Supporting Information

Penicilazaphilones D and E: Two New Azaphilones from a Sponge-Derived Strain of the Fungus *Penicillium sclerotiorum*

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List of Supporting Information

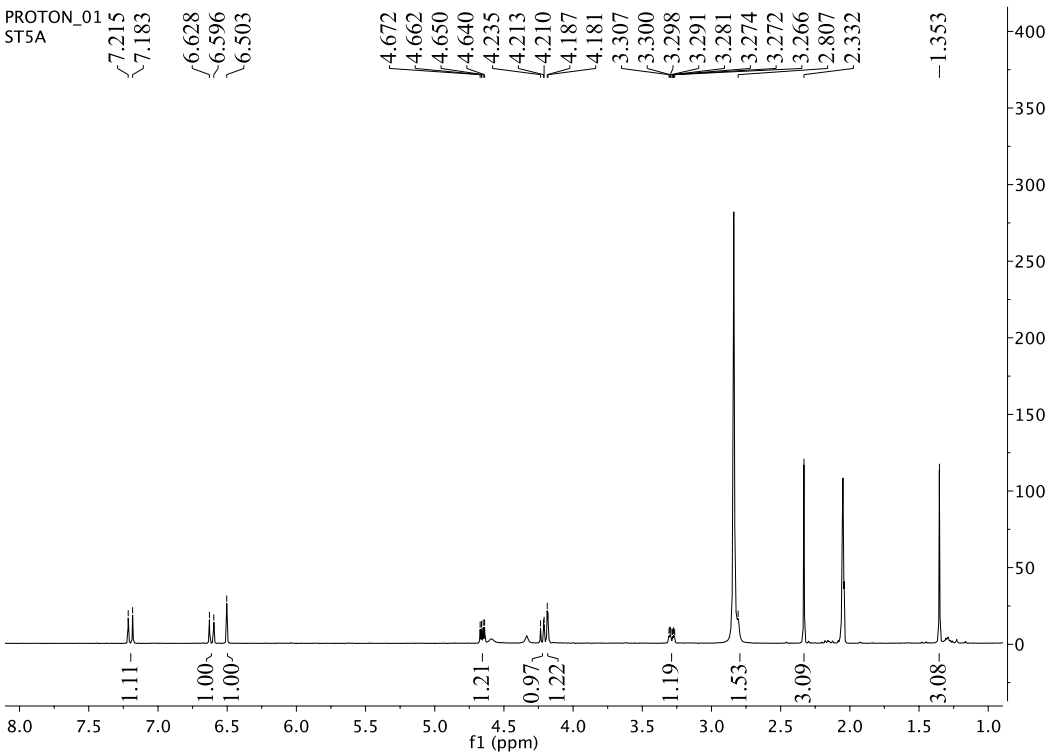

Figure S1. ^{1}H NMR (500 MHz, acetone-d_6) spectrum of compound **1**

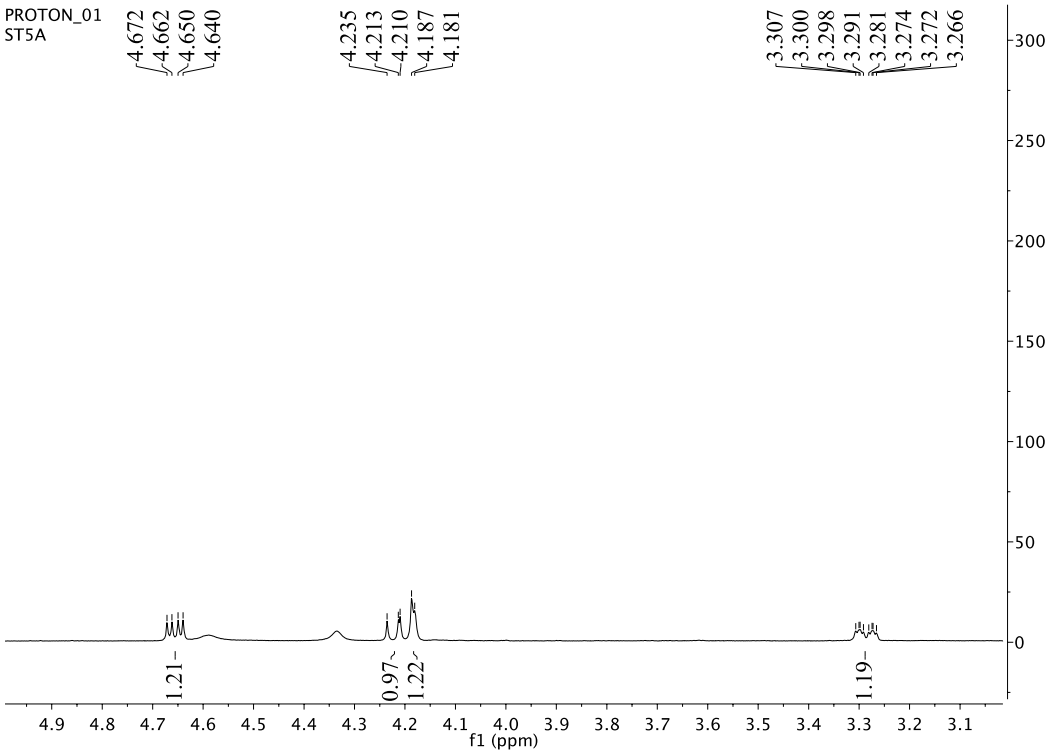

Figure S2. Partial ^{1}H NMR (500 MHz, acetone-d_6) spectrum of compound **1**

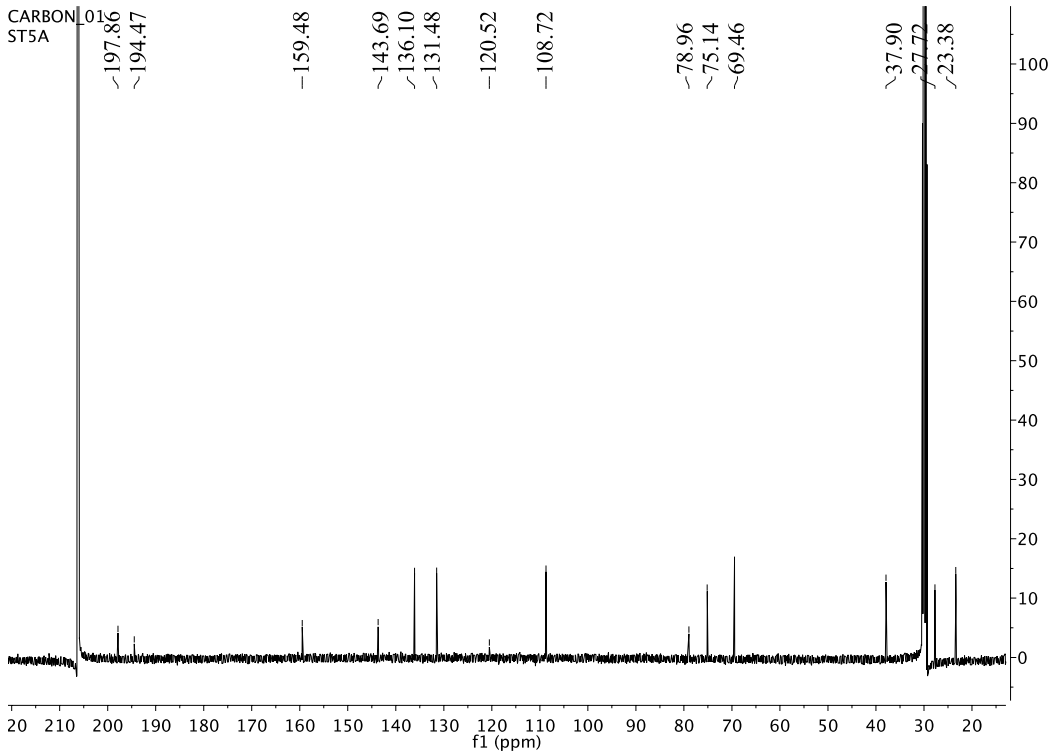

