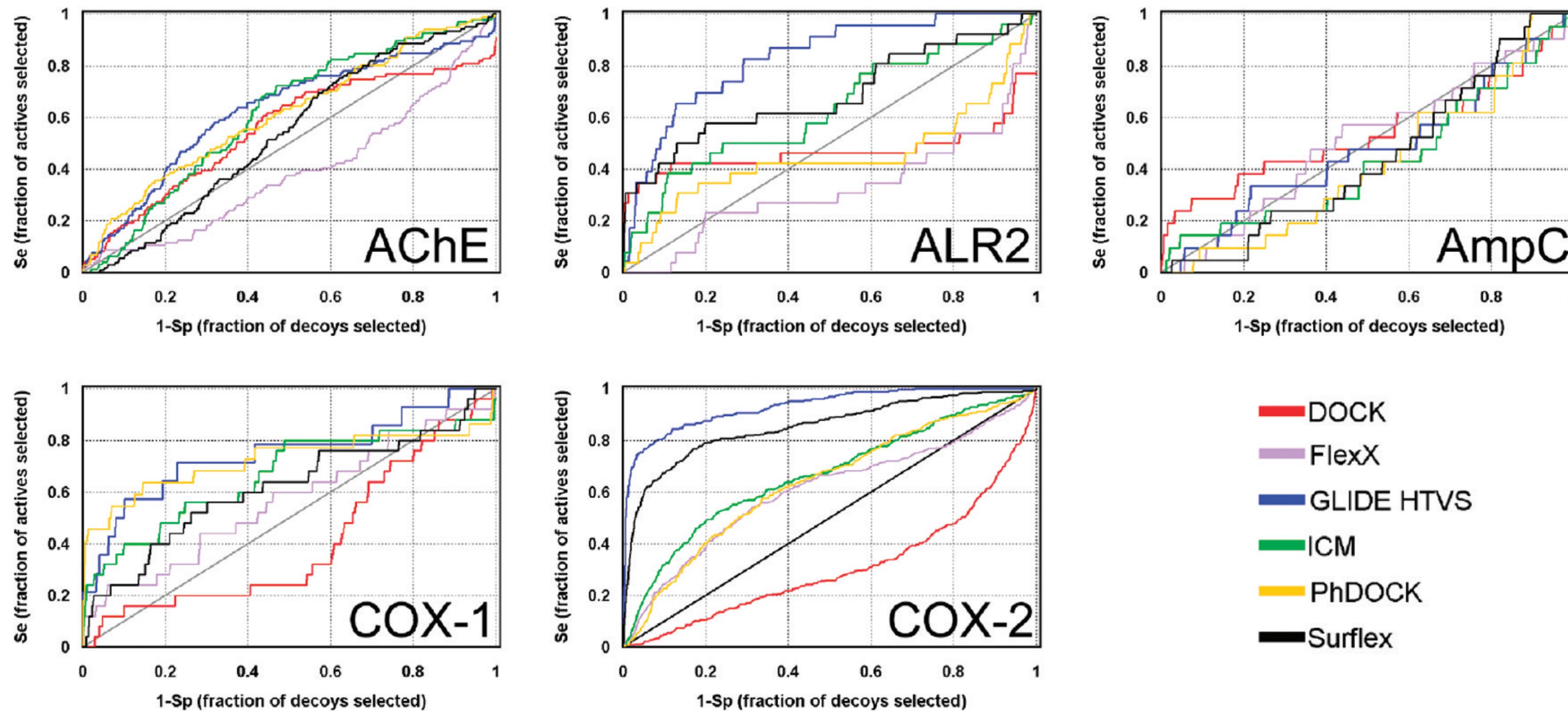


Molecular docking is often an unreliable binary classifier



Cross et al, 2009

Tour: Virtual screening of FDA-approved drugs against HIV protease