Supporting Information

Selective production of biobased phenol

from lignocellulose-derived alkylmethoxyphenols

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1. Extended results

1.1. TG analysis of the spent zeolite catalysts

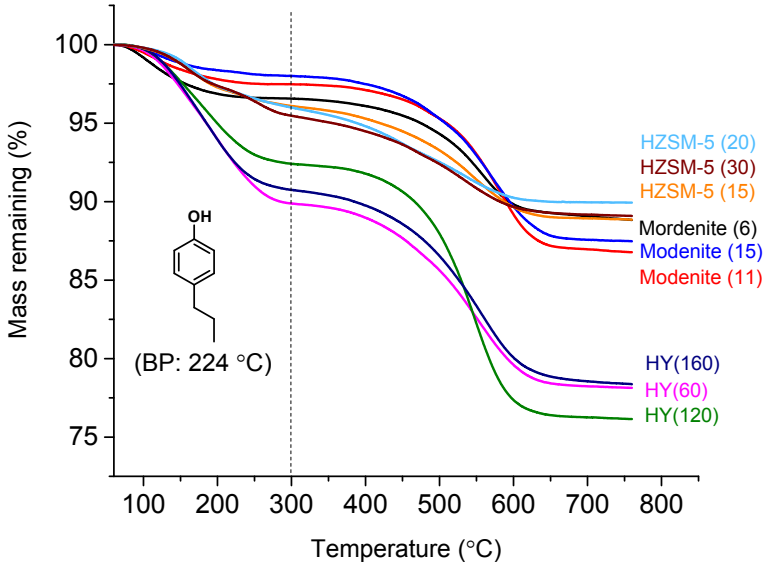

Figure S1. TG analysis of spent catalysts (the catalyst was washed with acetone and dried before measurement).

Catalyst	Si/Al ratio	Weight loss (%) (300-700 °C)
HZSM-5	15	7.1
HZSM-5	20	6.0
HZSM-5	30	6.3
Mordenite	6	7.7
Mordenite	11	10.5
Mordenite	15	10.8
HY	60	11.7
HY	120	16.3
HY	160	12.3

1. 2. Effect of feedstock to benzene ratio in transalkylation

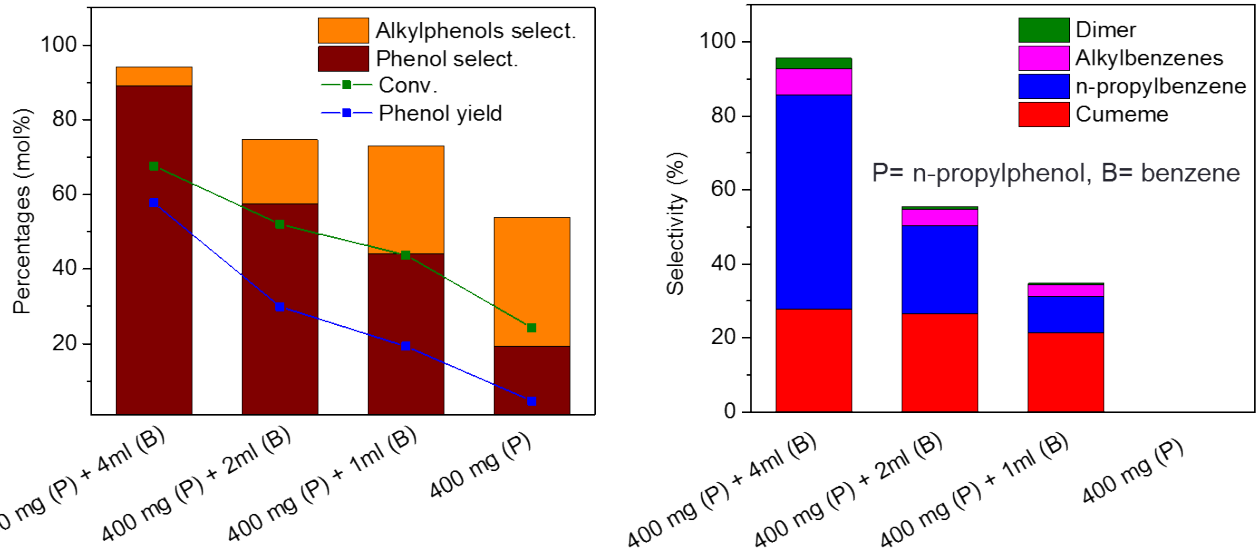

Figure S2. Influence of feedstock to benzene solvent ratio on product distributions over HZSM-5 (Si/Al 15) at 350°C for 2 h using a mini-batch autoclave (conditions: 400 mg 4-propylphenol, 40 mg catalyst).

