

## **Supporting information**

# **Selective isomerization-carbonylation of a terpene trisubstituted double bond**

**Hanna Busch, Florian Stempfle, Sandra Heß, Etienne Grau and Stefan Mecking\***

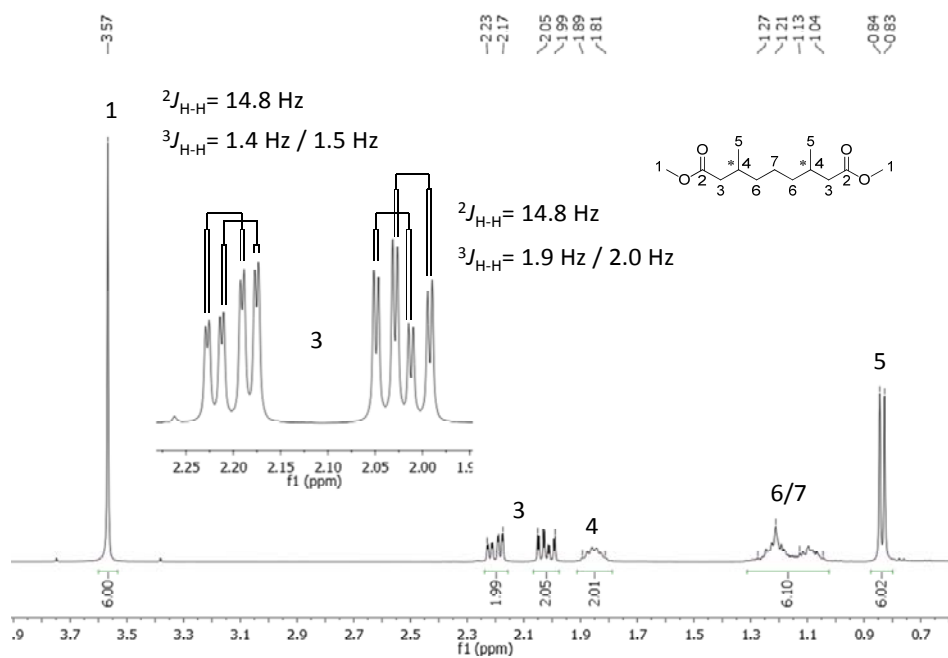


Figure S1:  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ ) of dimethyl 3,7-dimethylnonane-1,9-dioate (2).

