Supporting information

Effect of N-alkylation in N-carboxyanhydride (NCA) ring-opening polymerization kinetics

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1. N-Alkylated-N-Boc-glycine synthesis

The synthesis of the methyl, benzyl and Cbz-aminobutyl glycine derivatives were prepared in our previous work through a one-pot synthesis method[1] and Boc protected aminoacids were purchased from Sigma-Aldrich. The rest of the aminoacid precursors were synthesized as follows.

Synthesis of N-isopropyl-N-Boc-glycine: In a round bottom flask, isopropylamine (99%, 100 mmol, 8.27 mL, 1 equiv.) was solubilized in 200 mL of methanol. Glyoxylic acid (97%, 30 mmol, 2.85 g, 0.3 equiv.) was added and stirred for 30 min, then $NaBH_4$ (98%, 30 mmol, 1.16 g, 0.3 eq) was added and stirred 30 min. The previous action was repeated five times until no reactant was presented on thin-layer chromatography (TLC using as eluent $CHCl_2$-MeOH 60:40). An excess of 0.6 equiv. more of $NaBH_4$ was added to reduce the remaining imine and stirred for 30 min. Then, the solvent was evaporated *in vacuo*. To the previous mixture, 150 mL of water was added followed of the addition of K_2CO_3 (99%, 200 mmol, 27.92 g, 2 equiv.), 150 mL of dioxane and di-*tert*-butyl dicarbonate (99%, 200 mmol, 44.09 g, 2 equiv.), the mixture was stirred for 12 h at RT and the solvent was evaporated *in vacuo*. Then, 100 mL of water were added and three extractions with 100 mL of diethyl ether were performed. The pH of the aqueous phase was decreased around pH = 3 using 6 M HCl, added drop by drop. Four extractions with 100 mL of ether were done, the organic phase was dried over sodium sulphate, filtered, and evaporated *in vacuo*. The product was evaporated until a volume of 15 mL, then the temperature was decreased and the solid was filtered, the solvent was evaporated and 200 mL of hexane was added, the mixture was kept on the fridge overnight. The solid was washed three times with 25 mL of hexane and dried. The product was isolated as a white crystalline powder in 75% yield (16.29 g). Melting point: 94-95 °C (Lit. 98°C).[2] ^{1}H-NMR, $CDCl_3$ 400 MHz δ: 1.11 (br, 6H, $2CH_3$), 1.46 (br, 9H, $3CH_3$), 3.85 (d, 2H, J=37.4 Hz CH_2), 4.20-4.46 (m, 1H, CH), 9.75 (br, 1H), COOH. In agreement with the literature.[34] ^{13}C-NMR, $CDCl_3$ 100 MHz δ: 20.55 ($2CH_3$), 28.44 ($3CH_3$), 43.39 (d, J=68 Hz CH), 46.18-48.01 (d, J=180 Hz, C), 80.73 (d, J=40.7 Hz, CH_2), 150.03 (COO), 176.78 (COOH).

Synthesis of N-propyl-N-Boc-glycine: The synthesis was performed similarly to the protocol described for compound *N*-isopropyl-*N*-Boc-glycine. The product was isolated as a clear viscous oil in 75% yield (16.29 g) starting from propylamine 99% (8.27 mL, 100 mmol). ^{1}H NMR, DMSO 400 MHz δ: 0.78-0.83 (m, 3H, CH_3), 1.34, 1.39 (d, J=18.5Hz, 9H, CH_3), 1.41-1.49 (m, 2H, CH_2), 3.12 (m, 2H, CH_2), 3.79-3.81 (m, 2H, CH_2), 12.47 (s, 1H). 13C NMR, DMSO 101 MHz δ: 11.06-11.12(m, CH_3), 20.92-21.30 (m, CH_2), 27.91-28.03 (m, $3CH_3$), 48.32-49.54 (m, CH_2+C), 57-47.39 (m, C), 78.66-78.75 (m, CH2), 154.70-155.04 (m, COO), 171.26-171.48 (m, COOH).

Synthesis of N-cyclohexyl-N-Boc-glycine: The synthesis was performed similarly to the protocol described for compound *N*-isopropyl-*N*-Boc-glycine. The product was isolated as a white crystalline powder in 77% yield (19.81 g) starting from cyclohexylamine 99% (11.58 mL, 100 mmol). Melting point: 99-101 °C (Lit. 103-104 °C).[3] ^{1}H-NMR, $CDCl_3$ 400 MHz δ: 0.95-1.36 (m, 5H, CH_2), 1.37-1.54 (m, 9H, CH_3), 1.57-1.86 (m, 5H, CH_2), 3.64-4.17 (m, 3H, CH_2+CH), 9.09 (br, 1H, COOH). In agreement with the literature.[33] ^{13}C-NMR, $CDCl_3$ 100 MHz δ: 25.61 (d, J=28.6 Hz, $2CH_2$),), 28.42 (s, $3CH_3$), 31.14 ($2CH_2$), 42.21 (CH_2), 54.39 (CH), 56.39 (C), 80.53 (CH_2), 154.97 (COO), 176.86 (s, COOH).

Synthesis of N-p-nitrobenzyl-N-Boc-glycine: The synthesis was performed similarly to the protocol described for compound *N*-isopropyl-*N*-Boc-glycine. The product was isolated as a yellowish crystalline powder in 70% yield (4.56 g) starting from *p*-nitrobenzylamine hydrochloride 97% (4.08 g, 21 mmol). Molecular weight: 310.31 g/mol. MS (Cl^+): m/z= 311.12 $[M+H]^+$. Melting point: 93 °C. ^{1}H-NMR, $CDCl_3$ 400 MHz δ: 1.46 (d, 9H, J=16.6 Hz, $3CH_3$), 3.96 (d, 2H, J=54.8 Hz, CH_2), 4.61 (d, 2H, J=16.6 Hz, CH_2), 7.41 (m, 2H, Ar), 8.22 (m, 2H, Ar), COOH missing in these experimental conditions. ^{13}C-NMR, $CDCl_3$ 100 MHz δ: 28.34 ($3CH_3$), 48.65 (d, J=13.8 Hz, C), 51.49 (d, J=71.1 Hz, CH_2), 81.89 (d, J=28.0 Hz,

CH_2), 124.05 (2CH), 128.34 (d, *J*=67 Hz, 2CH), 145.15 (d, *J*=21.2 Hz, C), 147.60 (C), 155.52 (m, COO), 174.18 (d, *J*=33.7 Hz, COOH).

Synthesis of N-(2-methylthio)ethyl-N-Boc-glycine: The synthesis was performed similarly to the protocol described for compound *N*-isopropyl-*N*-Boc-glycine. The product was isolated as a yellow viscous oil in 63% yield (15.70 g) starting from 2-(methylthio)ethylamine 97% (9.59 mL, 100 mmol). Molecular weight: 249.33 g/mol. MS (Cl^+): *m/z*= 250.11 $[M+H]^+$. ^{1}H-NMR, $CDCl_3$ 400 MHz *δ*: 1.46 (d, 9H, *J*=18.6 Hz, $3CH_3$), 2.13 (br, 3H, CH_3), 2.67 (dd, 2H, *J*=12.2, 5.8 Hz, CH_2), 3.47 (dt, 2H, *J*=17.5, 7.2 Hz, CH_2), 4.03 (d, 2H, *J*=24.4 Hz, CH_2), COOH missing in these experimental conditions. ^{13}C-NMR, $CDCl_3$ 100 MHz *δ*: 15.64 (d, *J*=8.5 Hz, CH_3), 28.40 (d, *J*=14.5 Hz, $3CH_3$), 32.52 (d, *J*=24.0 Hz, CH_2), 48.40 (d, *J*=30.9 Hz, C), 49.93 (d, *J*=52.2 Hz, CH_2), 81.18 (d, *J*=22.9 Hz, CH_2), 155.46 (d, *J*=82.0 Hz, COO), 175.32 (d, *J*=59.4 Hz, COOH).

Synthesis of N-trifluoroethyl-N-Boc-glycine: The synthesis was performed similarly to the protocol described for compound *N*-isopropyl-*N*-Boc-glycine. The product was isolated as a white crystalline powder in 65% yield (16.71 g) starting from 2,2,2-trifluoroethylamine 99% (8.03 mL, 100 mmol). Molecular weight: 257.21 g/mol. MS (Cl^+): *m/z*= 258.09 $[M+H]^+$. Melting point: 82-85 °C. ^{1}H-NMR, $CDCl_3$ 400 MHz *δ*: 1.46 (d, 9H, *J*= 9.2 Hz, $3CH_3$), 3.92 (oct, *J*=17.5 Hz CH_2), 4.10 (d, 2H, *J*=23.4 Hz, CH_2), 8.19 (br, 1H, COOH). ^{13}C-NMR, CDCl3 100 MHz *δ*: 28.16 (d, *J*=3.5 Hz, $3CH_3$), 48.25-49.99 (m, CH_2), 56.39 (C), 85.52 (d, *J*=8.8 Hz, CH_2), 124.57 (q, *J*=280 Hz, CF_3), 154.94 (d, *J*=4.1 Hz, COO), 174.97 (d, *J*=28.2 Hz, COOH).