1.3. Effect of solvent for transalkylation

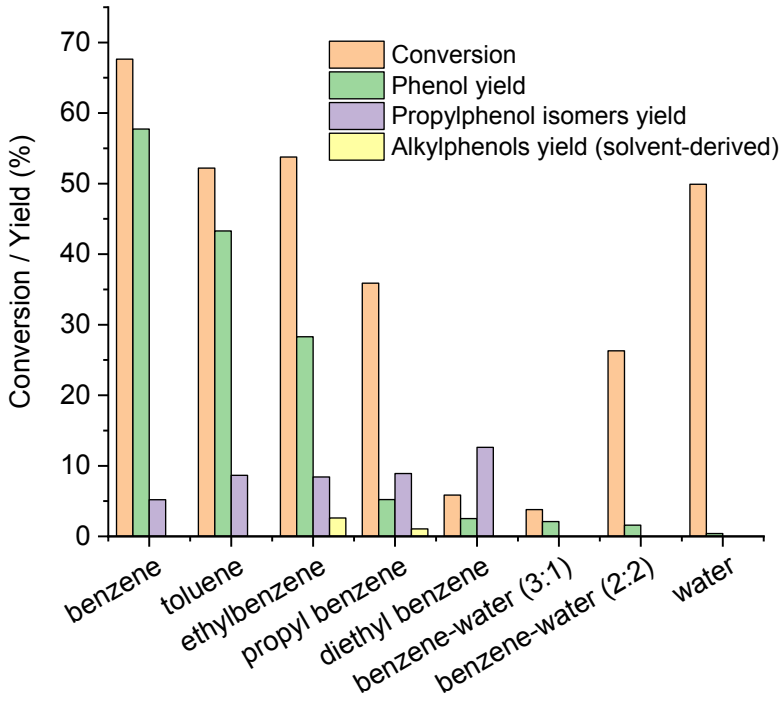

Figure S3. Influence of solvent on product distributions over HZSM-5 (Si/Al 15) at 350°C for 2 h using a mini-batch autoclave (conditions: 400 mg 4-propylphenol, 4 ml solvent, 40 mg catalyst).

1.4. Transalkylation of guaiacol and 4-propylguaiacol over HZSM-5

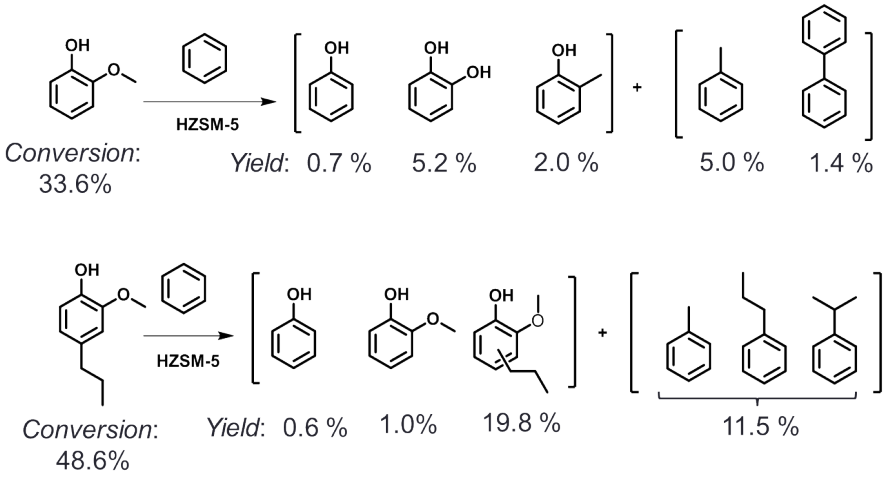

Figure S4. Transalkylation of guaiacol and 4-propylguaiacol over HZSM-5 (Si/Al 15) in benzene using a mini-batch autoclave (conditions: 400 mg feedstock, 4 ml benzene solvent, 40 mg catalyst, temperature 350 ^{o}C, 2h).

