Electronic Supplementary Information (ESI)

Phytochemical species intercalated into Layered Double Hydroxides: Structural Investigation and Biocompatibility Assays

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Materials

Reagents

p-Coumaric acid ($C_9H_8O_3$, Sigma), (*i*) main vibrational modes:[1] 1680 cm^{-1} (carbonyl stretching mode of the carboxyl group), 1447 and 1171 cm^{-1} (bending of the aromatic ring) and 930 cm^{-1} (OH bending, of the carboxyl group) and (*ii*) main chemical shifts: 172 ppm (C1a, carboxylic group), 157 ppm (C3a, styrene group) and 136 ppm (2b,6b, carbon from the aromatic ring). Magnesium chloride hexahydrate ($MgCl_2 \cdot 6H_2O$, Synth), aluminum chloride hexahydrate ($AlCl_3 \cdot 6H_2O$, Aldrich), zinc chloride ($ZnCl_2$, Aldrich), sodium hydroxide (NaOH, Merck), paraformaldehyde solution 4 % (Synth), historesin (Technovitz®7100, Kulzer), hematoxylin ($C_{16}H_{14}O_6$, Vetec), eosin ($C_{20}H_6Br_4Na_2O_5$, Vetec), Picrosirius red ($C_{45}H_{26}N_{10}Na_6O_{21}S_6$, Alfa Aesar), and polypropylene mesh (Prolene™, Ethicon) were used without further purification.

Physicochemical characterization of LDH-Cou

The *p*-coumaric acid salt exhibits its typical X-ray diffraction patterns, as shown in Fig. S1.[2,3]

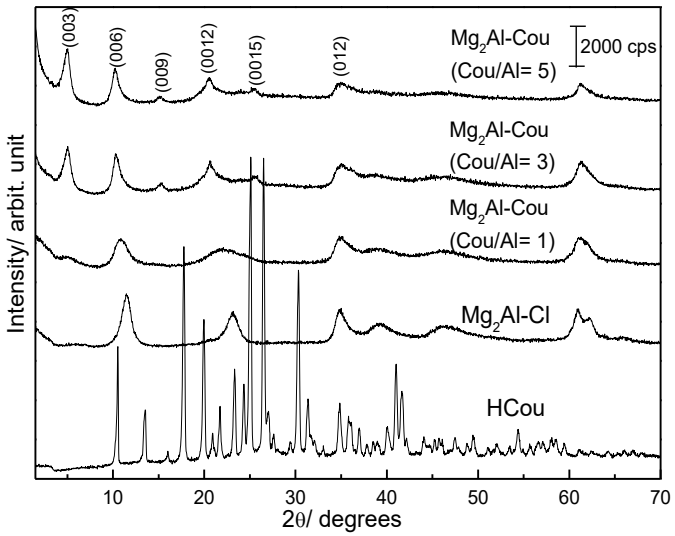


Fig. S1. PXRD patterns of HCou, Mg_2Al-Cl, and Mg_2Al-Cou with Cou/Al molar ratio equal to 1, 3 and 5.

Table S1: Interplanar distance (d_{hkl}) and 2θ (λ=1.54 Å) of Mg_2Al-Cou and Zn_2Al-Cou samples obtained from XRD data.

Mg_2Al-Cou (Cou/Al=1)		**Mg_2Al-Cou (Cou/Al=3)**		**Mg_2Al-Cou (Cou/Al=5)**		**Zn_2Al-Cou (Cou/Al=3)**		
2θ	**d(Å)**	**2θ**	**d(Å)**	**2θ**	**d(Å)**	**2θ**	**d(Å)**	**hkl**
5.13	17.21	5.04	17.51	5.04	17.51	5.13	17.20	(003)
10.86	8.14	10.26	8.61	10.26	8.61	10.20	8.66	(006)
-	-	15.36	5.76	15.06	5.88	15.33	5.77	(009)
-	-	20.61	4.30	20.52	4.32	20.55	4.32	(0012)
		25.83	3.45	25.14	3.54	25.77	3.45	(0015)
61.23	1.51	61.26	1.51	61.23	1.51	60.60	1.53	(110)/(113)

Table S2: Elemental analysis (CHN) data, metal contents and the percentage of H_2O (obtained from TGA curve) of LDH-Cou materials.

