Supplementary Materials: Bioactive Polycyclic Quinones from Marine *Streptomyces* sp. 182SMLY

Ying Liang, Xin Xie, Lu Chen, Shilun Yan, Xuewei Ye, Komal Anjum, Haocai Huang, Xiao-Yuan Lian and Zhizhen Zhang

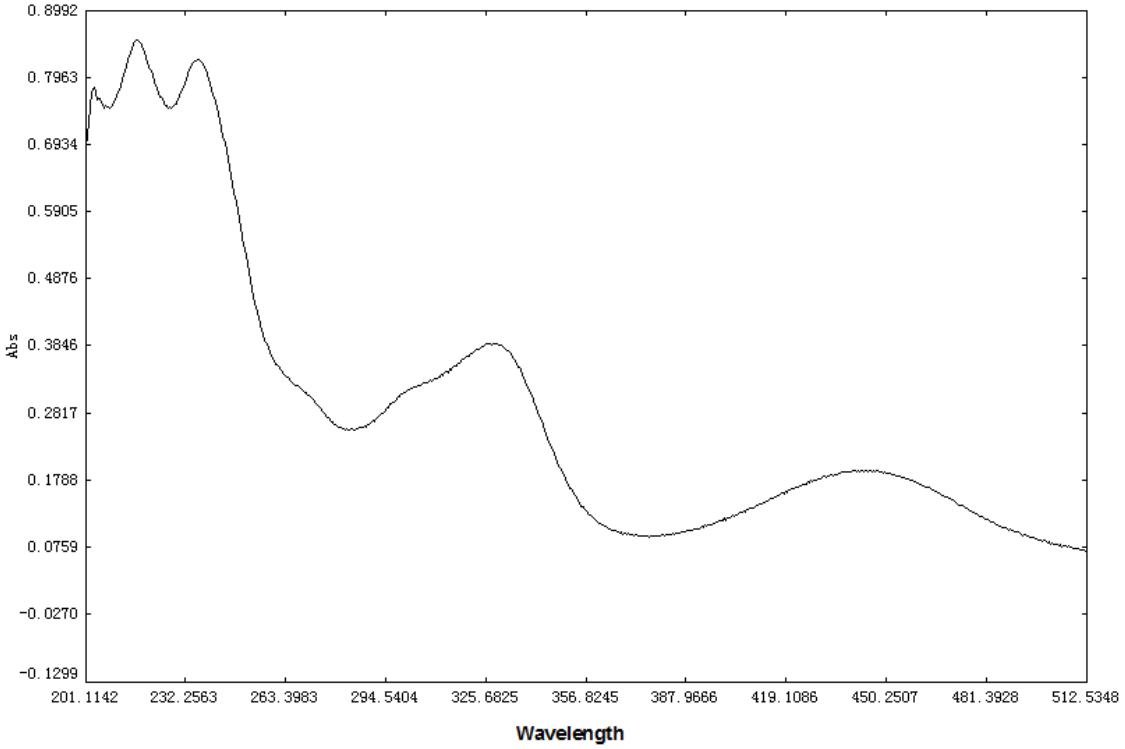

Figure S1. UV Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

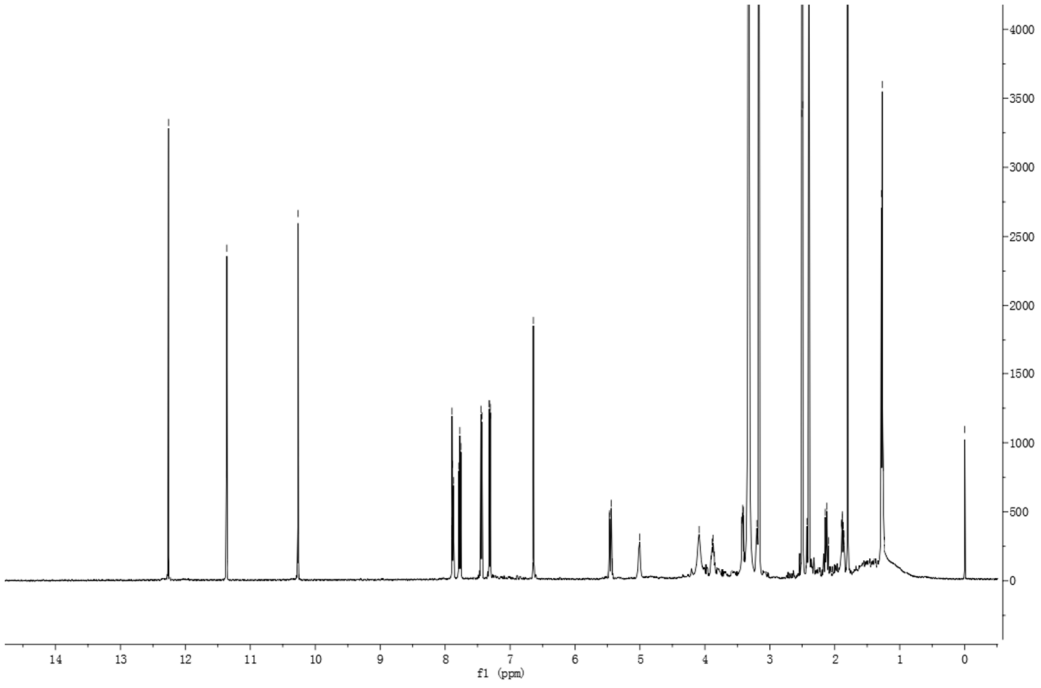

Figure S2. 1H NMR Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

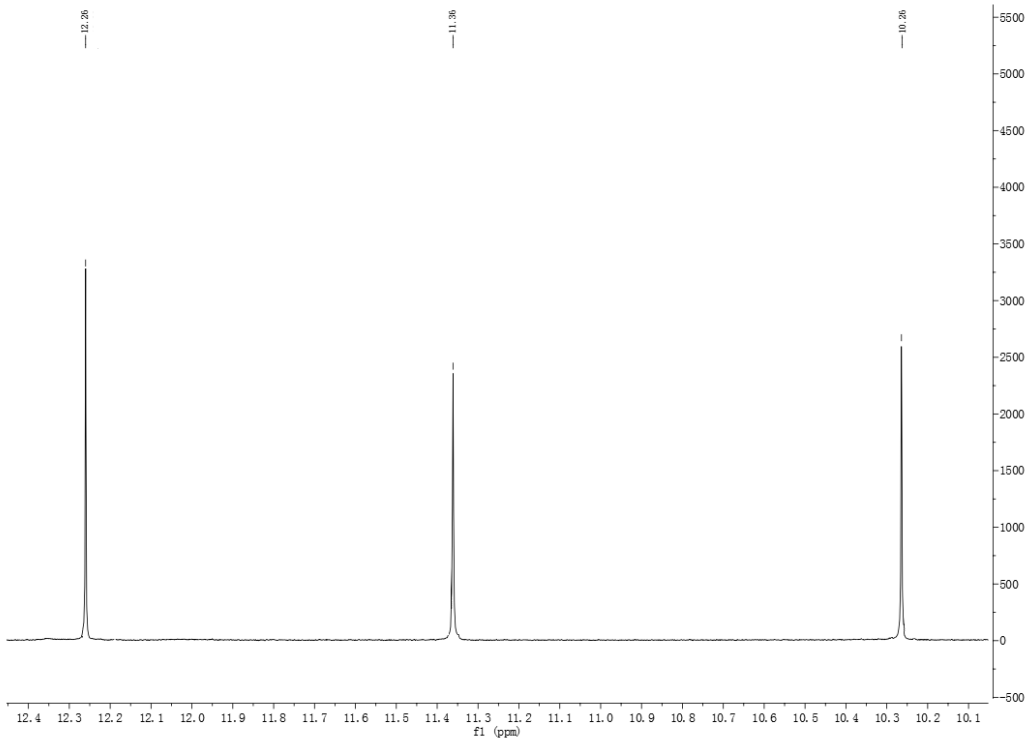

Figure S3. 1H NMR Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

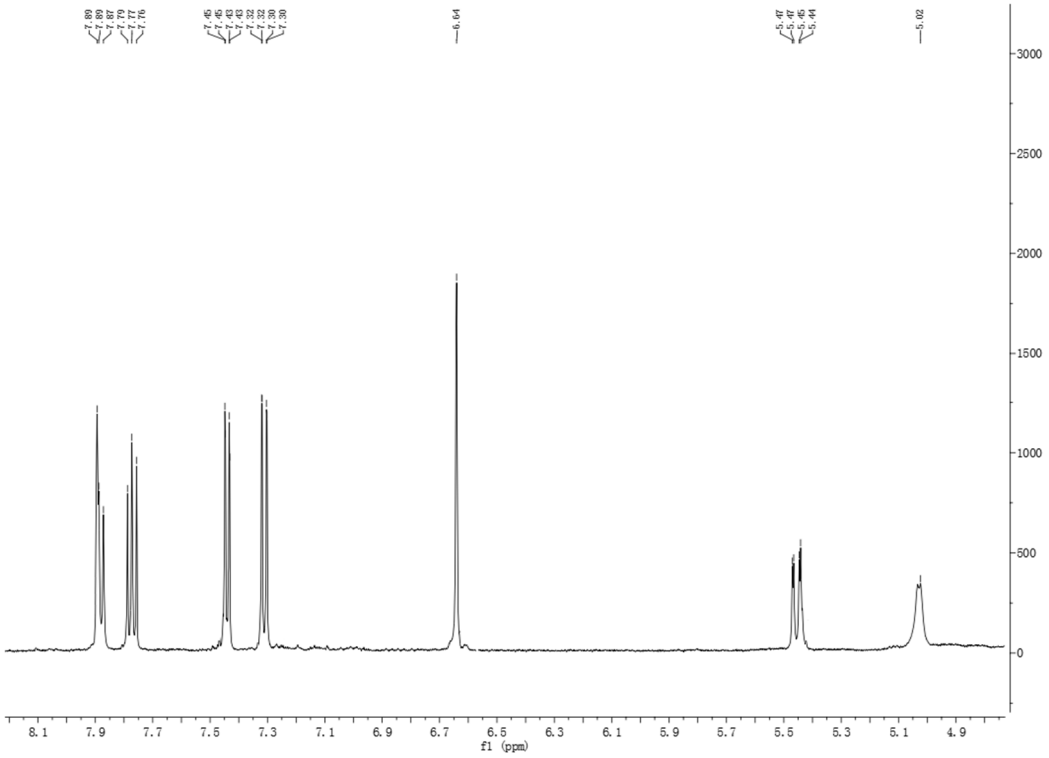

Figure S4. 1H NMR Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

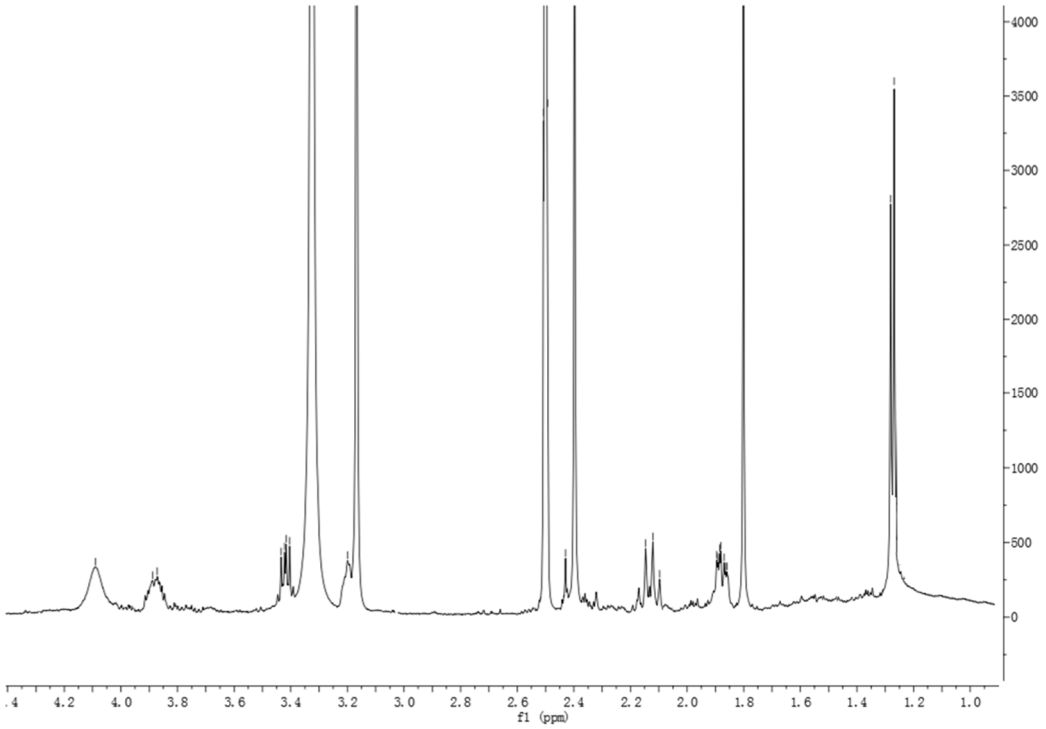

Figure S5. 1H NMR Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

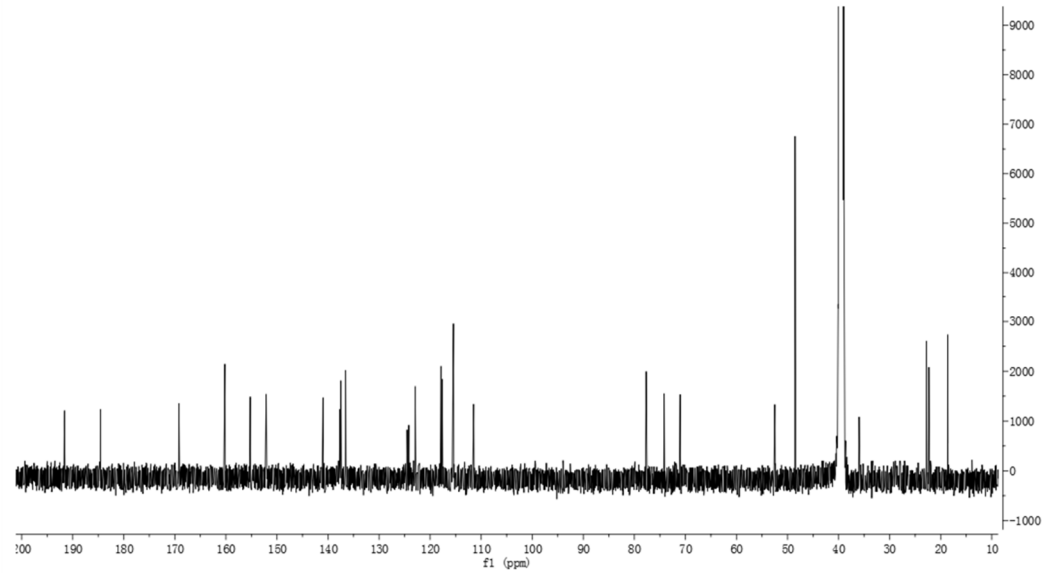

Figure S6. 13C-NMR of *N*-acetyl-*N*-demethylmayamycin (**1**).