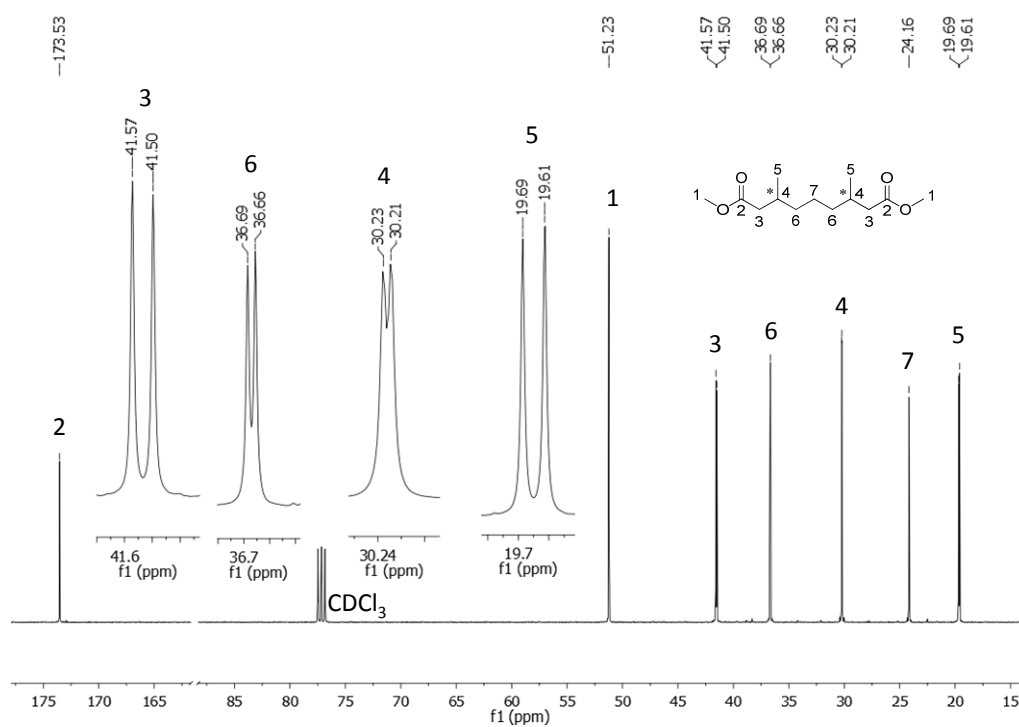


Figure S2:  $^{13}\text{C}$  ( $^1\text{H}$ ) NMR spectrum (100 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ ) of dimethyl 3,7-dimethylnonane-1,9-dioate (2).

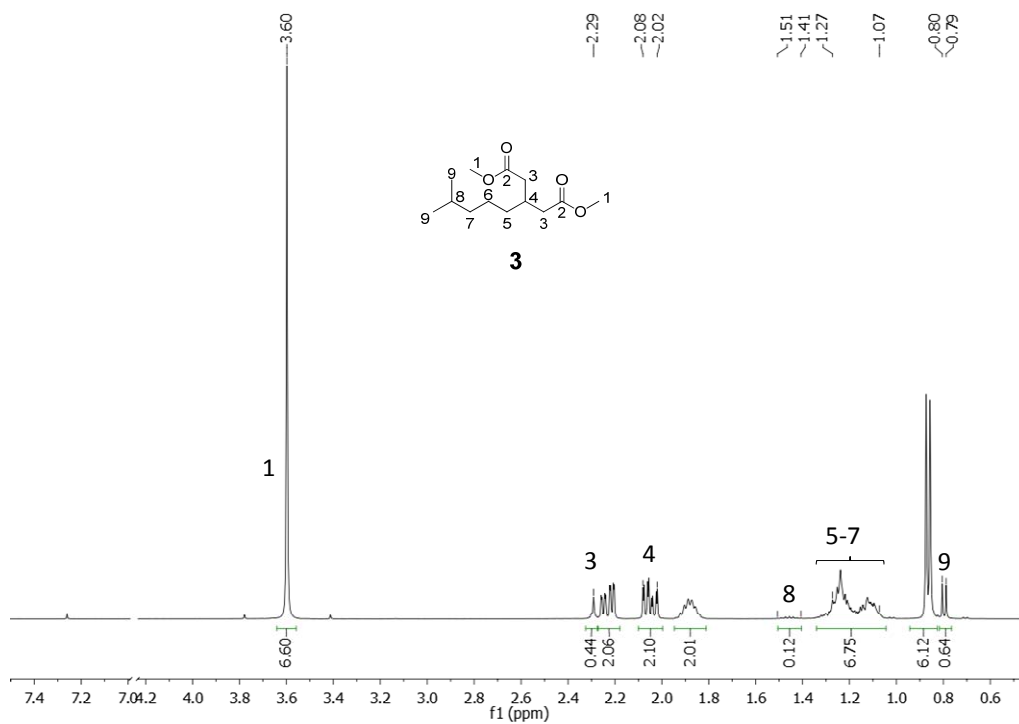


Figure S3:  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ ) of enriched dimethyl 3-(4-methylpentyl)pentanedioate (**3**) with dimethyl 3,7-dimethylnonane-1,9-dioate (**2**) (ratio 1:10).

