Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information for:

Aerobic oxidation of C_4-C_6 α,ω- diols to the diacids in base-free medium over zirconia-supported (bi)metallic catalysts.

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New Journal of Chemistry

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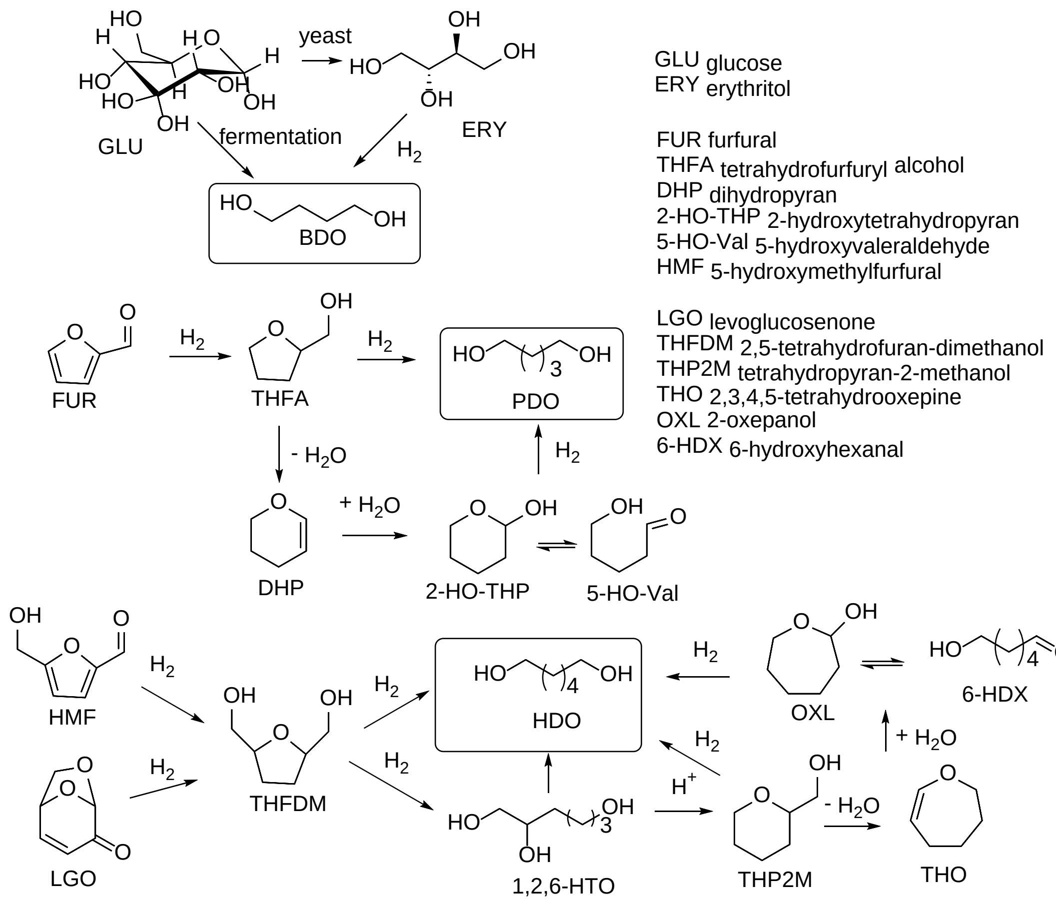
Fig. S4. Evolution of (▽) PDO conversion and yields of (◆) ALD, (▲) HA, (□) AA, and (●) DA versus time depending on NaOH amount ratio at 70°C under 40 bar of air over Au/ZrO_2: (a) NaOH =1 eq., (b) NaOH = 2 eq., (c) NaOH = 4 eq., (✳) carbon balance, and (★) TOC measurement.

Fig. S5. Reaction profile for HDO oxidation over Au/ZrO_2 in the presence of 2 eq. NaOH. (▽) HDO conversion and (◆) ALD, (▲) HA, (□) AA and (●) DA yields versus time at 70°C, 40 bar of air, (✳) carbon balance.



Scheme S1. Possible reaction networks to 1,4-butanediol (BDO), 1,5-pentanediol (PDO), and 1,6-hexanediol (HDO) from lignocellulosic biomass.

