polymers

MDPI

Supporting Information

Homoserine lactone as a structural key element for the synthesis of multifunctional polymers

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1. Synthesis of the thiolactone-lactone coupler (1)

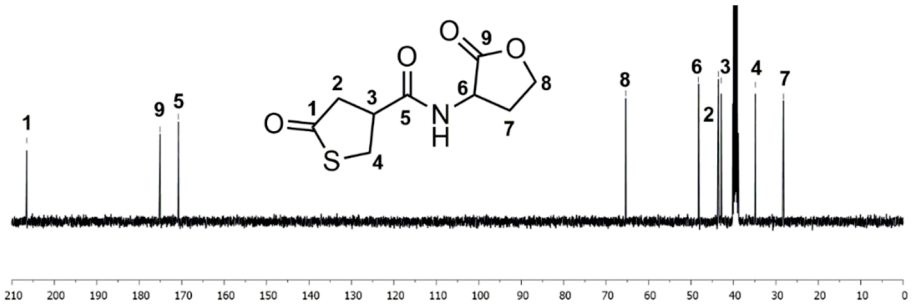

Figure S1. ^{13}C NMR spectrum of thiolactone-lactone (**1**) measured in DMSO-d_6.

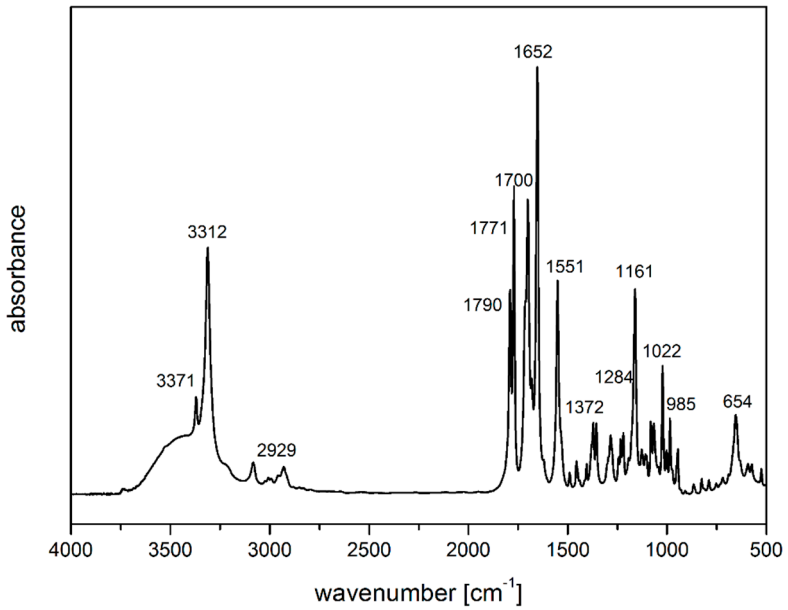

Figure S2. FTIR spectrum of thiolactone-lactone (**1**).

2. Model reaction of coupler 1 with hexylamine in a 1:1 molar ratio

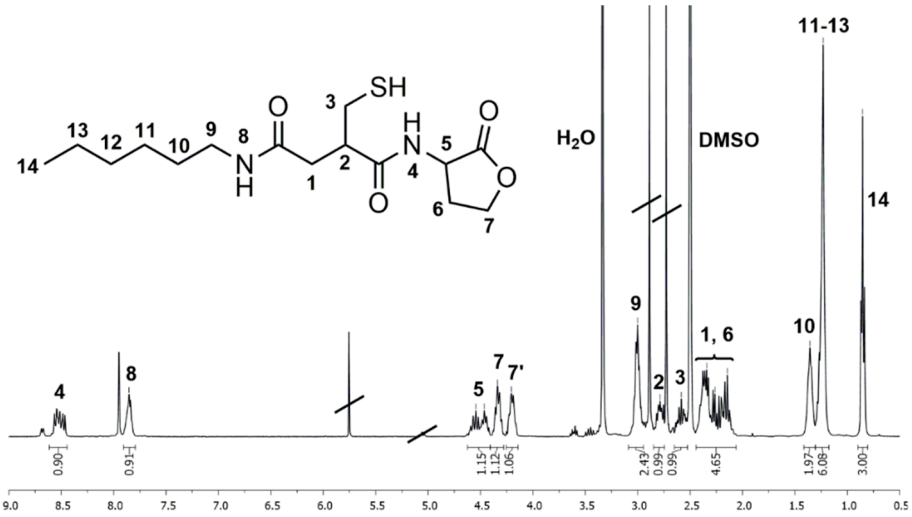

Figure S3. [1]H NMR spectrum of compound **2** measured in DMSO-d_6.

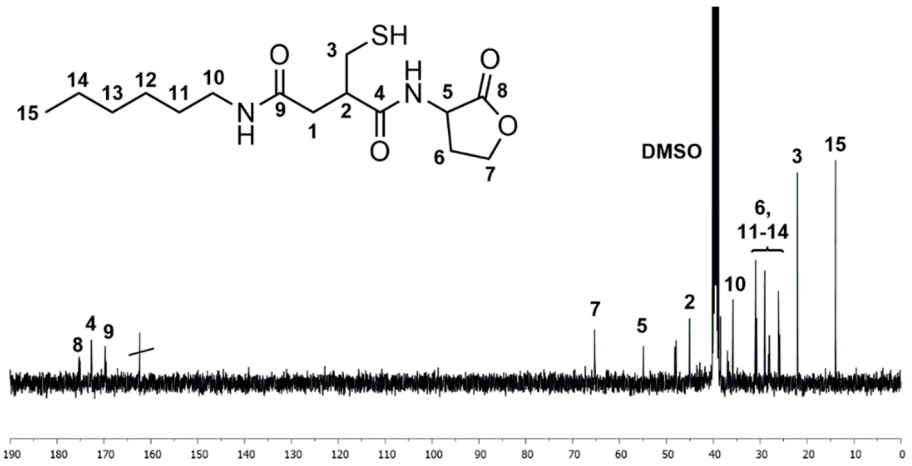

Figure S4. [13]C NMR spectrum of compound **2** measured in DMSO-d_6.

