Supporting Information

Metal Complexes of Tosyl Sulfonamides: Design, X-ray Structure, Biological Activities and Molecular Docking Studies

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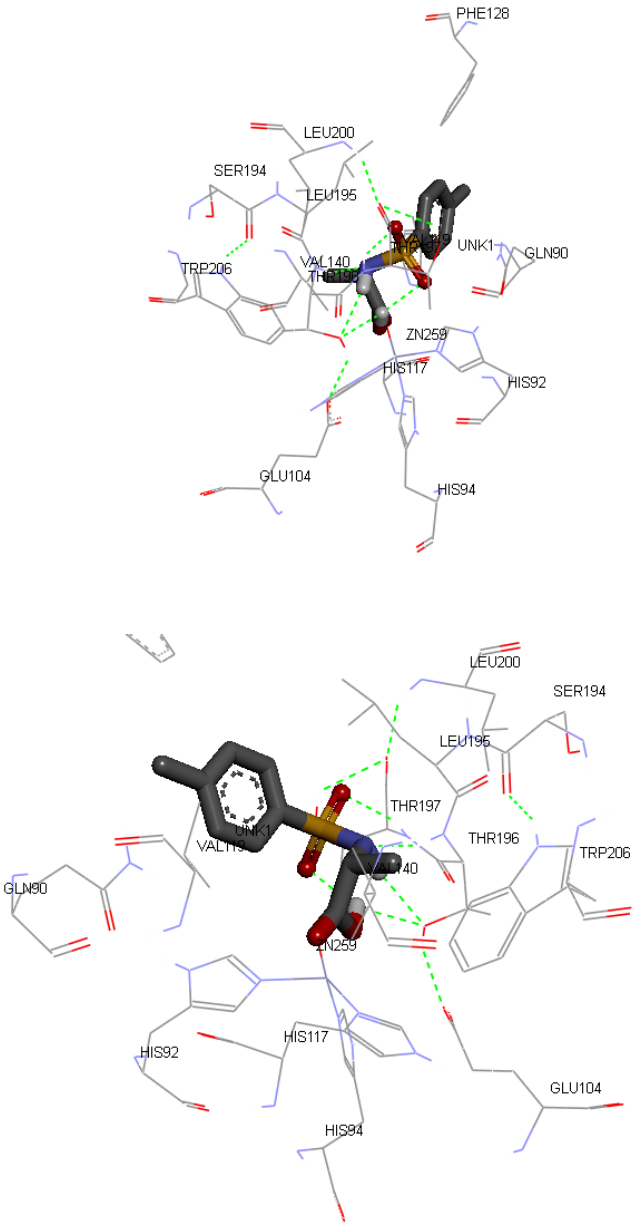

Figure S1. Binding site interactions of compound **NA1**.

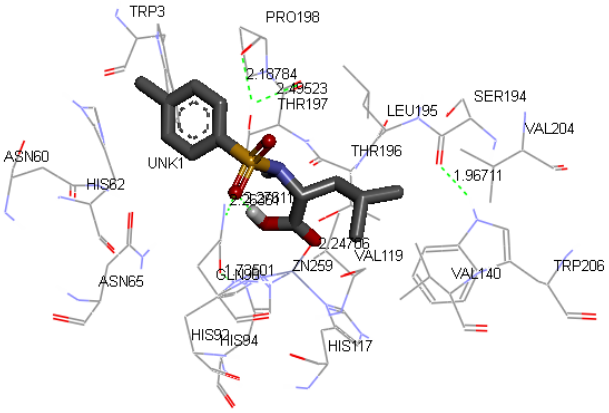

Figure S2. Binding site interactions of compound **NA2**.

