Two new catechins from Zijuan green tea enhance the fitness and lifespan of *Caenorhabditis elegans* via insulin-like signaling pathways

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Materials and instruments

The common column chromatographic materials contain Silica gel (Yantai Jiangyou Silicon Development Co., Ltd., Shandong, China), Toyopearl HW-40F (Tosoh Bioscience Shanghai Co., Ltd., Shanghai, China), Sephadex LH-20 (GE Healthcare Bio-Sciences AB, Sweden) were used in the column chromatography (CC). Human serum albumin (95%) was purchased from Sino Biological. CM7 sensor chips and coupling reagents [N-ethyl-N'-(dimethylaminopropyl)carbodiimide (EDC), N-hydroxysuccinimide (NHS), and ethanolamine hydrochloride] were purchased from GE Healthcare. Dimethyl sulfoxide (DMSO) was bought from Shanghai Sinopharm

Chemical Reagent Co., Ltd. (China). Trizol and SYBR Green reagent were purchased from Yuanye Biotechnology Co., Ltd (Shanghai, China).

The Agilent DD2 600 MHz instruments (Agilent, Inc., Santa Clara, CA, U.S.A.) with transcranial magnetic stimulation (TMS) were used to detect the ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra. Mass data were recorded on an Agilent 1290 UPLC with a photodiode detector array (PDA) coupled to a 6545 time-of-flight (TOF) mass spectrometer with electrospray ionization (ESI) source in negative mode (Agilent, Inc., Santa Clara, CA, U.S.A.). Semipreparative high-performance liquid chromatography (HPLC) was performed on a Waters e2695 instrument (Waters, Milford, MA, U.S.A.) combined with a Waters 2998 PDA detector. Freeze dryer (Freezone Labconco, U.S.A.). An iS50 FI-IR spectrometer instrument using KBr pellets (Thermo Co., Waltham, MA, U.S.A.) was used to record the Infrared (IR) spectrum. JASCO J-815 spectropolarimeter (Tokyo, Japan). Stereo Microscope

(Motic, Xiamen, China), Fluorescence microscope (Olympus, Tokyo, Japan). Bio-Rad MiniOption™ Real Time PCR Detection System (BioRad, Hercules, CA, U.S.A.).

NMR calculation

To establish the absolute configuration of **1**, the ECD spectra of (2*R*,3*R*,Glc-1*S*,Glc-2*R*,Glc-3*S*,Glc-4*S*,Glc-5*R*)-**1** and its enantiomer were calculated at the LC-wPBE/6-311G(d,p) level with the Gaussian 09 software.[1, 2]

The systematic random conformational analyses of all plausible stereoisomers of **1** and **2** were subjected to semiempirical PM3 quantum mechanical geometry optimizations using the BALLOON program. The stable conformers were optimized with B3LYP/6-31G(d) level (gas phase), followed with frequency calculation. The gauge-independent atomic orbital (GIAO) ^{13}C NMR was calculated at the mPW1PW91/6-311G(d,p) (IEFPCM) level of theory in DMSO.[1, 3] The calculated NMR data were analysed by using DP4+ probability to further confirm the relative configuration of **1** and **2**.

ECD calculation

The ECD calculation of **1** and **2** was performed as previously described.[4, 5] The conformation of **1** and **2** generated by BALLOON were subjected to semiempirical PM3 quantum mechanical geometry optimizations using the Gaussian 09 program. 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 LC-wPBE/6-311G(d,p) 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 0.25 eV. The spectra were combined after Boltzmann weighting according to their population contributions and UV correction was applied.

Assay of free radical scavenging activity

Briefly, 50 μL of compound solutions with a series of concentrations were pipetted into a 96-well plate (50 μL/well), and 200 μL of methanolic DPPH solution were added and mixed in each well. After 30 min incubation at room temperature in the dark, the absorbance (Abs) at 517 nm was measured by a microplate reader. The ABTS radical solution was generated by mixing potassium persulfate ($K_2S_2O_8$, 4.95 mM) well with ABTS (7.0 mM) at room temperature in the dark for 12 h. The ABTS solution was diluted with 0.2 M PBS (pH 7.4) to obtain a solution with Abs reading at 734 nm of 0.7 ± 0.02. Then 20 μL compound solution was mixed with 200 μL of ABTS solution, and Abs at 734 nm was measured after reaction at room temperature for 6 min. Ascorbic acid (VC) was used as a positive control. DPPH and ABTS

radical scavenging activity of the compound was calculated by the following formula: free radical scavenging activity (%) = (1- As/Ab) × 100

Molecular modeling and interaction analysis.

We used Autodock 4.2 Tools to simulate the interaction of HSA with the zijuanins E and F. The model of HSA (code ID: 1h9z) for simulation was obtained from the Protein Data Bank. Then we used ChemBio3D 14.0 to optimize the 3D structure of the compounds. The energy evaluation grid was located at the bottom of the active site gorge (37.463, 14.182, and 27.18) with grid points in the x-, y-, z-axes set to 60 × 60 × 60 Å and separated by 0.375 Å. The final results were assessed by two factors, binding constant (Ki) and binding energy (Ea). Population size was set to 150 with 2,500,000 energy evaluations(medium) and conformational searching was done using the Lamarckian genetic algorithm (LGA). The lowest energy conformation was used for further analysis. After protein docking, the resultant complexes were subjected to hydrogen bonding analysis. The binding affinity and interaction of compounds to HSA were studied by PyMOL and Discovery Studio visualizer.

SPR analysis

SPR measurements were performed using a BiacoreT200 instrument. For this experiment, CM7 sensor chips composed of carboxymethylated dextran covalently attached to a gold film were used. On the sensor chip surface were two flow channels: the sample channel (in which the protein will be immobilized) and the reference channel. During the analysis, the response of the detector relates to the dependency of

the SPR signal (expressed in arbitrary Resonance Units (RU)) versus time (t) in graphs called sensorgrams, where one RU corresponds to a 0.0001° shift in SPR angle. The output signal, or response, of the SPR is the difference of signals between the sample (with immobilized HSA) and reference (without immobilized HSA) channels.

Immobilization of HSA on the chip surface.

Immobilization of HSA on the chip surface was performed according to an amino coupling protocol. The protein was diluted with sodium acetate at pH 5.5, 5.0, 4.5, 4.0 to 10 μg/mL, and each was prepared at 100 μL. Through pre-enrichment experiment, determine pH 4.5 as the best coupling condition. Therefore, the ligand solution was diluted to 10 μg/mL with pH 4.5 sodium acetate, and 200 μL was used for the formal coupling operation. First, the CM7 chip was activated by injecting a freshly prepared mixture of EDC (0.4 M) and NHS (0.1 M) (1:1 v/v) at a flow rate of 10 μL/min for 7 min. The HSA, at a concentration of 10 μg/mL in immobilization buffer (10 mM sodium acetate at pH 4.5), was injected into the sample channel and allowed to react for 7 min at a flow rate of 10 μL/min, resulting in HSA immobilized densities averaging 4500 RU (RU values are proportional to bound HSA). HSA was coupled to the chip surface in the sample channel through covalent bonding between its amine groups and the carboxyl groups of the CM7 sensor chip. The remaining carboxyl groups were blocked by injecting a solution of ethanolamine hydrochloride at a flow rate of 10 μL/min. The HSA was immobilized only in the sample channel of the sensor chip to allow for monitoring of possible non-specific interactions between the

protein and the chip surface using the reference channel. The reference channel was activated with a 1:1 mixture of EDC/NHS and then treated with ethanolamine to block the carboxyl groups.

For the interaction experiments, the solutions of **1** and **2** were prepared in PBS-P buffer immediately before analysis. To obtain the sensorgrams of the interactions between the protein and **1** and **2**, a range of **1** and **2** concentrations were analyzed: 0.7815 to 25 μM (0.7815, 1.5625, 3.125, 6.25, 12.5, 25). The concentration ranges of **1** and **2** were chosen to obtain a linear relationship between the observed rate constant and the amount of substance of **1** and **2**. Compounds **1** and **2** were injected onto the HSA immobilized chip for 180 s at a flow rate of 20 μL/min. The PBS-P buffer flowing was injected for 200 s at a flow rate of 20 μL/min to regenerate the chip surface at the end of each experiment.

References:

1. Smith, S. G.; Goodman, J. M., Assigning Stereochemistry to Single Diastereoisomers by GIAO NMR Calculation: The DP4 Probability. *Journal Of The American Chemical Society* **2010,** *132* (37), 12946-12959.

2. Jin, P.; Yuan, X.; Ma, X.; Zheng, G.; Wang, R.; Sun, N.; Yao, G., Epoxymicranthols A-N, 5, 9-Epoxygrayanane Diterpenoids as Potent Analgesics from Rhododendron micranthum. *Chinese Journal of Chemistry* **2021,** *39* (7), 1997-2008.

3. Lang, H.; Guijuan, Z.; Yuanyuan, F.; Pengfei, J.; Biao, G.; Hanqi, Z.; Xiaomin, M.; Junfei, Z.; Guangmin, Y., Highly Oxygenated Dimeric Grayanane Diterpenoids as Analgesics: TRPV1 and TRPA1 Dual Antagonists from Rhododendron molle. *Chinese Journal of Chemistry* **2022**.

4. Feng, Y.; Zha, S.; Gao, B.; Zhang, H.; Jin, P.; Zheng, G.; Ma, Y.; Yao, G.,

Discovery of Kalmane Diterpenoids as Potent Analgesics from the Flowers of Rhododendron dauricum. *Chinese Journal of Chemistry* **2022**.

5. Zheng, G.; Kadir, A.; Zheng, X.; Jin, P.; Liu, J.; Maiwulanjiang, M.; Yao, G.; Aisa, H. A., Spirodesertols A and B, two highly modified spirocyclic diterpenoids with an unprecedented 6-isopropyl-3H-spiro[benzofuran-2,1'-cyclohexane] motif from Salvia deserta. *Organic Chemistry Frontiers* **2020,** *7* (20), 3137-3145.

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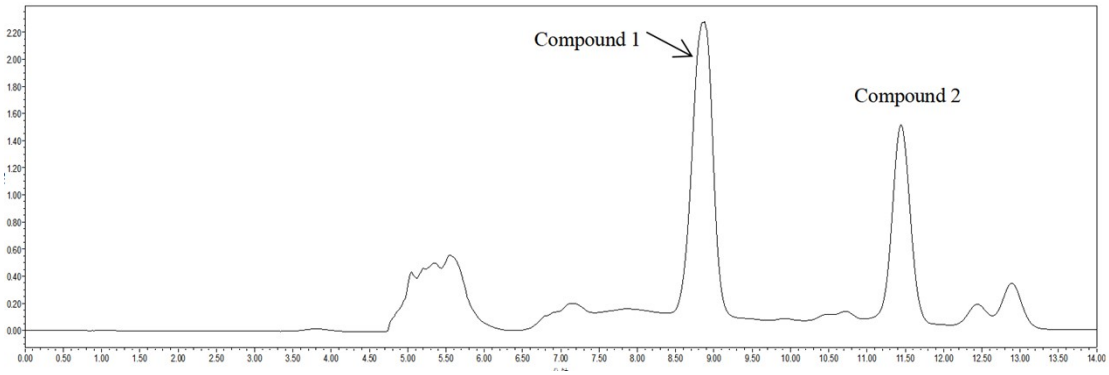
Table S11. Optimized coordinate of (Gal-4*R**)-**1** at B3LYP/6-31G (d) level in DMSO.

Table S12. DP4+ probability of ^{13}C NMR data of the isomers (**2**).

Table S13. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized (2*R*,3*R*,3‴*S*)-**2** at B3LYP/6-31G (d) level in DMSO

Table S14. Optimized coordinate of (2*R*,3*R*,3‴*S*)-**2** at B3LYP/6-31G (d) level in DMSO

Table S15. Optimized coordinate of (2*R*,3*R*,3‴*R*)-**2** at B3LYP/6-31G (d) level in DMSO



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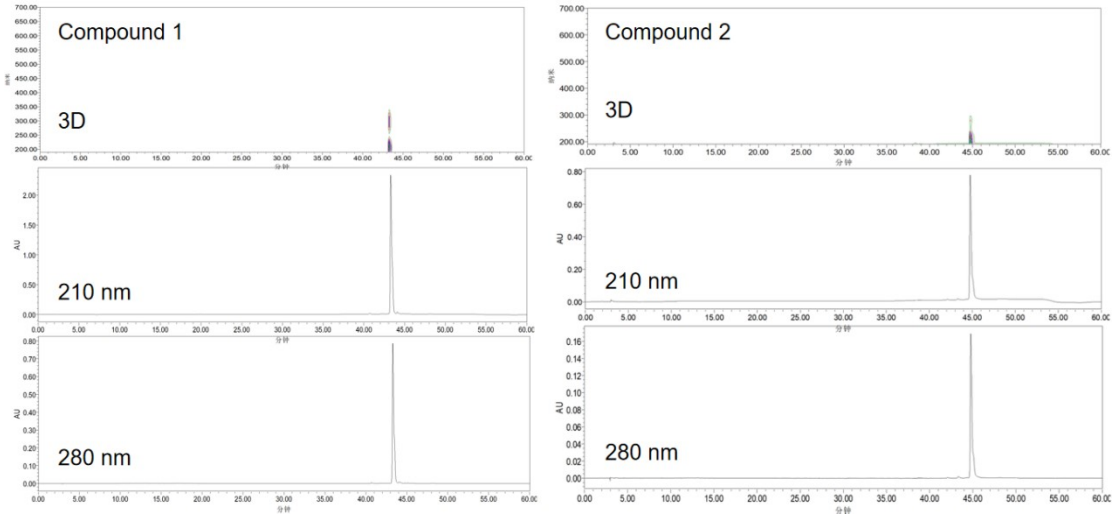


Fig. S2. Purity checks of **1** and **2** by HPLC (3D, 210, 280 nm).

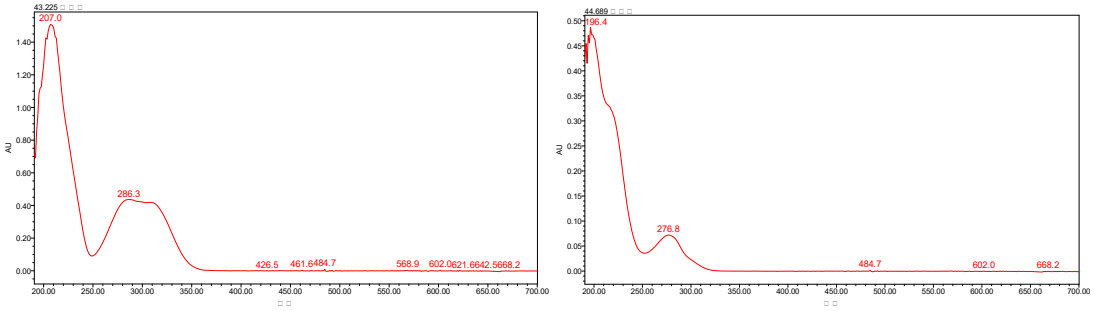
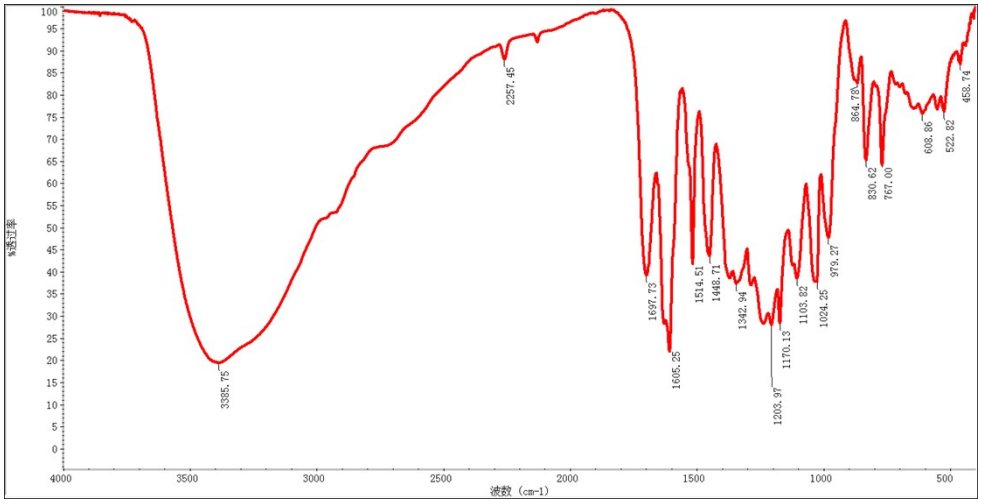


Fig. S3. UV of Compounds **1** and **2**.



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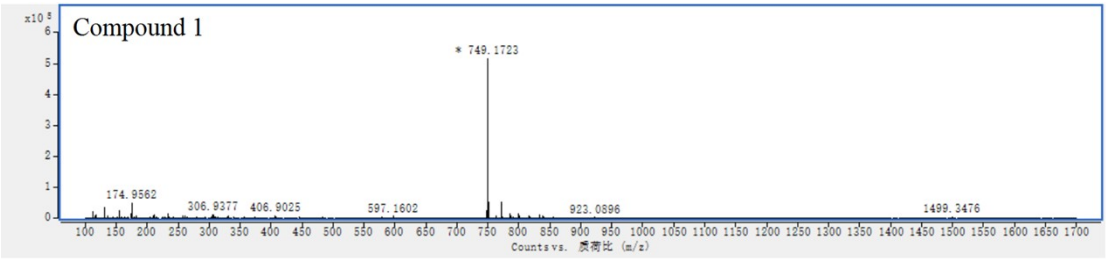


Fig. S5. ESI-HRMS^{-} of Compound **1**.

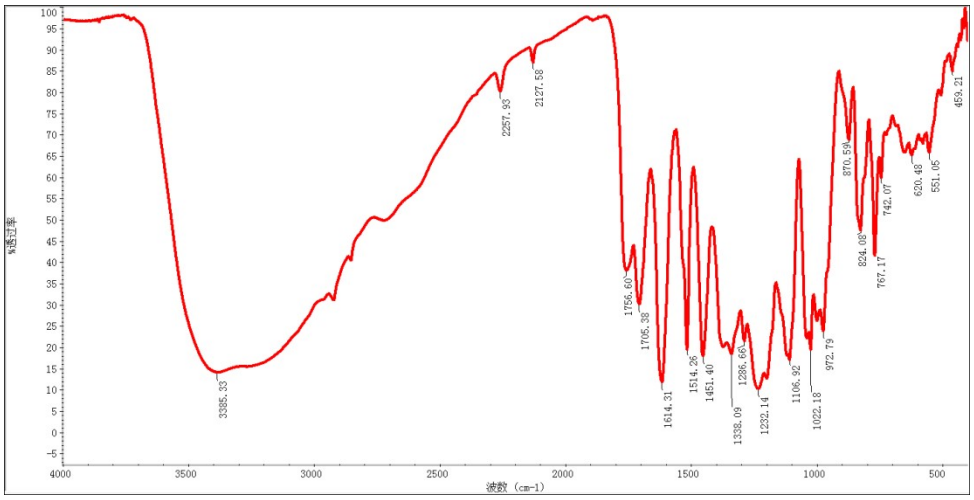


Fig. S6. IR of compound **2**.

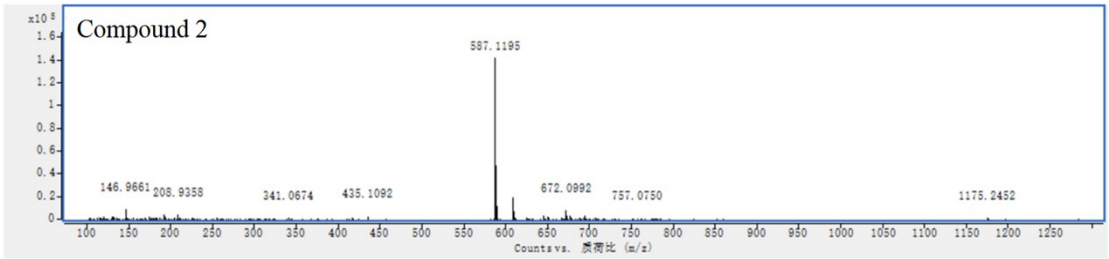


Fig. S7. ESI-HRMS$^-$ of Compound **2**.

