Supplementary information for

Investigating the Long-Term Kinetics of Pd Nanoparticles Prepared from Microemulsions and the Lindlar Catalyst for Selective Hydrogenation of 3-Hexyn-1-ol

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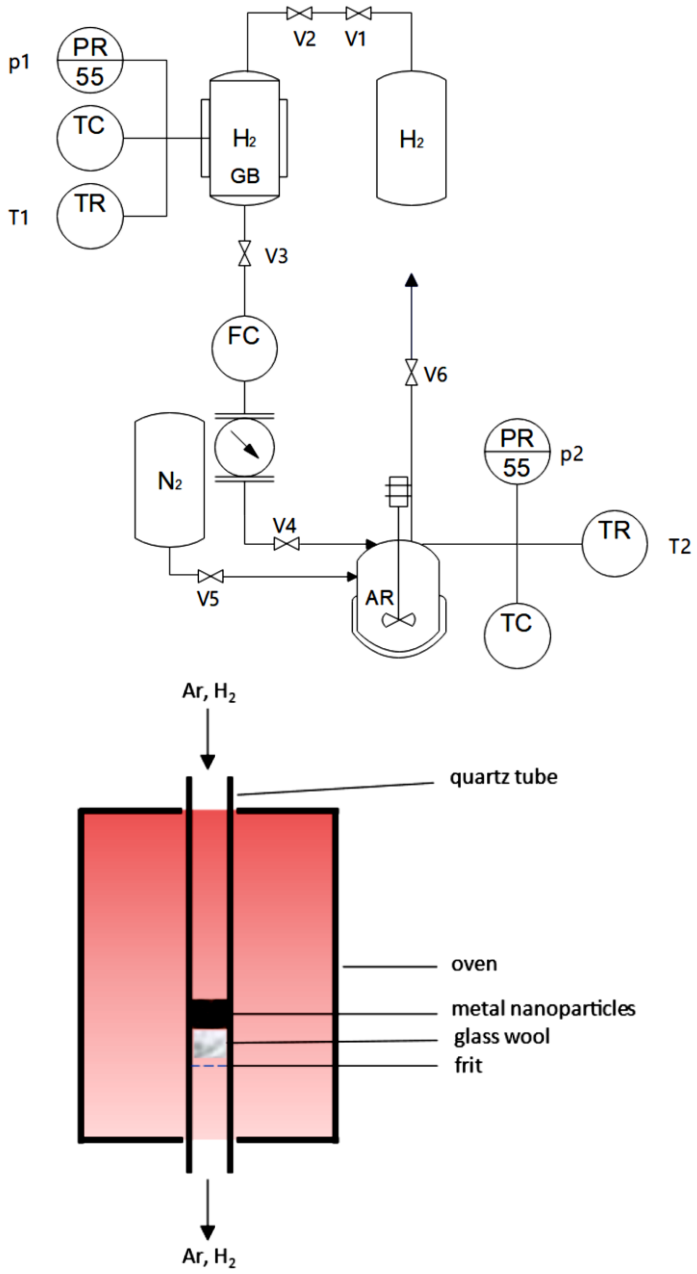

Scheme S1. Catalytic hydrogenation setup (top), and fixed-bed quartz reactor for sintering (bottom).