Figure S3. ^{13}C NMR (125 MHz, acetone-d_6) spectrum of compound **1**

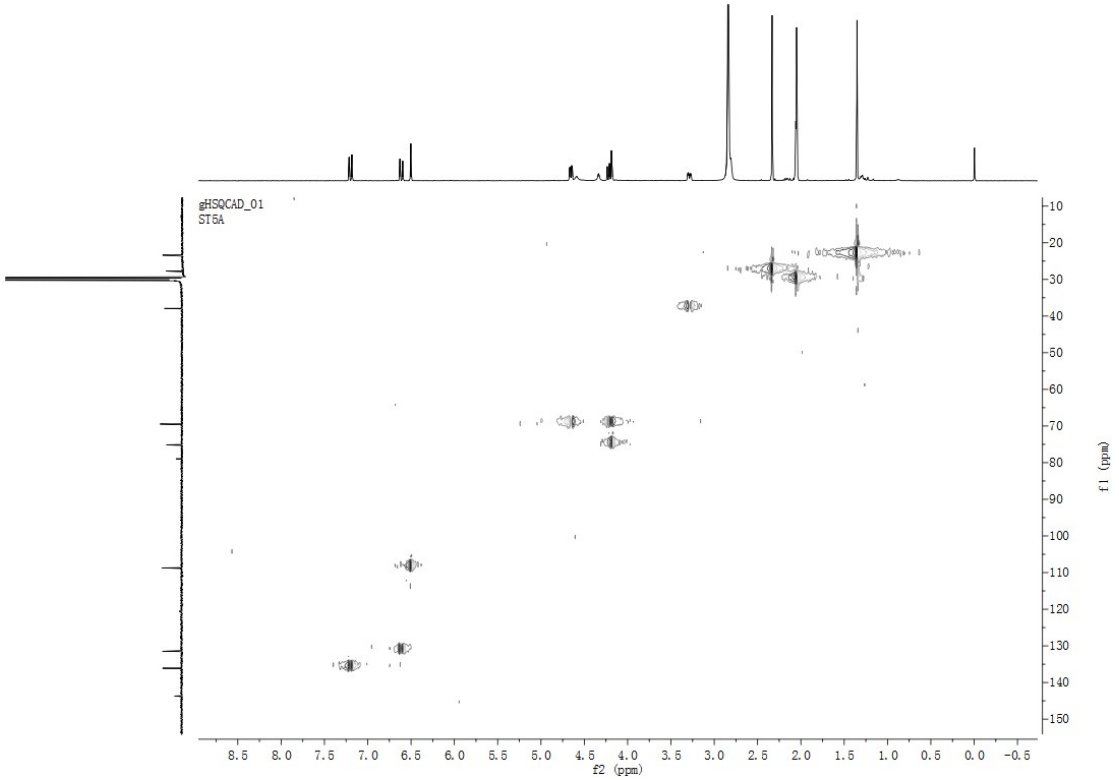

Figure S4. HMQC (acetone-d_6) spectrum of compound **1**

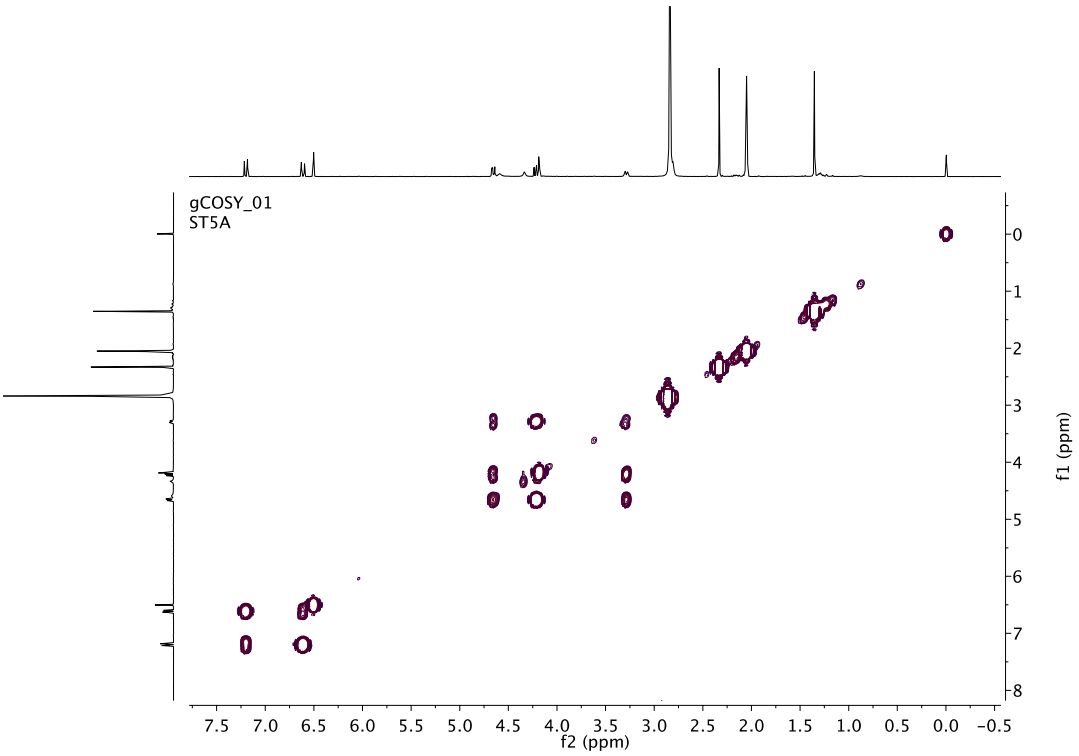

Figure S5. ^{1}H-^{1}H COSY (acetone-d_6) spectrum of compound **1**

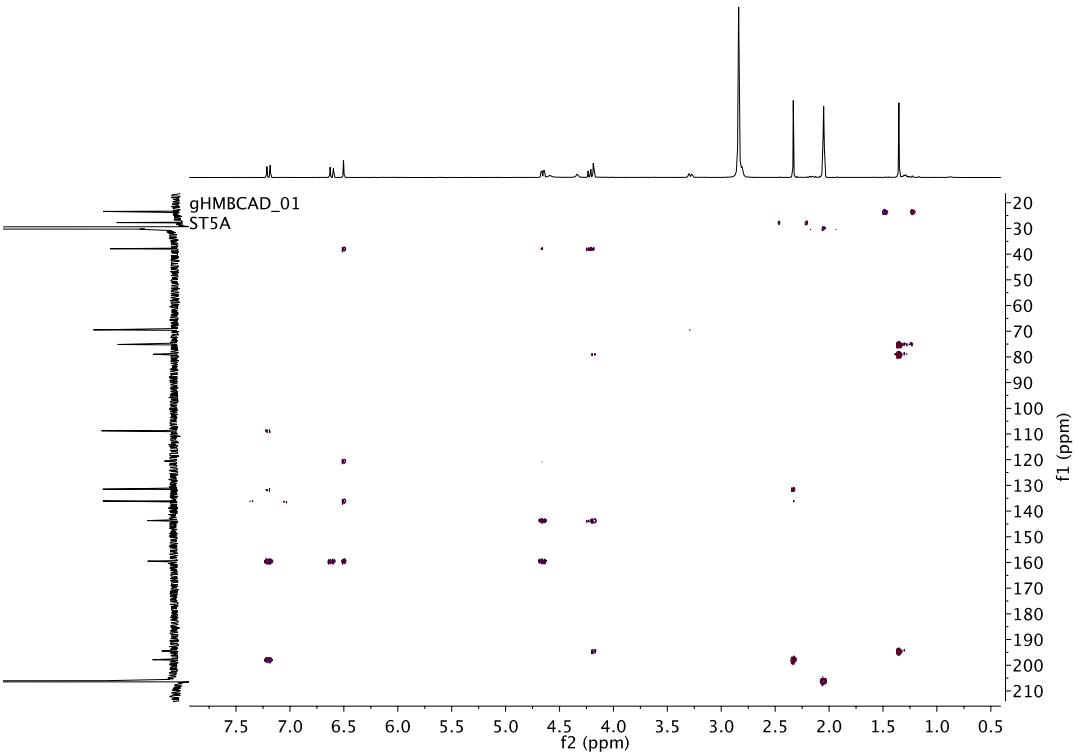

Figure S6. HMBC (acetone-d_6) spectrum of compound **1**

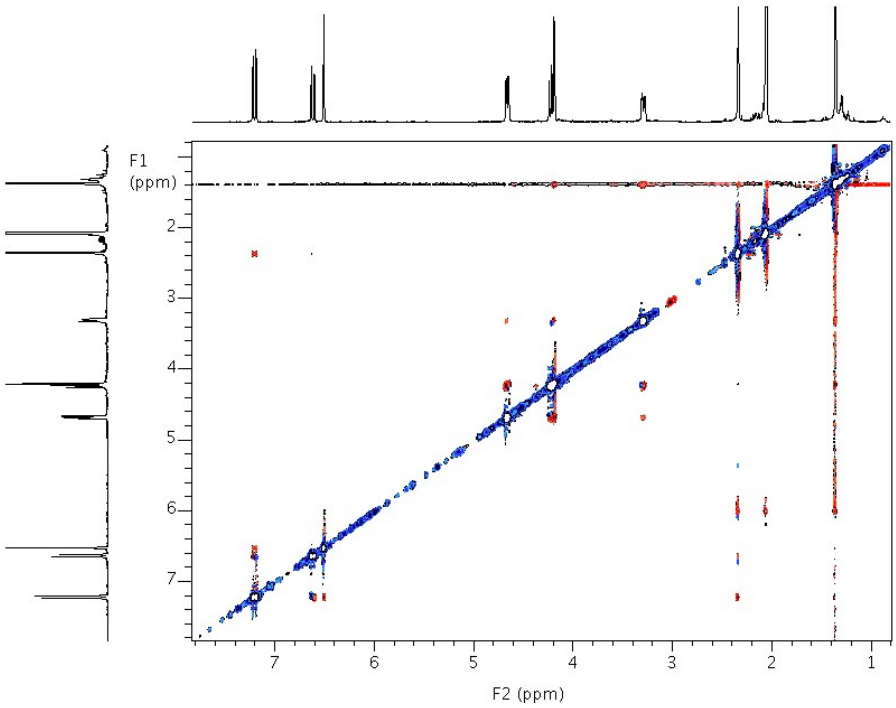

Figure S7. NOESY (acetone-d_6) spectrum of compound **1**

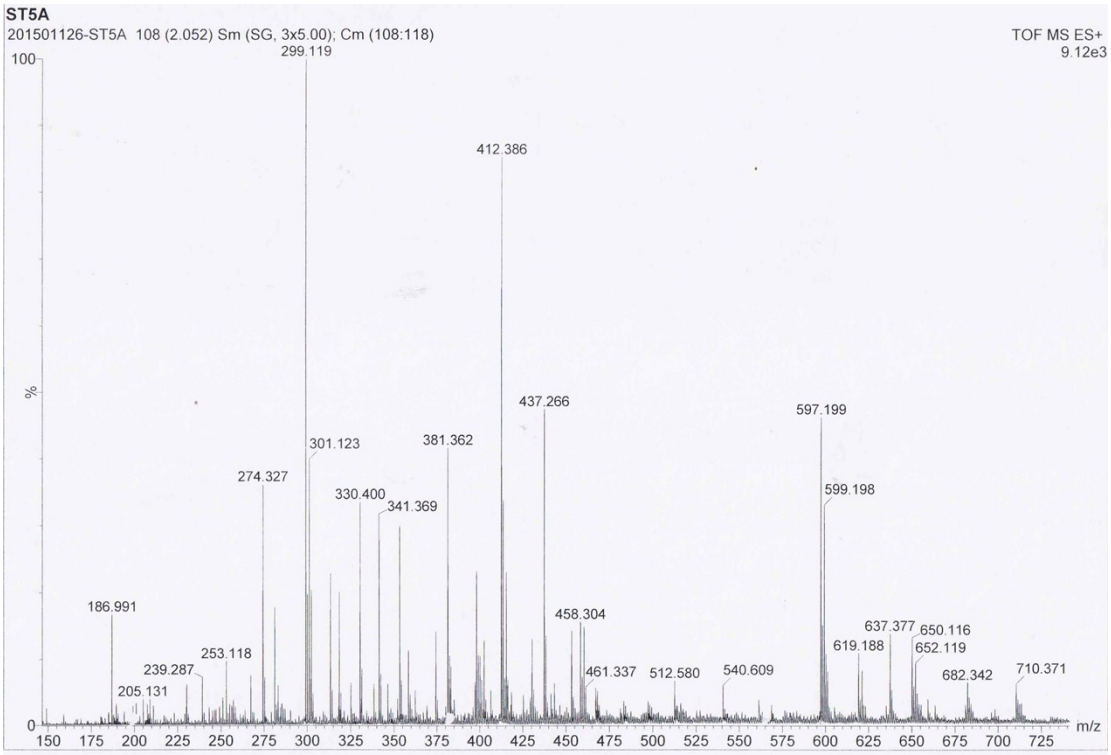