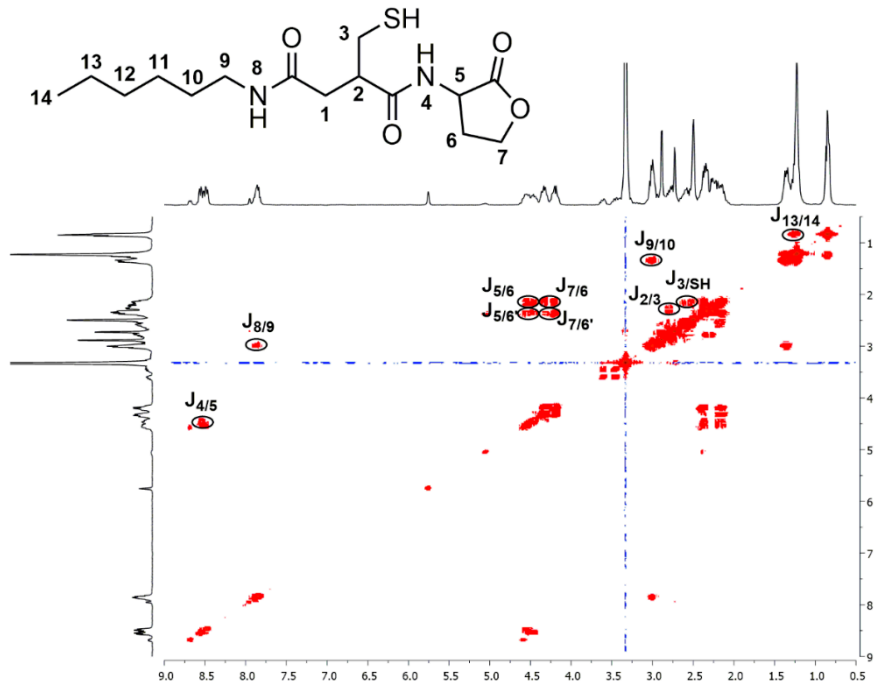

Figure S5. H,H-COSY NMR spectrum of compound **2** measured in DMSO-d_6.

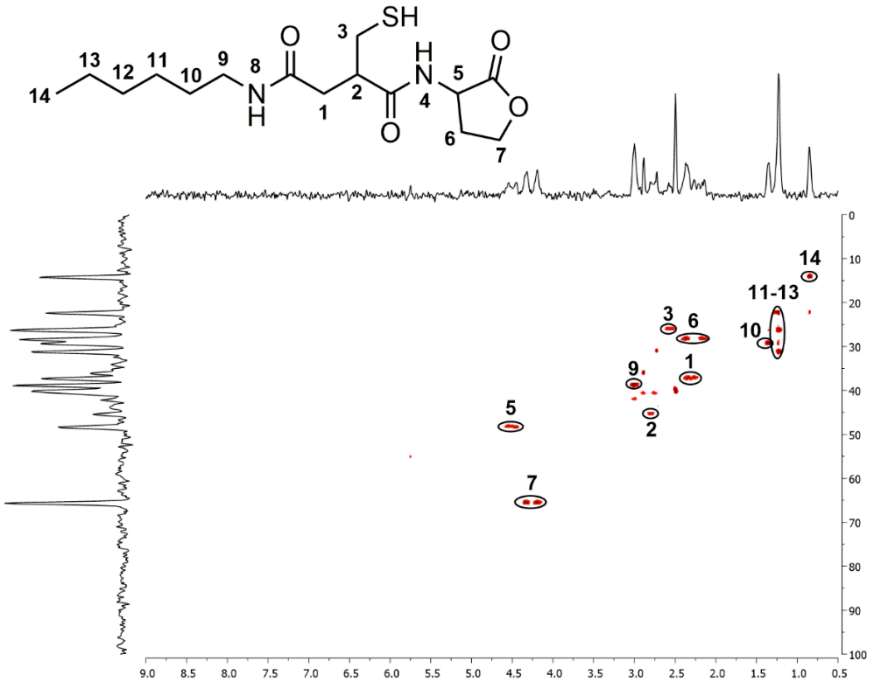

Figure S6. HSQC NMR spectrum of compound **2** measured in DMSO-d_6.

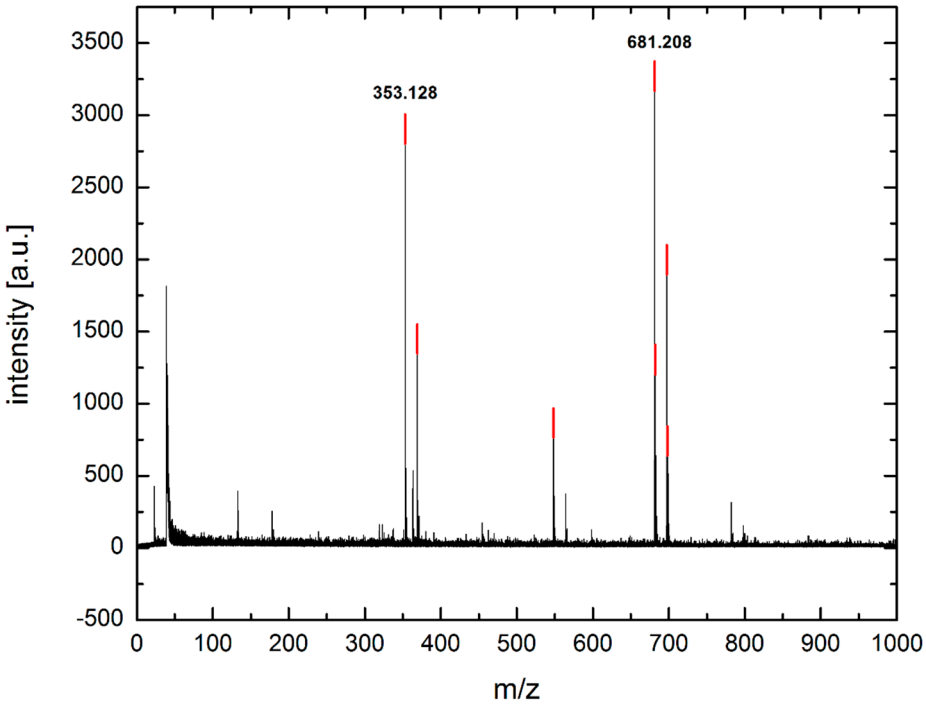

Figure S7. NALDI-TOF spectrum of compound **2**.

