Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Vapor-phase conversion of aqueous 3-hydroxybutyric acid and crotonic acid to propylene over solid acid catalysts

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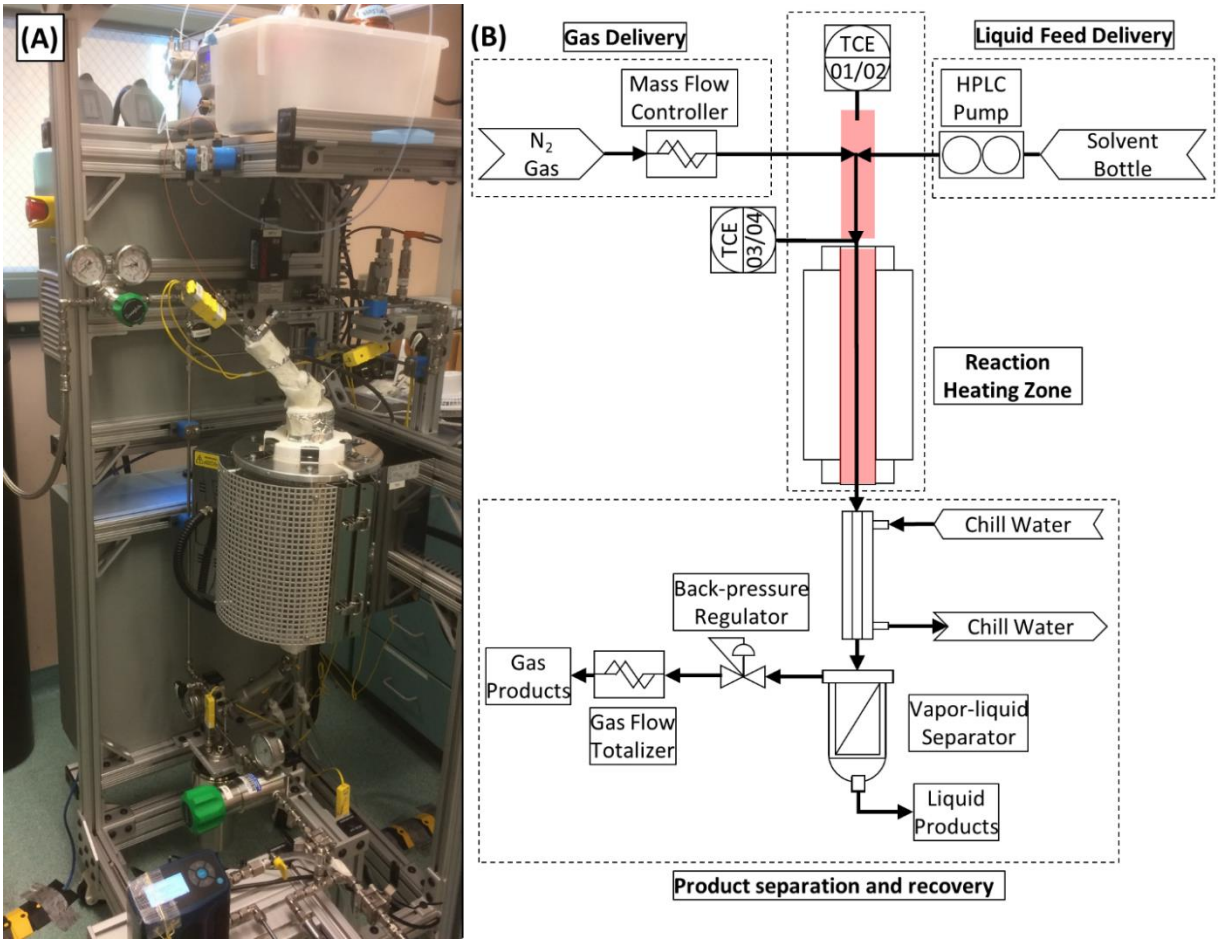

Figure S1. Fixed bed catalytic reactor used for performing experiments. (A) photograph and (B) general schematic.

