

Supporting Information

Nitric Oxide Inhibitory Dimeric Sesquiterpenoids from *Artemisia rupestris*

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Figure S1. The UV and MS Spectra Profiles of Disesquiterpeneoids in *A. rupestris*

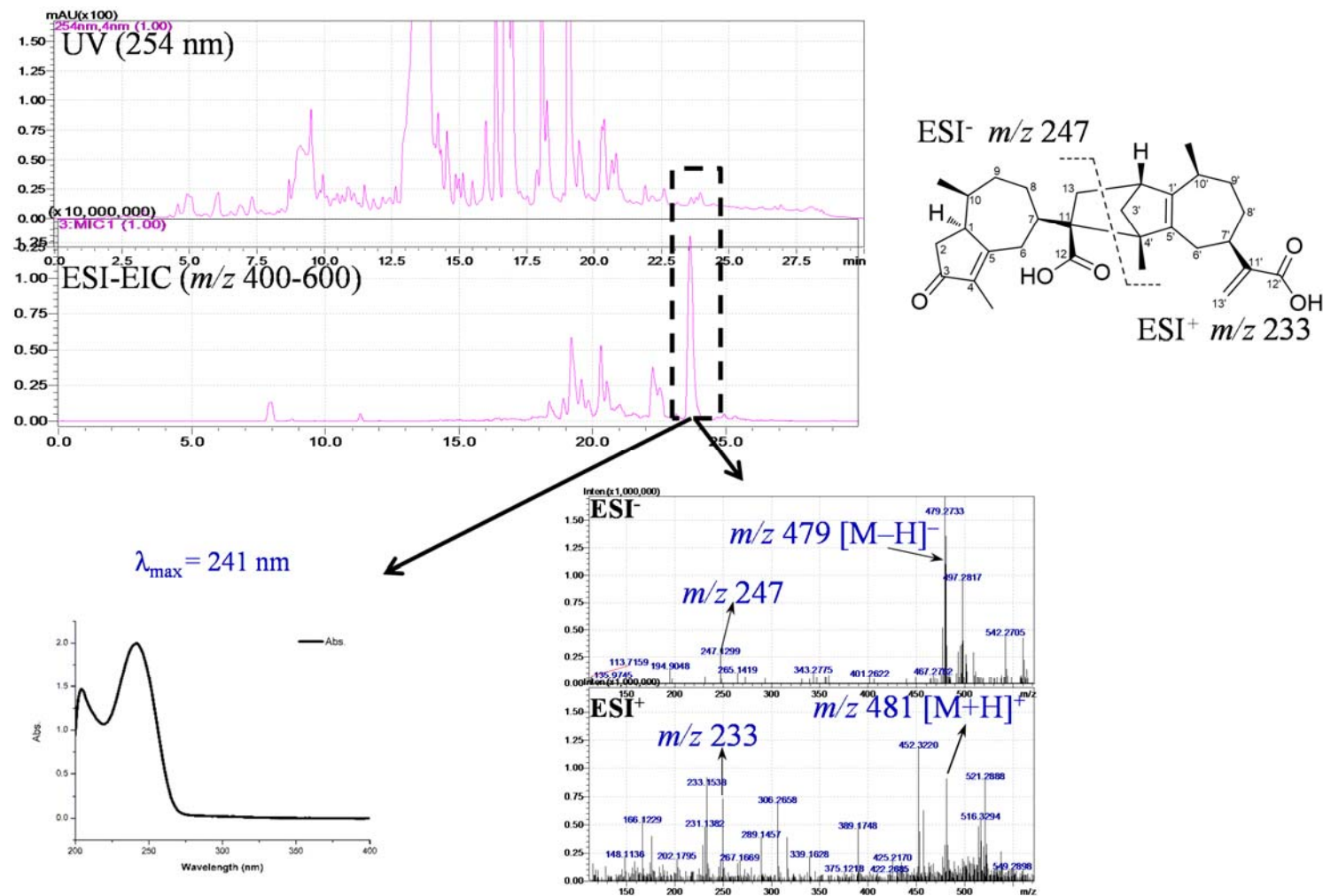


Figure S2. (-)-HRESIMS Spectrum of Compound 1

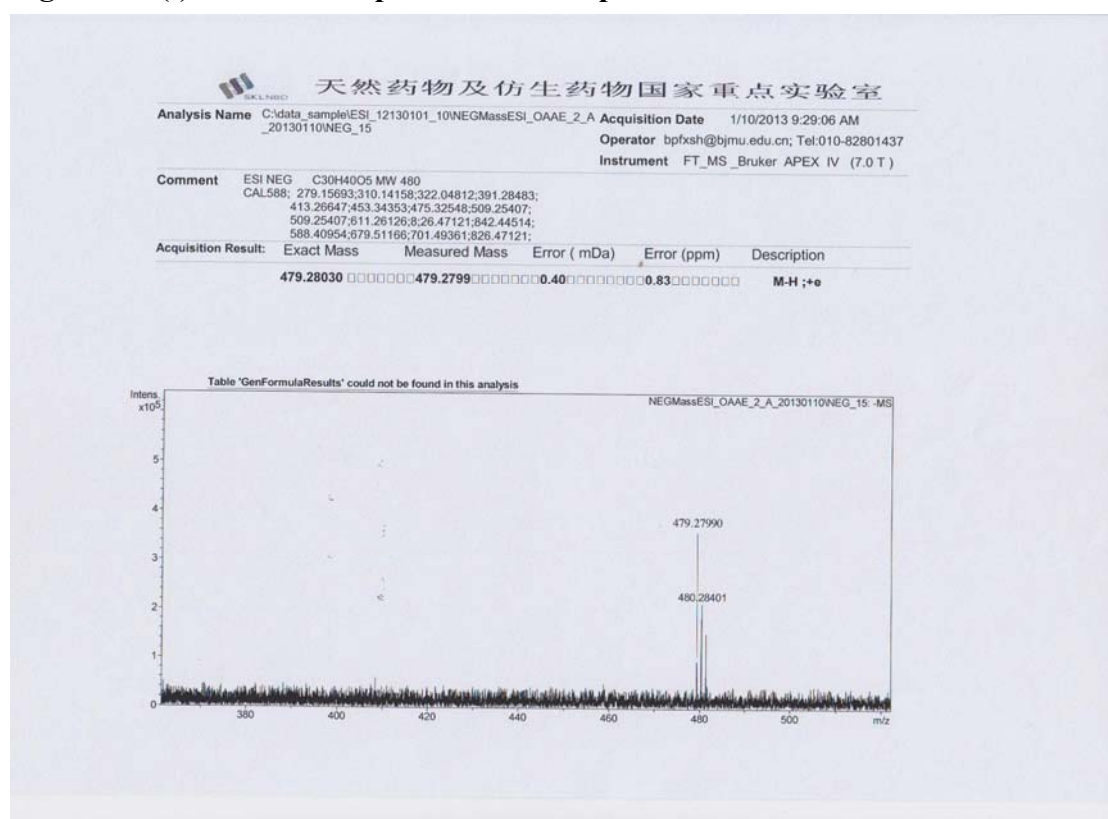


Figure S3. IR Spectrum of Compound 1

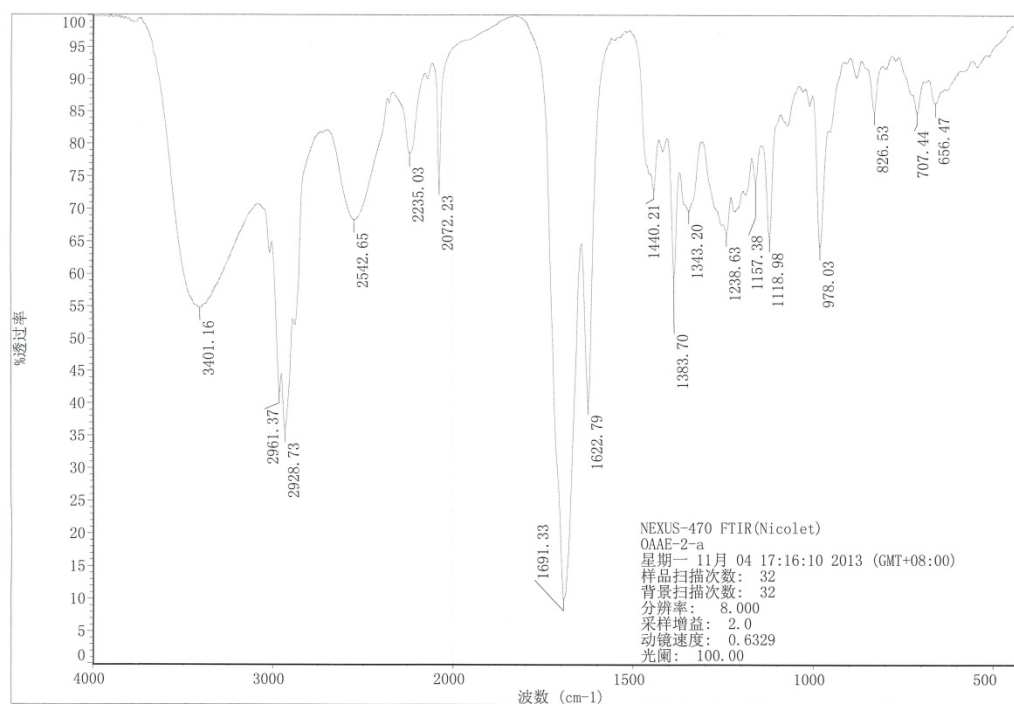


Figure S4. ^1H -NMR Spectrum of Compound 1 (500 MHz, CD_3OD)

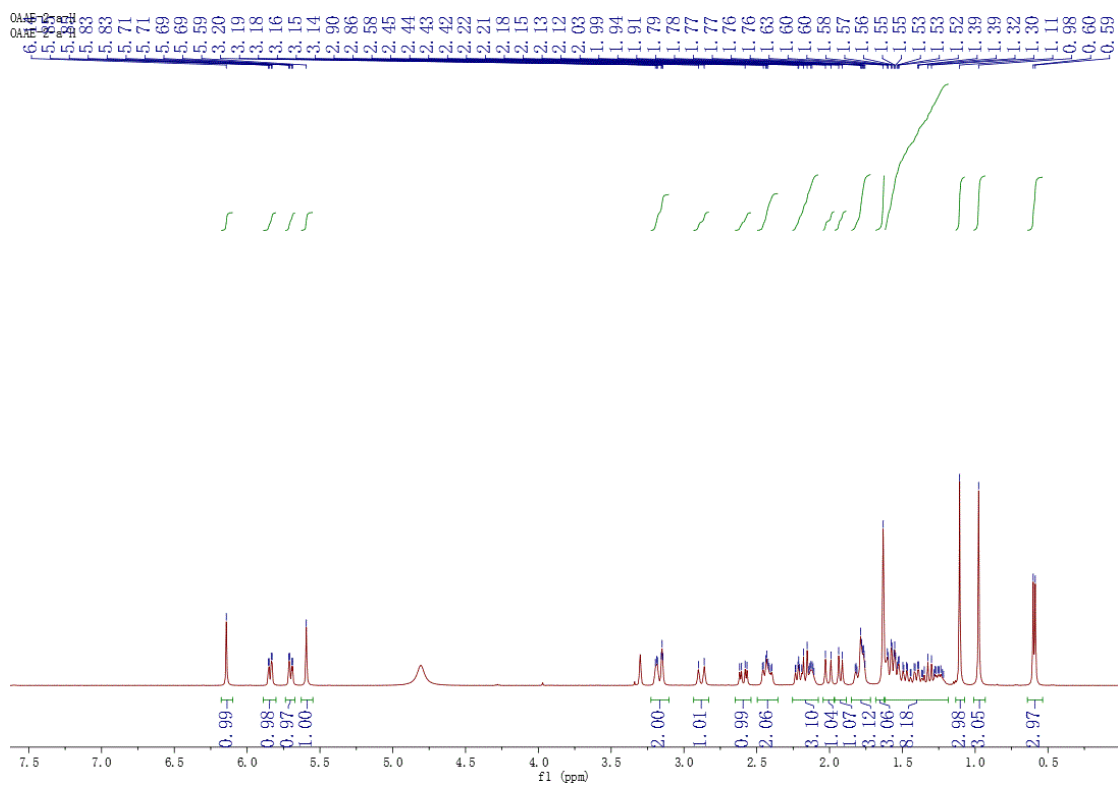


Figure S5. ^{13}C -NMR Spectrum of Compound 1 (125 MHz, CD_3OD)

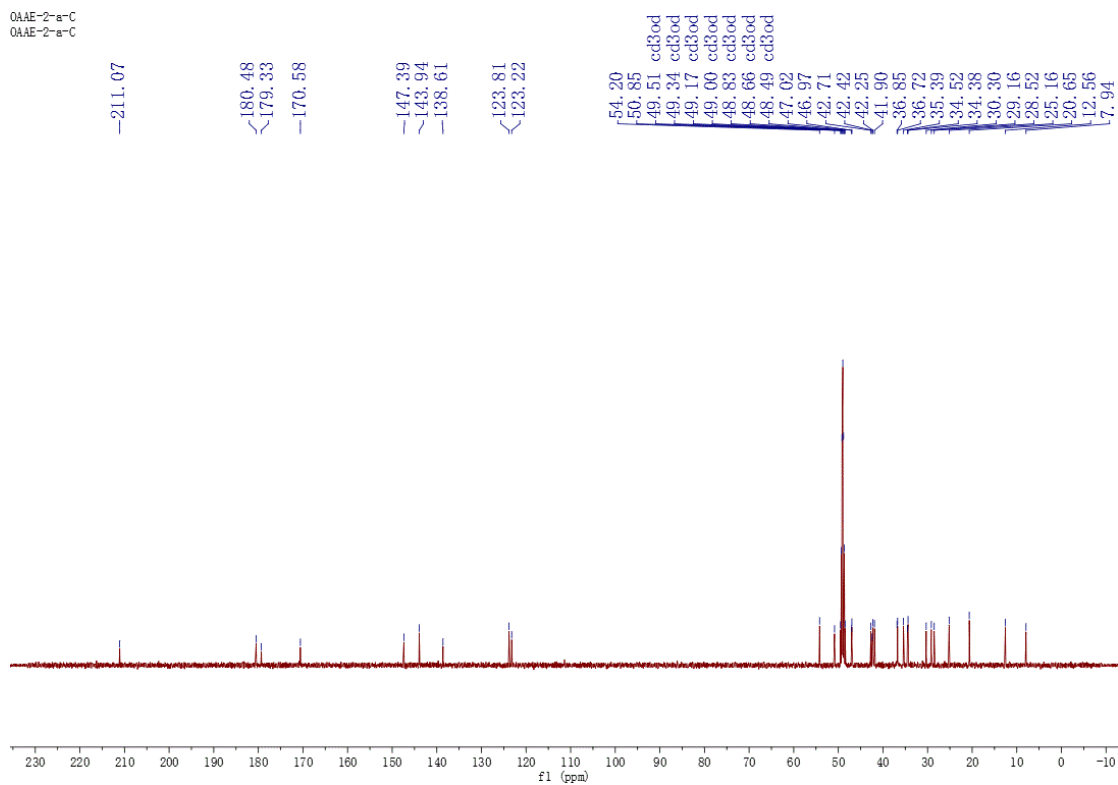


Figure S6. DEPT-135 Spectrum of Compound 1

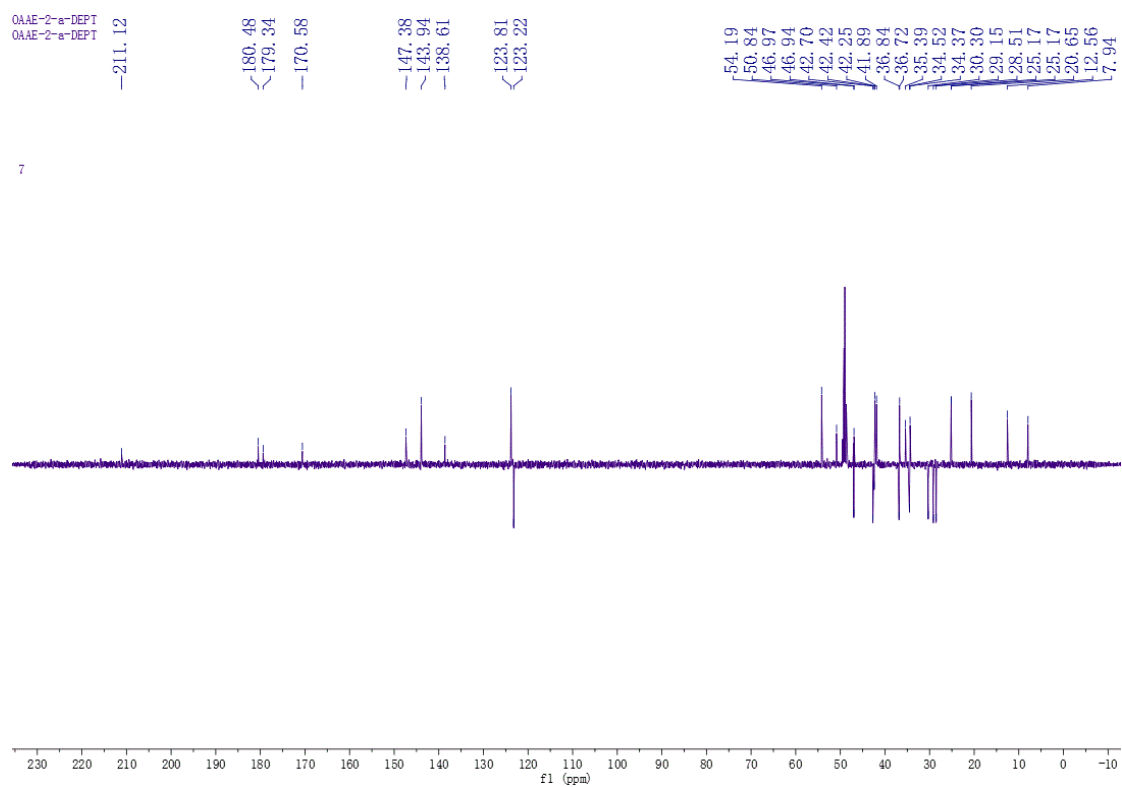


Figure S7. ^1H - ^1H gCOSY Spectrum of Compound 1

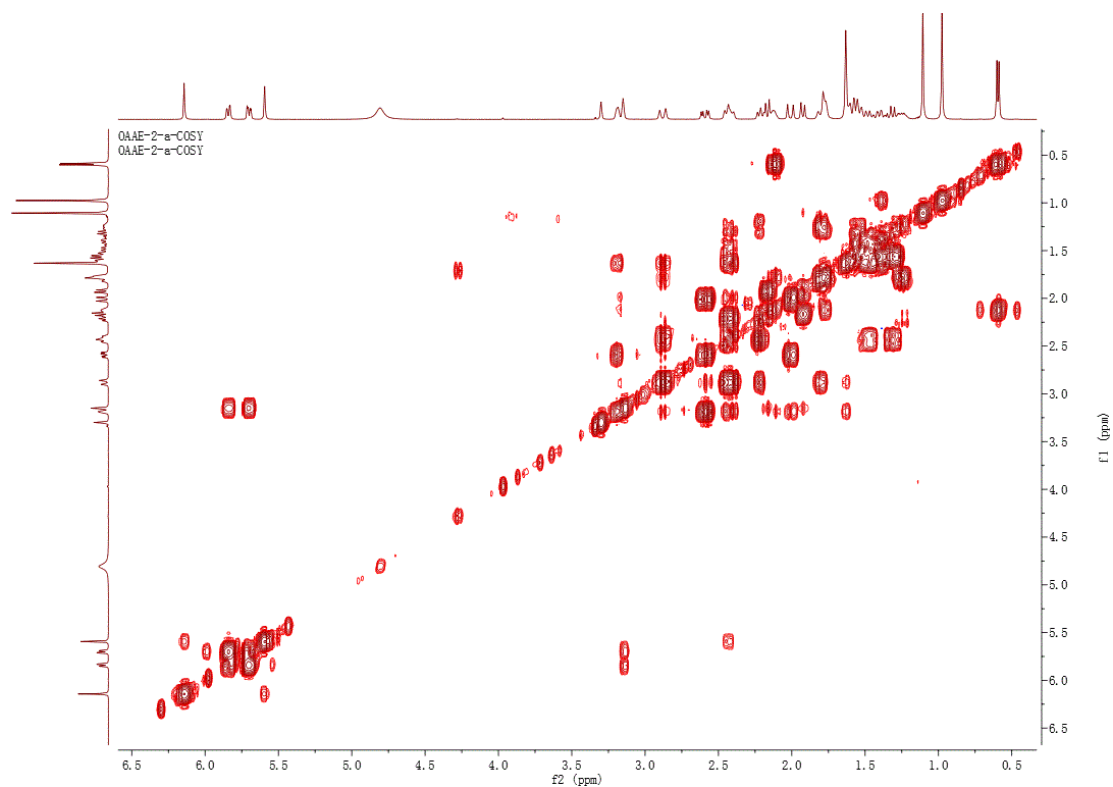


Figure S8. Multiplicity-edited gHSQC Spectrum of Compound 1

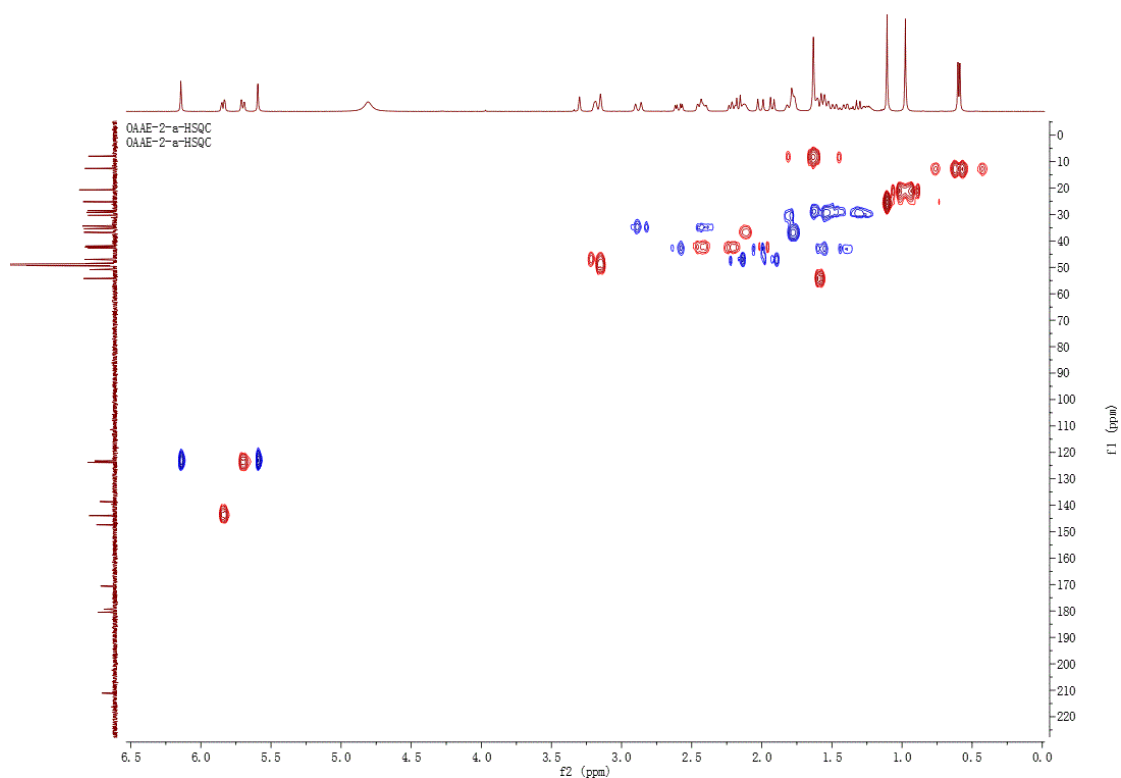


Figure S9. gHMBC Spectrum of Compound 1

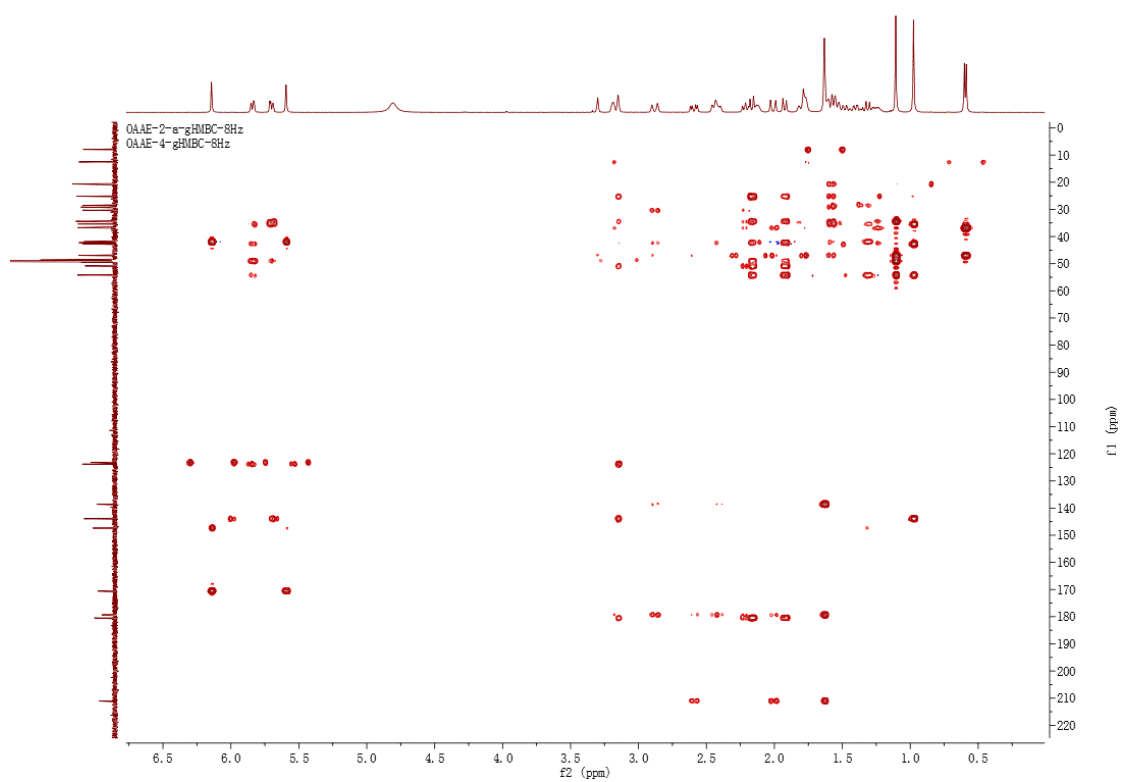


Figure S10. NOESY Spectrum of Compound 1

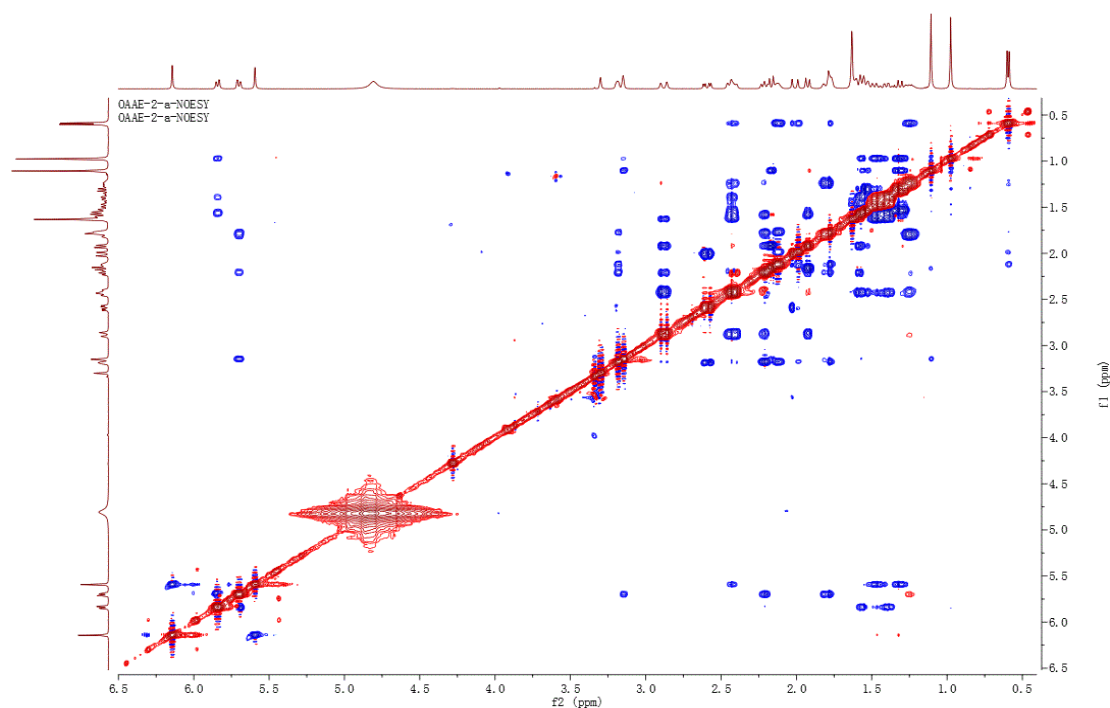


Figure S11. 1D NOE Spectra of Compound 1

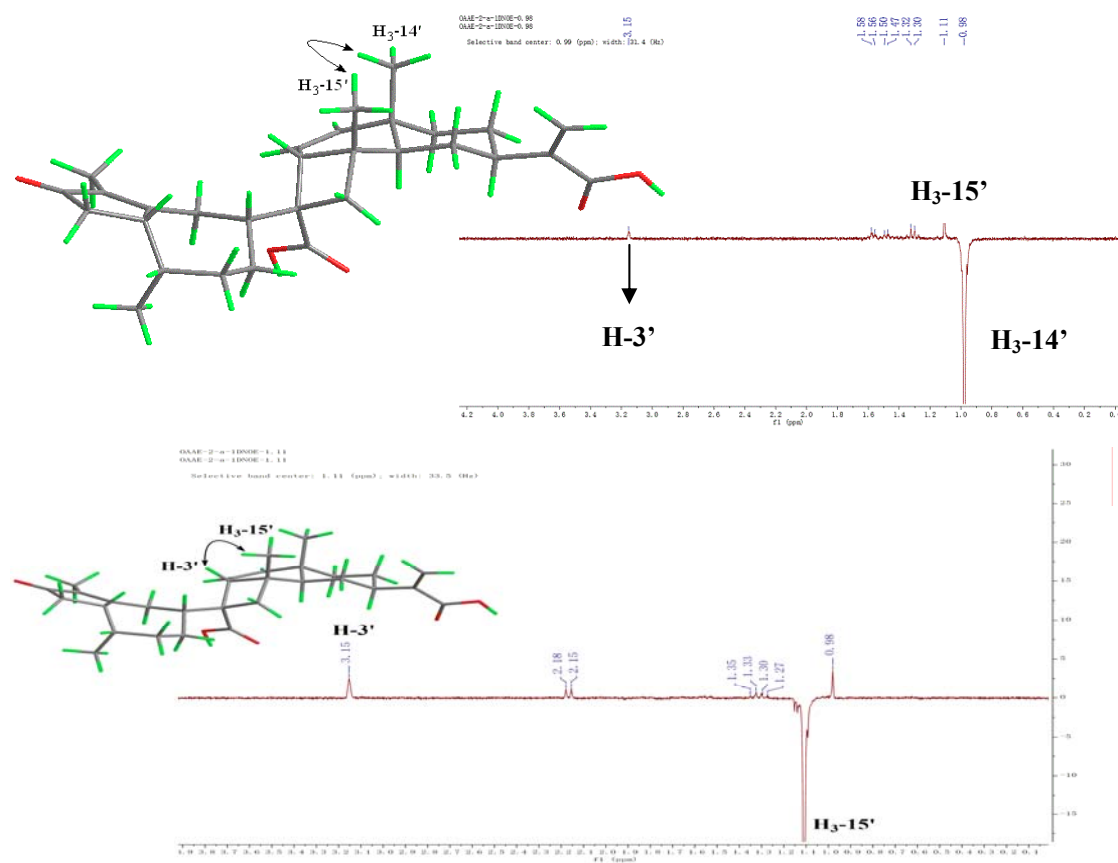


Figure S12. The Stable Conformers of Compound 1

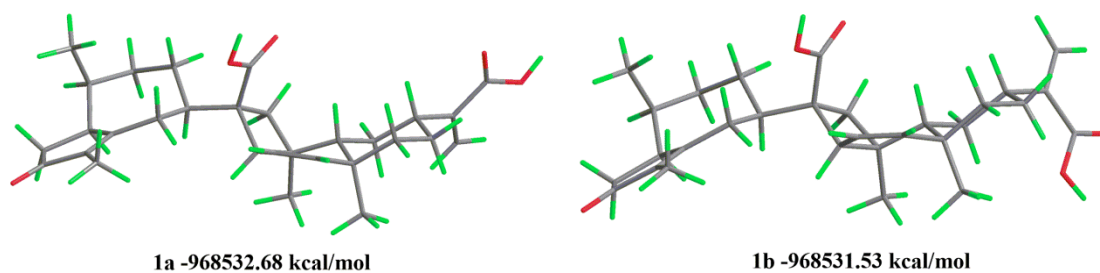


Table S1. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of **1**

Conf	$\Delta E_{6-31+G(d)}$ ^a	% ^b
1a	0	87.5
1b	1.15	12.5

^aRelative to 1a with $E_{6-31+G(d)} = -968532.68$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S13. The Stable Conformers of (1*S*,7*R*,10*S*,11*S*,3'*R*,4'*S*,5'*R*,7'*R*,10'*S*)-1

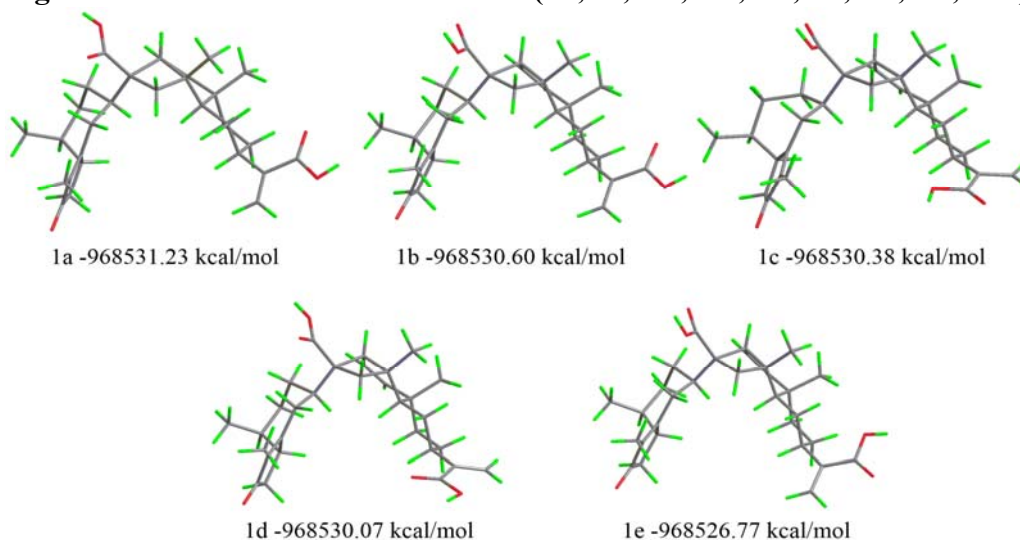


Table S2. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of (1*S*,7*R*,10*S*,11*S*,3'*R*,4'*S*,5'*R*,7'*R*,10'*S*)-**1**

Conf	$\Delta E_{6-31+G(d)}$ ^a	% ^b
1a	0	57.8
1b	0.62	20.1
1c	0.84	13.9
1d	1.16	8.1
1e	4.46	0.03

^aRelative to 1a with $E_{6-31+G(d)} = -968531.23$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S14. (-)-HRESIMS Spectrum of Compound 2

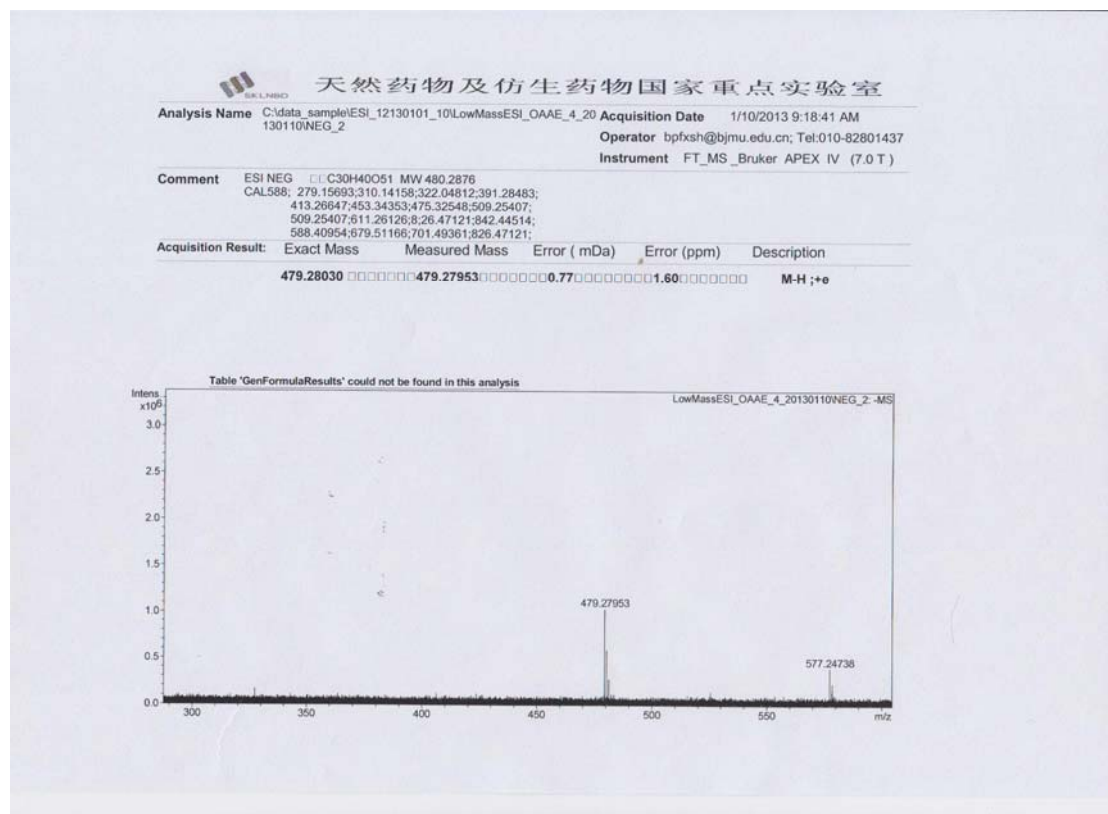
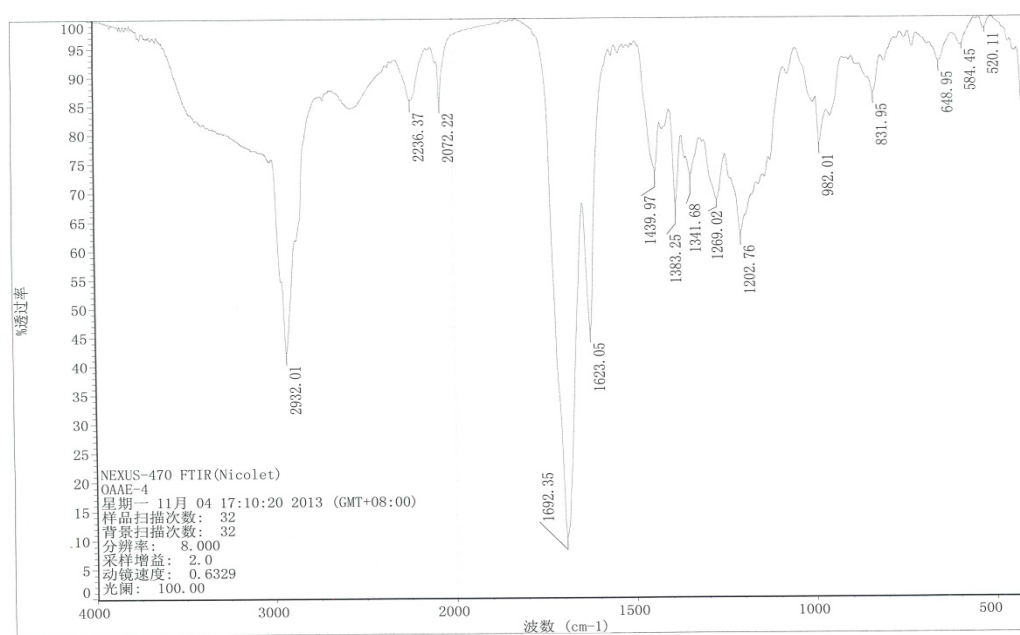


Figure S15. IR Spectrum of Compound 2



¹H NMR spectrum (CDCl₃) of compound 10a. The x-axis represents the chemical shift in ppm, ranging from 0.0 to 6.5. The spectrum shows several peaks, with integration values provided below the baseline. A list of chemical shifts (δ) is provided at the top of the spectrum.

Chemical shifts (δ): 4.81, 3.31, 3.30, 3.30, 3.20, 3.09, 2.85, 2.81, 2.60, 2.56, 2.55, 2.48, 2.31, 2.31, 2.30, 2.29, 2.28, 2.21, 2.19, 2.12, 2.10, 2.08, 2.03, 2.00, 1.99, 1.98, 1.88, 1.86, 1.83, 1.82, 1.74, 1.72, 1.70, 1.67, 1.64, 1.55, 1.35, 1.34, 1.34, 1.31, 1.31, 1.30, 1.28, 1.28, 1.24, 1.23, 1.23, 0.72, 0.61, 0.60.

Integration values (from left to right): 1.00, 1.00, 1.06, 1.06, 1.04, 1.04, 1.04, 2.15, 2.12, 2.21, 2.25, 2.16, 2.26, 3.03, 3.50, 1.19, 4.24, 1.10, 3.12, 3.15.

