Supplementary Information

Cicadamides A and B, *N*-acetyldopamine dimers from the insect *Periostracum cicadae*

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ECD calculated methods

Cell viability assay against cancer cells

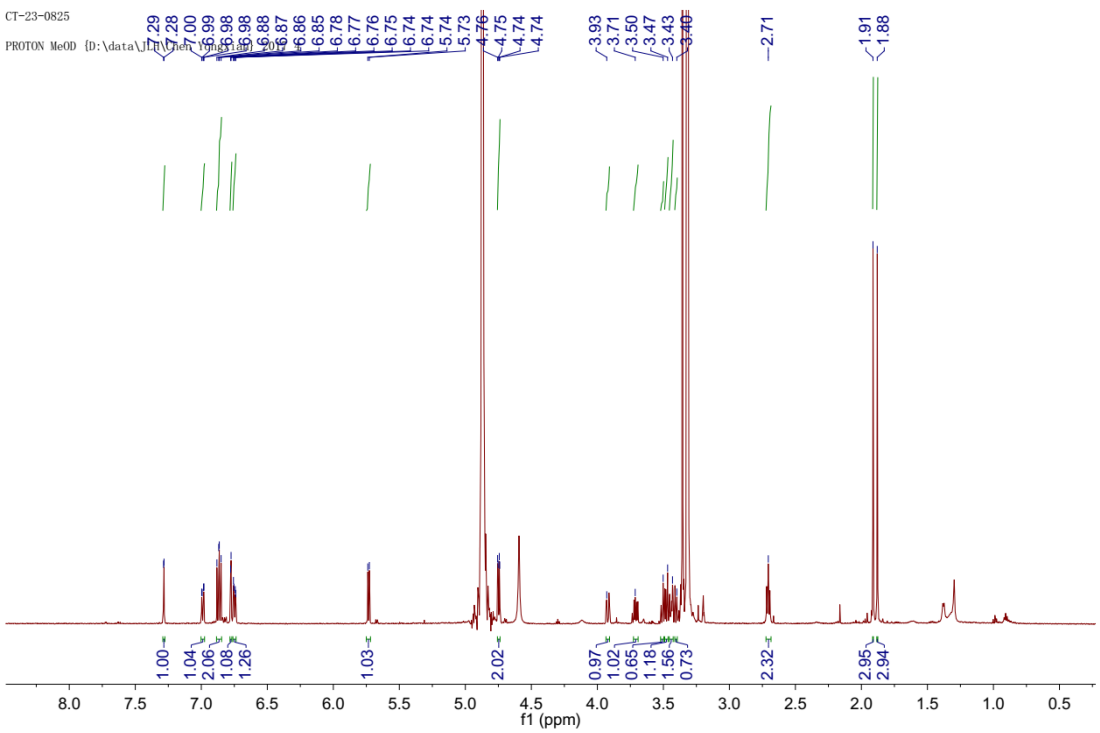


