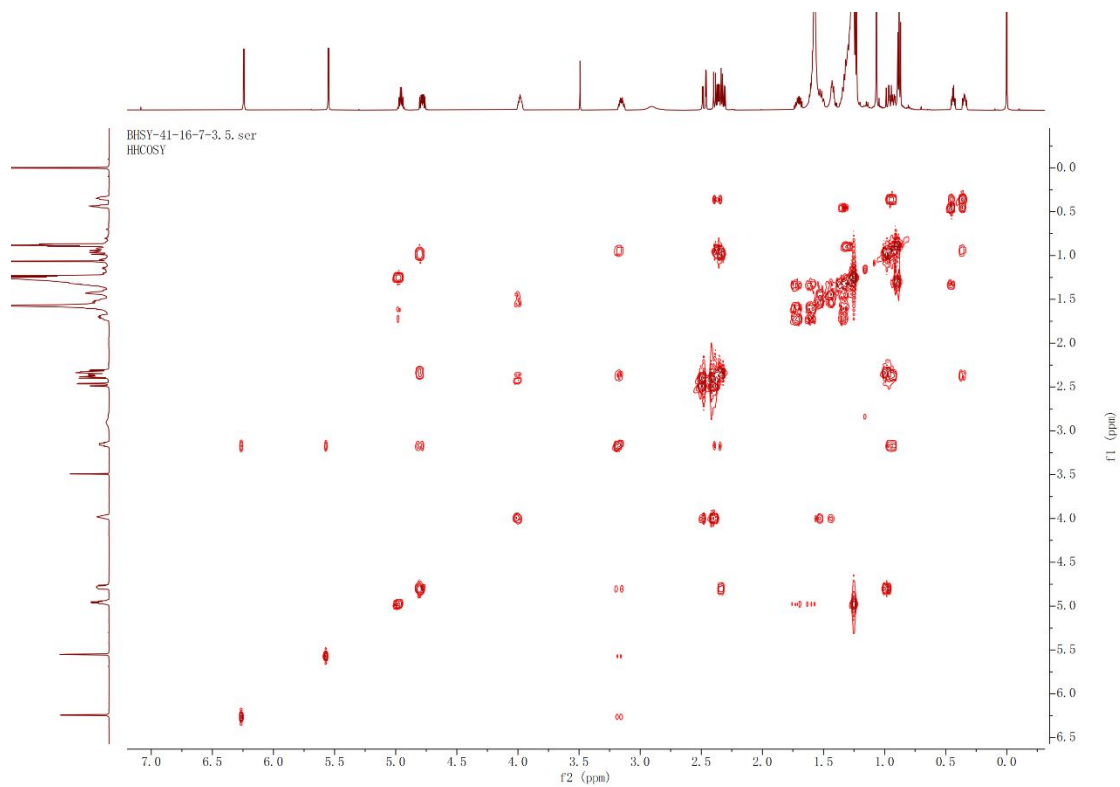


Figure S86. ^1H - ^1H COSY spectrum (600 MHz) of carabrolate I (**9**) in CDCl_3

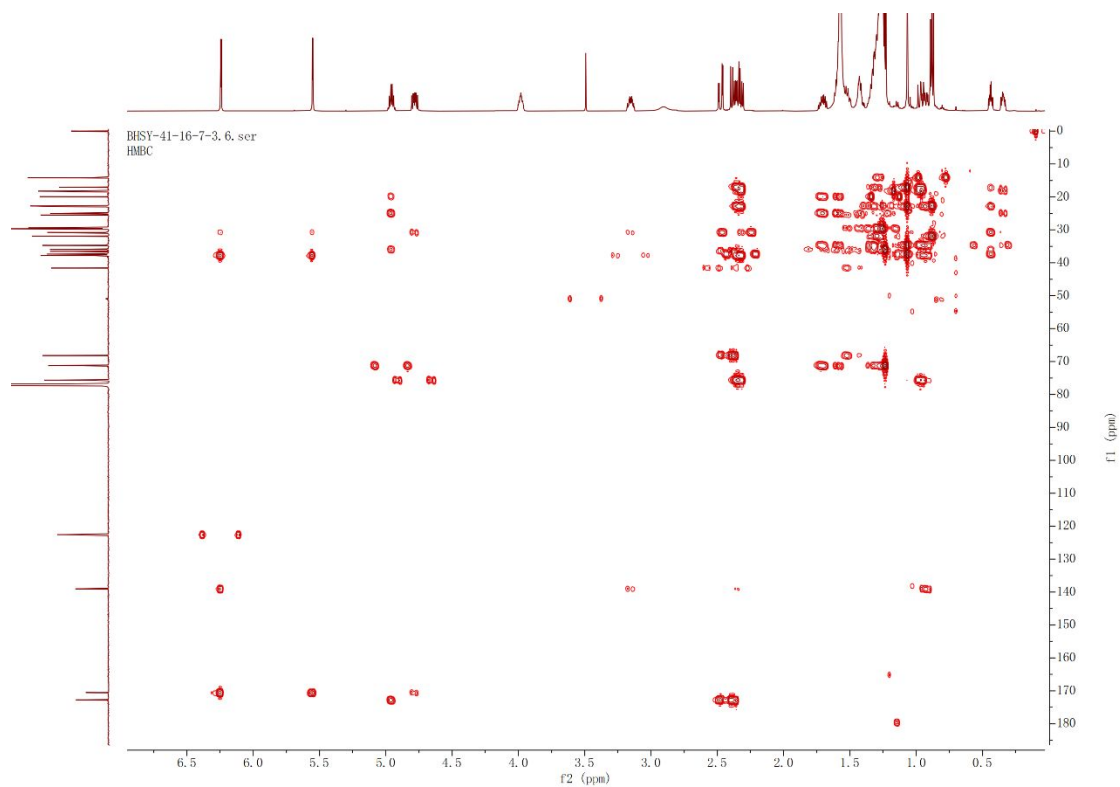


Figure S87. HMBC spectrum (600 MHz) of carabrolate I (**9**) in CDCl_3

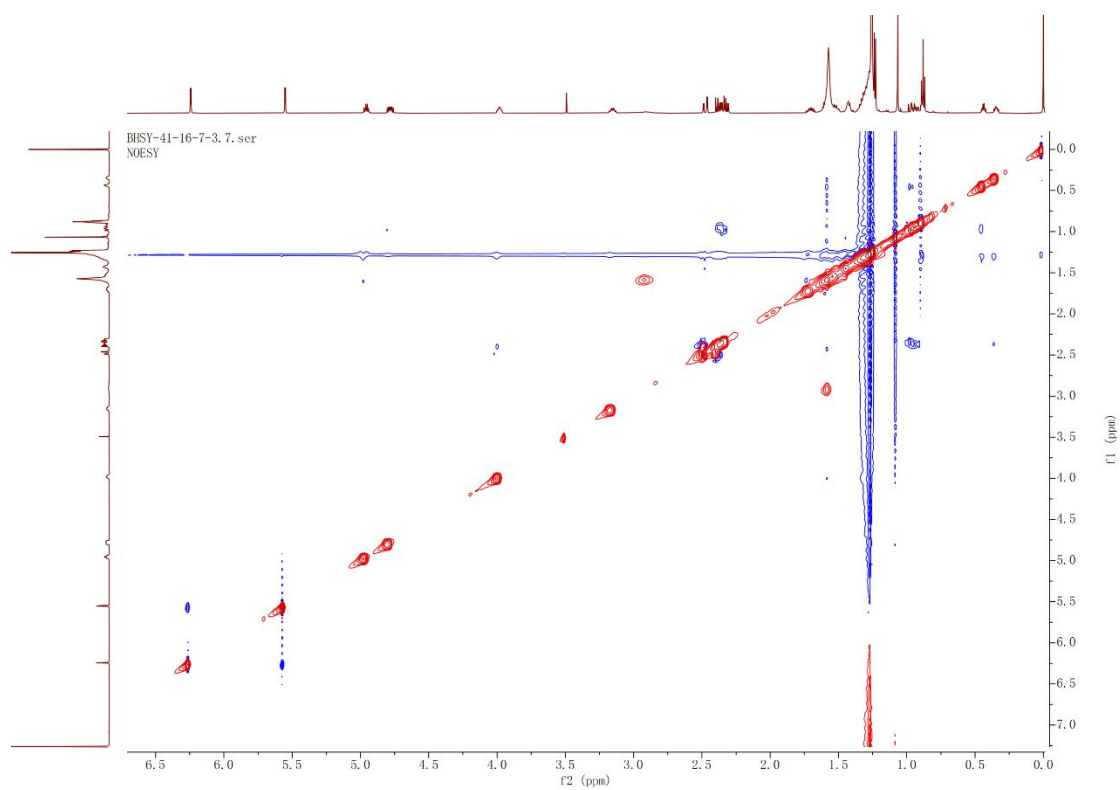


Figure S88. NOESY spectrum (600 MHz) of carabrolate I (**9**) in CDCl_3

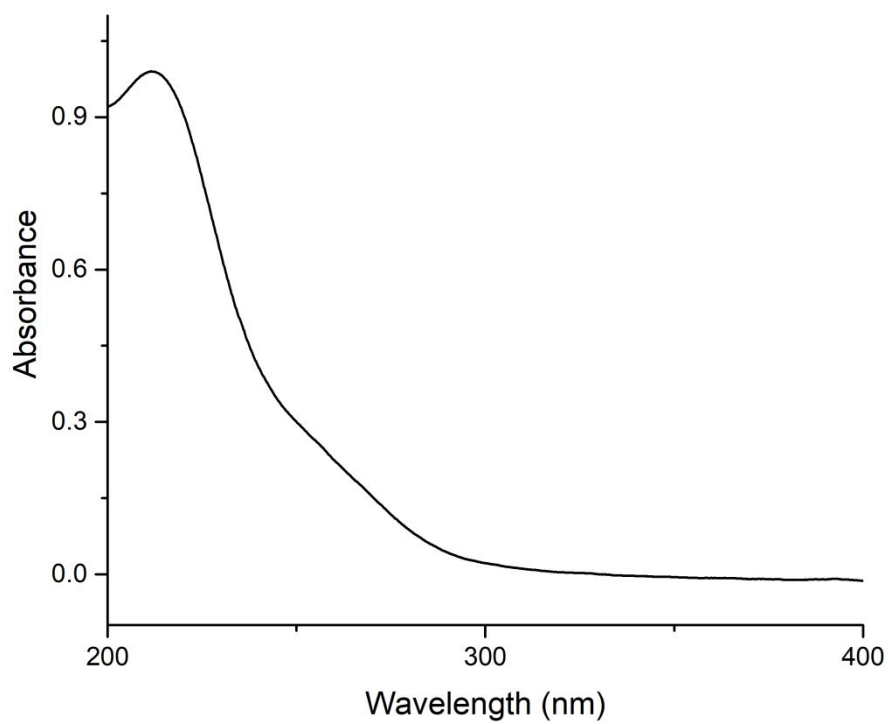


Figure S89. UV spectrum of carabrolate I (**9**) in MeOH

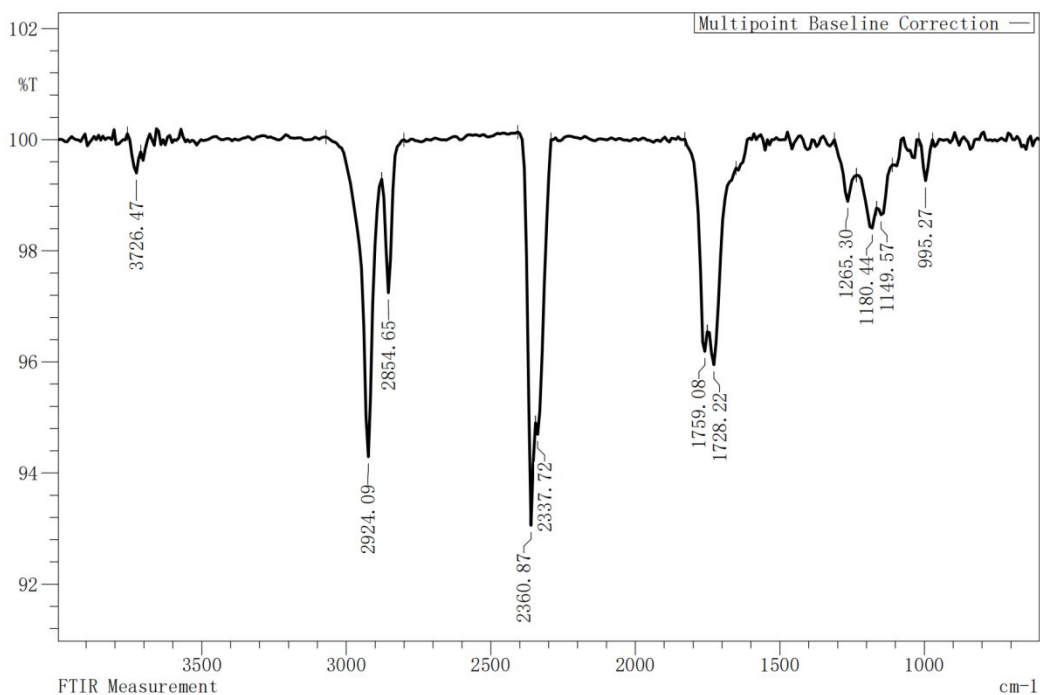
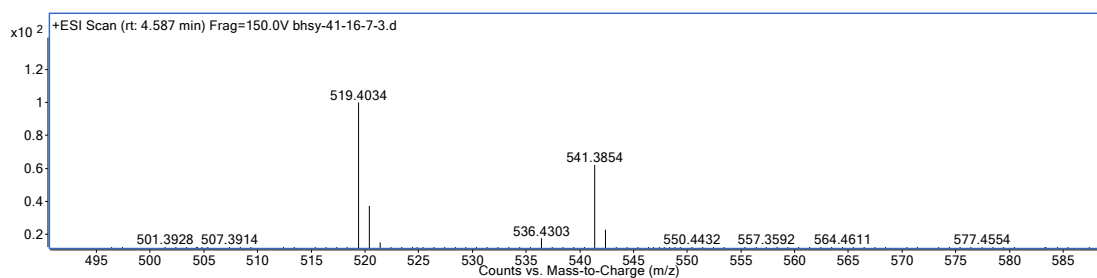


Figure S90. IR spectrum (film on KBr plate) of carabrolate I (9)



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	Ion Formula	m/z
C ₃₂ H ₅₄ O ₅	98.14	518.3961	518.3971	519.4044	1.93	C ₃₂ H ₅₅ O ₅	519.4034
C ₃₂ H ₅₄ O ₅	98.34	518.3962	518.3971	541.3863	1.82	C ₃₂ H ₅₄ NaO ₅	541.3854

Figure S91. HRESIMS spectrum of carabrolate I (9)

