

Target Name	EGFR
Target TTD ID	TTDS00355

Target Species	Human
Chemical Type	Anilinoquinolines
Mode of Action	Inhibitor
QSAR Model 1	$PA_{DFT} = -2.0703\varepsilon_{HOMO} - 0.7483\varepsilon_{LUMO} + 0.043W - 0.194MR + 2.0234I$ $- 0.036\Delta E_{nm} + 17.82$ $r^2_{CV} = 0.75r^2 = 0.80$
Molecular Descriptor	<p>Access the following web-servers to compute molecular descriptors: MoDel and e-dragon</p> <p>The ionization potential (IP), electron affinity (EA), charge (q), electron density (C) of an atom in a molecule, molecular weight (MW), molar refractivity (MR), indicator parameter (I), difference of softness ΔE_{nm}; All molecules having two substitutions at ring "A" were allotted values of $I = I$ and the reminder had $I = 0$.</p>
Reference	In silico QSAR studies of anilinoquinolines as EGFR inhibitors. <i>J Mol Model</i> (2010) 16:263–277