

Supplementary Materials for:

Article

Crude Glycerol Hydrogenolysis to Bio-Propylene Glycol: Effect of Its Impurities on Activity, Selectivity and Stability

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Supplementary Material S1

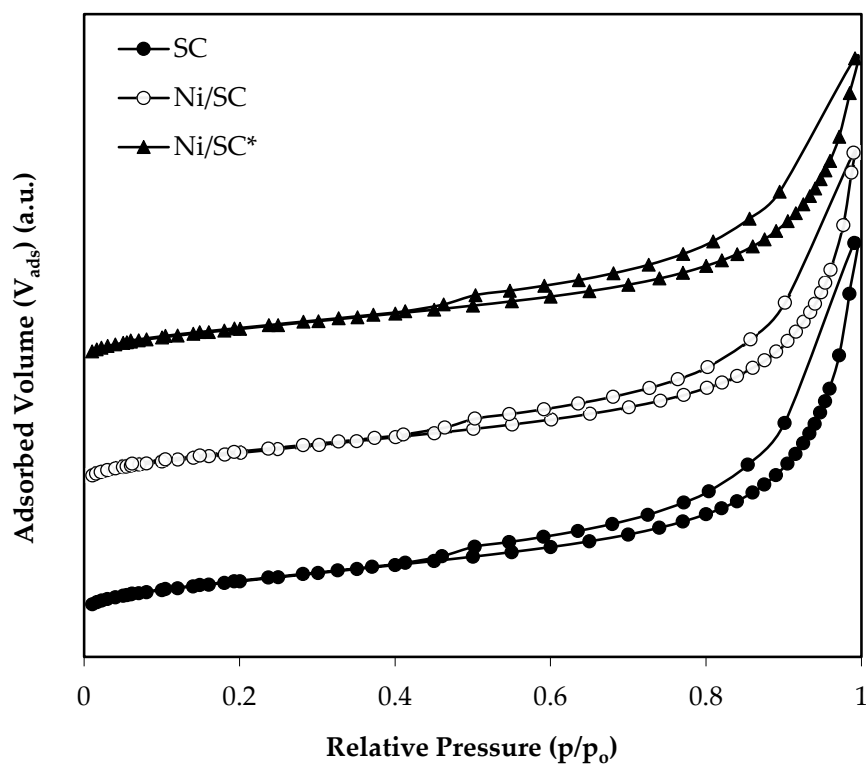


Figure S1. N₂ adsorption-desorption isotherms of SC (●), Ni/SC (○) and Ni/SC* (▲).

Supplementary Material S2

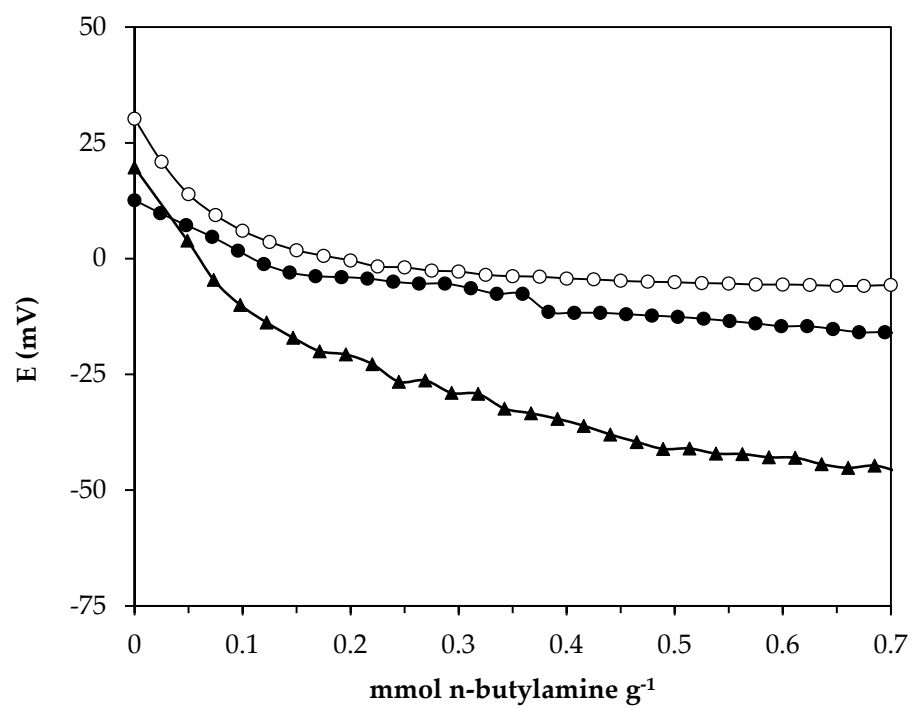


Figure S2. Potentiometric titration curves with n-butylamine in acetonitrile of SC (●), Ni/SC (○) and Ni/SC* (▲).

Supplementary Material S3

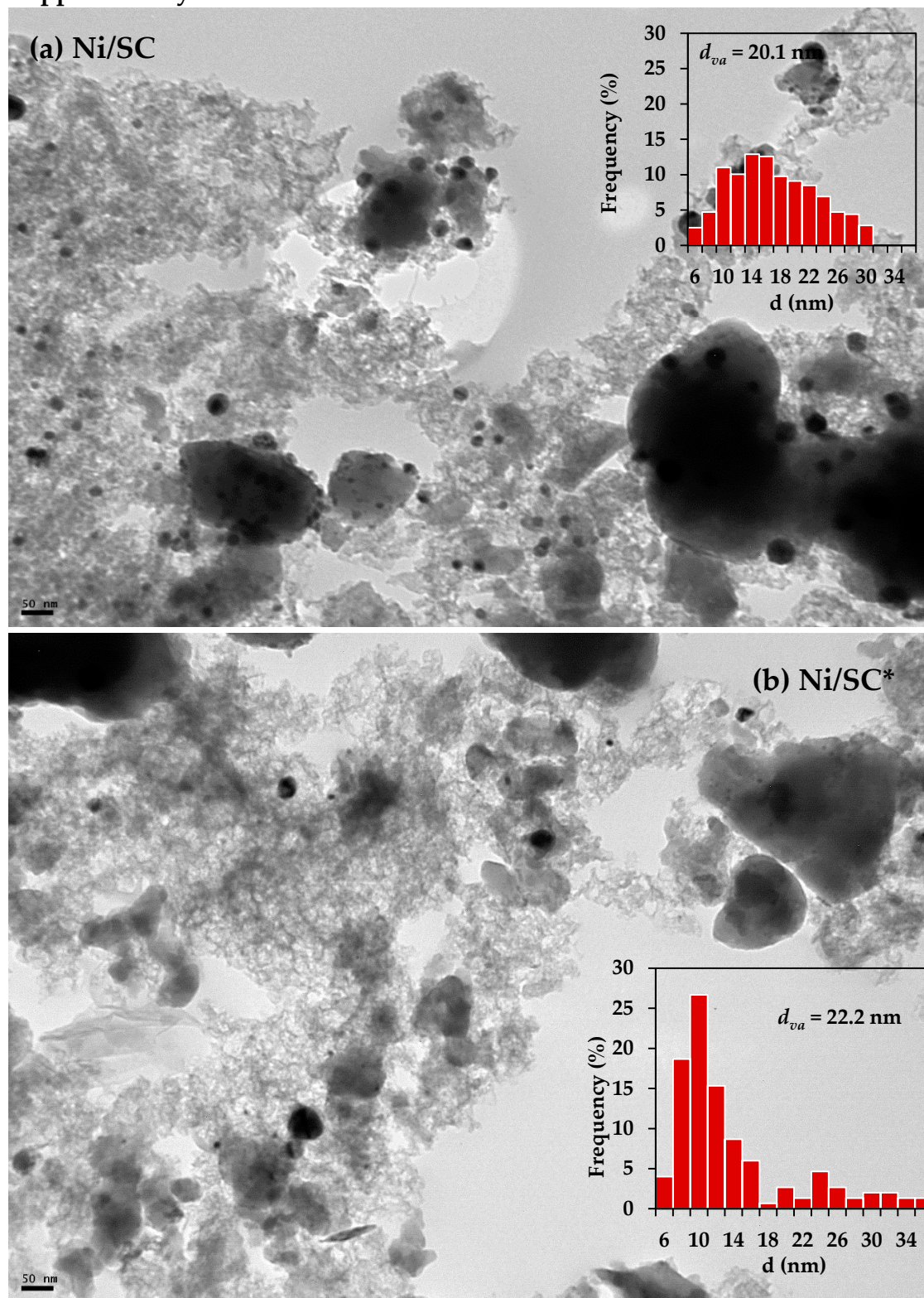


Figure S3. TEM micrographs for the reduced catalysts (a) fresh Ni/SC (b) used Ni/SC*

Supplementary Material S4

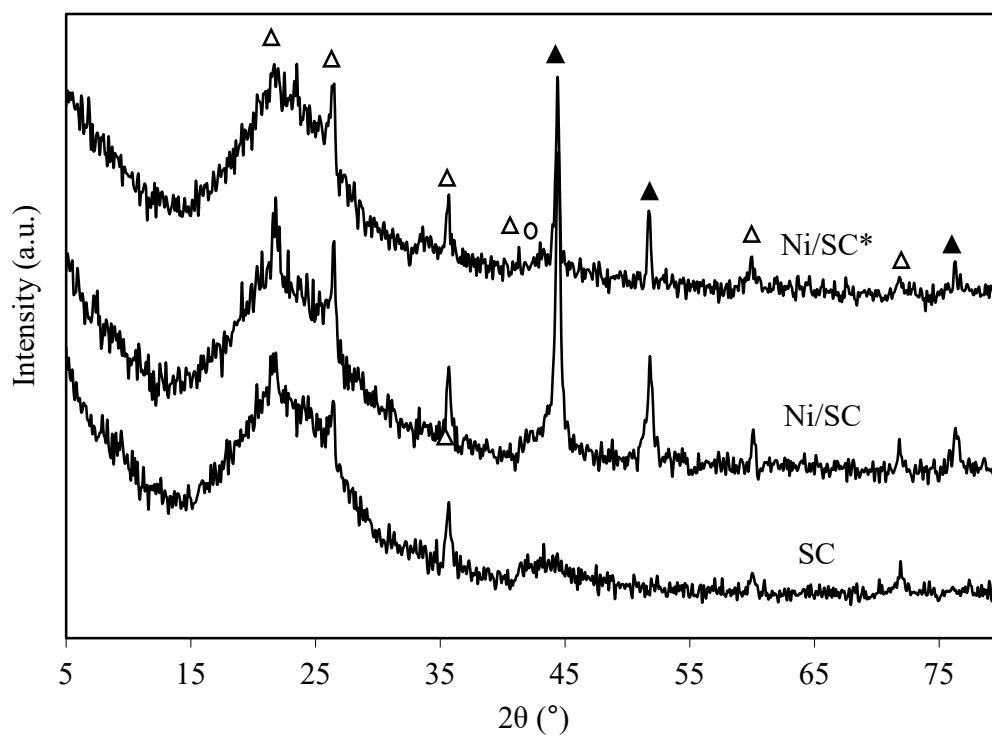


Figure S4. XRD patterns of SC, Ni/SC reduced fresh catalyst and used Ni/SC* catalyst. Symbols are referred to metallic nickel (▲), silicon carbide (Δ) and graphitic carbon (○).