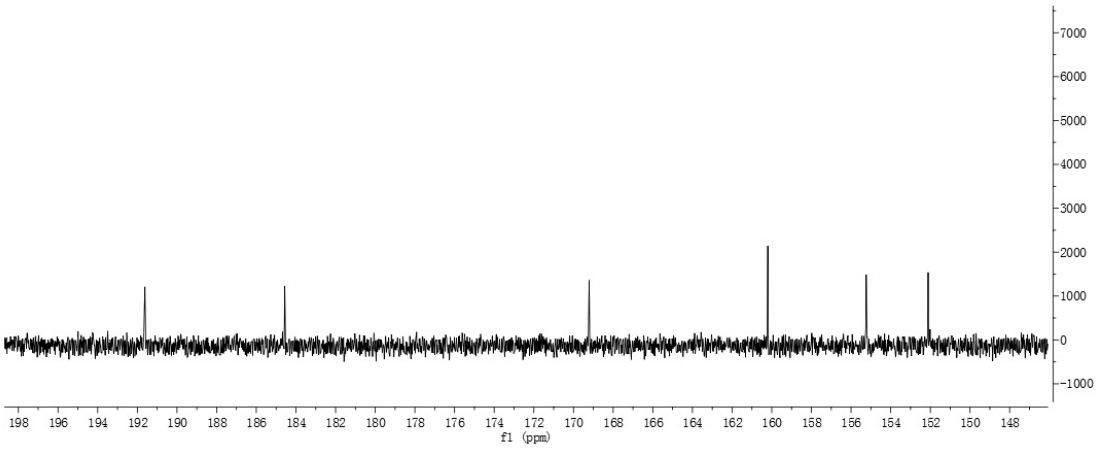

Figure S7. 13C-NMR of *N*-acetyl-*N*-demethylmayamycin (**1**).

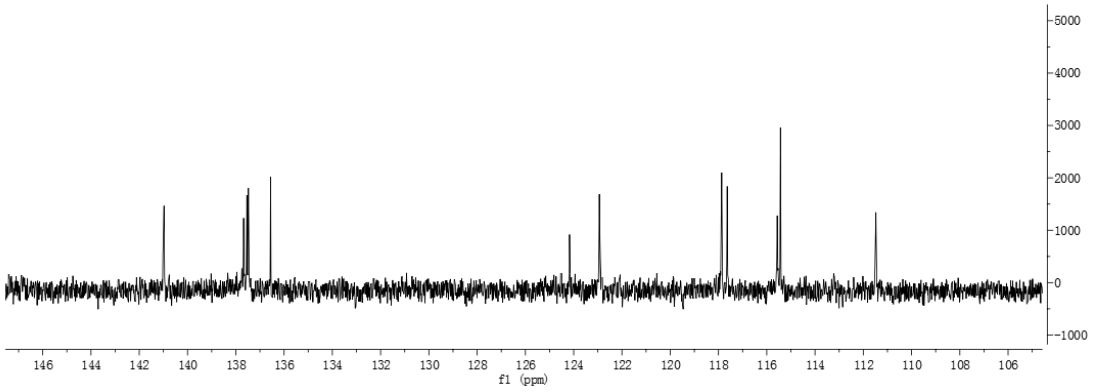

Figure S8. 13C-NMR of *N*-acetyl-*N*-demethylmayamycin (**1**).

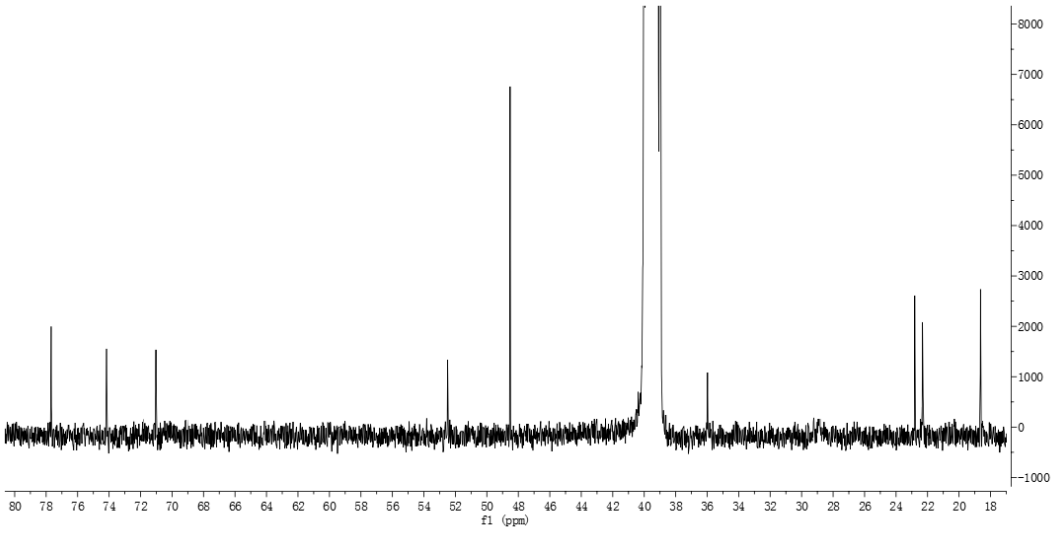

Figure S9. 13C-NMR of *N*-acetyl-*N*-demethylmayamycin (**1**).

