

Supplementary Information

New ethylated derivatives of sulfur and nitrogen-containing artifacts from *Tenodera sinensis* egg pod and their anti-renal fibrosis

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Analysis condition: Daicel Chiralpak IC column (250 mm × 4.6 mm, i.d., 5 μm), n-hexane/EtOH, 81:19, 0.05% TFA, flow rate: 1 mL/min.

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Detailed Isolation Procedures

The insect materials (30.0 kg), were pulverized and then extracted three times with 50% ethanol (200 L \times 48 h \times 1, 150 L \times 48 h \times 2) at room temperature. This process resulted in the production of the crude extract, weighing 2.1 kg. Afterwards, the extract was fractionated using a macro-porous resin (Rohm Haas AMBERLITETTM XADTM 16N, USA) column, and carefully eluted with EtOH/H₂O (0%–100%) to produce six fractions (Fr.A–Fr.F). Fr.D (57.1 g) was fractionated into seven parts (Fr.D.A–Fr.D.G) by using a MCI gel CHP 20P column (MeOH/H₂O, 10%–100%).

Fr.D.C. (400.0 mg) was gel filtered through Sephadex LH-20 (MeOH) to give three parts (Fr.D.C.1–Fr.D.C.3). The third part (98.2 mg) was fractionated into six parts (Fr.D.C.3.1–Fr.D.C.3.6) by using a semi-preparative HPLC (MeCN/H₂O, 11%, 0.05% HCOOH). Compound **6** (1.53 mg, t_R = 13.2 min; flow rate: 3 mL/min) was obtained from Fr.D.C.3.5 (4.2 mg) by using a semi-preparative HPLC (MeOH/H₂O, 34%, 0.05% HCOOH).

Fr.D.D (737.4 mg) was subjected to Sephadex LH-20 (MeOH) to give five parts (Fr.D.D.1–Fr.D.D.5). Fr.D.D.5 (83.4 mg) was cut by a semi-preparative HPLC (MeCN/H₂O, 18%, 0.05% HCOOH) to afford eight parts (Fr.D.D.5.1–Fr.D.D.5.8). Among them, Fr.D.D.5.7 is compound **7** (5.7 mg, t_R = 23.7 min; flow rate: 3 mL/min), and Fr.D.D.5.8 is **24** (5.7 mg, t_R = 24.6 min; flow rate: 3 mL/min). Fr.D.D.5.3 (8.1 mg) was purified by a semi-preparative HPLC (MeOH/H₂O, 14%, 0.05% HCOOH) to afford **19** (1.3 mg, t_R = 24.8 min; flow rate: 3 mL/min).

Fr.D.E (5.5 g) was passed through Sephadex LH-20 (MeOH) to provide five fractions (Fr.D.E.1–Fr.D.E.5). Fr.D.E.2 (1.2 g) was cut by an ODS column (MeOH/H₂O, 15%–100%) to give eight parts (Fr.D.E.2.1–Fr.D.E.2.8). Fr.D.E.2.2 (103.8 mg) was segregated by using preparative HPLC (MeCN/H₂O, 5%–100%, 0.05% HCOOH) to afford six parts (Fr.D.E.2.2.1–Fr.D.E.2.2.6). Fr.D.E.2.2.6 (5.9 mg) was purified by semi-preparative HPLC (MeCN/H₂O, 19%) to afford **22** (1.8 mg, t_R = 20.2 min; flow rate: 3 mL/min). Fr.D.E.3 (2.1 g) was cut by an ODS column (MeOH/H₂O, 30%–100%) to give five parts (Fr.D.E.3.1–Fr.D.E.3.5). **16** (2.4 mg, t_R = 19.9 min; flow rate: 3 mL/min) was purified from Fr.D.E.3.2 (51.7 mg) by semi-preparative HPLC (MeCN/H₂O, 15%, 0.05% HCOOH). Fr.D.E.3.3 (696.4 mg) was filtered through Sephadex LH-20 (MeOH) to produce four parts

(Fr.D.E.3.3.1–Fr.D.E.3.3.4). Of which, Fr.D.E.3.3.2 (497.3 mg) was cut into eight parts (Fr.D.E.3.3.2.1–Fr.D.E.3.3.2.8) by preparative HPLC (MeOH/H₂O, 10%–100%, 0.05% HCOOH). **5** (7.6 mg, t_R = 7.3 min; flow rate: 3 mL/min) was purified from Fr.D.E.3.3.2.2 (102 mg) by semi-preparative HPLC (MeCN/H₂O, 27%, 0.05% HCOOH). **21** (2.5 mg, t_R = 22.7 min; flow rate: 3 mL/min) and **13** (2.2 mg, t_R = 24.8 min; flow rate: 3 mL/min) was purified from Fr.D.E.3.3.2.3 (69.6 mg) by semi-preparative HPLC (MeCN/H₂O, 17%, 0.05% HCOOH). **15** (6.7 mg, t_R = 24.5 min; flow rate: 3 mL/min) was purified from Fr.D.E.3.3.2.4 (111.2 mg) by semi-preparative HPLC (MeCN/H₂O, 19%, 0.05% HCOOH). And **20** (3.8 mg, t_R = 31.4 min; flow rate: 3 mL/min) was purified from Fr.D.E.3.3.2.8 (6.0 mg) by semi-preparative HPLC (MeCN/H₂O, 17%, 0.05% HCOOH). Fr.D.E.4 (361.4 mg) was passed through preparative HPLC (MeCN/H₂O, 10%–100%, 0.05% HCOOH) to provide six fractions (Fr.D.E.4.1–Fr.D.E.4.6). Of which, Fr.D.E.4.3 (24.4 mg) was subjected to semi-preparative HPLC (MeCN/H₂O, 21%, 0.05% HCOOH) to afford **18** (6.5 mg, t_R = 20.9 min). Fr.D.E.4.4 (48.4 mg) was purified by semi-preparative HPLC (MeCN/H₂O, 19%, 0.05% HCOOH) to obtain **8** (3.6 mg, t_R = 19.5 min; flow rate: 3 mL/min) and **1** (3.5 mg, t_R = 36.1 min). Fr.D.E.4.5 (56.3 mg) was subjected to semi-preparative HPLC (MeCN/H₂O, 23%, 0.05% HCOOH) to provide three fractions (Fr.D.E.4.5.1–Fr.D.E.4.5.3). Among them, Fr.D.E.4.5.2 is **23** (19.9 mg, t_R = 14.0 min; flow rate: 3 mL/min). Compound **9** (3.8 mg, t_R = 23.9 min; flow rate: 3 mL/min) was purified from Fr.D.E.4.6 (29.1 mg) by semi-preparative HPLC (MeCN/H₂O, 20%, 0.05% HCOOH).

Fr.D.F (8.6 g) was sub-fractionated into five parts (Fr.D.F.1–Fr.D.F.5) through Sephadex LH-20 (MeOH). Among them, Fr.D.F.2 (3.1 g) was subjected to an ODS column (MeOH/H₂O, 20%–100%) to give five parts (Fr.D.F.2.1–Fr.D.F.2.5). Fr.D.F.2.5 (668.2 mg) was passed through preparative HPLC (MeCN/H₂O, 5%–100%, 0.05% HCOOH) to provide six fractions (Fr.D.F.2.5.1–Fr.D.F.2.5.6). **Compound 3** (2.0 mg, t_R = 19 min; flow rate: 3 mL/min) was purified from Fr.D.F.2.5.1 (85.4 mg) by semi-preparative HPLC (MeCN/H₂O, 18%, 0.05% HCOOH). Fr.D.F.3 (1.2 g) was subjected to a silica gel column eluting with CH₂Cl₂/Me₂CO (20:1–0:1) to afford nine portions (Fr.D.F.3.1–Fr.D.F.3.9). Fr.D.F.3.5 (121.4 mg) was passed through Sephadex LH-20 (MeOH) to obtain five portions (Fr.D.F.3.5.1–Fr.D.F.3.5.5). **4** (1.7 mg, t_R = 15.2 min; flow rate: 3 mL/min) was purified from Fr.D.F.3.5.3 (31.0 mg) by semi-preparative HPLC (MeCN/H₂O, 25%, 0.05% HCOOH). Fr.D.F.3.5.4 (31.0 mg)

was subjected to semi-preparative HPLC (MeCN/H₂O, 26%, 0.05% HCOOH) to afford **17** (2.3 mg, t_R = 15.2 min; flow rate: 3 mL/min) and **14** (3.9 mg, t_R = 19.4 min). Fr.D.F.3.6 (87.5 mg) was filtered through Sephadex LH-20 (MeOH) to afford three parts (Fr.D.F.3.6.1–Fr.D.F.3.6.3). Fr.D.F.3.6.2 (15.8 mg) was submitted to semi-preparative HPLC (MeCN/H₂O, 23%, 0.05% HCOOH) to obtain **2** (2.4 mg, t_R = 18.6 min). Compound **10** (8.1 mg, t_R = 12.7 min; flow rate: 3 mL/min) was purified from Fr.D.F.5 (102.1 mg) by semi-preparative HPLC (MeOH/H₂O, 51%, 0.05% HCOOH).

Fr.D.G (6.4 g) was cut to give three parts (Fr.D.G.1–Fr.D.G.3) through Sephadex LH-20 (MeOH). Fr.D.G.2 (1.9 g) was submitted to a silica gel column eluting with CH₂Cl₂/MeOH (40:1–0:1) to afford four portions (Fr.D.G.2.1–Fr.D.G.2.4). Fr.D.G.2.4 (572.3 mg) was divided into four parts (Fr.D.G.2.4.1–Fr.D.G.2.4.4) through Sephadex LH-20 (MeOH). Fr.D.G.2.4.4 (196.2 mg) was purified by a semi-preparative HPLC (MeCN/H₂O, 25%, 0.05% HCOOH) to afford compound **11** (21.6 mg, t_R = 39.6 min; flow rate: 3 mL/min). Fr.D.G.3 (750.0 mg) was cut by preparative HPLC (MeOH/H₂O, 20%–100%, 0.05% HCOOH) to give thirteen parts (Fr.D.E.3.1–Fr.D.E.3.13). **12** (2.1 mg, t_R = 19.5 min; flow rate: 3 mL/min) was purified from Fr.D.G.3.12 (20.2 mg) by semi-preparative HPLC (MeCN/H₂O, 29%, 0.05% HCOOH).

Afterwards, compounds **1**, **2**, and **3** are racemates, and were subjected to chiral HPLC (flow rate: 1 mL/min). These separations afforded (–)-**1** (1.7 mg, t_R = 9.7 min) and (+)-**1** (1.3 mg, t_R = 14.3 min) (n-hexane/ethanol containing 0.05% TFA in ethanol, 81:19) (Figure S12); (+)-**2** (1.4 mg, t_R = 36.5 min) and (–)-**2** (1.1 mg, t_R = 41.2 min) (n-hexane/ethanol containing 0.05% TFA in ethanol, 93:7) (Figure S24); (–)-**3** (0.8 mg, t_R = 10.4 min) and (+)-**3** (1.3 mg, t_R = 18.5 min) (n-hexane/ethanol containing 0.05% TFA in ethanol, 81:19) (Figure S33).

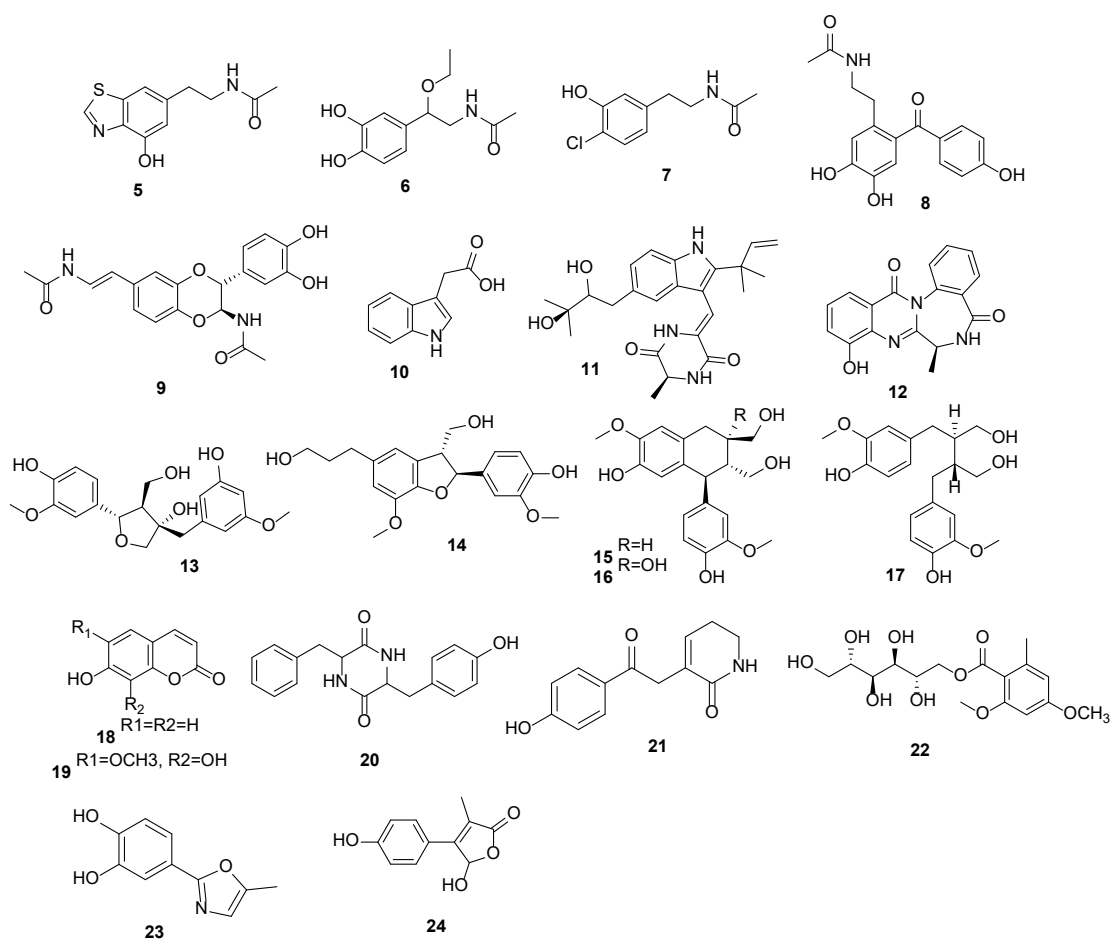


Figure S1. Structures of compounds 5–24.

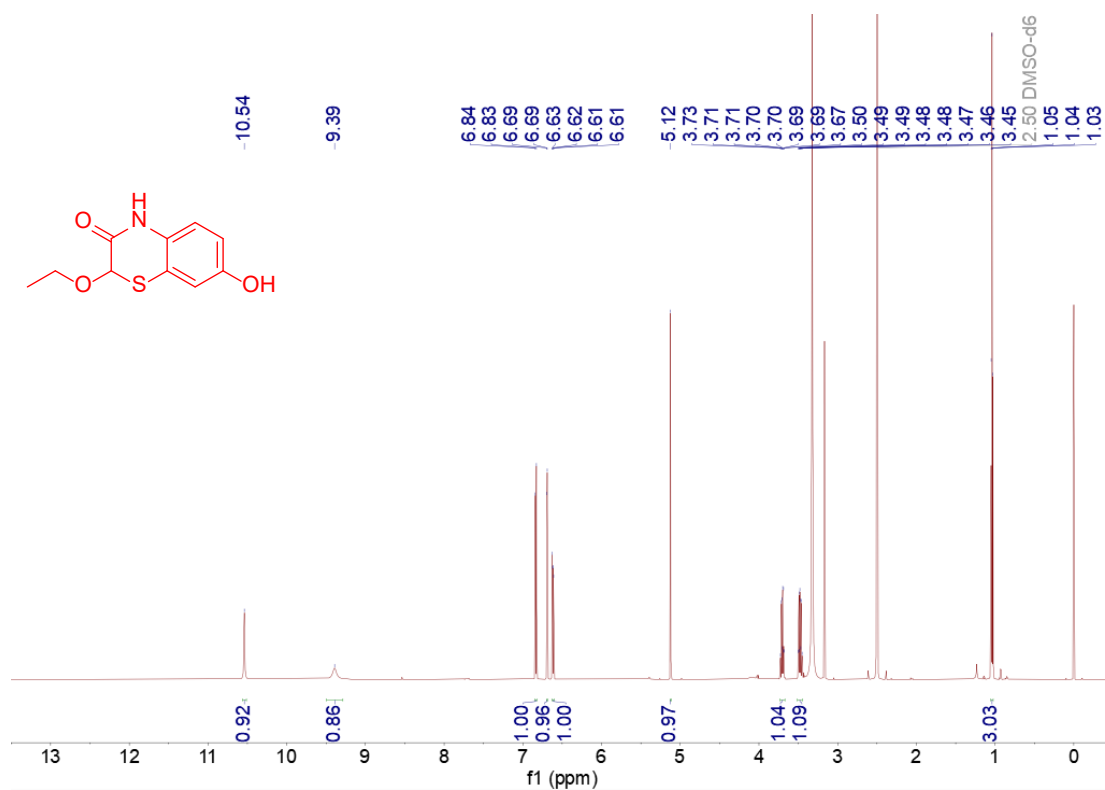


Figure S2. ¹H NMR (500 MHz) spectrum of **1** in DMSO-*d*₆.

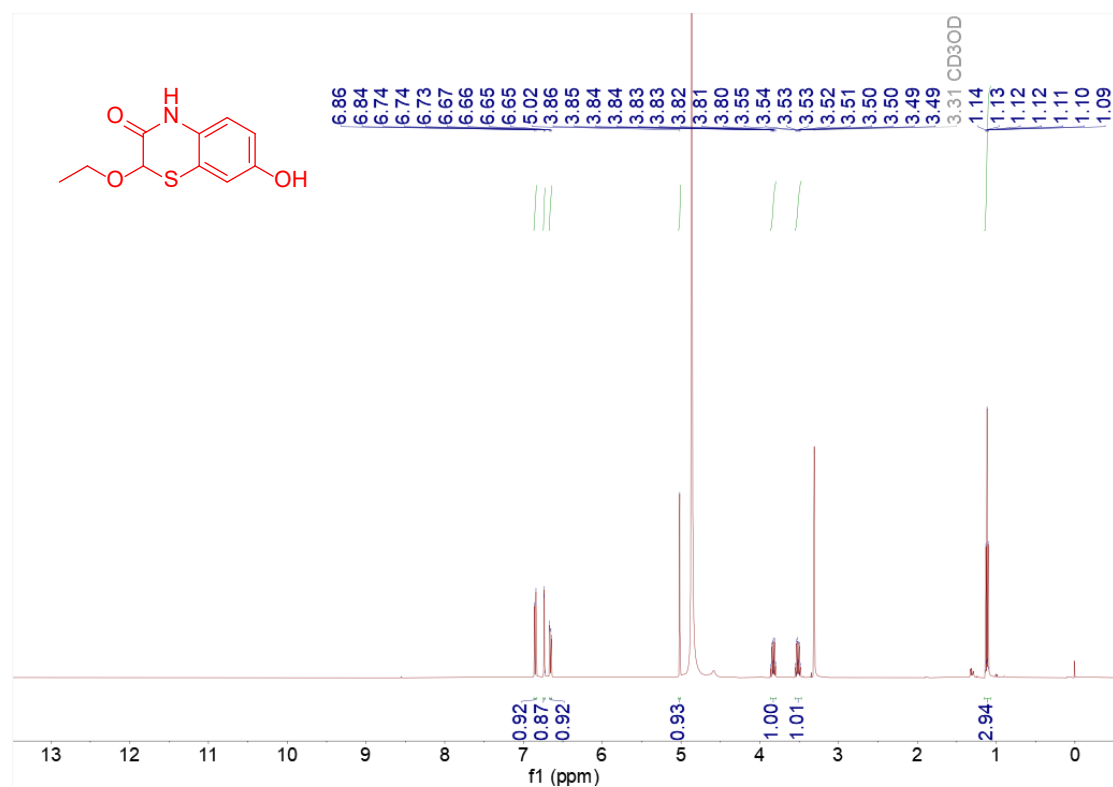


Figure S3. ¹H NMR (500 MHz) spectrum of **1** in methanol-*d*₄.

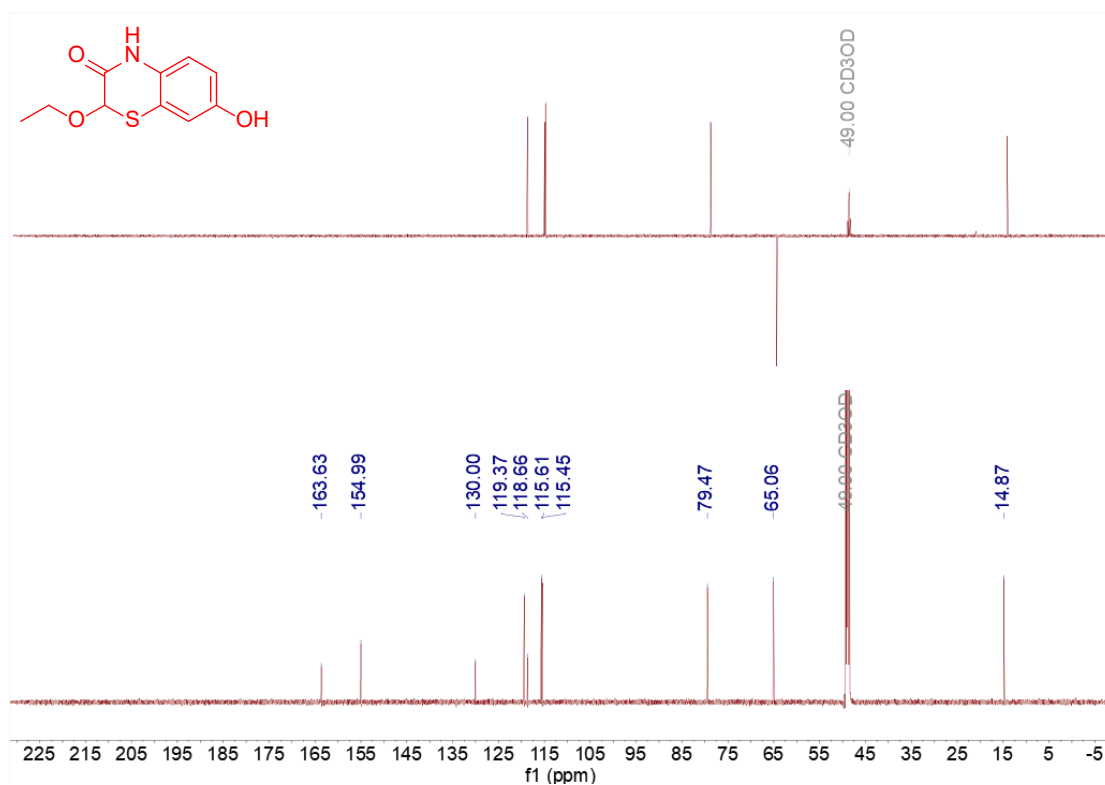


Figure S4. ¹³C NMR and DEPT-135 (150 MHz) spectra of **1** in methanol-*d*₄.