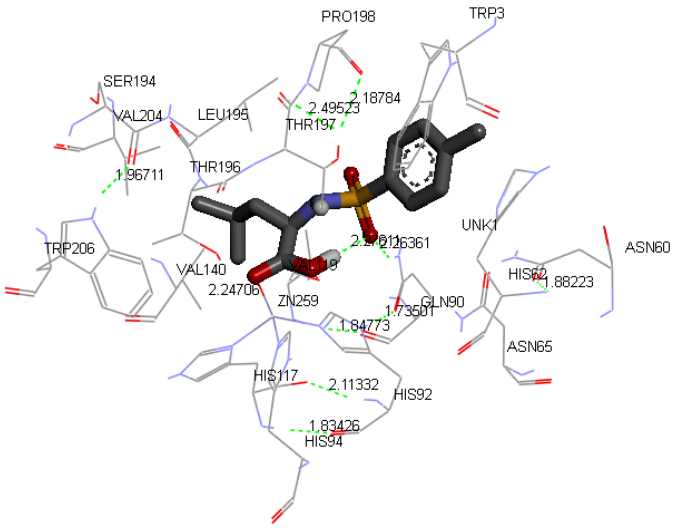

Figure S3. Binding site interactions of compound **NA3**.

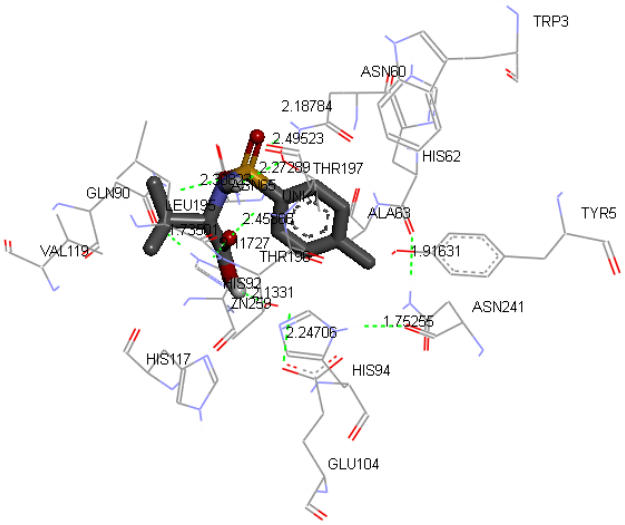

Figure S4. Binding site interactions of compound **NA4**.

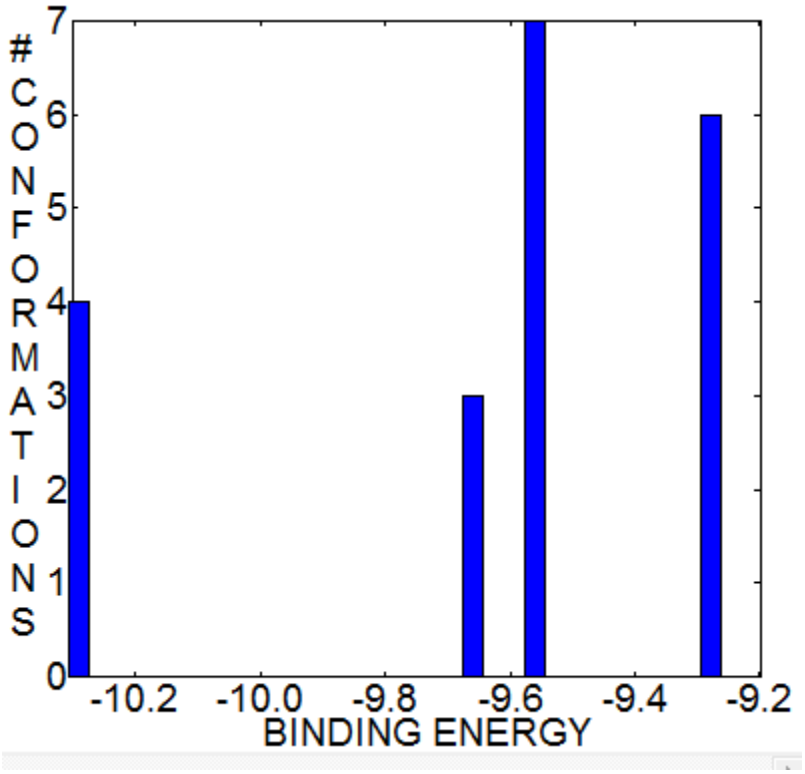

Figure S5. Clustering histogram of compound **NA1**.