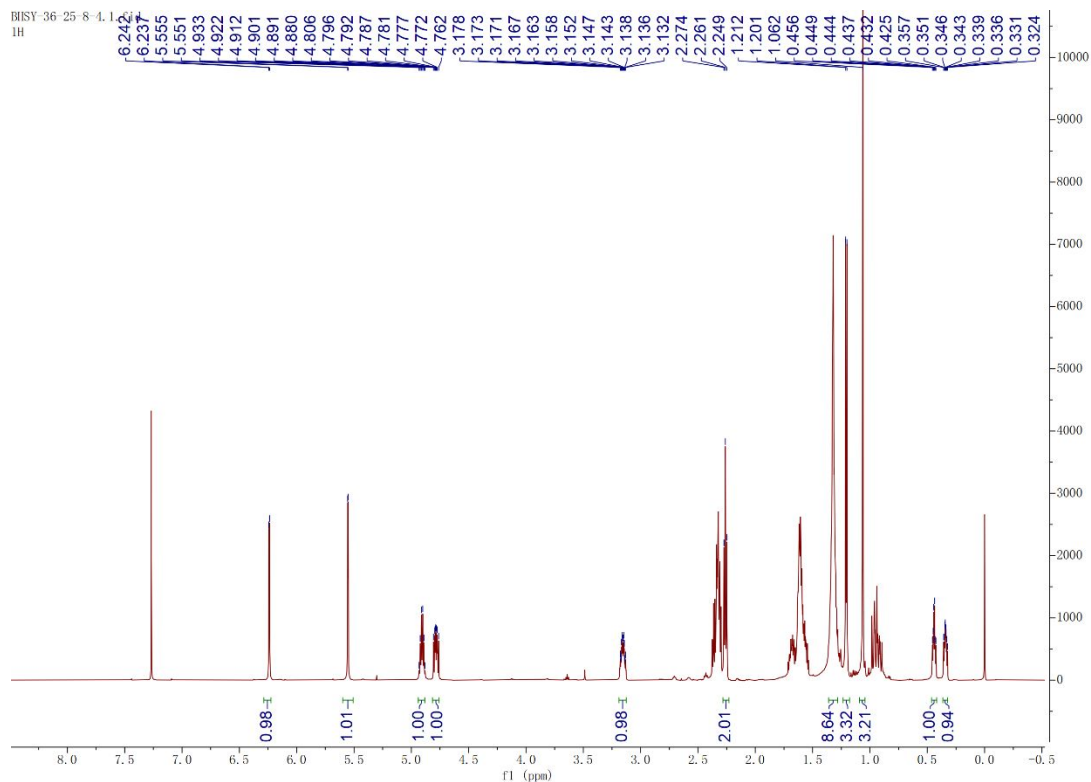


Figure S92. ^1H NMR spectrum (600 MHz) of carabrolate J (**10**) in CDCl_3

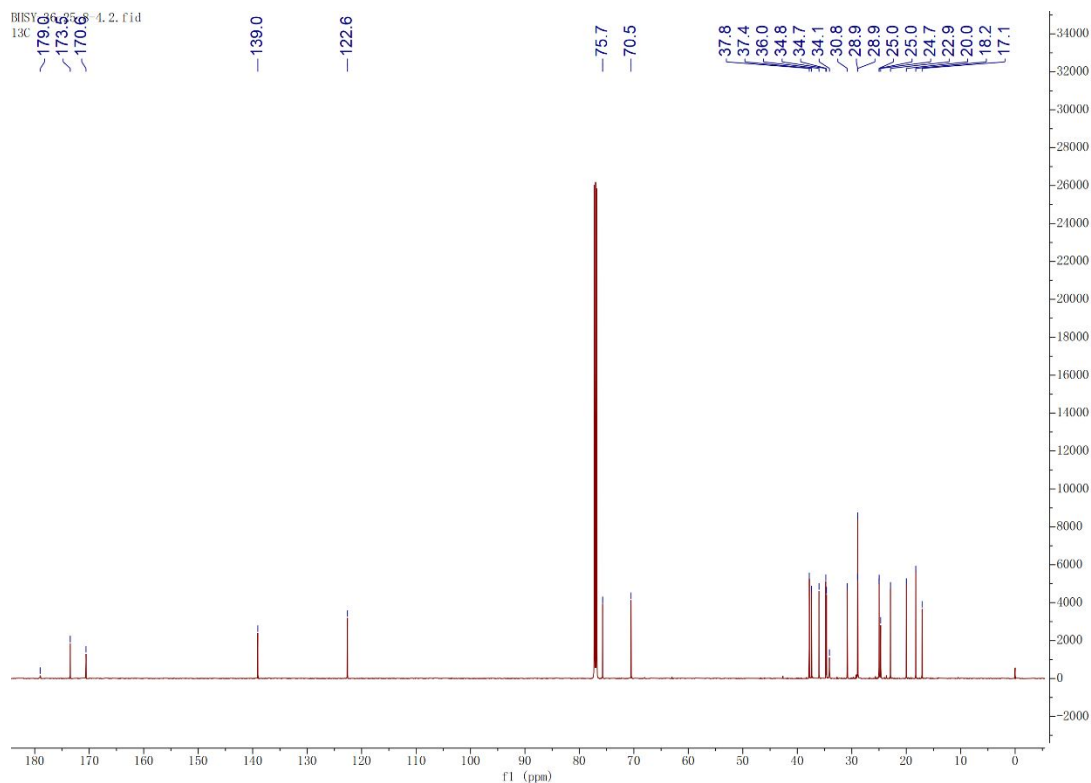


Figure S93. ^{13}C NMR spectrum (150 MHz) of carabrolate J (**10**) in CDCl_3

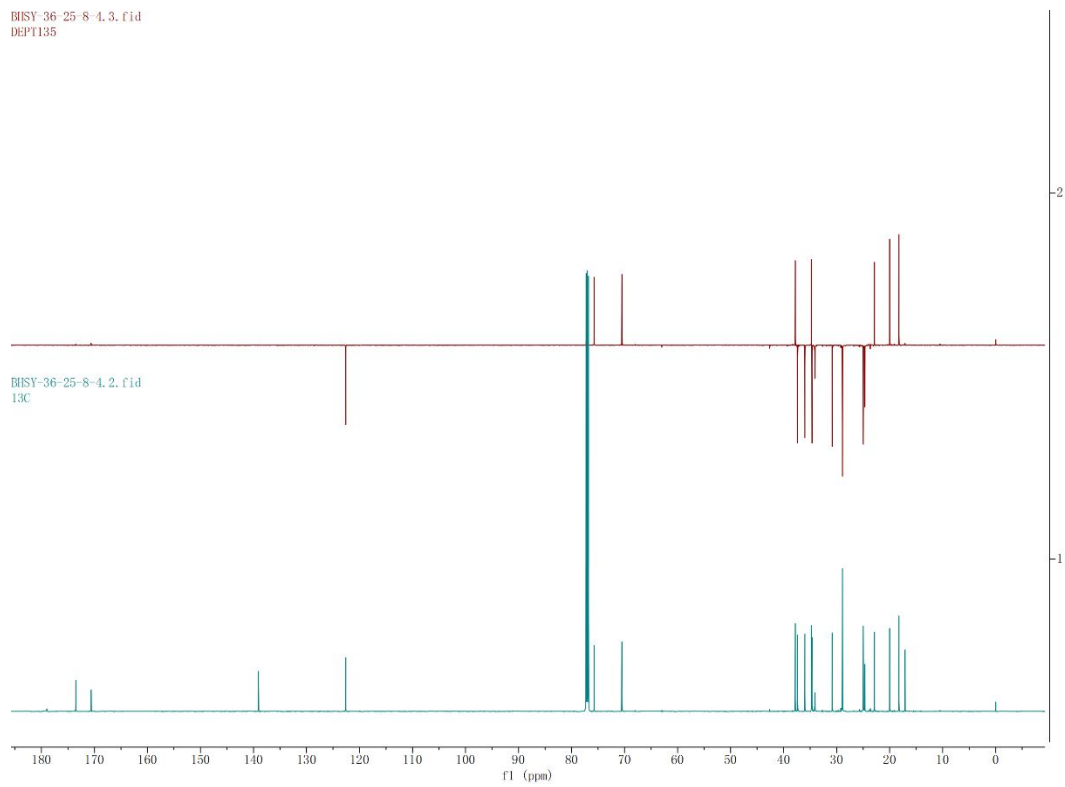


Figure S94. DEPT 135 spectrum (150 MHz) of carabrolate J (**10**) in $CDCl_3$

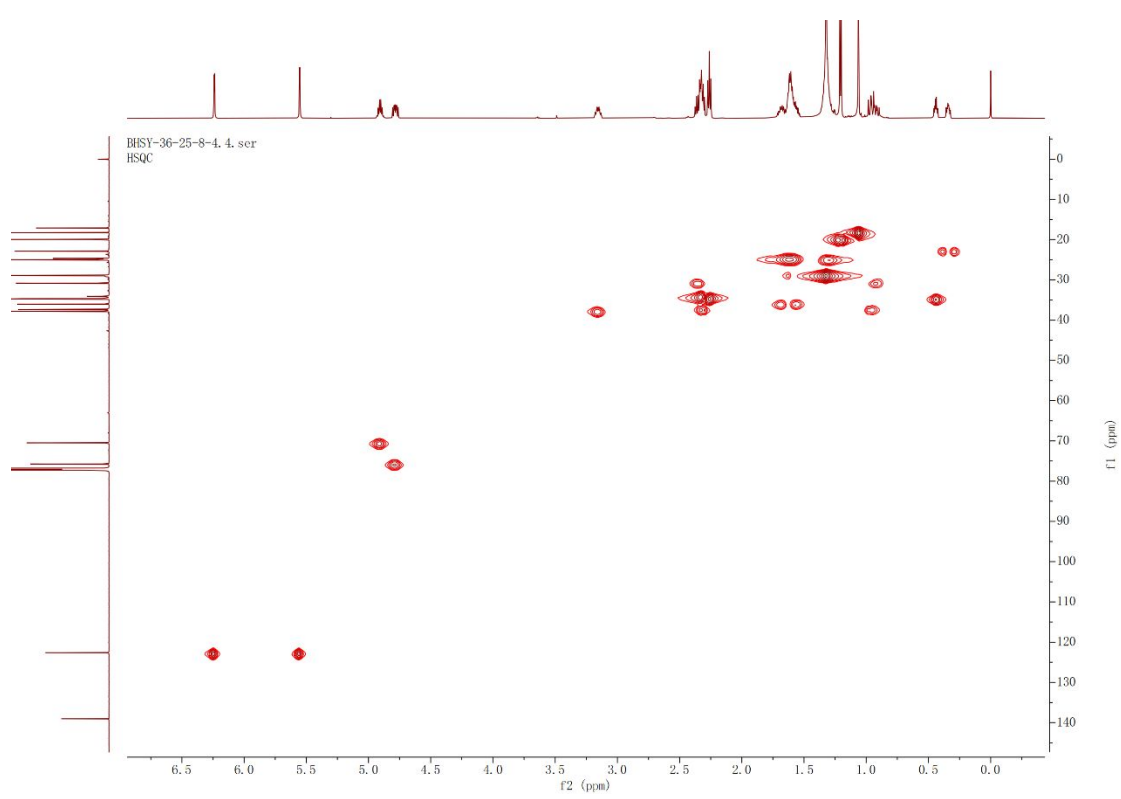


Figure S95. HSQC spectrum (600 MHz) of carabrolate J (**10**) in $CDCl_3$

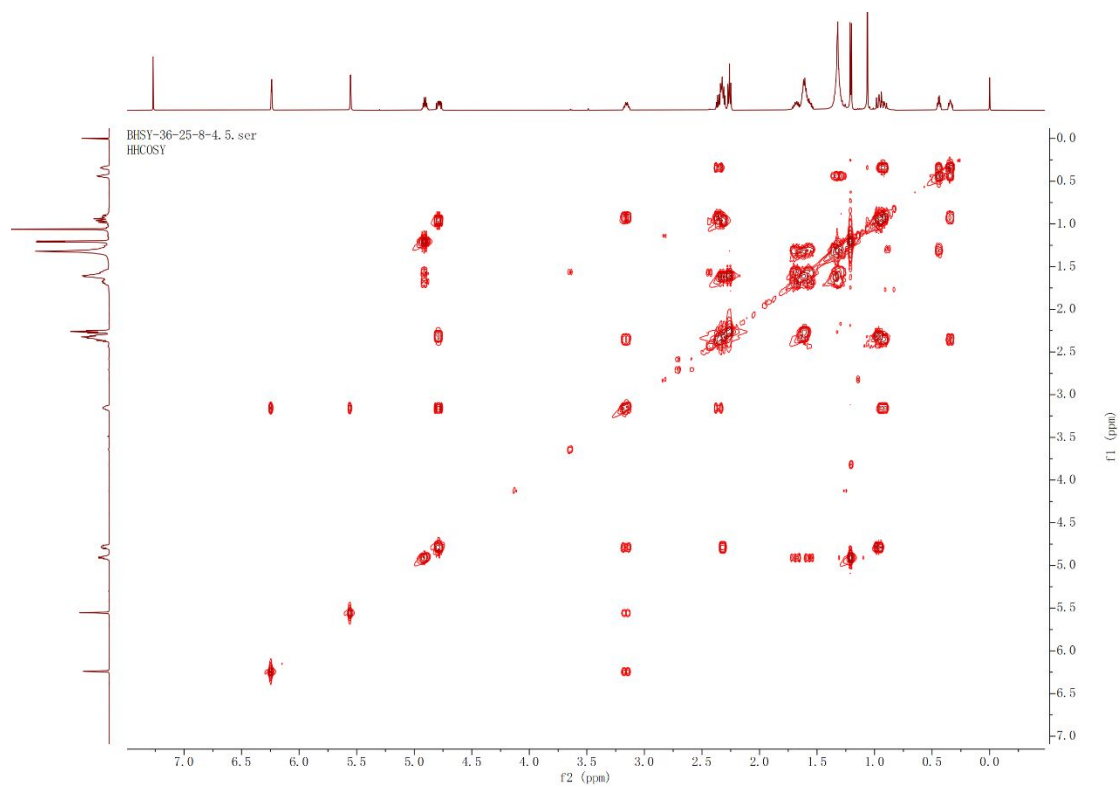


Figure S96. ^1H - ^1H COSY spectrum (600 MHz) of carabrolate J (**10**) in CDCl_3

