

Docking and Experimental Studies for Removal of Anthraquinone Dye by Modified Low Sulphonated Lignin †

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† Presented at International e-Conference on Green Chemistry and Engineering towards Sustainable Development – An Industrial Perspective (16-18 June 2021), Surat, Gujarat, India

Received: 5.06.2021; Revised: 10.06.2021; Accepted: 12.06.2021; Published: 15.06.2021

Abstract: Dyes and pigments are the major constituents of effluents generated from industries known to cause detrimental effects on environmental and human health. Among the numerous techniques available for the removal of dyes, adsorption is the simplest and inexpensive method. Lignin is a major component of lignocellulosic biomass, largely produced as a byproduct from paper and pulp industries. Due to the presence of many functional groups on lignin and various chemical activation, lignin can be used as a natural adsorbent. In this study, commercial low sulfonated lignin was modified by Mannich reaction and was characterized using FTIR, SEM, TGA. The docking study was carried out to understand the active site involved in the dye-adsorbent interactions. The results of the theoretical studies were collaborated by the batch experiments for adsorption of Reactive Blue 19. It was observed that the modified lignin showed high removal efficiency compared to the unmodified lignin. Moreover, the docking study was useful in illustrating the adsorption mechanism.

Keywords: lignin; docking; Mannich reaction and removal efficiency.

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Funding

This research received no external funding.

Acknowledgments

I would like to extend my special thanks to the National Institute of Technology, Karnataka (NITK) for providing me with sophisticated facilities such as FTIR, SEM, and TGA and Department of Chemical Engineering, NITK for their administrative support, including purchasing all the supplies for this study.

Conflicts of Interest

The authors declare no conflict of interest.