

Personalized prediction of EGFR mutation-induced drug resistance in lung cancer

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Supplementary information

Supplementary Table 1. Binding free energies and their components

This table lists the binding free energies and their components for EGFR mutants (including the WT protein) with inhibitors gefitinib or erlotinib. These components encompass energy components of Van der Waals forces (VDW), electrostatic interactions (EEL), and the polar (EPB) and non-polar (ENPOLAR) terms of the solvation free energies.

Mutation	gefitinib					erlotinib				
	A VDW	B EEL	C EPB	D ENPOLA	TOTAL	A VDW	B EEL	C EPB	D ENPOLA	TOTAL
Wild-Type	-50.2296	-11.1671	38.9803	-35.4615	-57.8778	-50.6681	-20.8587	43.3936	-33.3898	-61.523
delE709_T710insD	-44.6069	-13.964	39.4971	-31.4007	-50.4746	-53.6351	-19.6767	42.6918	-35.3254	-65.9455
delE746_A750	-50.5251	-22.0131	46.8522	-34.3009	-59.9869	-50.1603	-19.8216	41.8836	-33.8104	-61.9088
delE746_A750insAP	-51.9638	-15.1619	43.2361	-34.7622	-58.6518	-53.8646	-27.055	51.9279	-35.456	-64.4478
delE746_S752insV	-48.8281	-13.0112	41.0875	-34.0521	-54.804	-55.6001	-15.3985	37.3355	-35.9611	-69.6242
delE746_T751insA	-47.837	-13.729	43.0336	-33.4805	-52.0129	-54.0127	-18.2783	45.4917	-35.4571	-62.2566
delE746_T751insI	-50.4453	-29.1852	48.0859	-35.7435	-67.2881	-51.8367	-24.4881	48.8697	-34.6179	-62.0731
delE746_T751insV	-51.9404	-31.1156	45.7566	-36.121	-73.4205	-48.3525	-22.6061	43.5498	-32.3339	-59.7426
delE746_T751insVA	-49.1903	-12.9124	41.4606	-33.8416	-54.4837	-51.7018	-23.5795	47.7204	-33.9372	-61.4981
delL747_A750insP	-43.9295	-14.4339	41.8619	-31.2248	-47.7263	-51.5153	-19.9035	44.7871	-33.7622	-60.394
delL747_A755insSKG	-49.5679	-29.6112	43.0473	-35.1745	-71.3063	-55.103	-17.8136	40.1929	-35.7582	-68.4818
delL747_K754insANKG	-40.4989	-14.9861	37.8217	-29.4278	-47.0911	-52.3439	-20.8041	42.4109	-34.0711	-64.8083
delL747_P753insS	-48.5144	-8.1678	39.0625	-33.2823	-50.902	-52.276	-17.6311	39.7891	-34.2095	-64.3275
delL747_T751	-48.3858	-28.1914	41.512	-34.4295	-69.4947	-50.8573	-23.0883	49.1875	-34.1398	-58.8978
delL747_T751insP	-50.0991	-29.8346	47.6035	-36.2848	-68.6149	-55.2224	-20.6304	43.2604	-36.4882	-69.0806
delT751_I759insN	-41.8782	-8.3131	29.7125	-28.0847	-48.5636	-48.6189	-15.2223	40.6432	-31.2655	-54.4634
delT751_I759insS	-39.9473	-12.1323	35.9476	-27.9353	-44.0673	-52.4828	-21.6551	48.2974	-34.7362	-60.5767
dulA767_V769	-48.2267	-29.3215	43.4074	-34.5519	-68.6928	-45.8776	-15.6426	37.882	-30.7301	-54.3683
dulH773	-52.2024	-13.9438	42.2407	-35.3819	-59.2875	-51.4803	-23.9338	43.9719	-33.5343	-64.9766
dulN771_H773	-48.8178	-9.2522	38.4781	-34.2916	-53.8835	-53.2489	-24.3099	48.3375	-34.9052	-64.1266
dulS768_D770	-51.0018	-29.4648	41.0202	-36.7985	-76.245	-53.1133	-17.3574	35.9135	-34.6236	-69.1808
E709A_G719A	-48.2037	-12.671	43.3123	-34.6407	-52.203	-51.5416	-21.6045	43.8046	-34.89	-64.2316
E709K_L858R	-51.1386	-26.5117	39.5874	-35.8846	-73.9475	-53.4238	-16.8942	38.2251	-35.629	-67.722
G719A	-50.831	-12.1123	42.9616	-35.2798	-55.2615	-54.594	-21.4969	44.2138	-35.8647	-67.7419
G719A_L858R	-51.2702	-24.9909	38.0397	-36.5486	-74.77	-40.8519	-12.6117	30.7745	-27.5597	-50.2489
G719A_L861Q	-50.015	-13.0452	42.705	-34.5537	-54.9089	-52.1044	-17.057	42.0316	-34.637	-61.7669
G719C_S768I	-49.137	-13.7779	44.3125	-34.9308	-53.5332	-52.1466	-25.0559	48.8176	-35.1527	-63.5377
G724S	-50.0229	-29.1782	43.808	-34.7247	-70.1177	-52.2282	-25.4595	46.2447	-34.3403	-65.7834
G724S_L861Q	-48.5007	-28.2794	42.7513	-35.353	-69.3818	-51.5827	-18.7275	43.1828	-33.5062	-60.6336
K757R	-43.5618	-8.2131	37.2485	-30.2061	-44.7325	-53.4485	-22.6986	46.0288	-35.3252	-65.4435
L858R	-51.914	-26.6512	38.5811	-36.8522	-76.8363	-51.9583	-17.1889	37.3161	-35.0457	-66.8767
L858R_L861F	-50.64	-24.7729	39.3362	-34.5994	-70.676	-49.8005	-16.274	40.0645	-32.401	-58.411
L861Q	-52.9783	-14.3818	41.1706	-36.0401	-62.2296	-51.6732	-17.2987	35.5735	-33.1594	-66.5579
L861R	-49.7817	-15.9736	43.86	-34.0732	-55.9686	-48.8189	-17.7707	38.5243	-32.4751	-60.5404
R776H_L858R	-49.61	-27.9452	43.7866	-35.2183	-68.9869	-49.7391	-16.8023	39.8449	-32.6329	-59.3294
R831H	-51.0384	-30.234	45.0242	-35.3571	-71.6053	-54.2734	-15.6523	35.8019	-35.5799	-69.7037
S768I_V774M	-49.7211	-9.8949	37.34	-34.394	-56.67	-53.1199	-21.532	42.7696	-34.8986	-66.7809
T854A_L858R	-47.5049	-20.0659	37.8568	-33.7666	-63.4806	-47.7159	-14.8403	40.2891	-32.0103	-54.2773