Figure S1. ^{1}H NMR spectrum of **1** in methanol-d_4

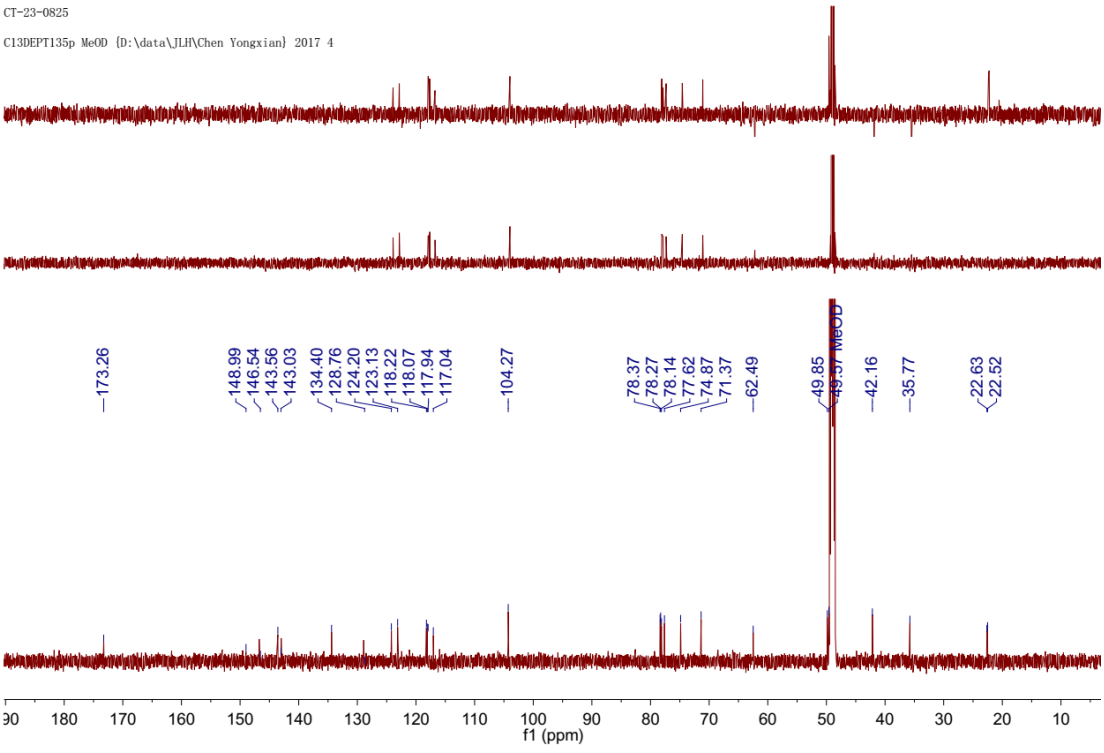


Figure S2. ^{13}C NMR and DEPT specta of **1** in methanol-d_4

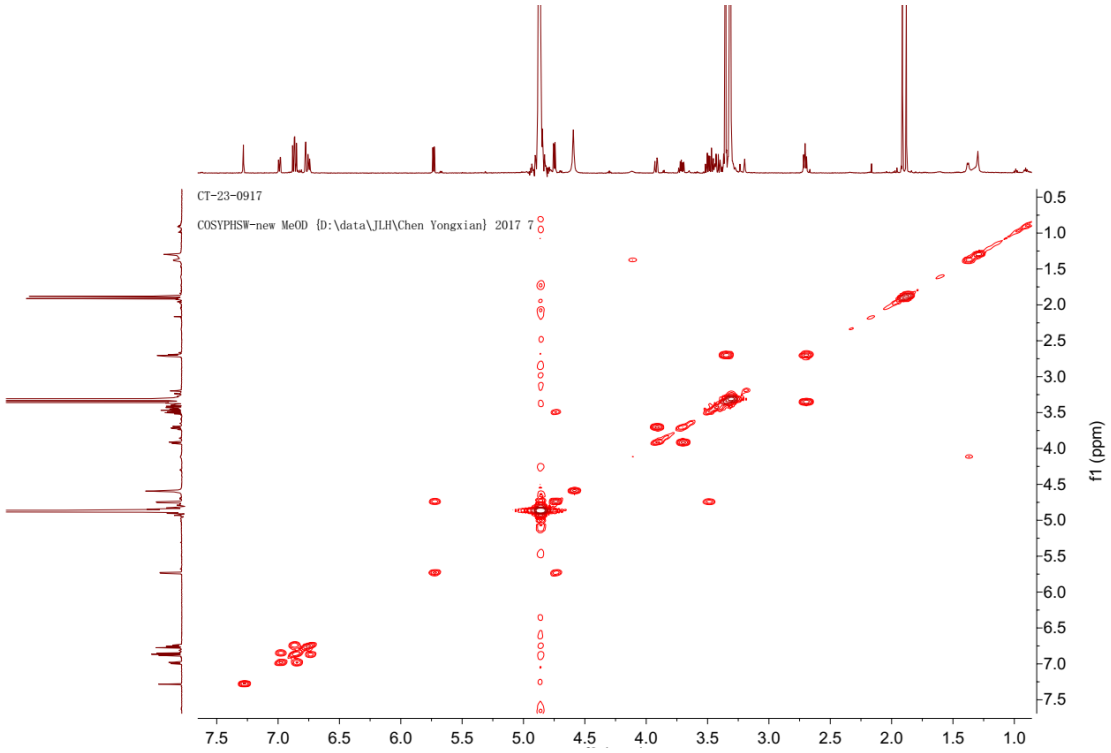


Figure S3. ^{1}H-^{1}H COSY spectrum of **1** in methanol-d_4

