

Supplementary Information:

Influence of synthesis methodology on the properties and catalytic performance of tin, niobium, and tin-niobium oxides in fructose conversion

Thatiane Veríssimo dos Santos Martins, Dhara Beatriz de Amorim Pryston, Simoni Margareti Plentz Meneghetti* and Mario Roberto Meneghetti*

Group of Catalysis and Chemical Reactivity, Institute of Chemistry and Biotechnology, Federal University of Alagoas, Av. Lourival Melo Mota, Tabuleiro do Martins, Maceió 57072-970, Brazil

* Correspondence: : simoni.plentz@gmail.com (S.M.P.M.); mrm@qui.ufal.br (M.R.M.)

Fructose conversion, yield and selectivity of each product formed

Fructose conversion was calculated by the ratio between the difference in the initial fructose concentration minus the concentration of the final fructose and the initial concentration, according to Equation (S1), in which C(%) = fructose conversion; C₀ = initial concentration of fructose (mol/L); C_f = final concentration of fructose (mol/L).

$$C (\%) = \left(\frac{C_0 - C_f}{C_0} \right) \times 100 \quad (S1)$$

The yield of each soluble product obtained and duly identified was calculated according to Equation (S2), in which R_i (%) = Yield of product i; C_i = concentration obtained from product i (mol/L); C₀ = initial fructose concentration.

$$R_i (\%) = \left(\frac{C_i}{C_0} \right) \times 100 \quad (S2)$$

The selectivity of each product was calculated according to Equation (S3), in which S_i (%) = Selectivity of product i; C_i = concentration of product i; C_{i1}, C_{i2}, C_{i3}, C_{i4}, C_{i5} = concentration of other products (mol/L).

$$S_i (\%) = \left(\frac{C_i}{C_{i1} + C_{i2} + C_{i3} + C_{i4} + C_{i5}} \right) \quad (S3)$$