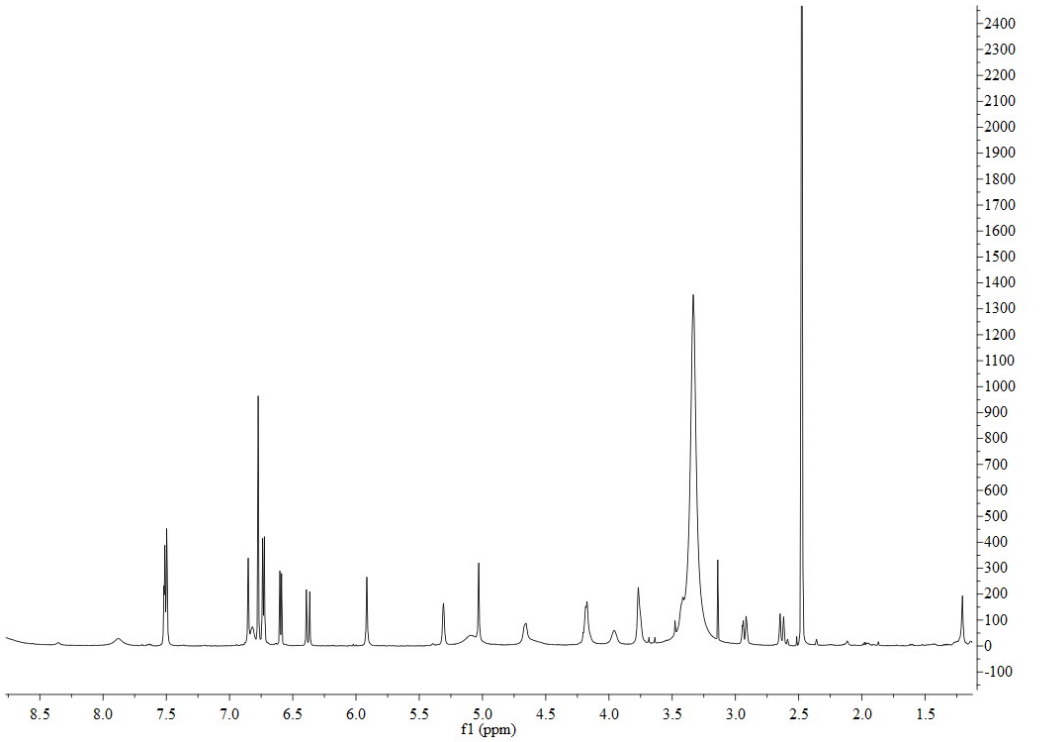


Fig. S8. ^{1}H NMR of compound **1** in DMSO-d_6.

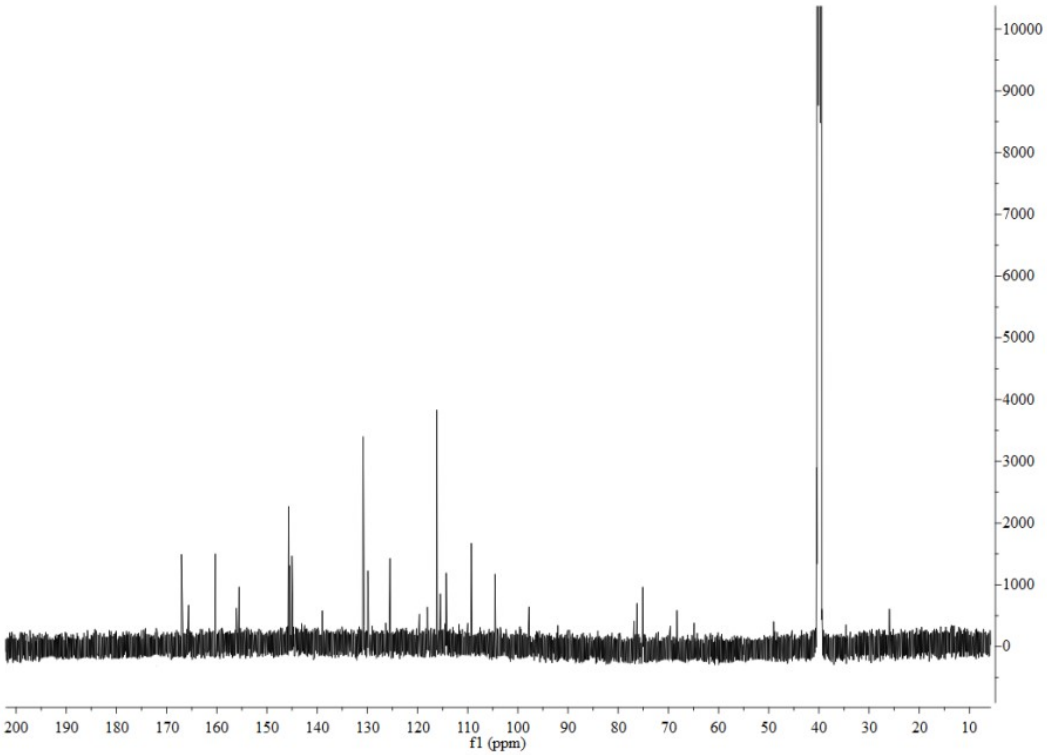


Fig. S9. ^{13}C NMR of compound **1** in DMSO-d_6.

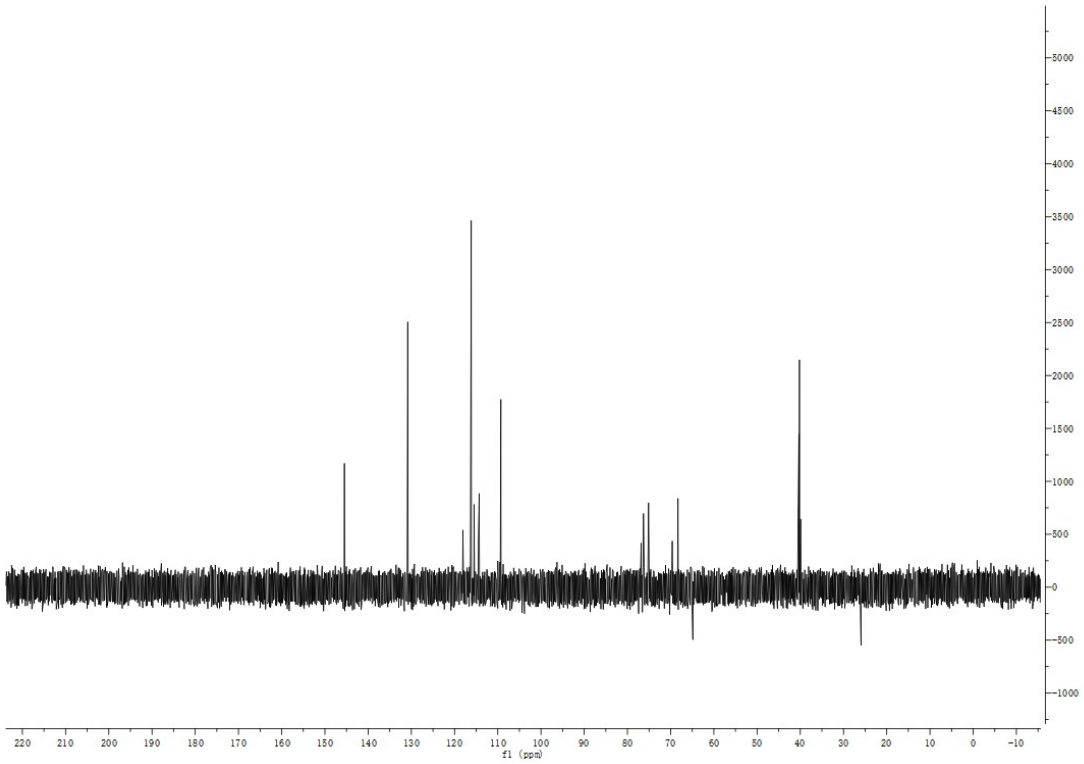


Fig. S10. DEPT-135 of compound **1** in DMSO-d_6.

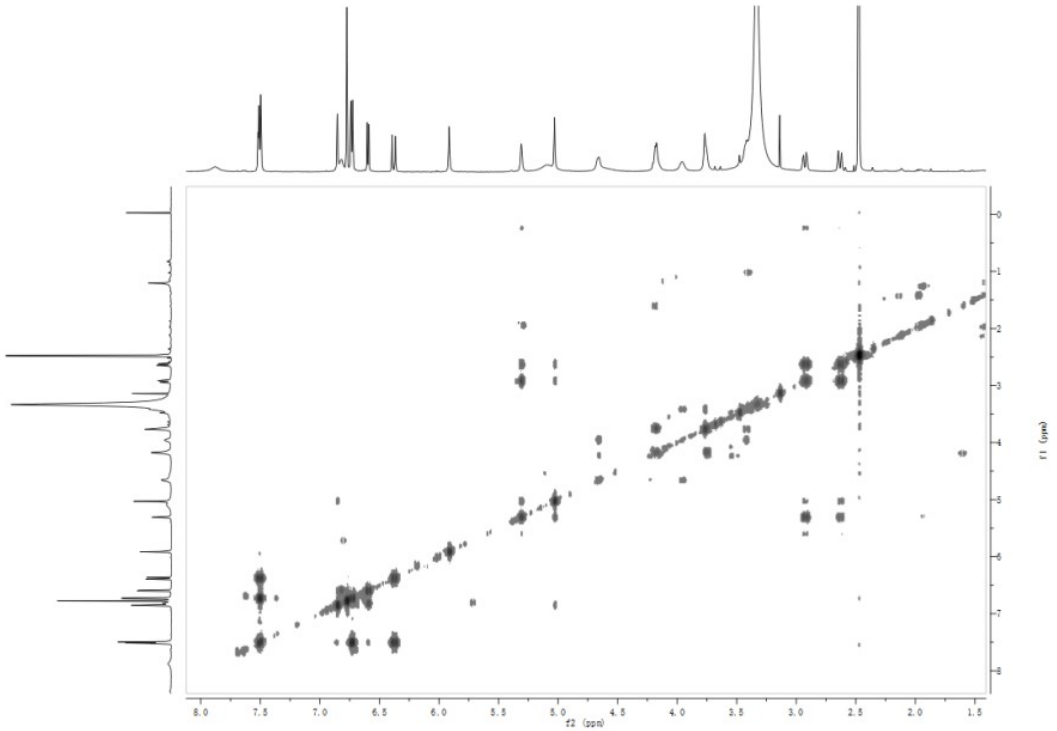


Fig. S11. ^{1}H-^{1}H COSY of compound **1** in DMSO-d_6.

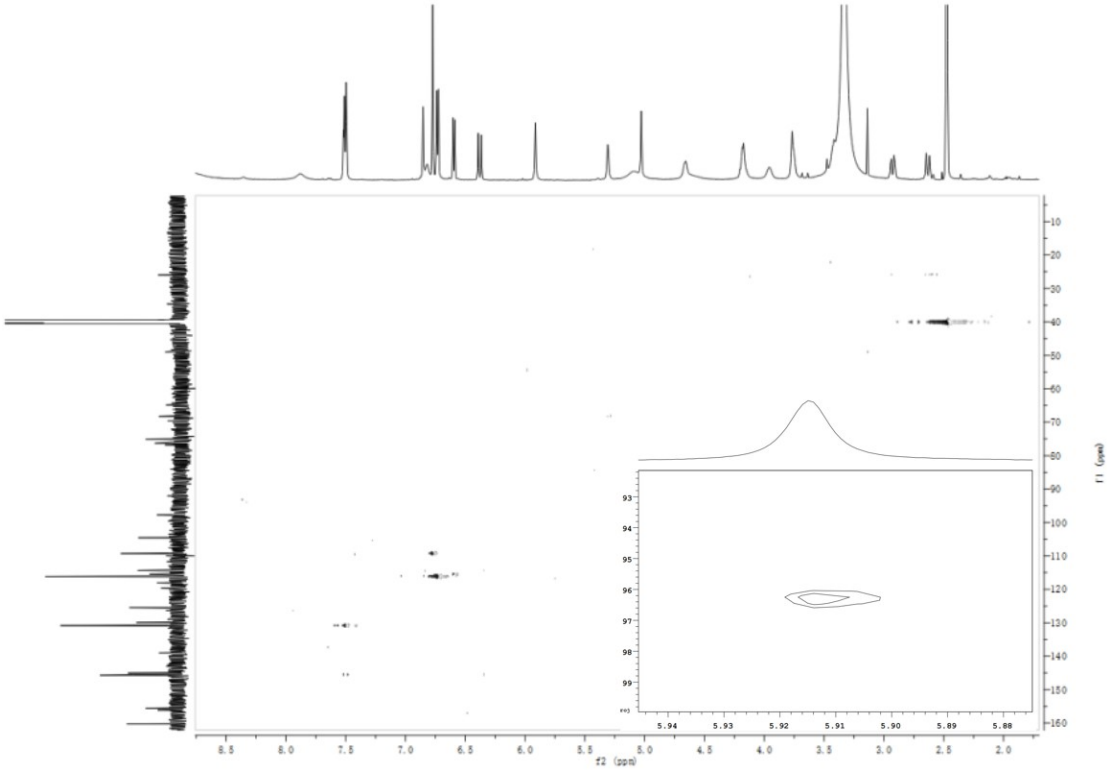


Fig. S12. HSQC of compound **1** in DMSO-d_6.

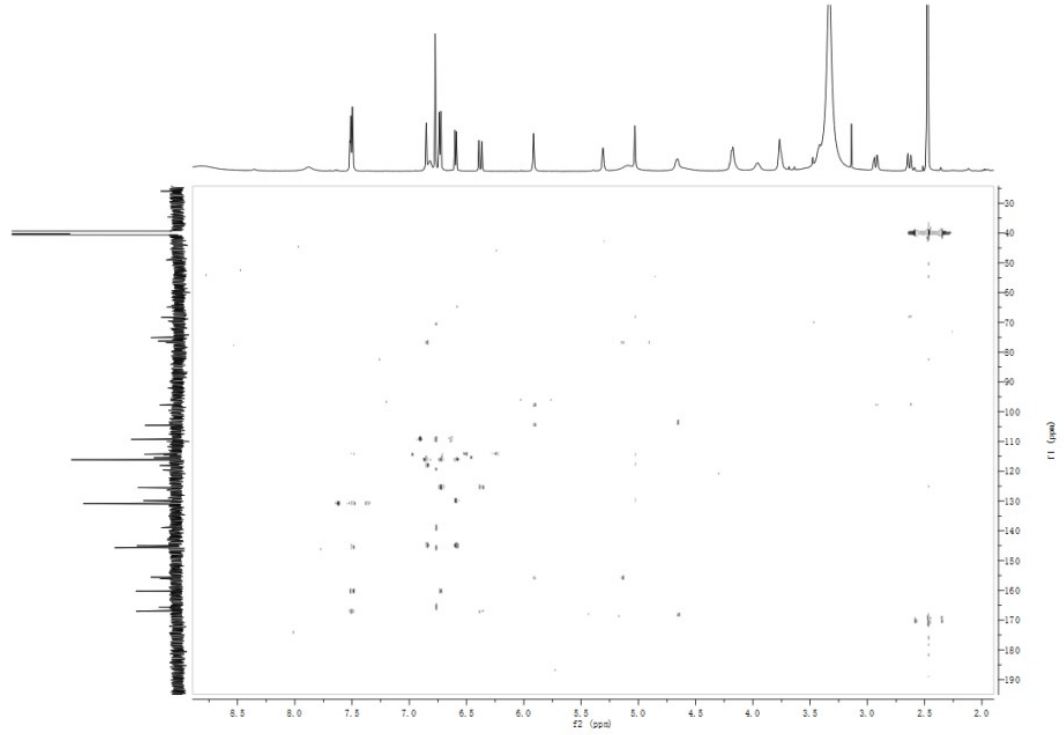


Fig. S13. HMBC of compound **1** in DMSO-d_6.

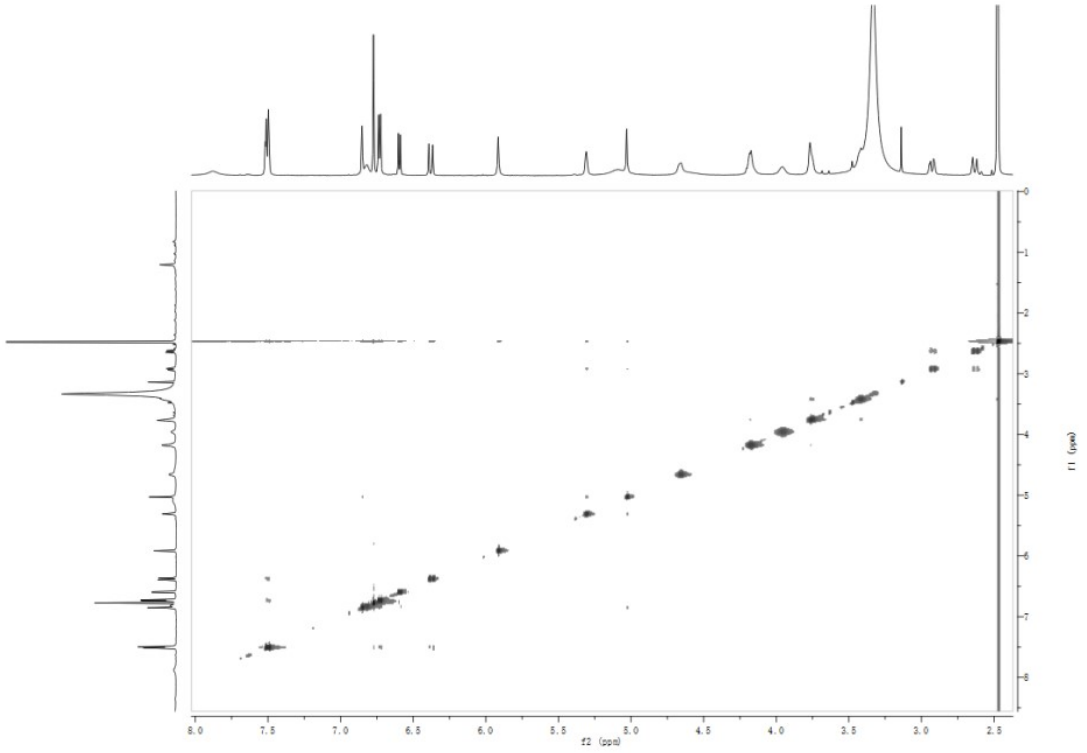


Fig. S14. ROESY of compound **1** in DMSO-d_6.

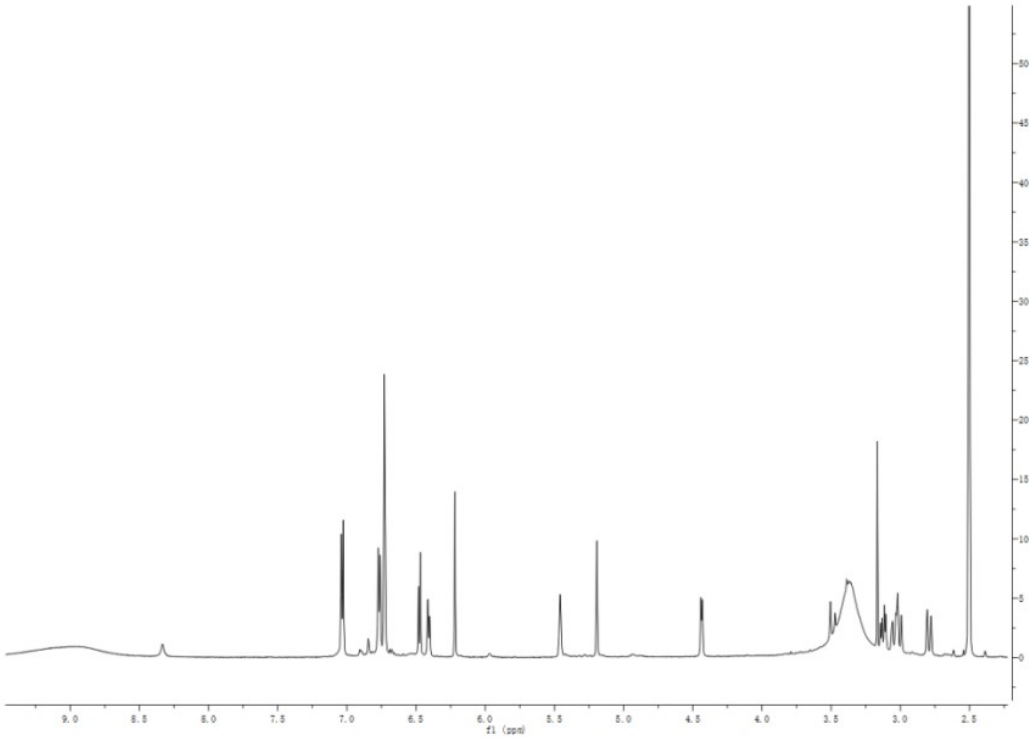


Fig. S15. ^{1}H NMR of compound **2** in DMSO-d_6.

