

Supporting Information

**Synthesis of jet fuel range high-density polycycloalkanes with vanillin
and cyclohexanone**

Haofei Gao,^{a,b} Fengan Han,^b Guangyi Li,^b Aiqin Wang,^{b,c} Yu Cong,^b Zhizhou Li,^{*a} Wei Wang^{*a} and
Ning Li^{*b,d}

^a Shaanxi Key Laboratory of Catalysis, School of Chemistry and Environment Science, Shaanxi University of Technology, Hanzhong 723001, China.

^b CAS Key Laboratory of Science and Technology on Applied Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China.

^c State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China.

^d Dalian National Laboratory for Clean Energy, Dalian 116023, China.

Correspondence and requests for materials should be addressed to N. L. (E-mail: lining@dicp.ac.cn)

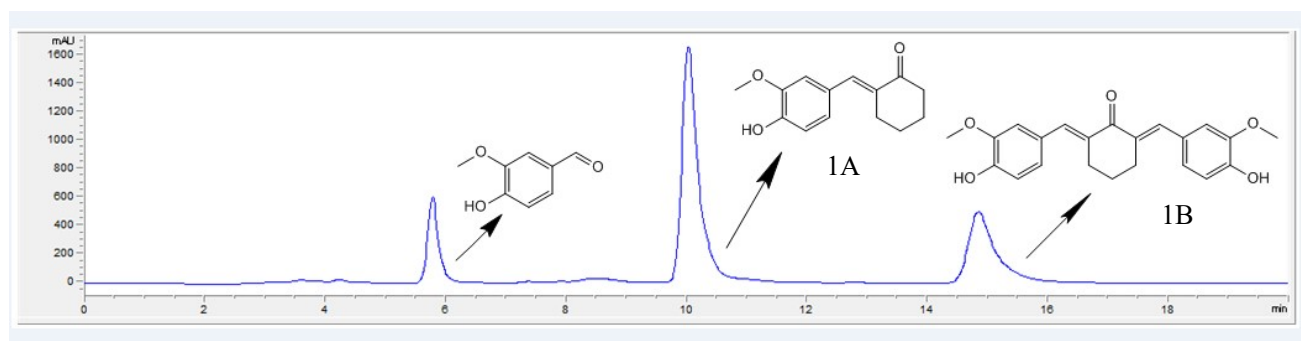


Figure S1. High performance liquid chromatography (HPLC) of the products from the aldol condensation of vanillin and cyclohexanone. Reaction conditions: 423 K, 4 h; 5 mmol vanillin, 15 mmol cyclohexanone and 0.05 g STNF were used in the test.

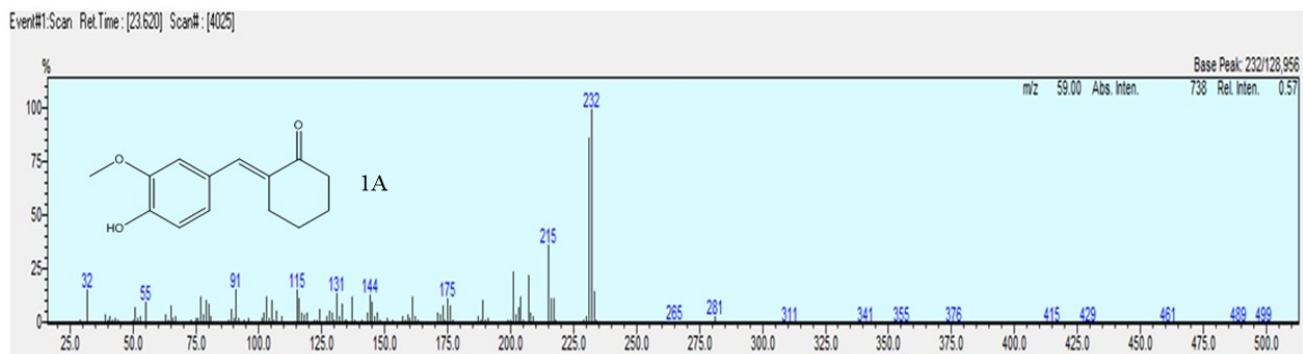


Figure S2. Mass spectrogram of **1A** from the aldol condensation of vanillin and cyclohexanone.

