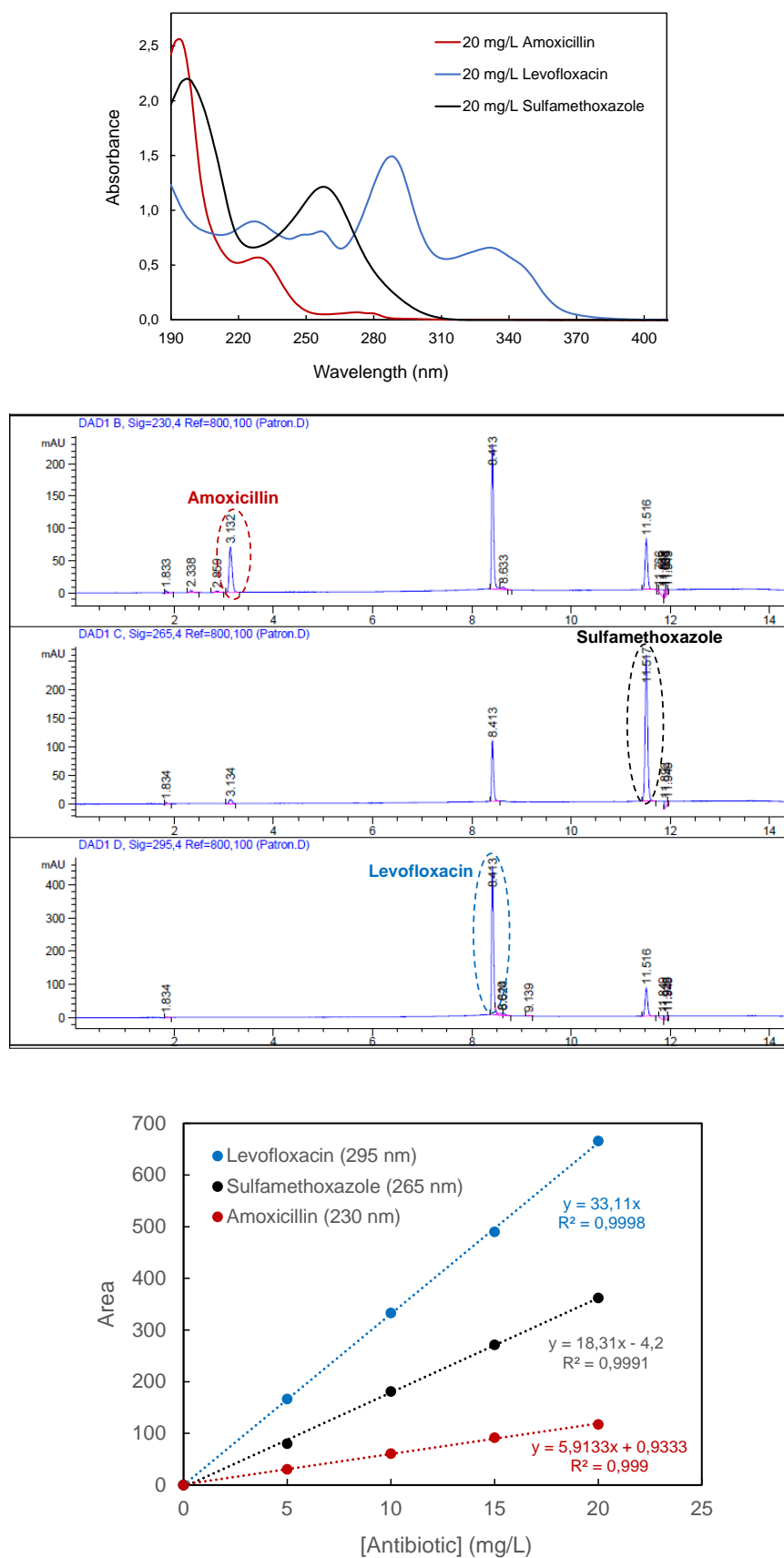


# SUPPLEMENTARY MATERIAL

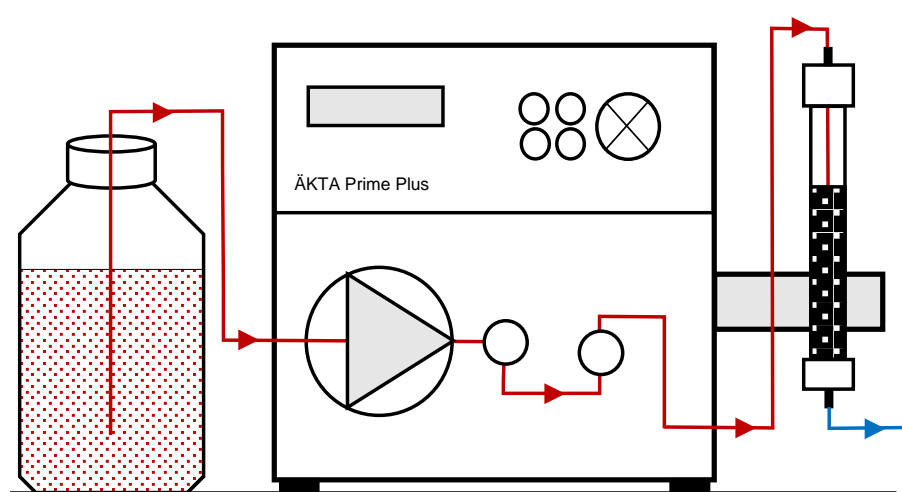
J.M. Obón<sup>\*</sup>, J.A. Fernández-López, M. Alacid, J.M. Angosto

Departamento de Ingeniería Química y Ambiental.  
Universidad Politécnica de Cartagena. Spain

