

Research Article

Predicting the Adsorption Efficiency Using Machine Learning Framework on a Carbon-Activated Nanomaterial

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Due to the excessive use of paracetamol (PCM), a significant amount of its metabolite has been released into the surroundings, and its removal from the surroundings must happen quickly and sustainably. Multicomponent adsorption modelling is difficult because it is challenging to anticipate the relationships among the adsorbates in this artificial intelligence-based modelling, a choice among different algorithms. Utilizing various algorithms, many studies assessed the single and binary adsorption of paracetamol on activated carbon. The present study implements that the effectiveness of PCM adsorption on a carbon-activated nanomaterial was predicted using an artificial neural network, a machine learning technology. As a factor of adsorbent particle size, adsorbent dosage, training time, and starting concentrations, the adsorption capacity for each medicinal ingredient was examined. SEM was used to analyze a nanomaterial that had been chemically altered with orthophosphoric acid (FTIR). To determine the residual proportion of PCM in solvent, batch adsorption of PCM was then carried out at various operation conditions, including contact time, temperatures, and initial dosage. The adsorption effectiveness of paracetamol on carbon-activated nanoparticle was calculated using experimental results. Thus, by using machine learning framework, the adsorption efficiency of paracetamol on a carbon-activated nanomaterial was predicted.

1. Introduction

Pharmaceutical substances are now understood to be developing contaminants with detrimental effects on both the surroundings and public health. Pharmaceutical contaminants are quickly emerging as new contaminants and are accumulated in sewage and aquatic systems. As a result, 300 million tons of industrial and medicinal chemicals are released into the environment annually. These contaminants

are dangerous for the ecosystem because they are nonbiodegradable and extremely poisonous and have a unique molecular size. In order to prevent medicines' negative impacts on the ecosystem, people, and aquatic environments, it is imperative that they are removed from sewage. The research states that paracetamol and nimesulide bioactive chemicals were found in small amounts in the waterways of South American countries. For example, due to its hepatotoxic consequences and gastrointestinal harms, the promotion

and intake of nimesulide were forbidden in various nations [1], while 4-aminophenol, an extremely dangerous and carcinogenic chemical that causes genetic defects and cellular deaths, could be produced when paracetamol is broken down. In the United States and Europe, paracetamol is the most typical cause of acute liver failure (ALF). A hyperacute structure governs both injury and recovery, with maximum hepatocyte damage occurring 72 hours after a single consumption and possible recovery occurring at a similarly rapid pace. The rapidity and magnitude of the disease, the possibility of recovering without LT, and the existence of complex psychosocial factors in the majority of patients make organ transplants for acetaminophen-induced acute liver failure frequently present considerable challenges and issues despite sensible renal transplant recipient results [2]. Regarding nanomaterial structures, characteristics, adsorption, and catalysis, this viewpoint illustrates and discusses the problems of general interest for the implementations and viewpoints of ML in the field of NM. NMs have created new opportunities for nanomedicine and healthcare development. Comprehending the nanomaterial foundation for use in biomedical application is their interfacial interactions with life. ML offers significant advantages in precisely determining and anticipating biochemical functions to the characteristics of both known and unknown molecules, which aid in the discovery of new functional nanomaterials and the prevention of negative consequences. Machine learning techniques lack comprehensibility (i.e., are ambiguous in their physical, chemical, or biological meaning), particularly deep learning systems with high prediction performance comparing to chemical, pharmaceutical, and biological molecular. Likewise, machine learning databases are still in their development. Additionally, they go over how to encourage the use of learning algorithm, create datasets in the realm of commodities, and create open to interpretation algorithms (e.g., white box models). Additional facets of the application of ML to advance nanotechnology are offered towards the conclusion of this viewpoint, for example, nanopattern image classification [3].

Although modelling techniques like multilinear regression models and linear correlativity are frequently used to describe the adsorption process, they are only somewhat accurate and applicable. In contrast, data-driven machine learning techniques are an effective tool that might be utilized to investigate the intricate connection among adsorption capacities and biochar characteristics. Methods can be classified, predicted, optimized, and clustered using ML. To hasten the completion of pharmaceutical adsorption processes using biochar, ML has been employed. Nevertheless, given this field's relative youth, there is not much information now available. A component is moved from the liquid stage to the interface of a solid through the charge transport procedure termed as adsorption, where it is subsequently bound by either physical, chemical, or a combination of the two. Studies have concentrated on using inexpensive, environmentally acceptable compounds to remove MPs, such as chitosan and bentonite. Chitosan's glucose molecules contain several hydroxyl groups, making it more hydrophilic and technically excellent for inorganic and

organic adsorption. Hydrogel structures have a great deal of interest in chitosan, a natural cationic copolymer. This polymer is biocompatible and biodegradable due to its hydrophilic nature and the capacity of degradation via human enzymes, two biological qualities typically required for biological devices. The main component of bentonite is the clay mineral montmorillonite. Pollutant removal from water has frequently employed low-cost adsorption as a criterion. Upgraded organ bentonite absorbed about 81% of the AMX [4]. Adsorbent architectures, fluid characteristics, impurity frameworks, operational circumstances, and system control are only a few of the variables that play a role in the adsorption mechanism. Silica gel, alumina, clays, composites, zeolites, activated carbon, biomasses, and biological and polymeric substances are just a few of the elements that have been utilized as adsorbents to remove toxins from aquatic environment. So over the last ten years, work on the use of carbon-based nanomaterials as adsorbents has grown quickly. The distinctive qualities and variety of carbon-based nanostructures, as well as the emergence of new possibilities in numerous subspecialties of chemical, economics, and construction, are the primary driving forces behind the development of this discipline. The capacity of carbon-based product to adsorb a wide range of water contaminants, including hazardous metallic ions, medications, insecticides, transition metals, and other both inorganic and organic chemicals, could be achieved using a number of processes [5]. The usual pollutants are simply concentrated and moved to other stages when using absorbance as a water treatment process.

The connections among adsorbed molecules and adsorbent are what define and rely on the adsorption phenomenon. The kind of the adsorptive (protein kinase, polarization, functioning, diameter, and molecular mass), the adsorption (chemical bonding and pore size and composition), and the solution circumstances all affect how well a carbon-based adsorbent absorbs chemical substances (ionic strength, pH, and temperature). Van der Waals, induced-dipole, dipole-dipole, and hydrogen bonding donor-acceptor interactions, as well as the liquid phase, are what cause different chemicals to bind to different adsorbents and accumulate there. Hydrogen and other chemical bonds, together with covalent and electrostatic contacts, the hydrophobic action, and other interactions, all play crucial parts in the adsorption process. AC, carbon nanofibers, carbon nanotubes, graphene, biochar, and carbon aerogels are all components of CBMs. A variety of CBMs utilized in the adsorption process are shown in Figure 1 [6].

