Handout, ChEMBL training, 30 Jan 2023

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ChEMBL Best Practice:

First steps:	Use the web interface for initial exploration, then progress onto the API
Get started with API:	Look at some example URLs: e.g. return all compounds: https://www.ebi.ac.uk/chembl/api/data/molecule
Check data output	Remember to spot check the API output e.g. For one compound: have I captured all relevant data? Are activity data for both parent and salt drug forms present?
Schema:	A schema description is available at e.g. https://www.ebi.ac.uk/chembl/api/data/activity/schema (although it can be easier to examine an actual example instead)
Try it out interactively:	Use our interactive API documentation https://www.ebi.ac.uk/chembl/api/data/docs

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Links

Webinars:

- ChEMBL Webinar: https://www.ebi.ac.uk/training/events/guide-explore-drug-compounds-and-their-biological-targets-using-chembl/
- ChEMBL quick tour: https://www.ebi.ac.uk/training-beta/online/courses/chembl-quick-tour/

Documentation:

- ChEMBL web services: https://chembl.gitbook.io/chembl-interface-documentation/web-services
- UniChem documentation: https://chembl.gitbook.io/unichem/ , Beta: https://chembl.gitbook.io/unichem/unichem-2.0/

FTP sites:

- UniChem: ftp://ftp.ebi.ac.uk/pub/databases/chembl/UniChem/data/
- ChEMBL: https://ftp.ebi.ac.uk/pub/databases/chembl/ChEMBLdb/releases/

Contact us: chembl-help@ebi.ac.uk, unichem@ebi.ac.uk

Blog: https://chembl.blogspot.com/

FAQs:
https://chembl.gitbook.io/chembl-interface-documentation/frequently-asked-questions

Standardiser code on GitHub:

https://github.com/chembl/ChEMBL_Structure_Pipeline/blob/master/chembl_structure_pipeline/standardizer.py

ChEMBL31 Schema
https://ftp.ebi.ac.uk/pub/databases/chembl/ChEMBLdb/latest/chembl_31_schema.png