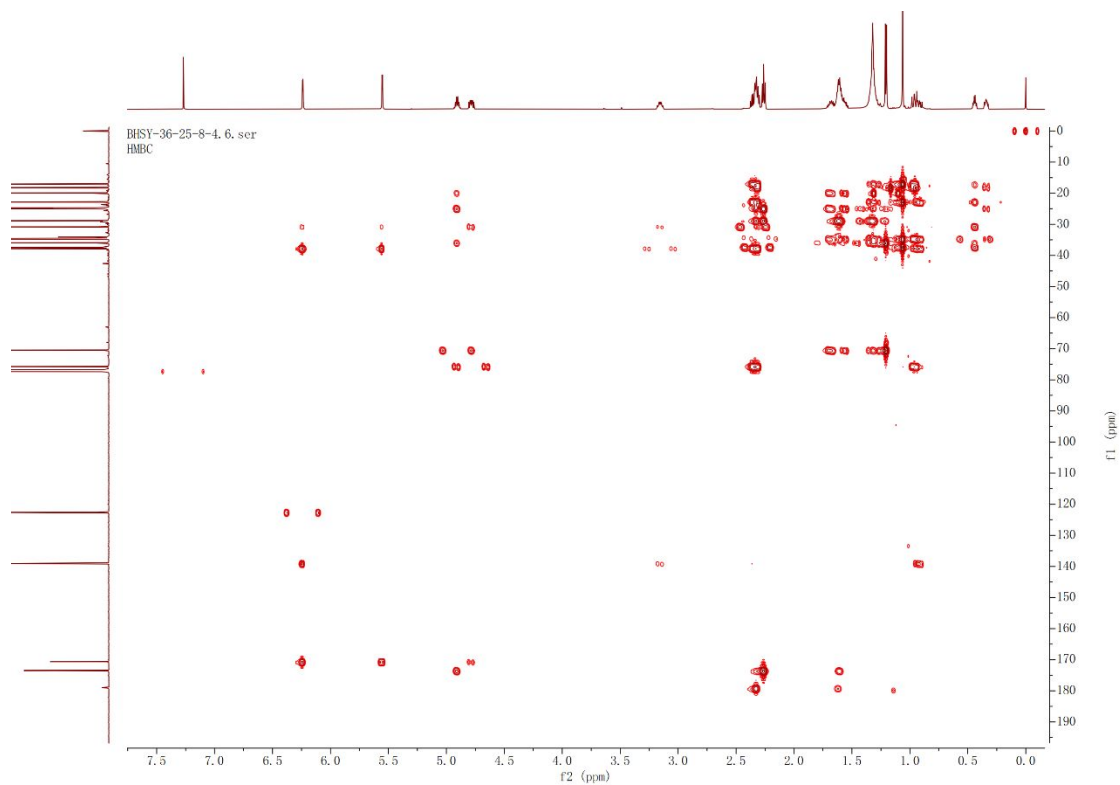


Figure S97. HMBC spectrum (600 MHz) of carabrolate J (**10**) in CDCl_3

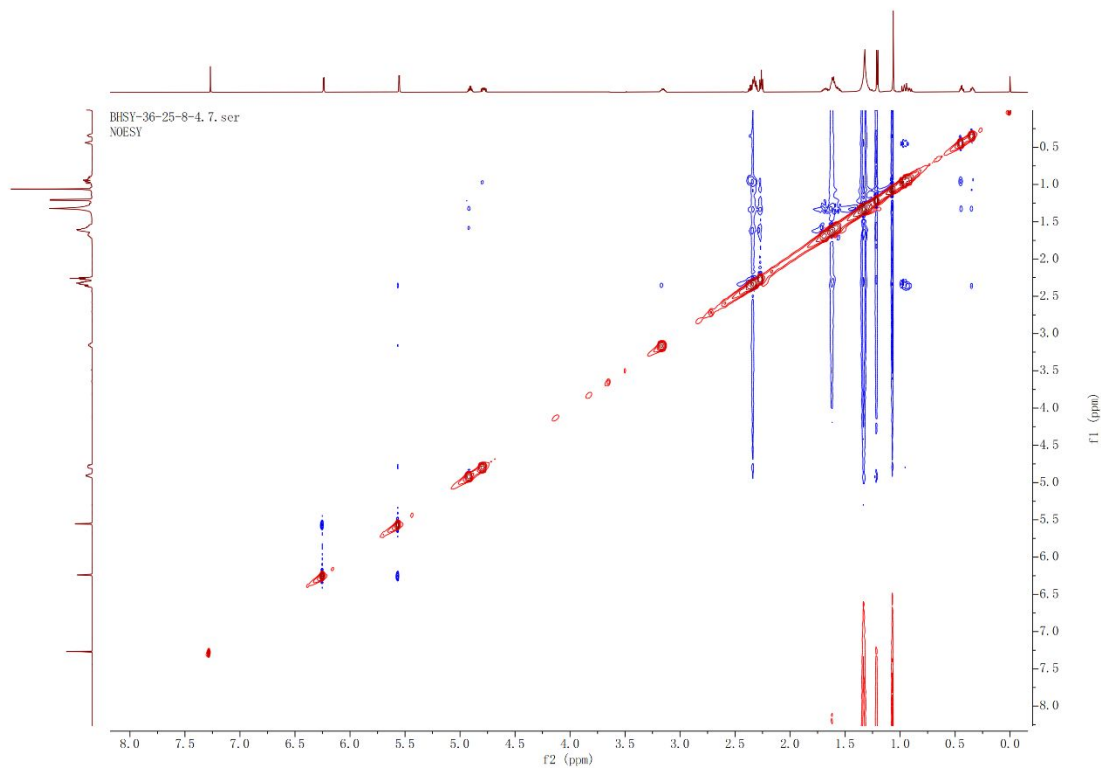


Figure S98. NOESY spectrum (600 MHz) of carabrolate J (**10**) in CDCl₃

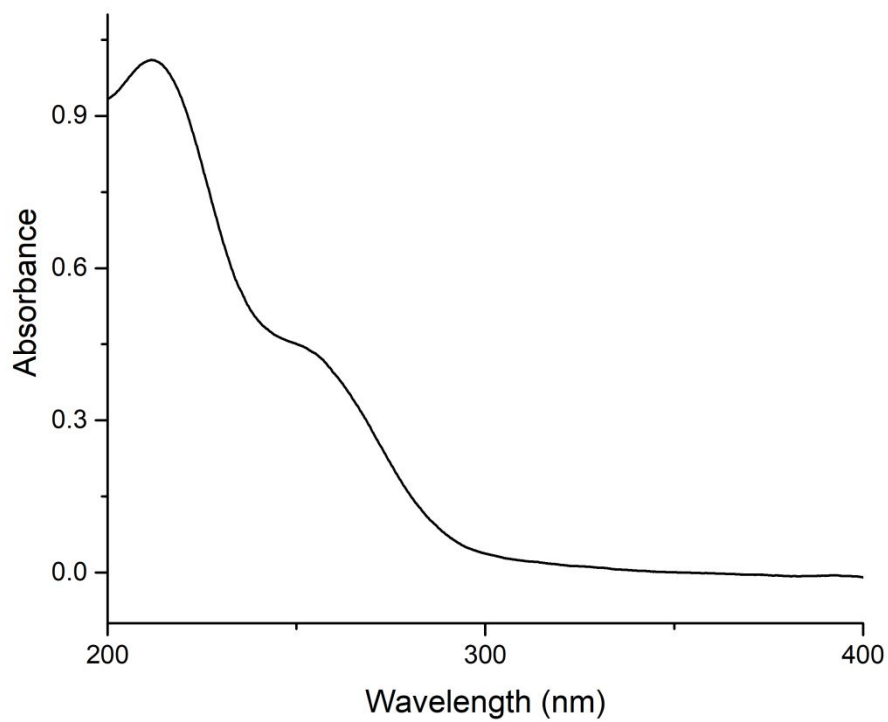


Figure S99. UV spectrum of carabrolate J (**10**) in MeOH

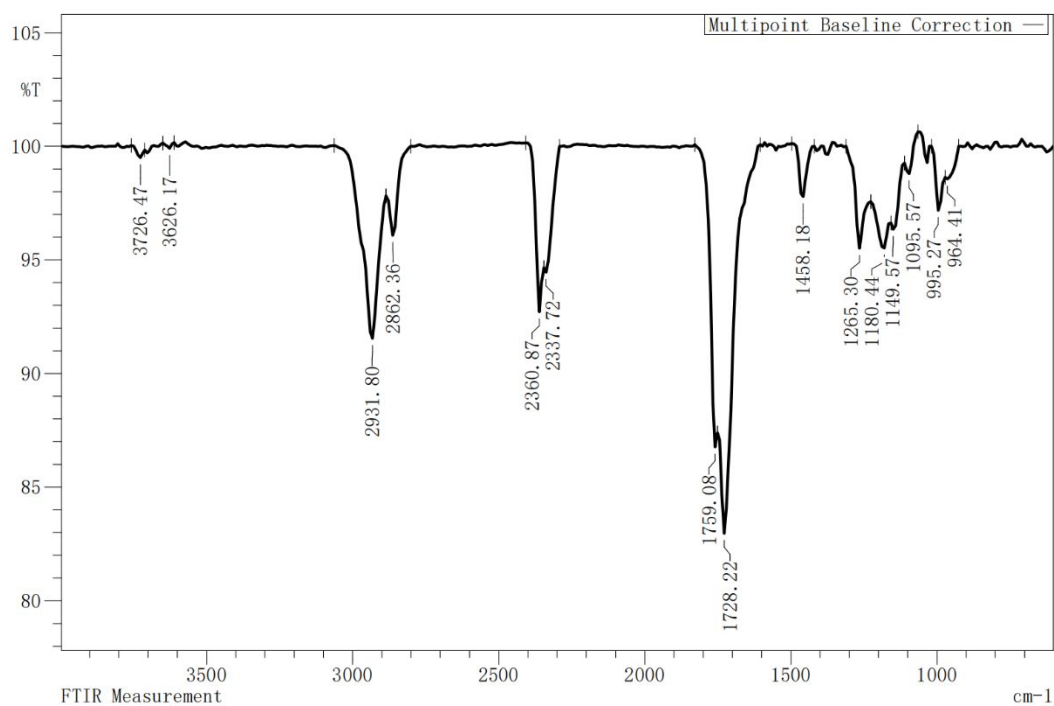
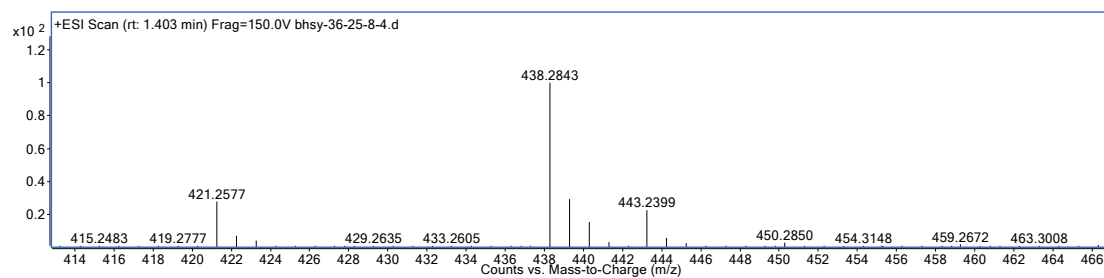


Figure S100. IR spectrum (film on KBr plate) of carabrolate J (10)



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	Ion Formula	m/z
C ₂₄ H ₃₆ O ₆	98.62	420.2504	420.2512	421.2585	1.82	C ₂₄ H ₃₇ O ₆	421.2577
C ₂₄ H ₃₆ O ₆	98.79	420.2505	420.2512	438.285	1.7	C ₂₄ H ₄₀ NO ₆	438.2843

Figure S101. HRESIMS spectrum of carabrolate J (10)

