Chemical Biology Resources @EMBL-EBI

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EMBL-EBI

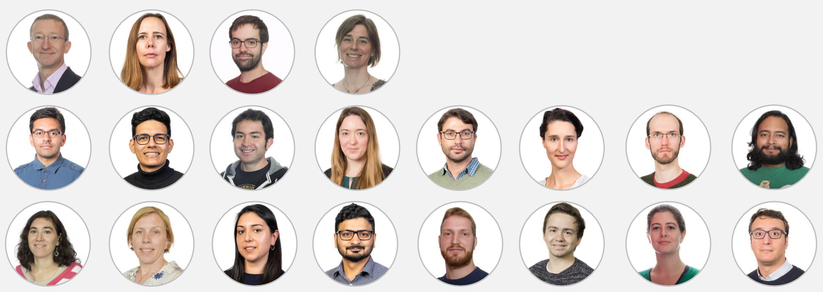
2004 ChEBI ~60K structures

2009 ChEMBL >2m structures

2013 UniChem Links ~40 resources >175m structures

2014 SureChEMBL >20m structures

Chemical Biology Resources Team

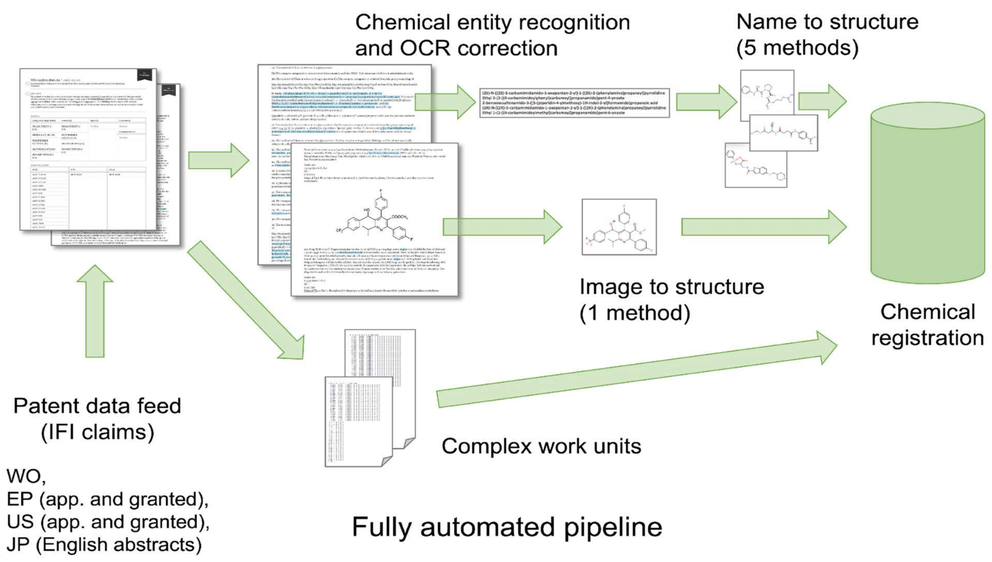


SureChEMBL Facts

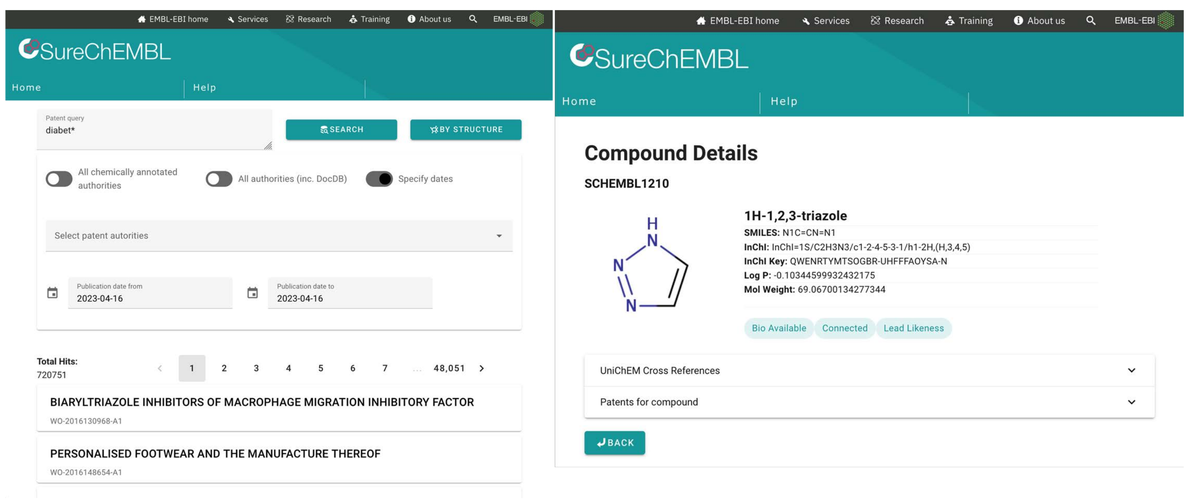
145M Patents | 26M Documents | 24.5M Chemicals | 105K BioAnnotations

