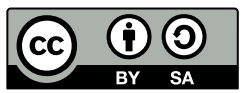
Crystallography Open Database (COD)

Saulius Gražulis

Vilnius, 2024

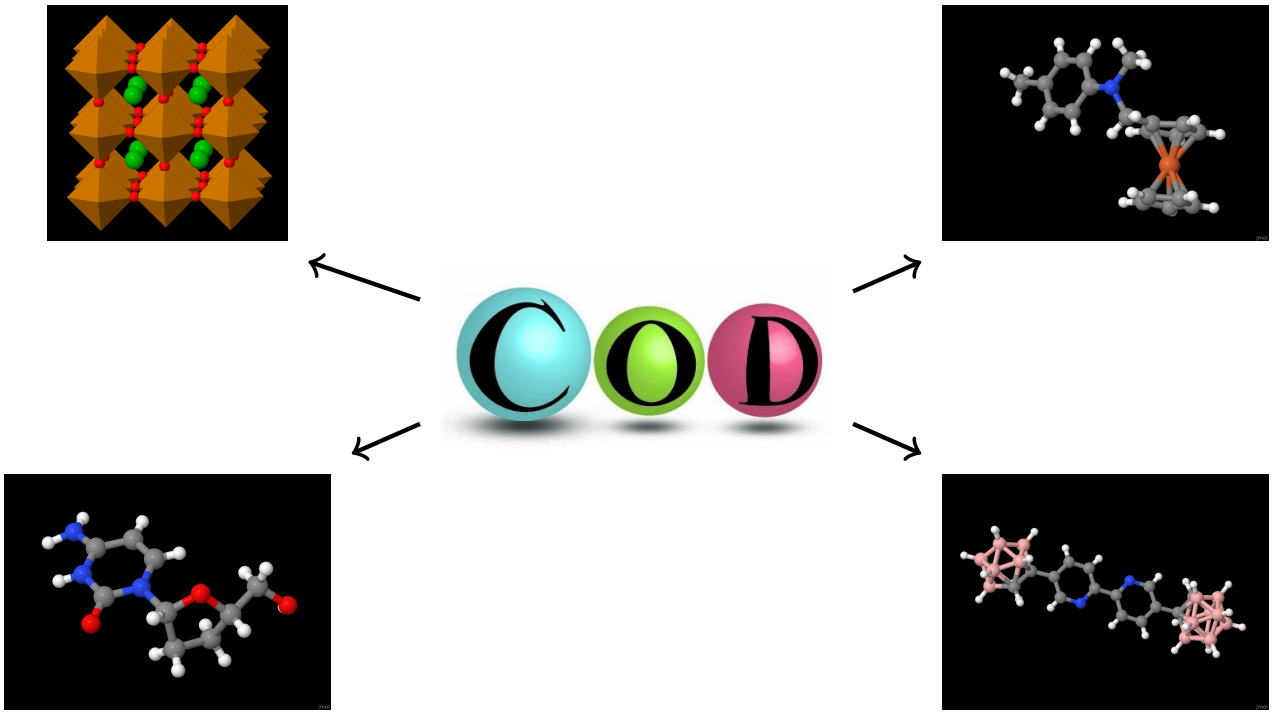
Vilnius University Institute of Biotechnology

Id: slides.tex 2572 2024-02-22 16:47:37Z saulius February 22, 2024



COD contents

https://www.crystallography.net/cod



510 995 records as of 2024-02-22, available under **CC0 License**

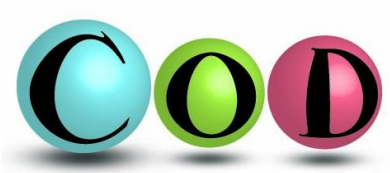
All data are presented in a standardised, machine-readable form (Gražulis et al. 2009; Gražulis et al. 2012), in CIF (Hall et al. 1991) format.

Accessing the COD

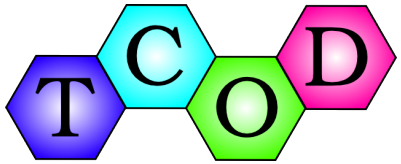
COD data can be accessed:

1. Via the Web page:
   https://www.crystallography.net/cod/7159763.html
2. Via the COD REST API:
   https://www.crystallography.net/cod/7159763.cif
   https://www.crystallography.net/cod/result?text=perovskite
3. Via the OPTIMADE API (Andersen et al. 2021):
   https://www.crystallography.net/cod/optimade/structures?filter=elements+HAS+"U"
4. Via SQL:
   ```
   mysql -u cod_reader -h sql.crystallography.net cod -e \
   'select file from data where formula = "- H2 O -"'
   ```
5. By downloading to your computer using Subversion, `rsync` or simple Web download:
   https://wiki.crystallography.net/howtoobtaincod

