Drug research enhanced by fragment screening libraries

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Professor Ron Quinn, Director of Griffith University's Eskitis Institute for Drug Discovery. Credit: Griffith University

Generation of fragment screening libraries could enhance the analysis and application of natural products for medicinal chemistry and drug

discovery, according to Griffith University's Professor Ronald Quinn.

In a paper entitled 'Capturing Nature's Diversity' and published in the peer-reviewed journal *PLOS ONE*, the Director of Griffith's Eskitis Institute for Drug Discovery and his co-authors propose a novel approach to capturing the structural diversity of nature for medical research and implementation.

"In a field where some research is still being conducted in the same way as it has for decades, fragment-based screening is a modern, fast and highly efficient process," says Professor Quinn.

"It offers a particularly tantalising approach to drug discovery by virtue of the fact that a small number of compounds represents a vast proportion of all known natural products."

Professor Quinn says natural products have a huge range of "molecular recognition building blocks" embedded within them.

In this study, researchers identified fragment-sized natural products from a known database, the Dictionary of Natural Products, and then investigated their structural diversity via atom type, atom function and scaffold analysis.

In the end they presented 422 structural clusters—comprised of approximately 2800 natural products—for application in chemical biology and drug discovery.

Professor Quinn contends these naturally-derived fragments could be used as the starting point for a highly diverse library with scope for further elaboration due to their minimal structural complexity.

"Natural products have long been recognised for contributing invaluable

chemical diversity to the design of molecular screening libraries," he says.

"However, fragment-based screening broadens research scope, informs biological application and modernises natural product discovery.

"This is an exciting possibility that should continue to be explored. It is another example of the Eskitis Institute's determination to trial and apply new techniques in the study of natural products for drug discovery and design."

More information: *PLOS ONE*, dx.plos.org/10.1371/journal.pone.0120942

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