# Supplementary Materials

# Conversion of sugar di-ketals to bio-hydrocarbons through the catalytic cracking over Beta catalysts in fixed and fluidized catalytic beds

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## SUMÁRIO

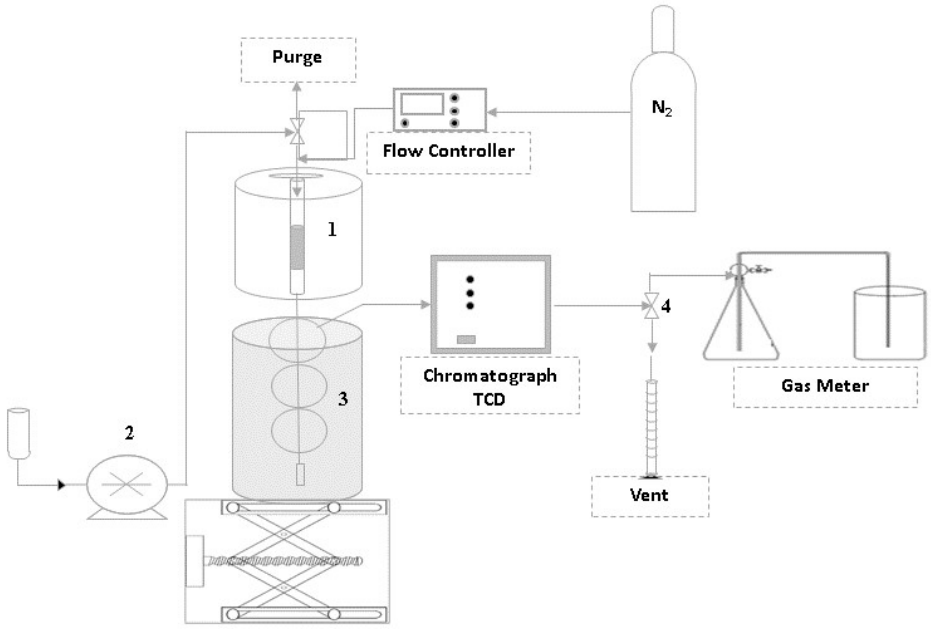
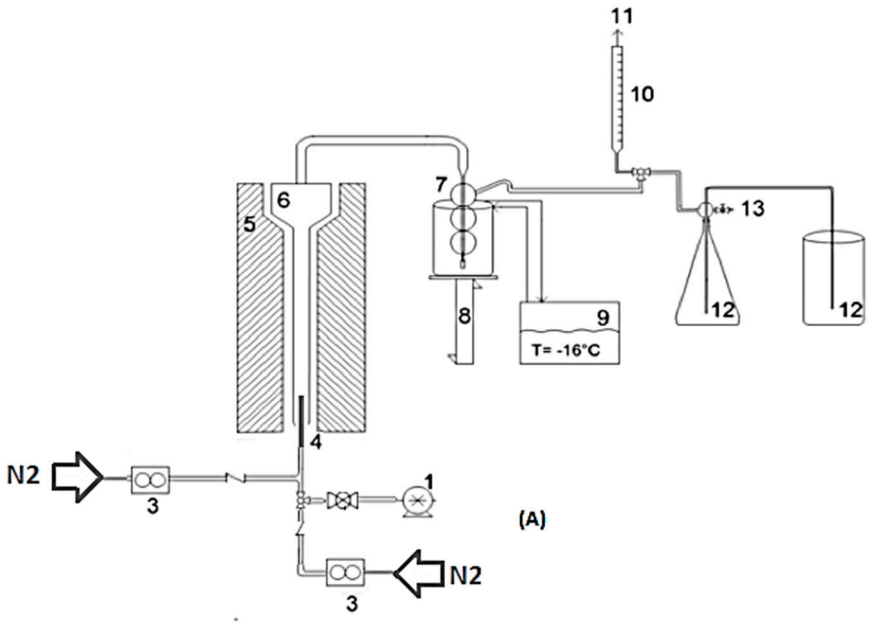



**Figure S1.** Schematic of the Fixed Bed Unit used in the DX/n-hexane experiments




Legend: 1 e 2 - syringe pump; 3 – Flowmeter; 4 - Injection tube; 5- Oven; 6 – Reactor; 7 – Condenser; 8 – Elevator; 9 – Chiller; 10 – Gas meter; 11 – Vent; 12 - Liquid entrainment gas meter; 13 - Gas recovery valve

**Figure S2.** Schematic of the Fluid Catalytic Cracking (FCC) Unit used in the DX/n-hexane experiments

**Table S1.** Table of identifie compounds of the general composition of Bio-petroleum (BP) from LC-HRMS analysis on positive ESI mode; Normalized intensity (a.u.) area [1].

