Bayesian Active Drug Discovery

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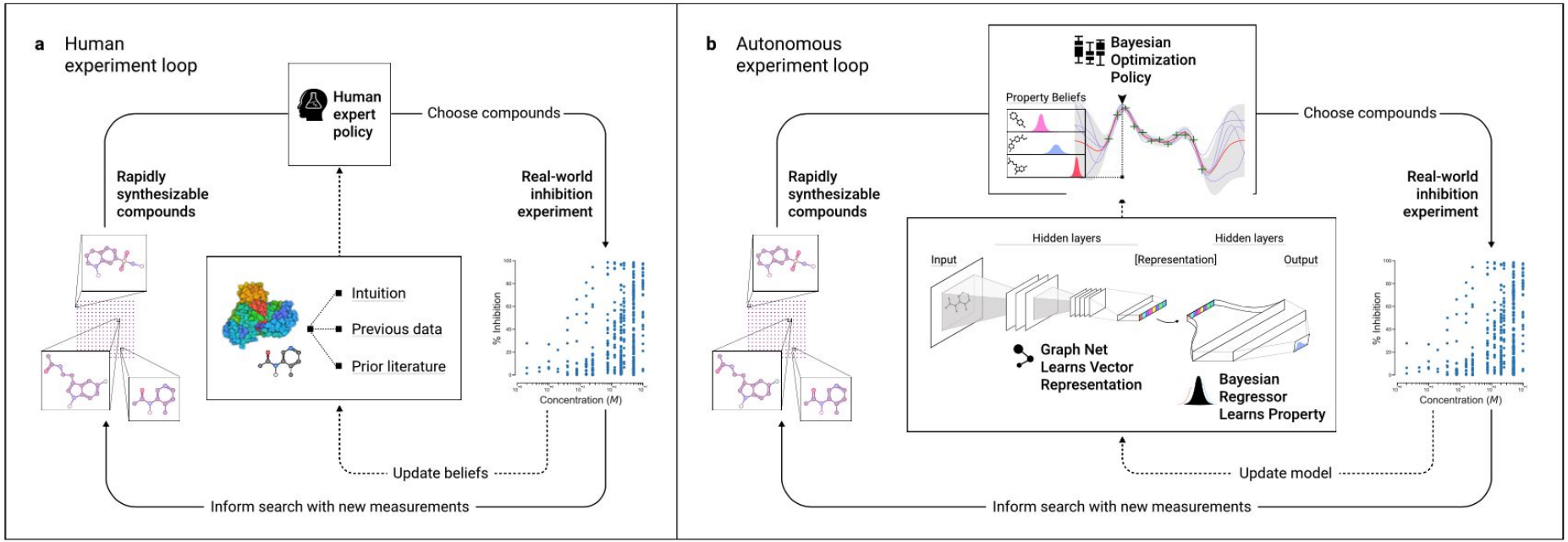
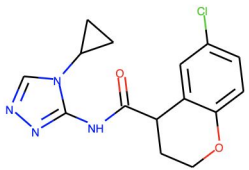
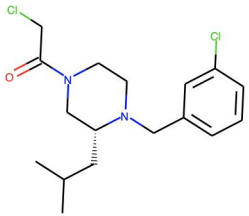
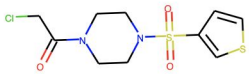


Image	Molecule	IC50 Curves	IC50 (µM) - Fluorescence	IC50 (µM) - RapidFire	Trypsin IC50 (µM)	pIC50 (µM) - Fluorescence
	JAG-UCB-a3ef7265-20 O=C(Nc1nncn1C1CC1)C1CCOc2ccc(Cl)cc21 Enamine MolPort Mcule Assayed	Fluorescence RapidFire	0.60	> 99		6.22
	DAN-LON-a5fc619e-3 CC(C)C[C@@H]1CN(C(=O)CCl)CCN1Cc1ccccc(Cl)c1 piperazine-chloroacetamide Chloroacetamide Assayed	Fluorescence RapidFire	0.78		> 99	6.11
	MAT-POS-ee51dedd-2 O=C(CCl)N1CCN(S(=O)(=O)c2ccsc2)CC1 piperazine-chloroacetamide Enamine Chloroacetamide Assayed	Fluorescence RapidFire	1.63	> 99	> 99	5.79

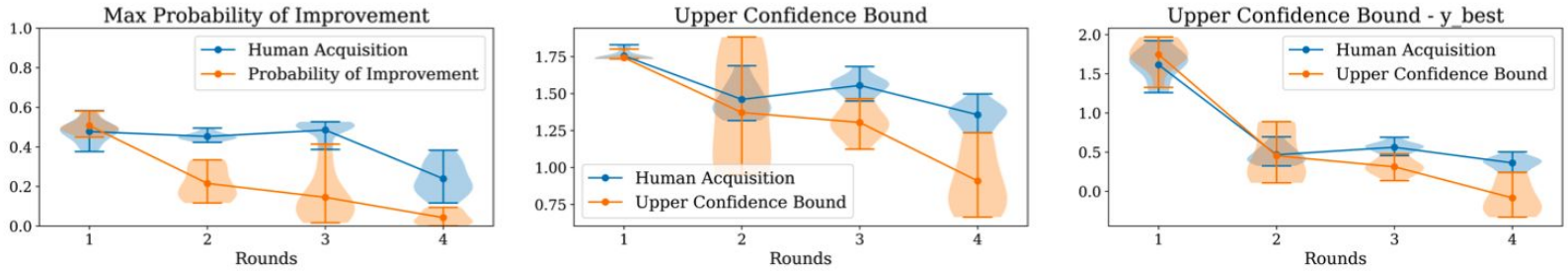


Figure 3: **Bayesian optimization acquisition rule is less prone to be overoptimistic.** Max probability of improvement, max upper confidence interval, and the difference between the max upper confidence interval and the current best candidate, plotted against rounds of acquisition.