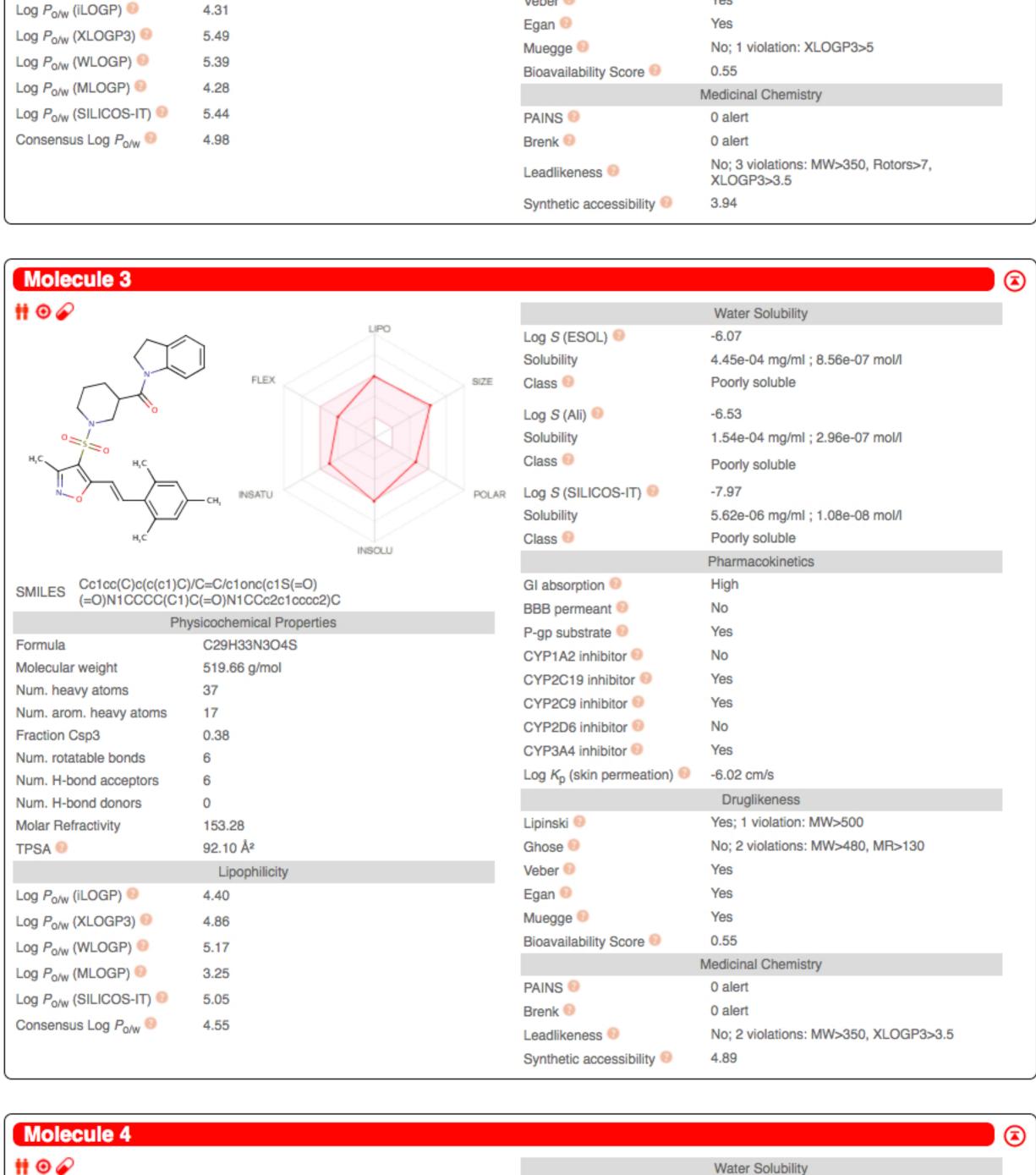


Molecule 1



Log S (ESOL) 0

Solubility

Class

Solubility

Class

Solubility

Class

Log S (Ali) 69

Log S (SILICOS-IT) 0

SIZE

POLAR

INSOLU

FLEX

INSATU

-6.61

-7.59

-9.97

Poorly soluble

Poorly soluble