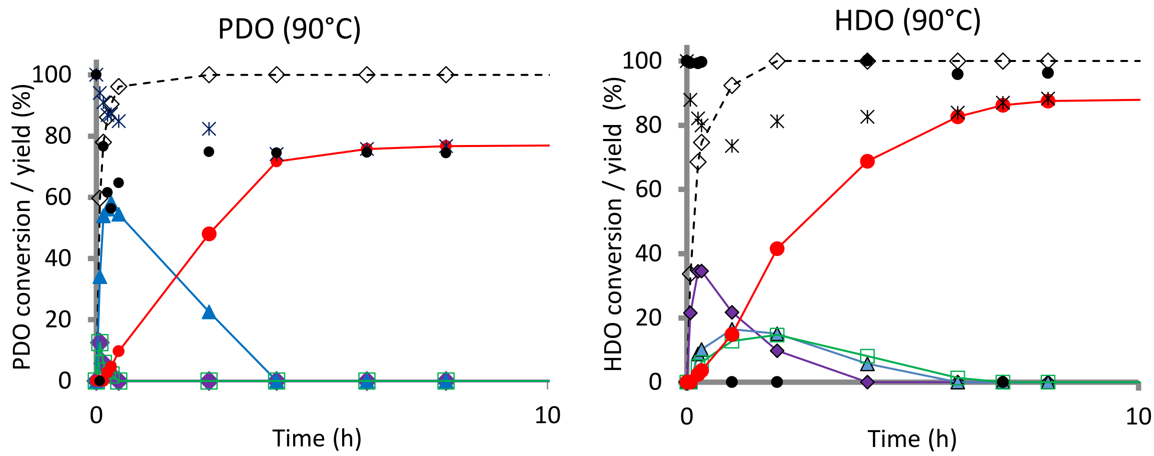
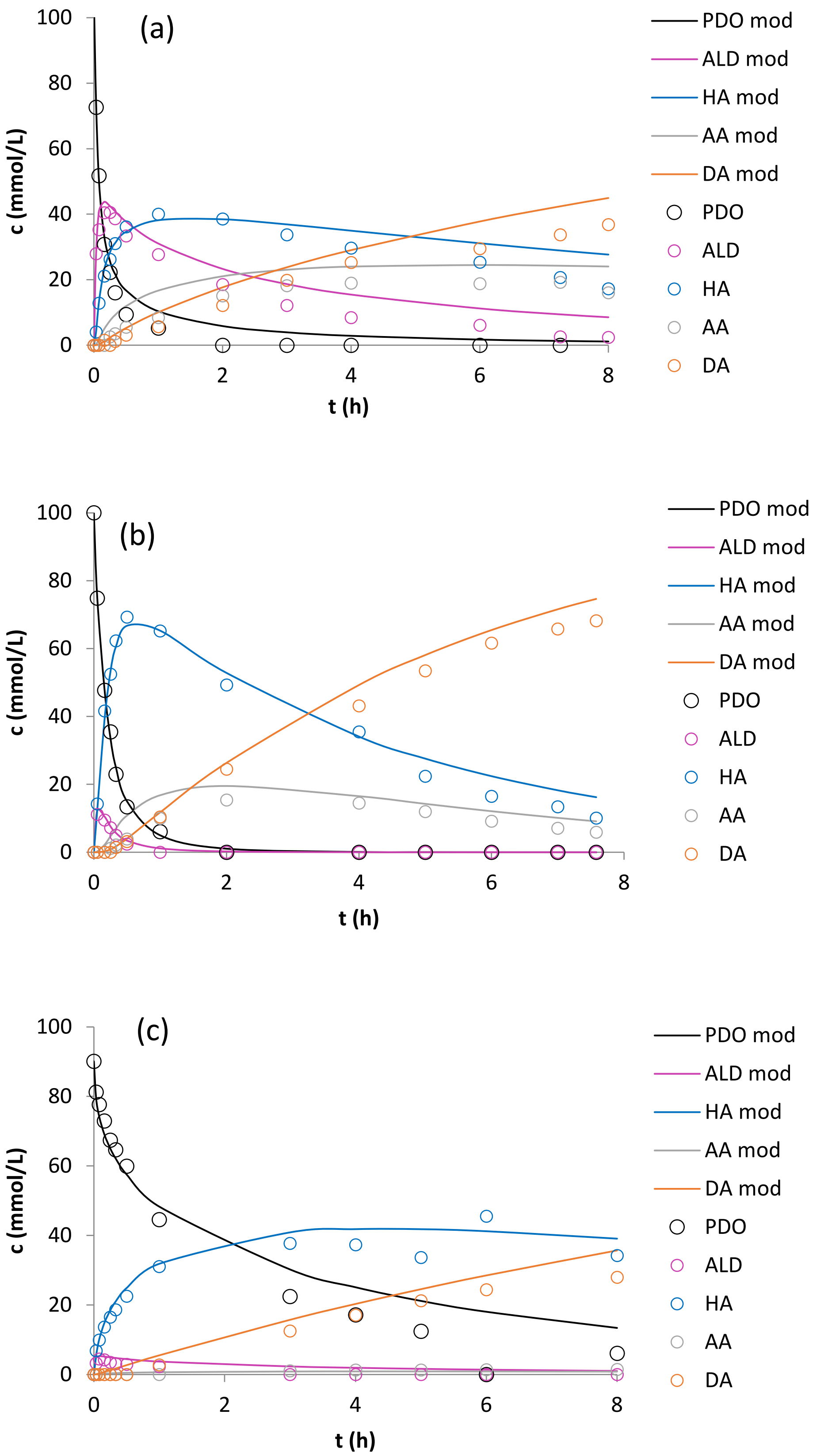


