Supporting Information

Emeriones A–C: Three Highly Methylated Polyketides with Bicyclo[4.2.0]octene and 3,6-dioxabicyclo[3.1.0]hexane Functionalities from *Emericella nidulans*

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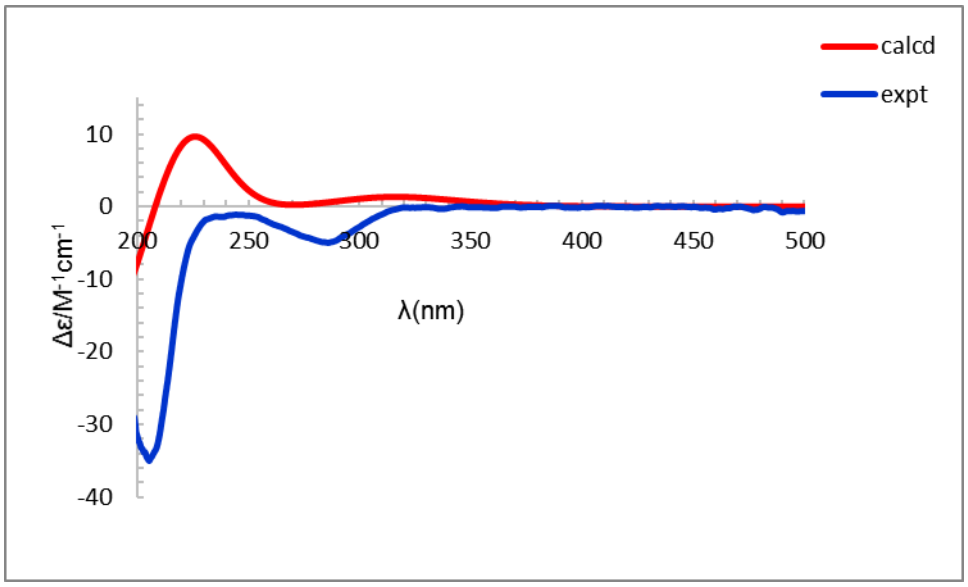

Figure S1. Experimental and calculated ECD spectra of **3**.

Experimental section:

Ceneral experimental procedures

Optical rotations were determined with a PerkinElmer PE-341 polarimeter (PerkinElmer, Waltham, MA, USA). UV spectra were measured by a PerkinElmer Lambda 35 spectrophotometer (PerkinElmer, Inc.). IR spectra were recorded with a Bruker Vertex 70 FT-IR spectrophotometer (Bruker, Karlsruhe, Germany). ECD data were obtained using a JASCO-810 spectrometer. NMR spectra were recorded on a Bruker AM-400 NMR spectrometer (Bruker, Karlsruhe, Germany). High-resolution electrospray ionization mass spectrometry (HRESIMS) data were acquired using a Bruker micrOTOF II spectrometer. Compounds were purified by a Dionex HPLC system semipreparative HPLC equipped with an Ultimate 3000 DAD detector (Thermo Fisher, Scientific, Germany). Chemical shifts are expressed in ppm with reference to the DMSO (δ_H 2.50/δ_C 39.52) signals. Single-crystal X-ray diffraction experiments were carried out with a Bruker APEX DUO diffractometer using graphite-monochromated Cu Kα radiation. Silica gel (80-120 mesh, 100-200 mesh, and 200-300 mesh, Qingdao Marine Chemical Inc., Qingdao, People′s Republic of China), and Sephadex LH-20 (GE Healthcare Bio-Sciences AB, Sweden) were used

in the chromatography processes. Thin-layer chromatography (TLC) was performed with silica gel 60 F_{254} and RP-C_{18} F_{254} plates. Fractions were monitored by TLC, and spots were visualized by spraying heated silica gel plates with 10% H_2SO_4 in EtOH.

Fungal Material

The fungus *Emericella nidulans* was isolated from the Annelida Whitmania pigra Whitman in 1-Dec-2017, Qichun County, Hubei Province, China. NCBI BLAST analysis of the partial 16S rRNA sequence of *E. nidulans* (deposited in GeneBank with an accession number MK828368) is 100% identical to *Emericella nidulans* (KC800583.1).

Fermentation, Extraction, and Isolation.

The fungus *Emericella nidulans* was fermented on a solid-substrate medium (rice30 kg) for 28 days at 28 ℃. Then the mycelia and rice medium were extracted with ethanol, and the solvent was removed in vacuo to yield 200 g of organic residue. The crude extract was chromatographed over silica gel (80–120 mesh) and eluted with a gradient system of petroleum ether-EtOAc (30:1→0:100, v/v) to give five fractions (Fr.1–Fr.5). Fr.3 (2.0 g) was further fractionated on a silica gel column eluted with CH_2Cl_2/MeOH (80:1–0:1) to obtain six major fractions (Fr.3.1–Fr.3.6) based on the TLC analysis. Fraction 3.3 (0.8 g) was further refined by a Sephadex LH-20 CC and isostatically eluted with MeOH to obtain fractions 3.3.1–3.3.3. Fr.3.3.2 (0.4 g) and Fr.3.3.3 (0.2 g) was further separated via semipreparative HPLC (MeOH–H_2O, 85/15, v/v) to afford compounds **1** (7.5 mg; t_R 13.2 min), **2** (4.7 mg; t_R 13.2 min), and **3** (1.2 mg; t_R 9.0 min), respectively.

Compound **1**: Colorless crystal, $[\alpha]^{25}_{D}$ −7.7 (*c* 0.13, CH_2Cl_2); UV (MeOH) λ_{max} (log ε) 216 (4.07) nm; CD (MeOH) λ_{max} ($\Delta\varepsilon$) 223 (-26.6), 283 (−2.5) nm; IR (KBr) ν_{max} = 3437, 2972, 2932, 1708, 1632, 1452, and 1380 cm^{-1}; ^1H and ^{13}C NMR data (DMSO) see Table 1; HRESIMS $[M + Na]^+$ *m/z* 495.3077 (calcd $C_{29}H_{44}O_5Na$ for 495.3086).

Compound **2**: Colorless crystal, $[\alpha]^{25}_{D}$ −4.9 (*c* 0.65, CH_2Cl_2); UV (MeOH) λ_{max} (log ε) 211 (4.07) nm; CD (MeOH) λ_{max} ($\Delta\varepsilon$) 223 (+31.4), 285 (-1.2) nm; IR (KBr) ν_{max} = 3454, 2969, 2927, 1711, 1629, 1456, and 1381 cm^{-1}; ^1H and ^{13}C NMR data (DMSO)

see Table 1; HRESIMS $[M + Na]^+$ *m/z* 495.3093 (calcd $C_{29}H_{44}O_5Na$ for 495.3086).

Compound **3**: white powder, $[\alpha]^{25}_D$ −48.5 (*c* 0.16, CH_2Cl_2); UV (MeOH) λ_{max} (log ε) 205 (4.11) nm; CD (MeOH) λ_{max} ($\Delta\varepsilon$) 285 (−1.8) nm; IR (KBr) ν_{max} = 3430, 2972, 2928, 1709, 1630, 1455, and 1381 cm^{-1}; ^1H and ^{13}C NMR data (DMSO) see Table 1; HRESIMS $[M + Na]^+$ *m/z* 511.3026 (calcd $C_{29}H_{44}O_6Na$ for 511.3036).

X-ray crystallographic data:

Crystal data for compound **1**: $C_{29}H_{44}O_5$, M = 472.64, monoclinic, a = 9.662(2) Å, b = 11.0994(3) Å, c = 13.8485(3) Å, α = 90 °, β = 104.868(2) °, γ = 90 °, V = 1435.41(6) $Å^3$, T = 293(2) K, space group $P2_1$, Z = 2, μ(CuKα) = 0.579 mm^{-1}, 30316 reflections measured, 5718 independent reflections (R_{int} = 0.0419). The final R_1 values were 0.0434 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1285 ($I > 2\sigma(I)$). The final R_1 values were 0.0501 (all date). The final $wR(F^2)$ values were 0.1348 (all date). The goodness of fit on F^2 was 1.078. Flack parameter = 0.09(9). (CCDC 1839898)

Crystal data for compound **2**: $C_{29}H_{44}O_5$, M = 472.64, monoclinic, a = 11.3616(3) Å, b = 10.2680(3) Å, c = 12.1676(3) Å, α = 90 °, β = 96.7930(10) °, γ = 90 °, V = 1409.52(7) $Å^3$, T = 296(2) K, space group $P2_1$, Z = 2, μ(CuKα) = 0.590 mm^{-1}, 17705 reflections measured, 4964 independent reflections (R_{int} = 0.0291). The final R_1 values were 0.0349 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0995 ($I > 2\sigma(I)$). The final R_1 values were 0.0350 (all date). The final $wR(F^2)$ values were 0.0996 (all date). The goodness of fit on F^2 was 1.035. Flack parameter = 0.01(3). (CCDC 1839903)

The crystallographic data for compounds **1** and **2** were collected using a Bruker APEX-II CCD with a graphite monochromator using CuKα radiation. The structures were refined with the SHELXTL refinement package using least squares minimization. The data can be obtained freely from the Cambridge Crystallographic Data Centre by visiting sites of www.ccdc.com.ac.uk/conts/retrieving.html.

Bioactivity Assay:

RAW 264.7 cells were obtained from the Boster Biological Technology Co., Ltd (Wuhan, China) and maintained in DMEM containing 10% fetal bovine serum (FBS) (Gibco BRL Co, Grand Island, NY, USA) at 37 ℃ in humidified incubator containing

5% CO_2. All tested compounds were dissolved in DMSO (the final concentration of DMSO was less than 0.25% in assay). Cell viability was evaluated by the CCK-8 method after 24 h incubation with test compounds of 40 μM. RAW 264.7 cells were seeded into 48-well plates (1×10^5 cells/wells) for 24 h and then pretreated with different concentrations (1−40 μM) of test compounds. After being incubated for 3 h, the cells were stimulated with 100 ng/ml LPS (final concentration) for another 24 h. Indomethacin was used as the positive control in the experiment. NO content in the supernatant was measured using Griess reagent. The absorbance at 540 nm was measured on a microplate reader. All the experiments were performed in three independent replicates.

In TNF-α stimulations, RAW 264.7 cells were plated at a density of 8×10^3 cells/wells in 96-well plates for 24 h. The cells were pretreated with different concentrations (1−40 μM) concentrations of test compounds and then stimulated with 100 ng/ml LPS (final concentration) for another 12 h in incubator. Dexamethasone was used as the positive control in the experiment. TNF-α levels in the supernatant were measured by the ELISA test according to manufacturer's instructions (Boster Biological Technology Co., Ltd Wuhan, China). Concentrations of cytokines were calculated using the cytokines standard calibration curve.

Detailed computational procedures:

ECD calculation for compound 3:

The conformations of **3** generated by BALLOON[1, 2] were subjected to semiempirical PM3 quantum mechanical geometry optimizations using the Gaussian 09 program[3]. Duplicate conformations were identified and removed when the root-mean-square (RMS) distance was less than 0.5 Å for any two geometry-optimized conformations. The remaining conformations were further optimized at the B3LYP/6-31G(d) level in MeOH with the IEFPCM solvation model using Gaussian 09, and the duplicate conformations emerging after these calculations were removed according to the same

RMS criteria above. The harmonic vibrational frequencies were calculated to confirm the stability of the final conformers. The electronic circular dichroism (ECD) spectrum were calculated for each conformer using the TDDFT methodology at the B3LYP/6-311++G(d,p)//B3LYP/6-31G(d) level with MeOH as solvent by the IEFPCM solvation model implemented in Gaussian 09 program. The ECD spectra for each conformer were simulated using a Gaussian function with a bandwidth σ of 0.45 eV. The spectra were combined after Boltzmann weighting according to their population contributions and UV correction was applied[4].

(1) And, M. J. V.; Johnson, M. S., Generating Conformer Ensembles Using a Multiobjective Genetic Algorithm. *J. Chem. Inf. Model.* **2007,** *47*, 2462-2474.
(2) Puranen, J. S.; Vainio, M. J.; Johnson, M. S., Accurate conformation-dependent molecular electrostatic potentials for high-throughput in silico drug discovery. *J. Comput. Chem.* **2010,** *31*, 1722-1732.
(3) Frisch MJT, G. W. S., H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. *J.*, **2009**, Gaussian 09, Revision D 01, Gaussian, Inc, Wallingford, CT.
(4) Zhu, H. J., *Organic Stereochemistry: Experimental and Computational Methods*. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim: Germany, **2015**.

Table S1. Important thermodynamic parameters (a.u.) and Boltzmann distribution of the optimized compound **3** at B3LYP/6-31G(d) level in methanol.

Conformation	**Internal Energy**	**Ratio**
1	-1582.45	48.64%
2	-1582.44	9.72%
3	-1582.44	7.46%
4	-1582.44	5.26%
5	-1582.44	4.94%
6	-1582.44	3.67%
7	-1582.44	2.91%
8	-1582.44	2.91%

9	-1582.44	2.53%
10	-1582.44	2.28%
11	-1582.44	2.14%
12	-1582.44	1.94%
13	-1582.44	1.84%
14	-1582.44	1.43%

Table S2. Optimized coordinates of compound **3** at B3LYP/6-31G(d) level in methanol.

Conformation 1				Conformation 2			
C1	-0.967	3.651	-1.225	C1	0.722	2.721	-1.493
C2	0.274	3.633	-0.723	C2	1.637	2.436	-0.559
C3	2.272	0.093	0.437	C3	1.515	-1.075	-0.091
C4	1.231	0.426	-0.353	C4	0.917	-0.549	0.992
C5	-3.431	-2.804	0.374	C5	-4.598	-1.485	0.412
C6	0.267	3.295	0.748	C6	1.101	2.681	0.833
C7	-0.111	0.618	0.364	C7	-0.308	0.358	0.95
C8	-1.847	1.989	0.491	C8	-1.209	2.167	0.052
C9	4.359	-1.068	1.104	C9	3.582	-1.727	-1.33
C10	4.245	-2.139	-1.036	C10	4.777	-1.856	0.748
C11	-2.053	3.342	-0.225	C11	-0.605	3.177	-0.948
C12	3.749	-0.09	0.104	C12	2.596	-2.142	-0.241
C13	-0.428	1.966	1.129	C13	-0.19	1.912	1.204
C14	-1.573	0.642	-0.279	C14	-1.332	0.619	-0.247
C15	4.644	-2.334	0.423	C15	4.907	-1.526	-0.735
C16	1.528	4.086	-1.411	C16	3.08	2.115	-0.798
C17	1.359	0.584	-1.85	C17	1.343	-0.838	2.419
C18	3.026	-2.958	-1.458	C18	5.035	-0.68	1.688
C19	-3.467	3.586	-0.732	C19	-1.58	3.693	-1.998
C20	4.49	1.255	0.089	C20	1.919	-3.486	-0.567
C21	-0.38	1.799	2.652	C21	-0.651	2.337	2.603
C22	-1.775	0.641	-1.8	C22	-1.046	0.144	-1.676
C23	4.681	-3.694	1.067	C23	5.987	-0.619	-1.262
C24	-3.893	-5.281	0.627	C24	-5.418	-3.35	-1.045
C25	-4.995	-3.903	-1.206	C25	-7.038	-1.55	-0.265
C26	-0.97	-2.548	0.111	C26	-2.259	-2.27	0.886
C27	-3.722	-4.115	-0.357	C27	-5.597	-1.859	-0.678
C28	-2.338	-1.895	-0.194	C28	-3.117	-1.339	0.017
C29	-2.49	-0.453	0.347	C29	-2.777	0.164	0.142
O1	-4.082	-2.491	1.366	O1	-4.938	-1.32	1.575
O2	-0.515	4.352	1.389	O2	0.746	4.101	0.868
O3	5.716	-1.422	0.782	O3	4.62	-2.703	-1.537
O4	4.007	-0.724	-1.175	O4	3.44	-2.374	0.911
O5	-1.901	4.339	0.863	O5	-0.329	4.371	-0.116