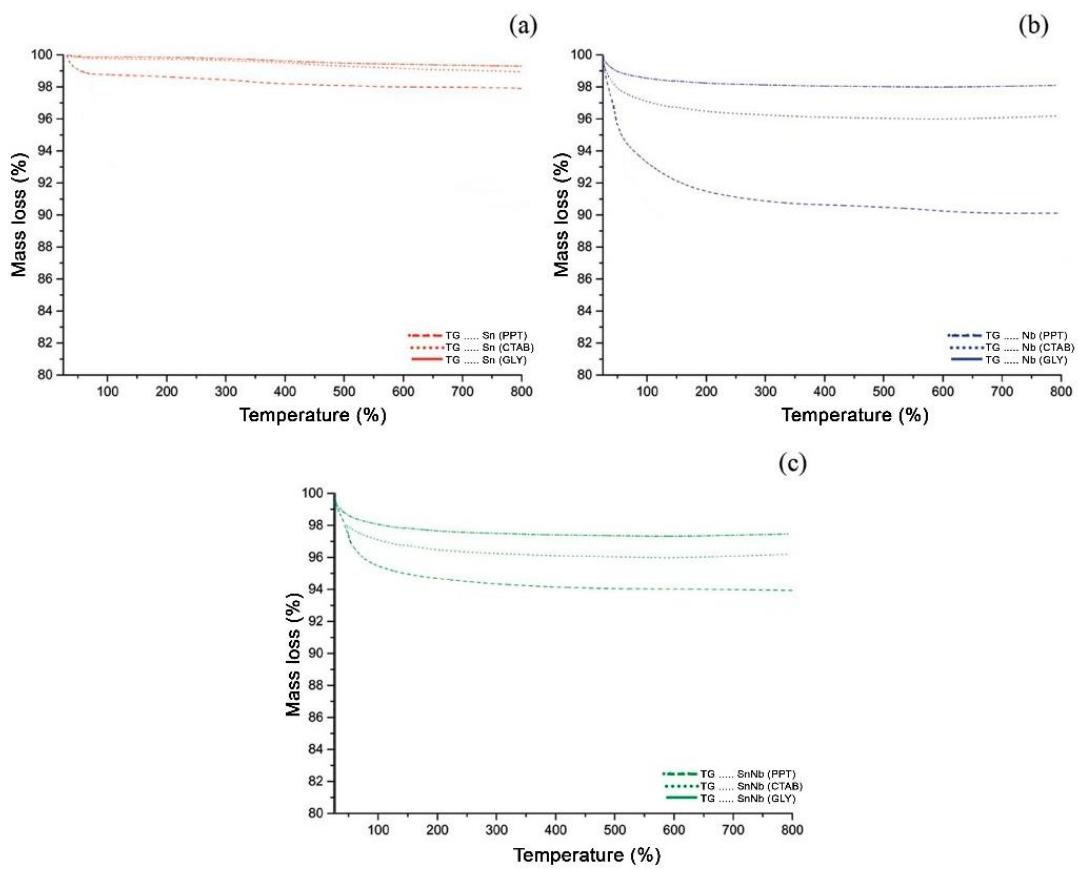


Figure S1. Thermal profiles (TG) of the catalysts: (a) Sn(PPT), Sn(CTAB) and Sn(GLY); (b) Nb(PPT), Nb(CTAB) and Nb(GLY) and (c) SnNb(PPT), SnNb(CTAB) and SnNb(GLY).

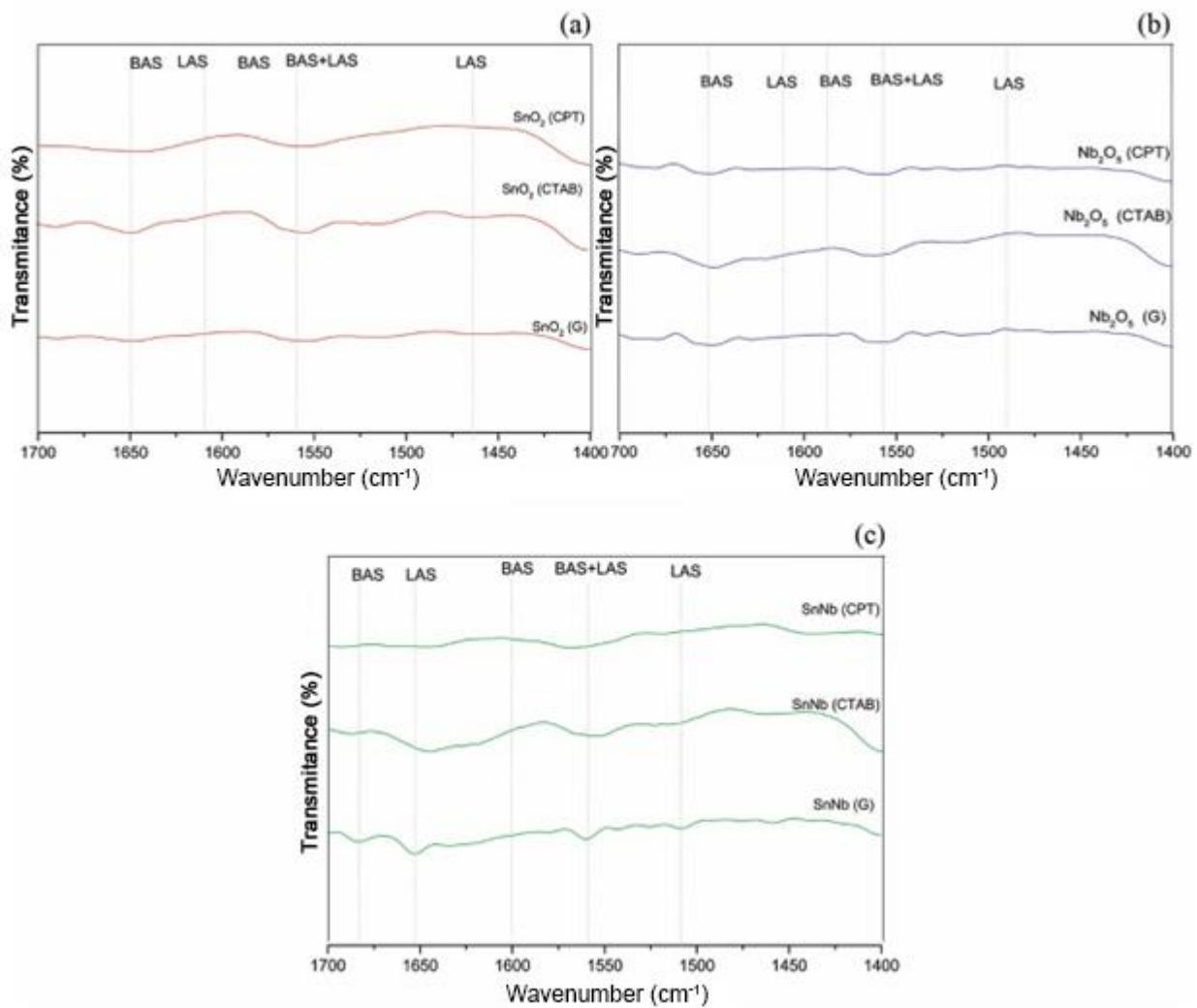
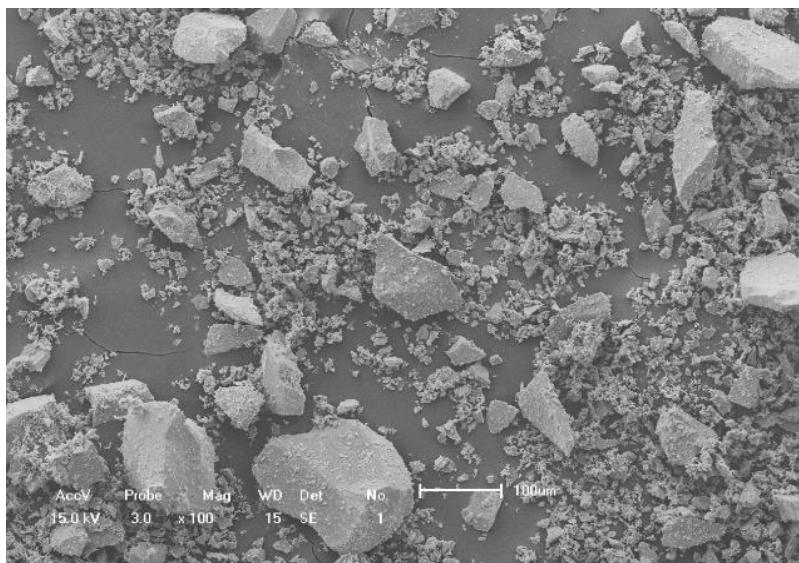
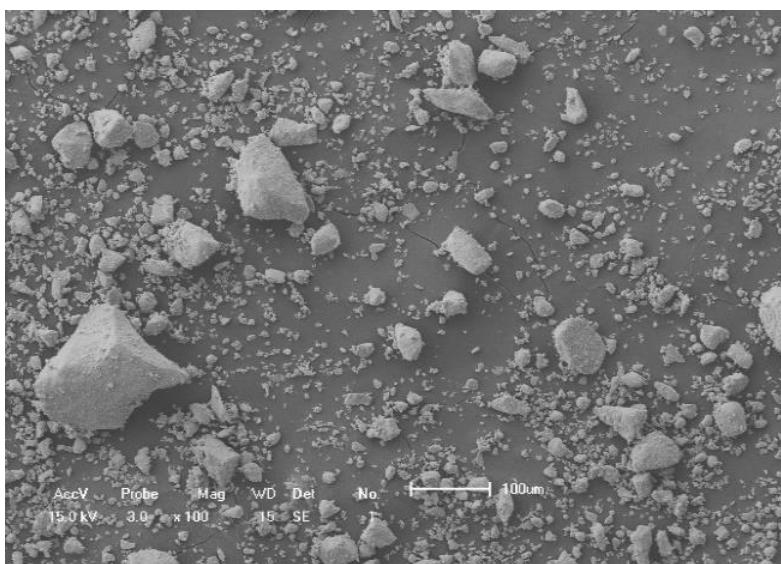


