Supporting Information for

Anti-inflammatory Dimeric 2-(2-Phenylethyl)chromones from the Resinous Wood of *Aquilaria sinensis*

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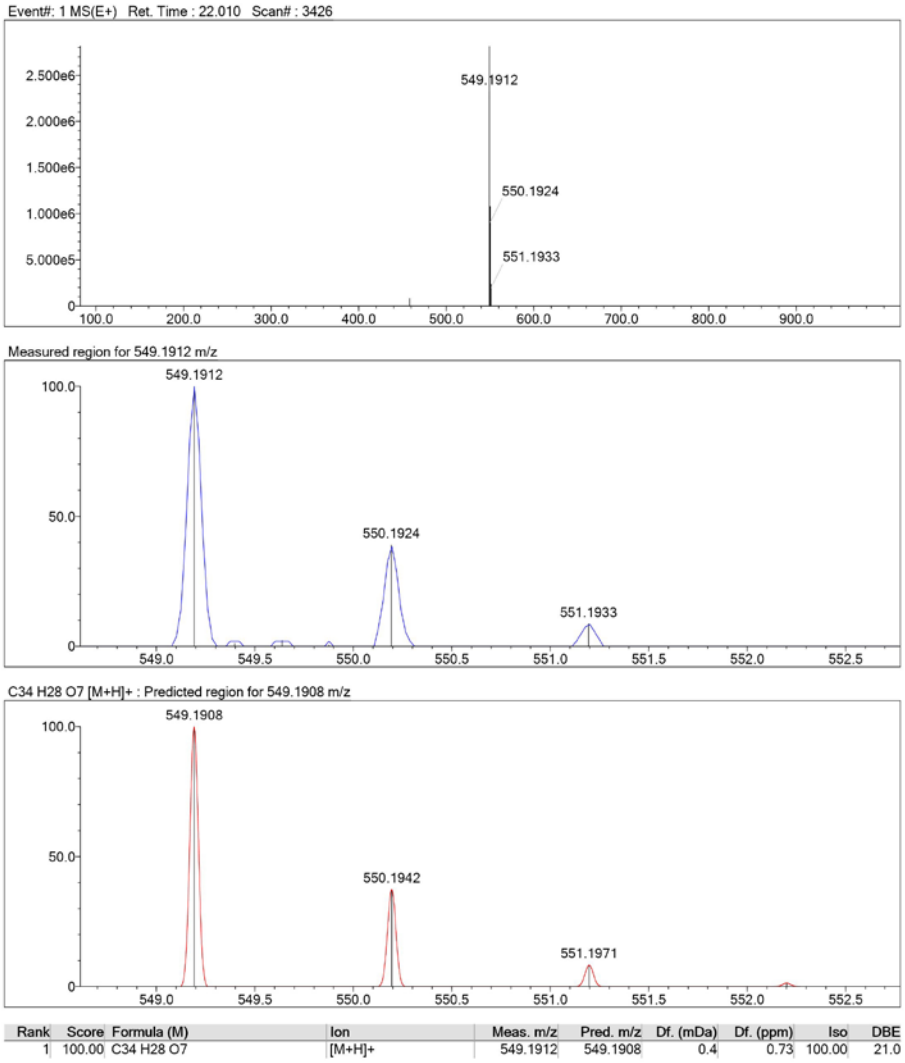
1. MS, UV, IR, and NMR Spectra of New Compounds



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	100.00	C34 H28 O7	[M+H]+	549.1912	549.1908	0.4	0.73	100.00	21.0