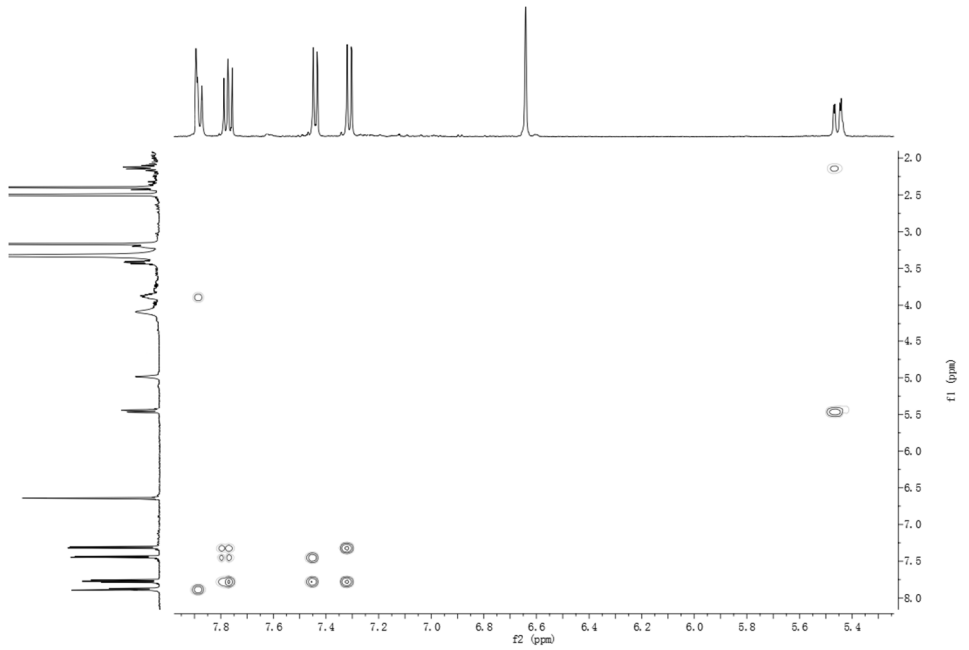

Figure S10. 1H-1H COSY Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

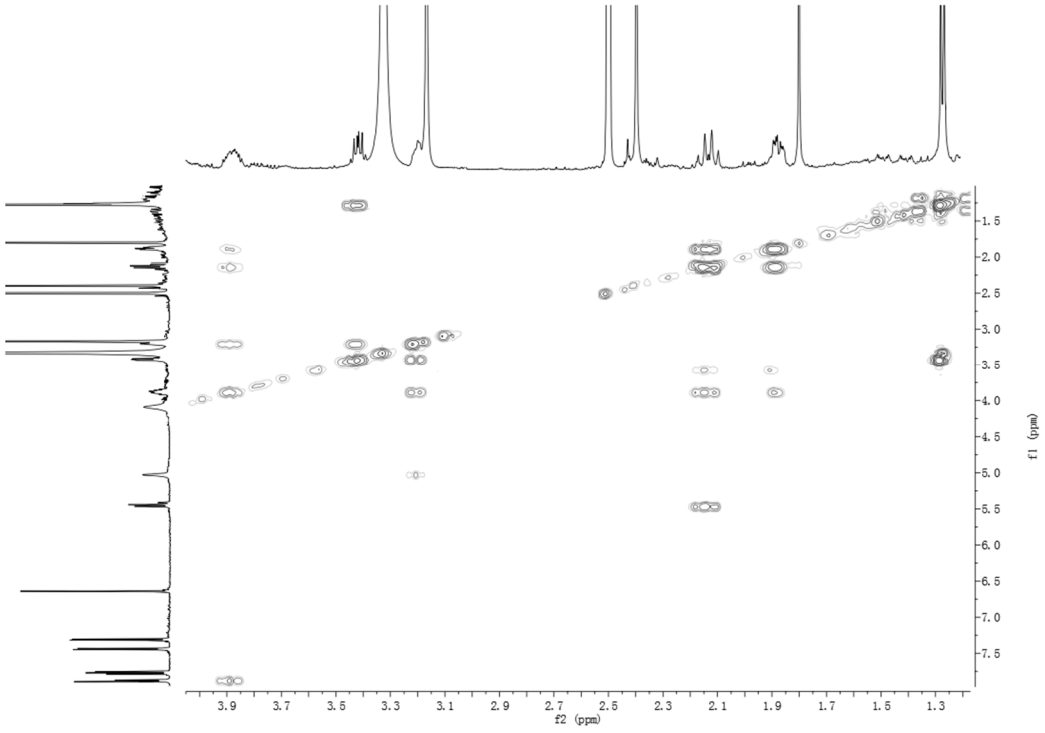

Figure S11. 1H-1H COSY Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

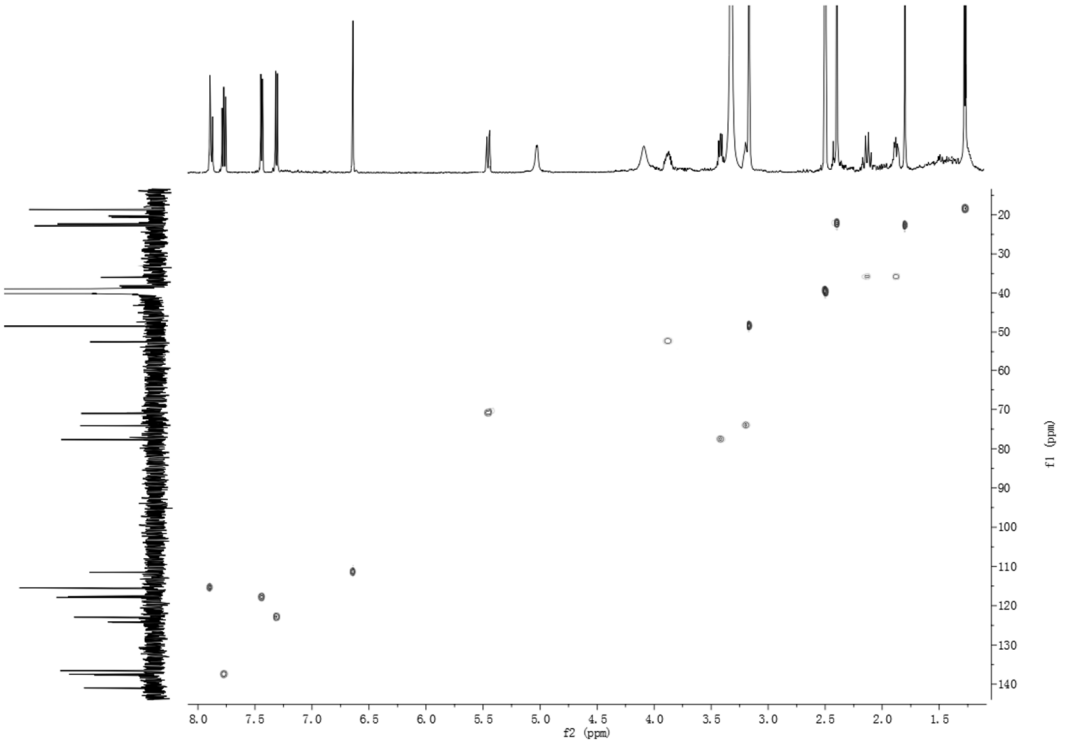

Figure S12. HSQC Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

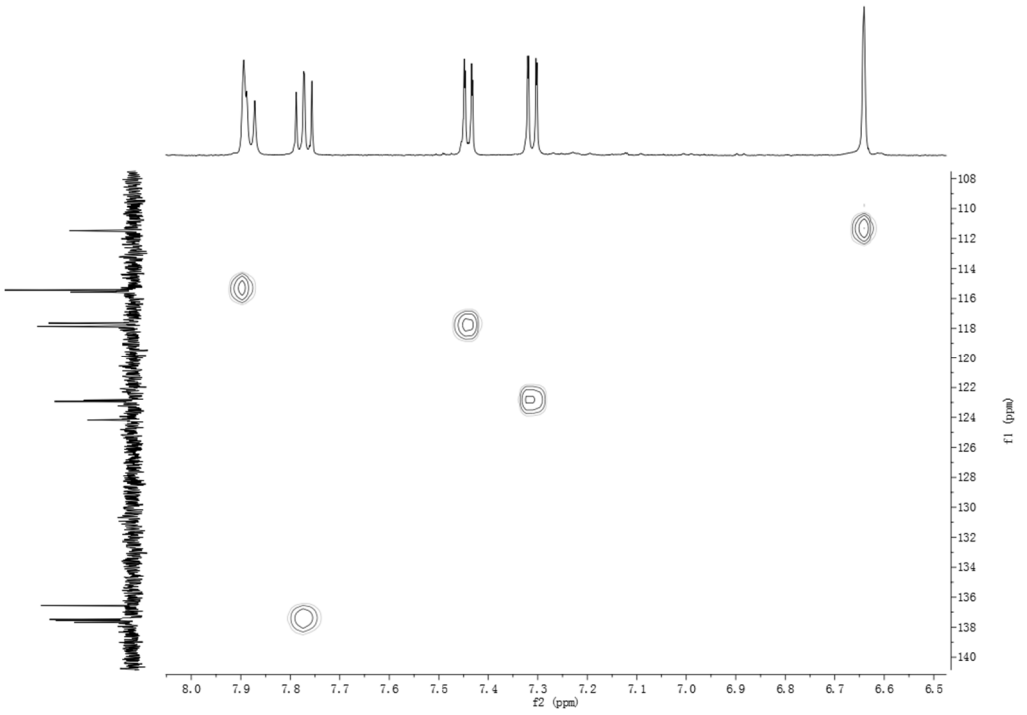

Figure S13. HSQC Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

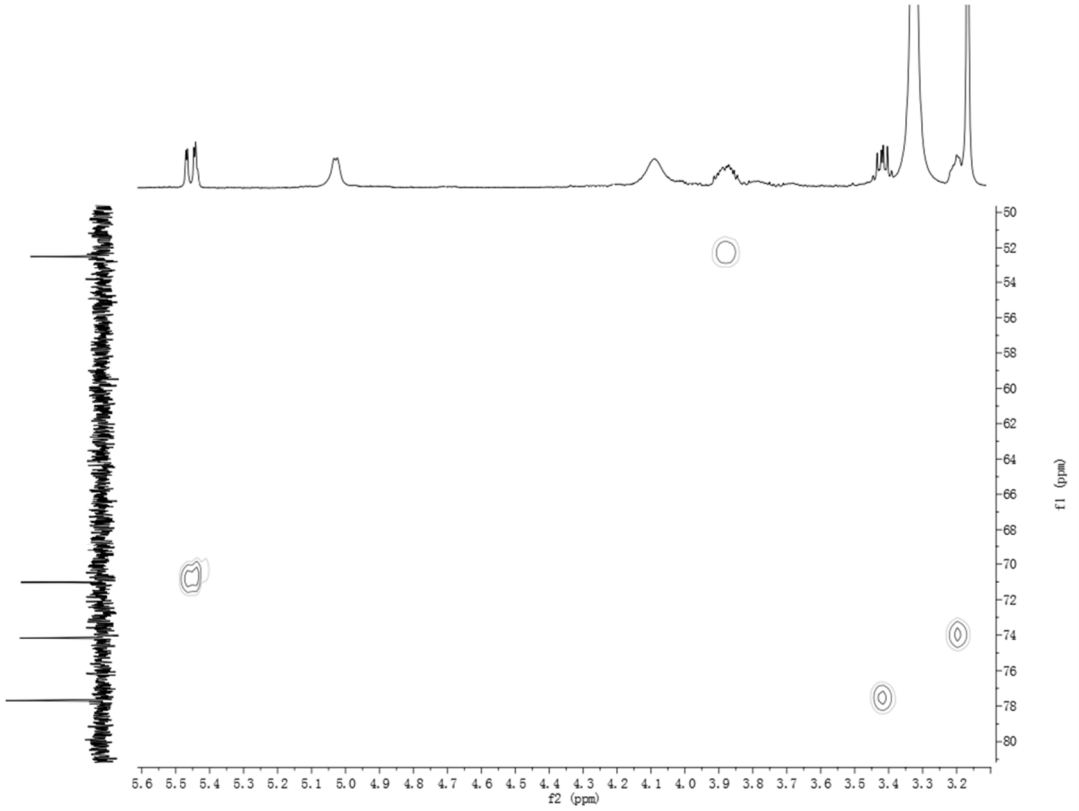

Figure S14. HSQC Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

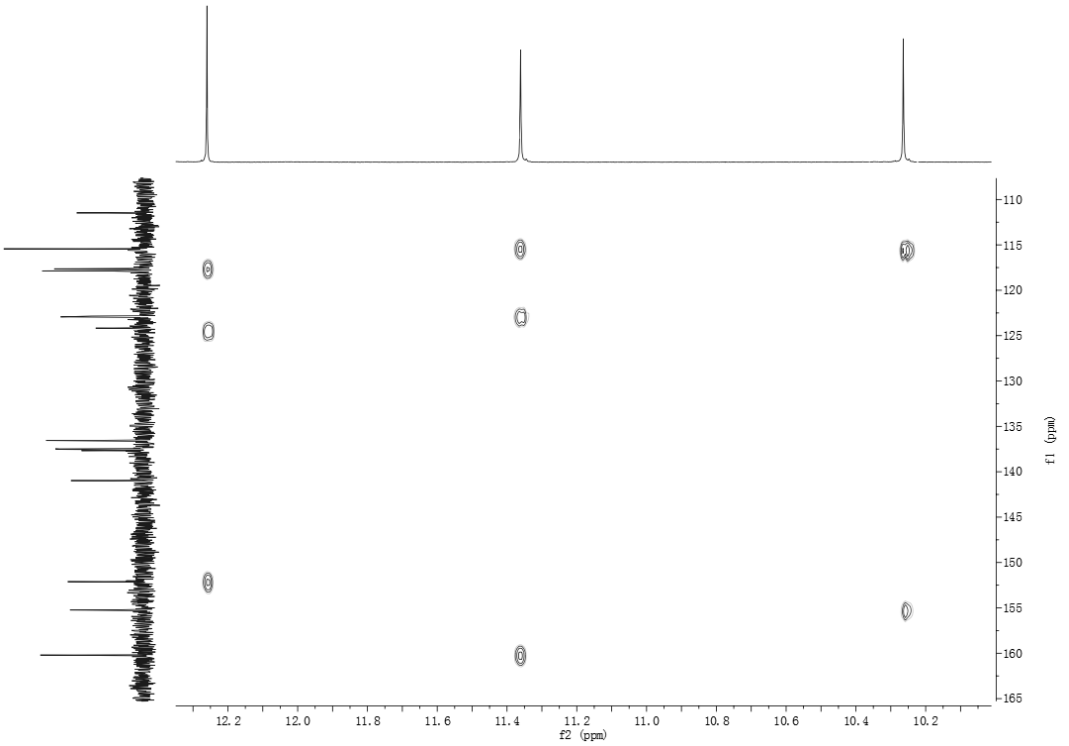

Figure S15. HMBC Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

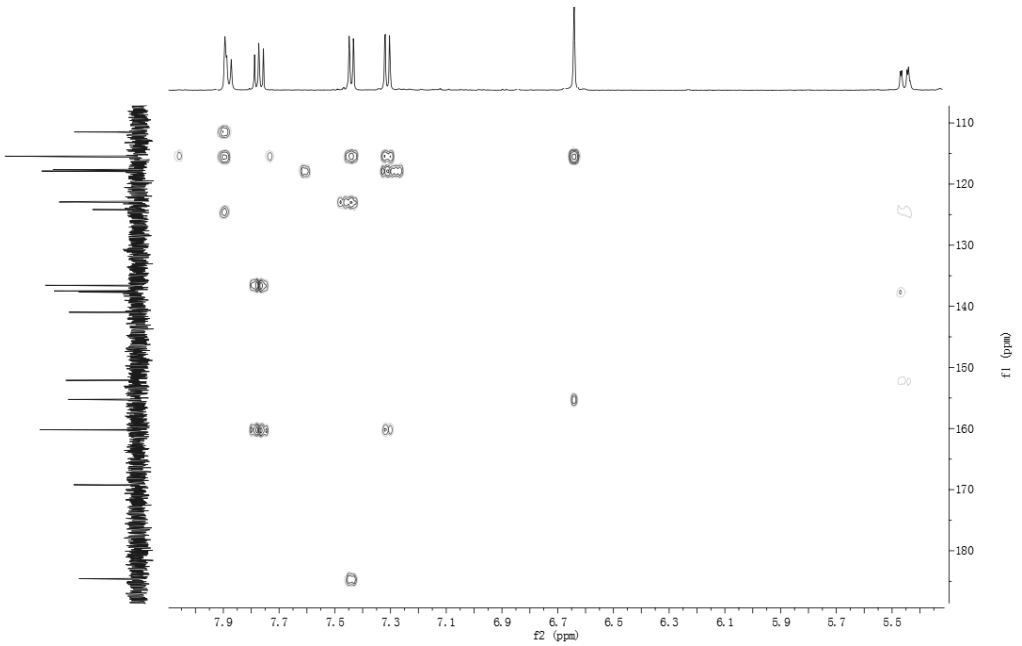

Figure S16. HMBC Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

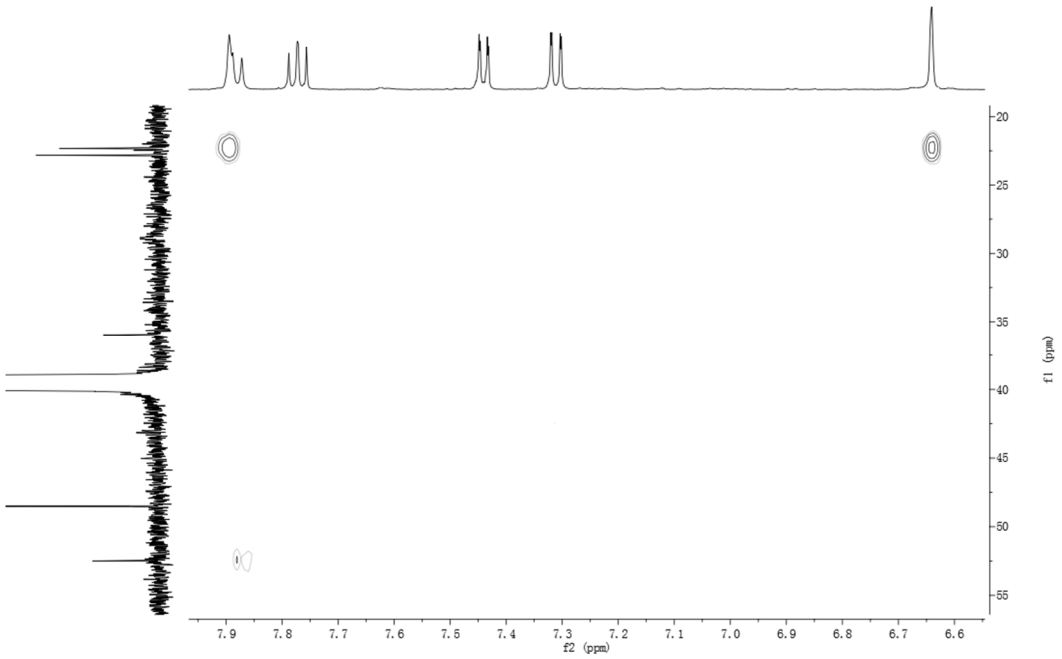

Figure S17. HMBC Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

