Supporting Information of "Sugar ketals as a platform molecule to overcome the limitation of converting biomass into green-hydrocarbons in typical refinery"

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1 Fluid catalytic cracking (FCC) results of pure n-hexane and mixture up with DX

1.1 Catalyst properties

Supplementary Table 1: Commercial catalyst properties based on ZSM-5 used in the cracking process.

Properties of commercial catalyst	
Superficial area S_{BET} (m2.g^{-1})	136
Apparent density (g.mL^{-1})	0.7
Pore volume$_s$ (ml.g^{-1})	0.34
Alumina (wt.%)	20.6
Iron (wt.%)	0.16
sodium (wt.%)	0.08

1.2 Data of FCC

Supplementary Table 2: Material balance: gas, liquid and coke in wt.% of the total feed of DX and n-hexane mixtures

	Mass injected,g	Feed	Product wt% in relation to feed				Conv.		Coke/ cat. (wt.%)
			Gas (%)	Liquid (%)	Coke (%)	Total (%)	n-C$_6$	DX	
FCC Catalyst based on ZSM-5	6.55	n-C$_6$	28	67	2.5	97	47	-	0.8
	7.29	30%DX	30	66	2.8	99	30	100	1.0
	7.79	50%DX	35	65	4.7	104	31	100	1.8
	8.29	70%DX	28	67	7.0	102	4	95	2.8
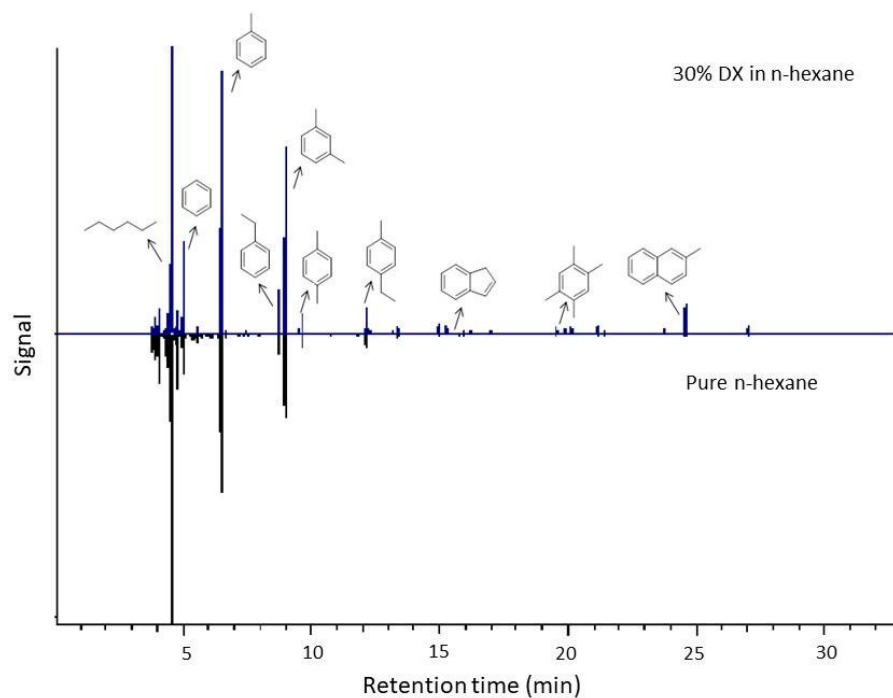
Supplementary Fig. 1. Liquid products of 30 wt.% of DX in n-hexane and liquid products of pure n-hexane. A higher relative intensity of aromatics and lower amount of lights products are observed from the mixture compared to pure n-hexane.
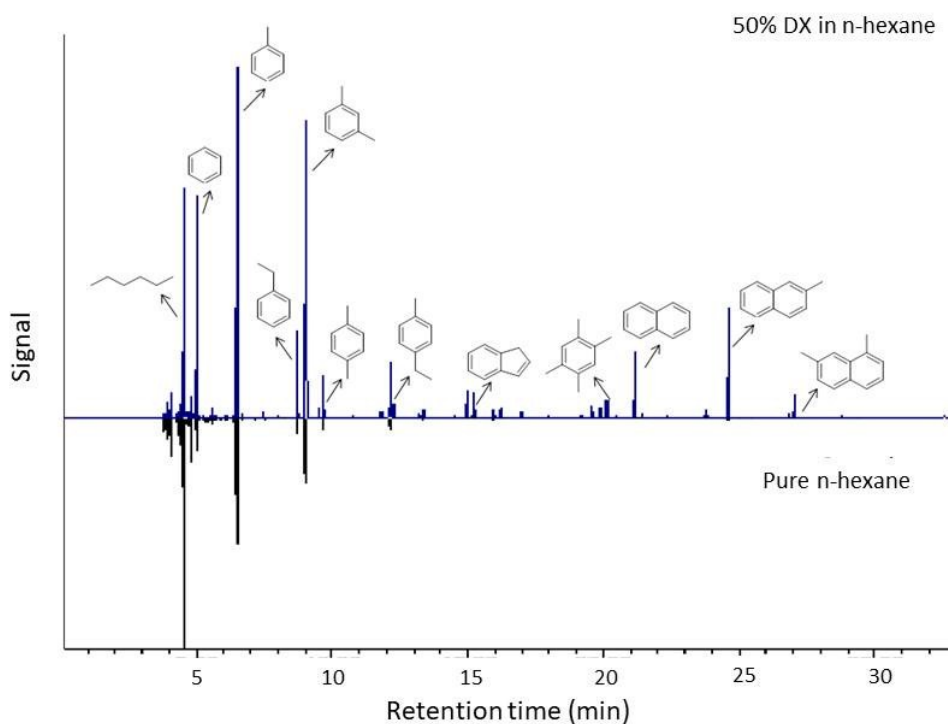
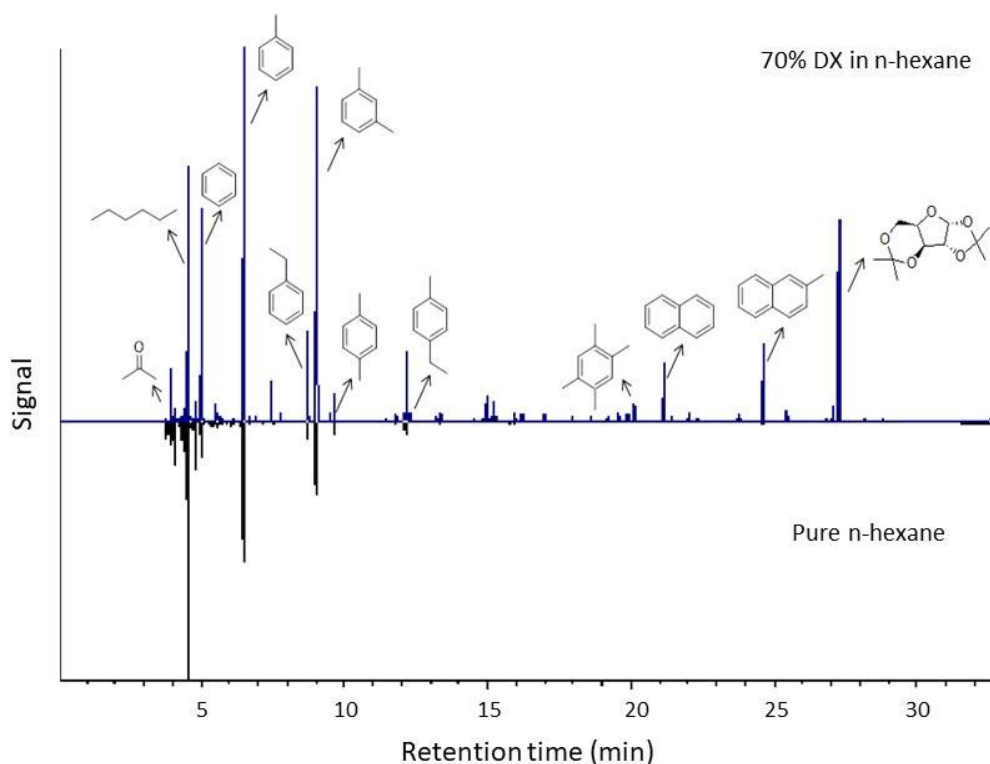**Supplementary Fig. 2.** Liquid products of 50 wt.% of DX in n-hexane and liquid products of pure n-hexane. The highest relative intensity *of* aromatics was observed.