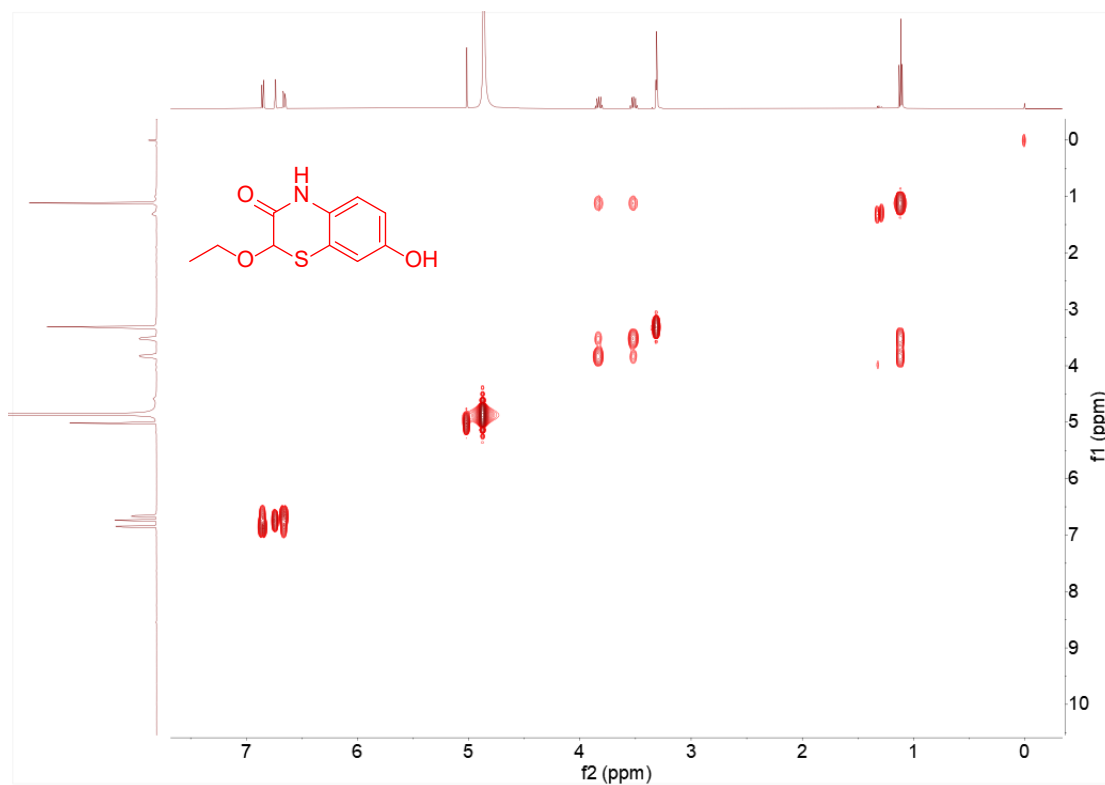


Figure S5. ¹H-¹H COSY (600 MHz) spectrum of **1** in methanol-*d*₄.

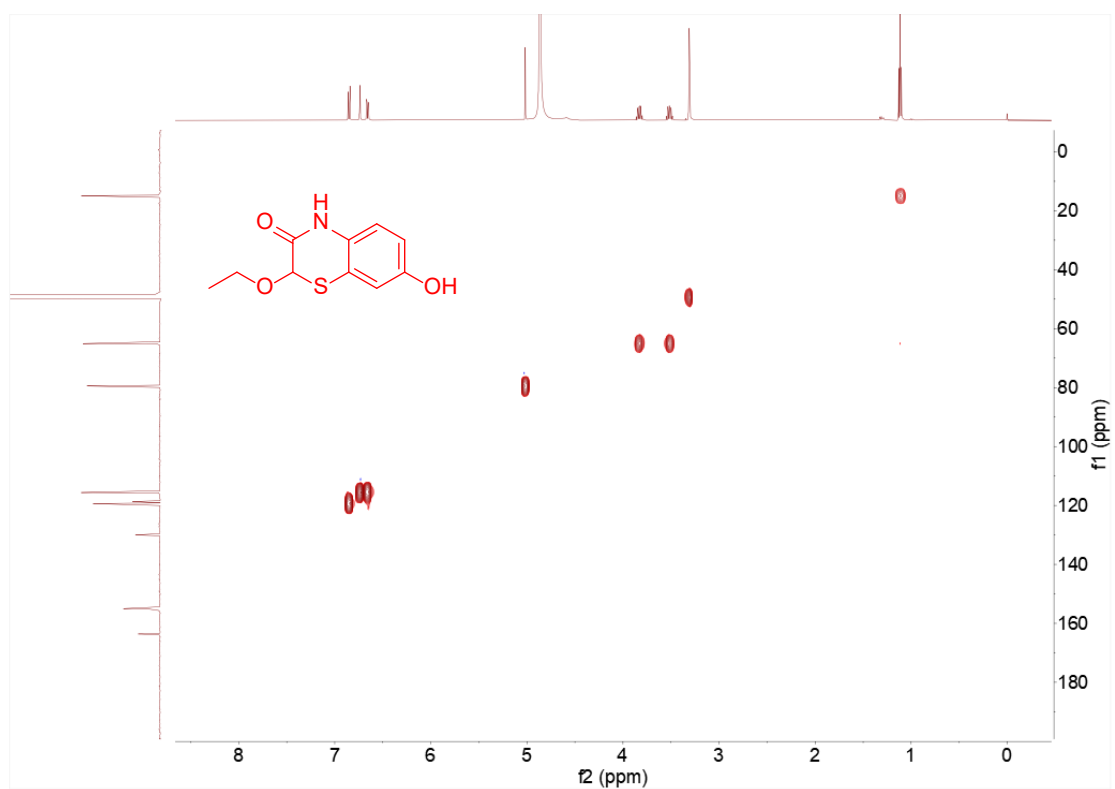


Figure S6. HSQC (600 MHz) spectrum of **1** in methanol- d_4 .

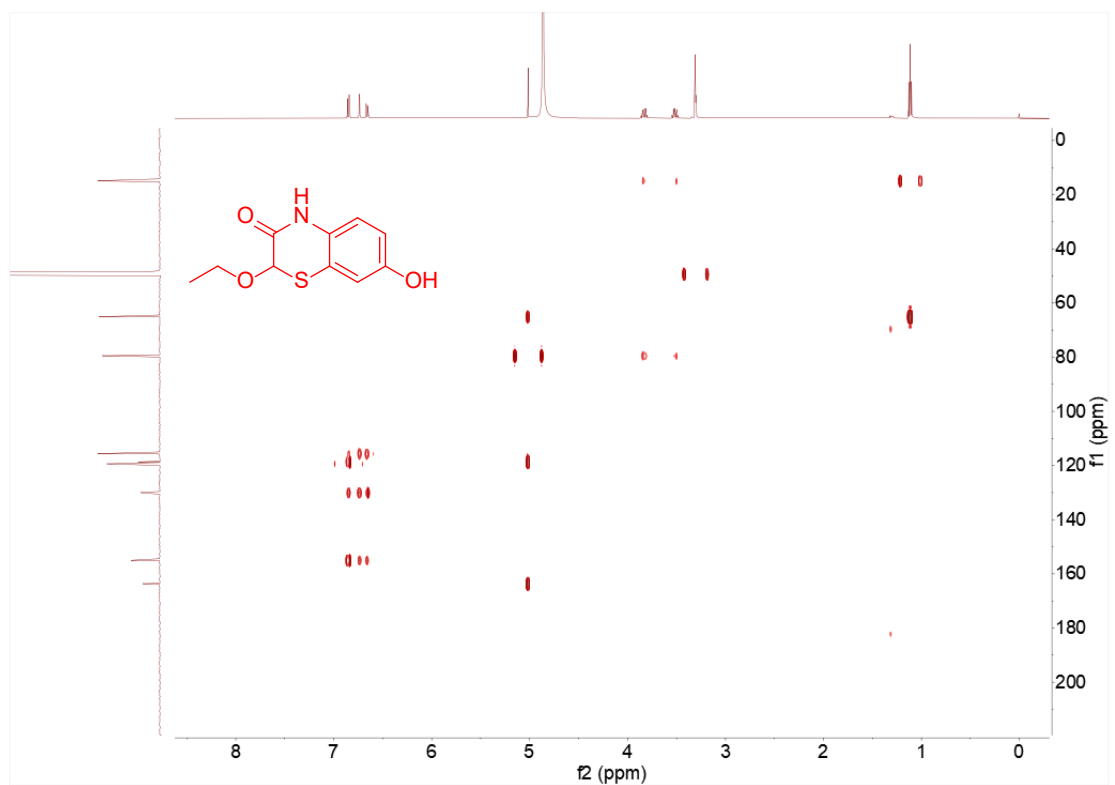


Figure S7. HMBC (600 MHz) spectrum of **1** in methanol- d_4 .

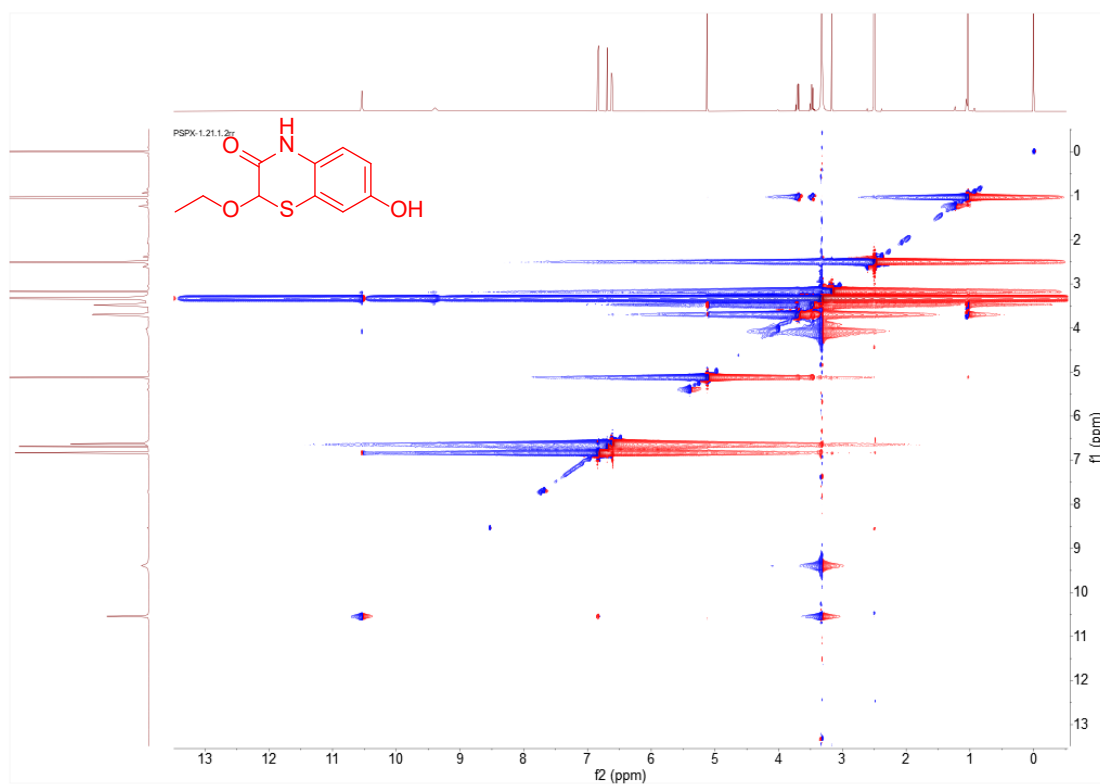


Figure S8. ROESY (600 MHz) spectrum of **1** in DMSO- d_6 .

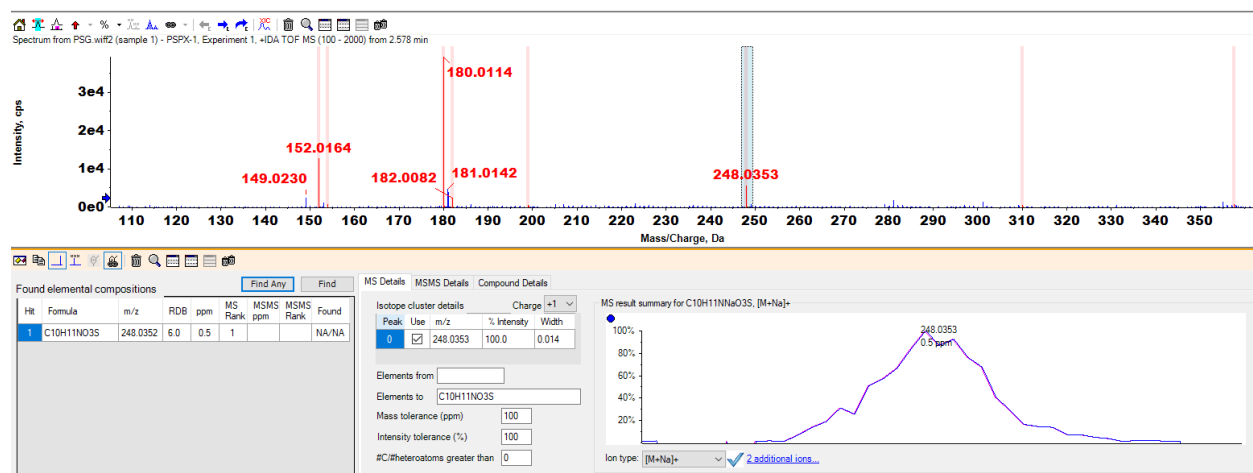


Figure S9. HRESIMS of **1**.

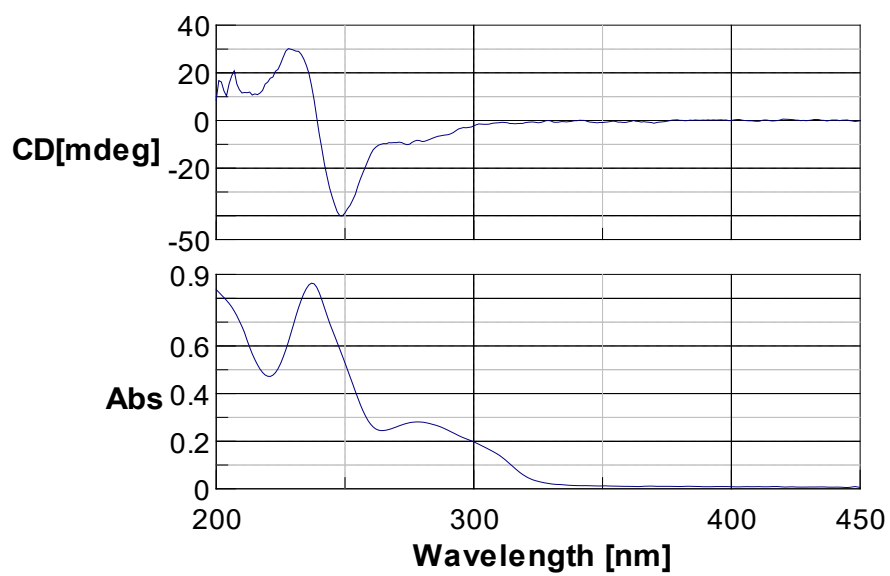


Figure S10. CD and UV spectra of (-)-1.

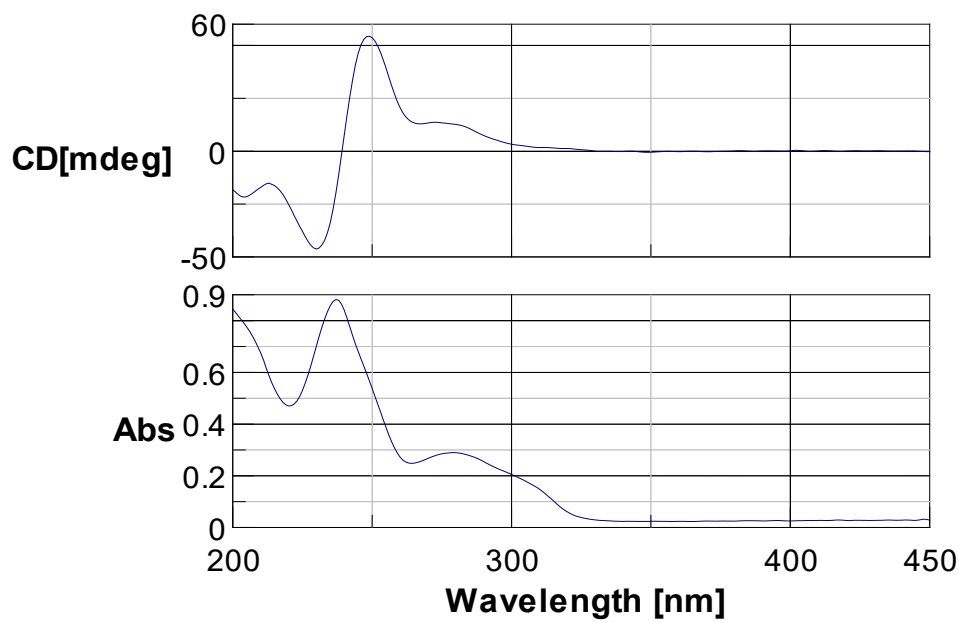


Figure S11. CD and UV spectra of (+)-1.

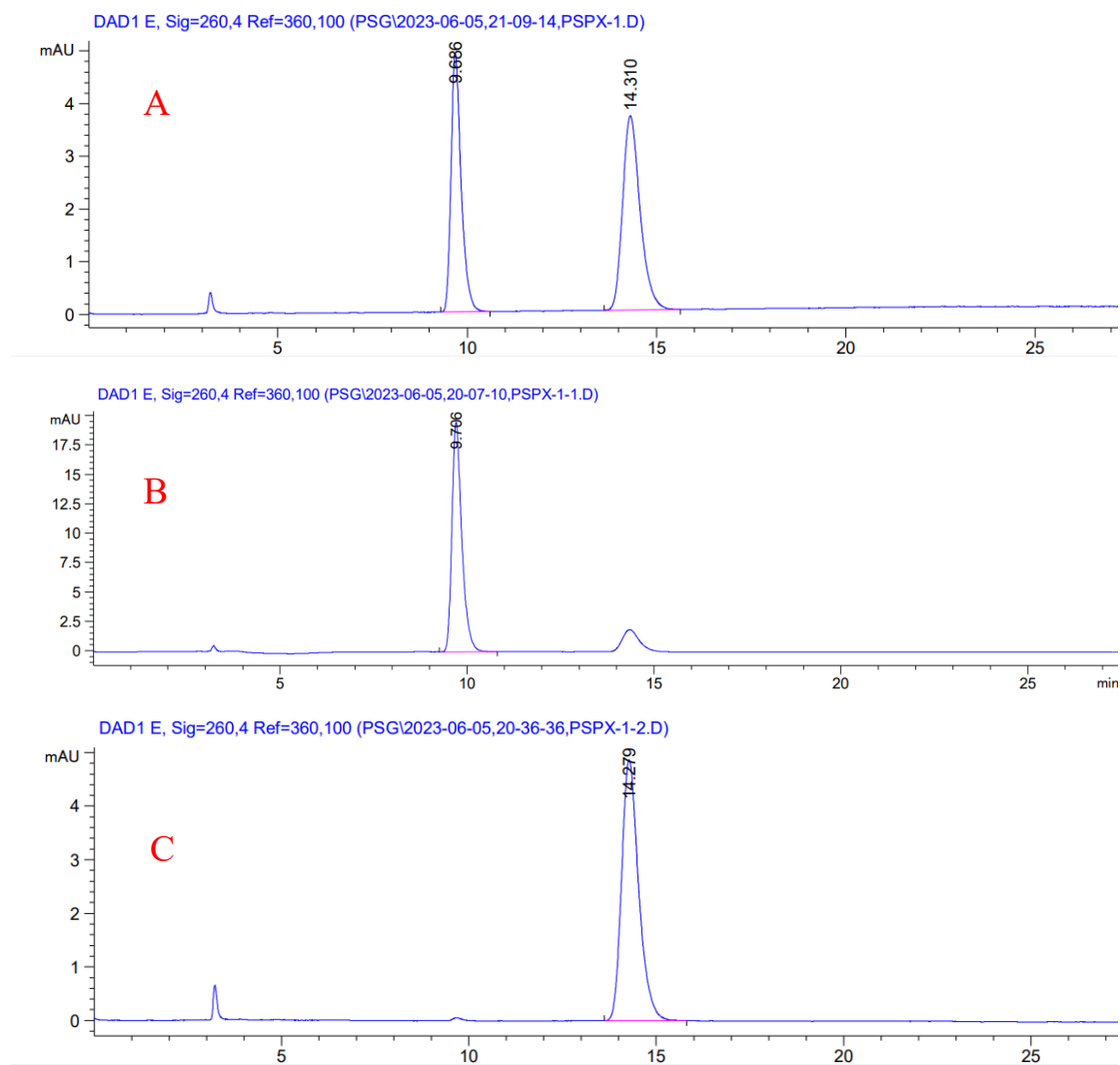


Figure S12. (A) Chiral HPLC chromatogram of **1**;

(B) Chiral HPLC chromatogram of (–)-**1**;

(C) Chiral HPLC chromatogram of (+)-**1**.

Analysis condition: Daicel Chiralpak IC column (250 mm × 4.6 mm, i.d., 5 μm), n-hexane/EtOH, 81:19, 0.05% TFA, flow rate: 1 mL/min.

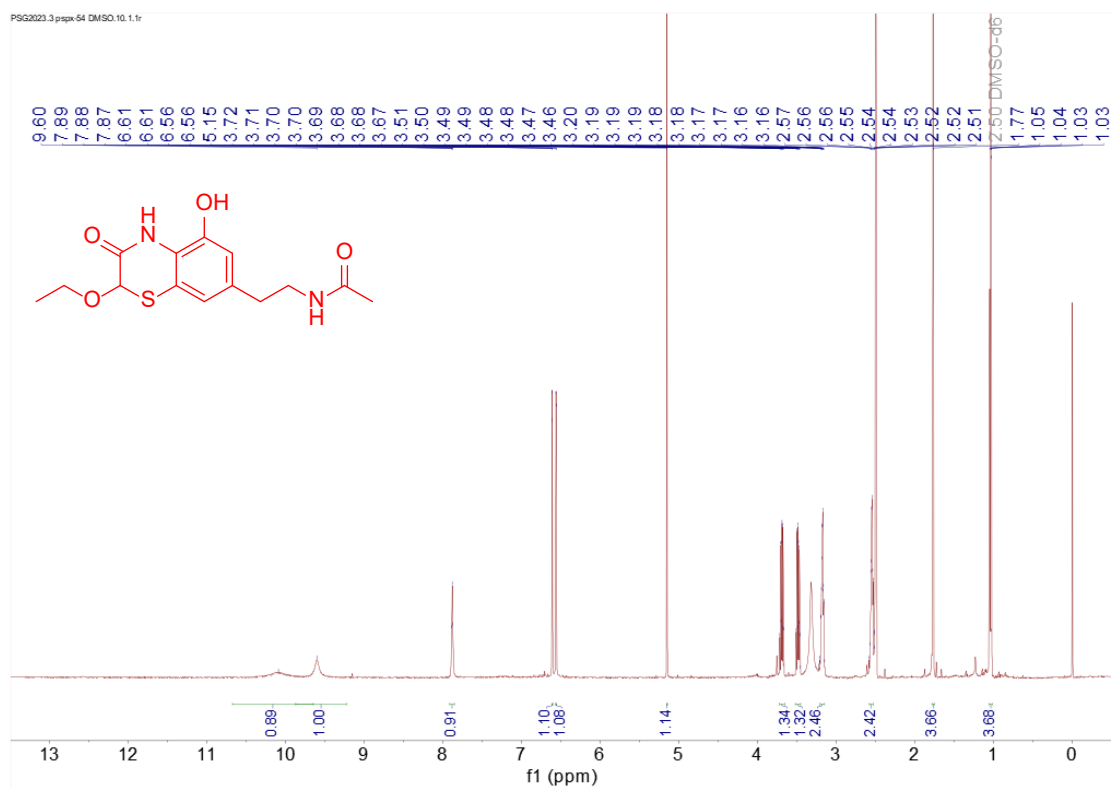


Figure S13. ¹H NMR (500 MHz) spectrum of **2** in DMSO-*d*₆.

