Supporting Information

Pyrimidine Nucleosides from *Streptomyces* sp. SSA28

Cheng-Dong Xu, Hao-Jian Zhang, Zhong-Jun Ma*

Institute of Marine Biology and Pharmacology, Ocean College, Zhejiang University, Zhoushan 316021, People's Republic of China;

*Corresponding author E-mail: mazj@zju.edu.cn

Table of Contants

Cytotoxicity Assay

HCT-116 cells were revived in McCoy's 5A medium supplemented with 10% FBS in a humidified atomosphere containing 5% CO_2 at 37 ℃. Removing the culture supernatants, cells were maintained in new medium and added into 96-well plates. Cells (5×10^3 cells/well) were incubated in the atomosphere containing 5% CO_2 at 37 ℃ for 24 hours. Then cells were added with test compounds (20 μg/mL, dissolved in DMSO) by half dilution method to give the terminal concentration of 10, 5, 2.5, 1.25 and 0.625 μg/mL, incubating for 24 hours. 100 μL of TCA (10%) was added into each wells after removing the supernatants, and then kept for 24 hours at 4 ℃. Removing TCA and washing for 5 times by water, cells were mixed with 80 μL of SRB of each well and kept for 20 mins. Then 100 μL of Tris solution (10 mmol/L) was added into each well after removing supernatants. OD values were measured by ELIASA under 515 nm, and then the IC_{50} values were calculated.

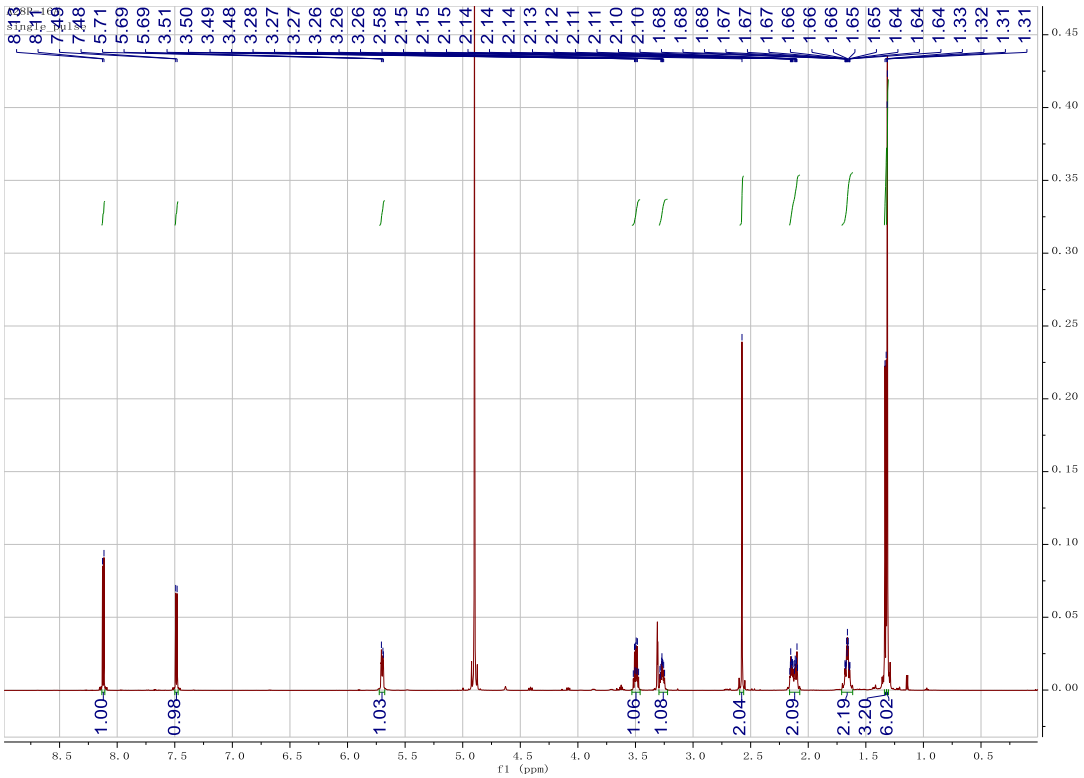


Figure S1. ^{1}H NMR spectrum of **1**

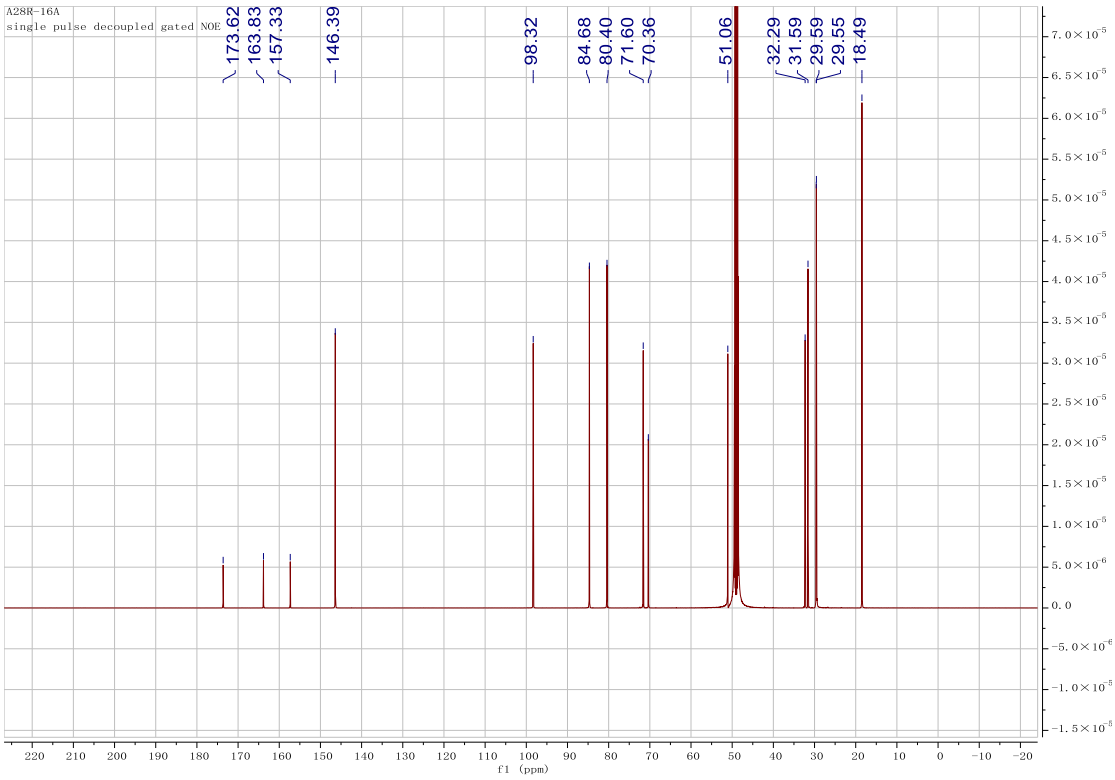


Figure S2. ^{13}C NMR spectrum of **1**

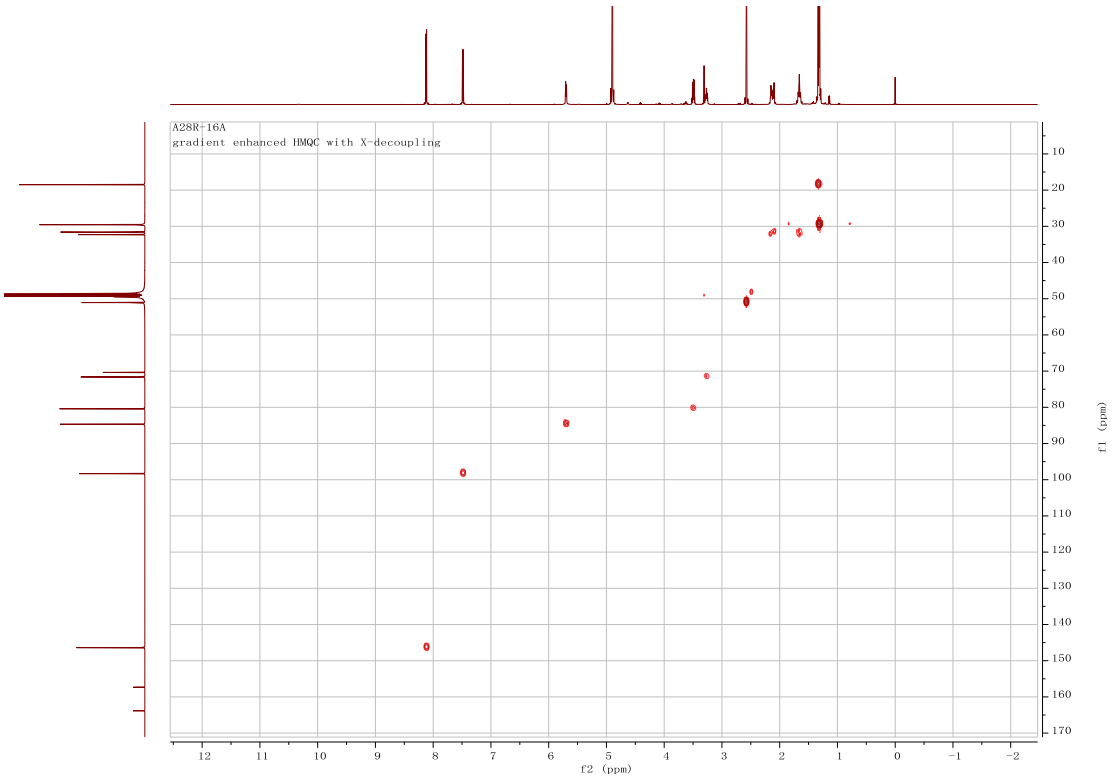


Figure S3. HSQC spectrum of **1**

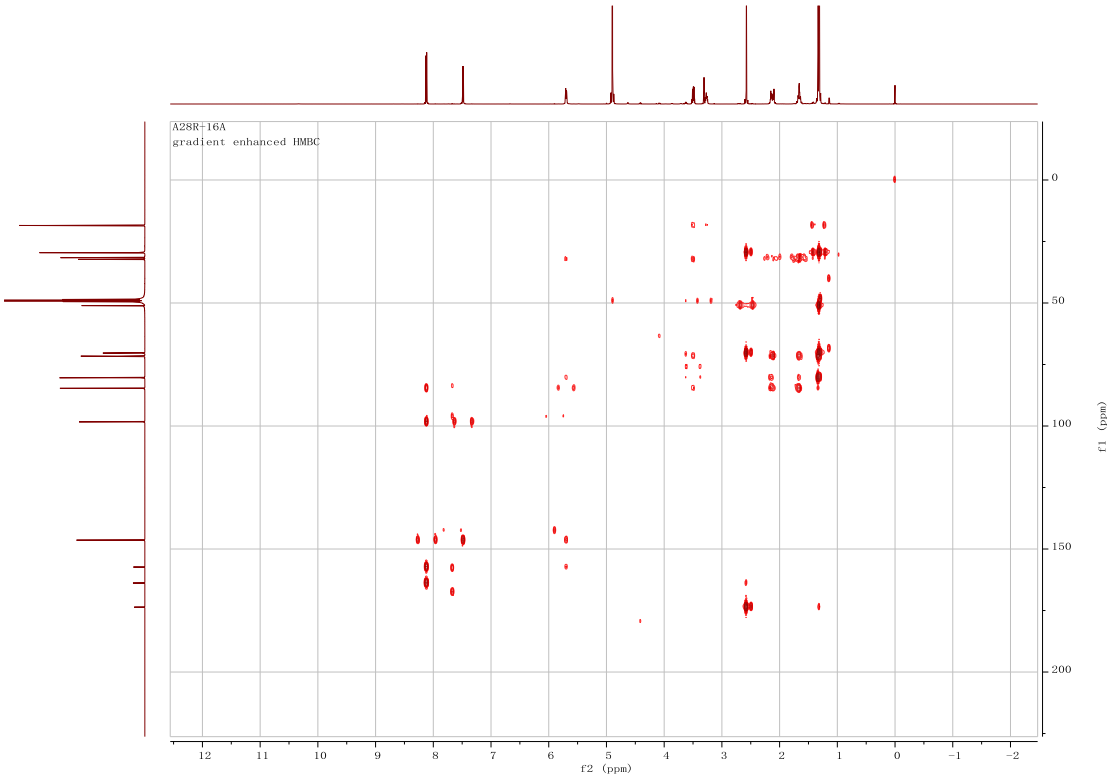


Figure S4. HMBC spectrum of **1**

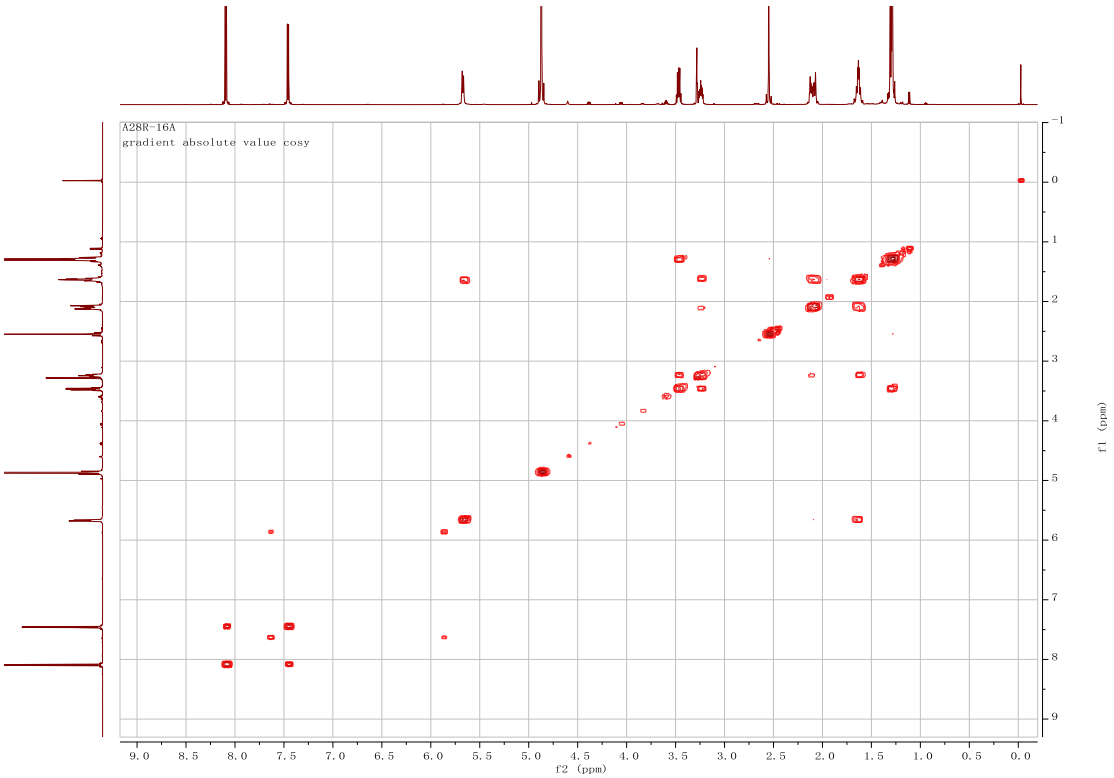


Figure S5. ^{1}H-^{1}H COSY spectrum of **1**

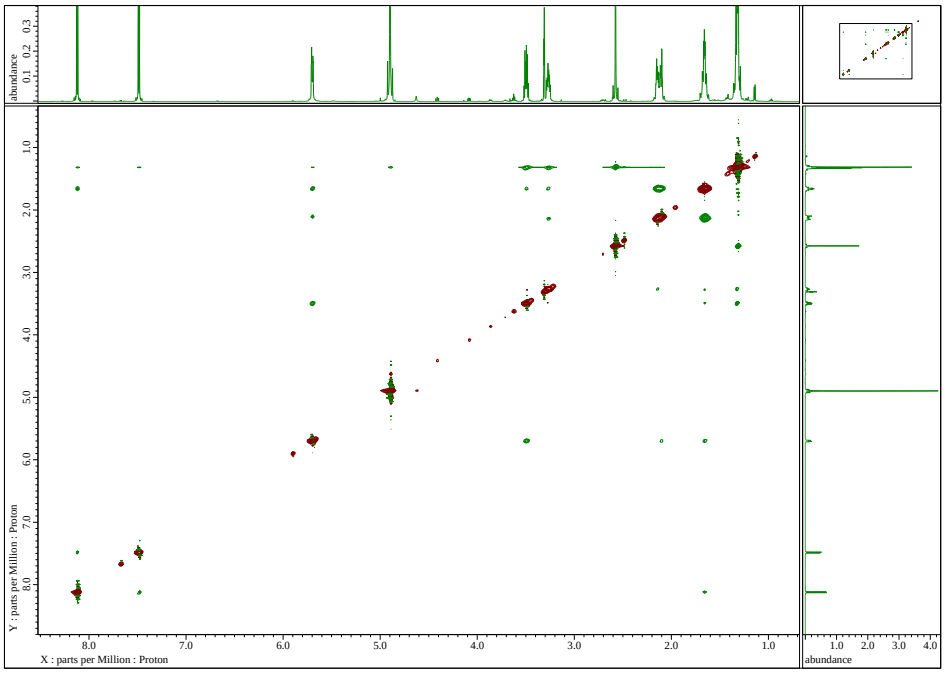


Figure S6. NOESY spectrum of **1**

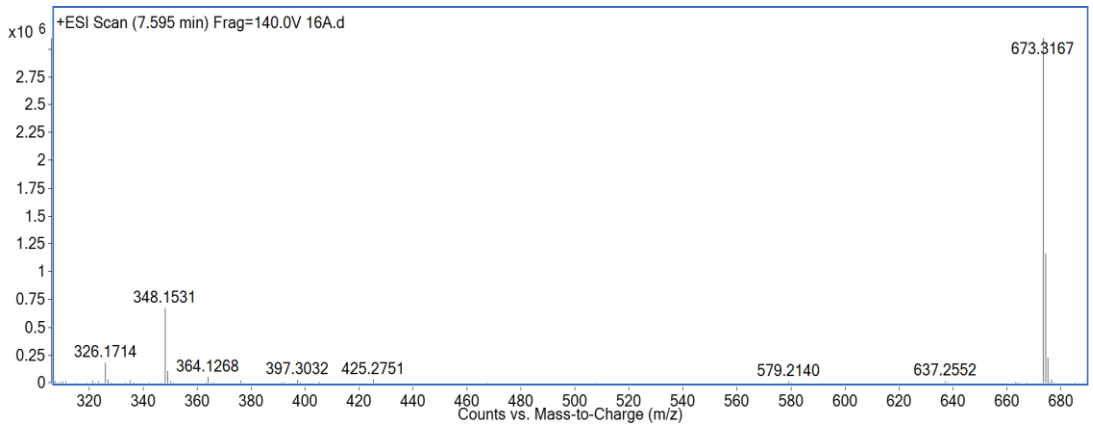


Figure S7. HRESIMS spectrum of **1**

Figure S8. IR spectrum of **1**.

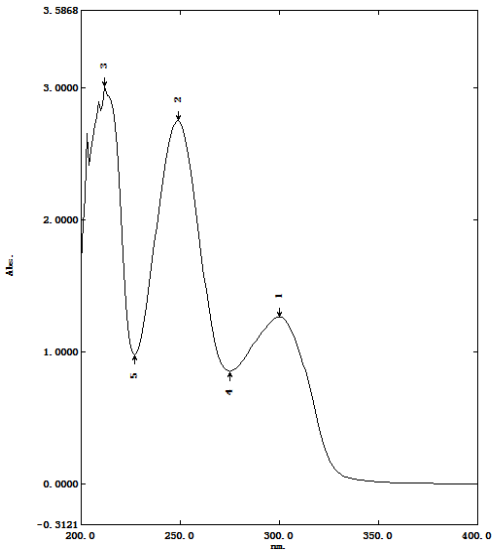


Figure S9. UV spectrum of **1**.

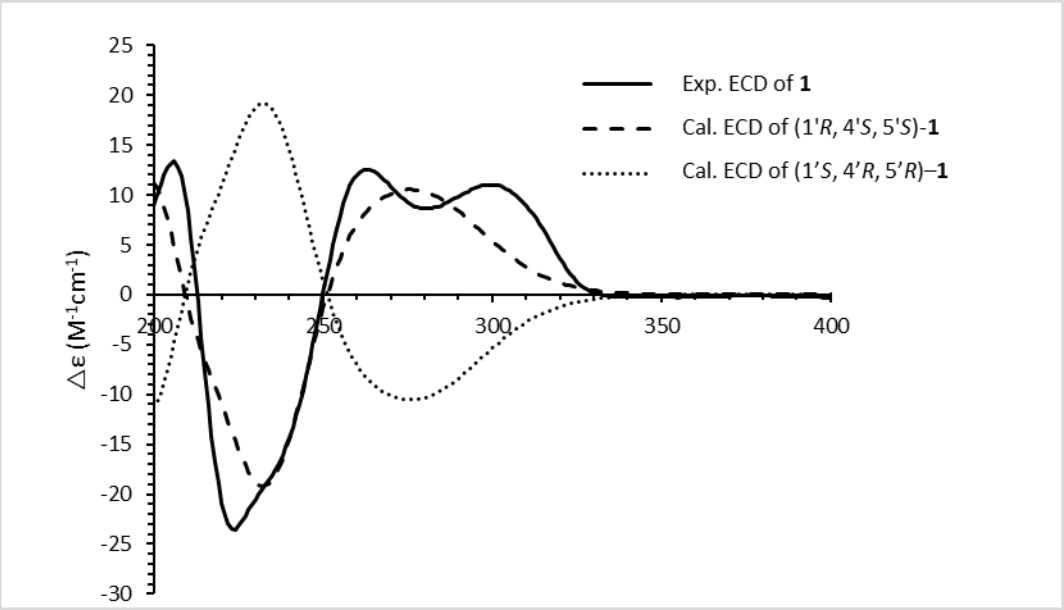


Figure S10. CD spectrum of **1**.

