

**Table 1.** Molecular scoring of canthin-6-one (**Cant**) interacting with target proteins.

Target 1: MAPK14							
Ligand	Estimated Free Energy of Binding (kcal/mol)	Estimated Inhibition Constant (Ki μM)	vdW + H-bond + dissolving Energy (kcal/mol)	Electrostatic Energy (kcal/mol)	Total Intermolecular Energy (kcal/mol)	Frequency (%)	Intert Surface
Cant	-7.07	6.60	-7.04	-0.03	-7.07	20	388.484
Mesa	-3.57	2.43	-4.25	-0.19	-4.44	10	359.758
Sulfa	-4.75	327.15	-6.98	-0.22	-7.20	20	618.697
Target 2: TLR8							
Cant	-7.41	3.68	-7.40	-0.02	-7.41	40	557.879
Mesa	-4.33	675.08	-5.25	-0.08	-5.33	10	426.459
Sulfa	-4.79	309.92	-6.26	-0.49	-6.75	10	685.389
Sulfa- Sulfasalazine, Mesa - Mesalazine. MAPK1 - Mitogen-Activated Protein Kinase 1, TLR8 - Toll-like receptor 8,							