With its benefits of high effectiveness, reduced energy usage, and broad scalability for various pressure and heat ranges, adsorption with adsorbent material to transiently collect carbon dioxide from flue gas generated in the coal combustion of fossil fuels has attracted immense attention. Zeolites, porous polymers, covalent organic frameworks, metal organic frameworks, and porous carbon materials are some of the commonly researched solid adsorbents for carbon dioxide collection. Porous carbon materials (PCMs) stand out among the others because of their copious and adaptable porous architectures, simple manufacturing and

rejuvenation, excellent good thermal stability, cheap and accessible raw ingredients, and superior resistance to water vapor. The kind and quantity of activating agents, the thermochemical transformation techniques, and the process temperature all had a significant impact on the final physicochemical attributes of PCMs. The stimulation processes sped up the breakdown of carbon antecedents and helped rearrange transitional byproducts to create porous carbon frameworks. Numerous investigations have shown that this family of porous carbons has outstanding carbon dioxide adsorption capacity [7].

According to the investigator, more research is needed on continuous flow studies to comprehend the adsorption capability and to take into account the adsorption of several pollutants. According to a new analysis, the effectiveness of medication elimination by biochar adsorption differs and depends substantially on a number of variables, including the physicochemical qualities of biochar, the reaction environment, and the kind of medicines involved. These difficulties have made it necessary to create various methods and data-driven techniques to comprehend the adsorption capability and forecast the effectiveness of pharmacological removal, particularly for complicated pollutants. Due to their beneficial morphological, biochemical, electrical, and optical properties, nanoparticles have received a lot of research attention in a variety of sectors, including food technology, power, technology, and pharmaceuticals [8]. Metal organic structures have attracted interest recently in contrast to other rigid nanoparticle transports because of their well-structured organization, exceptionally large surface area, high porosity, variable pore size, and simple chemical functionalization. A repetitive, hollow architecture resembling a cage is created in a metal by the linking of ions or ions in clusters by organic compounds. The examination of preclinical nanocomposite safety and risk management has made extensive use of intelligence approaches. Adverse effects of nanoparticles on living things, such as people, animals, algae, plants, and the ecosystem at various points along the food chain, could be mitigated by proper nanomaterial engineering. Evaluations before product release (presymptomatic) are necessary to forestall the use of dangerous nanoparticles (nanotechnology). An index case can spread the disease to close contacts without showing symptoms at the time of exposure. The main factor still preventing the widespread application of nanomaterials in consumer goods, particularly in healthcare, is higher nanotoxicity in environmental compartments and during clinical studies [9].

Utilizing ANN, multiple studies have modelled the adsorption effectiveness of various pollutants. For the purpose of predicting the effectiveness of activated carbon powder in eliminating chromium (VI) from wastewater, investigation created a three-layer feed-forward neural network. Adsorbent dosage, solution pH, contact period, and beginning concentration are among the attribute values. The ideal number of invisible neurons for the hidden layer was determined to be 10, which also produced the least mean square error result. In the first version of their investigation, the backpropagation technique altered the activation functions of tansig, satlin, and poslin at the hidden units.

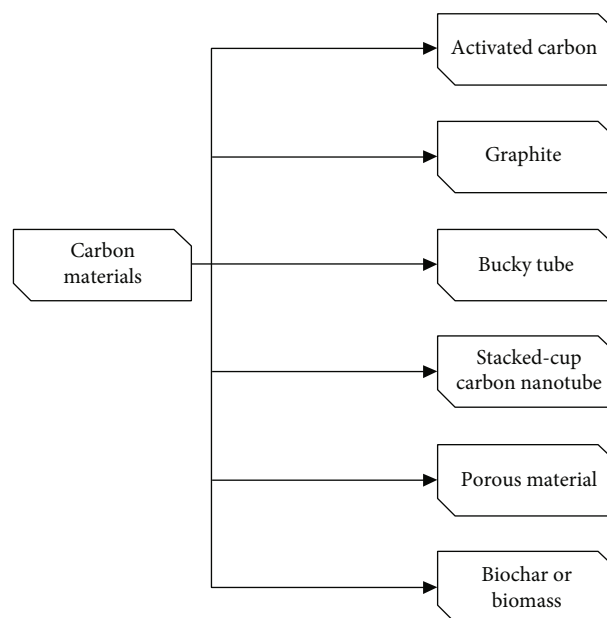


FIGURE 1: Several CBMs that can be used in adsorption techniques.

This is an example of a neural transfer function. Transfer functions are functions that determine the output of a layer based on the net input of that layer. At the output nodes, purelin activation function was utilized. Based on R^2 and mean square error values, the optimal method, activation function, and number of hidden neurons were chosen. When contrasting several forecasting systems for the efficacy of walnut, azo dyes [10]. In this research, a three-layer structure with a tansig converter at the concealed layer and endorphin transfer function at the output nodes was built. Size of the particles, beginning pH, dye concentration, training time, and temperatures are the five input factors that make up the material's input neurons. The quantity of dye deposited serves as the output neuron. Using trial and error, the researchers were able to choose the 25 hidden neurons that best suited the model for the adsorption mechanism. Nevertheless, a three-layered architecture with a 5-25-1 network arrangement was produced as a result. Composite adsorption is difficult to simulate since, in contrast to reactions among the adsorbent and the many adsorbents, operating factors significantly affect the adsorption mechanism. In this regard, multiphase network prediction has been achieved successfully using artificial neural networks (ANN). ANN seems to be more flexible than other traditional processes and has been utilized to anticipate isotherms, kinetic breakthrough curves, and operational efficiencies because it adjusts instantly from empirical observations without imposing assumptions about the thermodynamic framework that impacts the adsorption process [11].

This study looked into how paracetamol adsorbs on activated carbon in both single and binary aqueous environments. At various operational situations, the multicomponent state's antagonism and synergic impacts were demonstrated. For artificial neural network improvement of adsorption capability, independent parameters such as initial concentration,

adsorbent dose, adsorbent particle size, and starting intensity were employed as input data (output data). To find the best ANN, other network architectures and training procedures were also tested.

