Hydrotreating of guaiacol and acetic acid blends over Ni_2P/ZSM-5 catalyst: elucidating molecular interactions during bio-oil upgrading

S. Gutierrez-Rubio[a], I. Moreno[a,b*], D.P. Serrano[a,b], J.M. Coronado[a*+]

[a] *Thermochemical Processes Unit. IMDEA Energy Institute, Avda. Ramón de la Sagra 3, Móstoles, Madrid, Spain*

[b]*Chemical and Environmental Engineering Group, ESCET, Universidad Rey Juan Carlos, c/ Tulipán s/n, Móstoles, Madrid, Spain*

[+] Present address: Instituto de Catálisis y Petroleoquímica, CSIC, c/ Marie Curie, 2, Cantoblanco, Madrid, E28049. Spain.

Table S1. Chromatographic response factors in the relevant concentration range of the main chemicals identified during the hydrotreating of guaiacol and acetic acid blends.

Chemical	**Response factor**
Guayacol	9.28
Acetic Acid	27.81
Cyclohexane	6.44
Methyl Acetate	19.07
Ethyl Acetate	15.48
Anisole	8.95
Guaiacol Acetate	12.67
Phenol	7.94
Ethyl Guaiacol	7.32
Ethyl Cyclohexane	7.29
Ethanol	16.48
Acetone	14.84
Catechol Acetate	14.03
Diacetoxybenzene	15.81
Catechol	10.66
Ethyl Catechol	10.43
Apocynin	11.47
Others	11.47
2 Ethyl Phenol	7.32

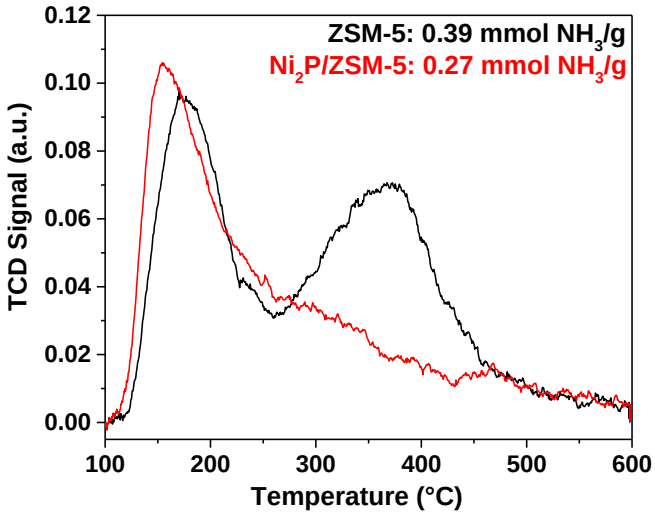

Figure S1. NH_3-TPD profiles of the raw ZSM-5 zeolite and the Ni_2P/ZSM-5 catalyst.