Supplementary Table 3: Liquid products of 50 wt.% of DX in n-hexane FCC test.

Retention time (min)	Compound	Area (%)
1.681	-	0.06
1.707	-	0.08
2.087	1-Propene, 2-methyl	0.06
2.304	1-Propene, 2-methyl	0.23
2.412	2-Butene, (E)-	0.14
2.525	Acetone	0.15
2.711	Cyclopropane, 1,2-dimethyl-, cis-	0.12
3.234	Cyclopropane, ethyl	0.01
3.562	2-Pentene, (E)-	0.85
3.945	-	0.05
4.114	1,3-Cyclopentadiene	0.14
4.243	-	0.07
4.456	Cyclopentene	0.14
4.707	-	0.07
4.869	1-Pentanol, 2-methyl	0.42
5.393	-	0.02
6.231	-	0.05
6.768	Pentane, 3-methyl	0.11
7.054	-	0.07
7.512	-	0.03
7.807	1-Pentene, 2-methyl	0.24
8.069	-	0.07
8.410	-	0.02
8.891	Hexane	60.85
9.021	1,3-Pentadiene, 3-methyl-, (E)-	0.01
9.128	2-Pentene, 3-methyl-, (E)-	0.06
9.285	-	0.07
9.471	-	0.04
9.809	Cyclopentane, methyl	0.10
10.186	1,3-Cyclopentadiene, 5-methyl	0.32
10.379	1,3-Cyclopentadiene, 5-methyl	0.03
10.576	Cyclopentene, 3-methyl	0.04
10.768	-	0.03
11.434	Benzene	3.97
12.687	2,4-Hexadien-1-ol	0.04
13.204	Cyclohexene	0.03
13.862	1,3-Pentadiene, 2,3-dimethyl	0.10
13.942	1,3-Pentadiene, 2,3-dimethyl	0.12
14.181	1,3,5-Heptatriene, (E,E)-	0.03
15.554	Cyclopropane, trimethyl-methylene	0.08
15.915	1-Ethylcyclopentene	0.02
16.540	Toluene	13.46

16.945	Cyclohexene, 1-methyl	0.06
18.519	Furan, 2,3,5-trimethyl	0.06
19.421	1,4-Dimethyl-1-cyclohexene	0.02
20.428	Ethylbenzene	1.09
20.845	Benzene, 1,3-dimethyl	9.72
21.442	Styrene	0.12
21.647	p-Xylene	0.53
22.832	Benzene, propyl-	0.02
23.899	Benzene, 1-ethyl-2-methyl	0.09
24.228	Benzene, 1-ethyl-4-methyl	1.08
25.215	Benzene, 1-ethenyl-3-methyl	0.08
25.315	Benzene, 1-ethyl-3-methyl	0.19
25.852	2H-Pyran-3(4H)-one, dihydro-6-methyl	0.03
26.250	Benzene, 1-ethenyl-3-methyl	0.05
26.586	-	0.04
26.707	Indene	0.49
26.919	Benzene, 1-propynyl	0.36
27.197	-	0.02
27.339	Phenol, 2-methyl	0.34
28.211	Benzene, 1-methyl-3-propyl	0.10
28.320	-	0.02
28.912	Phenol, 3-methyl	0.04
29.234	-	0.03
29.662	-	0.07
29.745	-	0.05
30.025	Benzene, 1-methyl-2-(2-propenyl)	0.11
30.279	Benzene, (1-methyl-2-cyclopropen-1-yl)	0.16
30.441	1,4-Dihydronaphthalene	0.25
30.750	-	0.03
31.329	Naphthalene	0.82
32.168	Naphthalene, 1,7-dimethyl	0.03
33.519	1H-Indene, 2,3-dimethyl	0.15
34.533	Naphthalene, 2-methyl	0.93
37.889	-	0.03
38.430	Naphthalene, 1,7-dimethyl	0.17

Supplementary Figure 3. Liquid products of 70 wt.% of DX in n-hexane and liquid products of pure n-hexane. Similar observations on aromatic formation (compared with previously figures 1 and 2). Also DX was not fully converted.