**\*Corresponding author e-mail:** josemaria.obon@upct.es (José María Obón)

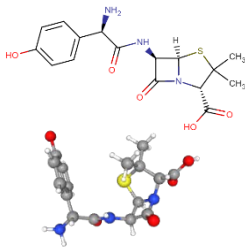
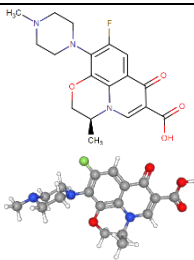
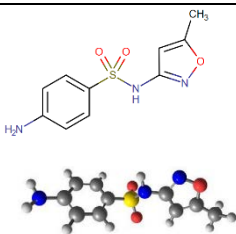


**Figure S1.** Spectra of antibiotics, a typical HPLC chromatogram, and HPLC quantification curves



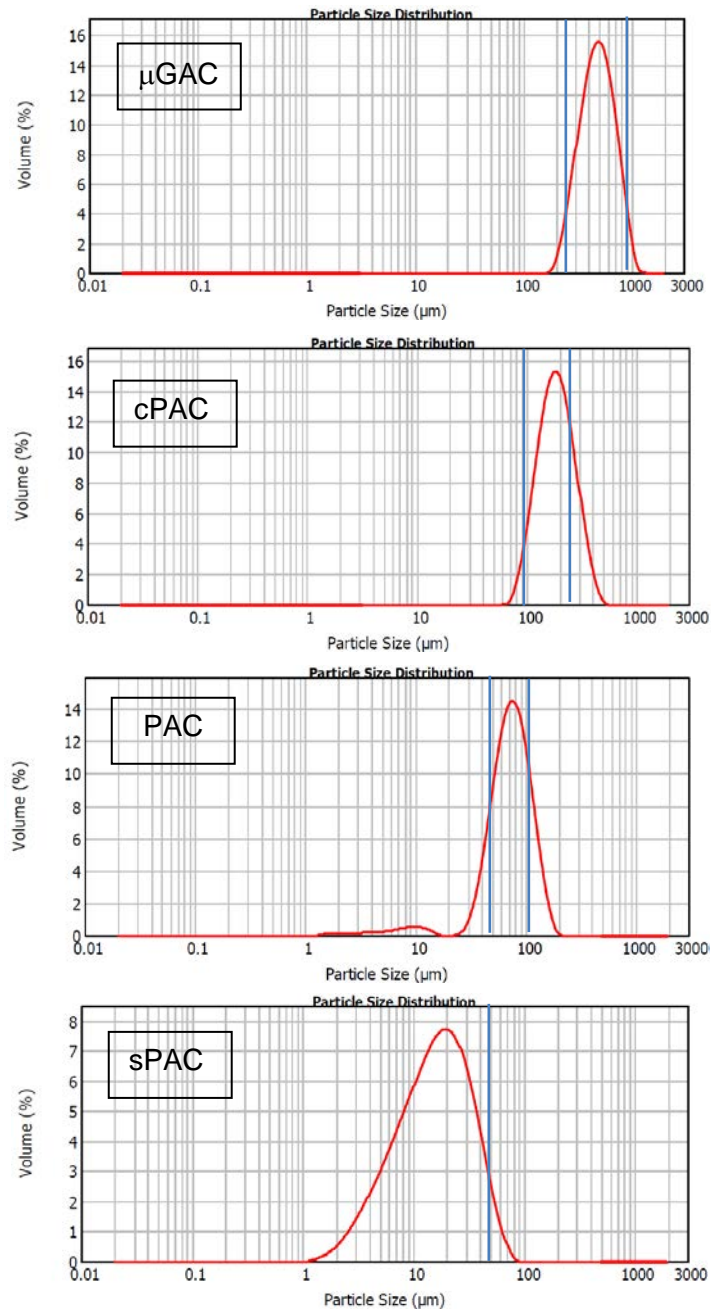
**Figure S2.** Experimental set-up of the studied fixed bed adsorber

**Table S1.** Antibiotic properties.

Property	Amoxicillin	Levofloxacin	Sulfamethoxazole
Chemical structure			
Molecular formula	$C_{16}H_{19}N_3O_5S$	$C_{18}H_{20}FN_3O_4$	$C_{10}H_{11}N_3O_3S$
M (g/mol)	365.4	361.4	253.3
Polar surface area ( $\text{\AA}^2$ )	132.9	73.3	107
Melting point ( $^{\circ}\text{C}$ )	194	220-225	166-169
Water solubility (mg/L)	3430	1000	459
pKa <sub>1</sub> / pKa <sub>2</sub> / pKa <sub>3</sub>	2.4 / 7.4 / 9.6 (carboxyl, amine, phenol)	6.1 / 8.1 (carboxyl, piperazine amine)	1.8 / 5.6 (amine, sulphonamide)

[DrugBank Online | Database for Drug and Drug Target Info](#) (Drugbank online)

