QUANTUM
pharmaceuticals

Quantum pKa calculation module

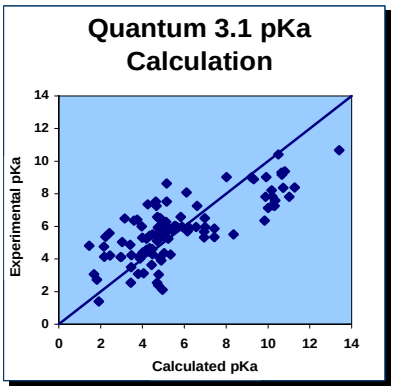
Key Capabilities

QUANTUM pKa module identifies all possible ionized species of a given small molecule and calculates their concentration in the whole range of pH (from 0 to 14).

Molecular protonation states predictions by QUANTUM

pKa is a very important for drug discovery. pKa of a drug determines concentration of its charged and neutral form at a given pH. This in turn influences drug solubility, distribution between polar and hydrophobic media, absorption and penetration through cell membrane and blood-brain barrier.

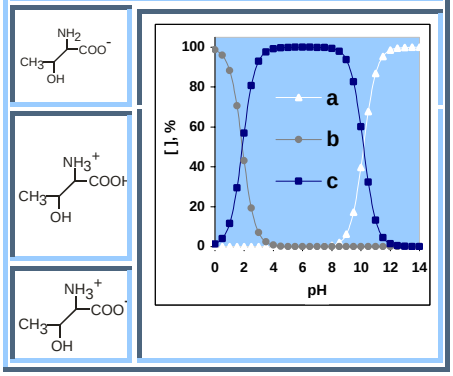
The identification of proper protonation states at a given value of ambient pH involves a careful thermodynamical analysis of proton affinity to a given molecule in aqueous environment. From a computational chemistry point of view, pKa calculations are a benchmark for quantum mechanical and free salvation energy calculations. The figure below summarizes the results of QUANTUM calculations and shows the correlation between experimental and predicted values of pKa dissociation constants a set of reactions involving more than a hundred of organic acids and bases.



If all possible protonation states of the molecule are identified and all corresponding dissociation constants are accurately calculated, then the proper protonation state of the molecule can be singled out for any given value of pH.

The following figure is an example of a typical calculation report and illustrates the titration analysis for a particular chemical compound: 2-amino-3-hydroxypropionic acid. The concentrations of different protonated states are represented as functions of pH.

Example: Titration curves for 2-amino-3-hydroxypropanoic acid.



As can be seen from the Figure at neutral pH 2-amino-3-hydroxypropionic acid is in its neutral state "c".

Technologacal advantage

QUANTUM uses QUANTUM Mechanics to calculate electronic densities and dissociation energies. The water environment is simulated with the help of our continuous solvation model

The main advantage of QUANTUM is its ability to calculate accurately pKa for absolutely novel types of molecules. Due to the use of most accurate first principles based calculations no any training sets are used in QUANTUM software.

While the performance of some statistically based QSAR pKa calculators can be excellent for molecules with chemical structures similar to that used in the training set they may fail badly for novel compounds with the structure and properties different from what they had in training sets. But at the same time the innovative novel compounds are the key focus of biotechnology industry.

QUANTUM will exactly reproduce the true physical picture for any randomly taken molecule, even a novel one, very different from those used in our QUANTUM verification study.

Software Description

The software runs both under Windows XP and Linux OSes (see technical requirements below). Users can choose either to import structures from any popular third-party formats or draw their structures using an array of tools including pre-made chemical templates. QUANTUM software includes user friendly chemical drawing tool.

QUANTUM software does not require molecules in a three dimensional format or optimized to minimum energy geometry. Necessary optimization will be done during calculation.

TRY IT FREE ONLINE

You can easily see how our pKa module works. Upload a small molecule and perform the modeling (http://q-lead.com). Note that free on-line version can be limited in its functionalities compared to the full pKa module.

Web-Based Services

In case a customer prefers ordering services rather than acquiring software QUANTUM offers opportunity to submit customer's library of compounds through the web interface in sdf, .mol2, .hin or .pdb formats and get the result of the calculations shortly. Full confidentiality and customer's IP protection are guarantied.

The online version of the pKa software has most of the functionality of the stand-alone version.

Software/Hardware Requirements

Linux:

Linux-32/64-bit Intel compatible CPU, glibc >2.3 Glibc 2.3 Python 2.4 wxPython 2.6;

Windows:

Windows 2000, Windows XP

Hardware:

Processor: Intel P4 or higher, AMD Athlon 64 (with SSE support) or higher Memory: at least 1 GB RAM Disk Space: 1 GB

References:

1)P.Fedichev, L. Men'shikov, *Long-Range Interactions of Macroscopic Objects in Polar Liquids*, ArXiv:cond-mat/0601129.pdf, submitted for publication.
2) P. Fedichev, L. Men'shikov, A. Vinnik, *Novel ab initio molecular modeling tools for drug discovery*, submitted for publication.
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