Novartis Institute for Biomedical Research

Putting RDKit in the hands of the users in a corporate environment: Leveraging the power of Datagrok

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21st of September, 2023

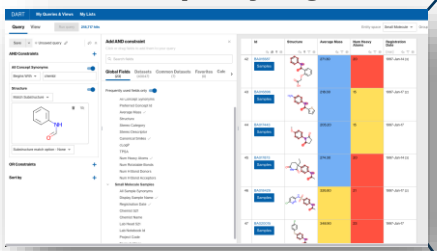
12th RDKit UGM

NOVARTIS | Reimagining Medicine

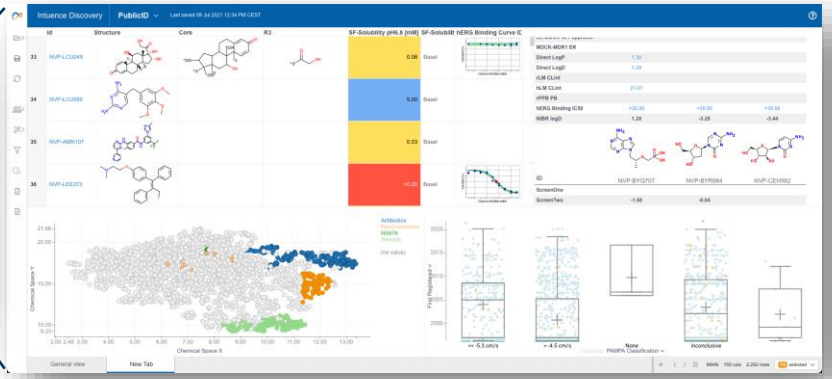
The Intuence product suite

Datagrok
KNIME
Spotfire
Python
…

Data querying

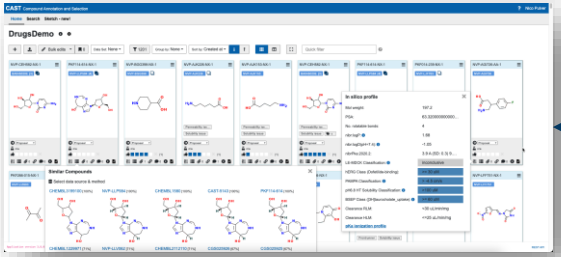


Interactive dashboards, decision-making:
Intuence Discovery



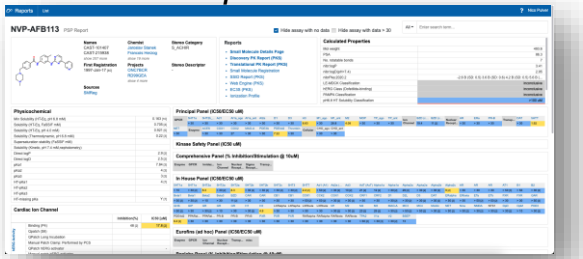
Data warehouse