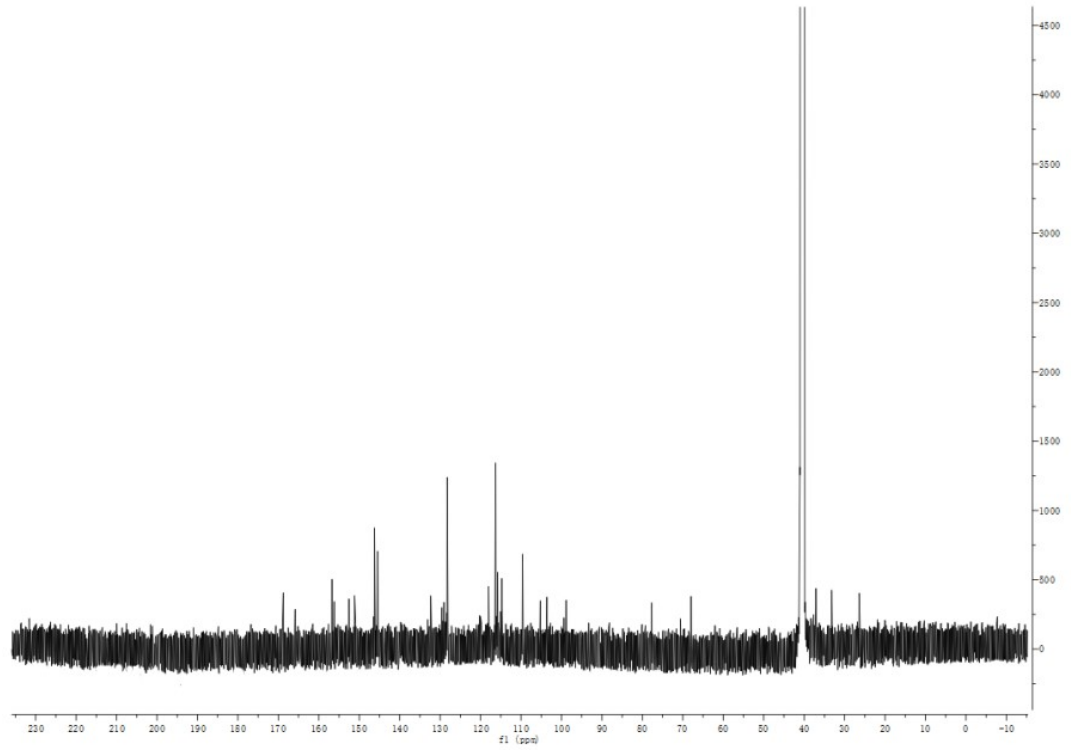


Fig. S16. ^{13}C NMR of compound **2** in DMSO-d_6.

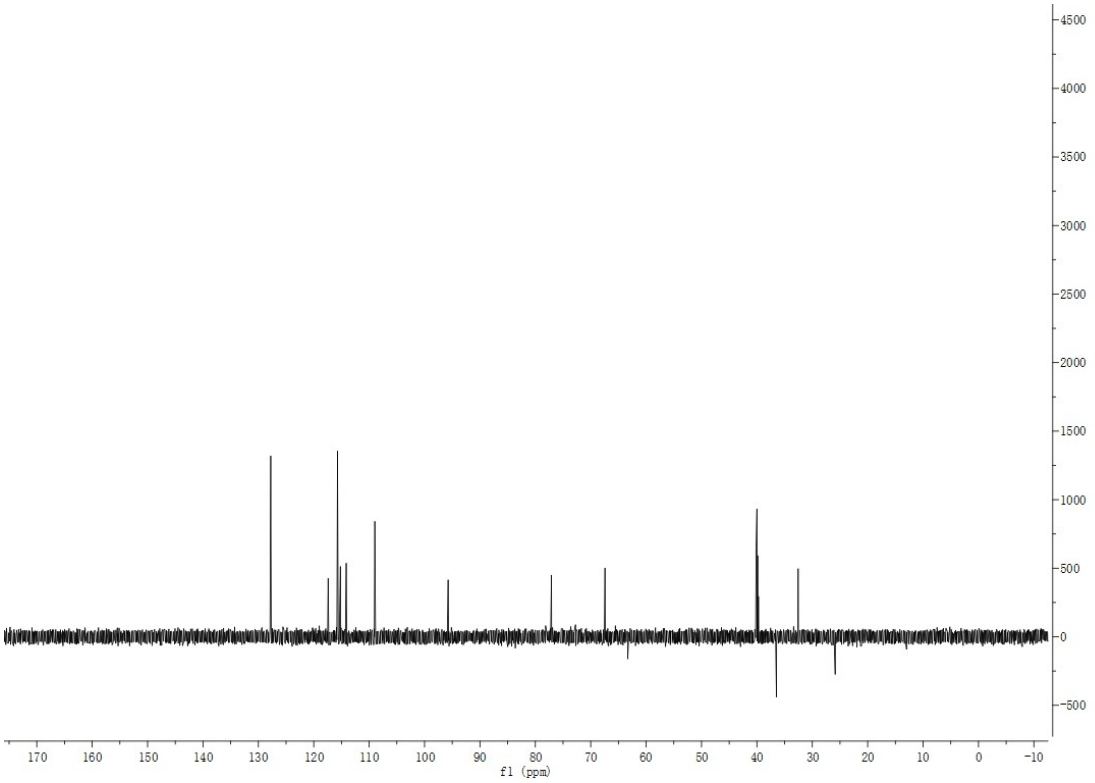


Fig. S17. DEPT-135 of compound **2** in DMSO-d_6.

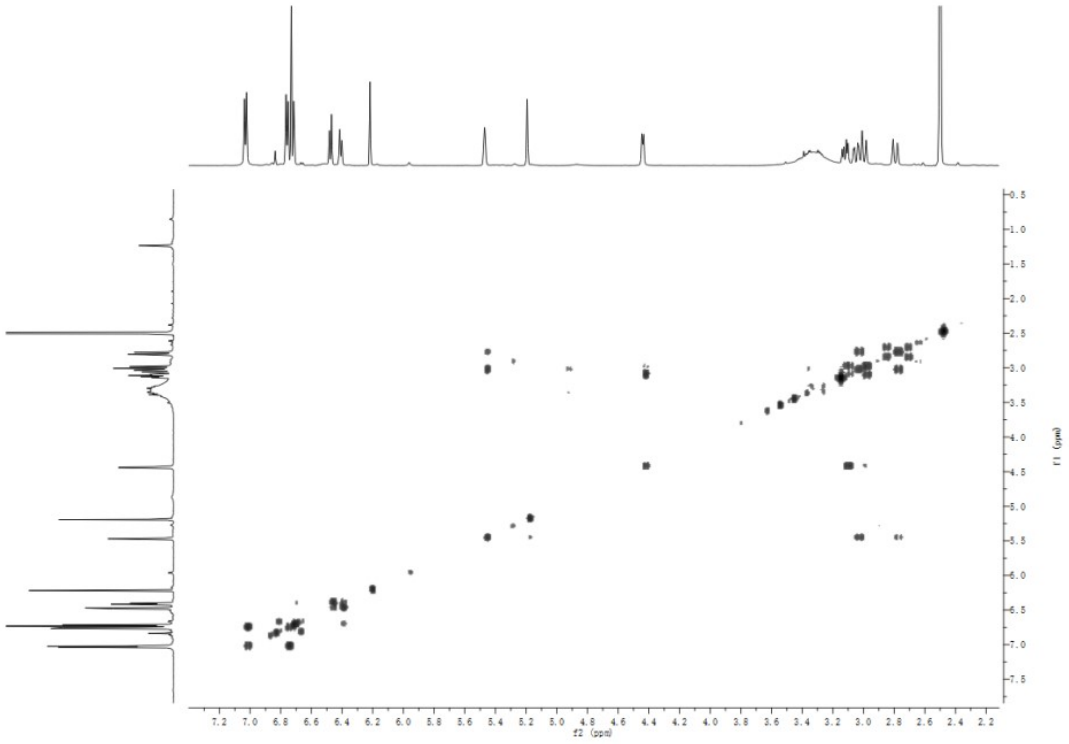


Fig. S18. ^{1}H-^{1}H COSY of compound **2** in DMSO-d_6.

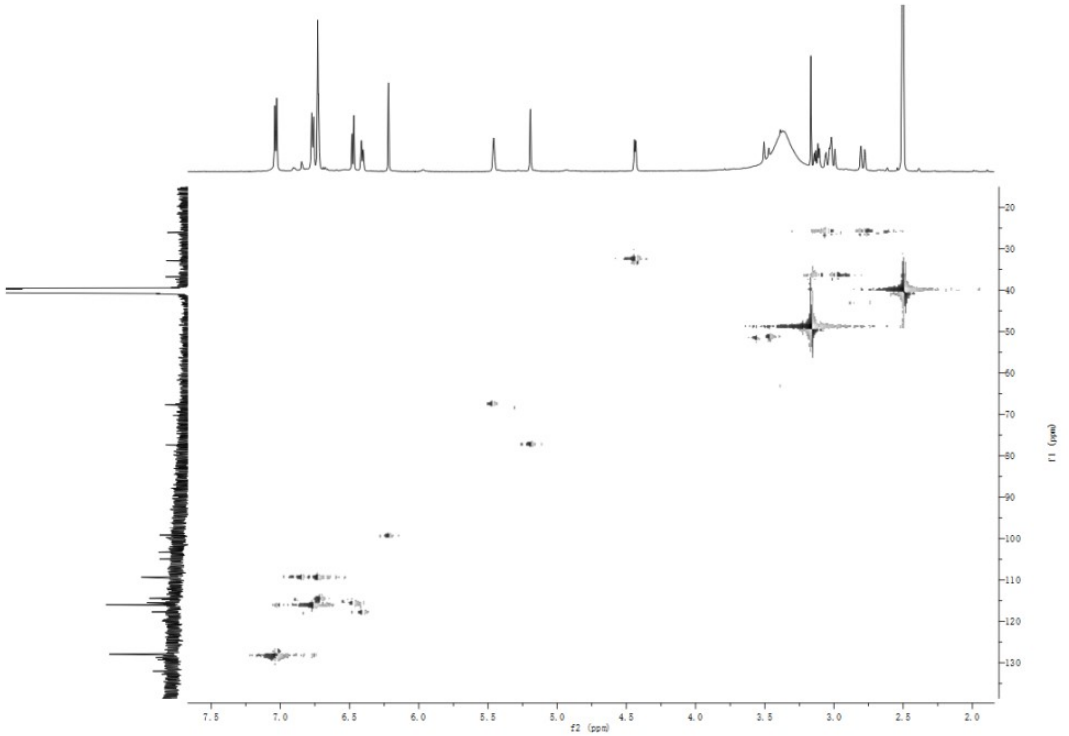


Fig. S19. HSQC of compound **2** in DMSO-d_6.

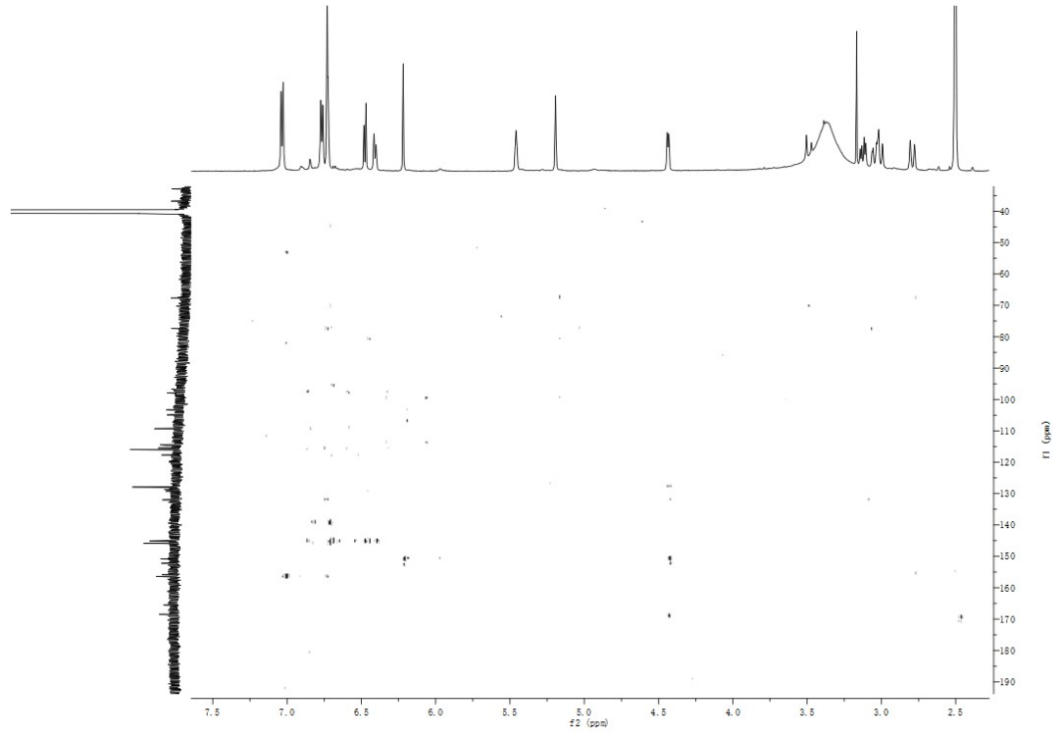


Fig. S20. HMBC of compound **2** in DMSO-d_6.

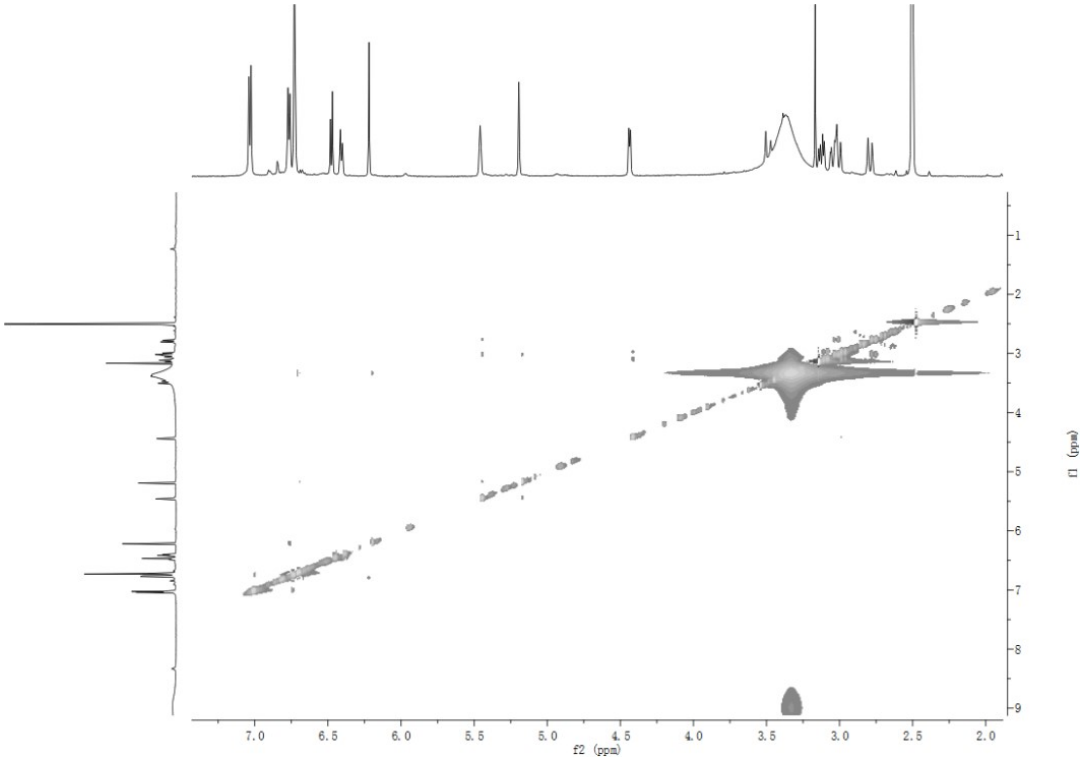


Fig. S21. ROESY of compound **2** in DMSO-d_6.

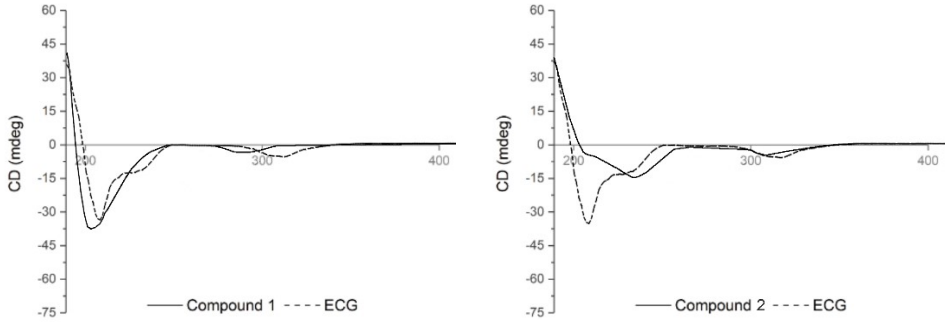
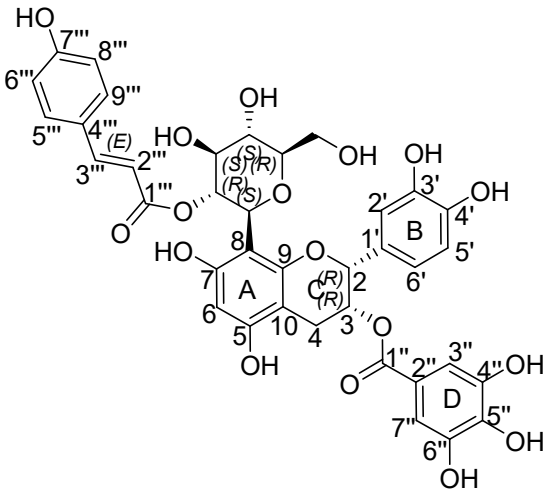


Fig. S22. CD of compounds **1**, **2**, and **ECG**.



Compound 1

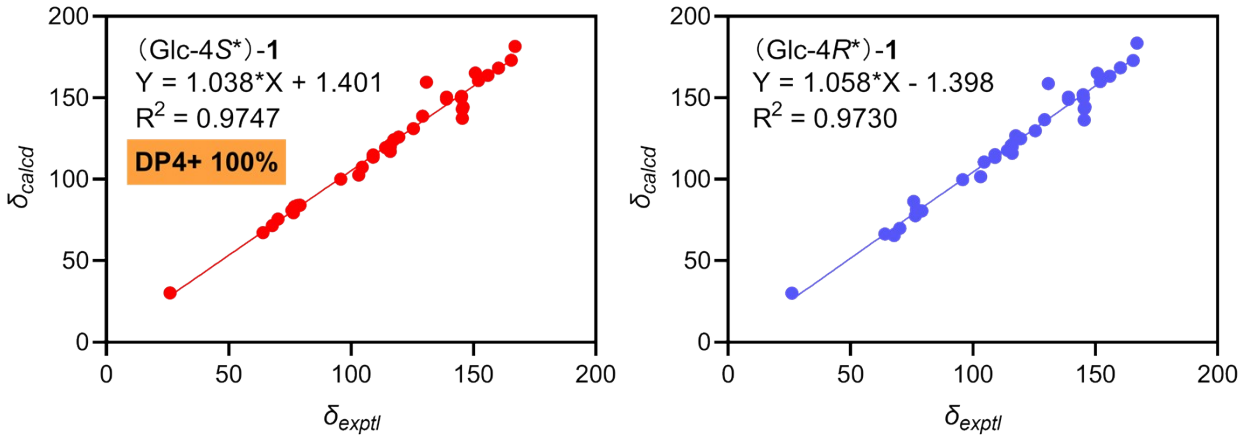


Fig. S23. Linear correlation plots between the experimental and calculated ^{13}C NMR data for (Glc-4*S**)-**1** and (Gal-4*R**)-**1**.

