

Supporting information

Exploring the potential waste biomass of Olive as additive to layer double hydroxide/poly urethan as effective and safe agent in the adsorption of drug residues: bioremediation approaches

Table S1 Previous studies in the open literature reporting adsorbents for Cefotaxime removal.

Adsorbent	pH	Adsorbent dose	Equilibrium (min)	time	q _{max} (mg/g) or %R	Reference
hybrid green nanocomposite polymeric beads doped with nano sulfated zirconia	6	11.68 mg of beads composite with 2.5wt.% of SZrO ₂	3.58h		659	[32]
novel NiFe ₂ O ₄ -COF-chitosan-terephthalaldehyde nanocomposites film (NCCT)	4	-	-		309.26	[33]
nanocatalysts TiO ₂	4	0.2 g/L	90 min		removal efficiency 68%	[34]
Biochar supported bimetallic nanoparticles	5	Co/Fe 0.8g/L	-		removal efficiency (99.23%)	[35]
Chitosan Film	4		25hr		1003.64 mg/g	[36]
TiO ₂ and SiO ₂ Nanoparticles Modified Polyether sulfone Membrane	7	2.50 g/L	120 min		6.15 mg/g	[8]
LDH/PU/O-Pom	5	0.09	-		250 mg/g	This work
O-Pom	5	0.07	-		163.23mg/g	This work

Table S2 Band frequencies from the FTIR spectra of O-Pom, LDH/PU, and LDH/PU/O-Pom

Wavenumber	Function group	Band assignments
3431 cm ⁻¹	(OH) stretching	Broad peak indicates the presence of hydroxyl (OH) groups

	3247cm ⁻¹	=CH stretching	Associated with the stretching vibration of =CH bonds
	2921cm ⁻¹ , 2852 cm ⁻¹	C-H stretching	Two Peaks are attributed to stretching vibrations of C-H bonds in aliphatic compounds.
	1714 cm ⁻¹	C=O stretching	Stretching vibration of carbonyl (C=O) groups.
	1643cm ⁻¹	C=C stretching	Associated with the stretching vibration of C=C bonds in conjugated systems.
	1544 cm ⁻¹	Aromatic C=C stretching	This peak further confirms the presence of aromatic compounds
	1029 cm ⁻¹	C-O	The bending vibrations of C-O
	603 cm ⁻¹	C-H bonds	This peak further supports the presence of aromatic compounds and aliphatic chains in pomace.
	3446cm ⁻¹	(OH) stretching	In LDH/PU, it could indicate the presence of interlayer water molecules or hydroxide ions, Additionally, it might suggest the presence of hydroxyl-containing functional groups in the PU compound
LDH/PU	1629 cm ⁻¹	stretching vibration of water molecules	stretching vibration of water molecules or hydroxide ions in the interlayer region of LDHs.
	1103cm ⁻¹	C-O	stretching vibrations of C-O bonds
	686cm ⁻¹	M-O	In LDHs like Zn-Al-LDH, the metal cations (such as zinc and aluminum) are coordinated with oxygen and hydroxide ions in a layered structure. The bending vibrations of metal-oxygen-hydroxide bonds typically occur in the region of 700-600 cm ⁻¹ in the FTIR spectrum.
	3452cm ⁻¹	(OH) stretching	It suggests the presence of hydroxyl-containing functional groups, possibly from both the pomace and the LDH component.
	3182cm ⁻¹	=C-H stretching	It further confirms the presence of hydroxyl-containing compounds in the sample
	(2935 cm ⁻¹ , 2852 cm ⁻¹)	C-H stretching	Stretching vibrations of C-H bonds in aliphatic compounds, such as lipids or carbohydrates present in the pomace
LDH/PU/O-Pom	1637cm ⁻¹	stretching vibration of C=C bonds in conjugated systems	Suggesting the presence of aromatic compounds in both the pomace and LDH
	1400cm ⁻¹	vibrations of C-H bonds	Correspond to the bending vibrations of C-H bonds in alkanes or methyl groups present in both the pomace and LDH
	(1143 cm ⁻¹ , 1035 cm ⁻¹)	C-O stretching vibrations	Correspond to carbohydrates or esters from the pomace component

613 cm⁻¹

M-O

Vibrations of metal-oxygen-hydroxide bonds

Table S3: Adsorption isotherm fitting parameters for drug adsorption onto O-Pom and LDH/O-Pom

Model	Parameter	O-Pom	LDH/PU/O-Pom
Langmuir $q_e = \frac{q_{max} K_L C_e}{1 + K_L C_e}$	q_{max}	163.23	25.00E+01
	K_L	1.60 E-03	1.00 E-03
	R^2	0.99	0.99
	AIC	81.04	73.54
	$1/n$	0.89	0.79
Freundlich $q_e = K_f C_e^{1/n}$	K_f	0.35	0.52
	R^2	0.99	0.99
	AIC	69.23	63.91
	q_{MLF}	99.80	179.70
	K_{LF}	3.90E-3	1.80E-3
Langmuir-Freundlich $q_e = \frac{q_{max}(K_{LF}C_e)^{MLF}}{1 + (K_{LF}C_e)^{MLF}}$	M_{LF}	1.40	1.19
	R^2	0.99	0.99
	AIC	76.43	73.23
	q_{max}	1.00E+2	161.30
	K_s	3.00E-4	4.90E-5
Sips $q_e = \frac{q_{max} K_s (C_e)^{1/ns}}{1 + K_s (C_e)^{1/ns}}$	$1/n$	1.40	1.23
	R^2	0.99	0.99
	AIC	76.43	73.25
	K_R	0.22	0.22
	a_R	5.80	1.78
Redlich-Peterson $q_e = \frac{K_R C_e}{1 + a_R C_e^{BR}}$	R^2	0.99	0.99
	AIC	76.43	73.25
	K_T	0.25	0.45
	a_T	6.10 E-3	5.77
	N	0.82	2.10
Fritz-Schlunder $q_e = \frac{K_T C_e}{(a_T + C_e^Z)^{1/Z}}$	R^2	0.99	0.99
	AIC	76.43	73.25
	q_{mFSS}	8.27	2.98
	K_1	0.13	0.05
	K_2	0.42	1.00E-4
	m_1	0.75	1.09
	m_2	0.03	1.32
	R^2	0.98	0.99
	AIC	88.43	91.91
	$Q_n(\text{mg/g})$	534.56	211.60
Khan $qe = \frac{Q_m b_K C_e}{(1 + b_K C_e)^{a_K}}$	b_K	4.90 E-5	1.0E-3
	a_K	2.65	0.64
	R^2	0.99	0.99
	AIC	76.43	73.25

