

## Adsorbent screening for glycidyl methacrylate extraction: A preliminary study using density functional theory

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### ABSTRACT

The difficulty in detecting glycidyl esters (GE), a potentially carcinogenic contaminant group in palm oil, remains a concern for the palm oil producers. The inefficient sample preparation step due to insufficient knowledge on GE interaction with extraction adsorbents is a challenge in improving the GE detection. This work aims to study the adsorption of glycidyl methacrylate (GM; a representative of GE) on adsorbents commonly used for chemical extraction (long-chain hydrocarbon, primary secondary amine and silica) based on the density functional theory. Gaussian 09W software (B3LYP/LanL2DZ) was used for chemical structure optimization and frequency calculation. GM adsorptions were generally found to be nonspontaneous. N - propylethylenediamine (PED; primary secondary amine type of adsorbent) is the most promising adsorbent for extracting GM. The adsorption on PED does not involve any bond breaking and formation, and only physisorption is expected to occur. The process is exothermic and can be referred as the most spontaneous among the non-spontaneous. The more negative  $\Delta E_{ads}$  also implies that the adsorbed GM is more stable on the PED surface than on C18 (long-chain hydrocarbon adsorbent). With that said, the silicon dioxide (silica type of adsorbent) was ruled out as chemical reaction were observed between the adsorbate and the adsorbent.

### KEYWORDS

Adsorption; bond angles; bond lengths; chemical engineering; contamination; density functional theory; Gaussian processes; vegetable oils

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