**Supplementary information**

**Structural identification of novel pyrimidine derivatives as epidermal growth factor receptor inhibitors using 3D QSAR, molecular docking and MMGBSA analysis: a rational approach in anticancer drug design**

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**Supplementary Figure 1.** Superimposition of co-crystalized gefitinib (sky) and re-docked co-crystalized gefitinib (purple) in the binding site of EGFRL858R/T790M protein (PDB ID: 4I22).

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 **(A) (B)**

**Supplementary Figure 2.** Binding interactions in between EGFRL858R/T790M protein and newly designed compounds. (A) Compound N4; (B) Compound N1.