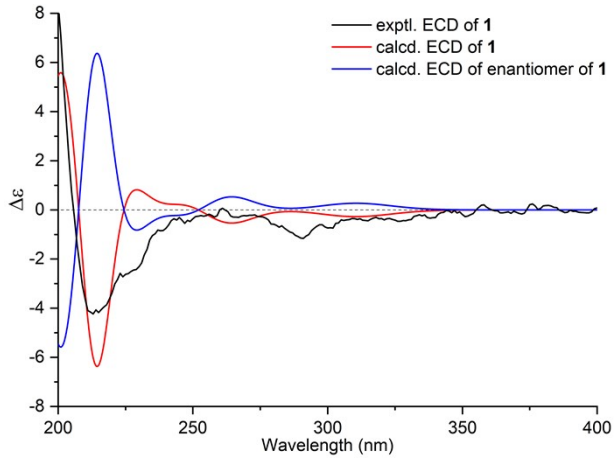


Fig. S24. The experimental and calculated ECD spectra of (Glc-4*S**)-**1** and its enantiomer (Gal-4*R**)-**1**.

Compound 2

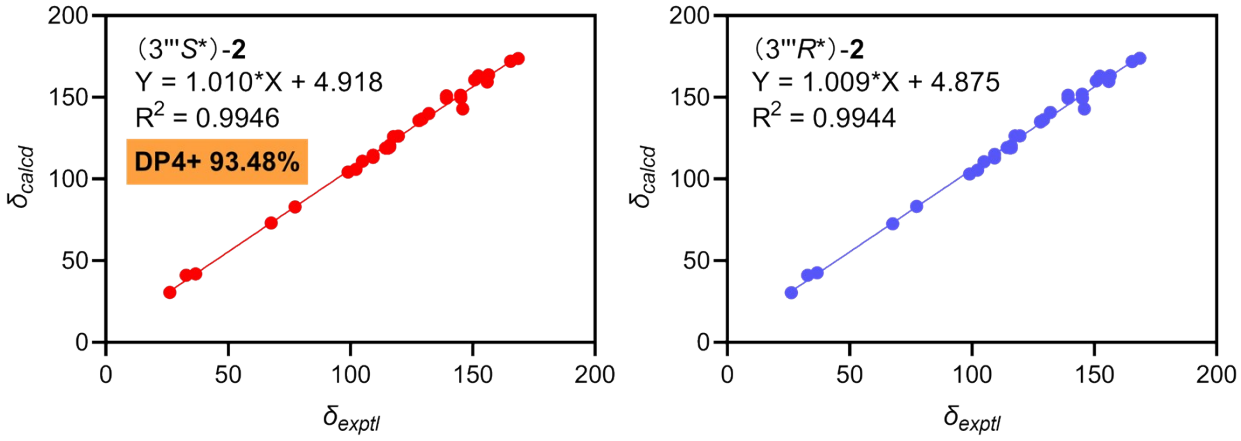


Fig. S25. Linear correlation plots between the experimental and calculated ^{13}C NMR data for (3‴*S**)-**2** and (3‴*R**)-**2**.

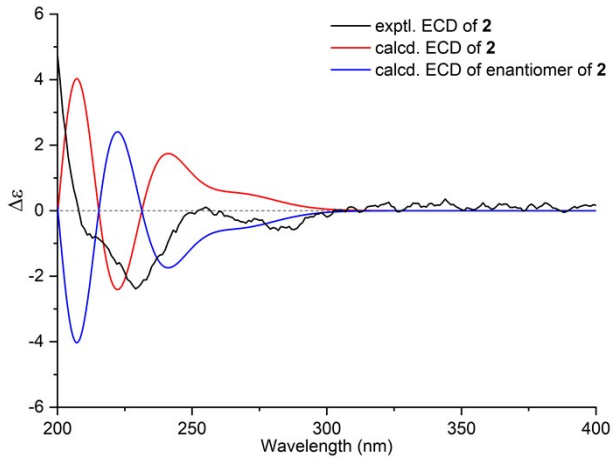


Fig. S26. The experimental and calculated ECD spectra of (3‴*S**)-**2** and its enantiomer (3‴*R**)-**2**.

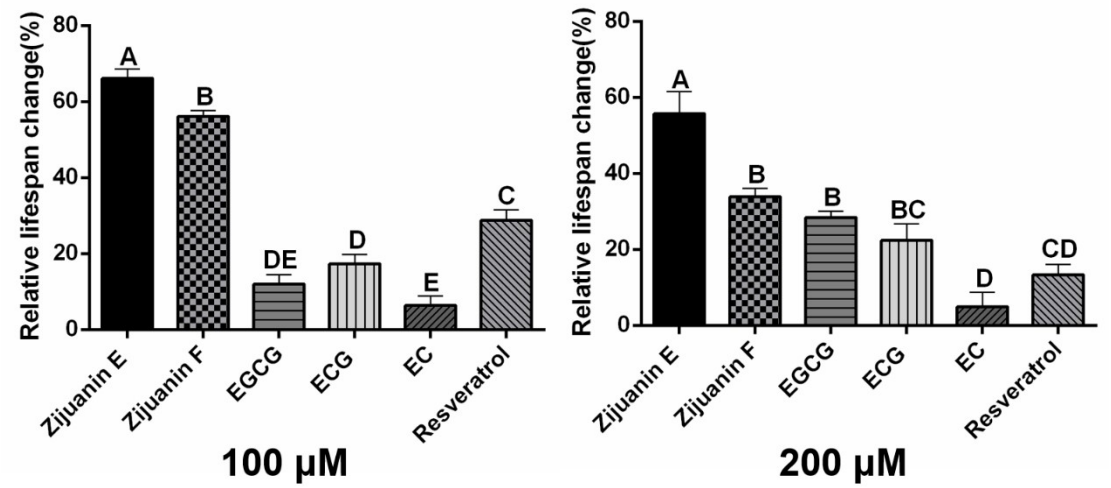


Fig. S27. Effect of zijuanins E, F, EGCG, ECG, EC, and resveratrol on the lifespan of *C. elegans*. Comparing the mean of each column with the mean of every other column by Tukey multiple comparisons. Means with different letters are significantly different at $p < 0.01$.

Table S1. ^{1}H and ^{13}C NMR Data of Compounds 1, 2, and ECG[a].

No.	1		2		ECG	
	δ_C	δ_H (J, Hz)	δ_C	δ_H (J, Hz)	δ_C	δ_H (J, Hz)
2	76.9	5.06, s	77.4	5.19, s	76.5	5.02 br s
3	67.8	5.34, br s	67.6	5.46, br s	69.1	5.34 br s
4	26.1	2.66, d (16.2)	26.2	2.79, d (16.8)	25.7	2.67 d (14.4)
		2.95, dd (16.2, 4.2)		3.04，dd (16.8, 4.2)		2.93 dd (14.4,3.6)
5	155.9		155.9		156.5	
6	95.8	5.94 s	104.9		95.6	5.93 s
7	150.8		150.8		156.6	
8	104.6		99.1	6.22 s	94.4	5.82 s
9	152.1		152.3		155.7	
10	103.2		102.3		97.3	
1′	129.3		129.3		129.4	
2′	114.2	6.88 d (1.8)	114.4	6.73 d (1.8)	114.3	6.85 d (1.2)
3′	145.2		145.2		144.7	
4′	145.1		145.1		144.7	
5′	115.6	6.62 d (7.8)	115.5	6.47 d (7.8)	115.1	6.64 d (8.4)
6′	117.5	6.82 dd (3.6, 7.8)	117.6	6.41 d (8.4)	117.6	6.73 d (8.4)
1″	165.5		165.5		165.2	
2″	119.5		119.6		119.2	
3″	109.1	6.80 s	109.3	6.73 s	108.6	6.82 s
4″	139.0		139.3		138.6	
5″	145.8		145.9		145.5	
6″	139.0		139.3		138.6	
7″	109.1	6.80 s	109.3	6.73 s	108.6	6.82 s
1‴	167.1		168.6			
2‴	116.0	6.38 d (15.6)	36.7	3.00, d (15.6) 3.12 dd (15.6, 6.6)		
3‴	130.8	7.51 d (15.6)	32.8	4.44 d (6.6)		
4‴	125.5		132.0			

5‴	145.5	7.50 d (8.4)	128.0	7.03, d (8.4)
6‴	116.1	6.73, d (8.4)	116.0	6.76, d (8.4)
7‴	160.3		156.5	
8‴	116.1	6.73 d (8.4)	116.0	6.76 d (8.4)
9‴	145.5	7.50 d (8.4)	128.0	7.03 d (8.4)
Glc 1	76.5	5.09 s		
2	75.8	4.67 br s		
3	78.1	4.18 s		
4	70.2	3.96 s		
5	79.2	3.96 s		
6	64.1	3.76 s		

[a]^{1}H at 600 MHz and ^{13}C NMR at 150 MHz in DMSO-d_6. s, single peak; d, double peaks; m, multipeaks. ECG, (−) epicatechin-3-*O*-gallate.

Table S2. List of primers used in *C. elegans*.

Gene	Forward primer	Reverse primer
act-1	CCAGAAGAGCACCCAGTC	TGATGTCACGGACGATTT
daf-2	GCCCGAATGTTGTGAAAACT	CCAGTGCTTCTGAATCGTCA
daf-16	ATCGTGTGCTCAGAATCC	ATGAATATGCTGCCCTCC
sod-3	AGAACCTTCAAAGGAGCTGATG	CCGCAATAGTGATGTCAGAAAG
sir-2.1	TGGCTGACGATTCGATGGAT	ATGAGCAGAAATCGCGACAC
skn-1	CACGCCGTCAGCGAAGTA	ATGCTCGGTGAGTATTGG

Table S3. Effect of zijuanins E, F, EGCG, ECG, EC, and resveratrol on the lifespan of *C. elegans*.

	Concentrations	Mean lifespan(d) ±SEM	Max lifespan(d) ±SEM	N (trials/n)	Change %
Control	0	18.3 ± 0.9		113	
Zijuanin E	50	26.9 ± 1.1	32.3 ± 0.9	126	47.1
	100	30.6 ± 0.3	35.0 ± 0.8	110	67.4
	200	28.5 ± 1.1	35.3 ± 2.0	103	56.3
	400	25.5 ± 1.8	34.0 ± 3.7	106	39.8
	1000	17.0 ± 0.3	22.7 ± 0.5	127	-6.9
Zijuanin F	50	21.9 ± 0.5	27.3 ± 0.5	114	19.8
	100	28.5 ± 0.4	33.3 ± 0.5	105	55.8
	200	24.5 ± 0.4	29.7 ± 1.2	109	33.9
	400	22.1 ± 0.6	29.3 ± 1.9	128	21.0
	1000	14.1 ± 0.3	19.3 ± 0.5	101	-22.9
EGCG	50	19.9 ± 1.3	24.3±1.3	119	2.8
	100	20.7 ± 0.3	24.3±1.3	110	7.4
	200	23.5 ±0.3	26.7±0.5	125	21.5
	400	20.4 ±1.1	25.0±1.6	106	5.9
	1000	16.0 ± 0.9	19.7 ± 0.5	102	-17.0
ECG	50	21.2 ± 0.4	25.3 ± 0.5	113	9.7
	100	21.6 ± 0.4	25.3 ± 0.5	127	12.0
	200	22.4 ± 0.8	25.3 ± 0.5	124	15.9
	400	19.8 ± 0.3	27.7 ± 0.5	110	2.6
	1000	15.2 ± 0.1	19.7 ± 0.5	105	-21.3
EC	50	19.1 ± 0.5	24.6 ± 0.9	114	4.3
	100	19.6 ± 0.4	25.7 ± 1.2	118	7.1
	200	19.2 ± 0.7	23.7 ± 0.9	106	4.9
Resveratrol	50	20.1 ± 0.4	23.0 ± 0.8	116	9.8
	100	23.4 ± 0.4	25.3 ± 0.5	105	27.9
	200	20.8 ± 0.4	24.3 ± 0.5	127	13.8

Table S4. Antioxidant effects of zijuanins E and F *in vitro*.

	DPPH IC_{50} (μM)	ABTS IC_{50} (μM)
Zijuanin E	1.89 ± 0.003[a]	5.77 ± 0.11 [a]
Zijuanin F	9.31 ± 0.017[a]	19.13 ± 0.19 [a]
Ascorbic acid	55.81 ± 0.506[b]	101.83 ± 1.99 [b]

Table S5. Effect of zijuanins E and F (100 μM) on the resistance to heat shock, UV and PQ damage in *C. elegans*.

	Compound (100 μM)	Mean lifespan(h) ±SEM	N (trials/n)	Change %
Heat	Control	7.4 ± 0.3	138	
	Zijuanin E	10.9 ± 0.5	136	47.2
	Zijuanin F	9.9 ± 0.2	126	33.0
	Compound (100 μM)	Mean lifespan(d) ±SEM	N (trials/n)	Change %
UV	Control	5.1 ± 0.5	106	
	Zijuanin E	8.9 ± 0.5	111	75.0
	Zijuanin F	6.8 ± 0.2	104	33.6
	Compound (100 μM)	Mean lifespan(d) ±SEM	N (trials/n)	Change %
PQ	Control	5.1 ± 0.4	128	
	Zijuanin E	8.8 ± 0.2	102	74.9
	Zijuanin F	7.1 ± 0.2	115	40.3

Table S6. Effects of zijuanins E and F (100 μM) on the lifespan of *daf-2* (e1370), *daf-16* (mu86), *sir-2.1* (ok434), and *skn-1* (zu135) mutants.

	Compound (100 μM)	Mean lifespan(d) ±SEM	N (trials/n)	Change%
daf-2 (e1370)	Control	36.3 ± 0.3	138	
	Zijuanin E	34.1 ± 1.1	136	-6.2
	Zijuanin F	32.9 ± 0.4	126	-9.5
daf-16 (mu86)	Control	18.4 ± 0.3	106	
	Zijuanin E	17.9 ± 0.3	111	-2.6
	Zijuanin F	17.9 ± 0.3	104	-2.9
sir-2.1 (ok434)	Control	18.7 ± 0.6	107	
	Zijuanin E	17.7 ± 0.3	112	-5.2
	Zijuanin F	18.8 ± 0.1	110	0.5
skn-1 (zu135)	Control	15.3 ± 0.4	128	
	Zijuanin E	15.2 ± 0.2	102	-0.7
	Zijuanin F	15.3 ± 0.2	115	-0.1

Table S7. Affinity parameters of interactions between zijuanins E and F and HSA based on the steady-state analysis.

Compound	K_D (μM)	Rmax (RU)	Offset (RU)	Chi2 (RU2)
1	2.32	136.6	-27.27	0.24
2	25.08	38.70	26.33	0.13

Table S8. DP4+ probability of ^{13}C NMR data of the isomers (**1**).

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311G(d,p)	Shielding Tensors

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	–	–	–	–	–	–
sDP4+ (C data)	99.99%	0.01%	–	–	–	–
sDP4+ (all data)	99.99%	0.01%	–	–	–	–
uDP4+ (H data)	–	–	–	–	–	–
uDP4+ (C data)	100.00%	0.00%	–	–	–	–
uDP4+ (all data)	100.00%	0.00%	–	–	–	–
DP4+ (H data)	–	–	–	–	–	–
DP4+ (C data)	100.00%	0.00%	–	–	–	–
DP4+ (all data)	100.00%	0.00%	–	–	–	–

Table S9. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized (Glc-4*S**)-**1** at B3LYP/6-31G (d) level in DMSO.

Conformation	Gibbs free energies (Hartree)	Boltzmann distribution
1	-2708.576146	46.35%
2	-2708.576013	40.25%
3	-2708.574307	6.60%
4	-2708.563775	0.00%
5	-2708.573874	4.17%
6	-2708.573439	2.63%

Table S10. Optimized coordinate of (Glc-4*S**)-**1** at B3LYP/6-31G (d) level in DMSO.

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	3.728712	-1.81948	1.131676	O	-5.39928	-3.68111	1.683739
C	3.535469	-3.20052	1.091472	O	4.778158	0.748304	0.535317
C	2.783244	-3.75365	0.059016	C	5.185539	2.121007	0.6845
C	2.221384	-2.96057	-0.95164	C	4.462261	2.699094	1.898055
C	2.437606	-1.5783	-0.88808	C	2.958091	2.628617	1.633567
C	3.183075	-0.97464	0.144738	C	2.493342	1.209938	1.289352
C	1.328595	-3.558	-2.01305	C	6.704685	2.100167	0.795777
C	0.364786	-2.48691	-2.52022	O	4.865858	4.039461	2.098447
C	1.167975	-1.24527	-2.92649	O	2.221288	3.198789	2.714349
O	1.904168	-0.71818	-1.81102	O	7.299794	1.546949	-0.36251
C	3.38019	0.523672	0.213104	H	3.992044	-3.81622	1.86105
O	4.465081	-1.32855	2.170471	H	1.906879	-3.95453	-2.85992
C	0.338917	-0.12546	-3.51765	H	0.763355	-4.40232	-1.60837
O	-0.52142	-2.11452	-1.44841	H	-0.22425	-2.84496	-3.36704
O	2.556269	-5.09921	-0.02825	H	1.890262	-1.58612	-3.68352

C	-0.00321	-0.16559	-4.87196	H	3.162037	0.979677	-0.75829
C	-0.79945	0.836785	-5.43175	H	4.829544	-0.46974	1.872871
C	-1.24441	1.887781	-4.63767	H	2.931871	-5.53121	0.754524
C	-0.89203	1.939593	-3.27992	H	0.350903	-0.97688	-5.50288
C	-0.1109	0.93446	-2.72373	H	-1.06483	0.803741	-6.48658
O	-1.31839	2.984392	-2.50111	H	0.166296	0.989115	-1.67879
O	-2.02109	2.936924	-5.07911	H	-1.81138	3.593889	-3.07763
C	-1.64594	-2.8754	-1.29612	H	-2.21149	2.82918	-6.02291
O	-2.04581	-3.63751	-2.15511	H	-0.64134	-1.5802	0.906327
C	-2.28653	-2.67634	0.027009	H	-4.03679	-3.79233	-0.57257
C	-1.6299	-1.9919	1.063764	H	-3.55449	-1.86297	4.30343
C	-2.25483	-1.87711	2.302207	H	-0.9789	-0.66749	3.163312
C	-3.51923	-2.4448	2.501759	H	-2.27129	1.168829	2.665557
C	-4.16702	-3.13397	1.470352	H	-1.03214	2.167429	0.033367
C	-3.54859	-3.25167	0.229548	H	-3.0159	2.804801	-0.7204
O	-4.15928	-2.34225	3.708734	H	-5.27087	3.628048	-1.32224
O	-1.74182	-1.24358	3.403539	H	-6.76232	2.409299	2.520406
C	-3.58606	2.14534	1.266354	H	-4.51514	1.587141	3.132104
C	-2.28824	1.644441	1.686884	H	-8.01015	3.403174	0.860773
C	-1.12062	1.695705	1.00532	H	-5.63733	-3.50839	2.610628
C	0.105003	1.149973	1.581764	H	4.901951	2.678612	-0.22013
O	0.219982	0.57936	2.667853	H	4.710036	2.079492	2.780037
O	1.162215	1.342642	0.753536	H	2.744335	3.279804	0.777753
C	-3.82387	2.726581	0.000668	H	2.460189	0.584497	2.18629
C	-5.08219	3.18662	-0.34883	H	7.069975	3.125092	0.894943
C	-6.14732	3.078533	0.559046	H	6.992291	1.547269	1.706567
C	-5.93748	2.500945	1.816465	H	4.186288	4.436661	2.671301
C	-4.67092	2.041194	2.156811	H	2.136681	2.53086	3.415868
O	-7.35903	3.549831	0.156418	H	6.869203	0.687475	-0.50338
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-3.73395	1.736894	1.254561	O	5.386703	3.628374	1.799893
C	-3.55506	3.120292	1.281956	O	-4.75914	-0.81294	0.543021
C	-2.81867	3.732611	0.271749	C	-5.14752	-2.1972	0.616447
C	-2.25918	2.997605	-0.78327	C	-4.39986	-2.83696	1.783445
C	-2.46234	1.611902	-0.78793	C	-2.90037	-2.72735	1.505661
C	-3.19058	0.949037	0.220519	C	-2.46105	-1.28366	1.241482
C	-1.37994	3.657076	-1.81944	C	-6.66503	-2.20337	0.749429
C	-0.41712	2.620371	-2.39459	O	-4.78101	-4.19341	1.904902
C	-1.21987	1.398253	-2.85729	O	-2.14143	-3.35023	2.540973
O	-1.93164	0.804587	-1.75925	O	-7.28394	-1.59133	-0.36606
C	-3.36898	-0.55306	0.213797	H	-4.00943	3.691535	2.086332
O	-4.45413	1.186905	2.27483	H	-1.96863	4.097863	-2.63671
C	-0.39595	0.318407	-3.52358	H	-0.8138	4.47999	-1.37387
O	0.48243	2.195091	-1.35428	H	0.160506	3.026443	-3.22746
O	-2.60528	5.082987	0.250689	H	-1.95746	1.775759	-3.58134
C	-0.12841	0.40075	-4.89254	H	-3.15893	-0.95509	-0.78297
C	0.66337	-0.56524	-5.51914	H	-4.81063	0.338362	1.940585

