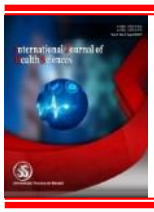


**International Journal of Health Sciences**
Available online at www.sciencescholar.us
Vol. 7 No. 3, December 2023, pages: 165-175
e-ISSN: 2550-696X, p-ISSN: 2550-6978
https://doi.org/10.53730/ijhs.v7n3.14657

# Molecular Docking of Lectins as a Biosorbent for Removal of Textile Dyes from Wastewater Media

**Afaf Amara-Rekkab** [a]

*Manuscript submitted: 18 August 2023, Manuscript revised: 09 October 2023, Accepted for publication: 27 November 2023*

***Corresponding Author*** [a]

***Keywords***

*binding affinity;*
*environment ;*
*health;*
*lectins;*
*molecular docking;*

**Abstract**

The molecular docking of lectins as biosorbents for textile dye removal from wastewater media is a topic of great significance in the fields of environmental and health science. Textile dyes are highly toxic and persistent, posing a serious threat to aquatic ecosystems and human health. Therefore, finding an effective and sustainable method for their removal is crucial. Lectins, which are proteins found in plants and animals, have been extensively studied for their ability to bind with specific sugar molecules. This unique property makes them potential candidates for biosorption applications. Molecular docking techniques allow scientists to study the interaction between lectins and textile dyes at the molecular level, providing valuable insights into their binding affinity and efficiency. By understanding the molecular interactions between lectins and textile dyes, researchers can design more efficient biosorbents that can selectively remove these harmful compounds from wastewater media. In addition, molecular docking studies can help optimize the conditions under which this process occurs, such as pH levels or temperature. Three textile dyes were docked on the lectins of Cupressus sempervirensto to evaluate the binding affinity of these drugs. The least binding energies between the lectins and bemacid blue, brilliant green and black acid 60 were - 8.7, -5.0, and -5.7 Kcal/mol, respectively, with the identification of several bending sites of our biosorbent. In conclusion, the results showed that Cupressus sempervirens could be advantageously used as a low-cost biosorbent for the removal of our dyes in wastewater treatment.



[a] Laboratory of Separation and Purification Technologies, Department of Chemistry, Faculty of Sciences, University of Tlemcen — 13000, Algeria & Institute of Science and Technology, Department of Hydraulics, University center of Maghnia Zouia maghnia street— 13000, Algeria.

**Contents**



## 1 Introduction

Textile dyes have been used for centuries to add vibrant colors and patterns to fabrics. However, the effects of these dyes on both human health and the environment are a growing concern. The chemicals used in textile dyes can have detrimental effects on both (Gadipelly et al., 2014; Dias et al, 2015).

Firstly, the health implications of textile dyes cannot be ignored. Many of these dyes contain toxic substances such as heavy metals, carcinogens, and allergens. These chemicals can be absorbed through the skin when wearing dyed clothing or through inhalation when working in dyeing factories. Prolonged exposure to these toxins has been linked to various health issues including skin allergies, respiratory problems, and even cancer (de Jong et al., 2016; Altintig et al., 2017; Ahmad et al., 2015; Tsuboy et al., 2007; Metin et al., 2013).

Furthermore, textile dyeing processes contribute significantly to environmental pollution. The wastewater generated during dyeing contains high levels of toxic chemicals that are often discharged into rivers and lakes without proper treatment. This not only contaminates water sources but also affects aquatic life and ecosystems. Additionally, the energy-intensive processes involved in dyeing contribute to greenhouse gas emissions and climate change (Yaseen & Scholz, 2019; Nandi et al., 2009; Ghaedi et al., 2011; Geissen et al., 2015; Djebbari et al., 2022).

To mitigate these negative effects, the textile industry must adopt more sustainable practices. This includes using natural or organic dyes that are free from harmful chemicals and implementing eco-friendly wastewater treatment systems. Consumers also play a vital role by choosing products made from environmentally friendly materials and supporting brands that prioritize sustainability.