Figure S1. HRESIMS spectrum of compound **1**

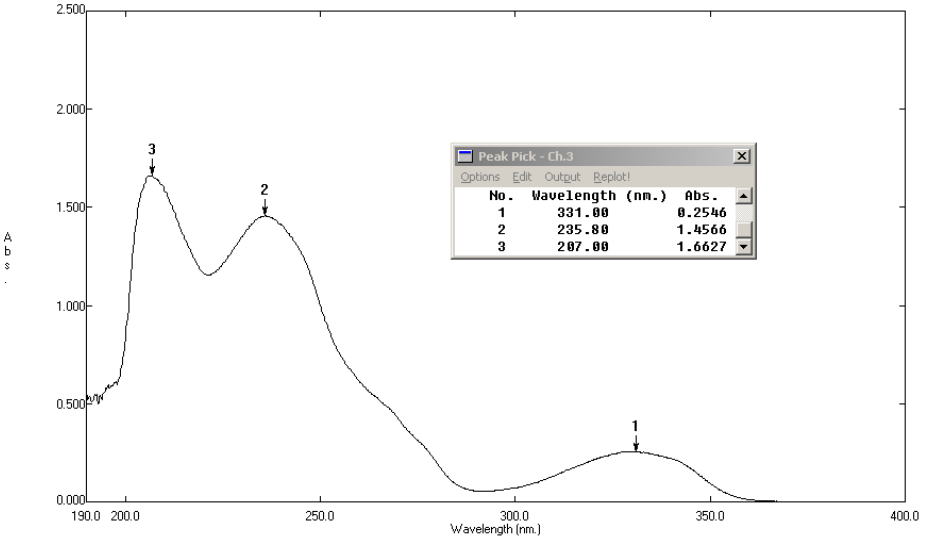


Figure S2. UV spectrum of compound **1**

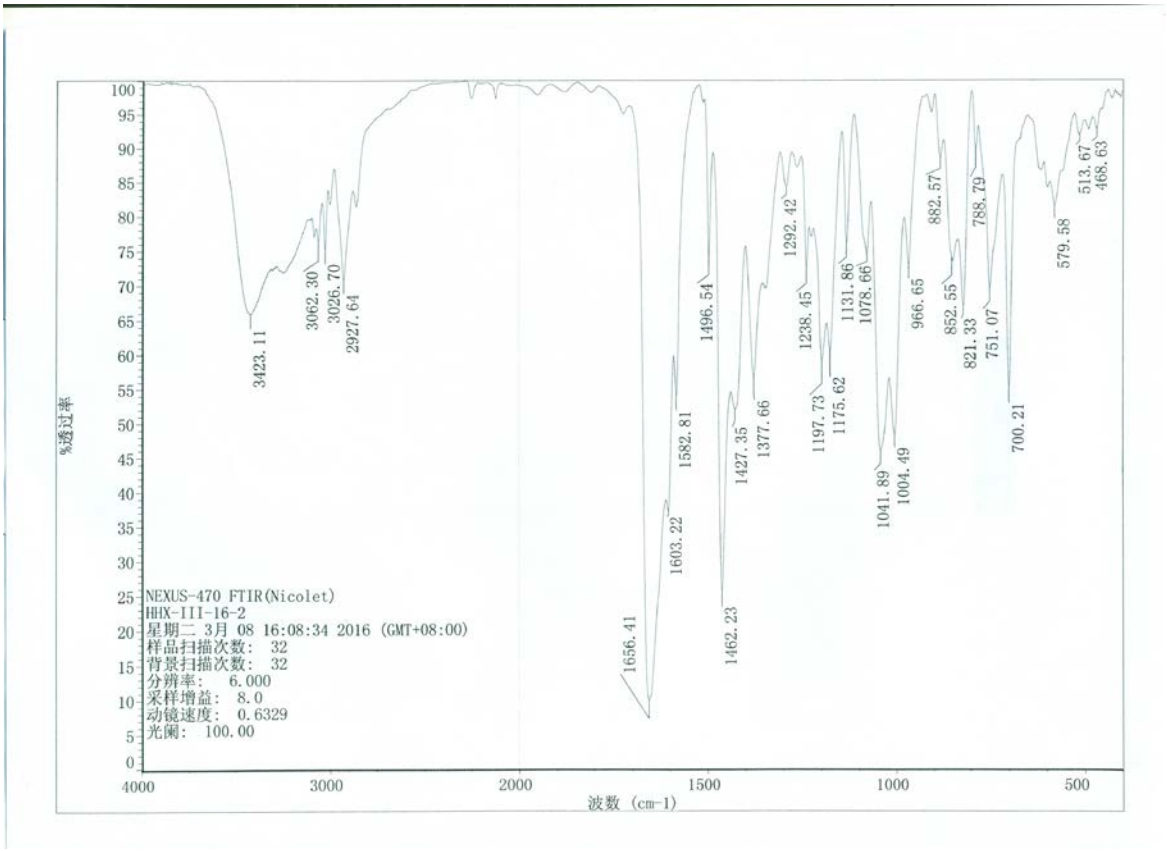


Figure S3. IR spectrum of compound **1**

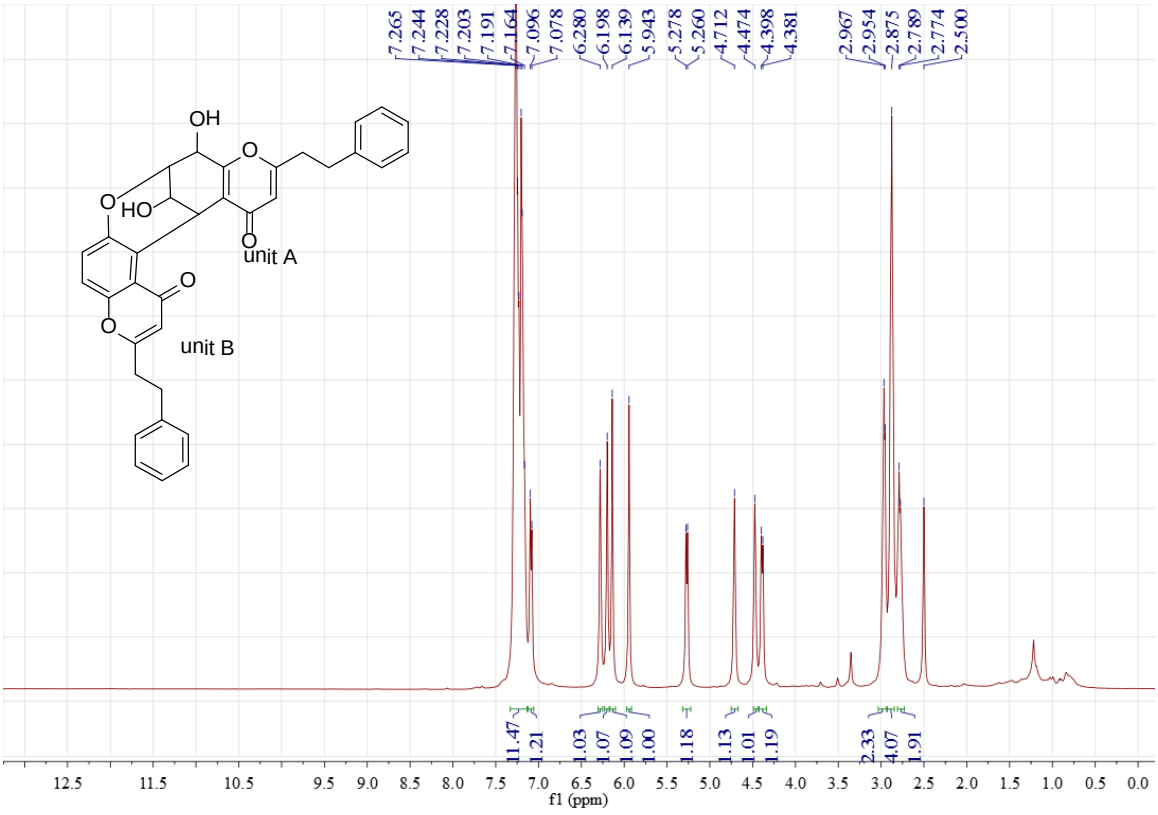


Figure S4. ^{1}H NMR spectrum of compound **1** in DMSO-d_6

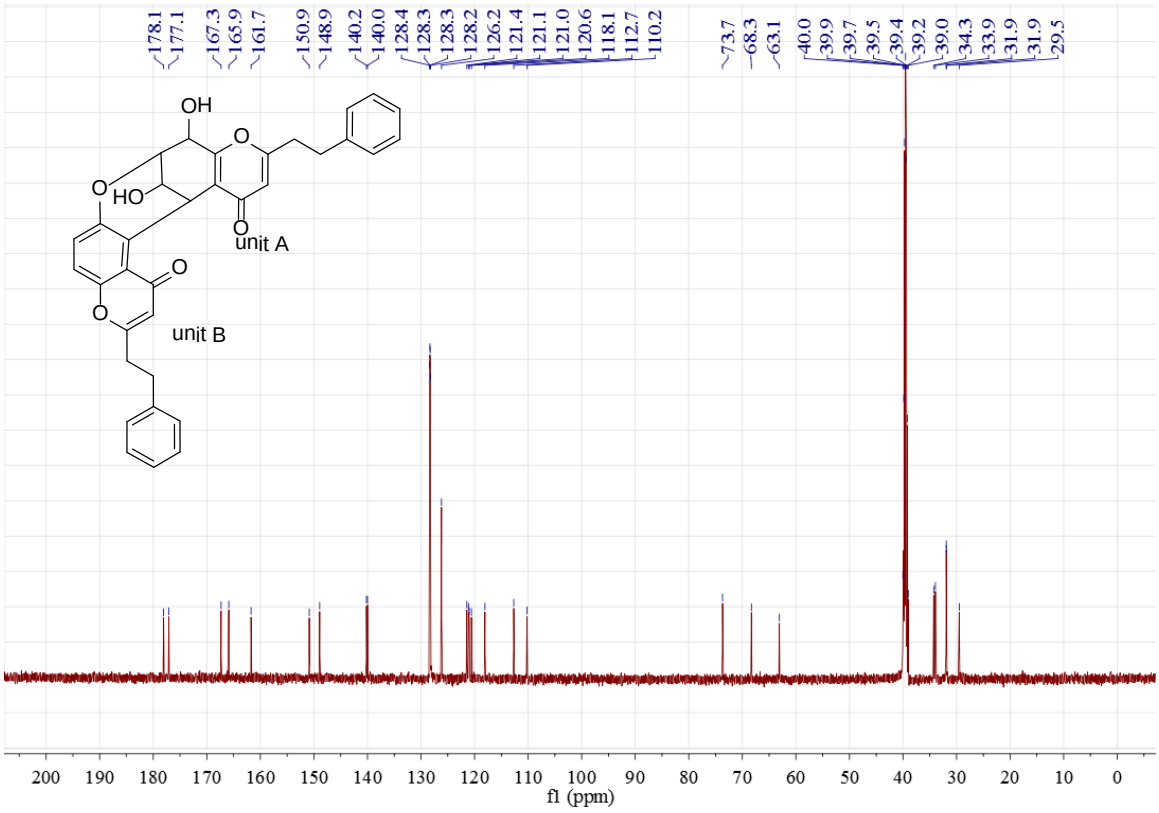


Figure S5. ^{13}C NMR spectrum of compound **1** in DMSO-d_6

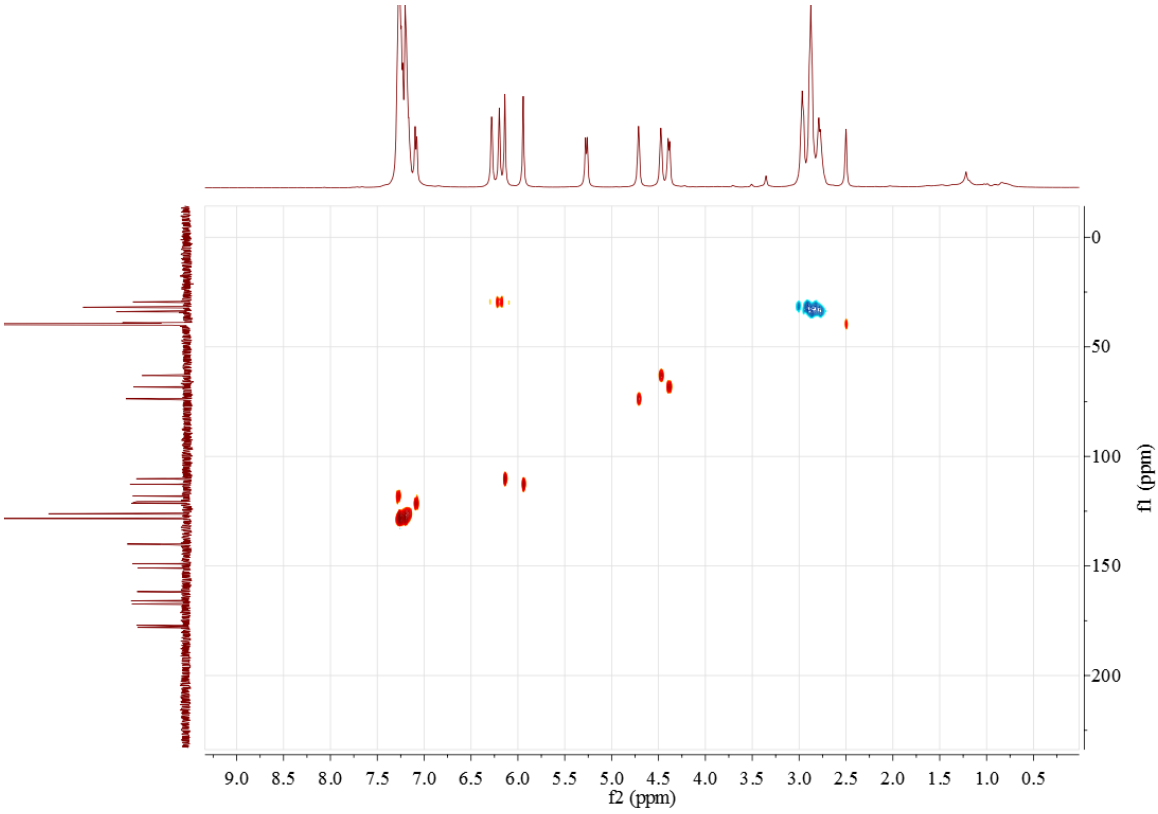


Figure S6. gHSQC spectrum of compound **1** in DMSO-d_6

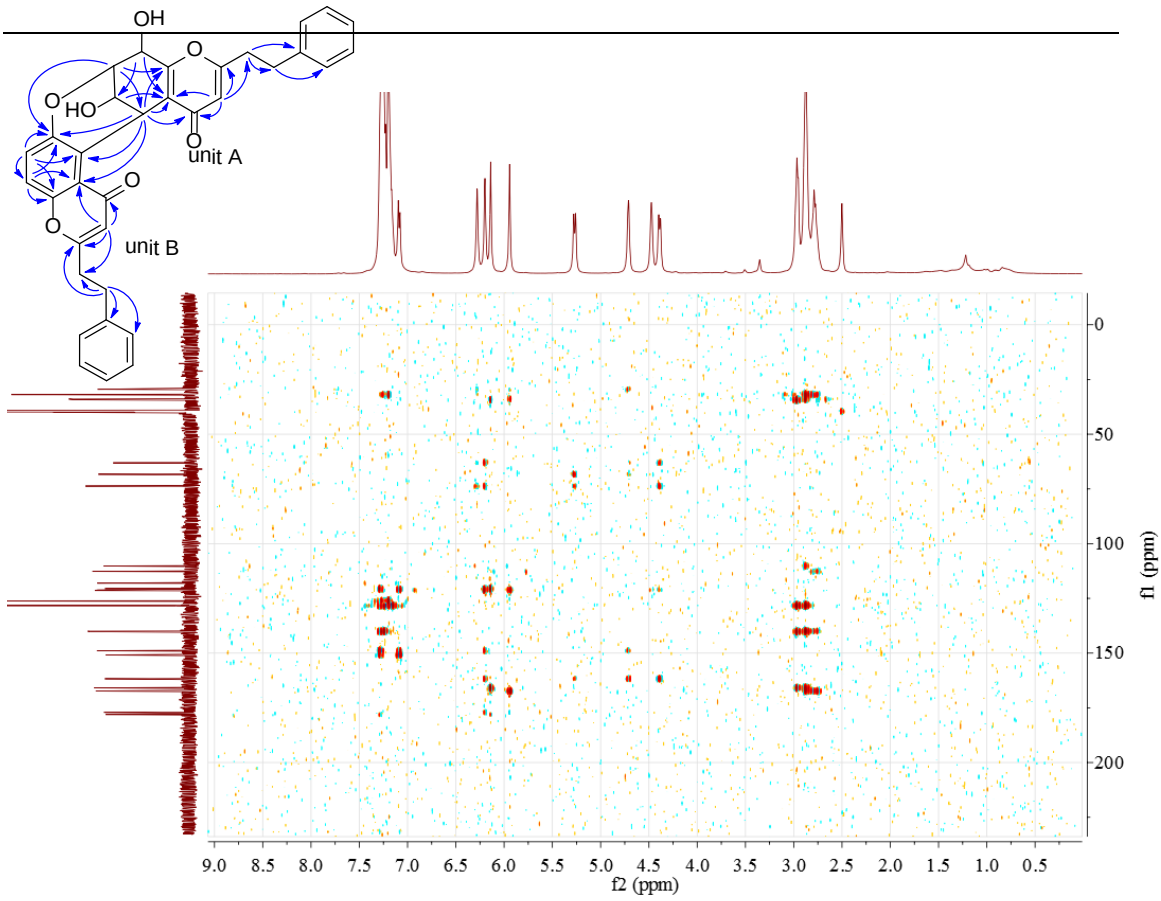


Figure S7. gHMBC spectrum of compound **1** in DMSO-d_6

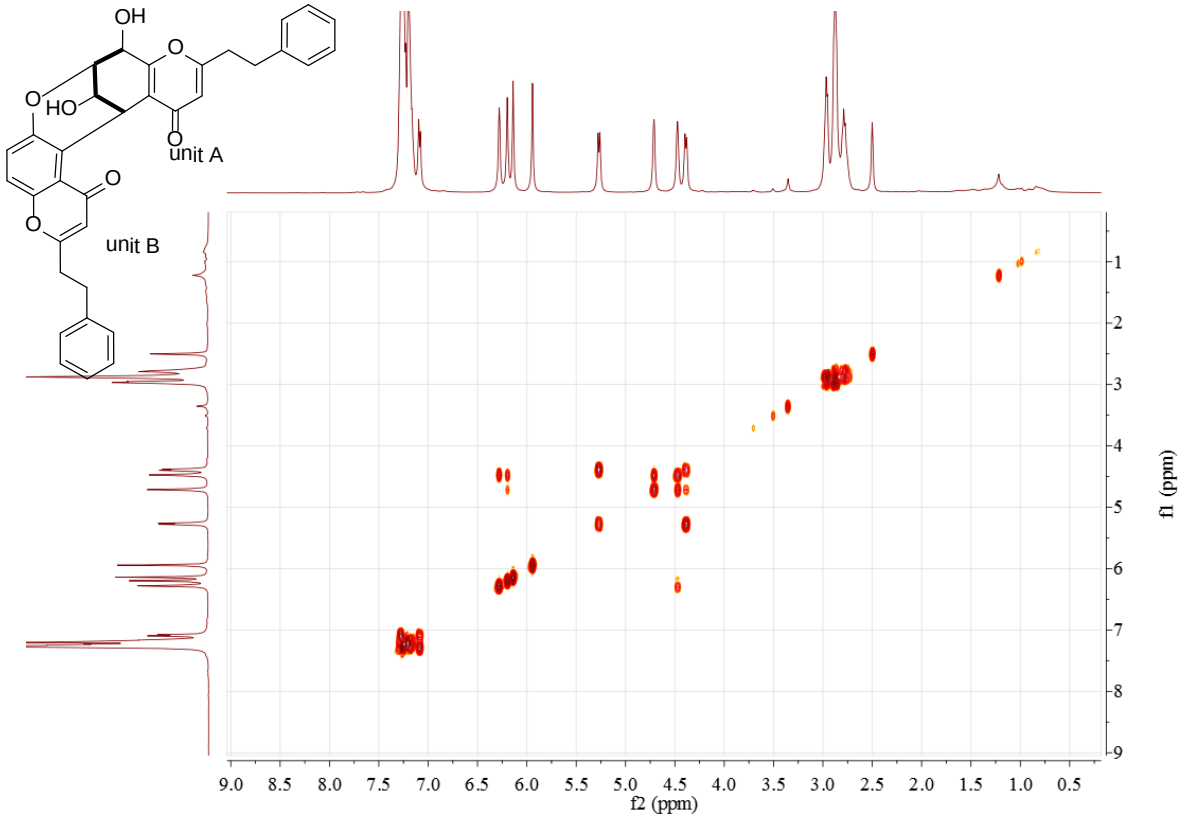


Figure S8. ^{1}H-^{1}H COSY spectrum of compound **1** in DMSO-d_6

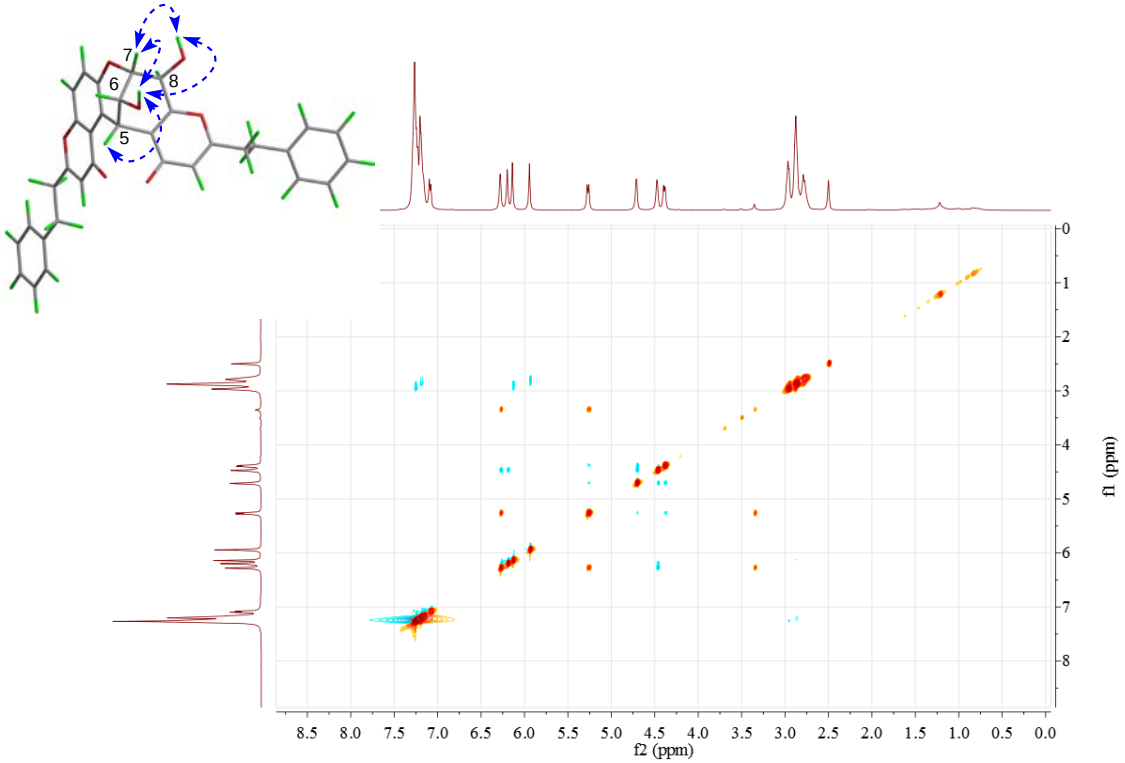


Figure S9. ROESY spectrum of compound **1** in DMSO-d_6

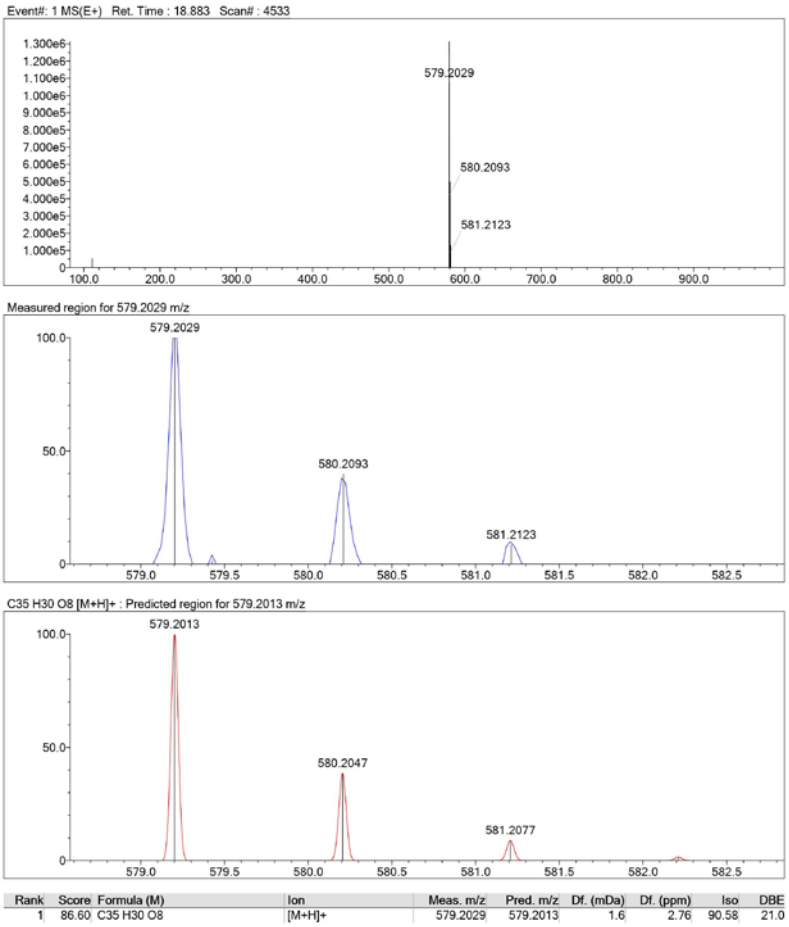


Figure S10. HRESIMS spectrum of compound **2**

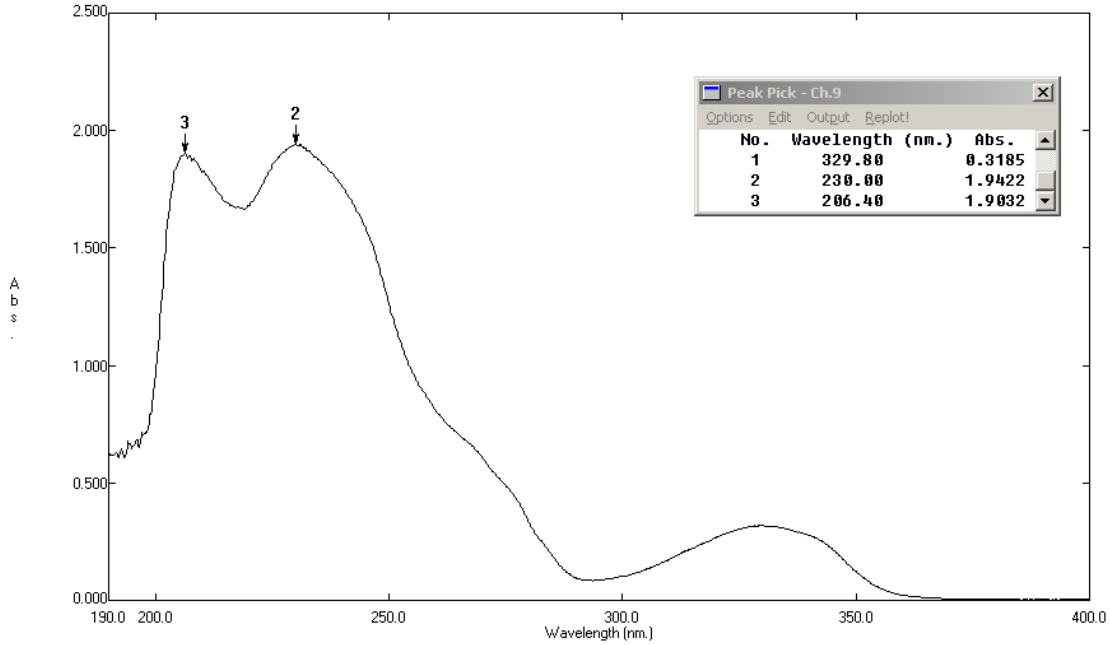


Figure S11. UV spectrum of compound **2**

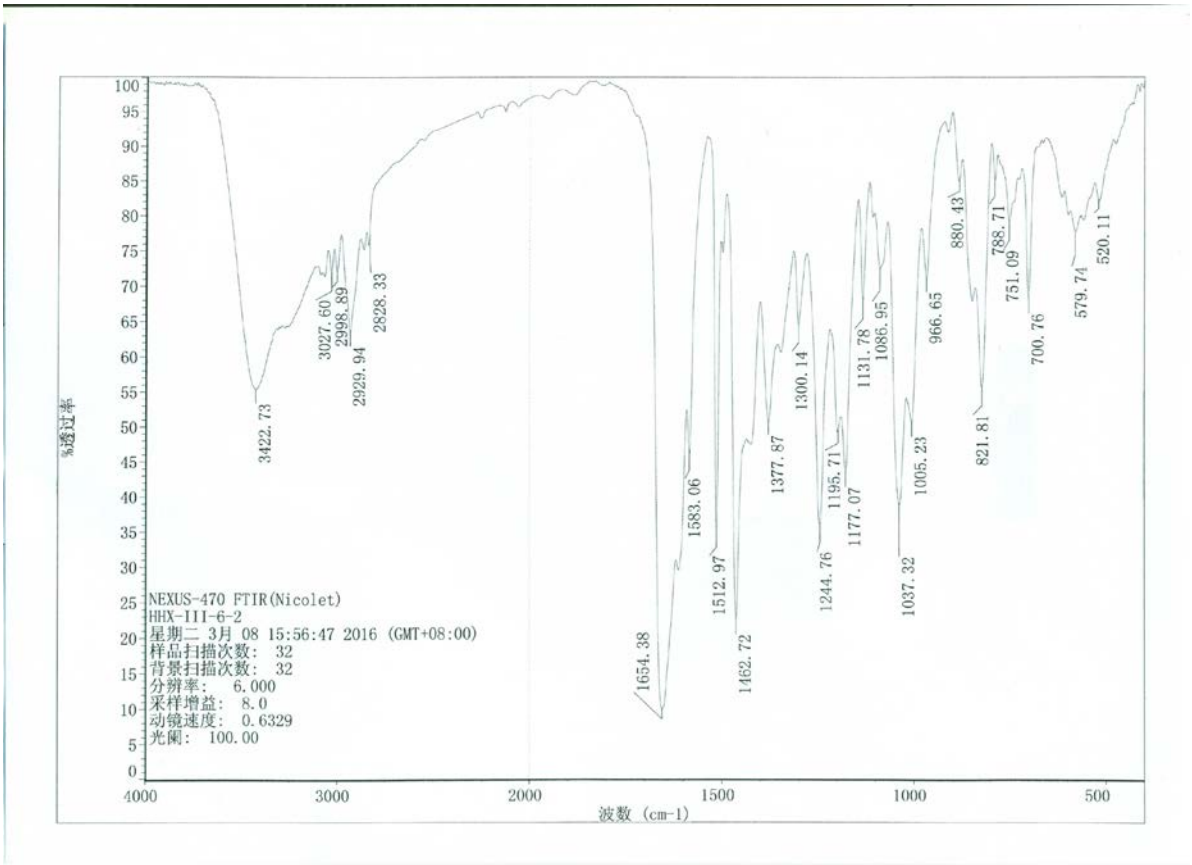


Figure S12. IR spectrum of compound **2**

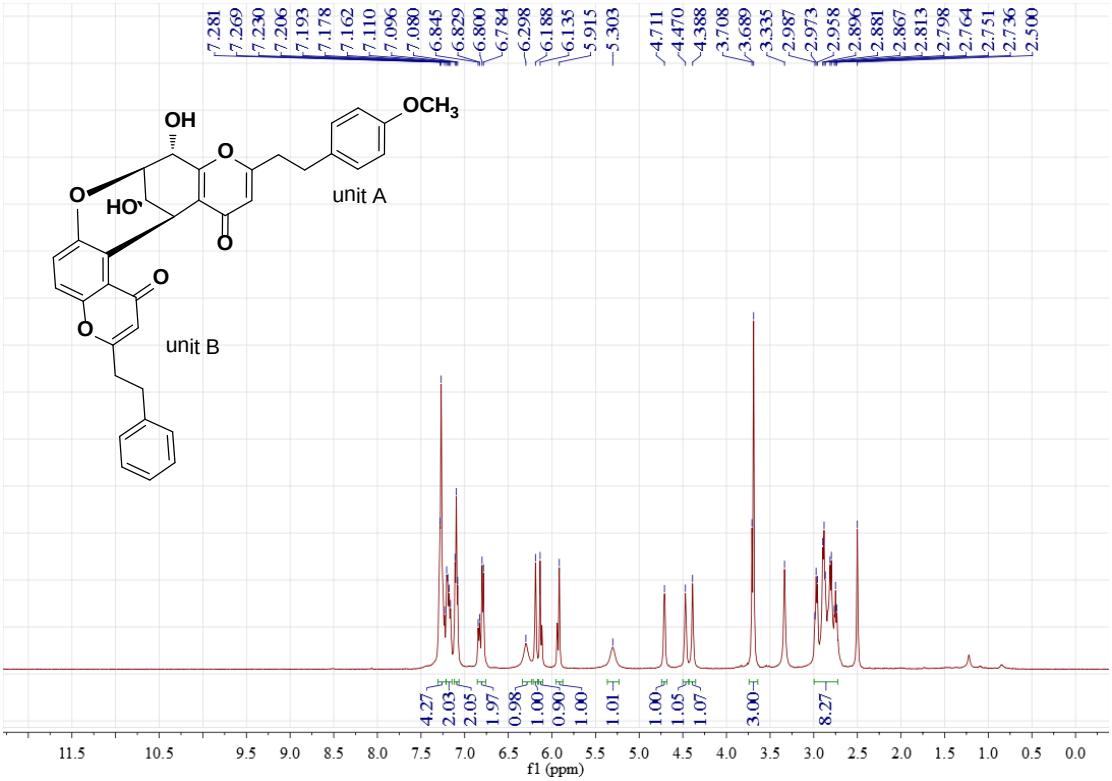


Figure S13. ^{1}H NMR spectrum of compound **2** in DMSO-d_6

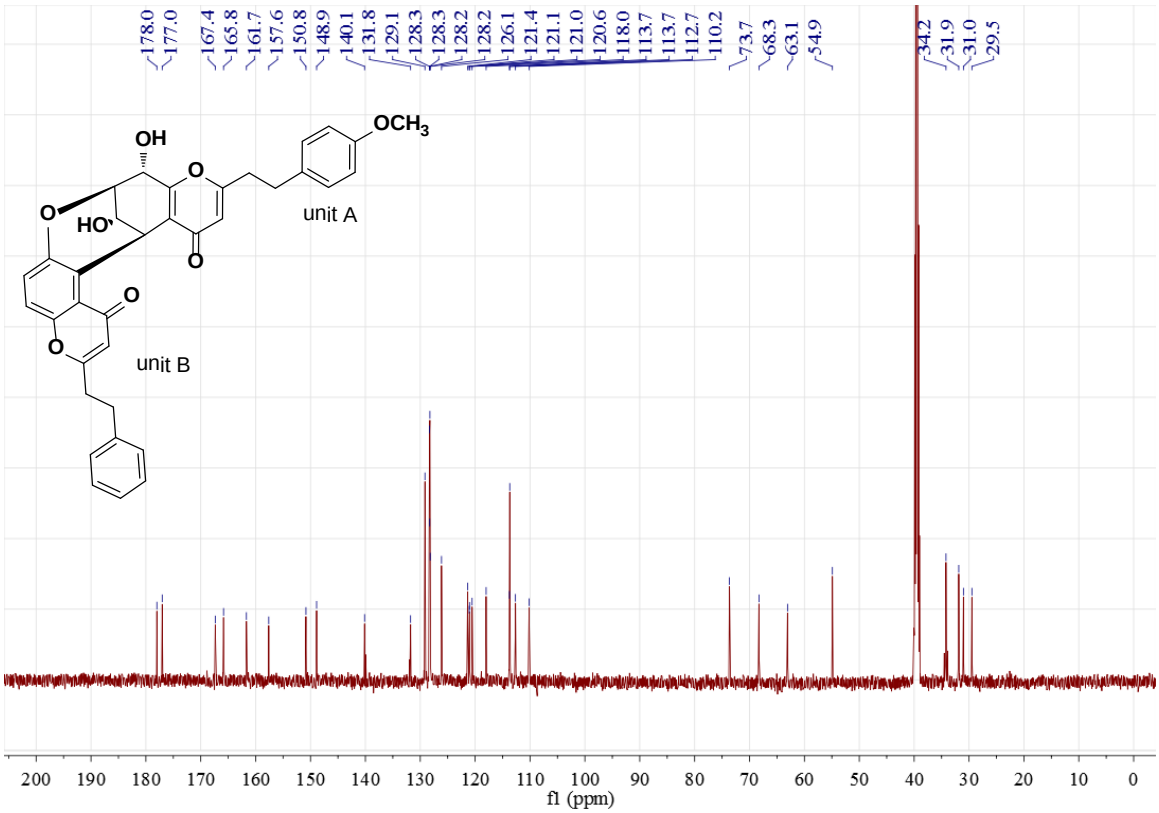


Figure S14. ^{13}C NMR spectrum of compound **2** in DMSO-d_6

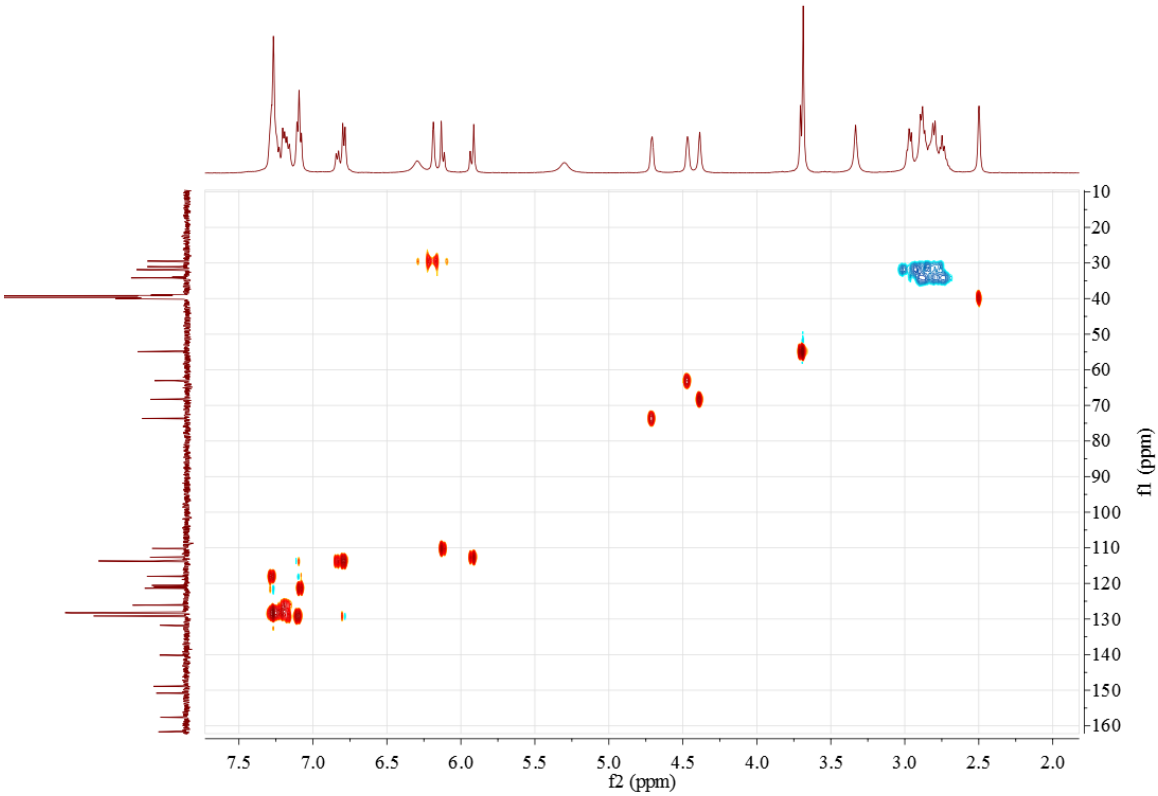


Figure S15. gHSQC spectrum of compound **2** in DMSO-d_6

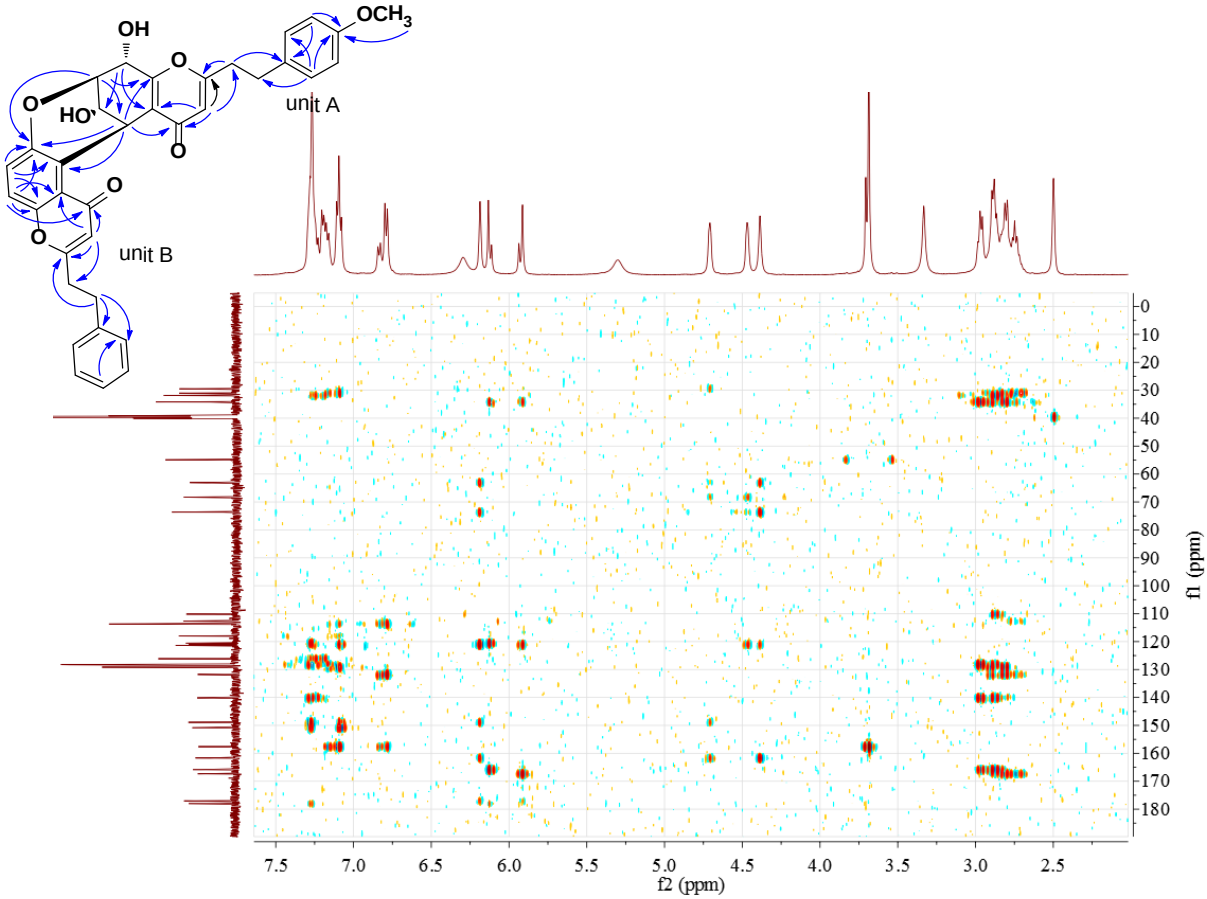


Figure S16. gHMBC spectrum of compound **2** in DMSO-d_6

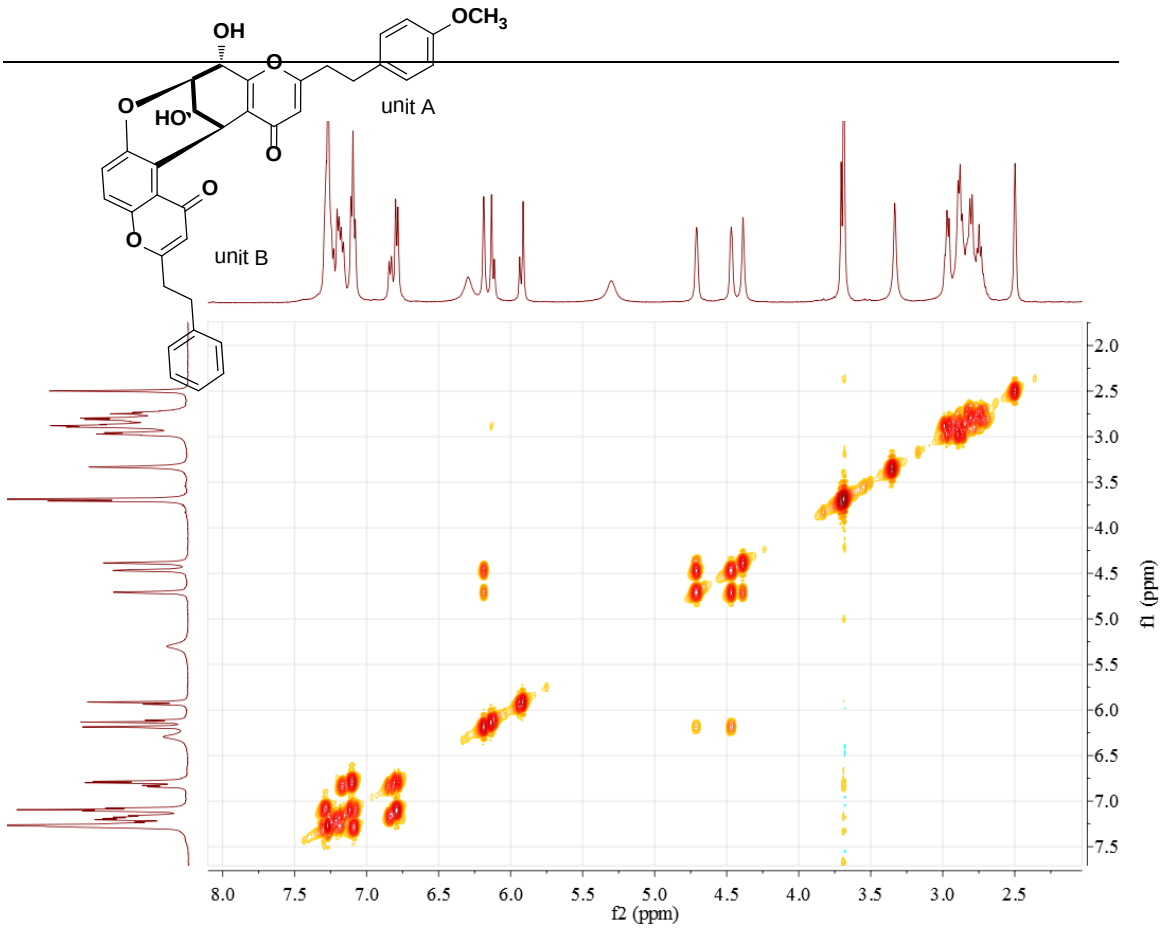


Figure S17. ^{1}H-^{1}H COSY spectrum of compound **2** in DMSO-d_6

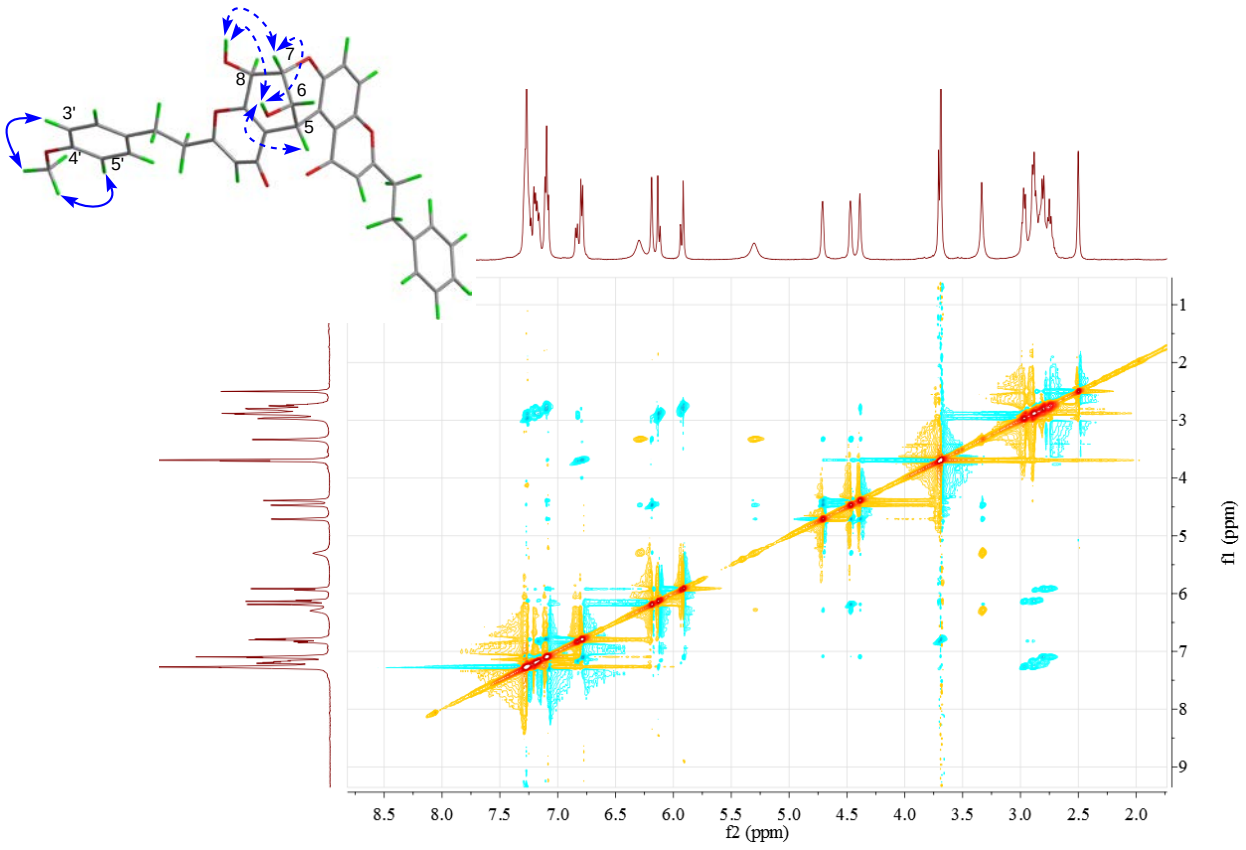


Figure S18. ROESY spectrum of compound **2** in DMSO-d_6

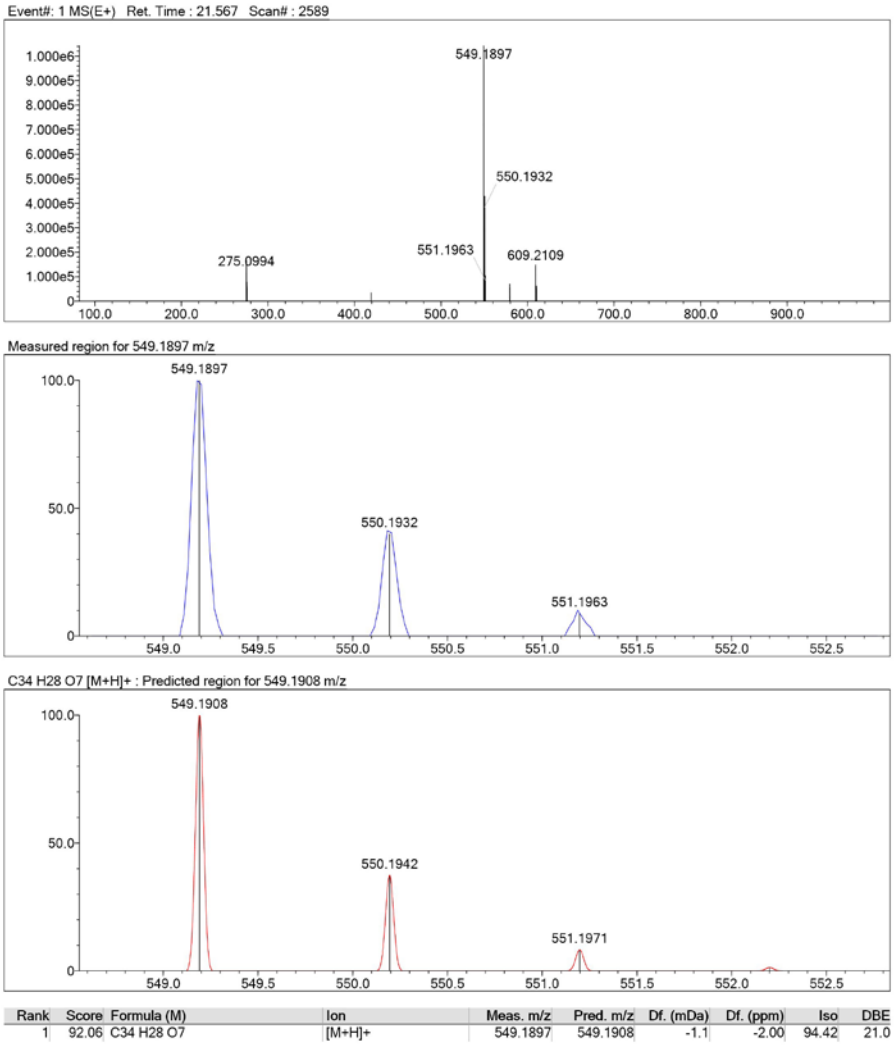


Figure S19. HRESIMS spectrum of compound **3**

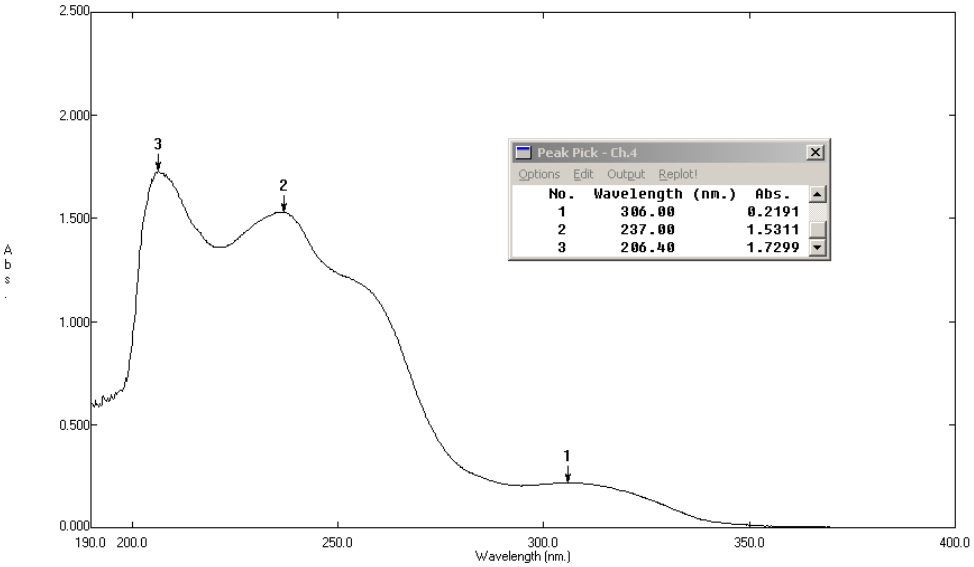


Figure S20. UV spectrum of compound **3**

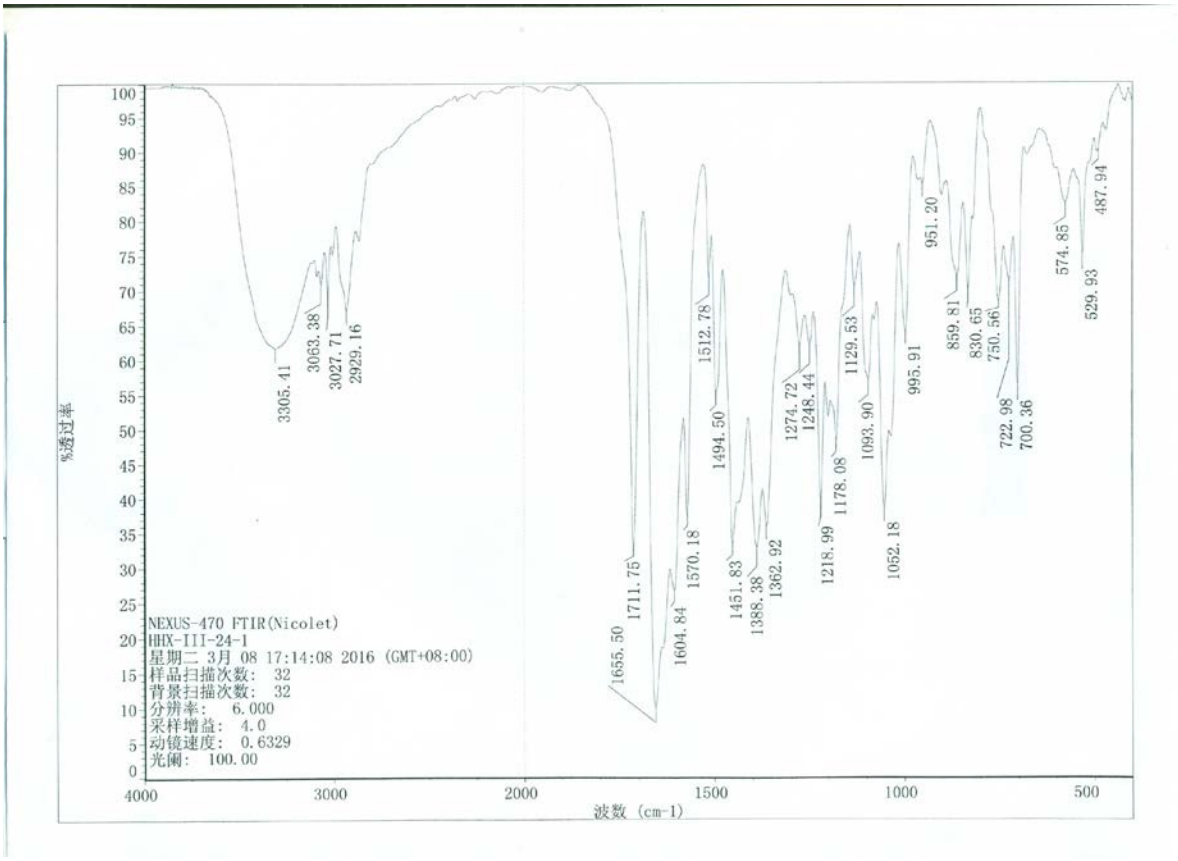


Figure S21. IR spectrum of compound **3**

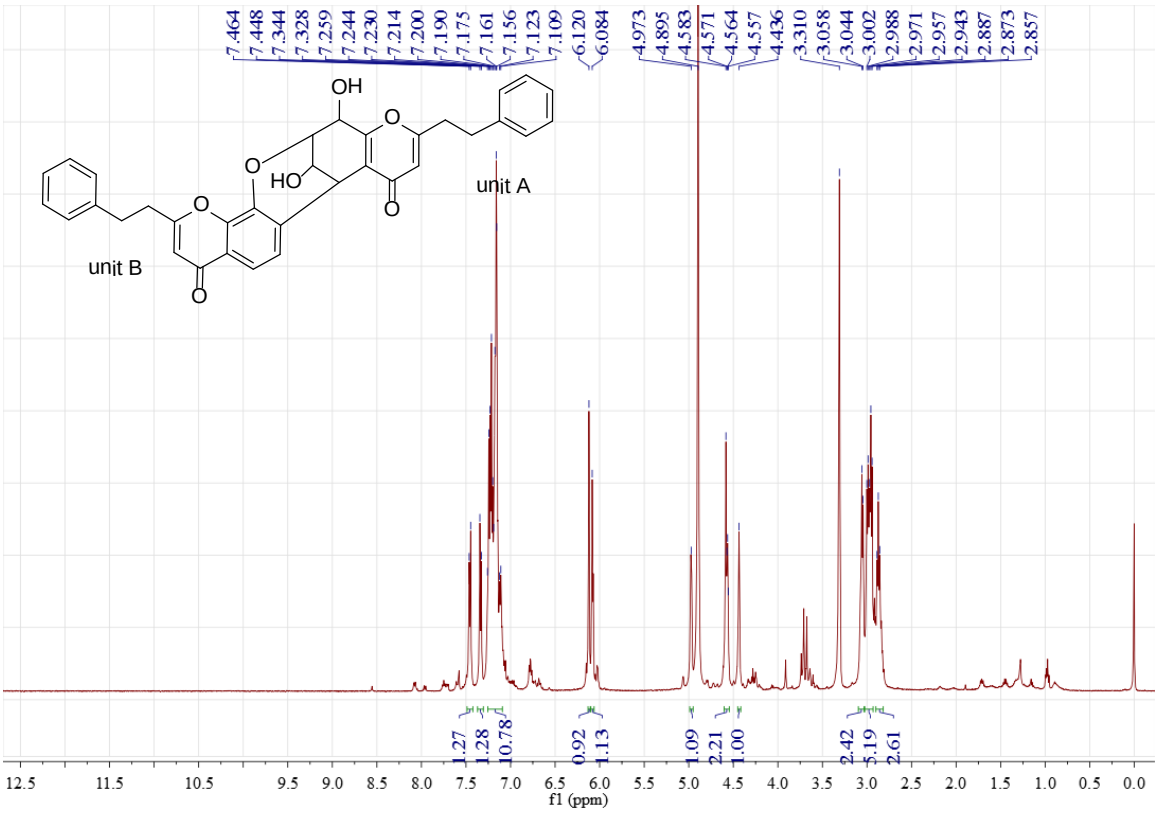


Figure S22. ^{1}H NMR spectrum of compound **3** in methanol-d_4

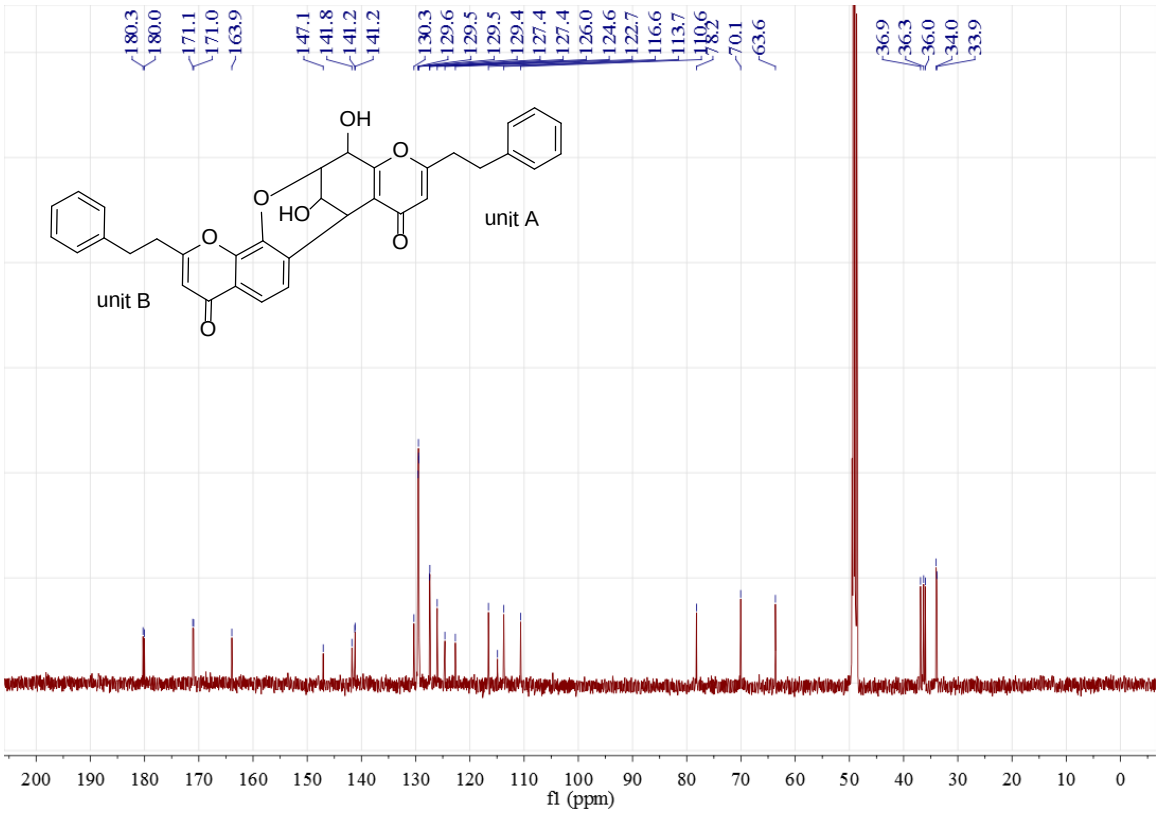


Figure S23. ^{13}C NMR spectrum of compound **3** in methanol-d_4

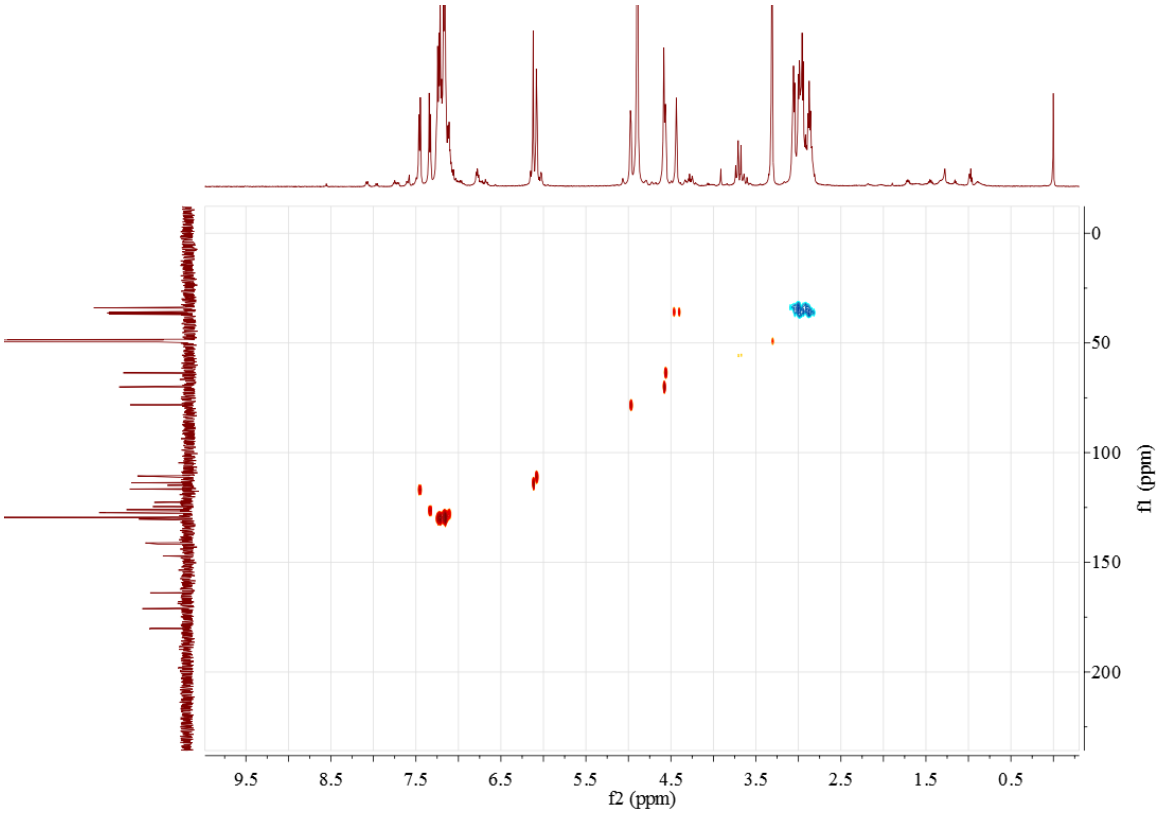


Figure S24. gHSQC spectrum of compound **3** in methanol-d_4

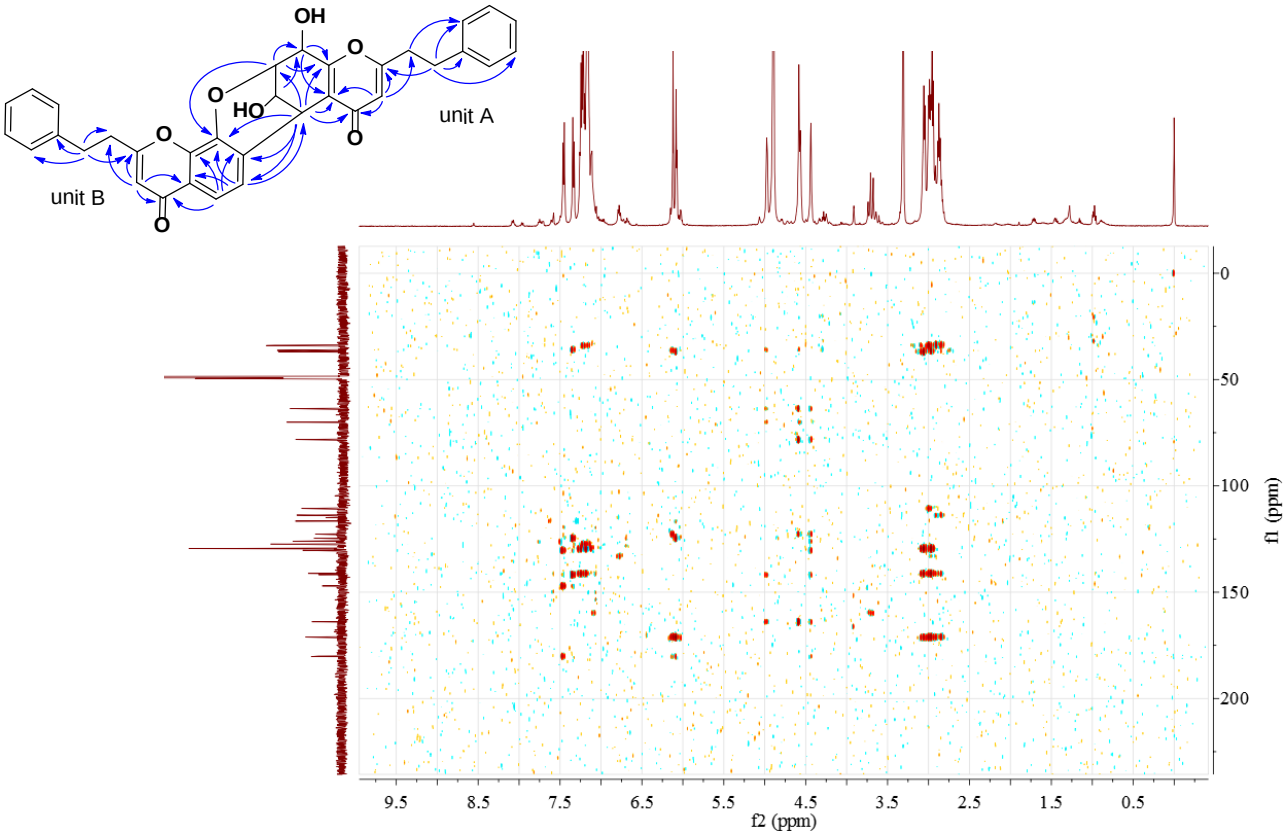


Figure S25. gHMBC spectrum of compound **3** in methanol-d_4

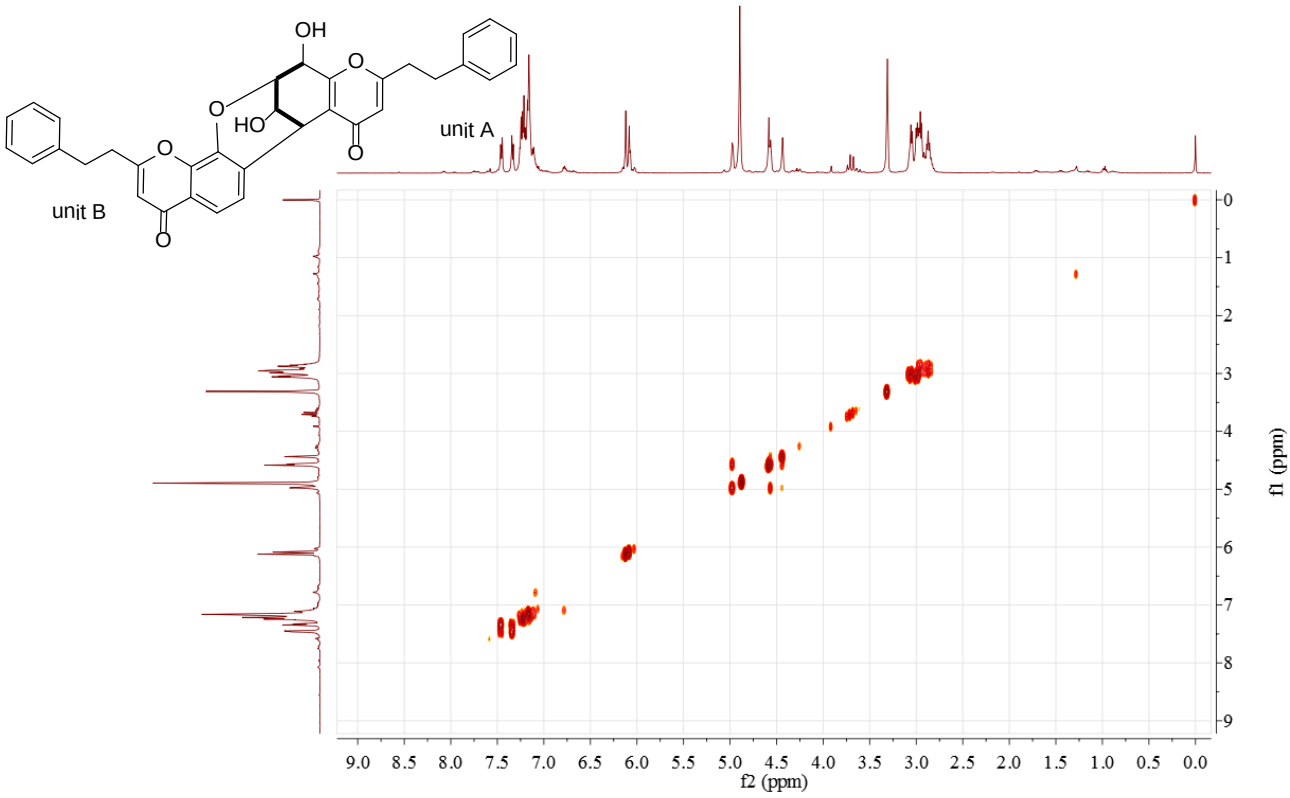


Figure S26. ^{1}H-^{1}H COSY spectrum of compound **3** in methanol-d_4

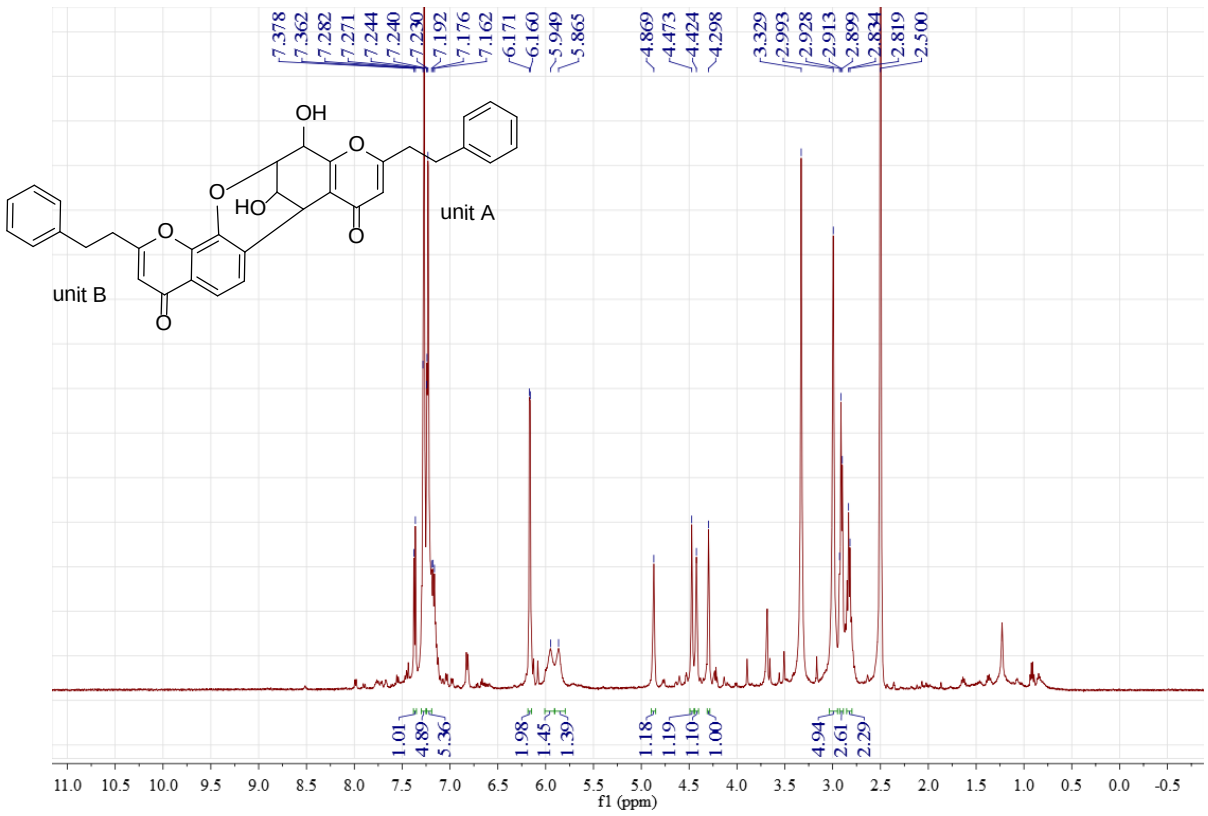


Figure S27. ^{1}H NMR spectrum of compound **3** in DMSO-d_6

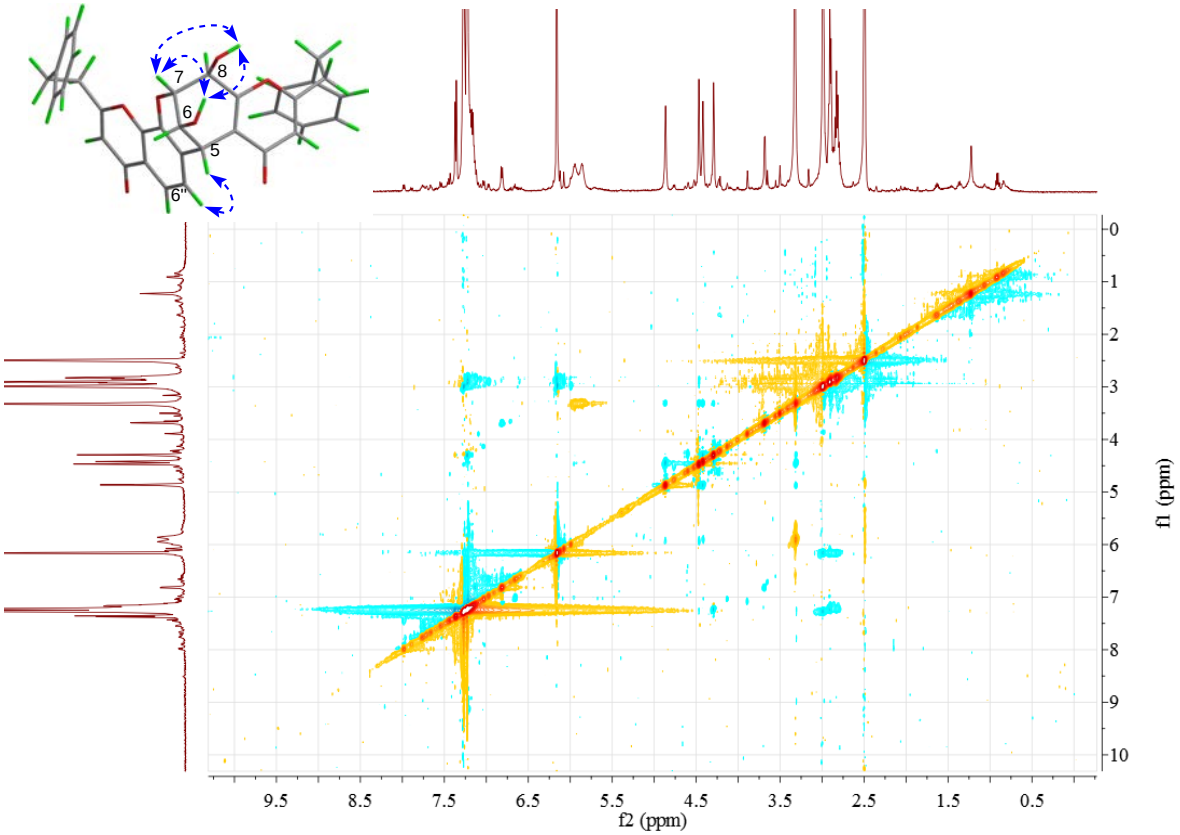
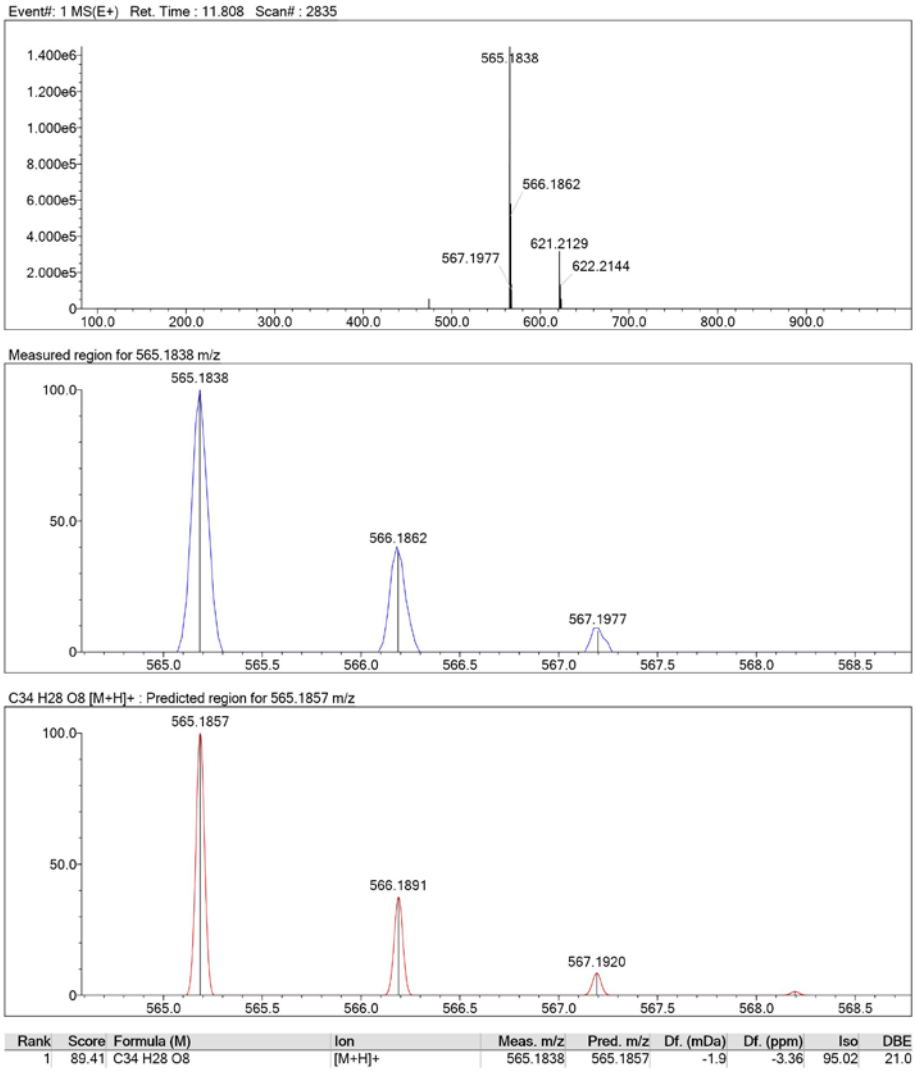


Figure S28. ROESY spectrum of compound **3** in DMSO-d_6



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	89.41	C34 H28 O8	[M+H]+	565.1838	565.1857	-1.9	-3.36	95.02	21.0

