

Labeled

observations

Acquisition

(b) Tasks

Molecular optimization

clcc(c(cc1N)C(=0)Nc2cc(ncc2F)NC(=0)C3CC3)Cl,
...,
clcc(c(cc1N)Cl)C(=0)Nc2cc(ncc2F)NC(=0)C3CC3F

LLM-enabled B



Protein optimization

AAAA, ..., LVIL

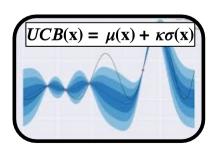
LLM-enabled







(c) Approaches

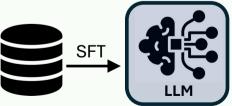


Statistical BO



LLM

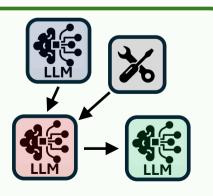
LLM-based approaches



Predicted

observations

Finetuned LLM



Agentic LLM workflows