* Treatment and Prophylaxis - Original Paper
* [Published: 11 April 2020](https://link.springer.com/article/10.1007%2Fs00436-020-06668-6#article-info)

Imidazole derivatives as antiparasitic agents and use of molecular modeling to investigate the structure–activity relationship

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[*Parasitology Research*](https://link.springer.com/journal/436) **volume 119**, pages1925–1941 (2020)[Cite this article](https://link.springer.com/article/10.1007%2Fs00436-020-06668-6#citeas)

* **332**Accesses
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Abstract

Toxoplasmosis is a common parasitic disease caused by *Toxoplasma gondii*. Limitations of available treatments motivate the search for better therapies for toxoplasmosis. In this study, we synthesized a series of new imidazole derivatives: *bis*-imidazoles (compounds 1–8), phenyl-substituted 1*H*-imidazoles (compounds 9–19), and thiopene-imidazoles (compounds 20–26). All these compounds were assessed for in vitro potential to restrict the growth of *T. gondii*. To explore the structure–activity relationships, molecular analyses and bioactivity prediction studies were performed using a standard molecular model. The in vitro results, in combination with the predictive model, revealed that the imidazole derivatives have excellent selectivity activity against *T. gondii* versus the host cells. Of the 26 compounds screened, five imidazole derivatives (compounds 10, 11, 18, 20, and 21) shared a specific structural moiety and exhibited significantly high selectivity (> 1176 to > 27,666) towards the parasite versus the host cells. These imidazole derivatives are potential candidates for further studies. We show evidence that supports the antiparasitic action of the imidazole derivatives. The findings are promising in that they reinforce the prospects of imidazole derivatives as alternative and effective antiparasitic therapy as well as providing evidence for a probable biological mechanism.

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