Isocyanate-free urethanediol itaconates as biobased liquid monomers in photopolymerization-based 3D printing

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SUPPORTING INFORMATION

Scheme S1. Chemical structure of the different isomers of UDO₃ formed by aminolysis of propylene carbonate with 1,4-diaminobutane.

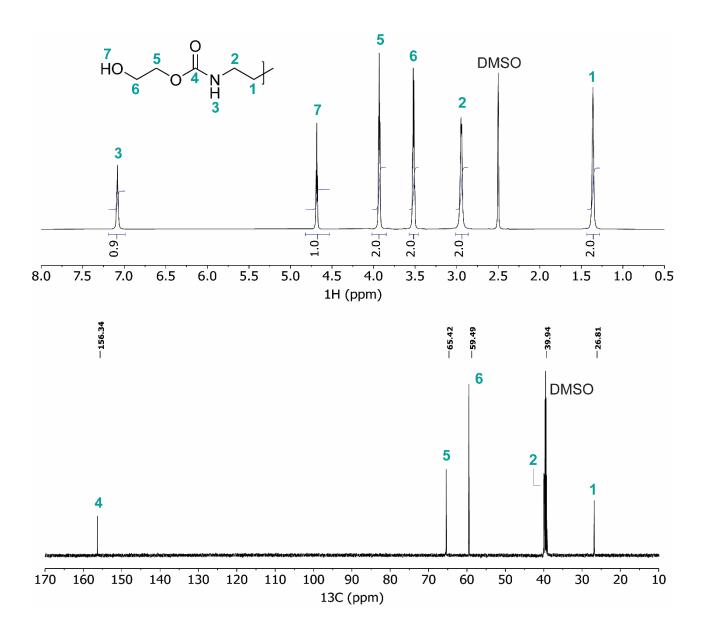


Figure S1. 1 H- (600 MHz, DMSO- d_6 , top) and 13 C- (150 MHz DMSO- d_6 , bottom) NMR spectra of UDO₂. The signal corresponding to carbon 2 is partially overlapped with the septuplet of DMSO, but still distinguishable.

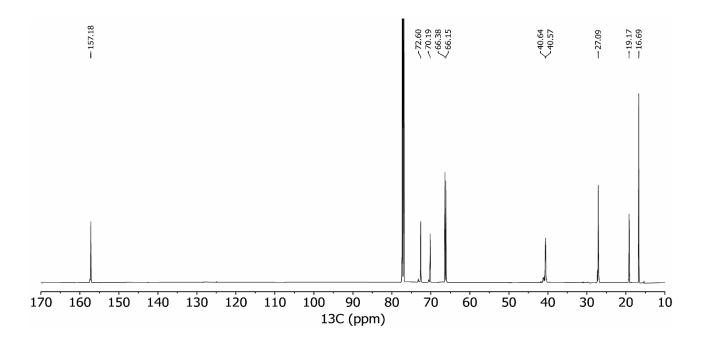


Figure S2. ¹³C-NMR spectrum (150 MHz, CDCl₃) of UDO₃.

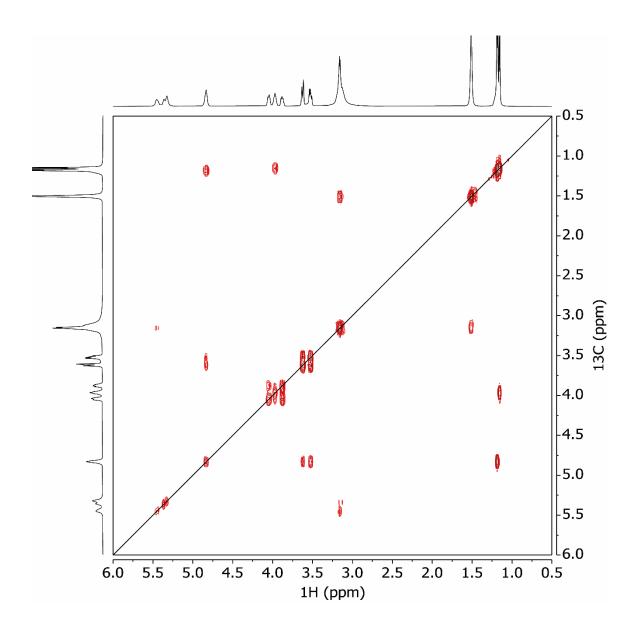


Figure S3. ¹H-¹H COSY (600 MHz, CDCl₃) NMR analysis of the diurethane diols UDOs.

