Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information

Systematic Investigation the Impact of the Level of Oxidation at Sulfur and the Configuration of R/S-sulfoxide on the solid structure

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Figure S1. The Chemical shift of the product obtained by oxidation with 30% H_2O_2 (up) and NaClO (down); pink background represents the different areas of chemical shift for these two compounds.

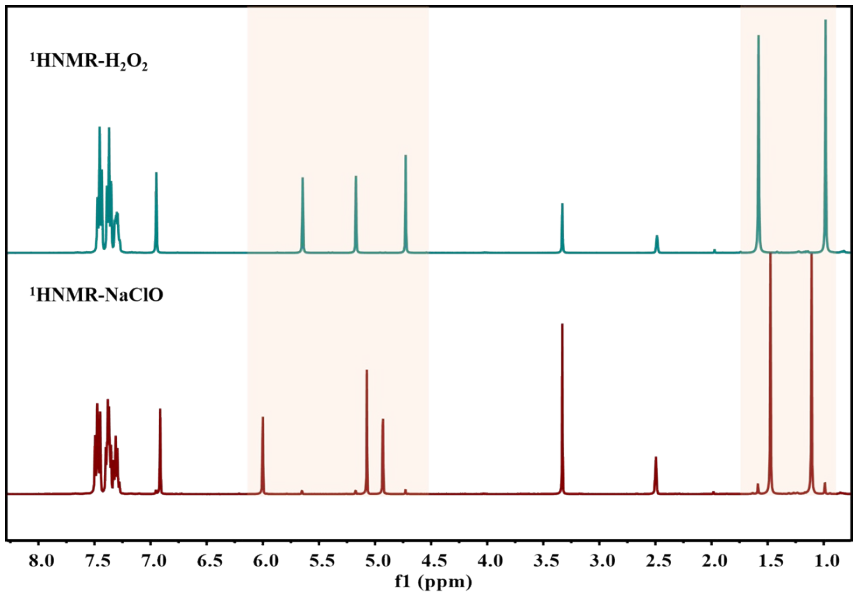

Figure S2. The existence of Br···C and Br···O interactions was due to the σ-hole of Br atom as shown by light blue to red area on Hirshfield surfaces.

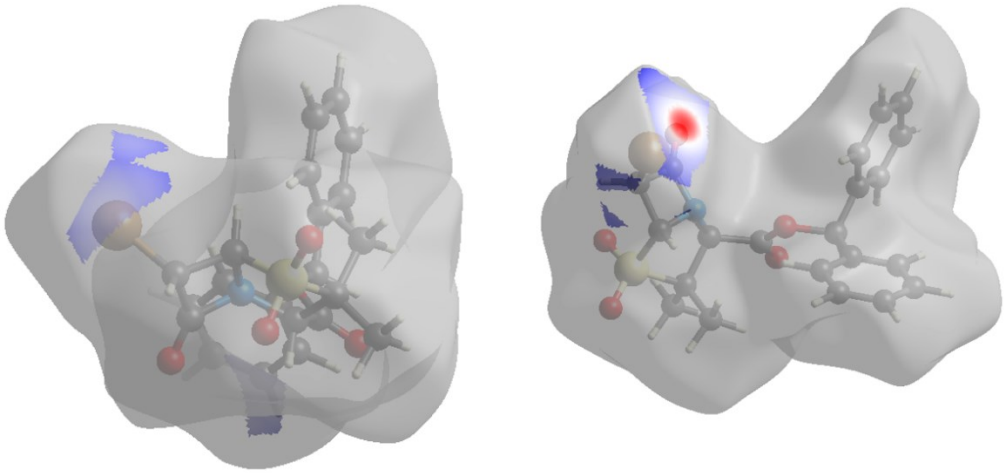

Figure S3. The electrostatic potential of bromine atom.