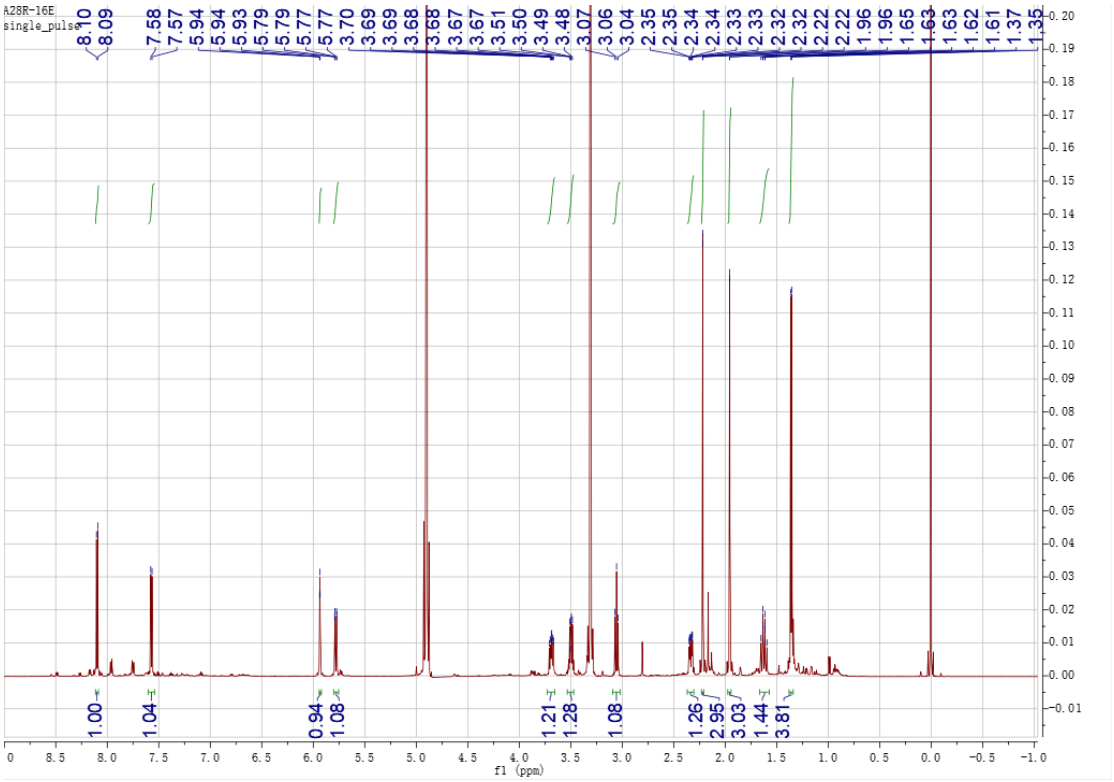


Figure S11. ^{1}H NMR spectrum of **2**

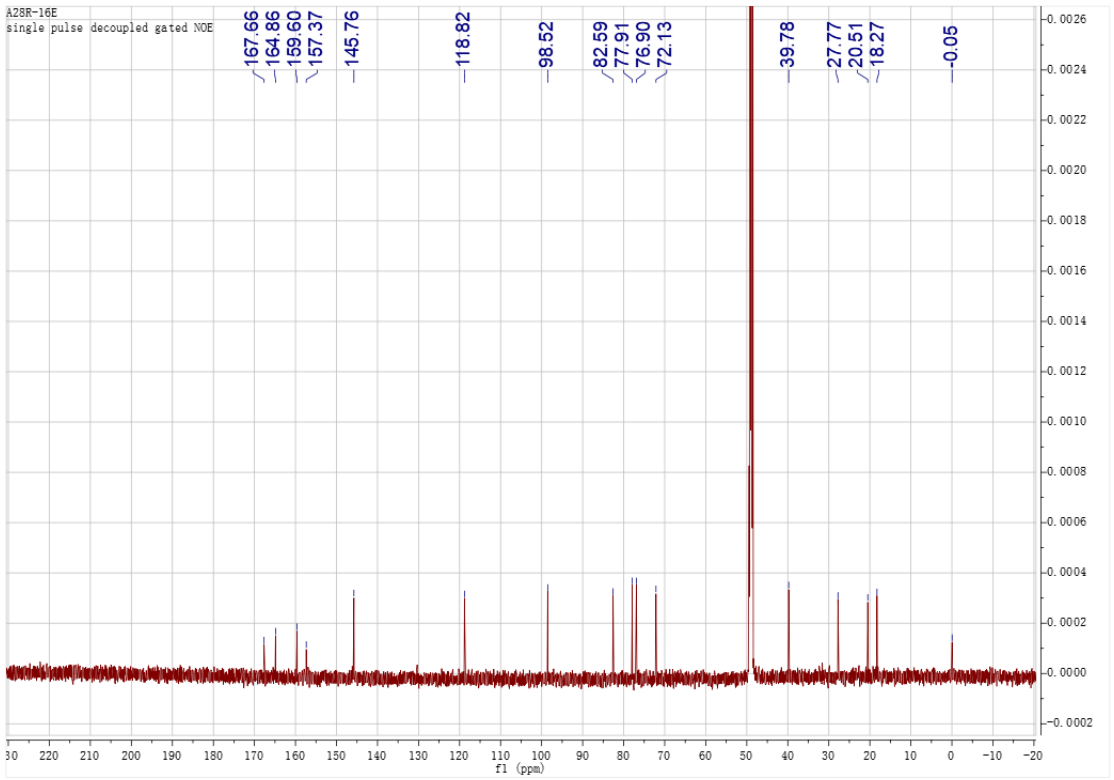


Figure S12. ^{13}C NMR spectrum of **2**

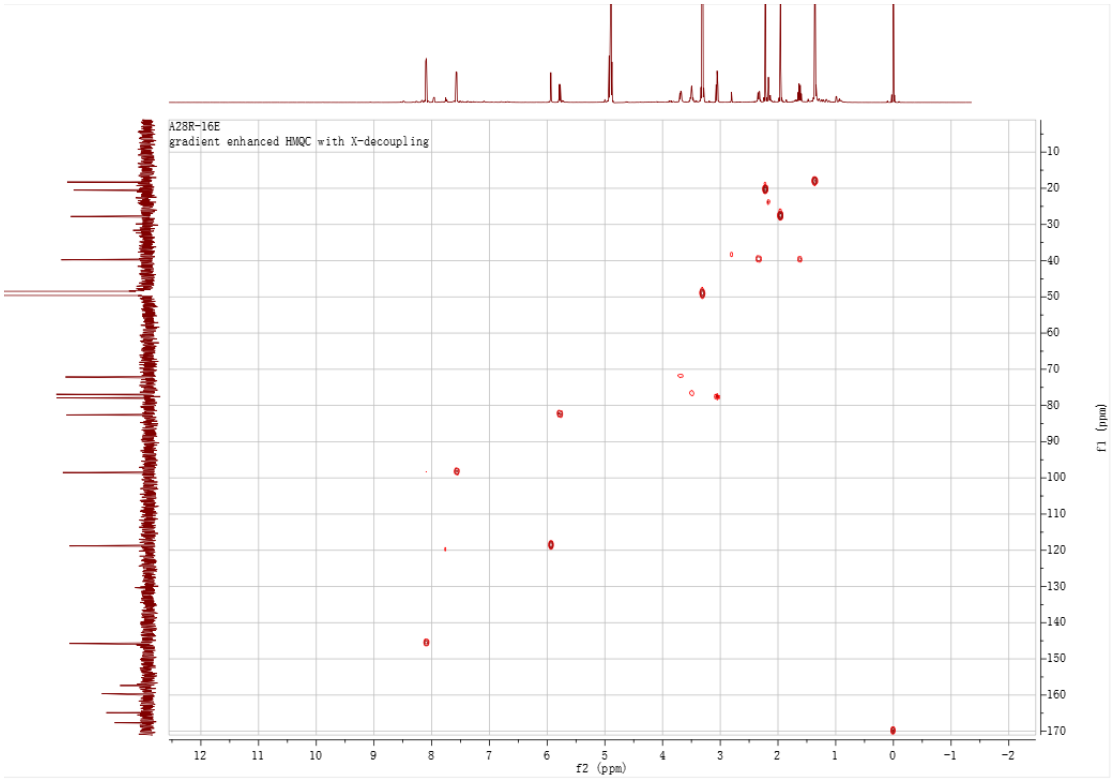


Figure S13. HSQC spectrum of **2**

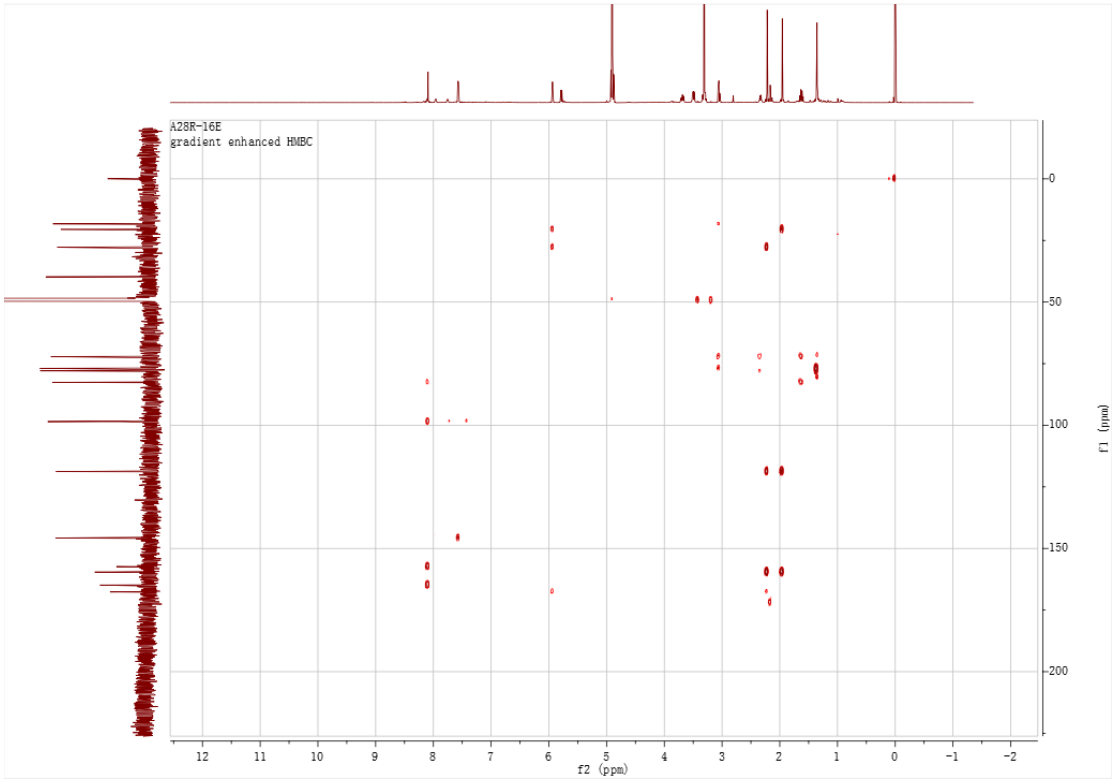


Figure S14. HMBC spectrum of **2**

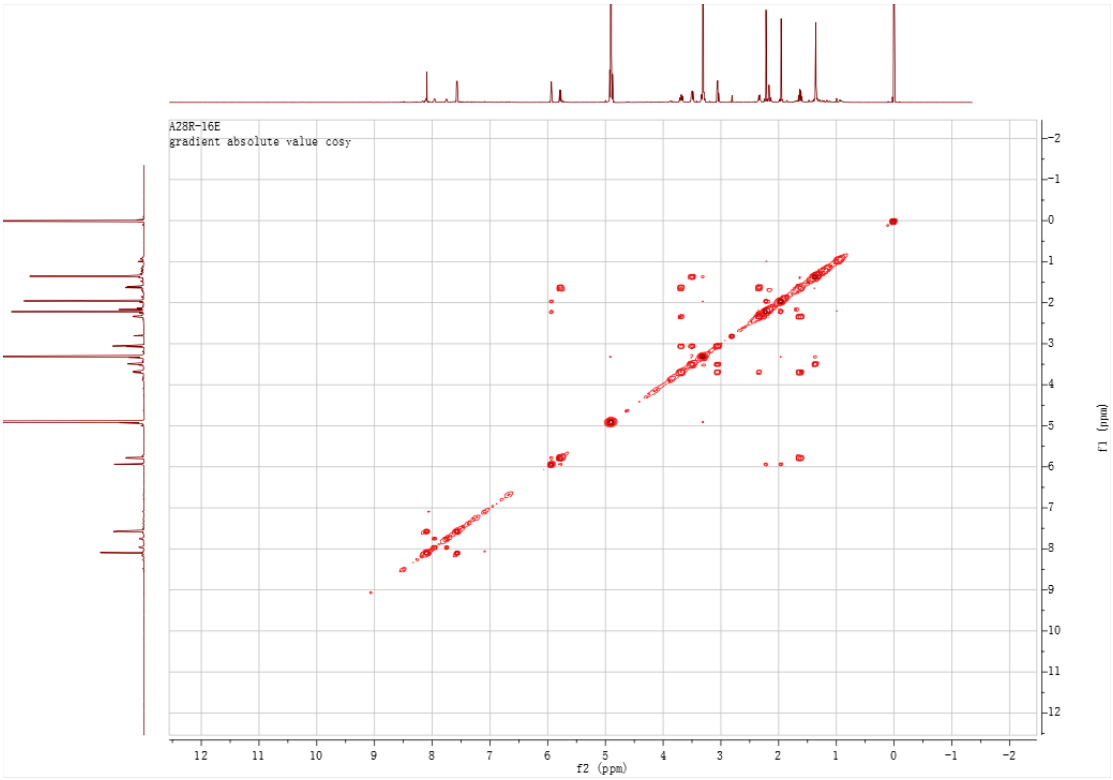


Figure S15. ^{1}H-^{1}H COSY spectrum of **2**

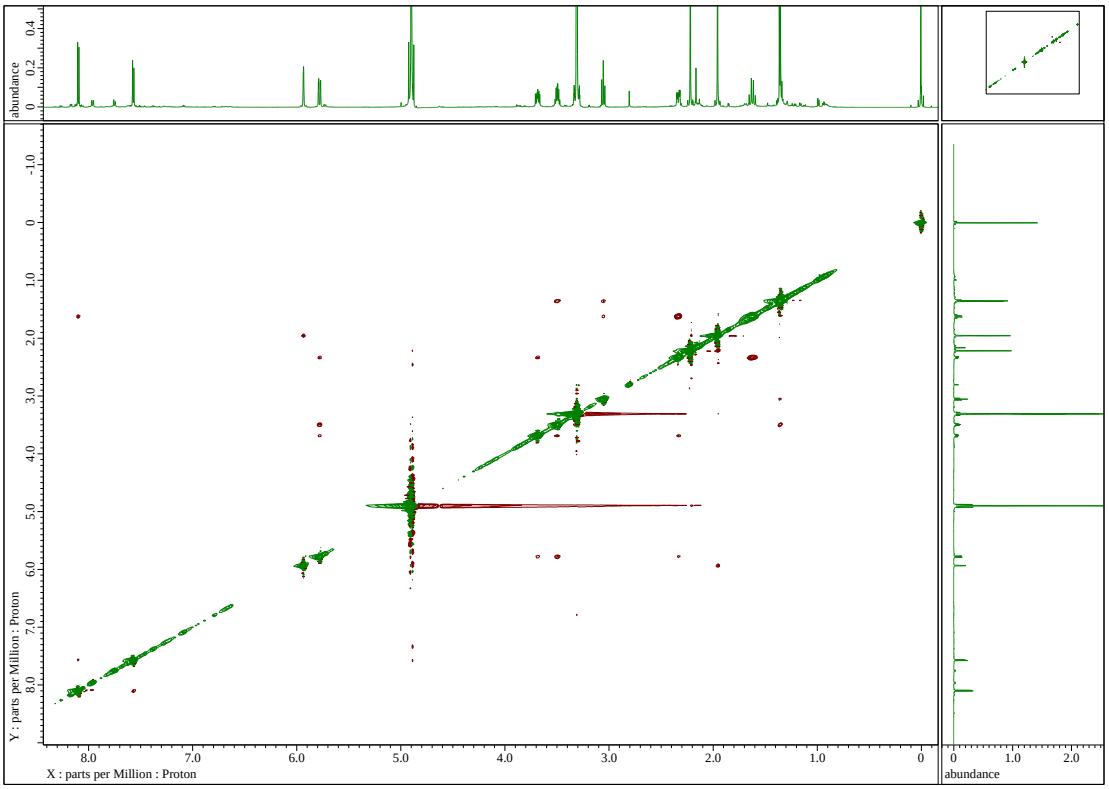


Figure S16. NOESY spectrum of **2**

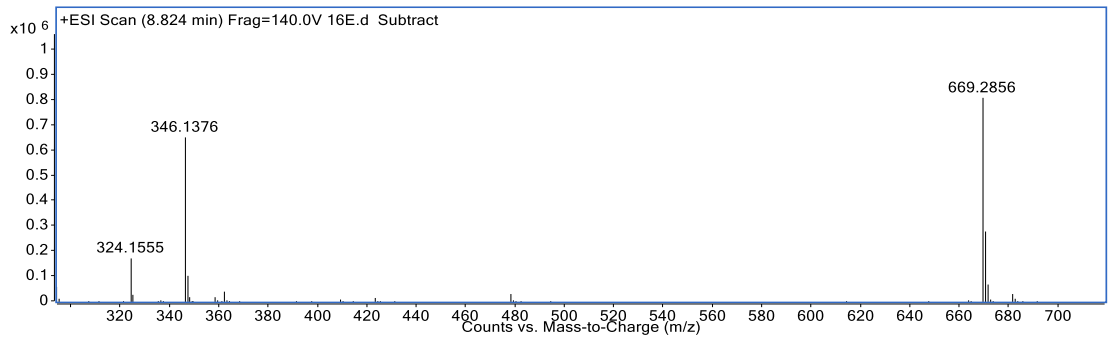


Figure S17. HRESIMS spectrum of **2**

Figure S18. IR spectrum of **2**

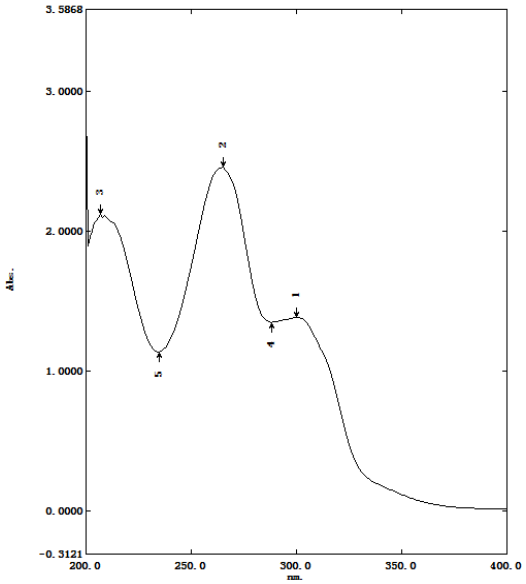


Figure S19. UV spectrum of **2**

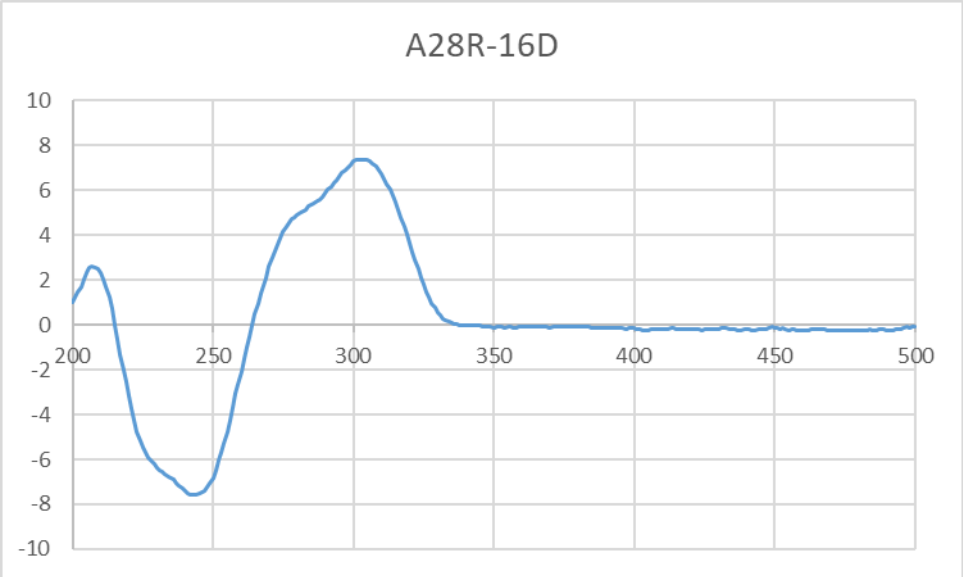


Figure S20. CD spectrum of **2**

Figure S21. ^{1}H NMR spectrum of **3**

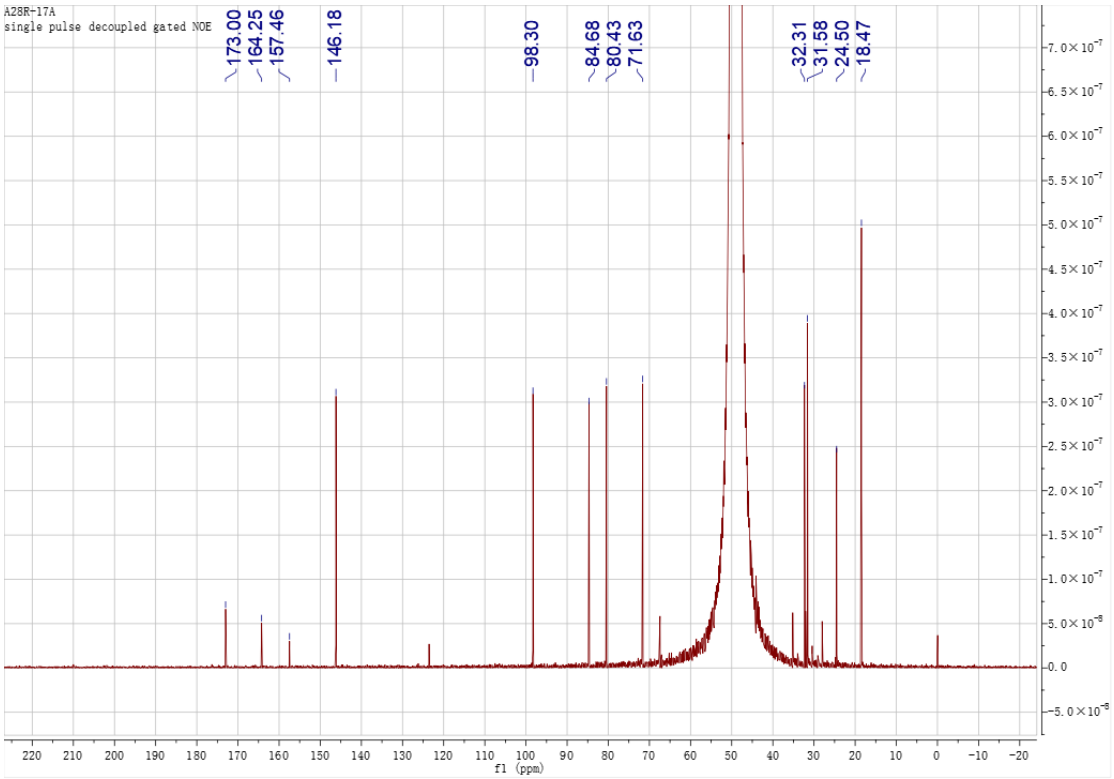


Figure S22. ^{13}C NMR spectrum of **3**

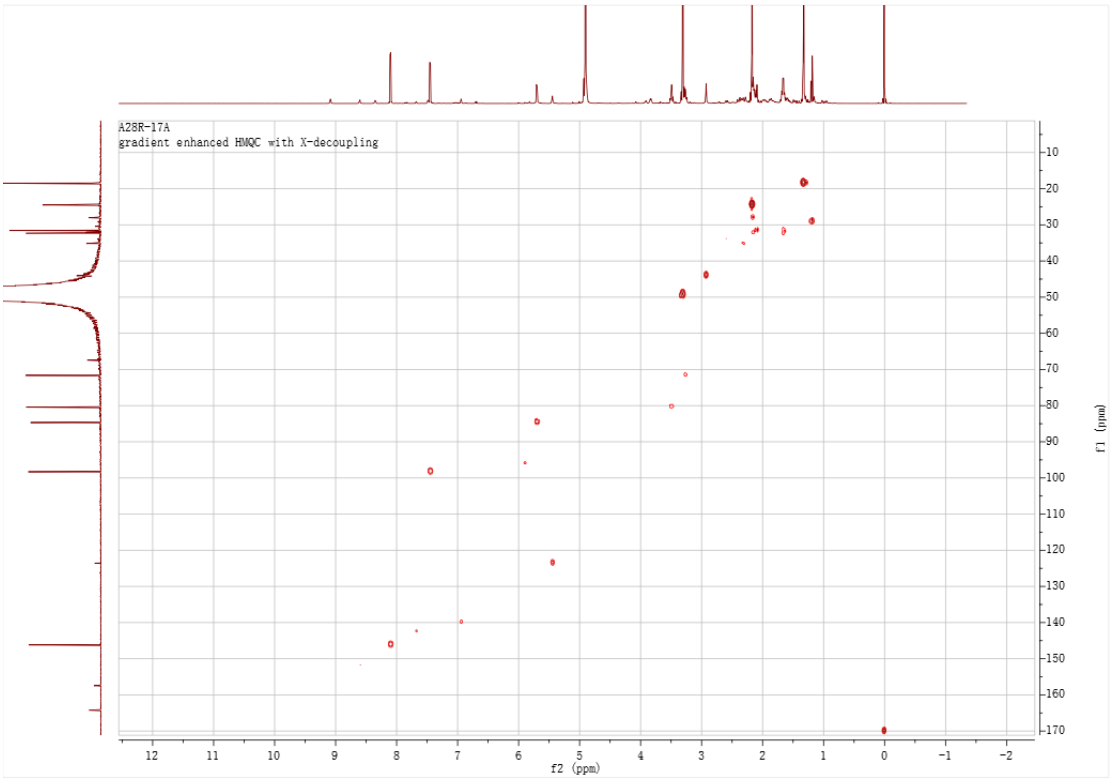


Figure S23. HSQC spectrum of **3**

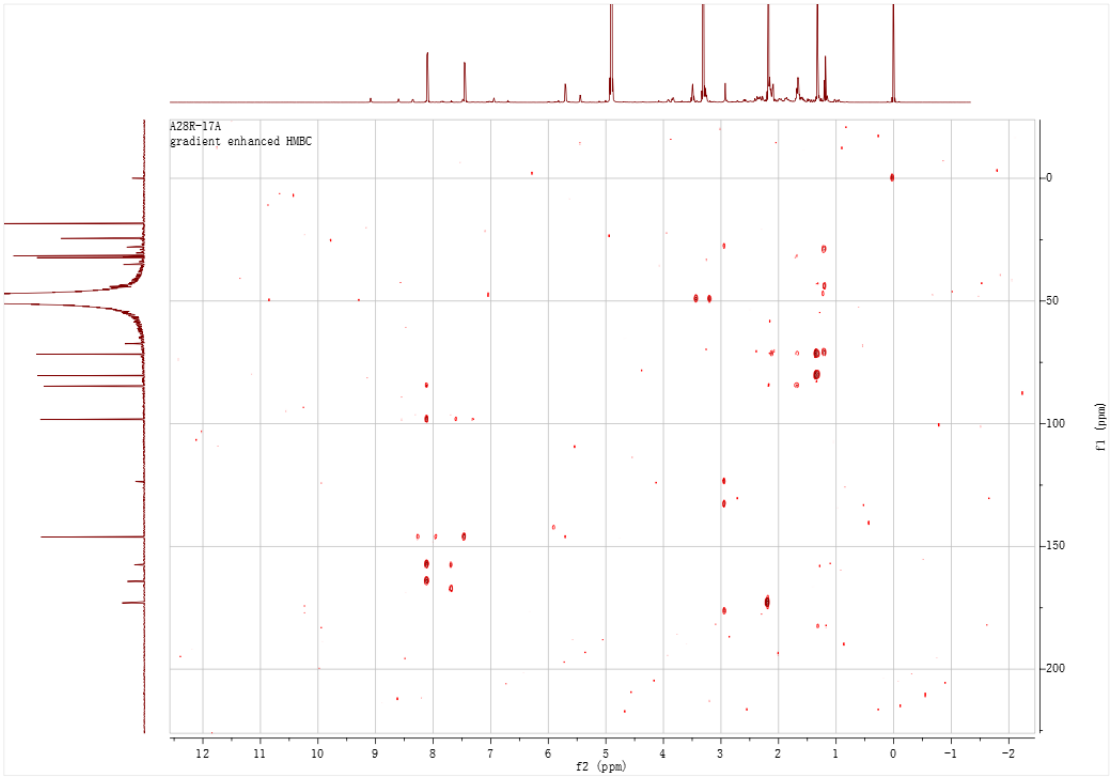


Figure S24. HMBC spectrum of **3**

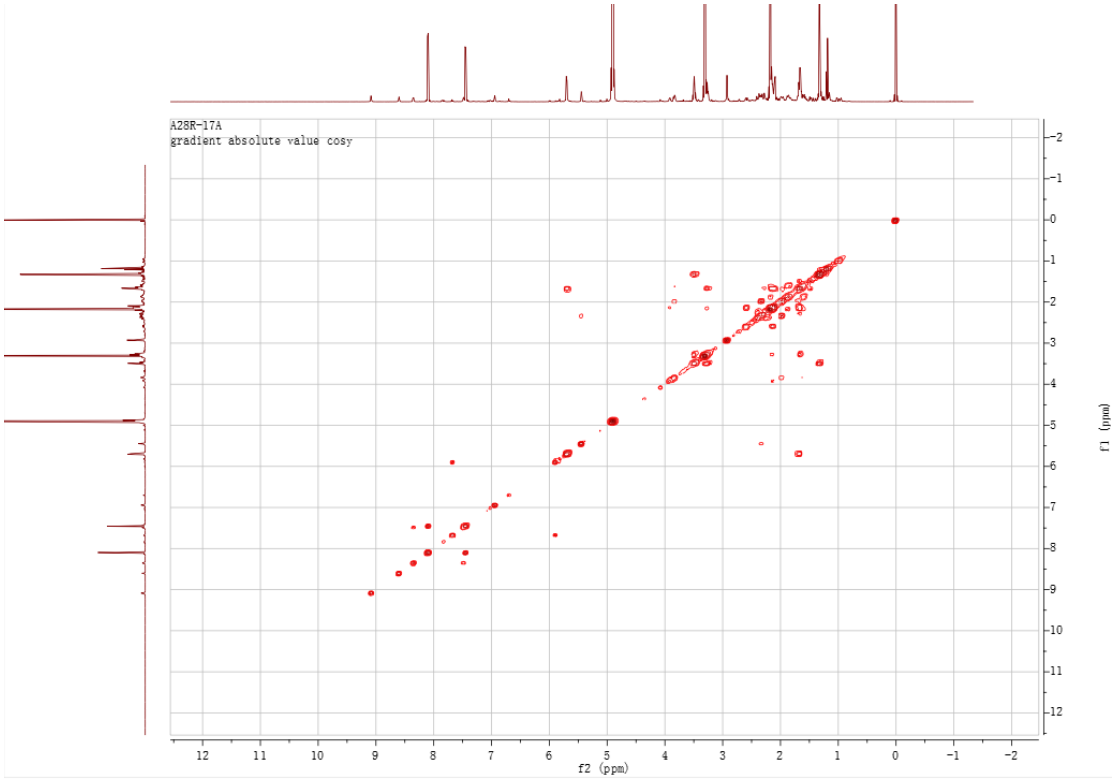


Figure S25. ^{1}H-^{1}H COSY spectrum of **3**

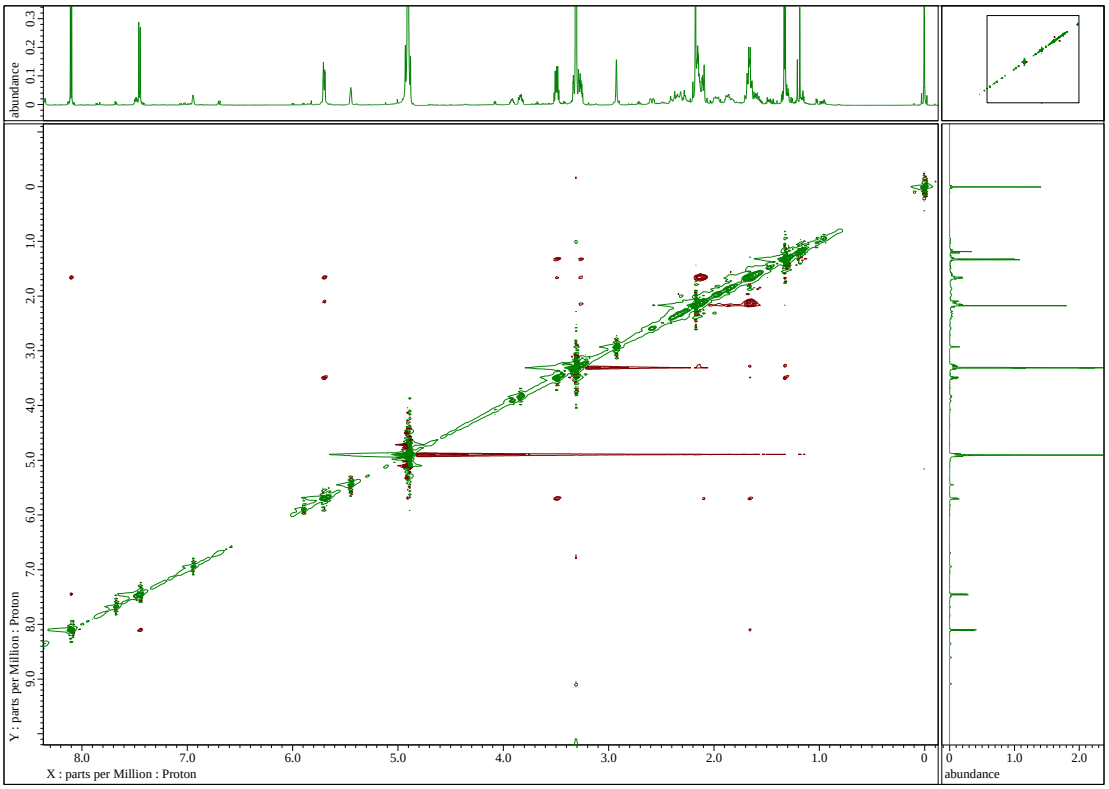


Figure S26. NOESY spectrum of **3**

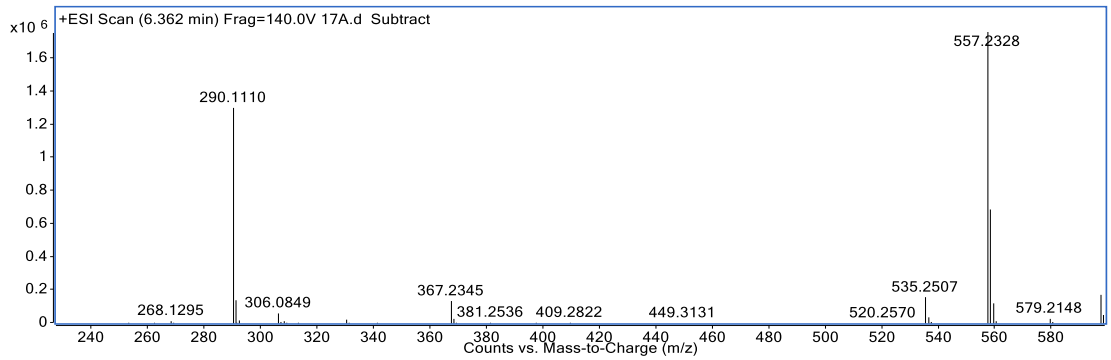


Figure S27. HRESIMS spectrum of **3**

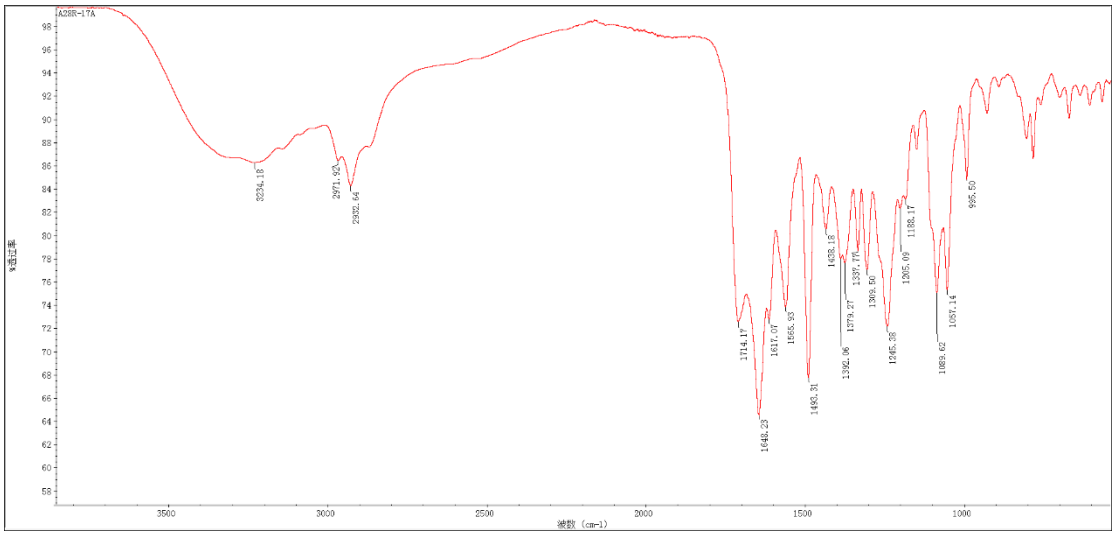


Figure S28. IR spectrum of **3**

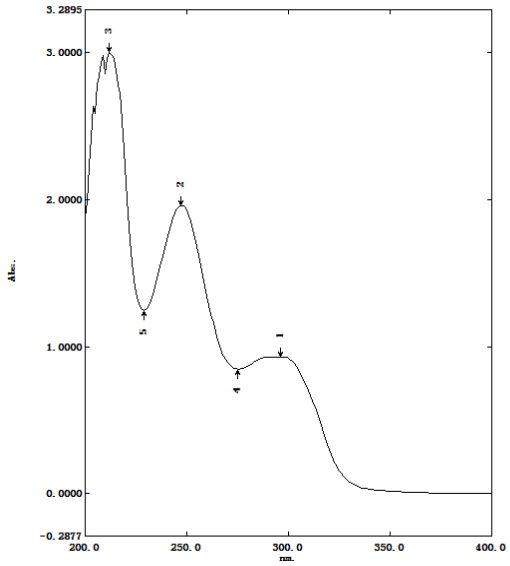


Figure S29. UV spectrum of **3**

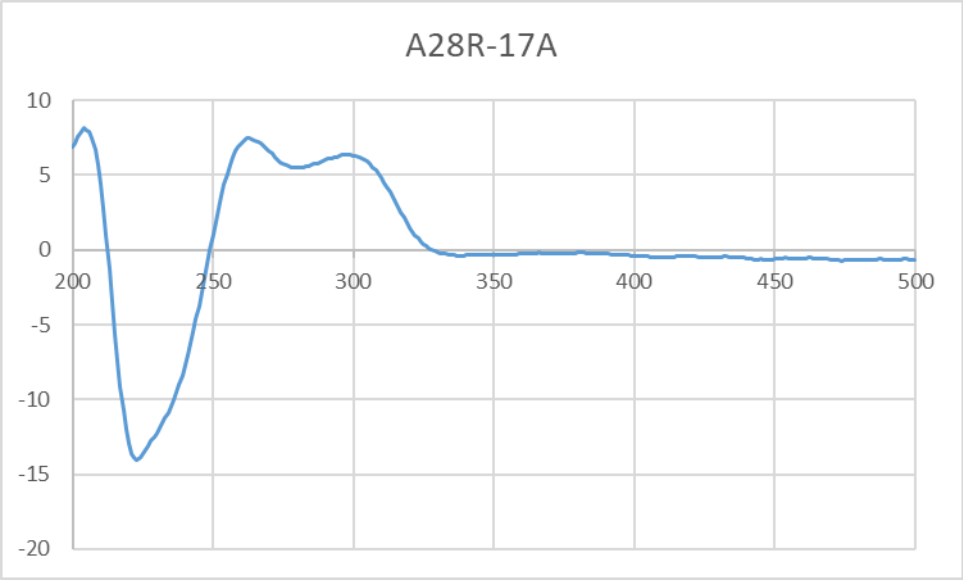


Figure S30. CD spectrum of **3**

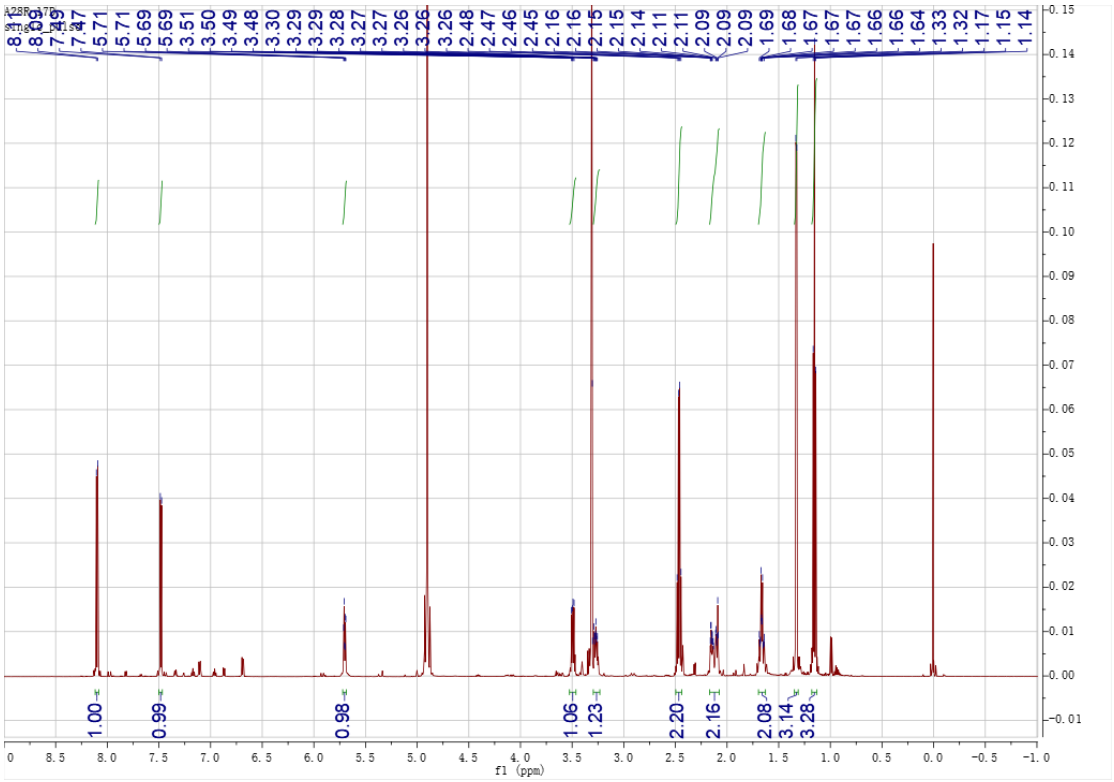


Figure S31. ^{1}H NMR spectrum of **4**

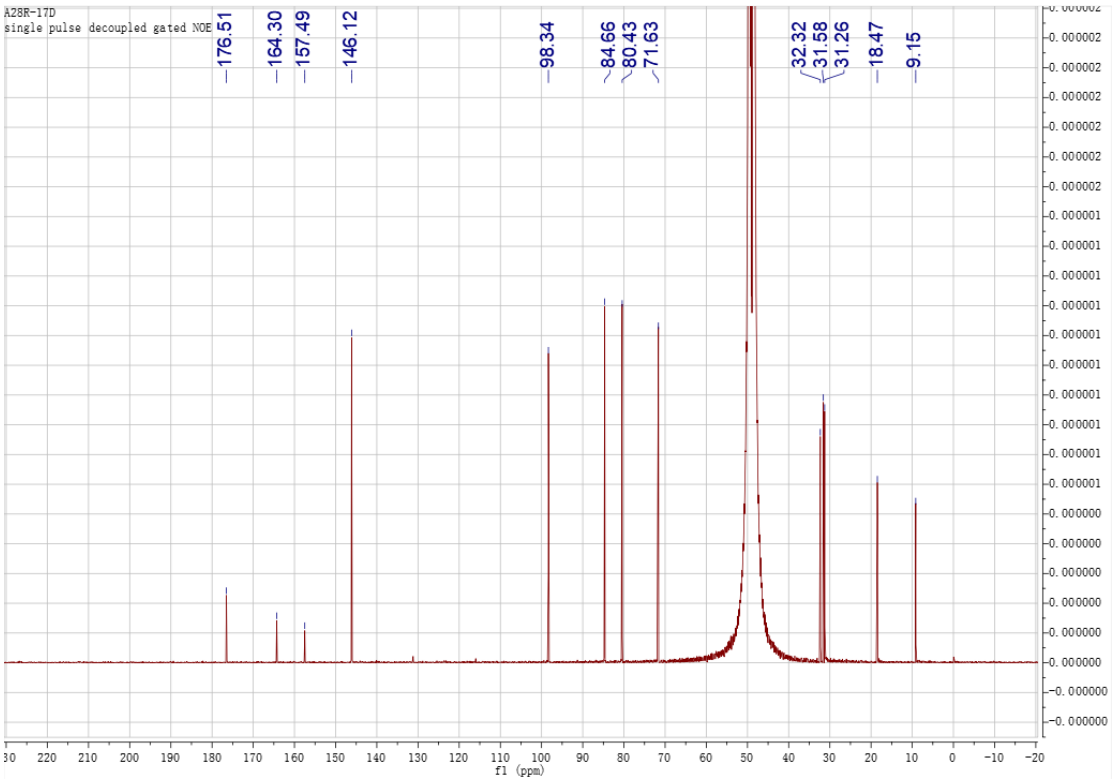


Figure S32. ^{13}C NMR spectrum of **4**

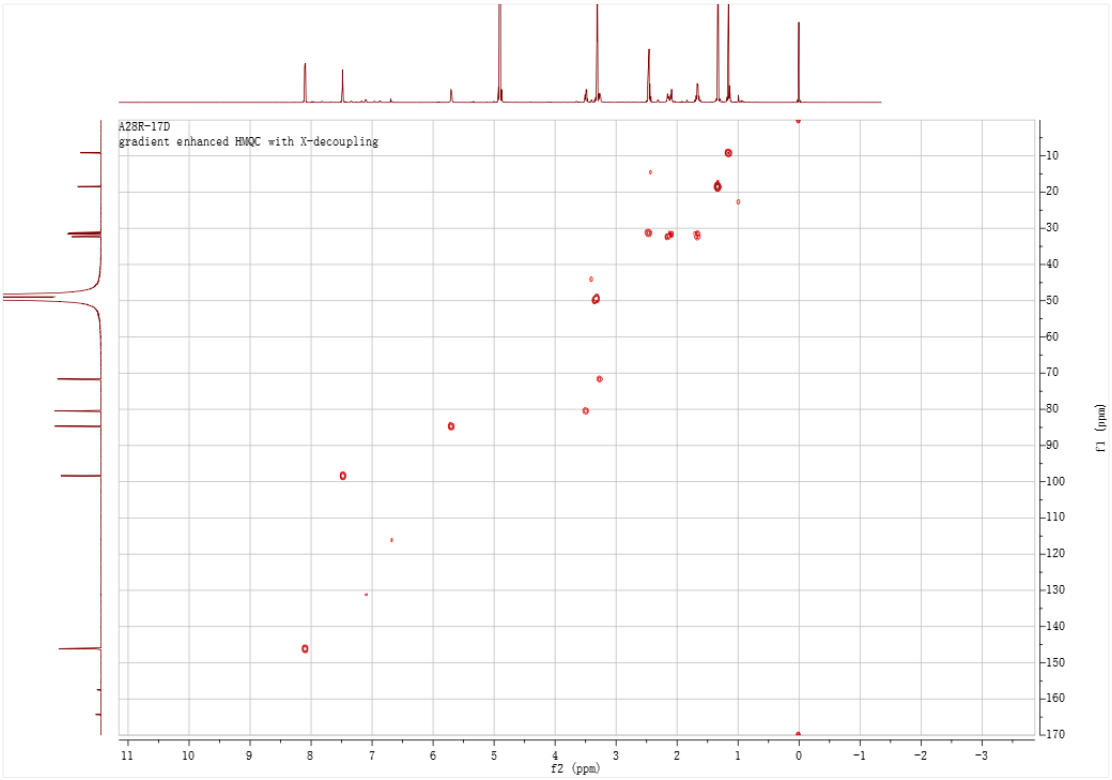


Figure S33. HSQC spectrum of **4**

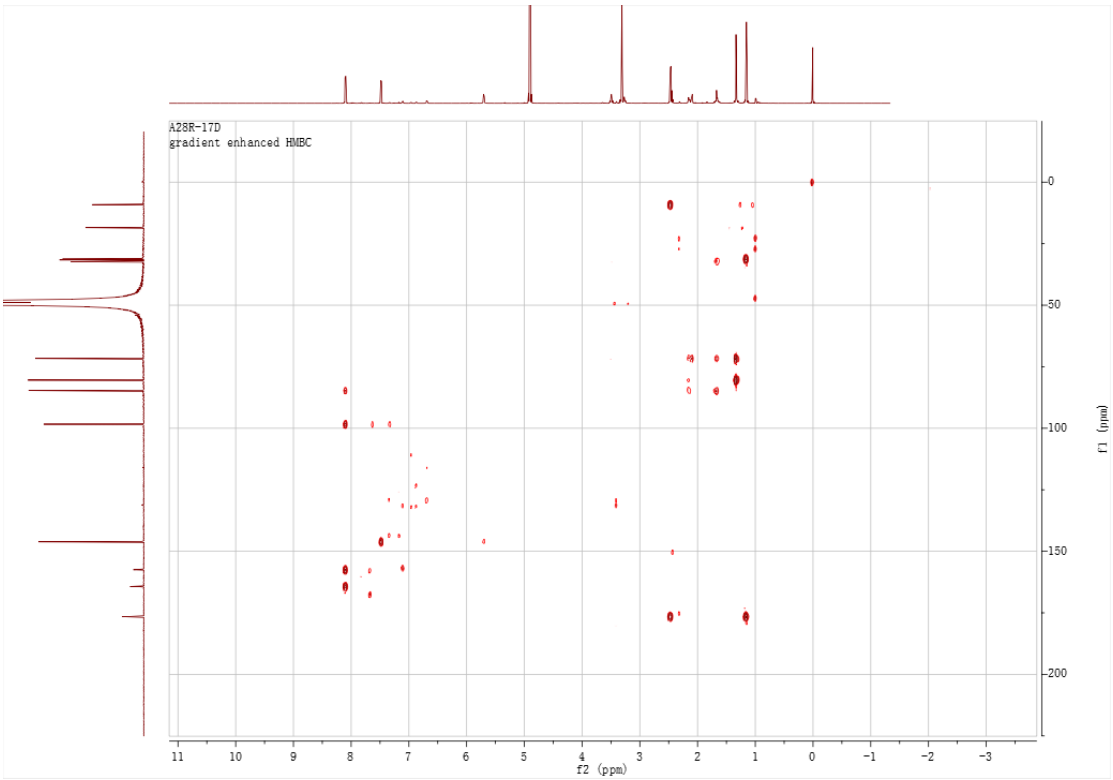


Figure S34. HMBC spectrum of **4**

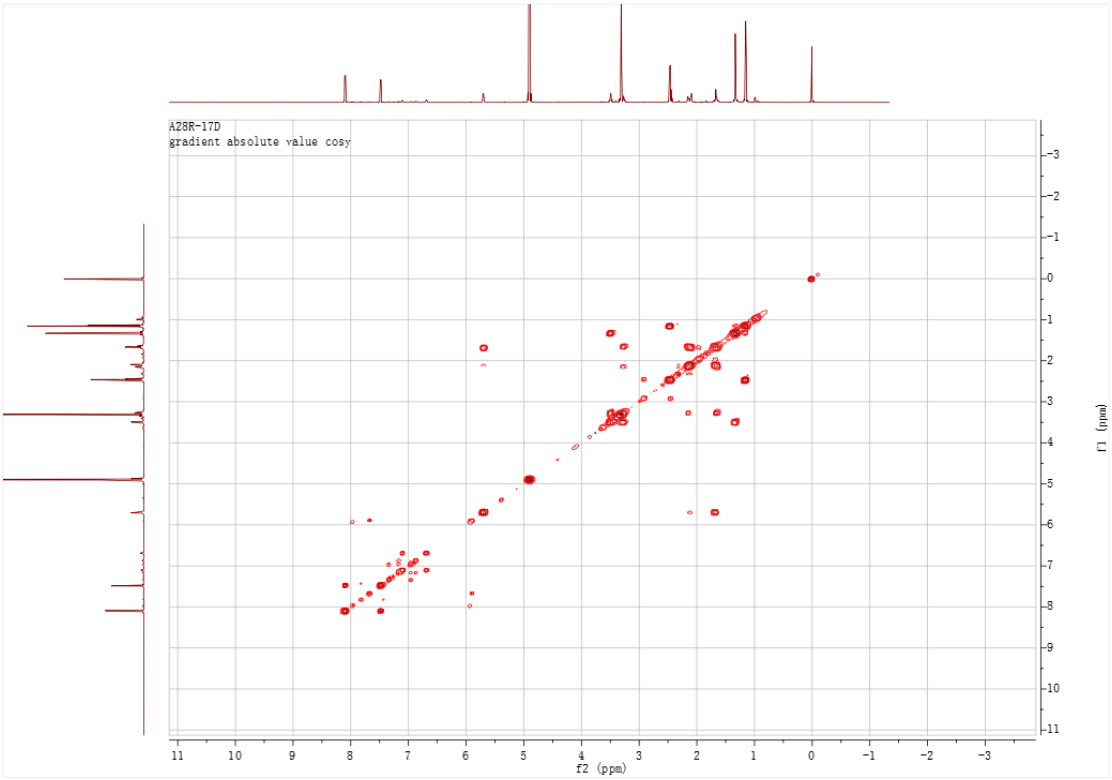


Figure S35. ^{1}H-^{1}H COSY spectrum of **4**

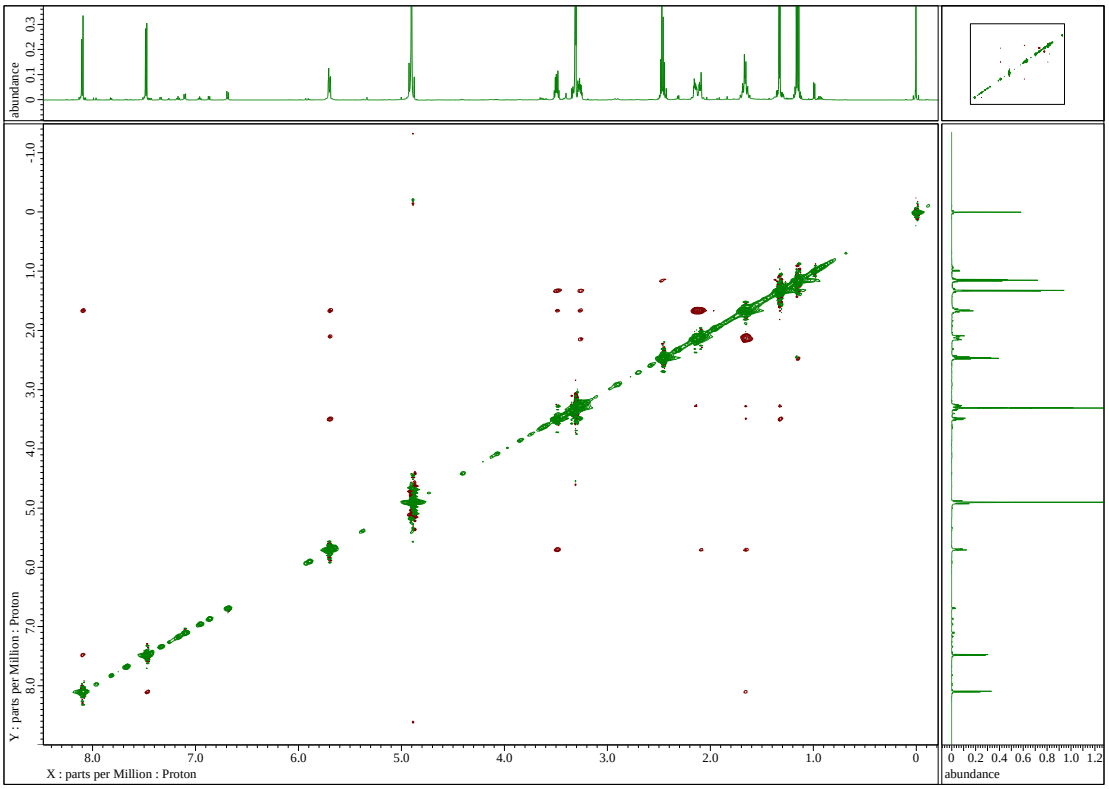


Figure S36. NOESY spectrum of **4**

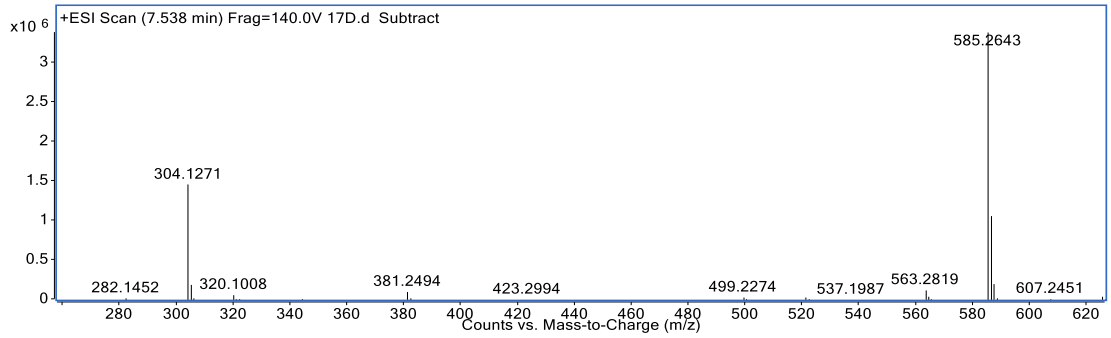


Figure S37. HRESIMS spectrum of **4**

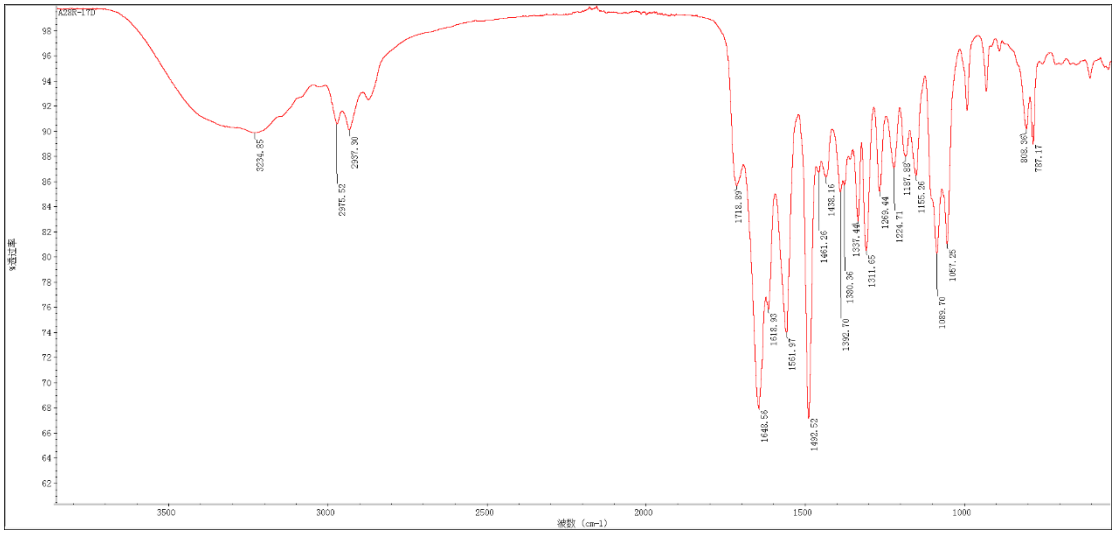


Figure S38. IR spectrum of **4**

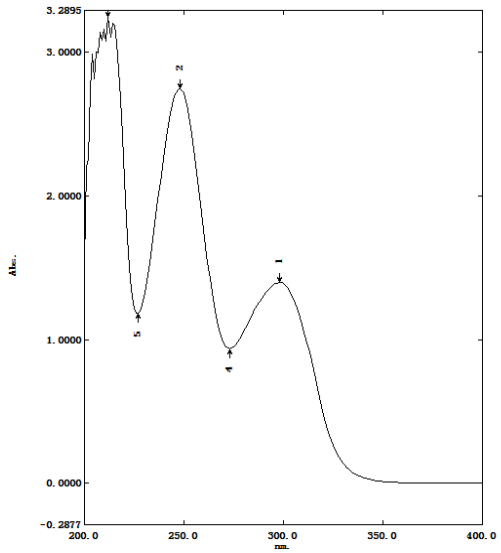


Figure S39. UV spectrum of **4**

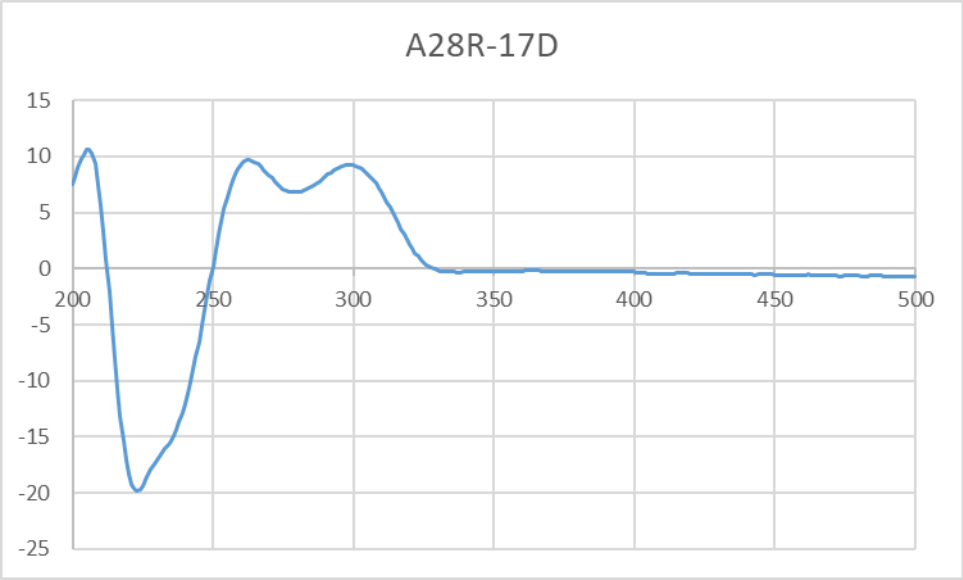


Figure S40. CD spectrum of **4**

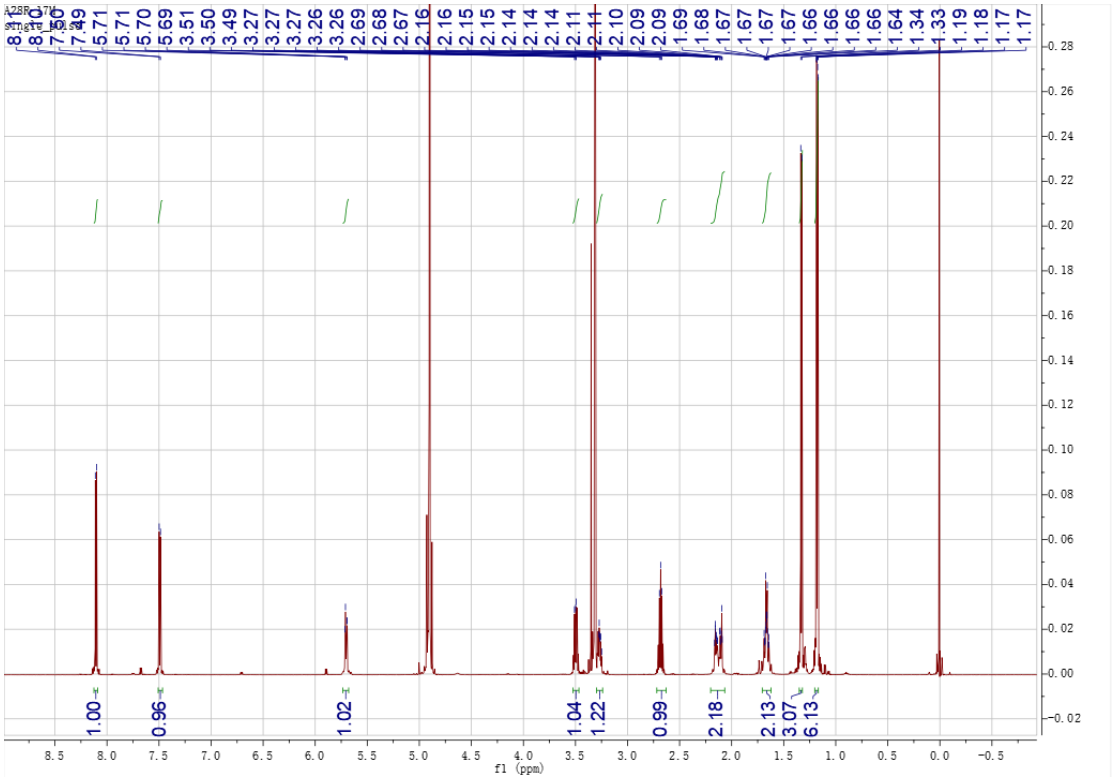


Figure S41. ^{1}H NMR spectrum of **5**

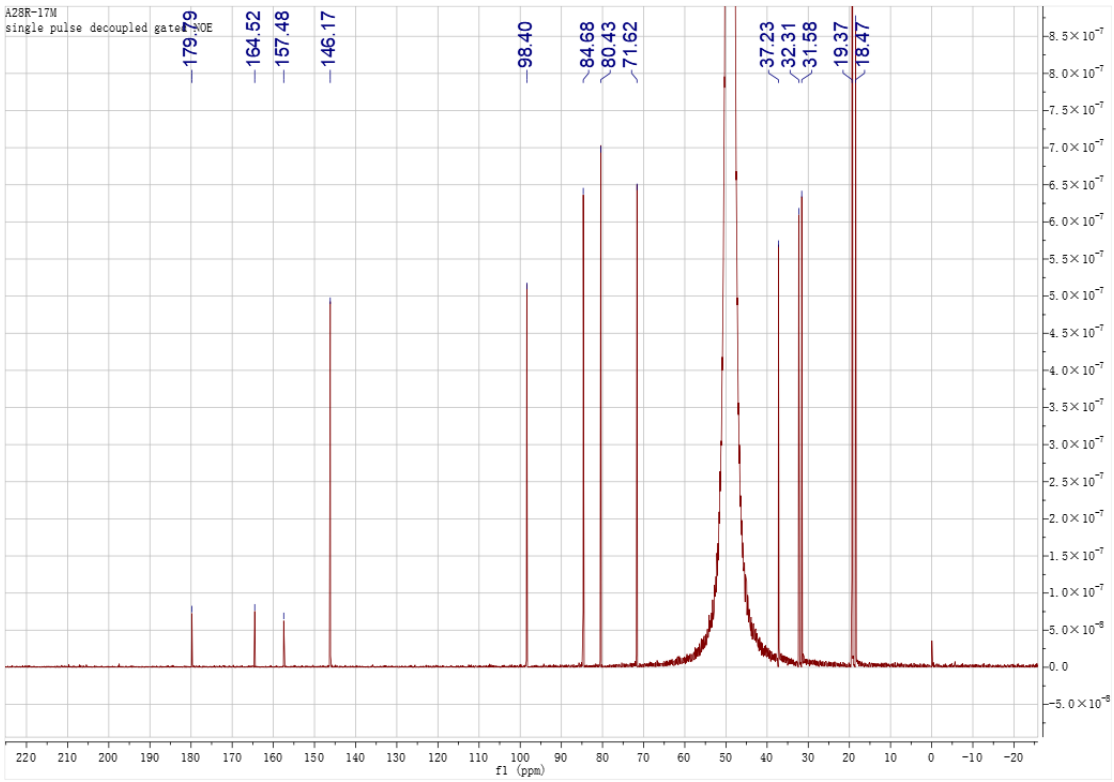


Figure S42. ^{13}C NMR spectrum of **5**

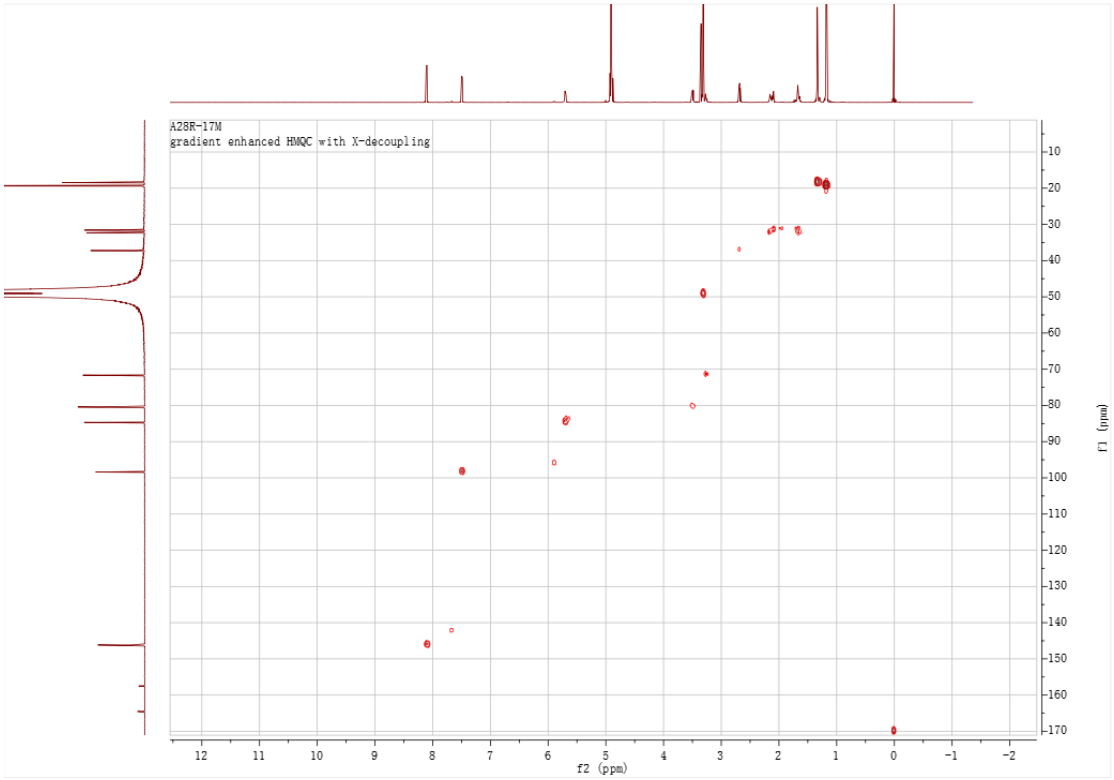


Figure S43. HSQC spectrum of **5**

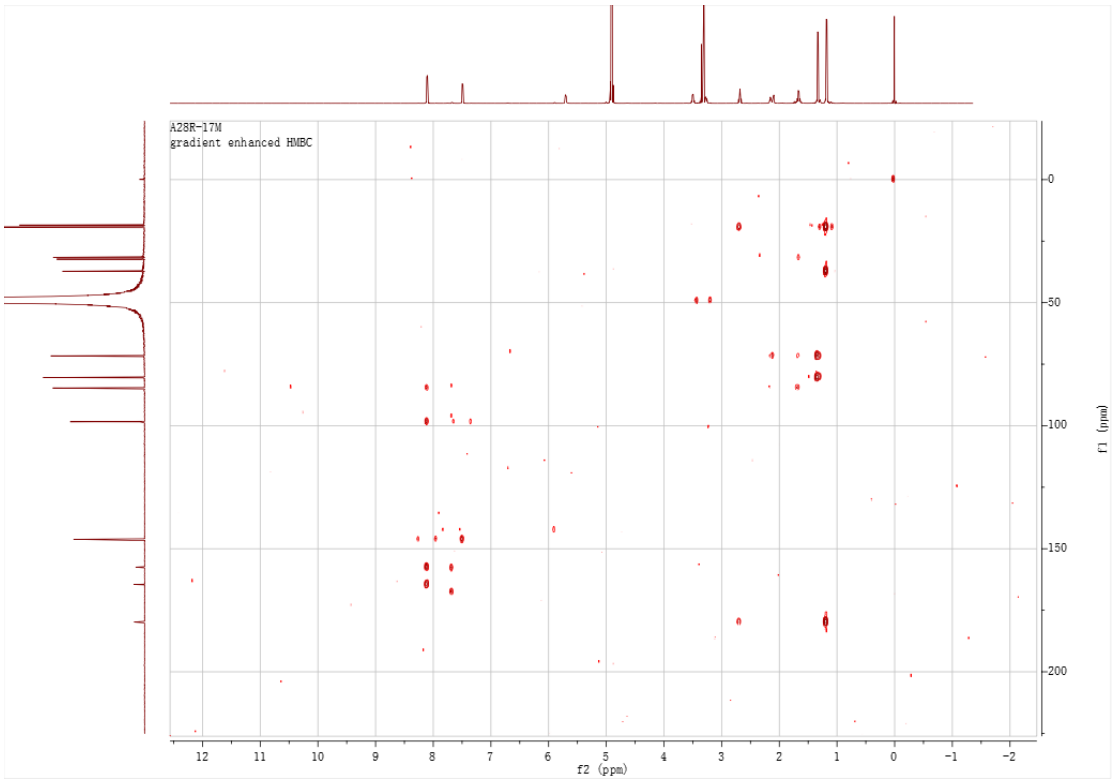


Figure S44. HMBC spectrum of **5**

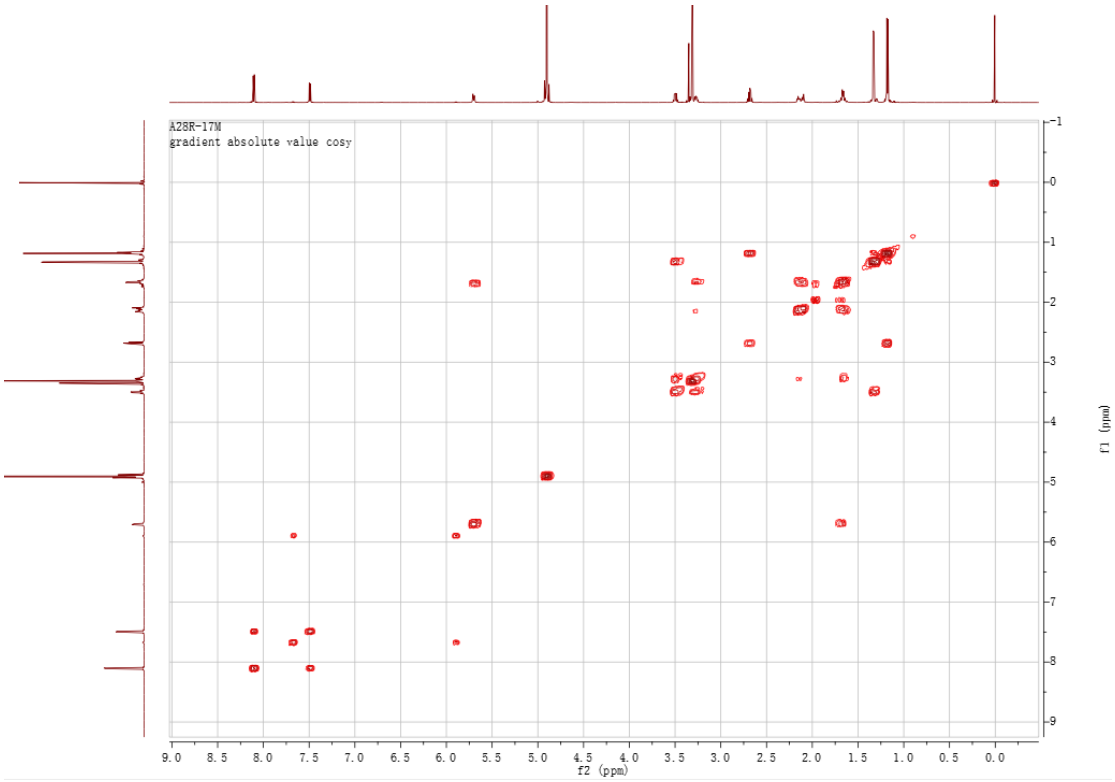


Figure S45. ^{1}H-^{1}H COSY spectrum of **5**

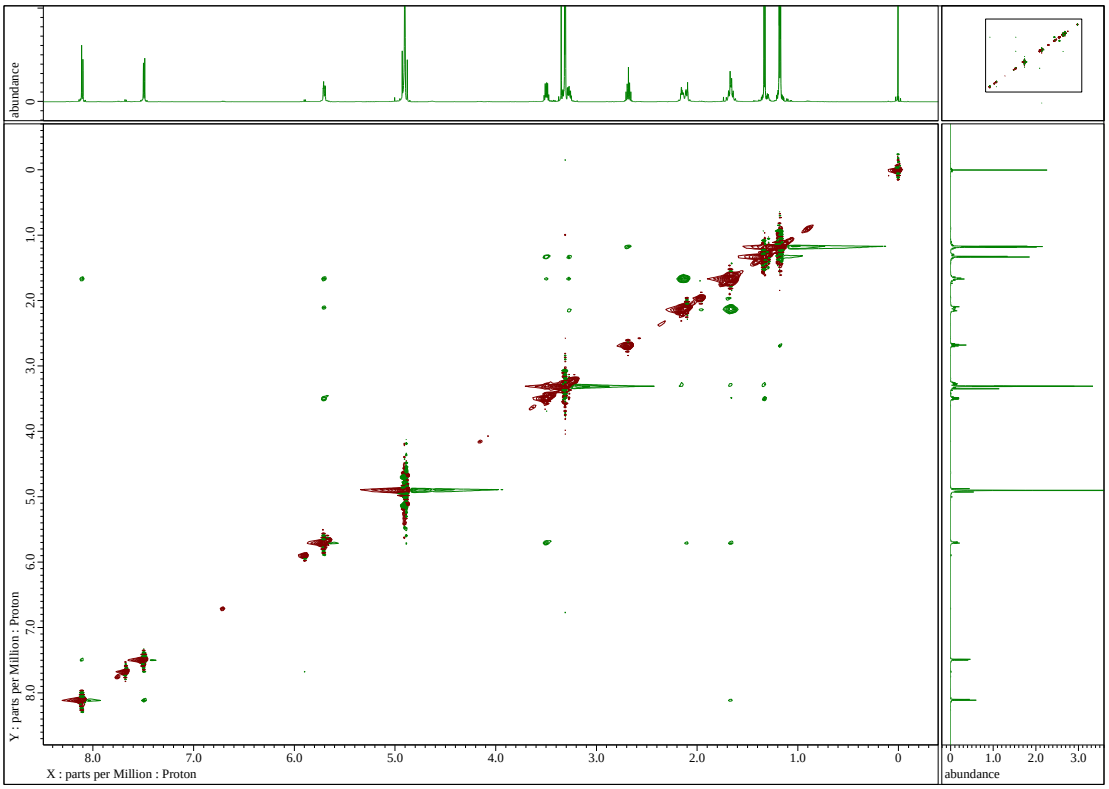


Figure S46. NOESY spectrum of **5**

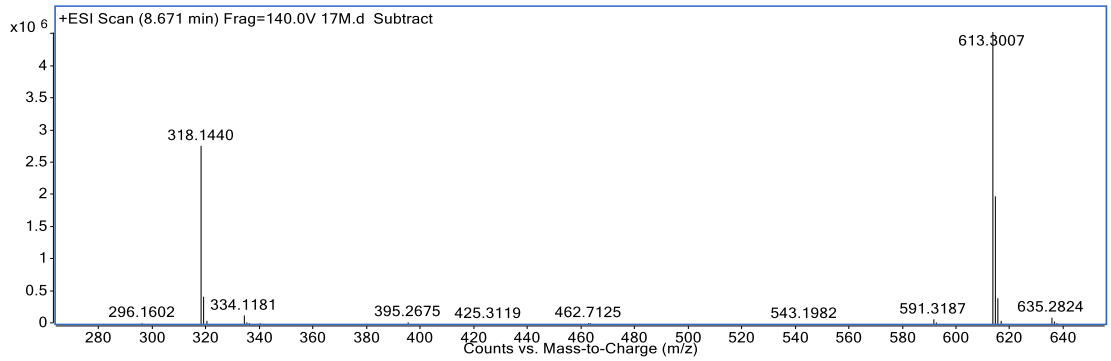


Figure S47. HRESIMS spectrum of **5**

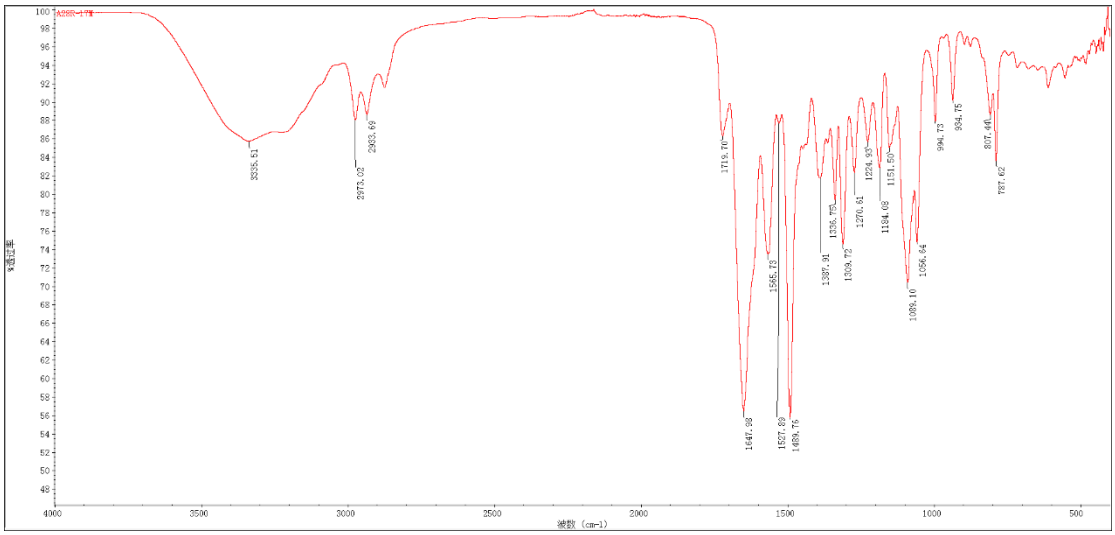


Figure S48. IR spectrum of **5**

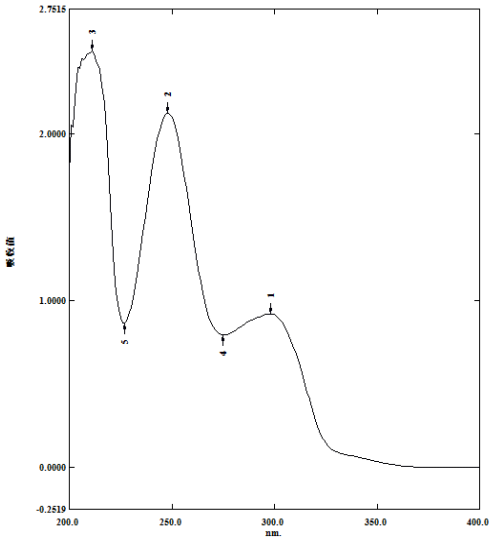


Figure S49. UV spectrum of **5**

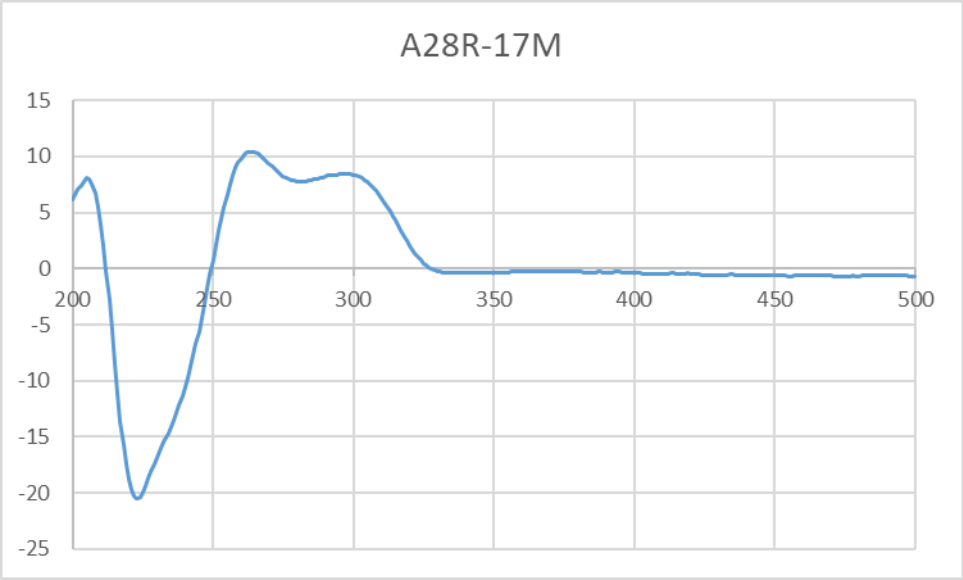


Figure S50. CD spectrum of **5**

