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Supplementary Materials: On the Effect of Microwave energy on Lipase-Catalyzed Polycondensation Reactions

Alessandro Pellis, Georg M. Guebitz and Thomas J. Farmer

Table S1. Solvent-free reactions catalyzed by Novozym 435[®] after 4 h of reaction.

| Entry (n°) | Diester (A) | Diol (B) | Heating | | T (°C) | Vessel Open/Close | Conversion (%) * | M _w (Da) ^λ | M _n (Da) ^λ | PDI ^λ |
|------------|-------------|----------|---------|----------|--------|-------------------|------------------|----------------------------------|----------------------------------|------------------|
| | | | MW | Oil Bath | | | | | | |
| Blank | DMA | BDO | + | | 50 | Open | - | - | - | - |
| Blank | DMA | BDO | | + | 50 | Close | - | - | - | - |
| 2 | DMA | BDO | + | | 50 | Close | 39 | 509 | 483 | 1.054 |
| 2 | DMA | BDO | | + | 50 | Close | 40 | 515 | 488 | 1.055 |
| 4 | DMS | BDO | + | | 50 | Open | 44 | 546 | 456 | 1.197 |
| 4 | DMS | BDO | | + | 50 | Open | 47 | 599 | 528 | 1.134 |
| 7 | DMS | BDO | + | | 50 | Open | 11 | 391 | 335 | 1.167 |
| 7 | DMS | BDO | | + | 50 | Open | 46 | 611 | 543 | 1.125 |

* Calculated via ¹H-NMR spectra; ^λ Calculated via GPC. Abbreviations: DMA: dimethyl adipate; DMS: dimethyl succinate; BDO: 1,4-butanediol.

Table S2. Reactions in organic media catalyzed by Novozym 435[®] after 4 h of reaction.

| Entry (n°) | Diester (A) | Diol (B) | Heating | | T (°C) | Conversion (%) * | M _w (Da) ^λ | M _n (Da) ^λ | PDI ^λ |
|------------|-------------|----------|---------|----------|--------|------------------|----------------------------------|----------------------------------|------------------|
| | | | MW | Oil Bath | | | | | |
| Blank | DMS | BDO | + | | 38 | - | - | - | - |
| Blank | DMS | BDO | | + | 38 | - | - | - | - |
| 9 | DMS | BDO | + | | 30 | 39 | 373 | 330 | 1.130 |
| 9 | DMS | BDO | | + | 30 | 38 | 303 | 287 | 1.056 |
| 11 | DMS | BDO | + | | 38 | 45 | 480 | 399 | 1.203 |
| 11 | DMS | BDO | | + | 38 | 46 | 479 | 391 | 1.225 |
| 13 | DMS | BDO | + | | 38 | 47 | 553 | 514 | 1.076 |
| 13 | DMS | BDO | | + | 38 | 48 | 530 | 505 | 1.050 |

* Calculated via ¹H-NMR spectra; ^λ Calculated via GPC. Abbreviations: DMA: dimethyl adipate; DMS: dimethyl succinate; BDO: 1,4-butanediol.

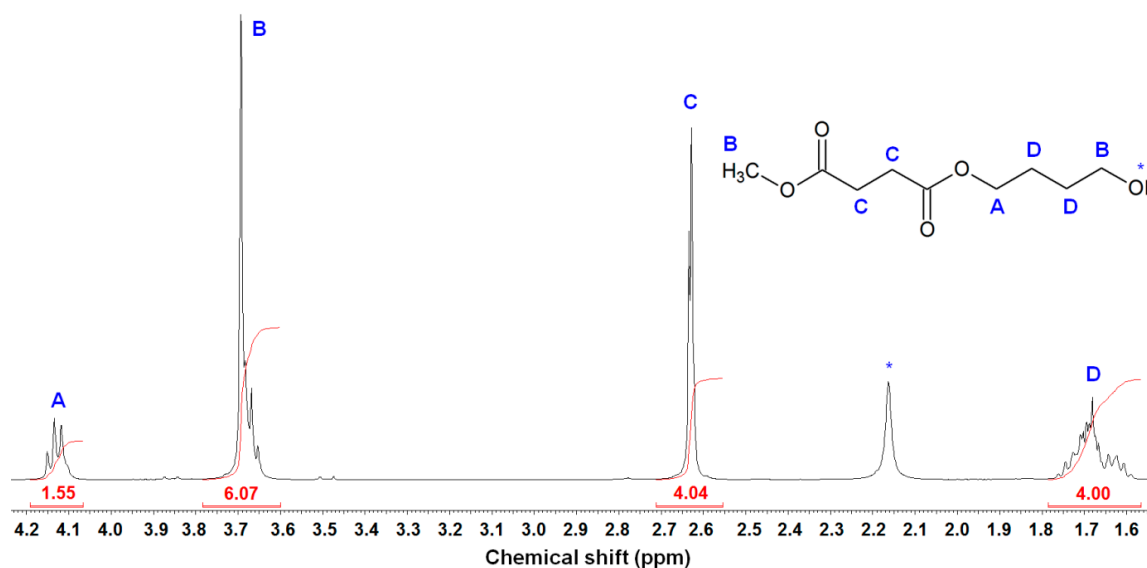


Figure S1. ¹H-NMR spectrum of the polycondensation products of DMS with BDO catalyzed by 10% w/w Novozym[®] 435 at 4 h. Entry 2 Table 1 and Table S1.

