AntiBase - A Natural Products Database for Rapid Structure Determination

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Analytical natural products' research is a job with high risk: More than 110,000 natural products (about 20,000 from microorganisms) are known, and every year more than 2000 new compounds (600 from microorganisms) are added. The chance to isolate a new metabolite is decreasing therefore, but increasing is the probability to re-isolate compounds which are already known. AntiBase helps to minimise this risk.

AntiBase is a comprehensive database of more than 21,000 natural compounds from microorganisms and higher fungi, including yeasts, ascomycetes, basidiomycetes, lichens, algae, and of quinones and carotenoids from other sources. The collection covers even the most recent work and contains information from the primary and secondary literature. All the data have been critically examined and, where necessary, corrected. AntiBase is carefully maintained and regular updates are available.

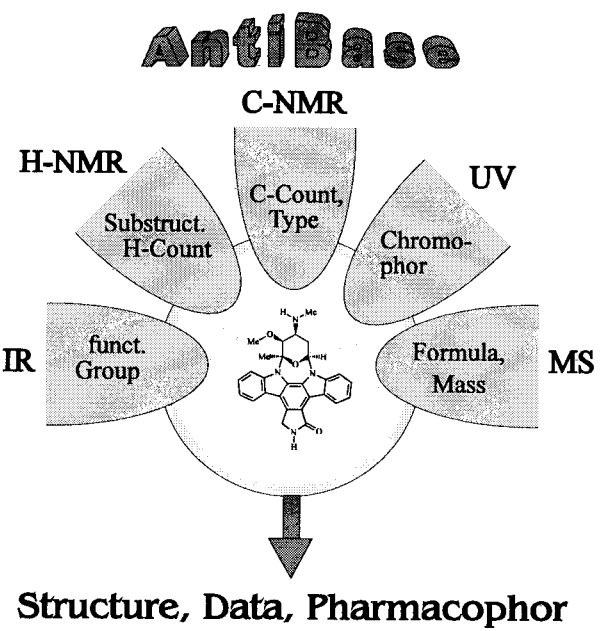
AntiBase contains:

- chemical structures
- CAS Registry numbers
- information on origin and isolation
- structure-connected ^{13}C-data
- biological activity
- names and synonyms
- natural sources
- physical properties
- other spectral data (UV, NMR, IR)
- literature references

AntiBase is designed for use with MDL's ChemBase or ISIS/Base. Structure or substructure searches can be combined with text searches and range searches of numerical data. By linking structural information with a wide range of spectroscopic and microbiological properties, it is possible to identify these types of natural products quickly and reliably.

Using the powerful search capabilities of ChemBase or ISIS/Base, simple NMR spectra are very often sufficient for structure identification: Even a search by the number of quaternary C atoms, which is easily determined from ^{13}C spectra, or the number of carbonyl, methine or methylen groups is possible. Also coupling patterns or signal shifts and multiplicities from ^{1}H NMR spectra can usually be translated into suitable sub-structures.

In addition to experimental data, AntiBase contains more than 17,000 SpecInfo-generated high quality ^{13}C-NMR spectra. This makes it very easy to search for distinct spectral data and to get structural hints also for new compounds.



Structure identification by overlapping fragmentary information with AntiBase

One of the most remarkable features of AntiBase is its capability in peptide identification. As also amino acid fragments can be used for a sub-structure search, the result of an amino acid determination after hydrolysis of a peptide, and perhaps determination of the N-terminal acid is sufficient in many cases to evaluate unambiguously most of the more than 1500 peptides in the data base.

AntiBase is distributed by Chemical Concepts, Boschstraße 12, D-69469 Weinheim, Germany.