

Supporting Information

Electrocatalytic cross-coupling of biogenic di-acids for the sustainable production of fuels

F. Joschka Holzhäuser,^a Guido Creusen,^b Gilles Moos, Manuel Dahmen,^c Andrea König,^d Jens

Artz,^a Stefan Palkovits^a and Regina Palkovits^{a,*}

a Institut für Technische und Makromolekulare Chemie, RWTH Aachen University, Aachen, Germany. [*palkovits@itmc.rwth-aachen.de]

b Institut für Makromolekulare Chemie, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany.

c Institut für Energie- und Klimaforschung Modellierung von Energiesystemen, Forschungszentrum Jülich, Jülich, Germany

d Aachener Verfahrenstechnik - Process Systems Engineering, RWTH Aachen University, Aachen, Germany

- 1. Calculations**
- 2. Experimental photographs**
- 3. NMR spectra**
- 4. Additional charts**
- 5. Total faradaic efficiency charts**

1. Calculations

Calculation of charge chronoamperometry (Q = charge, I = current, t = time):

$$Q = \int_x^y I dt$$

Calculation of charge potentiometry:

$$Q = It$$

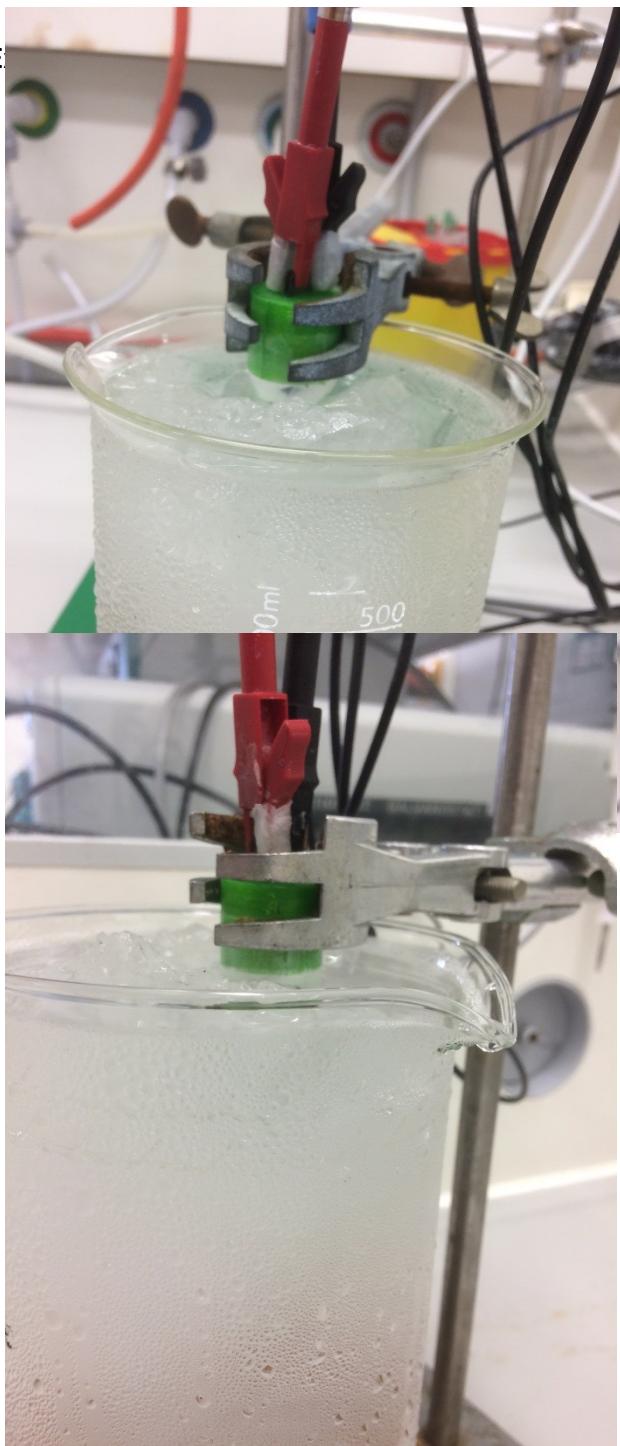
Calculation of the faradiac efficiency (n_{mol} = amount of total product amount in mol, n = number of electrons transferred, F = Faraday constant):

$$F_{eff} = \frac{n_{mol} n F}{Q} \cdot 100\%$$

For 1 faradaic equivalent the equation becomes ($n_{mol-spl}$ = simplified factor [dimensionless]):