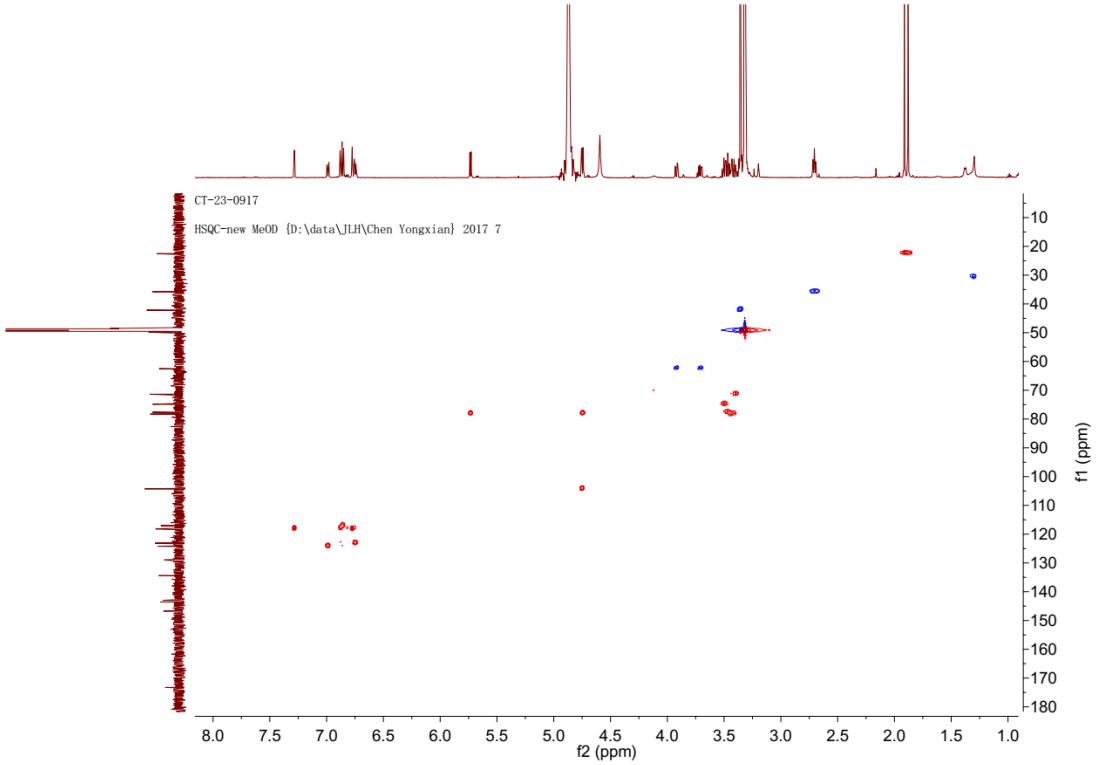


Figure S4. HSQC spectrum of **1** in methanol-d_4

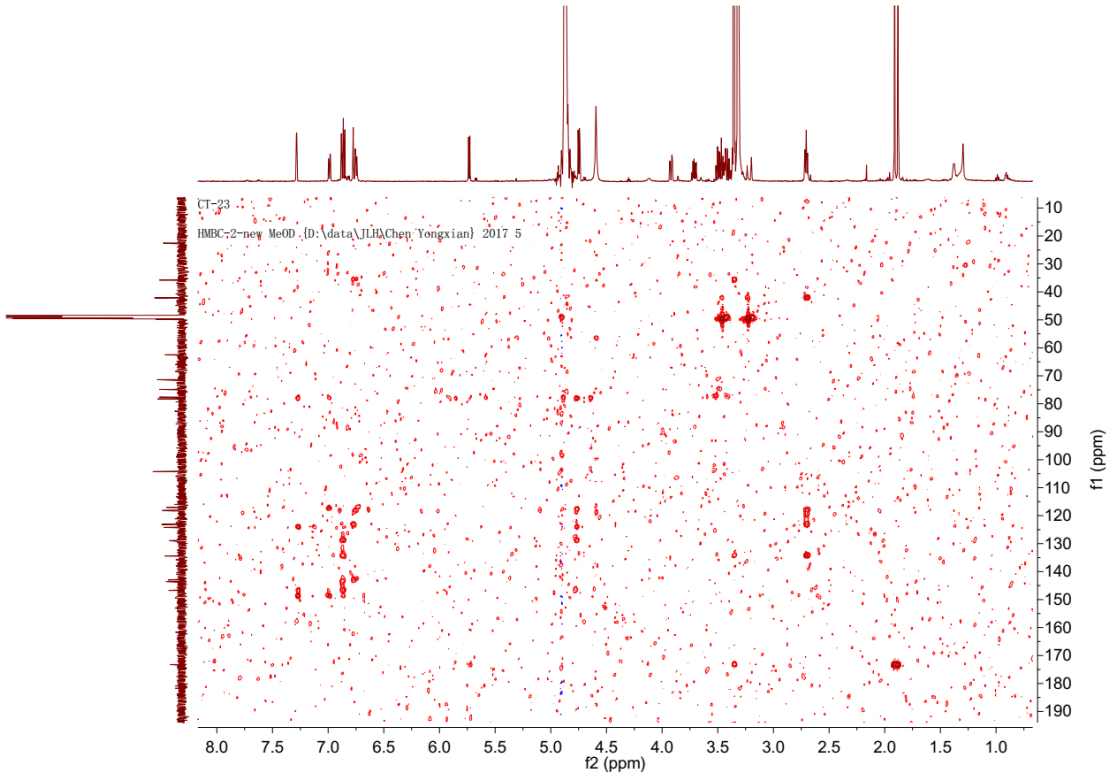


Figure S5. HMBC spectrum of **1** in methanol-d_4

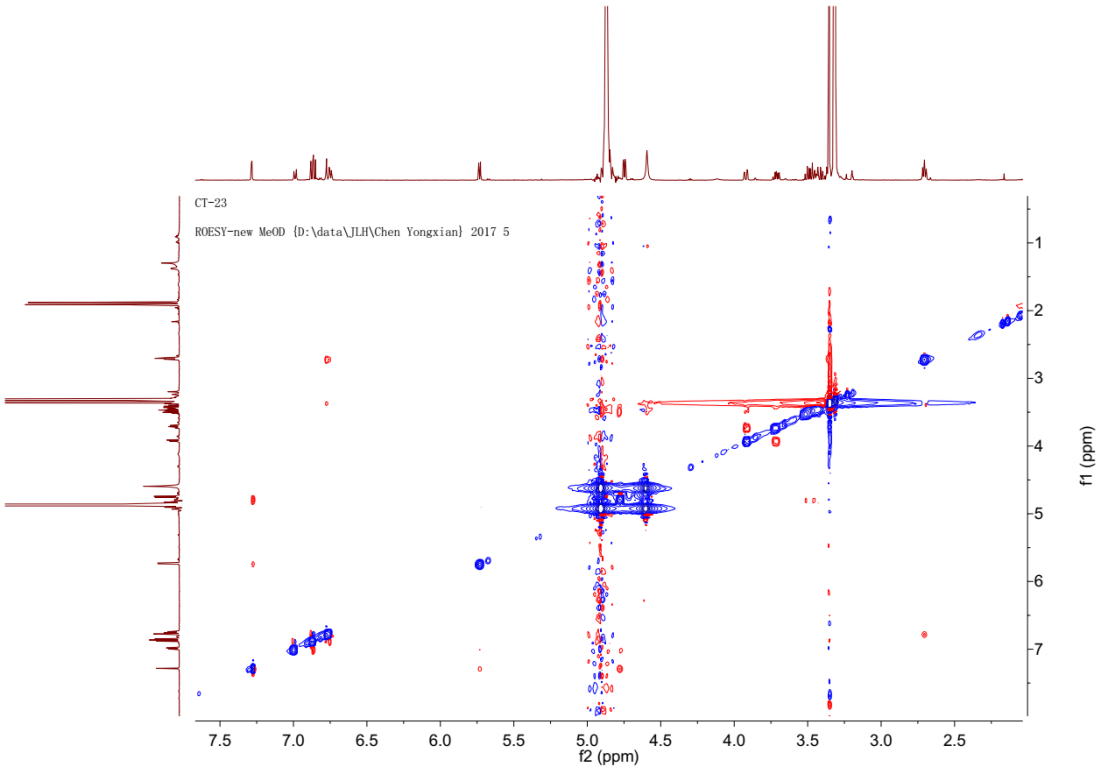
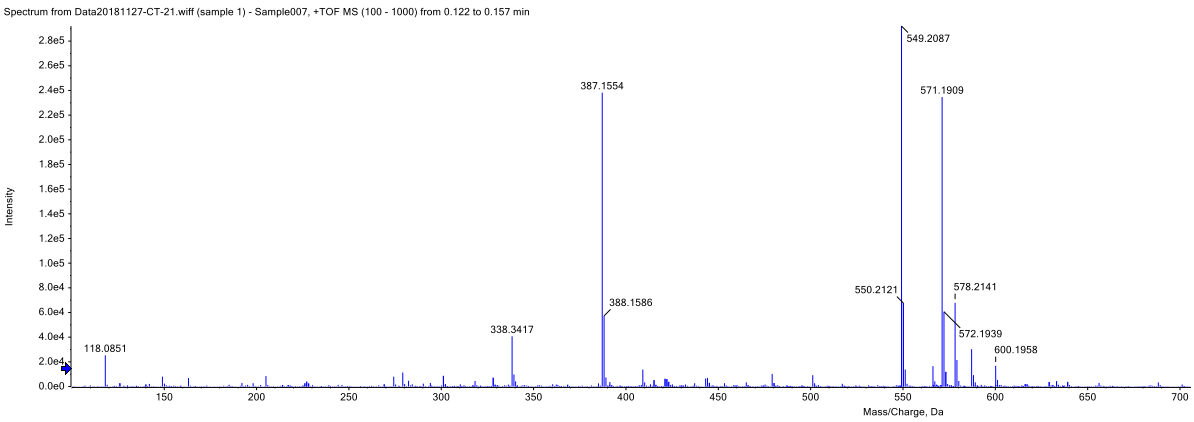