Supplementary Material S5

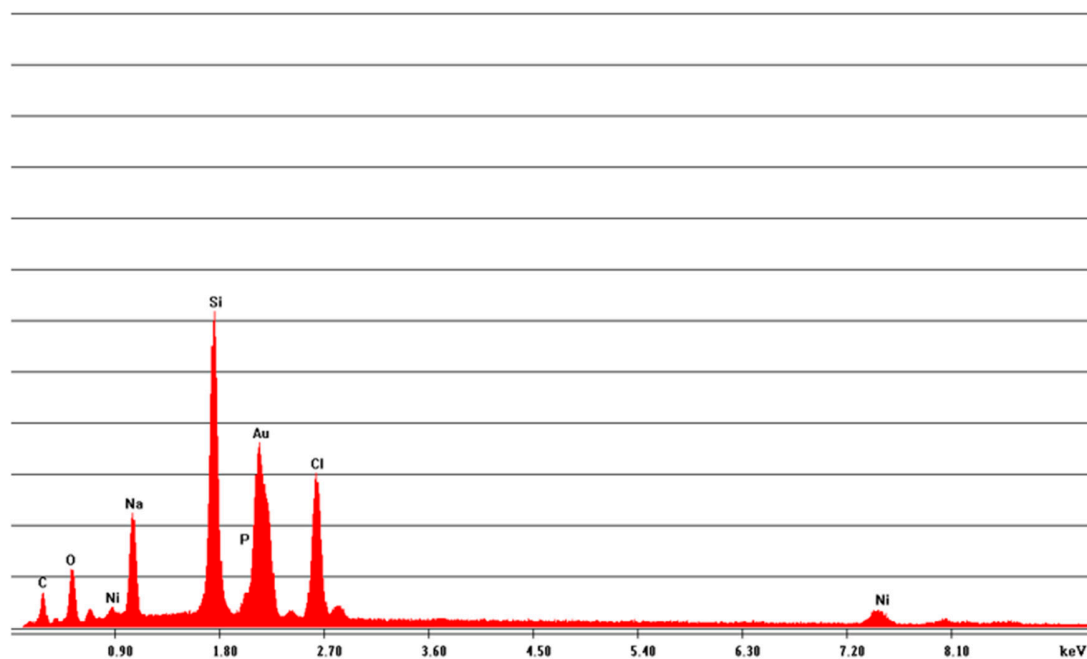


Figure S5. Analysis of elements by SEM-EDAX for the used catalyst after three reaction cycles in the presence of the crude glycerol sample D. Reaction conditions: 30 wt.% aqueous glycerol solution, 260 °C, 2 MPa, 2 h, $m_c/m_{gly} = 0.24$ (mass ratio).

Supplementary Material S6

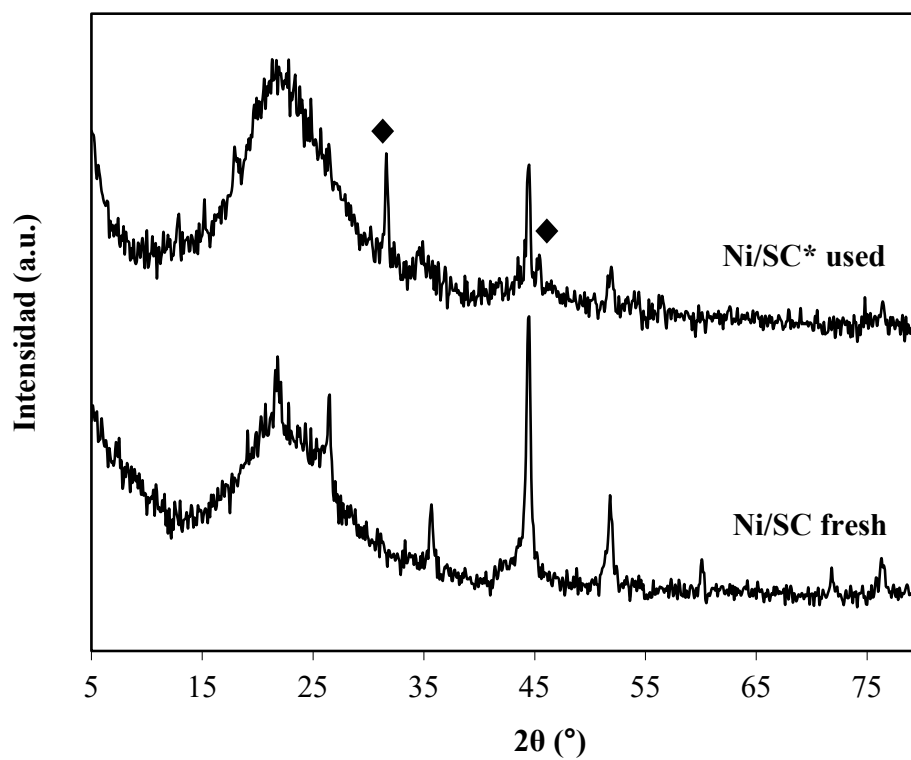


Figure S6. XRD patterns of Ni/SC reduced fresh catalyst and used Ni/SC* catalyst. Symbols are referred to planes (2 0 0) at 31.69° and (2 2 0) at 45.45° of crystalline cubic NaCl (♦) (JCPDS 05-0628).

Supplementary Material S7

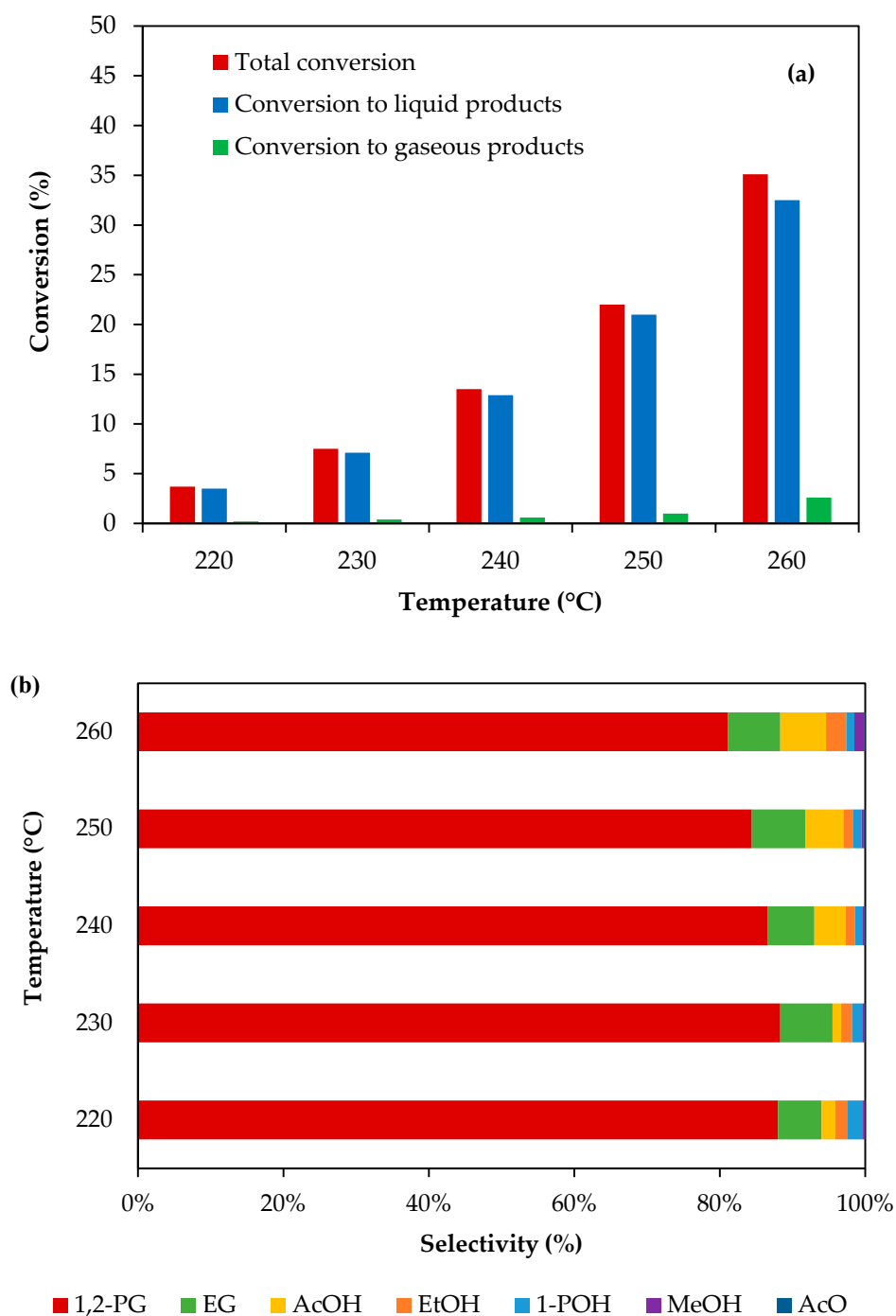


Figure S7. (a) Glycerol conversion vs temperature (b) Selectivity to liquid products vs temperature. Reaction conditions: 30 wt.% aqueous glycerol solution, 2 h, 2 MPa H₂, m_c/m_{gly} = 0.24 (mass ratio).