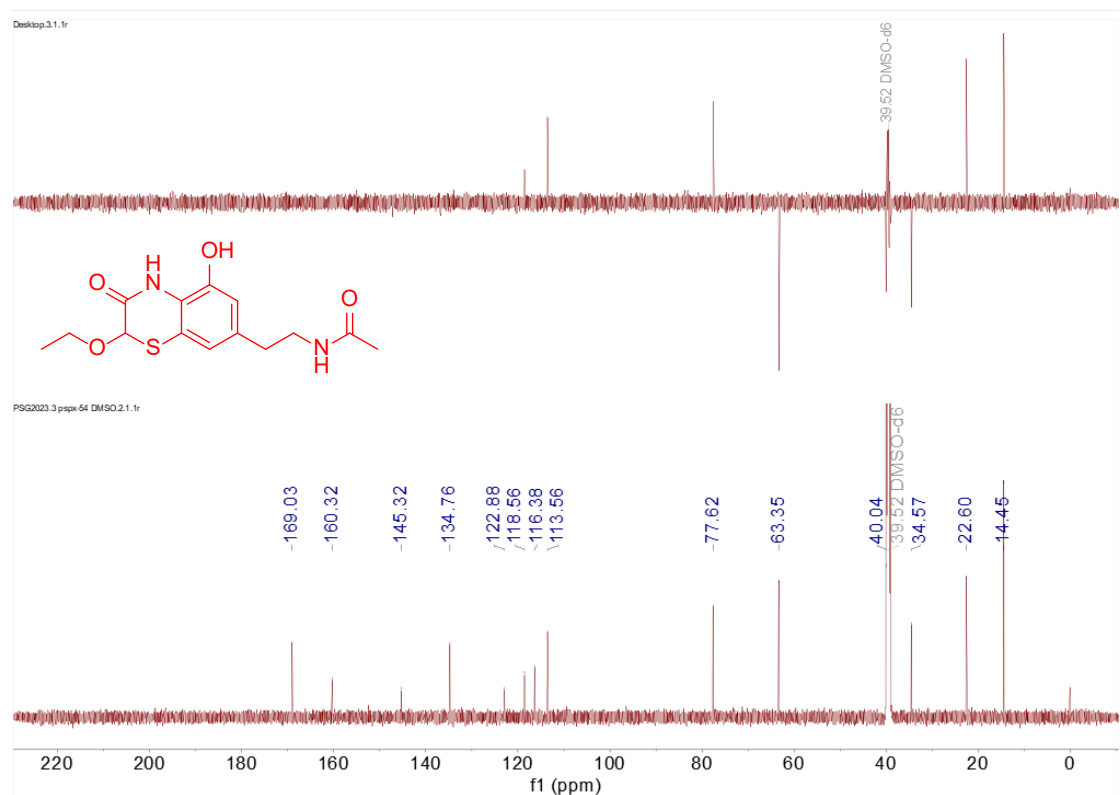


Figure S14. ¹³C NMR and DEPT-135 (150 MHz) spectra of **2** in DMSO-*d*₆.

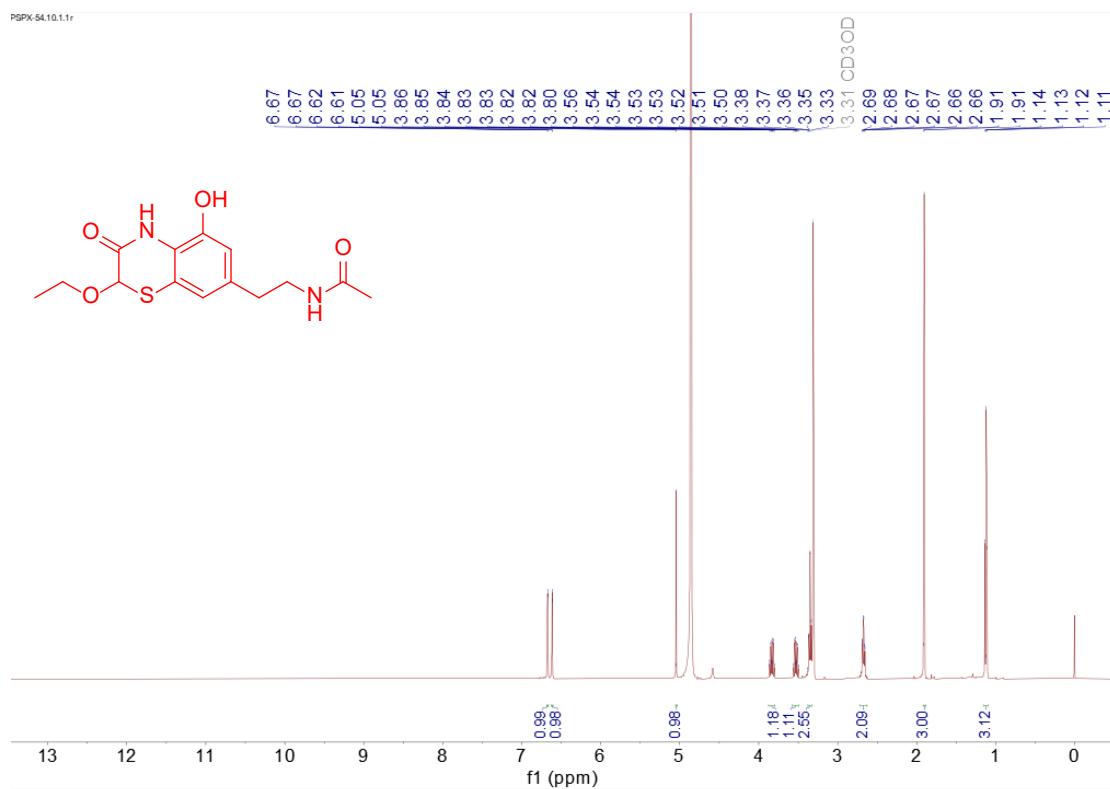


Figure S15. ¹H NMR (500 MHz) spectrum of **2** in methanol-*d*₄.

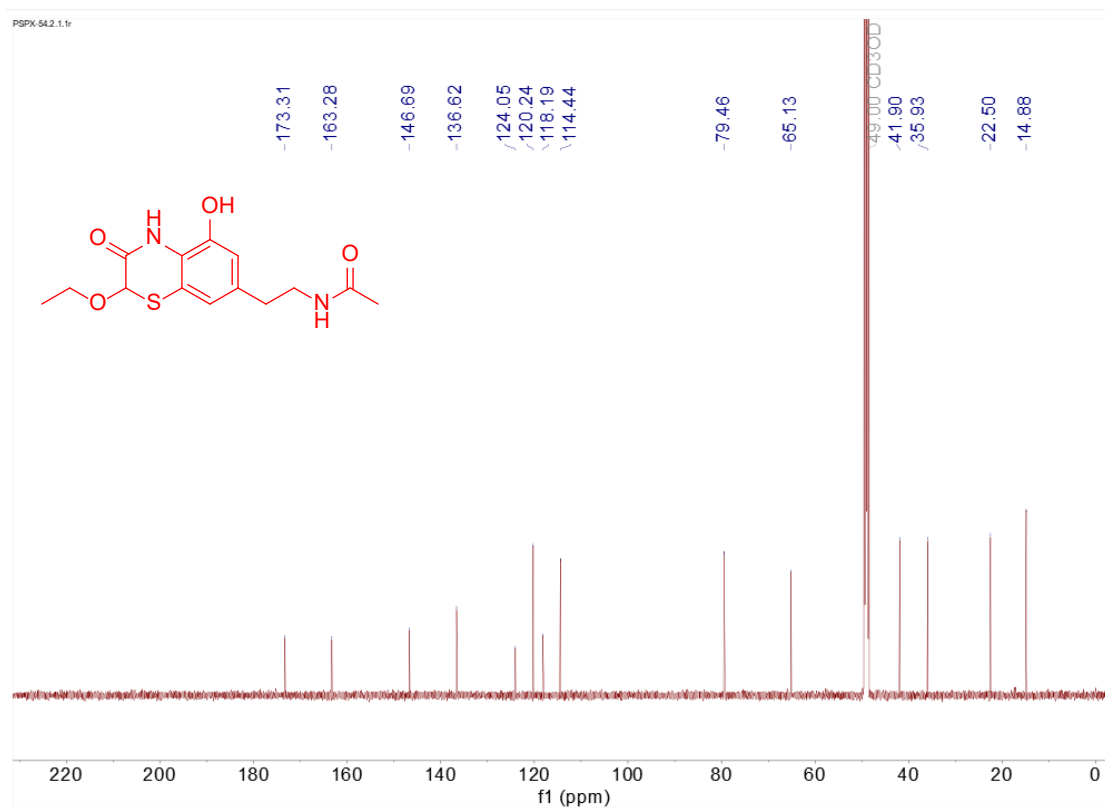


Figure S16. ¹³C NMR (150 MHz) spectrum of **2** in methanol-*d*₄.

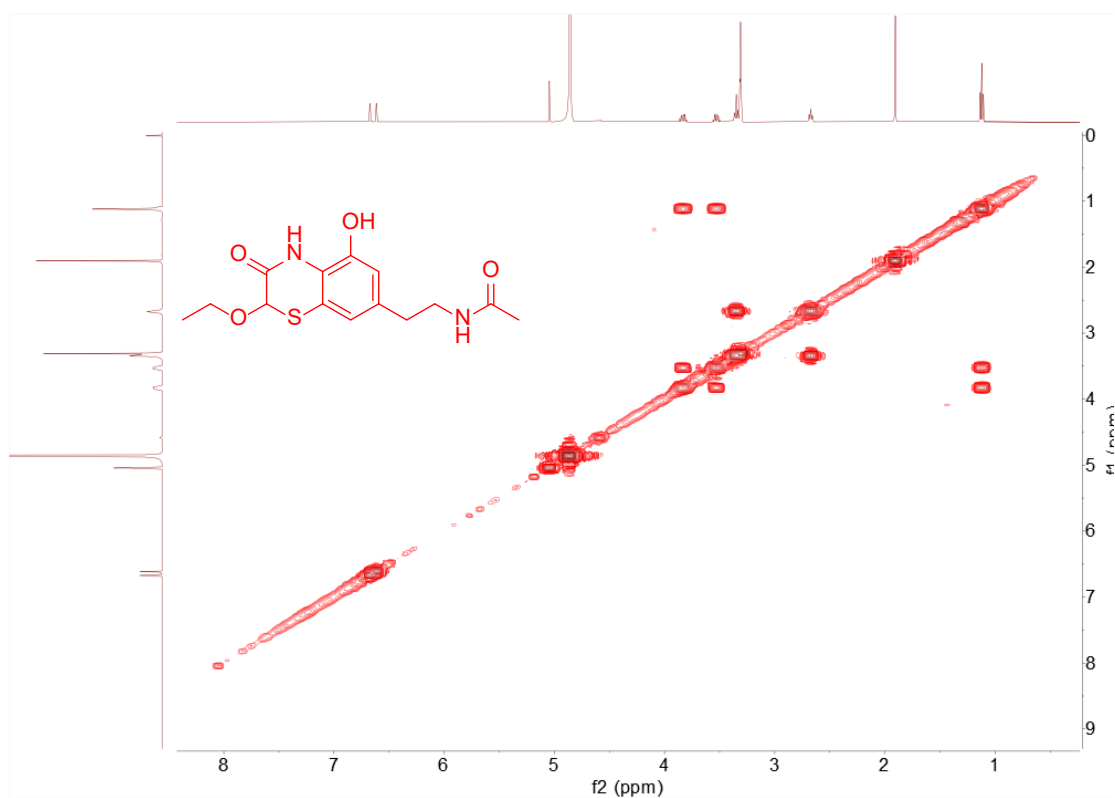


Figure S17. ^1H - ^1H COSY (600 MHz) spectrum of **2** in methanol- d_4 .

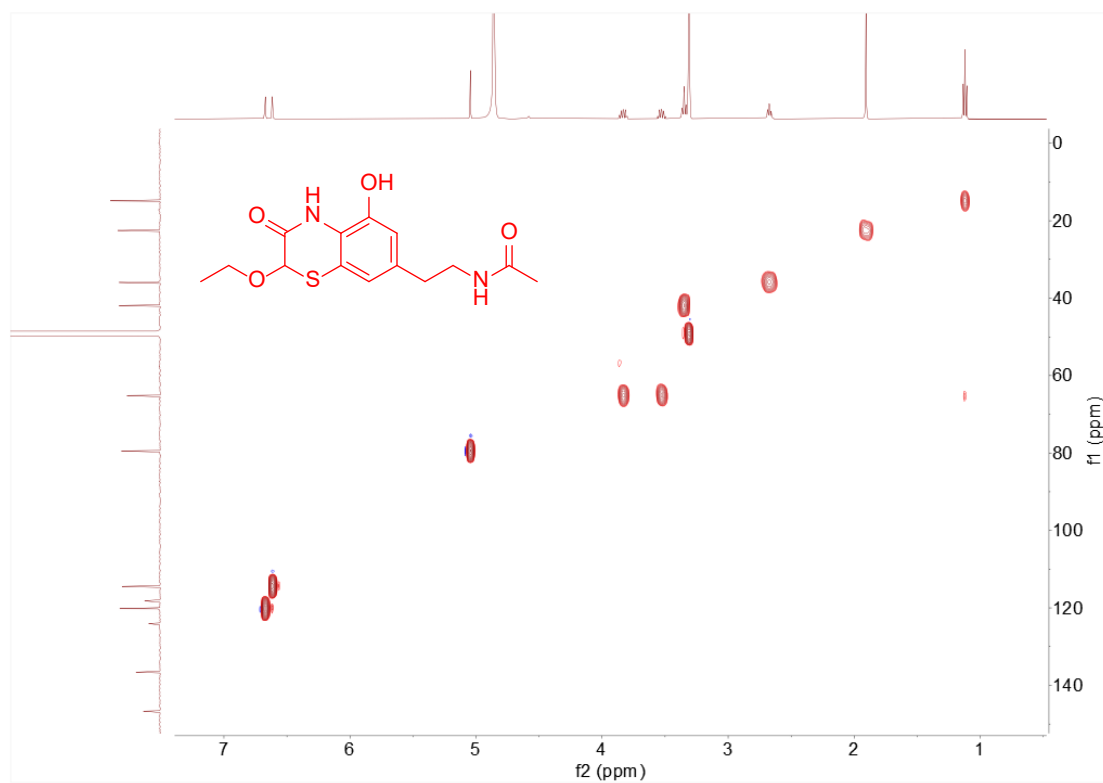
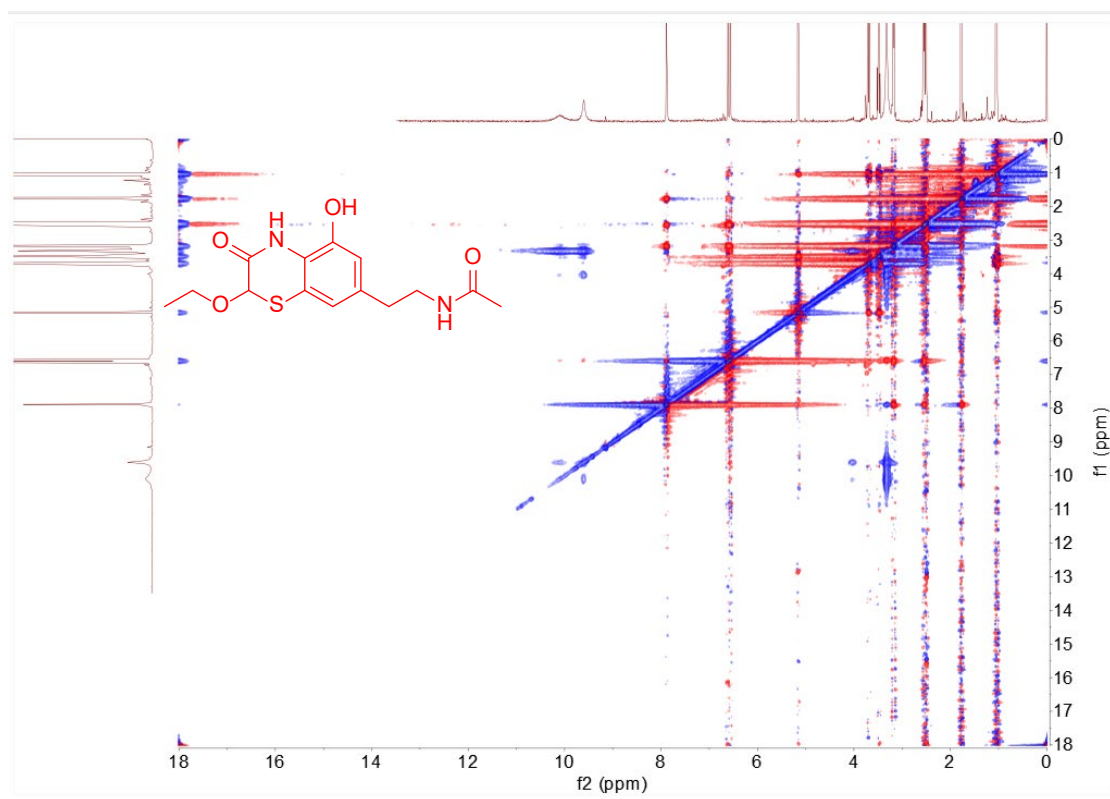
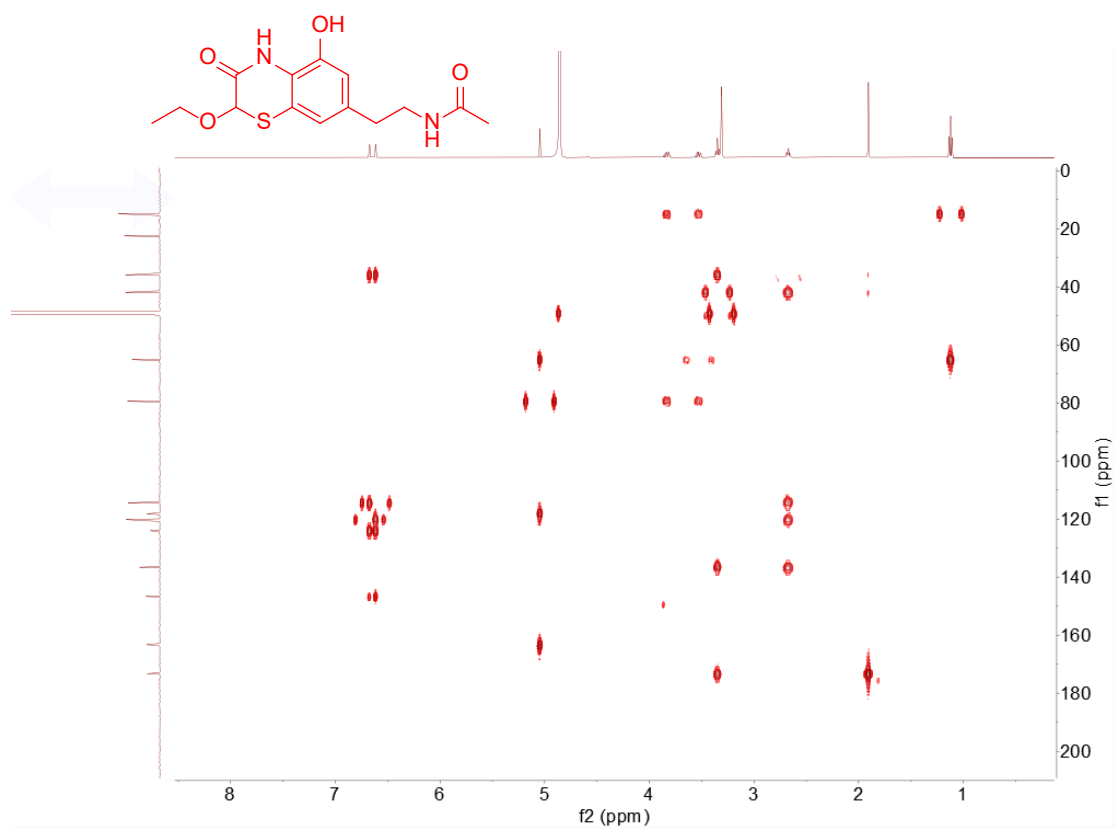


Figure S18. HSQC (600 MHz) spectrum of **2** in methanol- d_4 .



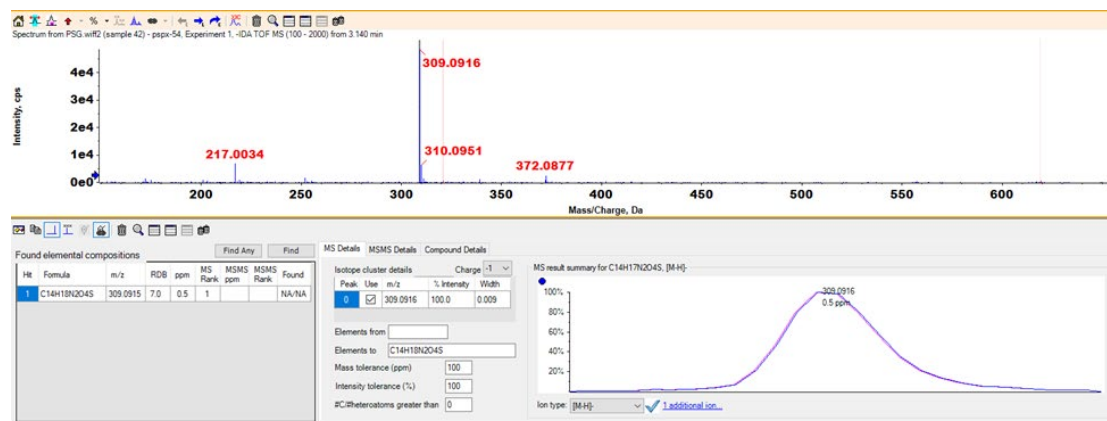


Figure S21. HRESIMS of **2**.