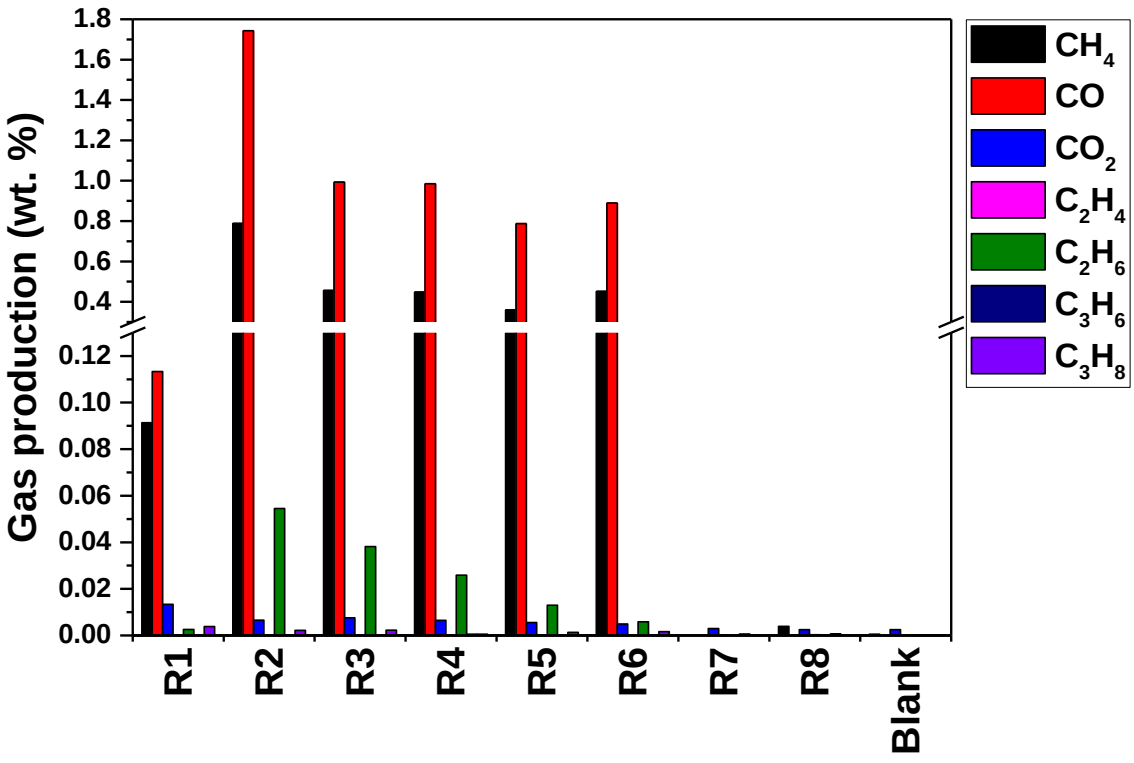

Figure S2. Gas production in catalytic reactions performed in this work. See Table 1 for reference of the of the tests conditions.

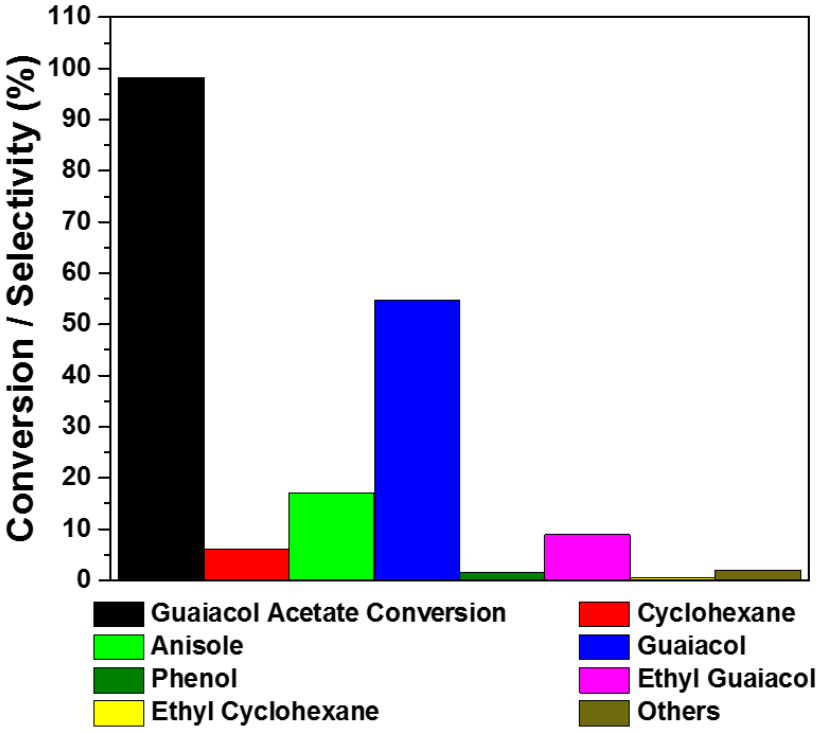

Figure S3. Conversion and products selectivity in catalytic HDO reaction of guaiacol acetate (R11) at 260 ºC and 40 bar H_2.

