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Experimental Study and Theoretical Modelling Based on DFT of the Elimination of Ceftriaxone by an Activated Carbon Synthesized from Grape Seeds Waste

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EXPERIMENTAL STUDY AND THEORETICAL MODELLING BASED ON DFT OF THE ELIMINATION OF CEFTRIAXONE BY AN ACTIVATED CARBON SYNTHESIZED FROM GRAPE SEEDS WASTE

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An activated carbon (AC) developed from grape seeds waste was characterized using various physico-chemical techniques to assess its structural and textural properties, then used for the removal of ceftriaxone (CFTX), an emerging pollutant, from aqueous solutions. Batch adsorption experiments were conducted, coupled with a theoretical study based on DFT (density functional theory) study, performed at the B3LYP level with a 6-311G (d,p) base, in order to study molecular geometries, electronic properties and molecular electrostatic potentials, to clarify the adsorption mechanism of CFTX on AC. The results revealed that the prepared AC had a well-established porosity offering a large exchange surface. Adsorption studies revealed that kinetic data aligned well with the PSO model, while equilibrium data were best described by the Freundlich isotherm and the multilayer STAT1 model. Thermodynamic analysis indicated endothermal and favorable adsorption, mainly controlled by chemical interactions. Moreover, the regeneration studies showed the difficult desorption of CFTX, supporting a chemisorption mechanism. The results of DFT calculations indicated that the adsorption of CFTX is favorable on AC functionalized with $-CHO$ and $-COOH-OH-CHO$, with adsorption energies of $-13.07 \text{ kcal mol}^{-1}$ and $-4.47 \text{ kcal mol}^{-1}$, respectively. AIM (atoms in molecules), NCI (non-covalent interactions) and RDG (reduced density gradient) analyses revealed that strong hydrogen-bond interactions mainly govern the adsorption mechanism. According to the obtained results, the produced AC is considered as a high-performance alternative material for the removal of CFTX from aqueous environments. In addition, a thorough understanding of the adsorption process resulted from integrating theoretical and experimental approaches.

Keywords Activated carbon, Adsorption, Ceftriaxone, DFT

In recent years, population growth and accelerated industrialization have led the emergence of new types of pollutants. These emerging contaminants are an environmental and health concern¹. Among them, drug residues, especially antibiotics, are of increasing disquiet related to their persistence in the natural environments, their ability to bioaccumulate in living organisms and their resistance to biodegradation. Antibiotics used in human² and veterinary³ medicine have recently been founded in different aquatic environments, such as wastewater, surface water, groundwater and sometimes even in drinking water. This is mainly due to human and animal excretions, discharges from the pharmaceutical industries and hospitals, as well as runoff from agricultural activities⁴. Even at low concentrations, their presence represents a significant risk, particularly for global public health through the spread of infections that are difficult to treat^{5,6}.

Ceftriaxone (CFTX), a third-generation cephalosporin antibiotic, is one of the most widely used antimicrobial agents worldwide, thanks to its broad efficacy against several types of bacterial infections, including those affecting the respiratory and urinary tract⁷. Despite its clinical efficacy combined with its relatively low cost, its extensive use leads to worrying environmental impacts⁸. Recently, studies have shown the detection of CFTX in wastewater treatment plant effluents, at significant concentrations reaching up to $15 \mu\text{g L}^{-1}$ in urban and hospital wastewater, indicating its widespread diffusion and persistence^{9,10}. CFTX is described as an emerging pollutant of concern¹, due to its ability to promote bacterial resistance, which therefore requires effective treatment methods to minimize its impact on ecosystems and public health by reducing their quantity in the aquatic environment¹¹. Due to the ineffectiveness of conventional treatments to completely remove antibiotics or other drugs from wastewater⁸, various sophisticated purification technologies have been developed, namely ultrafiltration¹², advanced oxidation processes (AOP)¹³, adsorption¹⁴, and biodegradation¹¹.

However, these techniques have certain environmental and economic drawbacks, such as the generation of secondary pollutants, high cost and complexity of use¹⁵. Adsorption stands out among these techniques as a promotional method due to its simplicity of implementation, low operation cost, and its ability to effectively remove a wide variety of contaminants, including drugs, dyes, or even complex organic compounds¹⁶, from an aquatic environment¹⁷.

Activated carbon (AC) is a highly efficient adsorbent widely employed in the purification and treatment of water and air by adsorption of various pollutants¹⁸. Its adsorption properties, such as well-developed porosity, a high specific surface area and strong adsorption capacity, enable it to can be recognized as high-performance adsorbent material, suitable for the elimination of different types of contaminants¹⁷. In addition, several studies have shown that AC can be modified or functionalized to improve its effectiveness in removing various organic and inorganic contaminants¹⁹.

However, the elevated cost of commercially available ACs, often derived from renewable raw materials, emphasizes the necessity of exploring alternative sustainable and low-cost alternatives for the production of ACs. Recently, many attempts have been made to study the use of agricultural waste and renewable biomass as precursors for AC synthesis²⁰. Among these unconventional sources, grape seeds, an abundant by-product of the wine industry, have attracted considerable attention because of their abundance, accessibility, and high carbon composition²¹. The production of AC from agro-industrial wastes, including lotus stalks²², wood and fishing kernels²³, coconut shells²⁴, pomegranate wood²⁵, and clusters of empty palm fruits¹⁵, is a potentially attractive production route from an economic and environmental point of view. These wastes also constitute promoters for the production of AC due to their abundance and effectiveness in removing various pharmaceutical contaminants from water²⁶.

Several studies have demonstrated the effectiveness of AC derived from waste as a high-performance adsorbent for the elimination of pharmaceutical products present in water. In a study by Grisales-Cifuentes, Claudia et al.²⁷ studied the adsorption of acetaminophen using activated carbon from palm oil, with an elimination efficiency reaching 7.3 mg g⁻¹. In another study, Bagheri, Afrouz, et al.²⁸ explored the elimination of ketoprofen by activated carbon derived from nutshell, obtaining an elimination capacity of 444 mg g⁻¹. Chen, Yue, et al.²⁹ developed activated carbon from corn cobs

for the adsorption of levofloxacin from water, with a removal efficiency of 56.6 mg g⁻¹. In another study by Chen, Jiaqi, et al.³⁰ adsorbents derived from lotus leaves were used to remove norfloxacin, the result shows an elimination efficiency reaching 91.7 mg g⁻¹.

The chemical composition, structural properties of the AC material³¹, physicochemical characteristics of the adsorbed molecules, and the nature of molecular interactions formed with the surface of the adsorbent³², have a major impact on the adsorption mechanism and capacity. In this context, the evaluation of adsorption mechanisms uses advanced quantum chemistry methods. These approaches are particularly effective for analyzing interactions at the molecular level³³. In recent years, simulations relying on density functional theory (DFT) have been studied to investigate intermolecular interactions and their effects on molecular properties. These simulations provide precise information on molecular configurations, adsorption sites and also the energies of the bonds formed^{34,35}. Understanding the adsorption of CFTX on AC from examining the impact of various function groups exists on the AC surface is the objective of this study. Theoretical calculations based on (DFT) applying the B3LYP approach coupled to the 6-311G (d, p) basis set were used to study the interactions formed between CFTX in these functional groups by estimating the adsorption energies, while determining the most stable molecular configurations.

This study mainly introduces two key novelties. First, it presents the development of AC derived from grape seeds, a new and sustainable biomaterial for the elimination of CFTX in water, thus contributing to green chemistry and waste valorization. Secondly, this research combines the experimental analysis of adsorption with density functional theory (DFT) based modeling, offering a theoretical framework for a thorough understanding of the adsorption mechanisms of CFTX on functionalized activated carbon surfaces. This dual approach is relatively unexplored in the context of CFTX adsorption, providing new insights into interactions at the molecular level.

Considering the above, this study focuses on the evaluation of CFTX removal, by the use of AC produced from grape seed waste, present in aqueous solution. The structural and textural proprieties of the developed adsorbents were determined using various analytical methods. An equilibrium, kinetic and thermodynamic study was performed in order to examine the adsorption process. A desorption study was executed to evaluate

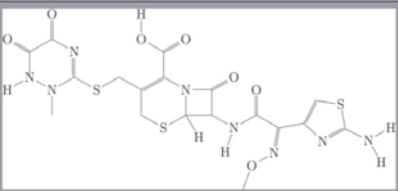
the regeneration of these materials. In addition to the experimental tests, quantum chemistry calculations based on DFT were conducted. This combination of experimental and theoretical approaches not only validates the results obtained but also allows for a better understanding of the retention mechanisms.

Materials and methods

Materials

Grape seeds waste from the AGRILAND® agro-food industry, based in Mitbasta, Kairouan, Tunisia, were employed as the raw material for AC production. Phosphoric acid H_3PO_4 (85% (W)) was used as the chemical activation agent. Ceftriaxone (CFTX), an injectable solution with a purity of more than 97% (UNIMED®), was selected for the adsorption experiments. The characteristics and chemical structure of CFTX are shown in Table 1³⁶.

Table 1. CFTX characteristics and chemical structure.

	
Structure	
Chemical formula	$C_{18}H_{18}N_8O_7S_3$
Molecular weight (g mol ⁻¹)	554.6
Water solubility (g L ⁻¹)	0.105
pK _a	3, 3.2 and 4.1

TEST NO	Settings			Answers	
	X ₁ Impregnation rate	X ₂ Temperature (°C)	X ₃ Time (min)	Y ₁ Iodine Index II ₂ (mg g ⁻¹)	Y ₂ Methylene blue index MBI (mg g ⁻¹)
1	1.5	600	120	467.01	0.60
2	1.5	400	180	614.22	0.23
3	2	400	120	583.76	0.28
4	1.5	400	60	578.68	0.24
5	1	400	120	609.14	1.20
6	1	600	60	558.38	0.51
7	2	600	60	573.61	0.81
8	1.5	600	120	548.23	0.57
9	2	600	180	609.14	1.07
10	1.5	600	120	548.23	0.85
11	1.5	800	60	659.90	1.11
12	2	800	120	634.52	1.19
13	1.5	800	180	736.04	1.21
14	1	600	180	507.62	0.47
15	1	800	120	710.66	1.05

Table 2. BBD experimental design matrix with response results.

Activated carbon preparation

Approximately 200 g of grape seeds waste were soaked in a diluted H_3PO_4 solution for 24 h at room temperature. The impregnation was carried out according to different impregnation rates defined as the mass ratio between the activating agent and the precursor, ranging from 1 to 2. The pyrolysis of the impregnated and dried material was then performed in a controlled tubular furnace, under a continuous nitrogen flow (3 L min⁻¹), at temperatures between 400 and 800 °C, for a duration varying from 60 to 180 min. Once cooled, the obtained AC underwent a washing with hot distilled water until neutrality to remove activation agent residues and unwanted impurities. Finally, the material was dried at 100 °C for 4 h.

In this study, the preparation of AC was performed under optimized conditions, namely the impregnation rate (X₁), temperature (X₂, in °C), and pyrolysis time (X₃, in minutes), obtained from the analysis of the experimental results using the Box – Behnken Design (BBD), based on the Response Surface Methodology (RSM). Figure S1 visually illustrates the final optimization diagram resulting from this analysis, indicating the optimal operating conditions for the AC preparation: temperature = 800 °C, time = 180 min and impregnation rate = 2. The iodine index II₂ (Y₁, expressed in mg g⁻¹) and methylene blue index MBI (Y₂, expressed in mg g⁻¹) taken as process responses were maximized. The experimental design was performed using Minitab 20.3 statistical software. The Table 2 presents the experimental design with the corresponding results.

Physical and chemical characterization of AC

In a previous study³⁷, the textural properties of the prepared AC were characterized by analysis of N₂ adsorption/ desorption at 77 K, measured with a surface analyzer (Micromeritics ASAP 2020). The specific surface area was evaluated by the BET method (Brunauer–Emmett–Teller)³⁸. The BJH approach (Barrett–Joyner–Halenda) was used to analyze the pore size distribution³⁹. Scanning electron microscopy (SEM) coupled with energy-dispersive X-ray spectroscopy (SEM–EDX) (Thermo Scientific Apreo S) was employed to analyze the surface morphology and elemental composition of AC. In addition, high-resolution X-ray diffraction (XRD) was used to study the crystal structure of AC.

The analysis of acid and basic functional groups on the AC surface was evaluated by Boehm titration⁴⁰.

1.5 g of AC was mixed with 0.05 M solutions of NaOH, Na₂CO₃, NaHCO₃, and HCl. After stirring for 24 h, the remaining excess acid or base was titrated with NaOH or HCl (0.05 M), respectively. The quantification of functional groups is based on neutralization reactions.

The pH_{pzc} was carried out following the method described by Lopez-Ramon et al.⁴¹. A 0.01 M NaCl solution was mixed with 0.15 g of AC whose initial pH was adjusted to values between 1 and 12. After stirring for 48 h, the change in pH values (ΔpH), was plotted as a function of the initial pH. The pH_{pzc} corresponds to the point where pH_{initial} is equal to pH_{final}.

Adsorption study

The study of CFTX adsorption on AC was carried out by a batch adsorption method. For the experiments, an optimal mass of 0.2 g AC (Fig. S2) was mixed with CFTX solutions of 20 mL volume and at concentrations varying from 4 and 20 mgL⁻¹, at room temperature and constant pH (Fig. S3). All the experiments were performed under constant stirring at 150 rpm, with samples taken at intervals of 3 to 360 min until equilibrium was achieved. The thermodynamic study was conducted between 30 °C and 40 °C, by determining the main parameters, notably the standard Gibbs free energy (ΔG°), standard enthalpy (ΔH°), and entropy (ΔS°). After each experimental run, the residual CFTX concentrations were determined by UV-vis spectrophotometer (CamSpec M501) at 240 nm. The following equations, including removal percentage (Eq. 1)⁴², as well as the retention capacity measured at equilibrium (Eq. 2)⁴², and at any given time in the process (Eq. 3)⁴², were used to determine the amount of CFTX retained by AC:

$$R = (\%) \frac{(ff_0 - ff_e)}{ff_0} \cdot 100 \quad (1)$$

$$q_e \text{ (ffig} \cdot \text{g}^{-1}) = \frac{(C_0 - C_{e,i})}{ff_i} \cdot V \quad (2)$$

$$q_t \text{ (ffig} \cdot \text{g}^{-1}) = \frac{(C_0 - C_{t,i})}{ff_i} \cdot V \quad (3)$$

Thermodynamic (Langmuir, Freundlich, BET_{n-finite}, and BET_{n-infinite}) and statistic (STAT1, STAT2, and STAT3) models were used to adjust the equilibrium isotherm data. Table 3 summarizes the fundamental equations and parameters associated with these models employed to analyze CFTX adsorption on AC. Adsorption kinetic were evaluated using the pseudo-first-order (PFO)⁴³, pseudo-second-order (PSO)⁴⁴, and intraparticle

diffusion⁴⁵ models.

The selection of the best fit for the kinetic and isotherm models was generally performed using the linear correlation coefficient R². However, because of potential bias in the results, the Chi-square (χ²) and sample-adjusted Akaike information criterion (AIC_c) were also used in addition to the correlation coefficients.

The AICc is expressed as follows (Eq. 4)⁴⁶:

$$\text{AICc} = n \ln \left(\frac{\text{SSR}}{n} \right) + 2k + \left(\frac{2k+1}{n-k-1} \right) + n \ln (2\pi) + n \quad (4)$$

n represents the number of data points, k is the number of parameters in the model and SSR refers to the residuals sum of squares, which is also used to calculate R².

The formulation of the Chi-square (χ²) is expressed as follows (Eq. 5)⁴⁷:

$$\chi^2 = \sum_{i=1}^n \frac{(q_{\text{exp},i} - q_{\text{mod},i})^2}{q_{\text{mod},i}} \quad (5)$$

n corresponds to the number of data points used for calculation.

Desorption study

Desorption tests were carried out to evaluate the efficiency of adsorbent recovery. For this purpose, 0.2 g of the adsorbent charged with CFTX, obtained from the isothermal study at different concentrations, was agitated in 20 mL of distilled water. The desorption efficiency (%) was determined using the following equation (Eq. 6)⁵¹:

$$\text{Desorption efficiency} = (\%) \frac{q_{\text{des}}}{q_{\text{ads}}} \cdot 100 \quad (6)$$

q_{des} and q_{ads} represent the quantities of desorbed and adsorbed CFTX (mg g⁻¹), respectively.

DFT modelling

Molecular modeling was performed to study the interactions and chemical reactivity of CFTX during its adsorption onto the AC surface. Optimization of molecular geometries was performed using Density Functional Theory (DFT) with the exchange-correlation function B3LYP, associated with the bases 6-311G (d, p). The B3LYP functional, is commonly used as it offers a favorable compromise between accuracy and computational efficiency, which then allows it to be adapted to a variety of molecular systems⁵². This hybrid functional is a combination between the three-parameter Becke exchange functional and the gradient-

	Expression	Parameter signi>cance	References
=ermodynamic models			
☒Langmuir	$q_e = \frac{q_{\max} k_L C_e}{1 + k_L C_e}$	$q_{\max}$ (mg g ⁻¹): maximum adsorption capacity of CFTX K_L (L mg ⁻¹): Langmuir constant associated with binding energies	48
☒Freundlich	$q_e = k_F C_2^{1/n_F}$	K_F (mg g ⁻¹) (L mg ⁻¹) ^{1/n_F}): Freundlich constant related to the adsorption capacity n_F : degree of surface irregularity	49
$q_e = q_{\max,1} \frac{k_L C_e \left[1 - (n+1)(K_S C_e)^n + n(K_S C_e)^{n+1} \right]}{(1 - K_S C_e) \left[1 + \left(\frac{K_L}{K_S} - 1 \right) K_S C_e - \left(\frac{K_L}{K_S} \right) (K_S C_e)^{n+1} \right]}$ ☒BET _{n;nite}		$q_{\max,1}$ (mg g ⁻¹): maximum adsorption capacity of CFTX on the ;rst layer n : maximum number of adsorbed layers $k_L = \frac{a_1}{b_1} e^{\frac{E_L}{RT}}$ (L mg ⁻¹): adsorption equilibrium constant for the ;rst layer $k_S = \frac{a_2}{b_2} e^{\frac{E_S}{RT}}$ (L mg ⁻¹): adsorption equilibrium constant for the upper layers, where E_L and E_S (J mol ⁻¹): adsorption heat on the ;rst and upper layers a_1 and b_1 : rate constants for adsorption and desorption on the ;rst layer a_2 and b_2 : rate constants for adsorption and desorption on the upper layers	50
☒BET _{n-in>nite}	$q_e = q_{\max,1} \frac{K_L C_e}{(1 - K_S C_e)(1 - K_S C_e + K_L C_e)}$		
Statistic models			

Table 3. Equations and parameter significance for thermodynamic and statistic isotherm models.

	Expression	Parameter significance	References
STAT ₁	$q_e = \frac{q_{\max,1}}{\left[\left(\frac{C_1}{C_e}\right)^m - \left(\frac{C_1}{C_2}\right)^m + 1\right] \left[1 - \left(\frac{C_e}{C_2}\right)^m\right]}$	$q_{\max,1}$ (mg g ⁻¹): maximum adsorption capacity of CFTX on the first layer m , steric parameter where:	50
STAT ₂	$q_e = q_{\max,1} \frac{\left(\frac{C_e}{C_1}\right)^m + 2\left(\frac{C_e}{C_2}\right)^{2m}}{\left[1 + \left(\frac{C_e}{C_1}\right)^m + 2\left(\frac{C_e}{C_2}\right)^m\right]}$		
STAT ₃	$q_e = q_{\max,1} \frac{\left(\frac{C_e}{C_1}\right)^m + 2\left(\frac{C_e}{C_2}\right)^{2m}}{\left[1 + \left(\frac{C_e}{C_1}\right)^m + \left(\frac{C_e}{C_2}\right)^{2m}\right]}$		

corrected Lee–Yang–Parr correlation functional.

The accuracy of calculations, for non-covalent interactions was improved by applying the Grimme D3BJ dispersion correction⁵³. Due to the limitation of standard DFT calculations in describing the various

interactions formed between adsorbate molecules and the adsorbent surface, this correction is important to integrate long-range Van der Waals forces. The influence of solvents was simulated using the CPCM (Conductor-like Polarizable

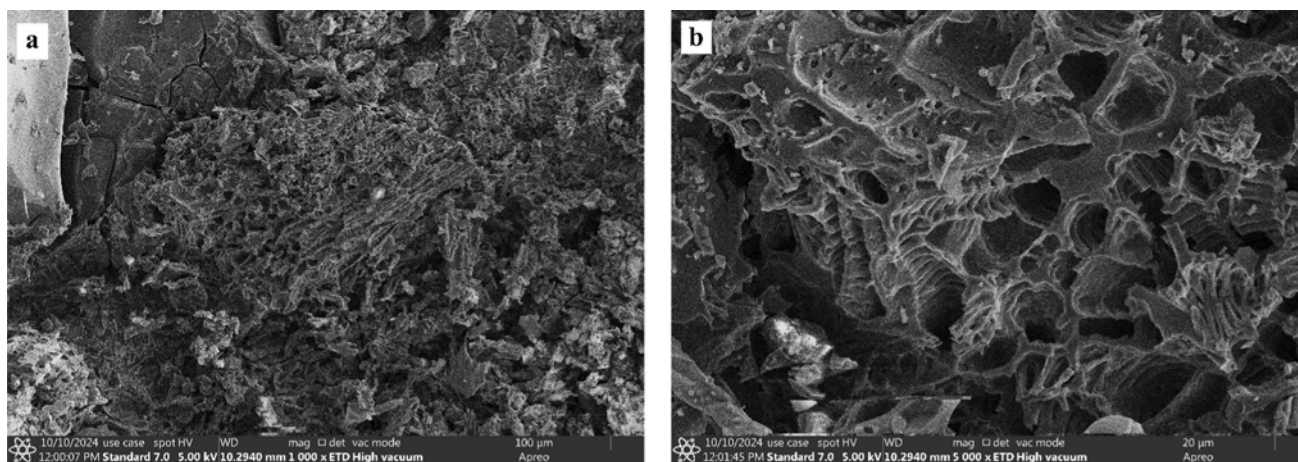


Fig. 1. SEM micrographs of the prepared AC, at magnifications of 1000x (a) and 5000x (b).