Sample	**M^{II}/Al[a)]**	**%C**	**%H_2O**	**%/ w/w**
Mg_2Al-Cou (Cou/Al=1)	2.39	13.4	16.2	19.9
Mg_2Al-Cou (Cou/Al=3)	2.18	20.9	16	31.3
Mg_2Al-Cou (Cou/Al=5)	1.93	21.5	18.2	32.4
Zn_2Al-Cou (Cou/Al=3)	2.15	23.6	7.0	34.8

a) molar ratio where M^{II} = Mg or Zn;

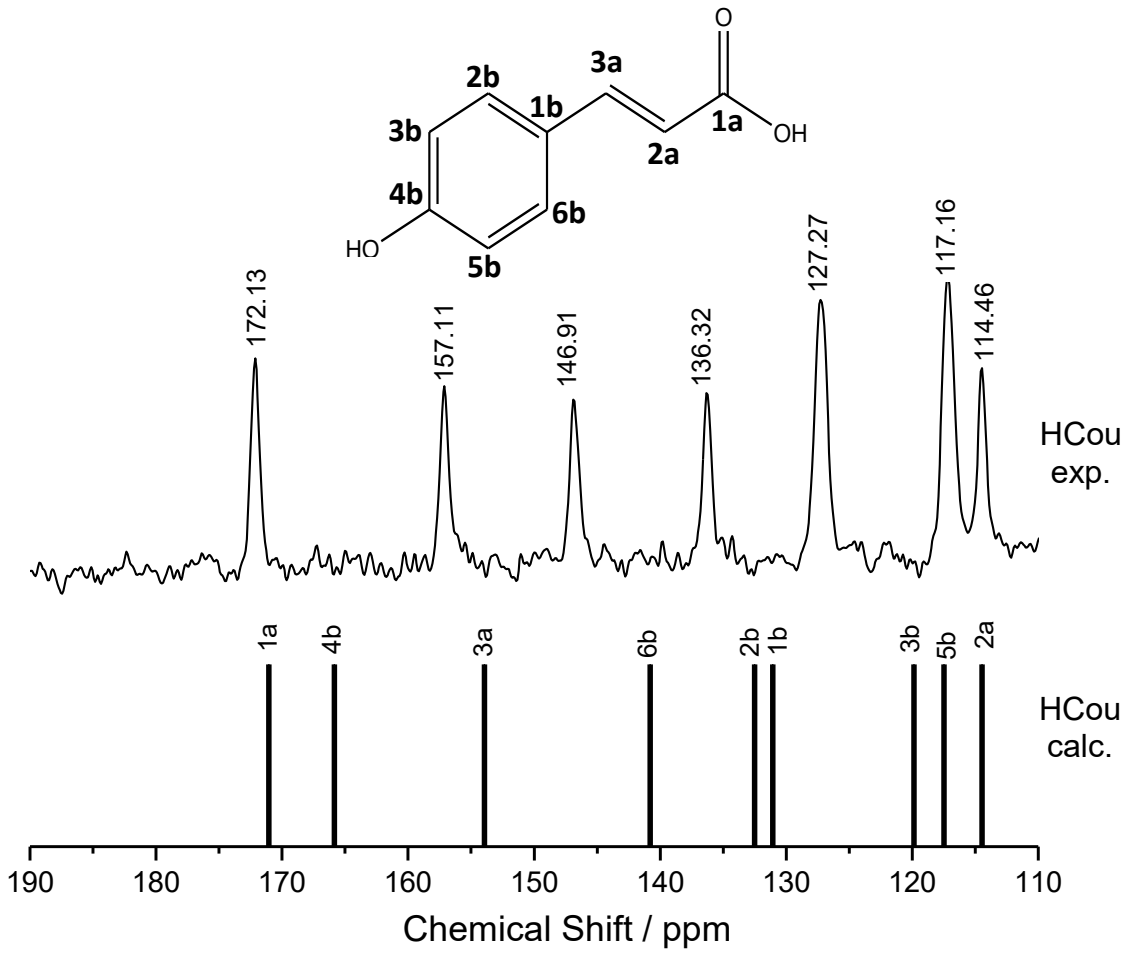


Fig. S2. ^{13}C NMR spectra of experimental and calculated HCou.

