ABSTRAK

FITRI SONDARI. 2025. **ANALISIS POTENSI SENYAWA AKTIF PURWOCENG (*Pimpinella pruatjan* Molk.) SEBAGAI KANDIDAT ANTIKANKER PADA OVARIUM SECARA *IN SILICO* UNTUK SUMBER BELAJAR BIOLOGI.** Jurusan Pendidikan Biologi, Fakultas Keguruan dan Ilmu Pendidikan, Universitas Siliwangi, Tasikmalaya.

Kanker ovarium merupakan salah satu kanker dengan tingkat mortalitas tinggi. Terapi konvensional sering menimbulkan efek samping, sehingga diperlukan alternatif berbahan alami yang lebih aman. Purwoceng (*Pimpinella pruatjan* Molk.) mengandung metabolit sekunder yang berpotensi sebagai antikanker melalui penghambatan PARP2. Penelitian ini bertujuan untuk mengetahui hasil analisis potensi senyawa aktif Purwoceng sebagai kandidat antikanker ovarium secara *in silico* untuk sumber belajar biologi. Metode penelitian ini yaitu *in silico screening* melalui *molecular docking* dengan analisis deskriptif kuantitatif. Hasil GC-MS sampel kalus Purwoceng mengidentifikasi 40 senyawa metabolit sekunder, 3 diantaranya dijadikan ligan uji karena berpotensi sebagai antikanker yaitu *Phen-1,4-diol 2,3-dimethyl-5-trifluoromethyl-*, *Phorbol*, dan *9-Hexadecenoic acid*. Ligan kontrol yang digunakan adalah *3-aminobenzamide* dengan protein target yaitu PARP2 (PDB ID: 3KCZ). Hasil analisis *molecular docking* menunjukkan *Phorbol* memiliki afinitas terbaik (-9.3 kcal/mol), diikuti *Phen-1,4-diol 2,3-dimethyl-5-trifluoromethyl-* (-7.5 kcal/mol), keduanya lebih baik dibandingkan ligan kontrol (-6.5 kcal/mol). Analisis fisikokimia menunjukkan seluruh ligan uji memenuhi *Lipinski's Rule of Five*. Analisis farmakokinetik menunjukkan bahwa tidak ada ligan uji yang memenuhi seluruh parameter secara optimal. *Phen-1,4-diol, 2,3-dimethyl-5-trifluoromethyl-* teridentifikasi sebagai inhibitor CYP1A2, *Phorbol* merupakan substrat P-gp dan memiliki permeabilitas kulit rendah, sedangkan *9-hexadecenoic* acid memiliki nilai total *clearance* yang paling tinggi, sehingga diprediksi mengalami eliminasi yang lebih cepat dari dalam tubuh. Berdasarkan analisis toksisitas, *9-hexadecenoic acid* tergolong sangat toksik (kelas 2), *Phen-1,4-diol 2,3-dimethyl-5-trifluoromethyl-* berada pada kategori toksik sedang (kelas 4), dan *Phorbol* tidak toksik secara akut (kelas 6) tetapi memiliki aktivitas imunotoksik dan mutagenik. Secara keseluruhan, *Phen-1,4-diol 2,3-dimethyl-5-trifluoromethyl-* merupakan kandidat paling potensial sebagai antikanker ovarium. Penelitian ini menghasilkan *booklet* sebagai sumber belajar biologi.

Kata Kunci: Purwoceng; *in silico*; PARP2; *molecular docking*; antikanker ovarium.

ABSTRACT

FITRI SONDARI. 2025**.** ***ANALYSIS OF THE POTENTIAL ACTIVE COMPOUNDS OF PURWOCENG (Pimpinella pruatjan*** **Molk*.) AS ANTI-CANCER CANDIDATES IN THE OVARY IN SILICO FOR BIOLOGY LEARNING RESOURCES.*** *Department of Biology Education, Faculty of Teacher Training and Education, Siliwangi University*, Tasikmalaya.

Ovarian cancer is one of the cancers with a high mortality rate. Conventional therapy often causes side effects, so safer natural alternatives are needed. Purwoceng (Pimpinella pruatjan Molk.*) contains secondary metabolites that have the potential to act as anticancer agents through PARP2 inhibition. This study aims to determine the results of the analysis of the potential of Purwoceng active compounds as ovarian anticancer candidates in silico for biology learning resources. This research method is in silico screening through molecular docking with quantitative descriptive analysis. The results of GC-MS of Purwoceng callus samples identified 40 secondary metabolite compounds, 3 of which were used as test ligands because they have the potential to act as anticancer agents, namely Phen-1,4-diol 2,3-dimethyl-5-trifluoromethyl-, Phorbol, and 9-Hexadecenoic acid. The control ligand used was 3-aminobenzamide with the target protein being PARP2 (PDB ID: 3KCZ). The results of molecular docking analysis showed that Phorbol had the best affinity (-9.3 kcal/mol), followed by Phen-1,4-diol 2,3-dimethyl-5-trifluoromethyl- (-7.5 kcal/mol), both of which were better than the control ligand (-6.5 kcal/mol). Physicochemical analysis showed that all test ligands met Lipinski's Rule of Five. Pharmacokinetic analysis showed that none of the test ligands met all parameters optimally. Phen-1,4-diol, 2,3-dimethyl-5-trifluoromethyl- was identified as a CYP1A2 inhibitor, Phorbol is a P-gp substrate and has low skin permeability, while 9-hexadecenoic acid had the highest total clearance value, so it is predicted to experience faster elimination from the body. Based on toxicity analysis, 9-hexadecenoic acid is classified as highly toxic (class 2), Phen-1,4-diol 2,3-dimethyl-5-trifluoromethyl- is in the moderate toxic category (class 4), and Phorbol is not acutely toxic (class 6) but has immunotoxic and mutagenic activities. Overall, Phen-1,4-diol 2,3-dimethyl-5-trifluoromethyl- is the most potential candidate as an ovarian anticancer. This research produces a booklet as a biology learning resource.*

Keywords**:** Purwoceng; *in silico*; PARP2; *molecular docking*; *ovarian anticancer*.