

Machine Learning Guided Design of Metal–Ligand Complexes for Photocatalysis

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INTRODUCTION

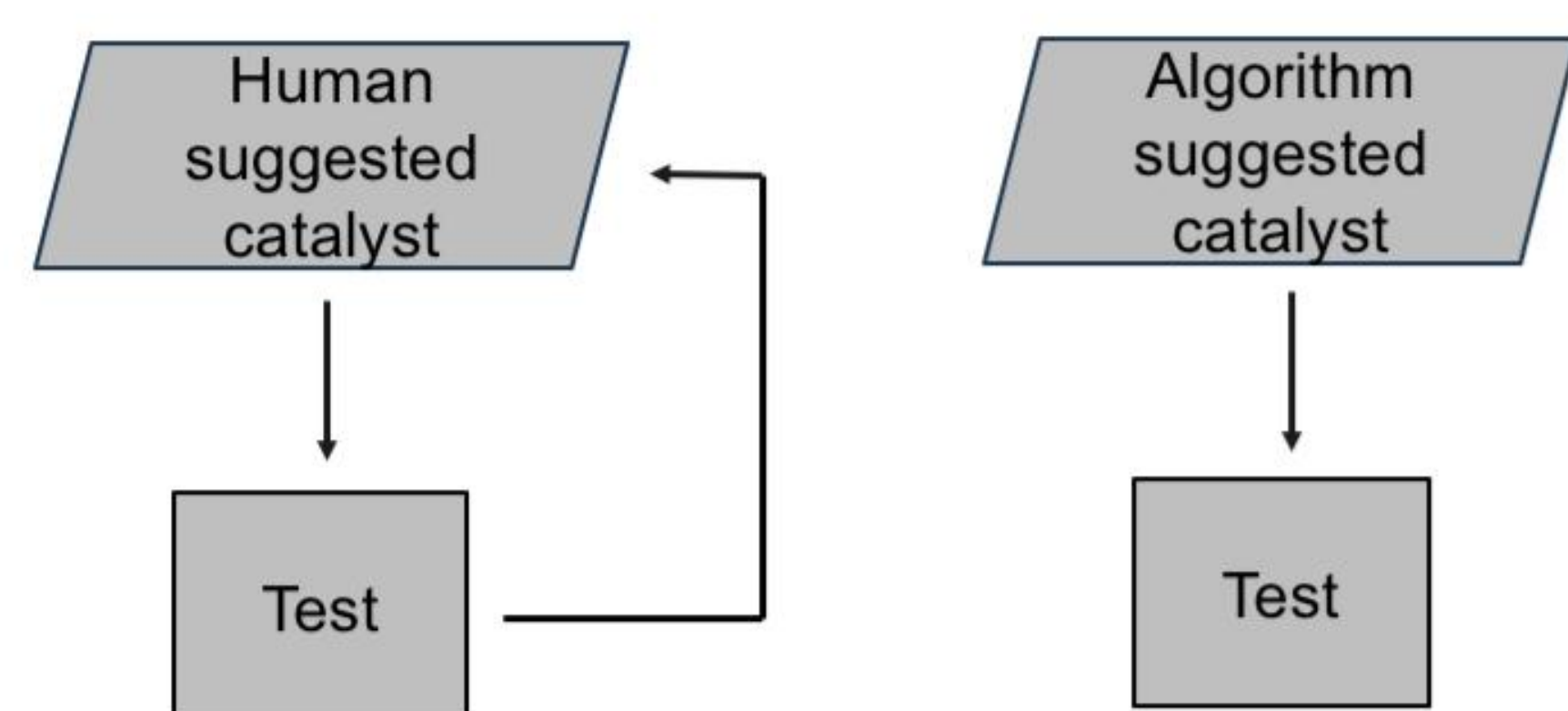


Figure 1: Comparison of traditional trial-and-error catalyst discovery (left) and machine learning guided catalyst discovery (right).

Photoredox catalysis enables transformations that are difficult or inaccessible under thermal conditions. However, identifying suitable photocatalysts remains challenging, as their photophysical and redox properties must match the reaction's energetic requirements. Machine learning can link reaction energetics with catalyst design by predicting key parameters from simple reaction representations, allowing candidate photocatalysts to be proposed prior to experimental testing. Unlike traditional trial-and-error screening, which may require testing hundreds or thousands of catalysts, this workflow suggests a small set of promising candidates, reducing experimental time and resource costs.

