Mentimeter

Intro to AI/ML

Let's recap the basic concepts from m0

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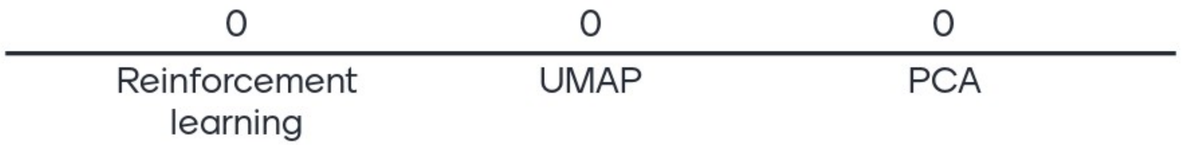
I want to find groups of similar molecules in my dataset, what will I do?



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For unsupervised learning, I need labelled data

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If I have a small dataset and a very complex model, I might risk having...

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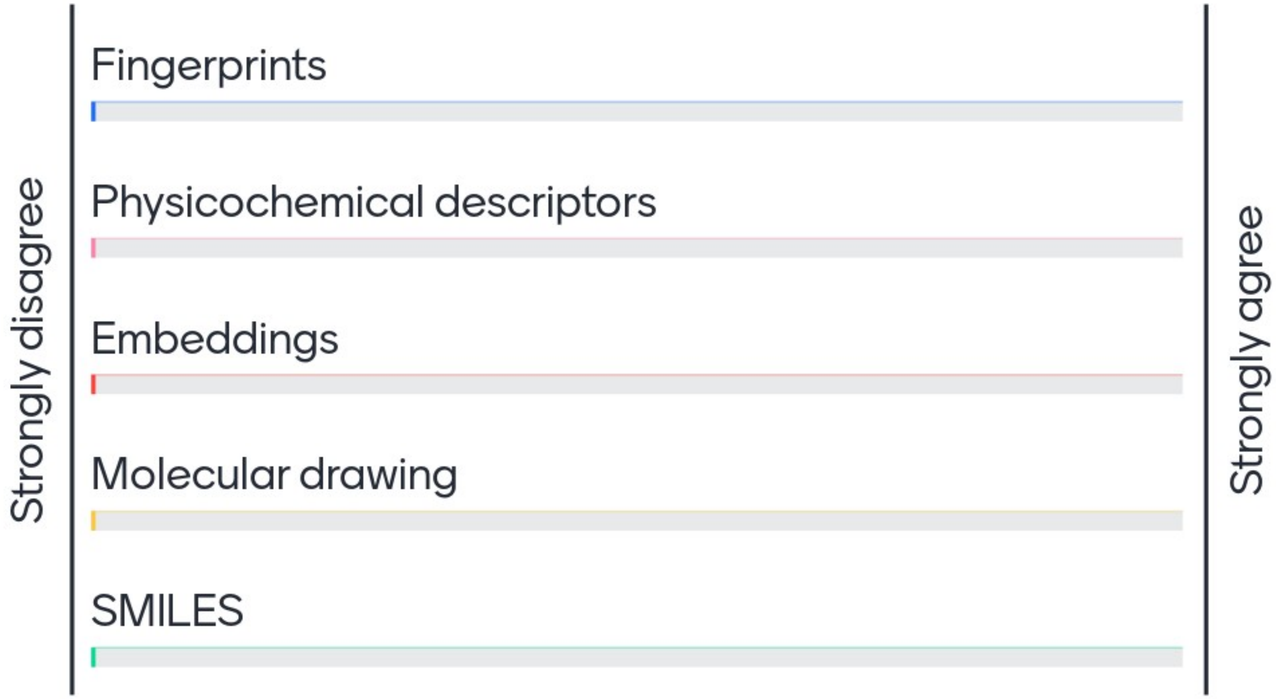
What can I use to describe molecules for ML?



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Which of the following is NOT true about SMILES?

0

It provides a way to represent chemical structures as text strings

0

It can accurately represent 3D structures

0

It is used in cheminformatics databases and tools

0

Different molecules can have more than one valid SMILES representation

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Which databases can I use to find bioassay data?

Waiting for responses ...

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Which physicochemical properties can help me analyse a chemistry dataset?