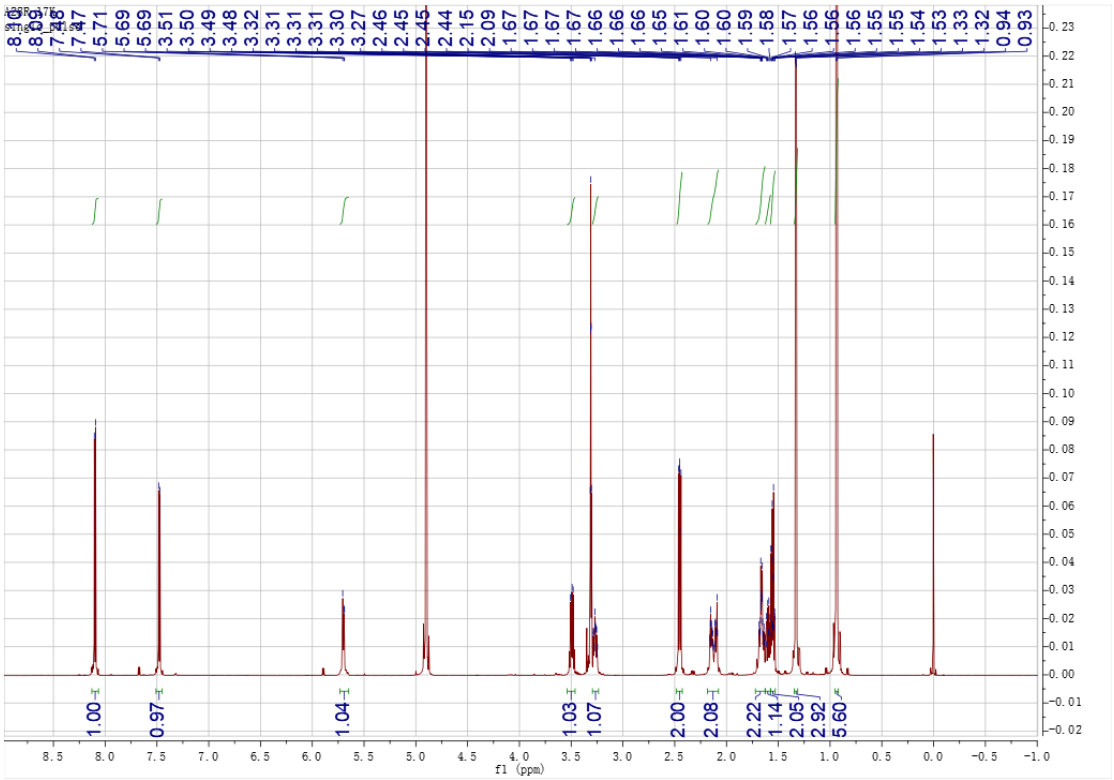


Figure S51. ^{1}H NMR spectrum of **6**

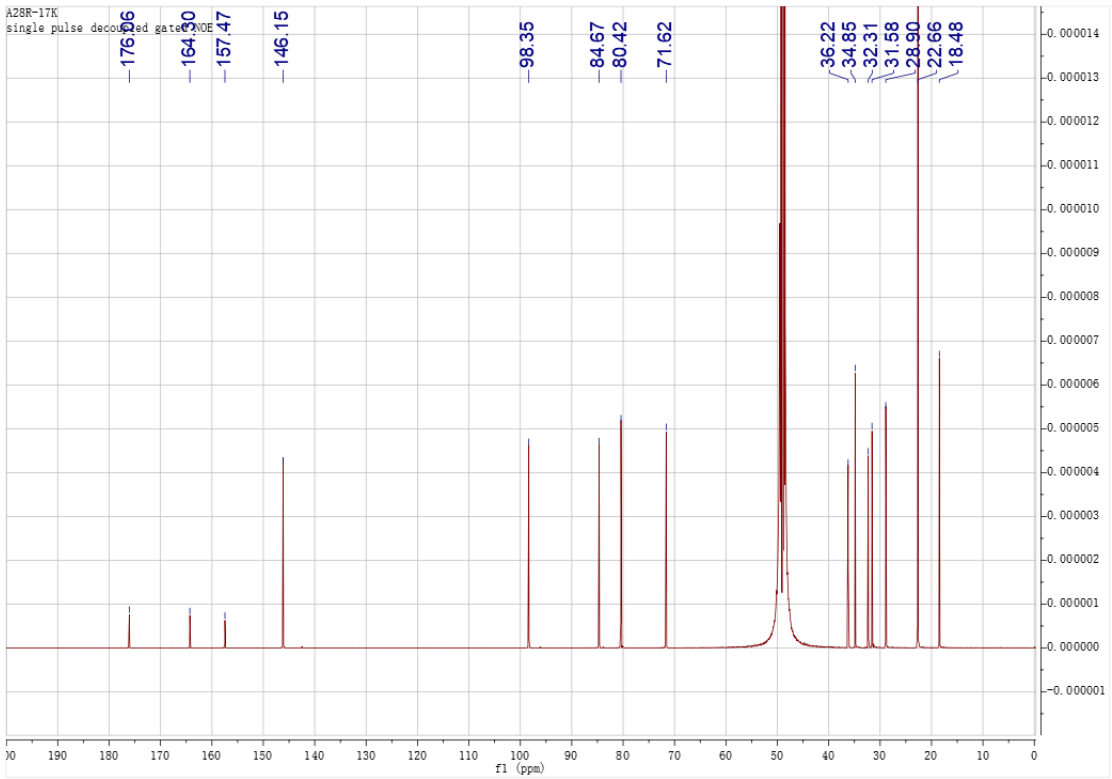


Figure S52. ^{13}C NMR spectrum of **6**

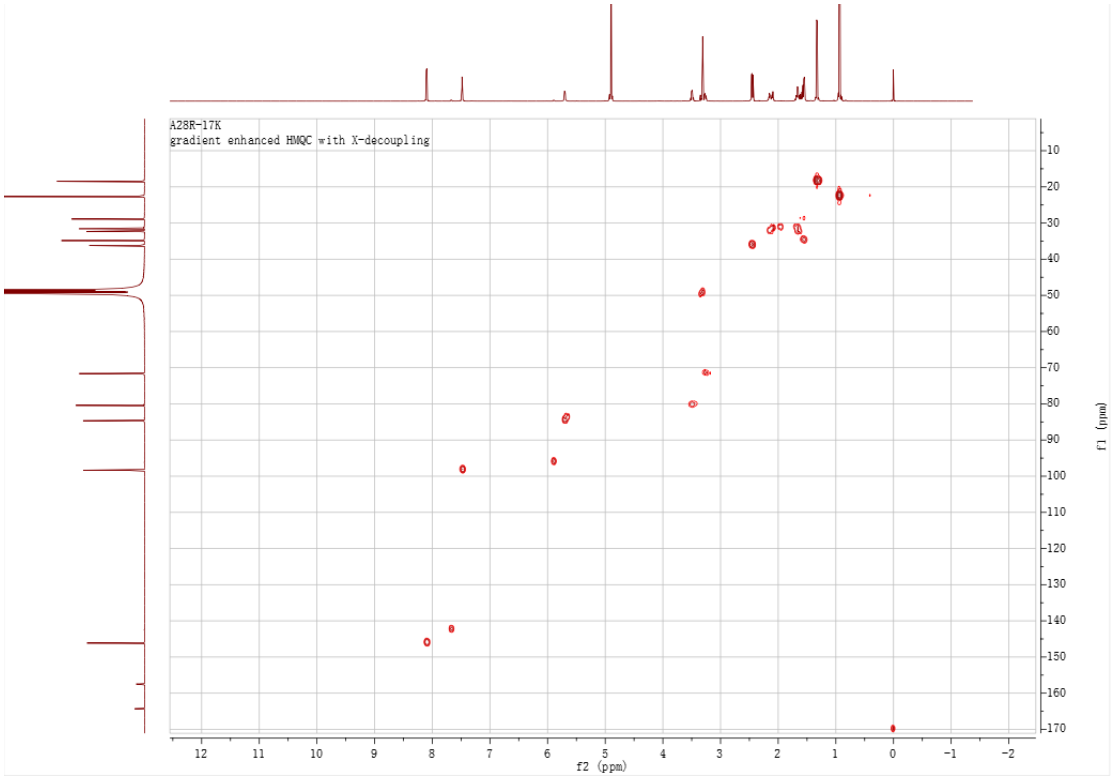


Figure S53. HSQC spectrum of **6**

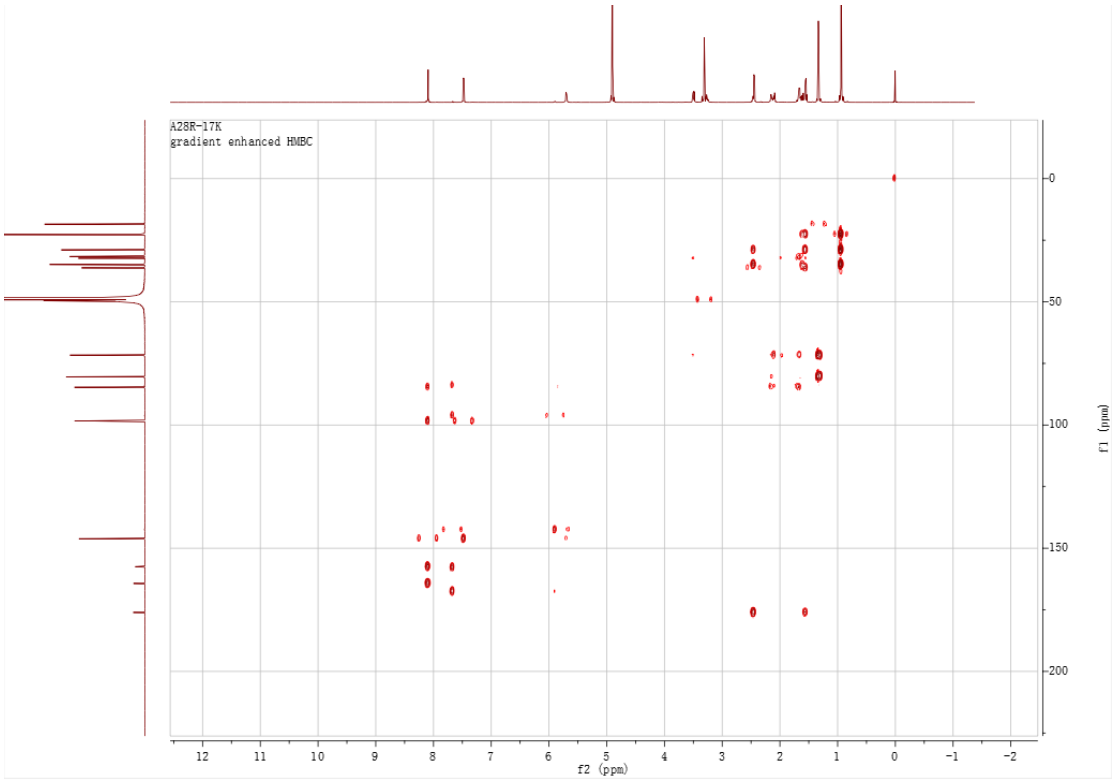


Figure S54. HMBC spectrum of **6**

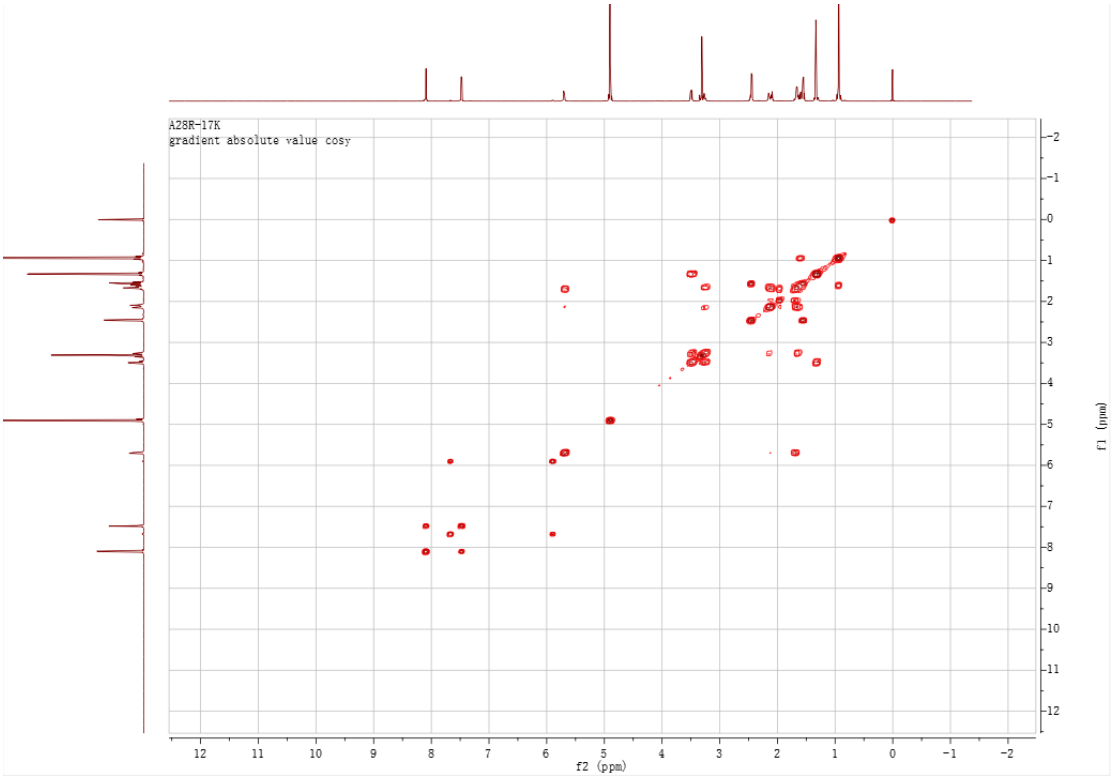


Figure S55. ^{1}H-^{1}H COSY spectrum of **6**

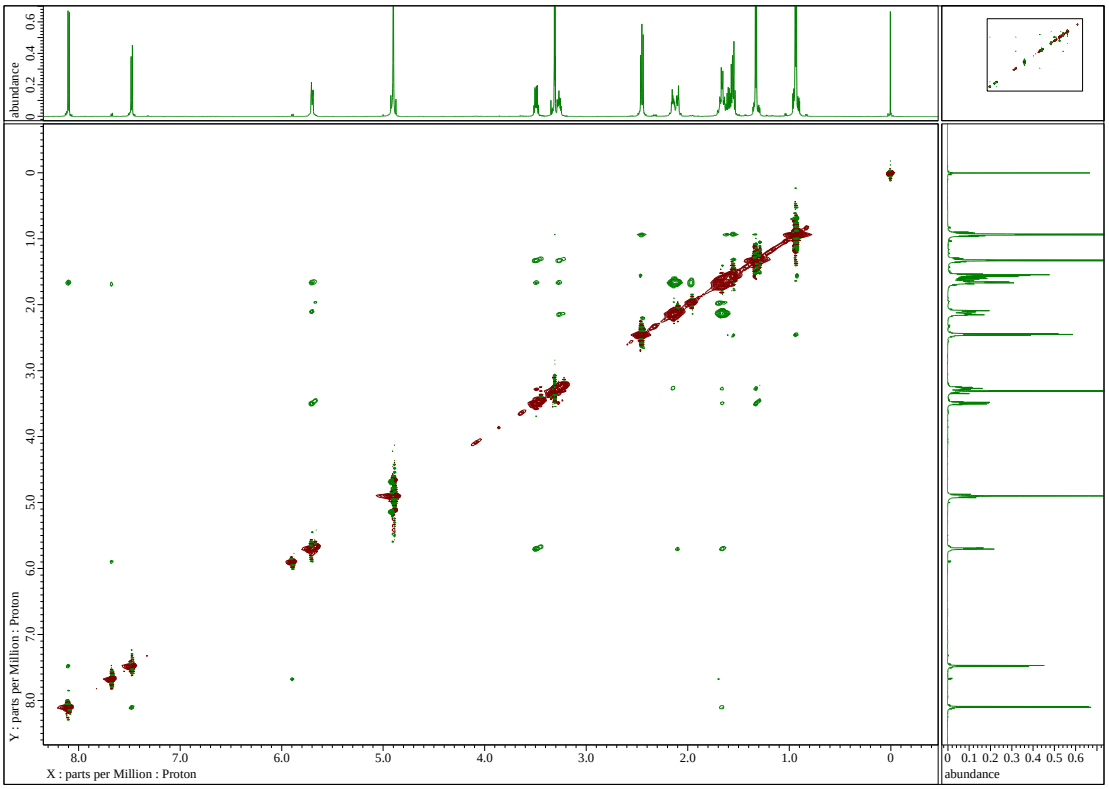


Figure S56. NOESY spectrum of **6**

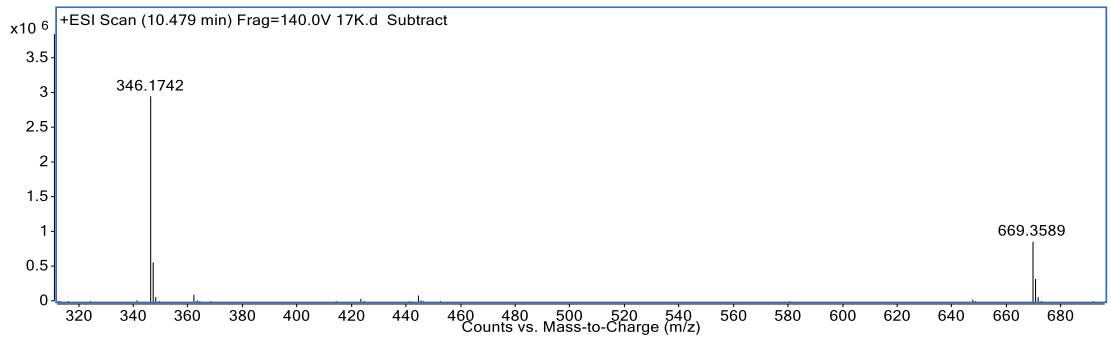


Figure S57. HRESIMS spectrum of **6**

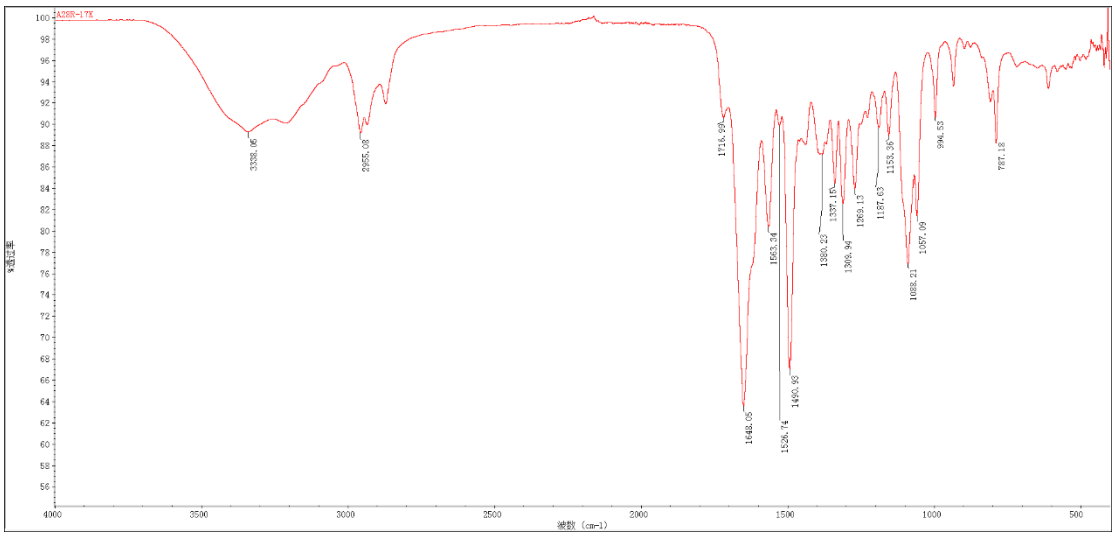


Figure S58. IR spectrum of **6**

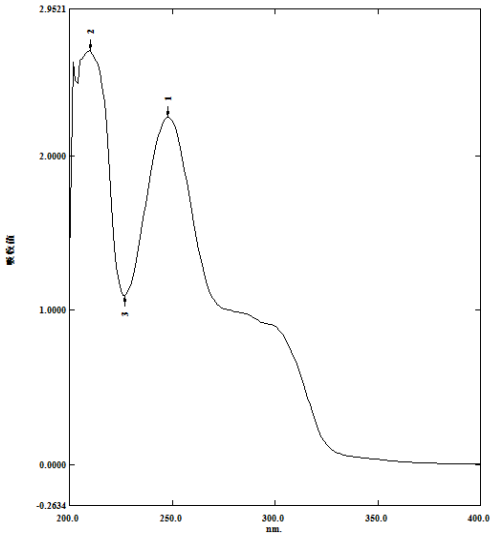


Figure S59. UV spectrum of **6**

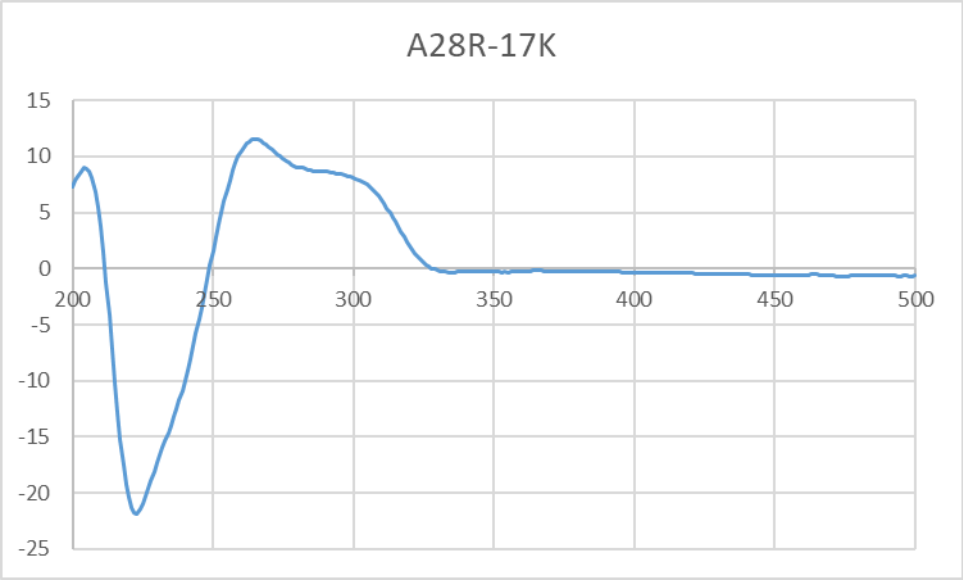


Figure S60. CD spectrum of **6**

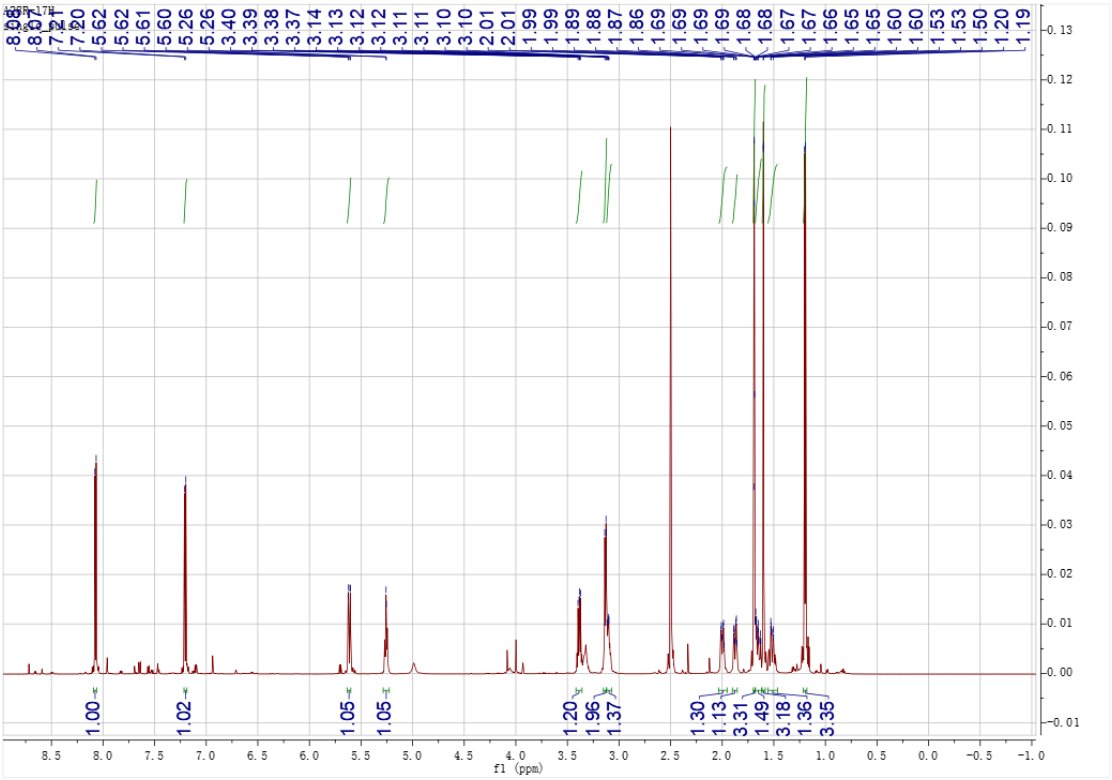


Figure S61. ^{1}H NMR spectrum of **7**

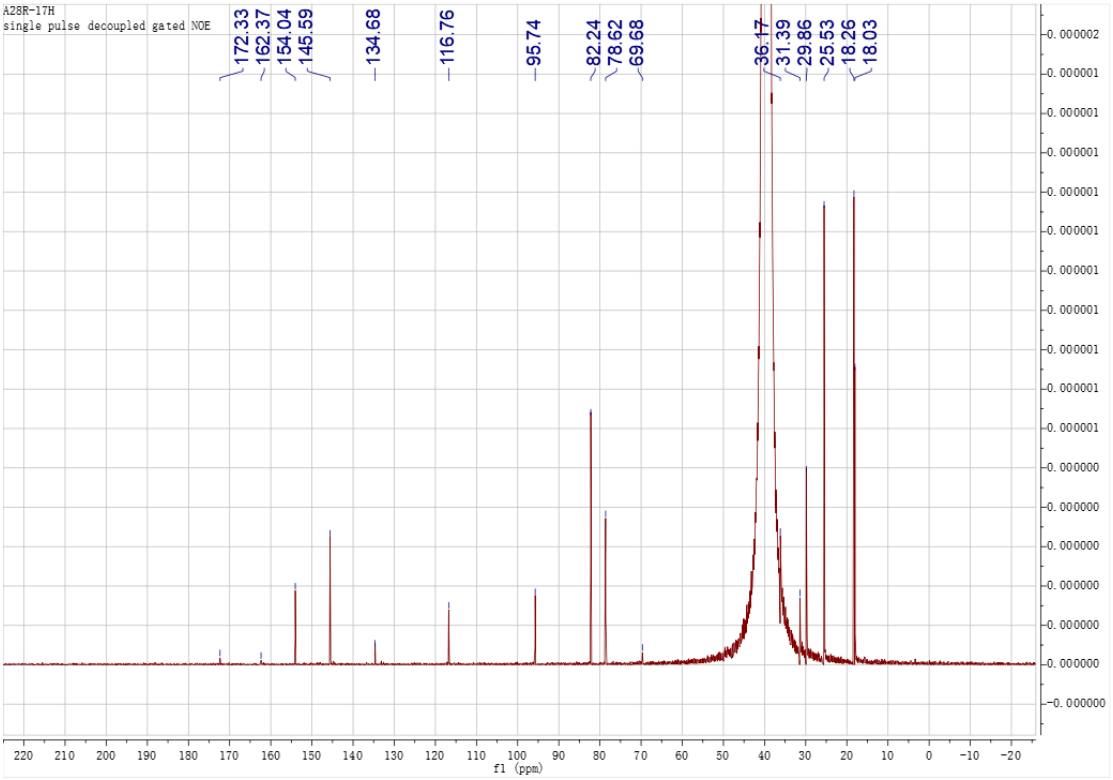


Figure S62. ^{13}C NMR spectrum of **7**

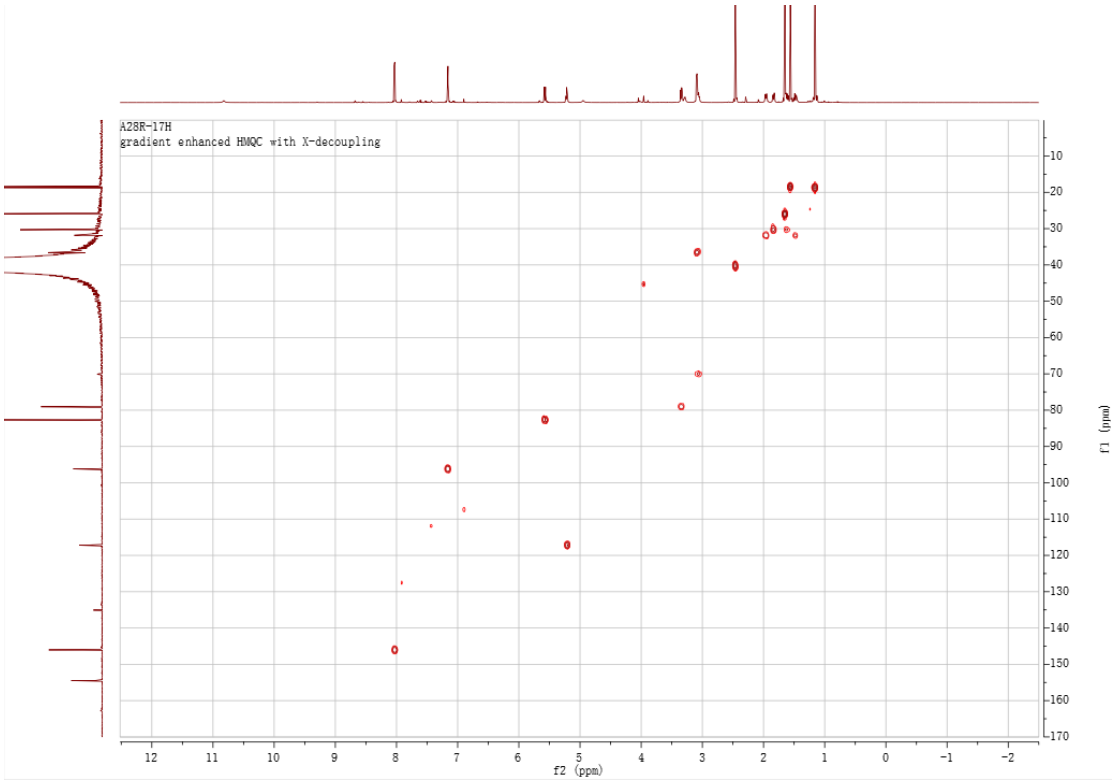


Figure S63. HSQC spectrum of **7**

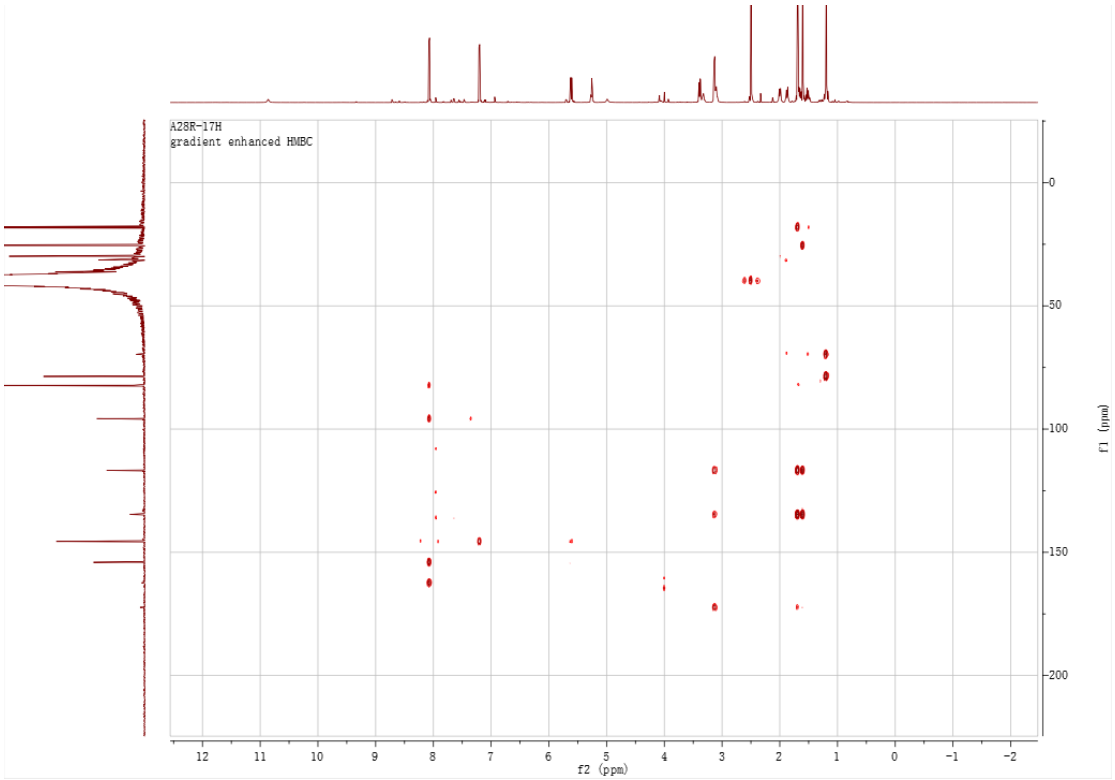


Figure S64. HMBC spectrum of **7**

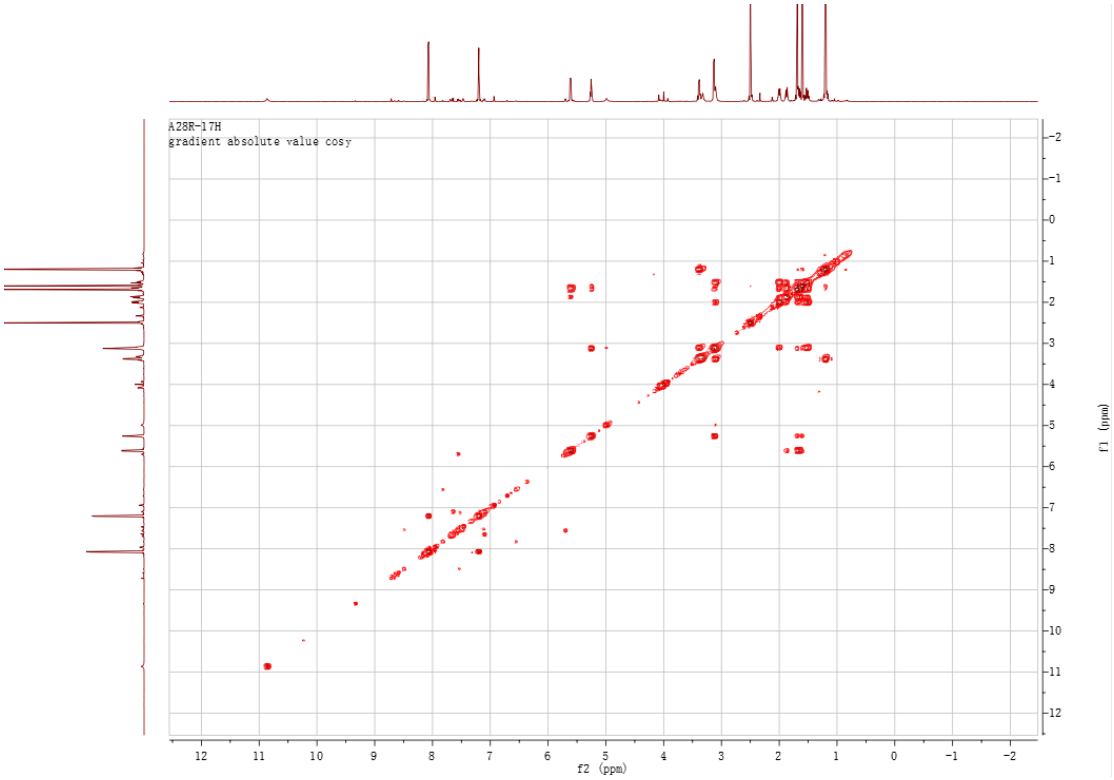


Figure S65. ^{1}H-^{1}H COSY spectrum of **7**

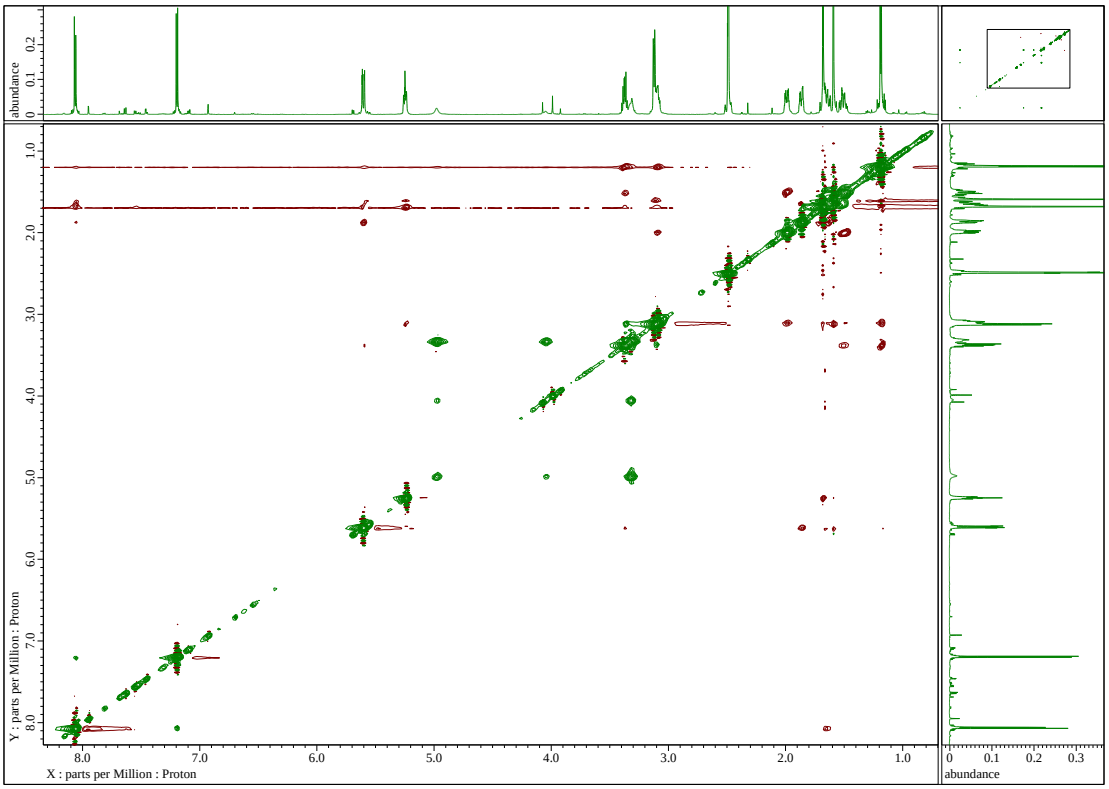


Figure S66. NOESY spectrum of **7**

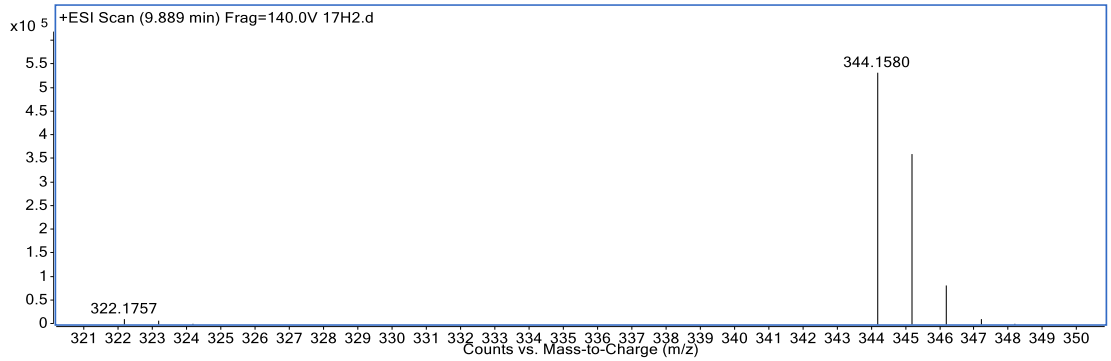


Figure S67. HRESIMS spectrum of **7**

Figure S68. IR spectrum of **7**

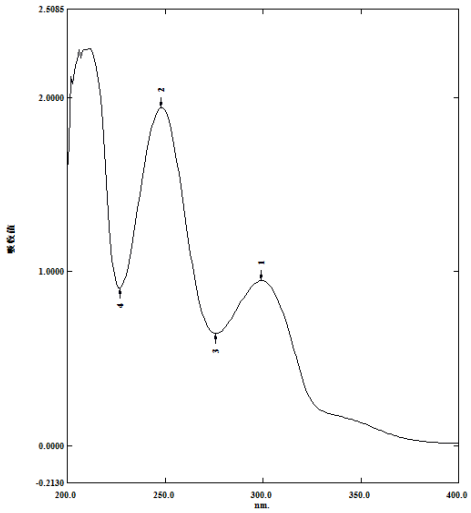


Figure S69. UV spectrum of **7**

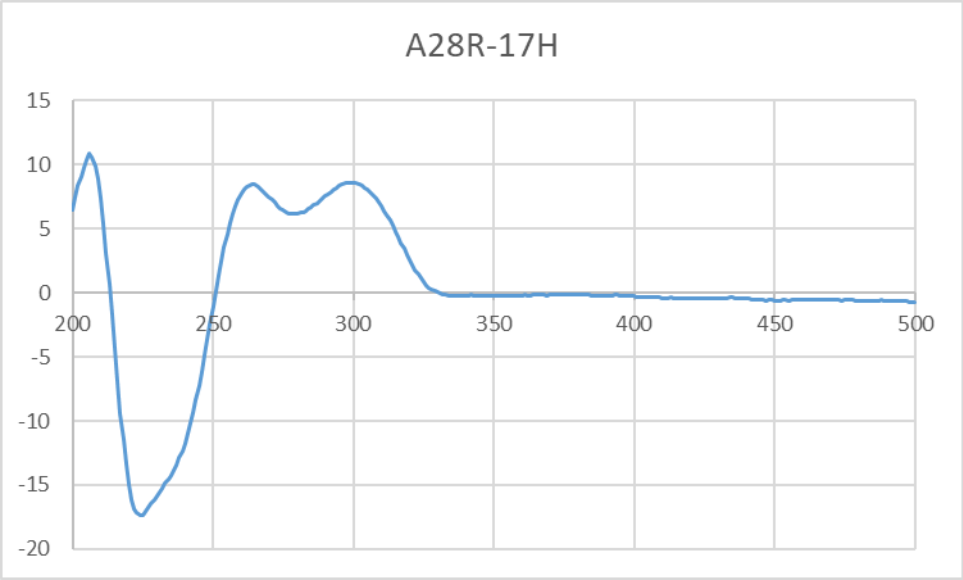


Figure S70. CD spectrum of **7**

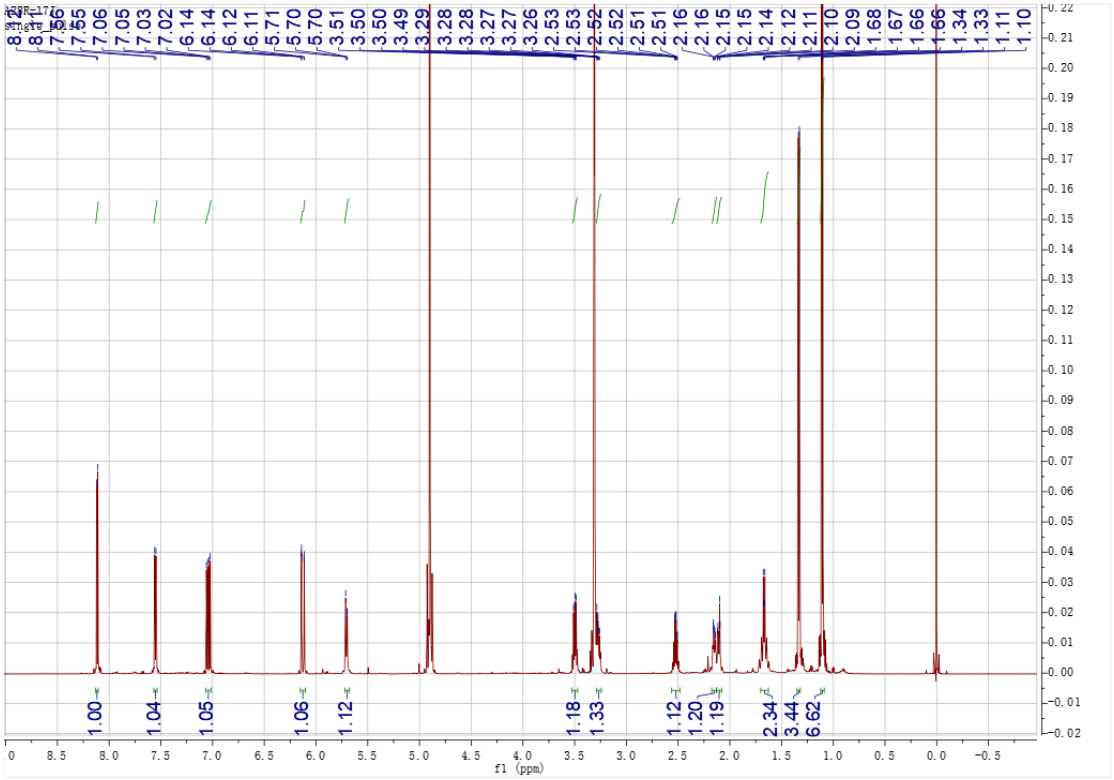


Figure S71. ^{1}H NMR spectrum of **8**

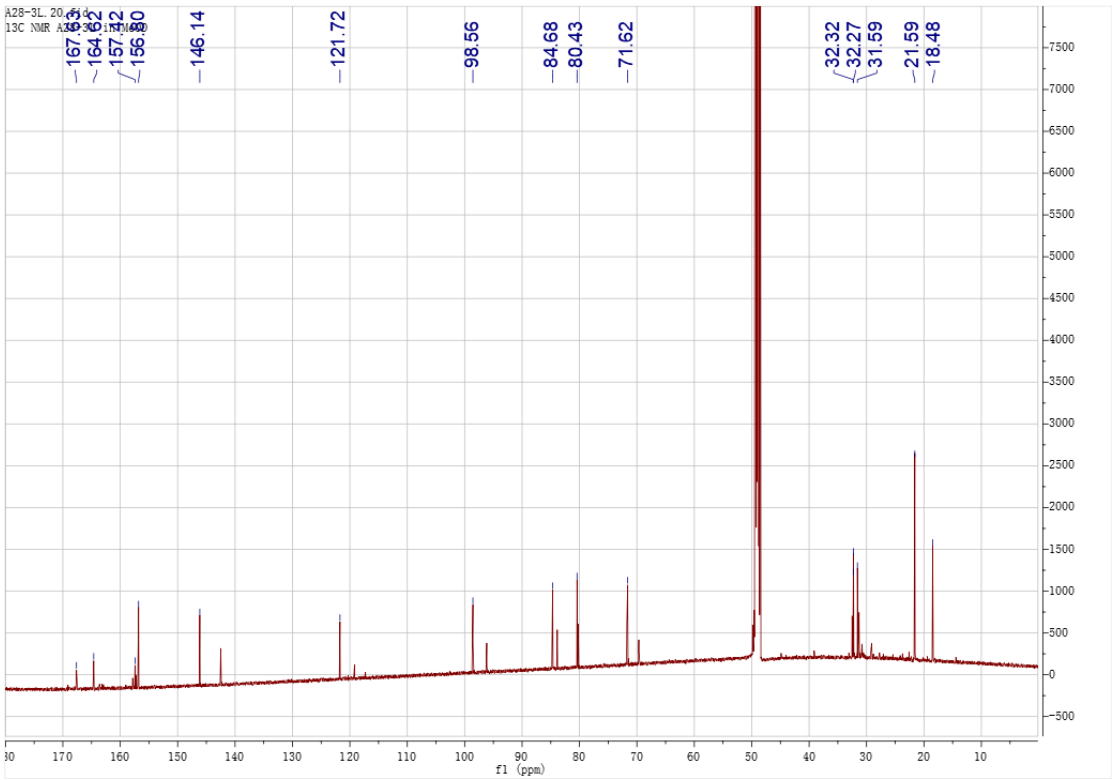


Figure S72. ^{13}C NMR spectrum of **8**

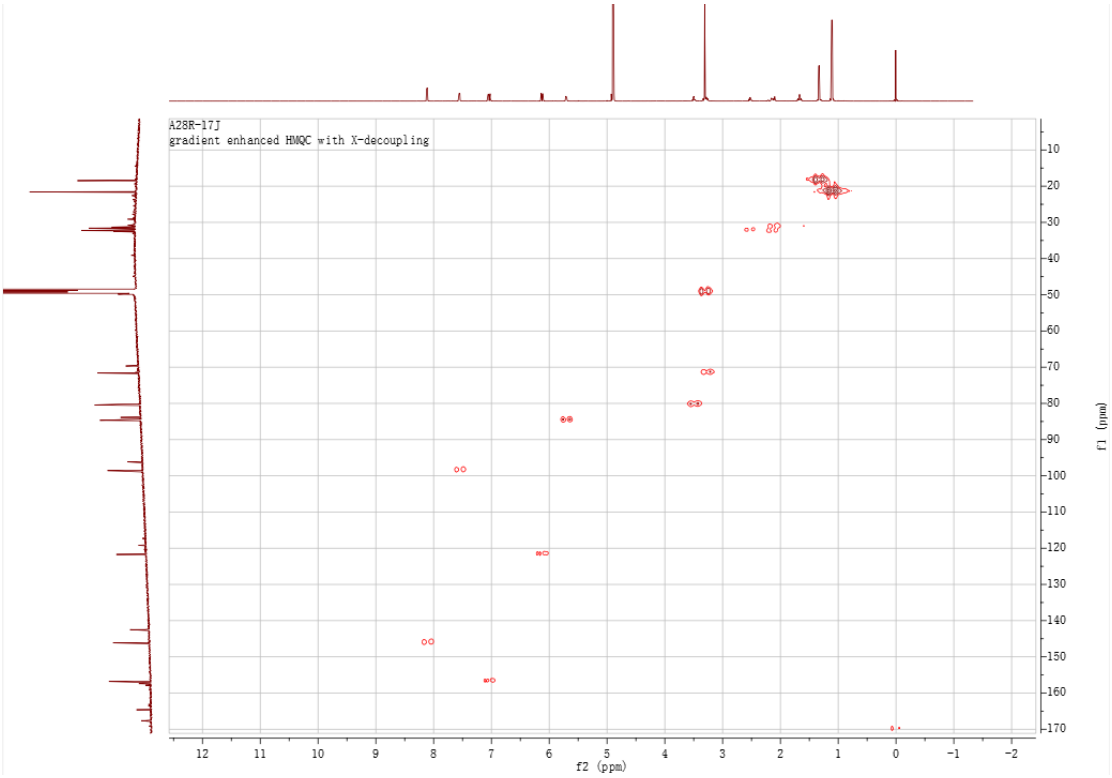


Figure S73. HSQC spectrum of **8**

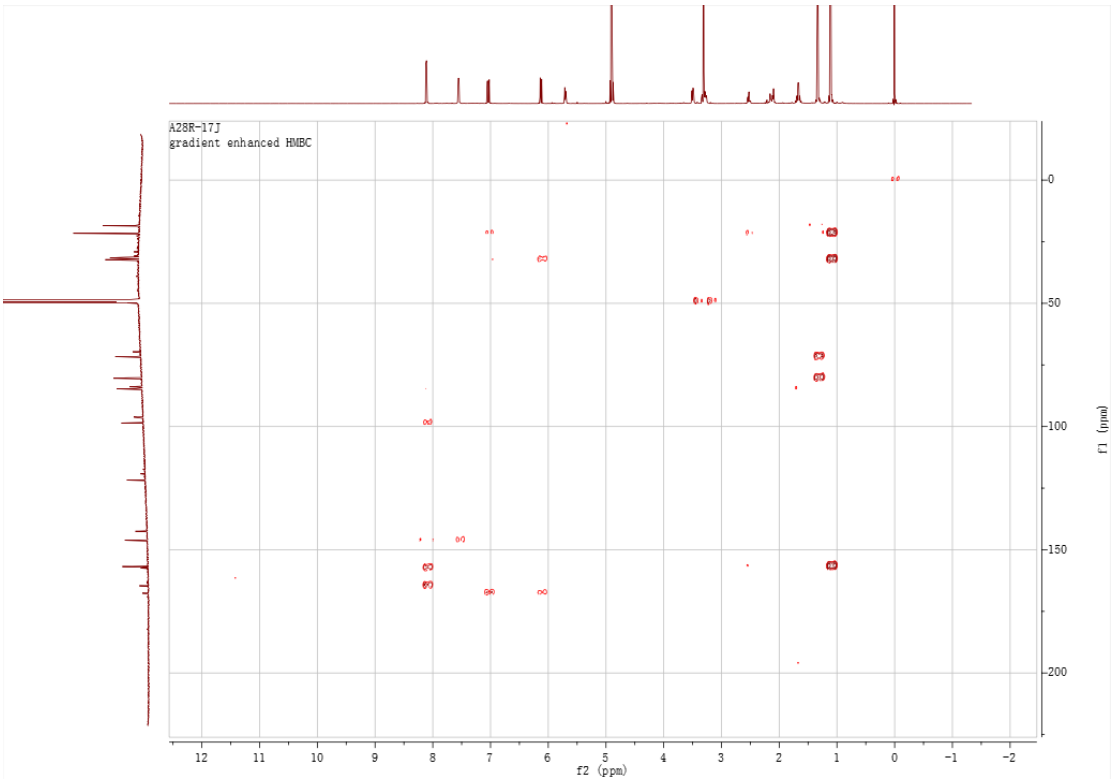


Figure S74. HMBC spectrum of **8**

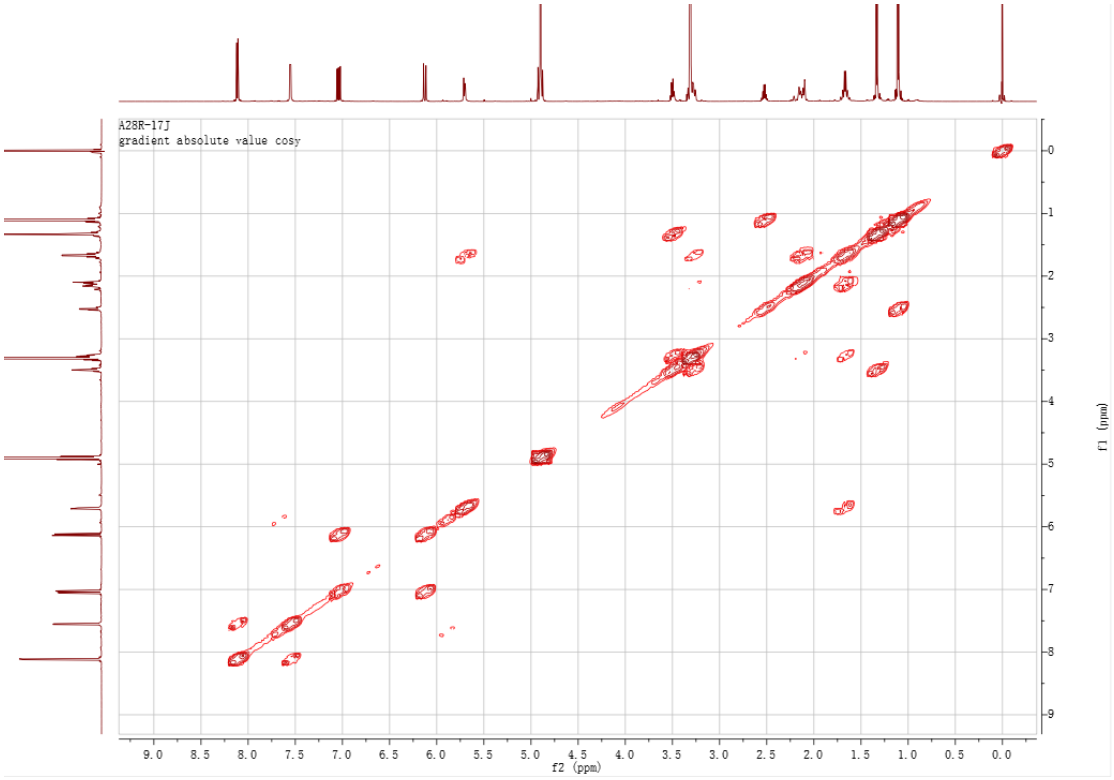


Figure S75. ^{1}H-^{1}H COSY spectrum of **8**

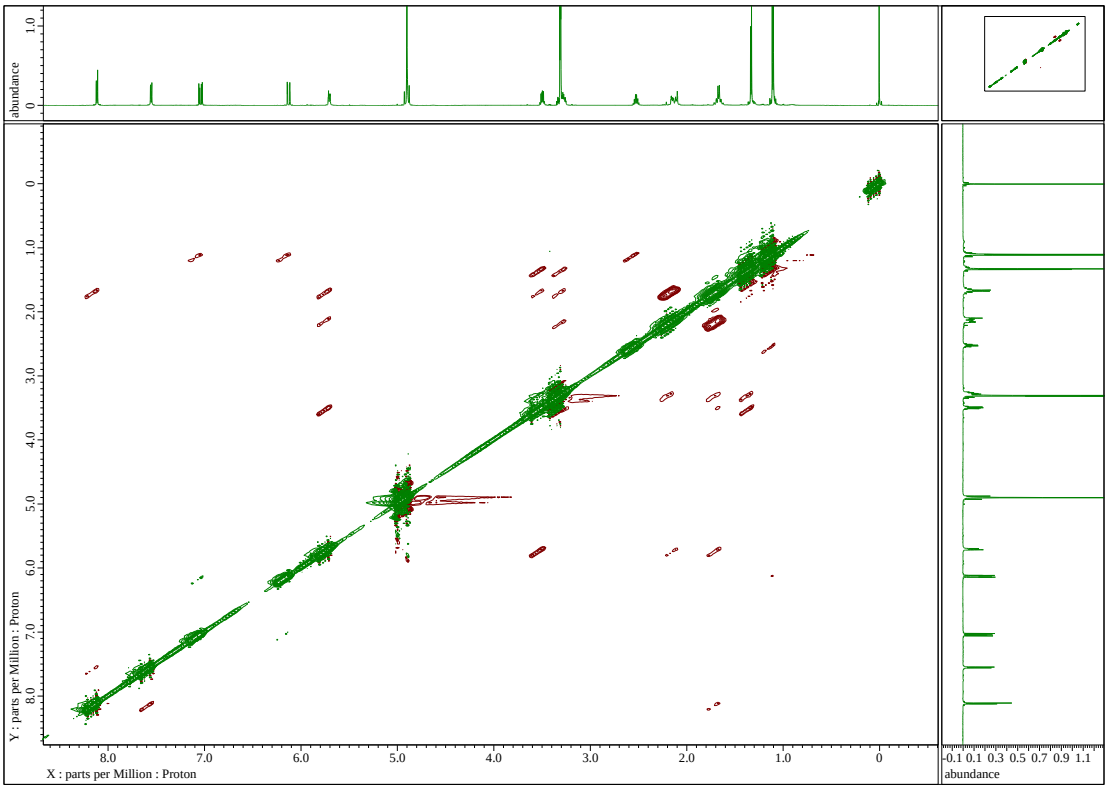


Figure S76. NOESY spectrum of **8**

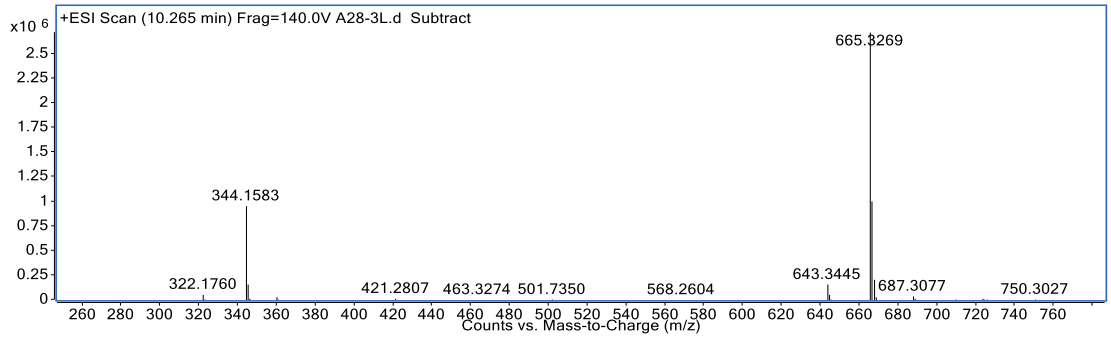


Figure S77. HRESIMS spectrum of **8**

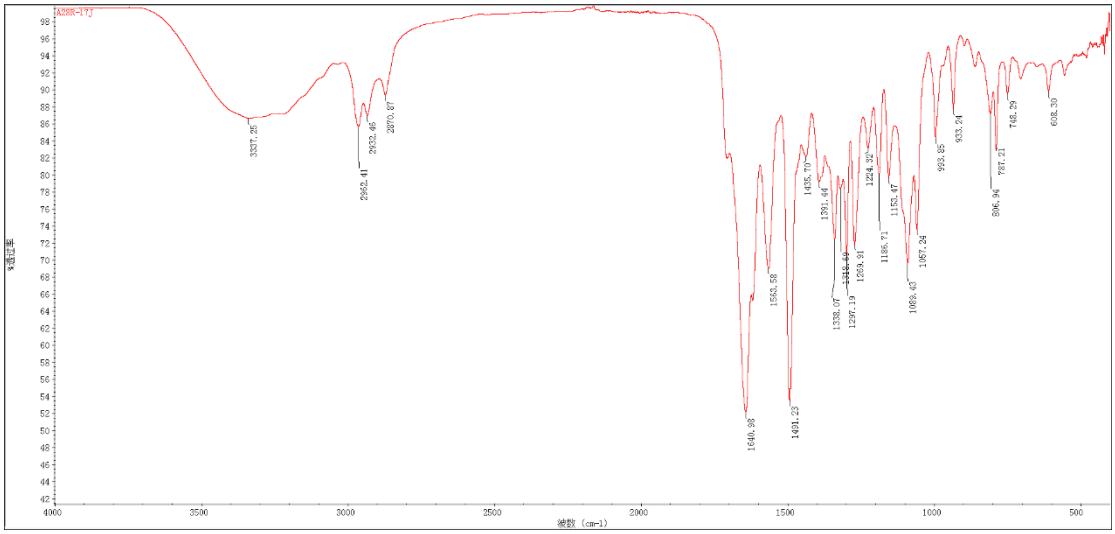


Figure S78. IR spectrum of **8**

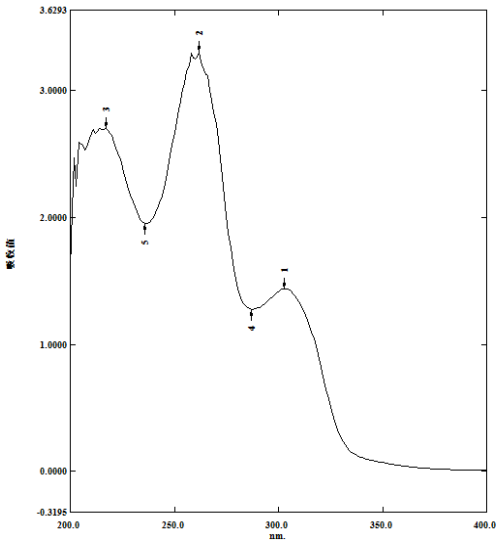


Figure S79. UV spectrum of **8**

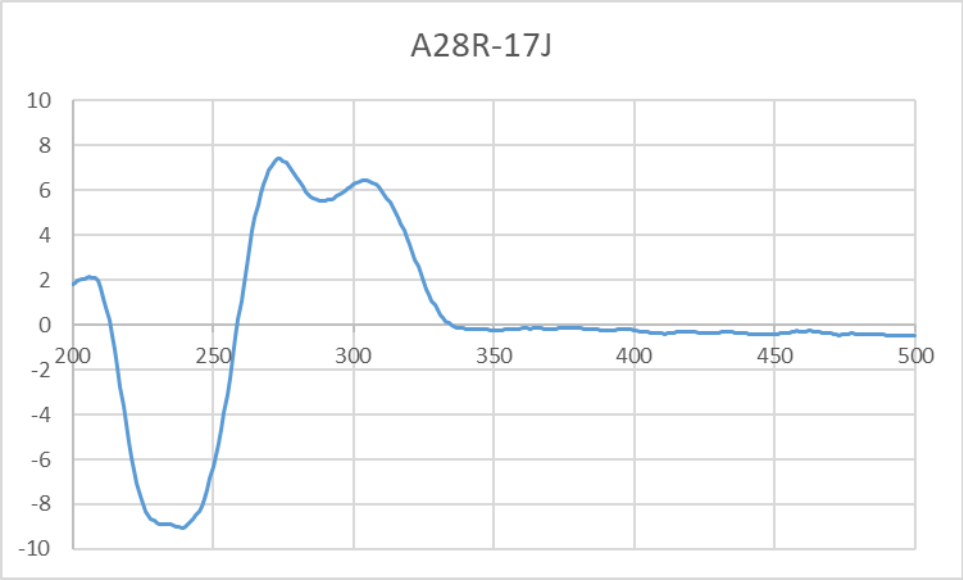


Figure S80. CD spectrum of **8**

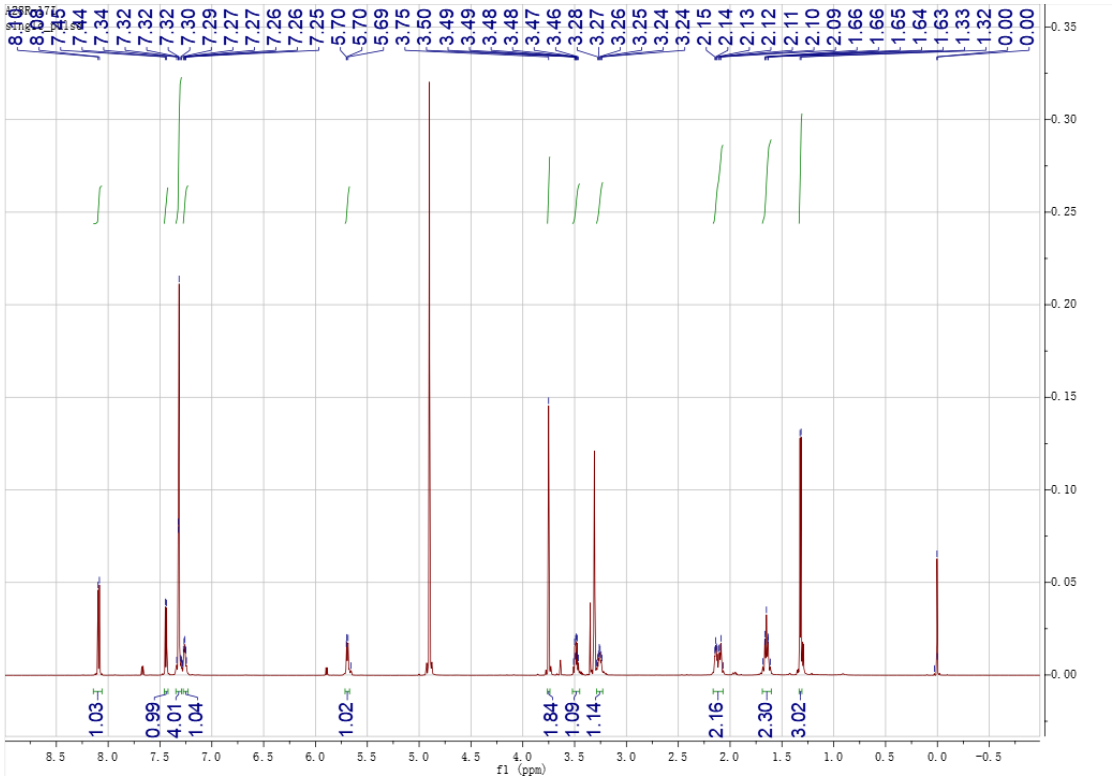


Figure S81. ^{1}H NMR spectrum of **9**

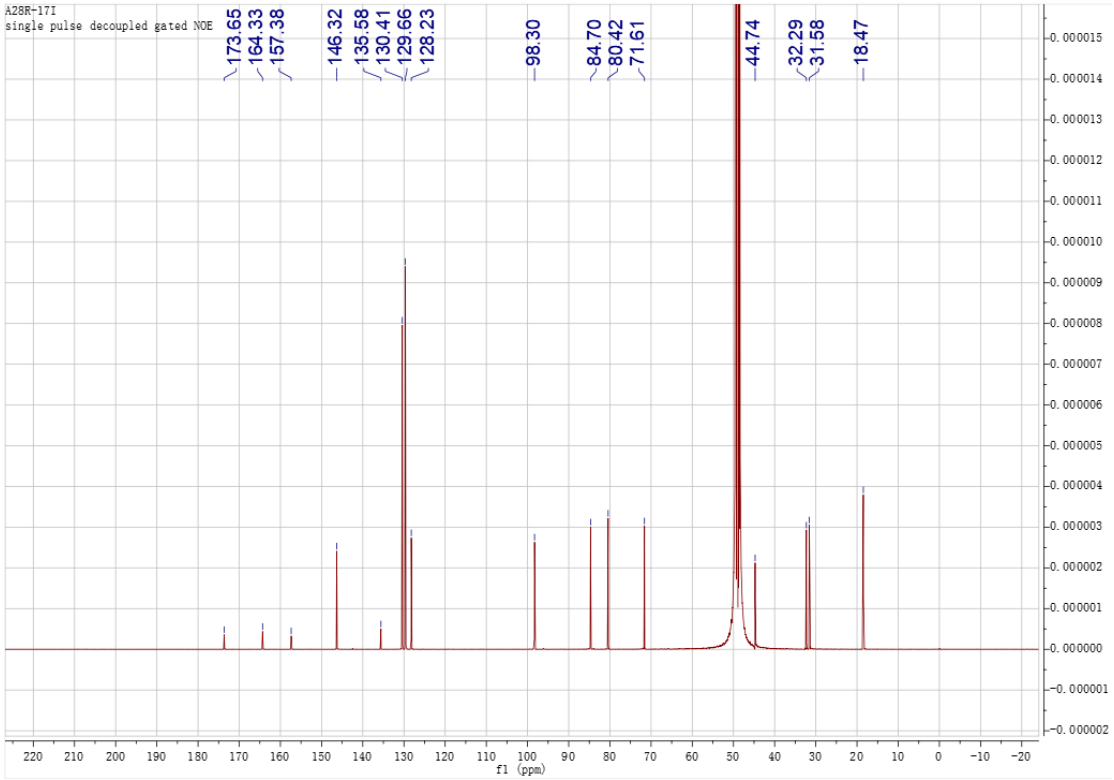


Figure S82. ^{13}C NMR spectrum of **9**

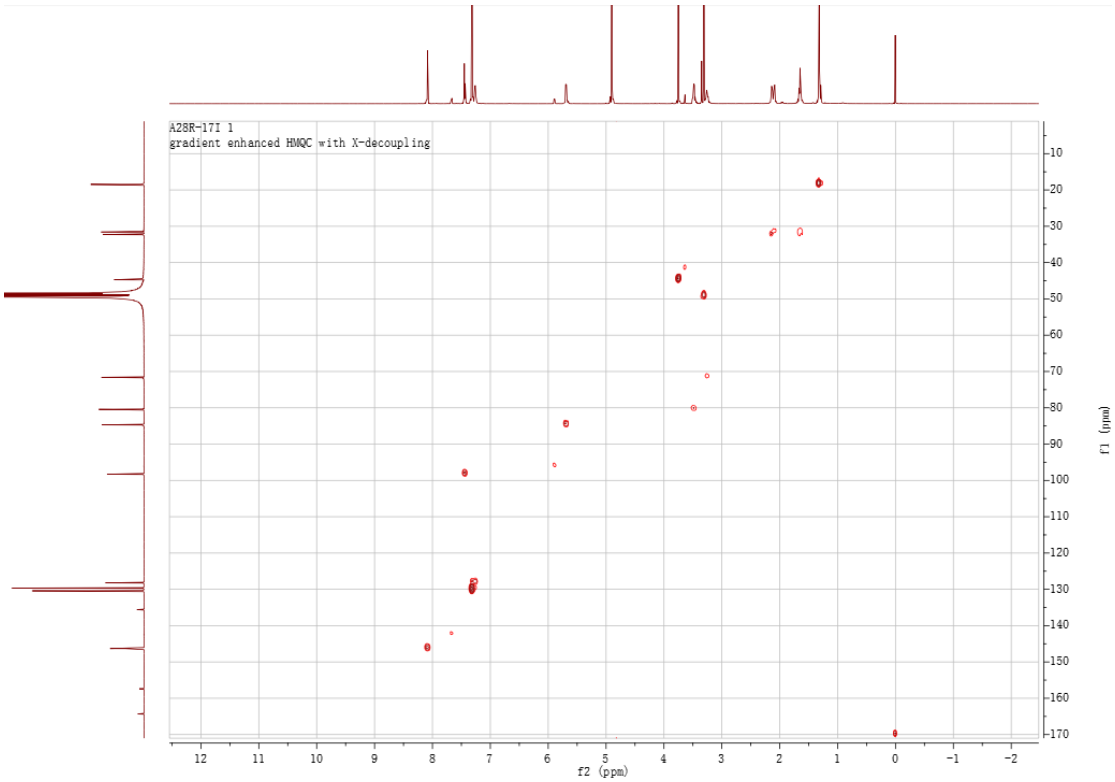


Figure S83. HSQC spectrum of **9**

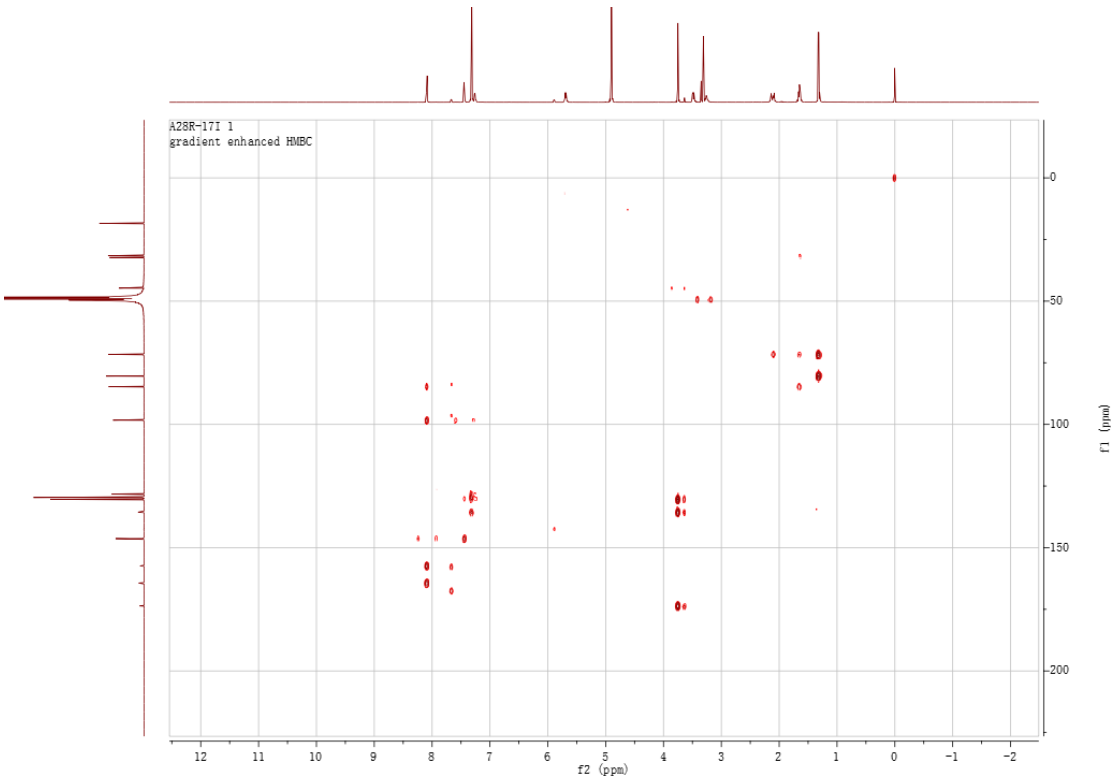


Figure S84. HMBC spectrum of **9**

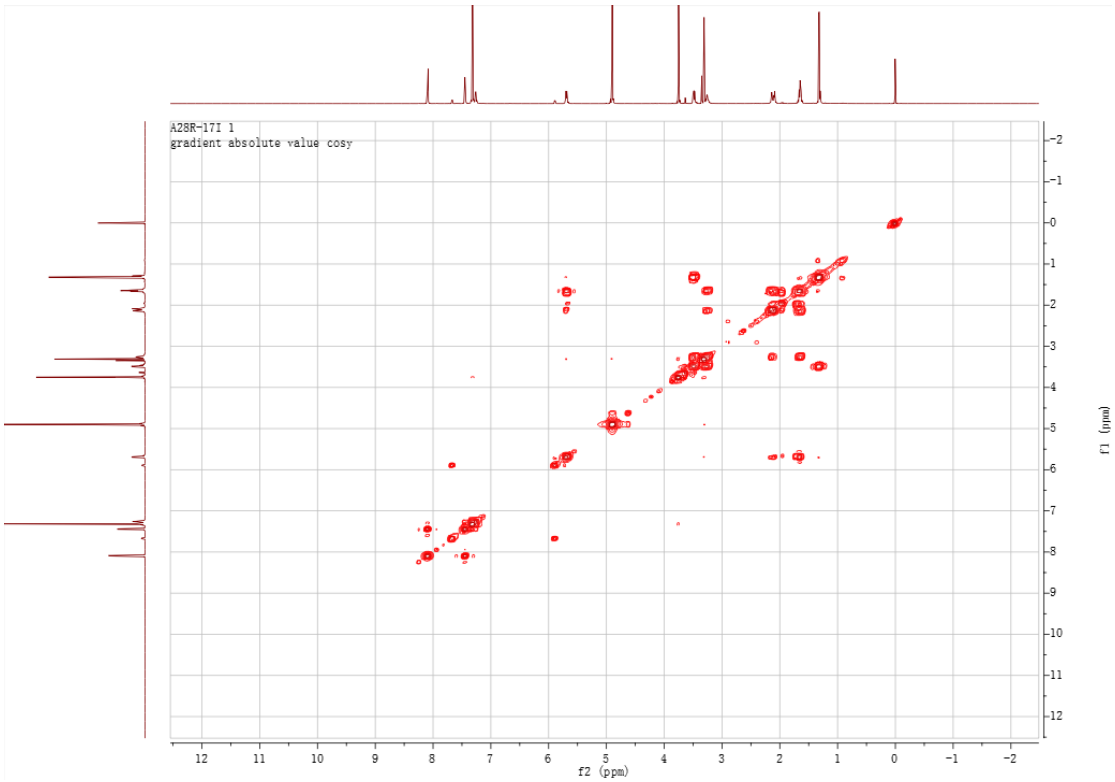


Figure S85. ^{1}H-^{1}H COSY spectrum of **9**

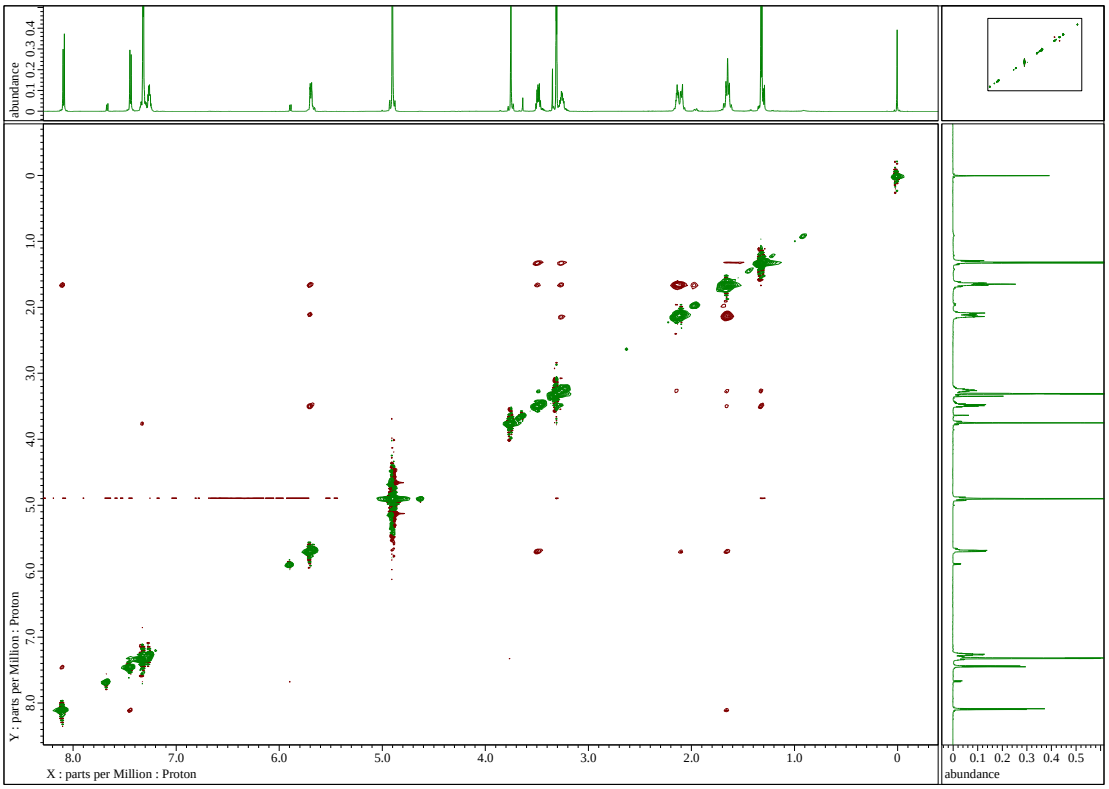


Figure S86. NOESY spectrum of **9**

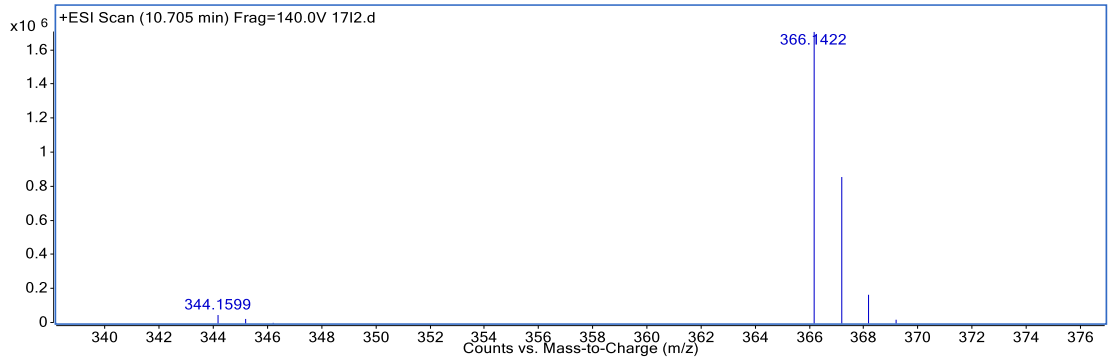


Figure S87. HRESIMS spectrum of **9**

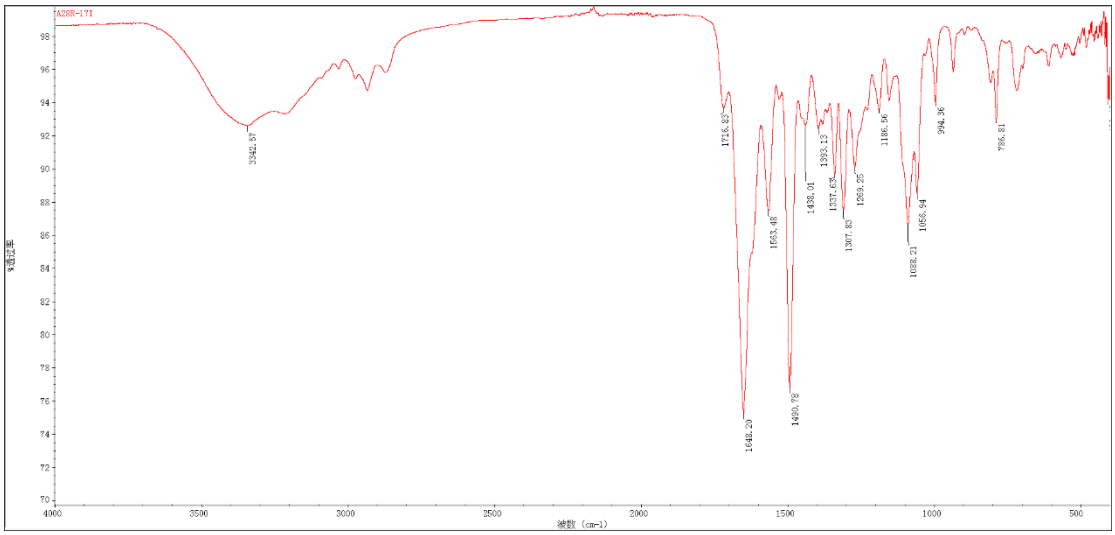


Figure S88. IR spectrum of **9**

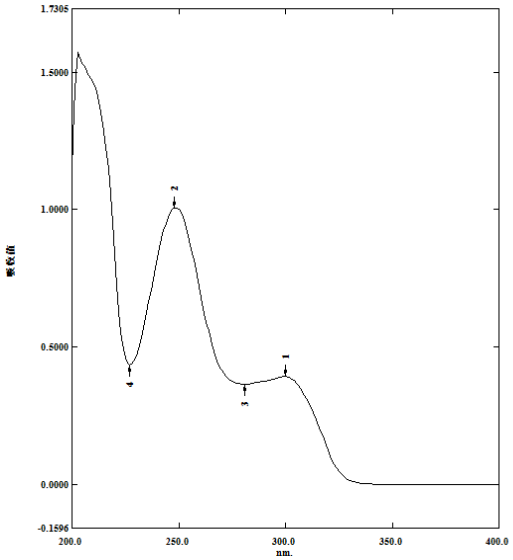


Figure S89. UV spectrum of **9**

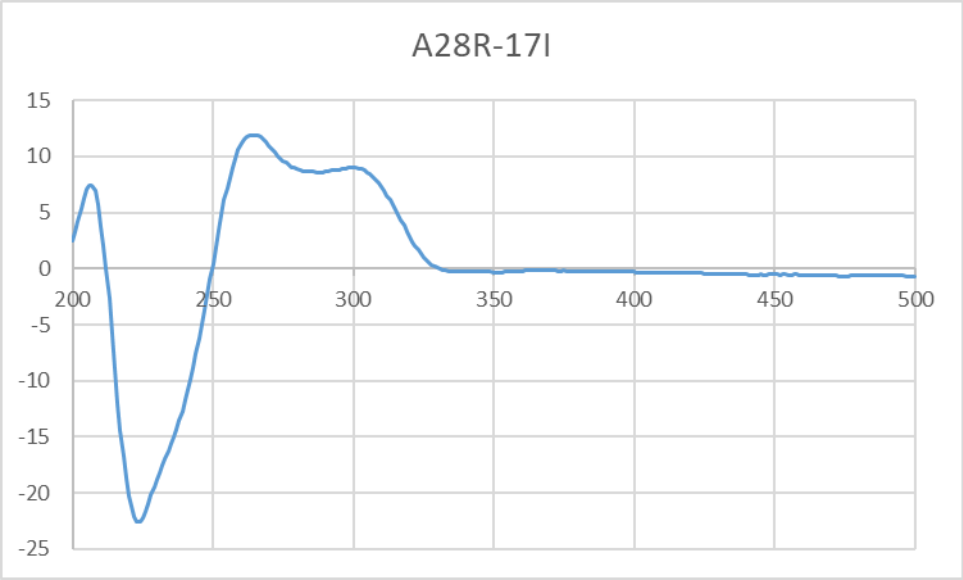


