Supporting Information

Synthesis of high-density jet fuel with creosol and formaldehyde

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Characterization of catalyst

Nitrogen adsorption was carried out at 77 K with an ASAP 2010 apparatus to determine the specific Brunauer–Emmett–Teller (BET) specific surface area (S_{BET}) of the catalysts. Before the measurements, the samples were evacuated at 573 K for 6 h.

Temperature programmed desorption of NH_3 (NH_3-TPD) of acidic zeolite support was carried out on a Micromeritics Autochem 2910 chemisorption apparatus. Typically, about 0.1 g of the sample was placed in a quartz reactor. Before the test, the catalyst was pretreated at 573 K under He flow for 0.5 h. After being cooled down in He flow to 373 K and the stabilization of baseline, the NH_3 was injected into the reactor by manual pulse until the saturated adsorption of catalyst. The catalyst was purged in He flow for 10 min to remove the physically adsorbed NH_3. The pulse signal was detected by a thermal conductivity detector (TCD), and the adsorption amount of NH_3 was calculated. Programmed temperature desorption of NH_3 was carried out in He flow at a heating rate of 10 K min^{-1} from 373 K to 1073 K. The desorbed NH_3 was monitored by OminiStar mass spectrometer.

The X-ray diffraction (XRD) patterns of the Ru-based HDO catalysts were collected by a PW3040/60X' Pert PRO (PANAlytical) diffractometer. The TEM images of the Ru-based HDO catalyst were obtained by a JEM-2100F scanning transmission electron microscopy (STEM).