Compound	C	O	Mg	Al	Si	P	K	Ca	Fe	Cu
Weight (%)	69.41	19.25	0.52	0.28	0.33	6.71	0.44	2.87	0.10	0.08

Table 4. EDX elemental analysis of prepared AC.

Continuum Model)⁵⁴. The optimized geometries were validated as local minima by the absence of imaginary frequencies in the corresponding Hessian matrices.

To deepen the understanding of the adsorption mechanisms, key quantum chemistry descriptors, such as the highest energy occupied molecular orbital (HOMO, EH) and the lowest unoccupied molecular orbital (LUMO, EL), as well as the energy gap ($E_{\text{gap}} = E_{\text{L}} - E_{\text{H}}$), were analyzed on the basis of DFT calculations. Using the HOMO and LUMO values, some reactivity descriptors for all molecules (adsorbate and adsorbent) were determined, in particular the electron chemical potential (μ), global hardness (η), and electrophilic index (ω) using equations (Eq. 7)⁵⁵, (Eq. 8)⁵⁵ and (Eq. 9)⁵⁵ respectively:

$$\mu = -\frac{E_{\text{L}} + E_{\text{H}}}{2} \quad (7)$$

$$\eta = \frac{E_{\text{L}} - E_{\text{H}}}{2} \quad (8)$$

$$\chi = \frac{\mu^2}{2\eta} \quad (9)$$

The adsorption energies (E_{ads}), which reflect adsorption that is more favorable as their values are high, were calculated for all adsorbate/adsorbent complexes using the following equation (Eq. 10)^{56,57}:

$$E_{\text{ads}} = E_{\text{CFTX+AC}} - (E_{\text{CFTX}} + E_{\text{AC}}) \quad (10)$$

where E_{CFTX} is the total energy of CFTX; E_{AC} represents the total energy of AC and $E_{\text{CFTX+AC}}$ corresponds to the total energy of the CFTX/AC complex.

The theoretical simulations were conducted using the Gaussian 09 software. The modelling and visualization of the structures were performed using VMD⁵⁸ and Gauss View⁵⁹ software, respectively.

The interaction types between CFTX and AC are best described using the Reduced Density Gradient and Non-Covalent Interactions (NCI and RDG)⁶⁰ and the theory of Atoms In Molecules (AIM)⁶¹. The Multiwfn software⁶², a multifunctional wave function analysis program, was used to perform AIM NCI, and RDG topological analyses.

Experimental results and interpretation Structural and physicochemical characterization of AC

Morphological and textural characteristics

The prepared AC had a large exchange surface of 543 m² g⁻¹, supported by the presence of micropores representing 87% of the total pore volume (0.240 cm³ g⁻¹)³⁷ (Fig. S4). A well-established porosity offering a large exchange surface have a fundamental importance in assessing the effectiveness of adsorbents in water treatment, because they promote the existence of active sites on the AC surface and allow a better penetration and diffusion of contaminants through pores⁵⁸.

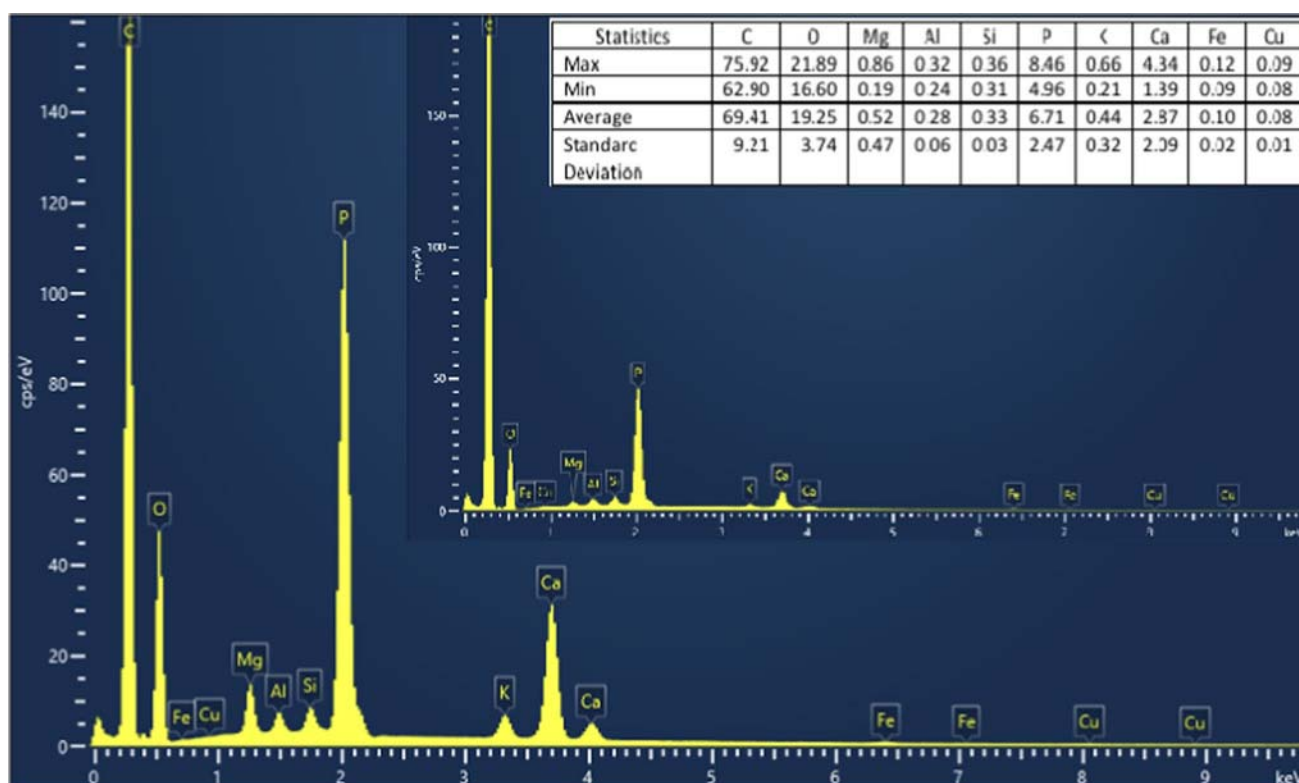


Fig. 2. EDX spectrum of the prepared AC.

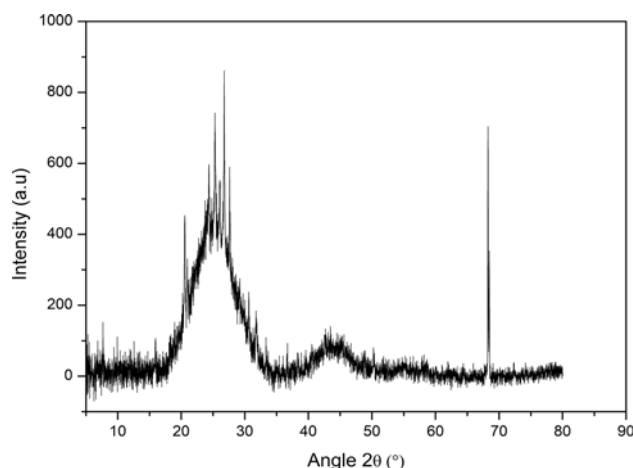


Fig. 3. XRD diagram of the AC.

The morphological characteristics of the AC surface were studied using a SEM analysis. As illustrated in Fig. ¹, the micrographs reveal a rough surface dotted with cavities presenting a varied morphology with irregular shape and size. The formation of these cavities results from the vaporization of the volatile compounds generated by the activation agent H_3PO_4 during carbonization, which leads to the expansion of existing pores and/or the formation of new pores⁶³. These cavities constitute channels facilitating the access of

adsorbed molecules to microporous and mesoporous regions of carbon. Similar results have been reported in previous researches⁶⁴, which also highlighted surfaces with comparable characteristics.

The elemental composition of AC, determined by energy diffusion X-ray (EDX) analysis and presented in Table 4, and Fig. 2, shows that carbon and oxygen are the main constituents of AC, with percentages of 69.41% and 19.25%, respectively. These elements indicate the presence of organic functional groups which can act as adsorption sites. Adsorbents with high carbon content are well known for their efficiency in removing various

Acid functions				Total basicity	pH _{pzc}
Carboxylic	Lactonic	Phenolic	Total acidity		
0.95	0.55	1.49	2.99 (±0.02)	2.37 (±0.03)	2.5

Table 5. Acid and basic functional groups on the prepared AC surface determined by Boehm titration and pHPZC value.

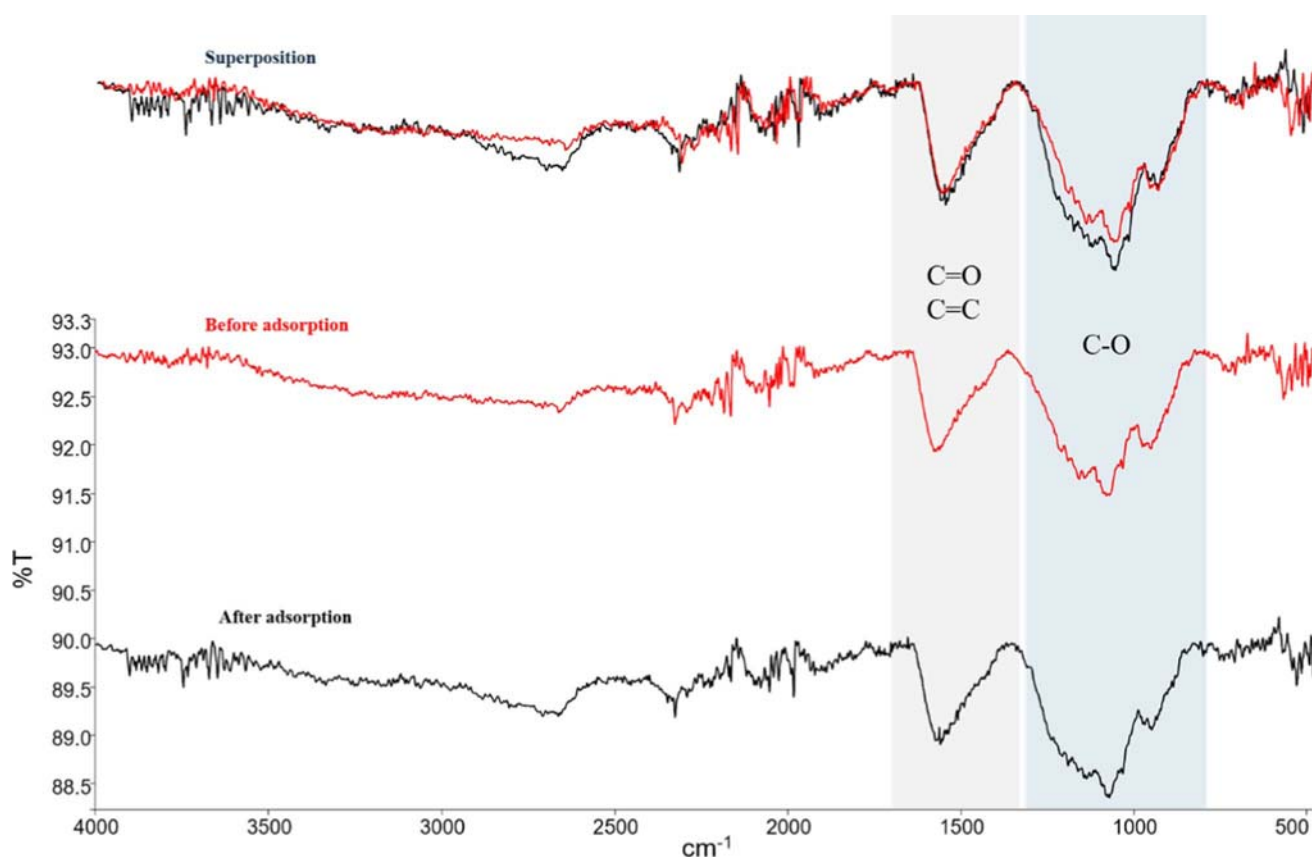


Fig. 4. FTIR spectra of AC before and after adsorption of CFTX.

contaminants. In addition, phosphorus detection can be attributed to the use of phosphoric acid (H_3PO_4) during activation⁶⁵. Other elements, such as magnesium, aluminum, potassium, and calcium, have also been identified. The carbon X-ray diffraction (XRD) diagram shown in Fig. 3 shows strong and wide peaks at approximately 25° and 45° , attributed to the Bragg reflections (002) and (100) of amorphous carbon^{66,67}. These drawings reveal the partially graphitic structure of AC. The presence of similar peaks indicates a high degree of disorder, which is typical of carbon materials. Comparable results have been obtained in other studies working on AC derived from agro-industrial waste⁶⁸.

Surface chemical characteristics

For surface chemistry, pH at the zero charge point (pH^{PZC}), is a key parameter in adsorption mechanisms. The pH^{PZC} was measured at about 2.5, indicating a predominance of acidic character on the AC surface. Below this pH value, the AC surface is acidic, promoting the adsorption of negatively charged particles. In contrast, when the pH exceeds the pH^{PZC} , the surface moves to a basic nature, facilitating interactions with

cationic species. In the case of CFTX, its behavior in solution changes according to its three acid dissociation constants ($\text{pK}_a = 3.0, 3.2, \text{ and } 4.1$). Thus it can exist in different stable ionic forms depending on the pH of the solution. These ion-shaped transitions cause changes in the electron configuration, allowing them to establish specific interactions with the AC surface.

The quantification results of the sites potentially responsible for drug residue adsorption are presented in Table 5. These data show that the surface has a slight acidity, mainly attributed to the existence of carboxylic, lactonic, and phenolic functional groups. In addition, the total basicity value (2.37 meq g^{-1}) was lower than the total acidity value (2.99 meq g^{-1}), this confirms the acid character of the AC.

The analysis of the IR spectrum (Fig. 4) of the raw processed activated carbon (before adsorption) showed mainly two bands. A band around 1600 cm^{-1} corresponds to the elongation vibration of the C=O group (carbonyls) or aromatic type vibrations C=C, and a wide band in the region $1000\text{--}1200 \text{ cm}^{-1}$, related to the elongation vibrations of the C–O group (carboxylic

and phenolic).

This observation corroborates the results of the Boehm assay, confirming the presence of polar functional groups likely to interact with CFTX molecules through hydrogen bonds or electrostatic interactions.

Adsorption studies

Adsorption kinetics

Adsorption kinetics experiments were performed to estimate the CFTX elimination rate of the aqueous solution and to better understand the adsorption mechanism of the adsorbents. Figure S5 illustrates the adsorption capacities of AC plotted against the contact time for varying initial concentrations of CFTX. The results showed that adsorption occurred rapidly during the first 30 min, then gradually slowed down to equilibrium after approximately 180 min with maximum adsorbed amounts ranging from 0.37 mg g⁻¹ to 1.36 mg g⁻¹ for initial CFTX concentrations of 4 and 20 mg L⁻¹, respectively. This can be explained by the abundance of unoccupied active sites at the beginning of the process, whose availability decreases over time, suggesting a saturation of the adsorbent surface⁶⁷. Furthermore, this relatively low adsorption capacity achieved can also be explained by the complexity of the CFTX molecule, comprising several functional groups, thus limiting its interaction with the carbon surface of the elaborated AC. Thus, its size and high spatial configuration may not be fully adapted with the pores of AC, despite its developed porosity and high specific surface area. However, although other materials^{69,70} have revealed better adsorption performances due to their very porous structures and large specific surfaces, the AC developed remains advantageous in terms of its low-cost synthesis from agro-industrial waste and their relatively simple preparation process.

To identify the most suitable kinetic model for describing CFTX retention on AC, the experimental adsorption data were adjusted in a non-linear manner using PFO, PSO, and intra-particle diffusion models. The parameters listed in Table 6 indicate that adsorption is most accurately represented by the PSO model, for all concentrations investigated. Indeed, it is distinguished by the highest values of the correlation coefficient (R^2) and the smallest values of chi-square (χ^2) and corrected Akaike Information Criterion (AIC_c). In addition, the q_e values calculated using this model are presents a great similarity with experimental data, thus confirming that the kinetics mainly follows a pseudo-second-

order model. This suggests a chemisorption process characterized by strong interaction forces⁶⁸. These results are consistent with another study⁷¹, indicating as well that the PSO model provides the best suited for describing antibiotics removal on AC derived from waste.

Although the analysis of FTIR spectra before and after adsorption does not reveal significant modifications, it nevertheless suggests the involvement of the C–O group in the adsorption mechanism, through the observation of a slight increase in the intensity of the characteristic band of the C–O, located in the region 1000–1200 cm⁻¹.

Adsorption isotherm

Adsorption isotherms represent the equilibrium correlation between the quantity of adsorbate retained by the adsorbent (q_e) and its concentration in the solution (C_e), at a fixed temperature. These isotherms offer information about the surface characteristics of the adsorbent and the affinity between the adsorbent and adsorbate, helping

to understand the retention mechanisms of pharmaceutical compounds in aqueous environments.

The experimental equilibrium data for CFTX adsorption on AC were fitted to various models, including thermodynamic (Langmuir, Freundlich, BET^{n-finite}, and BET^{n-infinite}) and statistical (STAT1, STAT2, and STAT3) models. The fitting curves of these models are illustrated

	Ceftriaxone concentration (mg L ⁻¹)						
	4	6	8	10	12	16	20
q_e (mg g ⁻¹)	0.37	0.55	0.61	0.77	0.92	1.22	1.36
Models	0.37	0.56	0.66	0.83	0.97	1.31	1.44
	0.05	0.04	0.03	0.02	0.02	0.01	0.01
	0.92	0.91	0.92	0.91	0.93	0.96	0.91
	—	—	—	—	—	—	—
	51.40	36.74	32.50	23.57	24.61	24.39	8.31
	0.23	0.54	0.62	1.12	0.74	1.08	2.83
	0.39	0.61	0.73	0.92	1.10	1.59	1.66
	0.20	0.11	0.06	0.03	0.02	0.00	0.01
	0.95	0.94	0.95	0.94	0.96	0.97	0.93
	—	—	—	—	—	—	—
	63.19	46.82	42.12	32.61	35.72	30.54	13.88
	0.07	0.20	0.25	0.49	0.30	0.62	1.55
	0.08	0.13	0.12	0.14	0.11	0.05	0.16
	0.02	0.03	0.04	0.04	0.05	0.07	0.08
	0.82	0.85	0.90	0.93	0.96	0.97	0.95
	—	—	—	—	—	—	—
	38.99	29.63	32.11	33.51	36.55	31.43	24.06
	0.20	0.26	0.23	0.21	0.18	0.14	0.27

Table 6. Parameters of kinetic models for various initial concentrations of CFTX.

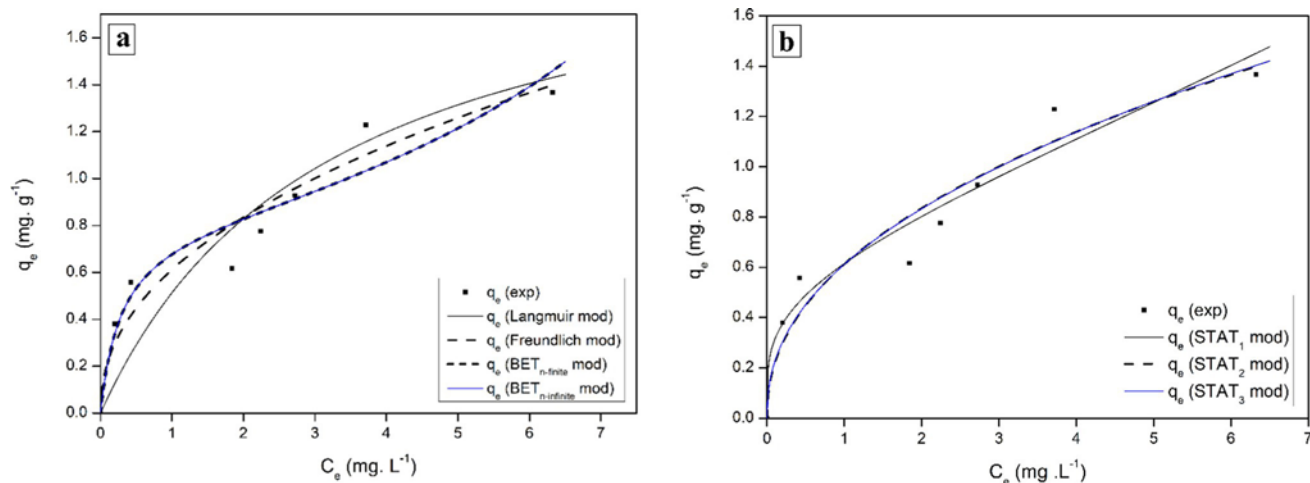


Fig. 5. Isotherms of experimental and thermodynamic adsorption (a) versus statistical (b) modelled CFTX on AC.