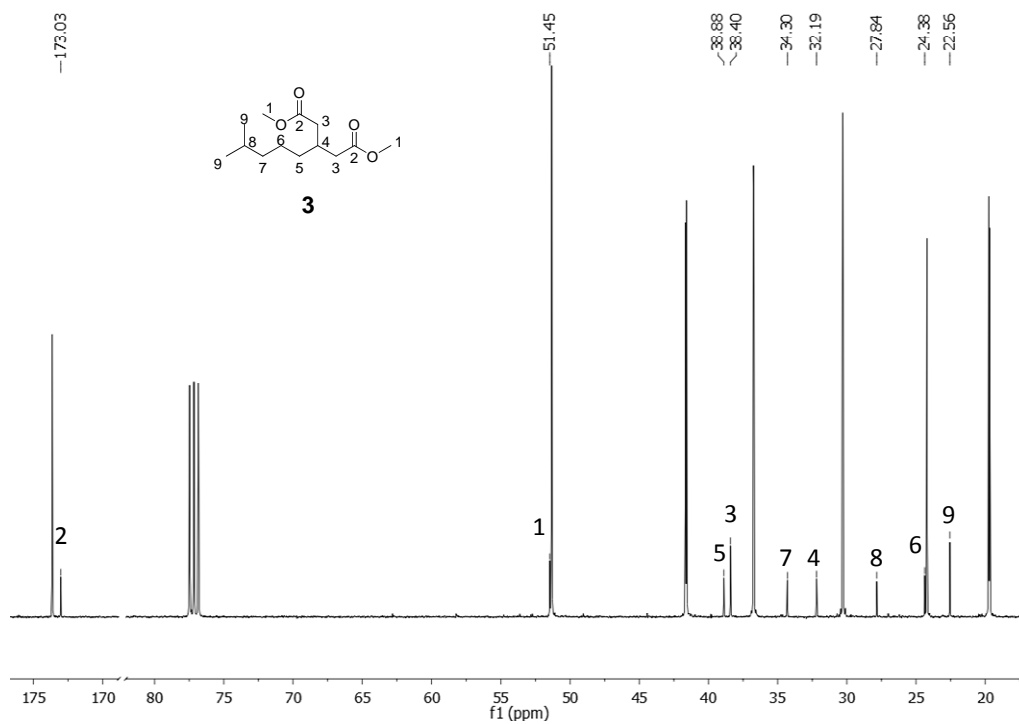


Figure S4:  $^{13}\text{C}$   $\{^1\text{H}\}$  NMR spectrum (100 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ ) of enriched dimethyl 3-(4-methylpentyl)pentanedioate (**3**) with dimethyl 3,7-dimethylnonane-1,9-dioate (**2**) (ratio 1:10).