The use of textile dyes has significant consequences for both human health and the environment. Manufacturers must prioritize sustainable practices to minimize these negative impacts. By doing so, we can ensure a healthier future for both ourselves and our planet (Chandarana et al., 2021; Dahri et al., 2015; Brillas et al., 1998; Liang et al., 2005; Ferreira et al., 2006; Ibrahim et al., 2018; Flórez-Castillo et al., 2020).

The use of lectins for the removal of metals and dyes has gained significant attention in recent years due to their unique properties and potential applications in environmental remediation. Lectins, a class of proteins found abundantly in plants, can bind specifically to carbohydrates. This property makes them ideal candidates for the removal of heavy metals and dyes from contaminated water sources (Małecki et al., 2012).

Lectins can be immobilized onto various solid supports such as activated carbon, silica gel, or magnetic nanoparticles. Once immobilized, they can be easily separated from the solution after metal or dye-binding occurs. The binding mechanism involves lectin-carbohydrate interactions, where lectins recognize specific carbohydrate moieties present on metal ions or dye molecules.

Several studies have demonstrated the effectiveness of biosorbents (Druzian et al., 2021; Fabbricino et al., 2016; Gautam et al., 2020) in removing heavy metals like lead, cadmium, and mercury from aqueous solutions. The high affinity and selectivity of biosorbents toward these metals make them efficient sorbents for water treatment processes. Similarly, biosorbents have also shown promising results in removing synthetic dyes commonly used in textile industries (Gonzalez et al., 2015; Kazemi et al., 2020).

Furthermore, lectin-based approaches offer several advantages over conventional methods such as low cost, ease of regeneration, and eco-friendliness. Lectin-based adsorbents can be regenerated by simply washing with appropriate solutions without losing their binding capacity. Additionally, the use of natural

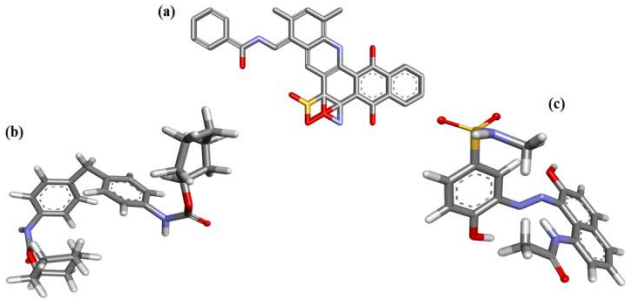
materials like plant-derived lectins reduces the reliance on synthetic chemicals that may pose environmental risks.

The liquid-solid extraction by lectins for the removal of metals and dyes presents a promising approach towards sustainable environmental remediation. Further research is needed to optimize their performance and explore their potential applications on a larger scale. Nonetheless, this emerging field holds great promise for addressing water pollution challenges effectively while minimizing adverse impacts on ecosystems.

## 2 Materials and Methods

*Dyes*

The bemacid blue (BB), brilliant green (BG) and black acid 60 (BA) are used as dyes. They were supplied to us by the textile factory (SWATEX) located in Tlemcen, Algeria. Their molecular structure is given in Scheme. 1.




Scheme. 1: Chemical structure of Ligans prepared for Molecular Docking: Bemacid Blue (BB) (a), Brilliant green (BG) and Black acid 60 (c)

*Docking analysis of dyes*

The principle of docking molecular is a fundamental concept in the field of computational chemistry. It involves predicting the binding affinity and orientation of a small molecule, known as a ligand, to a larger macromolecule, such as a protein or DNA. This technique plays a crucial role in drug discovery and design.

Docking molecular relies on algorithms that simulate the interaction between the ligand and macromolecule. These algorithms take into account various factors, including electrostatic interactions, hydrogen bonding, and hydrophobicity. By analyzing these interactions, we can predict how well a ligand will bind to its target macromolecule.

One of the key challenges in docking molecular is accurately representing the three-dimensional structure of both the ligand and macromolecule. This requires sophisticated modelling techniques that consider flexibility and conformational changes.