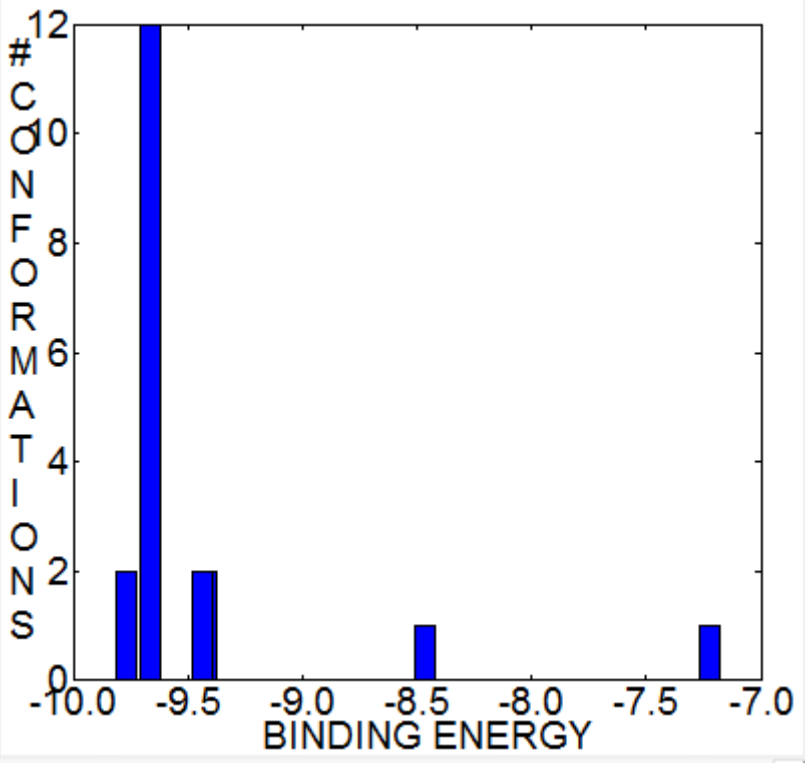

Figure S6. Clustering histogram of compound **NA2**.