	Model parameters	CFTX	R ²	AIC _c	χ ²
Thermodynamic models					
Langmuir	q _{max} (mg g ⁻¹)	2.15	0.89	− 1.35	0.92
	K _L (L mg ⁻¹)	0.31			
Freundlich	n _F	2.23	0.94	− 8.15	0.14
	K _F ((mg g ⁻¹)/ (mg L ⁻¹) ^{1/n})	0.61			
BET ^{n-finite}	n	51.41	0.93	− 1.76	0.10
	q _{max} (mg g ⁻¹)	0.39			
	K _L (L mg ⁻¹)	7.20			
	K _S (L mg ⁻¹)	0.07			
BET ^{n-infinite}	q _{max} (mg g ⁻¹)	0.78	0.93	− 5.01	0.10
	K _L (L mg ⁻¹)	3.63			
	K _S (L mg ⁻¹)	0.07			
Statistic models					
STAT ₁	m	0.15	0.95	− 7.33	0.08
	q _{max} (mg g ⁻¹)	0.44			
	C ₁ (mg L ⁻¹)/ ΔE ⁰ ₁ (kJ mol ⁻¹)	15.67/ 0.59			
	C ₂ (mg L ⁻¹)/ ΔE ⁰ ₂ (kJ mol ⁻¹)	35.02/ − 1.96			
STAT ₂	m	0.45	0.94	− 5.40	0.14
	q _{max} (mg g ⁻¹)	2.47			
	C ₁ (mg L ⁻¹)/ ΔE ⁰ ₁ (kJ mol ⁻¹)	21.13/ − 0.13			
	C ₂ (mg L ⁻¹)/ ΔE ⁰ ₂ (kJ mol ⁻¹)	11.29/ 1.52			
STAT ₃	m	0.41	0.94	− 5.62	0.13
	qmax (mg g-1)	13.17			
	C ₁ (mg L ⁻¹)/ ΔE ⁰ ₁ (kJ mol ⁻¹)	1797.31/ − 10.96			
	C ₂ (mg L ⁻¹)/ ΔE ⁰ ₂ (kJ mol ⁻¹)	1275.33/ 0.83			

Table 7. Thermodynamic and statistic model parameters for CFTX adsorption isotherms.

in Fig. 5 and the corresponding adjusted parameters are listed in Table 7, along with statistical analysis criteria (nonlinear regression coefficients (R²), Akaike information criterion corrected for sample size (AIC_c), and chi-square (χ²)) to assess the adequacy of the model.

The results of the modelling show that the Freundlich thermodynamic model and the multilayer statistical model STAT₁ are most appropriate for describing the adsorption of CFTX on the prepared AC compared to other models tested. Indeed, these two models have the highest regression coefficients (R²= 0.94 for Freundlich and R²= 0.95 for STAT₁) as well as the lowest values of chi-square and the corrected Akaike information criterion for small samples (χ²= 0.14 and AIC_c = - 8.15 for Freundlich and χ²=0.08 and AIC_c = - 7.33 for STAT₁). These indicators (R², χ², AIC_c) confirm their better adequacy to experimental data.

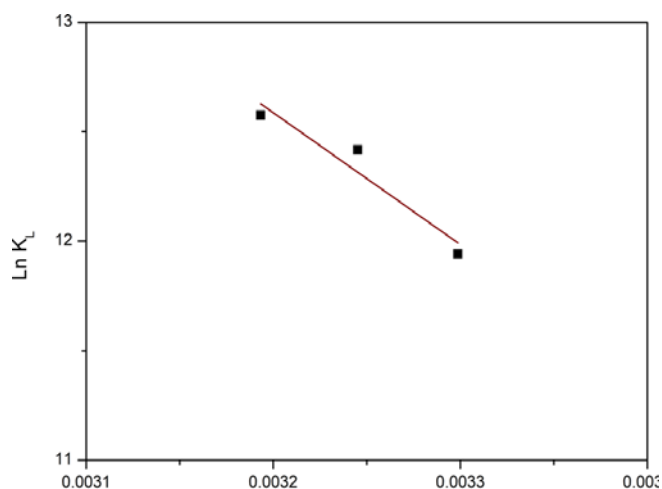


Fig. 6. Ln KL versus 1/T diagram.

Temperature (°C)	ΔG° (kJ mol ⁻¹)	ΔH° (kJ mol ⁻¹)	ΔS° (kJ mol ⁻¹ K ⁻¹)
30	-30.22	50.11	0.26
35	-31.55		
40	-32.87		

Table 8. Thermodynamic parameters (ΔG° , ΔH° , and ΔS°) of CFTX retention on AC.

Freundlich's model describes multilayer adsorption on heterogeneous surfaces with variable binding energies⁷². The intensity parameter, $1/n$, is essential for interpreting the adsorption behavior: If $n=1$ the adsorption is linear, indicating homogeneous sites with no interaction between adsorbed molecules. $1/n < 1$, the adsorption is favorable, with increased adsorption capacity and the formation of new adsorption sites. In contrast, when $1/n > 1$, the adsorption becomes unfavorable due to weaker adsorption bonds and reduced adsorption capacity.

By applying the nonlinear Freundlich equation, $1/n$ value of 0.44 was obtained, suggesting that the CFTX retention on the produced AC is favorable. This result is consistent with observations of the AC's SEM images, which clearly reveal the heterogeneity of its structure. In addition, the Freundlich curve shows that the adsorption has not reached saturation of AC, suggesting a multilayer adsorption process⁷³.

The STAT₁ statistical model, founded on a statistical physics approach applied to type II isotherms (according to the Brunauer, Emmett, and Teller classification), also assumes multilayer adsorption on the AC surface. It allows us to determine a stoichiometric coefficient ($m = 0.15$), representing the average number of CFTX molecules adsorbed as aggregates per adsorption site. This value reflects significant adsorbate-adsorbate interactions, as well as heterogeneity in the distribution of adsorbed molecules^{74,75}. In addition, the STAT1 model provides energy parameters for monolayer (for $n = 1$) and multilayer (for $n > 1$) adsorption. Indeed, it allows to

estimate the adsorption energies ΔE^0 (monolayer) and ΔE^0 (multilayer). For a CFTX saturation concentration of 20 mg L⁻¹, the calculated adsorption energies are $\Delta E^0 = 0.259$ kJ mol⁻¹ and $\Delta E^0 = -1.96$ kJ mol⁻¹. These results suggest that monolayer adsorption (CFTX-AC interactions) is endothermic in nature ($\Delta E^0 > 0$), while the

multilayer adsorption process (CFTX-CFTX interactions) is exothermic ($\Delta E^0 < 0$). 1

Adsorption thermodynamics

The study of the thermodynamic behavior of CFTX retention on AC allows the evaluation of key thermodynamic parameters, such as ΔG° , ΔH° , and ΔS° , thus providing information on the energetic variations during adsorption, as well as the feasibility and spontaneity of this process. These thermodynamic parameters were determined by applying the following equations (Eq. 11–13)⁷⁶:

$$\Delta G^\circ = -R \ln(K_L) \quad (11)$$

$$\Delta G^\circ = \Delta H^\circ - T \Delta S^\circ \quad (12)$$

$$\ln K_L = \frac{\Delta S^\circ}{R} - \frac{\Delta H^\circ}{R} \frac{1}{T} \quad (13)$$

where R (8.314 J mol⁻¹ K⁻¹) is the universal gas constant, T (K) is the absolute temperature and K_L is the thermodynamic equilibrium constant determined from the Langmuir isotherm. ΔG° (kJ mol⁻¹) represents the Gibbs free energy change, ΔH° (kJ mol⁻¹) is the enthalpy change, and ΔS° (kJ mol⁻¹ K⁻¹) is the entropy change.

According to the Van't Hoff equation (Eq. 13), ΔS° and ΔH° were determined from the slope and the intercept, respectively, of the linear plot of $\ln(K_L)$ as a function of $(1/T)$ (Fig. 6). The measured thermodynamic parameters are summarized in Table 8.

The negative ΔG° values indicate that the retention of CFTX on AC is thermodynamically favorable and can occur spontaneously, without requiring external energy input⁷⁷. Moreover, the increasingly negative ΔG° values with rising temperature suggest that the retention process becomes more favorable at higher temperatures.

The positive ΔH° value indicates that the adsorption process is endothermic, implying that higher temperatures enhance the adsorption of CFTX on AC⁷⁸. This endothermic behavior is explained by the increased mobility of the adsorbed molecules across the external boundary layer and into the internal pores of the adsorbent. A similar endothermic behavior was also observed in a previous study on the antibiotics adsorption on AC⁷⁹. The nature of the adsorption process can be interpreted according to the magnitude of ΔH° . A ΔH° value between 0 and 40 kJ·mol⁻¹ indicates physisorption, while a value between 40 and 800 kJ·mol⁻¹ is indicative of chemisorption⁸⁰.

Based on this and considering the obtained ΔH° value ($50.11 \text{ kJ}\cdot\text{mol}^{-1}$), the CFTX adsorption on AC can be classified as a chemisorption process. These results corroborate the conclusions of the kinetic study.

The positive ΔS° value ($0.26 \text{ kJ mol}^{-1} \text{ K}^{-1}$) indicates an increase in the randomness at the adsorbent surface during CFTX retention, reflecting a strong affinity of AC for CFTX⁸¹.

Study of desorption

The stability and reusability of an adsorbent are key parameters for its practical use in various fields. The durability of AC prepared from grape seeds waste was evaluated through an adsorption–desorption regeneration test which is shown in Fig. 7. The results show that the desorbed quantity stabilizes at approximately 0.11 mg g^{-1} from an initial concentration of 8 mg L^{-1} , suggesting that only a limited fraction of the adsorbed CFTX can be desorbed. In addition, the desorption rate significantly decreases from 25% to 6.46% when the CFTX concentration increases from 4 to 20 mg L^{-1} . This behavior indicates that the adsorption becomes less reversible at higher concentrations, likely due to the establishment of stronger interactions between CFTX and the prepared AC, which makes desorption more difficult and reduces the efficiency of the recovery process. These observations corroborate the results achieved by kinetic and thermodynamic studies, which suggest a chemisorption mechanism. These findings also highlight the importance of retention mechanisms when designing adsorbent materials for remediation applications, while highlighting the challenges associated with the regeneration of AC saturated with a high amount of adsorbate.

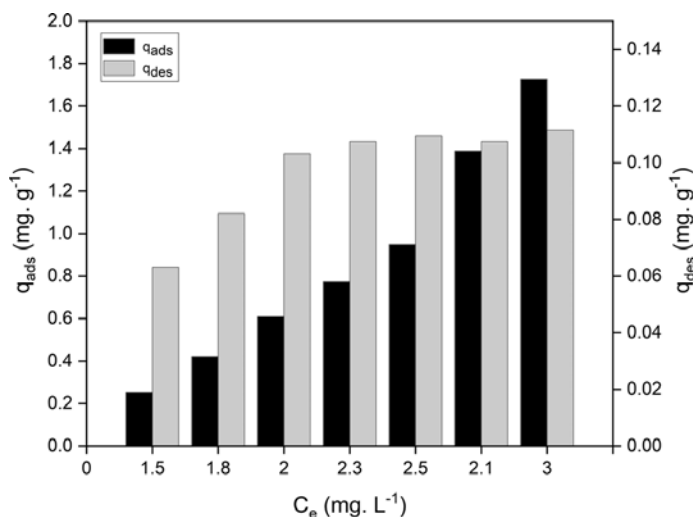


Fig. 7. Study of CFTX desorption.

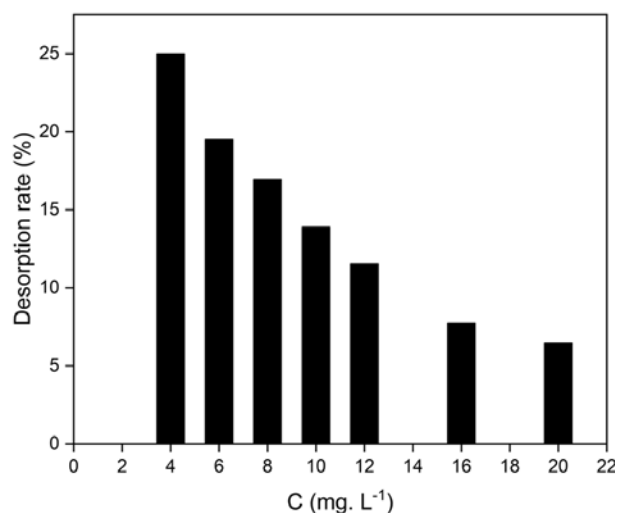
DFT modelling

Theoretical calculations of the interactions that occur in the presence of AC require a precise understanding of its atomic structure. In this study, four cycles of fused benzene (the chrysene) were used to model the AC surface. To assess the impact of functional groups, $-\text{OH}$, $-\text{CHO}$, and $-\text{COOH}$ groups were incorporated into the active sites, and selected based on the Boehm titration results^{82,83}.

Study of global reactivity of molecules

The electronic properties of Ceftriaxone (CFTX) and functionalized activated carbon (AC) were studied to investigate molecular interactions and affinity between adsorbate and adsorbent. Figure 8 shows the molecular electrostatic potential (MEP) and the positions of the HOMO and LUMO orbitals of the optimized AC models. These models are designated as follows: AC (unfunctionalized AC), AC–COOH (AC functionalized with $-\text{COOH}$), AC–OH (AC functionalized with $-\text{OH}$), AC–CHO (AC functionalized with $-\text{CHO}$) and AC–COOH–OH–CHO (AC functionalized with $-\text{COOH}$, $-\text{OH}$, and $-\text{CHO}$), as well as Ceftriaxone (CFTX) molecule.

MEP is a well-established calculation method for studying chemical reactivity and variations in electron density within a molecule. It allows us to predict the reactive sites that are favorable to nucleophilic and electrophilic attacks⁸⁴. The MEP map represents, through a color gradient, the regions where the electrostatic potential is negative, positive, and neutral; where the red color indicates the areas of most negative potential (electron-rich) favorable to electrophilic



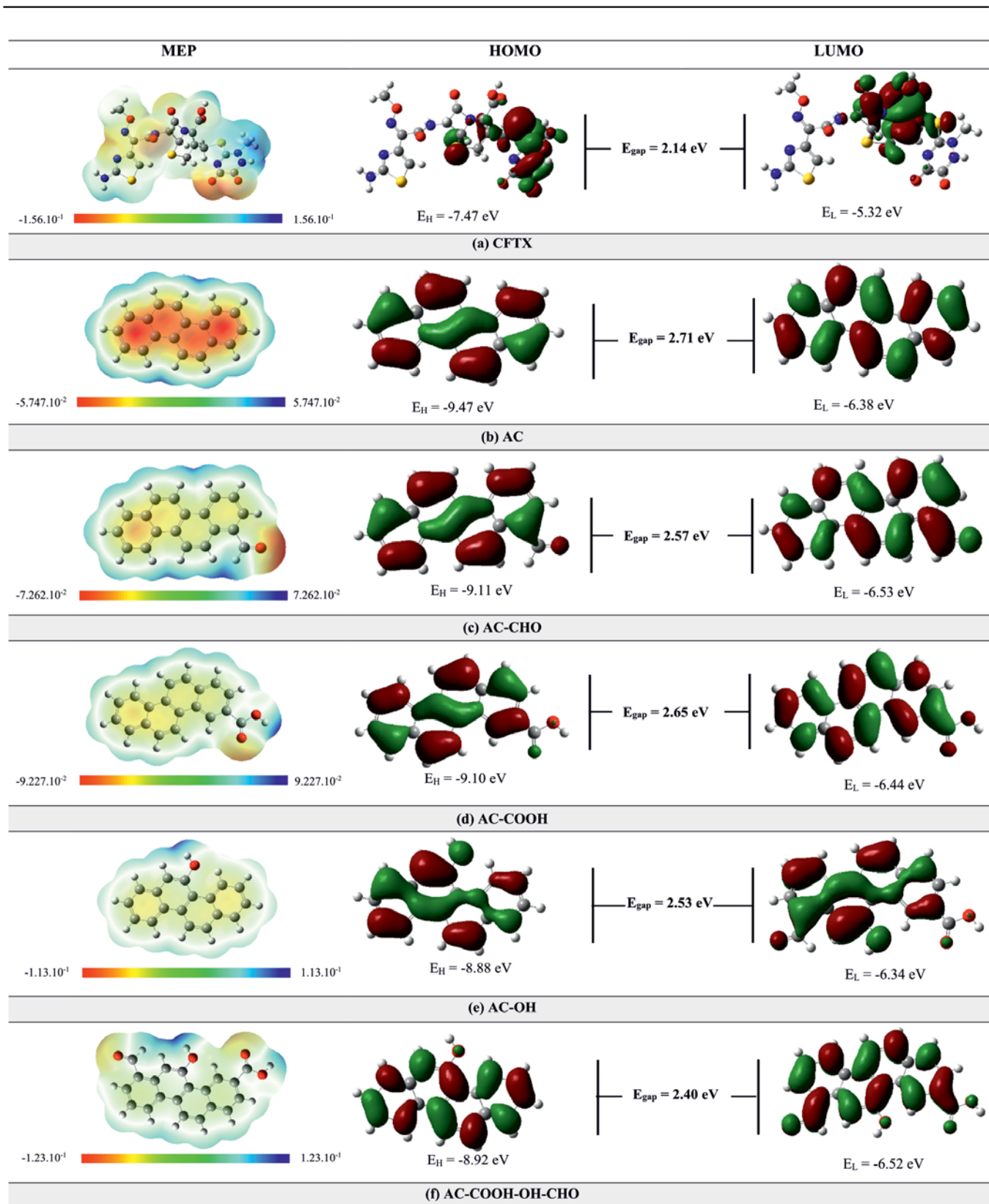


Fig. 8. MEP (e/au^3 scale) and HOMO/LUMO molecular orbital mapping of optimized geometric structures of: (a) CFTX, (b) AC, (c) AC-CHO, (d) AC-COOH, (e) AC-OH and (f) AC-COOH-OH-CHO, calculated by DFT at the level of B3LYP/6-311G (d, p).

attacks while the blue color corresponds to the most positive potential (electron-poor), associated with nucleophilic reactivity. Regions with neutral potential are shown in green⁸⁵.

Quantum chemical parameters	Energy gap (E_{gap} , eV)	Chemical potential (μ , eV)	Global hardness (η , eV)	Electrophilicity index (ω , eV)
MONOMERS				
CFTX	2.14	6.39	1.07	19.03
AC	2.71	7.74	1.35	22.11
AC-CHO	2.57	7.82	1.28	23.76
AC-COOH	2.65	7.77	1.32	22.77
AC-OH	2.53	7.61	1.26	22.84
AC-COOH-OH-CHO	2.40	7.72	1.20	24.84
DIMERS				
CFTX_AC	1.22	6.90	0.61	38.95
CFTX_AC-CHO	0.88	7.03	0.44	55.77
CFTX_AC-COOH	1.03	6.92	0.51	46.25
CFTX_AC-OH	1.25	6.86	0.62	37.56
CFTX_AC-COOH-OH-CHO	0.99	7.00	0.49	49.48

Table 9. Quantum chemical descriptor values for monomers (CFTX molecule and functionalized AC models before adsorption) and for dimers (CFTX/AC complexes representing the molecular situation after adsorption).

On the MEP map (Fig. 8 a), it is observed that the electron-rich zones of CFTX are concentrated mainly around carbonyl groups ($-\text{C}=\text{O}$), which are likely to interact with the functional groups of AC, acting as preferred adsorption sites. On the other hand, electron-

poor areas are located near hydrophobic groups. For functionalized ACs, the $-\text{CHO}$, $-\text{COOH}$, and $-\text{OH}$ groups have electron-rich zones, promoting electrostatic interactions and hydrogen bonds with CFTX.

The analysis of the frontier molecular orbitals, namely the HOMO and LUMO, is fundamental for a better understanding of chemical reactivity at the atomic level. It allows to study the charge transfer mechanisms during adsorption, by identifying regions of a molecule that can give or accept an electron, respectively⁸⁶. The HOMO and LUMO energy gap (E_{gap}) influences the reactivity and chemical stability of a molecule, a narrower gap usually corresponds to a higher reactivity. As shown in Fig. 8, CFTX has an energy gap of 2.14 eV, indicating a

moderate reactivity, with HOMO orbitals located on the electron donor amine groups and LUMO orbitals on the carbonyl acceptors. In contrast, the unfunctionalized AC shows a higher energy gap (2.71 eV), reflecting a lower intrinsic reactivity. However, the functionalization of carbon gradually reduces the energy gap, reaching 2.40 eV, for AC-COOH-OH-CHO, suggesting an increased reactivity due to the synergy between the functional groups. Chemical descriptors, such as chemical potential (μ), global hardness (η), and electrophilic index (ω) provide additional information on the stability and reactivity of molecules. A high overall hardness (η) indicates lower reactivity, while a high electrophilic index (ω) suggests a greater ability to accept electrons⁸⁷. Gap energies (E_{gap}) and the chemical descriptors for CFTX and functionalized carbons are calculated and summarized in Table 9.