The metal dispersions on the surfaces of Ru-based catalysts were measured with a Micromeritics AutoChem II 2920 Automated Catalyst Characterization System by CO-chemisorption. These values correspond to the ratio of surface metal atoms to total metal atoms assuming that the stoichiometry of adsorbed CO to surface metal atom is one. Before the tests, the samples were dried in He flow at 393 K for 0.5 h and cooled down in He flow to 323 K. After the stabilization of baseline, the CO adsorption was carried out at 323 K by the pulse adsorption of 10% CO in He.

General experimental details for NMR and GC-MS analysis

^{1}H NMR and ^{13}C NMR spectra were recorded at room temperature in CDCl$_3$ on Bruker AVANCE III 400 MHz instrument. The chemical shifts for ^{1}H NMR were recorded in ppm downfield using the peak of CDCl$_3$ (7.26 ppm) as the internal standard. The chemical shifts for ^{13}C NMR were recorded in ppm downfield using the central peak of CDCl$_3$ (77.16 ppm) as the internal standard.
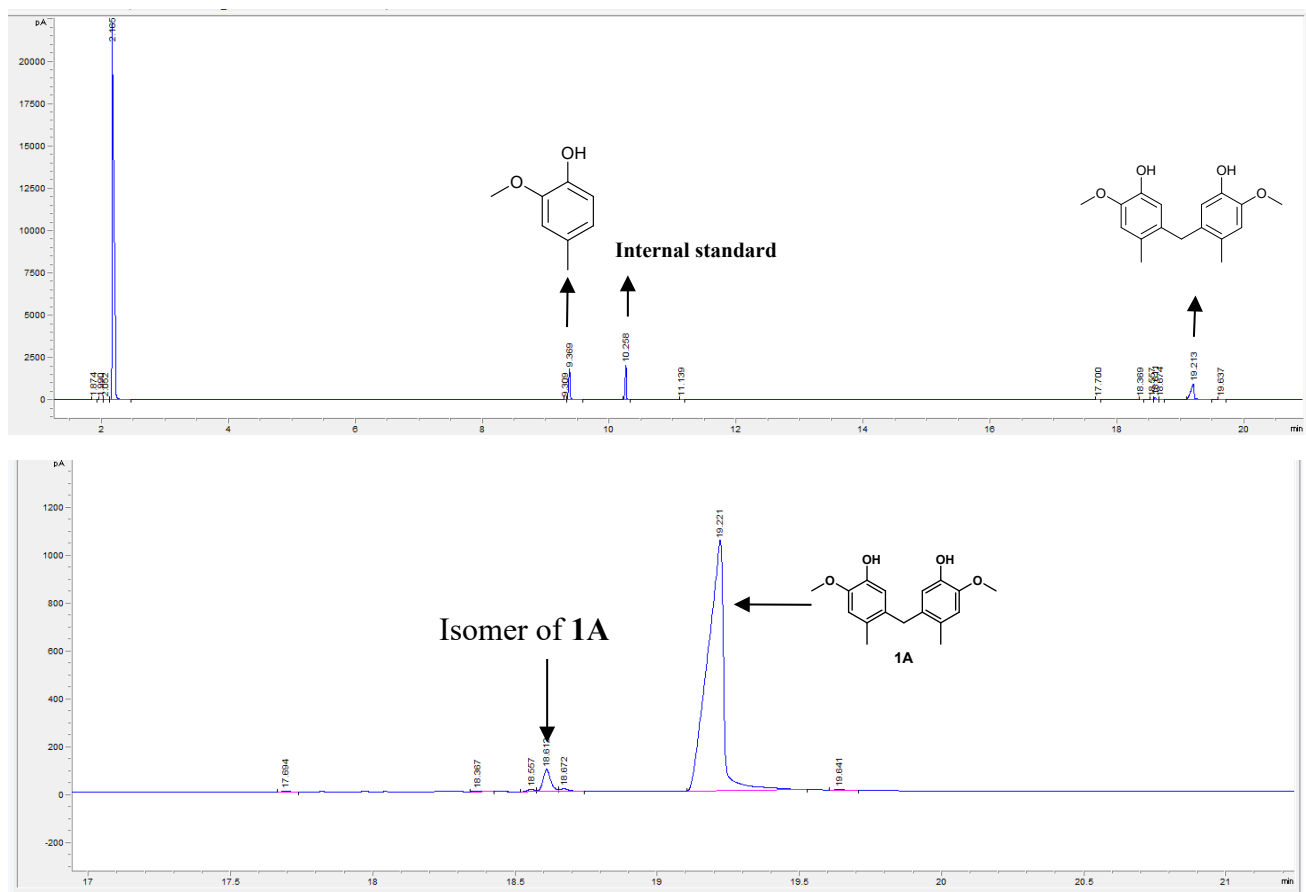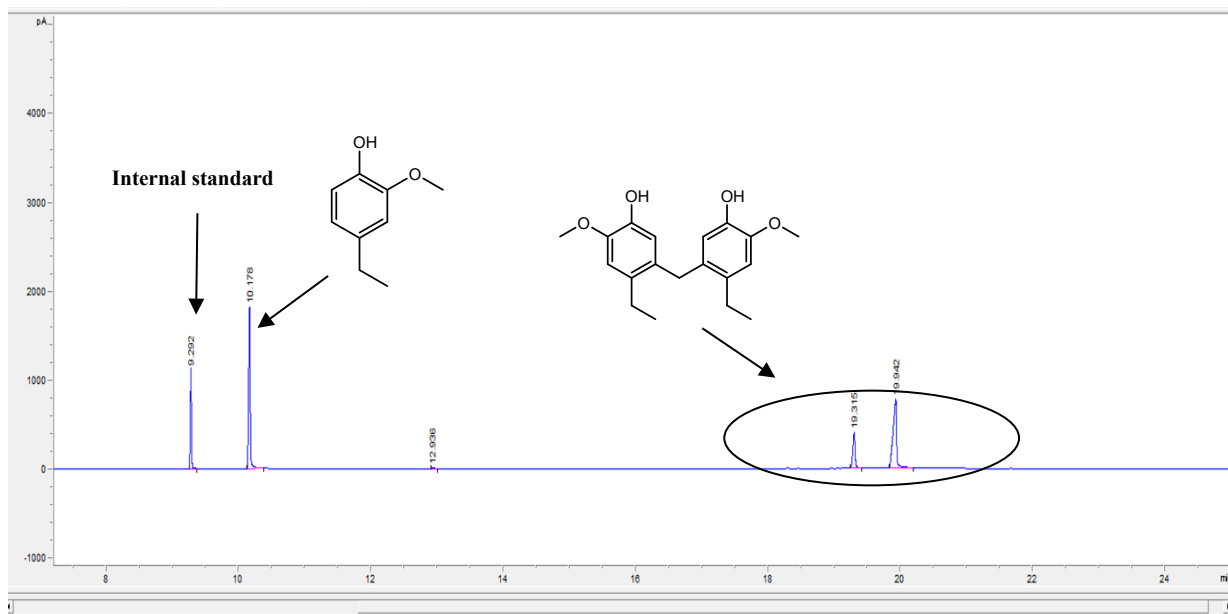
Figure S1. Gas chromatogram of the phenolic aldehyde condensation product of creosol and formaldehyde. Reaction conditions: 343 K, 6 h; 20 mmol creosol, 10 mmol formaldehyde and 0.05 g 40% HPW/SiO$_2$ catalyst were used in the test.
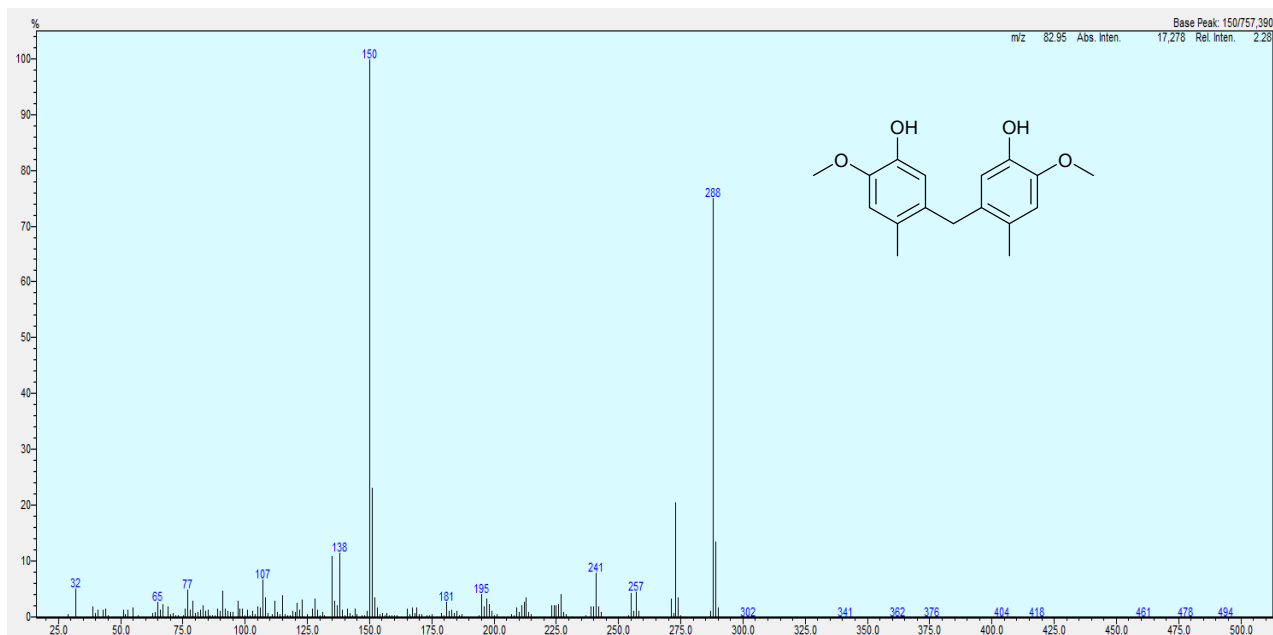
Figure S2. Mass spectrogram of **1A** from the phenolic aldehyde condensation of creosol and formaldehyde.
