Mcule - Chemical Probes Portal subset

The Chemical Probes Portal[1] is a public resource which enables scientists to find and use small-molecule reagents – so-called Chemical Probes – to interrogate protein targets in biomedical research and drug discovery. Hundreds of compounds have been evaluated and reviewed by a diverse group of experts in the field of chemical biology, medicinal chemistry, pharmacology and related disciplines. This is to provide advice and recommendations about how to best use these tools for a given protein target.

In the Mcule - Chemical Probes Portal subset, we have collected compounds from the Mcule aggregated catalogs that have an equivalent Chemical Probes Portal entity with at least a 3-star rating on the Chemical Probes Portal from the maximum rating of 4 about its in-cell or *in vivo* performance. The dataset contains the following data for each entry:

SMILES (in Mcule BD), Mcule_ID, Chemical Probes Portal ID, Probe name, Rating in cell, Rating in organism, Number of Ratings, URL, Target name, Target class, Target subclass, Published on, Uniprot ID, InChI key, SMILES (in Chemical Probes DB), PAINS, Toxicophore, canSAR ID, Reference (PMID), Mechanism of action, Potency value, Potency assay, Potency value in cells, Potency assay (cells), Potency in cells, Organism, Dose, Control compound

More details about the data types can be found here.

Reference:

[1]*Albert A Antolin, Domenico Sanfelice, Alisa Crisp, Eloy Villasclaras Fernandez, Ioan L Mica, Yi Chen, Ian Collins, Aled Edwards, Susanne Müller, Bissan Al-Lazikani, Paul Workman,* The Chemical Probes Portal: an expert review-based public resource to empower chemical probe assessment, selection and use, *Nucleic Acids Research*, Volume 51, Issue D1, 6 January 2023, Pages D1492–D1502

If you would prefer other molecular format or further filtering - feel free to contact us at support@mcule.com.

Our professional laboratory services include

- Transferring samples to plates/vials as solid or DMSO solution
- Solubility characterization
- Temperature controlled shipping
- Quality control via LC-MS & NMR (on demand)

Please also reach out to our cheminformatics experts with projects related to

- Screening library building/expansion
- Generation of synthetically feasible chemical spaces based on your building blocks
- Filtering the Mcule database based on your criteria