O6	-3.837	-0.013	0.136	O6	-3.744	0.81	-0.704
H1	-1.212	3.976	-2.234	H1	0.921	2.729	-2.562
H2	2.066	-0.017	1.503	H2	1.115	-0.805	-1.063
H3	1.25	3.403	1.219	H3	1.87	2.608	1.609
H4	-0.122	-0.154	1.137	H4	-0.917	-0.011	1.783
H5	-2.656	1.892	1.219	H5	-2.14	2.614	0.423
H6	4.123	-0.993	2.164	H6	3.234	-1.206	-2.22
H7	5.09	-2.373	-1.696	H7	5.462	-2.676	1.003
H8	1.919	4.993	-0.93	H8	3.351	1.157	-0.343
H9	1.344	4.314	-2.465	H9	3.728	2.881	-0.35
H10	2.32	3.332	-1.352	H10	3.303	2.063	-1.869
H11	2.403	0.589	-2.162	H11	0.505	-1.264	2.986
H12	0.873	1.496	-2.202	H12	1.624	0.09	2.937
H13	0.873	-0.251	-2.37	H13	2.186	-1.524	2.463
H14	2.183	-2.791	-0.78	H14	4.83	-0.984	2.719
H15	3.259	-4.029	-1.472	H15	4.396	0.176	1.452
H16	2.719	-2.665	-2.466	H16	6.082	-0.361	1.631
H17	-3.562	4.6	-1.133	H17	-1.908	2.867	-2.636
H18	-4.195	3.453	0.073	H18	-1.102	4.45	-2.628
H19	-3.701	2.873	-1.528	H19	-2.461	4.137	-1.524
H20	4.319	1.8	1.023	H20	1.234	-3.385	-1.415
H21	4.13	1.875	-0.738	H21	1.345	-3.829	0.3
H22	5.564	1.087	-0.035	H22	2.681	-4.232	-0.811
H23	-0.752	2.695	3.158	H23	-0.736	3.425	2.673
H24	0.65	1.621	2.99	H24	0.058	2	3.369
H25	-0.988	0.947	2.974	H25	-1.628	1.901	2.84
H26	-1.368	-0.265	-2.26	H26	-0.972	-0.947	-1.724
H27	-1.307	1.494	-2.29	H27	-0.128	0.559	-2.089
H28	-2.847	0.667	-2.022	H28	-1.876	0.443	-2.325
H29	5.004	-3.606	2.109	H29	5.905	-0.533	-2.349
H30	5.385	-4.352	0.544	H30	6.979	-1.02	-1.023
H31	3.695	-4.168	1.047	H31	5.914	0.383	-0.827
H32	-4.695	-5.066	1.339	H32	-5.654	-3.993	-0.189
H33	-2.973	-5.465	1.194	H33	-4.397	-3.577	-1.371
H34	-4.147	-6.198	0.085	H34	-6.095	-3.615	-1.864
H35	-5.854	-3.69	-0.56	H35	-7.323	-2.126	0.622
H36	-5.212	-4.809	-1.783	H36	-7.728	-1.804	-1.077
H37	-4.883	-3.072	-1.911	H37	-7.162	-0.488	-0.029
H38	-0.768	-2.552	1.188	H38	-2.364	-2.018	1.946
H39	-0.16	-2.008	-0.386	H39	-1.202	-2.217	0.613
H40	-0.937	-3.584	-0.241	H40	-2.582	-3.31	0.759
H41	-2.892	-4.332	-1.039	H41	-5.331	-1.262	-1.56
H42	-2.478	-1.889	-1.283	H42	-3.01	-1.621	-1.035

H43	-2.293	-0.484	1.429	H43	-2.964	0.453	1.187
H44	-4.377	-0.562	0.731	H44	-3.764	1.753	-0.48
Conformation 3				Conformation 4			
C1	3.247	-1.239	-1.504	C1	2.673	-1.942	-1.595
C2	2.987	-2.156	-0.564	C2	1.893	-2.768	-0.886
C3	-0.768	-1.835	-0.113	C3	-1.263	-0.727	-0.505
C4	0.037	-1.48	0.904	C4	-0.529	-1.074	0.566
C5	-1.012	4.092	0.358	C5	0.28	3.752	-0.178
C6	3.253	-1.613	0.821	C6	2.212	-2.69	0.59
C7	0.907	-0.232	0.927	C7	0.791	-0.404	0.924
C8	2.709	0.696	0.047	C8	2.924	-0.312	0.332
C9	-2.909	-2.794	0.822	C9	-3.361	-2.267	-0.299
C10	-3.78	-2.246	-1.346	C10	-4.462	-0.191	0.187
C11	3.704	0.093	-0.97	C11	3.636	-1.128	-0.771
C12	-1.789	-2.97	-0.201	C12	-2.627	-1.154	-1.031
C13	2.463	-0.334	1.192	C13	2.076	-1.28	1.216
C14	1.164	0.825	-0.24	C14	1.671	0.596	0.047
C15	-4.118	-2.329	0.137	C15	-4.481	-1.693	0.457
C16	2.664	-3.602	-0.787	C16	0.939	-3.786	-1.435
C17	0.085	-2.214	2.232	C17	-0.952	-2.084	1.621
C18	-3.777	-0.824	-1.906	C18	-4.066	0.655	1.397
C19	4.207	1.063	-2.03	C19	4.666	-0.351	-1.58
C20	-1.168	-4.373	-0.198	C20	-2.514	-1.449	-2.533
C21	2.872	0.131	2.594	C21	2.472	-1.336	2.696
C22	0.705	0.566	-1.681	C22	1.36	0.889	-1.424
C23	-5.213	-1.5	0.755	C23	-5.107	-2.274	1.697
C24	-2.914	5.66	0.939	C24	-1.185	5.749	-0.67
C25	-2.085	5.403	-1.453	C25	-1.894	3.413	-1.376
C26	-1.653	1.819	1.135	C26	0.763	3.736	2.242
C27	-2.339	4.692	-0.104	C27	-1.157	4.257	-0.311
C28	-0.782	2.597	0.12	C28	0.602	2.826	0.994
C29	0.729	2.26	0.185	C29	1.866	1.931	0.838
O1	-0.158	4.804	0.877	O1	1.141	4.13	-0.971
O2	4.665	-1.236	0.842	O2	3.619	-3.062	0.722
O3	-4.009	-3.699	0.609	O3	-4.713	-2.418	-0.777
O4	-2.485	-2.864	-1.475	O4	-3.544	-0.019	-0.91
O5	4.916	-0.174	-0.159	O5	4.465	-2.096	-0.015
O6	1.451	3.159	-0.666	O6	2.983	2.671	0.354
H1	3.228	-1.439	-2.573	H1	2.692	-1.903	-2.682
H2	-0.745	-1.256	-1.026	H2	-0.848	0.025	-1.162
H3	3.209	-2.382	1.599	H3	1.712	-3.464	1.18
H4	0.513	0.33	1.783	H4	0.562	0.11	1.87
H5	3.143	1.636	0.397	H5	3.705	0.216	0.888

H6	-2.686	-2.552	1.858	H6	-2.86	-3.193	-0.032
H7	-4.479	-2.863	-1.926	H7	-5.444	0.135	-0.182
H8	1.742	-3.892	-0.272	H8	-0.077	-3.63	-1.053
H9	3.465	-4.243	-0.394	H9	1.24	-4.8	-1.142
H10	2.545	-3.821	-1.853	H10	0.903	-3.743	-2.528
H11	-0.564	-3.09	2.268	H11	-2.032	-2.116	1.762
H12	-0.208	-1.546	3.052	H12	-0.507	-1.836	2.59
H13	1.101	-2.556	2.461	H13	-0.624	-3.101	1.373
H14	-3.384	-0.837	-2.928	H14	-3.965	1.701	1.093
H15	-3.15	-0.156	-1.305	H15	-3.11	0.327	1.818
H16	-4.792	-0.413	-1.937	H16	-4.831	0.601	2.179
H17	3.387	1.347	-2.695	H17	4.168	0.411	-2.186
H18	4.996	0.598	-2.63	H18	5.211	-1.024	-2.25
H19	4.603	1.972	-1.567	H19	5.382	0.147	-0.919
H20	-0.551	-4.545	0.687	H20	-1.816	-2.274	-2.713
H21	-0.539	-4.495	-1.084	H21	-2.146	-0.566	-3.065
H22	-1.965	-5.123	-0.228	H22	-3.496	-1.717	-2.932
H23	3.959	0.223	2.671	H23	3.469	-1.769	2.813
H24	2.535	-0.58	3.36	H24	1.767	-1.949	3.272
H25	2.43	1.105	2.827	H25	2.481	-0.335	3.139
H26	-0.383	0.626	-1.781	H26	0.465	1.504	-1.544
H27	1.02	-0.408	-2.053	H27	1.221	-0.018	-2.012
H28	1.126	1.336	-2.334	H28	2.189	1.454	-1.862
H29	-5.008	-0.431	0.648	H29	-4.613	-1.907	2.603
H30	-5.302	-1.732	1.82	H30	-5.032	-3.365	1.679
H31	-6.176	-1.711	0.275	H31	-6.167	-2.002	1.757
H32	-2.197	6.459	1.156	H32	-2.221	6.094	-0.76
H33	-3.144	5.145	1.879	H33	-0.677	5.926	-1.623
H34	-3.837	6.115	0.566	H34	-0.689	6.356	0.096
H35	-1.67	4.719	-2.203	H35	-1.971	2.358	-1.095
H36	-1.383	6.233	-1.322	H36	-1.384	3.484	-2.343
H37	-3.026	5.803	-1.845	H37	-2.913	3.796	-1.5
H38	-1.288	1.968	2.158	H38	1.685	4.32	2.158
H39	-1.645	0.749	0.915	H39	0.827	3.117	3.142
H40	-2.695	2.153	1.101	H40	-0.077	4.425	2.366
H41	-3.053	3.88	-0.28	H41	-1.665	4.104	0.649
H42	-1.16	2.384	-0.888	H42	-0.274	2.185	1.159
H43	1.053	2.417	1.225	H43	2.144	1.637	1.858
H44	1.366	4.03	-0.24	H44	2.633	3.253	-0.35
Conformation 5				Conformation 6			
C1	1.879	-2.327	-1.604	C1	-0.412	-2.661	-1.716
C2	1.323	-2.973	-0.571	C2	-1.391	-2.466	-0.825
C3	-1.421	-0.207	0.61	C3	-1.205	0.987	0.153

C4	-0.388	-0.727	1.297	C4	-0.742	0.239	1.169
C5	0.57	3.672	-0.435	C5	3.741	1.868	-0.269
C6	2.111	-2.76	0.699	C6	-0.979	-2.917	0.558
C7	1.055	-0.273	1.118	C7	0.47	-0.682	1.093
C8	2.876	-0.532	-0.112	C8	1.401	-2.39	0.034
C9	-3.721	0.177	-0.28	C9	-3.151	1.869	-1.139
C10	-4.186	-2.16	-0.009	C10	-4.544	1.688	0.809
C11	3.119	-1.543	-1.256	C11	0.852	-3.235	-1.137
C12	-2.915	-0.323	0.913	C12	-2.272	2.078	0.091
C13	2.277	-1.279	1.121	C13	0.299	-2.255	1.129
C14	1.687	0.5	-0.124	C14	1.581	-0.829	-0.041
C15	-4.481	-0.932	-0.862	C15	-4.53	1.605	-0.713
C16	0.18	-3.94	-0.619	C16	-2.798	-2.052	-1.13
C17	-0.584	-1.651	2.482	C17	-1.329	0.256	2.569
C18	-3.478	-3.281	-0.764	C18	-4.929	0.392	1.518
C19	3.88	-0.991	-2.453	C19	1.894	-3.648	-2.167
C20	-3.276	0.461	2.186	C20	-1.578	3.452	0.065
C21	3.107	-1.213	2.409	C21	0.631	-2.878	2.49
C22	0.925	0.644	-1.444	C22	1.429	-0.16	-1.409
C23	-4.919	-1.04	-2.299	C23	-5.559	0.819	-1.482
C24	-1.323	4.839	0.78	C24	4.905	4.101	-0.418
C25	-1.469	4.439	-1.728	C25	2.487	3.846	-1.149
C26	1.991	4.059	1.574	C26	4.321	1.118	2.008
C27	-0.937	3.91	-0.393	C27	3.571	3.384	-0.153
C28	1.248	2.979	0.748	C28	3.249	1.004	0.891
C29	2.271	1.873	0.335	C29	2.984	-0.494	0.568
O1	1.244	4.061	-1.389	O1	4.305	1.394	-1.253
O2	3.457	-3.265	0.439	O2	-0.669	-4.341	0.428
O3	-5.141	0.089	-0.069	O3	-4.158	2.888	-1.282
O4	-3.385	-1.688	1.096	O4	-3.218	2.116	1.186
O5	4.076	-2.51	-0.673	O5	0.473	-4.52	-0.499
O6	3.22	2.362	-0.609	O6	4.039	-1.068	-0.199
H1	1.541	-2.415	-2.634	H1	-0.524	-2.516	-2.788
H2	-1.201	0.479	-0.199	H2	-0.695	0.907	-0.801
H3	1.786	-3.405	1.521	H3	-1.808	-2.918	1.274
H4	1.209	0.362	2.004	H4	1.016	-0.439	2.015
H5	3.84	-0.056	0.093	H5	2.305	-2.893	0.39
H6	-3.38	1.038	-0.852	H6	-2.723	1.49	-2.065
H7	-5.121	-2.544	0.421	H7	-5.232	2.485	1.123
H8	0.509	-4.942	-0.313	H8	-3.51	-2.827	-0.817
H9	-0.239	-4.011	-1.628	H9	-2.935	-1.874	-2.201
H10	-0.623	-3.645	0.067	H10	-3.061	-1.134	-0.594
H11	-0.237	-1.169	3.407	H11	-2.146	0.968	2.659

H12	0.002	-2.571	2.377	H12	-0.552	0.507	3.303
H13	-1.627	-1.941	2.605	H13	-1.705	-0.738	2.846
H14	-2.58	-2.913	-1.272	H14	-4.822	0.52	2.6
H15	-4.144	-3.727	-1.51	H15	-4.294	-0.444	1.209
H16	-3.18	-4.066	-0.062	H16	-5.973	0.134	1.31
H17	4.136	-1.799	-3.147	H17	2.734	-4.158	-1.686
H18	4.801	-0.496	-2.132	H18	2.279	-2.761	-2.68
H19	3.265	-0.261	-2.987	H19	1.454	-4.317	-2.913
H20	-2.952	1.504	2.097	H20	-0.838	3.503	-0.741
H21	-2.784	0.027	3.061	H21	-1.065	3.626	1.016
H22	-4.359	0.439	2.339	H22	-2.323	4.237	-0.09
H23	2.541	-1.618	3.258	H23	0.686	-3.967	2.419
H24	3.378	-0.181	2.653	H24	-0.134	-2.625	3.236
H25	4.03	-1.791	2.307	H25	1.592	-2.511	2.864
H26	0.12	1.381	-1.382	H26	1.44	0.931	-1.328
H27	0.48	-0.297	-1.772	H27	0.506	-0.445	-1.915
H28	1.608	0.994	-2.224	H28	2.266	-0.445	-2.055
H29	-5.093	-0.042	-2.711	H29	-5.368	0.903	-2.555
H30	-5.852	-1.612	-2.378	H30	-6.566	1.203	-1.281
H31	-4.161	-1.541	-2.908	H31	-5.54	-0.24	-1.207
H32	-0.868	5.829	0.662	H32	5.67	3.812	0.312
H33	-1.023	4.433	1.75	H33	4.768	5.185	-0.355
H34	-2.41	4.968	0.795	H34	5.278	3.856	-1.417
H35	-1.041	5.421	-1.956	H35	2.78	3.599	-2.175
H36	-2.558	4.541	-1.682	H36	2.356	4.931	-1.078
H37	-1.22	3.766	-2.555	H37	1.519	3.377	-0.944
H38	2.817	4.473	0.989	H38	5.234	0.599	1.703
H39	2.401	3.609	2.484	H39	3.947	0.653	2.925
H40	1.331	4.879	1.87	H40	4.572	2.159	2.238
H41	-1.391	2.93	-0.183	H41	3.229	3.62	0.862
H42	0.48	2.521	1.381	H42	2.324	1.458	1.27
H43	2.845	1.667	1.248	H43	3.023	-1.016	1.533
H44	2.747	3.007	-1.173	H44	4.28	-0.394	-0.867
Conformation 7				Conformation 8			
C1	0.853	2.789	-1.457	C1	0.612	2.978	1.064
C2	1.741	2.456	-0.512	C2	-0.641	2.826	0.62
C3	1.405	-1.144	-0.065	C3	-2.607	-0.127	0.358
C4	0.904	-0.486	0.995	C4	-1.42	-0.695	0.634
C5	-4.653	-1.31	0.188	C5	4.755	-1.691	-0.088
C6	1.196	2.716	0.874	C6	-0.663	2.29	-0.793
C7	-0.297	0.45	0.942	C7	-0.157	-0.34	-0.124
C8	-1.122	2.296	0.052	C8	1.49	1.101	-0.396
C9	3.409	-1.935	-1.324	C9	-5.046	0.163	0.045

C10	4.669	-2.064	0.717	C10	-5.011	-2.178	-0.464
C11	-0.463	3.292	-0.928	C11	1.678	2.557	0.087
C12	2.44	-2.258	-0.19	C12	-3.981	-0.506	0.908
C13	-0.131	1.996	1.217	C13	0.065	0.935	-1.022
C14	-1.295	0.761	-0.265	C14	1.249	-0.105	0.59
C15	4.763	-1.787	-0.78	C15	-5.663	-0.846	-0.821
C16	3.166	2.054	-0.734	C16	-1.887	3.287	1.314
C17	1.415	-0.651	2.414	C17	-1.282	-1.877	1.575
C18	5.058	-0.889	1.612	C18	-4.099	-2.731	-1.559
C19	-1.398	3.86	-1.987	C19	3.094	2.928	0.505
C20	1.701	-3.588	-0.434	C20	-4.151	-0.181	2.396
C21	-0.6	2.424	2.612	C21	0.023	0.593	-2.517
C22	-1.004	0.299	-1.699	C22	1.185	0.2	2.094
C23	5.868	-0.955	-1.373	C23	-6.281	-0.592	-2.17
C24	-6.267	-3.182	0.732	C24	7.257	-1.994	-0.363
C25	-6.003	-2.303	-1.642	C25	6.015	-0.093	-1.508
C26	-2.4	-2.064	0.942	C26	4.003	-1.506	2.22
C27	-5.291	-2.609	-0.305	C27	6.101	-0.994	-0.253
C28	-3.149	-1.123	-0.031	C28	3.704	-1.002	0.784
C29	-2.76	0.37	0.098	C29	2.233	-1.283	0.329
O1	-5.344	-0.442	0.713	O1	4.54	-2.779	-0.616
O2	0.899	4.148	0.916	O2	0.065	3.274	-1.596
O3	4.387	-2.972	-1.532	O3	-6.376	-0.306	0.325
O4	3.303	-2.469	0.952	O4	-4.288	-1.922	0.755
O5	-0.152	4.468	-0.079	O5	1.468	3.364	-1.137
O6	-3.605	1.151	-0.756	O6	2.179	-1.587	-1.065
H1	1.068	2.791	-2.523	H1	0.872	3.438	2.014
H2	0.95	-0.954	-1.03	H2	-2.628	0.683	-0.367
H3	1.95	2.608	1.66	H3	-1.655	2.325	-1.253
H4	-0.925	0.088	1.765	H4	-0.005	-1.193	-0.795
H5	-2.057	2.752	0.389	H5	2.28	0.884	-1.12
H6	3.06	-1.424	-2.219	H6	-4.956	1.214	-0.224
H7	5.301	-2.927	0.967	H7	-5.777	-2.923	-0.213
H8	3.854	2.761	-0.25	H8	-2.582	2.456	1.482
H9	3.406	2.02	-1.802	H9	-2.419	4.032	0.708
H10	3.366	1.065	-0.307	H10	-1.654	3.739	2.283
H11	2.201	-1.4	2.479	H11	-2.23	-2.402	1.697
H12	0.592	-0.936	3.083	H12	-0.932	-1.565	2.566
H13	1.811	0.298	2.801	H13	-0.544	-2.592	1.19
H14	4.871	-1.149	2.658	H14	-3.57	-3.613	-1.183
H15	4.481	0.01	1.375	H15	-3.355	-1.99	-1.869
H16	6.124	-0.66	1.505	H16	-4.681	-3.034	-2.437
H17	-0.889	4.63	-2.576	H17	3.16	3.999	0.721