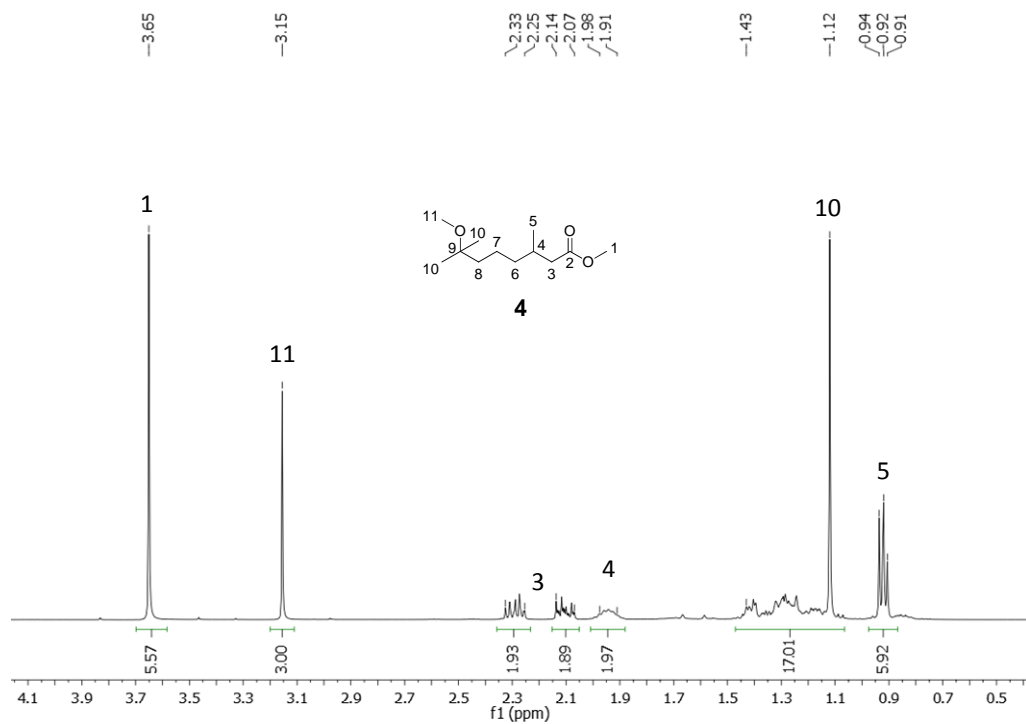


Figure S5:  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ ) of enriched methyl 7-methoxy-3,7-dimethyloctanoate (**4**) with dimethyl 3,7-dimethylnonane-1,9-dioate (**2**) (ratio 3:1).