The results obtained from docking studies can provide valuable insights into drug-target interactions. They can help identify potential lead compounds for further development or optimize existing drugs by predicting their binding affinity and suggesting modifications. Despite its immense potential, docking molecular has limitations. The accuracy of predictions heavily relies on the quality of input data and force fields used in simulations. Additionally, it may not capture all aspects of complex biological systems accurately.

The docking molecular is an essential tool in computational chemistry for predicting ligand-macromolecule interactions. Its applications range from drug discovery to understanding biological processes at a molecular level. Continued advancements in this field will undoubtedly contribute to significant breakthroughs in pharmaceutical research and development.

Molecular docking studies were performed to establish the plausible binding interfaces of ligands with the active sites of our biosorbent's enzymes and to validate experimental results. Lectins were previously synthesized in our biosorbent by Necib et al. (2015).

The AUTODOCK 4.2 program was used to conduct docking studies (Morris et al., 2009; Kausar et al., 2021; Bensegueni et al., 2019). Lectins' structure was obtained from the Protein Data Bank. Bemacid Blue's 3D structures in PDB format were created using the ChemDraw database and AutoDock Tools, which inserted polar hydrogen atoms into the amino acid residues and eliminated water molecules. Next, the AUTOGRID tool was run with the protein in PDBQT format as an input. Blind docking was used to accomplish rigid ligand docking. Discovery Studio Visualizer was used to display the results (Lee et al., 2020; El-Shwiniy et al., 2022; Bensegueni et al., 2019).

## 3 Results and Discussions

*Bemacid Blue*

Molecular docking allowed us to identify the different active sites of our biosorbent which are: ALA 70, SER 68, TYR 65, LYS 55 and GLN 57. Bemacid blue was complexed inside active sites of Lectins by showing many important interactions as presented in Figures 1, 2 and 3.

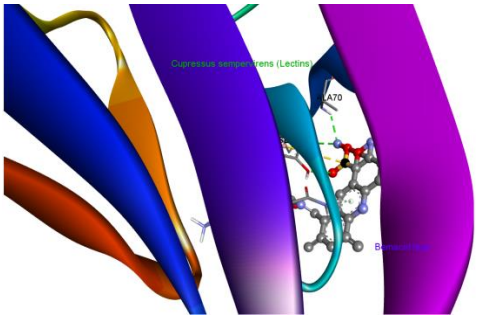


Figure 1. Details of the interaction between Bemacid blue with the protein's active site of the Lectins