2. Related Works

In this research, a unique activated carbon with built-in capacities to really remove acetaminophen and ketoprofen from fluids was created using the endocarp of the *Butia capitata* species as a precursor material. The activated carbon showed a mostly microporous structure with a median pore diameter of 1.23 nanometer, a considerable pore capacities of $0.449\text{ cm}^3\text{ g}^{-1}$, and a significant particular contact region of $820\text{ m}^2/\text{g}$. In accordance with the adsorption kinetics of both medications, the combination reached equilibrium after 120 minutes for ketoprofen and 170 minutes for acetaminophen. The best matches for the substance were provided by the Elovich concept and the pseudo-second-order framework, correspondingly. According to the findings from the adsorption equilibrium, the maximal adsorption capacities for the drugs ketoprofen and paracetamol were determined to be 108.79 mg g^{-1} and 100.60 mg g^{-1} , correspondingly. The Freundlich and Langmuir theories, in turn, offered the most appropriate statistical adjustments for the adsorption of ketoprofen and paracetamol, respectively. The Langmuir isotherm is used for monolayer adsorption on homogeneous surfaces, while the Freundlich isotherm suites are used for multilayer adsorption on heterogeneous sites. The thermal study verified that the processes for given parameter were exothermic and endothermic, respectively. The results of the recycling tests showed that the average reduction for elimination proportion for ketoprofen and paracetamol for the adsorbent was only 1.88% and 1.57%, respectively. According to cost estimates, the cost of 1 kilogram of activated carbon is 2.39 USD at the very least. Finally, the substance demonstrated extremely effective adsorptive action, removing 84.82% of a synthetic combination combining various salts and medicinal chemicals [12].

Concomitant adsorption of medicinal drugs is difficult to achieve for the purpose of water and wastewater treatment in a practical setting. Activated carbon was utilized in this examination in the role of an adsorbent so that researchers could look into the possibility of paracetamol and nimesulide being adsorbed at the same time. The findings of the study demonstrated that CSH can serve as a reliable, cost-effective, and environmentally friendly feedstock for the production of AC, which can then be utilized for the effective removal of paracetamol from an aqueous environment. In order to assess the variations in adsorption behavior, single adsorption tests were also carried out. For example, nimesulide (196.32 mg g^{-1}) has a larger single adsorption capacity in AC than paracetamol (58.21 mg g^{-1}). It is worth noting that nimesulide atoms were adsorbed into active sites that had earlier been inhabited by paracetamol particles during binary adsorption. This displacement effect, caused by the competing of drug molecules at increasing drug dosages, severely inhibited the adsorption of paracetamol on AC while promoting the adsorption of nimesulide. Since nimesulide is more hydrophobic than paracetamol ($\log K_{ow} =$

0.49), the AC and nimesulide have a stronger attraction for one another. In addition, it seemed from Fourier transform spectra taken both prior to and after adsorption that nimesulide was adsorbed by H bonding, whereas paracetamol was adsorbed by different hydrogen bonding and other dispersion connections. The single equilibrium isotherm models for both medicines were transformed by the Langmuir equation. To forecast the binary adsorption of paracetamol and nimesulide on AC, the expanded Langmuir model was employed. Finally, exothermic, advantageous, impulsive adsorption with lower adsorption vitalities that favoured physisorption was predicted by the dynamic simulation [13].

Due to their minuscule size, pharmaceuticals in wastewater are quickly evolving into new emergent contaminants that threaten both humans and the aquatic ecology. Due to its low affordability, adaptability, and recyclability, adsorption is proving to be a viable method for the extraction of pharmaceuticals from untreated wastewater. Adsorbents are porous substances that are frequently employed to eliminate medicinal contaminants via adsorption. Examples of adsorbents include silicon, kaolin, resinous, and carbon-based substances including charcoal, carbon nanotubes, and activated carbon. Among these, biochar is a newly developed, economical, and environmentally beneficial sorbent. Although modelling techniques like multilinear regressions and linear correlativity are frequently used to describe the adsorption behavior, they are only somewhat accurate and applicable. On the other hand, machine learning techniques are a potent tool that might be utilized to investigate the intricate connection among adsorption capacities and biochar characteristics. This paper offers a summary of current achievements in the study of drug adsorption onto biochar using machine learning techniques. An overview to various ML techniques is given, along with information on their benefits and drawbacks. The difficulties and potential outcomes of applying machine learning to the investigation of the adsorption mechanism are also discussed. In order to evaluate the elimination of medical products from wastewater utilizing charcoal or carbon black, the approach on assessing the potential of machine learning methods was developed by [1].

A category of porous carbons formed from biomass waste was created in recent years as an outcome of the creation of sophisticated materials. These carbons are employed for carbon capture and environmentally friendly waste treatment. Studying the adsorption process of carbon dioxide into the atmosphere is challenging due to the wide variety of characteristics it possesses due to its various textures, functional group existence, pressure, and temperature ranges. These characteristics have a variety of effects on the adsorption of carbon dioxide and provide significant difficulties in the procedure. To meet this numerous goal requirement, researchers use a machine learning forecasting models, carefully modelling the carbon dioxide absorption as a consequence of constituent and texturing aspects as well as adsorbed factors. The ML classification assists in the classification of various porous carbon materials throughout testing and validation. The results of the simulation show that the suggested method is more effective to previous methods for classifying the general porous nature of carbon

dioxide-adsorbed compounds. Therefore, Soft Computing Methods for Predicting Carbon Residue in Biomass Wastes [14]. With the development of nanotech, researchers are witnessing a shift in the global economy and deep infiltration of synthetic chemicals ranging from essentials to cutting-edge electronics, healthcare, and pharmaceuticals. Nanoproducts should be closely controlled to prevent undesirable consequences as they may produce undesirable adverse effects. The shortcomings of conventional safety assessment techniques are highlighted by the toxicological and safety measures that would arise in relation to the rapid integration of nanoparticles with various functions and properties into consumer items. The simulations and modelling of nanobio relations are presently expected to benefit from artificial intelligence and machine learning algorithms, and this extends to the postmarketing monitoring of nanotechnology in the actual life. In order to gain unique insights on the perturbations of sensitive bioactivities following integration with nanoparticles, ML could be combined with biology and nanoparticles. The possibility of integrating integrative omics with learning algorithms in assessing nanoparticles security and threats evaluation is discussed in this paper, along with the advice for regulatory bodies. As a result, omics with computational integration were used to evaluate the danger and toxicity of nanoparticles [4].

The computation complexity of using molecular computation for adsorbent screening makes it impractical for the new material development. Techniques for machine learning (ML) that have been trained on the essential characteristics of a material may be able to offer fast and accurate testing techniques. Prior work concentrated on developing structural characteristics for machine learning. In this work, architectural properties and the usage of pharmacological descriptions for adsorption evaluation were combined. To forecast methane ingestion on fictitious metal organic architectures, assessments of the structural and chemical characteristics along with different ML methods, such as decision tree, support vector machine, Poisson's regression, and random forest, were conducted. Machine learning models were compared on the residual 92% of the given database, which included 130,398 MOFs, after being trained on 8% of it to demonstrate their predictive power. With an R^2 of 0.98 as well as a mean absolute percentage inaccuracy of about 7%, the random forest technique with cross validation of tenfold beats the other ML techniques if both mechanical and chemical parameters were used as inputs. On a single personal computer, the training and forecasting employing random forest approach for estimating the adsorption capacity of all 130,398 MOFs took about 2 hours, which is a considerable amount faster than actual chemical computations on powerful computational complexes. As a result, the metal organic framework (MOF) methane adsorption efficiency forecast method using machine learning utilizing combined structural and chemical descriptors was developed by [15].

