What’s new in MetaboScape 2024

One integrated solution for processing and interpreting of MS based Phenomics, non-targeted Metabolomics, Lipidomics and MALDI Imaging data

Outline

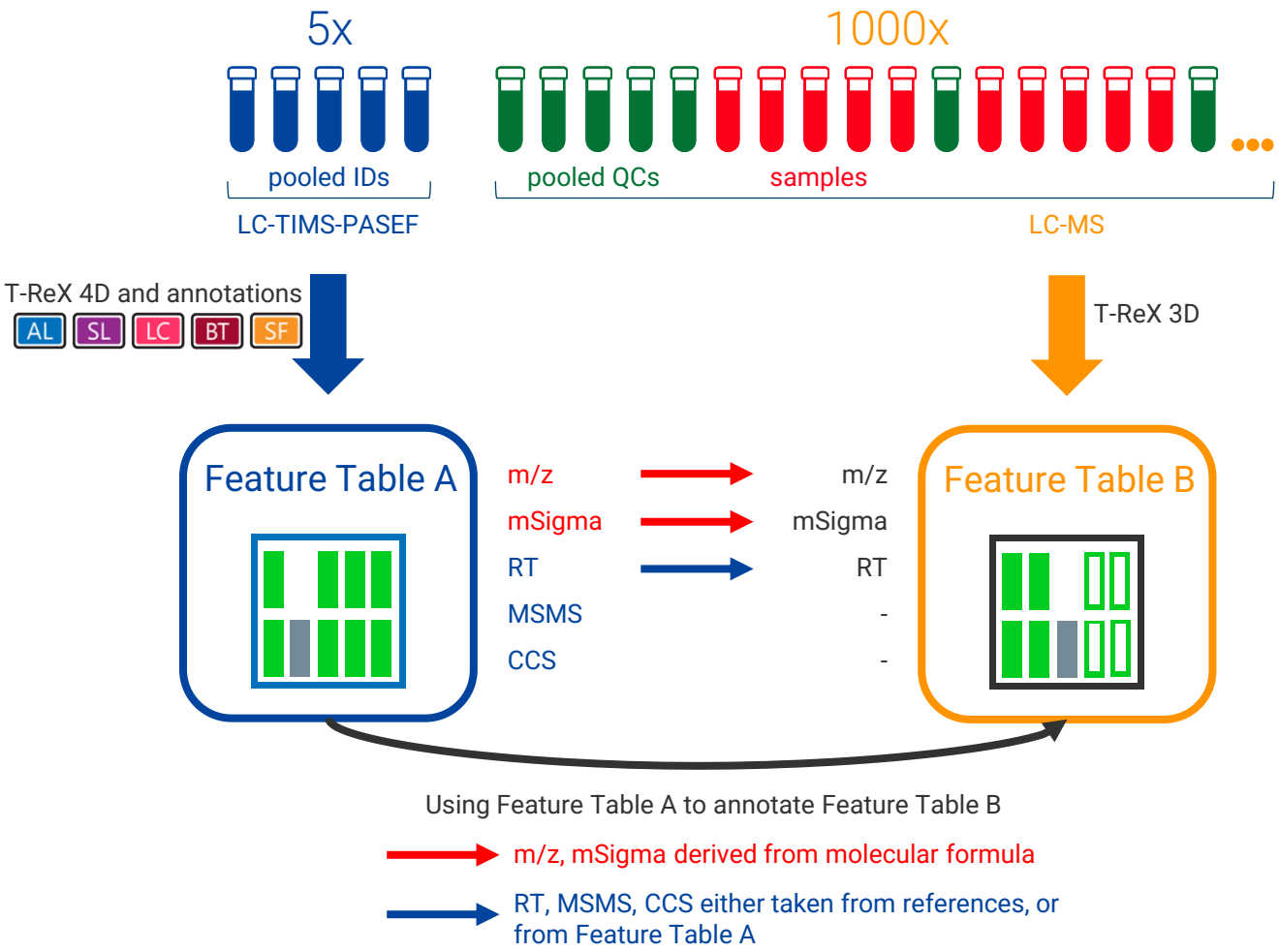
01 Combine Confidence and Speed using the Sample Characterization Workflow