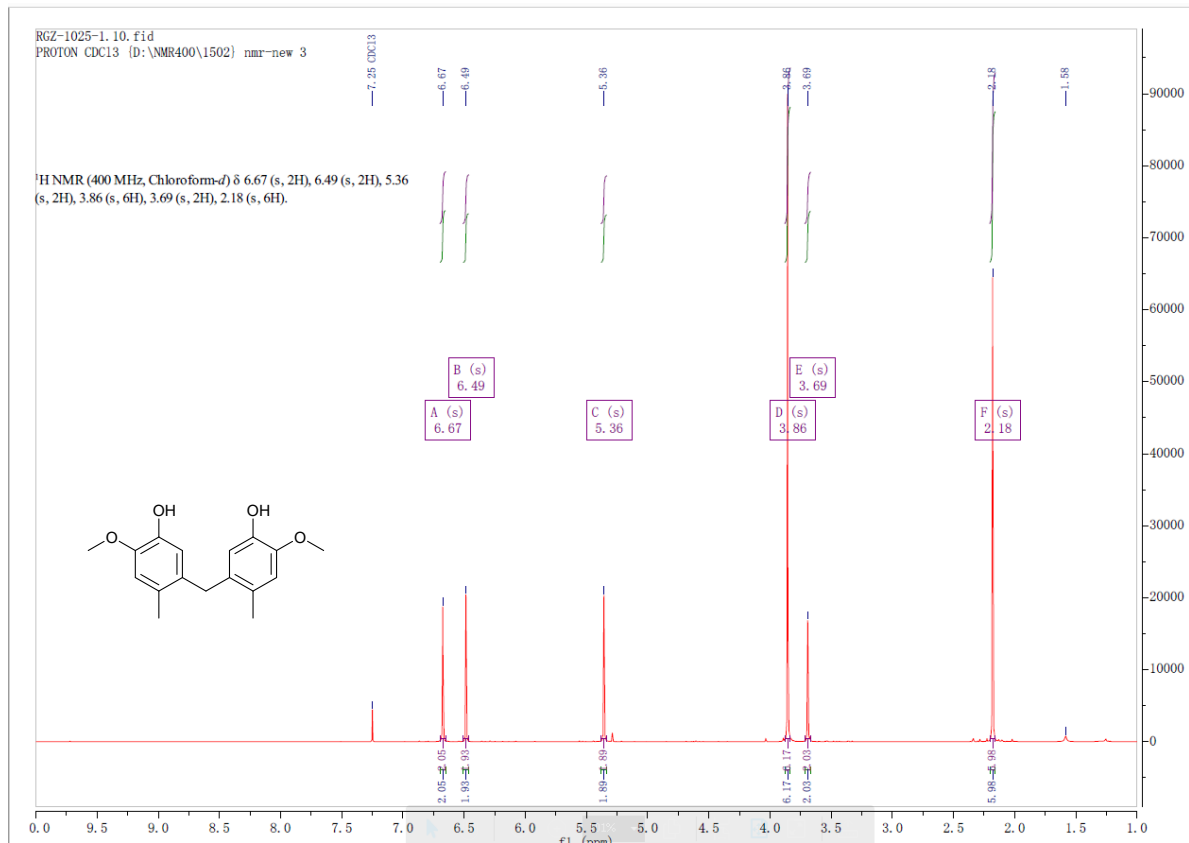
Figure S3. ¹H-NMR and ¹³C-NMR spectra of the **1A** generated from the phenolic aldehyde condensation of creosol and formaldehyde.
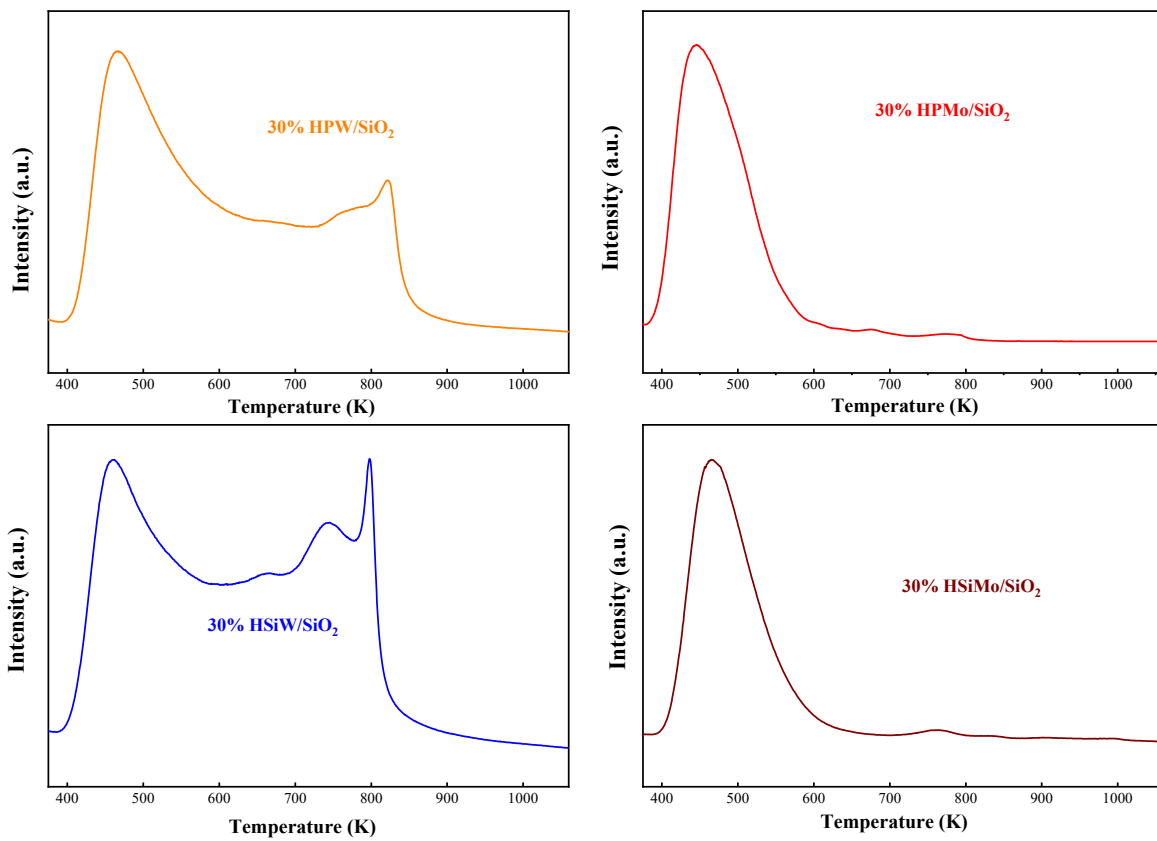
Figure S4. NH$_3$-TPD profiles of SiO$_2$ loaded heteropolyacids.