Figure S29. HRESIMS spectrum of compound **4**

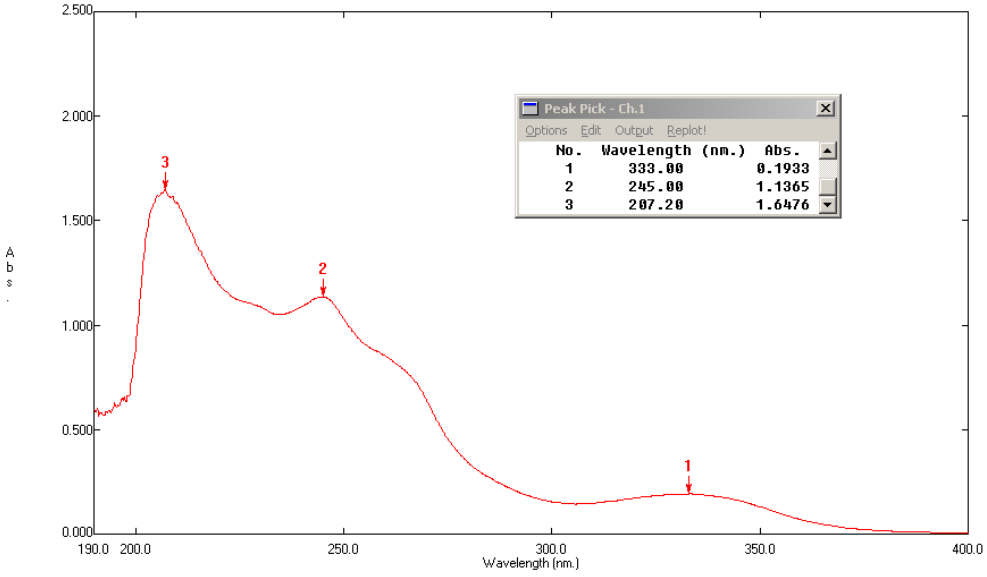


Figure S30. UV spectrum of compound **4**

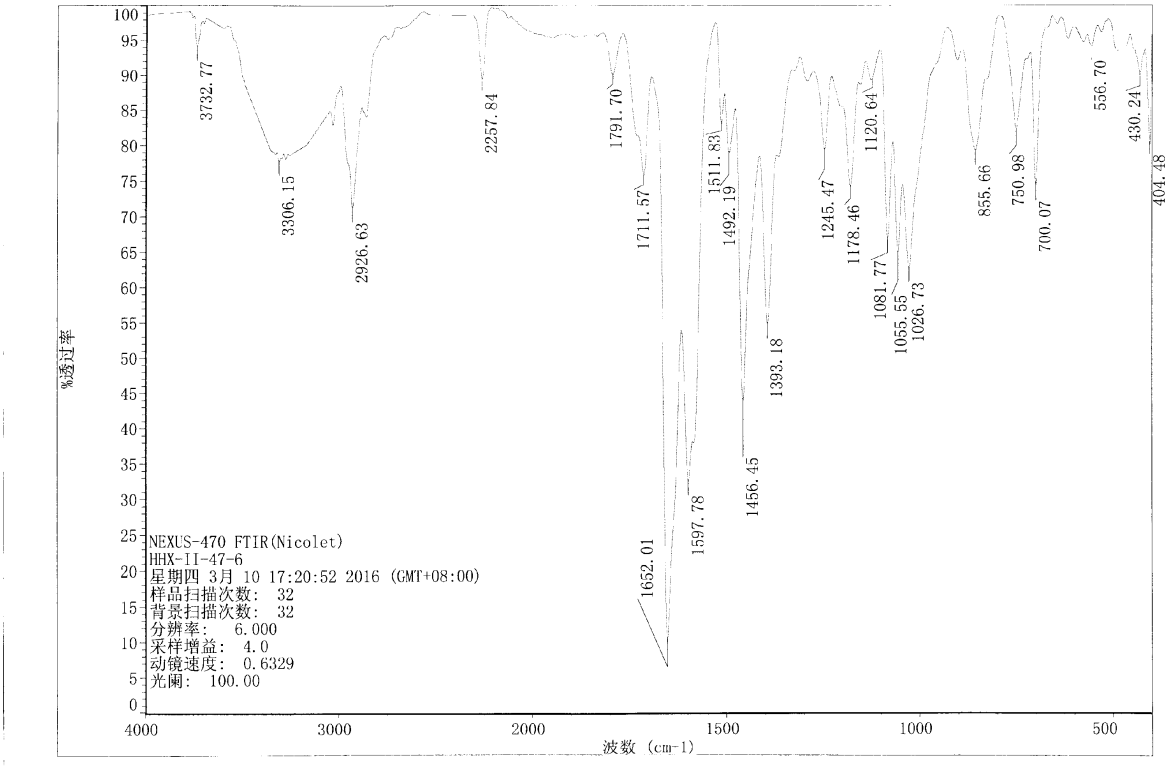


Figure S31. IR spectrum of compound **4**

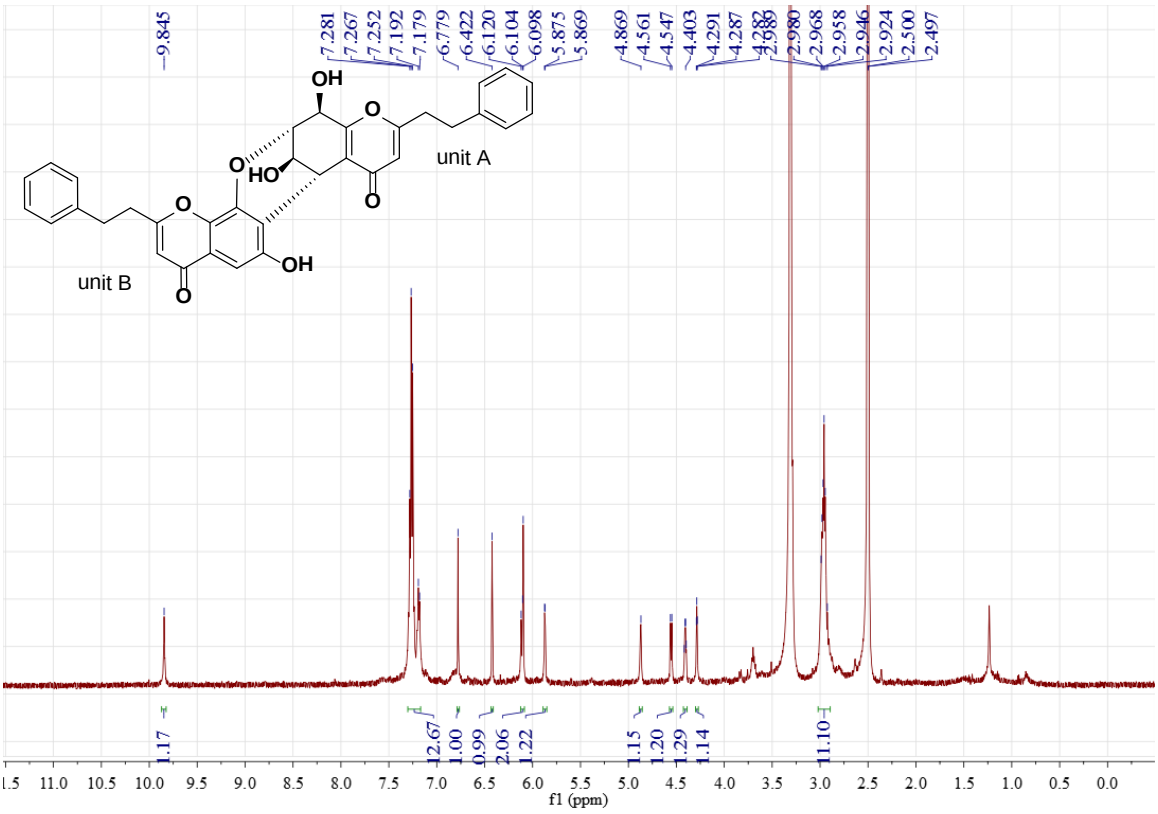


Figure S32. ^{1}H NMR spectrum of compound **4** in DMSO-d_6

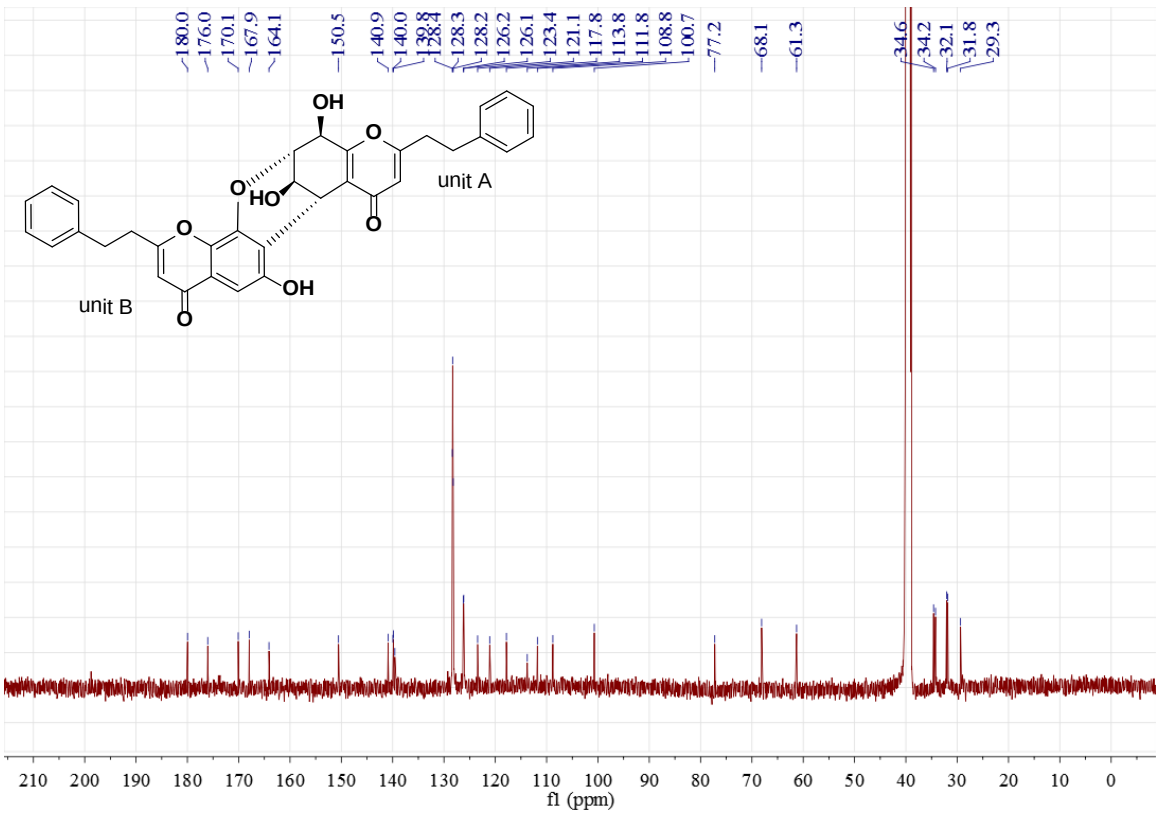


Figure S33. ^{13}C NMR spectrum of compound **4** in DMSO-d_6

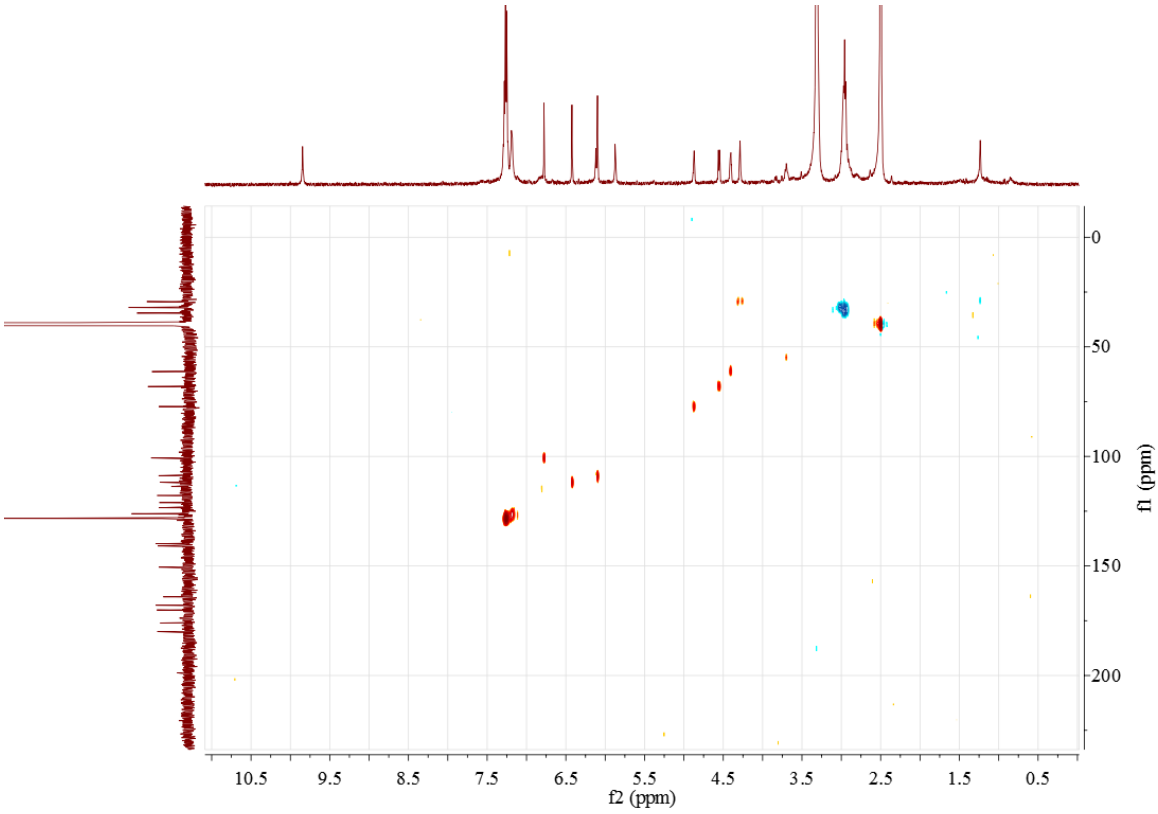


Figure S34. gHSQC spectrum of compound **4** in DMSO-d_6

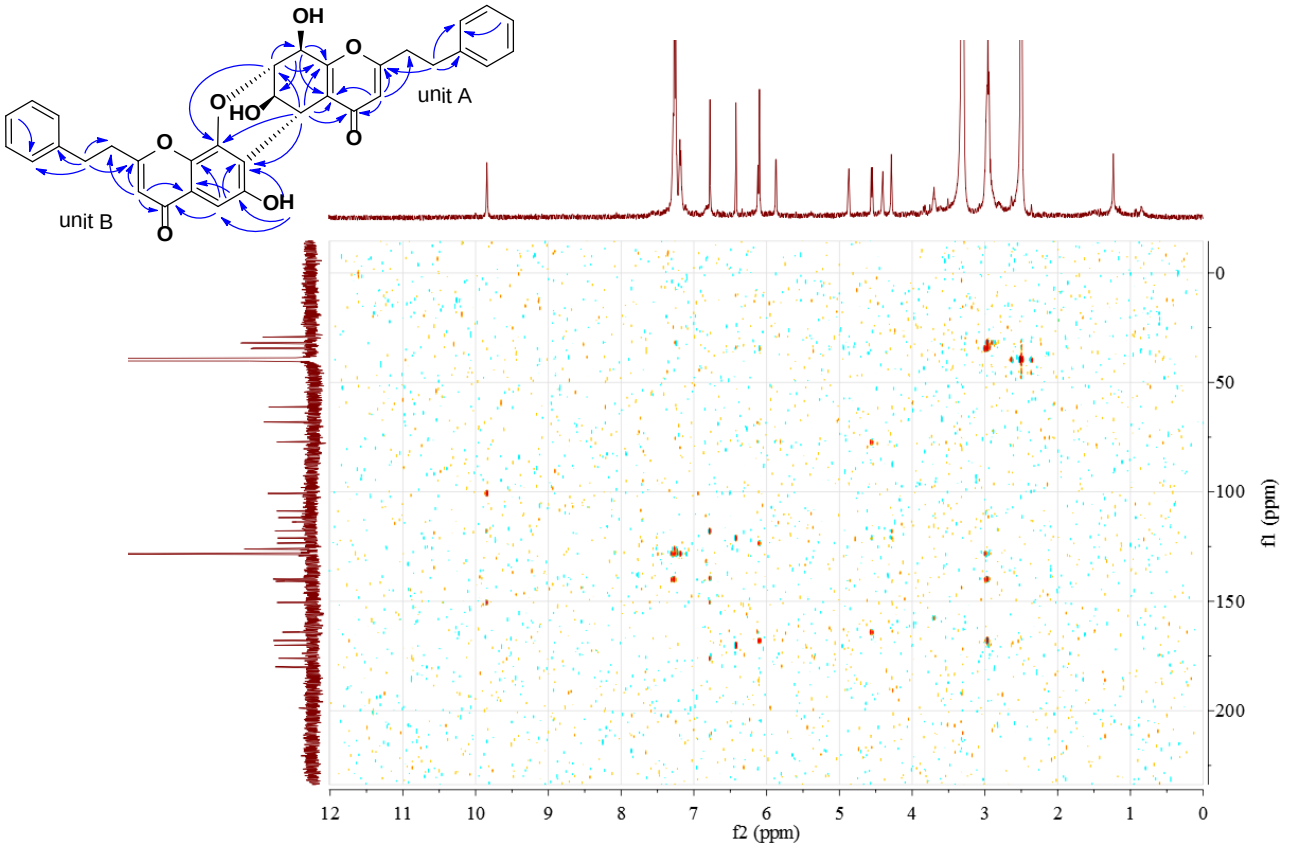


Figure S35. gHMBC spectrum of compound **4** in DMSO-d_6

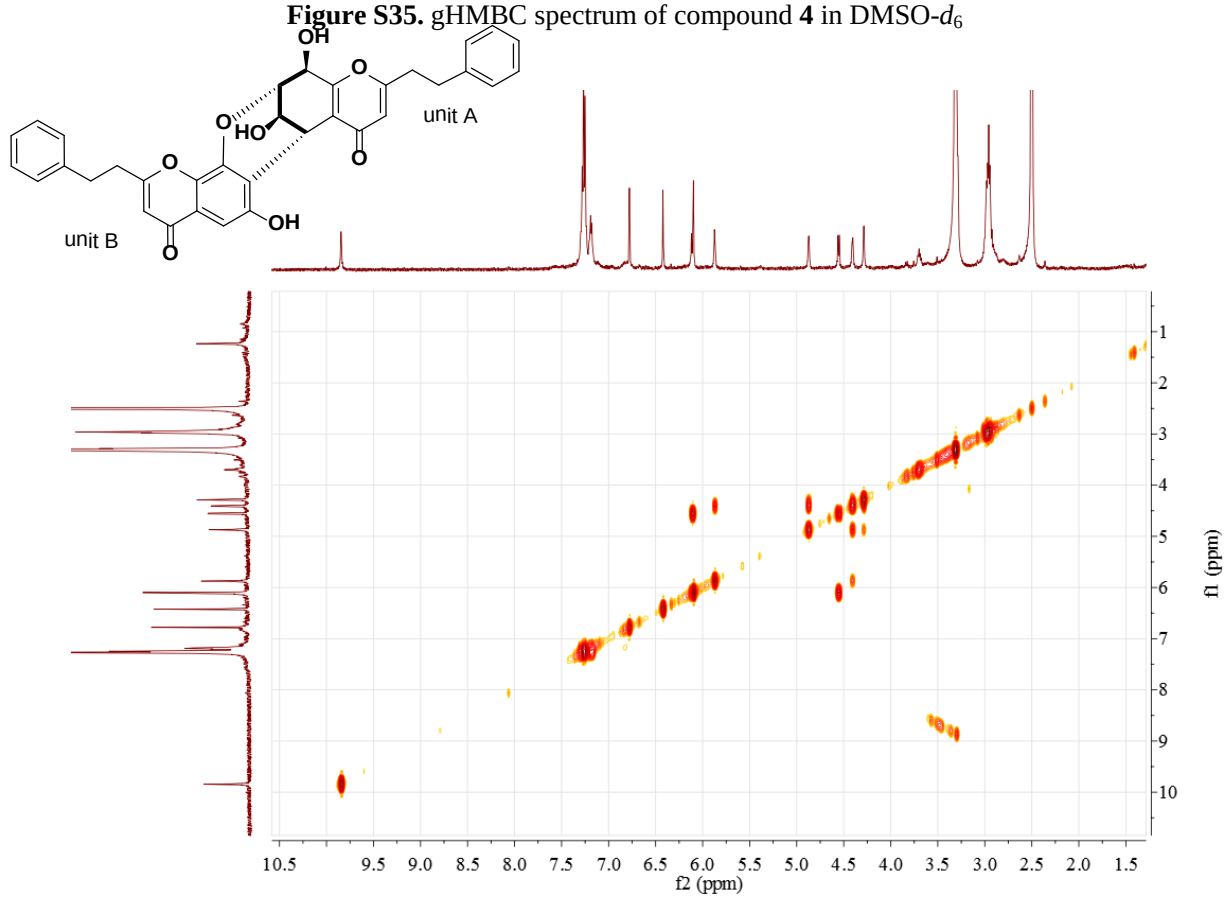


Figure S36. ^{1}H-^{1}H COSY spectrum of compound **4** in DMSO-d_6

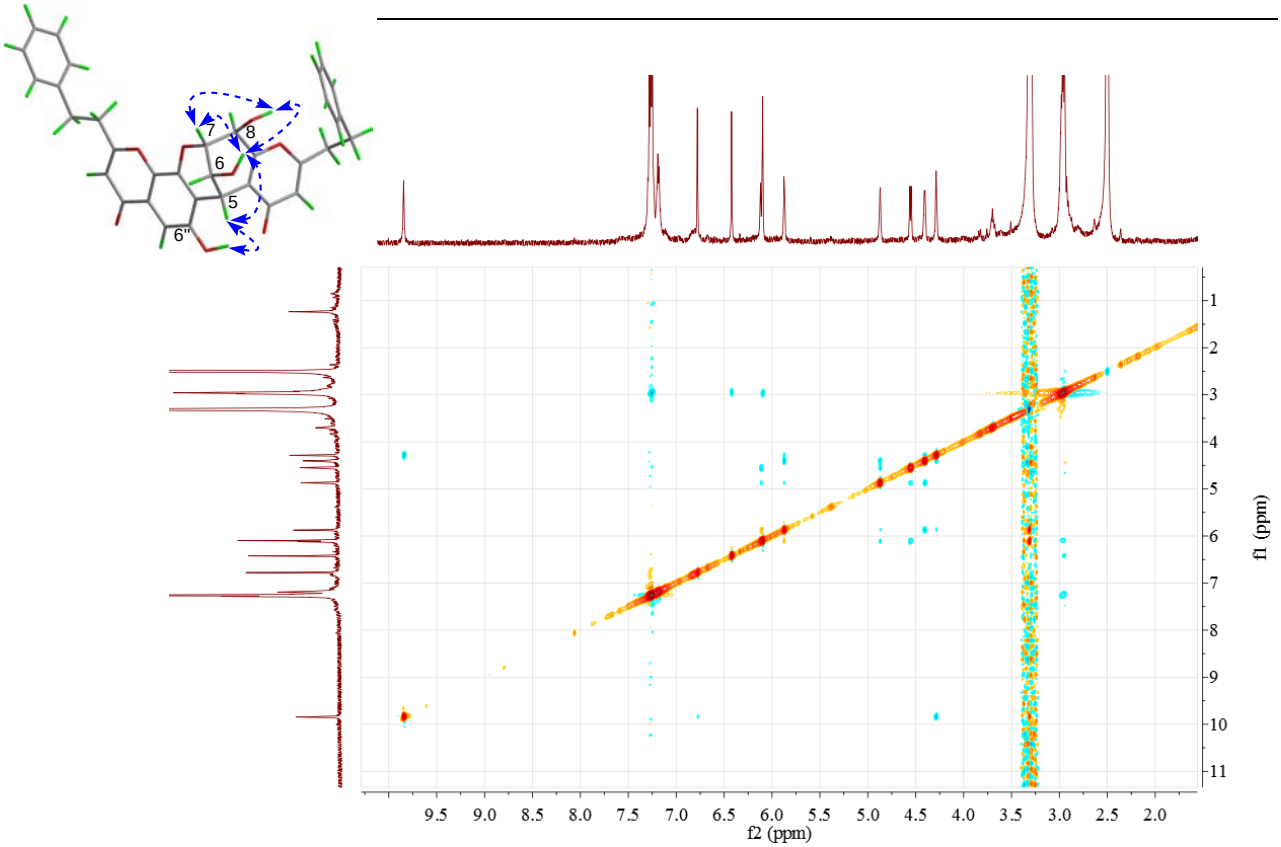
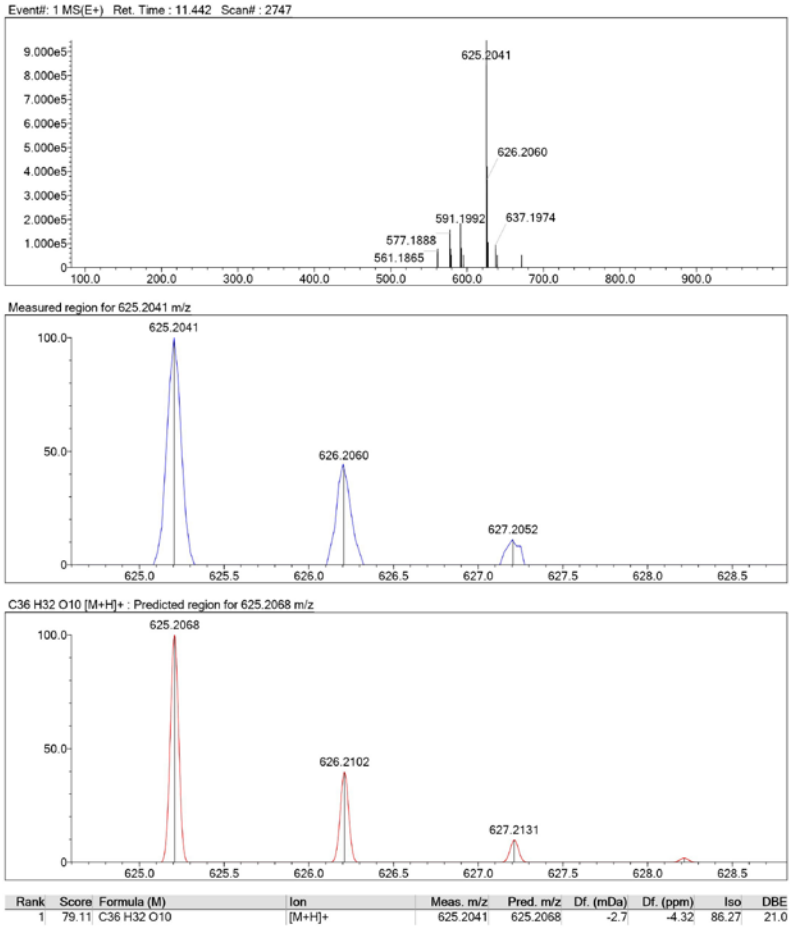


Figure S37. ROESY spectrum of compound **4** in DMSO-d_6



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	79.11	C36 H32 O10	[M+H]+	625.2041	625.2068	-2.7	-4.32	86.27	21.0