0AAE-4-C
0AAE-4-C

—211.04

—180.01
—178.81
—170.64

—147.54
—140.22
—138.31

—123.29
—120.82

56.85
47.22
43.38
42.46
42.26
41.63
41.53
40.44
38.22
36.65
36.44
35.48
34.08
31.75
30.82
27.97
27.32
21.82
18.10
12.31
7.89

f1 (ppm)

Figure S18. DEPT-135 Spectrum of Compound 2

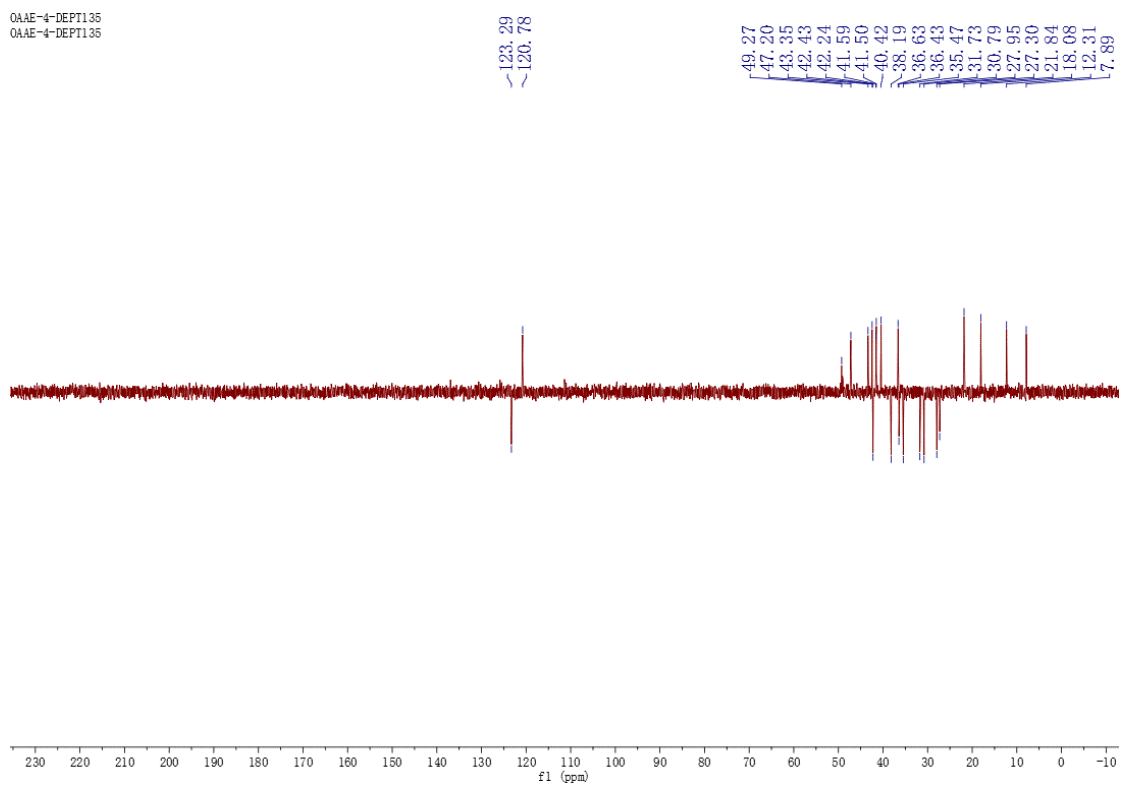


Figure S19. ^1H - ^1H gCOSY Spectrum of Compound 2

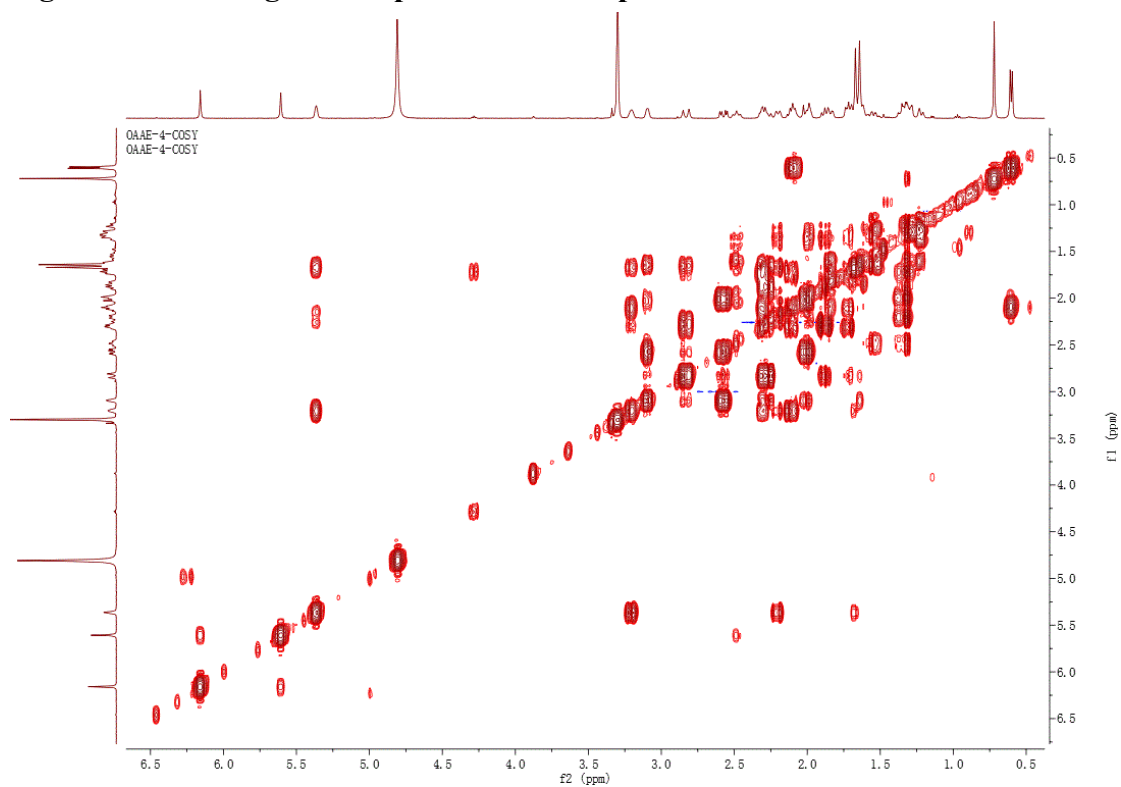


Figure S20. Multiplicity-edited gHSQC Spectrum of Compound 2

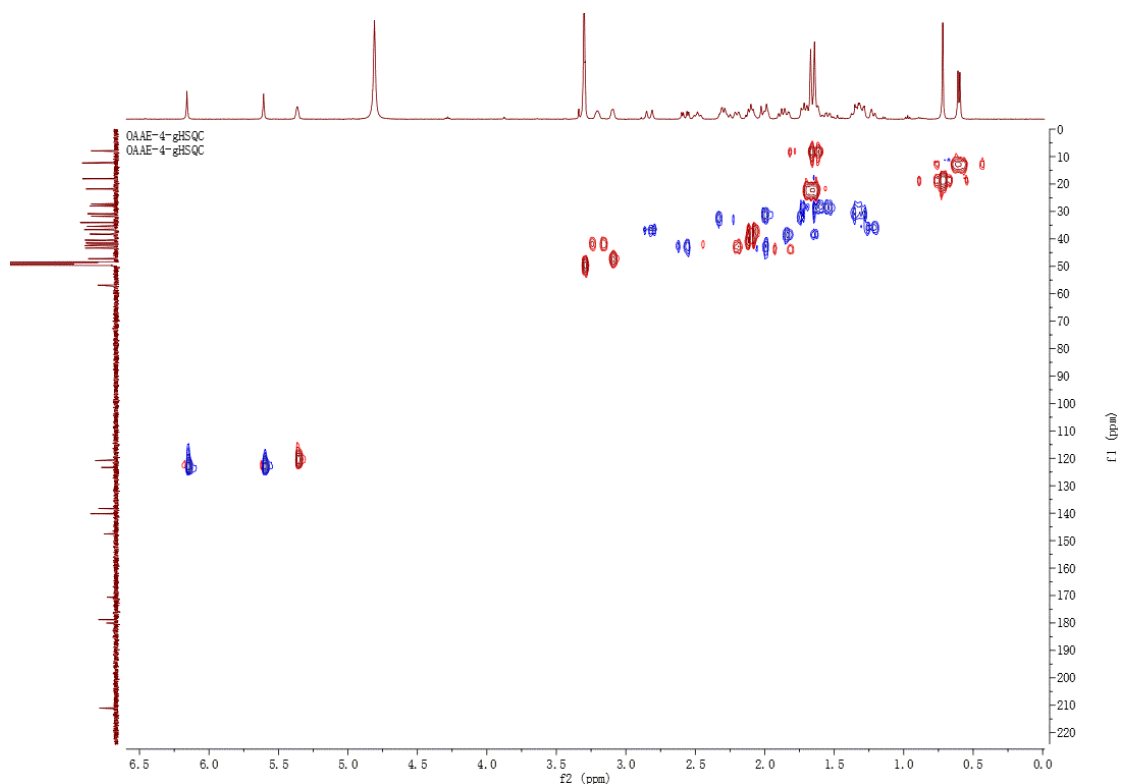


Figure S21. gHMBC Spectrum of Compound 2

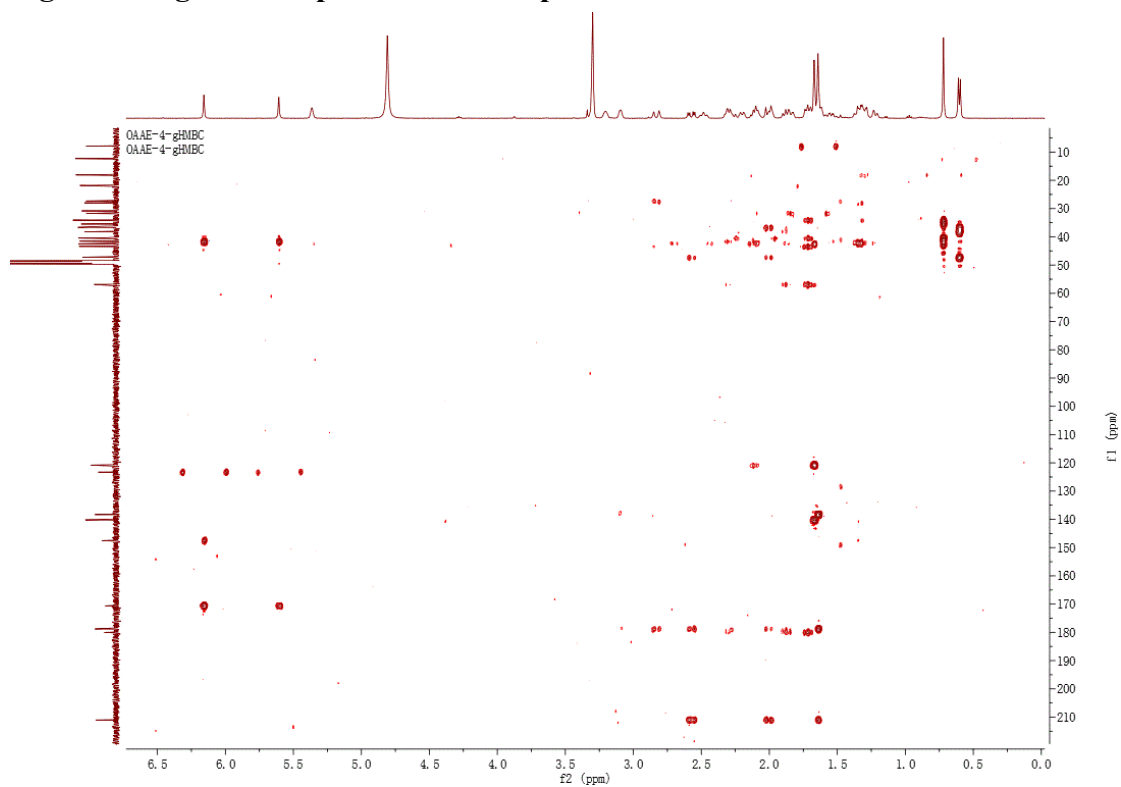


Figure S22. NOESY Spectra of Compound 2

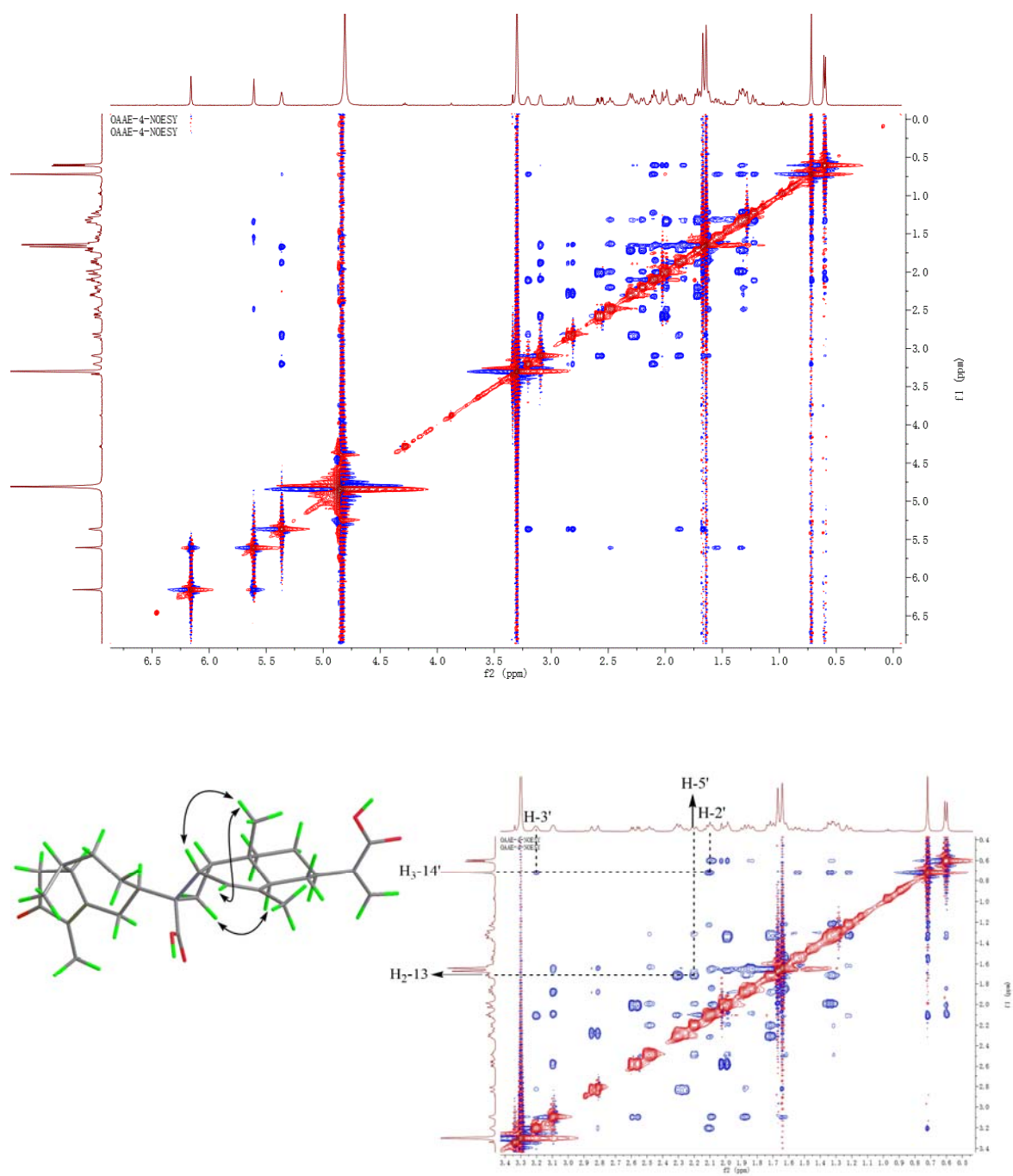


Figure S23. The Stable Conformers of Compound 2

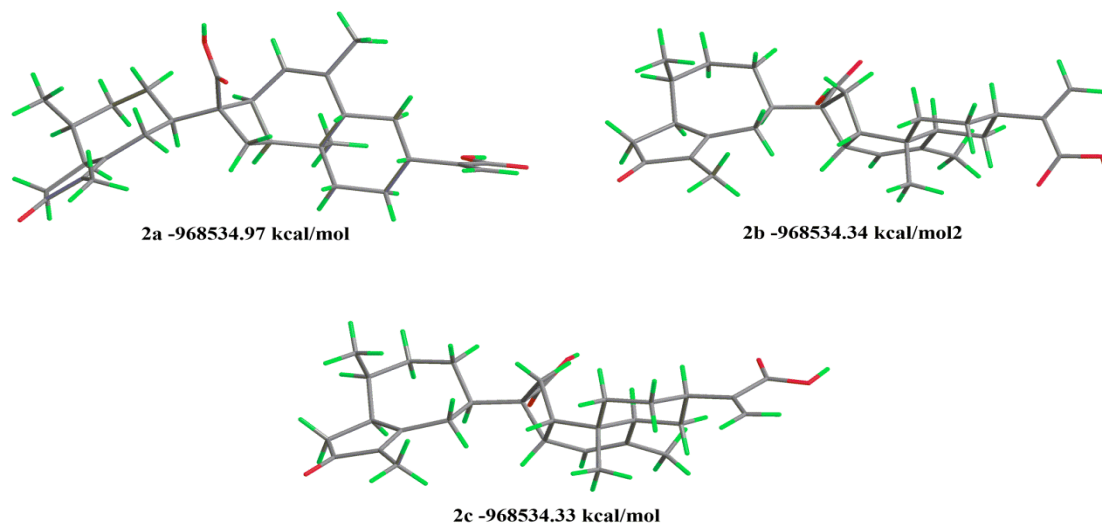


Table S3. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of **2**

Conf	$\Delta E_{6-31+G(d)}$ ^a	% ^b
2a	0	59.3
2b	0.63	20.5
2c	0.64	20.2

^aRelative to 2a with $E_{6-31+G(d)} = -968534.97$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S24. The Stable Conformers of (1*S*,7*R*,10*S*,11*R*,1'*S*,2'*S*,5'*S*,7'*R*,10'*S*)-2

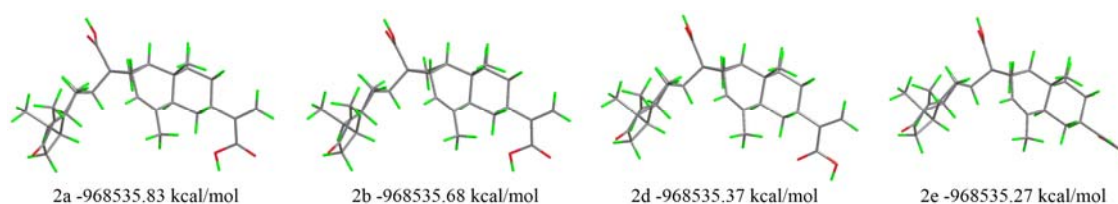


Table S4. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of (1*S*,7*R*,10*S*,11*R*,1'*S*,2'*S*,5'*S*,7'*R*,10'*S*)-**2**

Conf	$\Delta E_{6-31+G(d)}$ ^a	% ^b
2a	0	38.1
2b	0.14	29.8
2c	0.46	17.4
2d	0.56	14.7

^aRelative to 2a with $E_{6-31+G(d)} = -968535.83$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S25. (+)-HRESIMS Spectrum of Compound 3

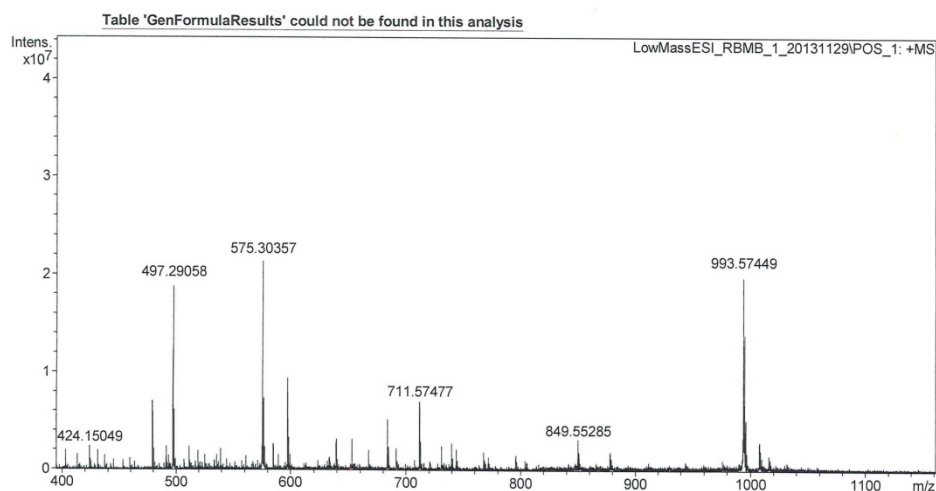
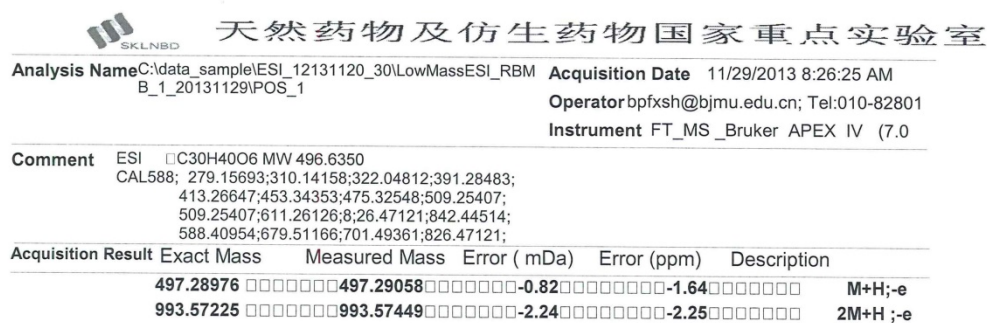


Figure S26. IR Spectrum of Compound 3

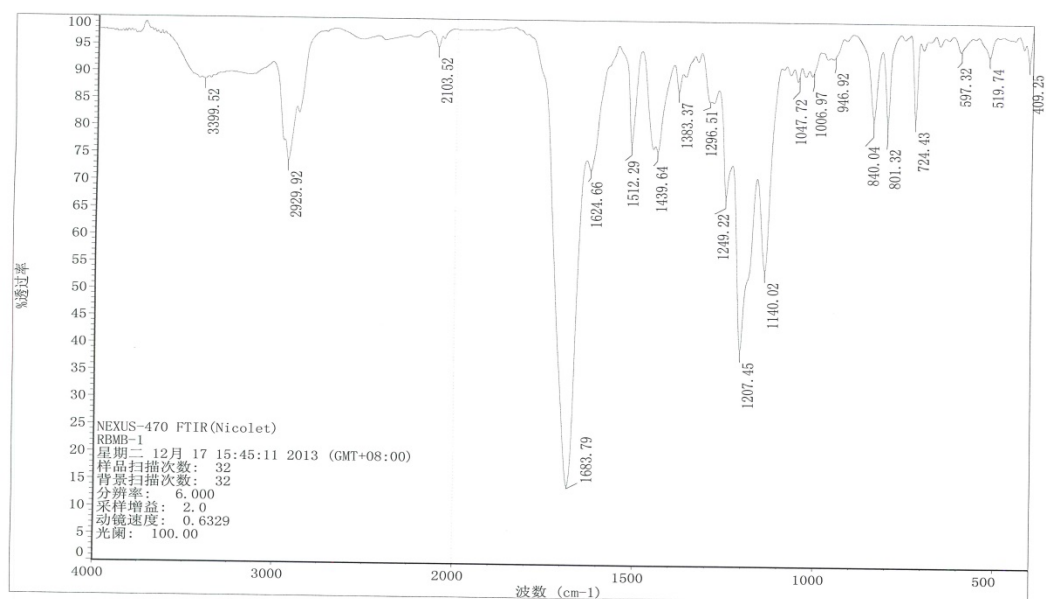


Figure S27. ^1H -NMR Spectrum of Compound 3 (500 MHz, CD_3OD)

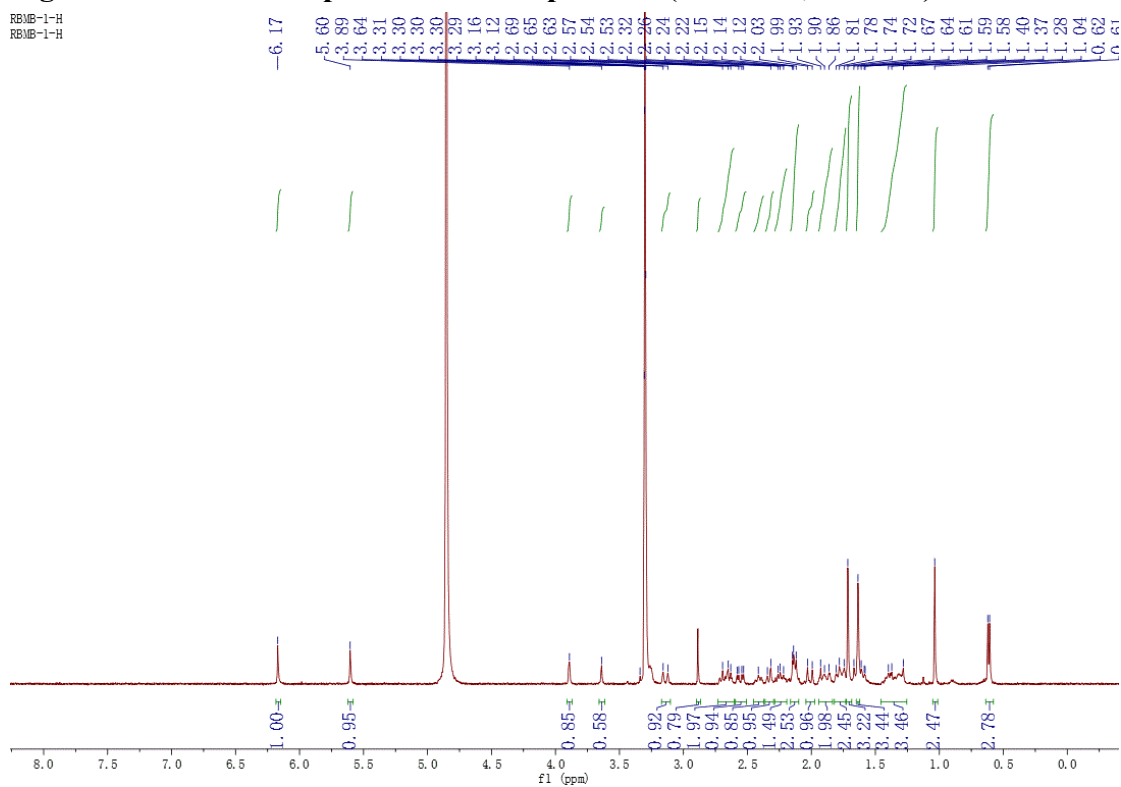


Figure S28. ^{13}C -NMR Spectrum of Compound 3 (125 MHz, CD_3OD)

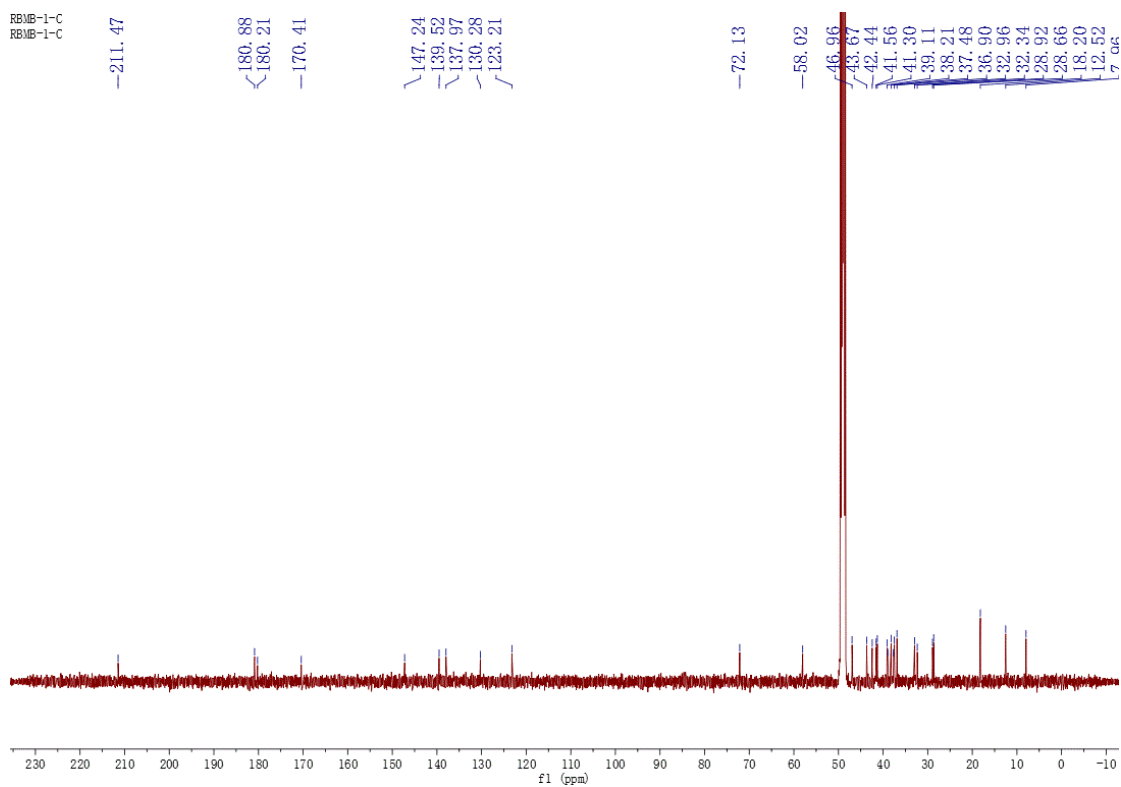


Figure S29. DEPT-135 Spectrum of Compound 3

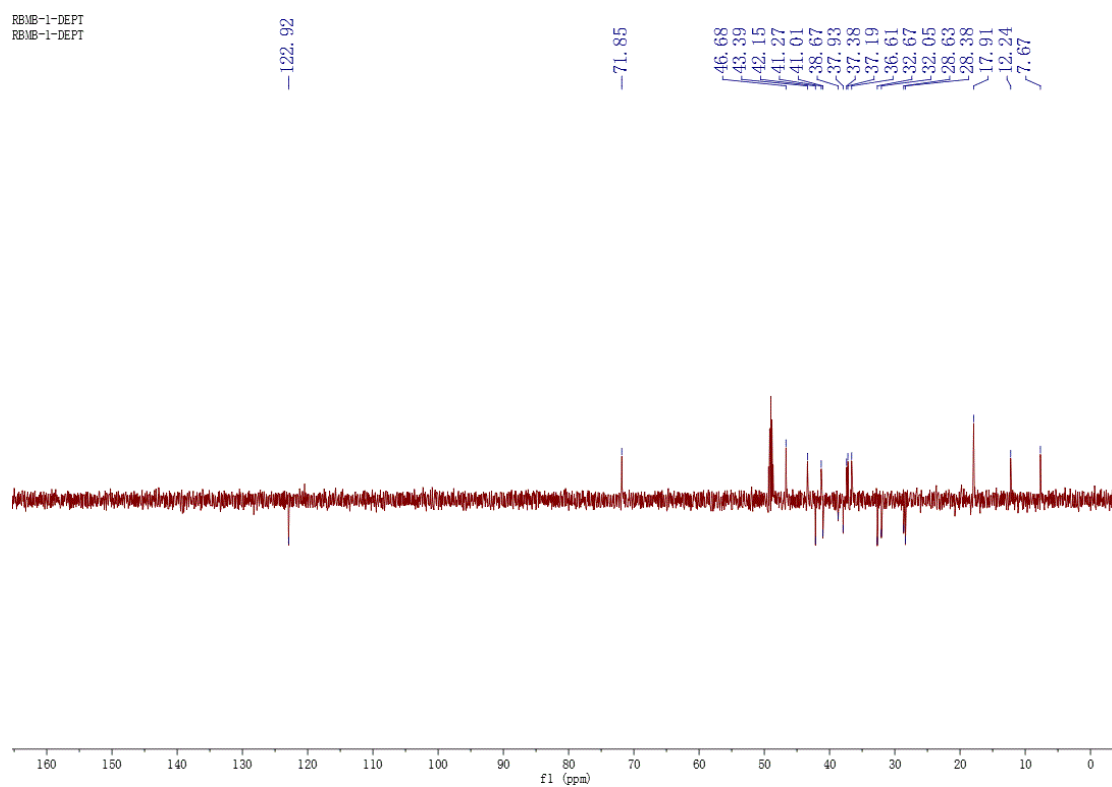


Figure S30. ^1H - ^1H gCOSY Spectrum of Compound 3

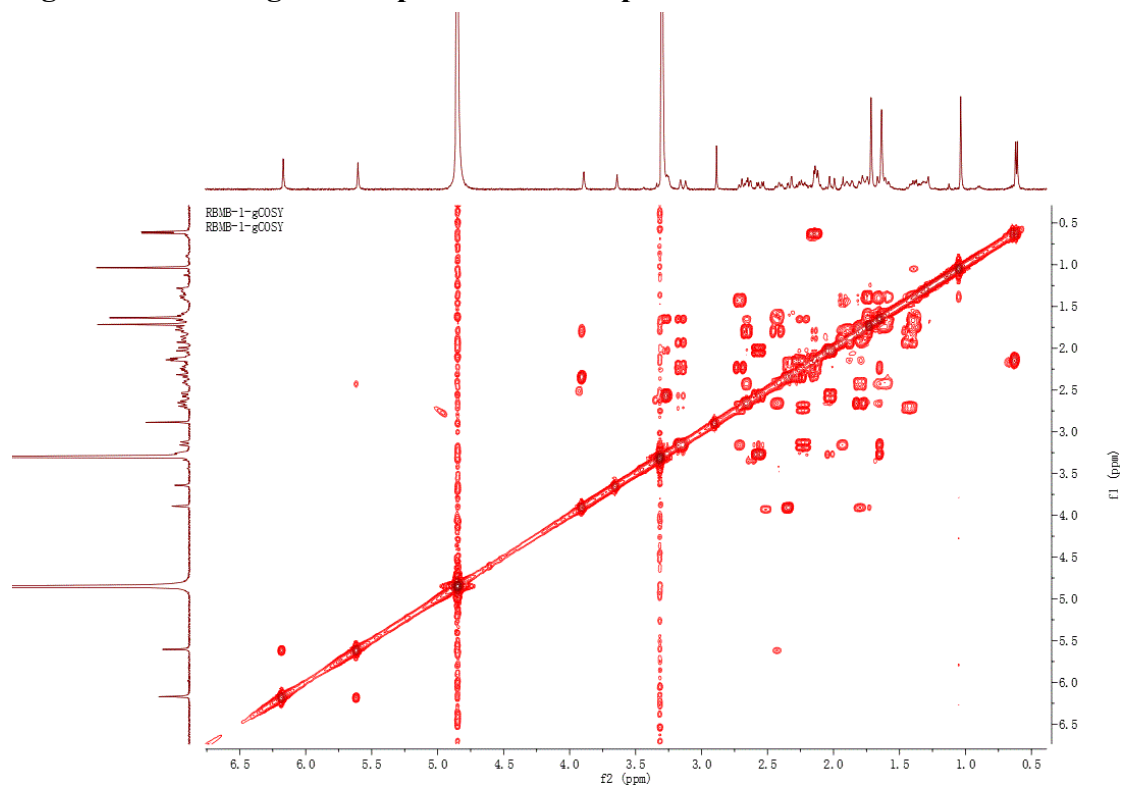


Figure S31. Multiplicity-edited gHSQC Spectrum of Compound 3

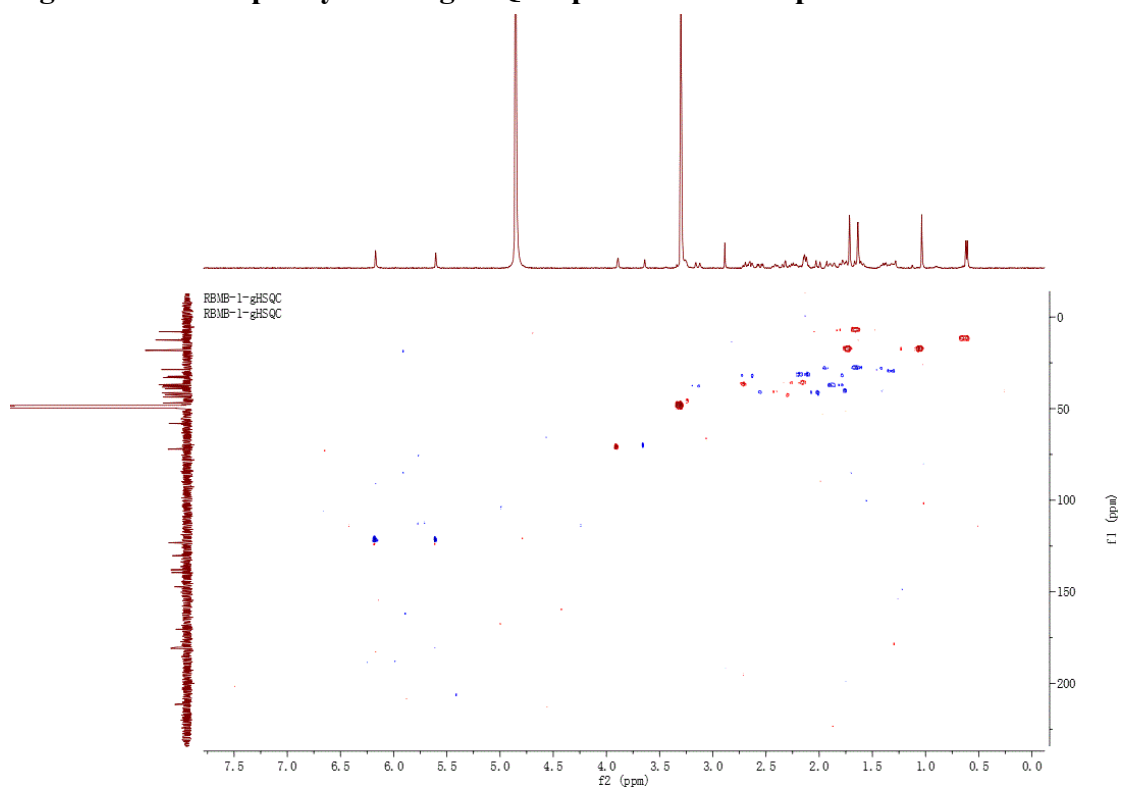


Figure S32. gHMBC Spectrum of Compound 3

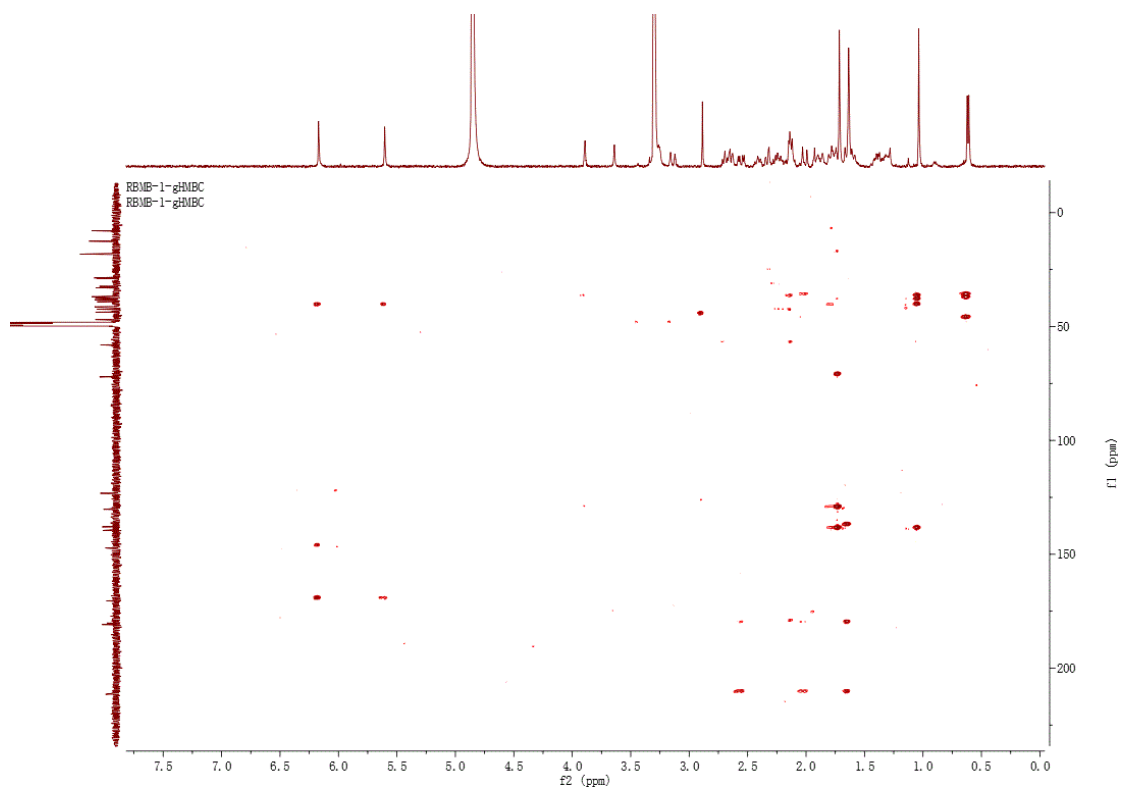


Figure S33. NOESY Spectra of Compound 3

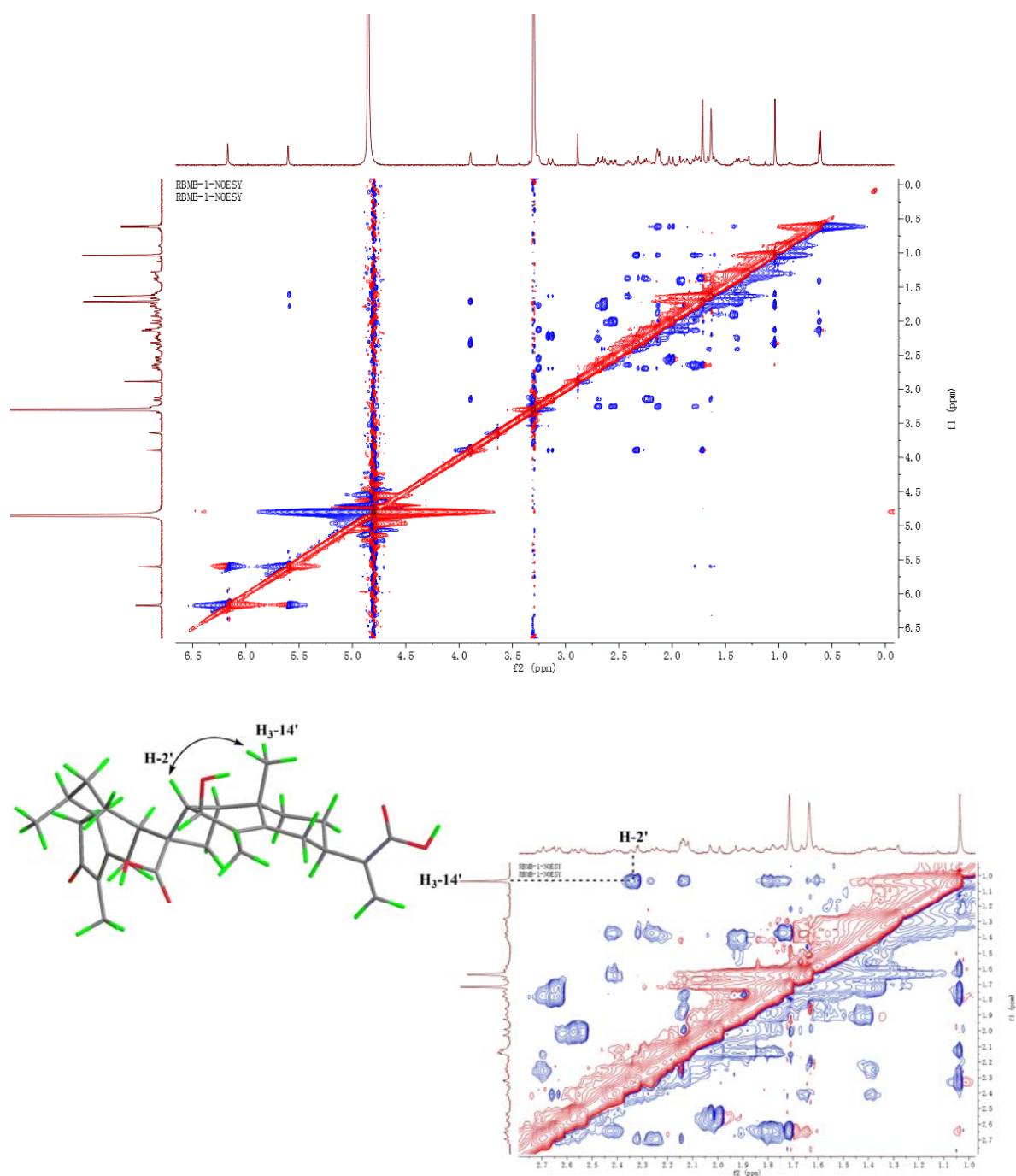


Figure S34. The Stable Conformers of Compound 3

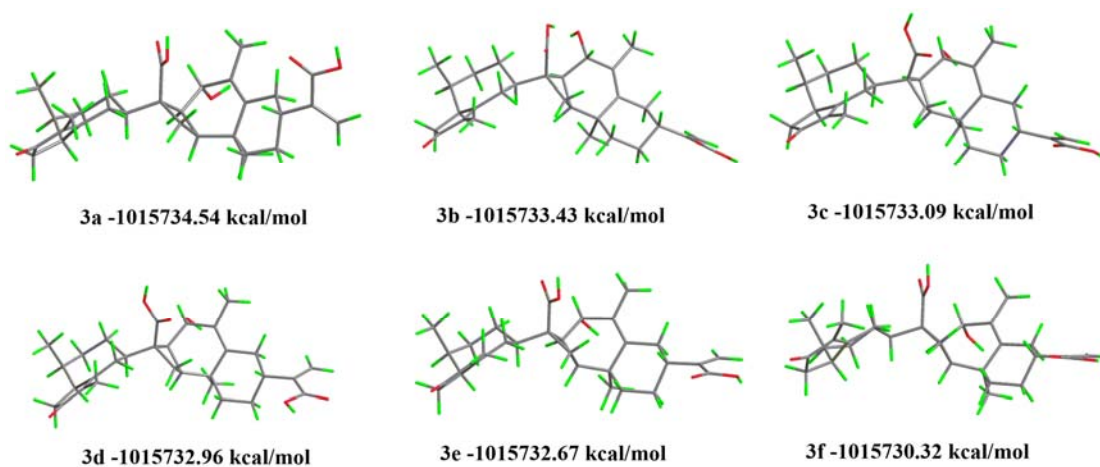


Table S5. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of **3**

conf	$\Delta E_{6-31+G(d)}^a$	% ^b
3a	0	74.1
3b	1.12	11.2
3c	1.45	6.4
3d	1.58	5.1
3e	1.87	3.1
3f	4.23	0.1