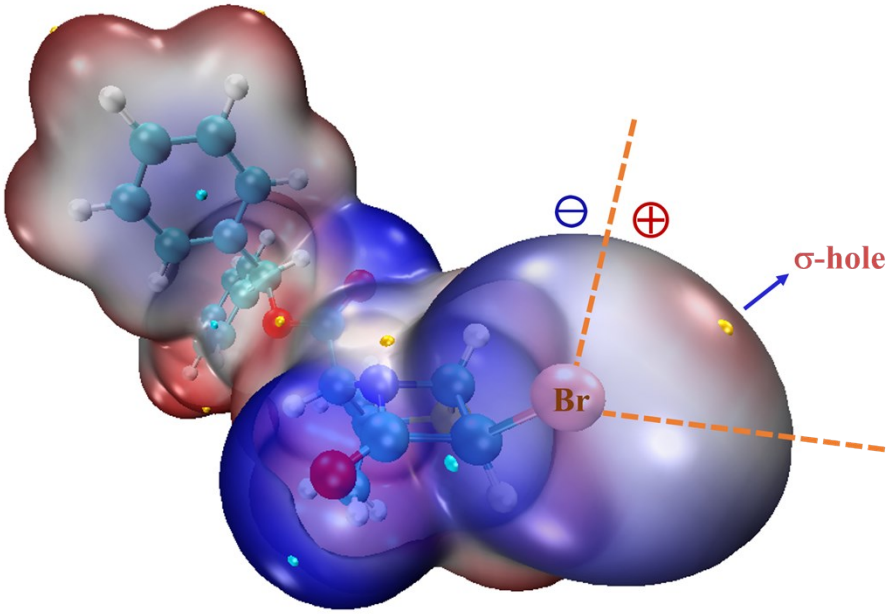

Figure S4. DSC curves of compounds 3-6 measured at the heating rates of 10 ^{o}C min^{-1}.