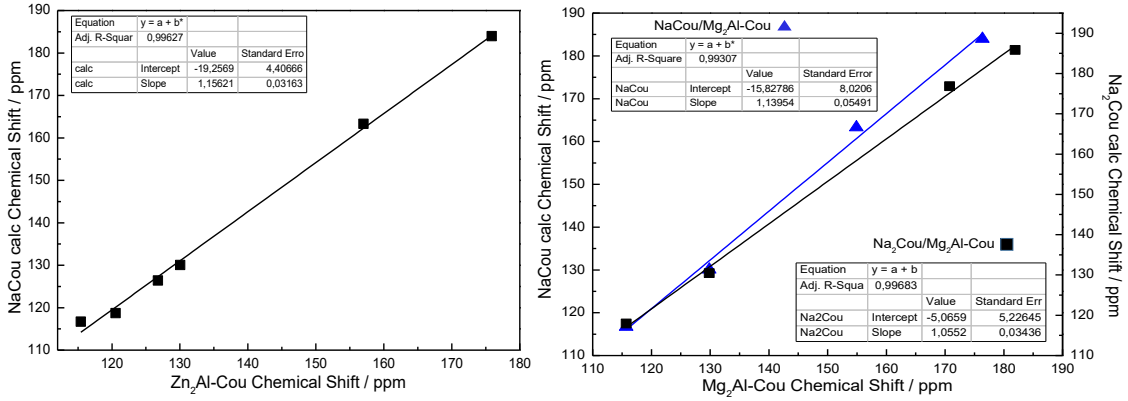


Fig. S3. Linear correlation of the ^{13}C NMR spectra chemical shifts: (A) Zn_2Al-Cou and calculated NaCou and (B) Mg_2Al-Cou with calculated NaCou and Na_2Cou.

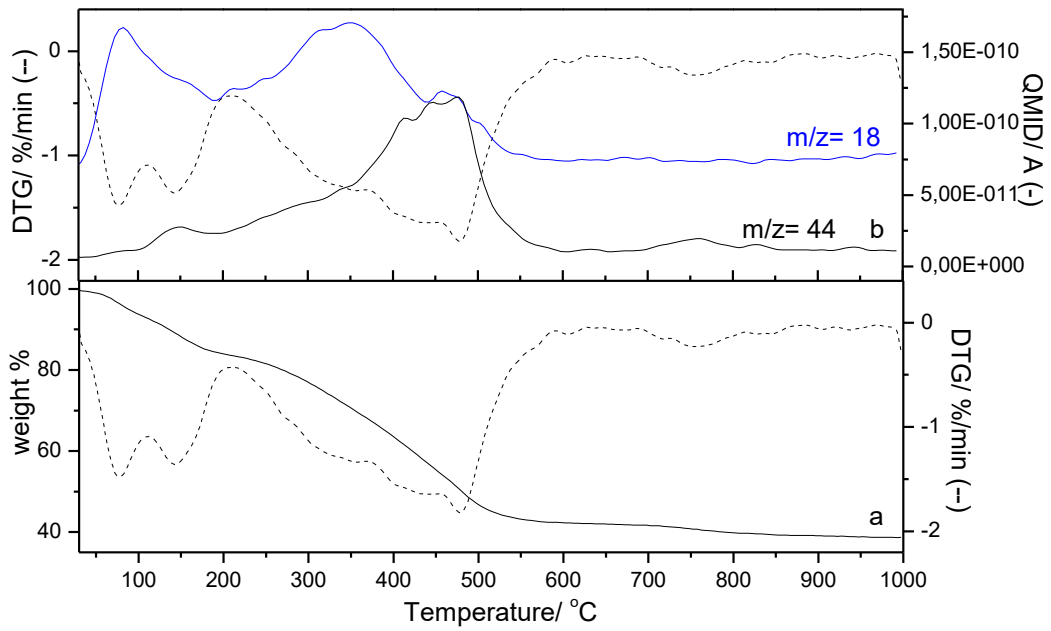


Fig. S4. (a) TGA (-) and DTG (--) and (b) DTG (--) and MS (-) curves of Mg_2Al-Cou (Cou/Al=3) sample.

