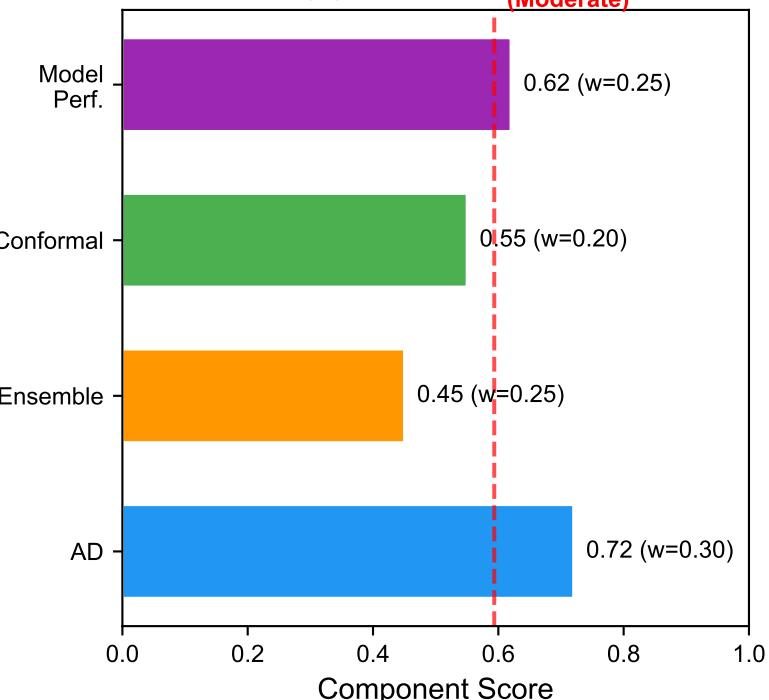


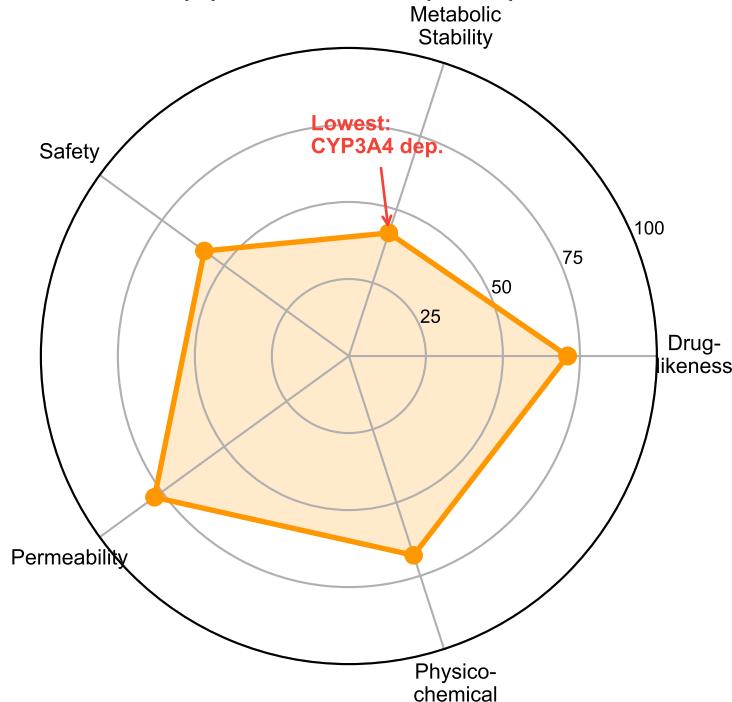
## (A) Physicochemical Properties

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  
PRI = 0.59 (Moderate)



(C) CDS = 62/100 (Good)



## (D) DDI Assessment

DDI Risk Score	72/100 (High)
Classification	CYP3A4 Victim Drug
Major pathway	CYP3A4 (single)
<b>Contraindicated with:</b>	
Ketoconazole (strong CYP3A4 inh.)	
Itraconazole (strong CYP3A4 inh.)	
<b>Dose adjust with:</b>	
Diltiazem (moderate CYP3A4 inh.)	
Verapamil (moderate CYP3A4 inh.)	
<b>Clinical risk:</b>	
Rhabdomyolysis	

## (E) AOP Mapping: Mitochondrial Dysfunction → DILI (AOP:25)