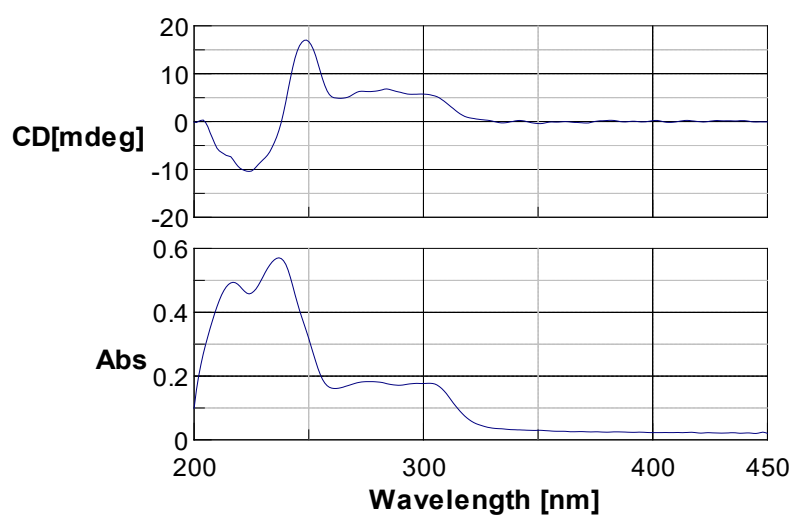


Figure S22. CD and UV spectra of (+)-**2** in methanol.

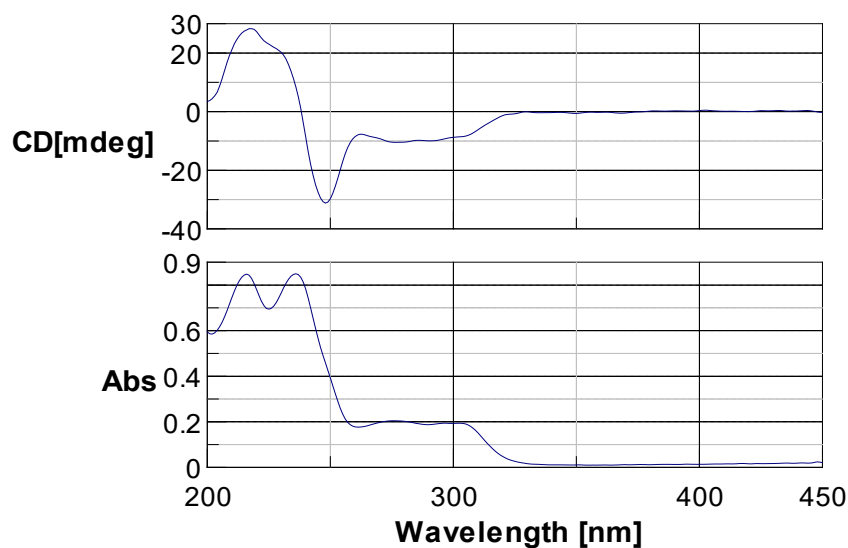


Figure S23. CD and UV spectra of (-)-**2** in methanol.

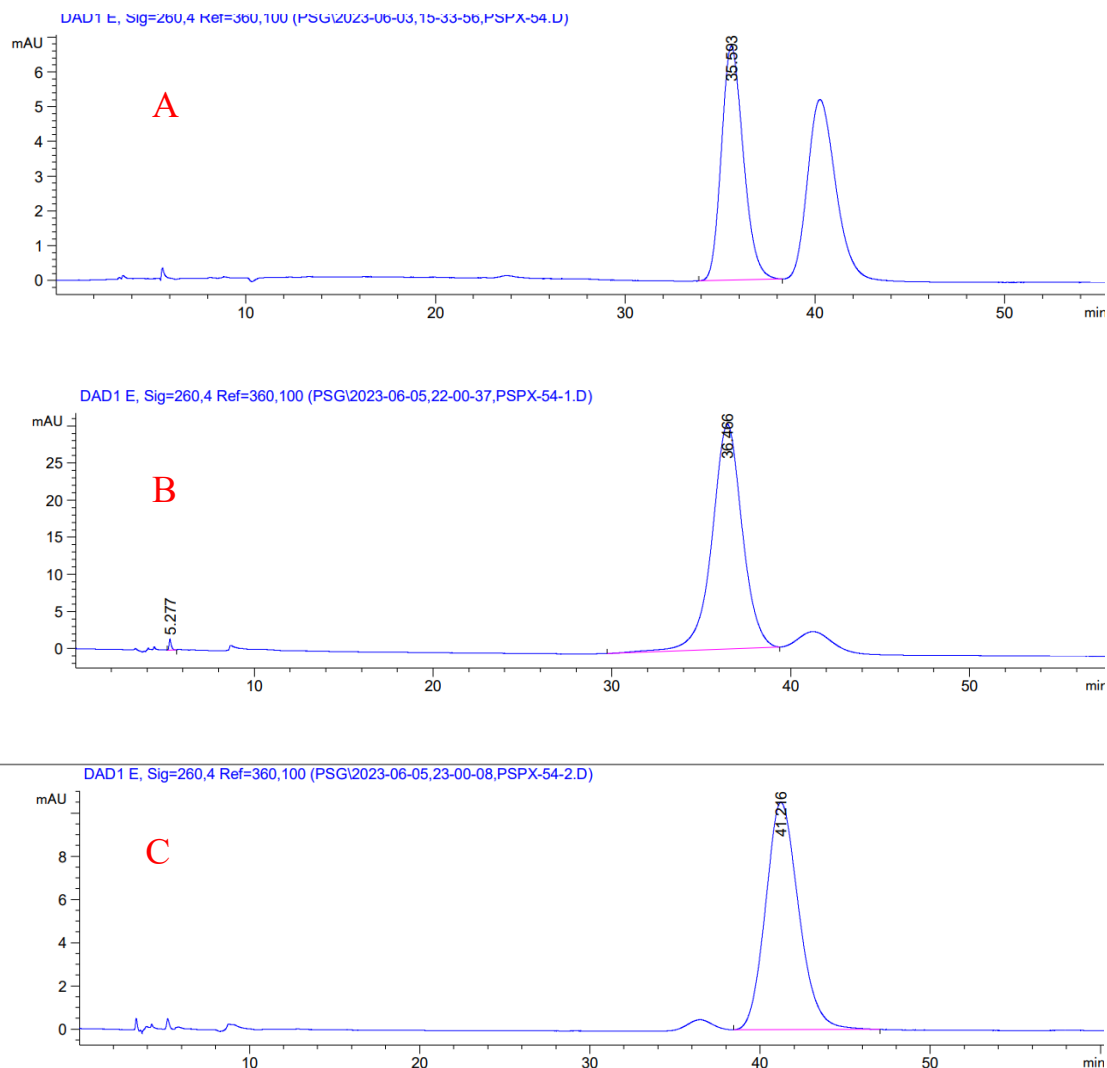


Figure S24. (A) Chiral HPLC chromatogram of **2**;

(B) Chiral HPLC chromatogram of (+)-**2**;

(C) Chiral HPLC chromatogram of (–)-**2**.

Analysis condition: Daicel Chiralpak IC column (250 mm × 4.6 mm, i.d., 5 μm), n-hexane/EtOH, 93:7, 0.05% TFA, flow rate: 1 mL/min.

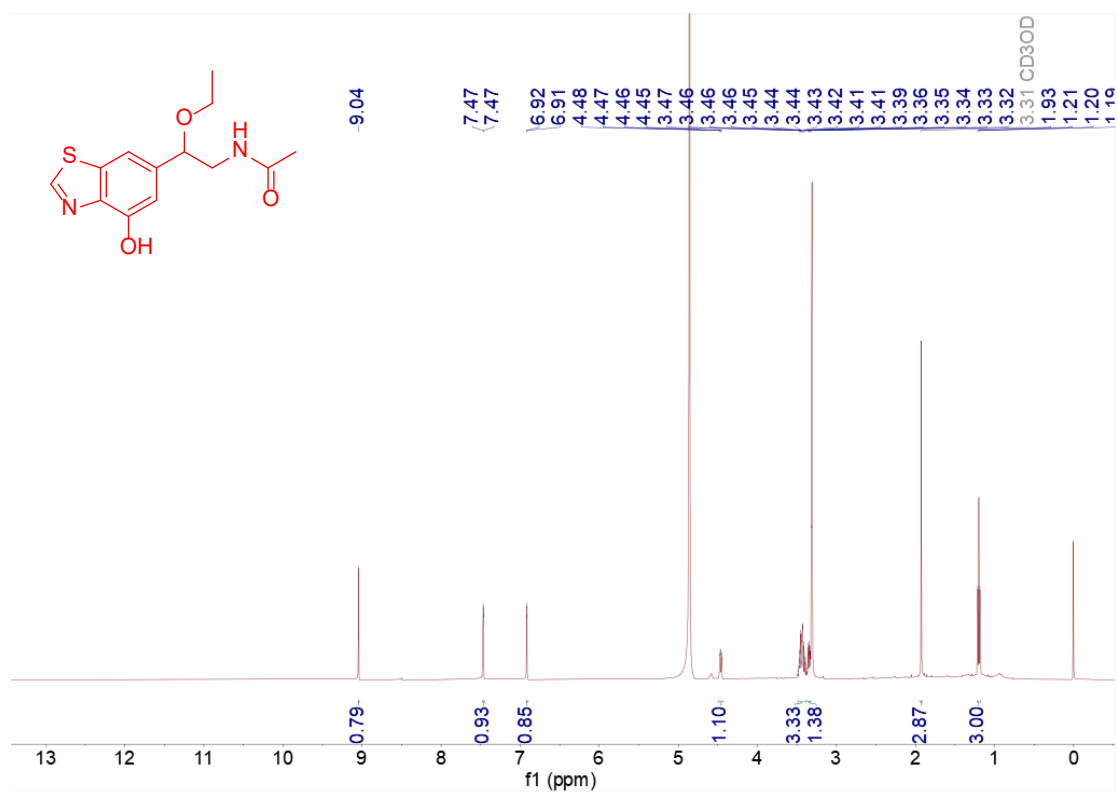


Figure S25. ¹H NMR (500 MHz) spectrum of **3** in methanol-*d*₄.

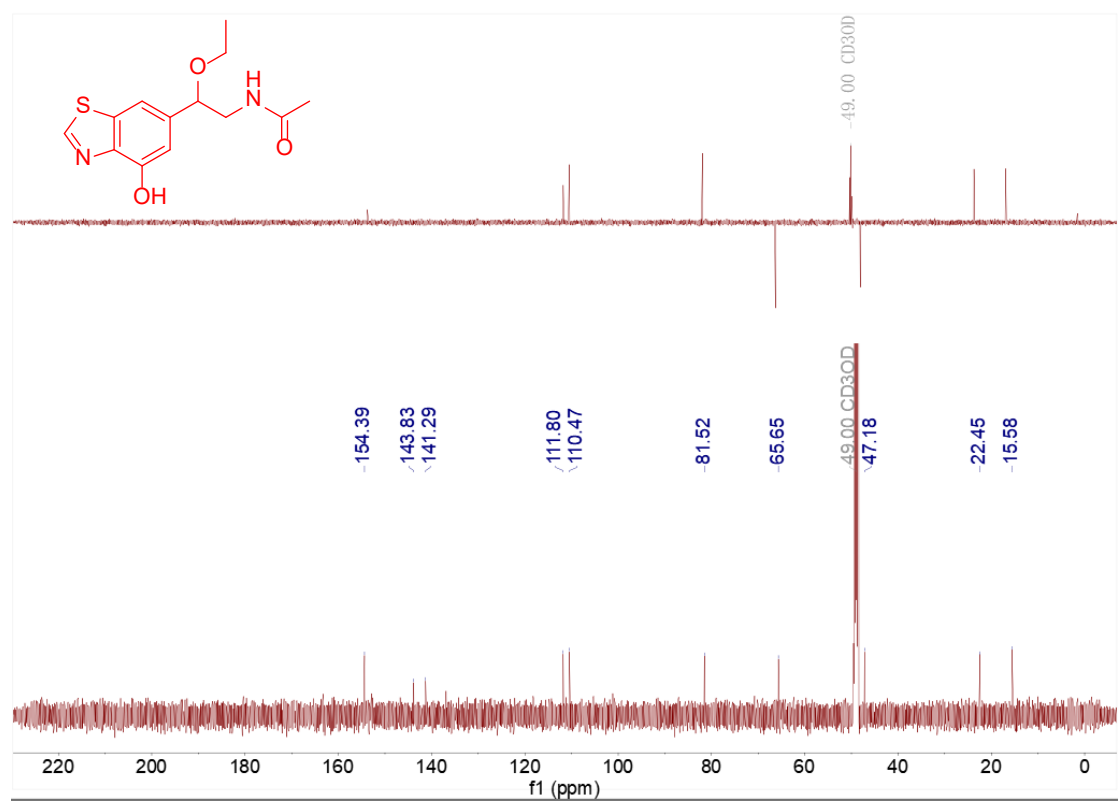


Figure S26. ¹³C NMR and DEPT-135 (150 MHz) spectra of **3** in methanol-*d*₄.

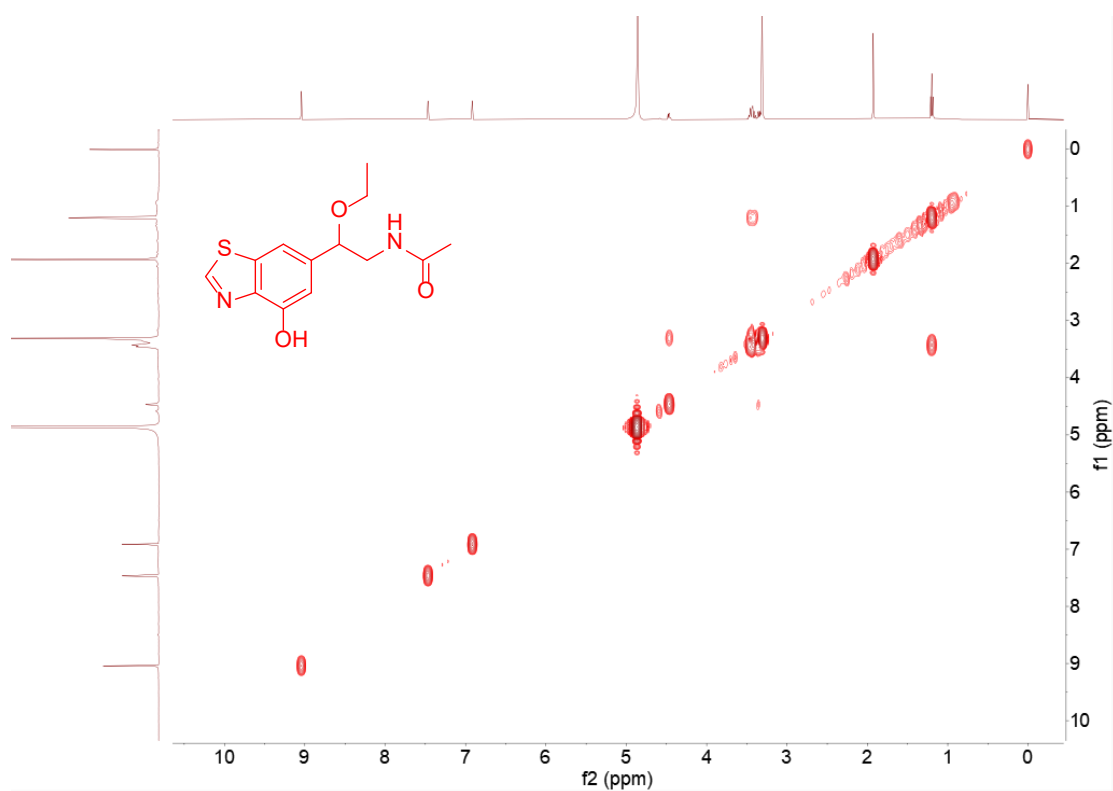


Figure S27. ^1H - ^1H COSY (600 MHz) spectrum of **3** in methanol- d_4 .

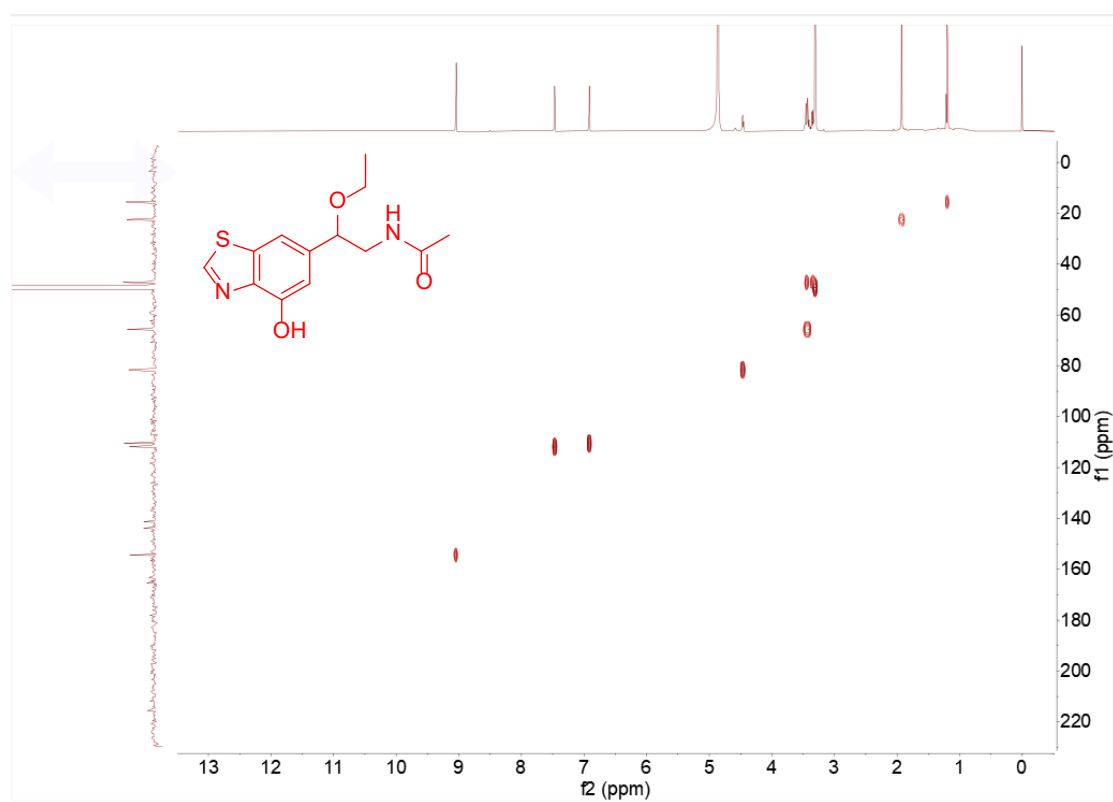


Figure S28. HSQC (600 MHz) spectrum of **3** in methanol- d_4 .

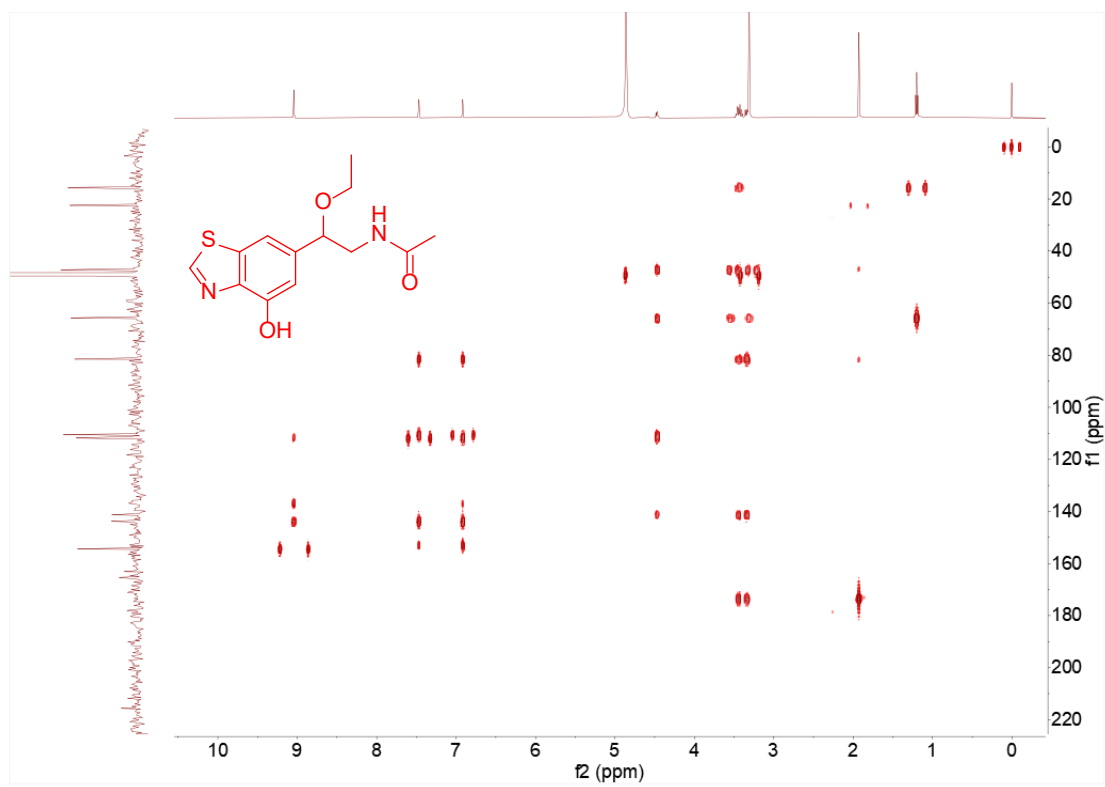


Figure S29. HMBC (600 MHz) spectrum of **3** in methanol-*d*₄.

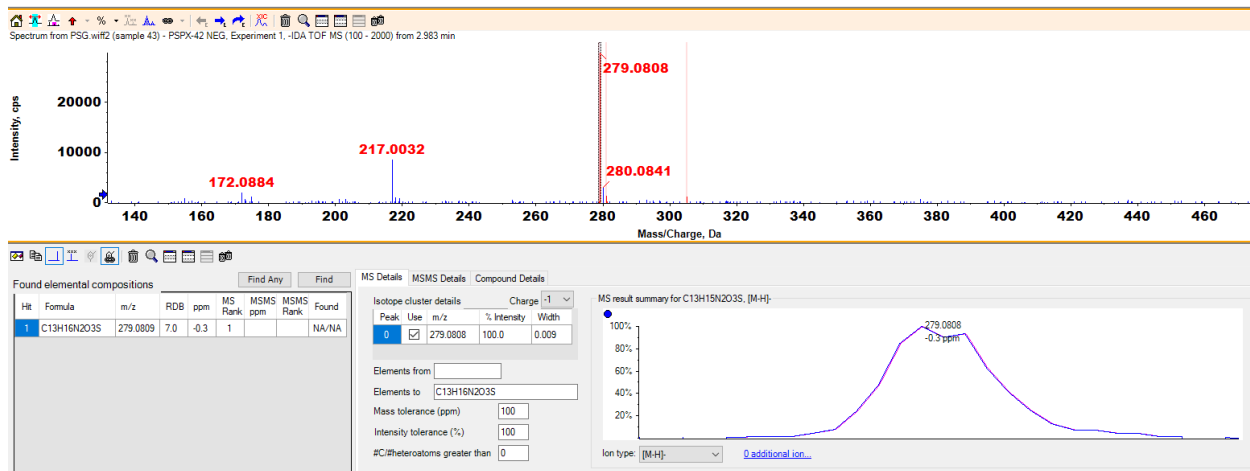


Figure S30. HRESIMS of **3**.

