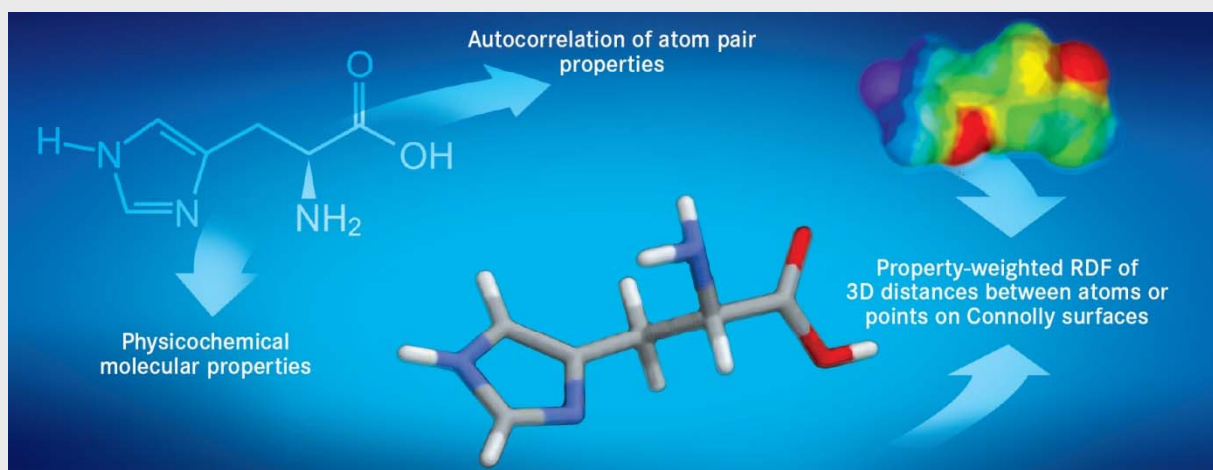


ADRIANA.Code

Fast Calculation of Physicochemical Descriptors

ADRIANA.Code calculates a series of molecular descriptors that can be applied in the area of *in silico* discovery and optimization of new chemical entities. **ADRIANA.Code** comprises a unique combination of methods that encode fundamental physicochemical effects and clear-cut geometric features of molecules.

The molecular descriptors calculated by **ADRIANA.Code** are ready to be used with data analysis software for the modeling and prediction of physical, chemical and biological properties of chemical compounds.

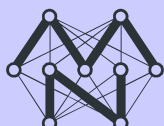


Key Features

- Fast and reliable conversion of compound datasets into uniform descriptors encoding structural and physicochemical features of molecules
- Internal generation of 3D structures based on **CORINA**
- Unique empirical methods for the internal calculation of atomic properties, *e.g.*, partial charges based on the Gasteiger-Marsili algorithm
- Applicable to a broad range of organic chemistry

Areas of Application

- Drug design, *e.g.*, lead identification and optimization
- Property prediction, *e.g.*, ADME/Tox properties or in QSAR/QSPR studies
- Similarity perception, *e.g.*, in ligand-based virtual screening experiments
- Classification and clustering of compounds according to a certain property under investigation
- Analysis of results and data of high-throughput screening
- Simulation of infrared and ^1H NMR spectra



Molecular Networks
Inspiring Chemical Discovery

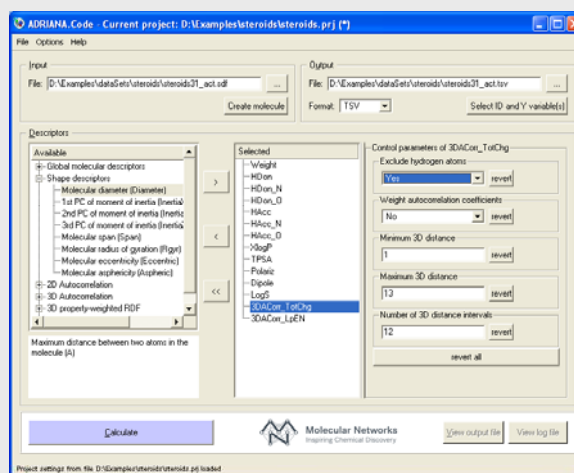
ADRIANA.Code

Fast Calculation of Physicochemical Descriptors

ADRIANA.Code calculates molecular descriptors on different levels of sophistication and resolution that can be selected and adapted to the needs of the user. Chemical compounds are represented from the constitution (2D) through the 3D structure to the surface of a molecule. At each level, a wide range of physicochemical effects can be considered.

ADRIANA.Code descriptors provide a uniform representation of molecules comprising different scaffolds and varying number of atoms. Therefore, the descriptors are directly amenable to data analysis methods such as techniques for similarity perception, statistical and pattern recognition methods or neural networks.

All methods implemented in **ADRIANA.Code** are optimized for speed and accuracy and are rapid enough to calculate descriptors for datasets comprising millions of compounds.



Technical Features

- Graphical user interface and optional batch mode execution
- Interface to the neural networks package **SONNIA** (also available from Molecular Networks) and Microsoft® Excel®
- Interface for integration into internal IT environments and workflows
- Also available as component for Accelrys Pipeline Pilot®

System Requirements

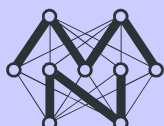
ADRIANA.Code is available for Microsoft® Windows® platforms and x86 Linux systems (32 and 64 bit).

References

- J. Gasteiger
J. Med. Chem. **2006**, *49*, 6429-6434.
- L. Terfloth, J. Gasteiger
in *The Practice of Medicinal Chemistry*, 2nd Edition, C.G. Wermuth (Editor), Elsevier, Amsterdam, NL, **2003**, 131-145.

Test Version

A 30 days evaluation copy of **ADRIANA.Code** 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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