Increasing the adoption of machine learning technologies by chemists with graphical and programmatic interfaces

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@acvaucher

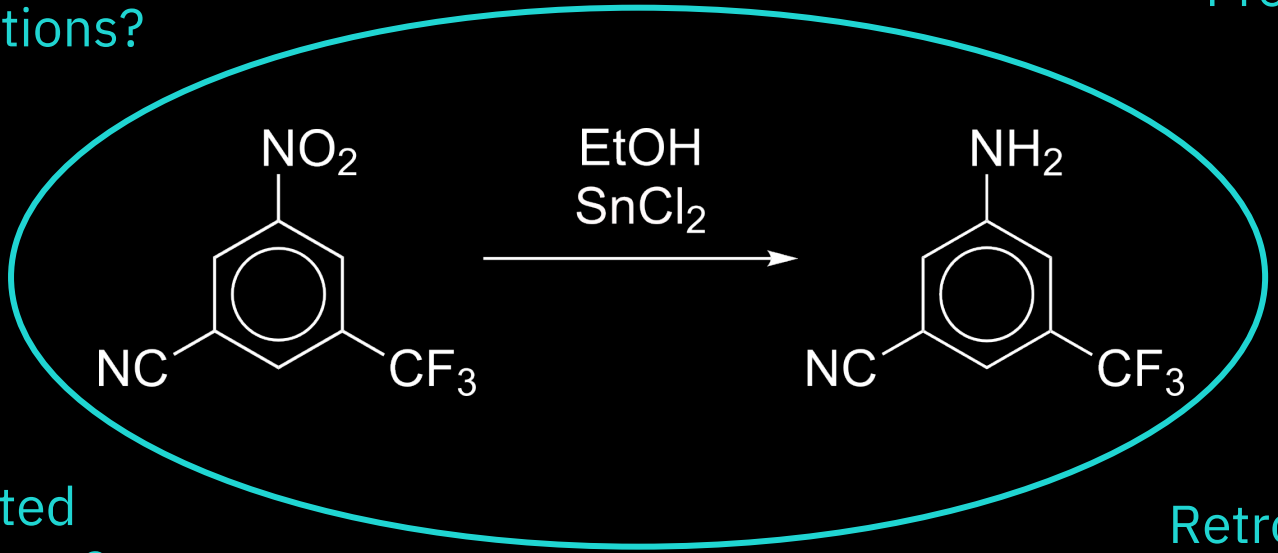
ACS Spring 2023
March 26, 2023

IBM **Research**

AI and chemical reactivity

Experimental conditions?

Product?



Related reactions?

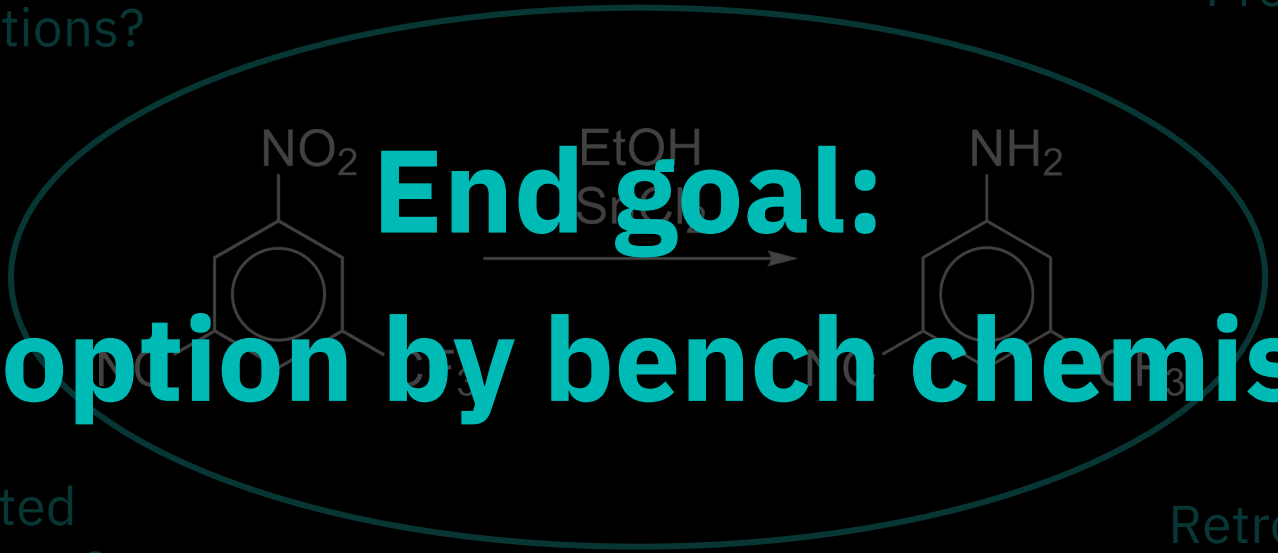
Retrosynthesis?

Yield?

AI and chemical reactivity

Experimental conditions?

Product?



End goal:

Adoption by bench chemists

Related reactions?

Retrosynthesis?

Yield?

Outline

1. AI models for chemistry
2. Building a user interface and API
3. Use cases and special considerations
4. Challenges and outlook

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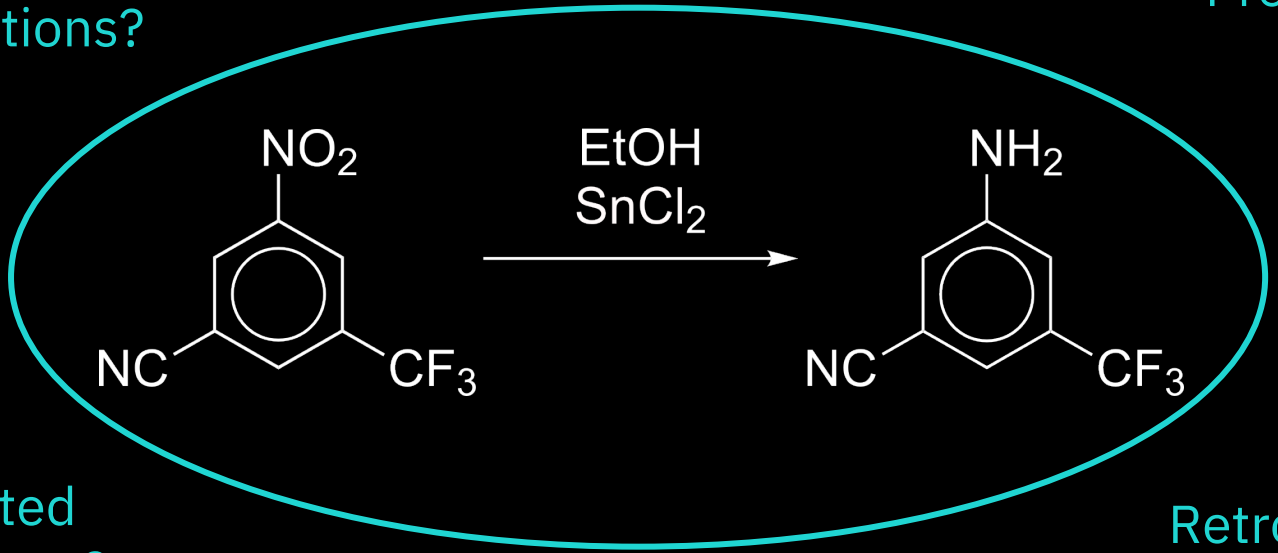
AI and chemical reactivity