SureChEMBL Pipeline

- SureChEMBL is a publicly available large-scale resource that contains compounds extracted on a daily basis from the full text, images and attachments of patent documents, through an automated text and image-mining pipeline



New SureChEMBL UI



SureChEMBL New Architecture Features

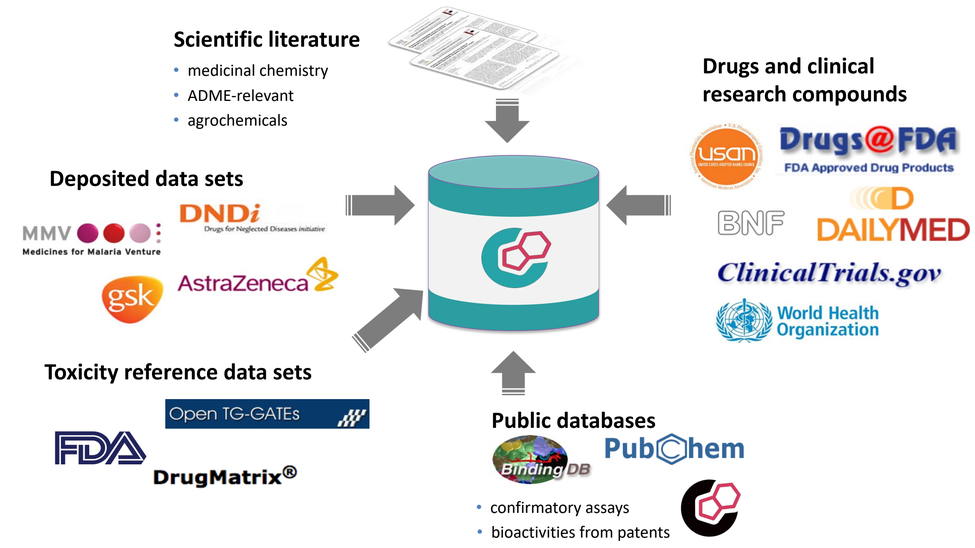
- Scalable Kubernetes Microservice Architecture
- Pipeline Moved from AWS SQS to Kafka
- No Lucene Dependency
- Modern Mobile Friendly UI(Aligned with EBI Standards)
- Biological Annotations in Data Exports
- Public API

ChEMBL facts

15,398 Targets | 2,399,743 Distinct compounds | 20,334,684 Activities | 88,630 Publications | 215 Deposited Datasets