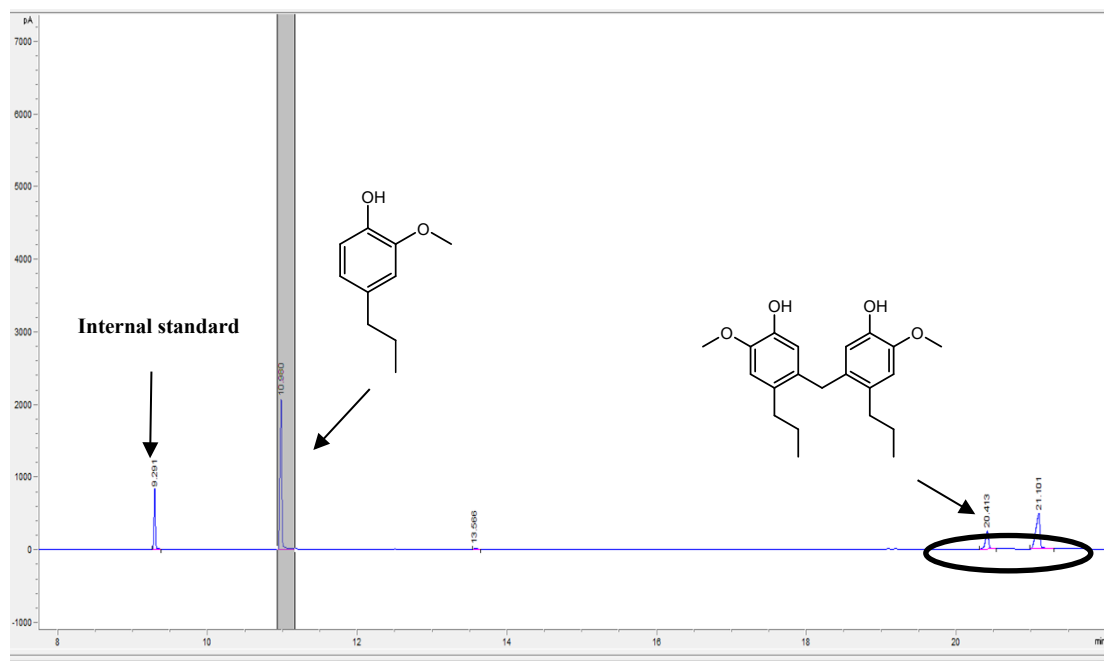
Figure S5. Gas chromatogram of the phenolic aldehyde condensation product of 4-ethyl guaiacol and formaldehyde. Reaction conditions: 373 K, 6 h; 20 mmol 4-ethyl guaiacol, 10 mmol formaldehyde and 0.15 g 40% HPW/SiO$_2$ catalyst were used in the test.
