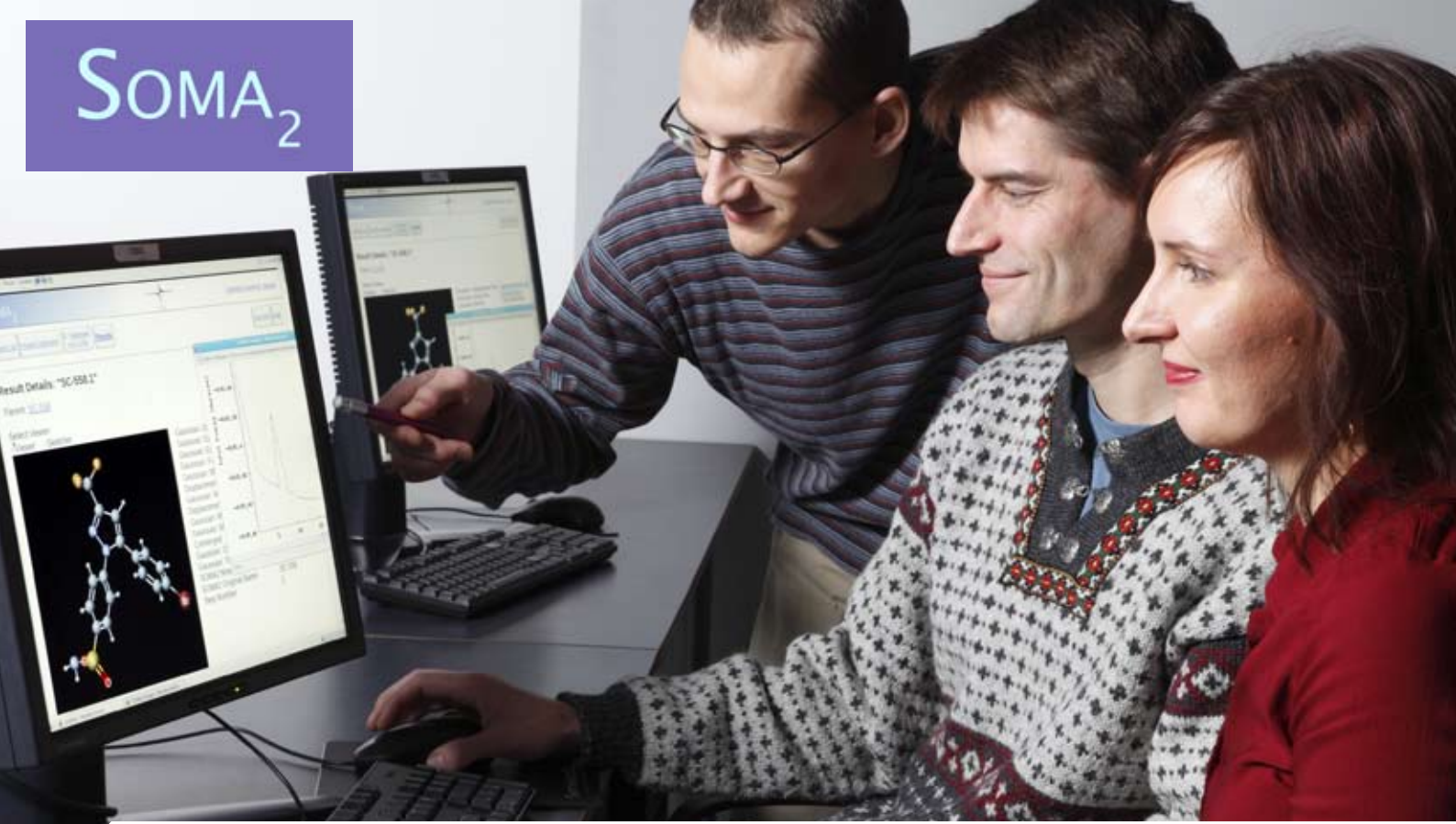


APPLICATION SERVICES



SOMA2



SOMA2 – Gateway to versatile molecular modeling

SOMA2 is WWW-browser operated molecular modeling workflow environment developed and maintained by CSC. It is an intuitive and versatile modeling environment for computational drug discovery and general molecular modeling. SOMA2 is distributed under the GPL open source license.

Full scale modeling environment

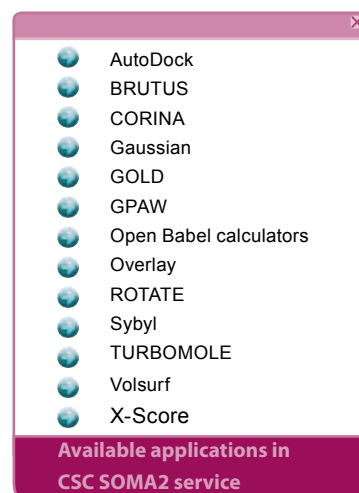
The SOMA2 environment offers a secure and personalized full scale molecular modeling environment. It facilitates inputting molecular data, submitting and controlling jobs, visualization and analysis of the results. It also helps organizing and storing the computed data. SOMA2 is easily upgraded to make use of most molecular modeling applications.

Gateway to other applications

SOMA2 environment makes use of different scientific applications installed in the computing system. The scientific applications are easily configured and automatically executed via the SOMA2 environment. In addition, the SOMA2 environment offers a possibility to construct unique application workflows where several programs can be automatically run one after another.

Easy to use

No technical or Linux/Unix skills all are required to use computational tools with SOMA2. It automates repeating work and eliminates redundant work. Advanced users benefit from automatically generated files, which can be saved for later use.



For more information

www.csc.fi/soma

Kinnunen, T., Nyrönen, T., Lehtovuori, P., SOMA2 - Open Source Framework for Molecular Modelling Workflows, Chemistry Central Journal, 2(Suppl 1):P4 (2008).

Lehtovuori, P. Nyrönen, T., SOMA - Workflow for Small Molecule Property Calculations on a Multiplatform Computing Grid, J. Chem. Inf. Model., 46(2) (2006) 620-625.