SKRINING POTENSI SENYAWA BIOAKTIF IKAN SIDAT (*Anguilla bicolor bicolor)* SEBAGAI IMUNOMODULATOR MENGGUNAKAN PENDEKATAN *IN SILICO*

SKRIPSI

diajukan sebagai salah satu syarat untuk memperoleh gelar Sarjana Sains
Program Studi Biologi Departemen Pendidikan Biologi

Oleh

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UNIVERISTAS PENDIDIKAN INDONESIA

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Sebuah skripsi yang diajukan untuk memenuhi salah satu syarat memperoleh gelar Sarjana Sains pada Program Studi Biologi, Departemen Pendidikan Biologi, Fakultas Pendidikan Matematika dan Ilmu Pengetahuan Alam

LEMBAR PENGESAHAN

KHANSA BIANTARI ALIKA

SKRINING POTENSI SENYAWA BIOAKTIF IKAN SIDAT (*Anguilla bicolor bicolor)* SEBAGAI IMUNOMODULATOR MENGGUNAKAN PENDEKATAN *IN SILICO*

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LEMBAR PERNYATAAN

Dengan ini penulis menyatakan bahwa skripsi berjudul "Skrining Potensi Senyawa Bioaktif Ikan Sidat (*Anguilla bicolor bicolor*) Sebagai Imunomodulator Menggunakan Pendekatan *In Silico*" beserta seluruh isinya adalah benar-benar karya penulis. Penulis tidak melakukan penjiplakan atau pengutipan dengan cara-cara yang tidak sesuai dengan etika ilmu yang berlaku dalam masyarakat keilmuan. Atas pernyataan ini, penulis siap menanggung risiko/sanksi apabila di kemudian hari ditemukan adanya pelanggaran etika keilmuan atau ada klaim dari pihak lain terhadap keaslian karya penulis.

Bandung, Juli 2022

Yang membuat pernyataan,

Khansa Biantari Alika

KATA PENGANTAR

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Penulis

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ABSTRAK

Skrining Potensi Senyawa Bioaktif Ikan Sidat (*Anguilla bicolor bicolor*) Sebagai Imunomodulator Menggunakan Pendekatan *In Silico*

Dalam kehidupan sehari-hari, manusia terpapar patogen berbahaya dan polutan lingkungan yang dapat mempengaruhi status kesehatan dan homeostasis tubuh. Namun, ketersediaan antibodi tidak menjamin bahwa tubuh akan terlindungi karena dapat terjadinya ketidakseimbangan respon imun, sehingga dikembangkan kelas molekul tertentu yang secara keseluruhan disebut imunomodulator. Spektrum bioaktivitas peptida organisme laut yang luas memiliki potensi *nutraceutical* dan nilai obat tinggi. Ikan sidat (*Anguilla bicolor bicolor*) mengandung berbagai potensi sebagai senyawa bioaktif yang belum diketahui keterlibatannya dalam mekanisme kekebalan tubuh. Penelitian ini bertujuan untuk mengidentifikasi aktivitas senyawa bioaktif dari ikan sidat secara *in silico* khususnya sebagai imunomodulator yang mampu mengaktifkan dan meningkatkan sistem kekebalan tubuh. Identifikasi potensi senyawapada ikan sidat dilakukan melalui penambatan molekuler terhadap protein gen MAPK3, SRC, MAPK1, dan AKT1 yang diperoleh melalui konstruksi jaringan protein-protein dengan Cytoscape 3.8.2. Orabilitas senyawa sebagai kandidat obat didapatkan dengan aturan "Lipinski Rule of Five". Nilai afinitas pengikatan tertinggi pada MAPK3, SRC, MAPK1, dan AKT1 ditunjukkan berturut-turut oleh Uridine-5-Monophosphate dengan nilai -7.3 kkal/mol, All-Trans-Retinal dengan nilai -8 kkal/mol, All-Trans-Retinal dengan nilai -8.4 kkal/mol, dan Chenodeoxycholic Acid 3-Sulfate dengan nilai -7.1 kkal/mol. Seluruh senyawa kecuali Cholesteryl Sulfate memenuhi aturan "Lipinski Rule of Five". Kandidat senyawa berhasil tertambat dengan berikatan pada sisi aktif protein dan memodulasi aktivasi jalur persinyalan protein MAPK3, SRC, MAPK1, dan AKT1 dalam mempertahankan kesehatan sistem kekebalan tubuh sebagai dasar dari skrining senyawa sebagai pengembangan obat imunomodulator.

