Electronic Supplementary Material (ESI) for Green Chemistry.

Supplementary Information

Selective production of bicyclic alkanes as high-density fuel additives by coupling lignocellulose-derived furanics and phenolics

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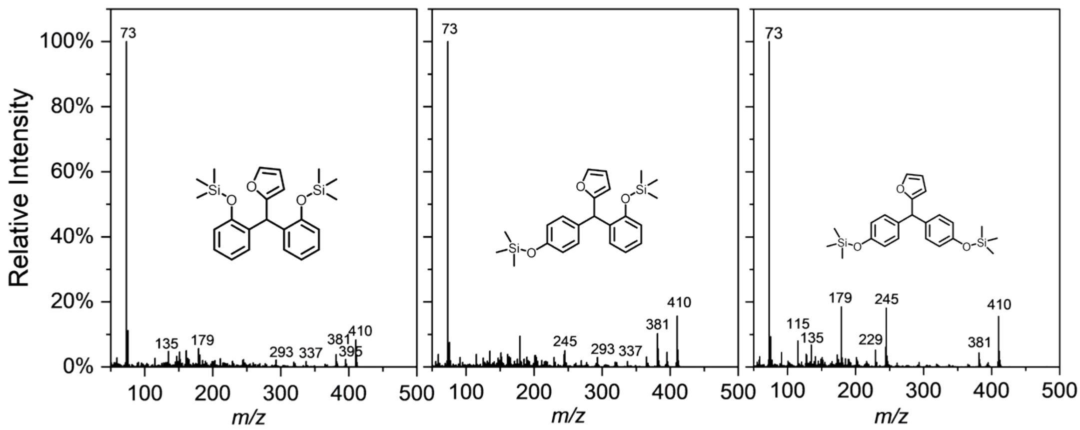

Fig. S1. GC-MS of FPP-PF and its isomers.

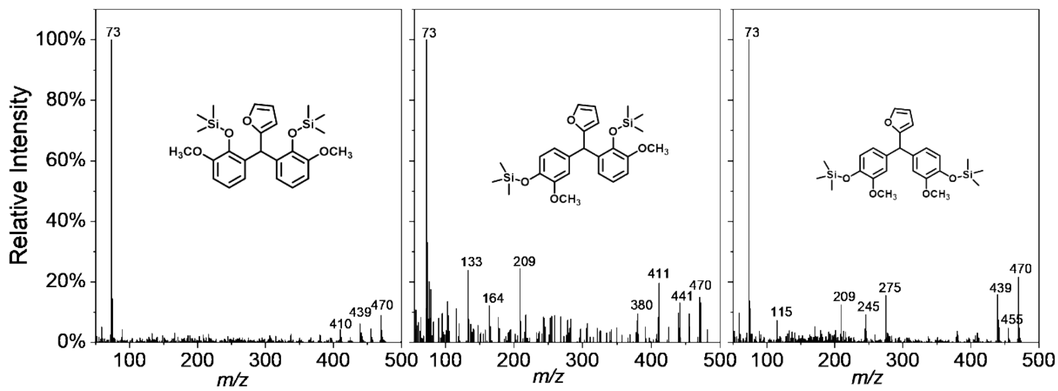

Fig. S2. GC-MS of FPP-GF and its isomers..

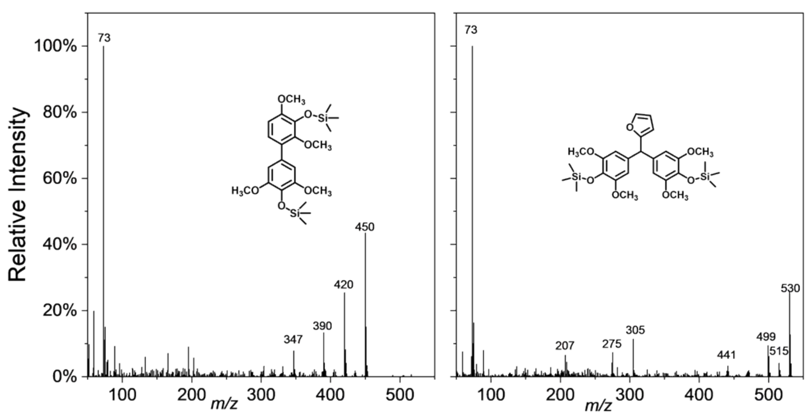

Fig. S3. GC-MS of syringol self-coupling product and FPP-SF.

