

1.2: Brief History of Cheminformatics

when are you going to finish the database sections?

Introduction

There are multiple surveys on the history of cheminformatics. As these are owned by publishing companies we can not share them online. See you instructor if you do not have access, as we do have the ability to share them within our class rooms.

Restricted Access Sources

1. [Cheminformatics: a history](#), by Peter Willet. *WIREs Comput Mol Sci* 2011, 1: 46-56. doi: 10.1002/wcms.1
 - o 11 pages with 91 references published in 2011.
 - Abstract: This paper gives a brief history of the development of chemoinformatics since the first studies in the late 1950s and early 1960s of methods for searching databases of chemical molecules and for predicting their biological and chemical properties. Topics, and associated key papers, that are discussed include: structure, substructure, and similarity searching; the processing of generic chemical structures and of chemical reactions; chemical expert systems; the identification of qualitative and quantitative structure–activity relationships in both two and three dimensions; pharmacophore analysis; ligand–protein docking; molecular diversity analysis; and drug-likeness studies. Brief mention is also made of other important areas such as computer-assisted synthesis design and computer-assisted structure elucidation.
2. [Chemoinformatics - An Introduction for Computer Scientists](#), by Nathan Brown, *ACM Comput. Surv.* 41, 2, Article 8 (February 2009), DOI: 10.1145/1459352.1459353
 - o 28 pages, 75 references, published in
 - Excellent introductory article, sections 1.4 (Origins of Chemoinformatics) and 2 (Chemistry and Graph Theory) are interesting reads.
3. [Chemoinformatics: Past, Present, and Future](#), by William Lingran Chen. *Journal of Chemical Information and Modeling* **2006** 46 (6), 2230-2255. DOI: 10.1021/ci060016u
 - o 26 pages with 332 references, published in 2006.
 - Abstract: The history of chemoinformatics is reviewed in a decade-by-decade manner from the 1940s to the present. The focus is placed on four traditional research areas: chemical database systems, computer-assisted structure elucidation systems, computer-assisted synthesis design systems, and 3D structure builders. Considering the fact that computer technology has been one of the major driving forces of the development of chemoinformatics, each section will start from a brief description of the new advances in computer technology of each decade. The summary and future prospects are given in the last section.

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