Virtual molecules, new ideas, annotations

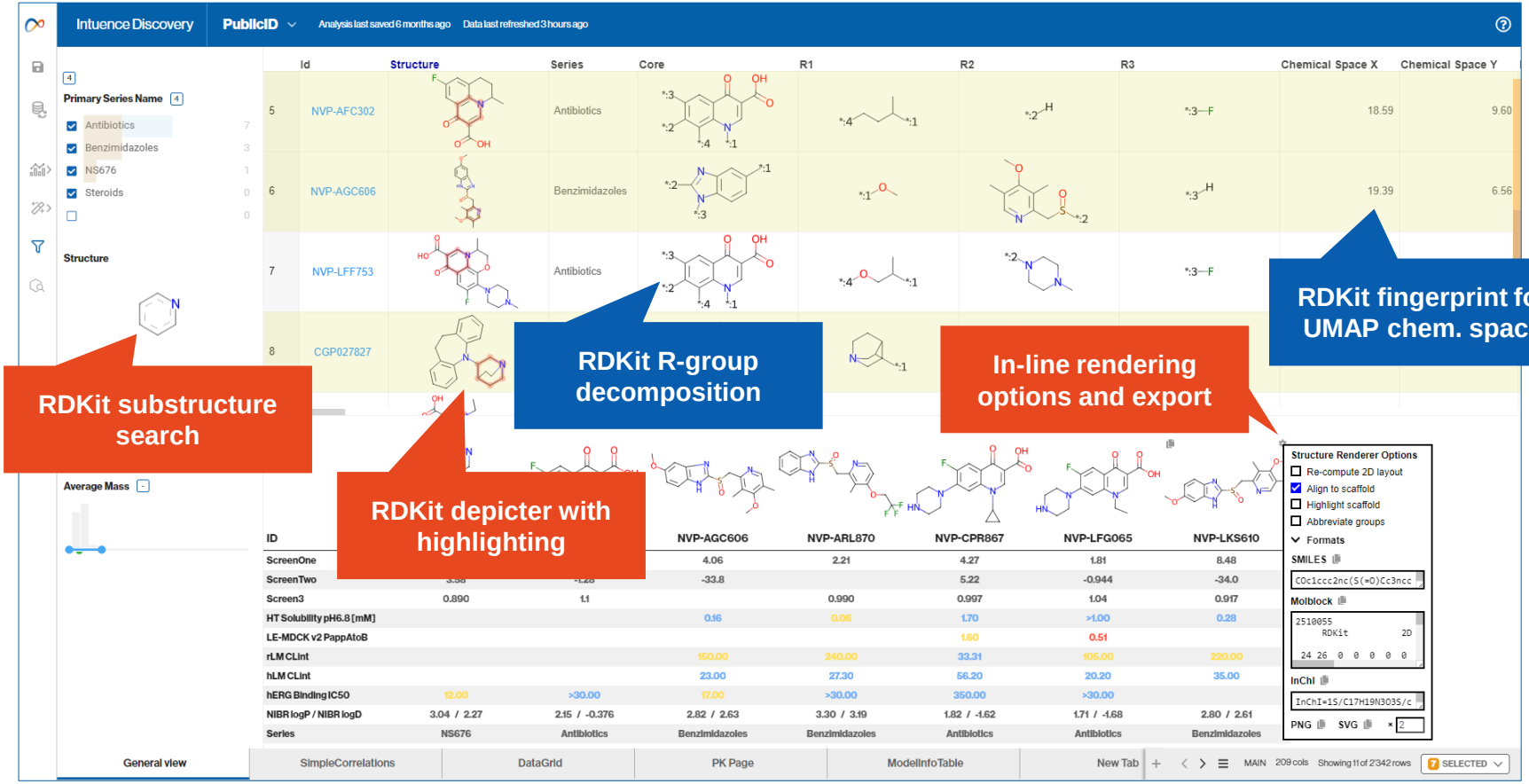


ML & Data science

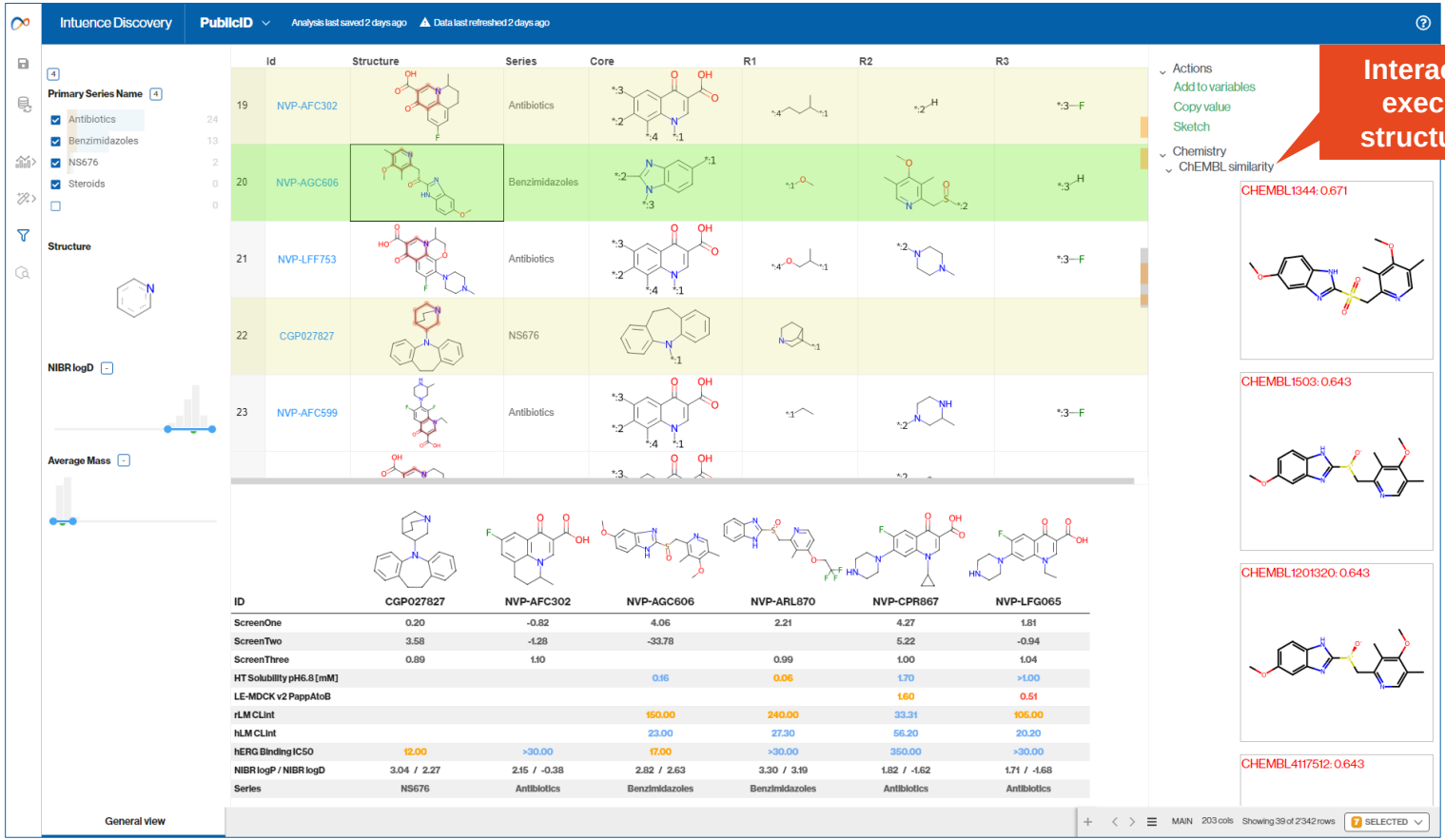
“One-pager” reports:
Intuence Reports



Intuence Discovery: RDKit in back- & front-end

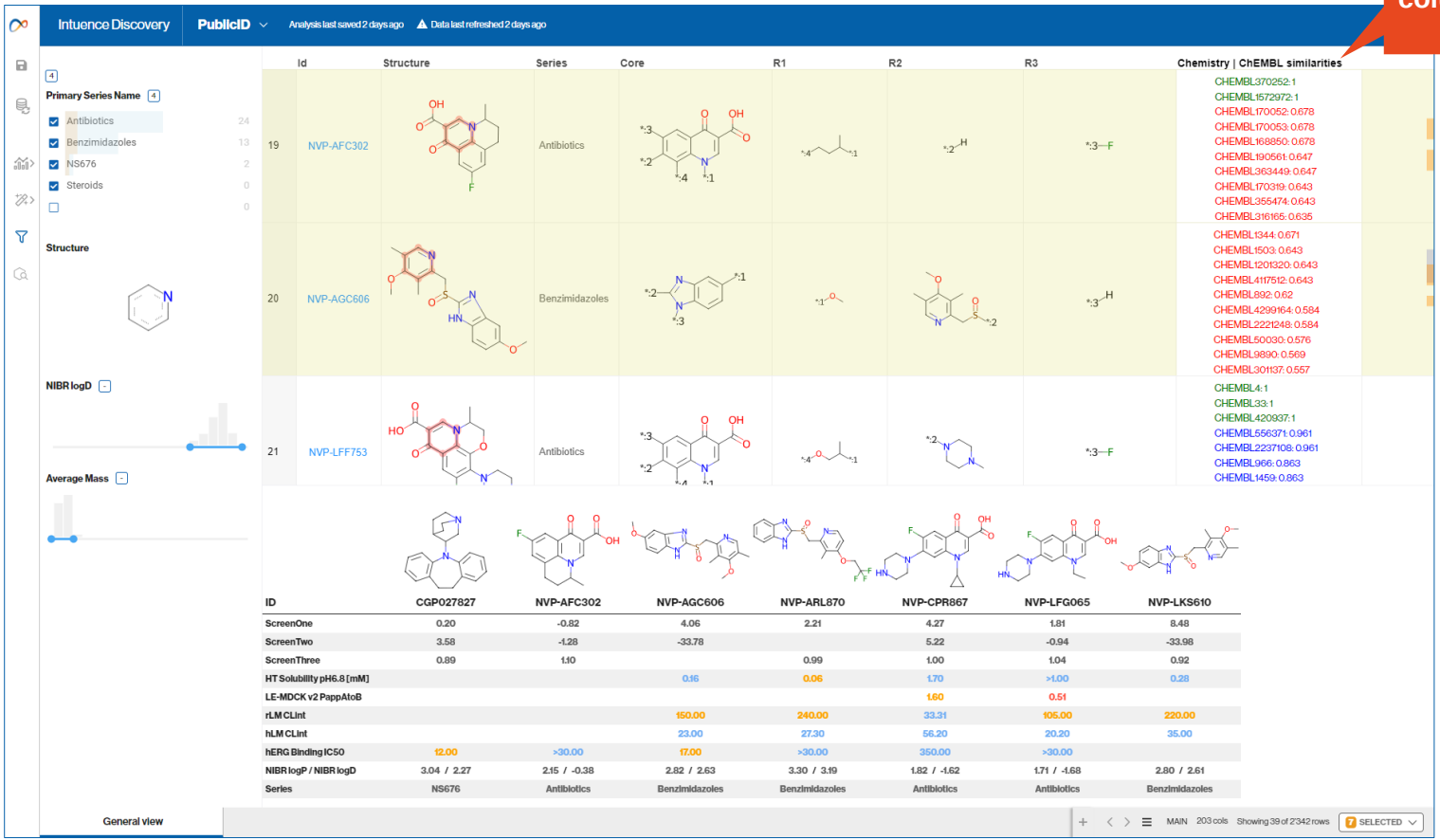


Leveraging RDKit.js in Datagrok

