Supporting Information

Production of aromatics from biomass by computer-aided selection of the zeolite catalyst

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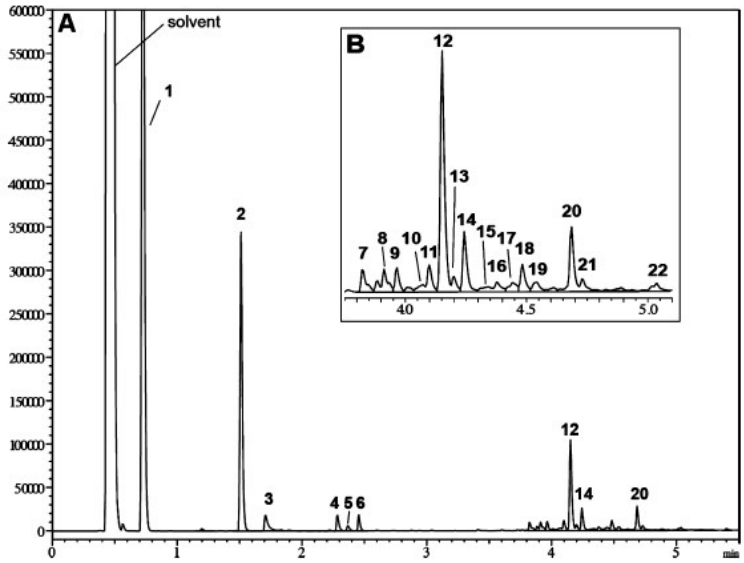
Figure S1: Gas chromatogram of all liquid products achieved from reaction of 2,5-dimethylfuran and ethylene (left) and list of products (right). Reproduced from ACS Catal, 2013, 3, 41.



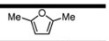
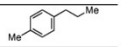
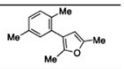
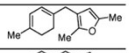
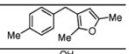
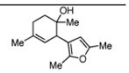
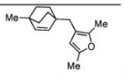
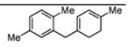
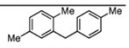
com-pound	area % 493 K	area % 528 K	chemical formula	chemical structure
1	88.9	70.3	C_6H_8O	
2	5.3	15.9	C_8H_{10}	
3	0.3	1.4	$C_6H_{10}O_2$	
4	0.0	0.9	$C_8H_{12}O$	
5	0.4	0.3	$C_8H_{12}O$	
6	0.3	0.8	$C_{10}H_{14}$	
7	0.2	0.4	$C_{14}H_{18}O$	n.d.
8	0.1	0.3	$C_{14}H_{18}O$	n.d.
9	0.1	0.4	$C_{14}H_{20}O_2$	n.d.
10	0.2	0.2	$C_{14}H_{16}O$	
11	0.3	0.5	$C_{14}H_{20}O_2$	n.d.
12	1.9	4.2	$C_{14}H_{18}O$	
13	0.2	0.1	$C_{14}H_{16}O$	
14	0.7	1.0	$C_{14}H_{20}O_2$	
15	0.1	0.2	$C_{16}H_{18}$	n.d.
16	0.2	0.2	$C_{14}H_{20}O_2$	n.d.
17	0.2	0.3	n.d.	n.d.
18	0.2	0.5	$C_{16}H_{22}O$	
19	0.2	0.3	$C_{14}H_{16}O_2$	n.d.
20	0.1	1.2	$C_{16}H_{20}$	
21	0.1	0.4	$C_{16}H_{18}$	
22	0.1	0.2	$C_{14}H_{16}O_2$	n.d.

