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Profiling Metabolit Antibakteri Jamur Endofit Rimpang Kunyit Hitam (Curcuma caesia Roxb.) Menggunakan Pendekatan Bioactivity-Guided Molecular Networking Berbasis LC-HRMS/MS
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PROFILING METABOLIT ANTIBAKTERI JAMUR ENDOFIT RIMPANG KUNYIT HITAM (*Curcuma caesia* Roxb.) MENGGUNAKAN PENDEKATAN *BIOACTIVITY-GUIDED MOLECULAR NETWORKING* BERBASIS LC-HRMS/MS

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INTISARI

Peningkatan prevalensi bakteri *multidrug-resistan* (MDR) telah mengurangi efektivitas antibiotik yang tersedia sehingga diperlukan sumber kandidat antibakteri baru, salah satunya dari metabolit sekunder jamur endofit. Penelitian ini bertujuan mengidentifikasi jamur endofit dari rimpang kunyit hitam (*Curcuma caesia* Roxb.), mengevaluasi aktivitas antibakterinya, dan memprioritaskan kandidat metabolit antibakteri melalui pendekatan *bioactivity-guided molecular networking* berbasis LC-HRMS/MS. Jamur endofit diisolasi, difermentasi, kemudian diekstraksi dari biomassa miselium dan supernatan kultur. Aktivitas antibakteri diuji berdasarkan nilai *minimum inhibitory concentration* (MIC) terhadap *Pseudomonas aeruginosa* MDR dan *Bacillus subtilis* MDR. Ekstrak paling aktif difraksinasi dan dianalisis dengan LC-HRMS/MS, kemudian data metabolom diproses melalui *feature-based molecular networking* dan anotasi komputasional.

Sebanyak empat isolat jamur endofit berhasil diisolasi dari rimpang *C. caesia*. Isolat CC-Hi yang teridentifikasi sebagai anggota *Aspergillus* section *Nigri* dipilih sebagai isolat prioritas berdasarkan aktivitas antibakteri, massa ekstrak, dan profil kromatogram HPLC-DAD. Ekstrak miseliumnya (CC7) menunjukkan aktivitas terhadap *P. aeruginosa* MDR dan *B. subtilis* MDR dengan nilai MIC sebesar 500 µg/mL, sedangkan fraksi F2 dan F4 menunjukkan peningkatan aktivitas terhadap *B. subtilis* MDR dengan nilai MIC sebesar 125 µg/mL. Analisis LC-HRMS/MS mendeteksi 742 fitur metabolit, dan integrasi data bioaktivitas, distribusi fitur, *molecular networking*, serta anotasi komputasional memprioritaskan kandidat metabolit putatif, antara lain *Aspergillicin A*, *Maculosin*, *Gancidin W*, *Cyclomethyltryptophan*, dan *20-Hidroxyfusarin C*, yang termasuk dalam kelompok peptida siklik, diketopiperazina, poliketida, alkaloid, dan furanokumarin.

Penelitian ini menunjukkan bahwa *bioactivity-guided molecular networking* berbasis LC-HRMS/MS efektif untuk memprioritaskan kandidat metabolit antibakteri dari jamur endofit rimpang *C. caesia*. Hasil ini menjadi dasar untuk isolasi senyawa murni, elusidasi struktur, dan validasi bioaktivitas lebih lanjut.

Kata kunci: *Curcuma caesia*; jamur endofit; aktivitas antibakteri; LC-HRMS/MS; *molecular networking*; metabolomik.

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LC-HRMS/MS-BASED BIOACTIVITY-GUIDED MOLECULAR NETWORKING FOR ANTIBACTERIAL METABOLITE PROFILING OF ENDOPHYTIC FUNGI FROM BLACK TURMERIC (*Curcuma caesia* Roxb.) RHIZOMES

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ABSTRACT

The increasing prevalence of multidrug-resistant (MDR) bacteria has reduced antibiotic effectiveness, highlighting the need for new antibacterial candidates from endophytic fungal secondary metabolites. This study aimed to isolate and identify endophytic fungi associated with black turmeric (*Curcuma caesia* Roxb.) rhizomes, evaluate their antibacterial activity, and prioritize putative antibacterial metabolite candidates using an LC-HRMS/MS-based bioactivity-guided molecular networking approach. Endophytic fungi were isolated, fermented, and extracted from mycelial biomass and culture supernatants. Antibacterial activity was evaluated against MDR *Pseudomonas aeruginosa* and *Bacillus subtilis* using the minimum inhibitory concentration (MIC) method. The most active extract was fractionated and analyzed by LC-HRMS/MS, followed by feature-based molecular networking and computational annotation.

Four endophytic fungal isolates were successfully obtained from *C. caesia* rhizomes. Isolate CC-Hi was identified as a member of *Aspergillus* section *Nigri* and selected based on antibacterial activity, extract yield, and HPLC-DAD chromatographic profile. Its mycelial extract (CC7) exhibited antibacterial activity against MDR *P. aeruginosa* and MDR *B. subtilis* with an MIC of 500 µg/mL, whereas fractions F2 and F4 showed enhanced activity against MDR *B. subtilis* with an MIC of 125 µg/mL. LC-HRMS/MS analysis detected 742 metabolite features, and integration of bioactivity data, feature distribution, molecular networking, and computational annotation effectively prioritized putative antibacterial metabolite candidates, including Aspergillicin A, Maculosin, Gancidin W, Cyclomethyltryptophan, and 20-Hydroxyfusarin C, representing the metabolite classes of cyclic peptides, diketopiperazines, polyketides, alkaloids, and furanocoumarins.

This study demonstrates that LC-HRMS/MS-based bioactivity-guided molecular networking is effective for prioritizing putative antibacterial metabolite candidates from endophytic fungi associated with *C. caesia* rhizomes. These findings provide a foundation for future isolation of pure compounds, structural elucidation, and biological activity validation.

Keywords: *Curcuma caesia*; endophytic fungi; antibacterial activity; LC-HRMS/MS; molecular networking; metabolomics