Experimental conditions?

Product?

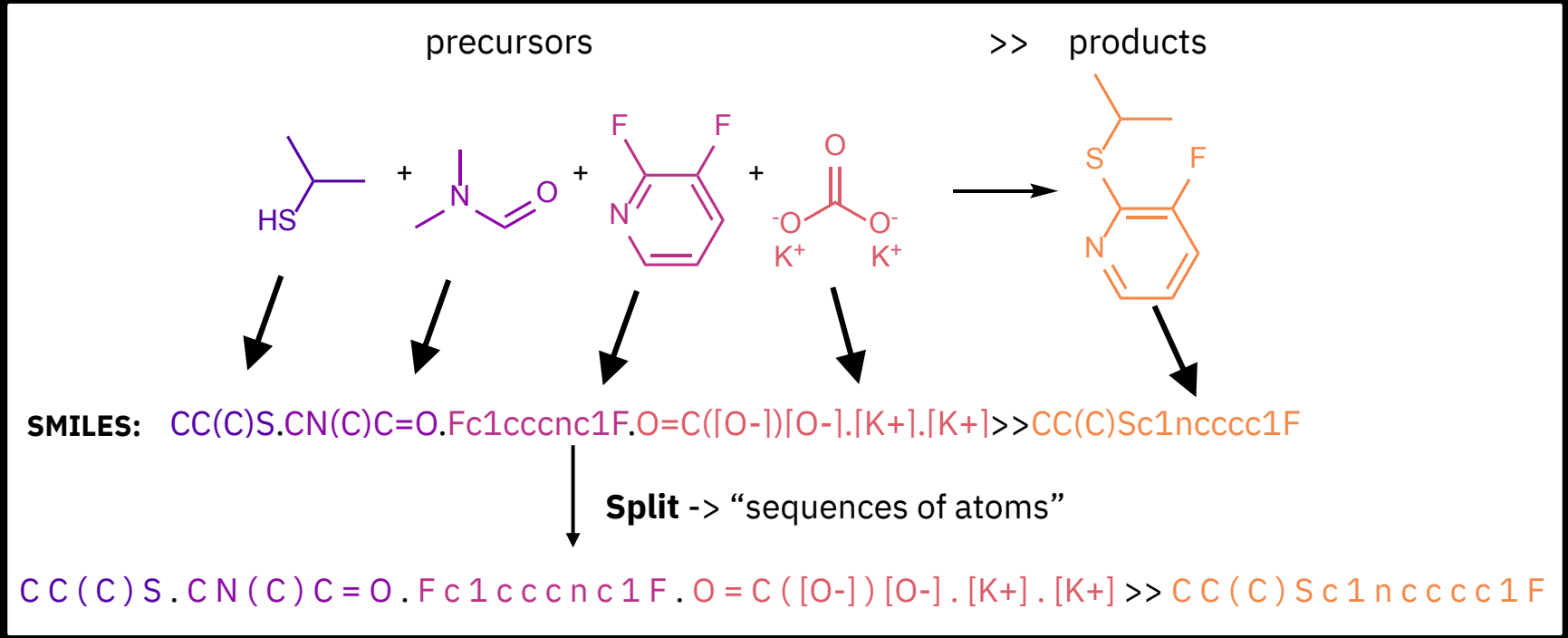


Related reactions?

Retrosynthesis?

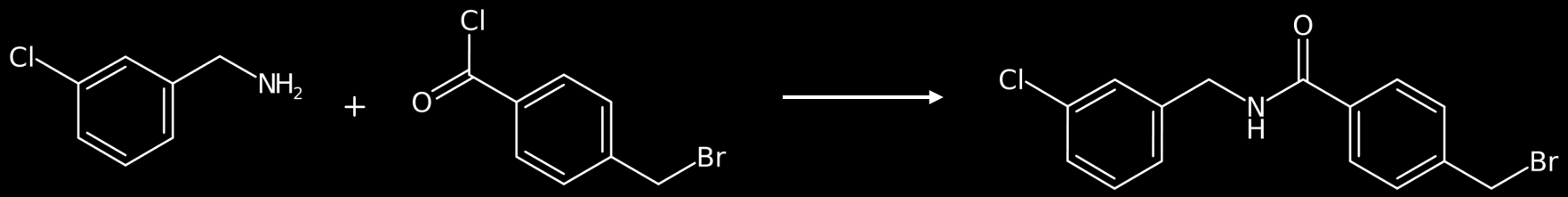
Yield?

Atoms as letters, molecules as words



→ Borrow AI methods developed for human languages

Reaction prediction



Textual representation (SMILES)

NCc1cccc(Cl)c1 O=C(Cl)c1ccc(CBr)cc1 O=C(NCc1cccc(Cl)c1)c1ccc(CBr)cc1

“Sentence of atoms”

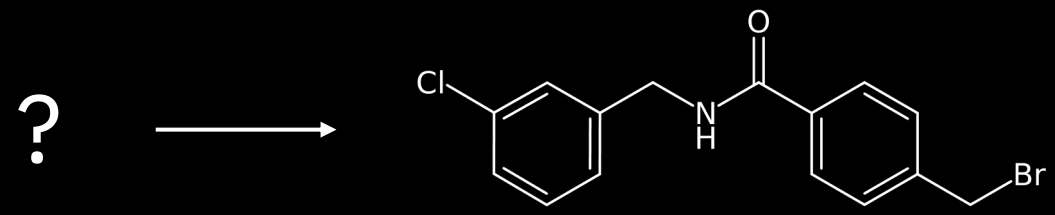
“Translation”

N C c 1 c c c c (Cl) c 1 . O = C (Cl) c 1 c c c (C Br) c c 1 → O = C (N C c 1 c c c c (Cl) c 1) c 1 c c c (C Br) c c 1

Molecular Transformer

Schwaller, P.; Laino, T.; Gaudin, T.; Bolgar, P.; Hunter, C. A.; Bekas, C. & Lee, A. A., *ACS Cent. Sci.*, **2019**, *5*, 1572-1583.

