Supplementary informations of in silico study on identification of novel MALT1 allosteric inhibitors

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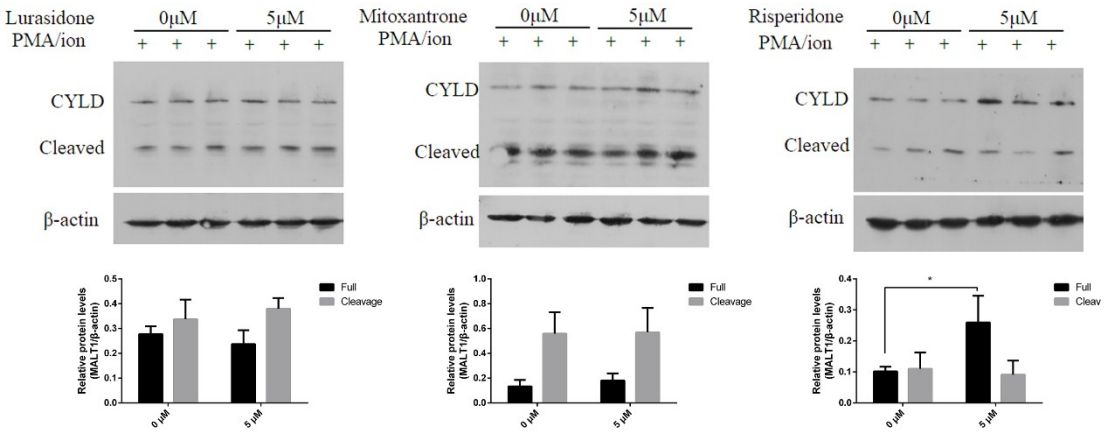
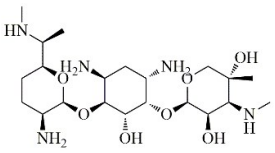
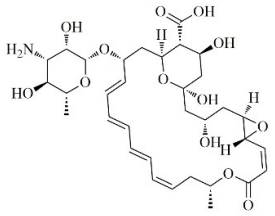
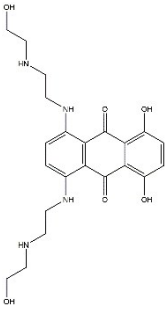
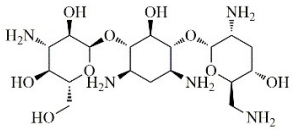
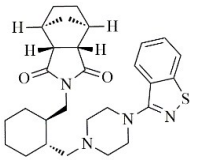
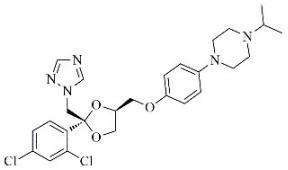
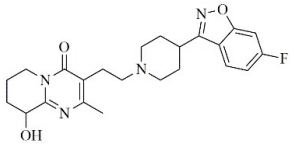
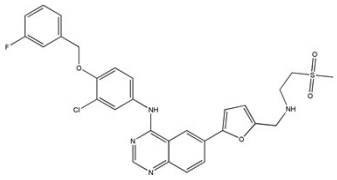
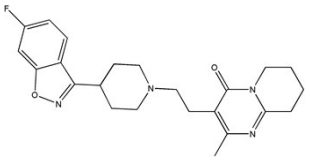
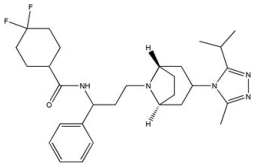


Figure S1 Compounds have no effect on the cleavage of MALT1 substrate CYLD. Jurkat cells were treated with lurasidone, mitoxantrone and risperidone for 12 h and then stimulated with PMA/ionomycin for 120 min. Histogram showed the quantification of immunoblot that normalized with β-actin. Per test group has three independent experiments. Data was shown as mean ± SD, *P< 0.05.

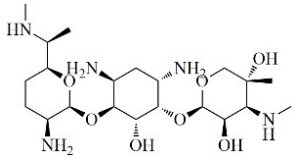
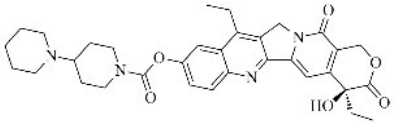
Table S1 Properties of the top 10 compounds that bind to the allosteric site after virtual screening

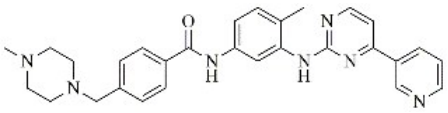
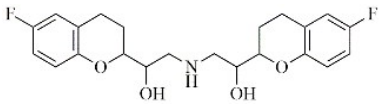
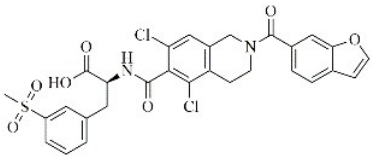
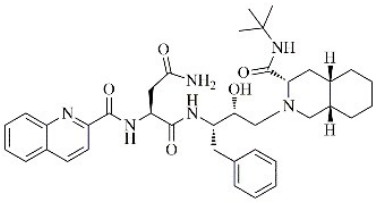
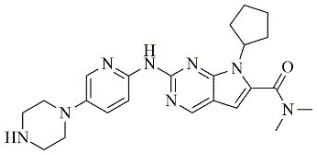
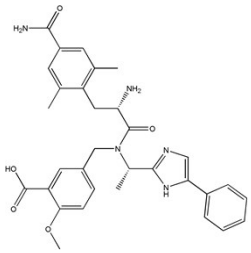
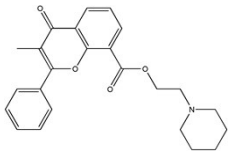
ZNIC ID	Chemical Name	Chemical structure	poses	Energy* (kcal/mol)
ZINC000242437513	Gentamicin		5	-18.55
ZINC000169621220	Natamycin		1	-16.05
ZINC000003794794	Mitoxantrone		6	-14.35

ZINC000008214692	Tobramycin		9	-14.21
ZINC000003927822	Lurasidone		6	-13.56
ZINC000003873936	Zazole		4	-13.47
ZINC000001481956	Paliperidone		3	-13.16
ZINC000001550477	Lapatinib		8	-13.12
ZINC000000538312	Risperdal		2	-13.07
ZINC000100003902	Maraviroc		6	-13.03

*Estimated free energy of binding of virtual screening results by AutoDock program.

Table S2 Properties of the top 10 compounds that bind to the catalytically active site after virtual screening

ZNIC ID	Chemical Name	Chemical structure	poses	Energy* (kcal/mol)
ZINC000242437513	Gentamicin		7	-13.6
ZINC000001612996	Irinotecan		5	-13.5

ZINC000019632618	Imatinib		4	-12.39
ZINC000001999441	Nebivolol		6	-12.24
ZINC000084668739	Lifitegrast		2	-11.7
ZINC000026664090	Saquinavir		10	-11.63
ZINC000072316335	Ribociclib		4	-11.63
ZINC000169621220	Natamycin		4	-11.56
ZINC000014210876	Eluxadoline		10	-11.51
ZINC000000608382	Flavoxate		5	-11.49

*Estimated free energy of binding of virtual screening results by AutoDock program.