



Pubchem_12124

Structure information

SMILES

CC(=O)NC1=CC(=CC=C1)O

Formula

C₈H₉NO₂

Molecular weight: 151.16 Da

LogP: 1.35

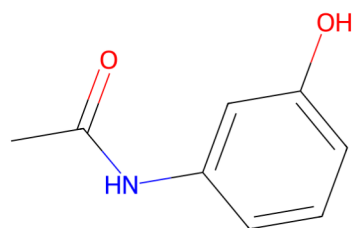
Num H-bond donors: 2

Num H-bond acceptors: 2

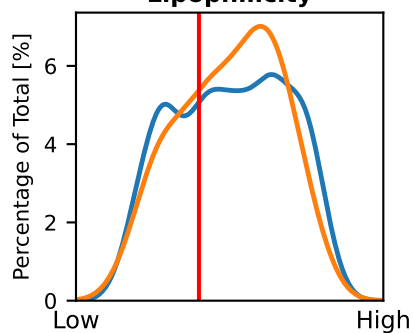
TPSA: 49.33 Å²

QED: 0.64

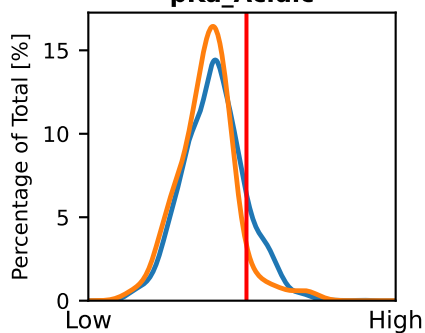
