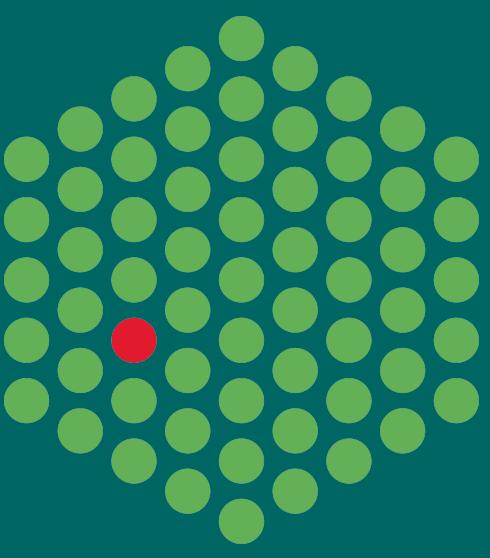


Enhancing small molecule information in the Protein Data Bank in Europe

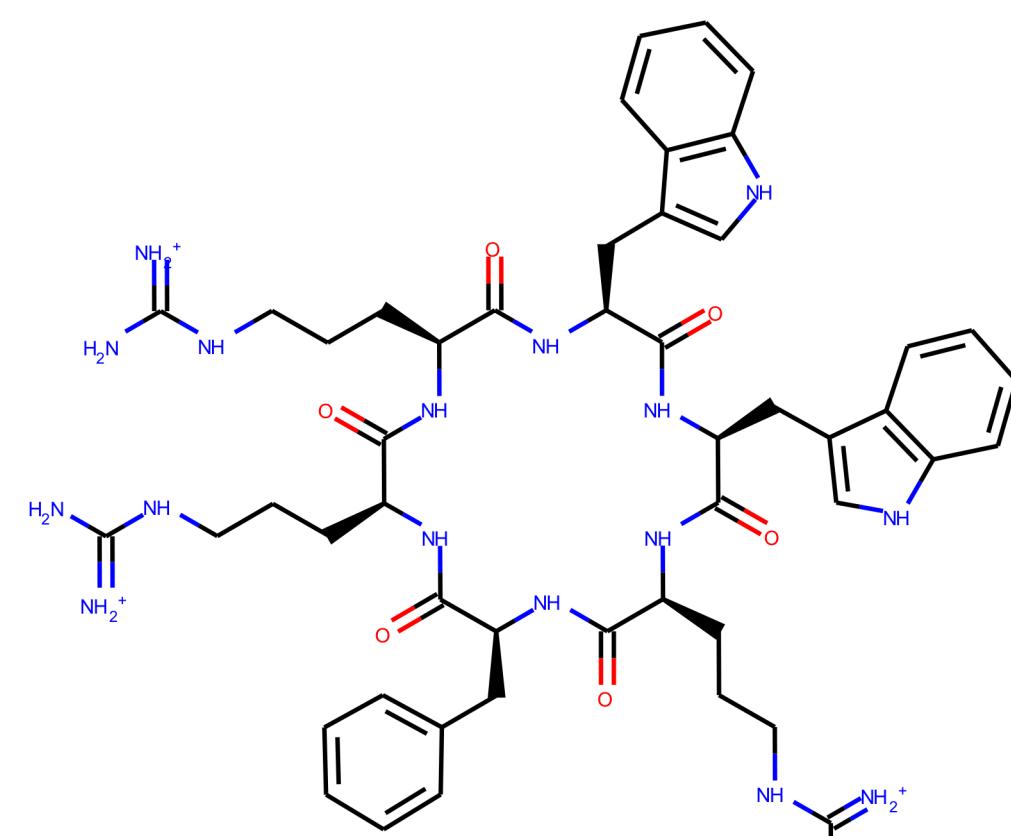
EMBL-EBI



PDBe-KB consortium, presented by Lukáš Pravda¹

¹ European Molecular Biology Laboratory (EMBL), European Bioinformatics Institute (EMBL-EBI), Cambridge, UK