3. Methodology

3.1. Absorbates. Dermapele offered paracetamol ($C_8H_9NO_2$) in high purity (99%). To make work preparations, specific

TABLE 1: Paracetamol molecular characteristic.

Property	Paracetamol	
	Pore volume ($cm^3 \cdot g^{-1}$)	Average pore size (nanometer)
Size of particle		
150	0.205	3.635
300	0.163	3.639
500	0.158	3.654
850	0.145	3.622

quantities of each pharmaceutical ingredient were dissolved in deionized saline and ethyl alcohol (10% v/v). To adequately depict medicinal pollutants, ethyl alcohol was employed. Table 1 lists the molecular weight, acid dissociation logarithmic constants, and octanol/water partitioning ratios of every synthesized medication in addition to the three-dimensional chemical equation. Labor fluids were created using distilled water. Add both ethanol and water to enhance absorption. Analytical grade chemicals were the remaining ones.

3.2. Activated Carbon Nanomaterial Preparation. The precursor material chosen for activated carbon manufacture is determined by numerous variables, such as accessibility, hazardous and nonhazardous character, and manufacturing costs. Many investigations have found that composites with a high fixed carbon content and low ash content have superior structural and textural properties. Because of their high carbon content, plant-based substances have become widely used in the synthesis of activated carbon. Various parts of this plant have indeed been employed in various dimensions and manufacturing procedures, including the core, seed, flowers, branches, peels, fruits, shells, leaves, husks, and stones. Activated carbon from date beads was generated by pyrolysis at 300 degrees Celsius for 3 hours and tested for lead nitrate adsorption from aqueous systems, yielding an adsorption ability of 76.8 mg/g. Carbonization is typically employed prior to activation chosen antecedent substance, in which it endures a thermal treatment called as pyrolysis to enhance carbon content. Moisture and low molecule weight aromatics, light flavorings, and ultimately H_2 gas are released during the catalytic pyrolysis, producing a fixed carbonaceous framework [16]. The majority of the pores in the pyrolyzed carbonaceous substances are filled by tarry chemicals, which results in the substances having a low porosity. Tarry oxidation products are the name given to the byproducts that are created when nitric acid reacts with aniline in an oxidation reaction. As a result, an activation step is necessary to generate the nanocarbon's unique properties. According to studies, the choice of carbonization variables, particularly temperatures, heating duration, and dwelling duration, has a considerable impact on the permeability and adsorption efficiency of the finished piece. Thermal treatment processing has been utilized to transform the precursor material's saccharides into graphite discs with low particular surface region. Carbon materials generated in this manner need not milling prior to activated processing and often have a minimal ash concentration. Subsequent

physical, chemical, or physicochemical procedures are required to activate the carbonaceous material and enhance the amount of functional containing oxygen on the interfaces of the activated charcoal. Figure 2 summarizes the biomass transformation into activated carbon [17].

The activated carbons were produced from lignocellulosic materials in four phases. The approach is as follows: (i) Hempseed oil slurry and activation reagent concentrations (K_2CO_3 or KOH) were combined for 24 hours at 1000 rpm continual agitation. (ii) To produce the impregnated material, this solution was heated at $110^\circ C$ for 24 hours. (iii) The impregnated material was placed in a stainless rigid bed furnace with a 6 cm diameter and a 21 cm height. The impregnated material was pyrolyzed for 1 hour at temperatures of 600 and $800^\circ C$ with a nitrogen flow rate of 30 mL min^{-1} and a heating time of $5^\circ C \text{ min}^{-1}$. (iv) The carbonized sample was then rinsed multiple times using hot distilled water and then with cold distilled water until the pH of the filtrate reached neutral. To produce the activated carbons, the cleaned materials were heated at 110 degrees Celsius for 24 hours. Following that, the activated carbons were cooked in a hydrogen chloride solution on reflux to remove the contaminants and decrease the ash content of the activated carbons. They were again rinsed numerous times in hot distilled water and lastly with distilled cold water till no contaminants were identified. To produce the activated carbons, the rinsed particles were dried at 110 degrees Celsius for one day [18].

Biochars produced from soybean oil cake without chemical activation were identified as BC1 and BC2, correspondingly. SAC1 and SAC2 are the activated carbons generated through chemical treatment with K_2CO_3 at 600 and 800 degrees Celsius, correspondingly. SAC3 and SAC4 are the activated carbons generated through chemical treatment with KOH at 600 and 800 degrees Celsius, respectively.

The empirical procreation ratio was calculated using the following equation:

$$\text{Procreation ratio} = \frac{(\text{wt of sample after procreation}) - (\text{wt of waste biomass})}{\text{wt of waste biomass}} \quad (1)$$

In Equation (1), the procreation (impregnation) ratio is estimated by taking the difference of weight of impregnation and weight of waste biomass by weight of waste biomass in which "wt" denotes the weight.

The amount of activated carbon was calculated using the following equation:

$$\text{Yield} = \frac{\text{wt of activated carbon}}{\text{wt of waste biomass}} \times 100. \quad (2)$$

Using a surface analyzer and nitrogen gas adsorption, the precise surface areas of activated carbons made from soybean oil cake were determined (at 77 K). Novawin 2 software was used to compile data, and the t-plot method was employed to determine micropore volume. The micropo-

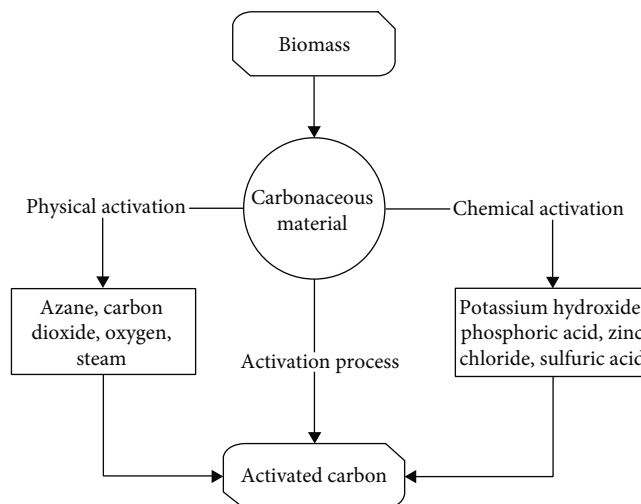


FIGURE 2: Carbon activation technique.

rous volumes and specific surface area of a sample can be calculated using the well-known t-plot approach by comparing the adsorption isotherm of the test to that of a benchmark nonporous material that has the exact surface chemistry.

