Supporting Information

Conformational Analyses of Thiirane-Based Gelatinase Inhibitors

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Syntheses of compounds 1-3

Compound **1** was synthesized according to the literature procedure developed in our laboratory.[1]

2-Bromo-1,3-dimethyl-5-phenoxybenzene (5b). The procedure was modified from that reported by Ma and Cai.[2] A mixture of 4-bromo-3,5-dimethylphenol (**4b**, 5.0 g, 25 mmol), 4-iodobenzene (5.6 mL, 50 mmol), Cs_2CO_3 (8.1 g, 25 mmol), *N*,*N*-dimethylglycine hydrochloride salt (1.0 g, 7.2 mmol), CuI (0.24 g, 1.3 mmol) in degassed 1,4-dioxane (50 mL) was heated at 90 ºC for 3.5 h under a nitrogen atmosphere. After dilution with water, the mixture was extracted with ethyl acetate. The combined organic layer was washed with water and brine, dried over anhydrous $MgSO_4$, and concentrated under reduced pressure. The resultant residue was purified by silica gel column chromatography (hexane to ethyl acetate/hexane = 1/20) to give the title compound as a colorless oil (2.5 g, 40%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.44 (s, 6H), 6.82 (s, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.9 Hz, 2 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 24.2, 118.8, 119.0, 121.2, 123.5, 129.9, 139.8, 155.9, 157.2; HRMS (FAB) calcd for $C_{14}H_{13}BrO$ (M^+) 276.0150, found 276.0147.

1-Chloro-3-(2,6-dimethyl-4-phenoxyphenylsulfanyl)-propan-2-ol (6b). This was prepared from **5b** according to a literature procedure developed in our laboratory.[1, 3] ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.54 (s, 6H), 2.73 (br. s., 1H), 2.83 (dd, *J* = 13.4, 7.2 Hz, 1H), 2.89 (dd, *J* = 13.4, 5.6

Hz, 1H), 3.66 (dd, *J* = 11.2, 5.8 Hz, 1H), 3.73 (dd, *J* = 11.2, 4.2 Hz, 1H), 3.85 (m, 1H), 6.78 (s, 2H), 7.05 (d, *J* = 8.4 Hz, 2H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.38 (t, *J* = 7.9 Hz, 2 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 22.4, 39.8, 48.4, 70.4, 118.1, 119.6, 123.9, 126.3, 130.0, 145.0, 156.5, 157.7; HRMS (FAB) calcd for $C_{17}H_{19}ClO_2S$ (M^+) 322.0794, found 322.0811.

2-(2,6-Dimethyl-4-phenoxybenzenesulfonylmethyl)-oxirane (7b). This was prepared from **6b** according to a literature procedure developed in our laboratory.[1,3] ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.53 (dd, *J* = 4.8, 2.4 Hz, 1H), 2.65 (s, 6H), 2.85 (t, *J* = 4.3 Hz, 1H), 3.23 (dd, *J* = 13.8, 4.8 Hz, 1H), 3.34 (m, 1H), 3.40 (dd, *J* = 14.0, 6.6 Hz, 1H), 6.72 (s, 2H), 7.07 (d, *J* = 7.6 Hz, 2H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 2 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 23.5, 45.9, 46.1, 59.7, 119.7, 120.7, 125.2, 129.9, 130.3, 143.2, 154.9, 161.1; HRMS (FAB) calcd for $C_{17}H_{19}O_4S$ ($M+H^+$) 319.1004, found 319.1000.

2-(2,6-Dimethyl-4-phenoxy-benzenesulfonylmethyl)-thiirane (3). This was prepared from **7b** according to a literature procedure developed in our laboratory.[1,3] ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.22 (m, 1H), 2.57 (m, 1H), 2.64 (s, 6H), 3.16 (m, 3H), 3.56 (dd, *J* = 13.4, 4.8 Hz, 1H), 6.72 (s, 2H), 7.07 (d, *J* = 7.8 Hz, 2H), 7.24 (m, 1H), 7.41 (t, *J* = 8.0 Hz, 2 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 23.5, 24.4, 26.1, 62.5, 119.8, 120.5, 125.1, 129.2, 130.3, 143.3, 154.9, 161.0; HRMS (FAB) calcd for $C_{17}H_{19}O_3S_2$ ($M+H^+$) 335.0776, found 335.0758.

Synthetic transformation of compound **4a** to compound **2** was done by same method for the synthesis of compound **3** from **4b**.

1-Bromo-2-methyl-4-phenoxybenzene (5a). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.38 (s, 3H), 6.73 (dd, *J* = 8.7, 2.7 Hz, 1H), 6.92 (d, *J* = 2.6 Hz, 1H), 7.02 (d, *J* = 8.4 Hz, 2H), 7.14 (t, *J* = 7.2 Hz, 1H), 7.36 (t, *J* = 7.7 Hz, 2H), 7.47 (d, *J* = 8.8 Hz, 1 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 23.3, 118.0, 118.4, 119.1, 121.3, 123.7, 130.0, 133.4, 139.6, 156.7, 157.1; HRMS (FAB) calcd for $C_{13}H_{11}BrO$ (M^+) 262.9993, found 262.9985.

2-(2-Methyl-4-phenoxybenzenesulfonylmethyl)-oxirane (7a). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.46 (dd, *J* = 4.5, 2.3 Hz, 1H), 2.59 (s, 3H), 2.75 (t, *J* = 4.3 Hz, 1H), 3.19 - 3.37 (m, 3H), 6.83 - 6.91 (m, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 7.20 (t, *J* = 7.4 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 2H), 7.93 (d, *J* = 8.8 Hz, 1 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 20.5, 45.7, 45.7, 58.7, 114.7, 120.4, 120.8, 125.0, 130.1, 130.8, 132.6, 140.8, 154.7, 162.3; HRMS (FAB) calcd for $C_{16}H_{17}O_4S$ ($M+H^+$) 305.0848, found 305.0846.

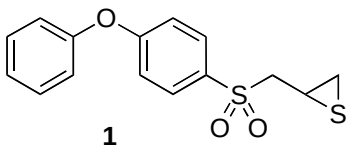
2-(2-Methyl-4-phenoxy-benzenesulfonylmethyl)-thiirane (2). ^{1}H NMR (500 MHz, $CDCl_3$) δ

2.20 (d, J = 5.0 Hz, 1H), 2.55 (d, J = 6.0 Hz, 1H), 2.64 (s, 3H), 3.08 (m, 1H), 3.22 (dd, J = 14.2, 7.8 Hz, 1H), 3.59 (dd, J = 14.3, 5.7 Hz, 1H), 6.92 (m, 2H), 7.10 (d, J = 8.4 Hz, 2H), 7.27 (t, J = 7.4 Hz, 1H), 7.45 (t, J = 7.8 Hz, 2H), 7.98 (d, J = 9.4 Hz, 1 H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 20.9, 24.4, 26.3, 62.0, 115.2, 120.6, 121.2, 125.3, 130.4, 133.3, 141.1, 155.0, 162.7; HRMS (FAB) calcd for $C_{16}H_{17}O_3S_2$ ($M+H^+$) 321.0619, found 321.0612.

References

1. Lim, I. T.; Brown, S.; Mobashery, S., *J. Org. Chem.* **2004,** *69*, 3572.
2. Ma, D. W.; Cai, Q., *Org. Lett.* **2003,** *5*, 3799.
3. Lee, M.; Bernardo, M. M.; Meroueh, S. O.; Brown, S.; Fridman, R.; Mobashery, S., *Org. Lett.* **2005,** *7*, 4463.
4. Reference 24. Case, D. A.; Darden, T. A.; T.E. Cheatham, I.; Simmerling, C. L.; Wang, J.; Duke, R. E.; Luo, R.; Merz, K. M.; Wang, B.; Pearlman, D. A.; Crowley, M.; Brozell, S.; Tsui, V.; Gohlke, H.; Mongan, J.; Hornak, V.; Cui, G.; Beroza, P.; Schafmeister, C.; Caldwell, J. W.; Ross, W. S.; Kollman, P. A. *AMBER 8*; University of California: San Francisco, 2004.
5. Reference 26. Frisch, M. J.; Trucks, G. W.; H. B. Schlegel; G. E. Scuseria; M. A. Robb; J. R. Cheeseman; J. A. Montgomery, J.; T. Vreven; K. N. Kudin; J. C. Burant; J. M. Millam; S. S. Iyengar; J. Tomasi; V. Barone; B. Mennucci; M. Cossi; G. Scalmani; N. Rega; G. A. Petersson; H. Nakatsuji; M. Hada; M. Ehara; K. Toyota; R. Fukuda; J. Hasegawa; M. Ishida; T. Nakajima; Y. Honda; O. Kitao; H. Nakai; M. Klene; X. Li; J. E. Knox; H. P. Hratchian; J. B. Cross; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03, Revision C.02*; Gaussian, Inc.: Wallingford, CT, 2004.