Current Release: ChEMBL 33

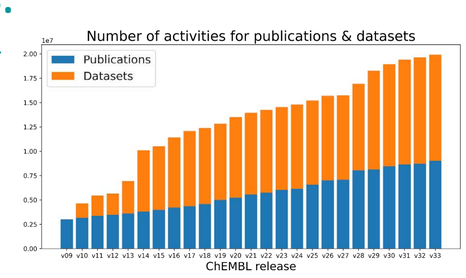
Last Update on 2023-05-31



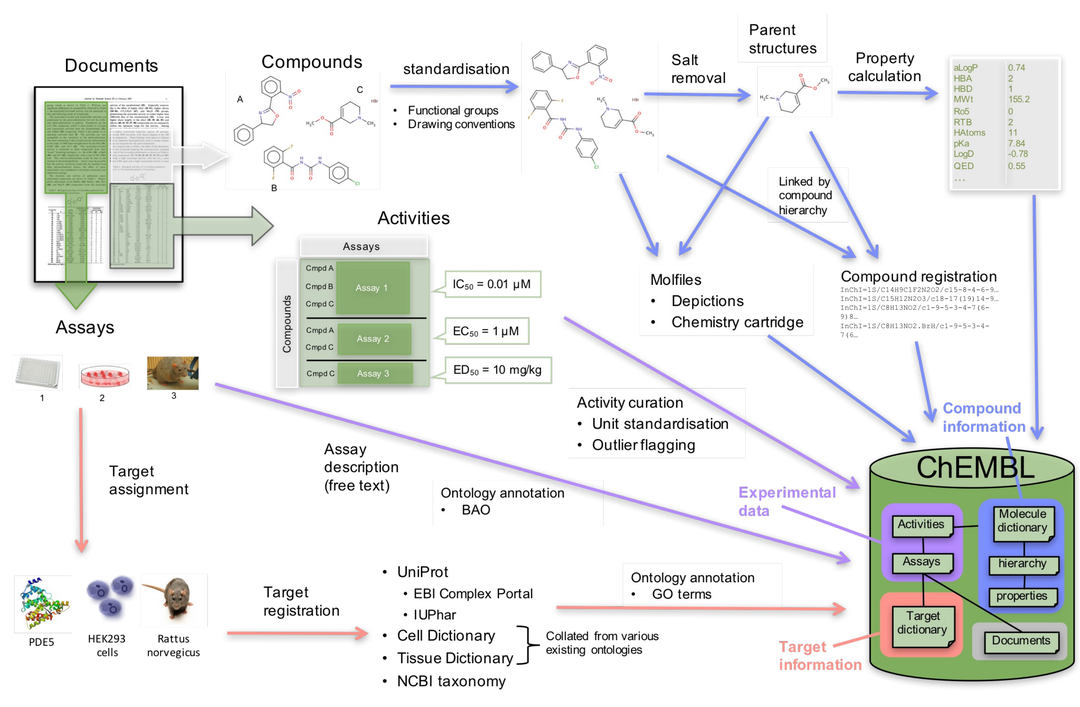
- ChEMBL integrates bioactivity data from diverse data sources
- Open, FAIR, extensively curated and high-quality drug-discovery data
- Bioactivities from Deposited Data Sets are now equal in number compared to those from published MedChem literature

New data & new features in ChEMBL 33:

- Bioactivity data on understudied SLC transporters from IMI-RESOLUTE
- New Chemical Probe data from IMI-EUbOPEN
- Flag for Natural Products: annotations from COCONUT
- Flag for Chemical Probes: from chemicalprobes.org
- Action_Type (e.g., inhibitor, substrate): now available for ca. 270K bioactivities!!



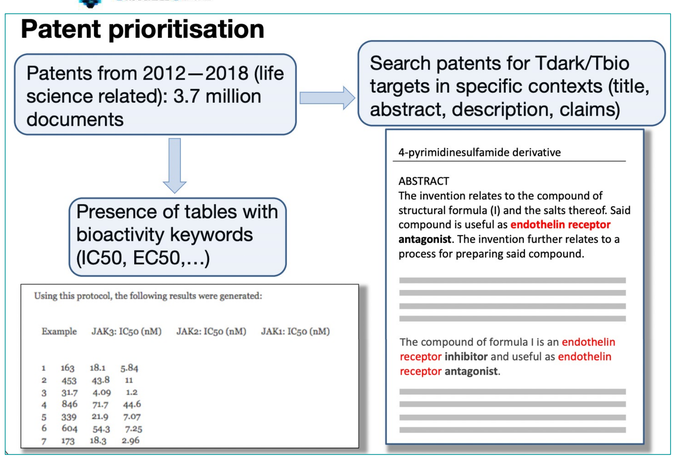
Curation & Standardization in ChEMBL



Patent data in ChEMBL

IDG Illuminating the Druggable Genome

BindingDB



ChEMBL contains bioactivity data for selected patents from **SureChEMBL** (www.surechembl.org) & **BindingDB**

Recently, 3.7 Mio life science relevant patents were prioritised in order to extract bioactivity data for T_{dark} & T_{bio} targets from **SureChEMBL**

190 patents had data for 152 T_{dark} & T_{bio} targets

76 T_{dark} & T_{bio} targets are annotated to at least 1 active compound (according to IDG activity cut-off's)

Open Targets | GLOBAL BIODATA COALITION | innovative medicines initiative | EUROPEAN COMMISSION | NIH | SGC | wellcome trust Strategic Award | EMBL-EBI

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