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Computer-aided rational molecular design of a new chitinase inhibitor

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Since chitinase is an essential enzyme for fungi, insects, and ticks, it appears to be a suitable target for developing new antibiotics or new pesticides. Recently, a new chitinase inhibitor, named argadin, was isolated [1], and its complex structure with chitinase was also reported [2]. In this study, we use structure-based drug design approach in order to design a new chitinase inhibitor with 14-membered ring macrolide skeleton, which has a potential availability for the oral administration. Our designed compound seems to be able to interact with chitinase in the fashion similar to argadin-chitinase interaction mode and have an affinity comparable to that of argadin.

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References

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[2] D.R. Houston, *et al., Proc. Natl. Acad. Sci. USA.*, **99** (14), 9127 - 9132 (2002).