Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supplementary Information

S1. Synthesis of covalent organic polymers

All the chemicals utilized in the present study were purchased from commercial vendors and utilized as received without any additional purification steps. The covalent organic polymer (COP) adsorbents functionalized with ethylenediamine (CBAP-1 (EDA) [CE]) and diethylenetriamine (CBAP-1 (DETA) [CD]) were synthesized using a Friedel-Crafts benzoylation approach; note that CBAP is a carbonyl-incorporated aromatic polymer. Briefly, 3.05 g of terephthaloyl chloride (99%; Sigma-Aldrich Corp., St. Louis, Missouri, USA) and 3.06 g of 1,3,5-triphenylbenzene (97%; Sigma-Aldrich Corp., St. Louis, Missouri, USA) were mixed in 180 mL of dichloromethane (99.8%; Sigma-Aldrich Corp., St. Louis, Missouri, USA) for 15 min under a constant nitrogen gas purge. Thereafter, 2 g of anhydrous aluminum chloride (98%; Sigma-Aldrich Corp., St. Louis, Missouri, USA) was added into the reaction solution and stirred for 12 h under reflux to yield a dark brown powder. Subsequently, the obtained powder was filtered and washed with 30 mL of dichloromethane and anhydrous methanol (99.8%; Sigma-Aldrich Corp., St. Louis, Missouri, USA), three times each. The powder was then dried at 130°C for 12 h under vacuum, and this sample was referred to as CBAP-1. The CBAP-1 (1 g) was then dissolved in methanol (40 mL) followed by the addition of 2 mL EDA ($\geq$ 99%; Sigma-Aldrich Corp., St. Louis, Missouri, USA) or DETA ($\geq$ 99%; Sigma-Aldrich Corp., St. Louis, Missouri, USA). The obtained mixture was stirred vigorously for 15 h at 80°C and then cooled to room temperature. Subsequently, excess sodium borohydride ($\geq$ 98%; Sigma-Aldrich Corp., St. Louis, Missouri, USA) was added to the solution, which was then stirred vigorously at room temperature for 10 h. The obtained powder was filtered and washed with 30 mL of methanol and distilled water, three times each. The powder was then dried at 130°C under vacuum for 12 h to obtain CE and CD, respectively.

S2. Adsorbent characterization

Fourier transform infrared (FTIR) spectroscopy was conducted using a PerkinElmer L1600400-IR spectrometer (Waltham, Massachusetts, USA) in the 400-4000 cm^{-1} range in attenuated reflectance mode. The powder x-ray diffraction (PXRD) results were obtained using an HR-XRD diffractometer (Rigaku Corp., Tokyo, Japan). The step size, 2θ range, and scan speed were 0.02°, 5-80°, and 4° min^{-1}, respectively. Thermogravimetric analysis (TGA) was conducted using an SDTQ600 Auto-DSCQ20 system (Eden Prairie, MN, USA) to determine the thermal stabilities of the applied adsorbents. The adsorbents were kept on an alumina pan and were heated at a ramping rate of 10°C min^{-1} from room temperature to 800°C (for COPs) or 600°C (for AC) under flowing nitrogen gas (100 mL min^{-1}). A Micrometrics ASAP 2010 system (Norcross, GA, USA) was utilized for Brunauer-Emmett-Teller (BET) analysis of the applied adsorbents and plotting the nitrogen adsorption-desorption isotherms at 77 K. The x-ray photoelectron spectroscopy (XPS) analysis was conducted using a K-alpha system (Thermo Fisher Scientific, Waltham, Massachusetts, USA) for assessing the surface chemistry of the applied adsorbents. The morphologies of COPs were determined using a field emission electron microscope (FE-SEM; TESCAN, Brno-Kohoutovice, Czech Republic). The morphology of activated carbon (AC) was determined using a NOVA nanoSEM-450 (Hillsboro, OR, USA).

