

# SuperStar 2.0 Release Notes

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## ***Introduction***

SuperStar version 2.0 is a full release of SuperStar.

If you require more information about these or any other SuperStar-related matters, please contact CCDC User Support at:

Email: [support@ccdc.cam.ac.uk](mailto:support@ccdc.cam.ac.uk)

Tel.: +44 1223 336022

Fax.: +44 1223 336033

SuperStar 2.0 features both a dedicated SYBYL (<http://www.tripos.com/>) interface and an interface via Hermes which is available for all supported platforms. For more information about using either of these interfaces please refer to the appropriate documentation:

Documentation can be found in:

`$(SUPERSTAR_ROOT)/superstar/docs/toc.html`

## ***Supported Platforms***

SuperStar version 2.0 is supported on the following platforms and operating systems:

- Windows - Intel compatible Windows 2000/XP/Vista
- Linux - Intel compatible, 32 bit:
  - RedHat Enterprise 4, 5
  - SuSE Linux Enterprise [Desktop|Server] 10
  - Debian 4.0

Note: As we add support for newer versions of Linux, support for older versions may have to be withdrawn.

## ***Important Notices***

- SuperStar 2.0 is intended to be used via the SuperStar interface in the Hermes visualisation

package. At the time of publication, the latest version of Hermes compatible with SuperStar is version 1.3 which can be obtained from

<http://www.ccdc.cam.ac.uk/pp/>

using your SuperStar username and password download details.

- SuperStar 2.0 may also be used via the included Sybyl 8.0 graphical interface, or via the command line using a previously constructed instructions file.

## ***New Features***

### Hermes Interface

- The Hermes interface of SuperStar can now handle small molecules as well as proteins.
- Shell correction is now implemented and is configurable.
- It is now possible to generate scatterplot maps and Connolly surfaces.
- It is now possible to specify a jobname.
- A user-defined output directory can be specified for output files.

## ***Modifications***

### Hermes Interface

- Default opacity levels have been modified such that 25% opacity level is fixed to apply at propensity 1.01 in all circumstances. The 100% opacity level is then applied at the highest propensity measured. Opacity of intermediate points are scaled accordingly.
- Probe types are now maintained between data sources (if an equivalent probe exists).
- Handling of multiple proteins has been improved.

## ***Support***

User guides for the Hermes and SYBYL interfaces to SuperStar can be found on the CCDC website in HTML and PDF format:

<http://www.ccdc.cam.ac.uk/support/documentation/>

Scientific and technical FAQs are also available from the CCDC website:

[http://www.ccdc.cam.ac.uk/support/faqs\\_downloads/](http://www.ccdc.cam.ac.uk/support/faqs_downloads/)

If you require more information about these or any other matters concerning SuperStar, please contact CCDC User Support.

## ***Validation***

SuperStar has been extensively validated using the CCDC/Astex validation set, which contains 305

protein-ligand complexes from the Protein Data Bank (PDB). See [http://www.ccdc.cam.ac.uk/products/life\\_sciences/validate/](http://www.ccdc.cam.ac.uk/products/life_sciences/validate/) and the SuperStar documentation for more information about the validation set and SuperStar validation results. Results have been published in:

**A New Test Set for Validating Predictions of Protein-Ligand Interaction**

J. W. M. Nissink, C. Murray, M. Hartshorn, M. L. Verdonk, J. C. Cole, R. Taylor  
*Proteins*, **49**, 457-471, 2002