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SHORT REPORT

Aromatic polyketides from the marine-derived fungus *Aspergillus unguis* PM03: α-glucosidase inhibitory activity, structure-activity relationship, molecular docking and ADMET evaluation

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Abstract: Chemical investigation of *Aspergillus unguis* PM03 yielded eight known aromatic polyketides, including unguinol (**1**), nidulin (**2**), 2,4-dichlorounguinol (**3**), 2-chlorounguinol (**4**), emeguisin B (**5**), aspergillusether A (**6**), guisinol (**7**), and isosclerone (**8**). Their structures were established by spectroscopic analysis and comparison with published data. All isolated compounds were evaluated for cytotoxicity against four human cancer cell lines (KB, Hep-G2, A549, and MCF-7) and for α-glucosidase inhibitory activity. None of the compounds exhibited significant cytotoxicity (IC_{50} > 128 μM). Compounds **1, 3, 5, 7**, and **8** inhibited α-glucosidase, with guisinol (**7**) showing the strongest activity (IC_{50} = 4.01 μM), followed by isosclerone (**8**) (11.39 μM), emeguisin B (**5**) (24.31 μM), unguinol (**1**) (26.28 μM), and 2,4-dichlorounguinol (**3**) (28.83 μM). To our knowledge, this is the first report of the α-glucosidase inhibitory activity of compounds **1**–**7**. A preliminary structure–activity relationship analysis suggested that the substitution pattern of the aromatic polyketides may affect their inhibitory activity. Molecular docking of compounds **1**–**7** and four aromatic polyketides previously isolated in our studies was performed against penicillin-binding protein 2a (PBP2a; PDB ID: 1MWT), together with in silico ADMET prediction to assess their pharmacokinetic properties.

Keywords: *Aspergillus unguis*, aromatic polyketide, depsidone, α-glucosidase inhibition, molecular docking, PBP2a

1 Fungal Source

The fungal strain PM03 was isolated from a sediment sample, collected at a depth of 9 m off Mui Nghe, Da Nang, Vietnam (16°07′81″ N, 108°19′96″ E), in May 2025. The sediment sample was collected during the 9th scientific expedition of the R/V *Akademik Oparin* in the Vietnamese marine waters. The taxonomy of the strain PM03 was identified by using 18S rRNA gene sequence analysis and compared with fungal 18S rRNA sequences in the GeneBank database by the NBCI Blast program. The ITS gene sequence of strain PM03 was deposited in GenBank under accession number PZ501680 and identified as *Aspergillus unguis*. Detailed information of the fungus identification was provided in the Supporting information.

2 Previous Studies

Marine-derived fungi have attracted considerable attention because of their remarkable biosynthetic capabilities and their ability to produce a wide variety of secondary metabolites with antibacterial, antifungal, antiviral, cytotoxic, anti-inflammatory, and enzyme inhibitory activities (Carroll et al., 2020, Carroll et al., 2022, Imhoff, 2016, Ji et al., 2025, Luo et al., 2025, Rateb & Ebel, 2011). Consequently, marine fungi have become a valuable resource for the discovery of lead compounds with potential pharmaceutical applications. Among fungal secondary metabolites,

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depsides and depsidones represent characteristic classes of aromatic polyketides that are frequently encountered in species of the genera *Aspergillus* and *Penicillium* (Khayat et al., 2023). Numerous members of these metabolite classes have been reported to exhibit diverse biological activities, including antibacterial, antifungal, cytotoxic, antiviral, and anti-inflammatory effects (Daletos et al., 2018, Wang et al., 2025, Wang & Ding, 2018, Yang et al., 2022). In particular, halogenated depsidones such as nidulin, unguinol, and emeguisin-type metabolites have demonstrated promising antibacterial activities against Gram-positive bacteria, highlighting these fungal aromatic polyketides as attractive scaffolds for antimicrobial drug discovery (Isaka et al., 2019, Sadorn et al., 2022, Yang et al., 2018). However, compared with their antimicrobial and cytotoxic activities, the α-glucosidase inhibitory potential of fungal depsides and depsidones has received considerably less attention (Ibrahim et al., 2018, Ibrahim et al., 2021). α-Glucosidase plays an important role in carbohydrate digestion and is a relevant target for controlling postprandial blood glucose levels (Proença et al., 2017, Van de Laar, 2008). Investigating the α-glucosidase inhibitory activity of these metabolites therefore provides an opportunity to explore an under-investigated aspect of their biological potential. To the best of our knowledge, the α-glucosidase inhibitory activities of compounds **1**–**7** have not previously been investigated.

