

Computer predicts anti-cancer molecules

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A new computer-based method of analyzing cellular activity has correctly predicted the anti-tumour activity of several molecules. Research published today in BioMed Central's open access journal *Molecular Cancer* describes 'CoMet' – a tool that studies the integrated machinery of the cell and predicts those components that will have an effect on cancer.

Jeffrey Skolnick, in collaboration with John McDonald, led a team from the Georgia Institute of Technology who have developed this new strategy. As Skolnick explains, "This opens up the possibility of novel therapeutics for cancer and develops our understanding of why such metabolites work. CoMet provides a deeper understanding of the molecular mechanisms of cancer".

The small molecules that are naturally produced in cells are called metabolites. Enzymes, the biological catalysts that produce and consume these metabolites are created according to a cell's genetic blueprints. Importantly, however, the metabolites can also affect the expression of genes. According to the authors "By comparing the gene expression levels of cancer cells relative to normal cells and converting that information into the enzymes that produce metabolites, CoMet predicts metabolites that have lower concentrations in cancer relative to normal cells".

The research proves that by adding such putatively depleted metabolites to cancer cells, they exhibit anticancer properties. In this case, growth of leukemia



cells was slowed by all nine of the metabolites suggested by CoMet. The future for this treatment looks bright, in McDonald's words, "While we have only performed cell proliferation assays, it is reasonable to speculate that some metabolites may also exhibit many other anticancer properties. These could be important steps on the road to a cure".

Source: BioMed Central

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