Supplementary Materials

Design, Construction, and Characterization of a New Regioisomer and Diastereomer Material Based on the Spirooxindole Scaffold Incorporating a Sulphone Function

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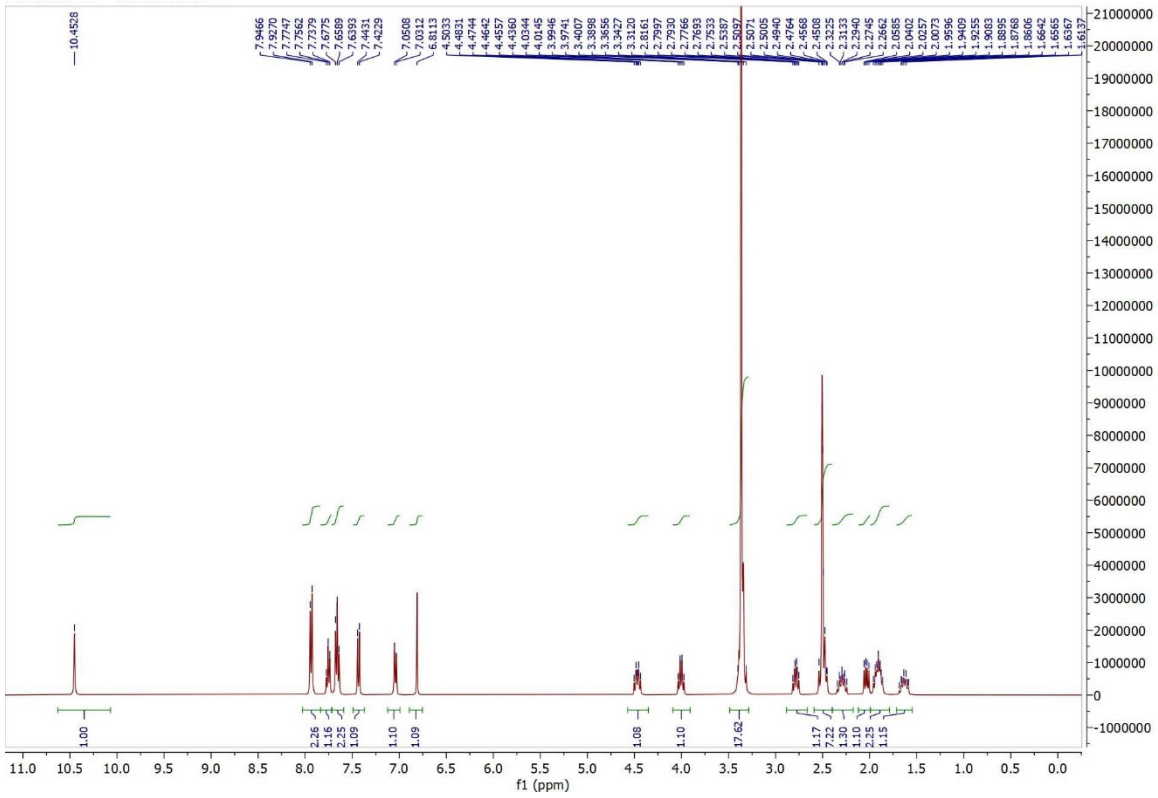