Synthesis of N-(Cbz-aminoethyl)-N-Boc-glycine: The synthesis was performed similarly to the protocol described for compound *N*-isopropyl-*N*-Boc-glycine. The product was isolated as a white powder in 60% yield (9.16 g) starting from *N-Cbz*-1,4-diaminoethane hydrochloride 99% (10.09 g, 43 mmol). Molecular weight: 352.39 g/mol. MS (Cl^-): *m/z*= 351.15 $[M-H]^-$. Melting point: 117 °C. ^{1}H-NMR, $CDCl_3$ 400 MHz *δ*: 1.42 (d, 9H, *J*=6.2 Hz, $3CH_3$), 3.21-3.50 (m, 4H, $2CH_2$), 3.90 (m, 2H, CH_2), 5.05-5.21 (m, 2H, CH_2), 5.53 (s, 1H, NH), 7.30-7.36 (m, 5H, Ar), COOH missing in these experimental conditions. ^{13}C-NMR, $CDCl_3$ 100 MHz *δ*: 28.31 (d, *J*=8.8 Hz, $3CH_3$), 39.89 (d, *J*=22.3 Hz, C), 48.80 (d, *J*=58.2 Hz, CH_2), 49.97 (d, *J*=44.7 Hz, CH_2), 67.20 (d, *J*=64.1 Hz, CH_2), 81.13 (d, *J*=27.2 Hz, CH_2), 128.21 (d, *J*=9.8 Hz, 2CH), 128.40 (CH), 128.63 (2CH), 136.56 (C), 155.98 (d, *J*=41.3 Hz, COO), 156.87 (d, *J*=42.9 Hz, COO), 174.03 (d, *J*=31.7 Hz, COOH)

2. Additional NCA synthesis

Synthesis of Glycine-NCA. In a clean and previously dried Shlenk flask *N*-Boc-glycine (2 g, 11.4 mmol, 1 equiv.) was dried during 15 min in the Schlenck line, then 32 mL of anhydrous THF were added, followed of thionyl chloride (1 mL, 13.7 mmol, 1.2 equiv.). The reaction was stirred for 4 h at RT. The solvent was evaporated using vacuum Schlenck line, washed three times with 35 mL of anhydrous hexane, the suspension was filtered using a cannula and the powder was dried. Then 90 mL of anhydrous ethyl acetate were added and the suspension was filtered over previously dried Celite. The system was washed with 60 mL of anhydrous ethyl acetate and the solution concentrated. The solution was filtered again over previously dried Celite and the system washed with 60 ml of anhydrous ethyl acetate. The solid was washed two times with 10 mL of dry diethyl ether and dried. The product was isolated as a white yellowish crystalline powder in 79% yield (700 mg). ^{1}H-NMR, DMSO-d_6 400 MHz δ: 4.20 (s, 2H, CH_2), 8.83 (s, 1H, NH). ^{13}C-NMR, DMSO-d_6 400 MHz δ: 46.26 (s, CH_2), 153.97 (s, NCOO), 169.40 (s, COO).

Synthesis of N-methyl-L-alanine NCA (mAla-NCA): In a dry Schlenk flask, *N*-Boc-*N*-methyl-L-alanine (1.00 g, 4.92 mmol, 1 eq) was dried under vacuum for 30 min. Then, 10 mL of anhydrous DCM were added, followed by phosphorus trichloride (0.52 mL, 5.9 mmol, 1.2 eq) and stirred under Ar. After complete conversion of amino acid into NCA, the reaction was dried under vacuum. The crude material was solubilized in 10 mL of DCM and was transferred, using a cannula, in a new Schlenk flask containing celite previously dried at 150 °C for 3 h under vacuum. The product was filtered in a new previously dried Schlenk flask, dry under and isolated as a white powder in 95% yield (0.6 g, 4.7 mmol). ^{1}H-NMR, $CDCl_3$ 400 MHz δ: 1.54 (d, *J* = 7.0 Hz, 3H, CH_3), 2.99 (s, 3H, NCH_3), 4.17 (q, *J* = 7.0 Hz, 1H, CH). ^{13}C-NMR, $CDCl_3$ 100 MHz δ: 15.24 (CH), 28.41 (NCH3), 57.03 (CH), 151.75 (COO), 169.37 (COON).

3. NNCA formation

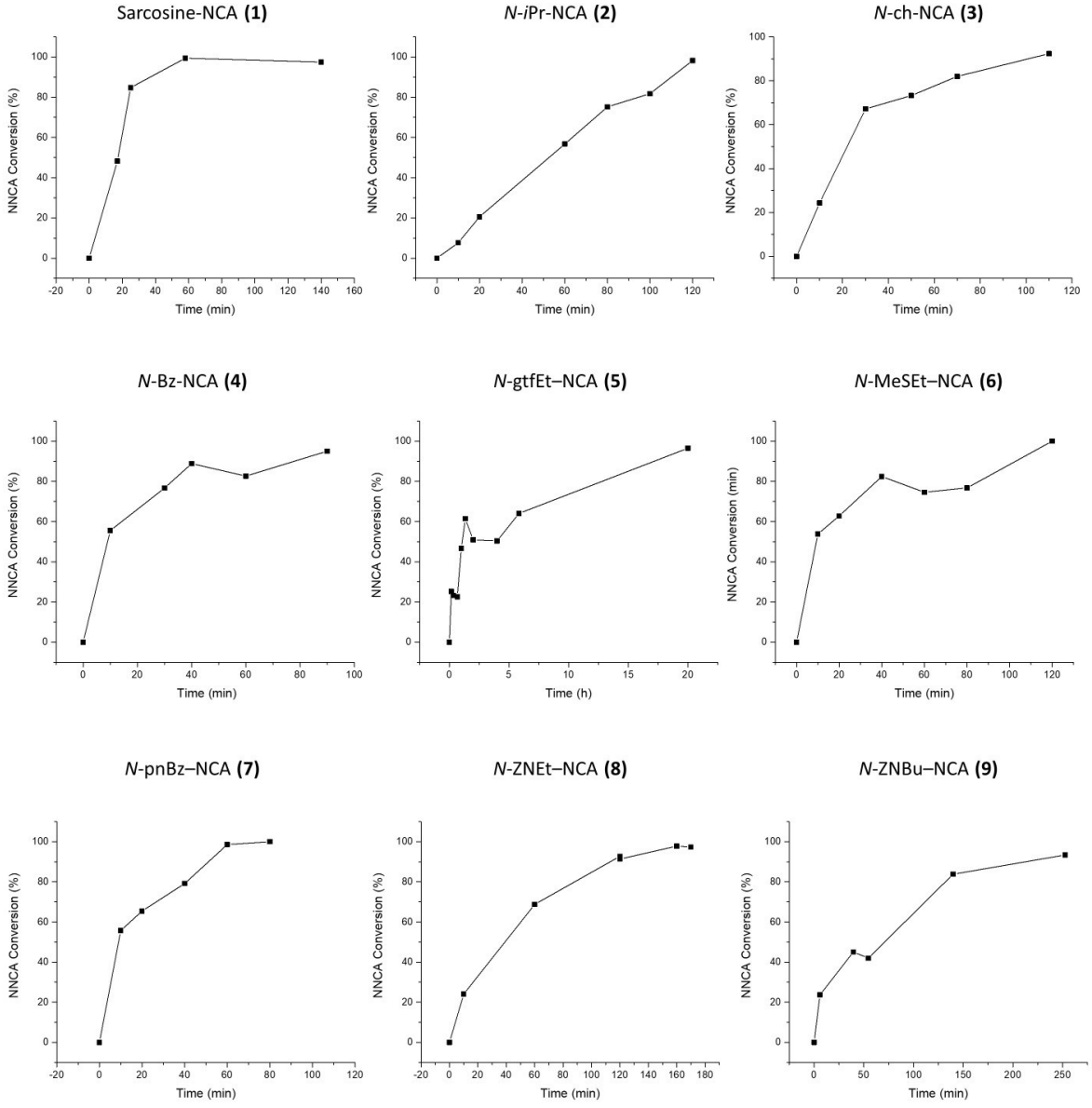


Figure S1. Kinetics experiments of NNCA formation from the cyclization of *N*-alkylated-*N*-Boc-glycine derivatives using $SOCl_2$.

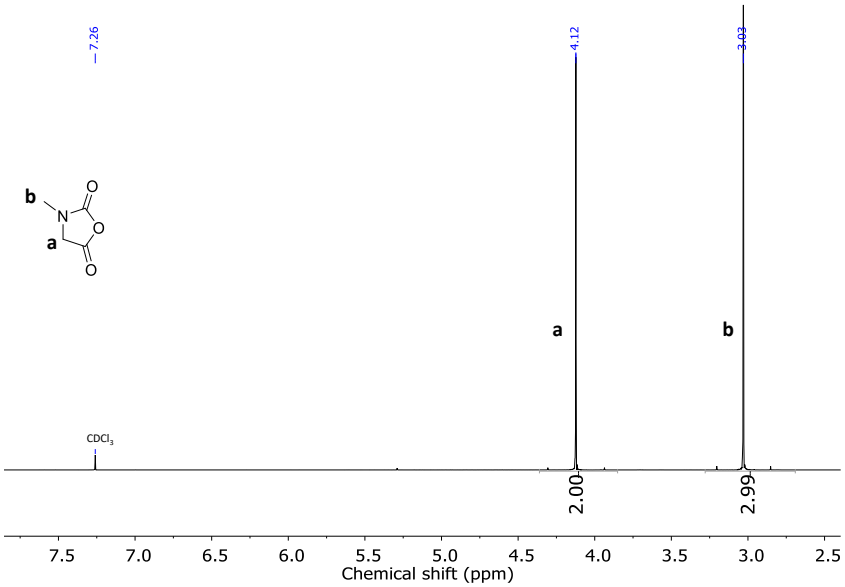


Figure S2A. ^{1}H-NMR of Sarcosine-NCA **(1)** in $CDCl_3$.

