

Supporting Information

Green synthesis of zinc oxide particles with apple-derived compounds and their application as catalysts in the transesterification of methyl benzoates

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$^1\text{H-NMR}$ scans were obtained using deuterated chloroform ($\text{CDCl}_3\text{-d}_6$) as solvent. Chemical shifts were expressed in parts per million (ppm) relative to tetramethylsilane. NMR spectra were recorded on a Bruker Avance 400 MHz (UltraShield Plus Magnet) spectrometers using the solvent peak as internal reference (CDCl_3 ; δ H 7.26. Multiplicities are indicated as s (singlet), d (doublet), t (triplet), q (quartet). Quantifications were performed upon integration of the selected peaks of the product against peaks of the substrate at 3.9 ppm.

Ethyl benzoylformate:

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 1.38 (t, CH_3 , 3H), 3.94 (s, OCH_3 , 3H), 4.41 (q, CH_2 , 2H), 7.47 (t, 2H), 7.65 (t, 1H), 8.00 (d, Ar, 2H).

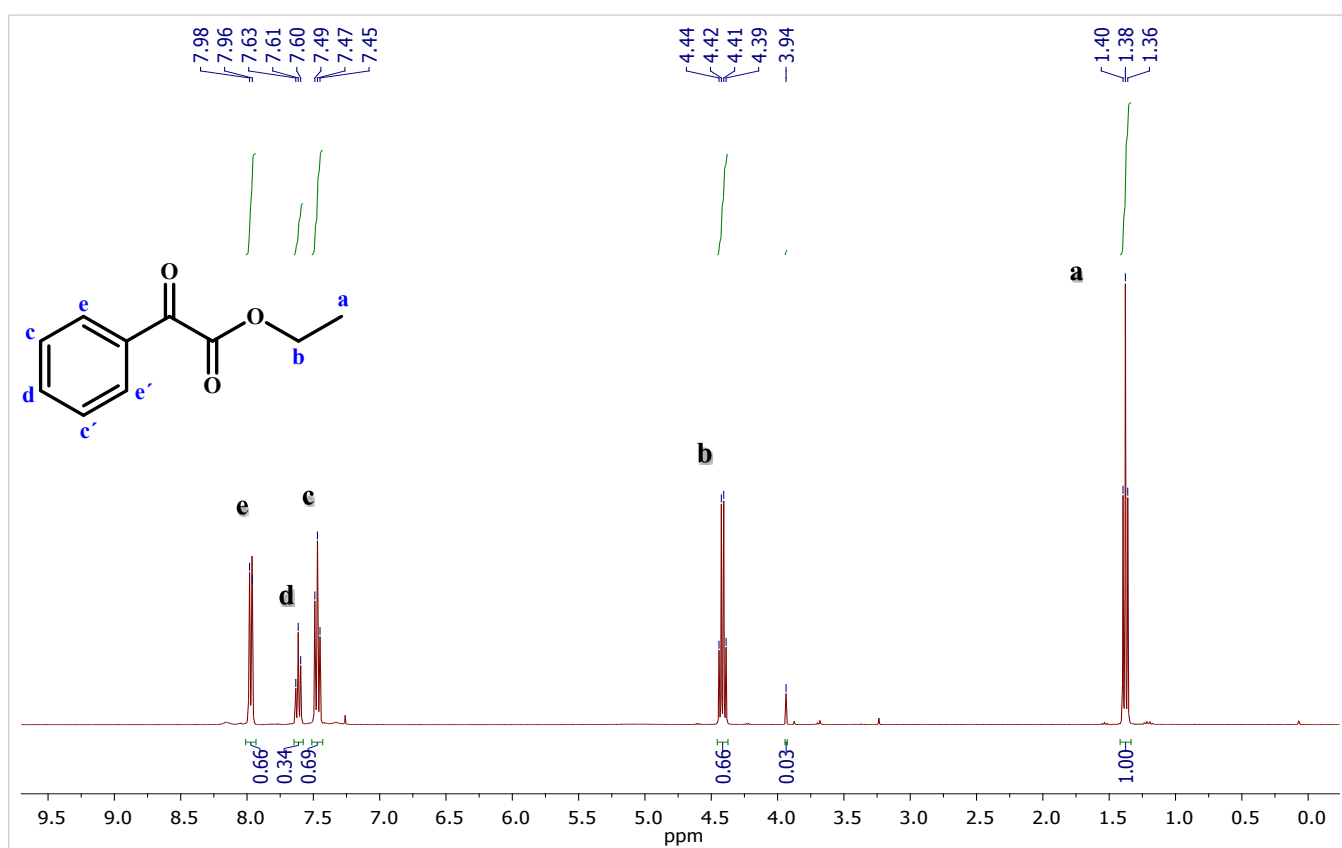


Figure S1. $^1\text{H-NMR}$ spectrum of ethyl benzoylformate (Table 2, entry 6).

Ethyl 4-nitrobenzoate:

^1H NMR (400 MHz, CDCl_3): δ 1.35 (t, 3H), 3.90 (s, 3H), 4.35 (q, 2H), 8.09 (t, 2H), 8.15 (t, 1H).