H18	-2.287	4.298	-1.524	H18	3.811	2.687	-0.286
H19	-1.721	3.061	-2.661	H19	3.376	2.38	1.409
H20	1.001	-3.502	-1.272	H20	-3.957	0.881	2.582
H21	1.133	-3.862	0.461	H21	-3.453	-0.764	3.003
H22	2.426	-4.376	-0.655	H22	-5.173	-0.413	2.708
H23	-0.647	3.513	2.691	H23	0.335	1.444	-3.128
H24	0.084	2.056	3.388	H24	-0.996	0.313	-2.817
H25	-1.595	2.021	2.828	H25	0.684	-0.252	-2.729
H26	-1.034	-0.792	-1.785	H26	1.146	-0.728	2.673
H27	-0.033	0.634	-2.063	H27	0.301	0.785	2.348
H28	-1.774	0.696	-2.368	H28	2.059	0.763	2.437
H29	5.751	-0.899	-2.459	H29	-6.699	0.418	-2.206
H30	6.847	-1.4	-1.156	H30	-7.089	-1.306	-2.367
H31	5.862	0.062	-0.97	H31	-5.539	-0.69	-2.969
H32	-5.753	-3.451	1.661	H32	7.111	-2.662	-1.217
H33	-6.75	-4.084	0.339	H33	7.337	-2.611	0.539
H34	-7.044	-2.45	0.972	H34	8.204	-1.462	-0.497
H35	-5.313	-1.889	-2.385	H35	5.865	-0.702	-2.407
H36	-6.814	-1.583	-1.487	H36	6.948	0.468	-1.624
H37	-6.431	-3.223	-2.053	H37	5.194	0.628	-1.444
H38	-1.33	-2.077	0.721	H38	3.812	-2.583	2.289
H39	-2.765	-3.092	0.859	H39	3.381	-0.999	2.959
H40	-2.536	-1.743	1.98	H40	5.049	-1.329	2.493
H41	-4.499	-3.339	-0.504	H41	6.259	-0.343	0.616
H42	-2.946	-1.462	-1.055	H42	3.9	0.076	0.749
H43	-2.94	0.667	1.142	H43	1.863	-2.151	0.899
H44	-4.491	1.085	-0.359	H44	2.78	-2.345	-1.189
Conformation 9				Conformation 10			
C1	0.747	-3.387	-1.34	C1	-0.948	3.604	-1.233
C2	-0.042	-3.624	-0.285	C2	0.29	3.585	-0.722
C3	-2.018	-0.447	-0.028	C3	2.297	0.077	0.442
C4	-1.155	-0.717	0.967	C4	1.259	0.388	-0.36
C5	2.563	3.391	-0.417	C5	-3.339	-2.832	0.478
C6	0.682	-3.356	1.013	C6	0.273	3.239	0.747
C7	0.361	-0.657	0.842	C7	-0.092	0.566	0.344
C8	2.104	-1.637	-0.102	C8	-1.833	1.93	0.465
C9	-3.996	0.811	0.915	C9	4.386	-1.064	1.136
C10	-4.285	1.512	-1.361	C10	4.297	-2.147	-0.999
C11	2.13	-2.902	-0.991	C11	-2.04	3.288	-0.242
C12	-3.543	-0.328	0.004	C12	3.779	-0.094	0.124
C13	1.249	-1.923	1.171	C13	-0.42	1.905	1.116
C14	1.246	-0.357	-0.451	C14	-1.548	0.586	-0.313
C15	-4.427	1.945	0.092	C15	4.683	-2.332	0.464

C16	-1.399	-4.258	-0.304	C16	1.547	4.044	-1.398
C17	-1.58	-1.002	2.395	C17	1.396	0.537	-1.858
C18	-3.21	2.273	-2.136	C18	3.085	-2.974	-1.426
C19	3.096	-2.844	-2.167	C19	-3.451	3.531	-0.758
C20	-4.271	-1.651	0.27	C20	4.51	1.255	0.109
C21	1.994	-1.814	2.506	C21	-0.387	1.73	2.638
C22	0.636	-0.297	-1.856	C22	-1.742	0.596	-1.833
C23	-4.387	3.393	0.504	C23	4.722	-3.687	1.117
C24	4.948	3.464	0.376	C24	-5.657	-3.845	0.6
C25	3.186	4.935	1.46	C25	-4.038	-4.509	-1.247
C26	0.403	2.634	0.616	C26	-0.91	-2.575	-0.112
C27	3.474	3.571	0.804	C27	-4.523	-3.376	-0.314
C28	1.492	2.289	-0.419	C28	-2.31	-1.962	-0.268
C29	2.149	0.904	-0.235	C29	-2.459	-0.53	0.296
O1	2.647	4.162	-1.361	O1	-3.18	-3.082	1.664
O2	1.837	-4.251	1.024	O2	-0.518	4.291	1.389
O3	-5.398	1.111	0.78	O3	5.747	-1.411	0.829
O4	-3.997	0.101	-1.311	O4	4.055	-0.734	-1.148
O5	2.73	-3.932	-0.114	O5	-1.901	4.276	0.854
O6	3.231	0.905	-1.181	O6	-3.845	-0.217	0.076
H1	0.475	-3.61	-2.369	H1	-1.187	3.934	-2.241
H2	-1.632	-0.257	-1.02	H2	2.082	-0.026	1.507
H3	0.123	-3.688	1.894	H3	1.251	3.347	1.227
H4	0.644	0.09	1.596	H4	-0.108	-0.215	1.109
H5	3.149	-1.411	0.147	H5	-2.634	1.848	1.21
H6	-3.579	0.931	1.911	H6	4.139	-0.984	2.193
H7	-5.248	1.614	-1.88	H7	5.149	-2.38	-1.65
H8	-1.373	-5.239	0.189	H8	1.934	4.948	-0.908
H9	-1.756	-4.401	-1.329	H9	1.37	4.278	-2.453
H10	-2.133	-3.65	0.235	H10	2.339	3.29	-1.339
H11	-2.662	-1.013	2.532	H11	0.912	-0.301	-2.375
H12	-1.163	-0.252	3.08	H12	0.913	1.448	-2.218
H13	-1.203	-1.974	2.735	H13	2.441	0.539	-2.163
H14	-2.252	2.266	-1.605	H14	2.235	-2.803	-0.758
H15	-3.508	3.315	-2.299	H15	3.322	-4.043	-1.429
H16	-3.064	1.804	-3.114	H16	2.788	-2.689	-2.44
H17	4.109	-2.608	-1.828	H17	-4.184	3.416	0.047
H18	2.778	-2.074	-2.876	H18	-3.687	2.81	-1.546
H19	3.119	-3.806	-2.69	H19	-3.541	4.54	-1.173
H20	-3.953	-2.11	1.21	H20	5.586	1.094	0
H21	-4.063	-2.353	-0.542	H21	4.323	1.806	1.038
H22	-5.349	-1.471	0.31	H22	4.156	1.867	-0.726
H23	2.733	-2.613	2.607	H23	-0.993	0.872	2.949

H24	1.297	-1.886	3.35	H24	-0.769	2.621	3.145
H25	2.515	-0.854	2.589	H25	0.641	1.555	2.983
H26	-0.011	0.575	-1.979	H26	-2.814	0.618	-2.056
H27	0.053	-1.184	-2.1	H27	-1.33	-0.306	-2.294
H28	1.442	-0.199	-2.591	H28	-1.276	1.454	-2.317
H29	-4.512	3.478	1.587	H29	5.434	-4.345	0.604
H30	-5.192	3.957	0.019	H30	3.739	-4.167	1.09
H31	-3.434	3.855	0.227	H31	5.034	-3.592	2.161
H32	5.184	4.235	-0.364	H32	-5.322	-4.656	1.255
H33	5.159	2.486	-0.068	H33	-6.016	-3.029	1.235
H34	5.605	3.603	1.242	H34	-6.5	-4.211	0.003
H35	3.357	5.745	0.743	H35	-3.661	-5.357	-0.664
H36	3.85	5.087	2.319	H36	-3.24	-4.177	-1.921
H37	2.152	5.007	1.816	H37	-4.87	-4.864	-1.864
H38	0.784	2.589	1.642	H38	-0.624	-2.627	0.943
H39	-0.446	1.951	0.538	H39	-0.154	-1.998	-0.65
H40	0.028	3.649	0.441	H40	-0.896	-3.594	-0.513
H41	3.261	2.783	1.534	H41	-4.877	-2.55	-0.945
H42	1.054	2.337	-1.421	H42	-2.58	-1.936	-1.328
H43	2.562	0.847	0.782	H43	-2.271	-0.586	1.378
H44	3.811	0.153	-0.981	H44	-4.08	0.539	0.636
Conformation 11				Conformation 12			
C1	0.285	3.297	-1.272	C1	0.132	3.28	-1.286
C2	1.418	2.718	-0.853	C2	1.292	2.761	-0.862
C3	1.719	-1.375	0.088	C3	1.787	-1.347	0.065
C4	0.882	-0.581	-0.61	C4	0.934	-0.572	-0.634
C5	-4.642	-1.516	0.439	C5	-4.473	-1.78	0.536
C6	1.346	2.366	0.613	C6	1.229	2.393	0.6
C7	-0.186	0.147	0.215	C7	-0.179	0.094	0.183
C8	-1.139	2.128	0.486	C8	-1.236	2.022	0.453
C9	4.019	-1.461	-0.99	C9	4.117	-1.296	-0.943
C10	4.689	-2.176	1.198	C10	4.756	-2.056	1.24
C11	-0.768	3.459	-0.204	C11	-0.934	3.379	-0.224
C12	2.874	-2.262	-0.375	C12	2.993	-2.168	-0.389
C13	0.161	1.461	1.022	C13	0.093	1.421	0.996
C14	-1.531	0.829	-0.315	C14	-1.552	0.705	-0.358
C15	5.123	-1.385	-0.03	C15	5.189	-1.204	0.053
C16	2.702	2.596	-1.618	C16	2.588	2.722	-1.616
C17	0.939	-0.445	-2.115	C17	1.017	-0.4	-2.134
C18	4.452	-1.313	2.437	C18	4.447	-1.249	2.501
C19	-1.956	4.316	-0.617	C19	-2.165	4.174	-0.637
C20	2.406	-3.436	-1.245	C20	2.605	-3.333	-1.31
C21	0.217	1.222	2.535	C21	0.149	1.18	2.509

C22	-1.82	0.988	-1.813	C22	-1.836	0.855	-1.856
C23	6.144	-0.282	0.05	C23	6.154	-0.059	0.201
C24	-6.607	-1.763	-1.053	C24	-6.991	-1.784	0.81
C25	-6.123	-3.555	0.687	C25	-5.887	-2.996	-1.136
C26	-2.331	-2.33	0.01	C26	-2.174	-2.472	-0.206
C27	-5.512	-2.54	-0.289	C27	-5.821	-1.785	-0.177
C28	-3.298	-1.141	-0.195	C28	-3.23	-1.358	-0.27
C29	-2.785	0.207	0.372	C29	-2.779	0.003	0.31
O1	-5.034	-0.997	1.479	O1	-4.355	-2.115	1.706
O2	1.143	3.634	1.315	O2	0.954	3.643	1.309
O3	5.205	-2.252	-1.192	O3	5.344	-2.025	-1.135
O4	3.489	-2.866	0.796	O4	3.599	-2.782	0.78
O5	-0.134	4.25	0.879	O5	-0.352	4.19	0.871
O6	-3.824	1.188	0.269	O6	-3.949	0.831	0.195
H1	0.151	3.73	-2.26	H1	-0.019	3.715	-2.271
H2	1.559	-1.461	1.162	H2	1.607	-1.465	1.132
H3	2.3	2.016	1.018	H3	2.198	2.09	1.01
H4	-0.482	-0.58	0.975	H4	-0.445	-0.651	0.937
H5	-1.866	2.369	1.266	H5	-1.958	2.232	1.252
H6	3.831	-0.695	-1.737	H6	3.915	-0.514	-1.669
H7	5.429	-2.953	1.43	H7	5.524	-2.808	1.466
H8	3.475	3.235	-1.168	H8	3.316	3.402	-1.154
H9	2.577	2.899	-2.662	H9	2.454	3.025	-2.659
H10	3.091	1.572	-1.596	H10	3.037	1.723	-1.599
H11	0.086	-0.953	-2.581	H11	0.205	-0.944	-2.631
H12	0.897	0.598	-2.434	H12	0.923	0.646	-2.433
H13	1.842	-0.889	-2.537	H13	1.953	-0.783	-2.544
H14	3.772	-0.481	2.223	H14	3.741	-0.437	2.295
H15	5.395	-0.902	2.814	H15	5.361	-0.817	2.922
H16	4.007	-1.924	3.229	H16	4.004	-1.907	3.255
H17	-2.63	4.477	0.229	H17	-2.839	4.315	0.213
H18	-2.515	3.812	-1.411	H18	-2.705	3.64	-1.424
H19	-1.618	5.288	-0.992	H19	-1.875	5.158	-1.021
H20	3.269	-4.035	-1.547	H20	3.505	-3.881	-1.604
H21	1.88	-3.09	-2.138	H21	2.089	-2.984	-2.208
H22	1.721	-4.068	-0.669	H22	1.936	-4.014	-0.775
H23	-0.685	0.71	2.887	H23	-0.726	0.617	2.852
H24	0.307	2.168	3.077	H24	0.183	2.127	3.055
H25	1.08	0.596	2.797	H25	1.043	0.6	2.773
H26	-2.787	1.485	-1.938	H26	-2.827	1.302	-1.986
H27	-1.88	0.021	-2.321	H27	-1.846	-0.115	-2.362
H28	-1.066	1.581	-2.33	H28	-1.109	1.485	-2.367
H29	7.099	-0.663	0.431	H29	7.116	-0.411	0.592

H30	5.809	0.52	0.716	H30	5.766	0.699	0.888
H31	6.316	0.142	-0.944	H31	6.331	0.411	-0.771
H32	-7.251	-1.221	-0.35	H32	-6.974	-2.68	1.44
H33	-6.18	-1.038	-1.754	H33	-6.95	-0.911	1.47
H34	-7.229	-2.461	-1.624	H34	-7.943	-1.761	0.27
H35	-6.719	-3.043	1.449	H35	-5.841	-3.938	-0.577
H36	-5.348	-4.138	1.197	H36	-5.069	-2.991	-1.865
H37	-6.774	-4.252	0.149	H37	-6.83	-2.978	-1.692
H38	-2.08	-2.454	1.069	H38	-1.878	-2.666	0.829
H39	-1.402	-2.183	-0.546	H39	-1.279	-2.221	-0.782
H40	-2.776	-3.267	-0.341	H40	-2.581	-3.403	-0.617
H41	-4.896	-3.068	-1.026	H41	-5.852	-0.872	-0.785
H42	-3.485	-1.033	-1.271	H42	-3.53	-1.198	-1.311
H43	-2.549	0.049	1.434	H43	-2.555	-0.156	1.375
H44	-4.51	0.892	0.893	H44	-3.837	1.601	0.775
Conformation 13				Conformation 14			
C1	-0.268	2.984	-1.644	C1	2.962	-2.075	-1.446
C2	0.939	2.54	-1.271	C2	1.895	-2.826	-1.142
C3	1.641	-1.161	0.473	C3	-1.714	-1.289	0.366
C4	0.639	-0.613	-0.243	C4	-0.65	-0.8	-0.301
C5	-3.995	-1.757	-0.057	C5	0.996	3.69	-0.145
C6	1.084	2.534	0.231	C6	1.691	-2.912	0.352
C7	-0.354	0.247	0.55	C7	0.568	-0.438	0.557
C8	-1.379	2.216	0.515	C8	2.77	-0.681	0.675
C9	3.723	-1.461	-0.963	C9	-4.095	-1.645	0.952
C10	4.821	-1.488	1.168	C10	-4.539	0.009	-0.722
C11	-1.175	3.363	-0.5	C11	3.688	-1.507	-0.253
C12	2.778	-2.092	0.057	C12	-3.057	-1.785	-0.159
C13	0.017	1.718	0.998	C13	1.55	-1.558	1.089
C14	-1.793	0.758	0.089	C14	1.82	0.462	0.154
C15	4.965	-1.07	-0.29	C15	-4.993	-0.533	0.629
C16	2.112	2.271	-2.165	C16	1.093	-3.672	-2.085
C17	0.445	-0.866	-1.72	C17	-0.655	-0.584	-1.796
C18	4.721	-0.314	2.142	C18	-3.907	1.399	-0.646
C19	-2.452	4.08	-0.917	C19	5.02	-0.848	-0.581
C20	2.275	-3.483	-0.352	C20	-2.973	-3.221	-0.691
C21	0.288	1.831	2.502	C21	1.387	-1.825	2.59
C22	-2.305	0.575	-1.342	C22	2.035	0.948	-1.281
C23	5.882	0.046	-0.716	C23	-5.74	0.315	1.623
C24	-4.382	-3.21	-2.095	C24	0.16	4.751	-2.288
C25	-3.599	-4.251	0.09	C25	-1.28	4.789	-0.192
C26	-3.903	-1.636	2.432	C26	0.872	3.621	2.345
C27	-3.557	-3.003	-0.822	C27	-0.223	4.008	-1.006