Num rotatable bonds: 1



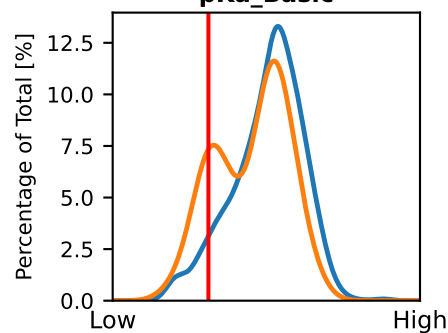
Lipophilicity



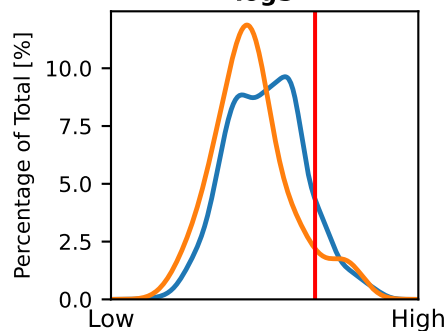
pKa_Acidic



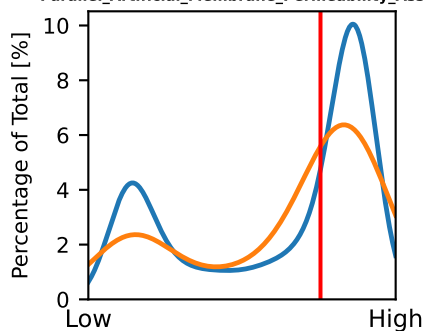
pKa_Basic



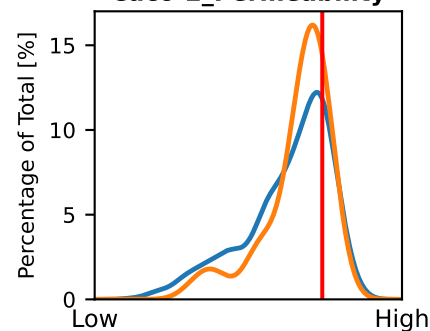
logS



Parallel_Artificial_Membrane_Permeability_Assay



Caco-2_Permability