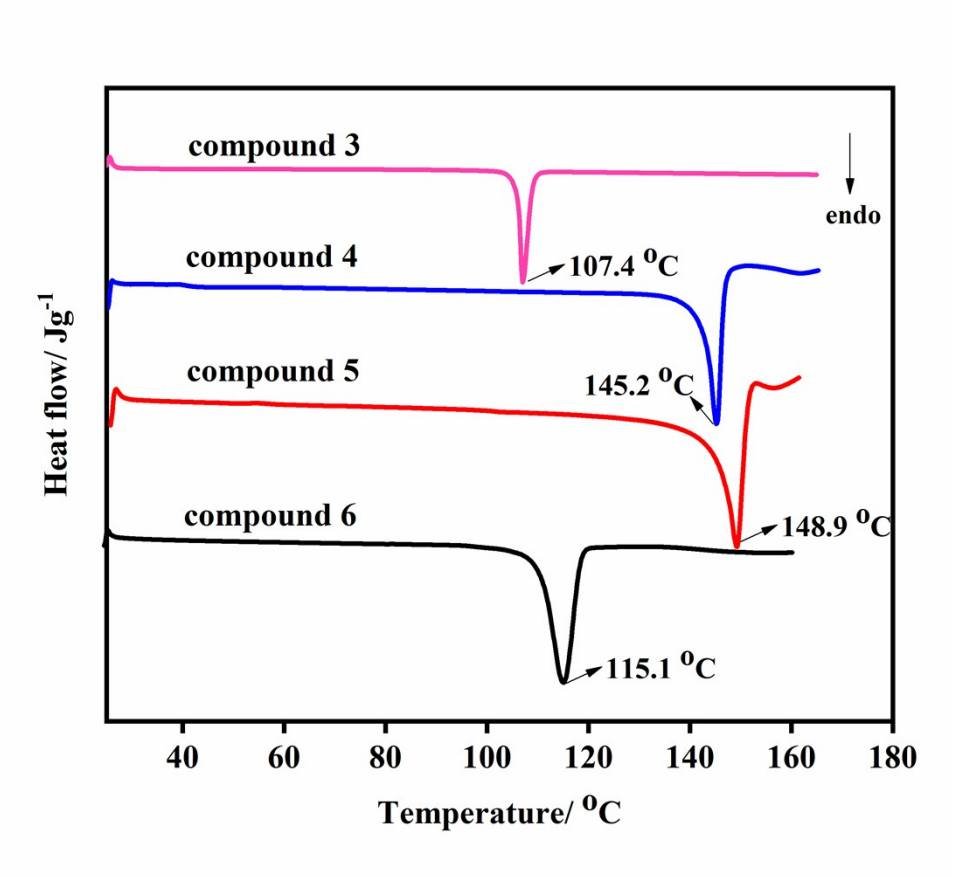

Figure S5. The Infrared Spectrums of compounds **3**-**6**.

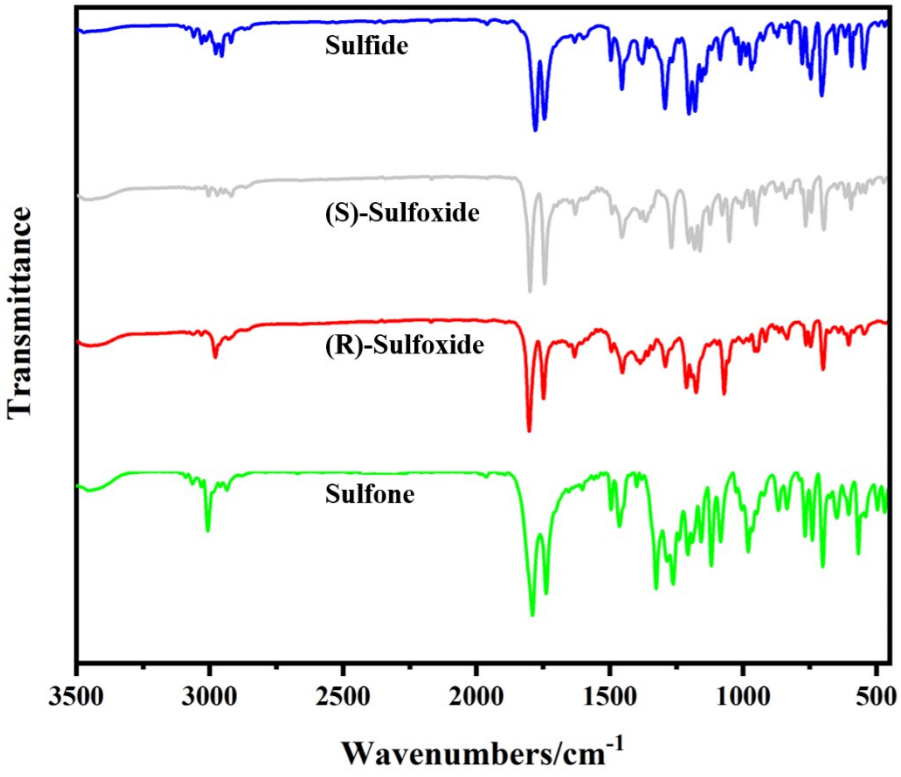

Figure S6. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of sulfide **3**.