Besides evaluating their antidiabetic potential, further understanding of the antibacterial properties of fungal aromatic polyketides is also of considerable interest. Methicillin-resistant *Staphylococcus aureus* (MRSA) remains a major antimicrobial-resistant pathogen, and penicillin-binding protein 2a (PBP2a) has been recognized as a relevant antibacterial target associated with *β*-lactam resistance (Chambers & DeLeo, 2009, Fishovitz et al., 2014, Lim & Strynadka, 2002, Turner et al., 2019). Molecular docking has been widely employed to investigate ligand-protein interactions and to provide molecular support for experimentally observed biological activities (Meng et al., 2011, Morris & Lim-Wilby, 2008). In the present study, PBP2a was selected as a representative antibacterial target to explore the potential interactions of fungal depsides and depsidones with a protein associated with MRSA resistance (Fishovitz et al., 2014, Handayani et al., 2023, Lim & Strynadka, 2002).

3 Present Study

Chemical investigation of the EtOAc extract of the marine-derived *Aspergillus unguis* PM03 led to the isolation of eight known compounds through successive chromatographic separations (Figure 1). The structures of the isolated compounds were established on the basis of their spectroscopic data analyses, including 1D and 2D NMR spectra (Supplementary Information), and by comparison with literature values. Accordingly, the compounds were identified as unguinol (**1**) (Kawahara et al., 1988a, Sadorn et al., 2022), nidulin (**2**) (Phainuphong et al., 2018), 2,4-dichlorounguinol (**3**) (Phainuphong et al., 2018), 2-chlorounguinol (**4**) (Kawahara et al., 1988a), emeguisin B (**5**) (Kawahara et al., 1988b), aspergillusether A (**6**) (Ganihigama et al., 2015, Zhang et al., 2014), guisinol (**7**) (Nielsen et al., 1999), and isosclerone (**8**) (Klaiklay et al., 2012) (Figure 1). Notably, compounds **1**–**7** represent depside/depsidone-derived polyketides, including two chlorinated compounds (**3** and **4**), highlighting the capacity of strain PM03 to produce structurally diverse aromatic polyketides. Considering the diverse biological activities previously reported for fungal aromatic polyketides, the isolated compounds **1**–**8** were subjected to cytotoxicity and α-glucosidase inhibition assays. Furthermore, comparative molecular docking studies toward PBP2a (PDB ID: 1MWT) were performed using the isolated compounds (**1**–**7**) together with several structurally related fungal depsides and depsidones reported by our research group (**9**–**12**) (Table S1) (Nguyen et al., 2023, Thi Hoang Anh et al., 2023), allowing a broader evaluation of structure-activity relationships within this class of aromatic polyketides. In addition, the pharmacokinetic properties of the investigated metabolites were preliminarily assessed through in *silico* ADME prediction to evaluate their drug-likeness and pharmacokinetic properties.