^aRelative to 3a with $E_{6-31+G(d)} = -1015734.54$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S35. Comparison of Experimental and Calculated ECD Spectra of 3

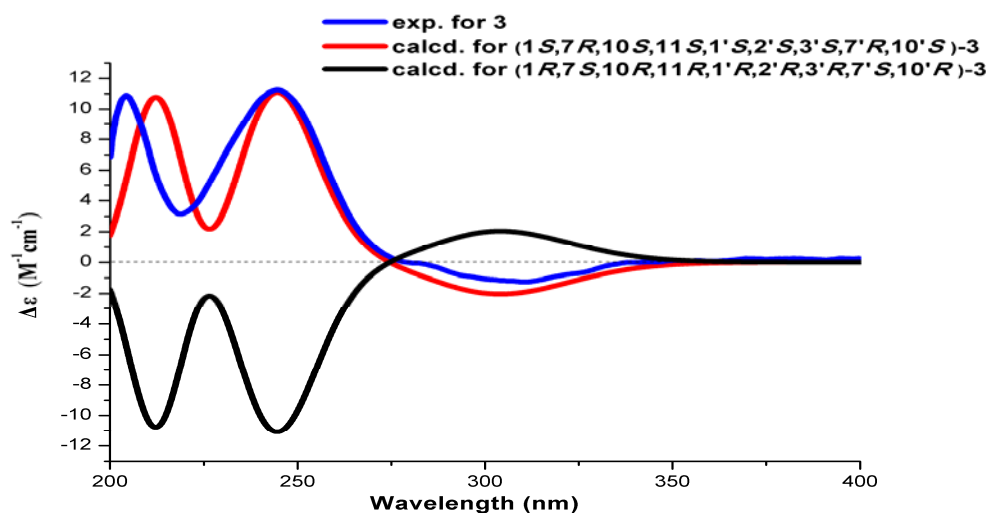


Figure S36. (-)-HRESIMS Spectrum of Compound 4

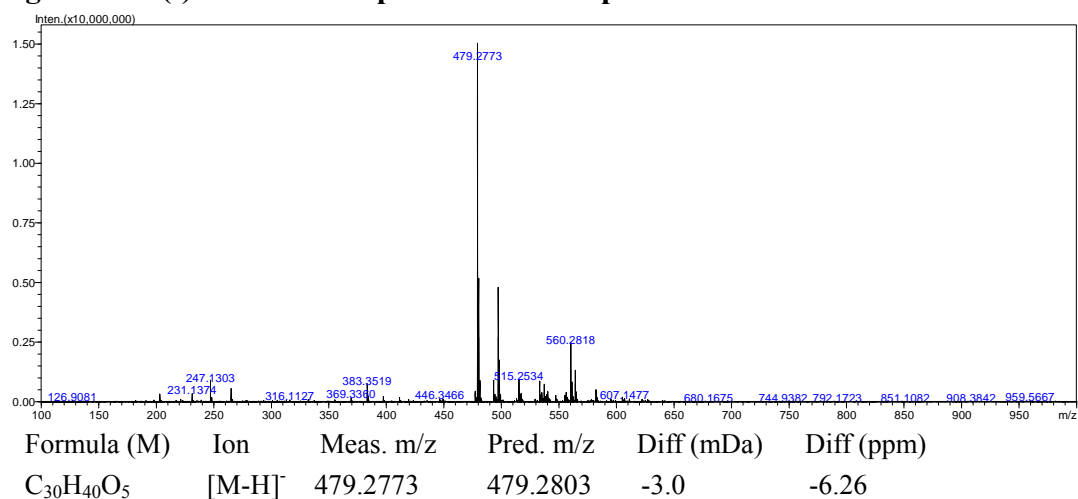


Figure S37. (+)-HRESIMS Spectrum of Compound 4

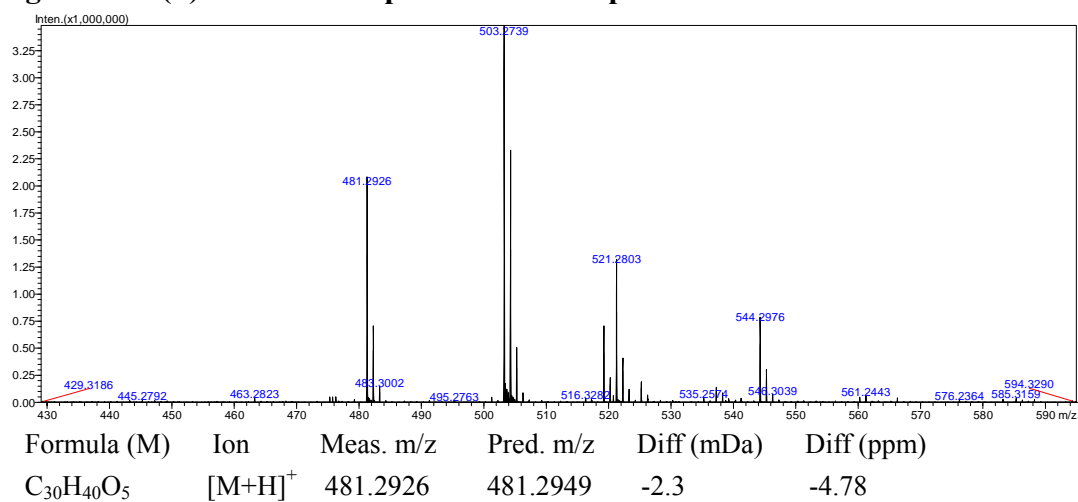


Figure S38. IR Spectrum of Compound 4

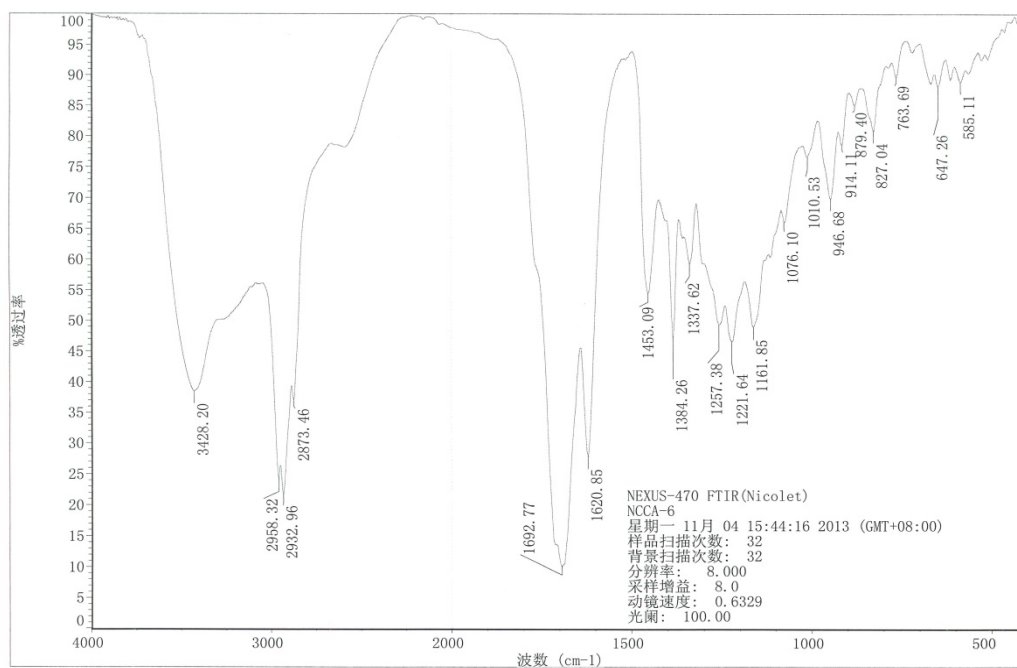
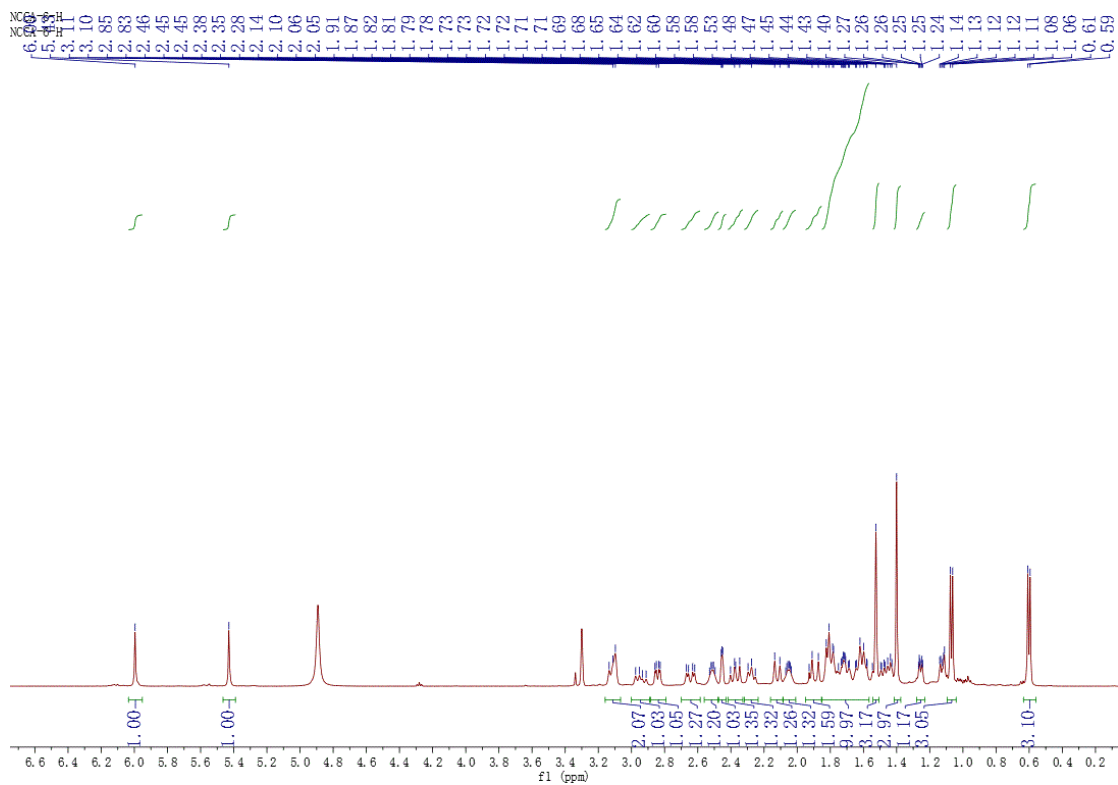


Figure S39. ¹H-NMR Spectrum of Compound 4 (500 MHz, CD₃OD)



NCCAcOAc
 NCCAcOAc

—211.29
 —180.01
 —179.23
 —169.81
 —152.57
 —148.38
 —138.11
 —138.08
 —121.86
 —63.20
 —61.48
 —56.48
 —49.51
 —48.51
 —48.28
 —49.17
 —49.00
 —48.83
 —48.66
 —47.67
 —45.16
 —43.17
 —42.65
 —40.53
 —38.11
 —37.54
 —36.28
 —35.81
 —34.73
 —33.66
 —32.75
 —32.22
 —18.81
 —18.67
 —12.42
 —8.29

f1 (ppm)

Figure S42. Multiplicity-edited gHSQC Spectrum of Compound 4

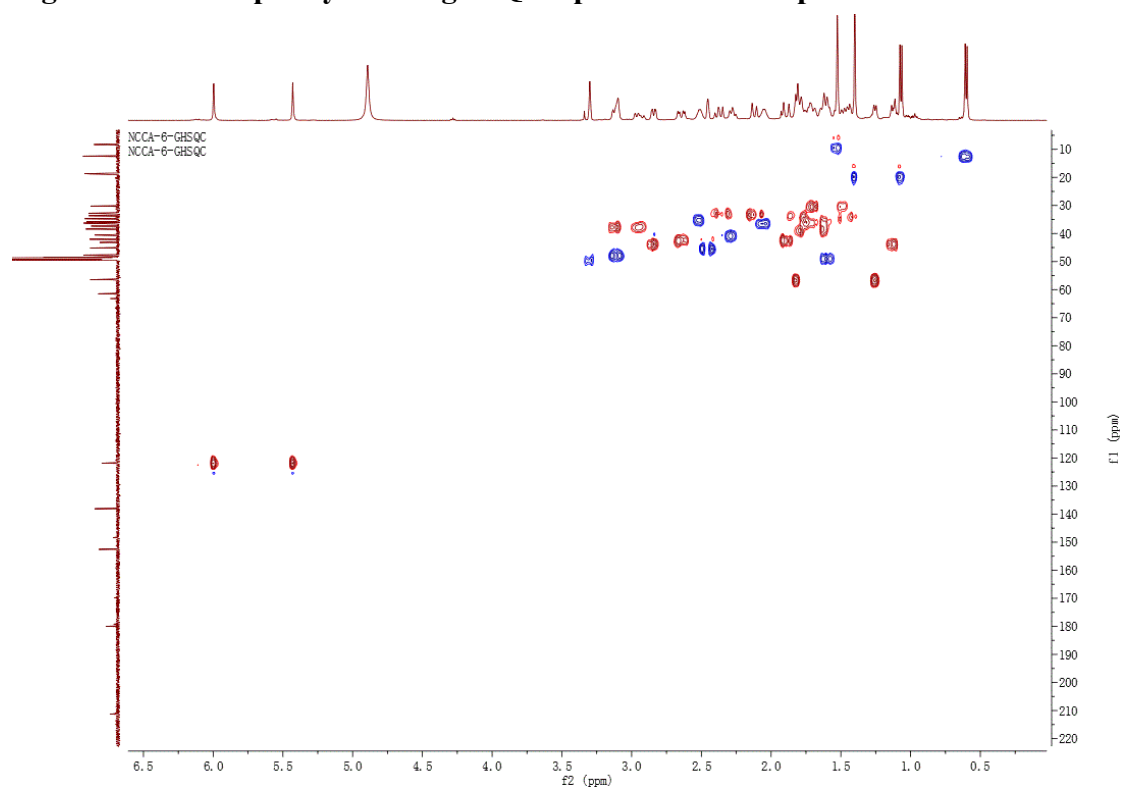


Figure S43. gHMBC Spectrum of Compound 4

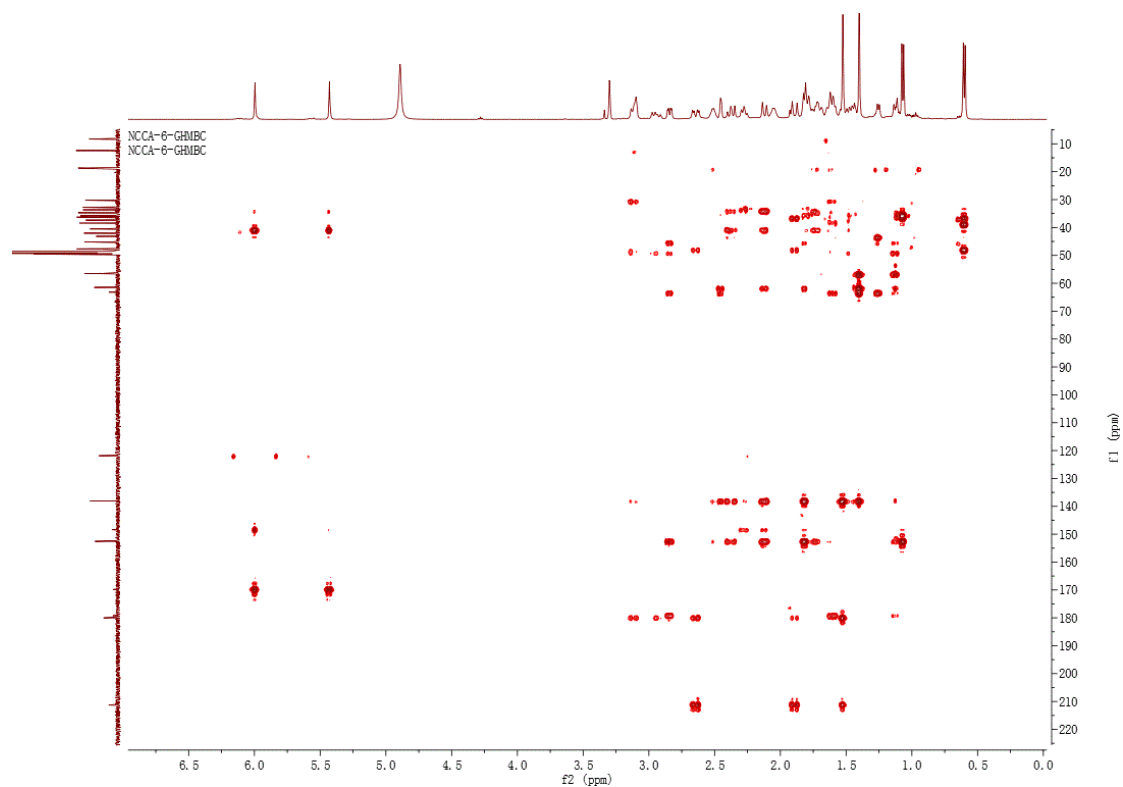


Figure S44. NOESY Spectrum of Compound 4

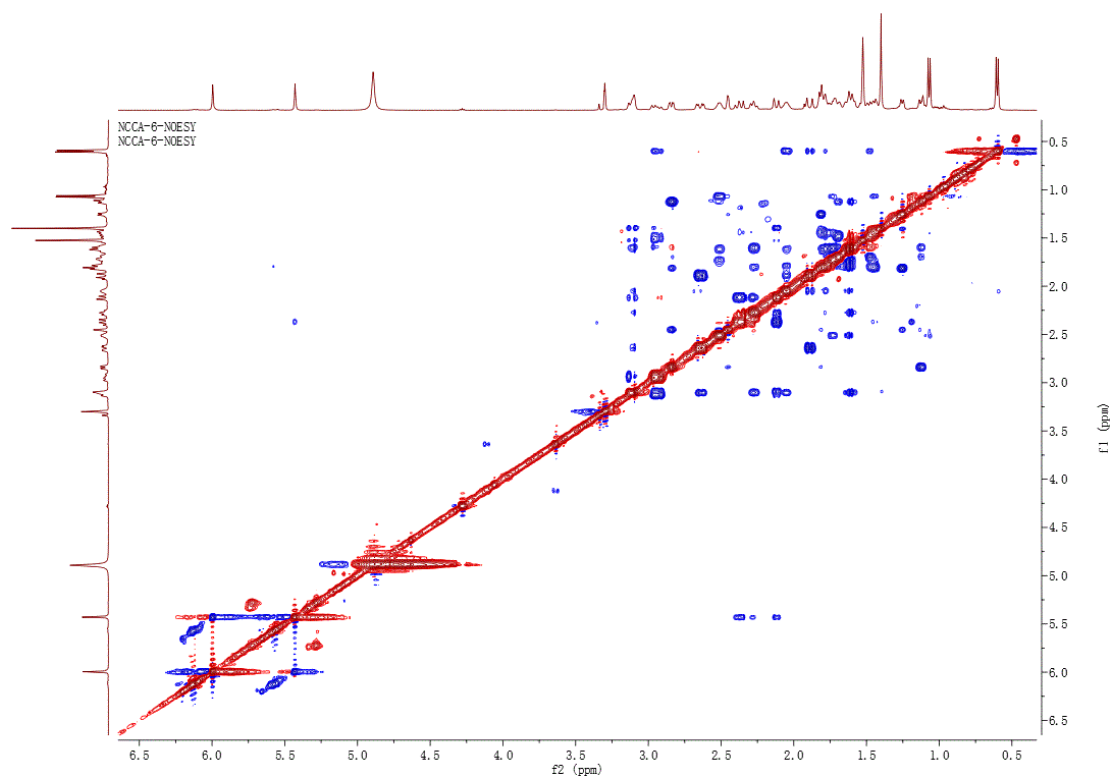


Figure S45. 1D NOE Spectrum of Compound 4

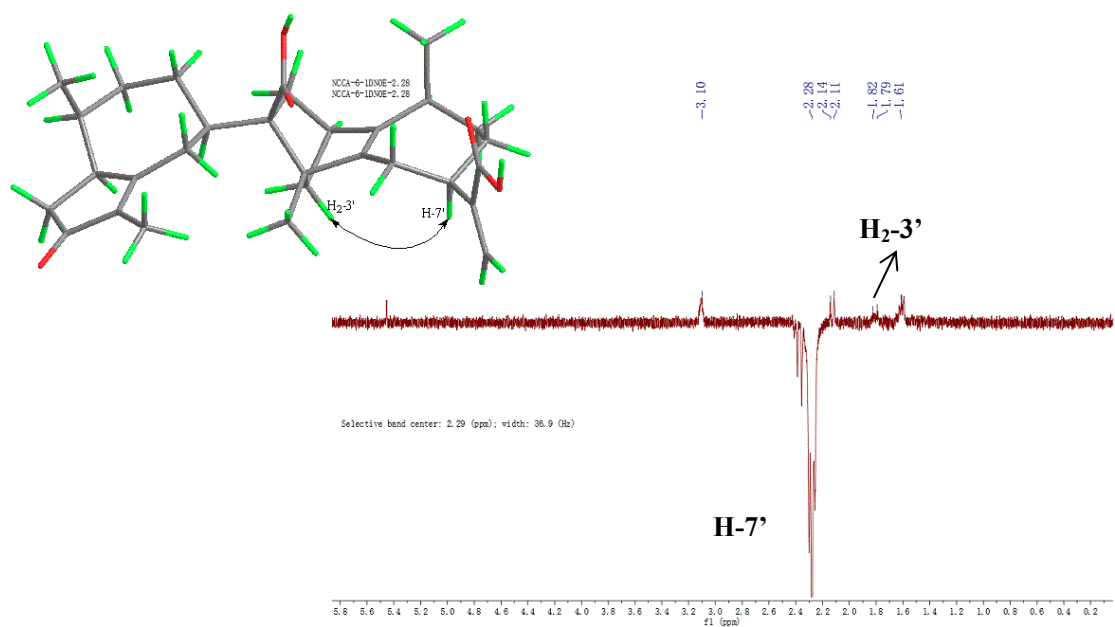


Figure S46. The Stable Conformers of Compound 4

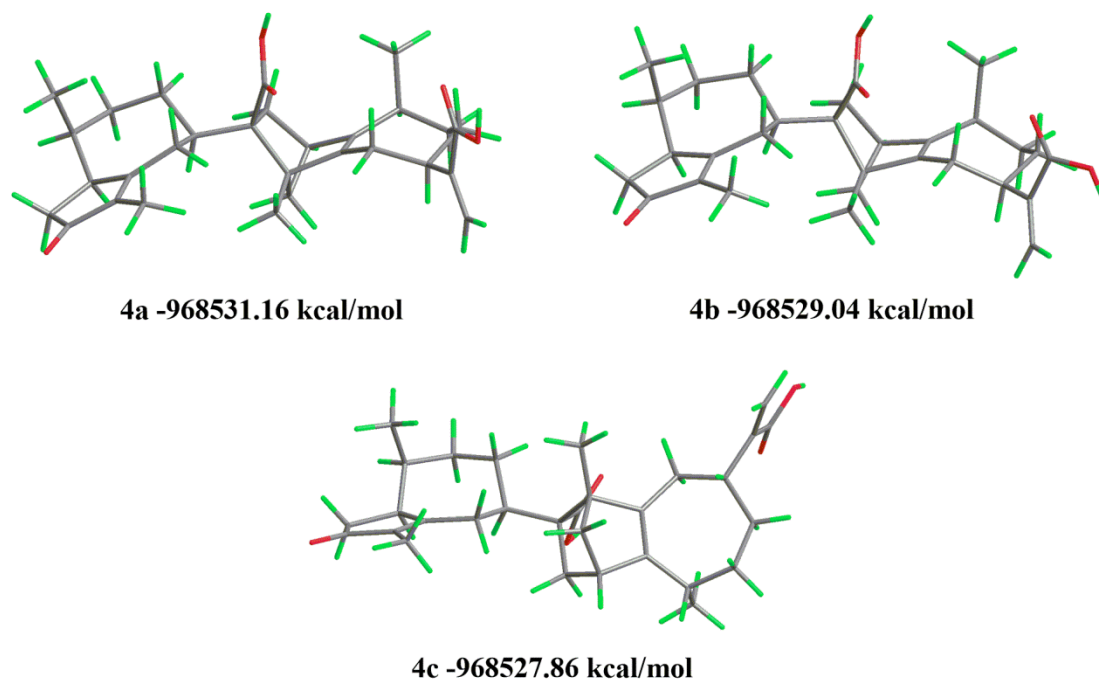


Table S6. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of **4**

conf	$\Delta E_{6-31+G(d)}$ ^a	% ^b
4a	0	96.9
4b	2.11	2.7
4c	3.30	0.4

^aRelative to 4a with $E_{6-31+G(d)} = -968531.16$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S47. The Stable Conformers of (1*S*,7*R*,10*S*,11*S*,2'*S*,4'*S*,7'*R*,10'*S*)-4

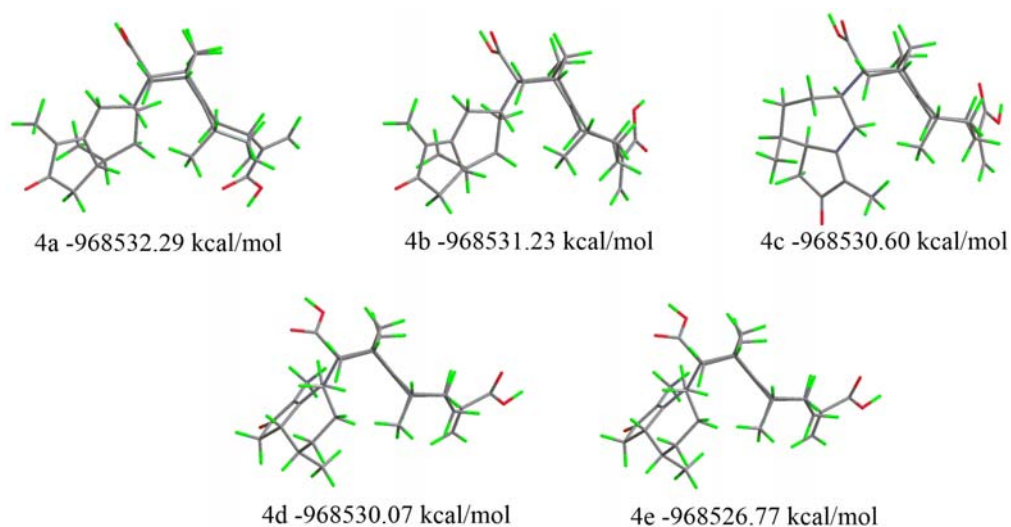


Table S7. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of (1*S*,7*R*,10*S*,11*S*,2'*S*,4'*S*,7'*R*,10'*S*)-4

conf	$\Delta E_{6-31+G(d)}$ ^a	% ^b
4a	0	80.2
4b	1.06	13.3
4c	1.68	4.6
4d	2.22	1.9
4e	5.52	<0.01

^aRelative to 4a with $E_{6-31+G(d)} = -968532.29$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S48. (+)-HRESIMS Spectrum of Compound 5

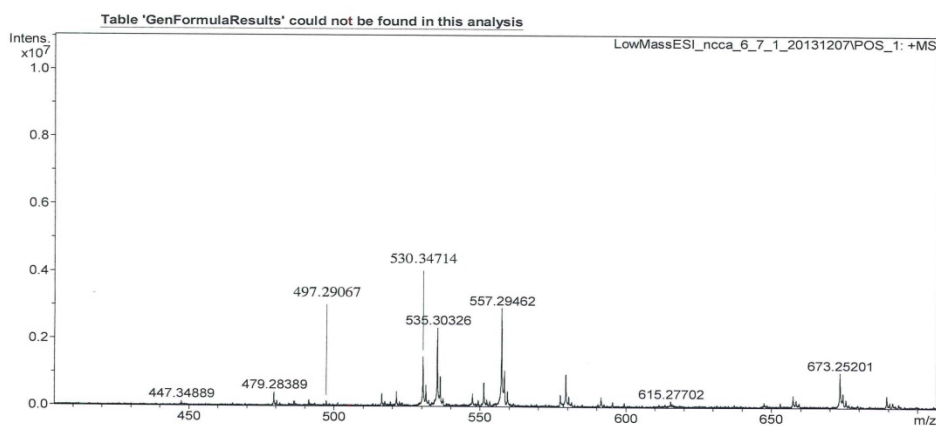
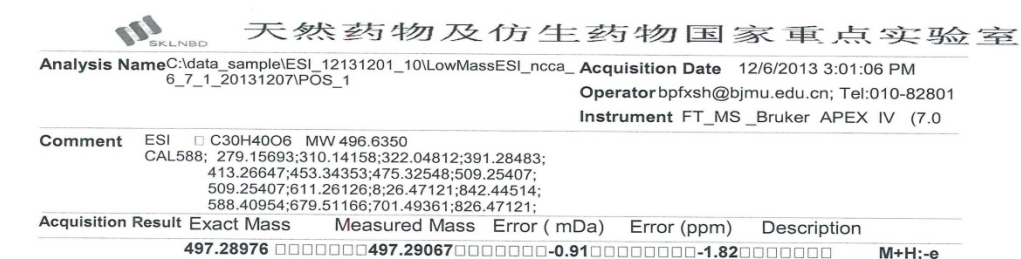


Figure S49. IR Spectrum of Compound 5

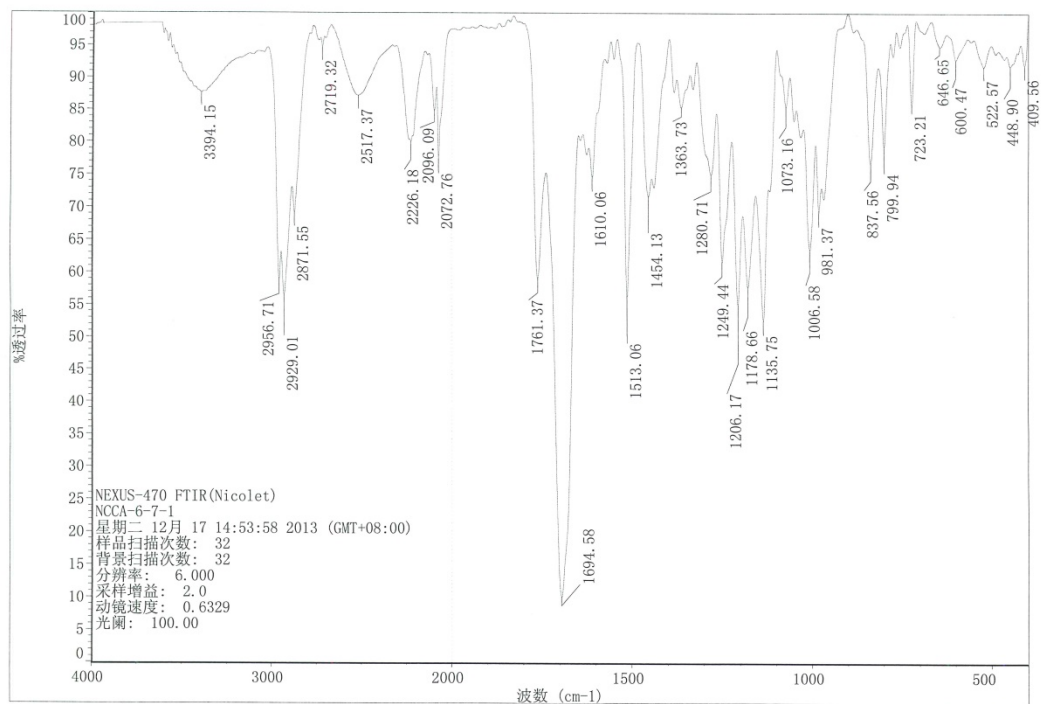


Figure S50. ^1H -NMR Spectrum of Compound 5 (500 MHz, CD_3OD)

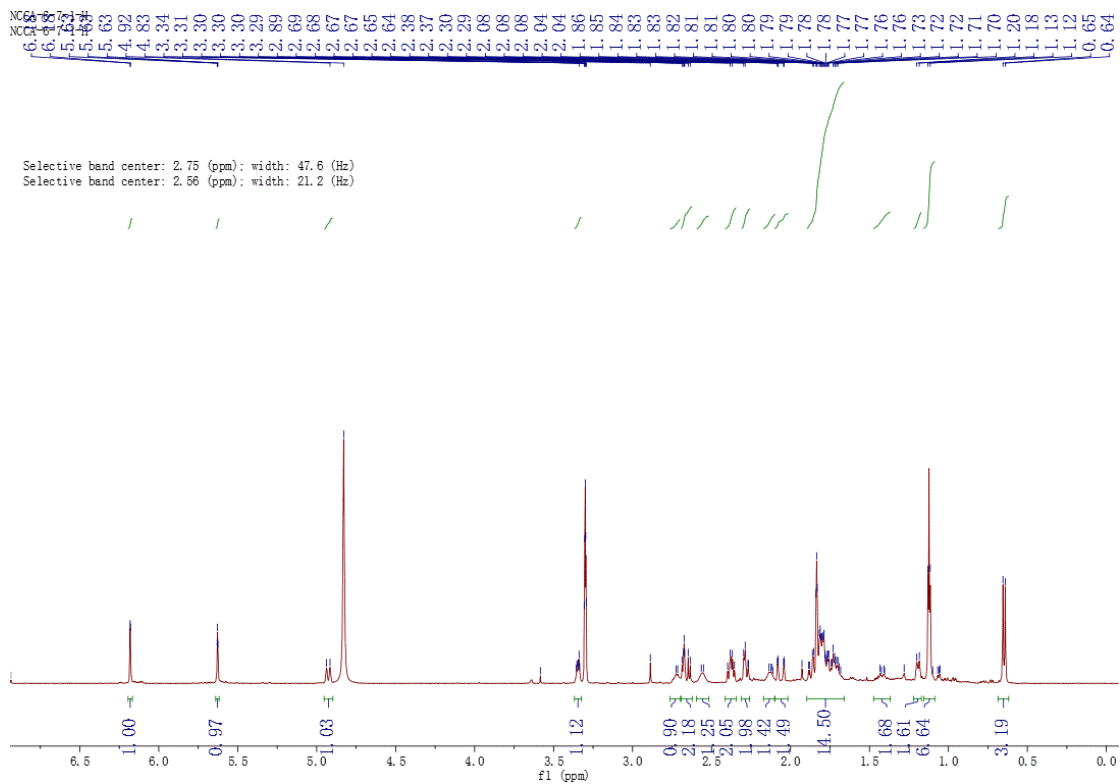


Figure S51. ^{13}C -NMR Spectrum of Compound 5 (125 MHz, CD_3OD)