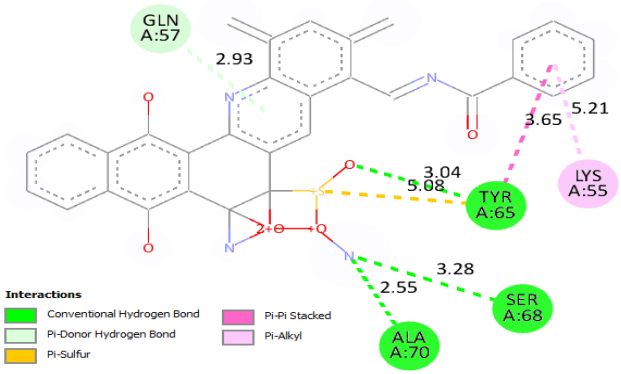



Figure 2. 2D of Lectins with Bemacid blue

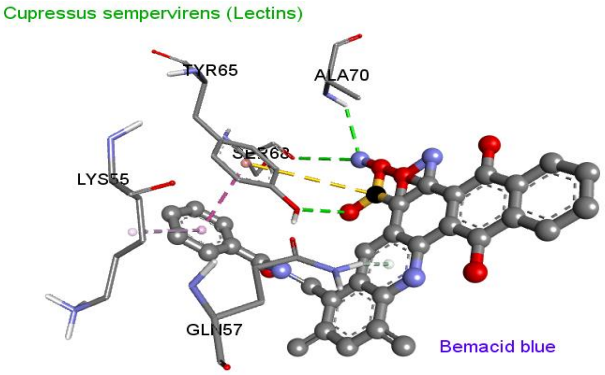



Figure 3. 3D of Lectins with Bemacid blue

It formed conventional hydrogen bond interactions with ALA 70 (2.55 ˚A), SER 68 (3.28 ˚A) and TYR 65 (3.04 ˚A) amino acid residues of Lectins. TYR 65 developed π–suplur (5.08 ˚A) interaction with the Bemacid blue. LYR 65 residue stabilized the ligand by forming π–π stacked (3.65 ˚A) interactions, the same result was observed by Lee et al. (2020). LYS 55 developed π-alkyl bonding (5.21 ˚A). Also, A π–donor hydrogen bond interaction is shown by GNL 57 (2.93 ˚A) contributed to stabilizing the ligand (El-Shwiniy et al., 2022) (Fig. 2 and 3).

*Brilliant green*

Brilliant green was complexed inside active sites of Lectins of cypressus by showing many important interactions as presented in Figures 4, 5 and 6.

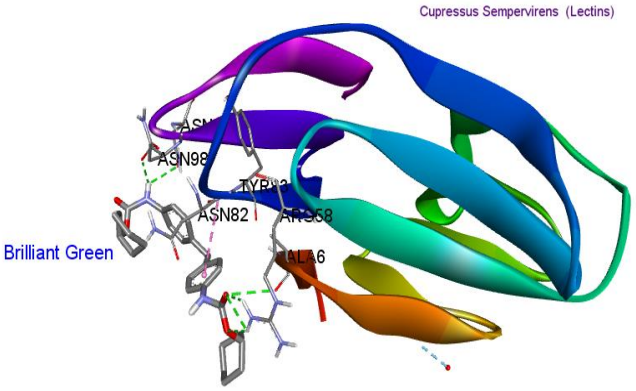



Figure 4. Details of the interaction between Brilliant green with the protein's active site of the Lectins

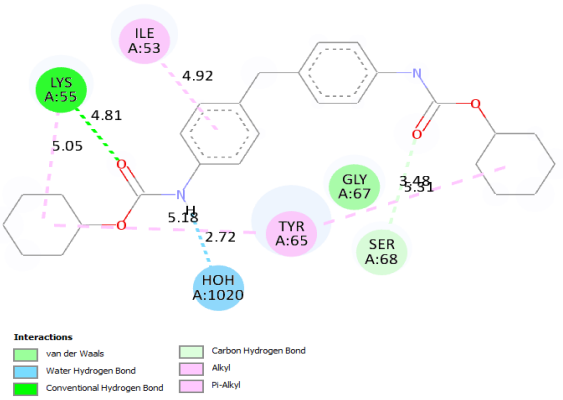



Figure 5. 2D of Lectins with Brilliant green

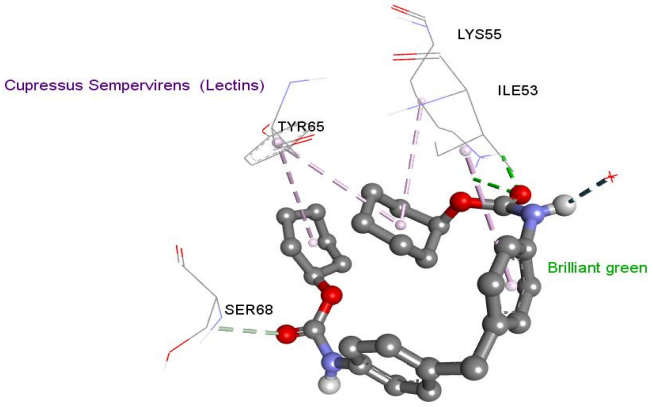



Figure 6. 3D of Lectins with Brilliant green

It formed a carbon-hydrogen bond with ASN 109 (3.42 ˚A) and ALA 102 (4.31˚A) amino acid residues of Lectins. ALA 105 (4.04 and 5.13˚A) and ILL 103 (4.04 ˚A) developed alkyl interaction with the Brilliant green. VAL 94 residue stabilized the ligand by forming pi-alkyl (4.93 ˚A) interactions (Fig. 5 and 6).