02 Improved Accuracy with CCS-Predict Pro 2024 & Prediction for Single Structures & CCS-Predict via REST API for custom use

03 Use the REST API to create MetaboScape projects from your favourite programming language

04 T-ReX Improvements for even higher quality

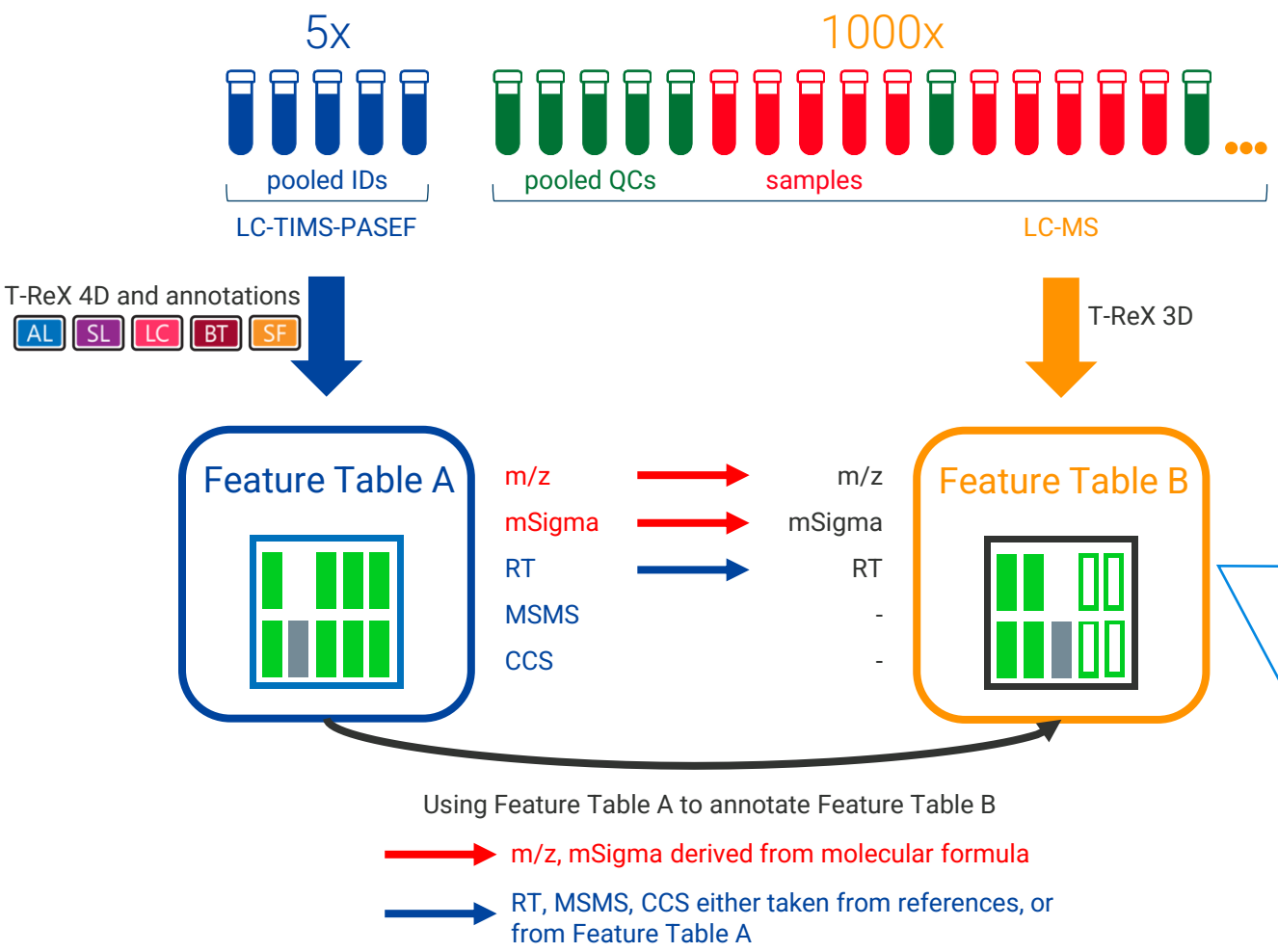
Combine Confidence and Throughput



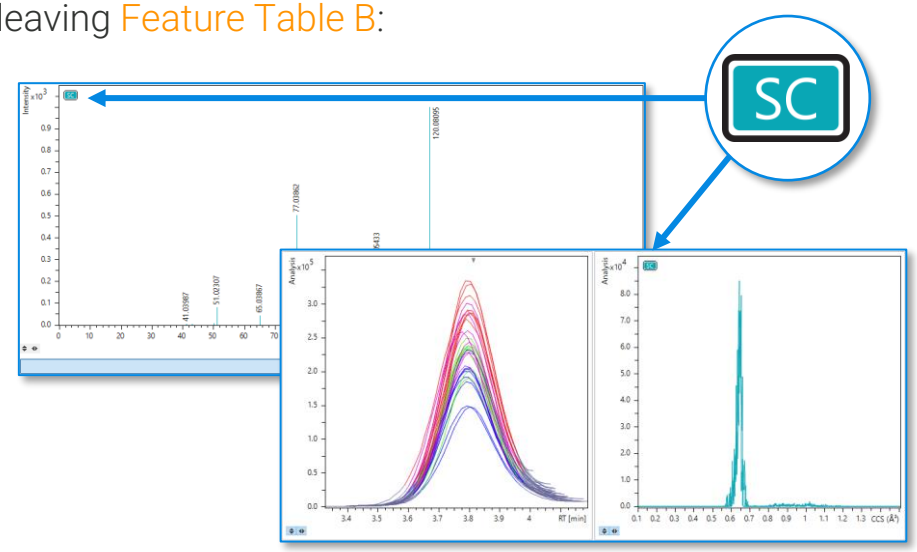
The Sample Characterization Table-based Annotation workflow allows separation of highly confident annotation and highly confident quantitation/high throughput.

- Create a Feature Table A from **pooled samples** acquired with a high-dimensional mode like LC-TIMS-PASEF, for the sake of sample characterization. Use the CCS and MSMS information for highly confident annotation.