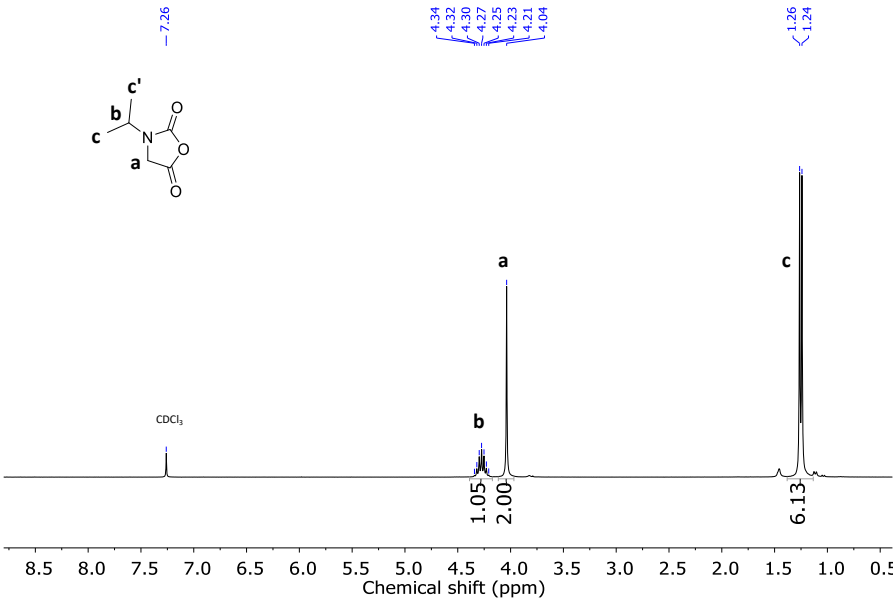


Figure S2B. ^{1}H-NMR of *N*-*i*Pr-NCA **(2)** in $CDCl_3$.

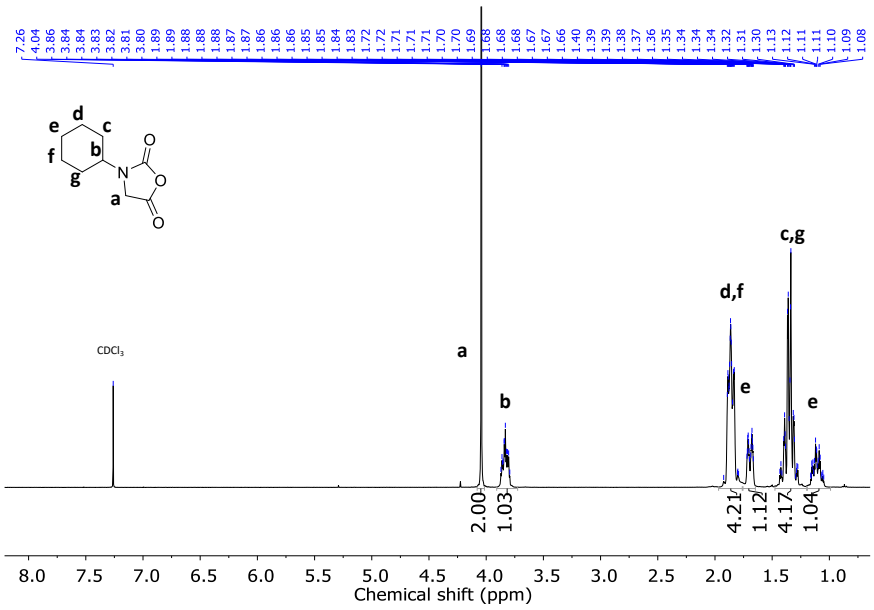


Figure S2C. ^{1}H-NMR of *N*-ch-NCA **(3)** in $CDCl_3$.

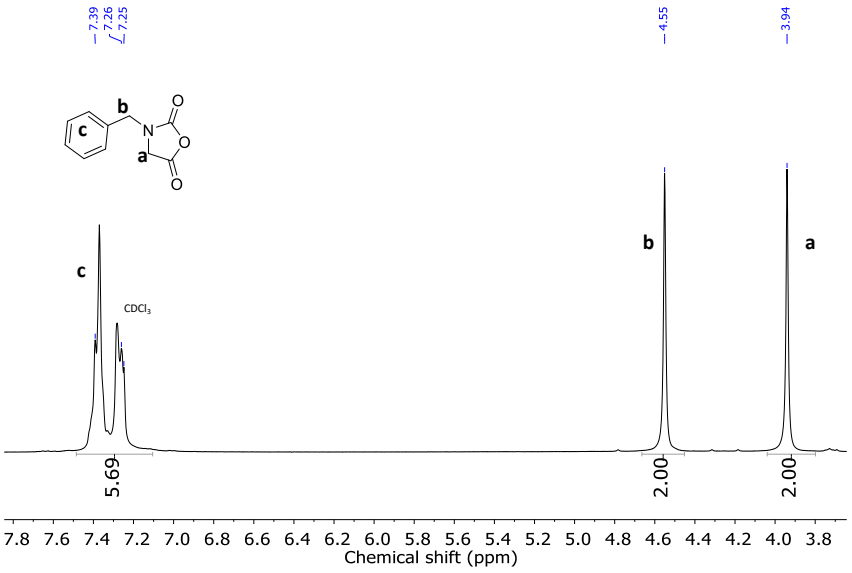


Figure S2D. ^{1}H-NMR of *N*-Bz-NCA **(4)** in $CDCl_3$.

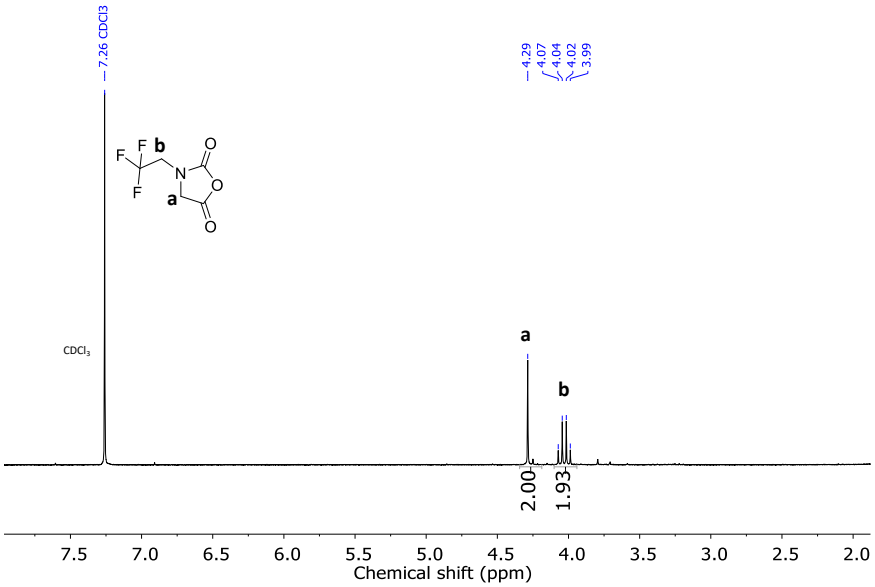


Figure S2E. ^{1}H-NMR of *N*-gtfEt–NCA **(5)** in $CDCl_3$.

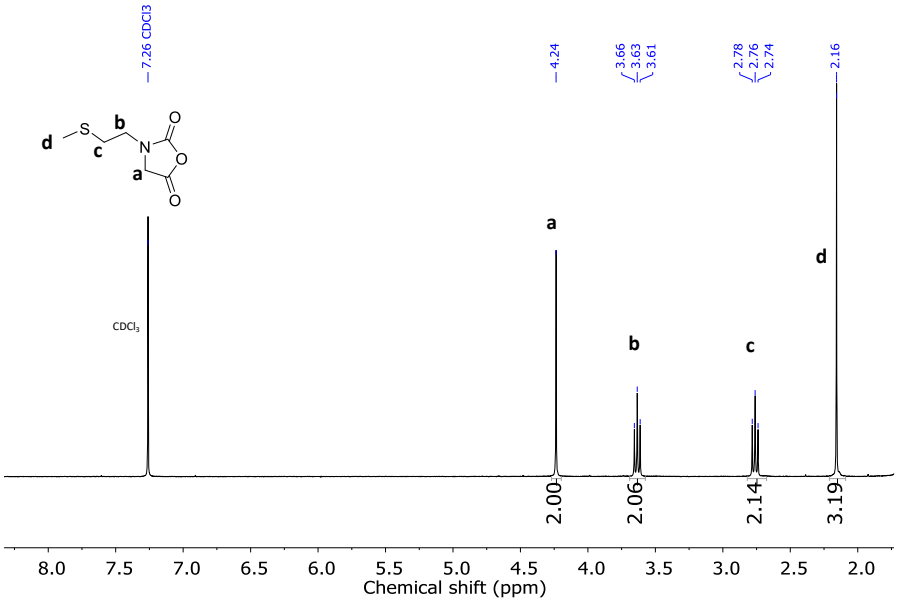


Figure S2F. ^{1}H-NMR of *N*-MeSEt–NCA **(6)** in $CDCl_3$.

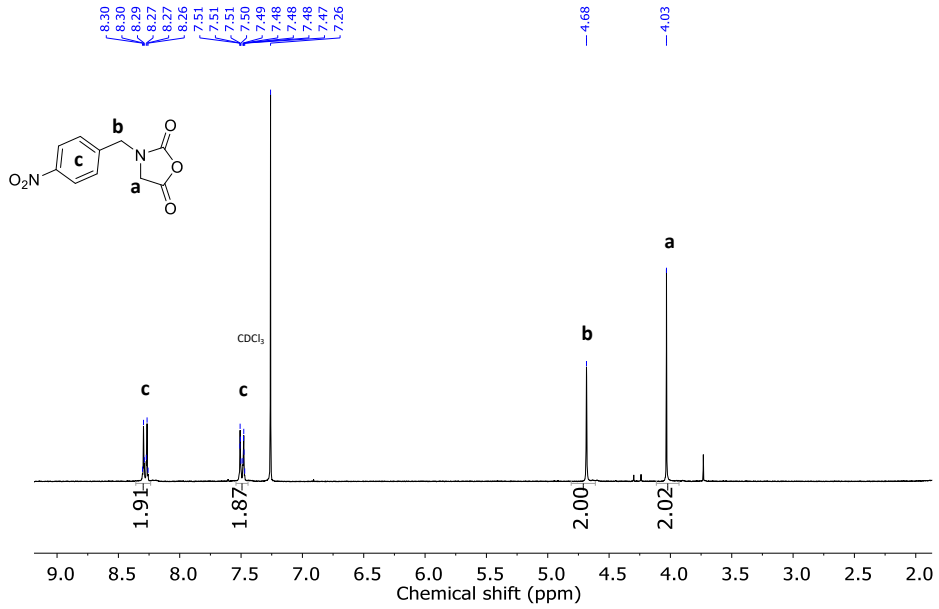


Figure S2G. ^{1}H-NMR of *N*-pnBz–NCA **(7)** in $CDCl_3$.