3.1 Cytotoxicity and α-glucosidase Inhibitory Activities

The isolated compounds were evaluated for their cytotoxic activities against four human cancer cell lines (KB, HepG2, A549, and MCF-7) and for α-glucosidase inhibitory activity (Table S2). None of the tested compounds exhibited significant cytotoxicity against the tested cell lines, with IC_{50} values exceeding 100 μM. These results suggest that the isolated compounds possess low cytotoxicity under the tested conditions and that their biological effects are unlikely to be associated with general cellular toxicity. In contrast, the isolated compounds displayed varying degrees of α-glucosidase inhibitory activity, with IC_{50} values ranging from 4.01 to 185.64 μM. Notably, guisinol (**7**) exhibited the strongest inhibition with an IC_{50} value of 4.01 ± 0.17 μM, followed by isosclerone (**8**) (11.39 ± 0.17 μM), emeguisin B (**5**) (24.31 ± 0.56 μM), unguinol (**1**) (26.28 ± 0.15 μM), and 2,4-dichloroguinol (**3**) (28.83 ± 0.51 μM). These compounds showed stronger inhibitory activity than the positive control acarbose (IC_{50} = 279.36 ± 11.23 μM), highlighting the potential of marine fungal aromatic polyketides as promising α-glucosidase inhibitors.

Preliminary structure-activity relationship analysis revealed that substitution patterns within the depsidone and depside skeletons markedly influenced inhibitory potency. Among the depsidones, unguinol (**1**) displayed considerably stronger activity than nidulin (**2**), suggesting that *O*-methylation at C-8 and additional chlorination may reduce α-glucosidase inhibition. Similarly, 2,4-dichloroguinol (**3**) was more active than 2-chloroguinol (**4**), indicating that the presence of an additional chlorine substituent may favour enzyme inhibition in this structural series. Comparison of compounds **1**–**4** further suggests that the free phenolic hydroxyl groups present in compounds **1** and **3** contribute positively to activity, whereas methylation of these functionalities appears detrimental. The prenylated depside guisinol (**7**) showed the highest inhibitory activity among all tested compounds, indicating that the depside

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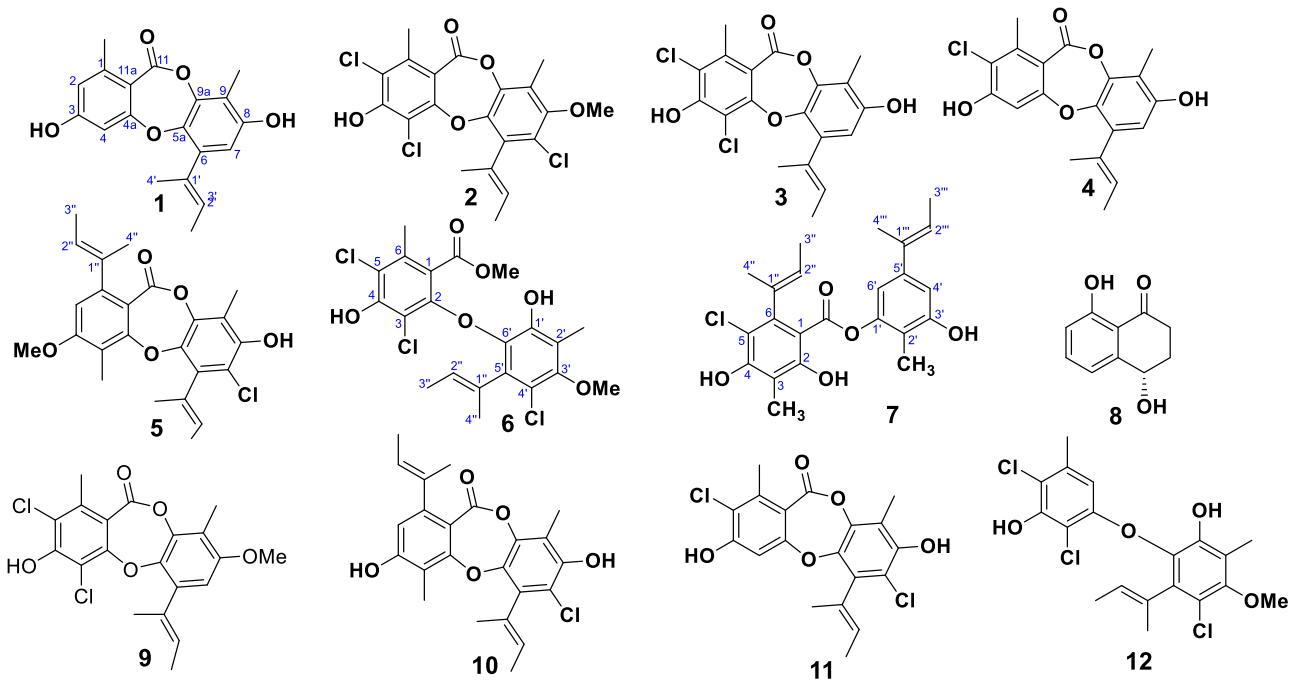