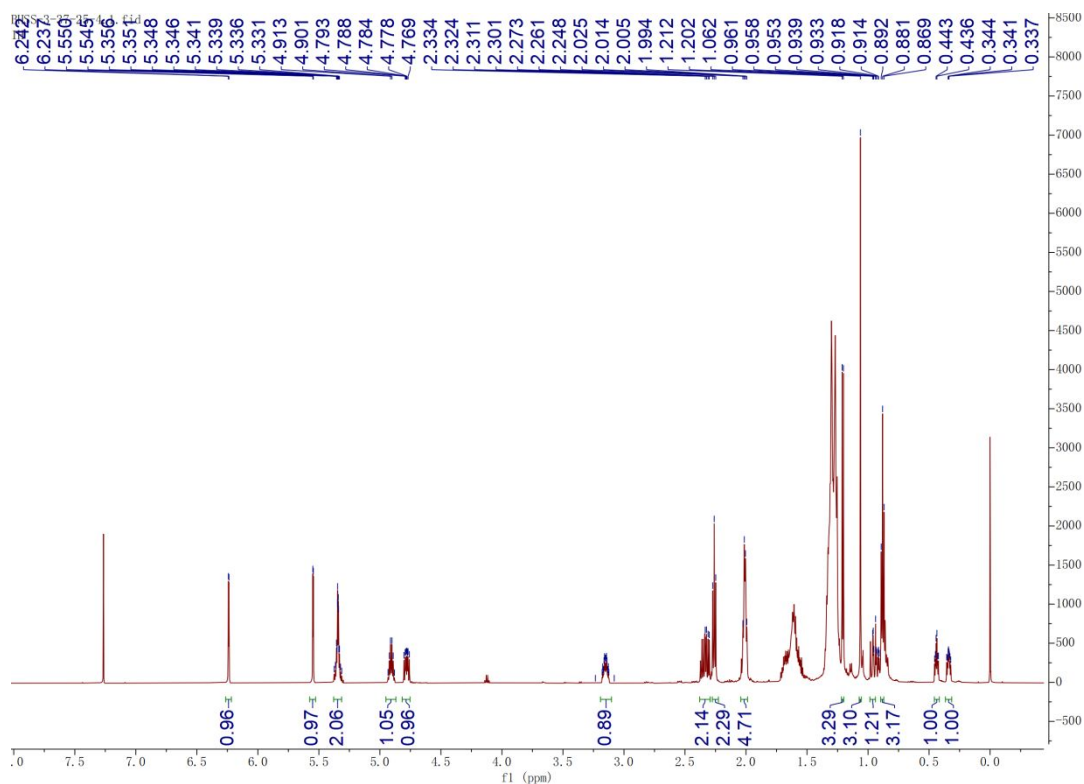


Figure S102. ^1H NMR spectrum (600 MHz) of carabrolate K (**11**) in CDCl_3

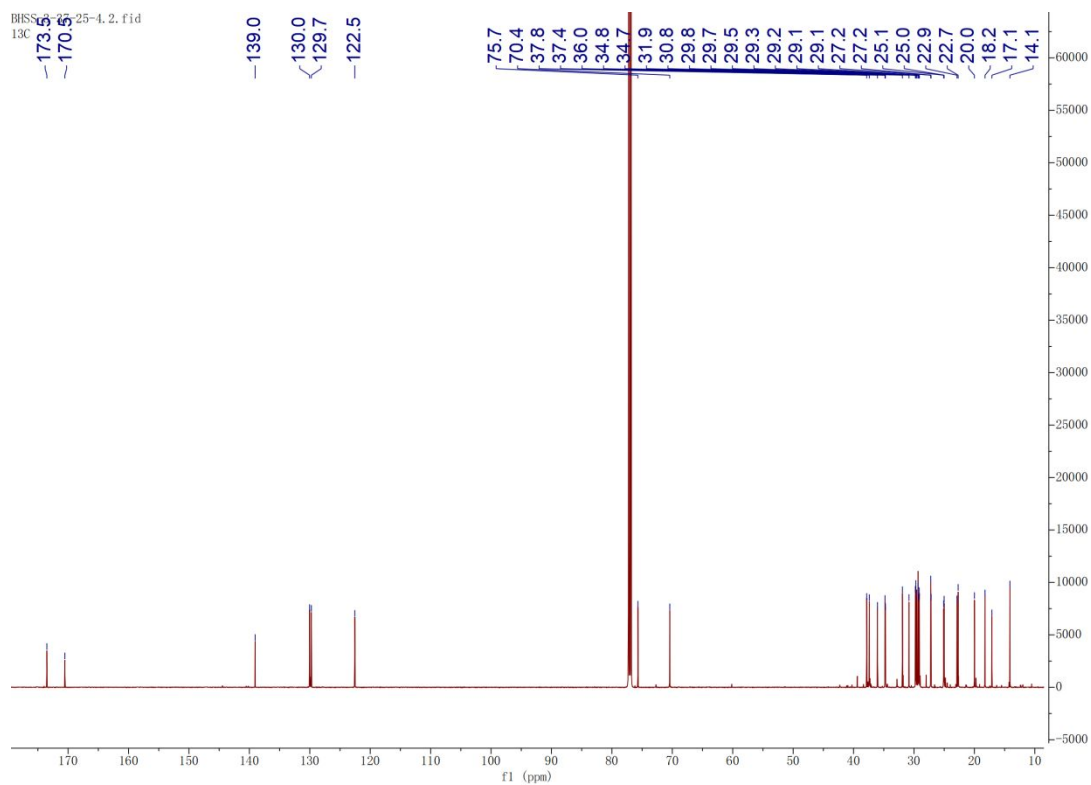


Figure S103. ^{13}C NMR spectrum (150 MHz) of carabrolate K (**11**) in CDCl_3

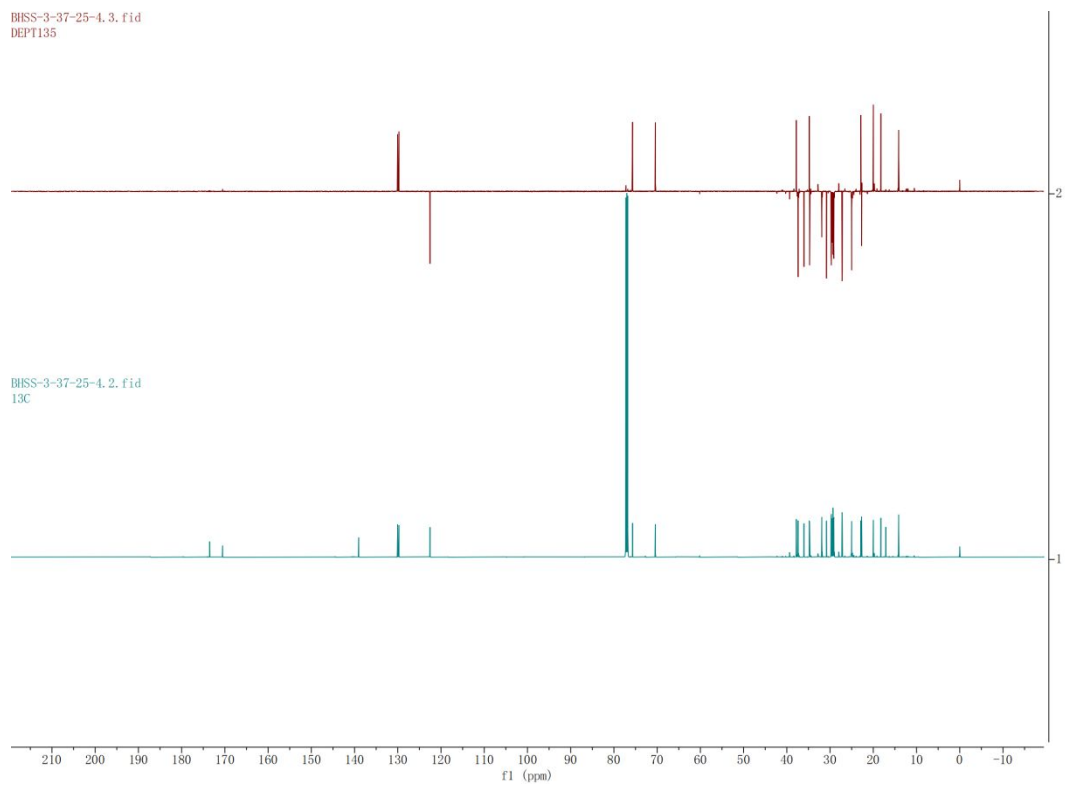


Figure S104. DEPT 135 spectrum (150 MHz) of carabrolate K (**11**) in CDCl_3

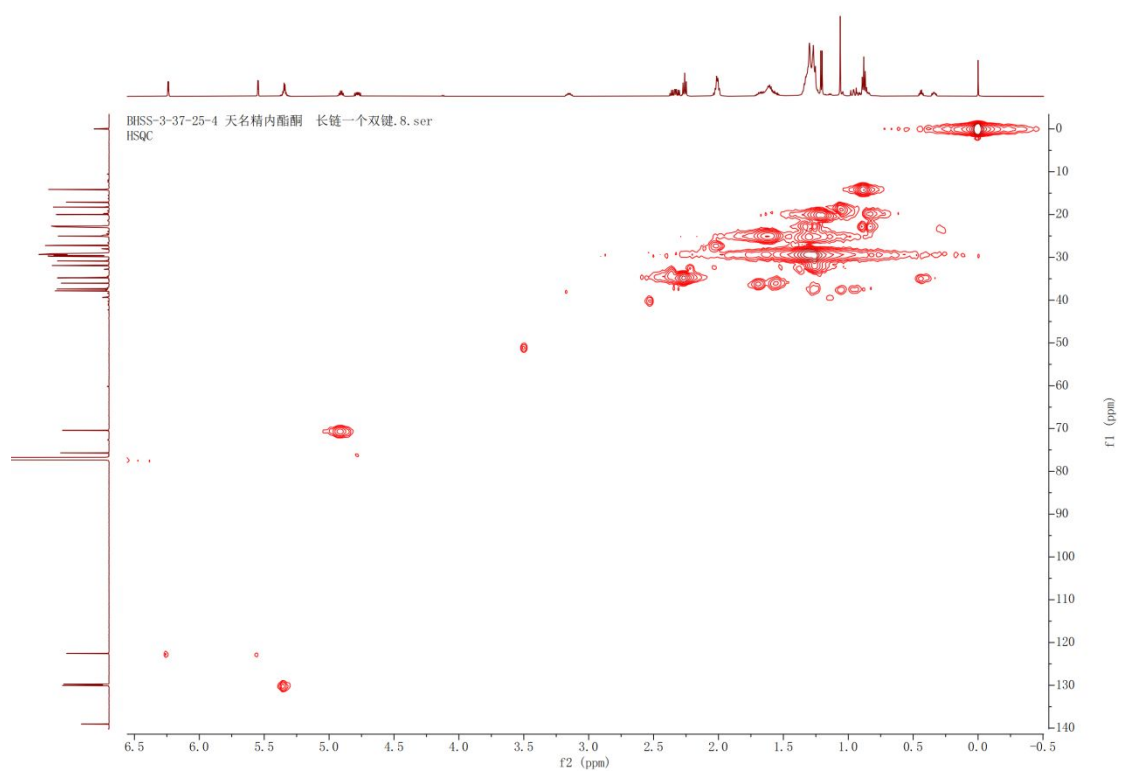


Figure S105. HSQC spectrum (600 MHz) of carabrolate K (**11**) in CDCl_3

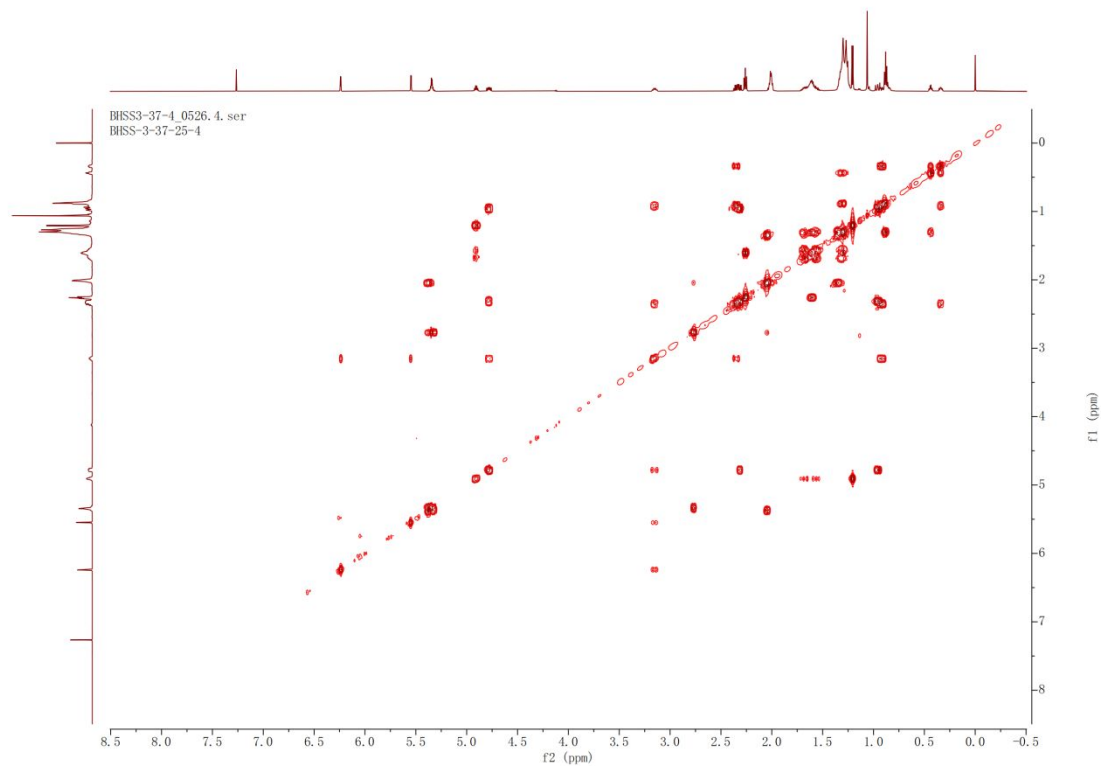


Figure S106. ^1H - ^1H COSY spectrum (600 MHz) of carabrolate K (**11**) in CDCl_3