Figure S90. CD spectrum of **9**

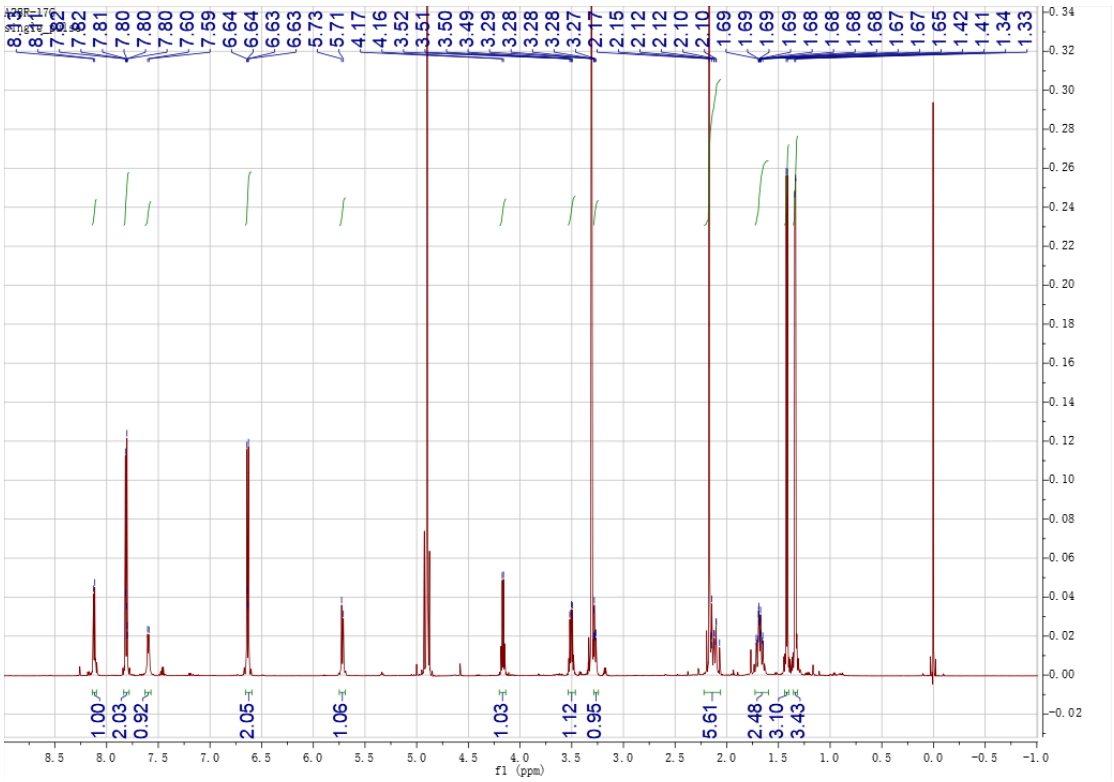


Figure S91. ^{1}H NMR spectrum of **10**

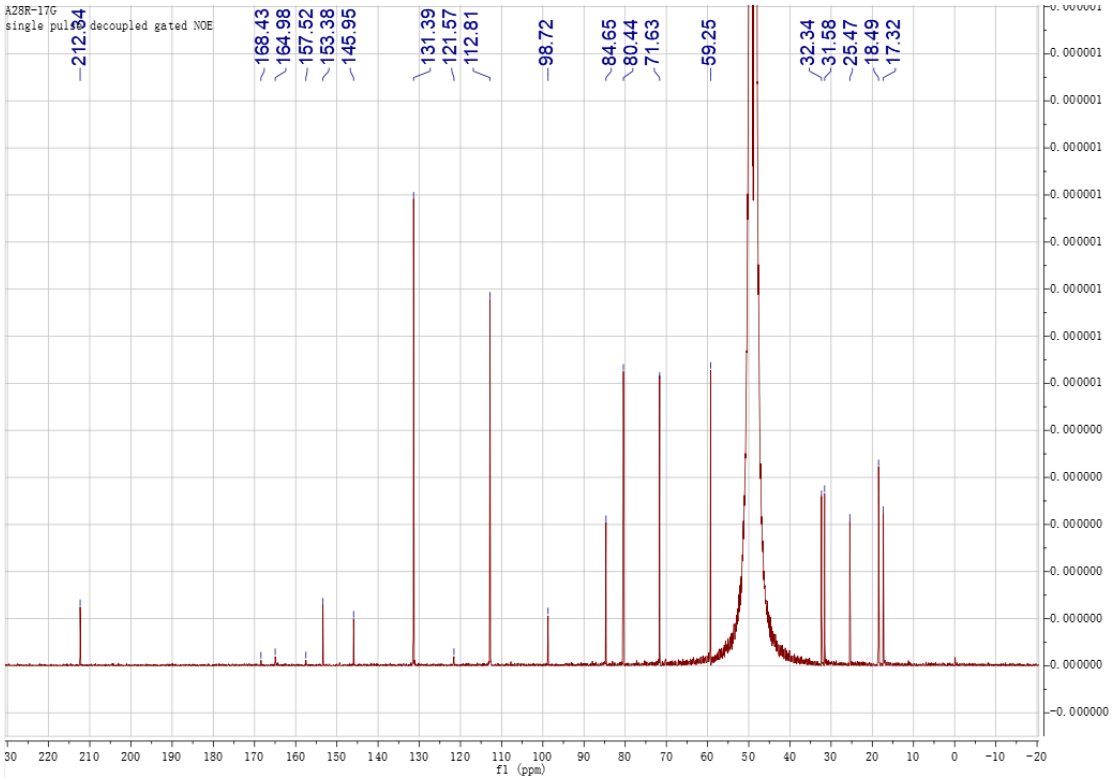


Figure S92. ^{13}C NMR spectrum of **10**

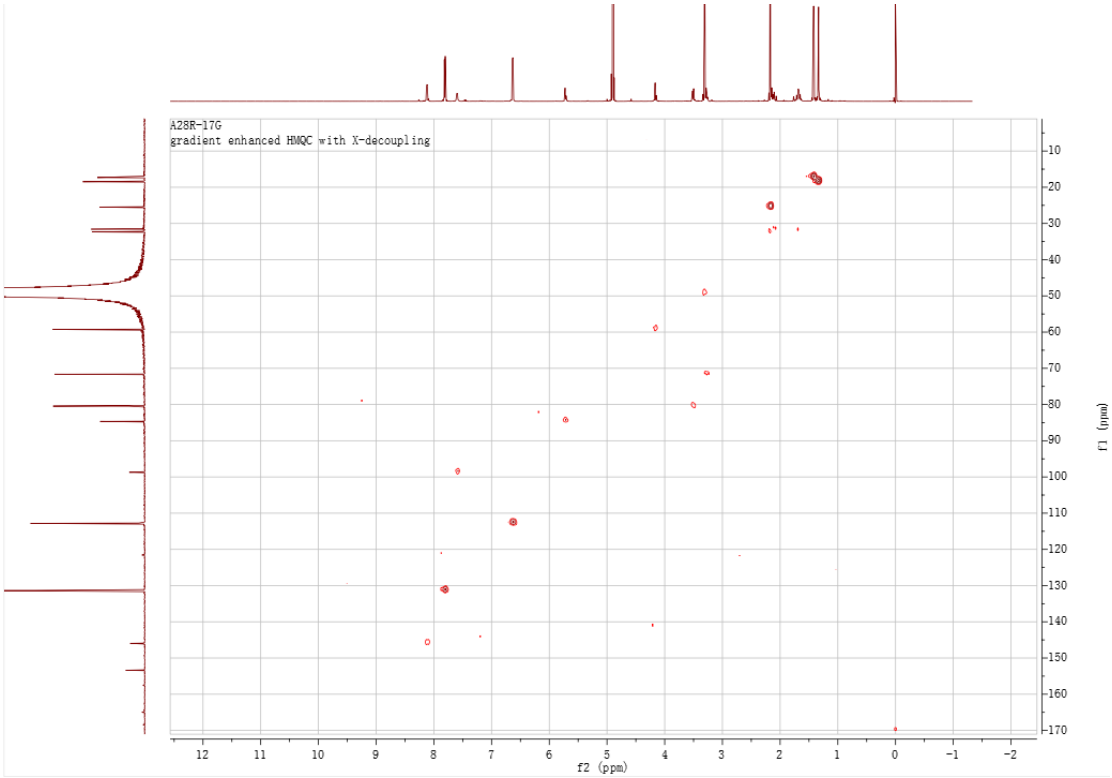


Figure S93. HSQC spectrum of **10**

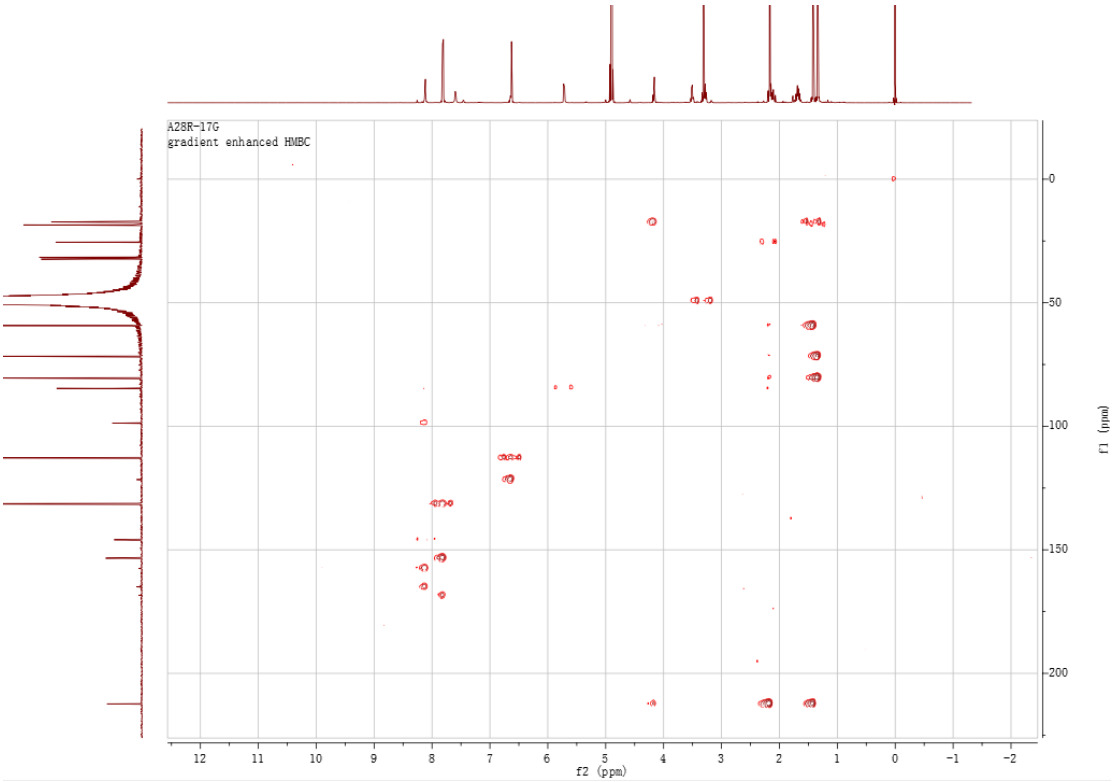


Figure S94. HMBC spectrum of **10**

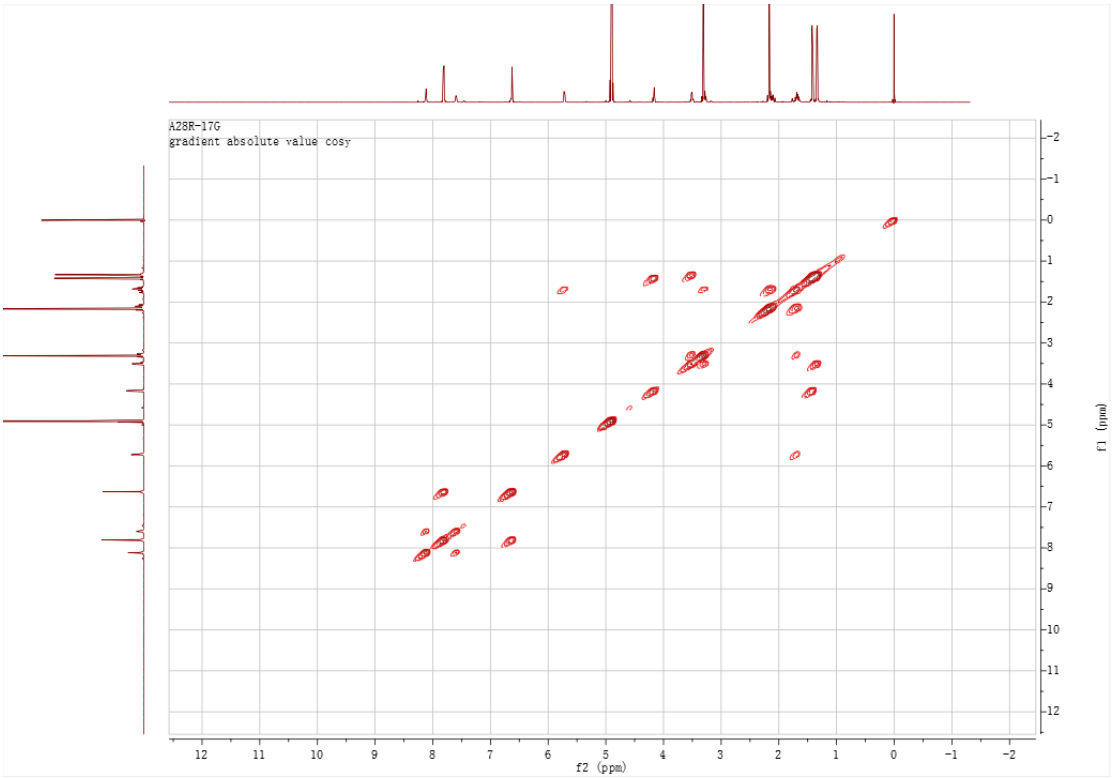


Figure S95. ^{1}H-^{1}H COSY spectrum of **10**

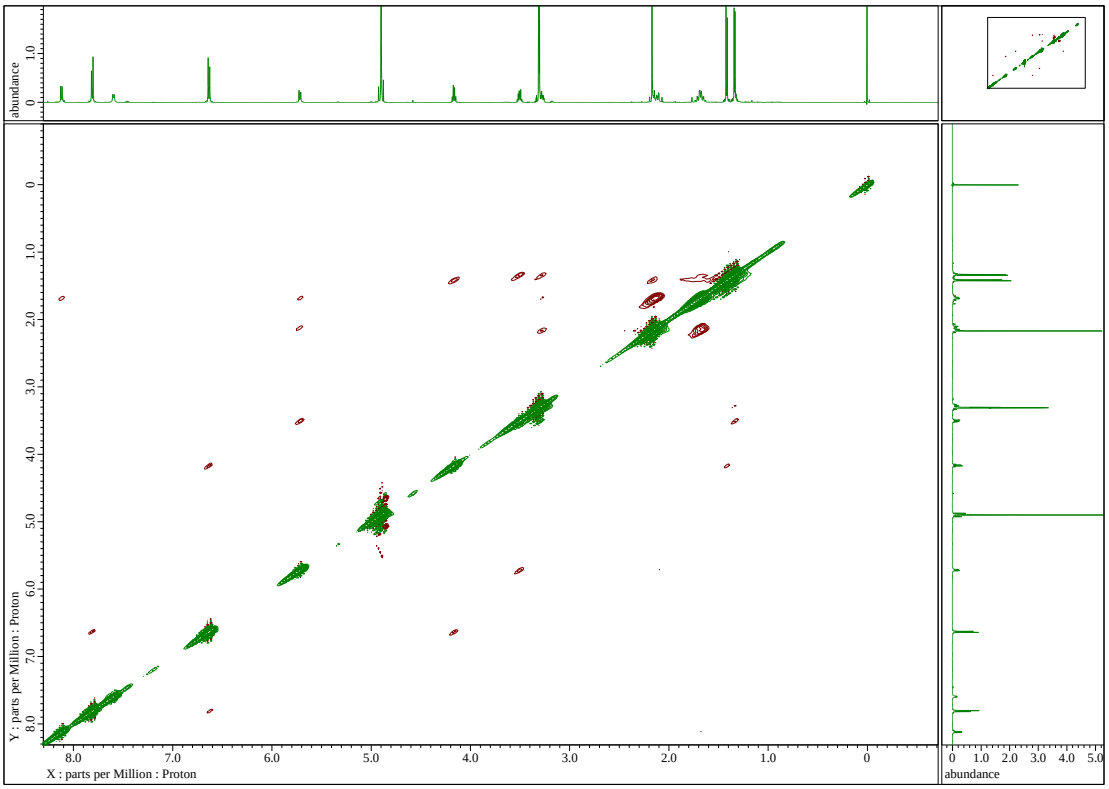


Figure S96. NOESY spectrum of **10**

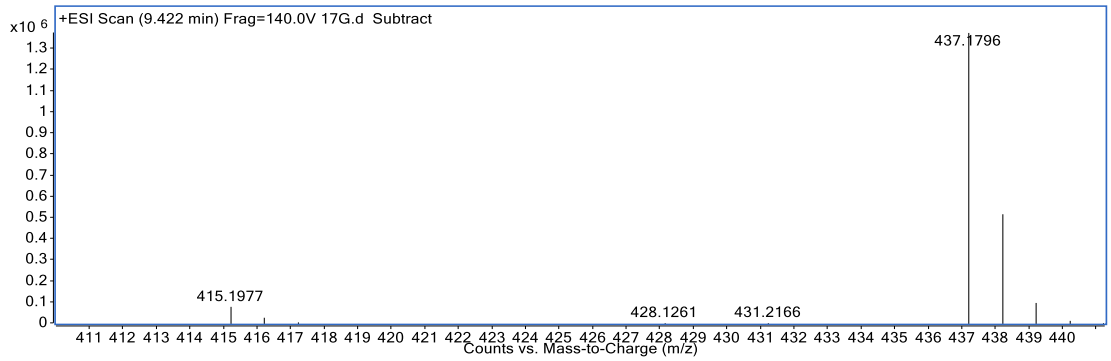


Figure S97. HRESIMS spectrum of **10**

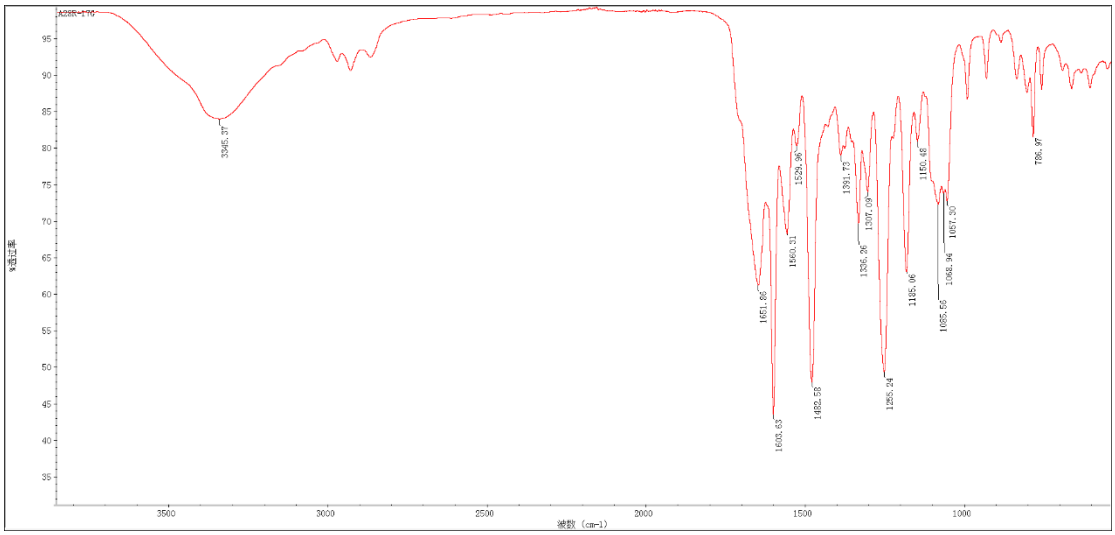


Figure S98. IR spectrum of **10**

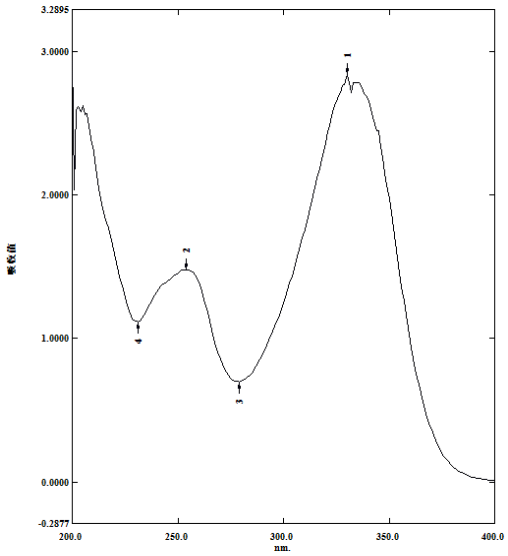


Figure S99. UV spectrum of **10**

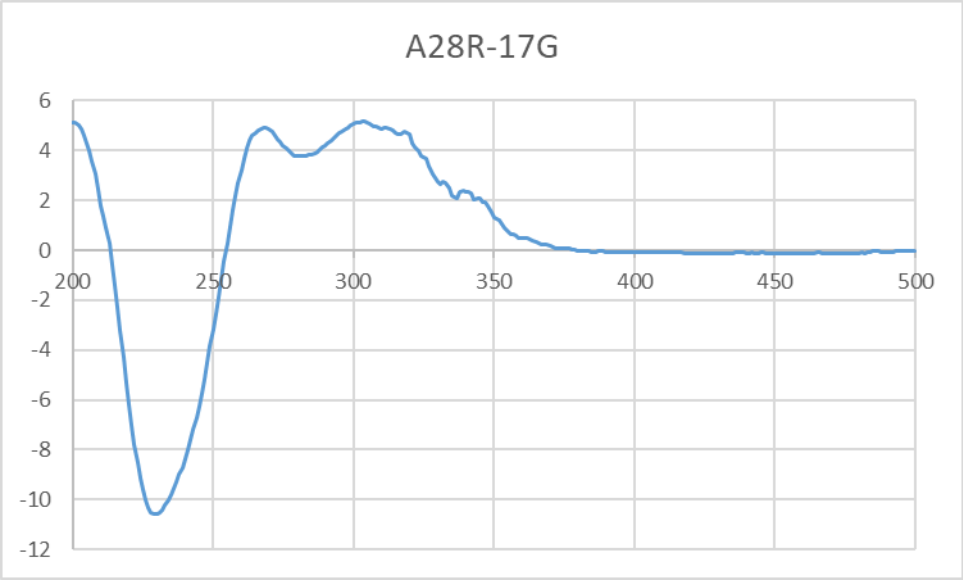


Figure S100. CD spectrum of **10**

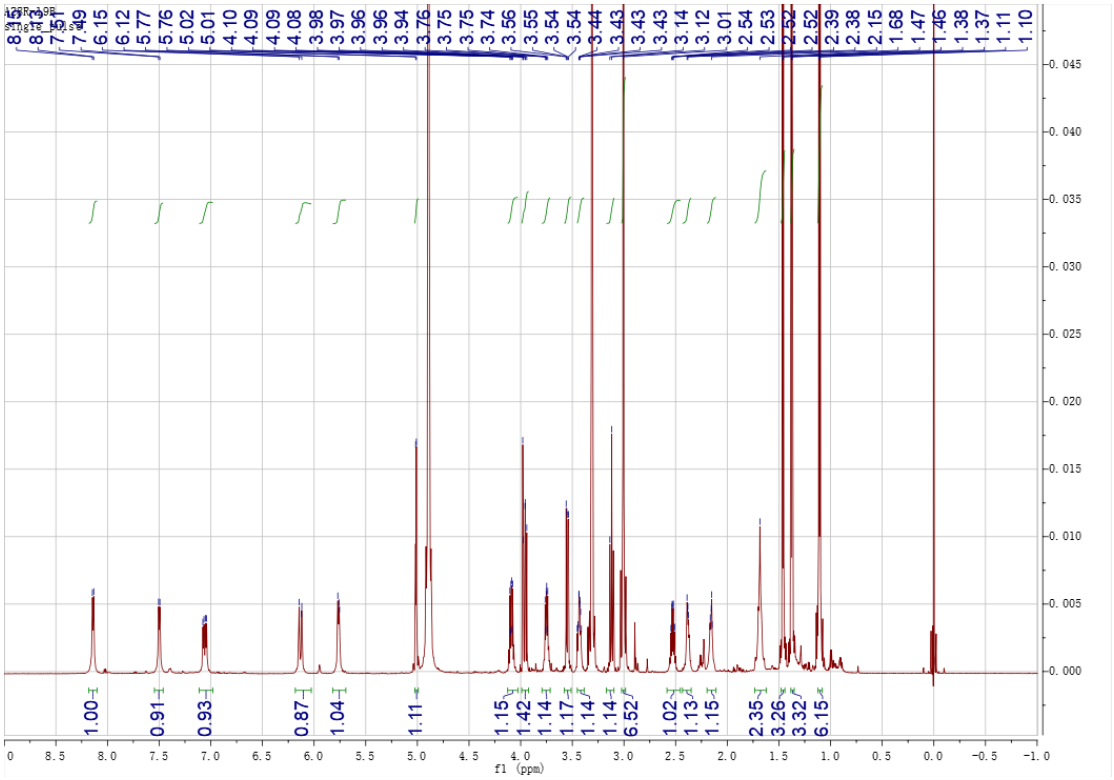


Figure S101. ^{1}H NMR spectrum of **11**

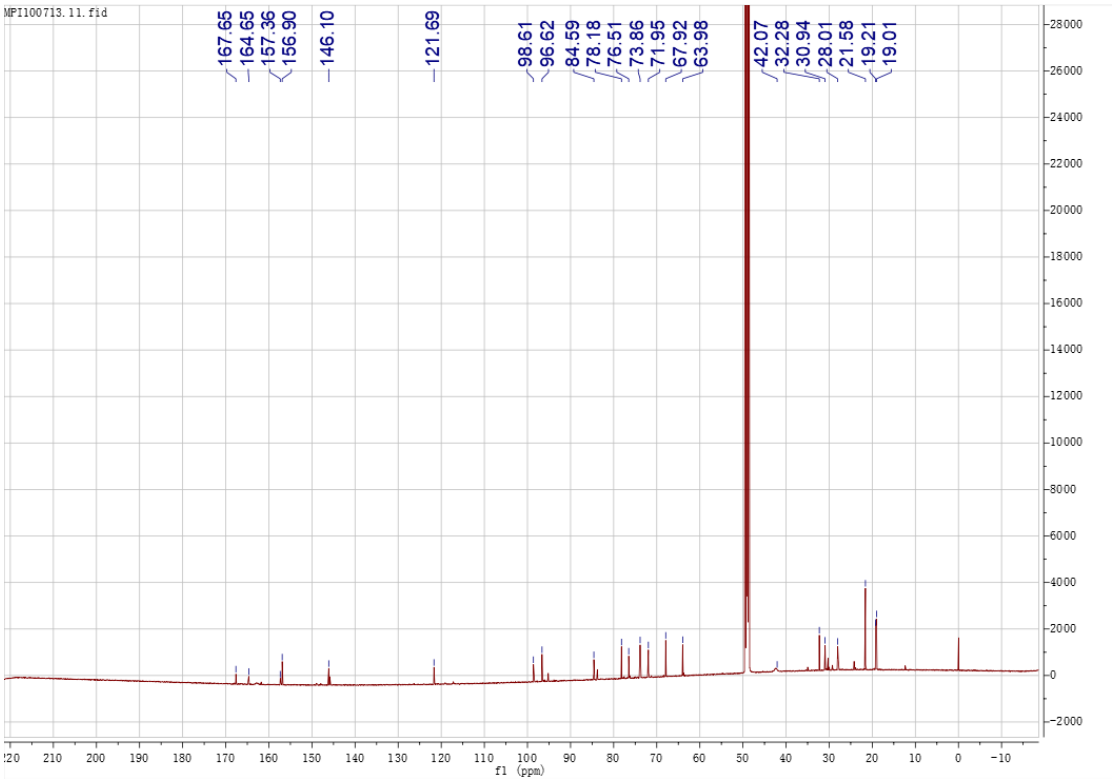


Figure S102. ^{13}C NMR spectrum of **11**

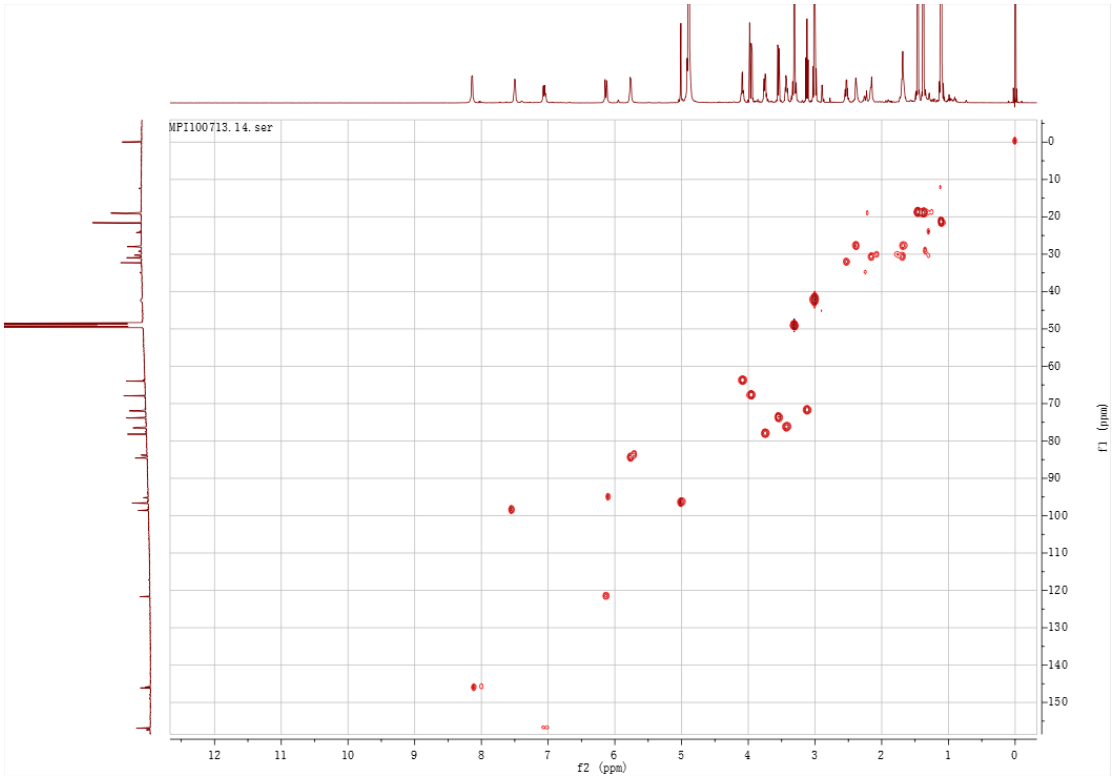


Figure S103. HSQC spectrum of **11**

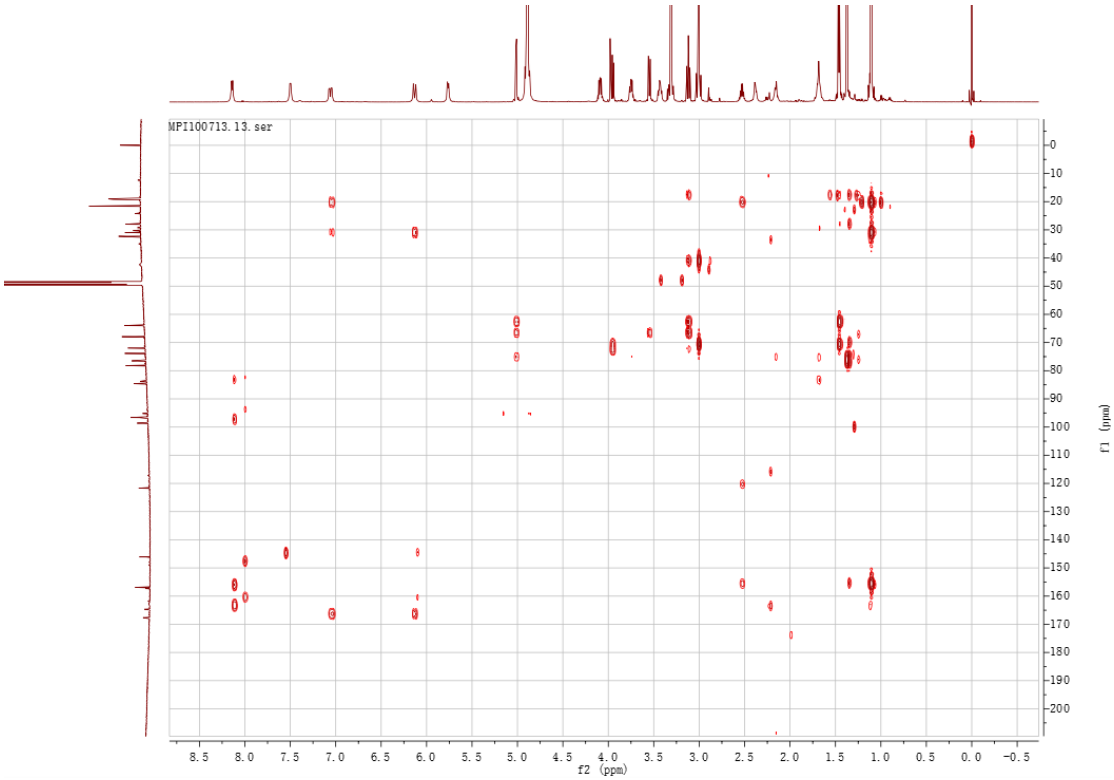


Figure S104. HMBC spectrum of **11**

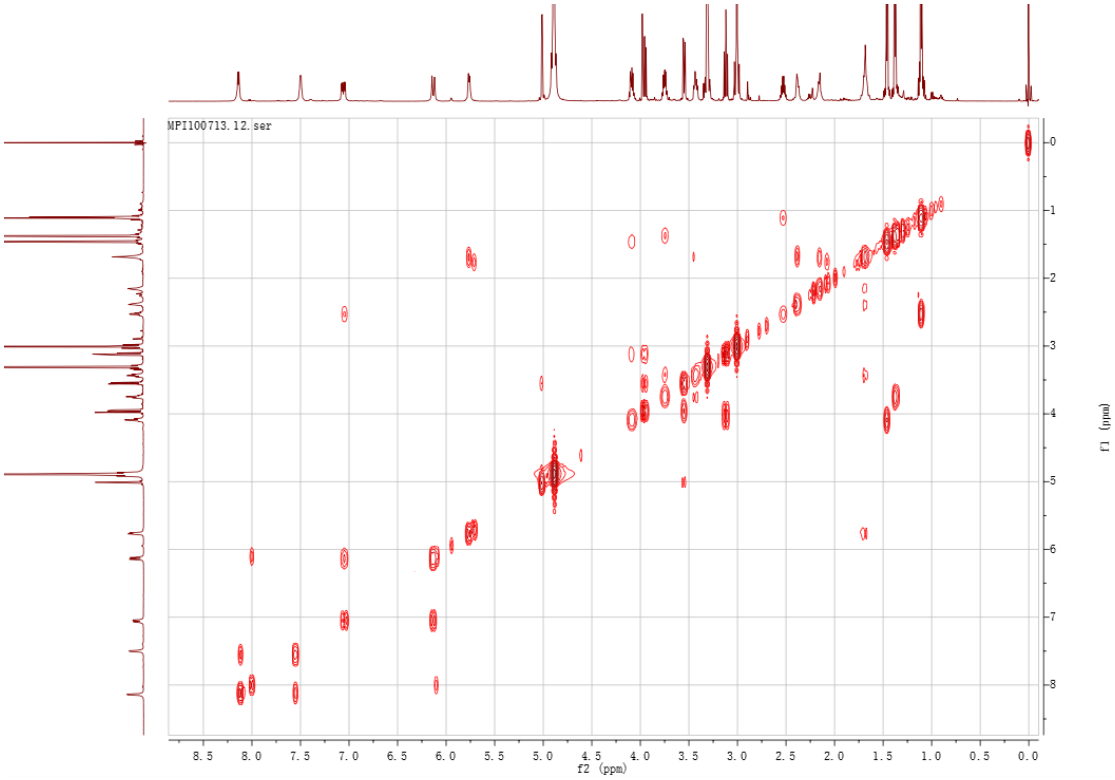


Figure S105. ^{1}H-^{1}H COSY spectrum of **11**

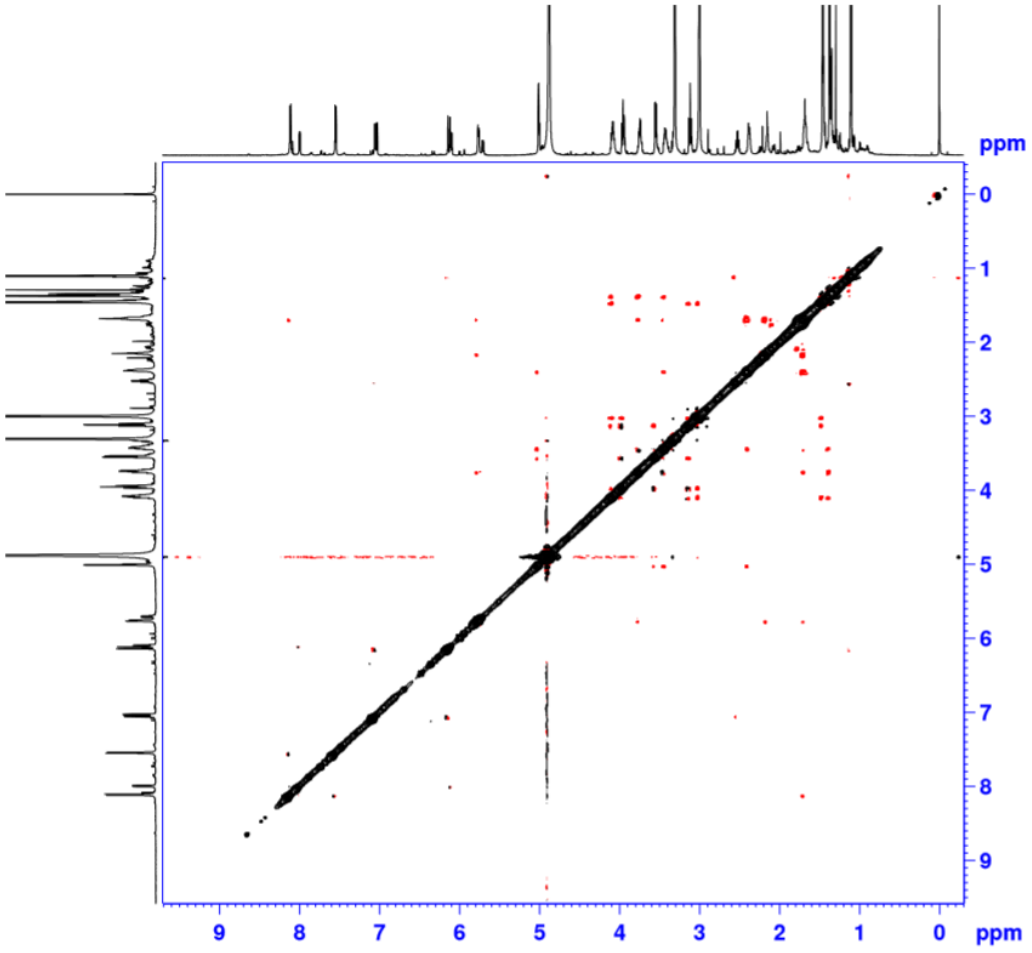


Figure S106. NOESY spectrum of **11**

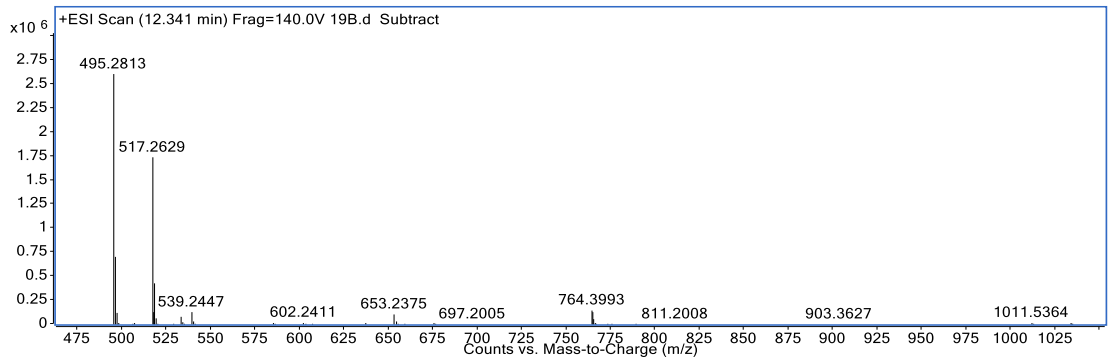


Figure S107. HRESIMS spectrum of **11**

Figure S108. IR spectrum of **11**

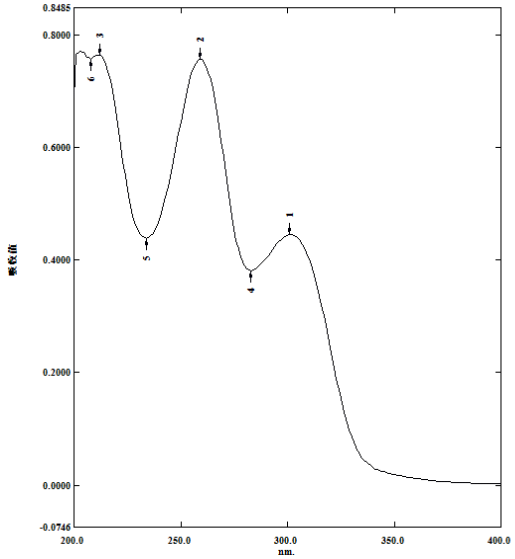


Figure S109. UV spectrum of **11**

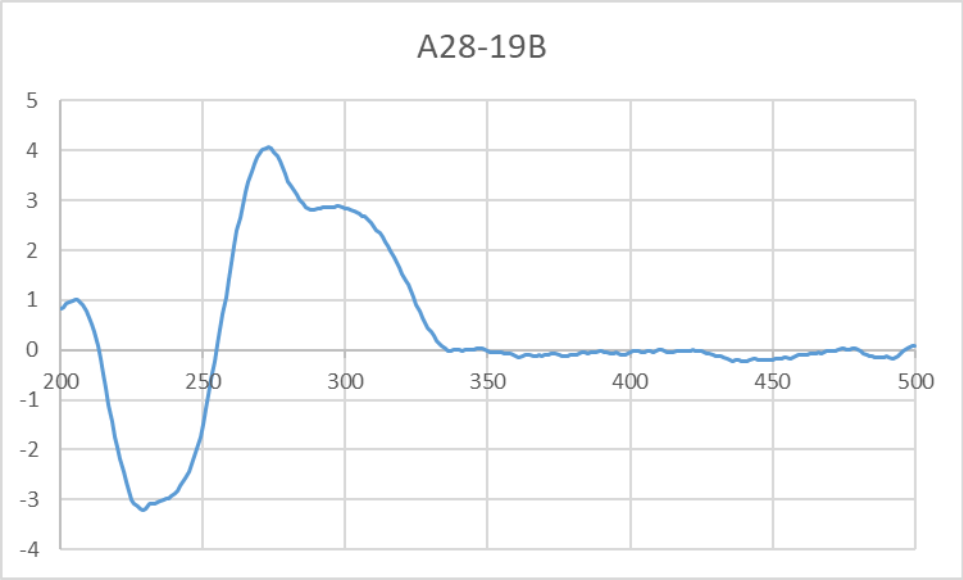


Figure S110. CD spectrum of **11**

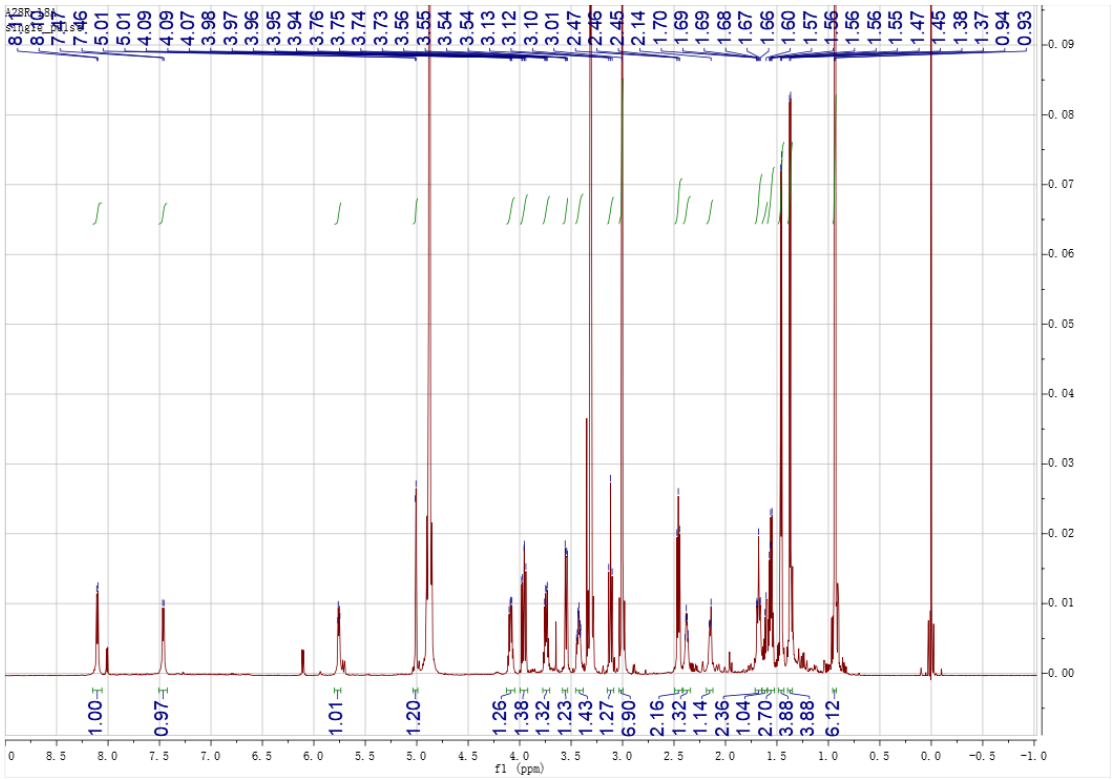


Figure S111. ^{1}H NMR spectrum of **12**

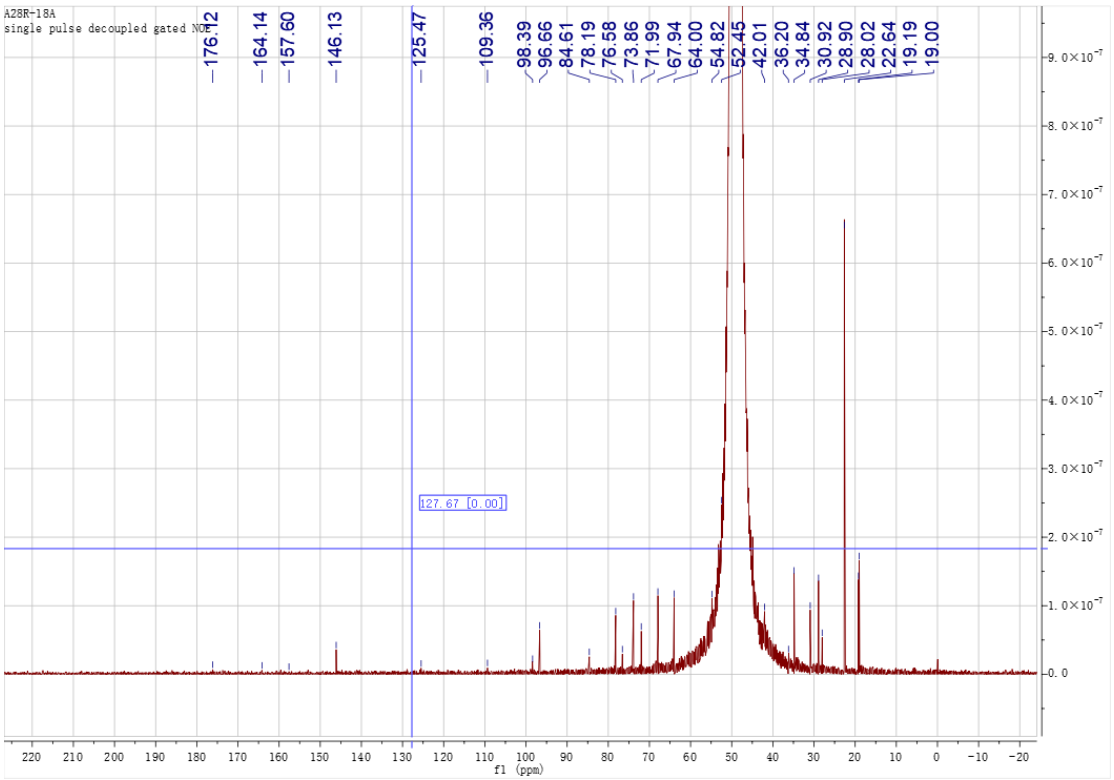


Figure S112. ^{13}C NMR spectrum of **12**

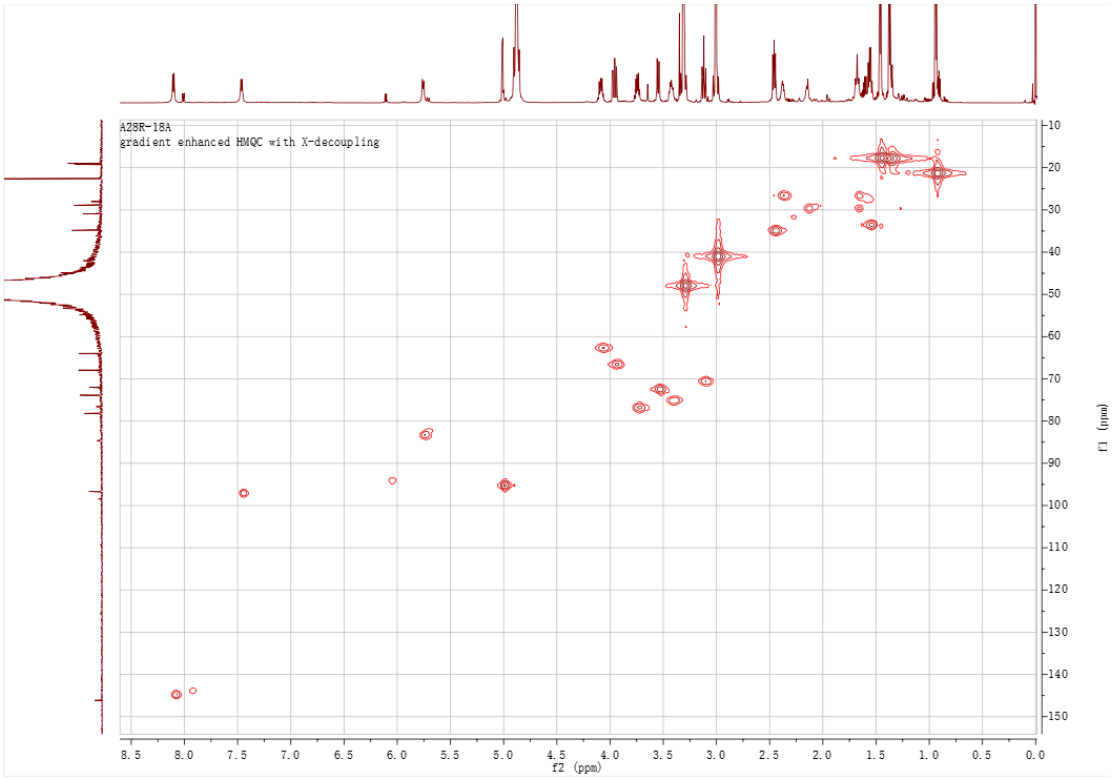


Figure S113. HSQC spectrum of **12**

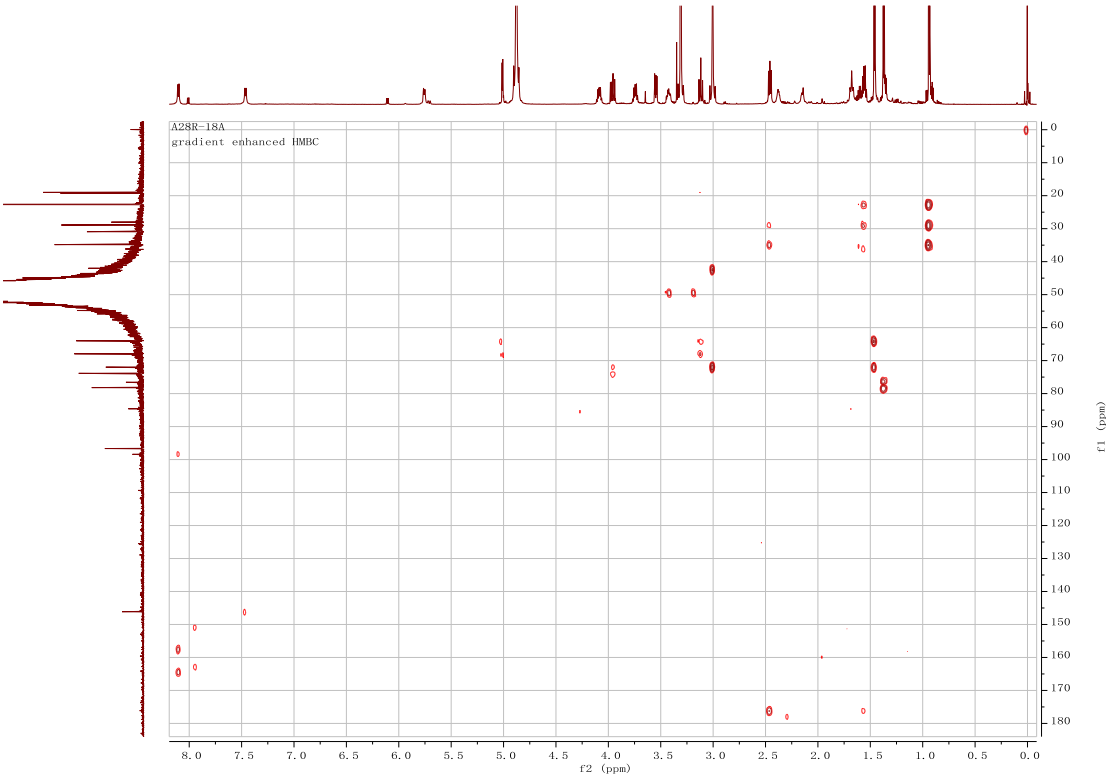


Figure S114. HMBC spectrum of **12**

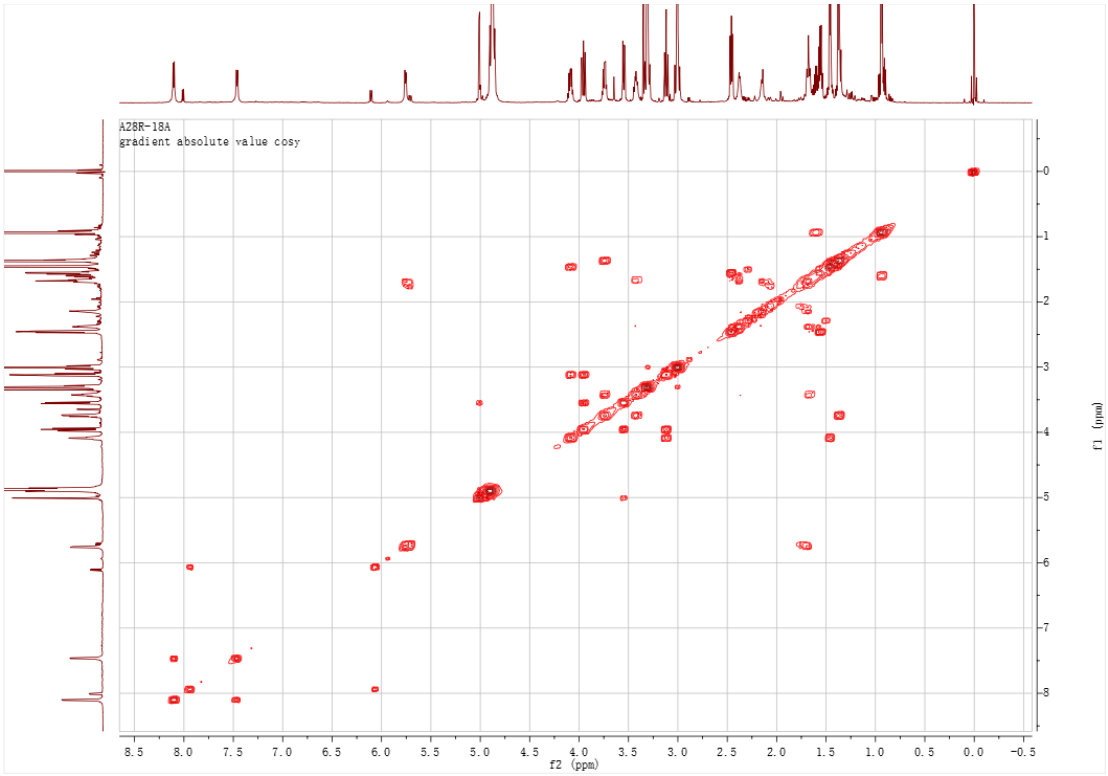


Figure S115. ^{1}H-^{1}H COSY spectrum of **12**

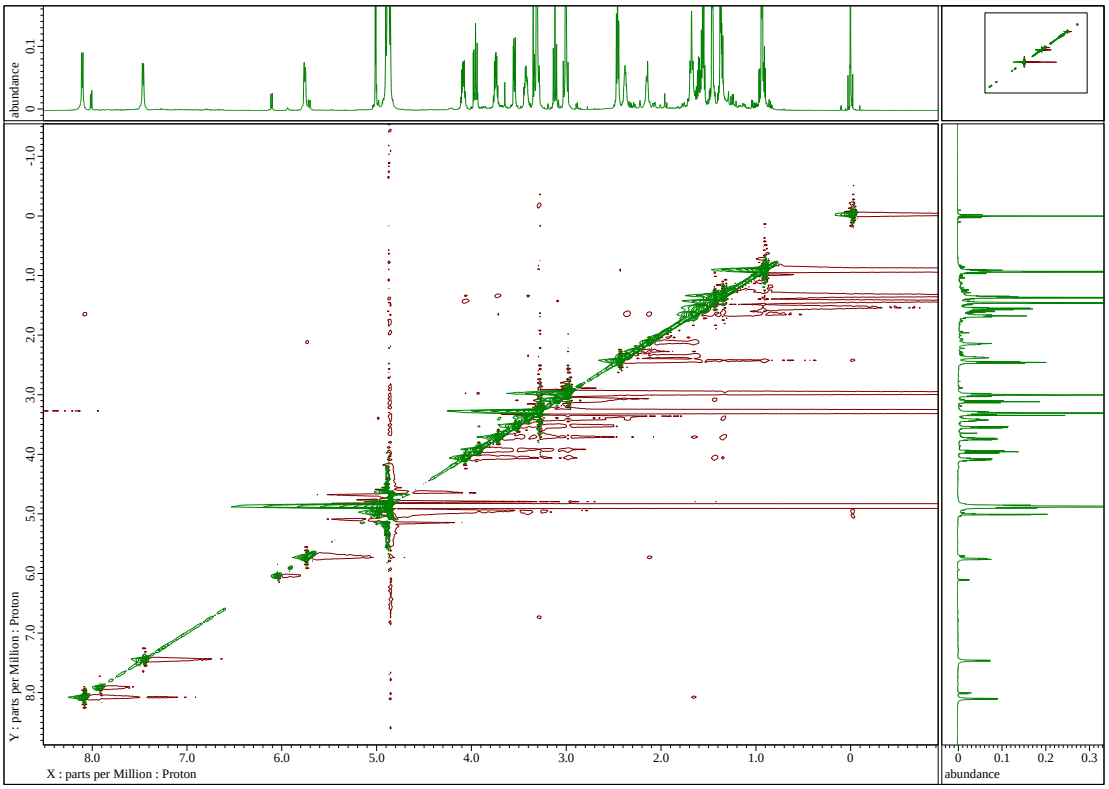


Figure S116. NOESY spectrum of **12**

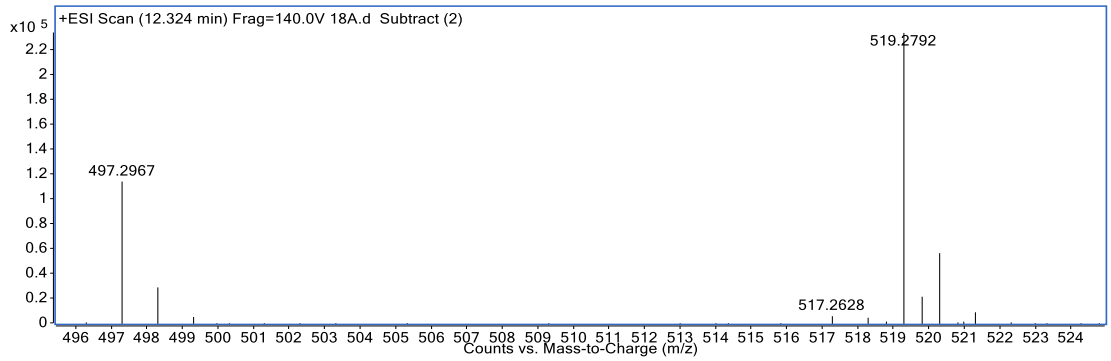


Figure S117. HRESIMS spectrum of **12**

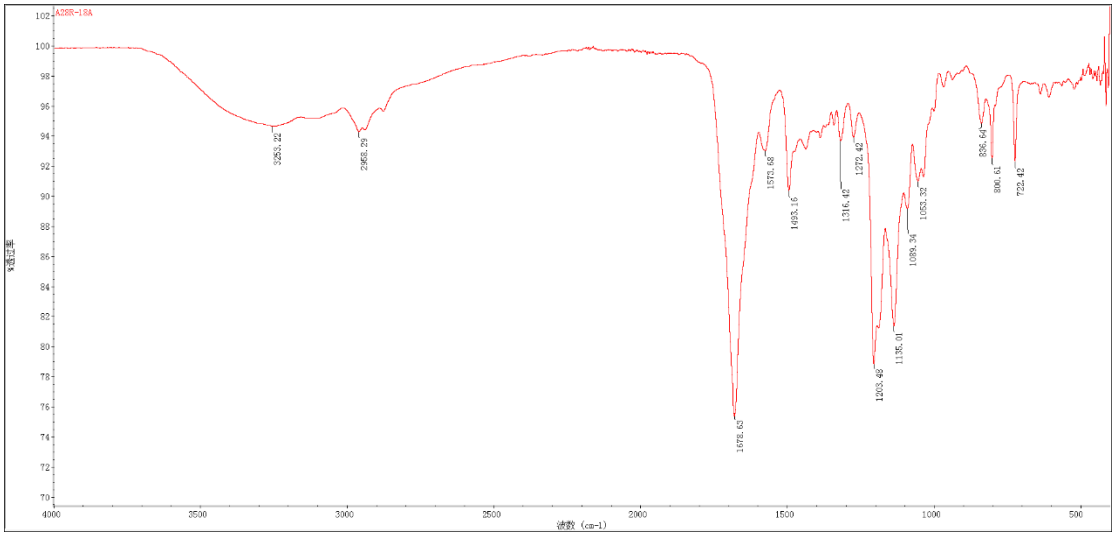


Figure S118. IR spectrum of **12**

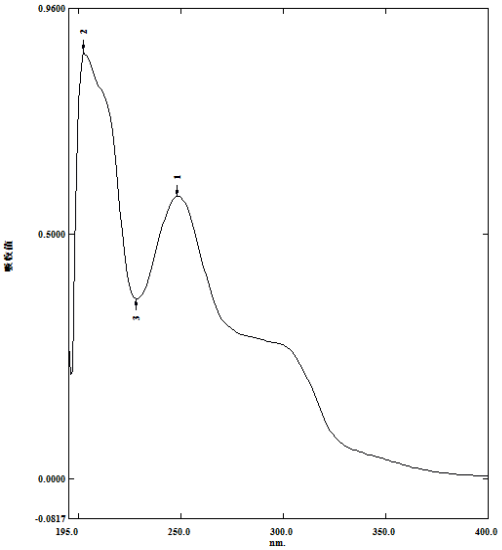


Figure S119. UV spectrum of **12**

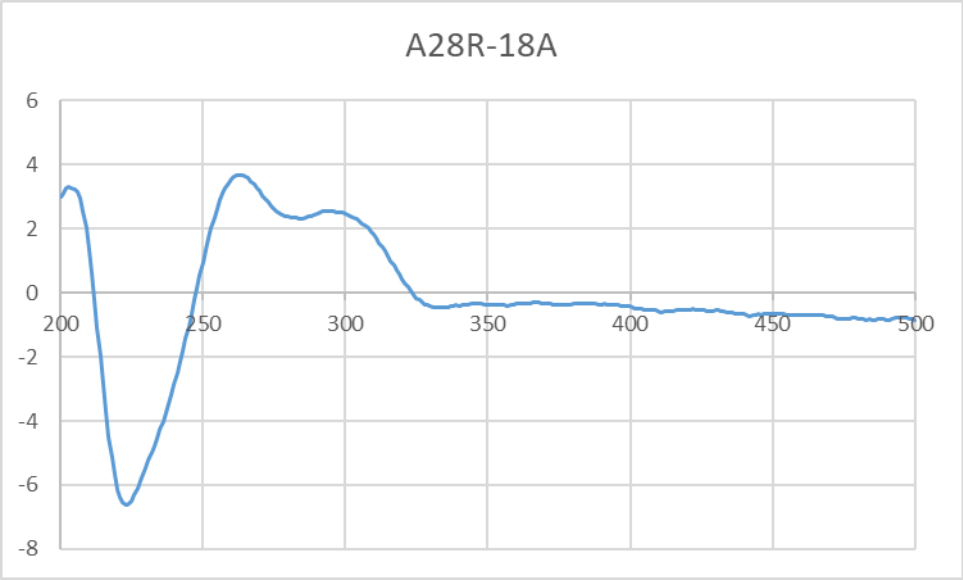


Figure S120. CD spectrum of **12**

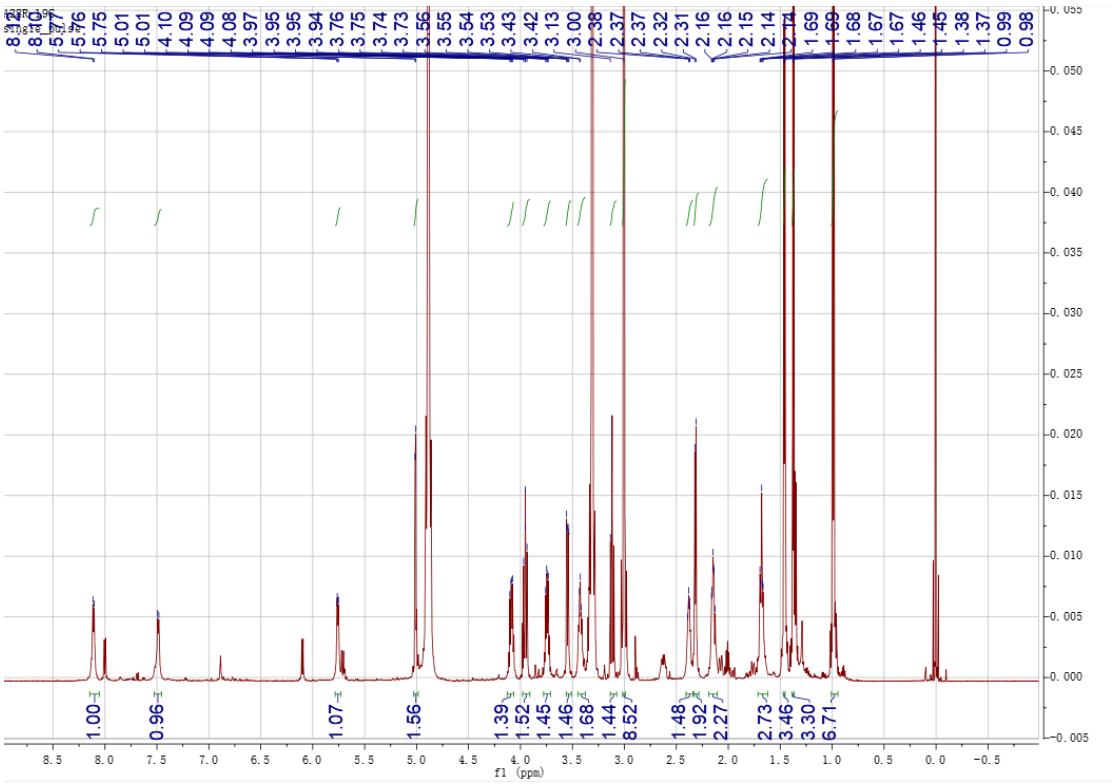


Figure S121. ^{1}H NMR spectrum of **13**

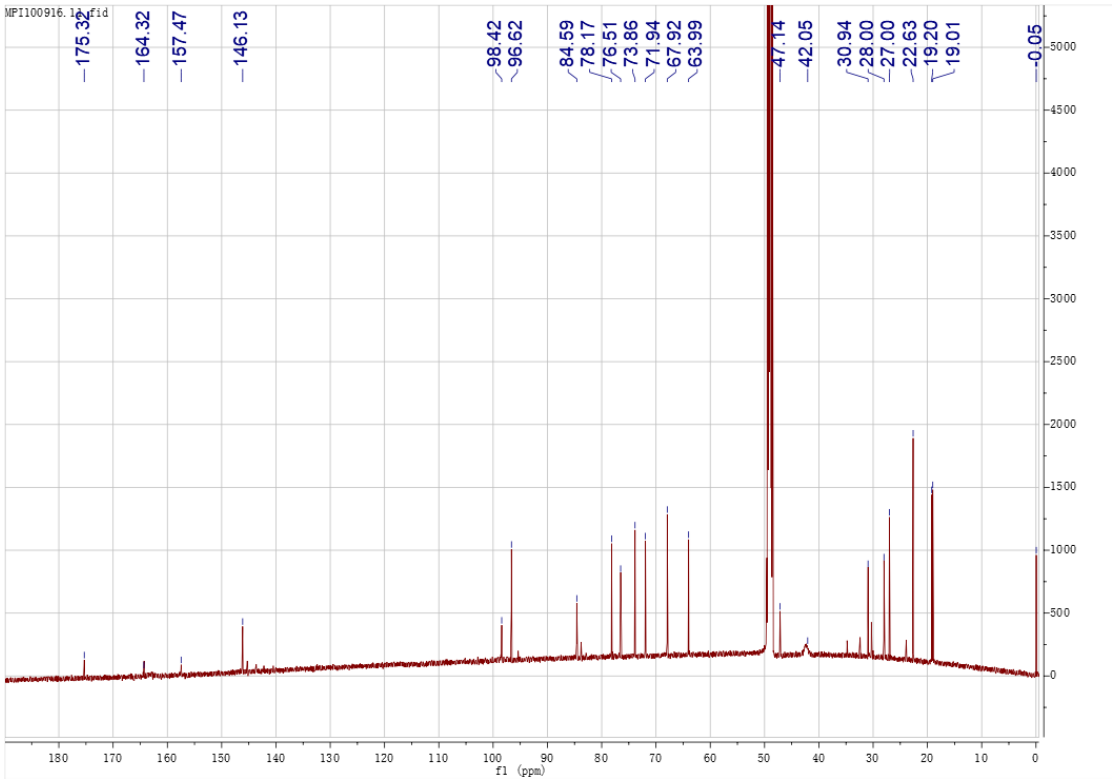


Figure S122. ^{13}C NMR spectrum of **13**

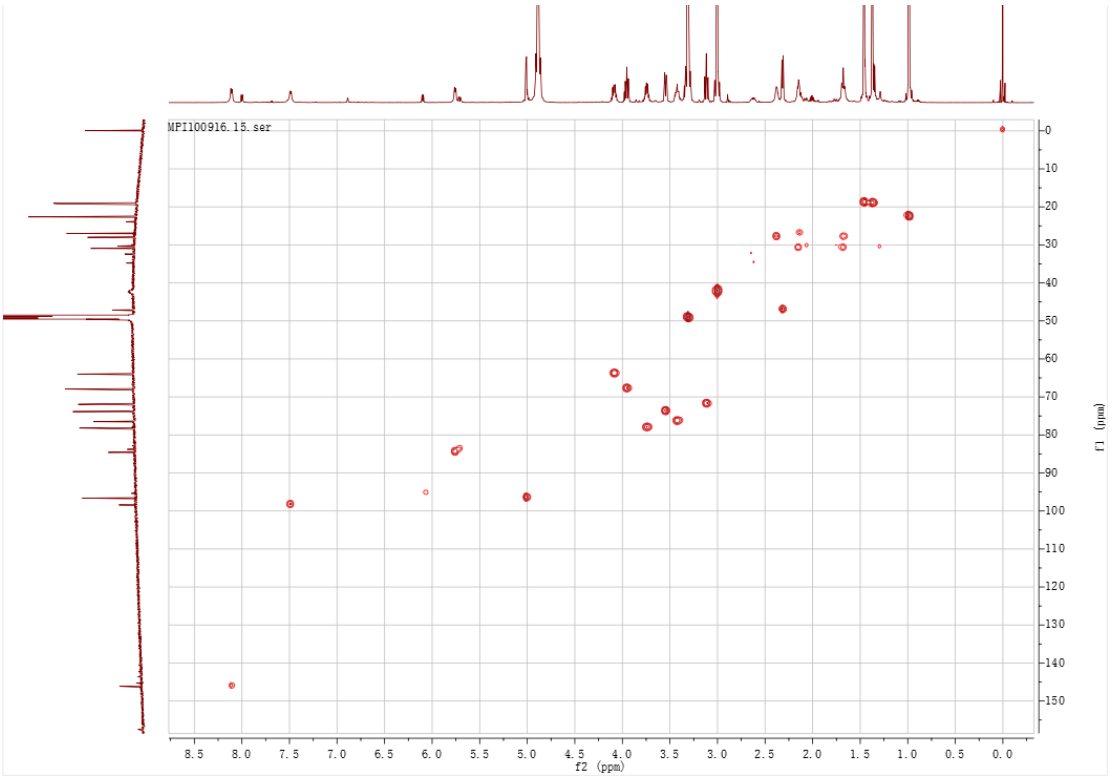


Figure S123. HSQC spectrum of **13**

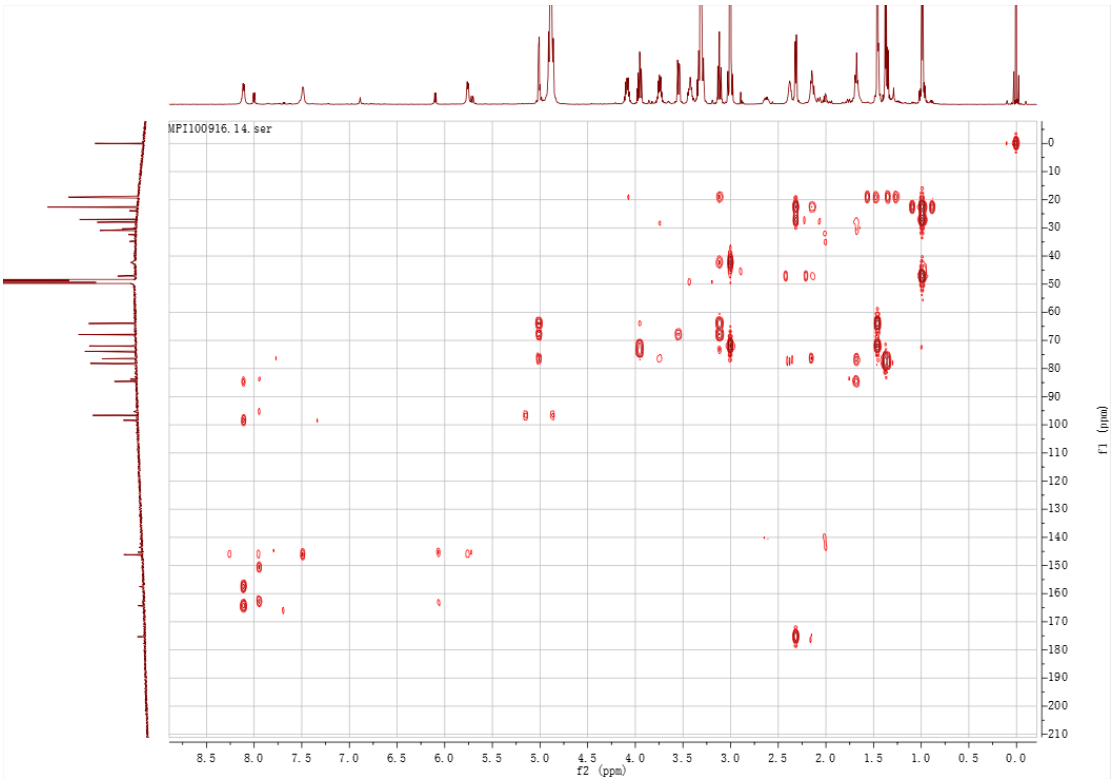


Figure S124. HMBC spectrum of **13**

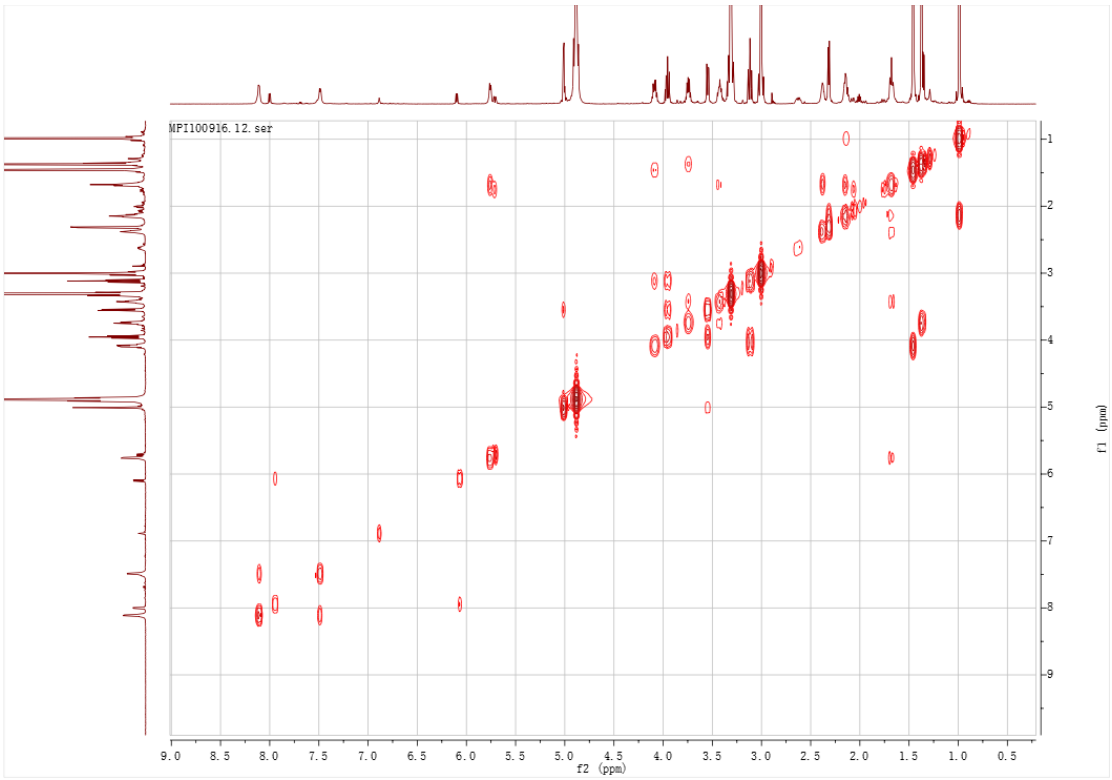


Figure S125. ^{1}H-^{1}H COSY spectrum of **13**

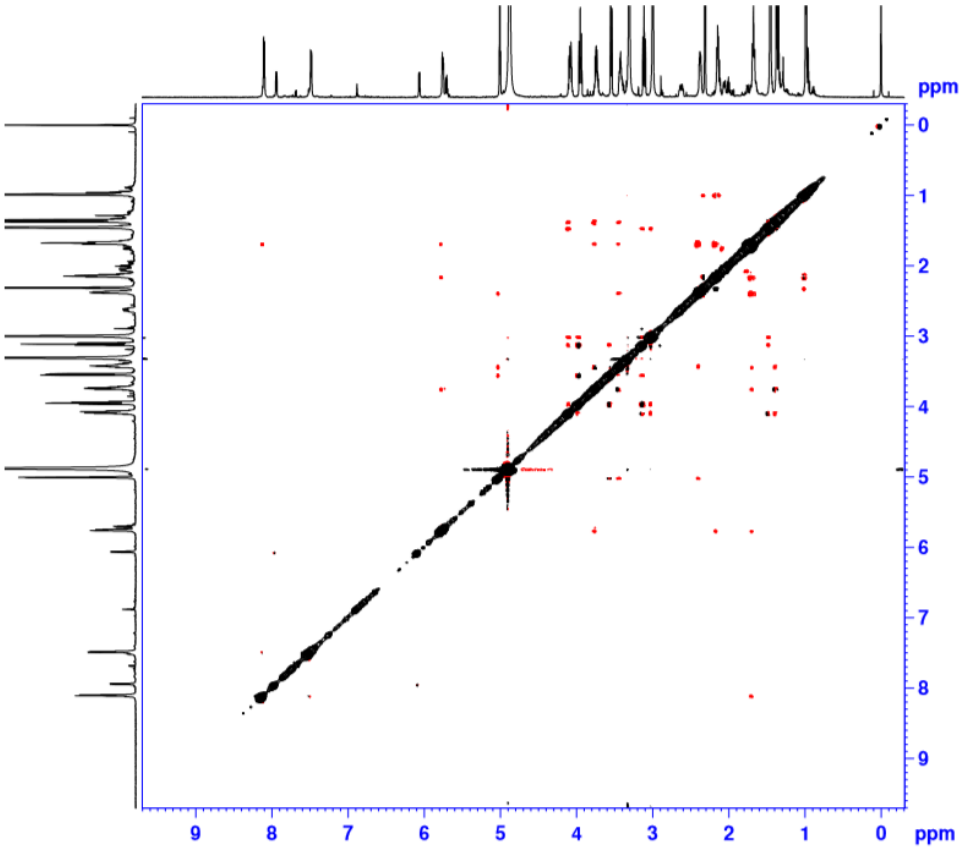


Figure S126. NOESY spectrum of **13**

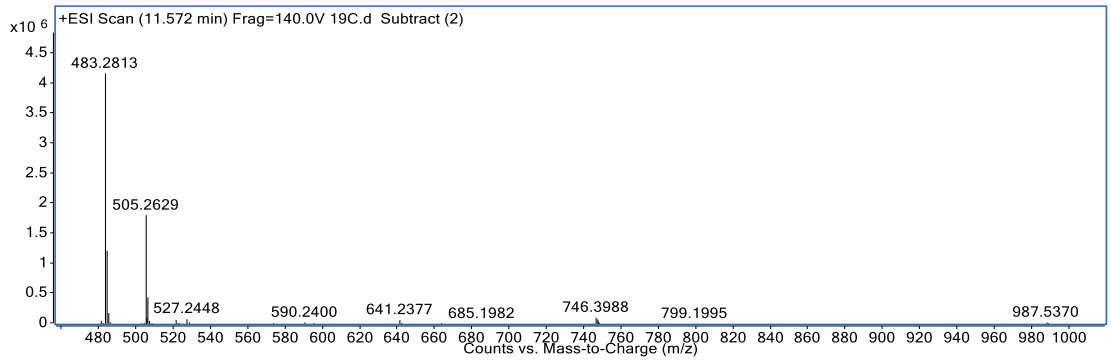


Figure S127. HRESIMS spectrum of **13**

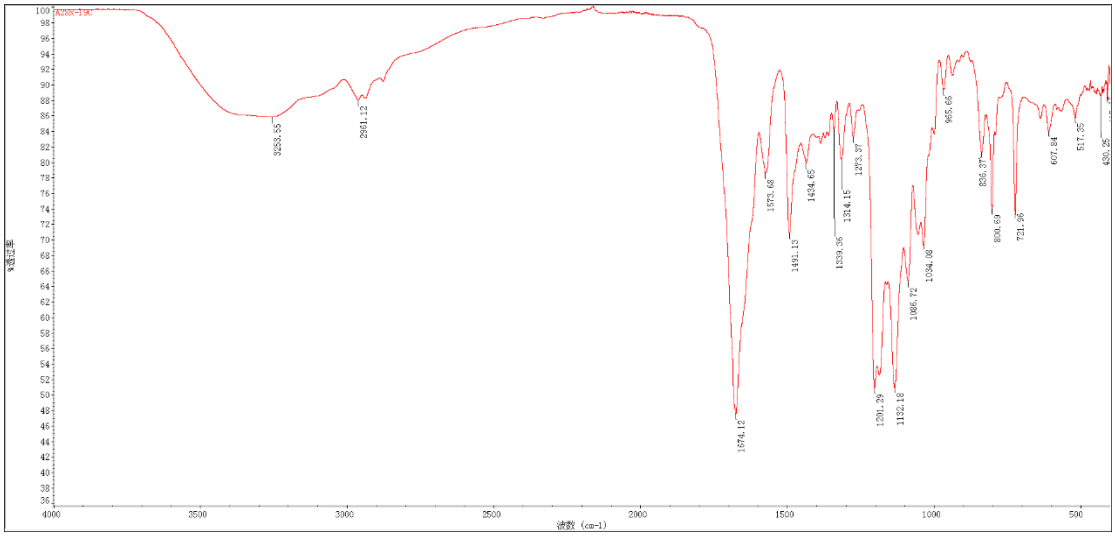


Figure S128. IR spectrum of **13**

