

## SUPPLEMENTARY MATERIALS

### Multifunctional Green Pigment with UV Protection Based on Capping Agent-Engineered Cr-Doped Hydroxyapatite Nanoparticles

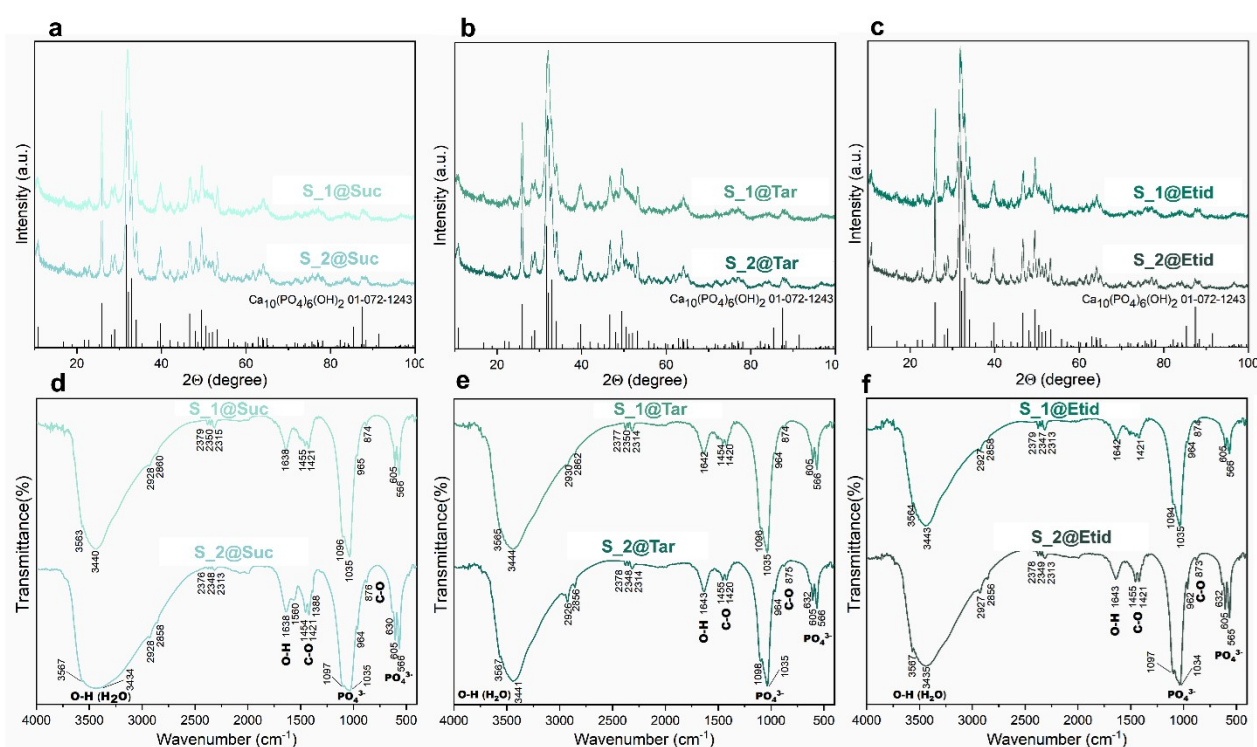
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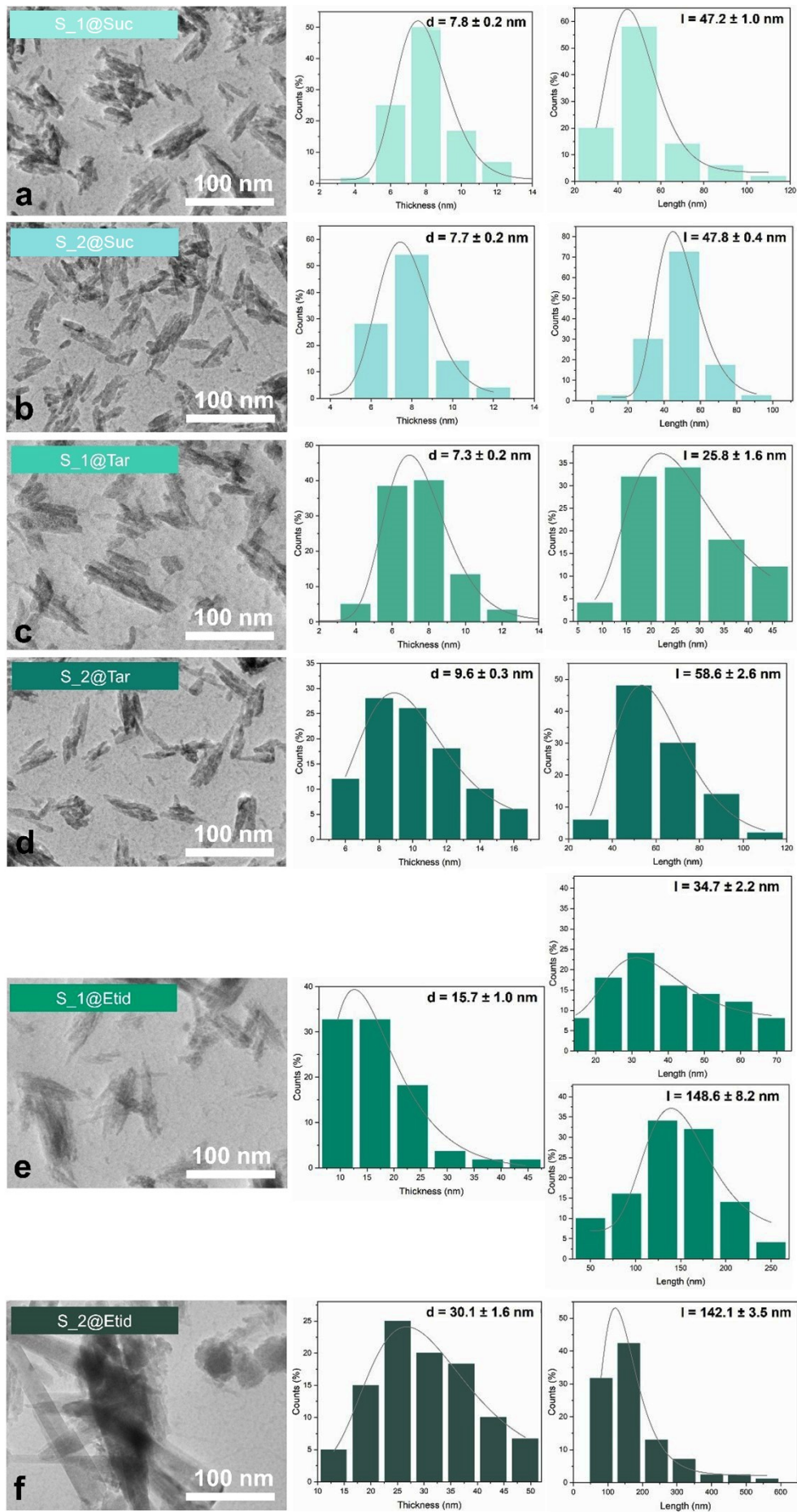