Adsorption mechanisms

Figure 9 presents the optimized complexes formed by the coordination of CFTX with both unfunctionalized and functionalized AC, along with their corresponding interaction energies. The energy gap values and related

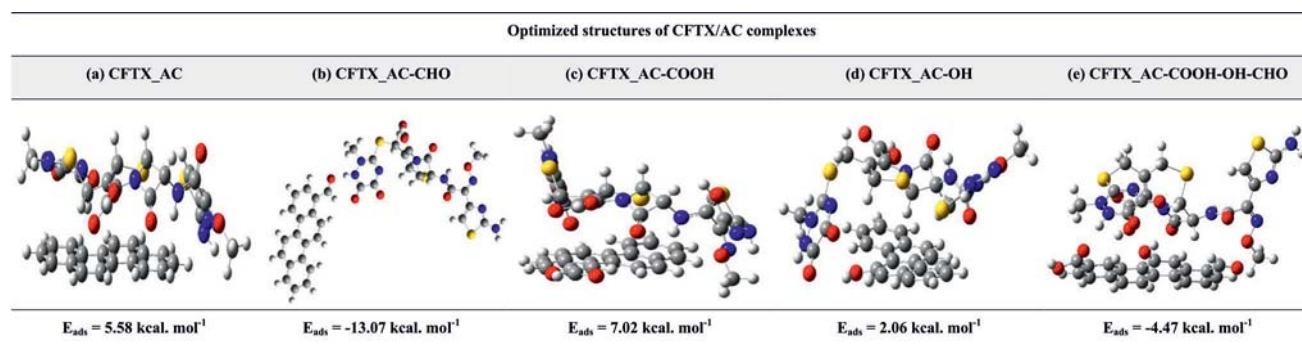


Fig. 9. Optimized structures of CFTX/AC complexes and their adsorption energies: (a) CFTX_AC, (b) CFTX_AC-CHO, (c) CFTX_AC-COOH, (d) CFTX_AC-OH and (e) CFTX_AC-COOH-OH-CHO.

chemical descriptors for each complex are summarized in Table 9.

After adsorption, a significant decrease in the energy gap is observed for all complexes, with the CFTX_AC-CHO complex exhibiting the lowest value at 0.88 eV. This reduction suggests enhanced stability of the adsorbed systems, attributed to efficient charge transfer from the HOMO of CFTX to the LUMO of the functionalized carbon surface. The calculated chemical potential (7.03 eV) and global hardness (0.44 eV) further confirm this stabilization, indicating increased reactivity and improved thermodynamic stability of the complexes post-adsorption.

The most negative adsorption energy recorded for the CFTX_AC-CHO complex ($-13.07 \text{ kcal mol}^{-1}$) confirms that this functional group promotes stronger interactions with CFTX, mainly via electrostatic interactions and hydrogen bonds. This result suggests that the functionalization of AC by the -CHO group

significantly improves the adsorption process, compared to the -OH and -COOH groups located on the AC surface.

The CFTX_AC-COOH-OH-CHO complex (Fig. 9e) also shows particularly favorable adsorption energy ($-4.47 \text{ kcal mol}^{-1}$), highlighting strong and synergistic interactions between the -COOH, -OH, and -CHO groups and the polar sites of the CFTX. This synergy results from the combination of the specific effects of each functional group, which increase the local electron density and thus facilitate interactions with CFTX.

AIM, NCI, and RDG analyses were employed to examine the intensity and nature of molecular interactions involved in adsorption within CFTX_AC-CHO and CFTX_AC-COOH-OH-CHO complexes. These methods provide a better understanding of interactions, particularly non-covalent bonds, thus contributing to the interpretation of adsorption mechanism and the stability of complexes formed⁸⁸.

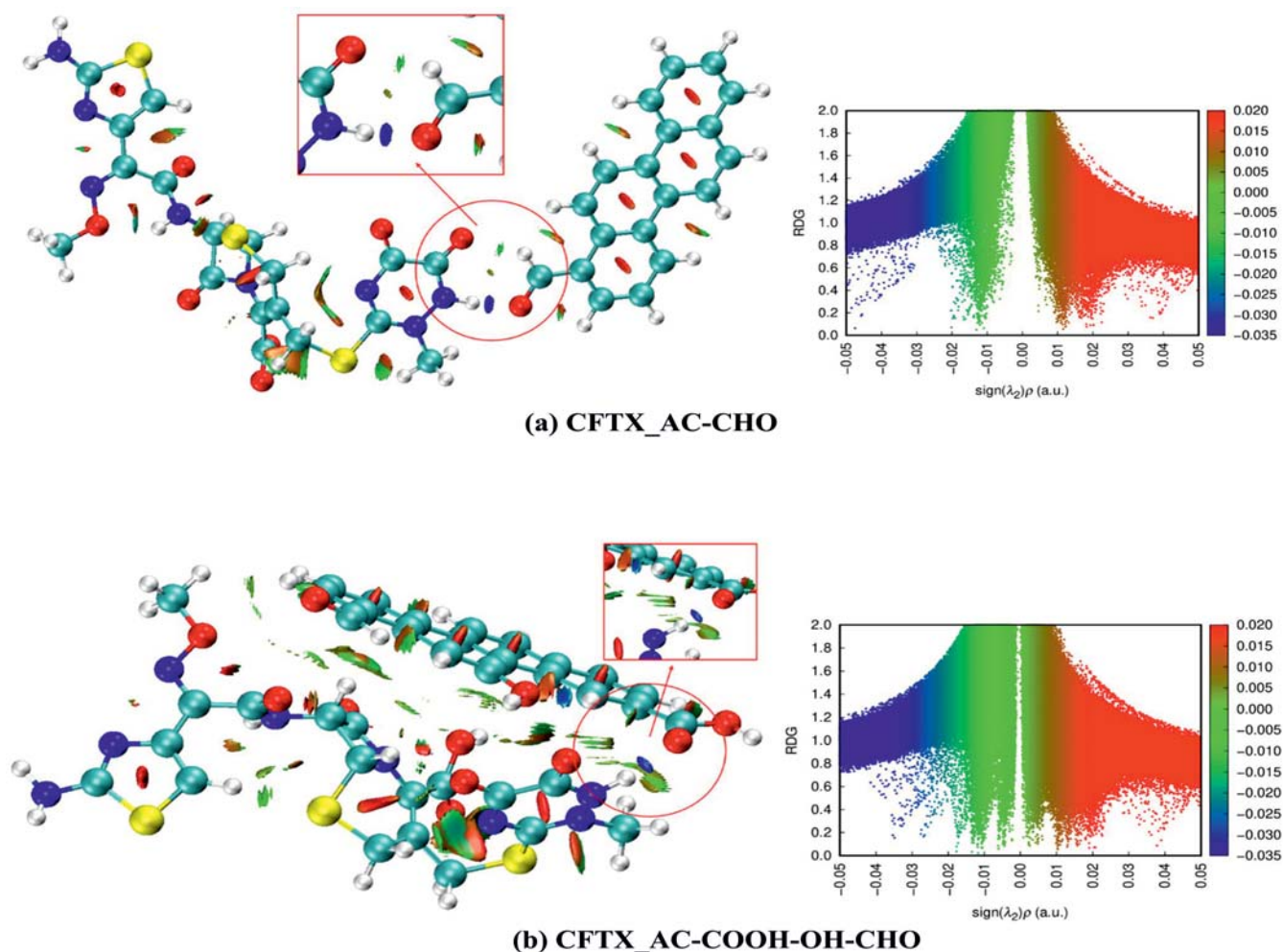


Fig. 10. NCI and RDG molecular graphs of CFTX_AC-CHO (a) and CFTX_AC-COOH-OH-CHO (b)

Non-covalent interactions can be visualized on the NCI and RDG maps. Green regions represent weakly attractive interactions, mainly of the Van der Waals type, while blue areas indicate stronger attractive interactions, such as hydrogen bonds, and the red zones reveal repulsive interactions, often attributed to steric hindrance. The NCI and RDG graphs of the two studied complexes, CFTX_AC-CHO and CFTX_AC-COOH-OH-COOH, are shown in Fig. 10.

In the CFTX_AC-CHO complex (Fig. 10a), small red spots indicating steric repulsion, are primarily observed at the center of the phenolic cycles of AC. A blue spot appears at the oxygen atom of the -CHO group in AC and the hydrogen atom of the CFTX, indicating the presence of a hydrogen bond in this region. In addition, low Van der Waals-type interactions, shown in green, are observed between CFTX and AC.

In the CFTX_AC-COOH-OH-CHO complex (Fig. 10b) there are also red spots, indicating steric repulsions, as well as blue zones corresponding to hydrogen bonds. The figure clearly shows green areas representing weak Van der Waals interactions between CFTX and AC.

AIM analysis corroborates these observations by identifying critical binding points (BCP, Bond Critical Points), which clearly confirms the presence of chemical interactions and bonds between the CFTX and the functional groups in the AC. Topological properties of intermolecular BCP, such as electron density $\rho(r)$, the Laplacian of electron density $\nabla^2\rho(r)$, total electronic energy density $H(r)$, Lagrangian kinetic energy $G(r)$ and potential energy density $V(r)$, have been determined to assess the nature and intensity of binding interactions between molecules. In addition, the intermolecular bond energies at BCP (E_{int}) and the hydrogen bond interaction energies (E_{HB}) were calculated using equations (Eq. 14)⁸⁹ and (Eq. 15)⁹⁰ respectively:

$$E_{int} = \frac{ff(r)}{2} \quad (14)$$

$$E_{HB} = -223.08 \cdot \rho(ff) + 0.7423 \quad (15)$$

Figure 11 illustrates the AIM molecular graph, highlighting the different BCP identified in the two complexes. The measured topological parameters associated with these BCP are listed in Table 10.

The results of the AIM reveal that, in the two studied complexes, the adsorption of CFTX on AC results from non-covalent interactions, characterized by low values of $\rho(r)$ at the level of the BCP and positive values of $\nabla^2\rho$

(r). These characteristics confirm the non-covalent nature of the interactions, mainly of hydrogen and Van der Waals bond type⁹¹.

In the CFTX_AC-CHO complex, two significant BCP (114 and 141) were identified, presenting low values of $\rho(r)$ and positive values of $\nabla^2\rho(r)$, indicating non-covalent hydrogen bond interactions. According to the classification proposed by Rozas et al.⁹², the strength of hydrogen bonds can be classified into three main types:

- (1) Strong hydrogen bond definite by $\nabla^2\rho(r) < 0$ and $H(r) < 0$;
- (2) Mean hydrogen bond characterized by $\nabla^2\rho(r) > 0$ and $H(r) < 0$;
- (3) Weak hydrogen bond when $\nabla^2\rho(r) > 0$ and $H(r) > 0$.

As shown in Table 10, the CFTX_AC-CHO complex is mainly stabilized by a moderate hydrogen bond between the H_{38} atom of the CFTX and the O_{85} atom of the -CHO group of the AC, as well as by a weaker interaction between H_{86} and O_8 . The $H_{38}-O_{85}$ bond, characterized by a higher hydrogen bond energy E_{HB} ($E_{HB} = -9.91$ kcal mol⁻¹), is significantly stronger than the $H_{86}-O_8$ bond ($E_{HB} = -1.99$ kcal mol⁻¹). These observations are corroborated by the total energy of the complex, estimated at -11.90 kcal mol⁻¹, which is almost equivalent to the adjusted adsorption energy found (-13.07 kcal mol⁻¹), confirming that the CFTX retention is primarily stabilized by hydrogen bonds.

In the CFTX_AC-COOH-OH-CHO complex, several BCP have been identified, revealing a diversity of interactions. The interactions at BCP 136, 141, 166, and 199 show moderate values of $\rho(r)$ and positive values of $\nabla^2\rho(r)$, suggesting non-covalent Van der Waals-like interactions or a very weak hydrogen bond, with low interaction energies between -0.67 kcal mol⁻¹ and -3.85 kcal mol⁻¹. The $H_{38}-O_{79}$ interaction at BCP₁₃₈ is distinguished by an EHB energy of -7.10 kcal mol⁻¹, representing the strongest hydrogen bond and significantly contributing to the stabilization of the complex.

In both complexes, the adsorption process is mainly governed by hydrogen bonds between a hydrogen atom of the CFTX (H_{38}) and an oxygen atom of the AC (O_{85} or O_{79}), presenting the highest bond energies. These results show that adsorption is optimized by diversification of non-covalent interactions, where hydrogen

bonds play an important role, while Van der Waals

interactions, although weaker, also contribute to overall stabilization, particularly in the CFTX_AC-COOH-OH-CHO complex.

The combined results of the AIM, NCI, and RDG analyses reveal that the retention mechanism of CFTX on AC is driven by hydrogen bonds and Van der Waals interactions. These interactions are essential for the stabilization of the formed complexes.

Conclusion

The present research focused on the elimination of Ceftriaxone (CFTX), an antibiotic considered as an emerging contaminant in aqueous solutions, through the employment of novel AC synthesized from grape

seeds waste. The synthesized carbon was characterized using various physico-chemical methods, which demonstrated well-established porosity offering a large exchange surface of $543 \text{ m}^2 \text{ g}^{-1}$. Batch adsorption studies, coupled with theoretical models, allowed us to elucidate the mechanisms of adsorption. Kinetic and equilibrium data demonstrated strong agreement with the PSO model and Freundlich's thermodynamic model, as well as with the multilayer statistical model STAT_1 , respectively. Thermodynamic parameters suggest that the adsorption process is promoted, endothermic, and mainly controlled by chemical interactions. Desorption studies confirmed a chemisorption mechanism between CFTX and AC, characterized by desorption, thus opening the possibility of exploring an alternative

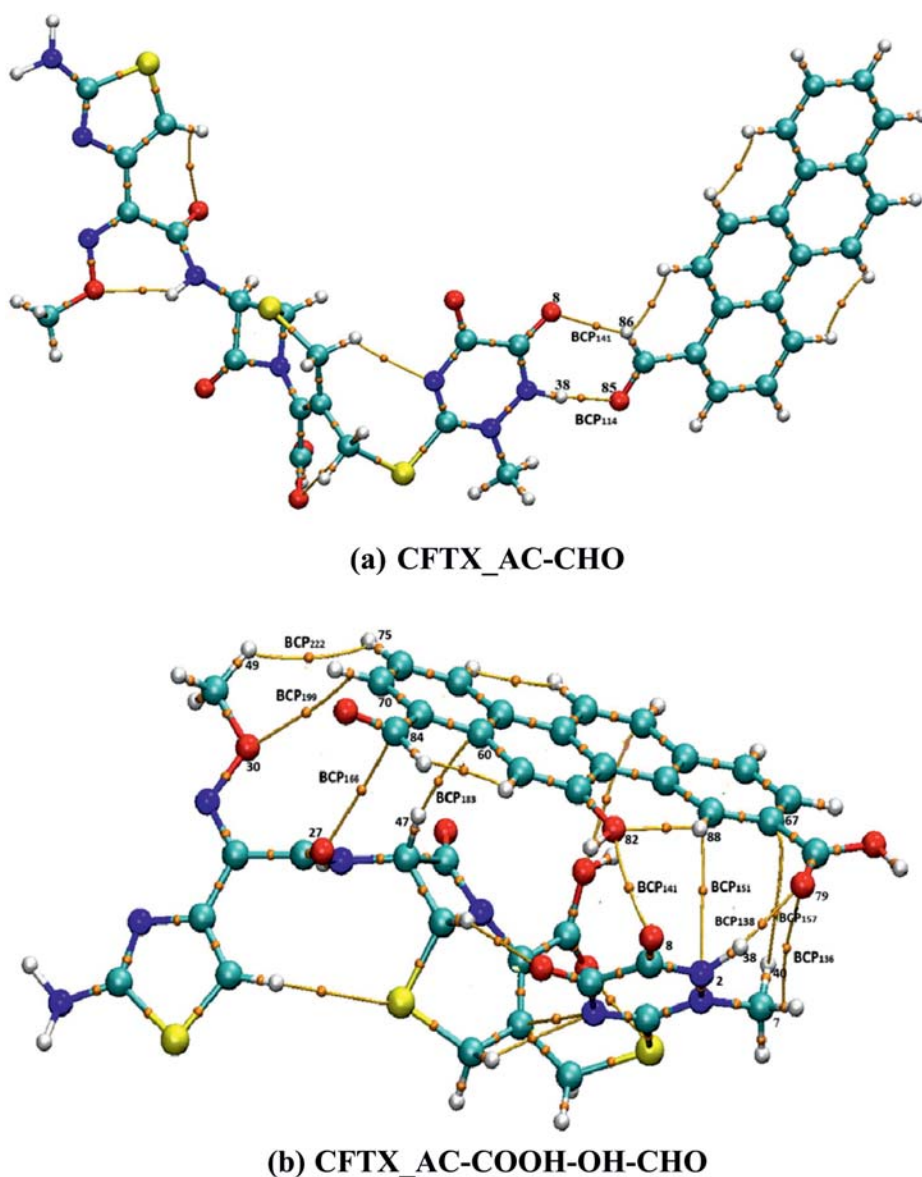


Fig. 11. AIM molecular graphs of the complexes CFTX_AC-CHO (a) and CFTX_AC-COOH-OH-CHO (b)

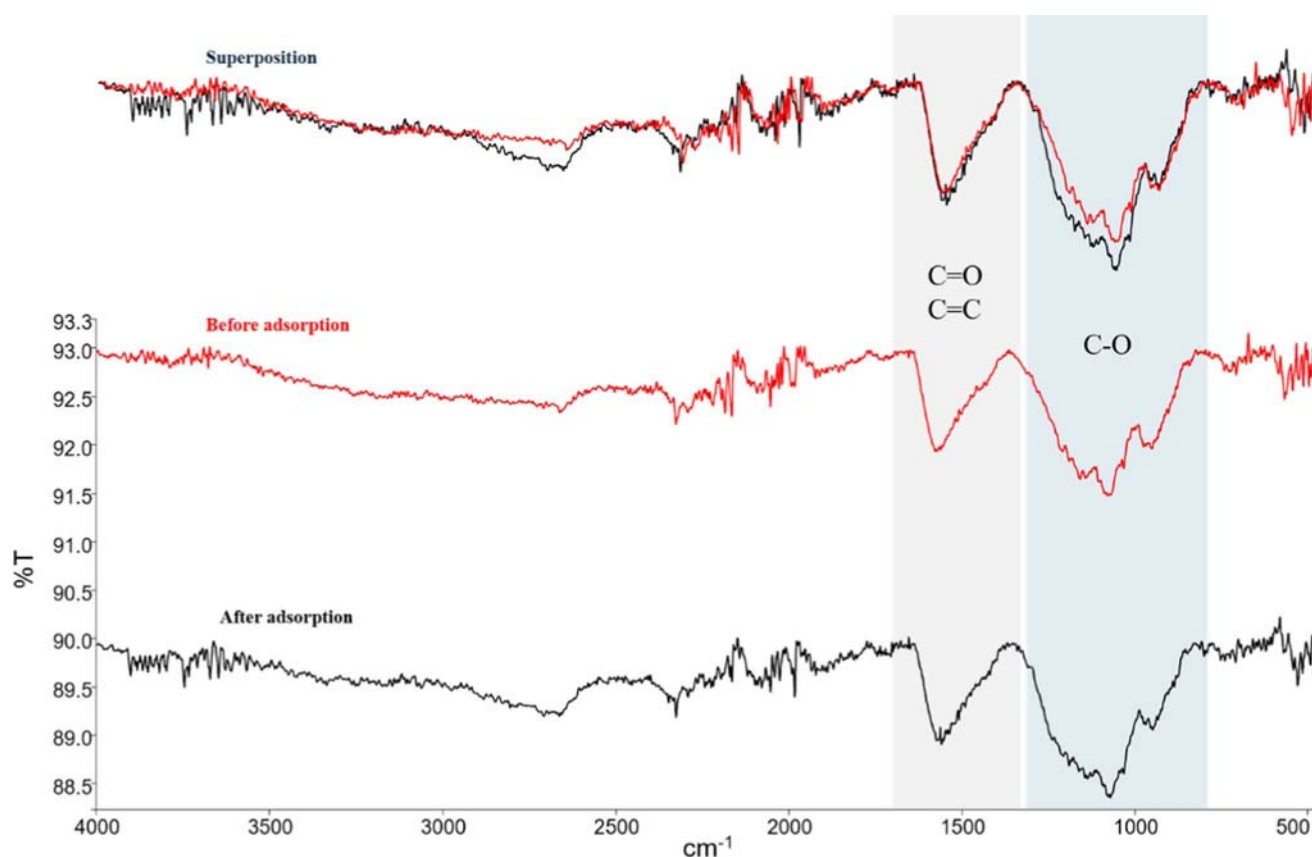


Fig. 4. FTIR spectra of AC before and after adsorption of CFTX.

contaminants. In addition, phosphorus detection can be attributed to the use of phosphoric acid (H_3PO_4) during activation⁶⁵. Other elements, such as magnesium, aluminum, potassium, and calcium, have also been identified. The carbon X-ray diffraction (XRD) diagram shown in Fig. 3 shows strong and wide peaks at approximately 25° and 45° , attributed to the Bragg reflections (002) and (100) of amorphous carbon^{66,67}. These drawings reveal the partially graphitic structure of AC. The presence of similar peaks indicates a high degree of disorder, which is typical of carbon materials. Comparable results have been obtained in other studies working on AC derived from agro-industrial waste⁶⁸.

Surface chemical characteristics

For surface chemistry, pH at the zero charge point (pH_{PZC}), is a key parameter in adsorption mechanisms. The pH_{PZC} was measured at about 2.5, indicating a predominance of acidic character on the AC surface. Below this pH value, the AC surface is acidic, promoting the adsorption of negatively charged particles. In contrast, when the pH exceeds the pH_{PZC} , the surface moves to a basic nature, facilitating interactions with

cationic species. In the case of CFTX, its behavior in solution changes according to its three acid dissociation constants ($\text{pK}_a = 3.0, 3.2, \text{ and } 4.1$). Thus it can exist in different stable ionic forms depending on the pH of the solution. These ion-shaped transitions cause changes in the electron configuration, allowing them to establish specific interactions with the AC surface.