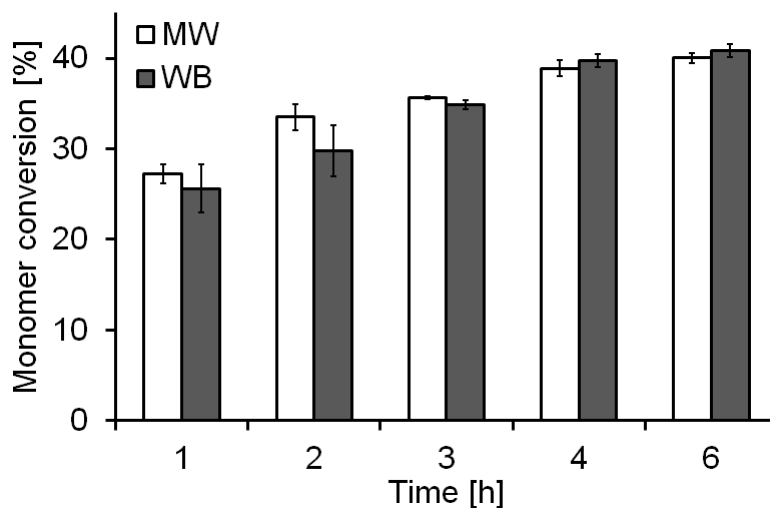


Figure S2. Time-course monitoring of the monomers conversion via $^1\text{H-NMR}$ spectra of the bulk reaction performed in a closed vessel at 50 °C without using the Power Max function.

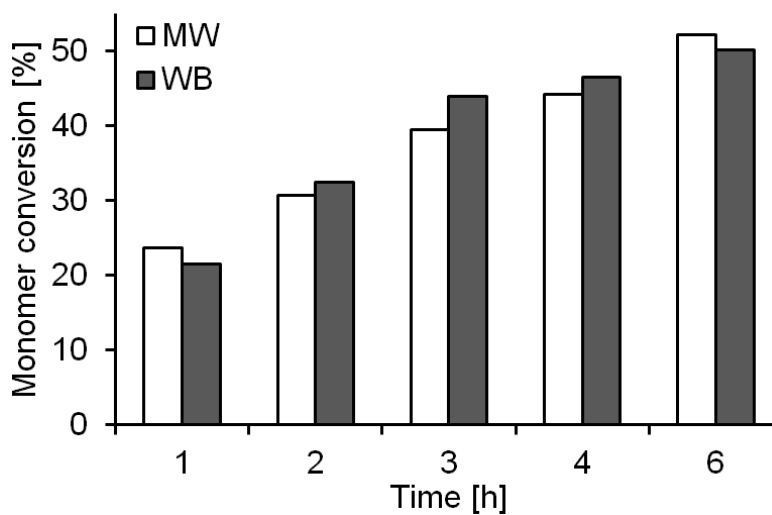


Figure S3. Time-course monitoring of the monomers conversion via $^1\text{H-NMR}$ spectra of the bulk reaction performed in an open vessel at 50 °C without using the Power Max function.

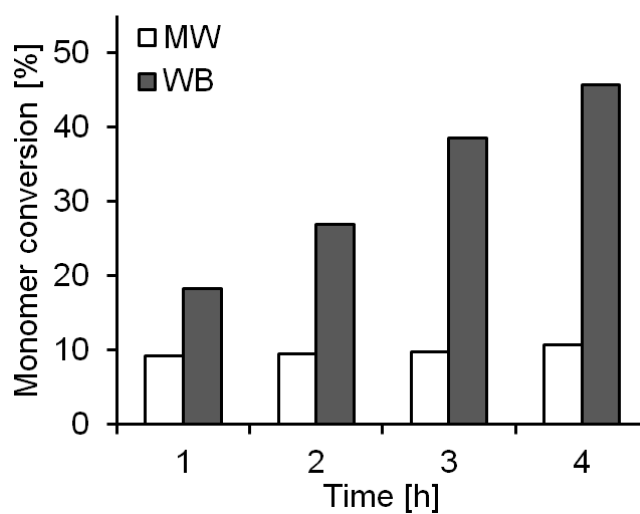


Figure S4. Time-course monitoring of the monomers conversion via $^1\text{H-NMR}$ spectra of the bulk reaction performed in an open vessel at 50 °C using the Power Max function.