



# Molecular Networks

Inspiring Chemical Discovery

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July 16, 2008

## New Features in **ADRIANA.Code** Version 2.2

Several new features have been implemented in order to improve and extend the functionality, the usability and the range of applications of **ADRIANA.Code**.

In the following, a brief description of the most significant improvements and features is given. For further information, please refer to the **ADRIANA.Code** user manual that can be downloaded free of charge from Molecular Networks' web server at [www.molecular-networks.com/software/adrianacode/adrianacode\\_manual.pdf](http://www.molecular-networks.com/software/adrianacode/adrianacode_manual.pdf).

- (1) The algorithms in **ADRIANA.Code** have been extended and improved to handle and process **charged molecules**. Especially, the routines for the calculation of atom charges ( $\sigma$  and  $\pi$ ) and electronegativities ( $\chi$ ) were newly parametrized for charged molecules.
- (2) The following molecular descriptors have been added to the category of **Global Molecular Descriptors**.
  - Number of rotatable bonds
  - Number of Lipinski's "Rule of 5" violations
  - Number of extended Lipinski's "Rule of 5" violations
  - Number of atoms
  - Number of tetrahedral stereocenters
  - Hendrickson molecular complexity
  - Gasteiger-Jochum ring complexity

Further details about all global molecular descriptors are given in section "Global Molecular Descriptors" on page 33 as well as in the Appendix B of the user manual.

- (3) A new descriptor category of **Size and Shape Descriptors** has been implemented. The following size- and shape-related descriptors can now be calculated.
  - Molecular diameter
  - Principle moment of inertia of the 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> principle axis
  - Molecular span
  - Molecular radius of gyration
  - Molecular eccentricity
  - Molecular asphericity

Further details about the newly implemented size- and shape-related descriptors are given in section "Size and Shape Descriptors" on page 34 as well as in the Appendix B of the user manual.