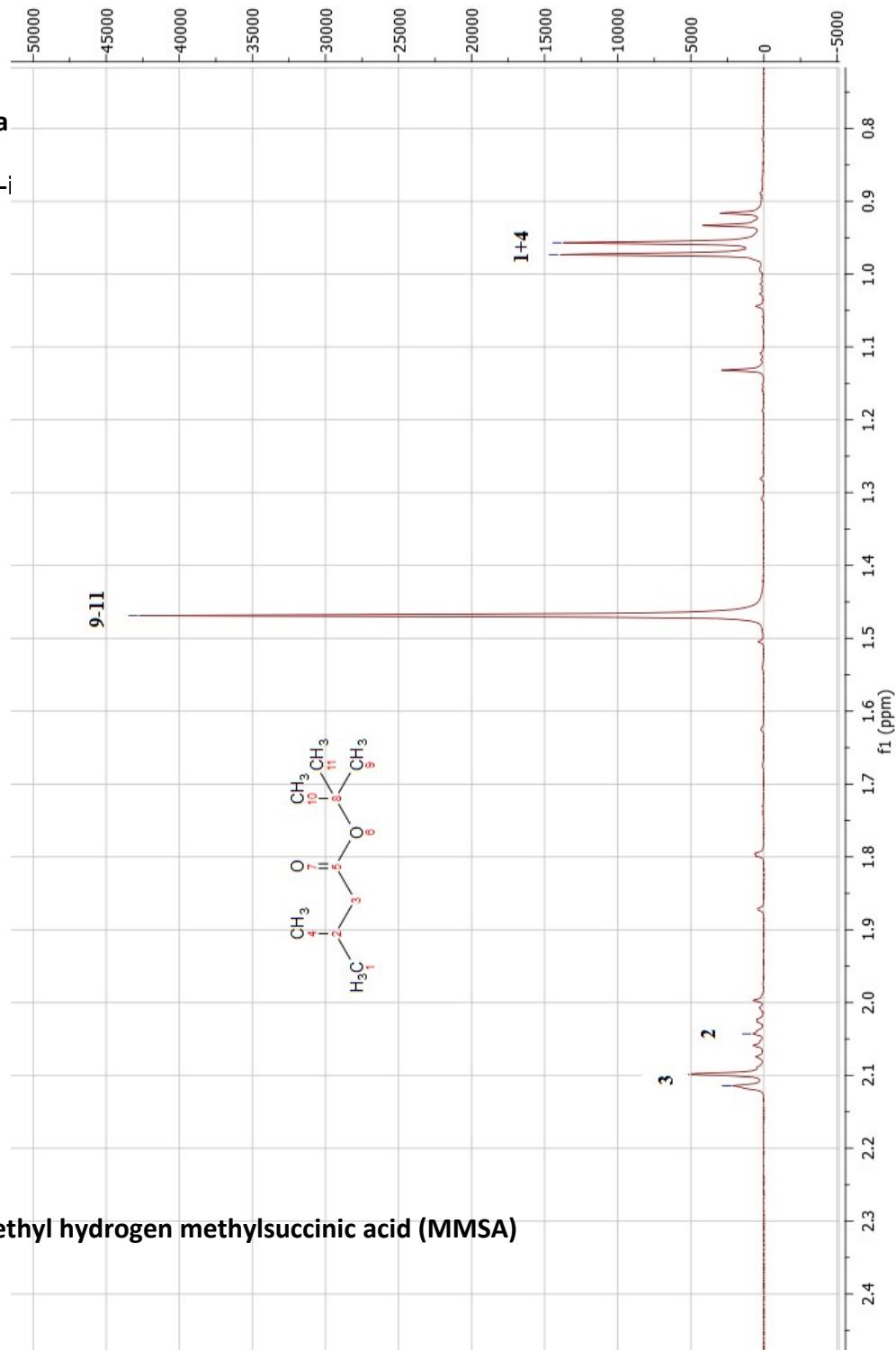
$$F_{eff} = n_{mol-spl} \cdot 100\%$$

2. E

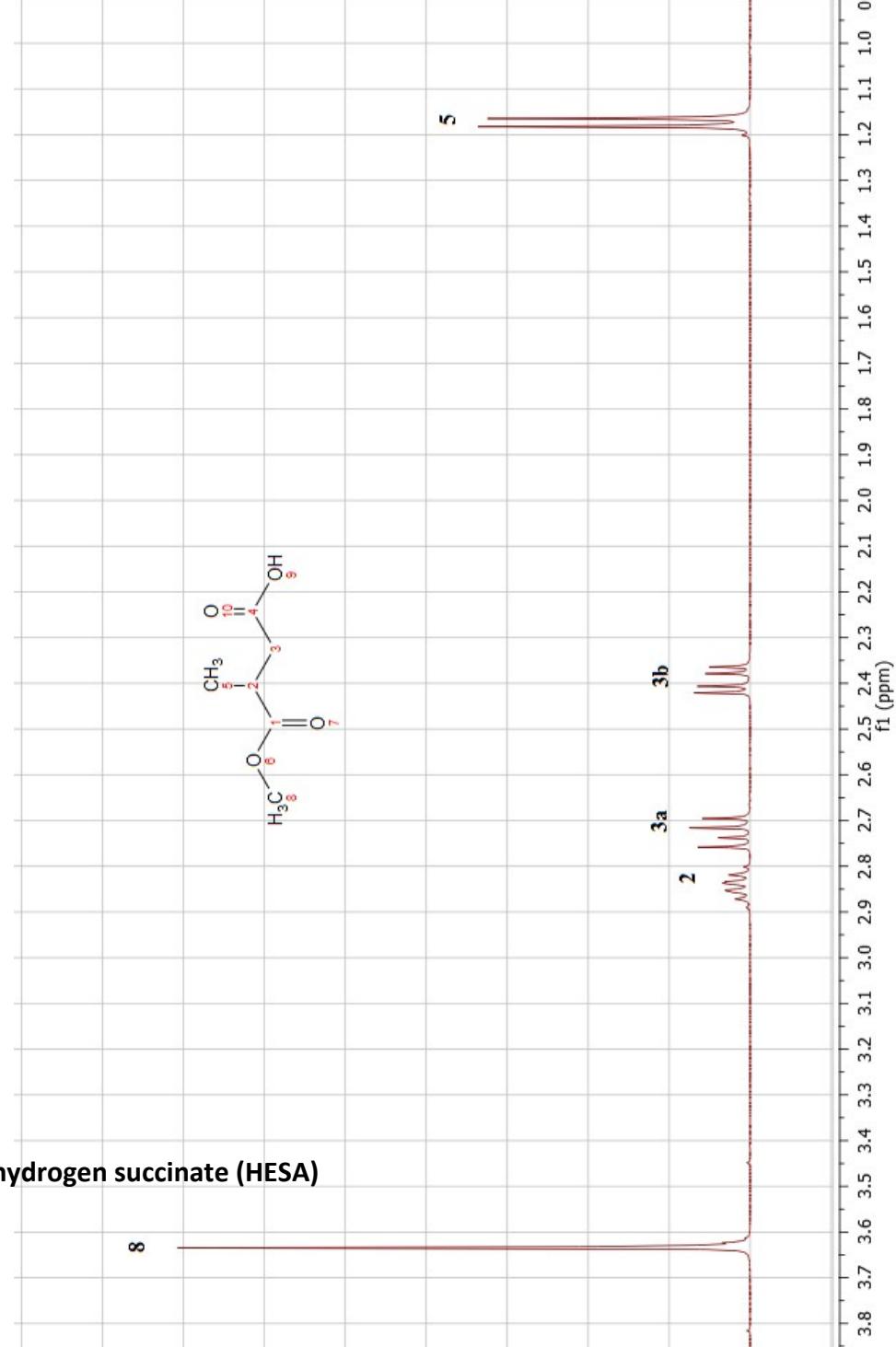
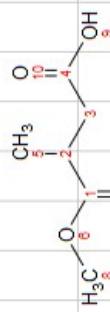