Supplementary Material S8

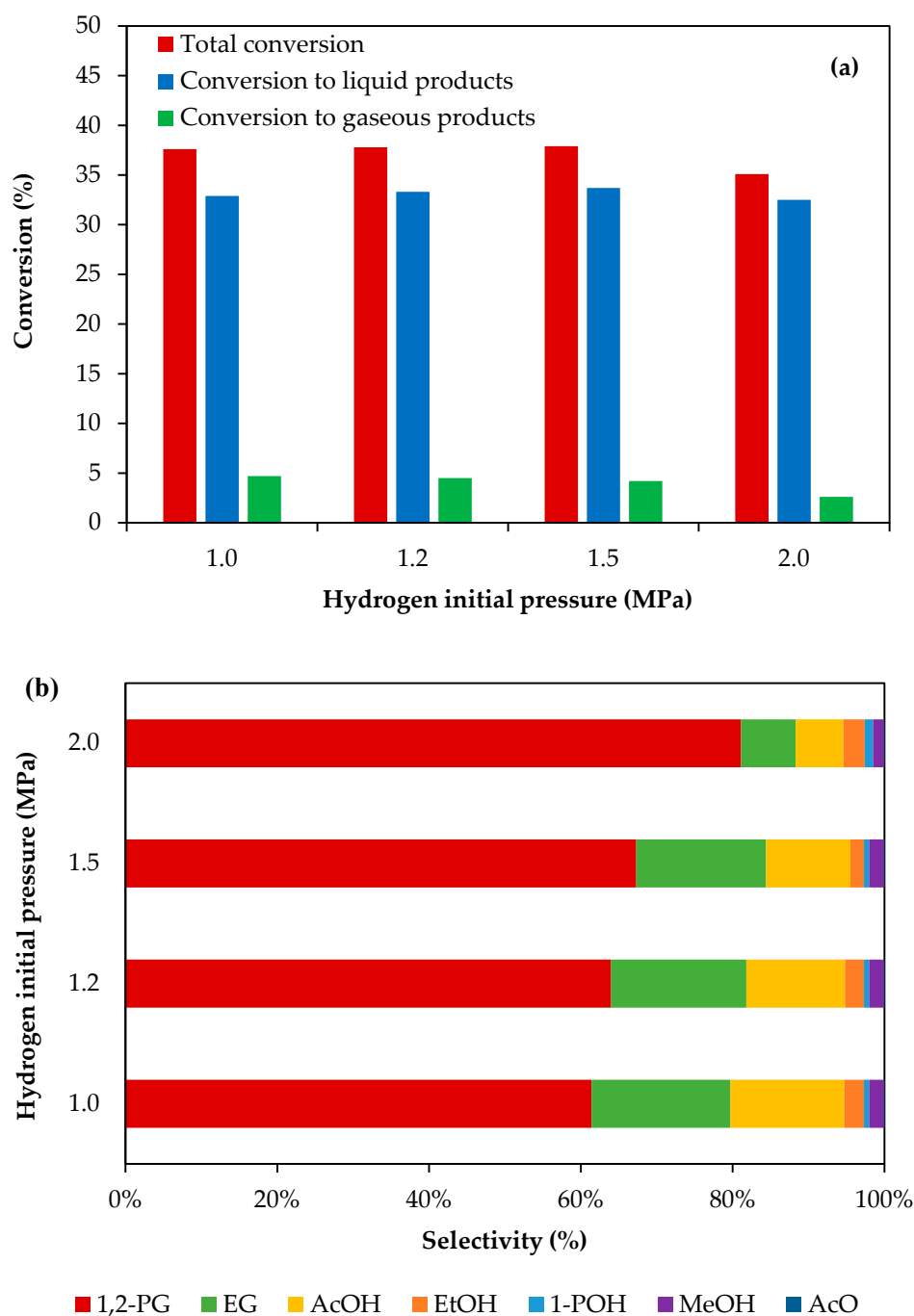


Figure S8. (a) Glycerol conversion vs partial pressure of H_2 (b) Selectivity to liquid products vs partial pressure of H_2 . Reaction conditions: 30 wt.% aqueous glycerol solution, 260 °C, 2 h, $m_c/m_{gly} = 0.24$ (mass ratio).