Figure S8. ESIMS spectrum of compound **1**

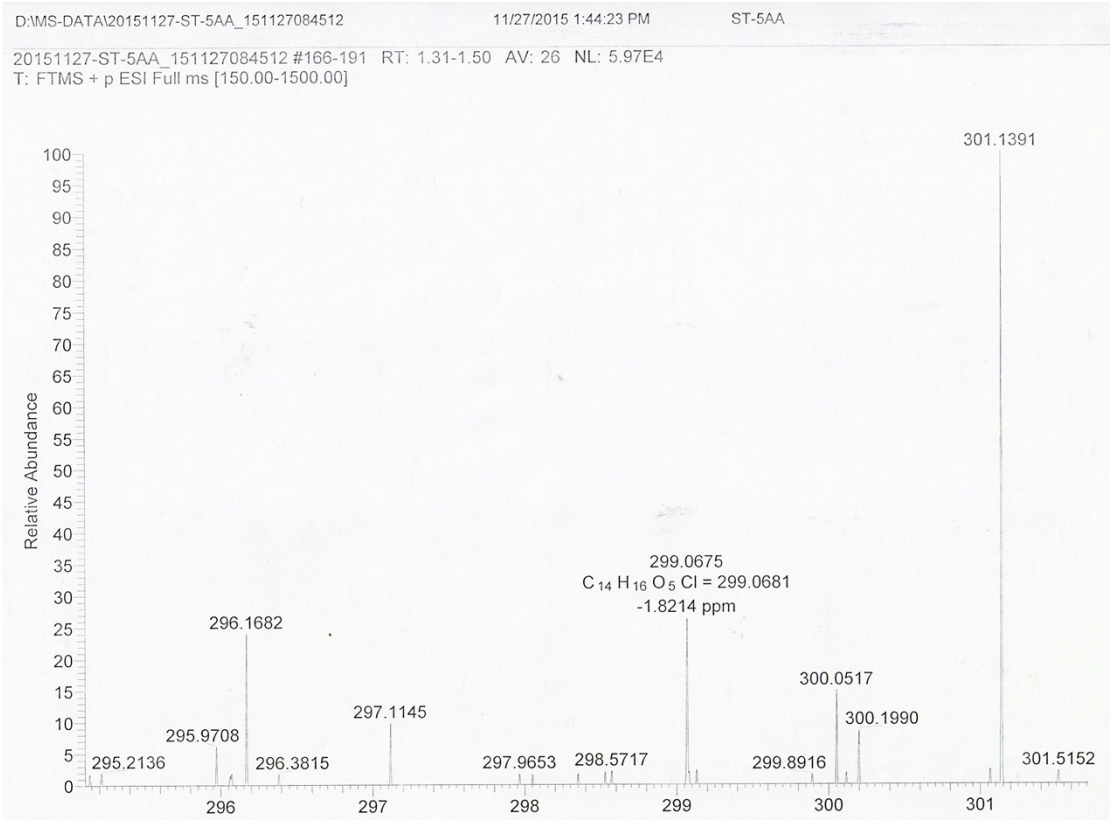

Figure S9. HRESIMS spectrum of compound **1**

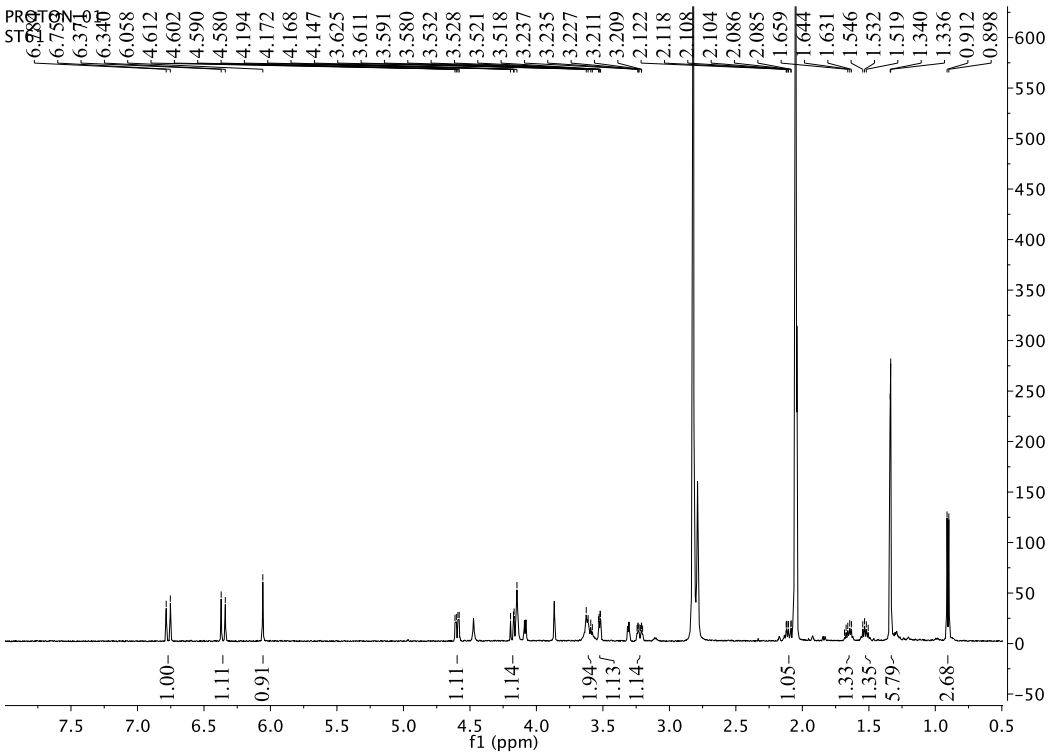

Figure S10. ^{1}H NMR (500 MHz, acetone-d_6) spectrum of compound **2**

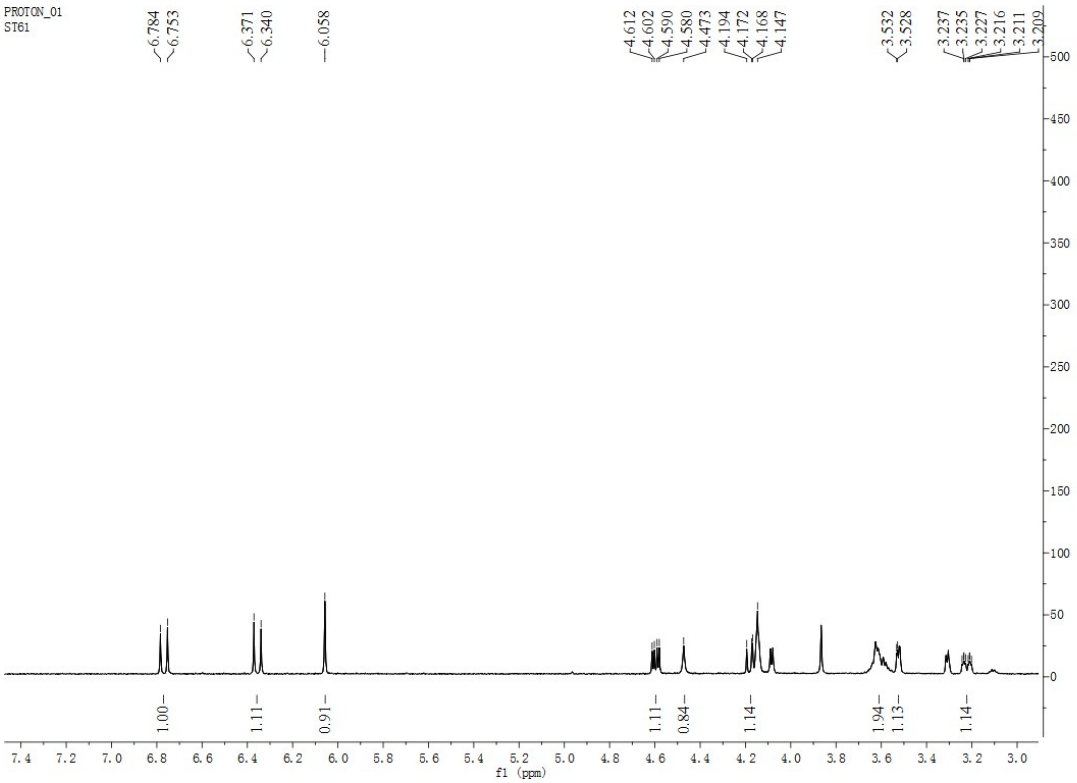

Figure S11. Partial ^{1}H NMR (500 MHz, acetone-d_6) spectrum of compound **2**

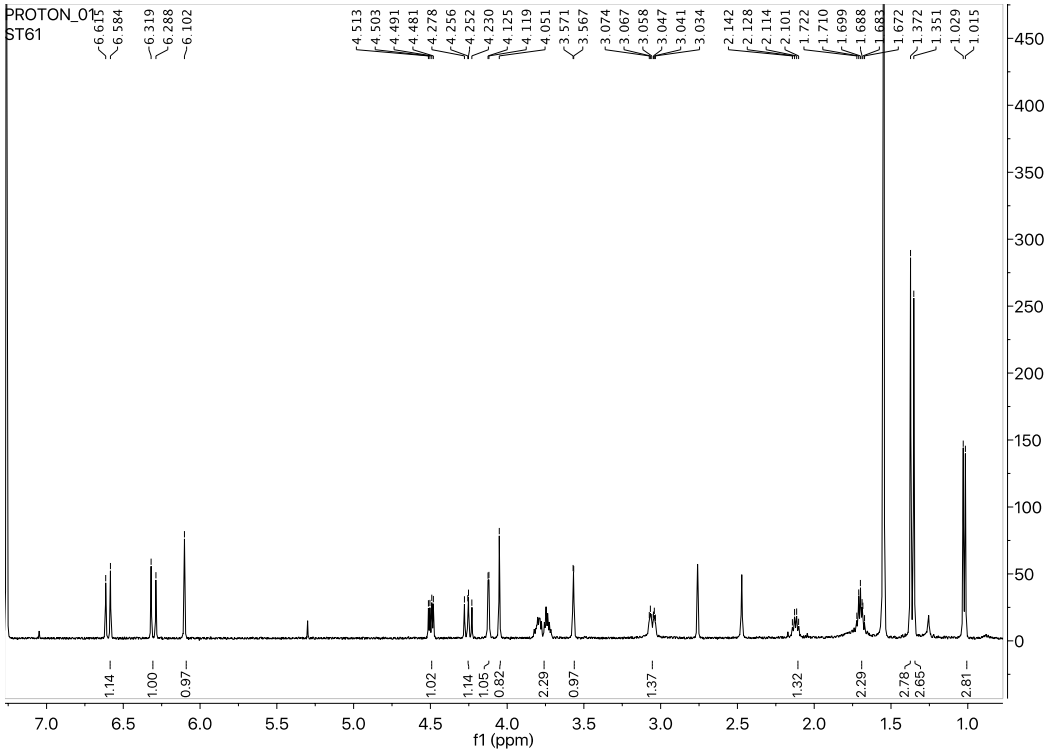

Figure S12. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **2**

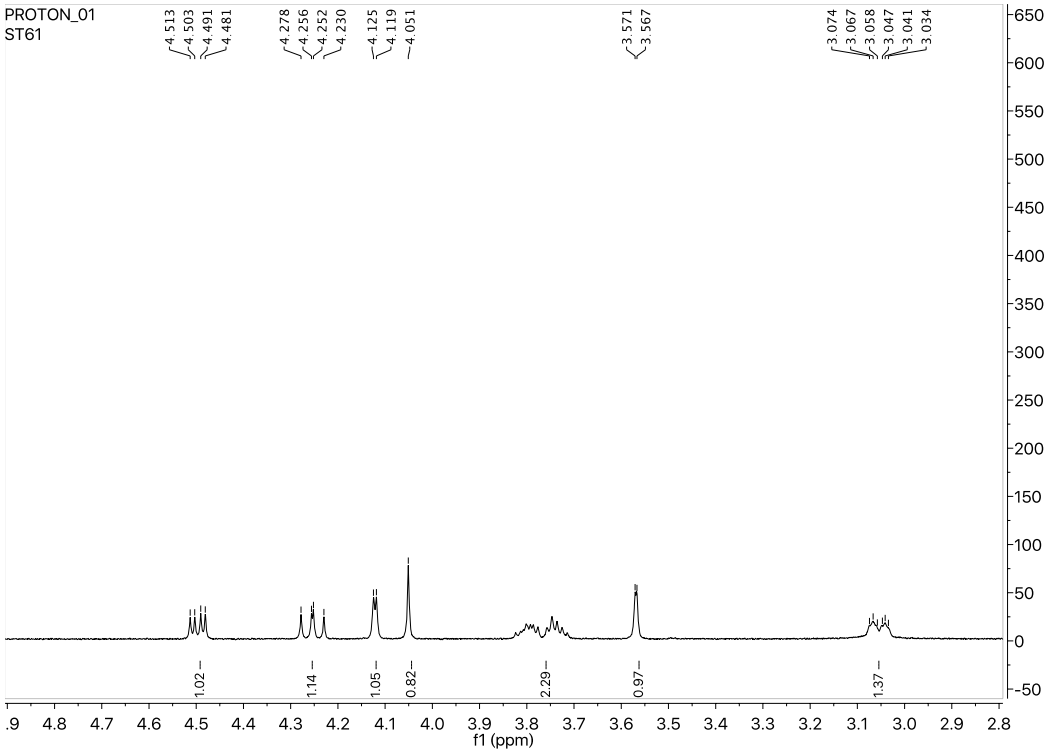