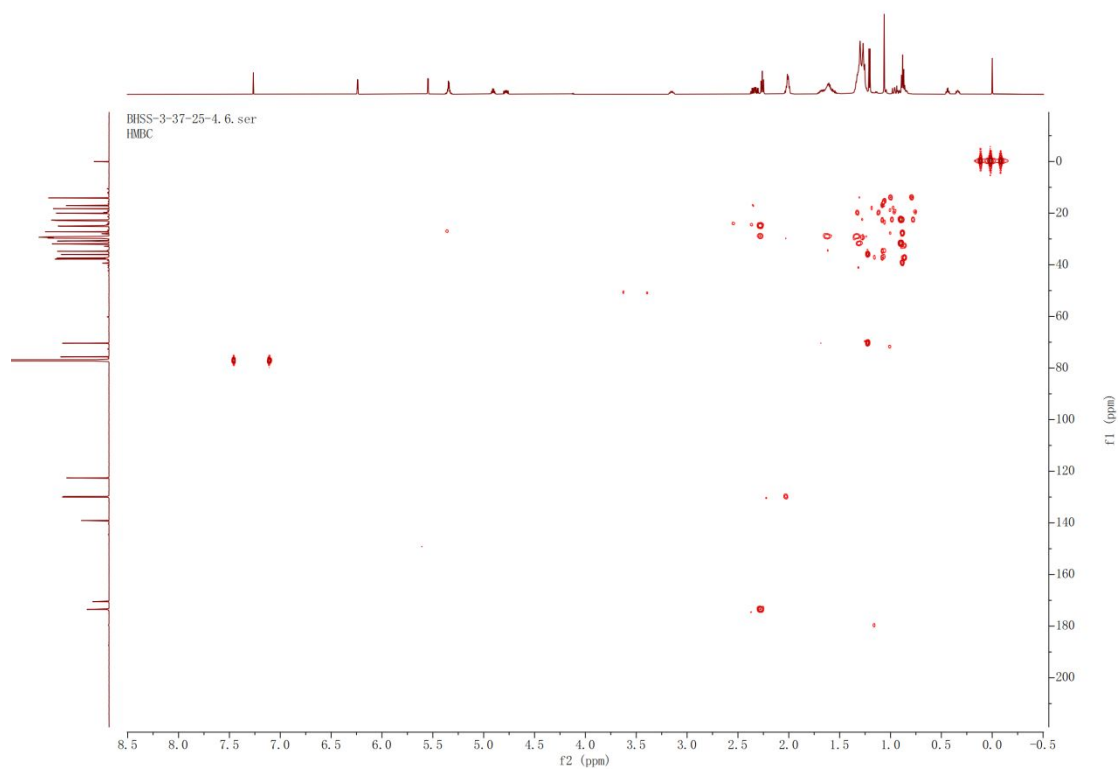


Figure S107. HMBC spectrum (600 MHz) of carabrolate K (**11**) in CDCl_3

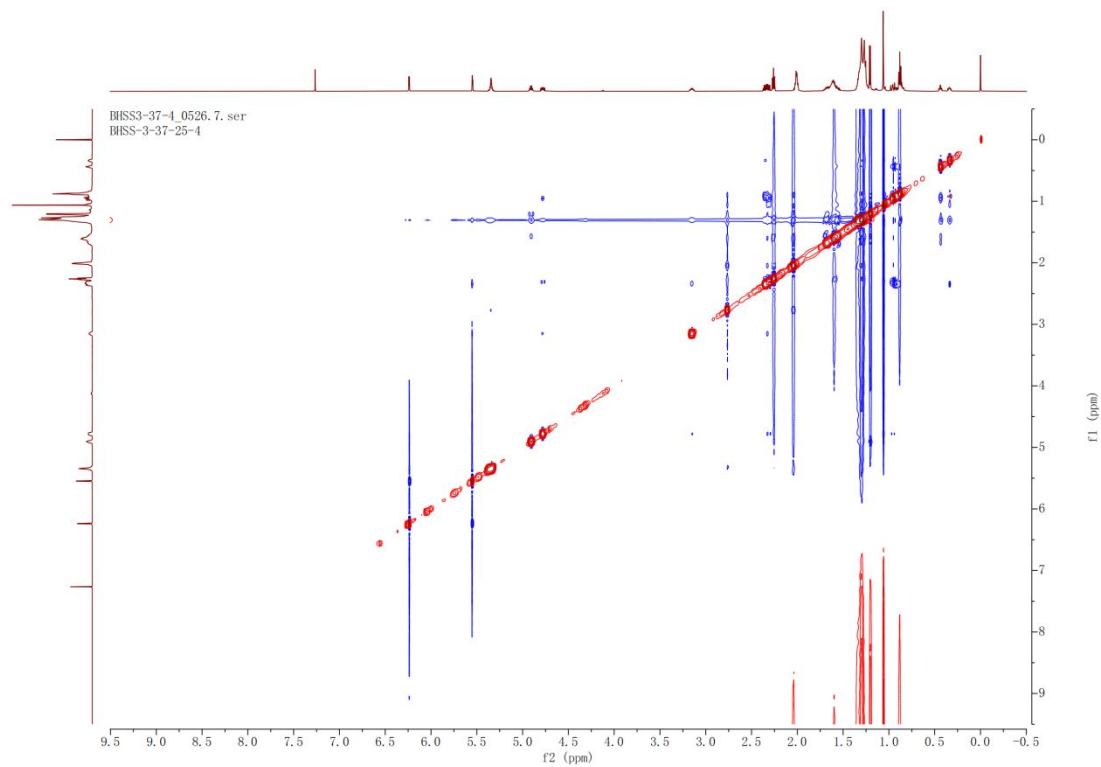


Figure S108. NOESY spectrum (600 MHz) of carabrolate K (**11**) in CDCl_3

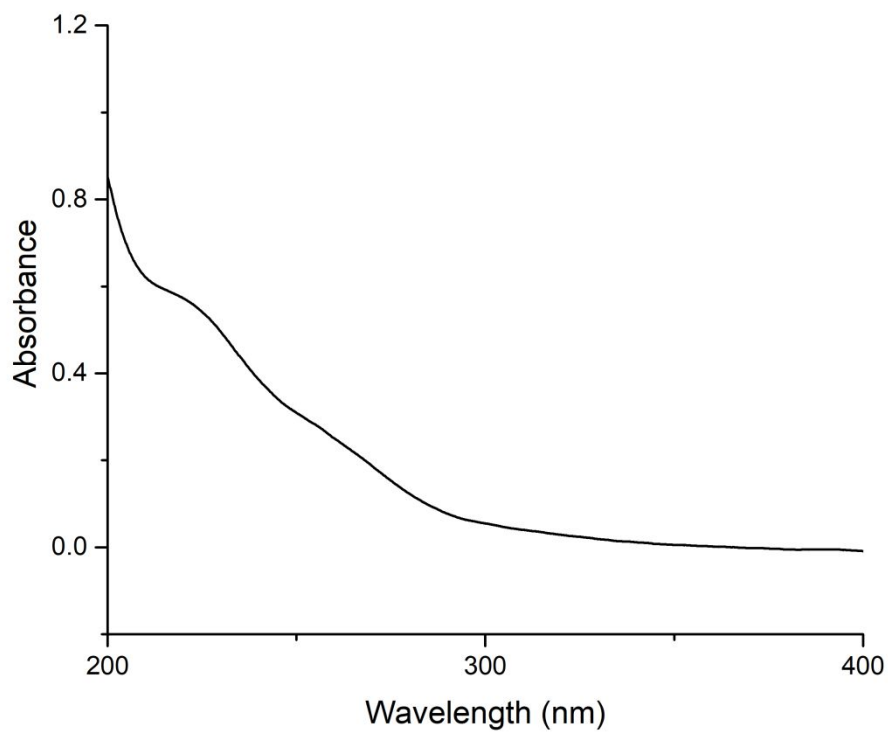


Figure S109. UV spectrum of carabrolate J (**10**) in MeOH

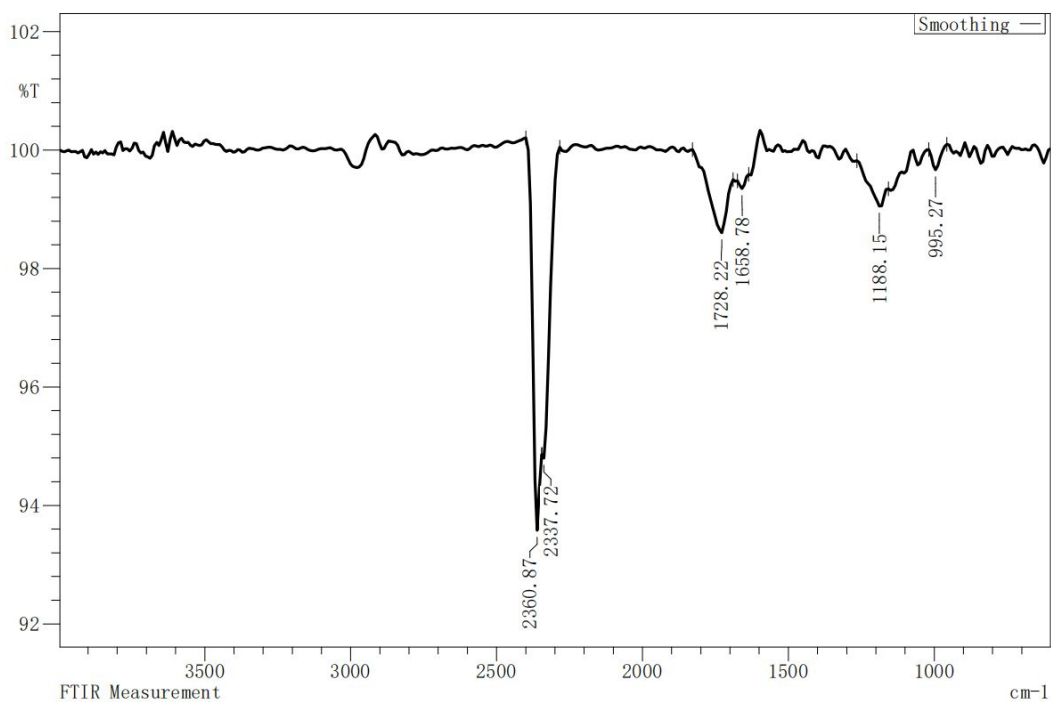
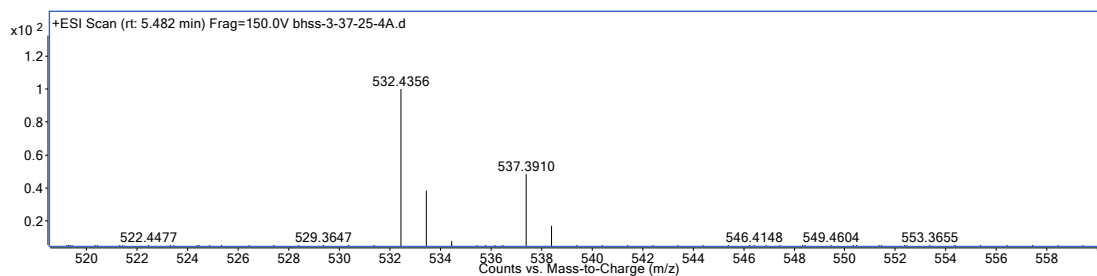
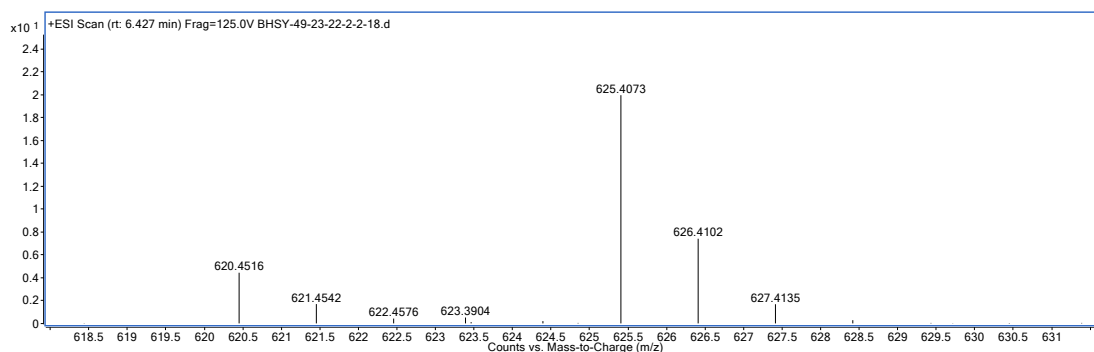


Figure S110. IR spectrum (film on KBr plate) of carabrolate K (**11**)



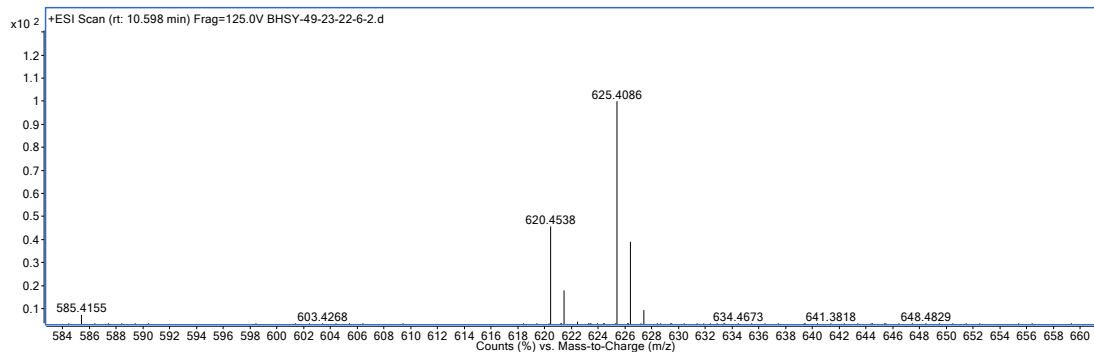
Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	Ion Formula	m/z
C ₃₃ H ₅₄ O ₄	99.64	514.4018	514.4022	532.436	0.85	C ₃₃ H ₅₈ NO ₄	532.4356
C ₃₃ H ₅₄ O ₄	99.65	514.4018	514.4022	537.3914	0.84	C ₃₃ H ₅₄ NaO ₄	537.391

