AlphaMol

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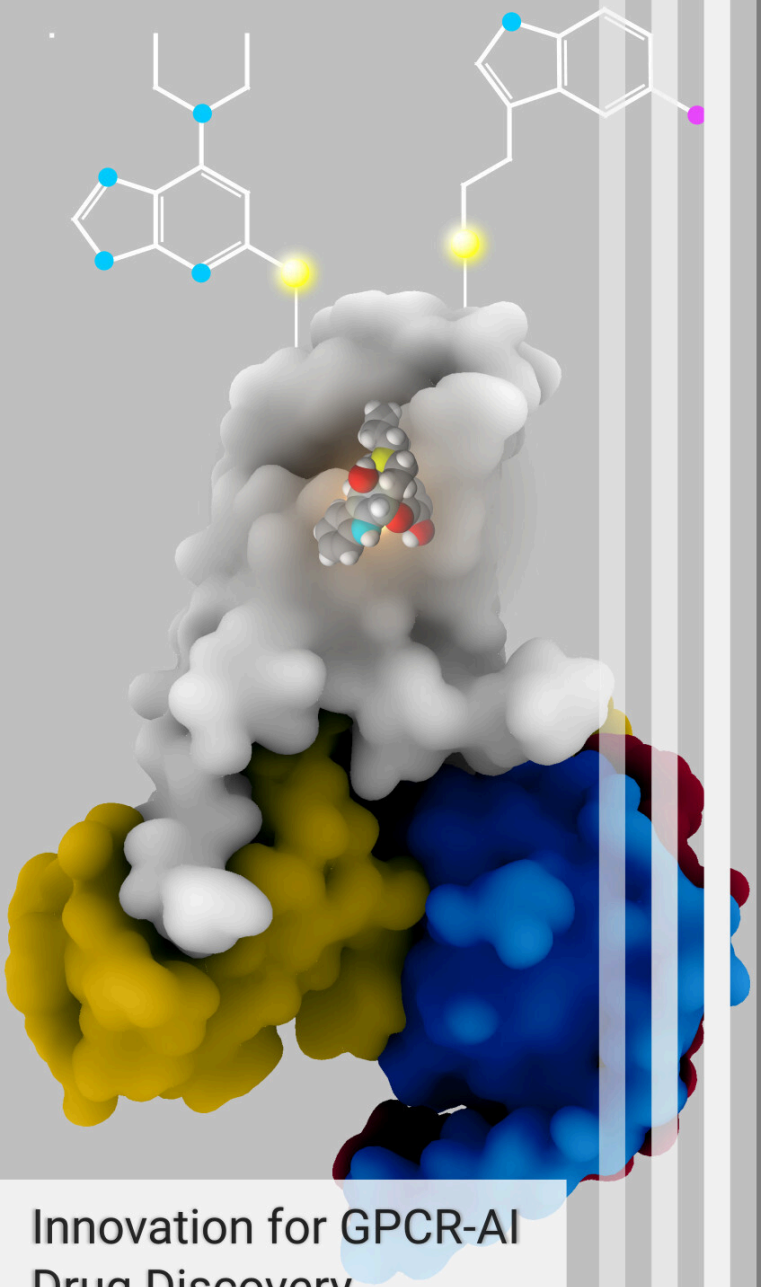

Innovation for GPCR-AI Drug Discovery

OUR TEAM

Dr. Shuguang Yuan
Co-founder

- PhD supported by the Marie Curie Fellowship and finished in KULeuven (Belgium), Polish Academy of Sciences & EPFL (Switzerland)
- 5 year CADD experience in big pharma
- Two FIC clinical drugs in three years
- H-index=32
- Top 2% scientist in the world

Dr. Horst Vogel
Co-founder

- Member of Swiss Academy of Sciences
- National Academy of Inventors USA
- 20+ years professorship and Emeritus professor at EPFL
- Long-term and intensive collaborations with Roche, Novartis and Nestle
- H-index=80
- Top 2% scientist in the world

WHAT WE DO

AlphaMol is mainly focusing on combining artificial intelligence with innovative biotechnology to advance G protein-coupled receptor (GPCR) drug discovery. GPCR is the most important target, of which about 40% of the marketed drugs are targeting.

Our team has more than 30-year history in the area of drug discovery and biotechnology development of GPCRs. Many important molecular mechanism and biotechnology were invented by our team.