S3. Tables and Figures

Order	Compounds	Short name	Formula	CAS No.	MW (g mol^{-1})	RF[a] (ng^{-1})	Linearity (R^2)	RSD[b] (%)	IDL[c] (ng)
1	Formaldehyde	FA	CH_2O	50-00-0	30.0	22973	0.9986	2.67	0.11
2	Acetaldehyde	AA	C_2H_4O	75-07-0	44.1	18487	0.9984	2.20	0.21
3	Propionaldehyde	PA	C_3H_6O	123-38-6	58.1	14273	0.9984	1.58	0.37
4	Butyraldehyde	BA	C_4H_8O	123-72-8	72.1	10910	0.9980	1.33	0.50
5	Isovaleraldehyde	IA	$C_5H_{10}O$	590-86-3	86.1	9745.6	0.9983	0.87	0.74
6	Valeraldehyde	VA	$C_5H_{10}O$	110-62-3	86.1	8926.8	0.9969	3.68	0.41

[a] Response factor

[b] Relative standard deviation

[c] Instrument detection limit

Table S1. Basic information for six target aldehydes and summary of related quality assurance datasets.

Table S2. Summary of the kinetic fitting results obtained for the adsorption of gaseous aldehydes onto AC.

Order	Aldehyde	Experimental maximum capacity (q_e, mg g^{-1})	Model	Kinetic model constants					Predicted maximum capacity (q_m, mg g^{-1})		Fitting parameters					
											[a]r^2			[b]Non-linear Chi-square test (χ^2)		
				K_1 (min^{-1})	K_2 (g mg^{-1} min^{-1})	$K_2q_m^2$ (h_0; mg g^{-1} min^{-1})	K_{ID} (mg g^{-1} min$^{-0.5}$)	c	PFO	PSO	PFO	PSO	IPD	PFO	PSO	IPD
1	FA	0.003	Linear	0.014	0.0008	0.001	0.02	-0.1	0.2	-1.4	0.873	0.999	0.948	0.048	0.000	0.050
2			Non-linear	0.0001	0.0001	0.002	-	-	13.5	4.4	0.997	0.995	-	0.001	0.001	-
3	AA	0.04	Linear	0.020	0.0013	0.02	0.14	-0.3	1.5	3.6	0.880	1.000	0.993	0.260	0.0003	0.030
4			Non-linear	0.008	0.0013	0.02	-	-	2.2	3.6	0.9998	0.9997	-			-
5	PA	0.2	Linear	0.070	1.87	0.19	0.002	0.3	0.3	0.3	0.497	0.458	0.138	0.207	0.018	0.002
6			Non-linear	2.550	4,651	447	-	-	0.3	0.3	0.000004	0.000004	-	0.003	0.003	-
7	BA	1.5	Linear	0.101	0.07	0.23	0.13	0.6	1.6	1.9	0.863	0.901	0.682	0.085	0.102	0.354
8			Non-linear	0.081	0.05	0.20	-	-	1.8	2.0	0.989	0.932	-	0.012	0.07	-
9	IA	6.7	Linear	0.024	0.0006	0.16	0.93	-1.2	9.2	16.7	0.960	0.995	0.993	0.516	0.046	0.084
10			Non-linear	0.017	0.0009	0.19	-	-	9.9	14.4	0.999	0.998	-	0.021	0.05	-
11	VA	7	Linear	0.027	0.0003	0.11	0.88	-1.5	9.6	21	0.790	0.990	0.991	4.192	0.061	0.074
12			Non-linear	0.012	0.0005	0.13	-	-	10.3	16.1	0.996	0.995	-	0.046	0.068	-

[a] r^2 is the correlation coefficient to determine the best-fitting isotherm. $r^2 = \frac{\sum(q_c - q_a)2}{\sum(\quad)\quad\sum(\quad)}$. Here, q_c and q_e are the calculated and experimental adsorption capacities, respectively. q_a is the average of q_e values.

[b] χ^2 is a statistical test to calculate the error between the predicted and experimental data. $\chi^2 = \sum_{i=1}^{n} \frac{(q_e - q_c)2}{qe}$. Here, 'n' is the run number.