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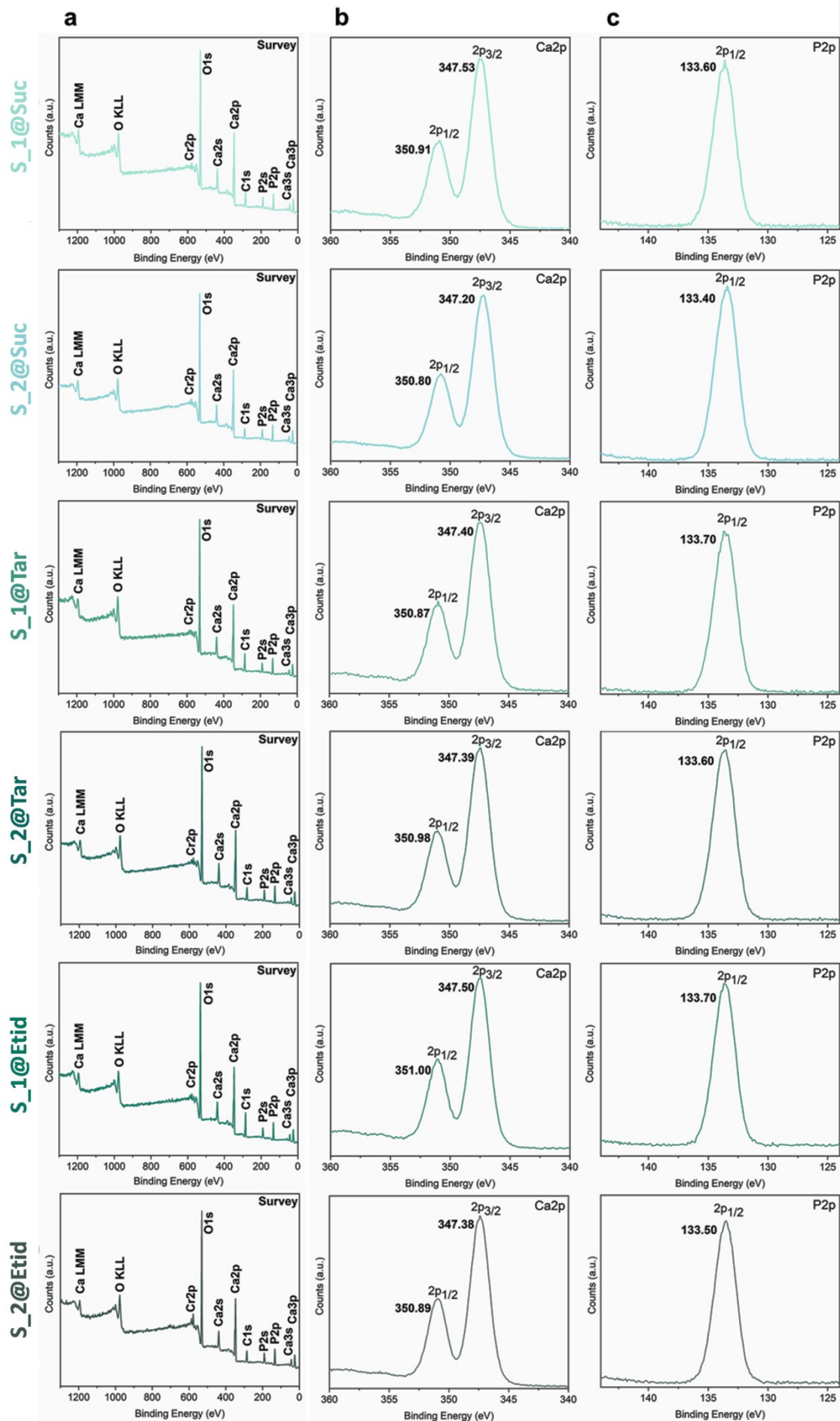
Email: dmitry.tka12@gmail.com