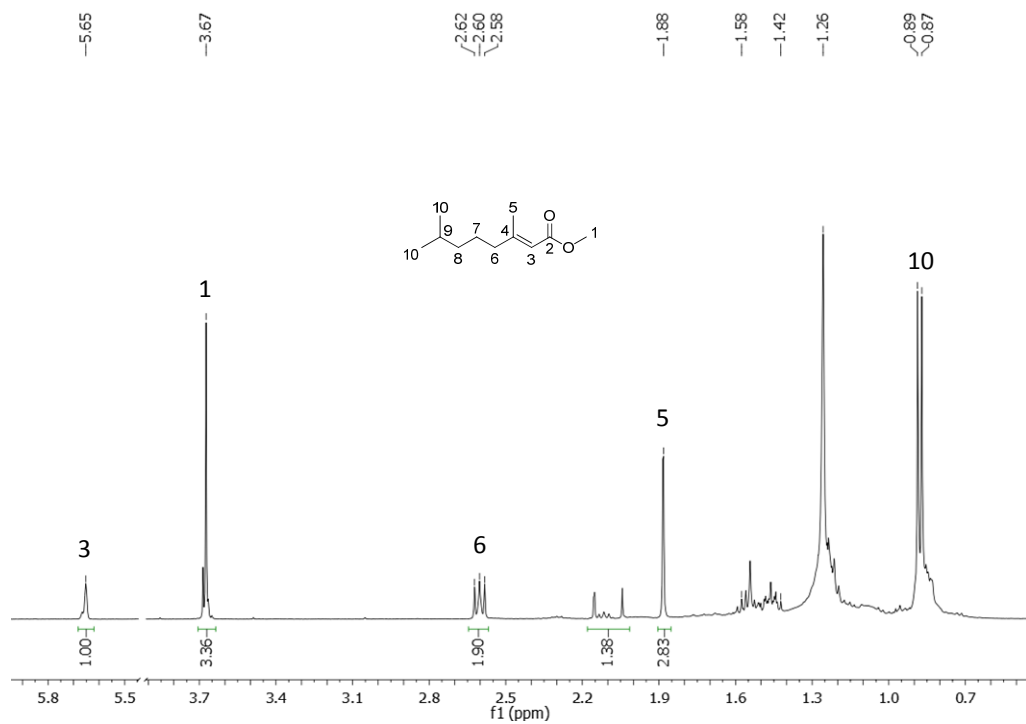
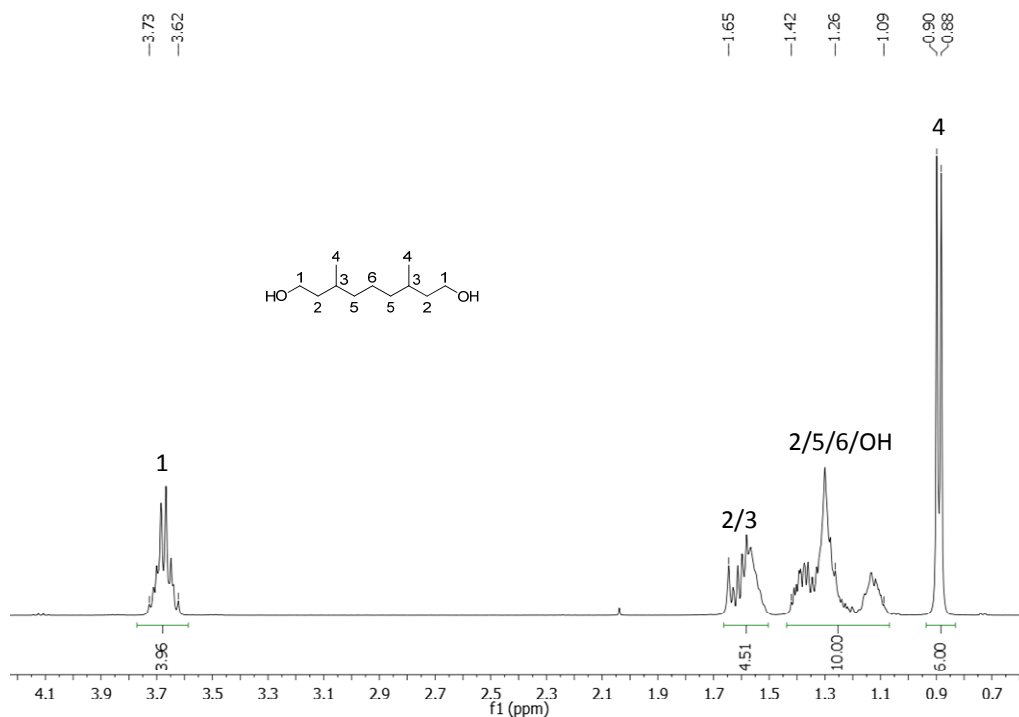
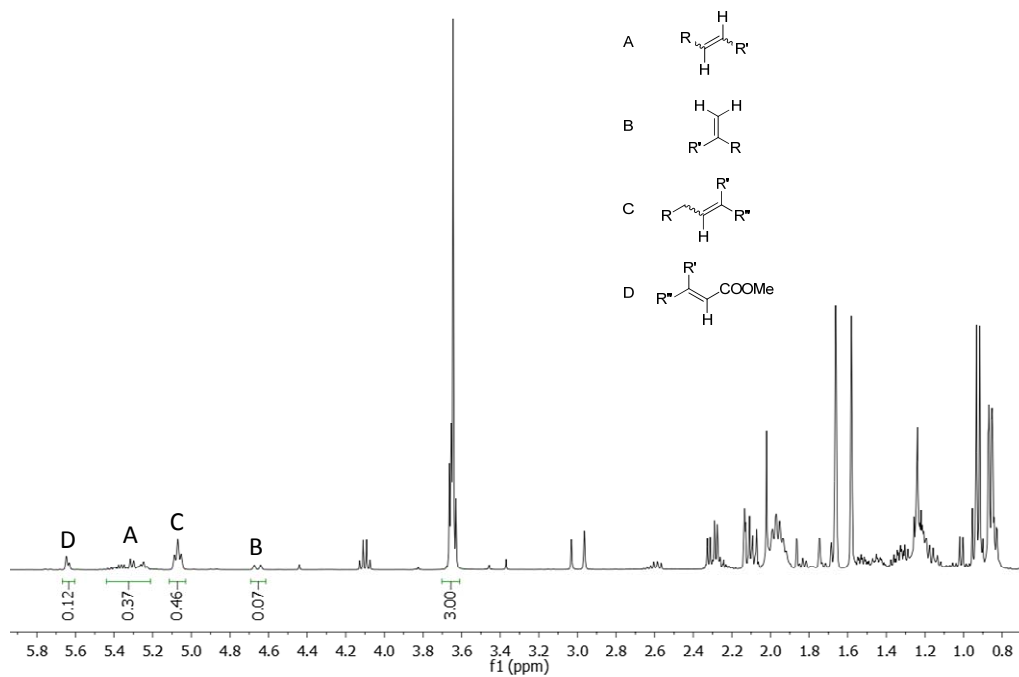


Figure S6:  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ ) of methyl 3,7-dimethyloct-2-enoate (**5**).