The quantification results of the sites potentially responsible for drug residue adsorption are presented in Table 5. These data show that the surface has a slight acidity, mainly attributed to the existence of carboxylic, lactonic, and phenolic functional groups. In addition, the total basicity value (2.37 meq g^{-1}) was lower than the total acidity value (2.99 meq g^{-1}), this confirms the acid character of the AC.

The analysis of the IR spectrum (Fig. 4) of the raw processed activated carbon (before adsorption) showed mainly two bands. A band around 1600 cm^{-1} corresponds to the elongation vibration of the C=O group (carbonyls) or aromatic type vibrations C=C, and a wide band in the region $1000\text{--}1200 \text{ cm}^{-1}$, related to the elongation vibrations of the C–O group (carboxylic

and phenolic).

This observation corroborates the results of the Boehm assay, confirming the presence of polar functional groups likely to interact with CFTX molecules through hydrogen bonds or electrostatic interactions.

Adsorption studies

Adsorption kinetics

Adsorption kinetics experiments were performed to estimate the CFTX elimination rate of the aqueous solution and to better understand the adsorption mechanism of the adsorbents. Figure S5 illustrates the adsorption capacities of AC plotted against the contact time for varying initial concentrations of CFTX. The results showed that adsorption occurred rapidly during the first 30 min, then gradually slowed down to equilibrium after approximately 180 min with maximum adsorbed amounts ranging from 0.37 mg g⁻¹ to 1.36 mg g⁻¹ for initial CFTX concentrations of 4 and 20 mg L⁻¹, respectively. This can be explained by the abundance of unoccupied active sites at the beginning of the process, whose availability decreases over time, suggesting a saturation of the adsorbent surface⁶⁷. Furthermore, this relatively low adsorption capacity achieved can also be explained by the complexity of the CFTX molecule, comprising several functional groups, thus limiting its interaction with the carbon surface of the elaborated AC. Thus, its size and high spatial configuration may not be fully adapted with the pores of AC, despite its developed porosity and high specific surface area. However, although other materials^{69,70} have revealed better adsorption performances due to their very porous structures and large specific surfaces, the AC developed remains advantageous in terms of its low-cost synthesis from agro-industrial waste and their relatively simple preparation process.

To identify the most suitable kinetic model for describing CFTX retention on AC, the experimental adsorption data were adjusted in a non-linear manner using PFO, PSO, and intra-particle diffusion models. The parameters listed in Table 6 indicate that adsorption is most accurately represented by the PSO model, for all concentrations investigated. Indeed, it is distinguished by the highest values of the correlation coefficient (R²) and the smallest values of chi-square (χ²) and corrected Akaike Information Criterion (AIC_c). In addition, the q_e values calculated using this model are presents a great similarity with experimental data, thus confirming that the kinetics mainly follows a pseudo-second-

order model. This suggests a chemisorption process characterized by strong interaction forces⁶⁸. These results are consistent with another study⁷¹, indicating as well that the PSO model provides the best suited for describing antibiotics removal on AC derived from waste.

Although the analysis of FTIR spectra before and after adsorption does not reveal significant modifications, it nevertheless suggests the involvement of the C–O group in the adsorption mechanism, through the observation of a slight increase in the intensity of the characteristic band of the C–O, located in the region 1000–1200 cm⁻¹.

Adsorption isotherm

Adsorption isotherms represent the equilibrium correlation between the quantity of adsorbate retained by the adsorbent (q_e) and its concentration in the solution (C_e), at a fixed temperature. These isotherms offer information about the surface characteristics of the adsorbent and the affinity between the adsorbent and adsorbate, helping

to understand the retention mechanisms of pharmaceutical compounds in aqueous environments.

The experimental equilibrium data for CFTX adsorption on AC were fitted to various models, including thermodynamic (Langmuir, Freundlich, BET_{n-finite}, and BET_{n-infinite}) and statistical (STAT1, STAT2, and STAT3) models. The fitting curves of these models are illustrated

	Ceftriaxone concentration (mg L ⁻¹)						
	4	6	8	10	12	16	20
q _e (mg g ⁻¹)	0.37	0.55	0.61	0.77	0.92	1.22	1.36
Models	0.37	0.56	0.66	0.83	0.97	1.31	1.44
	0.05	0.04	0.03	0.02	0.02	0.01	0.01
	0.92	0.91	0.92	0.91	0.93	0.96	0.91
	—	—	—	—	—	—	—
	51.40	36.74	32.50	23.57	24.61	24.39	8.31
	0.23	0.54	0.62	1.12	0.74	1.08	2.83
	0.39	0.61	0.73	0.92	1.10	1.59	1.66
	0.20	0.11	0.06	0.03	0.02	0.00	0.01
	0.95	0.94	0.95	0.94	0.96	0.97	0.93
	—	—	—	—	—	—	—
	63.19	46.82	42.12	32.61	35.72	30.54	13.88
	0.07	0.20	0.25	0.49	0.30	0.62	1.55
	0.08	0.13	0.12	0.14	0.11	0.05	0.16
	0.02	0.03	0.04	0.04	0.05	0.07	0.08
	0.82	0.85	0.90	0.93	0.96	0.97	0.95
	—	—	—	—	—	—	—
	38.99	29.63	32.11	33.51	36.55	31.43	24.06
	0.20	0.26	0.23	0.21	0.18	0.14	0.27

Table 6. Parameters of kinetic models for various initial concentrations of CFTX.

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S M: Writing—review and editing, Writing—original draft, Methodology, Investigation, Formal analysis, Data curation, Conceptualization, Software. HD: Writing—review and editing, Resources, Project administration, Methodology, Software, Investigation, Formal analysis, Conceptualization, Validation.

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Declarations

Competing interests

The authors declare no competing interests.

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Viridi's CO₂-capturing surfactant cuts carbon footprints for cosmetics

UK-based company Viridi has unveiled Vireya, the “world’s first” anionic surfactant that captures CO₂ as a principal feedstock. The surfactant aims to eliminate palm oil-derived feedstocks while increasing product performance, benefitting suppliers amid tightening regulations.

Personal Care Insights sits down with Dr. Daniel Stewart, CEO and co-founder of Viridi. Stewart tells us that Vireya’s performance characteristics will find many potential uses across personal care, cosmetics, and home care applications.

“It differentiates itself because CO₂ is a renewable raw material that is everywhere, yet it has never been used commercially in surfactants. The results of this innovative product makeup are ground-breaking improvements in product carbon footprint and performance.”

“The new improved version of Sodium Laureth Sulfate (SLES) means everything from shampoos and body washes to facial cleansers and makeup removers could benefit from Vireya. It provides good foaming, great cleansing, and improved skin mildness compared to SLES.”

The tech company notes that the surfactant becomes available at a suitable time for suppliers amid tightened regulations such as the EU Deforestation Regulation (EUDR) and supply volatility.

“Vireya marks a fundamental change in surfactant chemistry,” says Stewart. “By replacing palm-based feedstocks with captured carbon dioxide, we enable the industry to drastically reduce product carbon footprint, ensure compliance with tightening regulations, and deliver better-performing ingredients for consumer products.”

The surfactant is expected to be available for commercial deployment in 2026.



Viridi says the surfactant has a 70% reduction in product carbon footprint.

Reducing carbon footprint

Viridi says the surfactant has a 70% reduction in product carbon footprint.

“The major driver of a product’s carbon footprint is most often the carbon intensity of its ingredients. Vireya uses CO₂ as its principal ingredient instead of oil palm-derived raw materials. As CO₂ has a carbon intensity that is on average five times lower than the raw materials it replaces, this leads to a reduced product carbon footprint,” explains Stewart.

He says that Viridi anticipates only positive impacts on the environment from the surfactant.

“In addition to carbon footprint improvements, the replacement of oil palm-derived inputs is likely to have a positive effect on deforestation and biodiversity loss. In addition, manufacturers will be putting to work already generated waste CO₂ that might otherwise become new emissions.”

Stewart tells us that Vireya can be produced in manufacturers’ existing facilities, requiring no new infrastructure. “This enables fast and cost-effective adoption at scale and the possibility of quickly

introducing this breakthrough into consumer products.”

The personal care industry has recently seen a shift toward using captured carbon. Mibelle Group, LanzaTech, and the Fraunhofer Institute for Interfacial Engineering and Biotechnology IGB co-developed a CO₂-derived ingredient to replace palm oil in cosmetics and everyday products.

Meanwhile, Unilever recently announced its shift toward thermal renewable energy and has taken a step to lower emissions at its Oleochemical Indonesia facility in North Sumatra, to “inspire positive change in the palm oil industry.” The facility is the largest greenhouse gas-emitting site of the company’s global operations.



The company says the surfactant does not contain any 1,4-dioxane.

Skin mildness by 10-fold

Viridi says the surfactant showed 10 times increase in skin mildness in tests. “We have tested skin mildness — or more correctly, potential irritancy — using the ‘zein test,’ an in vitro method commonly used in the industry. It tests the product’s ability to break down zein, a plant-based protein like our skin’s keratin,” says Stewart.

“A low result in this test, as we achieved, suggests lower skin irritation potential. This is being validated by brand owners with whom Viridi is collaborating.”

Meanwhile, the company shares that it does not contain any 1,4-dioxane, a synthetic industrial chemical. The chemical is widely used as a stabilizer in various formulations and is frequently linked to chlorinated solvents. It is a byproduct or contaminant in consumer goods such as shampoo and laundry detergent. The US FDA has previously said 1,4-dioxane may be a trace contaminant in cosmetics and a potential carcinogen.

Source: Personal Care Insights

Indonesia takes another step towards B50 biodiesel



A general view of a palm oil plantation in Siak regency, Riau province, Indonesia, April 26, 2022. Picture taken with a drone on April 26, 2022.

Indonesia took another step towards launching biodiesel containing 50% palm-oil based biofuel (B50) by concluding laboratory tests, an energy ministry official said on Tuesday, as the country aims for implementation next year.

Palm-oil based biodiesel is currently mandated at 40% blend (B40) but Indonesia wants to increase the level to reduce its reliance on imports of fossil fuels.

The laboratory testing involved running an engine using the B50 fuel and was concluded in August. Officials will now carry out road tests, the energy

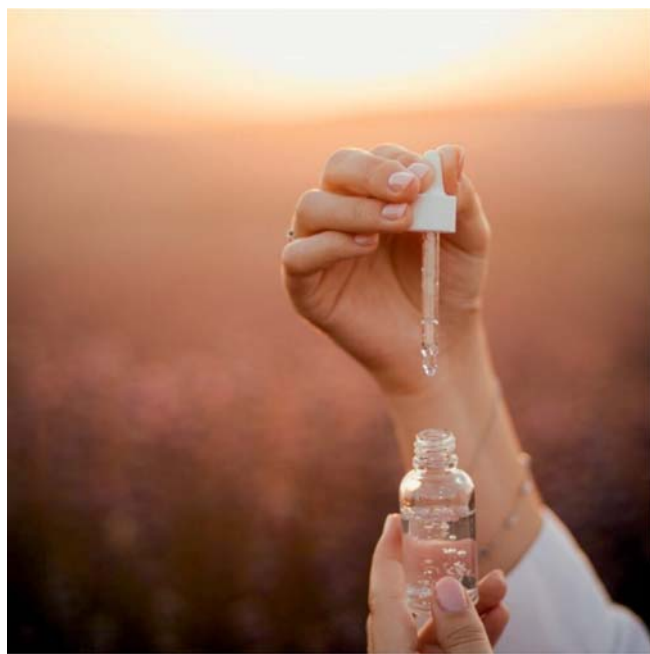
ministry's bioenergy director, Edi Wibowo, told Reuters. "Based on the test results we will move forward to launch road tests and testing on non-automotive machineries that run on diesel," he said.

The timing of the road test was still to be decided, he said.

Indonesia aims to make B50 mandatory in 2026, but it was unlikely to happen in January, a senior energy ministry official said in August. Adopting B50 would require 20.1 million kilolitres of palm-oil based biofuel a year for mixing with regular petroleum diesel, compared to 15.6 million KL with B40, energy ministry data shows.

Source: REUTERS

Sasol introduces bio-circular insect oil surfactant for cleaning industries



Sasol International Chemicals announced the launch of LIVINEX IO 7, a pioneering bio-circular surfactant. This innovative product is derived from insect oils and is palm-free and deforestation-free. It is now available for commercial use, primarily targeting the care chemicals markets across Europe.

LIVINEX IO 7 is the first nonionic surfactant of its kind in the fabric, home care, industrial, and institutional cleaning sectors. This patent-pending product transforms insect oil—by-product of [sustainable protein](#) production for animal feed—into a valuable chemical feedstock.

It offers a sustainable alternative to traditional oleochemicals derived from palm oil or other plant sources.

Louis Snyders, Vice President of Care Chemicals at Sasol, stated that LIVINEX IO 7 broadens Sasol's portfolio of sustainable offerings. He emphasized that the surfactant demonstrates Sasol's innovation skills and commitment to helping customers meet evolving sustainability requirements. LIVINEX IO 7 is a drop-in replacement for conventional C12-14-based chemistry, allowing easy integration into existing formulations.

Unlike other natural surfactants that often require reformulation, LIVINEX IO 7 can be seamlessly incorporated into current cleaning products. It is made from oil obtained from black soldier fly larvae, which is rich in fatty acids used to produce detergent-grade alcohols. Since insect oil chemistry matches that of vegetable oil, mature technology and existing manufacturing processes can be employed, avoiding land use change or food crop competition.

Snyders added that as global demand for sustainable products grows, Sasol plans to continue exploring and commercializing innovations like LIVINEX IO 7. The company aims to offer a diverse mix of high-performing synthetic and renewable solutions, aligning with its focus on sustainable resource use.

Sasol intends to expand its innovation pipeline to include insect oil-based products for the personal care industry. The company previously launched LIVINEX and CARINEX brands featuring sophorolipids in 2023.

Source: World Bio Market Insights

Biodiesel fuel blend could help future of farming and trucking

A new biodiesel blend, B-99, is made of soybeans and other oils. It is gaining traction, with the first two retail pumps in Iowa and Illinois.

A higher blend of biodiesel is catching the eye of a number of companies and the hopes of some farmers. Rob Shaffer grows soybeans in El Paso, Illinois. He said the biodiesel, B-99 or B-100, could boost demand for his crops and strengthen national energy independence. “With profits being challenging with input costs, cash rents, and lower commodity prices, anything we can help to stimulate demand means people buying our products, which helps the price go up,” he said. “It helps us farmers, you know, make ends meet and be able to hopefully pass my farm down to the 5th generation.”

The renewable fuel is made almost entirely, 99-100%, of soybeans, cooking oil, and animal fats. Heavy-duty trucks are able to run on the fuel with the addition of a three-part system created by Optimus Technologies. The retrofit starts the engine with regular diesel fuel, which generates heat to keep the biodiesel from gelling in cold conditions. The system then switches over to run on the renewable fuel.

Eric Dean, who works for the company, said the vector system allows nearly any Class 8 truck to switch from standard diesel to B-100 biodiesel. “We are the lowest cost way to decarbonize,” Dean said. “It’s the least amount of change to your daily operations.”

Partners for Pumps

The technology can already be spotted in semis refueling in two midwestern states. Pilot Flying J opened the first retail B-99 location in Decatur, Illinois, in March and the second location in Urbandale, Iowa, in May. The new fuel pumps are driven by connections with major companies like PepsiCo and ADM.

“What we’re doing is we’re leveraging the Pilot travel centers to help us kind of build that momentum with fueling our trucks,” said Brandon Rick, the Fleet and Sustainability Manager at Archer-Daniels Midland (ADM).

ADM started a B-100 pilot program in 2019. Rick said they tested five trucks for 18 months and found comparable fuel mileage, lower regeneration of their engines, and less ash accumulation in DPF filters. At the end of August, ADM said they had 50 trucks fitted with the technology running in Decatur. Rick estimates that in the company’s first full year, the fleet will reduce their carbon emissions by about 3,500 metric tons of CO₂. “In the Midwest, it really feels awesome to tell that story of that farmer who’s sending their soybeans,” Rick said. “Our crush facilities make soybean oil and then in turn we’re using that to make biofuels. That is a true circle for us, a closed loop of sustainability.”

PepsiCo has its B-99 fleet spread out across the central and eastern parts of the U.S. The company has over 700 trucks with the Optimus Technology, one of the largest private groups of trucks in the country.

PepsiCo over-the-road driver Brian Bassett said he’s been driving an altered truck for over two years and has put 200,000 miles on his vehicle. He said it’s one of numerous pushes by PepsiCo to be more sustainable. “There’s really no difference between a diesel and a biodiesel,” he said. “No change in power, no change in really fuel mileage. There is really no change at all.”

Source: WQAD.com

Sustainable Ultrasound-Enhanced Extraction of Apple Seed Oil

In recent years, the quest for environmentally friendly and efficient extraction methods has gained paramount importance within the field of food science

and sustainable development. The extraction of oils from various agricultural by-products has emerged as a promising avenue, not only for maximizing resource utilization but also for contributing to the circular economy.

A recent study by Wang et al. has brought significant insights into the extraction process of apple seed oil, showcasing innovative techniques that may revolutionize how we approach oil extraction from plant sources.

Apple seeds, often overlooked as agricultural waste, possess valuable oil that is packed with nutrients and bioactive compounds. This oil holds potential applications in cosmetics, food, and health-related industries due to its rich fatty acid profile and antioxidant properties. With the increasing demand for natural and functional ingredients, the efficient extraction of apple seed oil is more critical than ever.

The research spearheaded by Wang and colleagues' focuses on optimizing the extraction process using ultrasound-assisted enzymatic techniques combined with semi-bionic methods that utilize sustainable solvents.

The innovative approach taken by the researchers involves ultrasonic waves to enhance the enzymatic action during the extraction, allowing for higher yields in a shorter timeframe. This method capitalizes on the physical and chemical effects of ultrasound, which facilitates the breakdown of cell walls and releases oil more effectively than traditional extraction methods. This breakthrough not only increases the efficiency of the extraction but also reduces the energy costs associated with the process, which is a crucial factor when considering sustainability.

Moreover, the study highlights the use of sustainable solvents rather than conventional organic solvents that can have detrimental ecological effects. By employing greener alternatives, the extraction process aligns with the principles of green chemistry, aiming to minimize toxic waste and environmental impact. By optimizing the ratios and conditions of these solvents,

the researchers were able to improve oil quality while keeping the environmental footprint to a minimum, thus setting a benchmark for future studies in oil extraction.

The semi-bionic methodology introduced in this research signifies a blend between biological processes and advanced technology. This hybrid approach not only enhances extraction efficiency but also leverages the natural enzymatic activity of biological catalysts, promoting a sustainable practice that could transform various extraction processes across the food industry. The combination of these techniques presents a multifaceted strategy that could enhance the value of other agricultural residues, extending beyond apple seeds.

In conducting this research, the team meticulously analyzed several variables that influence oil yield and quality. Factors such as temperature, extraction time, and enzyme concentrations were systematically varied to ascertain the optimal conditions for maximum oil extraction. Such rigorous experimentation ensures that the methodologies proposed are grounded in scientific evidence, lending credibility to their potential for real-world application in the food processing sector.

Furthermore, the implications of this study reach beyond mere extraction; they provoke a broader discourse on agricultural waste management. By finding viable uses for by-products like apple seeds, we not only contribute to waste reduction but also generate high-value products. This aligns well with the overarching goal of promoting sustainability in agricultural practices, where every part of the plant is utilized rather than discarded.

The nutrient profile of apple seed oil, coupled with its health benefits, makes it an attractive target for food scientists and manufacturers alike. With rising consumer awareness regarding dietary health and wellness, the demand for oils that offer functional benefits is steadily increasing. Therefore, the capacity to extract high-quality oil in an environmentally

responsible manner positions apple seed oil as a competitive product in the marketplace.

As the research community continues to explore innovative techniques in the realm of oil extraction, Wang et al.'s findings serve as a pivotal reference point for future studies. Their work invites further exploration into other sustainable methods that can be incorporated into existing agricultural practices, reinforcing the importance of interdisciplinary collaboration between agriculture, chemistry, and food science.

Looking ahead, widespread adoption of these extraction methods could pave the way for a new era of food production that is not only profitable but also mindful of the planet's resources. The continued pursuit of sustainable practices within the food industry is vital for engendering a systemic change that prioritizes environmental responsibility alongside economic viability.

Through their interdisciplinary approach and commitment to sustainability, Wang and his team have opened doors to further research opportunities. Their findings lay the groundwork for additional innovation, inviting other researchers to explore the potential of ultrasound-assisted techniques in different sectors and for varying types of plant-based oils. Such collaboration is essential for tackling the grand challenges posed by food security and environmental degradation in the contemporary world.

Ultimately, the optimization of oil extraction processes, as evidenced by this study, symbolizes a

tangible step toward achieving a more sustainable future. As innovative methodologies take root in academia and industry, there lies a significant promise of reducing waste, maximizing resource use, and enhancing the nutritional value of products. The transformation of apple seeds from waste to wealth exemplifies the potential of scientific inquiry to effect meaningful change in our food systems.

The culmination of such research not only demonstrates technical proficiency but also a commitment to developing practices that are both innovative and eco-friendly. As industries gradually shift towards adopting sustainable practices, the groundwork laid by researchers like Wang et al. will serve as an invaluable asset in contextualizing and advancing our understanding of extraction in the age of environmental awareness.

In essence, this research represents a paradigm shift in how we valorize agricultural by-products, driving the conversation about sustainability within the food production industry. The integration of ultrasound-assisted enzymatic methods with sustainable solvents demonstrates a proactive approach towards fostering an ecological balance in extracting valuable resources while minimizing harm to our planet.