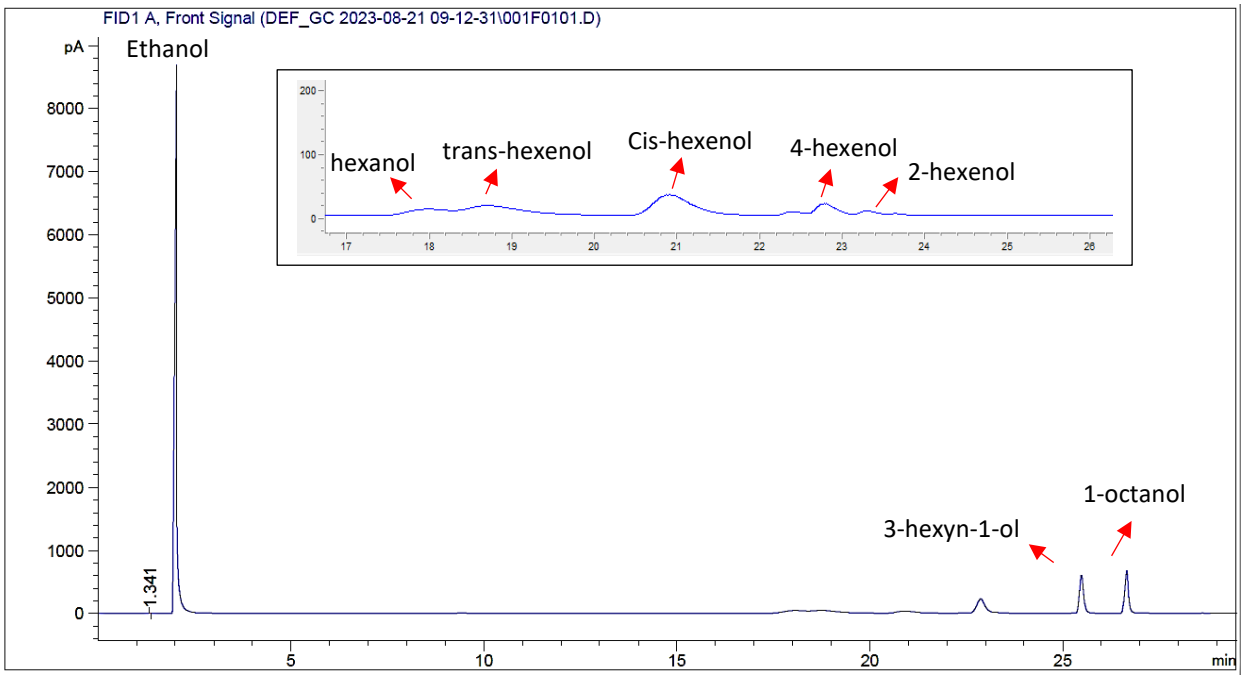

Figure S1. Possible product distribution pattern obtained by gas chromatography.