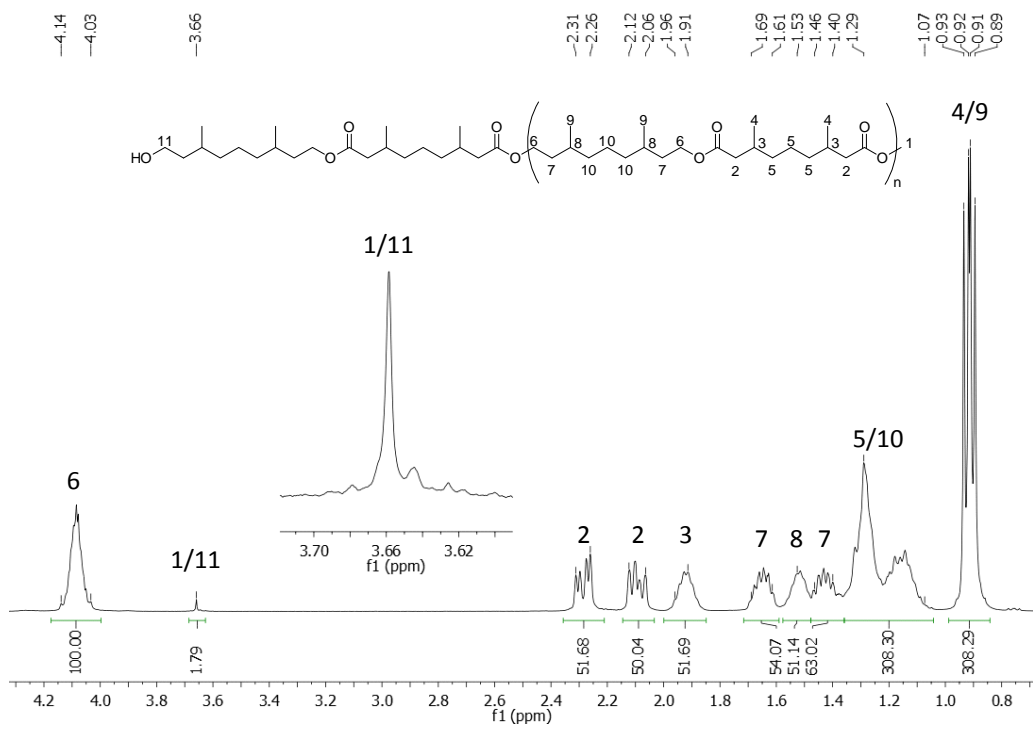


Figure S9: <sup>1</sup>H NMR spectrum (400 MHz, C<sub>2</sub>D<sub>2</sub>Cl<sub>4</sub>, 25 °C) of poly[1,9-(3,7-dimethyl)nonadiyl-1,9-(3,7-dimethyl)nonanedioate] (7). Insert shows enlargement of the end group region.