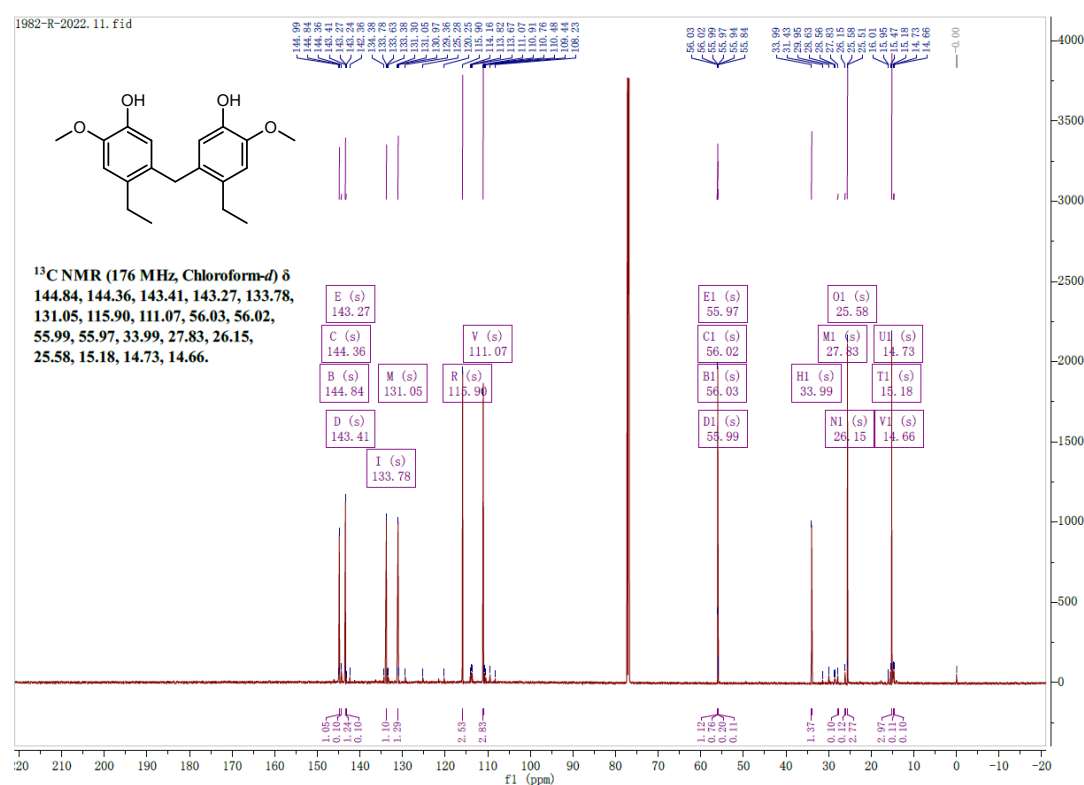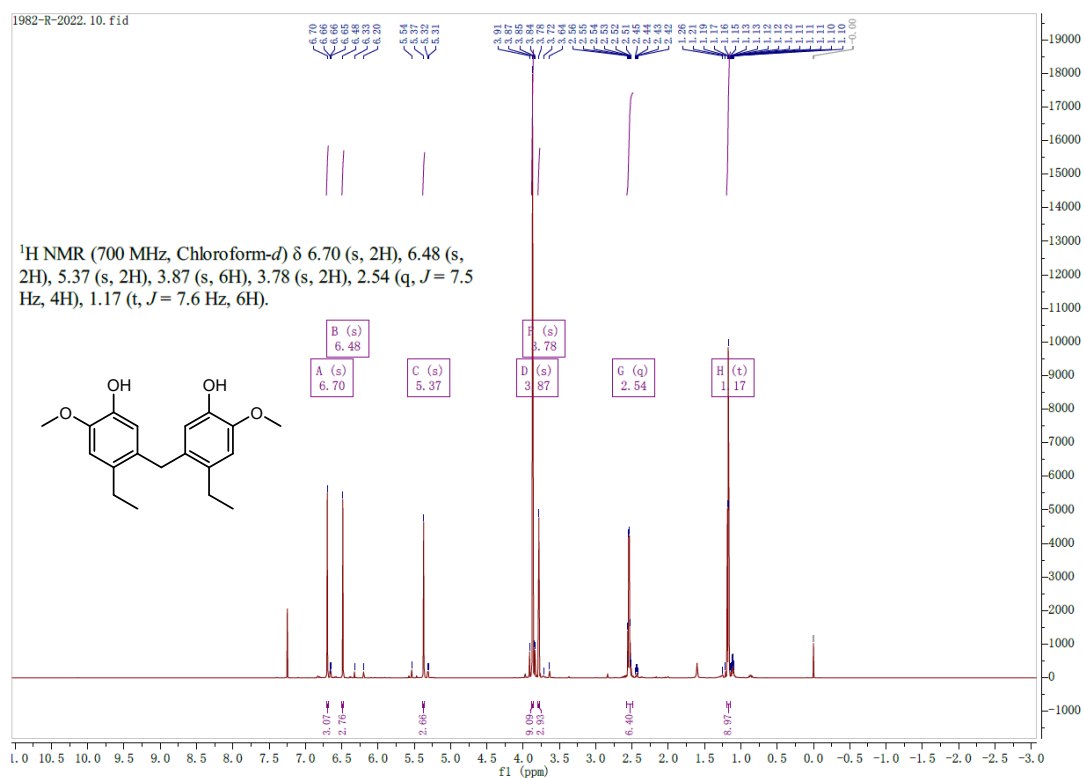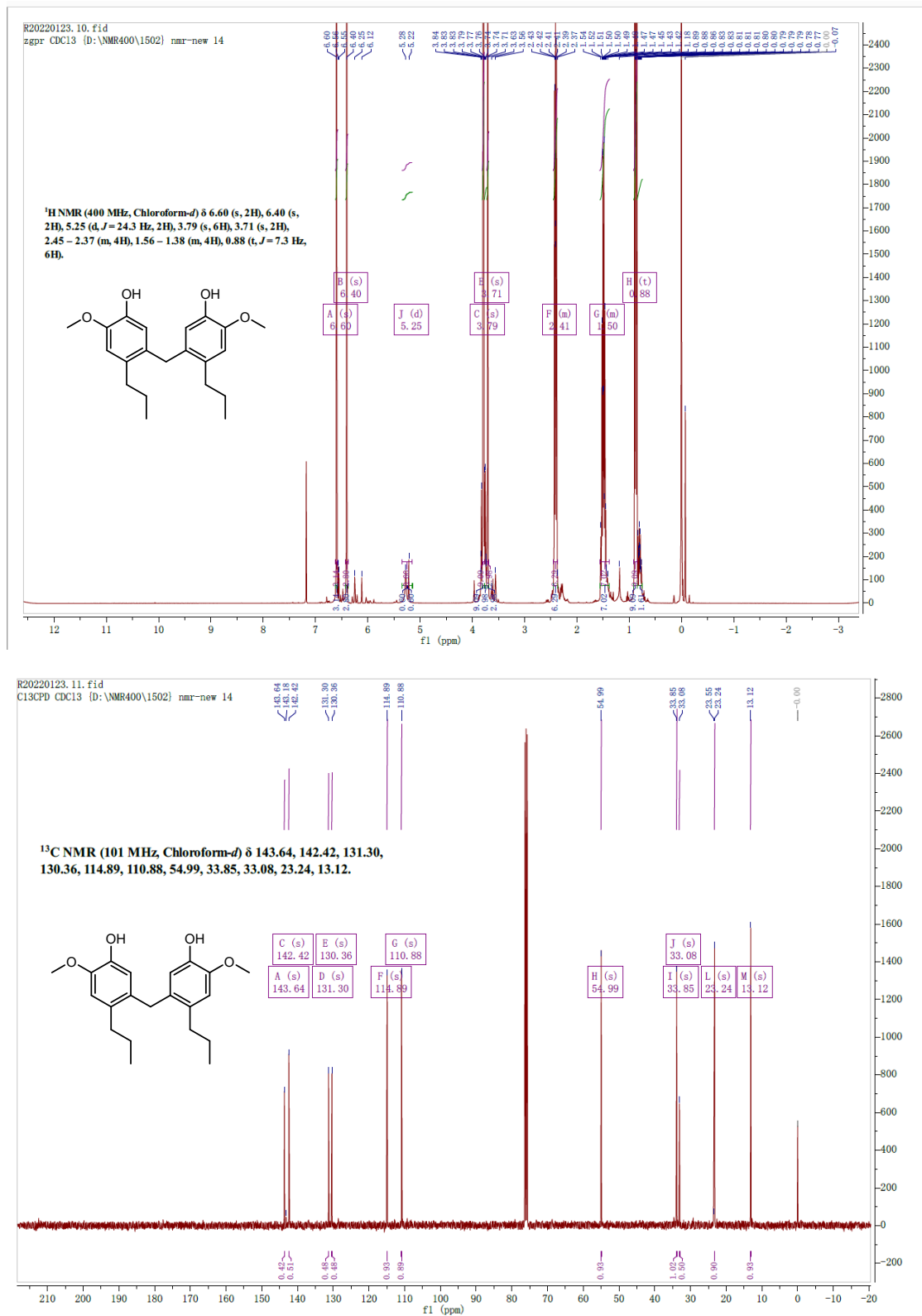
Figure S6. ^{1}H-NMR and ^{13}C-NMR spectra of the phenolic aldehyde condensation product of 4-ethyl guaiacol and formaldehyde.
