

## The development of molecular imprinting technology for caffeine extraction

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### Abstrak

Molecularly Imprinted Polymers (MIPs) is a type of macromolecule formed by application of molecularly imprinting technology, which creates cavities in synthetic polymeric matrices which are highly selective to an imprinted template. MIPs were synthesized experimentally using methacrylic acid (MAA), divinylbenzene-80 (DVB-80), azobisisobutyronitrile (AIBN) and methanol as a monomer, cross-linker, initiator and porogen, respectively. The Non-Imprinted Polymer (NIP) was produced simultaneously to serve as a control polymer. The rational design approach was theoretically conducted by Ab Initio Molecular Orbital Studies using Gaussian 09 computational software package at the theoretical level of DFT B3LYP/6-31 (d,p). The basis set is used to optimize the number of monomers and their binding site with the template. In both studies, MIPs were prepared with different ratios of template to monomer form a complex of 1:3, 1:4 and 1:5. Experimentally, the MIPs synthesized via precipitation polymerization technique produced homogenous spherical beads distribution where the complex 1:3 gave the best. Theoretical studies support this experimental finding where the complex 1:3 gave the highest interaction energy between caffeine and MAA, -45.29 kJ/mol followed by 1:4, -43.52 kJ/mol and 1:5, -43.11 kJ/mol.