C	1.178135	-1.62186	-4.77668	H	-2.97677	5.471221	1.057993
C	0.901316	-1.71592	-3.4037	H	-0.53805	1.216383	-5.48283
C	0.124629	-0.747	-2.78169	H	0.870755	-0.4994	-6.58539
O	1.397856	-2.76663	-2.67568	H	-0.09586	-0.83401	-1.72556
O	1.959215	-2.63733	-5.28566	H	1.861135	-3.35568	-3.29621
C	1.60669	2.951138	-1.17468	H	2.065757	-2.51935	-6.2414
O	1.994979	3.756648	-1.99875	H	0.633064	1.537586	0.970192
C	2.26173	2.687789	0.12957	H	3.998724	3.843405	-0.43218
C	1.621204	1.946769	1.13753	H	3.588497	1.66155	4.342677
C	2.260823	1.773939	2.361838	H	1.004593	0.511961	3.179338
C	3.52326	2.341171	2.576384	H	2.280739	-1.35281	2.637588
C	4.155784	3.084532	1.573373	H	1.074577	-2.12078	-0.08501
C	3.522619	3.260265	0.347082	H	3.09381	-2.61691	-0.88682
O	4.176685	2.185638	3.76954	H	5.338518	-3.38903	-1.52672
O	1.764892	1.083505	3.436387	H	6.76176	-2.68282	2.467425
C	3.614804	-2.2108	1.179504	H	4.496918	-1.89887	3.124579
C	2.312286	-1.74173	1.62166	H	7.482038	-3.75438	-0.80421
C	1.153894	-1.72855	0.922461	H	5.643114	3.400072	2.709768
C	-0.07494	-1.22755	1.531523	H	-4.86968	-2.69637	-0.32335
O	-0.19162	-0.73521	2.655279	H	-4.64568	-2.27738	2.705127
O	-1.13129	-1.36307	0.690844	H	-2.68885	-3.32213	0.609082
C	3.879912	-2.63704	-0.13803	H	-2.43178	-0.71029	2.172628
C	5.146253	-3.0702	-0.50366	H	-7.01576	-3.2372	0.793118
C	6.185801	-3.09002	0.438768	H	-6.94633	-1.70876	1.694993
C	5.946367	-2.66749	1.751782	H	-4.09133	-4.61338	2.448661
C	4.677977	-2.23274	2.106	H	-2.04416	-2.71952	3.274566
O	7.445231	-3.50558	0.132899	H	-6.86771	-0.71861	-0.46101
Conformation 3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.264149	1.978242	-0.13261	O	-5.19801	3.440962	-2.69451
C	4.119617	3.357131	0.033674	O	4.942873	-0.73595	0.254247
C	3.089818	3.844154	0.82886	C	5.281532	-2.08413	-0.09259
C	2.193062	2.984893	1.479208	C	4.867395	-2.2849	-1.5496
C	2.369763	1.60575	1.311845	C	3.35368	-2.17179	-1.66984
C	3.399983	1.067653	0.511135	C	2.808501	-0.88806	-1.0192
C	1.023823	3.53798	2.254495	C	6.784944	-2.26452	0.146791
C	-0.07971	2.492495	2.363664	O	5.303987	-3.56132	-2.00611
C	0.523968	1.163114	2.82064	O	3.050933	-2.25751	-3.05604
O	1.509157	0.696235	1.875892	O	7.167031	-3.62134	0.066614
C	3.532549	-0.42688	0.285695	H	4.82494	4.018215	-0.46161
O	5.272381	1.570657	-0.95104	H	1.318141	3.850233	3.266771
C	-0.46463	0.030881	3.049897	H	0.629767	4.432953	1.763398
O	-0.66533	2.291516	1.061519	H	-0.8522	2.829923	3.055365
O	2.891781	5.184607	1.018822	H	1.050708	1.373143	3.765624
C	-0.00611	-1.28735	3.158399	H	3.077766	-0.97502	1.117903
C	-0.88766	-2.33597	3.43543	H	5.470319	0.640933	-0.71194
C	-2.24437	-2.07885	3.614434	H	3.533269	5.673425	0.480271
C	-2.70951	-0.75989	3.505704	H	1.048602	-1.49924	3.022693

C	-1.83304	0.282984	3.232525	H	-0.53357	-3.35848	3.524461
O	-4.06507	-0.60589	3.687772	H	-2.24013	1.285264	3.13622
O	-3.12249	-3.09744	3.868034	H	-4.31324	0.319808	3.539175
C	-1.90634	2.794129	0.8237	H	-3.98525	-2.68541	4.049542
O	-2.58952	3.316018	1.68935	H	-0.54193	1.528818	-1.18138
C	-2.31895	2.605344	-0.5868	H	-4.1793	3.660546	-0.27378
C	-1.50592	1.906406	-1.49517	H	-2.99515	1.526441	-4.94207
C	-1.96065	1.697916	-2.79283	H	-0.57596	0.452801	-3.38843
C	-3.19755	2.221838	-3.19065	H	-1.87057	-1.48759	-2.64755
C	-3.99462	2.940869	-2.29154	H	-0.75787	-1.78289	0.209172
C	-3.56048	3.122139	-0.98173	H	-4.14997	-1.94439	-3.05143
O	-3.67088	2.037325	-4.46083	H	-6.36833	-2.81334	-2.34358
O	-1.30123	0.998309	-3.76831	H	-4.78376	-3.58784	1.585562
C	-3.20355	-2.26444	-1.13681	H	-2.60564	-2.73549	0.893418
C	-1.92391	-1.75175	-1.59241	H	-6.94718	-4.01653	0.909048
C	-0.80557	-1.56807	-0.85231	H	-5.30981	3.214588	-3.63371
C	0.435158	-1.11258	-1.46273	H	4.739865	-2.78478	0.560037
O	0.59346	-0.75556	-2.64024	H	5.333216	-1.48769	-2.15103
O	1.448835	-1.15569	-0.58318	H	2.92085	-3.02817	-1.12678
C	-4.2899	-2.30503	-2.0355	H	2.804199	-0.08232	-1.75731
C	-5.53281	-2.78619	-1.65193	H	7.343659	-1.63007	-0.56299
C	-5.71871	-3.25121	-0.34354	H	7.022854	-1.91812	1.157086
C	-4.65215	-3.22558	0.568395	H	4.915385	-3.6869	-2.88865
C	-3.41609	-2.73935	0.173046	H	2.180079	-1.84638	-3.21244
O	-6.95247	-3.71926	-0.01467	H	6.858382	-3.94596	-0.79813
Conformation 4							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-3.50419	-2.82275	-0.22815	O	2.75605	-2.83321	-3.05494
C	-2.99346	-4.06734	0.143389	O	-4.99402	-0.41346	-0.02817
C	-1.95991	-4.13067	1.073621	C	-5.74191	0.763937	-0.35541
C	-1.41353	-2.97391	1.647462	C	-5.52338	1.051483	-1.84196
C	-1.93176	-1.74071	1.237269	C	-4.04441	1.306772	-2.09868
C	-2.97419	-1.62642	0.292792	C	-3.19925	0.132347	-1.57958
C	-0.2944	-3.05314	2.65855	C	-7.20944	0.500618	0.000441
C	0.472967	-1.73436	2.739004	O	-6.29562	2.183117	-2.22944
C	-0.51301	-0.56374	2.828169	O	-3.91345	1.469967	-3.51286
O	-1.42476	-0.56394	1.711094	O	-7.98306	1.680995	-0.05523
C	-3.54953	-0.2865	-0.11952	H	-3.44438	-4.96368	-0.27274
O	-4.54414	-2.81939	-1.11285	H	-0.68494	-3.29591	3.657475
C	0.110185	0.823451	2.874656	H	0.399067	-3.85885	2.399743
O	1.27708	-1.6175	1.545669	H	1.136592	-1.72405	3.604814
O	-1.43446	-5.32297	1.491171	H	-1.11009	-0.74065	3.73758
C	1.268529	1.114614	3.604315	H	-3.22481	0.494924	0.572314
C	1.819015	2.400046	3.576668	H	-5.04931	-1.99737	-0.94298
C	1.233685	3.402465	2.807089	H	-1.86476	-6.04147	1.002223
C	0.060164	3.117482	2.095875	H	1.785036	0.342927	4.164225
C	-0.50711	1.854368	2.160432	H	2.730197	2.625057	4.122323
O	-0.45005	4.129442	1.311928	H	-1.40961	1.663476	1.600675

O	1.820825	4.635864	2.697817	H	-1.02474	3.720613	0.630937
C	2.627544	-1.56577	1.690398	H	1.225989	5.177689	2.149244
O	3.189013	-1.42843	2.761278	H	5.198634	-1.04226	1.249069
C	3.333866	-1.71161	0.390982	H	1.621459	-2.44004	-0.7221
C	4.701786	-1.39913	0.353947	H	6.339167	-1.93433	-2.97028
C	5.393536	-1.54163	-0.8416	H	6.861997	-0.26945	-0.9043
C	4.746641	-2.04341	-1.97487	H	0.752583	3.13911	-0.57421
C	3.386007	-2.3714	-1.93524	H	0.622679	0.47634	-2.11032
C	2.675563	-2.19249	-0.75167	H	2.909786	3.639261	0.371811
O	5.410585	-2.1696	-3.16328	H	5.36094	3.378171	0.421614
O	6.734458	-1.23255	-1.01973	H	5.153006	0.706827	-2.94557
C	2.608072	2.273648	-1.27982	H	2.692372	0.938472	-2.9812
C	1.15645	2.308903	-1.14761	H	7.161598	2.266013	-0.50868
C	0.294238	1.368162	-1.58777	H	3.427548	-2.92827	-3.752
C	-1.13671	1.447342	-1.27704	H	-5.38431	1.611758	0.246804
O	-1.69727	2.356879	-0.66749	H	-5.84055	0.164473	-2.41539
O	-1.77721	0.356968	-1.76276	H	-3.76807	2.229236	-1.58144
C	3.390508	2.998812	-0.36258	H	-3.38561	-0.72475	-2.23125
C	4.774726	2.853697	-0.33017	H	-7.60551	-0.29019	-0.66039
C	5.39412	1.995312	-1.23915	H	-7.2591	0.127479	1.027796
C	4.648053	1.343225	-2.2266	H	-6.01071	2.409179	-3.13149
C	3.268484	1.473246	-2.23265	H	-3.0327	1.830531	-3.6974
O	6.743742	1.713194	-1.18917	H	-7.82888	2.076861	-0.93144
Conformation 5							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	3.722819	-1.80548	1.154673	O	-5.34159	-3.8089	1.689191
C	3.544188	-3.1854	1.115135	O	4.760372	0.768959	0.551808
C	2.805493	-3.74816	0.078772	C	5.160295	2.143616	0.700609
C	2.234708	-2.95799	-0.93465	C	4.432759	2.718557	1.91316
C	2.439787	-1.57098	-0.87064	C	2.929409	2.640793	1.646278
C	3.175755	-0.96309	0.162115	C	2.471115	1.220364	1.300388
C	1.347201	-3.55072	-2.00701	C	6.67952	2.131052	0.813495
C	0.380846	-2.48121	-2.52024	O	4.829201	4.061202	2.113058
C	1.186015	-1.2396	-2.91902	O	2.187374	3.207604	2.725264
O	1.904129	-0.71201	-1.79628	O	7.278459	1.579742	-0.34378
C	3.364451	0.536503	0.227908	H	3.990305	-3.81314	1.876958
O	4.446463	-1.30228	2.196335	H	1.921739	-3.94749	-2.85755
C	0.358707	-0.12451	-3.52169	H	0.743879	-4.38331	-1.62154
O	-0.51504	-2.11573	-1.45783	H	-0.19605	-2.84571	-3.37254
O	2.669035	-5.10675	0.09881	H	1.91661	-1.58021	-3.66878
C	0.040047	-0.16245	-4.88166	H	3.145892	0.990161	-0.7445
C	-0.75307	0.836932	-5.45137	H	4.810638	-0.4447	1.896261
C	-1.21779	1.882342	-4.66127	H	2.170297	-5.3975	-0.67924
C	-0.8887	1.931759	-3.29729	H	0.410979	-0.96849	-5.5097
C	-0.11088	0.929549	-2.73141	H	-1	0.806239	-6.5107
O	-1.3341	2.970894	-2.52264	H	0.149146	0.982321	-1.68195
O	-1.99336	2.927884	-5.1116	H	-1.81971	3.580808	-3.10497
C	-1.60271	-2.92727	-1.28202	H	-2.16174	2.827065	-6.06037

O	-1.95269	-3.73883	-2.11824	H	-0.6572	-1.55263	0.897376
C	-2.25908	-2.72106	0.029739	H	-3.96576	-3.91023	-0.55806
C	-1.63178	-1.99552	1.057168	H	-3.56922	-1.89771	4.291188
C	-2.26481	-1.88559	2.292017	H	-1.0128	-0.64858	3.152043
C	-3.50961	-2.49496	2.494949	H	-2.29617	1.198524	2.660845
C	-4.12912	-3.22175	1.471912	H	-1.04984	2.173876	0.023475
C	-3.50101	-3.33817	0.236127	H	-3.03588	2.79256	-0.74574
O	-4.15624	-2.40041	3.697945	H	-5.28497	3.627313	-1.35365
O	-1.78034	-1.22143	3.386474	H	-6.77329	2.491301	2.515463
C	-3.60497	2.172631	1.253967	H	-4.53197	1.658013	3.133198
C	-2.31022	1.66694	1.678663	H	-8.0175	3.470175	0.843623
C	-1.14185	1.707351	0.997649	H	-5.5889	-3.63294	2.613103
C	0.081058	1.161199	1.58046	H	4.874721	2.699509	-0.20452
O	0.189356	0.592533	2.668163	H	4.682603	2.100785	2.795753
O	1.141907	1.350097	0.756851	H	2.71453	3.29122	0.79017
C	-3.84191	2.734412	-0.0206	H	2.434715	0.594721	2.196953
C	-5.09697	3.200831	-0.37346	H	7.039159	3.158076	0.911573
C	-6.15961	3.119382	0.540113	H	6.969377	1.580822	1.725054
C	-5.95056	2.561744	1.806632	H	4.147774	4.455013	2.686011
C	-4.68739	2.094917	2.15005	H	2.108969	2.541047	3.428836
O	-7.36802	3.595723	0.133694	H	6.857291	0.714861	-0.4799
Conformation 6							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-4.14179	2.036142	-0.32172	O	4.993778	4.233982	2.097184
C	-3.93134	3.340384	-0.77366	O	-4.93997	-0.67	-0.1209
C	-2.8738	3.602078	-1.6363	C	-5.33536	-1.90291	0.493553
C	-2.0132	2.586222	-2.07601	C	-4.90824	-1.82732	1.958509
C	-2.258	1.283088	-1.62548	C	-3.38979	-1.75785	2.046461
C	-3.31814	0.972367	-0.74607	C	-2.80997	-0.6403	1.164895
C	-0.81308	2.911169	-2.9305	C	-6.84924	-2.0547	0.304682
C	0.237515	1.812381	-2.8042	O	-5.38957	-2.9673	2.663629
C	-0.43547	0.453078	-2.98656	O	-3.07106	-1.5997	3.422706
O	-1.43936	0.237143	-1.97303	O	-7.29265	-3.34613	0.664489
C	-3.51742	-0.43366	-0.21108	H	-4.60791	4.122294	-0.44092
O	-5.1727	1.856937	0.549271	H	-1.08685	3.021257	-3.98964
C	0.482492	-0.75983	-2.98921	H	-0.37638	3.868695	-2.63225
O	0.815057	1.837971	-1.4847	H	1.024612	1.9621	-3.54452
O	-2.61236	4.861696	-2.10112	H	-0.95507	0.498667	-3.95736
C	-0.06463	-2.0374	-2.81737	H	-3.09012	-1.1644	-0.90643
C	0.744834	-3.17448	-2.89081	H	-5.40871	0.906497	0.514685
C	2.105208	-3.04293	-3.15008	H	-3.2307	5.482167	-1.68505
C	2.664445	-1.7688	-3.33427	H	-1.12493	-2.14799	-2.62191
C	1.854585	-0.639	-3.24753	H	0.313144	-4.16399	-2.75097
O	3.995691	-1.62666	-3.58559	H	2.335908	0.323579	-3.37892
O	3.000957	-4.09039	-3.22685	H	4.380818	-2.5167	-3.65467
C	1.903859	2.639442	-1.30157	H	2.526405	-4.93315	-3.16522
O	2.475543	3.193427	-2.22187	H	0.603645	1.618486	0.87428
C	2.291638	2.735516	0.126581	H	4.047312	3.903952	-0.34314

C	1.51517	2.139241	1.133707	H	2.884392	2.583035	4.623721
C	1.931687	2.230047	2.457758	H	0.577713	1.065026	3.257618
C	3.098663	2.937238	2.773535	H	1.857154	-0.96702	2.899841
C	3.85936	3.549487	1.770465	H	0.758944	-1.75599	0.131924
C	3.45917	3.44316	0.441589	H	2.651956	-2.68698	-0.42208
O	3.535357	3.046619	4.06703	H	4.865779	-3.62356	-0.95223
O	1.298468	1.672539	3.537477	H	6.33836	-2.33113	2.88137
C	3.208054	-1.96717	1.544349	H	4.116452	-1.39521	3.417114
C	1.918977	-1.40491	1.904763	H	7.580009	-3.42783	1.282616
C	0.801482	-1.36535	1.142141	H	5.084746	4.202778	3.064894
C	-0.44264	-0.81463	1.660558	H	-4.83695	-2.74641	-0.00711
O	-0.60233	-0.25256	2.755022	H	-5.33241	-0.90697	2.391457
O	-1.45438	-1.01492	0.801864	H	-2.99689	-2.71667	1.669449
C	3.449067	-2.60693	0.308763	H	-2.79316	0.295773	1.728794
C	4.689364	-3.13602	0.000619	H	-7.36601	-1.26157	0.872441
C	5.73869	-3.03827	0.92851	H	-7.08724	-1.91145	-0.7537
C	5.526	-2.40935	2.161628	H	-4.99277	-2.92948	3.550706
C	4.274071	-1.8846	2.459393	H	-2.20052	-1.16428	3.49458
O	6.935581	-3.57641	0.572375	H	-6.98273	-3.50149	1.57453

Table S11. Optimized coordinate of (Glc-4*R**)-**1** at B3LYP/6-31G (d) level in DMSO.