Supplementary Material S9

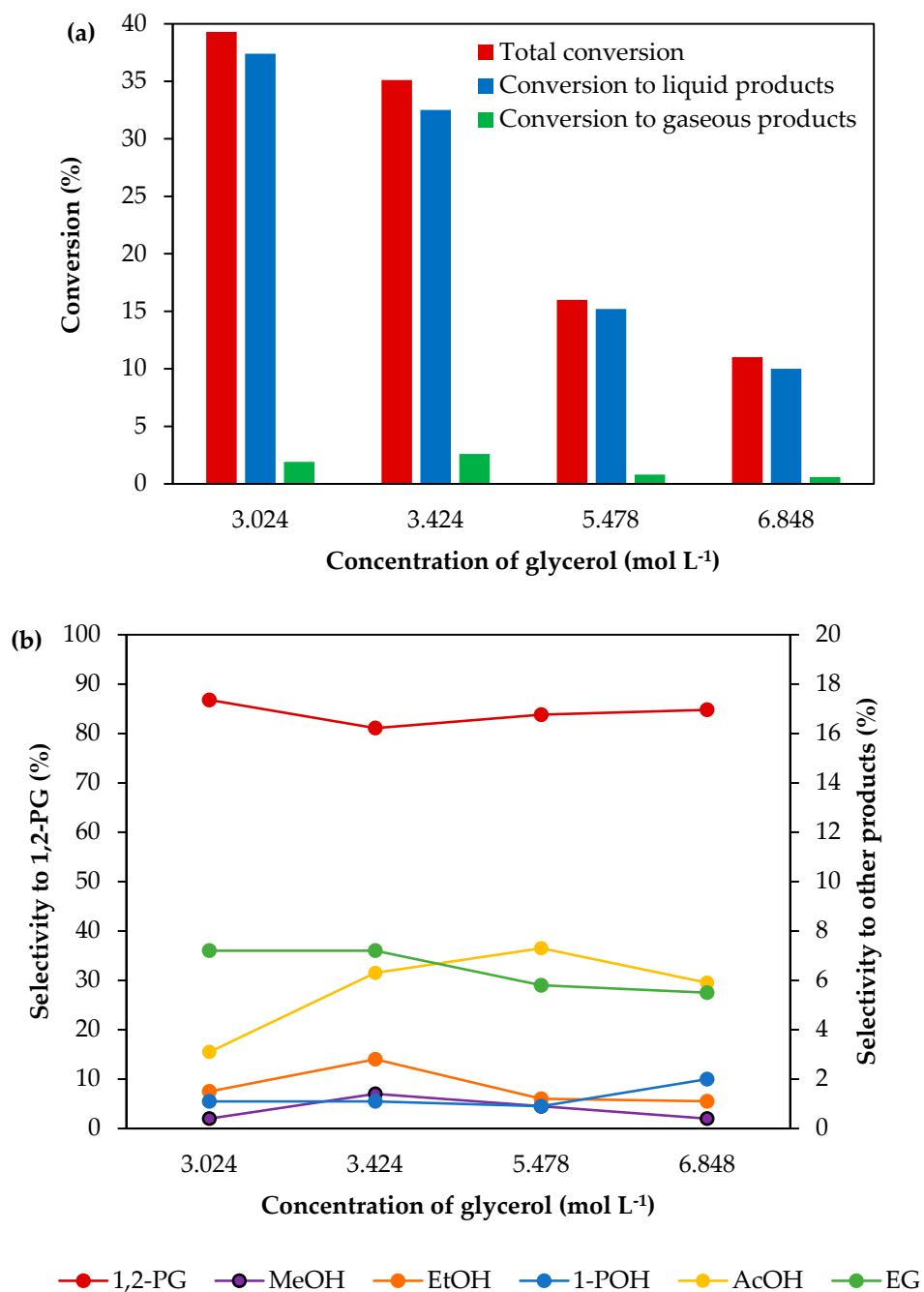
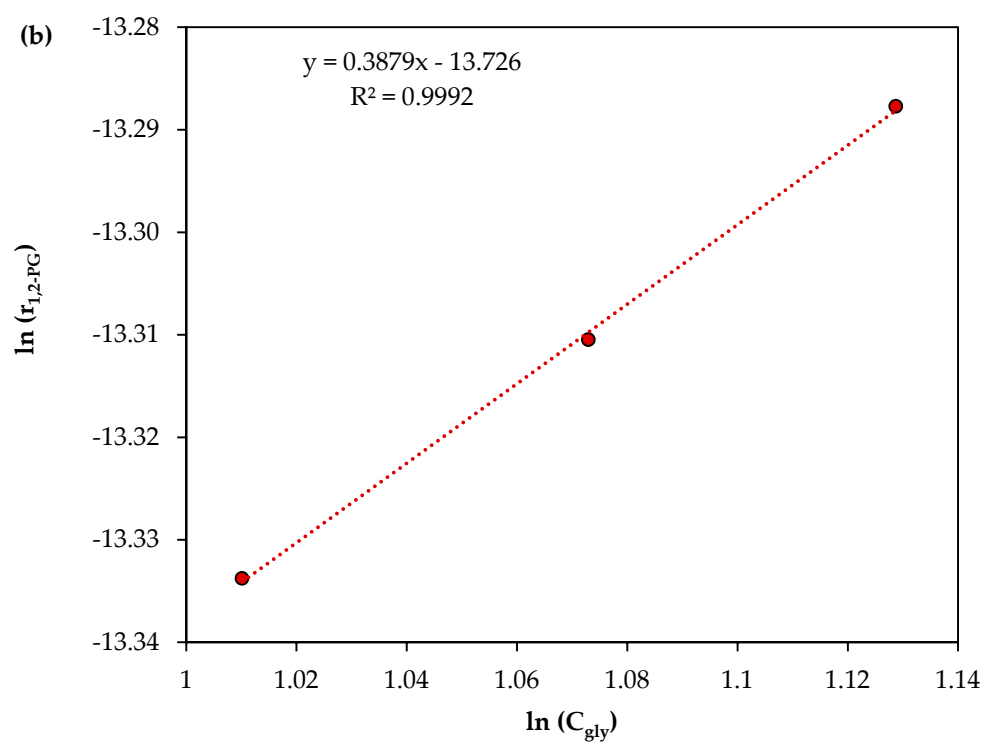
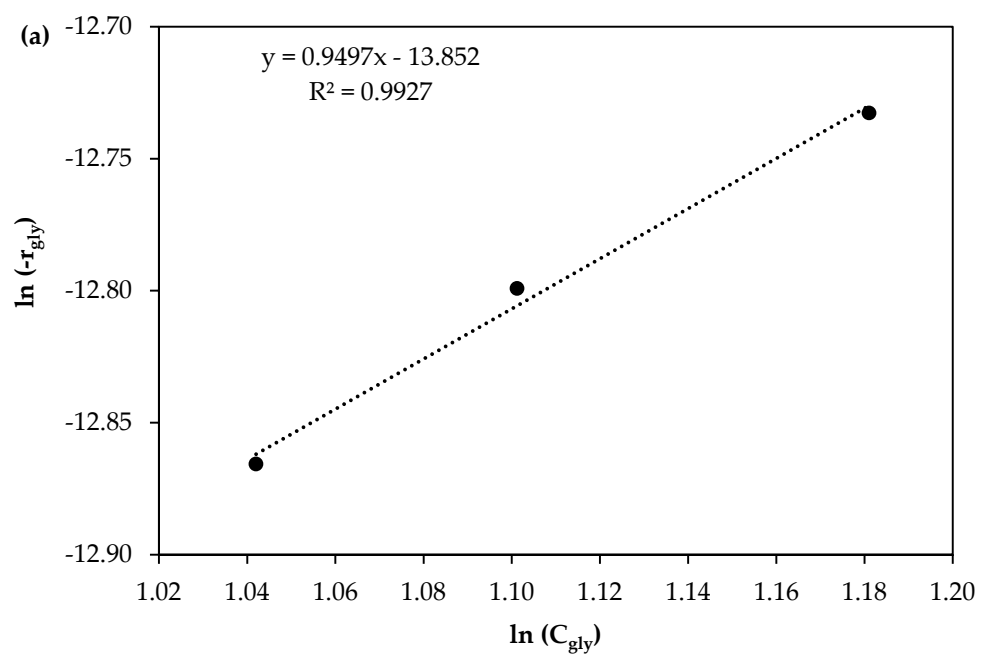
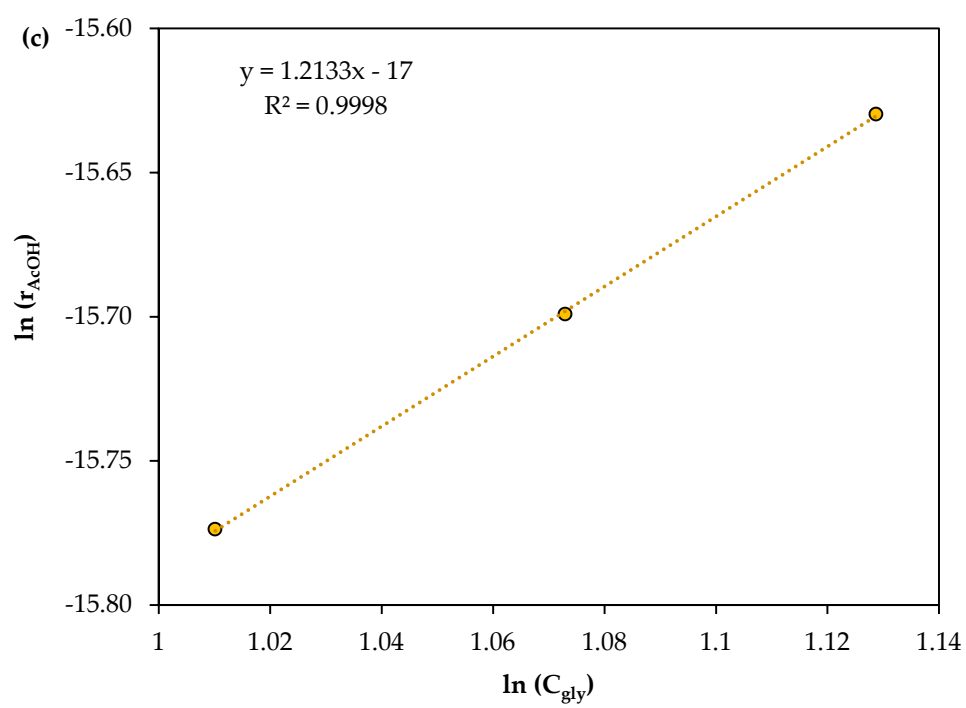
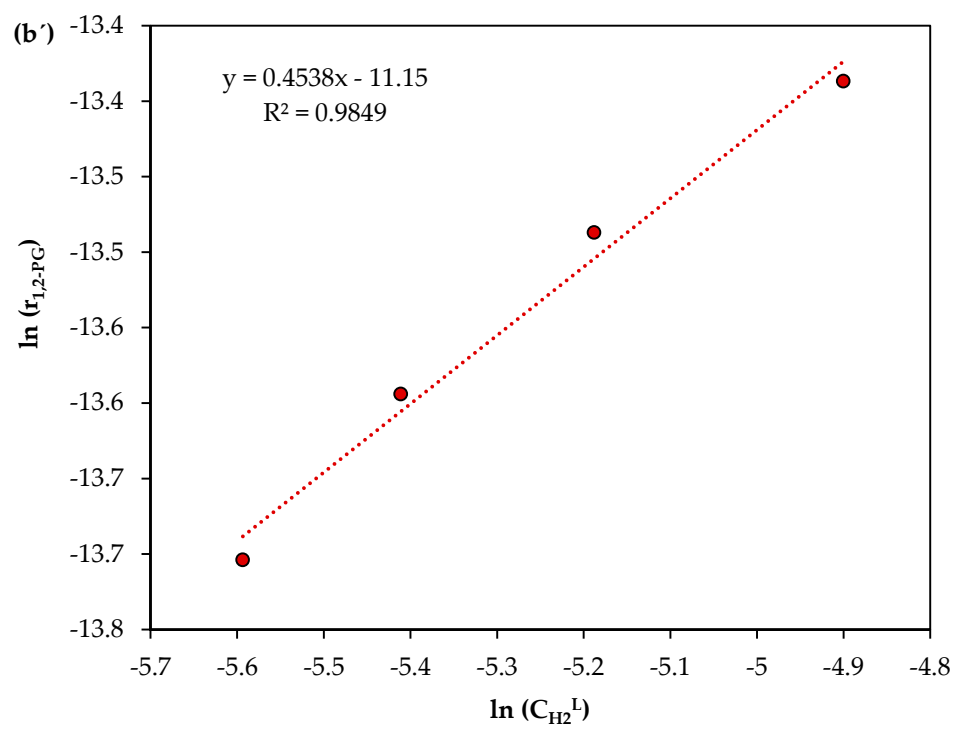
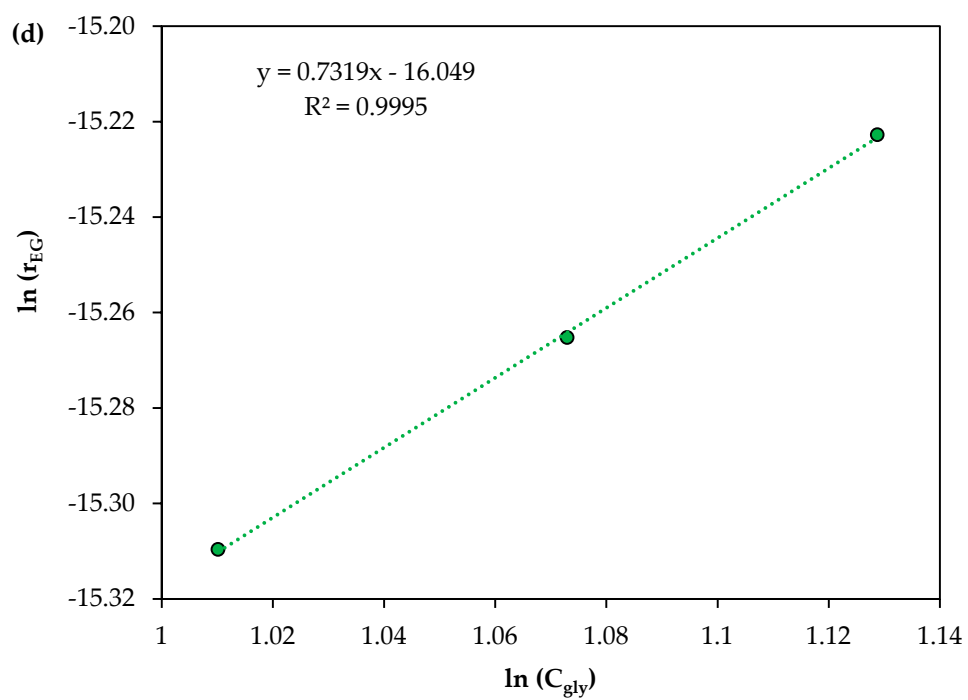
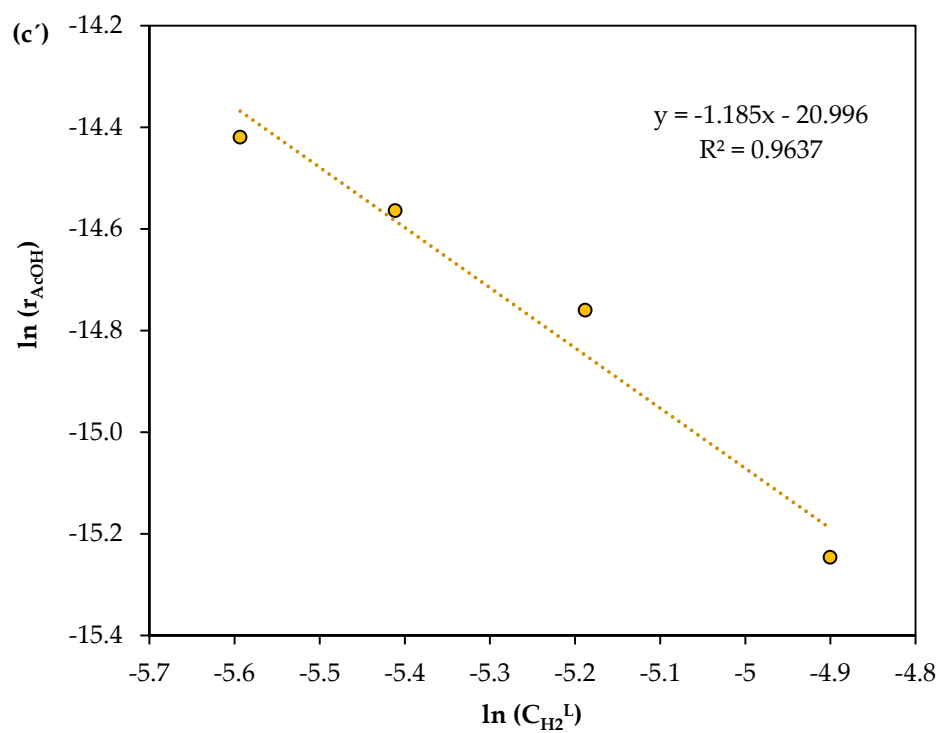