- Create a second Feature Table B from **individual samples**, acquired with e.g. LC-MS.
- Use the highly confident annotations from Feature Table A to annotate Feature Table B. This results in annotations in Feature Table B, referencing the CCS and MSMS annotation scores from Feature Table A.

Combine Confidence and Throughput



Review annotation criteria from Feature Table A without leaving Feature Table B:



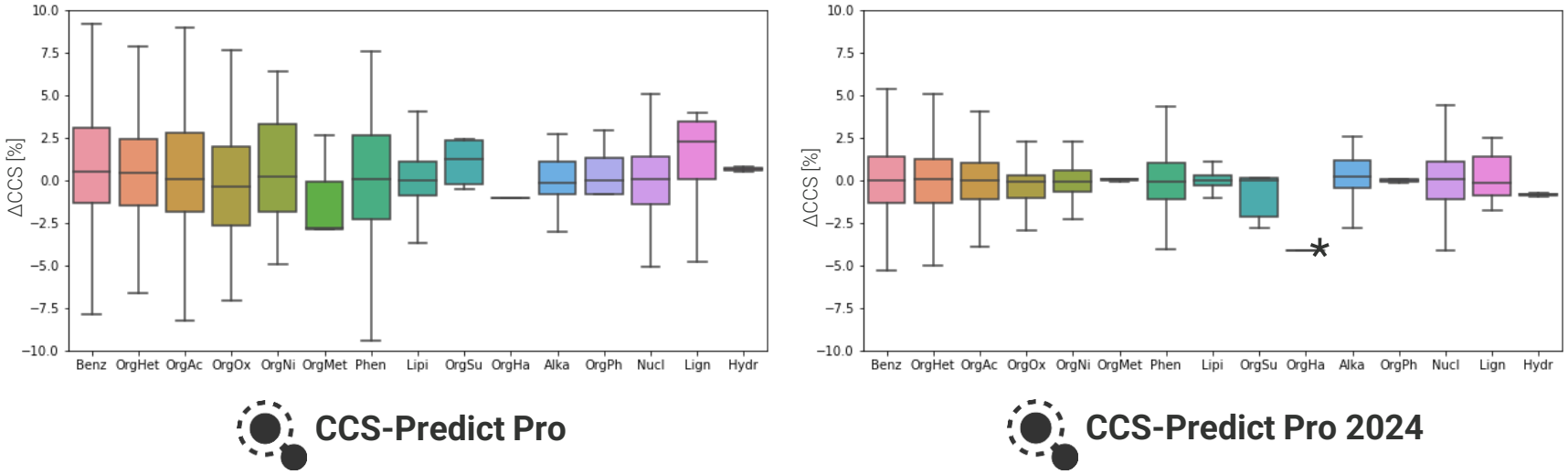
MS/MS spectra, EICs or EIMs that are references to Feature Table A are painted in turquoise and decorated with an SC icon, that allows to quickly navigate to the referenced Feature Table and Feature.

