

Synthesis, Nematicidal Activity, and Molecular Docking of Some 3-Isopropyl-1-methyl-1*H*-pyrazole-5-carboxamide Compounds

Yong-Hui Wen^{1,2}, Lin-Ru Han^{1,2}, Liang Han¹, Tian-Ming Xu², Xing-Hai Liu^{1*}, Wei-Li Peng^{2*}

¹College of Chemical Engineering, Zhejiang University of Technology, Hangzhou 310014, China

²Zhejiang Base of National Southern Pesticide Research Centre, Zhejiang Research Institute of Chemical Industry, Hangzhou 310023, China

ABSTRACT Seven 3-isopropyl-1-methyl-1*H*-pyrazole-5-carboxamide compounds were designed and synthesized. The structures of seven 3-isopropyl-1-methyl-1*H*-pyrazole-5-carboxamide compounds were confirmed by ¹H-nuclear magnetic resonance and MS. The primarily nematicidal activity results indicated that some of them exhibited moderate activity against *Meloidogyne incognita* at 10 ppm. Among them, compounds (*R*)-4-chloro-*N*-(1-(4-chlorophenyl)ethyl)-3-isopropyl-1-methyl-1*H*-pyrazole-5-carboxamide (5b) and 4-chloro-3-isopropyl-*N*,1-dimethyl-*N*-(3,4,5-trimethoxybenzyl)-1*H*-pyrazole-5-carboxamide (5g) exhibited the best activity. Furthermore, molecular docking results indicated that compound **5b** interacted with succinate dehydrogenase by hydrogen bond. It provided useful information for further design novel nematicides.

KEYWORDS Pyrazole carboxamide, Synthesis, Nematicidal activity, Molecular docking

How to cite this article: Wen, Y.H., Han, L.R., Han, L., Xu, T.M., Liu, X.H., Peng, W.L (2021) Synthesis, Nematicidal Activity, and Molecular Docking of Some 3-Isopropyl-1-methyl-1*H*-pyrazole-5-carboxamide Compounds. *Indian J. Heterocycl. Chem.* **2021**, *31*, 417–421.
(DocID: <https://connectjournals.com/01951.2021.31.417>)