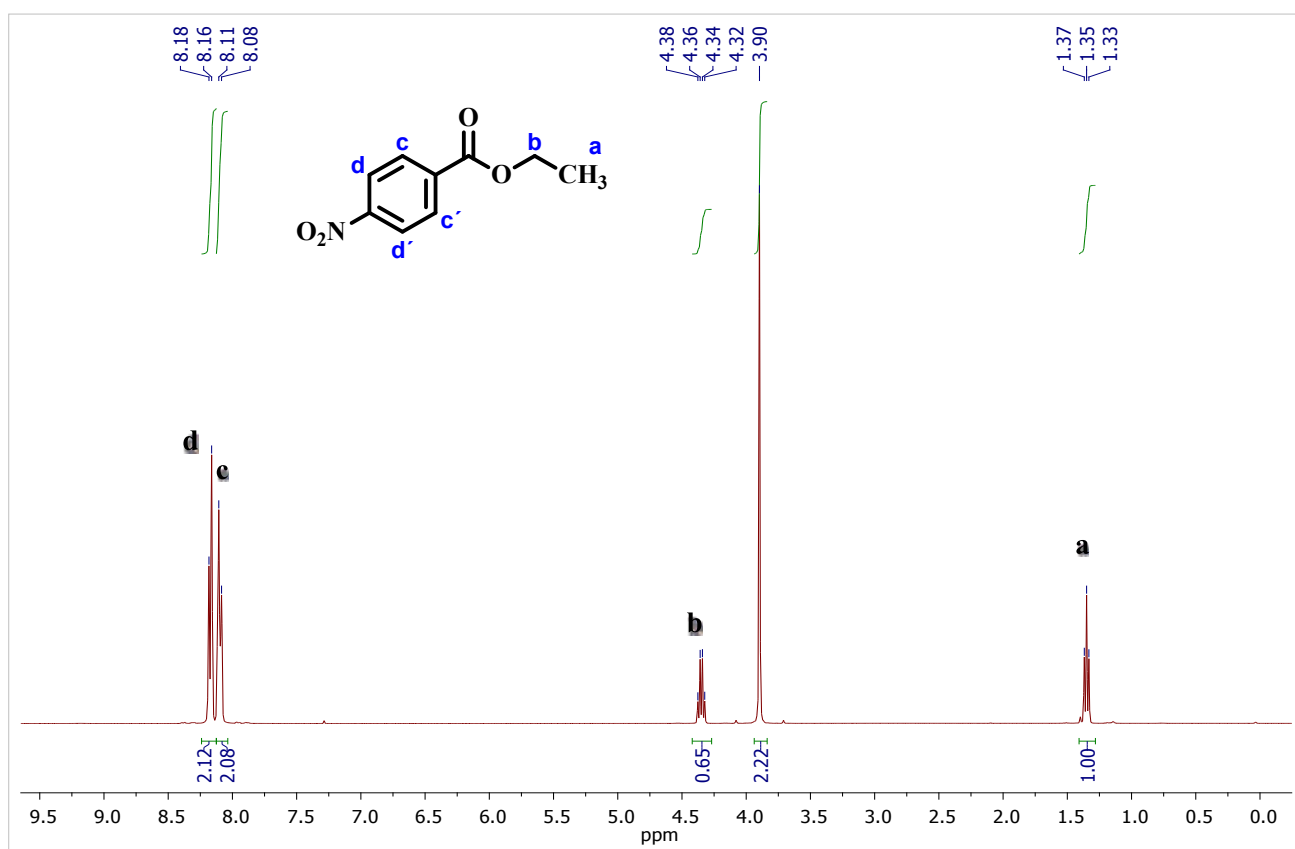


Figure S2. ^1H -NMR spectrum of ethyl 4-nitrobenzoate (Table 2, entry 18).

Table S1 – Elemental analysis determined by M.M. 8.6 (2009-05-06) (A.E.) method

Sample	N%	C%	H%
ZnONPs	0.71	5.18	<2.0
ZnOq	<0.5	4.35	<2.0

BET Analysis

Various information about the textural properties could be obtained through BET analysis. The specific surface area (S_{BET}) of the ZnO particles was determined from the nitrogen adsorption/desorption measurement applying the Brunauer-Emmett-Teller (BET) method.

The BET surface area and pore volume are presented in Table S2. The diameter of the ZnO particles can be calculated by using the following equation:

$$d_{BET} = \frac{6000}{\rho_{sample} \times S_{BET}} \quad (1)$$