If MS/MS spectra, EICs or EIMs are present in Feature Table B, they will not be overwritten, but displayed as found in Feature Table B.

Annotate with CCS-Predict Pro 2024 confidence!

The CCS-Predict Pro models for [M+H]+, [M-H]-, and [M+Na]+ have been trained with larger reference data sets, which have grown by 90%, 72% and 84% respectively, compared to the previous models.

Class-specific CCS prediction errors for the old and the new CCS-Predict Pro model for [M+H]+. Predictions were matched against references from both, training and test data.



CCS-Predict Pro

CCS-Predict Pro 2024

*Only six reference structures for compound class OrgHa

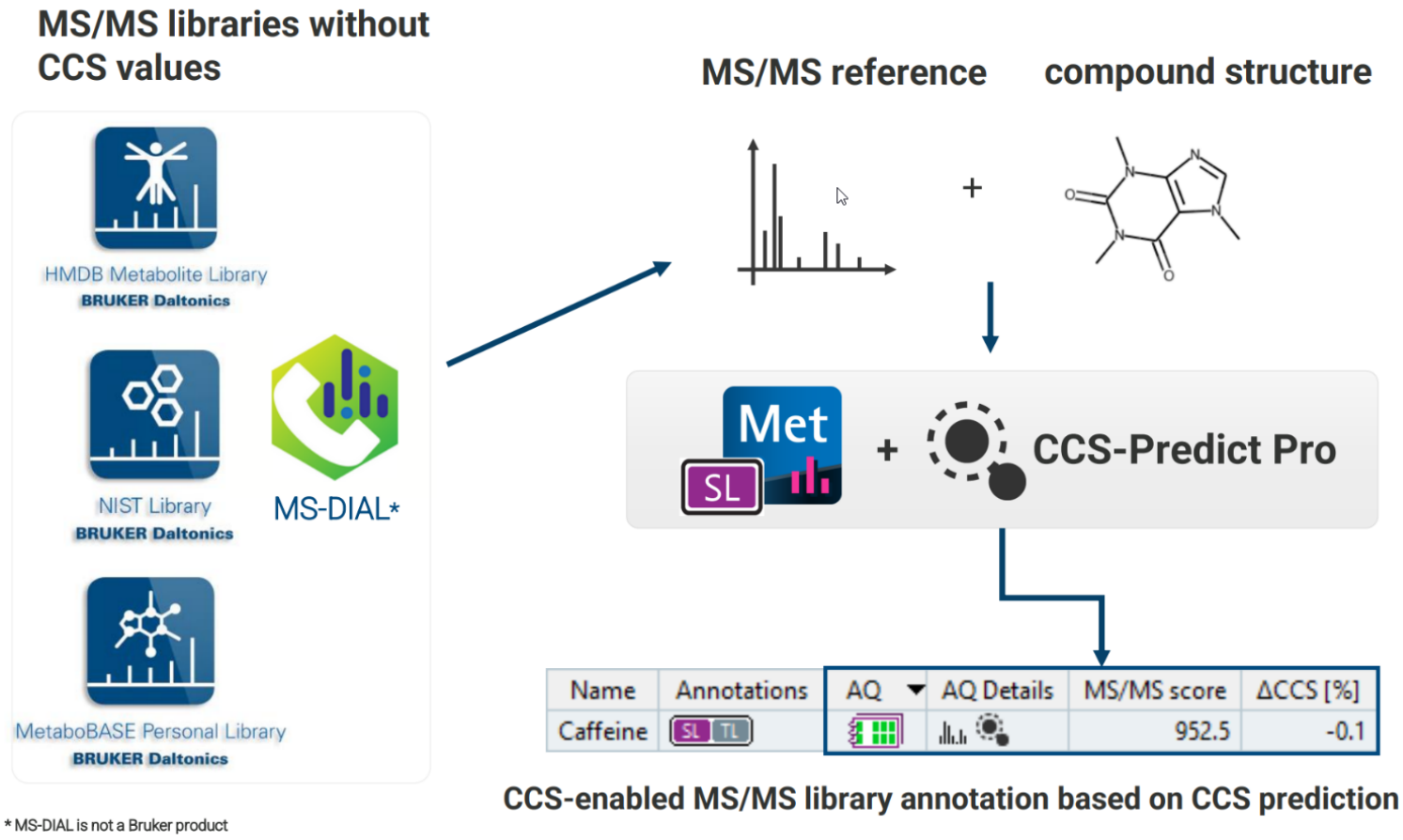
- Improvement in predictive accuracy across all main compound classes
- The three models for [M+H]+, [M+Na]+ and [M-H]- benefit from increased training data.