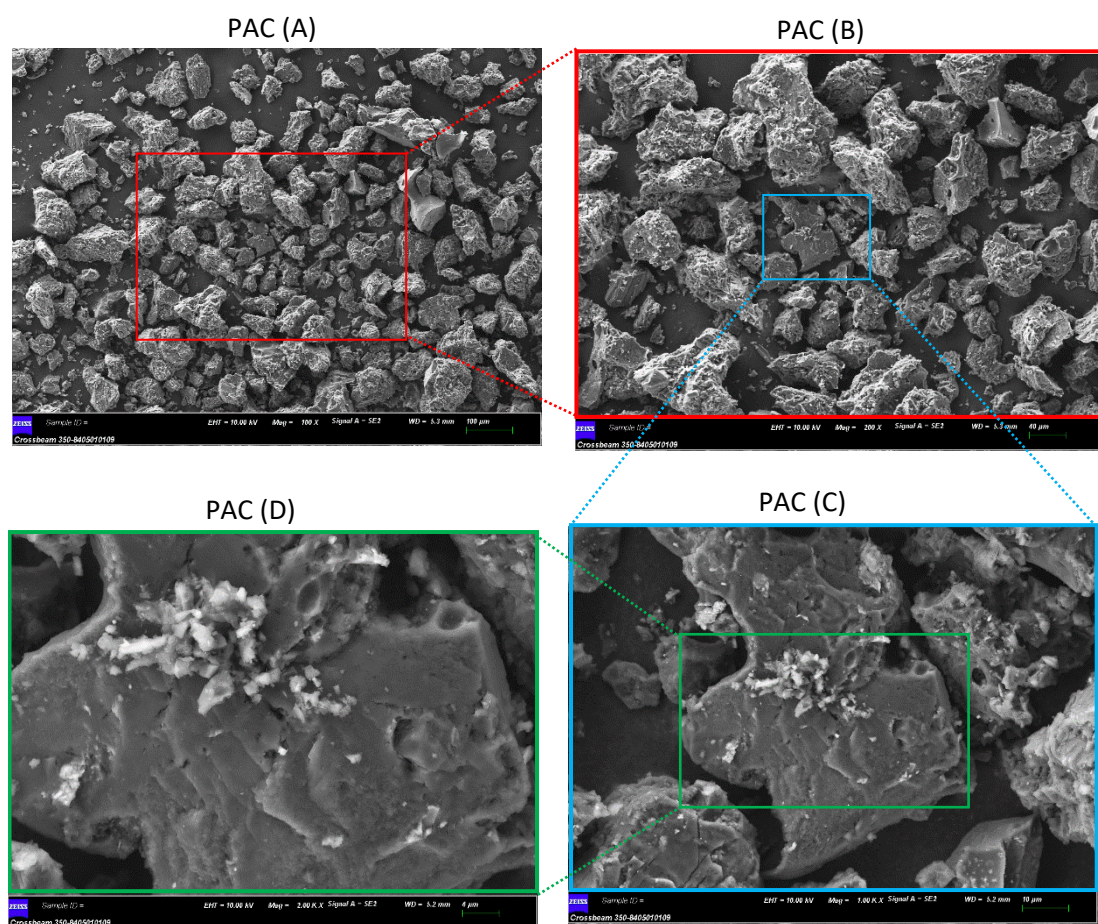
[PubChem \(nih.gov\)](#) (Pubchem)



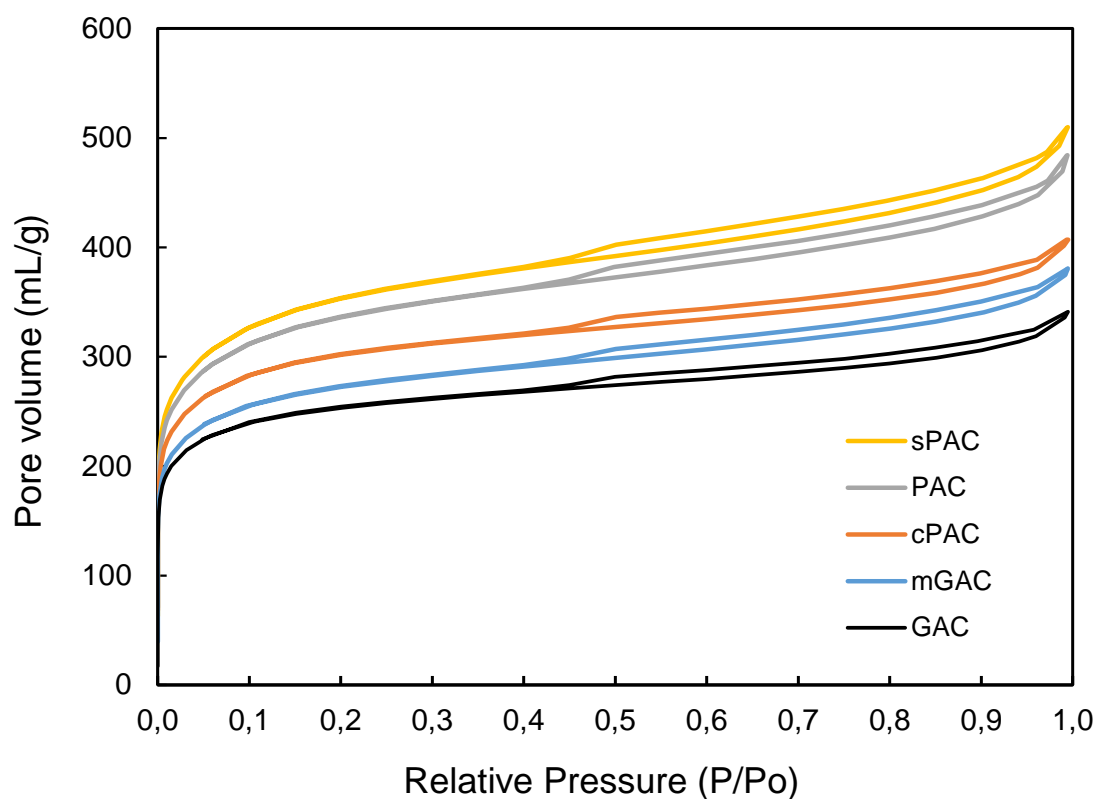
**Figure S3.** Particle size distribution curves of studied activated carbons.