3. NMR spectra

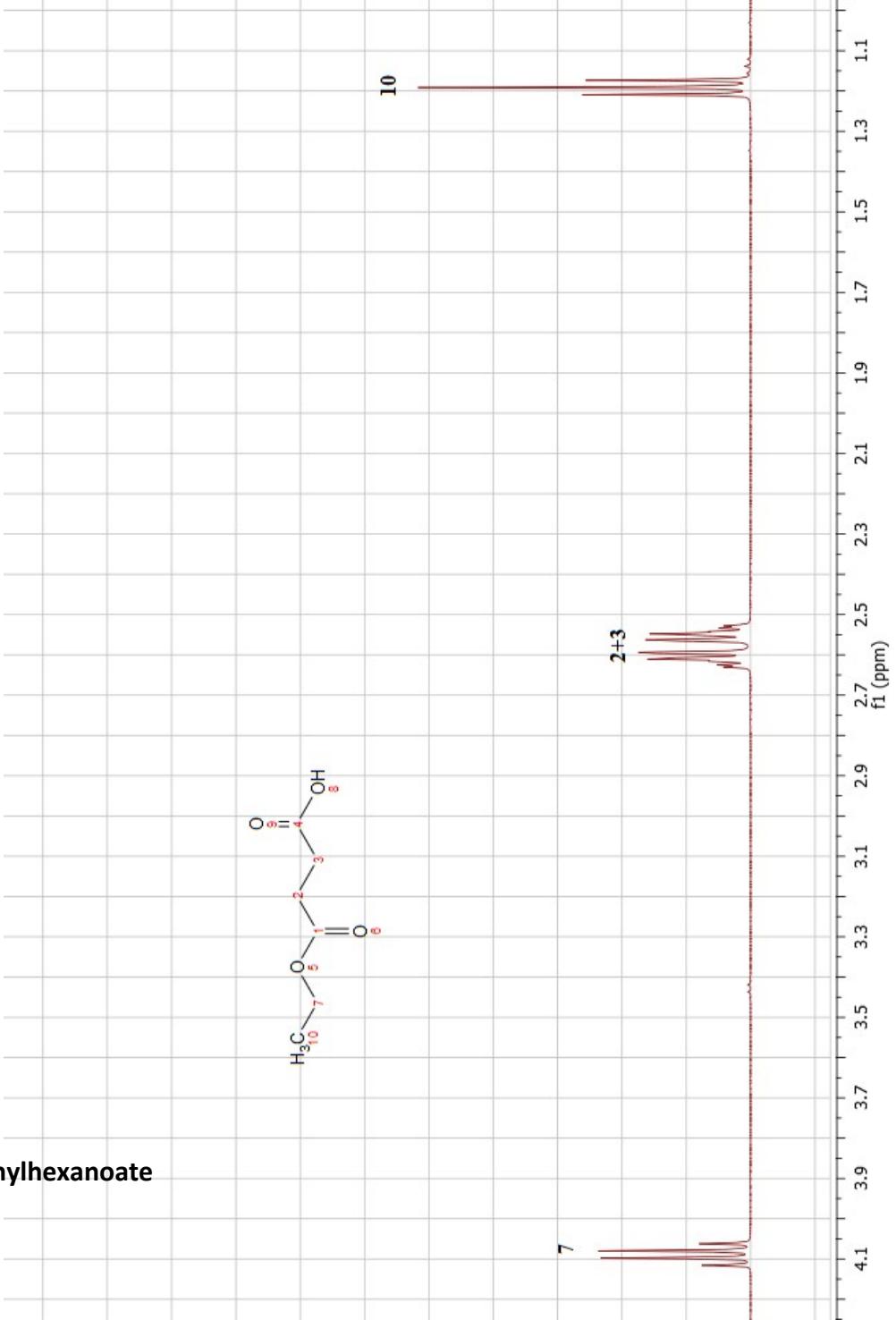
¹H-NMR: Tertbutyl-i

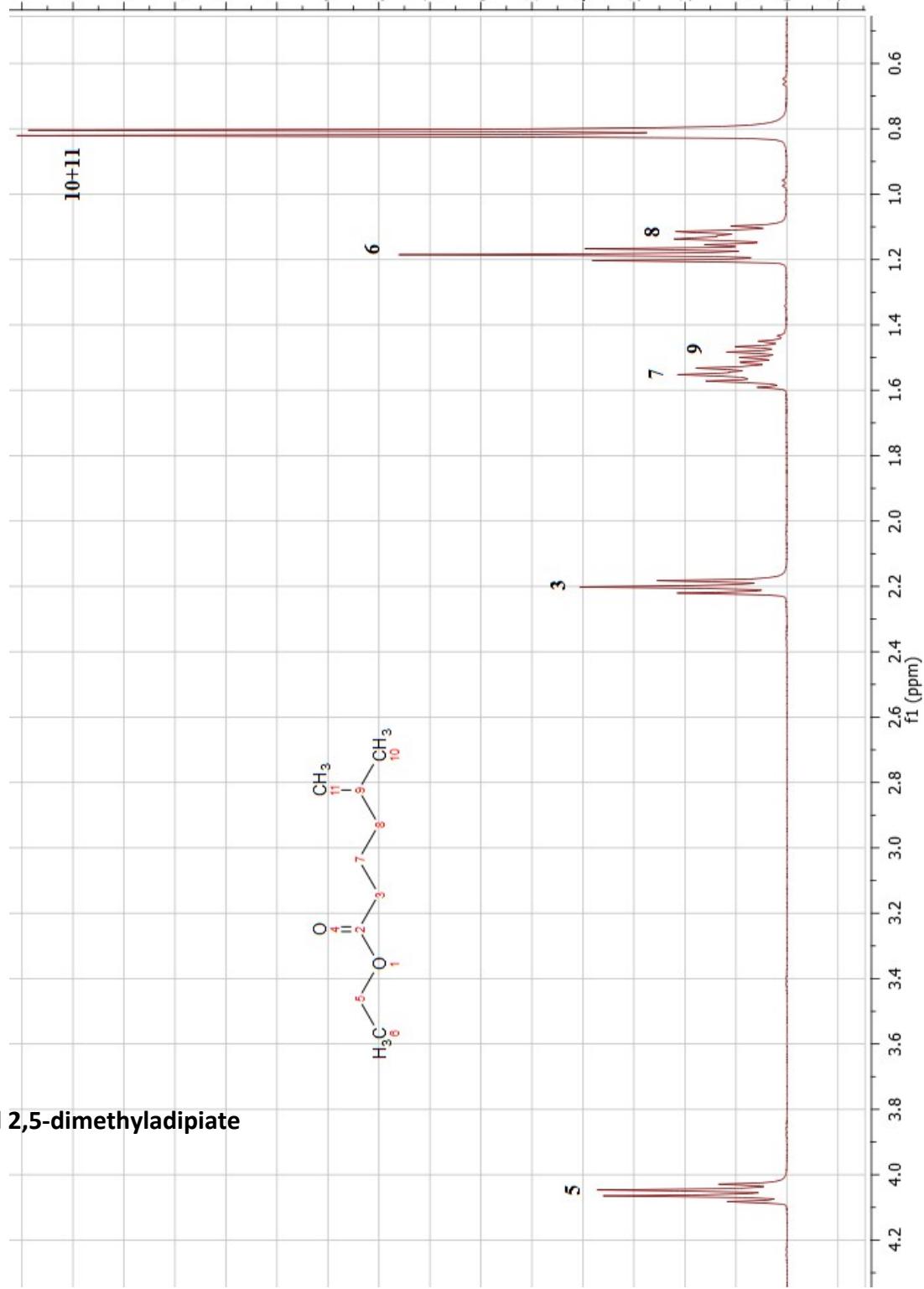


¹H-NMR: mono-Ethyl hydrogen succinate (HESA)



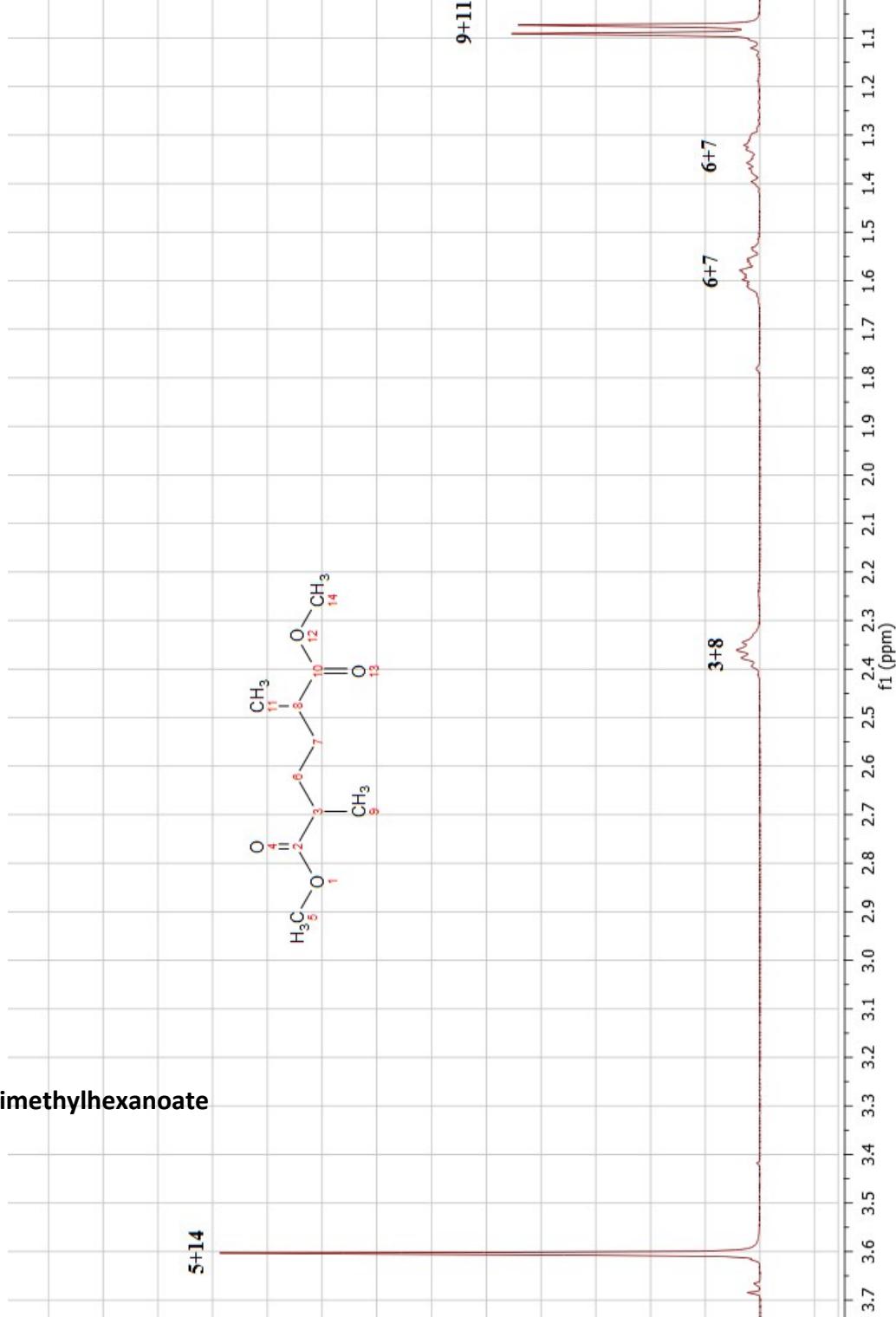
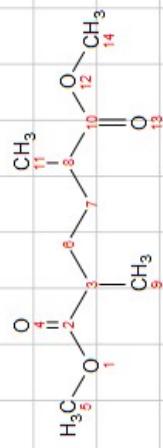
¹H-NMR: Ethyl 5-methylhexanoate



