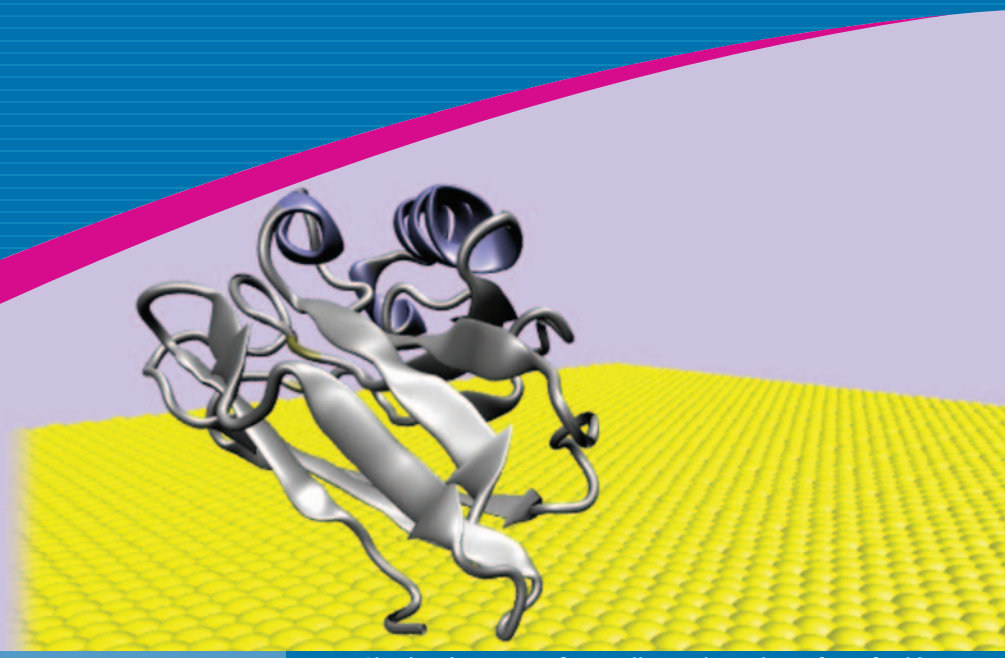
NEST 2006



Simulated structure of a metalloprotein on the surface of gold.
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PROSURF
NEST ADVENTURE

The PROSURF project is developing computational tools and basic scientific understanding to allow the remarkable surface-binding properties of proteins to be exploited in a variety of applications. Learning more about the chemistry and physics of protein-surface interactions will allow specific interactions to be designed and optimised. The outcome of this NEST Adventure project should lead to more successful exploitation of the powers of proteins in fields including nanotechnology, biomaterials and medicine.

Harnessing the powers of proteins

Proteins are the natural molecules which mediate most of the chemical processes that sustain living systems. They act as the catalysts (called enzymes) which accelerate biochemical reactions, and serve as structural materials, transport and messenger molecules, cellular receptors, portals and pumps, amongst other activities. One key to the varied activities of proteins is their ability to bind selectively to a huge variety of molecules. But selectivity is not limited to molecules: proteins can also discriminate between surfaces. The PROSURF project is developing tools and concepts to exploit the selective surface-binding properties of proteins in a wide range of applications.