Kata kunci: *Anguilla bicolor bicolor*, penambatan molekuler homeostasis imun, imunomodulator, pengembangan obat

ABSTRACT

Screening of Potential Eel (*Anguilla bicolor bicolor*) Bioactive Compounds as Immunomodulators by *In Silico* Approach

In daily life, humans are exposed to harmful pathogens and environmental pollutants that can affect health and homeostasis of the body. However, the availability of antibodies does not guarantee that the body will be protected because there could be a balance of immune responses, therefore a certain class called immunomodulators is developed. A wide spectrum of marine organism peptide bioactivity has high nutraceutical potential and medicinal value. Eel (*Anguilla bicolor bicolor*) has a lot of potential as bioactive compounds whose involvement in the immune mechanism is not yet known. This study aims to identify the activity of bioactive compounds from eel through in silico methods, especially as an immunomodulator to activate and enhance the immune system. Identification of potential compounds in eel was carried out by molecular docking of MAPK3, SRC, MAPK1 and AKT1 gene proteins which obtained by constructing a protein-protein network using Cytoscape 3.8.2. The orability of compounds as drug candidates were obtained by "Lipinski Rule of Five". The highest binding affinity values for MAPK3, SRC, MAPK1, and AKT1 are shown by Uridine-5-Monophosphate -7.3 kcal/mol, All-Trans-Retinal -8 kcal/mol, All-Trans-Retinal -8.4 kcal/mol, and Chenodeoxycholic Acid 3-Sulfate -7.1 kcal/mol. All compounds except Cholesterol Sulfate meet the "Lipinski Rule of Five" criterias. The candidate compounds successfully bind to the active site of protein targets and modulate the activation of MAPK3, SRC, MAPK1, and AKT1 proteins signaling pathways in maintaining the immune system as the the development of immunomodulatory drugs.

Keywords: *Anguilla bicolor bicolor,* molecular docking, immune homeostasis, immunomodulator, drug development

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LAMPIRAN

Lampiran 1. Konfigurasi Penambatan Molekuler

A) Reseptor Protein Gen MAPK3

grid2zoq - Notepad

File Edit Format View Help

```
receptor = 2zoq protein ready.pdbqt
ligand = 2zoq ligand ready.pdbqt

out = out2zoq.pdbqt

center_x = 28.903
center_y = 6.753
center_z = 18.399

size_x = 14
size_y = 12
size_z = 12

log = log.txt
num_modes = 9
exhaustiveness = 32
```

B) Reseptor Protein Gen SRC

grid2y9q - Notepad

File Edit Format View Help

```
receptor = 2y9q protein ready.pdbqt
ligand = 2y9q ligand ready.pdbqt

out = out2y9q.pdbqt

center_x = 52.690
center_y = 32.091
center_z = 9.526

size_x = 16
size_y = 18
size_z = 14

log = log.txt
num_modes = 9
exhaustiveness = 32
```

C) Reseptor Protein Gen MAPK1

grid2bdf - Notepad

File Edit Format View Help

```
receptor = 2bdf protein ready.pdbqt
ligand = 2bdf ligand ready.pdbqt

out = out2bdf.pdbqt

center_x = 13.615
center_y = 13.718
center_z = -9.961

size_x = 16
size_y = 14
size_z = 14

log = log.txt
num_modes = 9
exhaustiveness = 32
```

D) Reseptor Protein Gen AKT1

grid3ocb - Notepad

File Edit Format View Help

```
receptor = 3ocb protein ready.pdbqt
ligand = 3ocb ligand ready.pdbqt

out = out3ocb.pdbqt

center_x = 13.377
center_y = 0.171
center_z = 18.464

size_x = 14
size_y = 16
size_z = 14

log = log.txt
num_modes = 9
exhaustiveness = 32
```