Supplementary materials

Figure 1. Molecular docking analysis of the wild-type RhoA-GDP, mutant G17E-GDP and I86N-GDP complex with PLD1 protein. (A) Wild-type RhoA-GDP-PLD1 docking complex surface area (a) and superimpose structure (b) shows GDP in the pocket and H-bonds of interacting residues, respectively. (B) Mutant G17E-GDP-PLD1 docking complex surface area (a) and superimpose structure (b) shows GDP in the pocket and H-bonds of interacting residues, respectively. (C) Mutant I86N-GDP-PLD1 docking complex surface area (a) and superimpose structure (b) shows GDP in the pocket and H-bonds of interacting residues, respectively. (C) Mutant I86N-GDP-PLD1 docking complex surface area (a) and superimpose structure (b) shows GDP in the pocket and H-bonds of interacting residues, respectively. (C) Mutant I86N-GDP-PLD1 docking complex surface area (a) and superimpose structure (b) shows GDP in the pocket and H-bonds of interacting residues, respectively.



SNP ID	AA Substitution	I-Mutant	RI (Reliability Index)	DDG-Free energy change value (kcal/mol)
rs1057519951	E40K	Decrease	8	-0.81
rs1057519954	Y42S	Decrease	6	-1.35
rs1553631976	Y66H	Decrease	7	-1.38
rs1575647051	A61T	Decrease	8	-0.70
rs11552761	G17E	Decrease	1	-0.62
rs112304179	F171L	Decrease	3	-0.94
rs1381401434	I86N	Decrease	6	-2.19
rs1465894043	I151T	Decrease	9	-2.05
rs1575653732	V9G	Decrease	10	-2.06

 Table 1. Effect of nsSNPs on protein stability predicted by I-MUTANT 3.0