1. 5. Catalyst screening for demethoxylation

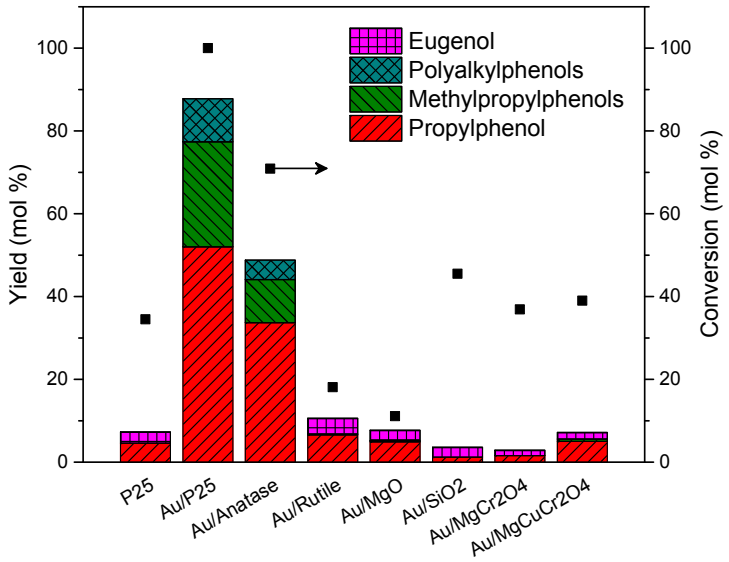

Figure S5. Influence of the support on the catalytic performance of supported Au nanoparticle catalysts for the demethoxylation of 4-propylguaiacol at 350°C for 2 h using a Parr batch autoclave (conditions: 3000 mg feedstock, 30 ml benzene, 100 mg catalyst, 50 bar H_2, 2 h reaction time)

1.6. XPS analysis of the Au/TiO_2 catalyst

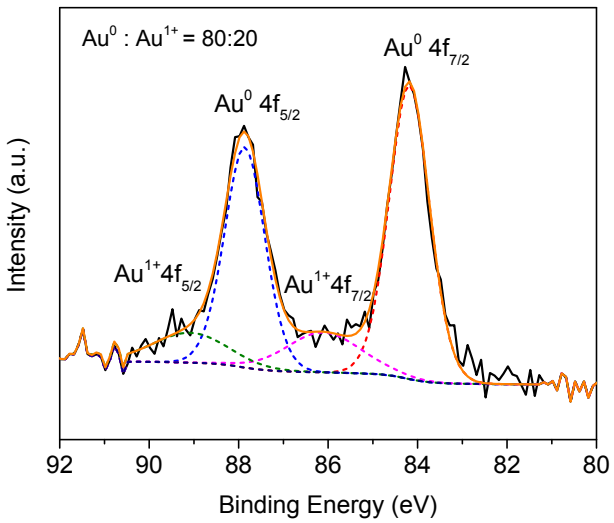

Figure S6. XPS spectra of Au 4f region of the calcined Au/TiO_2 (P25) catalyst.

The results show that after the calcination of Au/TiO_2 at 350°C, most of the Au nanoparticles are in the metallic form (~80%). The remainder of gold is in the 1+ oxidation state, which indicates the presence of gold oxide species.

