

Synthesis and molecular docking of ether mitsunobu reaction

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Abstrak

The Mitsunobu reaction is very important reaction for the synthesis of ether from phenol and alcohol. The [7-methoxy-2-(4-methoxyphenyl)-1-benzofuran-5-yl]methanol (2) was synthesised from vanillin by using series of known reactions such as Mannich reaction, acetylation, hydrolysis, Wittig reaction, hydroboration.

This methanol benzofuran derivative (2) condensed with 4-fluorophenol by using DEAD in THF. The final product 5-[(4-fluorophenoxy)methyl]-7-methoxy-2-(4-methoxyphenyl)-1-benzofuran (3) was characterised by using IR, NMR and mass spectra and study their biological activity by molecular docking using molecular docking software Glide. The activity of ether (3) was compared to their amine analogue.