EUMEDCONNECT2 Case Study
WISDOM: e-infrastructures speed up the hunt for new malaria drugs
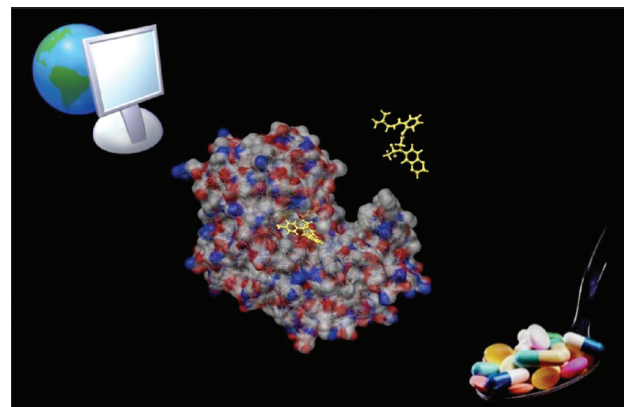
One of the commonest infectious diseases known to mankind, malaria kills more than one million of the world's poorest people every year, with some 500 million cases reported annually. Now the power of electronic research infrastructures (e-infrastructures) is being brought to bear on the urgent task of finding effective treatments for malaria, as well as for other major killers. The lengthy process of identifying drugs that might be effective has been speeded up by WISDOM, a massive biomedical data challenge involving the parallel use of 5000 computers in 27 countries - the equivalent of 420 years' computing for a single PC.

From October 2006 to January 2007, WISDOM benefited from EUMEDCONNECT – the research and education network for the Mediterranean – and EUMEDGRID - the Mediterranean grid infrastructure it supported. Computing centres across the Mediterranean were able to participate in such a ground-breaking international scientific endeavour for the first time. As a result of this work, scientists throughout the Mediterranean are now able to take part in world-class research to help fight these diseases.

A protein and its ligand before and after docking – innovative drug discovery thanks to high-speed networking and grid computing

Image courtesy of Ana Lucia Da Costa

A ground-breaking drug discovery process

Chemists have produced millions of compounds that could potentially be developed into effective drugs. WISDOM – Wide In Silico Docking on Malaria – is speeding up this process and offering hope to millions of malaria sufferers. WISDOM is also accelerating drug discovery for the treatment of another alarming killer – the virus H5N1, the cause of avian influenza. WISDOM uses in silico docking, where computers calculate the probability that molecules will 'dock' with proteins in the infective agent - virus, in the case of bird flu, or parasite for malaria. This lets researchers rule out the vast majority of potential drugs, allowing them to concentrate their laboratory testing on only the most promising compounds. As well as speeding up the screening process, this reduces the cost of developing new drugs to treat diseases.

WISDOM relies on the immense power of e-infrastructures – grids of thousands of co-ordinated computers around the world, supported by high-capacity state-of-the-art data communications networks like EUMEDCONNECT2 and GÉANT2, its multi-gigabit counterpart in Europe. Although the data challenge at the end of 2006 was mainly a collaboration between Asian and European laboratories and was primarily supported by the EGEE grid infrastructure (Enabling Grids for E-science), this data-intensive scientific initiative drew in a range of additional computing resources from around the world. Thanks to EUMEDCONNECT and EUMEDGRID, researchers across the Mediterranean were active participants in the study.

WISDOM: using the power of e-infrastructures to fight malaria

The first WISDOM data challenge – an initiative to discover drugs that might be effective against malaria – ran in summer 2005 and screened 41 million combinations ('dockings') in just six weeks, the equivalent of 80 years' work for a single PC; it identified over 30 leads and promised significant reductions in the development cost of new drugs. WISDOM uses the power of grid computing to screen molecules for their ability to disable a particular protein implicated in malaria.

'Docking' (the 'D' in WISDOM) refers to the way that molecules in a compound (ligands) attach to proteins in the infective agent of the malaria parasite. The aim of the research is to find ligands that bind in a particular way and to rule out those that don't. This process – 'virtual screening' – is a quick way of identifying compounds that might work effectively as anti-malarial drugs and allows medical researchers to focus their efforts far more narrowly on likely candidates.

Following on from the success of the first data challenge, a second study screened over 140 million dockings of compound and target proteins in a four-month period starting in October 2006.

EUMEDCONNECT2 – the research and education network for the Mediterranean

- providing high-capacity Internet connectivity for academic and scientific collaborations
- directly connecting southern and eastern Mediterranean partner countries: Algeria, Egypt, Jordan, Morocco, Palestine, Syria and Tunisia
- connecting other Mediterranean and European partners via GÉANT2
- taking forward Mediterranean region e-infrastructures pioneered by EUMEDCONNECT since 2004
- jointly funded by the European Commission and the Mediterranean partners to reduce the digital disparity between the Mediterranean and European regions

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A model of co-operation

WISDOM is a model for the kind of global co-operation in combating killer diseases that can be achieved by using advanced e-infrastructures: state-of-the-art data communications networks combined with the power of grid computing.

A wide range of global grid infrastructures supported the initiative. EGEE was involved (built on the GÉANT2 network and supported by the EU's FP6 funding programme), as well as peer grid infrastructures elsewhere in Europe (BioinfoGRID, Auvergrid, Embrace), in South America (EELA) and South East Asia (EUChinaGRID and the South East Asia Grid). EUMEDGRID enabled many Mediterranean scientists to make a contribution. EUMEDCONNECT allowed many smaller countries in the region – Morocco, Malta, Croatia and Cyprus, for example - to participate in a global research project of such breadth of scope for the first time, pointing the way to a future in which even more countries in the Mediterranean region can contribute to work of this kind.

The future

The success of WISDOM is leading to a growing interest in applying the technique to other major diseases that continue to pose a substantial threat to mankind – tuberculosis, diabetes and HIV. Together with malaria, these diseases are responsible for billions of cases and millions of deaths every year.

The size of the data challenge in the fight against these diseases means that the involvement of a broad range of countries is not a luxury, but a necessity. With EUMEDCONNECT2 now live and supporting powerful grid infrastructures like EUMEDGRID, future data challenges will involve an ever-widening group of Mediterranean countries, participating on an equal footing with the more established research centres in Europe and the rest of the world, strengthening the overall effort.

EUMEDGRID: empowering e-science across the Mediterranean

EUMEDGRID is the first distributed (grid) computing infrastructure supporting researchers in the Mediterranean. It is one of many collaborative applications that rely on the high-capacity links provided by EUMEDCONNECT2 and its predecessor network.

Although the EC-funded project has now come to an end (running for just over two years from January 2006) the pilot infrastructure it deployed remains in place and use and is being maintained on a best-effort basis by the Project Consortium, ensuring that Mediterranean countries are in a position to participate in world-class research in the years ahead.

As of March 2008, 25 sites across 13 countries, including Algeria, Egypt, Israel, Jordan, Morocco, Tunisia and Syria, benefited from the EUMEDGRID infrastructure.

Find out more

To learn more about WISDOM, visit: **wisdom.healthgrid.org**

Find out more about EUMEDCONNECT2 from: **www.eumedconnect2.net**

Find out more about GÉANT2 from: **www.geant2.net**

Find out more about EUMEDGRID from: **www.eumedgrid.org**

DANTE is a non-profit organisation that operates the GÉANT2 and EUMEDCONNECT2 networks. Further information about DANTE and its activities can be found at: **www.dante.net**

www.eumedconnect2.net