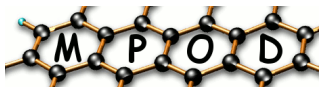
COD “sisters”



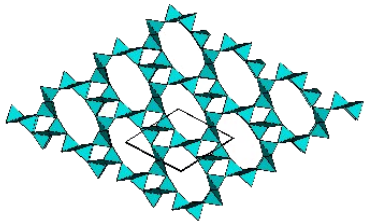
http://www.crystallography.net/cod
$>$ 500 000 entries



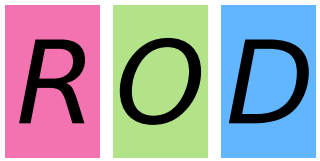
http://www.crystallography.net/tcod
$>$ 7400 entries (ready to grow to $>$ 10^7?)



http://mpod.cimav.edu.mx/
$>$ 300 entries



http://www.crystallography.net/pcod
$>$ 10^6 entries (ready to grow to $>$ 10^8?)



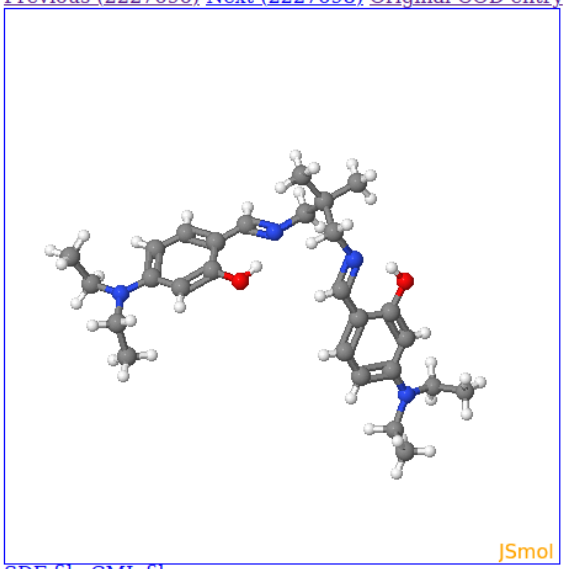
http://solsa.crystallography.net/rod/
$>$ 1100 entries

(Gražulis et al. 2009; Gražulis et al. 2012; Pepponi et al. 2012; Fuentes-Cobas et al. 2017; Mendili et al. 2019)

COD chemical repertoire

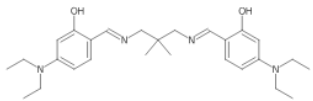
http://molecules.crystallography.net/

Previous (2227696) Next (2227698) Original COD entry



SDF file CML file

Reduced structural formula



Reduced canonical SMILES:

CCN(c1ccc(c(c1)O)/C=N/CC(C/N=C/c1ccc(cc1O)N(CC)CC)(C)C)CC **(x1)** PubChem

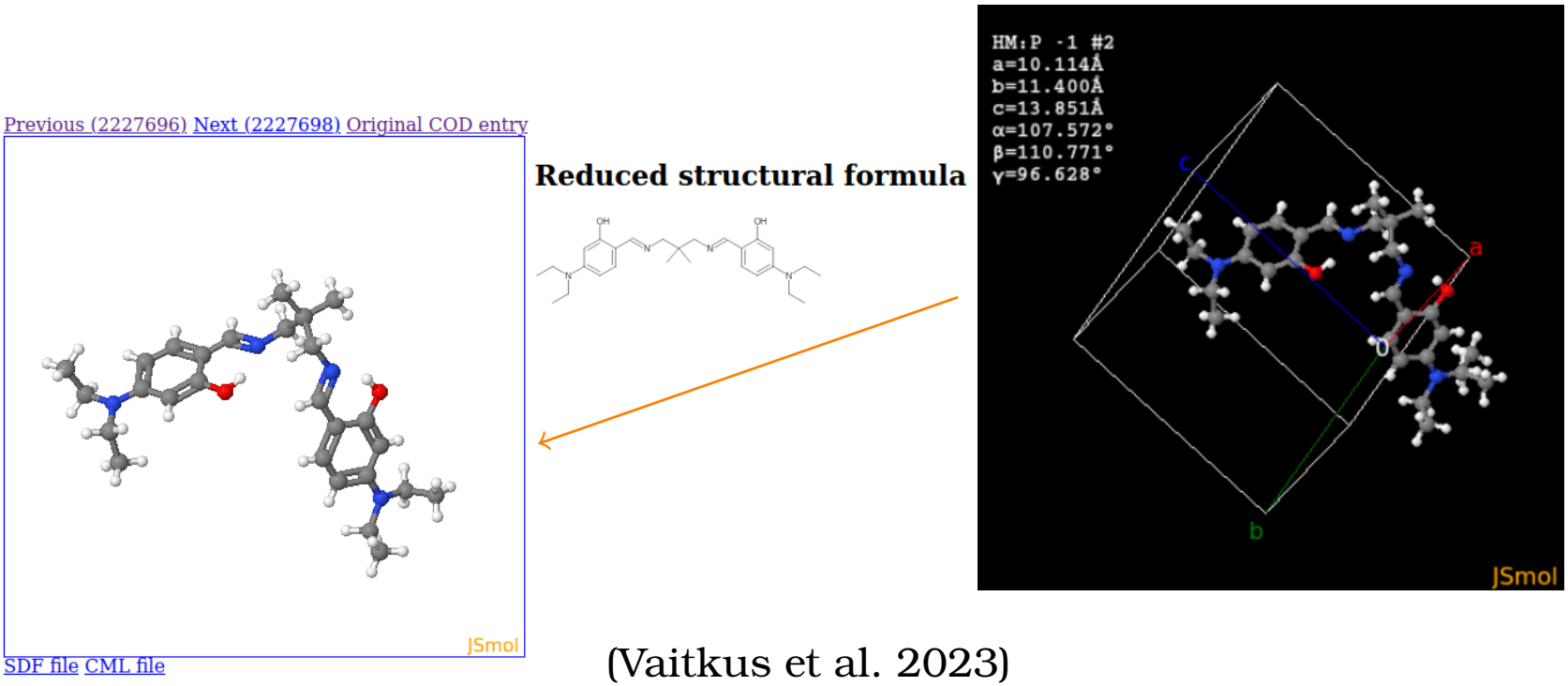
Unique components

SMILES	InChI
CCN(c1ccc(c(c1)O)/C=N/CC(C/N=C/c1ccc(cc1O)N(CC)CC)(C)C)CC	InChI=1S/C27H40N4O2/c1-7-30(8-2)23-13-11-21(25(32)15-23)17-28-19-27(5,6)2 /h11-18,32-33H,7-10,19-20H2,1-6H3/b28-17+,29-18+

See also poster by Merkys et al. (https://bit.ly/3BKZ5vG)

COD chemical repertoire

http://molecules.crystallography.net/



(Vaitkus et al. 2023)

Reduced canonical SMILES:

CCN(c1ccc(c(c1)O)/C=N/CC(C/N=C/c1ccc(cc1O)N(CC)CC)(C)C)CC **(x1)** PubChem

Unique components

SMILES	InChI
CCN(c1ccc(c(c1)O)/C=N/CC(C/N=C/c1ccc(cc1O)N(CC)CC)(C)C)CC	InChI=1S/C27H40N4O2/c1-7-30(8-2)23-13-11-21(25(32)15-23)17-28-19-27(5,6)2…/h11-18,32-33H,7-10,19-20H2,1-6H3/b28-17+,29-18+