Figure S38. HRESIMS spectrum of compound **5**

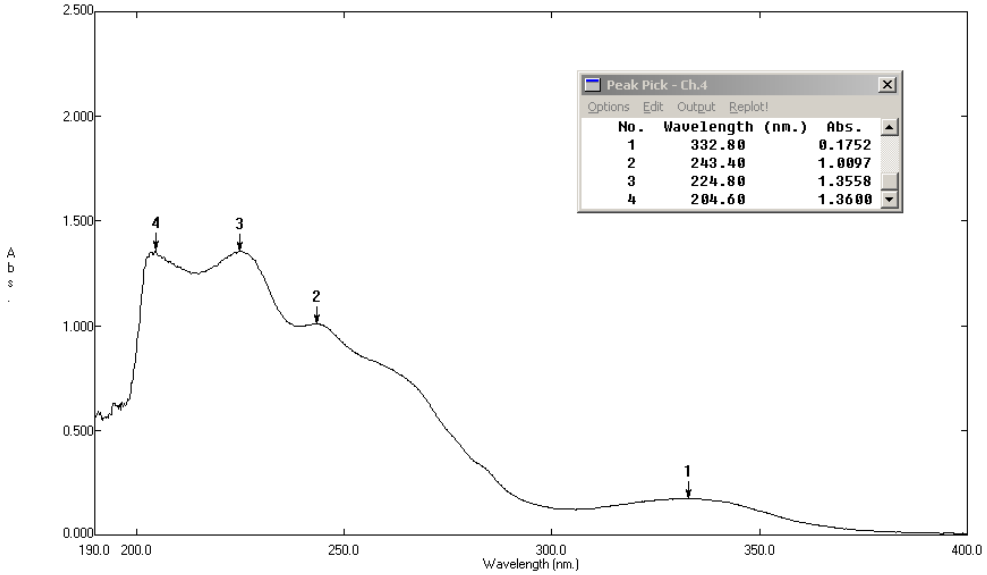


Figure S39. UV spectrum of compound **5**

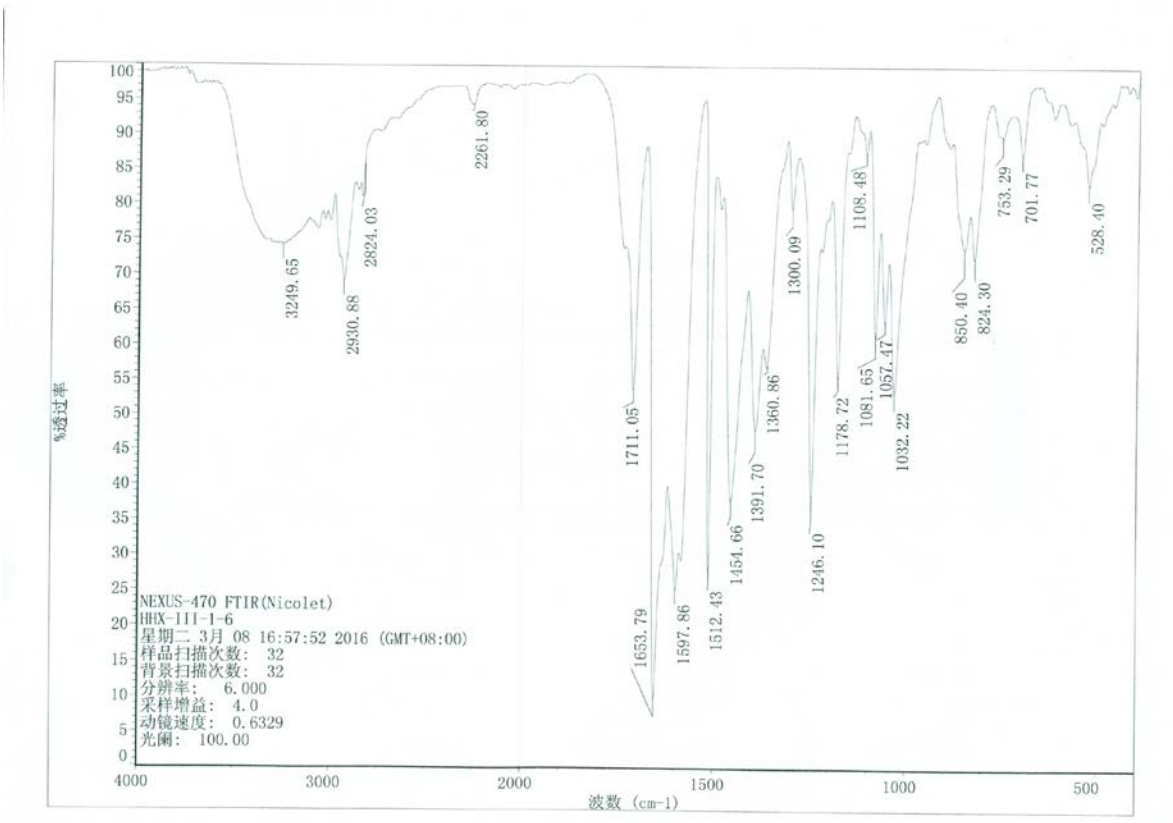


Figure S40. IR spectrum of compound **5**

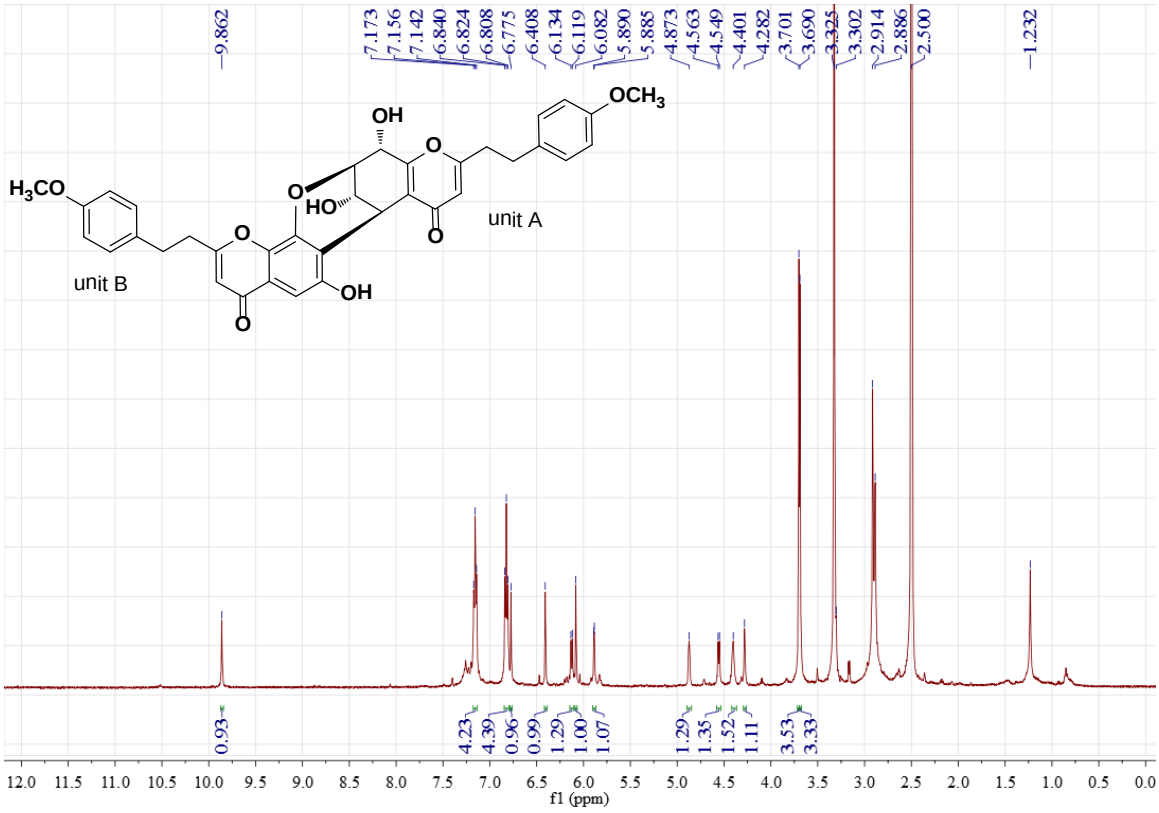


Figure S41. ^{1}H NMR spectrum of compound **5** in DMSO-d_6

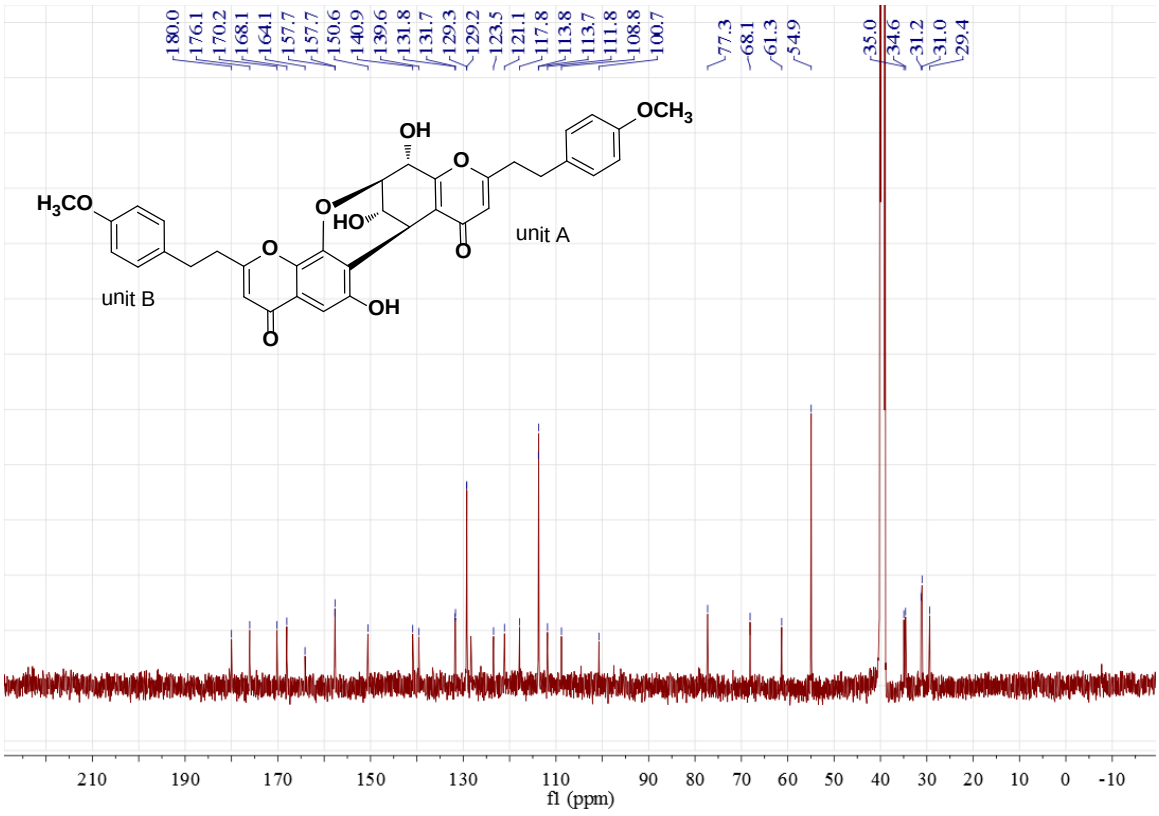


Figure S42. ^{13}C NMR spectrum of compound **5** in DMSO-d_6

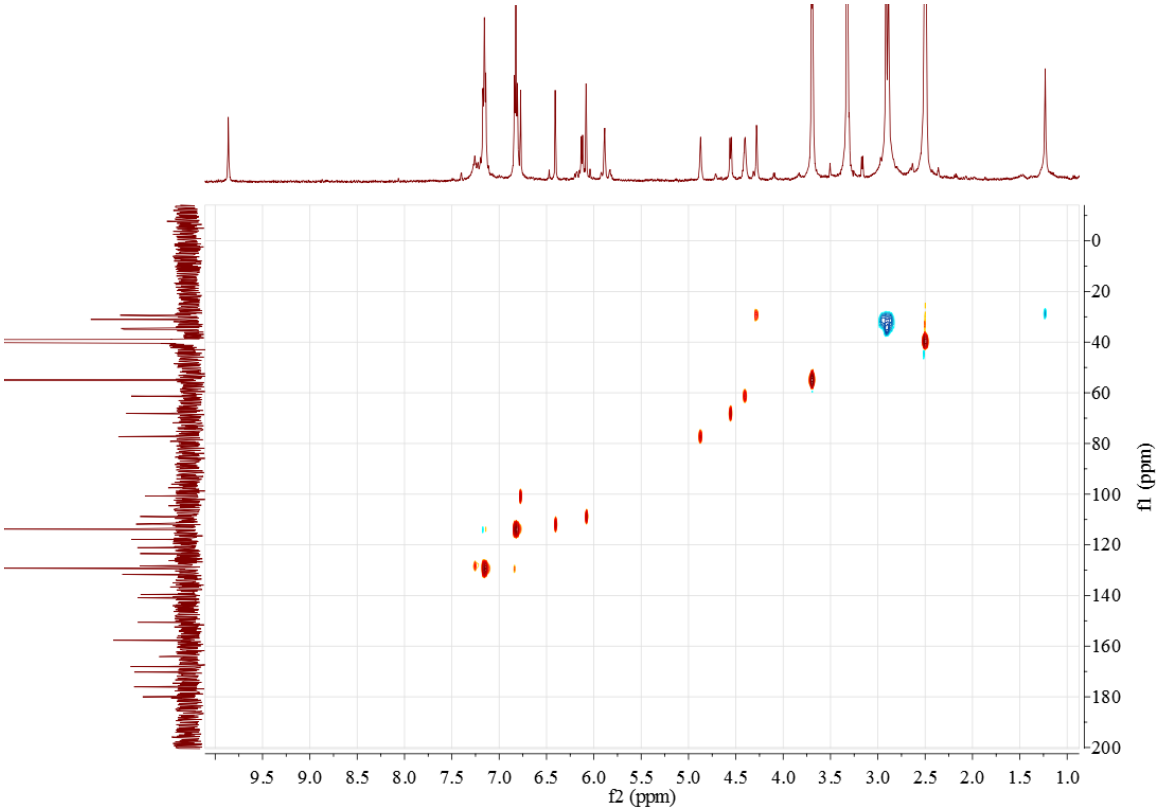


Figure S43. gHSQC spectrum of compound **5** in DMSO-d_6

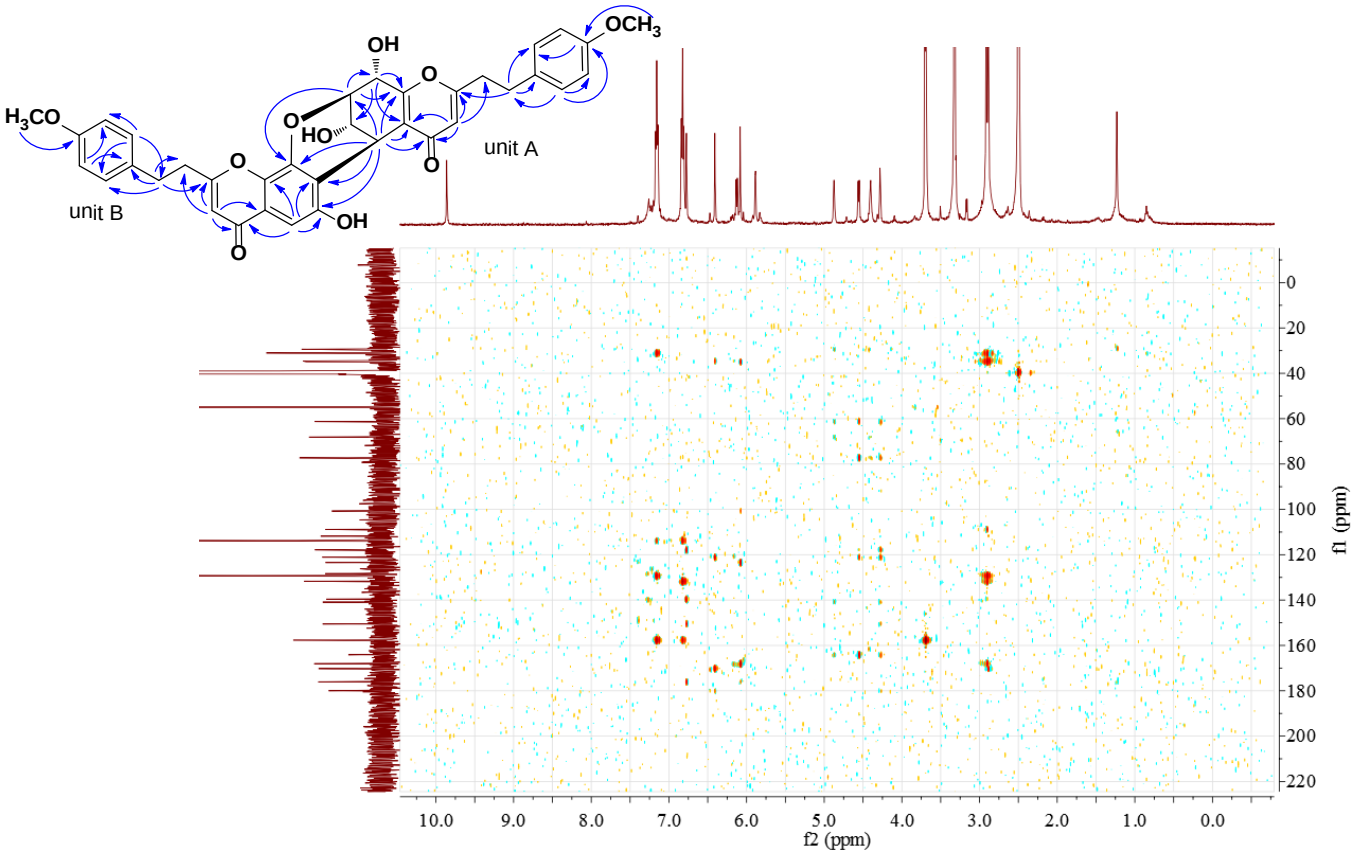


Figure S44. gHMBC spectrum of compound **5** in DMSO-d_6

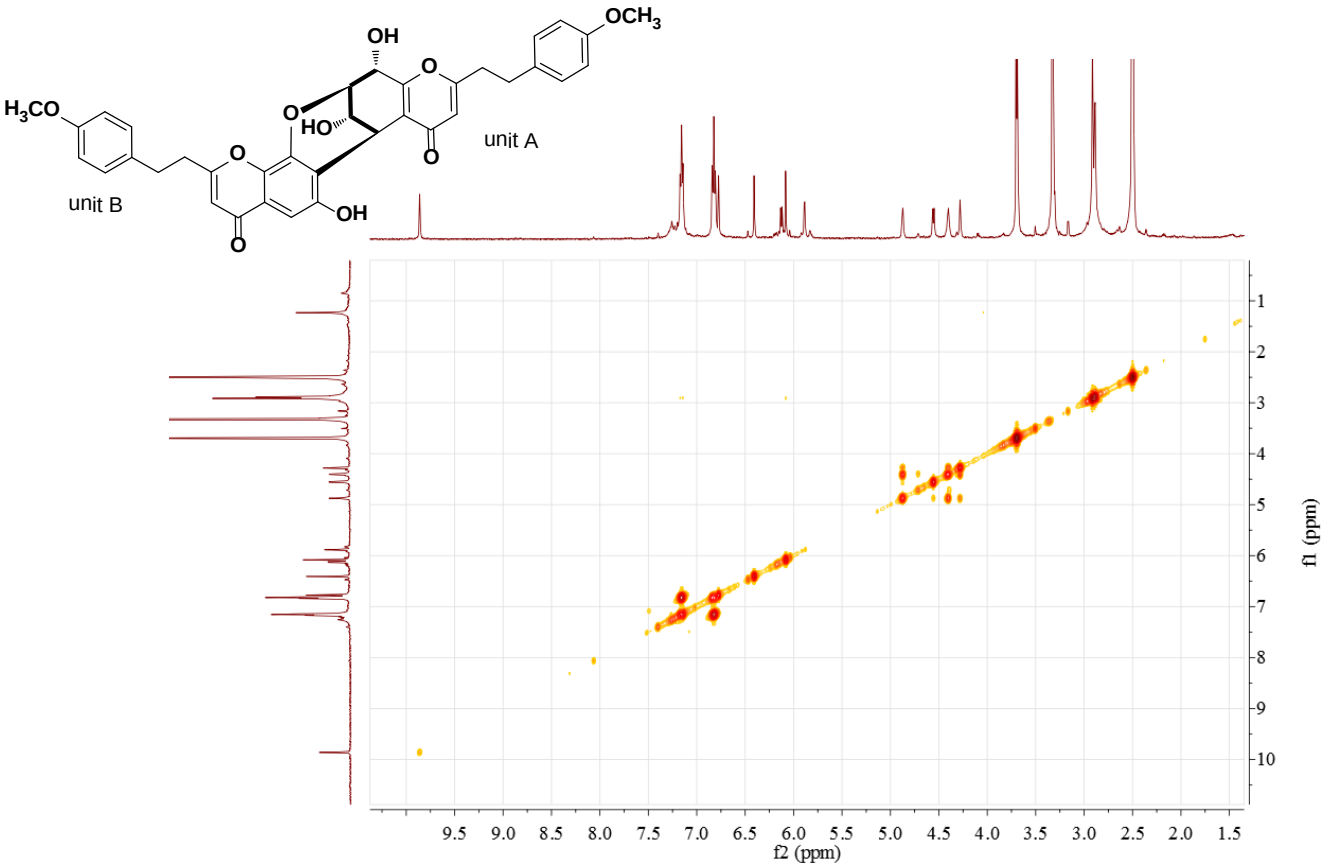


Figure S45. ^{1}H-^{1}H COSY spectrum of compound **5** in DMSO-d_6

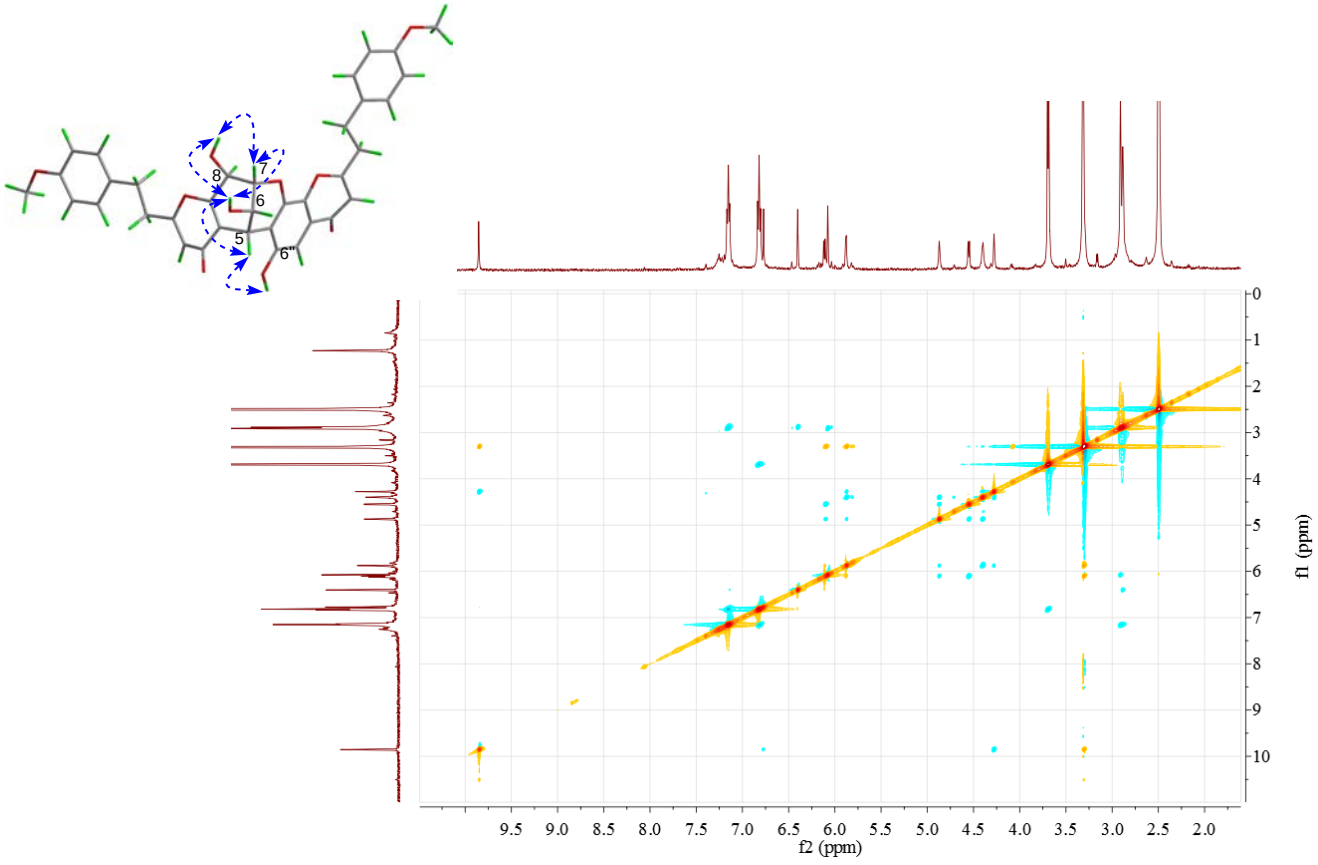


Figure S46. ROESY spectrum of compound **5** in DMSO-d_6

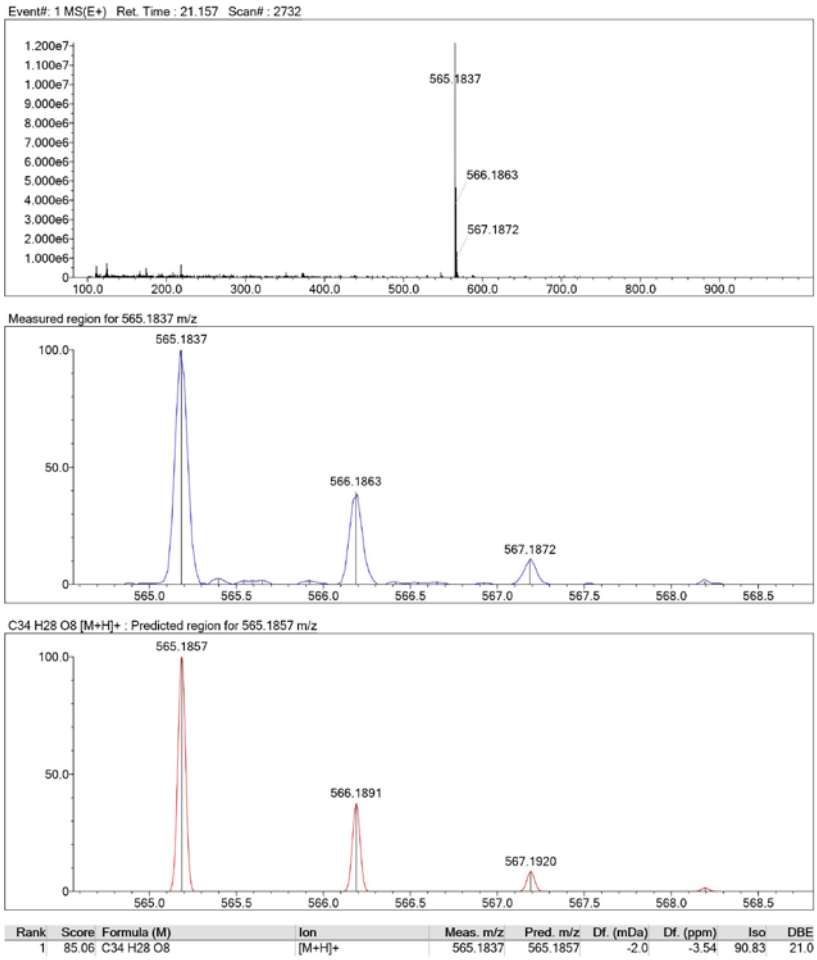


Figure S47. HRESIMS spectrum of compound **6**

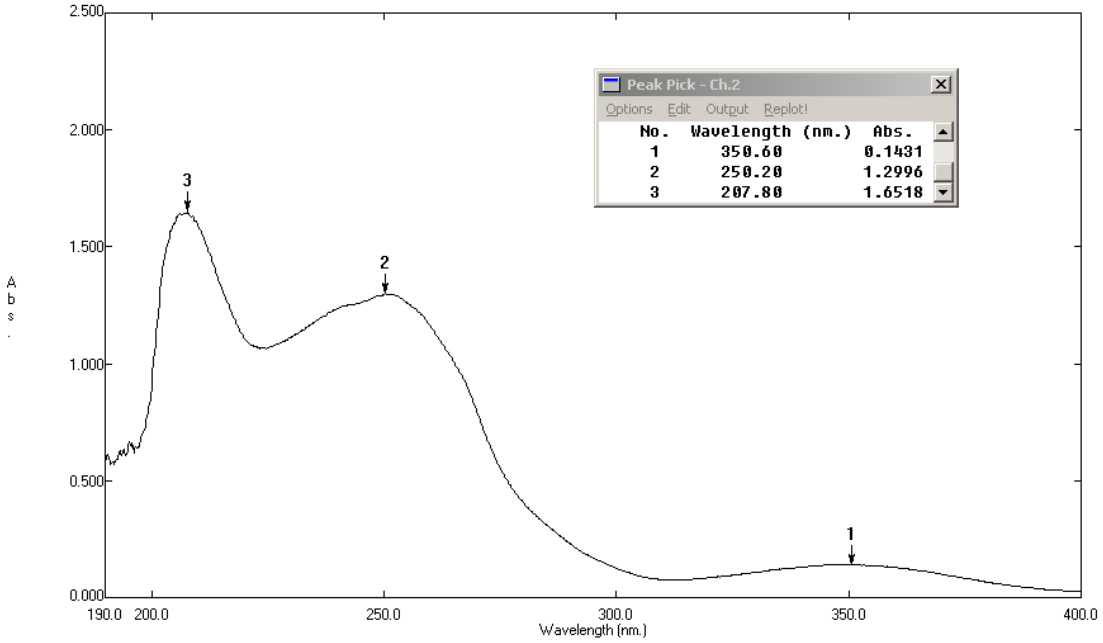


Figure S48. UV spectrum of compound **6**

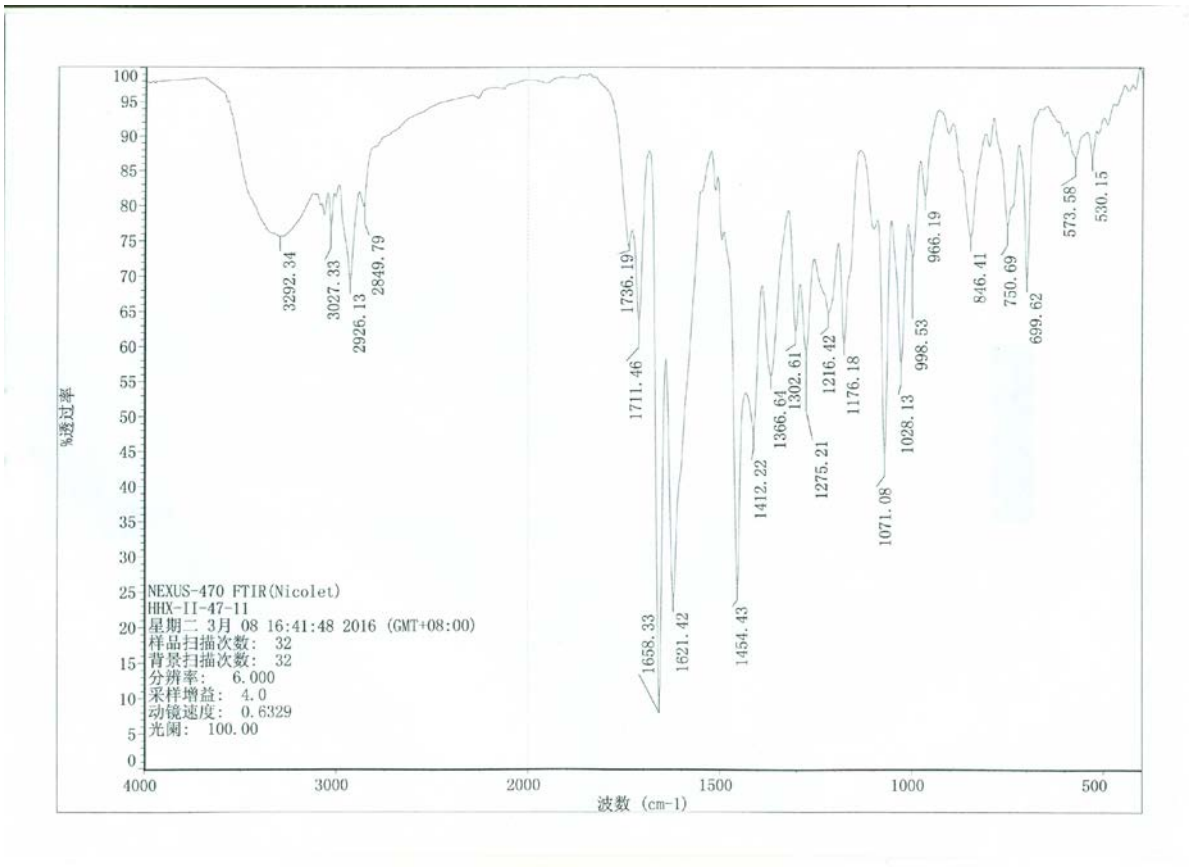


Figure S49. IR spectrum of compound **6**

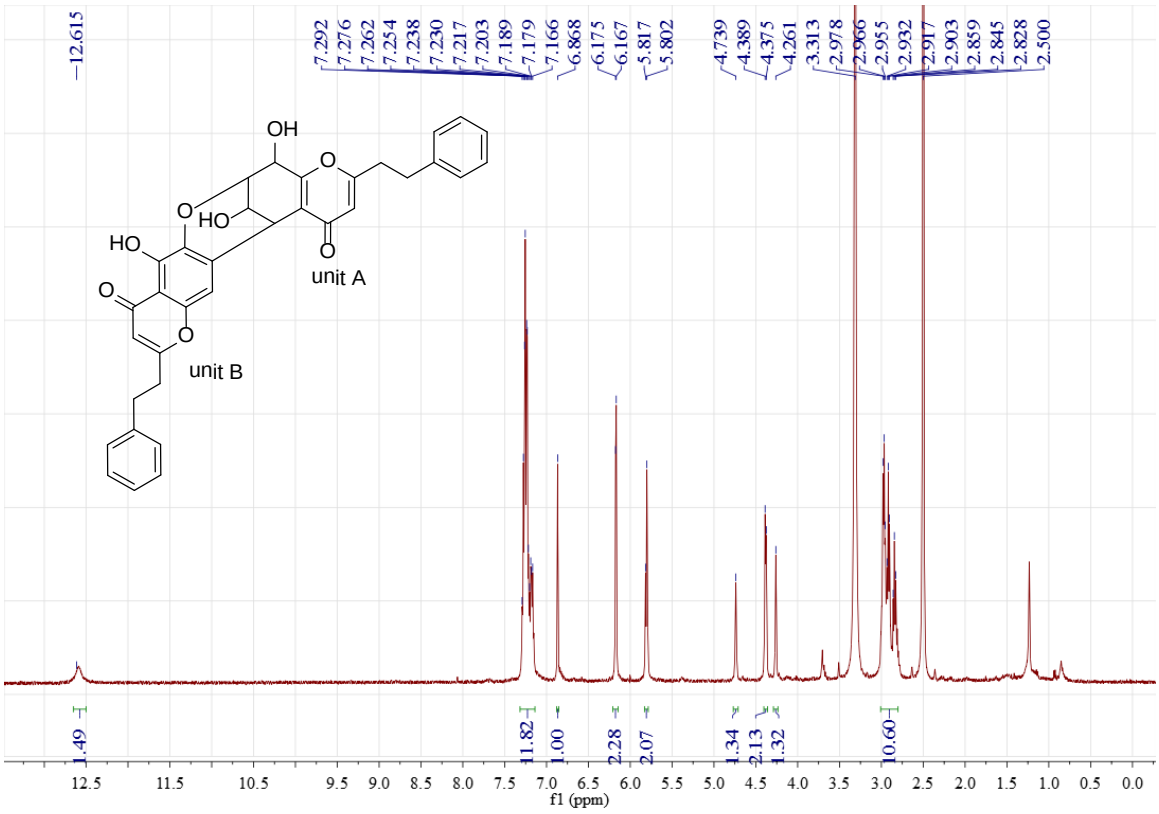


Figure S50. ^{1}H NMR spectrum of compound **6** in DMSO-d_6

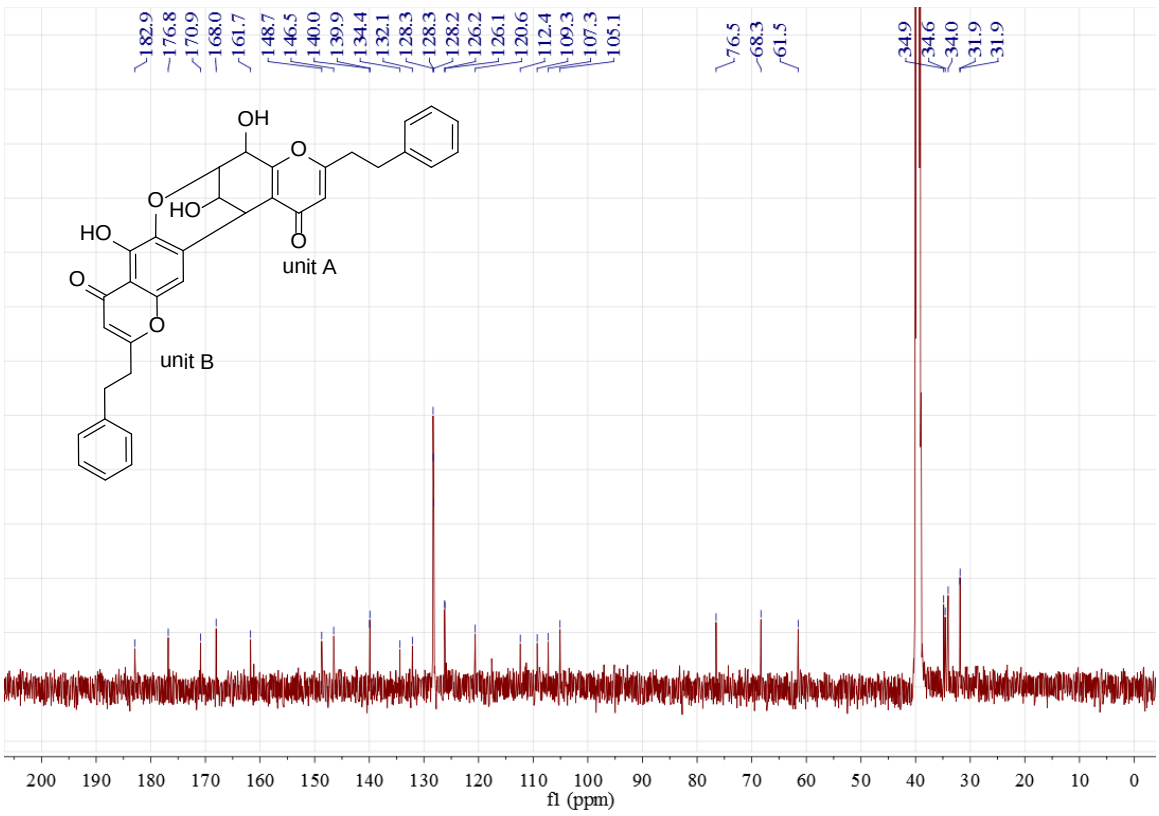


Figure S51. ^{13}C NMR spectrum of compound **6** in DMSO-d_6

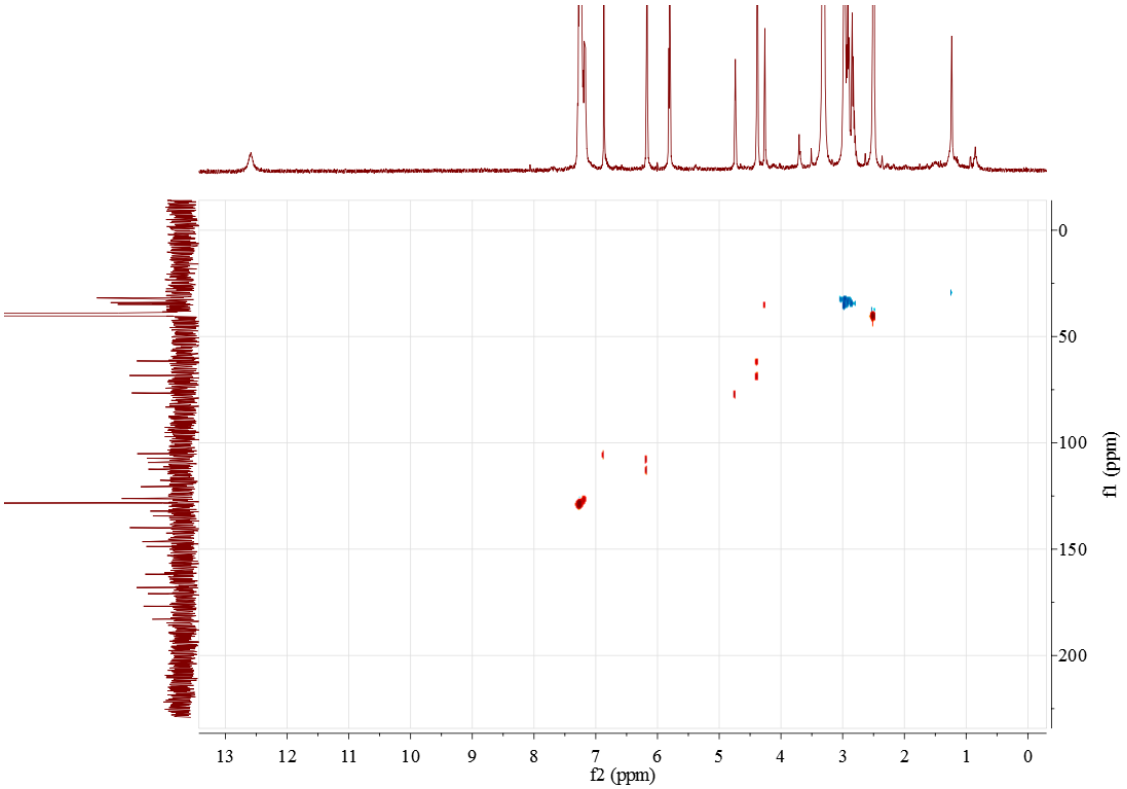


Figure S52. gHSQC spectrum of compound **6** in DMSO-d_6

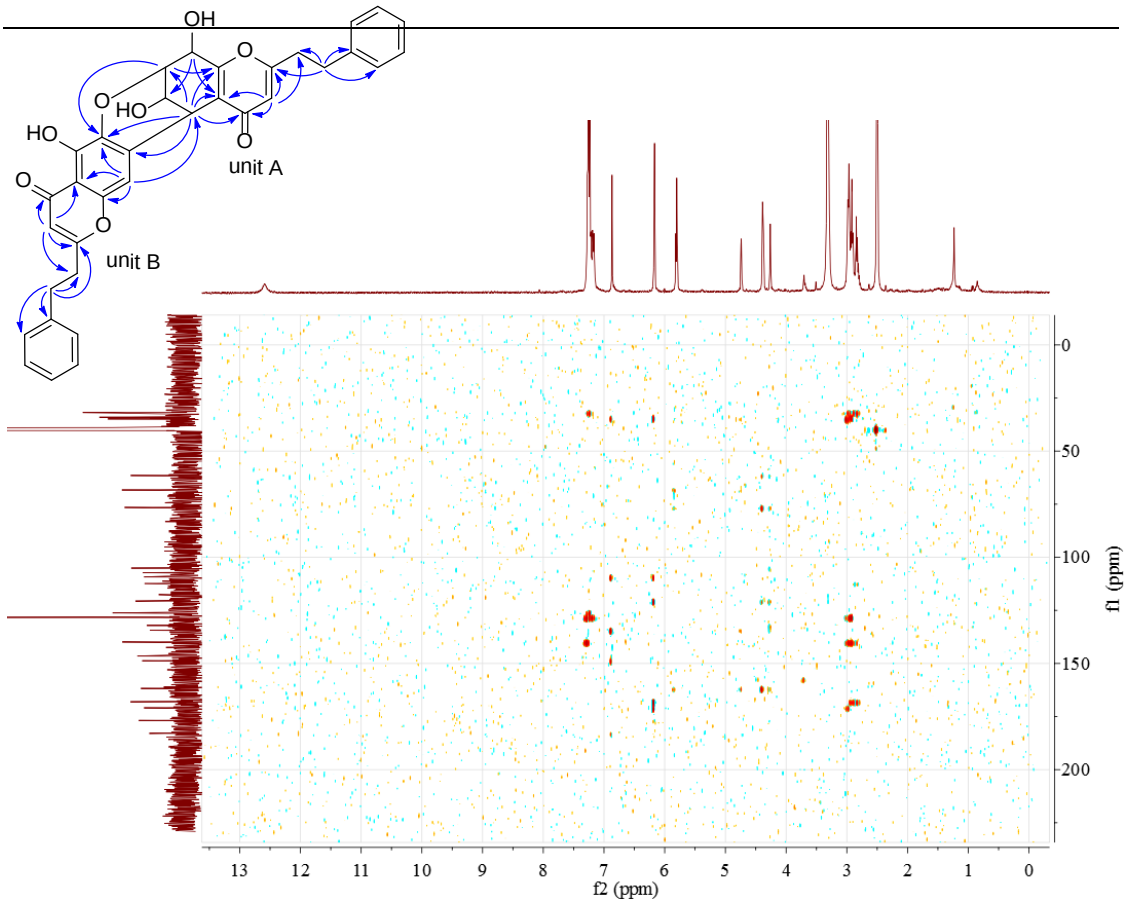


Figure S53. gHMBC spectrum of compound **6** in DMSO-d_6

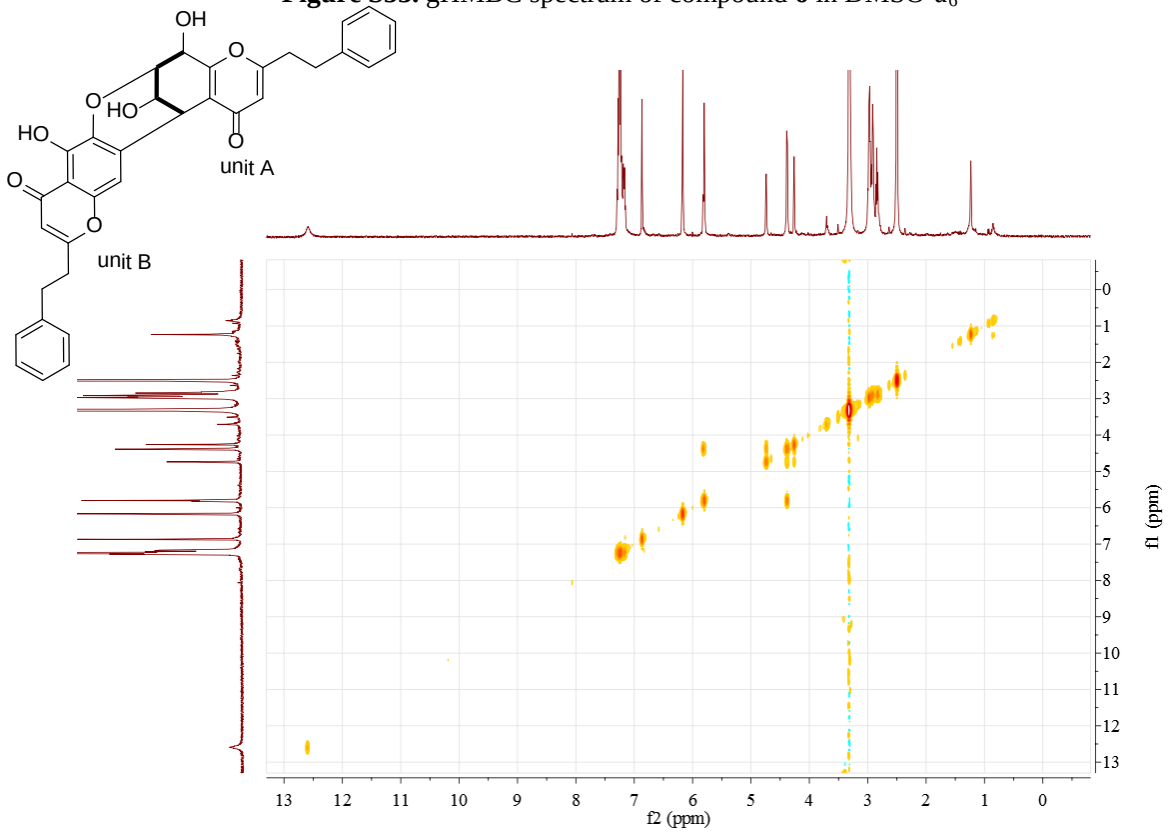


Figure S54. ^{1}H-^{1}H COSY spectrum of compound **6** in DMSO-d_6

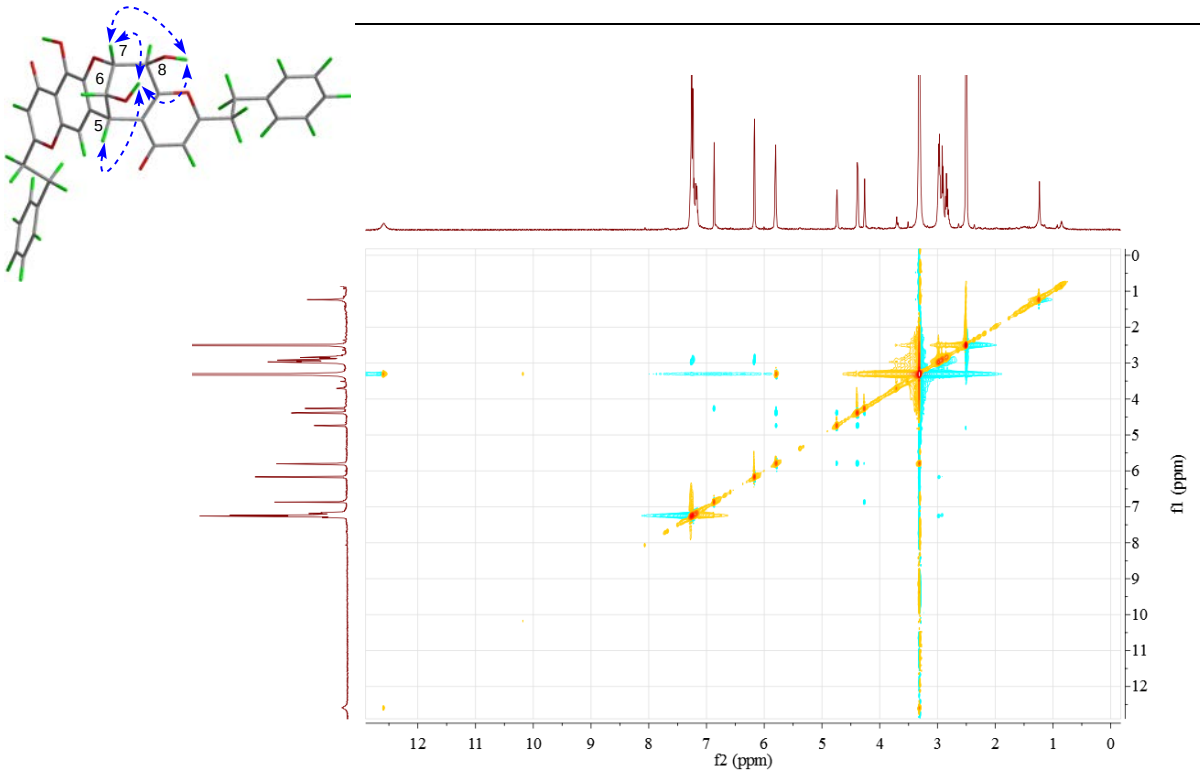