*Black Acid 60*

As shown in Figs. 7, 8, and 9, Black acid 60 was complexed inside the active areas of cypress lectins by exhibiting several significant interactions.

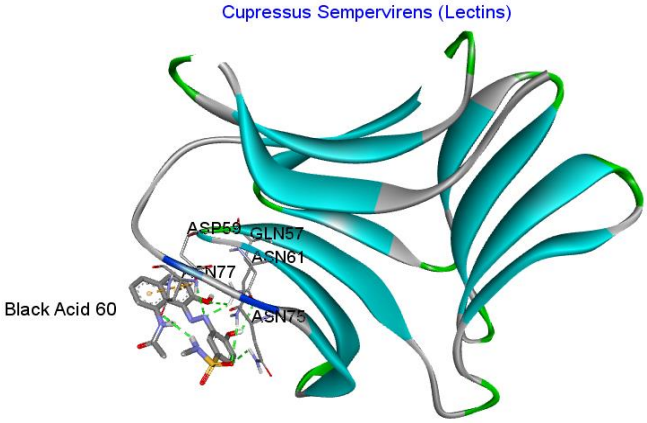



Figure 7. Details of the interaction between Black acid 60 with the protein's active site of the Lectins

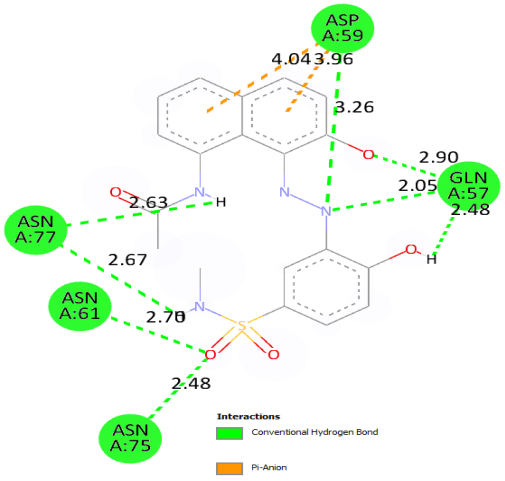



Figure 8. 2D of Lectins with Black acid 60

Black acid 60 developed eight converted hydrogen bonds (Fig. 8 and 9): ASN 77 (2.67 and 2.63˚A), ASN 61 (2.78 ˚A), ASN 75 (2.48 ˚A), GNL 57 (2.48, 2.05 and 2.90˚A) and ASP 59 (3.26 ˚A) amino acid residues of the biosorbent. ASP 59 developed two π–anion (3.96 and 4.04˚A) interactions with the Black acid 60.

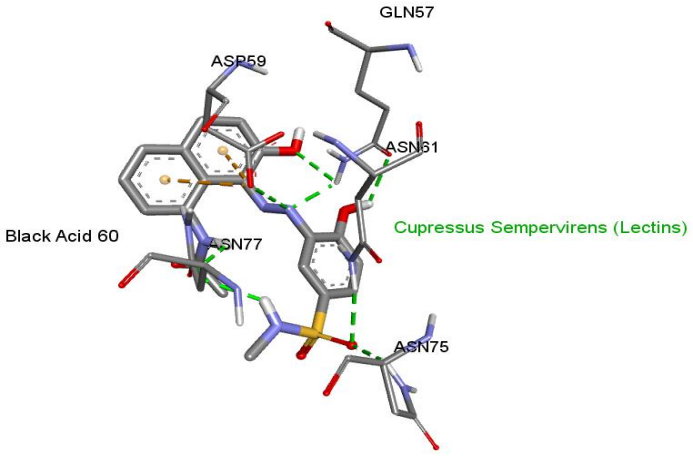



Figure 9. 3D of Lectins with Black acid 60

Based on the molecular docking calculation results [Table 1], every examined molecule has significance to the biosorbent that is being used. This implies that they could make thermodynamically advantageous up a complex (Bensegueni et al., 2019).