Fig. S1. Evolution of (◊) diol conversion and yields into (◆) ALD, (▲) HA, (□) AA and (●) DA from (a) PDO , (b) HDO over Au-Pt/ZrO_2 under 40 bar of air at 90°C and diol/metal = 100 in base-free medium, (⁎) Carbon balance, CB, and (•) TOC.


(a)
(b)
(c)
c (mmol/L)
t (h)
PDO mod
ALD mod
HA mod
AA mod
DA mod
PDO
ALD
HA
AA
DA

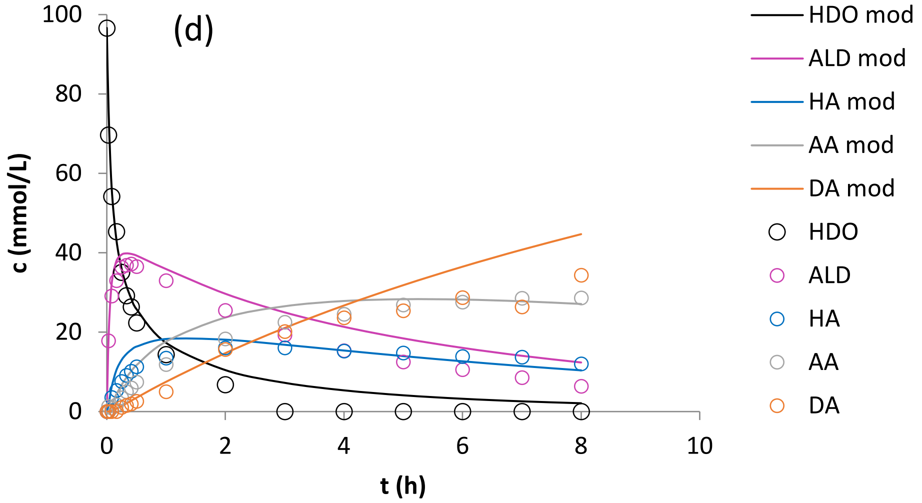
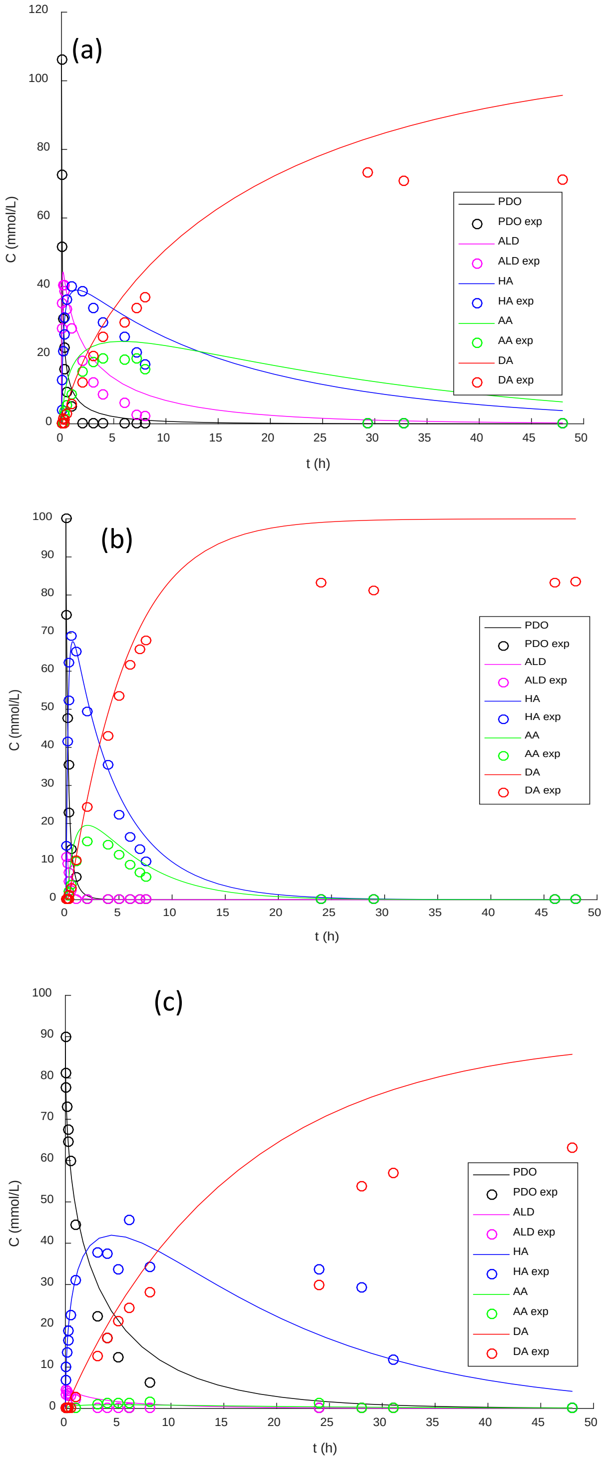