Retrosynthetic analysis

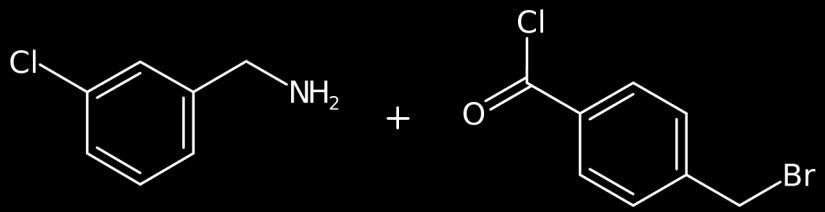


Similar approach, both sides switched

“Translation”

`O = C ( N C c 1 c c c c ( Cl ) c 1 ) c 1 c c c ( C Br ) c c 1` ⟹ `N C c 1 c c c c ( Cl ) c 1 . O = C ( Cl ) c 1 c c c ( C Br ) c c 1`

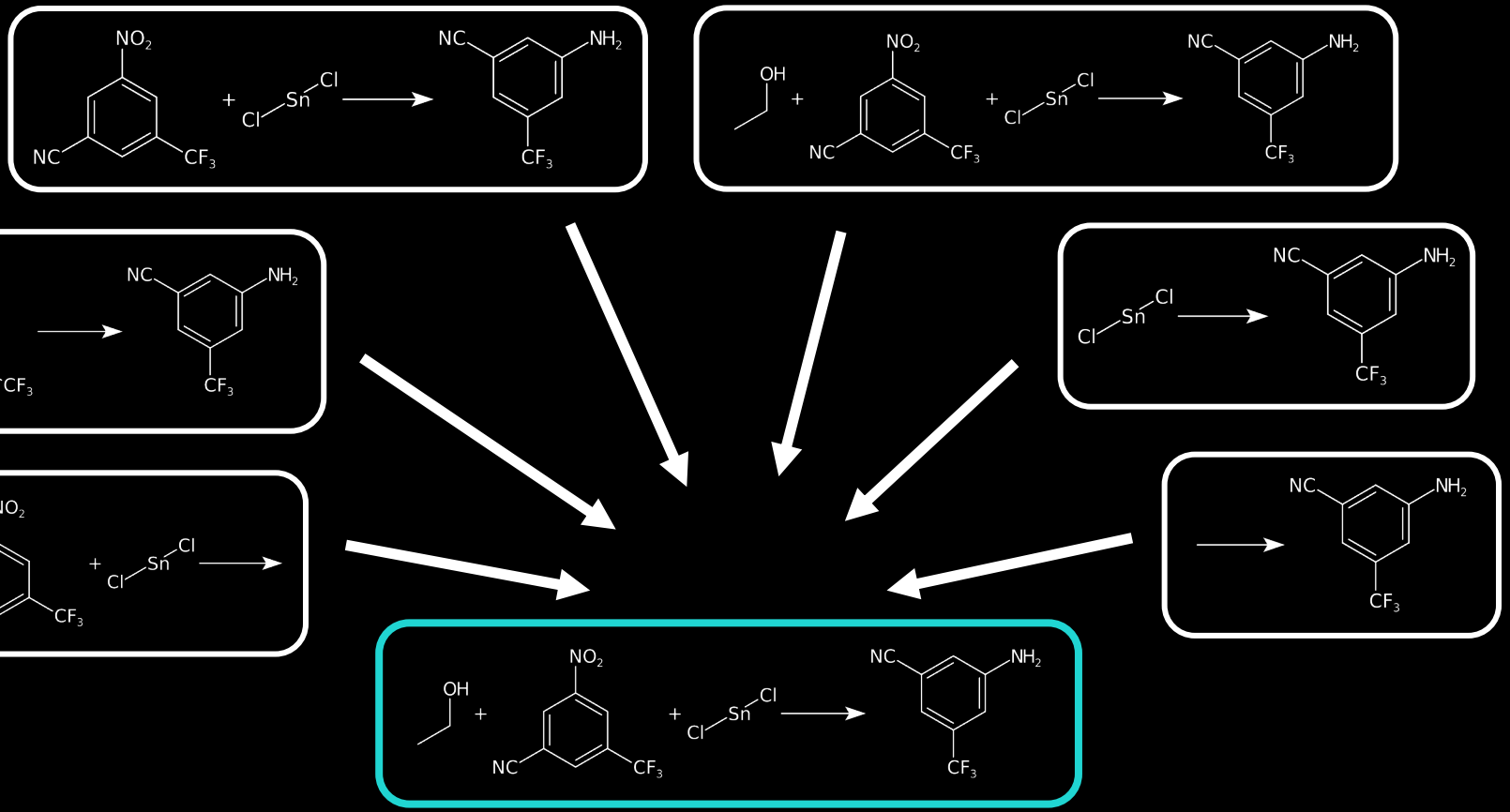
Transformer



Schwaller, P.; Petraglia, R.; Zullo, V.; Nair, V. H.; Haeuselmann, R. A.; Pisoni, R.; Bekas, C.; Iuliano, A. & Laino, T., *Chem. Sci.*, **2020**, *11*, 3316-3325.

