

Table S6. Molecular docking data of the synthesized pyrazine-thiazole analogues.

Analogues	S (Kcal/mol)	Rmsd	Interaction with ligand	Types of Interactions	Distance (Å)
2	-6.1099	1.1280	N 11 of thio-semi carbazone with Glu 123	H-donor	3.17
			N 16 of pyrimidine-ring with Lys 152	H-acceptor	2.89
			N 7 of 2° aromatic amine with 6-ring of Trp 52	H-pi	4.55
3	-7.0020	1.6525	N 11 of hydrazide moiety with Arg 205	H-donor	3.24
4a	-8.0078	1.1562	N 11 of hydrazide moiety with Arg 205	H-donor	3.05
			Methoxy-ring with Arg 205	pi-cation	3.50
4b	-8.1523	1.8728	N 11 of hydrazide moiety with Arg 205	H-donor	3.14
			C 18 of olefinic moiety with Glu 44	H-donor	3.32
4c	-7.9394	1.9990	N 11 of hydrazide moiety with Arg 205 Phenyl-ring with Arg 205	H-donor pi-cation	3.06 3.59
6a	-7.8517	1.3332	N 11 of hydrazide moiety with Arg 205	H-donor	3.14
6b	-8.2382	1.9889	N 11 of hydrazide moiety with Arg 205	H-donor	3.12
6c	-7.9533	1.1599	N 11 of hydrazide moiety with Arg 205	H-donor	3.10
8a	-6.7698	1.0625	N 11 of hydrazide moiety with Arg 205	H-donor	3.21
			S 13 of thiazole-ring with Arg 205	H-donor	3.90
8b	-7.5335	1.2370	N 11 of hydrazide moiety with Arg 205	H-donor	3.08
			S 13 of thiazole-ring with Arg 205	H-donor	3.70
9	-7.7557	0.7016	N 22 of pyrimidine-ring with Ser 179	H-acceptor	3.42
			Aniline-ring with Lys 152	pi-cation	4.42
11a	-7.9165	1.5625	N 11 of hydrazide moiety with Gln 149	H-donor	2.77
			S 13 of thiazole-ring with Gln 149	H-donor	3.04
			N 21 of pyrimidine-ring with Arg 205	H-acceptor	3.15
			pyrimidine-ring with Tyr 180	pi-H	3.66
11b	-8.5010	1.6461	N 11 of hydrazide moiety with Arg 205	H-donor	2.99
			O 33 of nitro--group with Lys 121	H-acceptor	3.22
11c	-7.7384	1.4935	N 11 of hydrazide moiety with Arg 205	H-donor	3.25
			Thiazole-ring with Lys 152	pi-cation	4.38
Erlotinib	-7.0792	1.8048	N 8 of pyrimidine-ring with Lys 152	H-acceptor	3.14