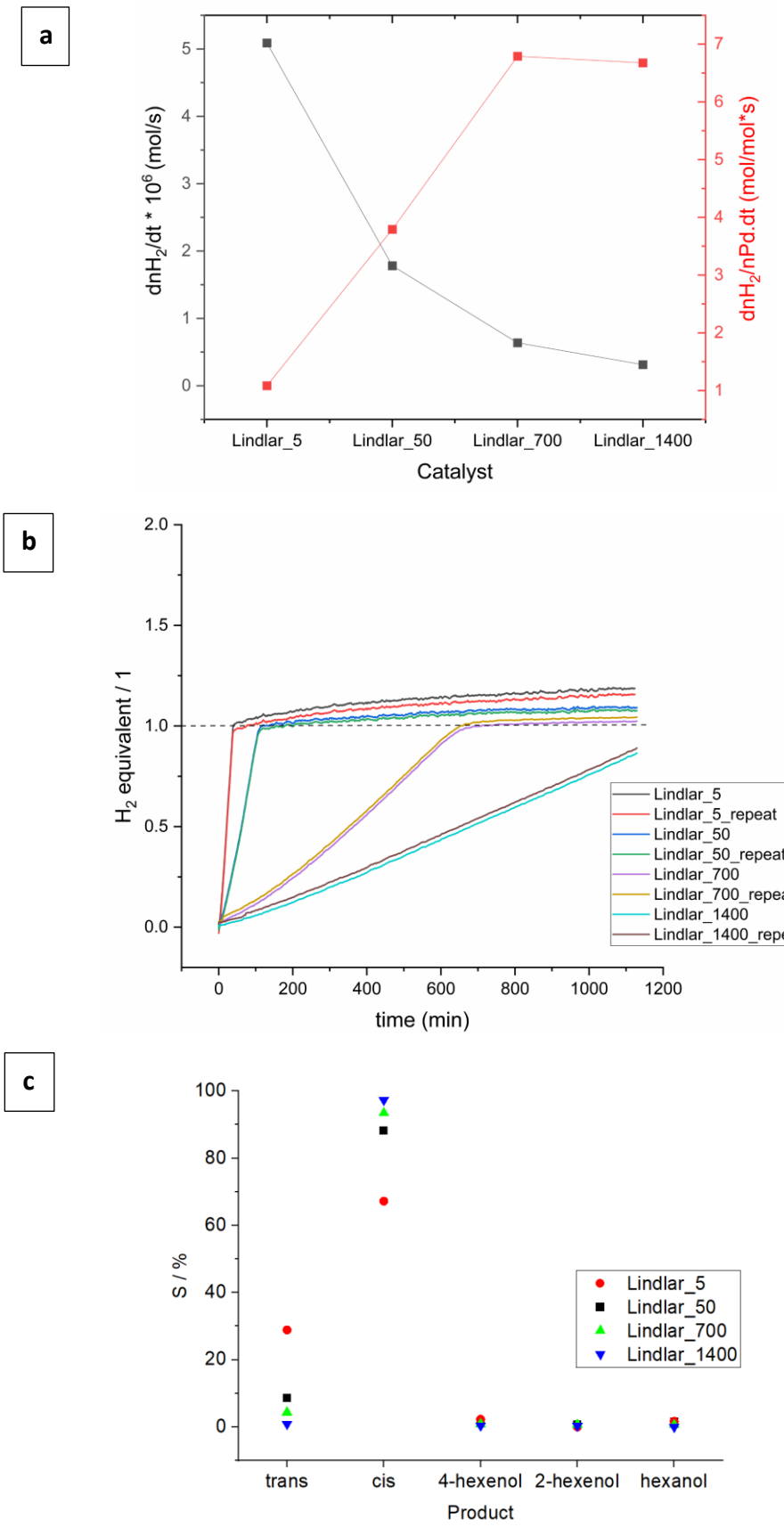

Figure S2. Catalytic hydrogenation of 3-hexyn-1-ol by Lindlar catalyst: activity (a), reproducibility (b), and average selectivity (c) at the end of the reaction (around 100 % conversion) at different $n_{alkynol}/A_{Pd}$ ratios.