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.345068	1.561468	-0.12801	O	-5.02886	3.95086	-2.08323
C	4.338912	2.916996	0.217756	O	4.834695	-1.21473	0.04432
C	3.406566	3.389176	1.132517	C	5.08241	-2.50023	-0.53335
C	2.463808	2.540007	1.730042	C	4.691534	-2.45725	-2.00705
C	2.511566	1.181843	1.3972	C	3.183685	-2.21927	-2.12052
C	3.451036	0.657556	0.485212	C	2.701382	-1.04971	-1.23587
C	1.371637	3.092373	2.611018	C	6.558278	-2.79043	-0.27193
C	0.182644	2.137812	2.634589	O	5.399548	-1.39194	-2.62481
C	0.677711	0.717598	2.916919	O	2.922797	-1.96095	-3.49606
O	1.598212	0.283978	1.895333	O	6.836103	-2.80338	1.116423
C	3.45793	-0.80804	0.108843	H	5.060007	3.576566	-0.25666
O	5.230372	1.205026	-1.09132	H	1.717537	3.251487	3.642599
C	-0.40036	-0.34846	3.038805	H	1.04547	4.070844	2.245288
O	-0.44648	2.139436	1.336734	H	-0.54296	2.456012	3.383748
O	3.343253	4.709676	1.487268	H	1.238506	0.770075	3.864202
C	-0.05581	-1.70358	2.967054	H	2.948325	-1.40174	0.875541
C	-1.02054	-2.70183	3.12903	H	5.318031	0.231163	-1.14136
C	-2.3478	-2.35778	3.371776	H	3.998964	5.202164	0.969567
C	-2.69793	-1.00171	3.448147	H	0.974482	-1.98408	2.778502
C	-1.73835	-0.00928	3.290526	H	-0.75454	-3.75325	3.077388
O	-4.03211	-0.75846	3.684167	H	-2.05919	1.027317	3.33739
O	-3.30795	-3.32341	3.510801	H	-4.20133	0.196	3.653003
C	-1.66048	2.735323	1.201974	H	-4.13086	-2.86627	3.757754
O	-2.28367	3.197776	2.14365	H	-0.44376	1.624299	-0.98837
C	-2.13048	2.72625	-0.20354	H	-3.91103	3.843024	0.300707

C	-1.39441	2.087952	-1.21649	H	-3.02618	2.178843	-4.61728
C	-1.90722	2.053171	-2.50897	H	-0.62584	0.804462	-3.30007
C	-3.12434	2.685574	-2.79425	H	-2.03147	-1.12358	-2.82029
C	-3.84381	3.342747	-1.78903	H	-0.89525	-1.88519	-0.06081
C	-3.35189	3.352749	-0.48731	H	-4.3288	-1.44122	-3.25237
O	-3.65291	2.670223	-4.05604	H	-6.5899	-2.2455	-2.60567
O	-1.32607	1.434662	-3.58423	H	-5.03467	-3.46462	1.221141
C	-3.3927	-1.99238	-1.38593	H	-2.8156	-2.67474	0.590418
C	-2.08621	-1.5199	-1.80752	H	-7.22149	-3.7094	0.528051
C	-0.94403	-1.5223	-1.08119	H	-5.18678	3.838773	-3.0363
C	0.318103	-1.07617	-1.65238	H	4.475461	-3.25941	-0.01389
O	0.485654	-0.55368	-2.76577	H	4.933247	-3.41671	-2.49112
O	1.339373	-1.33122	-0.81953	H	2.663396	-3.13015	-1.78572
C	-4.48443	-1.88568	-2.27254	H	2.711177	-0.13596	-1.83305
C	-5.75091	-2.32988	-1.92292	H	6.807286	-3.78484	-0.65637
C	-5.95684	-2.90307	-0.66124	H	7.172088	-2.05289	-0.80836
C	-4.88666	-3.02036	0.239332	H	4.893064	-1.18504	-3.43254
C	-3.62656	-2.5713	-0.12206	H	2.081623	-1.46699	-3.55562
O	-7.21361	-3.32937	-0.36479	H	6.531055	-1.94539	1.455267
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-3.70804	-2.46773	-0.08253	O	2.546867	-3.16441	-2.74563
C	-3.32112	-3.70662	0.435649	O	-4.97346	0.074802	-0.09277
C	-2.32573	-3.7649	1.407132	C	-5.63285	1.222675	-0.64417
C	-1.69337	-2.60843	1.886638	C	-5.42098	1.252363	-2.15512
C	-2.09389	-1.38489	1.341542	C	-3.92193	1.357406	-2.44211
C	-3.08975	-1.27744	0.34892	C	-3.15393	0.246412	-1.70818
C	-0.60363	-2.67579	2.930669	C	-7.09074	1.10619	-0.20654
C	0.270999	-1.42195	2.897894	O	-5.95154	0.054829	-2.70811
C	-0.61522	-0.17156	2.849036	O	-3.77755	1.207457	-3.85724
O	-1.50761	-0.21068	1.719445	O	-7.19811	1.094811	1.205413
C	-3.53111	0.057528	-0.20837	H	-3.8295	-4.60073	0.08603
O	-4.69275	-2.48237	-1.02376	H	-1.02929	-2.78228	3.938984
C	0.116088	1.160487	2.767171	H	0.024443	-3.5575	2.771437
O	1.0976	-1.48974	1.716072	H	0.921654	-1.37913	3.772645
O	-1.91859	-4.95118	1.954669	H	-1.23558	-0.20581	3.759546
C	1.277456	1.441001	3.495797	H	-3.11773	0.879341	0.380547
C	1.923552	2.673219	3.351864	H	-5.11805	-1.60101	-1.05922
C	1.431242	3.630733	2.468039	H	-2.39288	-5.67501	1.516927
C	0.255898	3.358382	1.755103	H	1.720966	0.696547	4.147689
C	-0.404	2.15259	1.930716	H	2.836995	2.887528	3.898067
O	-0.16427	4.318947	0.860346	H	-1.30599	1.970316	1.367462
O	2.110156	4.801952	2.253525	H	-0.76829	3.889997	0.218368
C	2.446379	-1.51058	1.880968	H	1.566477	5.329745	1.641981
O	3.001759	-1.31104	2.945279	H	5.054688	-1.21304	1.449892
C	3.158205	-1.81605	0.612456	H	1.412717	-2.50837	-0.4716
C	4.545469	-1.60465	0.576482	H	6.184476	-2.52336	-2.66184
C	5.240993	-1.8915	-0.59062	H	6.799261	-0.73699	-0.73322

C	4.574691	-2.43556	-1.69259	H	0.959189	3.102767	-0.90438
C	3.193549	-2.66189	-1.65296	H	0.68279	0.331038	-2.21054
C	2.482206	-2.33944	-0.50084	H	3.121369	3.545749	0.048424
O	5.243591	-2.7037	-2.8545	H	5.545034	3.12114	0.201778
O	6.603336	-1.69495	-0.76635	H	5.230694	0.161466	-2.90663
C	2.764956	2.056606	-1.48096	H	2.796133	0.5626	-3.04656
C	1.316697	2.201243	-1.3947	H	7.282992	1.798571	-0.55867
C	0.40223	1.284265	-1.77576	H	3.219859	-3.36502	-3.41844
C	-1.02549	1.47402	-1.50175	H	-5.20119	2.133427	-0.20041
O	-1.54434	2.456399	-0.97637	H	-5.92389	2.133965	-2.58403
O	-1.72106	0.380784	-1.91005	H	-3.56486	2.340104	-2.11963
C	3.573708	2.808294	-0.60886	H	-3.37156	-0.68968	-2.22482
C	4.942342	2.570431	-0.51748	H	-7.64871	1.978615	-0.5621
C	5.52096	1.58765	-1.3213	H	-7.53422	0.209008	-0.66109
C	4.755536	0.898718	-2.26828	H	-5.56071	-0.01789	-3.59714
C	3.39005	1.124873	-2.33294	H	-2.83733	1.06085	-4.04821
O	6.843957	1.21621	-1.20006	H	-6.61268	0.381349	1.509369
Conformation 3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-4.29941	-1.62157	-0.00682	O	5.075239	-3.98226	-1.78294
C	-4.26258	-2.94539	0.443904	O	-4.86457	1.145449	-0.04182
C	-3.32851	-3.32039	1.401087	C	-5.14584	2.376325	-0.7144
C	-2.4138	-2.40296	1.938117	C	-4.75079	2.232732	-2.18075
C	-2.49152	-1.07702	1.498465	C	-3.2368	2.02831	-2.27513
C	-3.43444	-0.64983	0.540613	C	-2.72741	0.939571	-1.30732
C	-1.31455	-2.85424	2.866352	C	-6.6297	2.644255	-0.47523
C	-0.14457	-1.87744	2.805221	O	-5.42719	1.103589	-2.71562
C	-0.66567	-0.4484	2.973022	O	-2.96402	1.677026	-3.6279
O	-1.6066	-0.1199	1.930231	O	-6.91024	2.753263	0.908279
C	-3.47769	0.782075	0.053458	H	-4.96229	-3.65835	0.017068
O	-5.18377	-1.36465	-1.00244	H	-1.65971	-2.92761	3.90775
C	0.390663	0.645823	2.9891	H	-0.9685	-3.85459	2.588941
O	0.478688	-1.97554	1.507795	H	0.590511	-2.11899	3.573407
O	-3.23621	-4.60727	1.858519	H	-1.21528	-0.43176	3.928117
C	0.019776	1.979197	2.77839	H	-2.98479	1.445734	0.772122
C	0.965276	3.006788	2.832673	H	-5.29952	-0.40062	-1.12807
C	2.299491	2.71649	3.105943	H	-3.87406	-5.1549	1.375079
C	2.675253	1.382692	3.326311	H	-1.01529	2.21896	2.562601
C	1.734683	0.360966	3.274515	H	0.679619	4.041632	2.669874
O	4.013154	1.1911	3.584597	H	2.075232	-0.6587	3.429524
O	3.237216	3.710555	3.134447	H	4.207024	0.241757	3.623368
C	1.700386	-2.56258	1.41525	H	4.081724	3.298586	3.388307
O	2.337192	-2.93491	2.386881	H	0.443477	-1.67584	-0.853
C	2.160681	-2.66674	0.009498	H	3.968904	-3.69674	0.592915
C	1.402697	-2.13686	-1.04846	H	3.011235	-2.48631	-4.44298
C	1.905853	-2.20274	-2.34358	H	0.599892	-1.04537	-3.22719
C	3.136767	-2.82676	-2.58335	H	2.011997	0.852227	-2.86556
C	3.877111	-3.37942	-1.53163	H	0.865828	1.912079	-0.21082

C	3.39392	-3.28851	-0.22975	H	4.335003	0.919716	-3.22331
O	3.659305	-2.90262	-3.84626	H	6.611851	1.673096	-2.63438
O	1.303282	-1.69209	-3.46316	H	5.05214	3.625753	0.872099
C	3.38034	1.830768	-1.51476	H	2.786029	2.876328	0.291184
C	2.064562	1.354113	-1.90083	H	7.86541	2.842726	-1.09895
C	0.915934	1.453914	-1.19221	H	5.216923	-3.96056	-2.74483
C	-0.34563	0.960933	-1.72645	H	-4.56052	3.188669	-0.25394
O	-0.50943	0.34501	-2.79176	H	-5.01815	3.145293	-2.73666
O	-1.36999	1.280391	-0.92028	H	-2.74193	2.974883	-2.00758
C	4.486193	1.514881	-2.32633	H	-2.71861	-0.01654	-1.8337
C	5.769401	1.934156	-1.99701	H	-6.90587	3.599594	-0.93322
C	5.973907	2.694646	-0.83894	H	-7.22131	1.85132	-0.95461
C	4.884899	3.02999	-0.01853	H	-4.9153	0.852819	-3.50736
C	3.612896	2.602592	-0.35499	H	-2.11576	1.192375	-3.64907
O	7.200769	3.140094	-0.45738	H	-6.57932	1.93302	1.310455
Conformation 4							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-4.12868	-1.7142	0.147187	O	4.941282	-4.71962	-0.84044
C	-4.08521	-2.93864	0.82152	O	-4.74593	0.996183	-0.38062
C	-3.1922	-3.11443	1.871605	C	-5.01823	2.086036	-1.26532
C	-2.32789	-2.09032	2.285689	C	-4.56646	1.700824	-2.66982
C	-2.4126	-0.86343	1.618428	C	-3.04682	1.512374	-2.6762
C	-3.3127	-0.63812	0.556667	C	-2.56052	0.614979	-1.51818
C	-1.26468	-2.34045	3.32625	C	-6.51296	2.364131	-1.12597
C	-0.10964	-1.36264	3.129203	O	-5.20759	0.483952	-3.02549
C	-0.66306	0.057527	3.032207	O	-2.72071	0.940811	-3.93806
O	-1.57539	0.183529	1.919281	O	-6.84316	2.70085	0.209494
C	-3.358	0.682958	-0.17771	H	-4.74592	-3.73601	0.493326
O	-4.96699	-1.65661	-0.91797	H	-1.65367	-2.23058	4.348813
C	0.36711	1.165775	2.893698	H	-0.88995	-3.36561	3.252668
O	0.558819	-1.6553	1.886463	H	0.603279	-1.44688	3.950799
O	-3.0951	-4.29985	2.548056	H	-1.24622	0.223385	3.952263
C	1.727192	0.968012	3.148262	H	-2.90093	1.472744	0.428426
C	2.636856	2.024273	3.045457	H	-5.10132	-0.7319	-1.20975
C	2.200983	3.293447	2.685279	H	-3.68911	-4.94442	2.133134
C	0.832992	3.503088	2.438762	H	2.107087	-0.01099	3.416981
C	-0.07113	2.454409	2.544811	H	3.694292	1.867752	3.232963
O	0.498346	4.794414	2.091585	H	-1.1245	2.628613	2.339976
O	3.094689	4.320335	2.546149	H	-0.46299	4.868432	1.994979
C	1.657663	-2.45981	1.937801	H	2.584229	5.121356	2.334467
O	2.157228	-2.82678	2.985969	H	0.615447	-1.75367	-0.49689
C	2.160365	-2.80625	0.586433	H	3.799157	-3.94978	1.40775
C	1.514442	-2.35036	-0.57552	H	3.166863	-3.42394	-3.79593
C	2.04369	-2.67773	-1.81977	H	0.84216	-1.60418	-2.93469
C	3.191473	-3.47681	-1.90107	H	2.22686	0.394776	-2.91353
C	3.823091	-3.94428	-0.74279	H	0.985098	1.788855	-0.46452
C	3.310919	-3.60196	0.505191	H	4.54164	0.600392	-3.31321
O	3.734613	-3.8188	-3.11005	H	6.784209	1.527392	-2.77686

O	1.545052	-2.28453	-3.03386	H	5.084239	3.639834	0.571566
C	3.533973	1.589772	-1.67894	H	2.884569	2.732195	0.045489
C	2.242885	1.025215	-2.02575	H	7.306899	3.676758	-0.0435
C	1.071654	1.194893	-1.36714	H	5.127705	-4.8465	-1.78644
C	-0.16608	0.610396	-1.85909	H	-4.46087	2.977238	-0.93296
O	-0.28899	-0.16325	-2.82174	H	-4.82465	2.499054	-3.38369
O	-1.22181	1.037307	-1.14568	H	-2.57481	2.500531	-2.55805
C	4.66112	1.268815	-2.46423	H	-2.52329	-0.41701	-1.87203
C	5.917588	1.779093	-2.17454	H	-6.78444	3.223164	-1.74813
C	6.078302	2.636563	-1.0779	H	-7.07768	1.491242	-1.48288
C	4.971868	2.975949	-0.2832	H	-4.6621	0.110564	-3.74314
C	3.722758	2.45783	-0.58448	H	-1.86544	0.47593	-3.84616
O	7.32781	3.112043	-0.83258	H	-6.52353	1.962067	0.753636
Conformation 5							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-3.82487	-1.44009	1.823321	O	2.636617	-4.13169	1.162741
C	-3.3899	-1.80961	3.099302	O	-5.18099	0.097203	-0.11626
C	-2.36655	-1.09185	3.708918	C	-5.85724	0.430556	-1.33515
C	-1.73965	-0.01073	3.071239	C	-5.61132	-0.66537	-2.36189
C	-2.18149	0.325651	1.787575	C	-4.10759	-0.80351	-2.64912
C	-3.23338	-0.35599	1.144814	C	-3.29346	-0.91381	-1.34387
C	-0.61988	0.748879	3.73889	C	-7.32069	0.633374	-0.95258
C	0.235634	1.484497	2.710485	O	-6.10778	-1.89004	-1.84296
C	-0.6685	2.216278	1.704792	O	-3.99066	-1.96634	-3.45418
O	-1.5838	1.32435	1.06118	O	-7.45811	1.672976	0.000453
C	-3.747	0.055962	-0.2147	H	-3.87986	-2.64116	3.597843
O	-4.82356	-2.18758	1.282793	H	-1.01612	1.482148	4.456676
C	0.076492	2.98195	0.622552	H	0.014615	0.070416	4.317017
O	1.060438	0.506472	2.043232	H	0.892571	2.208125	3.195679
O	-1.91732	-1.3979	4.965565	H	-1.25899	2.928409	2.305396
C	-0.18251	2.789862	-0.73659	H	-3.38005	1.056883	-0.46924
C	0.504457	3.527794	-1.70796	H	-5.25106	-1.68482	0.559025
C	1.46135	4.464872	-1.33307	H	-2.39021	-2.1835	5.281261
C	1.721607	4.661343	0.034272	H	-0.92452	2.062988	-1.04166
C	1.030751	3.940755	0.99744	H	0.29992	3.387699	-2.7652
O	2.685973	5.605784	0.312503	H	1.262824	4.112369	2.045711
O	2.142411	5.178494	-2.27545	H	2.897828	5.583696	1.257995
C	2.409553	0.686459	2.071903	H	2.743013	5.780414	-1.80291
O	2.942513	1.726526	2.415942	H	4.996033	0.559008	1.465193
C	3.143301	-0.53277	1.652013	H	1.449299	-1.88008	1.787996
C	4.515374	-0.40929	1.379953	H	6.210509	-3.60834	0.404254
C	5.233237	-1.53469	0.99741	H	6.755839	-0.90511	-0.04109
C	4.605178	-2.78326	0.938026	H	1.16501	-2.39363	-3.18192
C	3.241764	-2.91202	1.233631	H	0.438391	0.063015	-1.48134
C	2.506489	-1.78118	1.575583	H	3.550462	-2.95781	-3.05153
O	5.293137	-3.90128	0.564771	H	5.920171	-2.30398	-2.67058
O	6.580885	-1.54454	0.677466	H	4.656662	1.714236	-1.80042
C	2.748054	-1.00853	-2.58821	H	2.314735	1.072933	-2.16994

C	1.360042	-1.45826	-2.65908	H	6.838959	0.961485	-1.74034
C	0.317376	-0.8358	-2.07549	H	3.316057	-4.78403	0.920868
C	-1.04639	-1.36624	-2.16863	H	-5.45519	1.383565	-1.71539
O	-1.38141	-2.40411	-2.72896	H	-6.11786	-0.4077	-3.3065
O	-1.91042	-0.53078	-1.55093	H	-3.76383	0.093523	-3.19033
C	3.790849	-1.93401	-2.77735	H	-3.32583	-1.94846	-0.99208
C	5.118858	-1.57956	-2.56684	H	-7.89042	0.934398	-1.83771
C	5.420023	-0.27399	-2.17622	H	-7.73347	-0.31762	-0.58801
C	4.413141	0.689238	-2.07273	H	-5.66391	-2.57584	-2.37755
C	3.089985	0.320265	-2.27241	H	-3.07856	-2.31413	-3.34789
O	6.731088	0.000997	-1.83759	H	-6.86379	1.439372	0.732697
Conformation 6							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-4.11241	-1.73148	0.139327	O	4.933838	-4.7338	-0.80818
C	-4.06193	-2.95378	0.817156	O	-4.749	0.972644	-0.39849
C	-3.17302	-3.11936	1.872569	C	-5.02565	2.059408	-1.28558
C	-2.31958	-2.08698	2.28857	C	-4.56123	1.677729	-2.68688
C	-2.41124	-0.86292	1.617088	C	-3.03997	1.502797	-2.68294
C	-3.30761	-0.6477	0.550159	C	-2.55363	0.609889	-1.52168
C	-1.25929	-2.32402	3.335415	C	-6.52376	2.323731	-1.15615
C	-0.1103	-1.33871	3.138032	O	-5.18915	0.455192	-3.04672
C	-0.67348	0.077038	3.033672	O	-2.7	0.933961	-3.9426
O	-1.58482	0.191553	1.918241	O	-6.86576	2.658677	0.176763
C	-3.35957	0.672169	-0.18616	H	-4.71421	-3.75759	0.487767
O	-4.94591	-1.68331	-0.93022	H	-1.65362	-2.21127	4.355599
C	0.346188	1.193751	2.890822	H	-0.87691	-3.34681	3.269266
O	0.564175	-1.63241	1.898344	H	0.600893	-1.41397	3.962091
O	-3.06984	-4.30234	2.552501	H	-1.26025	0.24167	3.951618
C	1.710136	1.008484	3.132899	H	-2.91338	1.466486	0.422133
C	2.60908	2.072989	3.02114	H	-5.08588	-0.76019	-1.22427
C	2.158321	3.338309	2.664502	H	-3.65706	-4.95241	2.136509
C	0.78586	3.535249	2.431353	H	2.100835	0.033123	3.399533
C	-0.10727	2.478419	2.546331	H	3.669827	1.92745	3.198341
O	0.435279	4.823242	2.087299	H	-1.16416	2.643087	2.351673
O	3.041227	4.371251	2.517671	H	-0.52782	4.88792	2.002598
C	1.654054	-2.44803	1.955068	H	2.524985	5.168814	2.307638
O	2.143661	-2.82245	3.005128	H	0.627676	-1.73713	-0.48451
C	2.161191	-2.79843	0.605859	H	3.788172	-3.95265	1.435268
C	1.522698	-2.34016	-0.55904	H	3.172735	-3.43859	-3.77179
C	2.053666	-2.67391	-1.80088	H	0.857056	-1.60035	-2.92038
C	3.196381	-3.48055	-1.87668	H	2.234894	0.379712	-2.88222
C	3.820493	-3.95034	-0.71542	H	0.98635	1.81595	-0.46158
C	3.30634	-3.60234	0.530226	H	4.548953	0.536091	-3.25949
O	3.741357	-3.82839	-3.08376	H	6.788433	1.440852	-2.74597
O	1.561468	-2.27972	-3.0173	H	5.122783	3.691622	0.528434
C	3.543472	1.588592	-1.66493	H	2.895944	2.79488	0.017552
C	2.250169	1.025769	-2.00578	H	7.982652	2.81105	-1.33638
C	1.076365	1.209673	-1.3557	H	5.116199	-4.87138	-1.75346

C	-0.15808	0.617323	-1.84824	H	-4.47868	2.955882	-0.95023
O	-0.27296	-0.16277	-2.80698	H	-4.82163	2.47359	-3.40263
O	-1.21942	1.042876	-1.14323	H	-2.5775	2.495064	-2.56196
C	4.668733	1.229318	-2.43081	H	-2.50652	-0.42199	-1.87448
C	5.930662	1.735048	-2.14445	H	-6.7992	3.179577	-1.78095
C	6.094949	2.624882	-1.07499		-7.078	1.445258	-1.5158
C	4.986916	3.003527	-0.29939	H	-4.63547	0.086848	-3.76069
C	3.736801	2.490783	-0.59523	H	-1.84378	0.472469	-3.84346
O	7.299723	3.157784	-0.74037	H	-6.54217	1.923831	0.723894

Table S12. DP4+ probability of ^{13}C NMR data of the isomers (**2**).

