

(A) Physicochemical Properties

Simvastatin

CCC(C)(C)C(=O)OC1CC(O)C=C2C=CC(C)C...

MW:

418.6 Da

LogP:

4.68

TPSA:

72.8 A^2

HBD / HBA:

1 / 5

Rot. bonds:

7

Lipinski:

1 violation (LogP)

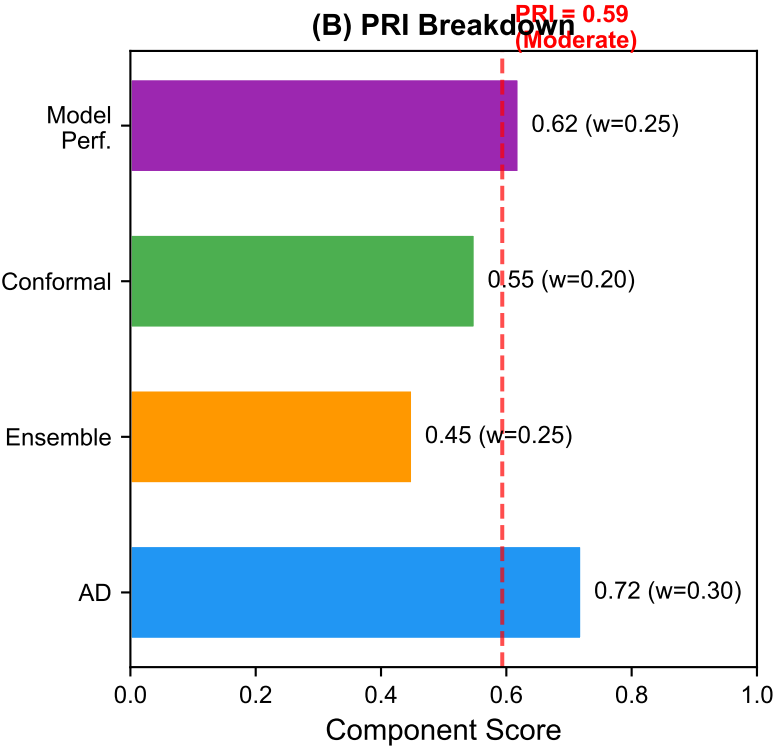
QED:

0.52

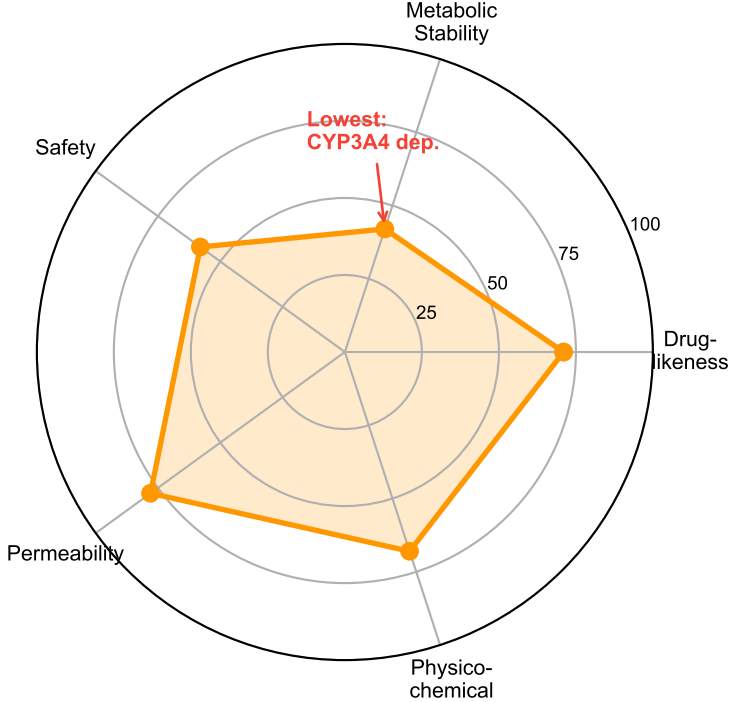
Fsp3:

0.69

(B) PRI Breakdown



(C) CDS = 62/100 (Good)



(D) DDI Assessment

DDI Risk Score

72/100 (High)

Classification

CYP3A4 Victim Drug

Major pathway

CYP3A4 (single)

Contraindicated with:

Ketoconazole (strong CYP3A4 inh.)  
Itraconazole (strong CYP3A4 inh.)

Dose adjust with:

Diltiazem (moderate CYP3A4 inh.)  
Verapamil (moderate CYP3A4 inh.)

Clinical risk:

Rhabdomyolysis

(E) AOP Mapping: Mitochondrial Dysfunction -> DILI (AOP:25)

