UNIVERSITY OF OXFORD

ChemBio Hub

Customising the ChemBio Hub ChemReg Data Model

- Tech Stack
- Installation for development
- Introduction to how the data model works
- Customising the data model to register compound batches
- Adding plugins for custom descriptors and data integrations
- Coming soon - export workflows for PubChem and ChEMBL

Tech Stack

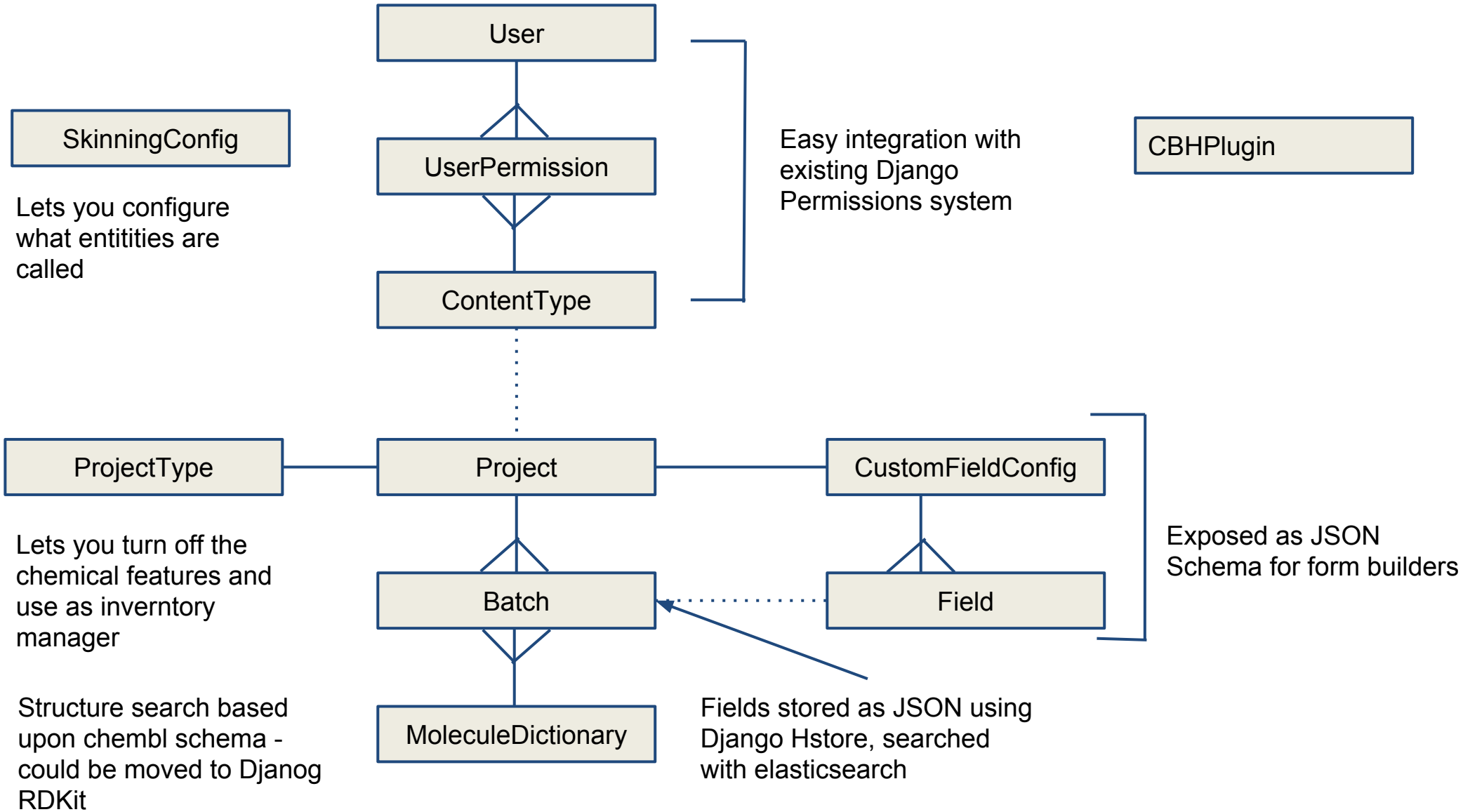
Tastypie Web Services

Open-Source Cheminformatics and Machine Learning

UNIVERSITY OF OXFORD

ChemBio Hub

Data Model



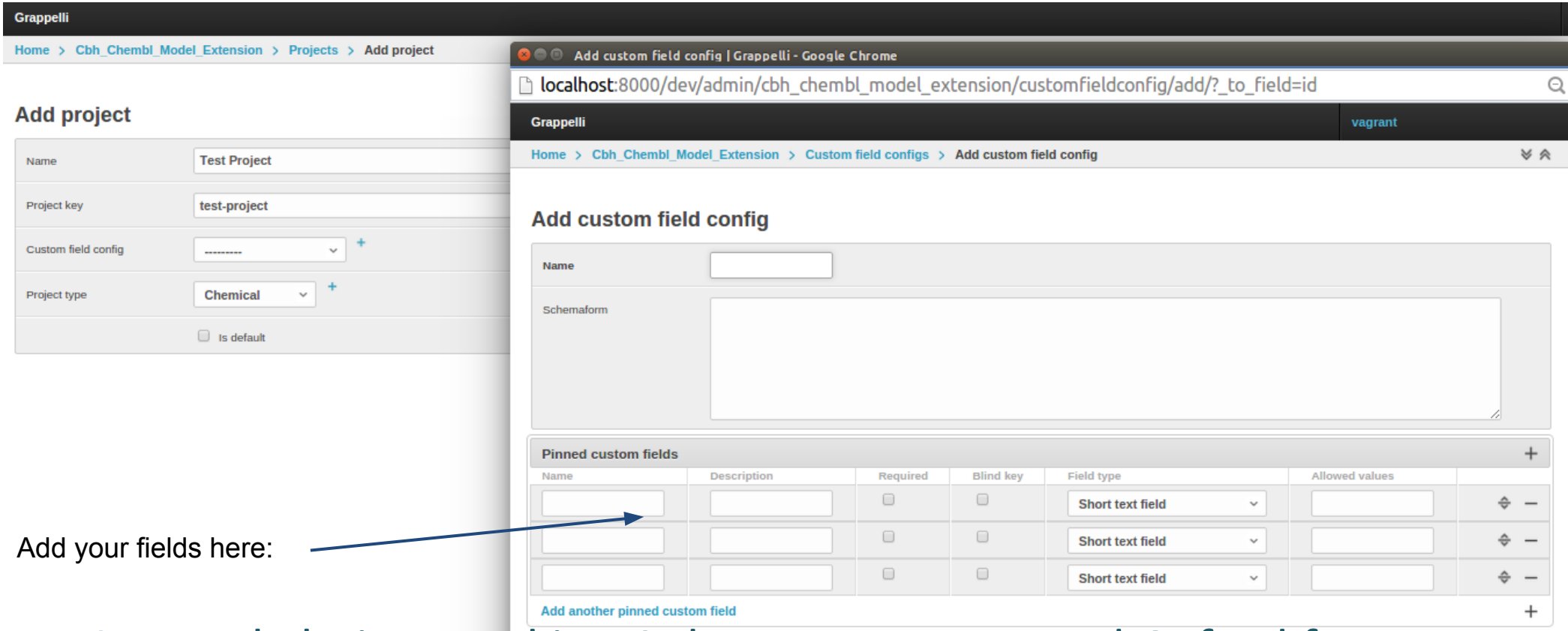
Tutorial

https://github.com/thesgc/chembiohub_ws/blob/master/turorial.md

UNIVERSITY OF OXFORD

ChemBio Hub

Customising the Data Model to Register Compound Batches



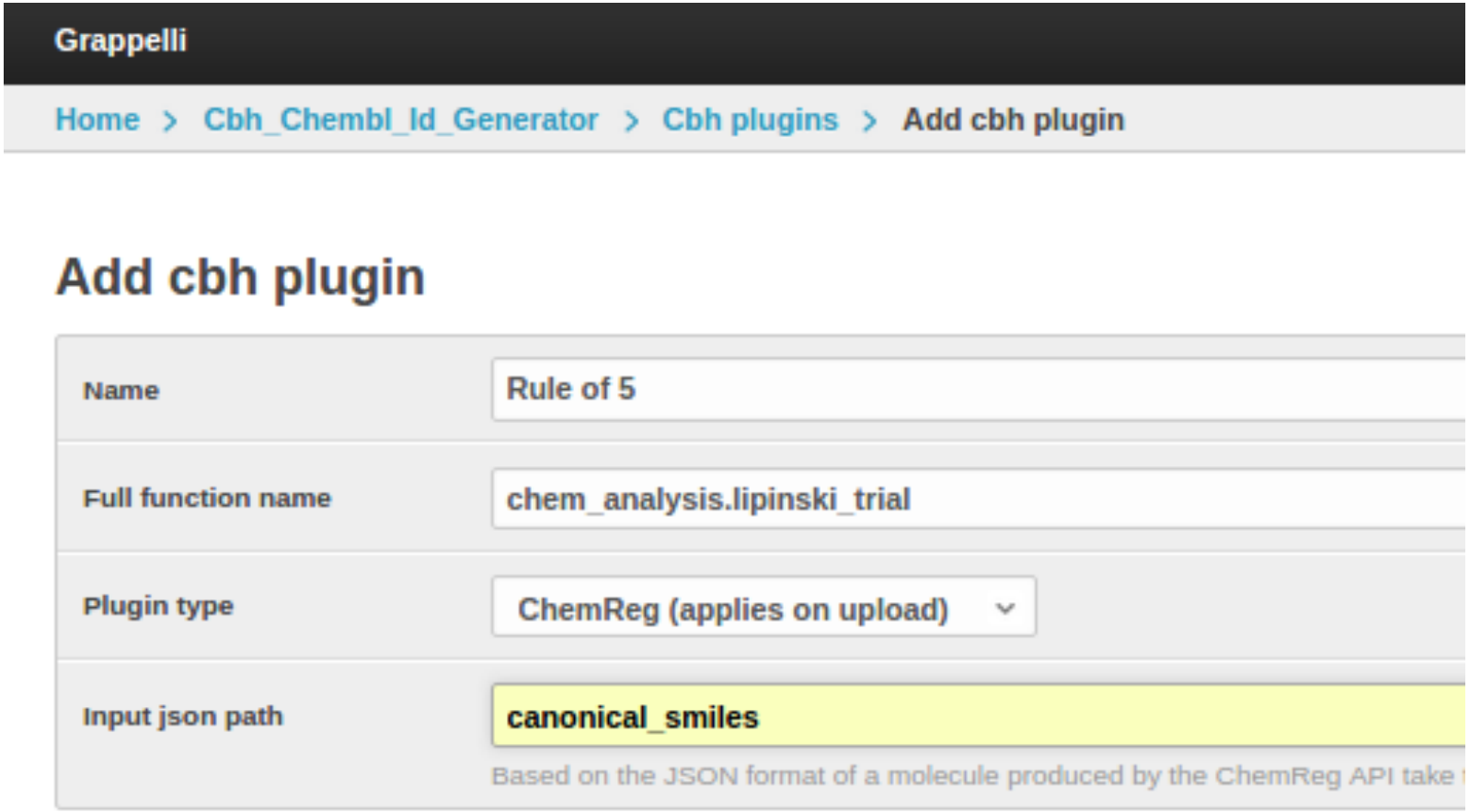
Add your fields here:

- Currently being used in 10 departments around Oxford for diverse areas such as materials science, plasmid studies and drug discovery chemistry

UNIVERSITY OF OXFORD

