

## APDbase: Amino acid Physico-chemical properties Database

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### Abstract:

Physico-chemical properties of amino acids can be used to study protein sequence profiles, folding and function. We collated 242 properties for the 20 naturally occurring amino acids and created a dataset. The dataset is available as a database named **APDbase** (Amino acid Physico-chemical properties Database). The database can be queried using either key words describing physico-chemical properties or pre-assigned database index number. The database contains corresponding references for each property value and facilitates deposition of new property values for processing and inclusion in the database.

**Availability:** The database is available for free at <http://www.rfdn.org/bioinfo/APDbase.php>

**Keywords:** physico-chemical properties; homology; amino acids; folding; function

### Background:

Proteins (composed of amino acids) constitute a major group of biological macromolecules that are key for the function of a living system. Protein evolution involves selection of sequences having functional advantage over random mutants. [1] Closely evolved proteins resemble the parent in their sequence, structure and function which are referred to as homologs. [2] Often multiple sequences (strings formed by different combinations of the 20 amino acid alphabets) have the same structure and function. This introduces functional redundancy to the sequence pool. Functional redundancy can be overcome by developing metrics for sequence comparison. Comparison of protein sequences should involve a metric for the 20 amino acids. Naturally occurring amino acids can be grouped based on their similarity of physico-chemical properties. In order to understand the conservation of residues in a protein sequence, it may be important to qualitatively and quantitatively measure the differences among residues. A collection of physico-chemical properties of amino acids will be helpful to study macroscopic properties of proteins (such as aggregation), perform sequence comparison or understand conservation of functionally important residues in a protein family (physico-chemical signatures).

### Methodology:

The site utilizes open-source software running on LINUX® platform to deliver the content. Flat files that contain indexed properties, author details and journal citations were created after curating the AAINDEX [3] database in DBGet (Japan) and ProtScale in Swiss Expasy.[4] We excluded properties that have missing values for any of the twenty amino acids and those that are less relevant to the study of protein sequence, structure and function. A search interface

is implemented in PHP driven by Zend engine. [5] Keyword search like hydrophobicity, charge, aromaticity and several others produces all listed properties in the dataset along with the journal citation. In order to facilitate future expansion, we have forms that the users can fill out to add new properties that will be audited for completion, accuracy and relevance by domain experts periodically. Numerical redundancy will be automatically avoided before incorporating into the dataset. A screen capture of the web-site is shown in Figure 1.

### Utility:

Protein sequence analysis, macroscopic property prediction, property motif identification and epitope prediction are of great interest to the biological community. Bioinformatics tools that perform such tasks are increasingly incorporating physico-chemical property based metric to increase their performance and to derive knowledge based rules. [6-8] APDbase was previously available as PDbase. [9] During 1999-2004 other groups have used this database for developing methods related to biological sequence analysis. [6] The previous database had 237 properties. The current dataset includes additional 5 properties that are PCP-descriptors derived elsewhere. [10]

### Limitations:

The dataset described here is a comprehensive sample of available properties for 20 naturally occurring amino acids. Nevertheless the dataset is not complete and requires regular updates. The dataset can be updated using property values derived from statistical analysis and experimental observations.

The screenshot shows the APDbase web interface in Microsoft Internet Explorer. The browser address bar shows <http://www.rfdn.org/bioinfo/APDbase.php>. The page title is "Amino acid physical chemical properties database". Below the title is the URL <http://www.rfdn.org/bioinfo/help.php> and navigation links: [ Query ] [ Add properties ] [ Help ] [ Author ].

The main content area is titled "Query Amino Acid Table". It features a search interface with the instruction "Specify either description or key, NOT both". There are two input fields: "Enter description to retrieve" (with the example "Hydrophobicity" and the text "E.g., Hydrophobicity index") and "Enter index" (with the example "15" and the text "E.g., 15"). An "OR" radio button is between the fields. Below the input fields are "SUBMIT" and "RESET" buttons. A black arrow points from the "SUBMIT" button to the search results table.

The search results are displayed under the heading "Search Results" with the text "Searching on description: Hydrophobicity". The results are shown in a table:

Index	1
Description	Hydrophobicity index (Argos et al., 1982)
Title	Structural prediction of membrane-bound proteins
Journal	Eur. J. Biochem. 128, 565-575 (1982)

Below the search results is a table titled "Matches found in" showing the hydrophobicity values for various amino acids:

Amino Acid	Value
A	0.61
R	0.6
N	0.06
D	0.46
C	1.07
Q	0
E	0.47
G	0.07
H	0.61
I	2.22
L	1.53
K	1.15
M	1.18
F	2.02
P	1.95
S	0.05
T	0.05
W	2.65
Y	1.88
V	1.32

At the bottom of the page is a section titled "Add Properties to PDBase". It includes a heading "Available descriptions" and a sub-heading "Enter information". There are four input fields: "Name of contributor" (with the text "Last, First"), "Affiliated with", "Description" (with the example "eg. Hydrophobicity (Fauschere & Phiska)"), and "Title".

**Figure 1:** A Screen capture of APDbase showing query and property value deposition interface is shown. This database can be queried using either amino acid property keyword or database index number. A search result for hydrophobicity is shown here as a sample

**Future Development:**

We are planning to incorporate a graphics tool that can cluster available properties into a dendrogram for visual inspection. This will help to visualize relatedness among clusters. The tool can be applied to generate physico-chemical profile for sequences of interest.

**Conclusion:**

APDbase is a dataset of physico-chemical properties of amino acids that will be converted as a tool to study protein sequence profiles.

**Acknowledgement:**

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