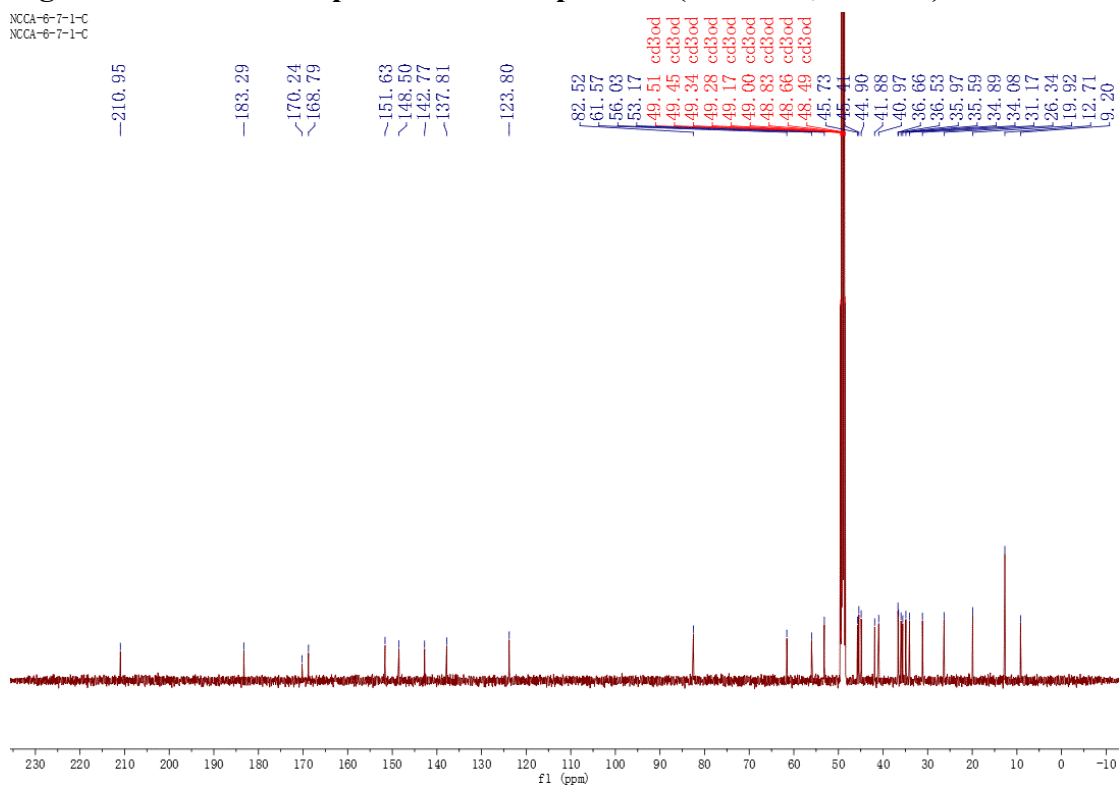


Figure S52. DEPT-135 Spectrum of Compound 5

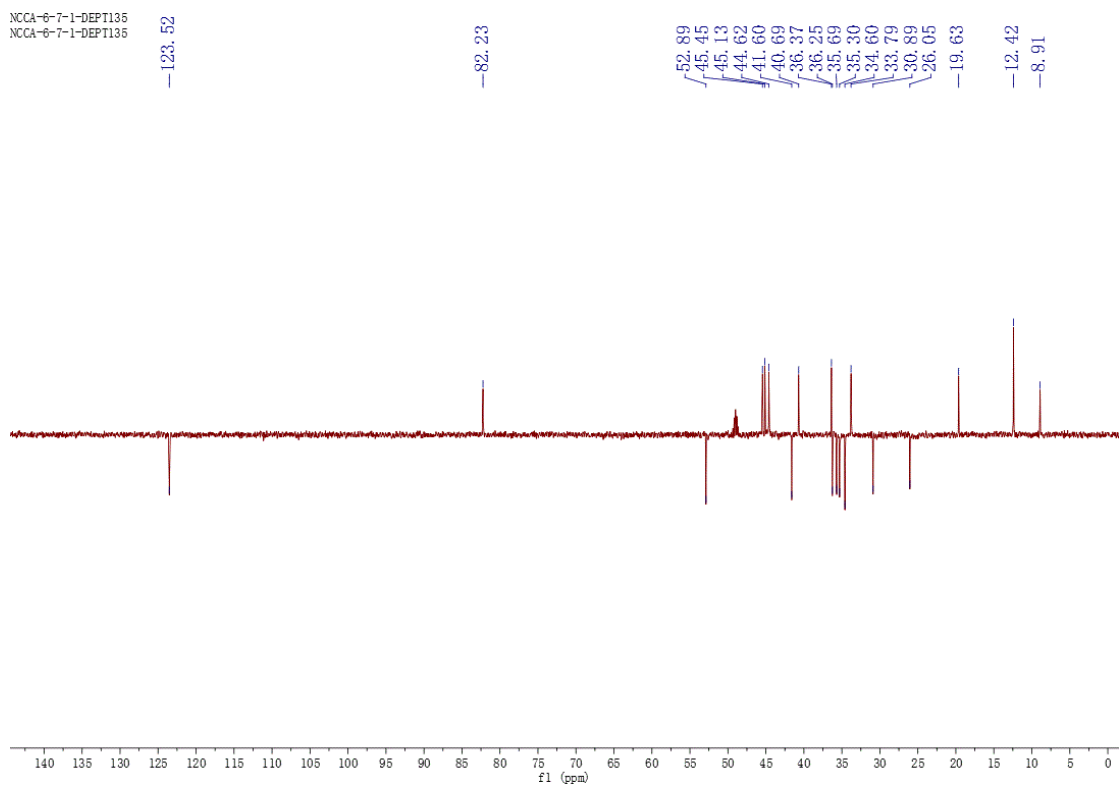


Figure S53. ^1H - ^1H gCOSY Spectrum of Compound 5

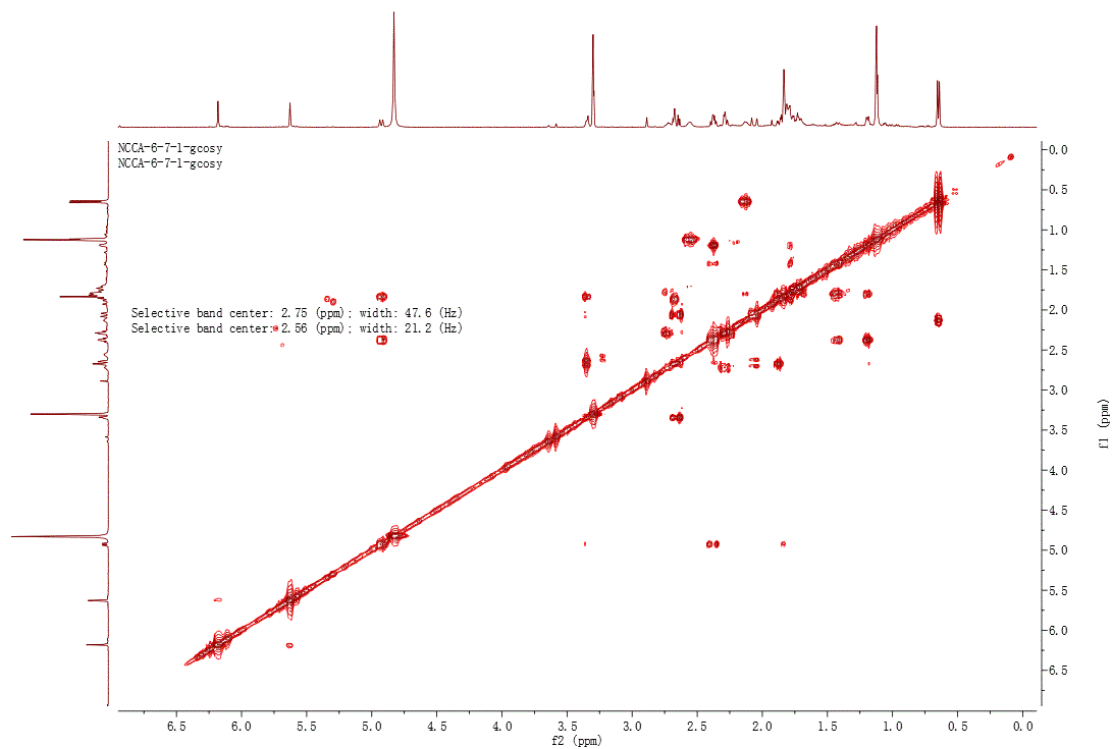


Figure S54. Multiplicity-edited gHSQC Spectrum of Compound 5

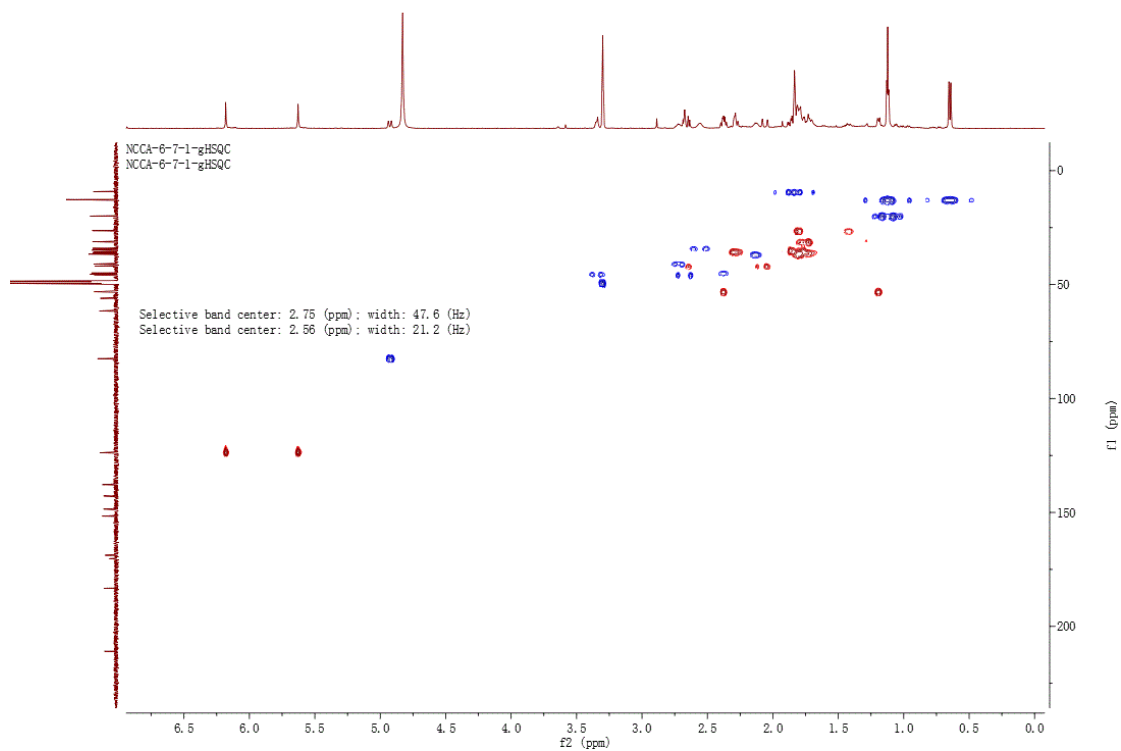


Figure S55. gHMBC Spectrum of Compound 5

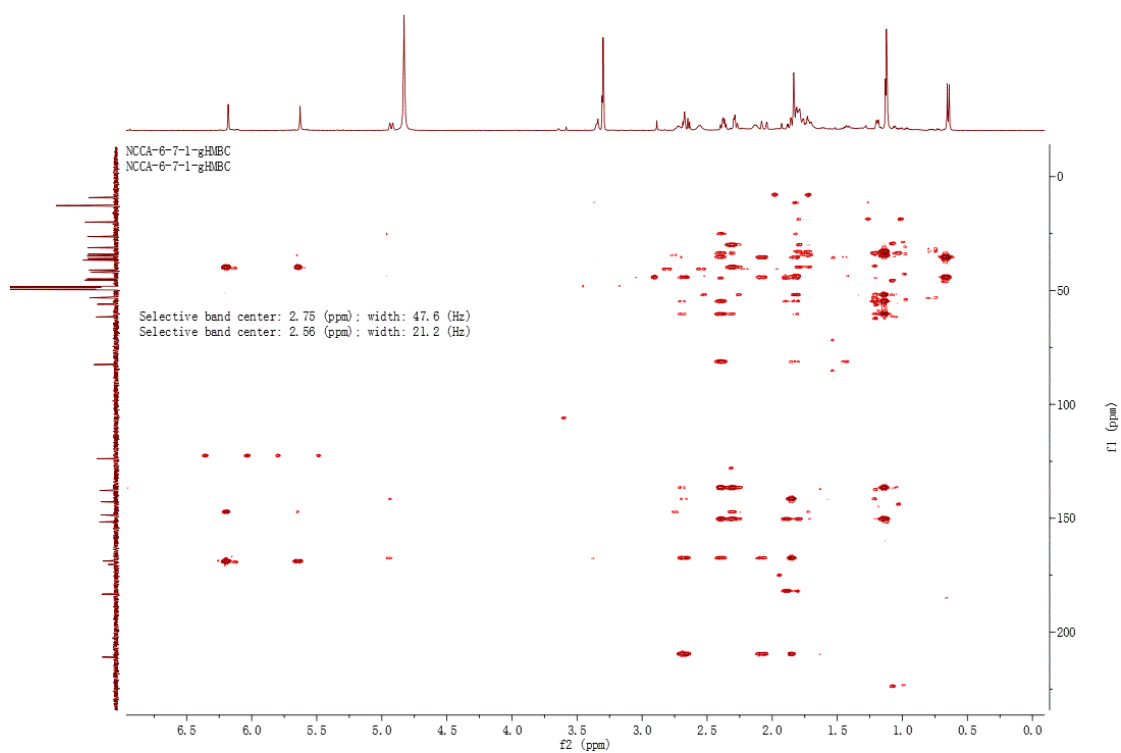


Figure S56. NOESY Spectrum of Compound 5

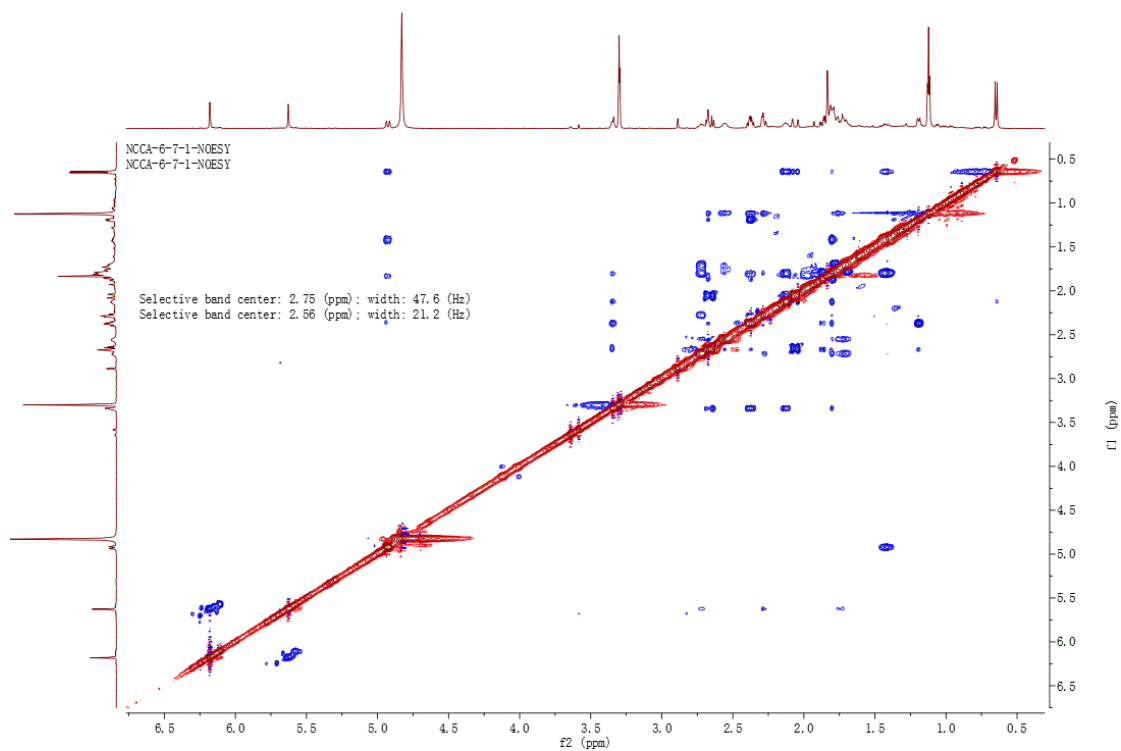


Figure S57. The Stable Conformers of Compound 5

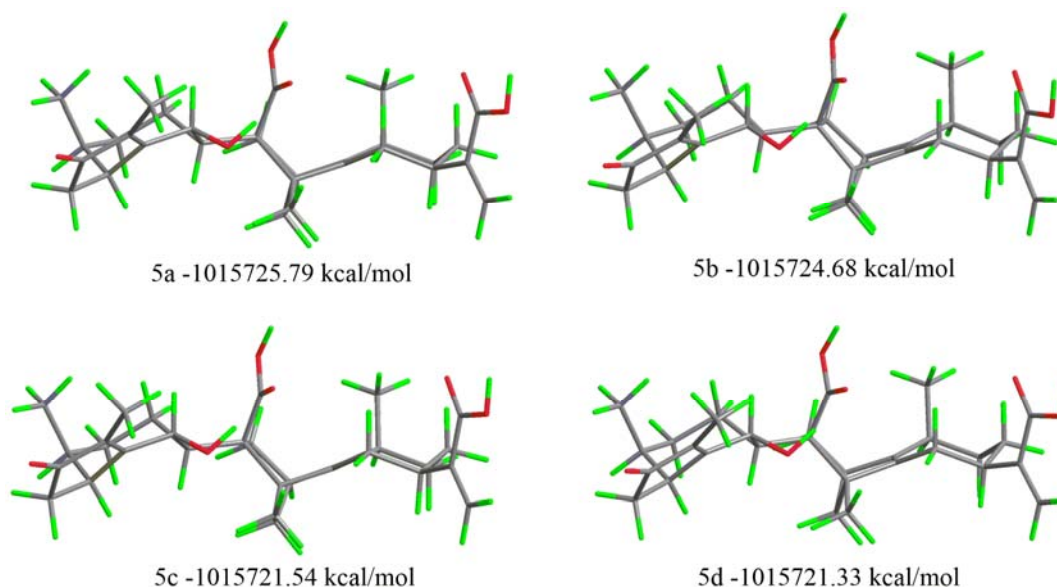


Table S8. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of **5**

conf	$\Delta E_{6-31+G(d)}$ ^a	% ^b
5a	0	86.7
5b	1.12	13.2
5c	4.25	0.07
5d	4.47	0.04

^aRelative to 5a with $E_{6-31+G(d)} = -1015725.79$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S58. Comparison of Experimental and Calculated ECD Spectra of 5

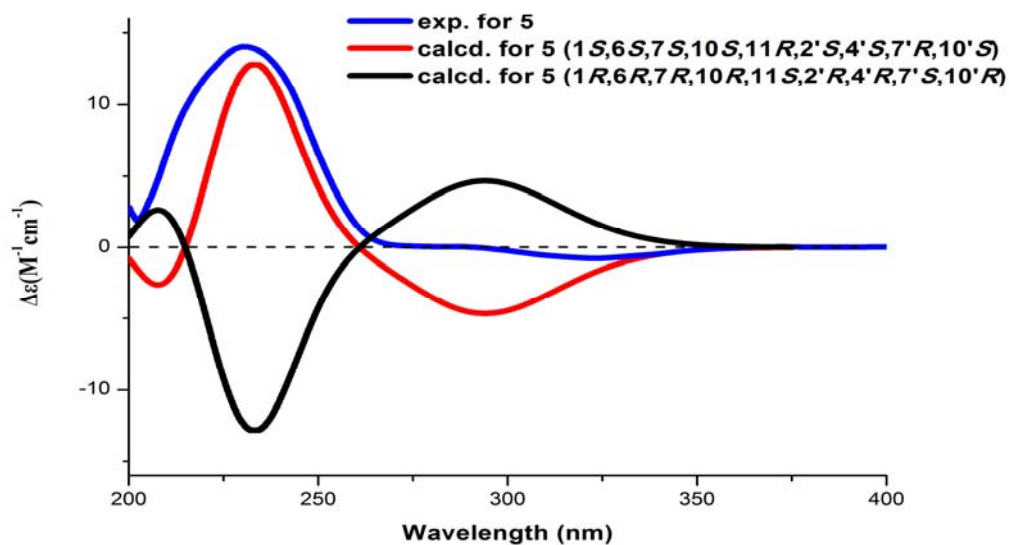


Figure S59. (+)-HRESIMS Spectrum of Compound 6

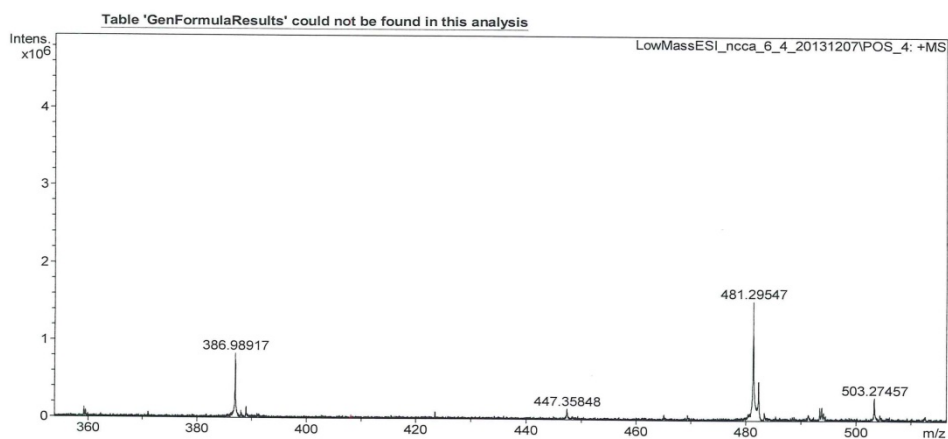


Figure S60. IR Spectrum of Compound 6

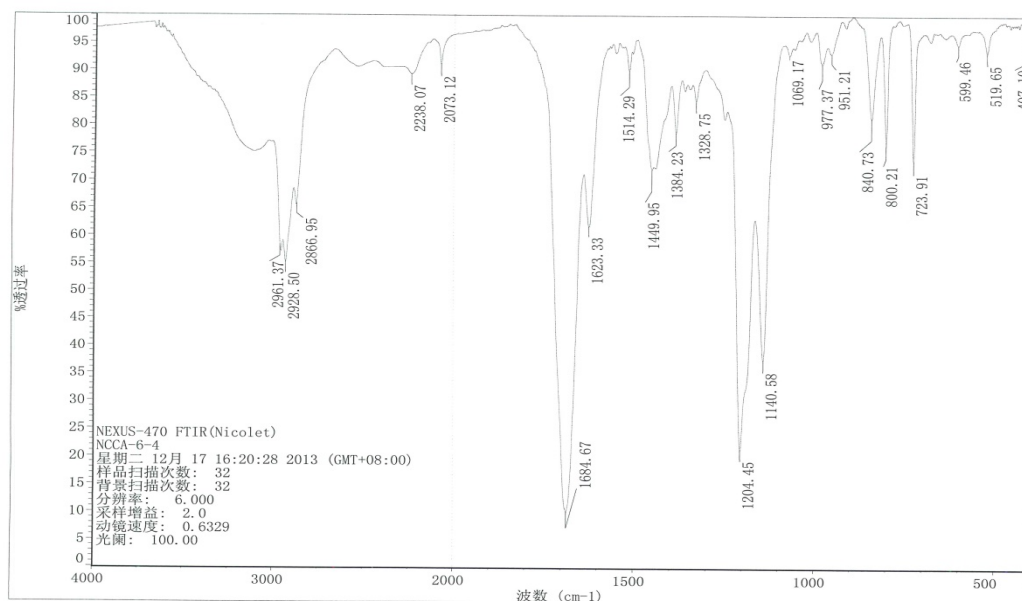


Figure S61. ^1H -NMR Spectrum of Compound 6 (500 MHz, CD_3OD)

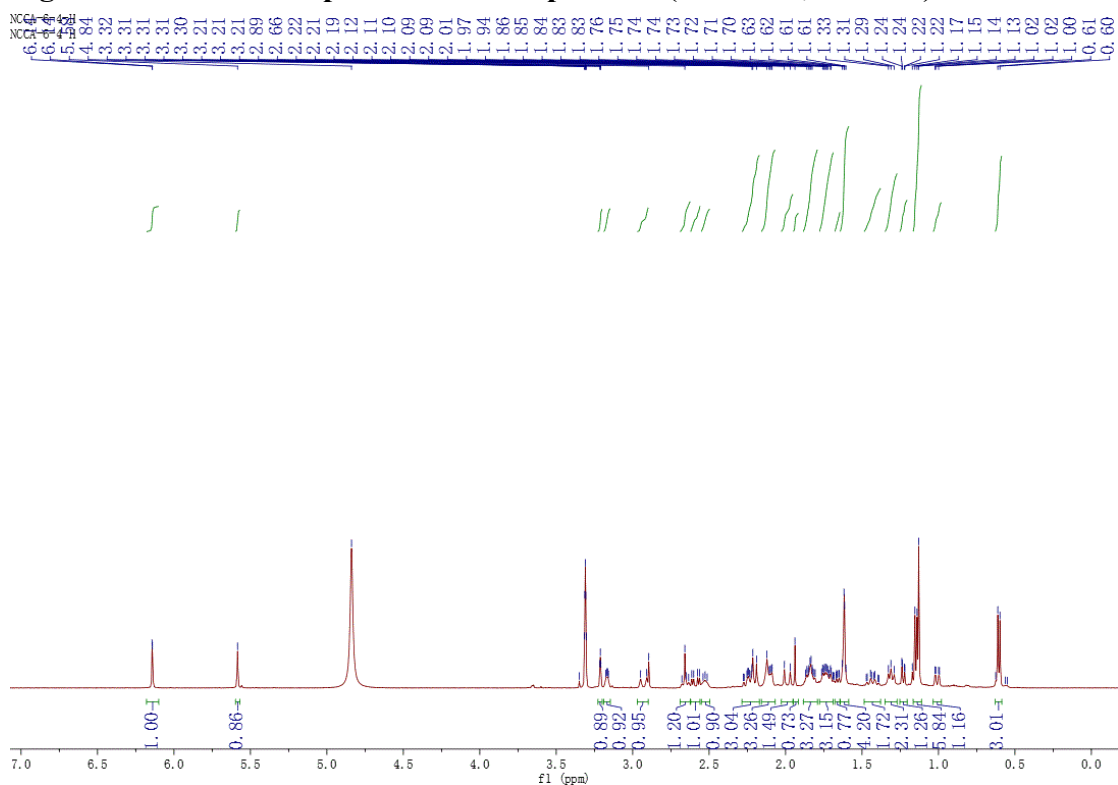


Figure S62. ^{13}C -NMR Spectrum of Compound 6 (125 MHz, CD_3OD)

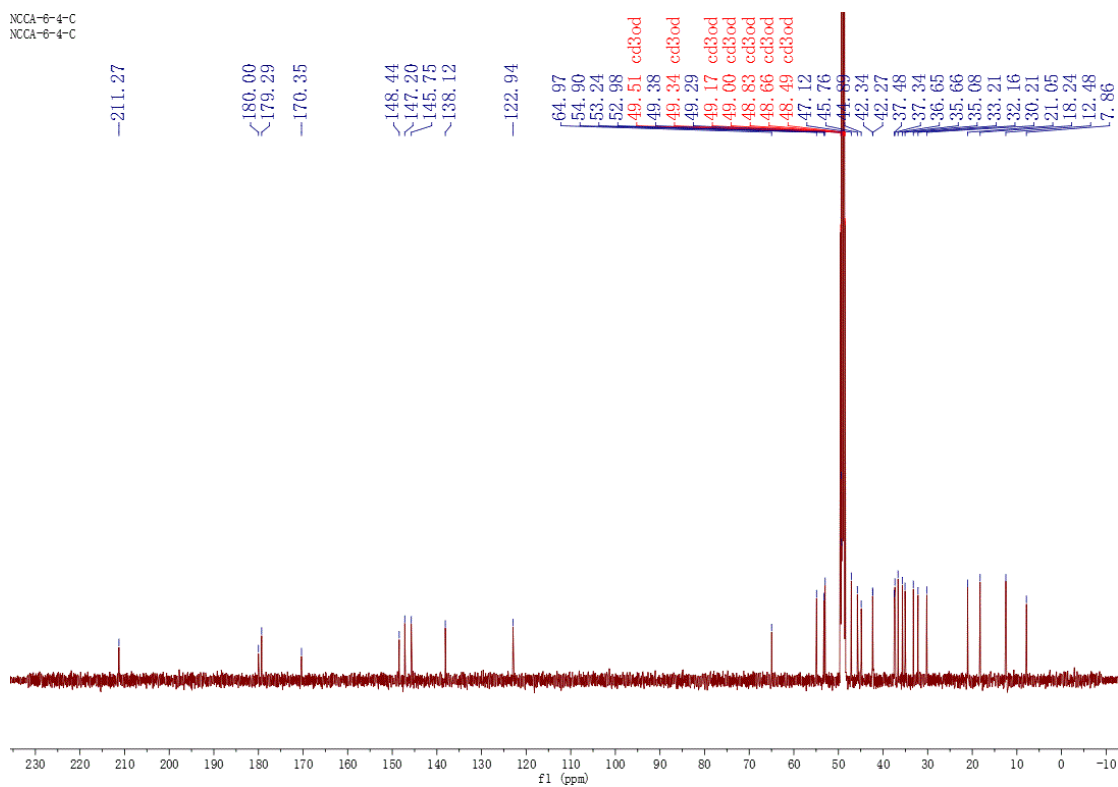


Figure S63. DEPT-135 Spectrum of Compound 6

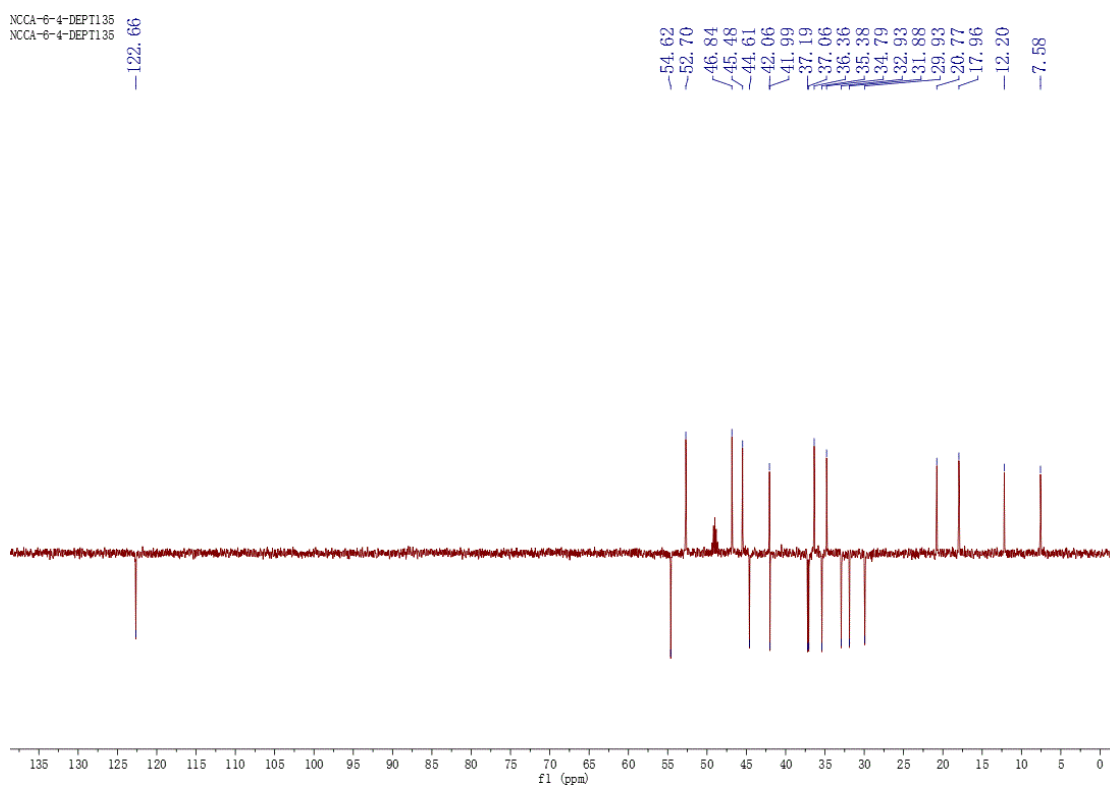


Figure S64. ^1H - ^1H gCOSY Spectrum of Compound 6

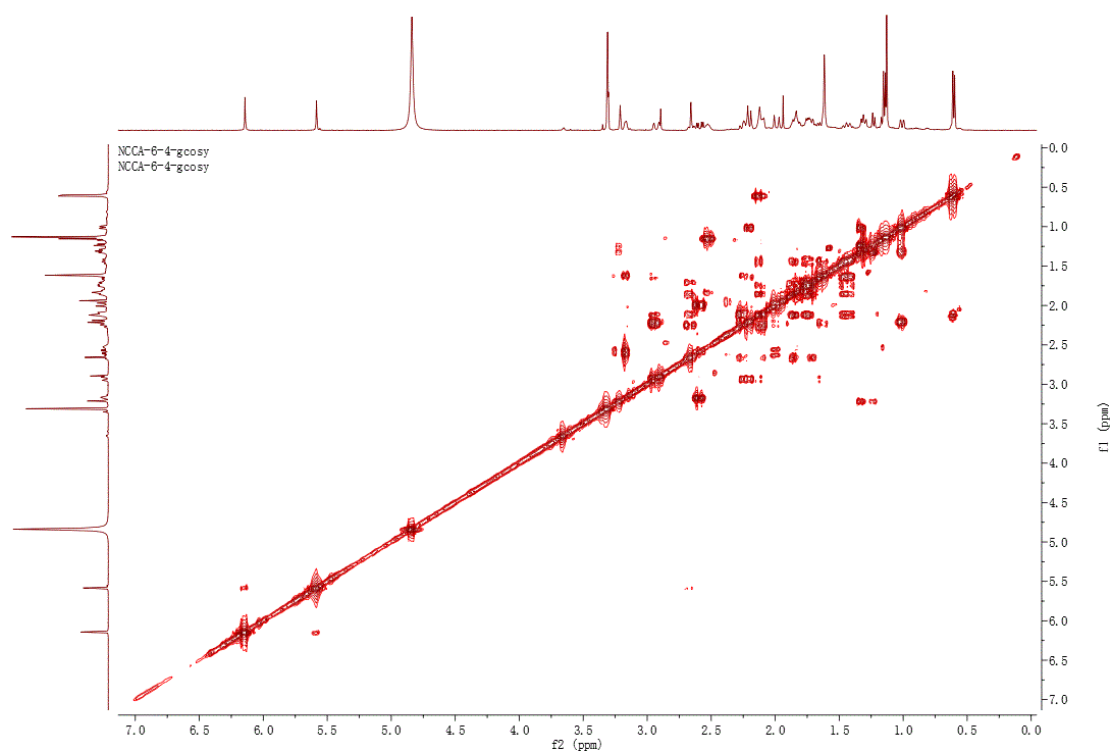


Figure S65. Multiplicity-edited gHSQC Spectrum of Compound 6

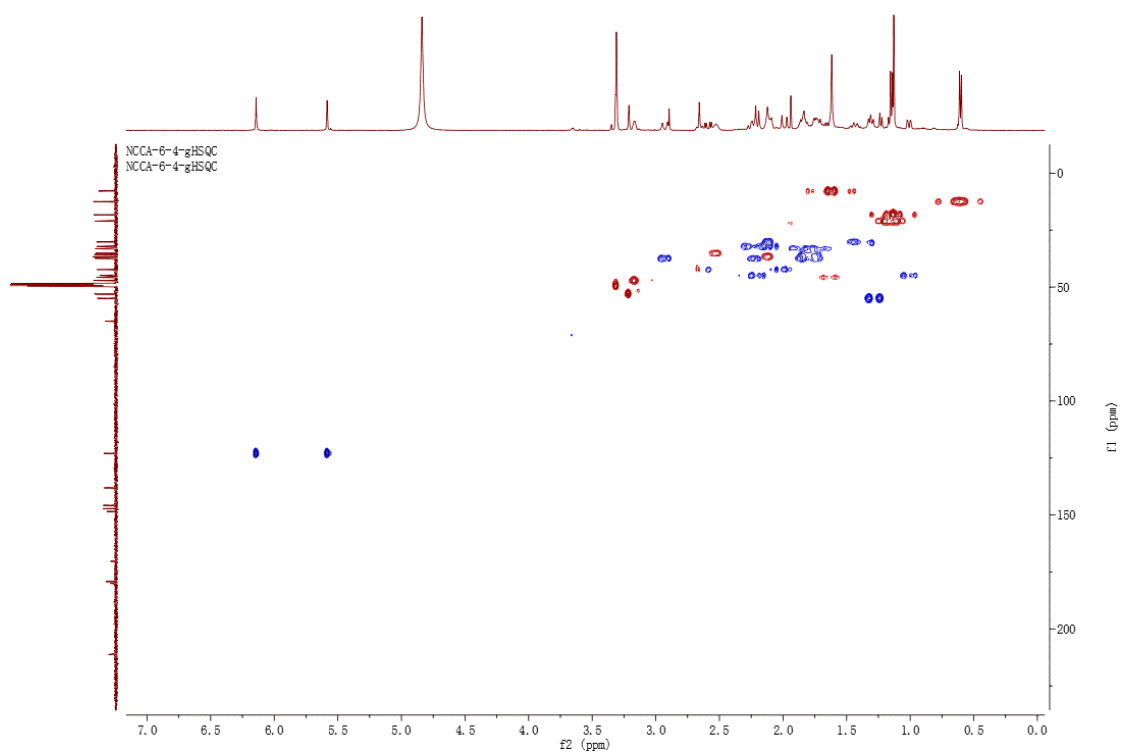


Figure S66. gHMBC Spectrum of Compound 6

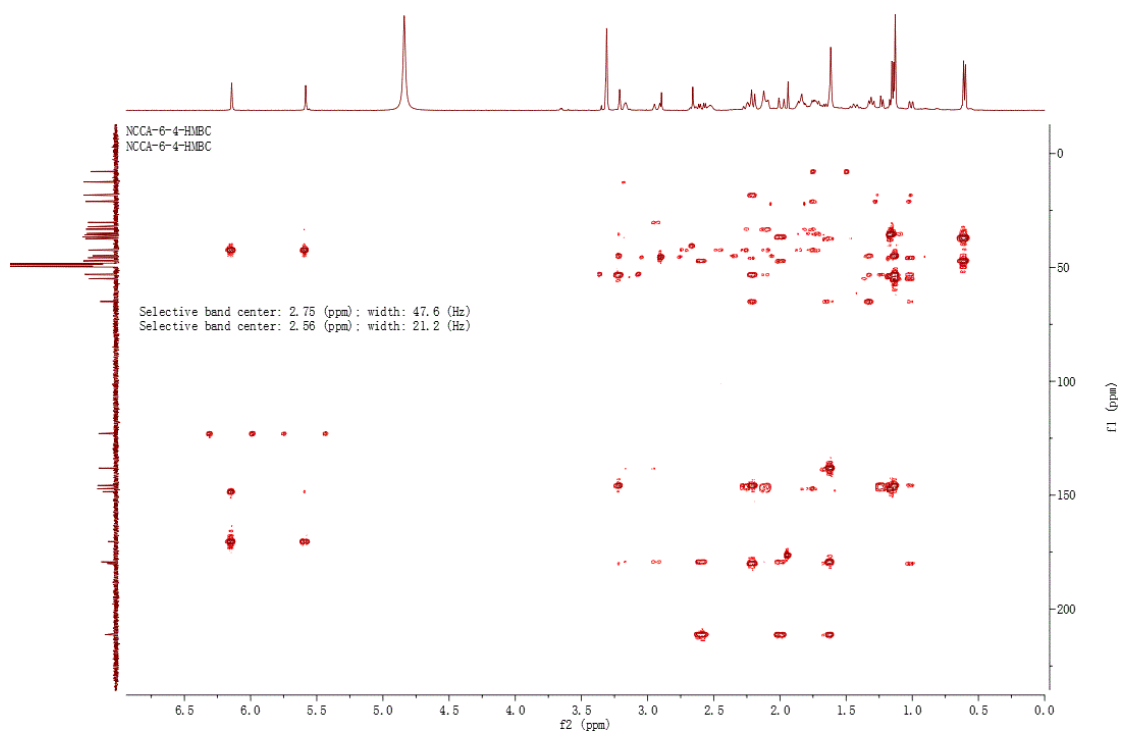


Figure S67. NOESY Spectra of Compound 6

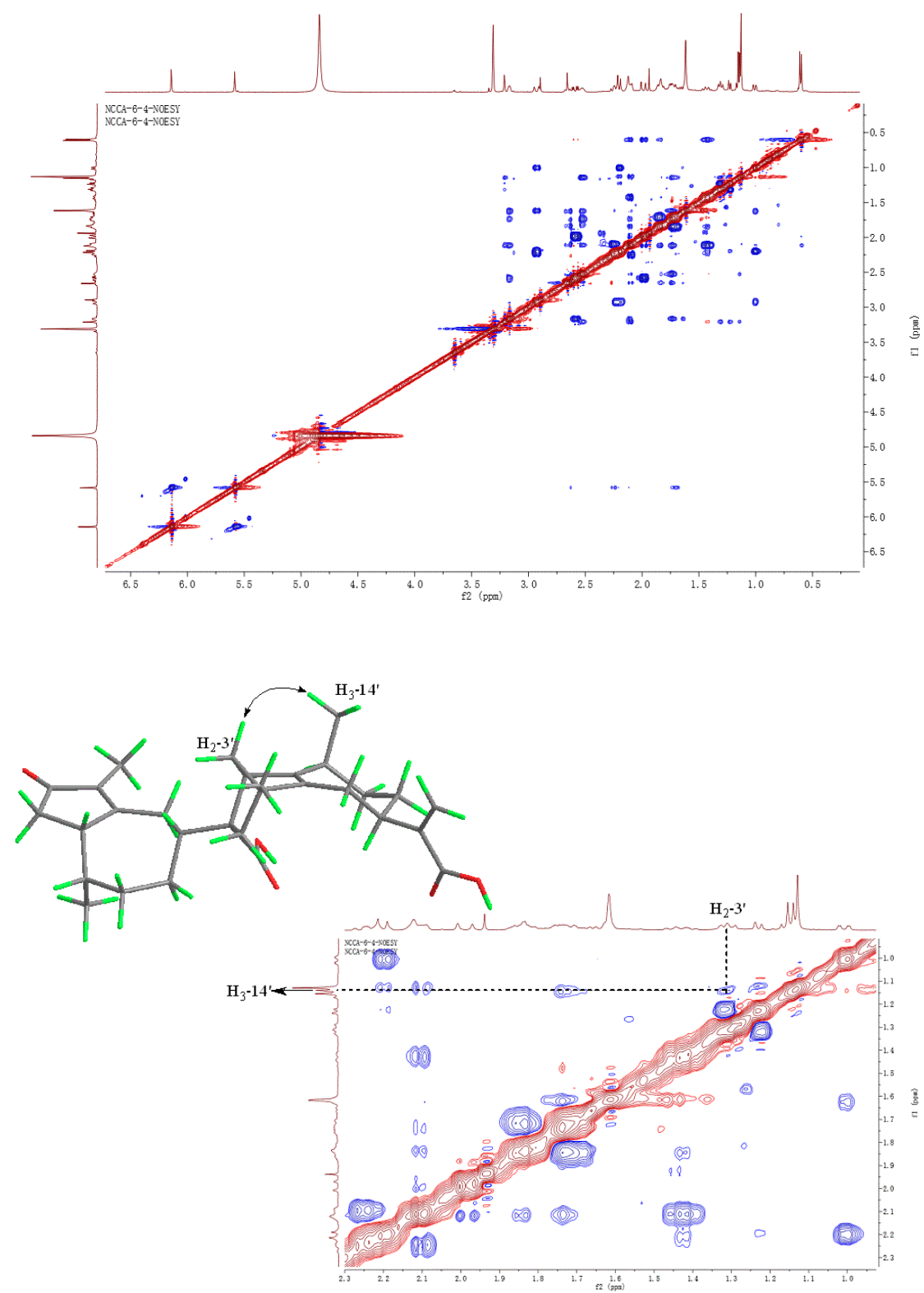


Figure S68. The Stable Conformers of Compound 6

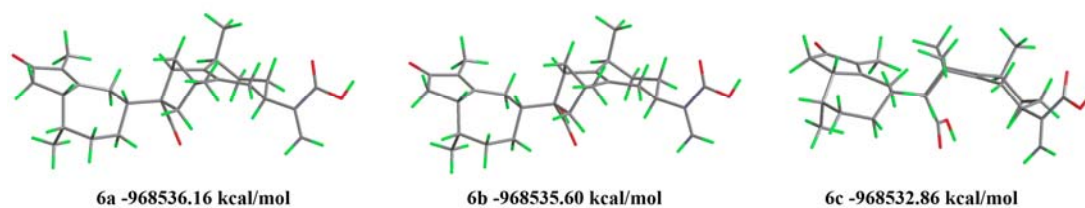


Table S9. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of **6**

conf	$\Delta E_{6-31+G(d)}$ ^a	% ^b
6a	0	71.8
6b	0.56	27.9
6c	3.30	0.3

^aRelative to 6a with $E_{6-31+G(d)} = -968536.16$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S69. Comparison of Experimental and Calculated ECD Spectra of 6

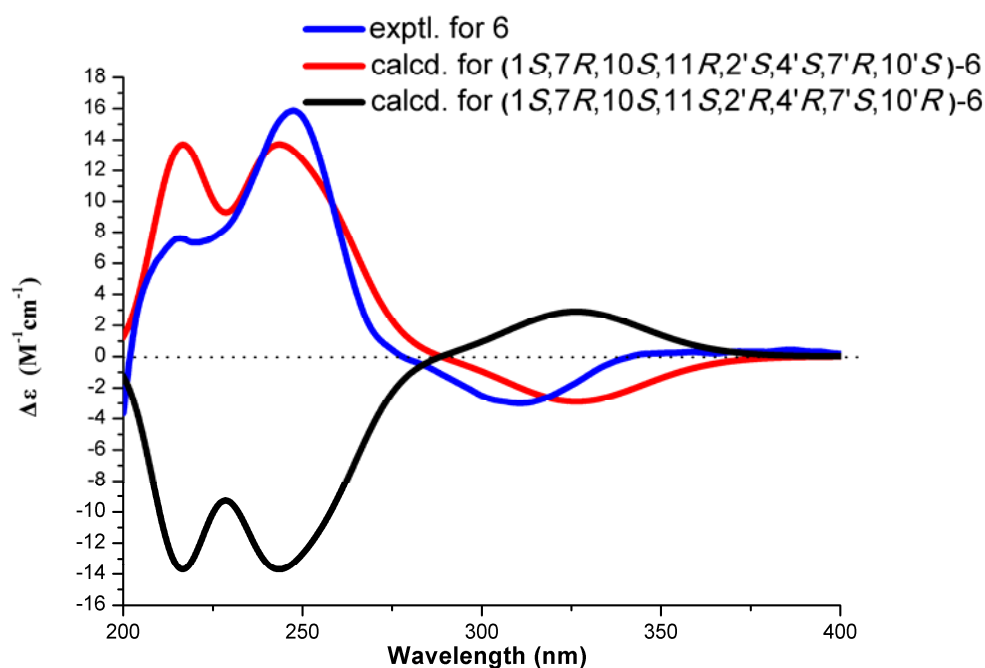


Figure S70. The Stable Conformers of (1*S*,7*R*,10*S*,11*S*,2'*S*,4'*S*,7'*R*,10'*S*)-6