Figure S13. Partial ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **2**

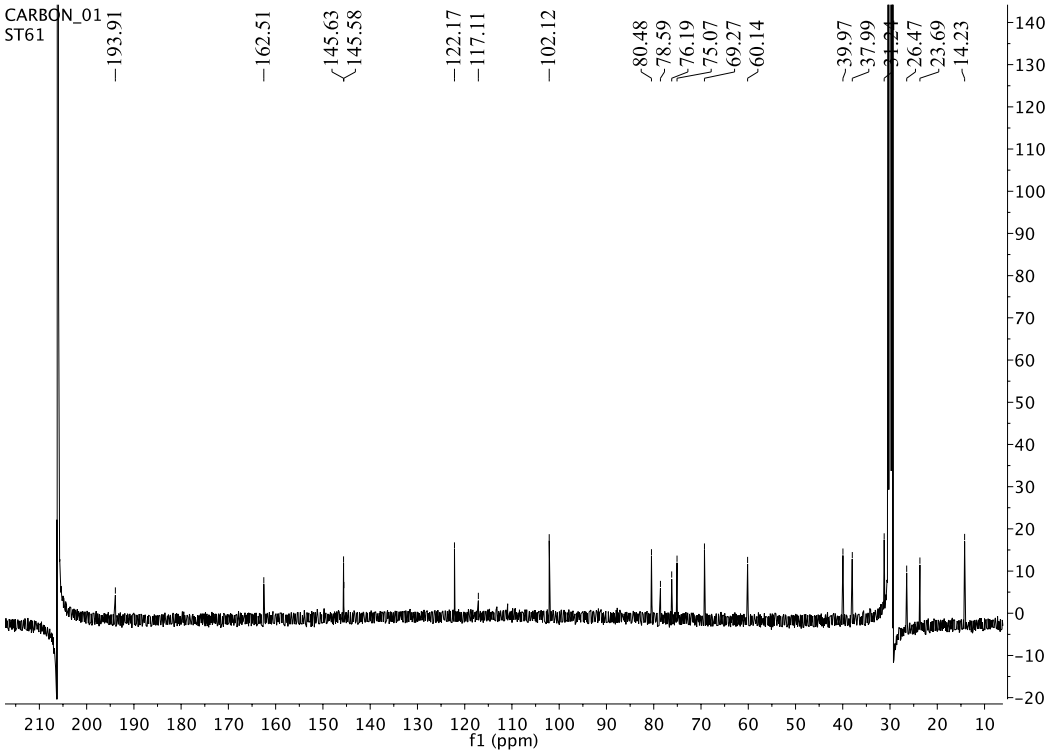

Figure S14. ^{13}C NMR (125 MHz, acetone-d_6) spectrum of compound **2**

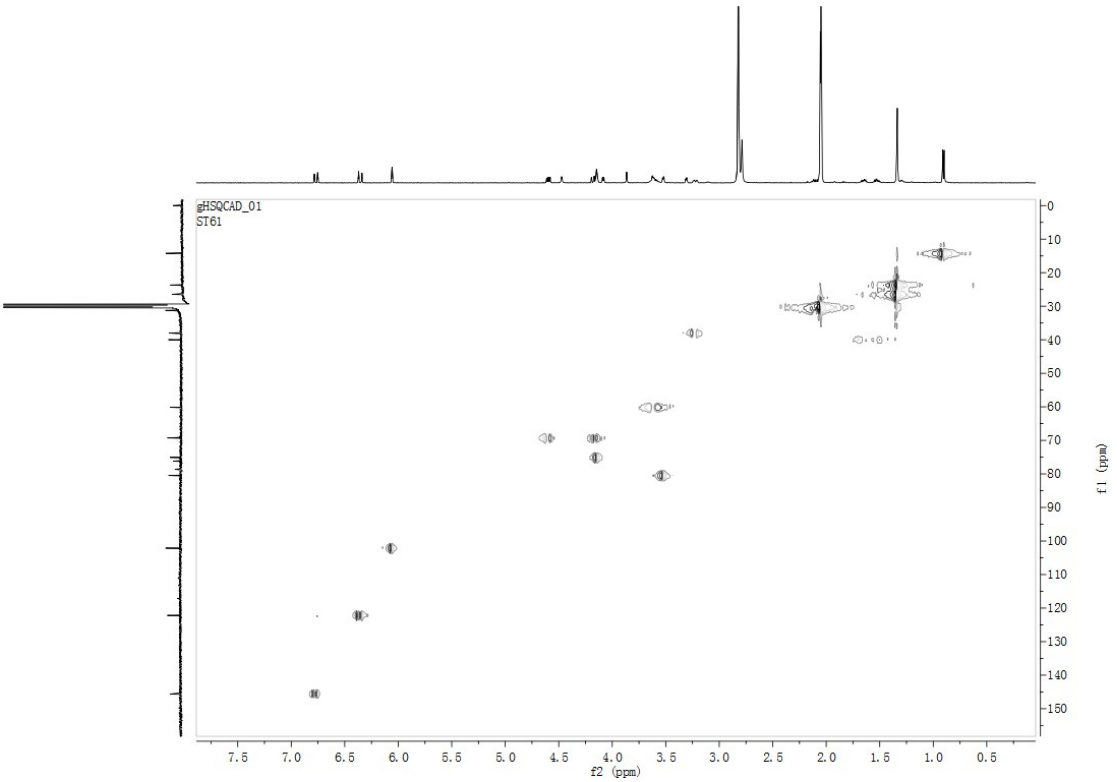

Figure S15. HMQC (acetone-d_6) spectrum of compound **2**

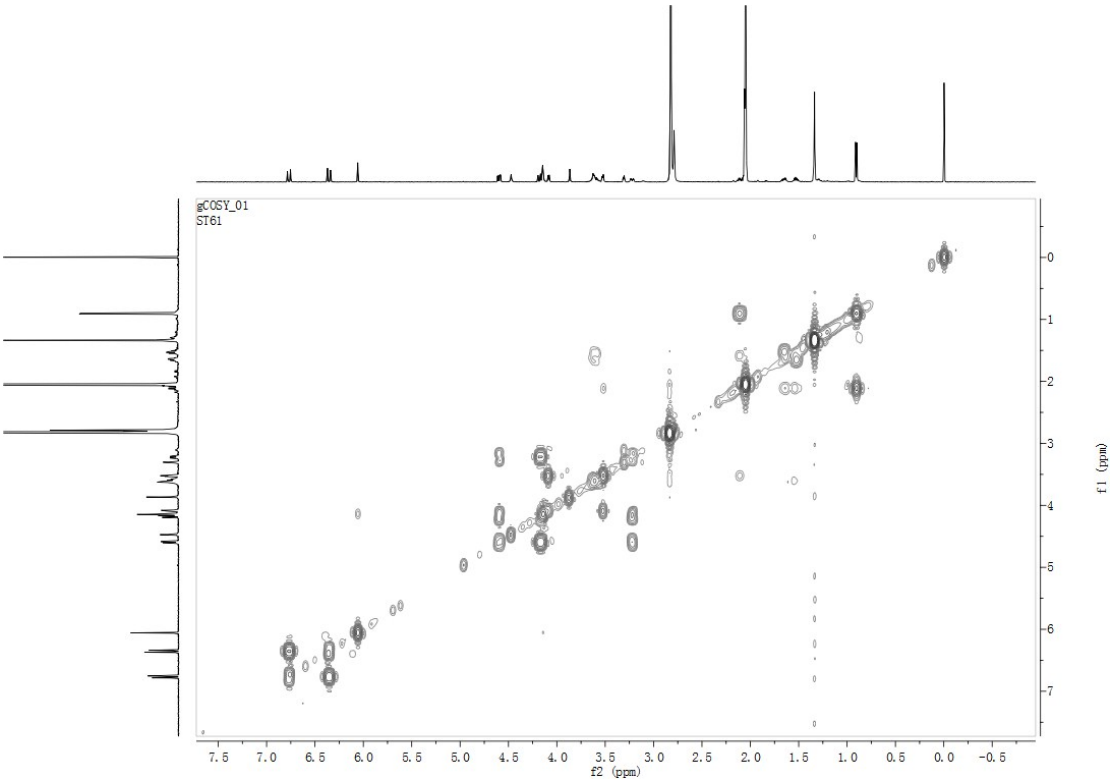

Figure S16. ^{1}H-^{1}H COSY (acetone-d_6) spectrum of compound **2**

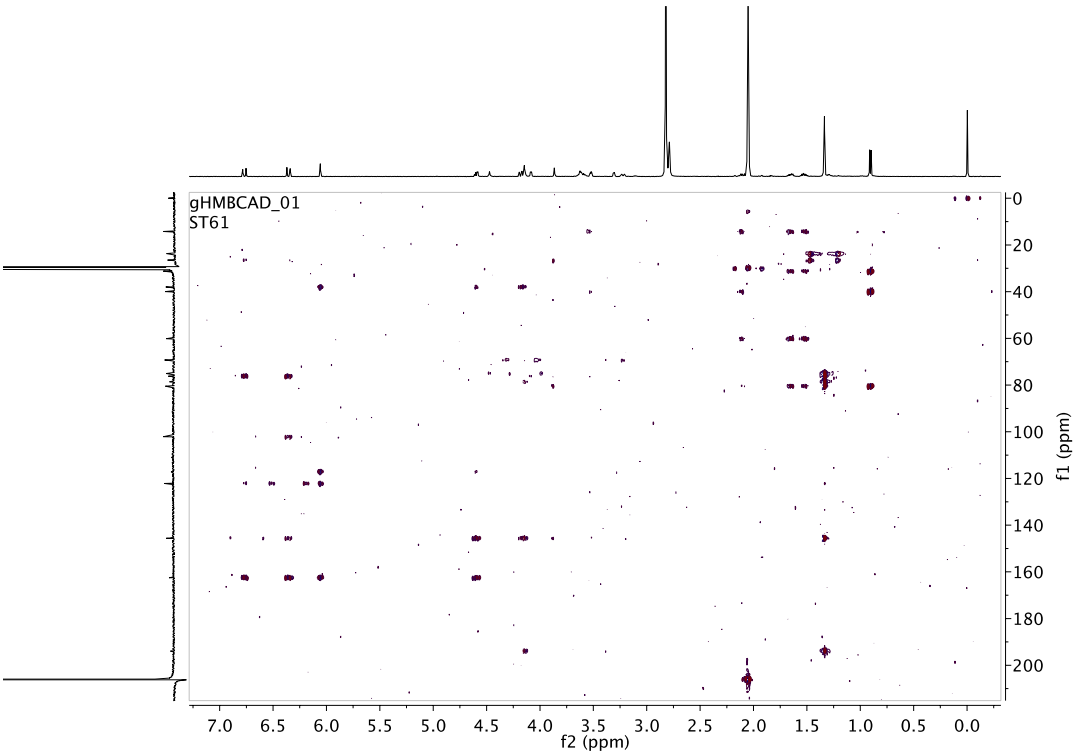

Figure S17. HMBC (acetone-d_6) spectrum of compound **2**