Superficial function classes of AC were detected utilizing Fourier spectra taken on a spectroscopy with 32 scans and a sensitivity of 4 cm^{-1} inside the region 5000 to 500 cm^{-1} , after the substance had been dispersed in potassium bromide. X-ray diffraction (XRD) utilizing copper-K monochromatic light in the 5° to 100° range confirmed the crystalline structures of AC. The primary application of the fast analytical technique known as X-ray powder diffraction (XRD) determines the phase of a crystalline material, and this approach can also reveal information on the unit cell dimensions. The outer layer and textural properties of AC were determined utilizing nitrogen gas adsorption behavior at 77 K done in a volumetric adsorption analyzer utilizing the Brunauer-Emmett-Teller and Barrett-Joyner-Halenda methods. The surface morphology was acquired using a scanning electron microscope after the samples were earlier metalized with gold. At varying pH value, the determination of point of zero charge is processed utilizing the adsorbent agent at the quantity of $1 \text{ gram} \cdot \text{L}^{-1}$ combined at 150 rpm and 298 Kelvin for one day. Using the Boehm titration, the oxygenated function groups of the adsorbent surface were generated with combination of adsorbent 1 g combined with 50 mL of hydrochloric acid, sodium hydroxide and sodium hydrogen carbonate with 0.1 molarity and sodium carbonate with 0.05 molarity.

3.3. Adsorbent Chemical Modification. 50 g of the previously prepared dry material was weighted with an analytical balance and moved to a glass vial. 600 cm^3 of 0.3 mol/dm^3 orthophosphoric acid was applied to the glass specimen; it was well stirred with a stirrer and cooked on a medium heat till the slush in the form of paste was created. Then, it was placed in a crucible. The material was therefore moved to a desiccator, which has been inserted in an oven that was heated to $500^\circ C$ for one hour, until charcoal emerged. The

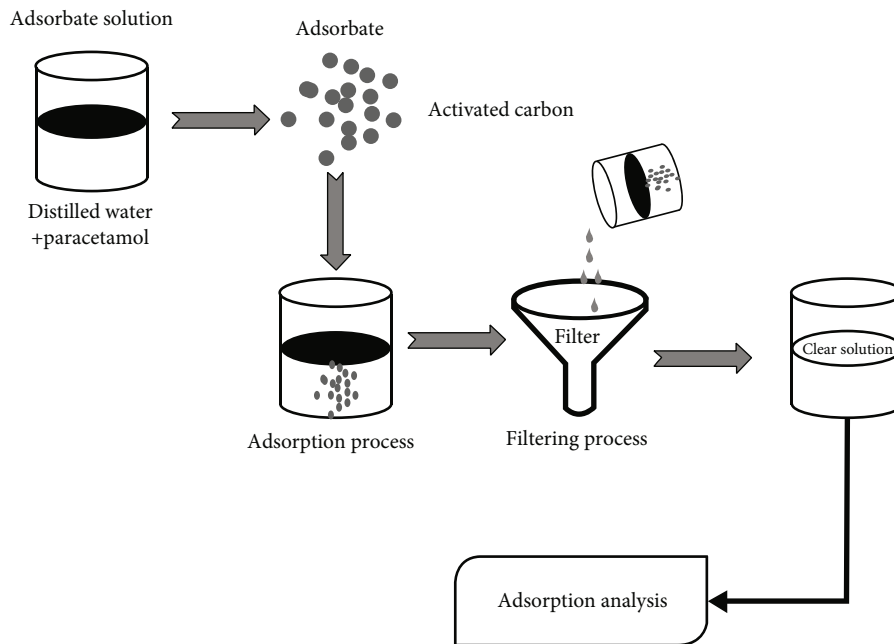


FIGURE 3: Adsorption process.

resulting charcoal was allowed to cool at room heating rate before being rinsed multiple times using distilled water till it reached a neutral pH. The cleaned charcoal was stored in an oven at 1050 degrees Celsius for four hours until it reached a consistent weight. After that, the charcoal was stored in an impermeable vessel for description and further adsorption investigations [19].

3.4. Adsorbate Solution Preparation. Adsorption is a surface phenomenon that affects only the adsorbent surface, and adsorbate must not enter the adsorbent's core. The adsorption process is depicted in Figure 3.

One gram of PCM was dissolved in one liter of filtered water to make a solution containing. To produce workable solution with concentrations of 10, 20, 30, 40, and 50 milligrams per liter, serial dilutions were performed. Because porous carbon materials are accessible in polar solvents, the experimental solutions were created with filtered water. A constant amount of adsorbent (0.1 g) was introduced to a series of 250 milliliter Erlenmeyer vials holding 100 milliliter of porous carbon material liquid with varying starting levels. The vials were shaken in an adiabatic liquid bath mixer at 200 revolutions per minute and at distinct temperature (30, 40, and 50 degree Celsius) until equilibrium was established. To measure the residual percentages, standard solutions were drained at periodically with a microfilter needle until homeostasis was attained. To avoid the interference of carbon particles, the solution was strained before examination. The test was permitted to continue until it achieved equilibrium [20].

At 298 Kelvin and 150 rpm, adsorption studies were carried out in a thermostat agitation. Activated carbon C with varying particle sizes between 15 and 800 μm and doses around 0.5 to 2.0 grams per liter was employed to neutralize paracetamol at a starting quantity of 0.1 $\text{mmol}\cdot\text{L}^{-1}$ and at the

acidity level of 8. The samples were extracted at predefined intervals of 5 min, 1 hour, 2 hours, and 5 hours; the stationary material was filtered out. The residual proportion in the liquid phase was determined using spectrophotometry at paracetamol's maximum wavelength ($\mu_{\text{max}} = 244 \text{ nm}$). All procedures were conducted out in triplicate ($x = 3$), and void checks were performed to ensure data repeatability and reliability. The standard deviation was no more than 3%. Equation (3) was used to compute the concentrations of paracetamol in the binary system. Lastly, Equation (5) was used to calculate the adsorption capability of each medicinal component (y):

$$C_U = \frac{k_{U2}Ug_1 - k_{U1}Ug_2}{k_{U2} - k_{U1}}, \quad (3)$$

where k_{U2} and k_{U1} are the paracetamol's calibrating variables (B) at 393 nm (1) and 244 nm (2) wavelengths, correspondingly, and Ug_1 and Ug_2 are the comparable acetaminophen absorbency readings.