Completing partial chemical equations

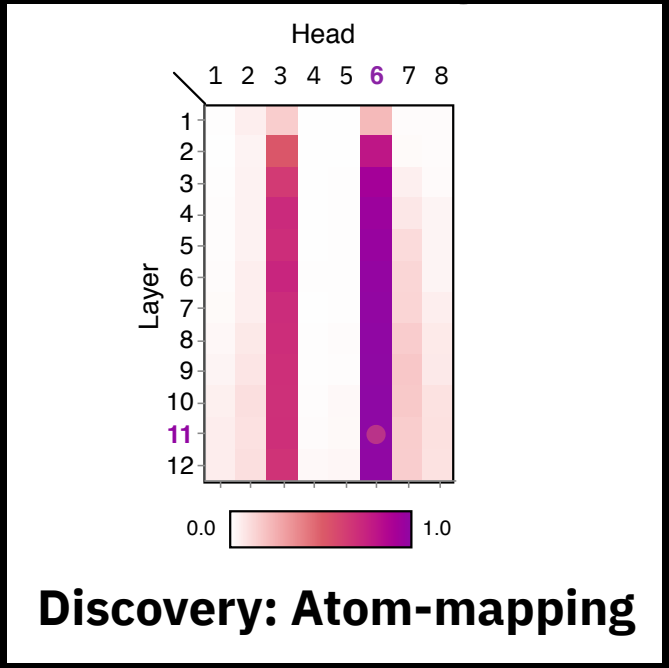
Example 3/5



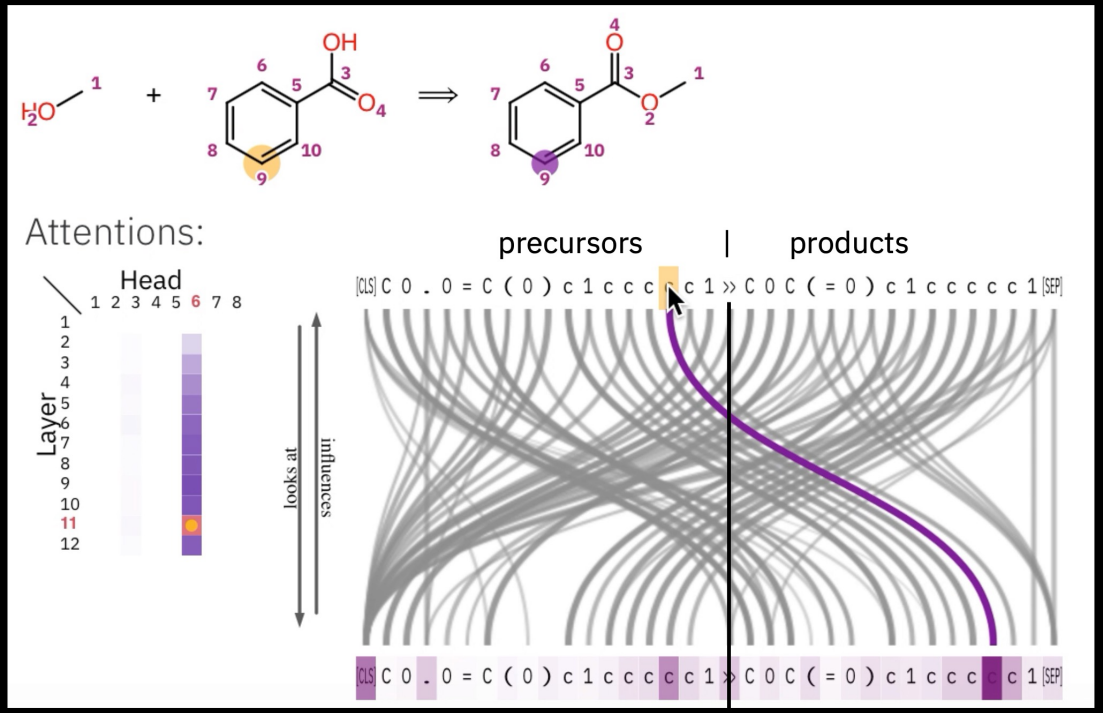
Vaucher, A. C.; Schwaller, P. & Laino, T., Chemrxiv.13273310, **2020**.