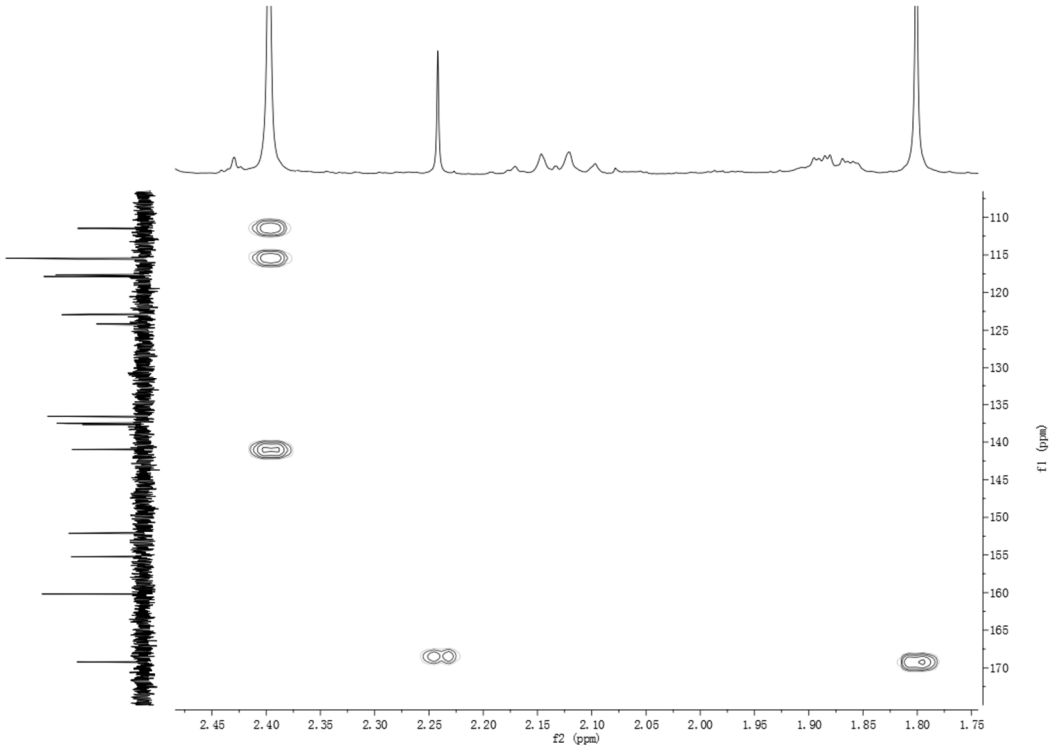

Figure S18. HMBC Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

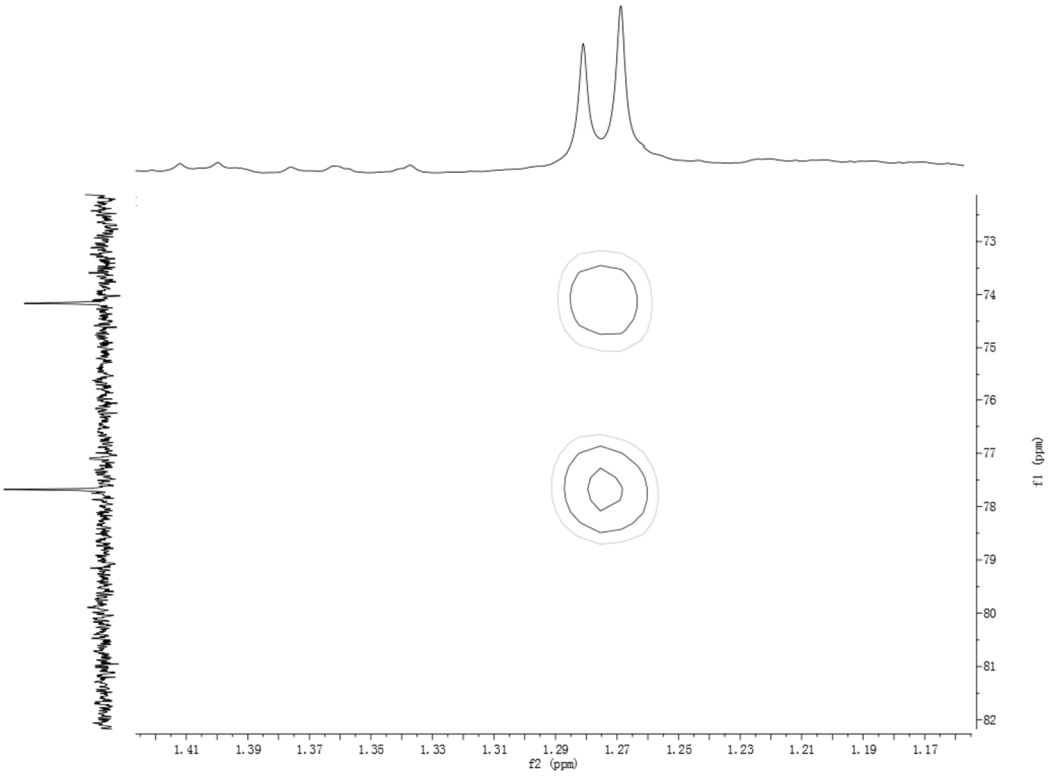

Figure S19. HMBC Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

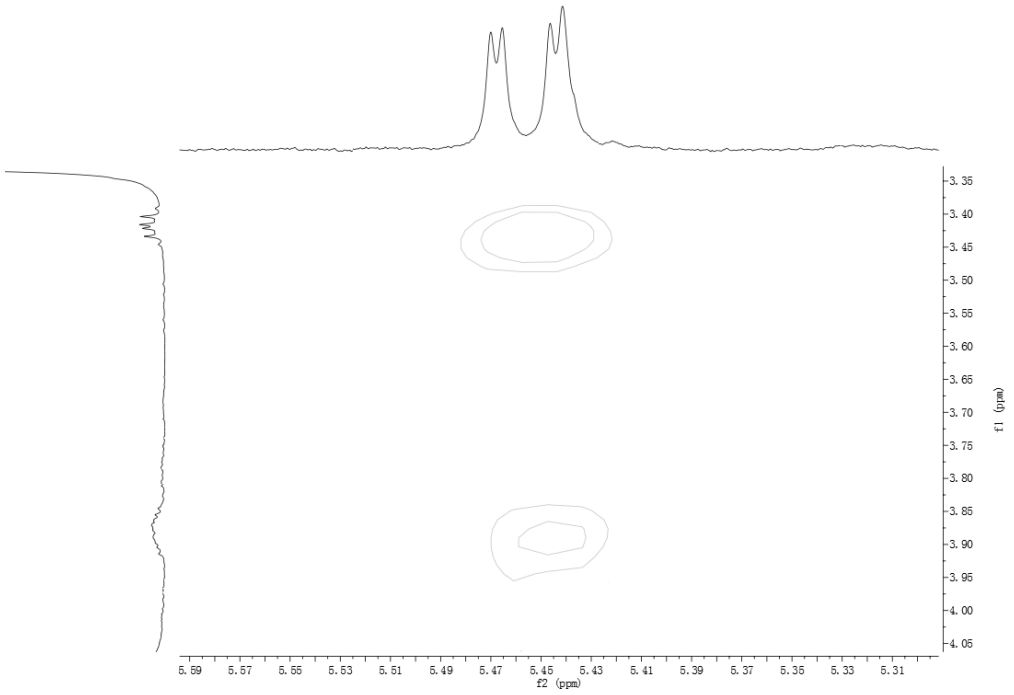

Figure S20. NOESY Spectrum of *N*-acetyl-*N*-demethylmayamycin (**1**).

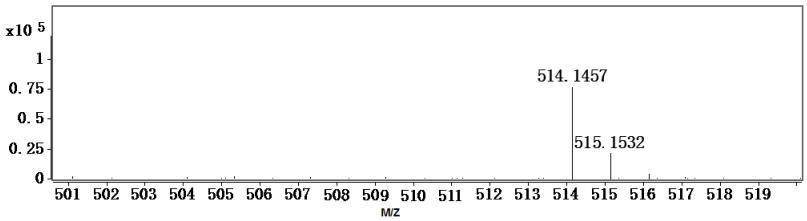

Figure S21. HRESIMS Data of *N*-acetyl-*N*-demethylmayamycin (**1**).

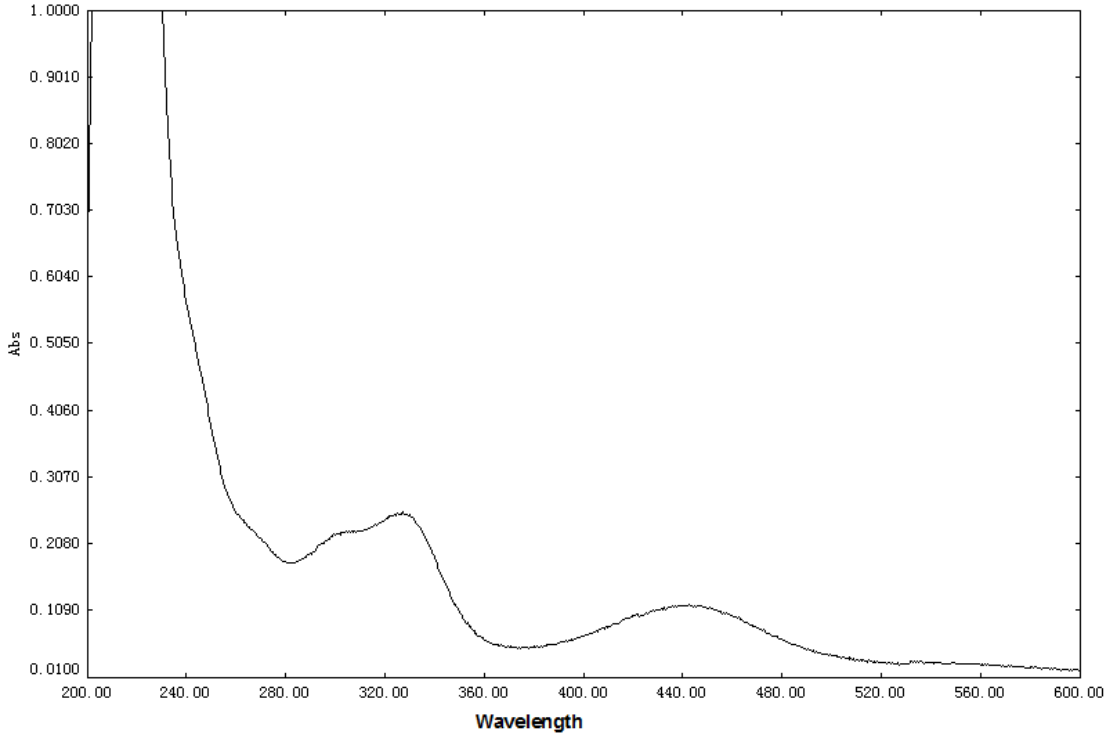

Figure S22. UV spectrum of Streptoanthraquinone A (**2**).

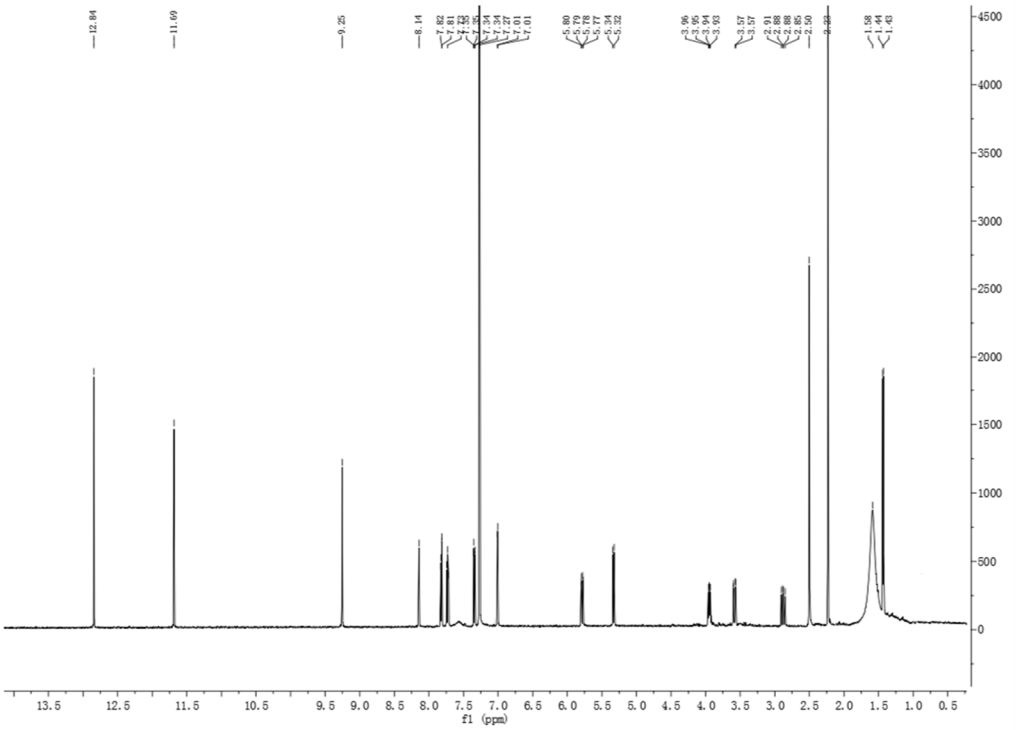

Figure S23. 1H-NMR of Streptoanthraquinone A (**2**).

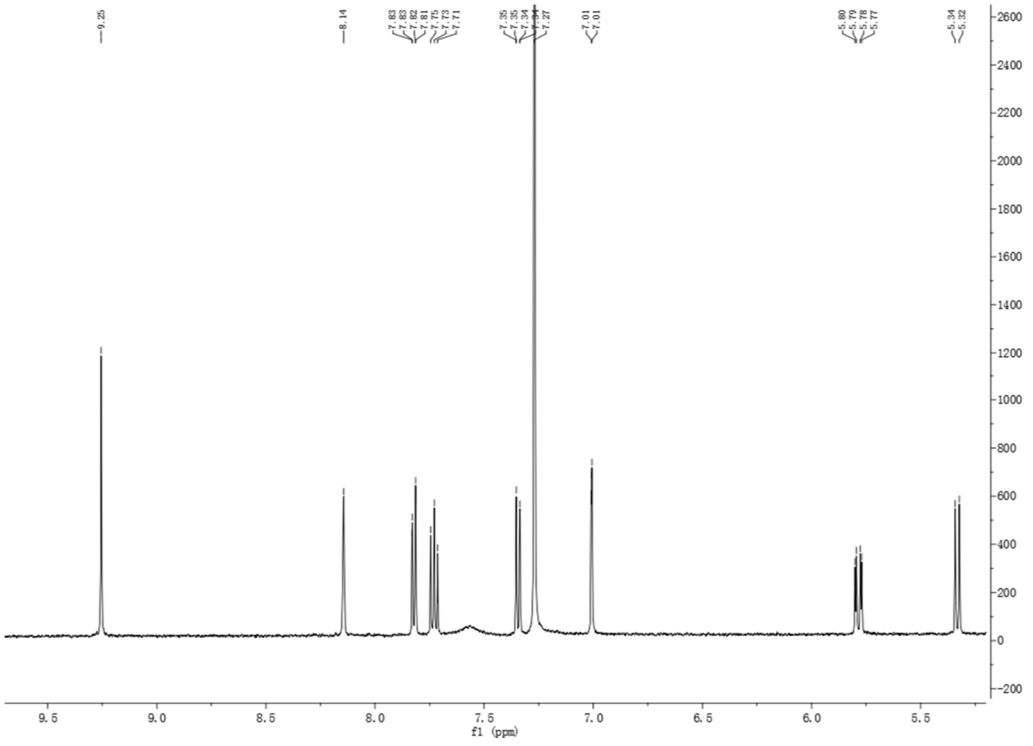

Figure S24. 1H-NMR of Streptoanthraquinone A (**2**).

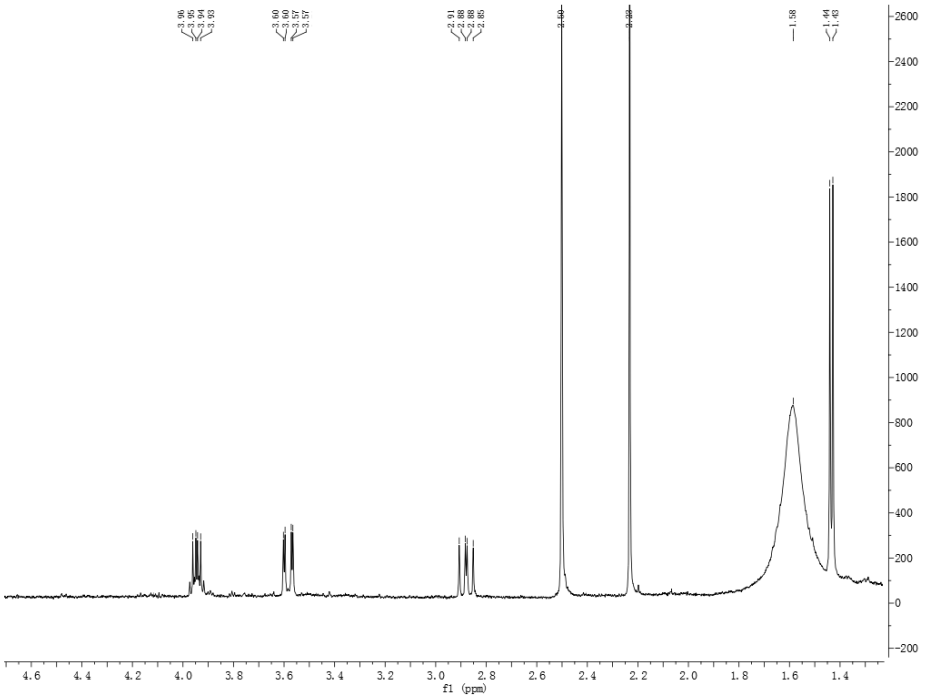

Figure S25. 1H-NMR Spectrum of Streptoanthraquinone A (**2**).