Supplementary Table 4: Gas products (fraction trapped in the Erlenmeyer) in molar % of the gas products.

	n-hexane	30%DX	50%DX	70%DX
H_2	0.2%	0.3%	0.3%	0.2%
Methane	2%	2%	3%	2%
Ethylene	8%	11%	11%	13%
Ethane	8%	9%	9%	3%
Propane	49%	34%	29%	14%
Propylene	15%	19%	15%	14%
Butanes	11%	9%	8%	3%
Butenes	5%	7%	6%	5%
CO	0%	4%	9%	21%
CO_2	0%	5%	9%	25%
Olefin/paraffin	0.4	0.7	0.7	1.6

Table 5. Yield of $CO + CO_2$ and H_2O (in wt.%) to total DX.

wt% of DX in nhexane	30 wt.DX%	50 wt.DX %	70 wt.DX %
[1] $CO + CO_2$,	8.5	11.9	17.7
[2] H_2O,	11.8	16.6	23.1
CO/CO_2	0.8	1	1.2
[1]/[2]	0.72	0.72	0.77

2 Hydroconversion results of pure n-hexane and mixture with DX

2.1 Catalyst properties

Surface area, average pore diameter and pore volume of the calcined catalyst were determined by N_2 adsorption in an adsorption-desorption equipment (Micromeritics ASAP-2020). The samples were dried at 120 °C and degassed at 200 °C for 2 h under vacuum before analysis. The surface area was obtained by the BET method and the average pore diameter and pore volume were obtained by BJH method. Energy dispersive X-ray spectrometry (EDX) analysis was performed with a Shimadzu EDX720 spectrometer in vacuum (< 30 Pa) to determinate the chemical compositions of the calcined catalysts.

Supplementary Table 6: Textural properties of catalysts used in the hydroconversion (Cu-Pd/HZSM-5 and Cu-Pd/HBEA).

Sample	S_{BET} $(m^2.g^{-1})$	S_{ext} $(m^2.g^{-1})$	V_p $(cm^3.g^{-1})$	V_{micro} $(cm^3.g^{-1})$	Pd (wt.%)	Cu (wt.%)	Si/Al
HZSM-5	396	101	0.21	0.12	-	-	23
Cu-Pd/HZSM-5	383	91	0.21	0.12	0.52	0.012	23
HBEA	654	221	0.85	0.18	-	-	25
Cu-Pd/HBEA	625	209	0.87	0.17	0.43	0.011	25

2.2 Data of hydroconversion process

Supplementary Table 7: Material balance (gas, liquid and coke) in wt.% of the total feed (DX and n-hexane mixture) obtained during the hydroconversion of 14.3%DX/n-hexane using Cu-Pd/HZSM-5 and Cu-Pd/HBEA. Cx- Product with x carbons. Px- are n-Paraffin with x carbons. Branched P_x are paraffins Isomers with x carbons. Nx- Naphthene with x carbons.

	Cu-Pd/HZSM-5		Cu-Pd/HBEA	
	n-hex	14.3%DX/n-hexane	n-hex	14.3%DX/n-hexane
Liquid (wt.%)				
P_{5-}	0.5	2.8	0.2	3.6
Branched P_6*	62.7	6.8	69.8	7.8
n-hexane	22.1	72.4	29.8	70.8
N_6**	0.2	0.7	0.2	0.9
Branched P_{7-8}	–	0.5	–	0.7
n-P_{7-8}	–	0.3	–	0.2
N_{7-8}	–	1.5	–	1.4
Branched P_{9+}	–	0.1	–	0.3
n-P_{9+}	–	0.2	–	0.1
N_{9+}	–	0.9	–	1.3
Aromatics C_{6-10}	–	0.4	–	0.8
Others	–	0.3	–	0.3
Total Liquid*	**85.6**	**86.8**	**88.6**	**88.3**
Gas** (wt.%)**				
CO + CO_2	–	1.6 (35.9%)	–	1.2 (27.8%)
C1-C3	1.8	1.1	1.3	0.8
Butanes*****	0.6	1.0	0.2	1.5
Pentanes******	0.4	0.6	0.1	0.9
Total Gas	**2.8**	**4.2**	**1.6**	**4.3**
Coke (wt.%)				
	< 0.1	0.5	< 0.1	0.6
Total	**88.4**	**91.2**	**90.2**	**92.8**

* Branched P_6 (2 and 3-methylpentane and 2,2-dimethylbutane).
** Including methyl-cyclopentane and cyclohexane.
*** Note that olefins were not produced. Also, P_{9+} and N_{9+} products reach carbon number up to 12 (only traces amounts). The aromatics products were produced mainly with 7 to 10 carbons.
**** In brackets: Distribution of gas products (%).
***** Including n-butane and i-butane.
****** Including 2-methylbutane and pentane.

Supplementary Table 8: Liquid products distribution (% of total liquid products) obtained during the hydroconversion of pristine n-hexane and 14.3%DX in n-hexane using Cu-Pd/HZSM-5 and Cu-Pd/HBEA. Cx- Product with x carbons. Px- Paraffin with x carbons. Nx- Naphthene with x carbons.

	Cu-Pd/HZSM-5		Cu-Pd/HBEA	
	n-hexane	14.3% DX/ n-hexane	n-hexane	14.3% DX/ n-hexane

Conversion (%)				
DX	–	100	–	100
n-hexane	78	16	79	18
Liquid products distribution (%)				
Propane	0.1	0.3	< 0.1	0.1
Butanes*	0.3	8.2	0.1	11.4
Pentanes**	0.3	11.0	0.2	9.1
Total C_5^-	0.7	19.5	0.3	20.6
Branched P_6***	98.8	47.5 (51.2)	99.3	44.8 (52.5)
N_6****	0.4	4.7	0.4	5.0
Branched P_{7-8}	< 0.1	3.7	–	1.1
n-P_{7-8}	< 0.1	2.0	–	4.1
N_{7-8}	–	10.2	–	8.0
Branched P_{9+}	–	0.4	–	1.5
n-P_{9+}	–	0.7	–	0.6
N_{9+}	–	6.5	–	7.7
Total C_{7+}	–	23.5	–	23.0
Aromatics C_{6-10}	–	2.6	–	4.6
Others	–	1.8	–	2.0

* Including n-butane and i-butane.
** Including 2-methylbutane and pentane.
*** In brackets: branched P_6 (2 and 3-methylpentane and 2,2-dimethylbutane) estimated supposing that n-hexane behaves equally when converted pure in the mixture with DX. Note that these values are higher for both tests.
**** Including methyl-cyclopentane and cyclohexane.

Supplementary Table 9: Liquid composition at different reaction times obtained from the hydroconversion of n-hexane at 250 ºC using Cu-Pd/HBEA.

       To assure that C_{7+} is exclusively produced from DX, n-hexane conversion was examined after different reaction times.