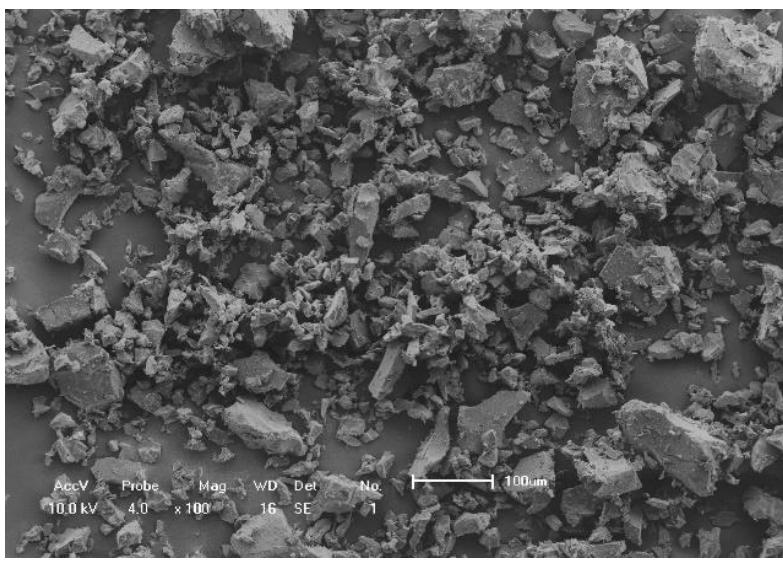
Figure S2. FTIR spectra using pyridine as probe molecule: (a) Sn(PPT), Sn(CTAB) and Sn(GLY); (b) Nb(PPT), Nb(CTAB) and Nb(GLY) and (c) SnNb(PPT), SnNb(CTAB) and SnNb(GLY).