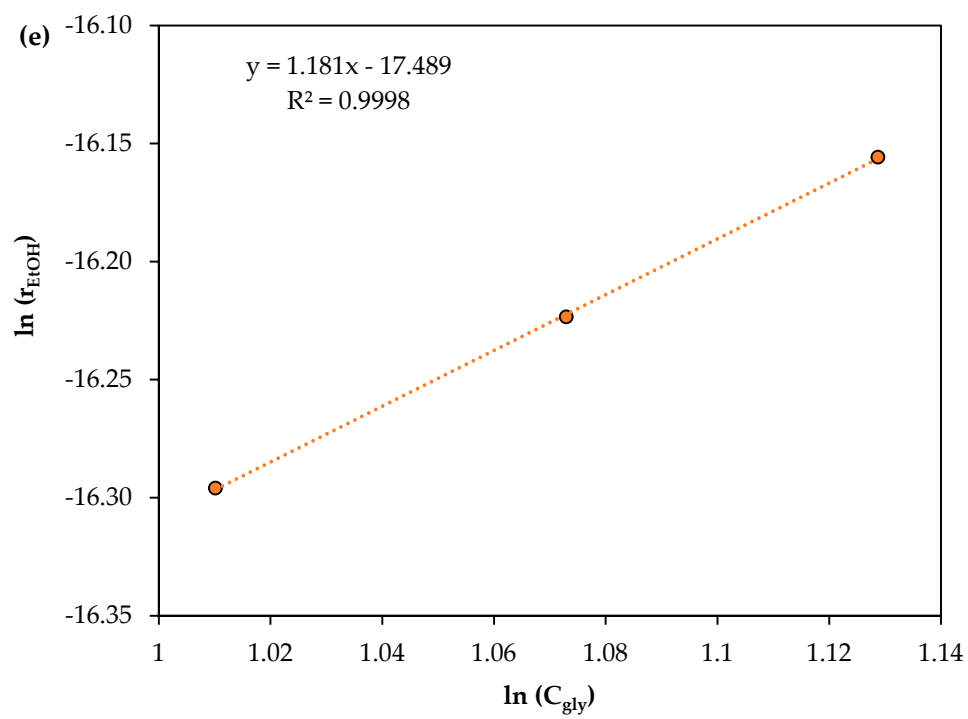
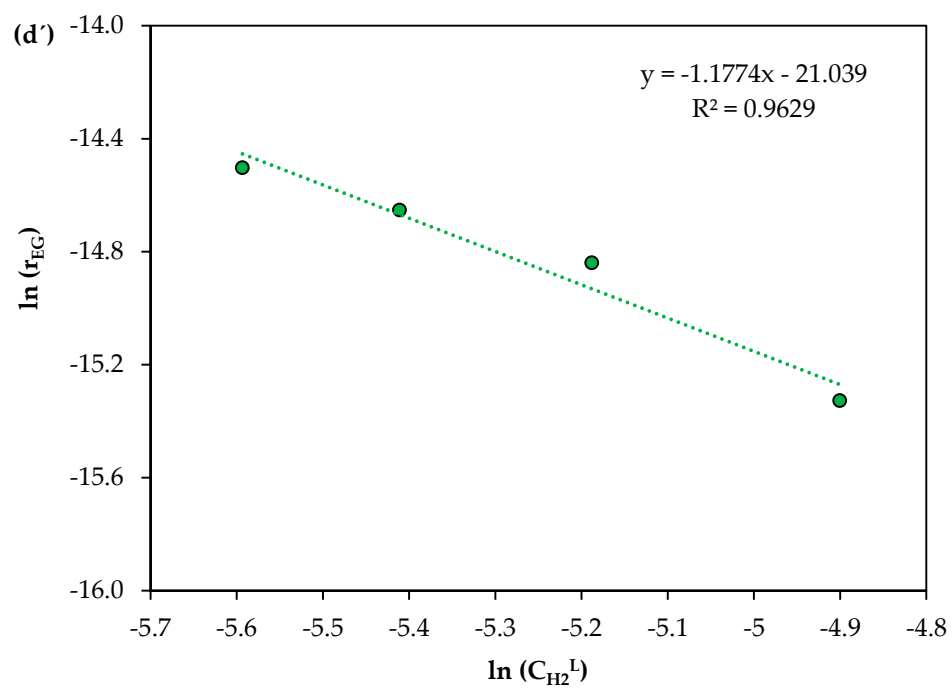
Figure S9. (a) Glycerol conversion vs glycerol initial concentration (b) Selectivity to liquid products vs initial glycerol concentration. Reaction conditions: 30-80 wt.% aqueous glycerol solutions, 260 °C, 2 MPa de H₂, 2 h, m_c/m_{gly} = 0.08-0.24 (mass ratio).