CCS-Predict Pro 2024 fully integrated into your workflow

MetaboScape CCS-enables annotation with

- TL **Target List**
- SL **Spectral Library**
- BT **Biotransformer**

if structural information is available



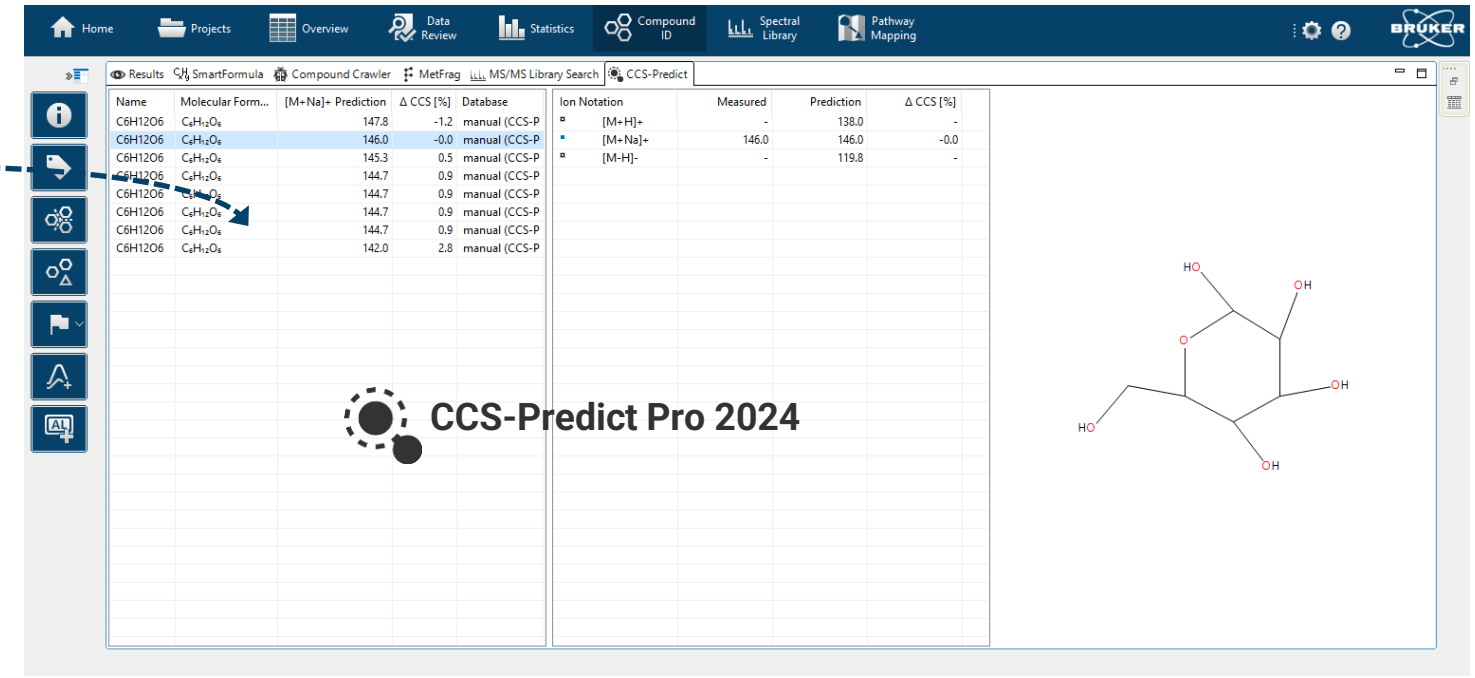
CCS-enabled MS/MS library annotation based on CCS prediction