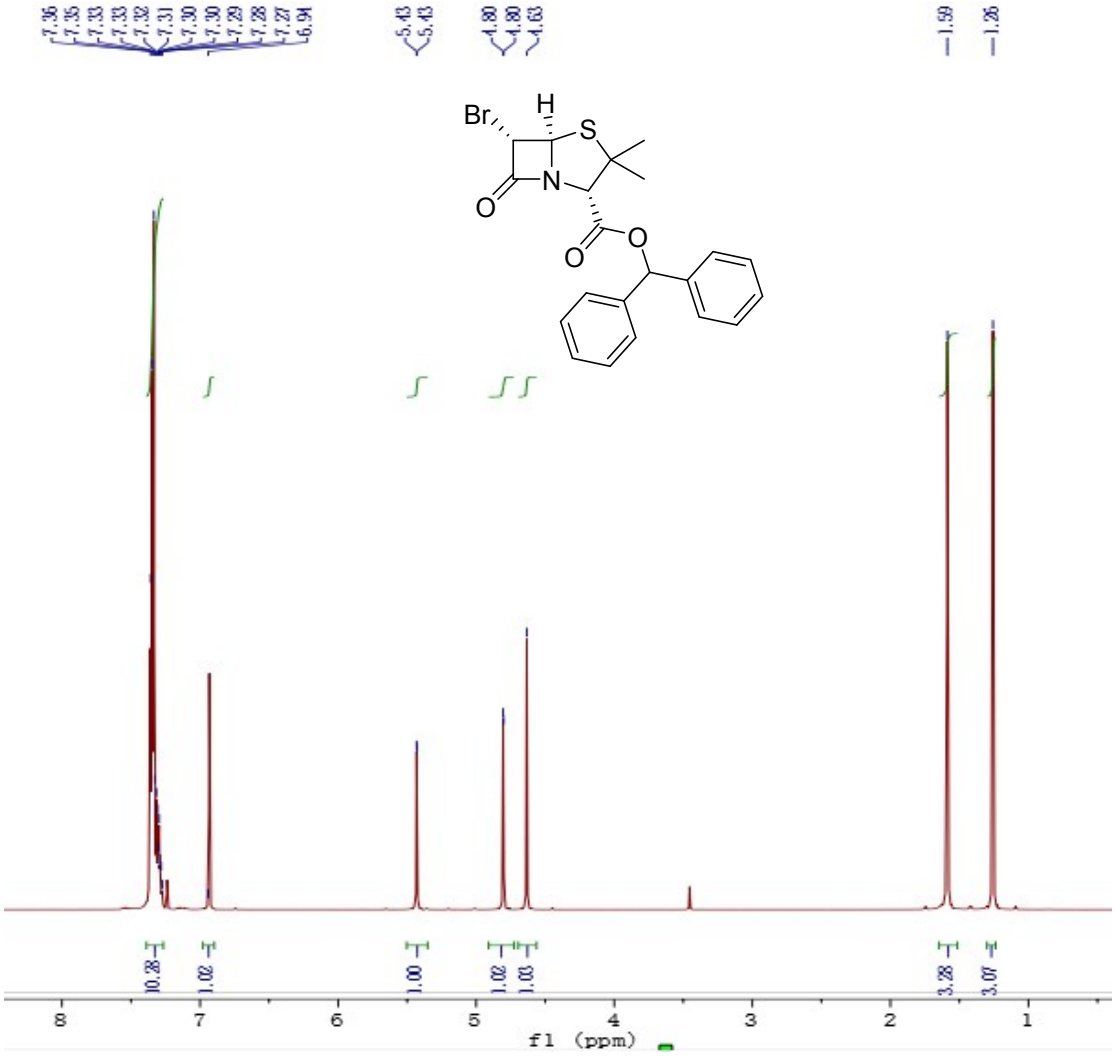

Figure S7. ^{13}CNMR spectrum (400 MHz, $CDCl_3$) of sulfide **3.**