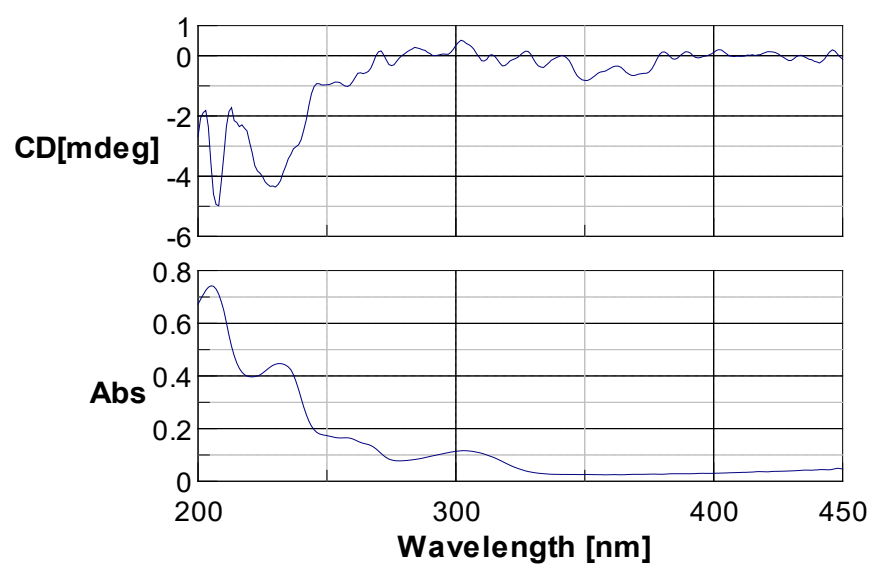


Figure S31. CD and UV spectra of (-)-3 in methanol.

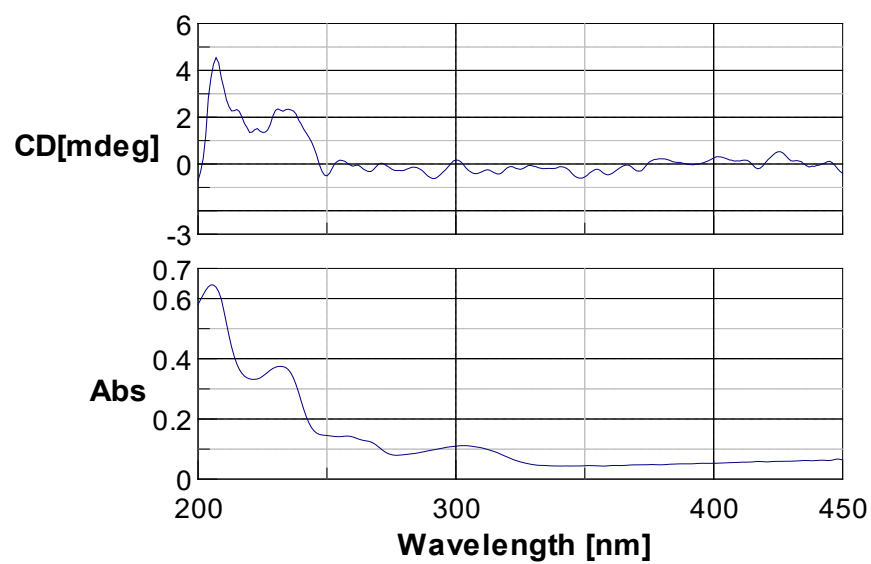


Figure S32. CD and UV spectra of (+)-3 in methanol.

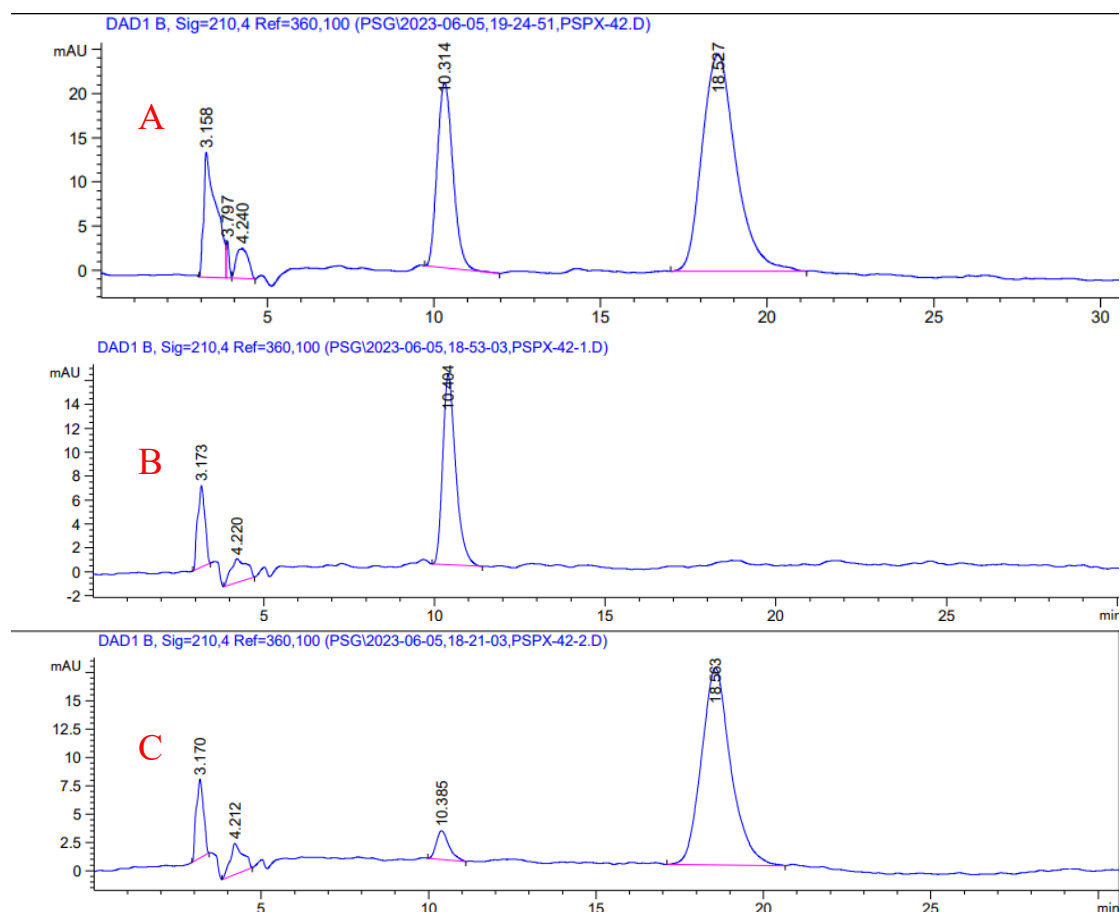


Figure S33. (A) Chiral HPLC chromatogram of **3**;

(B) Chiral HPLC chromatogram of (–)-**3**;

(C) Chiral HPLC chromatogram of (+)-**3**.

Analysis condition: Daicel Chiralpak IC column (250 mm × 4.6 mm, i.d., 5 μm), n-hexane/EtOH, 81:19, 0.05% TFA, flow rate: 1 mL/min.

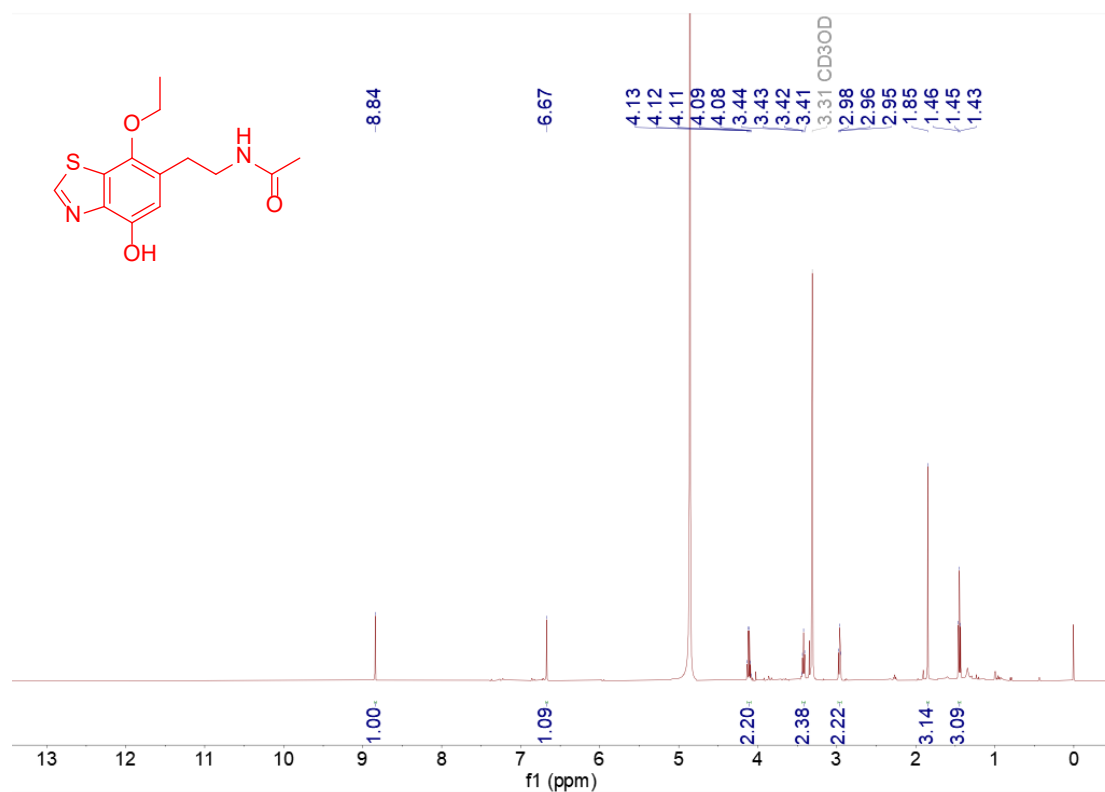


Figure S34. ¹H NMR (500 MHz) spectrum of **4** in methanol-*d*₄.

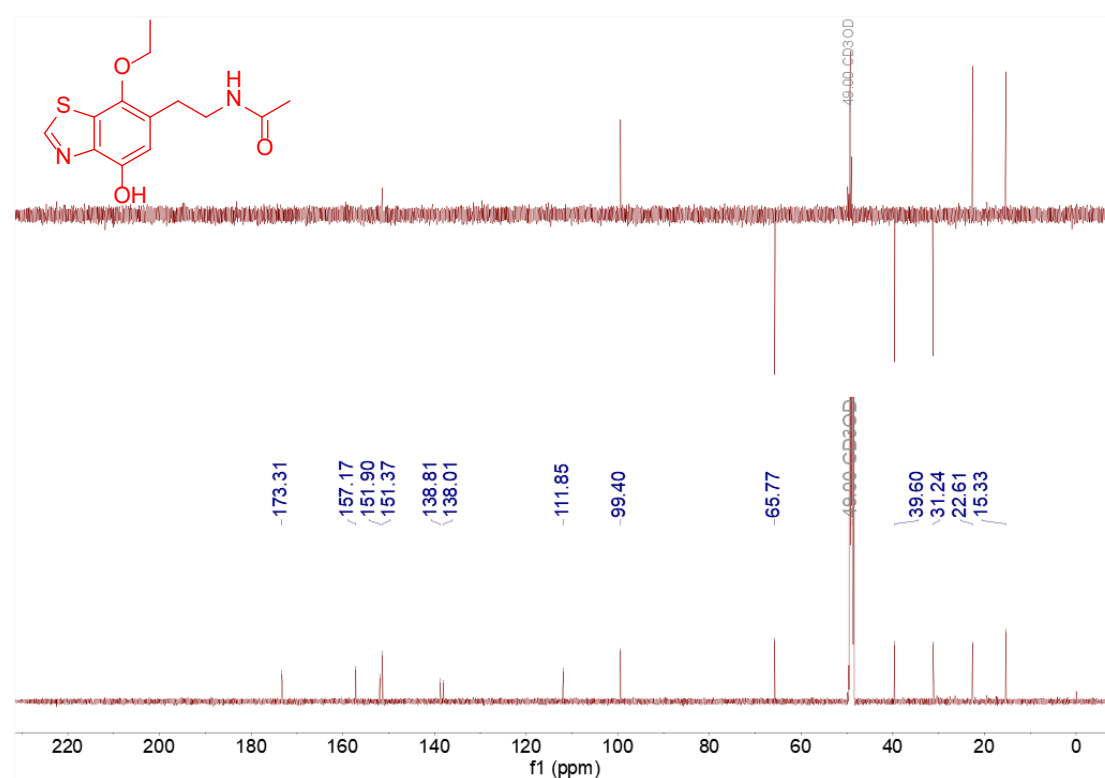


Figure S35. ¹³C NMR and DEPT-135 (150 MHz) spectra of **4** in methanol-*d*₄.

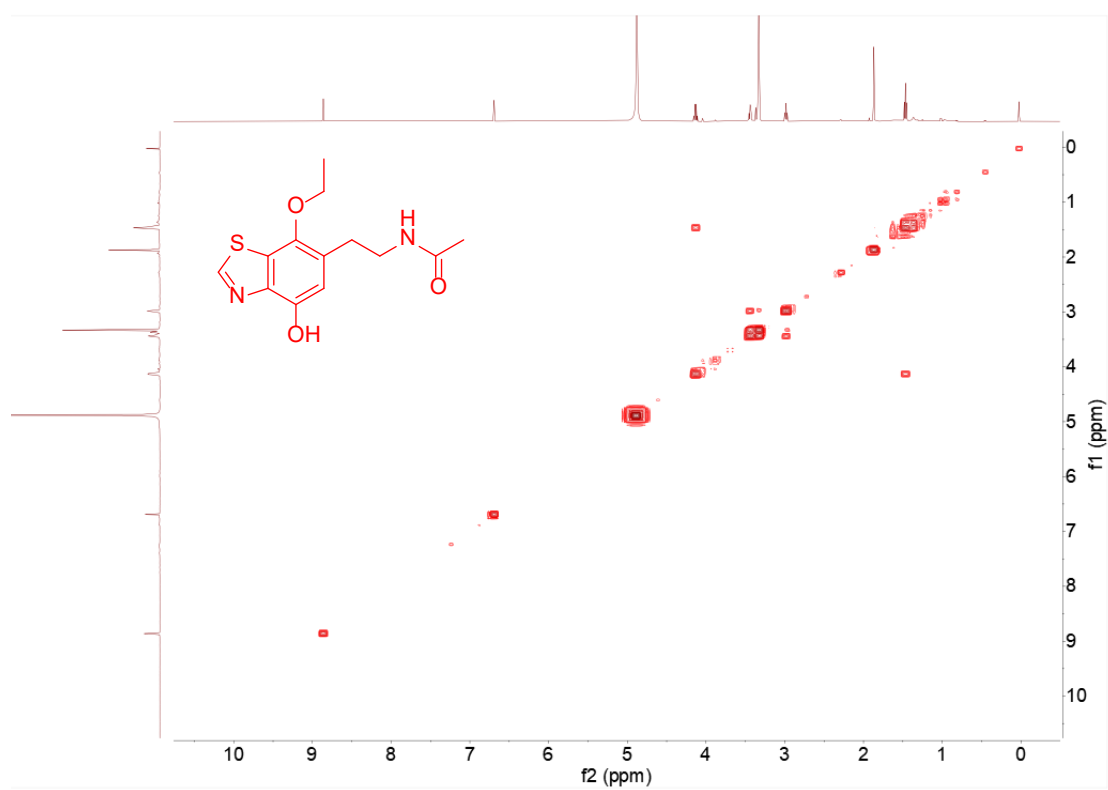


Figure S36. ^1H - ^1H COSY (600 MHz) spectrum of **4** in methanol- d_4 .

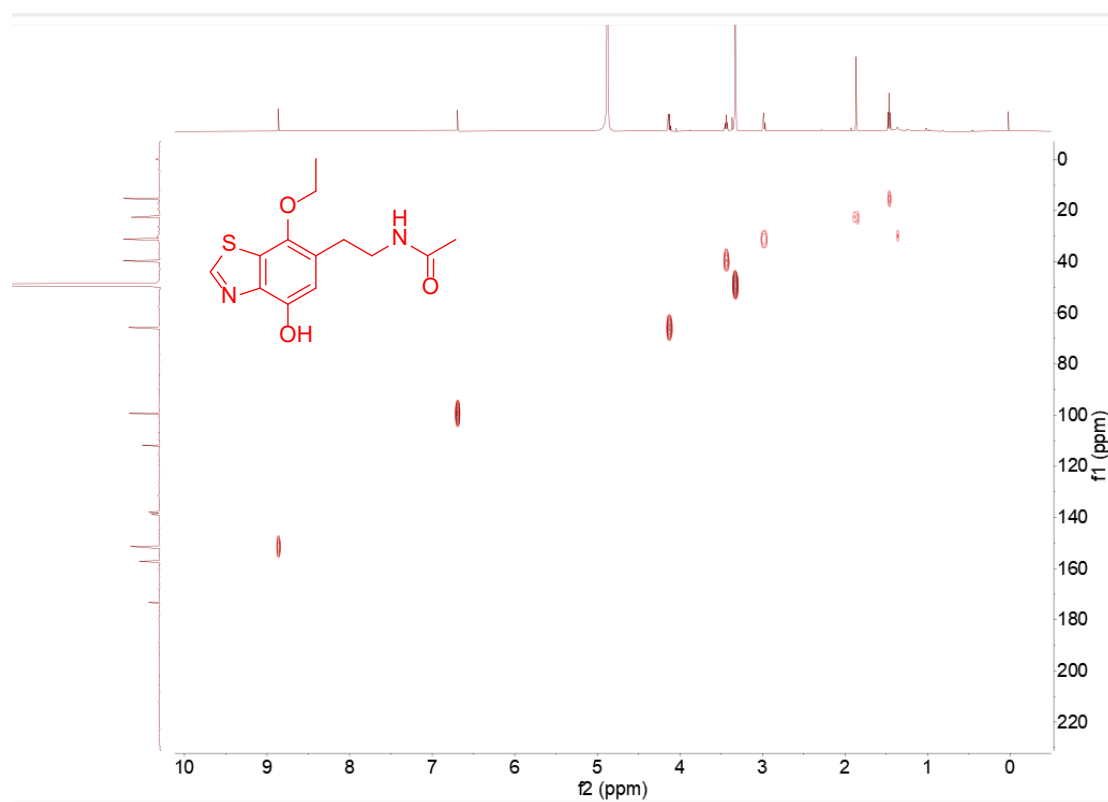


Figure 37. HSQC (600 MHz) spectrum of **4** in methanol- d_4 .

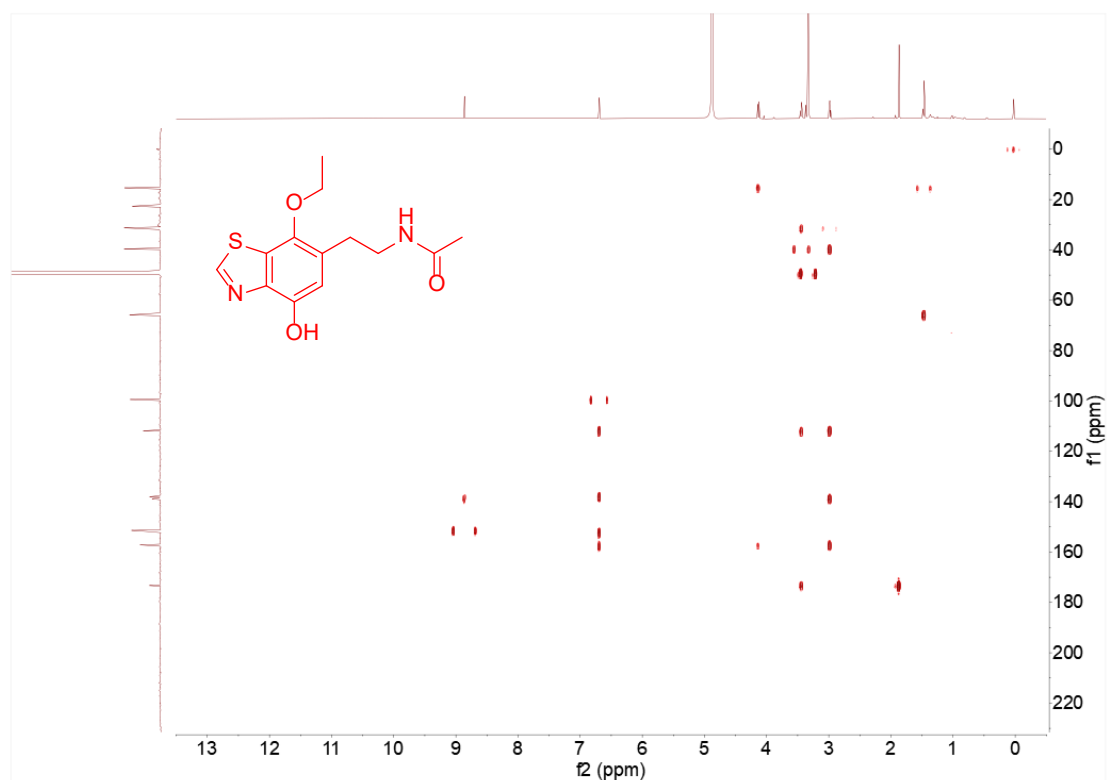


Figure S38. HMBC (600 MHz) spectrum of **4** in methanol- d_4 .

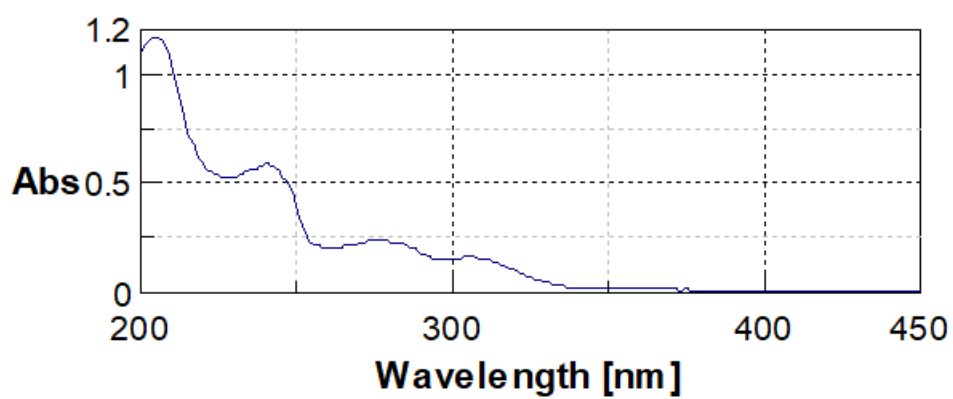


Figure S39. UV spectrum of **4** in methanol.

