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**Prediksi Mekanisme Aksi Senyawa Bioaktif Bekatul Beras Hitam (Oryza sativa L.) Sebagai Antidiabetes
Mellitus Tipe 2 Berbasis Data Mining, Network Pharmacology, dan Molecular Docking**
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INTISARI

Diabetes mellitus tipe 2 (DMT2) merupakan penyakit metabolik kronis yang ditandai dengan peningkatan glukosa darah akibat gangguan sekresi insulin, resistansi insulin, atau kombinasi keduanya. Bekatul beras hitam (*Oryza sativa* L.*)* diketahui mengandung senyawa bioaktif yang berpotensi sebagai antidiabetes alami. Penelitian ini bertujuan untuk mengeksplorasi mekanisme senyawa bioaktif bekatul beras hitam terhadap DMT2 melalui pendekatan *data mining*, *network pharmacology*, dan *molecular docking*.

Penelitian ini diawali dengan *data mining* senyawa metabolit sekunder bekatul beras hitam melalui Google Scholar, PubMed, dan Scopus menggunakan kata kunci berbahasa Inggris, yaitu ("black rice bran") AND ("LC-HRMS" OR "LC-MS" OR "Antidiabetic") AND ("phytochemicals" OR "bioactive compounds" OR "compounds" OR "isolation" OR "metabolites"), serta kata kunci berbahasa Indonesia, yaitu ("bekatul beras hitam") AND ("LC-HRMS" OR "LC-MS" OR "antidiabetes") AND ("fitokimia" OR "senyawa bioaktif" OR "senyawa" OR "isolasi" OR "metabolit"). Senyawa yang diperoleh kemudian diseleksi menggunakan SwissADME dan ADMETlab. Target potensial senyawa diprediksi menggunakan SwissTargetPrediction, TargetNet, dan PharmMapper, kemudian diintegrasikan dengan target penyakit DMT2 dari *database* NCBI GEO. Analisis *network pharmacology* dilakukan melalui identifikasi *overlapping target*, analisis *protein-protein interaction* (PPI), serta *enrichment analysis Gene Ontology* (GO) dan *Kyoto Encyclopedia of Genes and Genomes* (KEGG). Verifikasi interaksi senyawa dengan target protein dilakukan menggunakan pendekatan *molecular docking* melalui perangkat lunak MOE.

Hasil penelitian menunjukkan diperoleh 80 senyawa bioaktif dari bekatul beras hitam. Sebanyak 25 senyawa memenuhi kriteria, namun cyanidin-3-O-glucoside (C3G) tetap diikutsertakan karena merupakan antosianin utama pada bekatul beras hitam dan memiliki relevansi biologis sebagai antidiabetes. Analisis mengidentifikasi 6 protein target, yaitu AGTR1, CBS, PTGS2, PDGFRA, CRABP2, dan KIT. Hasil *molecular docking* menunjukkan bahwa C3G memiliki afinitas ikatan yang kuat dan stabil terhadap seluruh protein target dengan nilai RMSD < 2 Å. Senyawa bioaktif bekatul beras hitam diprediksi bekerja melalui mekanisme antiinflamasi, antioksidan, dan modulasi jalur resistansi insulin pada DMT2.

Kata kunci: antosianin, bekatul beras hitam, bioinformatika, hiperglisemia*, in silico*.

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ABSTRACT

Type 2 diabetes mellitus (T2DM) is a chronic metabolic disease characterized by elevated blood glucose levels caused by impaired insulin secretion, insulin resistance, or a combination of both. Black rice bran (*Oryza sativa* L.) is known to contain bioactive compounds with potential as natural antidiabetic agents. This study aimed to explore the mechanism of action of bioactive compounds from black rice bran against T2DM using *data mining*, *network pharmacology*, and *molecular docking* approaches.

The study was initiated by *data mining* of secondary metabolites from black rice bran through Google Scholar, PubMed, and Scopus using English keywords, namely ("black rice bran") AND ("LC-HRMS" OR "LC-MS" OR "antidiabetic") AND ("phytochemicals" OR "bioactive compounds" OR "compounds" OR "isolation" OR "metabolites"), as well as Indonesian keywords, namely ("bekatul beras hitam") AND ("LC-HRMS" OR "LC-MS" OR "antidiabetes") AND ("fitokimia" OR "senyawa bioaktif" OR "senyawa" OR "isolasi" OR "metabolit"). The identified compounds were subsequently screened using SwissADME and ADMETlab. Potential targets were predicted using SwissTargetPrediction, TargetNet, and PharmMapper, and then integrated with T2DM-related targets obtained from the NCBI GEO database. *Network pharmacology* analysis was conducted through overlapping target identification, protein–protein interaction (PPI) analysis, and enrichment analysis of Gene Ontology (GO) and Kyoto Encyclopedia of Genes and Genomes (KEGG). Verification of compound–target interactions was performed using *molecular docking* analysis through the Molecular Operating Environment (MOE) software.

The results identified 80 bioactive compounds from black rice bran. A total of 25 compounds met the criteria, but cyanidin-3-O-glucosi*de* (C3G) was still included due to its role as the major anthocyanin in black rice bran and its biological relevance as an antidiabetic compound. The analysis identified six target proteins, namely AGTR1, CBS, PTGS2, PDGFRA, CRABP2, and KIT. *Molecular docking* results demonstrated that C3G exhibited strong and stable binding affinities toward all target proteins with RMSD values < 2 Å. Overall, the bioactive compounds of black rice bran are predicted to exert antidiabetic effects through anti-inflammatory, antioxidant, and insulin resistance modulation mechanisms in T2DM.

Keywords: anthocyanin, black rice bran, bioinformatic, hyperglycemia, in silico.