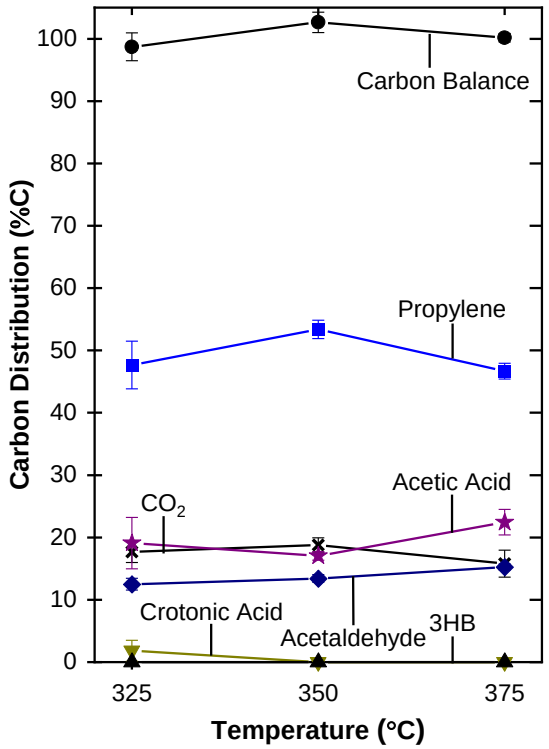

Figure S2. Effect of varying reactor bed temperature on carbon selectivity during vapor-phase conversion of 3HB over SIAL 3113 (as %C of inflow 3HB feed). Reaction conditions: WHSV of 3HB of 0.1 h^{-1}, 40 sccm N_2 at 55 psig (gaseous products sampled at atmospheric pressure), 4 h time-on-stream. Data points with error bars show the mean of duplicate reactions with min/max values.

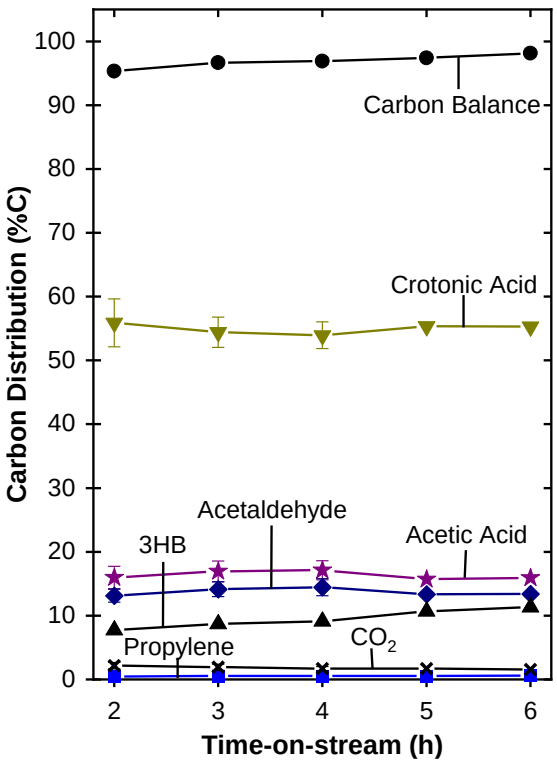

Figure S3. Carbon selectivity (as %C of inflow 3HB feed) results for 3HB "blank" reaction (no catalyst present) shown for the first 6 h time-on-stream. Reaction conditions: 350 °C, 0.3 mL/min of 2 wt% aqueous 3HB, 40 sccm N_2 at 55 psig (gaseous products sampled at atmospheric pressure). Data points with error bars show the mean of duplicate reactions with min/max values where duplicates were performed (up to 4 h).