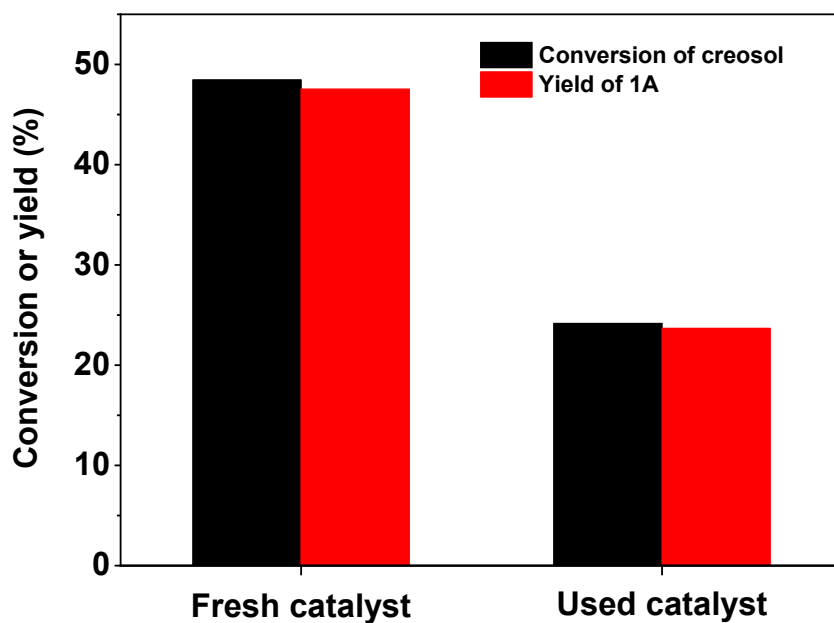
Figure S7. Gas chromatogram of the phenolic aldehyde condensation product of 4-propyl guaiacol and formaldehyde. Reaction conditions: 373 K, 6 h; 20 mmol 4-propyl guaiacol, 10 mmol formaldehyde and 0.15 g 40% HPW/SiO$_2$ catalyst were used in the test.

Figure S8. ^{1}H-NMR and ^{13}C-NMR spectra of the phenolic aldehyde condensation product of 4-propyl guaiacol and formaldehyde.

Figure S9. Creosol conversion and the yield of **1A** over the fresh and used 40% HPW/SiO$_2$ catalysts. Reaction conditions: 343 K, 1 h; 20 mmol creosol, 10 mmol formaldehyde and 0.1 g catalyst were used in the test.
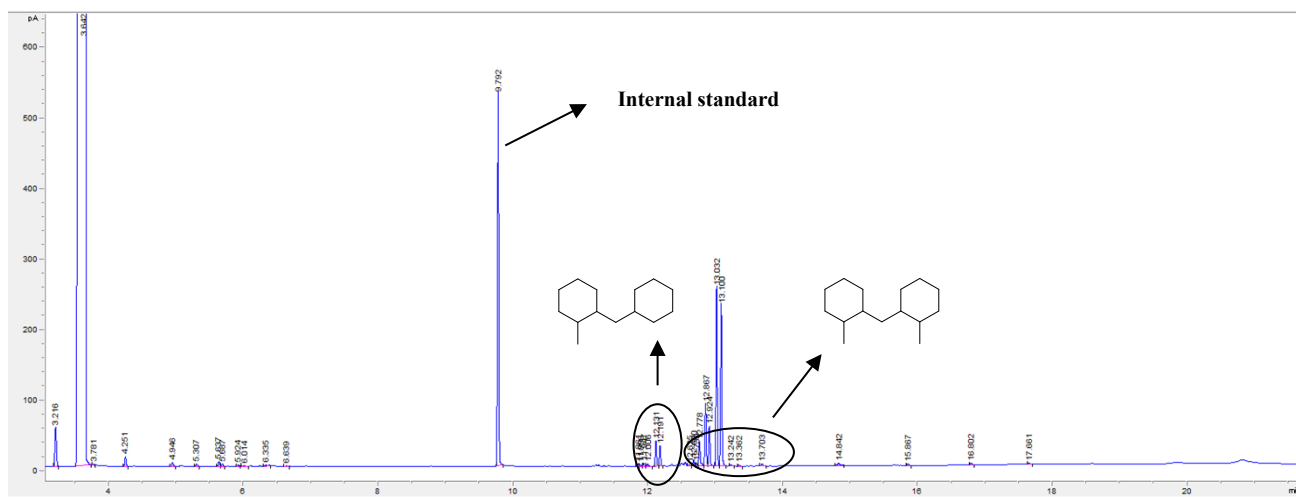
Figure S10. Gas chromatogram of the product from the HDO of **1A**. Reaction conditions: 473 K, 5 h, 4 MPa H_2; 0.2 g substrate, 0.1 g Ru/H-ZSM-5, 40 mL cyclohexane solvent were used for the test.