Table S1. Identified signals of the NALDI-TOF measurement of the addition product of the addition one equivalent hexylamine to the thiolactone-lactone coupler (**1**). Reported signals describe masses of $[M + Na^+]$ (MW = 22.99 g · mol^{-1}).

Product	m/z (calculated)	m/z (found)	intensity [a.u.]
2	353.15	353.128	2902
Disulfide of **2**	681.29	681.208	3270

3. Model reaction of coupler 1 with hexylamine in a 1:2 molar ratio

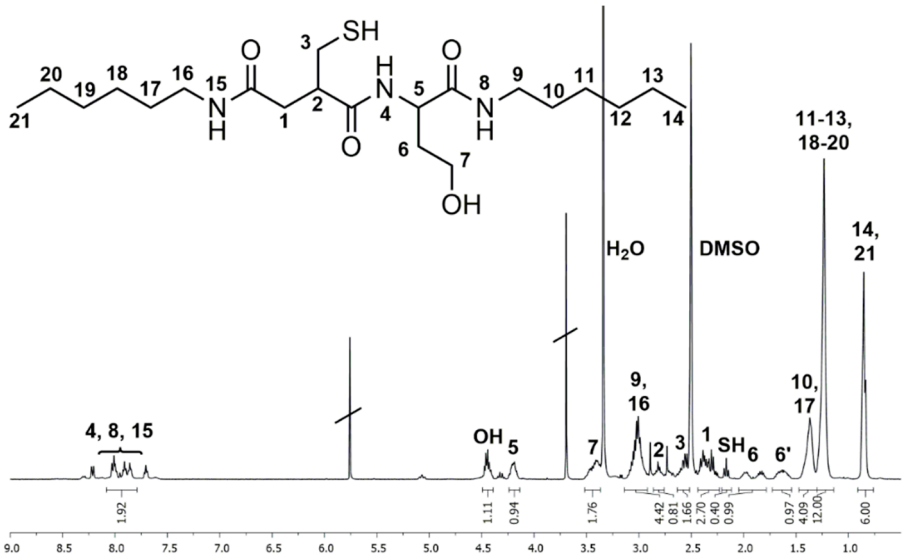

Figure S8. ^{1}H NMR spectrum of compound **3** measured in DMSO-d_6.

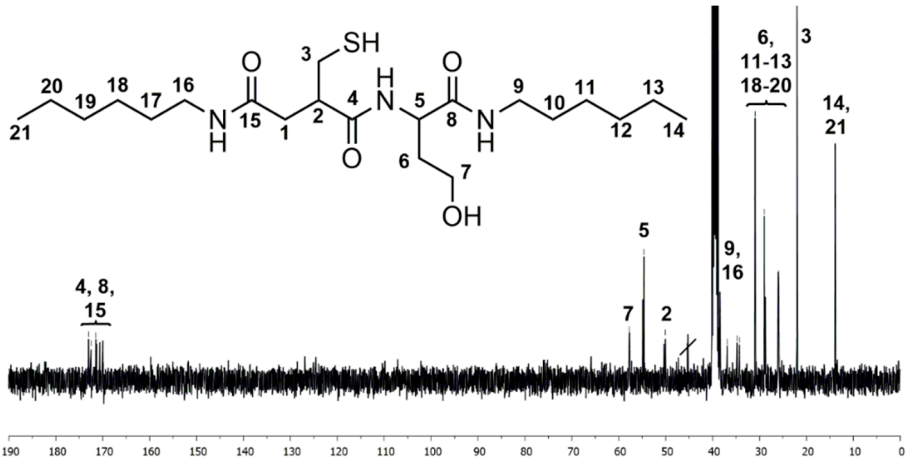

Figure S9. ^{13}C NMR spectrum of compound **3** measured in DMSO-d_6.

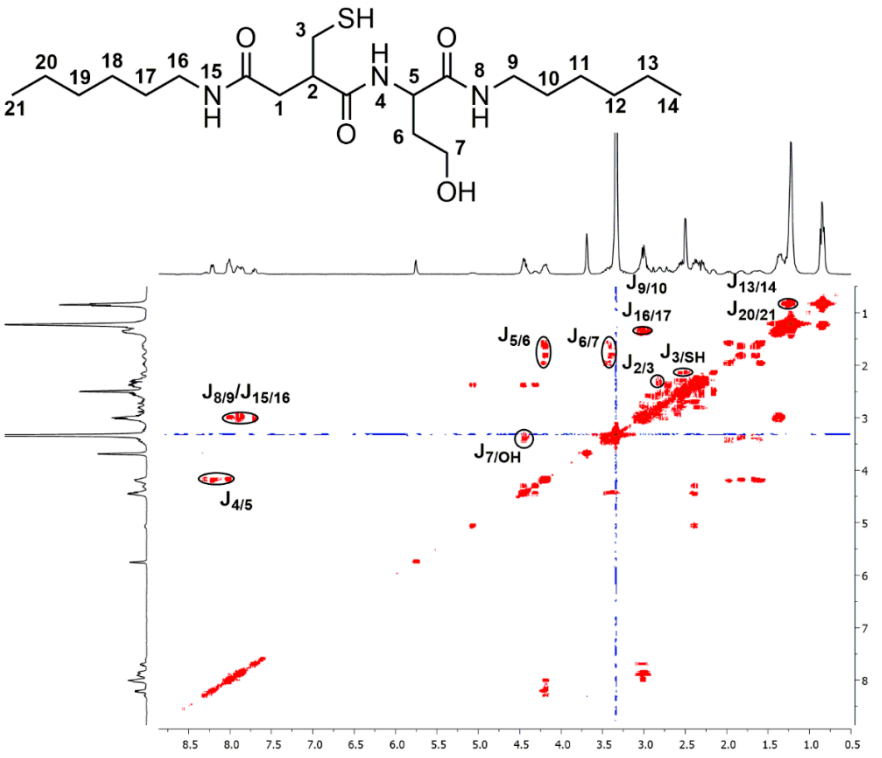

Figure S10. H,H-COSY NMR spectrum of compound **3** measured in DMSO-d_6.