METHOD

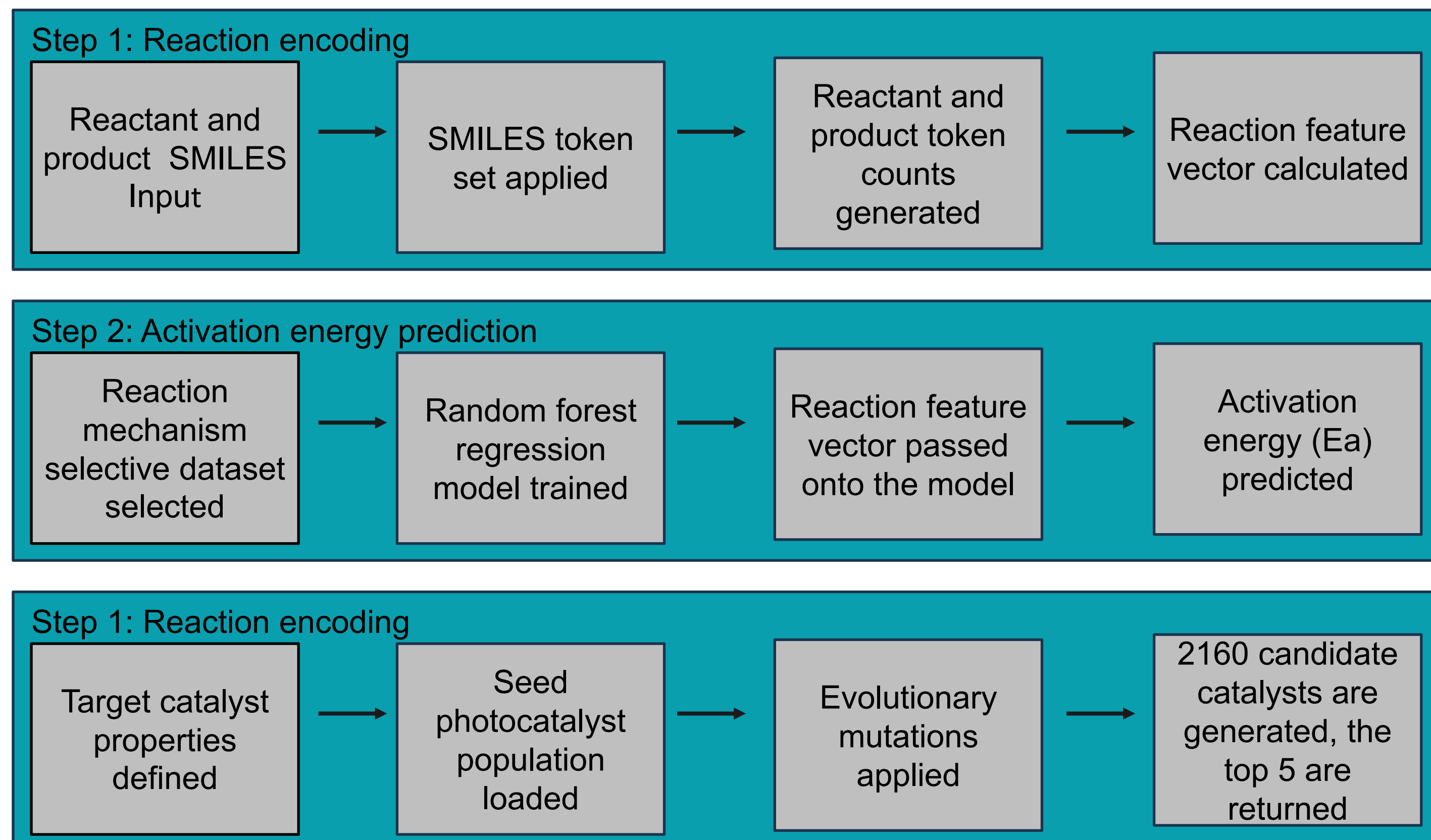
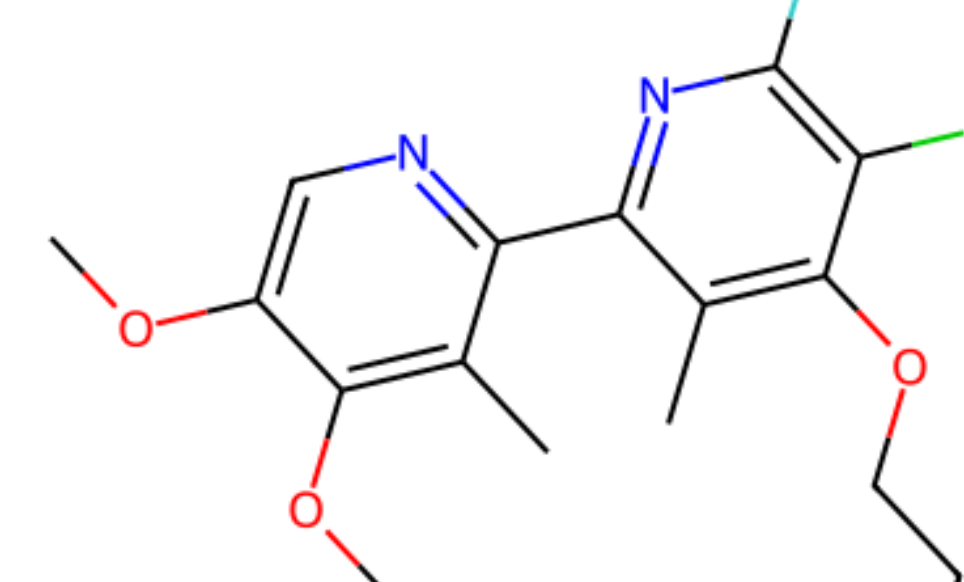
