## Is there life after AlphaFold2? A tool is only as good as the question it answers

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## Abstract

AlphaFold2 has caused a big stir. A problem that many people were working on for many, many years suddenly seemed solved: Modelling the protein structure from its sequence. A critical note is that AlphaFold is not yet very good at placing side chain atoms, so drug design isn't helped very much yet. But many other fields will be helped. In human genetics the two main questions are WHICH mutation is causally related to a genetic disease, and HOW the mutation causes its effect. But other fields, which include proteins that cannot be modelled, will not benefit at all: signalling by natively unfolded proteins, ab initio designed proteins, amyloidoses, etc. So, in summary, a few people world-wide lost their jobs, but you still have an equally great future ahead of you.

## About the presenter

Professor Gert Vriend has been involved in several European projects directed toward bioinformatics data and software interoperability. The concepts worked out in these EU projects are deeply embedded in most of his recent software products. Most recently they involved EMBRACE NoE for software and data interoperability in bioinformatics. He has been a teacher in a series of UNIDO, EMBO, EMBL and EMBnet courses, and he gives about a dozen invited seminars each year.

## EDUCATION and CAREER:

Prof. Vriend studied biochemistry at the university of Utrecht, in the Netherlands and got his PhD in 1983 at the agricultural university of Wageningen, the Netherlands. His PhD project was a study of assembly process of plant viruses, using NMR, EPR, etc. He post-doc-ed in Purdue, Indiana, USA on the Xray structure of the common cold virus, and in Groningen, the Netherlands, where he worked on several structures while starting the WHAT IF project. In 1989–1999 he worked at the EMBL in Heidelberg, Germany, where he continued working on (and with) the WHAT IF program.

In the summer of 1999 he took up a position at the Radboud University in Nijmegen, the Netherlands, where he built-up the CMBI (Center for Molecular and Biomolecular Informatics). At the CMBI Gert continued working on fundamental and applied aspects of protein structure (homology modelling, structure quality, visualization, molecular dynamics, ligand interactions) and of information technology (data mining, information systems). In 2007, a move of the CMBI from the science faculty to the Medical Centre of the Radboud University, allowed for more emphasis on the application of bioinformatics in biomedical research; this resulted in the design and implementation of a series of widely used products like:

- HOPE to automatically determine the molecular effects of (normally disease causing) mutations;
- MRS to get fast and flexible access to dozens of biomedically relevant data collections;
- NewProt, a portal for protein engineering.

Many of Prof. Vriend's students have used software developed in the CMBI to start their own companies. Elmar Krieger runs YASARA GmbH; Henk-Jan Joosten runs Bio-Prodict BV; Chris Spronk runs several companies on NMR consultancy, on educational video design, etc. Together with Prof. Malgorzata Kotulska, Prof. Vriend co-supervised one of our PhD students, Paweł Woźniak, who was awarded his doctorate degree in 2018.