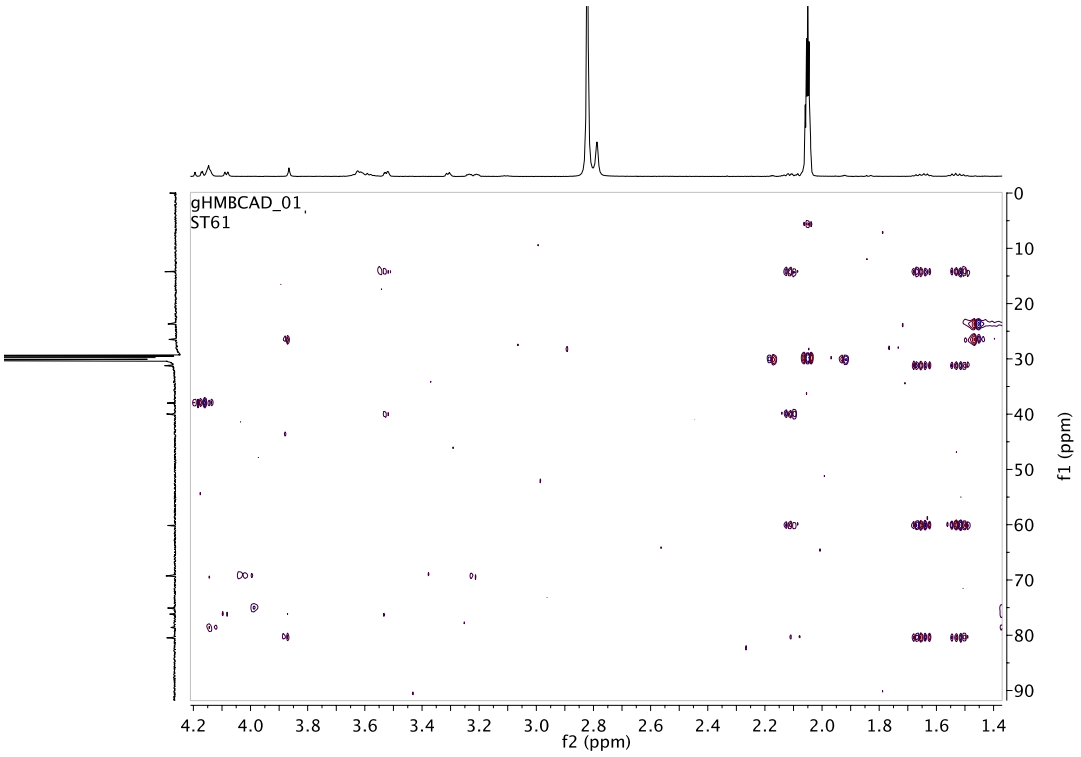

Figure S18. Partial HMBC (acetone-d_6) spectrum of compound **2**

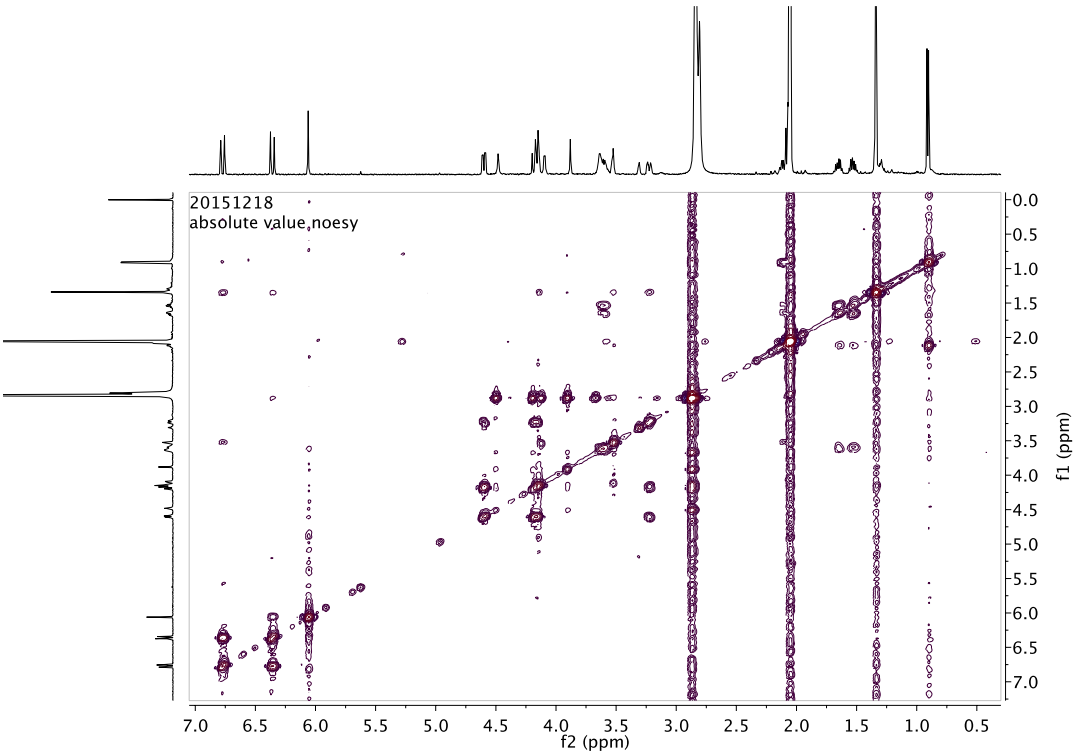

Figure S19. NOESY (acetone-d_6) spectrum of compound **2**

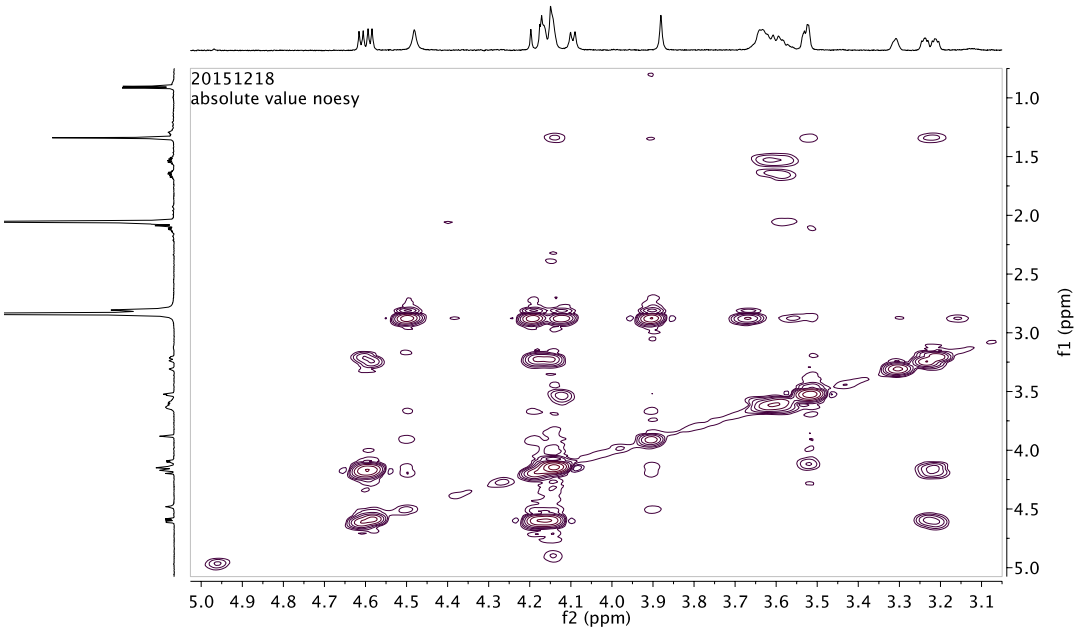

Figure S20. Partial NOESY (acetone-d_6) spectrum of compound **2**

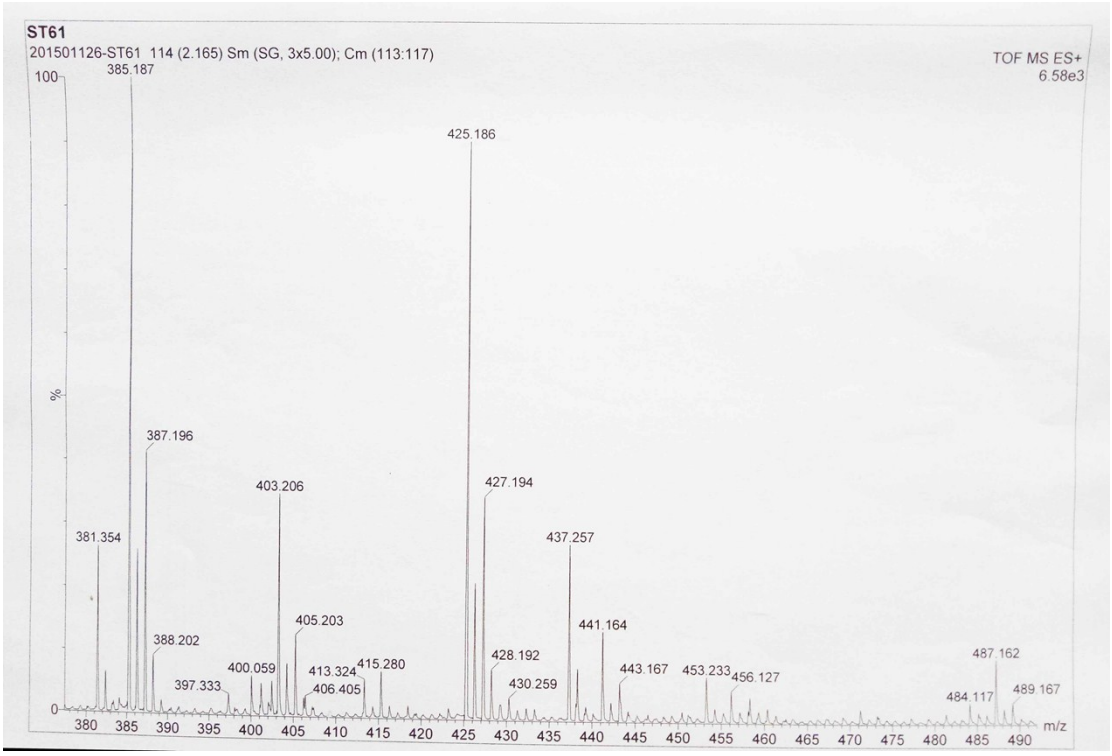

Figure S21. ESIMS spectrum of compound **2**

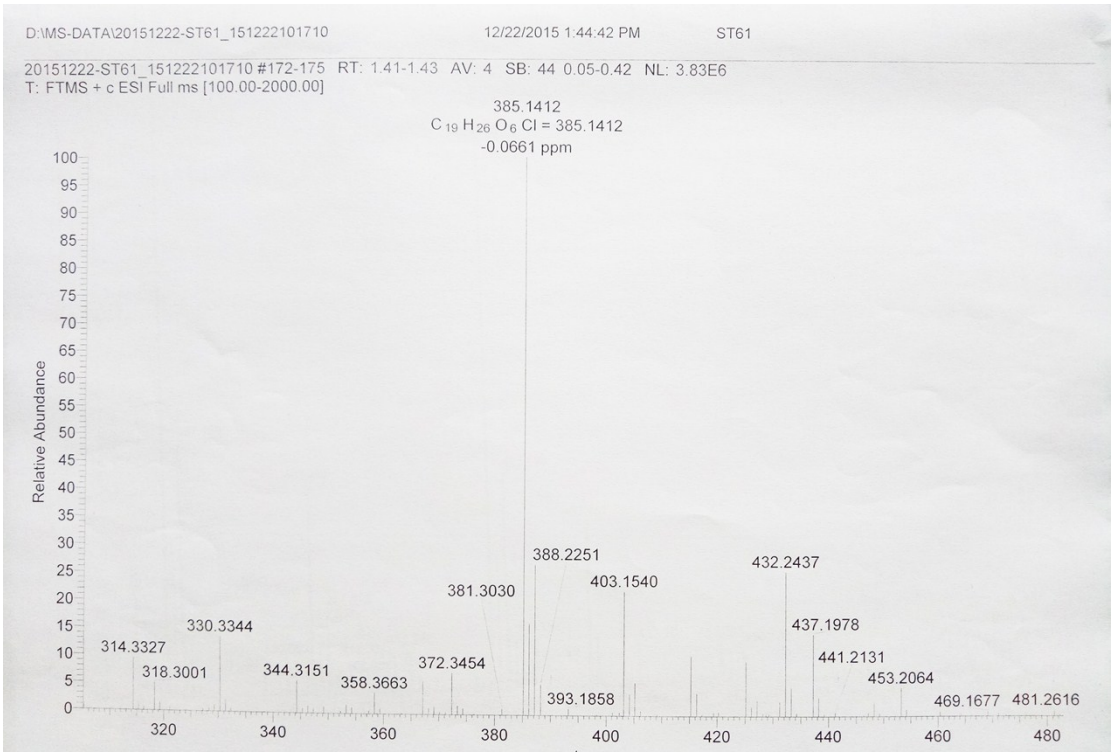

Figure S22. HRESIMS spectrum of compound **2**