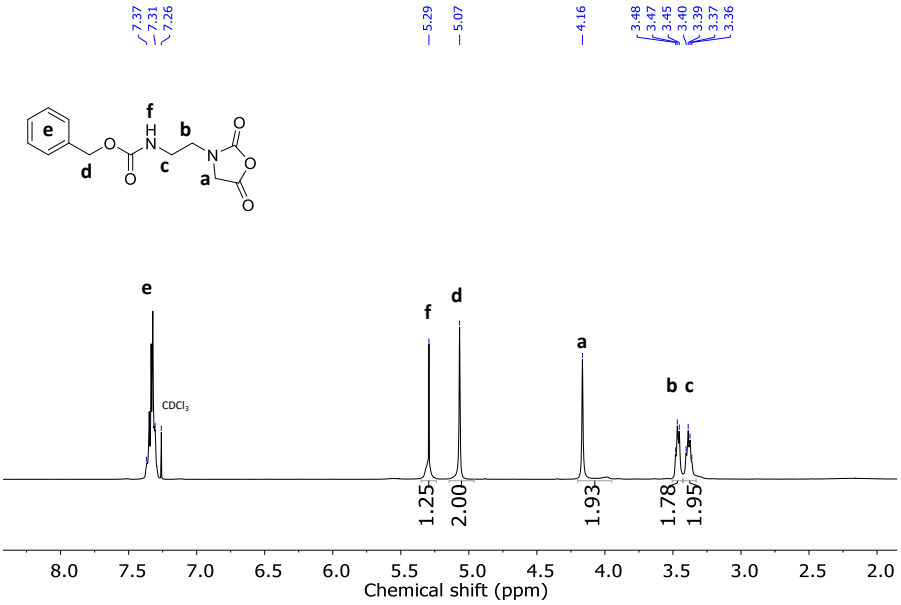


Figure S2H. ^{1}H-NMR of *N*-ZNEt–NCA **(8)** in $CDCl_3$.

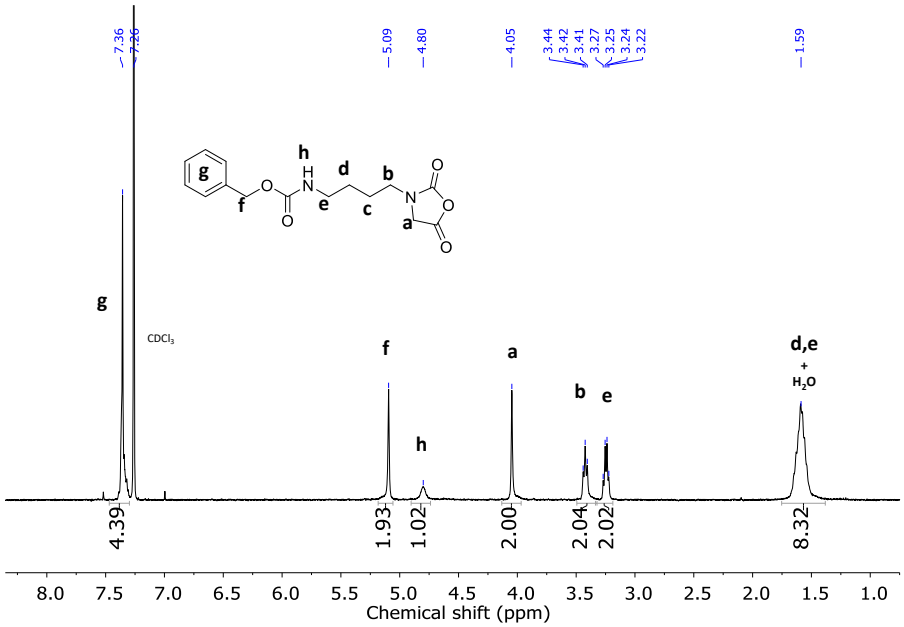


Figure S2I. ^{1}H-NMR of *N*-ZNBu–NCA **(9)** in $CDCl_3$.

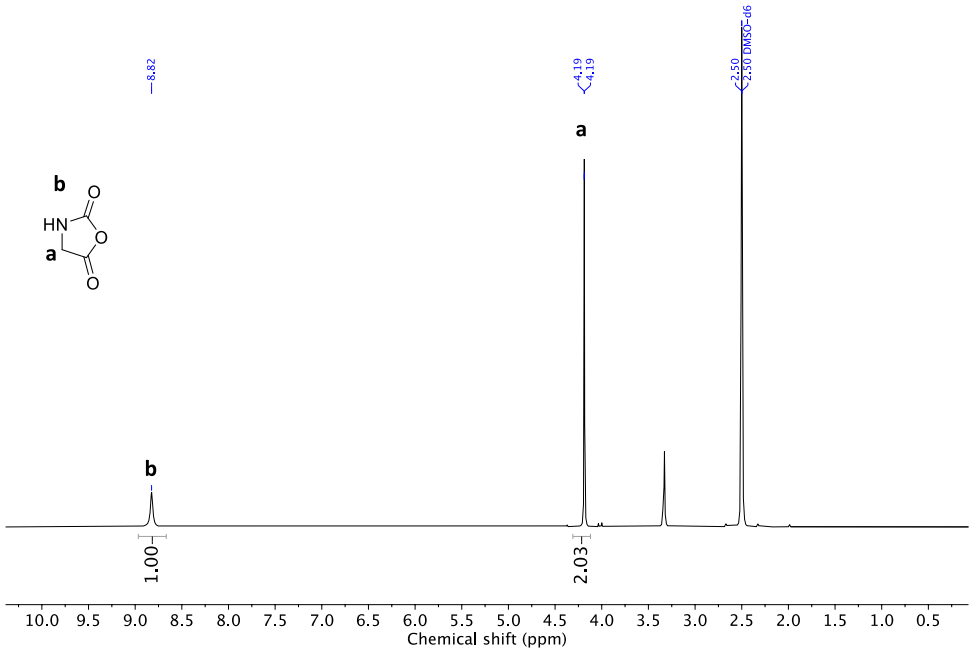


Figure S2J. ^{1}H-NMR of Glycine-NCA in $CDCl_3$.

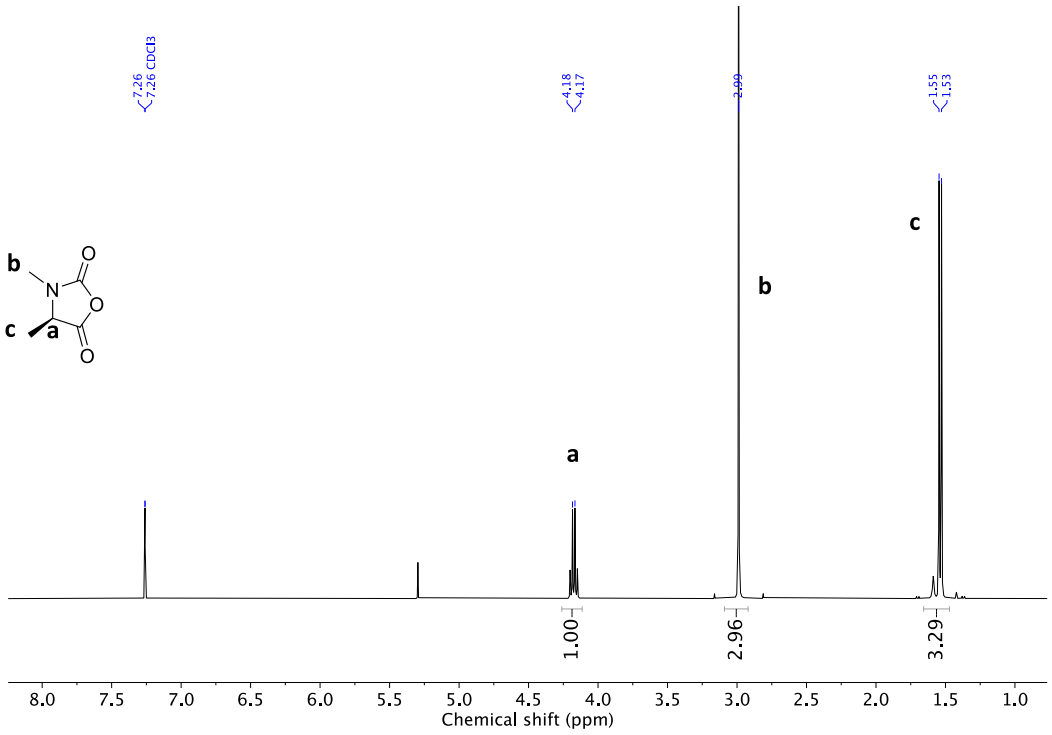


Figure S2K. ^{1}H-NMR of MeAla-NCA in $CDCl_3$.