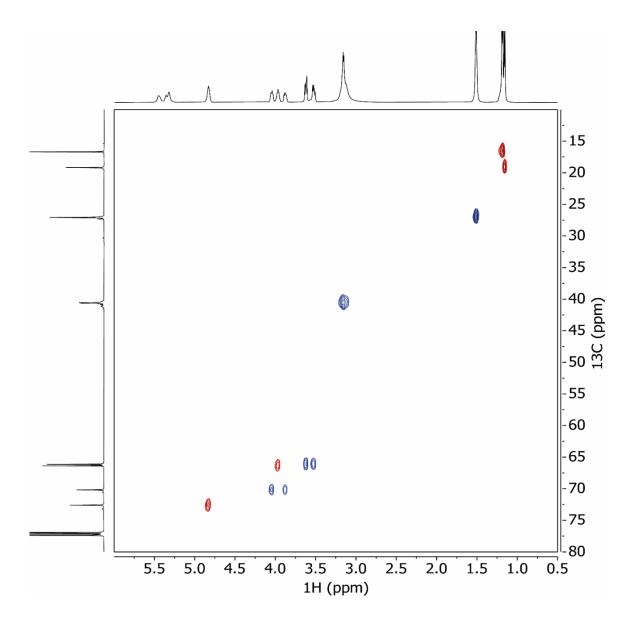


Figure S4. ¹H-¹³C HSQC (600 MHz, CDCl₃) NMR analysis of the diurethane diols UDOs. Positive peaks are colored red and are related to CH and CH₃ groups, while negative peaks are colored blue and are related to CH₂ groups.

$$HO \underbrace{\begin{array}{c} 5a & 4a \\ 0 & 3 \\ 0 & 1 \end{array}}_{6a} \underbrace{\begin{array}{c} 0 \\ N \\ 1 \end{array}}_{1} \underbrace{\begin{array}{c} 2 \\ N \\ 1 \end{array}}_{1} \underbrace{\begin{array}{c} 6b \\ N \\ 4b \end{array}}_{1} \underbrace{\begin{array}{c} 0 \\ N \\ 1 \end{array}}_{1} \underbrace{\begin{array}{c} 2 \\ N \\ 1 \end{array}}_{1} \underbrace{\begin{array}{c} 2$$

| | ¹ H (ppm) | ¹³ C (ppm) |
|----|----------------------|-----------------------|
| 1 | 1.50 | 27.09 |
| 2 | 3.16 | 40.64 and 40.57 |
| 3 | - | 157.18 |
| 4a | 3.87 and 4.04 | 70.19 |
| 4b | 3.51 and 3.61 | 66.15 |
| 5a | 3.97 | 66.38 |
| 5b | 4.83 | 72.60 |
| 6a | 1.16 | 19.17 |
| 6b | 1.18 | 16.69 |

Table S1. NMR spectral attributions for UDO₃.