This groundbreaking study stands as an impetus for future research and development in oil extraction methodologies, emphasizing a trajectory that prioritizes sustainability without sacrificing efficiency or quality in the quest for valuable resources.

Source: Bioengineer.com

IMPORTANT FIGURES

Table 01: Major Oilseeds: World Supply and Distribution (Commodity View)

Million Metric Tons

	2022/23	2023/24	2024/25	2025/26
Production				
Oilseed, Copra	6.05	6.27	6.12	5.92
Oilseed, Cottonseed	40.31	39.48	41.16	42.39
Oilseed, Palm Kernel	19.78	19.60	20.35	21.11
Oilseed, Peanut	49.81	50.02	51.87	51.24
Oilseed, Rapeseed	89.86	89.97	86.26	95.51
Oilseed, Soybean	378.21	396.45	427.89	427.60
Oilseed, Sunflowerseed	52.78	55.93	53.01	54.74
Total	636.79	657.72	686.65	698.51
Imports				
Oilseed, Copra	0.08	0.08	0.09	0.10
Oilseed, Cottonseed	1.37	1.19	0.93	1.04
Oilseed, Palm Kernel	0.16	0.19	0.22	0.23
Oilseed, Peanut	4.18	4.10	3.73	4.09
Oilseed, Rapeseed	20.07	18.26	20.00	17.58
Oilseed, Soybean	168.50	178.54	179.19	184.77
Oilseed, Sunflowerseed	3.77	2.54	2.61	3.22
Total	198.12	204.89	206.77	211.02
Exports				
Oilseed, Copra	0.10	0.09	0.08	0.09
Oilseed, Cottonseed	1.09	1.21	0.90	1.30
Oilseed, Palm Kernel	0.06	0.09	0.17	0.05
Oilseed, Peanut	4.85	4.80	4.66	4.75
Oilseed, Rapeseed	19.80	18.56	19.82	18.11
Oilseed, Soybean	171.76	177.76	184.17	186.57
Oilseed, Sunflowerseed	4.02	2.72	3.37	3.44
Total	201.68	205.23	213.17	214.31
Crush				
Oilseed, Copra	5.90	6.18	6.06	5.86
Oilseed, Cottonseed	30.22	31.41	31.26	31.31
Oilseed, Palm Kernel	19.77	19.46	20.22	21.11
Oilseed, Peanut	19.08	18.44	19.35	19.33
Oilseed, Rapeseed	82.11	84.68	84.61	88.72
Oilseed, Soybean	315.77	331.25	359.09	369.53
Oilseed, Sunflowerseed	51.36	52.26	48.25	49.63
Total	524.20	543.68	568.84	585.48
Ending Stocks				
Oilseed, Copra	0.07	0.06	0.06	0.05
Oilseed, Cottonseed	1.46	1.62	1.53	1.55
Oilseed, Palm Kernel	0.29	0.34	0.32	0.36
Oilseed, Peanut	4.32	3.85	4.04	4.31
Oilseed, Rapeseed	11.00	11.95	9.93	11.83
Oilseed, Soybean	101.83	115.13	125.91	125.13
Oilseed, Sunflowerseed	4.12	3.20	2.54	2.83
Total	123.08	136.13	144.33	146.07

Source: Foreign Agricultural Service/USDA Global Market Analysis

Table 02: Major Protein Meals: World Supply and Distribution (Commodity View)

Million Metric Tons

	2022/23	2023/24	2024/25	2025/26
Production				
Meal, Copra	1.96	2.04	2.00	1.93
Meal, Cottonseed	13.93	14.45	14.41	14.40
Meal, Fish	4.54	5.14	5.28	5.31
Meal, Palm Kernel	10.28	10.08	10.58	10.87
Meal, Peanut	7.62	7.38	7.78	7.76
Meal, Rapeseed	47.81	49.21	49.28	51.45
Meal, Soybean	248.39	259.86	281.74	290.33
Meal, Sunflowerseed	23.05	23.24	21.41	22.05
Total	357.57	371.39	392.48	404.10
Imports				
Meal, Copra	0.61	0.55	0.56	0.58
Meal, Cottonseed	0.20	0.19	0.23	0.19
Meal, Fish	3.36	3.62	3.95	3.79
Meal, Palm Kernel	7.70	7.41	7.26	7.93
Meal, Peanut	0.12	0.09	0.04	0.12
Meal, Rapeseed	9.30	9.93	10.15	10.92
Meal, Soybean	63.31	69.60	77.71	80.14
Meal, Sunflowerseed	8.55	10.16	7.75	7.88
Total	93.15	101.54	107.64	111.55
Exports				
Meal, Copra	0.56	0.54	0.53	0.55
Meal, Cottonseed	0.30	0.31	0.35	0.30
Meal, Fish	2.55	2.97	3.15	3.19
Meal, Palm Kernel	8.06	7.28	7.69	7.85
Meal, Peanut	0.18	0.12	0.10	0.16
Meal, Rapeseed	9.79	10.22	10.72	11.22
Meal, Soybean	67.07	74.22	83.04	83.95
Meal, Sunflowerseed	9.16	10.22	8.76	8.64
Total	97.66	105.88	114.34	115.85
Domestic Consumption				
Meal, Copra	2.01	2.02	2.02	1.98
Meal, Cottonseed	13.81	14.34	14.27	14.23
Meal, Fish	5.37	5.79	6.03	5.94
Meal, Palm Kernel	9.94	10.25	10.03	10.85
Meal, Peanut	7.58	7.34	7.73	7.73
Meal, Rapeseed	47.54	48.69	48.79	51.01
Meal, Soybean	247.04	255.09	272.78	285.57
Meal, Sunflowerseed	21.77	22.86	20.59	21.25
Total	355.06	366.40	382.22	398.54
Ending Stocks				
Meal, Copra	0.05	0.08	0.09	0.06
Meal, Cottonseed	0.11	0.10	0.11	0.18
Meal, Fish	0.25	0.24	0.29	0.27
Meal, Palm Kernel	0.62	0.57	0.69	0.79
Meal, Peanut	0.02	0.03	0.03	0.02
Meal, Rapeseed	1.26	1.50	1.43	1.58
Meal, Soybean	14.17	14.31	17.94	18.89
Meal, Sunflowerseed	1.81	2.13	1.93	1.97
Total	18.30	18.95	22.51	23.76

Source: Foreign Agricultural Service/USDA Global Market Analysis

Table 03: Major Vegetable Oils: World Supply and Distribution (Commodity View)

Million Metric Tons

	2022/23	2023/24	2024/25	2025/26
Production				
Oil, Coconut	3.71	3.88	3.83	3.70
Oil, Cottonseed	4.56	4.74	4.71	4.73
Oil, Olive	2.53	2.44	3.33	3.28
Oil, Palm	76.72	76.09	78.84	81.27
Oil, Palm Kernel	8.76	8.61	8.93	9.28
Oil, Peanut	6.20	6.00	6.31	6.31
Oil, Rapeseed	33.25	34.39	34.27	36.00
Oil, Soybean	60.73	64.01	70.06	71.81
Oil, Sunflowerseed	21.71	22.12	20.41	20.93
Total	218.16	222.27	230.71	237.31
Imports				
Oil, Coconut	1.93	2.18	1.86	1.92
Oil, Cottonseed	0.09	0.08	0.07	0.09
Oil, Olive	1.08	1.11	1.24	1.27
Oil, Palm	46.64	42.36	41.36	43.46
Oil, Palm Kernel	2.69	2.72	2.69	2.69
Oil, Peanut	0.39	0.34	0.47	0.37
Oil, Rapeseed	6.90	7.50	7.08	7.51
Oil, Soybean	10.98	10.53	14.30	12.78
Oil, Sunflowerseed	12.61	13.96	12.01	11.61
Total	83.30	80.77	81.06	81.70
Exports				
Oil, Coconut	2.18	2.47	2.24	2.01
Oil, Cottonseed	0.08	0.05	0.06	0.08
Oil, Olive	1.21	1.17	1.35	1.40
Oil, Palm	49.37	44.41	45.02	45.74
Oil, Palm Kernel	2.97	3.09	3.17	3.20
Oil, Peanut	0.35	0.37	0.59	0.44
Oil, Rapeseed	6.54	7.52	7.14	8.03
Oil, Soybean	11.74	11.81	15.26	14.13
Oil, Sunflowerseed	14.31	15.34	13.66	13.40
Total	88.75	86.23	88.48	88.43
Domestic Consumption				
Oil, Coconut	3.43	3.64	3.56	3.66
Oil, Cottonseed	4.57	4.72	4.73	4.72
Oil, Olive	2.58	2.48	3.14	3.04
Oil, Palm	73.82	75.05	76.18	78.53
Oil, Palm Kernel	8.48	8.23	8.44	8.69
Oil, Peanut	6.20	6.03	6.15	6.22
Oil, Rapeseed	32.71	34.35	34.38	35.53
Oil, Soybean	59.42	62.90	68.31	71.01
Oil, Sunflowerseed	19.55	21.07	19.10	19.26
Total	210.78	218.47	223.99	230.65
Ending Stocks				
Oil, Coconut	0.89	0.85	0.75	0.70
Oil, Cottonseed	0.15	0.19	0.18	0.20
Oil, Olive	0.53	0.42	0.50	0.60
Oil, Palm	16.99	15.98	14.98	15.44
Oil, Palm Kernel	0.96	0.96	0.97	1.05
Oil, Peanut	0.39	0.33	0.37	0.40
Oil, Rapeseed	3.44	3.46	3.29	3.25
Oil, Soybean	5.85	5.68	6.47	5.93
Oil, Sunflowerseed	3.22	2.89	2.55	2.44
Total	32.43	30.76	30.06	30.00

Source: Foreign Agricultural Service/USDA Global Market Analysis

Table 04: Major Oilseeds: World Supply and Distribution (Commodity View)

Million Metric Tons

	2022/23	2023/24	2024/25	2025/26
Production				
Brazil	166.91	160.29	179.56	187.94
United States	125.75	122.16	128.59	126.17
China	66.87	66.92	67.81	69.37
Argentina	31.45	54.24	59.10	56.73
India	42.31	41.39	42.83	41.77
Other	203.50	212.71	208.77	216.54
Total	636.79	657.72	686.65	698.51
Imports				
China	111.71	119.13	113.51	117.18
European Union	22.34	20.70	24.21	20.99
Mexico	8.14	7.86	7.85	8.32
Argentina	9.06	7.79	6.33	7.30
Turkey	4.02	3.71	5.02	5.30
Japan	5.49	5.41	5.57	5.71
Egypt	2.00	3.33	4.56	4.63
Thailand	3.34	3.53	4.29	4.32
Pakistan	1.50	1.89	2.60	3.61
Vietnam	2.21	2.51	2.83	3.29
Other	28.31	29.03	30.00	30.39
Total	198.12	204.89	206.77	211.02
Exports				
Brazil	95.92	104.52	103.59	115.62
United States	54.77	47.49	52.29	42.78
Canada	12.22	11.73	14.99	12.75
Argentina	5.11	6.13	9.61	10.13
Paraguay	6.50	8.00	6.43	8.22
Australia	6.98	6.62	5.75	6.26
Ukraine	8.37	7.28	7.39	4.65
Other	11.80	13.47	13.14	13.89
Total	201.68	205.23	213.17	214.31
Crush				
China	134.00	137.20	141.83	146.40
United States	64.16	66.23	70.43	75.39
Brazil	57.54	59.43	63.99	67.97
Argentina	34.60	40.58	48.44	47.30
European Union	48.25	48.29	46.92	47.21
India	34.78	35.63	35.64	34.11
Russia	24.50	25.70	26.23	27.60
Ukraine	15.68	18.55	15.70	15.10
Canada	11.73	12.69	13.09	13.70
Indonesia	13.25	12.59	13.44	13.82
Mexico	8.13	7.70	7.82	8.15
Pakistan	4.01	5.10	5.16	6.27
Turkey	6.03	5.18	6.14	6.15
Malaysia	5.08	5.38	5.20	5.52
Egypt	2.35	3.39	4.67	4.74
Other	60.11	60.06	64.15	66.08
Total	524.20	543.68	568.84	585.48
Ending Stocks				
China	36.71	48.35	48.95	48.21
Brazil	37.00	29.97	38.05	38.17
Argentina	18.34	25.38	25.94	24.58
United States	8.85	10.81	10.23	11.24
European Union	3.49	3.92	4.26	4.21
Other	18.70	17.70	16.90	19.67
Total	123.08	136.13	144.33	146.07

Source: Foreign Agricultural Service/USDA Global Market Analysis

Table 05: Major Protein Meals: World Supply and Distribution (Commodity View)

Million Metric Tons

	2022/23	2023/24	2024/25	2025/26
Production				
China	95.71	98.24	101.91	105.48
United States	49.93	51.43	55.27	59.11
Brazil	43.45	44.24	47.14	50.46
Argentina	25.58	30.16	35.86	34.75
European Union	30.74	30.82	30.26	30.33
Other	112.17	116.50	122.04	123.97
Total	357.57	371.39	392.48	404.10
Imports				
European Union	21.49	22.38	25.23	24.70
Vietnam	5.85	7.02	6.81	7.59
China	8.39	9.39	7.93	8.37
Indonesia	5.67	5.24	6.44	6.42
United States	4.31	4.29	4.95	5.09
Thailand	4.01	3.60	3.51	3.77
United Kingdom	2.76	3.26	3.87	3.91
Other	40.68	46.37	48.91	51.71
Total	93.15	101.54	107.64	111.55
Exports				
Argentina	21.92	26.07	31.47	30.83
Brazil	21.33	22.72	23.39	25.00
United States	13.39	14.75	16.78	18.17
Canada	5.70	5.98	6.17	6.28
Ukraine	4.60	5.78	4.99	4.83
Indonesia	5.87	4.92	5.29	5.41
Russia	3.82	4.30	4.16	4.34
Other	21.03	21.35	22.10	20.99
Total	97.66	105.88	114.34	115.85
Domestic Consumption				
China	103.04	106.32	108.62	112.00
European Union	49.53	50.08	52.44	53.03
United States	40.78	40.90	43.48	45.98
Brazil	21.95	22.38	23.26	24.74
India	17.59	18.15	18.02	18.14
Russia	8.93	9.36	9.83	10.36
Vietnam	7.25	8.05	8.79	9.48
Mexico	7.82	7.82	8.17	8.90
Indonesia	6.62	6.85	7.59	7.95
Thailand	6.26	6.02	6.00	6.58
Other	85.29	90.48	96.03	101.40
Total	355.06	366.40	382.22	398.54
SME				
China	96.11	99.39	102.29	105.64
European Union	42.18	42.67	45.71	46.00
United States	39.34	39.46	41.92	44.36
Brazil	21.58	21.93	22.76	24.21
India	14.94	15.37	15.34	15.38
Vietnam	6.77	7.64	8.37	9.02
Mexico	7.54	7.59	7.95	8.65
Other	95.63	100.58	107.12	113.12
Total	324.08	334.64	351.44	366.38
Ending Stocks				
Brazil	3.83	2.99	3.49	4.22
Argentina	2.59	2.47	2.94	2.69
European Union	1.27	1.72	2.49	2.32
China	0.94	0.79	0.94	1.28
Russia	0.71	0.75	0.83	1.01
Other	8.96	10.24	11.83	12.25
Total	18.30	18.95	22.51	23.76

Source: Foreign Agricultural Service/USDA Global Market Analysis

Table 06: Major Vegetable Oils: World Supply and Distribution (Commodity View)

Million Metric Tons

	2022/23	2023/24	2024/25	2025/26
Production				
Indonesia	51.10	48.81	51.74	53.11
China	30.41	31.06	32.40	33.27
Malaysia	20.59	22.03	21.61	22.55
European Union	18.33	18.48	18.25	18.49
United States	13.18	13.59	14.49	15.25
Brazil	11.94	12.57	13.56	14.40
Argentina	7.84	9.04	10.91	10.81
Other	64.77	66.70	67.75	69.44
Total	218.16	222.27	230.71	237.31
Imports				
India	17.12	15.85	16.29	16.54
China	11.35	9.14	7.51	8.37
European Union	9.17	9.62	8.01	8.62
United States	6.27	6.87	5.92	6.05
Pakistan	3.34	3.09	3.74	3.85
Turkey	2.75	2.41	2.12	2.33
Bangladesh	2.32	2.33	2.48	2.40
Egypt	1.64	1.81	1.80	2.00
Iran	1.75	1.34	1.74	1.28
Philippines	0.96	1.23	1.59	1.43
Other	26.63	27.10	29.88	28.83
Total	83.30	80.77	81.06	81.70
Exports				
Indonesia	30.25	24.46	25.49	25.90
Malaysia	16.64	17.82	16.98	17.67
Argentina	5.33	6.80	8.89	8.22
Russia	6.07	6.50	6.31	6.51
Ukraine	5.99	7.04	5.48	5.39
Canada	3.17	3.60	3.48	3.69
European Union	3.67	3.27	2.98	3.17
Other	17.64	16.76	18.87	17.88
Total	88.75	86.23	88.48	88.43
Domestic Consumption				
China	39.46	40.44	40.43	40.89
Indonesia	23.23	24.90	26.52	27.17
India	23.86	24.75	25.39	26.05
European Union	24.49	24.39	23.74	23.93
United States	19.27	20.13	19.05	20.55
Brazil	10.15	12.31	12.67	13.41
Malaysia	5.40	5.26	5.59	5.70
Pakistan	4.29	4.35	4.75	5.18
Russia	3.70	3.80	3.95	4.09
Bangladesh	3.12	3.18	3.43	3.57
Thailand	2.98	2.97	2.99	3.32
Mexico	3.17	3.13	3.18	3.28
Canada	1.73	2.19	2.34	3.01
Nigeria	2.66	2.71	2.88	2.94
Egypt	2.05	2.23	2.42	2.62
Other	41.22	41.74	44.66	44.96
Total	210.78	218.47	223.99	230.65
Ending Stocks				
Indonesia	5.64	5.24	5.07	5.20
India	4.37	4.63	4.69	4.29
Malaysia	2.87	2.56	2.74	2.83
China	3.73	3.32	2.44	2.35
European Union	2.10	2.55	2.08	2.09
Other	13.71	12.47	13.06	13.25
Total	32.43	30.76	30.06	30.00

Source: Foreign Agricultural Service/USDA Global Market Analysis

Table 07: Middle East Oilseeds and Products Supply and Distribution

Thousand Metric Tons

	2022/23	2023/24	2024/25	2025/26
Production				
Oilseed, Cottonseed	1,848	1,227	1,492	1,199
Oilseed, Rapeseed	470	470	475	475
Oilseed, Soybean	317	309	324	324
Oilseed, Sunflowerseed	1,946	1,595	1,399	1,299
Other	186	200	205	200
Total	4,767	3,801	3,895	3,497
Domestic Consumption				
Meal, Cottonseed	998	682	803	670
Meal, Soybean	9,746	11,748	12,622	12,660
Meal, Sunflowerseed	2,252	2,435	2,190	2,456
Other	1,250	1,075	1,137	1,235
Total	14,246	15,940	16,752	17,021
SME				
Meal, Cottonseed	809	553	651	543
Meal, Soybean	9,744	11,748	12,622	12,660
Meal, Sunflowerseed	1,502	1,624	1,461	1,638
Other	924	841	862	927
Total	12,978	14,765	15,595	15,768
Imports				
Meal, Cottonseed	12	32	11	29
Meal, Soybean	5,372	8,229	8,194	7,945
Meal, Sunflowerseed	1,059	1,519	1,198	1,370
Other	710	629	670	826
Total	7,153	10,409	10,073	10,170
Imports				
Oil, Palm	3,514	3,559	3,656	3,295
Oil, Rapeseed	148	111	135	107
Oil, Soybean	523	152	238	318
Oil, Sunflowerseed	3,617	3,405	3,617	3,075
Other	255	220	216	224
Total	8,057	7,447	7,862	7,019
Industrial Dom. Cons.				
Oil, Palm	245	240	255	245
Oil, Rapeseed	25	25	25	25
Oil, Soybean	55	50	50	50
Oil, Sunflowerseed	25	25	25	25
Other	37	40	35	42
Total	387	380	390	387
Food Use Dom. Cons.				
Oil, Palm	2,667	2,726	2,770	2,680
Oil, Rapeseed	379	320	360	340
Oil, Soybean	1,186	909	747	979
Oil, Sunflowerseed	3,073	3,505	3,285	3,355
Other	758	637	916	657
Total	8,063	8,097	8,078	8,011
Domestic Consumption				
Oil, Palm	2,912	2,966	3,025	2,925
Oil, Rapeseed	404	345	385	365
Oil, Soybean	1,246	964	827	1,059
Oil, Sunflowerseed	3,113	3,545	3,325	3,395
Other	795	677	951	699
Total	8,470	8,497	8,513	8,443