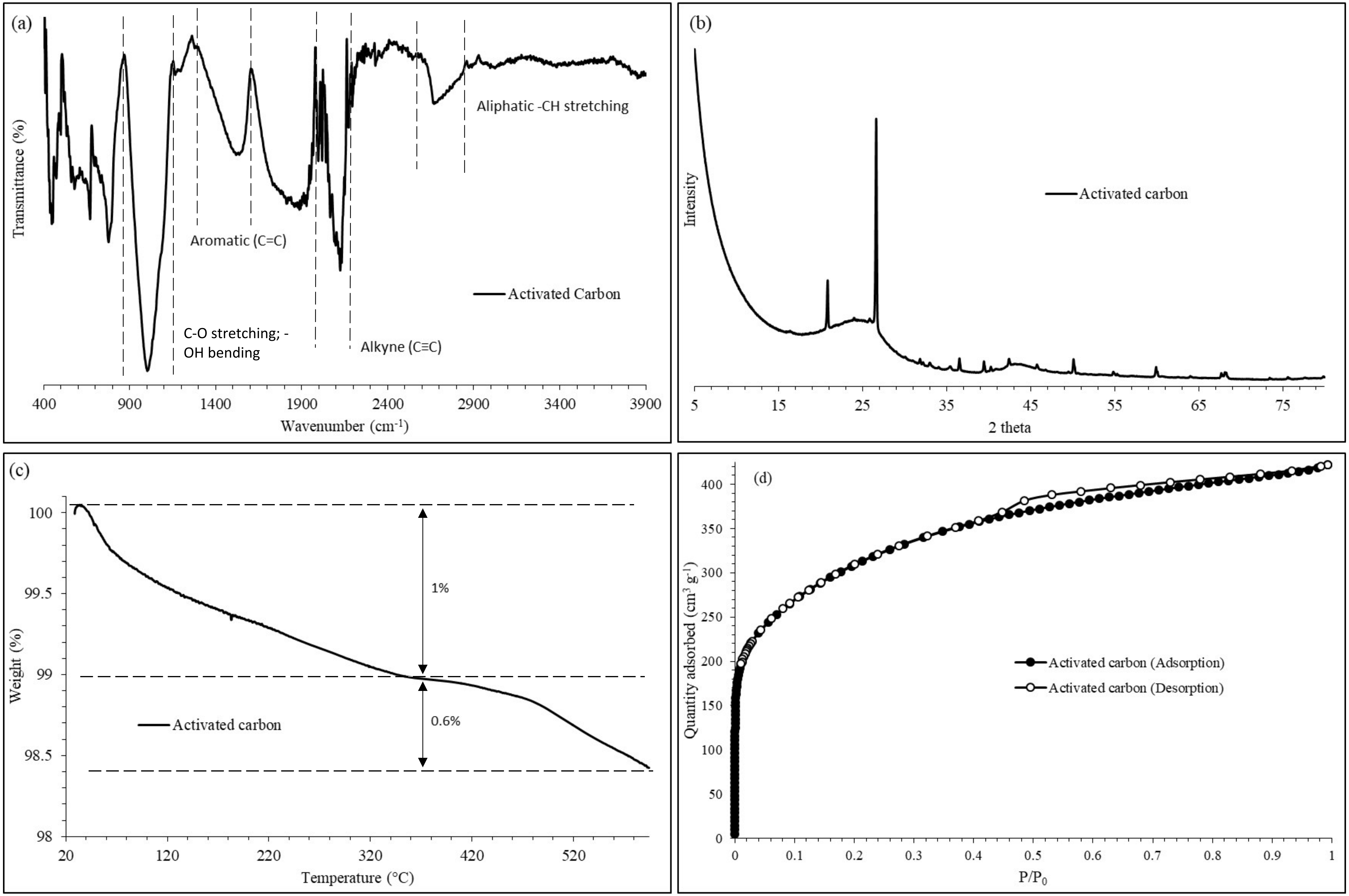

Figure S1. Characterization results of the AC: (a) FTIR spectra, (b) PXRD patterns, (c) TGA profiles, and (d) Nitrogen adsorption-desorption isotherms measured at 77 K.