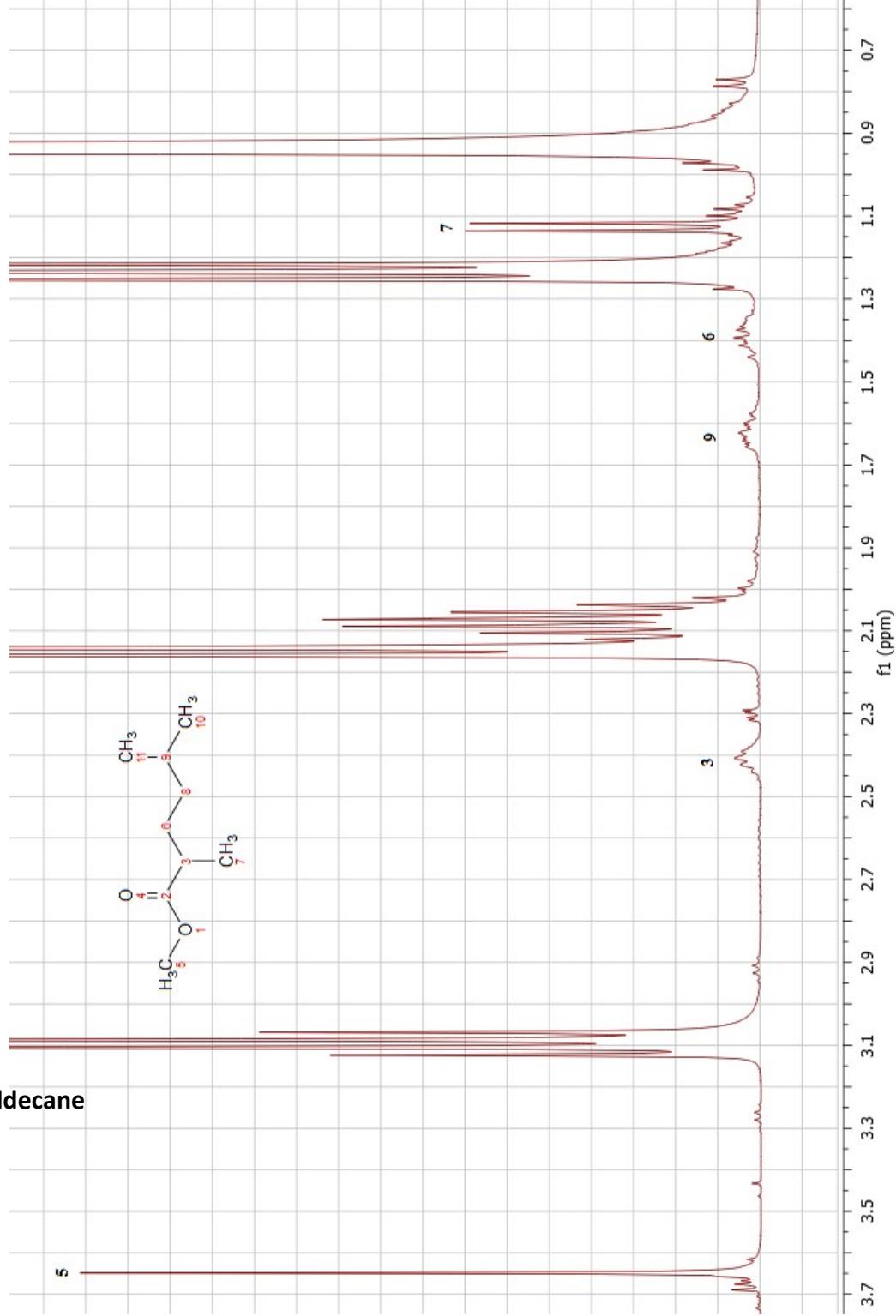


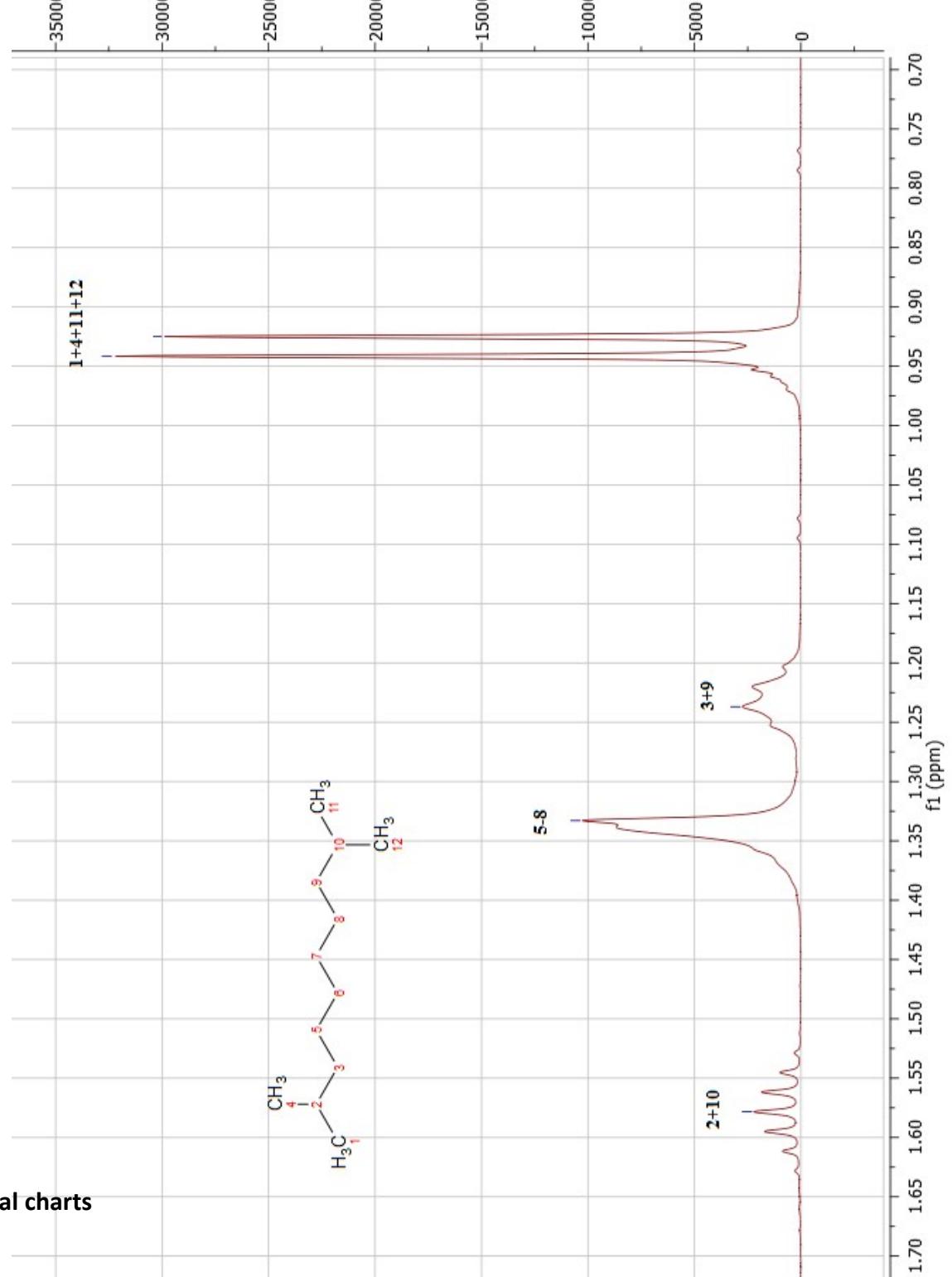
^1H -NMR: Dimethyl 2,5-dimethyladipate

¹H-NMR: Methyl 2,5-dimethylhexanoate



¹H-NMR: 2,9-Dimethyldecane





4. Additional charts

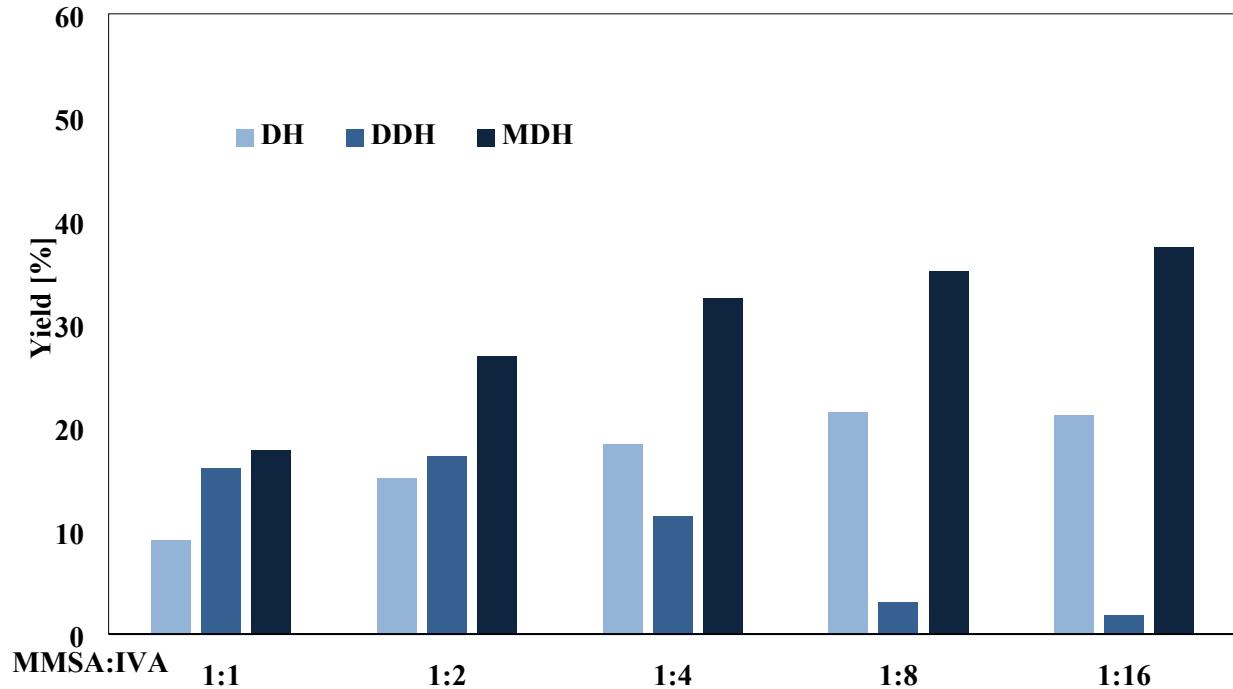


Figure 1a: Variation of different ratios of MMSA with IVA. Conditions: 0 °C, MeOH:H₂O 80:20, 1 farad equivalent, 0.1 M