Atom mapping: RXNMapper

Example 4/5



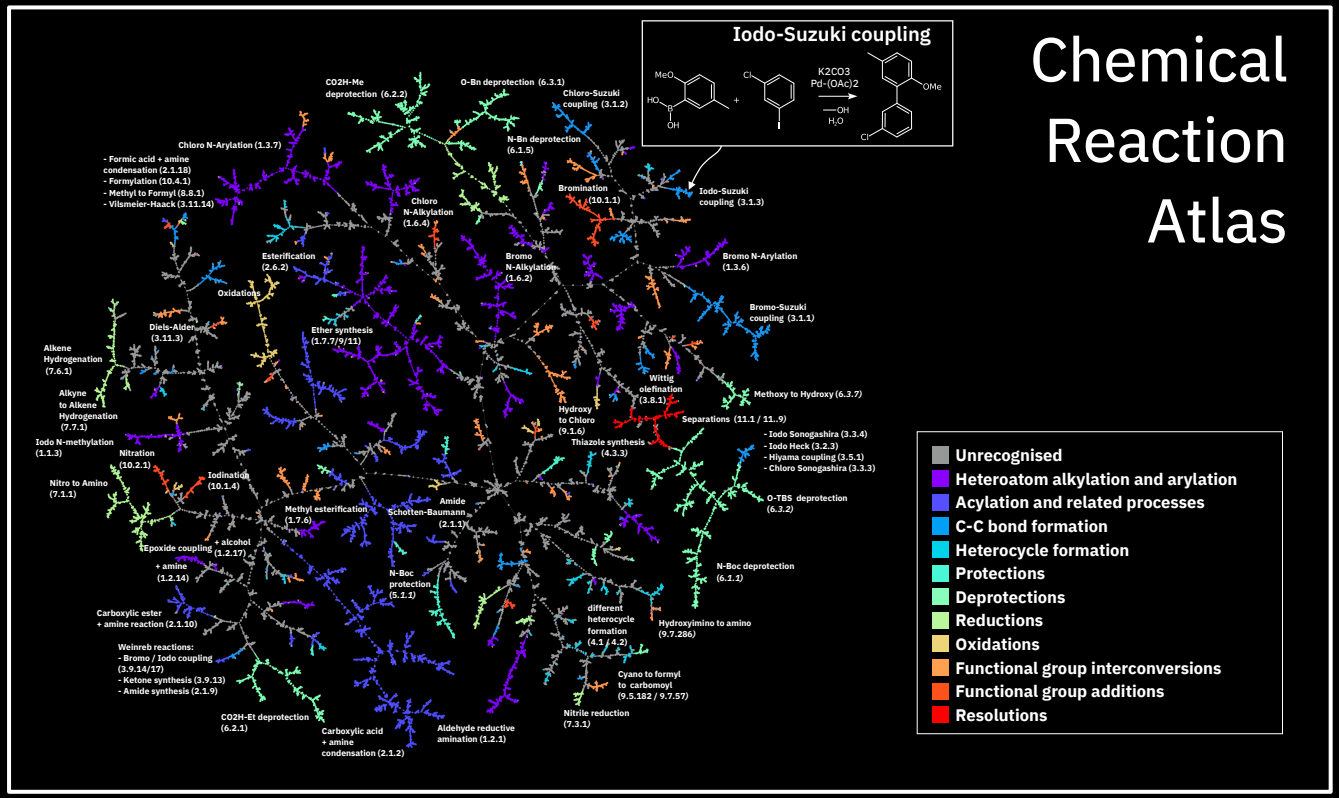
Discovery: Atom-mapping



Schwaller, P.; Hoover, B.; Reymond, J.-L.; Strobelt, H. & Laino, T., *Sci. Adv.*, **2021**, *7*, eabe4166.

Classifying and mapping reactions

Example 5/5



Schwaller, P.; Probst, D.; Vaucher, A. C.; Nair, V. H.; Kreutter, D.; Laino, T. & Reymond, J.-L., *Nat. Mach. Intell.*, **2021**, *3*, 144-152.

Outline

1. AI models for chemistry
2. Building a user interface and API
3. Use cases and special considerations
4. Challenges and outlook

Why provide interfaces to users?

- New applications of AI to chemistry every week
- Accessibility and reproducibility often limited

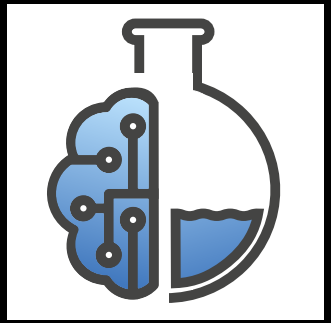
Model availability:

- Not available or limited availability (often)
- Open-source (often)
  - Easy to use?
  - Reproducible results?
- Web service (rare)

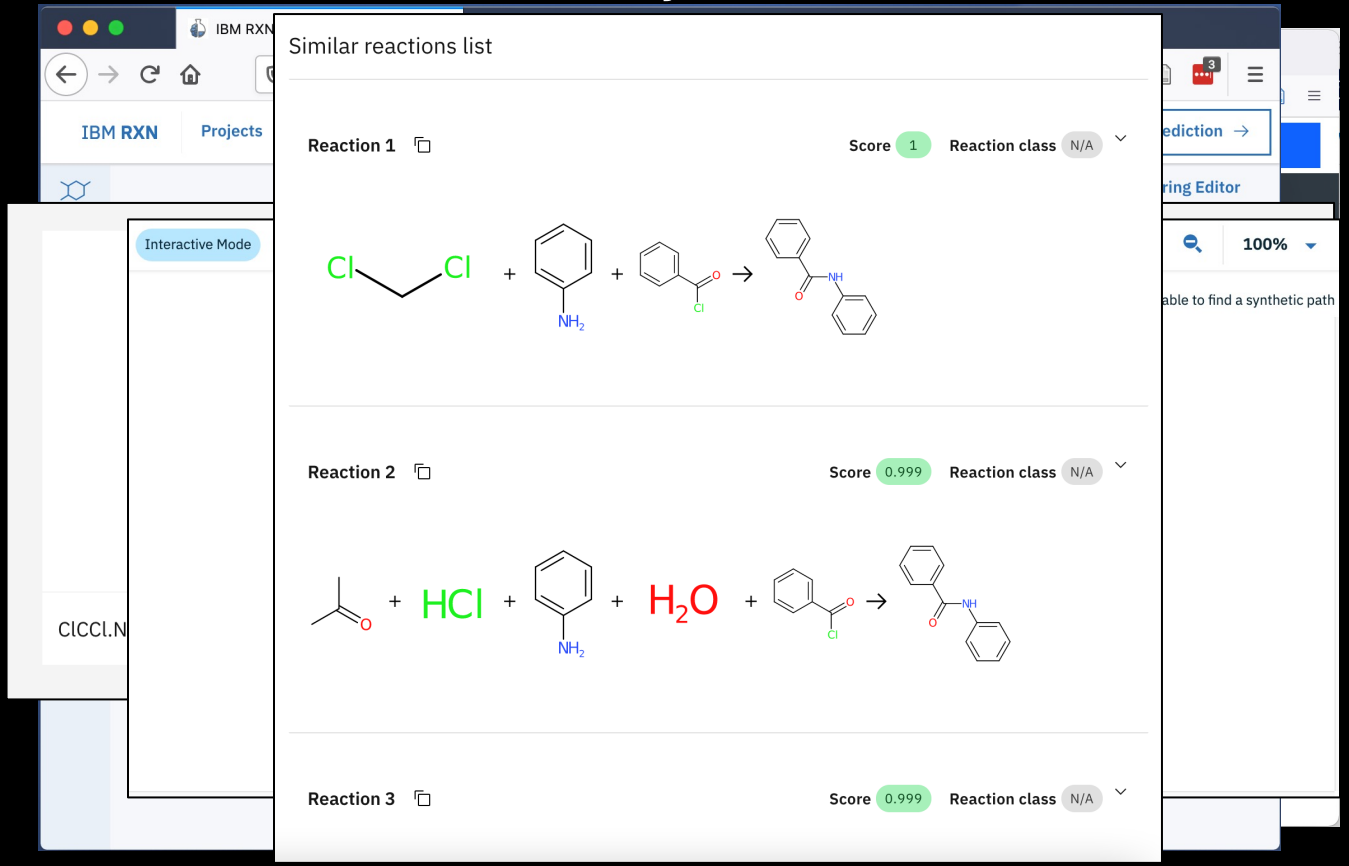
Consequence: limited use by the target audience (bench chemists)

User interfaces

- Challenges to make models more accessible:
  - Requires time
  - Requires expertise
- Starting in 2018: IBM RXN for chemistry



IBM RXN for chemistry



Freely available web platform

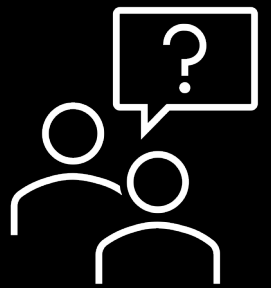
rxn.res.ibm.com

IBM RXN for chemistry

- Positive reception by the community

- At the beginning, limited to:
  - Use via web browser
  - Reaction outcome prediction model

- Quite soon, a user: “Can I access the API?”