Table 1
$\Delta G_{binding}$ values of the tested dyes

| Molecule | ΔG binding (kcal/mol) |
|---|---|
| Bemacid blue (BB) | -8.7 |
| Brilliant green (BG) | - 5.0 |
| Black acid 60 (BA) | -5.7 |

## 4 Conclusion

The use of molecular docking in this context has several advantages. Firstly, it allows for a more targeted approach towards developing biosorbents by identifying lectins with high binding affinities towards specific textile dyes. Secondly, it provides valuable information about the mechanism of dye-lectin interactions, aiding in the design of more efficient biosorption systems.

In conclusion, molecular docking of lectins as a biosorbent for textile dye removal from wastewater media holds great promise in addressing the growing concern over water pollution caused by these toxic compounds. By utilizing this technique, scientists can develop more effective and sustainable methods for treating industrial wastewater while minimizing its impact on the environment.

*Acknowledgements*
I am grateful to two anonymous reviewers for their valuable comments on the earlier version of this paper.

## References


Ahmad, A., Mohd-Setapar, S. H., Chuong, C. S., Khatoon, A., Wani, W. A., Kumar, R., & Rafatullah, M. (2015). Recent advances in new generation dye removal technologies: novel search for approaches to reprocess wastewater. *RSC advances*, *5*(39), 30801-30818.

Altıntıg, E., Altundag, H., Tuzen, M., & Sarı, A. (2017). Effective removal of methylene blue from aqueous solutions using magnetic loaded activated carbon as novel adsorbent. *Chemical Engineering Research and Design*, *122*, 151-163. https://doi.org/10.1016/j.cherd.2017.03.035

Bensegueni, R., Guergouri, M., Bensouici, C., & Bencharif, M. (2019). Synthesis, antioxidant, and anti-tyrosinase activity of some aromatic oximes: An experimental and theoretical study. *Journal of Reports in Pharmaceutical Sciences*, *8*(2), 195-203.

Brillas, E., Mur, E., Sauleda, R., Sanchez, L., Peral, J., Domènech, X., & Casado, J. (1998). Aniline mineralization by AOP's: anodic oxidation, photocatalysis, electro-Fenton and photoelectro-Fenton processes. *Applied Catalysis B: Environmental*, *16*(1), 31-42. https://doi.org/10.1016/S0926-3373(97)00059-3

Chandarana, H., Kumar, P. S., Seenuvasan, M., & Kumar, M. A. (2021). Kinetics, equilibrium and thermodynamic investigations of methylene blue dye removal using Casuarina equisetifolia pines. *Chemosphere*, *285*, 131480. https://doi.org/10.1016/j.chemosphere.2021.131480

Dahri, M. K., Kooh, M. R. R., & Lim, L. B. (2015). Application of Casuarina equisetifolia needle for the removal of methylene blue and malachite green dyes from aqueous solution. *Alexandria Engineering Journal*, *54*(4), 1253-1263. https://doi.org/10.1016/j.aej.2015.07.005

de Jong, L., Pech, N., de Aragão Umbuzeiro, G., & Moreau, X. (2016). Multi-scale biomarker evaluation of the toxicity of a commercial azo dye (Disperse Red 1) in an animal model, the freshwater cnidarian Hydra attenuata. *Water research*, *96*, 62-73. https://doi.org/10.1016/j.watres.2016.03.043

Dias, E. M., & Petit, C. (2015). Towards the use of metal–organic frameworks for water reuse: a review of the recent advances in the field of organic pollutants removal and degradation and the next steps in the field. *Journal of Materials Chemistry A*, *3*(45), 22484-22506.