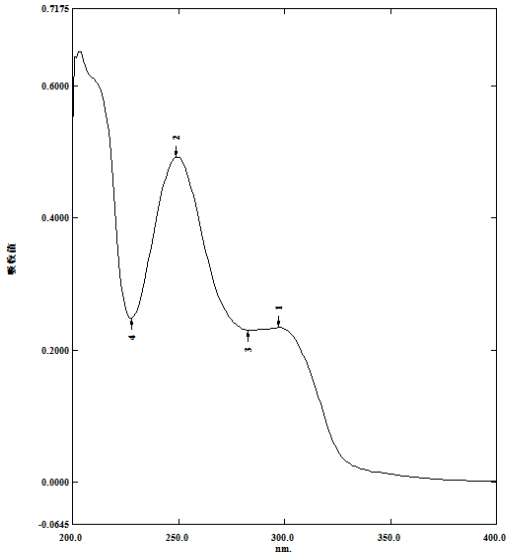


Figure S129. UV spectrum of **13**

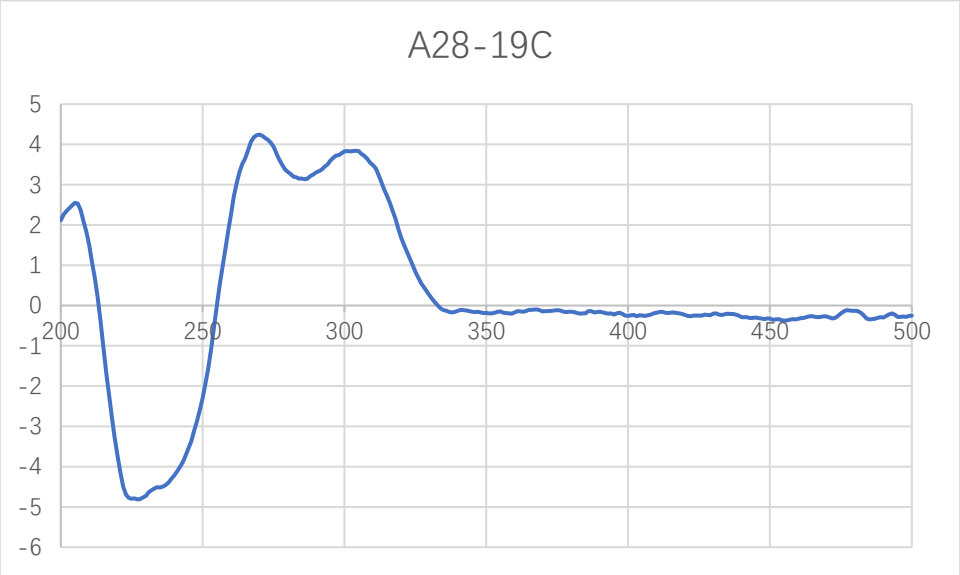


Figure S130. CD spectrum of **13**

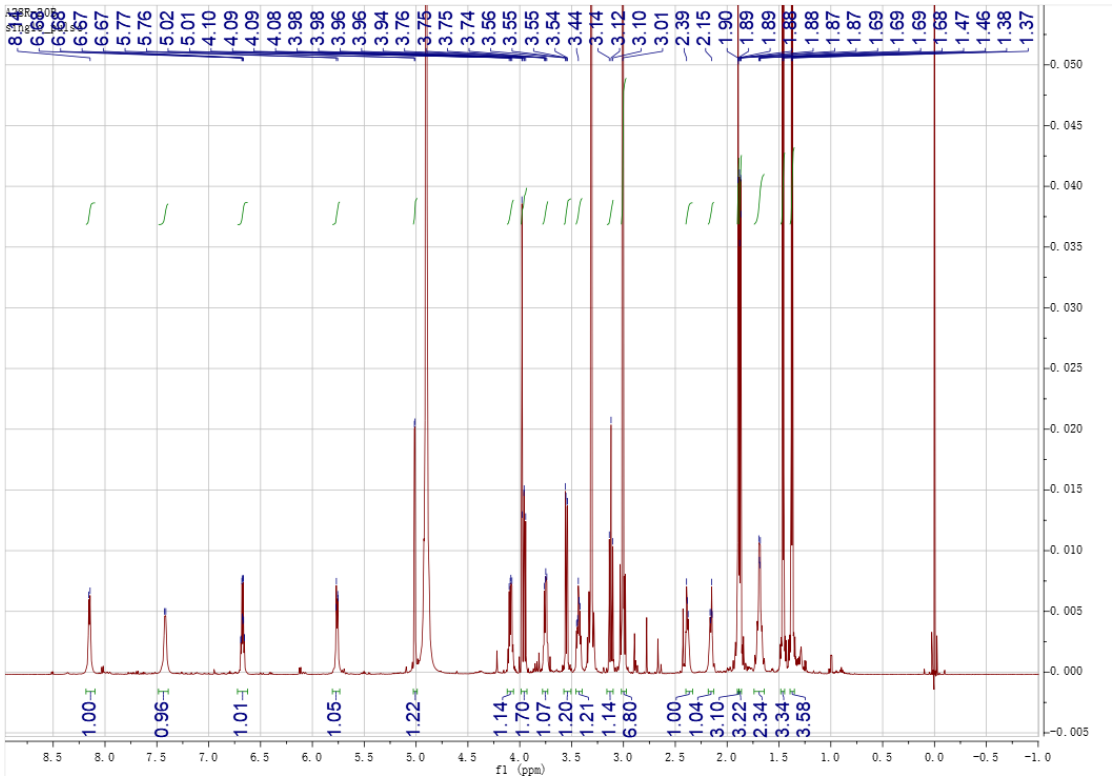


Figure S131. ^{1}H NMR spectrum of **14**

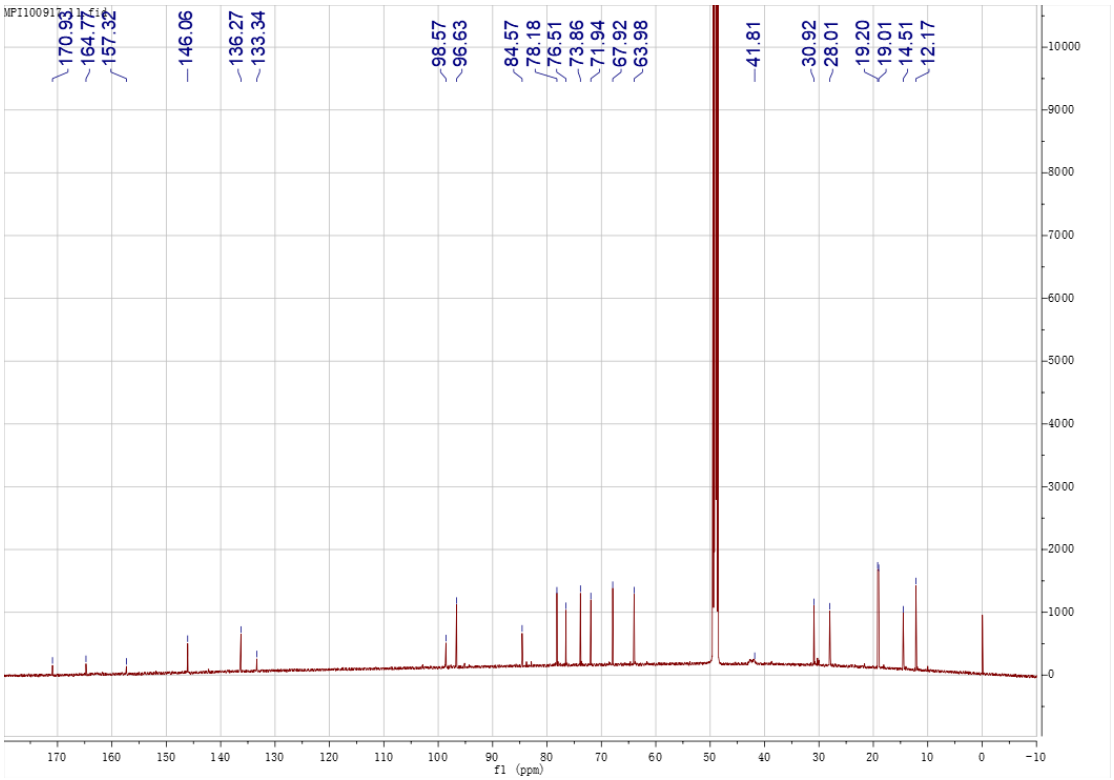


Figure S132. ^{13}C NMR spectrum of **14**

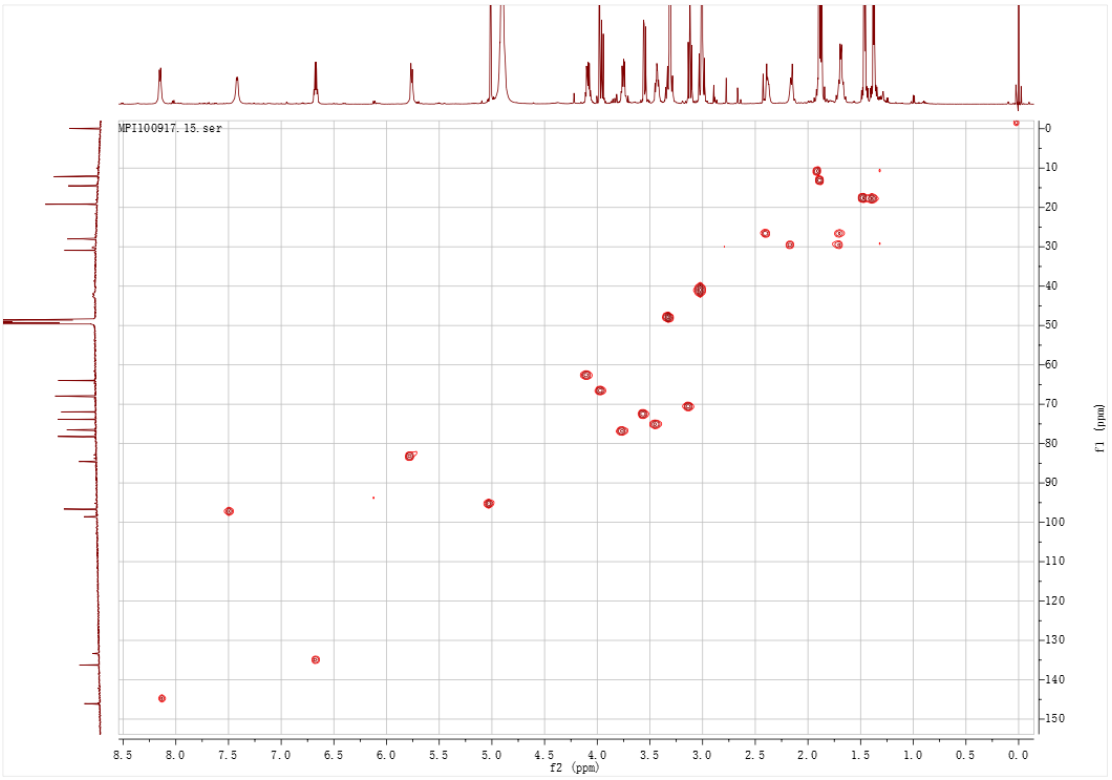


Figure S133. HSQC spectrum of **14**

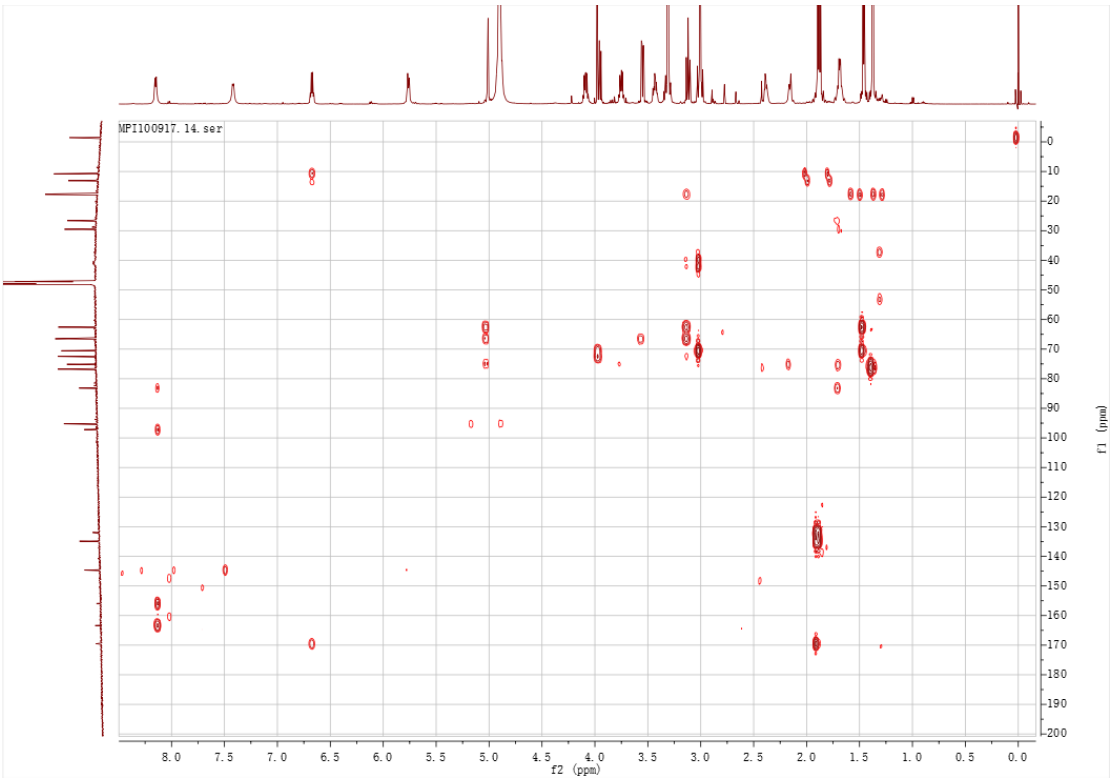


Figure S134. HMBC spectrum of **14**

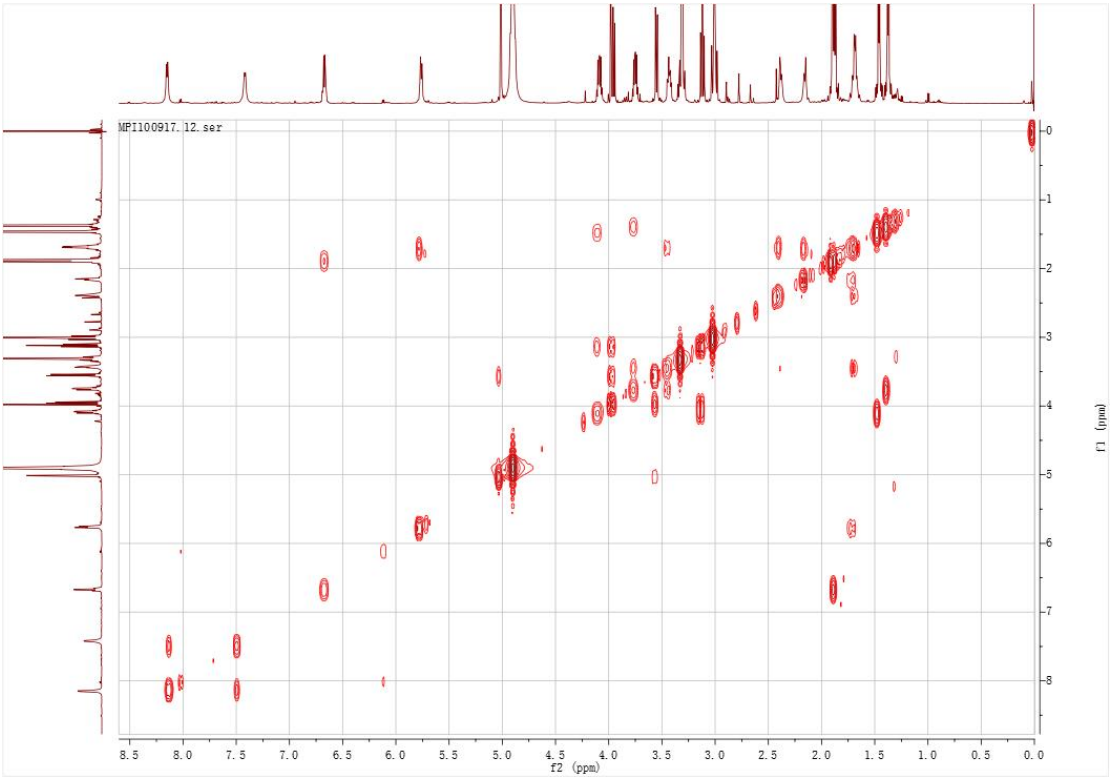


Figure S135. ^{1}H-^{1}H COSY spectrum of **14**

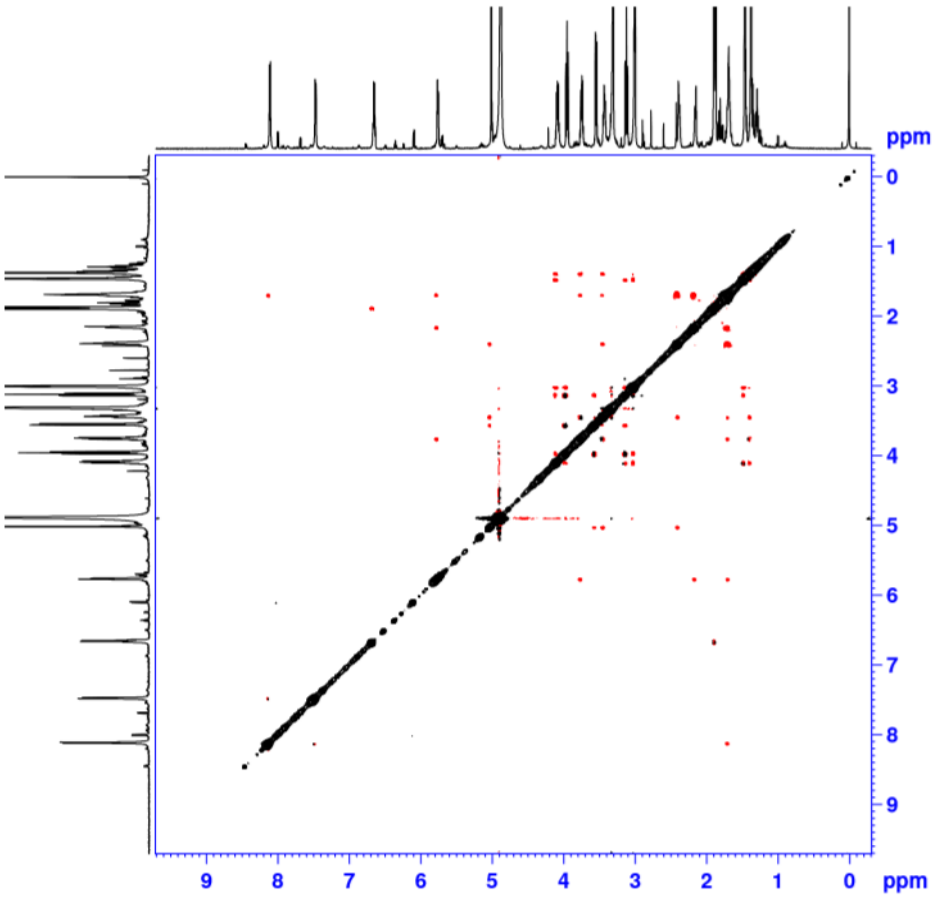


Figure S136. NOESY spectrum of **14**

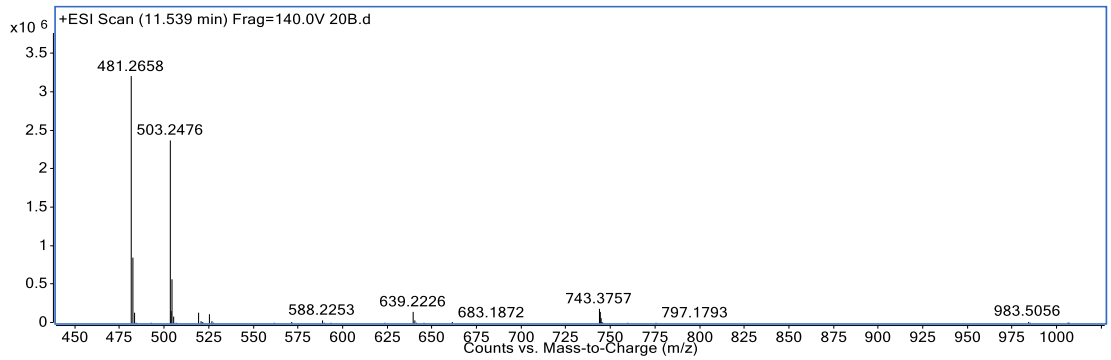


Figure S137. HRESIMS spectrum of **14**

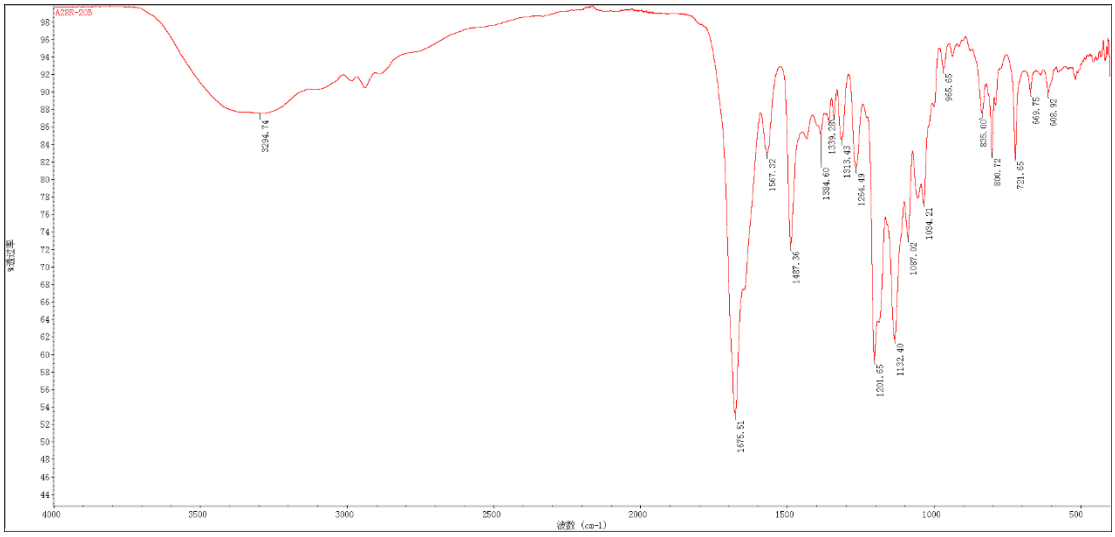


Figure S138. IR spectrum of **14**

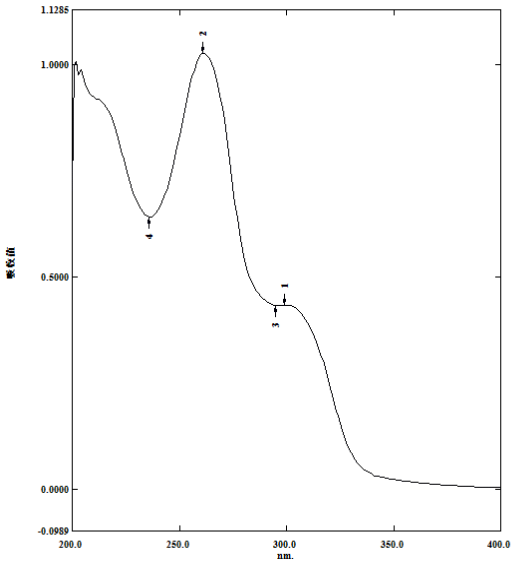


Figure S139. UV spectrum of **14**

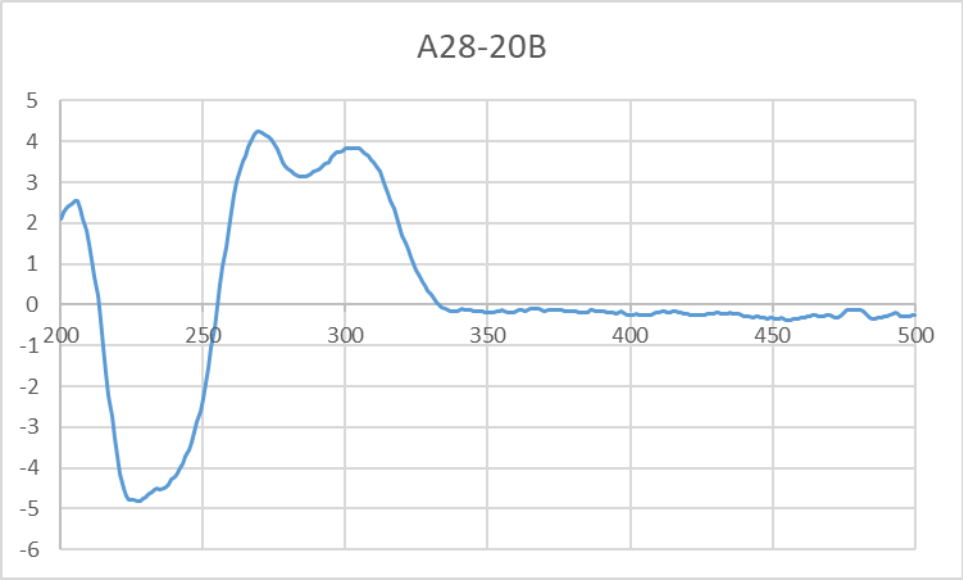


Figure S140. CD spectrum of **14**

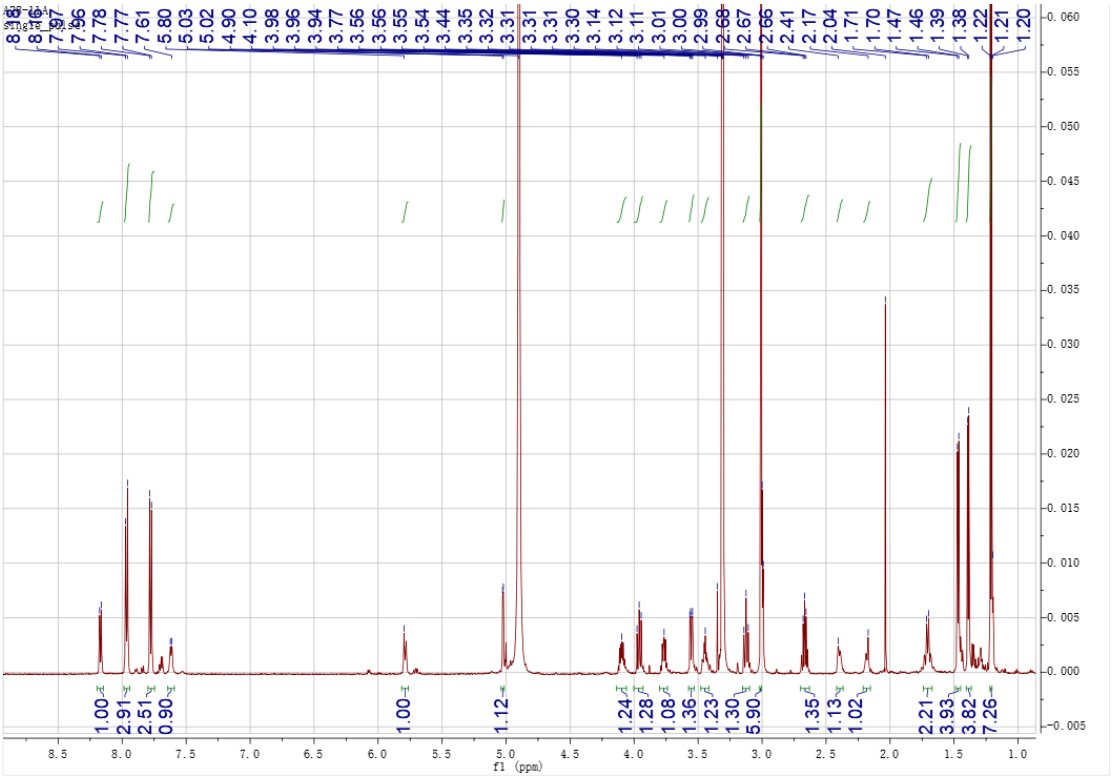


Figure S141. ^{1}H NMR spectrum of **15**

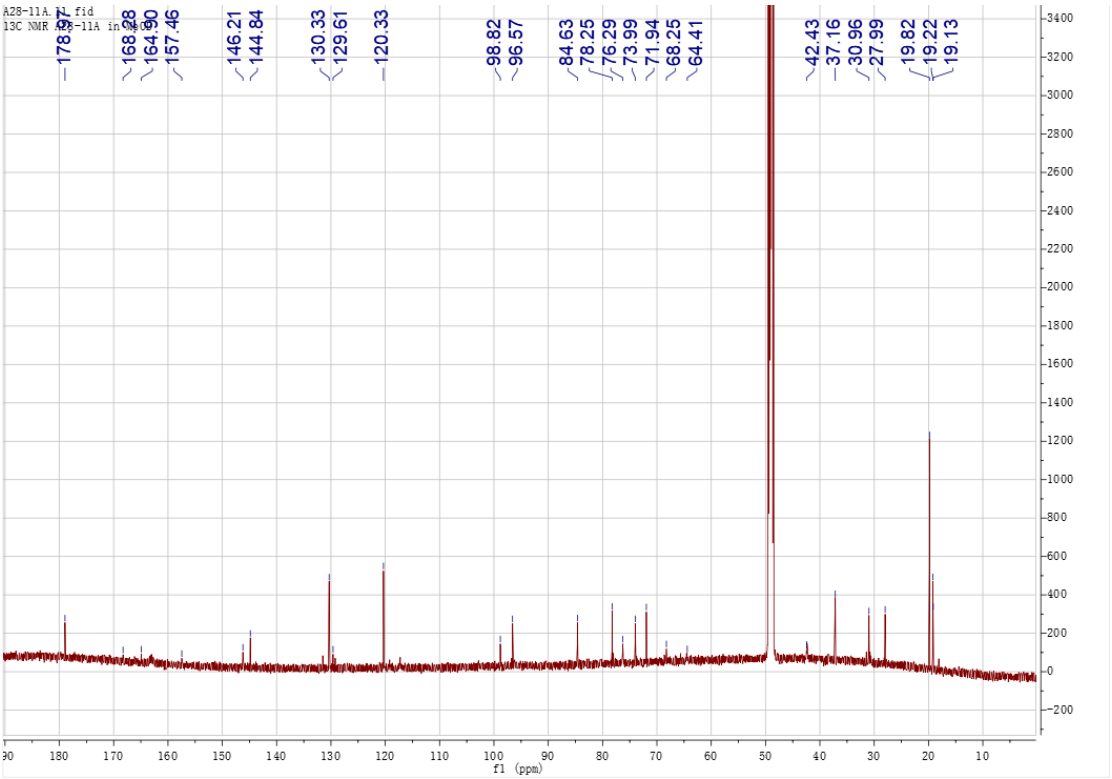


Figure S142. ^{13}C NMR spectrum of **15**

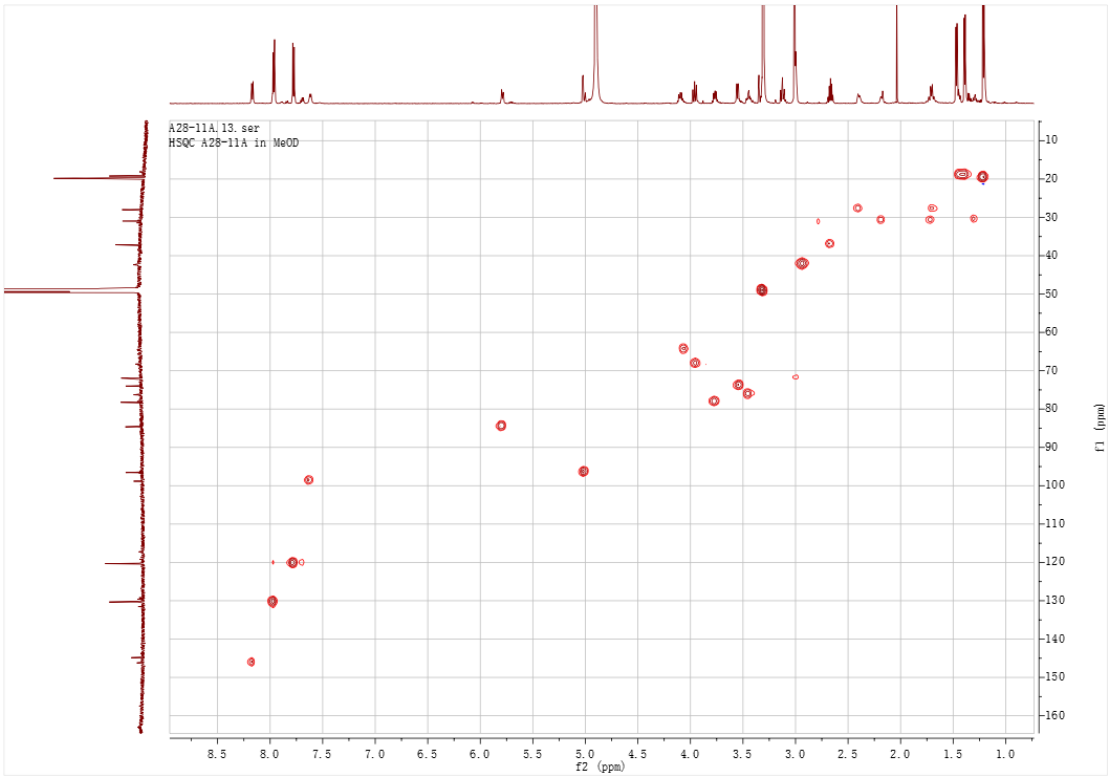


Figure S143. HSQC spectrum of **15**

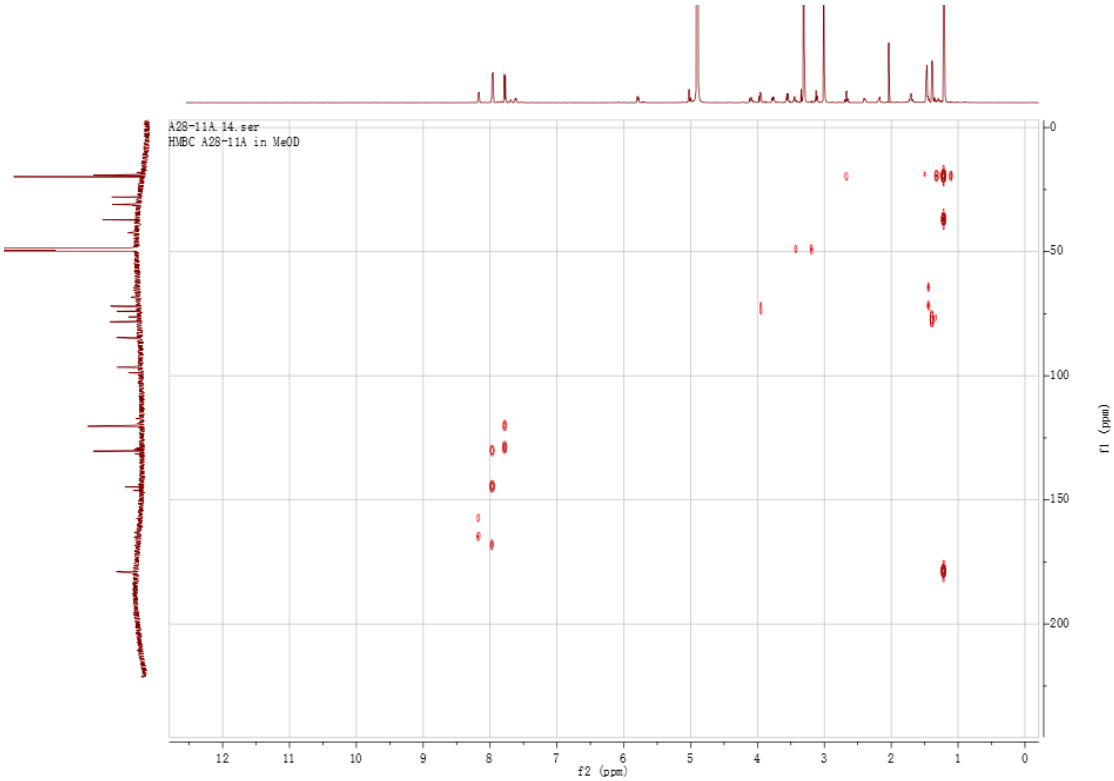


Figure S144. HMBC spectrum of **15**

Figure S145. ^{1}H-^{1}H COSY spectrum of **15**

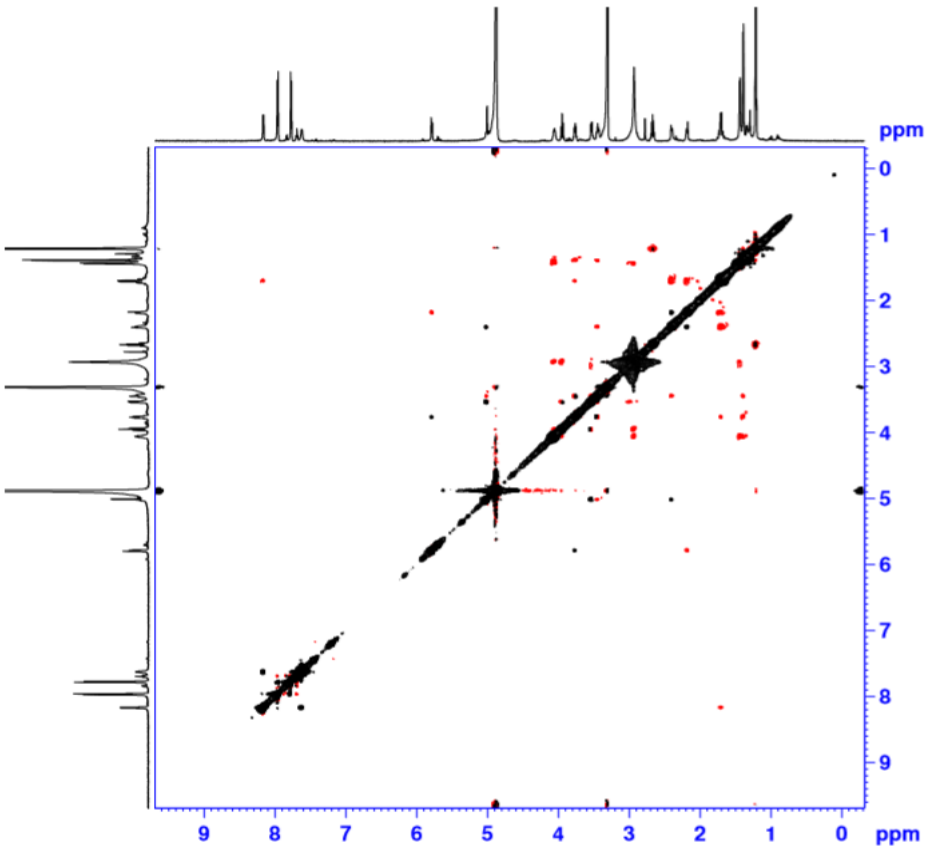


Figure S146. NOESY spectrum of **15**

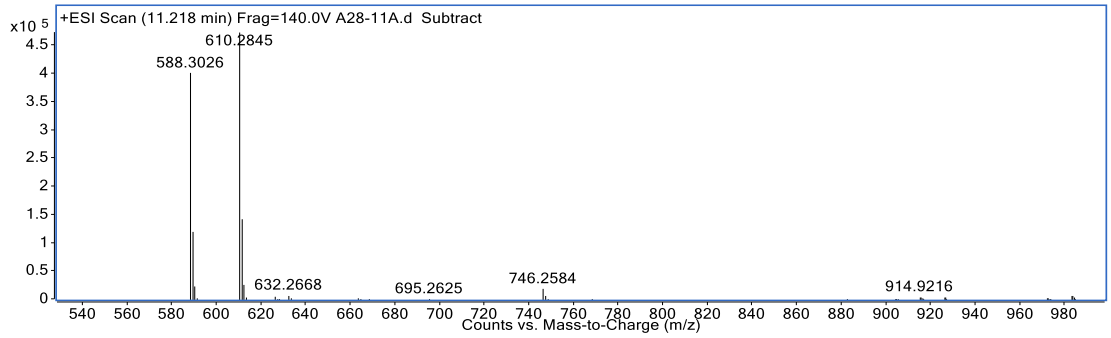


Figure S147. HRESIMS spectrum of **15**

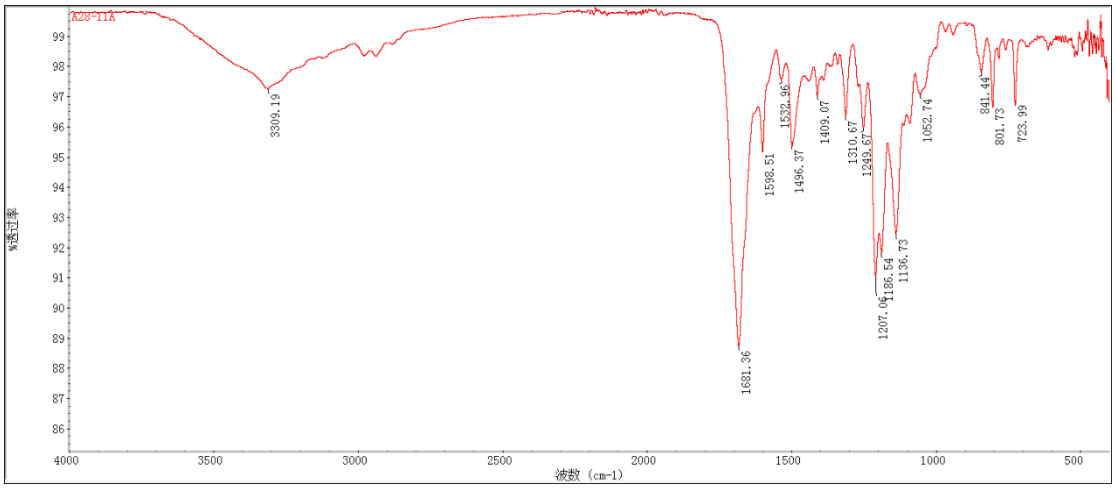


Figure S148. IR spectrum of **15**

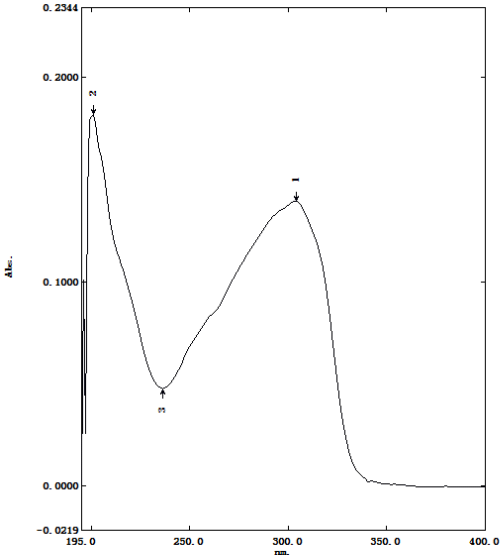


Figure S149. UV spectrum of **15**

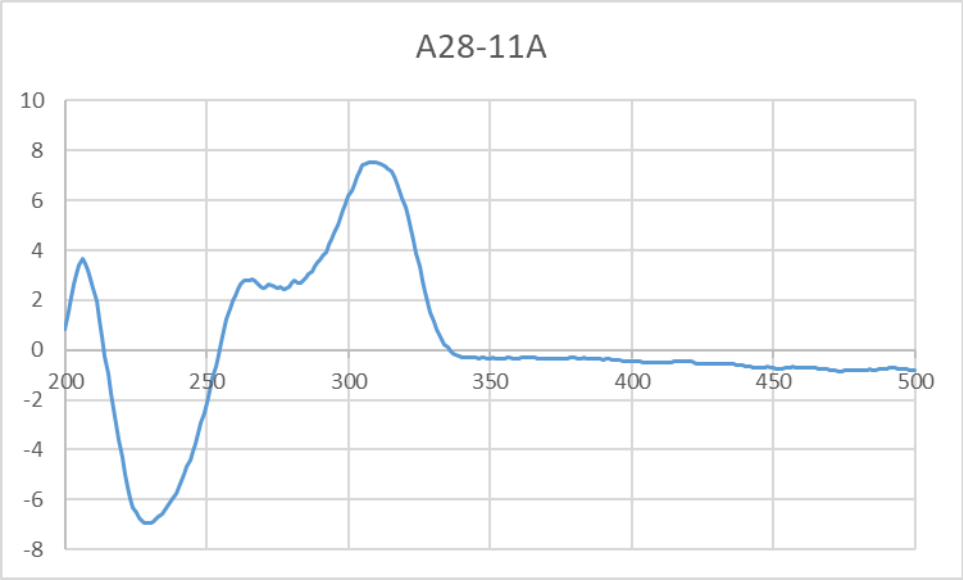


Figure S150. CD spectrum of **15**

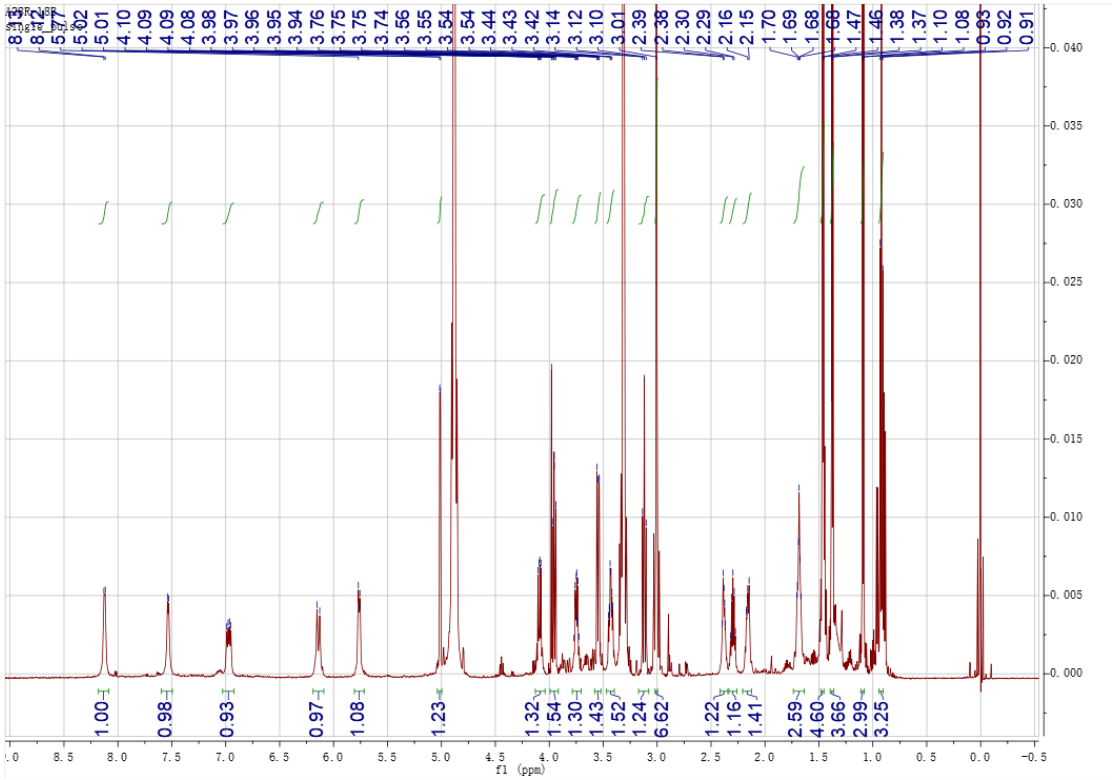


Figure S151. ^{1}H NMR spectrum of **16**

Figure S152. ^{13}C NMR spectrum of **16**

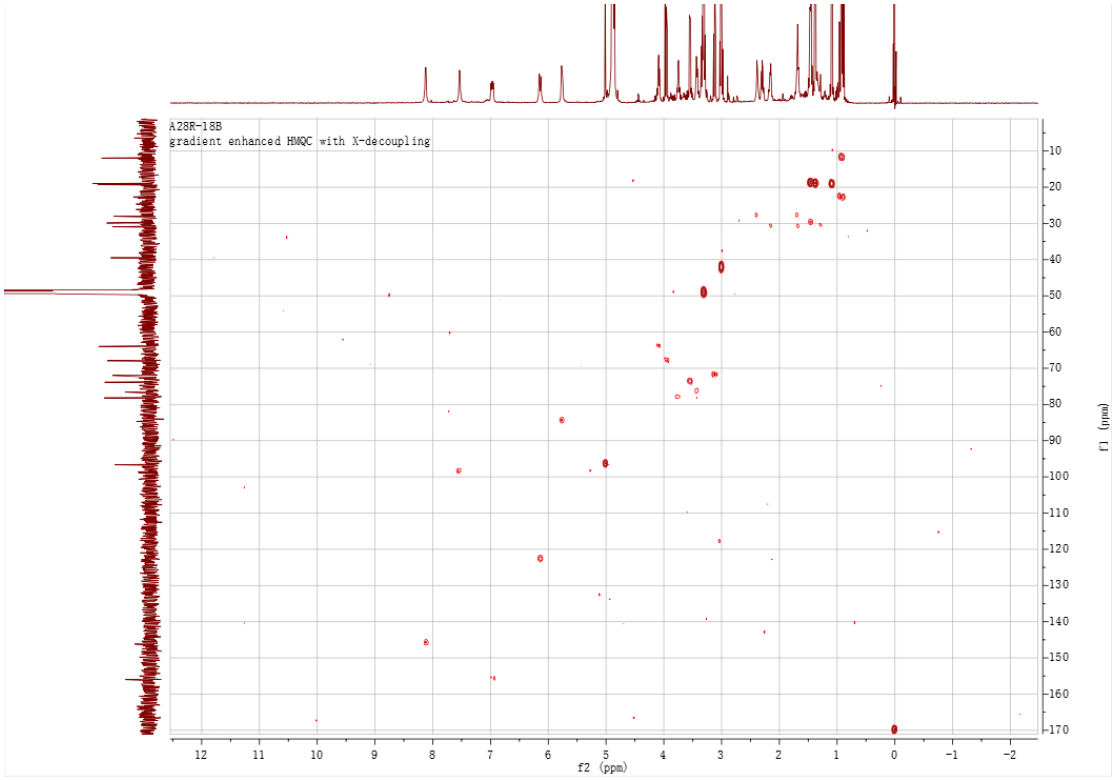


Figure S153. HSQC spectrum of **16**

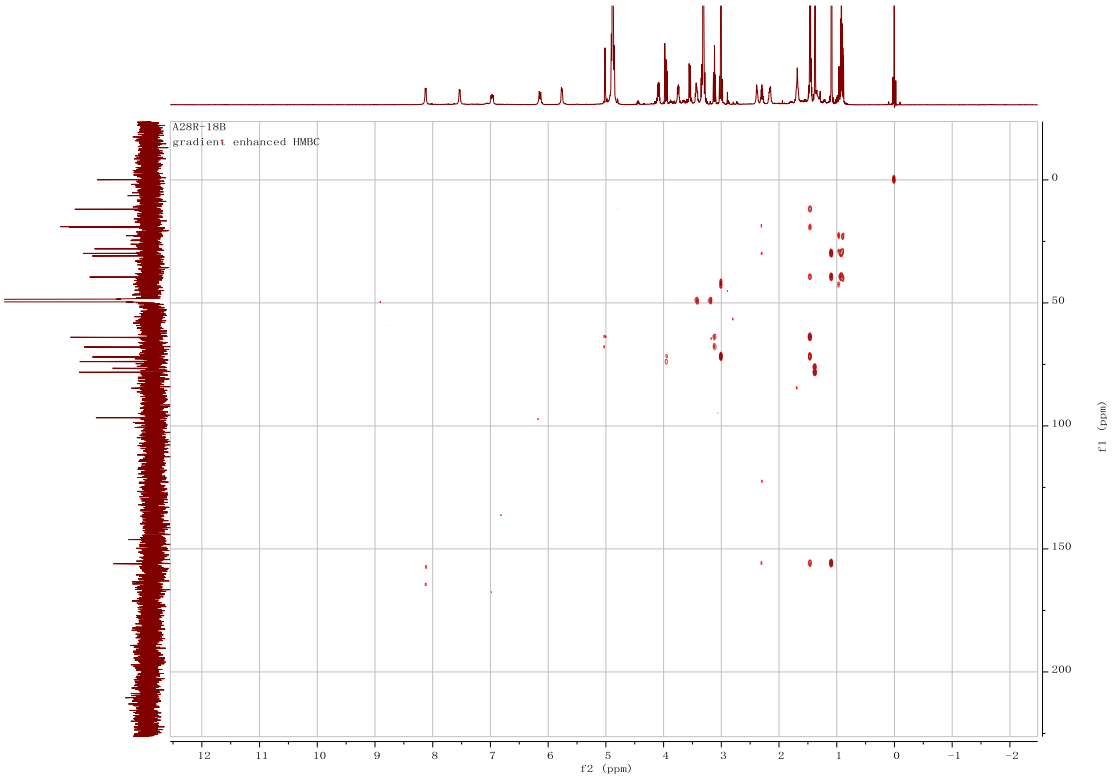


Figure S154. HMBC spectrum of **16**

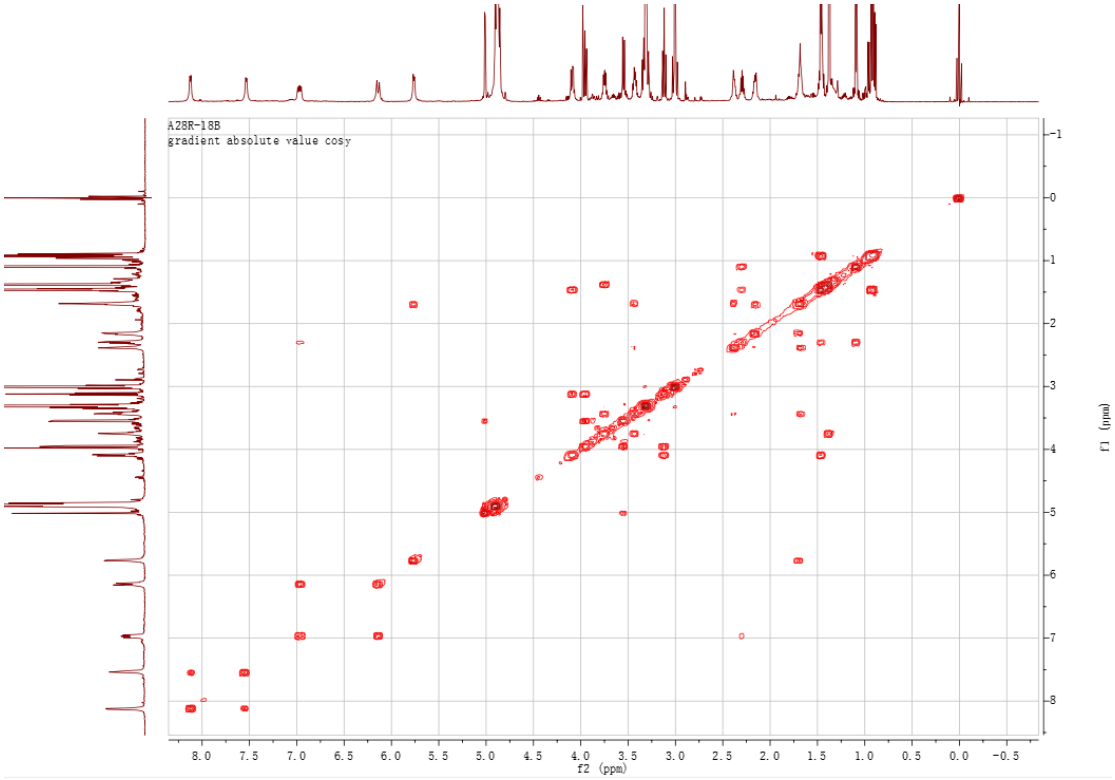


Figure S155. ^{1}H-^{1}H COSY spectrum of **16**

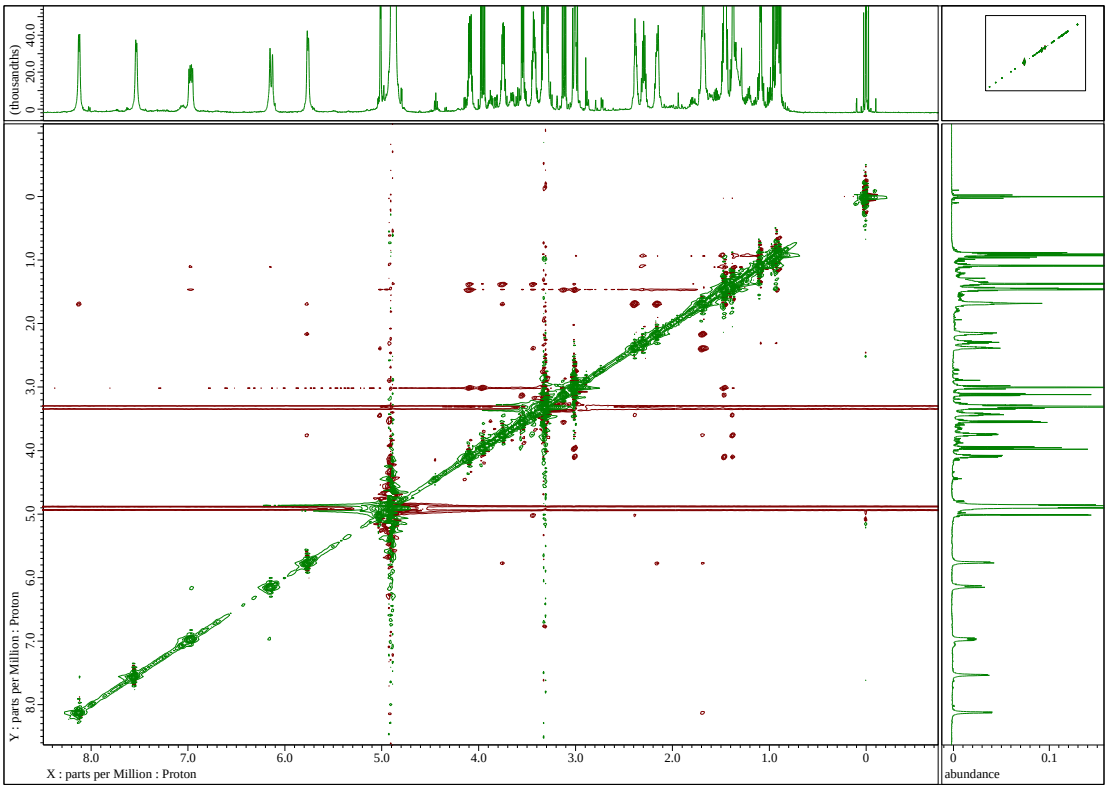


Figure S156. NOESY spectrum of **16**

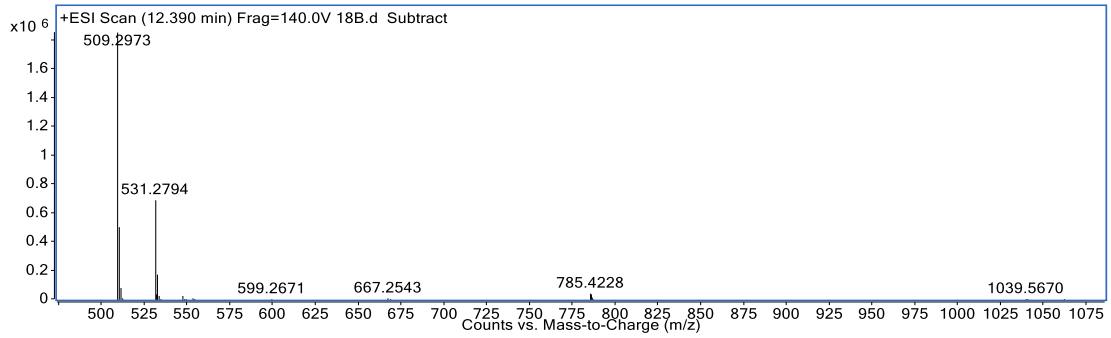


Figure S157. HRESIMS spectrum of **16**

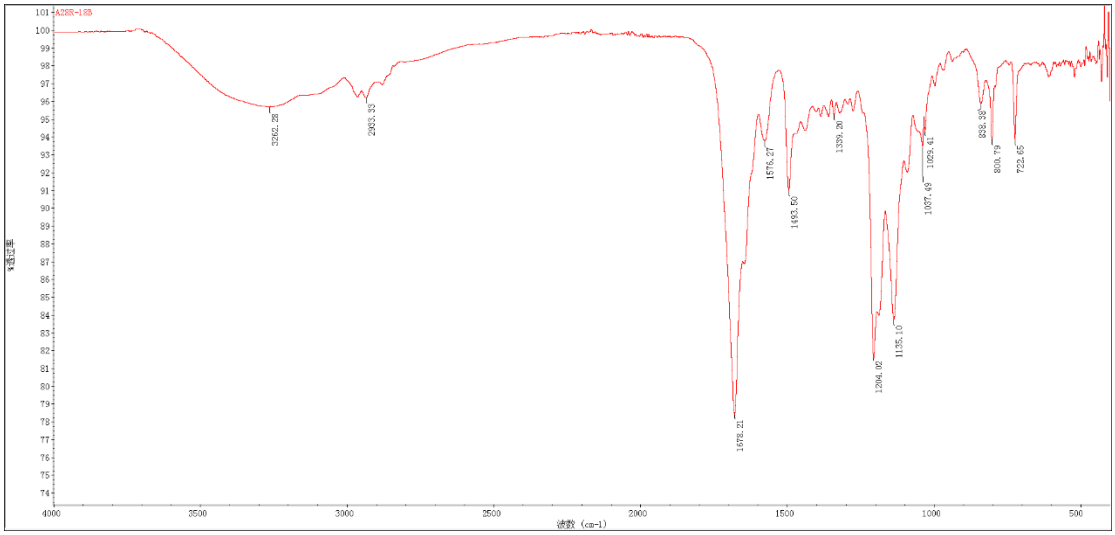


Figure S158. IR spectrum of **16**

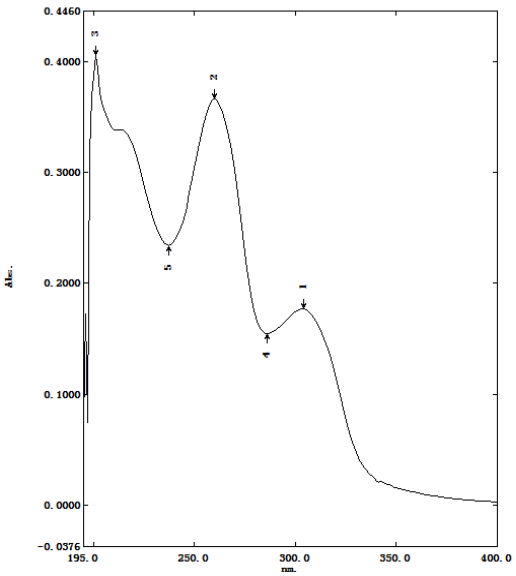


Figure S159. UV spectrum of **16**

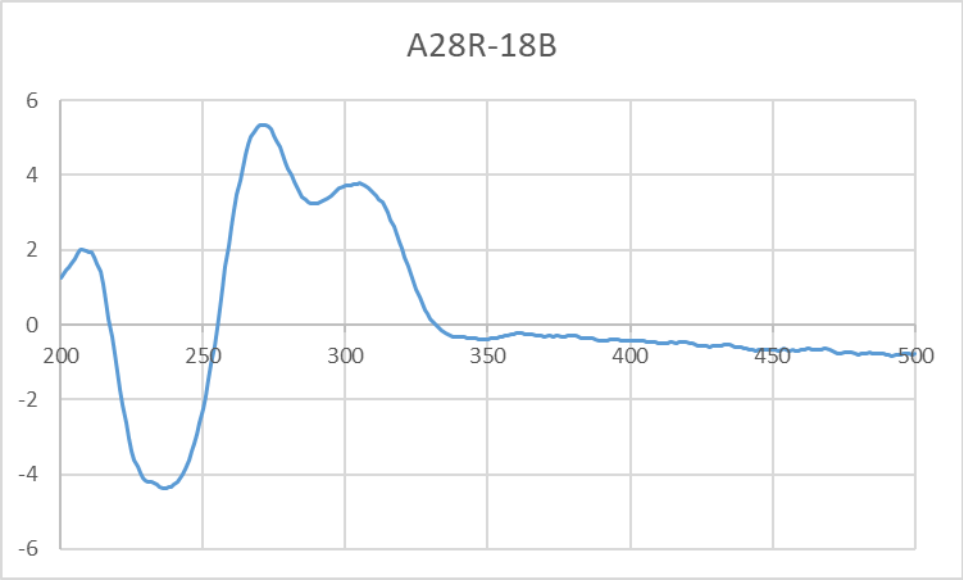


Figure S160. CD spectrum of **16**

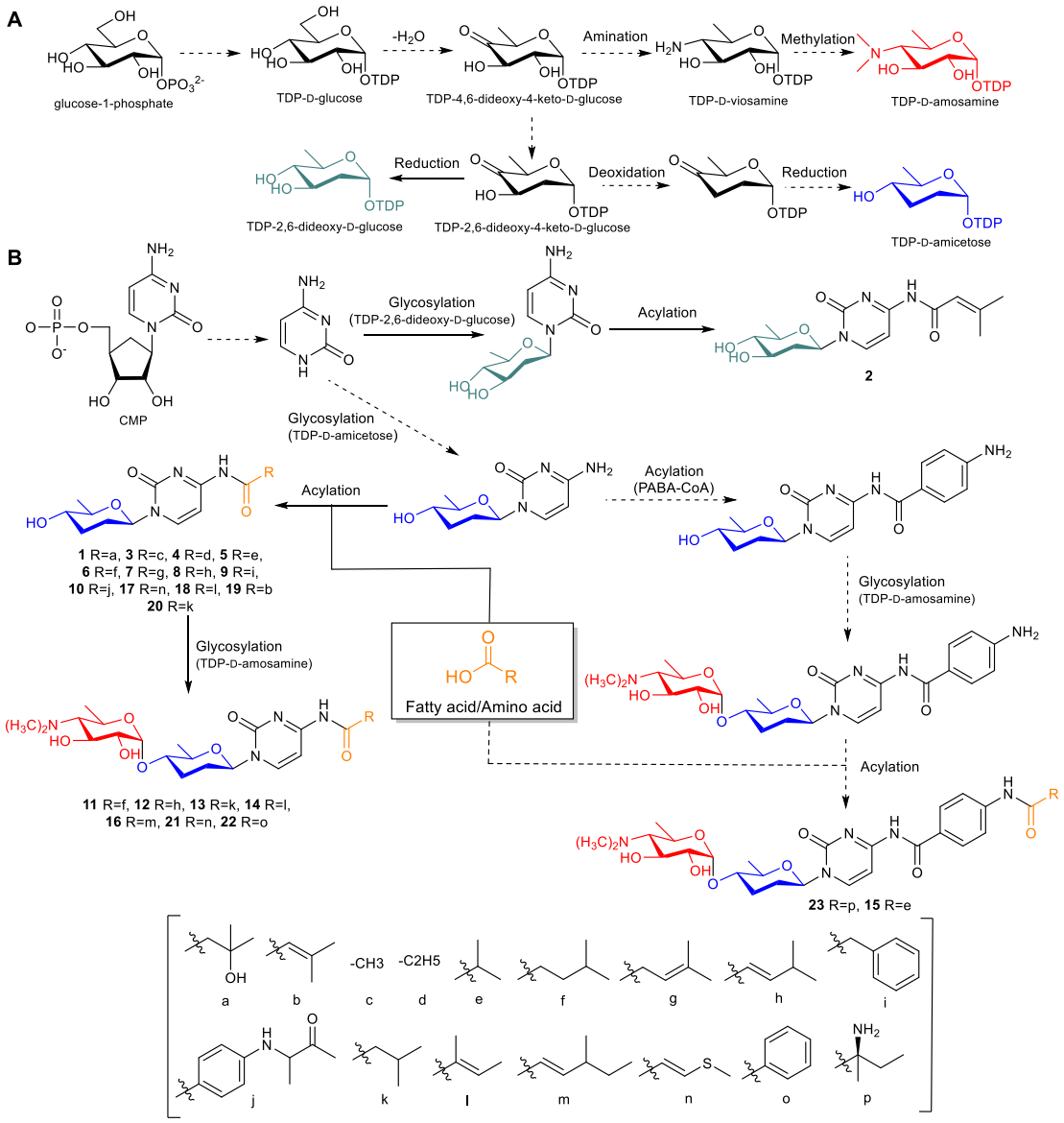


Figure S161. Proposed biosynthesis pathway of isolated compounds. (A) Deoxysugars biosynthesis. (B) Isolated compounds biosynthesis. The dashed-line arrows denote the biosynthesis steps based on the research reported before; The solid-line arrows represent the proposed biosynthesis pathway of isolated compounds.

ECD calculation details

1. Methods

