Development of New data analysis platform for medicinal chemists in Daiichi Sankyo

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Introduction

From 2018, Daiichi Sankyo has built new cheminformatics team and designed Data Driven Drug Discovery (D4) group engaged in close interactions with other groups participating in the DMTA cycle[1].
And we found that SAR visualization is one of the important task of D4.
Recently there are lots of tools for SAR analysis not only commercial packages. However, there are few tools can offer flexible SAR analysis environments for user and support idea sharing. To overcome the issue, we built new data analysis platform. Here we would like to present our internal effort to new SAR analysis platform with Datagrok[2].

What's and Why datagrok?

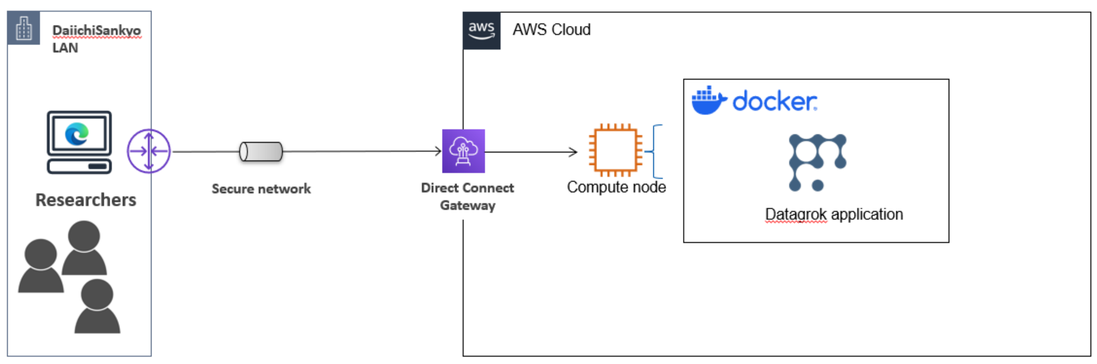
What's datagrok ?

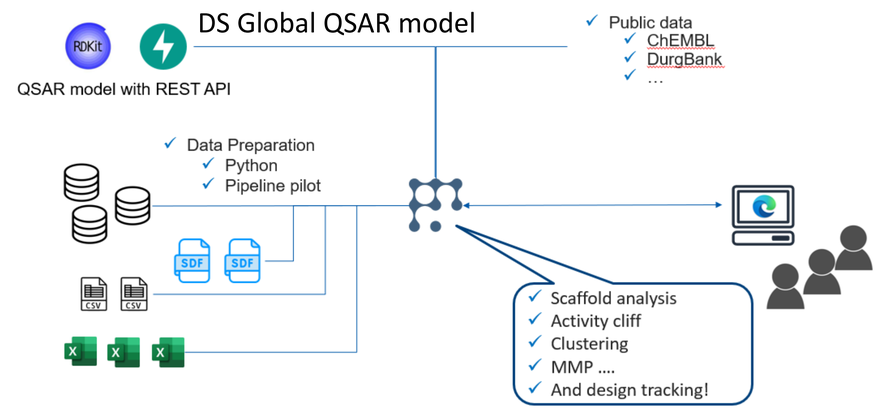
- A commercial package for data science
- A platform for turning data into actionable insights

Why datagrok ?

- Highly functionalized and faster performance
- Web based application implemented in internal environment
- Flexibility to incorporate third-party library
- Wide range of modalities are supported

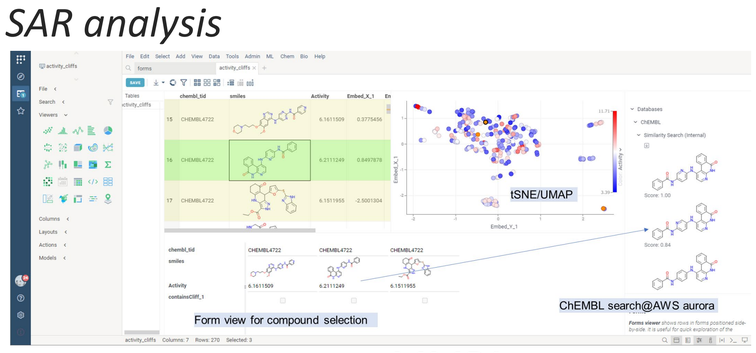
System architecture and current SAR analysis platform



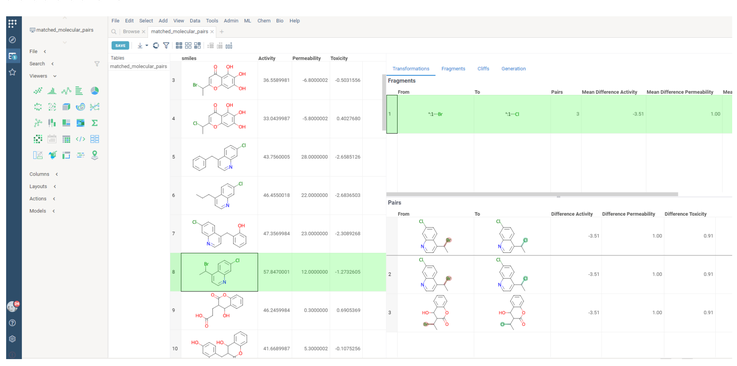


User can build their own favorite view from SAR table!