Table S1-1. Crystal data and structure refinement for compound **1**.



1

Identification code	dh11_1_0m	
Empirical formula	C15 H14 O3 S2	
Formula weight	306.38	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 5.40350(10) Å	α= 90°.
	b = 28.1118(6) Å	β= 95.7320(10)°.
	c = 9.3269(2) Å	γ = 90°.
Volume	1409.69(5) Å^3	
Z	4	
Density (calculated)	1.444 Mg/m^3	
Absorption coefficient	3.464 mm^{-1}	
F(000)	640	
Crystal size	0.36 x 0.19 x 0.09 mm^3	
Crystal color and habit	clear colorless block	
Diffractometer	Bruker SMART Apex CCD diffractometer	
Theta range for data collection	3.14 to 69.55°.	
Index ranges	-4<=h<=6, -32<=k<=32, -11<=l<=10	
Reflections collected	12650	
Independent reflections	2424 [R(int) = 0.0287]	
Observed reflections (I > 2sigma(I))	2266	
Completeness to theta = 69.55°	91.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7434 and 0.3677	
Solution method	XS (Sheldrick, 2001)	
Refinement method	XL (Sheldrick, 2001)	
Data / restraints / parameters	2424 / 0 / 200	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0366, wR2 = 0.0952	
R indices (all data)	R1 = 0.0392, wR2 = 0.0969	
Largest diff. peak and hole	0.424 and -0.332 e.Å^{-3}	

Table S1-2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for compound **1**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
S(1)	0.81010(9)	0.444237(17)	0.87821(5)	0.02256(16)
S(2)	0.65494(11)	0.57244(2)	0.61309(6)	0.03166(18)
O(1)	0.5727(3)	0.28873(5)	0.46374(14)	0.0261(3)
O(2)	1.0718(3)	0.45435(5)	0.87674(17)	0.0298(4)
O(3)	0.7156(3)	0.43243(5)	1.01242(16)	0.0291(3)
C(1)	0.4185(4)	0.25088(7)	0.4959(2)	0.0227(4)
C(2)	0.5027(4)	0.21787(8)	0.5993(2)	0.0276(5)
C(3)	0.3550(5)	0.17865(8)	0.6214(2)	0.0339(5)
C(4)	0.1257(5)	0.17325(8)	0.5413(2)	0.0351(6)
C(5)	0.0445(4)	0.20684(9)	0.4393(2)	0.0324(5)
C(6)	0.1905(4)	0.24614(8)	0.4155(2)	0.0263(5)
C(7)	0.6213(4)	0.32372(7)	0.5653(2)	0.0199(4)
C(8)	0.4711(3)	0.33211(7)	0.6754(2)	0.0198(4)
C(9)	0.5283(3)	0.36926(7)	0.7706(2)	0.0188(4)
C(10)	0.7361(3)	0.39734(7)	0.7553(2)	0.0184(4)
C(11)	0.8853(4)	0.38903(7)	0.6446(2)	0.0207(4)
C(12)	0.8274(4)	0.35236(7)	0.5491(2)	0.0218(4)
C(13)	0.6423(10)	0.49499(19)	0.8177(5)	0.0185(10)
C(13')	0.620(2)	0.4913(5)	0.7604(12)	0.020(2)
C(14)	0.7244(6)	0.50990(10)	0.6717(3)	0.0246(9)
C(14')	0.7422(14)	0.5376(3)	0.7714(8)	0.031(2)
C(15)	0.9476(5)	0.54217(10)	0.6721(3)	0.0403(6)

Table S1-3. Bond lengths [Å] and angles [°] for compound **1**.

S(1)-O(3)	1.4370(16)	S(1)-O(2)	1.4440(16)
S(1)-C(13)	1.754(5)	S(1)-C(10)	1.7666(19)
S(1)-C(13')	1.945(11)	S(2)-C(14')	1.795(7)
S(2)-C(15)	1.832(3)	S(2)-C(14)	1.868(3)
O(1)-C(7)	1.372(2)	O(1)-C(1)	1.402(2)
C(1)-C(2)	1.382(3)	C(1)-C(6)	1.383(3)
C(2)-C(3)	1.389(3)	C(2)-H(2)	0.9500
C(3)-C(4)	1.390(4)	C(3)-H(3)	0.9500

C(4)-C(5)	1.380(4)	C(4)-H(4)	0.9500
C(5)-C(6)	1.389(3)	C(5)-H(5)	0.9500
C(6)-H(6)	0.9500	C(7)-C(8)	1.391(3)
C(7)-C(12)	1.395(3)	C(8)-C(9)	1.386(3)
C(8)-H(8)	0.9500	C(9)-C(10)	1.391(3)
C(9)-H(9)	0.9500	C(10)-C(11)	1.392(3)
C(11)-C(12)	1.378(3)	C(11)-H(11)	0.9500
C(12)-H(12)	0.9500	C(13)-C(14)	1.532(6)
C(13)-H(13A)	0.9900	C(13)-H(13B)	0.9900
C(13')-C(14')	1.458(15)	C(13')-H(13C)	0.9900
C(13')-H(13D)	0.9900	C(14)-C(15)	1.509(4)
C(14)-H(14)	1.0000	C(14')-C(15)	1.521(8)
C(14')-H(14')	1.0000	C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900		

O(3)-S(1)-O(2)	119.15(9)	O(3)-S(1)-C(13)	104.54(18)
O(2)-S(1)-C(13)	108.2(2)	O(3)-S(1)-C(10)	108.42(9)
O(2)-S(1)-C(10)	107.41(9)	C(13)-S(1)-C(10)	108.78(16)
O(3)-S(1)-C(13')	115.8(4)	O(2)-S(1)-C(13')	108.8(4)
C(13)-S(1)-C(13')	15.9(3)	C(10)-S(1)-C(13')	93.9(4)
C(14')-S(2)-C(15)	49.6(3)	C(14')-S(2)-C(14)	38.5(3)
C(15)-S(2)-C(14)	48.13(12)	C(7)-O(1)-C(1)	118.24(15)
C(2)-C(1)-C(6)	121.8(2)	C(2)-C(1)-O(1)	119.83(19)
C(6)-C(1)-O(1)	118.22(18)	C(1)-C(2)-C(3)	118.9(2)
C(1)-C(2)-H(2)	120.6	C(3)-C(2)-H(2)	120.6
C(2)-C(3)-C(4)	120.1(2)	C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0	C(5)-C(4)-C(3)	120.1(2)
C(5)-C(4)-H(4)	120.0	C(3)-C(4)-H(4)	120.0
C(4)-C(5)-C(6)	120.5(2)	C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7	C(1)-C(6)-C(5)	118.6(2)
C(1)-C(6)-H(6)	120.7	C(5)-C(6)-H(6)	120.7
O(1)-C(7)-C(8)	123.03(18)	O(1)-C(7)-C(12)	116.04(17)
C(8)-C(7)-C(12)	120.88(18)	C(9)-C(8)-C(7)	119.44(18)
C(9)-C(8)-H(8)	120.3	C(7)-C(8)-H(8)	120.3
C(8)-C(9)-C(10)	119.50(18)	C(8)-C(9)-H(9)	120.3
C(10)-C(9)-H(9)	120.3	C(9)-C(10)-C(11)	120.94(18)