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COD chemical repertoire

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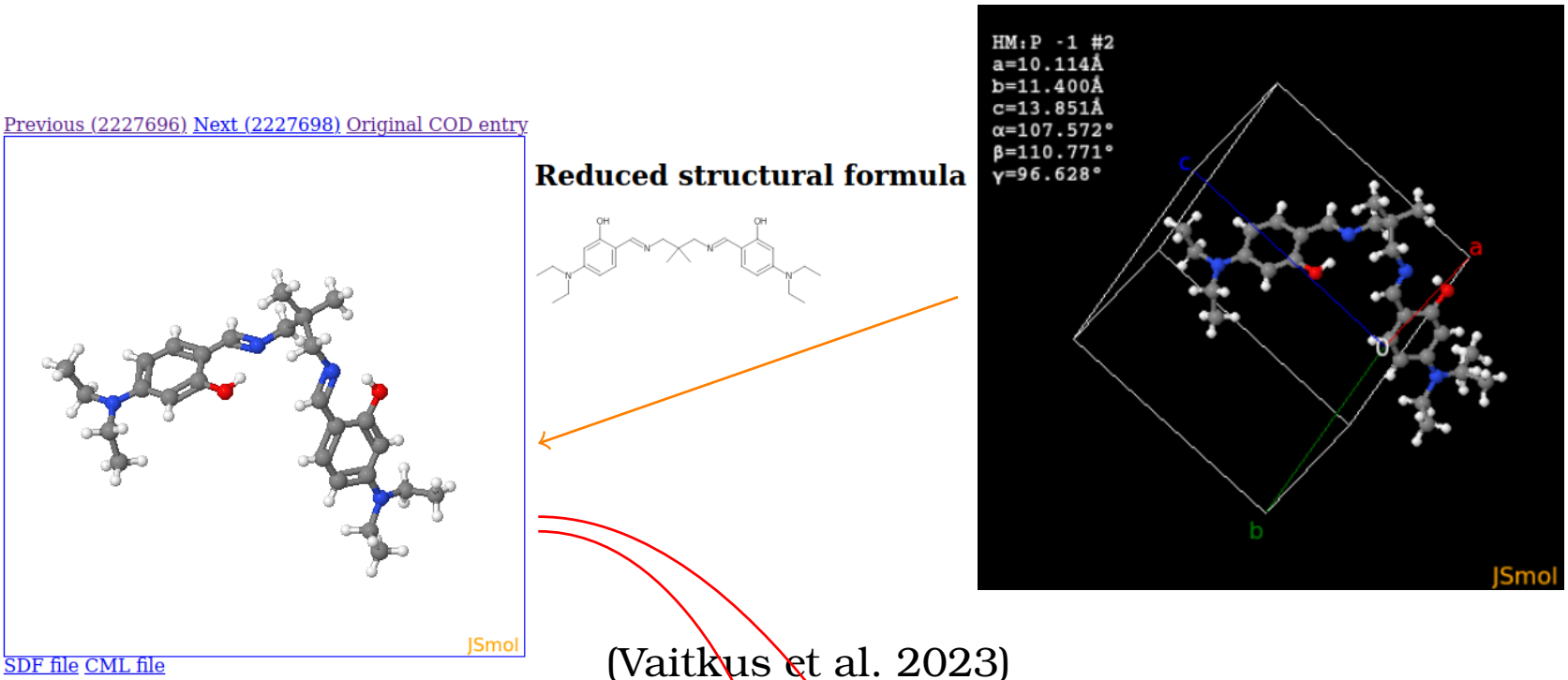

(Vaitkus et al. 2023)

See also poster by Merkys et al. (https://bit.ly/3BKZ5vG)

Acknowledgements

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QM community

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Giovanni Pizzi
Lubomir Smrcok
Linas Vilčiauskas
Rickard Armiento

VU MIF II (FMG)

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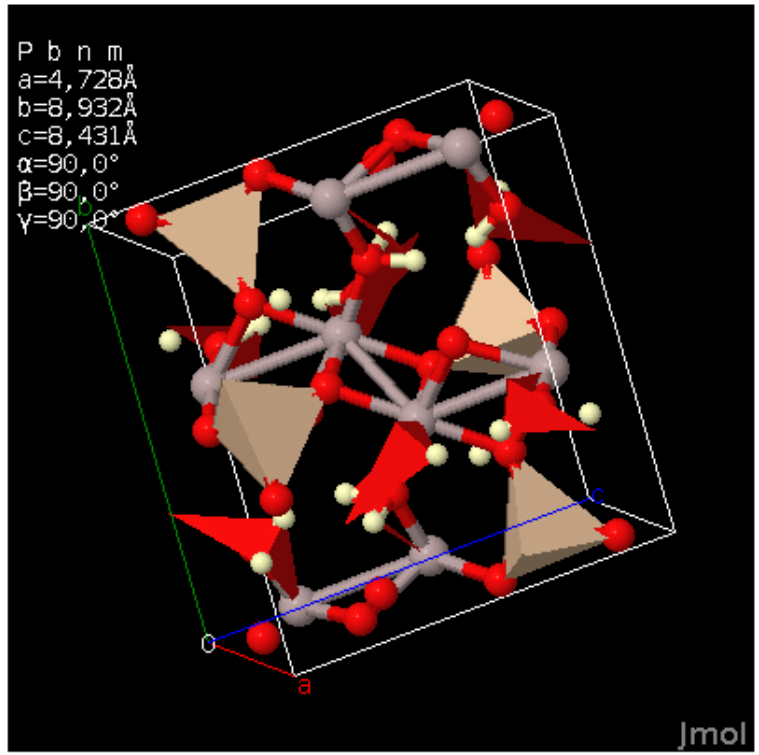
Thank you!



Coordinates	2207377.cif
Original IUCr paper	HTML

http://en.wikipedia.org/wiki/Topaz

http://www.crystallography.net/2207377.html

http://www.crystallography.net/cod/archives/2024/slides/MaRDA-meeting-repository-session/slides.pdf

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Vaitkus, Antanas et al. (Dec. 2023). "A workflow for deriving chemical entities from crystallographic data and its application to the Crystallography Open Database". In: *Journal of Cheminformatics* 15.1. ISSN: 1758-2946. DOI: 10.1186/s13321-023-00780-2.