

Using computer models to predict more effective therapies

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Scientists at Charité – Universitätsmedizin Berlin have used a computer simulation for predicting the effectiveness of various combination therapies for colon tumors. The study has been published in the current issue of the professional journal *Molecular Systems Biology*.

In most tumors, the communication between the individual cells is disturbed and the cells permanently receive growth and survival signals. For this reason, drugs are increasingly used in modern tumor therapy that targets those molecules to shut down these faulty signals. Hitherto, however, it has been difficult to predict the success of such a therapy, since the signal molecules are integrated into an extremely complex cellular network, which, moreover, reacts differently for each patient, depending on the mutations the tumor bears.

The research group headed by Nils Blüthgen, Charité Institute of Pathology, has now examined how the interconnection of such a [cellular network](#) affects the effectiveness of a therapy. For this purpose, the scientists created computer models to simulate the networks of various [colon cancer cells](#). The models were adapted to quantitative data from cell culture experiments. When analyzing their computer simulations, the researchers discovered that the cellular tumor networks exhibited strong feedback characteristics. This means that the cutting off of a particular signal molecule activates a receptor, which, in turn, then switches on [signal paths](#) that favor the survival of the tumor cell. In a further step, the computer model predicted a combination therapy using two drugs, which prevents the activation of survival signals, so making for a more

effective therapy. The scientists have tested these predictions on various cell models. "The remarkable thing is that the combination of two therapies is effective with a large number of different mutations, including the mutant oncogene KRAS. This is a gene, which is of key importance for the regulation of growth and differentiation processes, and for which no targeted therapy has been possible up to now", stated Nils Blüthgen. "However, it is still too early to say whether this behavior detected in the cell culture model can be applied to patients. Here, further investigations are necessary".

This approach undertaken by the researchers to combine computer models with quantitative data to simulate the behavior of networks is called system biology. It is considered a promising method of examining therapies and diagnostics for complex diseases. "Particularly when investigating the effect of inhibitors in complex networks, it is hardly possible to predict the network's response without the use of computer models", according to Blüthgen.

More information: Klinger, B., et al. Network quantification of EGFR signaling unveils potential for targeted combination therapy, *Molecular Systems Biology*, 9: 673, 2013.

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