Four new leads identified for anti-cancer drugs

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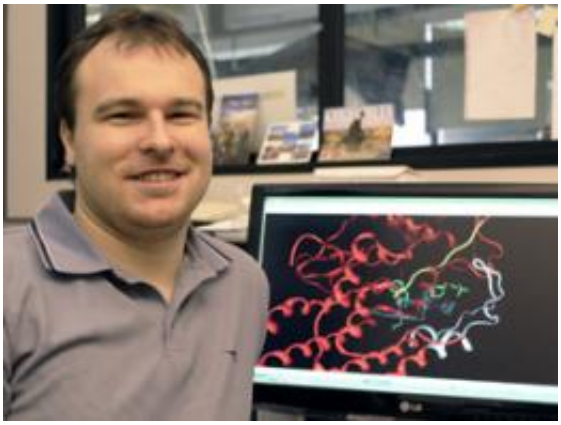

Four new anti-cancer drug leads have been identified in a research paper published online this week in *Bioorganic and Medicinal Chemistry*.

Lead author Jason Smith undertook a comprehensive study that combined existing knowledge of an enzyme with a specifically tailored computational chemistry approach to identify novel inhibitors. The enzyme (indoleamine 2,3-dioxygenase) has generated excitement amongst researchers over the last decade due to its increasingly recognised role as a drug target, particularly in cancer.

"Over the past ten years, scientists have learnt that compounds inhibiting this enzyme allow the immune system to attack cancer cells. They have

found that if you use these inhibitors alone, they slow tumour growth. Even more exciting is that in combination with chemotherapy, these inhibitors have the potential to destroy a tumour entirely," Smith explains.

After conducting virtual screening of a database of almost 60,000 compounds, Smith found 18 compounds that could hold potential as inhibitors of this enzyme. He then tested them in the lab and found four compounds with particularly exciting prospects.

Smith sees many strengths in the approach taken. "Computational chemistry means we don't have to spend years testing thousands of compounds in the lab. We can analyse all the potential compounds and narrow them down in a matter of 6 month's preparation and virtual screening, instead of years. In fact, after all the preparation and groundwork, the screening itself takes around 100 hours."

This research was conducted as part of a collaboration between the Department of Chemistry and Biomolecular Sciences at Macquarie University and the School of Medical Sciences/Pharmacology, University of New South Wales.

Although the leads are a way off from clinical trials, Smith and the team are excited about the future development of this research. Smith, a completing Master of Philosophy student, plans to continue study on these enzyme inhibitors as part of a Doctoral degree in 2012.

Provided by Macquarie University