Figure S111. HRESIMS spectrum of carabrolate K (**11**)



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	Ion Formula	m/z
C ₃₆ H ₅₈ O ₇	99.87	602.4178	602.4183	620.4521	0.8	C ₃₆ H ₆₂ NO ₇	620.4516
C ₃₆ H ₅₈ O ₇	99.98	602.4181	602.4183	625.4075	0.29	C ₃₆ H ₅₈ NaO ₇	625.4073

Figure S112. HRESIMS spectrum of the ketal of carabrolate E (5)



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	Ion Formula	m/z
C ₃₆ H ₅₈ O ₇	97.7	602.4195	602.4183	603.4255	-2.11	C ₃₆ H ₅₉ O ₇	603.4268
C ₃₆ H ₅₈ O ₇	98.18	602.4194	602.4183	625.4075	-1.87	C ₃₆ H ₅₈ NaO ₇	625.4086

Figure S113. HRESIMS spectrum of the ketal of carabrolate F (6)

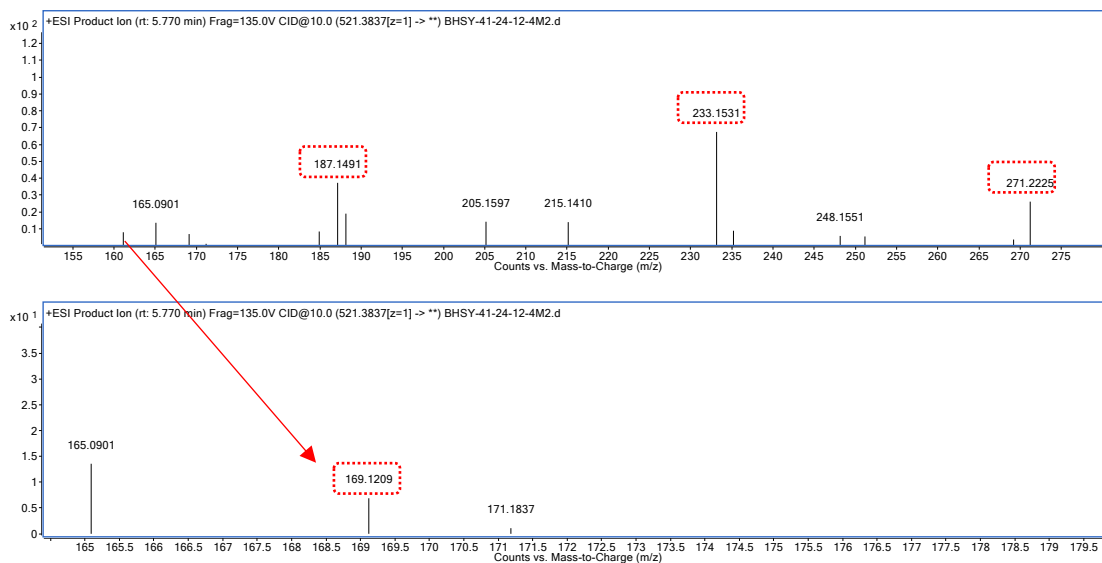


Figure S114. MS/MS spectrum (positive mode) of carabolate G (7).

