ABSTRACT

The effect of (-)-epicatechin (EC) derivatives is including (-)-epicatechin (EC), (-)-epicatechin gallate (ECG), (-)-epigallocatechin (EGC) dan (-)-epigallocatechin gallate (EGCG) to rifampicin (RIF) as first line medicine of anti-tuberculosis has been studied. From preliminary research in silico docking studies rerank score (RS) RIF to RNA Polymerase (RNAP) receptor (116V) is -117,2420, while the RS value of (-)epicatechin derivates to Fatty Acid Synthase (FAS) receptor (2VB7), namely, EC -92,994; ECG -135,821; EGC -95.458; and EGCG -125,695. In silico predicted that the (-)-epicatechin derivatives have anti-tuberculosis activity and is able to inhibit fatty acid synthase (FAS) in Mycobacterium tuberculosis and derivatives (-)-epicatechin contained in green tea is predicted can synergy with RIF as anti-tuberculosis by opening the way for RIF by changing the permeability bacterial cell membrane that is inhibit the fatty acid synthase (FAS), which are outside the Mycobacterium tuberculosis cells so that RIF more easily enter the cells and inhibit Mycobacterium tuberculosis RNA polymerase of Mycobacterium tuberculosis. Combination RIF and (-)-epicatechin derivatives have synergy effect as anti-tuberculosis and able to reduce Minimal Inhibitory Concentration (MIC) value of RIF. It has been found that the value of MIC RIF before combined with (-)-epicatechin derivatives is 5 ppm and after combined with EC, ECG, and EGCG, MIC RIF values into 0,5 ppm, after combined with EGC, MIC RIF values into 1 ppm. Constant improvement of lipophilic, electronic and steric and (-)-epicatechin derivatives indicates that there is no quantitative structure-activity relationship of anti-tuberculosis in linear and non linear regression.

Keywords: (-)-Epicatechin (EC) derivatives, rifampicin, anti-tuberculosis, QSAR, in silico.