C28	-3.153	-1.278	1.125	C28	0.834	2.76	1.059
C29	-2.868	0.258	1.109	C29	1.94	1.661	1.15
O1	-5.029	-1.16	-0.356	O1	2.09	4.198	-0.385
O2	0.908	3.923	0.654	O2	2.908	-3.53	0.88
O3	4.923	-2.232	-1.16	O3	-5.434	-1.912	0.502
O4	3.639	-2.31	1.209	O4	-3.611	-0.972	-1.226
O5	-0.447	4.394	0.278	O5	4.077	-2.669	0.582
O6	-4.07	1.013	1	O6	3.246	2.229	1.115
H1	-0.557	3.175	-2.674	H1	3.362	-1.963	-2.451
H2	1.658	-0.974	1.546	H2	-1.616	-1.385	1.449
H3	2.102	2.309	0.564	H3	0.914	-3.627	0.639
H4	-0.504	-0.31	1.481	H4	0.137	0.015	1.456
H5	-2.007	2.615	1.317	H5	3.387	-0.361	1.52
H6	3.343	-0.952	-1.844	H6	-3.861	-1.957	1.969
H7	5.658	-2.135	1.461	H7	-5.379	0.025	-1.429
H8	2.903	3.014	-1.991	H8	1.242	-4.737	-1.862
H9	1.83	2.316	-3.221	H9	1.386	-3.498	-3.125
H10	2.556	1.289	-1.965	H10	0.018	-3.478	-1.99
H11	-0.452	-1.472	-1.894	H11	-0.686	0.488	-2.032
H12	0.31	0.063	-2.279	H12	0.249	-0.981	-2.264
H13	1.283	-1.406	-2.163	H13	-1.529	-1.036	-2.263
H14	3.939	0.392	1.84	H14	-3.1	1.427	0.094
H15	5.672	0.226	2.204	H15	-4.655	2.154	-0.38
H16	4.478	-0.689	3.141	H16	-3.489	1.664	-1.622
H17	-3.012	4.416	-0.039	H17	5.542	-0.554	0.335
H18	-3.088	3.401	-1.492	H18	4.851	0.049	-1.183
H19	-2.219	4.948	-1.541	H19	5.659	-1.532	-1.148
H20	3.125	-4.11	-0.638	H20	-3.974	-3.578	-0.954
H21	1.574	-3.427	-1.188	H21	-2.543	-3.887	0.065
H22	1.761	-3.95	0.494	H22	-2.339	-3.261	-1.582
H23	-0.521	1.379	3.086	H23	1.427	-0.894	3.164
H24	0.383	2.878	2.804	H24	2.175	-2.488	2.957
H25	1.219	1.314	2.767	H25	0.419	-2.301	2.794
H26	-3.296	1.031	-1.431	H26	2.961	1.529	-1.334
H27	-2.405	-0.48	-1.613	H27	1.22	1.593	-1.622
H28	-1.657	1.037	-2.086	H28	2.115	0.129	-1.997
H29	6.917	-0.172	-0.428	H29	-6.679	0.681	1.192
H30	5.594	0.994	-0.25	H30	-5.147	1.182	1.929
H31	5.845	0.167	-1.802	H31	-5.978	-0.274	2.514
H32	-5.435	-3.385	-1.855	H32	0.6	5.727	-2.058
H33	-4.331	-2.336	-2.753	H33	0.89	4.186	-2.876
H34	-4.006	-4.078	-2.647	H34	-0.729	4.913	-2.906
H35	-4.62	-4.453	0.43	H35	-0.884	5.756	0.138

H36	-2.955	-4.145	0.968	H36	-1.618	4.235	0.689
H37	-3.251	-5.122	-0.474	H37	-2.155	4.979	-0.822
H38	-4.83	-1.062	2.502	H38	1.86	4.074	2.463
H39	-3.276	-1.39	3.296	H39	0.674	2.989	3.217
H40	-4.149	-2.7	2.485	H40	0.125	4.419	2.328
H41	-2.503	-2.84	-1.092	H41	-0.676	3.04	-1.268
H42	-2.194	-1.807	1.117	H42	-0.141	2.265	0.997
H43	-2.471	0.483	2.108	H43	1.834	1.235	2.156
H44	-4.677	0.491	0.437	H44	3.197	3.005	0.52

