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Antioxidant activity and *in vitro* and *in silico* gout inhibitory effect of benzylideneacetophenone derivatives

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Abstract. Chalcones were experimentally investigated for their ability to act as antioxidants and as xanthine oxidase inhibitors *in vitro* and *in silico*. The antioxidant ability of chalcone (benzylideneacetophenone, A) and 7 chalcone derivatives (1-phenyl-3(benzodioxolyl)-2-propen-1-one, B; 4'-nitro-4-dimethylaminochalcone, C; 4-nitro-4-methoxychalcone, D; 1(4'-nitrophenyl)-3(1,3-benzodioxolyl)-2-propen-1-one, E; 1-phenyl-3(γ-benzopyranoyl)-2-propen-1-one, F; 1-(4'-nitrophenyl)-3(γ-benzopyranoyl)-2-propen-1-one, G; 4-dimethylaminochalcone, H) was evaluated spectrophotometrically utilizing three methods: DPPH, copper chelation, and hydrogen peroxide scavenging. Also *in vitro* xanthine oxidase inhibitory activity and molecular docking using computer simulation were carried out. In the DPPH radical scavenging, samples A, B and G showed higher percentages of inhibiting DPPH as compared to the standard antioxidant gallic acid. The copper chelating ability of the compounds indicated that samples A, C, and F chelate copper efficiently than EDTA. The percent of hydrogen peroxide scavenging by chalcones indicated that samples C, D, G, and H are better antioxidants. Also, the *in vitro* xanthine oxidase inhibitory activity of chalcones showed that samples inhibited the enzyme but not as high as the reference drug allopurinol. The molecular docking studies revealed that samples C, E, F, and G had higher docking scores of -7.98, -8.51, -8.67 and -10.07, which were higher than -7.59 kcal/mol for allopurinol. Therefore, samples C, E, F, and G showed antioxidant and *in vitro* xanthine oxidase inhibition as well as better docking values. These results made these chalcones promising targets against xanthine oxidase or gout.

***Keywords*:** gout; chalcones; xanthine oxidase; molecular docking; antioxidants.

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