Equation (4) could be employed to calculate the quantity of adsorbed compound at optimized conditions, which corresponds to the adsorption capacity, Q_a and Q_b , which is the proportion of adsorbed component at random period b :

$$Q_a = \frac{(C_x - C_y) \cdot V_l}{W_t}, \quad (4)$$

$$Q_b = \frac{(C_x - C_b) \cdot V_l}{W_t}, \quad (5)$$

where C_x , C_y , and C_b (mg/L) are the adsorbate contents at the start, time b , and equilibrium, accordingly, V_l is the volume of solution (L), and W_t is the adsorbent weight (g).

3.5. Artificial Neural Network. In order to mimic the empirical findings in an effort to forecast the extraction efficiency of PCM using a neural network classifier, a feed-forward backpropagation train approach was selected as the appropriate method to use. It is important to remember that backpropagation (BP) is a feed-forward neural network, which means that it uses error propagation in the opposite way to update the weights of hidden layers. The deviation between actual output and the desired output, as calculated using the gradient descent algorithm, is the error. The research technique in this study was predicated on a component, i.e., one X variable at a period. This has been accomplished by holding the other two factors constant and varying a single input variable. 495 prototype examples were created from experiments conducted in this paper. The information was arbitrarily partitioned between the testing and training sets. 330 real numbers were utilized for training and the remainder for testing. Using Equation (6), the training and testing data were adjusted to decrease error.

$$X_i = \frac{A_i - A_{\min}}{A_{\max} - A_{\min}} \times (v_{\max} - v_{\min}) + v_{\min}, \quad (6)$$

where A_i is an input or output parameter and X_i is the normalized quantity of A_i , while A_{\min} and A_{\max} are the extreme values of A_i . In the research, A_i is adjusted to a ranging restriction defined by v_{\max} and v_{\min} . The input information and output information in this research were standardized among 0 and 1. After modelling, the results were reset to their original value. As illustrated in Figure 4, the experimental information was modelled in a three-layer artificial neural network (the network configuration contains input, hidden, and output layers).

Artificial neural network is commonly employed as a modelling tool to estimate complicated systems that cannot be modelled using traditional modelling techniques. They are commonly employed in categorization, pattern matching, and function approximation. There is no clear method for determining the artificial neural network structure and training procedure in tackling a specific problem. The structure and technique to be used in tackling a certain challenge are chosen through trial and error. This choice may, nevertheless, begin with a simple communication network and progress to a complicated network until an adequate compromise with tolerable minimum error is obtained. There are various network topologies in artificial neural network modelling [21]. The basic design is an MLP feed-forward neural network that uses a backpropagation training technique to train input data. If there is difference in the sequence of stages in the organization, the quantity of neurons within each layer, and/or transmission ratios at the source and destination nodes, there may be variability in the design. In this research, a three-layer ANN was developed, with an input layer (independent factor) having three synapses (interaction duration, operating temperature, and early dosage), a hidden units including seventeen neurons, and an outcome unit (dependent parameter) containing one neuron as in Figure 4. At the output and hidden layers

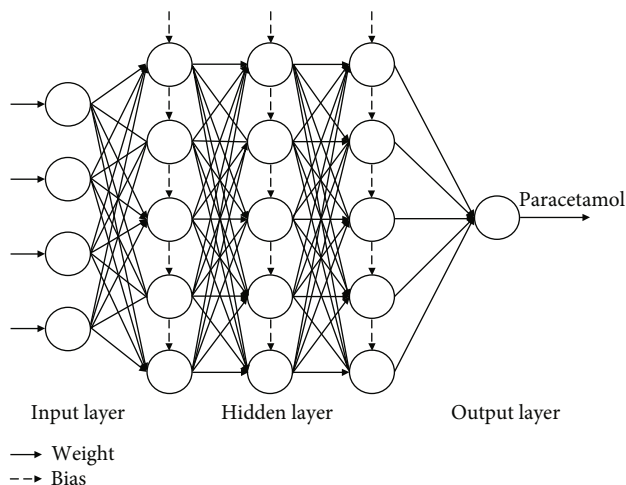


FIGURE 4: ANN processing.

of the neural system, a linear and nonlinear activation function was utilized in the topology. There were 495 experimental observation instances created. The database was randomly partitioned into training (70%) and testing (30%) subdatasets [9].

In order to correctly forecast data, it is crucial to determine how many hidden units and layers to employ in the artificial neural network modelling process. Optimal structures for artificial neural networks were found through exploration of varying numbers of hidden units and layers. The most significant positive Pearson linear correlation coefficient and the smallest mean square error were utilized to pick the best building design. One typical method of assessing linear relationships is the Pearson correlation coefficient (r). A coefficient measures the intensity and direction of a link between two variables and takes on a value between -1 and 1. For any given change in a given variable, there is an inverse and complementary shift in the other variable. Equations (7) and (8) were utilized to calculate the mean square error and the R^2 , respectively:

$$\text{Mean square error} = \frac{1}{N} \sum_{i=1}^N (x_i^{\text{AN}} - x_i^{\text{ex}})^2, \quad (7)$$

$$R^2 = \frac{\sum_{i=1}^N (x_i^{\text{ex}} - \bar{x}_i^{\text{ex}})(x_i^{\text{AN}} - \bar{x}_i^{\text{AN}})}{\sqrt{\sum_{i=1}^N (x_i^{\text{ex}} - \bar{x}_i^{\text{ex}})^2 \sum_{i=1}^N (x_i^{\text{AN}} - \bar{x}_i^{\text{AN}})^2}}, \quad (8)$$

where the normalized x_i^{ex} value is obtained, x_i^{AN} is the ANN prediction, \bar{x}_i^{AN} is the average values, and the quantity of empirical observations is N .

4. Result and Discussion

To determine the primary functional units contained in AC, the FTIR spectra were produced. Figure 5 shows a spectrum with bands about 3431 cm^{-1} , 2912 cm^{-1} , 1634 cm^{-1} , 1570 cm^{-1} , and 1112 cm^{-1} . The wave at 3430 cm^{-1} could be attributed to the bending frequencies of OH from $\text{C}_6\text{H}_6\text{O}$, $\text{C}_2\text{H}_2\text{O}$, and

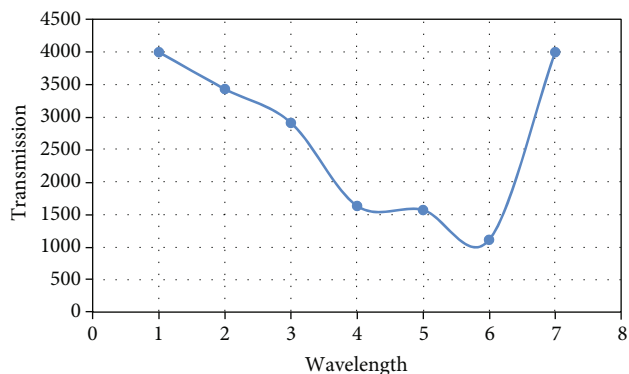


FIGURE 5: Activated carbon spectrum.