In the recent global GPCR-DOCK 2021 contest, we defeated Goolge's AlphaFold2 for the five nominated GPCR targets, with 60% higher accuracy. In 2022, AlphaMol obtained the best outstanding award in NVIDIA Inception contest for startups. In the same year, both co-founders of AlphaMol, Prof. Horst Vogel and Shuguang Yuan were in the list of "top 2%" scientists in the world.

Thanks to the outstanding GPCR-AI drug discovery platform, AlphaMol managed to develop several first-in-class PCCs within 3-9 months which usually takes 4-7 years to achieve.

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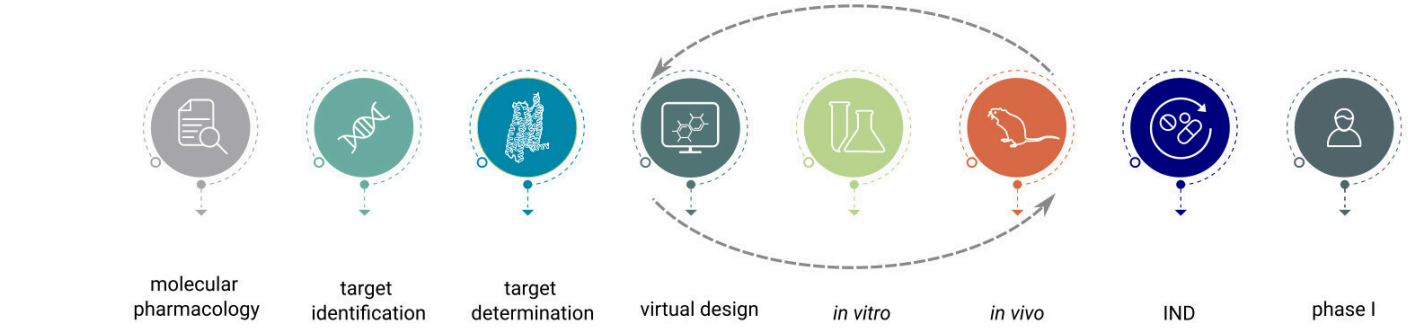
OUR ASSETS



GPCR PLATFORM

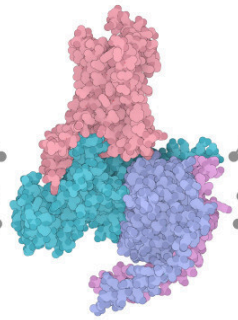
AlphMol has established a complete platform to advance GPCR drug discovery. It facilitate different stages of GPCR drug discovery including: new target identification, 3D model prediction, high-throughput virtual screening, lead-optimization, GPCRomx evaluation, lead optimization, biological activity testing in wet lab.

Ultimately, the preclinical drug candidates can be designed within a few months.

GPCR-GTP
Pharmacological network & signaling knowledge of GPCR

GPCR-3D
Accurate 3D model prediction for GPCR

GPCR-Screen
Dedicated platform to screen GPCR drug candiates

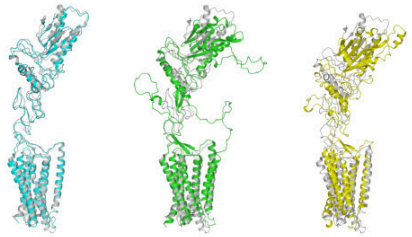


GPCRomx
Ligand binding heatmap across the whole GPCR family

GPCR-Lead
Lead optimization for GPCR in activity, ADMET, specificity, physical properties

GPCR-Chip
Measure direct interactions between GPCR & G proteins

Orphan GPCR Predictions



AlphaMol RMSD=3.6 Å | AlphaFold2 RMSD=53.9 Å | RosettaFold RMSD=58.3 Å

GPCR-DOCK 2021

Rank	Group code	Group name	Model	Ligand RMSD, A
1	8669	Seoul-Seok	3	2.09
2	8407	**AlphaMol**	2	2.46
3	8407	**AlphaMol**	3	2.48
4	2327	Copenhagen-Gloriam	4	2.58
5	8407	**AlphaMol**	1	2.58