Figure S6. ROESY spectrum of **1** in methanol-d_4



$[M+H]^+$ m/z 549.2087

Hit	Formula	m/z	RDB	ppm
1	C26H32N2O11	549.2079	12.0	1.5

Elments from ~ to C60H120O60N2

Mass tolerance 5 ppm

Figure S7. HRESIMS of **1**

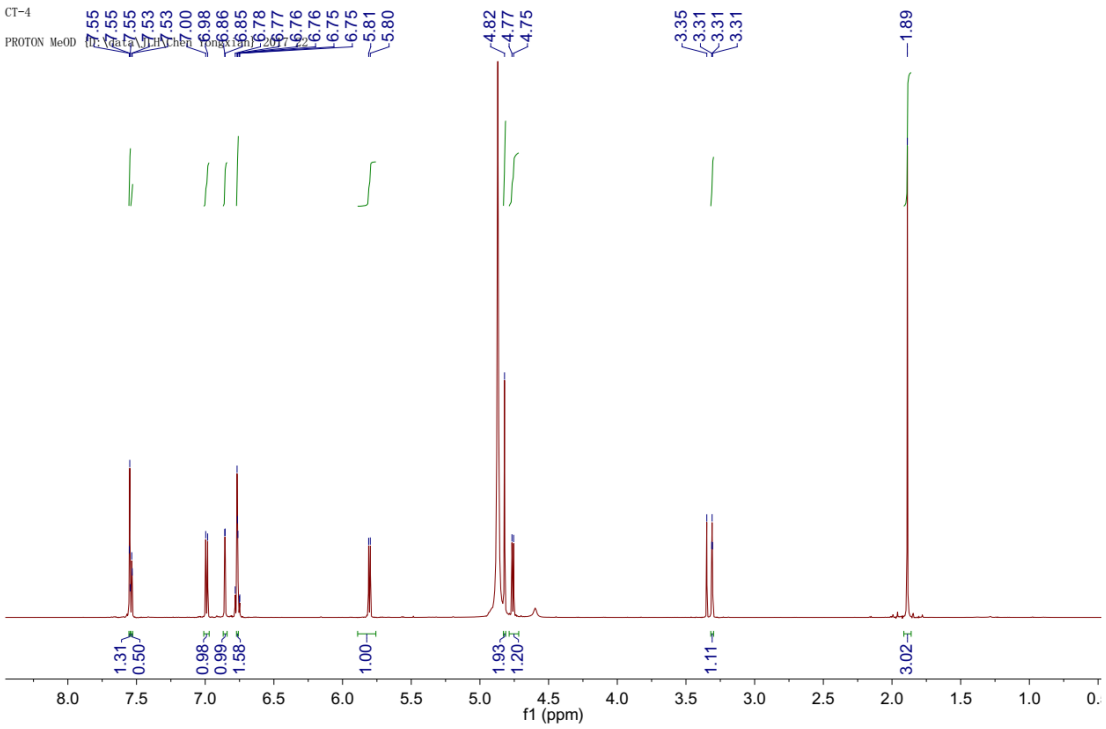


Figure S8. ^{1}H NMR spectrum of **2** in methanol-d_4

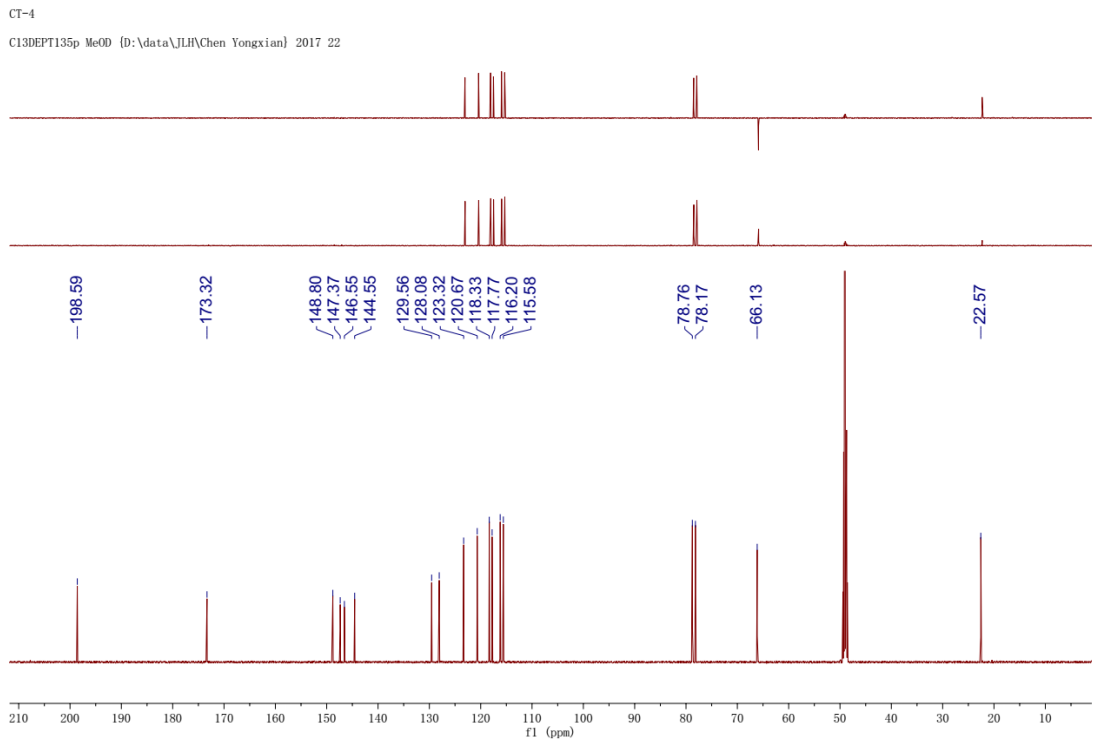


Figure S9. ^{13}C NMR and DEPT spectra of **2** in methanol-d_4

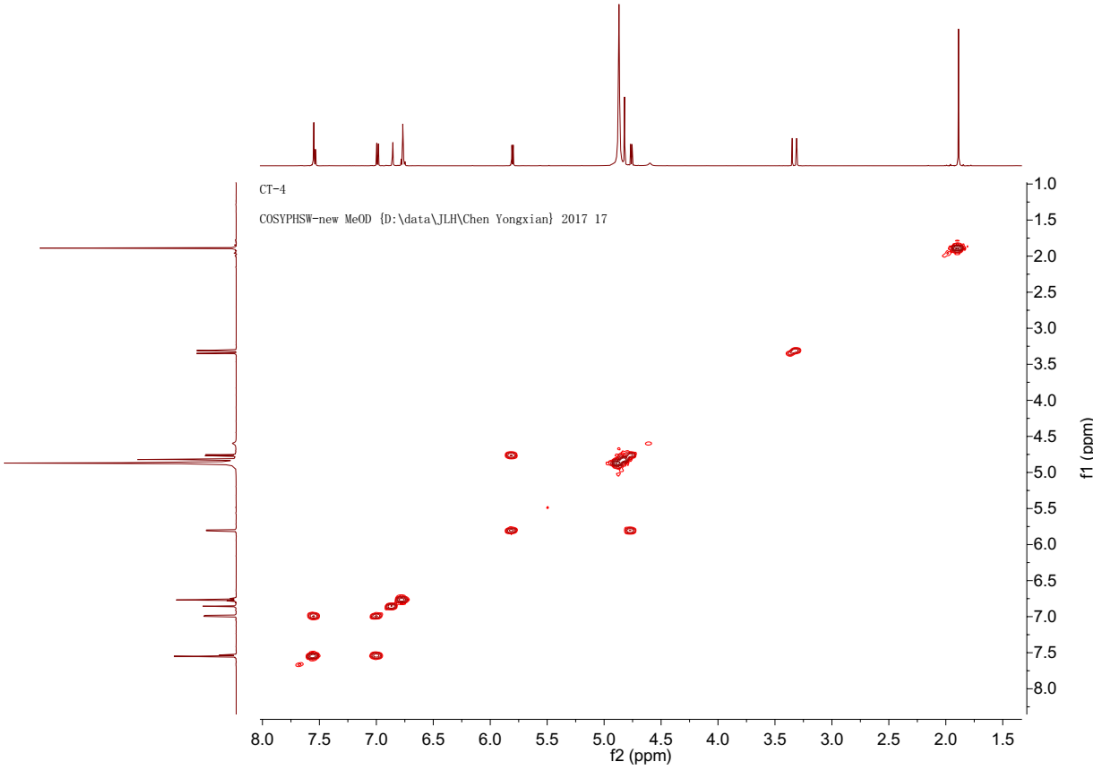