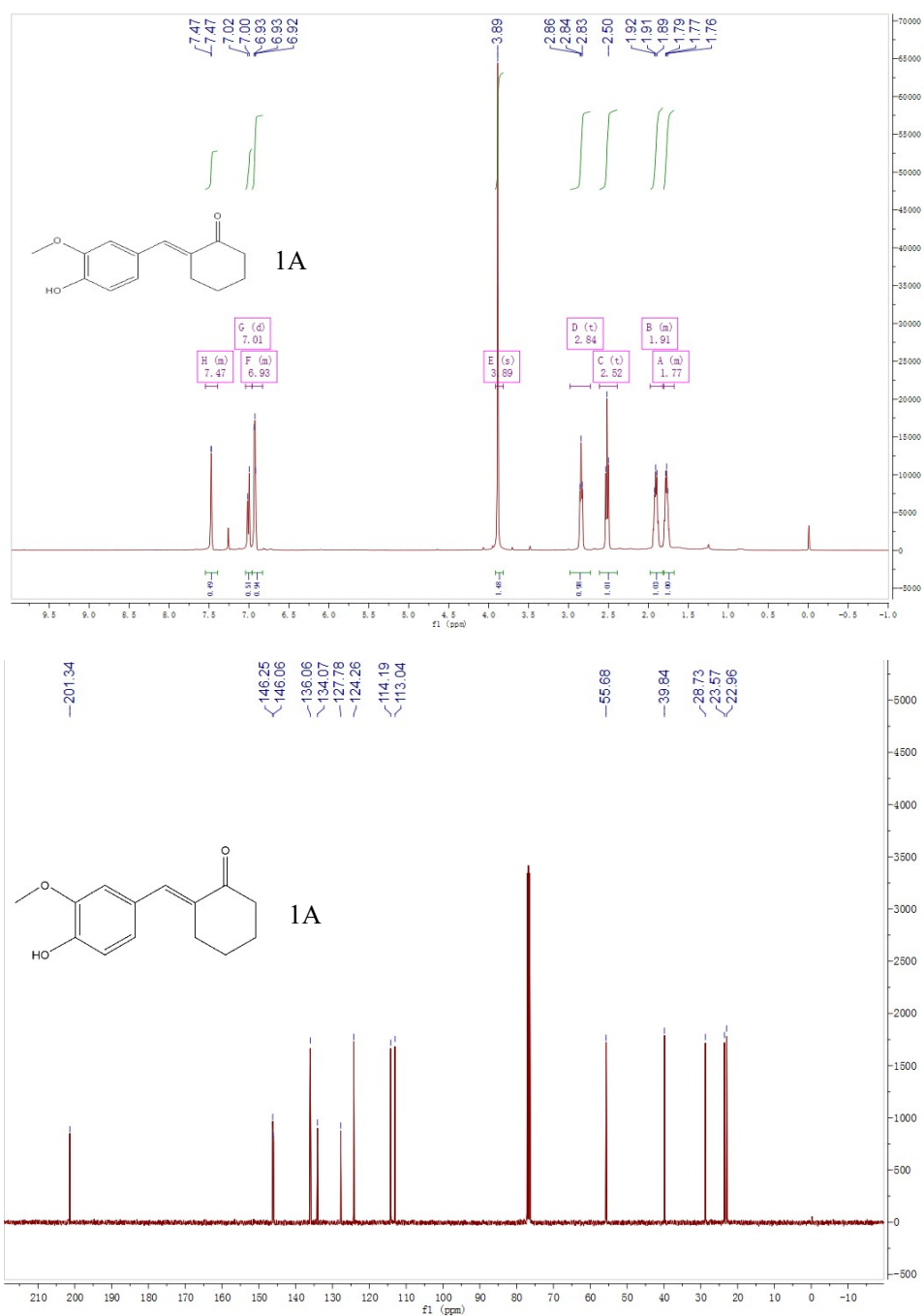


Figure S3. ^1H -NMR and ^{13}C -NMR spectra of the **1A** from the aldol condensation of vanillin and cyclohexanone.

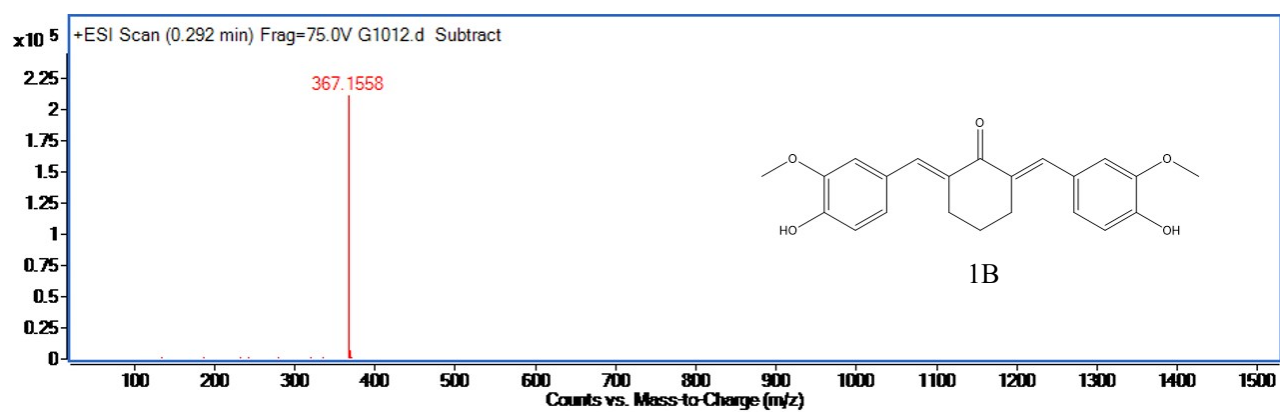


Figure S4. Mass spectrogram of **1B** from the aldol condensation of vanillin and cyclohexanone.