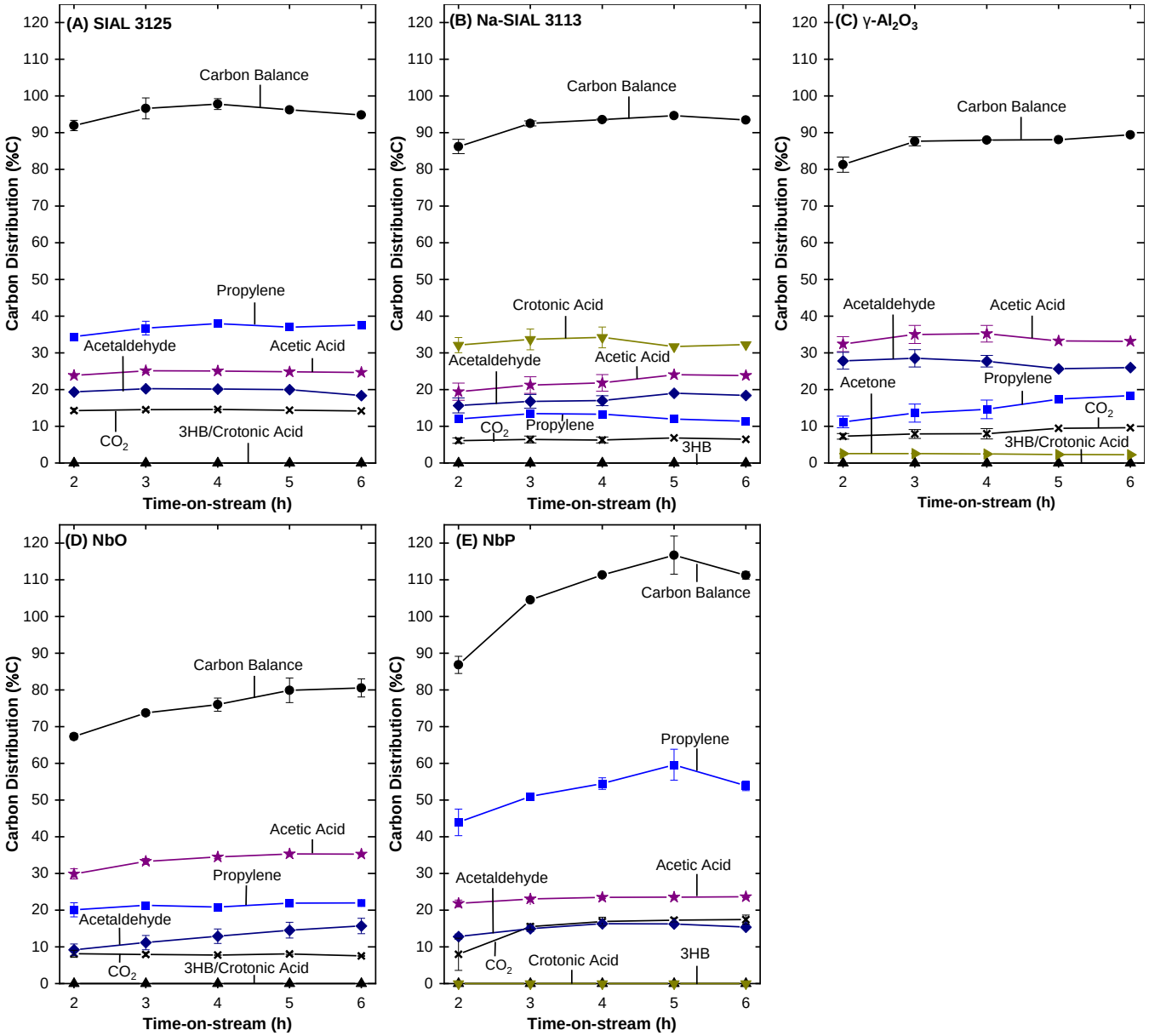

Figure S4. Detailed distribution of carbon products (as %C) during time-on-stream conversion of 3HB reaction over (A) SIAL 3125, (B) Na- SIAL 3113, (C) γ-Al_2O_3, (D) NbO, and (E) NbP corresponding to propylene yield data presented in **Figure 3a**. Reaction conditions: 350 °C, 0.1 h^{-1} WHSV, 40 sccm N_2 at 55 psig (gaseous products sampled at atmospheric pressure). Data points with error bars show the mean of duplicate reactions with min/max values where duplicates were performed.