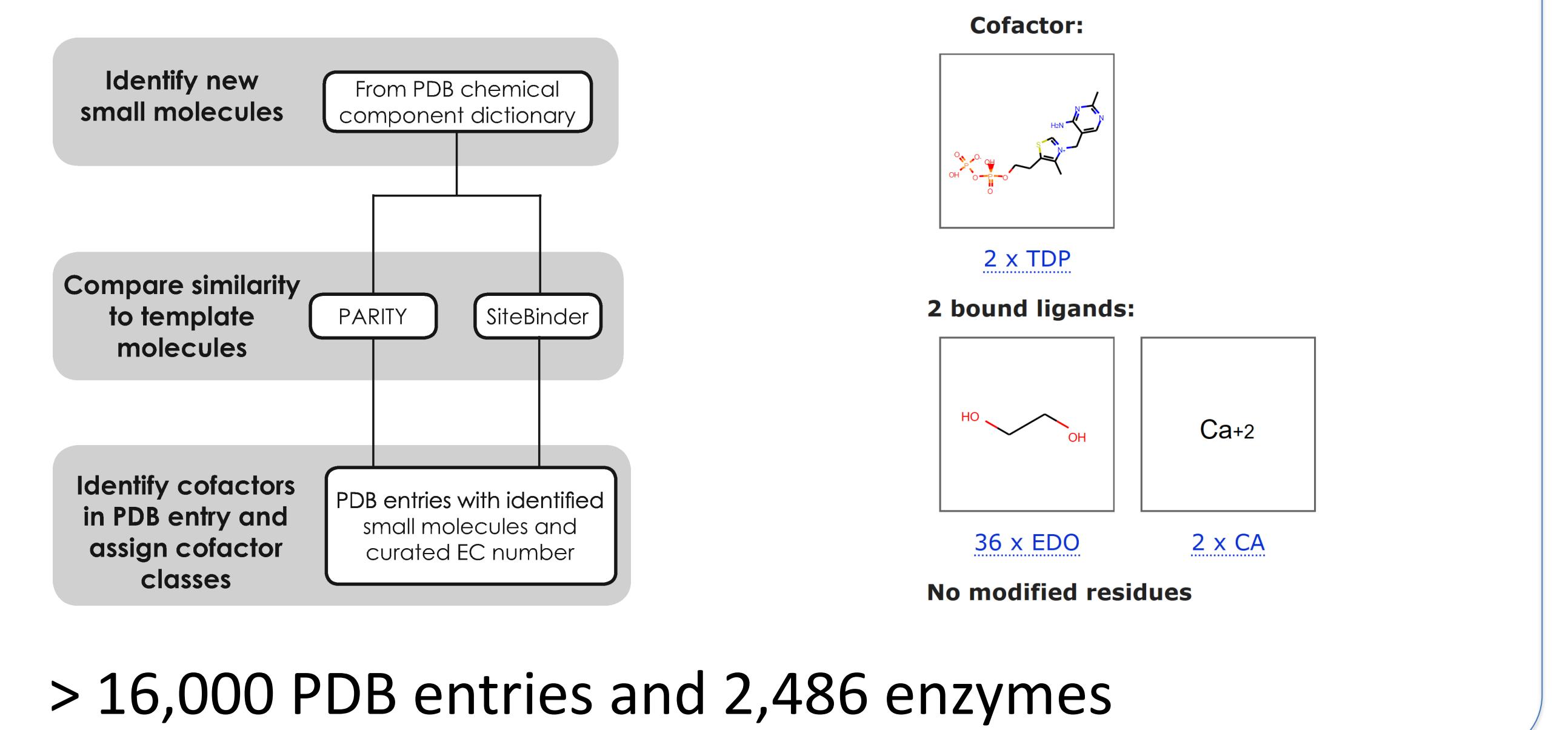
Computed properties



- Chemical components
- 2D, 3D coordinates
- Peptide reference dictionary
- Physicochemical properties