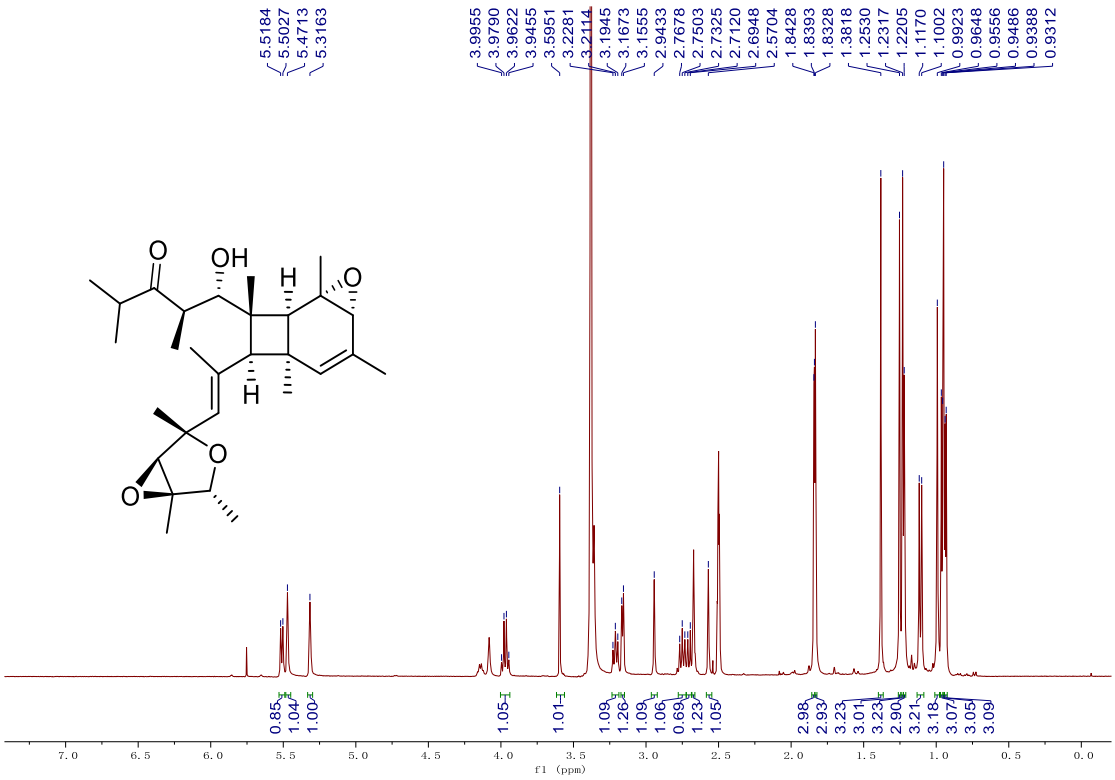

Figure S2. ^{1}H NMR spectrum of **1** recorded in DMSO-d_6

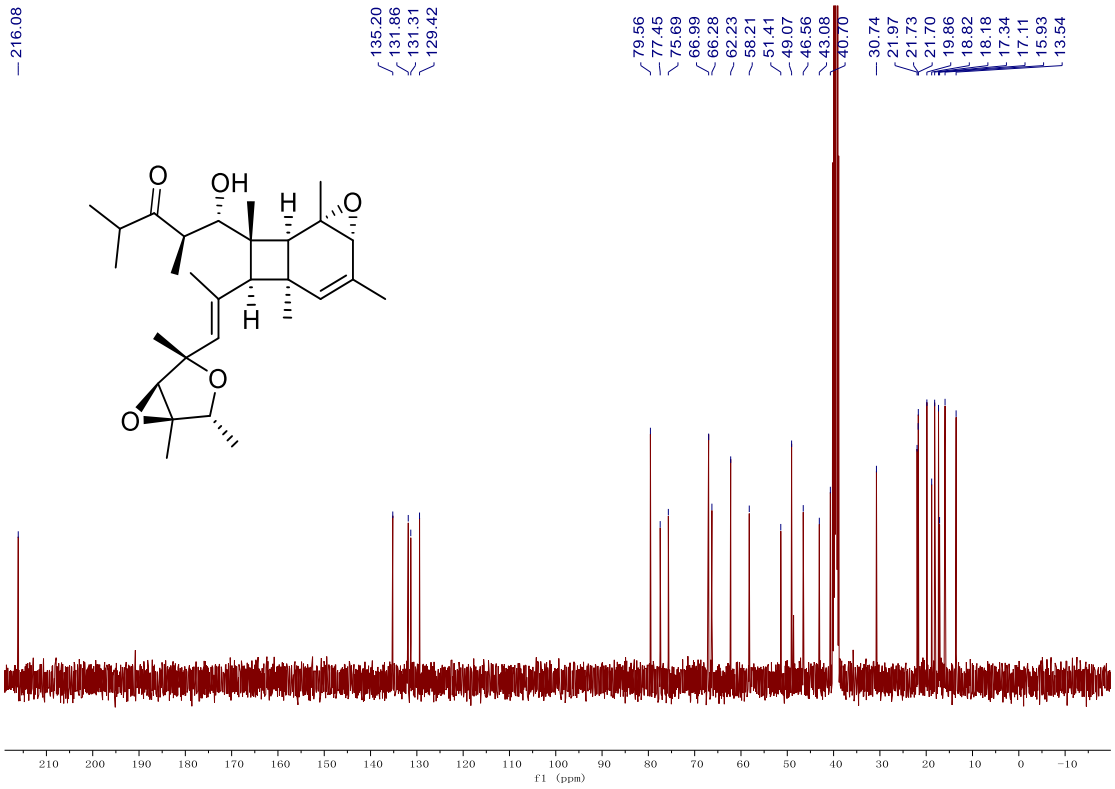

Figure S3. ^{13}C NMR spectrum of **1** recorded in DMSO-d_6

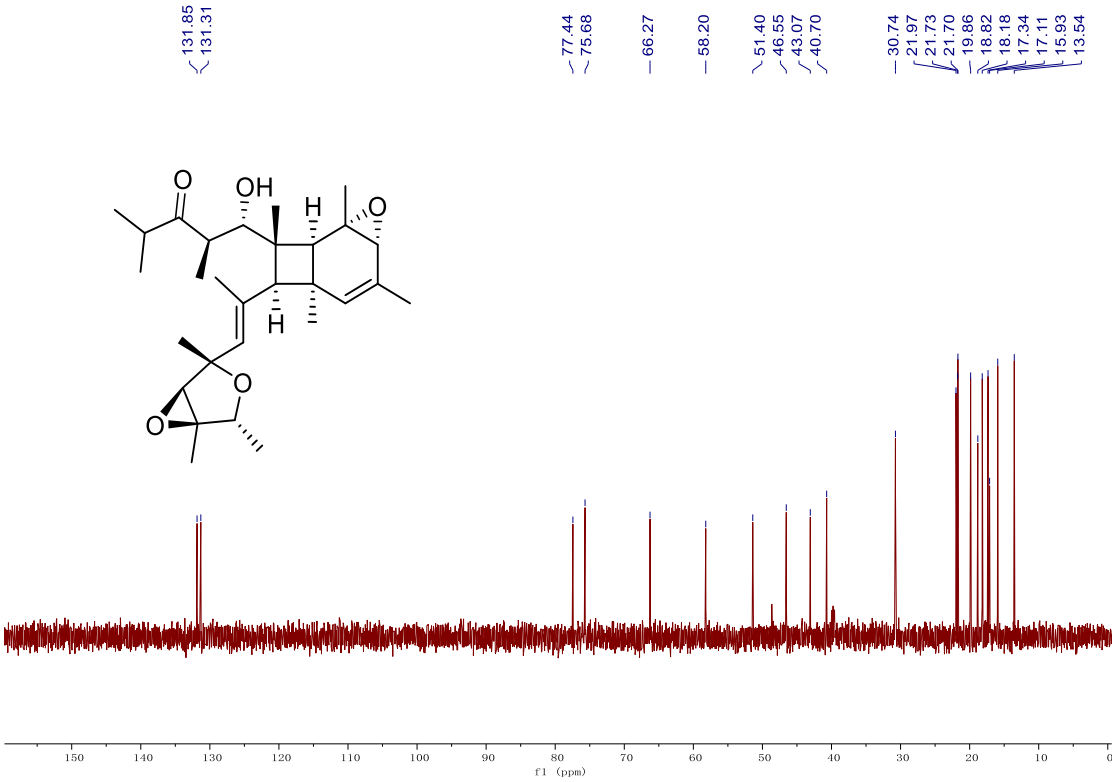

Figure S4. DEPT NMR spectrum of **1** recorded in DMSO-d_6

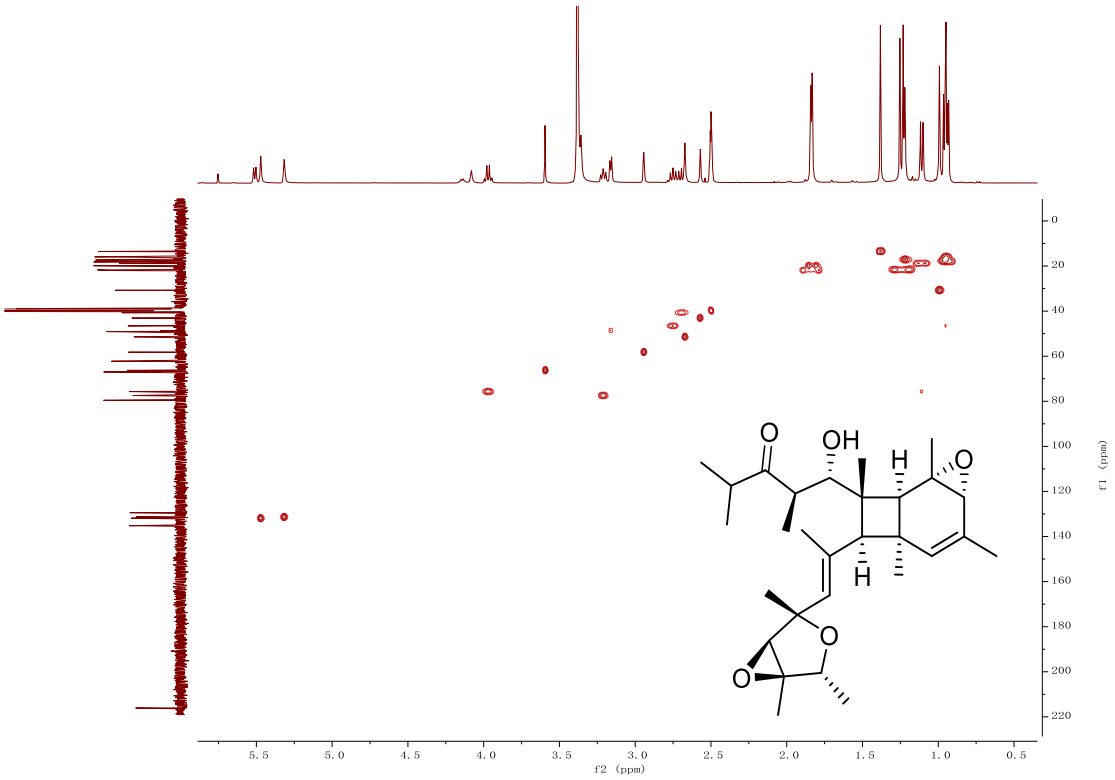

Figure S5. HSQC spectrum of **1** recorded in DMSO-d_6

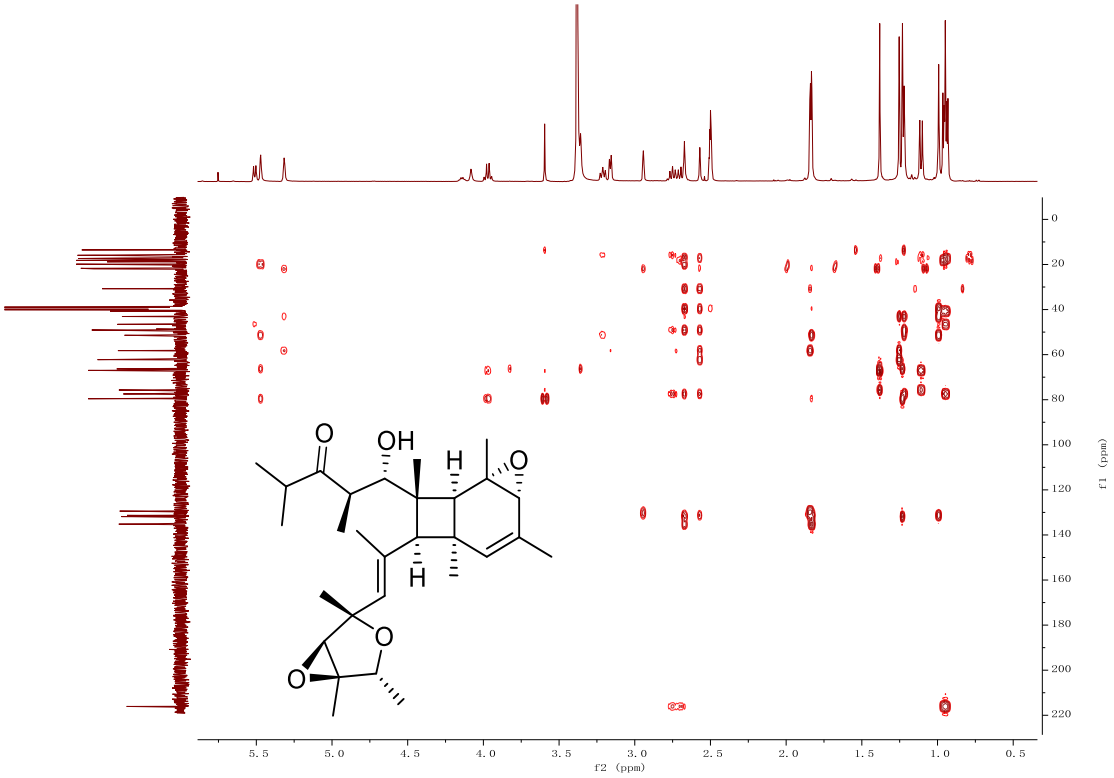

Figure S6. HMBC spectrum of **1** recorded in DMSO-d_6

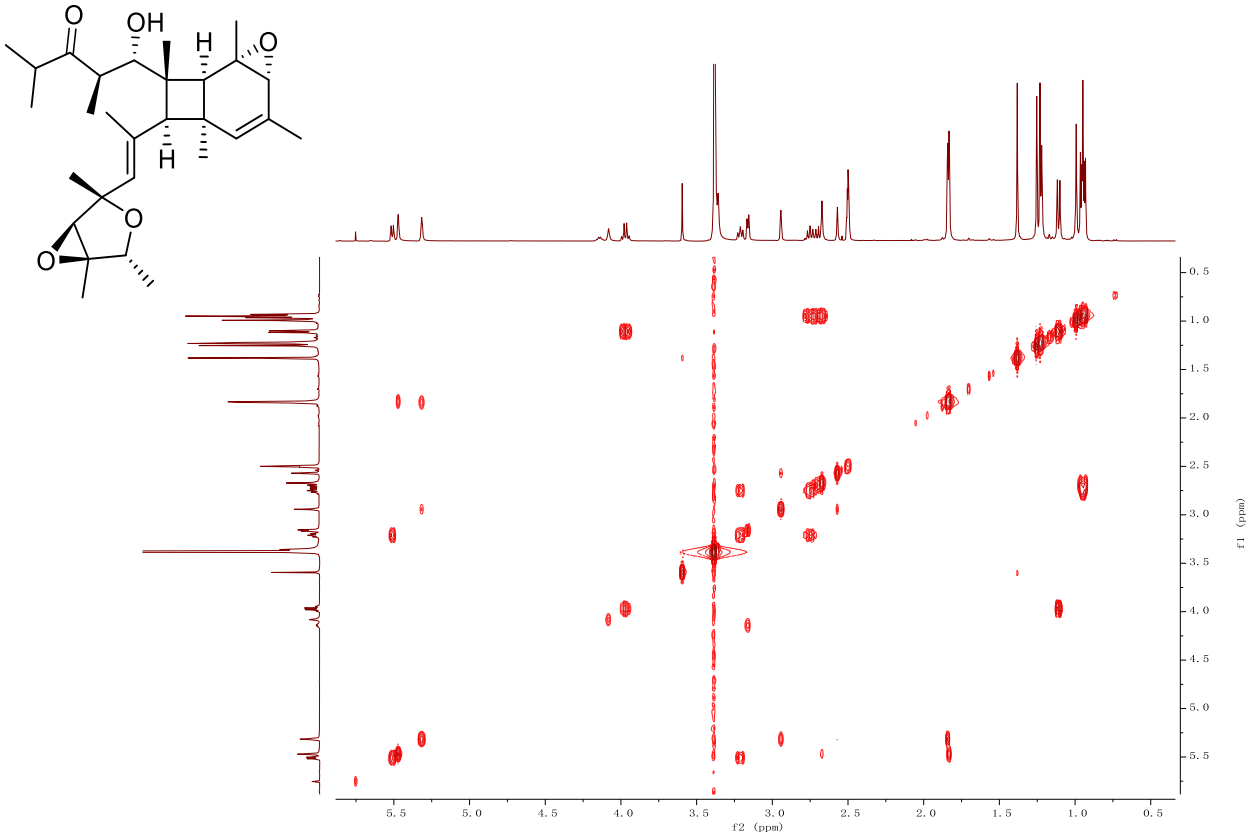

Figure S7. ^{1}H-^{1}H COSY spectrum of **1** recorded in DMSO-d_6

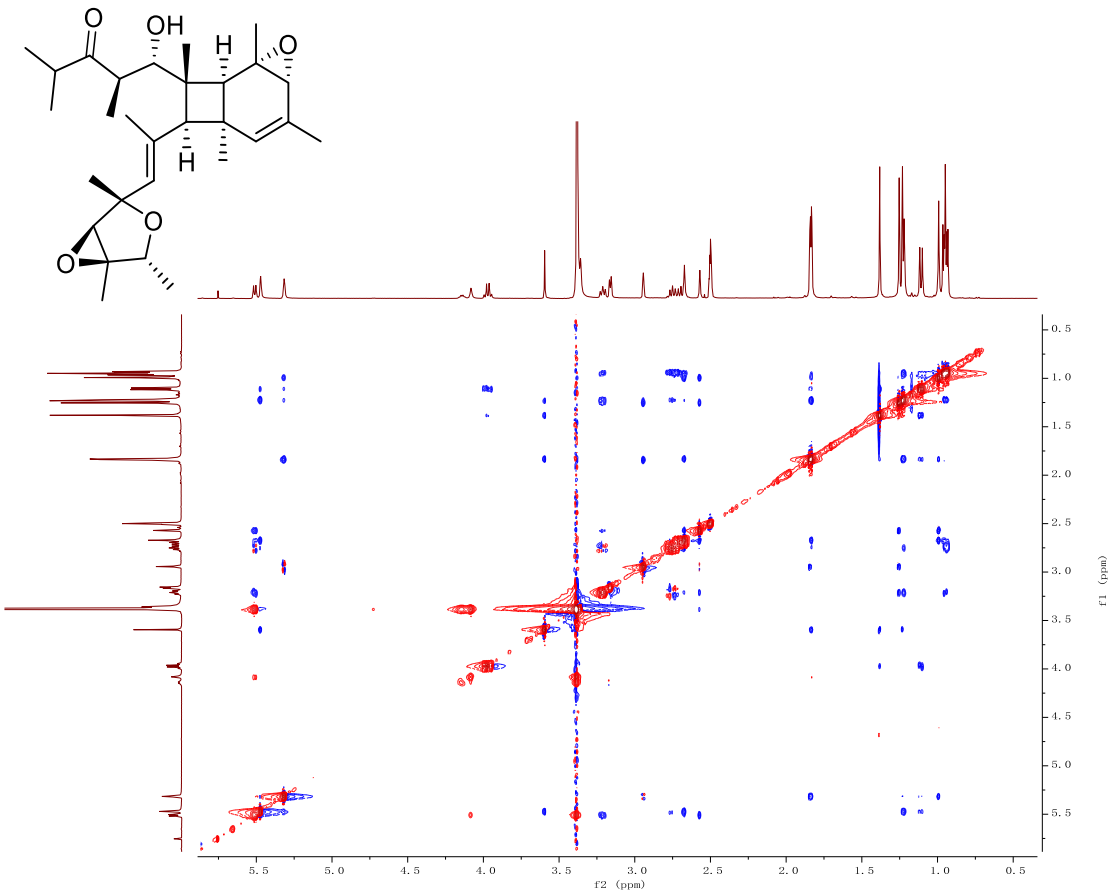

Figure S8. NOESY spectrum of **1** recorded in DMSO-d_6