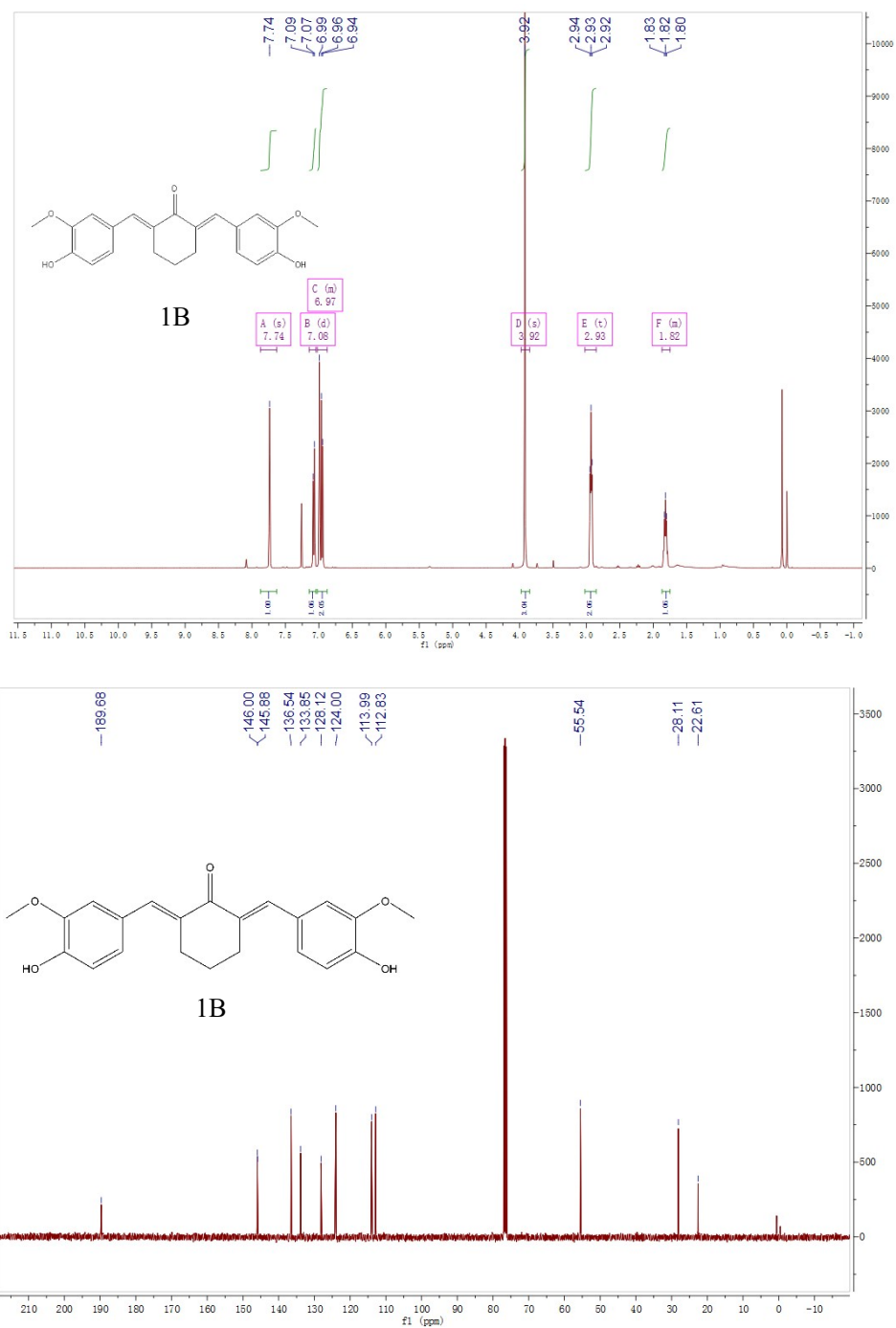


Figure S5. ¹H-NMR and ¹³C-NMR spectra of the **1B** from aldol condensation of vanillin and cyclohexanone.