1.7. Two-step demethoxylation-transalkylation

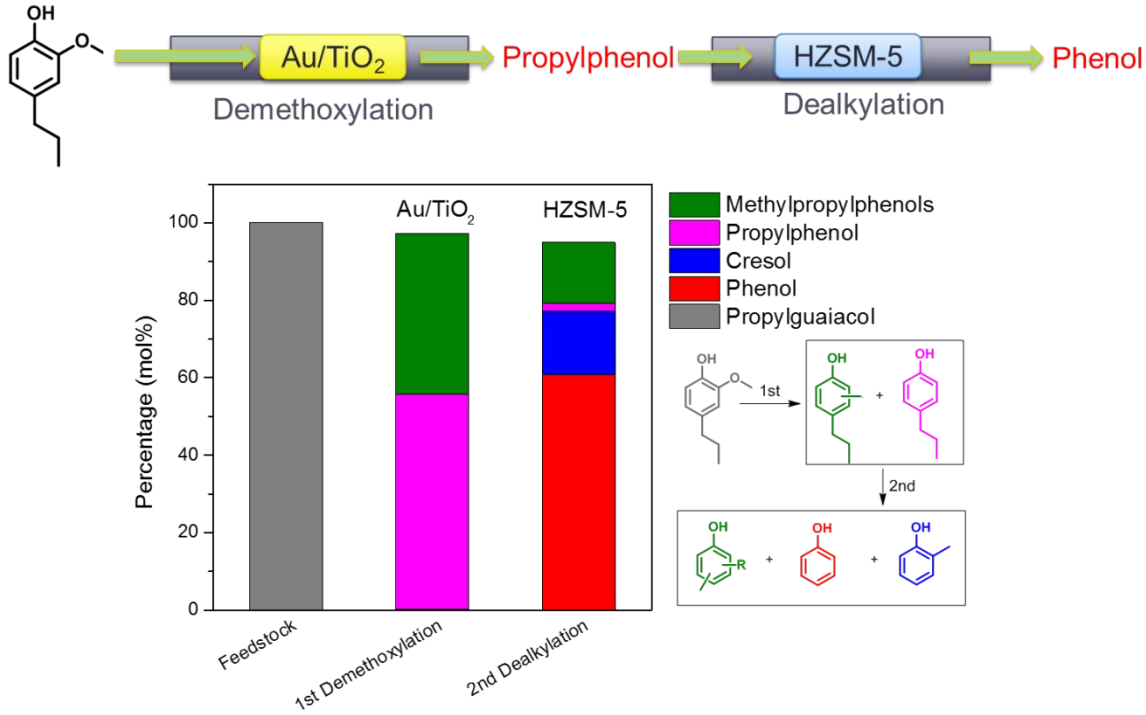

Figure S7. Two-step process for demethoxylation over Au/TiO_2 catalyst, followed by dealkylation into phenol over the HZSM-5 (Si/Al 15) in benzene using a fixed-bed reactor (conditions: 200 mg catalyst, 5 mol% feedstock in benzene, liquid feed rate 4.5 ml/h, gas feed rate 30 Nml/min H_2, temperature 350 ^oC, pressure 100 bar; the feedstock for the second step is obtained from the first demethoxylation step).