**Table S2.** Parameters of particle size distributions of studied activated carbons.

Parameter	GAC	μGAC	cPAC	PAC	sPAC
D[4,3] (μm)	1500	508	197	77	19
Span	-	0.976	1.019	1.089	2.103
Uniformity	-	0.300	0.317	0.350	0.654



**Figure S4.** SEM images of PAC using different magnifications 100, 200, 1000 and 2000 (A, B, C, D).



**Figure S5.** Adsorption-desorption isotherms of N<sub>2</sub> at 77 K

**Table S3.** Specific surface area and pore volumes of obtained activated carbons.

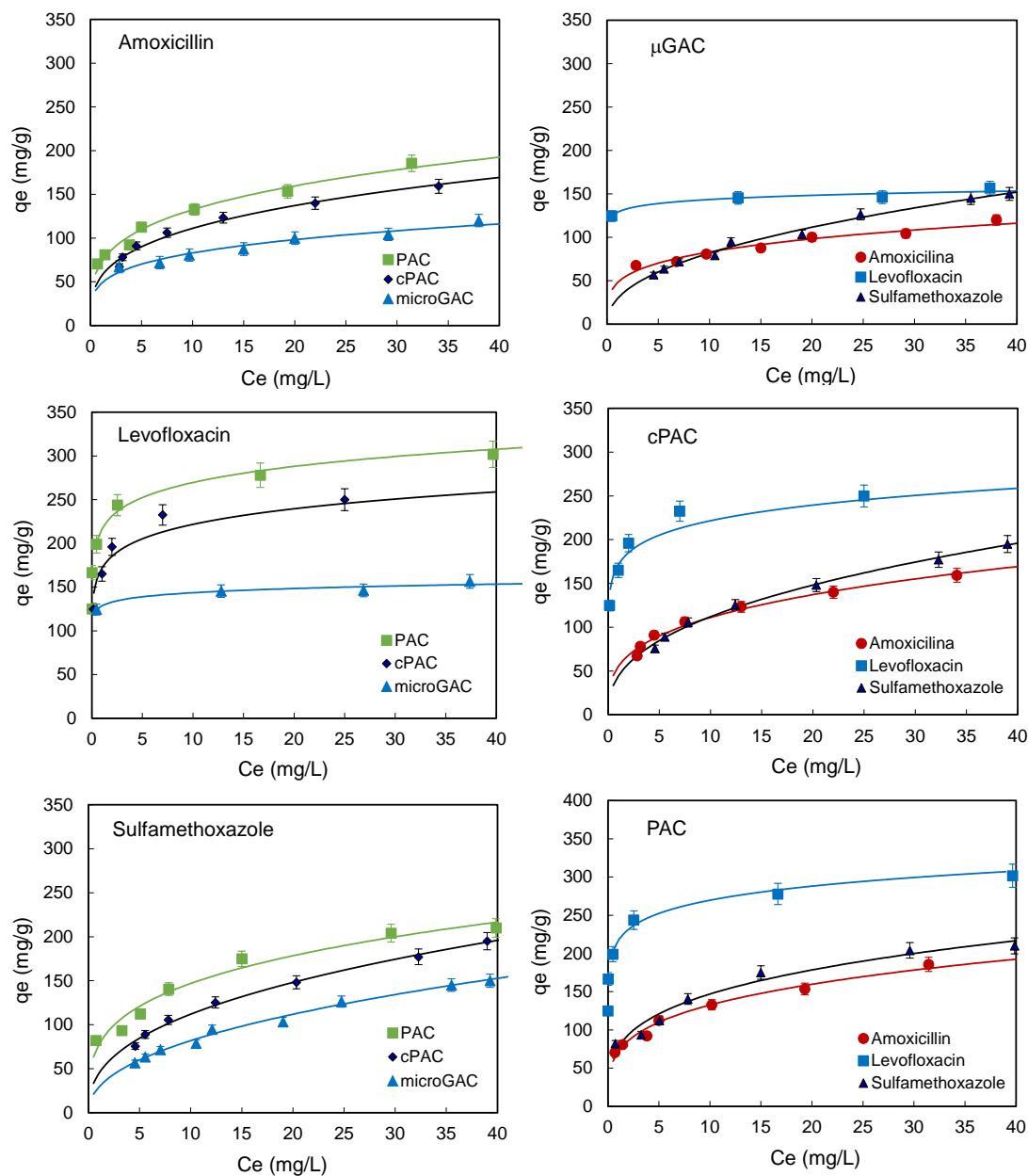
Parameter	GAC	$\mu$ GAC	cPAC	PAC	sPAC
$S_{\text{BET}}$ (m <sup>2</sup> /g)	942	1014	1125	1245	1318
$V_{\text{total}}$ (cm <sup>3</sup> /g)	0.492	0.550	0.590	0.693	0.733
$V_{\text{micro}}$ (cm <sup>3</sup> /g)	0.353	0.375	0.410	0.444	0.468
$V_{\text{meso}}$ (cm <sup>3</sup> /g)	0.139	0.175	0.180	0.249	0.265

$S_{\text{BET}}$  (m<sup>2</sup>/g) = BET surface area

$V_{\text{micro}}$  (cm<sup>3</sup>/g) = micropore volume (DR)