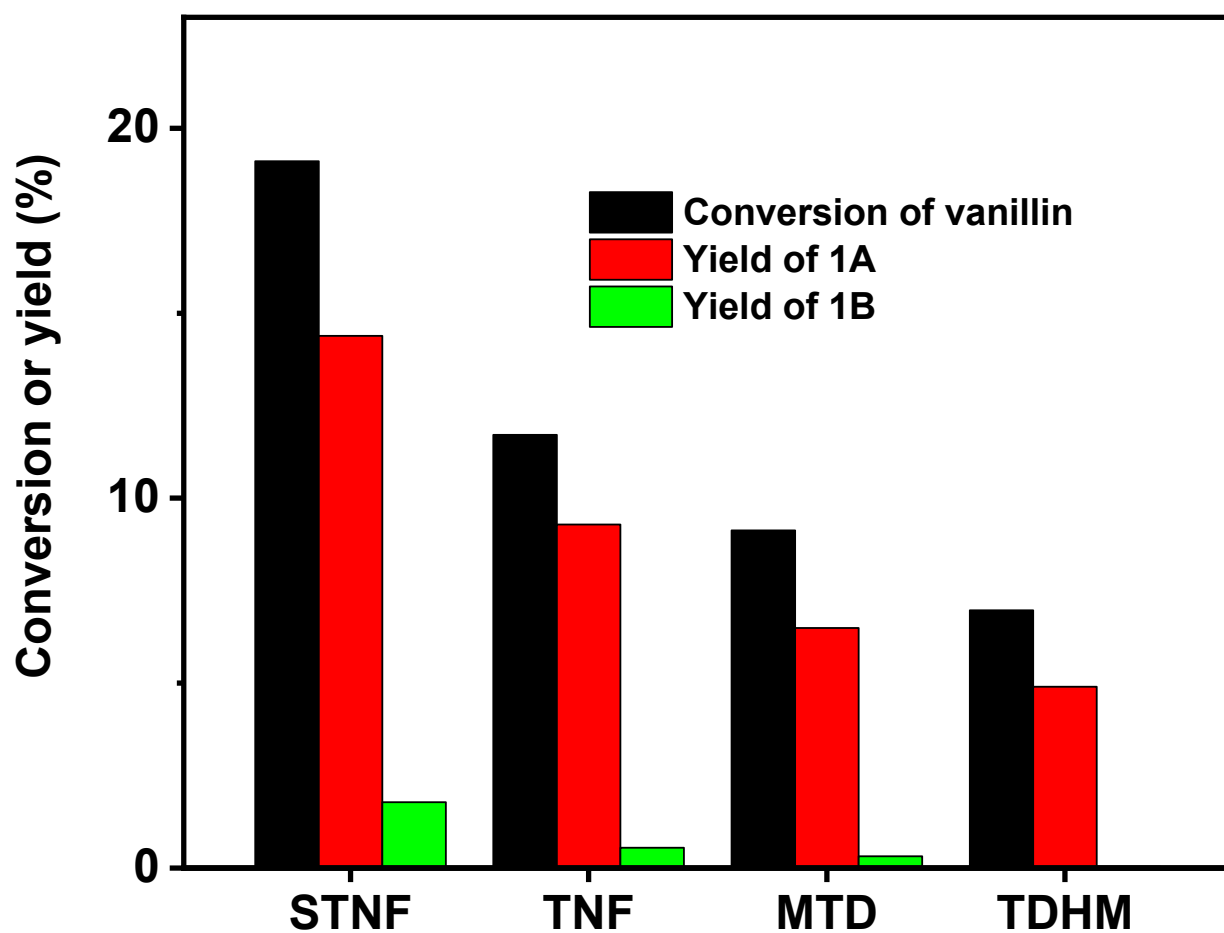


Figure S6. Conversion of vanillin and the yields of **1A** and **1B** over the titanium dioxide based nanometer material catalysts. Reaction conditions: 373 K, 4 h; 5 mmol vanillin, 5 mmol cyclohexanone and 0.025 g catalyst were used for each test.