Figure S1: ^{1}H-NMR of **4**

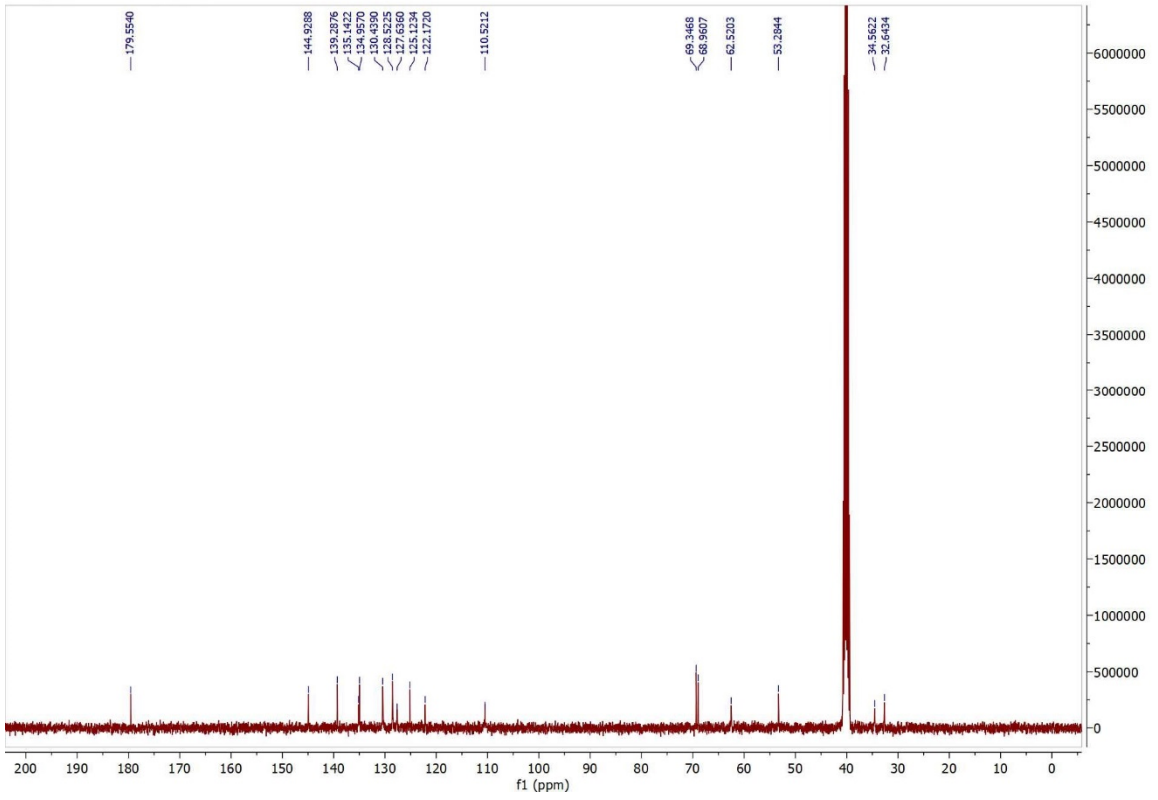

Figure S2: ^{13}C-NMR of **4**

Table S1 Bond angles [°] for **4**.

O(2)-S(1)-O(1)	119.28(6)
O(2)-S(1)-C(1)	108.39(6)
O(1)-S(1)-C(1)	108.02(6)
O(2)-S(1)-C(7)	106.77(6)
O(1)-S(1)-C(7)	109.58(6)
C(1)-S(1)-C(7)	103.72(6)
C(11)-N(1)-C(13)	116.85(10)
C(11)-N(1)-C(8)	107.66(10)
C(13)-N(1)-C(8)	108.31(9)
C(14)-N(2)-C(15)	110.89(10)
C(2)-C(1)-C(6)	121.58(13)
C(2)-C(1)-S(1)	119.30(11)
C(6)-C(1)-S(1)	119.12(10)
C(1)-C(2)-C(3)	118.24(14)
C(4)-C(3)-C(2)	120.47(15)
C(3)-C(4)-C(5)	120.73(14)
C(6)-C(5)-C(4)	119.79(14)
C(5)-C(6)-C(1)	119.16(13)
C(12)-C(7)-C(8)	104.39(10)
C(12)-C(7)-S(1)	115.51(8)
C(8)-C(7)-S(1)	113.29(8)
N(1)-C(8)-C(9)	105.17(10)
N(1)-C(8)-C(7)	105.06(9)
C(9)-C(8)-C(7)	119.19(10)
C(10)-C(9)-C(8)	101.79(10)
C(11)-C(10)-C(9)	101.50(11)
N(1)-C(11)-C(10)	103.17(10)
C(7)-C(12)-C(13)	101.92(9)
N(1)-C(13)-C(20)	116.52(10)
N(1)-C(13)-C(12)	104.97(9)
C(20)-C(13)-C(12)	115.92(10)
N(1)-C(13)-C(14)	105.45(9)
C(20)-C(13)-C(14)	101.48(9)
C(12)-C(13)-C(14)	112.18(10)
O(3)-C(14)-N(2)	125.92(11)
O(3)-C(14)-C(13)	125.63(11)
N(2)-C(14)-C(13)	108.44(10)
C(16)-C(15)-C(20)	122.50(11)
C(16)-C(15)-N(2)	127.33(11)
C(20)-C(15)-N(2)	110.07(11)
C(15)-C(16)-C(17)	116.41(11)
C(18)-C(17)-C(16)	123.00(12)
C(18)-C(17)-Cl(1)	119.25(10)
C(16)-C(17)-Cl(1)	117.75(10)
C(17)-C(18)-C(19)	119.12(12)
C(20)-C(19)-C(18)	119.41(11)
C(19)-C(20)-C(15)	119.45(11)
C(19)-C(20)-C(13)	131.61(11)
C(15)-C(20)-C(13)	108.63(10)

Table S2 The calculated geometric parameters of the studied compound **4**.

