ABSTRAK

STUDI *IN-SILICO* SENYAWA AKTIF JINTAN HITAM (*Nigella sativa L.*) TERHADAP RESEPTOR PPAR-γ (*Peroxisome Proliferator Activator Receptor-Gamma*) SEBAGAI ANTI KANKER TIROID

Penulis : Tiara Puspitasari Widhiastuti

Kanker tiroid merupakan salah satu jenis kanker yang menyumbang angka kematian sebesar 0,88% di Indonesia. Manajemen pengobatan kanker melalui kemoterapi obat trametinib menyebabkan efek samping serius jika digunakan dalam jangka waktu panjang, maka pemanfaatan senyawa aktif tanaman obat untuk mengurangi efek samping obat sintetis. Penelitian ini bertujuan untuk menganalisis potensi senyawa aktif dari tanaman *Nigella sativa L.* terhadap reseptor PPAR-γ sebagai kandidat obat antikanker tiroid melalui pendekatan *in-silico* metode *molecular docking*. Senyawa ligan didapatkan dari *PubChem* dan gugus reseptor didapatkan dari *Protein Data Bank*. *Software docking* yang digunakan adalah *Pyrx* dan *Biovia Discovery Studio Analizer*.

Variabel independen penelitian ini adalah senyawa *Alpha-linoleic acid*, *Arachidonic acid*, *Eicosadienoic acid*, *Myristic acid*, *Oleic acid*, *Palmitic acid* dan *Palmitoleic acid*, sedangkan variabel dependen *adalah binding affinity* dari *Alpha-linoleic acid*, *Arachidonic acid*, *Eicosadienoic acid*, *Myristic acid*, *Oleic acid*, *Palmitic acid* dan *Palmitoleic acid* terhadap reseptor PPAR-γ.

Data hasil pengujian *in-silico* menunjukkan nilai rata-rata *binding affinity* senyawa aktif *Nigella sativa L.* (ALA = -6.1 kkal/mol, AA = -6.3 kkal/mol, EDA = -5.8 kkal/mol, MA = -5.5 kkal/mol, OA = -5.7 kkal/mol, PA = -5.5 kkal/mol, POA = -5.8 kkal/mol) sedangkan trametinib sebagai kontrol positif menunjukkan affinitas sebesar -9.5 kkal/mol. Uji statistik menggunakan *Kruskal-Wallis* dengan koreksi *post-hoc Tukey* menunjukkan perbedaan yang signifikan antara senyawa *Nigella sativa L.* dengan trametinib (*p-value* < 0,05). Dengan demikian, senyawa aktif *Nigella sativa L.* berpotensi sebagai kandidat antikanker tiroid alternatif, meskipun masih menunjukkan aktivitas yang lebih rendah dibandingkan trametinib.

Kata Kunci : *Nigella sativa L.*, Kanker Tiroid, Trametinib, *Molecular Docking*, PPAR-γ.

ABSTRACT

IN-SILICO STUDY OF ACTIVE COMPOUNDS BLACK CUMIN (*Nigella sativa L.*) AGAINST PPAR-γ (*Peroxisome Proliferator Activator Receptor-Gamma*) RECEPTORS AS ANTI-THYROID CANCER

Writer : Tiara Puspitasari Widhiastuti

Thyroid cancer is one type of cancer that accounts for 0.88% of mortality in Indonesia. The management of cancer treatment through chemotherapy drug trametinib causes serious side effects if used in the long term, so the utilisation of active compounds of medicinal plants to reduce the side effects of synthetic drugs. This study aims to analyse the potential of active compounds from *Nigella sativa L*. plants against receptor PPAR-γ as candidates for anti-thyroid cancer drugs through an *in-silico* approach of molecular *docking* method. The ligand compounds were obtained from *PubChem* and the receptor clusters were obtained from *Protein Data Bank*. The *docking* software used *Pyrx* and *Biovia Discovery Studio Analizer*.

The independent variables of this study are the compounds *Alpha-linoleic acid*, *Arachidonic acid*, *Eicosadienoic acid*, *Myristic acid*, *Oleic acid*, *Palmitic acid* and *Palmitoleic acid*, while the dependent variables *are the binding affinity* of *Alpha-linoleic acid*, *Arachidonic acid*, *Eicosadienoic acid*, *Myristic acid*, *Oleic acid*, *Palmitic acid* and *Palmitoleic acid* to the receptor PPAR- γ.

The *in-silico* testing data showed the average binding affinity values of active compounds *Nigella sativa L*. (ALA = -6.1 kcal/mol, AA = -6.3 kcal/mol, EDA = -5.8 kcal/mol, MA = -5. 5 kcal/mol, OA = -5.7 kcal/mol, PA = -5.5 kcal/mol, POA = -5.8 kcal/mol) while trametinib as positive control showed an affinity of -9.5 kcal/mol. Statistical tests using *Kruskal-Wallis* with *Tukey's post-hoc* correction showed significant differences between the *Nigella sativa L*. compounds and trametinib (*p-value* <0.05). Thus, the active compound of *Nigella sativa L*. has the potential as an alternative anti-thyroid cancer candidate, although it still shows lower activity than trametinib.

Keywords: *Nigella sativa L*., Thyroid Cancer, Trametinib, Molecular Docking, PPAR-γ.