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Halogen Bonding Helps Design New Drugs

ScienceDaily (June 5, 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 employed in the area of materials science for some time, but is only now finding applications in the life sciences.

Scientists at the University of Tübingen, in cooperation with the MRC Laboratory of Molecular Biology in Cambridge / UK, have now demonstrated that halogen bonding can be used to identify potential drug candidates for cancer treatment. Dr. Rainer Wilcken and Prof. Frank Böckler in collaboration with Dr. Andreas Joerger and Prof. Sir Alan Fersht, have presented a new concept of pharmaceutical research: fragment-based development of lead compounds based on halogen bonding.

The method uses specially designed fragment libraries to screen for binders to biological target structures such as proteins or DNA in order to develop 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 (HEFLibs) in the *Journal of the American Chemical Society*.

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Story Source:

The above story is reprinted from materials provided by **Universitaet Tübingen**, via AlphaGalileo.

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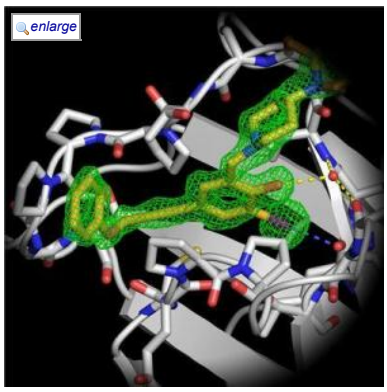
Journal Reference:

1. 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**. *Journal of the American Chemical Society*, 2012; 134 (15): 6810 DOI: 10.1021/ja301056a



Part of the crystal structure of the mutated tumor suppressor p53 bound to a reactivating small molecule 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. (Credit: Prof. Frank Böckler)

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