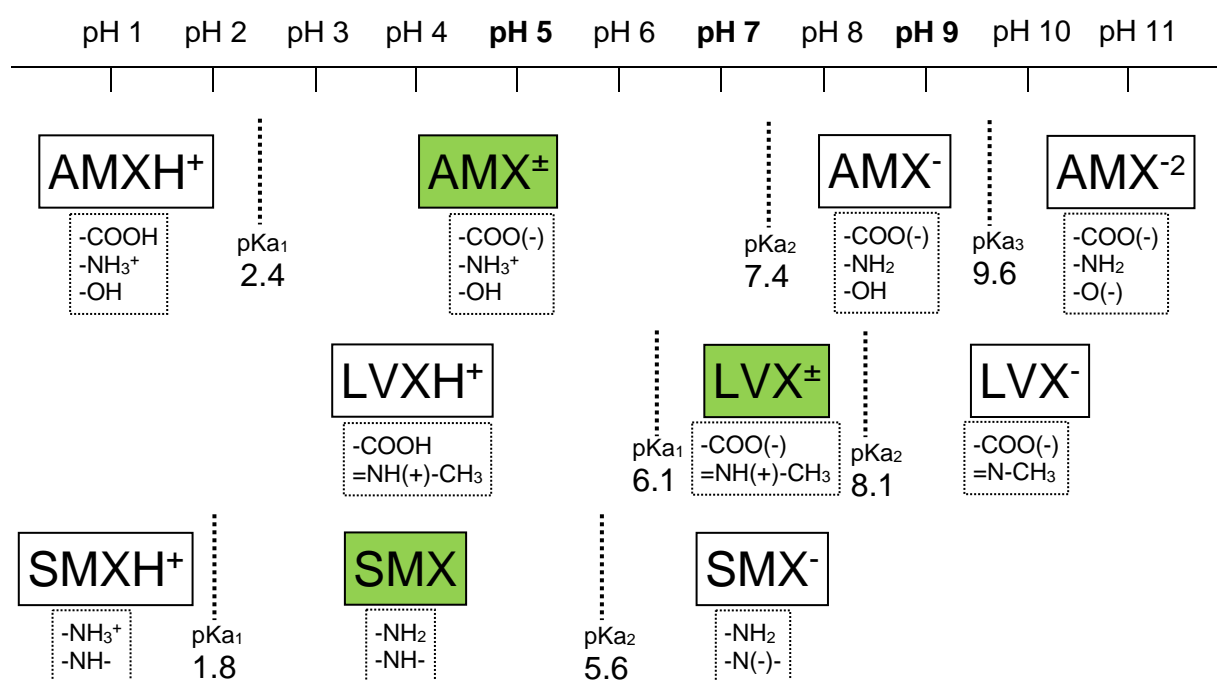
$V_{\text{total}}$  (cm<sup>3</sup>/g) = total pore volume

$V_{\text{meso}}$  (cm<sup>3</sup>/g) = mesopore volume =  $V_{\text{total}} - V_{\text{micro}}$

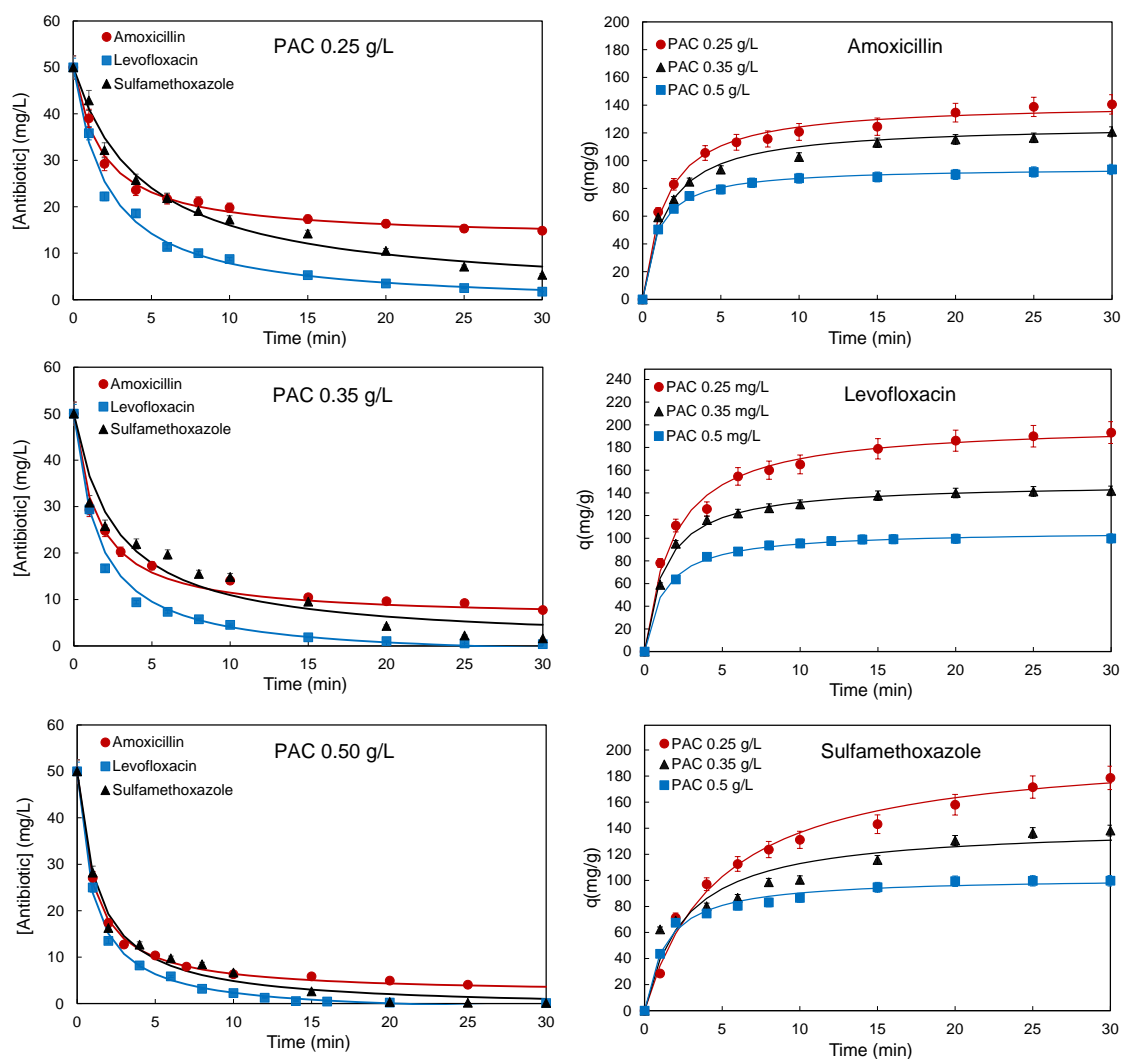


**Figure S6.** Isothermal adsorption of individual antibiotics on  $\mu$ GAC, cPAC, and PAC, fitted with Freundlich model.

