Structural characterization of naphthalene sulfonamides and a sulfonate ester and their *in vitro* efficacy against *Leishmania tarentolae* promastigotes

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Supplemental Information

Table S1: Crystallographic Data

	Compound **A**	Compound **B**	Compound **C**
Empirical formula	$C_{18}H_{15}NO_4S$	$C_{16}H_{12}ClNO_2S$	$C_{18}H_{14}O_5S$
Formula weight	341.37	317.78	342.35
crystal size (mm)	0.22×0.09×0.09	0.51×0.51×0.45	0.28×0.16×0.09
Temperature (K)	100(2)	297(2)	100(2)
crystal system	monoclinic	monoclinic	triclinic
space group	*C*2/*c*	$P2_1/n$	$P\bar{1}$
a (Å)	14.6257(9)	8.923(2)	7.9204(5)
b (Å)	14.7988(10)	9.1409(8)	8.7629(6)
c (Å)	15.0858(10)	17.8901(14)	11.5108(7)
α (°)	90	90	93.616(4)
β (°)	101.281(4)	97.508(10)	92.555(4)
γ (°)	90	90	103.286(4)
V (Å^3)	3202.1(4)	1446.7(4)	774.55(9)
Z	4	4	2
ρ_{calcd} (g/cm^3)	1.416	1.459	1.468
μ (mm^{-1})	0.224	0.411	0.235
F(000)	1424	656	356
Data / restraints / parameters	3264 / 1 / 226	3317 / 0 / 194	3695 / 0 / 222
R_1: [$I > 2\sigma(I)$] / all	0.0300 / 0.0358	0.0343 / 0.0483	0.0378 / 0.0473
wR_2: [$I > 2\sigma(I)$] / all	0.0792 / 0.0833	0.0960 / 0.1034	0.0972 / 0.1028
GOF on F^2	1.061	1.038	1.045
Largest peak/hole (e/Å^3)	0.344 / – 0.394	0.356 / – 0.332	0.698 / – 0.382
CCDC Number	1917626	1917627	1917628

Table S2: Bond lengths (Å) and angles (°)

Bond	Compound **A**	Compound **B**	Compound **C**
S11–C1	1.7694(11)	1.7682(17)	1.7629(17)
S11–O12	1.4376(10)	1.4287(13)	1.4253(12)
S11–O13	1.4376(11)	1.4337(12)	1.4291(12)
S11–N/O14	1.6316(12)	1.6382(15)	1.6021(12)
N/O14–C15	1.4188(16)	1.419(2)	1.4181(18)
O12–S11–O13	118.96(6)	118.11(8)	119.71(8)
C1–S11–N/O14	107.07(6)	106.71(7)	103.48(7)
S11–N/O14–C15	125.97(10)	124.13(12)	121.47(10)
C1–S11–N/O14–C15	65.53(12)	56.54(14)	71.86(12)

Table S3: Hydrogen-bond geometries for Compounds **A, B**, and **C** (Å, °)

Compound **A**				
D*—H···*A	***D*—H**	**H···*A***	***D*···*A***	***D*—H···*A***
C20—H20···O13	0.95	2.39	3.0255(17)	124
N14—H14···O12^{i}	0.851(19)	2.20(2)	3.0240(15)	163.3(17)
C9—H9···O12^{i}	0.95	2.58	3.4988 (18)	163
O24—H24···O23^{ii}	0.88(2)	1.76(2)	2.6335(14)	176(4)
Symmetry codes: (i) −*x*+3/2, −*y*+1/2, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*.				

Compound **B**				
D*—H···*A	***D*—H**	**H···*A***	***D*···*A***	***D*—H···*A***
N14—H14···O13^{i}	0.78(2)	2.36(2)	3.0824(19)	153(2)
C19—H19···O12^{iii}	0.93	2.6	3.380(2)	141
Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+1/2; (ii) −*x*−1/2, *y*+1/2, −*z*+1/2; (iii) *x*−1, *y*, *z*.				

Compound **C**				
D*—H···*A	***D*—H**	**H···*A***	***D*···*A***	***D*—H···*A***
O24—H24···O23^{i}	0.87(3)	1.77(3)	2.6411(17)	173(3)
C17—H17···O13^{ii}	0.95	2.53	3.432(2)	159
C21—H21*C*···O13^{ii}	0.98	3.05	3.762(2)	131
Symmetry codes: (i) −*x*+2, −*y*+3, −*z*+1; (ii) *x*+1, *y*, *z*.				

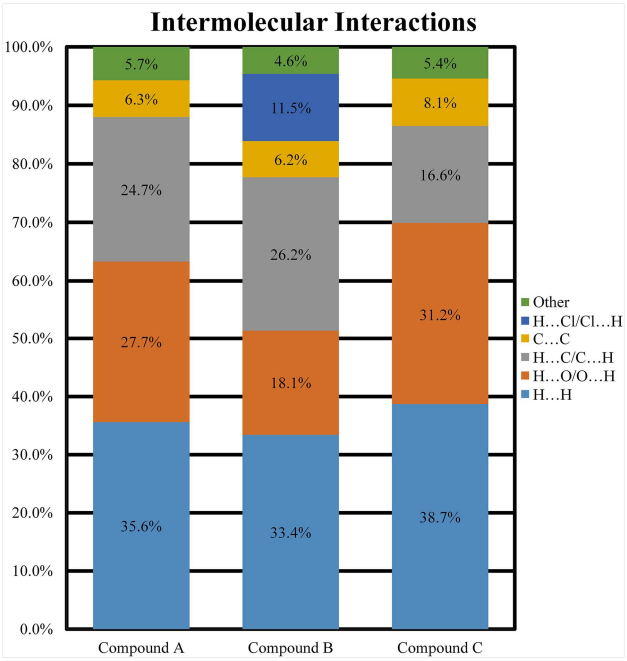

Figure S1. Hirshfeld surface contacts in compounds **A**, **B**, and **C**.