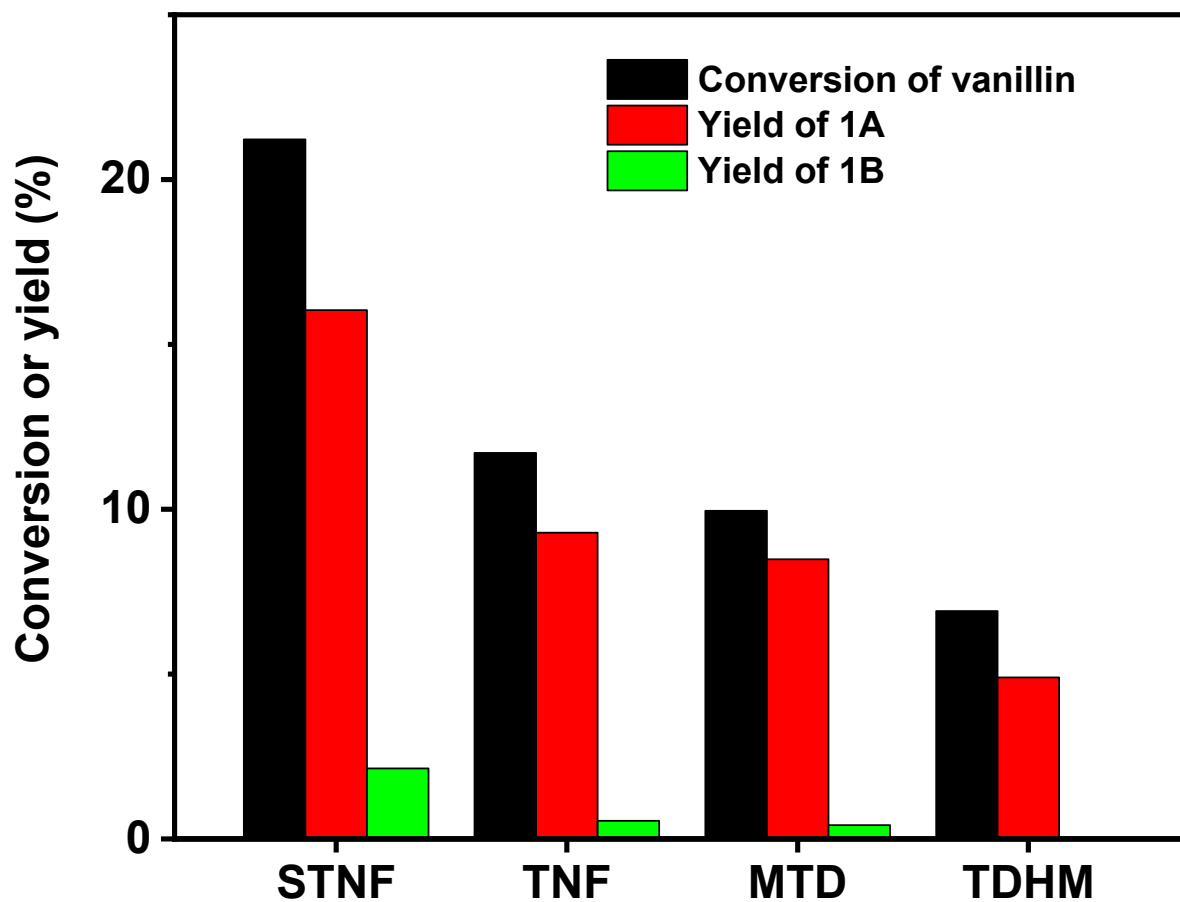


Figure S7. Conversion of vanillin and the yields of **1A** and **1B** over the titanium dioxide based nanometer material catalysts. Reaction conditions: 373 K, 4 h; 5 mmol vanillin, 5 mmol cyclohexanone were used in each tests. The surface areas of catalysts were fixed as 8.8 m² by controlling the masses of catalysts (0.032 g STNF, 0.025 g TNF, 0.049 g MTD, 0.025 g TDHM) according to their specific BET surface areas measured by N₂-physorption.

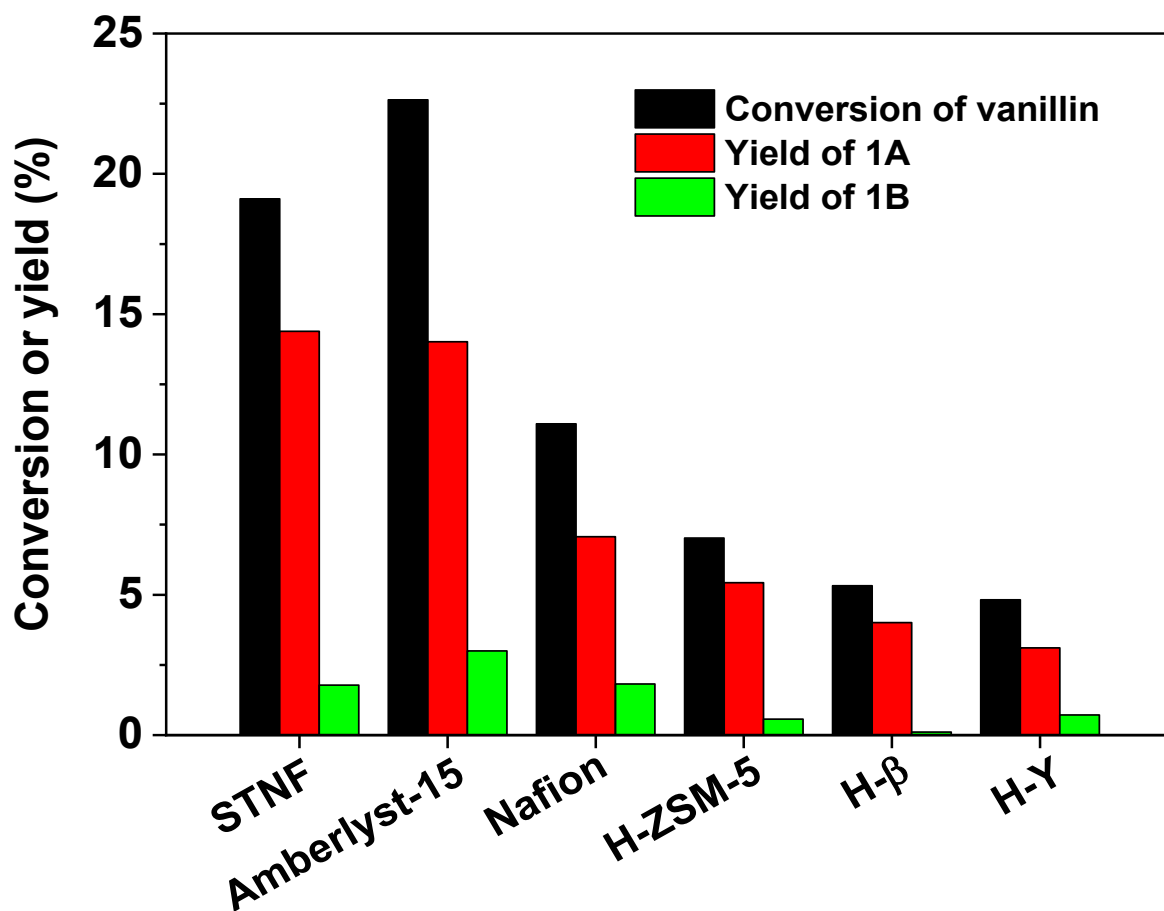


Figure S8. Conversion of vanillin and the yields of **1A** and **1B** over STNF and some commercial acid catalysts. Reaction conditions: 373 K, 4 h; 5 mmol vanillin, 5 mmol cyclohexanone, 0.025 g catalysts were used for each test.