1.8. Effect of temperature on one-step demethoxylation-transalkylation

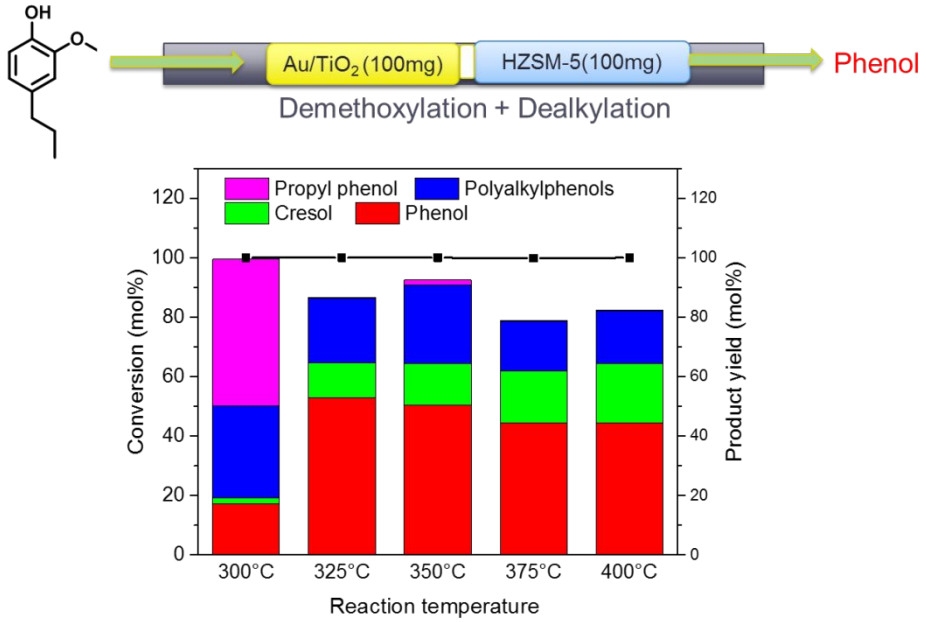

Figure S8. One-step process for demethoxylation and dealkylation over Au/TiO_2 and HZSM-5 (Si/Al 15) catalysts in benzene using a fixed-bed reactor at different temperatures (conditions: 100 mg Au/TiO_2 + 100 mg HZSM-5 catalysts, 5 mol% feedstock in benzene, liquid feed rate: 4.5 ml/h, gas feed rate 30 Nml/min H_2, pressure 100 bar, the yield are based on the averages of the 4-6 h time-on-stream).

1.9. Transalkylation of 4-propylphenol with benzene

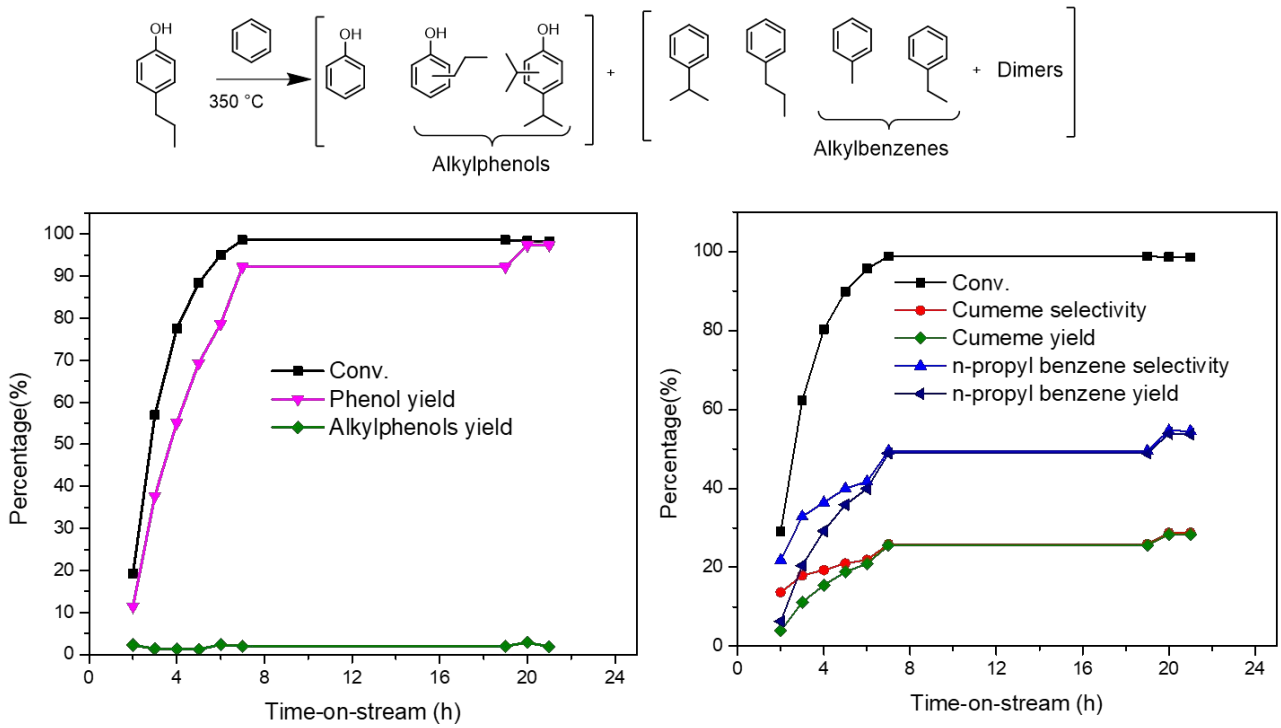

Figure S9. Catalytic dealkylation of 4-propylphenol into phenol over HZSM-5 (Si/Al 20) in benzene in a fixed-bed reactor (conditions: 200 mg HZSM-5, 5 mol% feedstock in benzene, liquid feed rate 2.3 ml/h, temperature 350 ^{o}C, pressure 50 bar corresponding to measured autogenous pressure of the liquid mixture).