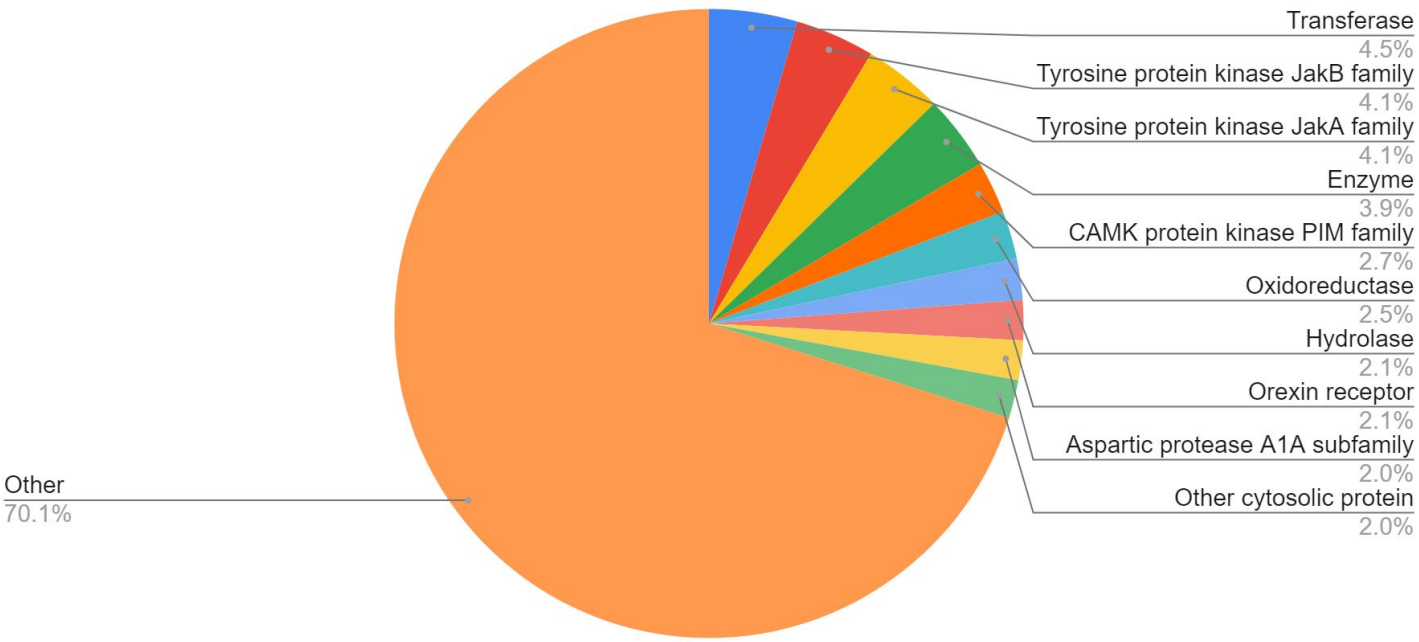
MCULE BIOACTIVITY LIBRARY

MCULE BIOACTIVITY LIBRARY CONTAINS PURCHASABLE MOLECULES POSSESSING ACTIVITY DATA ON AT LEAST ONE KNOWN TARGET IN THE SUBMICROMOLAR (<1 μM) CONCENTRATION RANGE.

The key features of the Mcule Bioactivity Library are the followings:

- The bioactivity data are derived from the ChEMBL database,
- Bioactivity data derived from multiple experiments are listed in separate columns
- Molecules are labeled with both Mcule and ChEMBL IDs.
- The number of covered protein classes is 336.

The distribution of the most frequent protein classes:



Click **here** to access the downloadable data file of the Mcule Bioactivity Library, inside the ZIP file you will find two CSV.GZ files one for all activities and one capped at maximum 100 activities/compound. If you would prefer another molecular format or a further customized library contact us at **support@mcule.com**.

The CSV files contains the following information:

Compound identification info:	Bioactivity data*:
• canonical SMILES strings	• **Target type:** TargetDictionary_target_type
• Mcule IDs	• **Target class:** ProteinClassification_pref_name
• ChEMBL IDs	• **Target ChEMBL ID:** TargetDictionary_chembl
	• **Target name:** TargetDictionary_pref_name
	• **Target's organism:** TargetDictionary_organism

*Column names in the header are identical to the names used in the ChEMBL database.

Please note that the salt forms, stereoisomers and charges may be different from the published molecules for which the activity data were measured. If you would like to check the forms of the original CHEMBL molecules you can do a look-up at https://www.ebi.ac.uk/chembl/g/#search_results/all using the enclosed ChEMBL IDs.

In the max100activity file we made an upper cap for the number of activities per compound because there are structures in the ChEMBL database with more than 100 activities (the max is above 2,500). This file can be more easily opened by Excel as a table.

Did you know?

Mcule provides professional laboratory services including:

- **Mcule Express Compound Inventory System™** - powered by robotized cold room sample storage
- **Mcule Client Portal™** - a cloud-based platform for real-time online sample management
- **Custom formatting** - Solid weighing, robotized dissolution and pipetting
- **Experimental sample characterization** - Structure identity, purity, solubility and reactivity analysis
- **Comprehensive logistic services**- Compound procurement, sample management, customs clearance and worldwide delivery

Mcule provides professional cheminformatics services including:

- **Custom library design** - using a wide range of ligand- and structure-based molecular modeling and cheminformatic approaches including physicochemical property calculations, molecular fingerprint based similarity and substructure searches, diversity selection, similarity clustering, scaffold hopping, toxicity filtering, PAINS and other unwanted substructure filters, molecular docking, etc. Custom library generation workflows can be applied on the Mcule Database or Mcule ULTIMATE database
- **Generation of synthetically feasible chemical universes** - based on specific building blocks and reaction rules

Mcule's Custom Solution Experts are ready to guide you through the selection and ordering process free of charge! If you have any questions or need any help, please feel free to contact us at **support@mcule.com.**