

DATABASE OF SYNTHETIC AMINO ACIDS **WITH APPLICATIONS IN NANOBIOLOGY AND NANOMEDICINE**

Synthetic amino acids are becoming more important every day within the fields of Nanobiology and Nanotechnology. At the same time, the number of these compounds is growing at a startling rate. We have developed a **database** that contains the **intrinsic conformational properties** of the synthetic amino acids that have been characterized via quantum-mechanical calculations.

Who is it aimed at?

- Companies in the biotechnology sector
- Companies in the pharmaceutical sector
- Companies in the chemistry industry
- Research groups

What is it for?

To **systematically search for solutions** to problems that arise within the different fields of **Nanoscience**.

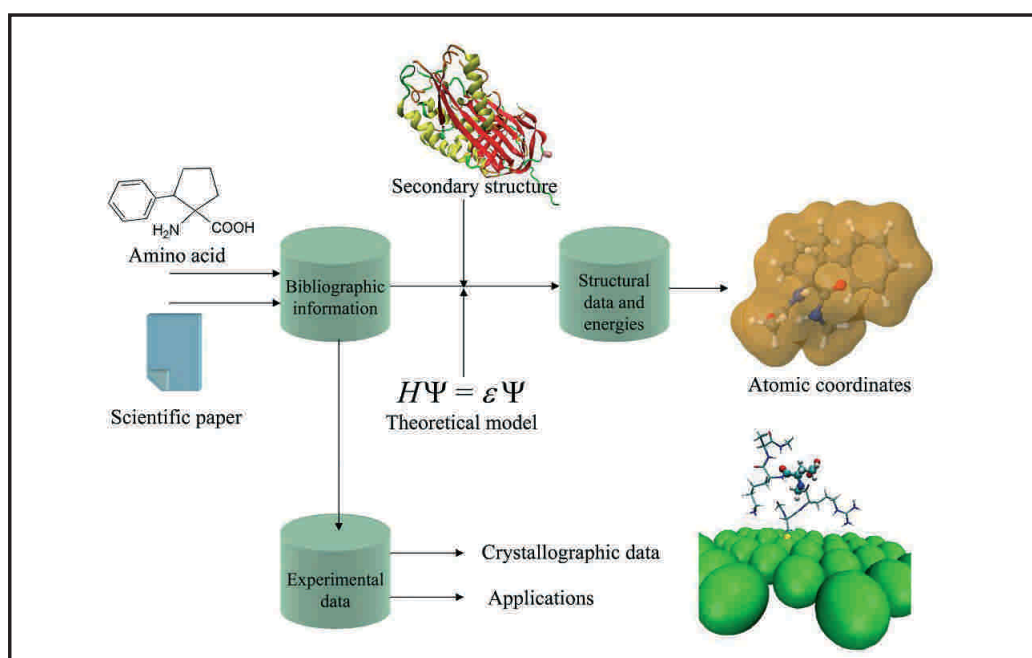
Examples:

- The protection of peptide systems from attack by proteases.
- Improving molecular recognition and the activity of antidiabetic and anticancer drugs.
- Establishing biosensor and protein nanostructures.
- The design of methods of diagnosis.
- The design of new polyamides with defined structures and controlled degradability, and nanotubular structures.
- The design of photovoltaic devices controlled by peptide foldamers and molecular actuators.
- The controlled design of bio-organic materials.

Characteristics of the technology

- In the database, the **amino acids are organized into different groups** according to the nature and the localization of the chemical modification introduced.
- Within each group, the following **information** is available for each amino acid:
 - the coordinates of the minimum energy obtained by quantum-mechanical calculations, the values of the relative energy and the distributions that are calculated based on these energies
 - identification of the accessible regions of the Ramachandran plot and their probability
 - bibliographical information about the available experimental data
 - the coordinates of the crystallized structures
 - applications in Nanobiology and Nanotechnology
- **Different criteria** can be used to **search for information** within the database, and these can be combined or applied individually.
- It works within a **graphic program** with a system of windows that makes both the searching and interpretation straightforward.
- This system of windows activates an external **3-dimensional graphic representation** program to visualize the minimums and the crystalline structures.

The database is accompanied by a program that can extract the **chemical and structural information** related to the selected amino acids in order to integrate it into **secondary structures and sequences defined by the user**; these can be **manipulated, minimized** and an **estimate of the energetic cost can be calculated** for the incorporation of the synthetic amino acid.



Flow diagram of the synthetic amino acid database with applications in Nanobiology and Nanotechnology.