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Synthesis, molecular docking and dynamic simulation studies of new 7-oxycoumarin derivatives as potential antioxidant agents

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Two new series of 4-styryl-7-oxycoumarin derivatives 3a-i and 4-styryl-7-oxycoumarin-8-Mannich bases 6a-r were designed and synthesized. Ten compounds were evaluated *in vivo* for their antioxidant activities against lipid peroxidation, Superoxide dismutase (SOD), glutathione-s-transferase (GST) and catalase (CAT) activities. Compounds 1, 6b, 3c and 6r displayed significant decrease in MDA, SOD and CAT enzyme levels in H2O2 treated rats. Free binding energy was estimated by docking, MM-PBSA and MM-GBSA. Molecular dynamics simulation followed by MM-GBSA calculation was correlated to the antioxidant effect. Compound 1 illustrated the highest MM-GBSA value (-20.38) and the best antioxidant effect.

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