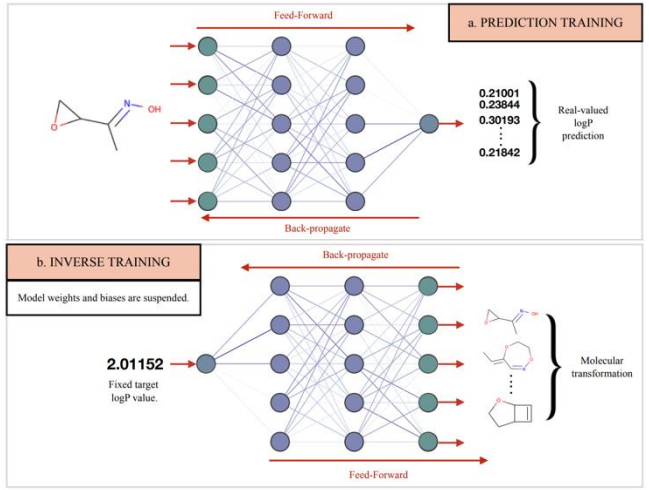
Examples of inverse molecular design

In the inverse molecular design methods, the regions of the chemical space that possess the desired properties are depicted and the compounds that occupy this space are generated.

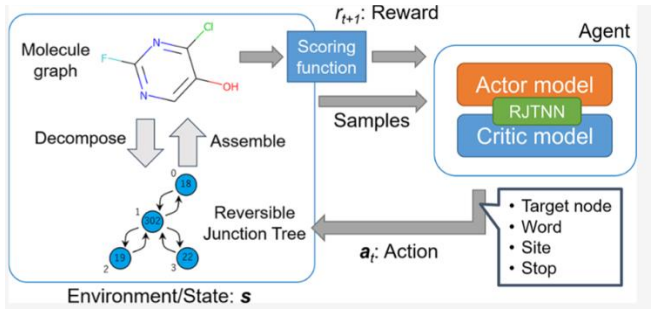
PASITHEA: Combining deep dreaming with molecular design

- A simple NN is trained to predict the target property using SELFIES. Next, the NN is trained in reverse order to generate novel molecules with the same weights and biases.
- The gradient with respect to the input's representation is calculated by minimising the error between the predicted property for each structure and the target property.



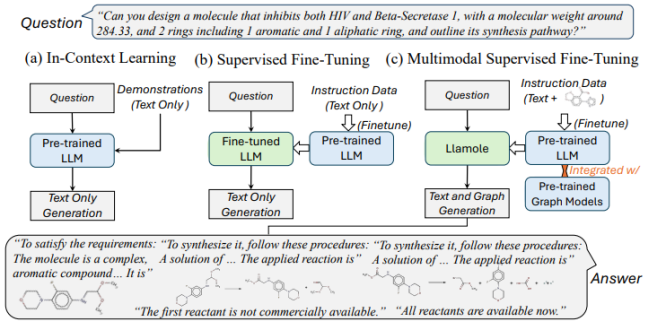
RJT-RL: Using reinforcement learning to perform molecular design

- The RJT representation was used as the state in RL. The RJT of s_t is modified by the agent, who then constructs it in step t+1. The policy is a probability distribution function for each action component (from an NN trained on RJT of s_t).
- The policy network was pretrained using the expert dataset to guide the RL exploration.



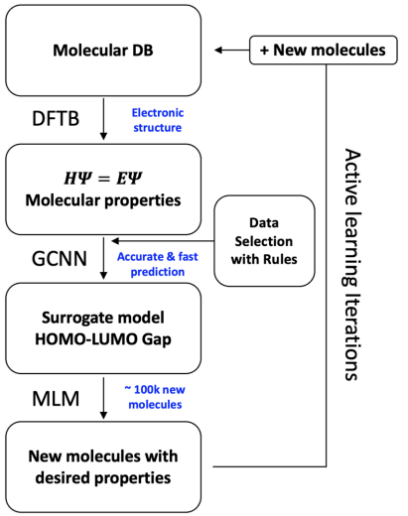
Llamole: Going beyond LLMs to perform molecular design

- Llamole merges LLMs and graph models in a multimodal autoregressive framework for molecular discovery (predicts the next token for both words and molecules).
- Llamole significantly outperforms 14 tested LLMs in molecular design.



HydraGNN: Combining generative and surrogate models for molecular design

- A surrogate model (HydraGNN) was trained to predict properties of interest using SMILES representation.
- Molecules are generated by mutating the selected molecular structure data using a pre-trained and validated masked language model (MLM).
- The surrogate model makes inaccurate predictions about novel molecules (active learning).



Reverse design relies on reversible and surjective representations.
Currently, various method are available for inverse design, ranging from molecular inceptionism to LLMs.