Monte Carlo conformational searches were carried out by means of the Spartan's 10 software using Merck Molecular Force Field (MMFF). The conformers with Boltzmann-population of over 5% were chosen for ECD calculations, and then the conformers were initially optimized at B3LYP/6-31+g (d, p) level in MeOH using the CPCM polarizable conductor calculation model. The theoretical calculation of ECD was conducted in MeOH using Time-dependent Density functional theory (TD-DFT) at the B3LYP/6-311+g (d, p) level for all conformers of compound **1**. Rotatory strengths for a total of 50 excited states were calculated. ECD spectra were generated using the program SpecDis 1.6 (University of Würzburg, Würzburg, Germany) and GraphPad Prism 5 (University of California San Diego, USA) from dipole-length rotational strengths by applying Gaussian band shapes with sigma = 0.3 eV.

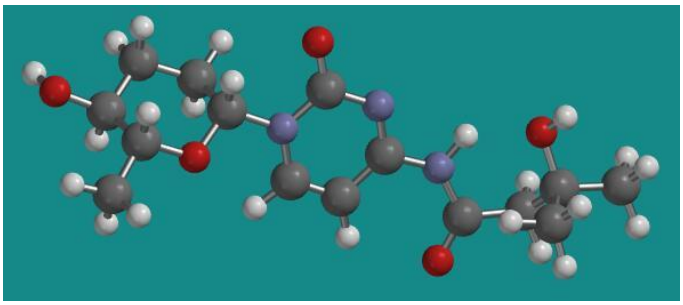
2. Results

Table S1 Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of compound **1**.

Conformers	In MeOH	
	ΔG	P (%)
1	0	35
2	0.21	32.1
3	2.19	10.8
4	3.0	10.4
5	4.51	5.7

[a]B3LYP/6-31+G(d,p), in kcal/mol. [b]From ΔG values at 298.15K.

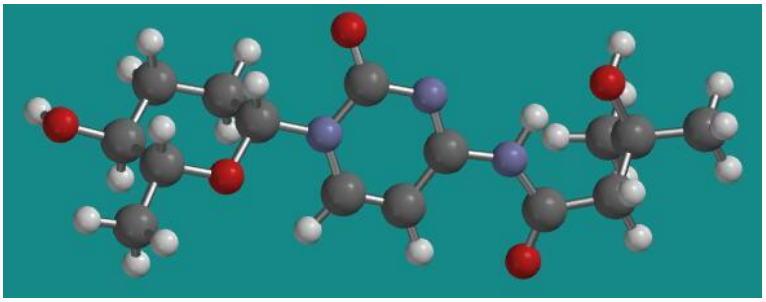
Table S2 Cartesian coordinates for the low-energy reoptimized MMFF conformers of compound **1** at B3LYP/6-311+G(d,p) level of theory in CH_3OH.



Conformer **1**, E(RB3LYP) -1125.9668502

1		Standard Orientation (Ångstroms)			
I	Atom	Type	X	Y	Z
1	7	0	0.872686	1.265504	0.116194
2	6	0	-0.46929	1.474305	0.253836
3	7	0	-1.33596	0.401571	-0.0812
4	6	0	-0.84531	-0.76517	-0.57414

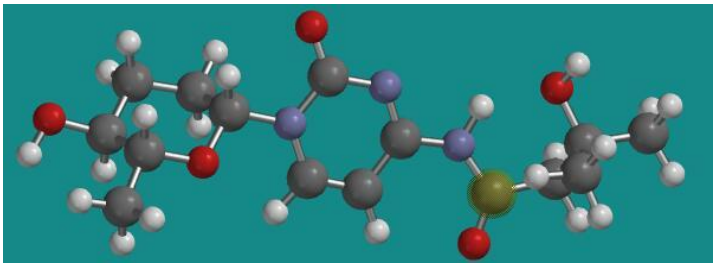
5	6	0	0.496157	-0.96443	-0.73934
6	6	0	1.338057	0.115412	-0.35512
7	6	0	-2.78859	0.582901	0.088695
8	8	0	-0.94884	2.545167	0.651012
9	7	0	2.72189	0.065791	-0.43827
10	6	0	3.544831	-0.96477	-0.85086
11	6	0	5.033153	-0.63264	-0.85211
12	6	0	5.628304	0.060129	0.394087
13	6	0	5.315043	-0.70708	1.685235
14	6	0	7.141413	0.226144	0.206925
15	8	0	5.010056	1.375399	0.434275
16	8	0	-3.28444	-0.64163	0.610999
17	6	0	-4.68902	-0.60007	0.940805
18	6	0	-5.49836	-0.30166	-0.3312
19	6	0	-5.0051	0.989947	-0.99312
20	6	0	-3.48769	0.942663	-1.22372
21	8	0	-6.87172	-0.20442	0.064275
22	8	0	3.128502	-2.05557	-1.23522
23	6	0	-5.02891	-1.93107	1.590496
24	1	0	-1.57885	-1.5263	-0.80802
25	1	0	0.890611	-1.89089	-1.12315
26	1	0	-2.90707	1.38748	0.820824
27	1	0	3.204329	0.898654	-0.09464
28	1	0	5.223262	0.009329	-1.72225
29	1	0	5.553942	-1.5766	-1.02307
30	1	0	5.73931	-1.71515	1.645587
31	1	0	5.75249	-0.19308	2.548039
32	1	0	4.23669	-0.79119	1.849057
33	1	0	7.638149	-0.74765	0.14983
34	1	0	7.568194	0.774157	1.053851
35	1	0	7.356619	0.783242	-0.70985
36	1	0	5.251198	1.815018	1.262531
37	1	0	-4.85644	0.22074	1.656262
38	1	0	-5.3691	-1.14719	-1.02386
39	1	0	-5.52617	1.148889	-1.94413
40	1	0	-5.25919	1.833862	-0.33829
41	1	0	-3.23557	0.186475	-1.97706
42	1	0	-3.11845	1.908177	-1.58378
43	1	0	-7.40642	-0.01996	-0.72048
44	1	0	-4.84541	-2.75681	0.894744
45	1	0	-4.41698	-2.08341	2.484231
46	1	0	-6.08202	-1.94713	1.880928



Conformer **2**, E(RB3LYP) -1125.9668518

2		Standard Orientation (Ångstroms)			
I	Atom	Type	X	Y	Z
1	7	0	0.872025	-1.01944	-0.69624
2	6	0	-0.46385	-1.29865	-0.68006
3	7	0	-1.3355	-0.29785	-0.17769
4	6	0	-0.8474	0.866561	0.322842
5	6	0	0.492287	1.134699	0.333979
6	6	0	1.333425	0.128825	-0.21635
7	6	0	-2.7865	-0.5589	-0.17643
