DISCUSSION PUBLISHERS
Research Center · Open Access Edition

Machine learning in chemoinformatics and drug discovery

YuChen Lo, Stefano Rensi, Wen Torng, Russ Biagio Altman

Discussion Research ID	DPR-2026-1138
Year	2018
Field	Computer Science
DOI	10.1016/j.drudis.2018.05.010
Author ORCID	0000-0002-9309-4098
Licence	CC-BY
Original source	Drug Discovery Today
Permanent link	https://discussionpublishers.com/research/83f9cef4-1832-4f52-93d3-25a442562435
Publisher	Discussion Publishers discussionpublishers.com

Republished by Discussion Publishers under the original CC-BY licence. Copyright remains with the original authors; please cite the original work.

Cite as: YuChen Lo, Stefano Rensi, Wen Torng, Russ Biagio Altman (2018). Machine learning in chemoinformatics and drug disc. Discu

Abstract

Chemoinformatics is an established discipline focusing on extracting, processing and extrapolating meaningful data from chemical structures. With the rapid explosion of chemical 'big' data from HTS and combinatorial synthesis, machine learning has become an indispensable tool for drug designers to mine chemical information from large compound databases to design drugs with important biological properties. To process the chemical data, we first reviewed multiple processing layers in the chemoinformatics pipeline followed by the introduction of commonly used machine learning models in drug discovery and QSAR analysis. Here, we present basic principles and recent case studies to demonstrate the utility of machine learning techniques in chemoinformatics analyses; and we discuss limitations and future directions to guide further development in this evolving field.

Keywords: machine learning, cheminformatics, drug discovery, QSAR, chemical data processing, chemical database

Full text

The complete text of this work is hosted by its original publisher.
Read it via the Discussion Publishers page:
https://discussionpublishers.com/research/83f9cef4-1832-4f52-93d3-25a442562435

Original record: https://doi.org/10.1016/j.drudis.2018.05.010
DOI: https://doi.org/10.1016/j.drudis.2018.05.010