Going beyond a user interface

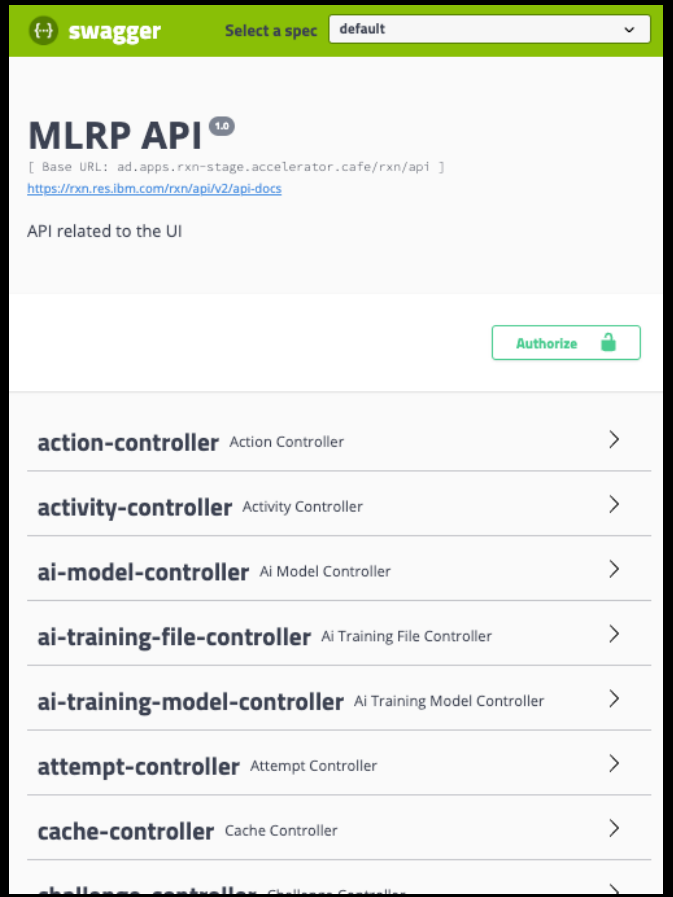
- User interface not always enough:
  - Automated predictions
  - Composability & modularity
  - Integration in other workflows
  - …

→ application programming interface (API)

IBM RXN API

- Same endpoints as for UI
- Direct use: not straightforward (authentication, etc.)

→ Python package for API wrapper



API wrapper on GitHub:
github.com/rxn4chemistry/rxn4chemistry

Launcher | rxn4chemistry_tour.ipynb

Markdown | Python 3 (ipykernel)

Running a reaction prediction is as simple as:

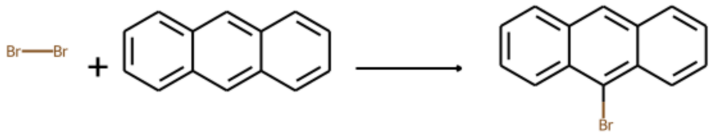
[5]:
```
predict_reaction_response = rxn4chemistry_wrapper.predict_reaction(
    'BrBr.c1ccc2cc3ccccc3cc2c1'
)
```

NOTE: we have set limitations on the number of calls per second and per minute in the public version of RXN for Chemistry. These limits can be tweaked or removed in on-premise deployments. Those limitations are currently set to 5 calls per minute, in most cases this is not a problematic limitation.

[6]:
```
predict_reaction_results = rxn4chemistry_wrapper.get_predict_reaction_results(
    predict_reaction_response['prediction_id']
)
```

[7]:
```
get_reaction_from_smiles(predict_reaction_results['response']['payload']['attempts'][0]['smiles'])
```

[7]:



It is possible to run reaction prediction in batches (not storing the information in any project) to use the service in a highthroughput fashion:

[8]:
```
predict_rection_batch_response = rxn4chemistry_wrapper.predict_reaction_batch(
```

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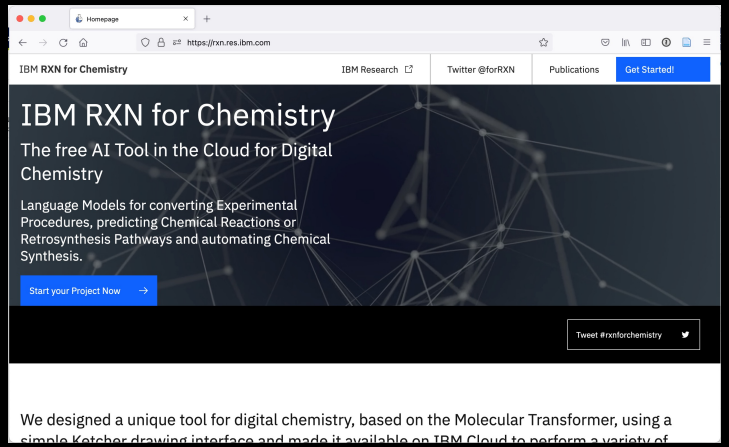
Current status

rxn.res.ibm.com



github.com/rxn4chemistry/rxn4chemistry

Status early 2023:
~35k registered users
~9M predictions

Use cases of IBM RXN

Chemical synthesis

Chemical reactivity screening

Education

... and others !

Use cases of IBM RXN

Chemical synthesis

Chemical reactivity screening

Education

... and others !

Use cases of IBM RXN

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Chemical reactivity screening

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... and others !