Waiting for responses

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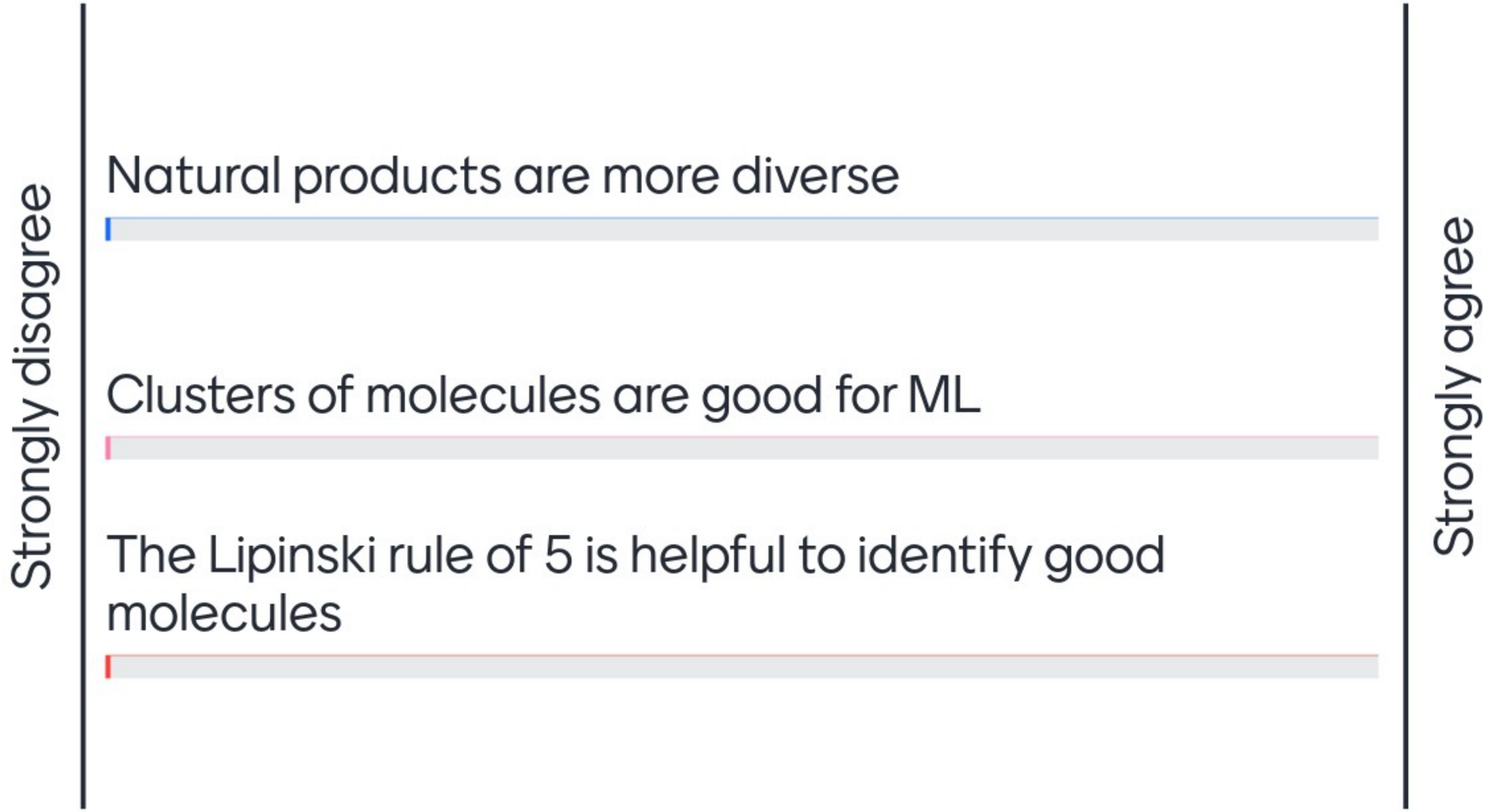
Rate the following...



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How can AI help in our exercise to select candidates?

Waiting for responses ...

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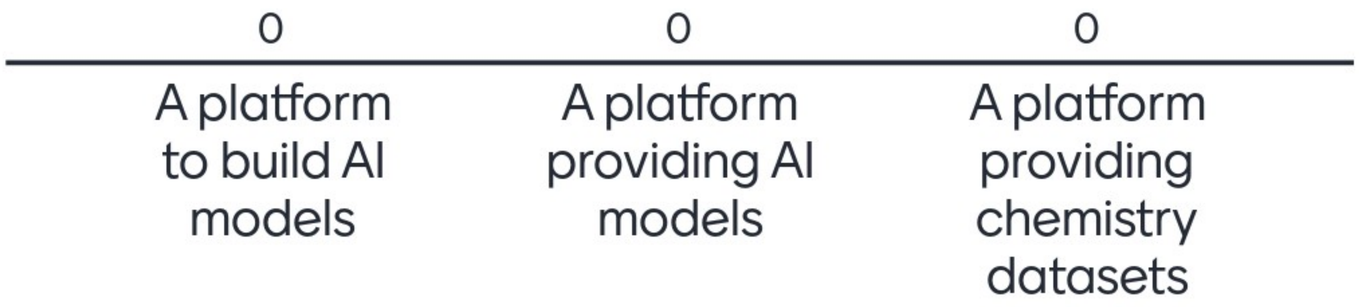
What is the Ersilia Model Hub



