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Computational Chemistry − the bridge between math, chemistry and medicine

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Computational chemistry exploits principles of computer science, physics and other interdisciplinary sciences to solve different chemical problems. The methods of computational chemistry can be based on the different approximations to Schrödinger equation (implementing principles of quantum mechanics) and/or upon the classical Newton mechanics. Therefore, it inevitably extensively exploits different complex mathematical tools.

Since physiological biochemical processes are based on physicochemical interactions and chemical reactions, methods of computational chemistry can be successfully applied for different medical tasks. Thus, so-called computational medicinal chemistry has arisen as a new science. It has to deal with computer-aided drug design, which is now widely used by different pharmaceutical companies. Drug design can shorten considerably time needed for discovery of efficient drug.

Moreover, methods of computational chemistry can be used in the explanation for the mechanisms of the physiological action of different chemicals. Found solutions have a lot of applications in medicine.