ChemBio Hub

Adding plugins for descriptors and data integrations



https://github.com/fergaljd/cyclops/blob/ef0e16a471027bfc48cea37c6ded617de36bc697/PepLibGen/Analysis/chem_analysis.py

Open to other plugin options e.g. Propbox, Zato ESB

ChemBio Hub AssayReg

- Make the data model tree-based
- Allow registration of peptides and proteins
- Allow export to ChEMBL and PubChem
- Data remapping will be via JSON patch language

https://github.com/thesgc/cbh_datastore_model/blob/master/cbh_datastore_model/models.py#L28

UNIVERSITY OF OXFORD

ChemBio Hub

ChemBio AssayReg

View Data >>

Study *last modified on Aug 13, 2015*

View Details | Add Study

Assay *last modified on Aug 13, 2015*

View Details | Add Assay

Activities *last modified on Aug 13, 2015*

Add Activity

Experiment ID	Purification ID	Protein Concetration	Plate Well ID	1st compound concentration	1st compound ID	1st compound name	Buffer ID	2nd compound concentration	2nd compound ID	2nd compound name	Tm valu

What we are looking for at RDKit UGM

- Use cases at other universities

- Help with registering similar molecules without annoying chemists (tick)

- Approaching the registration of peptides (tick)

- Speed up installation with conda to allow different VMs

- Get rid of the OpenBabel code (e.g. PAINS filters) so that we are fully Apache compliant (tick)
- Tell us where the documentation is poor and we will change
- https://github.com/thesgc/chembiohub_helpdesk/issues

Thanks

andrew.stretton@chembiohub.ox.ac.uk
chembiohub.ox.ac.uk

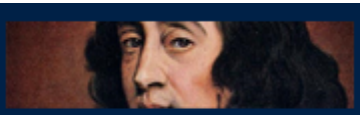
- Paul Barrett, Karen Porter, Brian Marsden, Adam Hendry and all the team at the SGC

- Many academics around Oxford

- ChEMBL team, especially Michal Nowotkna

- Funders

Nuffield Department of Medicine
Medical Sciences Division
Supported by wellcome trust
HIGHER EDUCATION FUNDING COUNCIL FOR ENGLAND hefce



To You for listening! Check out https://github.com/thesgc/chembiohub_ws