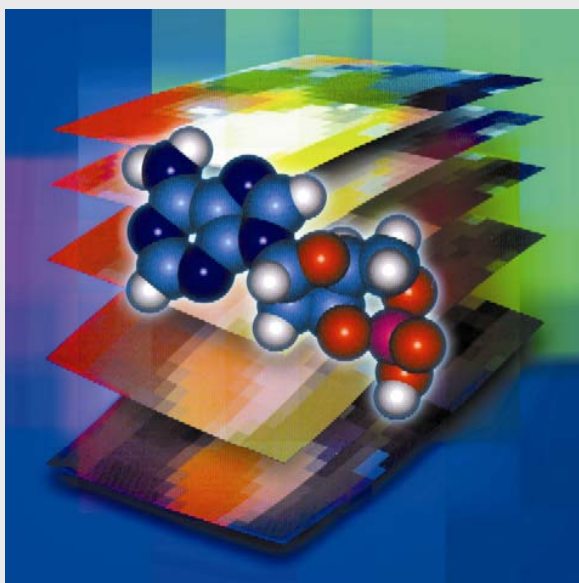


SONNIA

Data Analysis by Neural Networks

SONNIA offers an interactive and visual approach to the analysis of chemical structure and reaction information based on a self-organizing neural network technique. **SONNIA** can be utilized for the prediction of physical, chemical and biological properties of compounds and for analyzing chemical reaction information.



SONNIA enables computational chemists and chemoinformaticians to model complex relationships and to better understand their data. It allows the finding and optimization of new chemical entities with specific chemical or biological properties.

SONNIA provides highly interactive and visual methods and, thus, assists scientists in gaining knowledge from data faster. One-click access to the underlying data, such as chemical structure, reaction and related information, helps to quickly identify relationships between chemical objects and measured or calculated properties and to make better decisions about the next steps in any research project.

Key Features

- Analysis and visualization of large, multivariate chemical datasets including chemical structure and related information
- Classification, prediction and modeling of complex linear and non-linear chemical and biological relationships
- Highly interactive and intuitive graphical user interface
- Support of standard file formats for data and structure/reaction input (*e.g.*, TSV, MDL SD/RDFile, SMILES)
- Interface to the descriptor calculation package **ADRIANA.Code**

Areas of Application

- Qualitative and quantitative structure-activity and property relationships (QSAR/QSPR)
- Modeling of ADMETox properties
- Analysis of HTS data and results
- Hit identification and lead optimization
- Analysis of the similarity and diversity of combinatorial libraries and compound collections
- Selection of chemical descriptors
- Prediction of chemical reactivity and reaction classification
- Simulation of infrared spectra



Molecular Networks
Inspiring Chemical Discovery

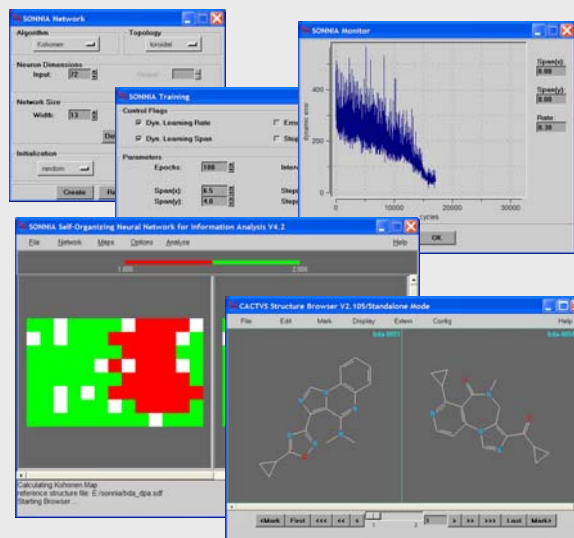
SONNIA

Data Analysis by Neural Networks

The data analysis engine of **SONNIA** contains both unsupervised and supervised learning methods, suitable either for classification or prediction of chemical data and objects.

Chemical datasets, characterized by a variety of molecular descriptors can be projected into a two-dimensional map by an unsupervised non-linear mapping technique. The projections are visualized as interactive 2D maps (Kohonen maps), color-coded by the property under investigation and fully linked to the underlying chemical information. This allows the chemical objects to be correctly assigned to a certain property class.

In addition, a supervised counter-propagation neural network technique can be applied to quantitatively predict properties.



Technical Features

- Graphical user interface and optional batch mode execution
- Interface for integration into company's internal IT environments and workflows
- Export of generated maps in standard graphics format
- Default but user-editable values for all control and learning parameters
- No limitations concerning number of molecules or objects

System Requirements

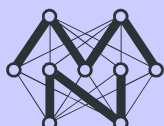
SONNIA is available for Microsoft® Windows® platforms and x86 Linux systems (32 and 64 bit).

References

- J. Zupan, J. Gasteiger, *Neural Networks in Chemistry and Drug Design*, 2nd Edition, Wiley-VCH, Weinheim, **1999**.
- L. Terfloth, J. Gasteiger in *The Practice of Medicinal Chemistry*, 2nd Edition, C.G. Wermuth (Ed.), Elsevier, Amsterdam, NL, **2003**, p. 131-145.
- J. Gasteiger, A. Teckentrup, L. Terfloth, S. Spycher *J. Phys. Org. Chem.* **2003**, *16*, 232-245.

Test Version

A 30 days evaluation copy of **SONNIA** is available free of charge in the Download Area of the web server of Molecular Networks at www.molecular-networks.com.



Molecular Networks
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