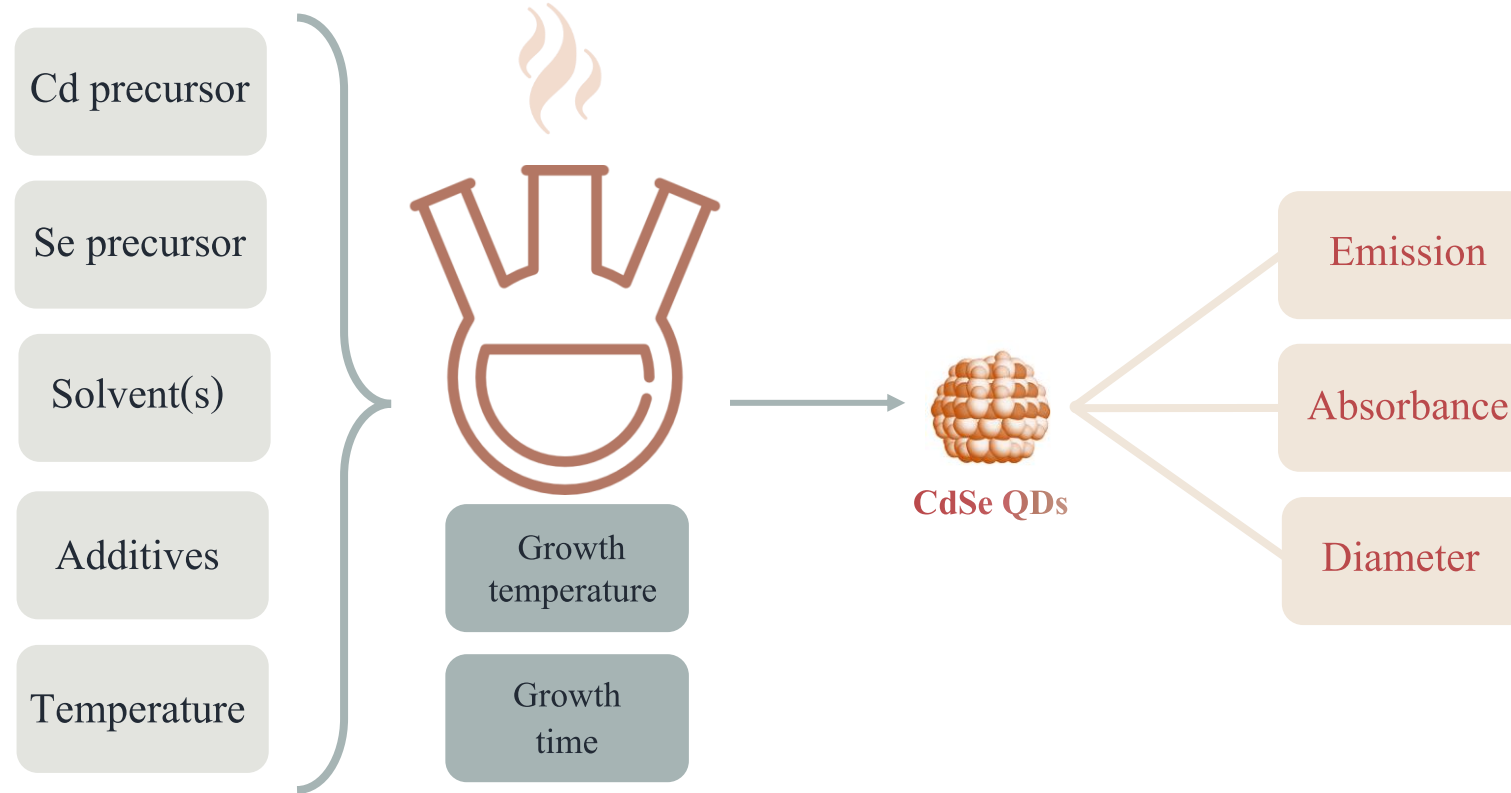


Hot Pots for Good Dots

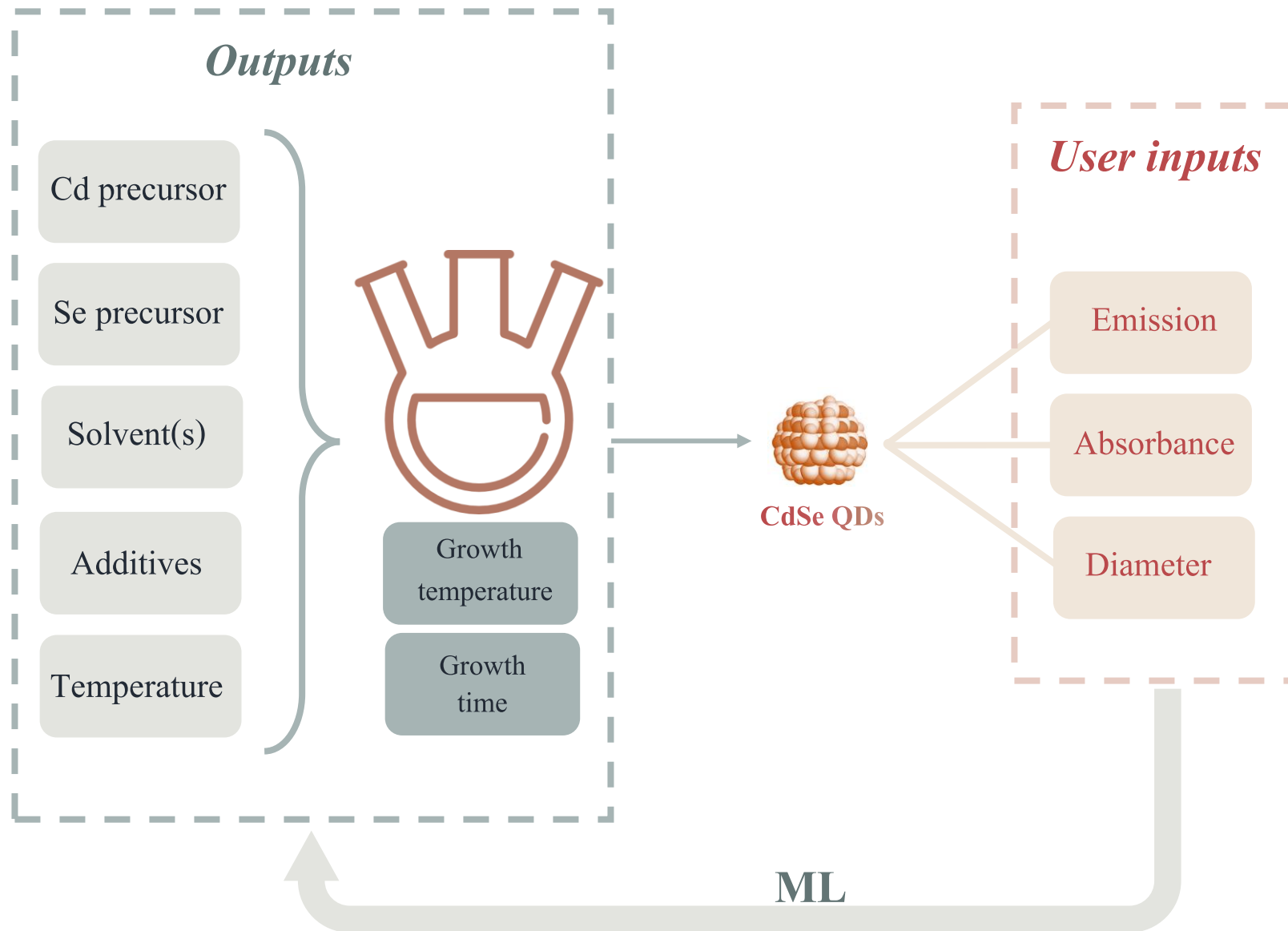
Typical synthesis of CdSe quantum dots (QDs)



User case 1

Story:

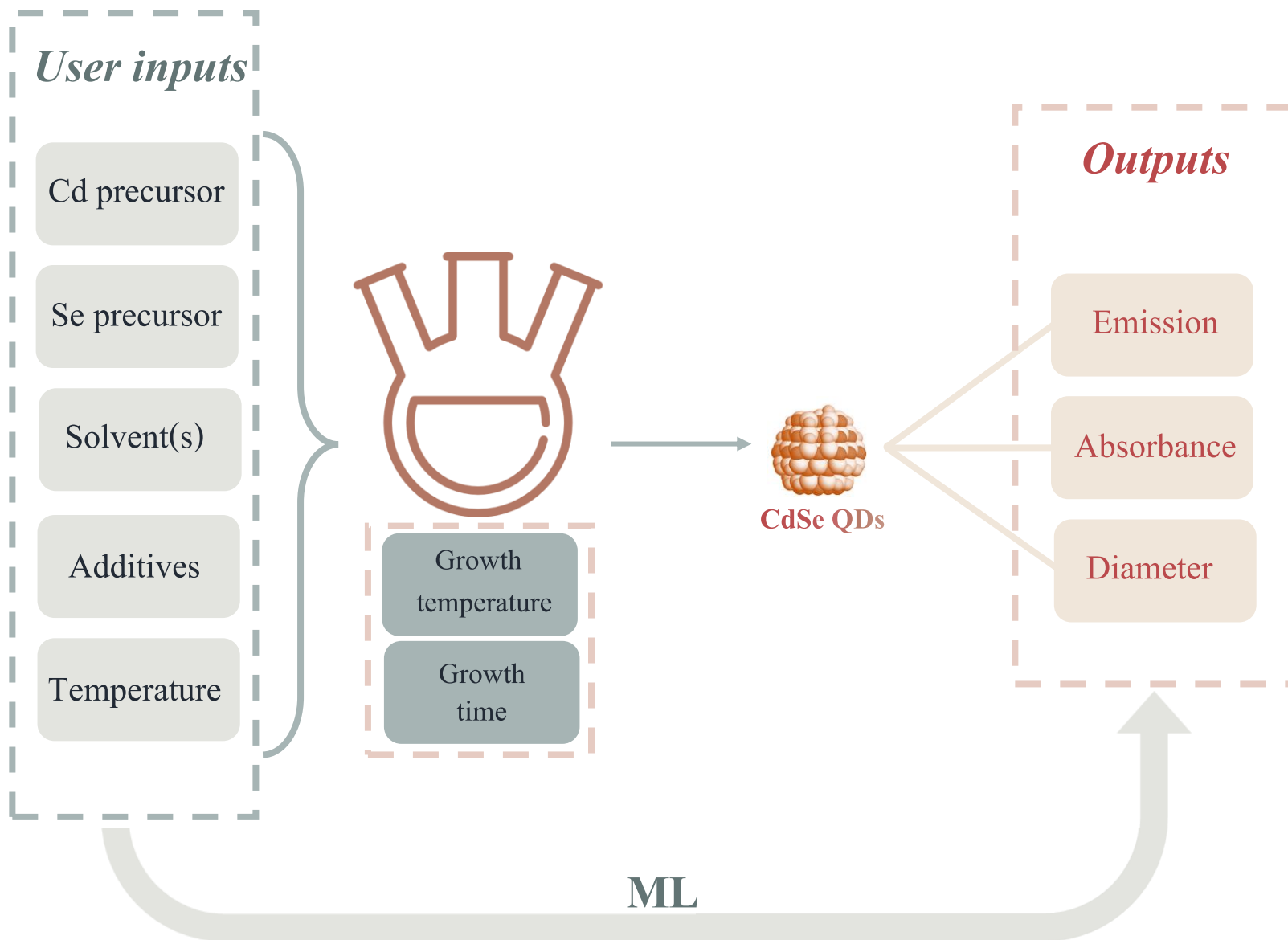
Alex is a chemistry undergrad student, and he needs to synthesize CdSe quantum dots for his grad student mentor. His mentor specifically requests that the material absorb and emit between 570-580 nm and are around 3nm in size. However, Alex is new to this field and is overwhelmed by all of the literature, some of which are contradicting. He doesn't know which procedure to follow and doesn't have time to read all of the papers. He can guess and modify an existing prep, but he cannot find one that suits his exact needs. Alex is confused.



User case 2

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.



User case 3

Story:

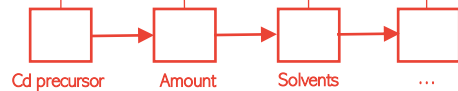
Zach is a demanding chemistry professor with a large group of grad students and undergrads studying synthesis and properties of colloidal nanocrystals. He knows that, despite the substantial improvement over the past decades, synthesising quantum dots is still too Edisonian (trial and error). **Zach** thinks that if he knew all of the existing literature, he could identify patterns and correlations and start to synthesise new quantum dots even more intentionally, systematically, and efficiently. **Zach** is curious.



User interface

User Case 1

INPUTS



(□, □, □, ...)

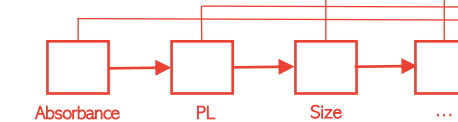
OUTPUTS

Predicted properties of quantum dots:

Absorbance PL Size

User Case 2

INPUTS



(□, □, □, ...)

OUTPUTS

A suggested CdSe QDs synthetic procedure

A citation of the procedure if matched

User Case 3

INPUTS

Desired correlations:
Time growth and size Temperature and PL
...

OUTPUTS

Links to graphs and discussions

Machine learning model

Machine learning algorithms

.sav

Study results



Dataset

Train

Test

Validation

.CSV

.exe