

**ANALISIS PENAMBATAN MOLEKULER SENYAWA AKTIF DARI IKAN SIDAT  
(*Anguilla bicolor bicolor*) SEBAGAI ANTI-COVID-19 SECARA IN SILICO**

**SKRIPSI**

diajukan untuk memenuhi sebagian syarat untuk memperoleh gelar Sarjana Sains  
Program Studi Biologi



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(*Anguilla bicolor bicolor*) SEBAGAI ANTI-COVID-19 SECARA IN SILICO**

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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

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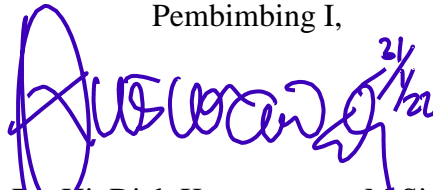
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**LEMBAR PENGESAHAN**  
**ANALISIS PENAMBATAN MOLEKULER SENYAWA AKTIF DARI**  
**IKAN SIDAT (*Anguilla bicolor bicolor*) SEBAGAI ANTI-COVID-19**  
**SECARA IN SILICO**

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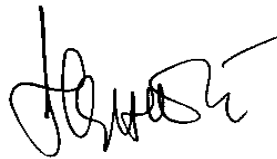
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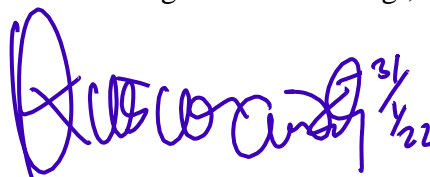
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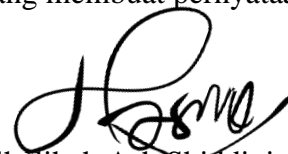


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## LEMBAR PENYATAAN

Dengan ini saya menyatakan bahwa skripsi/tesis/disertasi dengan judul **“ANALISIS PENAMBATAN MOLEKULER SENYAWA AKTIF DARI IKAN SIDAT (*Anguilla bicolor bicolor*) SEBAGAI ANTI-COVID-19 SECARA IN SILICO”** ini beserta seluruh isinya adalah benar-benar karya saya sendiri. Saya tidak melakukan penjiplakan atau pengutipan dengan cara-cara yang tidak sesuai dengan etika ilmu yang berlaku dalam masyarakat keilmuan. Atas pernyataan ini, saya siap menanggung risiko/sanksi apabila di kemudian hari ditemukan adanya pelanggaran etika keilmuan atau ada klaim dari pihak lain terhadap keaslian karya saya ini.

Bandung, Januari 2021  
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## ABSTRAK

### **Analisis Penambatan Molekuler Senyawa Aktif dari Ikan Sidat (*Anguilla bicolor bicolor*) sebagai Anti-COVID-19 secara In Silico**

Coronavirus disease 2019 (COVID-19) yang telah ditetapkan sebagai pandemi oleh organisasi kesehatan dunia (WHO), disebabkan oleh *Severe Acute Respiratory Syndrome Coronavirus 2* (SARS-CoV-2). Hingga saat ini pencarian kandidat obat COVID-19 terus diupayakan dalam mengurangi penyebaran virus ini. Ikan sidat telah diketahui memiliki kemampuan sebagai antipiretik, antiinflamasi, dan antibakteri, akan tetapi belum ada penelitian terkait ikan sidat sebagai antivirus. Protein yang memiliki peran dalam perkembangan virus dan pengikatan antara virus dengan sel inang, yaitu M<sup>pro</sup>, RBD dan ACE2 digunakan sebagai target dalam penelitian ini. Tujuan penelitian ini untuk mengetahui potensi senyawa yang ditemukan pada ikan sidat (*Anguilla bicolor bicolor*) sebagai inhibitor terhadap Sars-CoV-2. Struktur protein target dan senyawa pada ikan sidat diperoleh dari basis data Protein Data Bank dan Pubchem. Penambatan molekuler dilakukan dengan menggunakan AutodockTools 1.5.7 dan hasil interaksi yang terjadi divisualisasikan menggunakan Pymol dan Discovery Studio. Selain itu senyawa uji dianalisis dengan mengikuti aturan Lipinski's *Rule of Five* sebagai prediksi kemiripan obat dalam keamanan penggunaannya secara oral. Berdasarkan hasil penelitian menunjukkan dari 314 senyawa dari ikan sidat, enam diantaranya memiliki nilai afinitas ikatan yang kuat terhadap M<sup>pro</sup> dan RBD Sars-CoV-2 yaitu Chenodeoxycholic acid 3-sulfate dengan energi bebas tertinggi ( $\Delta G$  -8,1 kkal/mol), dan 2 diantaranya memiliki nilai afinitas ikatan yang kuat terhadap ACE2 dengan Carboprost dengan energi bebas tertinggi ( $\Delta G$  -7,6 kkal/mol). Penelitian merupakan prediksi secara komputasi sehingga diperlukan kajian lebih lanjut dalam skala laboratorium secara in vitro dan vivo.

**Kata kunci:** COVID-19, SARS-CoV-2, *Anguilla bicolor bicolor*, penambatan molekuler, metabolit sekunder

## ABSTRACT

### **Analysis In Silico of Molecular Docking of Active Compounds from Eel (*Anguilla bicolor bicolor*) as Anti-COVID-19**

Coronavirus disease 2019 (COVID-19), which has been designated as pandemic by the World Health Organization (WHO), is caused by *Severe Acute Respiratory Syndrome Coronavirus 2* (SARS-CoV-2). Exploring for COVID-19 drug candidates still continues to reduce the spread of the virus. Eel has been known to have antipyretic, anti-inflammatory, and antibacterial abilities, but there has been no research on eel as an antiviral. Proteins that have a role in viral development and binding between the virus and host cells, namely M<sup>pro</sup>, RBD and ACE2 were used as targets in this study. The purpose of this study is to determine the potential of compounds found in eel (*Anguilla bicolor bicolor*) as inhibitors of Sars-CoV-2. The structure of target proteins and compounds in eel was obtained from the Protein Data Bank and Pubchem databases. Molecular docking is done using AutodockTools 1.5.7 and the results of the interactions that occur are visualized using Pymol and Discovery Studio. In addition, the bioactive compounds were analyzed by following Lipinski's Rule of Five as a predictor of drug similarity in safety for oral use. Based on the results of the study, out of 314 compounds from eel, six of them had strong binding affinity values for M<sup>pro</sup> and RBD Sars-CoV-2, Chenodeoxycholic acid 3-sulfate which had the highest free energy ( $\Delta G$  -8.1 kcal/mol), 2 of them have a strong binding affinity for ACE2, Carboprost having the highest free energy ( $\Delta G$  -7.6 kcal/mol). This research is a computational prediction so that further studies are needed on a laboratory scale in vitro and in vivo.

**Keywords:** COVID-19, SARS-CoV-2, *Anguilla bicolor bicolor*, molecular docking, secondary metabolite

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