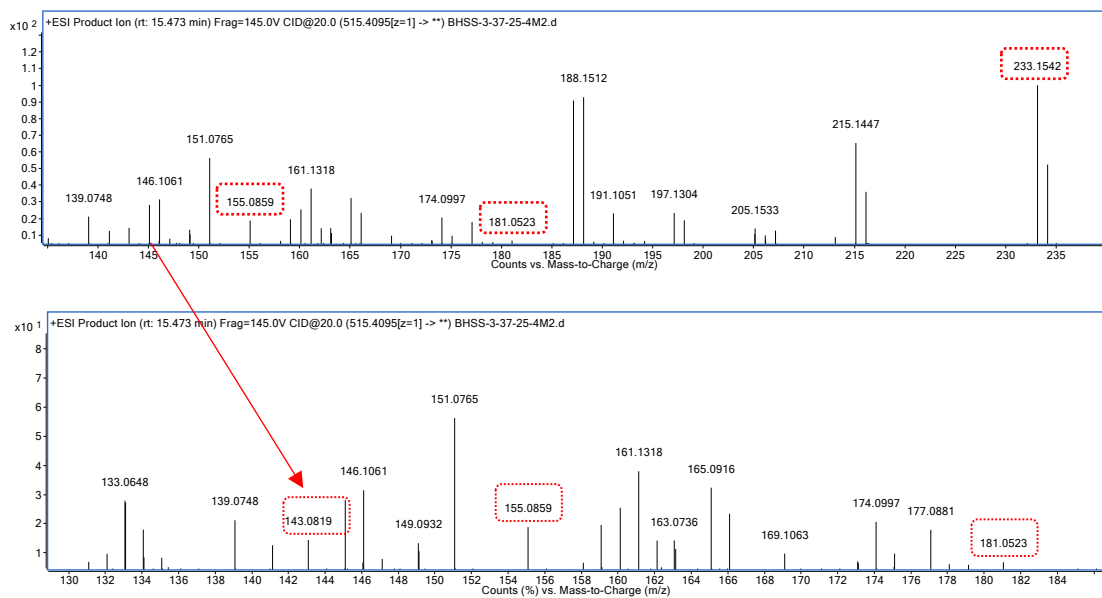


Figure S115. MS/MS spectrum (positive mode) of carabolate K (11).

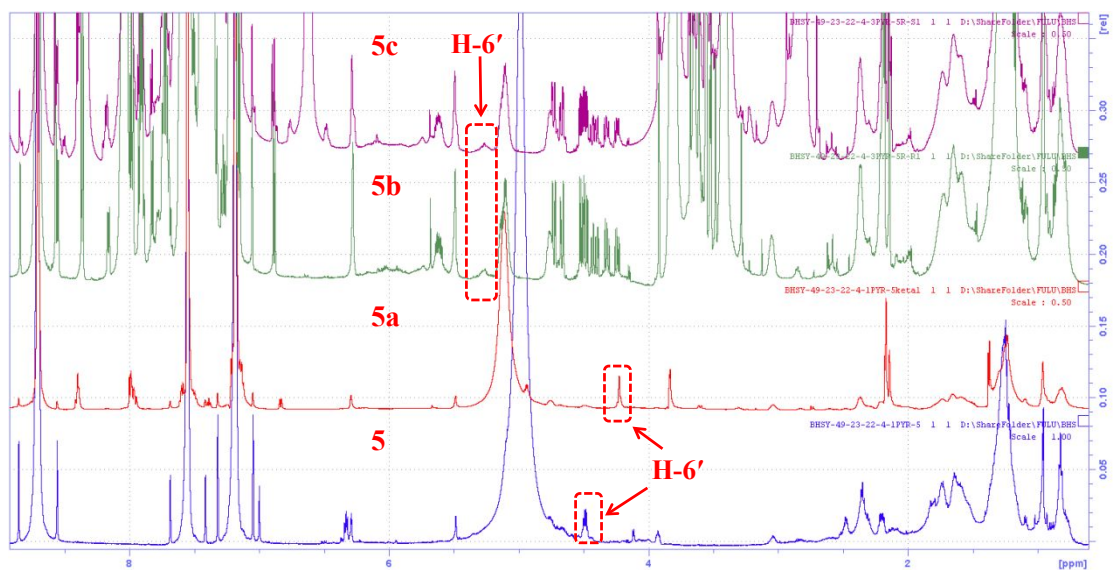


Figure S116. ^1H NMR spectra (600 MHz) of **5**, **5a**, **5b**, and **5c** in $\text{C}_5\text{D}_5\text{N}$. **5a**: the ketal of **5**; **5b**: (*S*)-MTPA esters of **5a**; **5c**: (*R*)-MTPA esters of **5a**.

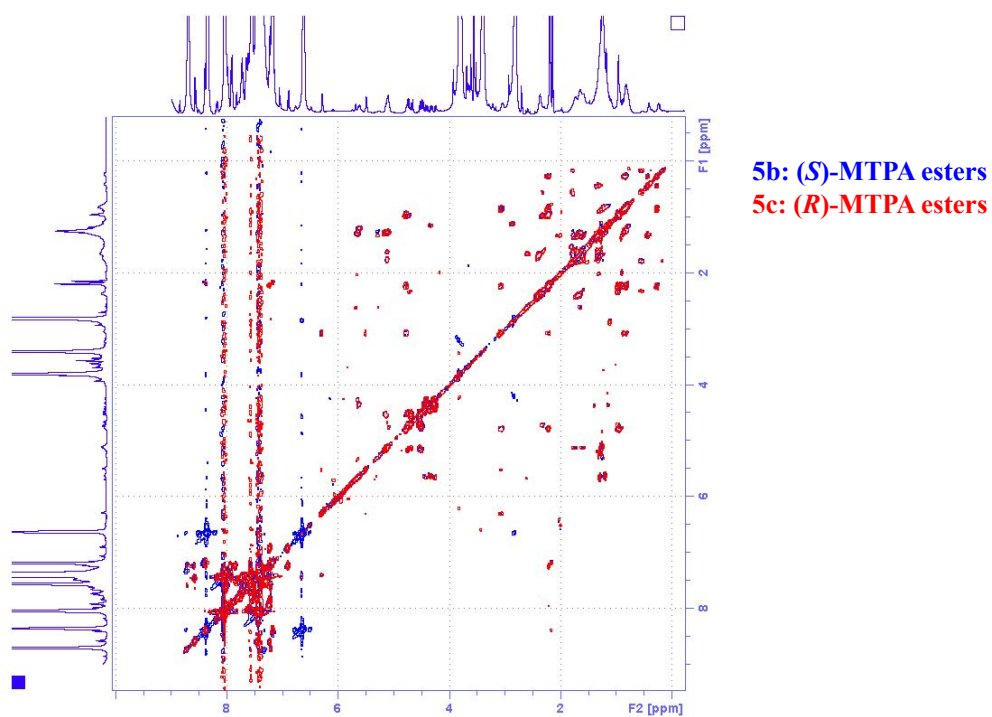


Figure S117. ^1H - ^1H COSY spectra (600 MHz) of **5b** and **5c** in $\text{C}_5\text{D}_5\text{N}$.

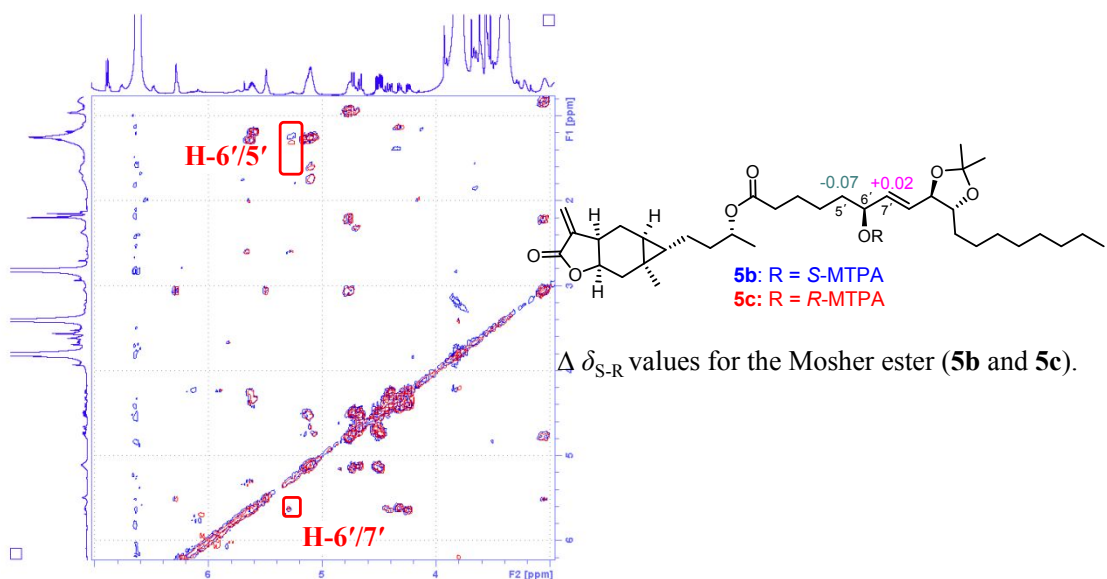


Figure S118. Enlarged ^1H - ^1H COSY spectra (600 MHz) of **5b** and **5c** in $\text{C}_5\text{D}_5\text{N}$.

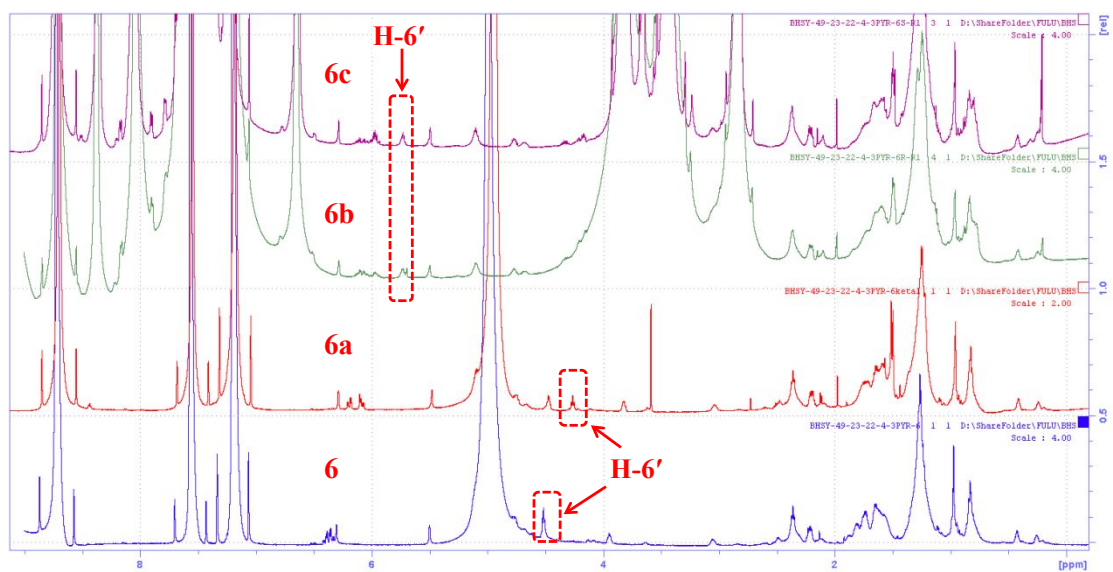


Figure S119. ^1H NMR spectra (600 MHz) of **6**, **6a**, **6b**, and **6c** in $\text{C}_5\text{D}_5\text{N}$. **6a**: the ketal of **6**; **6b**: (*S*)-MTPA esters of **6a**; **6c**: (*R*)-MTPA esters of **6a**.