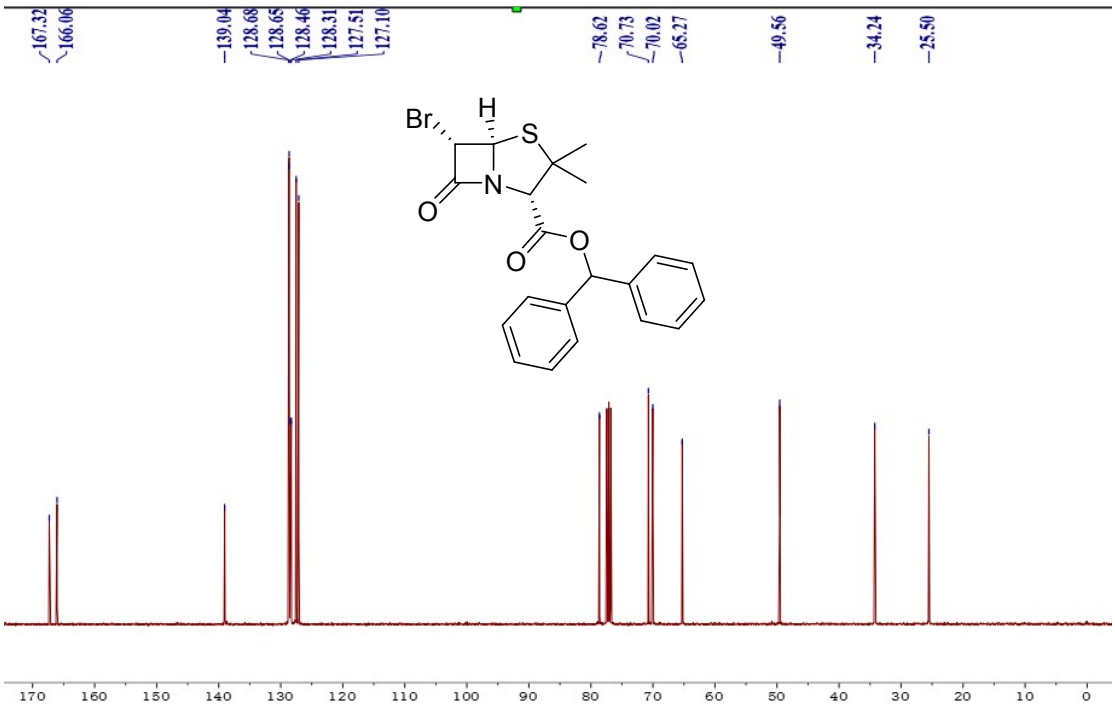

Figure S8. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of (S)-sulfoxides **4**.