where d_{BET} is the mean crystalline size (in nm), ρ_{sample} is the density of ZnO powder ($\rho_{ZnO} = 5.60 \text{ g/cm}^3$) and S_{BET} is the BET specific surface area (m^2/g). Applying Eq. (1), d_{BET} values were obtained for ZnO samples (Table S2). The BET surface area and pore volume are presented in Table (S2). The N_2 adsorption-desorption isotherms for ZnO NPs, ZnOq and ZnO are displayed in Fig. (S3)

Table S2 – BET surface area, total pore volume, BJH pore diameter and mean crystalline size of ZnO samples.

Sample	S_{BET} (m^2/g)	Total Pore Volume (cm^3/g)	BJH pore diameter (\AA)	d_{BET} (nm)	Type
ZnO	5	0.01408	180	214	II
ZnONPS	11	0.05713	279	97	II
ZnOq	17	0.04911	177	63	II

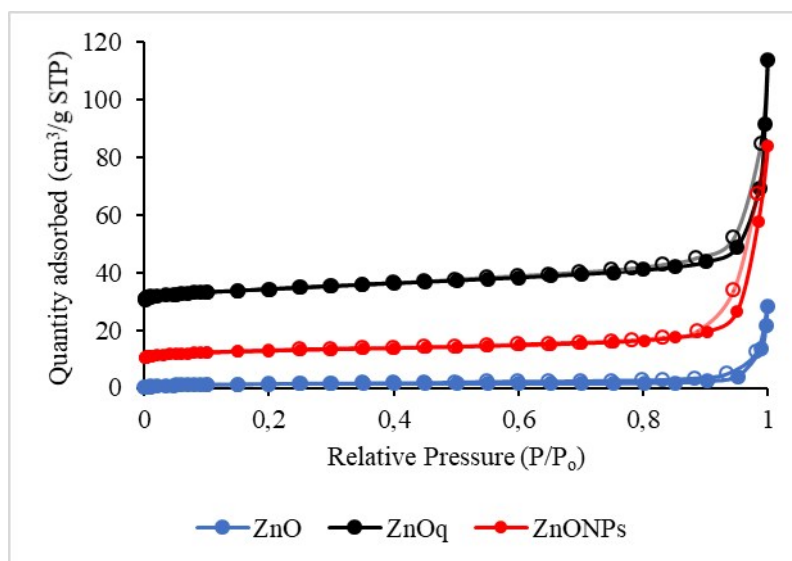


Figure S3 - N₂ adsorption/desorption isotherms of all the catalysts.