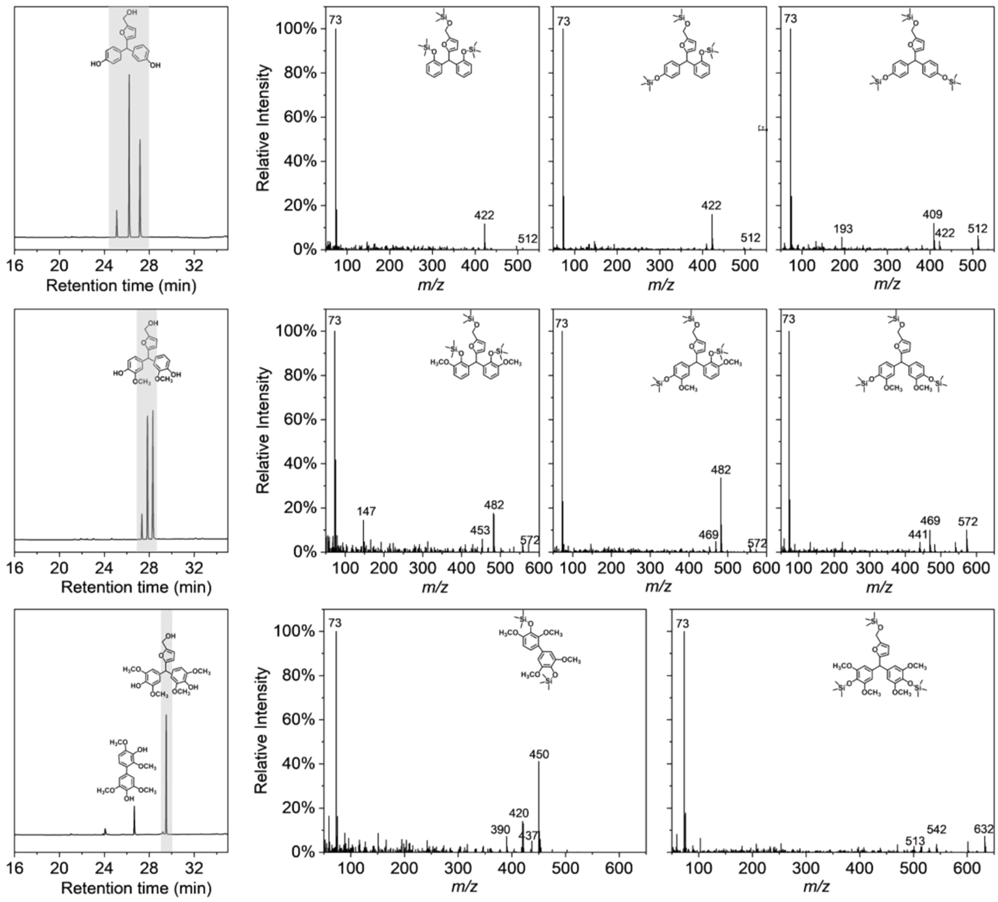

Fig. S4. GC chromatograms and GC-MS mass of FPP-PH, FPP-GH, and FPP-SH.