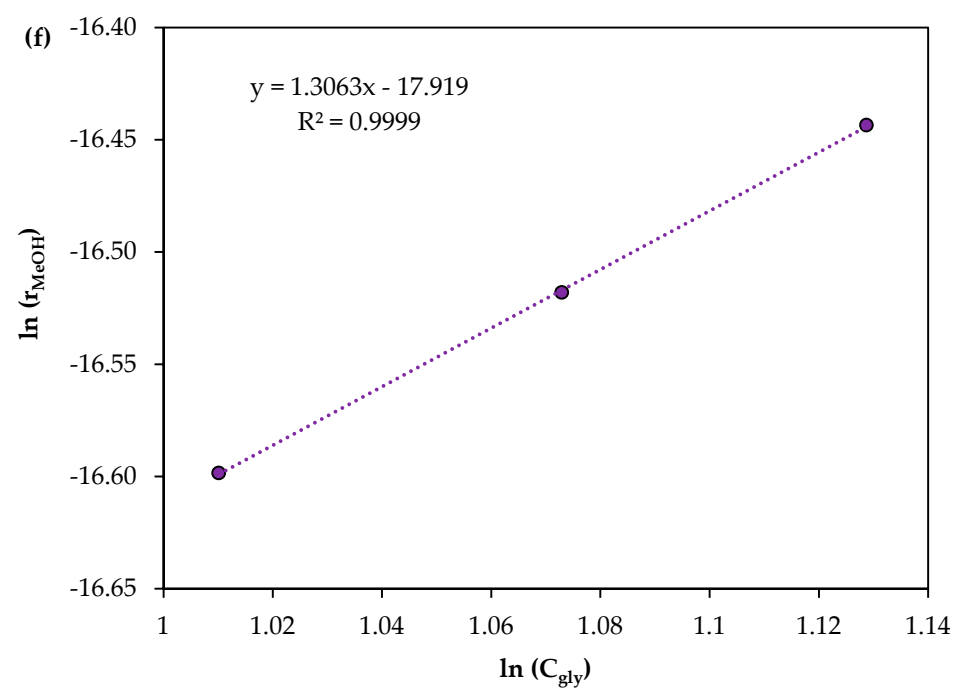
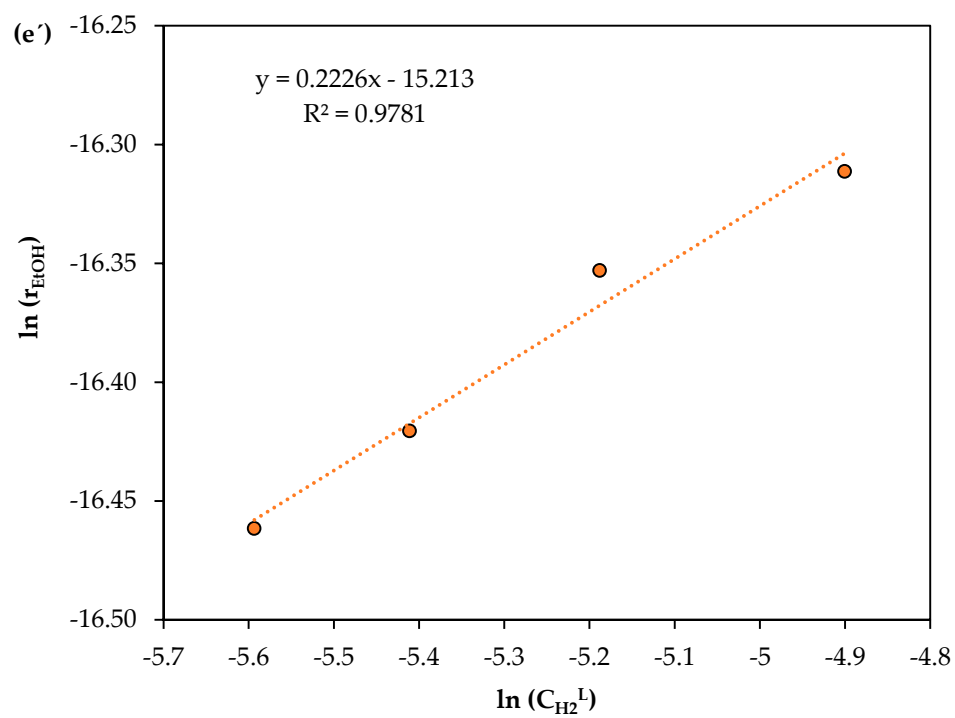
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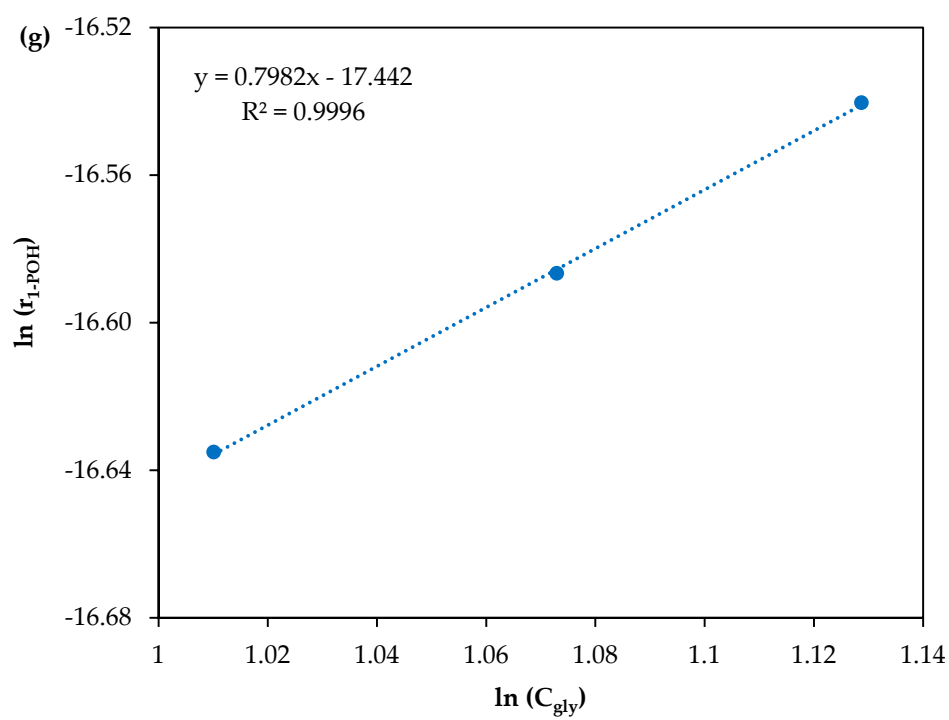
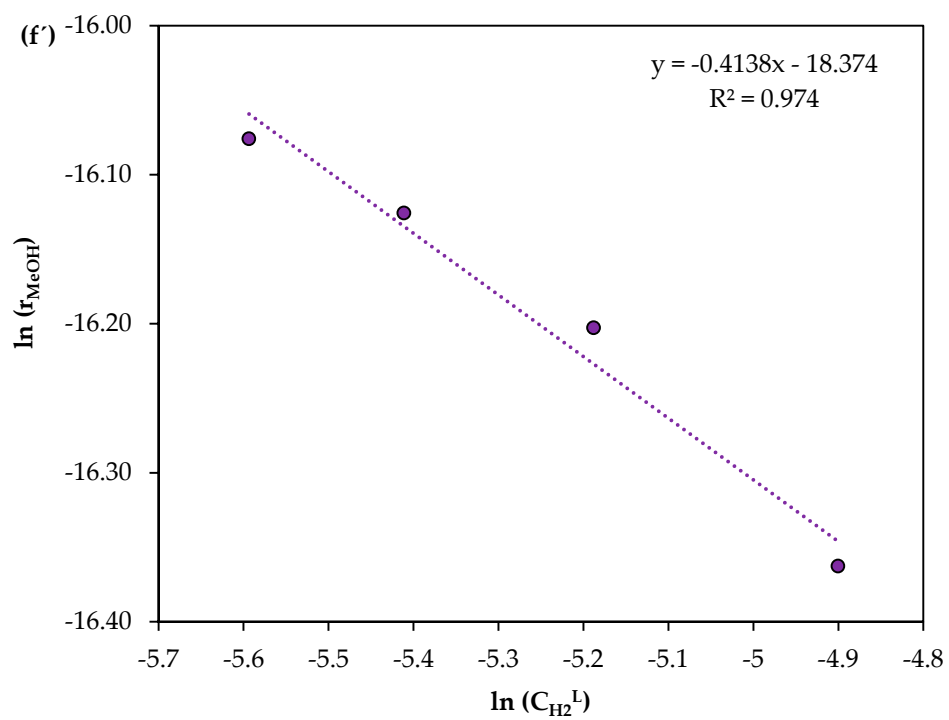