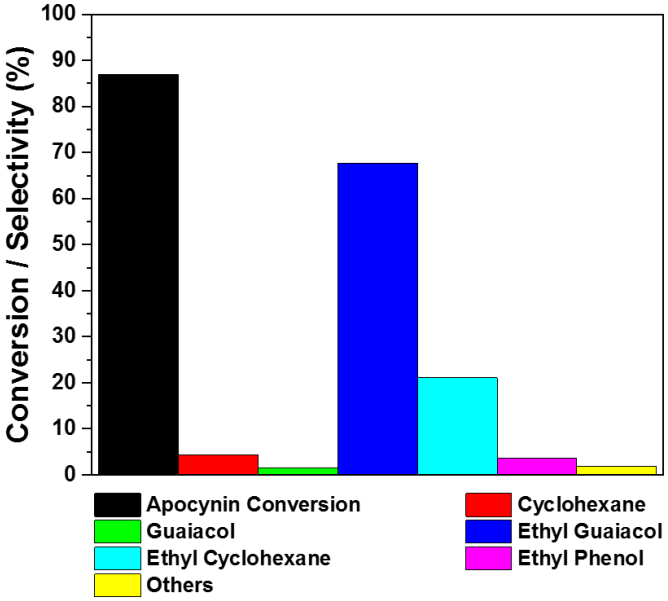

Figure S4. Conversion and products selectivity in catalytic HDO reaction of apocynin (R12) at 260 ºC and 40 bar H_2.

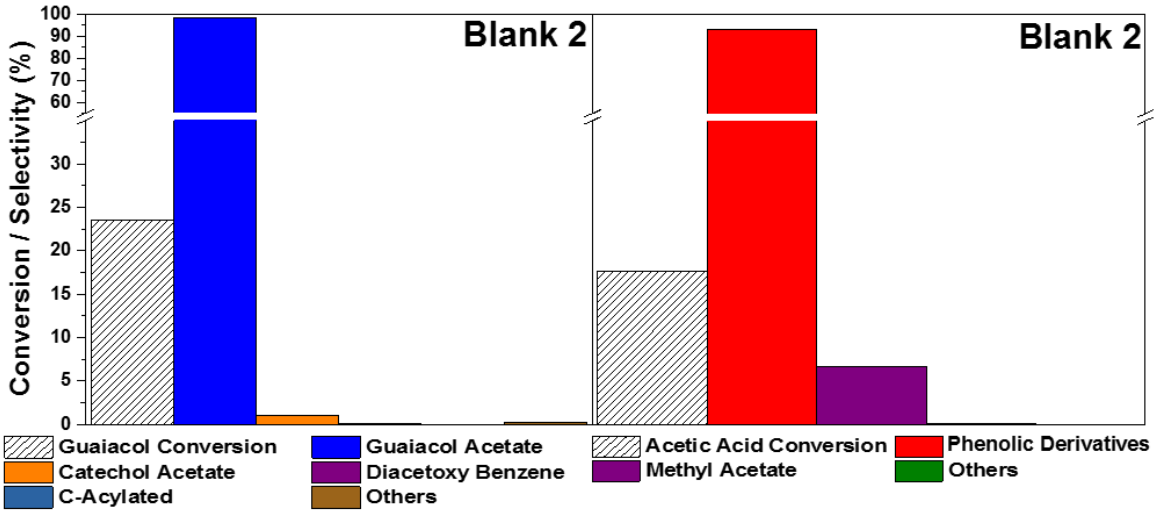

Figure S5. Conversion and products selectivity respect to guaiacol (Left) and acetic acid (Right) obtained in blank catalytic reaction of the blend at 260 ºC and hydrogen atmosphere (10 bar H_2) (Blank 2).