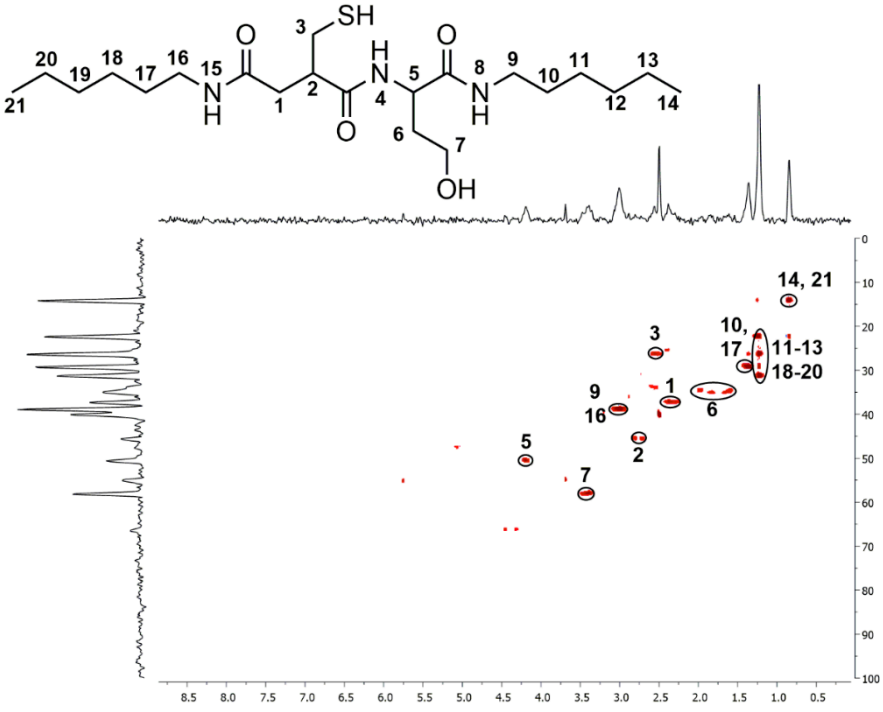

Figure S11. HSQC NMR spectrum of compound **3** measured in DMSO-d_6.

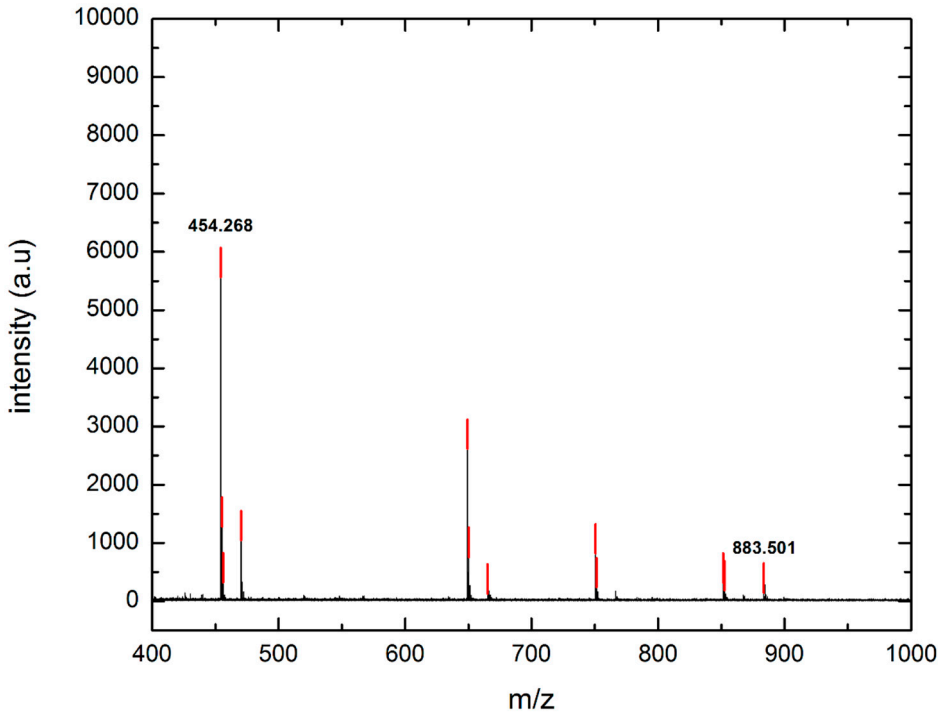

Figure S12. NALDI-TOF spectrum of compound **3**.

Table S2. Identified signals of the NALDI-TOF measurement of the addition product of the addition of two equivalents hexylamine to the thiolactone-lactone coupler (**1**). Reported signals describe masses of $[M + Na^+]$ (MW = 22.99 g · mol^{-1}).