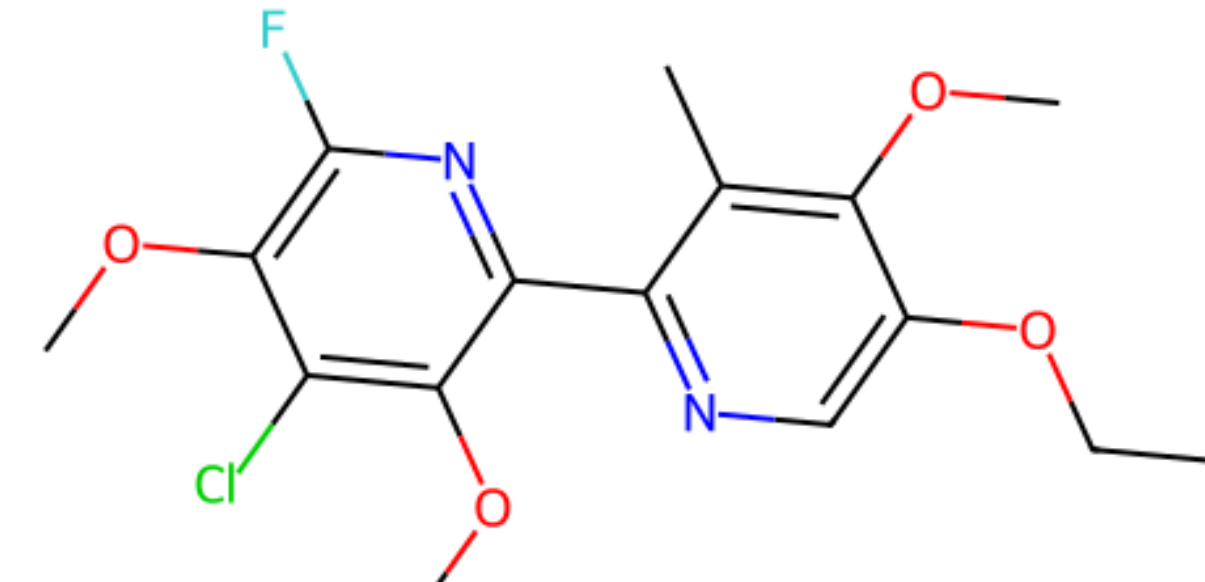
