

European Chemistry Congress

June 16-18, 2016 Rome, Italy

Data mining drug, chemical probe and their biological activity in PubChem

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The PubChem Project started in 2004 by the National Center for Biotechnology Information (NCBI) at NIH to provide an open repository for chemical structures and research data supporting open access. The PubChem databases experienced a tremendous growth over the past decade and now contain 150 million substance submissions, one million bioassay submissions and 200 million bioactivity outcomes. The biological test result in the BioAssay database largely consists of high throughput screening (HTS) data generated from the NIH efforts in the discovery of chemical probes, which may be used as tools for studying biological functions of proteins and genes. During the development of chemical tools, a compound library of over 400,000 compounds, including many drug molecules, were screened towards many biologically important and disease associated molecular targets and cell lines, producing a huge amount of information for pursuing drug repositioning. The chemical probes from the HTS campaigns demonstrated high selectivity and potency as agonists and antagonists for specific molecular targets. For many of these, the utility of the tools remain to be validated and utilized by researchers, and the mechanism of action may be further explored. Literature based bioactivity data, contributed by journal authors and curation projects, such as ChEMBL and PDBeBind, represents another important component of the BioAssay database. The integration of literature data and HTS greatly facilitates comparison to prior arts and systematic investigation on drugs and their potential targets. This presentation will provide an overview of the biological activity information in PubChem, and a review how these information are used by the community in drug discovery and development. Data in PubChem can be freely accessed and downloaded using the NCBI information retrieval system Entrez, with additional suite of services. PubChem welcomes further contributions from the community for sharing experimental and annotation data. Chemical structures and assay results can be deposited via the submission tool; new functions have been developed recently facilitating data management and release to synchronize with manuscript review and paper publication process.

Biography

Yanli Wang obtained her PhD in Computational Biology in 1995 from Peking University, China and completed Post-doctoral studies from the National Institute of Cancer and National Center for Biotechnology Information (NCBI) during 1995-1998. She is currently the lead Scientist of NCBI, primarily responsible for managing the PubChem BioAssay resource. She has published more than 40 papers in reputed journals.

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