Structural Insights on a Novel Anticancer Sulfonamide Chalcone

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Supplementary Information

Table S1: Experimental and Theoretical geometric parameters for 2,5-dichloro-N-{3-[(2E)-3-(4-nitrophenyl)prop-2-enoyl]phenyl}benzenesulfonamide. DFT calculations were performed with M062X/ 6311++G** theory level.

Bond	Lengths Å		Bond	Lengths Å	
	DRX	DFT		DRX	DFT
S1-O5	1.4252(3)	1.4526	N1-O2	1.1904(4)	1.2245
S1-O4	1.4262(3)	1.4565	N1-C1	1.4634(4)	1.4781
S1-N2	1.6122(3)	1.6896	C1-C6	1.3724(5)	1.3899
S1-C16	1.7733(3)	1.8197	C1-C2	1.3734(4)	1.3938
Cl2-C21	1.7155(4)	1.7515	C7-H7	0.9300	1.0871
Cl1-C18	1.7155(6)	1.7514	C13-C12	1.3814(5)	1.3898
O3-C9	1.2174(4)	1.2227	C13-H13	0.9300	1.0815
N2-C14	1.4204(4)	1.4253	C5-C6	1.3774(5)	1.3885
N2-HN1	0.8600	1.0143	C5-H5	0.9300	1.0840
C4-C5	1.3854(4)	1.4061	C3-C2	1.3764(4)	1.3852
C4-C3	1.3964(5)	1.4078	C3-H3	0.9300	1.0827
C4-C7	1.4664(5)	1.4624	C6-H6	0.9300	1.0811
C15-C14	1.3884(4)	1.3920	C2-H2	0.9300	1.0812
C15-C10	1.3894(4)	1.4004	C16-C17	1.3785(5)	1.3950
C15-H15	0.9300	1.0840	C16-C21	1.3965(7)	1.3988
C8-C7	1.3064(4)	1.3441	C17-C18	1.4046(6)	1.3891
C8-C9	1.4744(3)	1.4879	C17-H17	0.9300	1.0814
C8-H8	0.9300	1.0820	C12-H12	0.9300	1.0837
C9-C10	1.4974(4)	1.5010	C21-C20	1.3726(6)	1.3922
C11-C12	1.3734(4)	1.3936	C20-C19	1.3558(1)	1.3903
C11-C10	1.3894(4)	1.4000	C20-H20	0.9300	1.0824
C11-H11	0.9300	1.0821	C19-C18	1.3588(1)	1.3911
C14-C13	1.3894(4)	1.4014	C19-H19	0.9300	1.0823
N1-O1	1.1814(5)	1.2248			

Atoms	Angles (°)		Atoms	Angles (°)	
	DRX	DFT		DRX	DFT
O5-S1-O4	119.3414(2)	121.89	C2-C1-N1(3)	118.33	119.02
O5-S1-N2	105.8713(1)	105.30	C8-C7-C4(3)	127.43	127.55
O4-S1-N2	109.5314(1)	107.24	C8-C7-H7	116.3	116.42
O5-S1-C16	108.7515(2)	109.90	C4-C7-H7	116.3	116.03
O4-S1-C16	106.0715(2)	105.80	C12-C13-C14(3)	119.33	119.44
N2-S1-C16	106.6915(2)	106.64	C12-C13-H13	120.4	120.96
C14-N2-S1	127.52(2)	122.97	C14-C13-H13	120.4	119.60
C14-N2-HN1	116.3	114.59	C6-C5-C4(3)	121.73	121.36
S1-N2-HN1	116.3	109.36	C6-C5-H5	119.1	119.40
C5-C4-C3	118.13(3)	118.31	C4-C5-H5	119.1	119.23
C5-C4-C7	119.43(3)	118.38	C2-C3-C4(3)	121.13	121.04