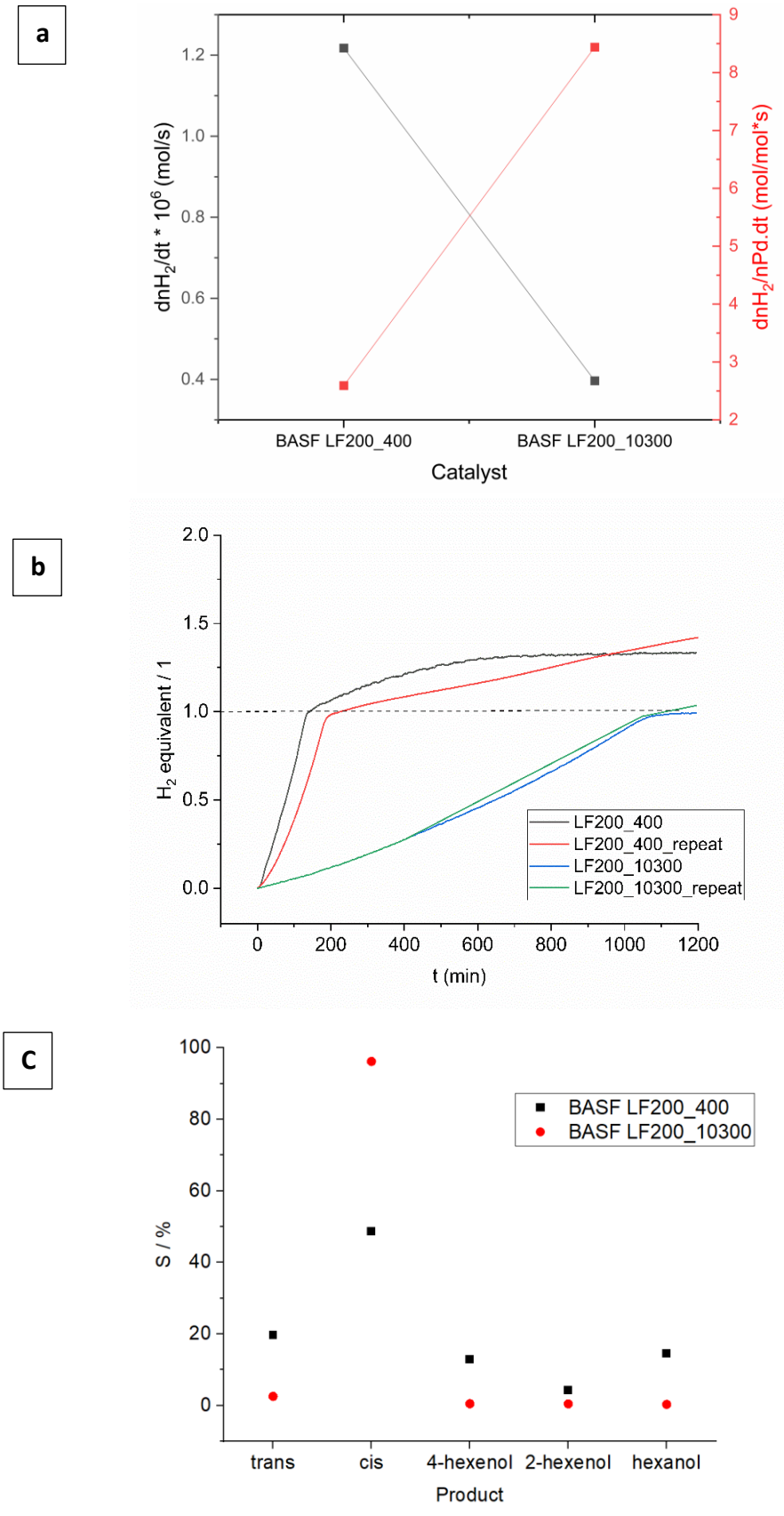

Figure S3. Catalytic hydrogenation of 3-hexyn-1-ol: activity (a) reproducibility (b), and average selectivity (c) of the BASF LF200 catalyst to different products at the end of the reaction (around 100 % conversion) at different $n_{alkynol}/A_{Pd}$ ratios.