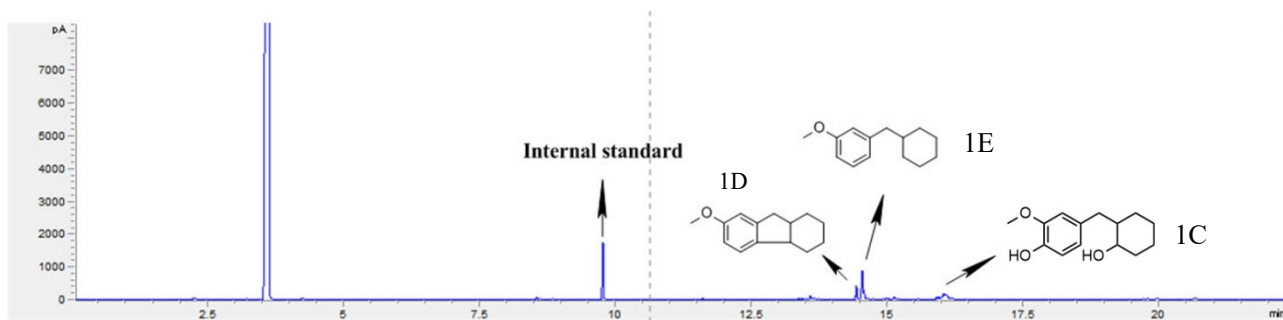


Figure S9. Gas chromatography of the product from the HDO of **1A** over the Pt/C catalyst. Reaction conditions: 443 K, 4 MPa H₂, 4 h; 5 mmol **1A** and 0.1 g Pt/C were used in the test.

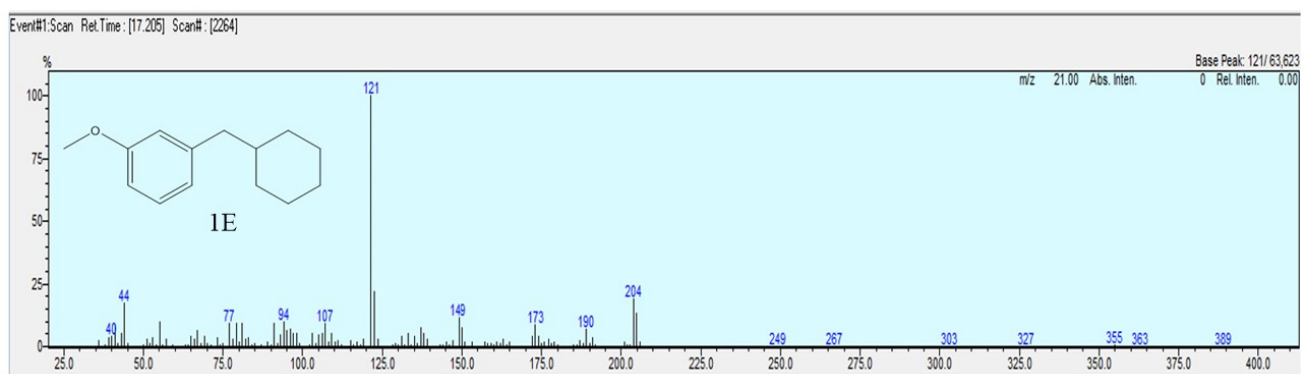
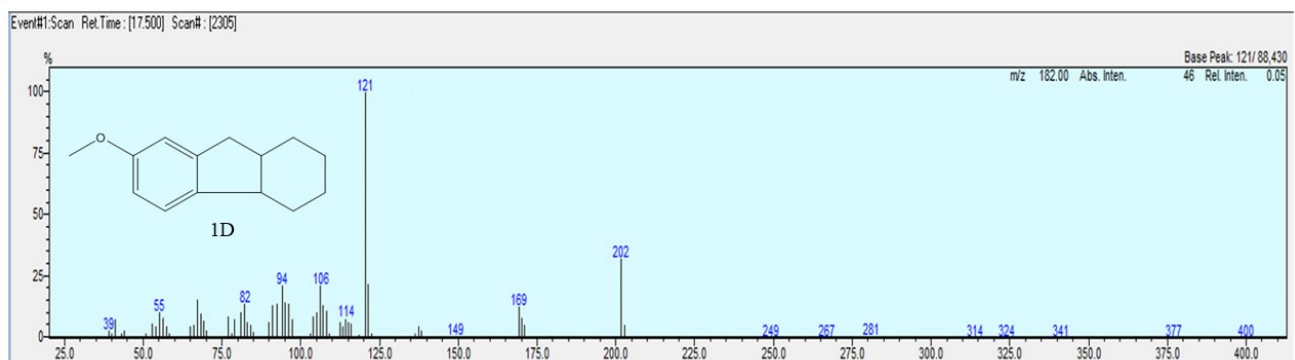
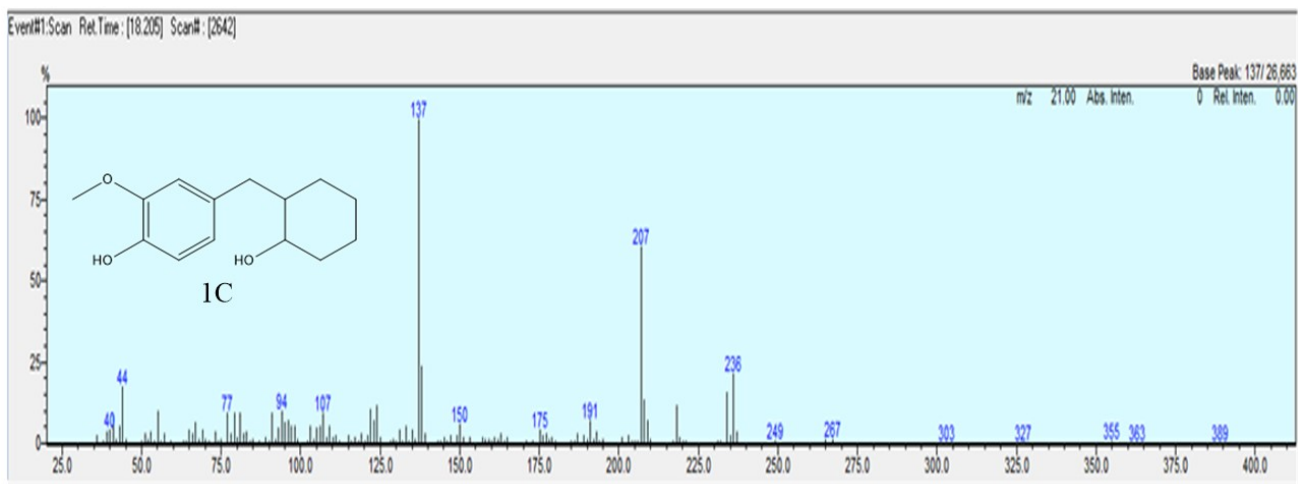