Figure S10. ^{1}H-^{1}H COSY spectrum of **2** in methanol-d_4

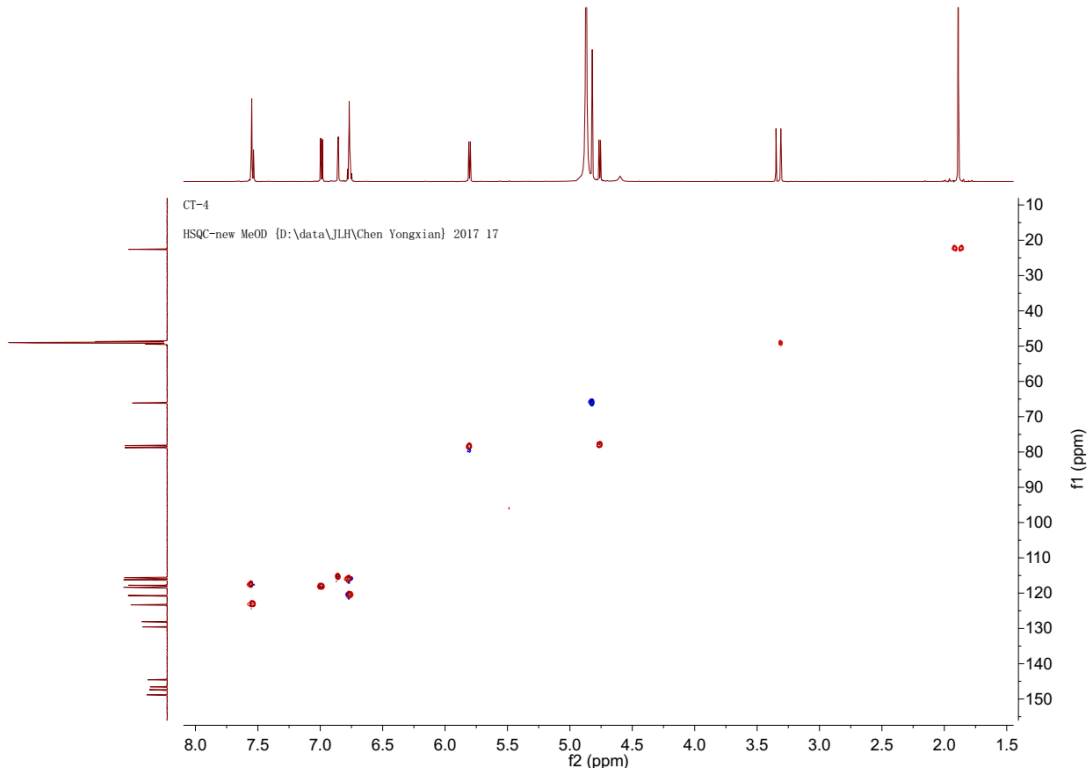


Figure S11. HSQC spectrum of **2** in methanol-d_4

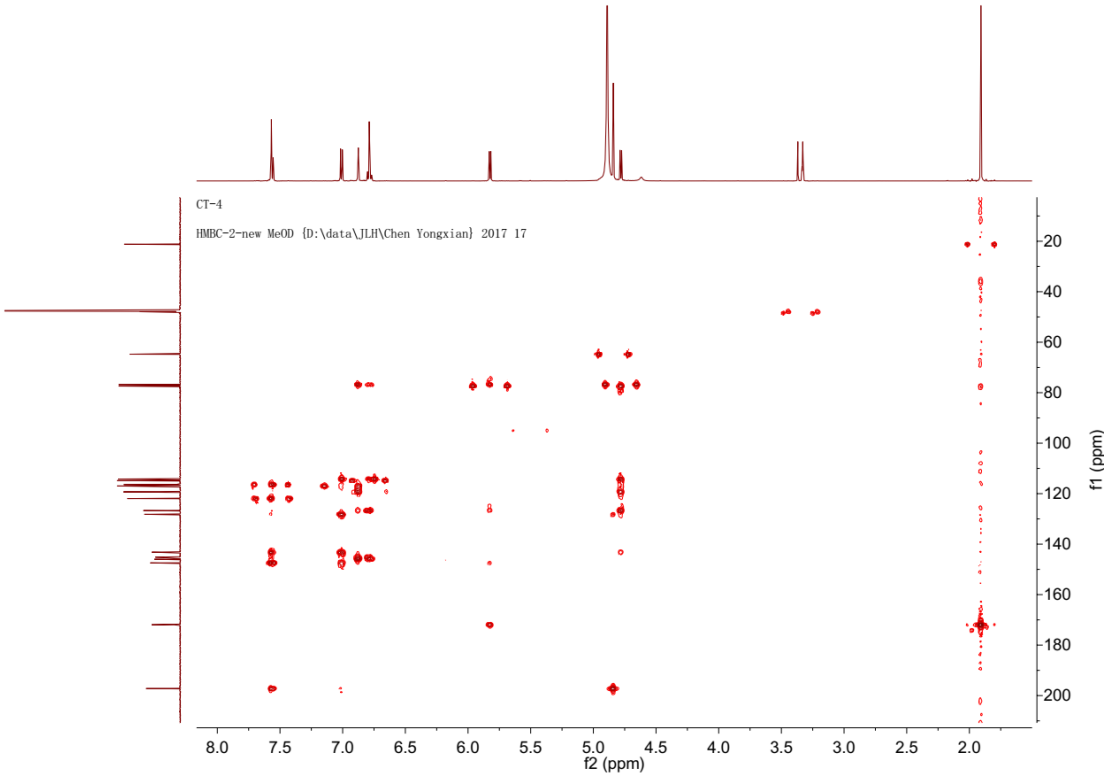
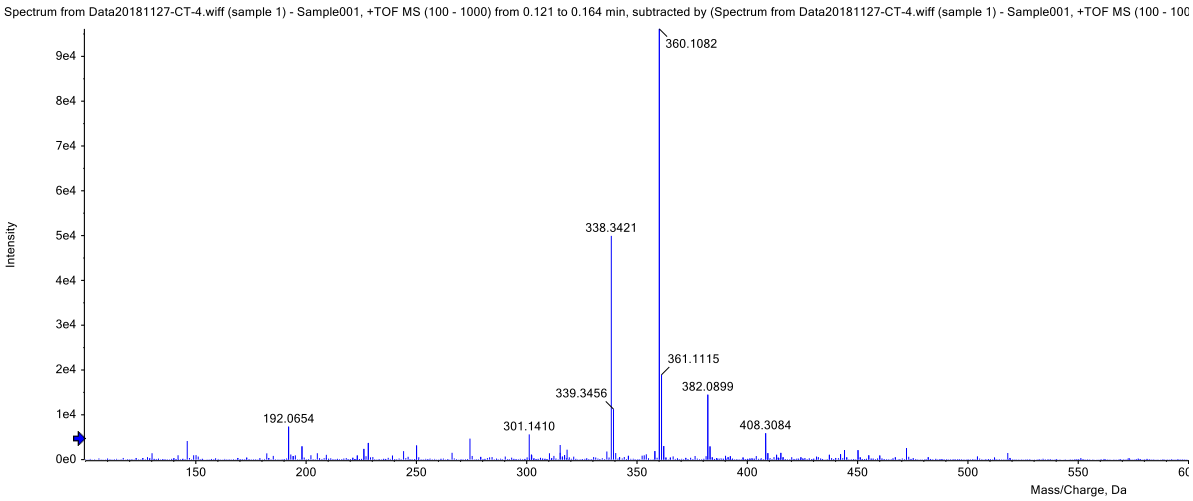