4. Sar-NCA monomer purification and kinetics of its ROP

During the NCA synthesis, the Leuchs method releases HCl and chlorinated byproducts that may persist even after recrystallization.[4–7] Acidic contaminants retard the ROP process,[8] and their elimination is therefore important to obtain an efficient and reproducible polymerization.[9] In this work, we specifically studied the kinetics of the ROP of Sar-NCA to optimize the purification step: a monomer without purification was used and compared to a monomer purified by crystallization and/or celite filtration. Sar-NCA was used in anhydrous DMF, under argon and at targeted ratio of M/I = 100 with allylamine. The ROP kinetics were monitored by following the disappearance of the NC=O stretching at 1850 cm^{-1} by FTIR analyses (**figure s2A**). The reaction time was longer without purification: the ROP of the non-purified monomer reached only 63% of conversion after 260 minutes whereas the ROP of the monomer purified by crystallization reached 77% after the same reaction time. Interestingly, the conversion was improved by replacing the crystallization step by filtration over celite (>97% conversion after 260 min). To determine the first-order rate coefficients, the data were fitted by NNLS using an exponential decay ($M_t = M_0.\exp(-kt)$), where the M_0 is the initial peak intensity and M_t is the intensity at time t: (**figure s2B**). Previous studies confirmed that the ROP of Sar-NCA follows a first-order kinetics rate: this indicates that the concentration of propagating species remains constant and supports the living character of the polymerization process.[8] We observed that the impurities generated during the NNCA synthesis induced lower kinetic rate constants and celite filtration showed a 2-4 fold increase in the first-order rate coefficients and afforded the fastest polymerization of Sar-NCA ($8.8 \times 10^{-3} \pm 0.4$ min^{-1}). As this method was the most effective in removing

acid contaminants, we used celite filtration to prepare all our other NNCA monomers before polymerization.

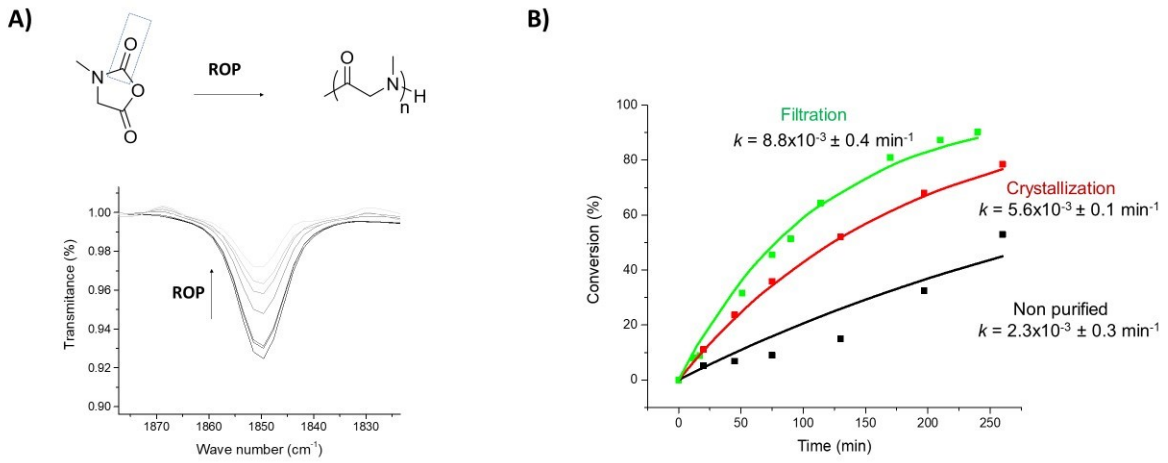
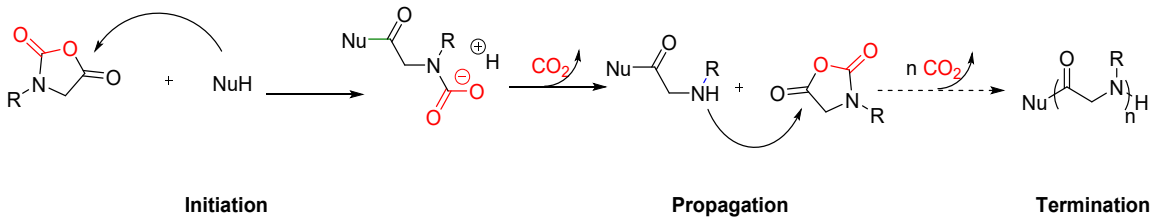


Figure S3. Kinetic experiments of Sar-NCA purified by Celite filtration, crystallization and without crystallization (ROP in DMF at 0.4 M and at M/I = 100). A) Disappearance over time of the stretching bond at 1850 cm^{-1} during the ROP, B) First-order kinetic plots.

5. Ring opening polymerization: additional procedures and characterizations



Scheme S1. Ring opening polymerization of NNCA monomers.

Synthesis of polyglycine (PGly). Glycine-NCA monomer (38.2 mg, 0.378x10^{-3} mol) was weighted in a glovebox under pure argon, introduced in a flame-dried Schlenck vessel, and dissolved with 0.944 mL of anhydrous DMF. A solution of allylamine (1.3 M in DMF) was prepared and 100 µL (0.018x10^{-3} mol) were added with an argon purged syringe. The solution was stirred at room temperature under argon until completion. The polymer was then recovered as a white solid by precipitation in THF and dried under high vacuum. Yield: 90% (20 mg). ^{1}H-NMR TFA-d 400 MHz δ (ppm): 3.86-3.99 (m, 2H, CH_2 allylamine), 3.80-4.42 (m, 32H, CH_2), 5.0-5.20 (m, 2H, CH_2 allylamine), 5.64-5.82 (m, 1H, CH allylamine). NH terminal missing in these experimental conditions.

*Synthesis of poly(N-methyl-L-Alanine) (*PNMeAla*). N*-Me-L-Ala-NCA monomer (0.05 g, 0.387x10^{-3} mol) was weighted in a glovebox under pure argon, introduced in a flame-dried Schlenk vessel, and dissolved with 1.0 mL of anhydrous DMF. A solution of allylamine (0.5 M in DMF) was prepared and 26 µL (1.3x10^{-5} mol) were added with an argon purged syringe. The solution was stirred at room

temperature under argon until completion. The polymer was then recovered as a white solid by precipitation in diethyl ether and dried under high vacuum. Yield: 79% (18 mg). ^{1}H-NMR $CDCl_3$ 400 MHz δ (ppm): 1.14-1.51 (m, 55H, CH_3), 2.65-3.21 (m, 56H, NCH_3), 3.75-3.96 (m, 2H, CH_2 allylamine), 4.94-5.53 (m, 18H, CH), 5.71-5.87 (m, 1H, CH allylamine). NH signals missing in these experimental conditions.

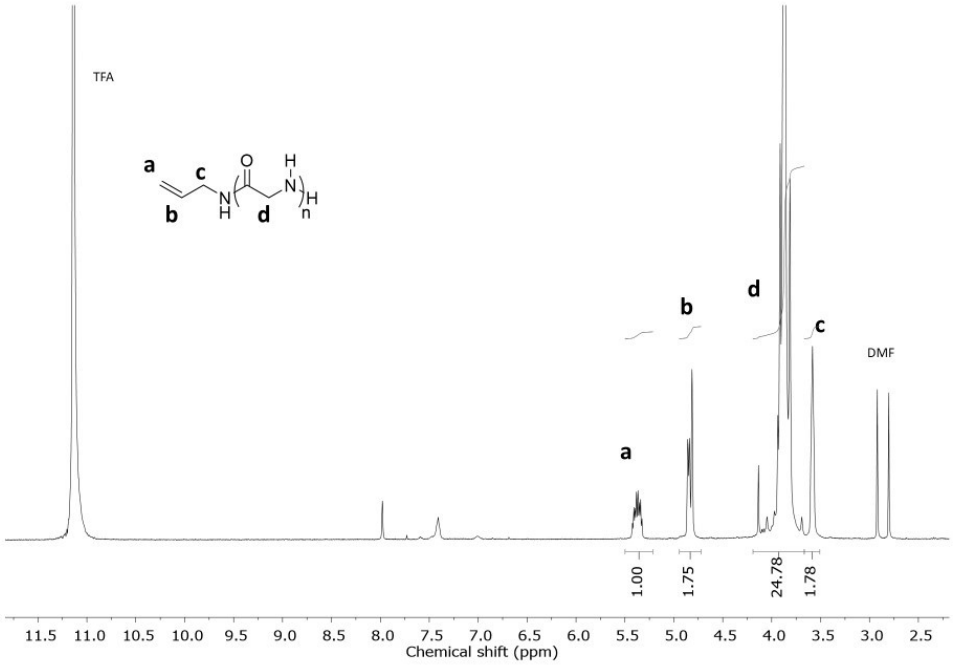


Figure S4. ^{1}H-NMR of PGly determined in TFA-d.

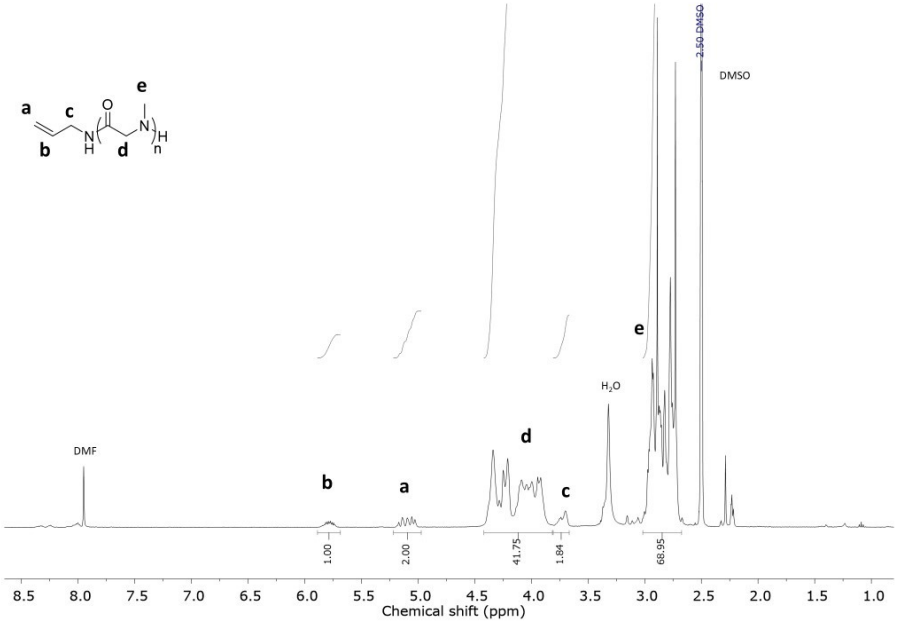


Figure S5. ^{1}H-NMR of PSar **1'** determined in DMSO-d.