Table S4: Summarization of the determined error functions for the non-linear adsorption isotherm models for O-Pom.

Function	Langmuir	Freundlich	Dubbin	Langmuir-Freundlich	Sips	Redlich-Peterson	Baudu	Fritz	Khan	Toth
SSE/ ERRSQ	52.72	23.394	295.25	19.115	19.12	11.08	19.427	125.25	41.829	66.03
X2	2.17	1.02	18.99	0.924	0.904	0.36	0.945	0.633	1.797	2.975
R2	0.992	0.997	0.958	0.998	0.997	0.998	0.997	0.983	0.994	0.991
Adjusted R ²	0.971	0.991	0.889	0.992	0.992	0.995	0.989	0.911	0.982	0.972
MAE	2.16	1.47	5.17	1.251	1.257	0.949	1.26	0.3.269	1.987	2.39
MAPE / ARE	11.198	6.728	29.09	7.419	7.35	4.22	7.51	20.080	10.249	13.26
RMSE	2.42	1.61	5.728	1.457	1.458	1.109	1.469	3.73	2.155	2.708
NRMSE	0.082	0.054	0.193	0.0497	0.049	0.037	0.05	0.127	0.0735	0.0924
HYBRID	20.157	8.65	37.40	11.129	11.02	6.33	13.52	45.18	15.37	19.89
MPSD	21.035	11.699	51.126	15.957	15.73	6.7	17.719	48.02	17.43	23.49
SAE / EABS	19.45	13.24	46.539	11.265	11.309	8.54	11.376	29.42	17.887	21.52
RMS	15.679	10.31	45.089	13.029	12.84	5.47	13.207	32.016	14.24	19.18
NSD	0.157	0.1030	0.450	0.130	0.128	0.055	0.132	0.322	0.14	0.192

Table S5: Summarization of the determined error functions for the non-linear adsorption isotherm models for LDH/PU/O-Pom

Function	Langmuir	Freundlich	Dubbin	Langmuir-Freundlich	Sips	Redlich-Peterson	Baudu	Fritz	Khan	Toth
SSE ERRSQ	44.41	47.107	133.43	31.98	32.35	30.19	33.56	31.45	38.05	28.98
X2	1.496	1.167	13.23	1.318	1.56	0.87	1.176	1.055	0.991	0.804
R2	0.994	0.993	0.98	0.995	0.995	0.996	0.995	0.996	0.995	0.995
Adjusted R ²	0.982	0.981	0.948	0.984	0.984	0.985	0.978	0.969	0.981	0.985
MAE	2.048	1.953	3.489	1.636	1.659	1.66	1.64	1.53	1.789	1.55
MAPE / ARE	9.24	7.558	31.39	8.65	9.61	7.419	7.78	7.19	7.695	6.87
RMSE	2.35	2.426	4.08	1.999	2.01	1.94	2.048	1.98	2.18	1.90
NRMSE	0.0978	0.101	0.169	0.082	0.083	0.081	0.085	0.082	0.0905	0.079
HYBRID	12.32	10.067	41.86	13.84	15.37	11.87	15.57	19.17	12.31	10.99
MPSD	13.596	11.32	57.81	19.43	21.87	12.52	19.43	21.24	12.34	12.51
SAE / EABS	16.389	15.63	27.92	13.089	13.28	13.29	13.13	12.27	14.34	12.40
RMS	11.77	9.80	50.06	15.36	17.29	9.89	13.74	13.004	9.75	9.89

Table S6: A summary of nonlinear kinetic models for O-Pom and LDH/PU/O-Pom for adsorption of Cefotaxime

Kinetic models	Equation	Parameters	O-Pom	LDH/PU/O-Pom
Pseudo first Order	$q_t = q_c (1 - e^{-k_1 t})$	K_1	1.80 E+05	1.86 E+05
		Q_c	30.00	31.90
		R^2	0.97	0.94
Pseudo second Order	$q_t = \frac{q_c^2 k_2 t}{1 + q_c k_2 t}$	K_2	1.03 E+06	1.03E+06
		Q_c	30.00	31.90
		R^2	0.97	0.94
Mixed 1,2 order	$q_t = q_c \frac{(1 - \exp(-kt))}{1 - f_2 \exp(-kt)}$	K	0.001	0.001
		Q_c	31.50	33.52
		F_2	0.99	0.99
		R^2	0.99	0.97
Avrami	$q_t = q_c [1 - \exp(-k_{av} t)^{n_{av}}]$	Q_c	30.00	31.90
		K_{av}	1.81	1.81
		n_{av}	1.71	1.71
		R^2	0.97	0.94
Intraparticle diffusion	$q_t = K_{ip} \sqrt{t} + C_{ip}$	K_{ip}	1.34	1.60
		C_{ip}	17.88	17.82
		R^2	0.39	0.49