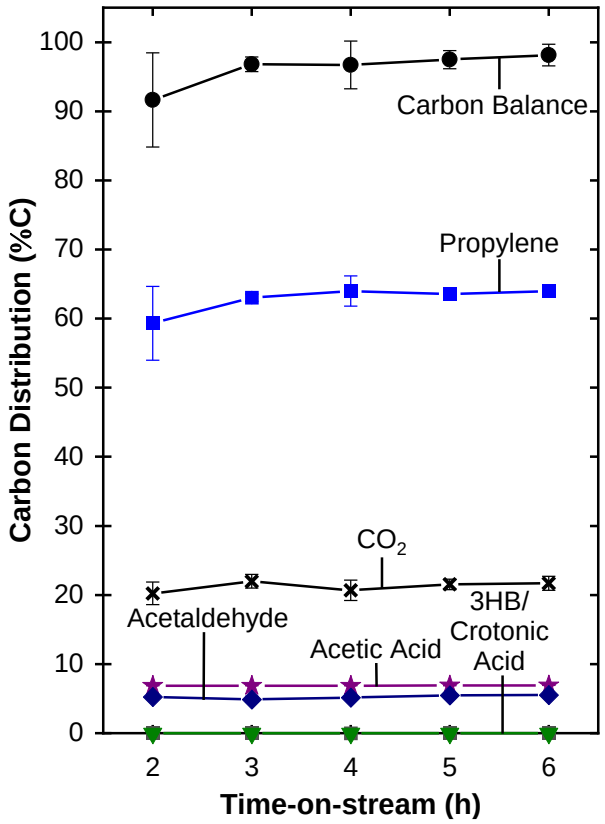

Figure S5. Distribution of carbon products (as %C of inflow crotonic acid feed) results for CA reaction over NbP. Reaction conditions: 350 °C, 0.1 h^{-1} WHSV, 40 sccm N_2 at 55 psig (gaseous products sampled at atmospheric pressure). Data points with error bars show the mean of duplicate reactions with min/max values. Horizontal dotted line indicates theoretical maximum yield of propylene from conversion of CA.