Computational challenge

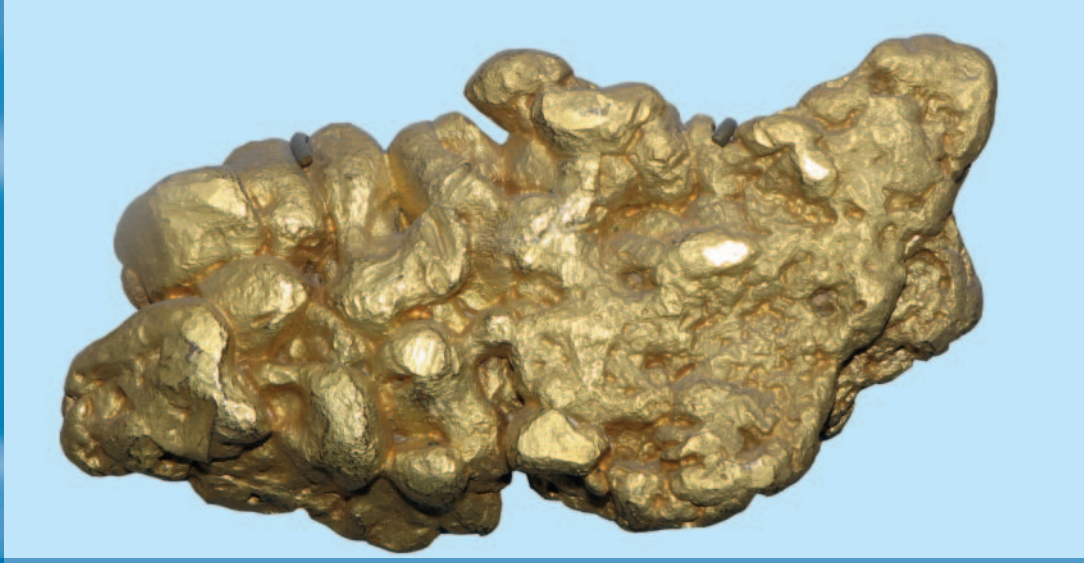
The ability of proteins to bind to natural and unnatural surfaces has been studied intensively in recent years. However, this experimental work has not yet provided a comprehensive understanding of the mechanisms of protein-surface interactions. Such understanding will be required to predict and control the use of protein-surface interactions in advanced research and industrial applications.

The objective of this NEST project is to provide the computational methods and basic scientific knowledge that will allow protein-surface interactions to be understood, predicted and controlled. One ultimate aim is to enable the rational design of novel proteins that will bind to specific surfaces, and the engineering of surfaces that will interact in a desired way with specific proteins. This is a very ambitious and novel undertaking to expand a currently underdeveloped field.

The partners intend to build on the success of existing computational tools that are used to analyse and predict the binding, or 'docking', between protein surfaces and small molecules such as drugs. Software developed during the project should be able to analyse protein structures and the structures of potential protein-binding surfaces, to predict the precise way in which the proteins will bind to the surfaces and how strong the binding will be. Success here will allow the effect of modifications to the proteins or surfaces to be explored, revealing ways to tailor the interactions until they optimally match the requirements for any industrial application.

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PROSURF
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Gold surfaces are among those binding surfaces most relevant to industrial applications.
© Steffen Foerster

AT A GLANCE

Official title
Computation Toolbox for Protein-Surface Docking

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Duration
36 months

Project Cost
€ 1 351 000

EU Funding
€ 1 000 000

Project reference
Contract No 28331 (NEST)

Web: http://cordis.europa.eu/nest

The project involves a mixture of theory, computation and experimental work, using the latest theoretical and computational innovations in the field. The partners will select a limited number of binding surfaces, including both metals and electrical insulators, reflecting the range of surfaces that may be most relevant to industrial applications. These surfaces will include gold, aluminium oxide and silica.

Gold is a prime candidate for a metallic material to be used in bio-electronics applications, while aluminium oxide is one of the ceramic materials exploited in biomaterials. The proteins initially chosen for study will be small molecules, known as 'peptides'. This work will hopefully reveal ways to extend the computational tools to larger proteins.

> This is a very ambitious and novel undertaking to expand a currently under-developed field.

From nanotechnology to medicine

The potential applications of the PROSURF project span biomedicine, pharmaceutics and industry, from nano-electronic components through to biomaterials for use in medicine and complex biosensor technology for environmental monitoring.

The project has the potential to give European industry a competitive advantage in some of the most exciting new and emerging technologies. It should open up a route to solve several urgent technological problems, such as how to create self-assembling nanotechnological devices and how to design biocompatible materials that can be incorporated into living systems (including humans) without rejection.

If the project yields an effective and validated protein-surface docking tool, it could take a significant step towards to the day when the full potential of protein activity can be harnessed for the industrial and medical exploitation of these remarkable natural materials. And it could allow us to go beyond the natural to create novel proteins that will bind and react in accordance with human design.

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SIXTH FRAMEWORK PROGRAMME