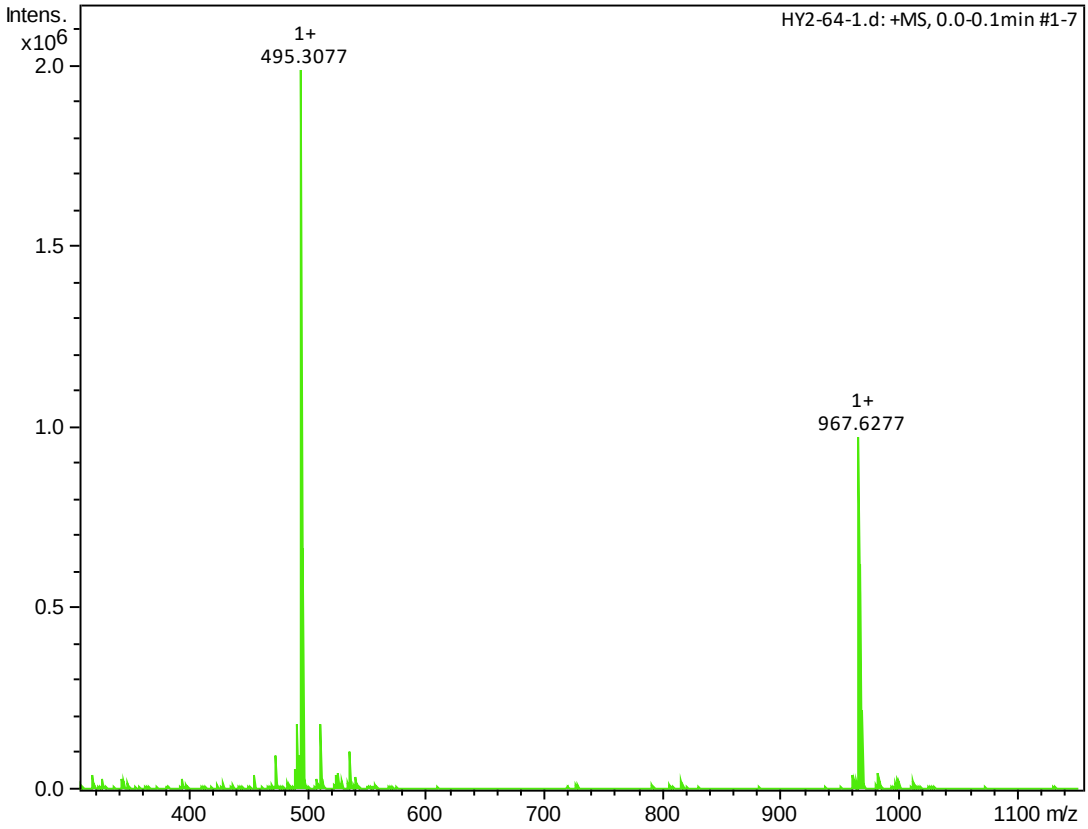

Figure S9. HRESIMS spectrum of **1**

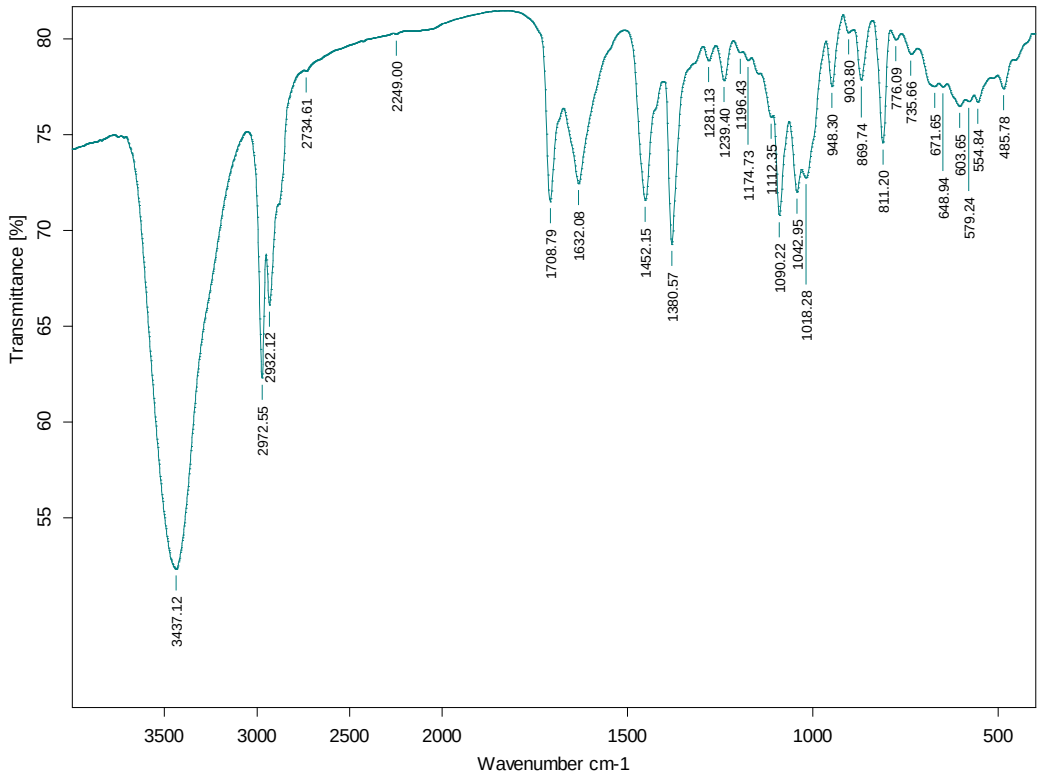

Figure S10. IR spectrum of **1**

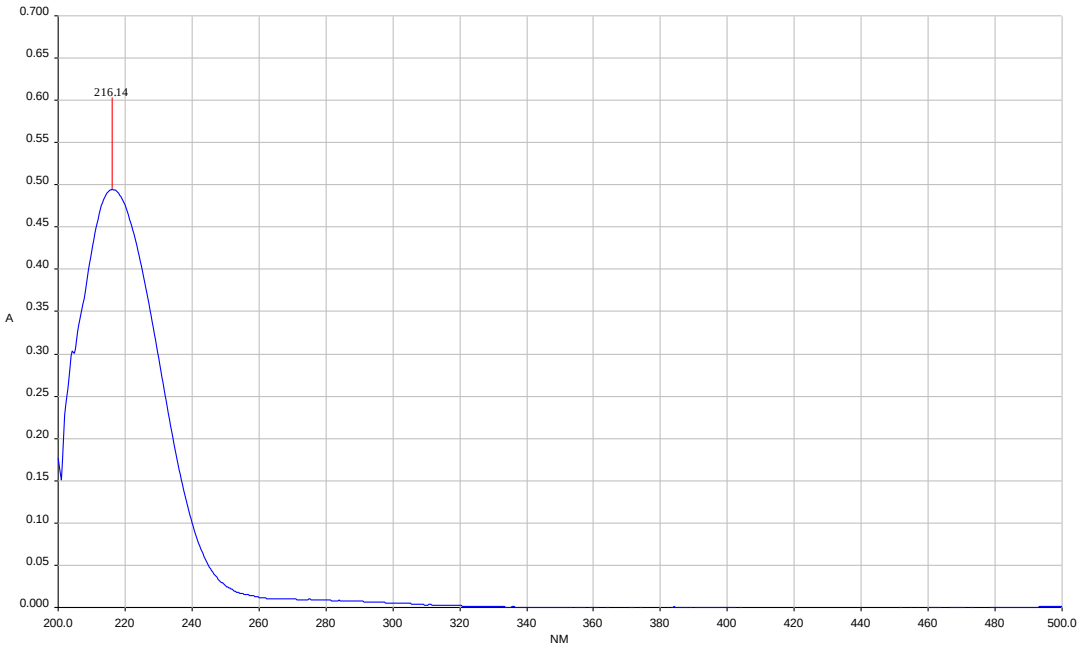

Figure S11. UV spectrum of **1**

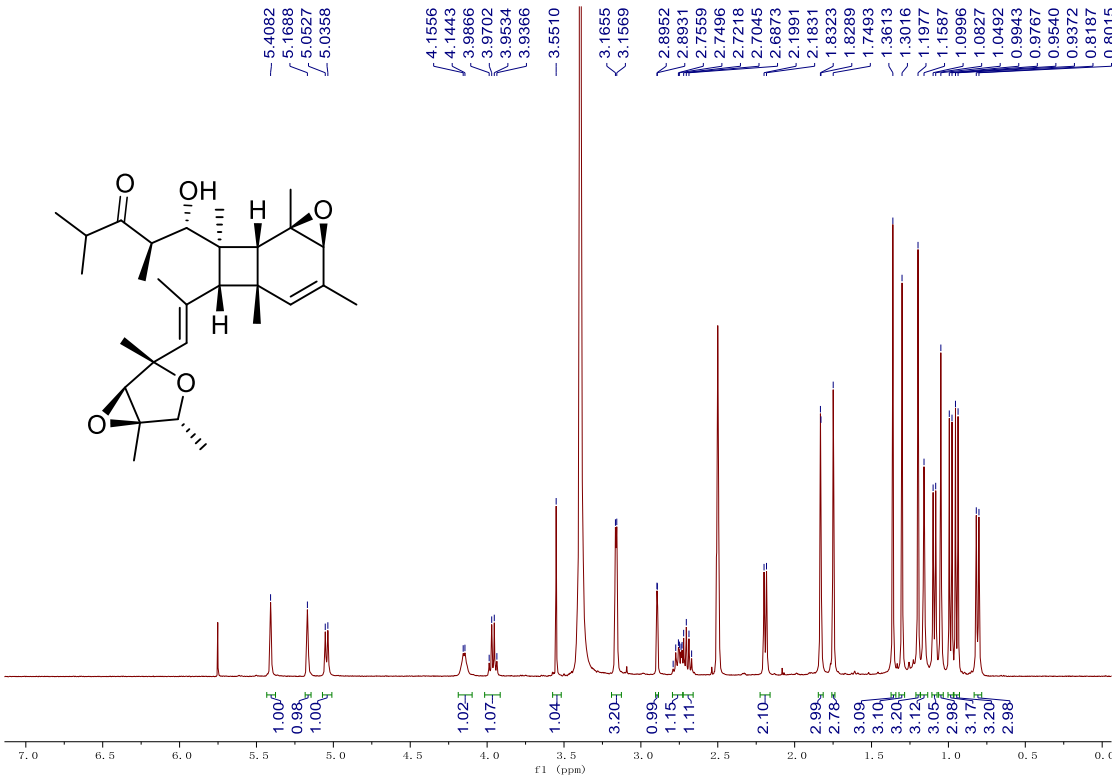

Figure S12. ^{1}H NMR spectrum of **2** recorded in DMSO-d_6

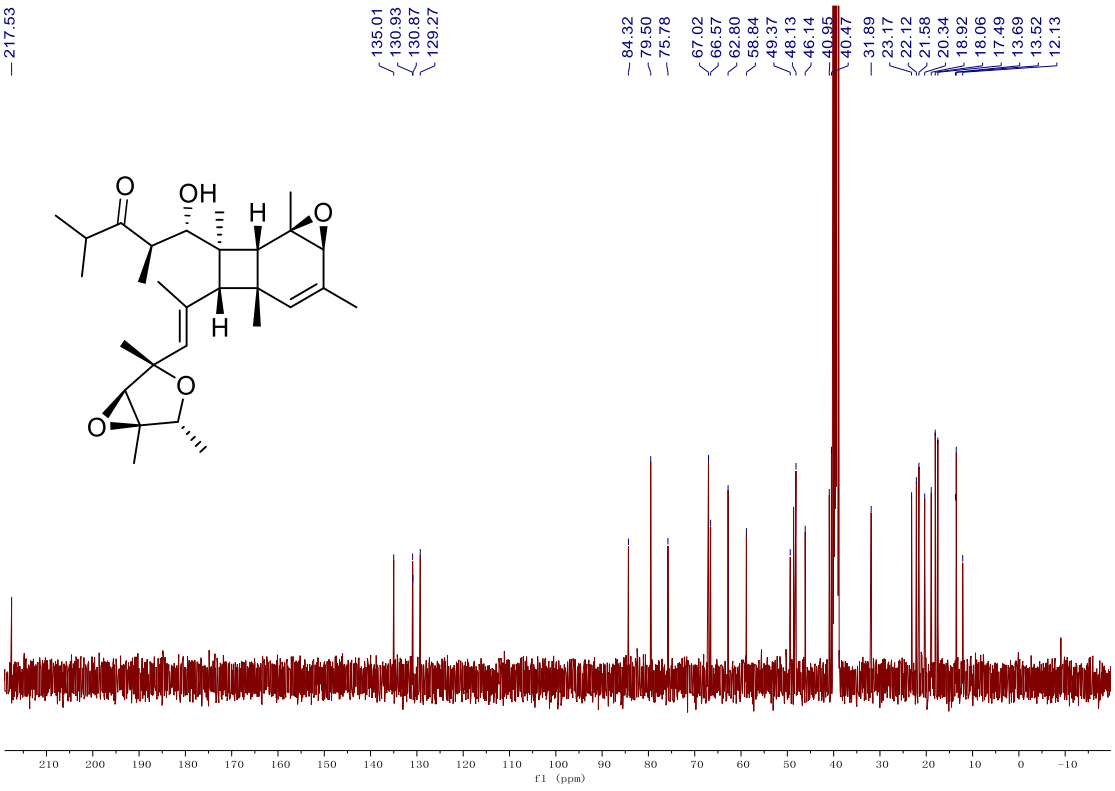

Figure S13. ^{13}C NMR spectrum of **2** recorded in DMSO-d_6

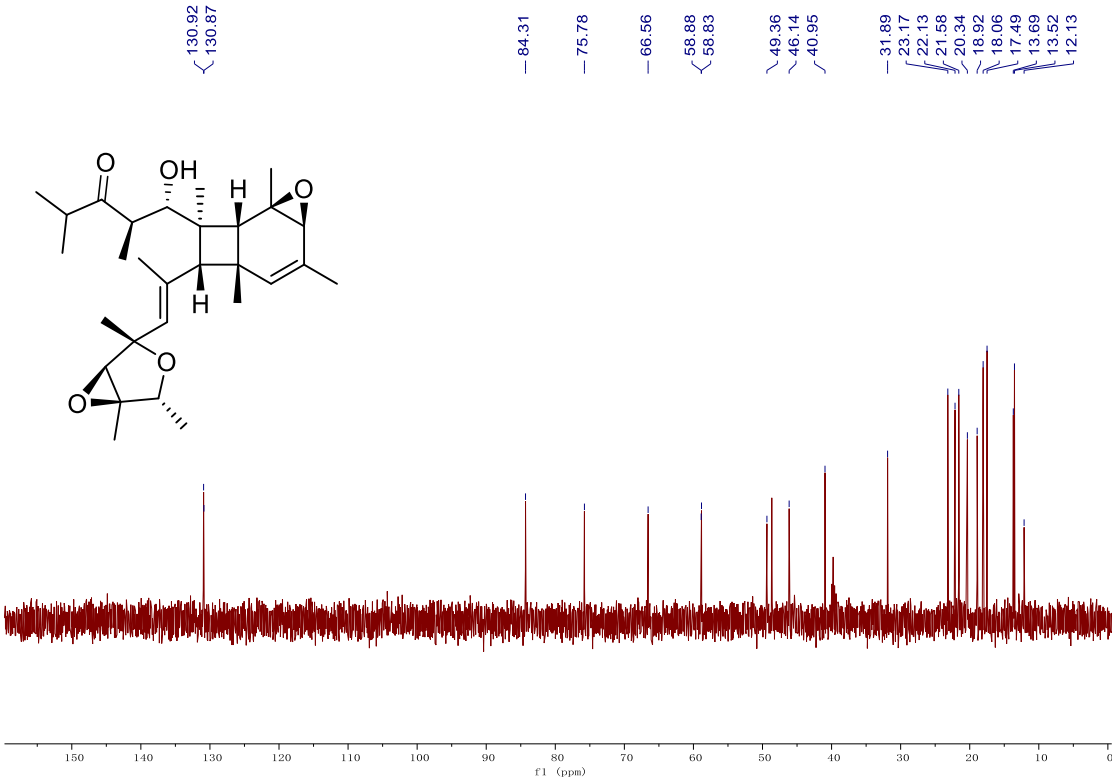

Figure S14. DEPT NMR spectrum of **2** recorded in DMSO-d_6

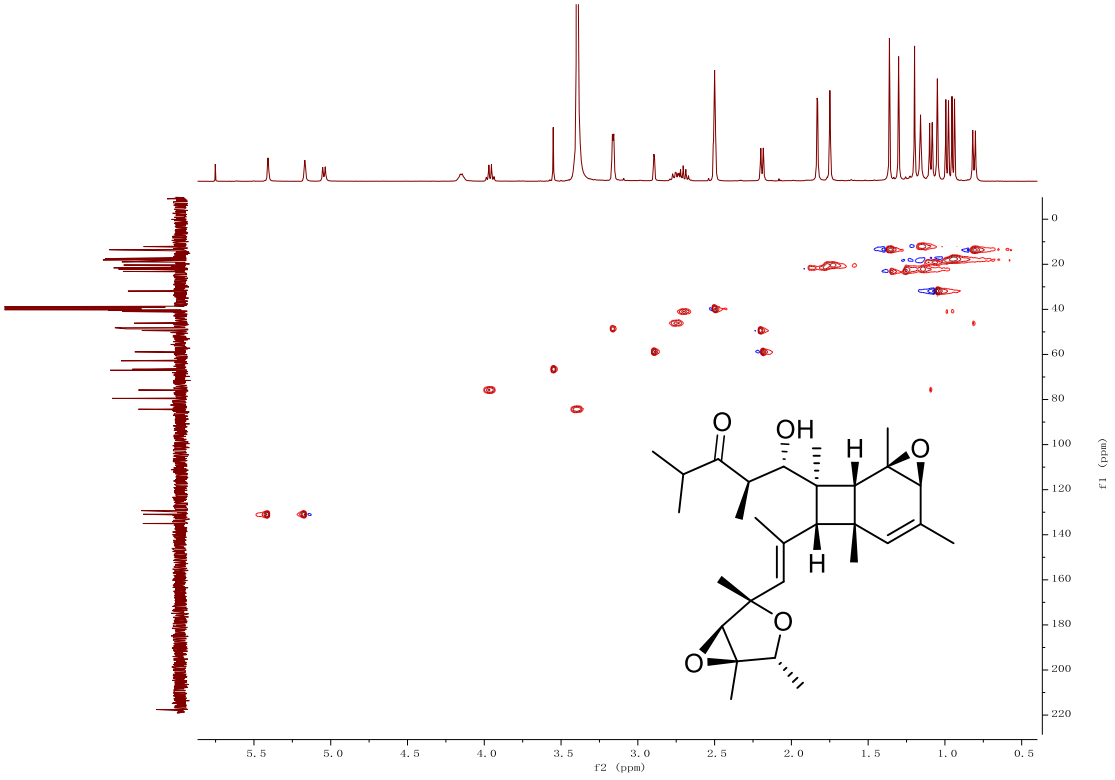

Figure S15. HSQC spectrum of **2** recorded in DMSO-d_6

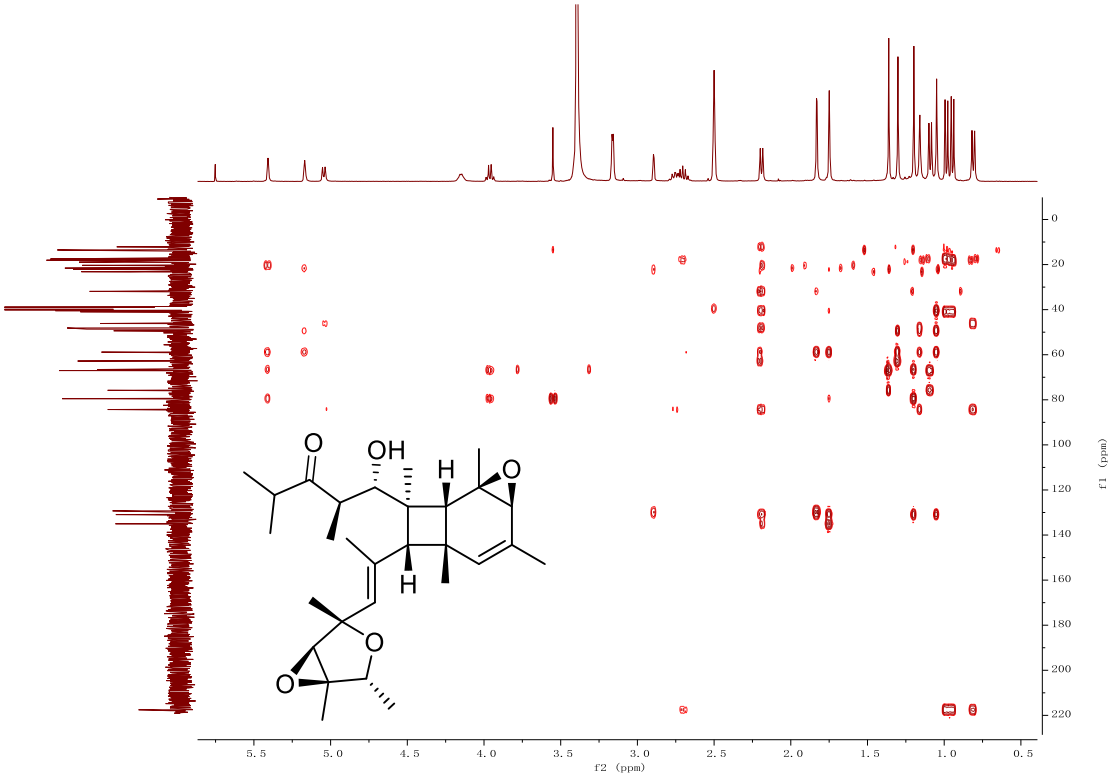

