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PubChem bioassay: A public information resource supporting medicinal chemistry and drug discovery research

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The PubChem Bioassay database, created in 2004 by National Center for Biotechnology Information (NCBI) at NIH, serves as a public repository of bioactivity data for drugs, chemical probes, small molecules, and screening results for RNAi reagents. The database currently contains over 1,000,000 bioassay protocols and more than 200 million of bioactivity outcomes for thousands of protein and gene targets and nearly three million substances. Information in PubChem can be freely accessed and downloaded using the NCBI information retrieval system Entrez and a suite of services provided by PubChem. This presentation will describe PubChem utilities. In addition, a recent bibliometric analysis on applications of the PubChem resource by the community will also be described, which indicates that PubChem has been utilized by a broad range of research fields in the past ten years, and is becoming an important information resource for a number of research fields such medicinal chemistry, drug discovery, chemical biology and cheminformatics. In particular, the analysis shows an increasing trend in supporting wet laboratory research towards lead development and drug discovery using the bioassay data. PubChem welcomes feedback on the usability of the information platform and welcomes contributions from the community by sharing data. Chemical structures and assay results can be deposited via the PubChem submission system.

Biography

Yanli Wang obtained her PhD in Computational Biology in 1995 from Peking University, China and completed Postdoctoral 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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