| Compounds of BP | | m/z[a] |
|---|---|---|
| Hexose acetals | Glucose monoacetal | 238.12817 |
| | Glucose diacetal | 278.15945 |
| | Diehexose triacetal | 480.24353 |
| | Pentose-hexose triacetal | 450.23322 |
| | Dipentose-hexose tetracetal | 622.30731 |
| Lignin derivatives | Feruloylquimic acid | 367.10364 |
| | p-Coumaroylquimic acid | 337.09329 |
| | p-Coumaric acid | 163.03923 |
| Pentose acetals | Xylose monoacetal | 208.11780 |
| | Xylose diacetal | 248.14908 |
| | Dipentose monoacetal | 340.15982 |
| | Dipentose diacetal | 380.19119 |
| | Dipentose triacetal | 420.22232 |
| | Tripentose triacetal | 552.26532 |
| | Tripentose tetracetal | 592.29645 |
| | Tetrapentose pentacetal | 764.37000 |
| Pentoses-acids acetals | Pentose-glucuronic acid monocetal | 384.14957 |
| | Pentose-ferulic acid monoacetal | 384.16483 |
| | Dipentose-ferulic acid diacetal | 539.21210 |
| | Dipentose-p-coumaric acid diacetal | 509.20230 |
| | Pentose-p-coumaric acid monoacetal | 335.11395 |
| Pentose-acetate acetals | Pentose monoacetal acetate | 250.12827 |
| | Dipentose monoacetal acetate | 382.17032 |
| | Dipentose diacetal acetate | 422.20169 |
| | Tripentose triacetal acetate | 594.27643 |

[a] Legend: m/z- Mass/charge

**Table S2**.Chromatographic factors employed for % mass of product of interest

| Compound types | Factor | Observations |
|---|---|---|
| Mono aromatics | 0.82 | Major product |
| Acetone | 0.28 | Major product |
| Other liquid oxygenates | 0.17 | Furans, phenols, products of aldo condensations, |
| Remaining products (RP) | 1.00 | Olefins, paraffins, poly-aromatics, unidentified Hidrocarbon |

**Table S3.** Gas yields obtained by catalytic cracking with 30% percentage change of DX/n-hexane in HBEA [a] and DHBEA [a].

| | Gas (%wt) | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | $H_2$ | $CH_4$ | $C_2H_4$ | $C_2H_6$ | $C_3H_8$ | $C_3H_6$ | $C_4H_{10}$ | $C_4H_8$ | CO | $CO_2$ | Total |
| **DHBEA** | 0.1 | 2.1 | 0.2 | 0.0 | 0.0 | 0.1 | 0.0 | 0.0 | 2.9 | 0.6 | **6.0** |
| **HBEA** | 0.2 | 2.3 | 0.4 | 0.1 | 0.2 | 0.7 | 0.3 | 0.3 | 6.1 | 2.1 | **12.8** |

[a] 500 mg of zeolite - WHSV ($16h^{-1}$) and reaction temperature of 500°C.

**Table S4.** Possibility of oxygenated compounds produced from DX/n-hexane reactions in the catalytic cracking of the Beta zeolite with steam treatment at 720°C (DHBEA)

| Content de DX- 30% | |
|---|---|
| **Oxygenates** | **Normalized Area (%)** |
| 2,3-dimethylfuran | 0.0250 |
| 2-Butanone | 0.0088 |
| 2-Cyclopenten-1-one | 0.0475 |
| 2-Cyclopenten-1-one, 2-methyl- | 0.0404 |
| 2-Cyclopenten-1-one, 3,4-dimethyl | 0.0098 |
| 3-Penten-2-one | 0.0093 |
| Benzofuran, 4,7-dimethyl- | 0.0070 |
| Bicyclo[3.3.0]oct-2-en-8-one, 3-methyl- | 0.0082 |
| Furan, 2,3,5-trimethyl- | 0.1289 |
| Methyl vinyl ketone | 0.0343 |
| 1H-Inden-1-one, 2,3,4,5,6,7-hexahydro | 0.0065 |
| 1-Methoxy-3-methyl-3-butene | 0.0069 |
| 1-Methoxyadamantane | 0.0126 |
| 2-(2-Hydroxyphenyl)buta-1,3-diene | 0.0039 |
| 2,4-Dimethylfuran | 0.0021 |
| 2-Cyclopenten-1-one, 2,3-dimethyl- | 0.0467 |
| 2-Cyclopenten-1-one, 3-methyl- | 0.0600 |
| 2-n-Butyl furan | 0.0196 |
| 2-n-Heptylcyclopentanone | 0.0314 |
| 2-Vinylfuran | 0.0042 |
| 4,5,6,7-Tetrahydro-3-methylbenzofuran | 0.0305 |