Source: Foreign Agricultural Service/USDA Global Market Analysis

Table 08: European Union Oilseeds and Products Supply and Distribution

Thousand Metric Tons

	2022/23	2023/24	2024/25	2025/26
Production				
Oilseed, Rapeseed	19,613	20,431	17,073	20,522
Oilseed, Soybean	2,610	2,811	2,911	2,854
Oilseed, Sunflowerseed	9,386	10,051	8,645	8,655
Other	526	344	400	385
Total	32,135	33,637	29,029	32,416
Domestic Consumption				
Meal, Rapeseed	13,800	13,900	13,100	14,000
Meal, Soybean	26,642	27,042	31,242	30,942
Meal, Sunflowerseed	6,860	7,110	6,260	6,160
Other	2,232	2,029	1,841	1,923
Total	49,534	50,081	52,443	53,025
SME				
Meal, Rapeseed	9,819	9,890	9,321	9,961
Meal, Soybean	26,600	27,000	31,200	30,900
Meal, Sunflowerseed	4,536	4,702	4,135	4,069
Other	1,230	1,075	1,050	1,070
Total	42,184	42,667	45,706	46,000
Imports				
Meal, Rapeseed	846	839	420	850
Meal, Soybean	15,997	16,564	20,609	19,600
Meal, Sunflowerseed	2,753	3,238	2,567	2,600
Other	1,892	1,736	1,633	1,648
Total	21,488	22,377	25,229	24,698
Industrial Dom. Cons.				
Oil, Palm	2,200	1,850	1,300	1,350
Oil, Rapeseed	6,975	7,050	6,750	6,900
Oil, Soybean	1,100	1,150	1,400	1,250
Oil, Sunflowerseed	550	550	475	500
Other	555	555	535	535
Total	11,380	11,155	10,460	10,535
Food Use Dom. Cons.				
Oil, Palm	2,150	1,880	1,800	1,900
Oil, Rapeseed	2,900	2,850	2,900	3,200
Oil, Soybean	1,250	1,425	1,550	1,400
Oil, Sunflowerseed	4,650	4,950	4,725	4,500
Other	1,887	1,852	2,089	2,177
Total	12,837	12,957	13,064	13,177
Domestic Consumption				
Oil, Palm	4,500	3,890	3,200	3,350
Oil, Rapeseed	9,925	9,950	9,700	10,150
Oil, Soybean	2,405	2,630	3,005	2,705
Oil, Sunflowerseed	5,213	5,513	5,213	5,013
Other	2,447	2,407	2,624	2,712
Total	24,490	24,390	23,742	23,930
Imports				
Oil, Palm	4,576	4,013	3,135	3,500
Oil, Rapeseed	391	463	295	500
Oil, Soybean	641	592	757	650
Oil, Sunflowerseed	2,103	3,022	2,411	2,475
Other	1,461	1,534	1,407	1,495
Total	9,172	9,624	8,005	8,620

Source: Foreign Agricultural Service/USDA Global Market Analysis

Table 09: China Oilseeds and Products Supply and Distribution

Thousand Metric Tons

	2022/23	2023/24	2024/25	2025/26
Production				
Oilseed, Peanut	18,330	19,231	19,000	18,400
Oilseed, Rapeseed	16,317	15,800	15,800	16,000
Oilseed, Soybean	20,284	20,840	20,650	20,900
Oilseed, Sunflowerseed	1,741	1,983	1,750	2,200
Other	10,196	9,069	10,611	11,871
Total	66,868	66,923	67,811	69,371
Imports				
Oilseed, Peanut	940	774	448	700
Oilseed, Rapeseed	5,335	5,486	4,600	4,000
Oilseed, Soybean	104,500	112,000	108,000	112,000
Oilseed, Sunflowerseed	266	183	132	125
Other	665	690	332	350
Total	111,706	119,133	113,512	117,175
Domestic Consumption				
Meal, Peanut	4,005	3,973	3,885	3,978
Meal, Rapeseed	13,512	14,519	14,639	14,084
Meal, Soybean	75,050	77,150	80,850	84,150
Other	10,472	10,678	9,249	9,788
Total	103,039	106,320	108,623	112,000
SME				
Meal, Peanut	4,502	4,466	4,367	4,471
Meal, Rapeseed	9,276	9,992	10,074	9,679
Meal, Soybean	73,900	76,000	79,700	83,000
Other	8,435	8,936	8,147	8,494
Total	96,112	99,394	102,288	105,644
Food Use Dom. Cons.				
Oil, Palm	3,100	2,800	1,800	2,600
Oil, Peanut	3,418	3,373	3,440	3,344
Oil, Rapeseed	8,800	9,700	10,350	10,000
Oil, Soybean	17,900	18,900	20,500	20,500
Oil, Sunflowerseed	1,803	1,419	717	793
Other	1,387	1,369	1,367	1,404
Total	36,408	37,561	38,174	38,641
Domestic Consumption				
Oil, Palm	5,400	5,000	3,300	4,100
Oil, Peanut	3,418	3,373	3,440	3,344
Oil, Rapeseed	8,800	9,700	10,350	10,000
Oil, Soybean	17,900	18,900	20,500	20,500
Oil, Sunflowerseed	1,803	1,419	717	793
Other	2,134	2,051	2,121	2,154
Total	39,455	40,443	40,428	40,891
Imports				
Oil, Palm	6,190	4,377	3,203	4,175
Oil, Peanut	292	247	347	250
Oil, Rapeseed	1,978	2,039	2,171	2,150
Oil, Soybean	365	381	296	300
Oil, Sunflowerseed	1,555	1,207	532	500
Other	967	884	956	995
Total	11,347	9,135	7,505	8,370

Source: Foreign Agricultural Service/USDA Global Market Analysis

Table 10: India Oilseeds and Products Supply and Distribution

Thousand Metric Tons

	2022/23	2023/24	2024/25	2025/26
Production				
Oilseed, Cottonseed	11,166	10,783	10,189	10,104
Oilseed, Peanut	6,300	6,000	7,100	7,500
Oilseed, Rapeseed	11,200	11,600	11,520	12,000
Oilseed, Soybean	12,411	11,875	12,882	11,027
Oilseed, Sunflowerseed	215	112	113	113
Other	1,022	1,021	1,021	1,021
Total	42,314	41,391	42,825	41,765
Domestic Consumption				
Meal, Cottonseed	4,443	4,409	4,329	4,207
Meal, Rapeseed	4,350	4,600	4,360	4,900
Meal, Soybean	6,625	7,075	7,185	6,830
Other	2,176	2,069	2,146	2,198
Total	17,594	18,153	18,020	18,135
SME				
Meal, Cottonseed	3,600	3,573	3,508	3,409
Meal, Rapeseed	3,095	3,273	3,102	3,486
Meal, Soybean	6,225	6,625	6,710	6,400
Other	2,021	1,903	2,015	2,086
Total	14,941	15,373	15,335	15,381
Food Use Dom. Cons.				
Oil, Cottonseed	1,315	1,290	1,285	1,265
Oil, Palm	8,300	8,340	8,150	8,475
Oil, Peanut	1,050	995	1,000	1,170
Oil, Rapeseed	3,600	3,900	3,925	4,000
Oil, Soybean	5,400	5,175	6,645	6,570
Oil, Sunflowerseed	2,750	3,525	2,900	3,050
Other	400	410	395	410
Total	22,815	23,635	24,300	24,940
Domestic Consumption				
Oil, Cottonseed	1,361	1,345	1,330	1,305
Oil, Palm	8,900	8,990	8,800	9,125
Oil, Peanut	1,060	1,005	1,010	1,180
Oil, Rapeseed	3,680	3,980	4,005	4,080
Oil, Soybean	5,400	5,175	6,645	6,570
Oil, Sunflowerseed	2,750	3,525	2,900	3,050
Other	710	730	695	740
Total	23,861	24,750	25,385	26,050
Imports				
Oil, Cottonseed	1	0	1	5
Oil, Palm	10,045	8,886	7,786	9,050
Oil, Peanut	0	0	0	0
Oil, Rapeseed	6	6	26	40
Oil, Soybean	3,968	3,308	5,471	4,250
Oil, Sunflowerseed	2,988	3,516	2,905	3,050
Other	111	131	98	145
Total	17,119	15,847	16,287	16,540

Source: Foreign Agricultural Service/USDA Global Market Analysis

THE RECENT APPLICATION OF PALM STEARIN IN FOOD INDUSTRY: A REVIEW

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Abstract

Palm oil is divided into two main fractions, namely solid fraction called palm stearin (PS) and liquid fraction called palm olein (PO). The separation of this fraction aims to increase the potential application of palm oil, especially palm stearin, which has flexible melting characteristics for various food industries. This review presents various uses of palm stearin for the food industry. The use of stearin is not only for fat-based food but also as a substitute material that can affect the physical and chemical characteristics of other food products. The more advanced the technology, the more research is developing the potential of stearin with various treatments, especially through interesterification technology. The uses of palm stearin for the food industry include polysaccharide-based coating substitutes, margarine, shortening, cocoa butter replacers, lard replacers, and emulsion products. Palm stearin has a good effect on the physicochemical, functional, sensorial properties of various food products.

Index Terms: Palm stearin, food industry, margarine, shortening, emulsion

1. Introduction

Oil palm plantations (*Elaeis guineensis* Jacq.) is a high productivity crop, which is the main potential to meet the world's vegetable oil needs. Commercially, there are two types of vegetable oil extracted from palm oil, namely crude palm oil (CPO) and palm kernel

oil (PKO). Both have different types of fatty acids so that each has different benefits for various industries. CPO is more widely used in food industries such as cooking oil, margarine and shortening, while PKO is more suitable in non-food sectors such as cosmetics [1], [2]. In processing, CPO is divided into two fractions, namely palm stearin (30-35%) and palm olein (65-70%). Palm stearin (PS) is solid at room temperature because it has a high amount of saturated fatty acids [2], [3]. PS has a slip melting point (SMP) of about 44-56°C [4]. It contains palmitic acid about 47-74%, oleic acid (16-37%), stearic acid (4-6%), linoleic acid (3-10%), and myristic acid (1-2%) [5]. The triglycerides composition of palm stearin was dominated by POP, PPP, and POO about 30.0%, 22.1%, and 16.3%, respectively [6]. The high melting point of palm stearin (44-56°C) can cause problems in the manufacture of edible fats such as shortening and margarine, which results in the product having low plasticity [7]. However, palm stearin has great potential if its melting point can be lowered as desired for the manufacture of various food products. This can be conducted by mixing other oils which have a lower melting point in order to obtain a fat mixture with more suitable melting properties. Modification through the hydrogenation, interesterification, and fractionation has been widely used to improve the plasticity of fats [8]. The modification method through enzymatic interesterification between palm stearin and other oils is a suitable and growing method for modifying the physical and chemical properties of the lipid [9]. The purpose of the treatment is to improve the functionality of stearin. Fats with extensive plastic range properties such as palm stearin are used in the

production of the bakery, shortening, and margarine [5], [8]. The use of stearin is not only for the manufacture of fat-based foods but as a substitute material that can affect the physical and chemical characteristics of food or supporting materials in the production of food produced.

2 Application of Palm Stearin in Food Industry

2.1 Coating substitution material

The coating material is generally made from polysaccharides, but they have the disadvantage of being very hygroscopic. Hygroscopic properties can cause agglomeration/clumping caused by increased water content during storage [10]. Improvement of hygroscopicity properties of the coating material can be conducted by the addition of material with hydrophobic properties such as stearin and beeswax, so it is expected that the substituted coating does not easily absorb water [11]. Palm oil can be used as the material in the encapsulation process, especially to improve the ability of film-forming or to form the outer layer of encapsulation. Specifically, palm stearin plays a role in the process of film formation because its high melting point makes stearin have a crystalline structure [12]. To increase the ability to form films, it also requires the addition of materials that can improve film properties such as beeswax. The addition of beeswax can improve film on microcapsules. Mixing palm stearin and beeswax will form stronger hydrophobic properties that increase the efficiency of the moisture barrier in the coating [13]. One of the coating material in the form of polysaccharide includes xanthan gum. Ding et al. [11] reported that the addition of stearin and beeswax with a ratio of 7:3 to xanthan gum can increase the efficiency of encapsulation and improve the wall system on the coating. That is because there is a synergistic effect between stearin and beeswax. Long fatty acid in palm stearin and beeswax form a stable layer on the surface of core material that has a high degree of polarity. The decrease in the hygroscopic level of xanthan gum causes the coating not easy to

absorb water vapor, and the coating is difficult to agglomerate. Therefore palm stearin and beeswax have the potential as suitable substitutes for coatings in the food industry [10]. Various solid lipids can also be used as coatings for the synthesis of nanostructured lipid carriers (NLCs) and solid lipid nanoparticles (SLNs) [14], [15]. Palm

stearin and palm olein have been used for α -carotene-loaded nanostructured lipid carriers. Rohmah et al. [16] reported that palm stearin could be prospectively developed as α -carotene-loaded nanostructured lipid carriers that produce NLC with an encapsulation efficiency of 91.2

2.2 Margarine

The formation of trans fatty acids produced due to the hydrogenation process in making margarine can increase the risk of coronary heart disease and increase the amount of cholesterol in the blood plasma [17], [18]. Therefore, the development of margarine manufacturing processes is carried out, including through blending or interesterification. The process does not change the level of saturation of fatty acids and does not produce trans fats. In addition, interesterification can improve the slip melting point (SMP) and solid fat content (SFC) fat produced [19], [20]. Interesterification changes the composition of triacylglycerol (TAG) through the redistribution of fatty acid positions, thereby improving the physicochemical properties of the resulting fat [17], [20]. Redistribution of fatty acid positions among the triacylglycerol (TAG) molecules also substantially improves lipid function. Sellami et al. [21] producing zero-trans margarine fat through enzymatic transesterification between palm stearin and palm olein obtained that transesterification results in redistribution to the triacylglycerol composition. The margarine obtained has good rheological behavior and is comparable to commercial margarine. Blending and interesterification processes in the production of trans fat-free margarine can also be carried out in a mixture of palm stearin, palm kernel oil, and soybean oil using sodium methoxide. The

results showed that interesterification in the mixture was effective in modifying or improving physicochemical properties [22]. Some researchers use a mixture of milk fat to obtain margarine or fats that have good physicochemical and flavor properties [23], [24]. The addition of stearin is important in the process of making margarine because the components in stearin can increase the plasticity of fats and contribute to providing solid properties [17]. The addition of soybean oil to palm stearin can increase the amount of monounsaturated and polyunsaturated fatty acids so that the resulting margarine is healthier. Thus the mixture of soybean oil and stearin contains saturated fatty acids that are dominated by palmitic acid (59.4%) [17], [20]. The content of fatty acids in the products produced has an effect on physical properties such as the crystal structure of fats. The high amount of palmitic acid increases the stability of β -crystals. Increased β -crystals improve the even distribution of small crystals in the polymorph structure so as to stabilize the air cavity and increase mouthfeel [17], [25]. According to the research of Naeli et al. [20], the interesterification between palm stearin, palm kernel oil (PKO), and soybean oil caused a change in the composition of triacylglycerol (TAG). TAG composition decreased in PPP, LLL, OOO, POP, POO, LLO, LnLL, and PLLn as well as an increase in PPLn, PLP, POS, PLO, and PLL. In addition, there was a decrease in some trisaturated (S3) and tri-unsaturated (U3), as well as an increase in monosaturated-disaturated (SU2) and disaturated-monosaturated (S2U). The interesterification process also significantly reduces the amount of free fatty acids from the margarine produced. The advantage of interesterification is that it can reduce the amount of saturated fatty acids, but there is no loss during the interesterification process. Interesterification also increases product stability against

oxidation. Interesterification can reduce slip melting points due to decreased trisaturated (S3) TAGs and increased monosaturated-disaturated (SU2) TAGs. slip melting point margarine obtained from

interesterification usually ranges from 23.6°C to 36.3°C, so that the resulting margarine melts completely at body temperature and can improve mouthfeel when consumed [20]. The microstructure of margarine shows a fine aqueous droplet that spreads between oil crystals/fats. The dispersion phase affects melting behavior, where an increase in the size of the droplet during storage causes a decrease in SFC below its critical point because solid fat is unable to withstand droplet unification, then the emulsion becomes unstable [25]. Ornlai et al. [18] reported the research on margarine from the interesterification of palm stearin and rice bran oil, it was found that the crystals formed had a smaller size (<10 μ m). The ratio of rice bran oil to palm stearin of 40:60 shows needle-shaped crystals in small size and no aggregate crystals. The crystals in small sizes and compact are suitable for use in the bakery because the crystals can spread and stabilize the air conditions during the creaming stage so as to produce a smooth texture. Crystal structure formed between margarine from interesterification and commercial margarine does not differ significantly. Adding rice bran oil to palm stearin reduces the size of the crystals [25].

2.3 Bakery shortening

Shortening is a fat-based food additive with a crystal structure. To increase the content of saturated fatty acids in shortening, some companies use the hydrogenation process so that it has the potential to produce trans fatty acids [2], [3]. Therefore, many companies are now starting to avoid the hydrogenation process. The alternative is to use sources of fat that are rich in saturated fatty acids such as palm stearin and the fraction of stearin from coconut oil or from palm kernel oil [26], [27]. Shortening for bakery products generally has solid fat content (SFC) between 15-25% at a temperature of 20°C with a melting point >38°C. Basically, palm oil has an SFC of around 22-25% at a temperature of 20°C. It shows a consistency similar to plastic cake shortening, so that palm oil itself has the ability to be shortening. The addition of palm kernel oil

(PKO) can also improve the ability of palm oil as a shortening [2]. According to Rudsari et al. [27], bakery shortening can be produced using palm stearin raw material. The functional characteristics of shortening can be improved by interesterification with ardeh oil (*Sesamum indicum*). The addition of ardeh oil improves the melting point in the resulting shortening. That is because ardeh oil increases the amount of unsaturated fatty acids. Interesterification reduces the slip melting point (SMP) due to changes in the formation of triacylglycerol (TAG) groups. The decrease in melting point during the interesterification process is due to an increase in di-unsaturated (SU2) TAGs and a decrease in trisaturated (S3) TAGs. Different ratios of palm stearin to ardeh oil produce shortening with different properties. The ratio of palm stearin to ardeh oil of 40:60 produces shortening that can be used on all bakery products because the shortening produced has a wide melting temperature range whereas the ratio of 50:50 produces shortening which is suitable for pie products because it can soften the dough while still providing a sense of flakiness [27].

2.4 Cocoa butter alternatives

Cocoa butter alternatives or cocoa butter replacers are made to replace the function of cocoa butter. Cocoa butter has a high price; therefore, the industry is replacing it with other vegetable fats that have lower prices, such as palm stearin. To improve the physical properties of the cocoa butter replacer produced, another vegetable fat was added to the oil palm stearin such as the addition of mango seed fat [28], addition of palm kernel oil [29], or the addition of Bambang (Mangifera pajang) kernel fat by the interesterification process [30]. Interesterification reaction will produce semi-solid fat that does not contain trans fatty acid residues. Stearin naturally forms a stable β crystal structure making it suitable for use as cocoa butter alternatives [31]. The resulting crystals are also small in size, shaped like a needle-shaped, and are numerous. Small crystals are more stable and have superior creaming properties [30]. The difference in the shape and size

of the crystal is affected by temperature, the ability of polymorphism, and chemical composition. The best crystallization is shown at the storage of 20-23°C. Triglycerides produce α -crystals (amorphous with small crystals), β -crystals (bulky shape or spherulitic) and β' -crystals (dominated by needle-shaped crystals). In palm stearin, crystals that form are stable in the β form, making it suitable for use in making chocolate and coatings [30]. Jahurul et al. [28] also succeeded in making Cocoa butter replacer by blending palm stearin with mango seed oil. Palm stearin is also used by Biswas et al. [29] by mixing palm kernel oil and palm mild fraction for confectionery filling.

2.5 Pig lard replacers

Lard from pigs is often used because of its sensory properties, mainly the taste and texture. Some countries, such as Japan, utilize lard from pigs to increase stickiness property in the meat consumed. The high saturated fatty acids in pork lard make the taste and texture of the final product preferred [32]. The addition of lard increases the content of triglyceride composition which is dominated by palmitic acid (25%) in food. However, excessive consumption of lard increases the risk caused by the accumulation of fat so that formulations that are similar in characteristics are needed but still safe for consumption. The lard formulation can be replaced with a mixture of some vegetable fats and conditioned to have similar characteristics. The mixture consists of palm oil, cocoa butter, avocado butter, and mee fat to replace liquid oil from pork oil; and a mixture of palm stearin, palm oil, soybean oil, cocoa butter, and mee fat to replace lard. All crystals form a β and β' structure that is dominated by a polymorph structure. This indicates that the fat produced is suitable as a lard substitution. Crystals with β structure will provide better products because they improve smooth mouthfeel and trap liquid oil because naturally, spherulitic crystals will form and allow as a lard replacer [32]. Palm stearin also could potentially be used to replace the portion of lard in frankfurter type beef sausages, where sausages

containing palm stearin have the same physical and sensory qualities compared to controls using lard [33].

2.5 Emulsion and other products

Various emulsion products develop rapidly, along with the needs of the food industry to obtain a stable food system.

Some researchers have used palm stearin for the synthesis of emulsion products. Arum et al. [34] synthesized emulsifiers from palm stearin through glycerolysis followed by cold-temperature fractionation. The results showed that emulsifiers from palm stearin contained about 91% monoacylglycerol and about 9% diacylglycerol. The emulsifier obtained has an emulsion capacity of 95.55% and has excellent stability. Subroto et al. [35] synthesized structured lipids containing mono- and diacylglycerol from a mixture of palm stearin and palm olein found that structured lipids produced by chemical glycerolysis-interesterification had an emulsion capacity of about 93.63% and had good stability. Whereas Wang et al. [36] studied the effect of adding palm stearin to glycerol monostearate-structured emulsions, it was found that palm stearin increased the stability of emulsions during storage at cold temperatures. Palm stearin can also be used for oleogel production. Ghosh et al. [37] produced oleogel from a mixture of palm stearin and cetyl caprylate, it was found that oleogel had a positive effect on in vivo testing. The research produced trans-free and quality oleogel because it provided good health effects. Whereas Das et al. [38] utilize palm stearin for mayonnaise production. A mixture of palm stearin and rice bran oil at a ratio of 3:7 produces a soft, creamy, and delicious mayonnaise.