Product	m/z (calculated)	m/z (found)	intensity [a.u.]
3	454.27	454.268	5819
Disulfide of **3**	883.53	883.501	403

4. Polyaddition reaction with of PEG-diamine to coupler 1

Table S3. Reagent ratios for the synthesis of **4a-d** (T = 90 °C, t = 16 h).

polymer	m_1 [g]	m_{MA} [g]	$m_{PEG\text{-}diamine}$ [g]	V_{DMF} [mL]	c [g · mol^{-1}]
7a	0.249	0.094	0.400	2.170	0.5
7b	0.100	0.038	0.161	0.436	1.0
7c	0.100	0.038	0.161	0.291	1.5
7d	0.100	0.038	0.161	-	-

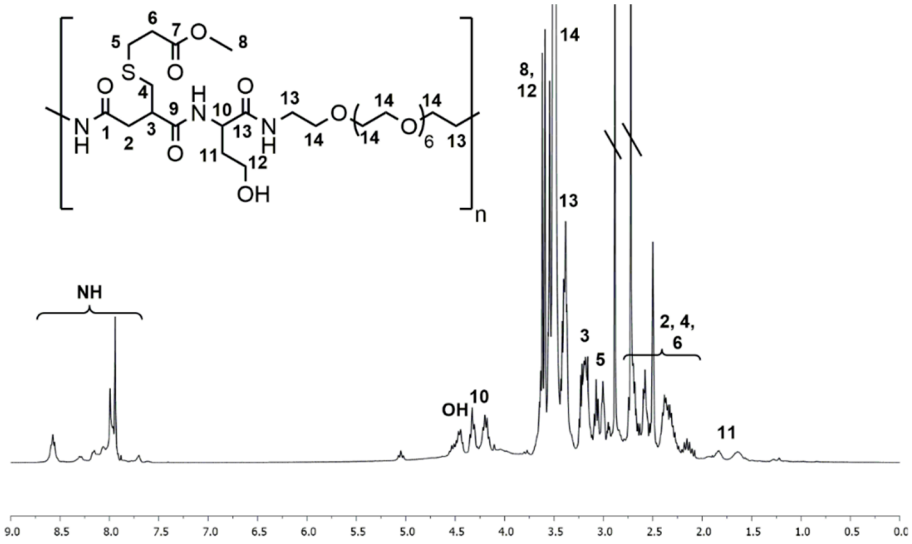

Figure S13. ^{1}H NMR spectrum of the reaction of thiolactone-lactone (**4**) with PEG-diamine measured in DMSO-d_6.

5. Synthesis of PG_{26} (5)

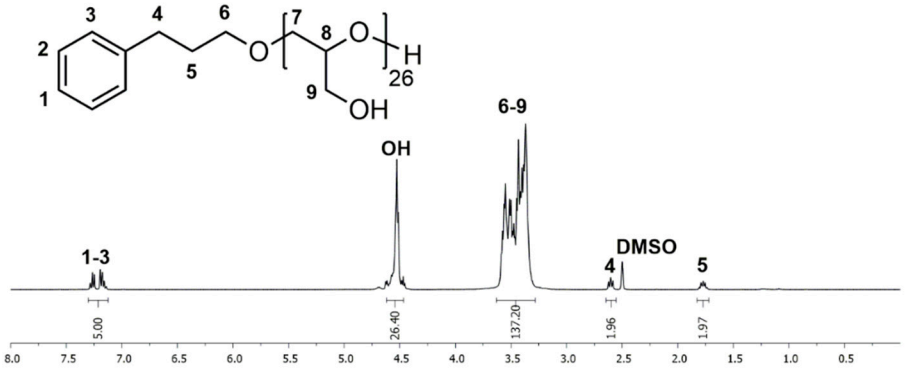

Figure S14. ^{1}H NMR spectrum of PG_{26} (**5**) measured in DMSO-d_6.

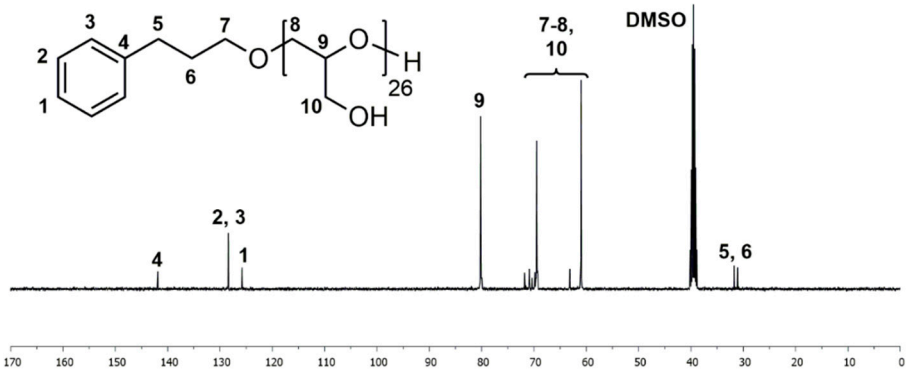

Figure S15. ^{13}C NMR spectrum of PG_{26} (**5**) measured in DMSO-d_6.

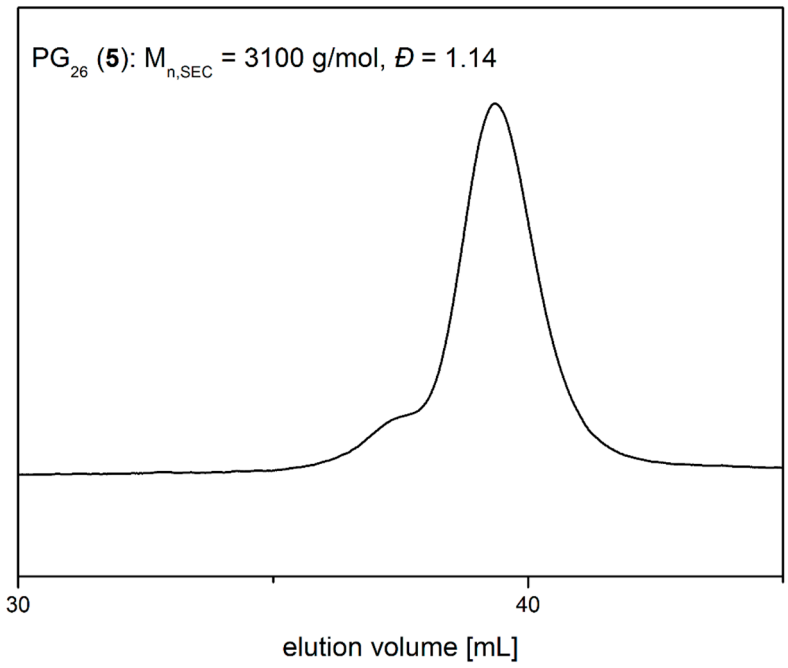

Figure S16. DMF-SEC traces of PG_{26} (**5**).