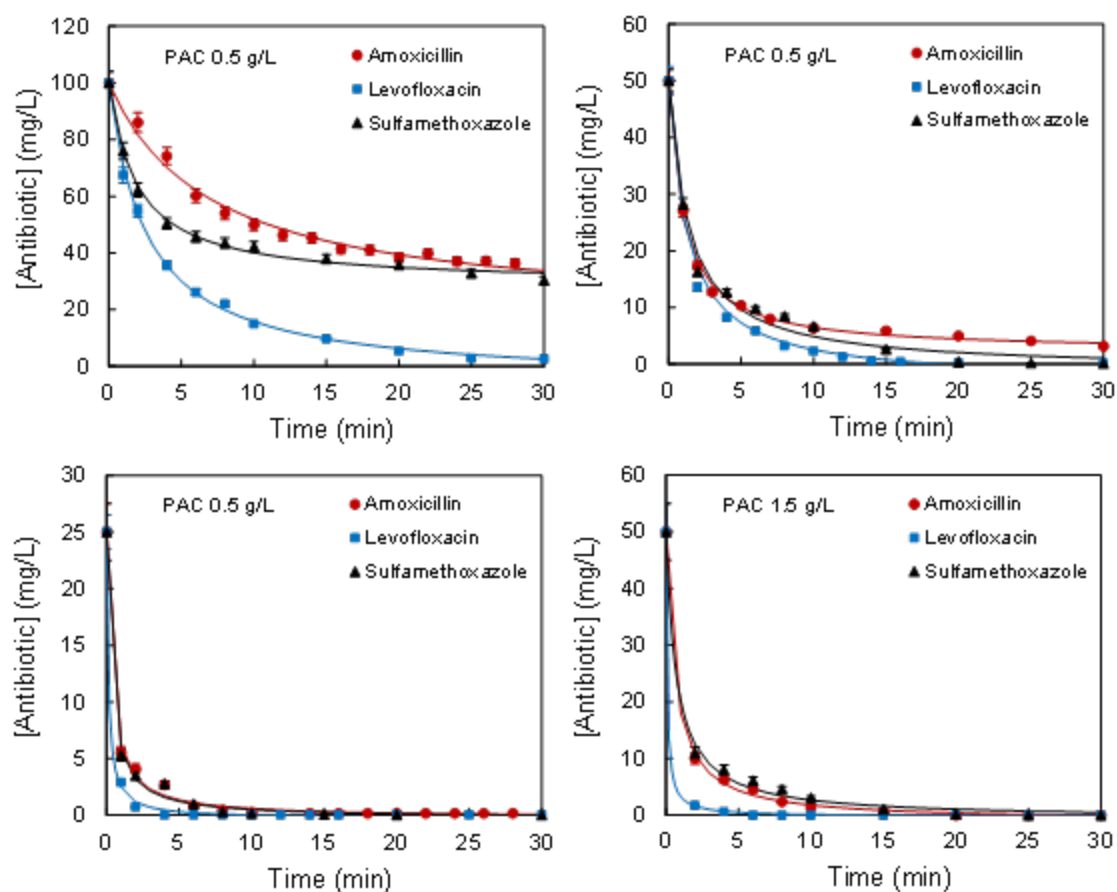




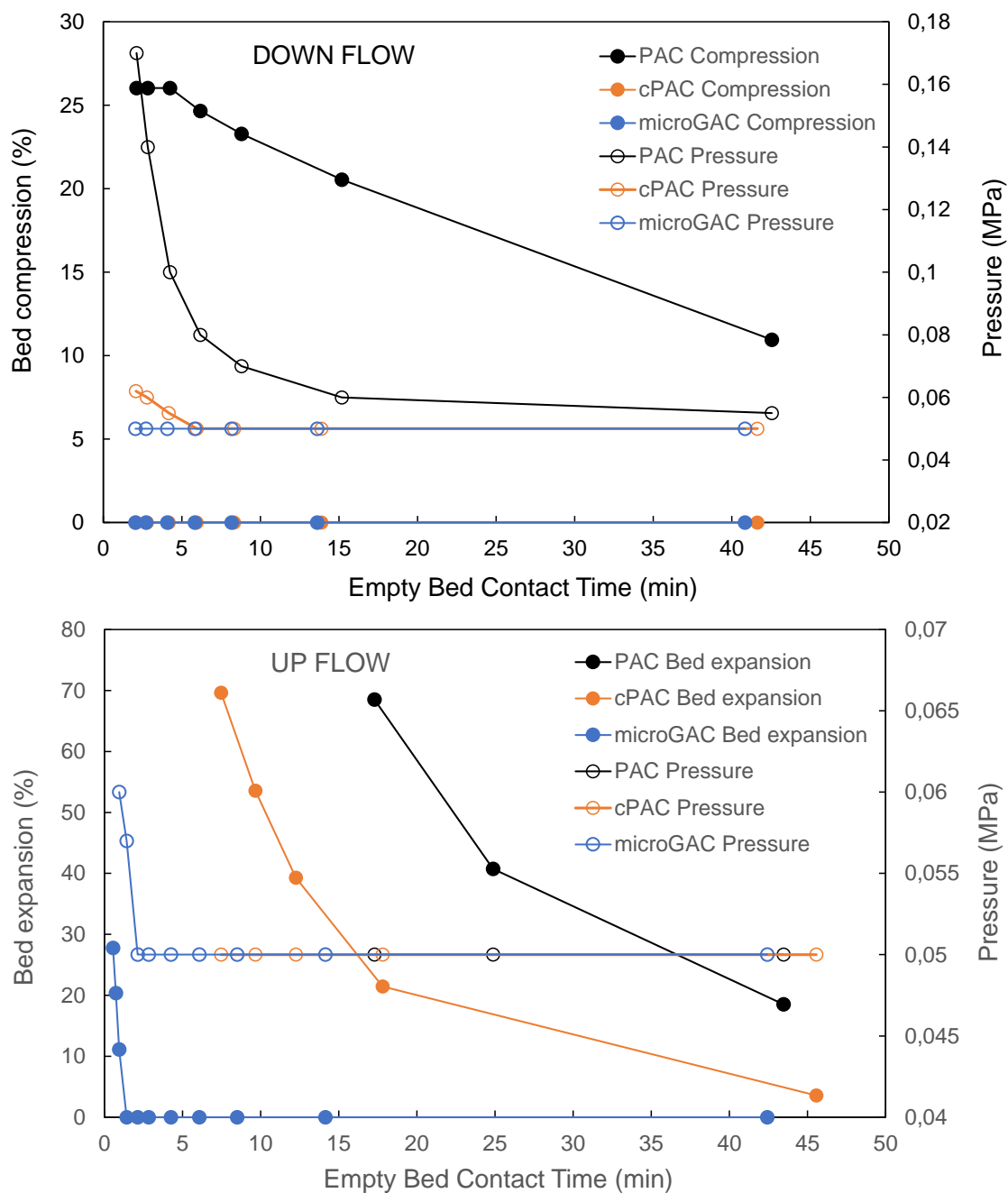
**Figure S7.** Distribution of molecular species at different pHs of amoxicillin (AMX), levofloxacin (LVX), and sulfamethoxazole (SMX). Green are structures at the pH of best adsorption.