* MS-DIAL is not a Bruker product

Try it out!
Easy CCS-Predict with drag-and-drop

In addition to the integration into automated workflows, MetaboScape's CCS-Predict in the Compound ID perspective allows to predict CCS values for structures via drag-and-drop. Choose from the CCS-Predict Pro 2024 and the CCS-Predict 4D-Lipidomics™ model.

InChI=1S/C6H12O6/c7-2-6(11)5(10)4(9)3(8)1-12-6/h3-5,7-11H,1-2H2/t3-,4+,5-,6+/m0/s1
InChI=1S/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3+,4+,5-,6+/m1/s1
InChI=1S/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4-,5-,6?/m0/s1
InChI=1S/C6H12O6/c7-1-3-4(9)5(10)6(11,2-8)12-3/h3-5,7-11H,1-2H2/t3-,4-,5+,6-/m1/s1
InChI=1S/C6H12O6/c7-1-2(8)4(10)6(12)5(11)3(1)9/h1-12H/t1-,2-,3-,4+,5-,6+
InChI=1S/C6H12O6/c7-1-3-4(9)5(10)6(11,2-8)12-3/h3-5,7-11H,1-2H2/t3-,4-,5+,6-/m1/s1
InChI=1S/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1
InChI=1S/C6H12O6/c7-1-3(9)5(11)6(12)4(10)2-8/h3,5-9,11-12H,1-2H2/t3-,5+,6-/m1/s1
InChI=1S/C6H12O6/c7-1-2(8)4(10)6(12)5(11)3(1)9/h1-12H/t1-,2-,3-,4+,5-,6+
InChI=1S/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6?/m1/s1



Drag and drop into CCS-Predict:

InChI text

SMILES text

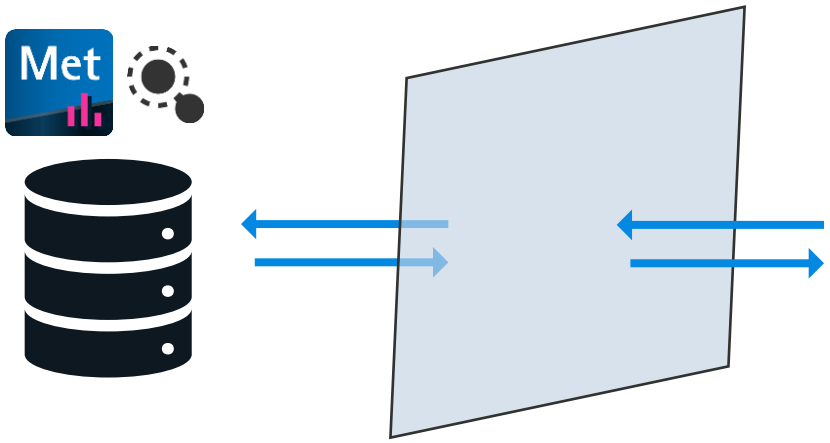
.mol file

.sdf file

Use CCS-Predict Pro in your own code

MetaboScape's CCS-Predict models now are accessible via the REST API via new endpoints.

