

## What is the National Grid Service?

The National Grid Service (NGS) aims to provide coherent electronic access for UK researchers to all computational and data based resources and facilities required to carry out their research, independent of resource or researcher location.

You can find further information about the NGS on its website at [www.ngs.ac.uk](http://www.ngs.ac.uk). The website contains a wide range of documentation including technical details, software listings, user case studies and online tutorials for self-guided learning.

## Keep in touch with the NGS

If you would like to be kept up to date with news from the NGS then join our mailing list to receive fortnightly news updates including events and training opportunities.

[www.jiscmail.ac.uk/lists/NGS-NEWS.html](http://www.jiscmail.ac.uk/lists/NGS-NEWS.html)

If you are a user of NGS resources then join our status mailing list to be kept up to date with service news and updates.

<http://www.jiscmail.ac.uk/lists/NGS-STATUS.html>

The NGS produces a quarterly newsletter containing a large variety of news about the NGS

including user case studies, NGS site news, application updates and conference reports. The latest edition of NGS News can be found on our website in the Outreach section or join our mailing list to receive an announcement when the latest edition is released.

## Contact the NGS

If you have any queries regarding the NGS or if you would like more information, then contact our helpdesk:

NGS Support Centre  
Email: [support@grid-support.ac.uk](mailto:support@grid-support.ac.uk)  
Tel: +44 (0) 1235 446 822

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Dr Brian Cheney  
University of Southampton

# Membrane Permeation



White Rose  
university consortium  
Universities of Leeds, Sheffield & York

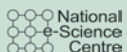


Science & Technology  
Facilities Council



Engineering and Physical Sciences  
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JISC

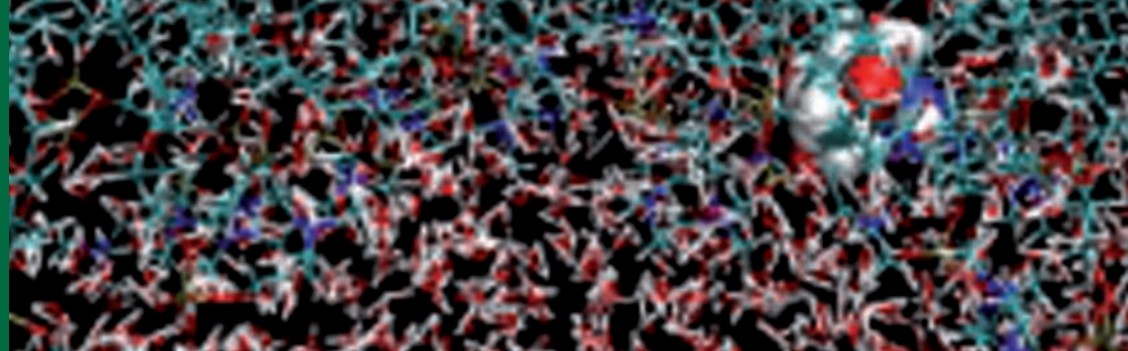


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[www.ngs.ac.uk](http://www.ngs.ac.uk)

Name: **Dr Brian Cheney**  
Institution: University of Southampton  
Research: **Membrane Permeation**



Drs Brian Cheney and Jonathan Essex research membrane permeation of small molecules at the University of Southampton. They are interested in learning what physical and chemical features make a molecule a good or bad permeant, and in developing ways to quantify and estimate a molecule's permeability. Besides being fascinating from a basic science perspective, membrane permeation also has important economic and applied science ramifications. Millions of pounds sterling are lost throughout the drug discovery process due to the pursuit of lead compounds that turn out to be dead ends. One of the many reasons an otherwise promising drug candidate might fail is due to low permeability and hence low absorption into the body through the epithelial membrane of the gastrointestinal tract.

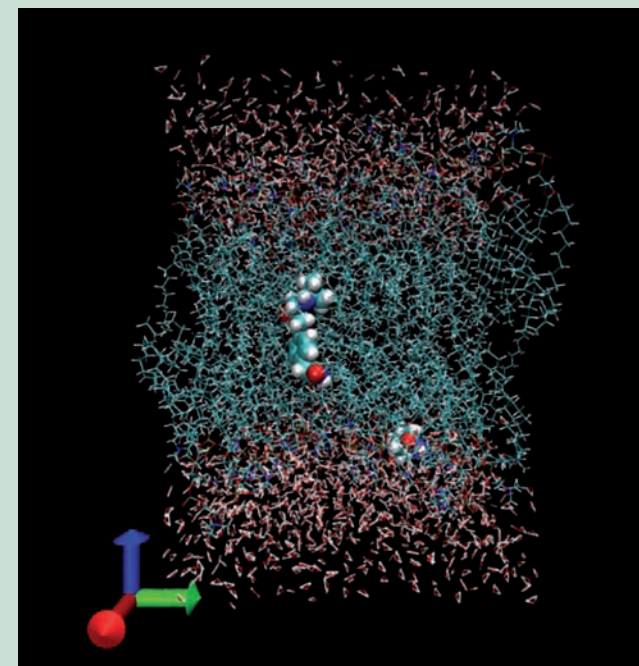
To estimate the thermodynamic and kinetic properties of small molecule permeation, the researchers turn to a

computational strategy that depends on all-atom classical molecular dynamics (MD) simulations of a drug permeating through a membrane. The MD simulations require many millions of time-steps and would take several years on a modern desktop computer for each drug studied.

With this kind of computationally intensive scientific challenge ahead of them, the researchers turned to the National Grid Service (NGS). They grid-enabled their modifications of the legacy molecular dynamics software package CHARMM, and collaborated with researchers at the University of Manchester and University College London to host their application on the NGS in the Application Hosting Environment. By using the NGS, the simulation time was cut from years per drug to about 2 weeks, allowing drug research to move forward much faster than would have otherwise been possible.

## Further information

Dept. of Chemistry,  
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[www.soton.ac.uk/chemistry](http://www.soton.ac.uk/chemistry)



*Simulation performed on the NGS of a drug permeating through a membrane.*