8	8	0	-0.93466	-2.37293	-1.07872
9	7	0	2.71127	0.259129	-0.31036
10	6	0	3.530622	1.29277	0.101957
11	6	0	5.007528	1.106629	-0.22883
12	6	0	5.662644	-0.25394	0.099218
13	6	0	7.157082	-0.18975	-0.23893
14	6	0	5.445634	-0.65879	1.562968
15	8	0	5.018428	-1.21273	-0.78381
16	8	0	-3.41255	0.668669	-0.52105
17	6	0	-4.84458	0.564184	-0.67064
18	6	0	-5.46249	0.104495	0.660566
19	6	0	-4.81346	-1.19978	1.136435
20	6	0	-3.28449	-1.06687	1.17749
21	8	0	-6.86768	-0.05395	0.430835
22	8	0	3.116779	2.310791	0.652725
23	6	0	-5.33823	1.922002	-1.14109
24	1	0	-1.58387	1.56861	0.692492
25	1	0	0.884304	2.058852	0.725788
26	1	0	-2.95855	-1.30867	-0.95494
27	1	0	3.194987	-0.55123	-0.70232
28	1	0	5.539697	1.899095	0.30045
29	1	0	5.126967	1.292306	-1.30422
30	1	0	7.669835	0.542846	0.392366

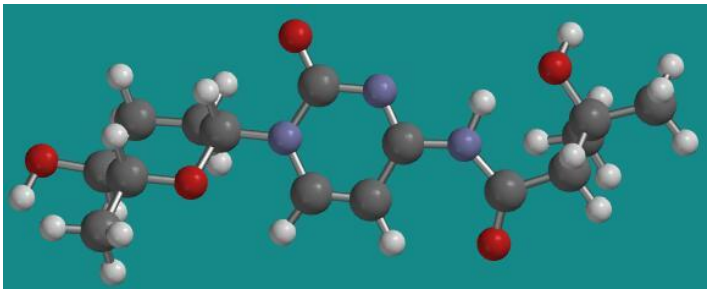
31	1	0	7.625213	-1.1658	-0.07235
32	1	0	7.302306	0.089022	-1.28699
33	1	0	5.922235	-1.62396	1.766245
34	1	0	4.381165	-0.74751	1.799156
35	1	0	5.889548	0.081635	2.235781
36	1	0	5.304283	-2.10694	-0.54686
37	1	0	-5.06118	-0.19976	-1.43429
38	1	0	-5.2943	0.896793	1.405701
39	1	0	-5.19524	-1.47075	2.127339
40	1	0	-5.10246	-2.00324	0.446346
41	1	0	-2.98014	-0.35523	1.954524
42	1	0	-2.81551	-2.02964	1.403486
43	1	0	-7.28832	-0.31879	1.260636
44	1	0	-6.41877	1.892236	-1.29919
45	1	0	-5.11475	2.69183	-0.39477
46	1	0	-4.85404	2.195654	-2.08293



Conformer **3**, E(RB3LYP) -1125.967008

3		Standard Orientation (Ångstroms)			
I	Atom	Type	X	Y	Z
1	7	0	0.87372	1.261917	0.116196
2	6	0	-0.46819	1.470419	0.254324
3	7	0	-1.33468	0.3965	-0.07704
4	6	0	-0.84419	-0.77104	-0.56797
5	6	0	0.49733	-0.97017	-0.73372
6	6	0	1.339135	0.110839	-0.35274
7	6	0	-2.78724	0.57949	0.09313
8	8	0	-0.94814	2.542031	0.649109
9	7	0	2.722938	0.061796	-0.43702
10	6	0	3.546269	-0.96983	-0.84599
11	6	0	5.034346	-0.63649	-0.85012
12	6	0	5.630136	0.062825	0.392126
13	6	0	5.319071	-0.69859	1.687238
14	6	0	7.142856	0.229632	0.202549

15	8	0	5.010533	1.377635	0.426697
16	8	0	-3.28735	-0.64716	0.605596
17	6	0	-4.69344	-0.59507	0.932546
18	6	0	-5.50393	-0.28585	-0.34285
19	6	0	-5.00191	1.000539	-0.99723
20	6	0	-3.48368	0.951347	-1.21724
21	8	0	-6.891	-0.09526	-0.03664
22	8	0	3.130419	-2.0626	-1.22528
23	6	0	-5.03748	-1.92561	1.583072
24	1	0	-1.57778	-1.53274	-0.79983
25	1	0	0.891805	-1.89735	-1.11576
26	1	0	-2.90447	1.378616	0.831512
27	1	0	3.20504	0.896369	-0.09707
28	1	0	5.223101	0.001414	-1.72354
29	1	0	5.55578	-1.58082	-1.01701
30	1	0	5.744349	-1.7064	1.651898
31	1	0	5.756903	-0.18011	2.54716
32	1	0	4.240979	-0.78305	1.852607
33	1	0	7.640686	-0.74384	0.149786
34	1	0	7.569897	0.782361	1.046284
35	1	0	7.356481	0.782416	-0.71721
36	1	0	5.252524	1.821763	1.252301
37	1	0	-4.85683	0.225886	1.648619
38	1	0	-5.38602	-1.12789	-1.04039
39	1	0	-5.52092	1.158614	-1.94779
40	1	0	-5.25897	1.844252	-0.34294
41	1	0	-3.22952	0.200877	-1.97572
42	1	0	-3.11122	1.919017	-1.56799
43	1	0	-7.30624	-0.95478	0.115167
44	1	0	-4.88771	-2.75199	0.879906
45	1	0	-4.40315	-2.09235	2.458226
46	1	0	-6.07876	-1.93361	1.918173

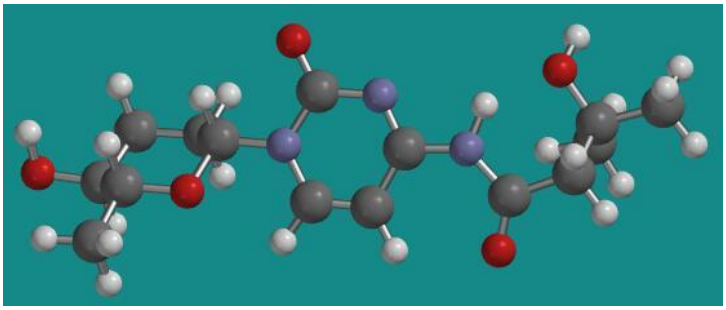


Conformer **4**, E(RB3LYP) -1125.9669817

4	Standard Orientation

		(Ångstroms)			
I	Atom	Type	X	Y	Z
1	7	0	0.873046	-1.01547	-0.70145