Sn(PPT)

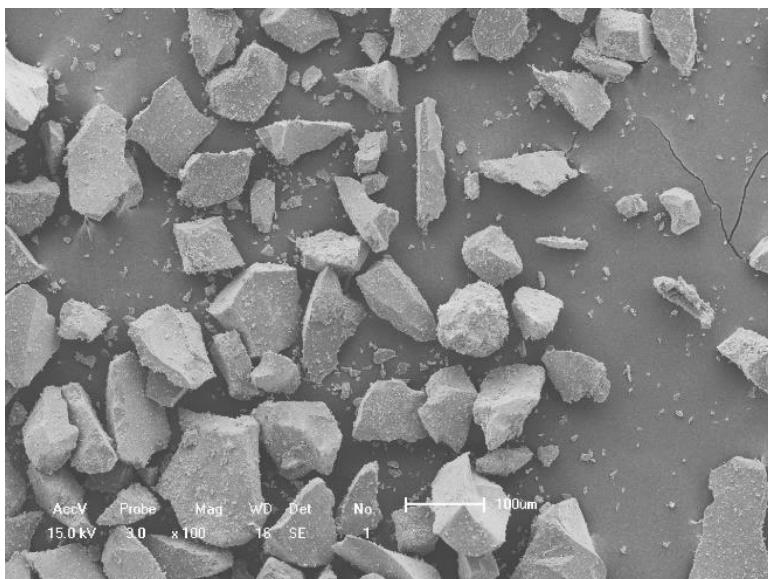


Sn(CTAB)

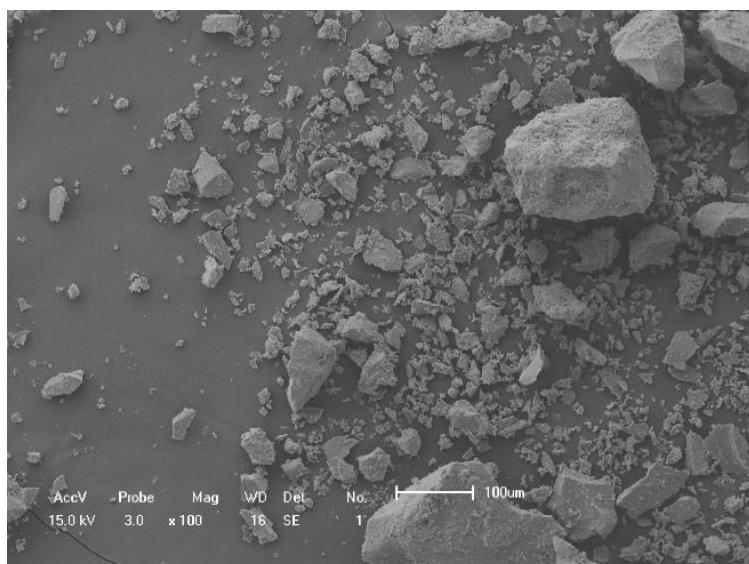


Sn(GLY)

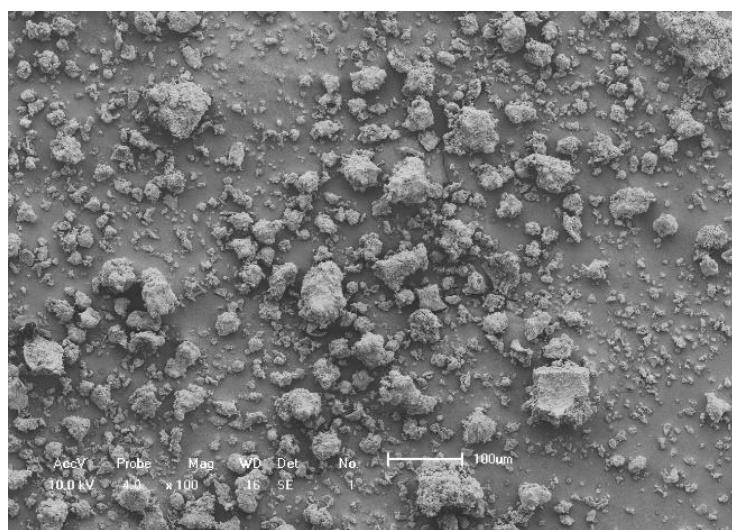
Figure S3. Scanning electron microscopy (SEM) images of the catalysts Sn(PPT), Sn(CTAB) and Sn(GLY).