Figure 1. The structures of compounds **1**–**12.** Compounds **1**–**8** were isolated from the marine-derived *A. unguis* PM03 in the present study, whereas compounds **9**–**12** were previously isolated and characterized by our research group and were included for comparative docking and structure-activity relationship analyses (Thi Hoang Anh et al., 2023)

skeleton may be more favorable for α-glucosidase inhibition than the corresponding depsidone skeleton. The enhanced activity of compound **7** may be attributed to the combination of multiple phenolic hydroxyl groups and a flexible depside linkage, which could facilitate productive interactions with the enzyme. In contrast, aspergillusether A (**6**), a highly substituted chlorinated depsidone bearing two methoxy groups, exhibited only weak activity (IC_{50} = 185.64 ± 4.43 μM), further supporting the unfavorable effect of extensive *O*-methylation on α-glucosidase inhibition. Overall, the results suggest that α-glucosidase inhibitory activity in this series is influenced by a delicate balance among halogenation, hydroxylation, and methoxylation patterns. Free phenolic hydroxyl groups appear to play a crucial role in maintaining activity, whereas excessive methylation generally diminishes inhibitory potency. The potent activity observed for guisinol (**7**), emeguisin B (**5**), unguinol (**1**), and 2,4-dichloroguinol (**3**) highlights these fungal aromatic polyketides as attractive scaffolds for the development of novel α-glucosidase inhibitors.

3.2 Comparative Antibacterial SAR Analysis

The antibacterial activities of compounds **1**–**7** have been reported previously by our research group (Nguyen et al., 2023, Thi Hoang Anh et al., 2023). For clarity and to facilitate comparative structure-activity relationship (SAR) analysis together with the subsequent molecular docking study, these antibacterial data are summarized in Table S1. Overall, the halogenated depsidones (**1**–**6**) exhibited moderate to potent antibacterial activities against the tested microorganisms, whereas the depside derivative guisinol (**7**) displayed the broadest antibacterial spectrum with minimum inhibitory concentration (MIC) values of 4 μg/mL against *E. faecalis*, *S. aureus*, *B. cereus*, and *S. enterica*. Among the depsidones, nidulin (**2**) showed the most potent antibacterial activity, suggesting that the combined presence of chlorine atoms and methoxy substitution may favor antibacterial potency. In contrast, the structurally related chlorinated analogues 2,4-dichlorounguinol (**3**) and 2-chlorounguinol (**4**) exhibited only moderate activities, indicating that chlorination alone is insufficient to determine antibacterial efficacy. Similarly, aspergillusether A (**6**) displayed weaker antibacterial activity than the other depsidones despite sharing the same core scaffold, suggesting that subtle differences in substitution patterns also influence biological activity. Collectively, these observations indicate that antibacterial activity within this family is governed by the combined effects of the aromatic scaffold and substituent pattern, providing a rationale for subsequent molecular docking studies toward PBP2a.

3.3 Molecular Docking Toward PBP2a Analysis

To further rationalize the previously reported antibacterial activities of this class of metabolites, molecular docking against penicillin-binding protein 2a (PBP2a) from methicillin resistant *S. aureus* strain (PDB ID: 1MWT) were performed using eleven structurally related aromatic polyketides (**1**–**7**, **9**–**12**). The results of docking analysis are described in Table S3 and major ligand-protein interactions are illustrated in Figure S20. Molecular docking revealed that all compounds exhibited favorable binding affinities

toward PBP2a, with binding energy ranging from –5.9 to –7.0 kcal/mol. Compounds **2** (nidulin), **4** (2-chlorounguinol), and **10** (emeguisin A) presented the highest binding energies (–7.0 kcal/mol), comparable to the reference control, penicillin (–7.0 kcal/mol) and streptomycin (–6.7 kcal/mol). The binding modes were mainly stabilized through hydrogen bonds, hydrophobic interactions, and π-related interactions with key residues, including Tyr446, Gln521, Glu602, Met641, Ser462, and Ser643.