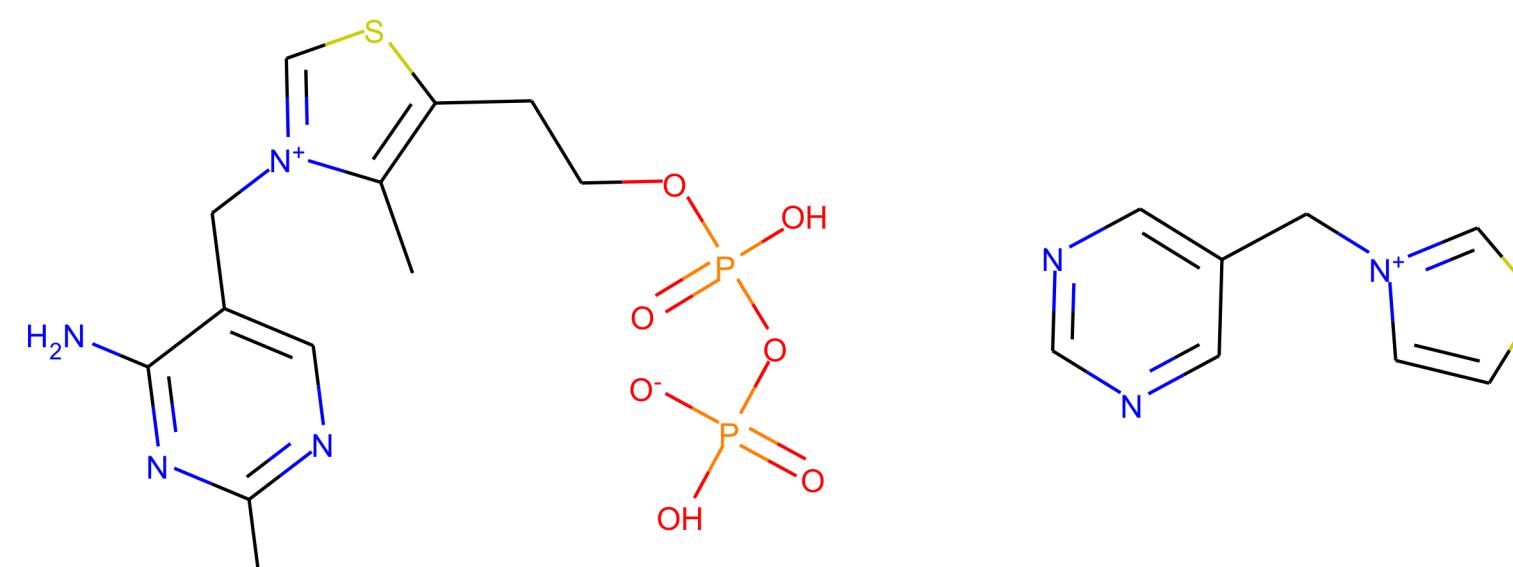


Cofactors



Scaffolds

Scaffold for ~ 28,000 chemical components

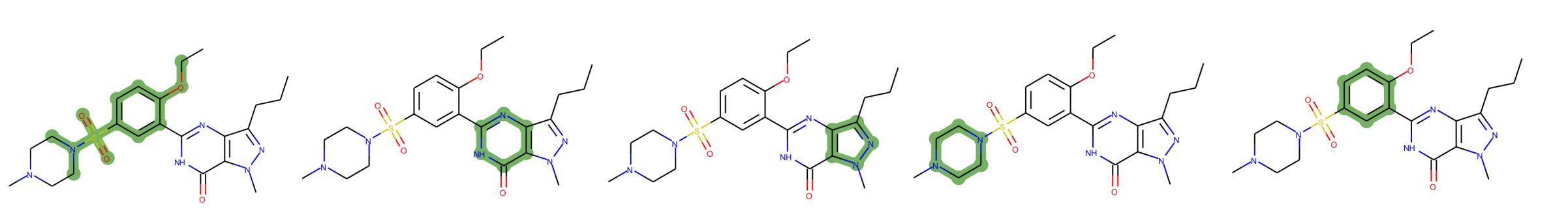


TDP Scaffold Generic

Fragments

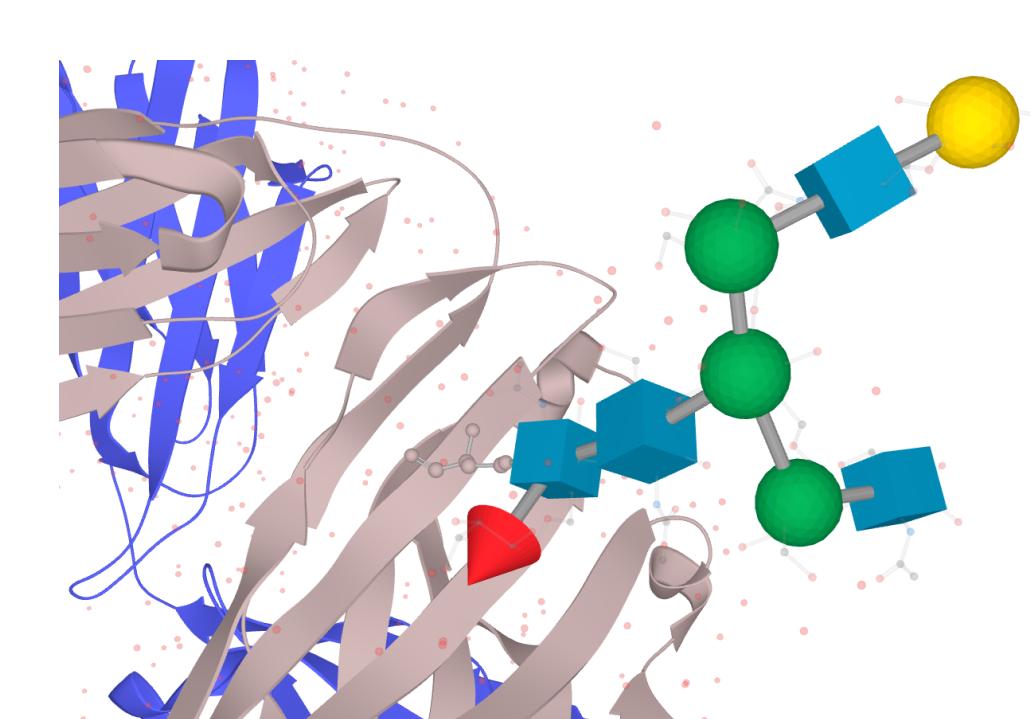
2,100 fragments

- 100 manually curated
- 1,300 from ENAMINE library
- 700 from DSI library



Glycans

3D-Symbol Nomenclature For Glycans (3D-SNFG)



COMING SOON

PDBe-KB Ligand Pages

PDBe-KB
Protein Data Bank in Europe Knowledge Base

Summary About 24 Structures 27 Interactions Functional annotations (1) Similar ligands (6) Publications (81) Feedback

PDBe-KB > 4-(4-METHYL-PIPERAZIN-1-YLMETHYL)-N-[4-METHYL-3-(4-PYRIDIN-3-YL-PYRIMIDIN-2-YLAMINO)-PHENYL]-BENZAMIDE

Synonyms: STI-571, Imatinib, Gleevec
Formula: C29H31N7O
3 Letter code: STI
InChI: InChI=1S/C29H31N7O/c1-21-5-10-25(18-27(21)34-29-31-13-11-26(33-29)24-4-3-12-30-19-24)32-28(37)23-8-6-22(7-9-23)20-36-16-14-35(2)15-17-38/h3-13,18-19H,14-17,20H2,1-2H3,(H,32,37)(H,31,33,34)
InChI Key: KTFUNOKKBV/MGRW-UHFQAYSA-N
SMILES: O=C(Nc3ccc(c(Nc2nc(c1ccncc1)ccn2)c3)Cc4ccc(cc4)CN5CCN(CC5)C

About 24 Structures 27 Interactions 1 Functional annotations 6 Similar ligands 81 Publications

Click to view in 3D

Similar ligands (6)

This section shows small molecules similar to STI. By default, all the ligands with >50 % similarity score with STI are shown. These ligands can further be filtered based on similarity score.