Figure S16. HMBC spectrum of **2** recorded in DMSO-d_6

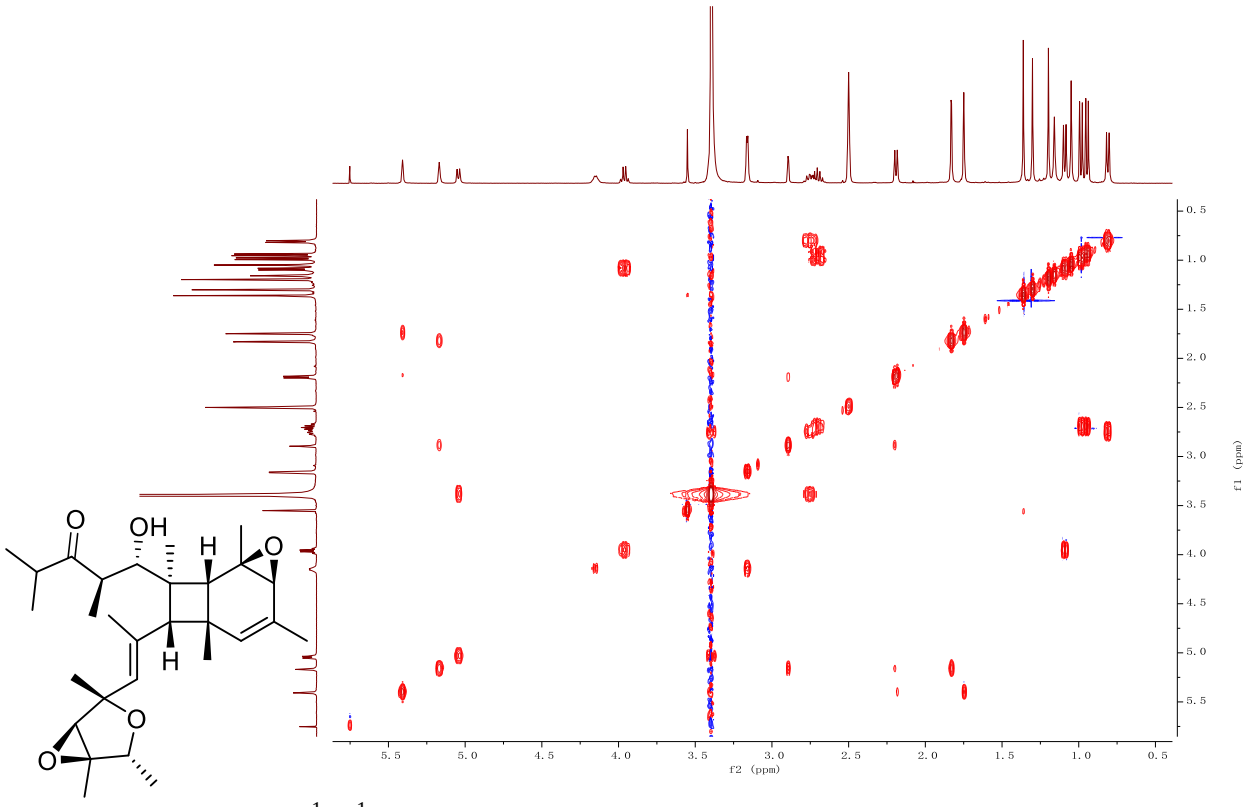

Figure S 17. ^{1}H-^{1}H COSY spectrum of **2** recorded in DMSO-d_6

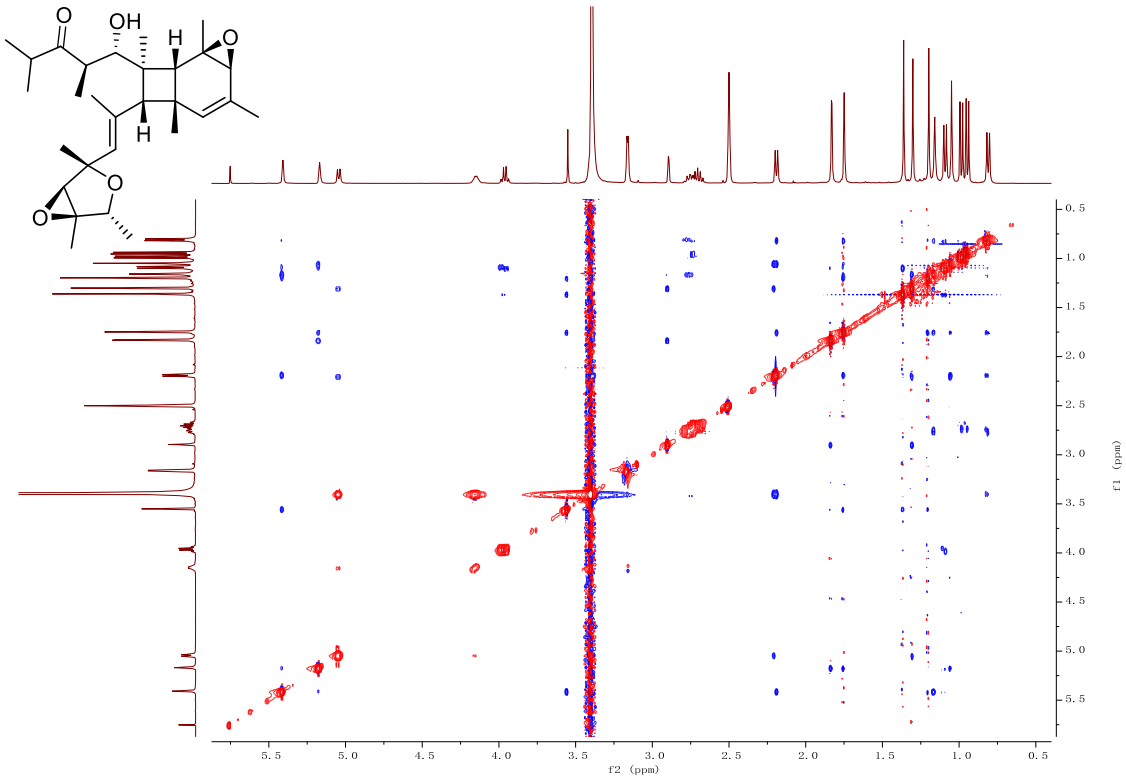

Figure S18. NOESY spectrum of **2** recorded in DMSO-d_6

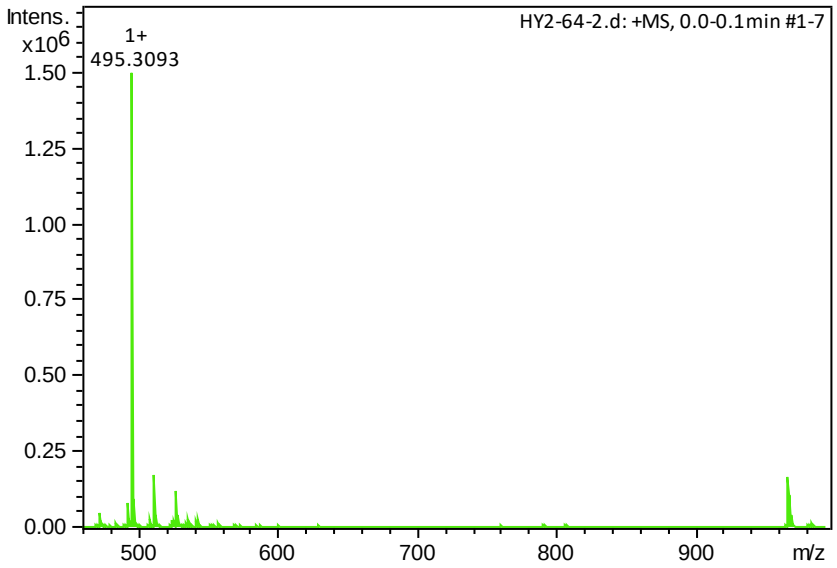

Figure S19. HRESIMS spectrum of **2**

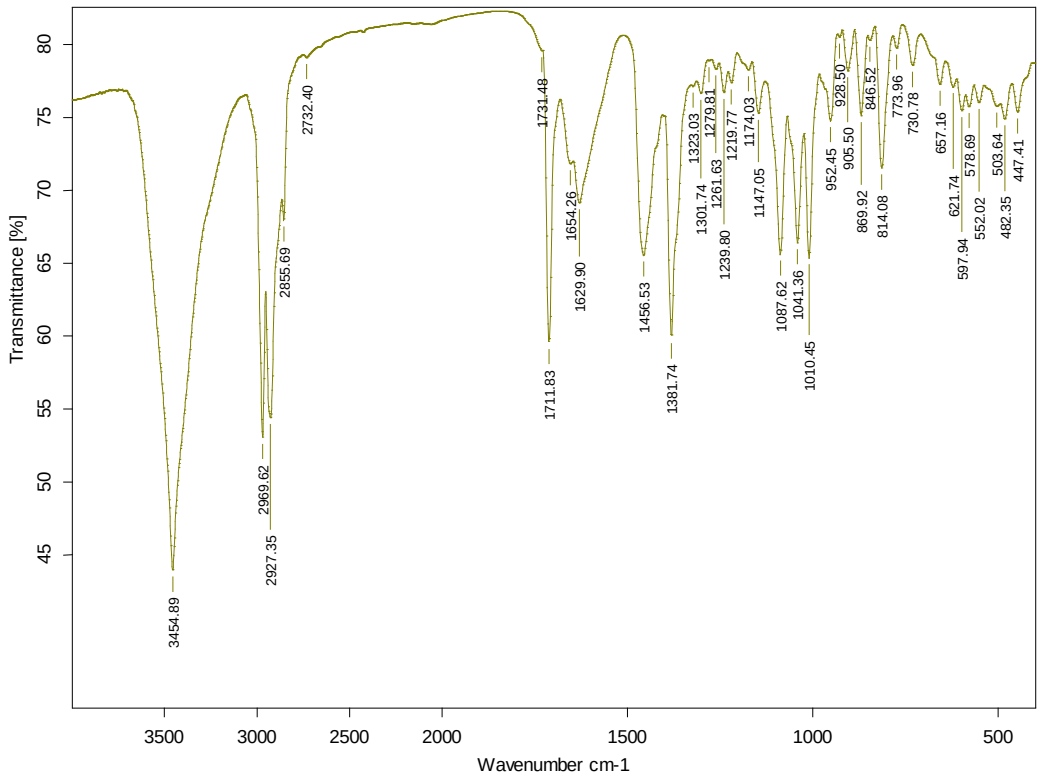

Figure S20. IR spectrum of **2**

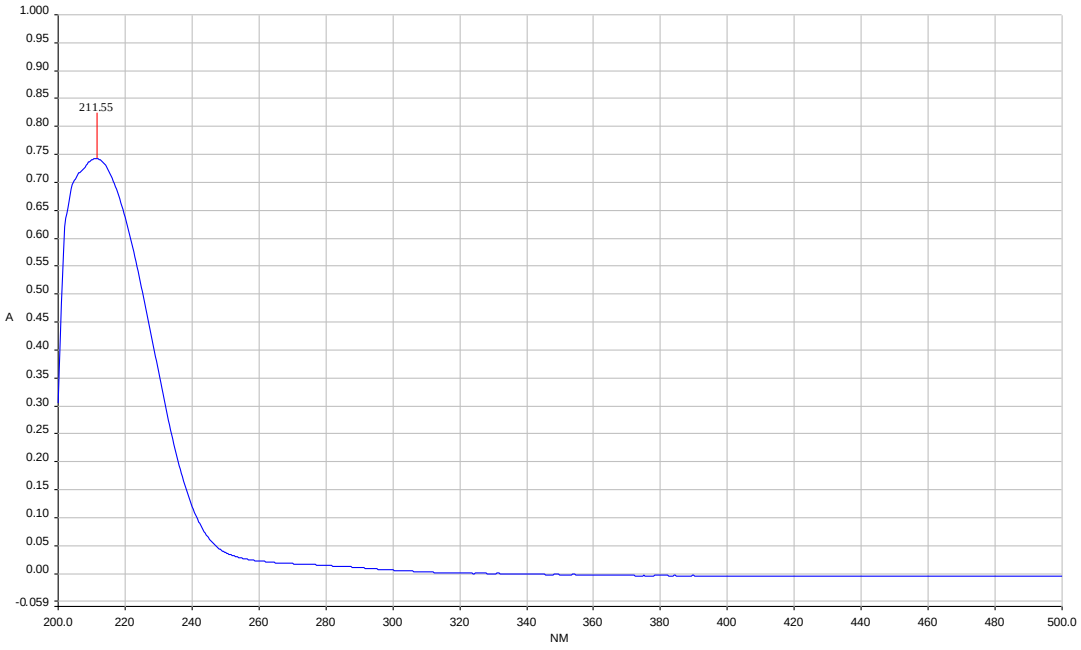

Figure S21. UV spectrum of **2**

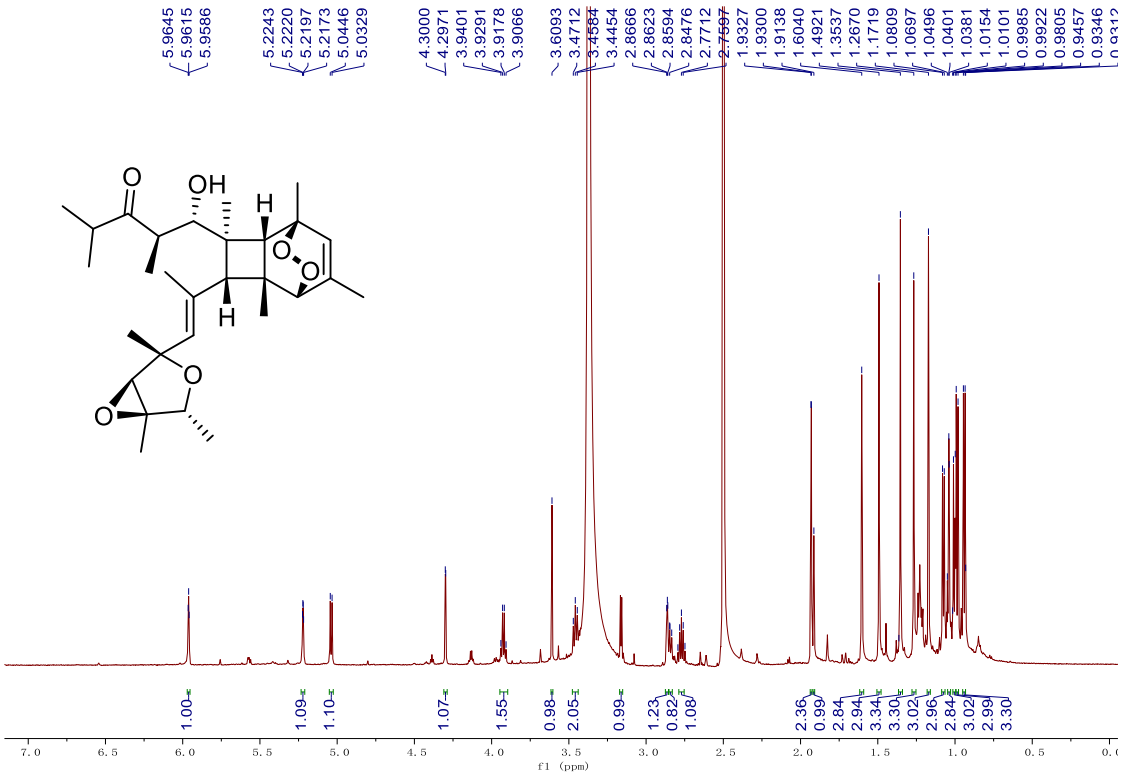

Figure S22. ^{1}H NMR spectrum of **3** recorded in DMSO-d_6

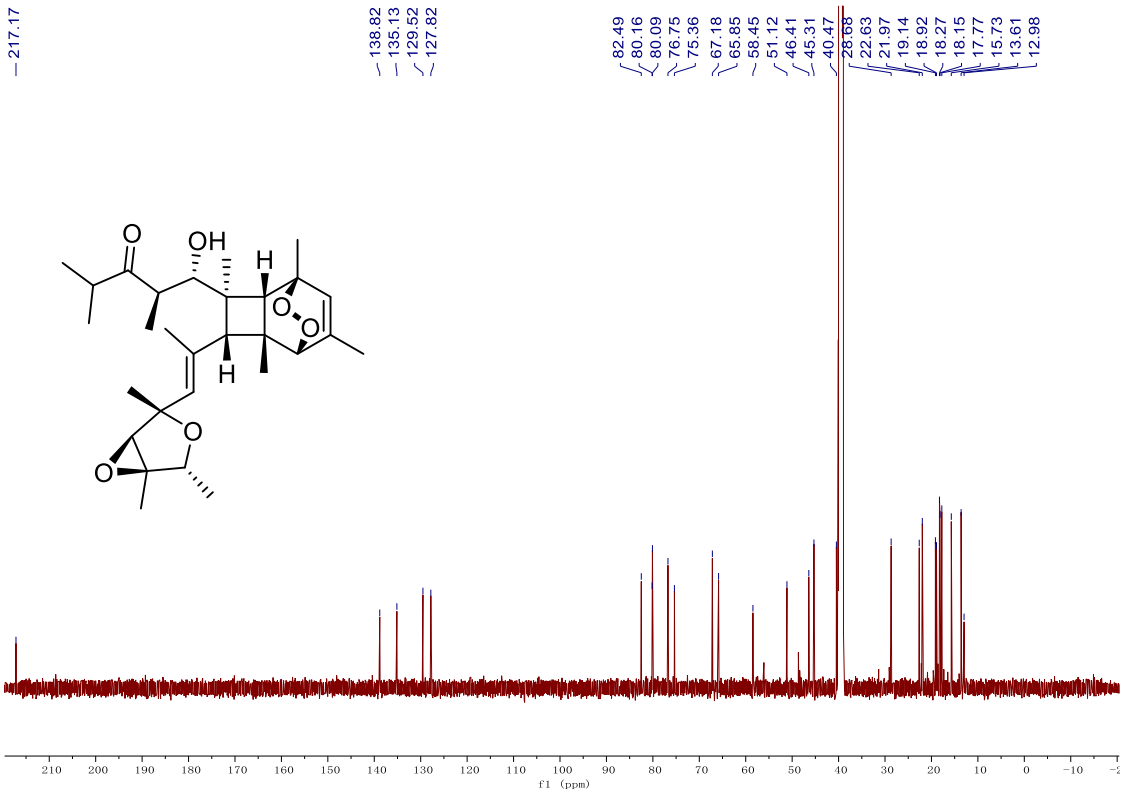

Figure S23. ^{13}C NMR spectrum of **3** recorded in DMSO-d_6

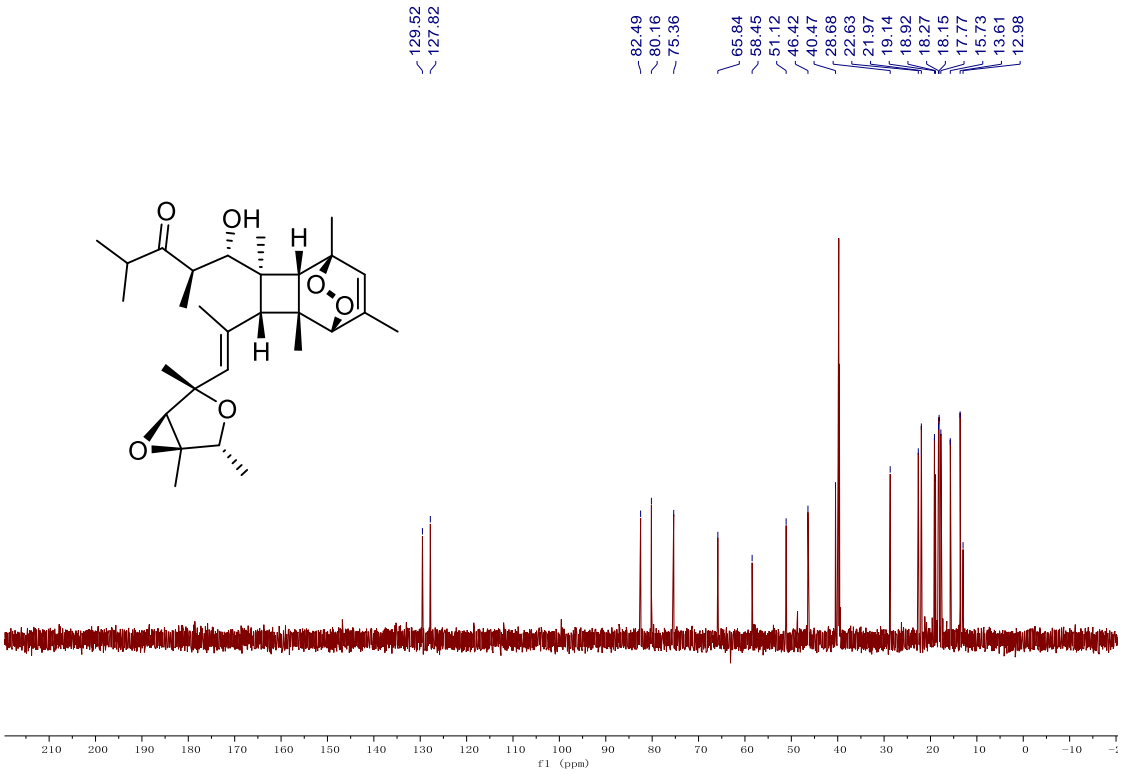

