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Jingfen Li, Dong Li, Yiming Xu, Zhenbo Guo, Xu Liu, Hua Yang, Lisheng Wang, Lichuan Wu

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**Design, synthesis, biological evaluation, and molecular docking of  
chalcone derivatives as anti-inflammatory agents**

Jingfen Li <sup>a,†</sup>, Dong Li <sup>b,†</sup>, Yiming Xu <sup>b</sup>, Zhenbo Guo <sup>b</sup>, Xu Liu <sup>b</sup>, Hua Yang <sup>b</sup>, Lisheng Wang <sup>b,\*</sup>, Lichuan Wu <sup>b,\*</sup>

<sup>a</sup> Department of Life Science, Huzhou Teachers' College, Huzhou, 313000, People's Republic of China

<sup>b</sup> School of Chemistry and Chemical Engineering, Guangxi University, Nanning, 530004, People's Republic of China

<sup>†</sup> The authors contributed equally to this work

\* Corresponding authors: Lisheng Wang, E-mail: [w\\_lsheng@163.com](mailto:w_lsheng@163.com), Daxue East Road, No.100, Nanning, Guangxi 530004, PR China  
Lichuan Wu, E-mail: [wulichuan@126.com](mailto:wulichuan@126.com), Daxue East Road, No.100, Nanning, Guangxi 530004, PR China

**Abstract:** In this study, two series of 35 new chalcone derivatives containing aryl-piperazine or aryl-sulfonyl-piperazine fragment were synthesized and their structures were characterized by <sup>1</sup>H, <sup>13</sup>C and ESI-MS. The *in vivo* and *in vitro* anti-inflammatory activities of target compounds were evaluated by using classical para-xylene-induced mice ear-swelling model and ELISA assays. Furthermore, docking studies were performed in COX-2 (4PH9). The *in vivo* anti-inflammatory assays indicated that most of the target compounds showed significant anti-inflammatory activities. Docking results revealed that the anti-inflammatory activities of compounds correlated with their docking results. Especially, compound **60** exhibited the most potent anti-inflammatory activity *in vivo* with the lowest docking score of -17.4 Kcal/mol and could significantly inhibit the release of LPS-induced IL-6 and TNF- $\alpha$  in a dose-dependent manner *in vitro*.

**Keywords:** inflammation, chalcone, derivatives, anti-inflammatory activity, COX-2

Inflammation is a complex biological process which seriously threatens human health. Exaggerated and prolonged inflammation may cause various diseases, such as arthritis, sepsis, and even cancer.<sup>1</sup> At present, the most widely used drugs in treating

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