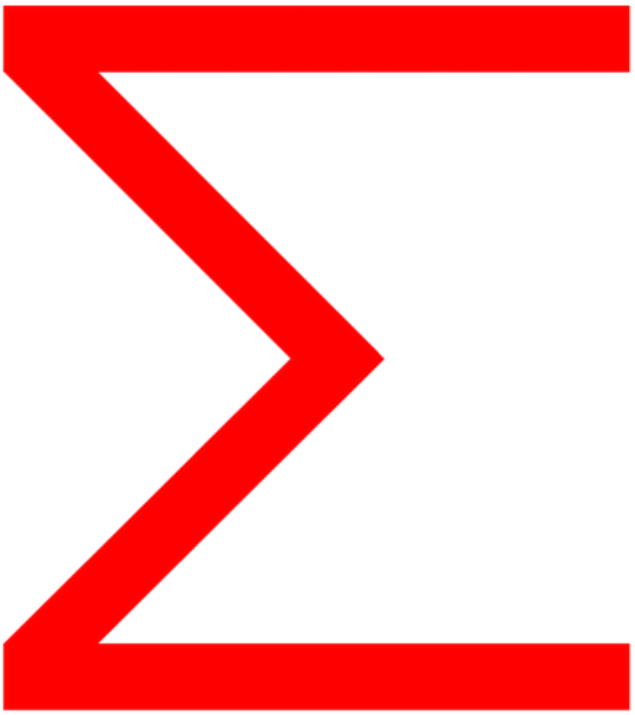
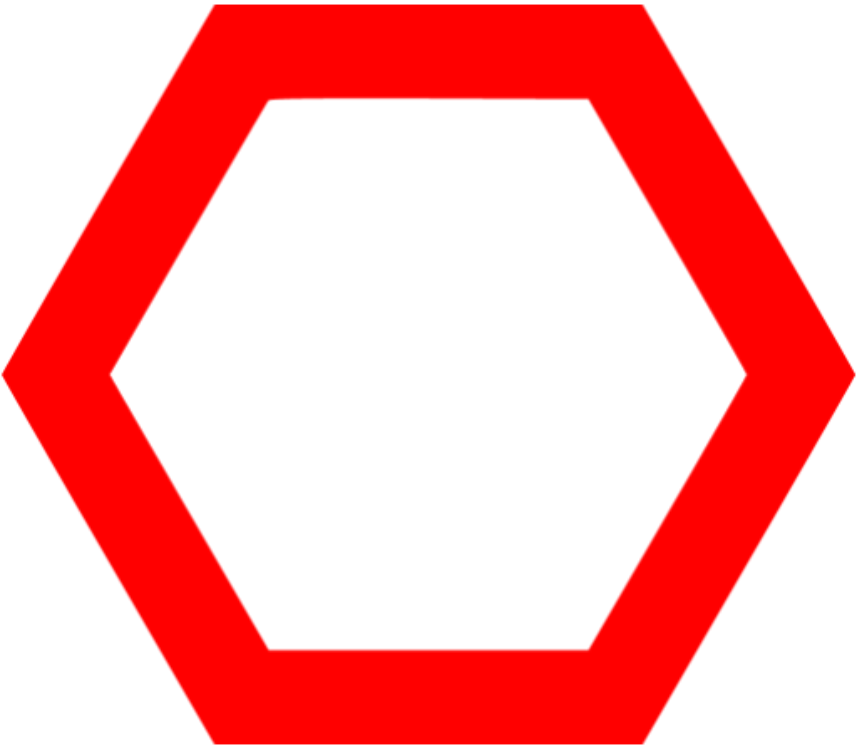
SwissDock