Djebbari, N. E., Amara, A., Didi, A., & Didi, M. A. (2022). Factorial Design Optimization Of Uranium (VI) Cloud Point Extraction With Triton X-100/TWEEN-40/D2EHPA/BMIMMESO 4. *Scientific Study & Research. Chemistry & Chemical Engineering, Biotechnology, Food Industry*, *23*(4), 333-343.

Druzian, S. P., Zanatta, N. P., Borchardt, R. K., Côrtes, L. N., Streit, A. F., Severo, E. C., ... & Dotto, G. L. (2021). Chitin-psyllium based aerogel for the efficient removal of crystal violet from aqueous solutions. *International Journal of Biological Macromolecules*, *179*, 366-376. https://doi.org/10.1016/j.ijbiomac.2021.02.179

El-Shwiniy, W. H., El-Desoky, S. I., Alrabie, A., & Abd El-wahaab, B. (2022). Spectrophotometric determination of Zr (IV), Hg (II) and U (VI) in solution with their analytical applications: Structural characterization and molecular docking of the solid complexes. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, *279*, 121400. https://doi.org/10.1016/j.saa.2022.121400

Fabbricino, M., & Pontoni, L. (2016). Use of non-treated shrimp-shells for textile dye removal from wastewater. *Journal of Environmental Chemical Engineering*, *4*(4), 4100-4106. https://doi.org/10.1016/j.jece.2016.08.028

Ferreira, H. S., Bezerra, M. D. A., & Costa Ferreira, S. L. (2006). A pre-concentration procedure using cloud point extraction for the determination of uranium in natural water. *Microchimica Acta*, *154*, 163-167.

Flórez-Castillo, J. M., Rondón-Villareal, P., Ropero-Vega, J. L., Mendoza-Espinel, S. Y., Moreno-Amézquita, J. A., Méndez-Jaimes, K. D., ... & Gómez-Duarte, O. G. (2020). Ib-M6 Antimicrobial peptide: Antibacterial activity against clinical isolates of Escherichia coli and molecular docking. *Antibiotics*, *9*(2), 79.

Gadipelly, C., Pérez-González, A., Yadav, G. D., Ortiz, I., Ibáñez, R., Rathod, V. K., & Marathe, K. V. (2014). Pharmaceutical industry wastewater: review of the technologies for water treatment and reuse. *Industrial & Engineering Chemistry Research*, *53*(29), 11571-11592.

Gautam, D., & Hooda, S. (2020). Magnetic graphene oxide/chitin nanocomposites for efficient adsorption of methylene blue and crystal violet from aqueous solutions. *Journal of Chemical & Engineering Data*, *65*(8), 4052-4062.

Geissen, V., Mol, H., Klumpp, E., Umlauf, G., Nadal, M., van der Ploeg, M., ... & Ritsema, C. J. (2015). Emerging pollutants in the environment: a challenge for water resource management. *International soil and water conservation research*, *3*(1), 57-65.

Ghaedi, M., Hossainian, H., Montazerozohori, M., Shokrollahi, A., Shojaipour, F., Soylak, M. U. S. T. A. F. A., & Purkait, M. K. (2011). A novel acorn based adsorbent for the removal of brilliant green. *Desalination*, *281*, 226-233. https://doi.org/10.1016/j.desal.2011.07.068

González, J. A., Villanueva, M. E., Piehl, L. L., & Copello, G. J. (2015). Development of a chitin/graphene oxide hybrid composite for the removal of pollutant dyes: adsorption and desorption study. *Chemical engineering journal*, *280*, 41-48. https://doi.org/10.1016/j.cej.2015.05.112

Ibrahim, M. K., Taghour, M. S., Metwaly, A. M., Belal, A., Mehany, A. B. M., Elhendawy, M. A., ... & Eissa, I. H. (2018). Design, synthesis, molecular modeling and anti-proliferative evaluation of novel quinoxaline derivatives as potential DNA intercalators and topoisomerase II inhibitors. *European journal of medicinal chemistry*, *155*, 117-134. https://doi.org/10.1016/j.ejmech.2018.06.004

Kausar, N., Murtaza, S., Nadeem Arshad, M., Munir, R., Saleem, R. S. Z., Rafique, H., Tawab, A. (2021). Synthesis, characterization, theoretical and molecular docking studies of mixed-ligand complexes of Cu(II), Ni(II), Co(II), Mn(II), Cr(III), UO2(II) and Cd(II). *Journal of Molecular Structure, 1244*, 130983.