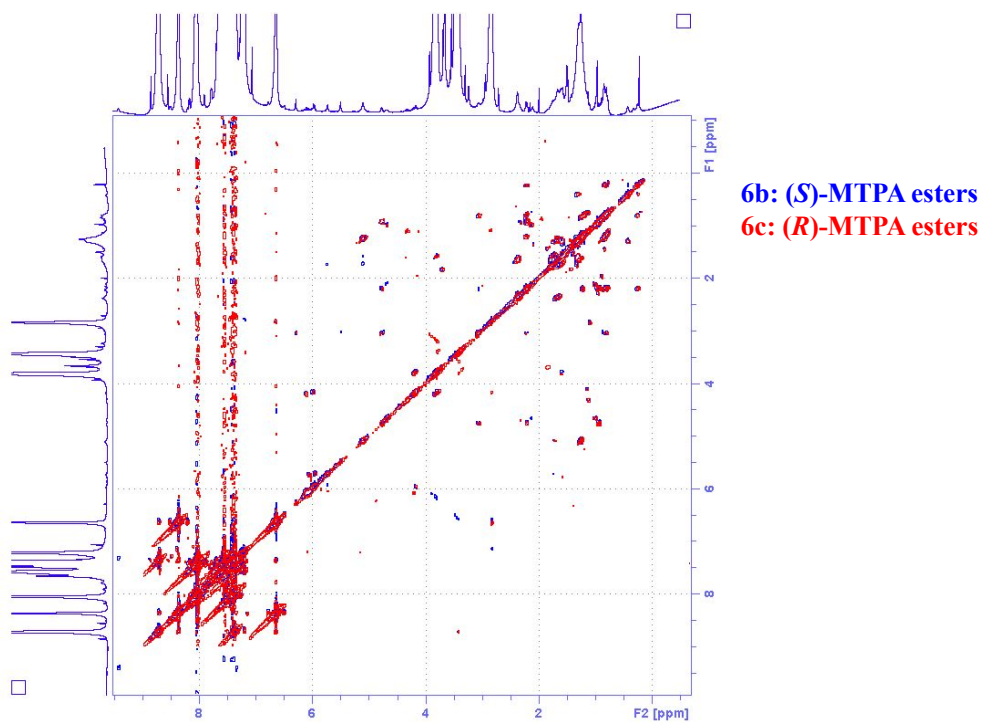


Figure S120. ^1H - ^1H COSY spectra (600 MHz) of **6b** and **6c** in $\text{C}_5\text{D}_5\text{N}$.

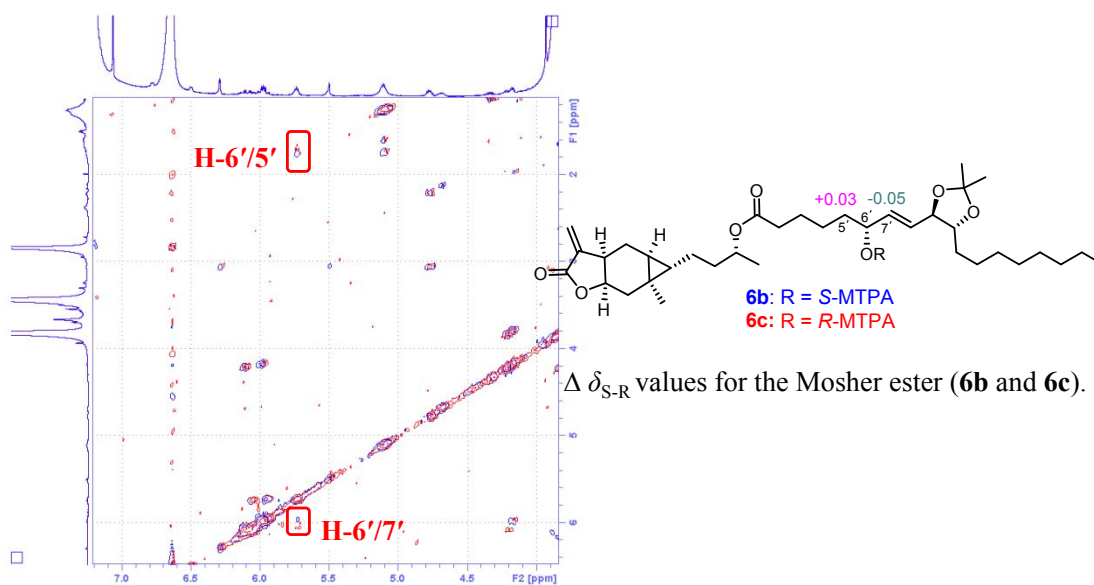


Figure S121. Enlarged ^1H - ^1H COSY spectra (600 MHz) of **6b** and **6c** in $\text{C}_5\text{D}_5\text{N}$.

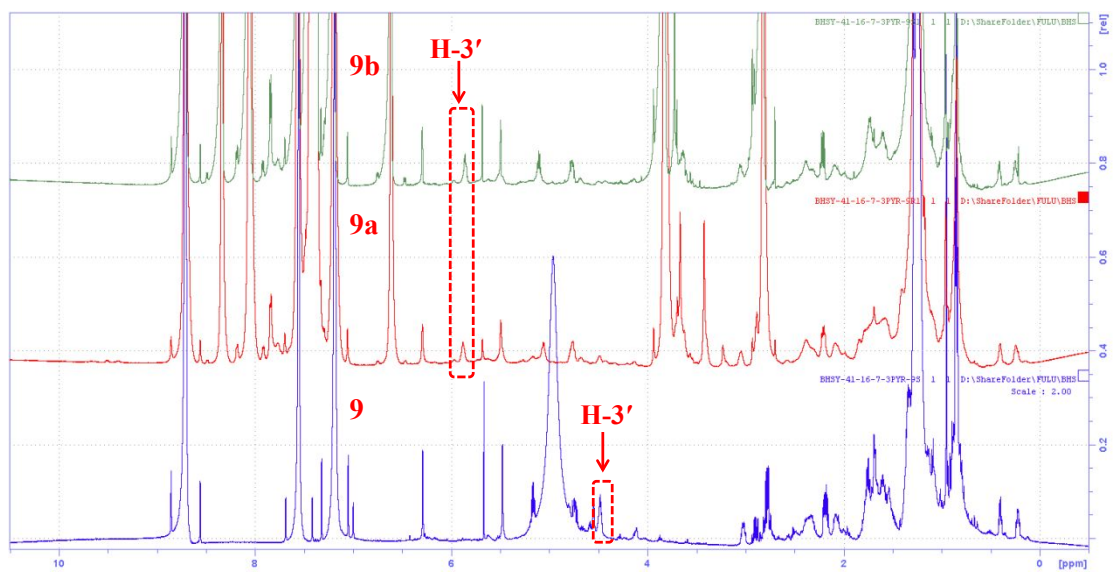


Figure S122. ^1H NMR spectra (600 MHz) of **9**, **9a**, and **9b** in $\text{C}_5\text{D}_5\text{N}$. **9a**: (*S*)-MTPA esters of **9**; **9b**: (*R*)-MTPA esters of **9**.

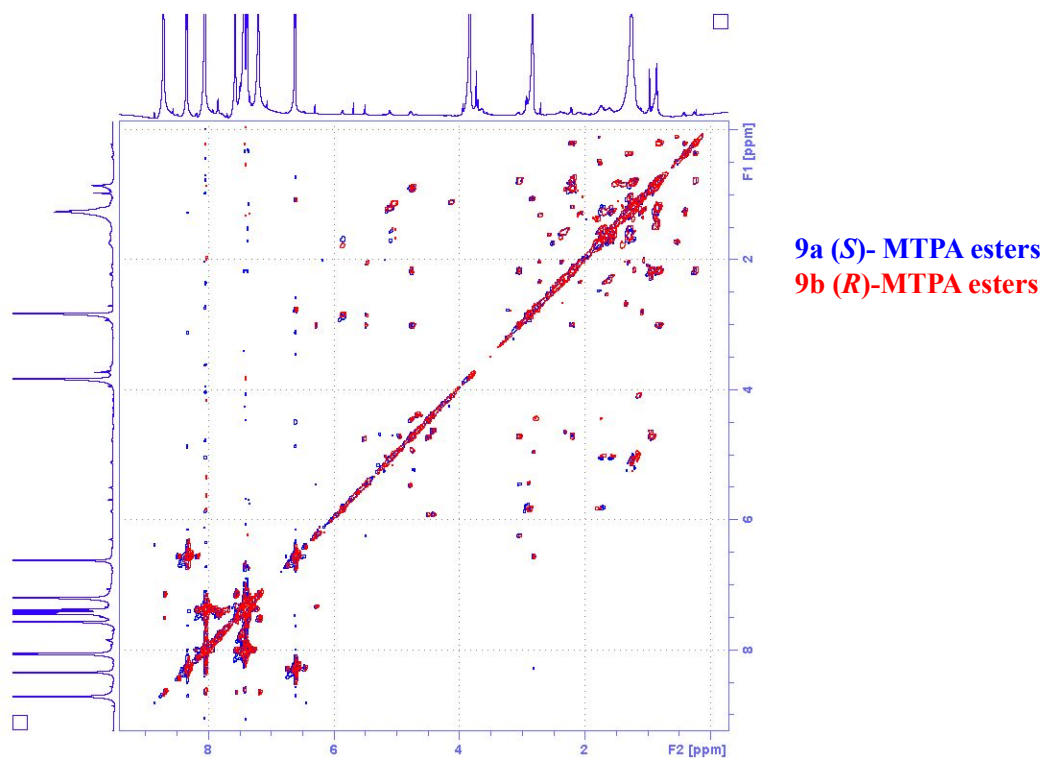


Figure S123. ^1H - ^1H COSY spectra (600 MHz) of **9a** and **9b** in $\text{C}_5\text{D}_5\text{N}$.

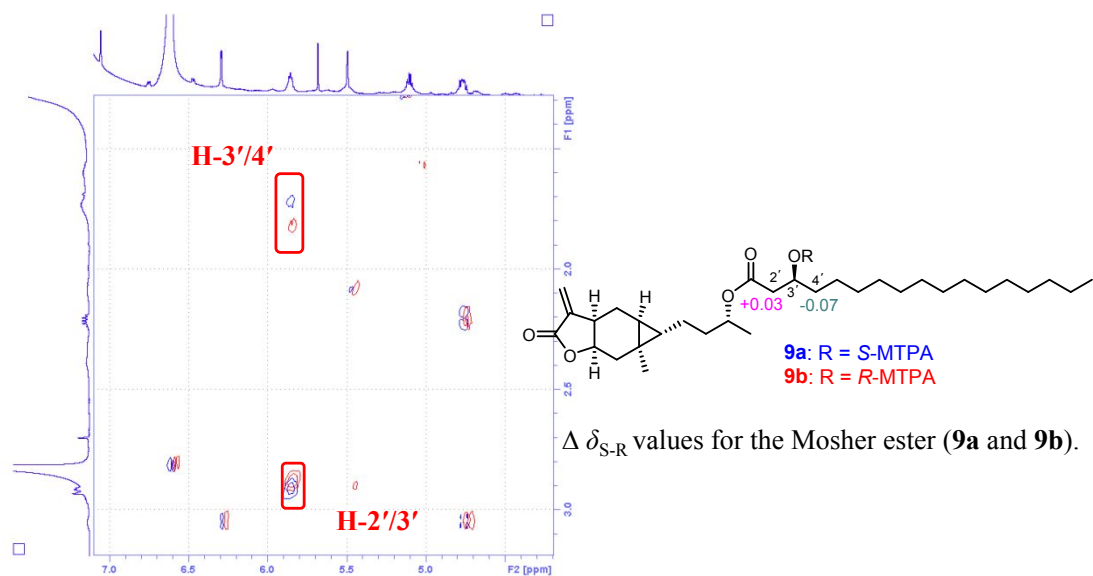


Figure S124. Enlarged ^1H - ^1H COSY spectra (600 MHz) of **9a** and **9b** in $\text{C}_5\text{D}_5\text{N}$.