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Special considerations

Data confidentiality

User feedback

Concept of users and projects

Symmetry UI-API

Special considerations

Data confidentiality

User feedback

Concept of users and projects

Symmetry UI-API

Special considerations

Data confidentiality

→ Portability is important

back

and projects

UI-API

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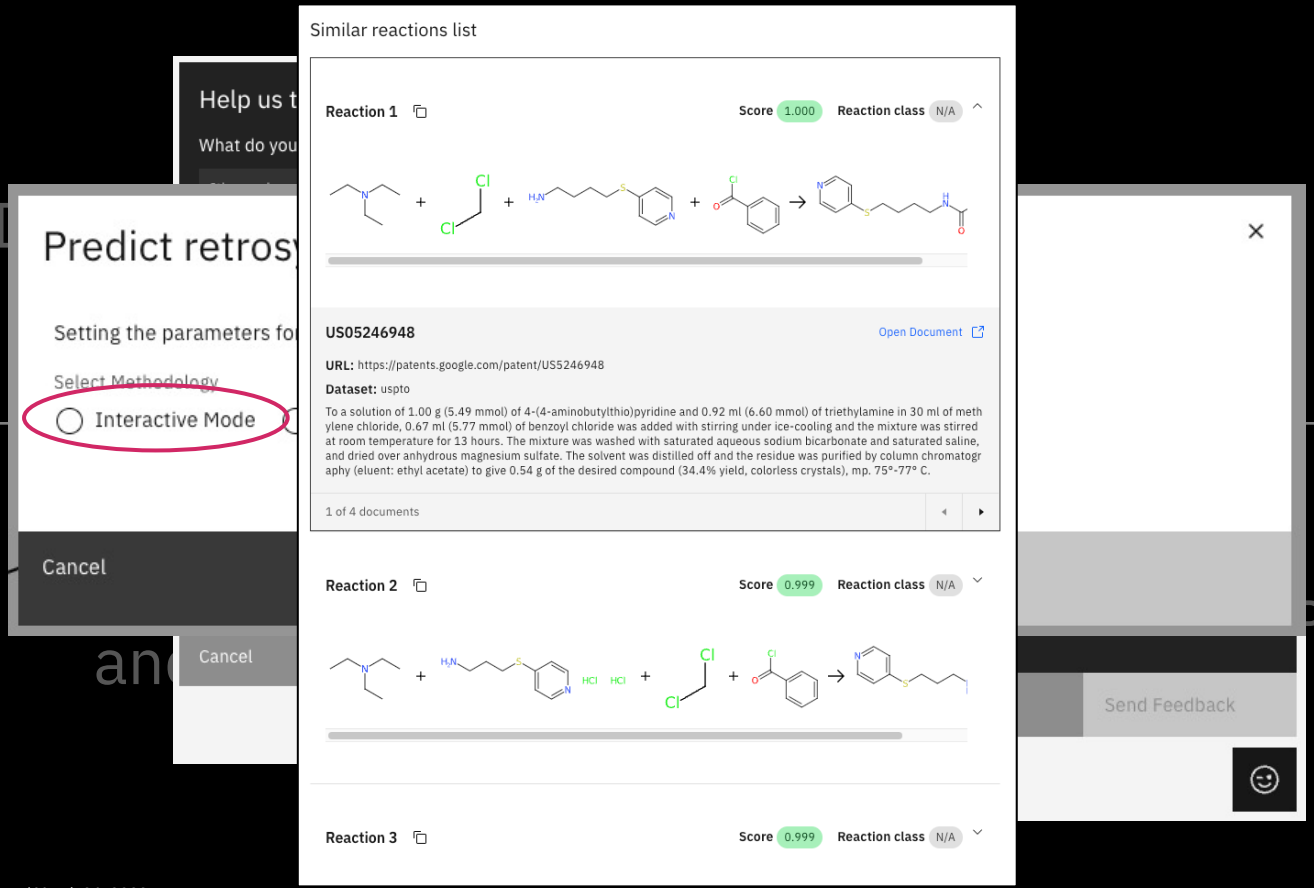

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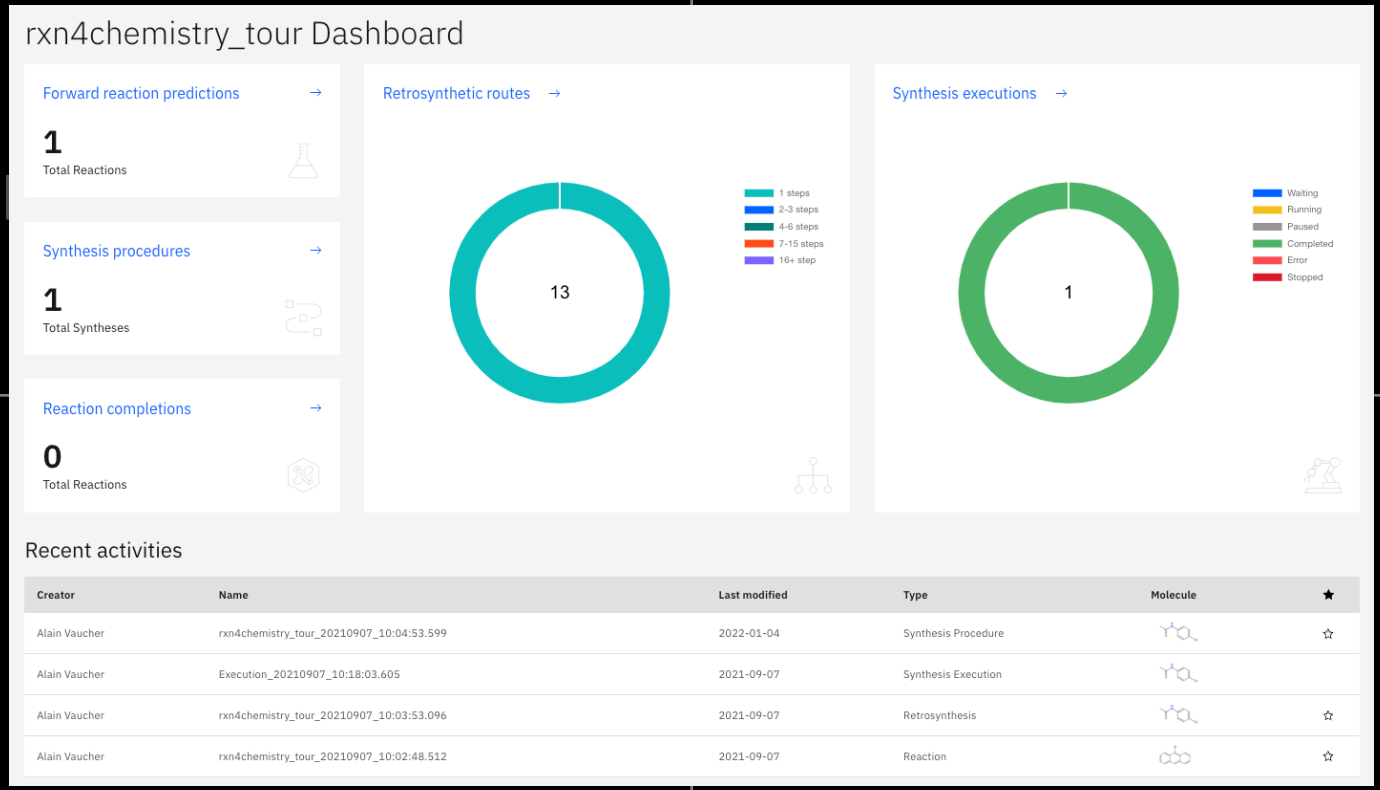