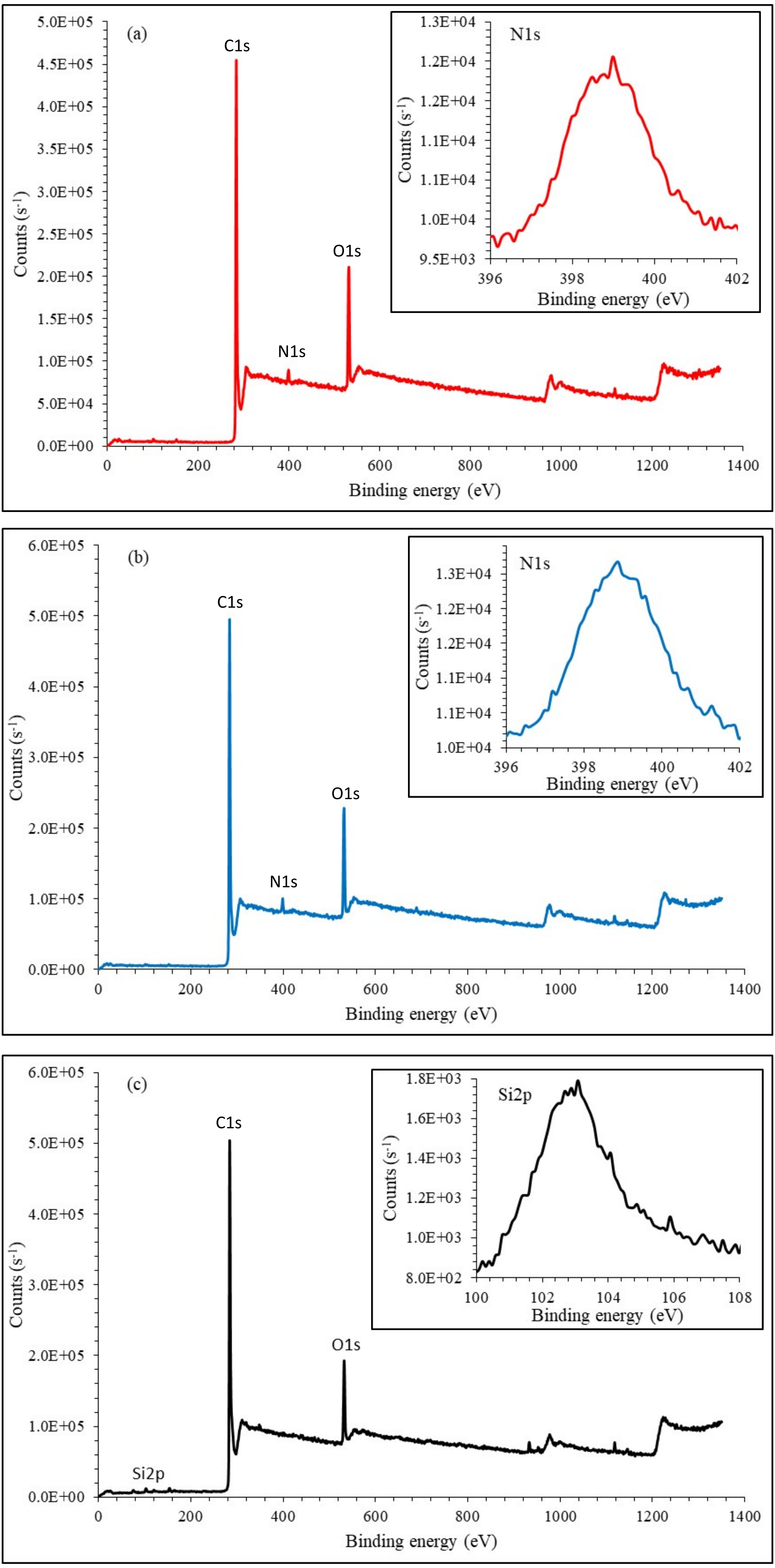

Figure S2. The wide-scan XPS profiles of the analyzed adsorbents: (a) CE, (b) CD, and (c) AC.