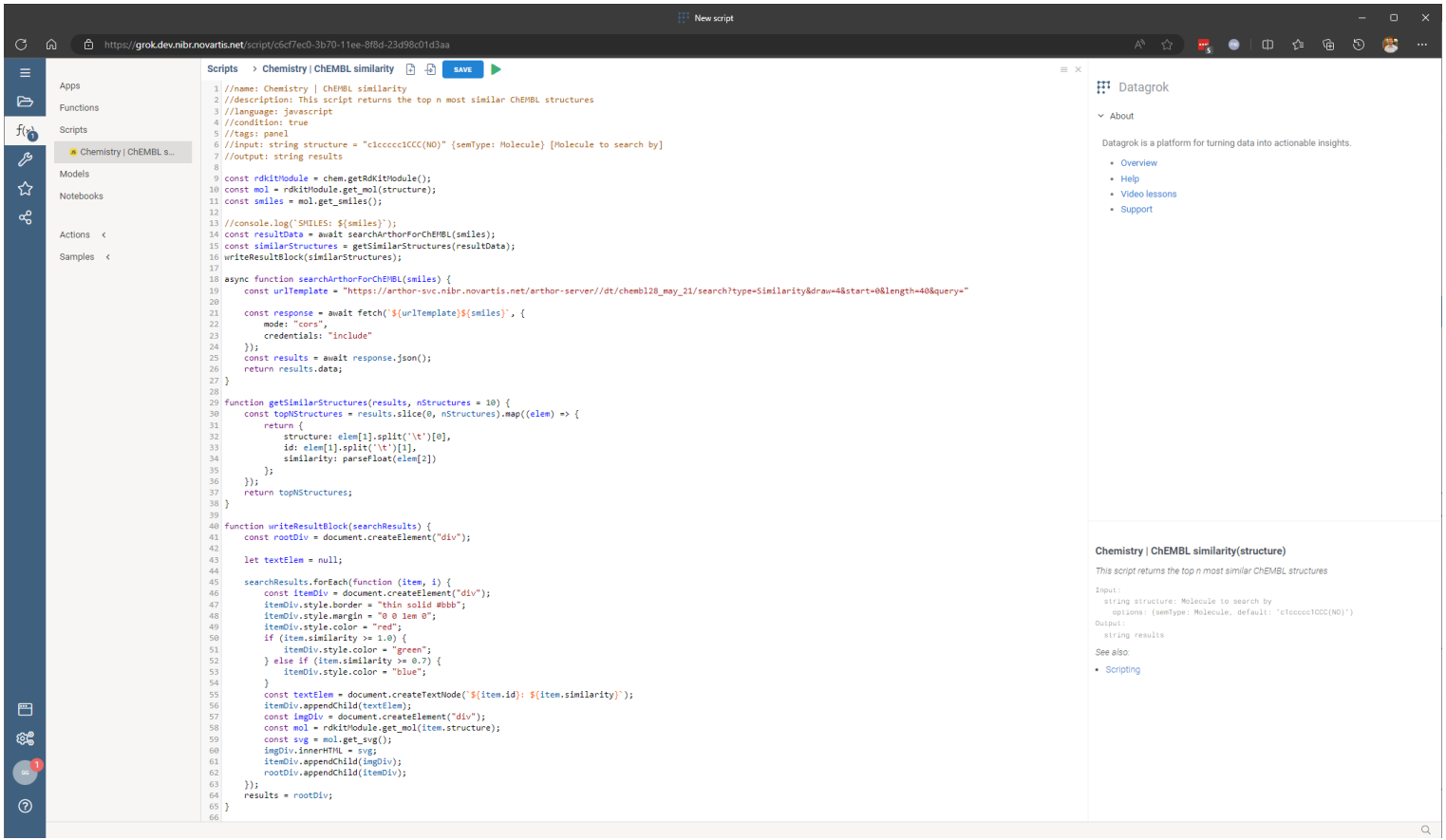


Leveraging RDKit.js in Datagrok

Adding script as a column (fetching while scrolling)



Leveraging RDKit.js in Datagrok



Acknowledgements

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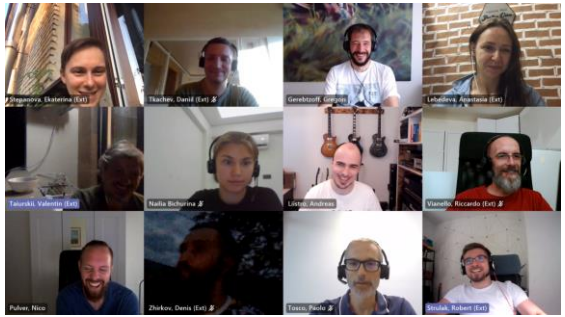

- Datagrok team
- Intuence user community
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- NIBR Global Discovery Chemistry & CADD
- NIBR Translational Medicine & PKS
- Greg Landrum & RDKit community
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Thank you

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