World Academy of Science, Engineering and Technology
International Journal of Environmental and Ecological Engineering
Vol:14, No:03, 2020

Prediction of Binding Free Energies for Dyes Removal Using Computational Chemistry

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Abstract : Dye removal is an environmental concern because the textile industries have been increasing by world population and industrialization. Adsorption is the technique to find adsorbents to remove dyes from wastewater. This method is low-cost and effective for dye removal. This work tries to develop effective adsorbents using the computational approach because it will be able to predict the possibility of the adsorbents for specific dyes in terms of binding free energies. The computational approach is faster and cheaper than the experimental approach in case of finding the best adsorbents. All starting structures of dyes and adsorbents are optimized by quantum calculation. The complexes between dyes and adsorbents are generated by the docking method. The obtained binding free energies from docking are compared to binding free energies from the experimental data. The calculated energies can be ranked as same as the experimental results. In addition, this work also shows the possible orientation of the complexes. This work used two experimental groups of the complexes of the dyes and adsorbents. In the first group, there are chitosan (adsorbent) and two dyes (reactive red (RR) and direct sun yellow (DY)). In the second group, there are poly(1,2-epoxy-3-phenoxy) propane (PEPP), which is the adsorbent, and 2 dyes of bromocresol green (BCG) and alizarin yellow (AY).

Keywords : dyes removal, binding free energies, quantum calculation, docking
Conference Title : ICEC 2020 : International Conference on Environmental Chemistry
Conference Location : London, United Kingdom
Conference Dates : March 12-13, 2020