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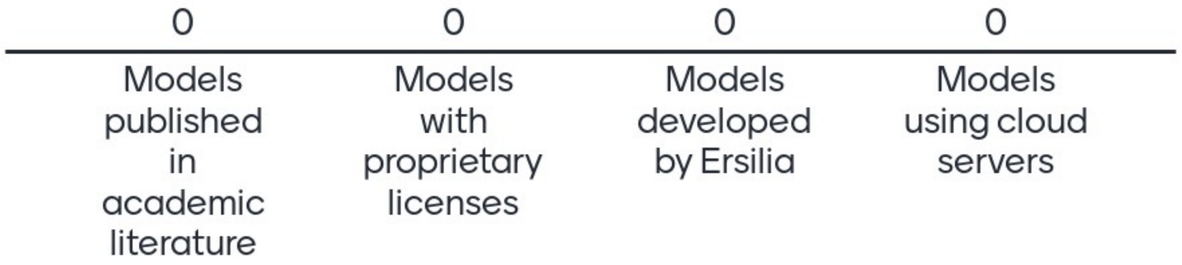
What kind of AI models we find in the Ersilia Model Hub?



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Selected Models from the Ersilia Model Hub!

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Antimalarial models available

Waiting for responses ...

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Antihelmintic models available

Waiting for responses ...

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Antibiotic models available
Waiting for responses

Cytotoxicity models available

Waiting for responses ...