C(9)-C(10)-S(1)	119.30(15)	C(11)-C(10)-S(1)	119.77(15)
C(12)-C(11)-C(10)	119.64(18)	C(12)-C(11)-H(11)	120.2
C(10)-C(11)-H(11)	120.2	C(11)-C(12)-C(7)	119.59(18)
C(11)-C(12)-H(12)	120.2	C(7)-C(12)-H(12)	120.2
C(14)-C(13)-S(1)	108.8(3)	C(14)-C(13)-H(13A)	109.9
S(1)-C(13)-H(13A)	109.9	C(14)-C(13)-H(13B)	109.9
S(1)-C(13)-H(13B)	109.9	H(13A)-C(13)-H(13B)	108.3
C(14')-C(13')-S(1)	111.0(7)	C(14')-C(13')-H(13C)	109.4
S(1)-C(13')-H(13C)	109.4	C(14')-C(13')-H(13D)	109.4
S(1)-C(13')-H(13D)	109.4	H(13C)-C(13')-H(13D)	108.0
C(15)-C(14)-C(13)	117.7(3)	C(15)-C(14)-S(2)	64.67(15)
C(13)-C(14)-S(2)	116.7(3)	C(15)-C(14)-H(14)	116.0
C(13)-C(14)-H(14)	116.0	S(2)-C(14)-H(14)	116.0
C(13')-C(14')-C(15)	112.6(7)	C(13')-C(14')-S(2)	110.5(6)
C(15)-C(14')-S(2)	66.5(3)	C(13')-C(14')-H(14')	118.8
C(15)-C(14')-H(14')	118.8	S(2)-C(14')-H(14')	118.8
C(14)-C(15)-C(14')	47.1(3)	C(14)-C(15)-S(2)	67.20(14)
C(14')-C(15)-S(2)	64.0(3)	C(14)-C(15)-H(15A)	117.0
C(14')-C(15)-H(15A)	163.6	S(2)-C(15)-H(15A)	117.0
C(14)-C(15)-H(15B)	117.0	C(14')-C(15)-H(15B)	76.9
S(2)-C(15)-H(15B)	117.0	H(15A)-C(15)-H(15B)	114.0

Table S1-4. Anisotropic displacement parameters (Å^2) for compound **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	0.0169(3)	0.0162(3)	0.0343(3)	-0.00175(19)	0.00154(19)	-0.00079(17)
S(2)	0.0353(3)	0.0297(3)	0.0295(3)	0.0066(2)	0.0005(2)	0.0023(2)
O(1)	0.0285(8)	0.0301(8)	0.0206(7)	-0.0037(6)	0.0060(5)	-0.0095(6)
O(2)	0.0183(8)	0.0243(8)	0.0464(9)	-0.0066(6)	0.0014(6)	-0.0017(6)
O(3)	0.0283(9)	0.0275(8)	0.0318(8)	-0.0078(6)	0.0037(6)	-0.0026(6)
C(1)	0.0239(11)	0.0235(11)	0.0220(9)	-0.0057(8)	0.0085(8)	-0.0035(8)
C(2)	0.0281(12)	0.0312(12)	0.0241(10)	-0.0038(9)	0.0051(8)	0.0000(9)
C(3)	0.0497(15)	0.0246(12)	0.0295(11)	-0.0029(9)	0.0144(10)	-0.0005(10)
C(4)	0.0442(15)	0.0273(12)	0.0370(12)	-0.0142(10)	0.0193(10)	-0.0141(10)
C(5)	0.0250(12)	0.0402(14)	0.0333(12)	-0.0167(10)	0.0085(9)	-0.0088(9)

C(6)	0.0238(12)	0.0303(12)	0.0254(10)	-0.0078(8)	0.0051(8)	0.0007(8)
C(7)	0.0196(10)	0.0220(10)	0.0176(9)	0.0029(7)	-0.0016(7)	0.0009(7)
C(8)	0.0149(10)	0.0226(10)	0.0217(9)	0.0043(8)	0.0008(7)	-0.0019(7)
C(9)	0.0168(10)	0.0200(10)	0.0196(9)	0.0041(7)	0.0013(7)	0.0013(7)
C(10)	0.0168(10)	0.0161(10)	0.0215(9)	0.0034(7)	-0.0018(7)	0.0015(7)
C(11)	0.0136(10)	0.0220(10)	0.0266(10)	0.0063(8)	0.0019(7)	-0.0005(7)
C(12)	0.0176(11)	0.0259(11)	0.0225(10)	0.0045(8)	0.0054(7)	0.0008(8)
C(13)	0.021(2)	0.0184(17)	0.016(2)	0.001(2)	0.000(2)	0.0019(12)
C(13')	0.020(4)	0.019(5)	0.021(6)	0.012(5)	-0.002(5)	0.008(3)
C(14)	0.0276(18)	0.0195(16)	0.0261(17)	0.0004(13)	-0.0002(12)	0.0046(12)
C(14')	0.038(5)	0.025(4)	0.028(4)	0.008(3)	-0.010(3)	-0.011(3)
C(15)	0.0275(14)	0.0510(16)	0.0425(14)	0.0190(12)	0.0038(10)	-0.0013(10)

Table S1-5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for compound **1**.

	x	y	z	U(eq)
H(2)	0.6590	0.2219	0.6542	0.033
H(3)	0.4108	0.1555	0.6914	0.041
H(4)	0.0248	0.1464	0.5567	0.042
H(5)	-0.1126	0.2030	0.3850	0.039
H(6)	0.1351	0.2693	0.3453	0.032
H(8)	0.3305	0.3125	0.6852	0.024
H(9)	0.4265	0.3755	0.8458	0.023
H(11)	1.0262	0.4085	0.6349	0.025
H(12)	0.9274	0.3466	0.4726	0.026
H(13A)	0.4618	0.4880	0.8077	0.022
H(13B)	0.6740	0.5212	0.8882	0.022
H(13C)	0.6030	0.4808	0.6586	0.024
H(13D)	0.4515	0.4940	0.7923	0.024
H(14)	0.7064	0.4852	0.5940	0.029
H(14')	0.7630	0.5539	0.8672	0.037
H(15A)	1.0628	0.5362	0.5979	0.048
H(15B)	1.0317	0.5513	0.7672	0.048

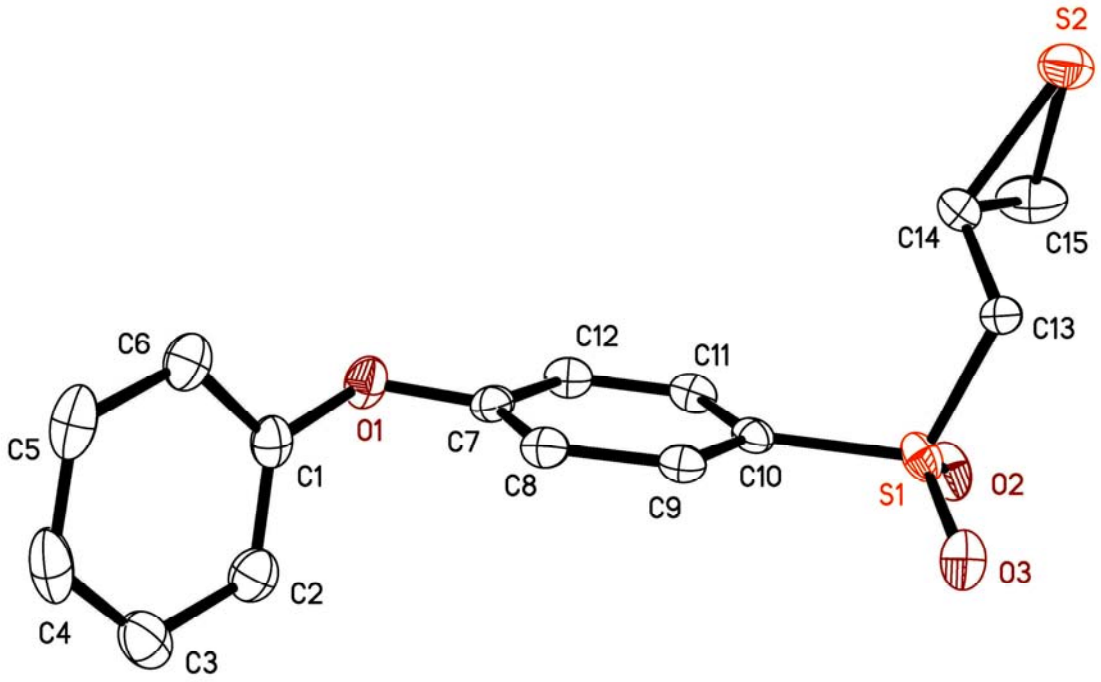
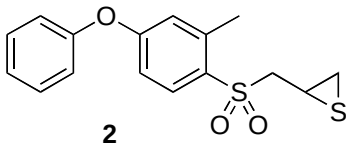


Figure S1. The ORTEP diagram of compound **1** is shown at 50% probability level. Hydrogen atoms are omitted for clarity.