NEt₃, 100 mAc⁻², WE: Pt, CE: Ti. Yield of MDH/ DDH related to MMSA, DH related to IVA (total Volume 5 mL).

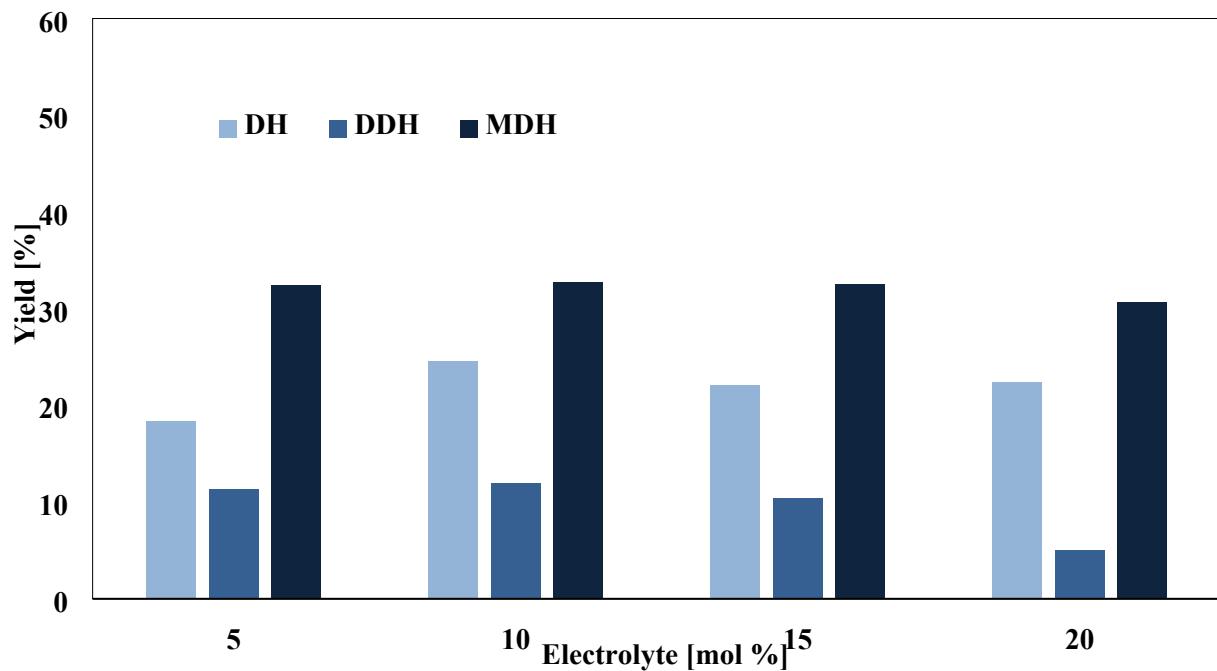


Figure 2a: Variation of the electrolyte concentration. Conditions: 0 °C, MeOH:H₂O 80:20, 1 farad equivalent, 100 mAc⁻², WE: Pt, CE: Ti, 0.33 M MMSA, 1.3 M IVA. Yield of MDH/ DDH related to MMSA, DH related to IVA (total Volume 5 mL).

