Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Identification of novel Src, Bcl-2 dual inhibitors by Pharmacophore Model, Molecular Docking, and Molecular Dynamics Simulations

Li-chuan Zhang[1], Hao-ran Zhang[1], Cheng-long Gao[1], Ri-lei Yu[2], Cong-min Kang[1]

[1.]College of Chemical Engineering, Qingdao University of Science and Technology, Qingdao, 266042 China

[2.]Key Laboratory of Marine Drugs, Chinese Ministry of Education, School of Medicine and Pharmacy, Ocean University of China, Qingdao, 266003 China

Table S1. Information about small molecules in the Src active validation set

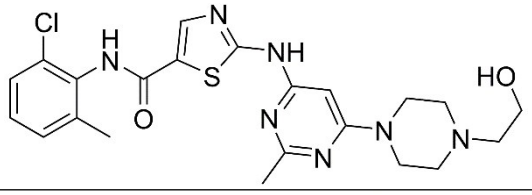
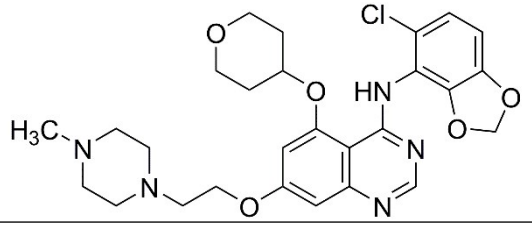
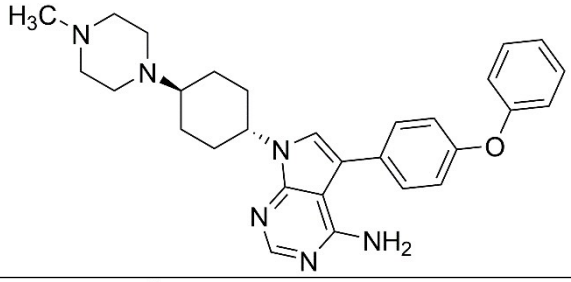
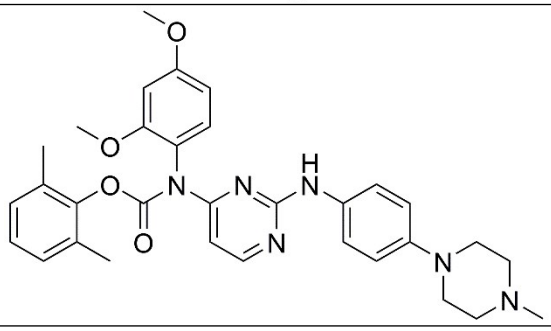
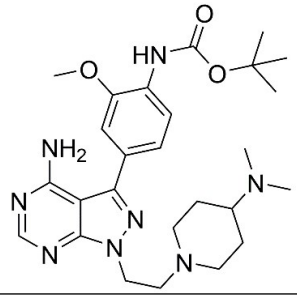
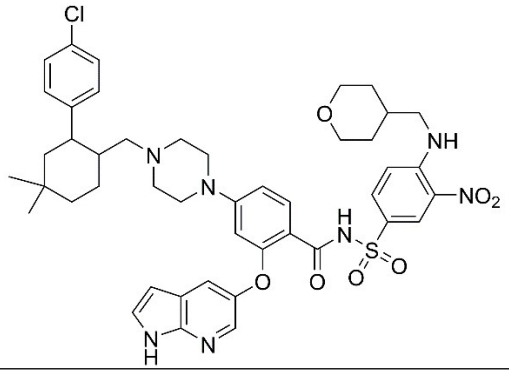
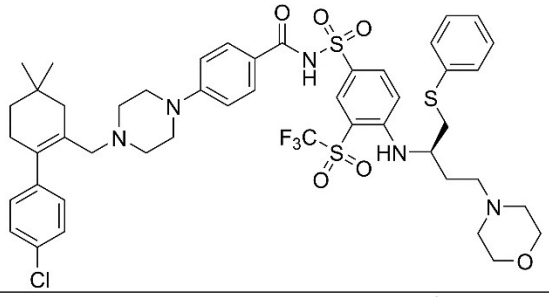
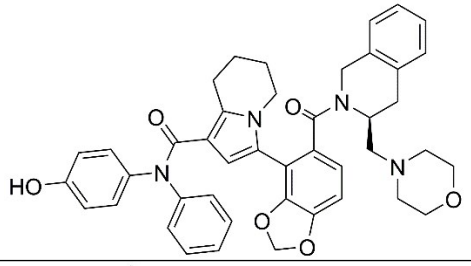
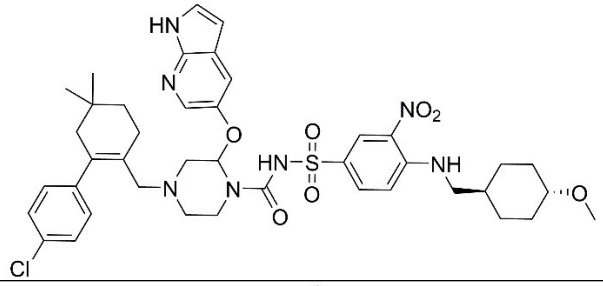
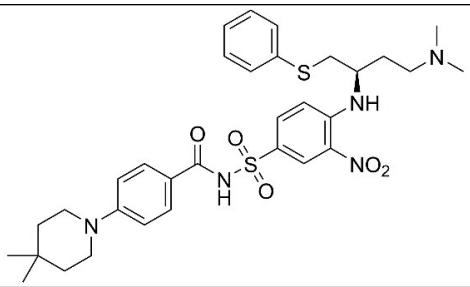
No.	Structure	Active
Dasatinib CAS 302962-49-8		Ki = 16pM
Saracatinib CAS 379231-04-6		IC50 = 2.7nM
A 419259 CAS 364042-47-7		IC50 = 9nM
WH-4-023 CAS 837422-57-8		IC50 = 6nM
eCF506 CAS 1914078-41-3		IC50 < 0.5nM