3 Conclusion

Palm stearin is a material that has high plasticity, so it is suitable for use in various food industries such as the bakery, shortening and margarine industries. Palm stearin can also be used as a mixture in polysaccharide-based coatings. The addition of palm

stearin to the coating material causes an increase in hydrophobic properties, which makes the coating material not easily undergo agglomeration during storage. In addition, palm stearin can be used as a raw material for the production of cocoa butter alternatives through a blending or interesterification. The interesterification process in palm stearin is also used in the production of trans fat-free margarine and shortening which has good physicochemical properties.

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Choosing the Right Gum for Baked Foods Depends on the Application



The bakery application and intended functionality are the key considerations in choosing the right gums/hydrocolloids for the job.

“For example, in breads, muffins and cakes, hydrocolloids are often used to control moisture, stabilize freeze-thaw cycles, replace gluten and provide texture,” said Lauren Standifer, project leader, applications and development, customized formulations, bakery, savory, confections and new ingredients, Ingredion Inc.

“In contrast, icings, frostings and glazes require hydrocolloids that provide structure, emulsify fat and air, control sugar bloom, manage moisture, and improve visual appearance. Each application demands a tailored approach to ensure the final product meets performance expectations and consumer preferences.”

The right choice also depends on the manufacturing process and how consumers will use the product. “For example, hydrocolloids like xanthan gum can improve dough handling, making sheeting and mixing easier on the line,” said Shiva Elayedath, principal technical services specialist, Cargill. “But we also need to consider how consumers will use the product. Is it ready-to-eat? Will consumers bake it at home? Will it need to withstand freeze-thaw cycles? Answers to those questions can also impact choices.”

In frozen doughs, a small amount of xanthan gum may be sufficient to hold moisture, he added, but in ready-to-eat frozen cakes, bakers often need a more complex combination of gums and starches that can provide structure during baking and retain moisture through storage.

“Hydrocolloids are also valuable in gluten-free and low-fat products,” Elayedath said. “In gluten-free formulas, they help provide structure that normally comes from gluten, while in low-fat products they can help deliver the mouthfeel fat would have provided.”

He also said that hydrocolloids play a key role in improving product stability by slowing starch retrogradation, which contributes to staling and moisture loss. This functionality is especially valuable during freeze-thaw cycles and throughout shelf life to maintain softness, texture and product quality.

The freezing and thawing process also play a role in determining which hydrocolloid will serve the application best, said Tim Cottrell, business development director, emulsifiers/texturants, Kerry. The speed of freezing and thawing, the length of time that it’s frozen, the speed and type of baking will all impact this choice. Even the moment in the process the product is frozen — par-baked, flash-baked, pre-proofed, post-proofed or post-baked — will be a determining factor.

“Reformulating with these technical solutions delivers high performance and quality results. However, they require specialist knowledge and expertise to navigate complexities,” he said. Formulators understand the importance of optimizing hydrocolloid usage, like making sure it’s in the best form for the application.

“For example, in soft cookie application, it is important to pre-hydrate the hydrocolloid before adding it with other ingredients,” said David Guilfoyle, senior manager for bakery/fats and oils, IFF. “Additionally, the pH of the dough or batter plays a critical role in hydrocolloid selection, as different hydrocolloids respond differently to varying pH levels.”

In addition to selecting the right gum for the bakery application and functional goals, formulators must also take into account regulations, including maximum usage levels and labeling requirements. “Front-of-pack claim goals may influence the choice as well, especially when aiming to meet consumer expectations or regulatory standards,” Standifer said.

Historically, bakers used aminated pectins, which don’t require calcium to gel but must be declared on ingredient statements as aminated pectin, Elayedath pointed out. “Cargill’s new UniPECTINE LMC-plus pectin offers a label-friendly alternative,” he said. “It functions effectively at higher pH levels and with less calcium dependence yet simply labels as pectin. It’s particularly well-suited for bake-stable, low-sugar, high-fruit fillings where both performance and consumer appeal matter.”

The point at which the hydrocolloid is added into a dough or batter is an important consideration. “Hydrocolloids are typically added early, before syrups, sugars and other ingredients that compete for water are incorporated,” Elayedath said. “Fat content is another consideration, as fats can coat hydrocolloids and prevent hydration — one more reason to add hydrocolloids early.”

He also mentioned that the type of flour being used in a product and the pH of a filling also play a role in the correct usage and choice of hydrocolloids. “In cakes and sweet baked goods, low-protein flours are best, as they support a softer, more moist texture,” Elayedath explained. “High-protein flours tend to make things tough and hold onto more water, making it hard to achieve the desired texture. “Some hydrocolloids are pH sensitive. In acidic fruit fillings, pectin performs best, while cream fillings may benefit from carrageenan,” he added.

Cottrell said in addition to water content and flour protein levels, sugars, fats, gluten-free flours, processing methods, baking time and clean label or allergen restrictions can all impact formulations. “Additional processing aids included in the formulation need to be considered — which may work synergistically with a hydrocolloid or gum, so a holistic view of the structure

of the formula is required by experts to determine the ideal solution,” he said.

The use of gums, or hydrocolloids, in baked foods can provide several advantages to formulators, including helping with the freeze-thaw cycle, viscosity and crumb structure, assisting with shelf life and more. But they must be chosen and added carefully to avoid any product quality issues.

Source: Baking Business.com

Chromatography-Driven Insights into Fat Replacement Effects in Frankfurters

Lard-derived diacylglycerol (DG) can replace pork fat in frankfurters, improving healthiness without compromising sensory quality. Replacing pork fat with purified glycerolized lard (PGL) enhances water content, lightness, yellowness, and protein thermal stability in frankfurters.

A study investigating the use of lard-derived diacylglycerol (DG) as a fat replacer on the flavor characteristics of frankfurters detected 50 volatile compounds in the samples analyzed using gas chromatography-mass spectrometry (GC-MS). Partial or total replacement of pork fat with homologous functional oils may help meet consumer demand for healthier meat products while preserving sensory quality. In a new study, researchers investigated the use of lard-derived diacylglycerol (DG) as a fat replacer and its effects on the flavor characteristics of frankfurters.

Gas chromatography-mass spectrometry (GC-MS) detected 50 volatile compounds in all the frankfurters used in the study (such as aldehydes, alcohols, terpenes, and aromatic hydrocarbons). In addition, electronic nose results showed that replacing pork fat with PGL affected the aroma of frankfurters. A paper based on this research was published in *Foods* (1).

Frankfurters usually contain high levels of animal fat (up to 20–30%), which play a part in improving cooking yield and offering the meat’s unique flavor, desired texture, solid structure, juiciness, and overall

acceptability (2). A great deal of evidence, however, reveals that increased intake of high-fat foods such as frankfurters can be detrimental to one's health (potentially leading to obesity and cardiovascular disease), as animal fat in general contains cholesterol and saturated fatty acids (3,4). Recent studies have concentrated on the reduction of fat content of frankfurters through the lowering of the amount of animal fat or the partial replacement of animal fat in the meat with plant oils, emulsion gels, emulsions, and gum (5-8).

However, compared to full-fat frankfurters, the reduced animal fat alternatives had lower consumer acceptability, flavor, and taste (particularly juiciness). Studies observed that the replacement of fat with porcine plasma protein-xanthan gum-based oleogels (PXOs) resulted in a reduction of flavor and interior color of frankfurters (9). Additional research reported that the high-proportion replacement of pork backfat with gelled emulsions prepared from hemp oil and buckwheat flour had a propensity toward disrupting the original flavor balance of the frankfurter (10). "Therefore," write the authors of the article, "there is an urgent need to identify healthy alternatives from homologous fat to traditional animal fat." (1)

The study revealed that replacing pork fat with purified glycerolized lard (PGL) at different levels (25%, 50%, and 100%) increased the water content and water activity, improved the lightness and yellowness values, and protein thermal stability, while decreasing the redness value of the frankfurters. Furthermore, substituting lard with PGL significantly increased the variety and content of flavor compounds in frankfurters. Of the identified 50 volatile compounds identified with GC-MS in this study, 7 were found to play an important part in the overall flavor profile of frankfurters based on odor activity value.

The researchers found that replacing lard with PGL increased the variety and content of volatile compounds in frankfurters. In addition, aldehydes (hexanal), alcohols (1-octen-3-ol), and terpenes [(+)-dipentene] could be regarded as the key volatile compounds that

distinguished frankfurters with different levels of PGL according to the OAV and variable importance in projection results. DG also improved the quality of frankfurters, which is specifically reflected in the increase in lightness and yellowness, water content and water activity, and protein thermal stability (1).

"Hence," write the authors of the study, "lard-derived DG may be a promising fat substitute for producing healthy and high-quality meat products." Future studies might focus on intelligent sensory techniques, such as the electronic tongue technology and gas chromatography-olfactometry (GC-O) (1).

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Source: *LCGC*

Sunflowers may be the Future of “Vegan Meat”

Sunflower flour emerges as a sustainable, nutrient-packed, and surprisingly meat-like plant protein innovation.

A collaboration between Brazilian and German researchers has led to a sunflower-based meat substitute that's high in protein and minerals. The new ingredient, made from refined sunflower flour, delivers excellent nutritional value and a mild flavor. Tests showed strong texture and healthy fat content, suggesting great potential for use in the growing plant-based food sector.



Researchers enriched the product with tomato powder, spices, and a mixture of fat sources made up of sunflower, olive, and linseed oils.

Researchers at the Institute of Food Technology (ITAL) and the University of Campinas (UNICAMP) in São Paulo, Brazil, working with colleagues from the Fraunhofer IVV Institute in Germany, have developed a new type of food made from sunflower flour that can serve as a substitute for meat.

The process begins by extracting oil from sunflower seeds. To make the resulting flour safe and digestible for humans, the outer husks and certain phenolic compounds must first be removed. These elements normally give the flour a darker color and make it harder for the body to absorb nutrients effectively.

Creating and Testing the Sunflower-Based Burgers

Researchers prepared two variations of the meat substitute. One was made from flour derived from roasted sunflower grains, while the other used textured sunflower protein. Both formulations were enhanced with tomato powder, spices, and a blend of sunflower, olive, and linseed oils to improve flavor and nutritional value.

The team shaped the mixtures into small burger patties and baked them. They then conducted sensory and physicochemical tests to evaluate the products' texture, flavor, and composition. Results revealed that the version made from textured sunflower protein had better consistency and higher levels of protein, along with

healthy fats such as monounsaturated fatty acids. It also contained impressive mineral levels, providing 49% of the recommended daily intake of iron, 68% of zinc, 95% of magnesium, and 89% of manganese.

Sustainable, Non-GMO Protein Potential

The study, supported by FAPESP, focused on sunflower meal because sunflower oil is already widely used in Europe, and sunflower cultivation is steadily increasing in Brazil. Another advantage is that the plant is not genetically modified, making it an appealing ingredient for consumers seeking non-GMO options.

Sunflower flour also offers a valuable source of plant-based protein, aligning with the growing global demand for sustainable and environmentally friendly food choices.

Mild Flavor and Strong Nutritional Profile

Maria Teresa Bertoldo Pacheco, a researcher at ITAL's Center for Food Science and Quality and lead author of the paper published in Food Research International, explained that removing the husks and phenolic compounds gives the flour a neutral flavor and aroma. "It should also be noted that, after removing the husks and phenolic compounds, the flour has a very neutral taste and aroma, especially compared to the various vegetable proteins on the market," she said.

Pacheco also highlighted the favorable balance of essential amino acids in the flour, which adds to its nutritional value. From a technological standpoint, she noted that creating a fibrous structure through processes like extrusion is key to achieving a product with a more authentic, meat-like appearance and texture.

TURMERIC (CURCUMA LONGA) RHIZOME ESSENTIAL OIL

Introduction:

The use of turmeric dates back nearly 4000 years to the Vedic culture in India, where it was used as a culinary spice and had some religious significance. It reached China by 700 AD, East Africa by 800 AD, West Africa by 1200 AD, and Jamaica in the eighteenth century. Turmeric has been used in folk medicine preparations over the centuries in different parts of the world. In Ayurvedic practices, turmeric is thought to have many medicinal properties, including strengthening the overall energy of the body, relieving gas, dispelling worms, improving digestion, regulating menstruation, dissolving gallstones, and relieving arthritis.

The plant is native to tropical South Asia and has been widely introduced and naturalized to many tropical and subtropical countries. India produces most of the world's supply, but turmeric is also cultivated in other countries in South, East and Southeast Asia as well as in the Americas.

Turmeric rhizomes contain two major classes of secondary metabolites: curcuminoids, which are responsible for the yellow color of the turmeric, and turmerones, which contribute to the characteristic aroma and flavor. While turmeric has been extensively studied along with curcumin, as one of the main active constituents, the interest and use of the essential oil of turmeric have been growing. Turmeric rhizomes contain about 0.5-6.0% essential oil. The oil of turmeric is traditionally used as an antacid, and in small doses, acts as a carminative, stomachic, appetizer, and tonic. It is used as a flavoring for food products and in animal feed. It has also been used in perfumes of heavy oriental character. Turmeric essential oil is widely utilized in cosmetic and pharmaceutical applications due to its antimicrobial, anti-inflammatory, antioxidant, and insect-repelling properties.

Botanical Name:

Curcuma longa L.; synonym: *Curcuma domestica* Valetton. Turmeric is a rhizomatous herbaceous



perennial flowering plant which belongs to the Zingiberaceae family and Curcuma genus.

Harvesting and Production :

Turmeric essential oil is produced from cultivated rhizomes. Growing conditions, such as water availability, sun exposure, and harvest time affect rhizome quality which can have subsequent effects on the quality of the essential oil.

After harvesting, the rhizomes are thoroughly cleaned with water to remove soil and debris. Fresh rhizomes are then cut into smaller pieces or pureed depending on the extraction process. Dried rhizomes are typically dehydrated whole and pulverized before essential oil extraction.

Turmeric essential oil is extracted from rhizomes via hydrodistillation and steam distillation methods. During hydrodistillation, pulverized dried rhizomes or pureed fresh rhizomes are mixed with water and boiled in the round bottom flask of a Clevenger apparatus or in the boiler of a manufacturing scale hydrodistillation system. The essential oil and water are collected in a condenser and subsequently separated.

In contrast, during steam distillation, the plant material is placed on a perforated plate and blasted with steam thereby evaporating the material's steam-volatile compounds. Then the evaporated water and volatile oil are collected in a condenser and are separated mechanically.

Following separation, both hydrodistilled and steam distilled oils are filtered and treated with anhydrous sodium sulfate, which acts as a drying agent to remove any remaining water in the essential oil. Hydrodistillation is by far the most common method for extracting turmeric essential oil on both laboratory and industrial scales, as it is more economical than steam distillation, which requires larger amounts of raw material and longer extraction times.

Harvesting Timing : Rhizomes are harvested when the plants mature (typically 7 to 10 months after planting), signaled by the yellowing and drying of the leaves.

Preparation : Harvested rhizomes are cleaned, cured

(often boiled or dried), and sliced or ground into a powder to optimize volatile oil release.

Yield : Dried rhizomes yield roughly 2.5% to 5.5% essential oil, which is higher than many other herbal extracts.

Extraction Methods :

Steam Distillation: The standard and most common commercial method, where steam passes through crushed or ground dried rhizomes to vaporize volatile compounds before condensing back into oil.

Hydrodistillation: Raw or powdered material is boiled directly in water, and the vapor is captured and separated.

Advanced Techniques: Modern methods like supercritical CO₂ extraction and molecular distillation yield higher purity and better retention of heat-sensitive active constituents.

Chemical Composition :

Primary Constituents: Dominated by sesquiterpenes, particularly α -turmerone (25–40%), α -turmerone (15–30%), and β -turmerone (10–20%).

Other Compounds: Contains curcylone, zingiberene, and α -curcumene.

Benefits and Uses :

Turmeric is a spice that comes from the ginger family. It has been used in India for thousands of years as both a spice and medicinal herb. Research has shown that turmeric contains compounds with medicinal properties. These compounds are called curcuminoids. The most important one is curcumin, which is the main active ingredient in turmeric.

While turmeric has several potential benefits, it should never be used as a replacement for medical treatment. It may also interact with certain medications. Therefore, always follow the doctor's advice.

1. Turmeric contains bioactive compounds: Turmeric contains several bioactive compounds, which have several potential benefits, such as

improving gut health and the immune system. Curcumin is also fat-soluble, which means it breaks down and dissolves in fat or oil.

2. Curcumin is a natural anti-inflammatory compound: Curcumin is a bioactive substance that can help fight inflammation, though very high doses are required to produce medicinal results.

3. Turmeric can increase the antioxidant capacity of the body: Oxidative damage is believed to be one of the causes behind aging and many diseases. It involves free radicals, highly reactive molecules which can cause damage to other cells in your body.

4. Curcumin can boost the development of new brain cells: Even in adulthood, brain neurons are capable of forming new connections, and in certain areas of the brain, they can multiply and increase in number.

5. Curcumin may lower your risk of heart disease: Heart disease is the number one Trusted Source cause of death in the world. Research suggests that curcumin may help protect against many steps in the heart disease process.

6. Turmeric may help prevent cancer: Many different forms of cancer appear to be affected by curcumin supplements. In fact, curcumin has been studied as a beneficial herb in cancer treatment and has been found to affect cancer growth and development.

7. Curcumin may be useful in treating Alzheimer's disease: Alzheimer's disease is the most common form of dementia and may contribute to up to 70% of dementia cases. It's known that inflammation and oxidative damage play a role in Alzheimer's disease, and curcumin has been found to be beneficial.

8. Arthritis patients respond well to curcumin supplements: There are several different types of arthritis, most of which involve inflammation in the joints. In a study on people with osteoarthritis, curcumin appeared to be more effective in relieving pain than a placebo.

9. Curcumin has benefits against depression:

Natural ways to cope with depression.

10. Curcumin may help delay aging and fight age-related chronic diseases: If curcumin can really help prevent heart disease, cancer, and Alzheimer's, it may have benefits for longevity as well. Given that oxidation and inflammation are believed to play a role in aging. It's a potent anti-inflammatory and antioxidant. It may also help improve symptoms of depression and arthritis.

11. Skin and Aromatherapy : Used in cosmetics to help soothe acne-prone skin, address hyperpigmentation, and promote relaxation when diffused.

Conclusions :

Turmeric (*C. longa*) rhizome essential oil represents a well-studied natural complex substance. Its quality is influenced by agricultural conditions, post-harvest processing, and distillation methodology. Comprehensive analytical evaluation of the essential oil confirms that turmerones are by far the major constituents in authentic rhizome oil, while monoterpene abundance is generally reduced in oil produced from ground turmeric compared to oil from fresh turmeric. A market survey revealed substantial variability among commercial products. Although some can be attributed to natural variability, some products were clearly diluted with non-essential oil material. Toxicological evidence demonstrates a favorable safety profile, with low acute toxicity, absence of dermal toxicity or genotoxicity, and good tolerability in both animals and humans. Pharmacological studies highlight diverse bioactivity properties, including anti-inflammatory, antimicrobial, neuroprotective, antioxidant, and anticancer effects, largely attributable to turmerone-rich fractions. Despite promising therapeutic potential, clinical evidence for turmeric essential oil remains limited. Altogether, the current body of evidence supports turmeric essential oil as a safe and multifunctional natural product with significant potential for therapeutic and nutraceutical applications.

Compiled by:
Dr. S. Adhikari

LAUGH AND LOUD

Q. Why is it so hard to get up in the morning?

A. Newton's First Law: A body at rest will remain at rest.

Q. What do you call a stern chemistry teacher?

A. A flask master.

Q. What type of science do crew teams study?

A. Oar-ganic chemistry.

Q. How to classify Science ?

A: If it moves, it is Biology

If it stinks, it is Chemistry

If it does not work , it is Physics

Q. What element was named after a beloved baseball catcher?

A. Yogi Berra-llium.

Q. Think like a Proton

A. Stay Positive.



Q. What do you give a man who has everything?

A. Penicillin..

Q. Why do cemeteries have fences around them?

A. Because everyone's dying to get in.

Q. Things I learn in Organic Chemistry?

A. Interesting Reactions

Nomenclatures

Deadly compounds and

Drawing of Hexagons.

MEMBERS' PAGE

COMING OF AGE

by R.C. ARORA (Ex. Manager Q.C. - S.F.F.I., New Delhi)



As many of us have found to our sorrow, our success in weight loss programmes tends to lessen with age. That's because our bodies change over time. Therefore, the approach to weight loss must differ with every passing decade. Here's how :

Weight loss in your 20s

At this age, weight loss can be very quick. That's because it's easier to deal with your appetite in the first place, and in the second place, your liver tends to be active and healthier than it's likely to be as you grow older. All exercise routines are suitable for you (provided of course that you suffer from no specific disorder) and your only mantra is to eat lots of fruit for skin that glows.

Weight loss in your 30s

If you are married and have kids, you will find that your metabolism has been affected by pregnancy. You are also likely to have loose skin and a flabby abdomen, which means toning exercises are a must. In terms of your diet, you should increase your intake of calcium, iron and vitamin B complex via foods like ragi, figs, spinach and fruit. Your mantra for this decade should be to cut down your intake of atta, and eat more whole grains to add fibre to your diet.

Weight loss in your 40s & 50s

Exercise should include a focus on de- stressing and this is best done with pranayam and yoga. Include lots of vegetable juices in your diet, cut down your intake of carbohydrates and increase your consumption of healthy pulses and legumes in sprout or chaat form. Make sure your food is not too oily, but since this is the age when body systems become drier, apply creams on your face and body, and have regular oil massages for your body and head. Drink lots of water, eat tofu and include alternative cereals like ragi and barley in your meals. Good sleep is a must.



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