Figure S55. ROESY spectrum of compound **6** in DMSO-d_6

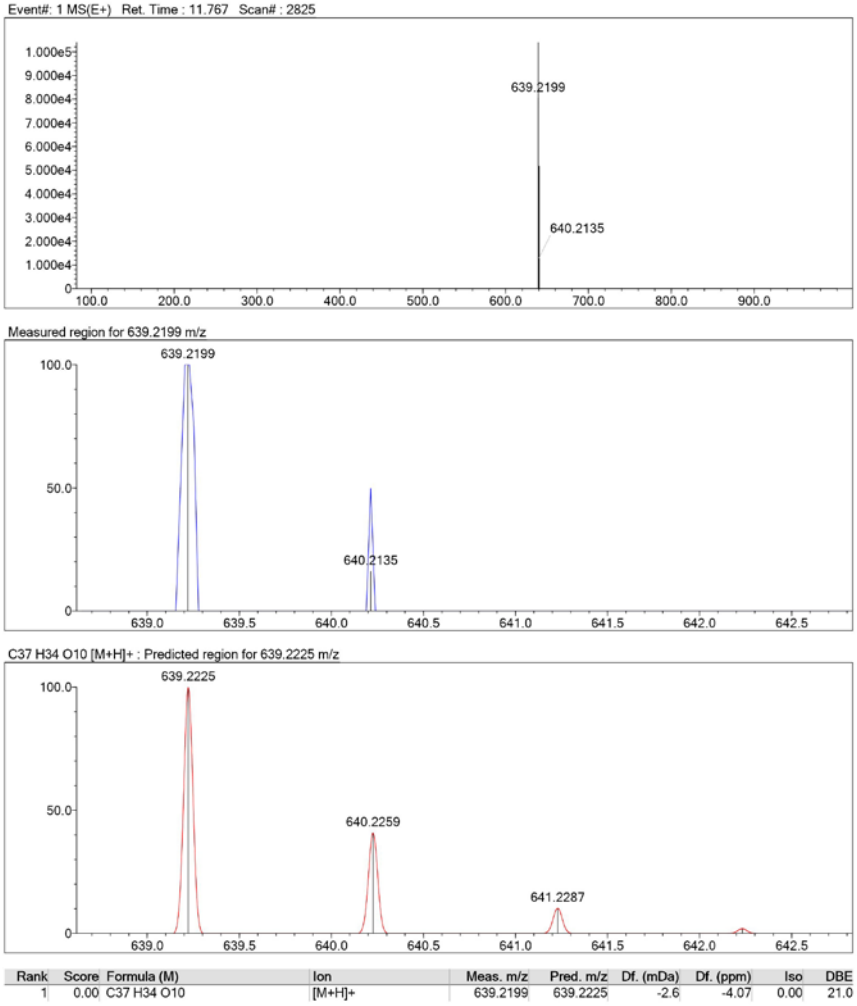


Figure S56. HRESIMS spectrum of compound **7**

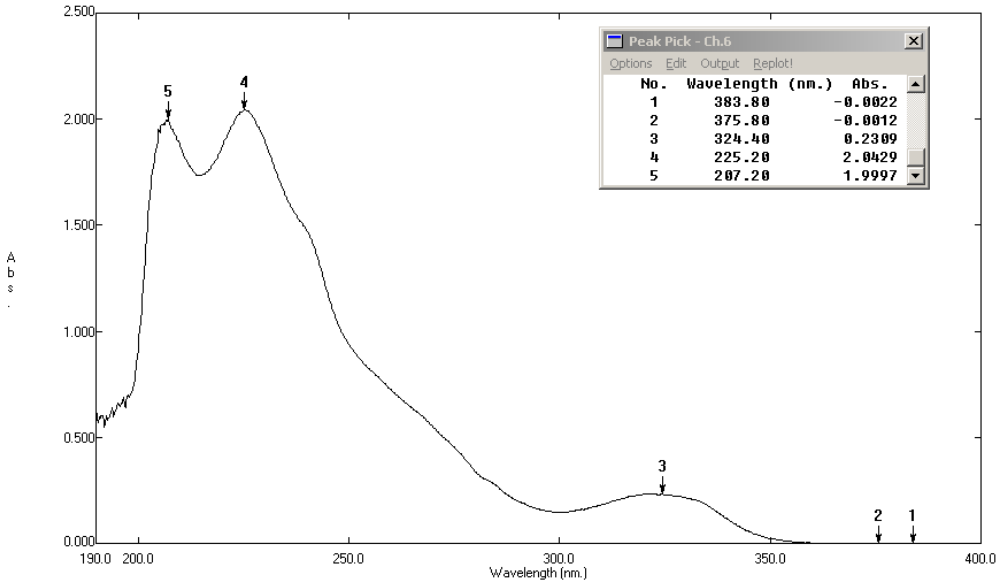


Figure S57. UV spectrum of compound **7**

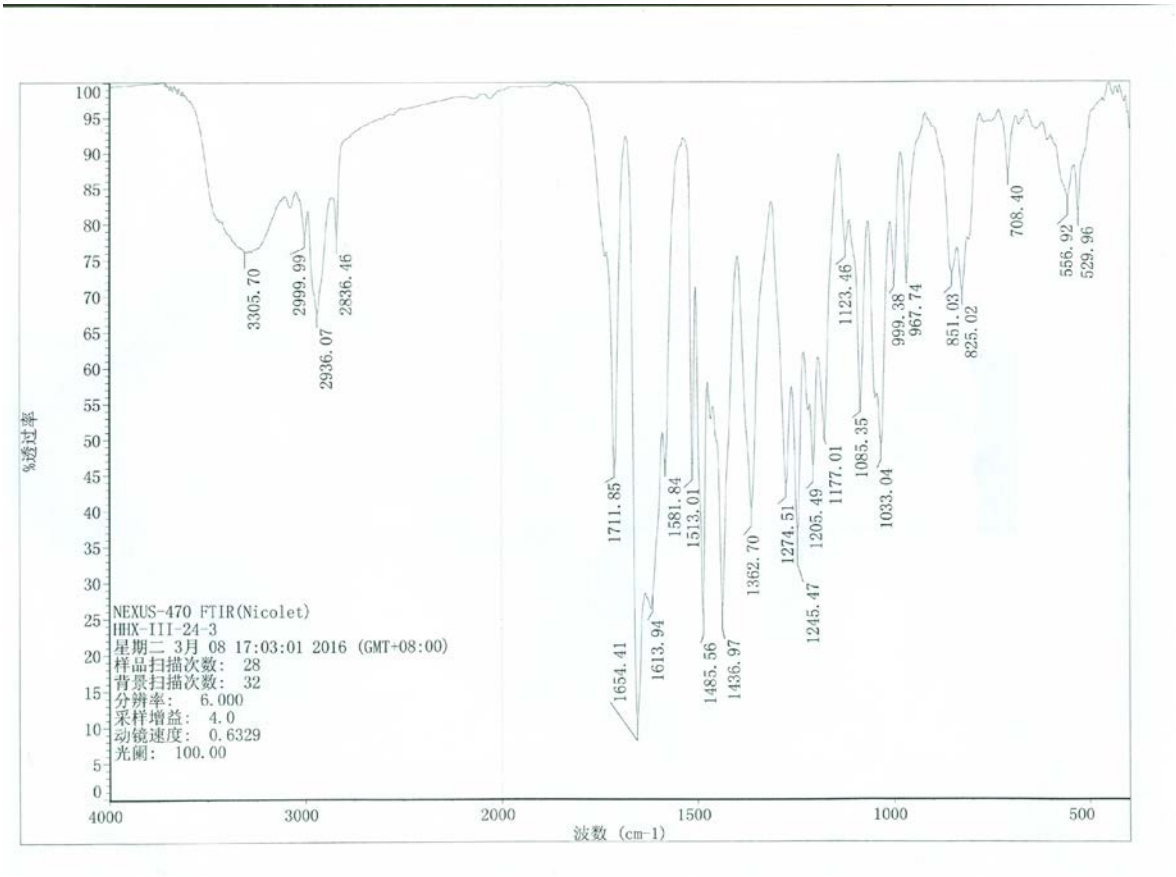


Figure S58. IR spectrum of compound **7**

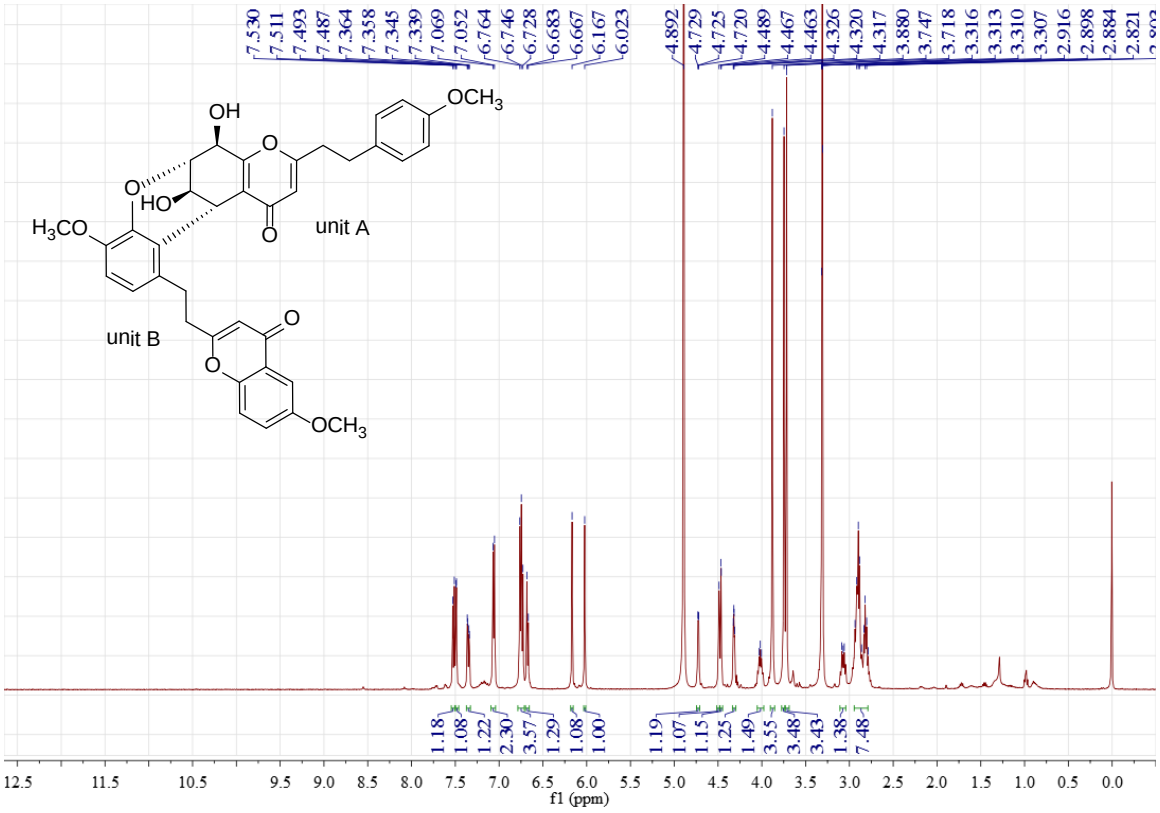


Figure S59. ^{1}H NMR spectrum of compound **7** in methanol-d_4

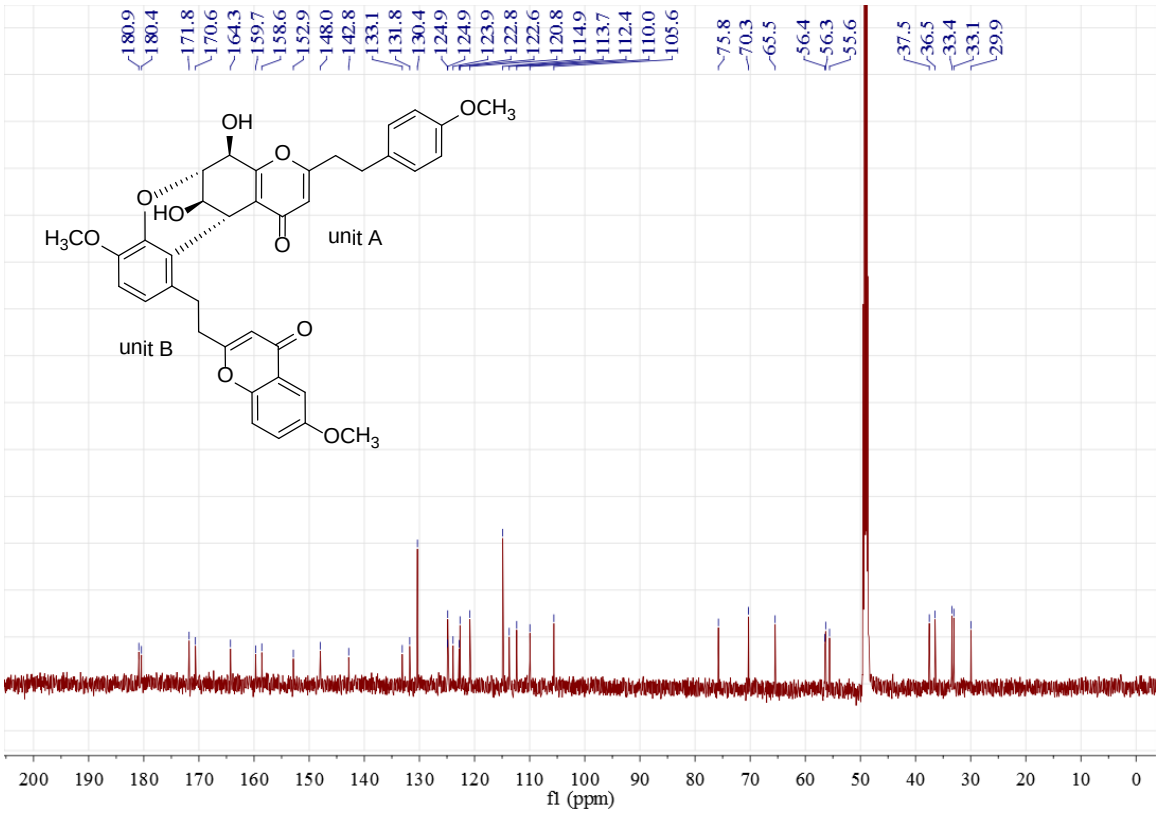


Figure S60. ^{13}C NMR spectrum of compound **7** in methanol-d_4

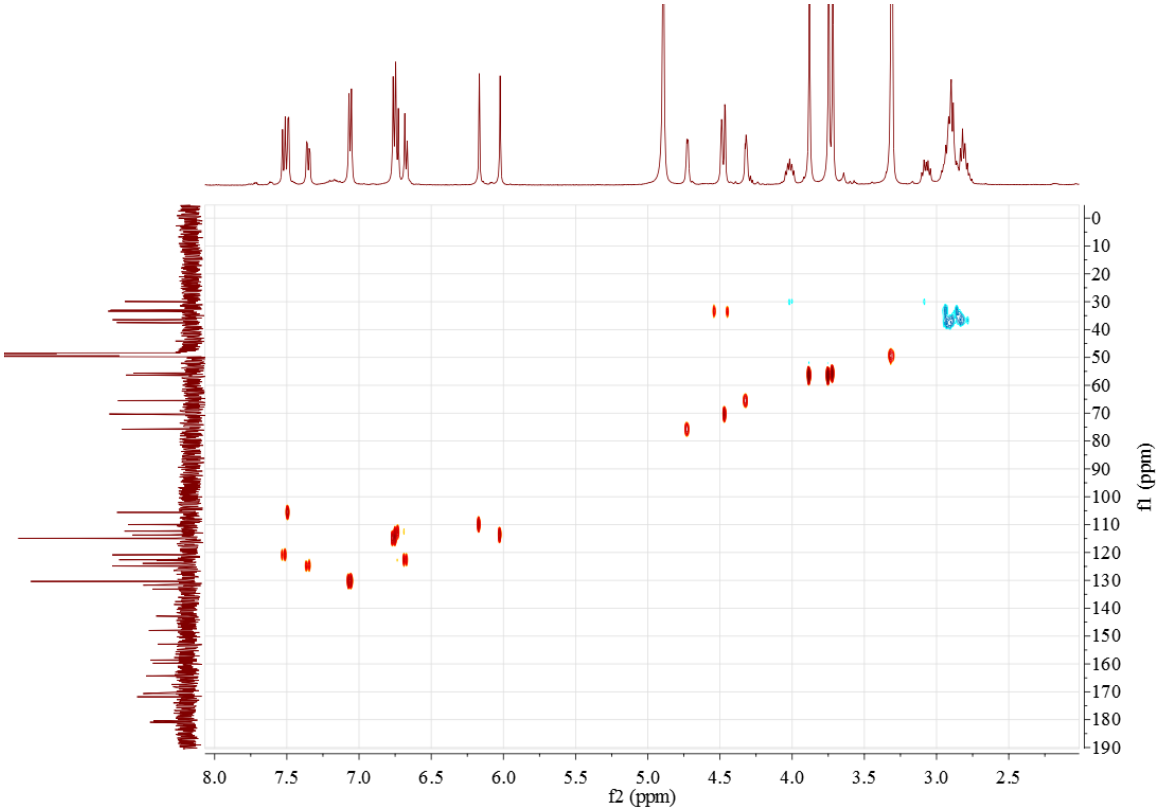


Figure S61. gHSQC spectrum of compound **7** in methanol-d_4

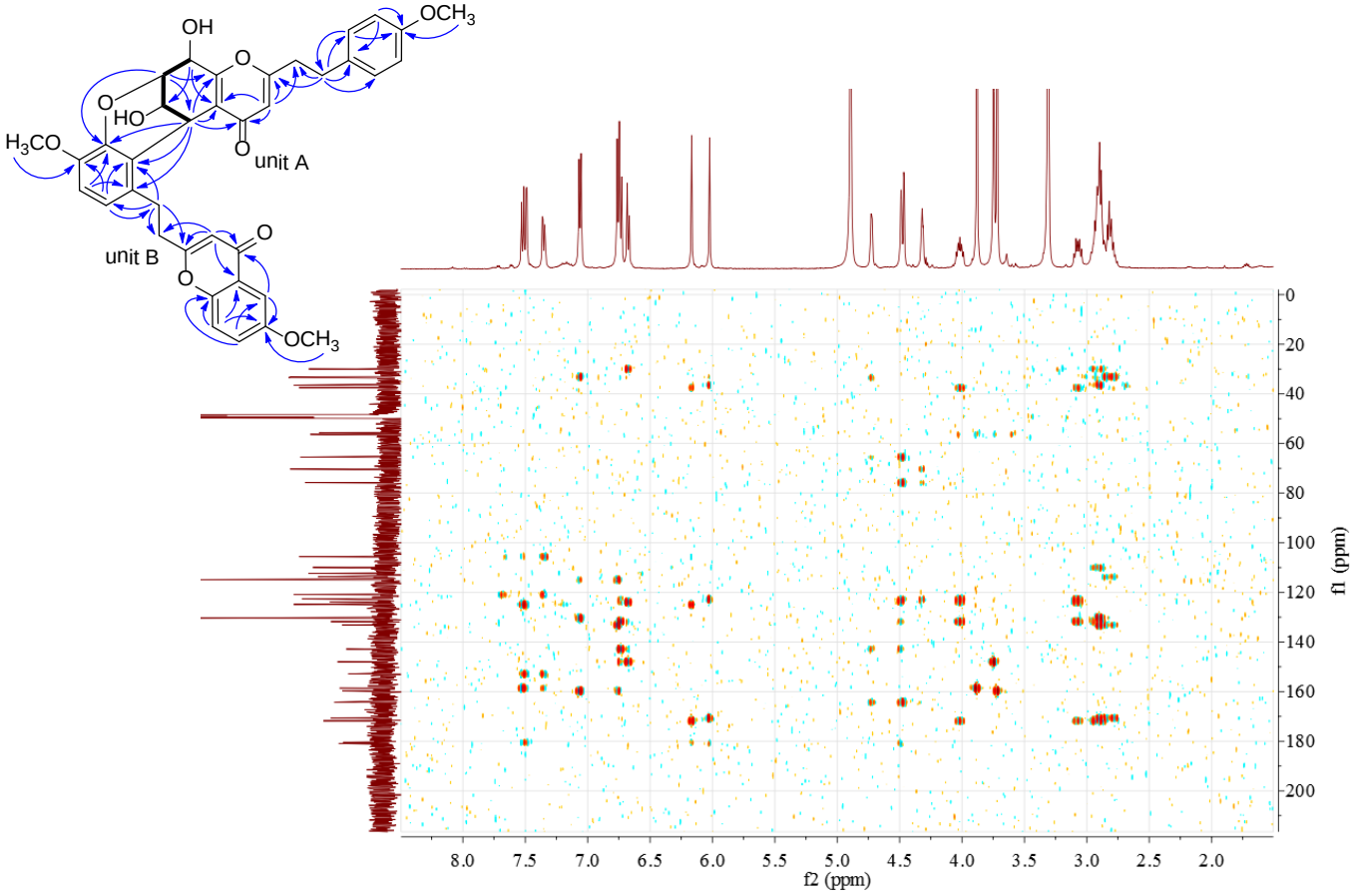


Figure S62. gHMBC spectrum of compound **7** in methanol-d_4

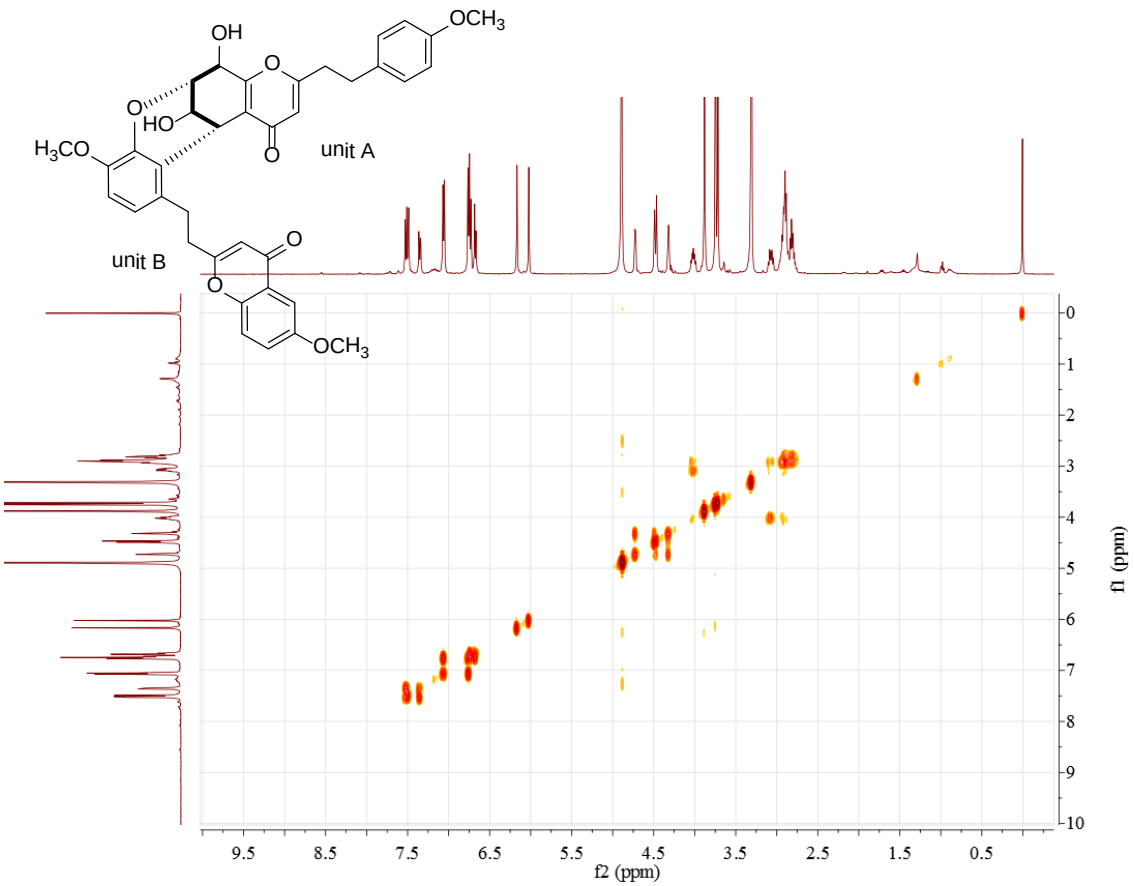


Figure S63. ^{1}H-^{1}H COSY spectrum of compound **7** in methanol-d_4

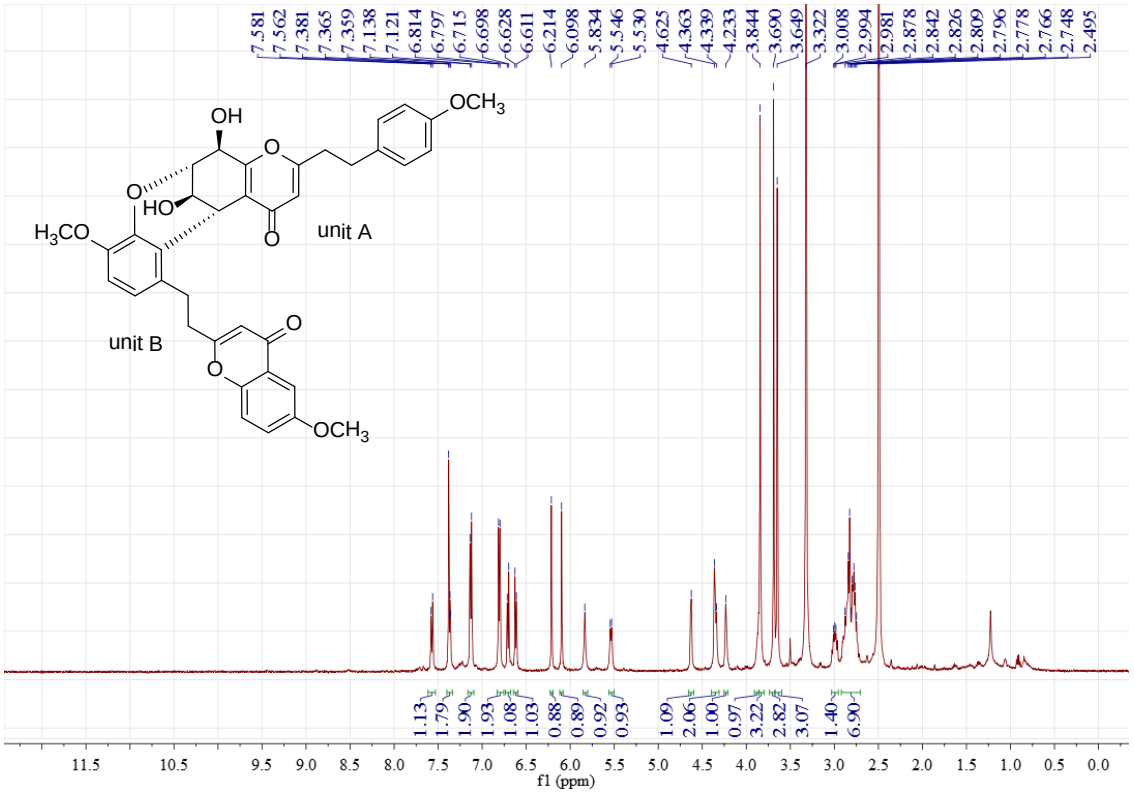


Figure S64 ^{1}H NMR spectrum of compound **7** in DMSO-d_6

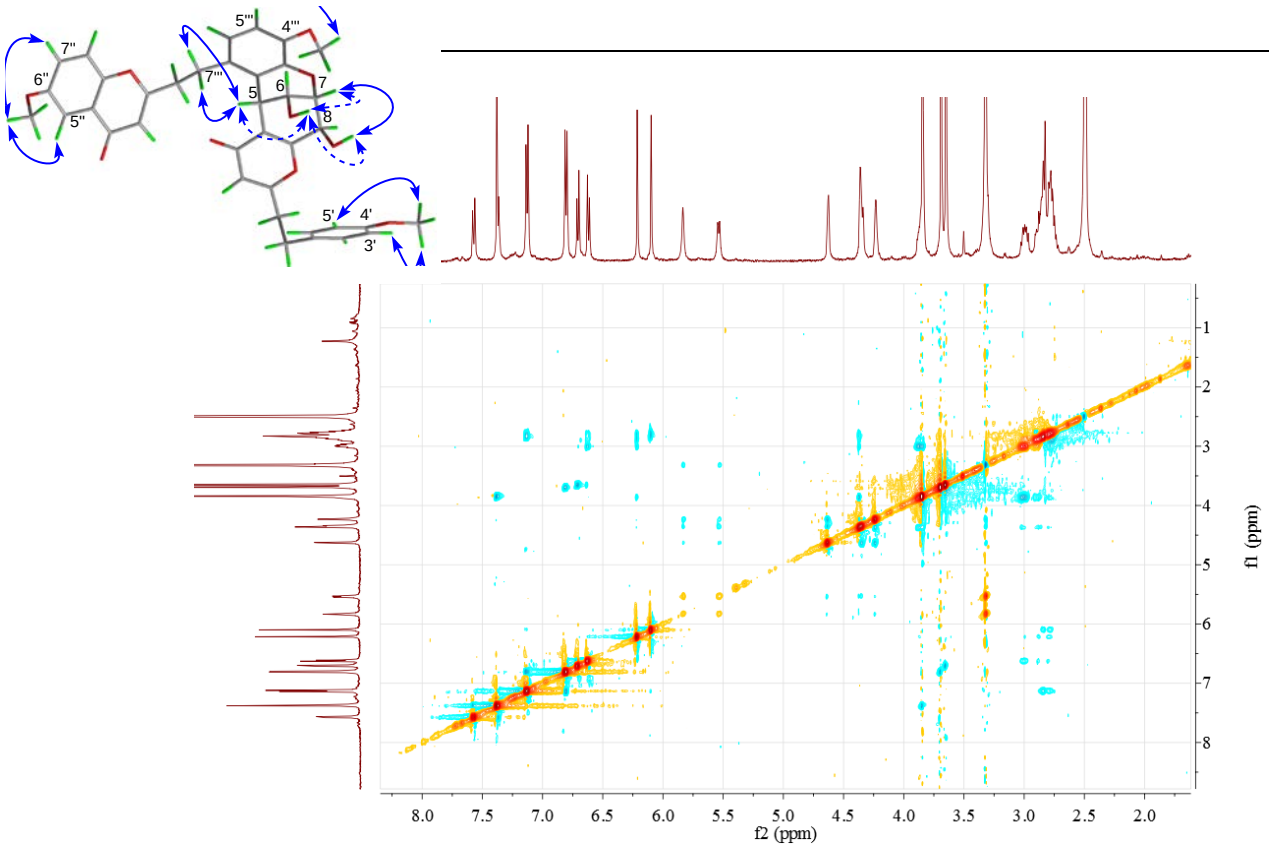


Figure S65. ROESY spectrum of compound **7** in DMSO-d_6

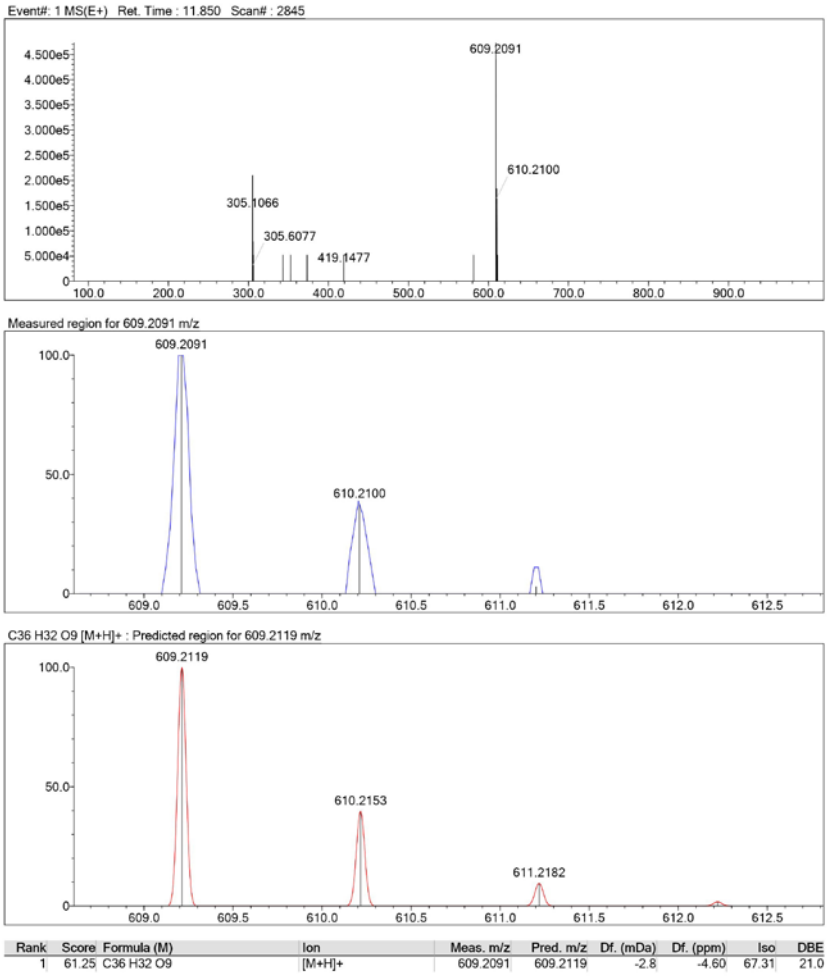


Figure S66. HRESIMS spectrum of compound **8**

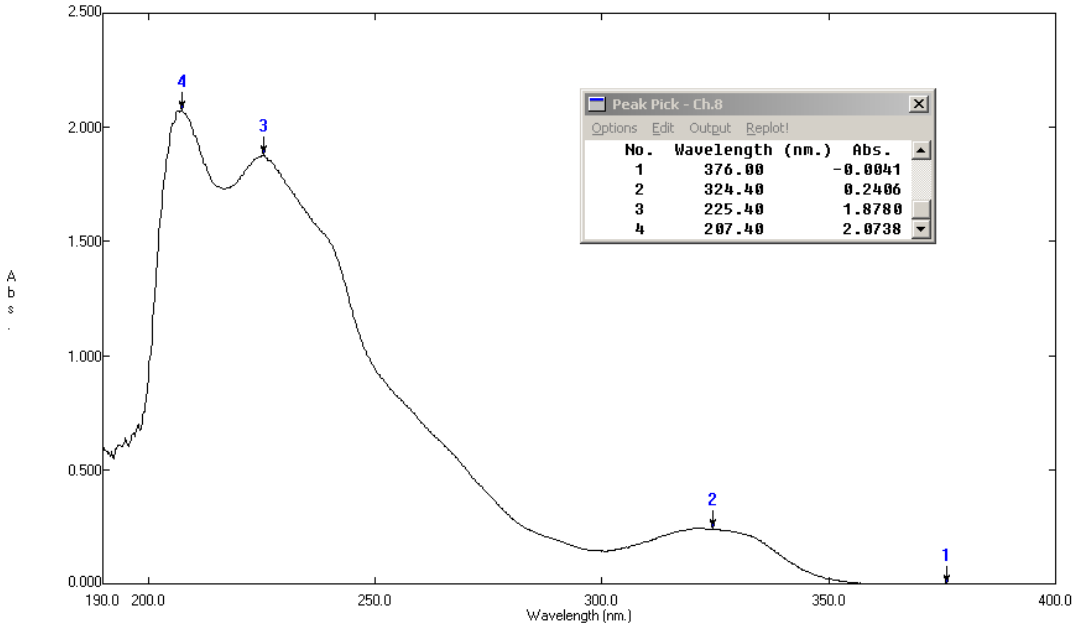


Figure S67. UV spectrum of compound **8**

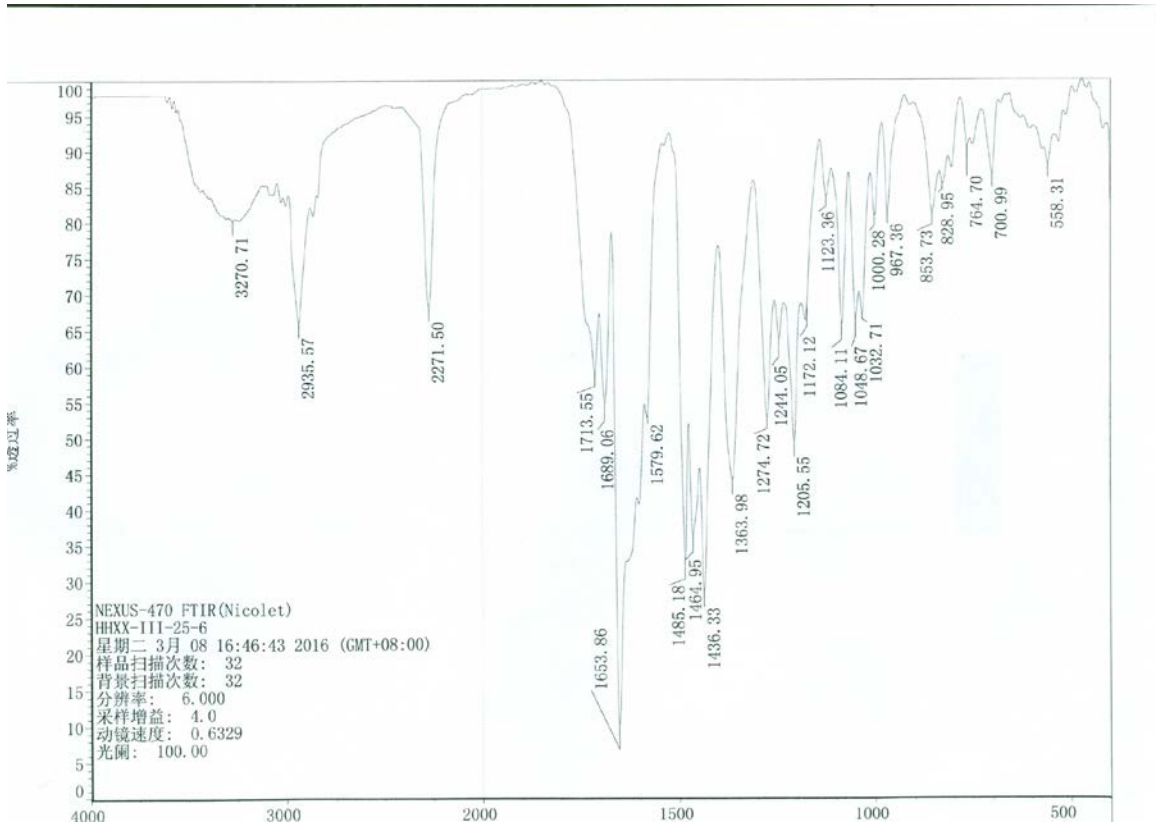


Figure S68. IR spectrum of compound **8**

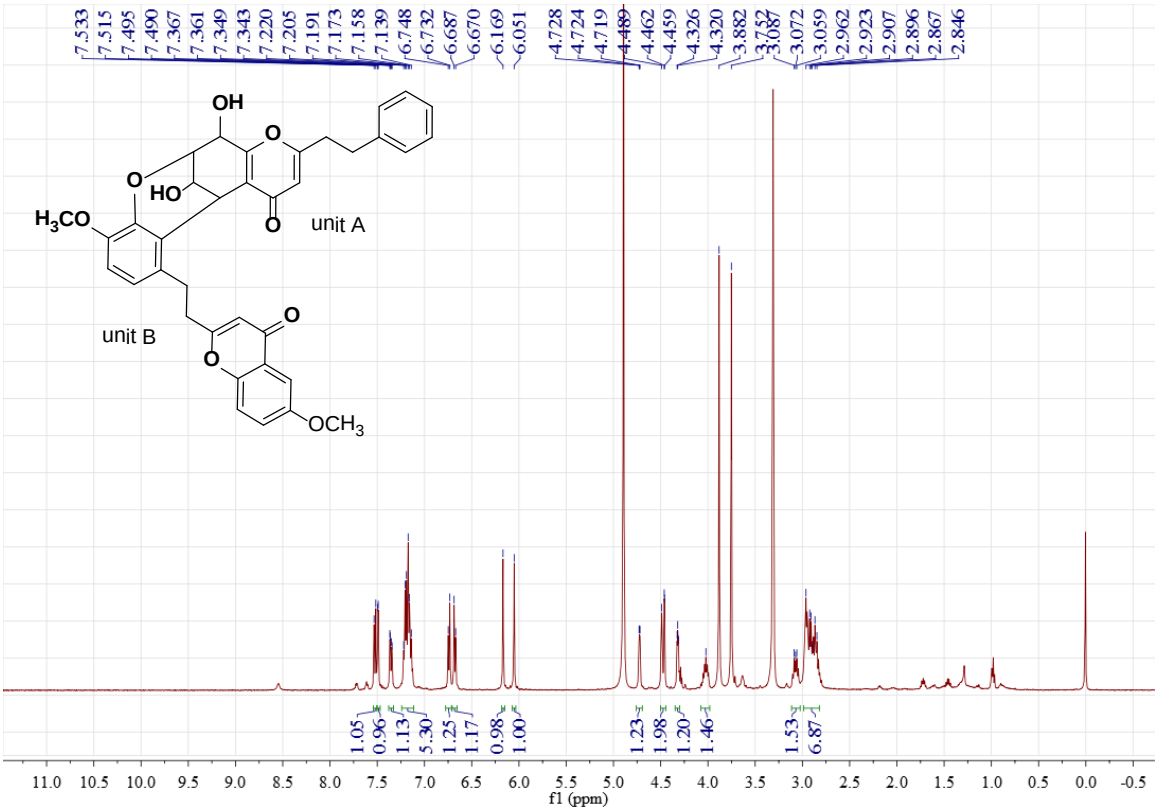


Figure S69. ^{1}H NMR spectrum of compound **8** in methanol-d_4

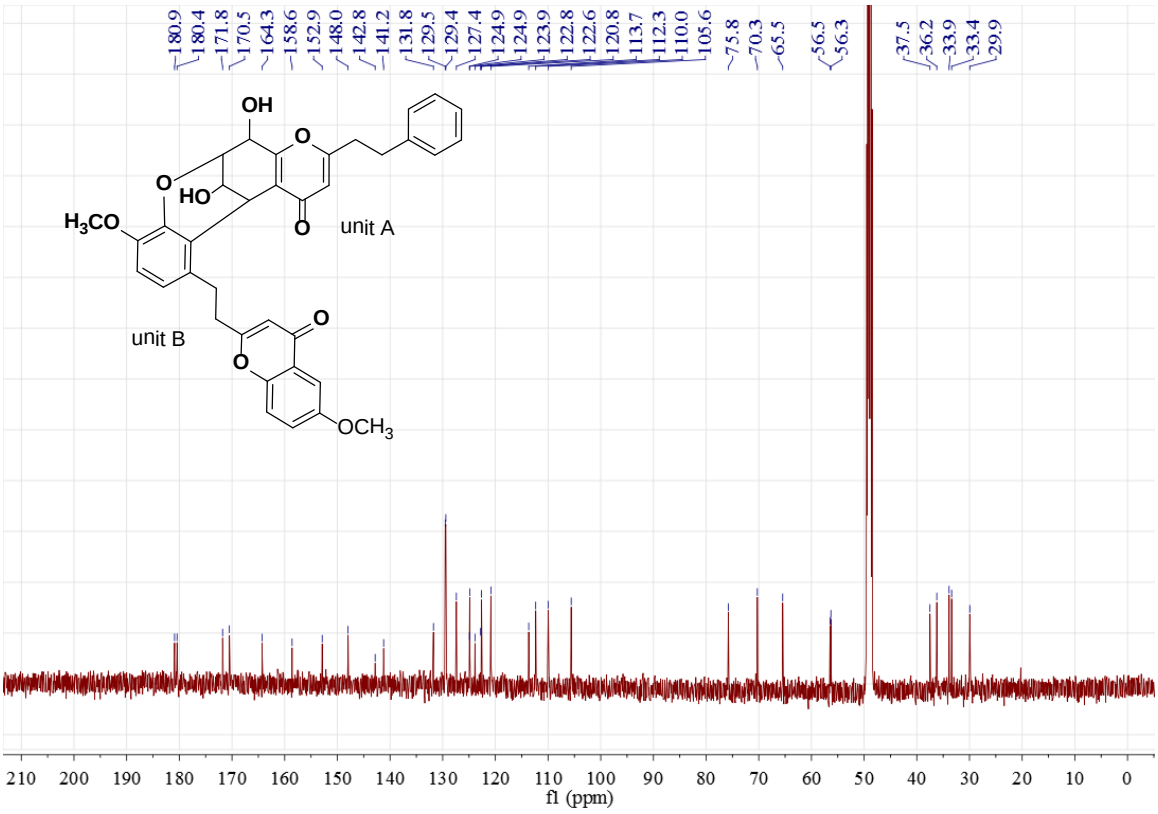


Figure S70. ^{13}C NMR spectrum of compound **8** in methanol-d_4

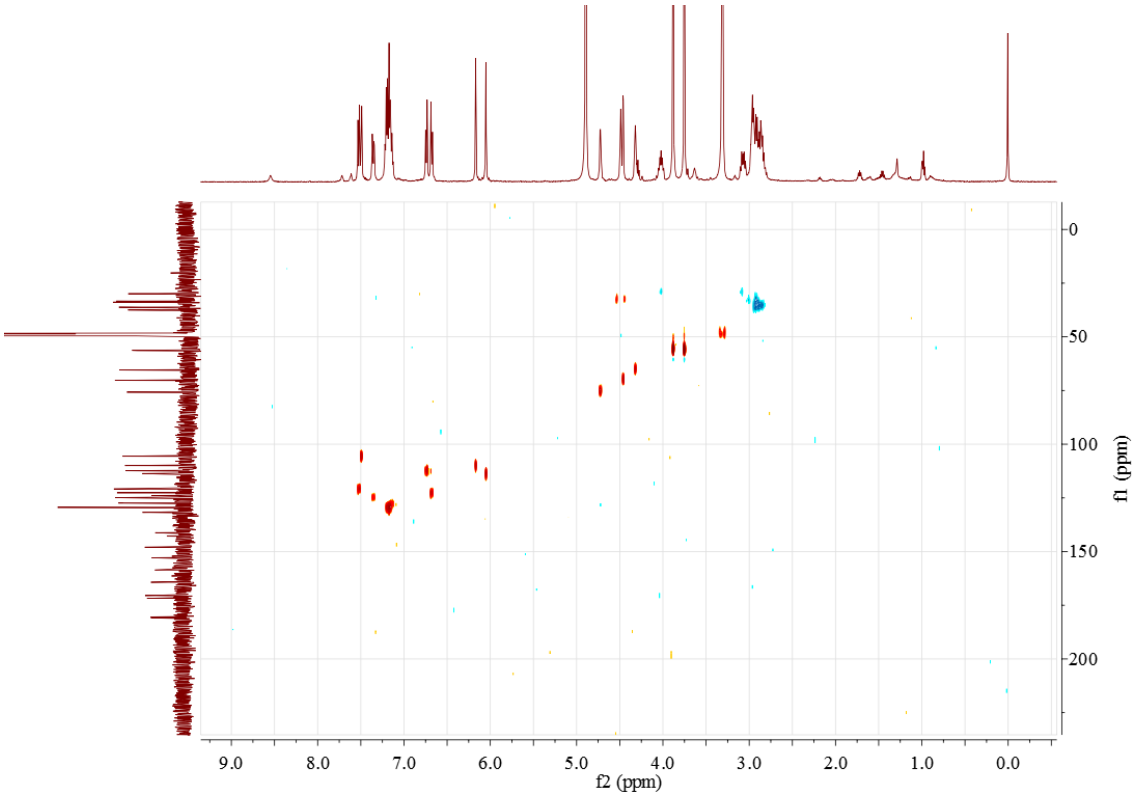


Figure S71. gHSQC spectrum of compound **8** in methanol-d_4

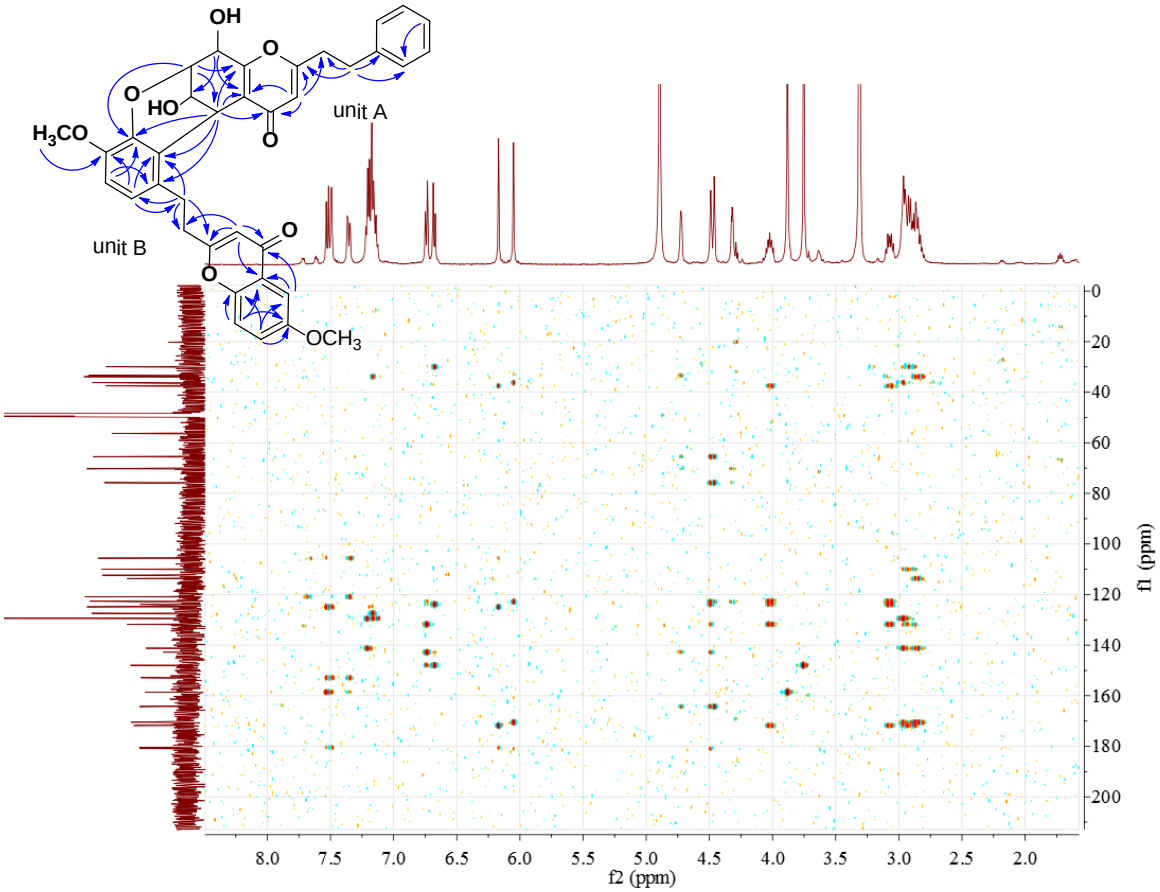


