Synthesis and structural analysis of the drug Aspirin using Jmol interface

Abstract

Aspirin is prepared by chemical synthesis from salicylic acid, through acetylation with acetic anhydride. The molecular weight of aspirin is 180.16g/mol. It is odourless, colourless to white crystals or crystalline powder. Aspirin is an oral non-steroidal anti-inflammatory drug (NSAID) that is rapidly absorbed from the stomach and the small intestine. The drug aspirin was synthesised in real time lab. The yield was about 66.3%. The 3D structure of the reactants and product were drawn in Jmol interface. The stimulated ^{1}HNMR spectra for the reactants and the product aspirin were generated from JSPEC view feature in Jmol. From the obtained stimulated spectrum of aspirin, the structure of the drug was examined.

Keywords:

Jmol, aspirin, drug, simulated ^{1}HNMR spectrum, 3D structure, reactants, products