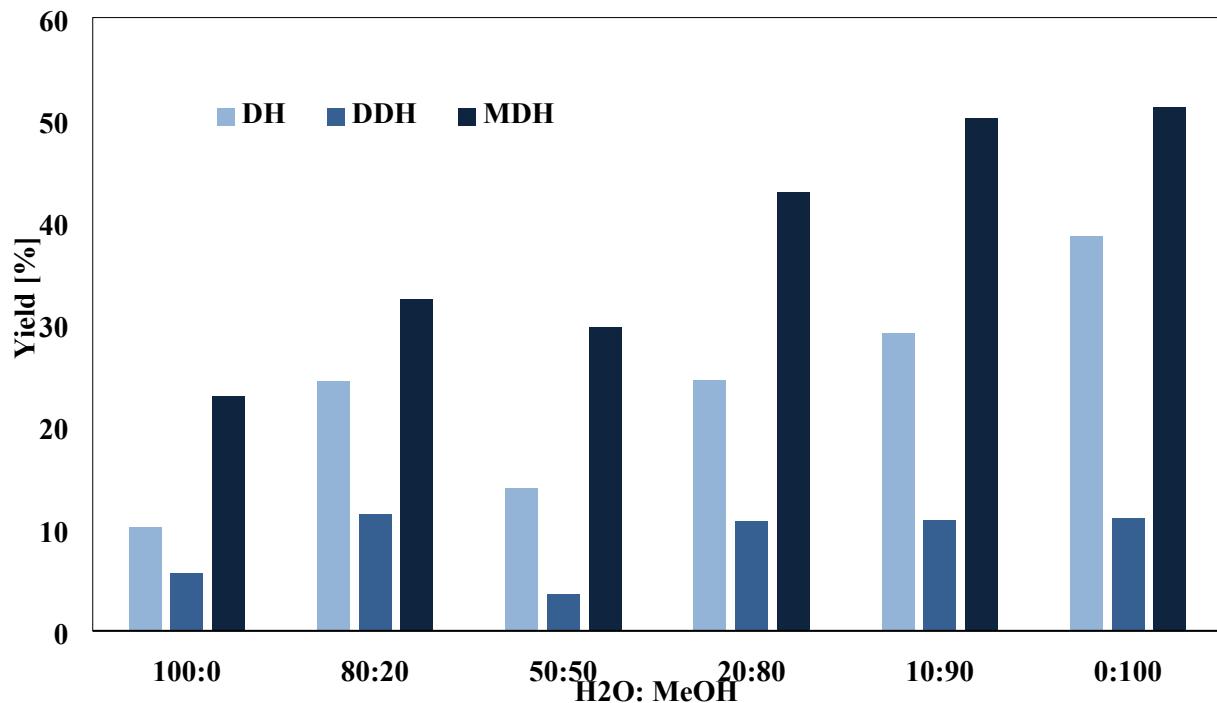


Figure 3a: Variation of the solvent mixture. Conditions: 0 °C, 1 farad equivalent, 100 mAc⁻², WE: Pt, CE: Ti, 0.33 M MMSA, 1.3 M IVA, 0.1 M NEt₃ (for 100% Water: 0.1 M MMSA, 0.4 M IVA). Yield of MDH/ DDH related to MMSA, DH related to IVA (total Volume 5 mL).

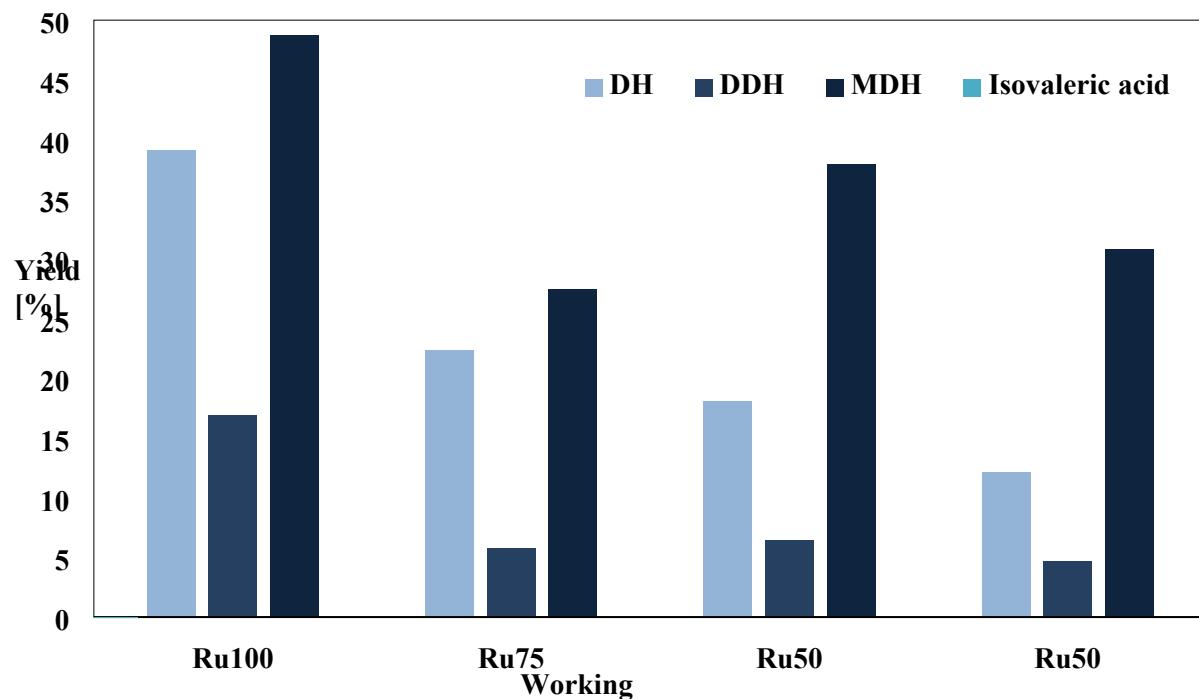
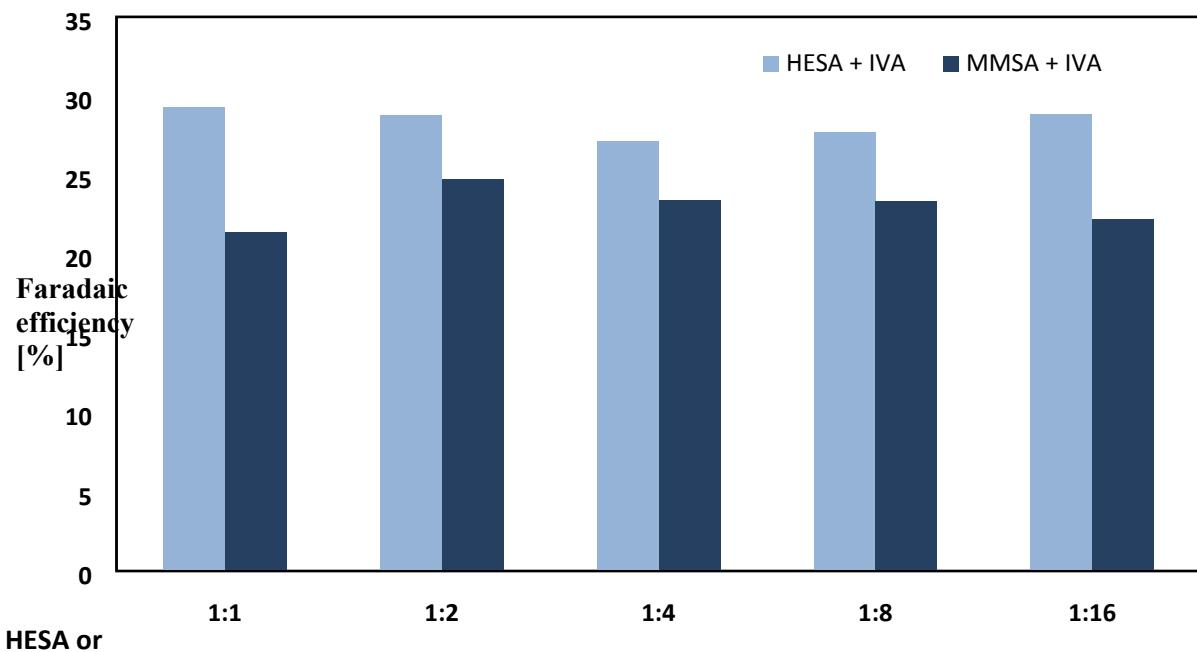
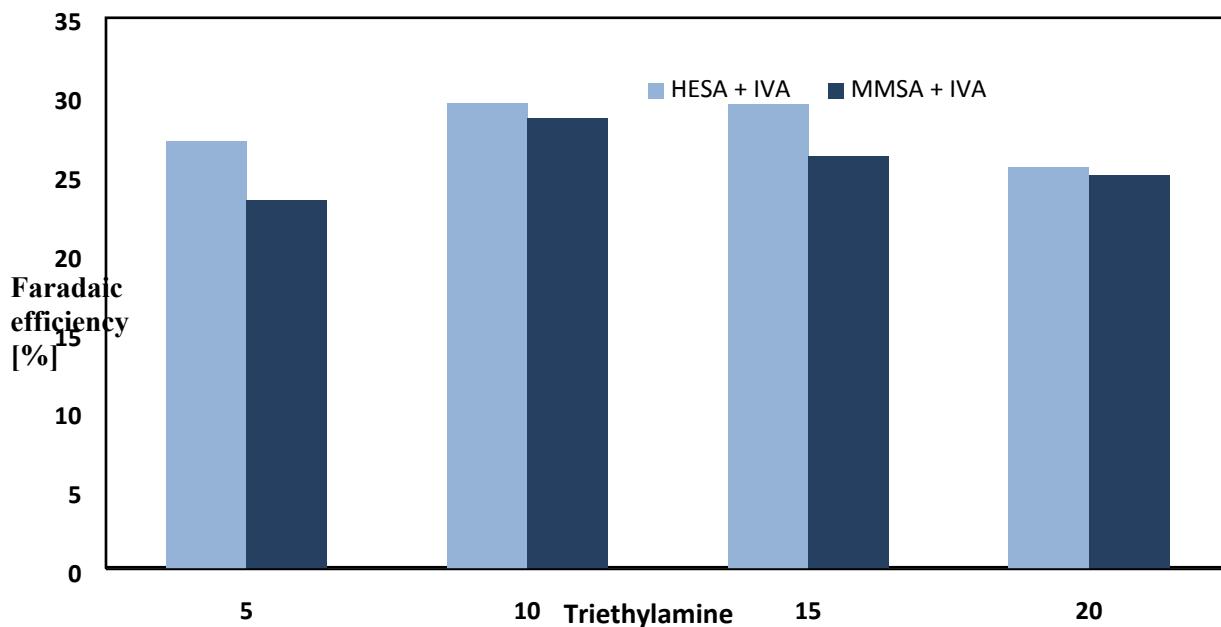