Figure S72. gHMBC spectrum of compound **8** in methanol-d_4

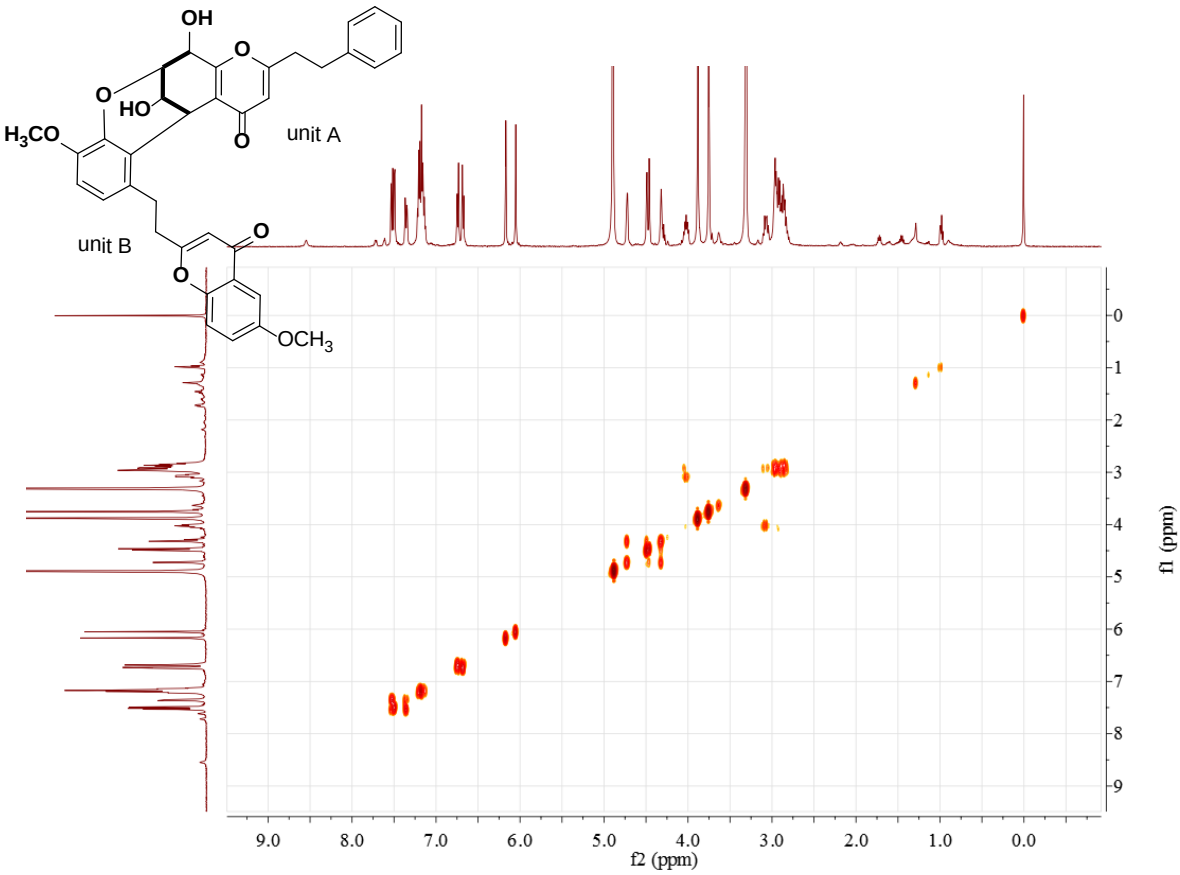


Figure S73. ^{1}H-^{1}H COSY spectrum of compound **8** in methanol-d_4

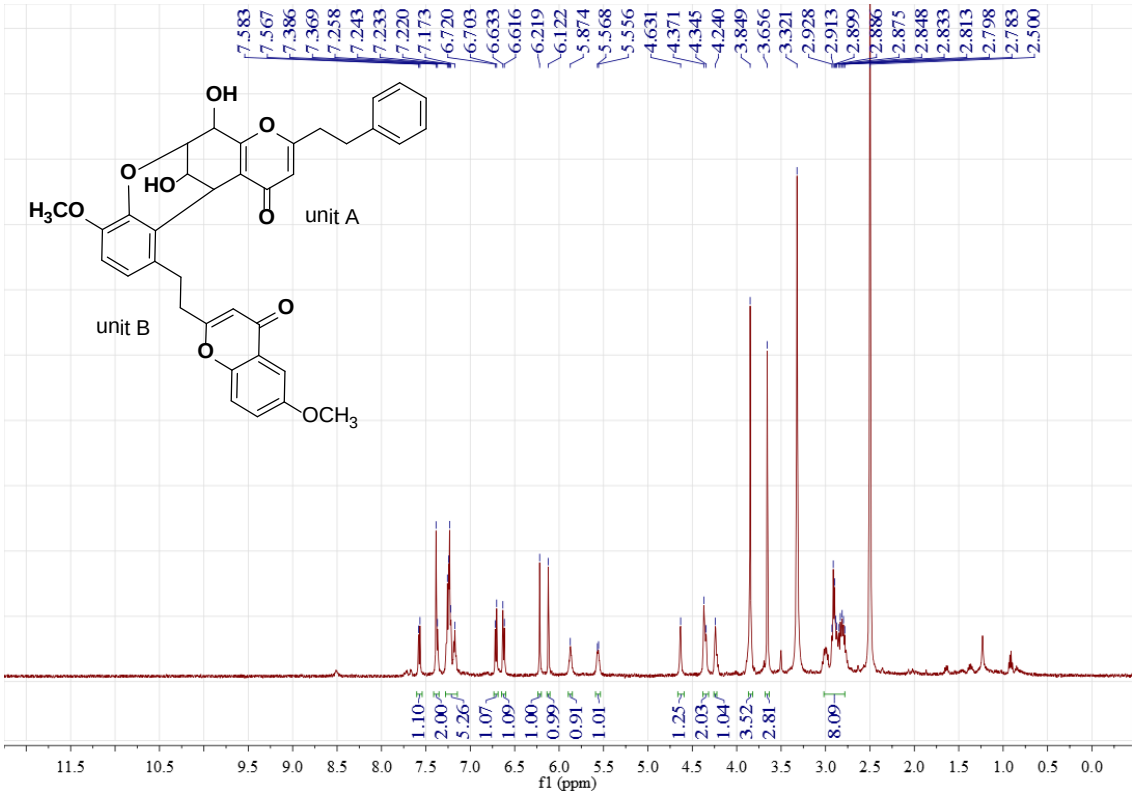


Figure S74. ^{1}H NMR spectrum of compound **8** in DMSO-d_6

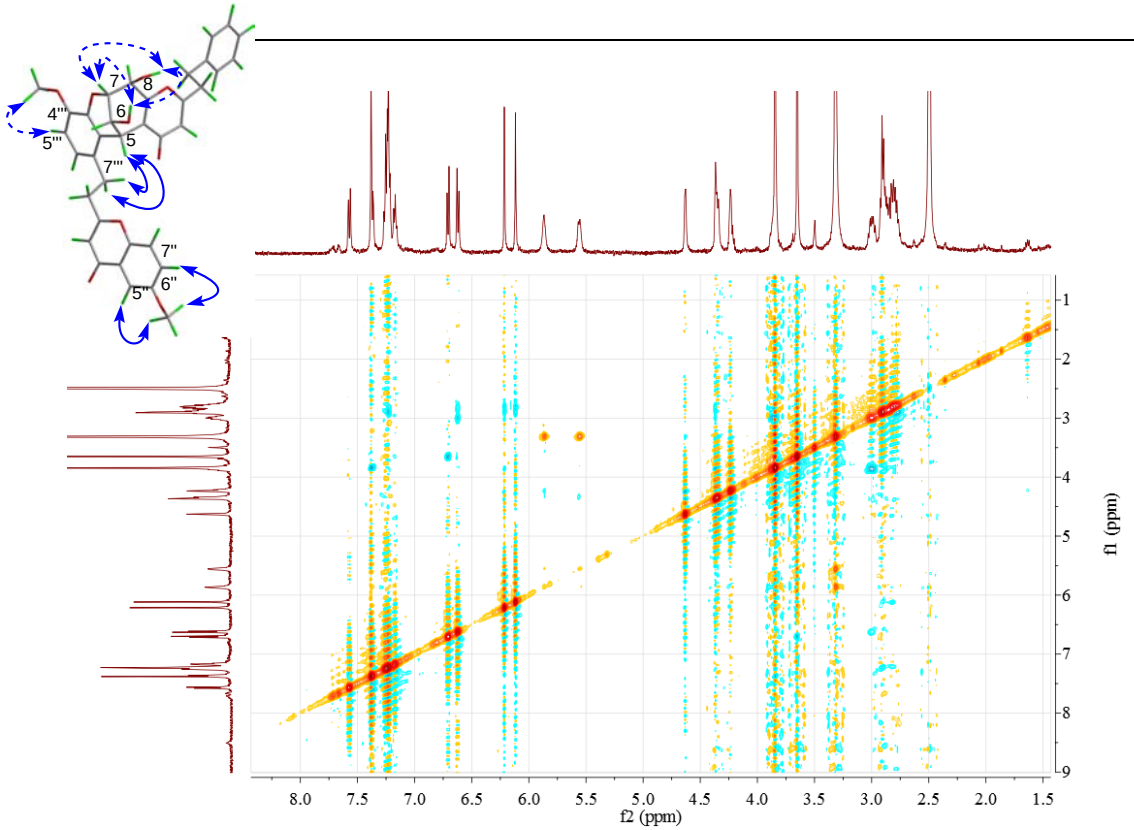


Figure S75. ROESY spectrum of compound **8** in DMSO-d_6

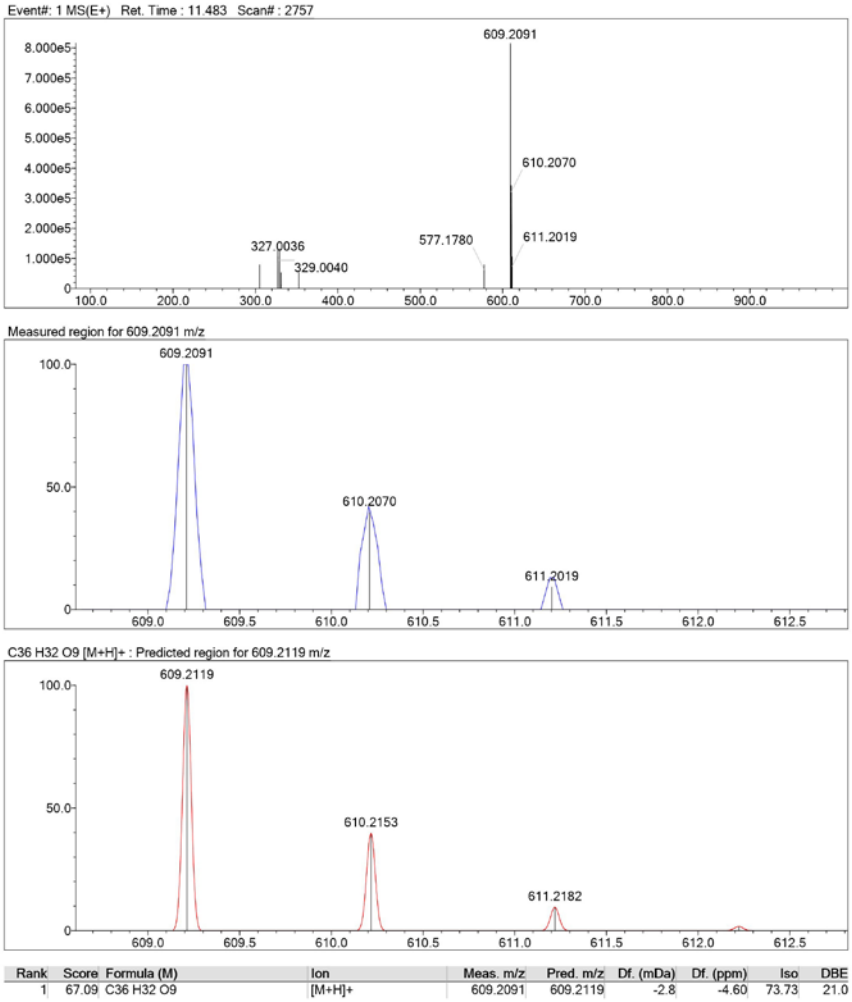


Figure S76. HRESIMS spectrum of compound **9**

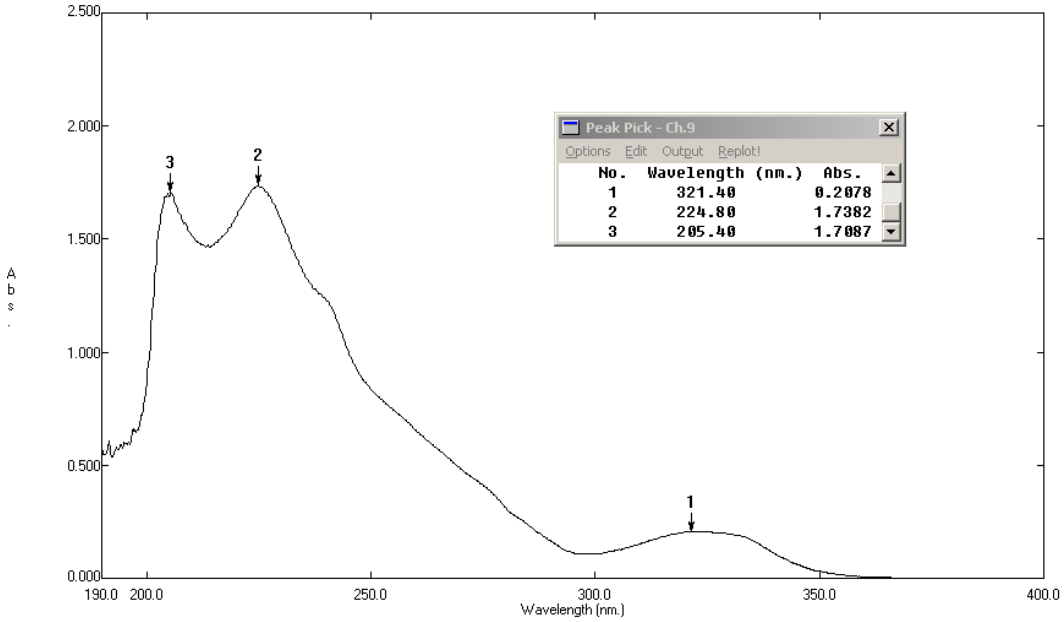


Figure S77. UV spectrum of compound **9**

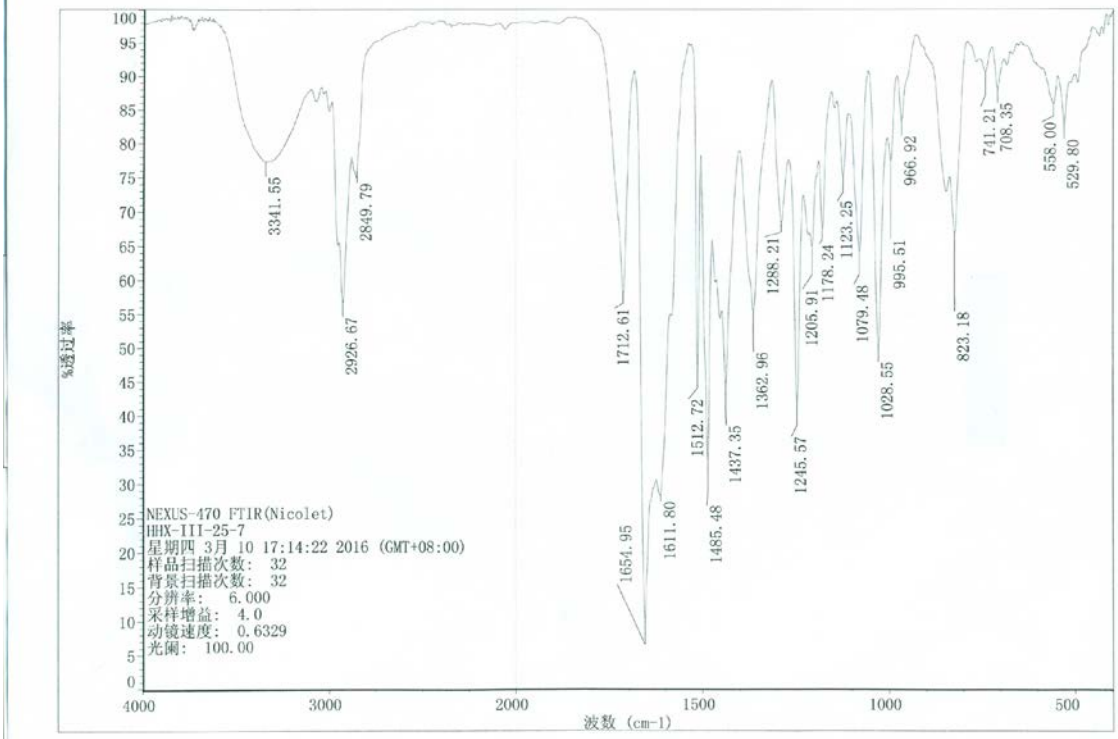


Figure S78. IR spectrum of compound **9**

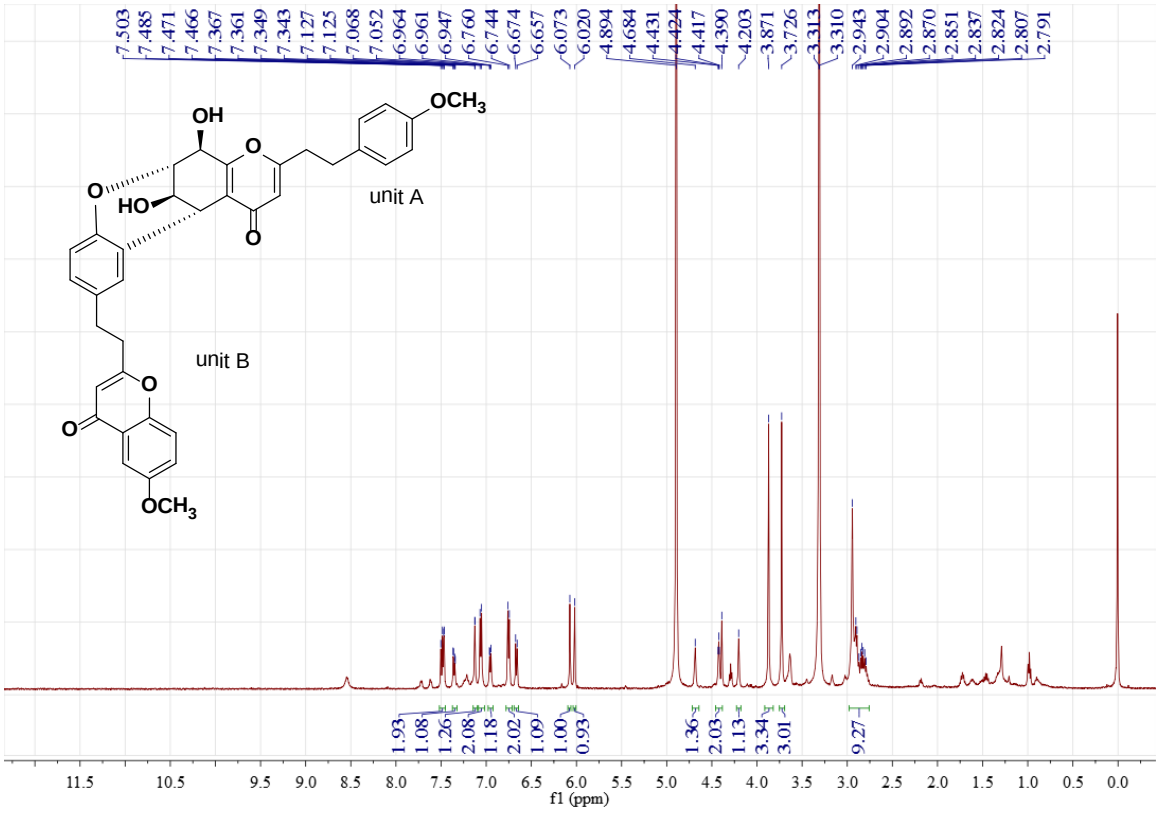


Figure S79. ^{1}H NMR spectrum of compound **9** in methanol-d_4

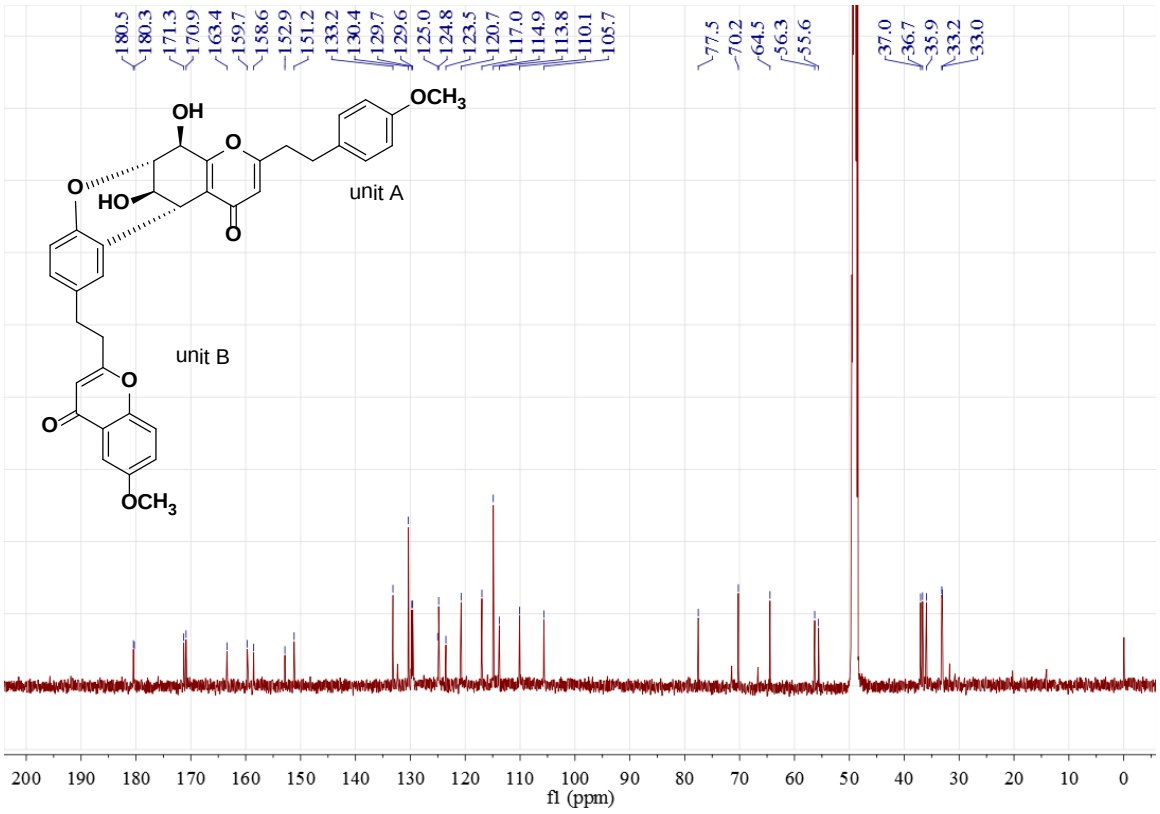


Figure S80. ^{13}C NMR spectrum of compound **9** in methanol-d_4

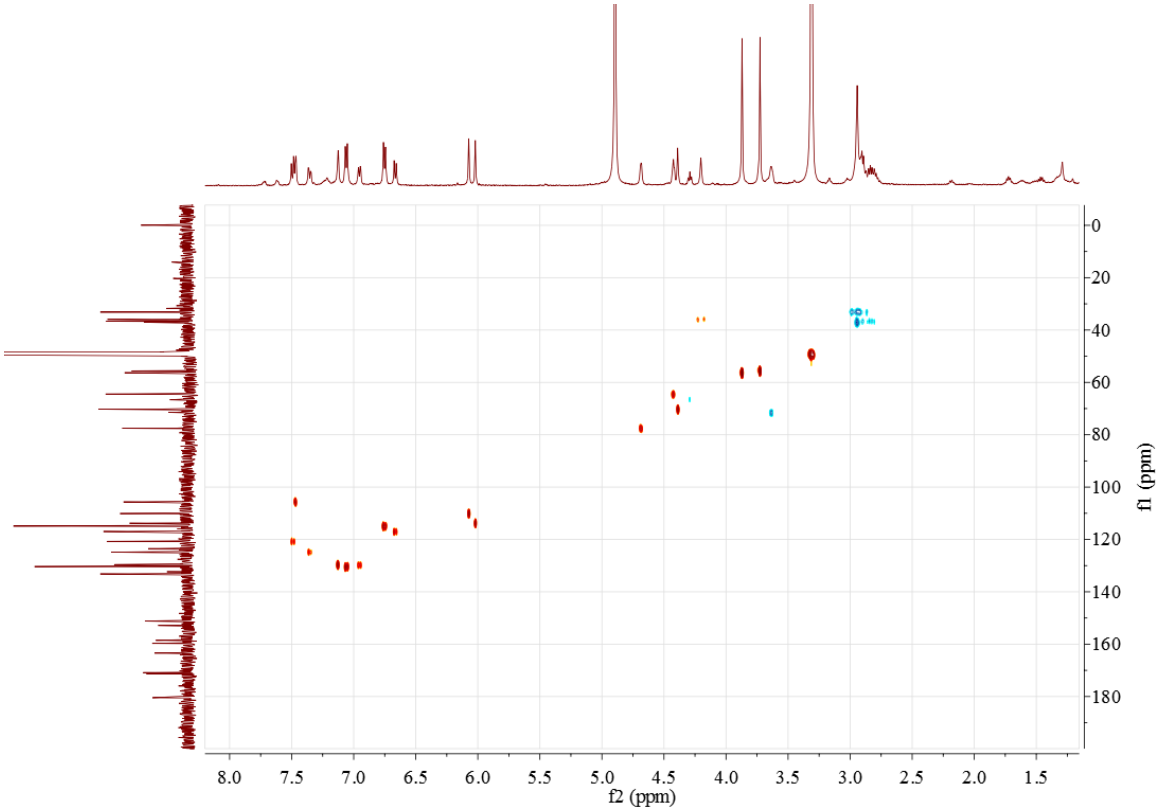


Figure S81. gHSQC spectrum of compound **9** in methanol-d_4

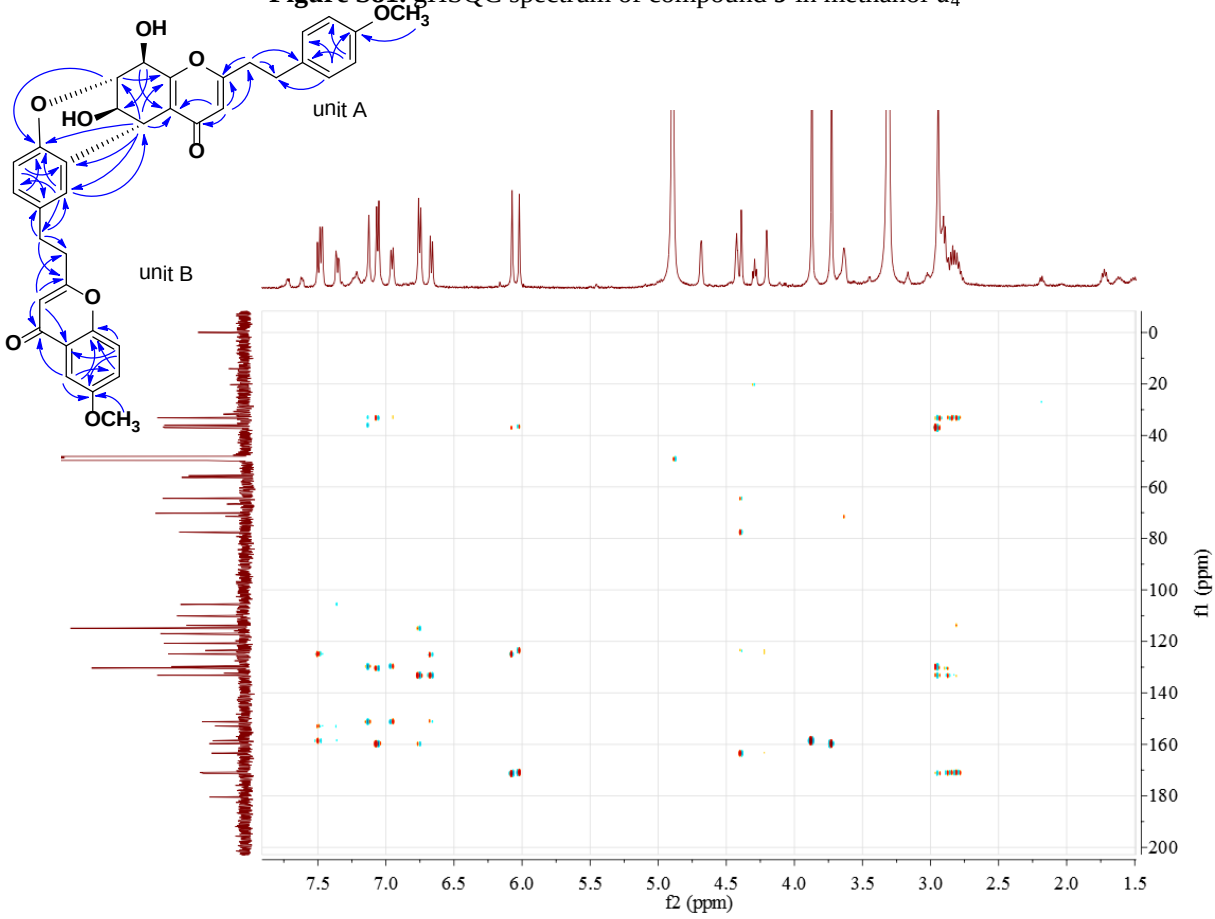


Figure S82. gHMBC spectrum of compound **9** in methanol-d_4

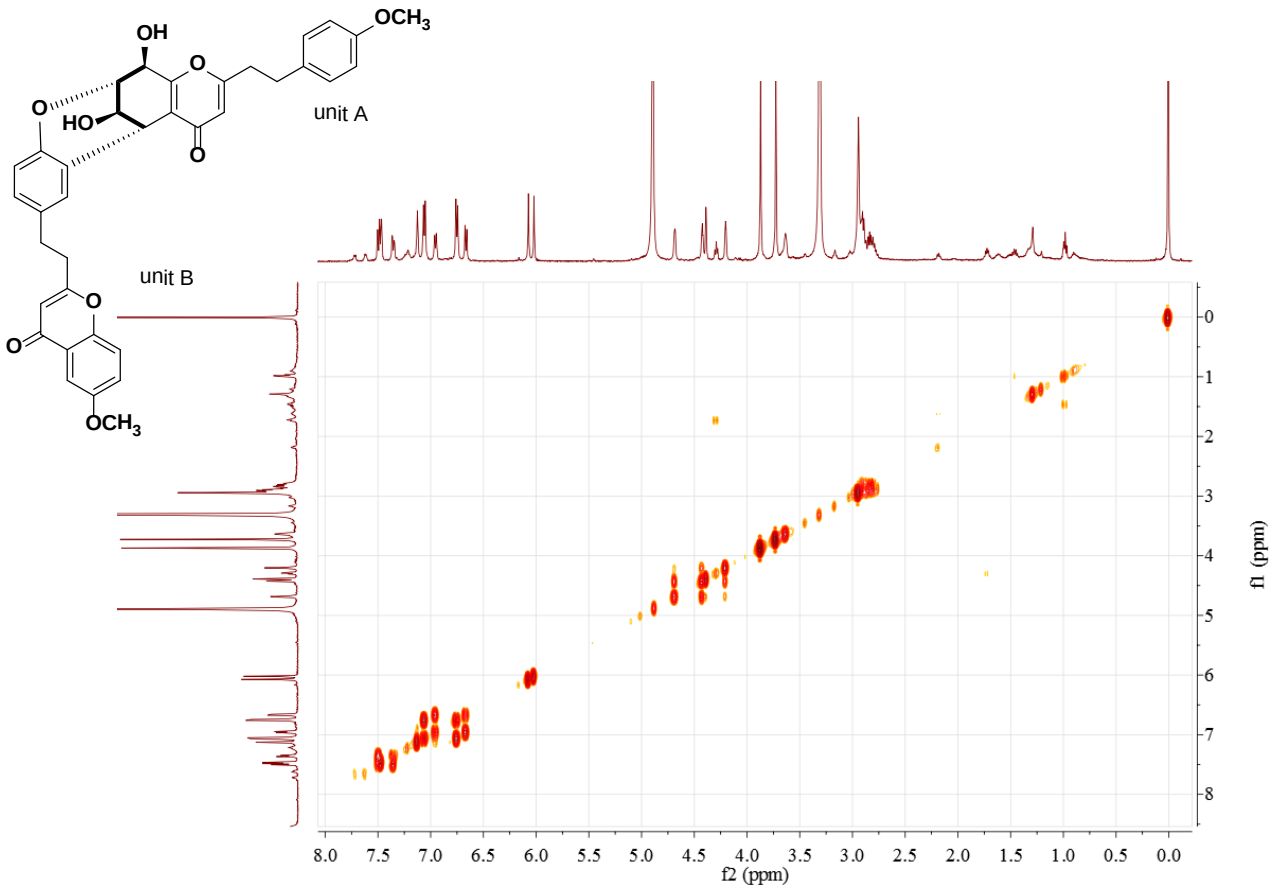


Figure S83. ^{1}H-^{1}H COSY spectrum of compound **9** in methanol-d_4

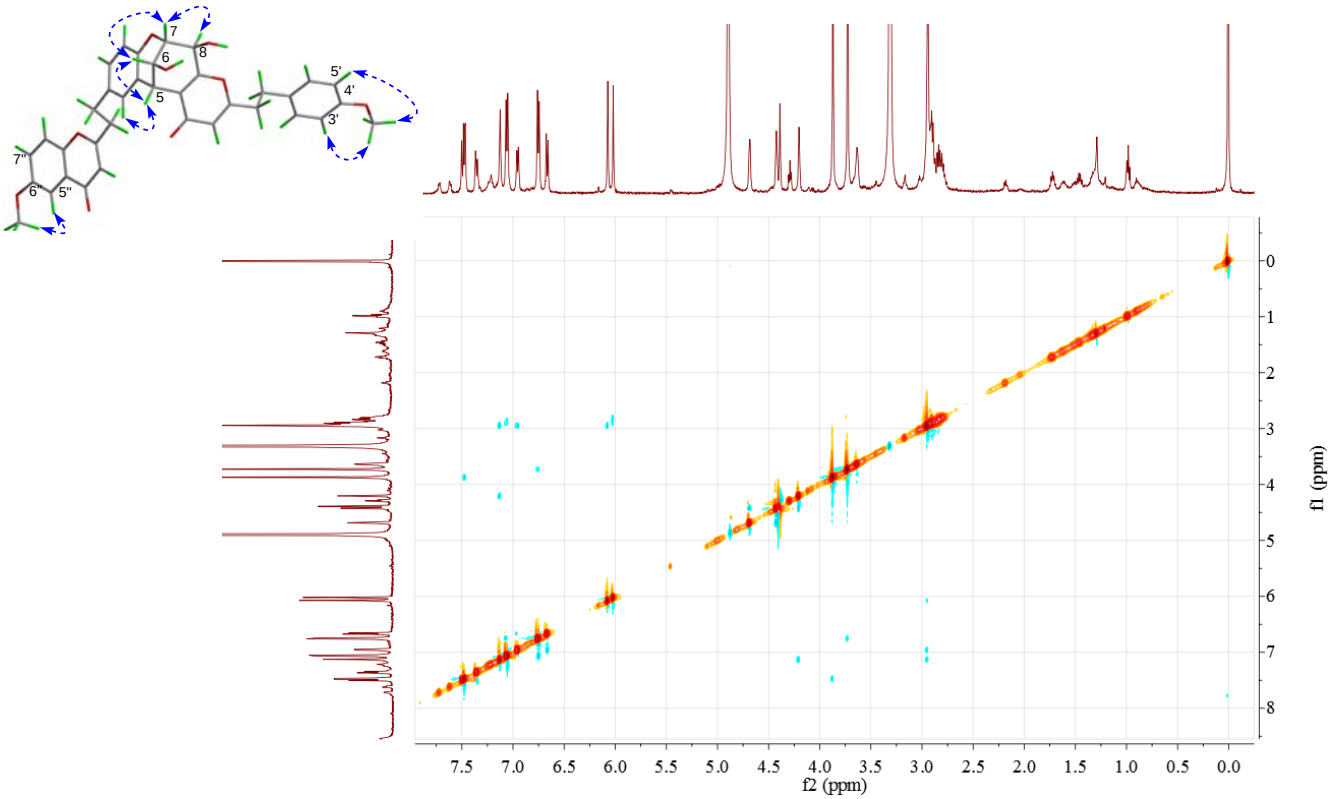


Figure S84. ROESY spectrum of compound **9** in methanol-d_4

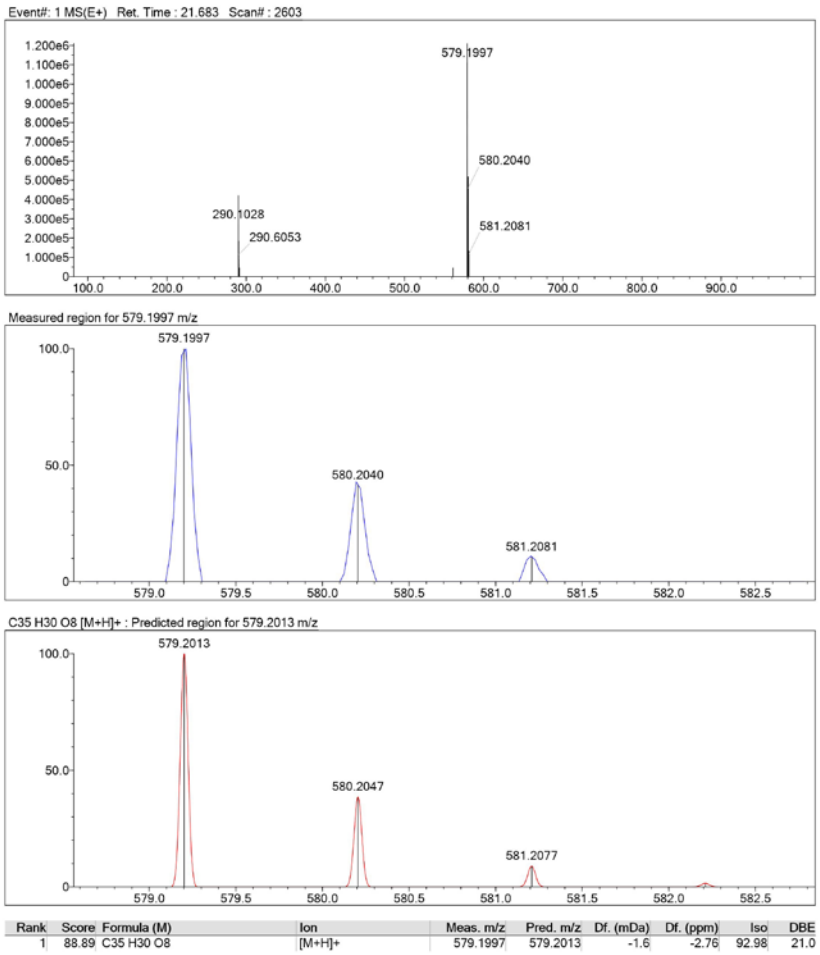


Figure S85. HRESIMS spectrum of compound **10**

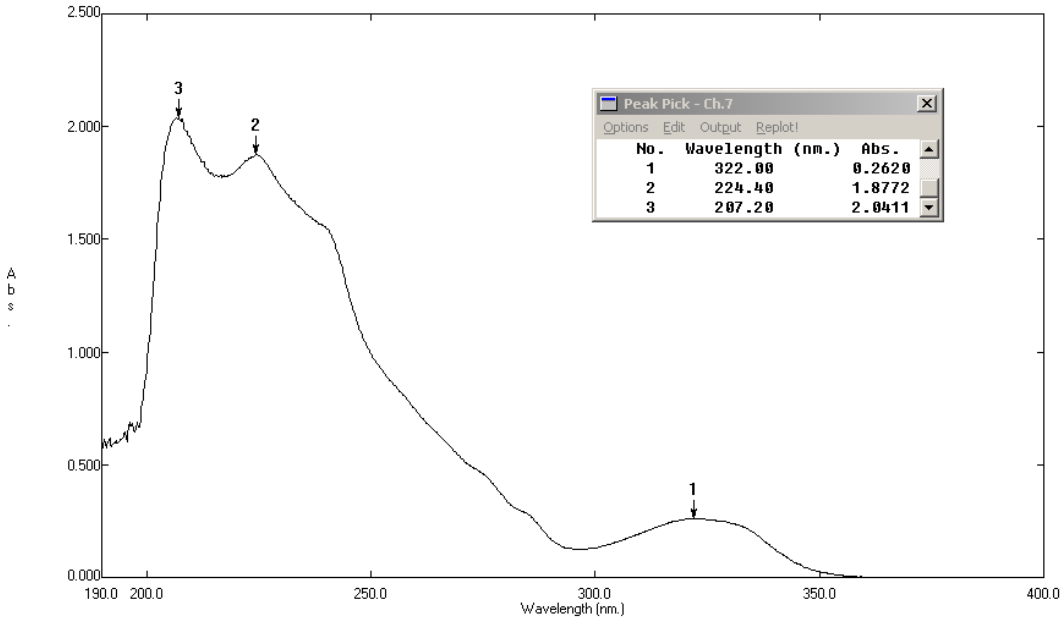


Figure S86. UV spectrum of compound **10**

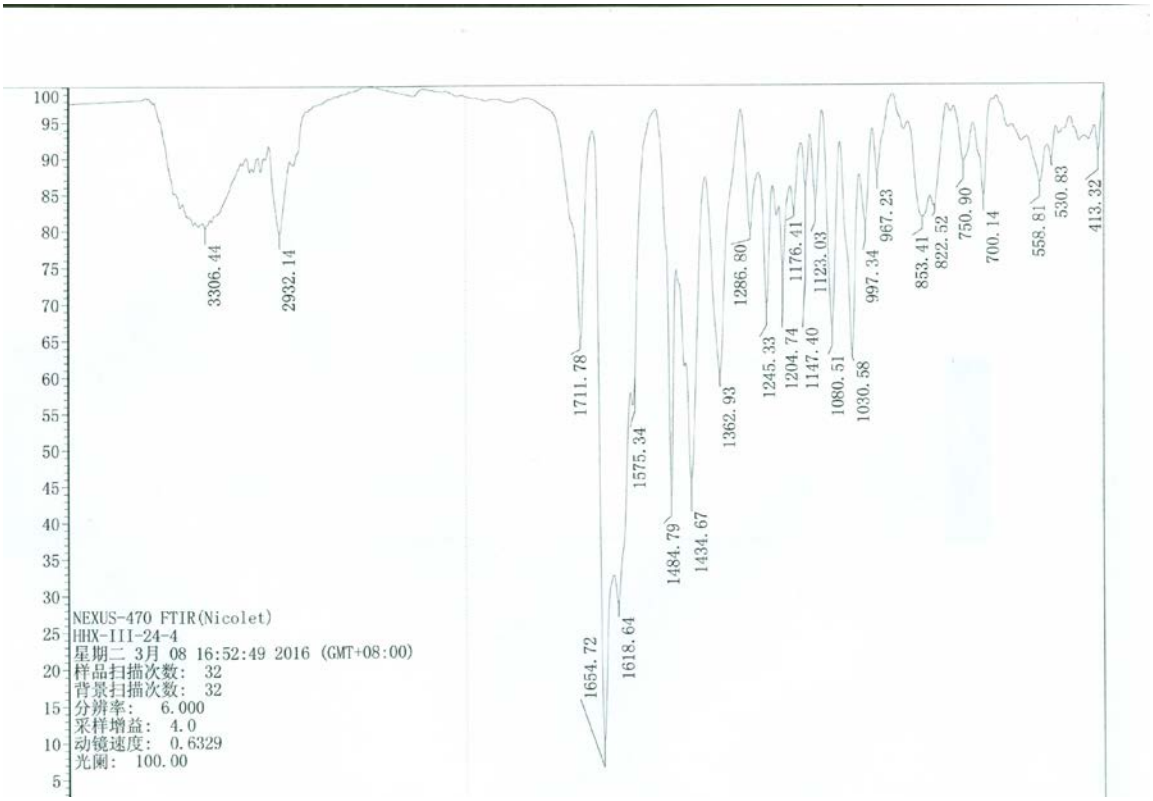


Figure S87. IR spectrum of compound **10**

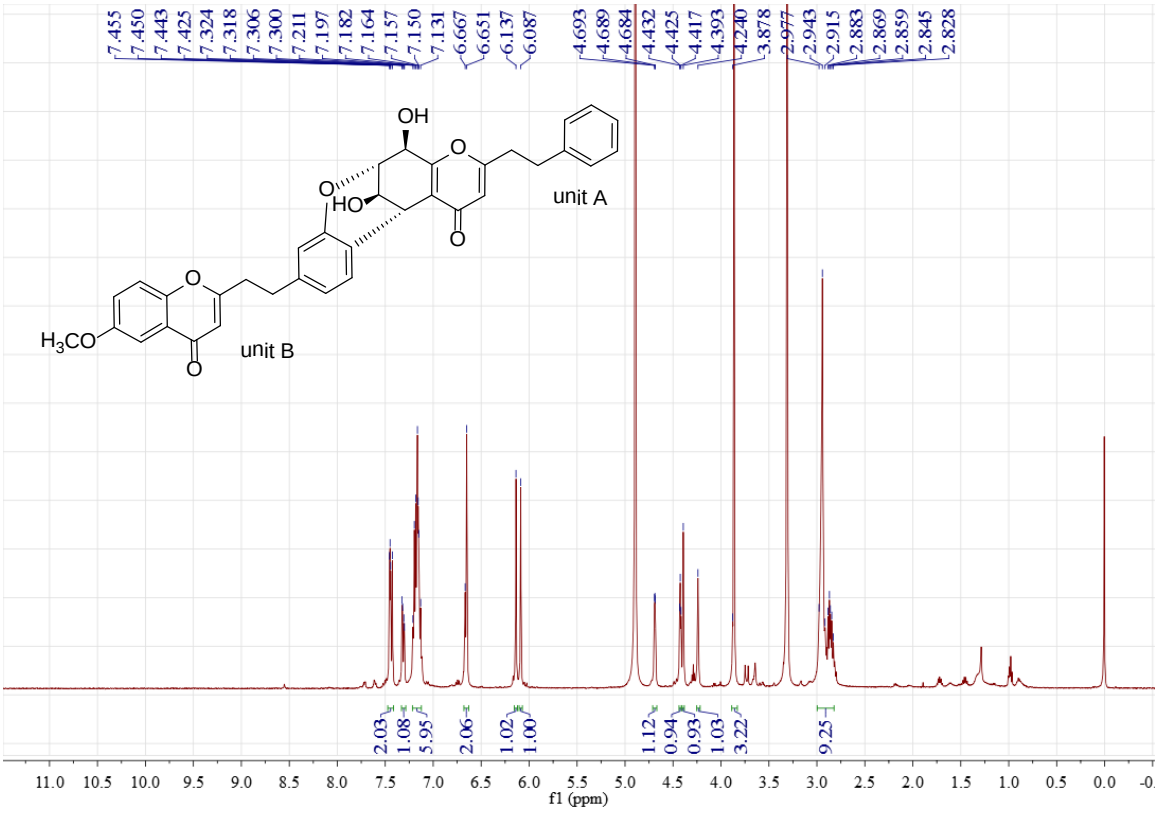


Figure S88. ^{1}H NMR spectrum of compound **10** in methanol-d_4

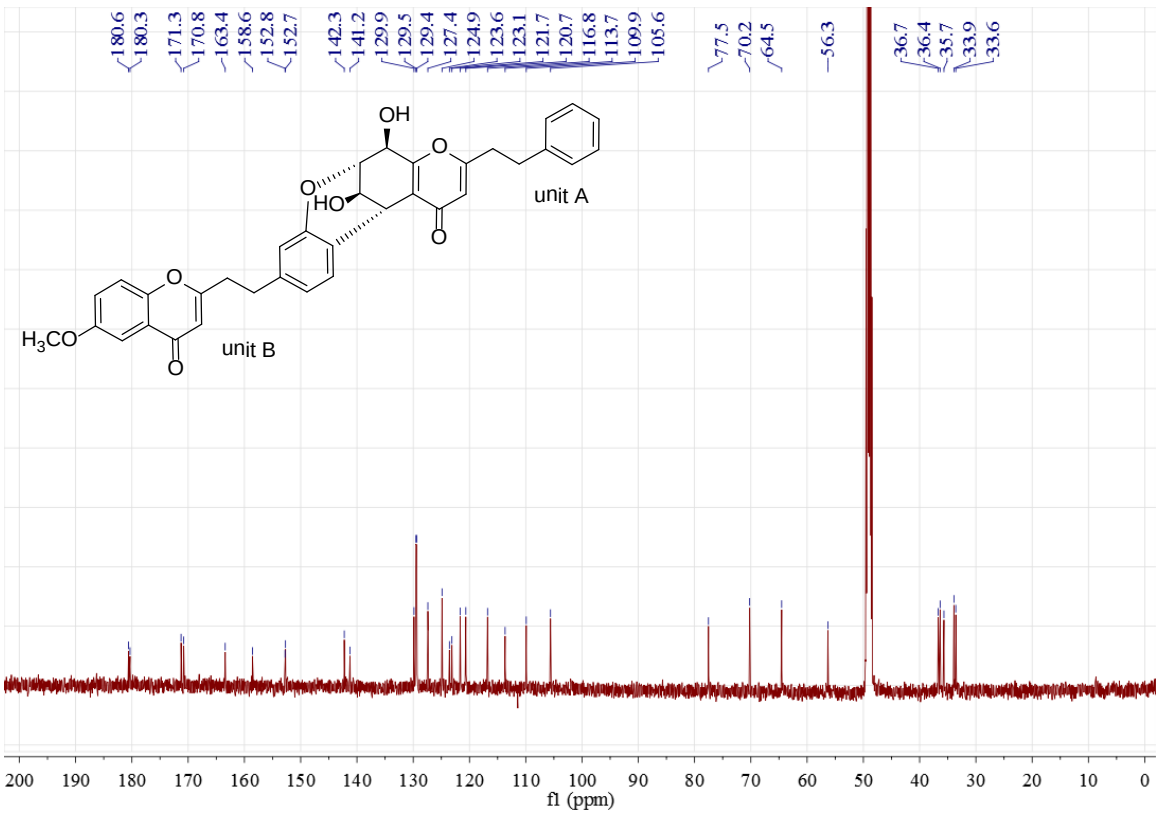


