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Structure-based discovery of new modulators targeting nuclear X receptor alpha for cancer therapy

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Retinoid X receptor-alpha (RXRα) is implicated in the regulation of many biological processes and also represents a unique intracellular target for pharmacologic interventions. Efforts on discovery of small molecules targeting RXRα have been primarily focused on the molecules that bind to its classical ligand-binding pocket (LBP). Using structure-based approach and in collaboration with a multi-disciplinary team, we have identified novel RXRα modulators that use new binding mechanisms to mediate the biological functions of RXRα. The new compounds can effectively suppress AKT activation and promotes apoptosis of cancer cells in a RXRα-dependent manner by inhibiting the interaction between a truncated RXRα and the p85α subunit of PI3K.

Biography

Ying Su, PhD, is computational chemist with over 15 years of experience on computer-aided drug design. She received her PhD from the University of California, San Diego. After a postdoctoral appointment at the Scripps Research Institute, she worked for several local biotech companies. She joined the Sanford-Burnham Medical Research Institute in 2005 to build and lead a HTS informatics and Cheminformticsgroup. She is co-author of over 40 peer-reviewed scientific publications.

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