AIffinity
MOLECULAR DESIGN

Enhancing Drug Discovery with Nuclear Magnetic Resonance & Artificial Intelligence

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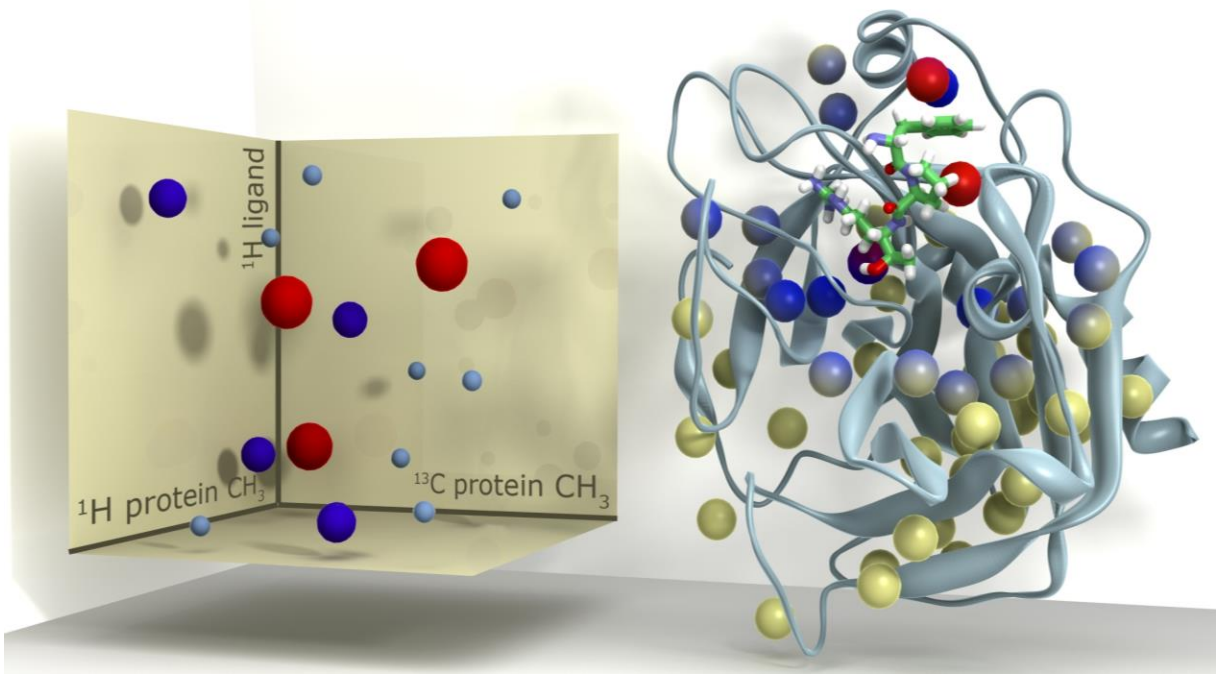
Nuclear Magnetic Resonance (NMR)

Applications:

1. Protein Structure Determination
2. Conformational Dynamics Studies
3. Molecular Interaction Studies
4. Drug screening



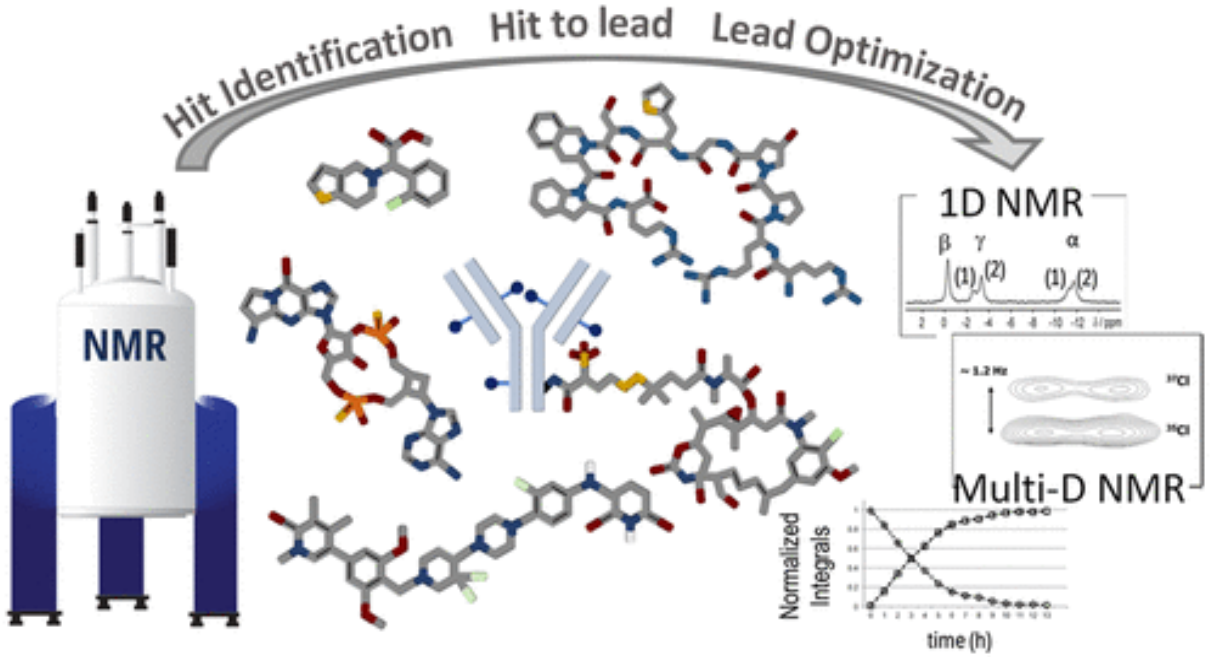
Challenges:

1. Technical Complexity
2. Instrumentation Cost
3. Resource Intensity
4. Protein Size Limitations

With **AI** and **Cheminformatics** we can navigate these challenges

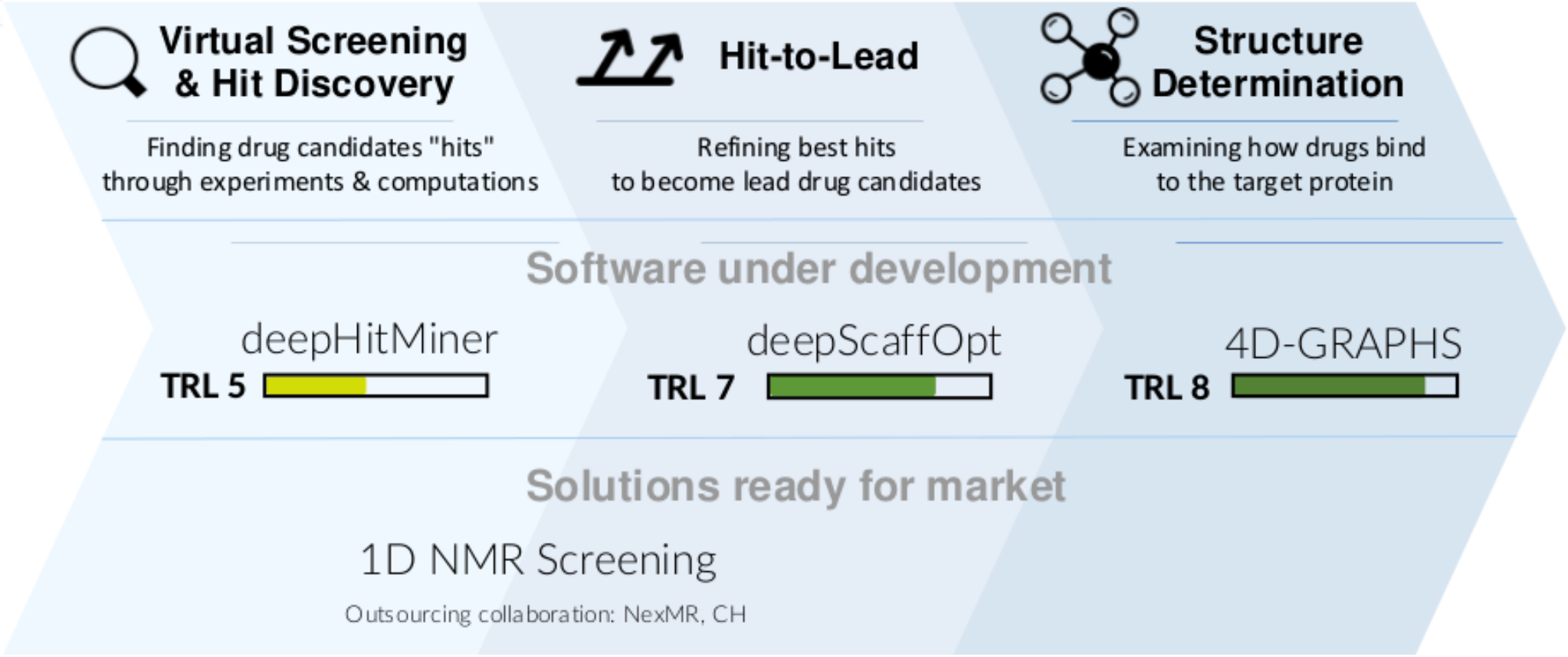
NMR in Drug Design

- Hit Identification and Hit-to-Lead.
- Interactions with ligands, peptides and other protein.
- Purity, solubility, and structural integrity of compounds.