**Figure S8.** Antibiotics adsorption kinetics at pH 7 with different PAC concentrations, fitted with second-order kinetic model.



**Figure S9.** Adsorption kinetics at pH 7 with different individual antibiotic concentrations using 0.5 g/L PAC, and an antibiotic's mixture with 1.5 g/L PAC concentration. Data fitted with pseudo-second order model.



**Figure S10.** Evaluation of operation conditions of fixed bed adsorbers packed with different activated carbons:  $\mu$ GAC, cPAC and PAC.

**Table S4.** Wastewater analysis

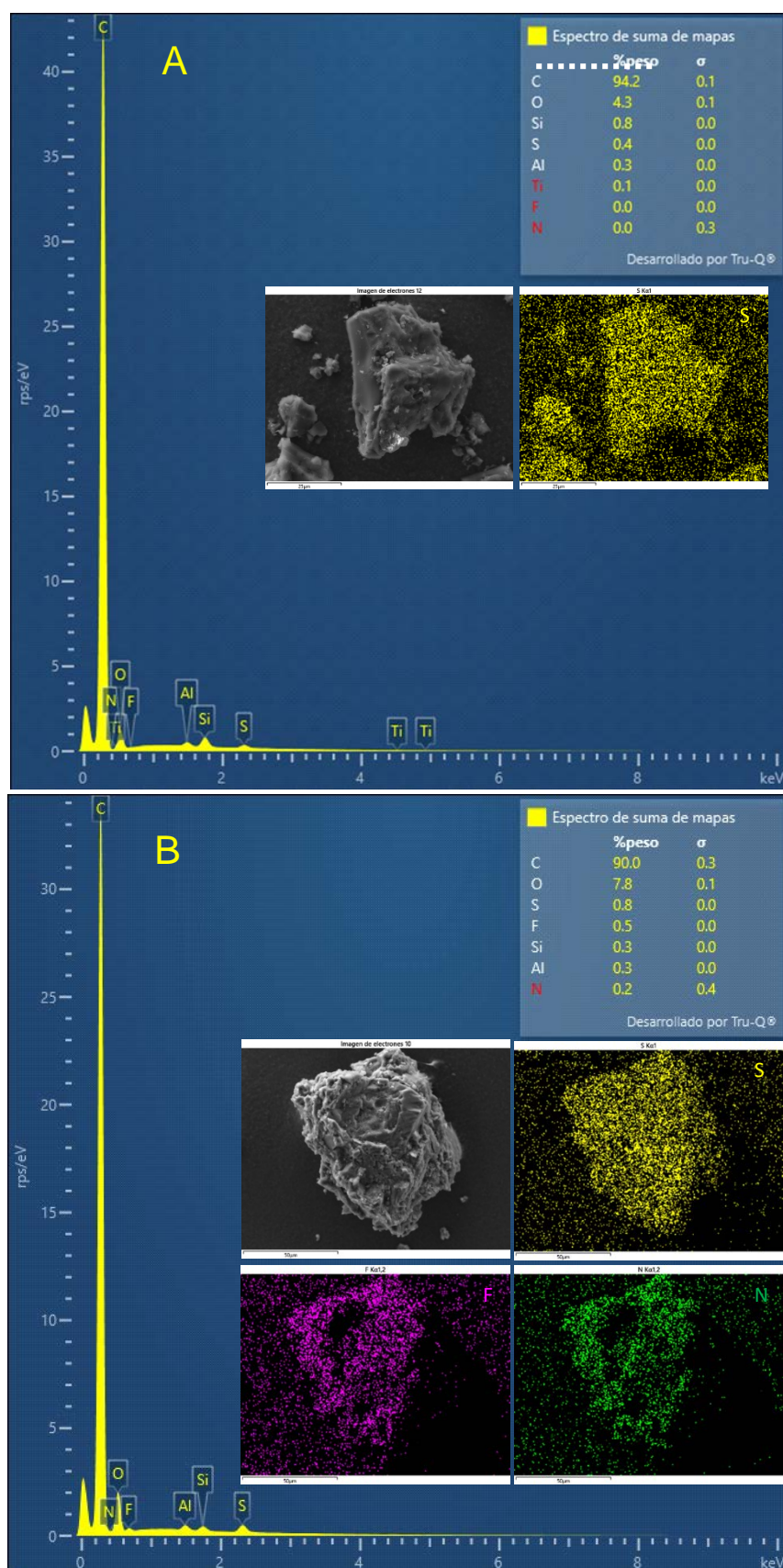
Analytical parameter	Value
pH	7.0
Conductivity ( $\mu\text{S}/\text{cm}$ )	120.0
BOD <sub>5</sub> ( $\text{mgO}_2/\text{L}$ )	10
Turbidity (NTU)	1
Cl <sup>-</sup> ( $\text{mg}/\text{L}$ )	44.24
Br <sup>-</sup> ( $\text{mg}/\text{L}$ )	0.67
F <sup>-</sup> ( $\text{mg}/\text{L}$ )	0.14
NO <sub>3</sub> <sup>-</sup> ( $\text{mg}/\text{L}$ )	14.29
NO <sub>2</sub> <sup>-</sup> ( $\text{mg}/\text{L}$ )	2.61
PO <sub>4</sub> <sup>3-</sup> ( $\text{mg}/\text{L}$ )	4.04
SO <sub>4</sub> <sup>2-</sup> ( $\text{mg}/\text{L}$ )	34.28
C <sub>2</sub> O <sub>4</sub> <sup>2-</sup> ( $\text{mg}/\text{L}$ )	<LD
Na <sup>+</sup> ( $\text{mg}/\text{L}$ )	28.29
K <sup>+</sup> ( $\text{mg}/\text{L}$ )	5.78
Li <sup>+</sup> ( $\text{mg}/\text{L}$ )	<LD
Ca <sup>2+</sup> ( $\text{mg}/\text{L}$ )	36.76
Mg <sup>2+</sup> ( $\text{mg}/\text{L}$ )	6.81
NH <sub>4</sub> <sup>+</sup> ( $\text{mg}/\text{L}$ )	1.23
Total Inorganic Carbon ( $\text{mg}/\text{L}$ )	12.22
Total Organic Carbon ( $\text{mg}/\text{L}$ )	4.79
Total Carbon ( $\text{mg}/\text{L}$ )	16.67
Total Nitrogen ( $\text{mg}/\text{L}$ )	5.68