Compound	Liquid composition (wt%)			
	0h	3h	6h	24h
Isobutane	−	−	−	< 0.1
Butane	−	−	< 0.1	< 0.1
Butane, 2-methyl-	0.2	0.2	0.2	0.1
Pentane	−	−	< 0.1	< 0.1
Butane, 2,2-dimethyl-	−	0.4	2.0	8.9
Pentane, 2-methyl-	0.2	8.7	23.9	38.9
Pentane, 3-methyl-	0.4	5.6	14.3	21.8
n-hexane	98.8	84.8	59.2	30.0
Cyclopentane, methyl-	0.3	0.3	0.3	0.2
Pentane, 3,3-dimethyl	−	< 0.1	< 0.1	< 0.1

Supplementary Table 10 presents an estimative of the product distribution (wt. %) in an n-hexane and DX basis obtained from hydroconversion of 14.3%DX/n-hexane using Cu-Pd/HZSM-5 and Cu-Pd/HBEA considering a mass balance of 100%. This estimative was based on some assumptions: the products distribution from n-hexane is not affected by DX; n-hexane has no contribution on coke formation; water formation (taking into account oxygen balance for total deoxygenation of the feed); C_6 isomers are only formed from n-hexane; the remaining mass of converted n-hexane will be C_{5-} compounds; thus the contribution of n-hexane (when mixture with DX) to C_{5-} fraction is obtained correcting by n-hexane converted, the contribution of DX to C_{5-} fraction can be obtained by subtracting the amount of C_{5-} fraction from n-hexane; C_{7+} compounds are exclusively formed from DX. These assumptions were made to just measured values and also to the values where the material balance corrected to 100% (presented in brackets).

Supplementary Table 10. Product distribution (wt. %) in an n-hexane and DX basis obtained from hydroconversion of 14.3%DX/n-hexane using Cu-Pd/HZSM-5 and Cu-Pd/HBEA.

	Cu-Pd/HZSM-5		Cu-Pd/HBEA	
	n-hexane basis	DX basis	n-hexane basis	DX basis
Coke	–	1.2	–	1.6
$CO+CO_2$	–	10.7	–	8.3
H_2O	–	24.3	–	26.7
Isomers C_6	67.2	–	61.2	–
C_{5-}	32.8	20.1 (30.9)*	38.8	14.0 (21.7)*
C_{7+}	–	31.7 (48.8)*	–	32.7 (50.4)*
Aromatics		3.5 (5.4)*		6.6 (10.2)*
Others	–	8.5	–	10.0

*in brackets: product distribution (wt. %) considering only C and H fraction of DX (35% discount based on O fraction)

2.3 Composition of liquid products

Supplementary Figures S4 and S5 display chromatogram of liquid phase obtained at the end of reaction carried out with 15gDX/90g n-hexane and 15g in the presence of Cu-Pd/HZSM-5 and Cu-Pd/HBEA respectively. Almost all compounds were identified. In the case of products from BEA catalyst (figure S5) the structures of the main compounds are illustrated in the figure. Yet, for products from ZSM-5 catalysts (figure S4), only representative structures were illustrated in figure S4. The other hydrocabons with similar retention times generally are isomers of the structure illustrated.

It could be observed Cu-Pd/HBEA gave more heavier aromatics, consistent with the larger pore and higher hidrogen transfer capacity of beta versus ZSM-5 zeolite.
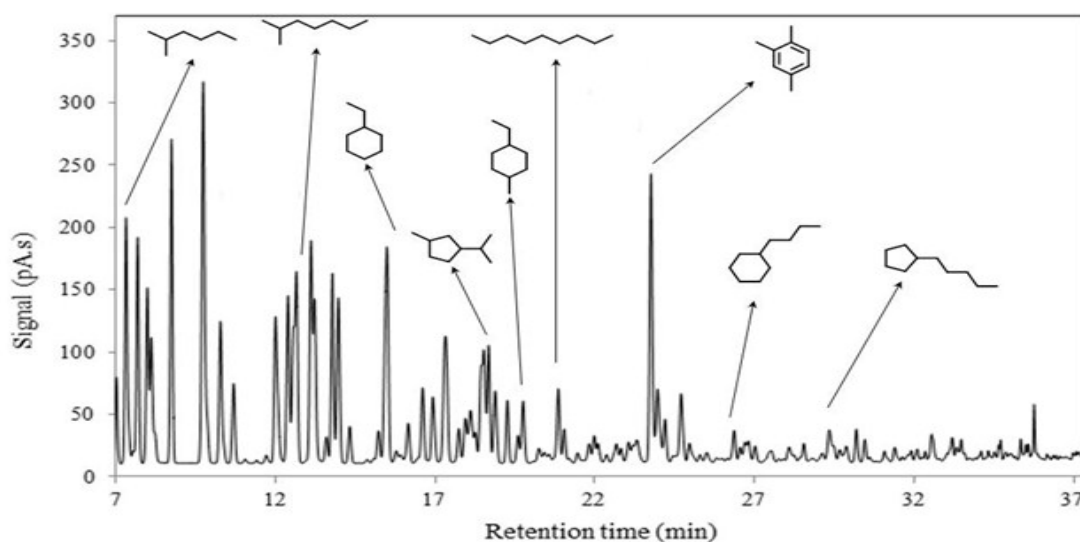
Supplementary Figure S4: Main products obtained from liquid phase produced by reaction carried out with 15gDX/90g n-hexane and 15g Cu-Pd/HZSM-5.
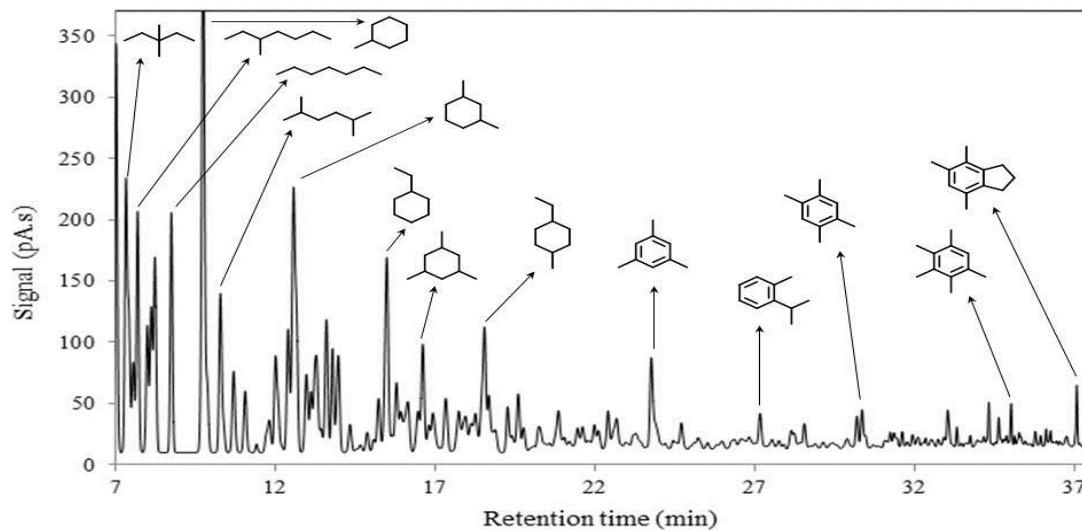
Supplementary Figure S5: Main products obtained from liquid phase produced by reaction carried out with 15gDX/90g n-hexane and 15g Cu-Pd/HBEA.

