Supplementary information to:

Kinetic modelling of reactions for the synthesis of 2methyl-5-ethyl pyridine

Emanuele Moioli^{*1,2,+}, Leo Schmid², Peter Wasserscheid¹, Hannsjörg Freund¹

¹Lehrstuhl für Chemische Reaktionstechnik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Egerlandstrasse 3, DE-91058 Erlangen, Germany

²Specialty Ingredients Research & Technology, Lonza Ltd., Lonzastrasse, CH-3930 Visp, Switzerland

⁺Current address: Paul Scherrer Institute, Forschungstrasse 111, CH-5232 Villigen, Switzerland

*Corresponding author: Emanuele Moioli, email: emanuele.moioli@fau.de

Analysis of the side products of the reaction para to MEP

The reaction para to MEP proceeds similarly to the reaction AAT to MEP, as analysed in detail in the main manuscript. Here, we report the analysis of the reaction side products with the Schulz-Flory model, in analogy to the main manuscript. Figure S1 shows the regression lines for the determination of the α values for the reaction from para, using 5 and 20 wt.-% initial concentrations, respectively. It can be observed that the results are quite similar to that of the AAT case which are reported in figure 5 in the main manuscript. In particular, it is possible to identify two areas for the linear regression below and above n=16, characterised by different values of α . Furthermore, in figure S2 we can observe that α_1 and α_2 increase with the initial concentration of para, exactly as in the case of AAT. Therefore, the model equation (4) derived in the main manuscript is valid for both, the reaction of AAT to MEP and the reaction of para to MEP.



Figure S1 Graph for the determination of the two parameters in the Schulz-Flory polymer distribution for the reaction para to MEP. The lines show the linear regression used for the determination of α . Experimental conditions: T=200°C, initial pressure: 1 bar, promoter/reactant ratio: 1:1 mol/mol.



Figure S2 Trend of α as a function of the initial para concentration. The dotted lines are the regression lines for the three data points of α_1 and α_2 calculated at various para initial concentrations. Experimental conditions: T=200°C, initial pressure: 1 bar, promoter/reactant ratio: 1:1 mol/mol.