Table S2-1. Crystal data and structure refinement for compound **2**.



2

Identification code	dh28_1_0m	
Empirical formula	C16 H16 O3 S2	
Formula weight	320.41	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 5.7744(2) Å	α= 85.695(2)°.
	b = 11.2258(4) Å	β= 78.737(2)°.
	c = 12.0078(4) Å	γ = 85.483(2)°.
Volume	759.59(5) $Å^3$	
Z	2	
Density (calculated)	1.401 Mg/m^3	
Absorption coefficient	3.239 mm^{-1}	
F(000)	336	
Crystal size	0.41 x 0.14 x 0.05 mm^3	
Crystal color and habit	clear colorlessplate	
Diffractometer	Bruker SMART Apex CCD diffractometer	
Theta range for data collection	3.76 to 69.72°.	
Index ranges	-5<=h<=6, -13<=k<=13, -14<=l<=14	
Reflections collected	8355	
Independent reflections	2649 [R(int) = 0.0174]	
Observed reflections (I > 2sigma(I))	2541	
Completeness to theta = 69.72°	92.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8445 and 0.3516	
Solution method	XS (Sheldrick, 2001)	
Refinement method	XL (Sheldrick, 2001)	
Data / restraints / parameters	2649 / 0 / 204	
Goodness-of-fit on F^2	1.247	
Final R indices [I>2sigma(I)]	R1 = 0.0423, wR2 = 0.1228	
R indices (all data)	R1 = 0.0442, wR2 = 0.1281	
Largest diff. peak and hole	0.532 and -0.401 $e.Å^{-3}$	

Table S2-2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for compound **2**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
S(1)	0.35231(11)	0.36437(5)	0.63090(5)	0.0262(2)
O(1)	0.1959(3)	-0.10901(17)	0.86923(19)	0.0406(5)
C(1)	0.3796(4)	-0.1950(2)	0.8808(2)	0.0251(5)
S(2)	0.11507(18)	0.13363(10)	0.48214(10)	0.0342(4)
C(14)	0.2520(14)	0.2765(5)	0.4400(6)	0.0295(11)
C(15)	0.0707(9)	0.2530(6)	0.3738(4)	0.0384(10)
S(2')	0.0546(7)	0.1897(5)	0.3693(3)	0.0413(13)
C(14')	0.249(5)	0.2474(19)	0.452(2)	0.0295(11)
C(15')	0.182(4)	0.1248(16)	0.4874(13)	0.0384(10)
O(2)	0.5987(3)	0.36156(17)	0.57707(18)	0.0368(5)
C(2)	0.5608(5)	-0.1718(2)	0.9354(2)	0.0291(6)
O(3)	0.2599(4)	0.46099(17)	0.7019(2)	0.0424(5)
C(3)	0.7254(5)	-0.2623(2)	0.9541(2)	0.0293(6)
C(4)	0.7109(5)	-0.3755(2)	0.9187(3)	0.0348(6)
C(5)	0.5305(5)	-0.3979(2)	0.8649(3)	0.0357(6)
C(6)	0.3636(5)	-0.3076(2)	0.8443(2)	0.0263(5)
C(7)	0.2461(5)	0.0006(2)	0.8150(2)	0.0275(5)
C(8)	0.0649(4)	0.0900(2)	0.8355(2)	0.0252(5)
C(9)	0.0881(4)	0.2047(2)	0.78407(19)	0.0222(5)
C(10)	0.3026(4)	0.2255(2)	0.7085(2)	0.0224(5)
C(11)	0.4827(4)	0.1359(2)	0.6874(2)	0.0268(5)
C(12)	0.4568(5)	0.0223(2)	0.7406(2)	0.0289(6)
C(13)	0.1855(5)	0.3692(2)	0.5211(2)	0.0297(6)
C(16)	-0.1125(5)	0.2985(2)	0.8124(2)	0.0294(6)

Table S2-3. Bond lengths [Å] and angles [°] for compound **2**.

S(1)-O(3)	1.435(2)	S(1)-O(2)	1.442(2)
S(1)-C(10)	1.769(2)	S(1)-C(13)	1.774(3)
O(1)-C(7)	1.373(3)	O(1)-C(1)	1.398(3)
C(1)-C(6)	1.383(3)	C(1)-C(2)	1.389(4)
S(2)-C(15)	1.835(5)	S(2)-C(14)	1.837(4)
C(14)-C(13)	1.457(8)	C(14)-C(15)	1.482(6)

C(14)-H(14)	1.0000	C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900	S(2')-C(15')	1.8025
S(2')-C(14')	1.8142	C(14')-C(15')	1.4689
C(14')-C(13)	1.64(3)	C(14')-H(14')	1.0000
C(15')-H(15C)	0.9900	C(15')-H(15D)	0.9900
C(2)-C(3)	1.373(4)	C(2)-H(2)	0.9500
C(3)-C(4)	1.384(4)	C(3)-H(3)	0.9500
C(4)-C(5)	1.377(4)	C(4)-H(4)	0.9500
C(5)-C(6)	1.385(4)	C(5)-H(5)	0.9500
C(6)-H(6)	0.9500	C(7)-C(12)	1.389(4)
C(7)-C(8)	1.390(4)	C(8)-C(9)	1.390(3)
C(8)-H(8)	0.9500	C(9)-C(10)	1.409(3)
C(9)-C(16)	1.508(3)	C(10)-C(11)	1.388(3)
C(11)-C(12)	1.388(3)	C(11)-H(11)	0.9500
C(12)-H(12)	0.9500	C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900	C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800	C(16)-H(16C)	0.9800

O(3)-S(1)-O(2)	118.01(13)	O(3)-S(1)-C(10)	110.08(12)
O(2)-S(1)-C(10)	107.50(11)	O(3)-S(1)-C(13)	107.44(13)
O(2)-S(1)-C(13)	107.19(12)	C(10)-S(1)-C(13)	105.95(12)
C(7)-O(1)-C(1)	119.94(19)	C(6)-C(1)-C(2)	121.1(2)
C(6)-C(1)-O(1)	117.4(2)	C(2)-C(1)-O(1)	121.3(2)
C(15)-S(2)-C(14)	47.6(2)	C(13)-C(14)-C(15)	115.9(6)
C(13)-C(14)-S(2)	115.6(5)	C(15)-C(14)-S(2)	66.1(3)
C(13)-C(14)-H(14)	116.6	C(15)-C(14)-H(14)	116.6
S(2)-C(14)-H(14)	116.6	C(14)-C(15)-S(2)	66.3(2)
C(14)-C(15)-H(15A)	117.1	S(2)-C(15)-H(15A)	117.1
C(14)-C(15)-H(15B)	117.1	S(2)-C(15)-H(15B)	117.1
H(15A)-C(15)-H(15B)	114.1	C(15')-S(2')-C(14')	47.9
C(15')-C(14')-C(13)	129(2)	C(15')-C(14')-S(2')	65.6
C(13)-C(14')-S(2')	124.0(17)	C(15')-C(14')-H(14')	110.3
C(13)-C(14')-H(14')	110.3	S(2')-C(14')-H(14')	110.3
C(14')-C(15')-S(2')	66.5	C(14')-C(15')-H(15C)	117.1
S(2')-C(15')-H(15C)	117.1	C(14')-C(15')-H(15D)	117.1
S(2')-C(15')-H(15D)	117.1	H(15C)-C(15')-H(15D)	114.1

