

# From fragments to the full picture with iNovacia

By Johan Falk

iNovacia continues to refine their services based on their unique library of over 300,000 compounds. Fragment based NMR screening and a strategic alliance with Provid Pharmaceuticals are the latest tools in iNovacia's portfolio.

**CONTRACT RESEARCH** iNovacia have with their chemical library been able to help clients identify leads for novel drugs. That ability is now further enhanced with the introduction of Fragment based NMR screening (FBS) technique.

"We have worked with it for quite some time now, but we have waited to introduce it to our clients until now," Peter Halkjaer-Knudsen, Senior VP of Alliances & Business Development at iNovacia says.

The reason for waiting with the introduction of this service was that originally the equipment was based at the Karolinska Institute but it is now situated in iNovacia's own labs.

"A building project at Karolinska made it impossible for us to continue there, since the vibrations from the building site interfered with our measurements," Peter Halkjaer-Knudsen says.

The FBS-technique is by no means something that the staff of iNovacia is only just learning. In fact Johan Schultz who is a member of the iNovacia team has just recently participated in the publishing of a book on the subject: *The Practical Aspects of Using NMR in Fragment-Based Screening in Fragment-Based Drug Discovery. A Practical Approach*, edited by Edward Zartler, to be published by John Wiley and Sons Ltd, as well as a number of articles since the inception of the technology (see e.g. *J Am Chem Soc*, 2002. 124: p. 11874-80).

"With FBS we can investigate if a molecule addresses the target protein either by interfering with or adhering to the active site," Johan Schultz says.

Only a relatively small number of fragments need to be screened since the hit rate will be much higher compared to traditional screening. This is a consequence of the fact that lower complexity fragments have a higher probability of matching a target protein binding site. Further, since the number of theoretically possible molecules

## "There is simply no time for procrastination anymore"

increases exponentially with the number of atoms in the molecules, screening a small fragment library, typically 102-103 compounds, samples substantially more chemical diversity space than a conventional HTS where typically 105-106 larger compounds are screened.

"We can explore the active site much better and find chemical motives that are not covered by current patents," Johan Schultz says.

### Starting at the correct place

The FBS-technique can be used either as a stand-alone investigation or as a complement to biochemical screening. The information gathered from how the fragment interact with the proteins can be used as

starting points in focused drug development, as well as a means to find areas of interest for immaterial rights.

"Using our expertise, a client with a pure, soluble and well characterised protein in low milligram quantities will get a very good description of the accessible areas of that protein and the types of compounds that will interact with it," Peter Halkjaer-Knudsen says.

To find a good starting point as early as possible is becoming more crucial in drug development, there is simply no time for procrastination anymore. The FBS-technique is one shortcut that iNovacia can provide, the other is the extensive chemical library the company disposes.

"Biotech and pharma are pressed for time, and might start development work already after finding the first lead in their own compound screening, even if they find only a single candidate. Instead of delaying their internal development process they have in some instances employed us to continue the screening and successfully



come up with back-up structures,” Peter Halkjaer-Knudsen says.

While the pharmaceutical company ploughs ahead with the leads that they have identified, iNovacia puts their 300,000 plus library to good use.

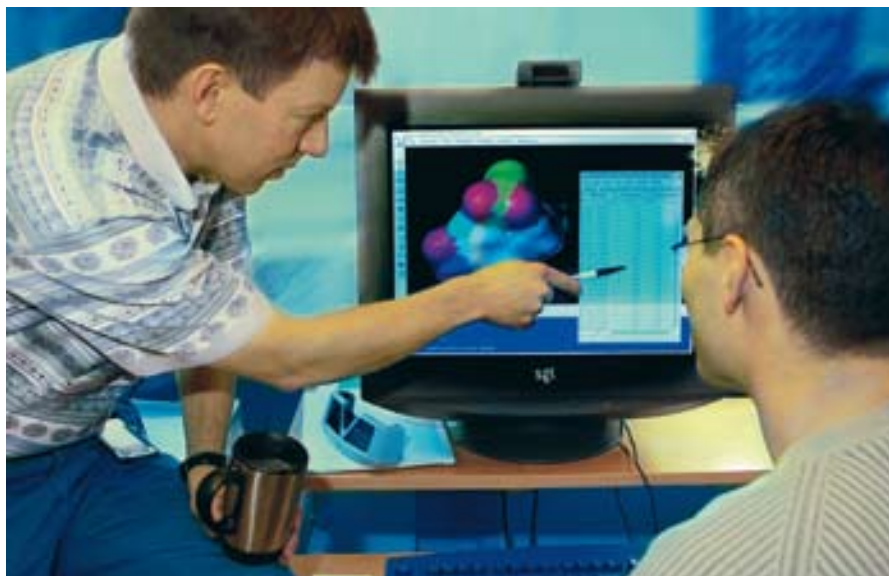
“It really proves our claims when our library of molecules can find other and new leads for our clients, even if they are big players in pharmaceuticals themselves,” Peter Halkjaer-Knudsen says proudly.

The library is continuously added to for even better diversity, both new fragments for FBS and more hit- or lead-like compounds for biochemical screening.

### Expanding the horizon

iNovacia took a big leap at the start of this year, both with the signing of a strategic alliance with the American drug discovery company Provid Pharmaceuticals, and also with the decision to establish a new base of operations in North Brunswick, New Jersey. It was certainly not a move without risks.

“It has been hard work, but it has paid off, we already have new contracts signed and the positive response from numerous clients in the US is very encouraging,” Peter Halkjaer-Knudsen says.



To not only establish a presence in the biggest biotechnology area in the USA, but also to do it successfully is a proof of concept for iNovacia. Another indication of what might be expected from the Swedish CRO comes from a medium-sized pharma, evaluation of costs to work with iNovacia.

“Even though the cost for a scientist in Asia is around 30% lower than for Stockholm, then if you take into account the travel cost, managing cost and the time-

lines for projects. It is actually cheaper in the long run to work with iNovacia, because the efficiency of our work is so high,” Peter Halkjaer-Knudsen states.

Not only are iNovacia now prepared to offer the FBS-technique in conjunction to their unique chemical library. They have extended their number of active sites with the added base of operation in North Brunswick, expanding their reach for their innovative screening techniques at continued cost efficiency. ❖

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