Filter by similarity score: < 50 % > 60 % > 70 % > 80 % > 90 %

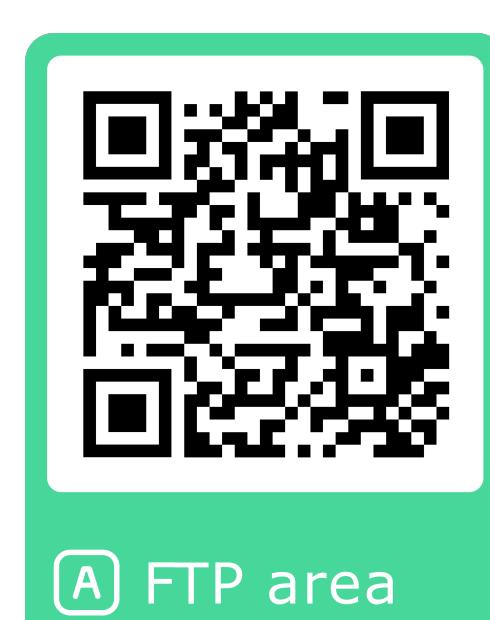
Ligand	Similarity Score	Description
MPZ	93% similar	Found in 1 PDB entry Mostly bound to P12931 (1)
PRC	64% similar	Found in 1 PDB entry Mostly bound to P00520 (1)
G65	56% similar	Found in 1 PDB entry Mostly bound to P16234 (1)
748	54% similar	Found in 1 PDB entry Mostly bound to P00519 (1)
66K	53% similar	Found in 1 PDB entry Mostly bound to P53779 (1)
406	52% similar	Found in 1 PDB entry Mostly bound to Q08345 (1)

Search: e.g. GLUTATHIONE
Select File Format: CSV JSON Download

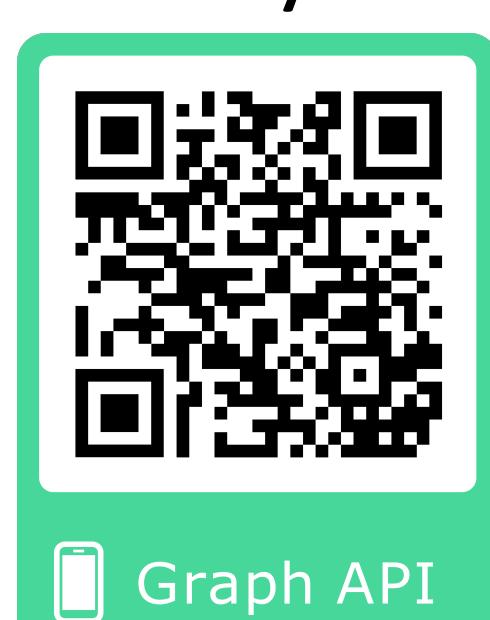
Show all items

Programmatic access

- ✓ Bulk download: Weekly release is available via FTP
- ✓ API: Protein-ligand interactions, small molecule functional annotations and much more are available over graph API
- ✓ pdbeccutils: Python 3.7 pip installable package that extends RDKit functionality



A FTP area



Graph API



python PIP

Feedback, please!

- ✓ We are in a process of designing Ligand Pages
- ✓ We'd really appreciate if you could spend a few moments to fill up a short questionnaire
- ✓ This will help us better understand the use small molecule data in your research