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3   Experimental

3.1 Catalyst preparation

For FCC, a commercial catalyst based on ZSM-5 was kindly provided by FCC.SA (Fabrica Carioca de Catalisadores).

For HDC process, zeolites (ZSM-5 with Si/Al ratio of 23 and BEA with Si/Al ratio of 23) used as support were kindly provided by Petrobras S.A. The acid form of the zeolites was obtained by ion exchange using a $(NH_4)_2SO_4$ 1M solution. Copper and palladium were introduced into the zeolite by incipient wetness impregnation using $Cu(NO_3)_2$ and $Pd(NO_3)_2.2H_2O$ as precursors. The amount of palladium precursor was estimated to obtain a 0.5 wt.% of Pd and copper precursor was estimated to obtain an atomic ratio of 1Cu:10Pd. The resulting catalysts were named Cu-Pd/HZSM-5 or Cu-Pd/HBEA.

3.2 Coke determination (thermogravimetric analysis)

For FCC and HDC process, the coke loading in the used catalysts was determined by thermogravimetric analysis in a Netzsch TG-IRIS apparatus.

Supplementary Figure S6 presents a thermogravimetric analysis example of Cu-Pd/HZSM-5 used for the hydroconversion of 14.3%DX/n-hexane. The used catalyst was heated from room temperature to 700 ºC according to the following profile of temperature: initially at 10 ºC.min^{-1} up to 250 ºC, plus 30 min at 250 ºC in nitrogen (for water determination) and a sequential heating until the final temperature in synthetic air for coke determination.

A1)

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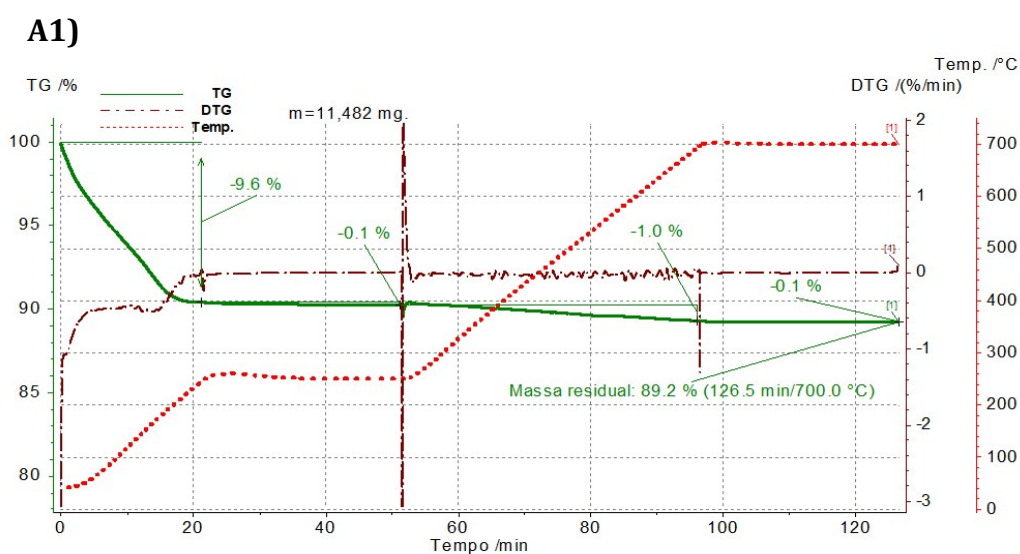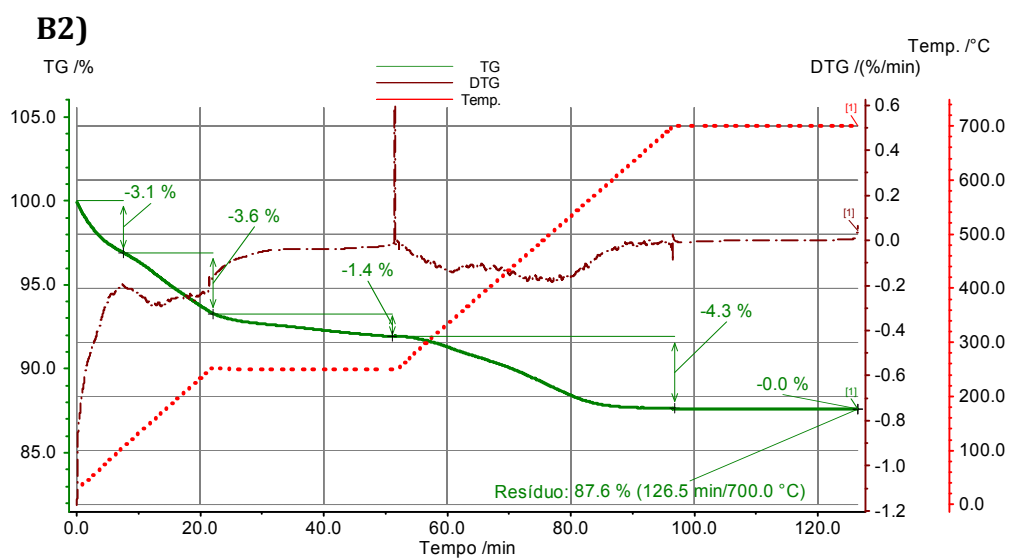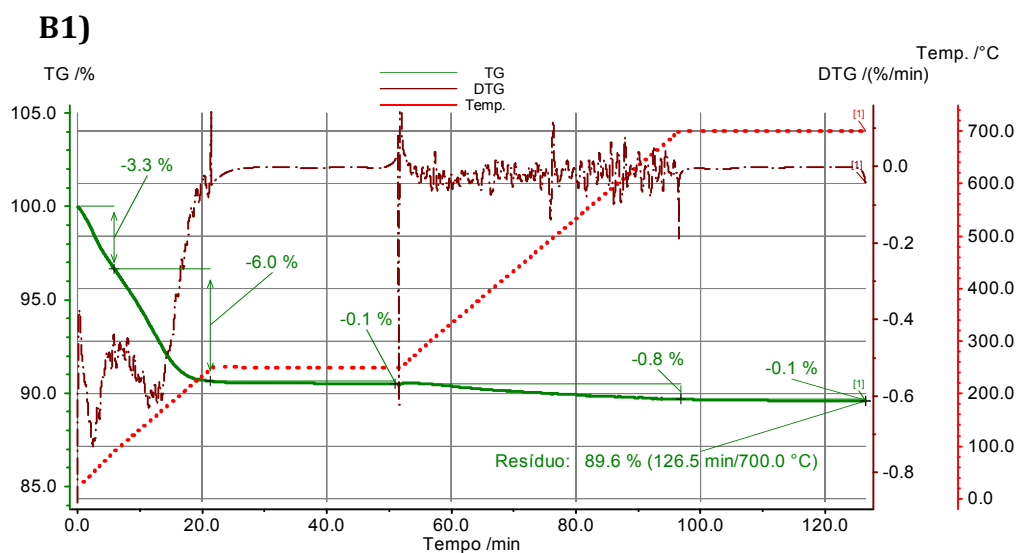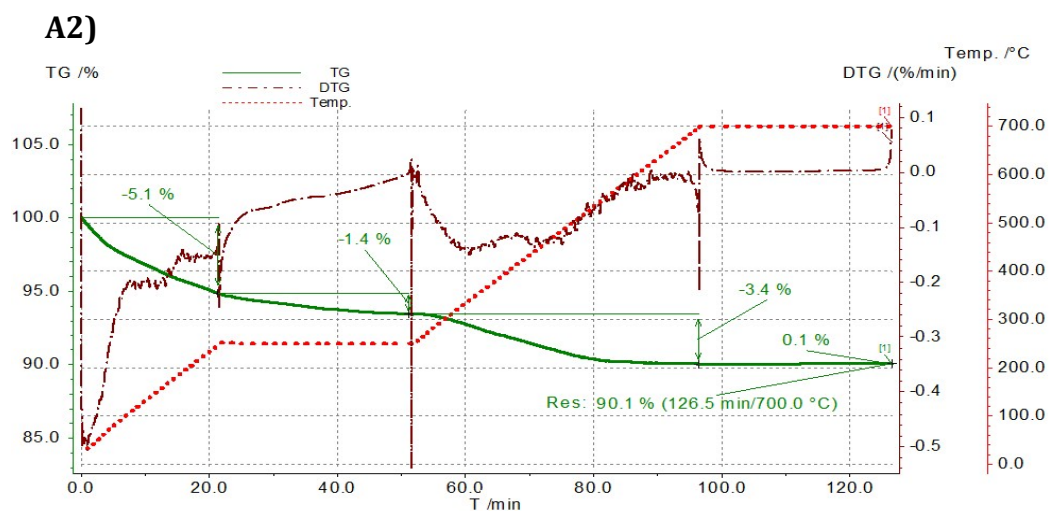
Supplementary Figure 6: Thermogravimetric analyses for **(A)** Cu-Pd/HZSM-5 and **(B)** Cu-Pd/HBEA used for the hydroconversion of **(1)** n-hexane and **(2)** 14.3%DX/n-hexane.