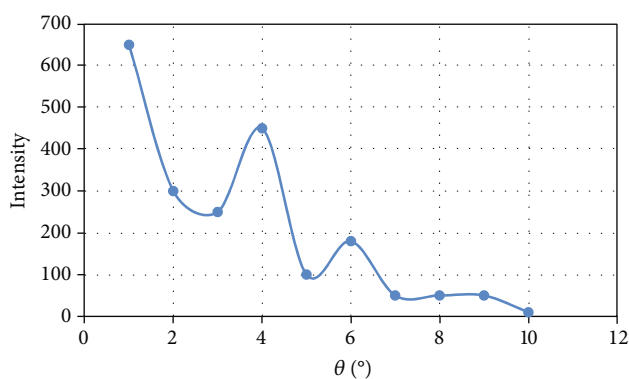


FIGURE 6: Diffraction pattern.

R-COOH existing as functional units of the activated carbon, or it could be explained by the occurrence of aquatic adsorption in the adsorbent. The bond found about 2912 cm^{-1} might be attributed to CH_2 and C-H asymmetrical stretching vibrations. The C=O asymmetric stretching vibrations of R-COOH are responsible for the wave at 1634 cm^{-1} . The aromatic ring of the AC structure's C=C stretching vibrations may be verified at 1568 cm^{-1} . Furthermore, the band at 1112 cm^{-1} can be attributable to hydroxyl CO bending vibration in $\text{C}_6\text{H}_6\text{O}$, $\text{C}_2\text{H}_2\text{O}$, and R-COOH.

Figure 6 depicts the diffraction patterns generated for AC. A very broad reflect similar to the reflect may be seen, with the peak location approximately $4 = 26^\circ$. Additionally, a reduced broad peak with an absorption peak of around $2 = 42^\circ$ was found to fit the planes. Figure 6 depicts an ordinary diffraction signal with disordered carbon network, demonstrating that activated carbon is crystalline. An oxidized form is often sufficient for adsorption applications because it contains more vacant spaces that enable medicinal compounds to enter the adsorbent.

0.1 gram of chemically modified orange peel was agitated with 150 mL of porous carbon material solution at various dosages between 15 milligrams per liter and 55 milligrams per liter during the research of the control of paracetamol adsorption on CMOP. The proportion of paracetamol removed in interaction with the improved adsorbent increased steadily in analyzed batch adsorption. The rise in proportion went from 56.66% at 10 milligrams per liter to

TABLE 2: Adsorption efficiency at 35 mg/L.

Period (seconds)	Performance	AN forecasting
240	80.15	4.74
600	83.58	77.58
1500	91.46	96.33
2400	98.97	96.58
3600	98.97	96.75
5400	98.97	96.99
7200	98.97	97.14
9900	98.97	97.29
12600	98.97	99.84
15300	98.97	99.97
18000	98.97	91.25

TABLE 3: Adsorption efficiency at 45 mg/L.

Period (seconds)	Performance	AN forecasting
240	89.93	0
600	92.34	69.14
1500	93.12	97.64
2400	93.22	97.70
3600	95.19	98.88
5400	95.46	99.94
7200	96.94	99.92
9900	99.36	97.71
12600	99.36	97.73
15300	99.36	98.96
18000	99.36	98.96

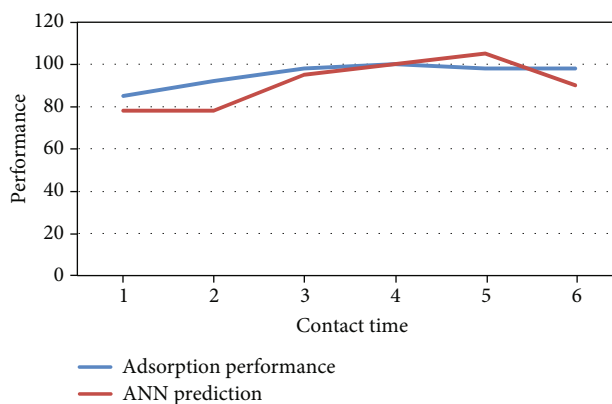


FIGURE 7: Adsorption performance at 15 mg/L.

99.36% at 45 milligrams per liter. At 55 milligrams per liter, there was a small drop to 98.5%. This may be owing to the adsorbent's accessible unoccupied pores leading in adsorption at lower amounts, as opposed to higher doses where adsorption might be determined by the amount of adsorbate diffusion along the adsorbent. The adsorption mechanism reached a steady as quickly as half an hour of adsorbate-adsorbent interaction at doses ranging from 10 to 30 mg/L, with the greatest inhibition efficiency at 35 mg/L and a

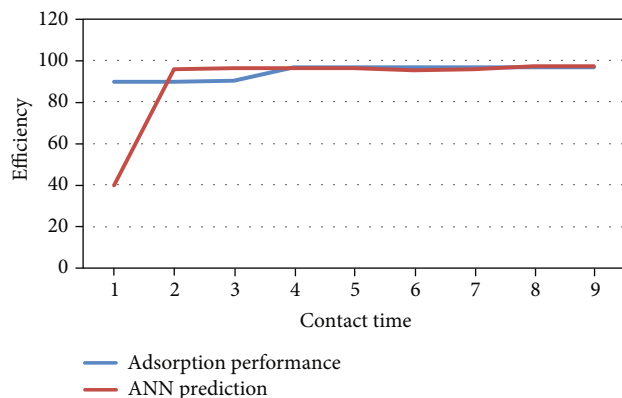


FIGURE 8: Adsorption performance at 45 mg/L.

reasonably stable removal number at all of these concentrations after the optimized conditions.

The adsorption mechanism, however, reaches homeostasis at 3 hours for porous carbon material concentrations of 40 mg/L with 99.35% clearance. With adsorption performance as a top concern, 40 milligrams per liter was determined to be the best dosage for the adsorption mechanism. Given the cost-effectiveness, 30 milligrams per liter was chosen as the appropriate dosage for the adsorption mechanism since it reached a steady in half an hour, implying that a lower temperature would be needed for the adsorption mechanism, as shown in Tables 2 and 3. The link among the testing outcome and the projected ANN result is depicted in Figures 7 and 8.