Figure S89. ^{13}C NMR spectrum of compound **10** in methanol-d_4

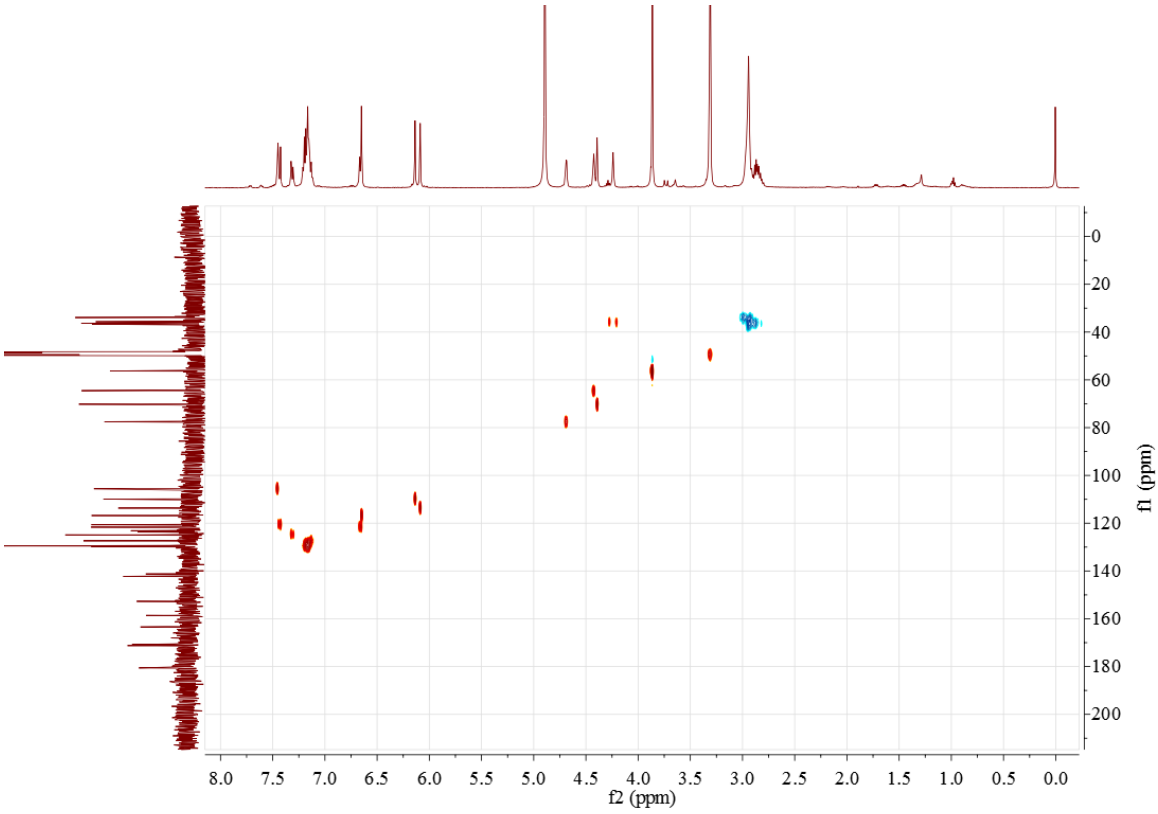


Figure S90. gHSQC spectrum of compound **10** in methanol-d_4

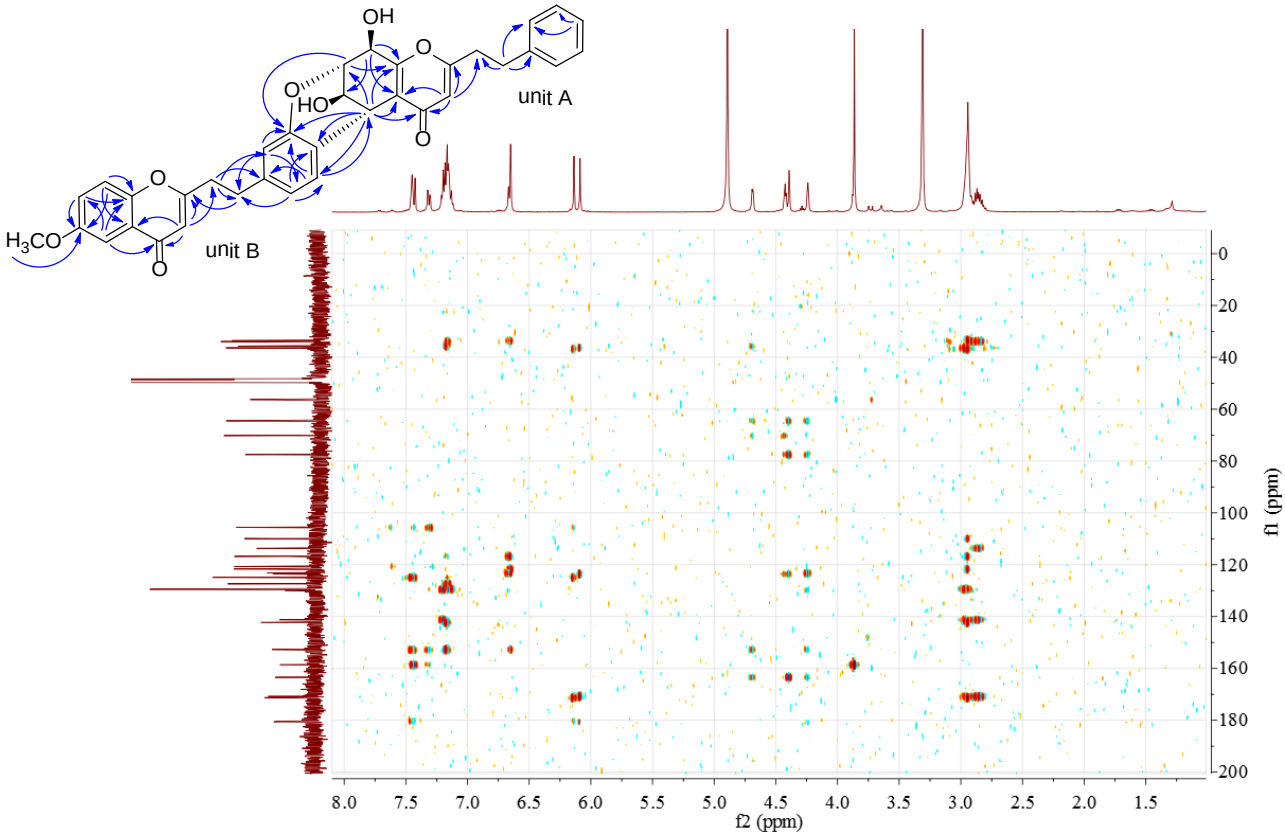


Figure S91. gHMBC spectrum of compound **10** in methanol-d_4

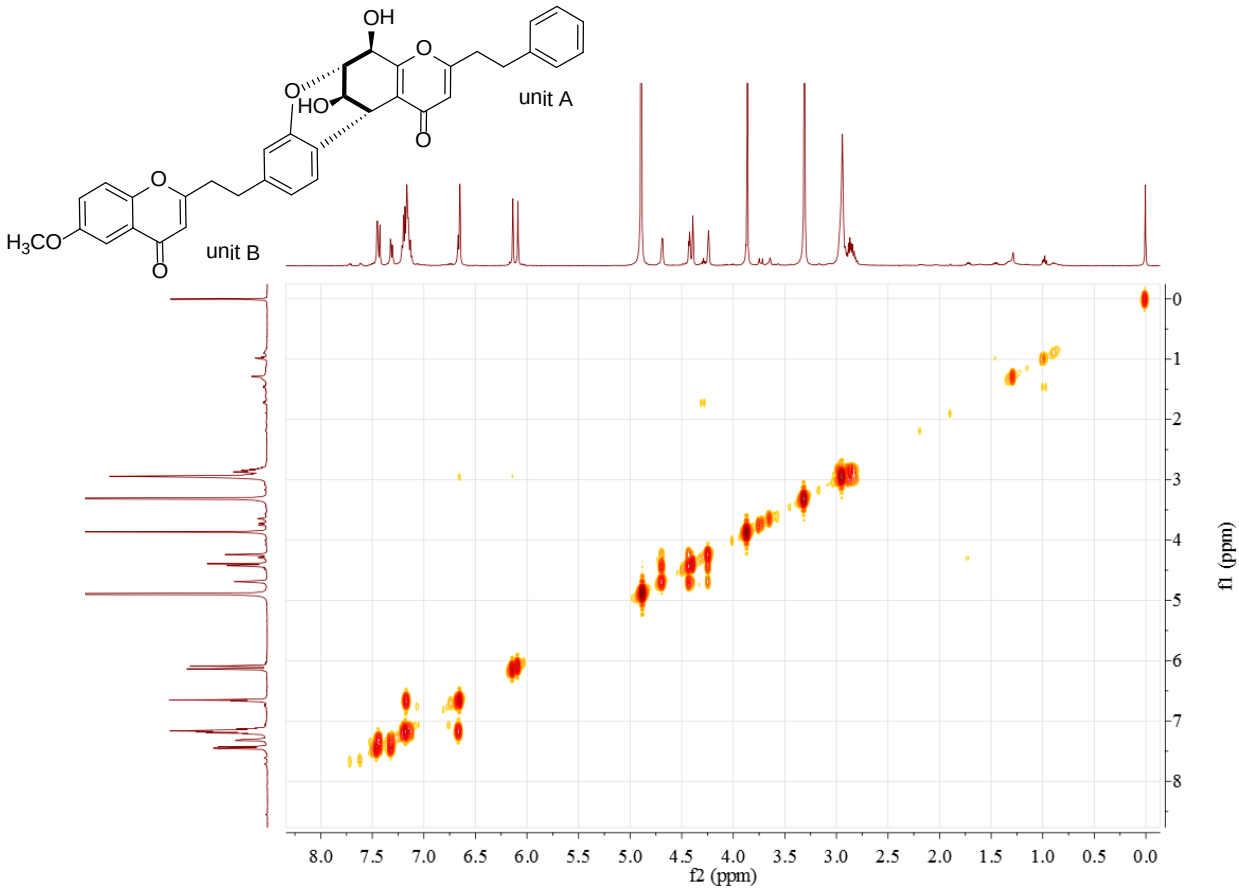


Figure S92. ^{1}H-^{1}H COSY spectrum of compound **10** in methanol-d_4

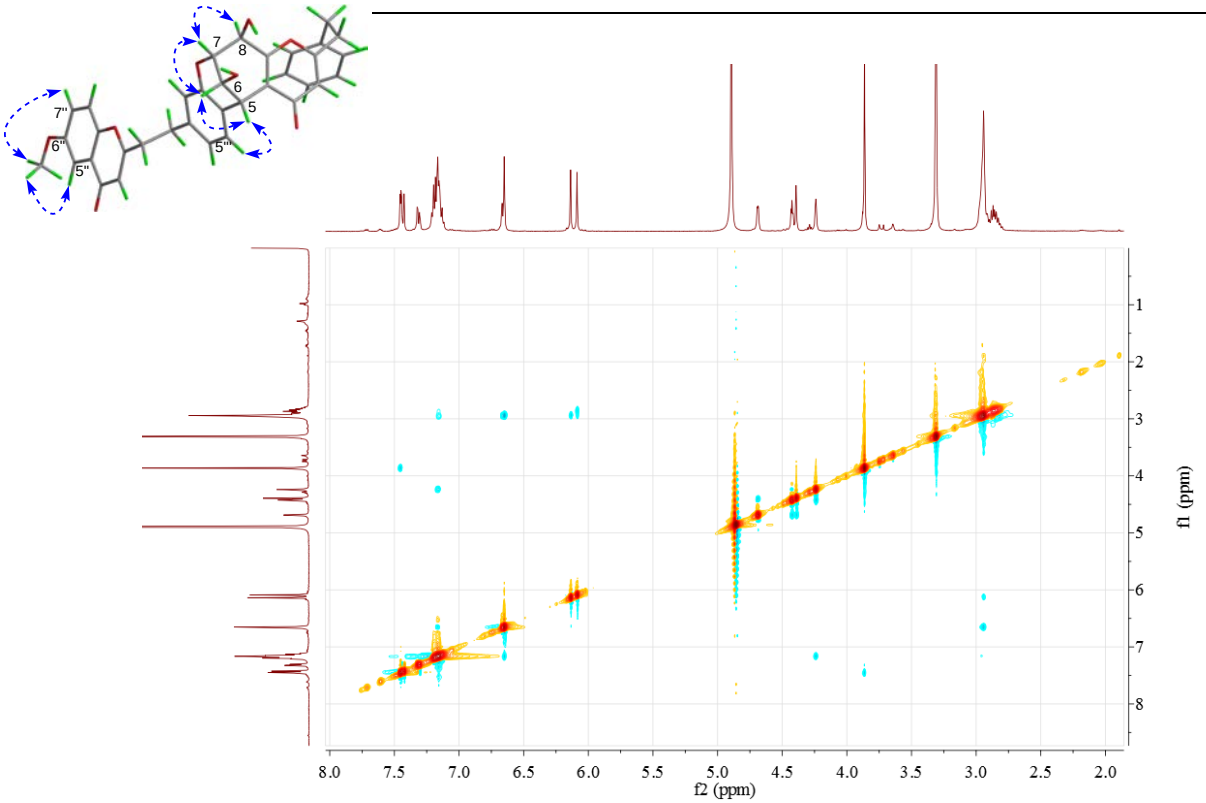


Figure S93. ROESY spectrum of compound **10** in methanol-d_4

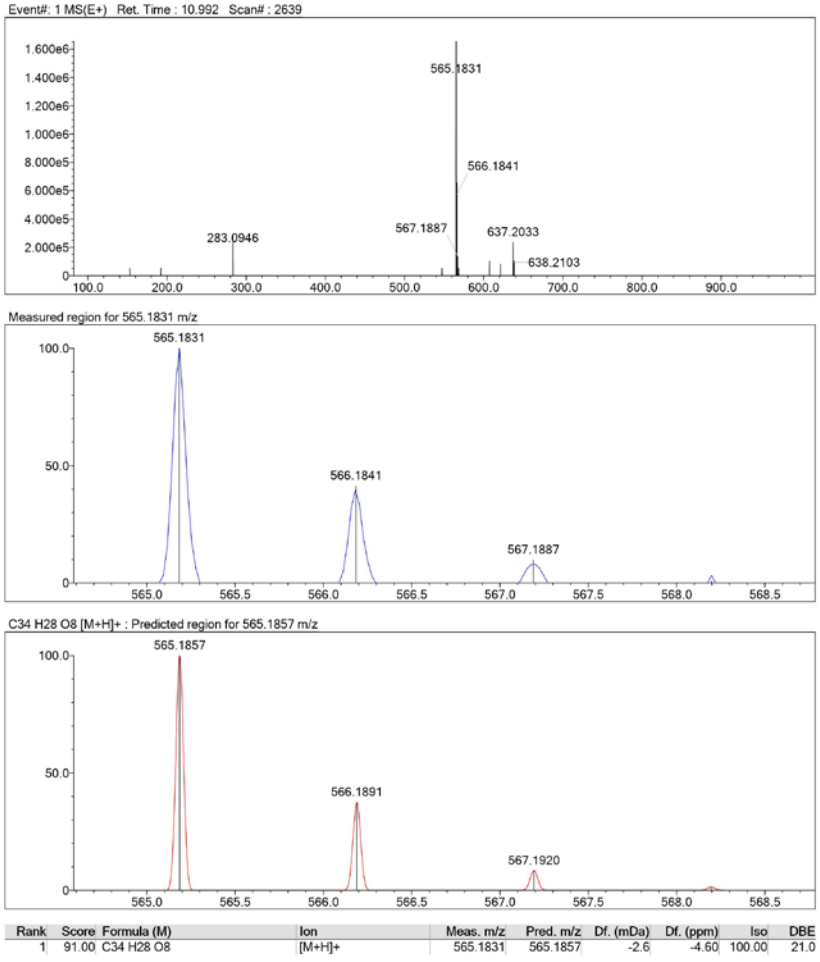


Figure S94. HRESIMS spectrum of compound **11**

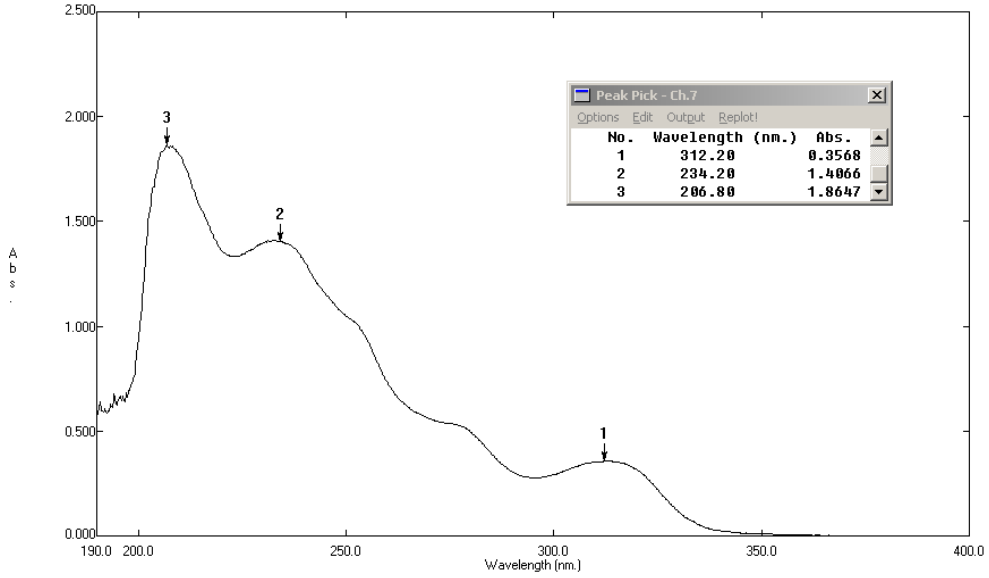


Figure S95. UV spectrum of compound **11**

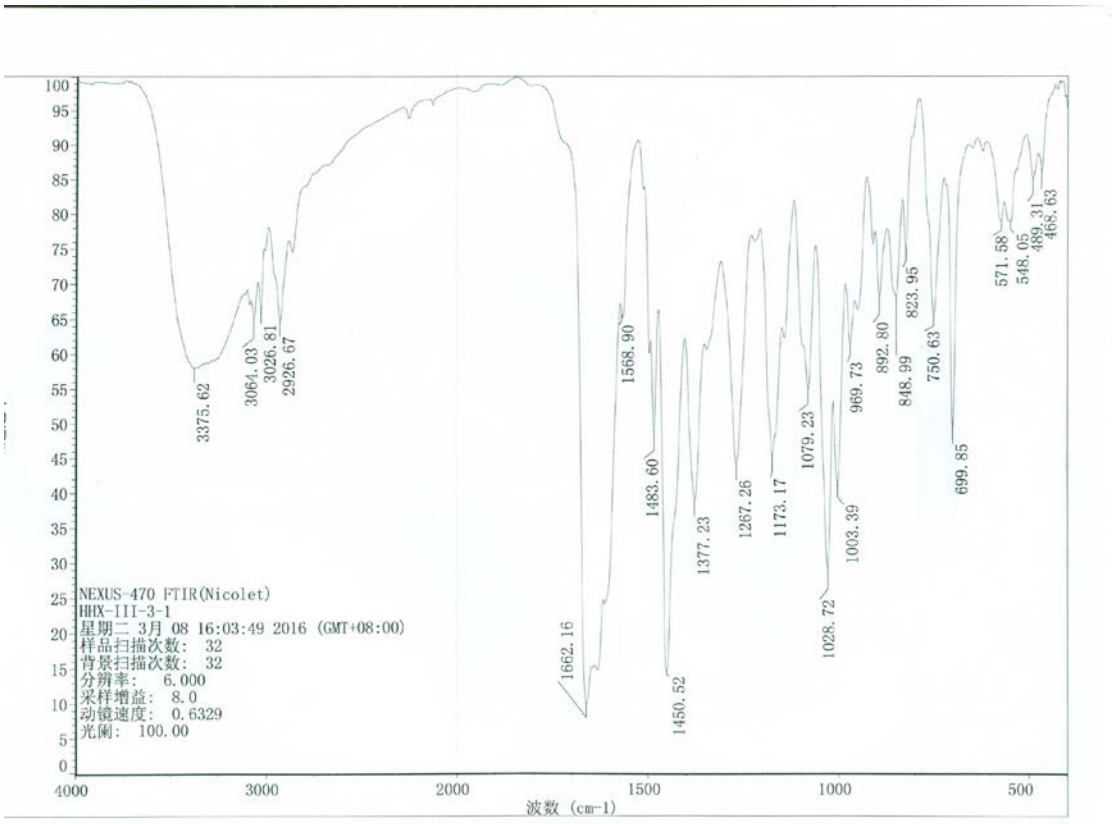


Figure S96. IR spectrum of compound **11**

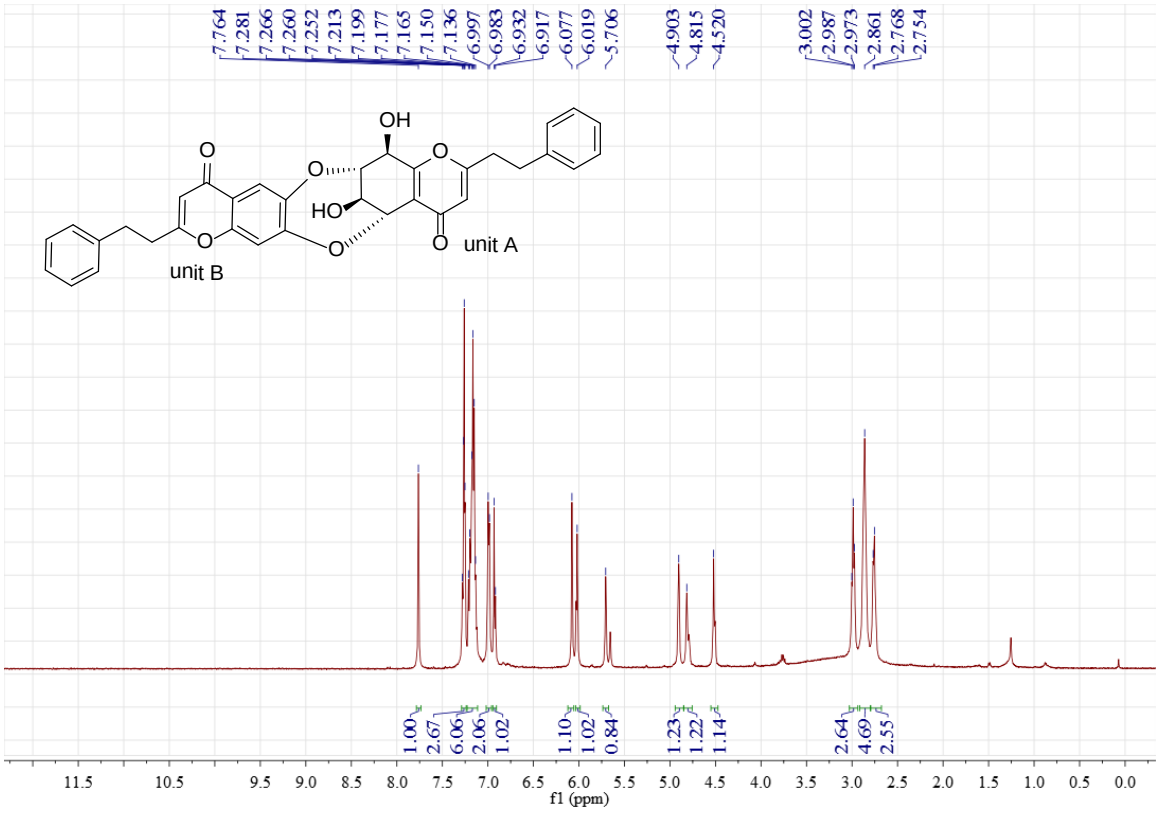


Figure S97. ^{1}H NMR spectrum of compound **11** in $CDCl_3$

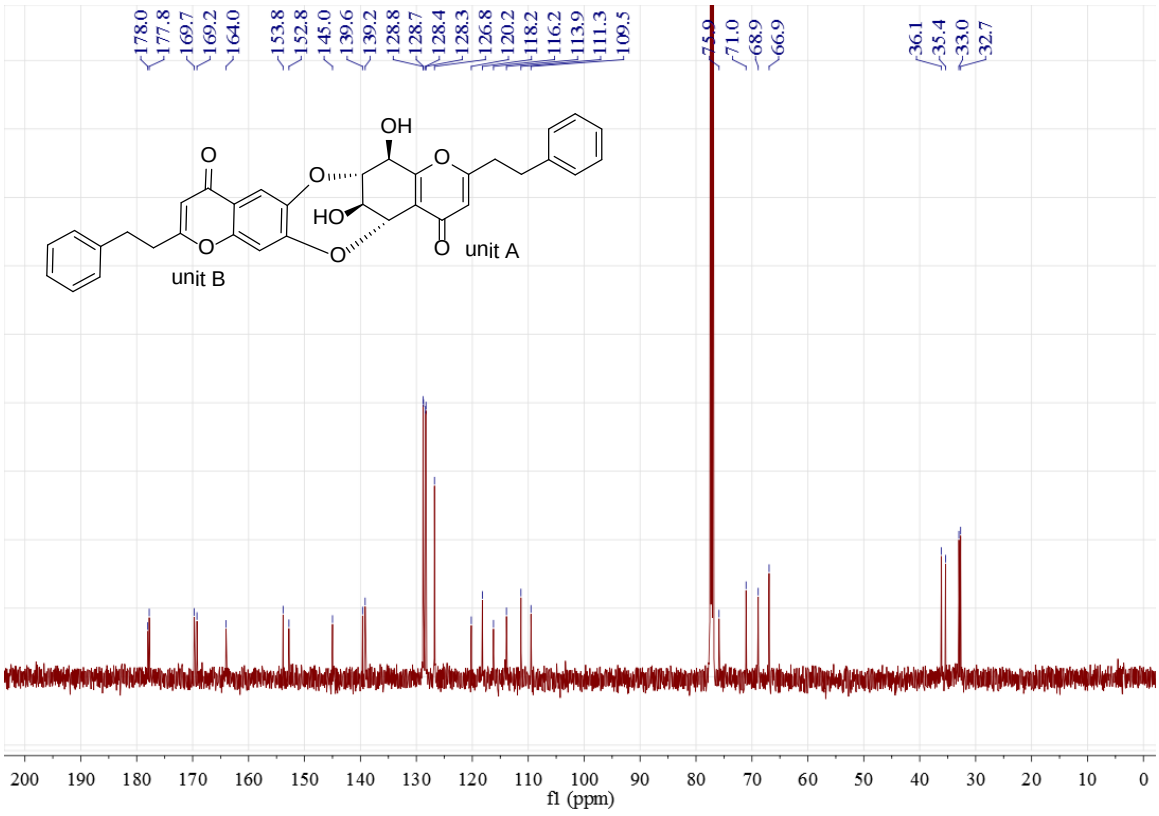


Figure S98. ^{13}C NMR spectrum of compound **11** in $CDCl_3$

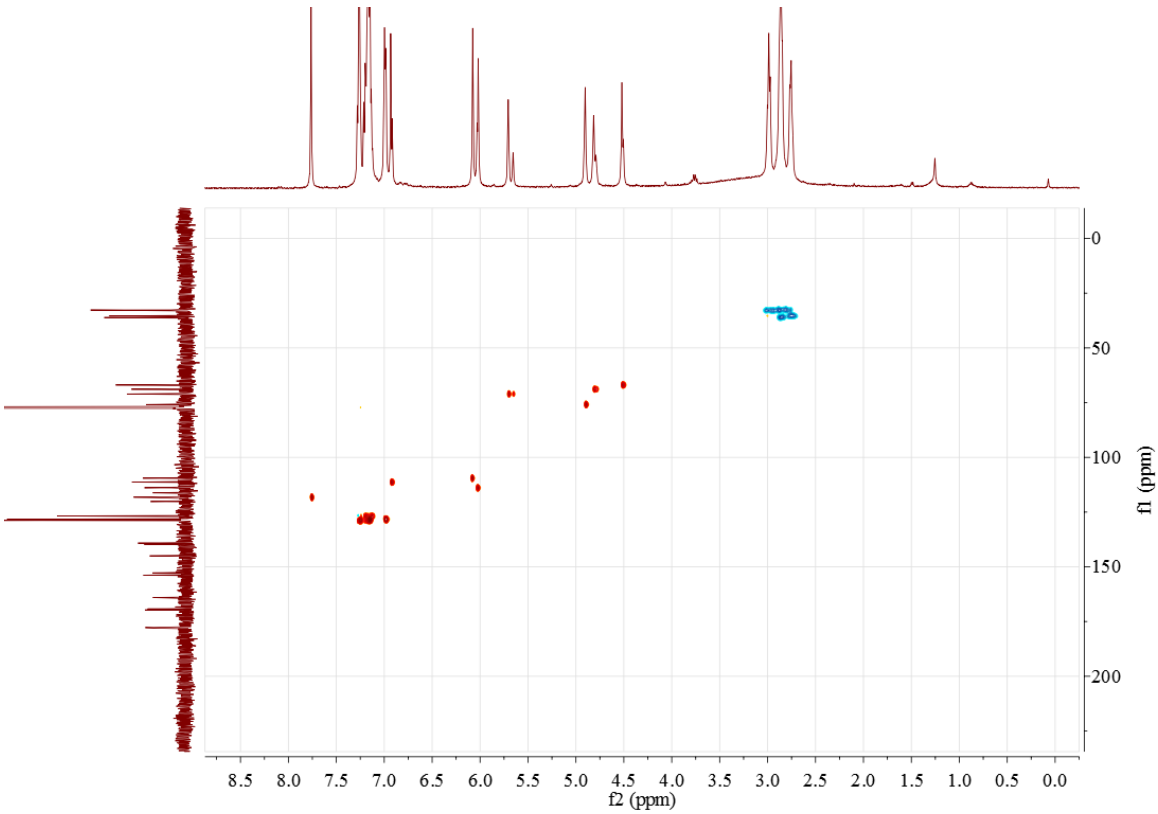


Figure S99. gHSQC spectrum of compound **11** in $CDCl_3$

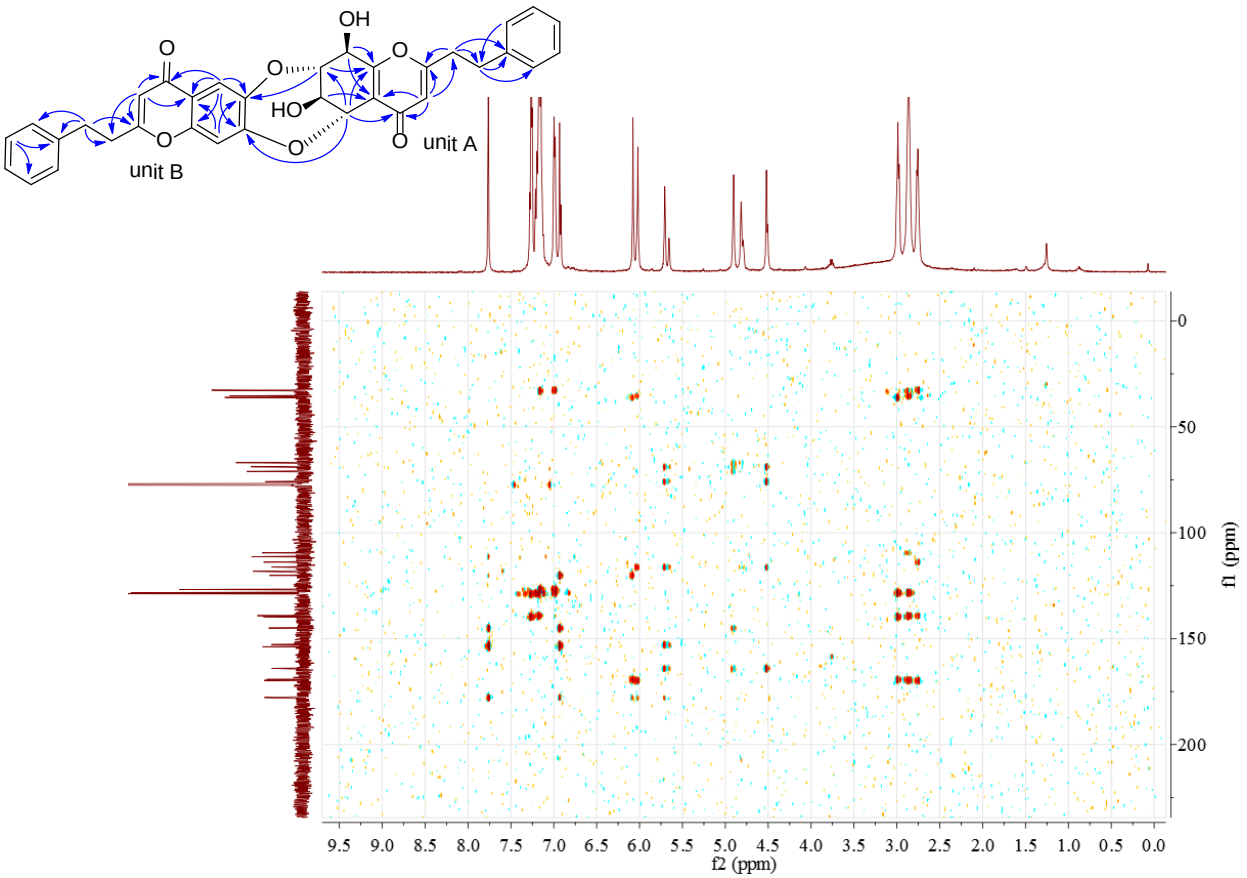


Figure S100. gHMBC spectrum of compound **11** in $CDCl_3$

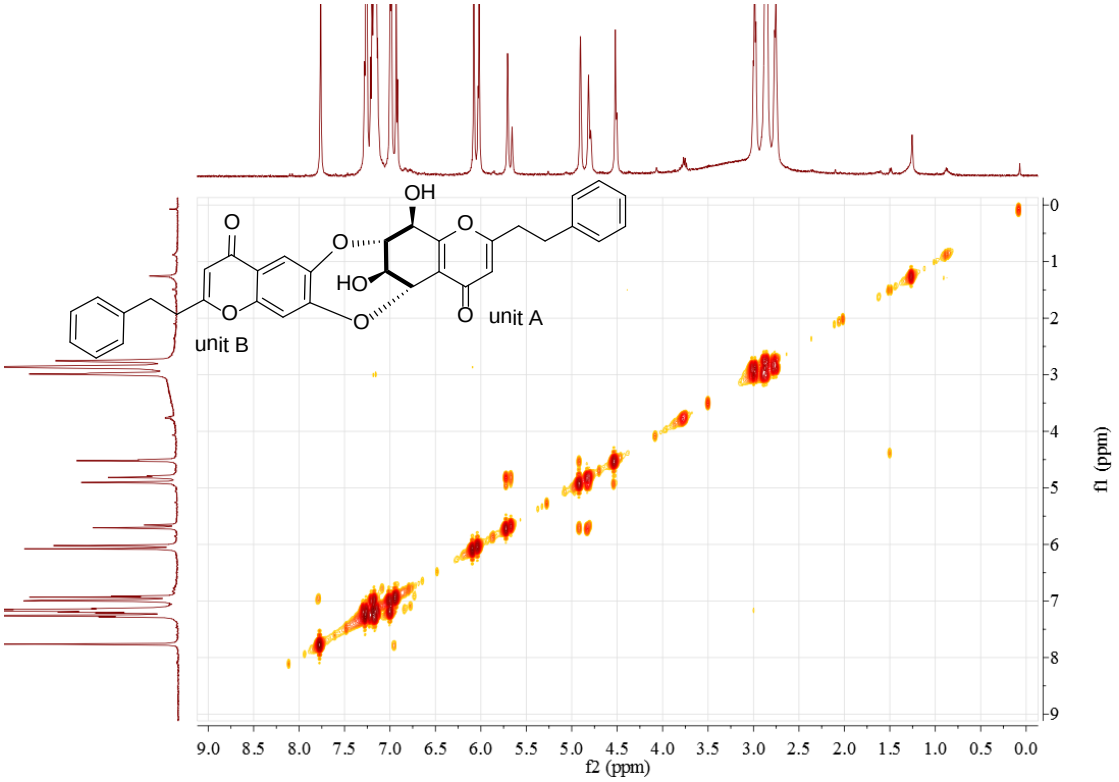


Figure S101. ^{1}H-^{1}H COSY spectrum of compound **11** in $CDCl_3$

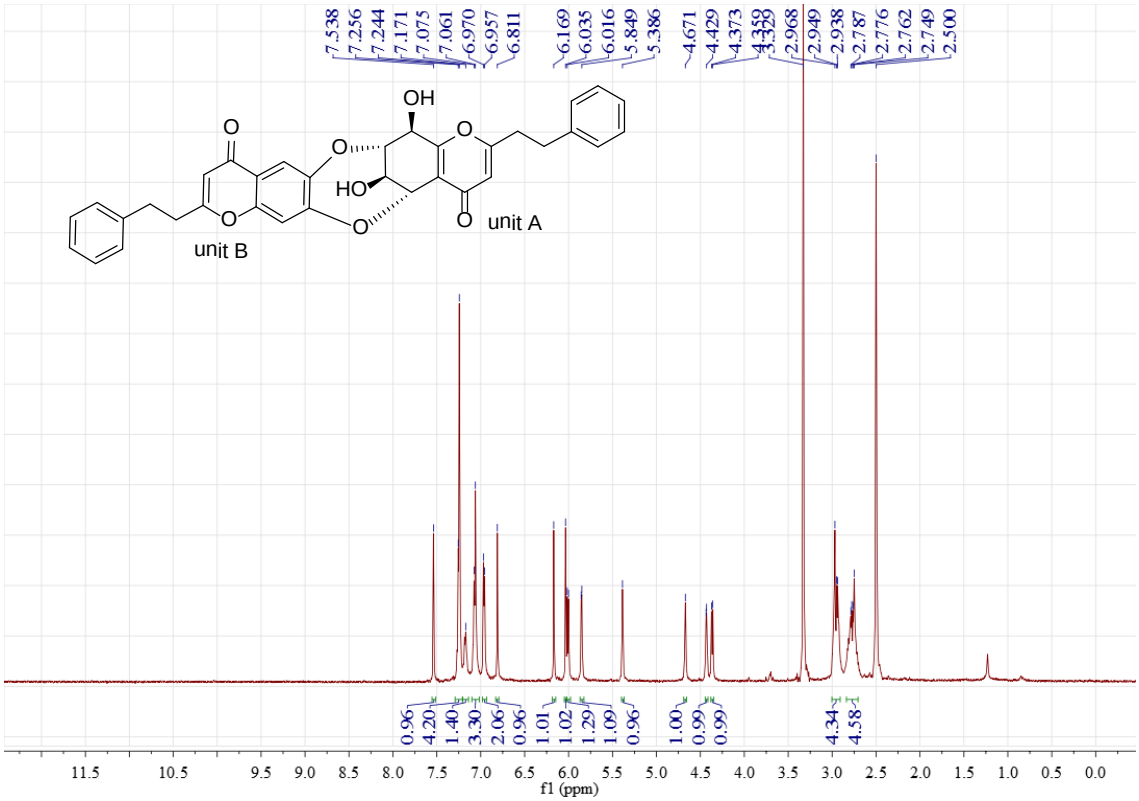


Figure S102. ^{1}H NMR spectrum of compound **11** in DMSO-d_6

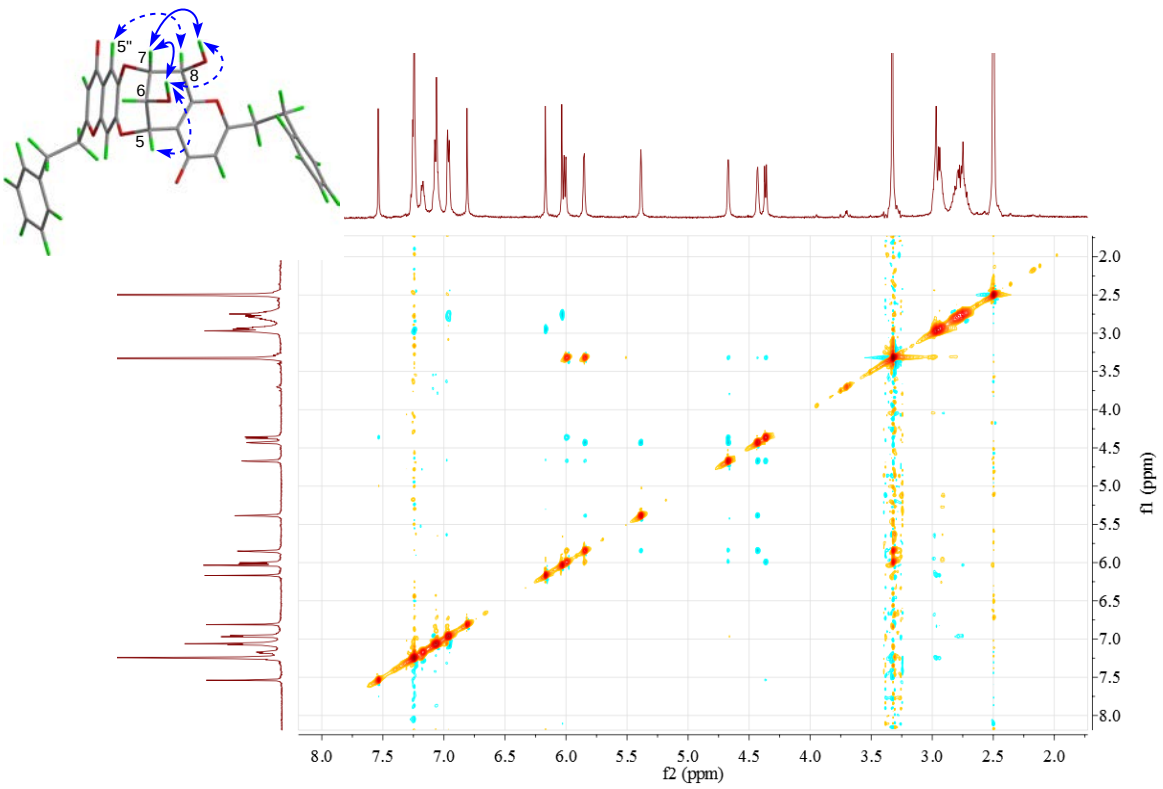
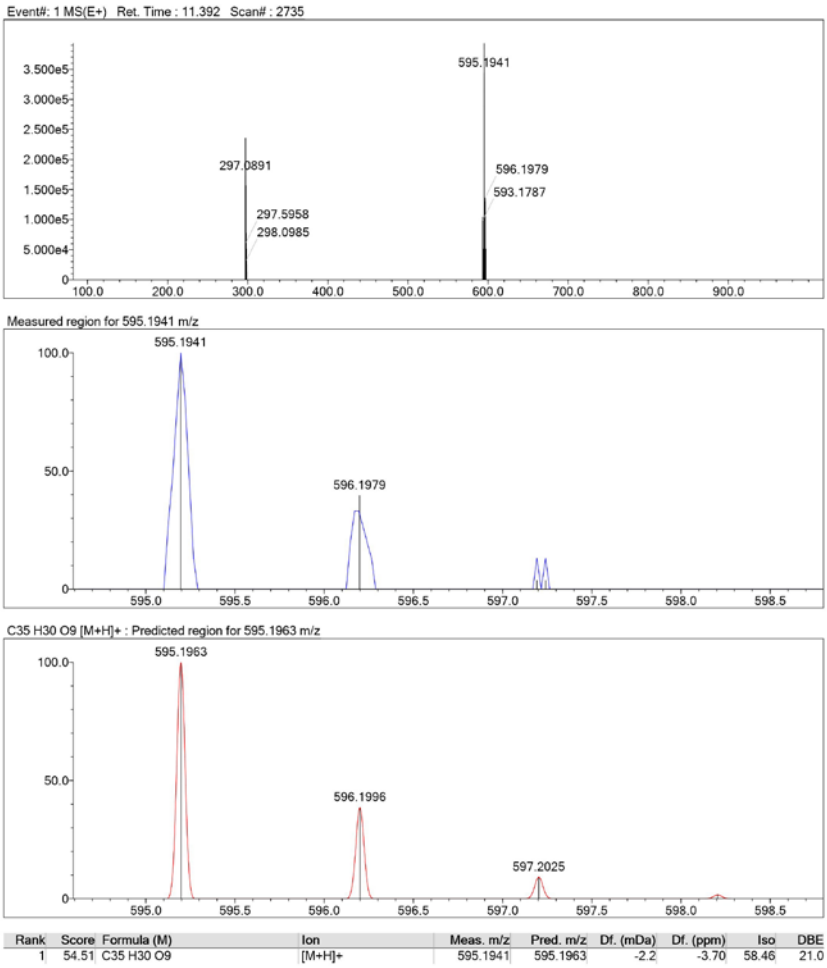


Figure S103. ROESY spectrum of compound **11** in DMSO-d_6



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	54.51	C35 H30 O9	[M+H]+	595.1941	595.1963	-2.2	-3.70	58.46	21.0