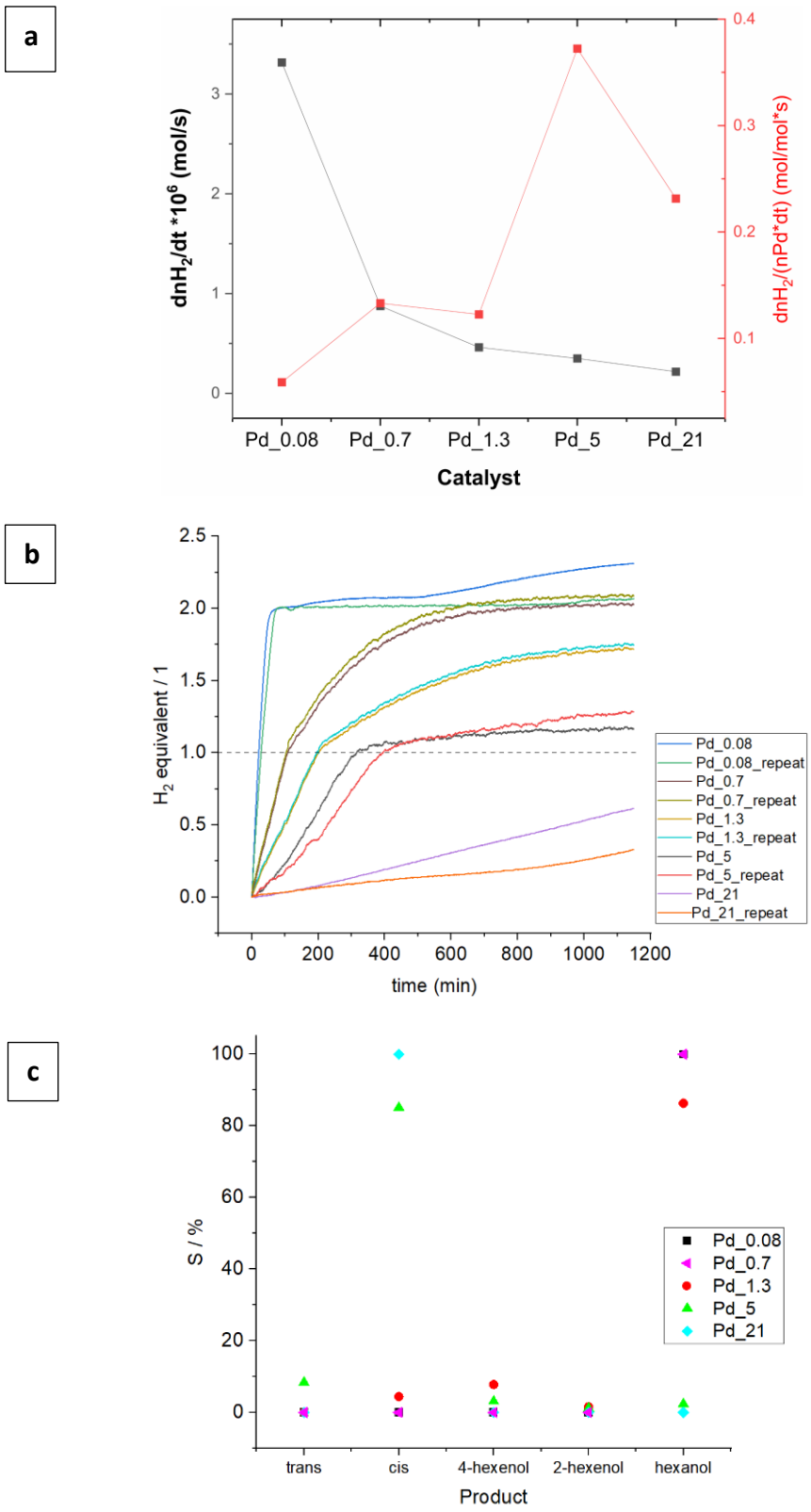

Figure S4. Catalytic hydrogenation of 3-hexyn-1-ol over Pd agglomerates: activity (a), reproducibility (b), and average selectivity at the end of the reaction (c) at different $n_{alkynol}/A_{Pd}$ ratios (all catalytic hydrogenation reactions could reach 99.99 % conversion, except Pd_21 which could reach around 60% at the end of 20 h).

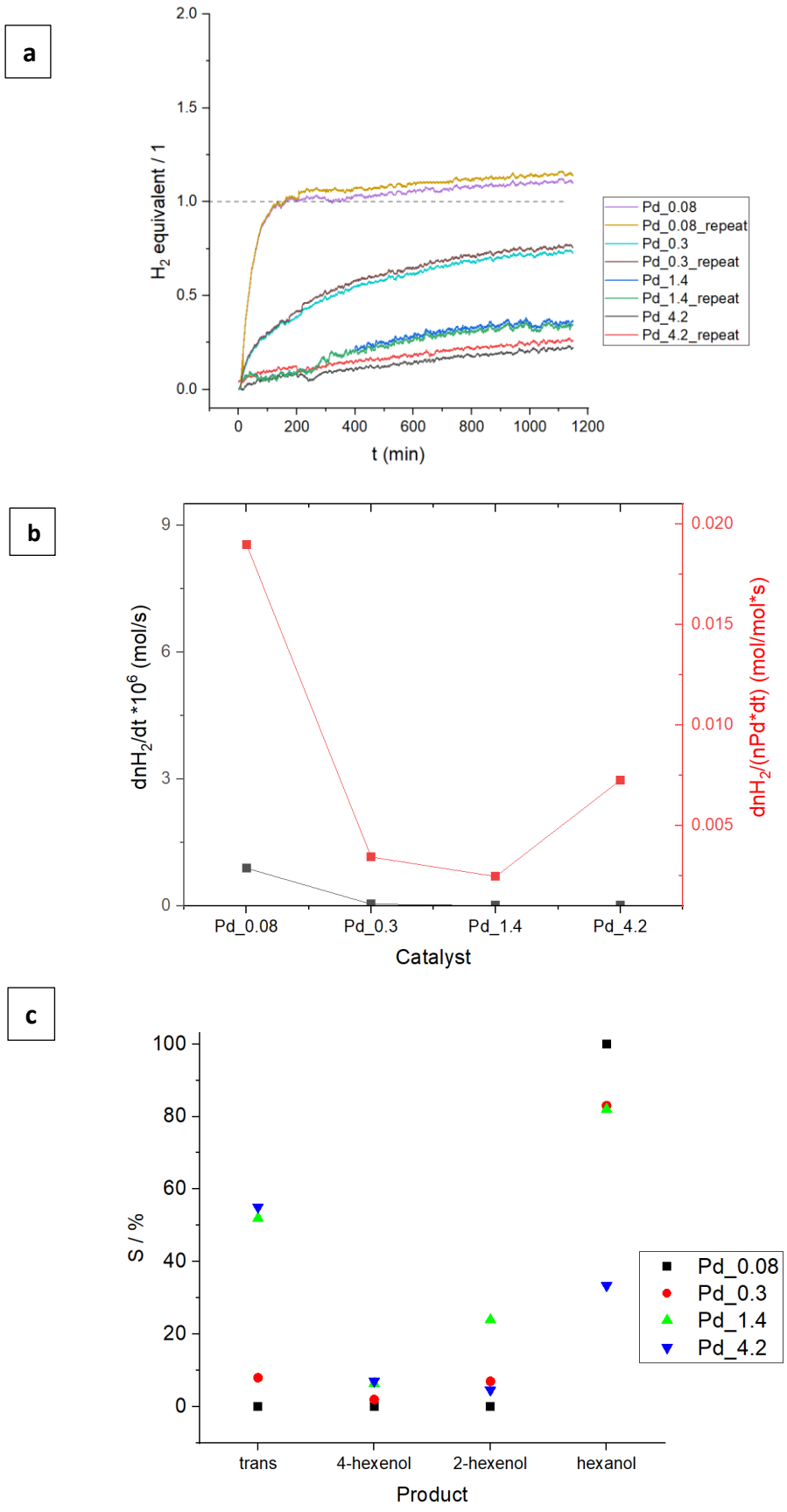

Figure S5. Long-term kinetics plots for catalytic hydrogenation of cis-3-hexen-1-ol by Pd agglomerates at different $n_{alkenol}/A_{Pd}$ ratios, T = 308 K, p = 0.3 MPa, and an agitation rate of 775 RPM, activity (a), reproducibility (b), and average selectivity (c) to different products at the end of the reaction. The conversion values after 20 hours for Pd_0.08, Pd_0.3, Pd_1.4 and Pd_4.2 were around 100 %, 75 %, 25 % and 10 %, respectively.