C(3)-C(2)-C(1)	119.3(2)	C(3)-C(2)-H(2)	120.3
C(1)-C(2)-H(2)	120.3	C(2)-C(3)-C(4)	120.2(2)
C(2)-C(3)-H(3)	119.9	C(4)-C(3)-H(3)	119.9
C(5)-C(4)-C(3)	120.0(2)	C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0	C(4)-C(5)-C(6)	120.6(2)
C(4)-C(5)-H(5)	119.7	C(6)-C(5)-H(5)	119.7
C(1)-C(6)-C(5)	118.6(2)	C(1)-C(6)-H(6)	120.7
C(5)-C(6)-H(6)	120.7	O(1)-C(7)-C(12)	123.7(2)
O(1)-C(7)-C(8)	115.3(2)	C(12)-C(7)-C(8)	121.0(2)
C(9)-C(8)-C(7)	121.7(2)	C(9)-C(8)-H(8)	119.2
C(7)-C(8)-H(8)	119.2	C(8)-C(9)-C(10)	116.8(2)
C(8)-C(9)-C(16)	119.0(2)	C(10)-C(9)-C(16)	124.2(2)
C(11)-C(10)-C(9)	121.5(2)	C(11)-C(10)-S(1)	116.36(18)
C(9)-C(10)-S(1)	122.07(18)	C(10)-C(11)-C(12)	120.7(2)
C(10)-C(11)-H(11)	119.6	C(12)-C(11)-H(11)	119.6
C(11)-C(12)-C(7)	118.3(2)	C(11)-C(12)-H(12)	120.8
C(7)-C(12)-H(12)	120.8	C(14)-C(13)-C(14')	11.0(9)
C(14)-C(13)-S(1)	115.7(3)	C(14')-C(13)-S(1)	109.7(5)
C(14)-C(13)-H(13A)	108.3	C(14')-C(13)-H(13A)	103.1
S(1)-C(13)-H(13A)	108.3	C(14)-C(13)-H(13B)	108.3
C(14')-C(13)-H(13B)	119.3	S(1)-C(13)-H(13B)	108.3
H(13A)-C(13)-H(13B)	107.4	C(9)-C(16)-H(16A)	109.5
C(9)-C(16)-H(16B)	109.5	H(16A)-C(16)-H(16B)	109.5
C(9)-C(16)-H(16C)	109.5	H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5		

Table S2-4. Anisotropic displacement parameters ($Å^2$) for compound **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	0.0223(4)	0.0198(3)	0.0383(4)	0.0049(2)	-0.0114(2)	-0.0051(2)
O(1)	0.0230(10)	0.0260(10)	0.0644(14)	0.0164(9)	0.0038(9)	0.0018(7)
C(1)	0.0242(13)	0.0194(11)	0.0279(12)	0.0042(9)	0.0017(9)	0.0001(9)
S(2)	0.0398(8)	0.0311(5)	0.0304(5)	-0.0094(4)	0.0019(4)	-0.0089(5)
C(14)	0.0249(15)	0.038(3)	0.023(2)	0.007(2)	0.0001(14)	-0.008(2)
C(15)	0.044(3)	0.045(3)	0.026(2)	-0.006(2)	-0.0065(15)	-0.003(2)
S(2')	0.037(2)	0.052(3)	0.0362(18)	-0.0122(18)	-0.0130(13)	0.0124(18)

C(14')	0.0249(15)	0.038(3)	0.023(2)	0.007(2)	0.0001(14)	-0.008(2)
C(15')	0.044(3)	0.045(3)	0.026(2)	-0.006(2)	-0.0065(15)	-0.003(2)
O(2)	0.0194(10)	0.0359(10)	0.0552(12)	0.0193(9)	-0.0131(8)	-0.0083(7)
C(2)	0.0344(15)	0.0242(12)	0.0270(12)	-0.0076(10)	0.0034(10)	-0.0084(10)
O(3)	0.0473(13)	0.0235(9)	0.0606(14)	-0.0050(9)	-0.0185(10)	-0.0048(8)
C(3)	0.0323(15)	0.0340(14)	0.0236(12)	0.0018(10)	-0.0087(10)	-0.0087(11)
C(4)	0.0353(16)	0.0246(13)	0.0468(16)	0.0031(11)	-0.0169(12)	0.0012(11)
C(5)	0.0362(16)	0.0236(13)	0.0503(17)	-0.0070(11)	-0.0142(12)	-0.0003(11)
C(6)	0.0276(14)	0.0279(12)	0.0253(12)	-0.0019(10)	-0.0090(10)	-0.0035(10)
C(7)	0.0238(13)	0.0233(12)	0.0337(13)	0.0047(10)	-0.0039(10)	-0.0016(9)
C(8)	0.0206(13)	0.0287(13)	0.0248(12)	0.0014(10)	-0.0017(9)	-0.0023(9)
C(9)	0.0225(13)	0.0240(12)	0.0213(11)	-0.0029(9)	-0.0075(9)	0.0004(9)
C(10)	0.0226(13)	0.0203(11)	0.0260(12)	0.0008(9)	-0.0088(9)	-0.0028(9)
C(11)	0.0196(13)	0.0252(12)	0.0330(13)	0.0056(10)	-0.0014(9)	-0.0013(9)
C(12)	0.0227(13)	0.0234(12)	0.0366(14)	0.0006(10)	0.0010(10)	0.0033(9)
C(13)	0.0209(13)	0.0335(14)	0.0341(14)	0.0119(11)	-0.0084(10)	-0.0030(10)
C(16)	0.0299(14)	0.0288(13)	0.0286(13)	0.0000(10)	-0.0067(10)	0.0051(10)

Table S2-5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for compound **2**.

	x	y	z	U(eq)
H(14)	0.4203	0.2716	0.3988	0.035
H(15A)	0.1273	0.2348	0.2933	0.046
H(15B)	-0.0802	0.3029	0.3878	0.046
H(14')	0.4144	0.2463	0.4073	0.035
H(15C)	0.0728	0.1131	0.5614	0.046
H(15D)	0.3071	0.0596	0.4713	0.046
H(2)	0.5707	-0.0939	0.9595	0.035
H(3)	0.8496	-0.2472	0.9916	0.035
H(4)	0.8256	-0.4378	0.9315	0.042
H(5)	0.5203	-0.4760	0.8416	0.043
H(6)	0.2407	-0.3226	0.8060	0.032
H(8)	-0.0783	0.0723	0.8859	0.030
H(11)	0.6253	0.1526	0.6360	0.032
H(12)	0.5801	-0.0390	0.7265	0.035
H(13A)	0.0167	0.3633	0.5567	0.036

H(13B)	0.2004	0.4482	0.4787	0.036
H(16A)	-0.2461	0.2621	0.8630	0.044
H(16B)	-0.1621	0.3315	0.7422	0.044
H(16C)	-0.0597	0.3628	0.8504	0.044

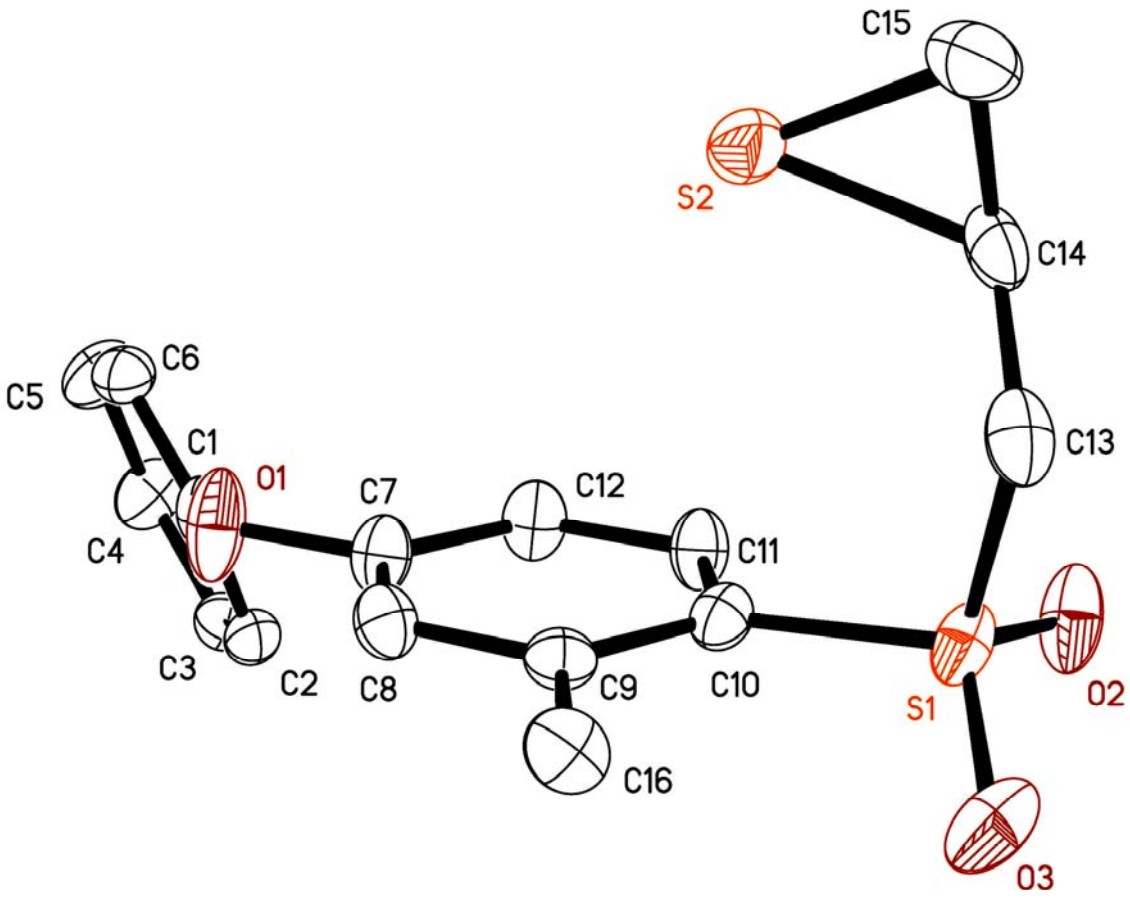
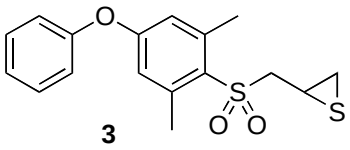