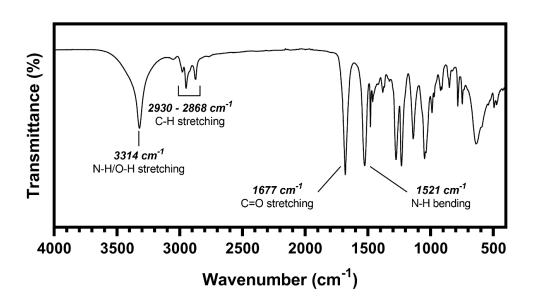


Figure S5. ATR-FTIR spectrum of UDO₃

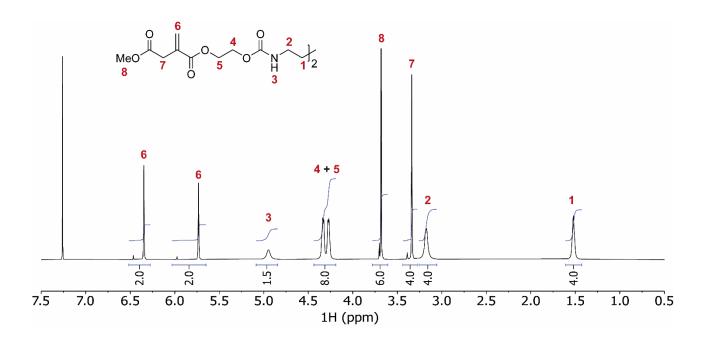


Figure S6. ¹H-NMR (400 MHz, CDCl₃) of UDO₂-I

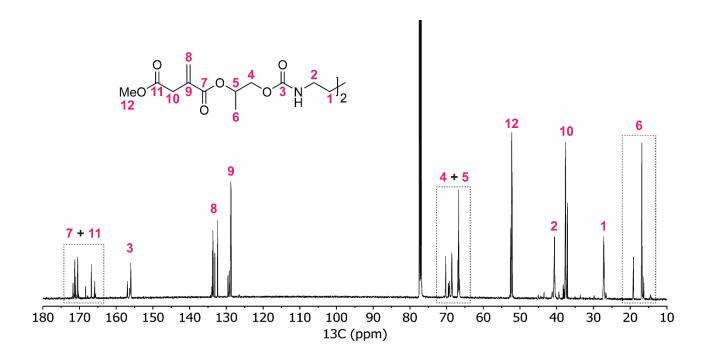


Figure S7. ¹³C-NMR (150 MHz, CDCl₃) of UDO₃-I.

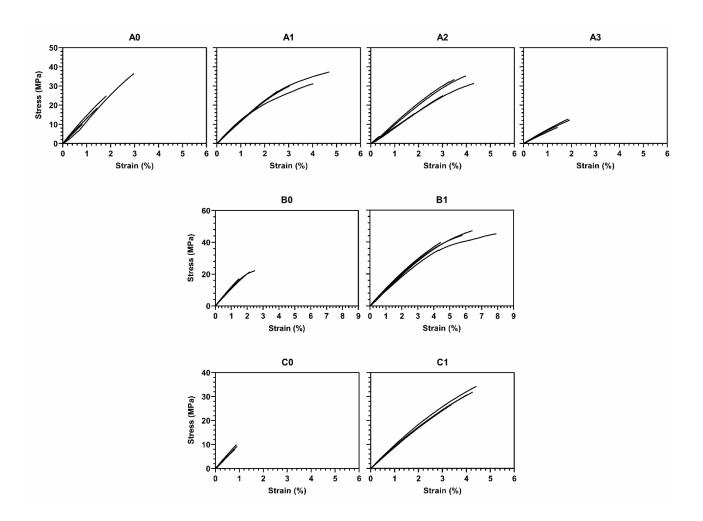


Figure S8. Tensile stress-strain curves.

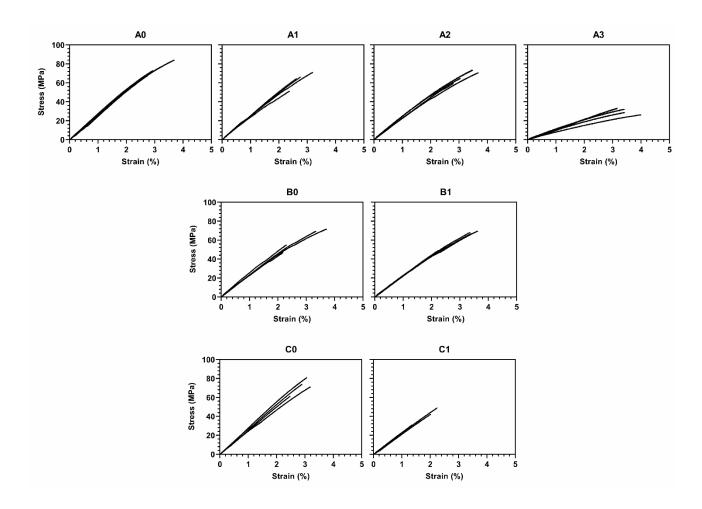


Figure S9. Flexural stress-strain curves