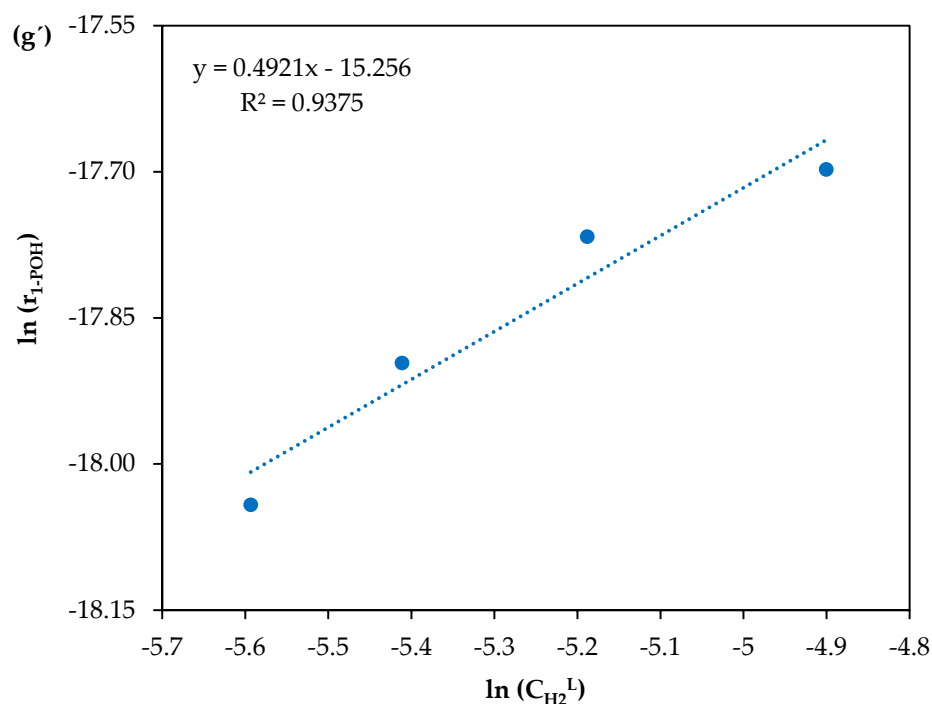
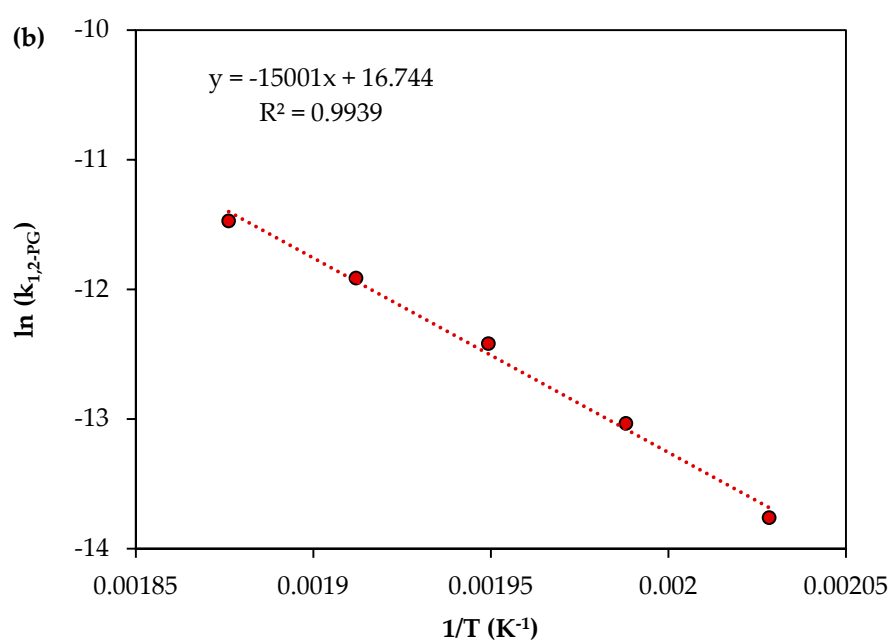
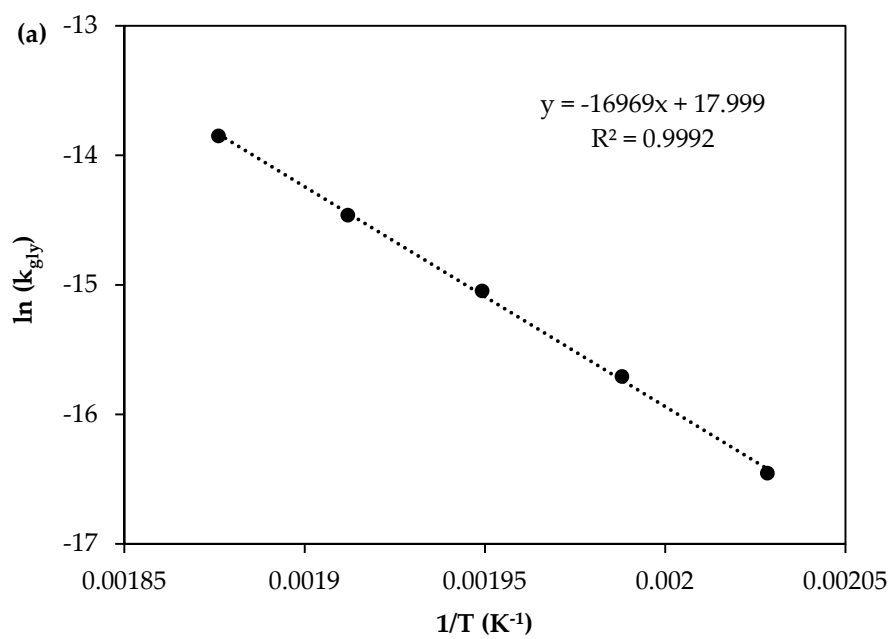
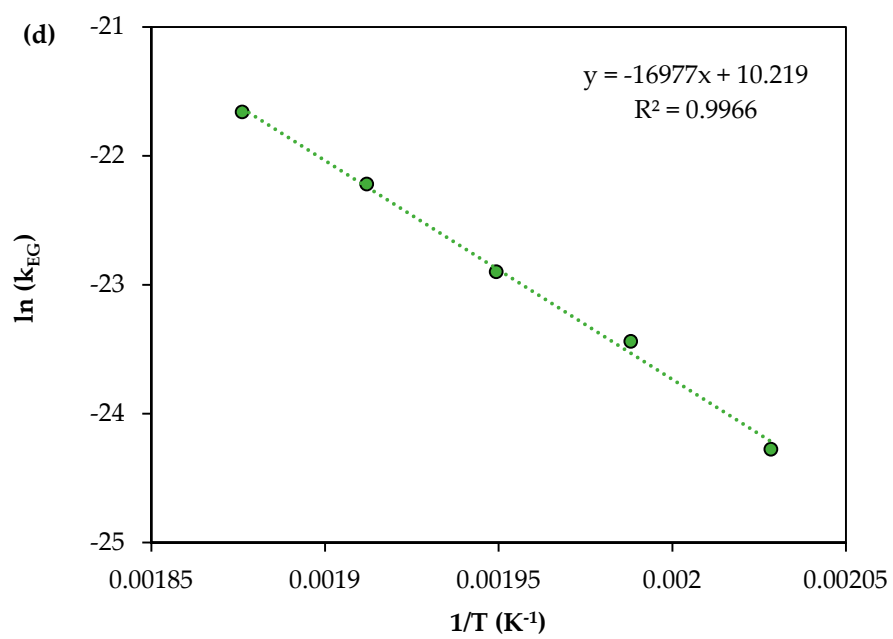
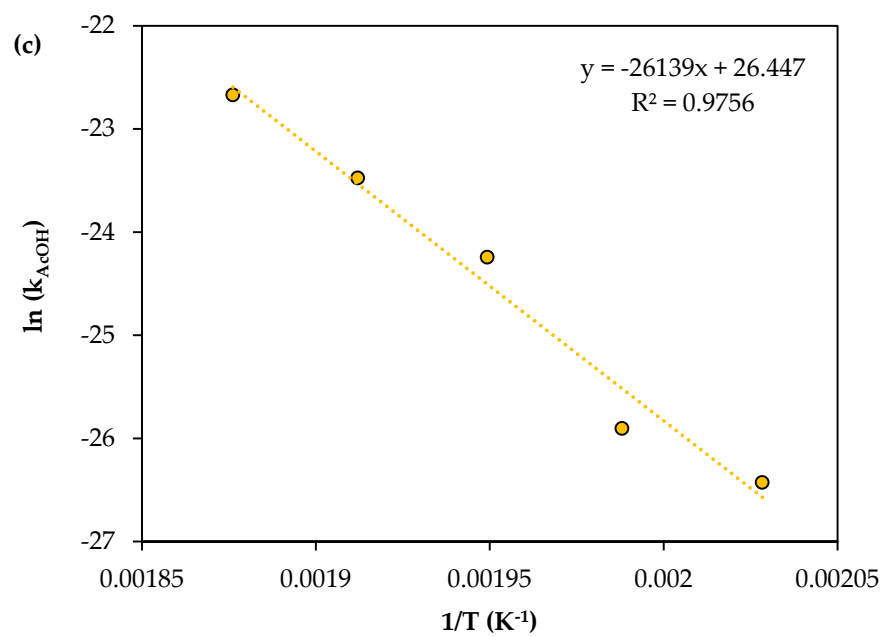
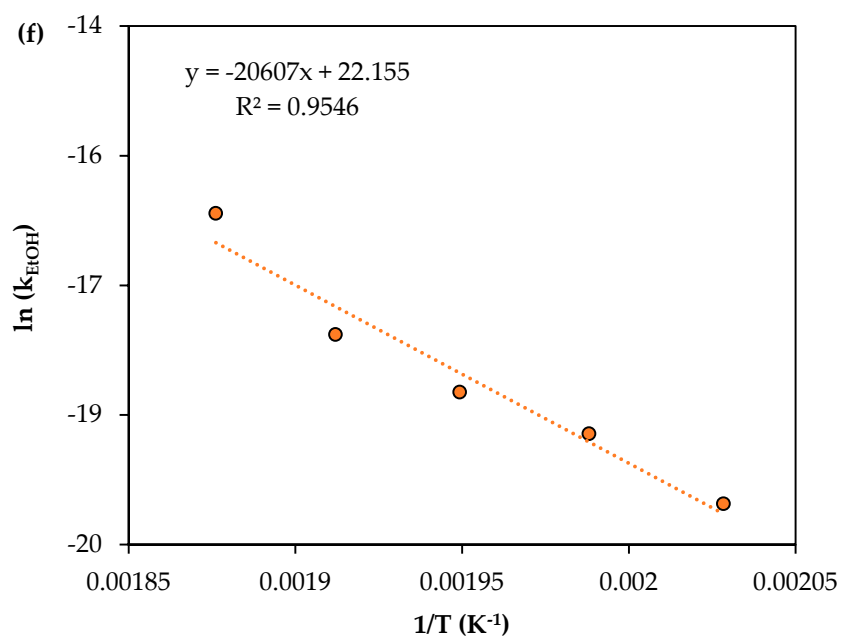
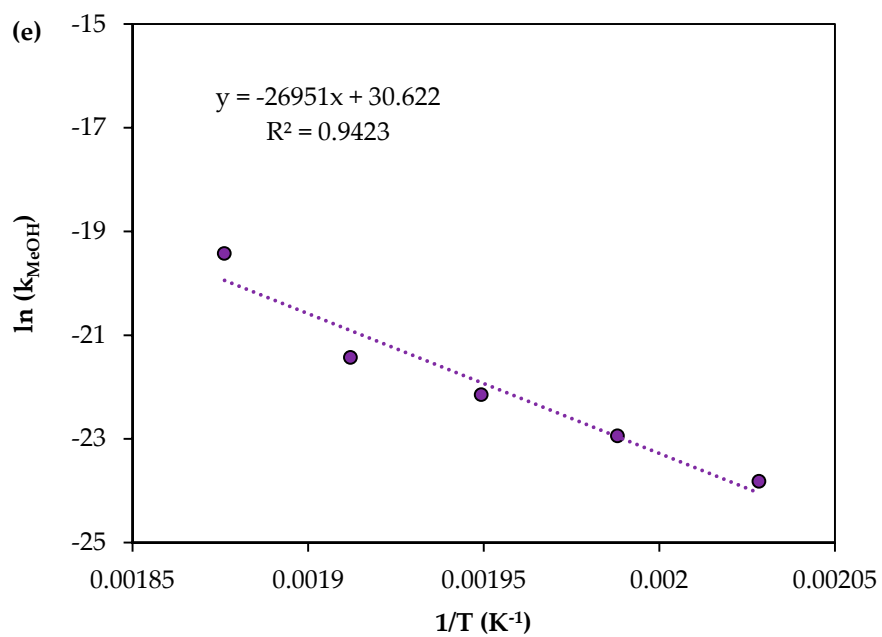


Figure S10. Fitting of experimental data by linear regression to obtain the reaction orders with respect to glycerol and hydrogen for **(a)** Gly **(b, b')** 1,2-PG **(c, c')** AcOH **(d, d')** EG **(e, e')** MeOH **(f, f')** EtOH **(g, g')** 1-POH. Reaction conditions: 30 wt.% aqueous glycerol solution, 260 °C, 1-2 MPa H_2 , 0.5-1 h, $m_c/m_{gly} = 0.24$ (mass ratio).

