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Wir bitten um Zusendung von Belegexemplaren! Danke.

Halogen Bonding Helps Design New Drugs

Pharmaceuticals researchers at the University of Tübingen present a new concept for the development of tumor treatments.

Tübingen, 31.05.2012

Halogens – particularly chlorine, bromine, and iodine – have a unique quality which allows them to positively influence the interaction between molecules. This “halogen bonding” has been used in the area of materials science for some time, but is only now finding applications in the life sciences. Yet halogen bonds make it possible to identify molecules which can be helpful in treating illness by influencing their biological target structure.

Scientists at the University of Tübingen have now demonstrated for the first time that halogen bonding can be used in cancer treatment. In doing so, Professor Frank Böckler and his team have presented a state-of-the-art method in pharmaceutical research: fragment-based development of leading compounds. The method uses fragment libraries to screen for biological target structures such as proteins or DNA, in order to form a basis for the development of new drugs.

To date, halogens – particularly the heavier bromine and iodine – have been underrepresented in such fragment libraries. Now, for the first time, scientists at the Pharmaceutical Institute at the University of Tübingen have described the design and application of halogen-enriched fragment libraries in the *Journal of the American Chemical Society* (DOI: 10.1021/ja301056a).

Publication: Rainer Wilcken, Xiangrui Liu, Markus O. Zimmermann, Trevor J. Rutherford, Alan R. Fersht, Andreas C. Joerger* & Frank M. Boeckler*: „Halogen-Enriched Fragment Libraries as Leads for Drug Rescue of Mutant p53“. *J. Am. Chem. Soc.*, 2012, 134 (15), pp 6810–6818 (DOI: 10.1021/ja301056a)

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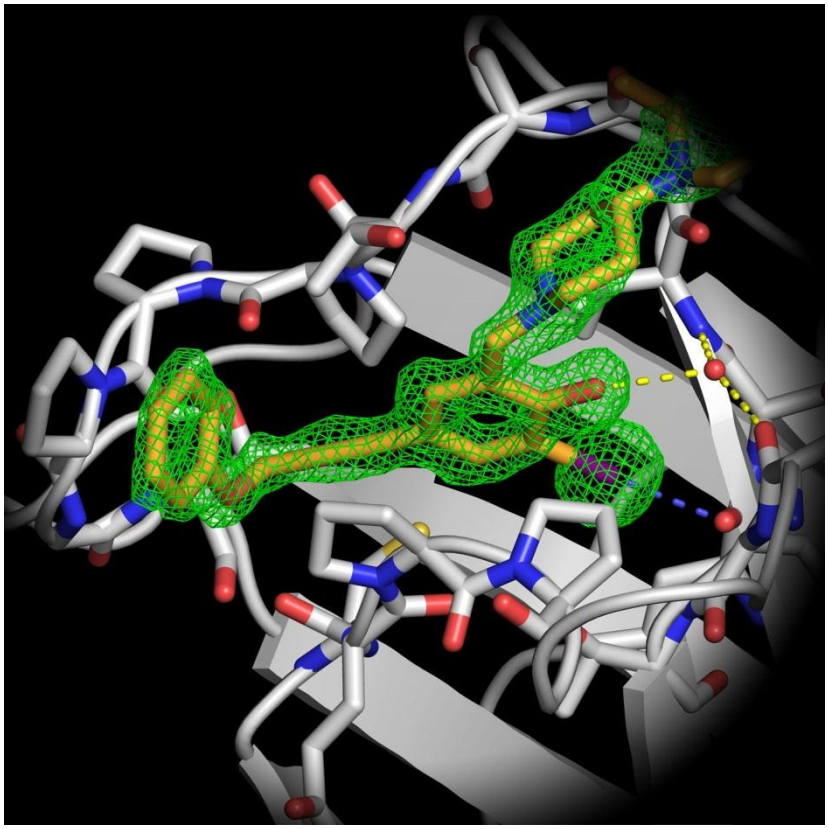

Part of the crystal structure of the mutated tumor suppressor p53, interacting with the binding pocket via a halogen bond (purple dotted line). Compounds of the new class of substances reactivate p53 in affected cancer cells.

Graphic: Prof. Frank Böckler