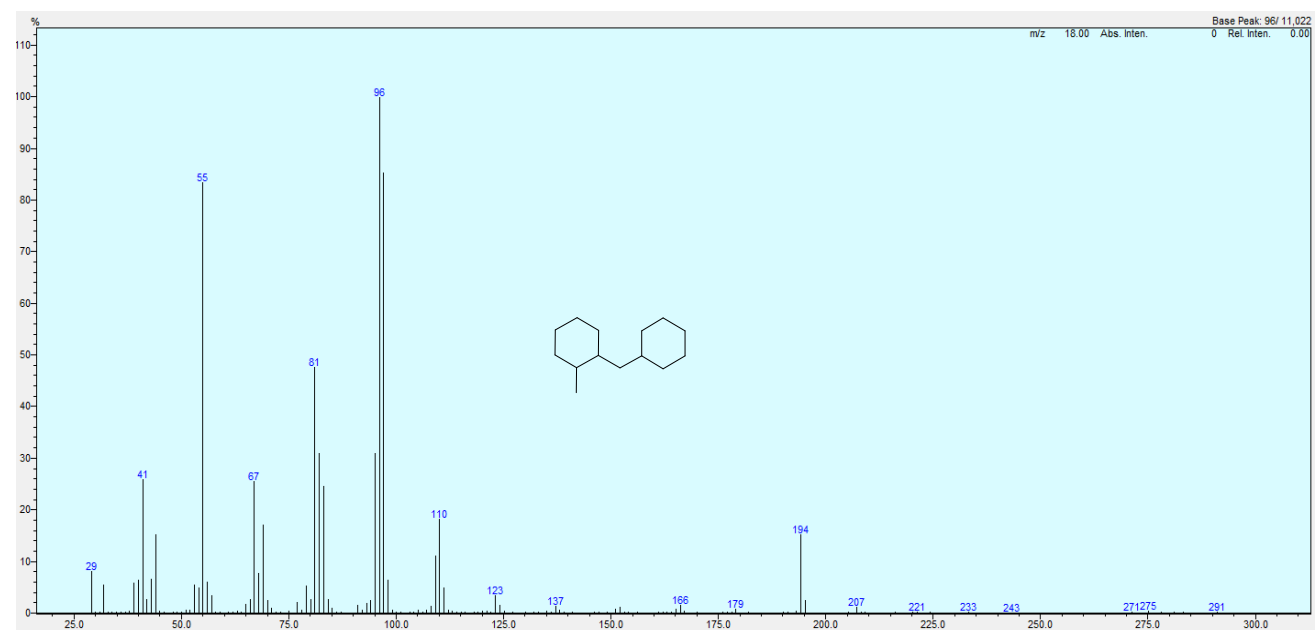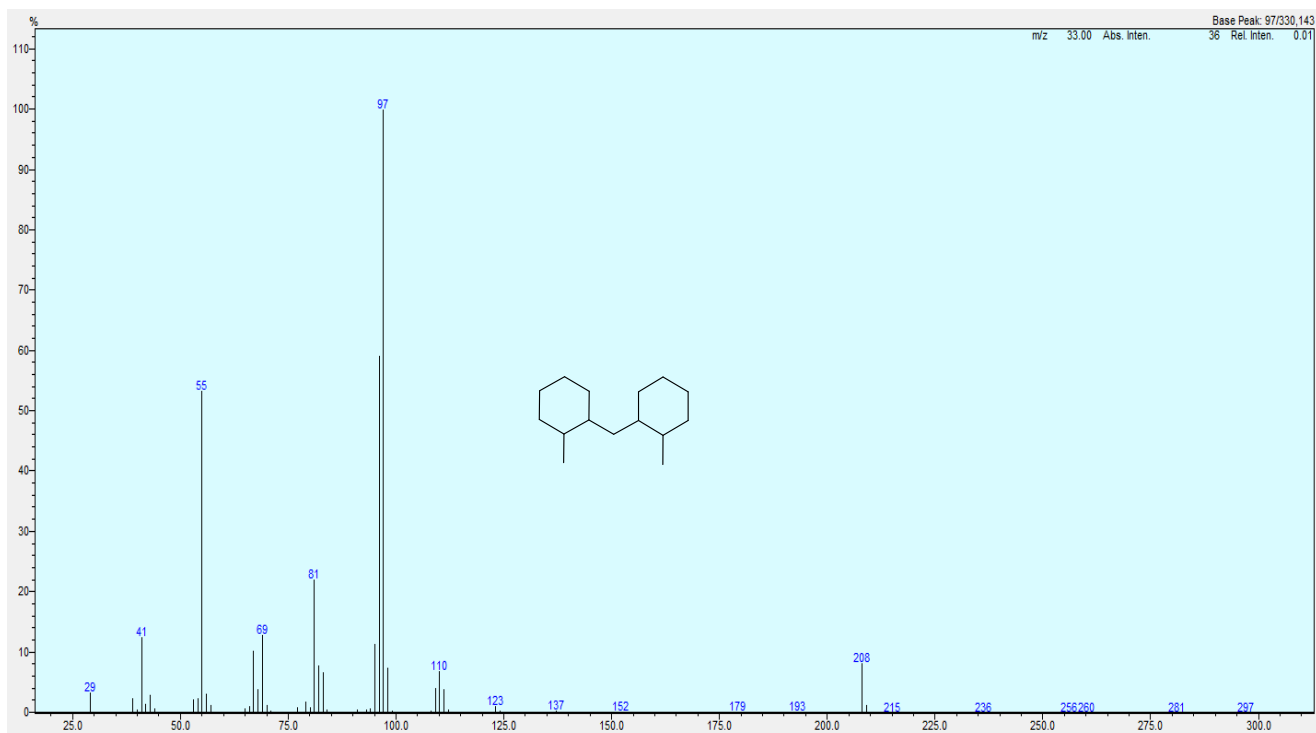
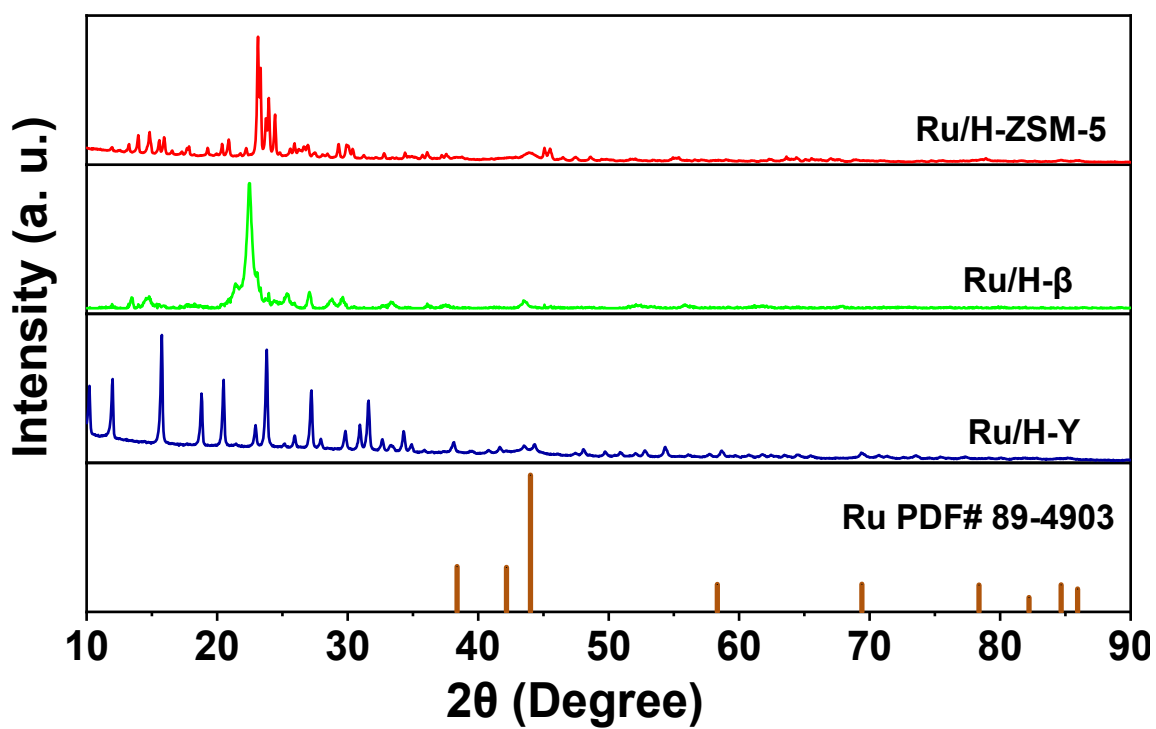**Figure S11.** Mass spectrograms of the C_{14} and C_{15} dicycloalkanes from the HDO of **1A**.

Figure S12. XRD patterns of the Ru-based HDO catalysts.