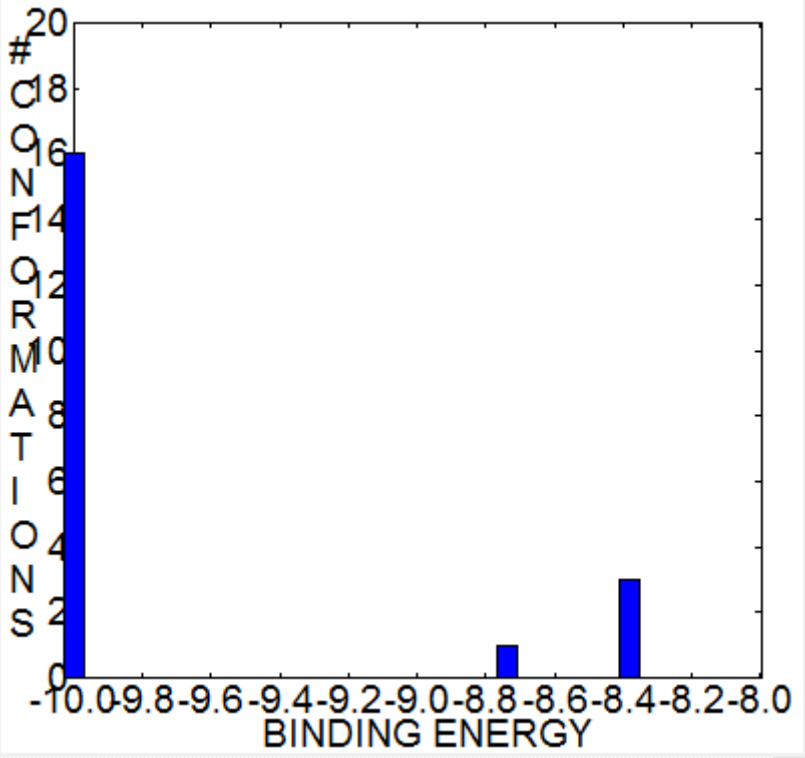

Figure S7. Clustering histogram of compound **NA3**.

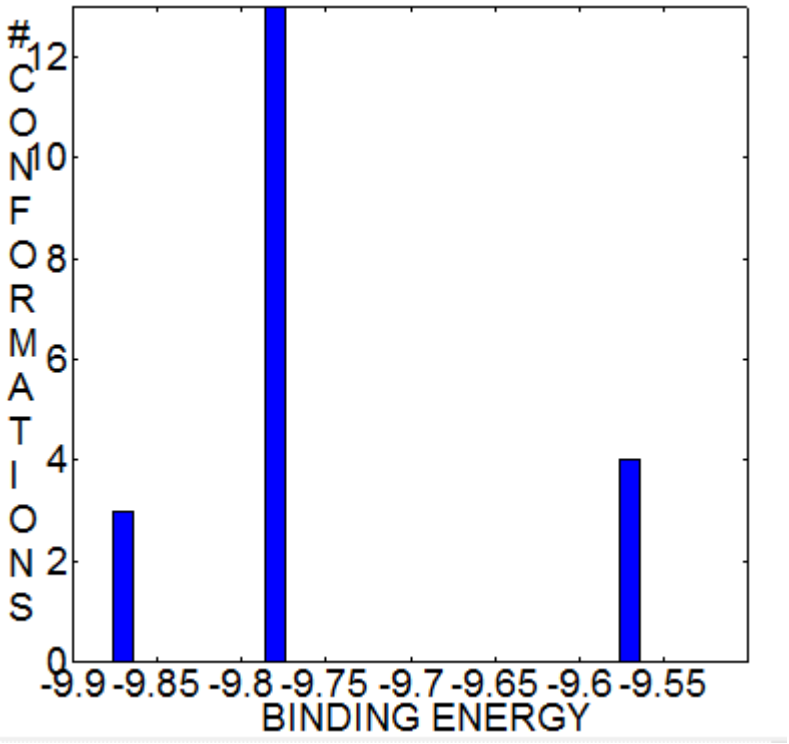

Figure S8. Clustering histogram of compound **NA4**.

Table S1 Crystal Data Collection and Refinement Parameters for compound **NA3**

Parameters	Compound (NA3)
Chemical formula	$C_{13}H_{19}NO_4S$
Cystal colour	Yellow
Fw; F (000)	285.35; 608
Temperature/K	100(2)
wavelength (Å)	0.71073
a/Å	5.51320(10)
b/Å	11.8110(2)
c/Å	21.7712(3)
α /°	90.00
β /°	90.00
γ /°	90.00
Volume/Å^3	1417.66(4)
ρ_{calcd} mg/mm^3)	1.337
μ (mm^{-1})	2.127
θ range (deg); completeness	4.06 − 70.98; 0.996
collected reflections; R_σ	18602; 0.0181
unique reflections; R_{int}	18602; 0.0253
R1[a]; wR2[b] [I > 2σ(I)]	0.0314; 0.0837
R1; wR2 [all data]	0.0320; 0.0841
Goodness-of-fit on F^2	1.042
largest diff peak and hole	0.370 and -0.403

