Table S1. Ten candidate compounds identified by *in silico* SBDS.

compound	ChemBridge IDs	IUPAC name	M.W.	cLogP	tPSA	GOLD score
1	7389795	4-methoxy-*N*-(4-{[(2-phenylethyl)amino]sulfonyl}phenyl)benzenesulfonamide	447	3.86	102	75.9
2	7788851	N^1-{4-[(diethylamino)sulfonyl]phenyl}-N^2-phenyl-N^2-(phenylsulfonyl)glycinamide	502	4.46	104	75.8
3	7780058	2-({3-[(2-ethoxybenzoyl)amino]benzoyl}amino)benzoic acid	404	4.70	105	72.4
4	7972614	*N*,*N*′-bis(4-methoxybenzyl)-1-[(4-methylphenyl)sulfonyl]-1H-1,2,4-triazole-3,5-diamine	494	3.18	107	71.1
5	6824862	*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)-2-{[5-(phenoxymethyl)-4-phenyl-4H-1,2,4-triazol-3-yl]thio}acetamide	527	1.42	96	70.8
6	7968391	*N*-1,3-benzothiazol-2-yl-2-({5-[3-(4-methoxy-2-methylphenyl)propyl]-4-methyl-4H-1,2,4-triazol-3-yl}thio)acetamide	468	4.31	82	70.4
7	6945187	3-[4-(4-bromophenyl)-1,3-thiazol-2-yl]-7-hydroxy-8-{[4-(2-hydroxyethyl)-1-piperazinyl]methyl}-2H-chromen-2-one	542	4.92	90	68.8
8	7355746	*N*-(2,4-dichlorobenzyl)-*N*-[(4-methylphenyl)sulfonyl]glycine	388	4.86	75	68.3
9	7917692	*N*-[(1-ethyl-2-oxo-1,2-dihydrobenzo[cd]indol-6-yl)sulfonyl]tryptophan	464	3.26	120	68.1
10	6082385	4-{4-[(phenoxyacetyl)amino]phenoxy}phthalic acid	407	3.58	122	68.0

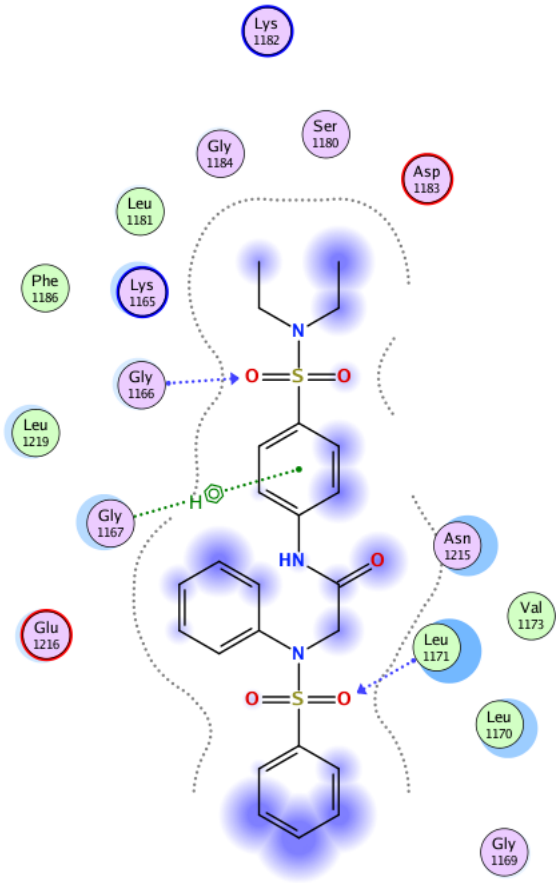

Figure S1. Ligand Interaction (LI) between IRβ and compound **2.** The data shows predicted interaction at 50 ns in the MD simulation. The dotted blue allows and green line represent hydrogen bonds and cation-π interaction, respectively. The blue crowds on compound **2** indicate hydrophobic interactions with the binding pocket.