

Publication

A Binary Ant Colony Optimization Classifier for Molecular Activities

JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)

ID 973987

Author(s) Hammann, Felix; Suenderhauf, Claudia; Huwyler, Jörg

Author(s) at UniBasel [Huwyler, Jörg](#) ; [Hammann, Felix](#) ; [Sünderhauf, Claudia](#) ;

Year 2011

Title A Binary Ant Colony Optimization Classifier for Molecular Activities

Journal Journal of Chemical Information and Modeling

Volume 51

Number 10

Pages / Article-Number 2690-6

Chemical fingerprints encode the presence or absence of molecular features and are available in many large databases. Using a variation of the Ant Colony Optimization (ACO) paradigm, we describe a binary classifier based on feature selection from fingerprints. We discuss the algorithm and possible cross-validation procedures. As a real-world example, we use our algorithm to analyze a Plasmodium falciparum inhibition assay and contrast its performance with other machine learning paradigms in use today (decision tree induction, random forests, support vector machines, artificial neural networks). Our algorithm matches established paradigms in predictive power, yet supplies the medicinal chemist and basic researcher with easily interpretable results. Furthermore, models generated with our paradigm are easy to implement and can complement virtual screenings by additionally exploiting the precalculated fingerprint information.

Publisher American Chemical Society

ISSN/ISBN 0095-2338

URL <http://www.ncbi.nlm.nih.gov/pubmed/21854036>

edoc-URL <http://edoc.unibas.ch/dok/A5849088>

Full Text on edoc No;

Digital Object Identifier DOI 10.1021/ci200186m

PubMed ID <http://www.ncbi.nlm.nih.gov/pubmed/21854036>

ISI-Number WOS:000296044200022

Document type (ISI) Journal Article