[a]R1=Σ(||Fo|-|Fc||)/Σ|Fo|

[b]wR2={Σ[w(Fo2–Fc2)2]/Σ[w(Fo2)2]}½

Table S2 Selected bond lengths (Å) for compound **NA3**

S1-O2	1.4252(14)	C5-H5C	0.9800
S1-O1	1.4344(13)	C6-C7	1.386(3)
S1-N1	1.6343(14)	C6-H6	0.9500
S1-C1	1.7736(18)	C7-H7	0.9500
O3-C9	1.209(2)	C8-C9	1.520(2)
O4-C9	1.323(2)	C8-C10	1.556(2)
O4-H4	0.8400	C8-H8	1.0000
N1-C8	1.452(2)	C10-C12	1.531(2)
N1-H1A	0.8800	C10-C11	1.547(3)
C1-C7	1.384(3)	C10-H10	1.0000
C1-C2	1.393(3)	C11-H11A	0.9800
C2-C3	1.388(3)	C11-H11B	0.9800
C2-H2	0.9500	C11-H11C	0.9800
C3-C4	1.392(3)	C12-C13	1.518(3)
C3-H3	0.9500	C12-H12A	0.9900
C4-C6	1.392(3)	C12-H12B	0.9900
C4-C5	1.512(3)	C13-H13A	0.9800
C5-H5A	0.9800	C13-H13B	0.9800
C5-H5B	0.9800	C13-H13C	0.9800

Table S3 Selected bond angles (˚) for compound **NA3**

O2-S1-O1	120.61(8)	C6-C7-H7	120.4
O2-S1-N1	107.97(8)	N1-C8-C9	110.95(14)
O1-S1-N1	104.60(8)	N1-C8-C10	110.73(14)
O2-S1-C1	107.83(9)	C9-C8-C10	109.34(14)
O1-S1-C1	107.96(8)	N1-C8-H8	108.6
N1-S1-C1	107.17(8)	C9-C8-H8	108.6
C9-O4-H4	109.5	C10-C8-H8	108.6
C8-N1-S1	119.78(12)	O3-C9-O4	124.60(16)
C8-N1-H1A	120.1	O3-C9-C8	122.97(17)
S1-N1-H1A	120.1	O4-C9-C8	112.40(14)
C7-C1-C2	120.82(17)	C12-C10-C11	110.46(16)
C7-C1-S1	119.88(14)	C12-C10-C8	110.63(15)
C2-C1-S1	119.25(14)	C11-C10-C8	111.32(15)
C3-C2-C1	119.20(17)	C12-C10-H10	108.1
C3-C2-H2	120.4	C11-C10-H10	108.1
C1-C2-H2	120.4	C8-C10-H10	108.1
C2-C3-C4	120.93(18)	C10-C11-H11A	109.5
C2-C3-H3	119.5	C10-C11-H11B	109.5
C4-C3-H3	119.5	H11A-C11-H11B	109.5

C6-C4-C3	118.58(18)	C10-C11-H11C	109.5
C6-C4-C5	120.62(18)	H11A-C11-H11C	109.5
C3-C4-C5	120.78(19)	H11B-C11-H11C	109.5
C4-C5-H5A	109.5	C13-C12-C10	113.32(16)
C4-C5-H5B	109.5	C13-C12-H12A	108.9
H5A-C5-H5B	109.5	C10-C12-H12A	108.9
C4-C5-H5C	109.5	C13-C12-H12B	108.9
H5A-C5-H5C	109.5	C10-C12-H12B	108.9
H5B-C5-H5C	109.5	H12A-C12-H12B	107.7
C7-C6-C4	121.32(18)	C12-C13-H13A	109.5
C7-C6-H6	119.3	C12-C13-H13B	109.5
C4-C6-H6	119.3	H13A-C13-H13B	109.5
C1-C7-C6	119.14(17)	C12-C13-H13C	109.5
C1-C7-H7	120.4	H13A-C13-H13C	109.5
		H13B-C13-H13C	109.5