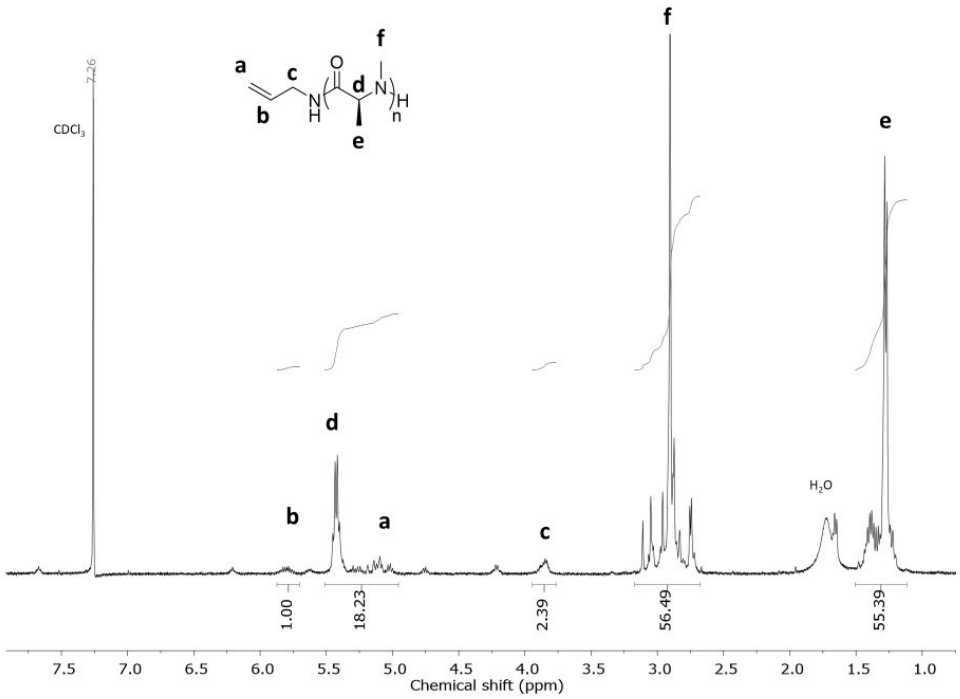


Figure S6. ^{1}H-NMR of P*N*MeAla determined in $CDCl_3$

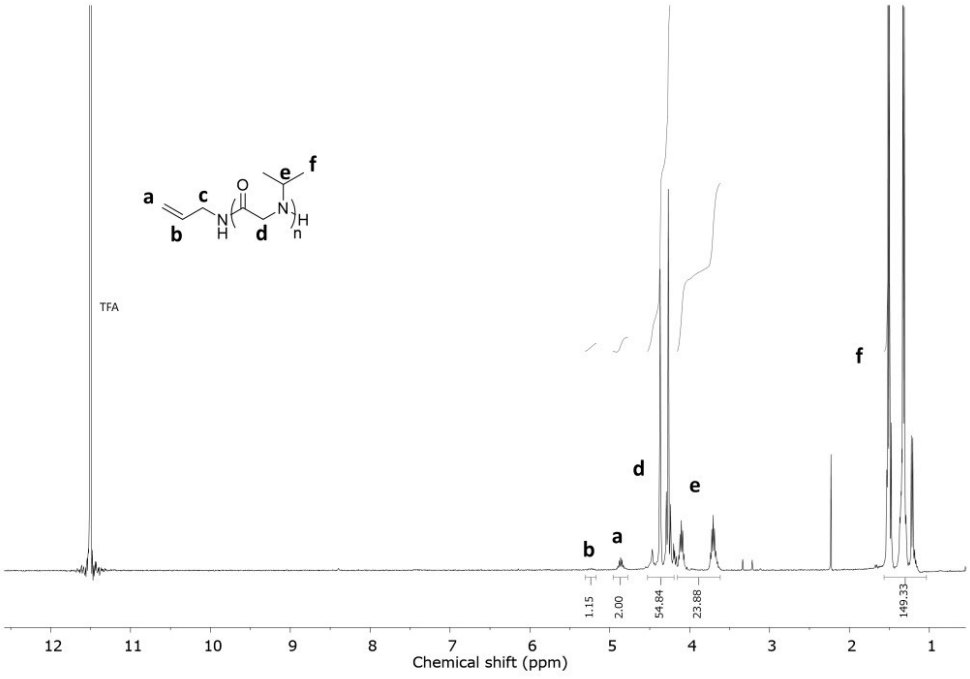


Figure S7. ^{1}H-NMR of P*N*iPr **2'** determined in TFA-d.

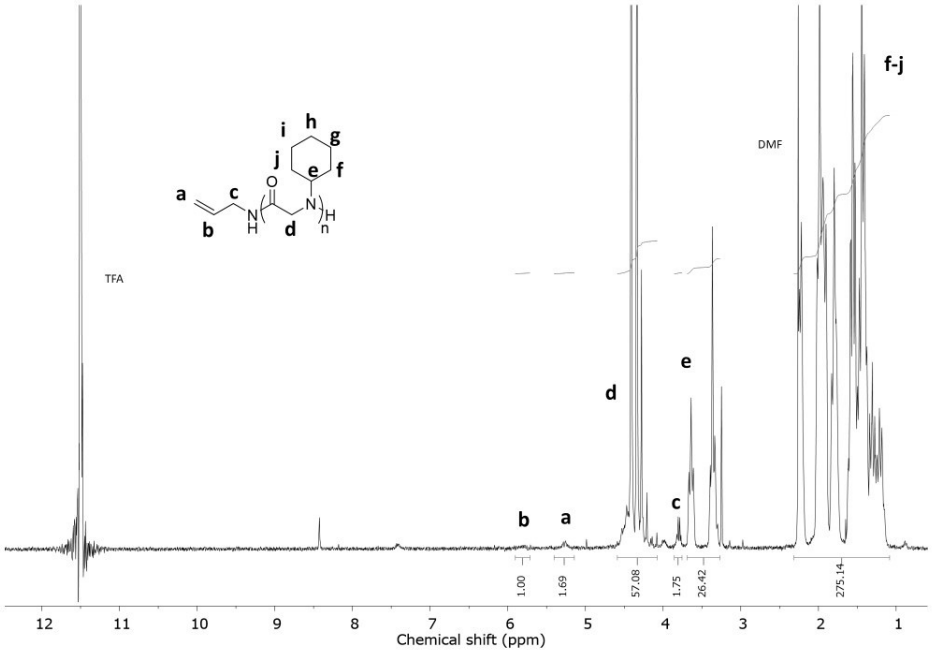


Figure S8. ^{1}H-NMR of P*N*ch **3'** determined in TFA-d.

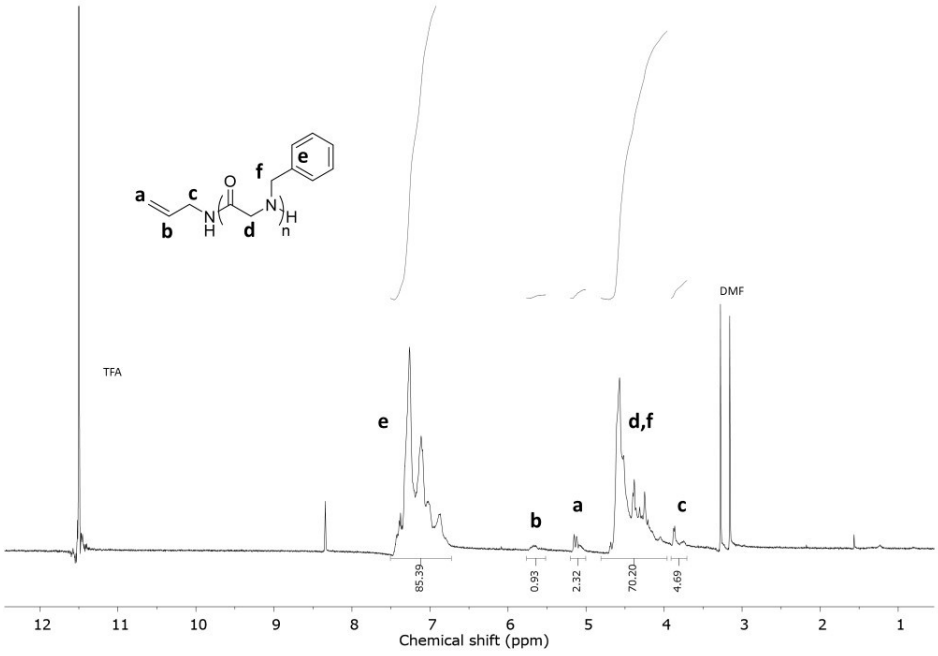


Figure S9. ^{1}H-NMR P*N*Bz **4'** determined in TFA-d.