Bond	**Calc.**	**Exp.**	**Bonds**	**Calc.**	**Exp.**
R(1-41)	1.758	1.74	A(1-41-39)	118.434	117.743
R(2-3)	1.478	1.445	A(1-41-42)	119.231	119.248
R(2-4)	1.474	1.44	A(3-2-4)	120.839	119.277
R(2-9)	1.804	1.765	A(3-2-9)	107.257	108.017
R(2-20)	1.828	1.787	A(3-2-20)	109.072	109.574
R(5-37)	1.216	1.221	A(4-2-9)	107.601	108.392
R(6-22)	1.493	1.505	A(4-2-20)	107.18	106.775
R(6-30)	1.472	1.491	A(9-2-20)	103.578	103.718
R(6-36)	1.477	1.499	A(2-9-10)	119.11	119.309
R(7-37)	1.382	1.361	A(2-9-18)	119.292	119.13
R(7-38)	1.397	1.405	A(2-20-22)	114.666	113.293
R(9-10)	1.397	1.389	A(2-20-33)	113.575	115.506
R(9-18)	1.396	1.392	A(5-37-7)	125.505	125.917
R(10-12)	1.394	1.396	A(5-37-36)	127.295	125.631
R(12-14)	1.397	1.378	A(22-6-30)	109.348	107.669
R(14-16)	1.396	1.386	A(22-6-36)	108.78	108.311
R(16-18)	1.395	1.386	A(6-22-20)	105.41	105.061
R(20-22)	1.567	1.55	A(6-22-24)	104.859	105.165
R(20-33)	1.533	1.529	A(30-6-36)	119.902	116.844
R(22-24)	1.545	1.535	A(6-30-27)	102.566	103.156
R(24-27)	1.536	1.53	A(6-36-33)	104.941	104.967
R(27-30)	1.53	1.519	A(6-36-37)	105.814	105.459
R(33-36)	1.547	1.536	A(6-36-46)	116.307	116.522
R(36-37)	1.562	1.555	A(37-7-38)	112.065	110.882
R(36-46)	1.516	1.509	A(7-37-36)	107.191	108.432
R(38-39)	1.389	1.382	A(7-38-39)	127.901	127.318

R(38-46)	1.407	1.401	A(7-38-46)	109.587	110.076
R(39-41)	1.399	1.392	A(10-9-18)	121.592	121.558
R(41-42)	1.393	1.385	A(9-10-11)	119.906	120.859
R(42-44)	1.402	1.401	A(9-10-12)	118.927	118.26
R(44-46)	1.388	1.385	A(9-18-16)	118.926	119.168
			A(9-18-19)	119.615	120.417
			A(10-12-14)	120.091	120.466
			A(12-14-16)	120.371	120.73
			A(14-16-18)	120.087	119.788
			A(16-18-19)	121.447	120.415
			A(22-20-33)	105.266	104.392
			A(20-22-24)	119.721	119.188
			A(22-24-26)	110.855	111.413
			A(22-24-27)	102.74	101.794
			A(26-24-27)	109.394	111.408
			A(24-27-30)	101.896	101.5
			A(27-30-31)	113.53	111.13
			A(27-30-32)	109.111	111.127
			A(31-30-32)	107.619	109.093
			A(33-36-37)	111.249	112.183
			A(33-36-46)	116.359	115.907
			A(37-36-46)	101.779	101.483
			A(36-46-38)	108.991	108.632
			A(36-46-44)	131.936	131.607
			A(39-38-46)	122.487	122.503
			A(38-39-41)	116.839	116.397
			A(38-46-44)	119.029	119.447
			A(40-39-41)	120.898	121.801
			A(39-41-42)	122.332	123.007

	A(41-42-44)	119.282	119.127
	A(42-44-46)	119.999	119.408

Table S3 The calculated and experimental chemical shifts (ppm) for the studied compound.

Atom	**(C.S)$_{Calc.}$**	**(C.S)$_{Exp.}$**	**Atom**	**(C.S)$_{Calc.}$**	**(C.S)$_{Exp.}$**
C 9	133.032	139.29	H 8	6.582	10.45
C 10	115.062	122.17	H 11	8.220	7.94
C 12	117.196	128.52	H 13	8.018	7.66
C 14	121.393	130.44	H 15	8.057	7.55
C 16	116.563	125.12	H 17	7.923	7.66
C 18	115.361	122.17	H 19	8.092	7.94
C 20	64.510	69.35	H 21	4.685	4.47
C 22	58.166	68.96	H 23	4.528	4.00
C 24	21.979	32.64	H 25	2.395	2.37
C 27	21.441	32.64	H 26	2.811	2.78
C 30	43.173	53.28	H 28	2.047	1.71
C 33	29.156	34.56	H 29	2.118	2.08
C 36	63.432	62.52	H 31	2.741	2.56
C 37	164.528	179.55	H 32	3.490	3.40
C 38	131.937	134.96	H 34	1.808	2.29
C 39	98.553	104.52	H 35	2.719	2.37
C 41	132.292	135.14	H 40	6.989	6.81
C 42	109.594	110.52	H 43	7.220	7.04
C 44	115.830	127.64	H 45	7.777	7.43
C 46	114.803	125.12			