ABSTRAK

ANALISIS BIOINFORMATIKA SENYAWA *ANDROGRAPHOLIDE* SEBAGAI ANTIKANKER PADA *SMALL CELL LUNG CANCER* (SCLC)

Klarisa Yuzar Mahardika[1], Nur Amalia Choironi[2], Sarmoko[2]

Latar Belakang : *Small Cell Lung Cancer* (SCLC) memiliki prognosis buruk, kelangsungan hidup rendah, dan cepatnya metastasis. Pembedahan bukan lini pertama dan terdapat resistensi kemoterapi sehingga diperlukan obat molekul kecil baru. *Andrographolide* memiliki aktivitas antikanker pada kanker paru NSCLC. Target *andrographolide* pada SCLC dan mekanismenya belum diketahui sehingga perlu dilakukan analisis bioinformatika.

Metodologi : Penelusuran data menggunakan STITCH, STRING, Swiss, dan NCBI. PTTGs dianalisis *gene ontology,* KEGG *pathway, drug association* kemudian Cytoscape sehingga didapatkan *top* 10 *hub genes*. Protein terpilih dilakukan *molecular docking* terhadap *andrographolide*. Tahapannya yaitu preparasi ligan-protein, validasi metode, dan *molecular docking*.

Hasil Penelitian : Target molekuler *andrographolide* terhadap SCLC secara bioinformatika yaitu IL6, TNF, MAPK3 (ERK1), CCL4, JAK2, IL1B, CXCL12, CSF2, IL10, dan MAPK1 (ERK2). TNF alfa, ERK1, JAK2, dan ERK2 memiliki RMSD $\leq$ 2Å dan terkait jalur pensinyalan MAPK, Nf-kB, dan JAK/STAT. Hasil *molecular docking* menunjukan nilai energi ikatan *andrographolide* pada TNF alfa yaitu -7,7 kkal/mol, ERK1 yaitu -2,3 kkal/mol, JAK2 yaitu -8,3 kkal/mol, dan ERK2 yaitu -8,9 kkal/mol. Jenis ikatannya yaitu ikatan hidrogen dan hidrofobik. TNF alfa dan ERK2 berpotensi dijadikan target karena energi ikatannya lebih kecil dibanding kontrol positif.

Kesimpulan : *Andrographolide* berpotensi menghambat SCLC dengan menargetkan TNF alfa dan ERK2

Kata kunci : *Small Cell Lung Cancer*, *andrographolide*, bioinformatika, antikanker.

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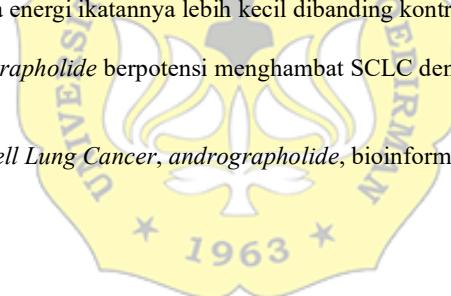
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ABSTRACT

BIOINFORMATICS ANALYSIS OF *ANDROGRAPHOLIDE* AS ANTICANCER IN *SMALL CELL LUNG CANCER* (SCLC)

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Background : *Small Cell Lung Cancer* (SCLC) has a poor prognosis, low survival, and rapid metastases. Surgery is not the first line, and chemotherapy is resistant, so new small-molecule drugs are needed. Andrographolide has anticancer activity in NSCLC lung cancer. The target of andrographolide in SCLC and its mechanism are unknown, so bioinformatic analysis is necessary.

Methodology : : Data searches were performed using STITCH, STRING, Swiss, and NCBI. PTTGs were analyzed for gene ontology, KEGG pathway, drug association then Cytoscape to obtain the top 10 hub genes. Molecular docking of andrographolide was carried out on selected proteins. The steps are ligand-protein preparation, method validation, and molecular docking.

Result : The molecular targets of andrographolide for SCLC in bioinformatics are IL6, TNF, MAPK3 (ERK1), CCL4, JAK2, IL1B, CXCL12, CSF2, IL10, and MAPK1 (ERK2). TNF alpha, ERK1, JAK2, and ERK2 have RMSD < 2Å and are involved in the MAPK, Nf-kB, and JAK/STAT signaling pathways. The results of molecular docking showed that the bond energy of andrographolide in TNF alpha was -7,7 kcal/mol, ERK1 was -2,3 kcal/mol, JAK2 was -8,3 kcal/mol, and ERK2 was -8,9 kcal/mol. The types of bonds are hydrogen and hydrophobic bonds. TNF alpha and ERK2 are potential targets because their binding energy is lower than the positive control.

Conclusion : Andrographolide potentially inhibits SCLC by targeting TNF alpha and EKR2.

Keywords: Small Cell Lung Cancer, andrographolide, bioinformatics, anticancer.

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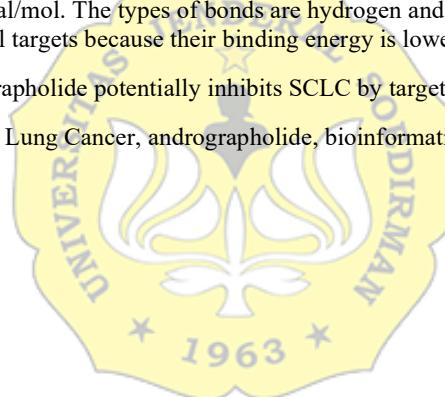
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