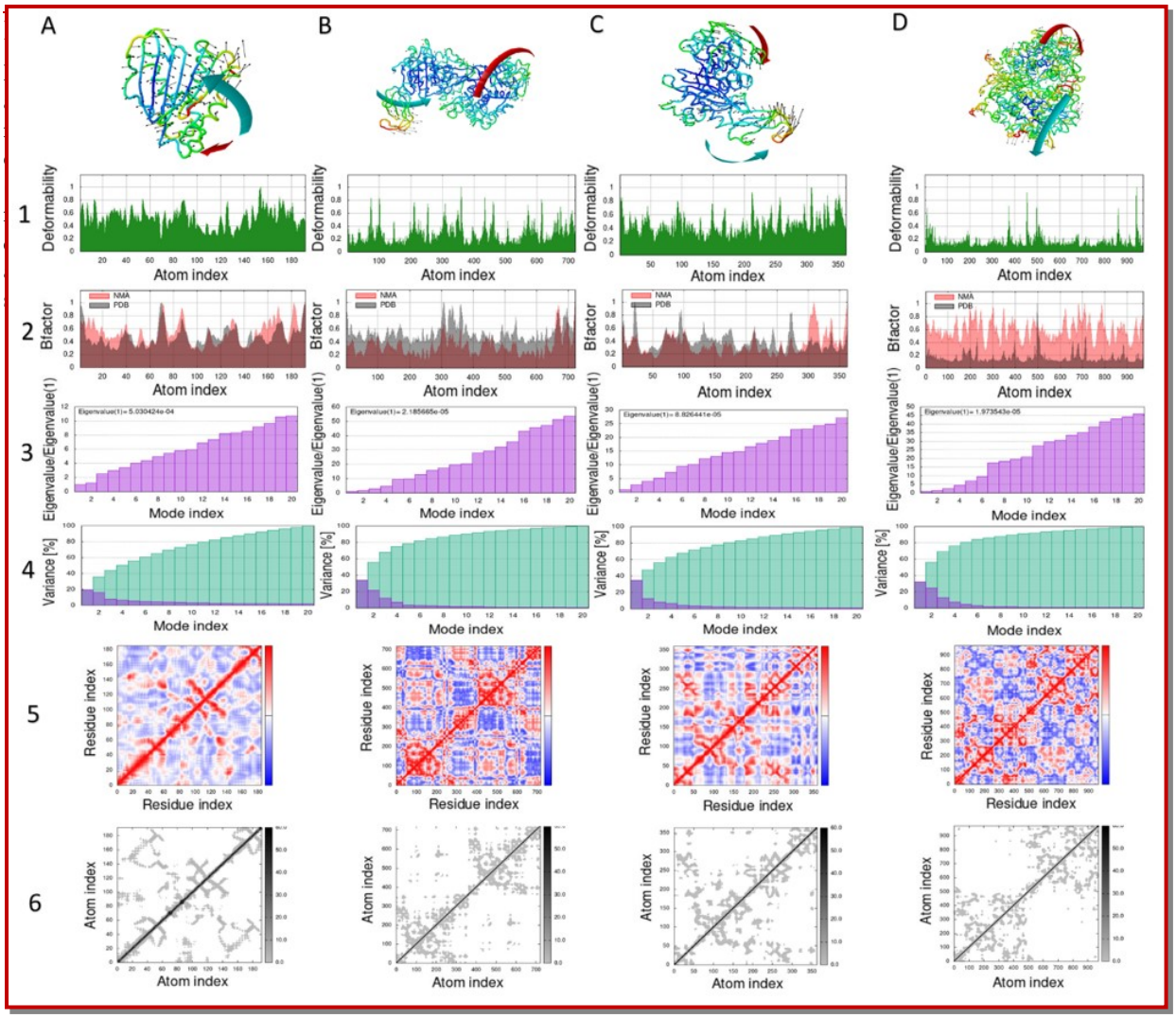
Supplementary Table I

Properties of a novel pyrazoline carboxamide from the SwissADME database

Physicochemical properties		Pharmacokinetics	
Formula	$C_{18}H_{20}N_4O$	GI absorption	High
Molecular weight	308.38 g/mol	BBB permeant	Yes
Number of heavy atoms	23	P-gp substrate	No
Number of heavy atoms	12	CYP1A2 inhibitor	No
Fraction Csp3	0.22	CYP2C19 inhibitor	Yes
Number of rotatable bonds	4	CYP2C9 inhibitor	Yes
Number of H-bond acceptors	2	CYP2D6 inhibitor	No
Number of H-bond donors	1	CYP3A4 inhibitor	No
Molar refractivity	99.53	Log K_p (skin permeation)	-6.58 cm/s
TPSA	61.93 Å²	Druglikeness	
Lipophilicity	Lipophilicity	Lipinski	Yes; 0 violation
Log $P_{o/w}$ (iLOGP)	2.69	Ghose	Yes
Log $P_{o/w}$ (XLOGP3)	2.25	Veber	Yes
Log $P_{o/w}$ (WLOGP)	1.90	Egan	Yes
Log $P_{o/w}$ (MLOGP)	2.59	Muegge	Yes
Log $P_{o/w}$ (SILICOS-IT)	1.94	Bioavailability score	0.55
Consensus Log $P_{o/w}$	2.27	Medicinal chemistry	
Water solubility		PAINS	2 alerts: anil_di_alk_D, anil_di_alk_E
Log *S* (ESOL)	-3.29	Brenk	0 alert
Solubility	1.58e-01 mg/mL; 5.11e-04 mol/L	Leadlikeness	Yes
Class	Soluble	Synthetic accessibility	3.46
Log *S* (Ali)	-3.19		
Solubility	2.01e-01 mg/mL; 6.51e-04 mol/L		
Class	Soluble		
Log *S* (SILICOS-IT)	-4.57		
Solubility	8.32e-03 mg/mL; 2.70e-05 mol/L		
Class	Moderately soluble		



Supplementary Figure 1: Molecular dynamic simulations of the enzyme-ligand complex. 1KZN-Pyr complex (A), 3HUN-Pyr complex (B), 7KCY-Pyr complex (C), and 5TZ1-Pyr complex (D), showing the 3D structure of the interaction, deformability plots, and B factor plots. Eigenvalue, and variance map. Correlation matrix, and elastic network model