6. Functionalization of polyglycidol (5) with DL-homoserine lactone hydrobromide

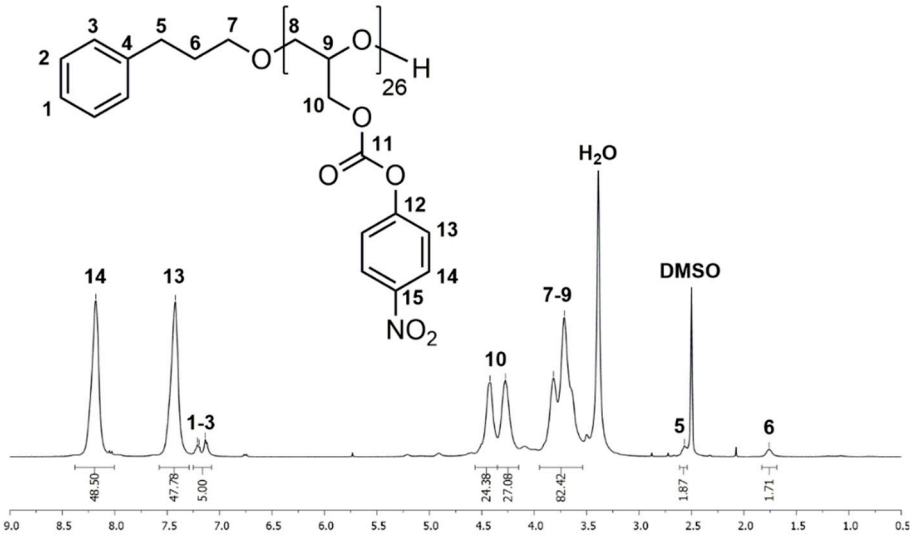

Figure S17. ^{1}H NMR spectrum of $P(G^{NPC})_{26}$ (**6**) measured in DMSO-d_6.

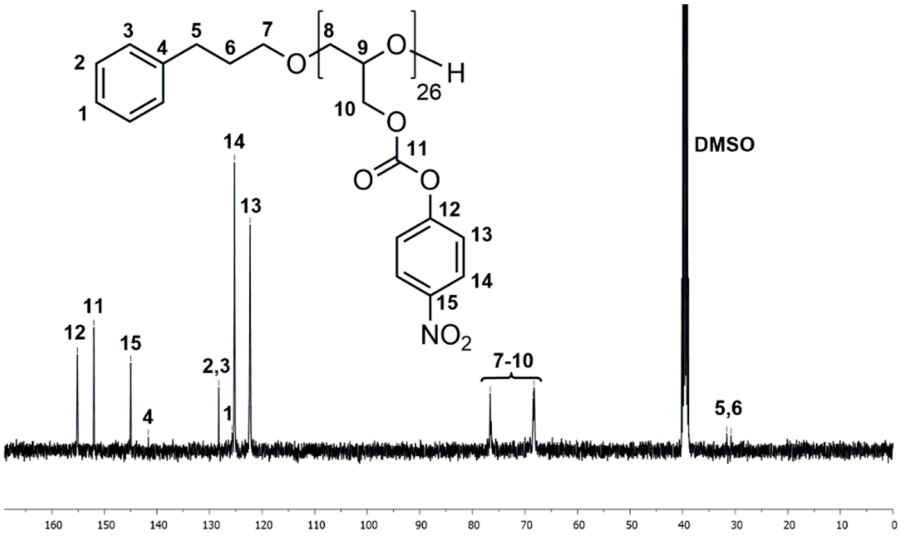

Figure S18. ^{13}C NMR spectrum of P(G^{NPC})$_{26}$ (**6**) measured in DMSO-*d*$_6$.

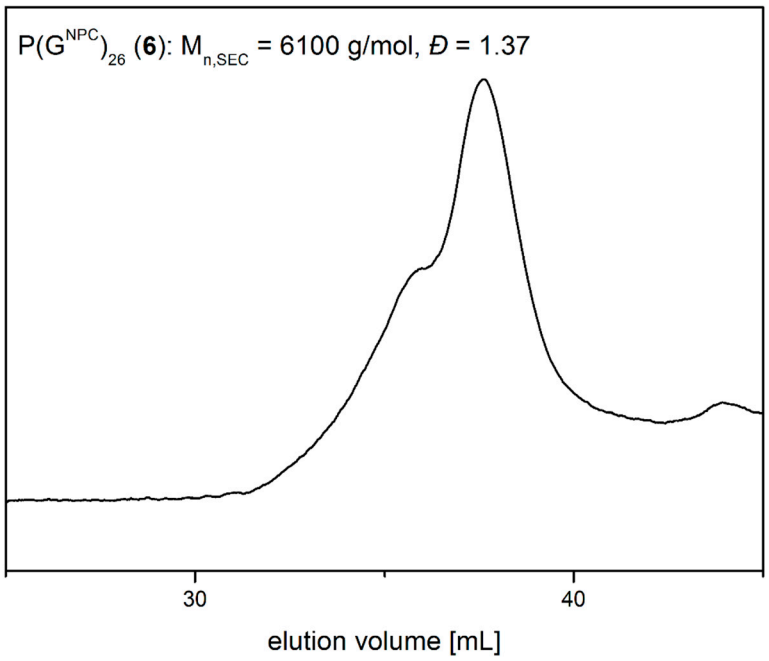

Figure S19. DMF-SEC traces of P(G^{NPC})$_{26}$ (**6**).