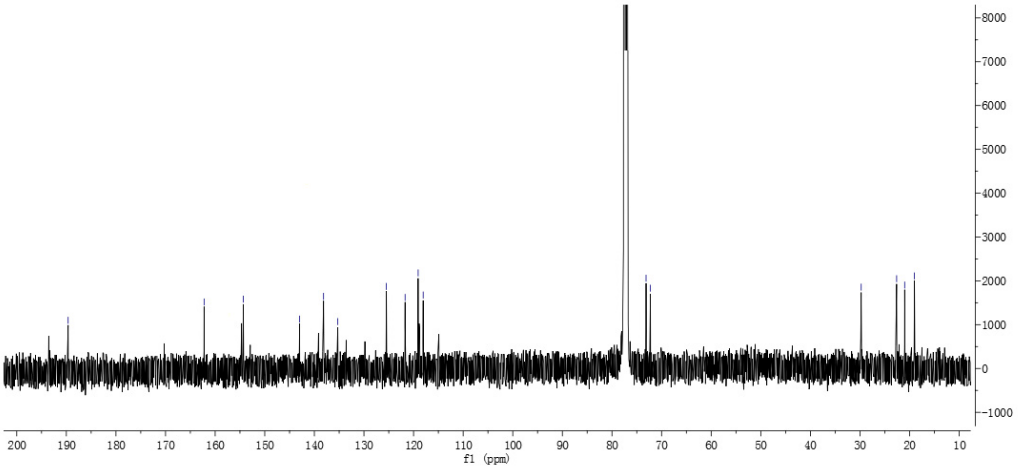

Figure S26. 13C-NMR Spectrum of Streptoanthraquinone A (**2**).

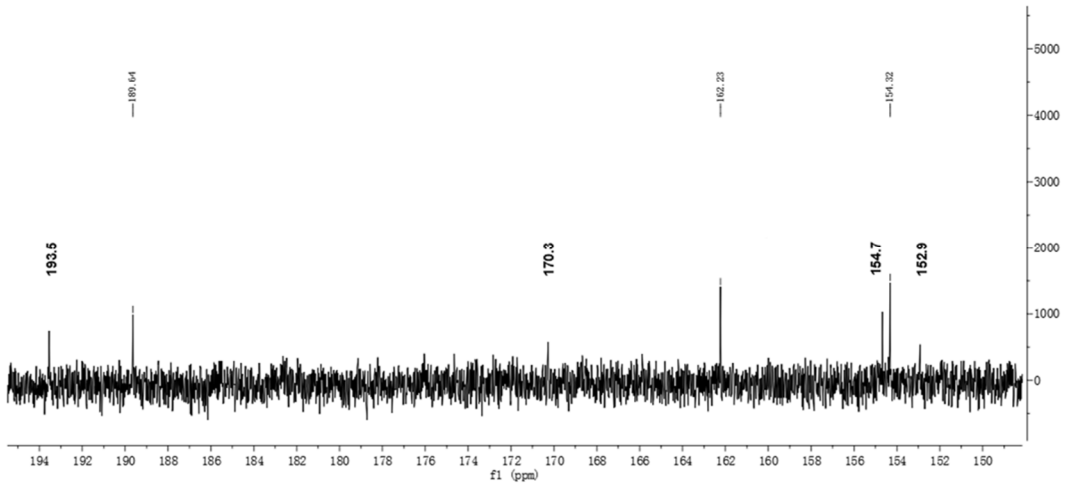

Figure S27. 13C-NMR Spectrum of Streptoanthraquinone A (**2**).

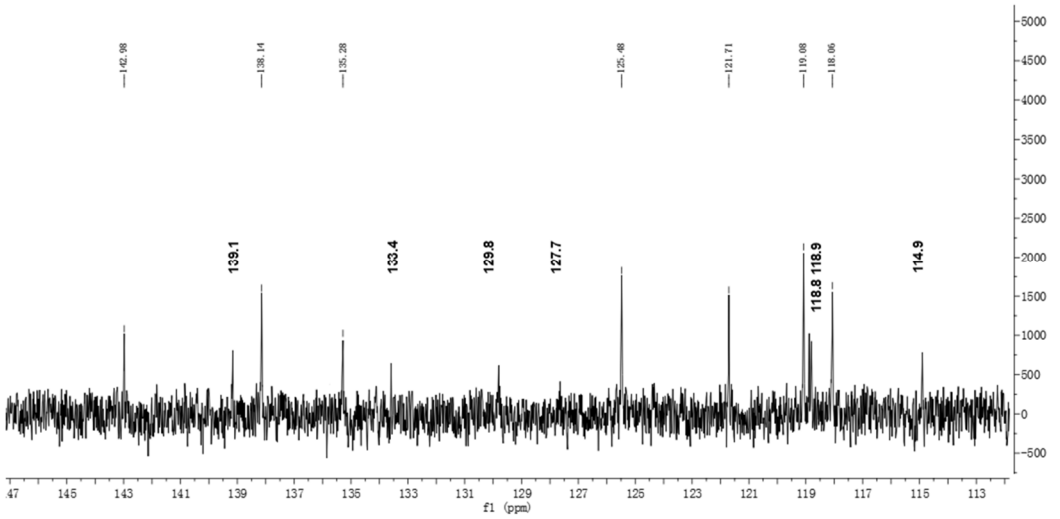

Figure S28. 13C-NMR Spectrumof Streptoanthraquinone A (**2**).

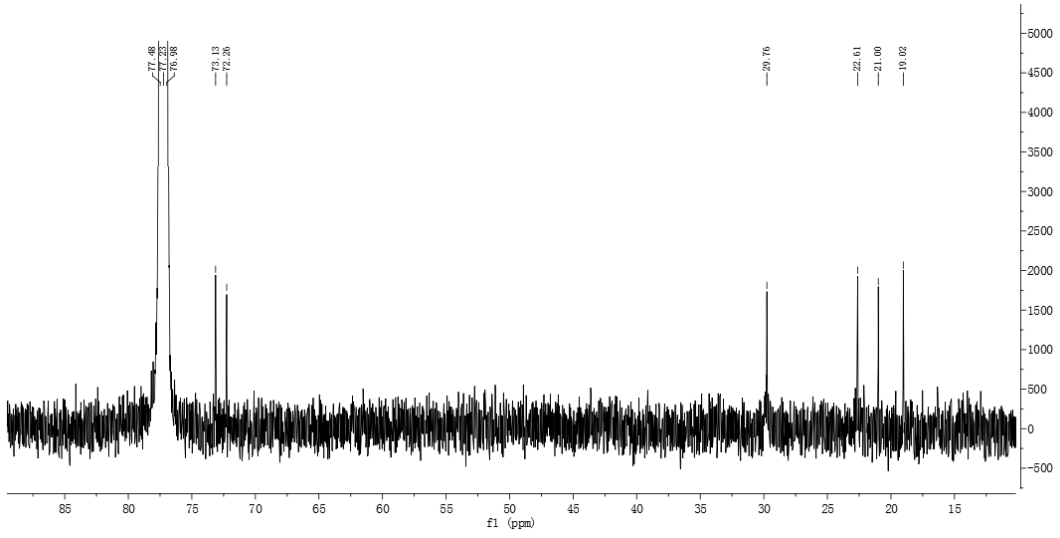

Figure S29. 13C-NMR of Streptoanthraquinone A (**2**).

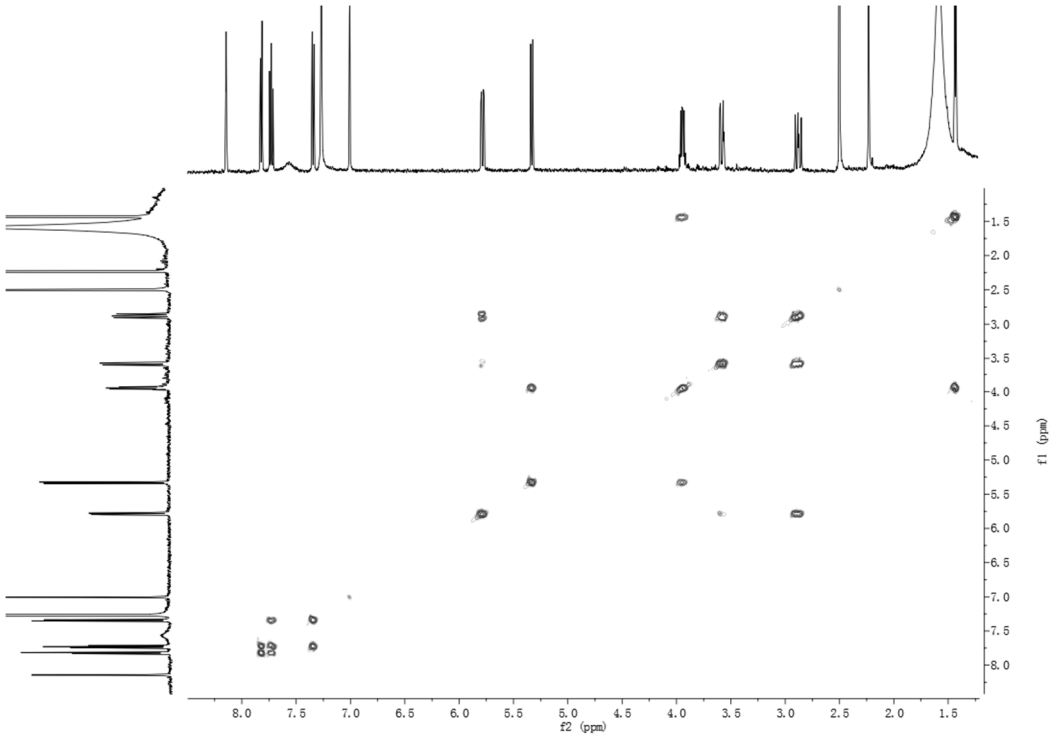

Figure S30. 1H-1H COSY of Streptoanthraquinone A (**2**).

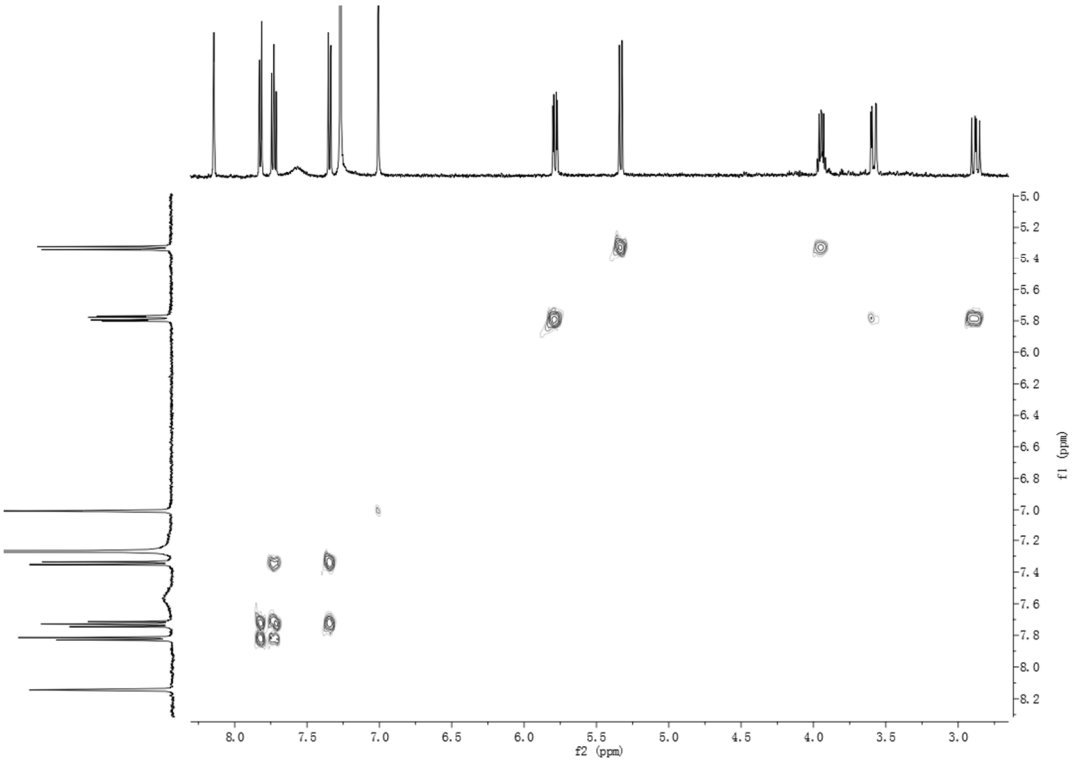

Figure S31. 1H-1H COSY of Streptoanthraquinone A (**2**).

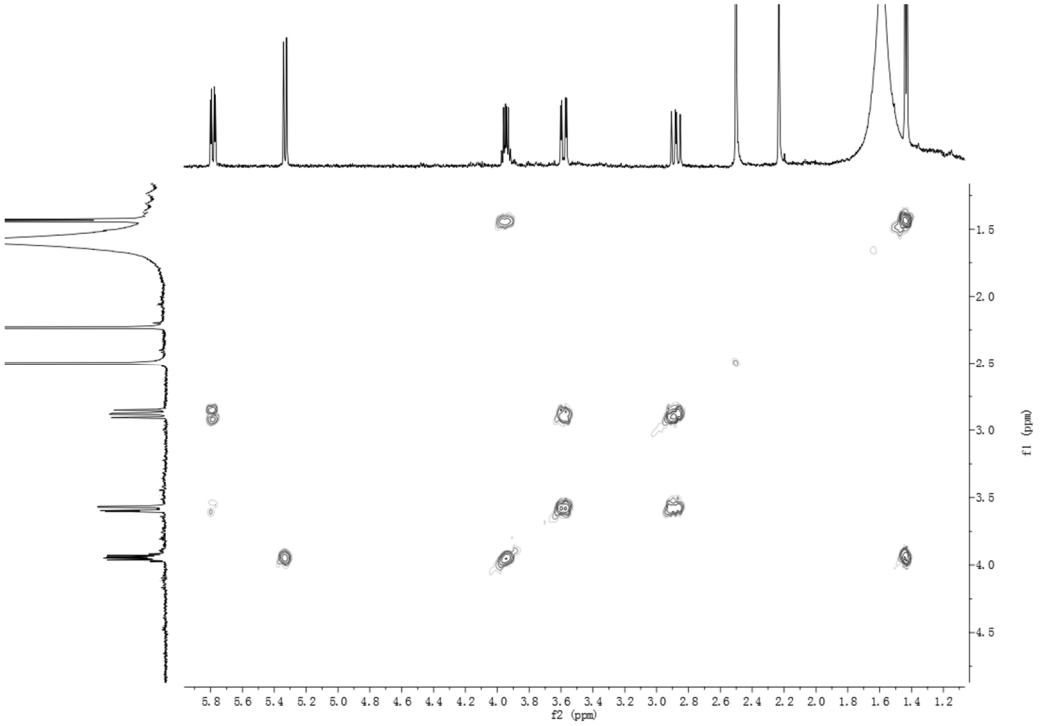

Figure S32. 1H-1H COSY of Streptoanthraquinone A (**2**).