**Fig. SM1.** X-ray diffraction patterns of modified Cr-HAP modified with succinic (a), tartaric (b) and HEDP acids (c) (solid line—Ca<sub>10</sub>(PO<sub>4</sub>)<sub>6</sub>(OH)<sub>2</sub>; ICDD card #01-072-1243). FTIR spectra of modified Cr-HAP samples modified with succinic (d), tartaric (e) and HEDP acids (f).



**Fig. SM2.** High-resolution TEM images, particle size distribution (diameter and thickness) of the samples. Row a: S\_1@Suc; row b: S\_2@Suc; row c: S\_1@Tar; row d: S\_2@Tar; row e: S\_1@Etid; row f: S\_2@Etid.



**Fig. SM3.** XPS survey spectra (column a), Ca1s (column b), and P2p (column c) of Cr-HAp nanoparticles modified with various organic acids.

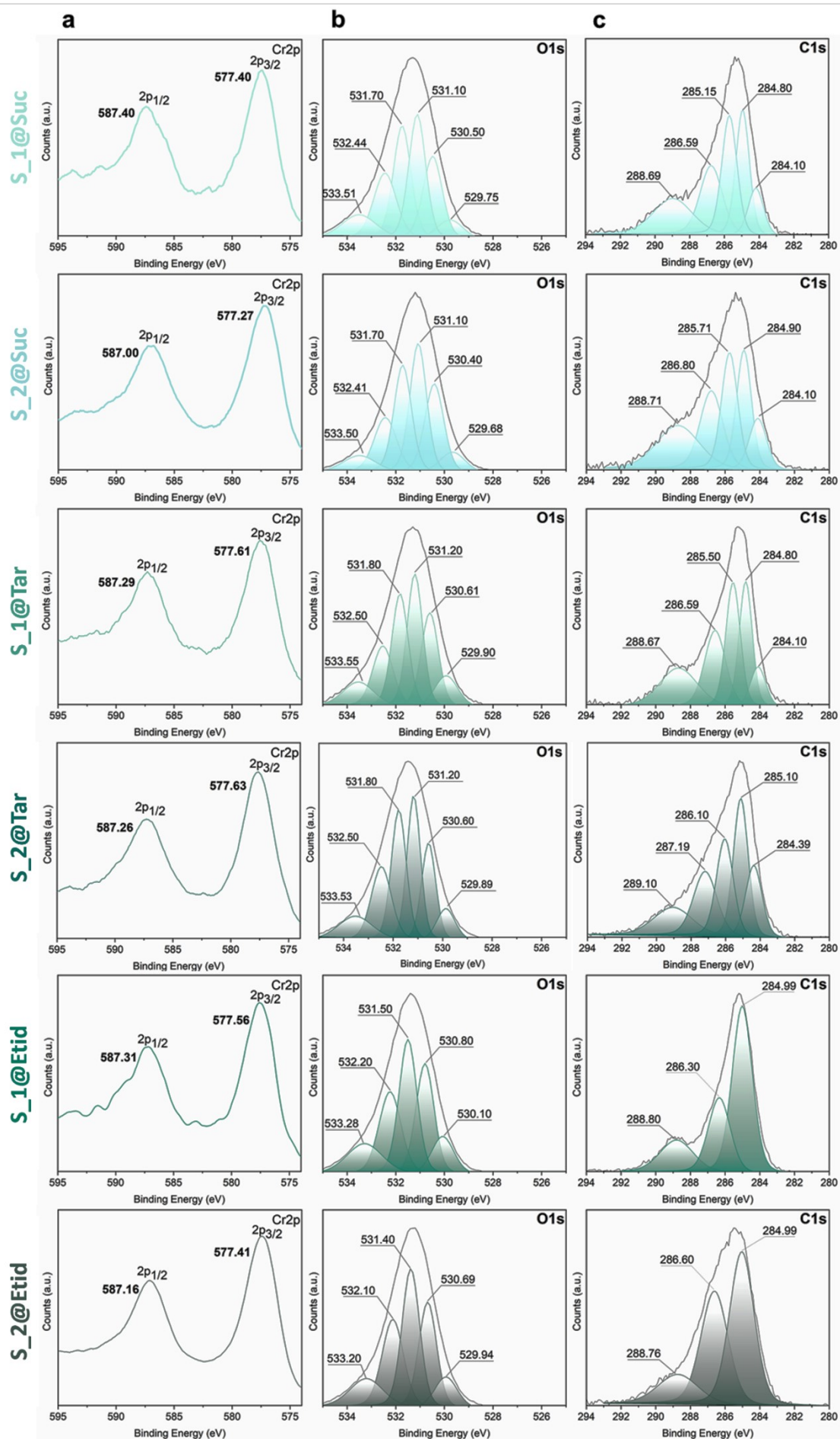
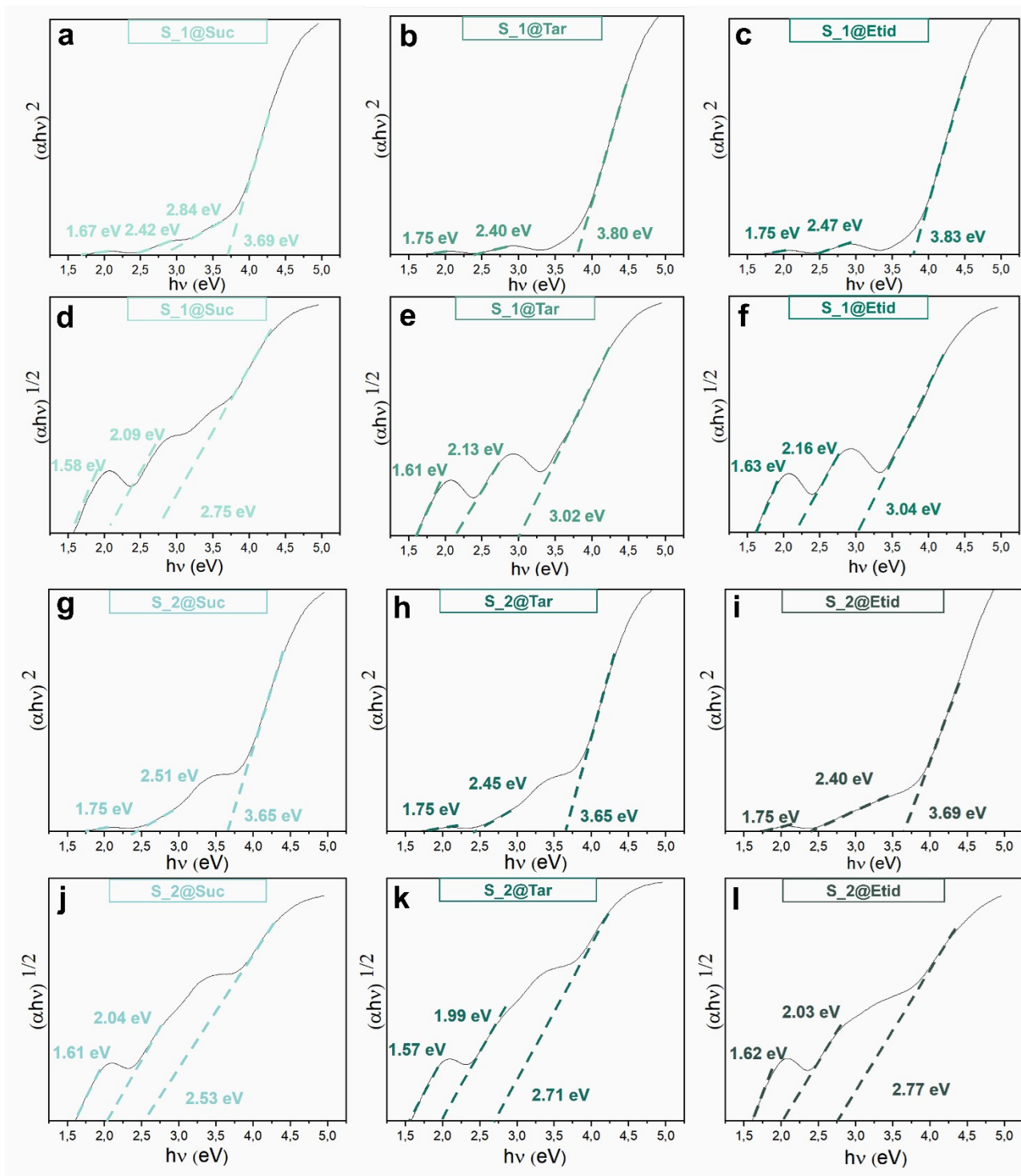
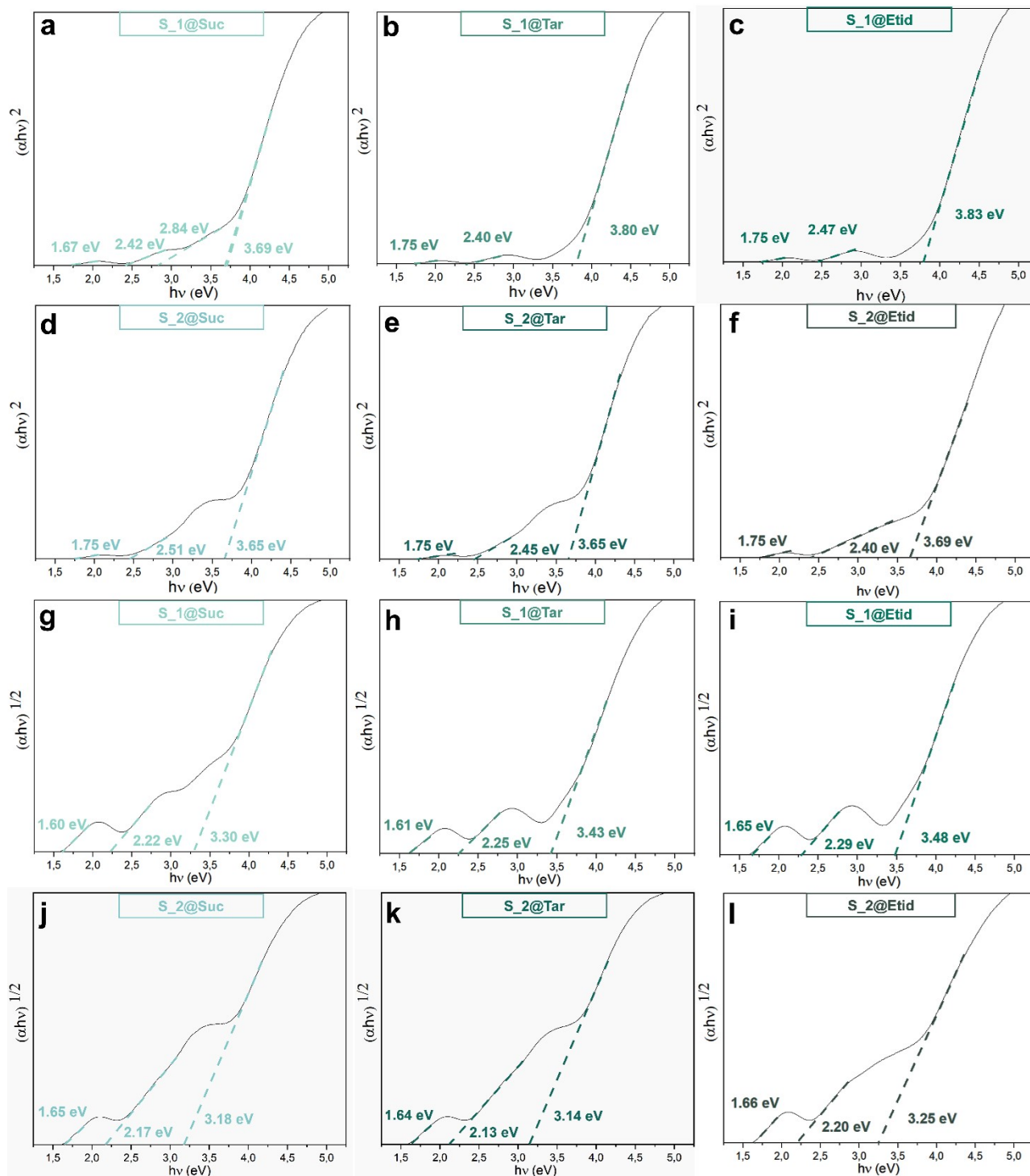