Table S2. Information about small molecules in the Bcl-2 active validation set

No.	Structure	Active
Venetoclax CAS 1257044-40-8		Ki = 0.01 nM
Navitoclax CAS 923564-51-6		Ki = 1 nM
S55746 CAS 1448584-12-0		Ki = 1.3 nM
BCL2-IN-1 CAS 1257044-75-9		Ki = 0.01 nM
A-385358 CAS 406228-55-5		Ki = 67 nM。

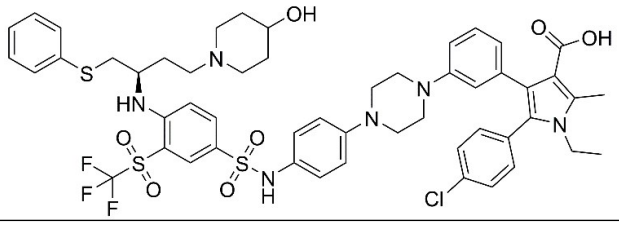
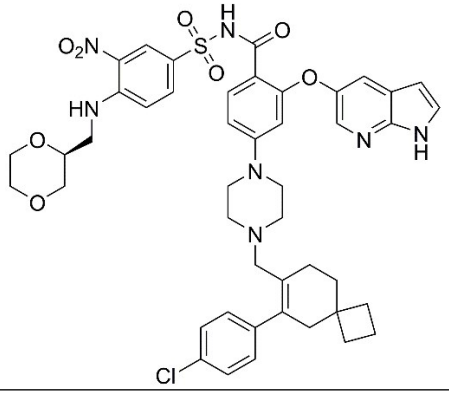
BM 957 CAS 1391107-54-2		IC50 = 5.4nM
Bcl-2/Bcl-xl inhibitor 1 CAS 2180923-05-9		IC50 = 2 nM

Table S3. The hydrogen bonding analysis of the last 10ns of MD simulation(T=300K)

Complex	Donor	Acceptor	Distance/Å	Angle/°	Occupancy/%
Compound1-Src	Compound1 (N41-H42)	GLU339(O)	2.883	14.29	90.54%
	Compound1 (N41-H42)	MET341(O)	3.152	14.95	0.03%
QTZ101-Src	QTZ101 (N41-H42)	GLU339(O)	3.023	13.45	0.01%
	QTZ101 (N41-H42)	MET341(O)	2.879	14.17	59.20%

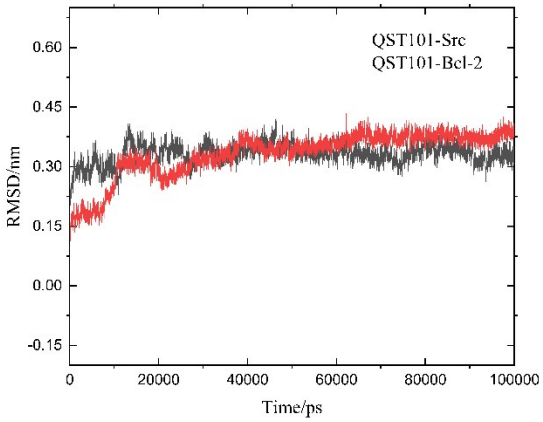


Figure S1. Root mean square deviation of protein backbone atoms (T = 310K).