Representative binding modes of compounds **2** (nidulin), **4** (2-chlorounguinol), and **10** (emeguisin A) and the docking binding poses of the remaining compounds are provided in the Supporting Information (Figures S20). These findings suggest that these metabolites can be favorably accommodated within the PBP2a binding pocket, supporting their potential antibacterial activity.

3.4 In silico ADME and Toxicity Prediction

To further evaluate the drug development potential of the isolated metabolites, *in silico* ADME and toxicity prediction was performed for compounds **1**–**7** together with the structurally related compounds **9**–**12**, using the SwissADME and Pro-Tox 3.0 platforms (Table S4). All compounds exhibited favorable physicochemical properties, including molecular weights below 500 Da, acceptable hydrogen-bond donor/acceptor counts, TPSA values below 90 Å^2, and no more than one Lipinski's rule-of-five violation, indicating generally favorable drug-likeness. The predicted ADMET profiles indicated that most compounds possessed acceptable drug-like properties, with high gastrointestinal absorption, no BBB permeability, and no cardiotoxicity, meanwhile no or only one Lipinski rule violation. However, several compounds exhibited high lipophilicity (logP > 5) and low aqueous solubility, which may limit oral bioavailability. In addition, inhibition of CYP2C9 and other CYP isoforms was predicted for several compounds, suggesting potential drug–drug interaction risks. Overall, compound **4** (2-chlorounguinol) demonstrated as one of the most favorable ADMET profiles by combining good oral absorption, absence of predicted hepatotoxicity, and minimal Lipinski violations, highlighting its potential for further pharmacological investigation.

In summary, chemical investigation of the marine-derived fungus *A. unguis* PM03 led to the isolation of eight known aromatic polyketides, including depsides, depsidones, a diphenyl ether derivative, and an isocoumarin. Evaluation of their biological activities revealed that several compounds, particularly guisinol (**7**), isosclerone (**8**), emeguisin B (**5**), unguinol (**1**), and 2,4-dichlorounguinol (**3**), exhibited potent α-glucosidase inhibitory activity, with IC_{50} values markedly lower than that of acarbose under the assay conditions. Notably, the α-glucosidase inhibitory activities of compounds **1**–**7** are reported for the first time. All isolated metabolites showed negligible cytotoxicity against the tested cancer cell lines, while molecular docking and structure-activity relationship analyses provided valuable insights into the previously reported antibacterial activities of fungal depsides and depsidones. Collectively, these results demonstrate that marine-derived fungal aromatic polyketides represent promising scaffolds for the discovery of potential α-glucosidase inhibitors.

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Author Contributions

The manuscript was written through the contributions of all authors. All authors have given approval to the final version of the manuscript. TLN: methodology, investigation, formal analysis, writing—original draft, review & editing; TDP: formal analysis, data curation, validation; VHT: investigation, methodology; LT: molecular docking, ADMET analysis, data curation; TVM: writing—review & editing; TTHV & THML: bioassays; VCP: resources, supervision, writing—review & editing; TMHD: conceptualization, supervision, project administration, funding acquisition, writing—review & editing.

Availability of Data and Materials

The authors declare that the data supporting the findings of this study are available within the paper and its Supplementary Information file. Should any raw data files be needed in another format they are available from the corresponding author upon reasonable request. Source data are provided with this paper.

Artificial Intelligence (AI) Statement

The authors utilized ChatGPT for enhancing language and correcting grammatical errors. All content generated with the assistance of AI was thoroughly reviewed, verified, and sanctioned by the authors, who assume complete responsibility for the precision and integrity of the final manuscript.

Conflicts of Interest

The authors declare that they do not have any conflict of interest.

Supporting Information

Supporting information accompanies this paper on http://www.acgpubs.org/journals/records-of-natural-products.

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