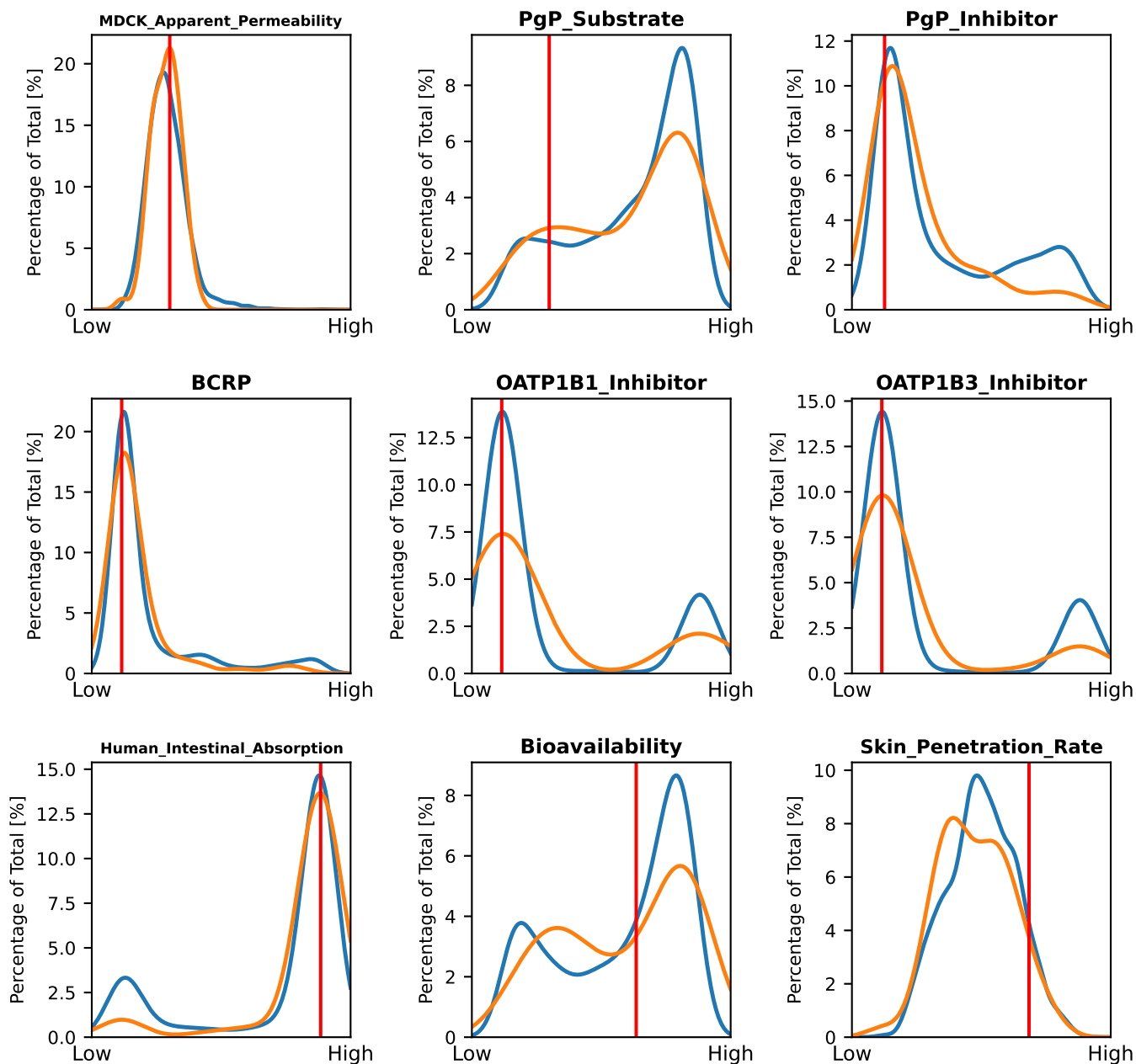


CONFIDENTIAL

— FDA approved small molecules — Drugs with similar indication — Your molecule



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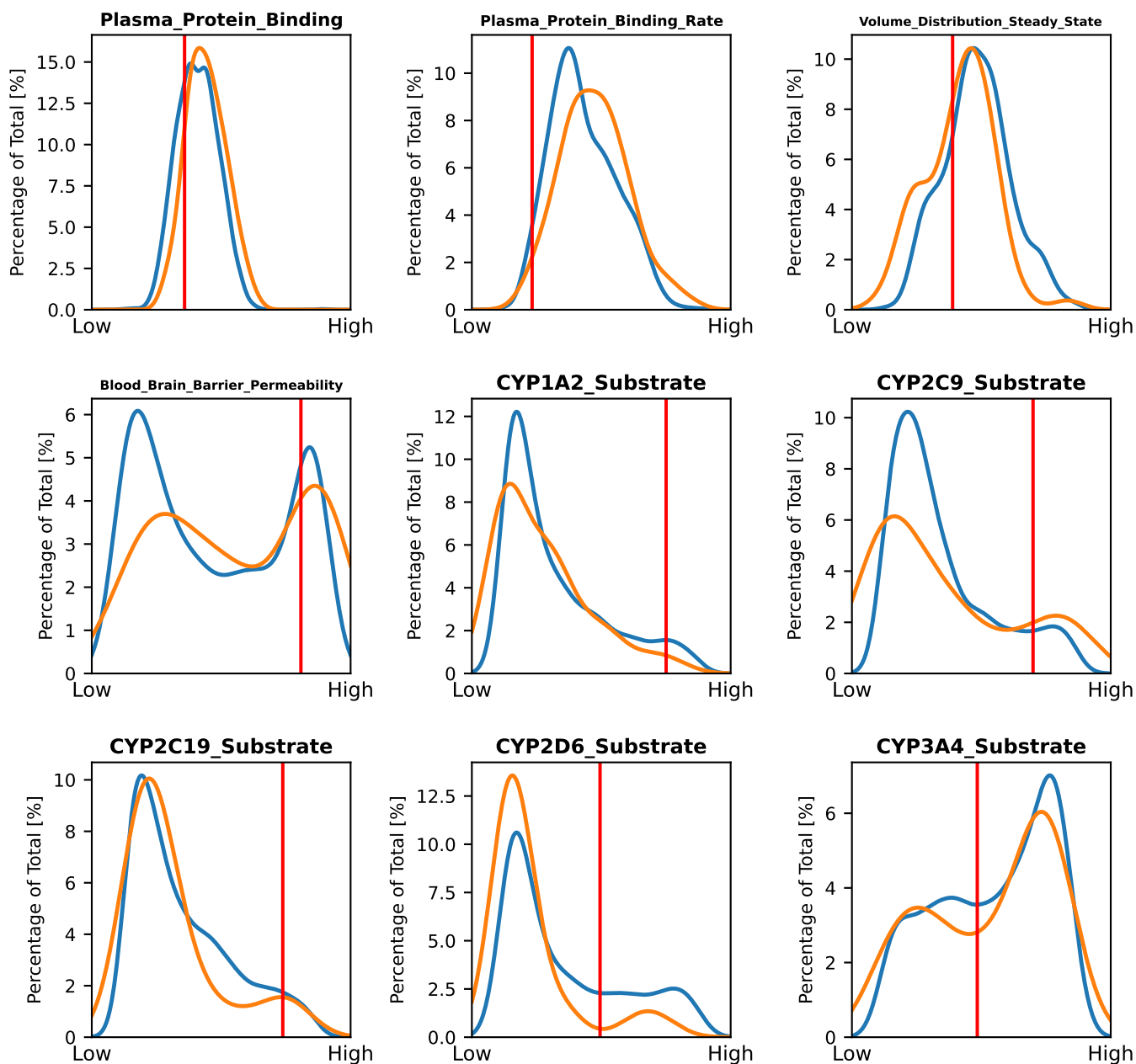


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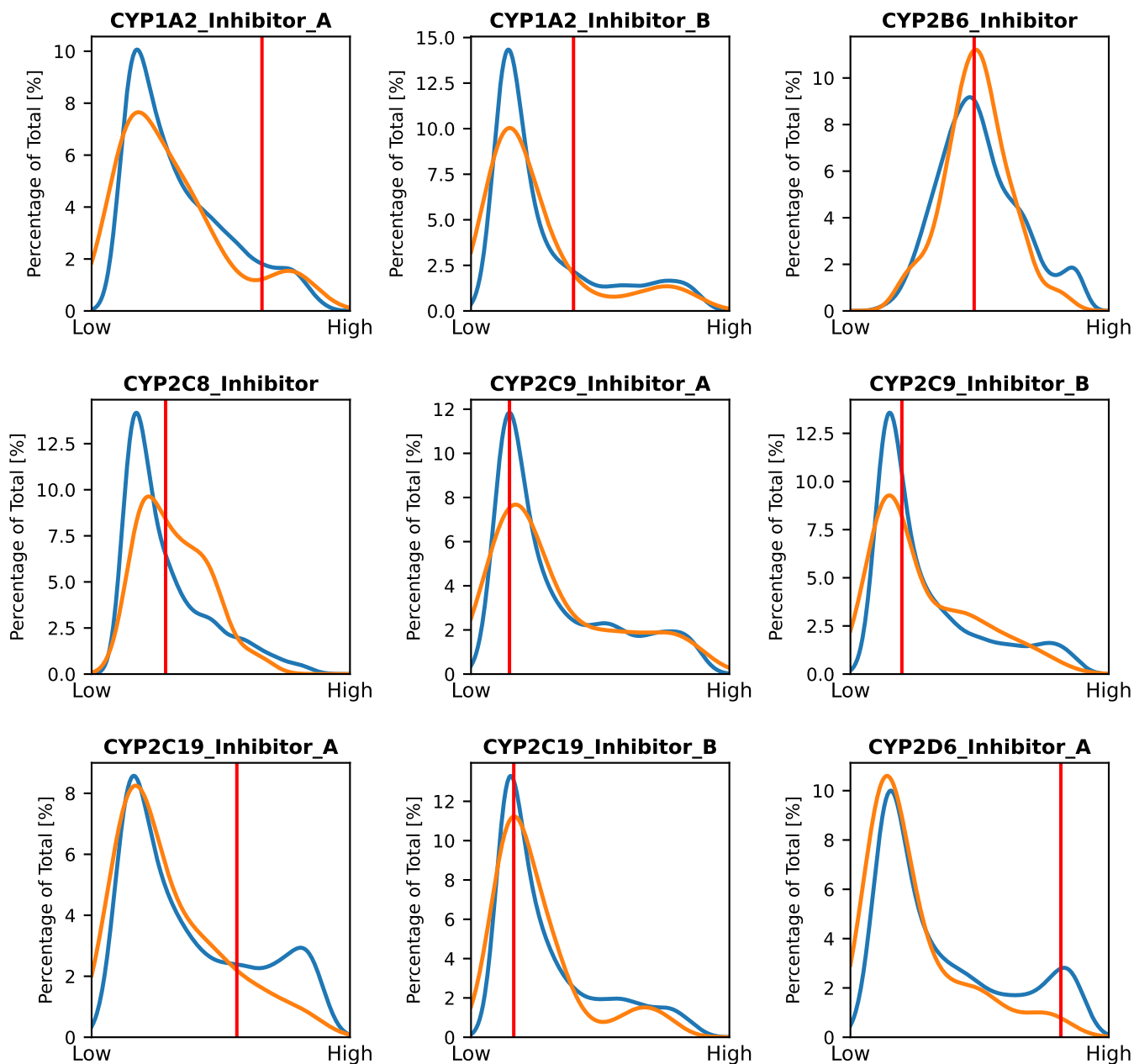