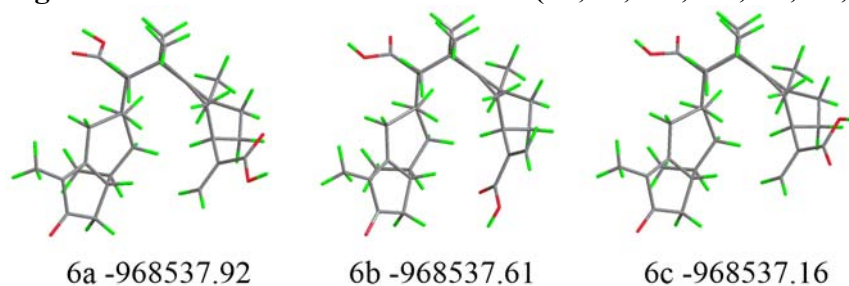


Table S10. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of (1*S*,7*R*,10*S*,11*S*,2'*S*,4'*S*,7'*R*,10'*S*)-6

conf	$\Delta E_{6-31+G(d)}$ ^a	% ^b
6a	0	53.6
6b	0.31	31.5
6c	0.76	14.9

^aRelative to 6a with $E_{6-31+G(d)} = -968537.92$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S71. Comparison of Experimental and Calculated ECD Spectra of (1*S*,7*R*,10*S*,11*S*,2'*S*,4'*S*,7'*R*,10'*S*)-6

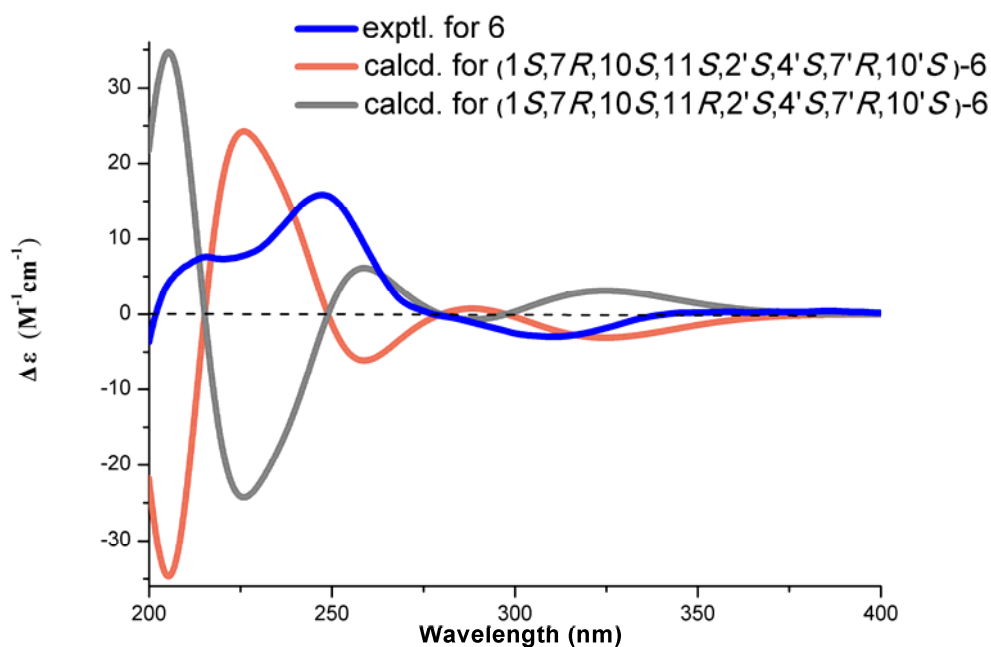


Figure S72. (-)-HRESIMS Spectrum of Compound 7

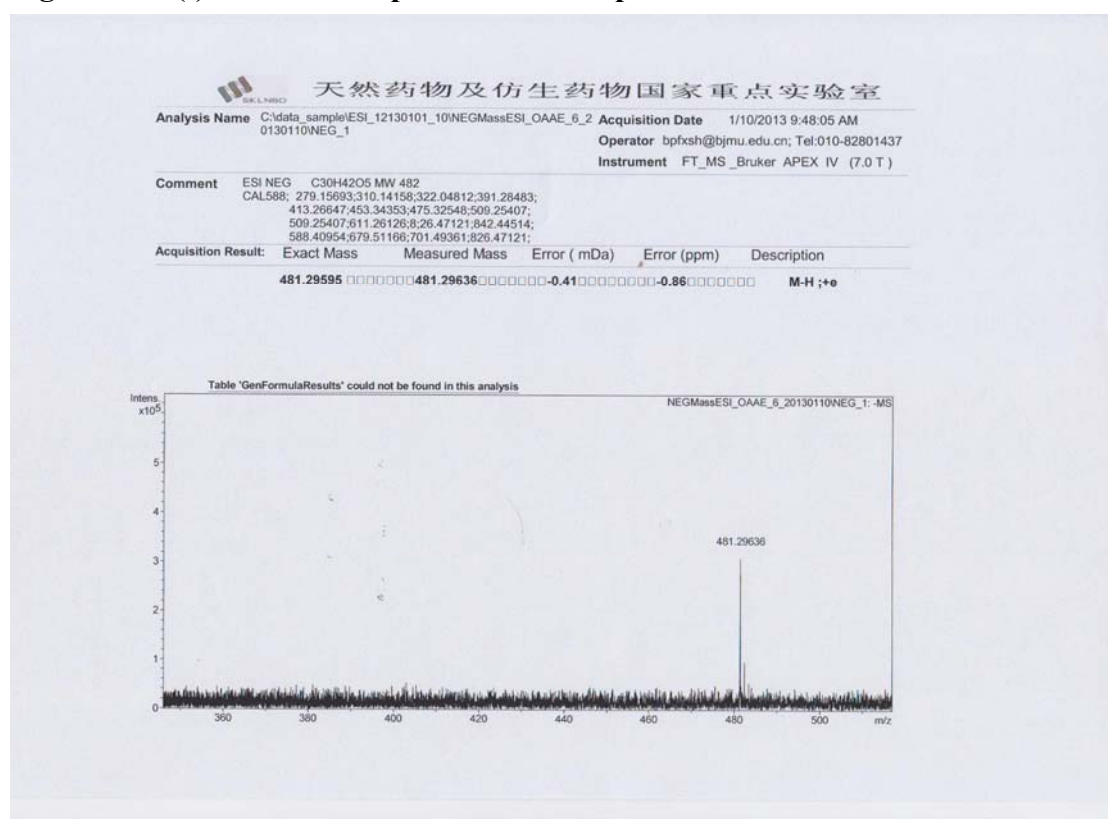


Figure S73. IR Spectrum of Compound 7

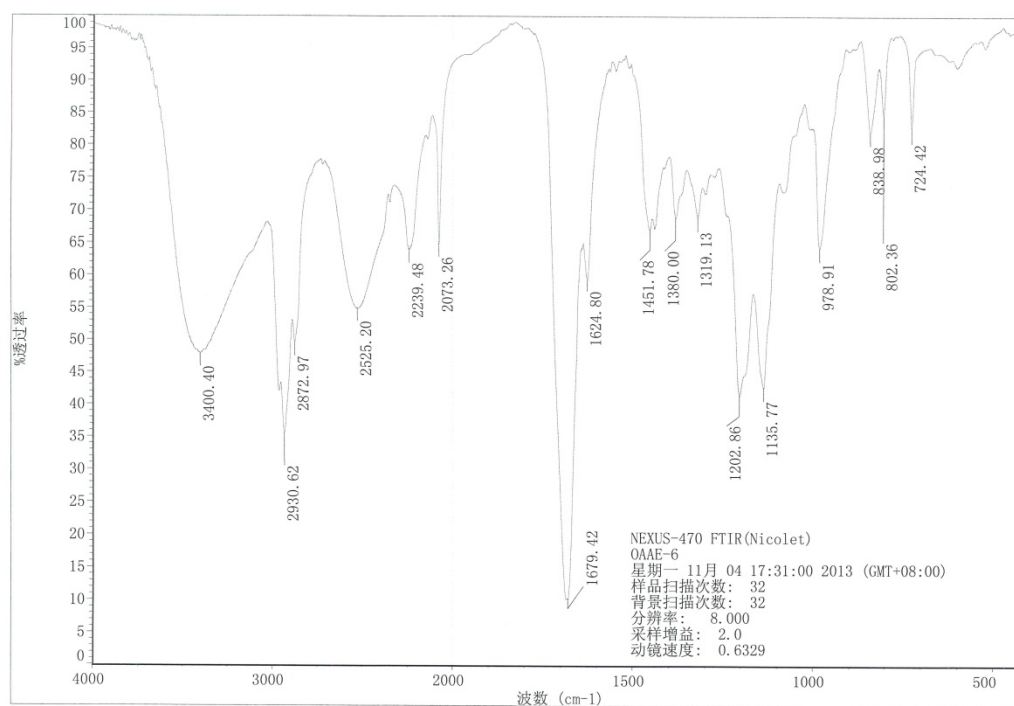


Figure S74. ^1H -NMR Spectrum of Compound 7 (500 MHz, CD_3OD)

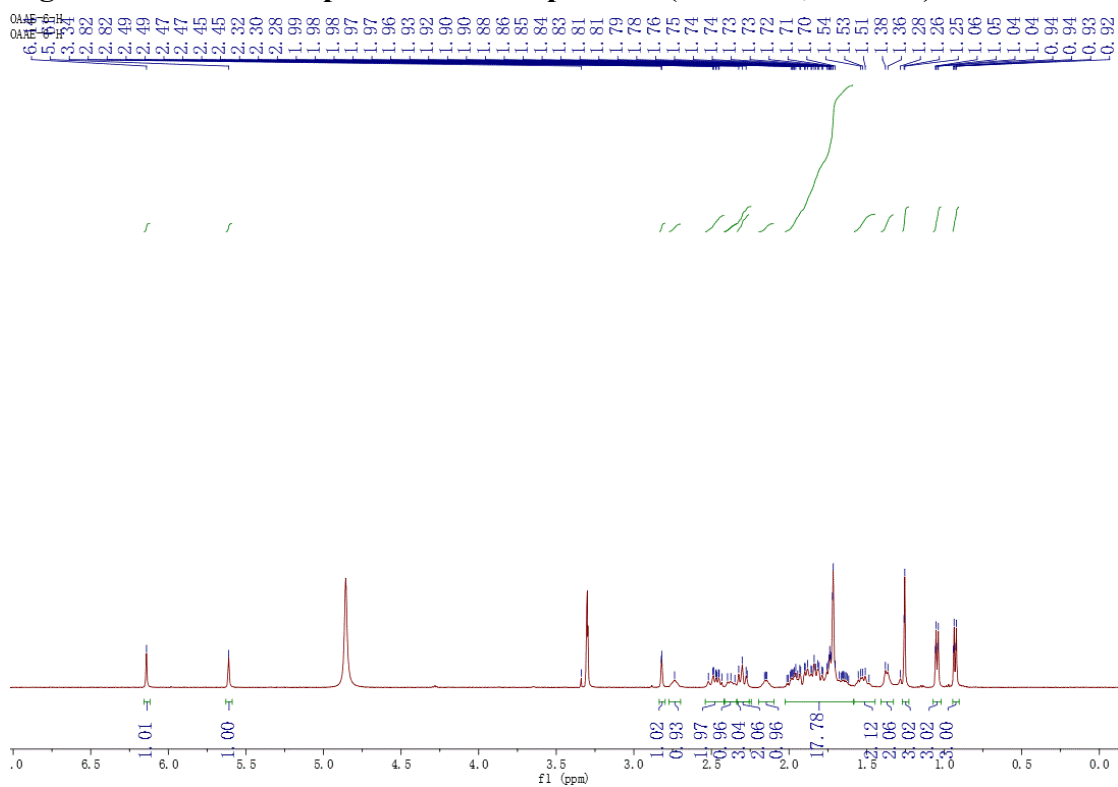


Figure S75. ^{13}C -NMR Spectrum of Compound 7 (125 MHz, CD_3OD)

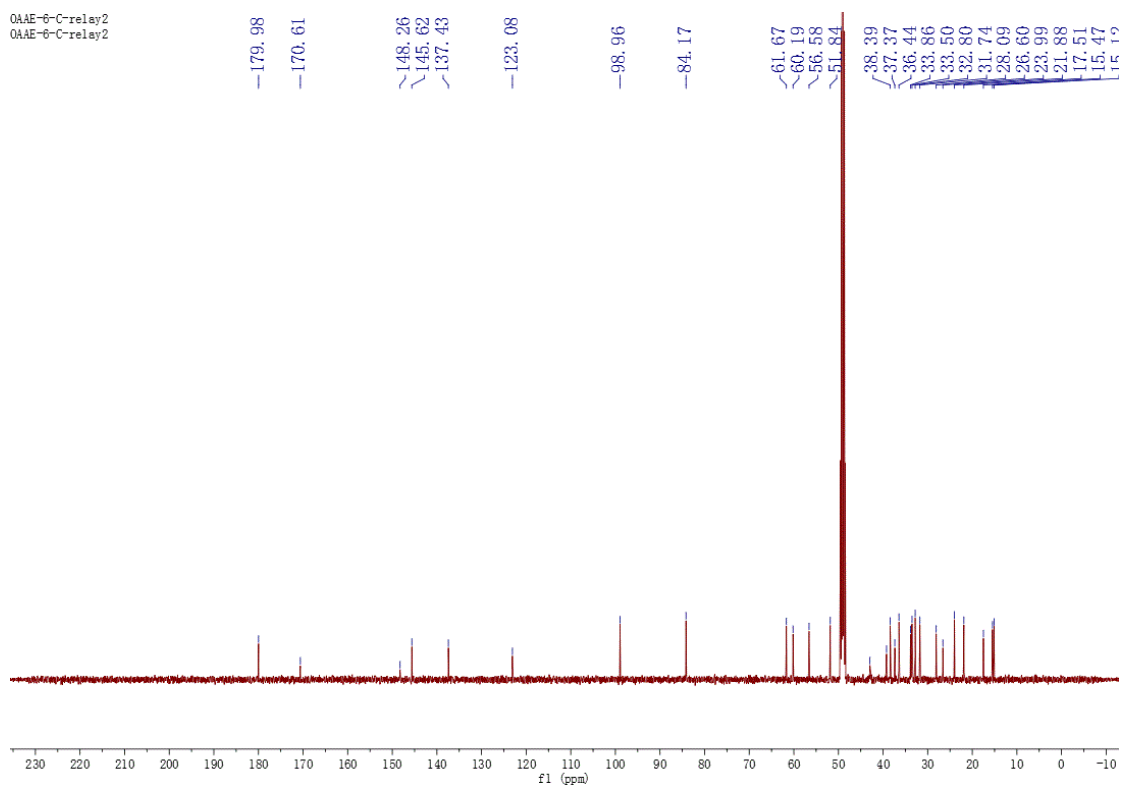


Figure S76. DEPT-135 Spectrum of Compound 7

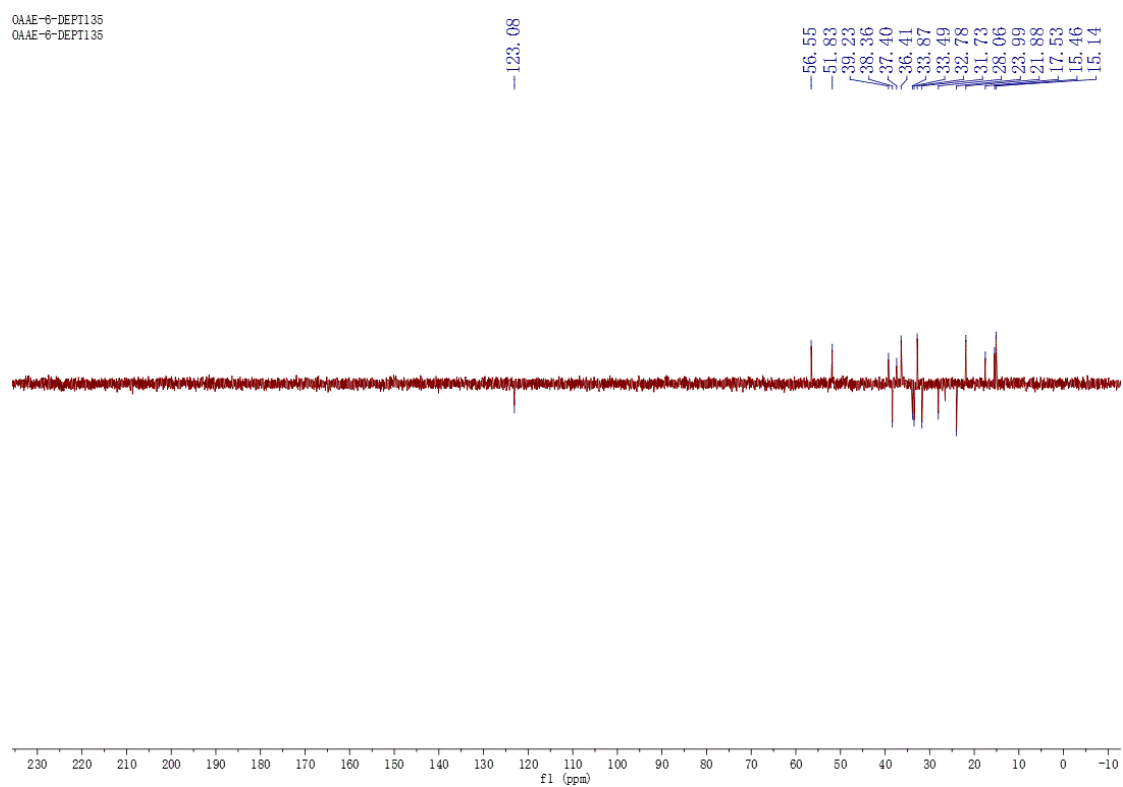


Figure S77. ^1H - ^1H gCOSY Spectrum of Compound 7

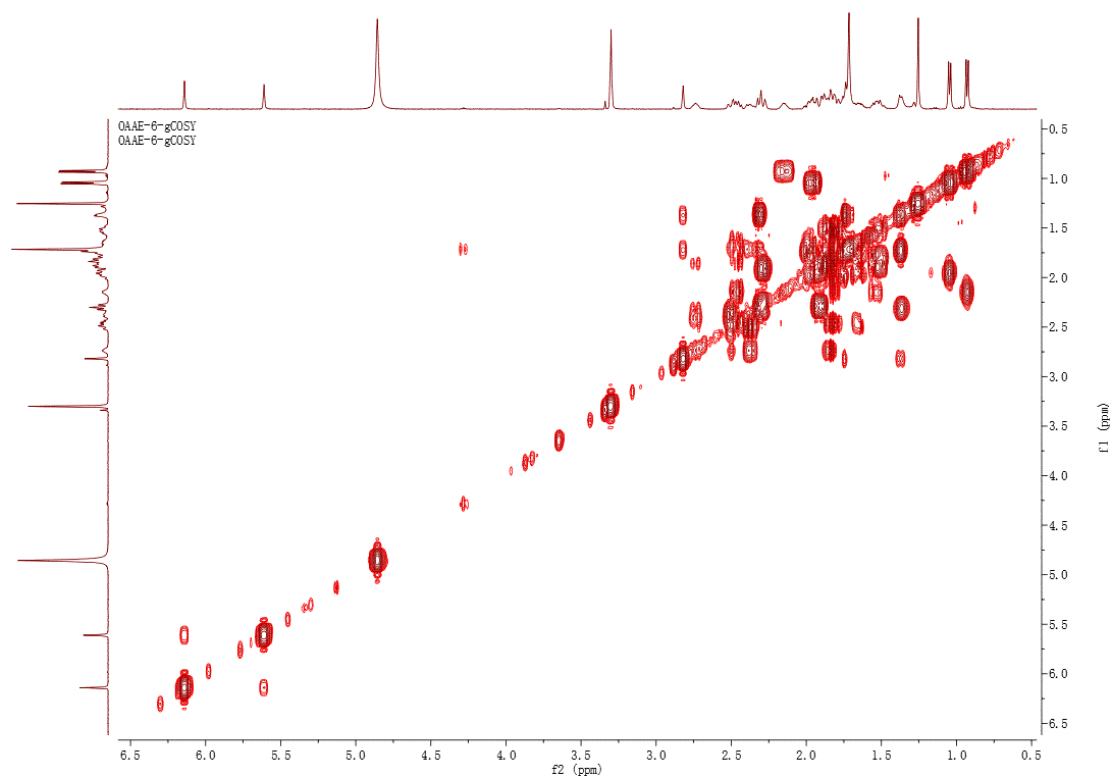


Figure S78. Multiplicity-edited gHSQC Spectrum of Compound 7

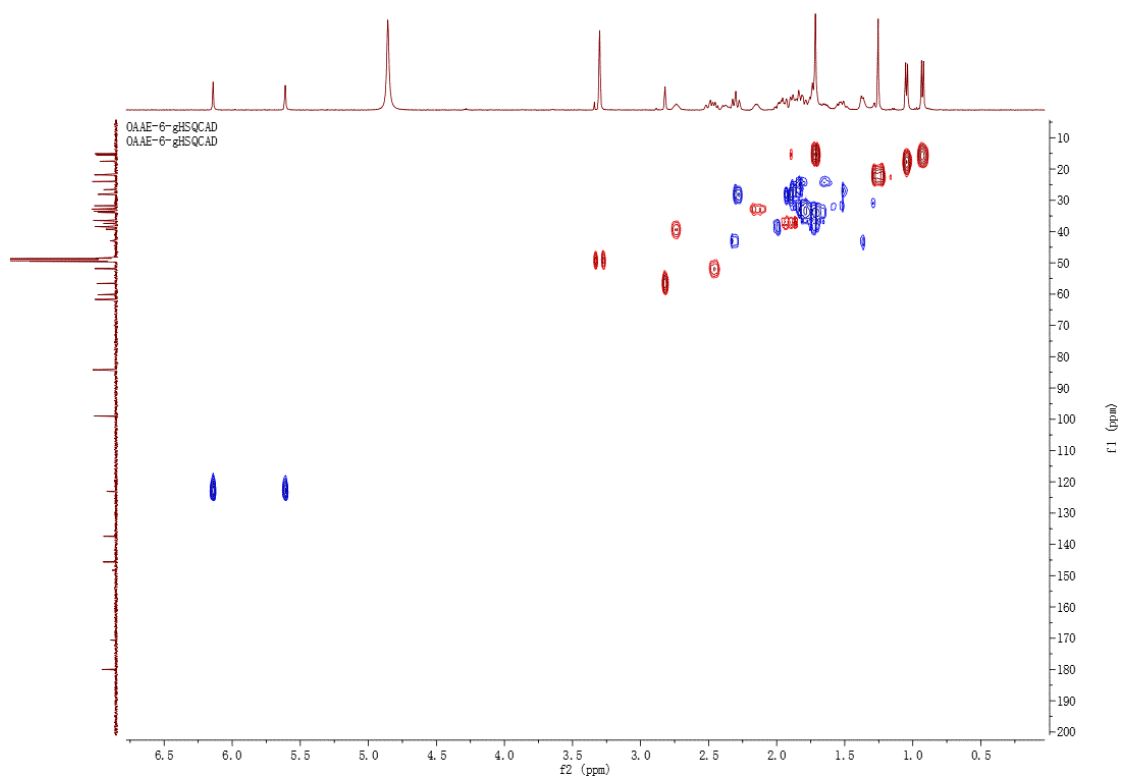


Figure S79. Selected Multiplicity-edited gHSQC Spectrum of Compound 7

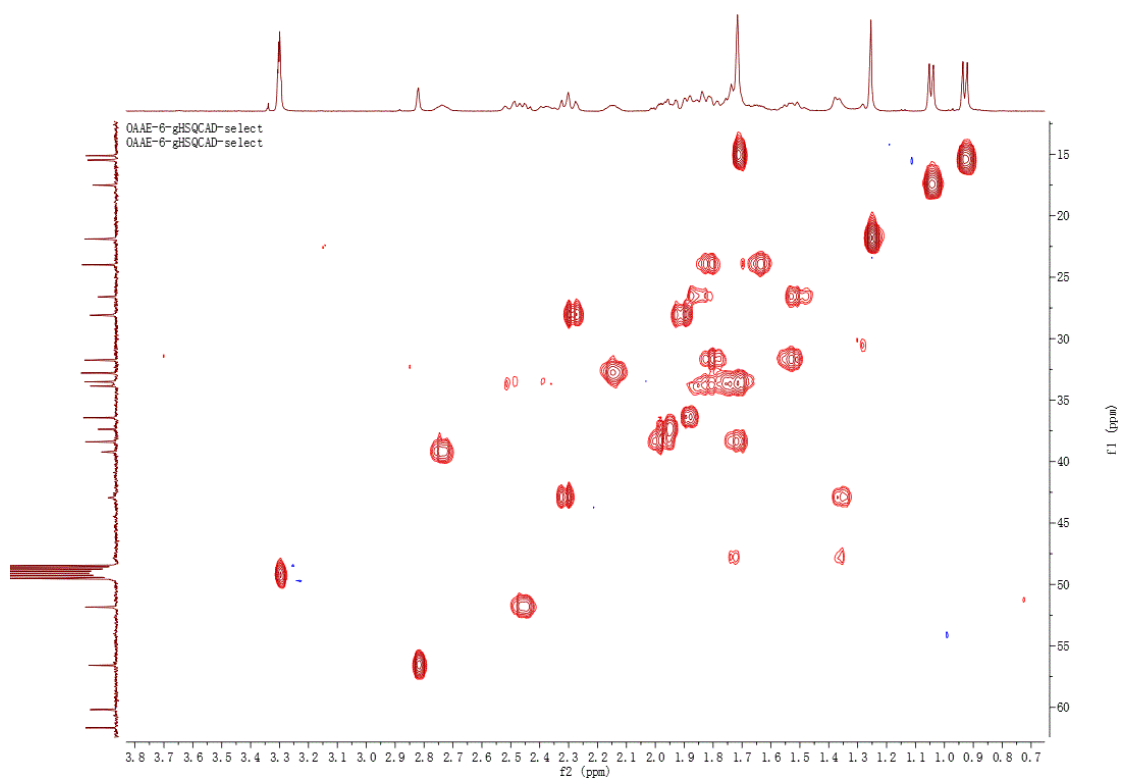


Figure S80. gHMBC Spectrum of Compound 7

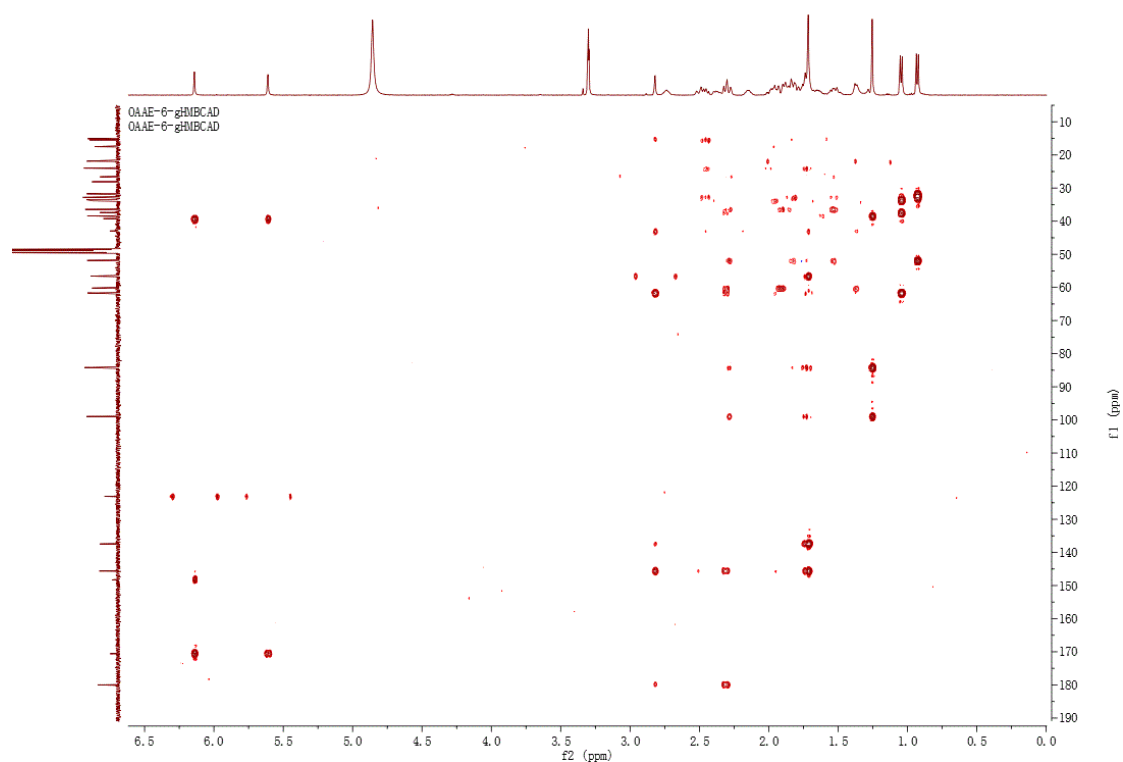


Figure S81. NOESY Spectrum of Compound 7

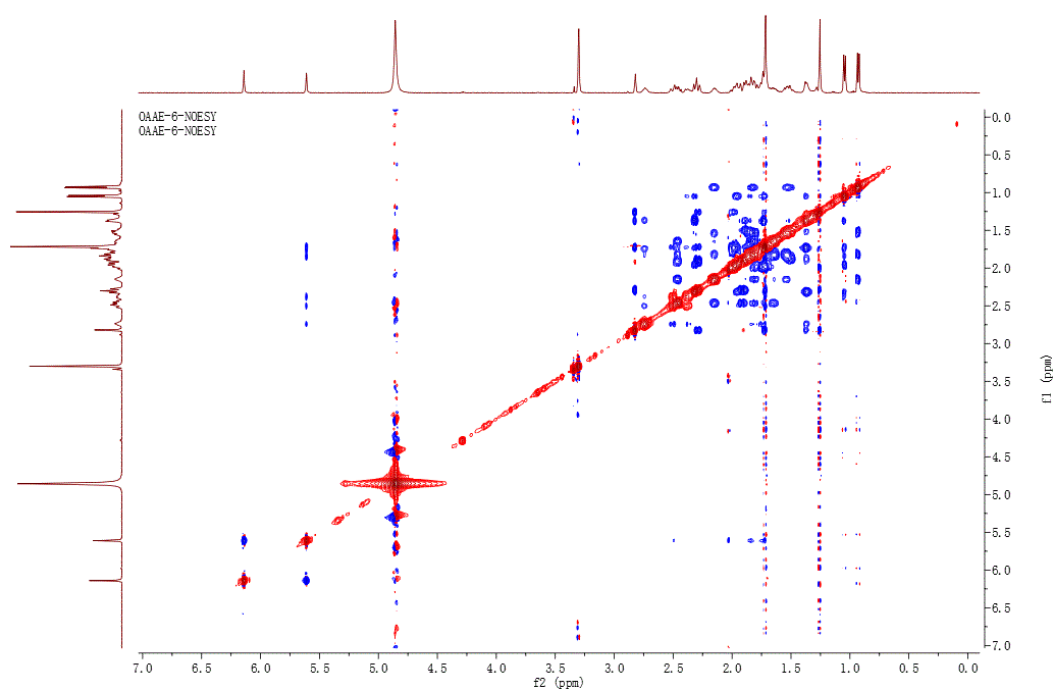


Figure S82. The Stable Conformers of Compound 7

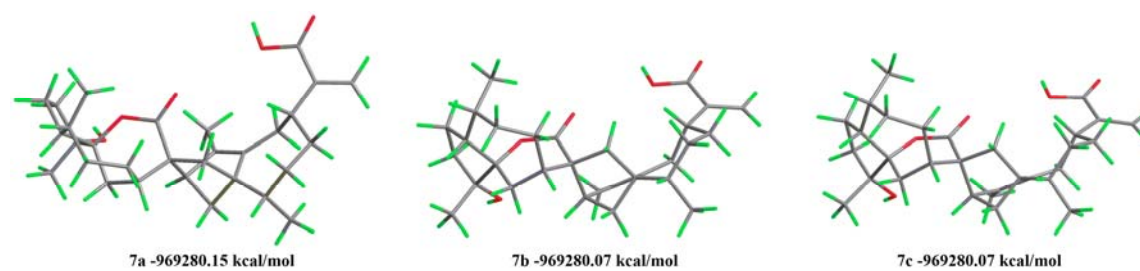


Table S11 B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of **7**

conf	$\Delta E_{6-31+G(d)}$ ^a	% ^b
7a	0	36.6
7b	0.08	31.7
7c	0.08	31.7

^aRelative to 7a with $E_{6-31+G(d)} = -969280.15$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S83 (-)-HRESIMS Spectrum of Compound 8