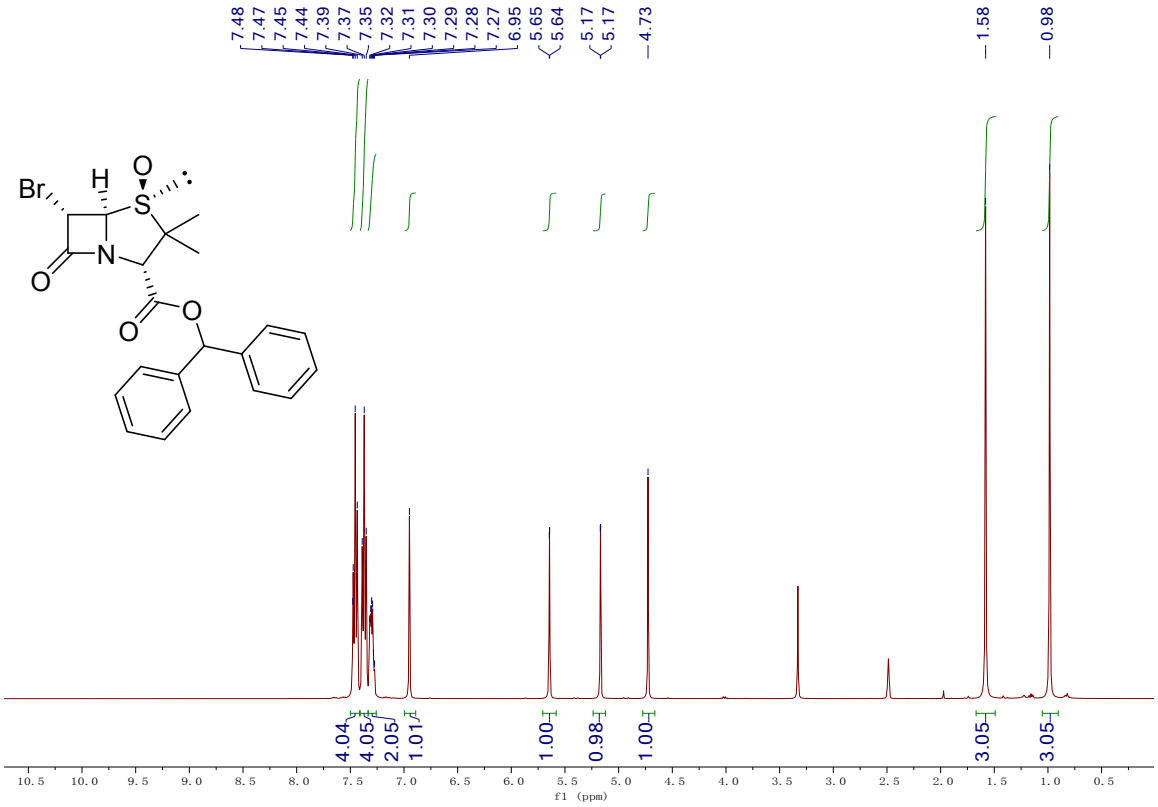

Figure S9. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of (R)-sulfoxides **5**.

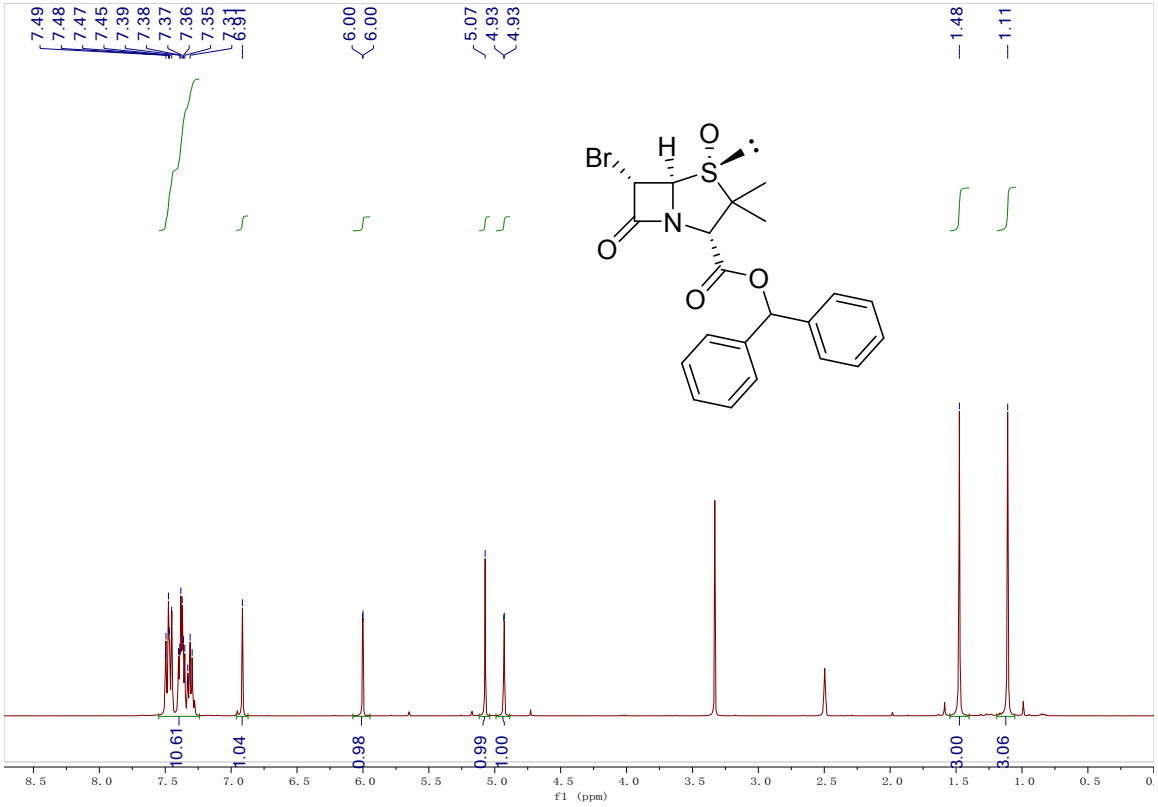

Figure S10. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of sulfone **6**.

