

Table S3 The time frames of each trajectory for binding free energy calculation

Wildtype ABL1		T315I ABL1	
Drug name	Time frame (ns)	Drug name	Time frame (ns)
Bethanechol	3~5	Bethanechol	10~12
Methacholine	10~12	Methacholine	12~14
Sorafenib	12~14	Plerixafor	10~12
Nilotinib	12~14	Ticlopidine	7~9
Chlorhexidine	8~10	Nicergoline	13~15
Imatinib	8~10	Ponatinib	12~14