Figure S10. Mass spectrograms of **1C**, **1D** and **1E** from the HDO of **1A**.

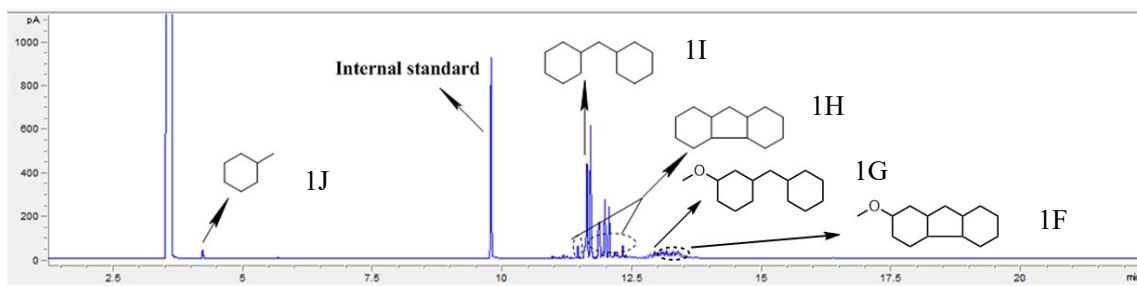


Figure S11. Gas chromatography of the product from the HDO of **1A**. Reaction conditions: 473 K, 6 MPa H₂, 4 h; 5 mmol vanillin, 0.1 g Pd/C and 1 g H-Y were used in the test.