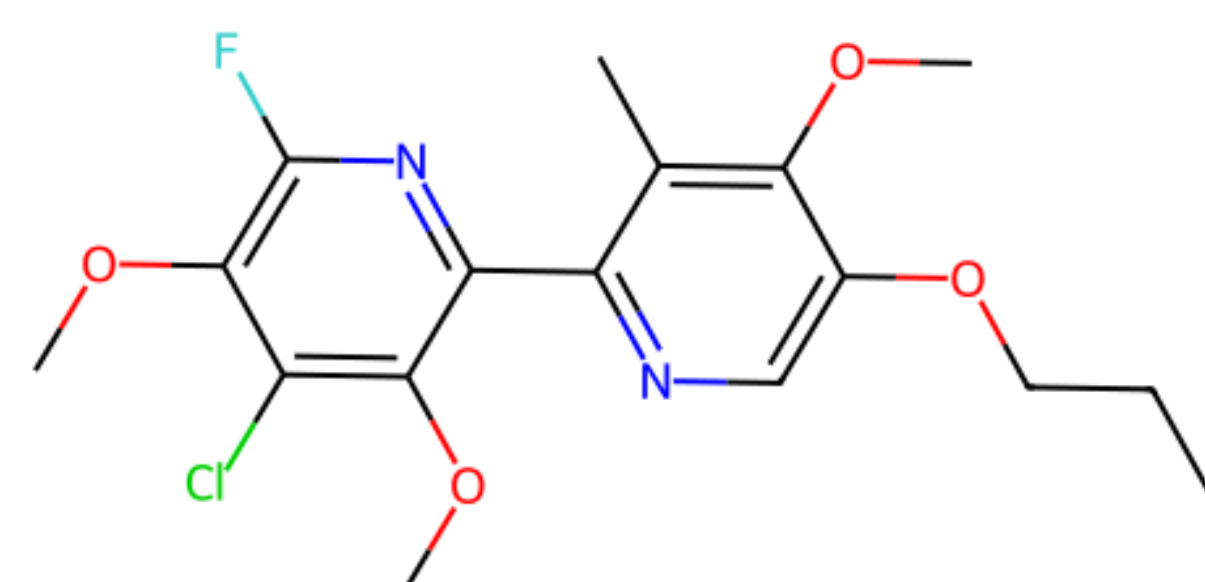
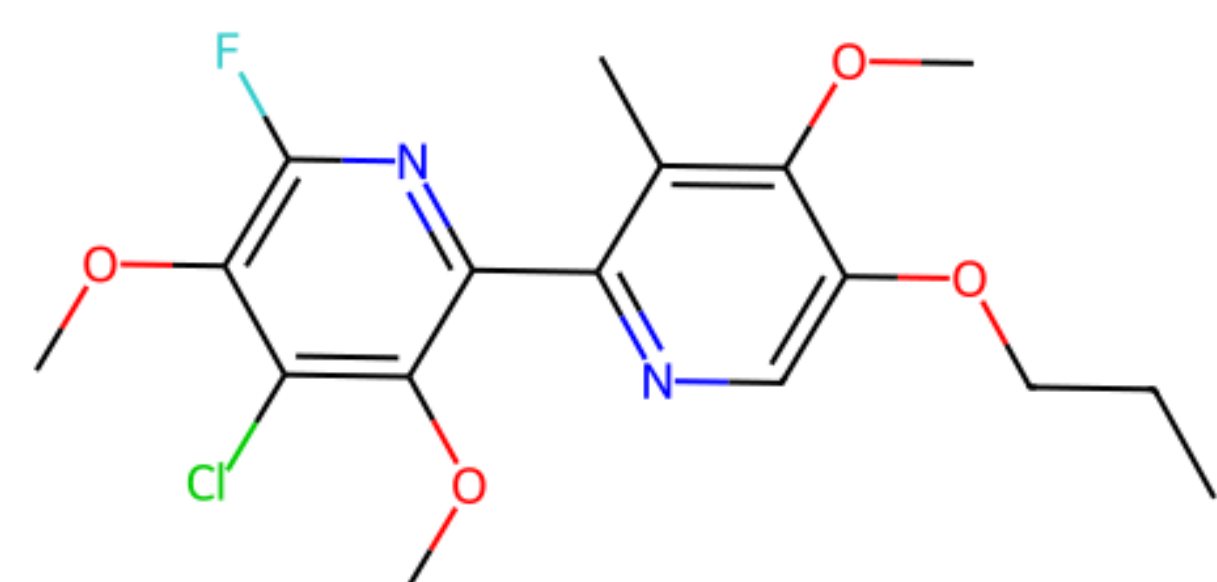