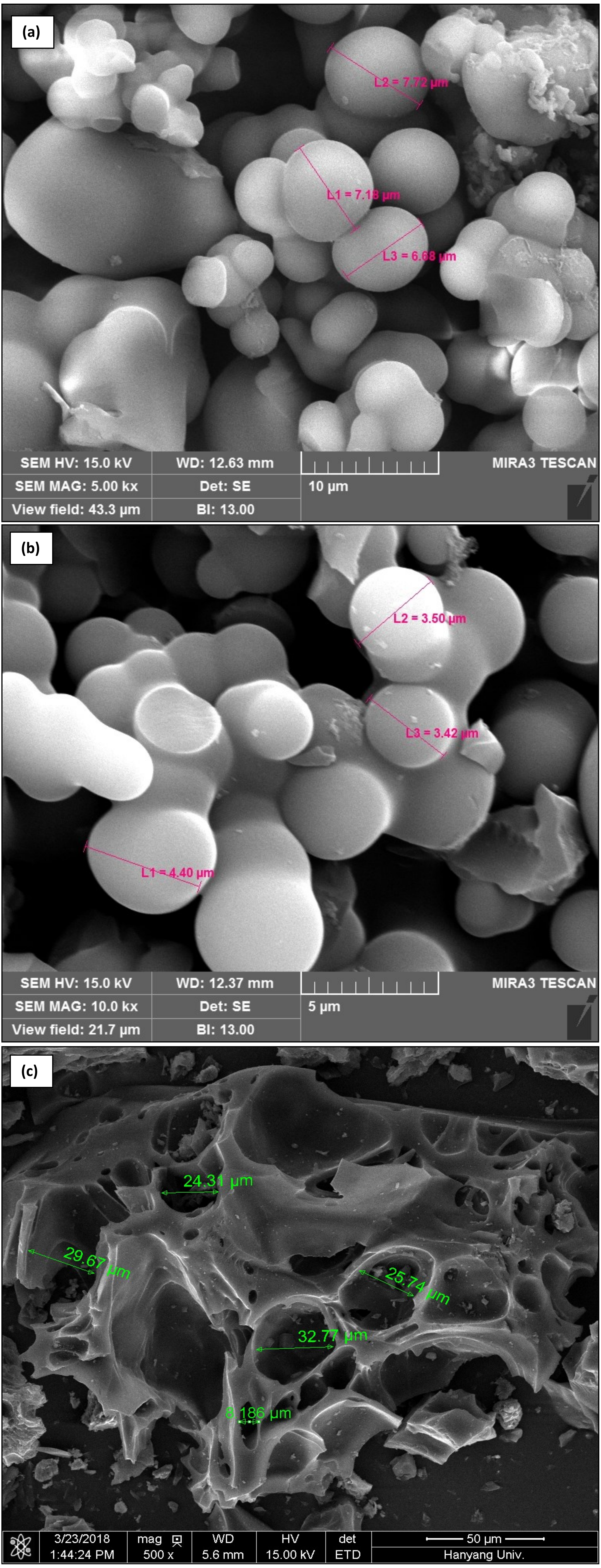

Figure S3. SEM images of the analyzed adsorbents: (a) CE, (b) CD, and (c) AC.