Nb(PPT)

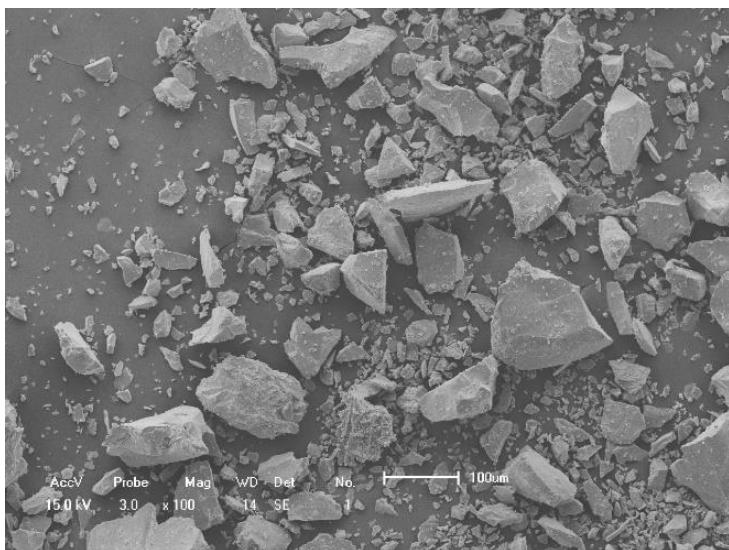


Nb(CTAB)

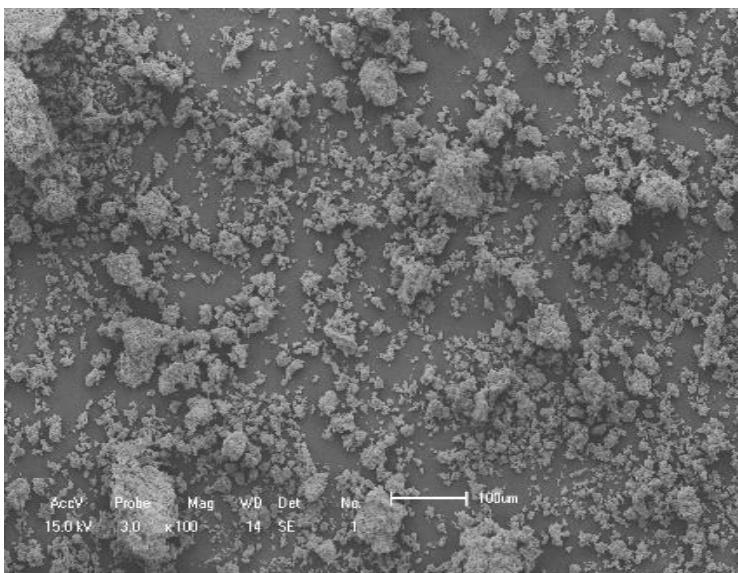


Nb(GLY)

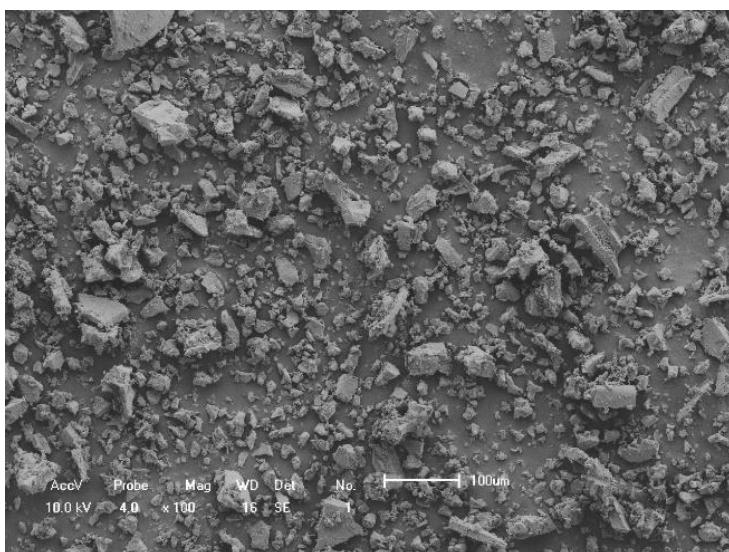
Figure S4. Scanning electron microscopy (SEM) images of the catalysts Nb(PPT), Nb(CTAB) and Nb(GLY).



SnNb(PPT)



SnNb(CTAB)



SnNb(GLY)

Figure S5. Scanning electron microscopy (SEM) images of the catalysts SnNb(PPT), SnNb(CTAB) and SnNb(GLY).