| | |
|---|---|
| 4,5-Dimethyl-3-heptanol | 0.0046 |
| 5-Methylene-1,3a,4,5,6,6a-hexahydropentalen-1-ol | 0.0070 |
| Acetone | 2.4195 |
| Benzofuran | 0.0054 |
| Benzofuran, 2-methyl- | 0.0123 |
| Cyclodecanone | 0.0283 |
| Cyclopentanone, 3,4-bis(methylene)- | 0.0056 |
| Furan | 0.0215 |
| Furan, 2,5-dimethyl- | 0.0698 |
| Furan, 2-ethyl- | 0.0059 |
| Furan, 2-ethyl-5-methyl- | 0.0283 |
| Furan, 2-methyl- | 0.0512 |
| Oxepine, 2,7-dimethyl- | 0.0041 |
| Phenol | 0.0519 |
| Phenol, 2-methyl- | 0.0069 |
| Phenol, 3-methyl- | 0.0512 |
| Propanal, 2-methyl- | 0.0045 |
| $\alpha$-D-Xylofuranose, 1,2:3,5-bis-O-(1-methylethylidene)- | 0.0389 |

**Table S5.** Possibility of oxygenated compounds produced from DX/n-hexane reactions in the catalytic cracking of the Beta catalyst with steam treatment at 720°C (DAD)

| **Content de DX- 30%** | |
|---|---|
| **Oxygenates** | **Normalized Area (%)** |
| Acetone | 0.0001228 |
| 1,2-Butanediol, 1-phenyl- | 0.0000899 |
| 1,3-Cyclobutanediol, 2,2,4,4-tetramethyl- | 0.0001018 |
| 1-Methoxy-1,3-cyclohexadiene | 0.0000343 |
| 2,3-Dimethylfuran | 0.0001448 |
| 2,4-Dimethylfuran | 0.0003798 |
| 2-Cyclohexen-1-one | 0.0000271 |
| 2-Cyclopenten-1-one, 2,3-dimethyl- | 0.0000375 |
| 2-Cyclopenten-1-one, 3-methyl- | 0.0000796 |
| 2-Propenal, 2-methyl-3-phenyl- | 0.0000526 |
| 3-Furaldehyde | 0.0001194 |

| | |
|---|---|
| 3-Methyl-1-dodecyn-3-ol | 0.0000513 |
| 3-Pentanone | 0.0000049 |
| Benzofuran | 0.0000410 |
| Benzofuran, 2-methyl- | 0.0001799 |
| Benzofuran, 7-methyl- | 0.0000282 |
| Benzyl methyl ketone | 0.0000090 |
| Cyclohexanol, 2-methylene-6-methyl- | 0.0004571 |
| Cyclopentanone | 0.0000149 |
| Dibenzofuran, 4-methyl- | 0.0000024 |
| Ethanone, 1-(2-furanyl)- | 0.0002463 |
| Furan, 2-(2-propenyl)- | 0.0000236 |
| Furan, 2,5-dimethyl- | 0.0004160 |
| Furan, 2-ethyl- | 0.0001420 |
| Phenol | 0.0001285 |
| Phenol, 2,3-dimethyl- | 0.0000091 |
| Phenol, 2,4-dimethyl- | 0.0000265 |
| Phenol, 2,5-dimethyl- | 0.0000176 |
| Phenol, 2-methyl- | 0.0000424 |
| Phenol, 3-(2-phenylethenyl)-, (E)- | 0.0000062 |
| Phenol, 3,4-dimethyl- | 0.0000084 |
| Phenol, 3-methyl- | 0.0000524 |
| Phenol, 4-(2-phenylethenyl)- | 0.0000094 |
| Tetramethylfuran | 0.0000298 |

**Table S6.** Yields to gas by percentage of DX obtained by catalytic cracking of n-hexane in FB and FCC, 30%DX/ n-hexane in the Beta catalyst hydrothermally treated at 720°C, 500 mg of zeolite at 500°C.

| | | Gas (%wt) | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **DX (30%)** | **Unit** | **$H_2$** | **$CH_4$** | **$C_2H_4$** | **$C_2H_6$** | **$C_3H_8$** | **$C_3H_6$** | **$C_4H_{10}$** | **$C_4H_8$** | **CO** | **$CO_2$** | **Total** |
| **DAD** | **FB** | 0.0 | 1.2 | 0.0 | 0.0 | 0.0 | 0.1 | 0.0 | 0.0 | 2.6 | 0.1 | 4.0 |
| | **FCC** | 1.1 | 3.4 | 0.2 | 0.1 | 0.0 | 0.4 | 0.0 | 0.1 | 3.1 | 1.6 | 10.0 |