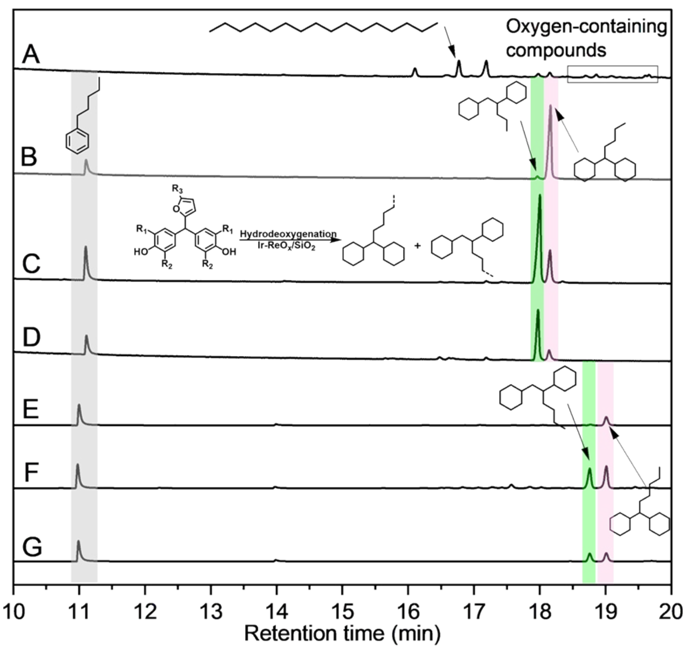

Fig. S5. Chromatograms of HDO products of FPPs. (A) FPP-SF, HDO conditions: Pd/C and H_3PO_4, 250 °C; (B) FPP-PF, HDO conditions: Ir-ReO_x/SiO_2, 180 °C; (C)FPP-GF, HDO conditions: Ir-ReO_x/SiO_2, 180 °C; (D) FPP-SF, HDO conditions: Ir-ReO_x/SiO_2, 200 °C; (E) FPP-PH, HDO conditions: Ir-ReO_x/SiO_2, 200 °C; (F) FPP-GH, HDO conditions: Ir-ReO_x/SiO_2, 200 °C; (G) FPP-SH, HDO conditions: Ir-ReO_x/SiO_2, 200 °C.

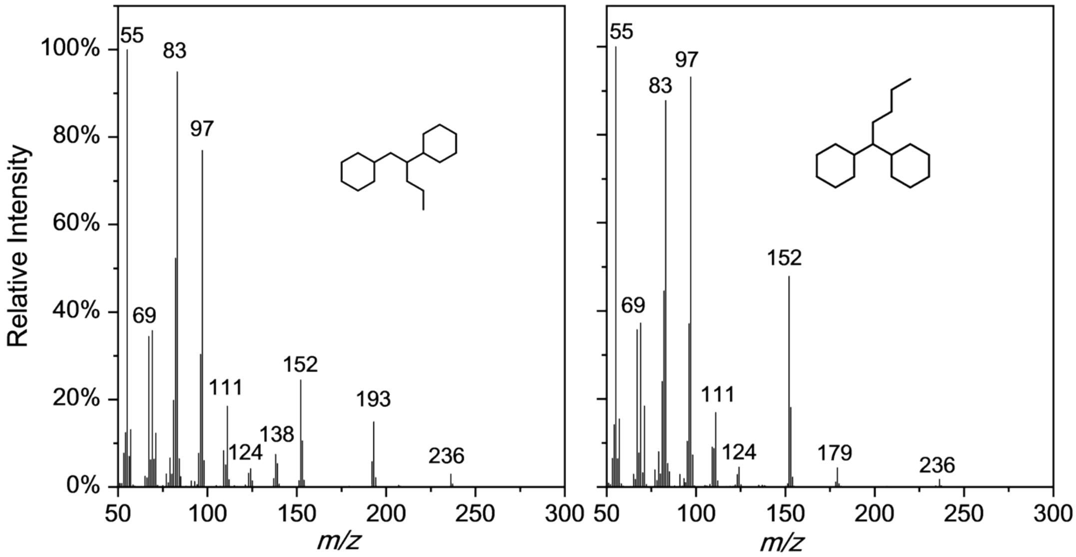

Fig. S6: GC-MS of C17-BCA.