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3.3 Gas products analysis

For the FCC, the amount of gas produced during the reaction was determined by water displaced from an Erlenmeyer (it was filled with saturated salt water to prevent gas solubilization). The volume displaced during the reaction is subtracted to the one in a pure nitrogen flow (always quantified before reaction). The gas composition was determined in the end of the reaction by taking three samples of the gas (inside the Erlenmeyer), as presented in Supplementary Figure S8. Typical gas products were H_2, CO, CO_2, methane and light hydrocarbon (up to C_4).

The gas chromatography analysis was done in an Agilent Technologies MicroGC 490. The main compounds were calibrated through injection of gas mixtures such as 10%(mole/mole) methane in helium, 10%(mole/mole) ethane in helium, 10%(mole/mole) CO_2 in helium, 10%(mole/mole) butane in helium. Retention times (RT) and molar response factors (MRF) obtained from these compounds were used to determine the RTs and MRFs for other compounds. The gas fraction in wt.% was determined by dividing the weight of total gas products by the mass of feed (DX + n-hexane). Then, gas product distribution (%) and yield (wt.%) were obtained by using the following equations:

$$\text{Gas product } i \text{ distribution } (\%) = \frac{\text{Micro GC area of product } i}{\text{Micro GC area of total products}} \times 100 \quad (\text{equation. 1})$$

$$\text{Yield of product } \boldsymbol{i} \textbf{ (wt. \%)} = \frac{\text{Gas product } i (\%) \times \text{weight of gas fraction}}{\text{weight of total feed}} \times 100$$

(equation 2)

For HDC process, only a few complete gas analysis was made since it represents a minor part of the product. However, some compositions were determined as follows. At the end of the run, the pressure inside the reactor were used to obtain the total number of moles using the ideal gas law and. Gas molar composition (%) was determined using MicroGC (Agilent Technologies MicroGC 490) and using both the gas calibration of each one of the Micro GC channels and respective gas MRF. By discounting the contribution of H_2 (reactant), each gas molar composition was multiplied by the total number of moles and finally the respective weight (g) of each gas was determined using molar mass (g/mole).

Gas product distribution (%) was determined by dividing the amount of each gas (g) for the total amount of gas products (g). The gas fraction (wt.%) was determined by dividing the weight of total gas products (g) by the mass (g) of feed (DX + n-hexane).

3.4   Liquid products, compound identification and quantification

For FCC and HDC process, the liquid amount was determined by weighing, and the material balance was determined in wt. of liquid / wt.% of feed (DX + n-hexane).

The identification of liquid products was obtained based on the library (NIST) of the GCxMS. Also some model compounds were co-injected to certify the measurement (like n-hexane, cyclohexane, n-butyl-cyclohexane, benzene, xylene, toluene, DX etc.).

Products quantification was carried out in a GCxFID, and the products were identified by a direct comparison (using the retention time) between GCxMS and GCxFID. The products yield were determined in three steps:

- Firstly, the selectivity (in wt.% of liquid product) of each product was determined. The FID areas (%) of a compounds were converted to wt.% using a correction factor (fc) of 0.82 for aromatic, 1.00 for naphthenes and paraffins and 0.70 for DX. Products selectivity was determined by discounting the amount of n-hexane (consider as diluent) in the liquid. Then, all areas were normalized and the selectivity (wt.%) of each product was obtained by equation 3.

