

MS5-P8 Needle Finder: A search engine for retrieving and evaluating hidden structural features and much more.

Wilhelm Stark¹, Nunzio Putrino², Karin Rügge³, Manfred Drozd⁴, Dominique Brodbeck¹, Markus Degen¹

1. Fachhochschule Nordwestschweiz
2. Future-IT-Com
3. Tradeware
4. peakmarks

email: wilhelm.stark@fhnw.ch

How can we retrieve hidden structural features in the world of bio-molecular structures in short time, without inspecting every single structure file manually? The task would turn in an impossible mission, if we do not merge together a powerful infrastructure, great ideas and improvements of data quality. Especially, if we take into account the steadily increasing amount of data.

We are developing a tool box, which allows users to find the details of a piece of information within over a billion rows secure, fast and reliable in minutes if not seconds. For this reasons we put the sample on two real-world questions. They consist in retrieving well defined amino acid patterns we know they must exist. But before we run the tests, we hadn't a clue where to find them in the over 100'000 protein structures. The content driven relational database is the core part of our tool box. Beside the facts that the programs have found the exact name of the PDB-files, they also spotted – as welcomed side effects – the exact position within each protein structure, the sets of coordinates, atom serial number and much more. Moreover, the program also listed exactly those rows which stored inconsistent patterns, instead of the expected resolutions of the protein structures. Let's estimate the time to be spent for the same tasks, in case we were requested to do it without the help of the needle finder. For the purpose of the calculation we establish as a basic assumption that it takes us one minute for the download of each PDB-file including a brief inspection of the file content. Having more than 100'000 PDB coordinate files to inspect by an eight hour working day we need more than 200 working days. The estimation does not include to keep track and to trace what we have done so far, not mentioning that any kind of calculation has been done. We simply cannot afford it any longer. What's about you?

	Manual download and inspection	Database
1 File	1 Minute	
100'000 Files	200 working days (8h/day)	5 minutes by sequential execution; less than 10 seconds by parallel processes

Figure 1.

Keywords: Biological Structures, information retrieval, bigdata, database,

MS5-P9 Structural and functional study of the antibody against influenza viruses' RNA polymerase to discover a new medicine for the influenza disease

Kanako Sugiyama¹, Hisashi Yoshida¹, Takeshi Urano², Sam-Yong Park^{1,3}

1. Influenza Drug Design Project, Kanagawa academy of science and technology
 2. Department of Biochemistry, Shimane University School of Medicine
 3. Department of Medical Life Science, Yokohama-city university
- email: pp-sugiyama@newkast.or.jp

As you know, the influenza virus causes the influenza disease. Especially some viruses called the high-pathogenic influenza virus leads death of a large number of farm animals and could be a factor of a human pandemic if it modified to have the ability of the infection to humans. We tried to discover a new medicine against influenza viruses. And then we found the structure of the binding region between RNA polymerase subunits of the H1N1 influenza A virus few years ago. The results of our study published in the papers below.^{1,2}

After that, we are studying more information about the RNA polymerase. We made some new antibodies against the RNA polymerase. One of it can repress the growth of several types of influenza A viruses. We introduce the structural and functional study of the anti-RNA polymerase antibody. The results of this research show a new possibility of a medicine against all kind of influenza A viruses.

1 Sugiyama, K. *et al.* Structural insight into the essential PB1-PB2 subunit contact of the influenza virus RNA polymerase. *The EMBO journal* **28**, 1803-1811 (2009).

2 Obayashi, E. *et al.* The structural basis for an essential subunit interaction in influenza virus RNA polymerase. *Nature* **454**, 1127-1131, (2008).

Keywords: Influenza virus, RNA polymerase, Antibody, Crystal structure