Figure S104. HRESIMS spectrum of compound **12**

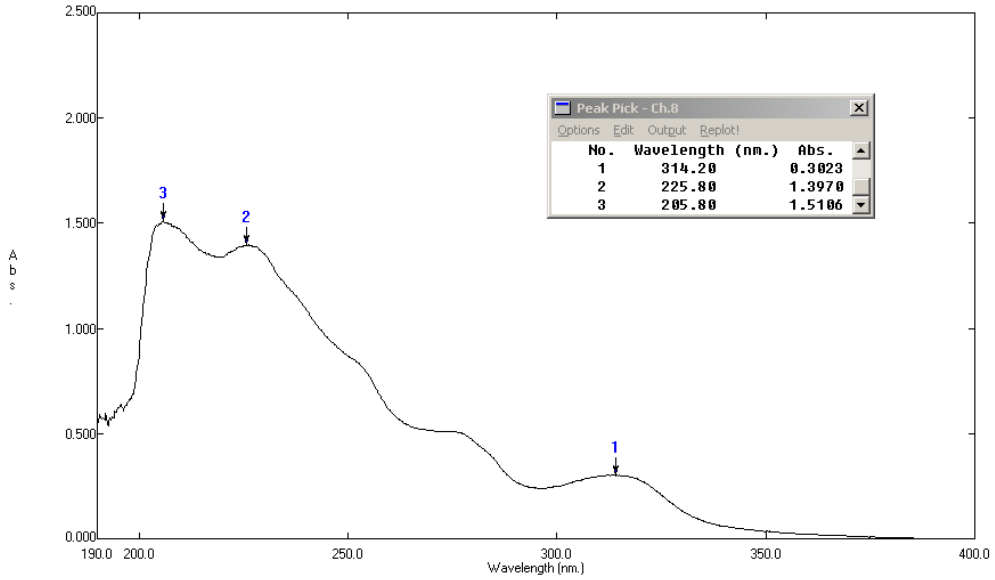


Figure S105. UV spectrum of compound **12**

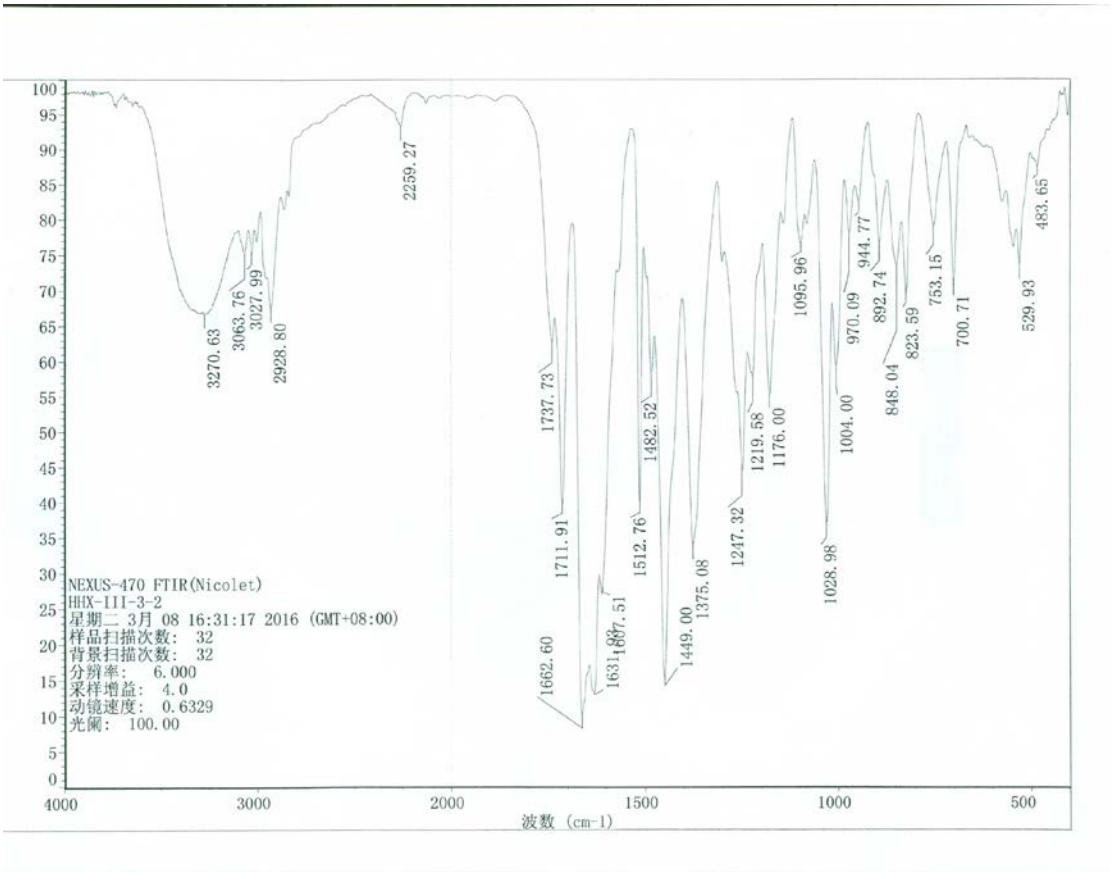


Figure S106. IR spectrum of compound **12**

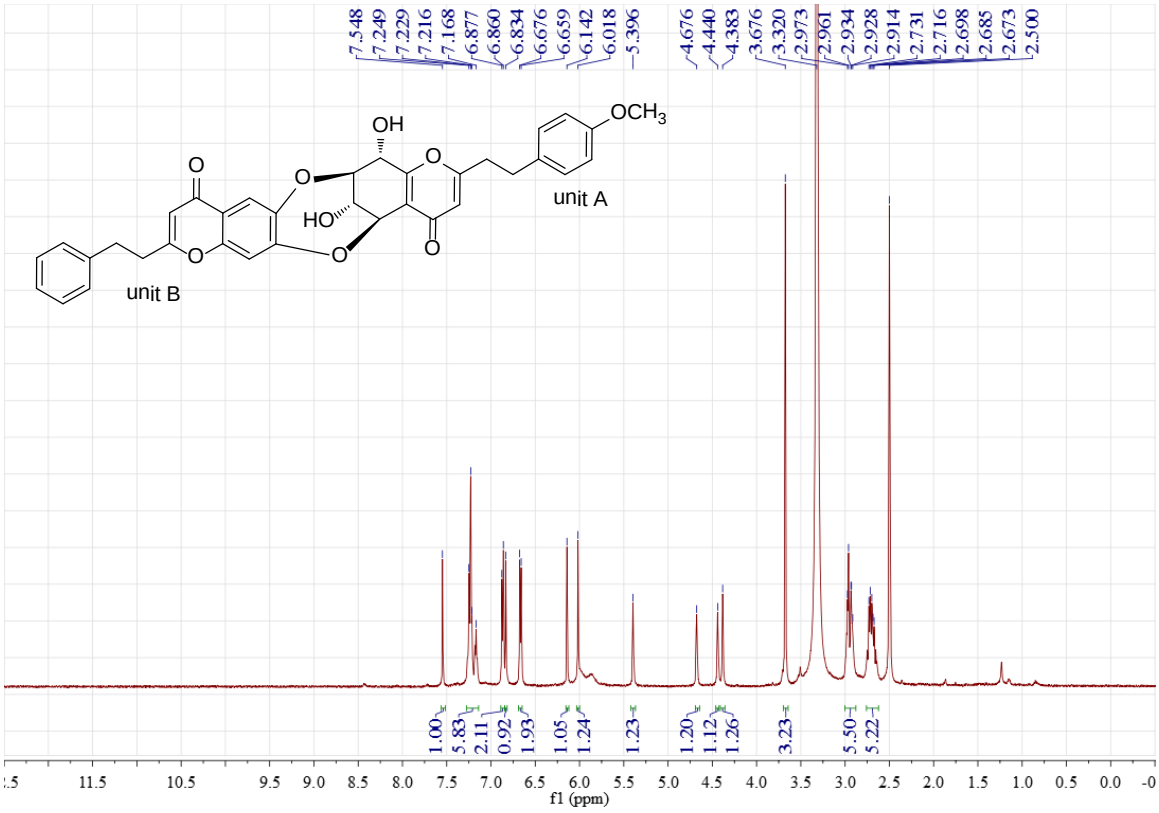


Figure S107. ^{1}H NMR spectrum of compound **12** in DMSO-d_6

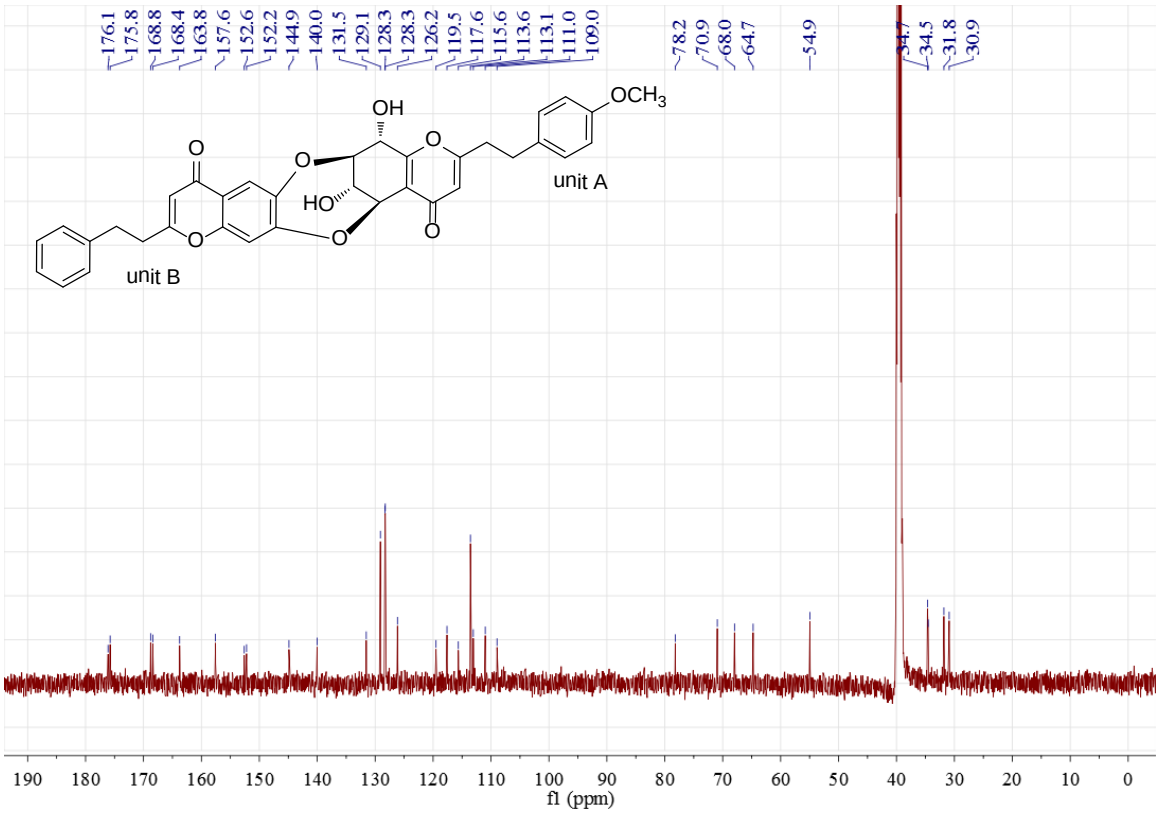


Figure S108. ^{13}C NMR spectrum of compound **12** in DMSO-d_6

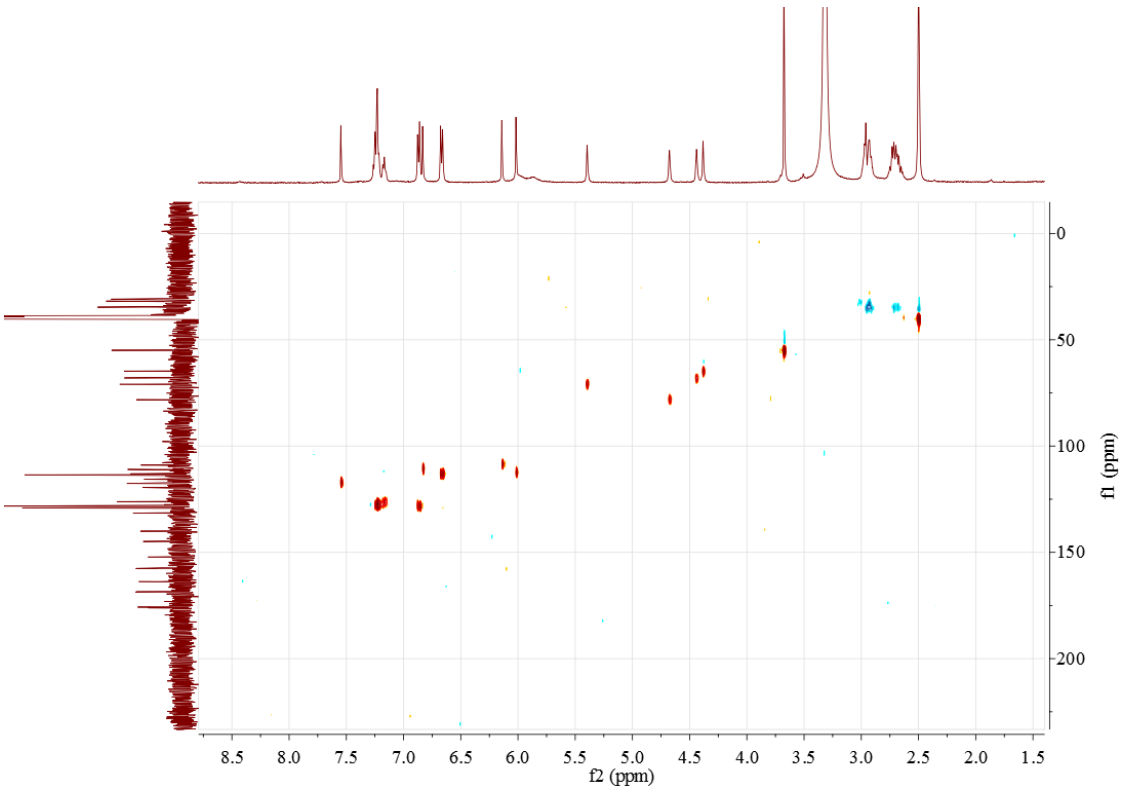


Figure S109. gHSQC spectrum of compound **12** in DMSO-d_6

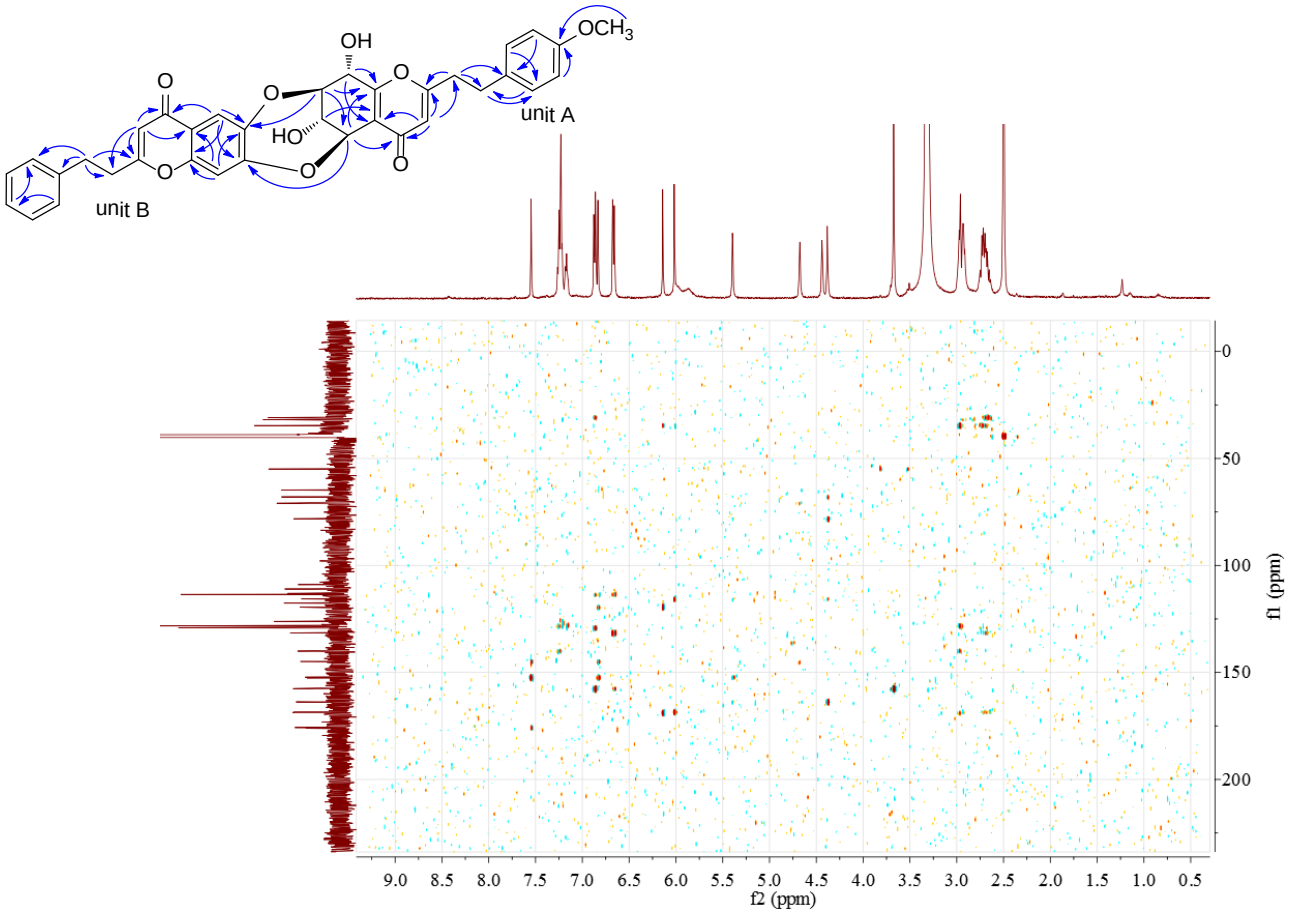


Figure S110. gHMBC spectrum of compound **12** in DMSO-d_6

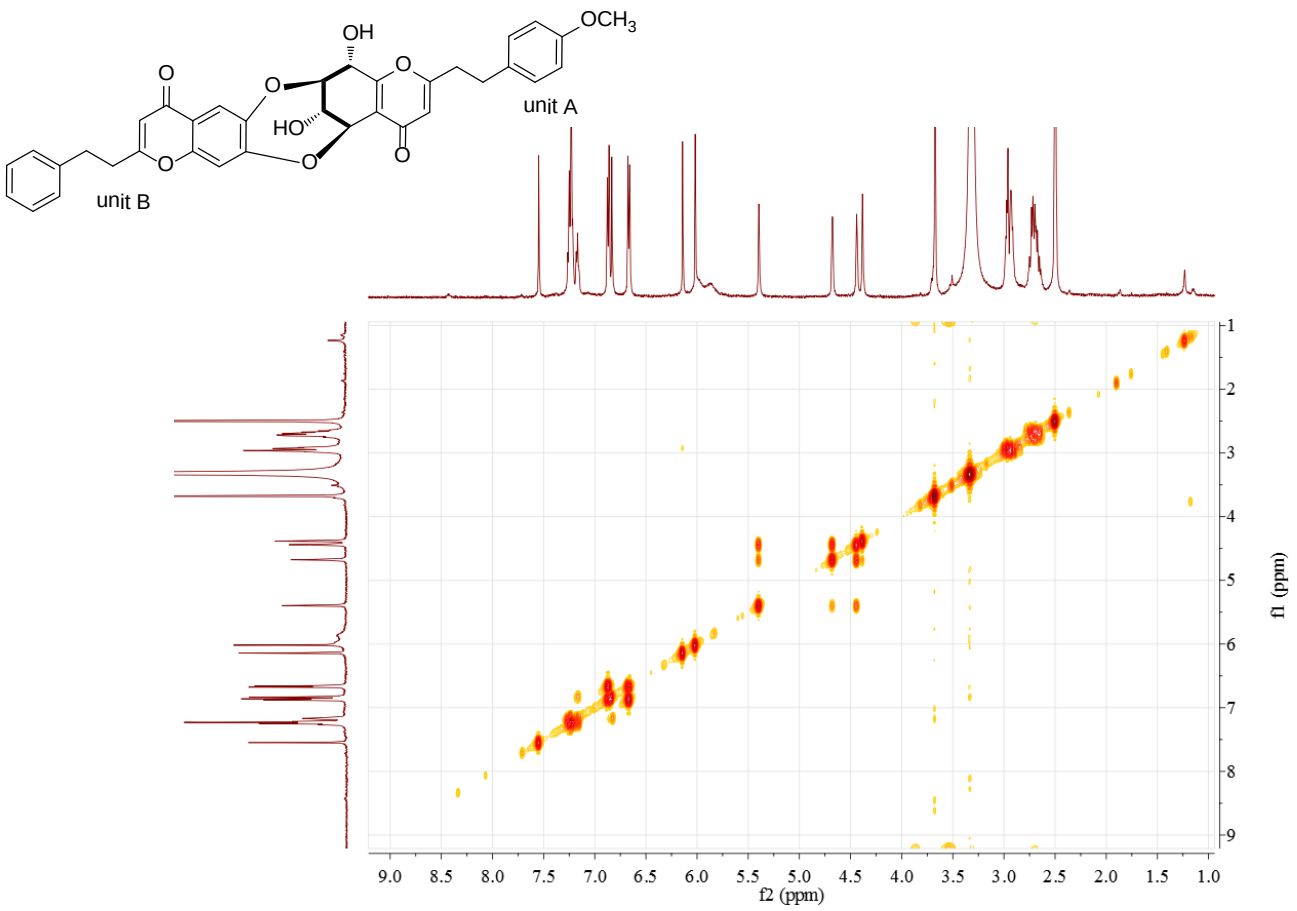


Figure S111. ^{1}H-^{1}H COSY spectrum of compound **12** in DMSO-d_6

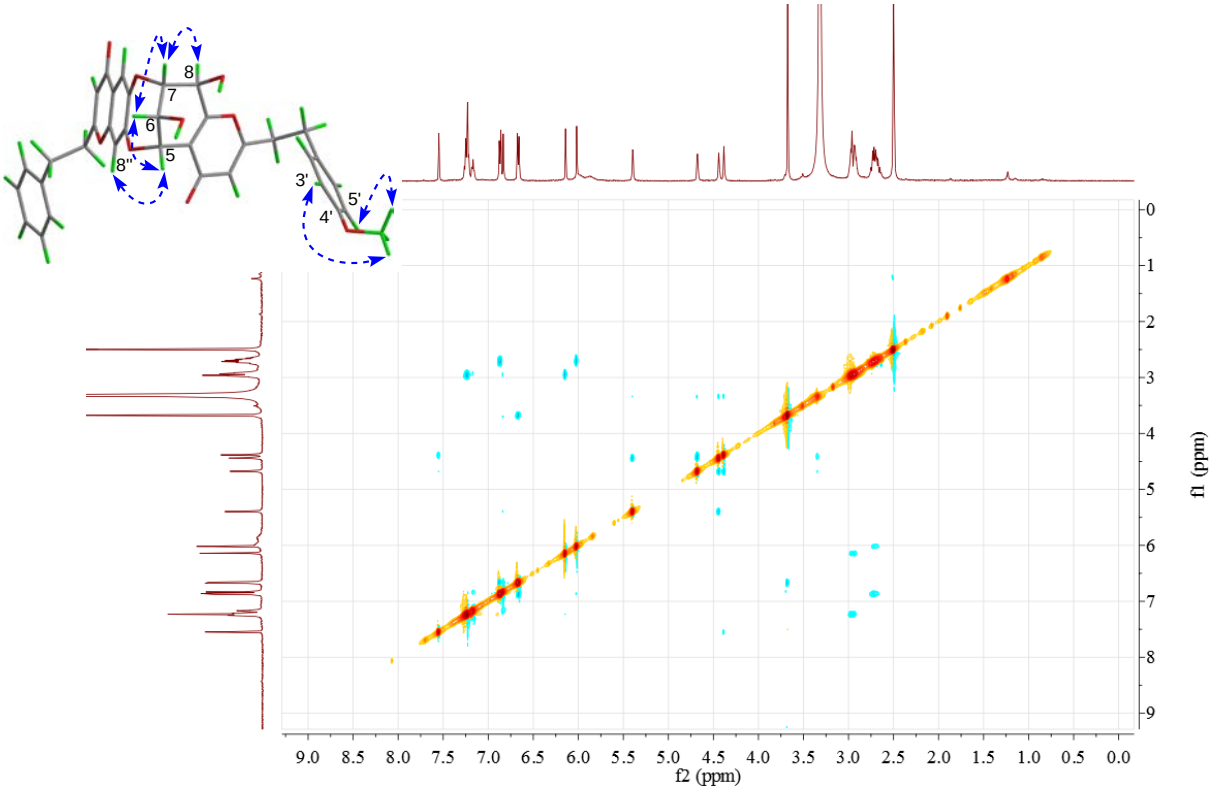


Figure S112. ROESY spectrum of compound **12** in DMSO-d_6

2. LCMS-IT-TOF base peak chromatograms

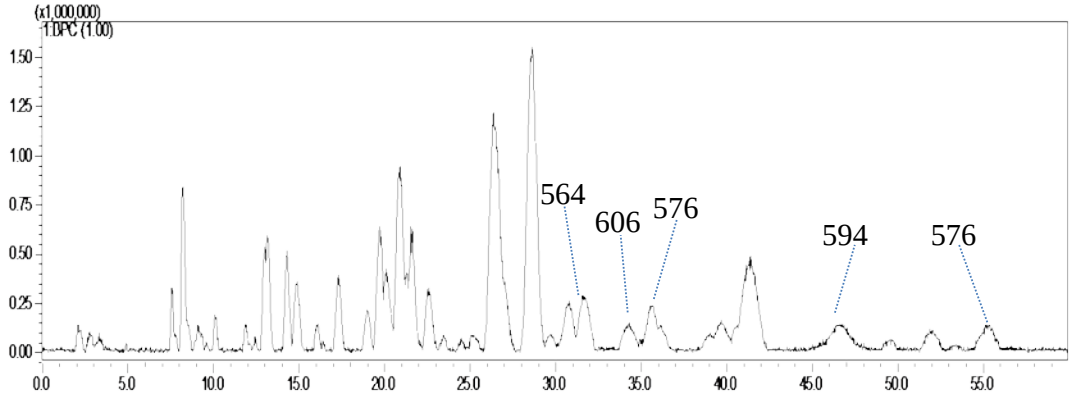


Figure S113. LCMS-IT-TOF base peak chromatogram (BPC) of subfraction H1a

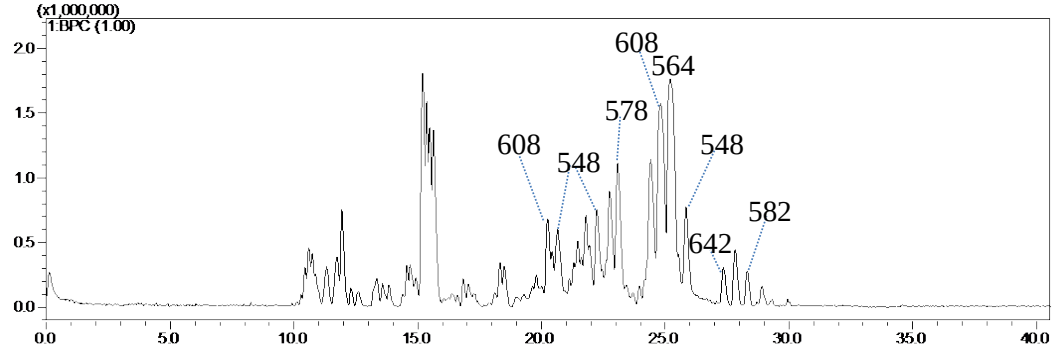


Figure S114. LCMS-IT-TOF base peak chromatogram (BPC) of subfraction H1c

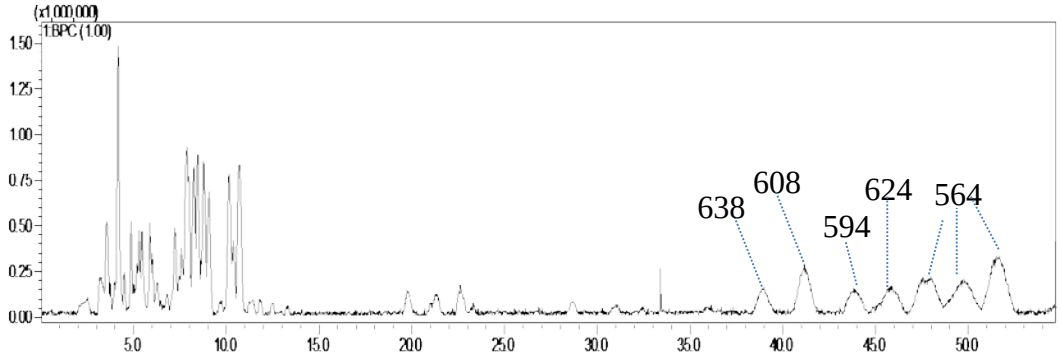


Figure S115. LCMS-IT-TOF base peak chromatogram (BPC) of subfraction H1d

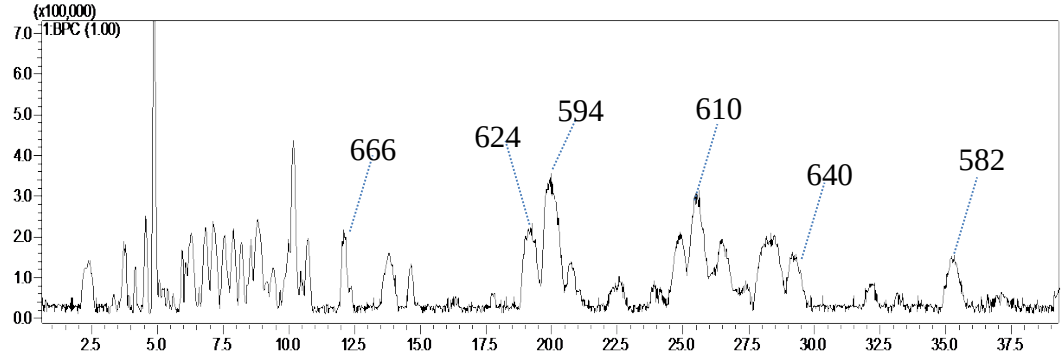


Figure S116. LCMS-IT-TOF base peak chromatogram (BPC) of subfraction H1e

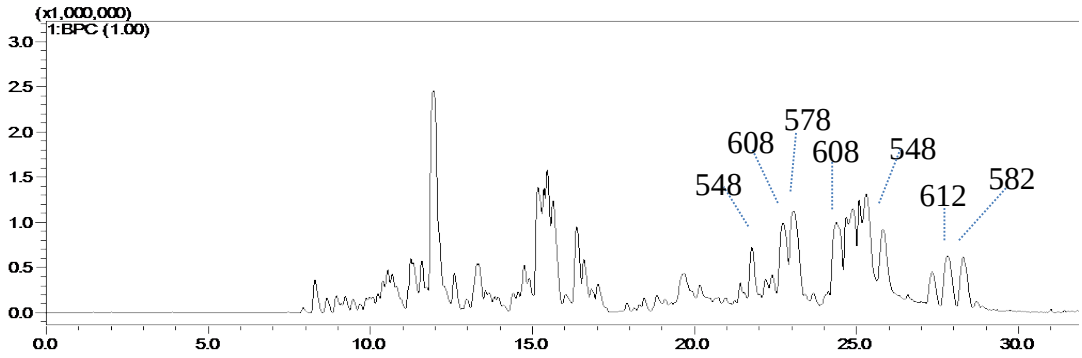


Figure S117. LCMS-IT-TOF base peak chromatogram (BPC) of subfraction H4

3. Chiral-phase HPLC Chromatograms

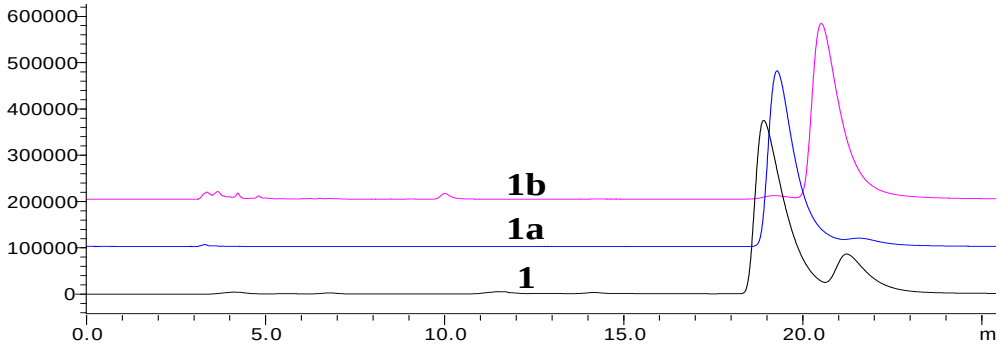


Figure S118. Chiral-phase HPLC chromatogram of compounds **1a** and **1b**

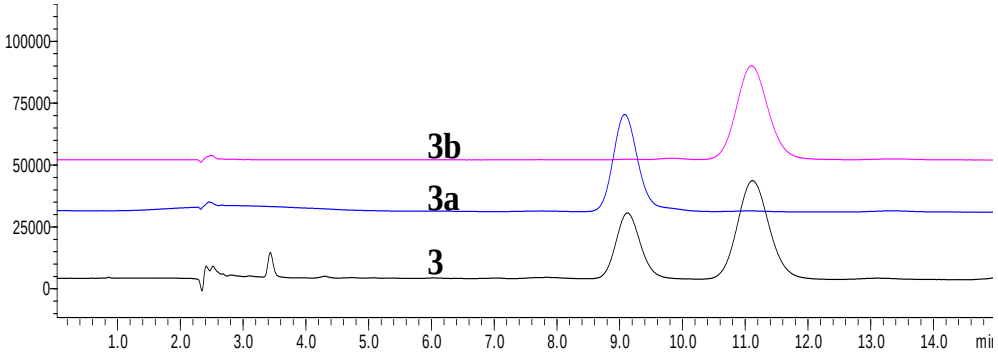


Figure S119. Chiral-phase HPLC chromatogram of compounds **3a** and **3b**

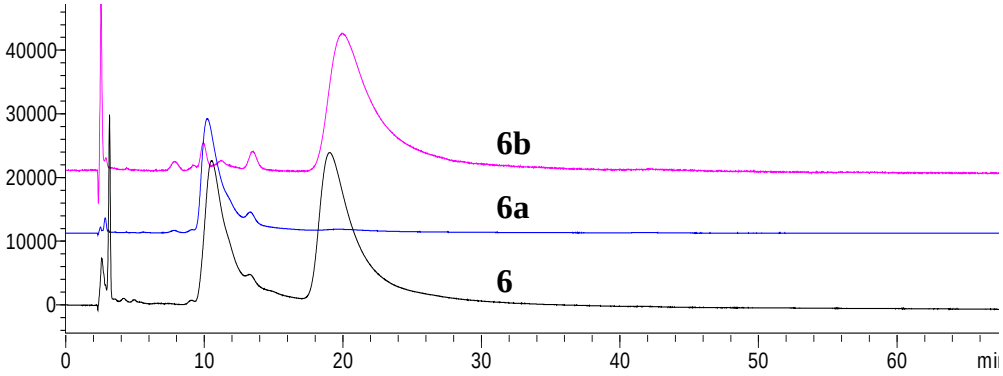


Figure S120. Chiral-phase HPLC chromatogram of compounds **6a** and **6b**

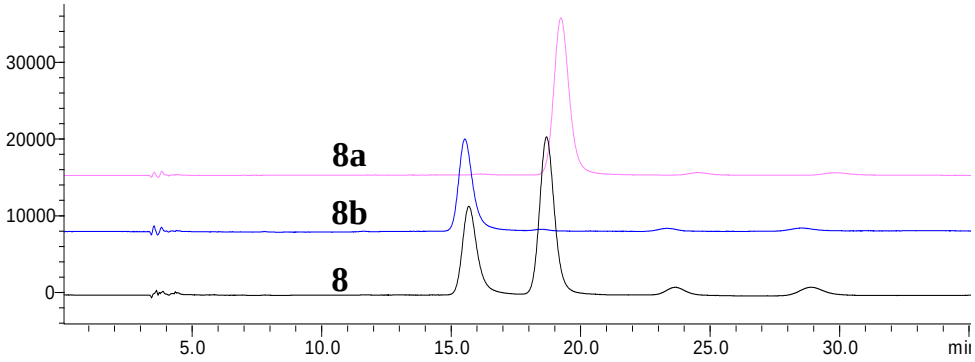


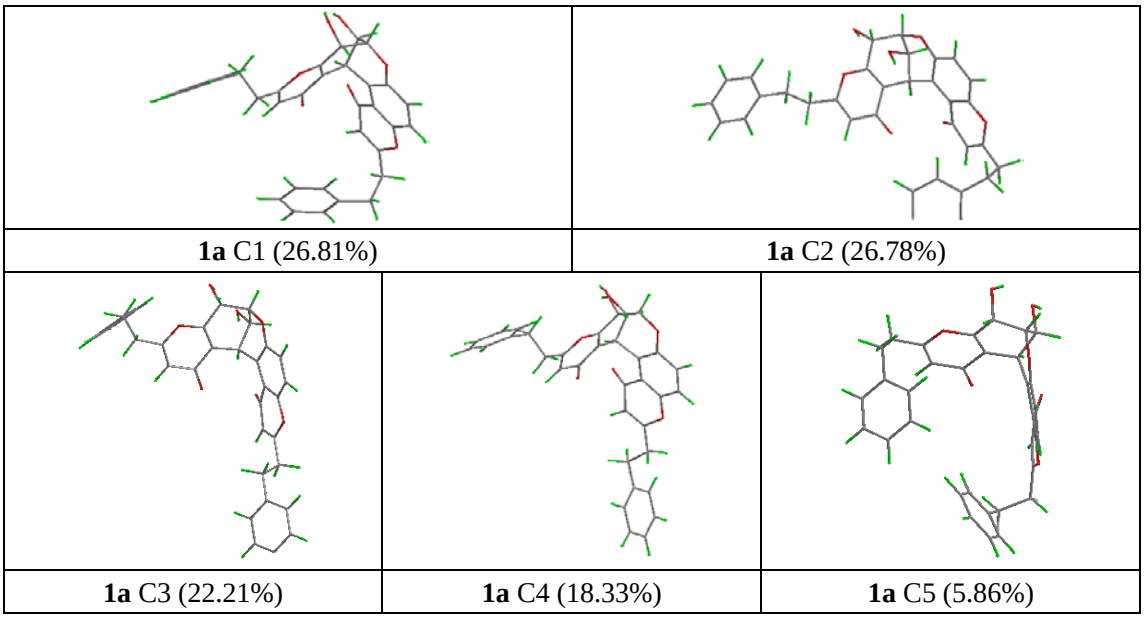
Figure S121. Chiral-phase HPLC chromatogram of compounds **8a** and **8b**

4. X-Ray Crystallographic Data

Table S122. X-ray Crystallographic Data for **1**

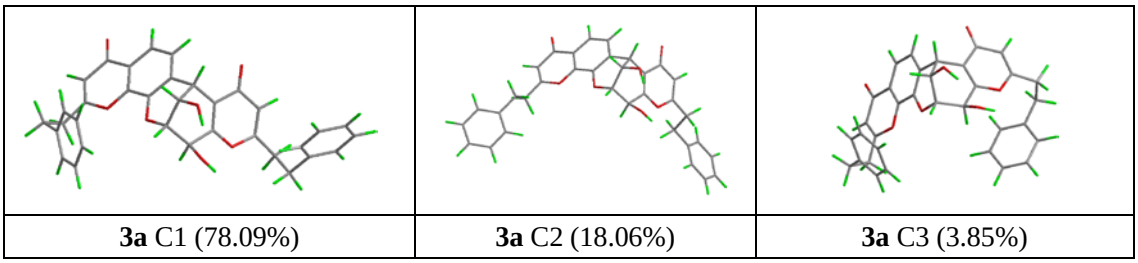
Identification code	exp_3891
Empirical formula	$C_{35}H_{32}O_8$
Formula weight	580.61
Temperature / K	107.2
Crystal system	triclinic
Space group	P-1
a / Å, b / Å, c / Å	9.6731(4), 11.8776(6), 13.3871(6)
α/°, β/°, γ/°	110.146(4), 98.926(4), 99.616(4)
Volume / $Å^3$	1385.60(11)
Z	2
ρ_{calc} / mg mm^{-3}	1.392
μ / mm^{-1}	0.808
F(000)	612
Crystal size / mm^3	0.20 × 0.17 × 0.07
2Θ range for data collection	7.22 to 141.96°
Index ranges	$-11 \le h \le 11$, $-14 \le k \le 14$, $-16 \le l \le 16$
Reflections collected	17394
Independent reflections	5259[R(int) = 0.0324 (inf-0.9Å)]
Data/restraints/parameters	5259/0/392
Goodness-of-fit on F^2	1.047
Final R indexes [I>2σ (I) i.e. F_o>4σ (F_o)]	R_1 = 0.0390, wR_2 = 0.1020
Final R indexes [all data]	R_1 = 0.0444, wR_2 = 0.1064
Largest diff. peak/hole / e $Å^{-3}$	0.321/-0.239
Flack Parameters	N
Hooft Parameter	N
Completeness	0.983

5. ECD Calculations



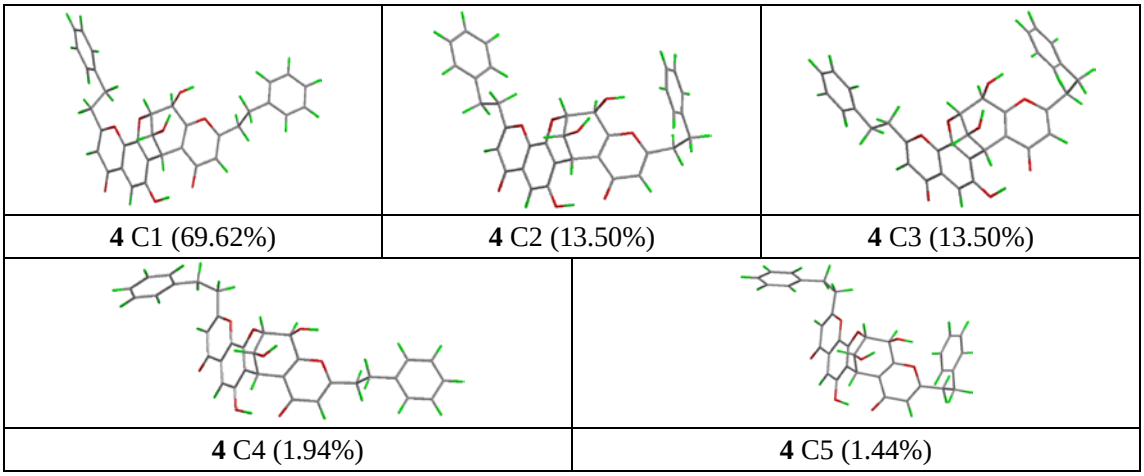
1a C1 (26.81%)	**1a** C2 (26.78%)	
1a C3 (22.21%)	**1a** C4 (18.33%)	**1a** C5 (5.86%)

Figure S123. DFT-optimized structures for low-energy conformers of (5*S*,6*R*,7*S*,8*R*)-**1a**



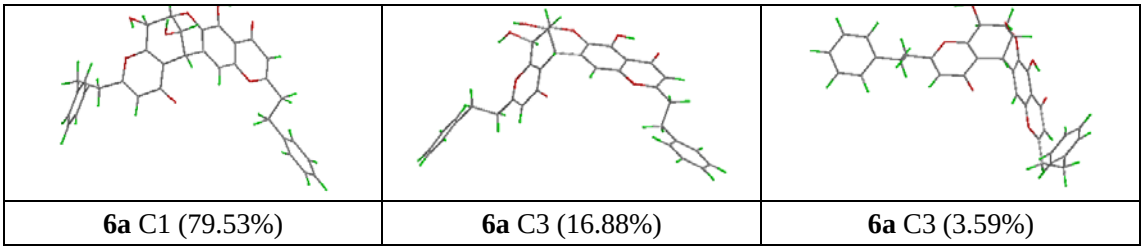
3a C1 (78.09%)	**3a** C2 (18.06%)	**3a** C3 (3.85%)

Figure S124. DFT-optimized structures for low-energy conformers of (5*S*,6*R*,7*S*,8*R*)-**3a**



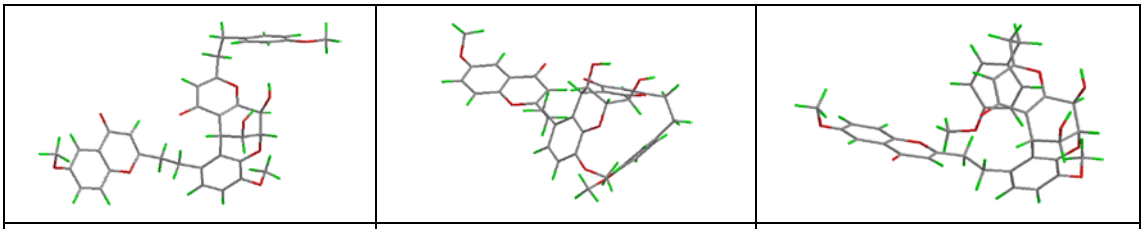
4 C1 (69.62%)	**4** C2 (13.50%)	**4** C3 (13.50%)
4 C4 (1.94%)	**4** C5 (1.44%)	

Figure S125. DFT-optimized structures for low-energy conformers of (5*S*,6*R*,7*S*,8*R*)-**4**

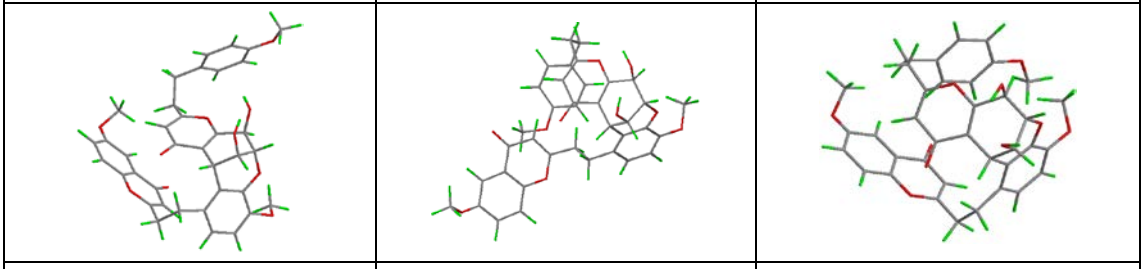


6a C1 (79.53%)	**6a** C3 (16.88%)	**6a** C3 (3.59%)

Figure S126. DFT-optimized structures for low-energy conformers of (5*R*,6*S*,7*R*,8*S*)-**6a**

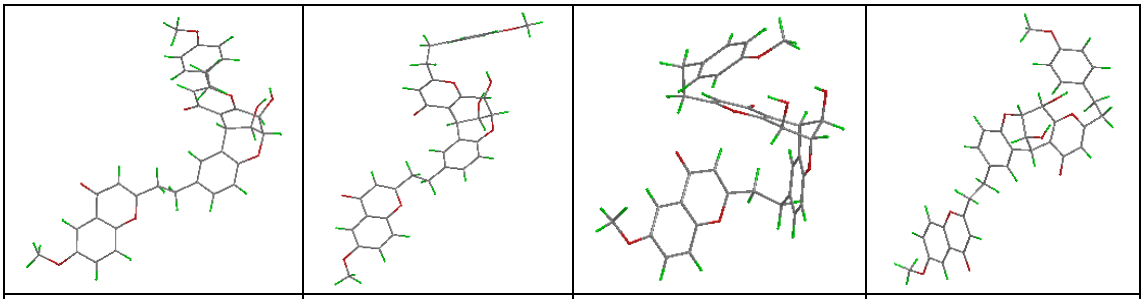


7 C1 (44.43%)	**7** C2 (37.01%)	**7** C3 (14.85%)



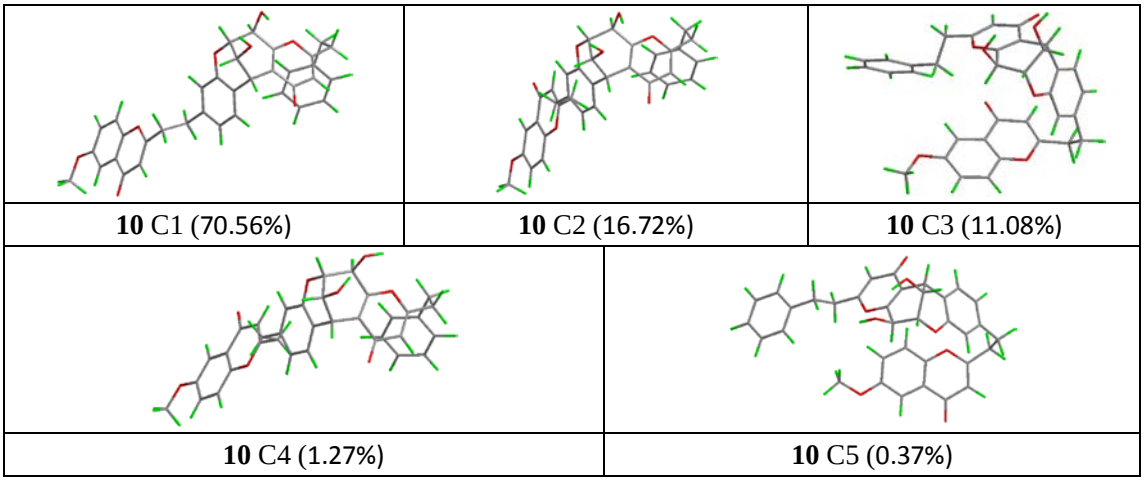
7 C4 (3.41%)	**7** C5 (0.17%)	**7** C6 (0.12%)

Figure S127. DFT-optimized structures for low-energy conformers of (5*R*,6*S*,7*R*,8*S*)-**7**



9 C1 (76.87%	**9** C2 (15.33%)	**9** C3 (4.67%)	**9** C4 (3.14%)

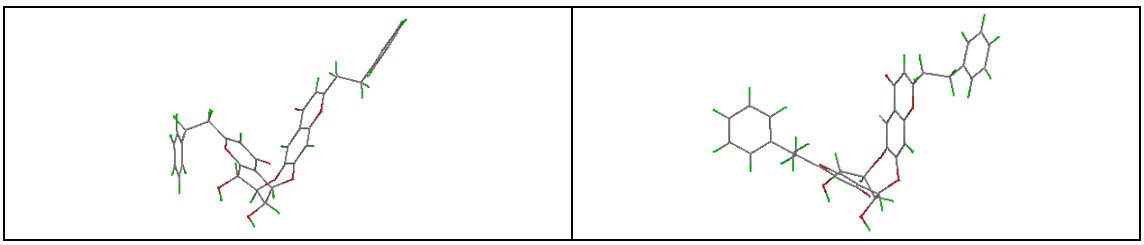
Figure S128. DFT-optimized structures for low-energy conformers of (5*S*,6*R*,7*S*,8*R*)-**9**



10 C1 (70.56%)	**10** C2 (16.72%)	**10** C3 (11.08%)

10 C4 (1.27%)	**10** C5 (0.37%)

Figure S129. DFT-optimized structures for low-energy conformers of (5*S*,6*R*,7*S*,8*R*)-**10**



11 C1 (67.33%)	**11** C2 (32.67%)

Figure S130. DFT-optimized structures for low-energy conformers of (5*S*,6*R*,7*S*,8*R*)-**11**

6. Experimental and calculated ECD spectra

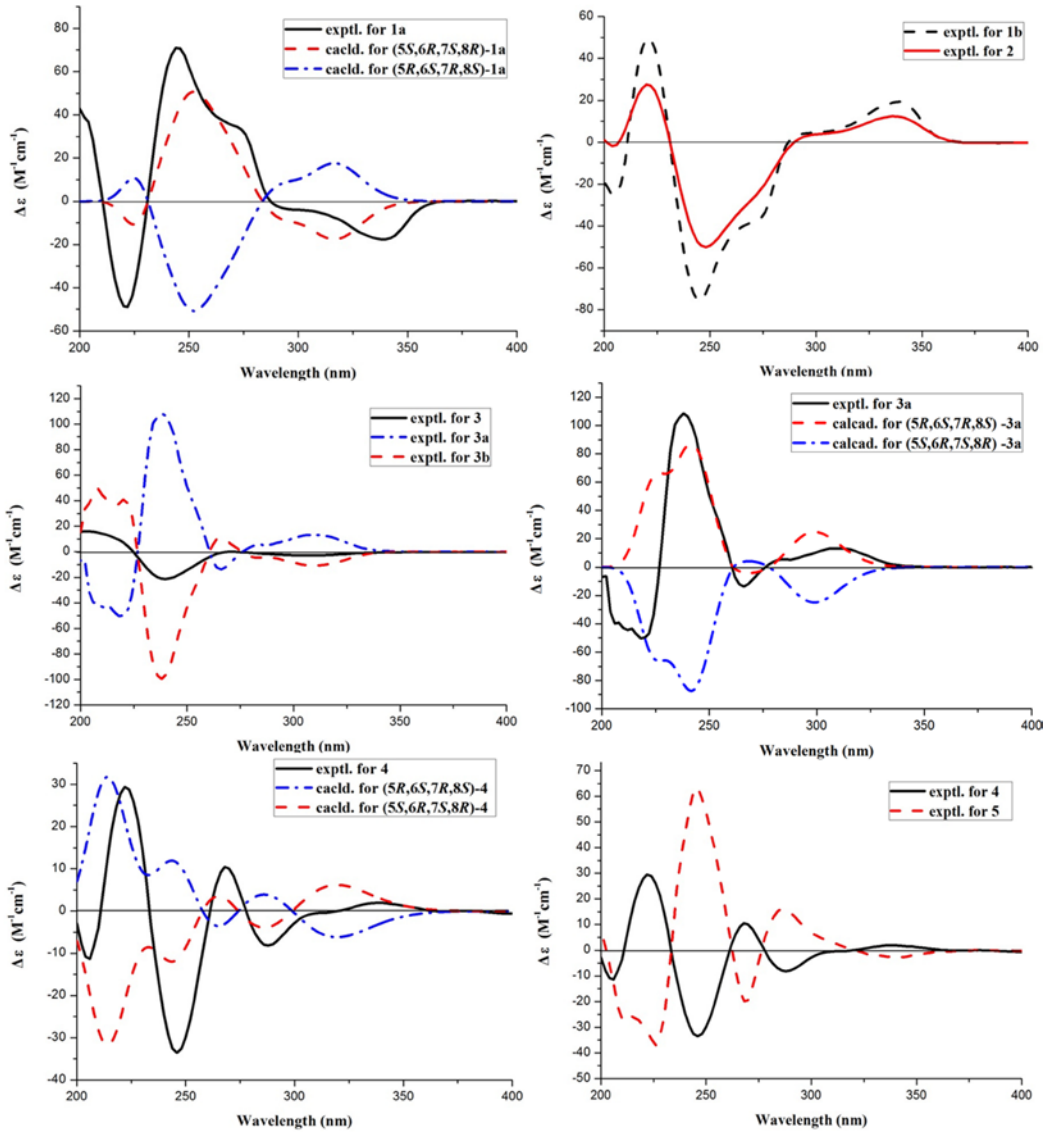


Figure S131. Experimental and calculated ECD spectra of compounds **2**–**5** (in MeOH)

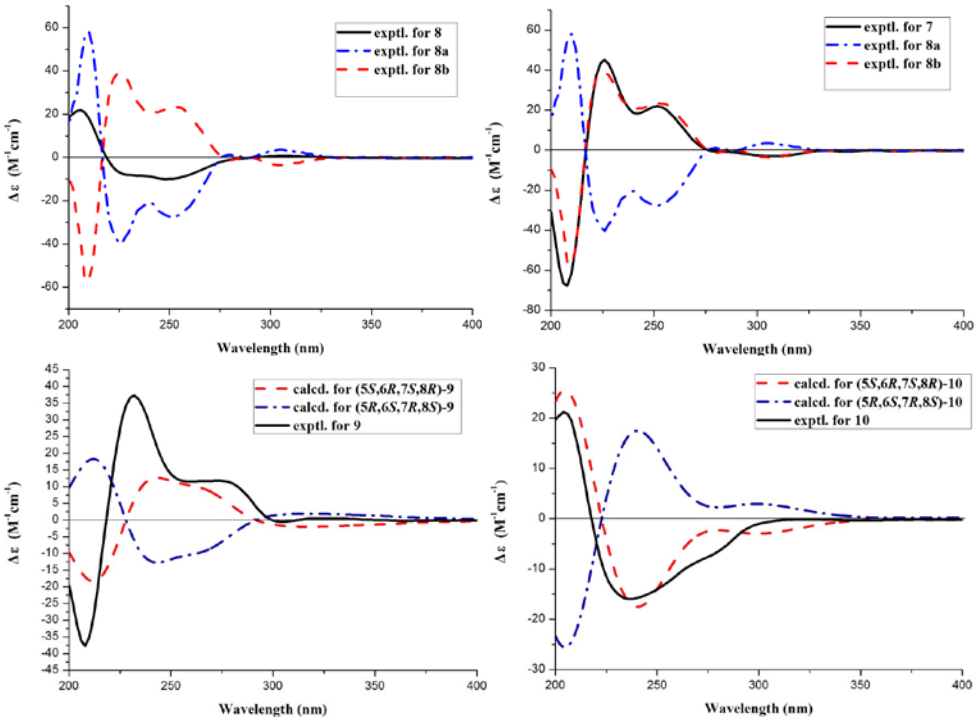


Figure S132. Experimental and calculated ECD spectra of compounds **7–10** (in MeOH)

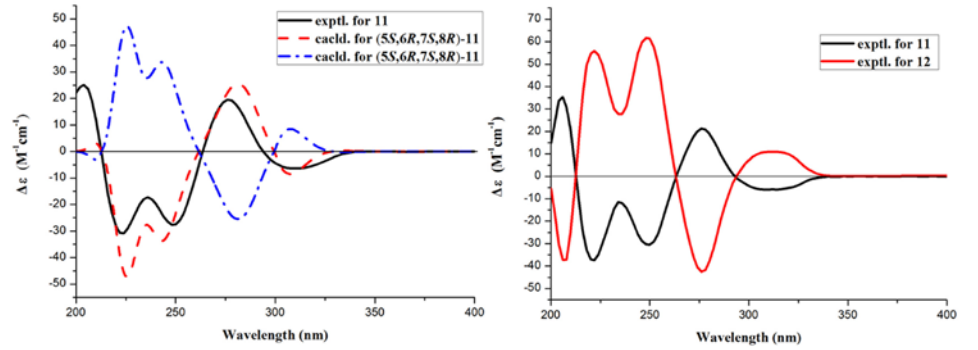


Figure S133. Experimental and calculated ECD spectra of compounds **11** and **12** (in MeOH)