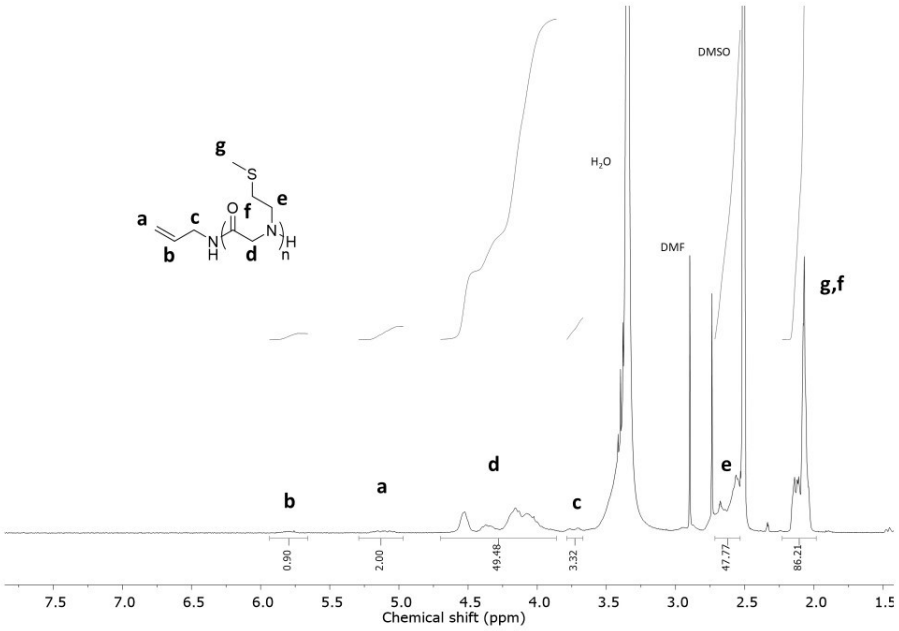


Figure S10. ^{1}H-NMR of P*N*mt **6'** determined in DMSO-d.

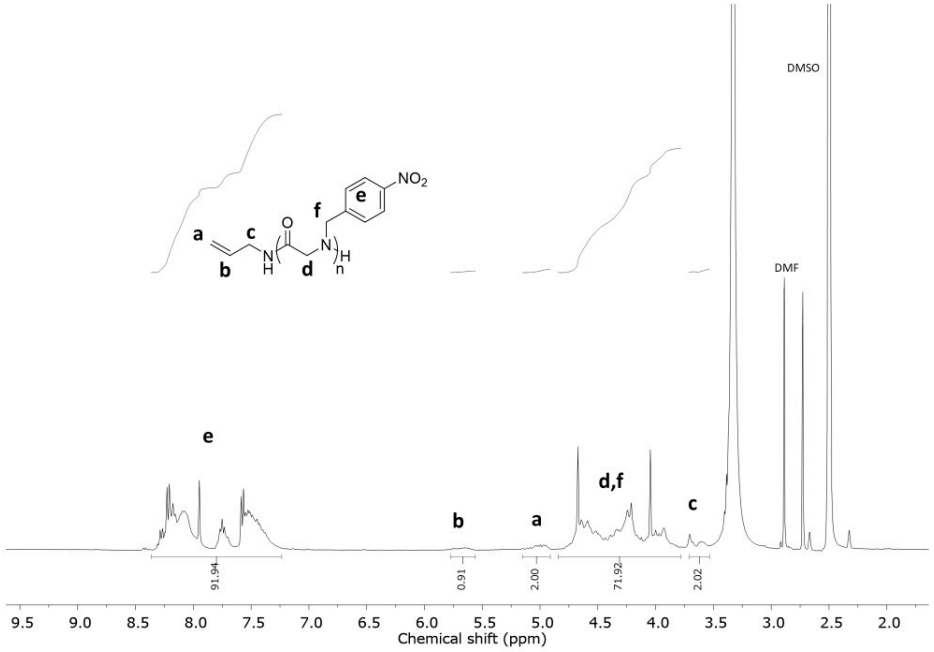


Figure S11. ^{1}H-NMR of P*N*pBzG **7'** determined in DMSO-d.

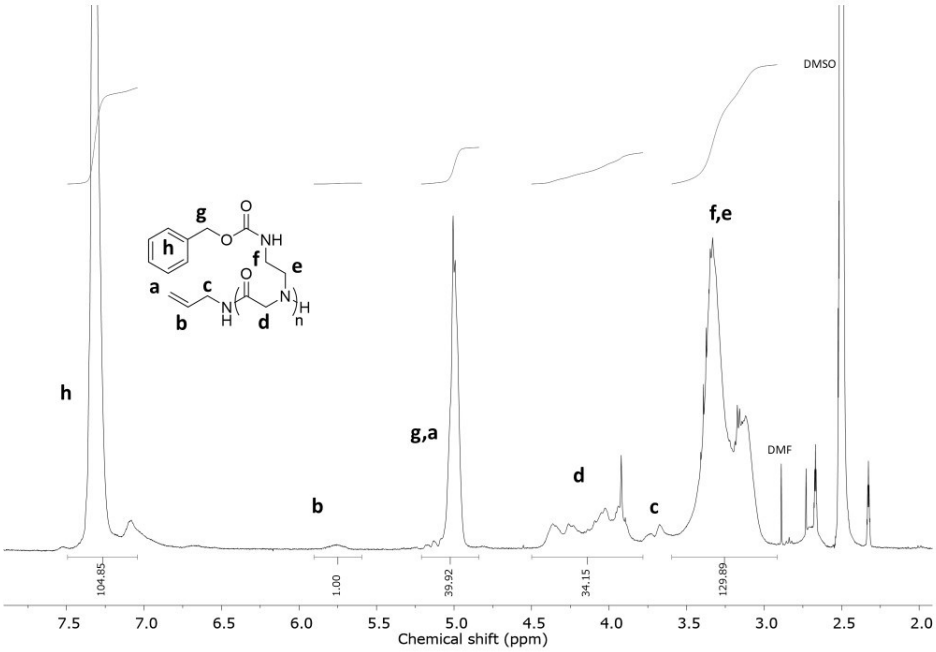


Figure S12. ^{1}H-NMR of P*N*zae **8'** determined in DMSO-d.

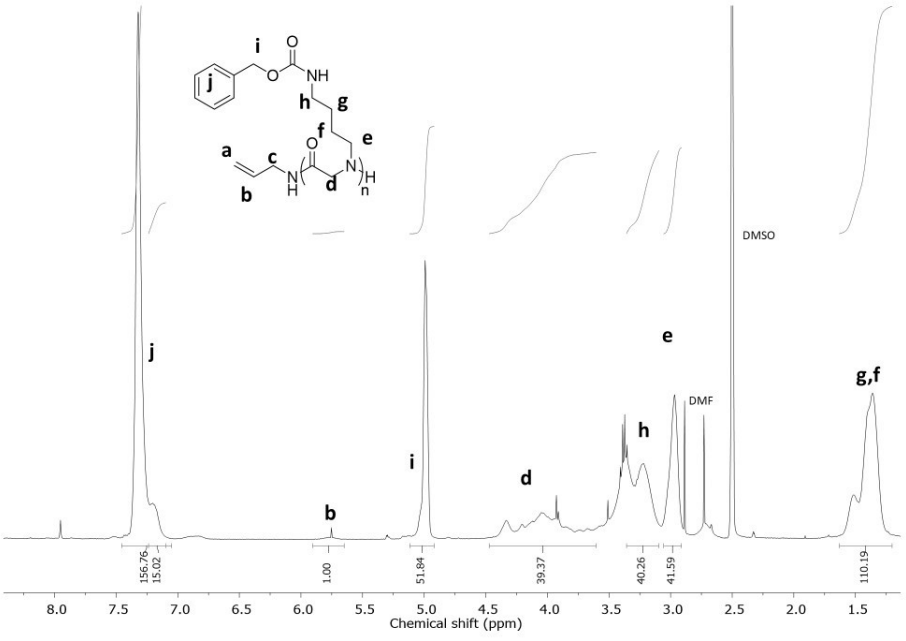


Figure S13. ^{1}H-NMR of P*N*Zab **9'** determined in DMSO-d.

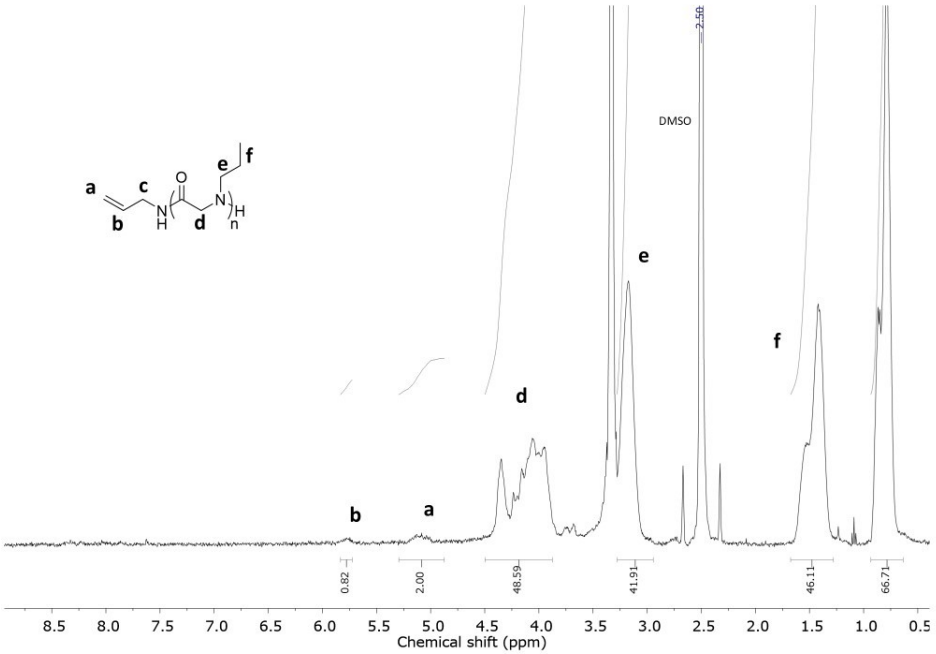


Figure S14. ^{1}H-NMR of P*N*Pr **10'** determined in DMSO-d.

