

Supplementary Materials

Table S1. The QM/MM + PB/SA calculated binding energies (ΔG_{ttl}) and mutation energies ($\Delta\Delta G_{\text{mtt}}$) of ATP molecule to wild-type EGFR kinase domain and its 68 NSCLC-related mutants (unit: kcal/mol)

EGFR kinase domain	ΔG_{ttl}	$\Delta\Delta G_{\text{mtt}}$
wild type	-8.90	0.00
V689M	-9.04	-0.14
L692F	-9.10	-0.20
G696E	-8.38	0.52
N700D	-8.52	0.38
L703V	-8.80	0.10
E709D	-8.74	0.16
E709Q	-9.14	-0.24
E709K	-9.68	-0.78
E709A	-9.38	-0.48
E709H	-9.52	-0.62
E709C	-9.30	-0.40
F712S	-9.24	-0.34
L718P	-8.24	0.66
G719C	-10.14	-1.24
G719A	-9.66	-0.76
G719R	-11.38	-2.48
G719S	-10.32	-1.42
S720P	-8.28	0.62
G721D	-7.06	1.84
G724S	-9.82	-0.92
W731R	-9.40	-0.50
P733S	-9.06	-0.16
V742A	-8.72	0.18
I744M	-8.44	0.46
N756D	-8.32	0.58
E758G	-10.64	-1.74
D761Y	-10.02	-1.12
A763V	-8.76	0.14
V765M	-8.72	0.18
V765A	-8.82	0.08
S768I	-8.56	0.34
S768C	-8.68	0.22
V769L	-9.18	-0.28
H773R	-9.88	-0.98
L777G	-8.66	0.24
G779S	-9.30	-0.40

T783A	-8.42	0.48
T790M	-11.44	-2.54
L798H	-9.76	-0.86
V802I	-7.98	0.92
R803W	-7.20	1.70
K806E	-7.38	1.52
Q812R	-9.58	-0.68
L814P	-8.62	0.28
N826S	-8.72	0.18
R831C	-8.48	0.42
R832H	-8.64	0.26
L833V	-9.20	-0.30
R836C	-7.42	1.48
A839T	-9.94	-1.04
V843I	-8.30	0.60
K846R	-8.00	0.90
T847I	-8.50	0.40
V851I	-8.56	0.34
D855G	-11.28	-2.38
F856L	-8.32	0.58
G857R	-10.80	-1.90
L858A	-8.38	0.52
L858W	-8.08	0.82
L858Q	-9.64	-0.74
L858K	-10.28	-1.38
A859I	-8.30	0.60
L861Q	-9.42	-0.52
G863D	-7.86	1.04
E865L	-9.72	-0.82
E868G	-9.58	-0.68
A871V	-8.38	0.52
A871T	-9.56	-0.66
