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Bansal H, Sharma A, Sharma V, Kumar V. Pharmacophore modeling studies on xanthones as monoamine oxidase-A inhibitors*. Bull. Pharm. Res.* 2011;1(1):15-21.

Abstract: Pharmacophore mapping studies were undertaken for a set of 42 xanthone as monoamine oxidase-A inhibitors. Five point pharmacophores with three hydrogen bond acceptor, and two aromatic ring as pharmacophoric features were developed. Amongst them the pharmacophore hypothesis AAARR1 yielded a statistically significant 3D-QSAR model with 0.81 as R-square value and was considered to be the best pharmacophore hypothesis. The developed pharmacophore model was externally validated by predicting the activity of test set molecules. The squared predictive correlation coefficient of 0.79 was observed between experimental and predicted activity values of test set molecules. The geometry and features of pharmacophore were expected to be useful for the design of selective MAO-A inhibitors.

Key words: Xanthone, Monoamine oxidase-A, Pharmacophore hypothesis, Regression coefficient.

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