Figure 4a: Screening of (Ru_xTi_{1-x})O₂ on titanium plates in comparison with Pt. Conditions: 0 °C, 1 farad equivalent, 100 mAc⁻², MeOH as solvent, CE: Ti, 0.33 M MMSA, 1.3 M IVA, 0.1 M NEt₃. Yield of MDH/ DDH related to MMSA, DH related to IVA (total Volume 2 mL).

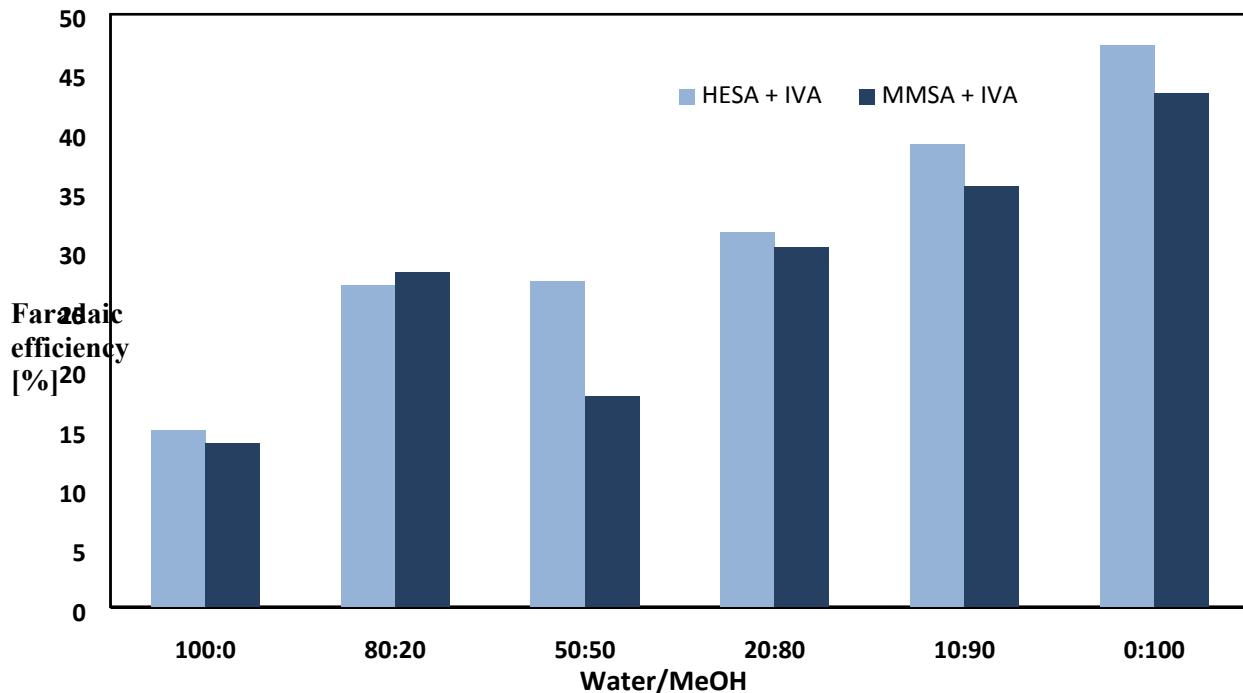
5. Total faradaic efficiency charts (Complete new Section!)



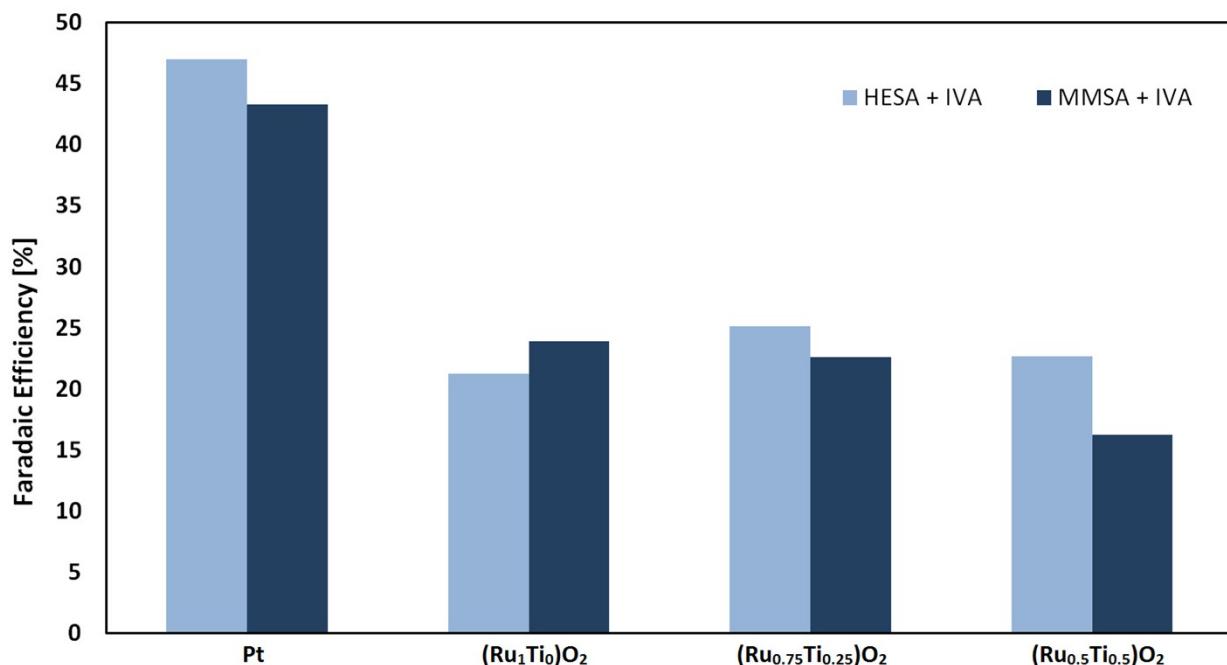
For Figure 1(left) + Figure 1a: Variation of different ratios of MMSA/HESA with IVA. Conditions: 0 °C, MeOH:H₂O 80:20, after 1 farad equivalent, 0.1 M NEt₃, 100 mAc⁻², WE: Pt, CE: Ti.



