

Bayesian Active Drug Discovery

Yuanqing Wang*, Manh Nguyen, Michael Retchin, John D. Chodera*, Theofanis Karaletsos*

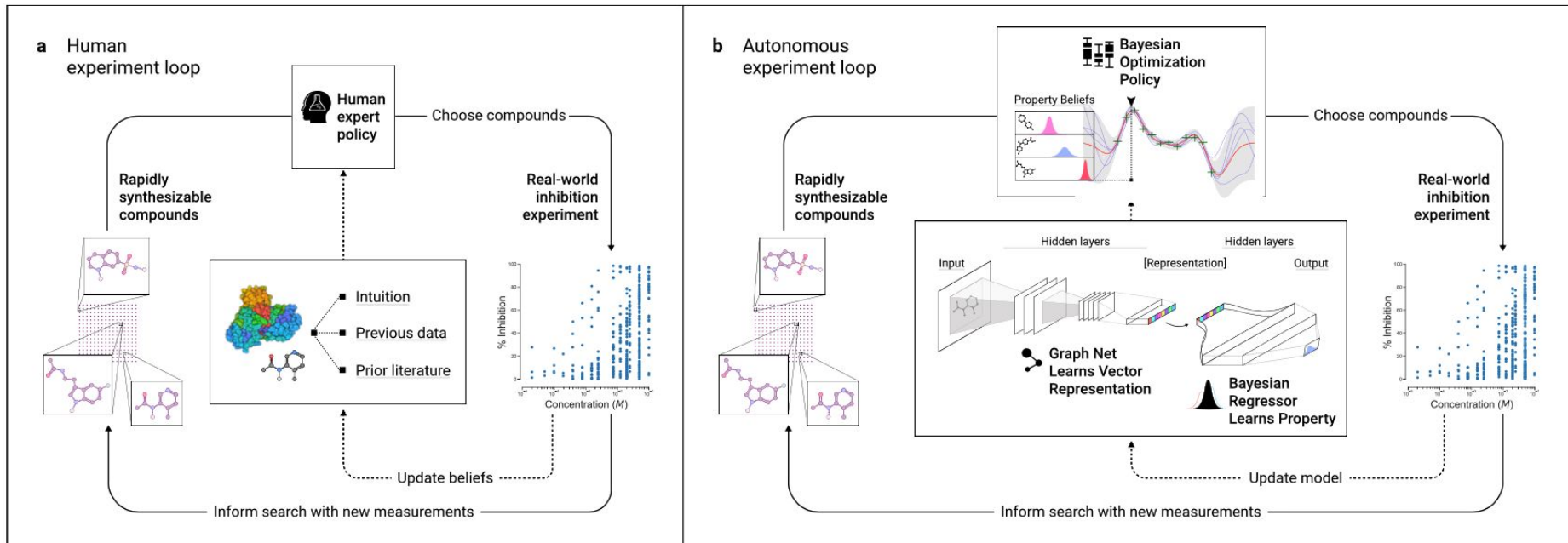


Image	↕	Molecule	↕	IC50 Curves	↕	IC50 (μM) - Fluorescence ↕	↕	IC50 (μM) - RapidFire ↕	↕	Trypsin IC50 (μM) ↕	↕	pIC50 (μM) - Fluorescence ↕
		<p>JAG-UCB-a3ef7265-20</p> <p><chem>O=C(Nc1nncn1C1CC1)C1CC0c2ccc(Cl)cc21</chem></p> <p>21</p> <p>Enamine MolPort</p> <p>Mcule Assayed</p>		<p>Fluorescence</p> <p>RapidFire</p>		0.60		> 99				6.22
		<p>DAN-LON-a5fc619e-3</p> <p><chem>CC(C)C[C@@H]1CN(C(=O)CCl)CCN1Cc1ccc(Cl)c1</chem></p> <p>piperazine-chloroacetamide</p> <p>Chloroacetamide Assayed</p>		<p>Fluorescence</p> <p>RapidFire</p>		0.78			> 99			6.11
		<p>MAT-POS-ee51dedd-2</p> <p><chem>O=C(CCl)N1CCN(S(=O)(=O)c2ccsc2)CC1</chem></p> <p>piperazine-chloroacetamide</p> <p>Enamine</p> <p>Chloroacetamide Assayed</p>		<p>Fluorescence</p> <p>RapidFire</p>		1.63		> 99	> 99			5.79

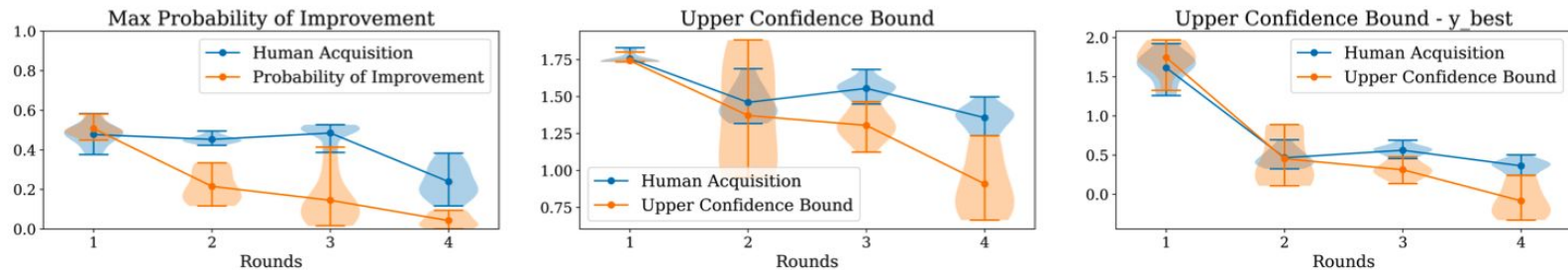


Figure 3: **Bayesian optimization acquisition rule is less prone to be overoptimistic.** Max probability of improvement, max upper confidence interval, and the difference between the max upper confidence interval and the current best candidate, plotted against rounds of acquisition.