Fig. S2. Comparison of experimental (points) and predicted (lines) concentration-time profiles for (a) PDO oxidation over Pt, (b) PDO over Au-Pt, (c) PDO over Au-Pd, and (d) HDO over Pt. Reaction conditions: 0.1 M diol, 70°C, 40 bar air, diol/metal molar ratio = 100.


(a)
C (mmol/L)
t (h)
PDO
PDO exp
ALD
ALD exp
HA
HA exp
AA
AA exp
DA
DA exp
(b)
C (mmol/L)
t (h)
PDO
PDO exp
ALD
ALD exp
HA
HA exp
AA
AA exp
DA
DA exp
(c)
C (mmol/L)
t (h)
PDO
PDO exp
ALD
ALD exp
HA
HA exp
AA
AA exp
DA
DA exp

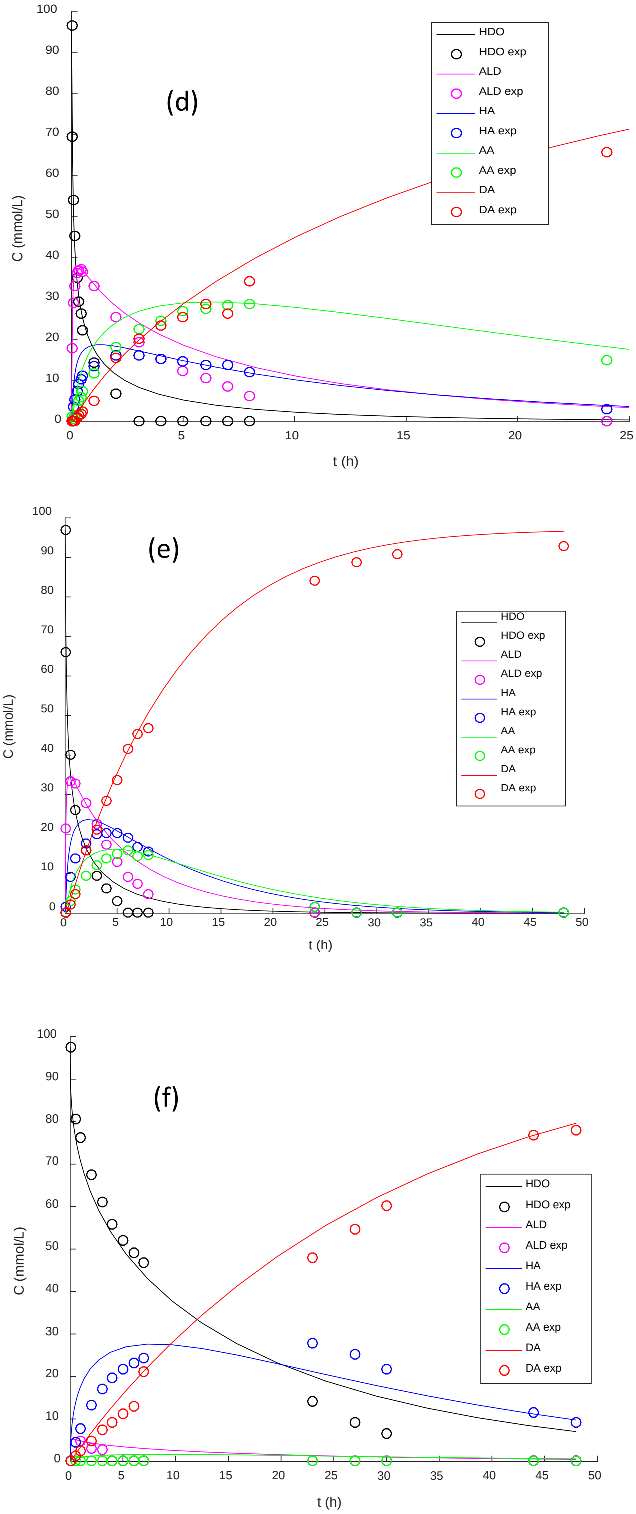
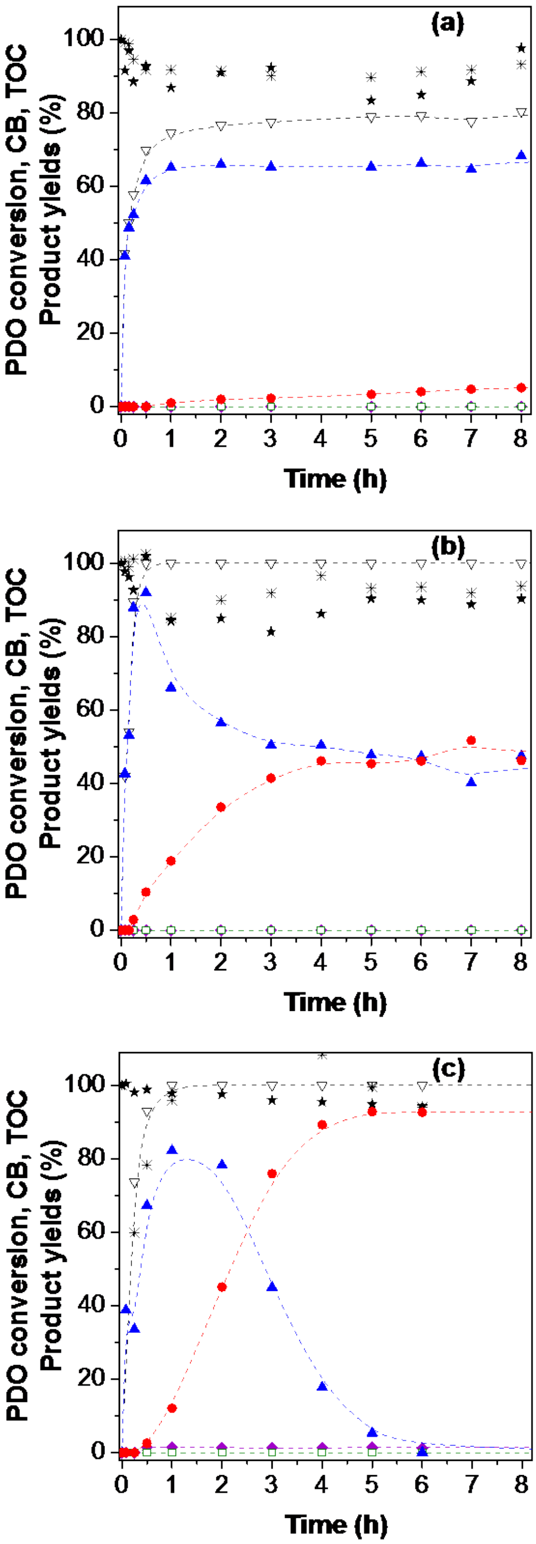


Fig. S3. Comparison of experimental (points) and predicted (lines) concentration-time profiles over the whole range of the reaction: PDO oxidation over (a) Pt, (b) Au-Pd, (c) Au-Pd, HDO over (d) Pt, (e) Au-Pt, (f) Au-Pd



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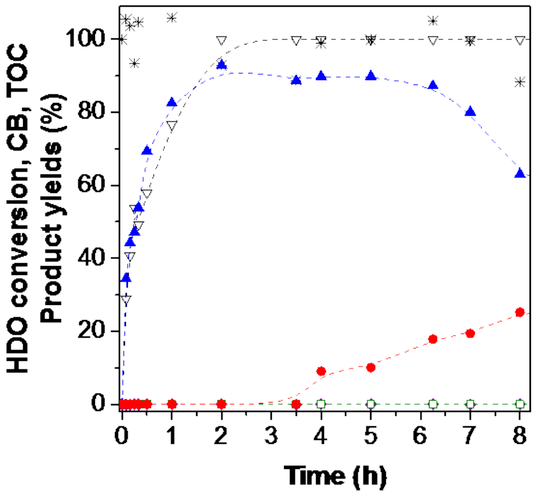

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