From the XRD results, no evident peaks of metallic Ru were observed in the patterns of the Ru-based catalysts, which means that Ru particles were well-dispersed on these catalysts.
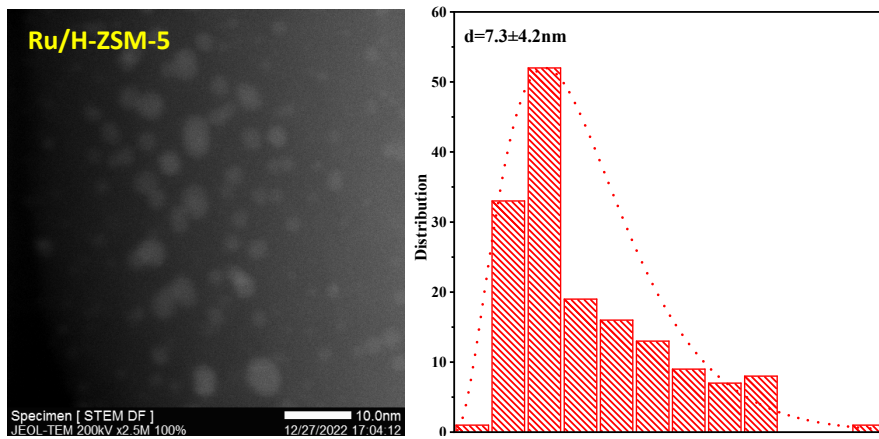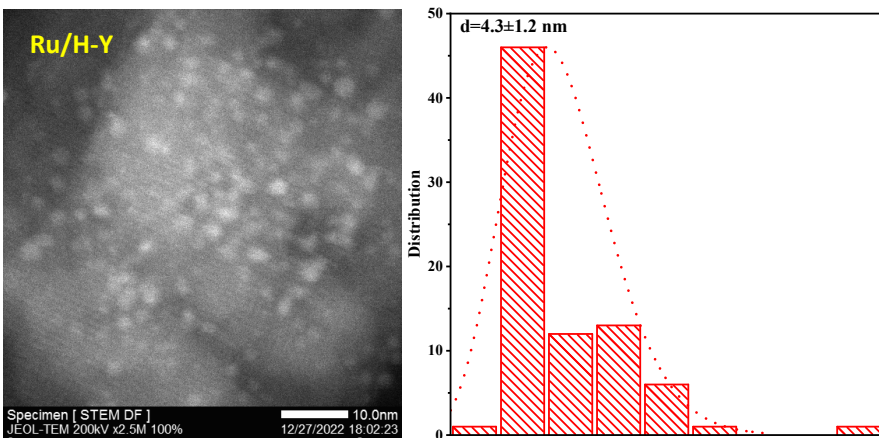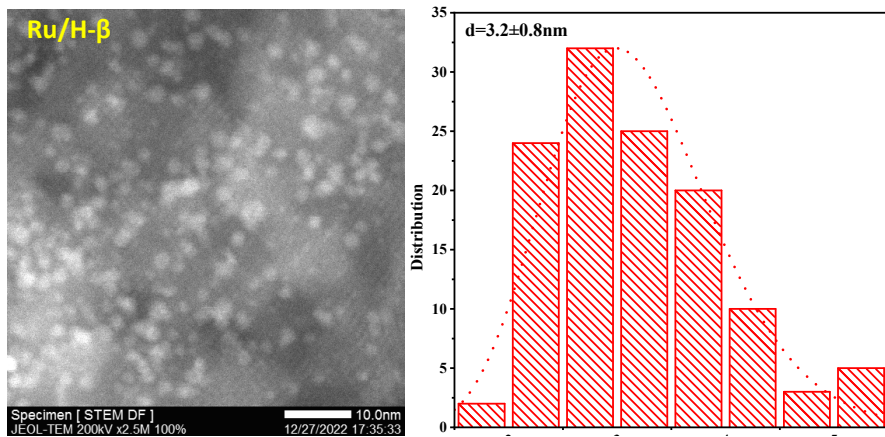
Figure S13. TEM images of the Ru-based HDO catalysts.