**Table S5.** Modelling breakthrough curves of fixed bed adsorbers packed with  $\mu$ GAC or cPAC using deionized water with 50 mg/L antibiotic concentrations as influent.

Activated carbon	Model	Model parameter	Antibiotic		
			Amoxicillin	Levofloxacin	Sulfamethoxazole
$\mu$ GAC	Bohart-Adams	$K_{BA}$ (cm <sup>3</sup> /mg min)	0.0406	0.0382	0.0260
		$q_m$ (mg/cm <sup>3</sup> )	29.63	43.87	29.10
		$R^2$	0.9844	0.9926	0.9917
	Thomas	$K_T$ (cm <sup>3</sup> /mg min)	0.0406	0.0382	0.0260
		$q_0$ (mg/g)	62.83	93.02	61.71
		$R^2$	0.9844	0.9926	0.9917
	Yoon-Nelson	$K_{YN}$ (h <sup>-1</sup> )	0.1217	0.1145	0.0781
		$\tau$ (h)	42	62	41
		$R^2$	0.9844	0.9926	0.9917
	Yan or modified dose-response	$\alpha'$ (-)	5.08	7.92	3.37
		$q_F$ (mg/g)	58.40	91.41	57.03
		$R^2$	0.9742	0.9840	0.9775
cPAC	Bohart-Adams	$K_{BA}$ (cm <sup>3</sup> /mg min)	0.0258	0.0458	0.0345
		$q_m$ (mg/cm <sup>3</sup> )	60.22	93.94	84.09
		$R^2$	0.9854	0.9663	0.9883
	Thomas	$K_T$ (cm <sup>3</sup> /mg min)	0.0258	0.0458	0.0345
		$q_0$ (mg/g)	127.70	199.20	178.31
		$R^2$	0.9854	0.9663	0.9883
	Yoon-Nelson	$K_{YN}$ (h <sup>-1</sup> )	0.0775	0.1373	0.1036
		$\tau$ (h)	85	133	119
		$R^2$	0.9854	0.9663	0.9883
	Yan or modified dose-response	$\alpha'$ (-)	8.15	21.13	11.90
		$q_F$ (mg/g)	126.70	189.12	173.58
		$R^2$	0.9826	0.9816	0.9980

**Table S6.** Modelling breakthrough curves of fixed bed adsorbers packed with cPAC using as influent wastewater with 50 mg/L antibiotic concentrations.

Model	Model parameter	Wastewater				Deionized water
		AMX	LVX	SMX	Total Ant	Total Ant
Bohart-Adams	$K_{BA}$ (cm <sup>3</sup> /mg min)	0.0362	0.031	0.0262	0.0083	0.0077
	$q_m$ (mg/cm <sup>3</sup> )	76.55	88.07	63.61	230.50	232.84
	$R^2$	0.9874	0.9757	0.9839	0.9791	0.9807
Thomas	$K_T$ (cm <sup>3</sup> /mg min)	0.0362	0.031	0.0262	0.0083	0.0077
	$q_0$ (mg/g)	162.33	186.75	134.90	488.85	493.75
	$R^2$	0.9874	0.9757	0.9839	0.9791	0.9807
Yoon-Nelson	$K_{YN}$ (h <sup>-1</sup> )	0.1086	0.0942	0.0786	0.0750	0.0694
	$\tau$ (h)	108	124	89	109	110
	$R^2$	0.9874	0.9757	0.9839	0.9791	0.9807
Yan or modified dose-response	$\alpha'$ (-)	11.27	9.94	8.76	7.86	6.94
	$q_F$ (mg/g)	157.84	184.98	134.79	472.88	481.75
	$R^2$	0.9677	0.9619	0.9767	0.9818	0.9621



**Figure S11.** Elemental analyses of a PAC particle determined by energy dispersive X-ray spectroscopy, before (A) and after (B) amoxicillin, levofloxacin, and sulfamethoxazole full adsorption.