Figure S2: Gas chromatogram with product identification

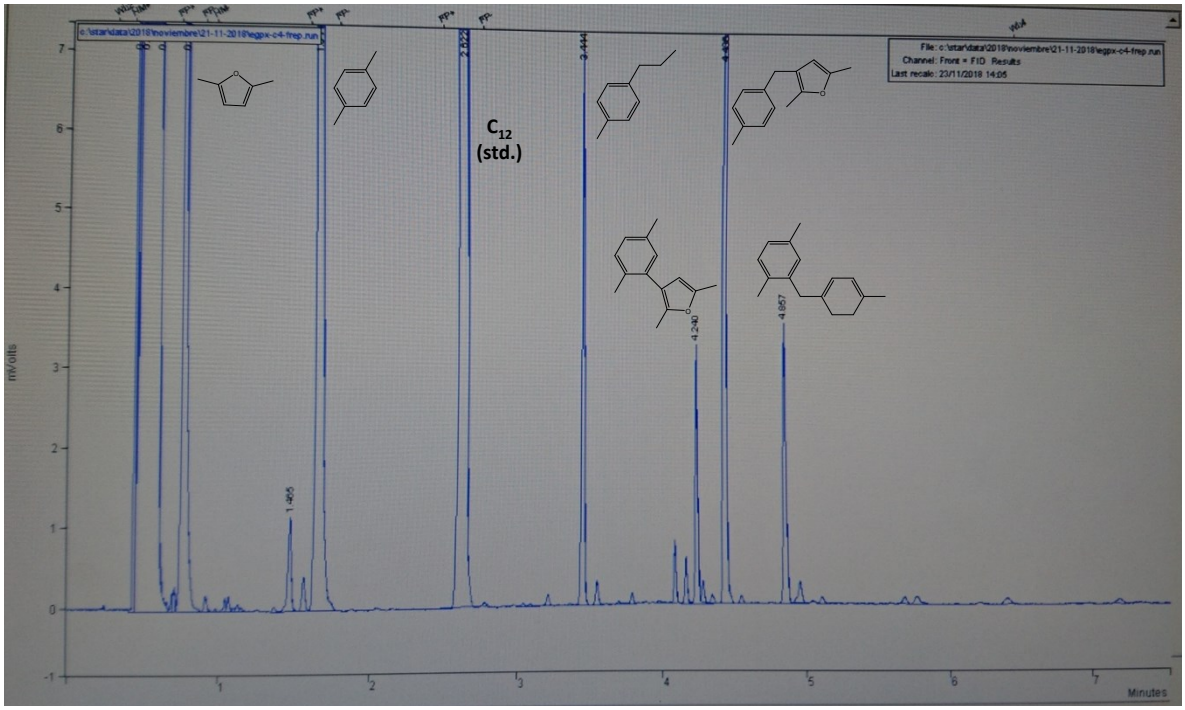


Table S1: ***Conversion and selectivity to main products for the Diels-Alder dehydration reaction using dimethylfuran (DMF) and ethylene after 3 h. Reaction conditions: 14.6 mmol DMF, 28.1 ml heptane and 30 mg of catalyst, at 52 bar and 240 ℃.***

Sample	t (h)	X_{DMF} (%)	$S_{P\text{-}XYL}$ (%)	S_{COND} (%)[a]	S_{ALKYL} (%)[b]	$Y_{P\text{-}XYL}$ (%)
USY	3	18	46	25	2	8
USY	20	32	46	26	2	15
Beta	3	26	49	24	1	13
Beta	20	45	46	19	2	21
MCM-22	3	18	35	17	3	6
DS-ITQ-2_L	3	37	45	24	2	16
DS-ITQ-2_L	20	64	50	21	4	32
DS-ITQ-2_H	3	49	44	23	2	22
DS-ITQ-2_H	20	78	55	17	5	43

[a] S_{COND}: This selectivity has been calculated considering the peaks assigned in the GC chromatogram to 3-(2,5-dimethylphenyl)-2,5-dimethylfuran, 2,5-dimethyl-3-(4-methylbenzyl)furan, and 1,4-dimethyl-2-((4-methylcyclohexa-1,3-dien-1-yl)methyl)benzene (see Figure S2).

[b] S_{ALKYL}: This selectivity has been calculated considering the peak assigned in the GC chromatogram to 1-methyl-4-propylbenzene (see Figure S2).