Figure S2. The ORTEP diagram of compound **2** is shown at 50% probability level. Hydrogen atoms are omitted for clarity.

Table S3-1. Crystal data and structure refinement for compound **3**.



3

Identification code	dh29_3_0m	
Empirical formula	C17 H18 O3 S2	
Formula weight	334.43	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 5.4528(3) Å	α= 88.396(2)°.
	b = 11.4721(5) Å	β= 81.581(2)°.
	c = 13.0581(6) Å	γ = 79.755(2)°.
Volume	795.16(7) $Å^3$	
Z	2	
Density (calculated)	1.397 Mg/m^3	
Absorption coefficient	3.117 mm^{-1}	
F(000)	352	
Crystal size	0.26 x 0.10 x 0.03 mm^3	
Crystal color and habit	clear colorlessneedle	
Diffractometer	Bruker SMART Apex CCD diffractometer	
Theta range for data collection	3.42 to 69.42°.	
Index ranges	-5<=h<=6, -13<=k<=13, -15<=l<=15	
Reflections collected	11197	
Independent reflections	2781 [R(int) = 0.0231]	
Observed reflections (I > 2sigma(I))	2639	
Completeness to theta = 69.42°	93.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9234 and 0.5002	
Solution method	XS (Sheldrick, 2001)	
Refinement method	XL (Sheldrick, 2001)	
Data / restraints / parameters	2781 / 18 / 305	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0592, wR2 = 0.1549	
R indices (all data)	R1 = 0.0612, wR2 = 0.1566	
Largest diff. peak and hole	0.616 and -0.469 $e.Å^{-3}$	

Table S3-2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for compound **3**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
S(1)	0.16676(14)	0.35453(6)	0.86467(7)	0.0416(3)
S(2)	0.50512(18)	0.29353(8)	1.15166(7)	0.0497(3)
O(1')	0.9599(14)	-0.0332(9)	0.6460(8)	0.058(3)
O(1)	0.8346(13)	0.0069(3)	0.5916(4)	0.071(2)
O(2)	0.1232(5)	0.4626(2)	0.8073(3)	0.0631(8)
O(3)	-0.0536(4)	0.3107(2)	0.9141(2)	0.0549(7)
C(1)	0.8492(10)	-0.1133(2)	0.5964(4)	0.0307(15)
C(2)	0.6807(7)	-0.1701(5)	0.5554(4)	0.0440(17)
C(3)	0.7163(8)	-0.2931(5)	0.5542(4)	0.0501(16)
C(4)	0.9203(12)	-0.3593(2)	0.5941(5)	0.0369(17)
C(5)	1.0887(9)	-0.3025(5)	0.6351(4)	0.052(2)
C(6)	1.0532(8)	-0.1795(6)	0.6363(4)	0.0482(16)
C(1')	0.9103(18)	-0.1361(7)	0.6123(6)	0.018(2)
C(2')	0.7442(15)	-0.1319(6)	0.5405(6)	0.030(3)
C(3')	0.6965(12)	-0.2363(10)	0.5025(7)	0.043(3)
C(4')	0.8149(19)	-0.3450(6)	0.5363(9)	0.053(4)
C(5')	0.981(2)	-0.3492(6)	0.6081(9)	0.047(4)
C(6')	1.0287(17)	-0.2447(10)	0.6461(6)	0.041(3)
C(7)	0.6724(10)	0.0795(3)	0.6606(3)	0.0348(14)
C(8)	0.6956(9)	0.1981(3)	0.6506(3)	0.0352(13)
C(9)	0.5350(9)	0.2824(3)	0.7147(3)	0.0276(11)
C(10)	0.3512(9)	0.2480(4)	0.7888(4)	0.0267(15)
C(11)	0.3280(10)	0.1294(4)	0.7988(5)	0.0326(18)
C(12)	0.4886(10)	0.0451(3)	0.7347(5)	0.0260(15)
C(7')	0.7652(16)	0.0499(7)	0.6873(7)	0.037(3)
C(8')	0.7996(15)	0.1670(7)	0.6765(6)	0.038(3)
C(9')	0.6174(16)	0.2569(6)	0.7244(6)	0.029(3)
C(10')	0.4008(15)	0.2297(8)	0.7831(7)	0.024(3)
C(11')	0.3664(15)	0.1126(9)	0.7939(9)	0.015(2)
C(12')	0.5486(17)	0.0227(7)	0.7460(9)	0.023(3)
C(13)	0.6055(11)	0.4031(4)	0.6961(3)	0.0627(12)
C(14)	0.1369(7)	0.0751(3)	0.8696(4)	0.0499(9)
C(15)	0.3474(6)	0.3795(3)	0.9622(2)	0.0369(7)

C(16)	0.4211(11)	0.2703(5)	1.0279(6)	0.0283(14)
C(16')	0.313(4)	0.286(2)	1.0475(16)	0.072(5)
C(17)	0.2267(9)	0.2477(4)	1.1174(4)	0.0344(12)
C(17')	0.4543(15)	0.1711(6)	1.0510(5)	0.024(2)

Table S3-3. Bond lengths [Å] and angles [°] for compound **3**.

S(1)-O(2)	1.431(3)	S(1)-O(3)	1.443(3)
S(1)-C(10)	1.681(3)	S(1)-C(15)	1.779(3)
S(1)-C(10')	1.962(7)	S(2)-C(16)	1.782(8)
S(2)-C(17)	1.810(5)	S(2)-C(16')	1.846(19)
S(2)-C(17')	2.031(7)	O(1')-C(7')	1.352(10)
O(1')-C(1')	1.355(9)	O(1)-C(7)	1.354(5)
O(1)-C(1)	1.366(4)	C(1)-C(2)	1.3900
C(1)-C(6)	1.3900	C(2)-C(3)	1.3900
C(2)-H(2)	0.9500	C(3)-C(4)	1.3900
C(3)-H(3)	0.9500	C(4)-C(5)	1.3900
C(4)-H(4)	0.9500	C(5)-C(6)	1.3900
C(5)-H(5)	0.9500	C(6)-H(6)	0.9500
C(1')-C(2')	1.3900	C(1')-C(6')	1.3900
C(2')-C(3')	1.3900	C(2')-H(2')	0.9500
C(3')-C(4')	1.3900	C(3')-H(3')	0.9500
C(4')-C(5')	1.3900	C(4')-H(4')	0.9500
C(5')-C(6')	1.3900	C(5')-H(5')	0.9500
C(6')-H(6')	0.9500	C(7)-C(8)	1.3900
C(7)-C(12)	1.3900	C(8)-C(9)	1.3900
C(8)-H(8)	0.9500	C(9)-C(10)	1.3900
C(9)-C(13)	1.506(5)	C(10)-C(11)	1.3900
C(11)-C(12)	1.3900	C(11)-C(14)	1.498(4)
C(12)-H(12)	0.9500	C(7')-C(8')	1.3900
C(7')-C(12')	1.3900	C(8')-C(9')	1.3900
C(8')-H(8')	0.9500	C(9')-C(10')	1.3900
C(9')-C(13)	1.698(8)	C(10')-C(11')	1.3900
C(11')-C(12')	1.3900	C(11')-C(14)	1.592(7)
C(12')-H(12')	0.9500	C(13)-H(13A)	0.96(5)
C(13)-H(13B)	0.93(5)	C(13)-H(13C)	0.85(5)