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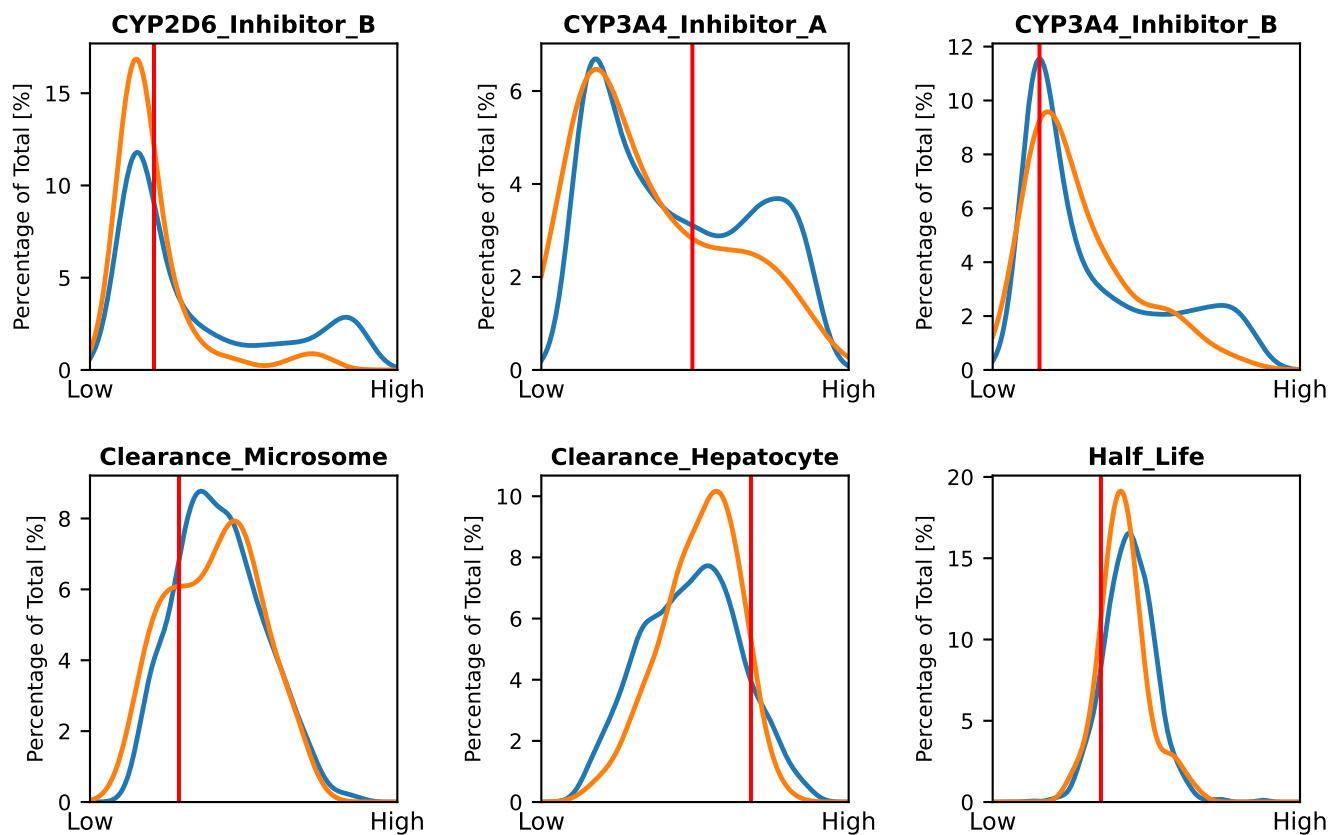


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