Supplementary Table S1

In silico evaluation by SwissADME (http://www.swissadme.ch/)

Molecule 1

SMILES CSCCCCN=C=S

Physicochemical Properties

Property	Value
Formula	C6H11NS2
Molecular weight	161.29 g/mol
Num. heavy atoms	9
Num. arom. heavy atoms	0
Fraction Csp3	0.83
Num. rotatable bonds	5
Num. H-bond acceptors	1
Num. H-bond donors	0
Molar Refractivity	47.71
TPSA	69.75 Å²

Lipophilicity

Property	Value
Log $P_{o/w}$ (iLOGP)	2.55
Log $P_{o/w}$ (XLOGP3)	2.96
Log $P_{o/w}$ (WLOGP)	2.23
Log $P_{o/w}$ (MLOGP)	2.86
Log $P_{o/w}$ (SILICOS-IT)	3.38
Consensus Log $P_{o/w}$	2.80

Water Solubility

Property	Value
Log S (ESOL)	-2.37
Solubility	6.80e-01 mg/ml ; 4.22e-03 mol/l
Class	Soluble
Log S (Ali)	-4.09
Solubility	1.32e-02 mg/ml ; 8.17e-05 mol/l
Class	Moderately soluble
Log S (SILICOS-IT)	-2.18
Solubility	1.06e+00 mg/ml ; 6.56e-03 mol/l
Class	Soluble

Pharmacokinetics

Property	Value
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.18 cm/s

Druglikeness

Property	Value
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: MW<200
Bioavailability Score	0.55

Medicinal Chemistry

Property	Value
PAINS	0 alert
Brenk	2 alerts: imine_1, thiocarbonyl_group
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	2.47