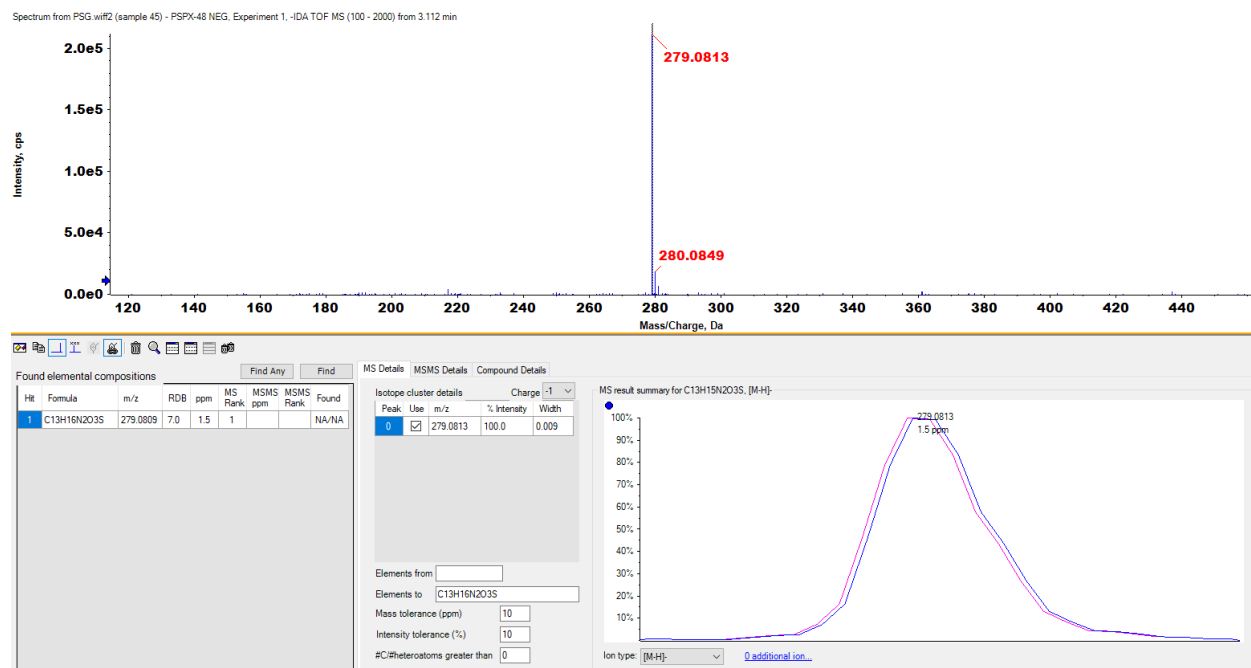


Figure S40. HRESIMS of **4**.

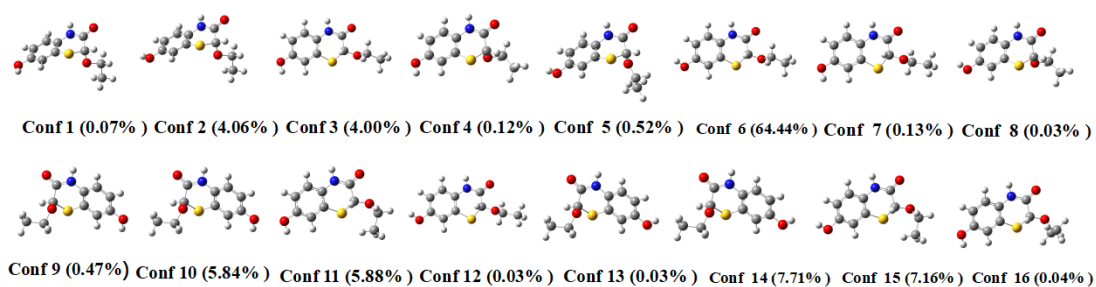


Figure S41. mPW1PW91/6-311+G(d,p) optimized lowest energy conformers for (**8R**)-**1**.

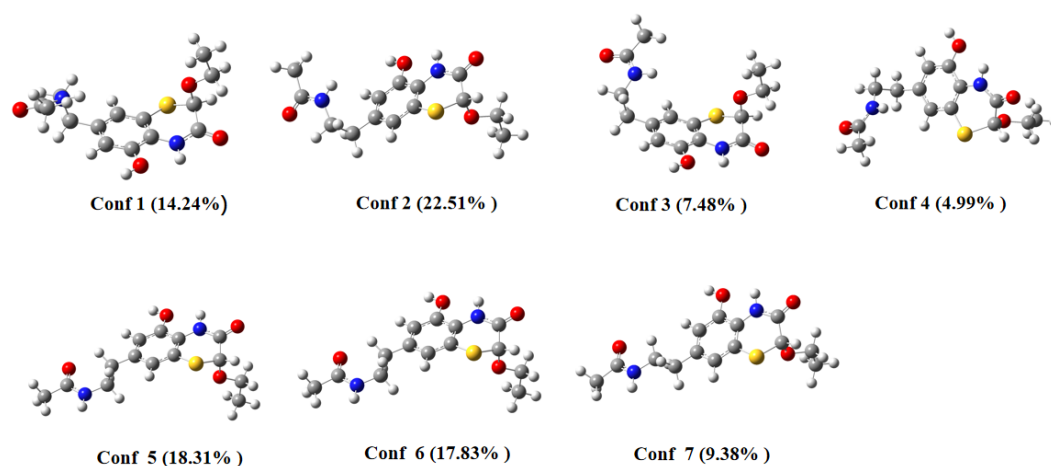


Figure S42. B3LYP/6-31G(d,p) optimized lowest energy conformers for (**8R**)-**2**.

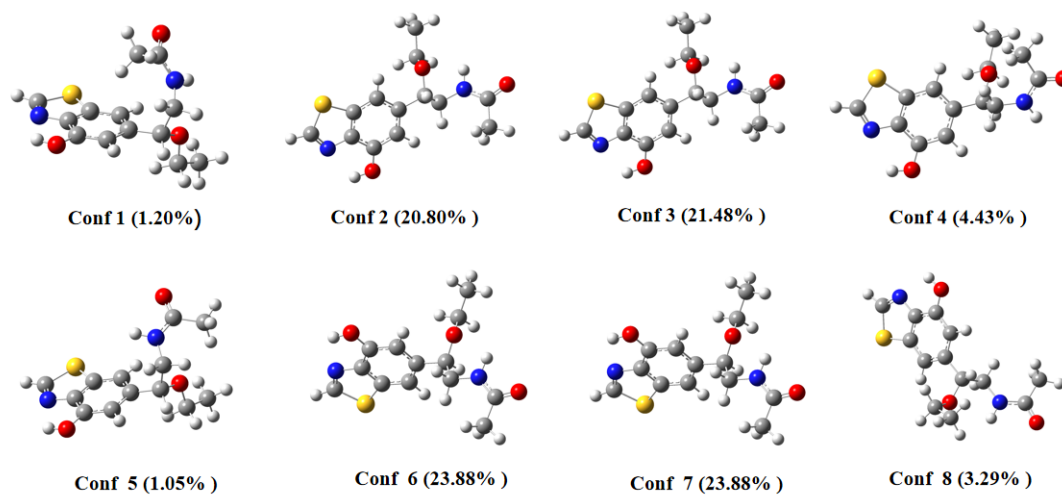


Figure S43. B3LYP/6-31G(d,p) optimized lowest energy conformers for (7*R*)-3.

HPLC-MS experiments of the crude extract and the compounds 1–4.

We have applied LC-MS (at positive ion mode) to confirmed that whether these new compounds are artificial products or not. By comparing the retention times (t_R) of HPLC profile and molecular weight of compounds 1–4 with that of the crude extract (raw materials were extracted with acetone and MeOH, respectively), which showed that compounds 1–4 were not detectable in the above extracts (data not shown), confirming that they are artificial products.

Extraction and analytical methods:

The dried and powdered insect bodies of *Mantidis Ootheca* (5.0 g) were smashed, then ultrasonic-assisted extraction respectively with acetone and MeOH (2 × 50 mL, 1 h). The LC-MS analyses of the extracts of *Mantidis Ootheca* in acetone and MeOH were performed on an Shimadzu LC-20AD AB SCIEX triple TOF X500R MS spectrometer (Shimadzu Corporation, Tokyo, Japan) using a C18 column (2.1 mm × 50 mm, i.d., 5 μm, Waters Corporation, Milford, MA, USA). The run started with 90% water and 10% acetonitrile, increasing to 100% acetonitrile in 50 min, held until 56.5 min, then returning to initial conditions and stabilizing up to 60 min. Taking compounds 1–4 as the standard samples by running the same LC-MS conditions as above.

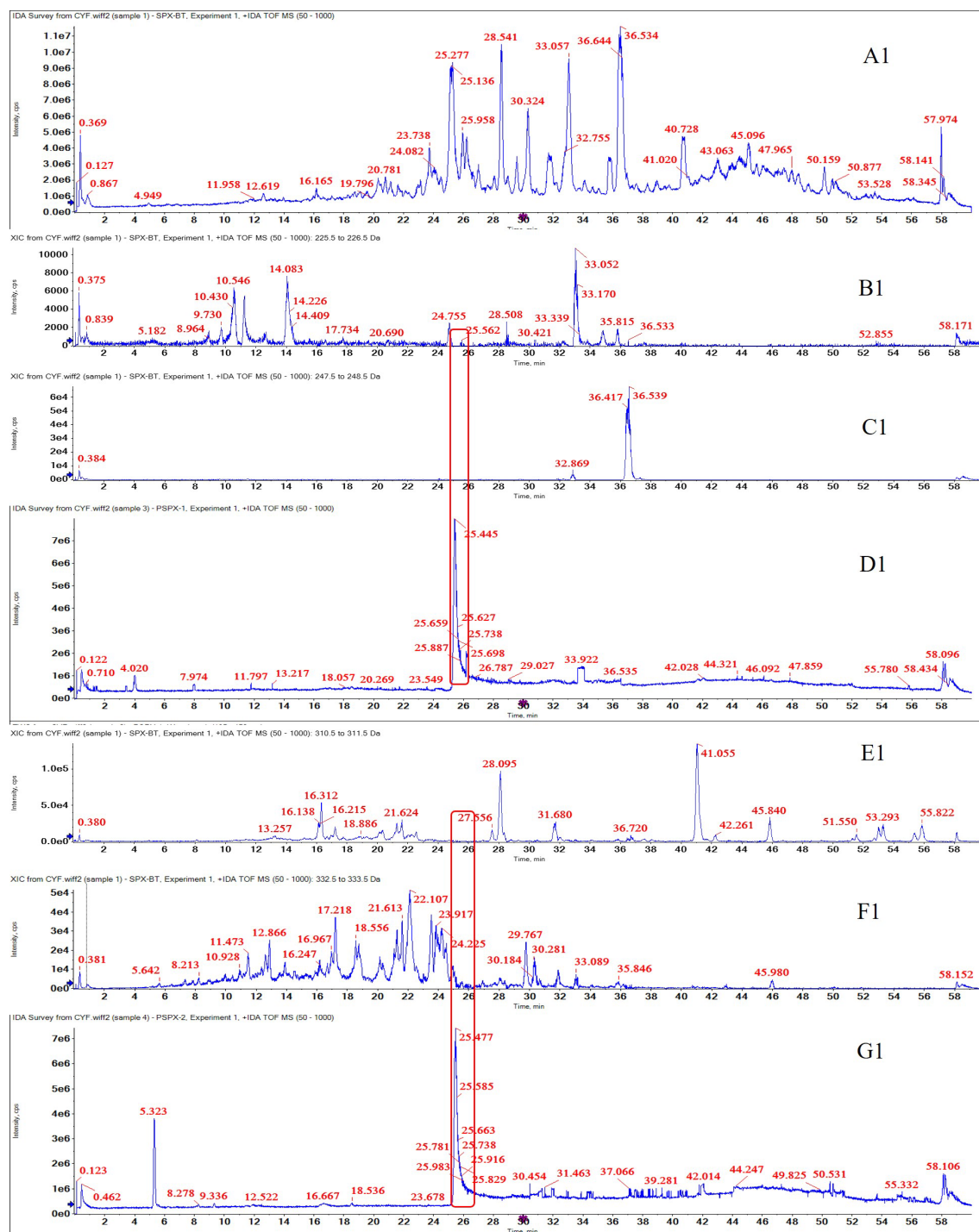


Figure S44. LC-MS chromatogram of the crude extract and the compounds (**1** and **2**). To check whether compounds **1** and **2** are natural products or artifacts, *Mantis Ootheca* was extracted with **acetone** (for details, see above Extraction). **A1**: HPLC chromatogram of crude extract; **B1**: LC-MS spectrum of crude extract targeting m/z 226; **C1**: LC-MS spectrum of crude extract targeting m/z 248; **D1**: HPLC chromatogram of compound **1**; **E1**: LC-MS spectrum of crude extract targeting m/z 311; **F1**: LC-MS spectrum of crude extract targeting m/z 333; **G1**: HPLC chromatogram of compound **2**;

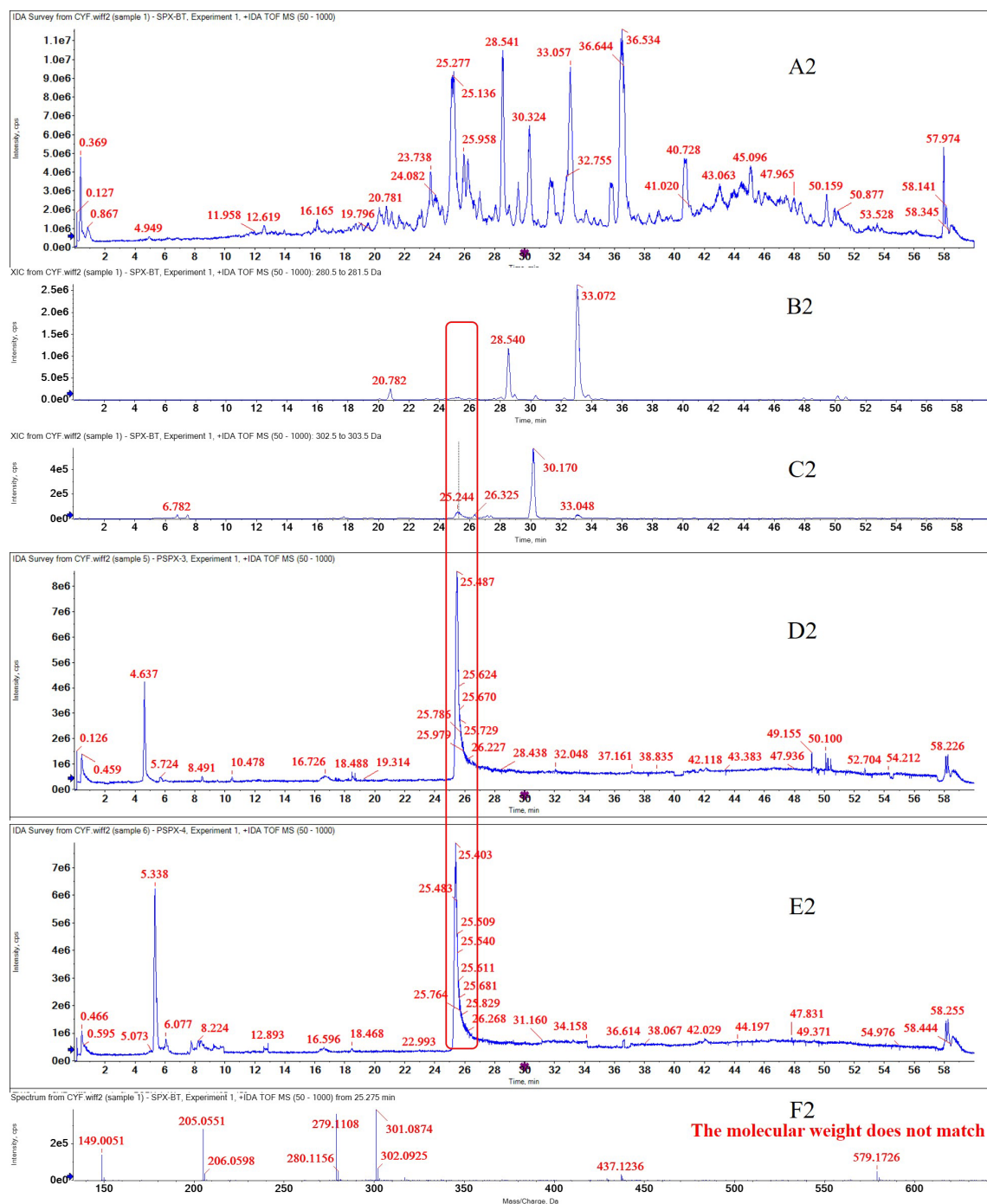


Figure S45. LC-MS chromatogram of the crude extract and the compounds (**3** and **4**). To check whether compounds **3** and **4** are natural products or artifacts, Mantidis Ootheca was extracted with **acetone** (for details, see above Extraction). **A2**: HPLC chromatogram of crude extract; **B2**: LC-MS spectrum of crude extract targeting m/z 281; **C2**: LC-MS spectrum of crude extract targeting m/z 303; **D2**: HPLC chromatogram of compound **3**; **E2**: HPLC chromatogram of compound **4**; **F2**: LC-MS spectrum of the fractions that from 25.2 minutes in **C2**;

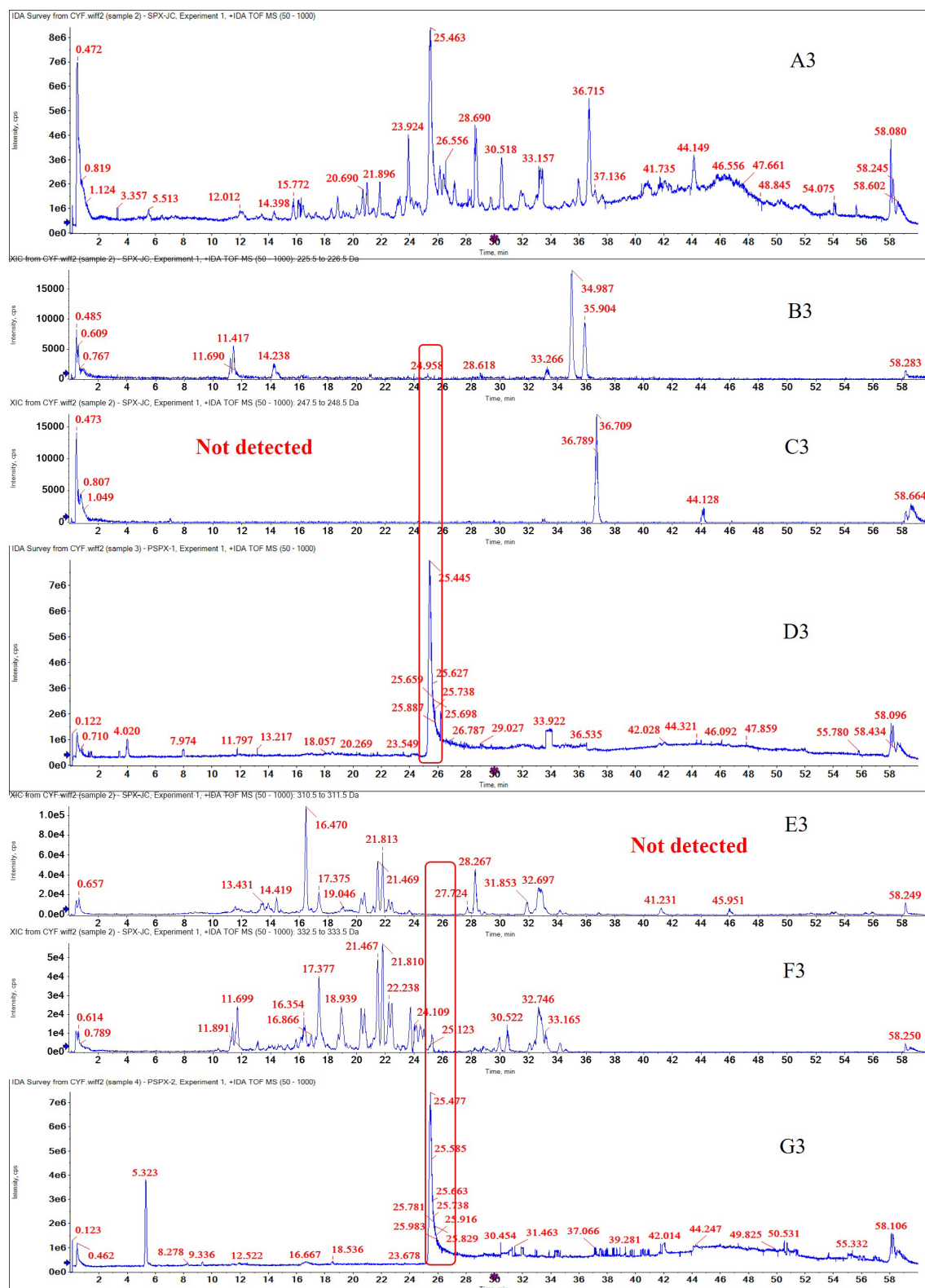


Figure S46. LC-MS chromatogram of the crude extract and the compounds (**1** and **2**). To check whether compounds **1** and **2** are natural products or artifacts, *Mantis Ootheca* was extracted with **MeOH** (for details, see above Extraction). **A3**: HPLC chromatogram of crude extract; **B3**: LC-MS spectrum of crude extract targeting m/z 226; **C3**: LC-MS spectrum of crude extract targeting m/z 248; **D3**: HPLC chromatogram of compound **1**; **E3**: LC-MS spectrum of crude extract targeting m/z 311; **F3**: LC-MS spectrum of crude extract targeting

m/z 333; **G3**: HPLC chromatogram of compound 2;

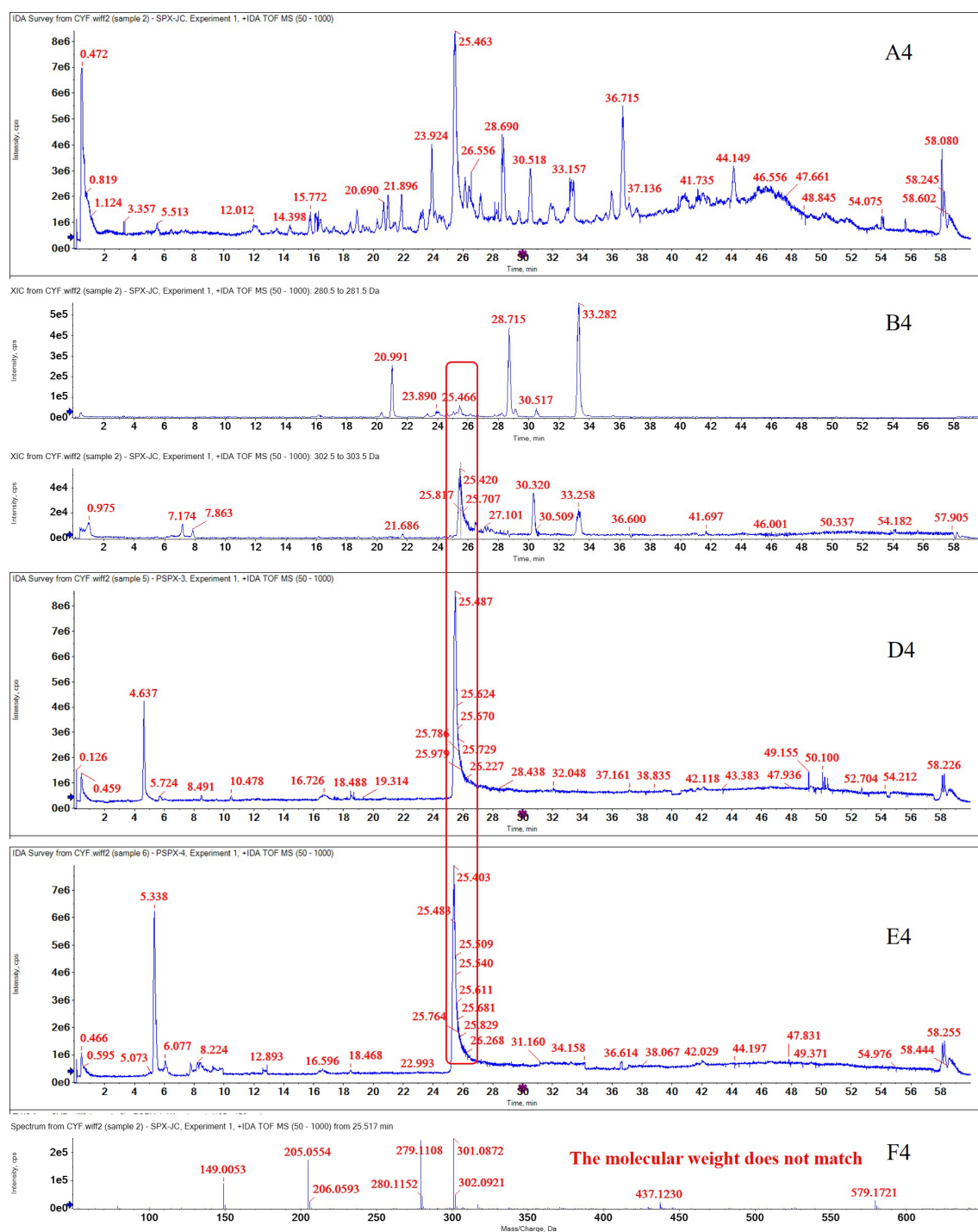


Figure S47. LC-MS chromatogram of the crude extract and the compounds (**3** and **4**). To check whether compounds **3** and **4** are natural products or artifacts, *Mantis Ootheca* was extracted with **MeOH** (for details, see above Extraction). **A4**: HPLC chromatogram of crude extract; **B4**: LC-MS spectrum of crude extract targeting m/z 281; **C4**: LC-MS spectrum of crude extract targeting m/z 303; **D4**: HPLC chromatogram of compound **3**; **E4**: HPLC chromatogram of compound **4**; **F4**: LC-MS spectrum of the fractions that from 25.5 minutes in **C4**;

Table S1 The Cartesian coordinates of the lowest energy conformers for (8*R*)-1.