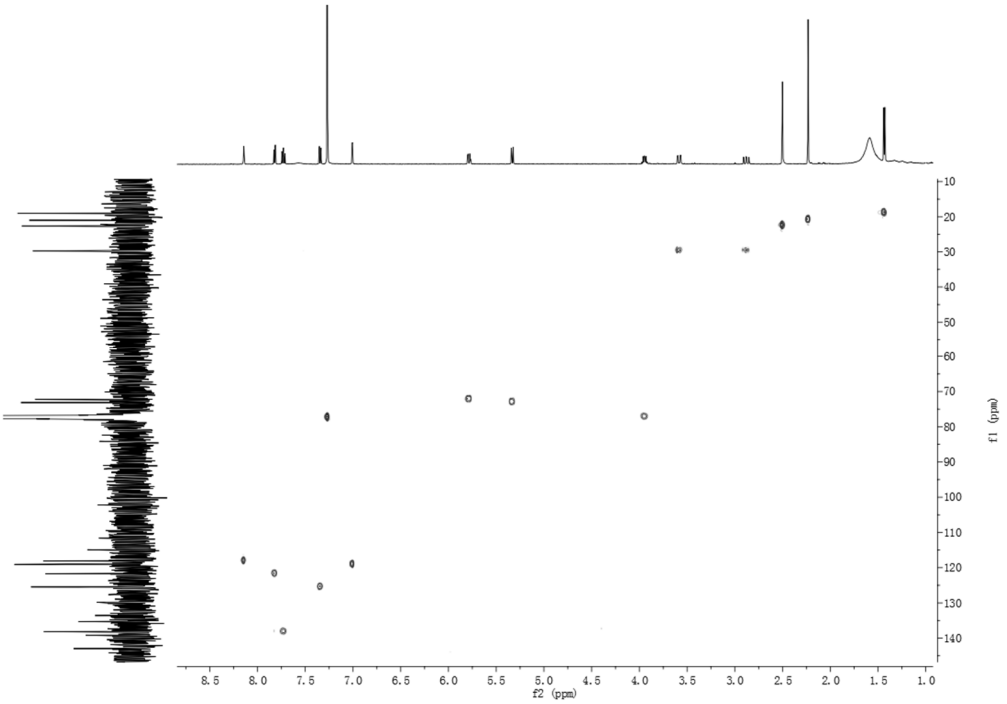

Figure S33. HSQC spectrum of Streptoanthraquinone A (**2**).

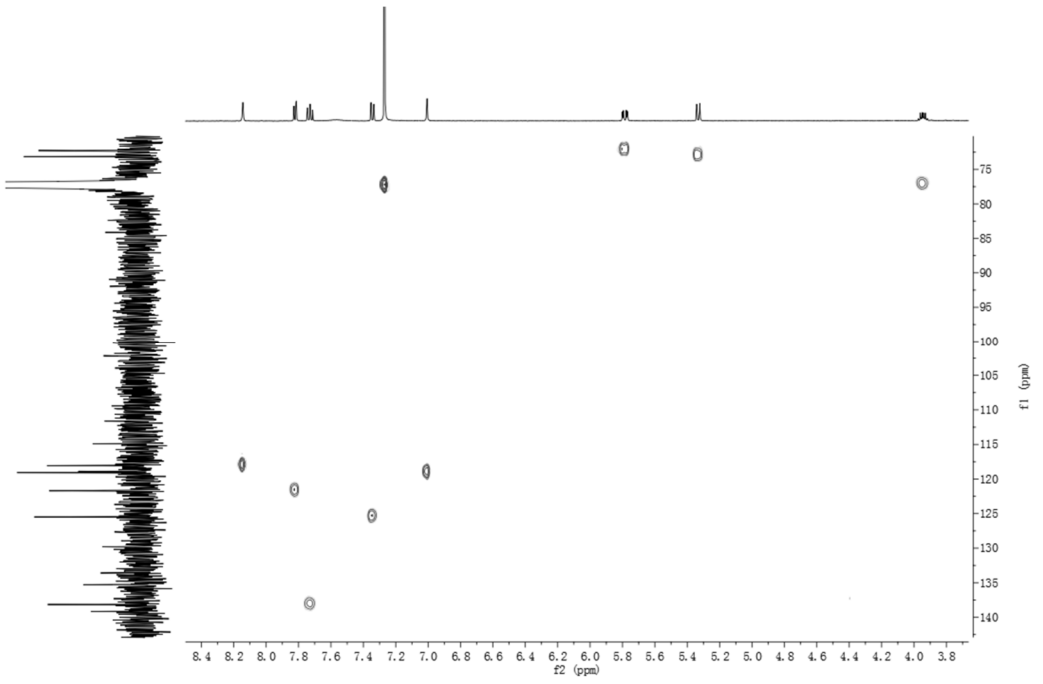

Figure S34. HSQC spectrum of Streptoanthraquinone A (**2**).

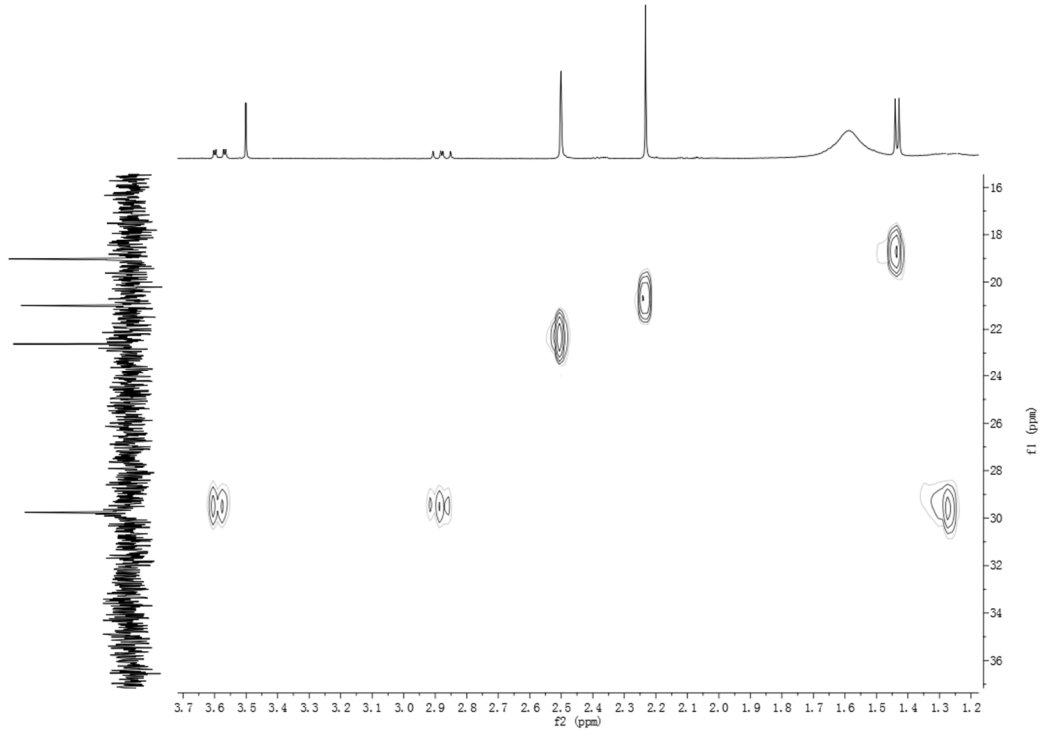

Figure S35. HSQC spectrum of Streptoanthraquinone A (**2**).

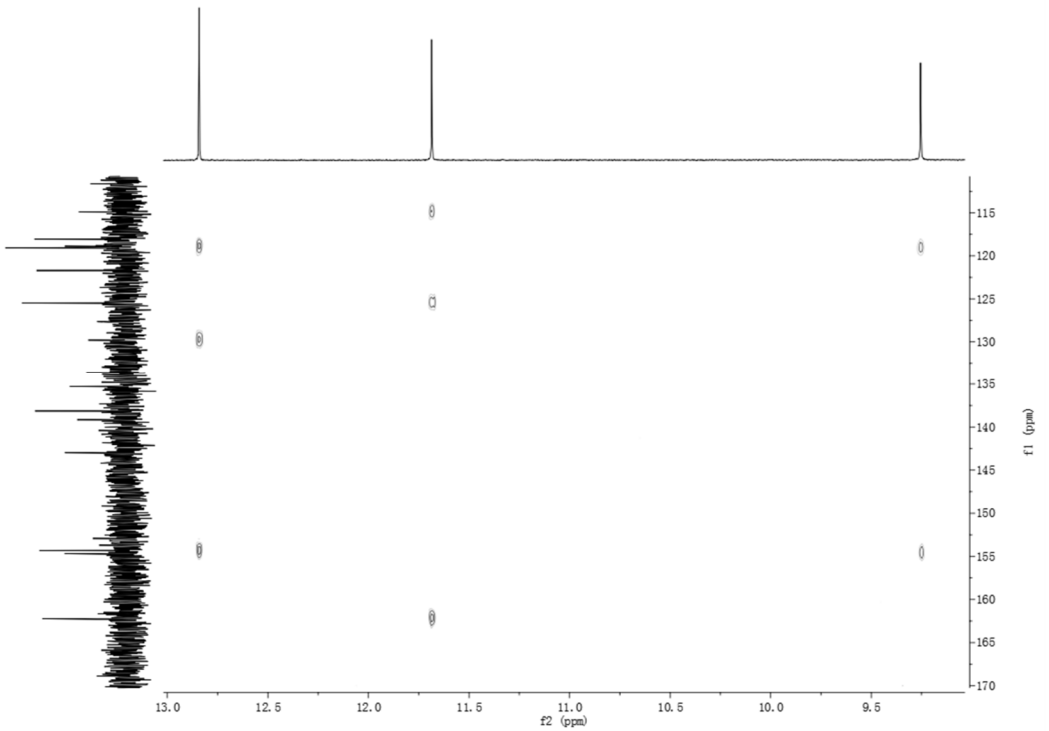

Figure S36. HMBC spectrum of Streptoanthraquinone A (**2**).

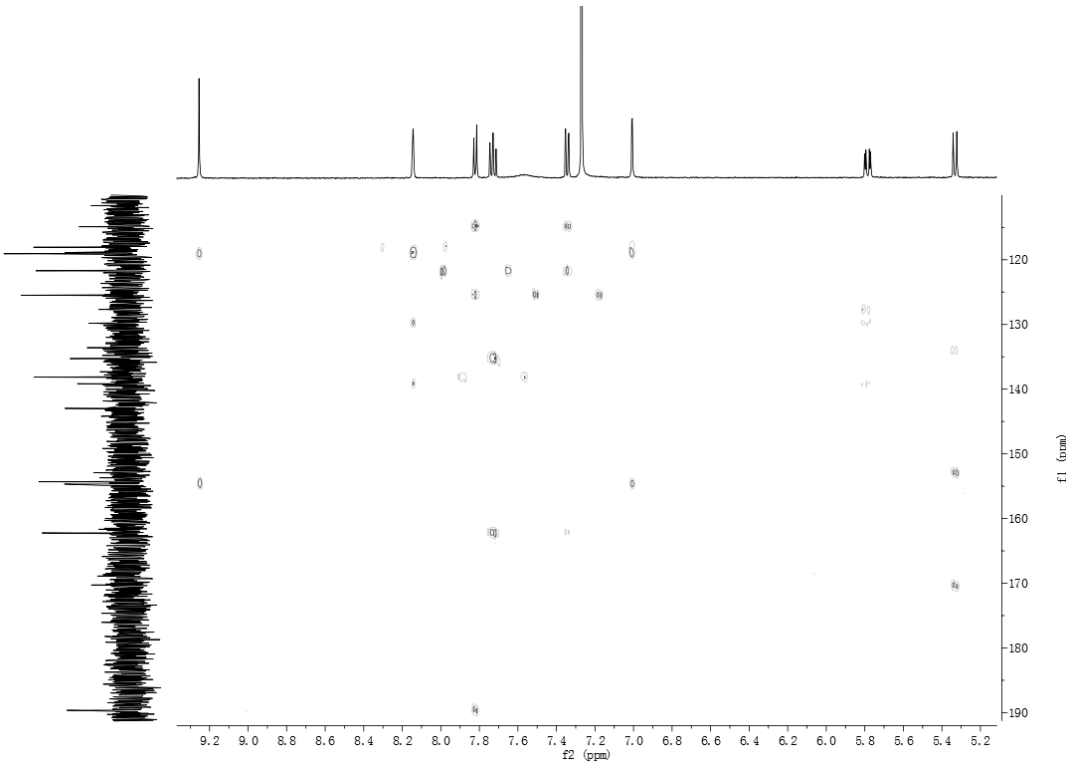

Figure S37. HMBC spectrum of Streptoanthraquinone A (**2**).

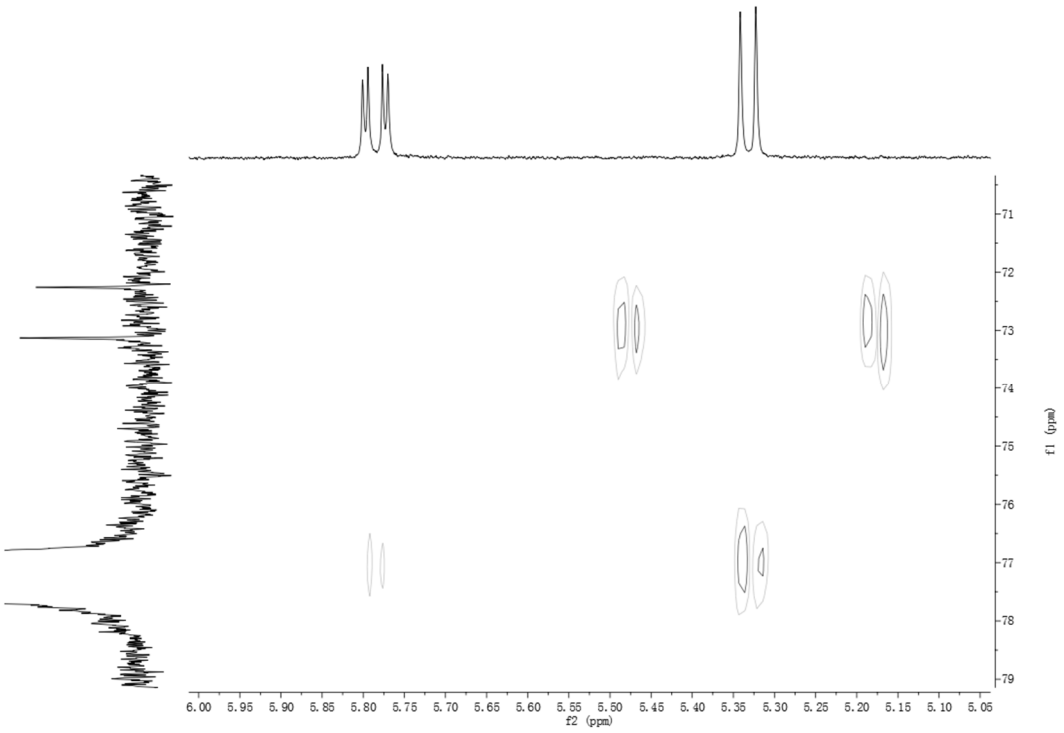

Figure S38. HMBC Spectrum of Streptoanthraquinone A (**2**).

