

NASKAH TUTORIAL

PREDIKSI PROFIL FARMAKOKINETIK SENYAWA DAN PENERAPAN ATURAN LIPINSKI MENGUNAKAN PKCSM

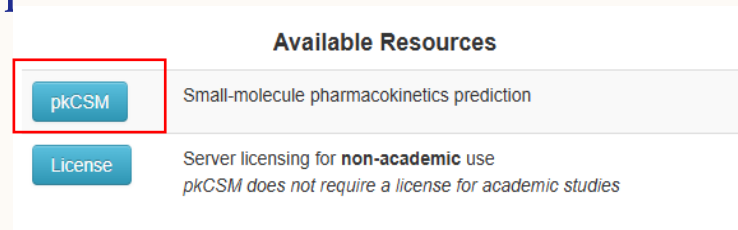
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FAKULTAS FARMASI DAN SAINS
PROGRAM STUDI FARMASI
UNIVERSITAS MUHAMMADIYAH PROF. DR. HAMKA
JAKARTA
JUNI 2023

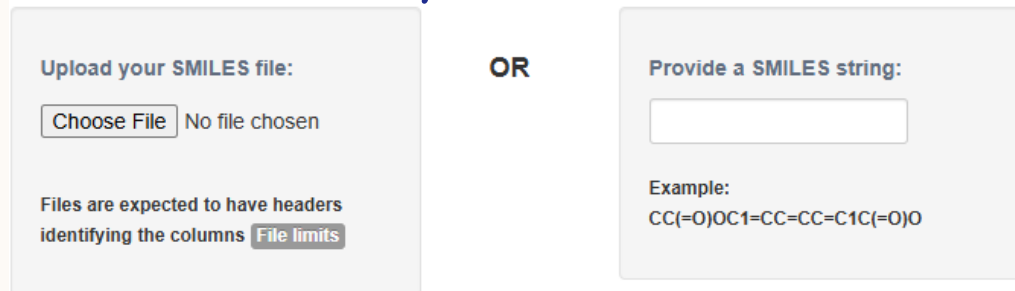
WEBSITE PKCSM

<https://biosig.lab.uq.edu.au/pkcsm/>

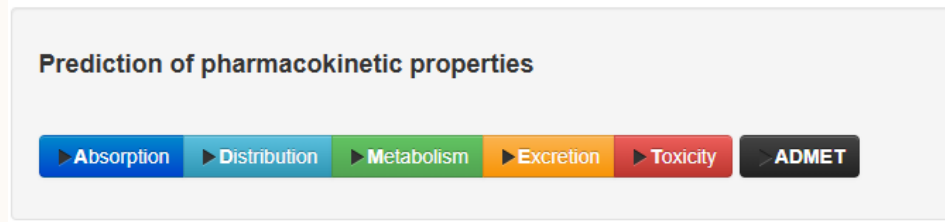
1. Buka website pkCSM
2. Pilih pkCSM



3. Masukkan file senyawa .smi atau canonical SMILES



4. Pilih satu per satu parameter farmakokinetik atau pilih langsung ADMET



Note: File senyawa dalam format .pdb dan .mol dapat diketahui Canonical Smiles-nya melalui website Online SMILES Translator and Structure File Generator (<https://cactus.nci.nih.gov/translate/>)

HASIL PENERAPAN ATURAN LIPINSKI

Molecule properties:

Descriptor	Value
Molecular Weight	180.159
LogP	1.3101
#Rotatable Bonds	2
#Acceptors	3
#Donors	1
Surface Area	74.757

HASIL PREDIKSI ADME

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Property	Model Name	Predicted Value	Unit
Absorption	Water solubility	-1.868	Numeric (log mol/L)
Absorption	Caco2 permeability	0.09	Numeric (log Papp in 10 ⁻⁶ cm/s)
Absorption	Intestinal absorption (human)	76.938	Numeric (% Absorbed)
Absorption	Skin Permeability	-2.715	Numeric (log Kp)
Absorption	P-glycoprotein substrate	No	Categorical (Yes/No)
Absorption	P-glycoprotein I inhibitor	No	Categorical (Yes/No)
Absorption	P-glycoprotein II inhibitor	No	Categorical (Yes/No)
Distribution	VDss (human)	-1.716	Numeric (log L/kg)
Distribution	Fraction unbound (human)	0.481	Numeric (Fu)
Distribution	BBB permeability	-0.332	Numeric (log BB)
Distribution	CNS permeability	-2.489	Numeric (log PS)
Metabolism	CYP2D6 substrate	No	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	No	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2C19 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2C9 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2D6 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP3A4 inhibitor	No	Categorical (Yes/No)
Excretion	Total Clearance	0.72	Numeric (log ml/min/kg)
Excretion	Renal OCT2 substrate	No	Categorical (Yes/No)

SYARAT PARAMETER ADME DAN PENERAPAN ATURAN LIPINSKI (PKCSM)

Parameter	Persyaratan	Parameter	Persyaratan
Absorption		Metabolism	
Water solubility	-	CYP2D6 substrate	-
Caco2 permeability	> 0,9	CYP3A4 substrate	-
Intestinal absorption (human)	> 30%	CYP1A2 inhibitor	-
Skin Permeability	≥ -2,5	CYP2C19 inhibitor	-
P-glycoprotein substrate	-	CYP2C9 inhibitor	-
P-glycoprotein I inhibitor	-	CYP2D6 inhibitor	-
P-glycoprotein II inhibitor	-	CYP3A4 inhibitor	-
Distribution		Excretion	
VDss (human)	≥ -0,15	Total Clearance (E1)	Higher is better
Fraction unbound (human)	-	Renal OCT2 substrate	-
BBB permeability	≥ -1	Lipinski's rule of five	
CNS permeability	≥ -3	Mr	≤ 500 Da
		log P	≤ 5
		hydrogen bond acceptors	≤ 10
		hydrogen bond donors	≤ 5

**THANK
YOU**