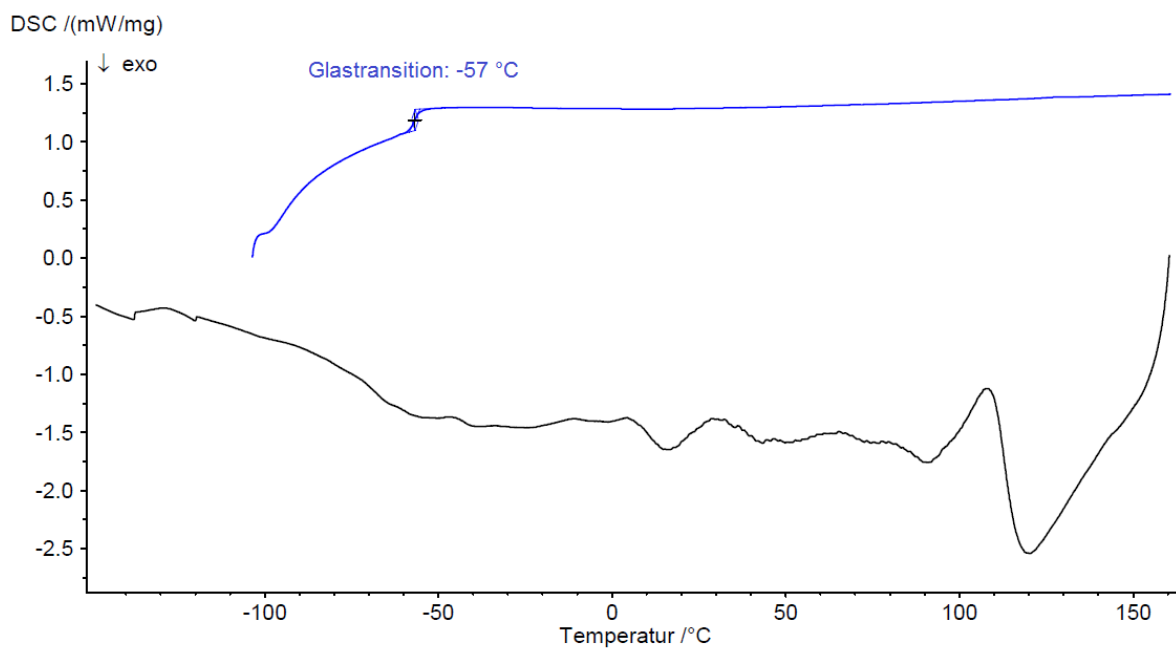


Figure S10: DSC trace of poly[1,9-(3,7-dimethyl)nonadiyl-1,9-(3,7-dimethyl)nonanedioate] (7).

**MW Averages**

Mp: 16965  
Mz: 45223

Mn: 8341  
Mz+1: 84223

Mv: 19015  
PD: 2.5745

Mw: 21474

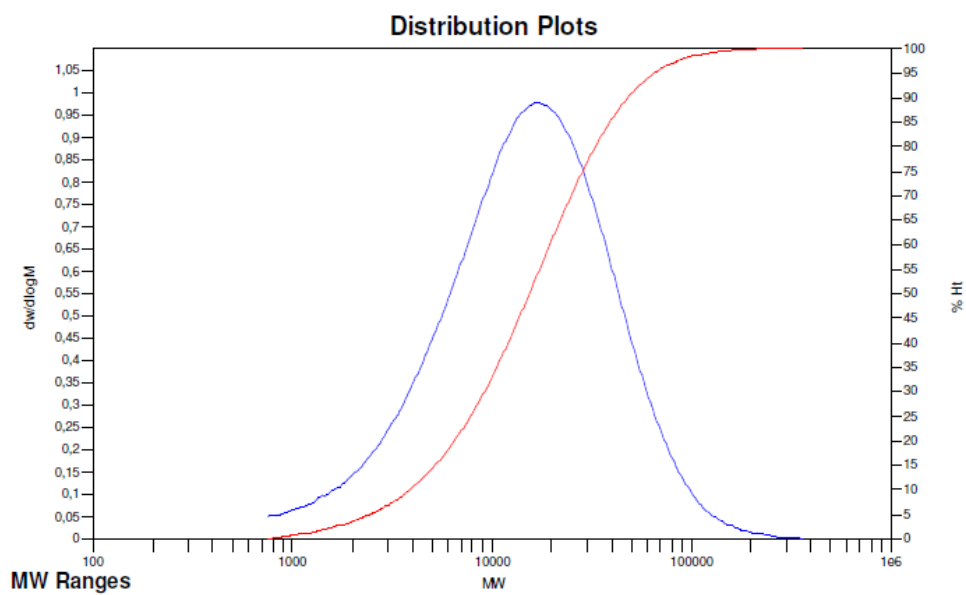


Figure S11: GPC trace of poly[1,9-(3,7-dimethyl)nonadiyl-1,9-(3,7-dimethyl)nonanedioate] (**7**) (TCB: 160 °C, vs. PE standards).