C(14)-H(14A)	0.95(4)	C(14)-H(14B)	0.91(5)
C(14)-H(14C)	0.87(5)	C(15)-C(16)	1.526(8)
C(15)-C(16')	1.54(2)	C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900	C(16)-C(17)	1.508(6)
C(16)-H(16)	1.0000	C(16')-C(17')	1.40(2)
C(16')-H(16')	1.0000	C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900	C(17')-H(17C)	0.9900
C(17')-H(17D)	0.9900		

O(2)-S(1)-O(3)	116.52(16)	O(2)-S(1)-C(10)	110.0(2)
O(3)-S(1)-C(10)	109.3(2)	O(2)-S(1)-C(15)	106.96(15)
O(3)-S(1)-C(15)	108.13(16)	C(10)-S(1)-C(15)	105.3(3)
O(2)-S(1)-C(10')	111.9(3)	O(3)-S(1)-C(10')	110.9(3)
C(15)-S(1)-C(10')	101.1(3)	C(16)-S(2)-C(17)	49.6(2)
C(16')-S(2)-C(17')	42.1(7)	C(7')-O(1')-C(1')	118.7(7)
C(7)-O(1)-C(1)	121.4(4)	O(1)-C(1)-C(2)	122.2(6)
O(1)-C(1)-C(6)	117.6(6)	C(2)-C(1)-C(6)	120.0
C(3)-C(2)-C(1)	120.0	C(3)-C(2)-H(2)	120.0
C(1)-C(2)-H(2)	120.0	C(2)-C(3)-C(4)	120.0
C(2)-C(3)-H(3)	120.0	C(4)-C(3)-H(3)	120.0
C(5)-C(4)-C(3)	120.0	C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0	C(4)-C(5)-C(6)	120.0
C(4)-C(5)-H(5)	120.0	C(6)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	120.0	C(5)-C(6)-H(6)	120.0
C(1)-C(6)-H(6)	120.0	O(1')-C(1')-C(2')	119.0(9)
O(1')-C(1')-C(6')	120.9(9)	C(2')-C(1')-C(6')	120.0
C(1')-C(2')-C(3')	120.0	C(1')-C(2')-H(2')	120.0
C(3')-C(2')-H(2')	120.0	C(2')-C(3')-C(4')	120.0
C(2')-C(3')-H(3')	120.0	C(4')-C(3')-H(3')	120.0
C(3')-C(4')-C(5')	120.0	C(3')-C(4')-H(4')	120.0
C(5')-C(4')-H(4')	120.0	C(6')-C(5')-C(4')	120.0
C(6')-C(5')-H(5')	120.0	C(4')-C(5')-H(5')	120.0
C(5')-C(6')-C(1')	120.0	C(5')-C(6')-H(6')	120.0
C(1')-C(6')-H(6')	120.0	O(1)-C(7)-C(8)	114.3(3)
O(1)-C(7)-C(12)	125.7(3)	C(8)-C(7)-C(12)	120.0
C(9)-C(8)-C(7)	120.0	C(9)-C(8)-H(8)	120.0

C(7)-C(8)-H(8)	120.0	C(8)-C(9)-C(10)	120.0
C(8)-C(9)-C(13)	111.1(3)	C(10)-C(9)-C(13)	128.7(3)
C(11)-C(10)-C(9)	120.0	C(11)-C(10)-S(1)	122.7(3)
C(9)-C(10)-S(1)	117.3(3)	C(10)-C(11)-C(12)	120.0
C(10)-C(11)-C(14)	128.3(3)	C(12)-C(11)-C(14)	111.6(4)
C(11)-C(12)-C(7)	120.0	C(11)-C(12)-H(12)	120.0
C(7)-C(12)-H(12)	120.0	O(1')-C(7')-C(8')	116.5(7)
O(1')-C(7')-C(12')	123.3(7)	C(8')-C(7')-C(12')	120.0
C(9')-C(8')-C(7')	120.0	C(9')-C(8')-H(8')	120.0
C(7')-C(8')-H(8')	120.0	C(10')-C(9')-C(8')	120.0
C(10')-C(9')-C(13)	114.6(5)	C(8')-C(9')-C(13)	124.0(5)
C(9')-C(10')-C(11')	120.0	C(9')-C(10')-S(1)	119.4(5)
C(11')-C(10')-S(1)	120.1(5)	C(12')-C(11')-C(10')	120.0
C(12')-C(11')-C(14)	117.6(6)	C(10')-C(11')-C(14)	122.0(7)
C(11')-C(12')-C(7')	120.0	C(11')-C(12')-H(12')	120.0
C(7')-C(12')-H(12')	120.0	C(9)-C(13)-H(13A)	115(3)
C(9')-C(13)-H(13A)	110(3)	C(9)-C(13)-H(13B)	105(3)
C(9')-C(13)-H(13B)	92(3)	H(13A)-C(13)-H(13B)	108(4)
C(9)-C(13)-H(13C)	108(3)	C(9')-C(13)-H(13C)	122(3)
H(13A)-C(13)-H(13C)	120(4)	H(13B)-C(13)-H(13C)	98(4)
C(11)-C(14)-H(14A)	113(3)	C(11')-C(14)-H(14A)	115(3)
C(11)-C(14)-H(14B)	113(3)	C(11')-C(14)-H(14B)	105(3)
H(14A)-C(14)-H(14B)	105(4)	C(11)-C(14)-H(14C)	112(3)
C(11')-C(14)-H(14C)	118(3)	H(14A)-C(14)-H(14C)	108(4)
H(14B)-C(14)-H(14C)	105(4)	C(16)-C(15)-S(1)	113.7(3)
C(16')-C(15)-S(1)	107.5(7)	C(16)-C(15)-H(15A)	108.8
C(16')-C(15)-H(15A)	129.8	S(1)-C(15)-H(15A)	108.8
C(16)-C(15)-H(15B)	108.8	C(16')-C(15)-H(15B)	91.8
S(1)-C(15)-H(15B)	108.8	H(15A)-C(15)-H(15B)	107.7
C(17)-C(16)-C(15)	116.0(4)	C(17)-C(16)-S(2)	66.1(3)
C(15)-C(16)-S(2)	117.5(4)	C(17)-C(16)-H(16)	116.0
C(15)-C(16)-H(16)	116.0	S(2)-C(16)-H(16)	116.0
C(17')-C(16')-C(15)	127.0(15)	C(17')-C(16')-S(2)	76.0(10)
C(15)-C(16')-S(2)	113.1(10)	C(17')-C(16')-H(16')	111.8
C(15)-C(16')-H(16')	111.8	S(2)-C(16')-H(16')	111.8
C(16)-C(17)-S(2)	64.2(4)	C(16)-C(17)-H(17A)	117.3

S(2)-C(17)-H(17A)	117.3	C(16)-C(17)-H(17B)	117.3
S(2)-C(17)-H(17B)	117.3	H(17A)-C(17)-H(17B)	114.4
C(16')-C(17')-S(2)	61.9(8)	C(16')-C(17')-H(17C)	117.6
S(2)-C(17')-H(17C)	117.6	C(16')-C(17')-H(17D)	117.6
S(2)-C(17')-H(17D)	117.6	H(17C)-C(17')-H(17D)	114.7