Figure S12. HMBC spectrum of **2** in methanol-d_4



[M+H]+ m/z 360.1082

Hit	Formula	m/z	RDB	ppm
1	C18H17NO7	360.1078	11.0	1.2

Elments from ~ to C60H120O60N

Mass tolerance 5 ppm

Figure S13. HRESIMS of **2**

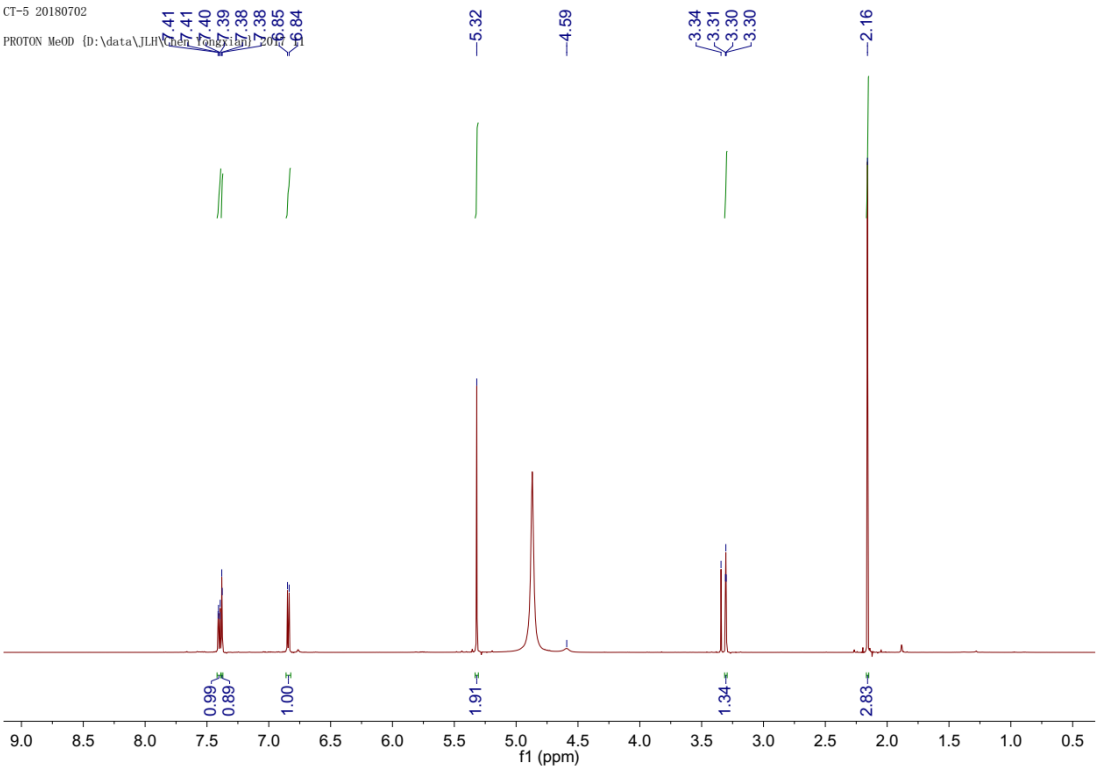


Figure S14. ^{1}H NMR spectrum of **6** in methanol-d_4

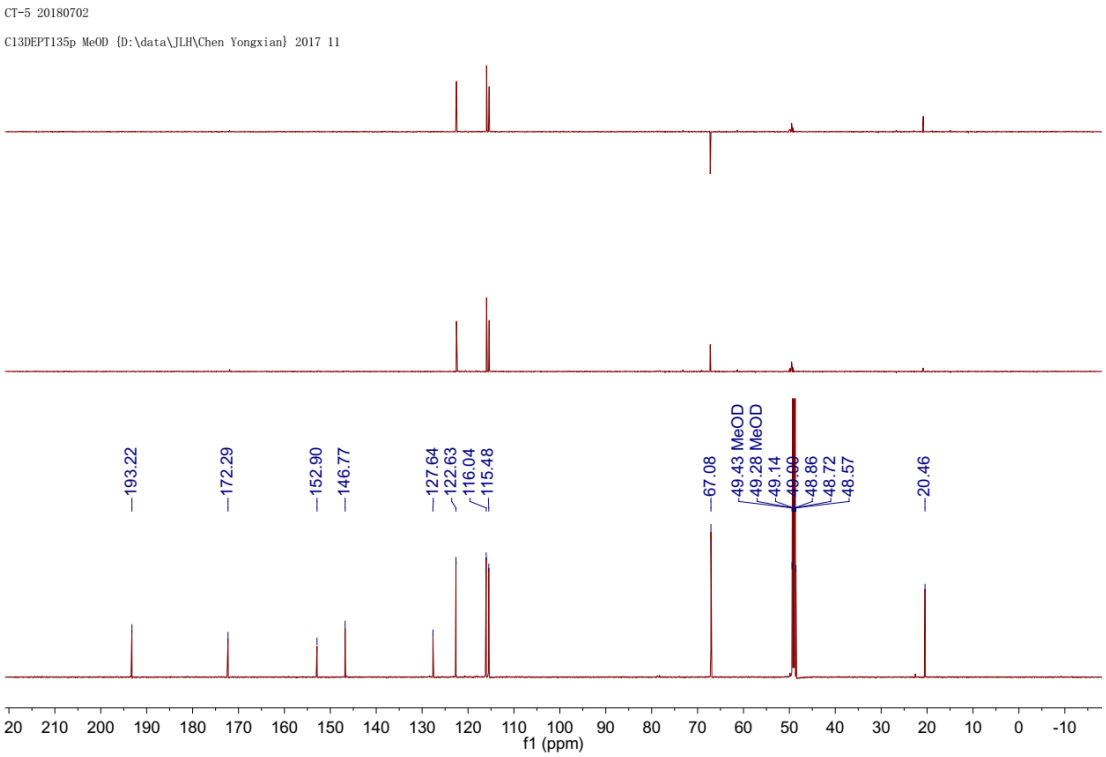


Figure S15. ^{13}C NMR and DEPT spectra of **5** in methanol-d_4

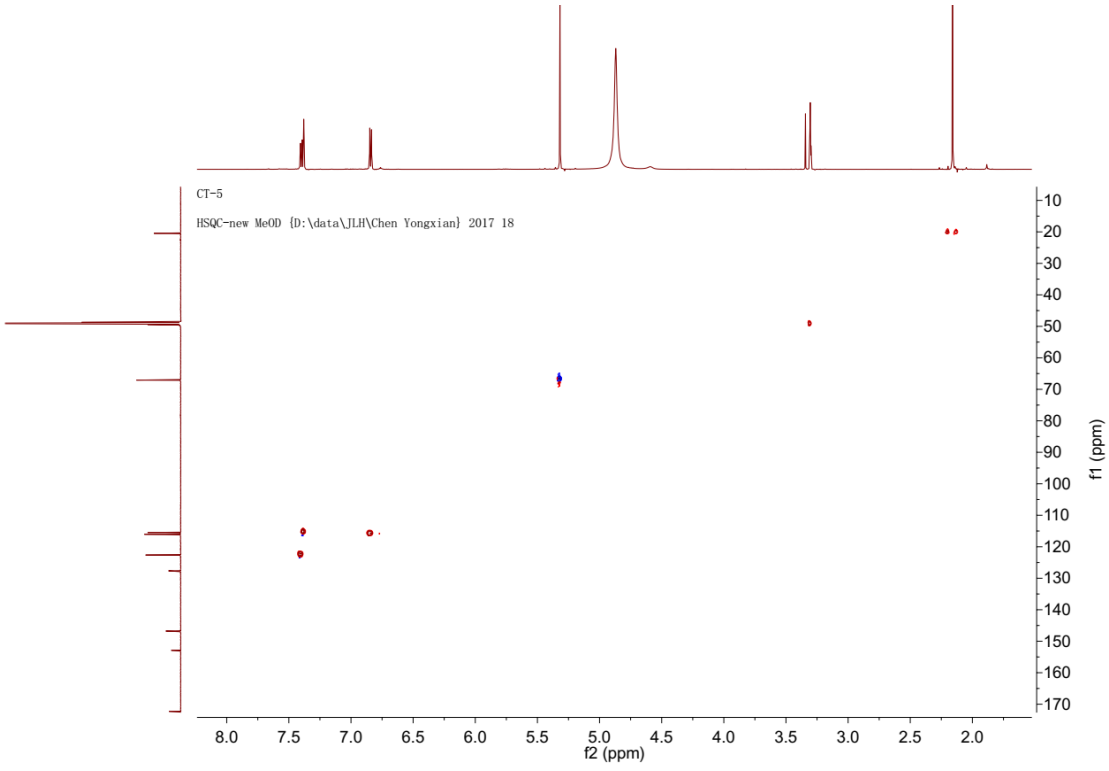


Figure S16. HSQC spectrum of **5** in methanol-d_4

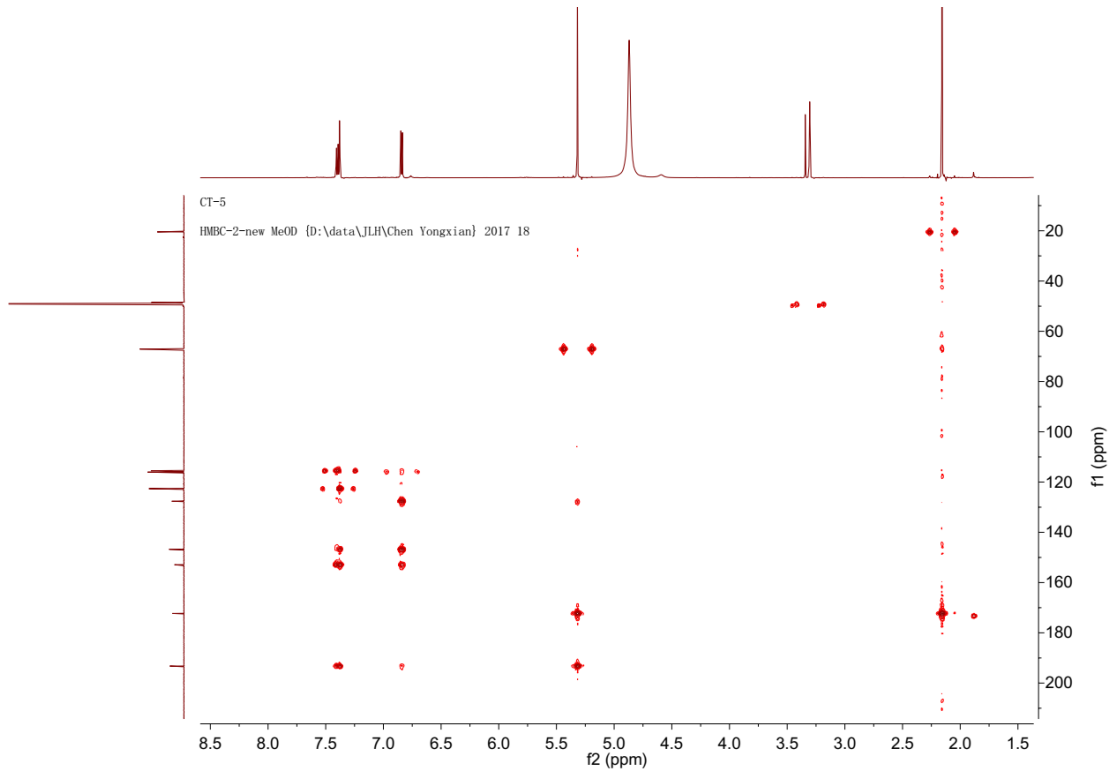


Figure S17. HMBC spectrum of **5** in methanol-d_4

ECD calculated methods

Molecular Merck force field (MMFF) and DFT/TDDFT calculations were performed with Spartan'14 software package (Wavefunction Inc., Irvine, CA, USA) and Gaussian09 program package (Frisch et al. 2010), Conflex conformational search generated low-energy conformers within a 10 kcal/mol energy was finished by software CONFLEX 7. The predominant conformers were optimized by DFT calculation at B3LYP/6-31G (d,p) level with the PCM in MeOH. ECD calculations further were conducted at the B3LYP/6-31G (d,p) level with the PCM in MeOH. For comparisons of the calculated curves and experimental CD spectra, the program SpecDis (Bruhn et al. 2013) was used.

References