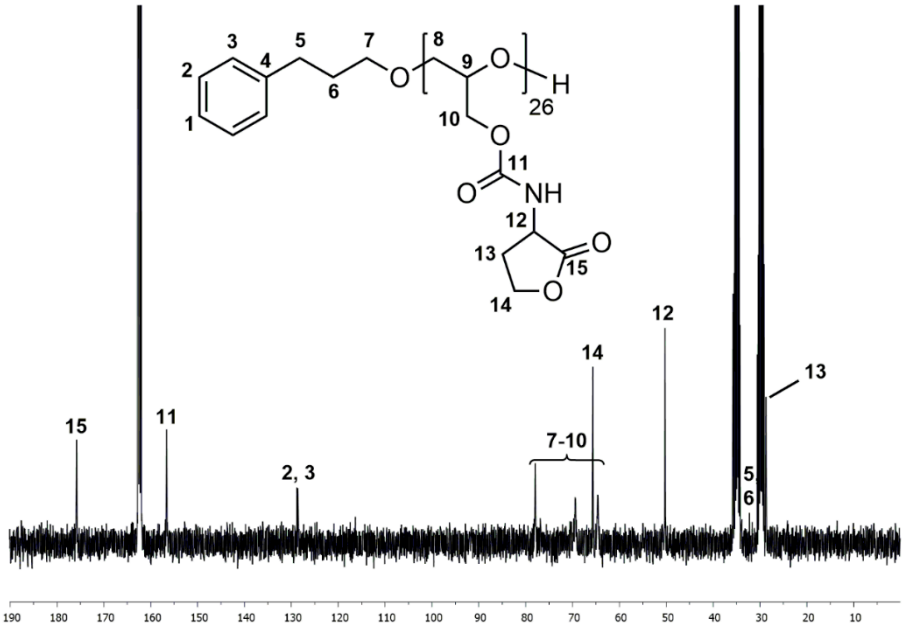

Figure S20. ^{13}C NMR spectrum of P(G^{HSL})$_{26}$ (**7**) measured in DMF-*d*$_7$.

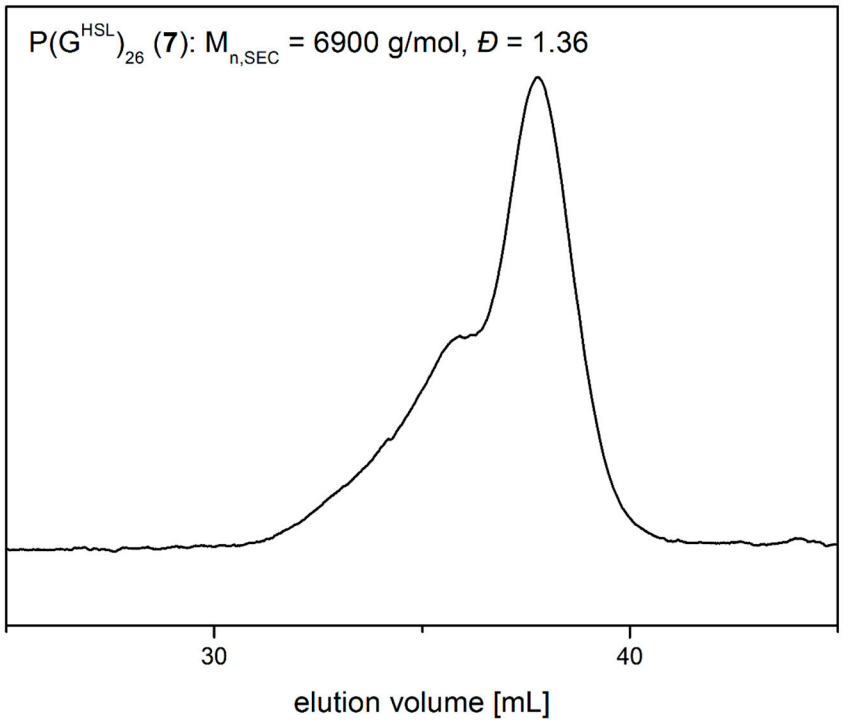

Figure S21. DMF-SEC traces of P(G^{HSL})$_{26}$ (**7**).

7. Ring-opening of P(G^{HSL})$_{26}$

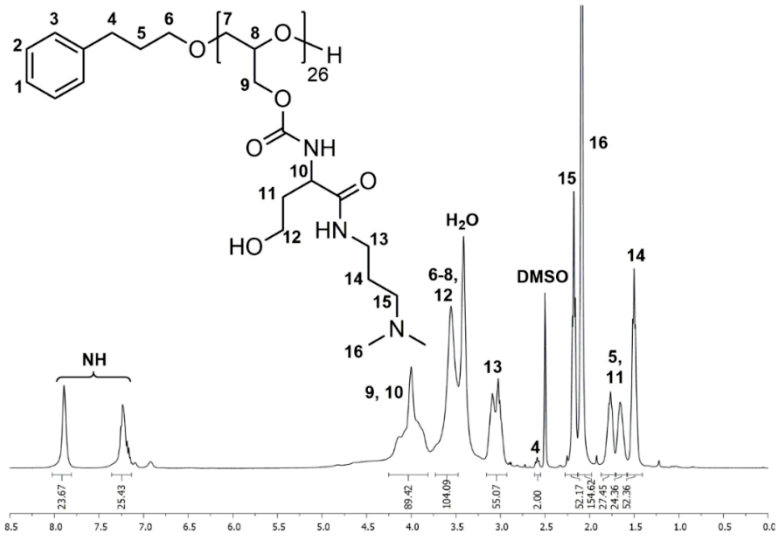

Figure S22. ^{1}H NMR spectrum of P(G^{HSL,o})$_{26}$ (**8**) measured in DMSO-*d*$_6$.

