

**S1 Table:** The list of different features used to build the empirical model for predicting novel resistance associated mutations in bedaquiline.

<b>Feature</b>	<b>Effect measured</b>	<b>Technique</b>	<b>p-value*</b>
mCSM_Stability	Protein stability	Graph based signatures	0.31
SDM	Protein stability	Graph based signatures	0.90
DUET	Protein stability	Graph based signatures	0.65
mCSM_PPI	Protein-protein interaction	Graph based signatures	0.68
DynaMut	Conformational flexibility	Normal mode analysis	0.60
$\Delta\Delta G$ ENCoM	Conformational flexibility	Normal mode analysis	0.66
$\Delta\Delta S$ ENCoM	Changes in Entropy	Normal mode analysis	0.66
mCSM_Lig	Ligand binding affinity	Graph based signatures	0.03
Distance from ligand binding site	Distance of the mutation from the drug (bedaquiline) binding site	Perl script (in-house)	$< 2.2e-16$
SNAP2	Effect of single nucleotide substitution	Neural Network	0.0002

\*Welch two sample t-test