# Prediction on mechanism design of molecularly imprinted polymer synthesis using oleic acid as a template

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**ABSTRACT**
Palm Fatty Acid Distillate (PFAD) consists of more than 80% of free fatty acids, primarily palmitic acid and oleic acid, which can be esterified and added to the biofuel and oleo-chemical industries as feedstock. Oleic Acid is also known as cis-9-octadecenoic acid has the chemical formula C18H34O2 or (CH3(CH2)7CHCH(CH2)7COOH). There have been numerous studies that demonstrate the nutritional value of oleic acid. The objectives of this research were to simulate the mechanism reaction design for Molecularly Imprinted Polymer (MIP) synthesis and to predict the bonding formed after synthesis by comparing the monomers and template. The mechanism and complexes formed were drawn according to the theoretical mechanism of MIP. The chemicals involved were allylthiourea as the monomer, oleic acid as the template, ethylene glycol dimethacrylate (EGDMA) as the cross-linker, 2,2-azobisisobutyronitrile (AIBN) as the initiator, and acetonitrile as porogenic solvent. The monomer, allylthiourea was compared with the other two monomers which are vinylpyridine and acrylamide in MIP synthesis prediction. On average, when the allylthiourea was used as the monomer, the bond length was quite similar for each connection of atoms (1.316 Angstrom). However, when the vinylpyridine and acrylamide were used as the monomers, the length of the bonds was not similar to each other. On top of that, the bond angles prediction for allylthiourea-oleic acid complex agreed with the molecular geometry shape was tetrahedral due to the average angle was 109.5o. Next, two different templates; oleic acid and palmitic acid; were compared in MIP synthesis prediction. The bond length for oleic acid was on average quite similar to each other (1.316 Angstrom) whereas for palmitic acid as the template the bond length was not similar. The palmitic acid-allylthiourea complex showed the angles reading was not synchronized to each other and quite unstable, unlike the oleic acid-allylthiourea complex. The results agree that oleic acid as the template was the best in this setting parameter for MIP synthesis.

**KEYWORDS**
Bond Angle, Bond Length, Molecularly Imprinted Polymer, Oleic Acid, Prediction

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