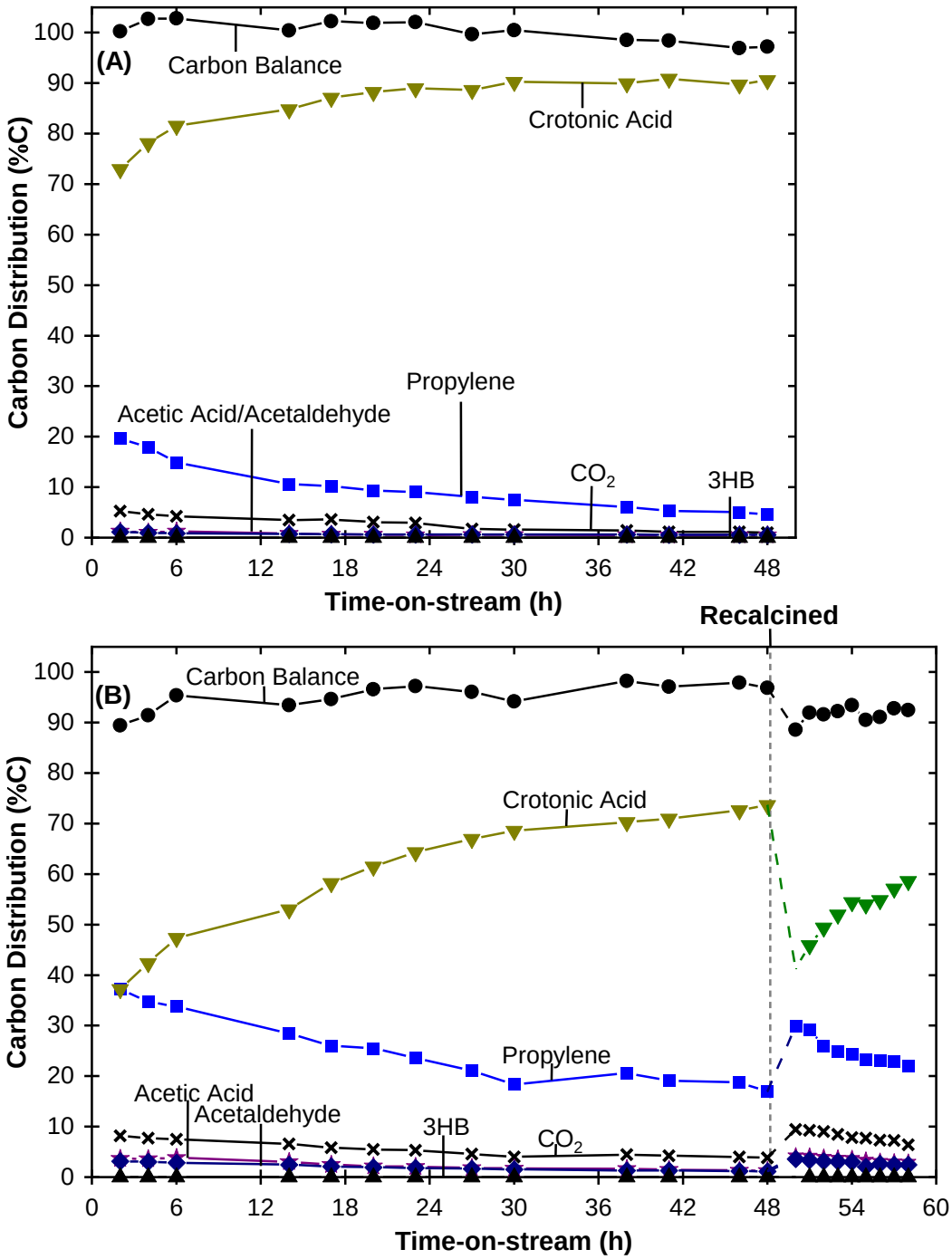

Figure S6. Detailed distribution of carbon products (as %C) during extended time-on-stream partial conversion of CA feeds for (A) SIAL 3113 and (B) NbP corresponding to the propylene yield data presented in **Figure 4.** Reaction conditions: 350 °C, 2.75 h^{-1} WHSV, 40 sccm N_2 at 55 psig (gaseous products sampled at atmospheric pressure). Recalcination conditions: 500 °C for 3 h (200 °C·h^{-1} heat rate).