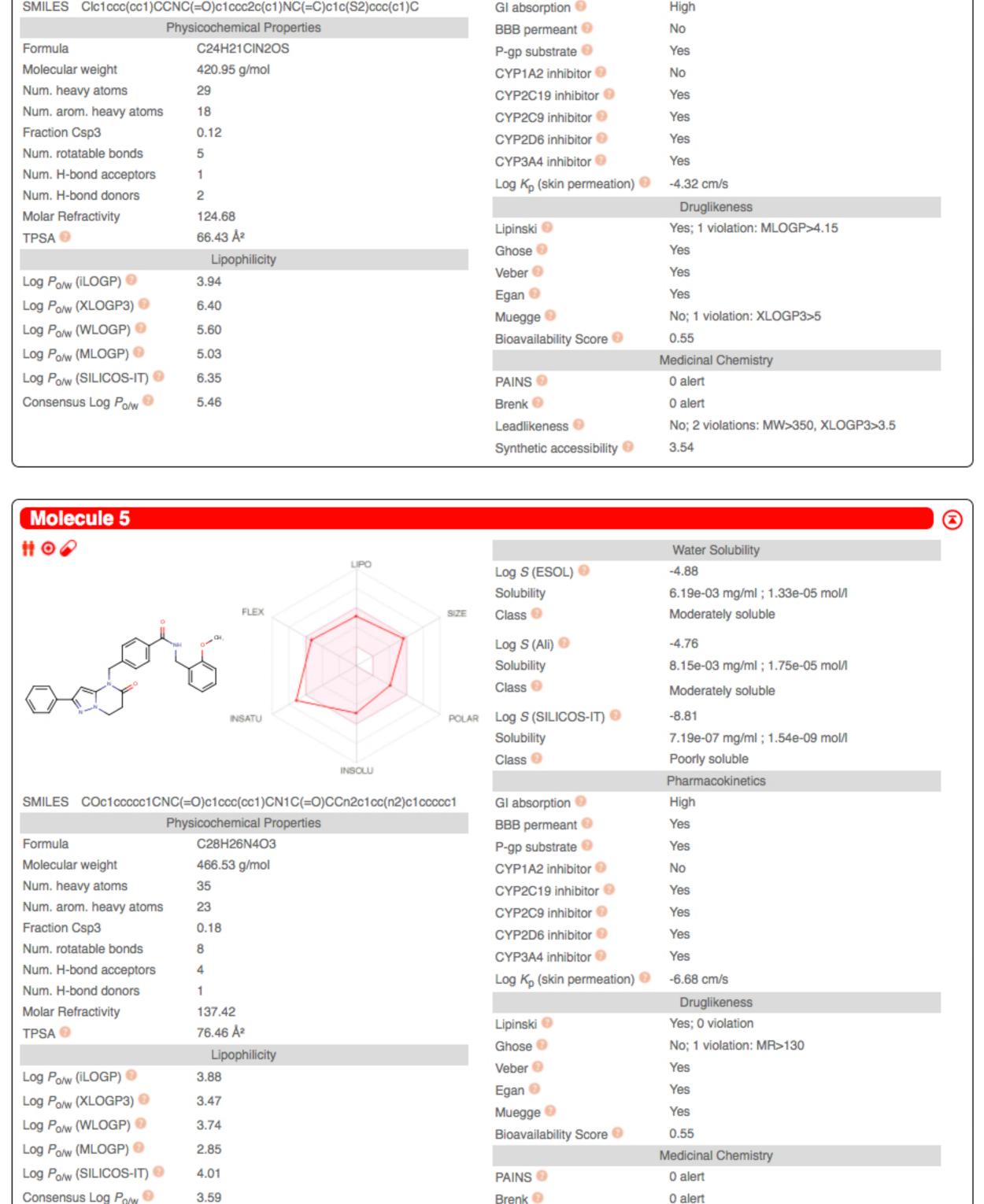
Poorly soluble

Pharmacokinetics

1.03e-04 mg/ml; 2.45e-07 mol/l

1.09e-05 mg/ml; 2.59e-08 mol/l

4.53e-08 mg/ml; 1.08e-10 mol/l



Leadlikeness @

Synthetic accessibility

No; 2 violations: MW>350, Rotors>7

3.58