

Trametinib modulates cancer multidrug resistance by targeting ABCB1 transporter

Supplementary Material

Supplementary Table 1: Summary of the potential residues in transmembrane (TM) domains of ABCB1 interacting with Trametinib in comparison with QZ59-RRR, QZ59-SSS and verapamil.

TM	Residue	QZ59-RRR	QZ59-SSS	Verapamil	Trametinib
1	His 60			x	
	Ala 63			x	
	Leu 64	x	x	x	
	Met 67		x		
	Met 68	x	x		x
	Phe 71	x	x		
2	Tyr114		x		
	Val121			x	
4	Ser218			x	
5	Met295		x		
	Phe299		x		x
	Ile302		x	x	x
	Tyr303		x		x
	Tyr306	x	x		x
6	Phe331				x
	Phe 332	x	x		x
	Leu 335		x	x	x
	Ile 336	x	x		x
	Ala 338			x	
	Phe 339	x	x		
7	Asn 717		x		x
	Gly718				x
	Gln 721	x	x		x
	Phe 724	x	x	x	x
	Ala725			x	x
	Phe 728	x	x		x
8	Phe 766		x		
9	Gln834				x
	Ala837			x	
	Asn838			x	x
10	Ile 864			x	
	Ala 867			x	
	Gly 868			x	
11	Phe938			x	
	Thr941			x	
	Met945		x		
	Tyr949	x	x		x
	Phe953		x		
12	Leu 971		x	x	
	Phe 974	x	x		
	Ser 975	x			x
	Val 978			x	

Phe979	x	x		x
Gly 980			x	
Ala 981			x	
Met 982	x	x		x
Ala983	x	x		x
Gln 986	x	x		x
Val987		x		x