



SOFTWARE

AntiBase 2012 - The Natural Compound Identifier

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Software
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Description

Progress in natural products chemistry today is progress in synthetic chemistry tomorrow. Structure determination of complex natural products delivers not only the most interesting, the most challenging targets for synthetic chemists, but is also the basis of new medical applications of the future. There is no doubt that natural product's isolation and structure identification is still one of the most important areas in chemistry.

An army of scientists tries to discover with unlimited effort a limited number of natural metabolites: More than 170.000 natural products are known today, and every year are added about 700 new structures just only from micro-organisms. This gives raise to a major problem in natural product chemistry: It is unavoidable that certain common compounds are re-isolated again and again, a handicap which costs time and money, and is a steady source of avoidable frustration

Antibase 2011, the Natural Compound Identifier, is a comprehensive database of more than 38,843 natural compounds from micro-organisms and higher fungi.

The data in AntiBase have been collected from the primary and secondary literature and then carefully checked and validated. AntiBase includes descriptive data (molecular formula and mass, elemental composition, CAS registry number); physico-chemical data (melting point, optical rotation); spectroscopic data (UV, ¹³C-NMR, IR and mass spectra); biological data (pharmacological activity, toxicity); information on origin and isolation and a summary of literature sources

A unique feature of AntiBase is the use of predicted ¹³C-NMR spectra for those compounds where no measured spectra are available. These spectra have been produced using the spectrum prediction program SpecInfo.

Calculated high resolution molecular masses are included in the new update

AntiBase is available in the database formats ISIS/Base (MDL) and ChemFinder (CambridgeSoft)

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