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311G(d,p)	Shielding Tensors

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	–	–	–	–	–	–
sDP4+ (C data)	76.82%	23.18%	–	–	–	–
sDP4+ (all data)	76.82%	23.18%	–	–	–	–
uDP4+ (H data)	–	–	–	–	–	–
uDP4+ (C data)	81.22%	18.78%	–	–	–	–
uDP4+ (all data)	81.22%	18.78%	–	–	–	–
DP4+ (H data)	–	–	–	–	–	–
DP4+ (C data)	93.48%	6.52%	–	–	–	–
DP4+ (all data)	93.48%	6.52%	–	–	–	–

Table S13. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized (2*R*,3*R*,3‴*S*)-**2** at B3LYP/6-31G (d) level in DMSO.

Conformation	Gibbs free energies (Hartree)	Boltzmann distribution
1	-2097.996924	31.62%
2	-2097.995891	10.58%
3	-2097.995651	8.21%
4	-2097.994293	1.95%
5	-2097.997211	42.87%
6	-2097.99514	4.77%

Table S14. Optimized coordinate of (2*R*,3*R*,3‴*S*)-**2** at B3LYP/6-31G (d) level in DMSO.

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.672515	0.317285	1.867839	O	-6.02486	-4.31166	-1.11247
C	3.115892	-0.43251	0.765897	O	3.99685	-2.55136	-2.56958
C	2.351298	-0.36299	-0.39745	C	5.658288	-0.55348	0.528149
C	1.183337	0.400859	-0.52275	C	5.76589	0.418458	-0.47764

C	0.79367	1.140584	0.600121	C	6.974684	1.052505	-0.74772
C	1.524165	1.099541	1.792937	C	8.113906	0.725628	-0.00514
C	0.364161	0.414501	-1.79201	C	8.027449	-0.2365	1.004857
C	-1.0276	0.990944	-1.53068	C	6.808371	-0.8636	1.261473
C	-0.92543	2.24851	-0.65396	O	9.275757	1.382224	-0.3072
O	-0.3255	1.926647	0.614211	H	1.181028	1.689507	2.638281
C	-2.24083	2.94154	-0.39178	H	0.85502	1.016945	-2.56919
O	-1.83171	0.033427	-0.80874	H	0.269806	-0.59152	-2.21155
C	-2.60958	4.053344	-1.15243	H	-1.52957	1.228843	-2.47026
C	-3.8442	4.678233	-0.95926	H	-0.25759	2.942076	-1.18657
C	-4.72215	4.199917	0.008014	H	-1.92948	4.4443	-1.90517
C	-4.34893	3.086276	0.782456	H	-4.1365	5.54298	-1.54639
C	-3.12543	2.462835	0.586215	H	-2.84577	1.609659	1.196678
O	3.426496	0.236834	3.006228	H	3.024394	0.796716	3.688226
O	2.735923	-1.03576	-1.55225	H	-4.97812	1.884594	2.157622
C	-2.62576	-0.7857	-1.54321	H	-6.38227	4.31802	0.914712
O	-2.67786	-0.75738	-2.75819	H	-4.40386	-2.51373	-2.42921
O	-5.28071	2.694077	1.718845	H	-2.58463	-1.09736	1.211762
O	-5.92603	4.806222	0.207682	H	-4.57758	-3.33381	3.133583
C	-3.42317	-1.70707	-0.69219	H	-6.29686	-4.83401	0.98047
C	-4.32723	-2.55682	-1.34695	H	4.439211	-1.71542	1.822411
C	-5.10286	-3.4303	-0.59703	H	5.033715	-3.08591	-0.28529
C	-4.9855	-3.46198	0.79656	H	3.348383	-3.13942	0.261225
C	-4.08006	-2.61502	1.446627	H	-6.04046	-4.23684	-2.07864
C	-3.29511	-1.73653	0.702623	H	4.890844	0.695969	-1.05838
O	-3.97015	-2.64845	2.805427	H	7.052816	1.803949	-1.52708
O	-5.733	-4.3063	1.571769	H	8.907074	-0.49041	1.594303
C	4.354961	-1.29889	0.813481	H	6.754438	-1.6058	2.055076
C	4.130604	-2.48693	-0.15311	H	9.979931	1.058639	0.275761
C	3.66203	-2.0587	-1.52532				
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.685151	0.168862	1.922944	O	-3.82484	-3.09801	2.757747
C	3.110738	-0.47672	0.750255	O	3.932315	-2.29913	-2.76943
C	2.309272	-0.33072	-0.38067	C	5.646439	-0.52358	0.427955
C	1.12264	0.41389	-0.40927	C	6.824411	-0.85731	1.111056
C	0.751985	1.049093	0.78198	C	8.023001	-0.1923	0.870884
C	1.518775	0.927308	1.946036	C	8.064421	0.836738	-0.07481
C	0.264365	0.513817	-1.64858	C	6.900338	1.188899	-0.76409
C	-1.13189	1.029711	-1.29894	C	5.706978	0.513709	-0.50974
C	-1.03162	2.210069	-0.32137	O	9.264062	1.463392	-0.27634
O	-0.38168	1.805558	0.89352	H	1.188345	1.436052	2.847338
C	-2.36272	2.832636	0.035958	H	0.716746	1.192614	-2.38518
O	-1.89295	-0.00349	-0.63954	H	0.179942	-0.45483	-2.14988
C	-3.12212	2.369335	1.112383	H	-1.66573	1.334389	-2.20113
C	-4.36742	2.940084	1.388196	H	-0.40187	2.966211	-0.81466
C	-4.85902	3.963669	0.586335	H	-2.73807	1.575184	1.740765
C	-4.10289	4.435872	-0.49972	H	-4.95796	2.58305	2.230106

C	-2.8596	3.870883	-0.76322	H	-2.28727	4.261128	-1.60061
O	3.474928	0.012054	3.028508	H	3.078041	0.496444	3.76886
O	2.672479	-0.89931	-1.59708	H	-5.44535	5.702985	-0.93534
C	-2.65522	-0.80127	-1.42948	H	-6.52329	4.211443	1.535737
O	-2.72494	-0.67622	-2.63801	H	-2.58008	-1.31719	1.292239
O	-4.57431	5.447049	-1.28406	H	-4.3292	-2.56213	-2.44482
O	-6.07073	4.594281	0.769456	H	-5.83532	-4.41962	-2.22915
C	-3.38659	-1.83432	-0.6518	H	-6.01817	-5.27964	0.769693
C	-3.24227	-1.96748	0.734922	H	4.491113	-1.81007	1.660988
C	-3.95588	-2.95684	1.408149	H	5.046099	-2.99532	-0.56626
C	-4.80906	-3.80753	0.695239	H	3.379523	-3.12915	0.022458
C	-4.94567	-3.66888	-0.68997	H	-4.38798	-3.84205	3.032328
C	-4.23888	-2.68716	-1.36997	H	6.803104	-1.65289	1.852851
O	-5.81235	-4.56651	-1.2715	H	8.930164	-0.45209	1.407442
O	-5.48775	-4.76408	1.401166	H	6.923655	1.992804	-1.49805
C	4.367207	-1.3172	0.691462	H	4.81305	0.8132	-1.04927
C	4.135973	-2.4287	-0.36016	H	9.151839	2.143599	-0.95843
C	3.618277	-1.90106	-1.67923				
Conformation 3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.691826	0.160607	1.915356	O	-5.83976	-4.54706	-1.2598
C	3.114266	-0.48697	0.742722	O	3.921941	-2.31752	-2.77757
C	2.310236	-0.34202	-0.38659	C	5.648645	-0.52806	0.419379
C	1.124436	0.403875	-0.41349	C	5.710408	0.502484	-0.53067
C	0.75715	1.041312	0.777588	C	6.895457	1.186291	-0.78345
C	1.526172	0.919953	1.940199	C	8.056568	0.851827	-0.07895
C	0.264391	0.504216	-1.65155	C	8.015633	-0.16788	0.87574
C	-1.12985	1.02464	-1.30077	C	6.819783	-0.84478	1.115369
C	-1.02507	2.205441	-0.32421	O	9.193598	1.55882	-0.36161
O	-0.37513	1.799542	0.89033	H	1.198449	1.430562	2.841444
C	-2.35396	2.832095	0.034131	H	0.717851	1.180501	-2.38973
O	-1.89322	-0.00595	-0.63964	H	0.176492	-0.46499	-2.1512
C	-3.11384	2.37131	1.111314	H	-1.66386	1.330044	-2.20258
C	-4.35718	2.945868	1.388076	H	-0.39349	2.959356	-0.81845
C	-4.84637	3.970759	0.586415	H	-2.73164	1.576151	1.739552
C	-4.08976	4.440457	-0.50038	H	-4.9481	2.59081	2.230568
C	-2.84838	3.871681	-0.76483	H	-2.27556	4.260102	-1.60272
O	3.483894	0.004948	3.019857	H	3.089297	0.492842	3.759129
O	2.669154	-0.91303	-1.60306	H	-5.4286	5.711779	-0.9349
C	-2.66296	-0.79877	-1.42716	H	-6.5088	4.223857	1.537538
O	-2.73731	-0.67239	-2.63526	H	-4.35027	-2.54976	-2.43725
O	-4.55881	5.452857	-1.28454	H	-2.57979	-1.3175	1.293836
O	-6.05608	4.605017	0.770523	H	-4.39502	-3.83387	3.038921
C	-3.39666	-1.8287	-0.64737	H	-6.04185	-5.26039	0.781473
C	-4.25639	-2.67626	-1.36288	H	4.497391	-1.81932	1.650877
C	-4.96586	-3.65469	-0.68092	H	5.052756	-3.00037	-0.57946
C	-4.82455	-3.79528	0.703603	H	3.38944	-3.14113	0.016087
C	-3.96395	-2.94988	1.413848	H	-5.86636	-4.39856	-2.21711

C	-3.24762	-1.96383	0.738651	H	4.81762	0.786859	-1.08027
O	-3.82844	-3.09299	2.762865	H	6.938147	1.982829	-1.51957
O	-5.50577	-4.74877	1.411367	H	8.912497	-0.42859	1.435528
C	4.371821	-1.32588	0.681805	H	6.801211	-1.63213	1.865852
C	4.141198	-2.43736	-0.36973	H	9.916714	1.224179	0.191129
C	3.614883	-1.91431	-1.68731				
Conformation 4							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.887305	0.65778	1.813447	O	-5.73815	-0.46036	2.169256
C	3.333078	-0.30372	0.891706	O	4.242268	-3.05047	-1.93678
C	2.558467	-0.49483	-0.25139	C	5.875474	-0.43413	0.673432
C	1.376496	0.208228	-0.52202	C	5.978887	0.266278	-0.53798
C	0.988395	1.165157	0.419685	C	7.176566	0.849753	-0.93891
C	1.727911	1.392566	1.585167	C	8.308519	0.74724	-0.12367
C	0.547826	-0.05456	-1.75569	C	8.225658	0.05921	1.089862
C	-0.85729	0.534588	-1.61998	C	7.017698	-0.52194	1.47571
C	-0.79994	1.944131	-0.99451	O	9.459481	1.343712	-0.56186
O	-0.14264	1.92312	0.279407	H	1.382539	2.144301	2.289426
C	-2.17151	2.554301	-0.78673	H	1.024439	0.384428	-2.64389
O	-1.70078	-0.25223	-0.75971	H	0.465544	-1.12443	-1.96118
C	-2.8049	3.244981	-1.82122	H	-1.32835	0.592972	-2.60572
C	-4.12062	3.696421	-1.67326	H	-0.21228	2.571687	-1.68186
C	-4.81404	3.435483	-0.49627	H	-2.28172	3.432921	-2.75519
C	-4.17916	2.747264	0.549123	H	-4.60886	4.238857	-2.48019
C	-2.86	2.341028	0.414858	H	-2.37045	1.835059	1.238102
O	3.650518	0.830282	2.935488	H	3.240502	1.510206	3.4921
O	2.947263	-1.38777	-1.24263	H	-5.75393	2.866268	1.619995
C	-2.35767	-1.31214	-1.31832	H	-6.48848	4.252134	-1.01873
O	-2.04948	-1.78743	-2.39336	H	-3.49675	0.027954	0.734603
O	-4.88406	2.433689	1.693142	H	-3.77124	-3.61051	-1.554
O	-6.11538	3.804585	-0.2445	H	-6.67042	-4.56786	0.296959
C	-3.49887	-1.75222	-0.4777	H	-7.15121	-2.13635	2.220397
C	-3.99221	-0.90694	0.525513	H	4.676667	-1.32037	2.185339
C	-5.14512	-1.25093	1.216043	H	5.288138	-3.0909	0.404726
C	-5.77883	-2.46764	0.946954	H	3.60532	-3.05376	0.9606
C	-5.27076	-3.3283	-0.03785	H	-5.36159	0.441259	2.119162
C	-4.14005	-2.96401	-0.76614	H	5.109398	0.368331	-1.18122
O	-5.90299	-4.50851	-0.29747	H	7.251732	1.389825	-1.87744
O	-6.91515	-2.85377	1.60681	H	9.099367	-0.01766	1.735152
C	4.585011	-1.12481	1.112165	H	6.966425	-1.04976	2.425547
C	4.37627	-2.4907	0.414983	H	10.16013	1.191419	0.091077
C	3.897046	-2.36337	-1.01307				
Conformation 5							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.719847	0.455673	1.694977	O	-5.91173	-4.46593	-0.96019
C	3.107154	-0.35828	0.614446	O	4.024094	-2.42315	-2.7343
C	2.317941	-0.31128	-0.53517	C	5.651874	-0.57051	0.542717
C	1.143749	0.442046	-0.64055	C	6.745062	-0.96135	1.331908

C	0.783282	1.206203	0.479176	C	7.994172	-0.36166	1.197689
C	1.562966	1.224326	1.638934	C	8.174562	0.653248	0.25258
C	0.288505	0.425379	-1.88577	C	7.096882	1.059284	-0.54269
C	-1.10356	0.985591	-1.5923	C	5.851444	0.45363	-0.39248
C	-0.99486	2.261294	-0.74364	O	9.416616	1.212137	0.157372
O	-0.34457	1.979619	0.507231	H	1.278681	1.850589	2.476261
C	-2.31693	2.929265	-0.44793	H	0.747027	1.024874	-2.68483
O	-1.87366	0.033069	-0.82875	H	0.196321	-0.58703	-2.28971
C	-2.7761	3.963975	-1.26592	H	-1.63564	1.198762	-2.52141
C	-4.01966	4.559304	-1.03996	H	-0.36265	2.958079	-1.3148
C	-4.81495	4.129213	0.017405	H	-2.16064	4.317624	-2.08956
C	-4.35012	3.093785	0.848419	H	-4.38217	5.365021	-1.67034
C	-3.11808	2.498491	0.619362	H	-2.76423	1.708193	1.274462
O	3.460279	0.506314	2.845067	H	4.377077	0.256057	2.644198
O	2.684629	-0.9928	-1.69312	H	-4.8376	1.990894	2.357228
C	-2.63823	-0.8419	-1.52882	H	-6.41517	4.265811	1.023787
O	-2.68462	-0.86714	-2.74448	H	-4.34509	-2.67253	-2.347
O	-5.20432	2.745385	1.871879	H	-2.61296	-1.02198	1.237296
O	-6.02639	4.708714	0.249807	H	-4.54338	-3.2355	3.246894
C	-3.40954	-1.7514	-0.64224	H	-6.18798	-4.89615	1.153927
C	-4.27645	-2.66305	-1.26336	H	4.303593	-1.74627	1.688835
C	-5.02698	-3.52833	-0.4793	H	5.012371	-3.02387	-0.44848
C	-4.92108	-3.49101	0.915058	H	3.317949	-3.0989	0.065668
C	-4.05309	-2.58193	1.531506	H	-5.92835	-4.42902	-1.9285
C	-3.29323	-1.71135	0.753166	H	6.618939	-1.75666	2.064487
O	-3.95533	-2.54711	2.891058	H	8.835005	-0.66412	1.813672
O	-5.64487	-4.32474	1.723592	H	7.230322	1.852662	-1.27595
C	4.305758	-1.27879	0.694764	H	5.023148	0.791632	-1.00897
C	4.104263	-2.43281	-0.31715	H	9.407452	1.890582	-0.53577
C	3.649869	-1.97267	-1.68364				
Conformation 6							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.73396	0.304021	1.760147	O	-5.71981	-4.69166	-1.13319
C	3.106054	-0.39174	0.595031	O	3.956874	-2.11035	-2.96076
C	2.278132	-0.25744	-0.52017	C	5.65185	-0.53372	0.422016
C	1.082924	0.469467	-0.51708	C	6.782552	-0.97968	1.124508
C	0.740177	1.112425	0.681722	C	8.014159	-0.3417	1.006986
C	1.55672	1.041425	1.81367	C	8.138289	0.769675	0.167171
C	0.18728	0.547511	-1.73153	C	7.022677	1.23199	-0.53998
C	-1.2078	1.037073	-1.34253	C	5.795392	0.58624	-0.40751
C	-1.10118	2.227131	-0.37778	O	9.365217	1.36325	0.084468
O	-0.40461	1.847913	0.818067	H	1.283481	1.575037	2.71628
C	-2.43464	2.822778	0.015911	H	0.603969	1.233034	-2.48289
O	-1.92722	-0.00482	-0.65104	H	0.106925	-0.42405	-2.22767
C	-3.13706	2.37015	1.134475	H	-1.77506	1.322967	-2.23048
C	-4.38698	2.913343	1.443487	H	-0.50514	2.992899	-0.89778
C	-4.93957	3.898255	0.633062	H	-2.70448	1.607113	1.769849
C	-4.24069	4.359402	-0.49527	H	-4.93281	2.565032	2.318531

C	-2.99269	3.82234	-0.79223	H	-2.46521	4.203629	-1.66259
O	3.510243	0.265067	2.886956	H	4.42492	0.057215	2.635096
O	2.622797	-0.81583	-1.74877	H	-5.63519	5.575873	-0.91114
C	-2.67702	-0.84019	-1.41284	H	-6.56897	4.132144	1.644565
O	-2.76459	-0.74413	-2.6231	H	-4.3071	-2.67422	-2.36889
O	-4.77236	5.333318	-1.28864	H	-2.56391	-1.28544	1.320304
O	-6.16147	4.499405	0.84604	H	-4.28347	-3.81592	3.13927
C	-3.37045	-1.87494	-0.60329	H	-5.8913	-5.35615	0.92792
C	-4.20341	-2.77006	-1.29223	H	4.369423	-1.84383	1.494724
C	-4.87502	-3.75484	-0.58171	H	5.029734	-2.90016	-0.77289
C	-4.72233	-3.85504	0.805099	H	3.354851	-3.06059	-0.21546
C	-3.8888	-2.96195	1.48891	H	-5.76327	-4.56213	-2.09262
C	-3.21033	-1.96917	0.784906	H	6.699946	-1.84891	1.77467
O	-3.7427	-3.06481	2.840155	H	8.884098	-0.68756	1.556095
O	-5.36676	-4.81296	1.540823	H	7.112187	2.100285	-1.19038
C	4.326947	-1.28537	0.549665	H	4.9371	0.968299	-0.95316
C	4.114968	-2.34457	-0.55884	H	9.315888	2.10922	-0.53353
C	3.607296	-1.76932	-1.86143				

Table S15. Optimized coordinate of (2*R*,3*R*,3‴*R*)-**2** at B3LYP/6-31G (d) level in DMSO.