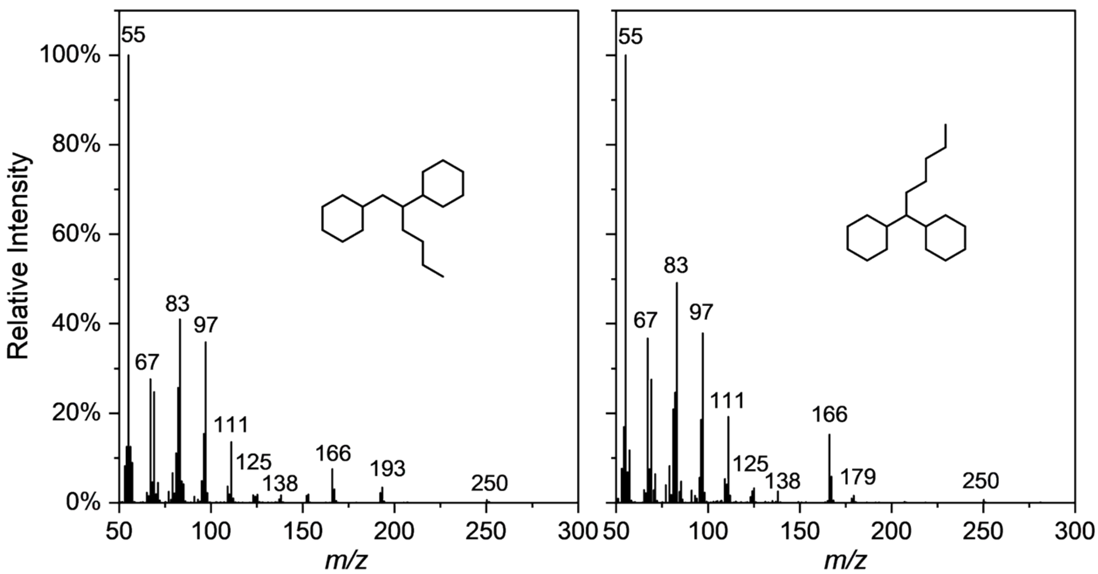

Fig. S7: GC-MS of C18-BCA.

Tab. S1 Parametric optimization of phenol-furfural coupling

Phenol/furfural (mol)	Temperature (°C)	NaOH (mg)	Reaction time (h)	FPP-PF yield
16/1	80	10	4	11.1%
16/1	80	10	8	25.1%
16/1	80	10	12	41.9%
16/1	80	10	24	56.3%
16/1	80	10	48	67.0%

Tab. S2 Parametric optimization of HDO of FPP

Time (h)	Temperature (°C)	Catalyst	BCA yield
6 [a]	250	Pd/C and H_3PO_4	24.9%
12 [a]	180	Pd/C and H_3PO_4	18.2%
6 [a]	250	Ru/C and H_3PO_4	<10.0%
6 [a]	250	Pt/C and H_3PO_4	<10.0%
6 [a]	200	Ir-Re/SiO_2	48.0%
18 [b]	200	Ir-Re/SiO_2	86.8%
18[c]	200	Ir-Re/SiO_2	94.2%
18[d]	200	Ir-Re/SiO_2	90.0%
18[e]	200	Ir-Re/SiO_2	90.7%

[a] 100 mg catalyst, 100 mg FPP; [b] 50 mg catalyst, 100 mg FPP; [c] the first recycling of Ir-Re/SiO_2; [d] the second recycling of Ir-Re/SiO_2, [e] the third recycling of Ir-Re/SiO_2.