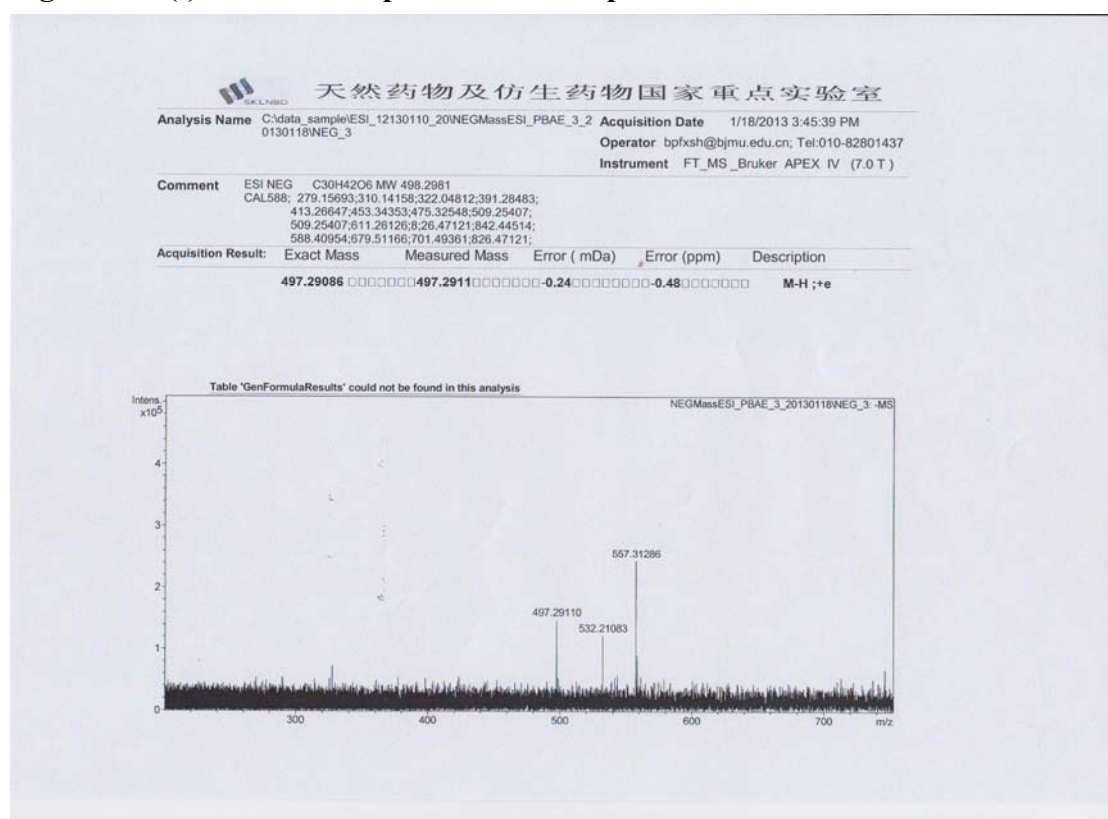


Figure S84 IR Spectrum of Compound 8

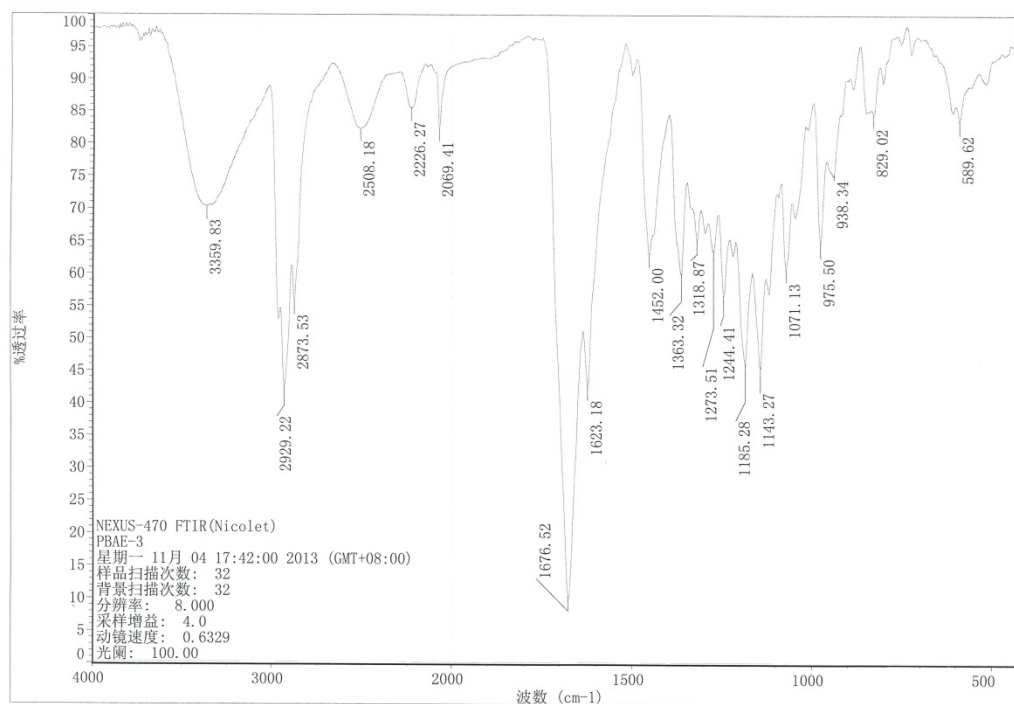


Figure S87 DEPT-135 Spectrum of Compound 8

PBAE-3-DEPT135
PBAE-3-DEPT135

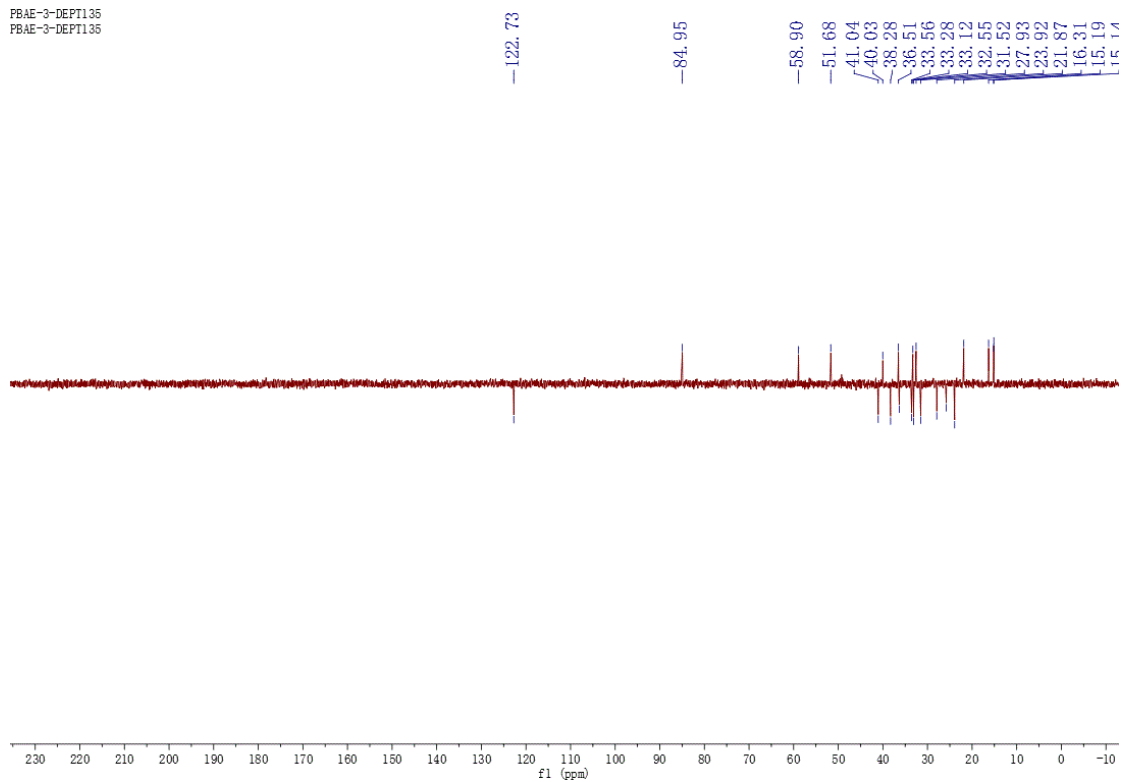


Figure S88. ^1H - ^1H gCOSY Spectrum of Compound 8

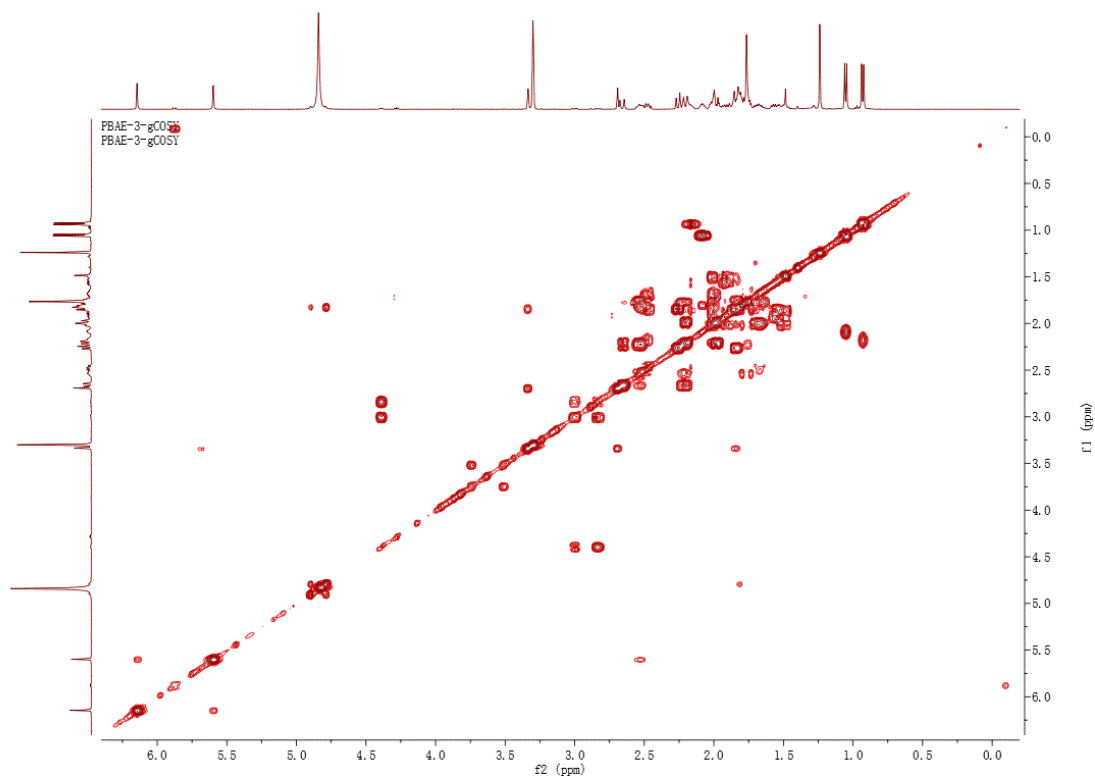


Figure S89. Multiplicity-edited gHSQC Spectrum of Compound 8

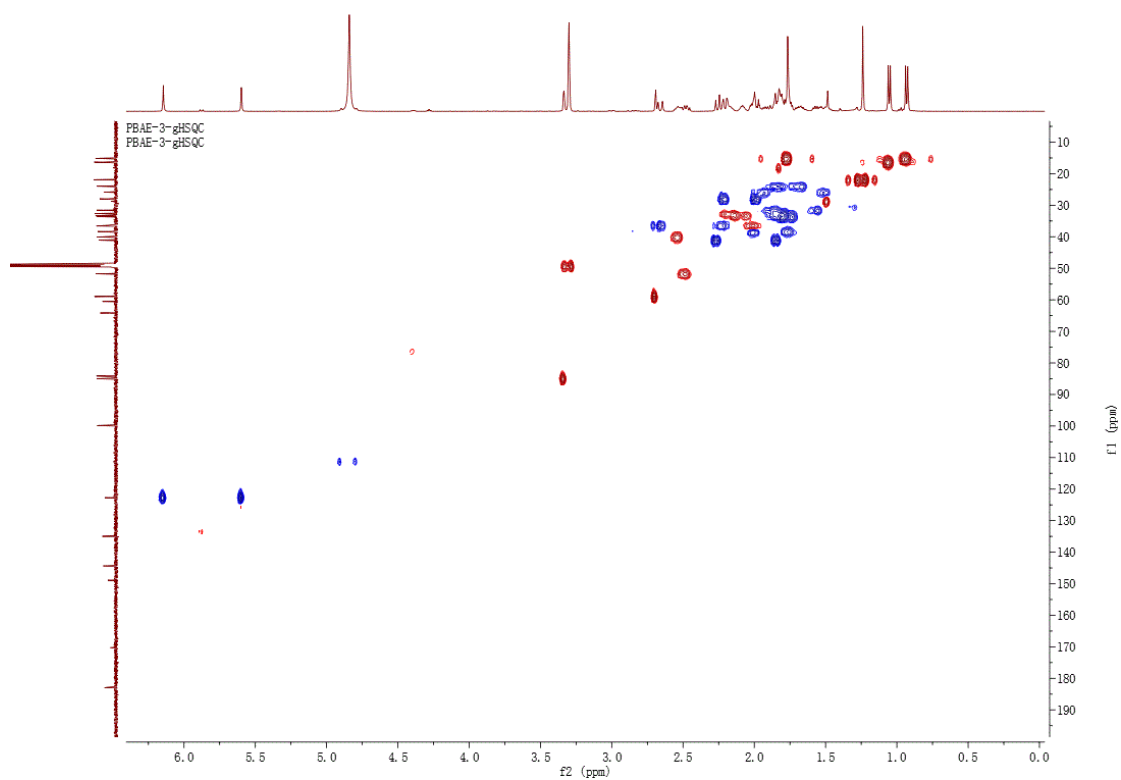


Figure S90. gHMBC Spectrum of Compound 8

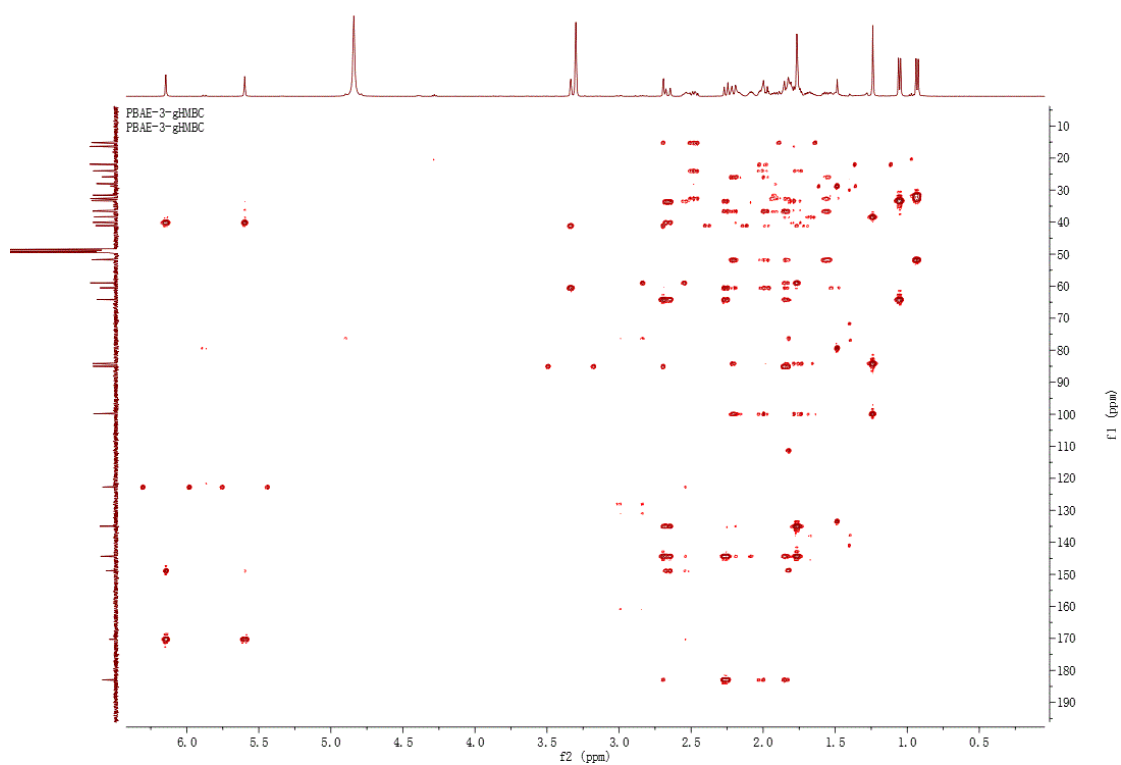


Figure S91. NOESY Spectrum of Compound 8

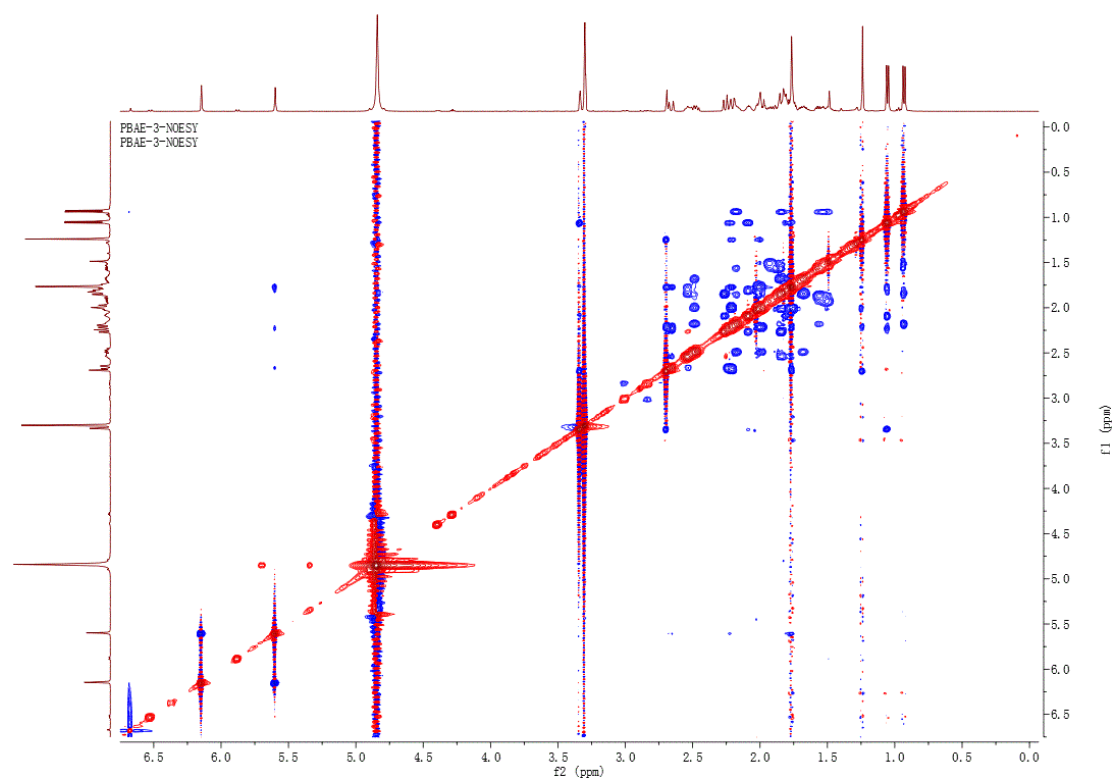


Figure S92. 1D-NOE Spectrum of Compound 8

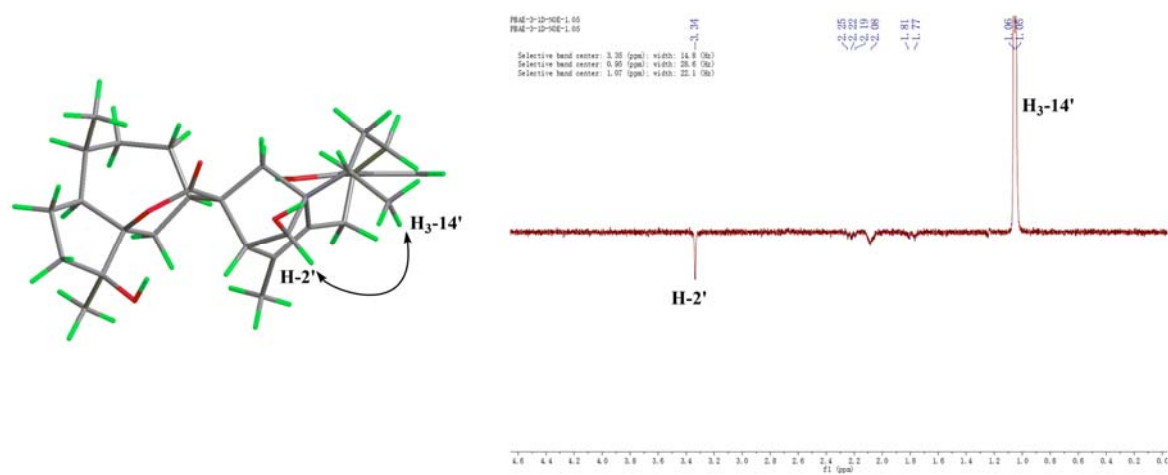


Figure S93. The Stable Conformers of Compound 8

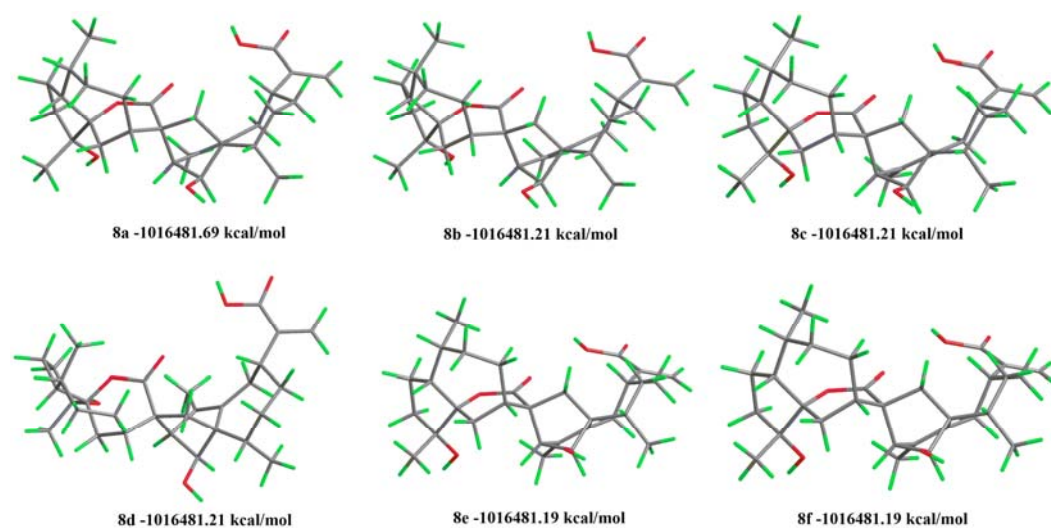


Table S12. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of **8**

Conf	$\Delta E_{6-31+G(d)}^a$	% ^b
8a	0	31.2
8b	0.81	13.9
8c	0.81	13.9
8d	0.82	13.8
8e	0.83	13.6
8f	0.83	13.6

^aRelative to 8a with $E_{6-31+G(d)} = -1016481.69$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S94. Comparison of Experimental and Calculated ECD Spectra of 8

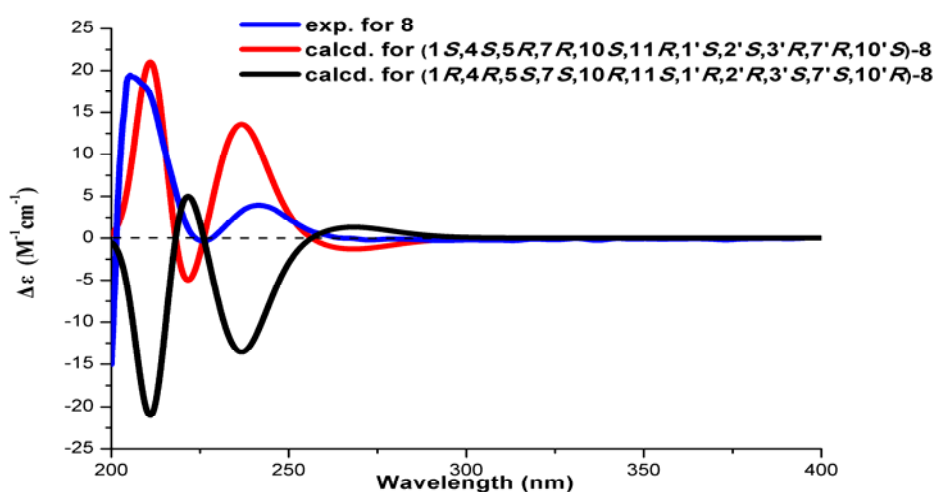


Figure S95. (+)-HRESIMS Spectrum of Compound 9

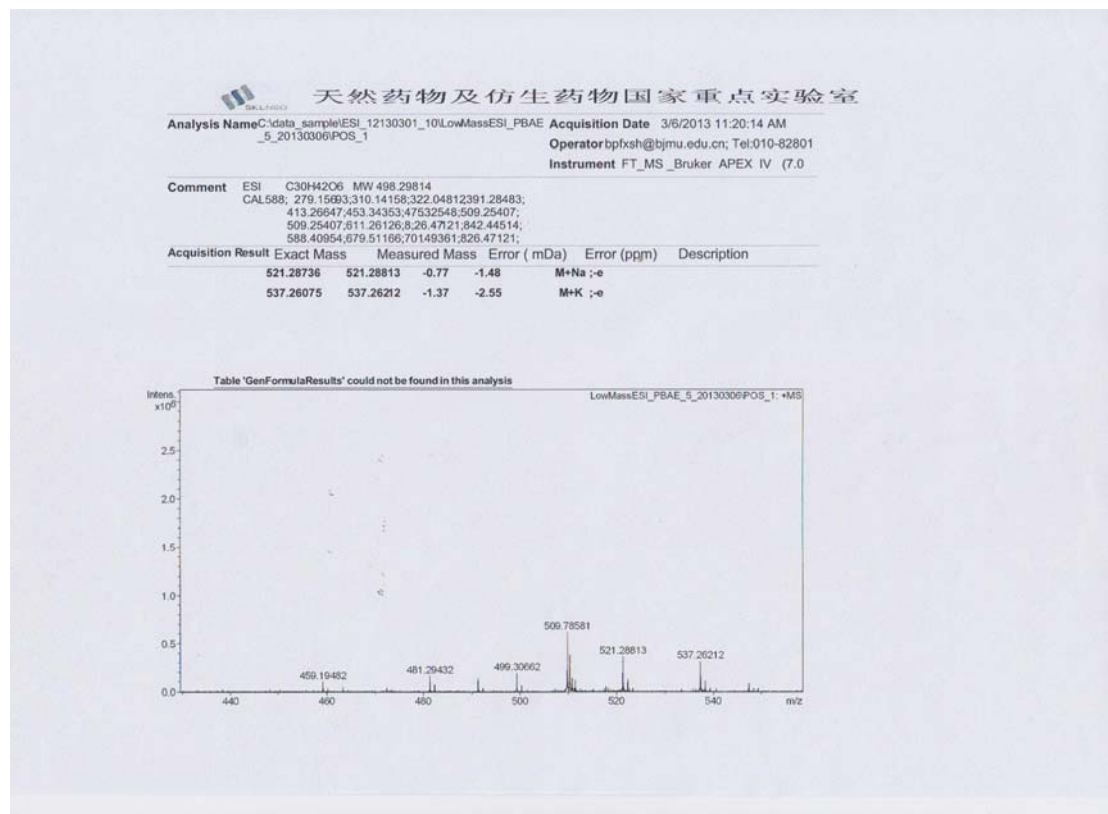


Figure S96. IR Spectrum of Compound 9

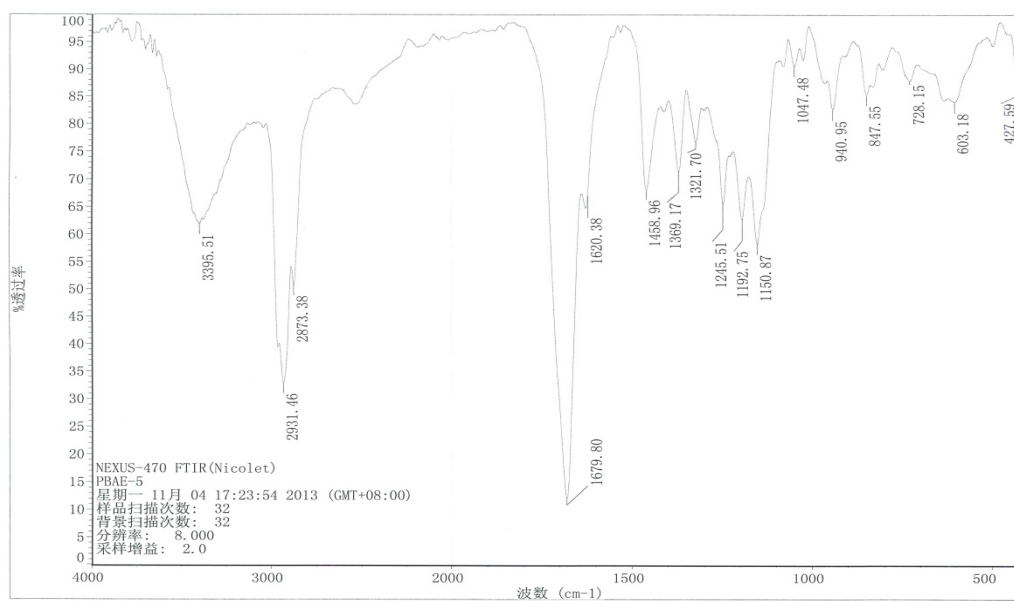


Figure S97. ^1H -NMR Spectrum of Compound 9 (500 MHz, CD_3OD)

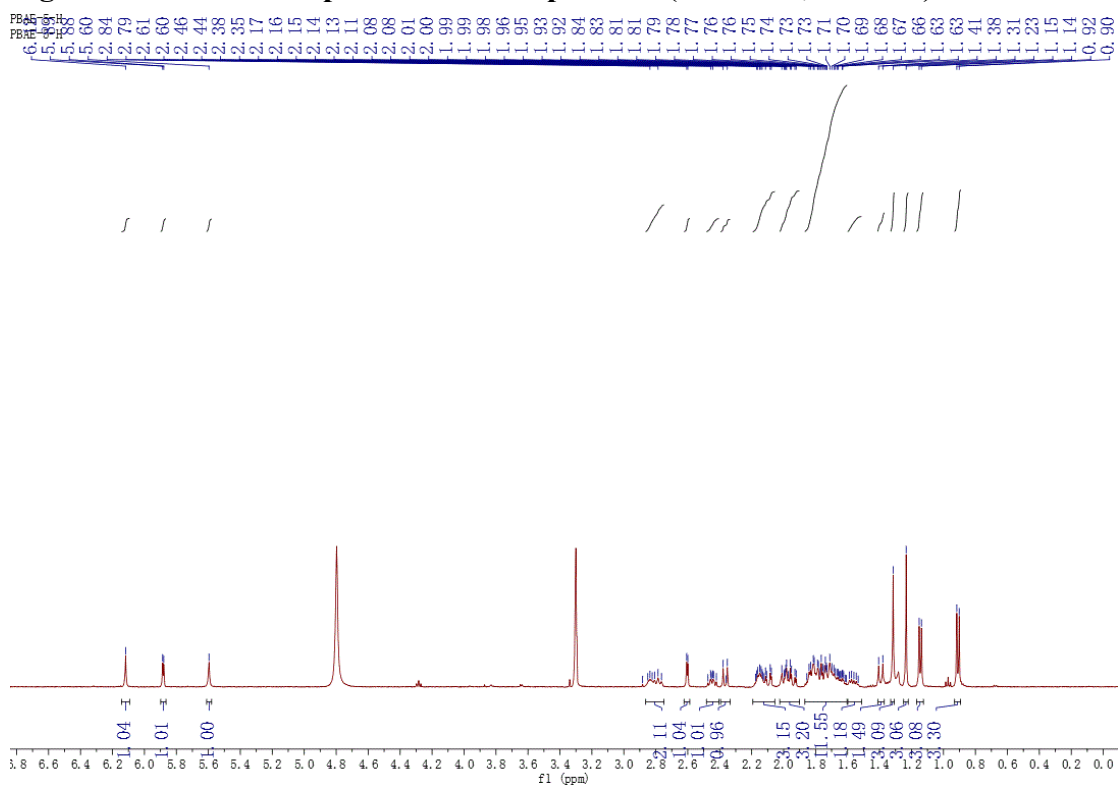


Figure S98. ^{13}C -NMR Spectrum of Compound 9 (125 MHz, CD_3OD)

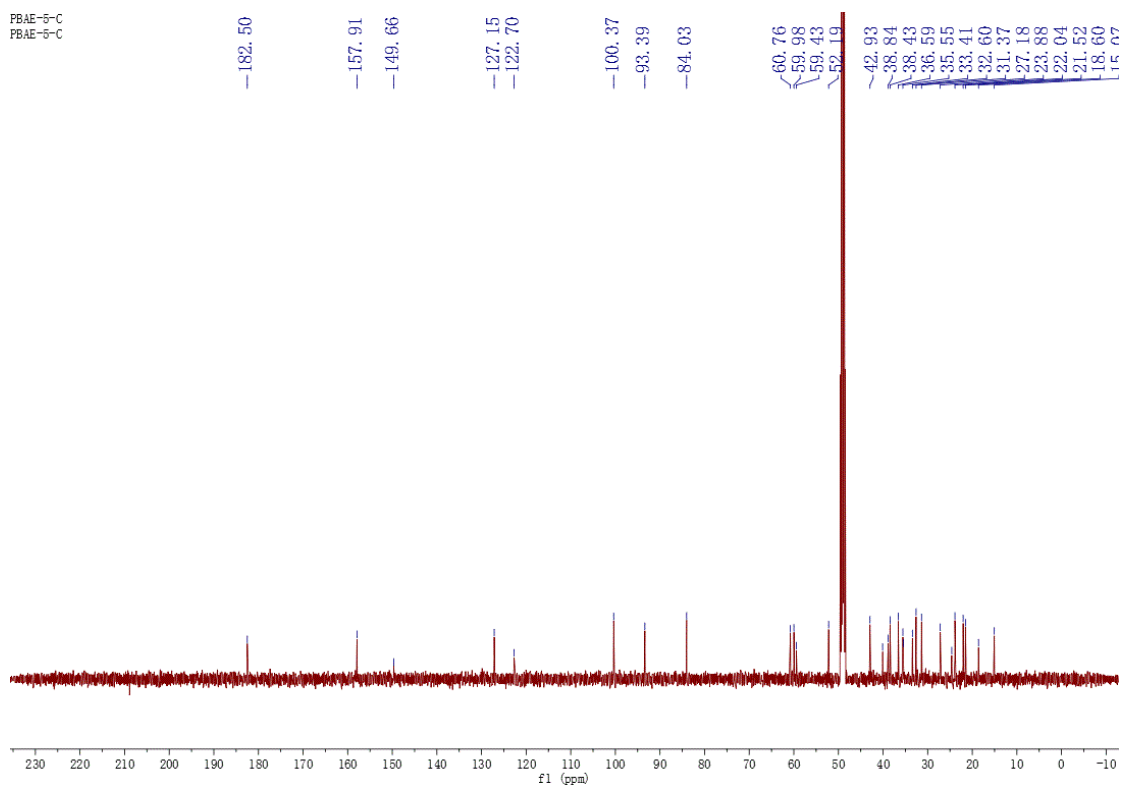


Figure S99. DEPT-135 Spectrum of Compound 9

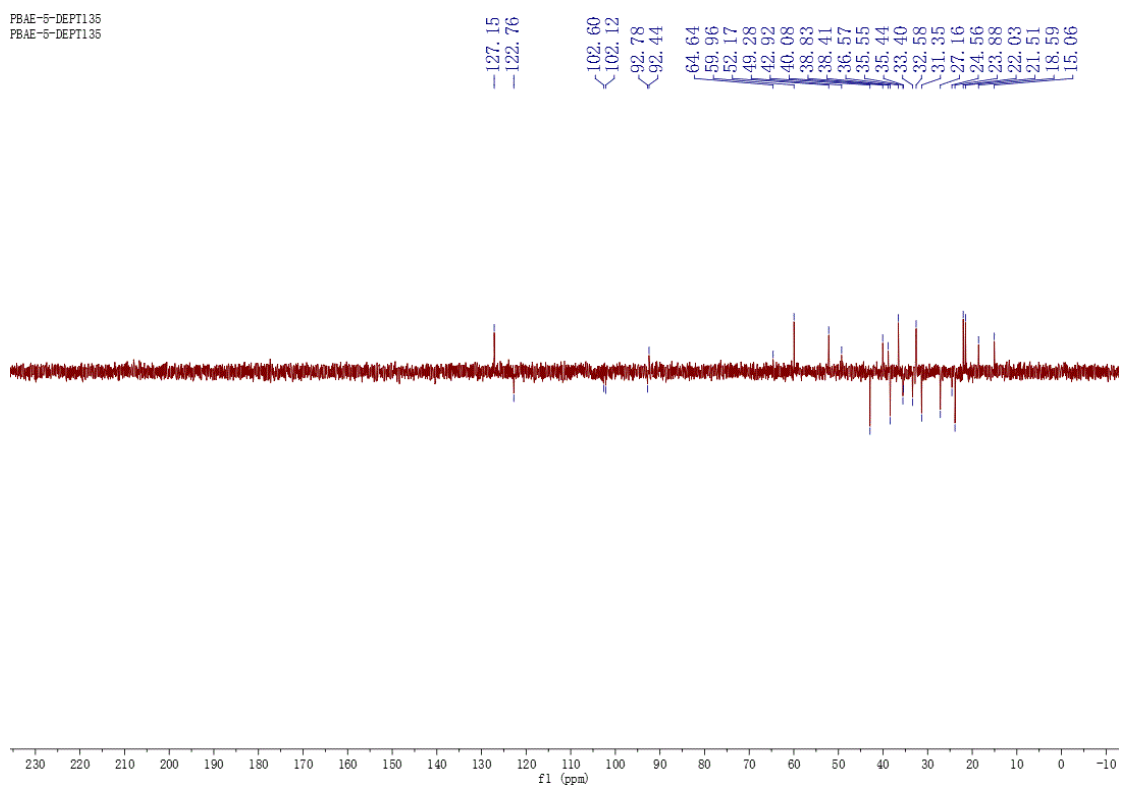


Figure S100. ^1H - ^1H gCOSY Spectrum of Compound 9

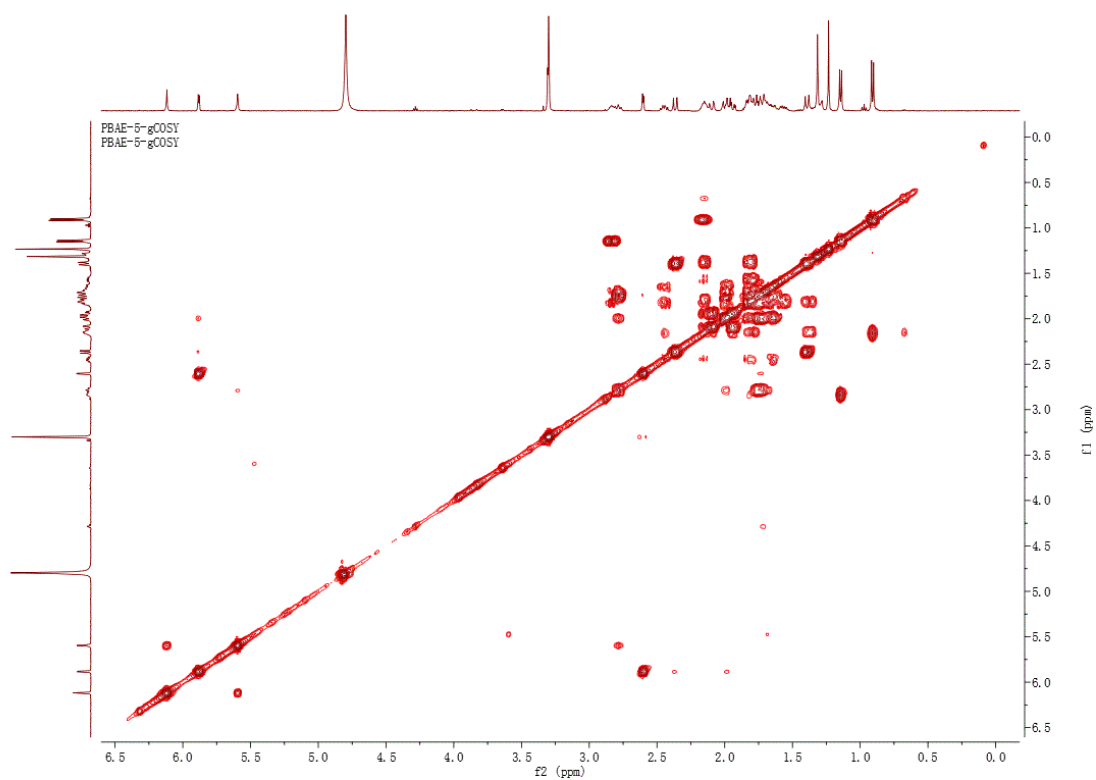


Figure S101. Multiplicity-edited gHSQC Spectrum of Compound 9

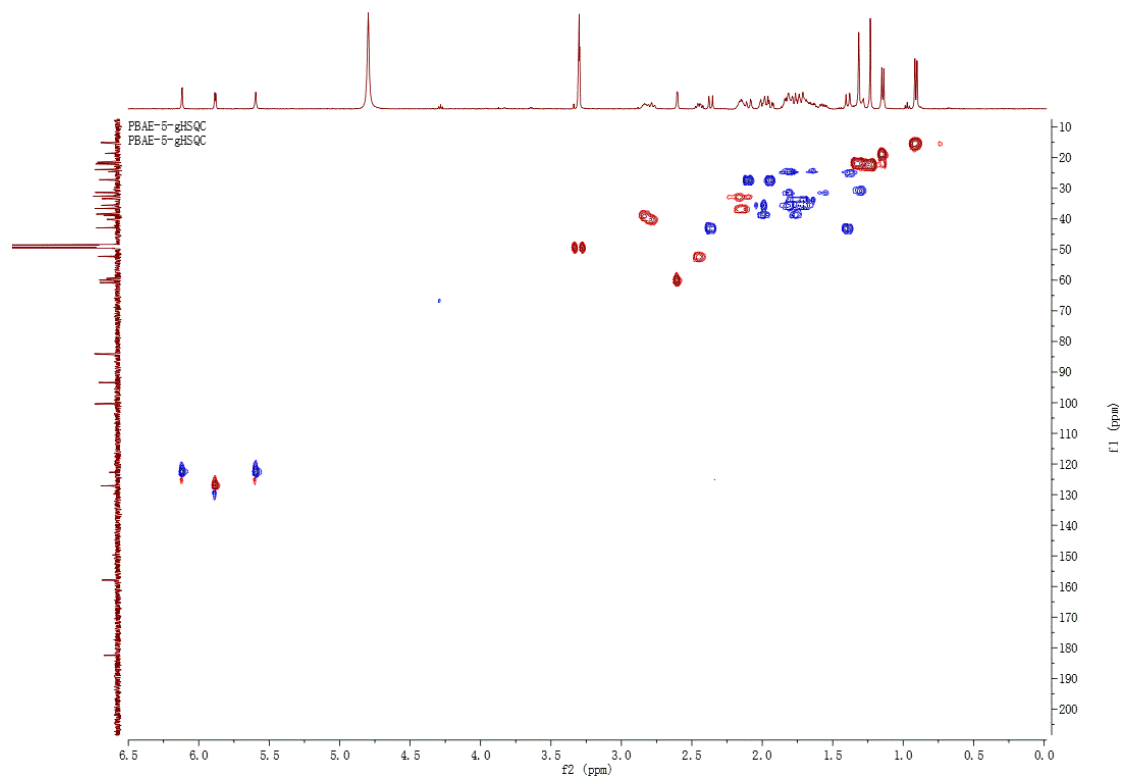


Figure S102. gHMBC Spectrum of Compound 9

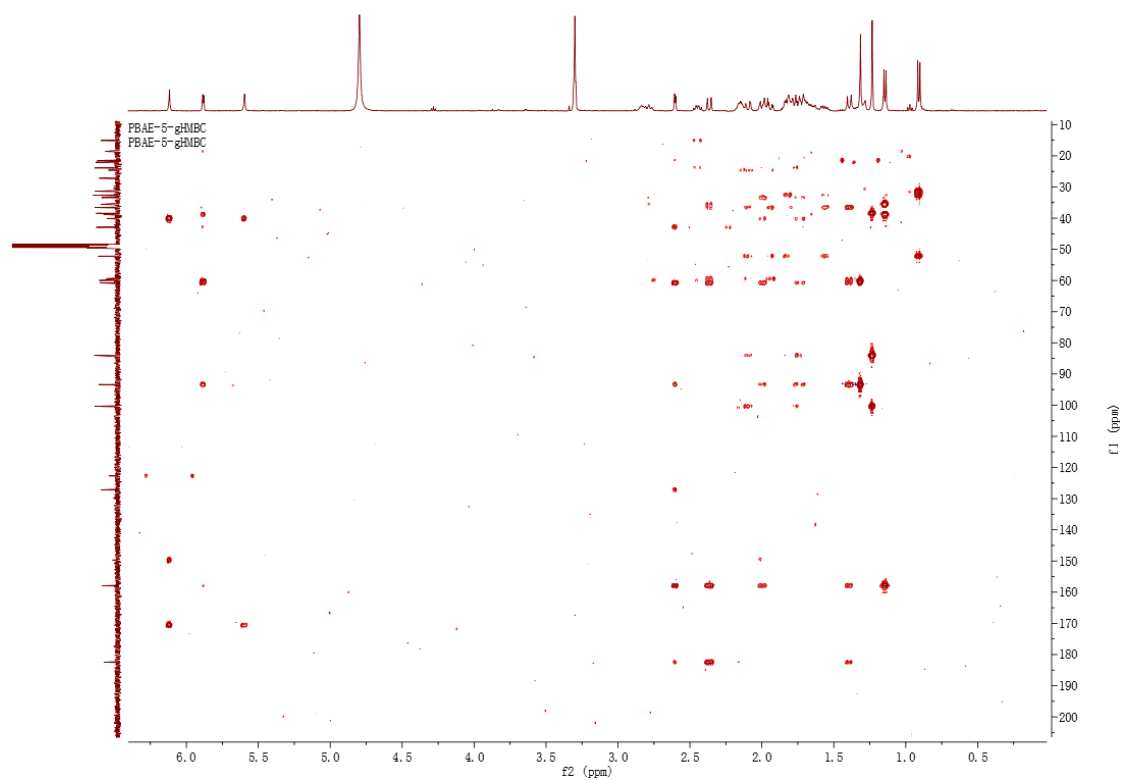


Figure S103. NOESY Spectra of Compound 9

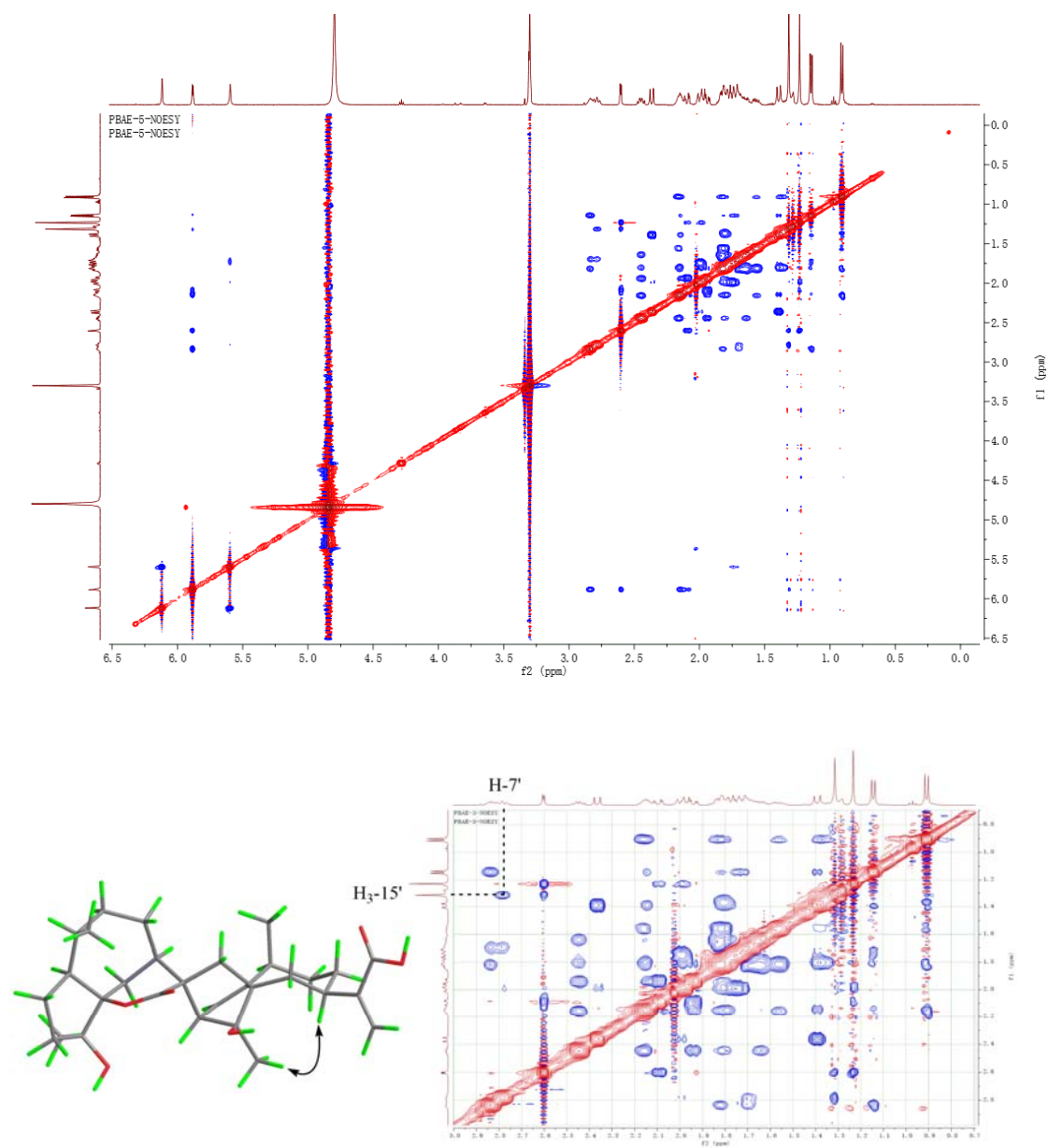


Figure S104. The Stable Conformers of Compound 9

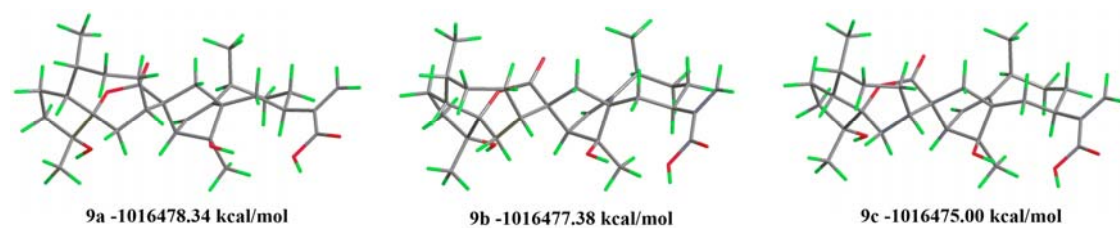


Table S13. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of **9**

conf	$\Delta E_{6-31+G(d)}$ ^a	% ^b
9a	0	83.3
9b	0.96	16.4
9c	3.34	0.3

^aRelative to **9a** with $E_{6-31+G(d)} = -1016478.34$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S105. Comparison of Experimental and Calculated ECD Spectra of **9**