5. Conclusion

A large majority of current research studies have shown a considerable improvement in the adsorption process of all altered activated carbons when compared to nonmodified, suggesting a tremendous promise for transformed activated carbon in eliminating heavy metals in the industry. Activated carbon has evolved from an intriguing alternative antecedent to a strong particular configuration, with cost-effectiveness and industrialization in consideration. Numerous physiological remodelling approaches for activated carbons have enormous commercial viability. In this research, ANN factors along with hidden neurons, training techniques, and backpropagation were investigated in order to build an ideal ANN structure for predicting adsorption performance. The effects of absorbent particle diameter, adsorbent dosages, and training duration were evaluated on every pharmaceutical reactor core adsorbed efficiency. The optimum adsorption efficiency for acetaminophen was found to be 98 percentage elimination for binary paracetamol adsorption, accordingly. As a consequence, nimesulide particles were linked with acetaminophen molecules throughout binary adsorption to lessen acetaminophen adsorption. As a result, even with the presence of simultaneous and antagonistic relationships, ANN could be utilized to ensure the smooth operation to forecast the adsorption capacity of these medicinal compounds.

Data Availability

The data used to support the findings of this study are included within the article. Further data or information is available from the corresponding author upon request.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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References

- [1] J. A. Okolie, S. Savage, C. C. Ogbaga, and B. Gunes, "Assessing the potential of machine learning methods to study the removal of pharmaceuticals from wastewater using biochar or activated carbon," *Total Environment Research Themes*, vol. 1-2, article 100001, 2022.
- [2] J. L. Speiser, C. J. Karvellas, B. J. Wolf, D. Chung, D. G. Koch, and V. L. Durkalski, "Predicting daily outcomes in acetaminophen-induced acute liver failure patients with machine learning techniques," *Computer Methods and Programs in Biomedicine*, vol. 175, pp. 111–120, 2019.
- [3] A. Spaltro, M. N. Pila, D. D. Colasurdo et al., "Removal of paracetamol from aqueous solution by activated carbon and silica. Experimental and computational study," *Journal of Contaminant Hydrology*, vol. 236, article 103739, 2021.
- [4] F. Ahmad, A. Mahmood, and T. Muhmood, "Machine learning-integrated omics for the risk and safety assessment of nanomaterials," *Biomaterials Science*, vol. 9, no. 5, pp. 1598–1608, 2021.
- [5] M. M. Sabzehmeidani, S. Mahnaee, M. Ghaedi, H. Heidari, and V. A. L. Roy, "Carbon based materials: a review of adsorbents for inorganic and organic compounds," *Materials Advances*, vol. 2, no. 2, pp. 598–627, 2021.
- [6] L. Spessato, K. C. Bedin, A. L. Cazetta et al., "KOH-super activated carbon from biomass waste: insights into the paracetamol adsorption mechanism and thermal regeneration cycles," *Journal of Hazardous Materials*, vol. 371, pp. 499–505, 2019.
- [7] X. C. Nguyen, Q. V. Ly, T. T. H. Nguyen, H. T. T. Ngo, Y. Hu, and Z. Zhang, "Potential application of machine learning for exploring adsorption mechanisms of pharmaceuticals onto biochars," *Chemosphere*, vol. 287, article 132203, Part 2, 2022.
- [8] A. Almuntashiri, A. Hosseinzadeh, U. Badeti et al., "Removal of pharmaceutical compounds from synthetic hydrolysed urine using granular activated carbon: column study and predictive modelling," *Journal of Water Process Engineering*, vol. 45, article 102480, 2022.
- [9] J. L. S. Fagundes and N. P. G. Salau, "Optimization-based artificial neural networks to fit the isotherm models parameters of

- aqueous-phase adsorption systems,” *Environmental Science and Pollution Research*, vol. 29, no. 53, pp. 79798–79807, 2022.
- [10] G. Alam, I. Ihsanullah, M. Naushad, and M. Sillanpää, “Applications of artificial intelligence in water treatment for optimization and automation of adsorption processes: recent advances and prospects,” *Chemical Engineering Journal*, vol. 427, article 130011, 2022.
- [11] W. Guo, J. Liu, F. Dong et al., “Deep learning models for predicting gas adsorption capacity of nanomaterials,” *Nanomaterials*, vol. 12, no. 19, p. 3376, 2022.
- [12] C. M. Kerkhoff, K. . Boit Martinello, D. S. P. Franco et al., “Adsorption of ketoprofen and paracetamol and treatment of a synthetic mixture by novel porous carbon derived from *Butia capitata* endocarp,” *Journal of Molecular Liquids*, vol. 339, article 117184, 2021.
- [13] P. S. Pauletto, S. F. Lütke, G. L. Dotto, and N. P. G. Salau, “Adsorption mechanisms of single and simultaneous removal of pharmaceutical compounds onto activated carbon: isotherm and thermodynamic modeling,” *Journal of Molecular Liquids*, vol. 336, article 116203, 2021.
- [14] P. Verma, J. Godwin Ponsam, R. Shrivastava et al., “Predicting carbon residual in biomass wastes using soft computing techniques,” *Adsorption Science and Technology*, vol. 2022, article 8107196, pp. 1–8, 2022.
- [15] M. Pardakhti, E. Moharreri, D. Wanik, S. L. Suib, and R. Srivastava, “Machine learning using combined structural and chemical descriptors for prediction of methane adsorption performance of metal organic frameworks (MOFs),” *ACS Combinatorial Science*, vol. 19, no. 10, pp. 640–645, 2017.
- [16] A. Abdolali, H. H. Ngo, W. Guo et al., “Characterization of a multi-metal binding biosorbent: chemical modification and desorption studies,” *Bioresource Technology*, vol. 193, pp. 477–487, 2015.
- [17] X.-Y. Huang, X.-Y. Mao, H.-T. Bu, X.-Y. Yu, G.-B. Jiang, and M.-H. Zeng, “Chemical modification of chitosan by tetraethylenepentamine and adsorption study for anionic dye removal,” *Carbohydrate Research*, vol. 346, no. 10, pp. 1232–1240, 2011.
- [18] M. Haroon, L. Wang, H. Yu et al., “Chemical modification of starch and its application as an adsorbent material,” *RSC Advances*, vol. 6, no. 82, pp. 78264–78285, 2016.
- [19] Q. Chen, X. Zheng, L. Zhou, and M. Kang, “Chemical modification of starch microcrystals and their application as an adsorbent for metals in aqueous solutions,” *BioResources*, vol. 14, no. 1, pp. 302–312, 2019.
- [20] D. Schwantes, A. C. Gonçalves, G. F. Coelho et al., “Chemical modifications of cassava peel as adsorbent material for metals ions from wastewater,” *Journal of Chemistry*, vol. 2016, Article ID 3694174, 15 pages, 2016.
- [21] P. S. Pauletto, S. F. Lütke, G. L. Dotto, and N. P. G. Salau, “Forecasting the multicomponent adsorption of nimesulide and paracetamol through artificial neural network,” *Chemical Engineering Journal*, vol. 412, article 127527, 2021.