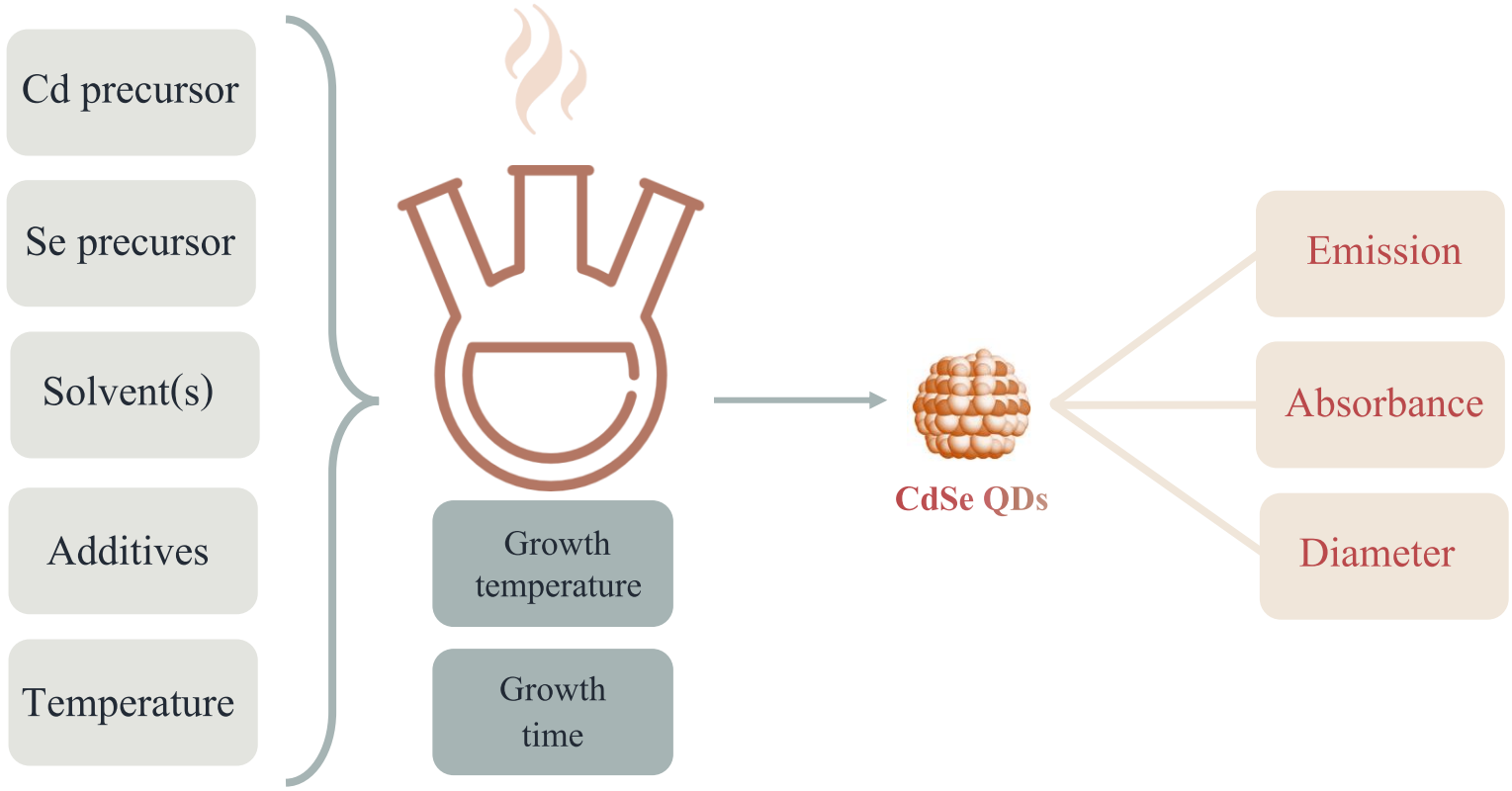
Hot Pots for Good Dots

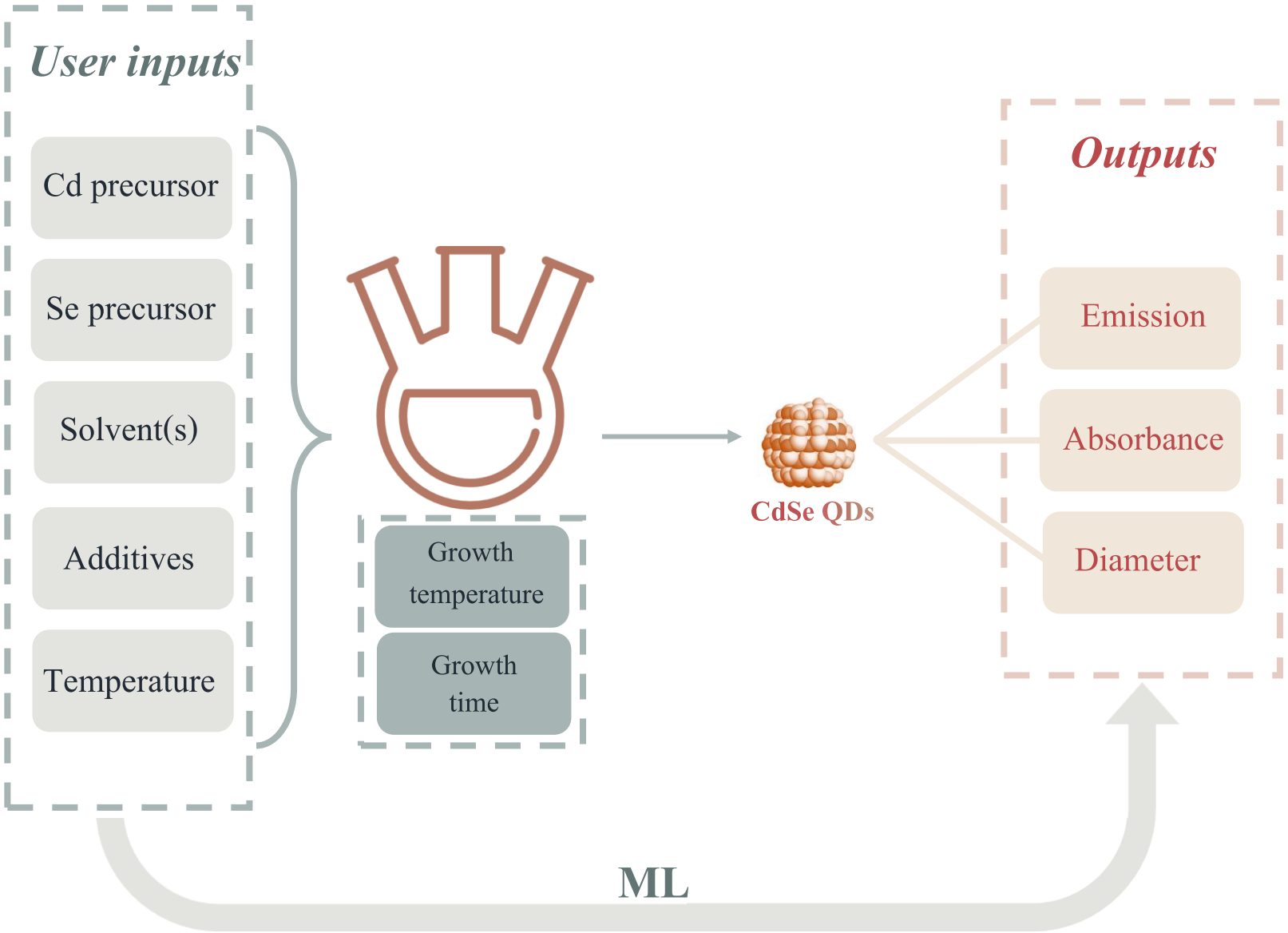
Typical synthesis of CdSe quantum dots (QDs)



Use case 1

Story:

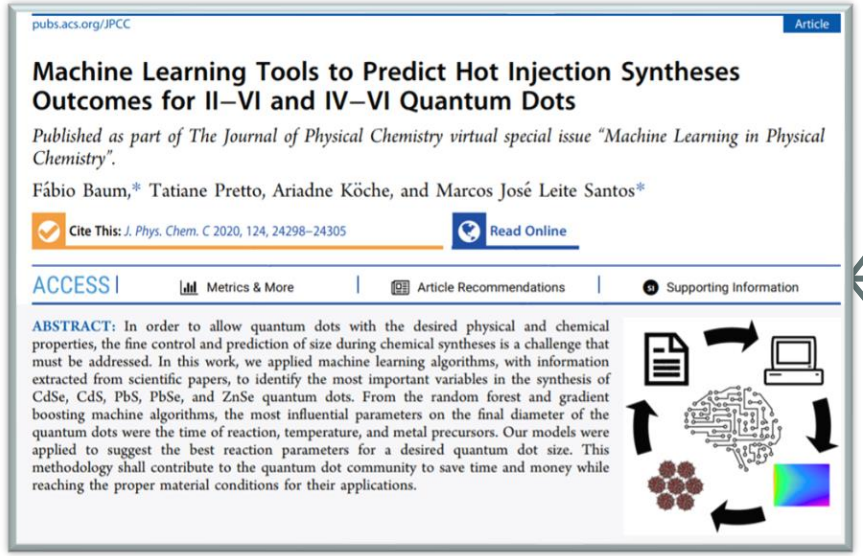
Clay is a chemistry grad student who has some experience with the synthesis of nanoparticles. He has already asked his undergrad to help him synthesize one batch of CdSe quantum dots. Clay needs to run a dozen more experiments modifying the conditions of the synthesis. He wants to adjust the temperature and the solvents of the reaction to see if the size, absorbance and emission are different. This specific set of experiments has never been reported before. But Clay can only come to the lab twice a week due to COVID. Clay knows that in group meeting on Friday, his PI will be mad if he doesn't have the data. Clay is frustrated.



Use case 2

Story:

Zach is a demanding chemistry professor. He's read the paper "*Machine Learning Tools to Predict Hot Injection Syntheses Outcomes for II-VI and IV-VI Quantum Dots*" and had some thoughts. Because this is the only paper about using machine learning for II-VI and IV-VI quantum dots syntheses in the literature, Zach wonder if there is a better model that can predict not only the diameter of the quantum dots, but also their max photoluminescence and max absorbance. Zach is curious.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Article

Machine Learning Tools to Predict Hot Injection Syntheses Outcomes for II–VI and IV–VI Quantum Dots

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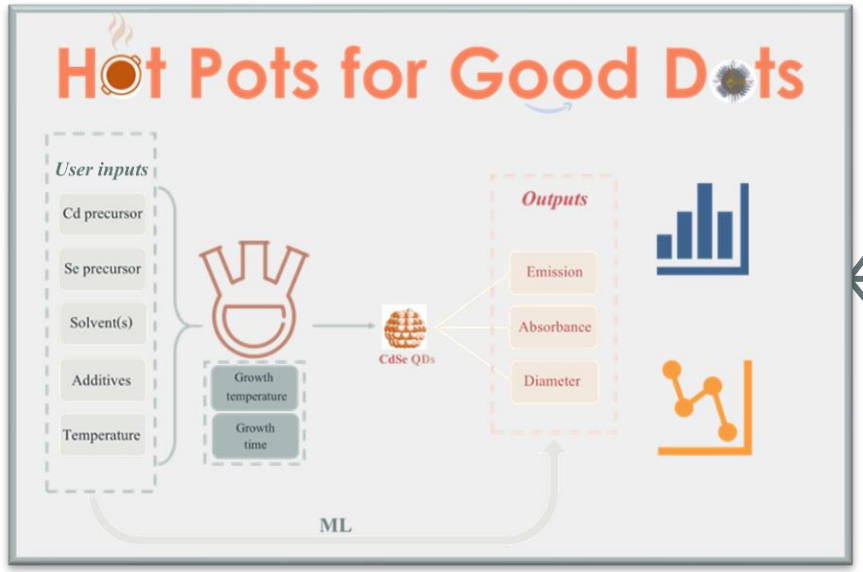
ABSTRACT: In order to allow quantum dots with the desired physical and chemical properties, the fine control and prediction of size during chemical syntheses is a challenge that must be addressed. In this work, we applied machine learning algorithms, with information extracted from scientific papers, to identify the most important variables in the synthesis of CdSe, CdS, PbS, PbSe, and ZnSe quantum dots. From the random forest and gradient boosting machine algorithms, the most influential parameters on the final diameter of the quantum dots were the time of reaction, temperature, and metal precursors. Our models were applied to suggest the best reaction parameters for a desired quantum dot size. This methodology shall contribute to the quantum dot community to save time and money while reaching the proper material conditions for their applications.