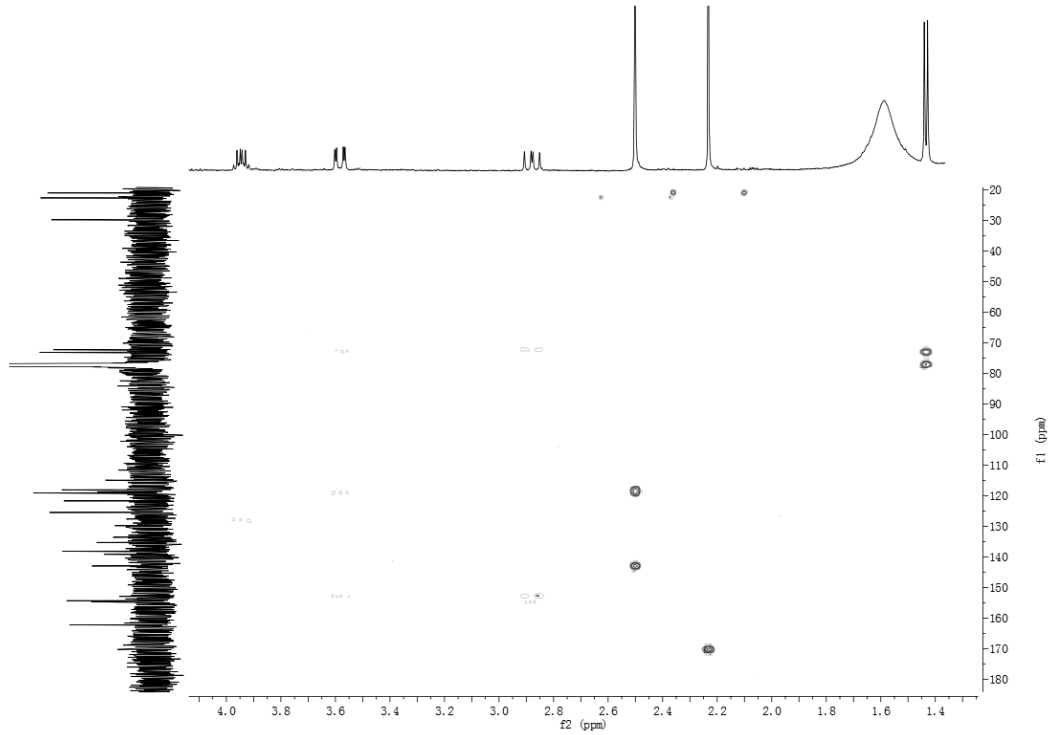

Figure S39. HMBC Spectrum of Streptoanthraquinone A (**2**).

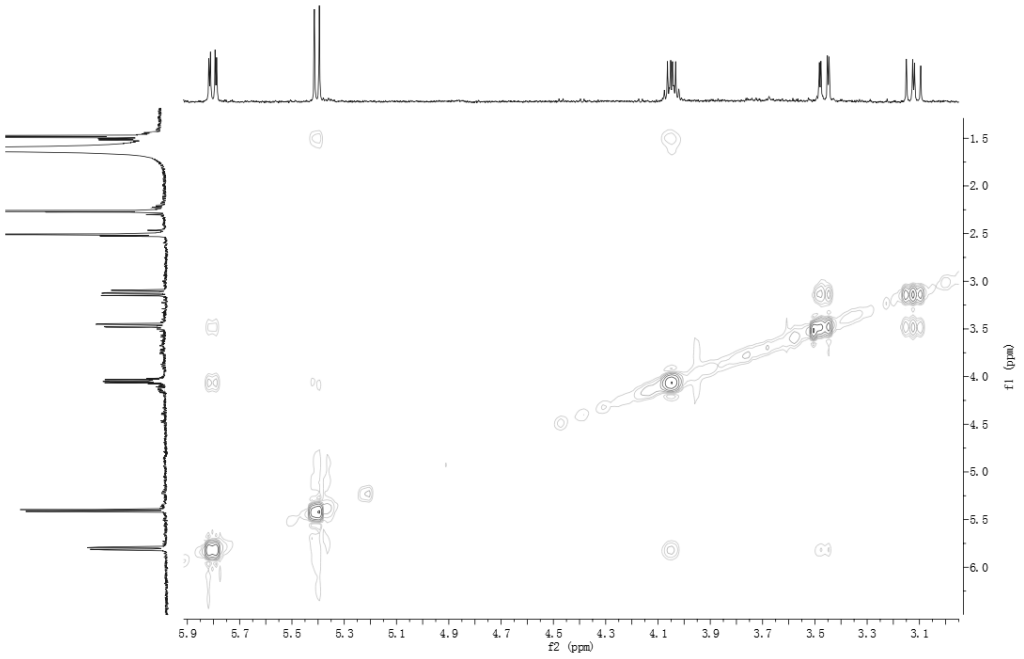

Figure S40. NOESY Spectrum of Streptoanthraquinone A (**2**).

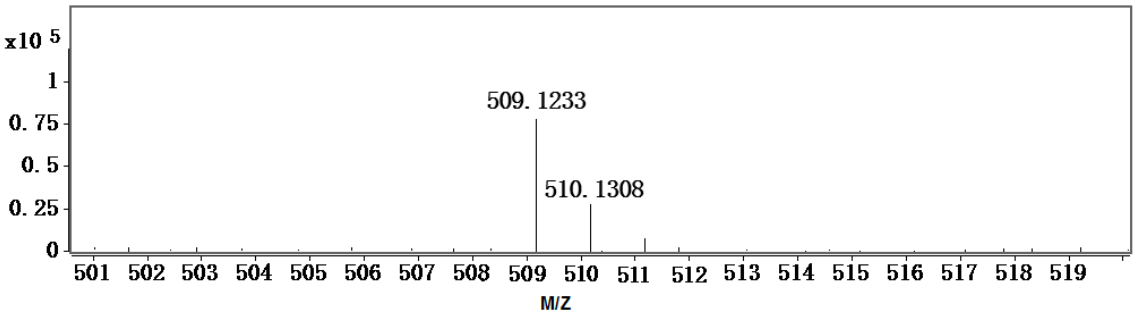

Figure S41. HRESIMS Spectrum of Streptoanthraquinone A (**2**).

TGCAGTCGAACGATGAAGCCCTTCGGGGTGGATTAGTGGCGAACGGGTGAGTAACACGT
GGGCAATCTGCCCTTCACTCTGGGACAAGCCCTGGAAACGGGGTCTAATACCGGATAACA
CTCTGTCCCGCATGGGACGGGGTTGAAAGCTCCGGCGGTGAAGGATGAGCCCGCGGCCT
ATCAGCTTGTTGGTGGGGTAATGGCCTACCAAGGCGACGACGGGTAGCCGGCCTGAGAG
GGCGACCGGCCACACTGGGACTGAGACACGGCCCAGACTCCTACGGGAGGCAGCAGTGG
GGAATATTGCACAATGGGCGAAAGCCTGATGCAGCGACGCCGCGTGAGGGATGACGGCC
TTCGGGTTGTAAACCTCTTTCAGCAGGGAAGAAGCGAAAGTGACGGTACCTGCAGAAGA
AGCGCC-GGCTAACTACGTGCCAGCAGCCGCGGTAATACGTAGGGCGCAAGCGTTGTCCG
GAATTATTGGGCGTAAAGAGCTCGTAGGCGGCTTGTCACGTCGGATGTGAAAGCCCGGG
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TTCCTGGTGTAGCGGTGAAATGCGCAGATATCAGGAGGAACACCGGTGGCGAAGGCGGA
TCTCTGGGCCATTACTGACGCTGAGGAGCGAAAGCGTGGGGAGCGAACAGGATTAGATA
CCCTGGTAGTCCACGCCGTAAACGTTGGGAACTAGGTGTTGGCGACATTCCACGTCGTCG
GTGCCGCAGCTAACGCATTAAGTTCCCCGCCTGGGGAGTACGGCCGCAAGGCTAAAACTC
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TGGTCGGTATACAGGTGGTGCATGG-CTGTCGTCAGCTCGTGTCGTGAGATGTTGGGTTAA
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ACCCCATGAAGTCGGAGTTGCTAGTAATCGCAGATCAGCATTGCTGCGGTGAATACGTTC
CCGGGCCTTGTACACACCGCCCGTCACGTCACGAAAGTCGGTAACACCCGAAGCCGGTGG
CCCAACCCC

Figure S42. 16S rDNA sequence of *Streptomyces* sp. 182SMLY.

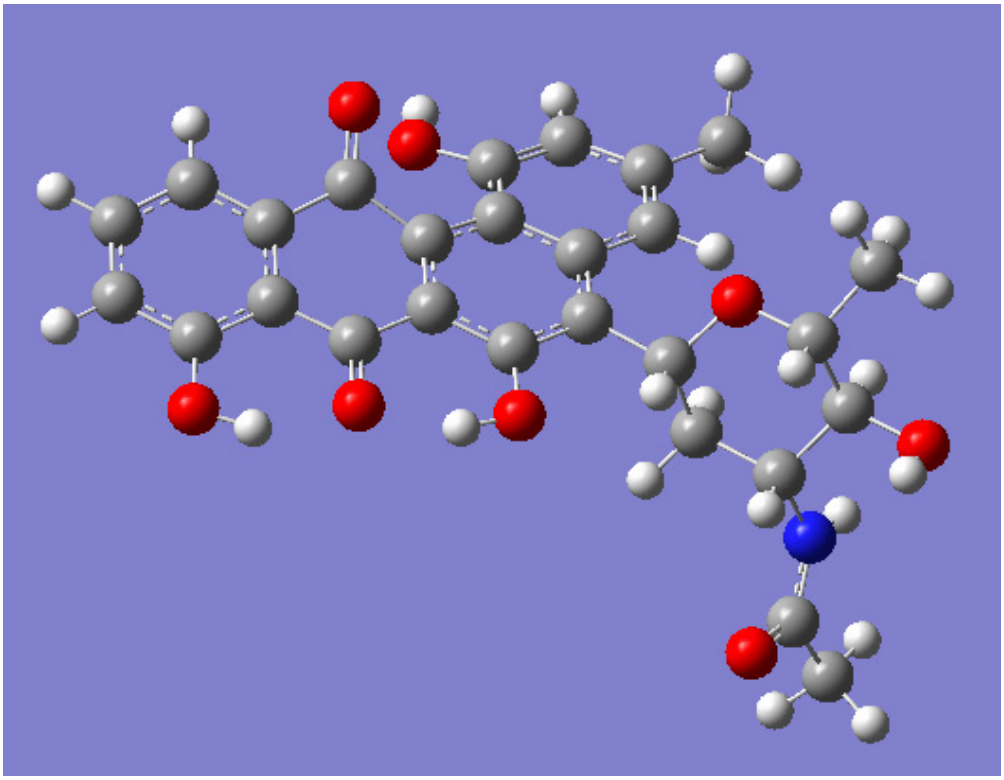

Figure S43. The Optimized Geometry of Conformer 1 of (1′*R*, 3′*R*, 4′*S*, 5′*R*)-**1**.

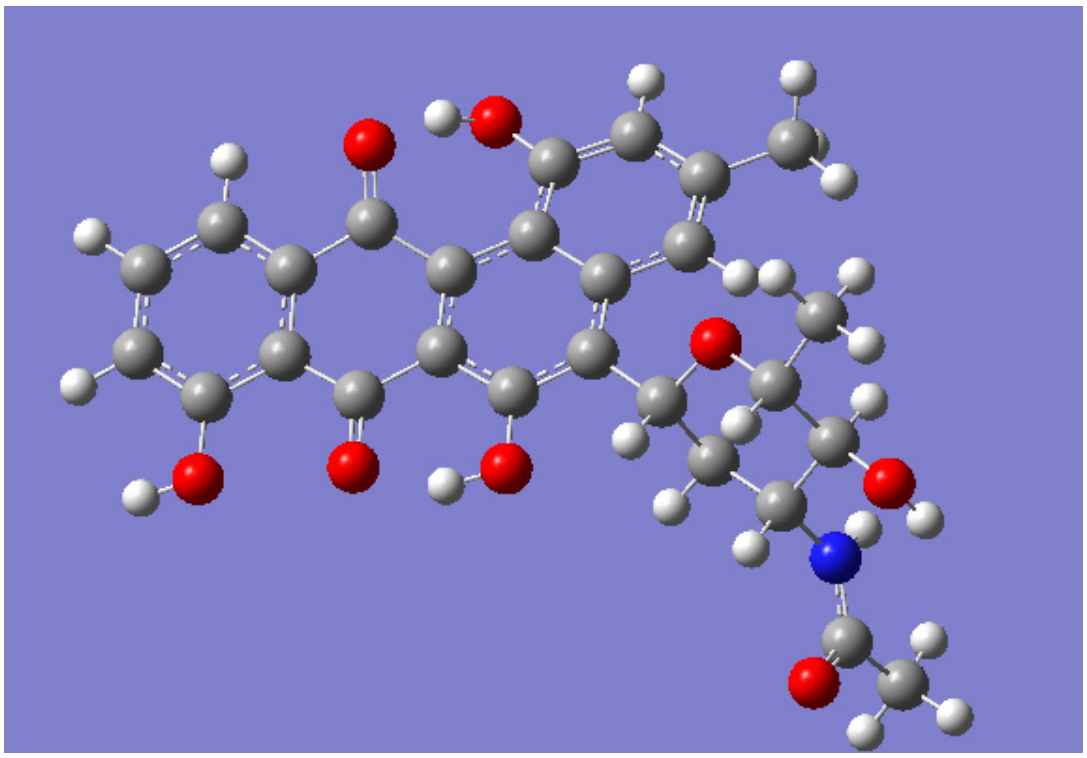

Figure S44. The Optimized Geometry of Conformer 2 of (1′*R*, 3′*R*, 4′*S*, 5′*R*)-**1**.