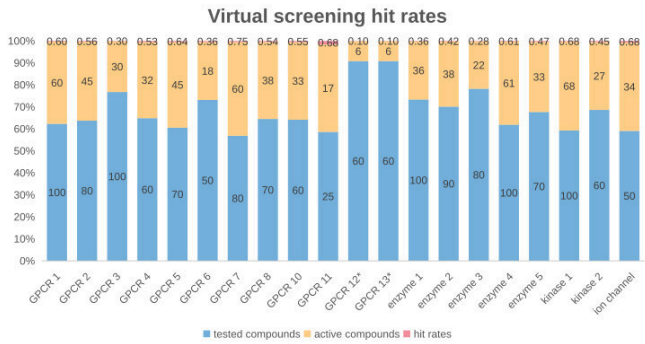
CryoEM Structure | Model by AlphaMol

GPCR-3D

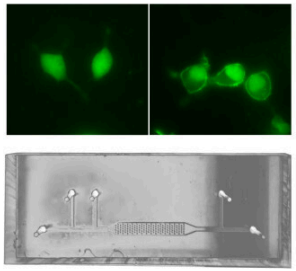
GPCR-3D could predicted different states of GPCR structure accurately. This was validated in the global "*GPCR-Dock 2021*"contest, where the overall accuracy of our models was 60% higher than that of AlphaFold2 for thefive nominated targets.

GPCR-Screen

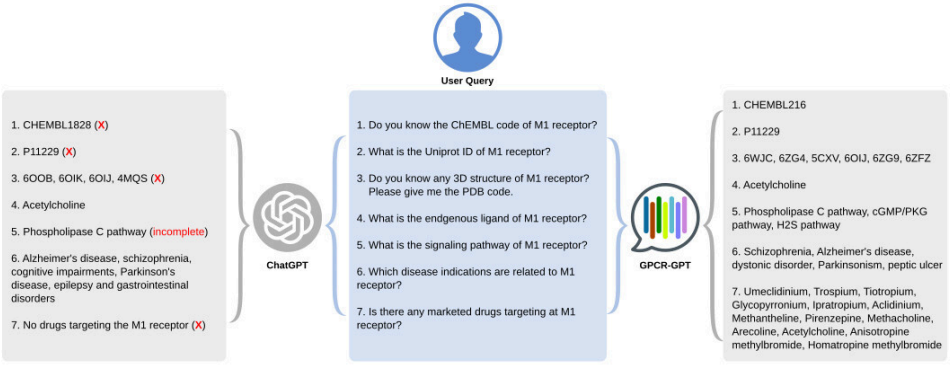
AlphaMol has established a dedicated platform **GPCR-Screen** for GPCR drug candidates screening. It combines AI as well as self-developed GPCR-Chip technonogy. It overcomes all major problems of secondary messages screening. The hit rates of our platform for GPCR screening are in the range of 10-80%.



GPCR-Chip in AlphaMol



GPCR-GPT



GPCR-GPT

Despite the widespread popularity of large language models such as ChatGPT, they often fall short in satisfying users in retrieving and answering domain-specific questions. With **GPCR-GTP in AlphaMol**, GPCR signaling network, downstream pathway, effectors, disease indications and many other related properties/questions can be accurately answered and summerized.

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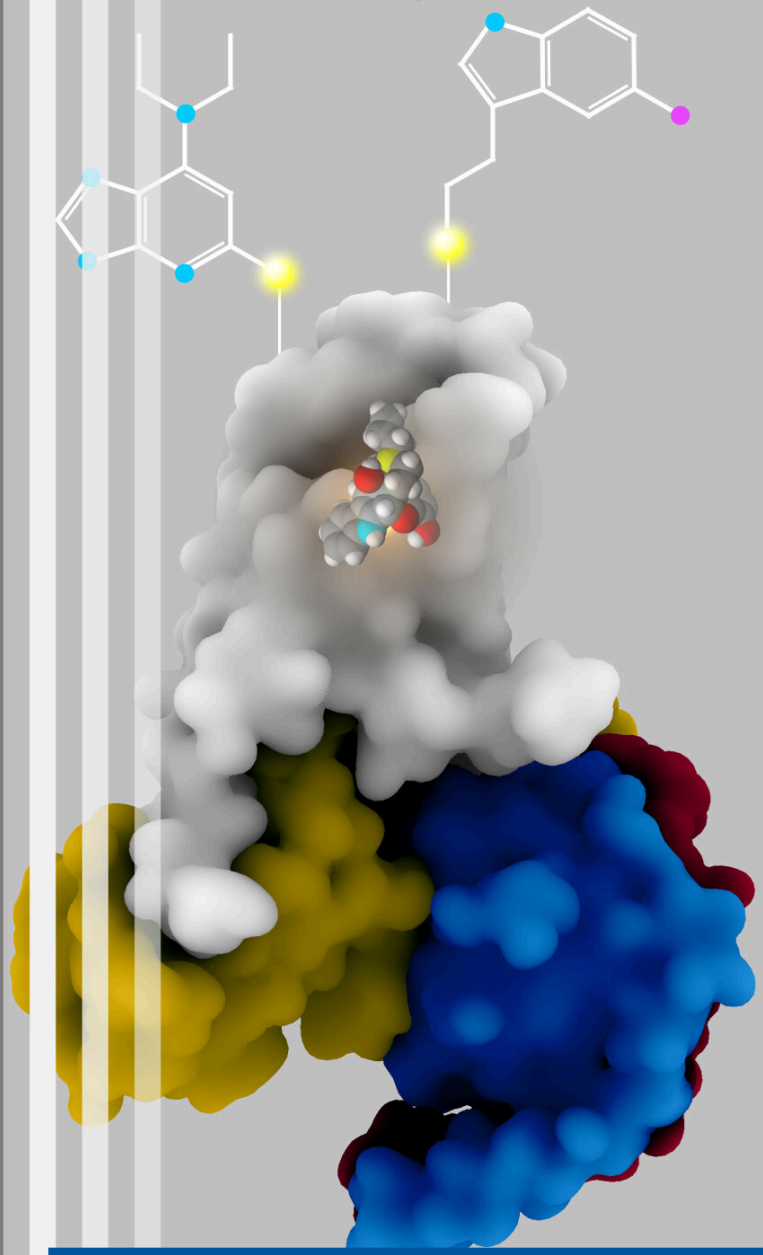