Conf 1	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.2202	-0.4539	-0.3002	C	-3.2231	-0.4586	-0.2956
C	-3.0682	0.6542	-1.1242	C	-3.0775	0.6518	-1.1193
C	-1.8691	1.3671	-1.1101	C	-1.8765	1.364	-1.1026
C	-0.8196	0.9565	-0.2816	C	-0.8237	0.9526	-0.277
C	-0.9836	-0.1566	0.5576	C	-0.9825	-0.1631	0.5586
C	-2.1937	-0.8613	0.5465	C	-2.1924	-0.865	0.5457
N	0.3568	1.7197	-0.2877	N	0.3505	1.7192	-0.2832
C	1.5436	1.371	0.3026	C	1.5393	1.3719	0.3046
S	0.2695	-0.6393	1.7291	S	0.2745	-0.6492	1.7233
O	2.4687	2.1891	0.3199	O	2.4613	2.1936	0.3218
C	1.7316	-0.0738	0.8048	C	1.7328	-0.0734	0.8018
O	2.0125	-0.9852	-0.2567	O	2.018	-0.9742	-0.268
C	3.3494	-0.8707	-0.7379	C	3.364	-0.8725	-0.7254
C	3.5515	-1.908	-1.8252	C	3.5659	-1.8888	-1.8323
O	-4.4109	-1.1164	-0.3446	O	-4.3803	-1.179	-0.2749
H	-3.8826	0.9633	-1.7739	H	-3.8811	0.9779	-1.7723
H	-1.7649	2.233	-1.7581	H	-1.7706	2.2332	-1.7467
H	-2.3265	-1.7162	1.203	H	-2.3417	-1.7258	1.1926
H	0.3619	2.6275	-0.7567	H	0.3539	2.6288	-0.7481
H	2.5584	-0.0783	1.5247	H	2.5599	-0.0774	1.5214
H	3.5191	0.1289	-1.1505	H	3.5579	0.133	-1.1122
H	4.0569	-1.0497	0.079	H	4.0547	-1.0822	0.0985
H	4.5677	-1.8598	-2.2265	H	4.5892	-1.8497	-2.2161
H	3.3727	-2.9154	-1.435	H	3.3633	-2.9013	-1.4679
H	2.8404	-1.7522	-2.6433	H	2.8712	-1.7023	-2.658
H	-4.3729	-1.8722	0.2653	H	-5.0042	-0.7953	-0.9128
Conf 3	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.5419	-0.4568	0.1939	C	-3.2769	-0.4822	-0.2819
C	-3.5482	0.9246	0.3401	C	-3.2354	0.8186	-0.7675
C	-2.3546	1.6375	0.2251	C	-2.0615	1.5633	-0.6501
C	-1.1548	0.9607	-0.0163	C	-0.9273	0.9955	-0.0605
C	-1.1557	-0.4336	-0.1709	C	-0.979	-0.3152	0.439
C	-2.3596	-1.142	-0.0684	C	-2.1639	-1.0535	0.3275
N	0.0125	1.7252	-0.1471	N	0.2202	1.7931	0.0533
C	1.297	1.2445	-0.2091	C	1.467	1.3601	0.4228
S	0.3204	-1.3305	-0.6034	S	0.3916	-1.0386	1.3185
O	2.2046	2.0435	-0.4555	O	2.3638	2.192	0.5936
C	1.549	-0.2342	0.1798	C	1.7445	-0.1532	0.486
O	2.8544	-0.7071	-0.1331	O	1.9489	-0.6951	-0.8189
C	3.8241	-0.3556	0.8491	C	3.2778	-0.5291	-1.3068
C	5.1773	-0.8536	0.3807	C	4.1764	-1.6506	-0.8162

O	-4.7331	-1.1096	0.3057	O	-4.4466	-1.1698	-0.4145
H	-4.4819	1.4455	0.5356	H	-4.1159	1.2524	-1.2341
H	-2.3762	2.7187	0.3337	H	-2.0439	2.5803	-1.0324
H	-2.3658	-2.2198	-0.2036	H	-2.2095	-2.0638	0.7232
H	-0.0629	2.7401	-0.247	H	0.1553	2.7941	-0.1413
H	1.384	-0.313	1.2623	H	2.6303	-0.3065	1.1117
H	3.8589	0.7291	0.9888	H	3.2236	-0.5737	-2.3995
H	3.5679	-0.8293	1.8032	H	3.6836	0.4525	-1.0404
H	5.9557	-0.6127	1.1102	H	5.1718	-1.5708	-1.2627
H	5.1582	-1.9379	0.2291	H	4.2839	-1.6293	0.2723
H	5.4421	-0.4018	-0.581	H	3.7502	-2.6253	-1.0754
H	-4.5897	-2.0589	0.1535	H	-4.3295	-2.0626	-0.049
Conf 5	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.1502	-0.6067	-0.158	C	-3.541	-0.4614	0.194
C	-3.1557	0.5091	-0.9872	C	-3.5541	0.9215	0.3343
C	-2.0209	1.3201	-1.0514	C	-2.3582	1.6326	0.2177
C	-0.8829	1.0019	-0.301	C	-1.1557	0.9567	-0.0204
C	-0.8889	-0.1208	0.5406	C	-1.1529	-0.4372	-0.1724
C	-2.0334	-0.9221	0.6093	C	-2.356	-1.1425	-0.0655
N	0.2191	1.8647	-0.3863	N	0.0104	1.7233	-0.1483
C	1.4711	1.6218	0.1184	C	1.2959	1.2444	-0.2051
S	0.483	-0.4994	1.6123	S	0.324	-1.3306	-0.6065
O	2.3143	2.5237	0.0837	O	2.2026	2.0474	-0.4433
C	1.8163	0.2064	0.6039	C	1.5499	-0.2351	0.1789
O	2.0903	-0.6046	-0.5427	O	2.8573	-0.701	-0.1372
C	3.1659	-1.5121	-0.3241	C	3.8236	-0.3608	0.8521
C	3.3341	-2.3598	-1.5694	C	5.1797	-0.8463	0.3793
O	-4.2381	-1.4224	-0.0597	O	-4.6849	-1.1955	0.295
H	-4.0266	0.7641	-1.583	H	-4.4773	1.4592	0.528
H	-2.0323	2.1926	-1.6995	H	-2.3767	2.7146	0.3227
H	-2.0656	-1.7901	1.2628	H	-2.3808	-2.222	-0.1942
H	0.1177	2.7674	-0.8532	H	-0.0642	2.738	-0.2483
H	2.7058	0.2982	1.2393	H	1.3861	-0.3174	1.2613
H	4.0872	-0.9515	-0.1311	H	3.8536	0.7219	1.0082
H	2.9487	-2.1553	0.5354	H	3.5671	-0.8498	1.7984
H	4.1548	-3.0723	-1.4486	H	5.9556	-0.6135	1.114
H	2.4142	-2.9131	-1.7859	H	5.1652	-1.9283	0.2113
H	3.5388	-1.7289	-2.4408	H	5.4448	-0.379	-0.5749
H	-4.9352	-1.0931	-0.6507	H	-5.4347	-0.5978	0.4506
Conf 7	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.496	-0.5446	-0.0095	C	-3.2767	-0.4916	-0.2755
C	-3.5773	0.8415	-0.0326	C	-3.2441	0.8094	-0.7644
C	-2.4081	1.6018	-0.0608	C	-2.0695	1.5553	-0.6481

C	-1.1597	0.9705	-0.048	C	-0.9308	0.9916	-0.0603
C	-1.0837	-0.4298	-0.0339	C	-0.9751	-0.3186	0.4393
C	-2.262	-1.1875	-0.0179	C	-2.1588	-1.0561	0.3301
N	-0.0192	1.7828	-0.0985	N	0.2132	1.7948	0.051
C	1.2805	1.3818	0.0814	C	1.4626	1.3673	0.4188
S	0.4695	-1.2923	-0.1424	S	0.4004	-1.0376	1.3129
O	2.1719	2.2126	-0.1114	O	2.3554	2.2045	0.5859
C	1.5476	-0.0427	0.6405	C	1.7475	-0.144	0.4827
O	2.8888	-0.509	0.7373	O	1.9565	-0.6781	-0.8251
C	3.649	-0.4118	-0.4641	C	3.2928	-0.529	-1.2975
C	4.9073	-1.242	-0.2901	C	4.1682	-1.6688	-0.807
O	-4.6643	-1.2462	0.011	O	-4.404	-1.2533	-0.362
H	-4.5489	1.3286	-0.0337	H	-4.1156	1.2577	-1.2314
H	-2.4878	2.6856	-0.0839	H	-2.0517	2.5729	-1.0295
H	-2.2072	-2.2725	-0.0208	H	-2.2196	-2.0691	0.7199
H	-0.1249	2.7787	-0.3066	H	0.1453	2.7953	-0.1431
H	1.2063	0.0099	1.6822	H	2.6341	-0.2923	1.1086
H	3.0836	-0.7834	-1.3245	H	3.2499	-0.5632	-2.3911
H	3.9341	0.6279	-0.6444	H	3.7107	0.4439	-1.0178
H	5.534	-1.1927	-1.185	H	5.17	-1.6	-1.2406
H	5.4881	-0.8878	0.5681	H	4.2625	-1.6597	0.2829
H	4.6536	-2.289	-0.0936	H	3.7303	-2.6343	-1.0808
H	-4.4633	-2.1971	0.0165	H	-5.097	-0.744	-0.8133
Conf 9	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 10	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.2239	0.0029	0.4189	C	3.3053	-0.3018	0.3347
C	2.9582	1.3637	0.3308	C	3.1638	1.0186	0.7424
C	1.6999	1.7969	-0.0879	C	1.9417	1.6686	0.5685
C	0.7062	0.8638	-0.4009	C	0.8599	0.9874	0.0011
C	0.9845	-0.5096	-0.3217	C	1.0121	-0.3433	-0.4191
C	2.253	-0.9378	0.0887	C	2.245	-0.9864	-0.2515
N	-0.5346	1.3495	-0.8373	N	-0.3389	1.6931	-0.1739
C	-1.6757	0.6076	-0.9998	C	-1.5459	1.1518	-0.5343
S	-0.2002	-1.7358	-0.8396	S	-0.291	-1.2157	-1.2664
O	-2.6725	1.1413	-1.4964	O	-2.4914	1.9079	-0.7781
C	-1.7229	-0.8246	-0.43	C	-1.7142	-0.376	-0.5097
O	-1.9383	-0.8628	0.9791	O	-1.889	-0.82	0.8368
C	-3.247	-0.454	1.37	C	-3.1727	-1.3756	1.1039
C	-3.1673	0.8789	2.09	C	-4.2427	-0.304	1.2108
O	4.4687	-0.3732	0.8281	O	4.5191	-0.8942	0.52
H	3.7302	2.085	0.585	H	4.0038	1.5412	1.1922
H	1.5068	2.8641	-0.1543	H	1.8456	2.7022	0.8899
H	2.4737	-1.9999	0.14	H	2.3687	-2.0122	-0.586
H	-0.63	2.3393	-1.0724	H	-0.3492	2.7056	-0.0376

H	-2.5323	-1.3649	-0.9349	H	-2.5825	-0.6232	-1.1317
H	-3.9413	-0.4022	0.5238	H	-3.4309	-2.1277	0.3497
H	-3.6288	-1.2115	2.0622	H	-3.0978	-1.8952	2.0649
H	-4.1527	1.182	2.4549	H	-5.1894	-0.7376	1.546
H	-2.4802	0.8163	2.9404	H	-3.9398	0.4758	1.9169
H	-2.7838	1.6622	1.4296	H	-4.415	0.1827	0.2464
H	4.5099	-1.3437	0.8578	H	4.4723	-1.8123	0.2049
Conf 11	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 12	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.4439	-0.5016	0.2248	C	-3.4966	-0.5467	-0.0089
C	-3.4617	0.851	0.5404	C	-3.5824	0.84	-0.0349
C	-2.2863	1.5971	0.4521	C	-2.4097	1.5972	-0.0637
C	-1.0919	0.9799	0.0665	C	-1.1599	0.966	-0.0493
C	-1.0816	-0.3847	-0.2587	C	-1.082	-0.4335	-0.0335
C	-2.2681	-1.1249	-0.1815	C	-2.2613	-1.1863	-0.0159
N	0.0556	1.7786	-0.0288	N	-0.0202	1.7794	-0.0989
C	1.3414	1.3361	-0.2157	C	1.2795	1.3792	0.0831
S	0.3807	-1.1915	-0.8755	S	0.4709	-1.2951	-0.1418
O	2.2249	2.1779	-0.4015	O	2.1692	2.2131	-0.1052
C	1.6353	-0.1737	-0.0322	C	1.5483	-0.0459	0.6393
O	2.9276	-0.5637	-0.4847	O	2.8927	-0.5046	0.7334
C	3.9697	-0.3155	0.4543	C	3.6427	-0.4281	-0.4759
C	4.121	-1.4917	1.4029	C	4.9247	-1.2165	-0.2819
O	-4.618	-1.1878	0.3174	O	-4.6141	-1.3265	0.0142
H	-4.3906	1.3246	0.8474	H	-4.5435	1.3452	-0.0376
H	-2.3171	2.6561	0.6943	H	-2.4849	2.6816	-0.0884
H	-2.2665	-2.178	-0.4482	H	-2.2269	-2.2733	-0.0164
H	-0.0391	2.7964	0.0041	H	-0.1244	2.7752	-0.3069
H	1.5367	-0.3882	1.039	H	1.2095	0.0055	1.6818
H	4.8964	-0.1998	-0.1172	H	3.0829	-0.8462	-1.3182
H	3.8048	0.616	1.0063	H	3.8974	0.6117	-0.6966
H	4.9703	-1.3393	2.0751	H	5.5439	-1.1821	-1.1826
H	3.2207	-1.6325	2.0086	H	5.5009	-0.816	0.5588
H	4.2762	-2.4195	0.8425	H	4.7015	-2.2624	-0.0463
H	-4.4696	-2.1081	0.042	H	-5.4009	-0.7568	0.0086
Conf 13	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 14	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.3057	-0.3216	-0.3257	C	3.2276	-0.0046	0.4193
C	-3.1783	0.9974	-0.7456	C	2.9679	1.3585	0.3336
C	-1.9578	1.6546	-0.5777	C	1.7079	1.7906	-0.0854
C	-0.8684	0.9852	-0.0077	C	0.7111	0.8593	-0.3988
C	-1.0081	-0.3431	0.4219	C	0.9846	-0.5145	-0.3193
C	-2.2372	-0.9915	0.2616	C	2.2525	-0.9404	0.0896
N	0.3251	1.7022	0.1585	N	-0.5278	1.349	-0.8364
C	1.5375	1.1728	0.5193	C	-1.6707	0.6101	-1.0007

S	0.3039	-1.2004	1.269	S	-0.2034	-1.7375	-0.8342
O	2.478	1.9392	0.7511	O	-2.6647	1.1484	-1.4984
C	1.7179	-0.353	0.5076	C	-1.7236	-0.8215	-0.431
O	1.8992	-0.7979	-0.8382	O	-1.9452	-0.8524	0.9776
C	3.1688	-1.3933	-1.0856	C	-3.2591	-0.453	1.3598
C	4.268	-0.351	-1.1892	C	-3.1918	0.8781	2.0843
O	-4.4805	-0.9994	-0.4643	O	4.4454	-0.4705	0.8171
H	-4.0106	1.5276	-1.1982	H	3.7274	2.0932	0.5823
H	-1.8655	2.6868	-0.9054	H	1.5127	2.8577	-0.1535
H	-2.3722	-2.0167	0.597	H	2.4902	-1.9997	0.1478
H	0.3289	2.7134	0.0149	H	-0.6216	2.3385	-1.0727
H	2.5892	-0.586	1.1309	H	-2.533	-1.36	-0.9378
H	3.3977	-2.1451	-0.3217	H	-3.9474	-0.4014	0.5087
H	3.0906	-1.919	-2.043	H	-3.6421	-1.215	2.0465
H	5.2094	-0.8137	-1.4993	H	-4.1816	1.1758	2.4416
H	3.998	0.4238	-1.9141	H	-2.5116	0.8163	2.9403
H	4.4336	0.149	-0.2304	H	-2.8061	1.6647	1.4291
H	-5.1309	-0.421	-0.8954	H	5.0213	0.2835	1.0247
Conf 15	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf16	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.4421	-0.5087	0.2229	C	-3.4833	-0.3244	0.2789
C	-3.4687	0.8456	0.5344	C	-3.4109	1.0569	0.4058
C	-2.2918	1.5917	0.4452	C	-2.1883	1.7045	0.2266
C	-1.0938	0.9767	0.0629	C	-1.0377	0.9628	-0.0597
C	-1.0779	-0.3875	-0.2611	C	-1.1182	-0.4313	-0.1941
C	-2.2627	-1.1266	-0.1803	C	-2.3515	-1.074	-0.027
N	0.0519	1.7785	-0.0281	N	0.1601	1.6634	-0.2535
C	1.3396	1.3387	-0.2095	C	1.4143	1.1167	-0.3679
S	0.3863	-1.1884	-0.8791	S	0.2873	-1.4106	-0.6796
O	2.2214	2.1845	-0.3855	O	2.3493	1.8676	-0.6589
C	1.6367	-0.1711	-0.0319	C	1.6065	-0.3678	0.0204
O	2.9314	-0.5522	-0.4861	O	2.8723	-0.8785	-0.3863
C	3.9702	-0.3149	0.4592	C	3.7788	-1.1303	0.6818
C	4.1191	-1.5022	1.3942	C	4.3447	0.1493	1.2711
O	-4.5676	-1.2745	0.291	O	-4.7004	-0.9123	0.4538
H	-4.3881	1.3352	0.8409	H	-4.306	1.6287	0.6363
H	-2.3211	2.6517	0.6848	H	-2.1484	2.7866	0.3207
H	-2.278	-2.1823	-0.4406	H	-2.4203	-2.1515	-0.1466
H	-0.0431	2.7959	0.0055	H	0.1343	2.6802	-0.3603
H	1.5388	-0.3899	1.0385	H	1.4998	-0.4212	1.1117
H	4.8986	-0.1918	-0.1078	H	3.2995	-1.746	1.4515
H	3.8027	0.61	1.0213	H	4.6022	-1.7204	0.2657
H	4.9661	-1.3572	2.071	H	5.11	-0.0774	2.0191
H	3.217	-1.6509	1.9952	H	4.7907	0.7704	0.4877

H	4.2769	-2.4232	0.8234	H	3.5635	0.7459	1.7517
H	-5.3168	-0.7171	0.5584	H	-4.6146	-1.8691	0.3059

Table S2 The Cartesian coordinates of the lowest energy conformers for (8*R*)-2.