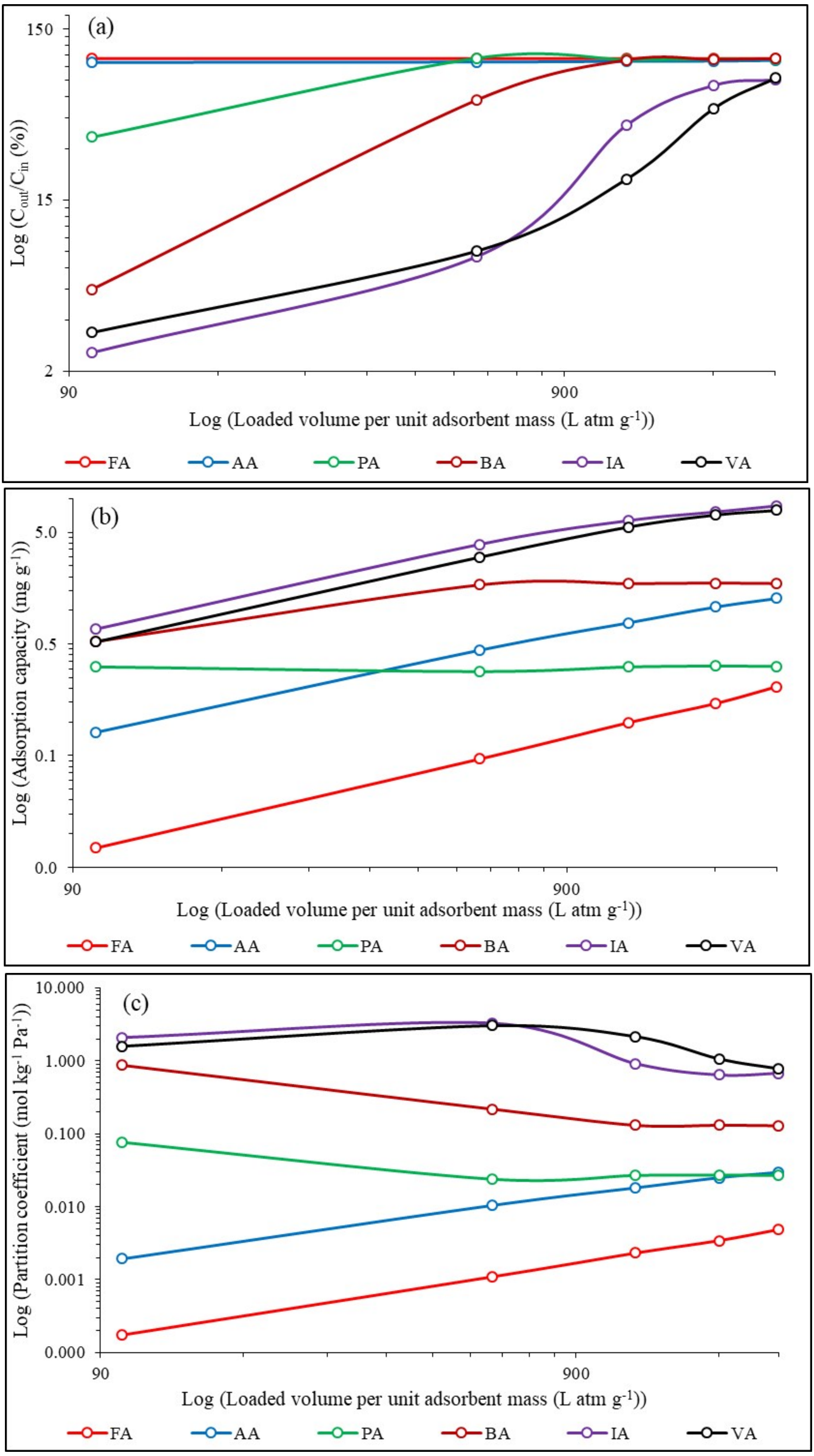

Figure S4. Performance of AC toward the gaseous aldehyde mixture. (a) Breakthrough profiles. (b) Evolution of adsorption capacity values as a function of the loaded G-WS volume. (c) Variations in the partition coefficient values with the loaded G-WS volume.

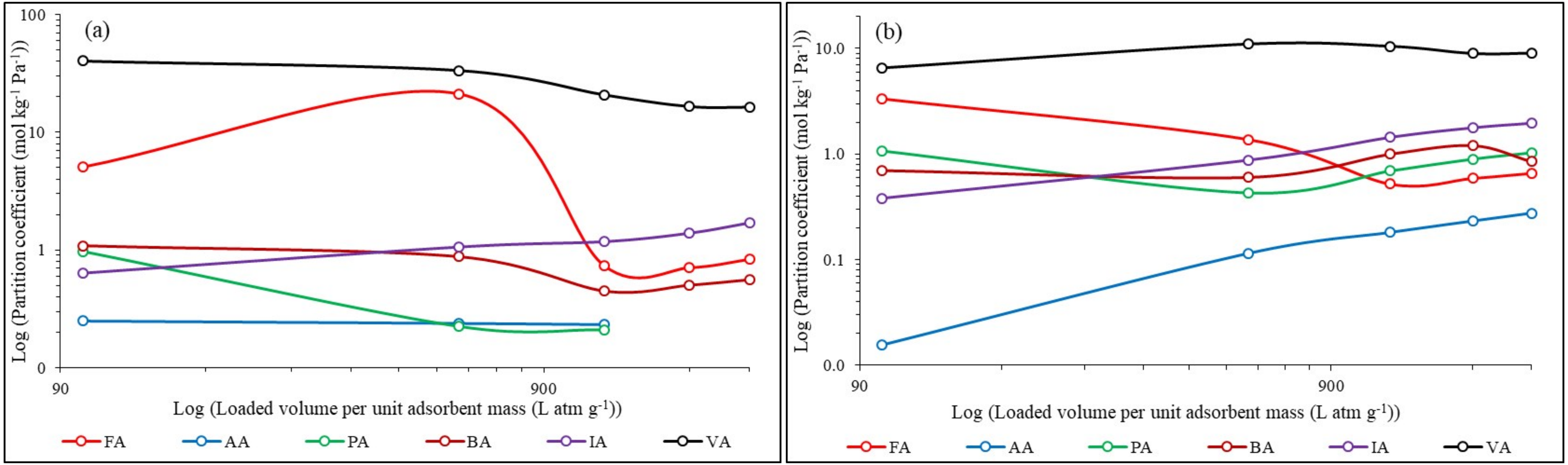

Figure S5. Variations in the partition coefficient values of the analyzed COPs with the loaded G-WS volume: (a) CE and (b) CD.