- Secondly, the amount of products in wt.% in the liquid was determined. Thus it was necessary to quantify n-hexane in the liquid fraction (as it is presented in high amount). The amount of products in mass (g) was obtained by subtracting the liquid mass by the n-hexane.

- Products yield (in wt% of the feed) was determined multiply the liquid mass by each product selectivity and divided by total feed, equation 4.

Liquid Product i (wt.%) $=$

$$\frac{\text{FIDarea of product } i \text{ x fc}}{\text{FIDarea of total liquid products}} \quad \text{(equation 3)}$$

Yield of Product i (wt. %) $=$

$$\frac{\text{Product } i \ (\%) \ \times \ \text{wt. of liquid fraction}}{\text{weight of total feed}} \text{x}100 \quad \text{(equation 4)}$$

For FCC liquid products, Figures 2b and 2c in the manuscript and are presented in wt.% of liquid products according to equation 5. Similarly, for a better understanding of HDC products (Figures 2d, 2e and 2f) all products (liquid and gas) were presented according to equation 6.

$$\text{Liquid product i (wt.\%)} = \frac{\text{Yield of liquid product } i}{\text{Yield of total liquid products}} \quad \text{(equation 5)}$$

$$\text{Product } i \ \text{(wt.\%)} = \frac{\text{Yield of product } i}{\text{Yield of total products}} \times \ 100 \quad \text{(equation 6)}$$
Total

3.5   GCxFID

The GCxFID analysis was performed on a gas chromatograph model 7890A GC System (Agilent Technologies Inc.) coupled to a flame ionization detector. The samples were injected by an automated liquid sampler model 7963A (Agilent Technologies Inc.). Injection chamber was maintained at 250 °C under a total flow of hydrogen equivalent to 55.3 mL/min. It was used a J&W DB1 capillary column (30 m x 250 µm x 0.25 µm ; 100% dimethylpolysiloxane) under a constant flow of hydrogen equal to 0.8mL/min. The oven program consisted of **1)** 30 °C for 0 min; **2)** 3 °C/min to 120 °C; 120 °C for 0 min; **3)** 10 °C/min to 250 °C; 250 °C for 0 min. FID was maintained at 300 °C under a hydrogen flow equal to 30 mL/min, air flow equal to 400 mL/min and make-up gas (nitrogen) flow equal to 25 mL/min. The volume of sample injected and split ratio have different values depending on the aim of analysis. For the n-hexane quantitation analysis the volume of sample injected was equal to 0.1µL associated to a split ratio equal to 200:1. For the determination of selectivity the volume of sample injected was equal to 1µL associated to a split ratio equal to 30:1.

3.6 GCxMS

The GCxMS analysis was performed on a gas chromatograph model 7890A GC System (Agilent Technologies Inc.) coupled to a mass spectrometer detector model 5975C GC/MSD containing a quadrupole and a triple axis detector (Agilent Technologies Inc.). The samples were injected by an automated liquid sampler model 7963A (Agilent Technologies Inc.). Injection chamber was maintained at 290 °C under a total flow of helium equivalent to 3 mL/min. The volume of sample injected was equal to 1µL with a split ratio equal to 200:1.

 It was used a Agilent J&W DB1-ms capillary column (30 m x 250 µm x 0.25 µm; 100% dimethylpolysiloxane) under a constant flow of helium equal to 3mL/min. The oven program consisted of **1)** 30 °C for 0 min; **2)** 3 °C/min to 120 °C; 120 °C for 0 min; **3)** 10 °C/min to 250 °C; 250 °C for 0 min.

MS detector operated on electron impact ionization mode at energy equal to 70 eV. MS source was maintained at 230 °C while quadrupole was maintained at 150 °C. The MSD operated on total ion monitoring set up with a mass range comprised of 45 to 400 Da. The identification of compounds was based on association of retention time and information provided by mass spectrum of a single peak compared with NIST library mass spectra database.

3.7   **N-hexane quantitative analysis**

All the reactions were carried out using n-hexane as a carrier liquid of DX. So, by discounting the n-hexane amount on the residual liquid phase obtained from the FCC and HDC of DX+n-hexane it is possible to determine the selectivity and yield of reaction products.

The n-hexane amount was measured through calibration with an internal standard by a gas chromatograph coupled to a flame ionization detector (GC-FID). Calibration solutions containing 25, 50, 75 and 100 µL of n-hexane and 975, 950, 925 and 900 µL of acetone were prepared. Finally, 100 µL of n-hexadecane was added as an internal standard to each previously prepared standard solution. Each compound (n-hexane, acetone and n-hexadecane) and product samples were weighted to obtain the percentage weight of each substance on its respective solutions.

A calibration graph was constructed with ordinate axis values of the ratio of areas of n-hexane and n-hexadecane multiplied by weight percentage of n-hexadecane (RA_{C6} x wt.%$_{C16}$/RA_{C16}) and abscissas the percentage weight of n-hexane (wt.%$_{C6}$) (Supplementary Fig. S7). The calibration curve ($y = 1.0986x - 0.1915$; $R^2 = 0.9998$) was generated by linear regression of points shown on Supplementary Fig. S7.
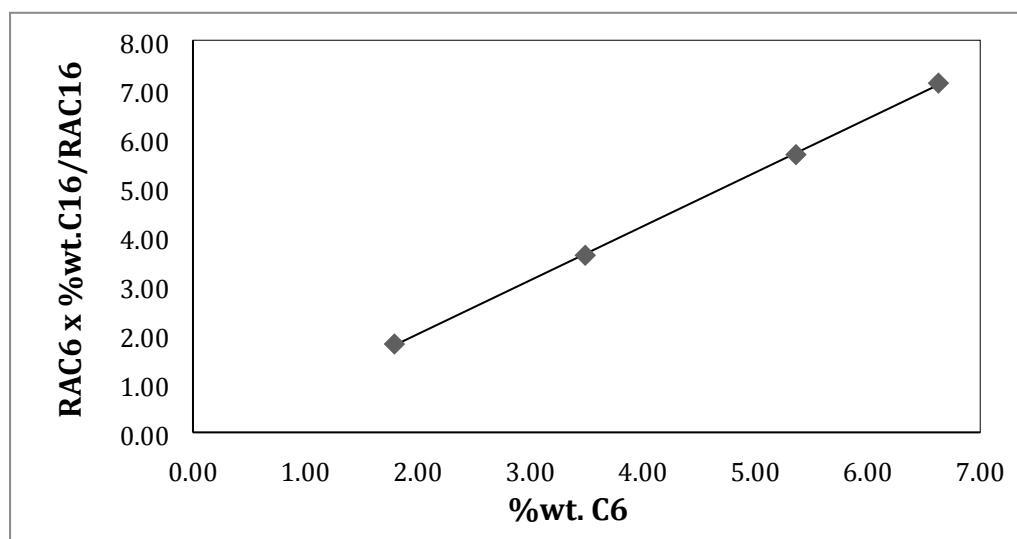
Supplementary Figure 7: Calibration curve used to determine the n-hexane percentage weight on different samples.