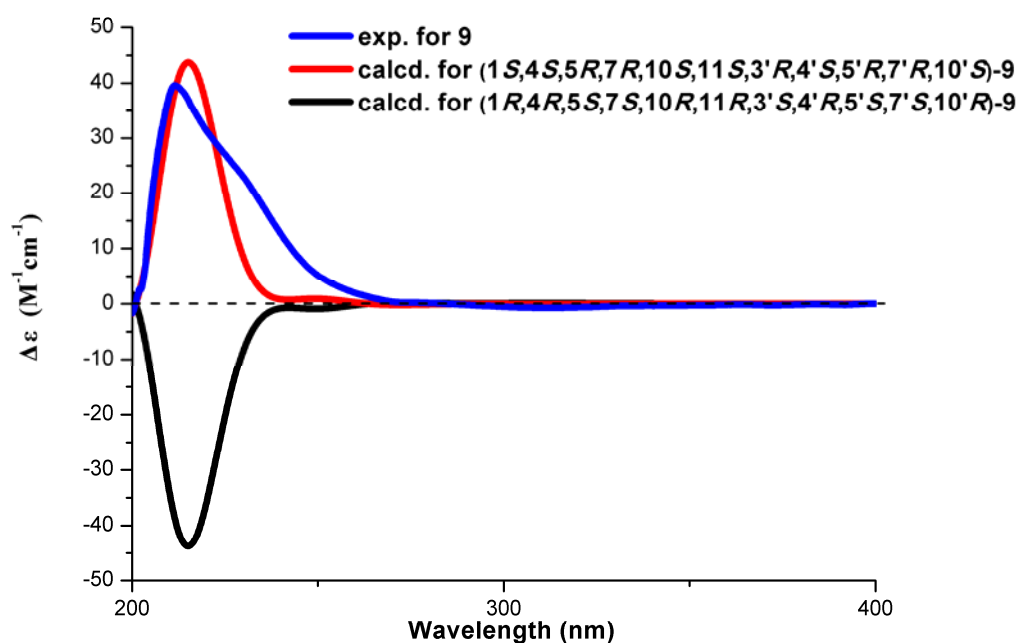


Figure S106. (-)-HRESIMS Spectrum of Compound 10

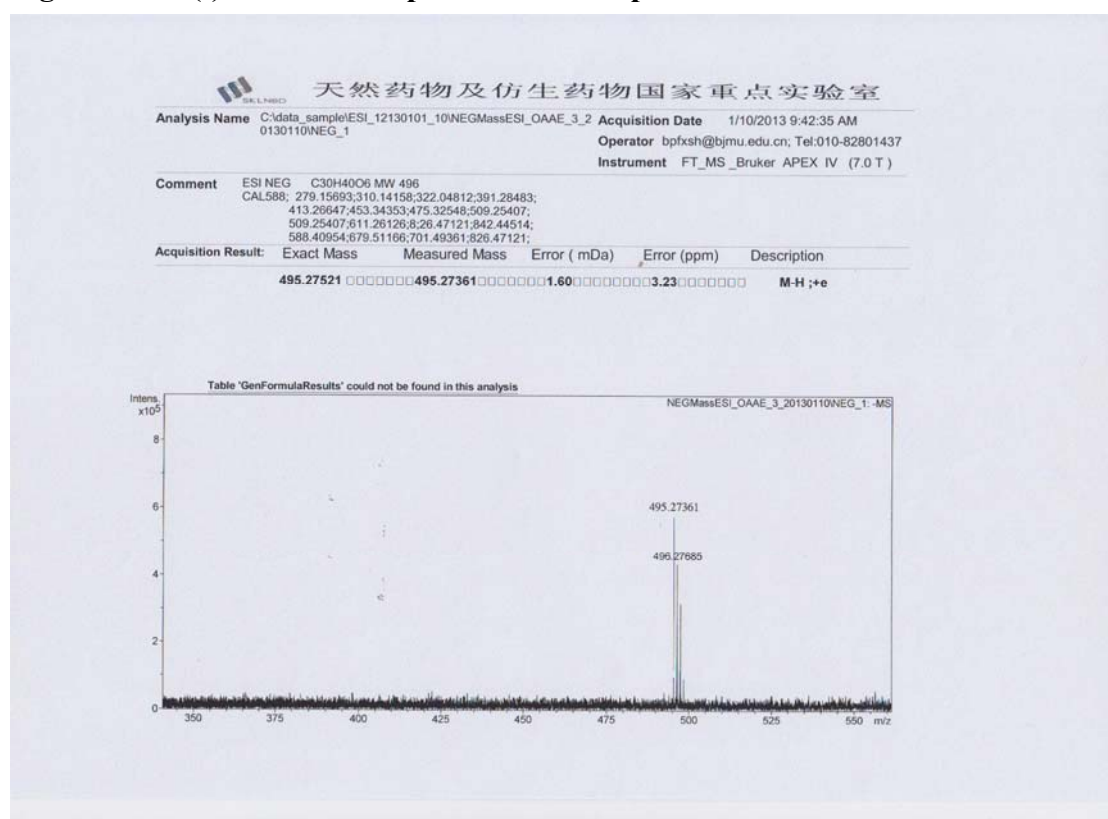
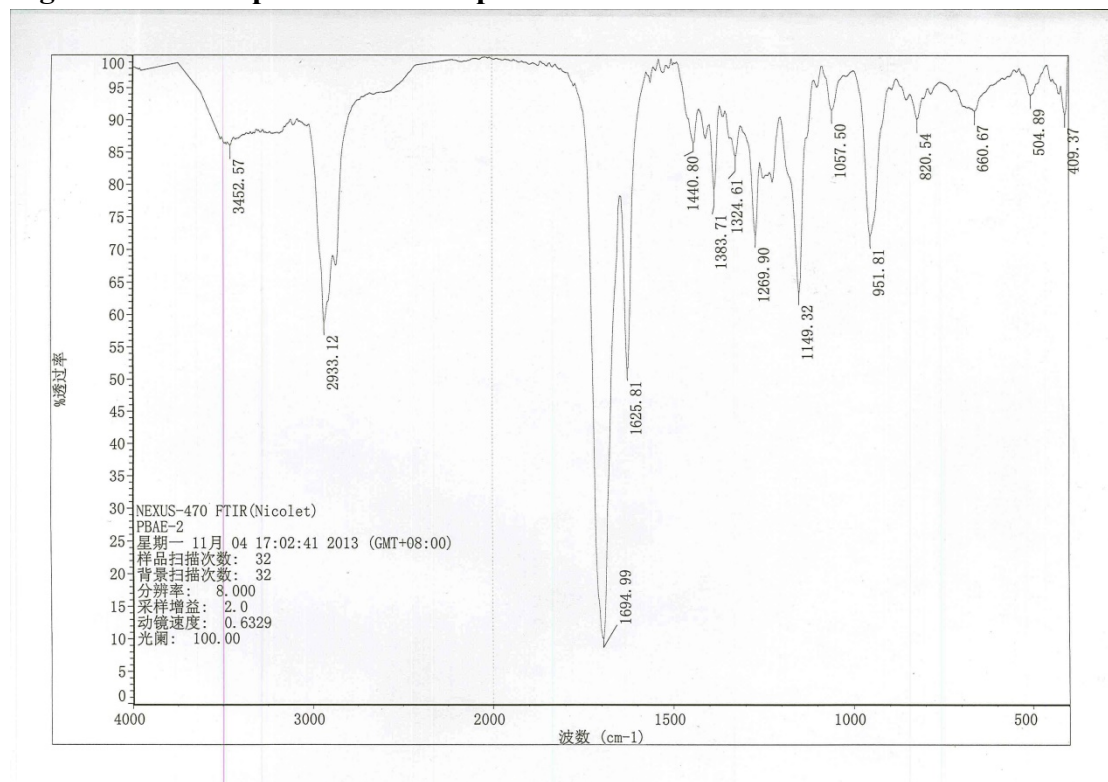


Figure S107. IR Spectrum of Compound 10



¹H NMR spectrum of compound 10a in CDCl₃. The x-axis is chemical shift (delta) in ppm, ranging from 0 to 7.5. The spectrum shows several peaks: a multiplet at ~7.2 ppm (2H), a doublet at ~6.1 ppm (1H), a doublet at ~5.6 ppm (1H), a doublet at ~5.4 ppm (1H), a doublet at ~5.2 ppm (1H), a doublet at ~4.8 ppm (1H), a doublet at ~3.2 ppm (1H), a doublet at ~3.0 ppm (1H), a doublet at ~2.8 ppm (1H), a doublet at ~2.6 ppm (1H), a doublet at ~2.4 ppm (1H), a doublet at ~2.2 ppm (1H), a doublet at ~2.0 ppm (1H), a doublet at ~1.8 ppm (1H), a doublet at ~1.6 ppm (1H), a doublet at ~1.4 ppm (1H), a doublet at ~1.2 ppm (1H), a doublet at ~1.0 ppm (1H), a doublet at ~0.8 ppm (1H), and a doublet at ~0.6 ppm (1H). Integration values are shown below the peaks: 2.18, 1.00, 1.02, 1.02, 1.03, 1.06, 1.11, 1.25, 1.13, 2.01, 1.21, 1.31, 2.64, 2.52, 1.63, 3.00, 3.12, 3.68, 3.29, 3.18.

13C NMR spectrum of compound 10a in CDCl₃. The x-axis represents the chemical shift in ppm, ranging from -10 to 230. The spectrum shows a triplet for the solvent CDCl₃ at 77.0 ppm. Numerous peaks are visible in the aliphatic region (10-40 ppm) and the carbonyl region (118-178 ppm). Peaks are labeled with their chemical shifts: 178.22, 170.46, 167.45, 148.13, 147.42, 143.22, 138.44, 124.06, 123.41, 118.10, 76.73, 74.53, 47.32, 42.34, 41.60, 40.48, 39.41, 39.27, 37.68, 36.97, 36.69, 35.00, 32.86, 30.13, 27.64, 21.40, 16.68, 12.36, 7.90, and 210.94.

Figure S110. DEPT-135 Spectrum of Compound 10

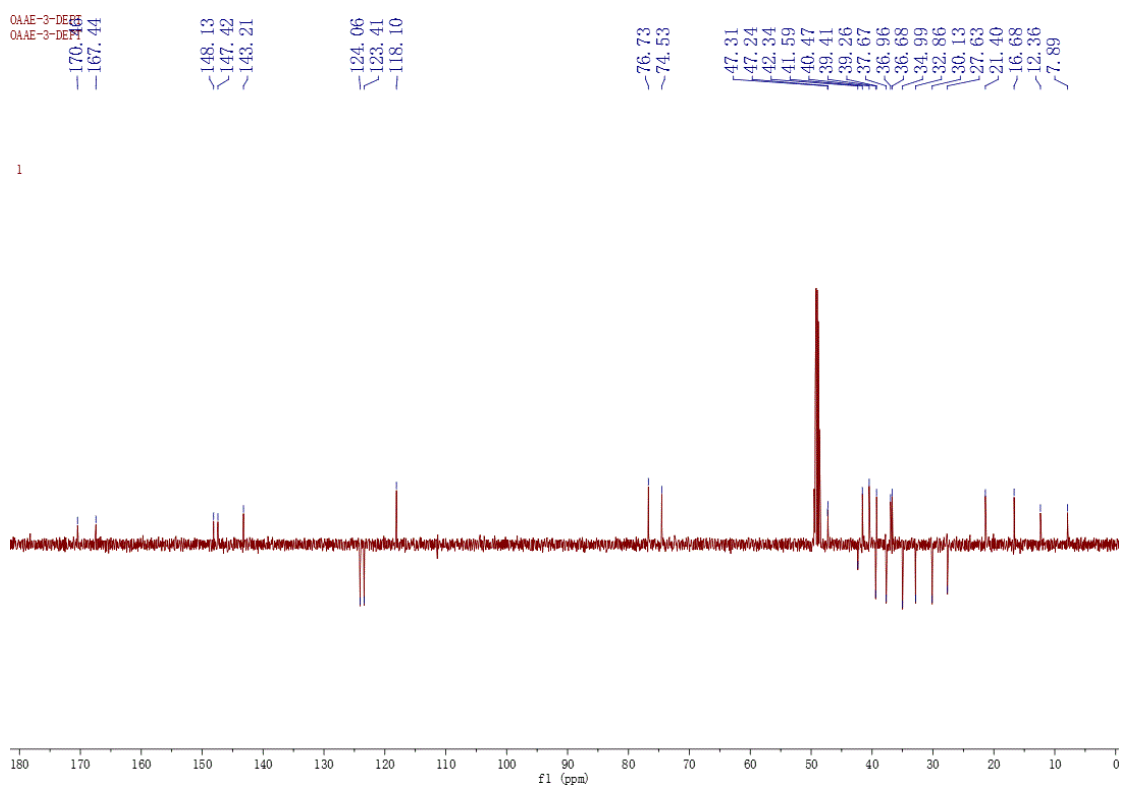


Figure S111. ^1H - ^1H gCOSY Spectrum of Compound 10

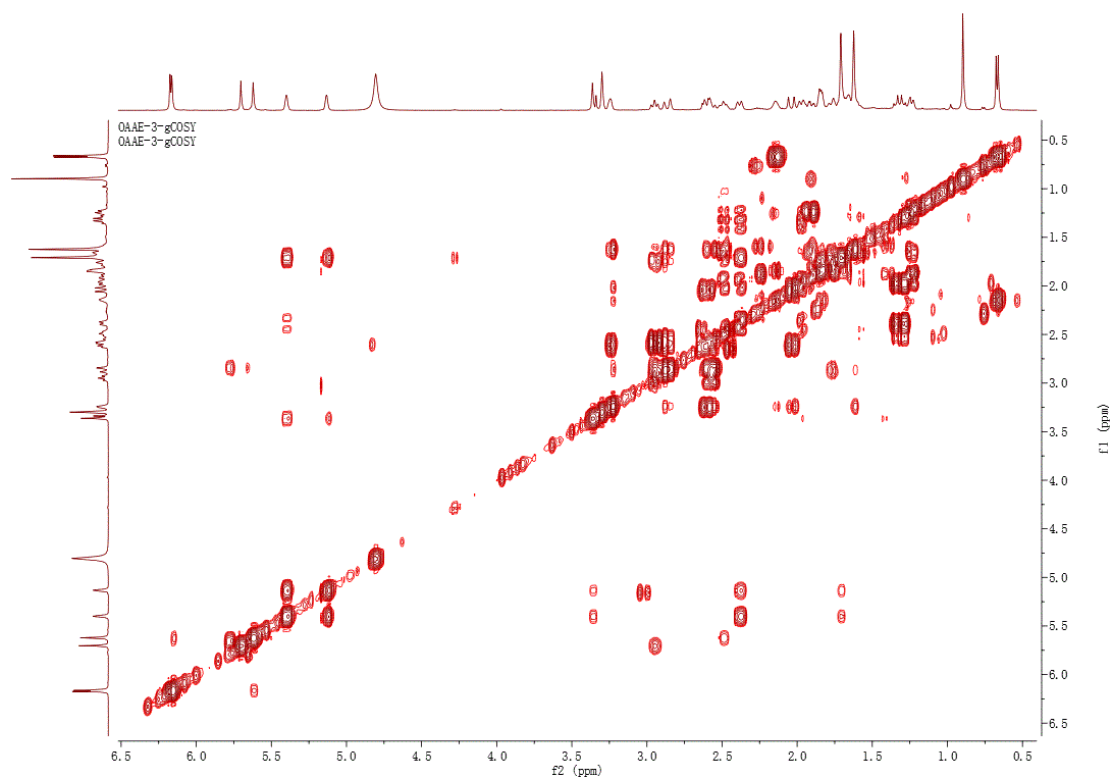


Figure S112. Multiplicity-edited gHSQC Spectrum of Compound 10

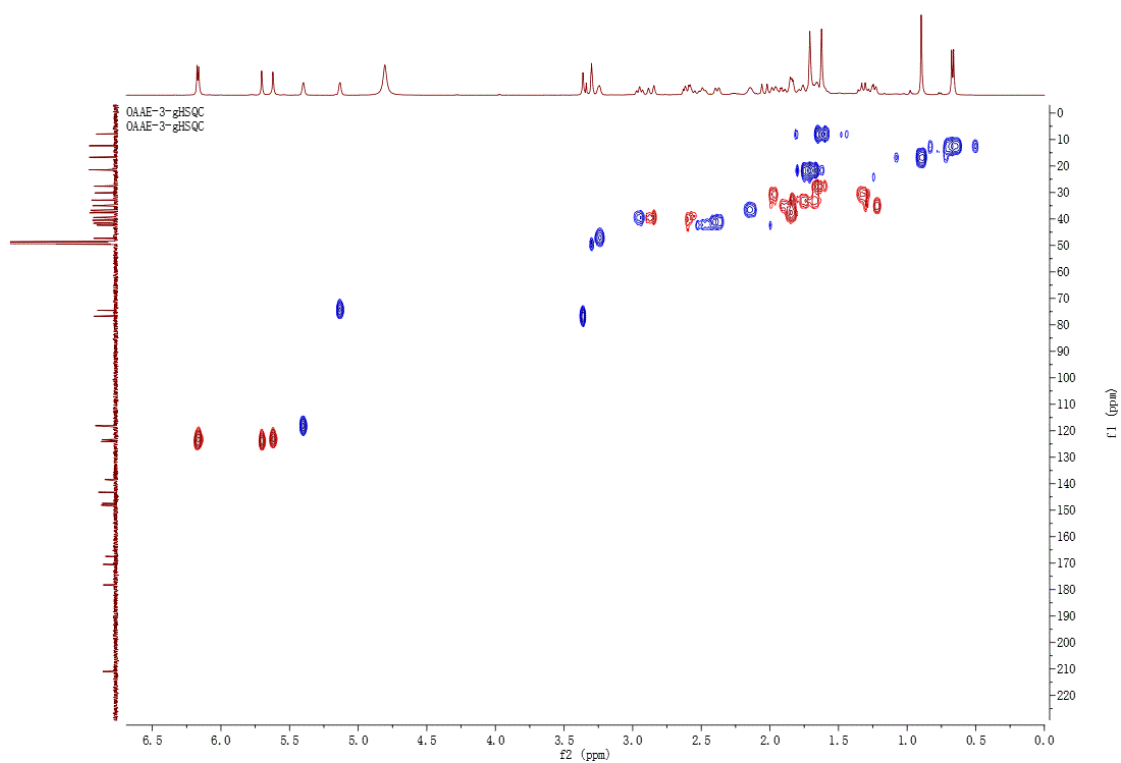


Figure S113. gHMBC Spectrum of Compound 10

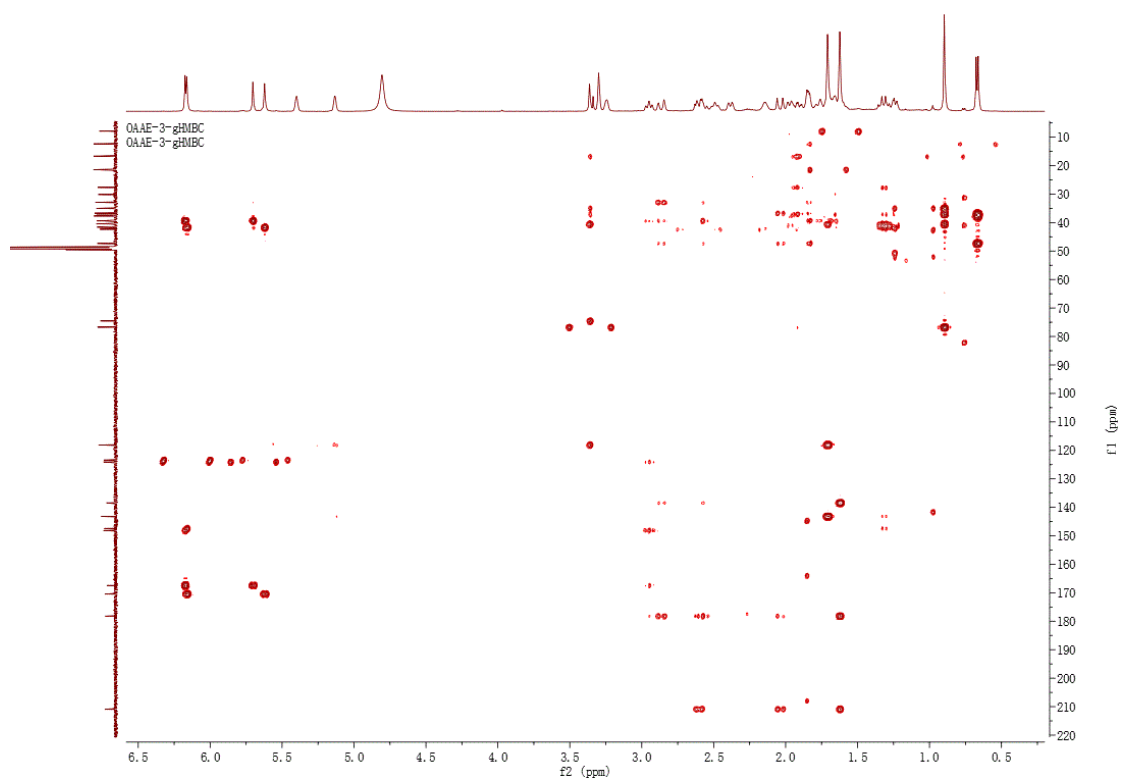


Figure S114. NOESY Spectra of Compound 10

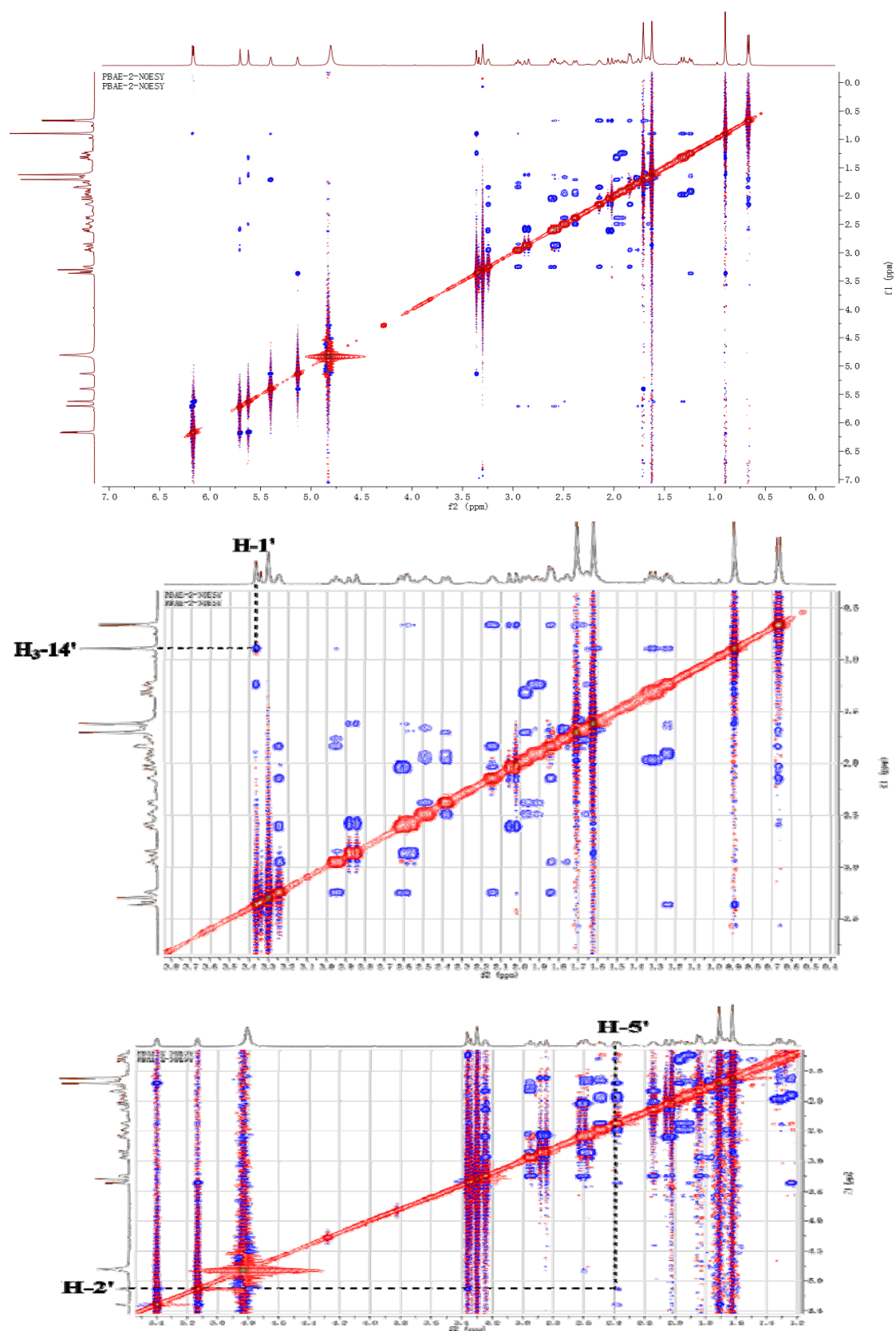


Figure S115. The Stable Conformers of Compound 10

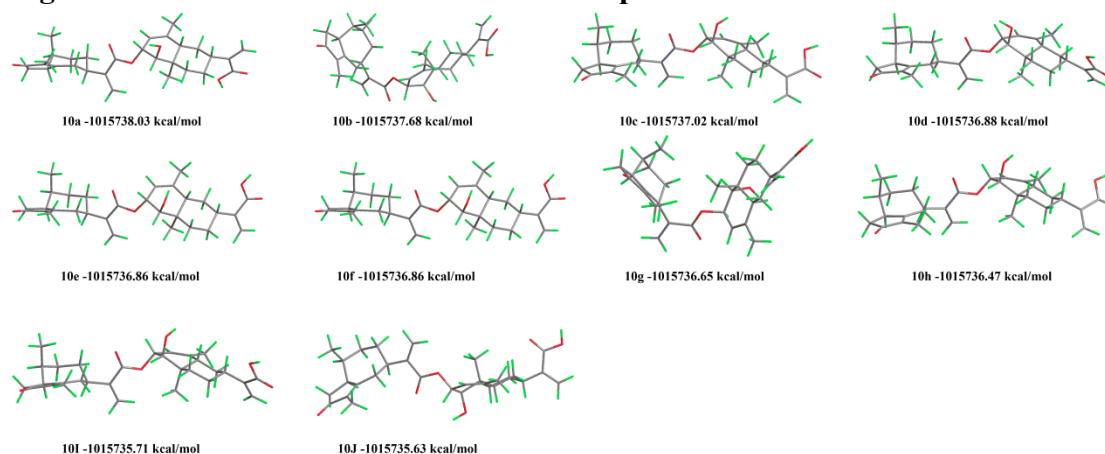


Table S14. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of **10**

conf	$\Delta E_{6-31+G(d)}$ ^a	% ^b
10a	0	42.2
10b	0.35	23.5
10c	1.01	7.6
10d	1.15	6.1
10e	1.16	5.9
10f	1.16	5.9
10g	1.38	4.1
10h	1.56	3.2
10i	2.31	0.8
10j	2.39	0.7

^aRelative to 10a with $E_{6-31+G(d)} = -1015738.03$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S116. Comparison of Experimental and Calculated ECD Spectra of **10**

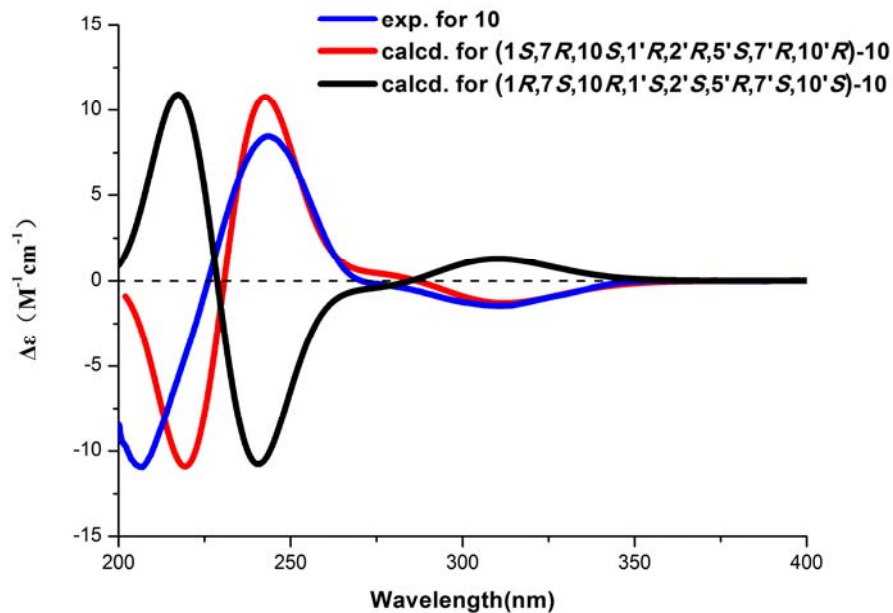


Figure S117. (+)-HRESIMS Spectrum of Compound **11**

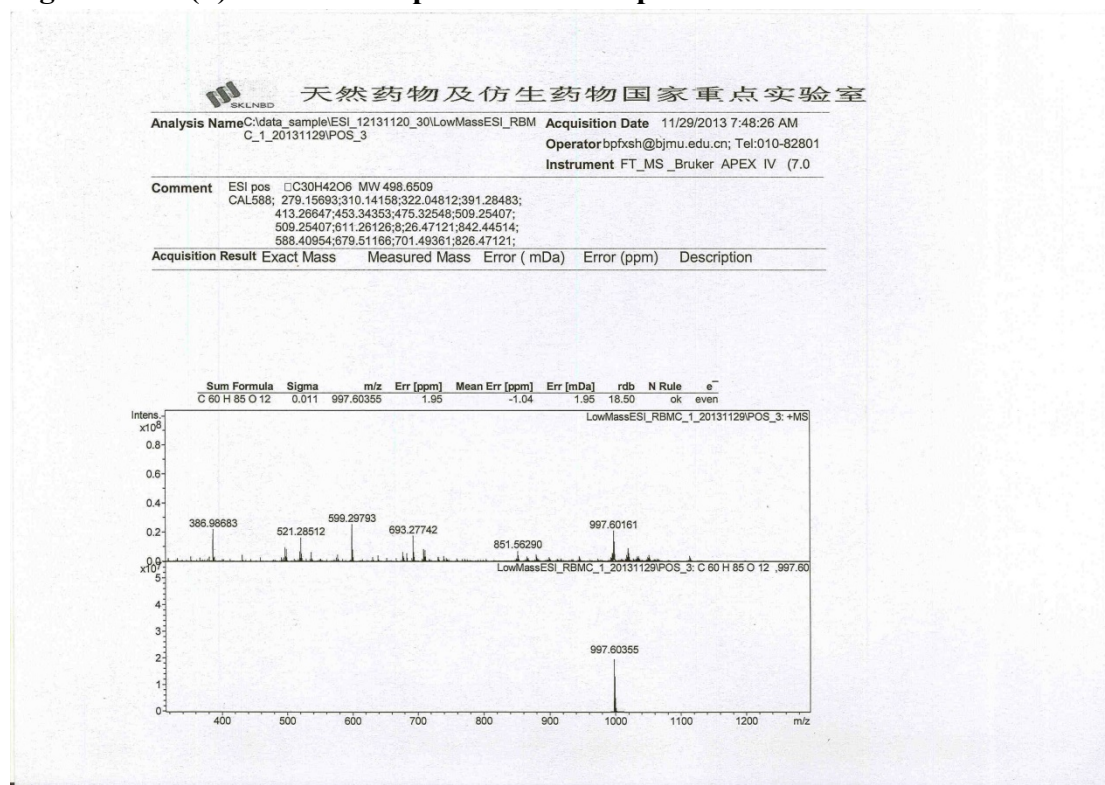


Figure S118. IR Spectrum of Compound 11

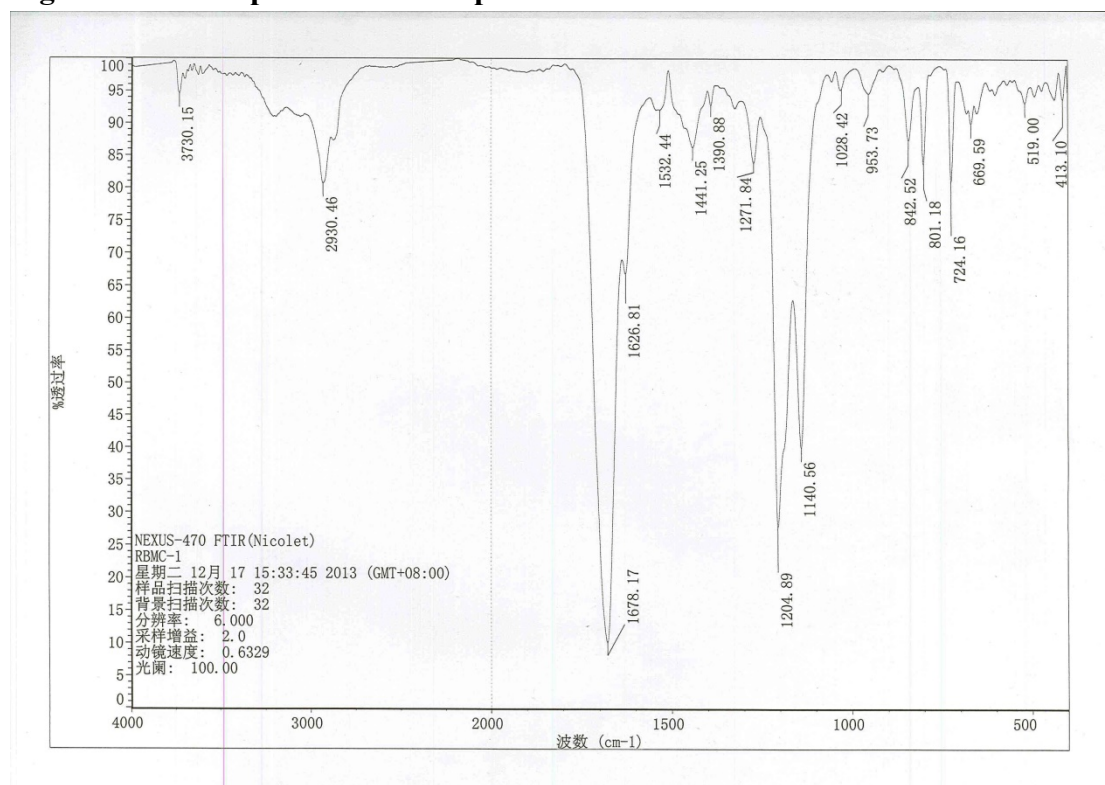


Figure S119. ¹H-NMR Spectrum of Compound 11 (500 MHz, CD₃OD)

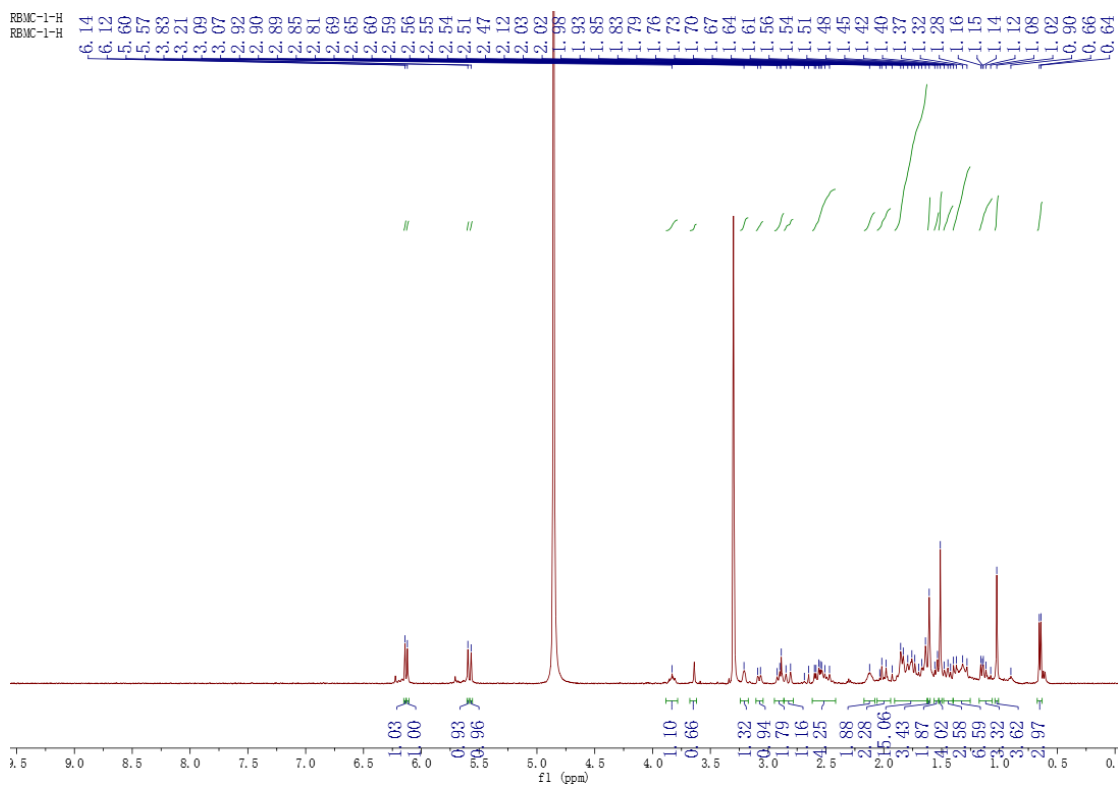


Figure S120. ^{13}C -NMR Spectrum of Compound 11 (125 MHz, CD_3OD)

