

## **In Silico Molecular Docking Study of Gallic Acid and its Derivatives as Inhibitor BRAF Colon Cancer**

**Aji Humaedi<sup>1,3\*</sup>, Ade Arsiyanti<sup>2</sup>, Maksum Radji<sup>1</sup>**

<sup>1</sup>Department of Pharmacy, Faculty of Pharmacy, Universitas Indonesia, Depok 16424, Indonesia

<sup>2</sup>Department of Chemistry, Faculty of Medicine, Universitas Indonesia, Depok 16424, Indonesia

<sup>3</sup>Department of Pharmacy, Faculty of Science and Pharmacy, University of Mathla'ul Anwar, Banten 42273, Indonesia

**Abstract:**Gallic acid is a phenolic acid compound that can be found in natural products and has been reported to have various biological activity against several cancer cell lines such as leukemia, lung cancer, and colon adenocarcinoma. This research is aimed to study the stability, affinity, and interaction of the gallic acid and its five derivatives compounds, namely, ethylgallate, benzylgallate, phenylethyl gallate, (2-hydroxy)-benzylgallate and 4-methoxy-(2-hydroxy)-benzylgallate as inhibitors of BRAF colon cancer by in silico molecular docking. Gallic acid and the five derivatives as a ligand were transformed into 3D structures, subsequently docking simulation process is performed against BRAF. In silico docking study showed the five derivatives have the Gibbs energy ( $\Delta G$ ) value lower than gallic acid, suggesting that the five derivatives have higher stability than gallic acid. Furthermore, compared to gallic acid, the five derivatives have a greater affinity and stronger interaction with the catalytic site of BRAF colon cancer. Among the five derivatives, (2-hydroxy)-benzylgallate has the highest stability and strongest interaction on BRAF colon cancer. Thus, (2-hydroxy)-benzylgallate could be developed as a potential inhibitor of BRAF and promising candidate for colon cancer drug.

**Keywords :**In silico, Gallic acid, Gallic acid derivatives, BRAF, colon cancer.

**AjiHumaedi *et al***/International Journal of ChemTech Research, 2017,10(1): 310-315.

\*\*\*\*\*