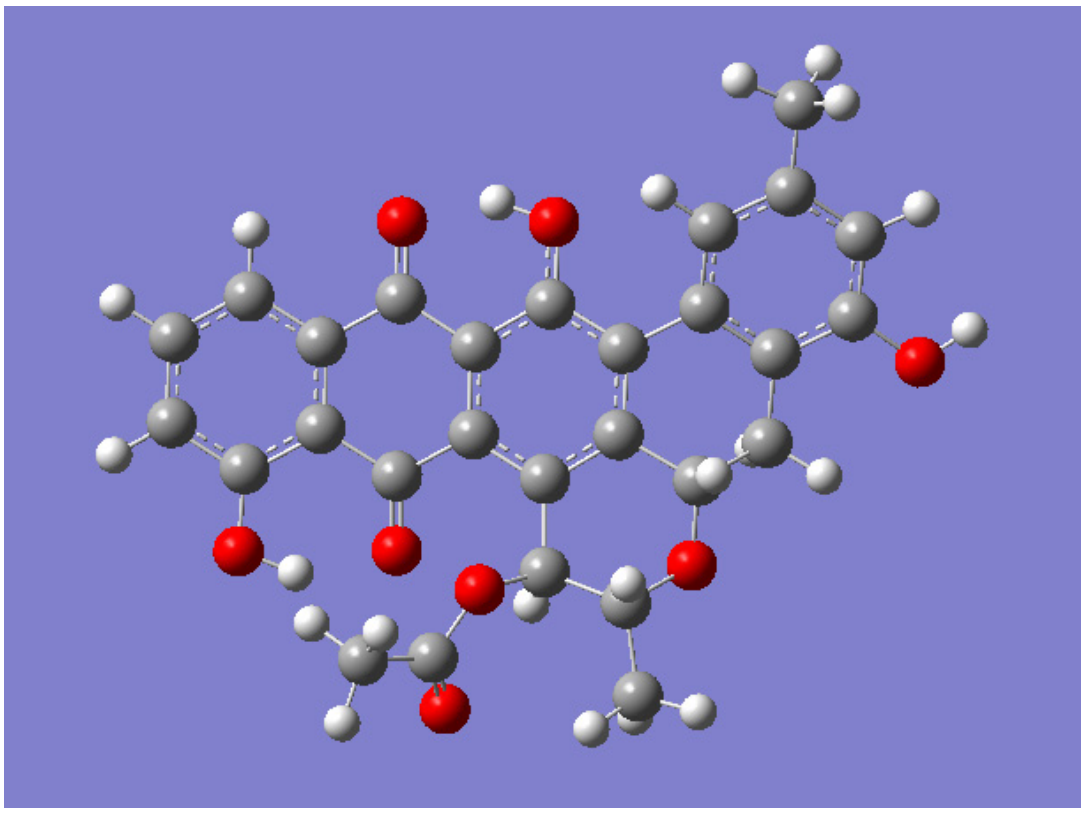

Figure S45. The Optimized Geometry of Conformer 1 of (6′*S*, 16′*R*, 17′*R*)-**2**.

Table S1. Sequences producing significant alignments.

Accession	Description	Max Score	Total Score	Query Coverage	Evalue	Ident
KF981731.1	*Streptomyces griseus* strain CB00830 16S ribosomal RNA gene	2542	2542	100%	0.0	100%
HQ6074 11.1	*Streptomyces pluricolorescens* strain 999 16S ribosomal RNA gene	2542	2542	100%	0.0	100%
FJ792544.1	*Streptomyces tricolor* strain cfcc3055 16S ribosomal RNA gene	2542	2542	100%	0.0	100%
EU7814 91.1	*Streptomyces sporovirgulis* strain L0801 16S ribosomal RNA gene	2542	2542	100%	0.0	100%
EU257232.1	*Streptomyces* sp. A15Ydz-AH 16S ribosomal RNA gene	2542	2542	100%	0.0	100%
EU119184.1	*Streptomyces* sp. HBUM74775 16S ribosomal RNA gene	2542	2542	100%	0.0	100%
JQ654447.1	*Streptomyces sporovirgulis* strain TGNBSA5 16S ribosomal RNA gene	2540	2540	99%	0.0	100%

Table S2. Optimized Z-Matrixes of Conformer 1 of (1′*R*, 3′*R*, 4′*S*, 5′*R*)-**1**. Standard orientation.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	−6.57339	−2.12099	−0.20611
2	6	0	−5.22477	−2.43785	0.036568
3	6	0	−4.27011	−1.3966	0.13893
4	6	0	−4.70468	−0.0561	0.032749
5	6	0	−6.04365	0.247081	−0.17531
6	6	0	−6.97149	−0.79675	−0.31107
7	6	0	−2.86044	−1.68059	0.384568
8	6	0	−3.71602	1.038823	0.209917
9	6	0	−2.27202	0.717085	0.000235
10	6	0	−1.87148	−0.59079	0.319624
11	6	0	−0.48253	−0.86923	0.52819
12	6	0	0.472659	0.146009	0.478701
13	6	0	0.090126	1.444061	0.018538
14	6	0	−1.29802	1.711967	−0.28777
15	1	0	−7.28637	−2.9349	−0.29543
16	1	0	−6.35685	1.283296	−0.24217
17	1	0	−8.017	−0.56637	−0.49496
18	6	0	−1.59956	2.946777	−0.96337
19	6	0	−0.63525	3.91536	−1.13266
20	1	0	−0.89969	4.839408	−1.64285
21	6	0	0.699535	3.701631	−0.71189
22	6	0	1.048479	2.479953	−0.17527
23	1	0	2.075766	2.299137	0.105377
24	6	0	1.717171	4.796356	−0.90129
25	1	0	1.451636	5.68382	−0.31185
26	1	0	2.716837	4.472867	−0.59592
27	1	0	1.764103	5.116145	−1.95009
28	8	0	−4.90258	−3.73863	0.162969
29	1	0	−3.93161	−3.78506	0.353745
30	8	0	−0.06274	−2.12326	0.812715
31	1	0	−0.86411	−2.71054	0.816762

Table S2. *Cont.*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
32	8	0	−4.07807	2.141094	0.616494
33	8	0	−2.49044	−2.86805	0.599146
34	6	0	2.742257	−0.56084	−0.44462
35	6	0	1.90254	−0.2594	0.807303
36	6	0	4.166068	−0.98135	−0.04063
37	1	0	2.783012	0.323388	−1.09103
38	1	0	1.853156	−1.17651	1.405948
39	6	0	4.784373	0.042681	0.922754
40	1	0	4.116066	−1.94762	0.473586
41	6	0	3.826852	0.325443	2.100374
42	1	0	4.963172	0.984245	0.387873
43	1	0	3.702804	−0.61233	2.669047
44	1	0	2.273241	−1.37088	−1.01425
45	8	0	2.541593	0.742557	1.614566
46	6	0	4.333989	1.422545	3.022094
47	1	0	3.63765	1.573466	3.853869
48	1	0	5.311092	1.151296	3.431983
49	1	0	4.435553	2.368802	2.477326
50	8	0	6.065794	−0.37494	1.390407
51	1	0	5.952001	−1.22804	1.845724
52	7	0	5.022492	−1.17524	−1.20512
53	6	0	5.237978	−2.37766	−1.78539
54	8	0	4.751606	−3.43154	−1.34226
55	6	0	6.11987	−2.37871	−3.01597
56	1	0	5.562763	−2.81981	−3.8497
57	1	0	6.465406	−1.38227	−3.30541
58	1	0	6.989353	−3.01848	−2.82809
59	1	0	5.419609	−0.34999	−1.63877
60	8	0	−2.83922	3.09323	−1.50742
61	1	0	−2.8735	3.936539	−1.99307

Table S3. Optimized Z-Matrixes of of Conformer 2 of (1′*R*, 3′*R*, 4′*S*, 5′*R*)-**1**. Standard orientation.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	−6.58576	−2.23913	−0.21749
2	6	0	−5.22579	−2.55237	−0.04242
3	6	0	−4.27982	−1.50782	0.094572
4	6	0	−4.74015	−0.17343	0.055855
5	6	0	−6.09174	0.123201	−0.10331
6	6	0	−7.0112	−0.91966	−0.24676
7	6	0	−2.84886	−1.74223	0.311116
8	6	0	−3.78984	0.955263	0.189873
9	6	0	−2.33905	0.722268	0.002378
10	6	0	−1.90314	−0.59576	0.252618
11	6	0	−0.51205	−0.85235	0.450178
12	6	0	0.427728	0.17939	0.405567
13	6	0	0.024236	1.477156	−0.02324

Table S3. *Cont.*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
14	6	0	−1.38345	1.768705	−0.23713
15	6	0	−1.68947	3.075246	−0.77638
16	6	0	−0.69239	3.996618	−1.02366
17	6	0	0.668964	3.718414	−0.77774
18	6	0	1.004104	2.478981	−0.28136
19	6	0	1.71302	4.764551	−1.06972
20	8	0	−4.82076	−3.84107	−0.00994
21	8	0	−0.05662	−2.09646	0.709259
22	8	0	−4.24635	2.069983	0.50507
23	8	0	−2.41961	−2.89666	0.519324
24	6	0	2.692389	−0.57965	−0.50735
25	6	0	1.860674	−0.21723	0.737271
26	6	0	4.116116	−0.96863	−0.08376
27	6	0	4.728307	0.115567	0.820584
28	6	0	3.790364	0.413961	2.001742
29	8	0	2.504198	0.811132	1.504147
30	6	0	4.289067	1.536586	2.897182
31	8	0	5.977485	−0.3077	1.362452
32	7	0	4.966122	−1.22137	−1.24279
33	6	0	5.616503	−2.38936	−1.4755
34	8	0	5.586704	−3.34562	−0.68646
35	6	0	6.390619	−2.46491	−2.77439
36	8	0	−2.93464	3.457681	−1.17896
37	1	0	−7.29863	−3.05292	−0.3242
38	1	0	−6.41542	1.15708	−0.12585
39	1	0	−8.06583	−0.69909	−0.38281
40	1	0	−0.99096	4.956632	−1.43617
41	1	0	2.04132	2.251979	−0.08619
42	1	0	1.520871	5.682519	−0.49946
43	1	0	2.717322	4.411127	−0.81706
44	1	0	1.705114	5.043858	−2.13126
45	1	0	−5.59062	−4.42412	−0.14314
46	1	0	−0.85518	−2.69767	0.712807
47	1	0	2.722391	0.270943	−1.1987
48	1	0	1.808763	−1.11037	1.370678
49	1	0	4.090491	−1.90175	0.486687
50	1	0	4.858397	1.041254	0.237173
51	1	0	3.677078	−0.51135	2.589953
52	1	0	2.219512	−1.41776	−1.03058
53	1	0	3.577903	1.714537	3.711067
54	1	0	5.256375	1.273315	3.334766
55	1	0	4.404831	2.465867	2.326833
56	1	0	6.56145	−0.51664	0.613089
57	1	0	6.353254	−1.53951	−3.35525
58	1	0	7.435235	−2.70826	−2.55295
59	1	0	5.984073	−3.28311	−3.37934
60	1	0	5.015243	−0.49768	−1.95105
61	1	0	−3.59531	3.090039	−0.54117

Table S4. Optimized Z-Matrixes of Conformer 1 of (6′*S*, 16′*R*, 17′*R*)-**2**. Standard orientation.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.715434	−2.26822	−0.43924
2	6	0	4.907718	−1.12172	−0.32309
3	6	0	3.495798	−1.25714	−0.24673
4	6	0	2.941269	−2.55743	−0.27372
5	6	0	3.752335	−3.68344	−0.38148
6	6	0	5.141711	−3.52954	−0.4691
7	6	0	2.640604	−0.07112	−0.13037
8	6	0	1.479828	−2.72632	−0.17092
9	6	0	0.615796	−1.54209	−0.11636
10	6	0	1.158195	−0.22385	−0.14482
11	6	0	0.281076	0.882229	−0.19481
12	6	0	−1.11021	0.646101	−0.21102
13	6	0	−1.67063	−0.62528	−0.03838
14	6	0	−0.78923	−1.7372	−0.05084
15	6	0	−3.14315	−0.76589	0.092731
16	6	0	−2.04477	1.817436	−0.458
17	6	0	−3.29621	1.381253	−1.21226
18	6	0	−3.94768	0.224891	−0.50216
19	6	0	−3.74617	−1.80542	0.826174
20	6	0	−5.34207	0.114805	−0.40165
21	6	0	−5.13518	−1.89043	0.94864
22	6	0	−5.93157	−0.92655	0.317593
23	8	0	−6.09359	1.075216	−1.03093
24	8	0	−1.3229	−2.96388	−0.04223
25	8	0	5.528483	0.070101	−0.30513
26	8	0	3.175277	1.052955	−0.02305
27	6	0	0.765313	2.32821	−0.16955
28	6	0	−0.30355	3.387558	−0.5613
29	8	0	1.167581	2.579442	1.217536
30	6	0	2.253035	3.341509	1.453634
31	6	0	2.611676	3.334517	2.915187
32	8	0	2.859282	3.9532	0.591719
33	8	0	−1.38358	2.78215	−1.26389
34	6	0	0.24281	4.482099	−1.46527
35	8	0	1.000038	−3.88376	−0.15981
36	6	0	−5.77549	−3.0129	1.730495
37	1	0	6.790955	−2.13312	−0.50554
38	1	0	3.302318	−4.66933	−0.39649
39	1	0	5.776606	−4.40639	−0.55875
40	1	0	−3.00473	1.103875	−2.23643
41	1	0	−3.13125	−2.54733	1.319522
42	1	0	−7.01691	−0.97613	0.390084
43	1	0	−7.0365	0.910262	−0.85759
44	1	0	−0.56319	−3.61983	−0.09372
45	1	0	4.815587	0.760657	−0.21666
46	1	0	1.748047	3.624039	3.523736
47	1	0	2.90227	2.320316	3.212403
48	1	0	3.44249	4.019933	3.093852

Table S4. *Cont.*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
49	1	0	1.647865	2.445419	−0.79431
50	1	0	−0.69079	3.824665	0.371479
51	1	0	0.641248	4.053682	−2.39233
52	1	0	−0.55699	5.184946	−1.72352
53	1	0	1.044201	5.027378	−0.96094
54	1	0	−3.97812	2.231517	−1.28916
55	1	0	−2.33394	2.275675	0.503258
56	1	0	−6.53505	−2.6356	2.425838
57	1	0	−6.2785	−3.72513	1.062556
58	1	0	−5.03038	−3.56936	2.308534