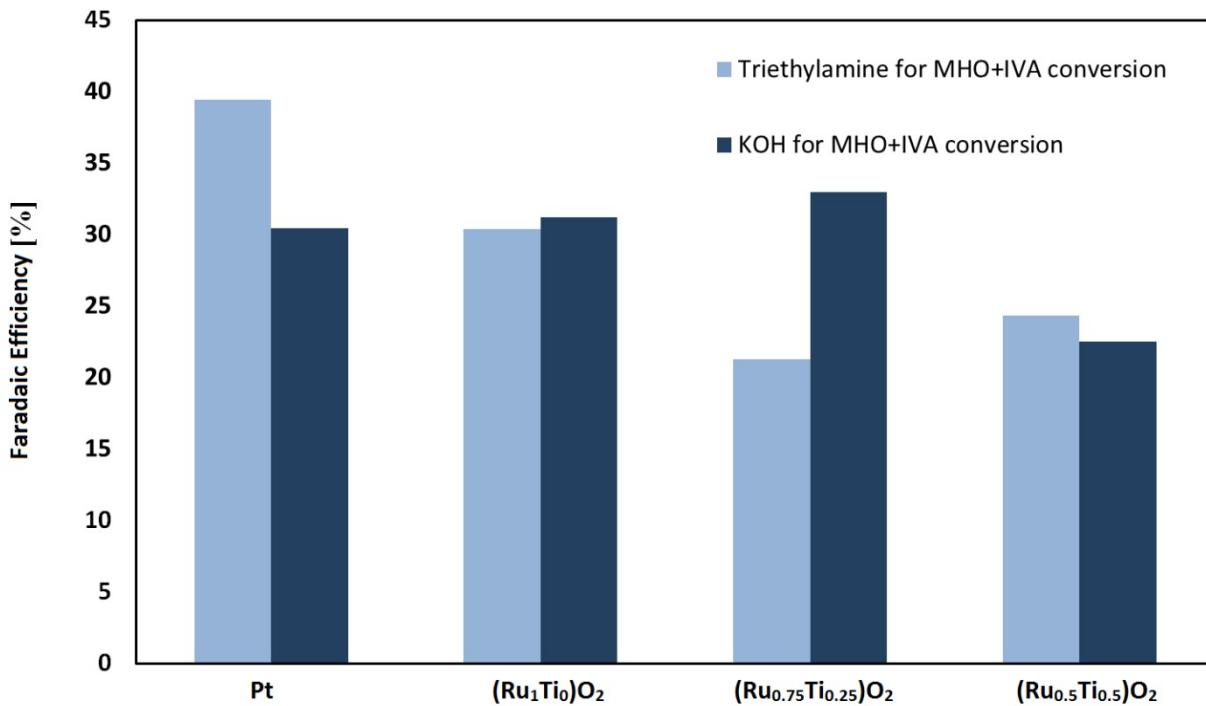
For Figure 1(right) + Figure 2a: Variation of the electrolyte concentration. Conditions: 0 °C, MeOH:H₂O 80:20, after 1 farad equivalent, 100 mAc⁻², WE: Pt, CE: Ti, 0.33 M MMSA/HESA, 1.3 M IVA.



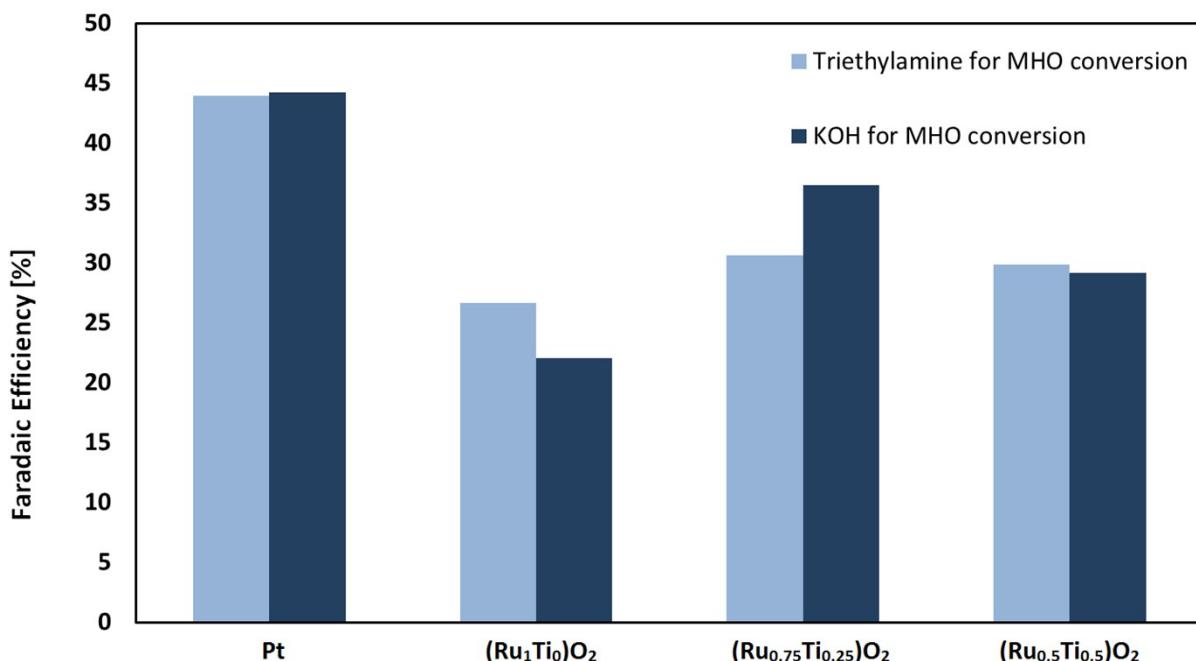
For Figure 2 + Figure 3a: Variation of the solvent mixture. Conditions: 0 °C, after 1 farad equivalent, 100 mAc m^{-2} , WE: Pt, CE: Ti, 0.33 M MMSA/HESA, 1.3 M IVA, 0.1 M NEt₃ (for 100% Water: 0.1 M MMSA/HESA, 0.4 M IVA).



For Figure 3 + Figure 4a: Screening of (Ru_xTi_{1-x})O₂ on titanium plates in comparison with Pt. Conditions: 0 °C, after 1 farad equivalent, 100 mAc m^{-2} , MeOH as solvent, CE: Ti, 0.33 M MMSA/HESA, 1.3 M IVA, 0.1 M NEt₃.



For Figure 4: Screening of $(\text{Ru}_x\text{Ti}_{1-x})\text{O}_2$ on Ti and Pt plates with different electrolytes. Left: Using 0.1 M NEt_3 as electrolyte and base. Right: Using 0.1 M KOH as electrolyte and base. General conditions: 0 °C, after 1 farad equivalent, 100 mA cm^{-2} , MeOH as solvent, CE: Ti, 0.33 M MHO, 1.3 M IVA.



For Figure 5: Screening of $(\text{Ru}_x\text{Ti}_{1-x})\text{O}_2$ on Ti and Pt plates with different electrolytes. General conditions: 0 °C, after 1 farad equivalent, 100 mA cm^{-2} , MeOH as solvent, CE: Ti, 1 M MHO.