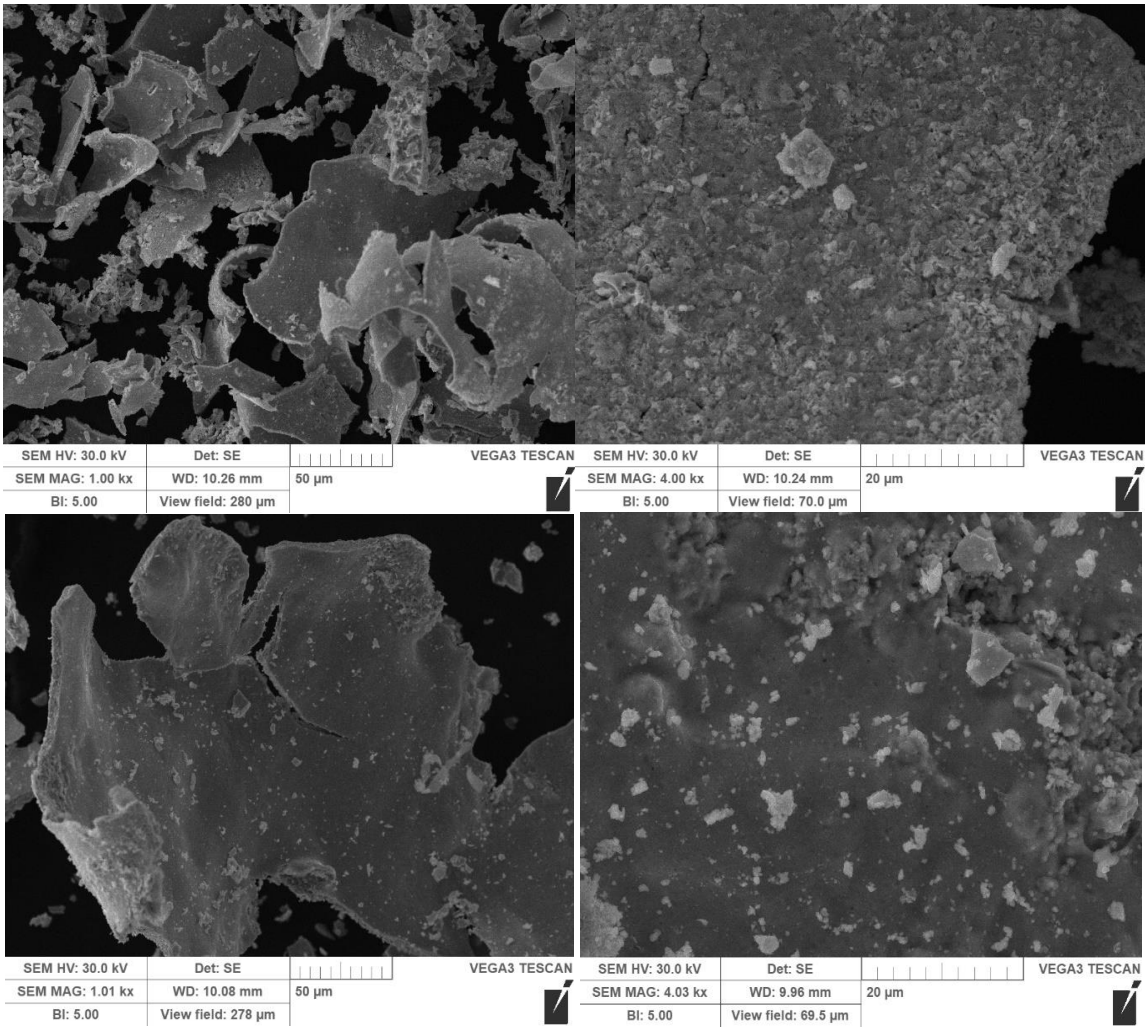

Figure S6. SEM micrographs of Pd_sin (623) particles (top) and Pd_sin (723) particles (bottom).