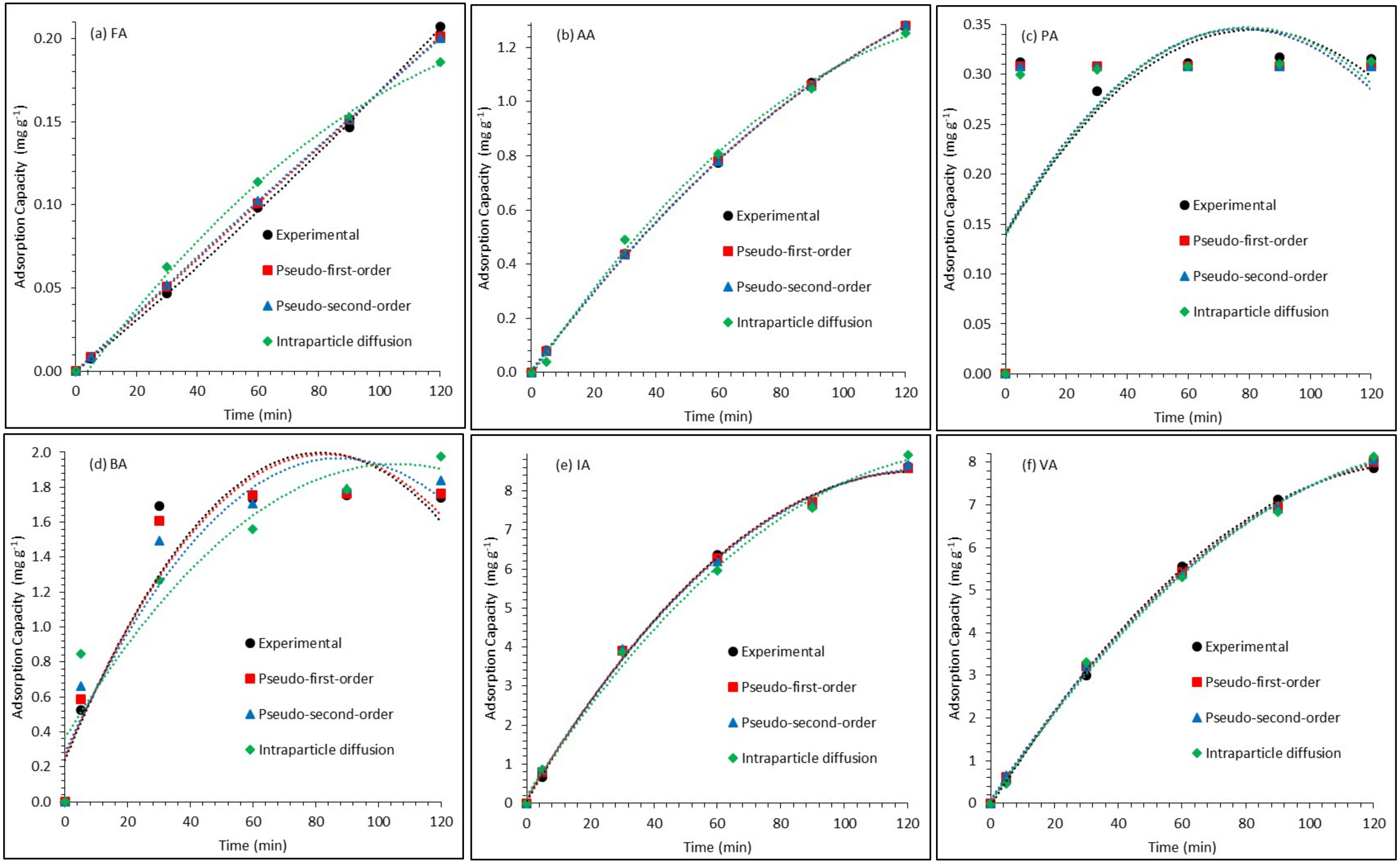

Figure S6. Non-linear PFO, non-linear PSO, and IPD kinetic fitting plots for the adsorption of gaseous aldehydes onto AC: (a) FA, (b) AA, (c) PA, (d) BA, (e) IA, and (f) VA.