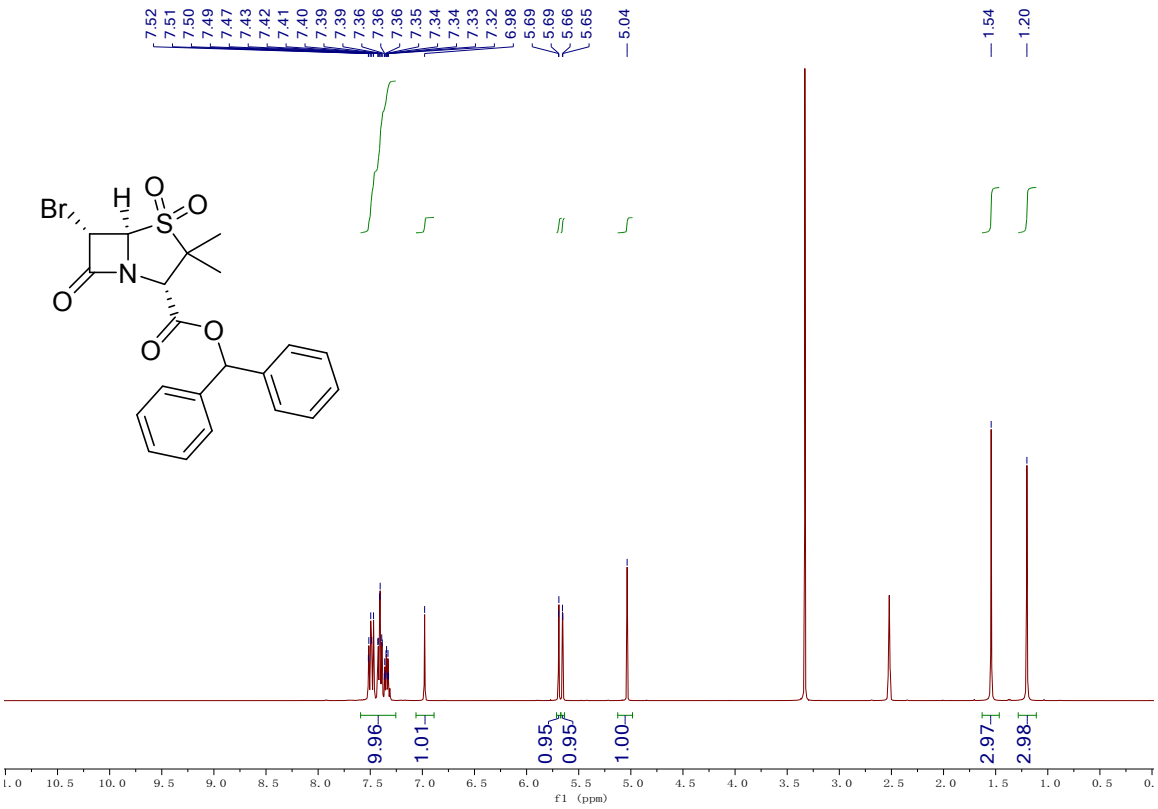

Table S1. Crystal data and structure refinement parametera for compounds **3-6**

Compound	**3**	**4**	**5**	**6**
Empirical formula	$C_{21}H_{20}BrNO_3S$	$C_{21}H_{20}BrNO_4S$	$C_{21}H_{20}BrNO_4S$	$C_{21}H_{20}BrNO_5S$
Molecular weight	446.35	462.35	462.35	478.35
Temperature (K)	293	293	150	293
Crystal system	orthorhombic	tetragonal	monoclinic	orthorhombic
Space group	$P2_12_12_1$	$P4_1$	$P2_1$	$P2_12_12_1$
a/ Å	5.9222(17)	11.0865(15)	6.4439(3)	7.8376(16)
b/ Å	13.176(4)	11.0865(15)	7.6636(4)	10.864(2)
c/ Å	26.122(8)	16.544(5)	20.6198(10)	24.590(5)
α/ deg	90	90	90	90
β/ deg	90	90	95.354(4)	90
γ/ deg	90	90	90	90
V/ Å^3	2038.3(11)	2033.4(8)	1013.85(8)	2093.8(7)
Z	4	4	2	4
D_{calcd} [mg/m^3]	1.454	1.510	1.515	1.517
θ_{range} [deg]	4.392-49.996	2.598-24.993	3.968-51.586	5.456-49.994
Reflns collected/ unique	10309/3570	10346/3550	3920/2897	10643/3669
R(int)	0.0616	0.0738	0.0431	0.0392

Abs coeff/mm^{-1}	2.140	2.151	2.157	2.095
F (000)	912	944	472	976
GOF	1.036	1.024	1.028	1.027
R_1/wR_2[I > 2σ(I)][a]	0.0467, 0.0863	0.0551, 0.1202	0.0683, 0.1848	0.0453, 0.1011
R_1/wR_2[all data]	0.0737, 0.0917	0.0715, 0.1248	0.0727, 0.1911	0.0603, 0.1058

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|\mathrm{Fo}|$, $wR^2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$.