SwissParam



SwissSidechain

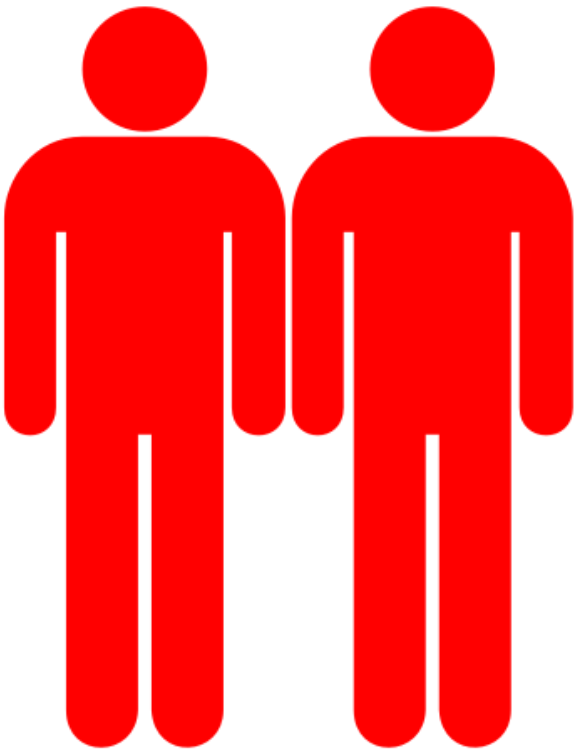
SwissBioisostere



SwissTargetPrediction

SwissADME

SwissSimilarity



Swiss Institute of Bioinformatics

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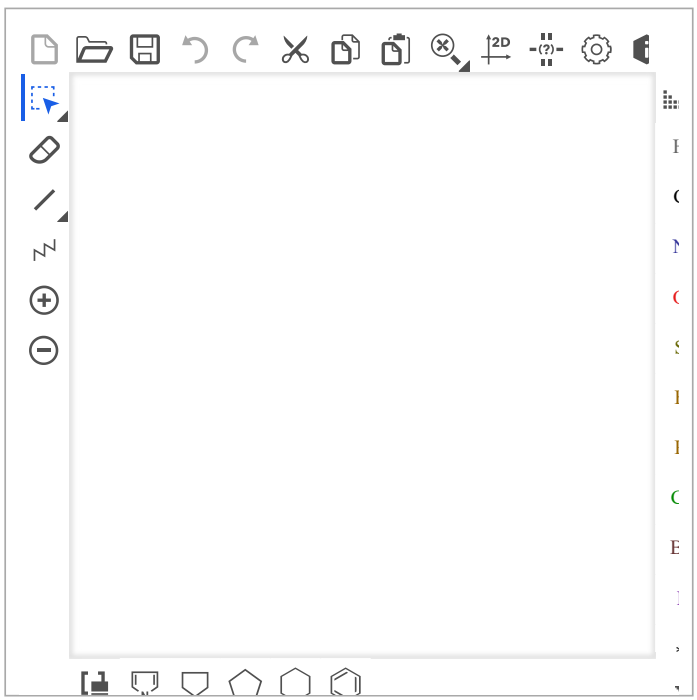
For information: We have changed the look and feel of our tool. However, we have **NOT** changed the underlying technologies and parameters. Consequently, this updated Web tool provides exactly the same results as the previous version.



Enter a list of SMILES here:

CN1C=NC2=C1C(=O)N(C(=O)N2C)C Caffeine

Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Powered by Chemaxon

Caffeine

SMILES Cn1cnc2c1c(=O)n(C)c(=O)n2C

Physicochemical Properties

Formula	C8H10N4O2
Molecular weight	194.19 g/mol
Num. heavy atoms	14
Num. arom. heavy atoms	9
Fraction Csp3	0.38
Num. rotatable bonds	0
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	52.04
TPSA	
Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	61.82 Å²

Lipophilicity

Log $P_{o/w}$ (iLOGP)

iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	1.79

Log $P_{o/w}$ (XLOGP3)

XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	-0.07

Log $P_{o/w}$ (WLOGP)

WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	-1.03

Log $P_{o/w}$ (MLOGP)

MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	0.22

Log $P_{o/w}$ (SILICOS-IT)

SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, https://www.silicos-it.be	-0.50

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-1.48
Solubility	6.50e+00 mg/ml ; 3.35e-02 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Very soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-0.78
Solubility	3.25e+01 mg/ml ; 1.67e-01 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Very soluble

Log *S* (SILICOS-IT)

SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, https://www.silicos-it.be	-0.67
Solubility	4.15e+01 mg/ml ; 2.14e-01 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble

Pharmacokinetics

GI absorption

Gatrointestinal absorption: according to the white of the BOILED-Egg	High

BBB permeant

BBB permeation: according to the yolk of the BOILED-Egg	No

P-gp substrate

P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No

CYP1A2 inhibitor

Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	No

Consensus Log $P_{o/w}$

Consensus Log $P_{o/w}$: 0.08
Average of all five predictions

CYP2C19 inhibitor

Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	No

CYP2C9 inhibitor

Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	No

CYP2D6 inhibitor

Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No

CYP3A4 inhibitor

Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	No

Log K_p (skin permeation)

Skin permeation: QSPR model implemented from Potts RO and Guy RH. 1992 Pharm. Res.	-7.53 cm/s

Druglikeness

Lipinski

Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation

Ghose

Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	No; 1 violation: WLOGP<-0.4

Veber

Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes

Egan Yes

Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med.	

Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	No; 1 violation: MW<200
Bioavailability Score	
Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.55
Medicinal Chemistry	
PAINS	
Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	0 alert
Brenk	
Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert
Leadlikeness	
Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 1 violation: MW<250
Synthetic accessibility	
Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penalties, trained on 12'782'590 molecules and tested on 40 external molecules (r^2 = 0.94)	2.03