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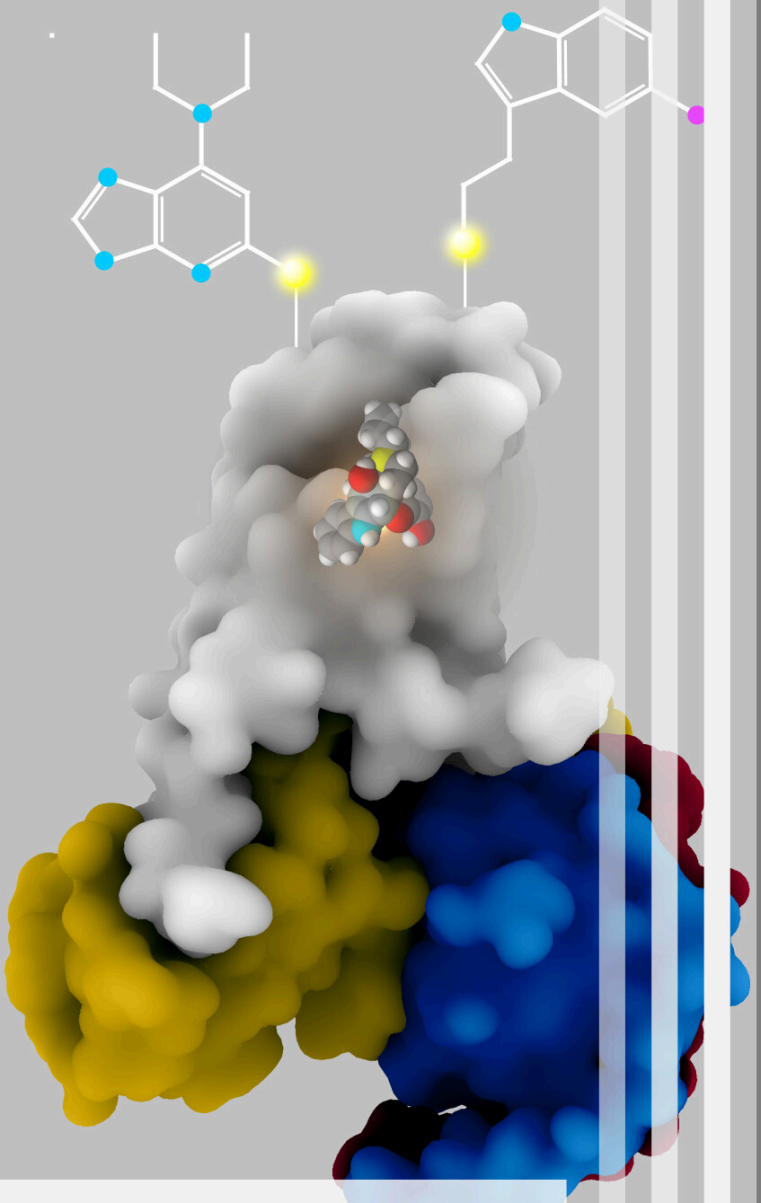

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OUR SCIENCE

Molecular mechanism

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