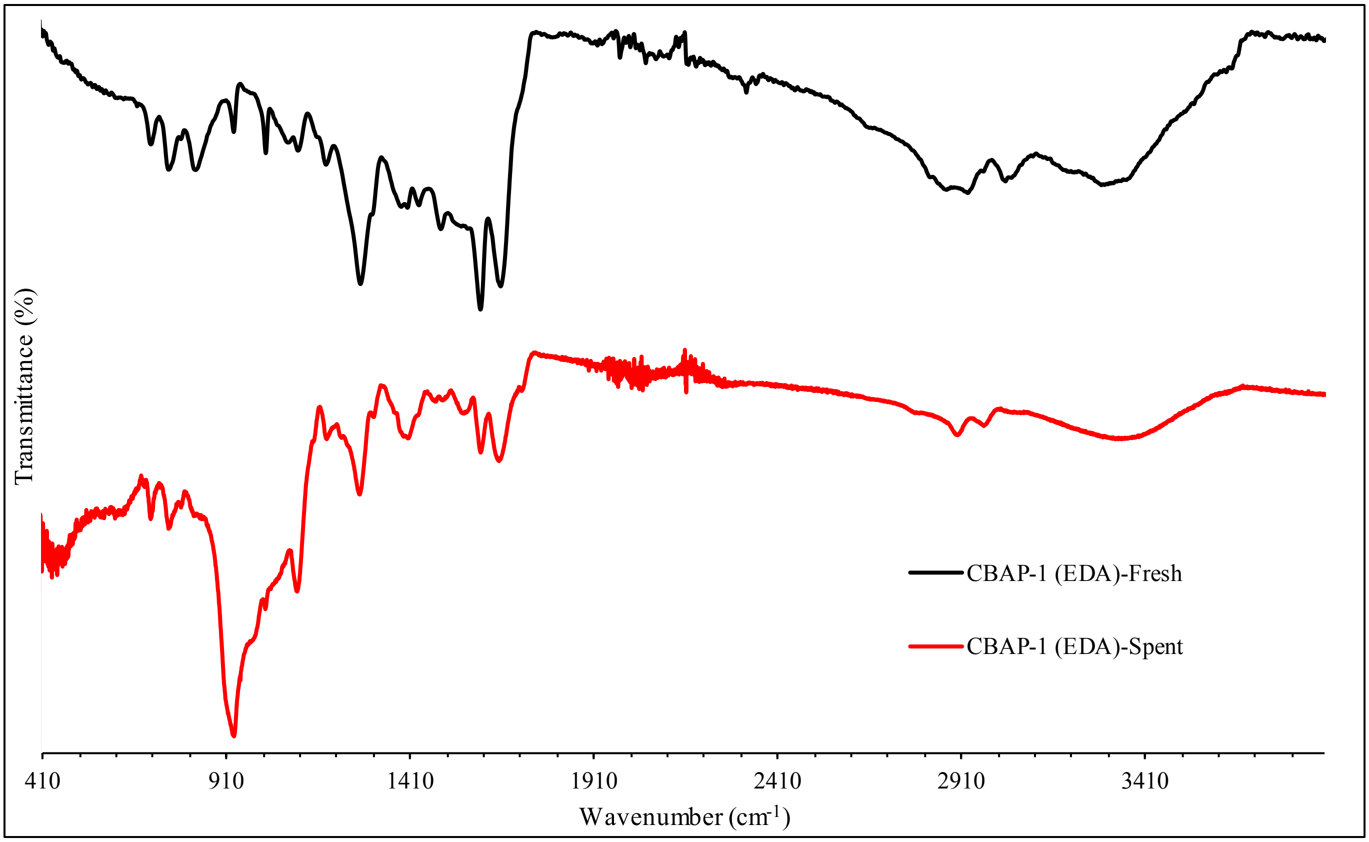

Figure S7. FTIR spectra of CE for FA adsorption before (fresh) and after use (spent).