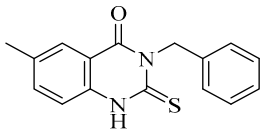
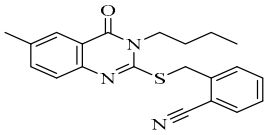
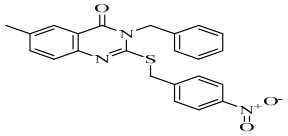
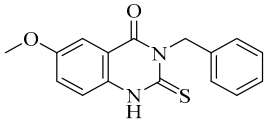
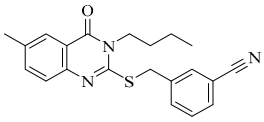
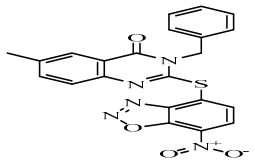
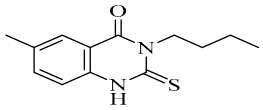
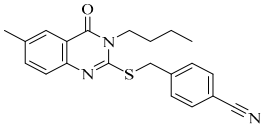
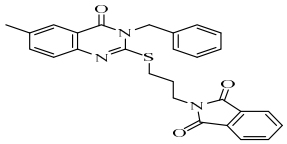
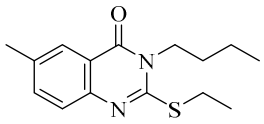
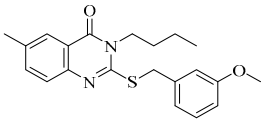
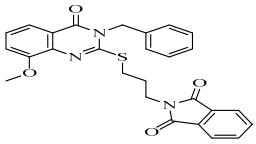
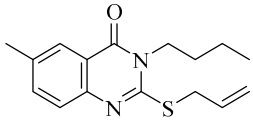
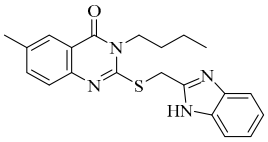
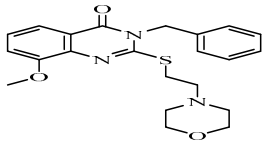
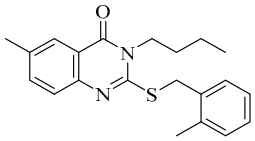
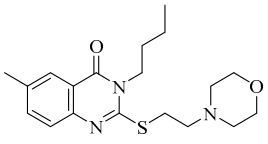
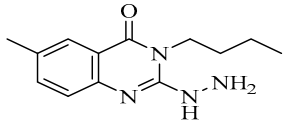
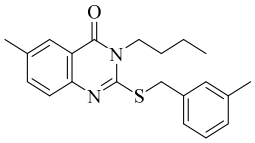
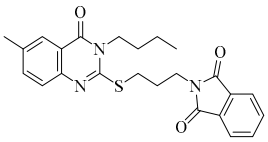
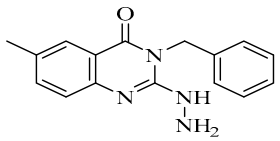
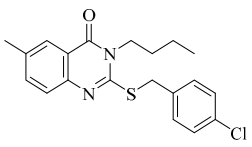
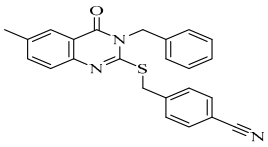
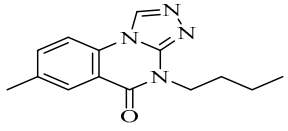
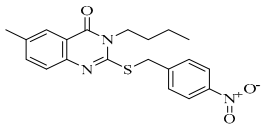
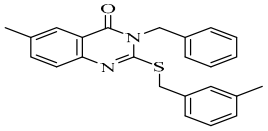
Table S1. Chemical structure and pIC_{50} values of the investigated quinazoline derivatives.

N°	Compounds	Pic50[1]	N°	Compounds	Pic50[1]	N°	Compounds	Pic50[1]
S1		5.314	S10		4.018	S19		5.456
S2		5.564	S11		5.292	S20		5.633
S3		5.420	S12		5.286	S21		5.592
S4		5.424	S13		5.304	S22		5.551
05		5.353	S14		4.755	S23		5.562
S6		5.301	S15		5.208	S24		5.252
S7		5.384	S16		5.533	S25		5.241
S8		5.385	S17		5.304	S26		5.314

S9		5.371	S18		5.491

1 pIC_{50} values determined against MDA-MB-231 cell line

Table S2. Key residue interactions of the selected quinazoline derivatives and the reference ligand within the EGFR active site (PDB ID: 3UG2).

Compound	Key Residue Interactions	Interaction Types
Gefitinib (Reference ligand)	Met793, Leu788, Gln791, Leu792, Met790, Pro794, Phe795, Cys797, Leu718, Met766, Ile744, Ala743, Ser719	Hydrogen bond (Met793), Halogen bond (Leu788), Hydrophobic interactions, Polar contacts
S26	Met793, Gln791, Thr854, Leu792, Met790, Cys775, Ala743, Leu844, Phe795, Pro794, Val726, Leu718	Hydrogen bond (Met793), Hydrophobic interactions, Polar contacts
S24	Met793, Gln791, Leu792, Met790, Cys775, Val726, Leu788, Ala743, Ile744, Cys797	Hydrogen bonds (Met793, Gln791), Hydrophobic interactions, Polar contacts
S16	Met793, Thr854, Gln791, Lys745, Arg776, Arg841, Asp855, Asn842, Leu792, Met790, Leu788, Cys775, Leu718, Leu844, Met766, Cys797, Ser719	Hydrogen bonds (Met793, Thr854), Hydrophobic interactions, Polar contacts, Electrostatic interactions

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