(1) Frisch, M. J.; Trucks, G. W.; Schlegel, 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.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; 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, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, revision C.01. Gaussian, Inc.: Wallingford CT, 2010.

(2) Bruhn, T.; Schaumlöffel, A.; Hemberger, Y.; Bringmann, G. *Chirality* 2013, *25*, 243–249.

Cell viability assay against cancer cells

Human cancer cell lines were obtained from the Cell Bank of China Science Academy (Shanghai, PR China), maintained in Dulbecco's modified Eagle's medium (DMEM) supplemented with 10% fetal bovine serum and 100 U/mL penicillin-streptomycin and incubated at 37 ℃ in an atmosphere of 5% CO_2. Cell viability was evaluated using the CCK-8 assay (Dojindo Laboratories, Tokyo, Japan) according to the manufacturer's instructions. Exponentially growing cells were seeded at $3-8\times10^3$ cells per well in 96-well culture plates for 24 h. Cells were exposed to increasing concentrations (0−80 μM) of compounds **1**, (+)-**2**, and (–)-**2** or 5-FU for 48 h. The equal volume of DMSO was used as the solvent control. CCK-8 solution (10 μL) was added to each well and incubated for another 1−4 h. Light absorbance of the solution was measured at 450 nm (Epoch 2; BioTek Instruments, Inc., Winooski, VT, USA). The IC_{50} values were

calculated using the PrismPad program (Version 5.0, GraphPad Software, San Diego, CA, USA).