Thus, the conversion of n-hexane, the yield (wt.%$_{RP}$) and mass (m$_{RP}$) of reaction products on liquid phase were calculated as described in equations 7, 8 and 9, respectively.

Conversion (%)

$$= \frac{\text{initial weight of n - hexane } - \text{ final weight of } n-hexane}{\text{initial weight of } n-hexane} \times 100 \text{ (eq. 7)}$$
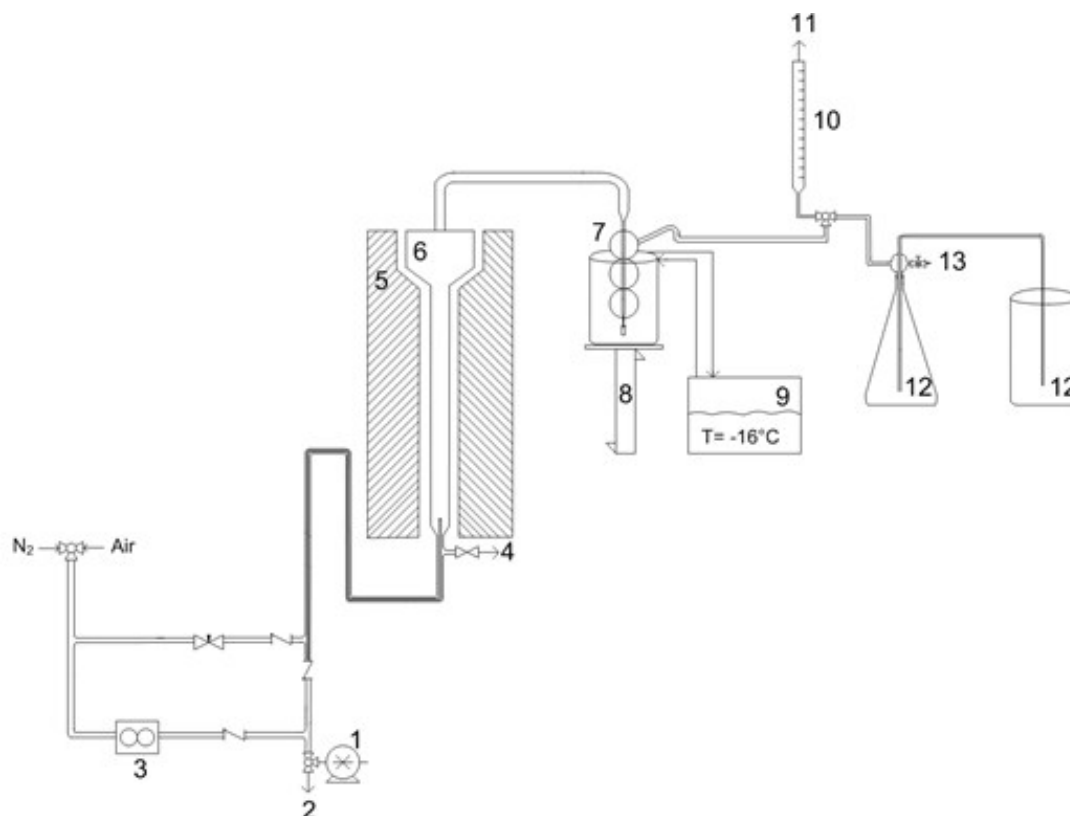
$$wt.\% \, rp = 100 - \%wt.C6 \qquad (equation\ 8)$$
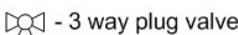
$$m_{RP} = \frac{wt.\%_{RP}}{100} x\, M_{RP} \qquad (equation\ 9)$$

where,

M$_{RP}$ = mass of liquid phase obtained at the end of reaction

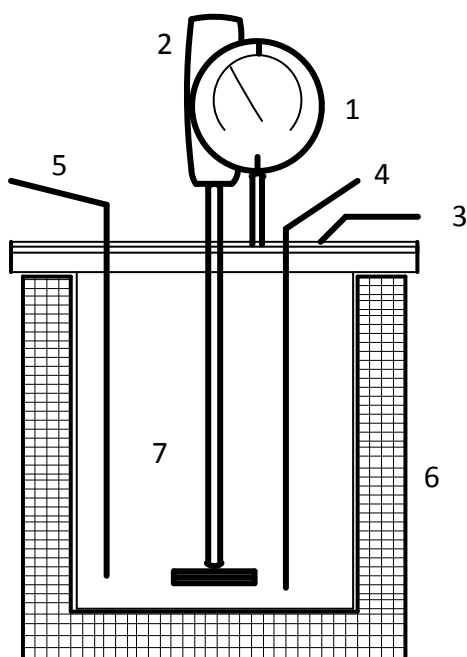## 4   Experimental apparatus for both FCC and hydroconversion.

Supplementary Figure 8. FCC hardware, reactor diameter 1.88 cm.
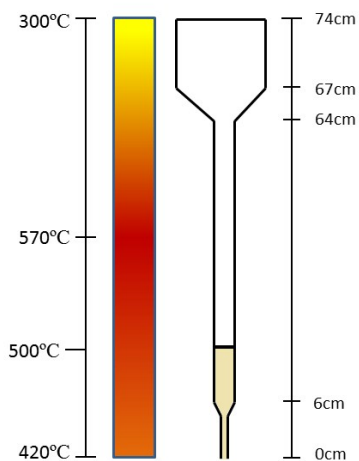
Supplementary Figure 9. Temperature profile of the reactor.

Supplementary Figure 10: Batch reactor used in hydroconversion. Legend: 1-manometer; 2-magnetic stirrer drive; 3-reactor gases outlet; 4-thermocouple; 5-reactor gases inlet; 6- oven; 7-Reactor.