



Avantium and AMS start collaboration to develop and commercialize Crystal Structure Prediction

Crystal Structure Prediction: a new service opening up exciting possibilities for the pharmaceutical industry

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Avantium and Avant-garde Materials Simulations (AMS) announced today that they have entered into a collaboration for the further development and commercialization of Crystal Structure Prediction (CSP) with AMS' GRACE software.

Pharmaceutical companies can use CSP to predict the crystal structures of their drug compounds. CSP provides an essential approach to significantly reduce the risk of missing a more stable crystal form.

In the partnership AMS will further develop the software to accelerate the calculations and broaden the range of compounds for which it can be used. AMS will also perform the predictions for third parties. Avantium will develop efficient experimental strategies to physically generate the predicted crystal forms and commercialize Crystal Structure Prediction as a stand-alone service or in combination with experimental programs.

CSP, as developed by AMS, is a breakthrough approach, showing for the first time that the reliable prediction of crystal forms is feasible. AMS in collaboration with the Institute of Pharmaceutical Innovation at the University of Bradford were the first participants ever to score a 4 out of 4 success rate at the 2007 CSP Blind Test.

The scope of applicability and the accuracy of CSP will continue to improve rapidly, says Marcus Neumann, Managing director of AMS. The next key challenge is to actually produce predicted but not yet observed forms by rational experiment design. With Avantium Pharma we have found the ideal partner to write the next chapter of the story.

The CSP technology is a great extension of our service portfolio, comments Guus Scheefhals, Chief Operating Officer of Avantium Pharma. The predictions will prevent overlooking the most stable crystal form, which will strengthen the IP position of our clients and will help to reduce the risk of crystal form inter-conversions in drug development.

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About AMS

Avant-garde Materials Simulations has focused on the development of novel algorithms for Crystal Structure Prediction since 2002. AMS has developed an empirical van der Waals correction for accurate lattice energy calculation in conjunction with third party DFT codes and owns proprietary software for the generation of tailor-made force fields and the statistically controlled generation and optimization of crystal structures.

AMS has a strong commitment to sustainable development and is based in one of Europe's most advanced ecological districts in Freiburg, Germany.

About Avantium

Avantium is a leading technology company in the area of advanced high-throughput R&D operating in the energy, chemicals and pharmaceutical industries. The company develops products and processes in the area of biofuels, bio-based chemicals and novel crystal forms of existing drugs by applying its proprietary, high-throughput R&D technology.

Avantium has demonstrated the potential of this technology by providing R&D services and tools to more than 70 companies worldwide. Avantium's customer base includes many of the world's largest energy, chemicals and pharmaceutical companies, such as BP, Shell, Sasol, Pfizer and GSK. Avantium has more than 100 employees; its offices and head quarters are based in Amsterdam, The Netherlands.

For more information

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