Kazemi, J., & Javanbakht, V. (2020). Alginate beads impregnated with magnetic Chitosan@ Zeolite nanocomposite for cationic methylene blue dye removal from aqueous solution. *International journal of biological macromolecules*, *154*, 1426-1437. https://doi.org/10.1016/j.ijbiomac.2019.11.024

Lee, J., Worrall, L. J., Vuckovic, M., Rosell, F. I., Gentile, F., Ton, A. T., ... & Strynadka, N. C. (2020). Crystallographic structure of wild-type SARS-CoV-2 main protease acyl-enzyme intermediate with physiological C-terminal autoprocessing site. *Nature communications*, *11*(1), 5877.

Liang, P., Li, J., & Yang, X. (2005). Cloud point extraction preconcentration of trace cadmium as 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone complex and determination by flame atomic absorption spectrometry. *Microchimica Acta*, *152*, 47-51.

Małecki, P. H., Rypniewski, W., Szymański, M., Barciszewski, J., & Meyer, A. (2012). Binding of the plant hormone kinetin in the active site of Mistletoe Lectin I from Viscum album. *Biochimica et Biophysica Acta (BBA)-Proteins and Proteomics*, *1824*(2), 334-338. https://doi.org/10.1016/j.bbapap.2011.10.013

Metin, A. U., Çiftçi, H., & Alver, E. (2013). Efficient removal of acidic dye using low-cost biocomposite beads. *Industrial & Engineering Chemistry Research*, *52*(31), 10569-10581.

Morris, G. M., Huey, R., Lindstrom, W., Sanner, M. F., Belew, R. K., Goodsell, D. S., & Olson, A. J. (2009). AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. *Journal of computational chemistry*, *30*(16), 2785-2791.

Nandi, B. K., Goswami, A., & Purkait, M. K. (2009). Removal of cationic dyes from aqueous solutions by kaolin: kinetic and equilibrium studies. *Applied Clay Science*, *42*(3-4), 583-590. https://doi.org/10.1016/j.clay.2008.03.015

Necib, Y., Bahi, A., Merouane, F., Bouadi, H., & Boulahrouf, K. (2015). Comparative study of a new lectin extracted from roots of plants: Cyperus rotundus, Pistacia lentiscus and Ruta graveolens. *World journal of pharmaceutical research*, *4*(1), 1720-1733.

Tsuboy, M. S., Angeli, J. P. F., Mantovani, M. S., Knasmüller, S., Umbuzeiro, G. A., & Ribeiro, L. R. (2007). Genotoxic, mutagenic and cytotoxic effects of the commercial dye CI Disperse Blue 291 in the human hepatic cell line HepG2. *Toxicology in vitro*, *21*(8), 1650-1655. https://doi.org/10.1016/j.tiv.2007.06.020

Yaseen, D. A., & Scholz, M. (2019). Textile dye wastewater characteristics and constituents of synthetic effluents: a critical review. *International journal of environmental science and technology*, *16*, 1193-1226.

## Biography of Author

**Mrs. Amara-Rekkab**
obtained her PhD from ABOU BEKR BELKAID University, Tlemcen, Algeria, in 2015. Since this year, she has been an Algerian lecturer in the Department of Chemistry. She has published over ten articles in highly regarded journals. His research focuses on environmental pollution, the extraction of heavy metals, and their toxicity. She also teaches desalination, water treatment, and wastewater treatment.
*Email: amarafaf@yahoo.fr*