Conf 1	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 2	X axis(Å)	Y axis(Å)	Z axis(Å)
O	-4.2787	-1.056	-1.1942	O	-3.8131	1.9904	-1.1752
C	-3.242	-0.791	-0.5776	C	-2.9726	1.1544	-0.829
N	-2.0416	-1.2533	-1.0432	N	-1.7788	1.5725	-0.3081
C	-0.8025	-1.1414	-0.3939	C	-0.6822	0.7566	0.0099
C	0.3472	-1.4927	-1.1107	C	0.3807	1.3326	0.7153
O	0.2074	-1.9109	-2.4087	O	0.2892	2.6523	1.0752
C	1.608	-1.4143	-0.5246	C	1.5096	0.5867	1.0444
C	1.7313	-1.0008	0.8087	C	1.5945	-0.7567	0.6541
C	3.0972	-0.8906	1.4483	C	2.8267	-1.5686	0.9846
C	3.571	0.5592	1.6048	C	3.7569	-1.7678	-0.2178
N	3.6653	1.2738	0.3452	N	4.2556	-0.5238	-0.7747
C	4.6943	1.0611	-0.5404	C	5.2469	0.2051	-0.1626
C	4.6039	1.8983	-1.7866	C	5.6185	1.4617	-0.9007
O	5.587	0.2398	-0.3625	O	5.7604	-0.1068	0.906
C	0.5747	-0.6801	1.5377	C	0.5382	-1.3279	-0.0739
C	-0.6919	-0.7444	0.9423	C	-0.6004	-0.5783	-0.3983
S	-2.1275	-0.4204	1.9447	S	-1.8518	-1.3208	-1.4251
C	-3.2466	0.1664	0.6321	C	-3.2851	-0.3565	-0.8437
O	-2.9001	1.5044	0.2725	O	-3.7038	-0.8449	0.4302
C	-3.9483	2.1714	-0.4267	C	-5.0245	-0.4299	0.7698
C	-3.5011	3.5935	-0.7041	C	-5.3891	-1.0557	2.1019
H	-2.0464	-1.7233	-1.9532	H	-1.6767	2.5758	-0.1287
H	1.0852	-2.1468	-2.7548	H	1.0584	2.8769	1.6262
H	2.5004	-1.6694	-1.0908	H	2.3326	1.0374	1.5936
H	3.0632	-1.3704	2.4345	H	3.3712	-1.0912	1.8085
H	3.8257	-1.4636	0.8616	H	2.5098	-2.5483	1.3638
H	2.8851	1.1274	2.2425	H	4.6164	-2.3769	0.0846
H	4.5582	0.5699	2.0806	H	3.2407	-2.2948	-1.0276
H	2.9178	1.9282	0.1037	H	3.8286	-0.1733	-1.6349
H	5.6042	2.037	-2.2057	H	5.5487	1.3139	-1.9821
H	3.9698	1.3882	-2.5166	H	4.9426	2.2672	-0.6015
H	4.181	2.8824	-1.5655	H	6.6474	1.7381	-0.6544
H	0.6624	-0.3824	2.5815	H	0.6063	-2.366	-0.3956
H	-4.251	0.1522	1.0713	H	-4.0771	-0.5306	-1.5816
H	-4.1553	1.6631	-1.3737	H	-5.0686	0.6604	0.8551
H	-4.8573	2.1831	0.1844	H	-5.7305	-0.7617	7.00E-04
H	-4.2757	4.1486	-1.2406	H	-6.3988	-0.766	2.406

H	-3.2753	4.1161	0.2314	H	-5.3375	-2.1479	2.0418
H	-2.5836	3.5993	-1.3018	H	-4.683	-0.7457	2.8794
Conf 3	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 4	X axis(Å)	Y axis(Å)	Z axis(Å)
O	-4.5205	0.5824	-0.4114	O	-4.0732	0.4491	-1.8286
C	-3.2984	0.4062	-0.4329	C	-3.0436	0.2219	-1.1856
N	-2.4641	1.4064	-0.0139	N	-2.1727	1.2438	-0.9226
C	-1.0629	1.4031	-0.0919	C	-0.9109	1.123	-0.3203
C	-0.3663	2.42	0.5723	C	-0.2434	2.2982	0.0453
O	-1.0856	3.3545	1.2715	O	-0.8635	3.4993	-0.1841
C	1.0253	2.4801	0.5337	C	1.0227	2.2541	0.6255
C	1.7404	1.526	-0.2018	C	1.6459	1.0172	0.8378
C	3.2528	1.5499	-0.2315	C	3.0336	0.9465	1.4363
C	3.875	0.777	0.9373	C	4.1388	1.0908	0.3839
N	3.6008	-0.6467	0.8831	N	4.1775	-0.0179	-0.5512
C	4.3365	-1.4979	0.0926	C	4.7992	-1.2052	-0.2427
C	3.8693	-2.9266	0.1428	C	4.6959	-2.2425	-1.3267
O	5.2657	-1.1318	-0.6185	O	5.3579	-1.4216	0.8269
C	1.0383	0.527	-0.8968	C	0.9845	-0.1602	0.45
C	-0.3591	0.4566	-0.8422	C	-0.2899	-0.1147	-0.1289
S	-1.1946	-0.7777	-1.8155	S	-1.0215	-1.6289	-0.7143
C	-2.6878	-0.9652	-0.7891	C	-2.7754	-1.1601	-0.5543
O	-2.3764	-1.7423	0.3682	O	-3.1634	-1.2204	0.8177
C	-3.5392	-2.2787	0.995	C	-4.5778	-1.2733	0.986
C	-3.0935	-3.1296	2.1683	C	-4.8736	-1.3953	2.4681
H	-2.9033	2.2341	0.3993	H	-2.4718	2.1871	-1.1865
H	-0.47	4.0019	1.6546	H	-0.3154	4.2108	0.1876
H	1.5604	3.2615	1.0659	H	1.5332	3.1699	0.9101
H	3.6063	1.1498	-1.19	H	3.1378	1.7458	2.1808
H	3.5919	2.5928	-0.1963	H	3.1466	0.0047	1.9875
H	4.9613	0.9212	0.9306	H	4.0036	2.0041	-0.2056
H	3.4927	1.1417	1.8969	H	5.1111	1.1545	0.8853
H	2.795	-1.0083	1.3985	H	3.6758	0.0732	-1.4373
H	3.5205	-3.1868	1.1462	H	3.7489	-2.7786	-1.2219
H	3.0522	-3.0626	-0.5707	H	4.741	-1.7776	-2.3157
H	4.6974	-3.5905	-0.1198	H	5.5265	-2.9479	-1.2367
H	1.5917	-0.2028	-1.4871	H	1.476	-1.1218	0.5951
H	-3.4098	-1.506	-1.4122	H	-3.3349	-1.9084	-1.1279
H	-4.1828	-1.4699	1.3548	H	-5.04	-0.3611	0.5958
H	-4.0972	-2.8959	0.2825	H	-4.9854	-2.1409	0.4557
H	-3.954	-3.5659	2.6831	H	-5.9512	-1.4406	2.6486
H	-2.4362	-3.9378	1.8308	H	-4.4077	-2.296	2.8814
H	-2.5202	-2.5302	2.8832	H	-4.4589	-0.5422	3.0154

Conf 5	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 6	X axis(Å)	Y axis(Å)	Z axis(Å)
O	-4.6774	1.4326	-0.0142	O	-4.6779	1.4319	-0.0115
C	-3.5827	0.8883	-0.1895	C	-3.5832	0.888	-0.1878
N	-2.4345	1.5629	0.1225	N	-2.435	1.5626	0.1244
C	-1.1241	1.1316	-0.1344	C	-1.1245	1.1318	-0.1336
C	-0.0715	1.859	0.4336	C	-0.0719	1.8589	0.4347
O	-0.3728	2.9382	1.2236	O	-0.373	2.9372	1.2258
C	1.2537	1.4957	0.2076	C	1.2533	1.496	0.2077
C	1.5435	0.4009	-0.6179	C	1.5429	0.402	-0.619
C	2.9758	-0.0112	-0.853	C	2.9752	-0.0096	-0.8552
C	3.481	-0.9506	0.2447	C	3.4817	-0.9485	0.2424
N	4.8756	-1.304	0.0634	N	4.876	-1.3024	0.06
C	5.8871	-0.4439	0.4258	C	5.888	-0.4377	0.4098
C	7.2668	-0.9859	0.171	C	7.2673	-0.9933	0.1838
O	5.6934	0.6773	0.8837	O	5.6954	0.6769	0.8838
C	0.4889	-0.3146	-1.2065	C	0.4882	-0.3131	-1.2078
C	-0.8446	0.045	-0.9691	C	-0.8452	0.046	-0.9694
S	-2.1345	-0.8297	-1.8311	S	-2.1353	-0.8281	-1.8316
C	-3.4784	-0.5885	-0.6242	C	-3.4787	-0.5883	-0.6239
O	-3.2943	-1.4769	0.478	O	-3.2939	-1.4777	0.4773
C	-4.476	-1.6327	1.2598	C	-4.4753	-1.6346	1.2595
C	-4.1902	-2.6449	2.352	C	-4.1888	-2.6478	2.3506
H	-2.5395	2.4678	0.5909	H	-2.54	2.467	0.5936
H	0.458	3.3229	1.5522	H	0.4579	3.3216	1.5545
H	2.0689	2.0543	0.6618	H	2.0686	2.0544	0.662
H	3.0684	-0.4975	-1.8328	H	3.0673	-0.496	-1.8348
H	3.6029	0.8872	-0.9146	H	3.6018	0.8892	-0.9174
H	3.3673	-0.4898	1.2332	H	3.3694	-0.4872	1.2309
H	2.9086	-1.8849	0.2466	H	2.909	-1.8826	0.2456
H	5.1055	-2.2199	-0.3275	H	5.1057	-2.2262	-0.312
H	7.2952	-2.0687	0.3224	H	7.5686	-1.5747	1.0591
H	7.5585	-0.7569	-0.8573	H	7.2892	-1.6346	-0.7019
H	7.974	-0.5208	0.8632	H	7.9712	-0.1702	0.033
H	0.7086	-1.1556	-1.8623	H	0.7078	-1.1534	-1.8645
H	-4.4016	-0.8501	-1.1545	H	-4.4021	-0.8496	-1.1541
H	-4.7586	-0.6775	1.7134	H	-4.7579	-0.6799	1.7141
H	-5.2972	-1.9916	0.6299	H	-5.2967	-1.9931	0.6296
H	-5.0713	-2.7998	2.9809	H	-5.0696	-2.8034	2.9798
H	-3.8916	-3.6054	1.919	H	-3.8901	-3.6077	1.9166
H	-3.3606	-2.3079	2.9823	H	-3.3589	-2.3111	2.9809
Conf 7	X axis(Å)	Y axis(Å)	Z axis(Å)				

O	-4.4674	1.486	-1.1003				
C	-3.4578	0.8422	-0.7977				
N	-2.3037	1.5045	-0.4805				
C	-1.0513	0.9187	-0.2403				
C	-0.031	1.7358	0.2606				
O	-0.3098	3.0555	0.5059				
C	1.2413	1.2245	0.5042				
C	1.5129	-0.1233	0.2325				
C	2.8954	-0.6791	0.4698				
C	3.8092	-0.4607	-0.7385				
N	5.1594	-0.9301	-0.4949				
C	6.0588	-0.1827	0.2308				
C	7.4102	-0.8275	0.3733				
O	5.785	0.8954	0.7473				
C	0.4987	-0.9351	-0.2994				
C	-0.7839	-0.422	-0.5346				
S	-1.9963	-1.4686	-1.3136				
C	-3.4994	-0.6917	-0.6362				
O	-3.6779	-1.1003	0.7196				
C	-5.0002	-0.8612	1.1953				
C	-5.0973	-1.3956	2.611				
H	-2.358	2.5247	-0.4081				
H	0.4858	3.4766	0.8743				
H	2.0305	1.8609	0.8979				
H	3.321	-0.2129	1.3675				
H	2.8313	-1.7501	0.7016				
H	3.4308	-1.0039	-1.6116				
H	3.8554	0.6023	-1.0036				
H	5.4469	-1.83	-0.8847				
H	7.4002	-1.4952	1.2388				
H	7.6661	-1.4005	-0.5225				
H	8.1691	-0.0537	0.518				
H	0.7115	-1.9761	-0.5373				
H	-4.328	-1.0725	-1.2448				
H	-5.214	0.2122	1.1957				
H	-5.7267	-1.375	0.5564				
H	-6.0983	-1.2352	3.0209				
H	-4.8728	-2.4671	2.6349				
H	-4.3661	-0.9023	3.2601				

Table S3 The Cartesian coordinates of the lowest energy conformers for (7*R*)-**3**

Conf 1	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 2	X axis(Å)	Y axis(Å)	Z axis(Å)
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O	1.9789	3.2723	-1.1155	O	-5.6653	-0.7342	-0.5814
C	1.9314	2.6416	-0.0613	C	-4.4748	-1.0368	-0.608
N	2.6007	1.4613	0.051	N	-3.5502	-0.1246	-1.0197
C	2.6314	0.5249	1.1698	C	-2.0984	-0.2636	-1.0609
C	1.9375	-0.824	0.858	C	-1.433	0.2902	0.218
O	2.5574	-1.3876	-0.3109	O	-1.6153	1.7168	0.2295
C	2.3881	-2.8019	-0.4033	C	-1.5652	2.267	1.5454
C	3.042	-3.2739	-1.6868	C	-1.7171	3.7712	1.4363
H	2.1289	-1.4935	1.7076	H	-1.9303	-0.1421	1.0966
C	0.4356	-0.6563	0.6776	C	0.0479	-0.0533	0.2283
C	-0.1078	-0.2935	-0.573	C	0.9676	0.7008	-0.5308
C	-1.4979	-0.1202	-0.6905	C	2.3274	0.3434	-0.5066
C	-2.3521	-0.299	0.397	C	2.7867	-0.7397	0.2426
C	-1.7887	-0.6611	1.6369	C	1.8492	-1.4825	0.9879
O	-2.587	-0.8455	2.7414	O	2.2497	-2.5616	1.7403
C	-0.4138	-0.8361	1.7765	C	0.4977	-1.1451	0.9807
N	-3.7037	-0.0964	0.1501	N	4.1514	-0.9884	0.1796
C	-3.859	0.2352	-1.1124	C	4.7102	-0.0973	-0.6086
S	-2.4372	0.3198	-2.0655	S	3.6675	1.0672	-1.3117
C	1.1546	3.1367	1.1266	C	-3.9904	-2.4016	-0.2028
H	3.094	1.1767	-0.8003	H	-3.9423	0.7908	-1.2584
H	3.6949	0.3394	1.3584	H	-1.8406	-1.3161	-1.2142
H	2.2027	0.982	2.0658	H	-1.7674	0.2995	-1.9412
H	1.3244	-3.061	-0.4149	H	-0.6099	2.0255	2.0231
H	2.866	-3.2857	0.4554	H	-2.3828	1.8551	2.147
H	2.9431	-4.3571	-1.7998	H	-1.6898	4.239	2.4243
H	4.1054	-3.0129	-1.6968	H	-2.6631	4.029	0.9488
H	2.5856	-2.7847	-2.5537	H	-0.916	4.1954	0.8219
H	0.538	-0.1396	-1.4351	H	0.6344	1.5528	-1.1196
H	-3.4965	-0.6735	2.4215	H	3.2182	-2.6143	1.6056
H	-0.019	-1.1112	2.7517	H	-0.1938	-1.7435	1.5696
H	-4.8317	0.4457	-1.5381	H	5.7738	-0.0915	-0.8096
H	0.6733	4.0868	0.877	H	-4.8287	-2.9844	0.1897
H	0.3792	2.417	1.3994	H	-3.578	-2.922	-1.0713
H	1.8282	3.2997	1.972	H	-3.2306	-2.3198	0.5786
Conf 3	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 4	X axis(Å)	Y axis(Å)	Z axis(Å)
O	-5.7893	-0.7362	-0.517	O	5.6254	0.7739	-0.7726
C	-4.6306	-1.1397	-0.5848	C	4.4941	0.3412	-0.9869
N	-3.5975	-0.2836	-0.3516	N	3.4238	1.1689	-0.8241
C	-2.1659	-0.5483	-0.4371	C	2.005	0.8502	-0.9516
C	-1.3659	0.3415	0.5382	C	1.3497	0.5261	0.4112
O	-1.6007	1.715	0.18	O	1.8147	-0.7587	0.8513

C	-1.3596	2.6159	1.2609	C	1.7745	-0.9056	2.2698
C	-1.5993	4.0274	0.7628	C	2.2457	-2.3046	2.6133
H	-1.7424	0.1719	1.556	H	1.654	1.2902	1.1394
C	0.115	0.0096	0.4561	C	-0.1647	0.5068	0.2709
C	0.909	0.518	-0.5938	C	-0.8214	-0.6135	-0.2814
C	2.2727	0.1789	-0.6438	C	-2.2218	-0.5904	-0.4067
C	2.8565	-0.6507	0.3133	C	-2.9749	0.5126	-0.0048
C	2.0429	-1.152	1.3492	C	-2.2974	1.6224	0.5386
O	2.569	-1.9767	2.3157	O	-2.9931	2.7359	0.9474
C	0.69	-0.8276	1.4197	C	-0.9109	1.6208	0.6741
N	4.2109	-0.9099	0.1494	N	-4.3482	0.4097	-0.1837
C	4.6386	-0.2775	-0.9205	C	-4.6216	-0.7619	-0.713
S	3.4789	0.6443	-1.7824	S	-3.2886	-1.7925	-1.027
C	-4.3016	-2.571	-0.9065	C	4.2564	-1.0701	-1.4469
H	-3.8825	0.6896	-0.2008	H	3.6877	2.1125	-0.5299
H	-1.9735	-1.607	-0.2373	H	1.5386	1.7351	-1.3991
H	-1.8842	-0.3411	-1.4762	H	1.8849	0.0146	-1.6481
H	-0.3281	2.5196	1.6154	H	0.7542	-0.757	2.6386
H	-2.0457	2.3928	2.0851	H	2.437	-0.1675	2.7348
H	-1.4316	4.7565	1.5604	H	2.2379	-2.4647	3.695
H	-2.6241	4.1371	0.3929	H	3.2607	-2.4726	2.2379
H	-0.9319	4.2588	-0.0739	H	1.603	-3.0543	2.14
H	0.4775	1.1708	-1.3497	H	-0.2565	-1.4881	-0.5966
H	3.5148	-2.0675	2.0789	H	-3.932	2.5236	0.7677
H	0.0961	-1.2352	2.2348	H	-0.426	2.497	1.0984
H	5.6688	-0.3307	-1.2486	H	-5.6339	-1.0687	-0.9427
H	-5.2177	-3.1046	-1.1757	H	5.2161	-1.587	-1.5408
H	-3.6113	-2.6204	-1.7528	H	3.6441	-1.6124	-0.7247
H	-3.8566	-3.0545	-0.0329	H	3.7687	-1.0685	-2.4251
Conf 5	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 6	X axis(Å)	Y axis(Å)	Z axis(Å)
O	-2.9473	2.9079	-0.6422	O	-5.4659	-1.4809	-0.1707
C	-3.1691	1.7075	-0.7937	C	-4.2564	-1.5332	-0.3798
N	-2.2327	0.9267	-1.401	N	-3.5939	-0.4306	-0.8288
C	-2.2429	-0.5195	-1.5961	C	-2.1635	-0.2691	-1.0695
C	-1.4932	-1.3199	-0.4994	C	-1.4432	0.3408	0.1534
O	-2.1772	-1.1518	0.7509	O	-1.8821	1.7027	0.2898
C	-1.9217	-2.2066	1.6771	C	-1.711	2.2116	1.6114
C	-2.6624	-1.8951	2.9625	C	-2.175	3.6546	1.6275
H	-1.5515	-2.3805	-0.7798	H	-1.7329	-0.2185	1.0529
C	-0.0308	-0.9068	-0.4008	C	0.0638	0.2816	-0.0403
C	0.3607	0.1749	0.417	C	0.8136	-0.6976	0.643
C	1.7184	0.5357	0.47	C	2.2056	-0.7501	0.4431

C	2.686	-0.1462	-0.2672	C	2.8589	0.136	-0.4134
C	2.2726	-1.2202	-1.0807	C	2.0889	1.1039	-1.0886
O	3.1869	-1.9229	-1.8302	O	2.6848	1.9988	-1.9454
C	0.9326	-1.5949	-1.1486	C	0.7103	1.1752	-0.9048
N	3.9907	0.3089	-0.1281	N	4.2341	-0.0255	-0.5214
C	3.9991	1.3251	0.7058	C	4.6083	-1.0226	0.2484
S	2.4871	1.7909	1.3646	S	3.3718	-1.8167	1.1302
C	-4.46	1.0764	-0.3516	C	-3.4646	-2.7926	-0.1599
H	-1.3906	1.4413	-1.6715	H	-4.1843	0.3992	-0.9381
H	-3.2814	-0.8603	-1.6449	H	-1.7311	-1.2382	-1.3371
H	-1.7803	-0.6997	-2.5729	H	-2.0777	0.394	-1.938
H	-0.8489	-2.288	1.8801	H	-0.6579	2.1593	1.907
H	-2.2817	-3.1545	1.2628	H	-2.3111	1.6221	2.3131
H	-2.5027	-2.6814	3.7055	H	-2.0672	4.0882	2.6257
H	-3.7369	-1.7985	2.7748	H	-3.2243	3.7258	1.3224
H	-2.3248	-0.9405	3.3794	H	-1.5953	4.2534	0.9173
H	-0.3767	0.7255	0.9984	H	0.3344	-1.4031	1.3169
H	4.0473	-1.4979	-1.6348	H	3.6374	1.7759	-1.9188
H	0.6551	-2.4282	-1.7899	H	0.1449	1.9393	-1.4352
H	4.9097	1.8475	0.9694	H	5.6422	-1.3334	0.3272
H	-5.0982	1.8384	0.1055	H	-4.1094	-3.5556	0.2858
H	-4.9856	0.6571	-1.2135	H	-3.0886	-3.1663	-1.1159
H	-4.2738	0.2959	0.388	H	-2.6308	-2.6042	0.5212
Conf 7	X axis(Å)	Y axis(Å)	Z axis(Å)	Conf 8	X axis(Å)	Y axis(Å)	Z axis(Å)
O	5.7019	-1.2745	-0.0504	O	5.5726	0.6055	-0.7757
C	4.5333	-1.4911	0.2611	C	4.3838	0.9153	-0.7913
N	3.5984	-0.511	0.12	N	3.446	-0.0051	-1.1515
C	2.1843	-0.5515	0.4756	C	1.9941	0.1394	-1.1618
C	1.3461	0.3741	-0.4326	C	1.3624	-0.3479	0.16
O	1.8077	1.7215	-0.2369	O	1.5451	-1.7721	0.2392
C	1.4612	2.5912	-1.314	C	1.6217	-2.2682	1.575
C	1.981	3.9775	-0.9891	C	3.0404	-2.1598	2.1056
H	1.5244	0.0904	-1.4786	H	1.8727	0.1379	1.0008
C	-0.1305	0.2484	-0.0936	C	-0.1203	-0.0125	0.1908
C	-0.9725	-0.5141	-0.9288	C	-1.0566	-0.818	-0.4911
C	-2.3345	-0.6327	-0.5951	C	-2.4175	-0.4657	-0.4511
C	-2.8692	-0.0209	0.5386	C	-2.8621	0.6615	0.2395
C	-2.0082	0.7328	1.3608	C	-1.9086	1.455	0.9082
O	-2.4857	1.3536	2.4907	O	-2.2943	2.5788	1.6004
C	-0.6573	0.865	1.0492	C	-0.5558	1.1237	0.8838
N	-4.2271	-0.2189	0.7529	N	-4.2296	0.8998	0.1996
C	-4.706	-0.9713	-0.2123	C	-4.8049	-0.0429	-0.5132

S	-3.5926	-1.4821	-1.4109	S	-3.7752	-1.2456	-1.1695
C	4.0817	-2.826	0.7852	C	3.9155	2.2973	-0.4277
H	3.9784	0.3951	-0.1729	H	3.8282	-0.9311	-1.3638
H	1.8196	-1.5817	0.4148	H	1.7365	1.1847	-1.3589
H	2.128	-0.2304	1.5221	H	1.6374	-0.464	-2.0045
H	0.3744	2.626	-1.4428	H	1.3364	-3.3247	1.54
H	1.9216	2.2311	-2.2404	H	0.9085	-1.7569	2.231
H	1.7433	4.6815	-1.7914	H	3.1179	-2.6164	3.0965
H	3.0664	3.9586	-0.8452	H	3.3608	-1.1163	2.18
H	1.5422	4.3442	-0.0552	H	3.742	-2.6601	1.43
H	-0.5861	-1.0043	-1.8188	H	-0.7352	-1.7045	-1.0337
H	-3.4399	1.137	2.5122	H	-3.2665	2.6181	1.4907
H	-0.0199	1.4599	1.701	H	0.1483	1.7621	1.4128
H	-5.7487	-1.2588	-0.2557	H	-5.8737	-0.0663	-0.6829
H	4.9527	-3.4659	0.9532	H	4.7659	2.8907	-0.0798
H	3.5554	-2.7022	1.7354	H	3.4831	2.7856	-1.305
H	3.4261	-3.3082	0.0553	H	3.1756	2.2499	0.3754