Written in R

Tested with 5 models

Predicting one output

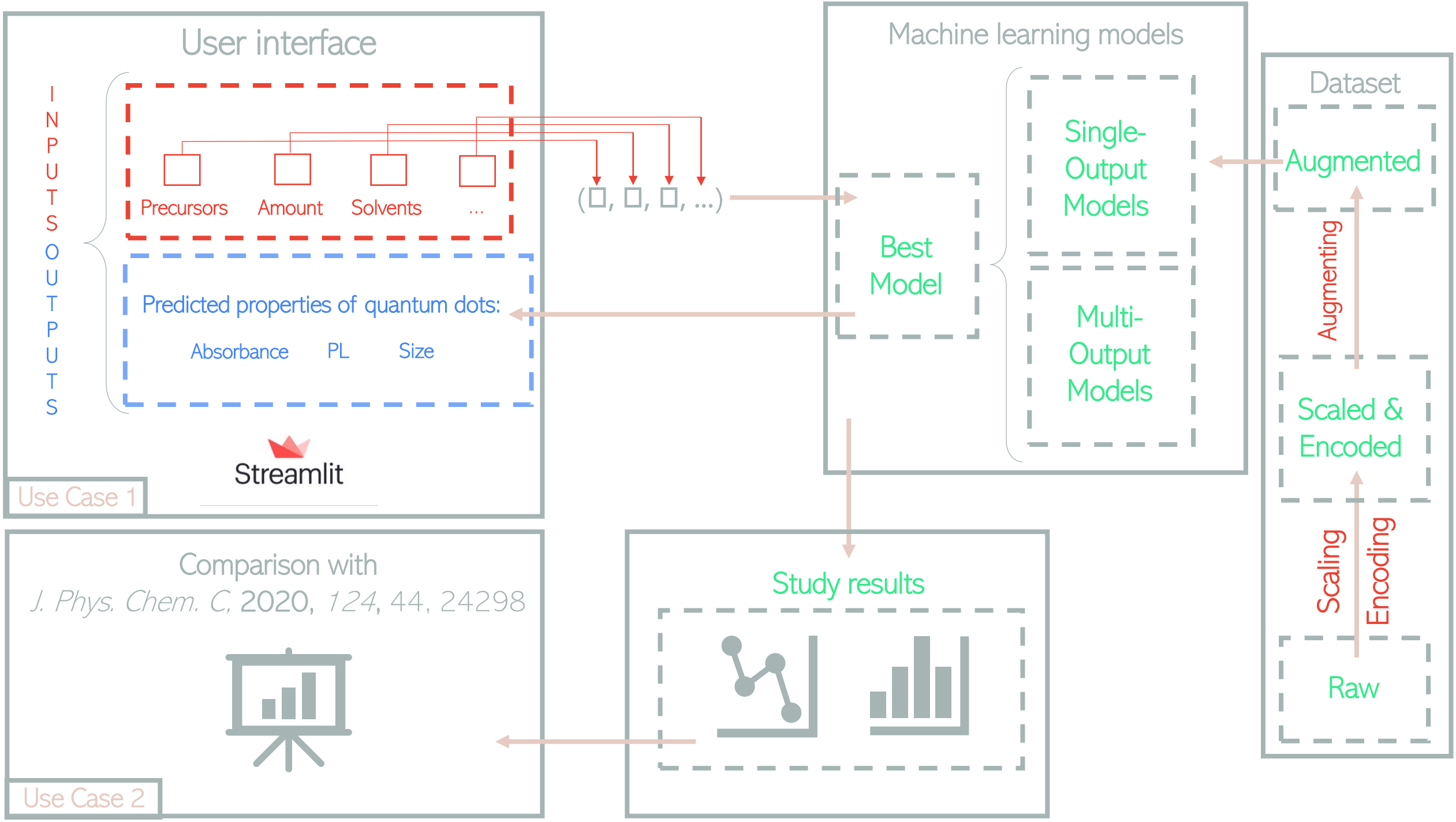
Vs.



Written in Python

Tested with 12 models

Predicting three outputs


User interface
INPUTS
OUTPUTS
Precursors
Amount
Solvents
...
Predicted properties of quantum dots:
Absorbance
PL
Size
Streamlit
Use Case 1
(□, □, □, ...)
Machine learning models
Best Model
Single-Output Models
Multi-Output Models
Dataset
Augmented
Augmenting
Scaled & Encoded
Scaling
Encoding
Raw
Study results
Comparison with
J. Phys. Chem. C, 2020, 124, 44, 24298
Use Case 2