datagrok

Cheminformatics in the browser

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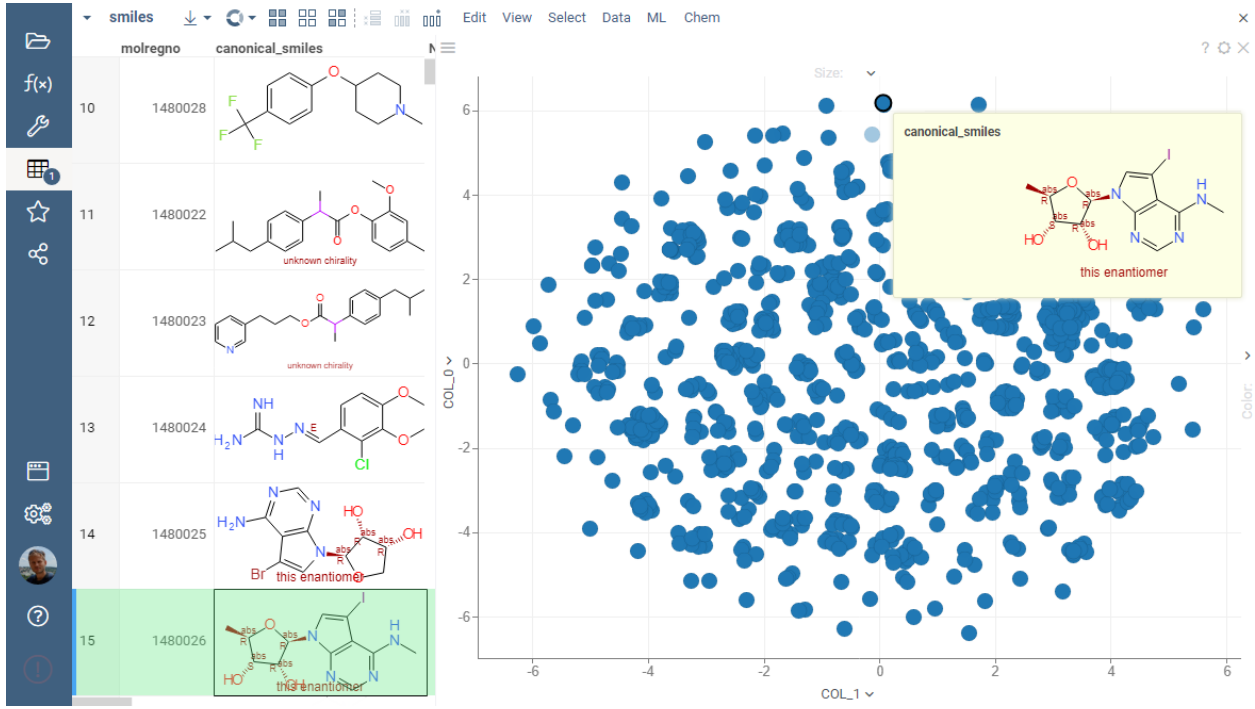
Datagrok: enterprise-ready life sciences platform

- Data access, exploratory data analysis, scientific computing, etc
- Analyzing big datasets completely in the browser
- Proprietary core, open-source plugin ecosystem
- Industry adoption
- Free for academia and personal use
- Domain-agnostic
- Cheminformatics as a plugin
- RDKit (WebAssembly or Python)

RDKit in the browser

- RDKit for cheminformatics: WebAssembly and Python
- Rendering
- Descriptors & fingerprints
- Substructure search
- Similarity & diversity analyses
- Activity cliffs
- SAR Viewer
- Sketching (OpenChemLib, MarvinJS, Ketcher)
- … + other community-built functionality (app store, JS API is provided)

Demo time!


smiles
Edit
View
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ML
Chem
molregno
canonical_smiles
10
1480028
11
1480022
unknown chirality
12
1480023
unknown chirality
13
1480024
14
1480025
this enantiomer
15
1480026
this enantiomer
Size:
canonical_smiles
this enantiomer
COL_0
COL_1
Color:

Thank you!

Acknowledgements

- Greg Landrum
- Paolo Tosco
- RDKit community
- Novartis Institutes for BioMedical Research
- All our users ☺

Run the platform right now in your browser: https://datagrok.ai