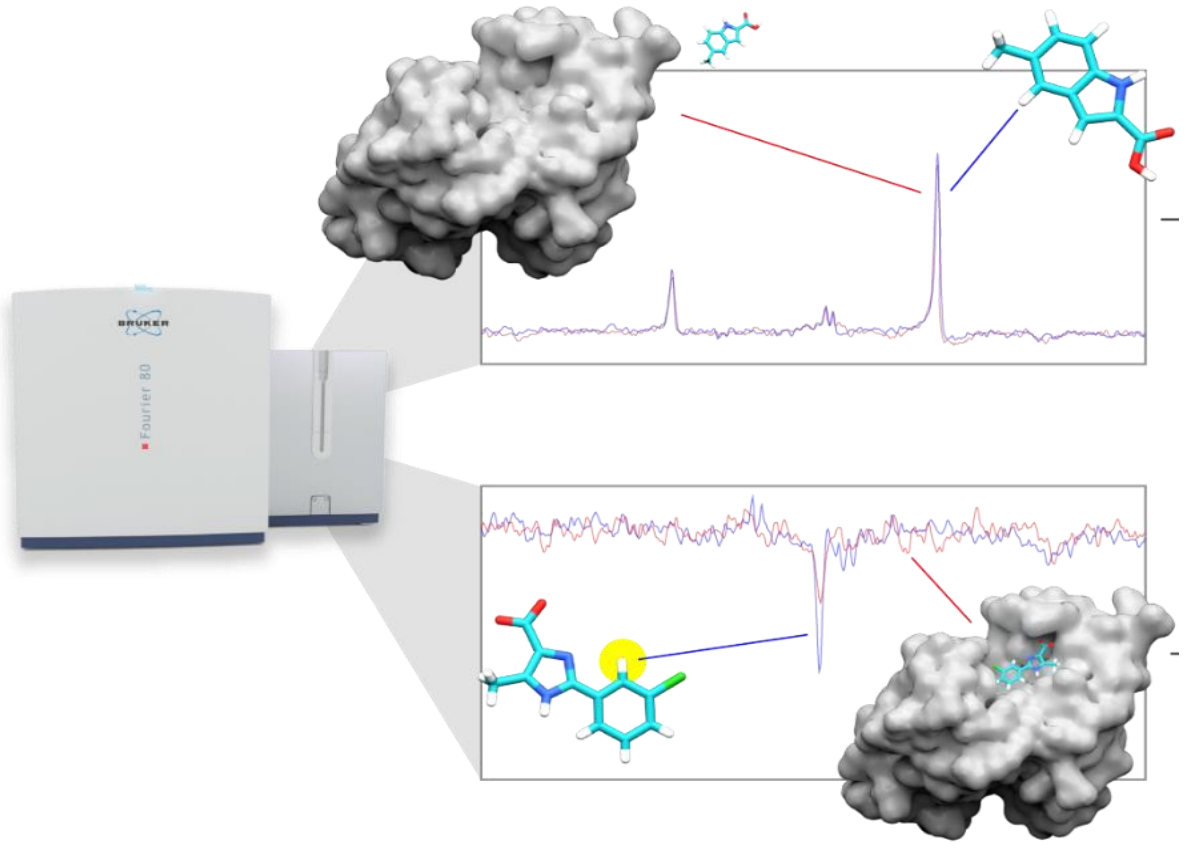
- Development of targeted protein degraders, cyclic dinucleotides, macrocyclic peptides, and antibody-drug conjugates.

Our solution: NMR-AI Integrated platform for Streamlined Target-to-Lead Process



1D NMR Screening

- No assay development.
- Independent of Protein 3D structure
- Gives the atoms of the small molecule that interact with the protein (**ligand epitope**)
- We develop both **Generative AI** and **Virtual Screening solutions** incorporating ligand epitope information.



Joint Drug Development powered by our NMR-AI tech

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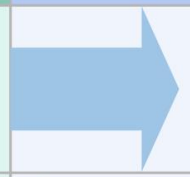
CEITEC Central European Institute of Technology BRNO | CZECH REPUBLIC

NEXMR

安宏生醫 AnHorn Medicines Innovation · New Therapeutics

MUNI SCI Department of Chemistry

Indication	Target	Drug type	Hit discovery	Hit to Lead	Lead Optimization	Pre-clinical Development
Prostate cancer	Androgen Receptor	PROTAC 				
Colorectal cancer	Epigenetic Regulator	Small mol. 				

AI|ffinity Team

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Open Position in Prague or Brno

Cheminformatics Developer

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