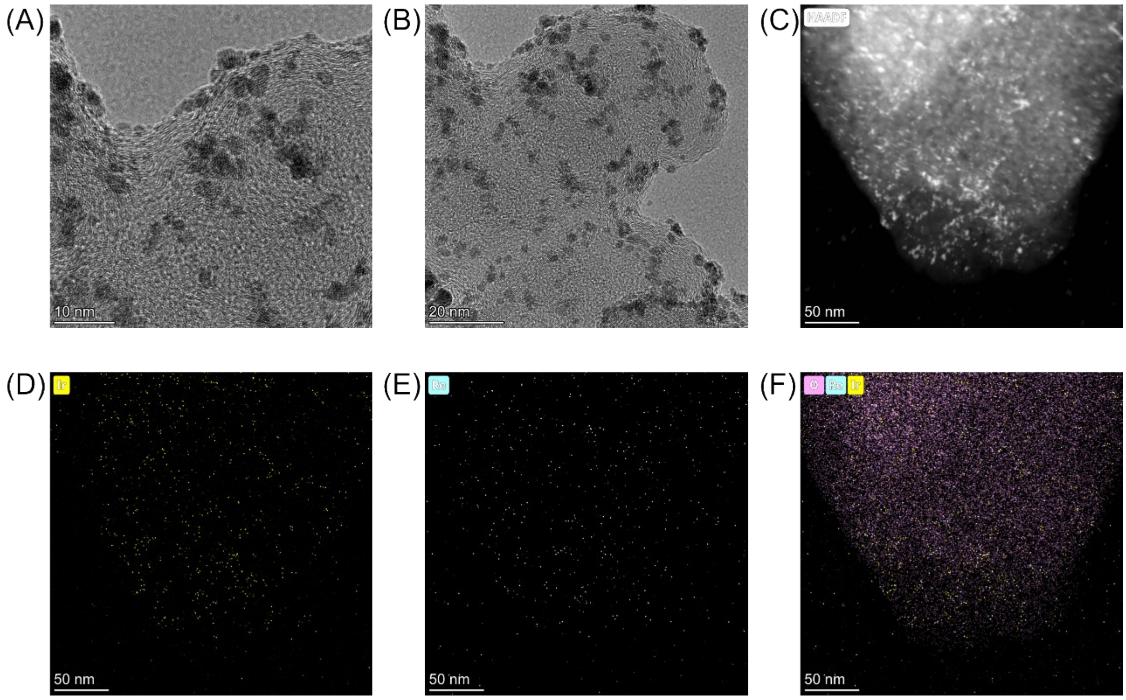

Fig. S8 (A) and (B) TEM image of Ir-ReO_x/SiO_2; (C), (D), (E)and (F) EDX mapping of Ir-ReO_x/SiO_2.

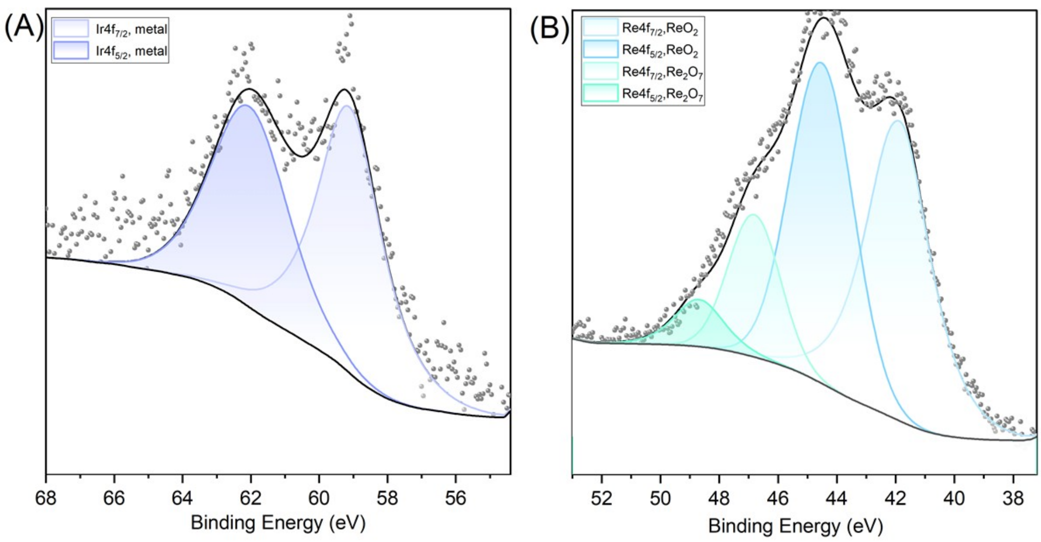

Fig. S9 XPS spectra of the Ir-ReO_x/SiO_2. (A) High-resolution Ir spectra of Ir-ReO_x/SiO_2; (B) High-resolution Re spectra of Ir-ReO_x/SiO_2.

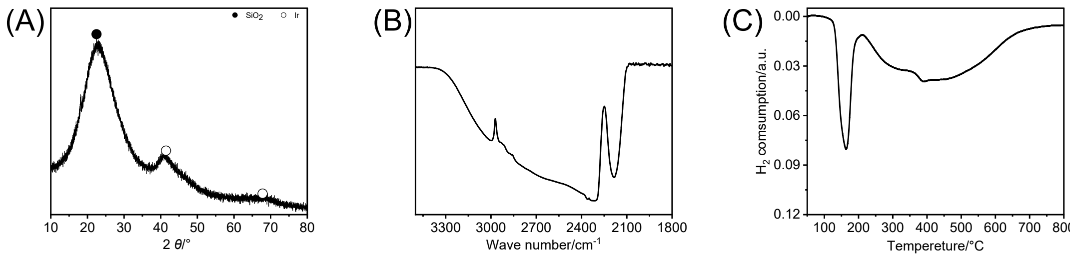

Fig. S10 (A) XRD Patterns of the Ir-ReO_x/SiO_2. (B) DRIFT spectra of CO adsorbed on the Ir-ReO_x/SiO_2 after the reduction at 200 °C. (C) TPR profiles of Ir-ReO_x/SiO_2. Conditions: sample (50 mg, calcined at 500 °C for 3 h) and H_2/Ar (10% v/v, 50 ml/min) at a heating rate of 10 °C /min.