Supplementary Material S11







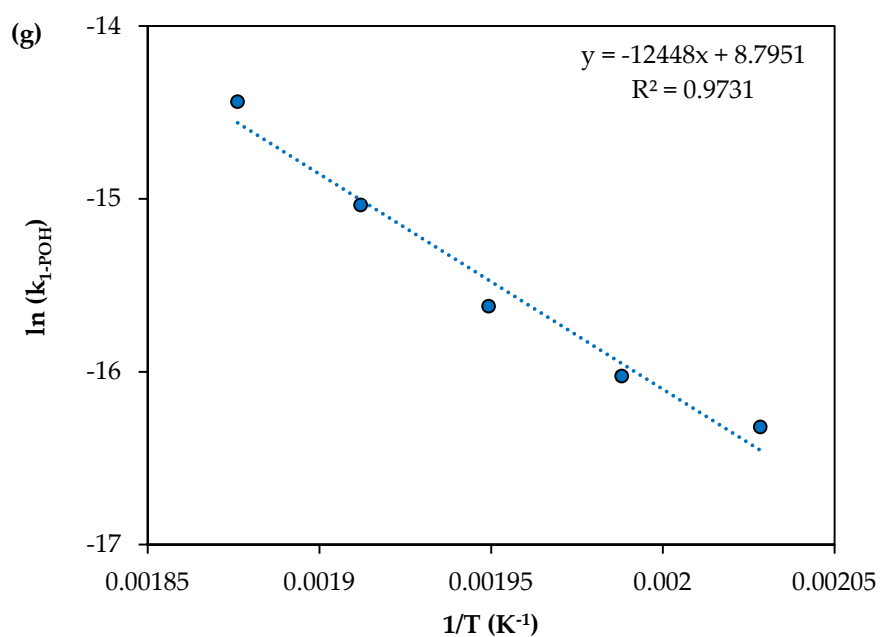
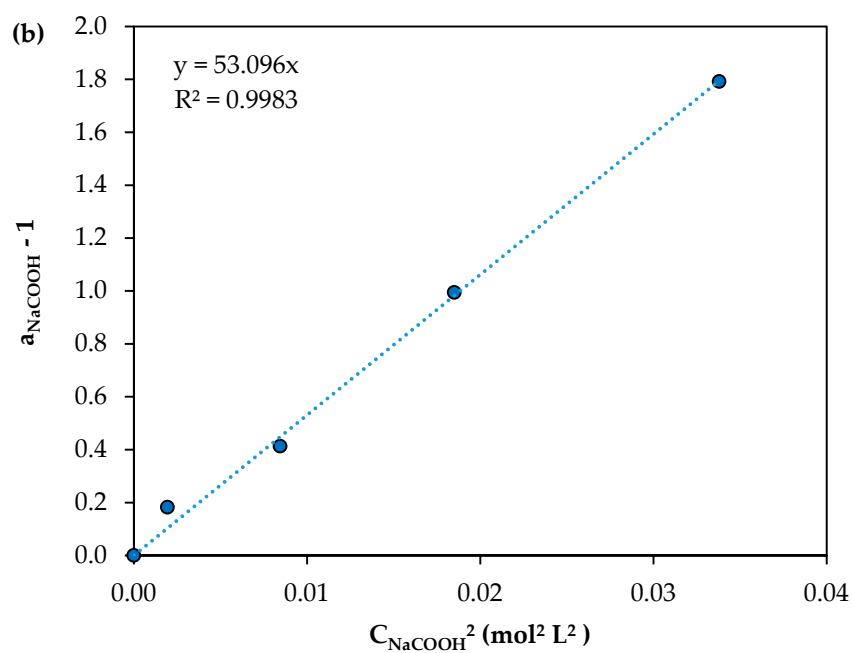
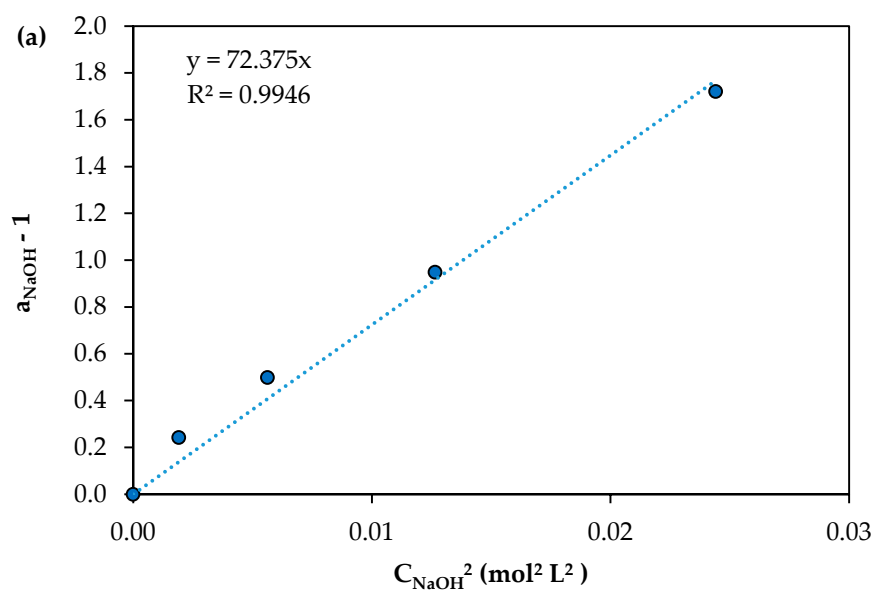


Figure S11. Fitting of experimental data by linear regression to obtain $\ln(k_{oj})$ y E_{aj} **(a)** Gly **(b)** 1,2-PG **(c)** AcOH **(d)** EG **(e)** MeOH **(f)** EtOH **(g)** 1-POH. Reaction conditions: 30 wt.% aqueous glycerol solution, 220-260 °C, 2 MPa H_2 , 2 h, $m_c/m_{gly} = 0.24$ (mass ratio).

Supplementary Material S12



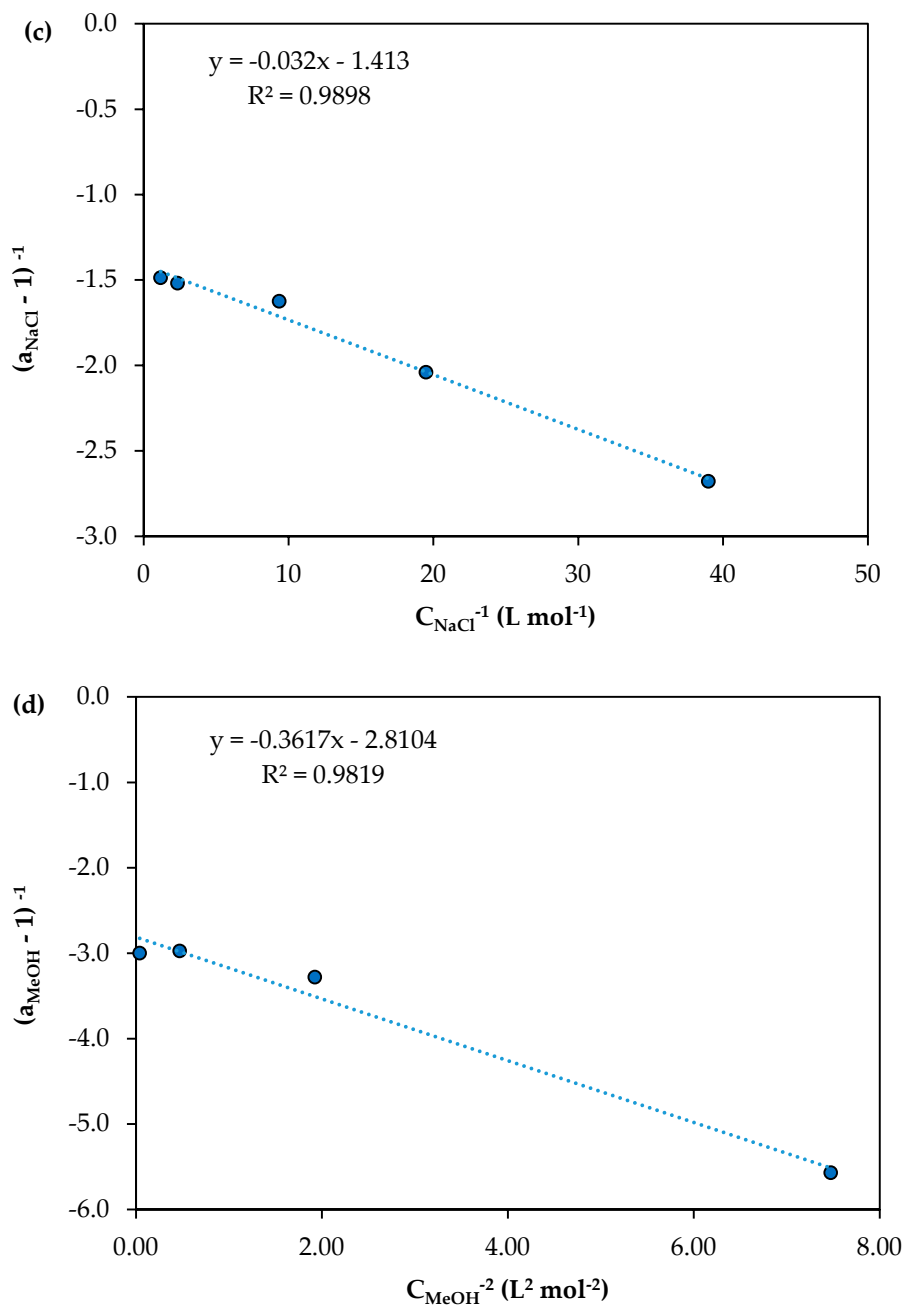


Figure S12. Fitting of experimental data by linear regression to obtain the individual activity factors (a_i) for (a) NaOH (b) NaCOOH (c) NaCl (d) MeOH. Reaction conditions: 30 wt.% aqueous glycerol solution, 260 °C, 2 MPa H_2 , 2 h, $m_c/m_{\text{gly}} = 0.24$ (mass ratio).