Table S2. Selected bond parameters for compounds **3-6**.

D-X···A	Symmetry code	D-X (Å)	X···A (Å)	D···A (Å)	D-X···A (°)
compound **3**					
C(15)-H(15)···S1[i]	-1+x, y, z	0.98	2.82	3.776(6)	163
C(20)-H(20)···C(5)	2-x, -1/2+y,1/2-z	0.98	2.82	3.751(7)	160
C(18)-H(18)···Br1	2-x, 1/2+y,1/2-z	0.96	3.00	3.915(6)	161
C(11)-H(11)···Br1	3/2-x, -y,1/2+z	0.93	3.06	3.872(6)	101
C(3)-H(3)···O2	3/2-x,1-y,1/2+z	0.93	2.70	3.620(7)	169
C(17)···O3	3/2-x,1-y,1/2+z	-	-	3.137(6)	-
compound **4**					
C(10)-H(10)···O(4)	1-x, 1-y, 1/2+z	0.93	2.54	3.373(11	149
C(11)-H(11)···O(3)	2-y, x, 1/4+z	0.93	2.56	3.478(11	171
C(17)···O2	1-y,1+x,1/4+z	-	-	3.017(9)	-
C(20)···O2	1-y,1+x,1/4+z	-	-	3.183(9)	-
S1···O2	1-y,1+x,1/4+z	-	-	3.077(6)	-
compound **5**					
C(12)-H(12)···O(3)	1+x, -1+y, z	0.93	2.42	3.312(11	161
C(18)-H(18B)···O(3)	x, -1+y, z	0.96	2.52	3.335(11	143
C(10)-H(20)···O(4)	-x, -1/2+y, -z	0.98	2.19	3.110(10	155
C20···O(4)	-x, -1/2+y, -z	-	-	3.110(10	-
Br1···O(4)	1-x, -1/2+y, -z	-	-	3.083(7)	-
compound **6**					
C(15)-H(15)···O(5)	1-x, -1/2+y, 3/2-z	0.98	2.45	3.380(6)	143
C(19)-H(19A)···O(3)	1-x, -1/2+y, 3/2-z	0.96	2.70	3.640(6)	166
C(19)-H(19B)···O(5)	1-x, -1/2+y, 3/2-z	0.96	2.60	3.359(6)	136
C(1)-H(1)···C(11)	1/2+x, 1/2-y, 1-z	0.98	2.80	3.652(6)	145
C(17)-H(17)···O(3)	2-x, -1/2+y, 3/2-z	0.98	2.21	3.180(5)	172

Br1···O(4)	2+x, y, z	-	-	3.155(3)	-