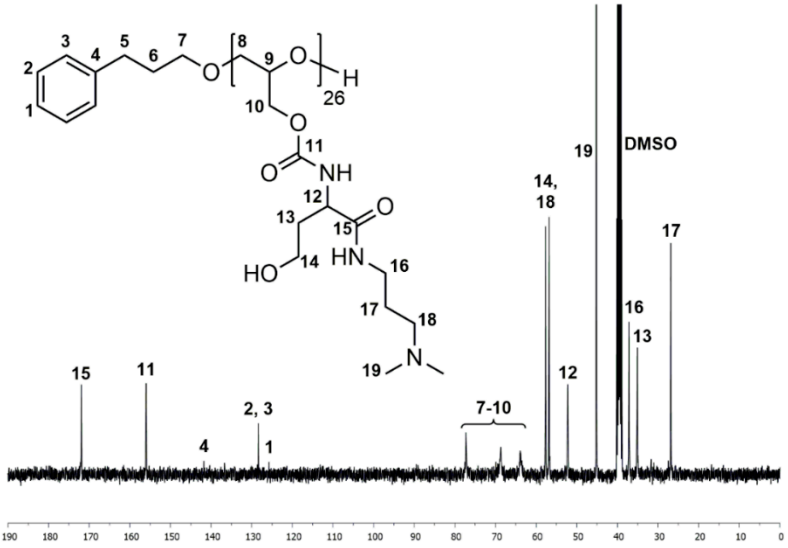

Figure S23. ^{13}C NMR spectrum of P(G^{HSL,o})$_{26}$ (**8**) measured in DMSO-*d*$_6$.

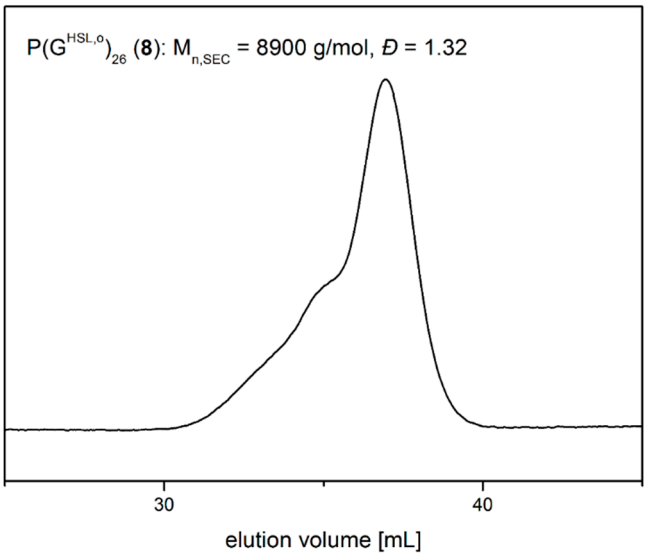

Figure S24. DMF-SEC traces of P(G^{HSL,o})$_{26}$ (**8**).

8. Quaternization of $P(G^{HSL,o})_{26}$

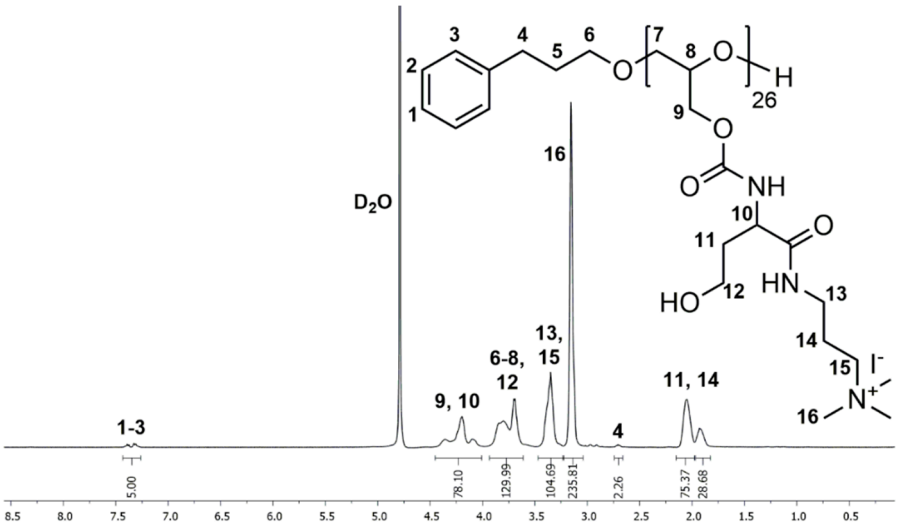

Figure S25. ^{1}H NMR spectrum of $P(G^{HSL,o,q})_{26}$ (**9**) measured in D_2O.

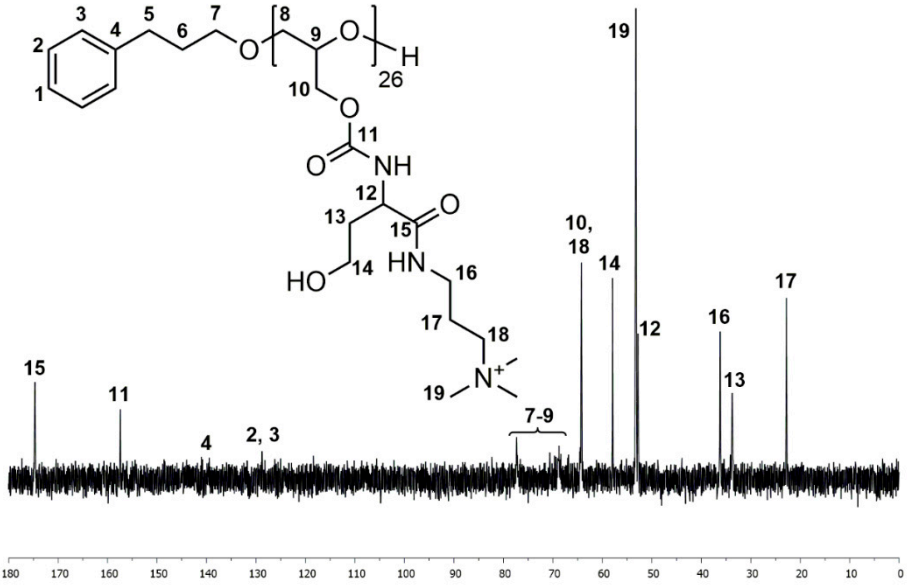

Figure S26. ^{13}C NMR spectrum of $P(G^{HSL,o,q})_{26}$ (**9**) measured in D_2O.