Lundbeck to test AI for treating brain disorders

Founded in 1915 with a foundation as a controlling shareholder, H. Lundbeck A/S has navigated a conservative path towards drug development. The company started as a machine manufacturer and then moved into pharmaceuticals in the 1980s to treat brain diseases. Along the way, it has adopted many new technologies. One of these is artificial intelligence, which is about to be tested for an expanded new role.

On 6 May, Lundbeck announced an agreement to collaborate with a new supercomputer project that is being run by a public-private consortium in Denmark. The partners are Nvidia Corp, the Novo Nordisk Foundation and the Danish government's export and investment fund. The project, called the Danish Centre for AI Innovation, was launched on 23 October 2024 and houses a supercomputer called Gefion. Gefion was built by Eviden, a subsidiary of the French company Atos SE, and uses chips provided by Nvidia.

The Danish AI centre is a public limited company that owns and operates Gefion whose revenue will be reinvested in the project. The largest shareholder is the Novo Nordisk Foundation with a stake of 85% with the remaining shares held by the government's export and import fund. Nvidia is not a shareholder but its tools underpin the project. These are the company's DGX SuperPOD servers and workstations using general-purpose computing on graphics processing units. To test the new system, the centre has selected six research projects that require high-level computation. Lundbeck is not one of the trialists but it will be one of the first pharmaceutical companies to use the system.

In an interview, Tarek Samad, head of research, explained how the company hopes to leverage Gefion to discover new molecules, both chemical and biological, and speed up the process of drug development. Dr Samad joined Lundbeck in 2021 from Immunitas Therapeutics Inc in the US where he was chief scientific officer. His research focus is on neuroimmunology. "This is an area that we are really excited about and that requires both biologics and small molecules. We believe that the AI approach with high computational power can be transformative," he said.

Neuroimmunology is a combination of neuroscience and immunology focusing on how the nervous system and immune system work together during development and how they respond to injuries and infections. Previously, scientists thought the systems operated independently of each other, but this concept has been disproven by subsequent research[1]. Multiple sclerosis is a common neuroimmune disease. Many other disorders falling into this category are rare.

Lundbeck already has a neuroinflammation project in Phase 1b that is being developed with partner AprilBio Co Ltd of South Korea. The collaboration started in 2021 and gives the Danish company exclusive rights to an antibody-like drug candidate that targets a pathway, CD40-CD40L, which plays a central role in the co-stimulation and regulation of the immune system. The product is being assessed as a potential treatment for thyroid eye disease.

Other AI partnerships in place include a 2024 collaboration with Iambic Therapeutics Inc of San Diego, US, to identify a small molecule therapeutic to treat migraine. But none of the existing partnerships compares in scale or resource to the new Danish AI centre.

"Lundbeck is an example of a pharma company that is interested in tapping into high computational power," Dr Samad said in the interview. There are multiple reasons for this interest, but one of the most important is the time it takes discover a new molecule, which is expected to shorten with AI. The second is achieving target engagement whether the molecule is an antagonist or an agonist. A third aspect is cost. According to an article published in *Nature Medicine* in January, the current cost of developing a new drug is approximately $2.6 billion over 12 to 15 years[2]. Meanwhile the success rate over the whole development cycle is less than 10%.

Whereas in the past, researchers used high throughput screening to scan chemical libraries with hundreds of thousands of molecules, AI scans virtual libraries potentially containing trillions of *in silico* molecules. "This is the revolution in drug discovery. Now that we have very powerful algorithms that can understand protein structure and sequences, depending on the questions, it [the computer] will suggest molecules that are likely to bind," Dr Samad said. Furthermore, the new computer will be able to identify which one or two molecules can simultaneously engage two or three targets at the same time, he added. Having said this, after a molecule has been identified, it still has to be tested and verified in a laboratory.

Lundbeck's current portfolio is about evenly divided between small molecules and biologics but the trend is leaning towards biologics. Until about a year or two ago it was more difficult to scan a virtual library for biologics because of their complex structure. This problem is being overcome slowly with the latest iterations of AI which can identify proteins by calculating sequences of amino acids[3]. As a result, Lundbeck will be able to select future drug modalities based on disease criteria, rather than on what AI can or cannot do well, Dr Samad said.

As a neuroscience company, Lundbeck is also working on strategies for helping its drugs cross the blood-brain barrier, a layer of cells that protect the brain from pathogens, but can also hamper the delivery of drugs. Lundbeck is using AI to fine-tune shuttles to cross this barrier. These.are currently in pre-clinical development.

References:

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2. Zhang, Kang et al, Artificial intelligence in drug development, *Nature Medicine* 20 January 2025.

3. Service, Robert, The AI revolution comes to protein sequencing, *Science*, 11 April 2025.

This article was written by the *MedNous* editor following an interview with Tarek Samad, head of research at H. Lundbeck A/S.