

## INTISARI

Penyakit kanker payudara merupakan salah satu penyakit kanker dengan prevalensi tertinggi di Indonesia. Data Kementerian Kesehatan RI (2015) melaporkan Daerah Istimewa Yogyakarta sebagai provinsi dengan prevalensi kanker payudara tertinggi sebesar 2,4%. Sel kanker mampu mensintesis *extracellular protease* seperti matriks metalloproteinase (MMP) untuk mendegradasi *extracellular matrix* (ECM) sehingga mempermudah invasi ke jaringan lain. Pada sel normal, MMP diekspresikan dalam proses pembengkakan dan penyembuhan luka, namun pada kanker payudara, subfamili MMP yang diekspresikan secara berlebihan untuk migrasi sel dan angiogenesis yaitu MMP-9. Tujuan penelitian ini untuk mensintesis analog purin dari *p*-nitroanilin, 3-bromopropionil klorida dan teofillin serta melakukan studi *in silico* terhadap PEX-9 dilakukan menggunakan penambatan molekul dengan perangkat lunak Autodock4.0. Hasil penelitian menunjukkan bahwa analog purin FUSD-002 dapat disintesis dari *p*-nitroanilin, 3-bromopropionil klorida dan teofillin. Hasil penelitian menunjukkan bahwa struktur analog purin dapat dijelaskan dengan uji <sup>1</sup>H-NMR dan LC-MS. Penambatan molekul FUSD-002 ke sisi aktif MMP-9 *hemopexin domain* (PEX-9) menghasilkan *free energy of binding* -8,68 kcal/mol dan Ki terprediksi 0,43  $\mu$ M, diasosiasikan sebagai adanya interaksi molekuler antara PEX-9 dan senyawa hasil sintesis.

**Kata kunci:** FUSD-002, penambatan molekul, PEX-9, sintesis

**ABSTRACT**

Breast cancer is one of the cancer diseases with the highest prevalence in Indonesia. In 2015, DIY is the province with that highest prevalence (2,4%), as reported by the Indonesian Ministry of Health. Cancer cell is able to synthesize extracellular protease e.g. matrix metalloproteinase (MMP), which degrades the extracellular matrix (ECM), therefore it enhances the invasion of the cancer cell to other tissues. In normal cell, MMP is expressed during inflammation as well as wound healing, but in breast cancer, subfamily of MMP (MMP-9) is expressed highly to facilitate cell migration and angiogenesis. This study aims to synthesize purine analog from *p*-nitroanilin, 3-bromopropionil chloride and theophylline. The ligan is then studied its molecular interaction with PEX-9 using molecular docking. The result shows that the structure of the purine analog has been confirmed by  $^1\text{H-NMR}$  and LC-MS. The docking study reveals that there are molecular interactions between the ligan (FUSD-002) with PEX-9 at the active site with free energy of binding -8,68 kcal/mol and predicated  $\text{Ki}$  0,43  $\mu\text{M}$ , is associated as a molecular interaction between PEX-9 and the synthesis compound.

**Keywords:** FUSD-002, molecular docking, PEX-9, synthesis