Fig. SM4. XPS spectra of Cr2p (column a), O1s (column b), and C1s (column c) of Cr-HAp nanoparticles modified with various organic acids.



**Fig. SM5.** Tauc plots with band gap values of Cr-HAp samples: Cr-HAp@Suc (a, d), Cr-HAp@Tar (b, e), Cr-HAp@Etid (c, f), Cr-HAp@Suc<sub>180</sub> (g, j), Cr-HAp@Tar<sub>180</sub> (h, k), Cr-HAp@Etid<sub>180</sub> (i, l), obtained from optical absorption spectra.



**Fig. SM6.** Kubelka-Munk plots with band gap values of Cr-Hap samples: Cr-Hap@Suc (a, d), Cr-Hap@Tar (b, e), Cr-Hap@Etid (c, f), Cr-Hap@Suc<sub>180</sub> (g, j), Cr-Hap@Tar<sub>180</sub> (h, k), Cr-Hap@Etid<sub>180</sub> (i, l), obtained from optical reflection spectra.

Table SM1. Direct and indirect electron transition energies obtained from Tauc and Kubelka-Munk plots.

Sample	Direct transitions (eV)		Indirect transitions (eV)	
	Absorption spectra	Reflection spectra	Absorption spectra	Reflection spectra
S_0	4.08, 2.55, 1.81	4.26, 2.55, 1.84	3.40, 2.24, 1.67	3.77, 2.33, 1.67
S_1@Suc	3.69, 2.84, 2.42, 1.67	2.75, 2.09, 1.58	3.80, 2.76, 2.41, 1.64	3.30, 2.22, 1.65
S_2@Suc	3.65, 2.51, 1.75	2.53, 2.04, 1.61	3.78, 2.42, 1.78	3.17, 2.11, 1.63
S_1@Tar	3.80, 2.40, 1.75	3.02, 2.13, 1.61	3.80, 2.41, 1.76	3.41, 2.24, 1.61
S_2@Tar	3.65, 2.45, 1.75	2.71, 1.99, 1.57	3.75, 2.40, 1.74	3.06, 2.17, 1.62
S_1@Etid	3.83, 2.47, 1.75	3.04, 2.16, 1.63	3.86, 2.46, 1.75	3.47, 2.28, 1.66
S_2@Etid	3.69, 2.40, 1.75	2.77, 2.03, 1.62	3.81, 2.42, 1.73	3.42, 2.24, 1.69

Table SM2. Calculated surface-acid interaction energies for S\_0.

Facet	001	100
<b>Suc</b> <i>E</i> (eV)	82.5	42.9
<b>Tar</b> <i>E</i> (eV)	66.5	25.9
<b>Etid</b> <i>E</i> (eV)	48.6	72.4

Table SM3. Hydrodynamic sizes (*HS*) and  $\zeta$ -potential ( $\zeta$ ) of modified Cr-HAp nanoparticles.

Sample	<i>HS</i> (nm)	$\zeta$ (mV)
S_1	166	-16.8
S_1@Suc	277	-16.7
S_2@Suc	1296	-6.2
S_1@Tar	602	-11.6
S_2@Tar	2338	-26.0
S_1@Etid	1919	-12.7
S_2@Etid	391	-35.6

Table SM4. Raw ICP-AES data of Cr doping levels.

Sample	Ca (mg/L)	Cr (mg/L)
S_1@Suc	71 ± 5	10.8 ± 0.3
S_2@Suc	52 ± 4	6.6 ± 0.6
S_1@Tar	49.0 ± 1.3	6.04 ± 0.28
S_2@Tar	55 ± 8	7.08 ± 0.17
S_1@Etid	66 ± 6	9.6 ± 0.3
S_2@Etid	60 ± 5	8.2 ± 0.3

## **References**

Multifunctional Cosmetics. Cosmetic Science and Technology Series, Volume 26. Marcel Dekker Inc., 2001.