

RANCANGAN BERBASIS KOMPUTER UNTUK POLIMER TERCETAK MOLEKUL KURKUMIN BERDASARKAN SIMULASI DINAMIKA MOLEKUL

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INTISARI

Penelitian rancangan pembentukan polimer tercetak molekul (*Molecular Imprinted Polymer*, MIP) kurkumin sebagai templat dengan monomer fungsional asam metakrilat (MAA) dan *crosslinker* etilen glikol dimetakrilat (EGDMA) menggunakan pemodelan dan simulasi dinamika molekul telah dilakukan. Kajian pemodelan dilakukan dengan menggunakan perhitungan mekanika kuantum semi-empiris PM3 dan perhitungan DFT (B3LYP) *basis set* 6-31G (d) digunakan sebagai optimasi dalam simulasi dinamika molekul. Pembentukan MIP diawali dengan optimasi struktur kurkumin dan MAA serta bahan pendukung lainnya. Kedua struktur kurkumin dan MAA yang telah teroptimasi kemudian dilakukan pemodelan untuk didapatkan informasi energi interaksi yang terjadi. Simulasi dilakukan dengan pembuatan polietilen glikol dimetakrilat pada suatu kotak yang kemudian dilakukan minimasi energi dan ekuilibrisasi sistem sehingga didapatkan hasil analisis ikatan hidrogen selama waktu simulasi.

Pada pembentukan MIP, interaksi kurkumin dan MAA ditinjau melalui interaksi non kovalen (ikatan hidrogen) pada sisi aktif templat. Rasio optimum dari struktur model antara kurkumin dan MAA melalui perhitungan semi-empiris PM3 adalah 1:3 dengan hasil energi interaksinya sebesar -1,130 kkal/mol. Pada simulasi dinamika molekul didapatkan rasio templat-monomer fungsional sebesar 1:2 dan terdapat 2 ikatan hidrogen yang terjadi dengan nilai okupansi tertinggi yaitu 20,79% pada jarak $2,77 (\pm 0,15) \text{ \AA}$ serta sudut $49,24^\circ (\pm 18,06)$ selama 5 ns. Oleh karena itu, rasio MIP yang direkomendasikan untuk dilakukan sintesis secara eksperimen adalah 1:2.

Kata kunci: asam metakrilat, kurkumin, MIP, pemodelan, dinamika molekul

COMPUTER-BASED DESIGN FOR MOLECULAR IMPRINTED POLYMER OF CURCUMIN BASED ON MOLECULAR DYNAMIC SIMULATIONS

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ABSTRACT

The design formation of Molecular Imprinted Polymer (MIP) of curcumin as a template and a functional monomer of methacrylic acid (MAA) coupled with ethylene glycol dimethacrylate (EDGMA) as crosslinker through the modeling and molecular dynamic simulations has been conducted. Study on modeling has been carried out using semi-empirical quantum mechanical calculation of PM3 and DFT (B3LYP) 6-31G (d) was used as an optimization in the molecular dynamics simulation. The formation of MIP was begun by optimizing both curcumin and MAA structure and other supporting materials. Both optimized structures of curcumin and MAA were further modeled to get the information of interaction energies that occurred. In the simulation was started with box preparation which was then minimized the energy and equilibration system to obtain the results of hydrogen bonding analysis during the simulation.

In the formation of MIP, interactions of curcumin and MAA were observed through non covalent interactions (hydrogen bond) on the active sites of template. The optimum ratio of the model structure between curcumin and MAA through the semi-empirical calculation of PM3 was obtained as 1:3 with its interaction energy of -1.130 kcal/mol. In the molecular dynamics simulations, the obtaining ratio of template-functional monomers was 1:2 and there were 2 hydrogen bonds that occurred with the highest occupancy value of 20.79% at 2.77 (± 0.15) Å with 49.24° (± 18.06) for the distance and angle respectively in 5 ns. Therefore, the recommended MIP for further experimental synthesis was 1:2.

Keywords: methacrylic acid, curcumin, MIP, modelling, molecular dynamics