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IIT Kanpur partners with Nobel Laureate David Bakerâ??s Lab for AI-guided drug discovery

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AI-guided design of novel proteins targeting key drug receptors

Researchers at the Indian Institute of Technology (IIT) Kanpur worked with the laboratory of Nobel Prize winner Prof. David Baker at the University of Washington to help design a new kind of small protein.

These proteins can block a group of receptors called GPCRs (G protein-coupled receptors), which are present on the surface of our cells and play a part in how many modern medicines act.

The study titled “De novo design of miniproteins targeting GPCRs” has been published in the journal *Nature*. It shows how artificial intelligence (AI) can be used to efficiently design and find the miniproteins that attach to specific GPCRs and change how they behave.

The team designed miniproteins for several GPCRs, including two called CXCR4 and CCR5. Both are being studied as possible drug targets for cancer and for viral infections such as HIV.

IIT Kanpur also contributed to visualising how one of these designed miniproteins attaches to the CXCR4 receptor. Using a powerful imaging technique called cryo-electron microscopy at its cryo-EM facility, researchers could see exactly how the two molecules fit together and how the miniprotein affects the receptor.

The findings of the study reveal that AI-based protein design is a practical tool for drug discovery. While these specific proteins are not medicines yet, and years of further testing lie ahead before it reaches the clinic, the study offers a workable method for designing targeted, protein-based treatments for receptors that have been difficult to target with drugs.