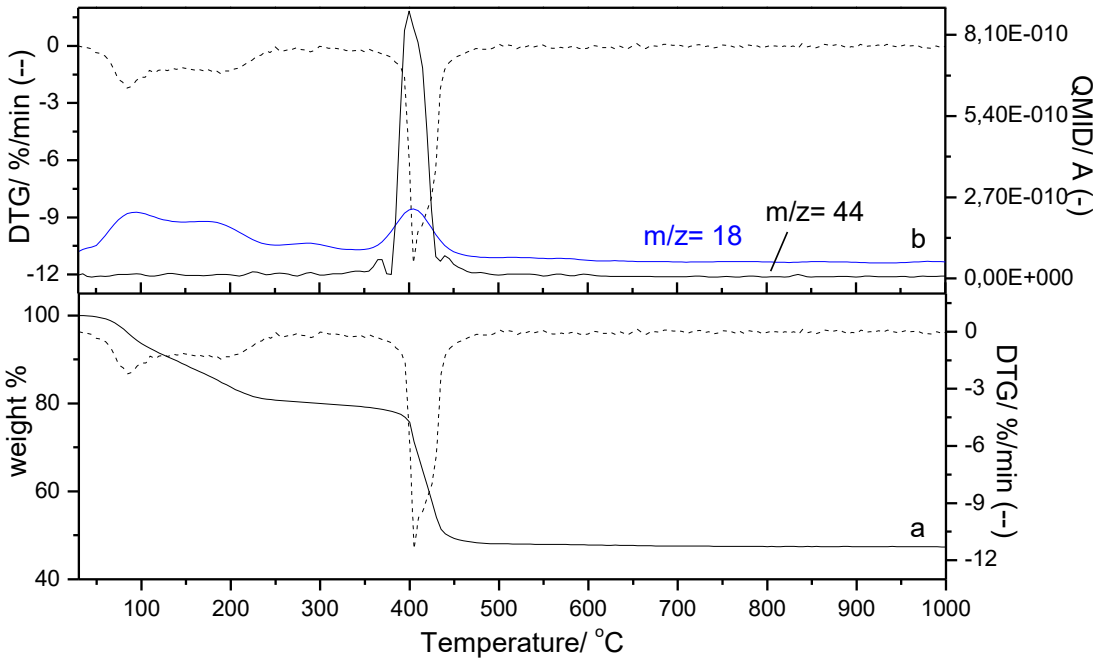
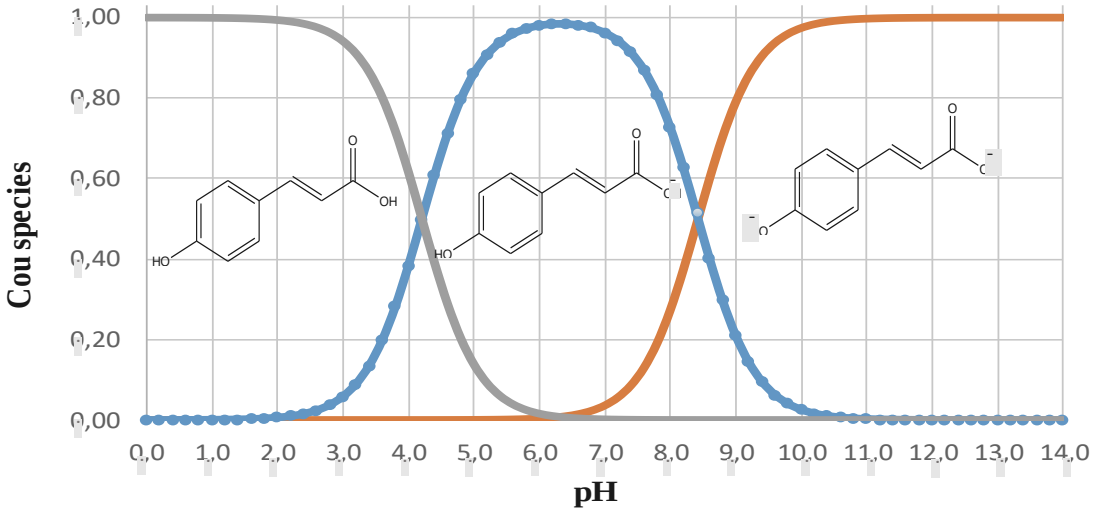
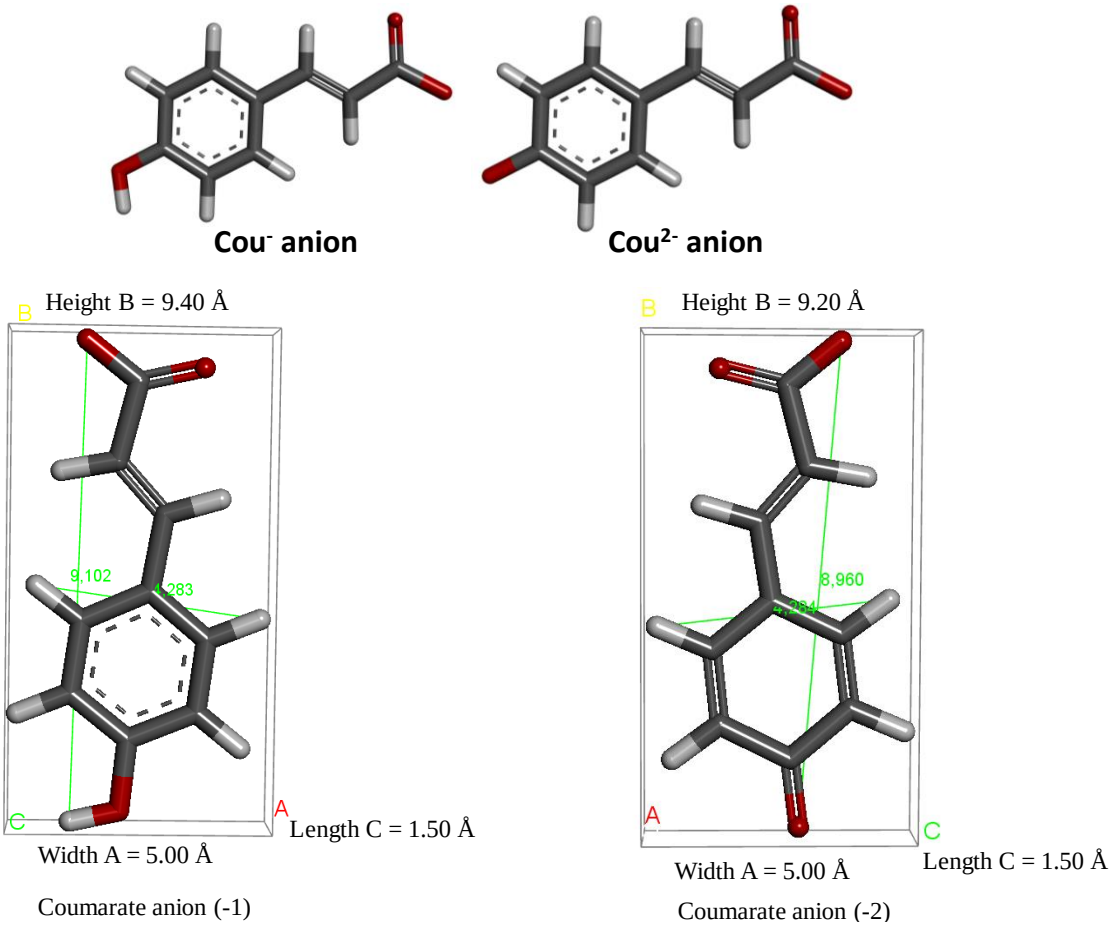


Fig. S5. (a) TGA (-) and DTG (--) and (b) DTG (--) and MS (-) curves of Zn_2Al-Cou (Cou/Al=3) sample.



(a)



(b)

Fig. S6. (a) Distribution of Coumaric acid and coumarate anions species as a function of pH value; (b) Schematic representation of Coumarate ions structure and dimensions achieved by DFT calculations.

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