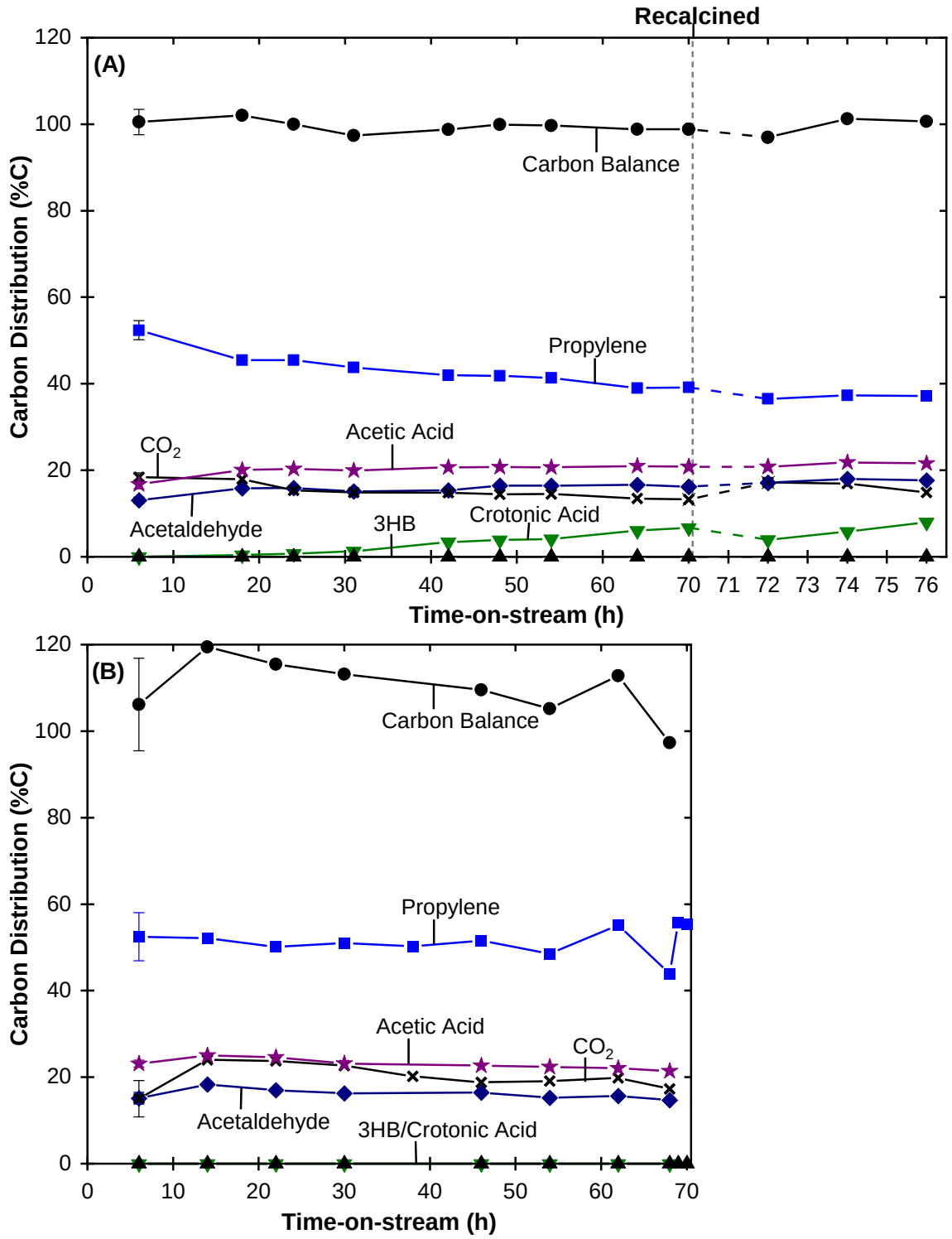

Figure S7. Detailed distribution of carbon products (as %C) during extended time-on-stream conversion of 3HB feeds for (A) SIAL 3113 and (B) NbP. SIAL 3113 subjected to recalcination at t = 70 h before continuing time-on-stream conversion measurements. Reaction conditions: 350 °C, 0.1 h^{-1} WHSV, 40 sccm N_2 at 55 psig (gaseous products sampled at atmospheric pressure). Recalcination conditions: 550 °C for 3 h (200 °C·h^{-1} heat rate).

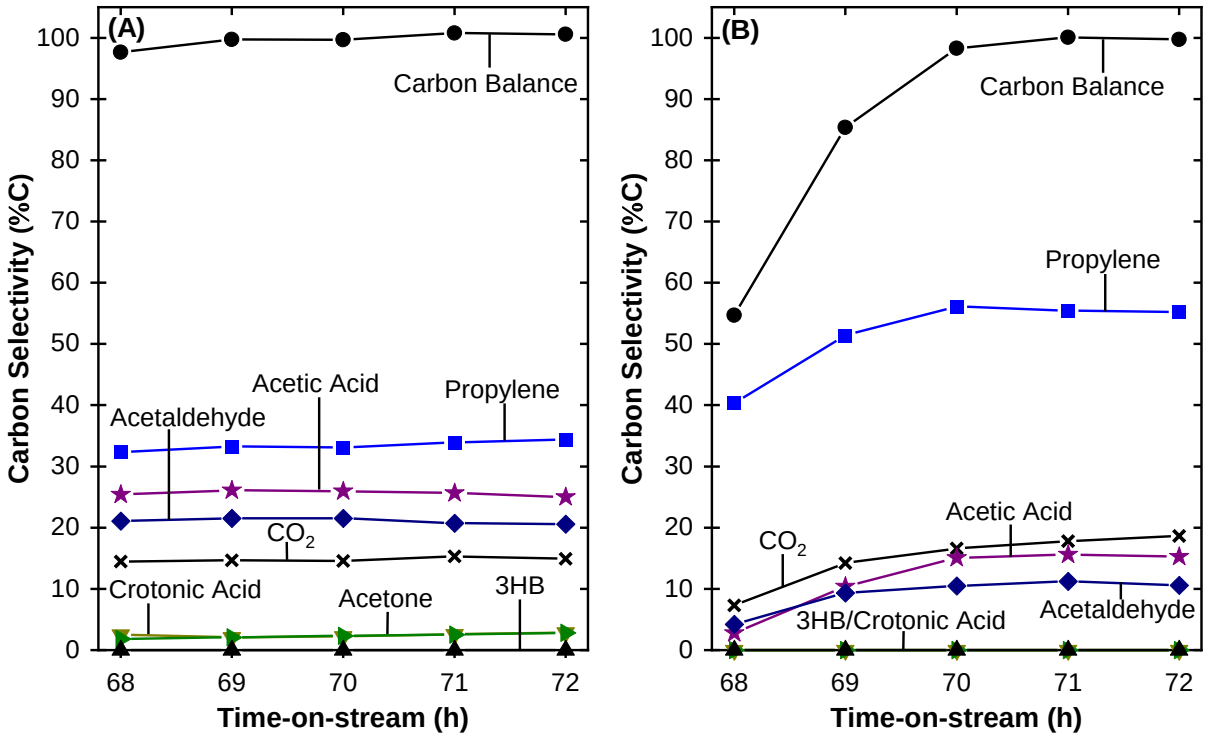

Figure S8. Carbon selectivity (as %C of inflow 3HB feed) of steam-treated SIAL 3113 (A) and NbP (B) for DYHD-DCBX of 3HB up to 6 h time-on-stream. Virgin catalysts were steam-treated for 66 h prior to starting 3HB feedstock (i.e., 68 h = 2 h time-on-stream of feedstock). Reaction conditions: 350 °C, 0.1 h^{-1} WHSV, 40 sccm N_2 at 55 psig (gaseous products sampled at atmospheric pressure).