Figure S24. DEPT NMR spectrum of **3** recorded in DMSO-d_6

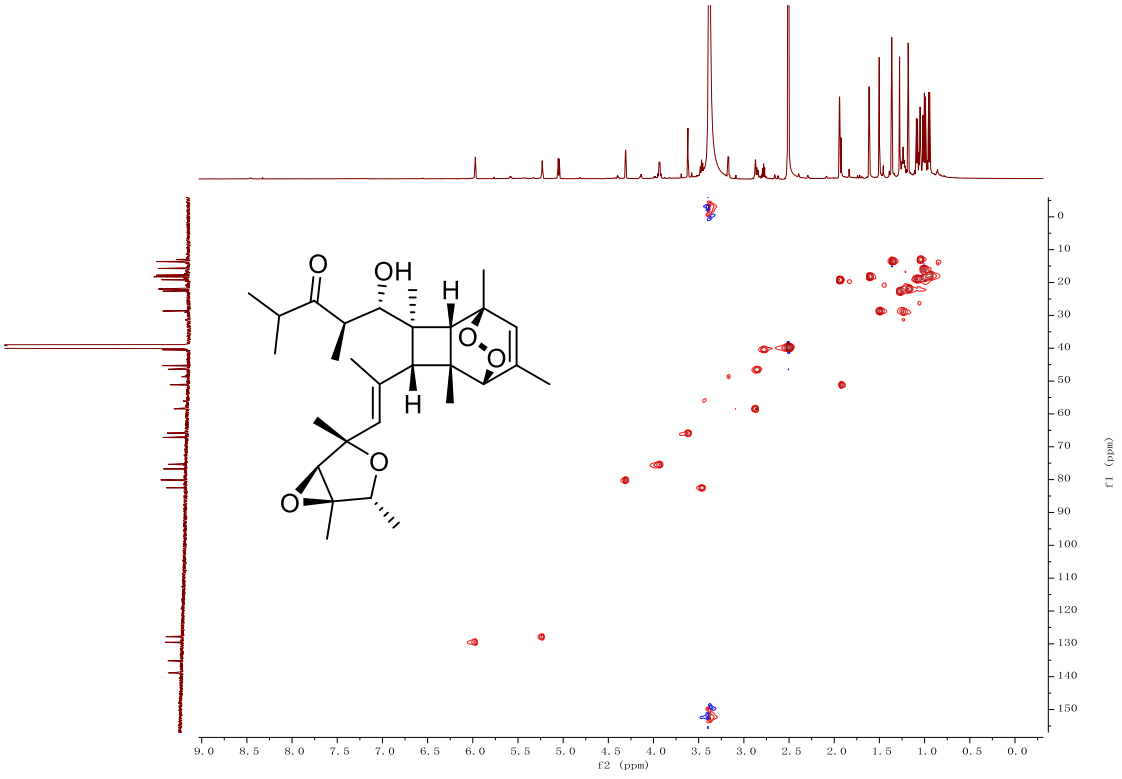

Figure S25. HSQC spectrum of **3** recorded in DMSO-d_6

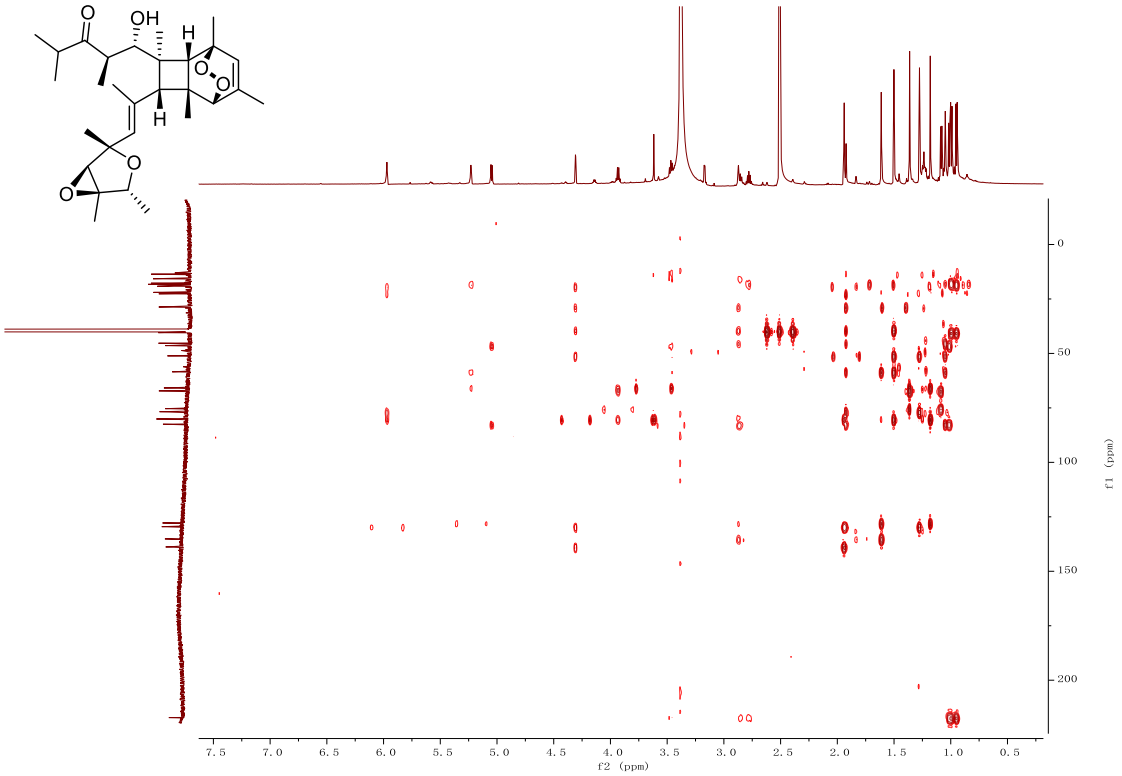

Figure S26. HMBC spectrum of **3** recorded in DMSO-d_6

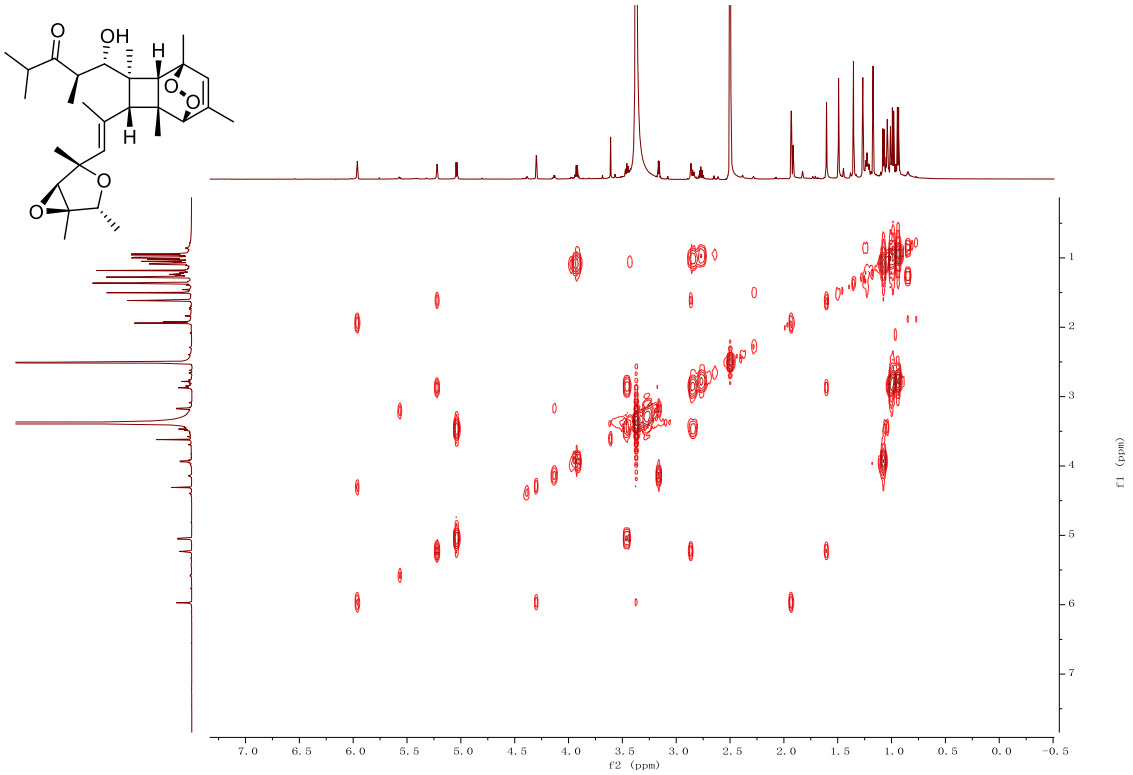

Figure S27. ^{1}H-^{1}H COSY spectrum of **3** recorded in DMSO-d_6

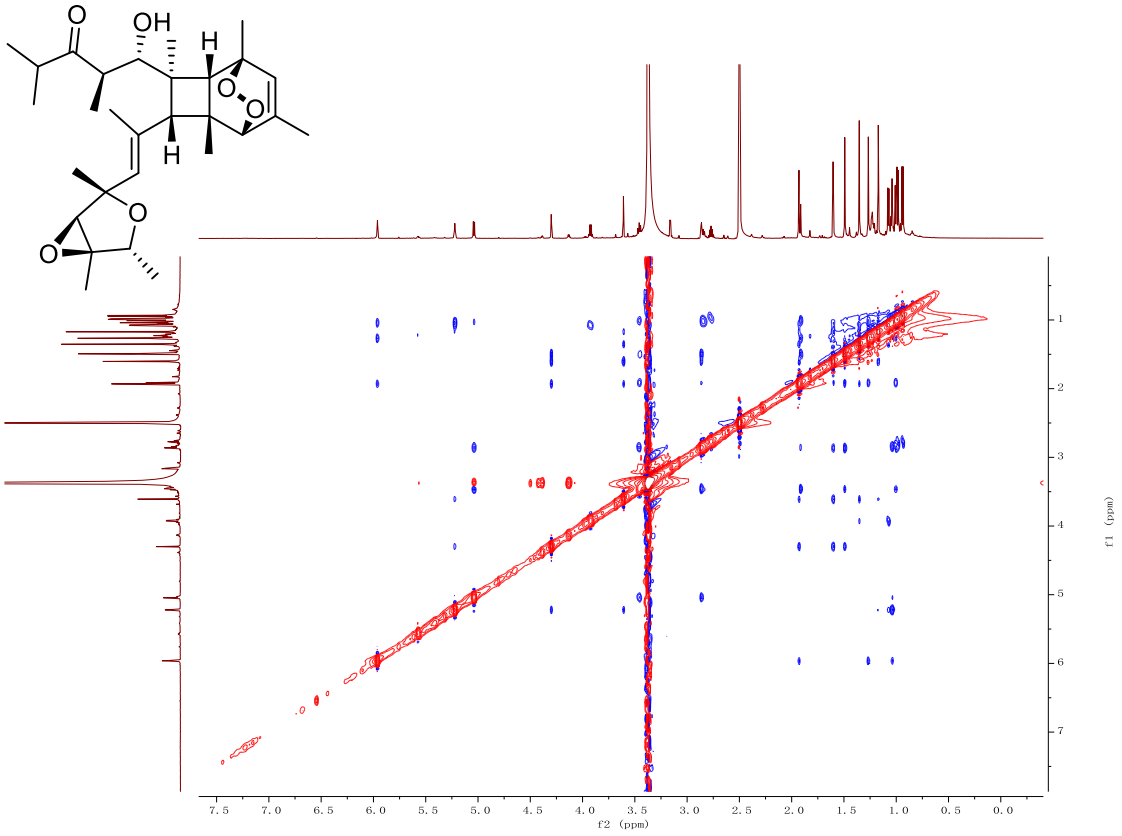

Figure S28. NOESY spectrum of **3** recorded in DMSO-d_6

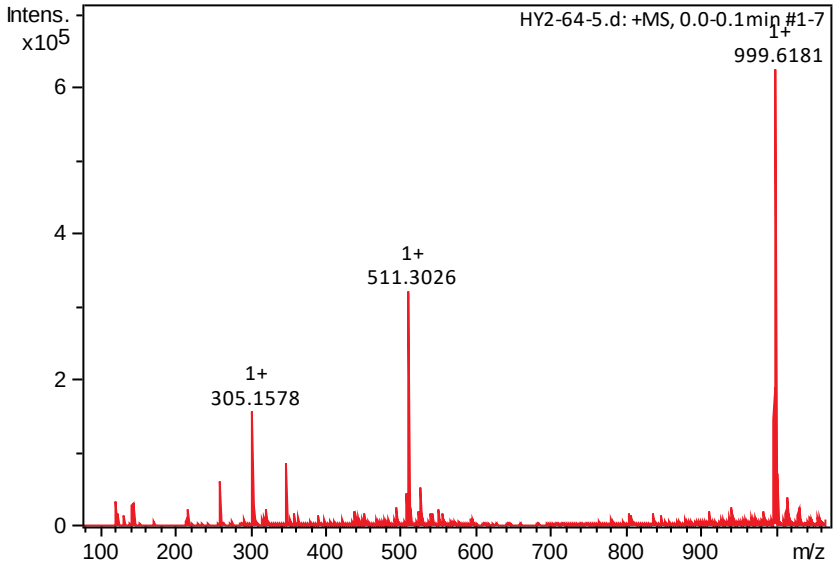

Figure S29. HRESIMS spectrum of **3**

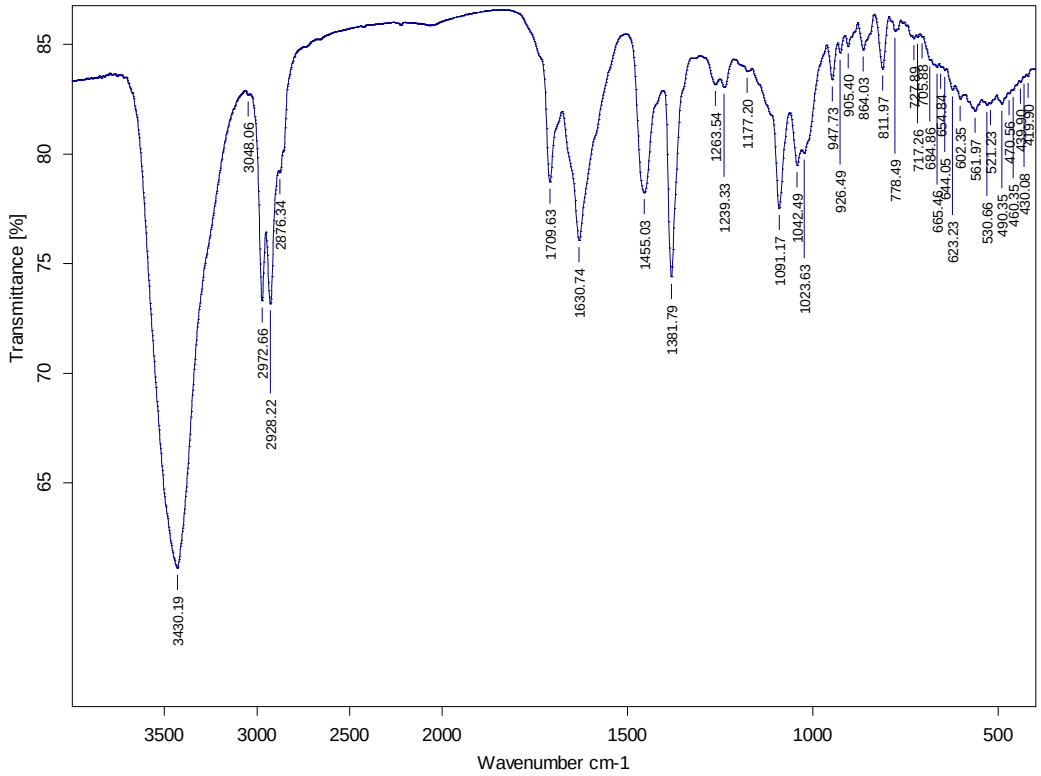

Figure S30. IR spectrum of **3**

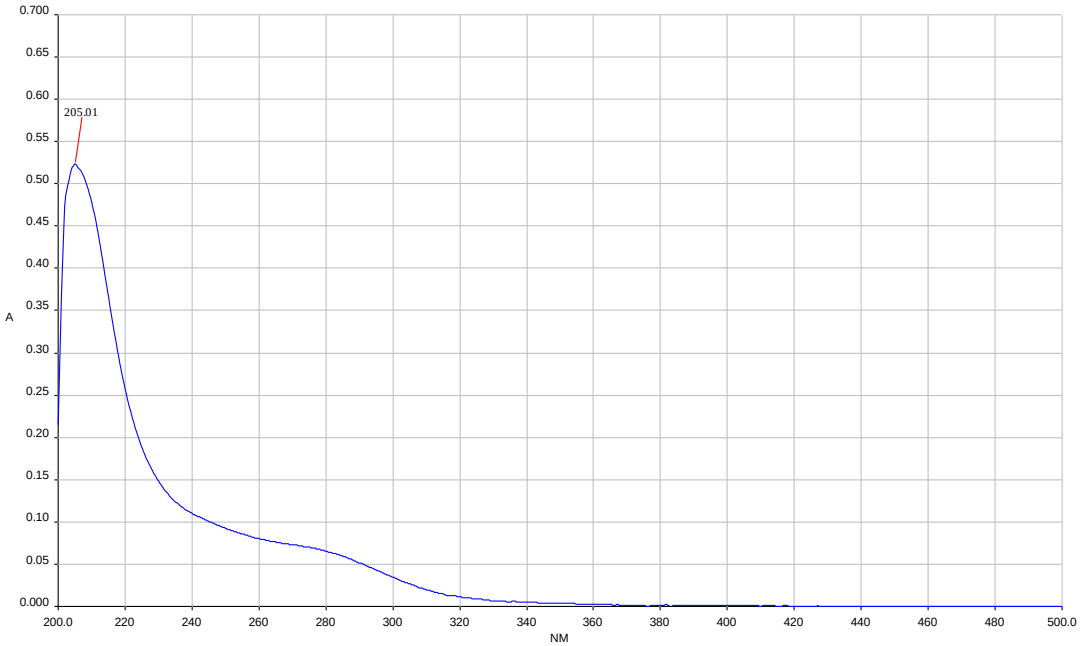

Figure S31. UV spectrum of **3**