

Supplementary Materials

Identification of Novel Src Inhibitors: Pharmacophore Based Virtual Screening, Molecular Docking and Molecular Dynamics Simulations

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ADME		Toxicity	
ID	Value	ID	Value
BBB	0.0103644**	algae_at	0.00280111**
Buffer_solubility_mg_L	81.6862**	Ames_test	mutagen
Caco2	18.8714	Carcino_Mouse	negative
CYP_2C19_inhibition	Non	Carcino_Rat	negative
CYP_2C9_inhibition	Non	daphnia_at	0.00222569**
CYP_2D6_inhibition	Non	hERG_inhibition	low_risk
CYP_2D6_substrate	Non	medaka_at	1.91433e-005**
CYP_3A4_inhibition	Inhibitor	minnow_at	4.47499e-005**
CYP_3A4_substrate	Substrate	TA100_10RLI	negative
HIA	97.409918	TA100_NA	negative
MDCK	0.0440467**	TA1535_10RLI	negative
Pgp_inhibition	Inhibitor	TA1535_NA	negative
Plasma_Protein_Binding	100.000000**		
Pure_water_solubility_mg_L	0.000456487**		
Skin_Permeability	-1.95856**		
SKlogD_value	5.861190**		
SKlogP_value	5.861190**		
SKlogS_buffer	-3.796760**		
SKlogS_pure	-9.049480**		

Figure S1. The ADMET prediction for ZINC3214460

ADME

ID	Value
BBB	0.449141
Buffer_solubility_mg_L	3735.39**
Caco2	26.6213
CYP_2C19_inhibition	Non
CYP_2C9_inhibition	Non
CYP_2D6_inhibition	Non
CYP_2D6_substrate	Substrate
CYP_3A4_inhibition	Non
CYP_3A4_substrate	Substrate
HIA	92.105528
MDCK	2.5236
Pgp_inhibition	Non
Plasma_Protein_Binding	34.897436
Pure_water_solubility_mg_L	432.56
Skin_Permeability	-4.56456
SKlogD_value	1.283610
SKlogP_value	1.283610
SKlogS_buffer	-2.026970**
SKlogS_pure	-2.963260

Toxicity

ID	Value
algae_at	0.0608198
Ames_test	mutagen
Carcino_Mouse	negative
Carcino_Rat	negative
daphnia_at	0.15396
hERG_inhibition	high_risk
medaka_at	0.0490291
minnow_at	0.250973
TA100_10RLI	negative
TA100_NA	positive
TA1535_10RLI	negative
TA1535_NA	negative

Figure S2. The ADMET prediction for ZINC1380384