Scientists devise screening method to aid RNA drug development research

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(Phys.org)—Scientists from the Florida campus of The Scripps Research Institute (TSRI) have developed a new method of screening more than three million combinations of interactions between RNA and small molecules to identify the best targets on RNA as well as the most promising potential drug compounds. This novel technology may lead to more efficient drug development.

The study was published in the October 9, 2012 issue of the journal *Nature Communications*.

RNA has multiple biological functions, including encoding and translating proteins from genes and regulating the amount of protein expressed under various cellular conditions. Recent studies have identified RNA as a "molecular switch" that controls cellular events such as gene expression, making RNA an attractive target for small molecules that serve as chemical genetics probes, analytical tools or potential drugs.

However, to date information on which small molecules bind to which parts (structural motifs) of RNA has been sparse, hampering this promising area of research and development. That's where the new study comes in.

"For the first time we have been able to probe what types of small molecules would be good lead drugs to target RNA by probing millions of RNA-ligand combinations," said Matthew Disney, an associate professor at TSRI who authored the study with graduate student Tuan

Tran. "In a viral genome, for example, RNA folds such as hairpin loops contribute to disease, but we don't know which hairpin loops should we focus on. In the study, we were able to define those RNA motifs, including hairpin loops, that bind to small molecules and the types of small molecules that bind to RNA."

Disney notes that larger, more chemically diverse small molecule libraries could be screened to provide additional ligands with an affinity for RNA recognition, plus additional RNA motifs preferred by small molecules. The new method could be used to create easily accessible small molecule libraries biased towards binding to RNA.

The new technology will also be used in a computer program designed by Disney that brings together information on the interaction between small molecules and RNA with data on the RNA folds present in segments of the human genome that contribute to specific human diseases.

More information: "Identifying the Preferred RNA Motifs and Chemotypes that Interact by Probing Millions of Combinations," www.nature.com/ncomms/journal/ … /abs/ncomms2119.html

Provided by Scripps Research Institute

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