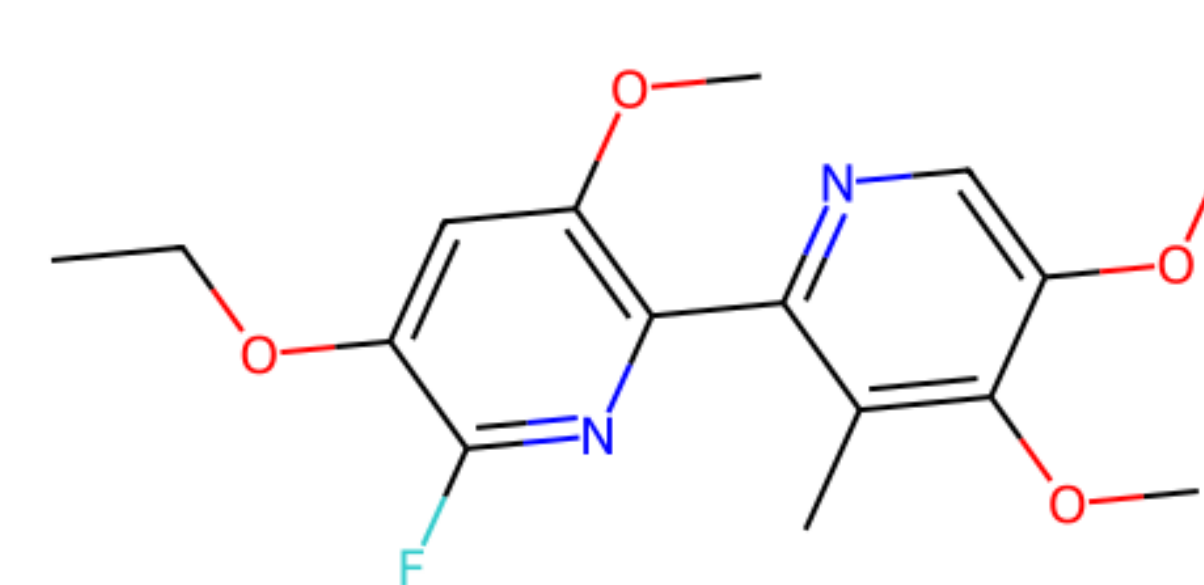
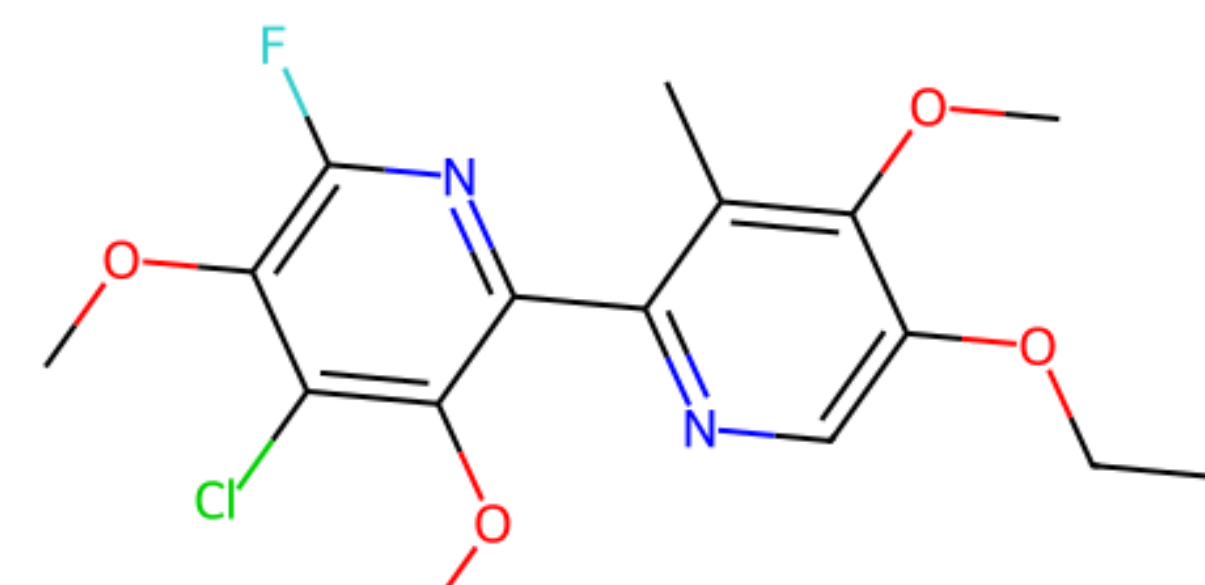
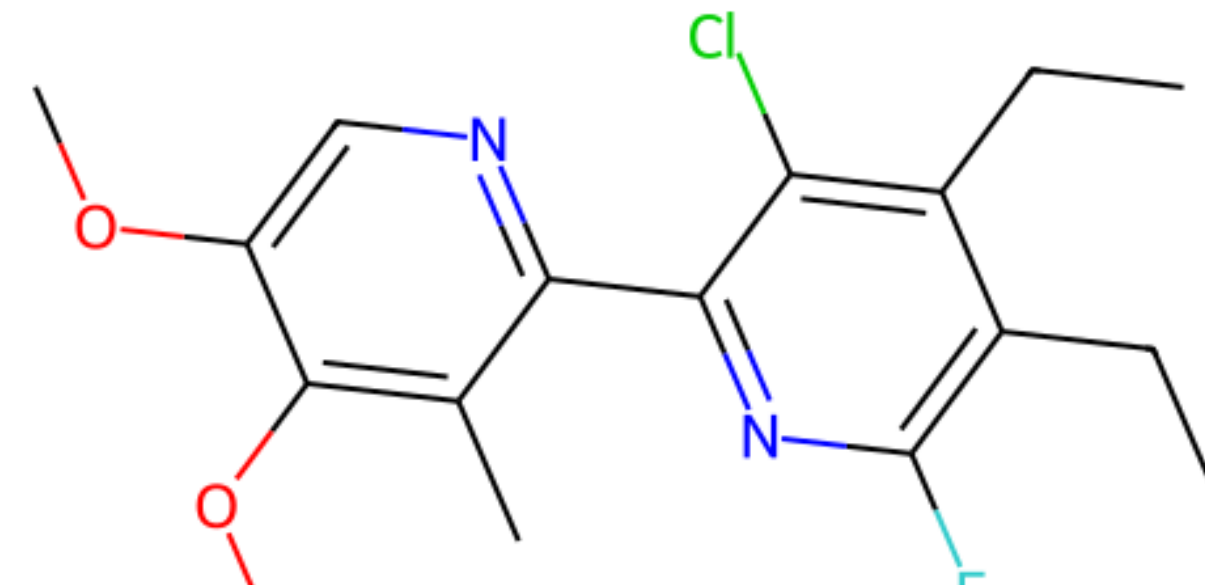