C3-C4-C7	122.53(3)	123.31	C2-C3-H3	119.4	118.77
C14-C15-C10	120.93(3)	120.69	C4-C3-H3	119.4	120.19
C14-C15-H15	119.5	121.00	C1-C6-C5(3)	118.13	118.53
C10-C15-H15	119.5	118.31	C1-C6-H6	120.9	119.77
C7-C8-C9	122.23(3)	120.20	C5-C6-H6	120.9	121.70
C7-C8-H8	118.9	121.25	C1-C2-C3(3)	118.53	118.88
C9-C8-H8	118.9	118.54	C1-C2-H2	120.7	119.54
O3-C9-C8	120.53(3)	121.05	C3-C2-H2	120.7	121.58
O3-C9-C10	120.03(3)	120.15	C17-C16-C21(3)	119.63	120.04
C8-C9-C10	119.53(3)	118.79	C17-C16-S1(3)	117.93	116.38
C12-C11-C10	119.93(3)	119.99	C21-C16-S1(3)	122.53	123.57
C12-C11-H11	120.1	119.01	C16-C17-C18(4)	118.94	119.47
C10-C11-H11	120.1	120.99	C16-C17-H17	120.6	119.32
C15-C14-C13	119.53(3)	119.90	C18-C17-H17	120.6	121.21
C15-C14-N2	116.73(3)	119.42	C11-C12-C13(3)	121.43	120.81
C13-C14-N2	123.83(3)	120.62	C11-C12-H12	119.3	119.81
O1-N1-O2	121.53(4)	124.80	C13-C12-H12	119.3	119.36
O1-N1-C1	119.43(3)	117.59	C20-C21-C16(4)	119.74	119.76
O2-N1-C1	119.13(3)	117.62	C20-C21-Cl2(4)	118.54	117.71
C15-C10-C11	119.03(3)	119.13	C16-C21-Cl2(3)	121.83	122.53
C15-C10-C9	117.43(3)	117.28	C19-C20-C21(5)	121.05	120.38
C11-C10-C9	123.63(3)	123.56	C19-C20-H20	119.5	120.24
C6-C1-C2	122.43(3)	121.87	C21-C20-H20	119.5	119.38
C6-C1-N1	119.33(3)	119.11	C20-C19-C18(6)	120.25	119.45
			C20-C19-H19	119.9	120.23
			C18-C19-H19	119.9	120.31
			C19-C18-C17(5)	120.65	120.90
			C19-C18-Cl1(5)	120.55	119.67
			C17-C18-Cl1(4)	118.95	119.43

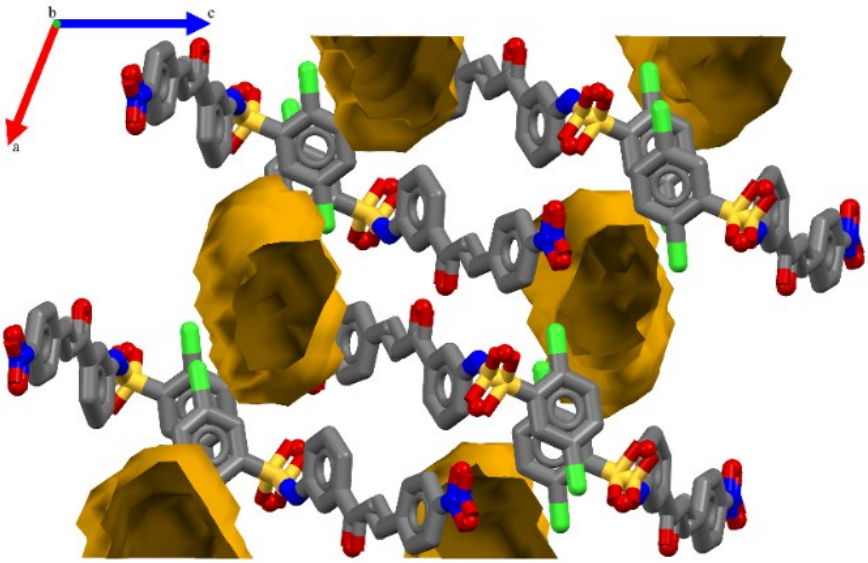

Figure S1: Crystal packing of BSC in view of [010] showing the solvent accessible voids (yellow)

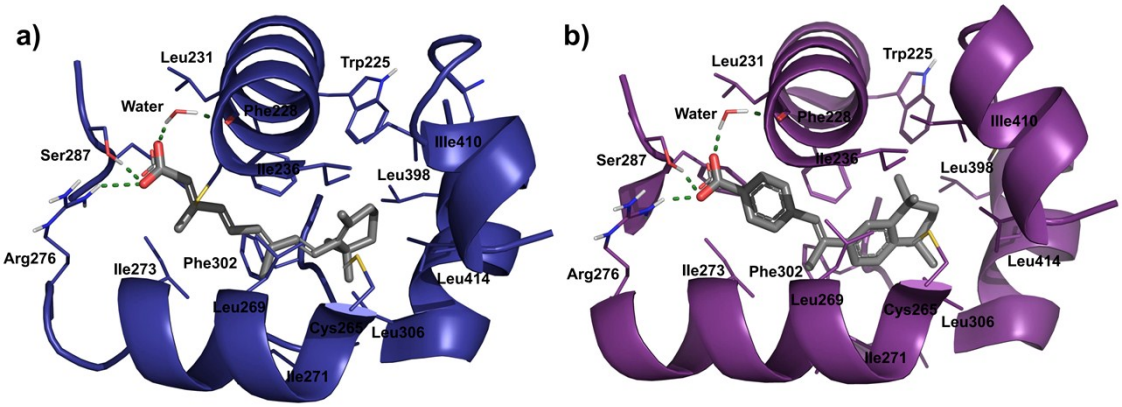

Figure S2. Intermolecular interactions of RARα (a, PDB ID = 3A9E) and RARβ (b, PDB ID = 4DM6) with their co-crystalized ligands.