GET	/ccspredict/models
POST	/ccspredict/models/{modelId}



MetaboScape server

REST interface

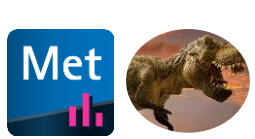
Your code (for example with python):

```
models = ccspredict.list_ccs_predict_models()
...

structure = metaboscape_client.Structure("SMILES","CC(C)C(CCCN(C)CCC1=CC(=C(C=C1)OC)OC)(C#N)C2=CC(=C(C=C2)OC)OC")
ion_predictions = ccspredict.predict_ccs("CCS-Predict_Pro_2024", body=structure)
for ion in ion_predictions:
    print(ion.ion_notation,': ',ion.predicted_ccs)

[M+H]+ :  206.58969106016252
[M-H]- :  222.53750677292976
[M+Na]+ :  226.36295962368797

structure = metaboscape_client.Structure("INCHI","InChI=1S/C27H38N2O4/c1-20(2)27(19-28,22-10-12-24(31-5)26(18-22)33
ion_predictions = ccspredict.predict_ccs("CCS-Predict_Pro_2024", body=structure)
for ion in ion_predictions:
    print(ion.ion_notation,': ',ion.predicted_ccs)

[M+H]+ :  206.58969106022255
[M-H]- :  222.5375067728079
[M+Na]+ :  226.36295962364431
```

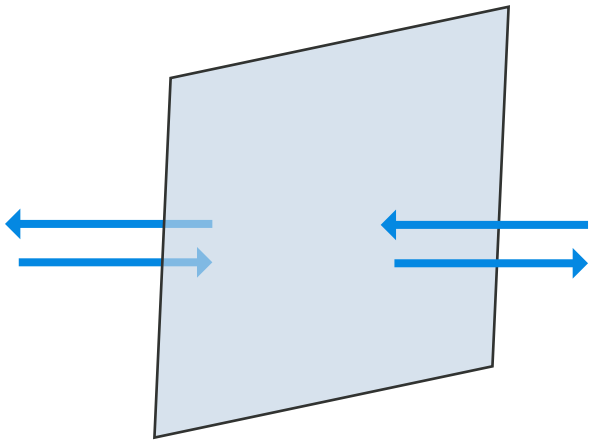
Connect your Lab to MetaboScape

Connect your data repository to MetaboScape with custom code, using the REST API.

POST /projects/create	GET /projects/taskstatus
POST /experiments/create	
POST /featuretable/create	



MetaboScape server



REST interface

Your code (for example with python):

```
project_yaml = Path("...\yourProjectDefinition.yaml").read_text()
projects_api = metaboscape_client.ProjectsApi(api_client)
response = projects_api.create_project(project_file=project_yaml)
```

```
...
```

```
projects_api.get_task_status(response.workflow_task_id)
```

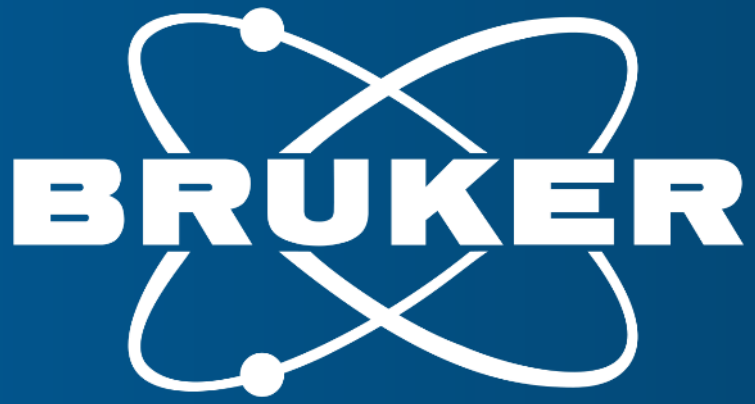
```
{'status': 'Running',
 'task_infos': [{'name': 'Processing',
                 'progress_value': 19.0,
                 'status': 'Running',
                 'task_id': '56391dcc-92d4-4a70-a7c0-c7576dcd4f16'},
                {'name': 'Target List',
                 'progress_value': 0.0,
```

Project Definition .yaml

Your repository

Improved Feature Finding Workflow

- Improved retention time alignment
- Improved merging of MSMS spectral peaks across scans
- Improved determination of peak start and end in T-ReX 3D
- If required, use calibration results created with Data Analysis



Innovation with Integrity