DFG-Forschungszentrum MATHEON
Mathematik für Schlüsseltechnologien

Berlin, 14.10.2010

Press relation

Mathematics ensures clean water

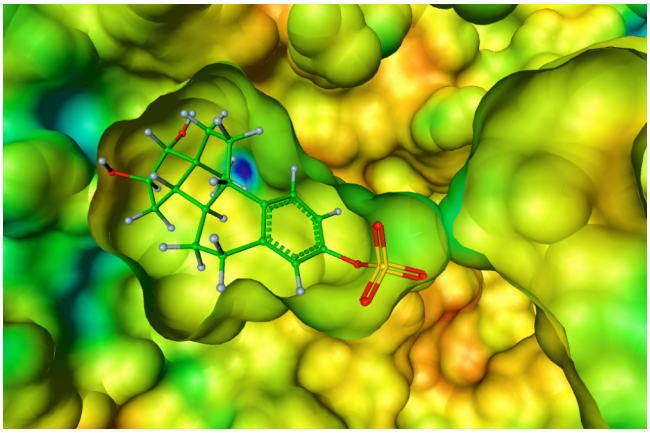
Reduction of medicine residues in drinking water

Drinking water is a vital prerequisite for all life on earth and is therefore probably our most important resource. However, this resource is also becoming increasingly scarce. Additionally, it is becoming increasingly polluted. Up to now, little attention has been paid to water pollution due to medicines. Although at present this is by no means dramatic, there is a noticeable accumulation of various medications in our water. Hardly any research is available with regard to the results of this unintentional medication for humans, plants and animals.

Because of this, at the instigation of the Federal Ministry of Health, in January the German Federal Environmental Agency (UBA) and the Institute for Socio-ecological Research (ISOE) invited experts from the health services, the pharmaceutical industry, utility companies, scientists, environmental associations and consumer organisations to a conference in Berlin on " The possibilities for action to reduce the introduction of human medications and their residue into unprocessed and drinking water". Amongst the 50 experts, Dr. Marcus Weber, an employee of the DFG Research Centre MATHEON was the only mathematician present.

As a result of this conference, a consensus paper has now been published with several highly practicable proposals whose implementation is planned in the near future. In several areas of the catalogue of measures, a significant mathematical involvement is planned, which should lead to previously unexpected results.

At MATHEON and in the Zuse Institute, Marcus Weber has been working on the mathematical prerequisites for a rapid and efficient simulation of molecules and their function in various medications for several years. Here, the so-called "key and lock principle" is used, by which computers can construct molecules so that they can predictably attach themselves to a harmful protein, block it and therefore render it harmless. Thanks to visualization and simulation the virtual molecule of the active ingredient can be modified in the computer until the optimum results are achieved.

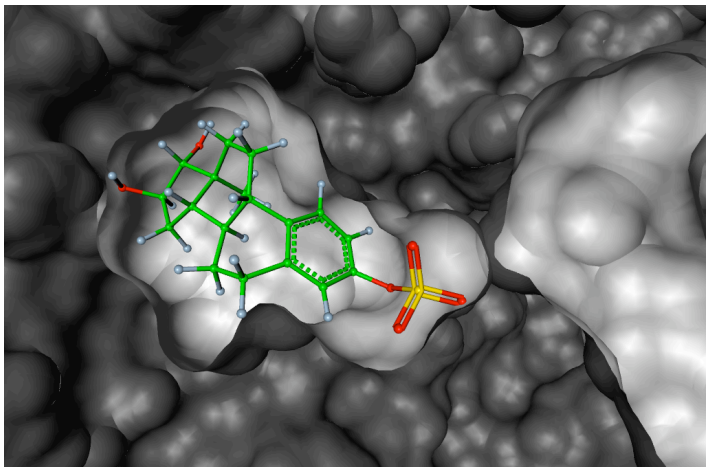


Computersimulation, in der untersucht wird, in welcher Weise das Flammschutzmittel HBCD durch sogenannte Cytochrome im Körper in andere Spurenstoffe umgewandelt wird.

This is a process which is accompanied by enormous difficulties, as both the molecule of the active ingredient and the harmful protein constantly change under certain influences, for example body temperature. Marcus Weber assumes that at present, throughout the world, up to 80 percent of the computing power of modern large computers is required simply for the simulation of molecules. Here, mathematics can help with new algorithms, which optimize the calculations and therefore the use of computing power. In this respect, Marcus Weber's previous work has certainly had a pioneering effect.

Of course, this research by Marcus Weber and his workgroup can also be used to great advantage and can lead to entirely new approaches for the simulation of hazardous substances which may enter the water cycle and have a detrimental effect on all forms of life if their concentrations are too high.

For example, at the conference in January it was recommended that the relevance of medications to drinking water should be taken into account even at their design stage. "It is not difficult to simulate not only the pharmaceutical effect of the actual medical ingredients in advance, but we can also consider their possible decomposition and transformation products", says Dr. Weber. In a further step, medications can also be developed with particular properties which increase their binding to sediments and active carbon. Such medicines would therefore be easier to remove from the water cycle. In addition it would be possible to ensure that the proportion of active ingredients which leaves the body unused is reduced or ideally completely eliminated.



Computersimulation zur Untersuchung der Auswirkung eines künstlich erzeugten Moleküls auf den Östrogenrezeptor und den Hormonzyklus. Mit solchen Studien wird versucht, das Gefahrenpotential von Spurenstoffen abzuschätzen.

A wide field in which Marcus Weber and his mathematical research could achieve great progress for the protection of untreated water is the assessment of the risk due to the effect of certain medication residues in drinking water. Many of these trace substances cannot be investigated in experiments on animals, as for this they would need to be isolated (or produced artificially in the laboratory), which is not yet possible for many forms of compounds. Marcus Weber believes that "with our algorithms we can create a virtual laboratory in which the toxicological effect of such decomposition products can be simulated. However, even for us this is a relatively new question, but it is a very interesting and certainly achievable challenge", says the mathematician. An additional success would also be that with the use of a mathematical basis for toxicological investigations, experiments with animals could be eliminated, restricted, or at least could be better planned.

Marcus Weber is convinced that the specialist conference and the resulting consensus paper is an important step towards the purification of water, the basis of our lives. "For me, this aspect is a further example of how our mathematical work can form the basis for successful measures, which above all protect nature."

Further information: Dr. Marcus Weber, DFG-Forschungszentrum MATHEON, Tel.: +49-30-8 41 85-189, E-mail: weber@zib.de
www.zib.de/Numerik/DrugDesign/index.en.html