2	6	0	-0.46299	-1.29373	-0.68592
3	7	0	-1.33446	-0.29162	-0.18596
4	6	0	-0.84625	0.873627	0.312306
5	6	0	0.493633	1.14117	0.323603
6	6	0	1.334715	0.133401	-0.22323
7	6	0	-2.78526	-0.55463	-0.18225
8	8	0	-0.9343	-2.36838	-1.08309
9	7	0	2.712894	0.261942	-0.31513
10	6	0	3.532947	1.294813	0.097584
11	6	0	5.01047	1.105099	-0.22847
12	6	0	5.661898	-0.25607	0.104536
13	6	0	7.15751	-0.19549	-0.22907
14	6	0	5.439516	-0.65748	1.568418
15	8	0	5.018617	-1.21548	-0.7785
16	8	0	-3.41547	0.67318	-0.51699
17	6	0	-4.84822	0.556526	-0.66155
18	6	0	-5.46321	0.089167	0.674573
19	6	0	-4.80562	-1.2075	1.144304
20	6	0	-3.27715	-1.0722	1.170315
21	8	0	-6.86552	-0.17018	0.529735
22	8	0	3.119417	2.314656	0.645233
23	6	0	-5.34851	1.91173	-1.13513
24	1	0	-1.58271	1.576608	0.68021
25	1	0	0.885825	2.06602	0.713605
26	1	0	-2.95844	-1.29953	-0.96526
27	1	0	3.196237	-0.55007	-0.70409
28	1	0	5.542647	1.897664	0.300657
29	1	0	5.133501	1.288135	-1.30391
30	1	0	7.669766	0.537274	0.402439
31	1	0	7.623118	-1.17217	-0.05915
32	1	0	7.306532	0.081018	-1.27719
33	1	0	5.913728	-1.6231	1.775155
34	1	0	4.374144	-0.7438	1.801372
35	1	0	5.882635	0.083525	2.24111
36	1	0	5.301826	-2.10974	-0.53861
37	1	0	-5.06205	-0.20991	-1.42333
38	1	0	-5.30385	0.878413	1.423617
39	1	0	-5.18269	-1.47397	2.136637
40	1	0	-5.09963	-2.01343	0.45884
41	1	0	-2.96746	-0.36541	1.949764

42	1	0	-2.80588	-2.03596	1.38694
43	1	0	-7.34735	0.667675	0.526078
44	1	0	-5.15278	2.682389	-0.38177
45	1	0	-4.84653	2.195779	-2.06431
46	1	0	-6.42388	1.877616	-1.33207



Conformer **5**, E(RB3LYP) -1125.96681310

5		Standard Orientation (Ångstroms)			
I	Atom	Type	X	Y	Z
1	7	0	0.870213	-1.01505	-0.69359
2	6	0	-0.46622	-1.29083	-0.67563
3	7	0	-1.33511	-0.28639	-0.17578
4	6	0	-0.84402	0.878345	0.32099
5	6	0	0.496396	1.143155	0.330383
6	6	0	1.334735	0.133523	-0.21735
7	6	0	-2.78648	-0.5456	-0.17241
8	8	0	-0.94027	-2.36508	-1.07066
9	7	0	2.712828	0.259858	-0.31251
10	6	0	3.535392	1.292064	0.096953
11	6	0	5.011692	1.100384	-0.23346
12	6	0	5.662377	-0.26172	0.097102
13	6	0	7.15694	-0.20312	-0.24149
14	6	0	5.444358	-0.66306	1.56166
15	8	0	5.01483	-1.22011	-0.78394
16	8	0	-3.41317	0.683287	-0.50915
17	6	0	-4.84595	0.574491	-0.66264
18	6	0	-5.47294	0.093352	0.66277
19	6	0	-4.80954	-1.20065	1.144785
20	6	0	-3.28109	-1.05925	1.18054
21	8	0	-6.89195	-0.05061	0.538142
22	8	0	3.124722	2.312834	0.644982
23	6	0	-5.34437	1.936652	-1.11485
24	1	0	-1.57859	1.583169	0.68915

25	1	0	0.890944	2.067524	0.719147
26	1	0	-2.96079	-1.29188	-0.95394
27	1	0	3.194044	-0.55302	-0.70236
28	1	0	5.546494	1.892107	0.294285
29	1	0	5.131674	1.283667	-1.3092
30	1	0	7.672259	0.528993	0.388262
31	1	0	7.621887	-1.18038	-0.07308
32	1	0	7.302854	0.07312	-1.29012
33	1	0	5.890854	0.077174	2.232971
34	1	0	5.917811	-1.62942	1.766653
35	1	0	4.379658	-0.74784	1.798238
36	1	0	5.298505	-2.11474	-0.54592
37	1	0	-5.0523	-0.17733	-1.4428
38	1	0	-5.33273	0.882722	1.410693
39	1	0	-5.19363	-1.46618	2.134744
40	1	0	-5.08541	-2.01716	0.461741
41	1	0	-2.98018	-0.34693	1.958248
42	1	0	-2.80662	-2.01976	1.404713
43	1	0	-7.08245	-0.83026	-0.00434
44	1	0	-5.1154	2.698142	-0.36161
45	1	0	-4.86909	2.222218	-2.05765
46	1	0	-6.42645	1.90811	-1.26375