SAR analysis

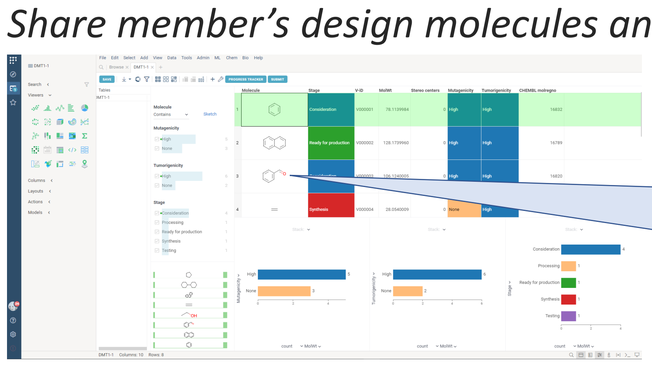


MMPA



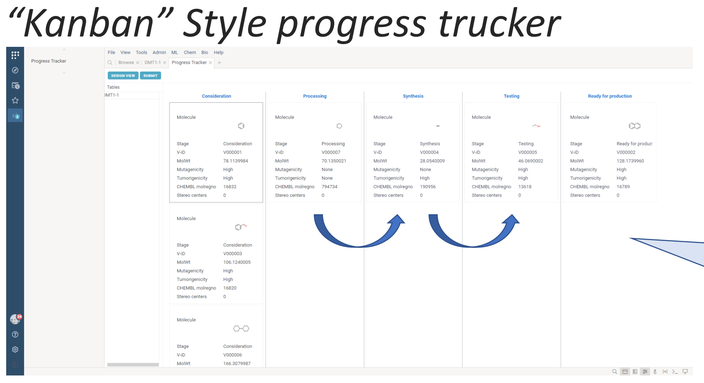
Share idea and progress of design with project member

Share member's design molecules and add ML predicted value



Hit Design Table is integrated in-house compound DB.
When the idea is synthesized, in-house compound ID will be retrieved from the DB.

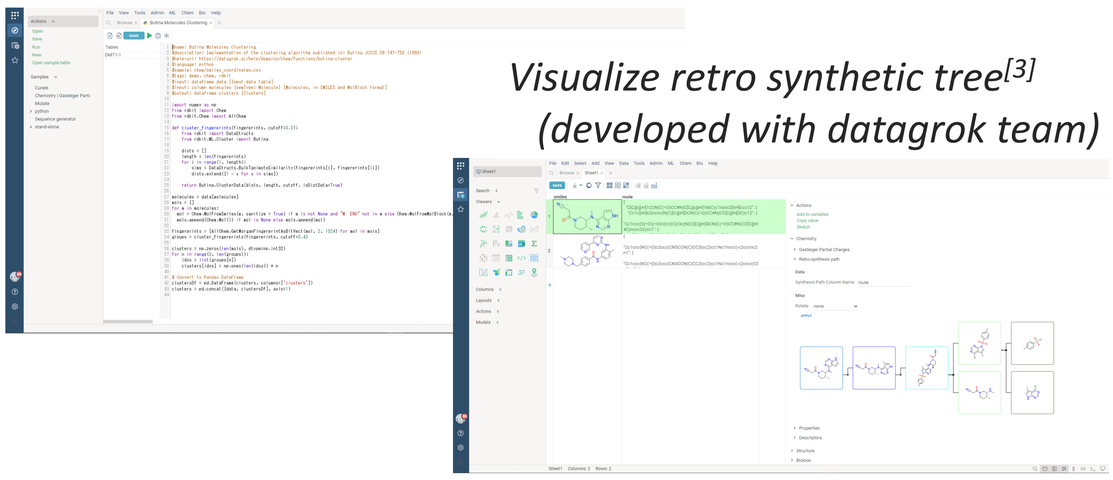
"Kanban" Style progress trucker



The status is updated by project member

Support multi languages for development Python, Javascript, R …

Develop new function with scripting



Visualize retro synthetic tree[3]
(developed with datagrok team)

Summary and future plan

Summary

- ✓ Built new SAR analysis and idea sharing platform in Daiichi Sankyo
- ✓ Integrated in-house data based QSAR model and scoring functions
- ✓ Provide idea sharing system to medicinal chemists
- ✓ Provide training for medicinal chemists

Future plan

- ✓ Integrate GPU docking to support drug design
- ✓ Expand support modalities not only small molecule but also others
- ✓ Integrate design tracker and in-house real compound DB

Acknowledgements

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- Vladyslav Hlushchenko
- Olena Ahadzhanian
- Davit Rizhinashvili
- Alexander Paramonov
- Pavlo Polovyi
- And community!

References

1.Drug Discov. Today, 27 (8) (2022), pp. 2065-2070
2.https://datagrok.ai/
3.https://spaya.ai/app

Conflict of Interests

All authors are employees of Daiichi Sankyo