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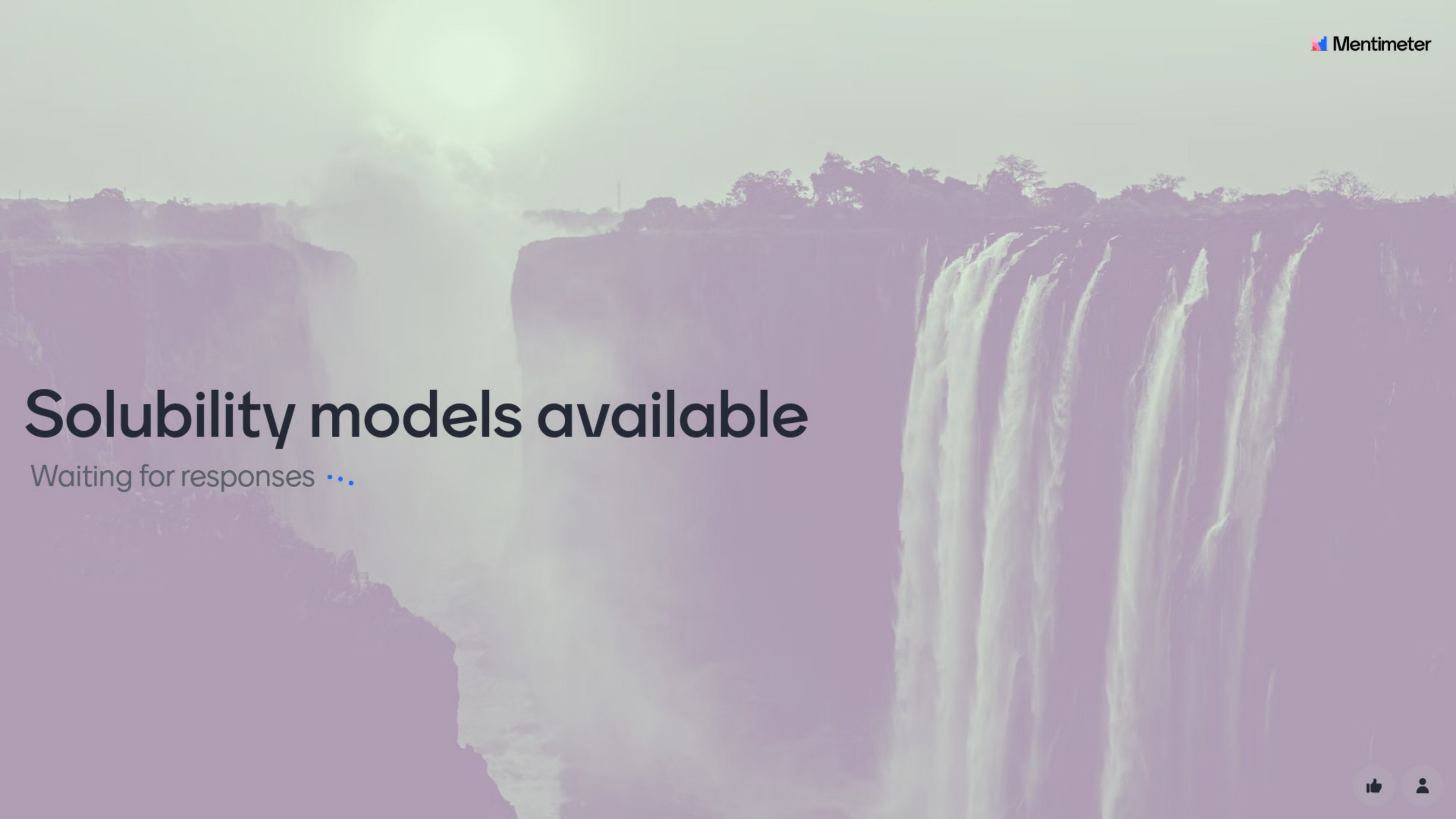
Cardiotoxicity models available
Waiting for responses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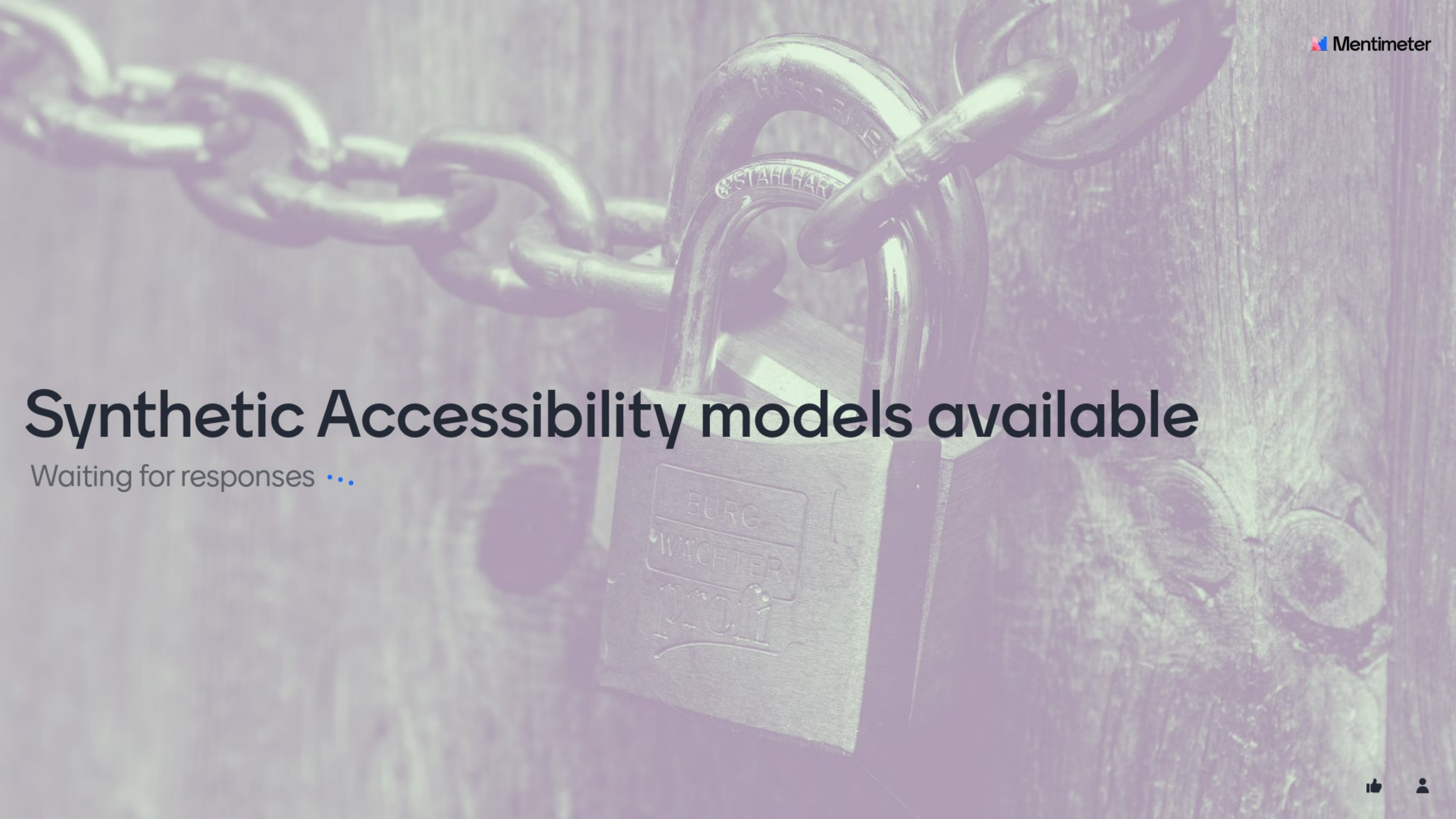
Solubility models available
Waiting for responses



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Synthetic Accessibility models available

Waiting for responses ...

Mentimeter

Natural product scoring models available

Waiting for responses ...