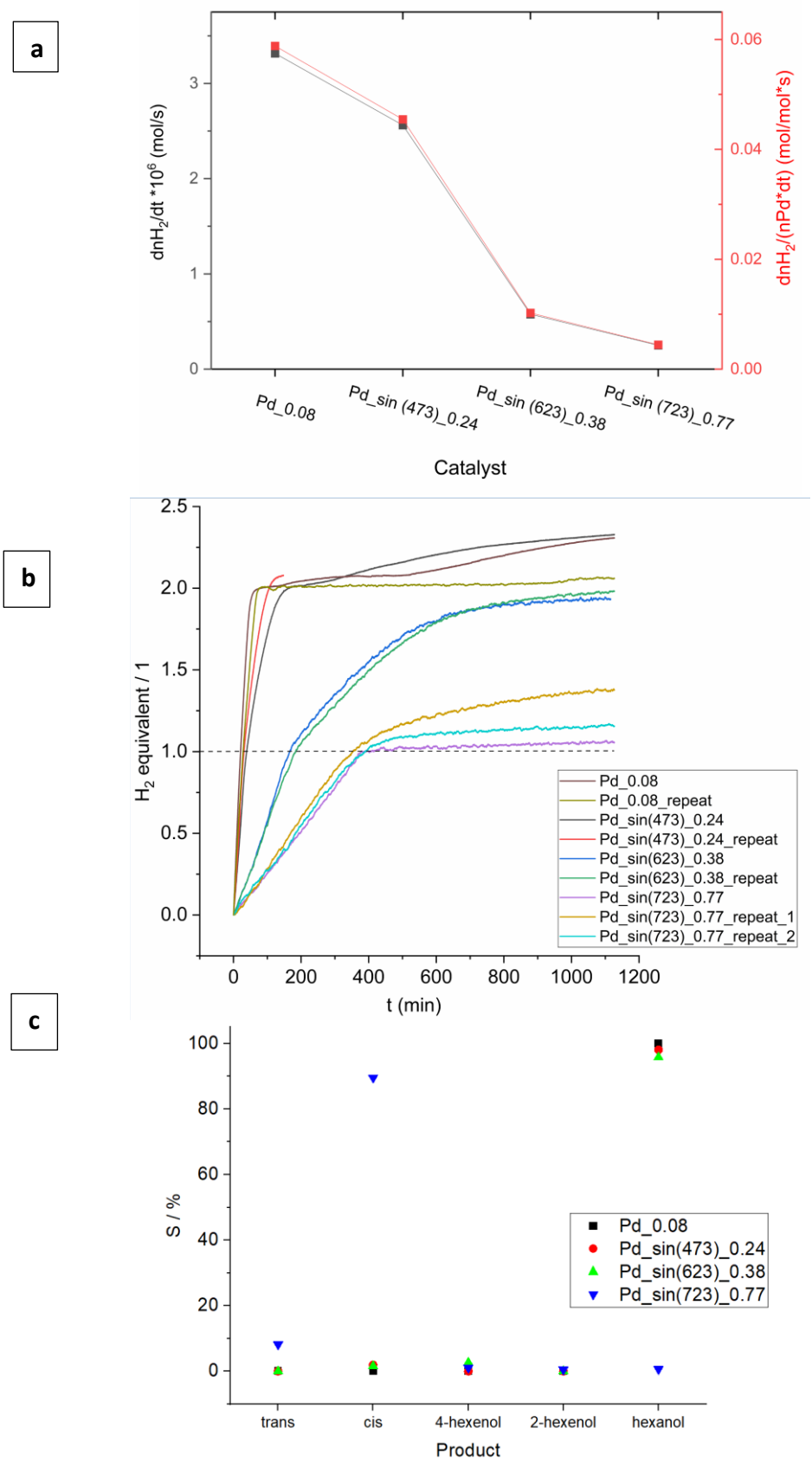

Figure S7. Catalytic hydrogenation of 3-hexyn-1-ol: activity (a), reproducibility (b), and average selectivity (c) of the sintered Pd aggregates at different $n_{alkynol}/A_{Pd}$ ratios (but at the same $n_{alkynol}/n_{Pd}$ molar ratio of 100).