Special considerations

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Concept of users and projects

Symmetry UI-API

Special considerations

Project list 14

Search by name

Name	Owner	Creation date	Reactions	Retrosynthetic routes	Synthesis	Reaction completion
reaction completion	Alain Vaucher	2023-02-13	0	0	0	1
[redacted]	Alain Vaucher	2023-02-13	0	0	0	5
[redacted]	Alain Vaucher	2023-02-10	0	0	0	1
[redacted]	Alain Vaucher	2022-02-24	0	3	0	0
[redacted]	Alain Vaucher	2022-02-17	0	35	18	0
[redacted]	Alain Vaucher	2021-11-30	0	1	0	0
[redacted]	Chiara Faralli	2021-10-19	13	137	19	0
[redacted]	Alain Vaucher	2021-10-13	1	14	1	0
[redacted]	Alain Vaucher	2021-09-08	1	0	0	0
[redacted]	Alain Vaucher	2021-09-07	1	13	1	0
[redacted]	Chiara Faralli	2020-10-21	0	16	15	0
[redacted]	Alain Vaucher	2020-09-28	0	7	3	0
[redacted]	Chiara Faralli	2020-06-15	6	4	1	0
[redacted]	Alain Vaucher	2020-06-11	42	171	42	13

Items per page: 20 | 1-14 of 14 items | 1 of 1 page

Projects

```
[26]: projects_response = rxn4chemistry_wrapper.list_all_projects()
      projects = projects_response["response"]["payload"]["content"]

[27]: print(len(projects))
```

```
14
```

```
[28]: from pprint import pprint
      pprint(projects[-1])
```

```
{'attempts': [],
 'computedFields': {},
 'createdBy': '6eec3679-b8de-40e2-b73e-0dcd1b9ccf1c',
 'createdOn': 1676273811483,
 'description': None,
 'embed': {},
 'id': '63e9e89350f97b001f83c766',
 'isFavorite': False,
 'metadata': {},
 'modifiedBy': '6eec3679-b8de-40e2-b73e-0dcd1b9ccf1c',
 'modifiedOn': 1676273811483,
 'name': 'reaction completion',
 'visibility': None}
```

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Challenges

Backward compatibility

Cost

API rate limits

Handling of API errors

Challenges

Backward compatibility

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Challenges

Backward comp

Cost

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https://xkcd.com/1172/

Challenges

Backward compatibility

Cost

API rate limits

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Challenges

Backward compatibility

Cost

API rate limits

Handling of API errors

Challenges

Backward compatibility

Cost

```
[7]: predict_reaction_response_1 = rxn4chemistry_wrapper.predict_reaction('BrBr.c1ccc2cc3ccccc3cc2c1')
     predict_reaction_response_2 = rxn4chemistry_wrapper.predict_reaction('BrBr.c1ccc2cc3ccccc3cc2c1CC')

ERROR:rxn4chemistry.response_handler:The service might be overloaded at the moment. Please try again.
ERROR:rxn4chemistry.response_handler:Full response: {"timestamp":1679481031108,"status":429,"error":"T
oo Many Requests","message":"Too many requests","path":"/rxn/api/api/v1/predictions/pr"}
```

API rate limits

Handling of API errors

Challenges

Backward compatibility

Cost

API rate limits

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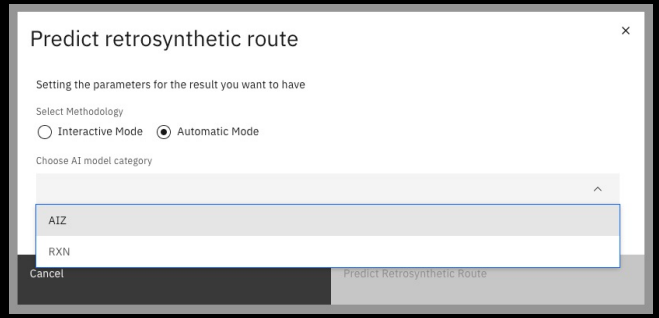
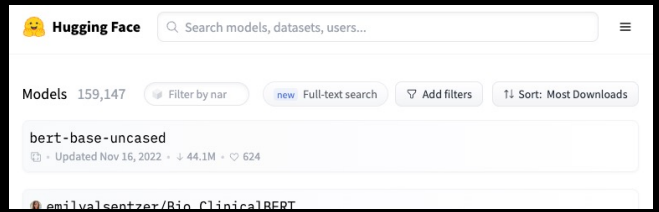
Outlook

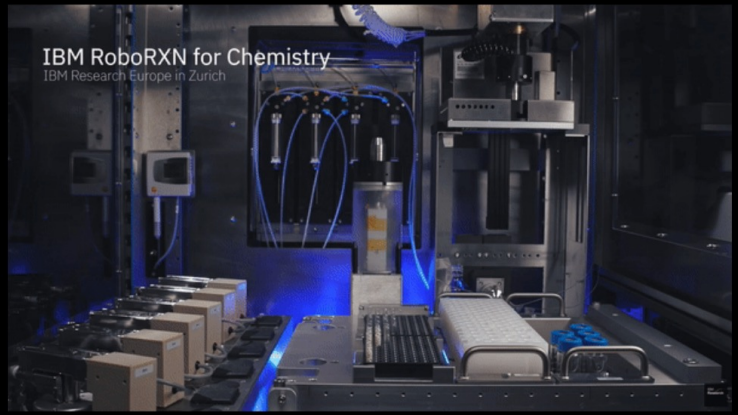
Integration of external models





Steering synthesis robot from the API

```
[5]: synthesis_execution = rxn4chemistry_wrapper.start_synthesis(synthesis_id)
```



Thank you for your attention!

Questions or comments

E-mail: ava@zurich.ibm.com

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Talks by other team members:
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Thank you for your attention!

Questions or comments

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