Table S1. ^{1}H NMR Data (500 MHz, δ in ppm, J in Hz) and ^{13}C NMR Data (125 MHz, δin ppm) for **5**

position	$\delta_C{}^a$, type	$\delta_H{}^a$ (J in Hz)
1	68.4, CH_2	4.21, m
		4.46, dd (11.1, 4.8)
3	161.5, C	
4	102.7, CH	6.06, s
4a	145.3, C	
5	116.7, C	
6	193.4, C	
7	77.8, C	
8	73.9, CH	4.07, d (2.3)
8a	37.0, CH	3.02, m
9	23.4, CH_3	1.34, s
1′	122.5, CH	6.25, d (15.5)
2′	144.4, CH	6.54, d (15.5)
3′	75.9, C	
4′	78.4, CH	3.45, m^b
5′	35.5, CH	1.65, m
6′	28.8, CH_2	1.38, m
		1.30, m
7′	11.9, CH_3	0.88, t (7.4)
8′	13.5, CH_3	0.93, d (6.7)
9′	23.5, CH_3	1.29, s

^{a}In $CDCl_3$. ^{b}Signal partially obscured

Table S2. Antibacterial activities of **3** against bacterial strains

strain	**MIC (μM)**	
	3	Ciprofloxacin
M. lysodeikticus	6.75	0.156
B. subtilis	6.75	0.156
B. cereus	12.5	0.078
M. luteus	12.5	0.313
B. megaterium	12.5	0.313
S. dysenteriae	12.5	0.156

ECD calculation details of compound 1

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 compounds **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 *e*V.