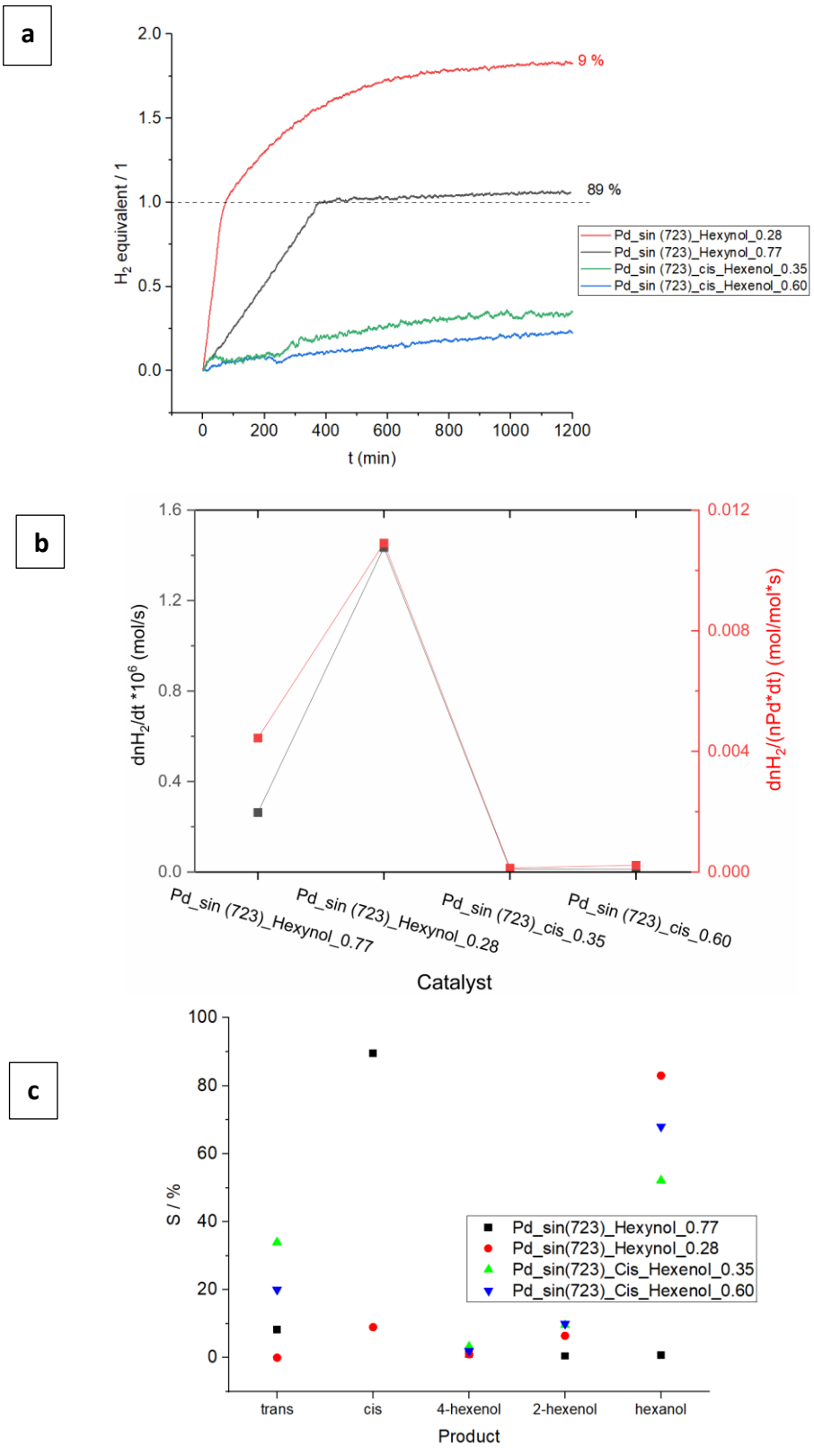

Figure S8. Long-term kinetics plots for catalytic hydrogenation of 3-hexyn-1-ol and cis-3-hexen-1-ol by Pd_sin (723) particles at different $n_{alkynol}/A_{Pd}$ ratios and T = 308 K, p = 0.3 MPa, and an agitation rate of 775 RPM (a): for the heyxnol substrate, at H_2 eq. = 1, the conversion value and also the selectivity to the cis-hexenol are considered to be around 100 %, while by further H_2 uptake isomer products are produced and the selectivity to the cis-hexenol drops to lower values. For the cis-hexenol substrate, the activity in both cases could not reach 100 %; activity (b), and average selectivity of the Pd_sin (723) aggregates to different products (c) at different $n_{alkynol}/A_{Pd}$ ratios at the end of the reaction. The numbers shown at the end of each curve in (a) give the average cis-hexenol selectivity.