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Computer Model to Identify Potential anti-Diabetic Compounds

A new computer model that helps screen potential anti-diabetic compounds has been developed and tested by researchers at the Bharati Vidyapeeth College of Pharmacy and Annasaheb Dange College of Pharmacy, Maharashtra in their recent study published in the journal of Molecular structure.

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Traditional method of screening and testing anti-diabetic drugs is expensive, laborious, and time consuming. Many labs across the globe have now shifted to computer-based or *in silico* approach to screen drugs.

Researchers at the Bharati Vidyapeeth College of Pharmacy and Annasaheb Dange College of Pharmacy, Maharashtra have developed a computer model for testing compounds for their potential anti-diabetic activity.

It tests the anti-diabetic activity of compounds by simulating the binding of the test compound with protein called PPARϒ- a family of receptor proteins involved in insulin sensitivity, and regulation and metabolism of fats. This protein has a significant therapeutic value in many metabolic disorders including diabetes.

The researchers have tested their model using 46 known anti-diabetic compounds and found that their model predicts the anti-diabetic potential of these anti-diabetic compounds in accordance with their known biological activity. The scientists proclaim, "… (The) model developed in this study will be a useful tool in identification and development of lead molecules with anti-diabetic activity".

If developed further, this model can also help researchers to design new molecules with desired biological activity against specific diseases and ailments.

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