Conformation 1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.58928	-2.10821	-1.58383	O	-3.59127	5.443697	1.743647
C	3.173349	-1.79609	-0.34489	O	4.493515	-0.99198	3.393552
C	2.315977	-1.6741	0.747491	C	5.174216	-0.20858	-0.49634
C	0.927198	-1.84825	0.676965	C	6.431331	-0.05242	-1.09788
C	0.398152	-2.1715	-0.57825	C	6.959586	1.204969	-1.37271
C	1.216331	-2.30007	-1.70618	C	6.225342	2.349021	-1.04443
C	0.031642	-1.66459	1.880125	C	4.968256	2.215929	-0.44822
C	-1.42882	-1.52048	1.45189	C	4.452744	0.947809	-0.18061
C	-1.77061	-2.55798	0.371816	O	6.783133	3.56414	-1.33586
O	-0.93939	-2.36636	-0.78759	H	0.760244	-2.55676	-2.65827
C	-3.21308	-2.55061	-0.07384	H	0.114091	-2.52091	2.564299
O	-1.64969	-0.21573	0.874697	H	0.329917	-0.78836	2.463328
C	-4.1137	-3.47637	0.457495	H	-2.09477	-1.63912	2.30863
C	-5.46365	-3.45308	0.098039	H	-1.53734	-3.54198	0.805639
C	-5.92582	-2.50386	-0.80779	H	-3.76492	-4.2296	1.159666
C	-5.01875	-1.5763	-1.35212	H	-6.16856	-4.16998	0.506792
C	-3.67964	-1.59679	-0.99079	H	-2.98795	-0.88136	-1.42497
O	3.439924	-2.23007	-2.64741	H	2.922783	-2.43801	-3.4409
O	2.796582	-1.31085	2.000582	H	-4.89958	-0.03765	-2.51387
C	-2.09618	0.759518	1.705829	H	-7.35189	-1.74147	-1.79606
O	-2.29807	0.588923	2.893132	H	-3.05883	2.954327	2.799051
O	-5.57036	-0.68358	-2.24519	H	-1.59873	1.397891	-0.945
O	-7.23951	-2.47627	-1.1685	H	-2.21115	4.520876	-2.53806
C	-2.31661	2.046057	0.995033	H	-3.37009	6.312761	-0.23599

C	-2.84329	3.107688	1.745934	H	5.174766	-2.30345	-0.84659
C	-3.07886	4.32674	1.125209	H	6.055164	-1.81248	1.530992
C	-2.79625	4.494511	-0.2346	H	4.879143	-3.12889	1.367305
C	-2.2676	3.434067	-0.98016	H	-3.75381	5.2509	2.679467
C	-2.02462	2.207416	-0.36557	H	7.009023	-0.93573	-1.3623
O	-1.9946	3.60141	-2.30559	H	7.930827	1.318985	-1.84389
O	-3.01626	5.679039	-0.88352	H	4.388342	3.102024	-0.19521
C	4.664376	-1.61152	-0.16875	H	3.46841	0.868939	0.271698
C	5.018969	-2.04203	1.275324	H	6.177005	4.264166	-1.0476
C	4.136703	-1.39493	2.318506				
Conformation 2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.578723	-2.11413	-1.58177	O	-3.52319	5.465597	1.756168
C	3.16281	-1.80547	-0.34208	O	4.481055	-1.0156	3.401377
C	2.305125	-1.6849	0.750305	C	5.163126	-0.21838	-0.49446
C	0.916194	-1.8568	0.678773	C	4.446785	0.941403	-0.16473
C	0.387096	-2.17648	-0.57736	C	4.955024	2.208728	-0.43379
C	1.205686	-2.30411	-1.70511	C	6.204192	2.342329	-1.04805
C	0.020105	-1.67285	1.881473	C	6.932477	1.199063	-1.38906
C	-1.43917	-1.52184	1.451488	C	6.409041	-0.06334	-1.11162
C	-1.78411	-2.55726	0.370454	O	6.655764	3.610402	-1.29478
O	-0.95047	-2.36871	-0.78795	H	0.749608	-2.55777	-2.65803
C	-3.22587	-2.54348	-0.07731	H	0.098328	-2.5312	2.563618
O	-1.65352	-0.21626	0.87449	H	0.32102	-0.79917	2.46705
C	-4.13	-3.46938	0.447782	H	-2.10656	-1.63818	2.307477
C	-5.47938	-3.44017	0.086544	H	-1.5557	-3.54256	0.803886
C	-5.93742	-2.48465	-0.81472	H	-3.78446	-4.22722	1.146586
C	-5.02682	-1.55688	-1.35284	H	-6.18709	-4.15697	0.490645
C	-3.68827	-1.58351	-0.98998	H	-2.99391	-0.86782	-1.41932
O	3.429433	-2.23498	-2.64584	H	2.911047	-2.43805	-3.43978
O	2.785372	-1.3257	2.004724	H	-4.90331	-0.00833	-2.50102
C	-2.08701	0.763288	1.7079	H	-7.35993	-1.71102	-1.79915
O	-2.28369	0.59395	2.896289	H	-3.01208	2.970761	2.808555
O	-5.57454	-0.65768	-2.24176	H	-1.60774	1.39331	-0.94811
O	-7.25058	-2.45084	-1.17695	H	-2.18938	4.523528	-2.53671
C	-2.29963	2.051382	0.998104	H	-3.30058	6.333068	-0.22432
C	-2.80542	3.12024	1.753108	H	5.164164	-2.31327	-0.84364
C	-3.03151	4.34165	1.133525	H	6.044188	-1.82166	1.534508
C	-2.76133	4.5044	-0.22944	H	4.871348	-3.14031	1.367651
C	-2.25378	3.43661	-0.97922	H	-3.66469	5.279771	2.696786
C	-2.01958	2.207841	-0.3656	H	3.469321	0.859558	0.301877
O	-1.99278	3.598757	-2.30757	H	4.396437	3.103446	-0.17766
O	-2.97299	5.690872	-0.87727	H	7.901545	1.29374	-1.8765
C	4.653951	-1.62133	-0.16563	H	6.983949	-0.94472	-1.38798
C	5.008567	-2.05291	1.277978	H	7.529013	3.556728	-1.71306
C	4.124814	-1.41144	2.323512				
Conformation 3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**

C	2.452753	-2.24659	-1.59962	O	-2.89013	5.853925	1.657338
C	3.012977	-1.99212	-0.33675	O	4.252354	-1.31254	3.453637
C	2.127659	-1.80243	0.723172	C	5.139755	-0.57309	-0.40272
C	0.732924	-1.85698	0.598621	C	6.429311	-0.51572	-0.95071
C	0.227357	-2.12602	-0.67889	C	7.066433	0.69652	-1.19623
C	1.074396	-2.31929	-1.77584	C	6.411876	1.894481	-0.89265
C	-0.19038	-1.60169	1.767354	C	5.124389	1.860106	-0.3501
C	-1.61249	-1.31947	1.281774	C	4.499406	0.636228	-0.11144
C	-2.00291	-2.31478	0.179491	O	7.075581	3.062438	-1.15393
O	-1.1123	-2.20154	-0.942	H	0.634849	-2.52875	-2.74707
C	-3.42092	-2.16023	-0.322	H	-0.21497	-2.46758	2.443982
O	-1.68571	0.002892	0.709062	H	0.163054	-0.7614	2.372063
C	-3.74078	-1.26829	-1.34807	H	-2.3209	-1.38109	2.110014
C	-5.06825	-1.1184	-1.75742	H	-1.88359	-3.31869	0.614848
C	-6.07627	-1.84898	-1.13853	H	-2.95611	-0.70225	-1.83487
C	-5.76468	-2.7482	-0.10501	H	-5.31798	-0.42711	-2.56041
C	-4.44021	-2.90053	0.29145	H	-4.22176	-3.611	1.084225
O	3.330663	-2.43479	-2.63111	H	2.828595	-2.58976	-3.44608
O	2.588754	-1.48668	1.996453	H	-7.58904	-3.23507	0.077004
C	-2.05606	1.010649	1.539143	H	-7.53952	-1.13983	-2.18217
O	-2.33584	0.843914	2.711592	H	-2.75857	3.288566	2.655496
O	-6.7468	-3.47654	0.499078	H	-1.38647	1.630739	-1.0787
O	-7.41347	-1.77787	-1.46412	H	-1.47524	4.850459	-2.59352
C	-2.07686	2.328742	0.85395	H	-2.46067	6.73078	-0.28354
C	-2.48058	3.435714	1.616214	H	4.98374	-2.66023	-0.76729
C	-2.51406	4.690595	1.0247	H	5.811575	-2.24754	1.644161
C	-2.14907	4.850097	-0.31619	H	4.541505	-3.46582	1.430176
C	-1.74505	3.74396	-1.07321	H	-3.11484	5.661732	2.580265
C	-1.7076	2.479689	-0.48858	H	6.945995	-1.44123	-1.1966
O	-1.38879	3.905666	-2.37908	H	8.062576	0.734092	-1.62593
O	-2.16824	6.070959	-0.93548	H	4.605903	2.788698	-0.11698
C	4.506178	-1.93155	-0.10416	H	3.493321	0.634631	0.297868
C	4.77063	-2.39331	1.349344	H	6.513425	3.807273	-0.88989
C	3.904532	-1.68053	2.363117				
Conformation 4							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.43409	-2.25615	-1.59548	O	-2.77531	5.881103	1.675035
C	2.994616	-2.00385	-0.33241	O	4.232547	-1.33319	3.46113
C	2.109291	-1.81117	0.727097	C	5.127342	-0.59402	-0.40237
C	0.714521	-1.86099	0.601773	C	4.496705	0.622135	-0.10237
C	0.208667	-2.12834	-0.67599	C	5.120778	1.842189	-0.34512
C	1.055686	-2.32437	-1.77247	C	6.4027	1.869951	-0.90294
C	-0.20861	-1.60172	1.76977	C	7.047004	0.669217	-1.2142
C	-1.62881	-1.31257	1.282453	C	6.40791	-0.5446	-0.96361
C	-2.02305	-2.30737	0.181132	O	6.969621	3.095387	-1.1266
O	-1.13094	-2.19983	-0.93984	H	0.615968	-2.532	-2.74403
C	-3.43991	-2.14693	-0.32183	H	-0.23807	-2.46771	2.446089
O	-1.69567	0.008678	0.707322	H	0.148027	-0.76334	2.37508

C	-3.75474	-1.25551	-1.34988	H	-2.33814	-1.37003	2.110323
C	-5.08123	-1.09959	-1.76011	H	-1.90879	-3.31131	0.617771
C	-6.09325	-1.82368	-1.14014	H	-2.96696	-0.69452	-1.83748
C	-5.78674	-2.72249	-0.10479	H	-5.32702	-0.40851	-2.56447
C	-4.46325	-2.88084	0.292568	H	-4.24879	-3.59067	1.087011
O	3.311731	-2.44756	-2.62705	H	2.80853	-2.59831	-3.44211
O	2.570397	-1.49764	2.000935	H	-7.61384	-3.19847	0.078217
C	-2.03603	1.023032	1.542656	H	-7.55283	-1.10562	-2.18277
O	-2.29604	0.860618	2.720329	H	-2.66939	3.314783	2.67278
O	-6.77295	-3.44459	0.500295	H	-1.41872	1.628126	-1.09124
O	-7.42996	-1.74633	-1.46654	H	-1.47304	4.848334	-2.60508
C	-2.05009	2.340304	0.856449	H	-2.36295	6.749778	-0.27372
C	-2.41412	3.455441	1.626788	H	4.962498	-2.68128	-0.76067
C	-2.43748	4.710241	1.034665	H	5.791338	-2.26502	1.650412
C	-2.10286	4.861547	-0.31507	H	4.519735	-3.48143	1.435962
C	-1.73871	3.7472	-1.08029	H	-2.96481	5.696131	2.607275
C	-1.71095	2.483114	-0.4949	H	3.495412	0.62307	0.318709
O	-1.41172	3.900678	-2.39463	H	4.627758	2.780712	-0.11227
O	-2.11347	6.081885	-0.9352	H	8.041353	0.681761	-1.65787
C	4.488074	-1.94884	-0.09935	H	6.918746	-1.47115	-1.21733
C	4.750372	-2.40925	1.354883	H	7.852221	2.967614	-1.50748
C	3.884719	-1.6962	2.368955				
Conformation 5							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.749456	-2.65766	-1.64405	O	1.867054	3.227174	-1.03093
C	2.365366	-2.51872	-0.39017	O	3.767977	-2.19519	3.401653
C	1.531058	-2.37169	0.716981	C	4.418286	-1.04298	-0.46636
C	0.134193	-2.32113	0.638985	C	5.460522	-0.84172	-1.38128
C	-0.42993	-2.42866	-0.6394	C	5.990036	0.423043	-1.62597
C	0.365054	-2.62221	-1.77512	C	5.478861	1.53114	-0.94494
C	-0.74652	-2.02527	1.830391	C	4.436223	1.355876	-0.02585
C	-1.98643	-1.27508	1.341319	C	3.913876	0.081174	0.202232
C	-2.67065	-2.082	0.225586	O	6.029547	2.752012	-1.21468
O	-1.7687	-2.32016	-0.87437	H	-0.11812	-2.70919	-2.74432
C	-3.92454	-1.44501	-0.32796	H	-1.05842	-2.94378	2.346904
O	-1.53211	-0.01901	0.803572	H	-0.20992	-1.42048	2.566019
C	-3.86355	-0.43373	-1.29048	H	-2.70105	-1.08305	2.144132
C	-5.03814	0.166269	-1.75056	H	-2.9311	-3.0551	0.666184
C	-6.27048	-0.23619	-1.24772	H	-2.90455	-0.12123	-1.68617
C	-6.34199	-1.25325	-0.28114	H	-4.99336	0.951662	-2.50294
C	-5.16977	-1.85294	0.166948	H	-5.2499	-2.6439	0.907667
O	2.580397	-2.81432	-2.72022	H	2.041712	-2.89691	-3.52235
O	2.056166	-2.18683	1.992935	H	-8.23291	-1.11828	-0.21889
C	-1.9386	1.13862	1.396991	H	-7.3447	1.014902	-2.25496
O	-2.80104	1.192822	2.248617	H	0.344109	1.133048	-0.12657
O	-7.54765	-1.66104	0.207408	H	-2.5376	3.708768	1.790477
O	-7.48583	0.284766	-1.63399	H	-0.76991	6.592882	0.643044
C	-1.179	2.304275	0.872757	H	1.665717	5.378127	-0.92451

C	-0.00867	2.129867	0.114306	H	4.329971	-3.10623	-0.968
C	0.695123	3.251925	-0.30678	H	5.266449	-2.8594	1.429667
C	0.226349	4.535127	-0.00656	H	4.028441	-4.09742	1.168881
C	-0.9448	4.703977	0.742764	H	2.218638	2.322079	-1.07449
C	-1.64157	3.585928	1.193522	H	5.864222	-1.69427	-1.92229
O	-1.39208	5.956972	1.036041	H	6.795272	0.568486	-2.33911
O	0.88821	5.662688	-0.41428	H	4.046686	2.210426	0.524903
C	3.867411	-2.44985	-0.2249	H	3.10437	-0.02355	0.919009
C	4.217064	-3.01421	1.170336	H	5.596215	3.423208	-0.66457
C	3.381465	-2.42993	2.28748				
Conformation 6							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.965289	-1.95337	-1.53167	O	-3.89623	5.138801	1.622545
C	3.53066	-1.51669	-0.32241	O	4.815355	-0.42415	3.358682
C	2.67932	-1.416	0.776782	C	5.35309	0.253736	-0.59461
C	1.311488	-1.72003	0.737901	C	4.560593	1.356846	-0.24264
C	0.803992	-2.16323	-0.48659	C	4.927821	2.653465	-0.58857
C	1.615938	-2.28204	-1.61959	C	6.107724	2.875286	-1.30616
C	0.414555	-1.5552	1.940381	C	6.908644	1.78987	-1.67162
C	-1.06028	-1.53893	1.535088	C	6.526964	0.496466	-1.31525
C	-1.35038	-2.63538	0.488964	O	6.420063	4.168554	-1.62566
O	-0.51248	-2.49249	-0.66611	H	1.174768	-2.63259	-2.54852
C	-2.78806	-2.62833	0.009299	H	0.568742	-2.37563	2.656051
O	-1.44691	-0.29291	0.929809	H	0.644071	-0.63686	2.485717
C	-3.77603	-3.31451	0.717461	H	-1.68698	-1.70455	2.416483
C	-5.12125	-3.20234	0.350186	H	-1.1223	-3.59901	0.969615
C	-5.48283	-2.38327	-0.71399	H	-3.50863	-3.93832	1.566446
C	-4.49225	-1.69769	-1.43401	H	-5.88768	-3.74245	0.902144
C	-3.15611	-1.8466	-1.09373	H	-2.39733	-1.33483	-1.6731
O	3.810896	-2.05402	-2.60205	H	3.304198	-2.34708	-3.37509
O	3.139815	-0.94901	2.002134	H	-5.81423	-0.93294	-2.57781
C	-1.81478	0.725883	1.763673	H	-7.39388	-2.65862	-0.58952
O	-1.56274	0.729015	2.952278	H	-2.42345	3.213081	2.647316
O	-4.85282	-0.83879	-2.45182	H	-2.95463	0.528822	-0.67852
O	-6.77051	-2.17357	-1.15082	H	-4.58389	1.228285	-2.23386
C	-2.58865	1.767713	1.044239	H	-5.39142	4.196838	-1.60326
C	-2.8409	2.994887	1.671201	H	5.566039	-1.84561	-0.83727
C	-3.64791	3.934476	1.03276	H	6.425008	-1.14193	1.494957
C	-4.23073	3.632362	-0.20732	H	5.395435	-2.58249	1.417783
C	-3.99069	2.397729	-0.81771	H	-4.48384	5.640016	1.031554
C	-3.1491	1.479299	-0.20754	H	3.634062	1.207227	0.304277
O	-4.63513	2.179299	-2.01039	H	4.311288	3.5034	-0.31373
O	-5.04796	4.57369	-0.77448	H	7.823911	1.952514	-2.23867
C	4.998124	-1.17499	-0.18441	H	7.15705	-0.3394	-1.6118
C	5.415683	-1.49273	1.271339	H	7.259076	4.177975	-2.11182
C	4.48568	-0.89525	2.303155				