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Warsaw, 31 January 2013

Biologistics: How fast do chemical trains move in living cells?

The rate of chemical processes in cells is dictated by the speed of movement (diffusion) of molecules needed for a given reaction. Using a versatile method developed at the Institute of Physical Chemistry of the Polish Academy of Sciences in Warsaw, researchers were able to predict for the first time the diffusion coefficients of all proteins in Escherichia coli. The achievement is important not only for biologists and chemists, but also for... transport companies.

Understanding of chemical foundations of life requires knowledge about the rate of chemical reactions in cells. The rates of these reactions depend on how fast the molecules taking part in reactions move (diffuse) in the cytoplasm. Prof. Robert Hołyst's research team from the Institute of Physical Chemistry of the Polish Academy of Sciences in Warsaw (IPC PAS) managed to determine – for the first time – the diffusion coefficients for virtually all the proteins occurring in *Escherichia coli*. The method developed by the researchers can also be used for other cells.

The movements of molecules in cells resemble a bit what's going on in railway stations. But the differences are obvious at first glance. "Regular trains leave stations at fixed times, whereas in cells transport processes take place virtually all the time. That's why it doesn't make sense to ask what time does the train with specific molecules leave the station. But it definitely makes sense to ask how fast the train with specific molecules is moving!", explains Prof. Robert Hołyst (IPC PAS).

Transport efficiency of chemical compounds in cells became inspiring for many transport companies. There's talk of biologistics as modelling vehicle or rail transport by looking up to what's going on inside the cells. Prof. Hołyst, however, has no illusions about that: "Everyone is delighted, for in cells the transport is so wonderfully resistant to perturbations. They forget, however, that the transport results from random fluctuations, in addition occurring in a small volume, where viscosity depends not only on the medium, but also on the size of the viscosity probe! I wish good luck all those who want to transfer processes occurring in physically so different environment to our roads. Biologistics works excellent, but inside cells only!".

Supported by grants from the National Science Center and the Ministry of Science and Higher Education as well as by programs from the Foundation for Polish Science, the research published in the "Bioinformatics" journal focused on the rate of diffusion of protein molecules in the *Escherichia coli* cytoplasm.

“The viscosity inside mammalian cells is relatively low, only 60 times higher than that of water. But bacteria are considerably smaller, everything is more crowded. The macroscopic viscosity there is up to 26,000 times higher than that of water. This is really dramatic difference!”, concludes Dr Tomasz Kalwarczyk (IPC PAS).

Earlier research of Prof. Hołyst’s team allowed for concluding that viscosity experienced by molecules is not only medium, i.e., solvent dependent, but also depends on the size and shape of molecules. Therefore, in the same medium, molecules differing in shape and size can experience very low viscosity (nanoviscosity) or macroscopic viscosity that is up to several thousand times higher. The previous methods for predicting diffusion coefficients in cytoplasm have not accounted for the effect.

Experimental determination of the diffusion rates of chemical compounds in bacterial cells is both time consuming and difficult. As a result, diffusion coefficients have been measured only for a very limited number of compounds in only some bacterial cells. That’s why the researchers from the IPC PAS developed a method for predicting diffusion coefficients for various compounds and media. For that purpose they used their own formulae, accounting for nanoviscosity and macroscopic viscosity, and a few dozens of diffusion coefficients of macromolecules in *Escherichia coli* taken from the literature. This was a basis for construction of a scale-dependent viscosity reference curve that could be used to determine diffusion coefficients of remaining compounds.

The database constructed at the IPC PAS contains diffusion coefficients for complete proteome of *Escherichia coli*. It includes over 6000 macromolecules, with about 4300 gene-expressed amino acid chains and their various, often multiple combinations (polymers), created both by the same chains (homomers), and by different amino acids (heteromers).

“Because of easy access to the literature data, we created a database only for molecules occurring in *Escherichia coli*. Our method could be, however, adapted for virtually any cell and every molecule, for instance for determining diffusion coefficients of sugars in mammalian cells”, stresses Dr Marcin Tabaka (IPC PAS).

This press release was prepared thanks to the NOBLESSE grant under the activity “Research potential” of the 7th Framework Programme of the European Union.

The Institute of Physical Chemistry of the Polish Academy of Sciences (http://www.ichf.edu.pl/) was established in 1955 as one of the first chemical institutes of the PAS. The Institute's scientific profile is strongly related to the newest global trends in the development of physical chemistry and chemical physics. Scientific research is conducted in nine scientific departments. CHEMIPAN R&D Laboratories, operating as part of the Institute, implement, produce and commercialise specialist chemicals to be used, in particular, in agriculture and pharmaceutical industry. The Institute publishes approximately 200 original research papers annually.

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SCIENTIFIC PAPERS:

”Biologistics – diffusion coefficients for complete proteome of Escherichia coli”; Tomasz Kalwarczyk, Marcin Tabaka, Robert Hołyst; Bioinformatics; doi: 10.1093/bioinformatics/bts537

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The database constructed at the Institute of Physical Chemistry of the Polish Academy of Sciences (IPC PAS) in Warsaw contains diffusion coefficients for complete proteome of *Escherichia coli*. Pictured above: Dr Tomasz Kalwarczyk is trying to deliver a message in a crowded environment. (Source: IPC PAS, Grzegorz Krzyżewski)

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The database constructed at the Institute of Physical Chemistry of the Polish Academy of Sciences (IPC PAS) in Warsaw contains diffusion coefficients for complete proteome of *Escherichia coli*. (Source: IPC PAS)

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Proteins' motion in a crowded environment. The database constructed at the Institute of Physical Chemistry of the Polish Academy of Sciences (IPC PAS) in Warsaw contains diffusion coefficients for complete proteome of *Escherichia coli*. (Source: IPC PAS)