

Table S3

ALDH1B1*2	DOPE score	-58565.9
(A86V)	Z score	-13.5002
	Minimization Energy	-393390
ALDH1B1*3	DOPE score	-58137.2
(L107R)	Z score	-13.5356
	Minimization Energy	-395944
ALDH1B1*5	DOPE score	-58403.7
(M253V)	Z score	-13.6703
	Minimization Energy	-406335
ALDH1B1*1	DOPE score	-58968.1
(WT)	Z score	-13.5177
	Minimization Energy	-395741