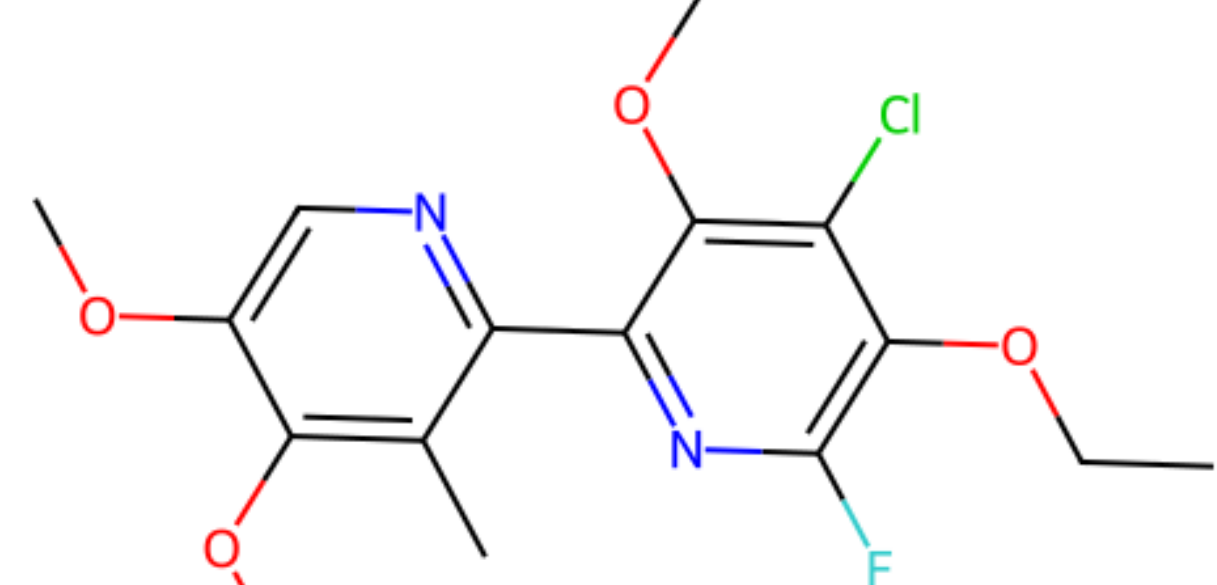
Figure 2: Machine learning workflow for photocatalyst discovery