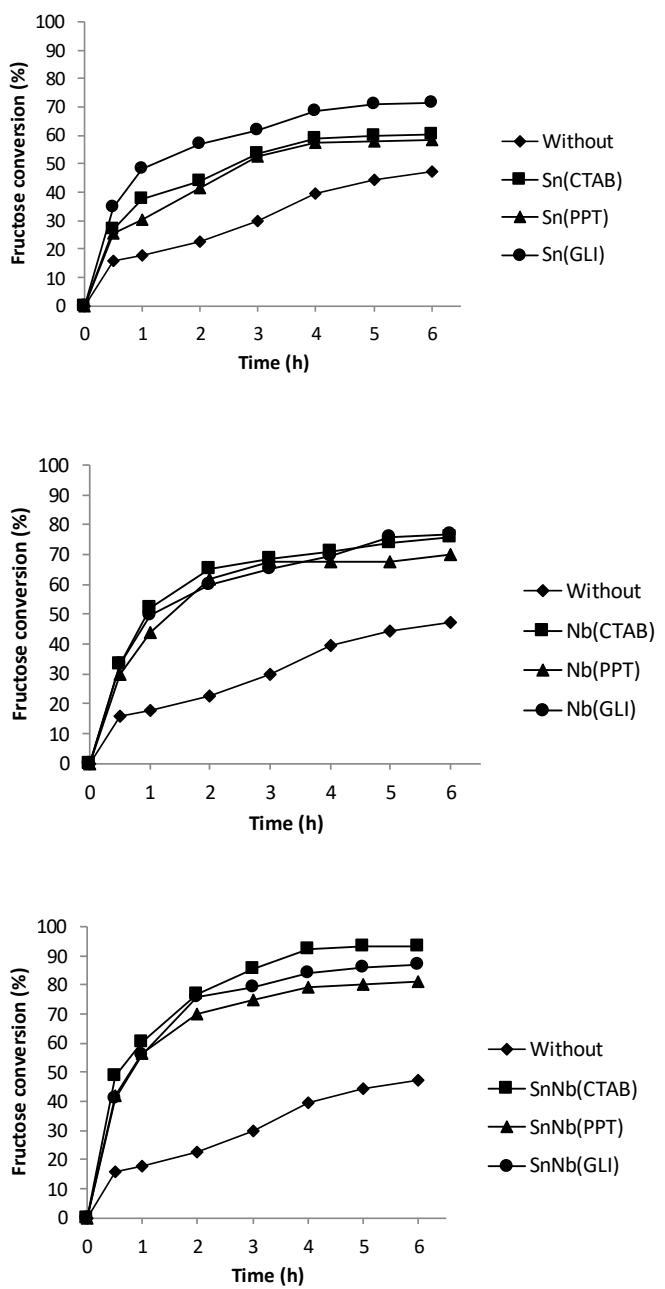


Figure S6. Fructose conversion at 150 °C using (a) Sn(PPT), Sn(CTAB) and Sn(GLY), (b) Nb(PPT), Nb(CTAB) and Nb(GLY) and (c) Nb(GLY) SnNb(PPT) SnNb(CTAB) and SnNb(GLY).