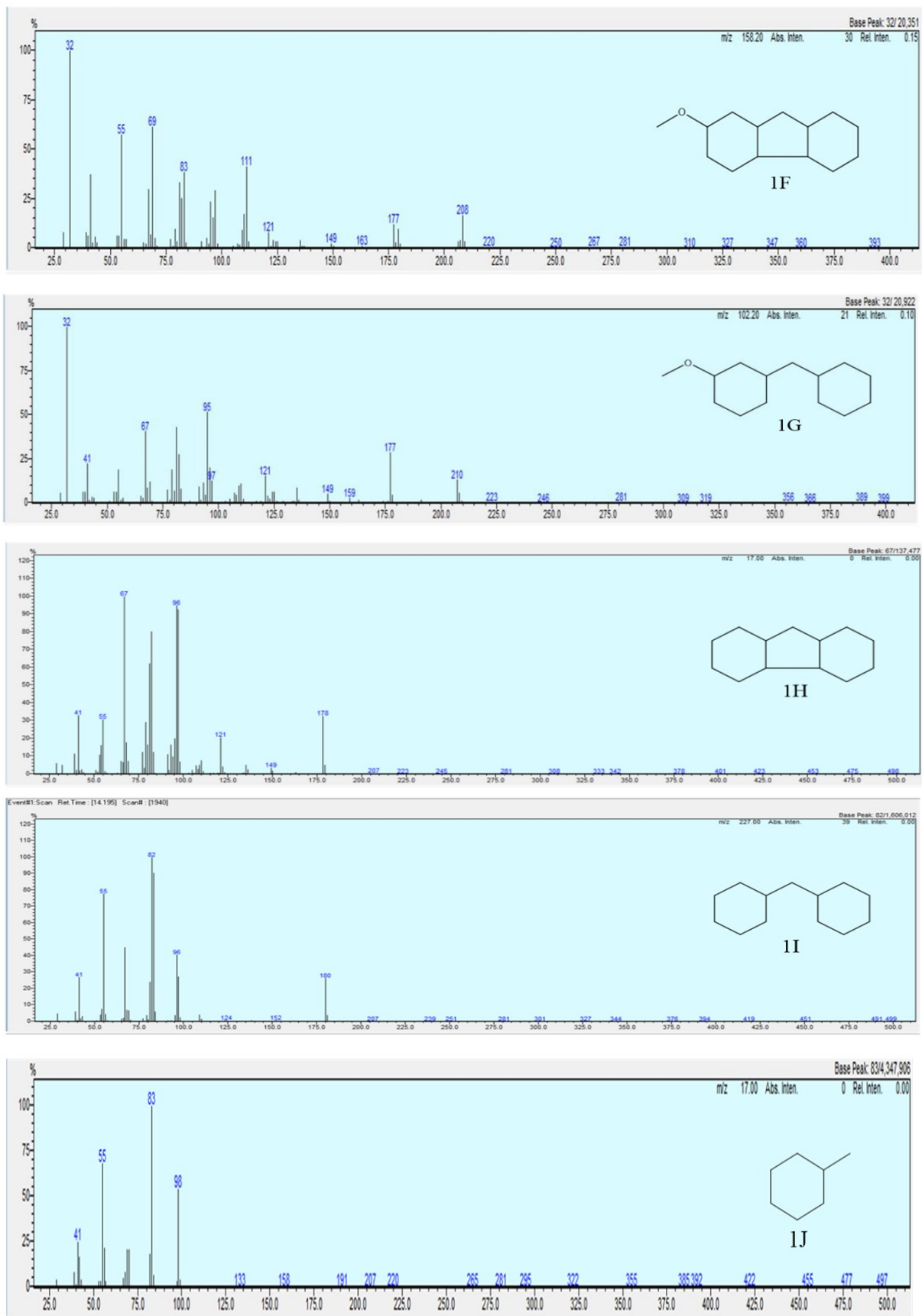


Figure S12. Mass spectrograms of 1F, 1G, 1H and 1J from the HDO of 1A.

Table S1. Metal dispersions and average particle sizes of the M/C catalysts measured by CO-chemisoption.

Catalyst	Metal dispersion (%)	Particle size (nm)
Pd/C	1.55	64.6
Ru/C	2.47	40.4
Pt/C	2.75	36.3

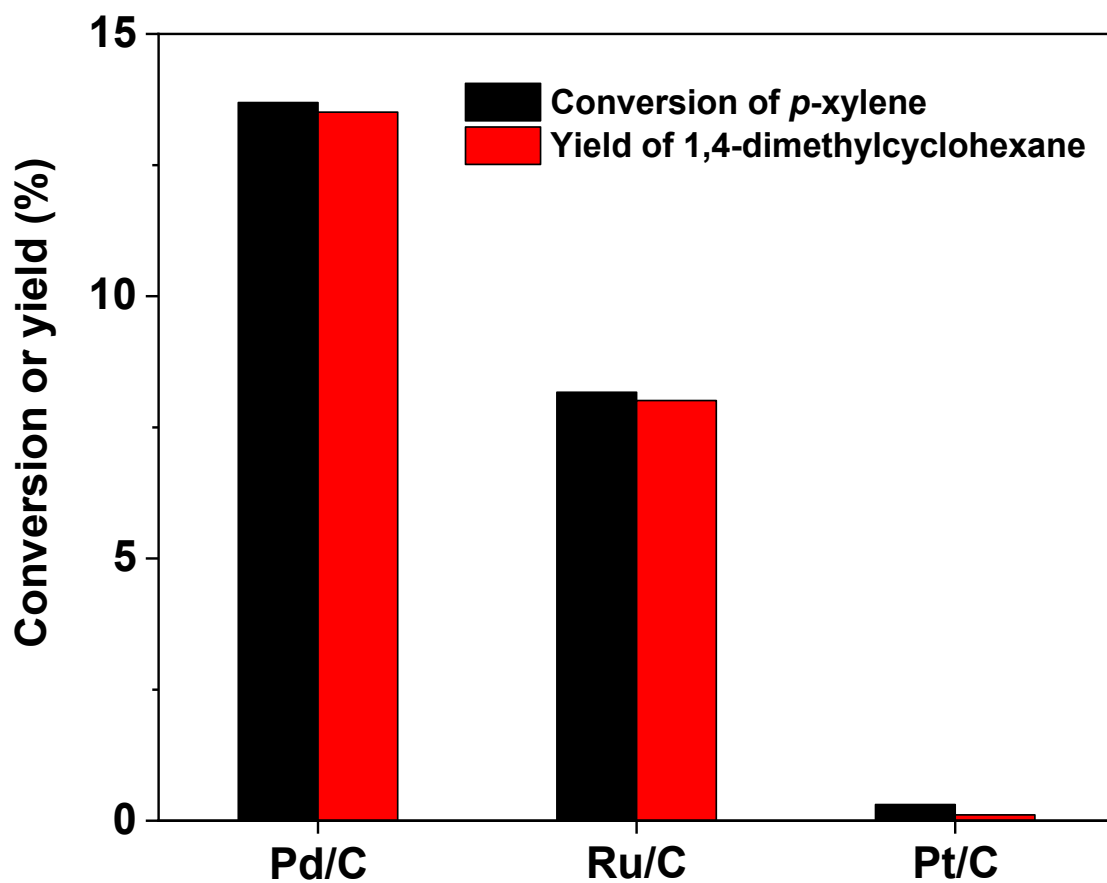


Figure S13. Conversion of *p*-xylene and the yield of 1,4-dimethylcyclohexane over the M/C catalyst (M = Pd, Ru, Pt). Reaction conditions: 2 MPa H₂, 413 K, 0.5 h; 5 mmol *p*-xylene, 10 mL cyclohexane (used as solvent) and 0.025 g catalyst were used in each test.