RESULTS & DISCUSSION

Example 1: Giese-Type Radical Addition to an Alkene



Example 2: Reductive Dehalogenation



Example 3: Photoredox-Mediated Substitution (S_N2-Type)

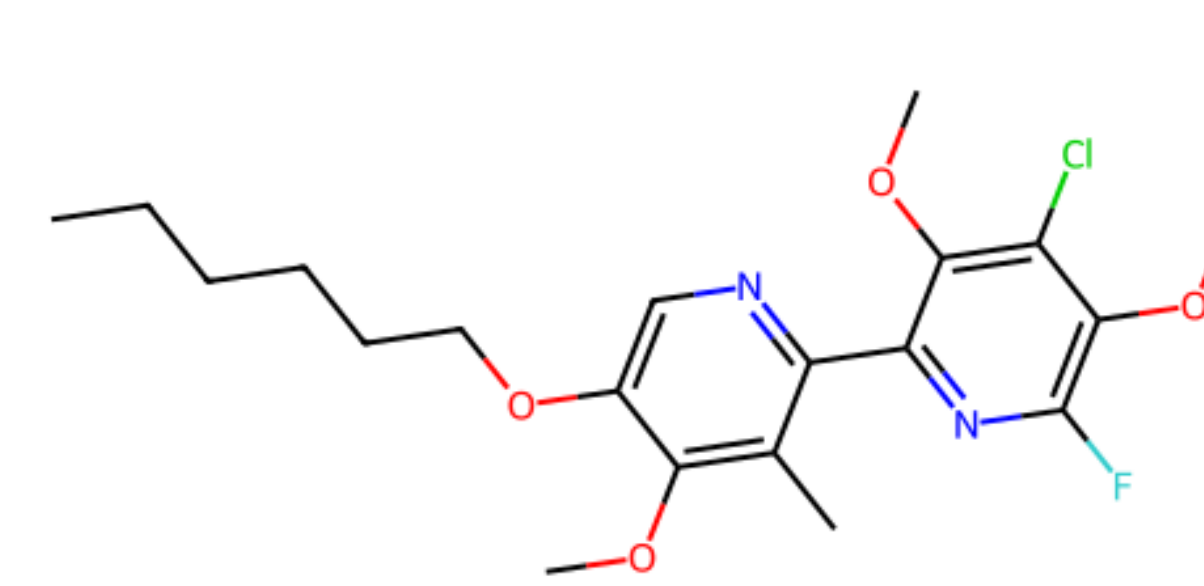
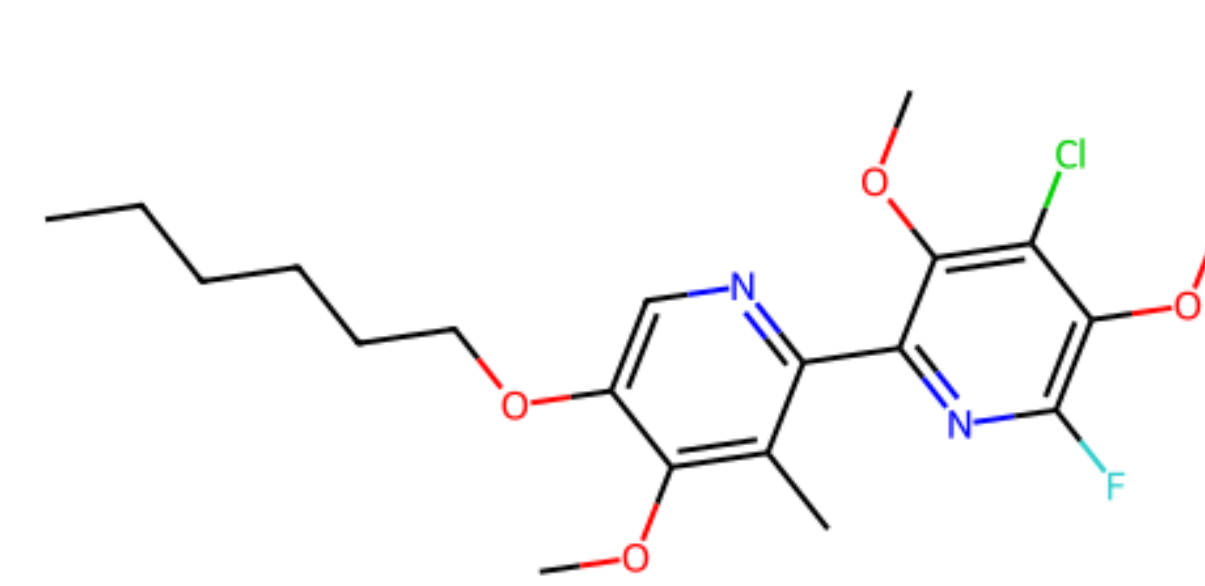
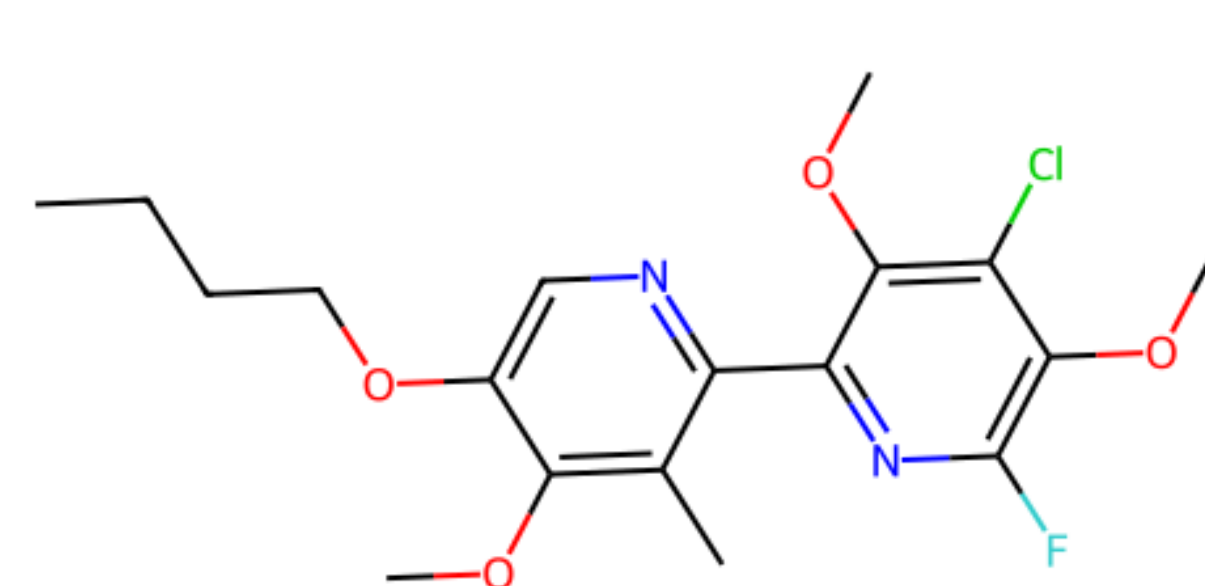
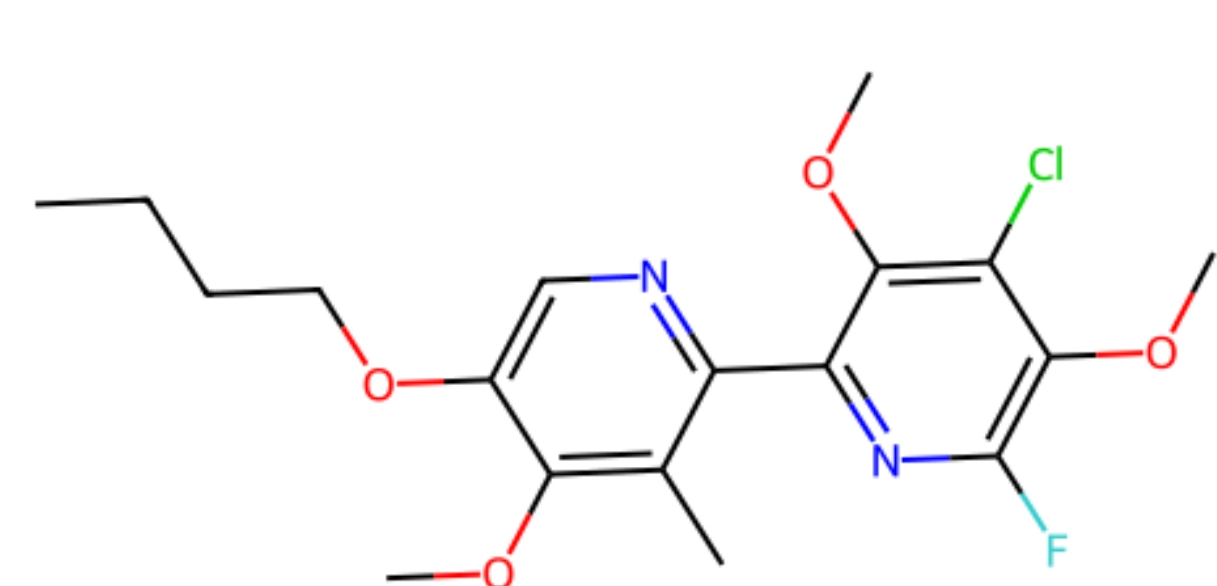


Figure 3: Example Photocatalysts Suggested by the Machine Learning Workflow

CONCLUSIONS

A machine learning workflow was developed to predict reaction activation energies and propose suitable photocatalysts. The model successfully generates chemically plausible catalyst candidates tailored to the energetic requirements of specific reactions.

Across representative transformations, the workflow consistently reduces a large catalyst search space to a small number of high-quality suggestions. The observed preference for Ru-based systems reflects both their favourable photophysical properties and biases within the training data.

These results demonstrate that reaction-driven modelling can be used to guide photocatalyst selection and provide a practical starting point for experimental investigation.

FUTURE WORK

- Incorporate solvent-dependent effects to improve reaction and catalyst predictions under realistic conditions.
- Account for metal coordination geometry and ligand field effects not captured by the current representation.
- Experimentally evaluate the top-ranked candidates suggested by the workflow.
- Introduce energetic constraints linked to electron transfer theory (e.g. driving force considerations) to improve physical interpretability of catalyst selection.
- Improve treatment of excited-state processes, including relaxation pathways and competing deactivation mechanisms.
- Explore strategies to reduce metal bias and promote greater diversity in catalyst suggestions.