

Novel algorithm predicts drug combinations to treat drug resistant fungal infections

July 14 2016

Scientists have created an algorithm that can identify drug combinations to treat fungal infections that have become resistant to current drug treatments. This new study, published in *PLOS Computational Biology*, represents a strategy for treating complex diseases and finding new uses for existing drugs.

Fungal infections are one of the leading causes of hospital-acquired infections and are therefore associated with high mortality rates due to growing populations of patients with [weakened immune systems](#). Unfortunately, drug resistance is common for fungus-causing diseases and so there is an urgent need to develop new therapies to overcome this.

Drug combinations have been widely used in biomedical research and medical practices for treating various diseases. In particular, synergistic drug combinations are an effective strategy to overcome drug resistance, increase treatment efficacy and decrease drug dosage to avoid toxicity. Traditionally, effective drug combinations have been identified through experimentally screening all possible combinations of a pre-defined set of drugs - which is expensive, time consuming and labour intensive.

The authors, led by Professor Yan Guiying from the Chinese Academy of Sciences, created a novel algorithm termed Network-based Laplacian regularized Least Square Synergistic drug combination prediction (NLLSS), to predict potential synergistic drug combinations. It does this by integrating different kinds of information such as known synergistic drug combinations, drug-target interactions and drug chemical

structures.

The study then uses NLLSS to predict antifungal synergistic drug combinations for the fungal pathogen *Candida albicans*. This pathogen causes candidiasis which develops into the fourth most common fungal blood stream infection among hospitalized patients in the United States - according to the Centers for Disease Control & Prevention. Using NLLSS, the scientists, led by Prof. Zhang Lixin from the Chinese Academy of Sciences, experimentally validated 7 out of 13 predicted antifungal synergistic drug combinations for *Candida albicans* - which could provide new treatments and work towards overcoming fungal [drug resistance](#) for this pathogen.

This research shows that NLLSS is an efficient strategy to identify potential synergistic antifungal combinations, explore new indications of existing drugs, and provide useful insights into the underlying molecular mechanisms of synergistic [drug combinations](#).

More information: *PLOS Computational Biology*,
[dx.plos.org/10.1371/journal.pcbi.1004975](https://doi.org/10.1371/journal.pcbi.1004975)

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