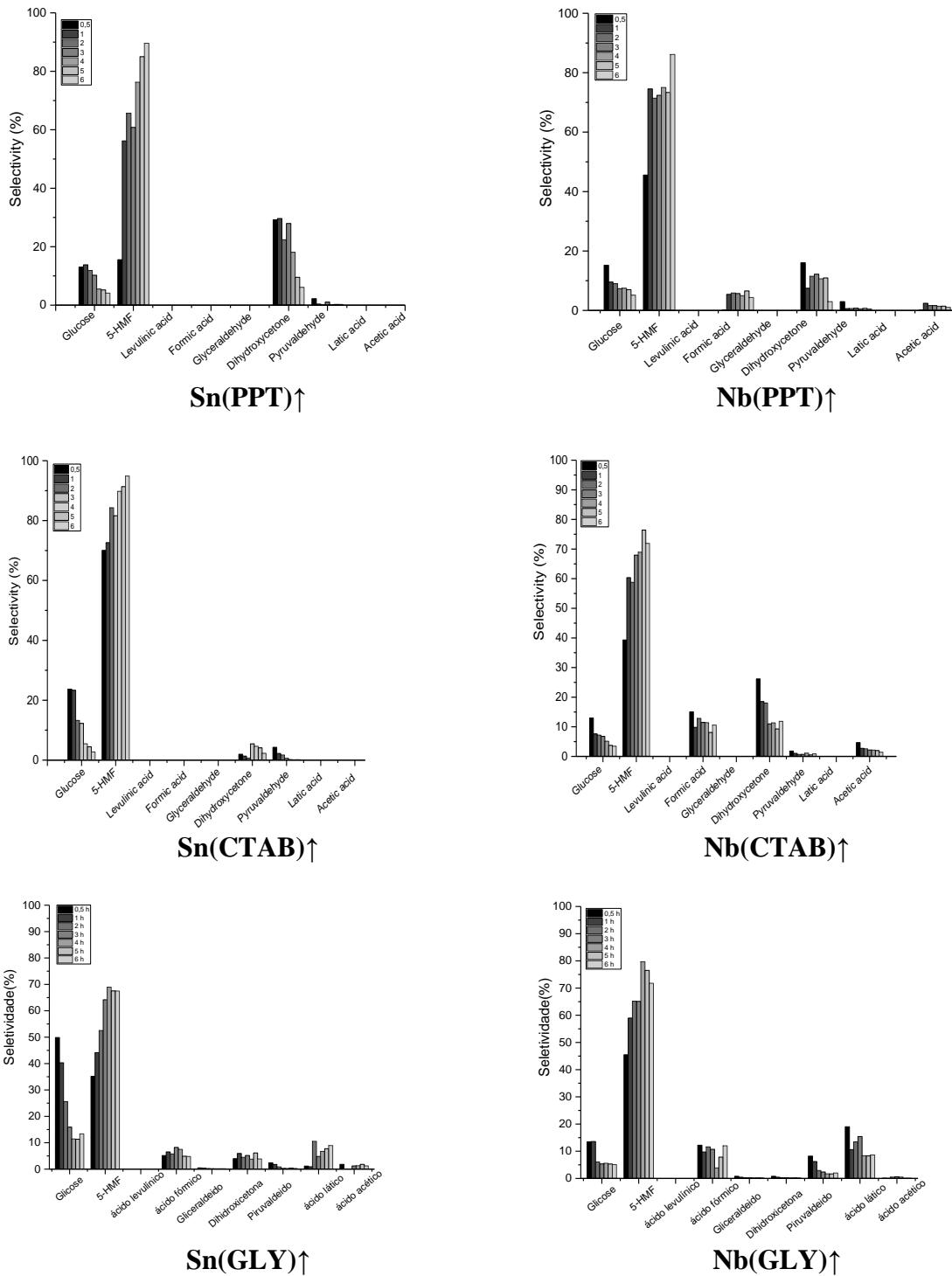


Figure S7. Selectivity for soluble products identified in the fructose conversion at 150 °C using 1.5×10^{-3} g of catalyst (a) Sn(PPT) and Nb(PPT); (b) Sn(CTAB) and Nb(CTAB); (c) Sn(GLY) and Nb(GLY).

Table S1: Yield (%) for soluble products identified in the fructose conversion at 150 °C in absence of catalyst or using 1.5 x 10⁻³ g of catalyst (a) Sn(PPT) and Nb(PPT); (b) Sn(CTAB) and Nb(CTAB); (c) Sn(GLY) and Nb(GLY).

