TABLE S1. Molecular docking data of the synthesized tricyanofuran-hydrazone chromophores

Derivative	**S (Kcal/mol)**	**Rmsd**	**Interaction with ligand**	**Types of Interactions**	**Distance (Å)**
(1) R= H	-6.5220	1.6759	N 11 of hydrazone moiety with Asp 245 N 24 of nitrile group with Val 169	H-donor H-acceptor	2.95 3.42
(2) R= 4-CH_3	-6.6246	1.5841	N 11 of hydrazone moiety with Asp 257 Phenyl ring with Gly 251	H-donor Pi-H	3.29 3.81
(3) R= 4-$(CH_2)_7CH_3$	-7.2496	1.6960	N 28 of nitrile group with Asn 282	H-acceptor	3.49
(4) R= 4-CF_3	-6.5070	1.5786	N 24 of nitrile group with Val 169	H-acceptor	3.37
(5) R= 3,5-$(NO_2)_2$	-7.0952	1.4723	N 22 of nitrile group with Lys 283	H-acceptor	3.014
Penicillin	-6.0265	1.4275	C 5 of thiazolidinone ring with Asp 245 O12 of carboxylic acid with Asp 245 S 7 of thiazolidinone ring with Ser 168 Phenyl ring with Lys 283	H-donor H-donor H-acceptor Pi- cation	3.06 3.35 2.86 3.30