Table S3-4. Anisotropic displacement parameters ($Å^2$) for compound **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S(1)	0.0300(4)	0.0258(4)	0.0698(6)	-0.0035(3)	-0.0108(3)	-0.0036(3)
S(2)	0.0524(6)	0.0478(5)	0.0494(5)	-0.0066(4)	0.0016(4)	-0.0166(4)
O(1')	0.028(4)	0.061(6)	0.084(7)	-0.052(5)	0.019(4)	-0.019(4)
O(1)	0.101(5)	0.0183(18)	0.074(3)	-0.0081(18)	0.057(3)	-0.015(2)
O(2)	0.0561(17)	0.0344(13)	0.106(2)	0.0098(13)	-0.0374(15)	-0.0068(11)
O(3)	0.0242(12)	0.0385(13)	0.100(2)	-0.0145(12)	-0.0011(12)	-0.0040(9)
C(1)	0.028(3)	0.021(2)	0.038(3)	0.002(2)	0.008(2)	0.000(2)
C(2)	0.040(4)	0.032(3)	0.060(4)	-0.002(3)	-0.020(3)	0.002(3)
C(3)	0.035(4)	0.046(4)	0.072(5)	-0.016(4)	-0.004(3)	-0.016(3)
C(4)	0.033(3)	0.021(3)	0.051(4)	-0.003(2)	0.014(3)	-0.005(2)
C(5)	0.050(5)	0.041(5)	0.060(4)	0.003(3)	-0.011(3)	0.006(3)
C(6)	0.042(4)	0.041(4)	0.063(4)	-0.013(3)	-0.009(3)	-0.007(3)
C(1')	0.017(3)	0.015(3)	0.020(3)	-0.0012(18)	-0.0012(18)	0.0003(19)
C(2')	0.018(5)	0.020(5)	0.053(7)	-0.004(4)	-0.005(4)	-0.006(4)
C(3')	0.031(5)	0.050(7)	0.050(6)	-0.020(6)	0.004(4)	-0.018(5)
C(4')	0.021(6)	0.035(6)	0.093(11)	-0.013(7)	0.025(7)	-0.005(4)
C(5')	0.042(8)	0.023(6)	0.072(10)	0.016(6)	0.008(6)	-0.007(5)
C(6')	0.027(6)	0.054(11)	0.041(6)	0.015(6)	-0.013(4)	-0.002(6)
C(7)	0.044(4)	0.019(2)	0.034(3)	-0.0035(18)	0.012(2)	0.001(2)
C(8)	0.046(3)	0.022(2)	0.034(3)	0.0046(19)	0.009(2)	-0.009(2)
C(9)	0.035(3)	0.016(2)	0.030(2)	0.0024(16)	-0.004(2)	0.0012(19)
C(10)	0.020(3)	0.015(2)	0.043(3)	-0.004(2)	0.000(2)	0.000(2)
C(11)	0.018(3)	0.029(3)	0.048(3)	-0.010(2)	0.005(2)	-0.002(2)
C(12)	0.024(3)	0.016(2)	0.038(3)	0.005(2)	-0.005(3)	-0.003(2)
C(7')	0.021(6)	0.040(6)	0.052(7)	-0.013(5)	0.002(4)	-0.014(4)
C(8')	0.039(6)	0.048(7)	0.028(5)	-0.011(4)	0.008(4)	-0.018(5)
C(9')	0.028(3)	0.029(3)	0.030(3)	-0.0006(19)	-0.0042(18)	-0.009(2)

C(10')	0.021(5)	0.023(5)	0.024(5)	-0.013(4)	-0.004(4)	0.010(4)
C(11')	0.017(3)	0.011(3)	0.018(3)	-0.0002(18)	-0.0033(18)	-0.0029(19)
C(12')	0.017(5)	0.013(4)	0.036(6)	-0.010(4)	-0.002(4)	0.007(4)
C(13)	0.104(4)	0.044(2)	0.046(2)	-0.0016(16)	0.005(2)	-0.043(2)
C(14)	0.0350(19)	0.0305(17)	0.080(3)	-0.0080(16)	0.0176(17)	-0.0151(13)
C(15)	0.0346(17)	0.0284(15)	0.0469(17)	-0.0112(12)	0.0011(13)	-0.0072(11)
C(16)	0.018(3)	0.026(3)	0.040(3)	-0.0050(18)	0.007(3)	-0.009(2)
C(16')	0.051(12)	0.113(15)	0.071(14)	-0.005(10)	-0.025(10)	-0.051(12)
C(17)	0.030(3)	0.038(2)	0.035(2)	-0.0050(19)	0.0094(19)	-0.0162(19)
C(17')	0.044(5)	0.010(4)	0.016(3)	-0.004(2)	-0.007(3)	0.006(3)

Table S3-5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for compound **3**.

	x	y	z	U(eq)
H(2)	0.5413	-0.1248	0.5281	0.053
H(3)	0.6012	-0.3319	0.5262	0.060
H(4)	0.9446	-0.4433	0.5933	0.044
H(5)	1.2282	-0.3477	0.6624	0.062
H(6)	1.1683	-0.1406	0.6643	0.058
H(2')	0.6633	-0.0576	0.5174	0.036
H(3')	0.5830	-0.2335	0.4535	0.052
H(4')	0.7823	-0.4164	0.5104	0.064
H(5')	1.0619	-0.4235	0.6312	0.057
H(6')	1.1422	-0.2476	0.6952	0.049
H(8)	0.8212	0.2216	0.5999	0.042
H(12)	0.4728	-0.0360	0.7415	0.031
H(8')	0.9476	0.1856	0.6364	0.046
H(12')	0.5251	-0.0574	0.7534	0.028
H(13A)	0.607(9)	0.447(4)	0.757(4)	0.075
H(13B)	0.768(10)	0.389(4)	0.660(4)	0.075
H(13C)	0.529(10)	0.436(4)	0.648(4)	0.075
H(14A)	0.130(8)	0.095(4)	0.940(4)	0.060
H(14B)	0.166(8)	-0.005(4)	0.868(3)	0.060
H(14C)	-0.013(9)	0.096(4)	0.853(3)	0.060
H(15A)	0.5025	0.4067	0.9289	0.044
H(15B)	0.2493	0.4437	1.0082	0.044

H(16)	0.5183	0.1986	0.9894	0.034
H(16')	0.1319	0.2878	1.0755	0.086
H(17A)	0.2072	0.1644	1.1318	0.041
H(17B)	0.0672	0.3055	1.1286	0.041
H(17C)	0.5917	0.1467	0.9932	0.029
H(17D)	0.3640	0.1071	1.0795	0.029

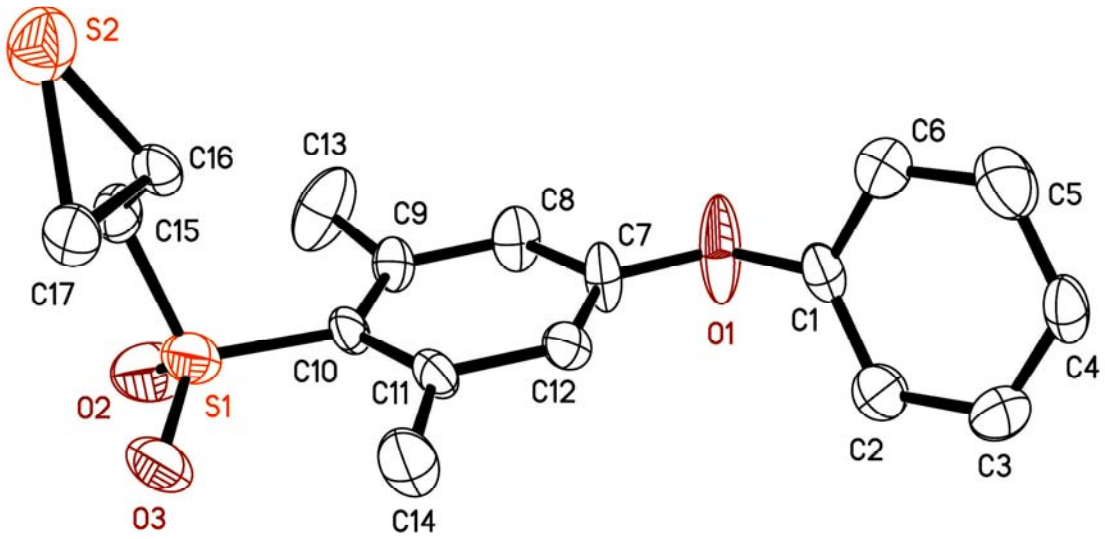


Figure S3. The ORTEP diagram of compound **3** is shown at 50% probability level. Hydrogen atoms are omitted for clarity.