Catalyst	Time (h)	Glucose	5-HMF	Levulinic acid	Formic acid	Glyceraldehyde	Dihydroxycetone	Pyruvaldehyde	Lactic acid	Acetic acid
Without	0.5	0.3	0.4	0	0	0	0	0	0	0
	1	0.2	1.0	0	0	0	0.3	0.1	0	0
	2	0.3	2.3	0	0	0	0.5	0.1	0	0
	3	0.5	3.5	0	0	0	0.6	0.1	0	0
	4	0.5	5.5	0	0	0	0.9	0	0	0
	5	0.5	6.6	0	0	0	0.7	0	0	0
	6	0.4	12.0	0	0	0	0.7	0.1	0	0
Sn(PPT)	0.5	0.2	0.2	0	0	0	1.1	0.03	0	0
	1	0.3	1.2	0	0	0	0.6	0.01	0	0
	2	0.5	2.6	0	0	0	0.9	0.01	0	0
	3	0.6	3.4	0	0	0	1.5	0.06	0	0
	4	0.4	5.7	0	0	0	1.3	0.01	0	0
	5	0.4	6.3	0	0	0	0.7	0.02	0	0
	6	0.6	12.2	0	0	0	1.1	0.03	0	0
Nb(PPT)	0.5	0.6	1.7	0	0	0	1.4	0.11	0	0
	1	0.5	4.2	0	0.31	0	0.4	0.03	0	0.1
	2	0.7	5.3	0	0.44	0	0.9	0.05	0	0.1
	3	0.6	6.0	0	0.47	0	1.0	0.06	0	0.1
	4	0.7	7.2	0	0.48	0	1.0	0.05	0	0.1
	5	0.7	7.4	0	0.66	0	1.1	0.07	0	0.1
	6	0.7	11.0	0	0.55	0	0.4	0.06	0	0.1
SnNb(PPT)	0.5	0.3	0.5	0	0	0.02	0.5	0.02	0.01	0
	1	0.3	1.8	0	0.4	0.02	0.6	0.07	0.02	0
	2	0.3	3.6	0	1.2	0.02	0.8	0.06	0.02	0.1
	3	0.4	4.4	0	1.8	0.02	0.9	0.06	0.02	0.1
	4	0.4	6.5	0	1.1	0.02	1.1	0.08	0.01	0.1
	5	0.4	7.8	0	2.0	0.02	0.7	0.04	0.02	0.1
	6	0.45	12.6	0	2.2	0.02	1.1	0.05	0.01	0.1
Sn(CTAB)	0.5	0.2	0.2	0	0	0.02	0	0.03	0	0
	1	0.3	0.5	0	0	0.02	0	0.02	0	0
	2	0.3	1.6	0	0	0.02	0	0.04	0	0
	3	0.4	2.5	0	0	0.02	0.2	0.02	0	0
	4	0.4	6.5	0	0	0.02	0.3	0.01	0	0
	5	0.4	9.1	0	0	0.02	0.4	0.01	0	0
	6	0.4	12.1	0	0	0.02	0.4	0.02	0	0
Nb(CTAB)	0.5	0.6	1.9	0	0.7	0	1.2	0.09	0	0.2
	1	0.6	4.9	0	0.8	0	1.5	0.08	0	0.2
	2	0.6	5.1	0	1.1	0	1.6	0.06	0	0.2
	3	0.7	7.0	0	1.2	0	1.1	0.07	0	0.2
	4	0.5	7.2	0	1.2	0	0.9	0.11	0	0.2
	5	0.4	8.5	0	0.9	0	1.0	0.06	0	0.1
	6	0.5	11.2	0	1.6	0	1.8	0.12	0	0.2
SnNb(CTAB)	0.5	0.4	3.2	0	0	0	0.3	0.02	0.02	0
	1	0.5	4.9	0	0.3	0	0.2	0.04	0.06	0
	2	0.7	6.2	0	0.7	0	0.5	0.05	0.11	0
	3	1	7	0	0.8	0	0.6	0.04	0.08	0
	4	0.9	8.8	0	0.8	0	0.2	0.07	0.09	0
	5	0.9	10.1	0	0.8	0	0.6	0.04	0.13	0
	6	0.7	14.4	0	1.9	0	1.3	0.05	0.14	0
Sn(GLY)	0.5	2.3	1.6	0	0.2	0	0.2	0.1	0.1	0.1
	1	2.5	2.7	0	0.4	0	0.4	0.1	0.1	0
	2	2.3	4.7	0	0.5	0	0.4	0.1	1.0	0
	3	2.1	8.3	0	1.1	0	0.7	0	0.6	0.2
	4	1.8	10.8	0	1.2	0	0.6	0	1.0	0.2
	5	1.9	11.0	0	0.8	0	1.0	0.1	1.3	0.3
	6	2.2	11.1	0	0.8	0	0.6	0	1.5	0.2
Nb(GLY)	0.5	0.4	1.3	0	0.4	0	0	0.2	0.5	0
	1	0.7	3.0	0	0.5	0	0	0.3	0.5	0
	2	0.7	7.6	0	1.4	0	0	0.3	1.6	0.1
	3	0.6	7.0	0	1.2	0	0	0.3	1.7	0.1
	4	0.7	10.1	0	0.5	0	0	0.2	1.1	0.1
	5	0.7	9.5	0	1.0	0	0	0.2	1.0	0
	6	0.9	12.1	0	2.0	0	0	0.3	1.4	0.1
SnNb(GLY)	0.5	0.7	2.4	0	0.1	0	0.2	0.1	0.5	0
	1	0.9	4.9	0	0.7	0	0.5	0.1	1.0	0
	2	0.9	7.9	0	0.4	0	1.5	0.1	1.8	0
	3	1	11.2	0	0.3	0	1.2	0.1	1.4	0
	4	1	11.1	0	0.6	0	0.5	0.1	1.2	0
	5	1.2	12.3	0	1.9	0	1.4	0.1	1.9	0
	6	0.8	13.8	0	1.2	0	0.9	0.1	1.8	0