2. Results

Table S1.2.1. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **1**.

Conformer	In MeOH	
	Δ*G*	P (%)
1a	0	50.16
1b	0.01	49.09
1c	2.48	0.75

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

Table S1.2.2**.** Cartesian coordinates for the low-energy reoptimized MMFF conformers of **1** at B3LYP/6-311+G(d,p) level of theory in CH_3OH

Conformer 1a		Standard Orientation (Ångstroms)			
I	Atom	Type	X	Y	Z
1.	6.	0.	-3.582630	0.471769	-0.018510
2.	6.	0.	-3.401356	-0.512333	1.154532
3.	6.	0.	-2.041455	-0.281164	1.838996
4.	6.	0.	-0.899754	-0.368276	0.823577
5.	6.	0.	-1.135359	0.448677	-0.439251
6.	6.	0.	-2.408115	0.788385	-0.818344
7.	6.	0.	0.435395	0.048615	1.440104
8.	6.	0.	1.294686	0.421024	-0.735925
9.	6.	0.	0.042491	0.756298	-1.190547
10.	8.	0.	-4.709500	0.922937	-0.235793
11.	6.	0.	-3.572813	-1.953798	0.641965
12.	8.	0.	-4.399845	-0.228686	2.133669
13.	8.	0.	-2.013853	1.006036	2.450940

14.	1.	0.	-0.808424	-1.420340	0.520507
15.	6.	0.	2.476440	0.584275	-1.563785
16.	6.	0.	3.732207	0.280085	-1.175336
17.	1.	0.	-1.902059	-1.058486	2.603595
18.	6.	0.	4.895266	0.465718	-2.084626
19.	8.	0.	1.518191	-0.089732	0.491520
20.	6.	0.	6.249950	0.110176	-1.521855
21.	8.	0.	4.758910	0.889255	-3.232620
22.	17.	0.	-2.703946	1.726249	-2.275754
23.	1.	0.	0.407740	1.091952	1.768072
24.	1.	0.	0.703435	-0.592116	2.280475
25.	1.	0.	-0.040903	1.215143	-2.167206
26.	1.	0.	-4.583811	-2.076380	0.244038
27.	1.	0.	-3.438961	-2.651936	1.473432
28.	1.	0.	-2.861893	-2.206120	-0.149293
29.	1.	0.	-5.137584	0.196077	1.659133
30.	1.	0.	-2.855788	1.099662	2.925740
31.	1.	0.	2.309824	0.972388	-2.564684
32.	1.	0.	3.924728	-0.108093	-0.179999
33.	1.	0.	7.028359	0.270719	-2.268715
34.	1.	0.	6.258078	-0.936427	-1.195116
35.	1.	0.	6.457347	0.719448	-0.633940

Conformer 1b		Standard Orientation (Ångstroms)			
I	Atom	Type	X	Y	Z
1.	6.	0.	-3.445264	0.181820	0.052531
2.	6.	0.	-3.237343	-0.492623	1.423525
3.	6.	0.	-1.913269	-0.023037	2.054147
4.	6.	0.	-0.740750	-0.265052	1.100626
5.	6.	0.	-0.990354	0.226235	-0.318584
6.	6.	0.	-2.270156	0.385682	-0.782396
7.	6.	0.	0.549100	0.367048	1.623315
8.	6.	0.	1.443618	0.292800	-0.568449
9.	6.	0.	0.187027	0.432612	-1.104503
10.	8.	0.	-4.591191	0.494200	-0.278658
11.	6.	0.	-3.308253	-2.021289	1.255615
12.	8.	0.	-4.277676	-0.056614	2.297618
13.	8.	0.	-1.980156	1.368943	2.354248
14.	1.	0.	-0.578116	-1.350268	1.047646
15.	6.	0.	2.637367	0.343277	-1.397638
16.	6.	0.	3.895596	0.218912	-0.922834
17.	1.	0.	-1.748073	-0.594357	2.978506

18.	6.	0.	5.115353	0.258114	-1.760343
19.	8.	0.	1.664336	0.089384	0.744918
20.	6.	0.	5.005309	0.448203	-3.257105
21.	8.	0.	6.214478	0.134054	-1.214608
22.	17.	0.	-2.581855	0.945652	-2.419491
23.	1.	0.	0.449066	1.453372	1.704837
24.	1.	0.	0.832976	-0.048188	2.590495
25.	1.	0.	0.102484	0.651072	-2.161153
26.	1.	0.	-4.299003	-2.296756	0.884132
27.	1.	0.	-3.155418	-2.499637	2.227448
28.	1.	0.	-2.562518	-2.402580	0.552989
29.	1.	0.	-5.026670	0.197985	1.728443
30.	1.	0.	-2.840100	1.514190	2.781373
31.	1.	0.	2.451973	0.482985	-2.457948
32.	1.	0.	4.072358	0.078705	0.139439
33.	1.	0.	4.431095	-0.367152	-3.710243
34.	1.	0.	6.005405	0.468036	-3.691521
35.	1.	0.	4.488625	1.384272	-3.494372

Conformer **1c**		Standard Orientation (Ångstroms)			
I	Atom	Type	X	Y	Z
1.	6.	0.	-3.368505	0.169148	0.225428
2.	6.	0.	-3.137804	-0.512087	1.589676
3.	6.	0.	-1.807680	-0.040777	2.205732
4.	6.	0.	-0.647963	-0.266542	1.233055
5.	6.	0.	-0.919000	0.233032	-0.178786
6.	6.	0.	-2.208254	0.388131	-0.621880
7.	6.	0.	0.643472	0.373678	1.739371
8.	6.	0.	1.507597	0.297622	-0.470959
9.	6.	0.	0.242913	0.449911	-0.981855
10.	8.	0.	-4.523173	0.472377	-0.087265
11.	6.	0.	-3.201968	-2.040030	1.413587
12.	8.	0.	-4.168994	-0.087568	2.480205
13.	8.	0.	-1.877710	1.347784	2.520998
14.	1.	0.	-0.477949	-1.349991	1.170526
15.	6.	0.	2.748252	0.325224	-1.242864
16.	6.	0.	2.839649	0.296486	-2.588252
17.	1.	0.	-1.625841	-0.620422	3.121931
18.	6.	0.	4.115377	0.343666	-3.341359
19.	8.	0.	1.747150	0.106966	0.844240
20.	6.	0.	5.434458	0.417363	-2.605953
21.	8.	0.	4.073059	0.322688	-4.573160

22.	17.	0.	-2.546005	0.960730	-2.251050
23.	1.	0.	0.537018	1.459553	1.821979
24.	1.	0.	0.945419	-0.039536	2.702018
25.	1.	0.	0.129606	0.687848	-2.030525
26.	1.	0.	-4.194639	-2.319533	1.050305
27.	1.	0.	-3.036076	-2.523468	2.380771
28.	1.	0.	-2.460661	-2.412210	0.701264
29.	1.	0.	-4.924969	0.169556	1.921164
30.	1.	0.	-2.732534	1.483749	2.961285
31.	1.	0.	3.646111	0.359545	-0.632024
32.	1.	0.	1.956318	0.233100	-3.217812
33.	1.	0.	5.490086	1.329432	-2.002014
34.	1.	0.	6.249163	0.416232	-3.330862
35.	1.	0.	5.552074	-0.433656	-1.926916