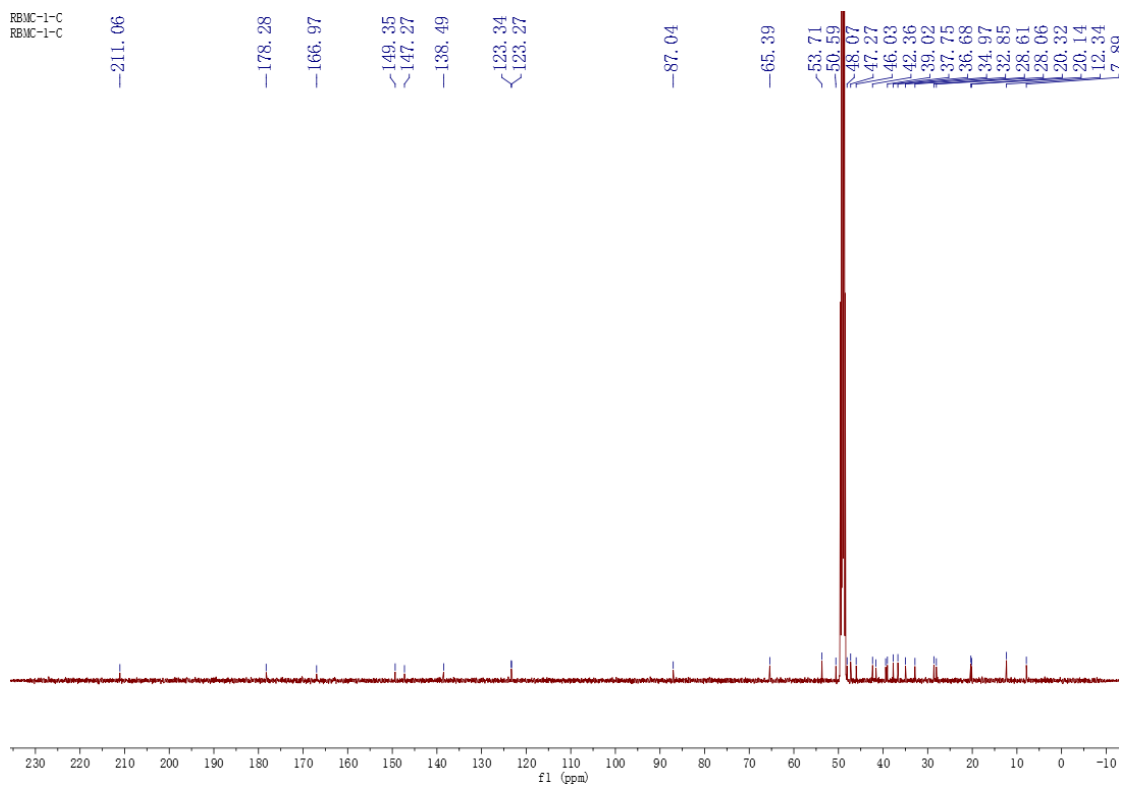


Figure S121. ^1H - ^1H gCOSY Spectrum of Compound 11

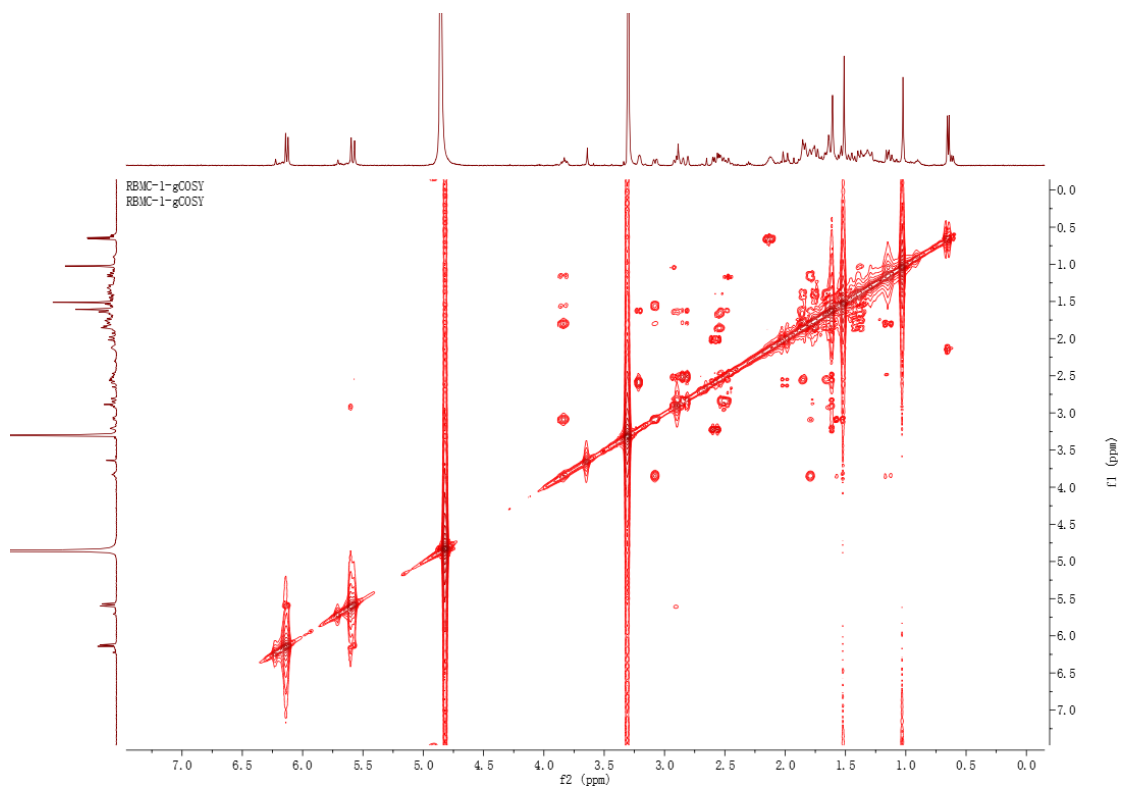


Figure S122. Multiplicity-edited gHSQC Spectrum of Compound 11

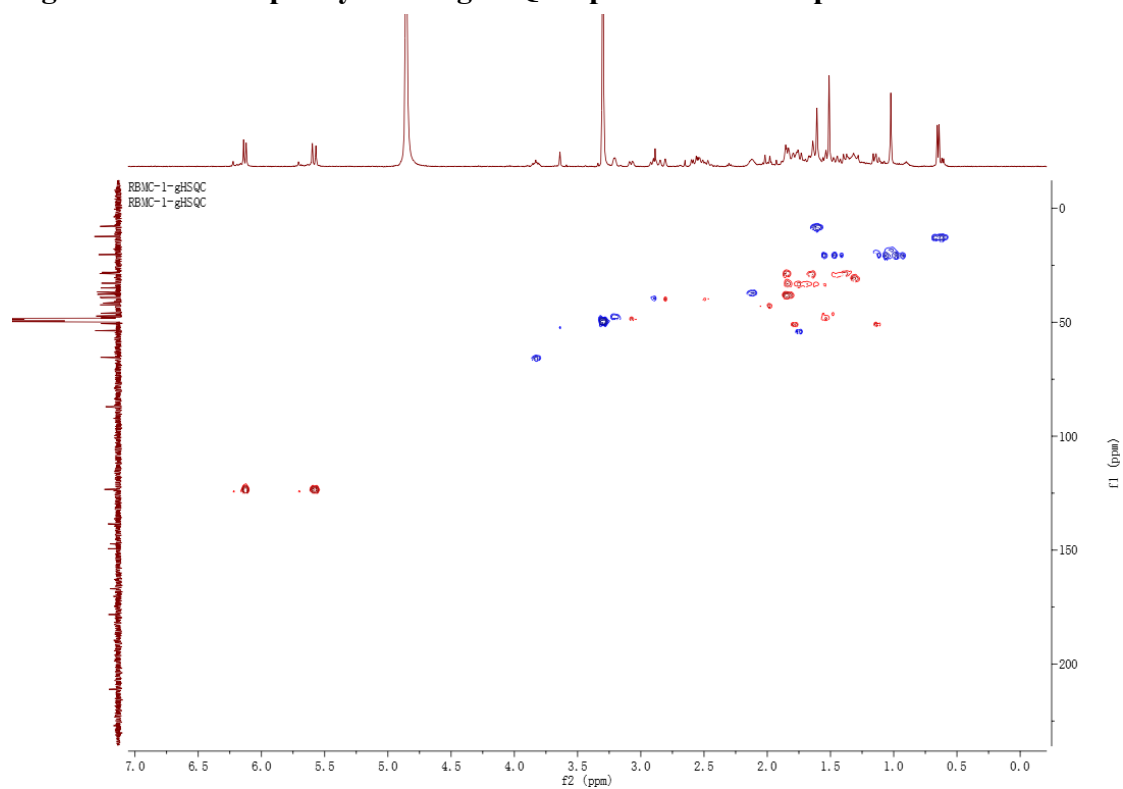


Figure S123. gHMBC Spectrum of Compound 11

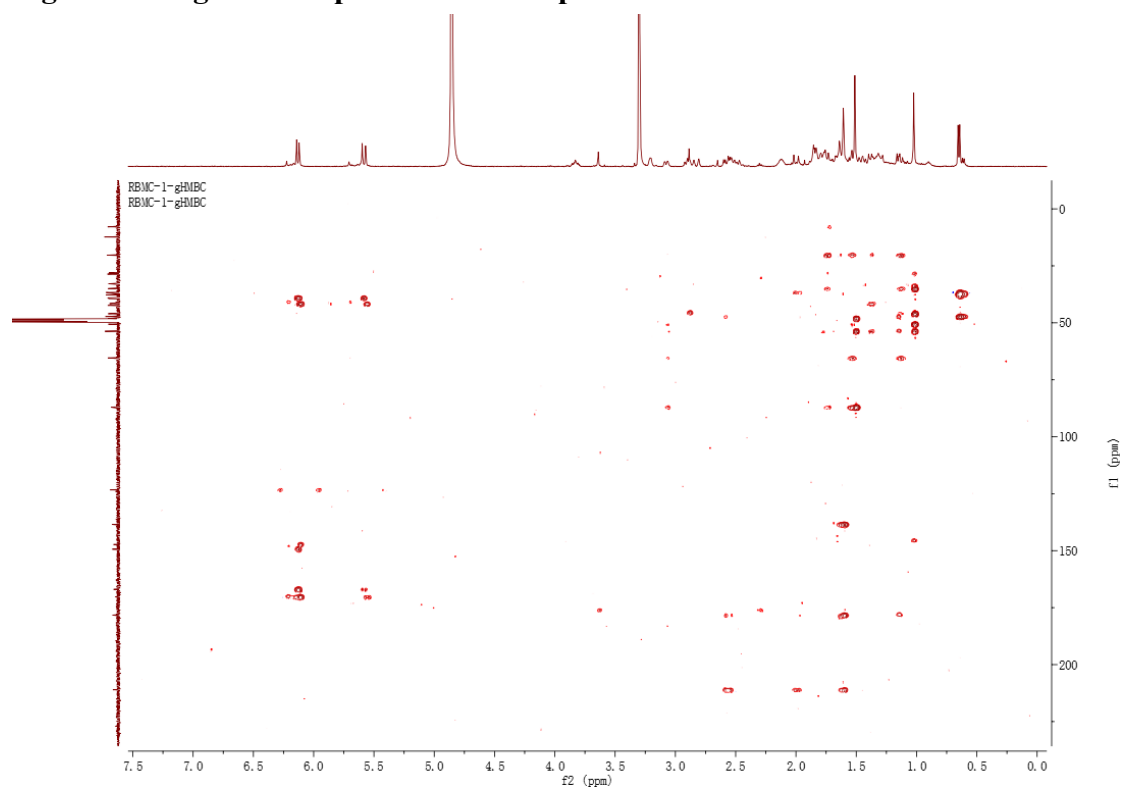


Figure S124. NOESY Spectra of Compound 11

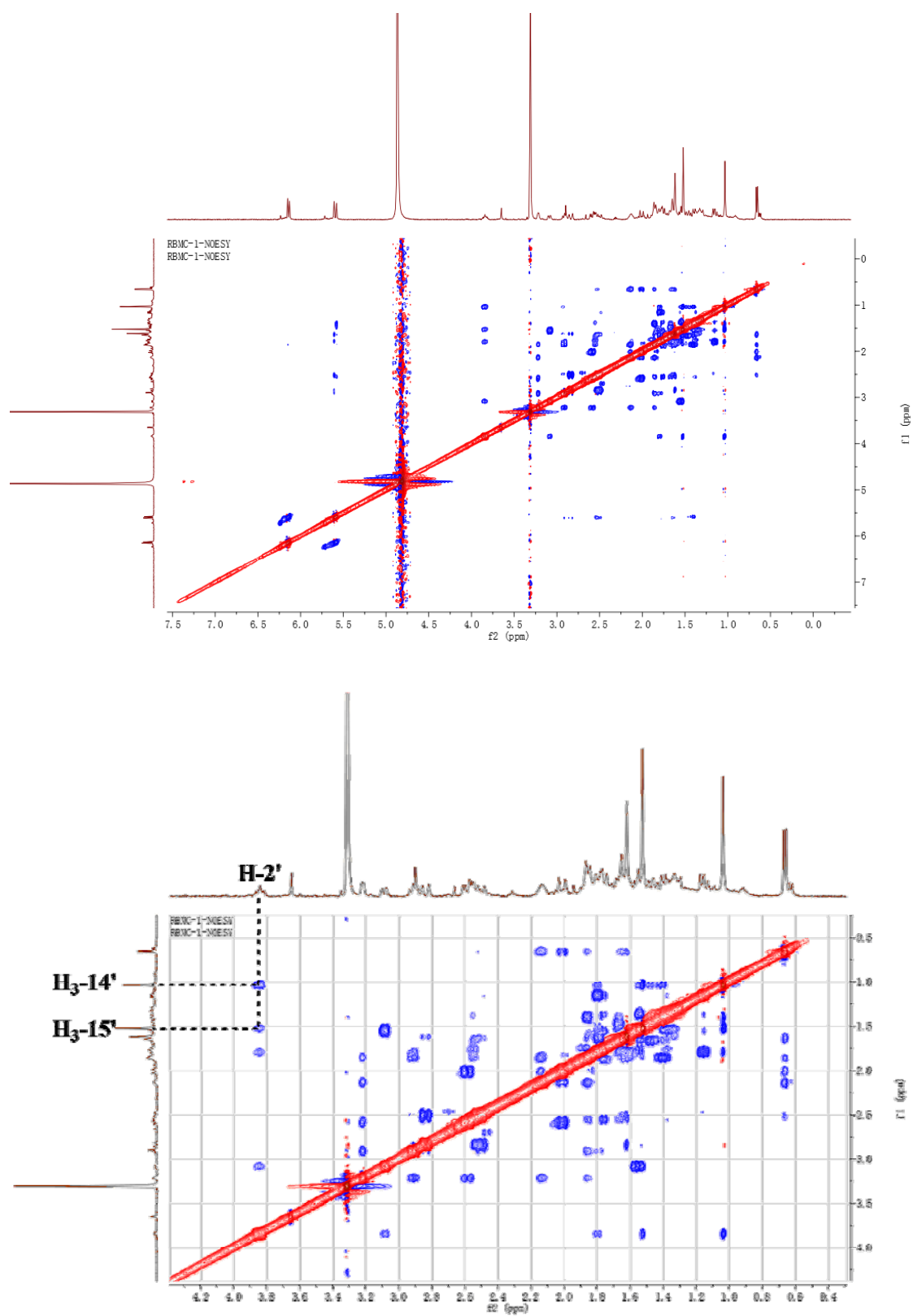


Figure S125. The Stable Conformers of Compound 11

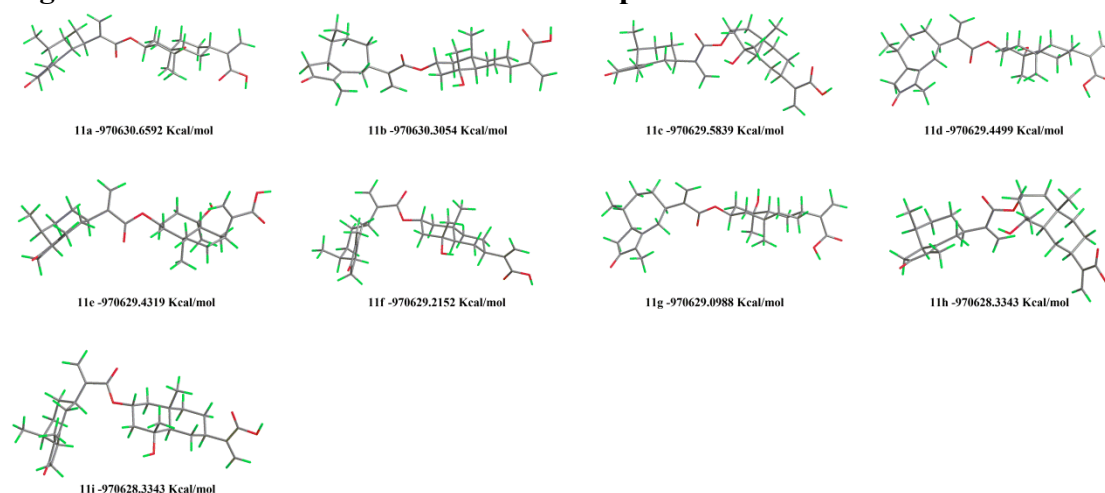


Table S15. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of **11**

conf	$\Delta E_{6-31+G(d)}$ ^a	% ^b
11a	0	46.2
11b	0.35	25.4
11c	1.07	7.5
11d	1.21	6.0
11e	1.23	5.9
11f	1.44	4.0
11g	1.56	3.3
11h	2.32	0.9
11i	2.40	0.8

^aRelative to 11a with $E_{6-31+G(d)} = -970630.66$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S126. Comparison of Experimental and Calculated ECD Spectra of **11**

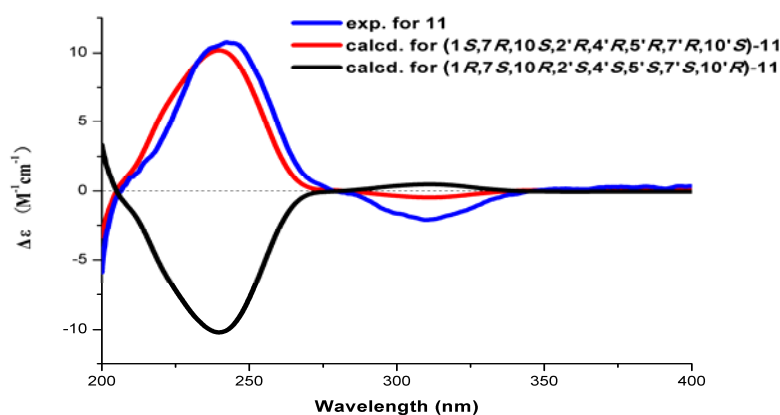


Figure S127. (+)-HRESIMS Spectrum of Compound 12

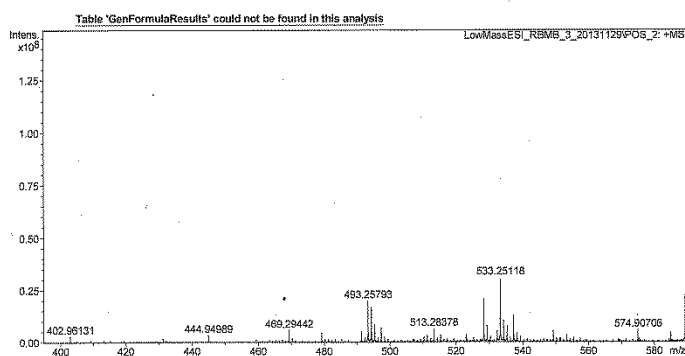


Figure S128. IR Spectrum of Compound 12

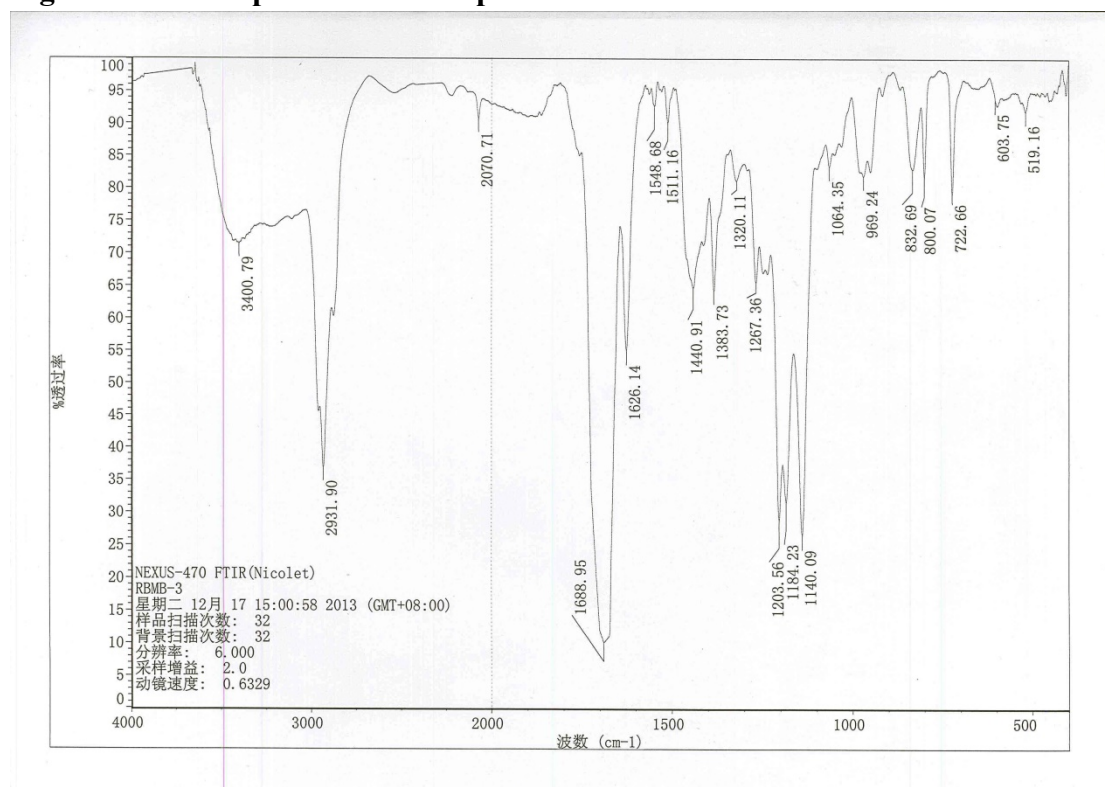


Figure S129. ^1H -NMR Spectrum of Compound 12 (500 MHz, CD_3OD)

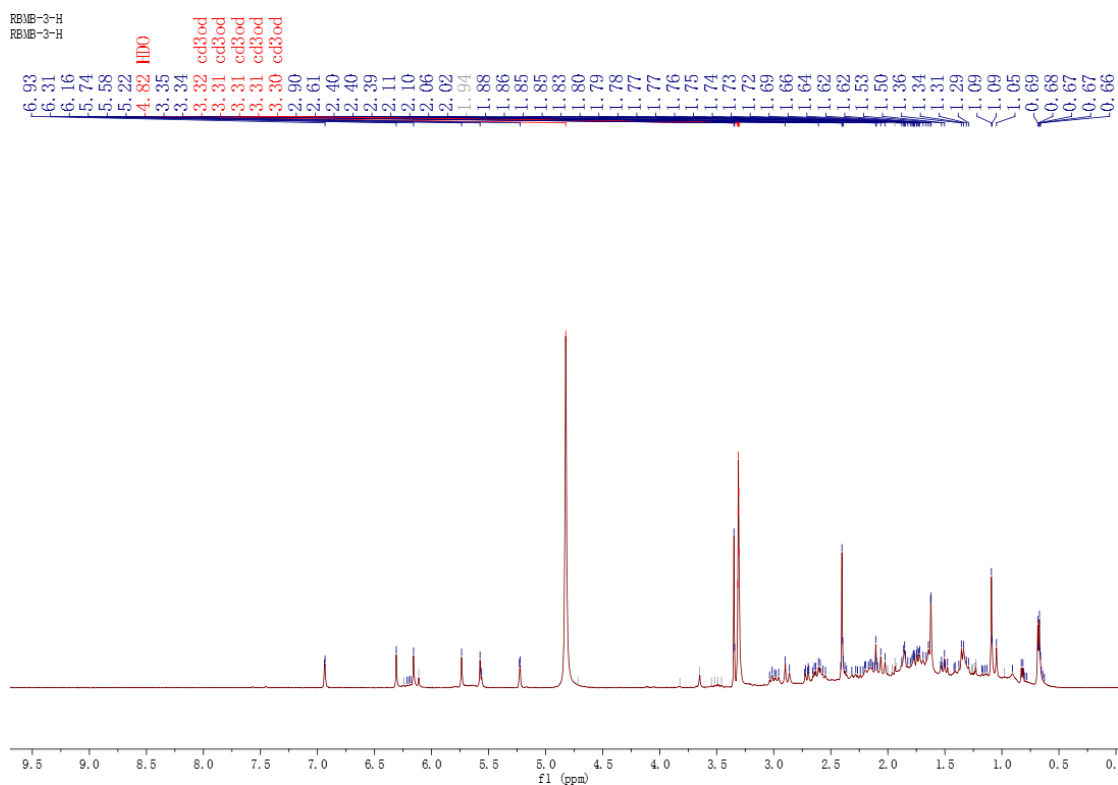
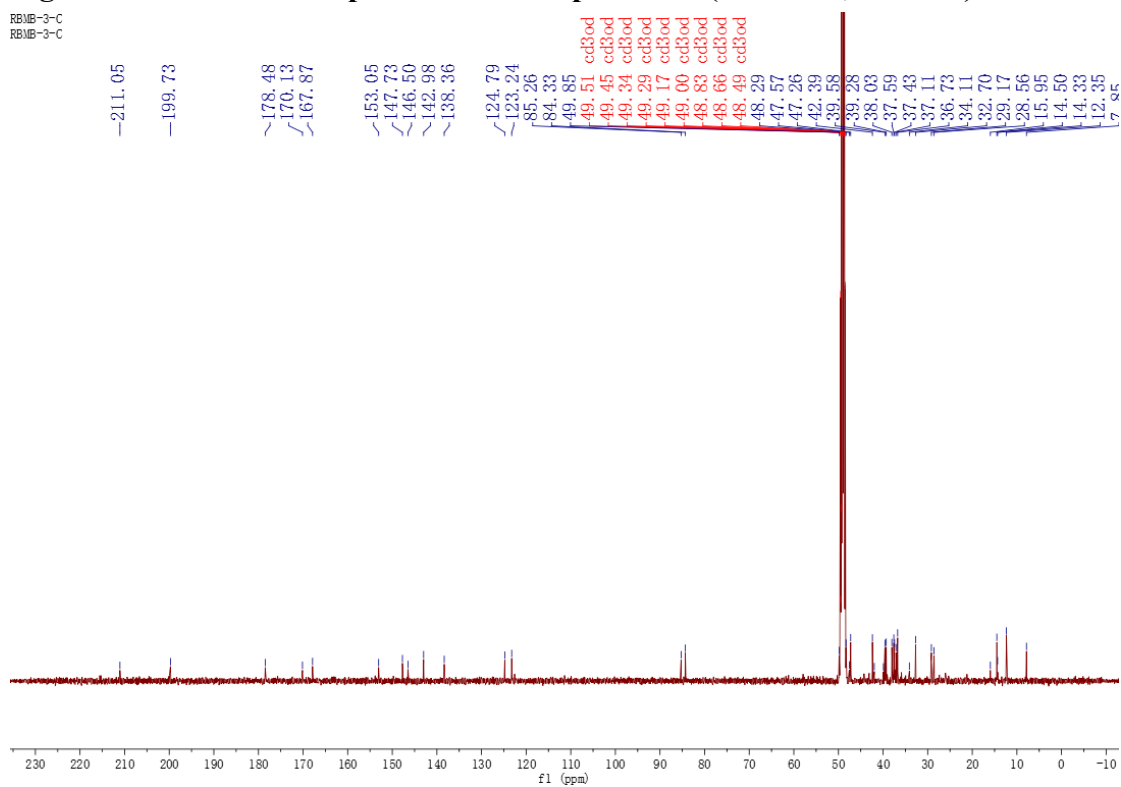


Figure S130. ^{13}C -NMR Spectrum of Compound 12 (125 MHz, CD_3OD)



RBMB-3-DEPT135
RBMB-3-DEPT135

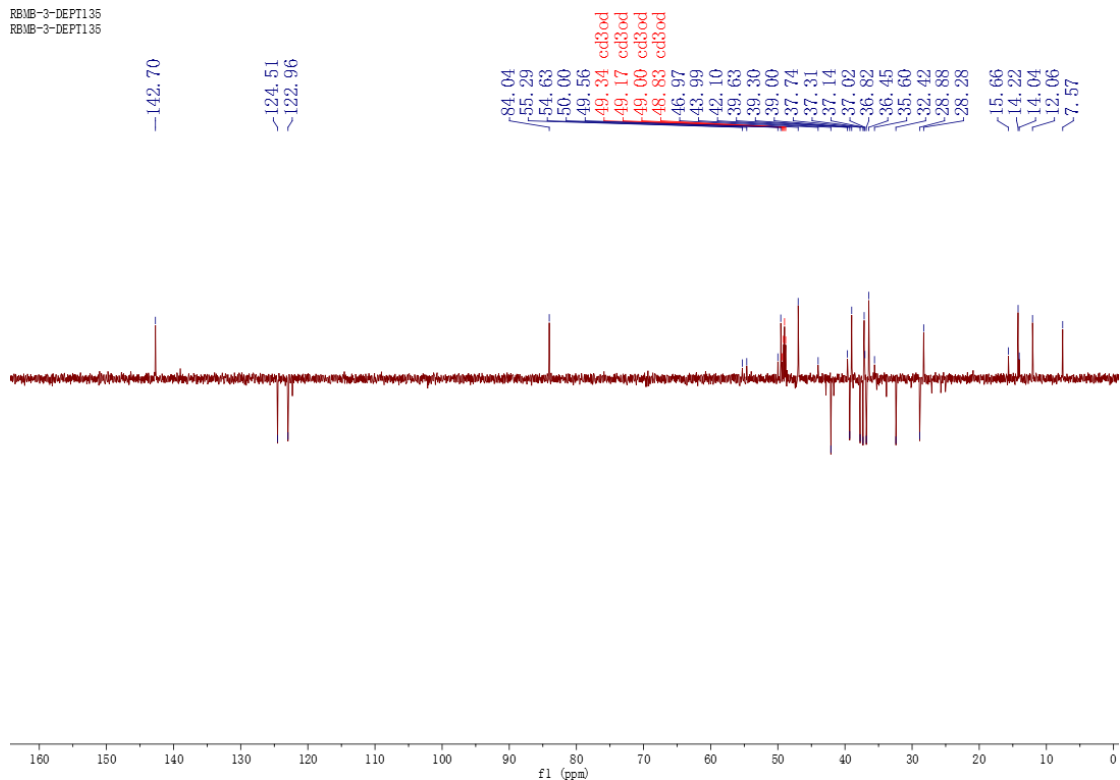
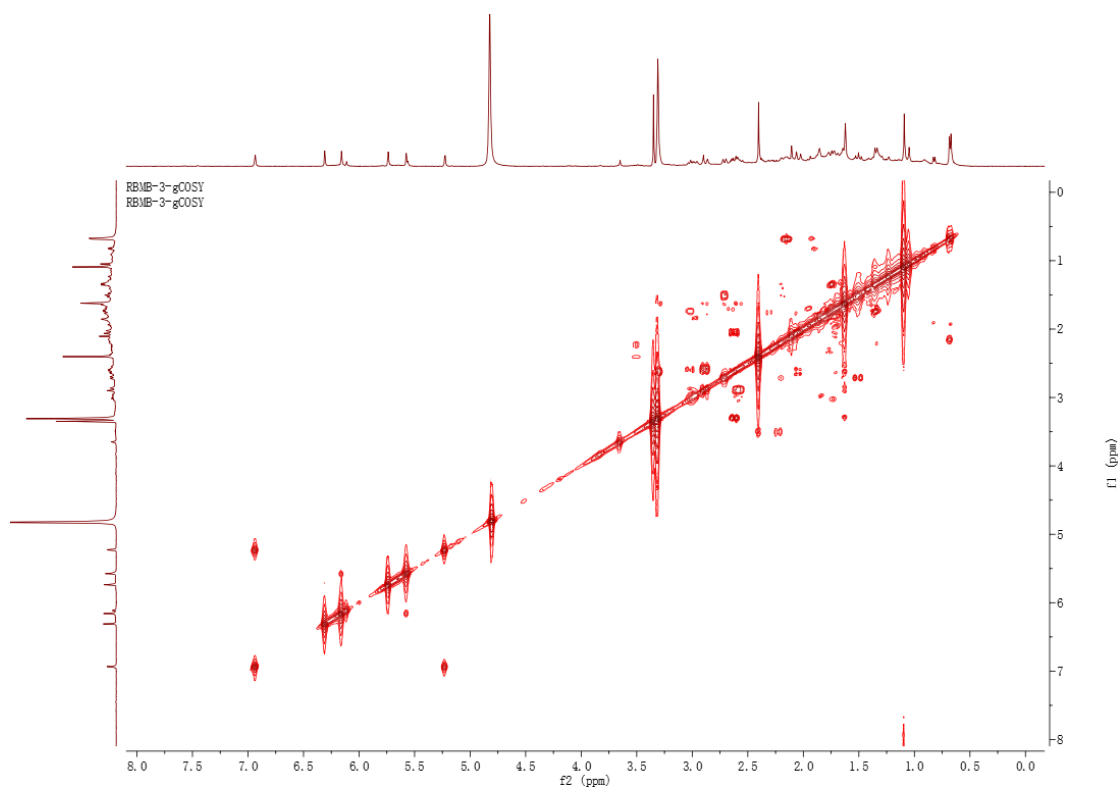
RBMB-3-gCOSY
RBMB-3-gCOSY

Figure S133. Multiplicity-edited gHSQC Spectrum of Compound 12

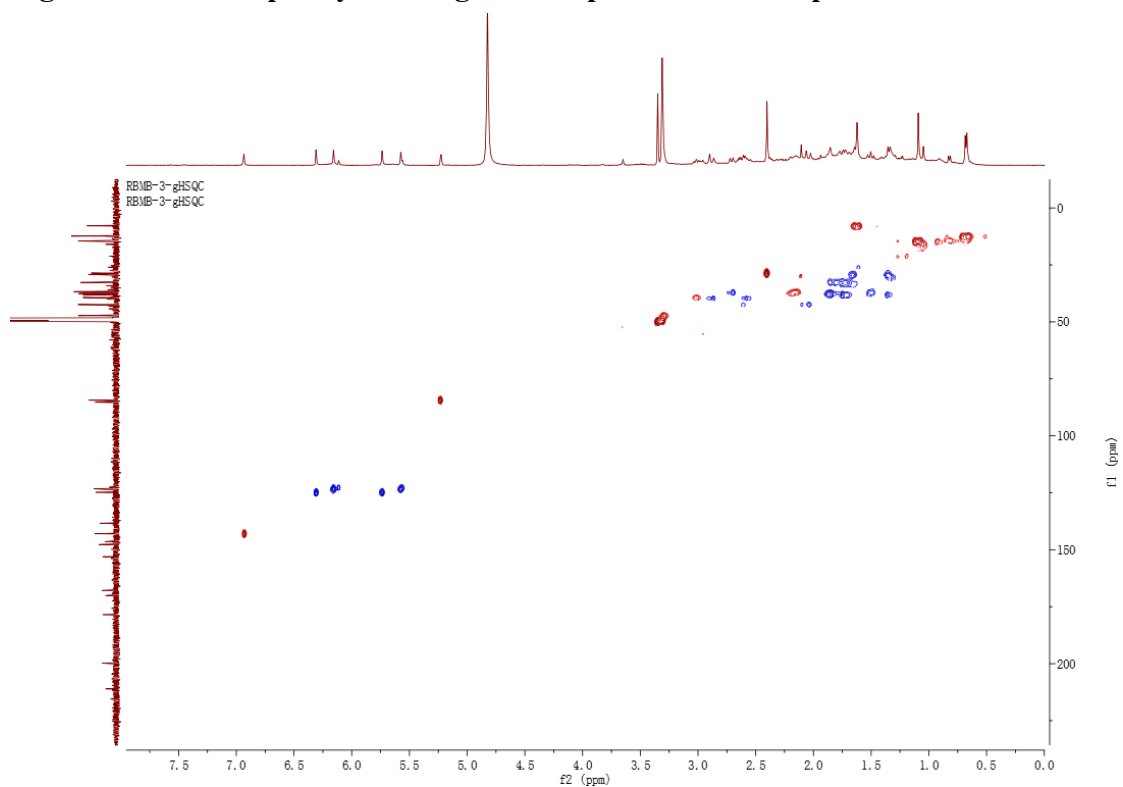


Figure S134. gHMBC Spectrum of Compound 12

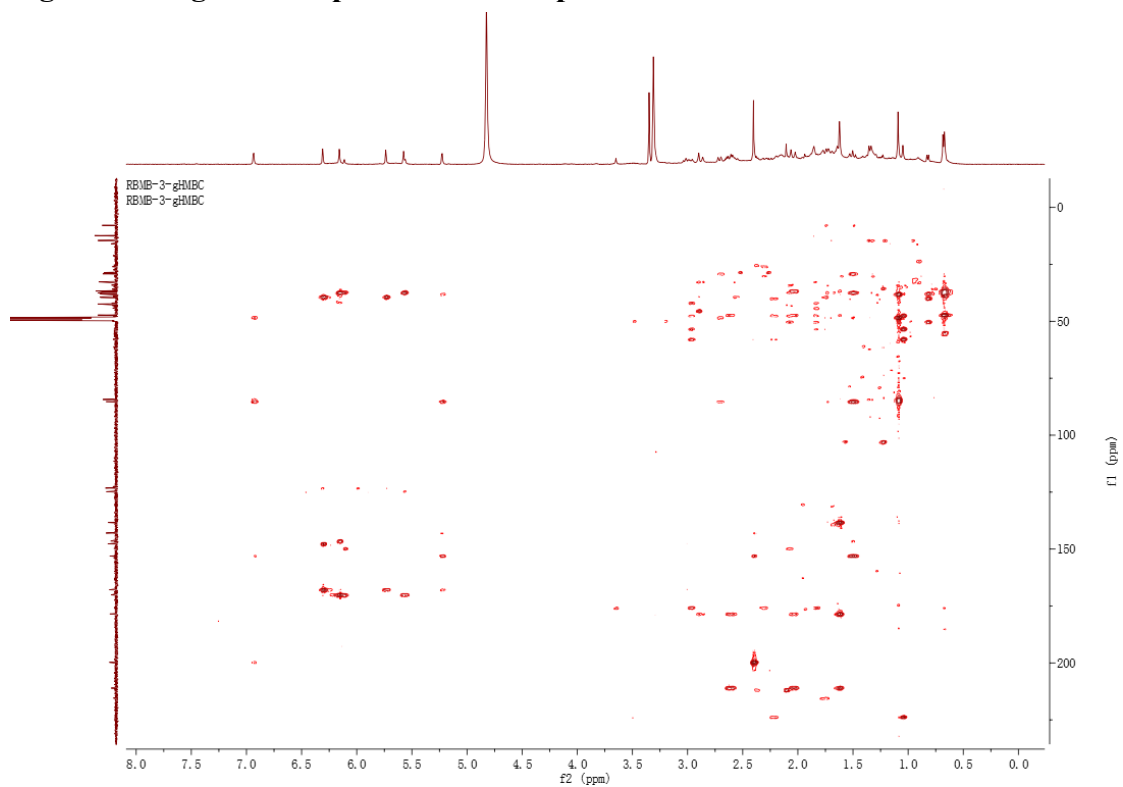


Figure S135. NOESY Spectra of Compound 12

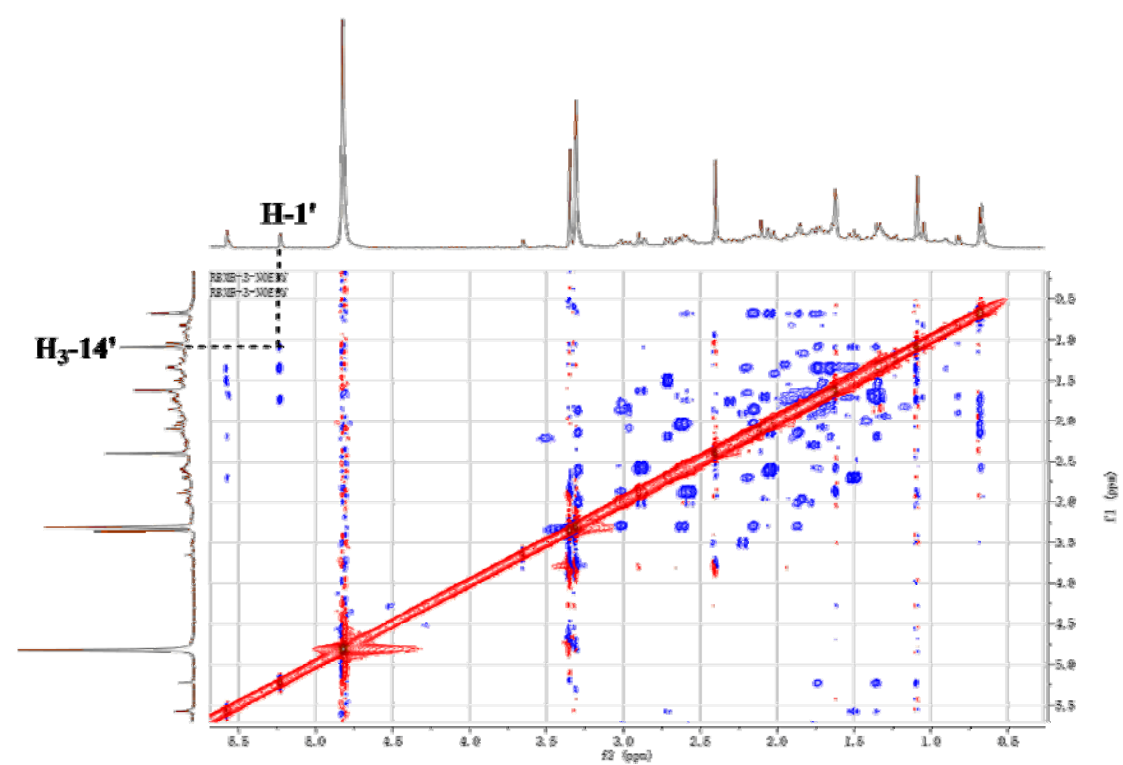
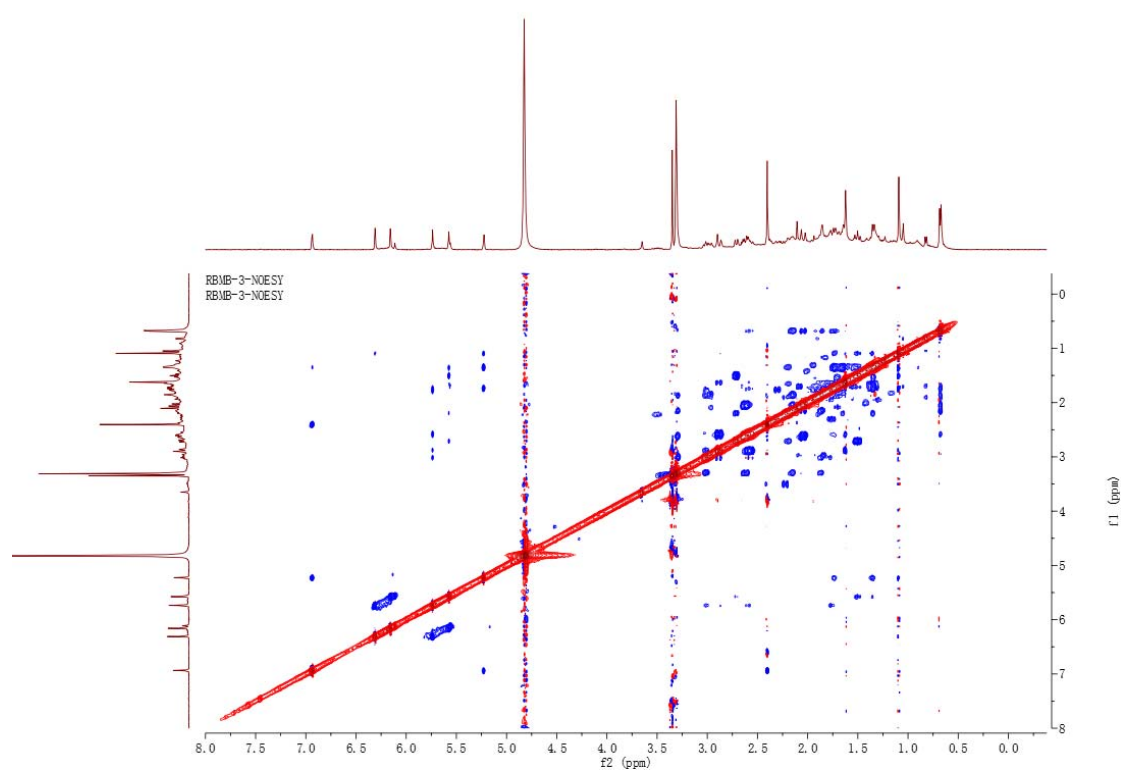


Figure S136. The Stable Conformers of Compound 12

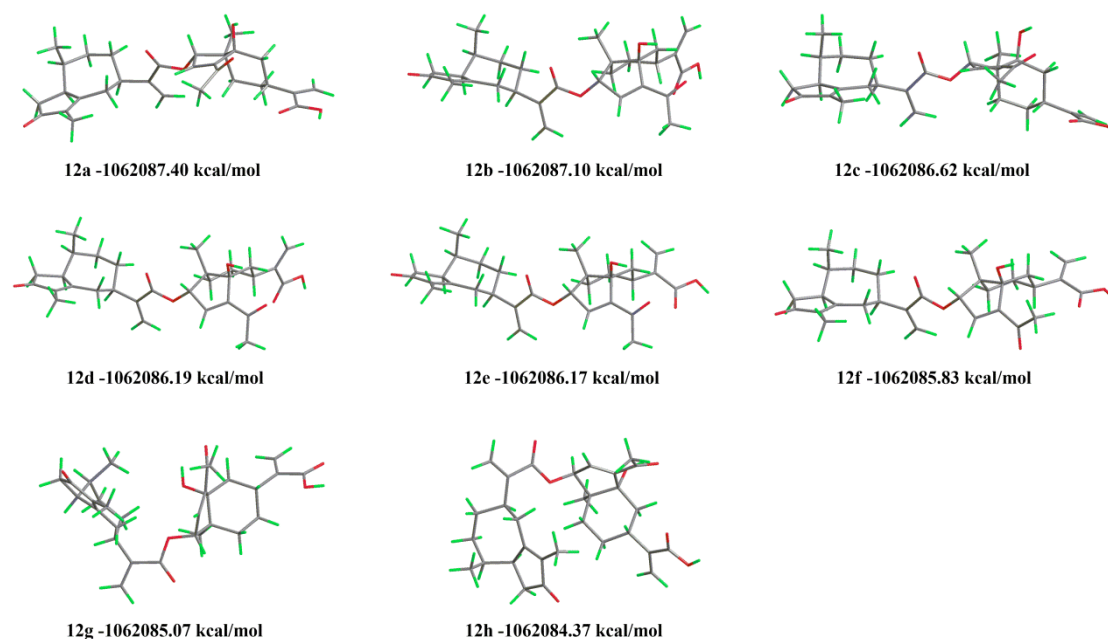


Table S16. B3LYP-Calculated Relative Energies (kcal/mol) and Conformational Population (%) for the Most Stable Conformers of **12**

conf	$\Delta E_{6-31+G(d)}^a$	% ^b
12a	0	44.7
12b	0.29	27.4
12c	0.77	12.1
12d	1.21	5.8
12e	1.23	5.6
12f	1.56	3.2
12g	2.32	0.9
12h	3.02	0.3

^aRelative to 12a with $E_{6-31+G(d)} = -1062087.40$ kcal/mol. ^bCalculated using free energy values from Gaussian 03W according to $\Delta G = -RT \ln K$.

Figure S137. Comparison of Experimental and Calculated ECD Spectra of 12