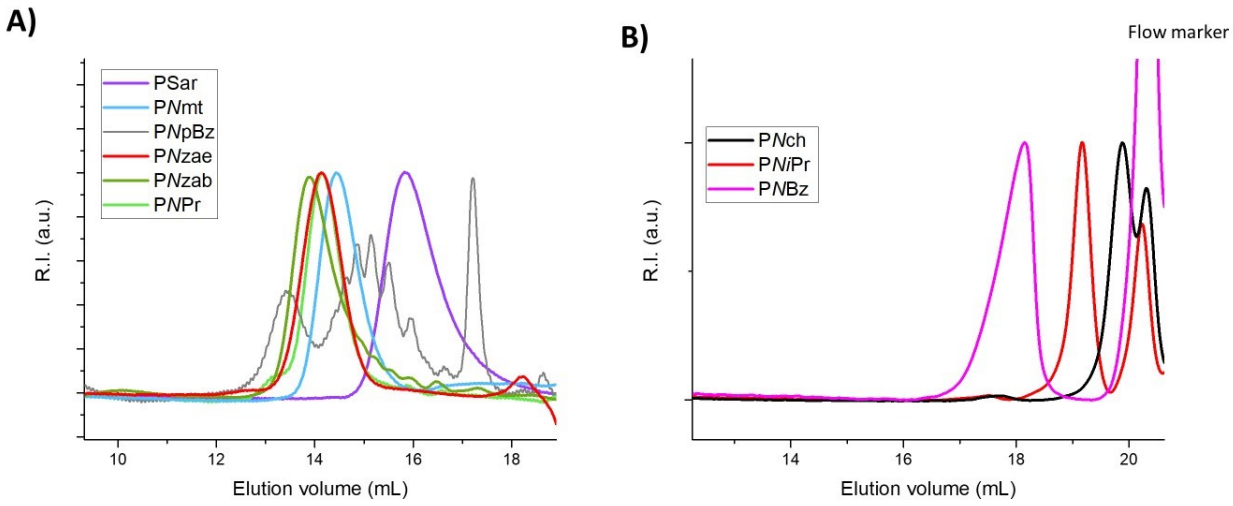


Figure S15. Refractive index-molar masses profiles of poly(*N*-substituted)glycines determined by size exclusion chromatography (SEC) using two different systems: a) DMF (LiBr 1%) and b) HFIP ($NaCF_3COO$ 1%).

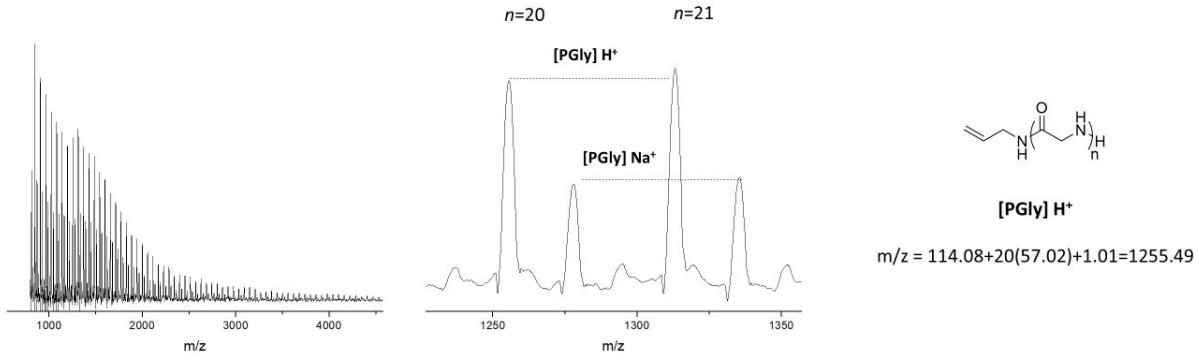


Figure S16. Identification of the PGLy by MALDI TOF using matrix 2,5- dihydroxybenzoic acid as matrix agent in MeOH (0.1M). Ratio 1:10

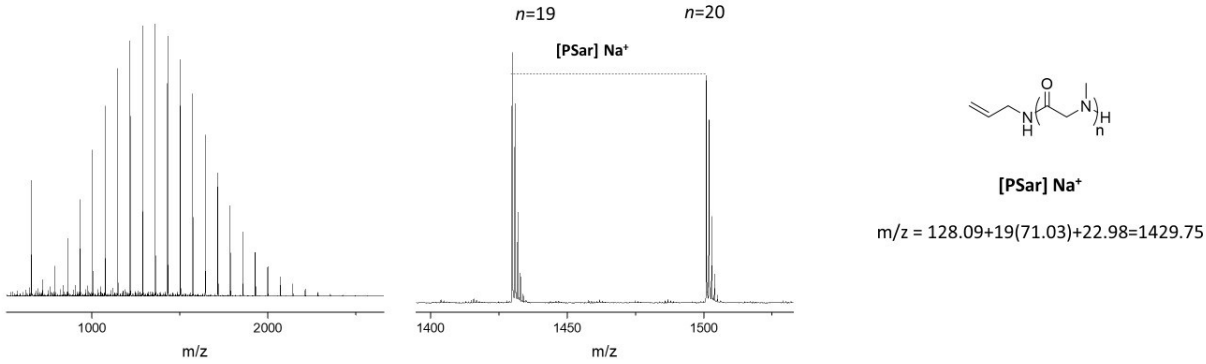


Figure S17. Identification of the PSar **1'** by MALDI TOF using α-CHCA as matrix agent.

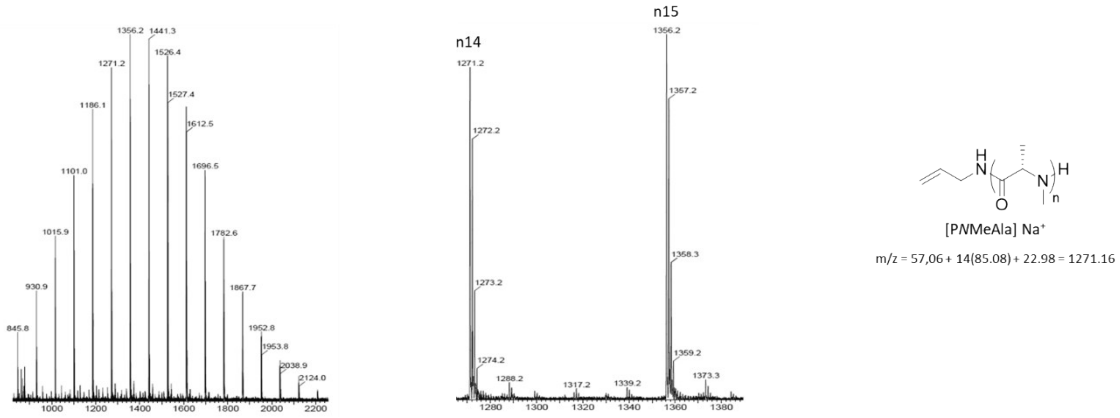


Figure S18. Identification of the P*N*MeAla by MALDI TOF using α-CHCA as matrix agent (P*N*MeAla/α-CHCA/NaI 1/3/1).

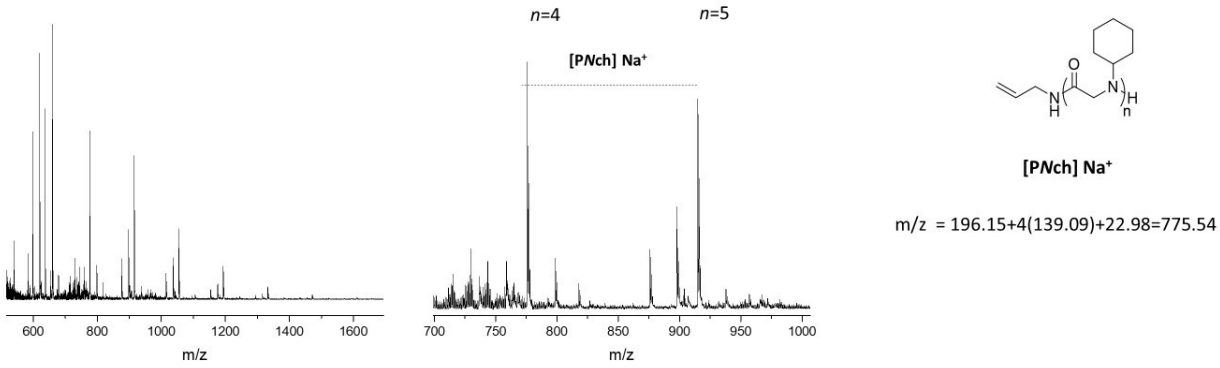


Figure S19. Identification of the P*N*ch **2'** by MALDI TOF using dithranol as matrix agent.

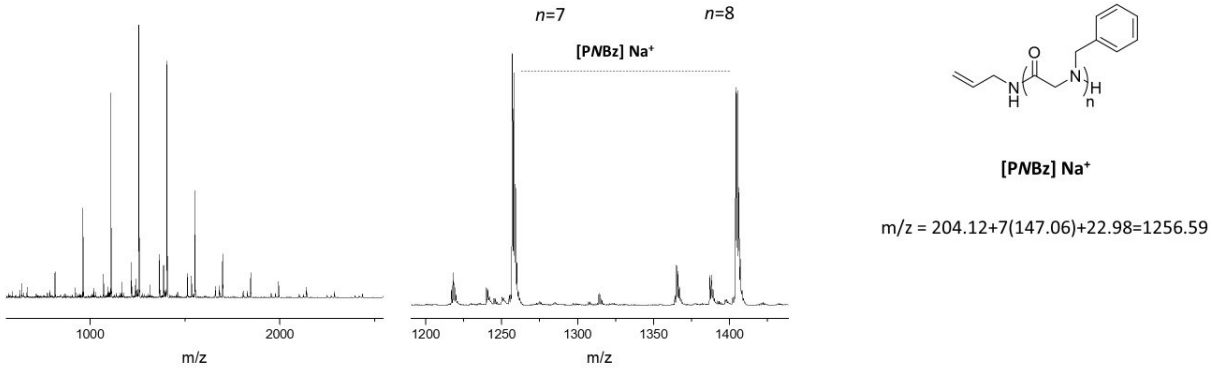


Figure S20. Identification of the P*N*BzG **4'** by MALDI TOF using α-CHCA as matrix agent.

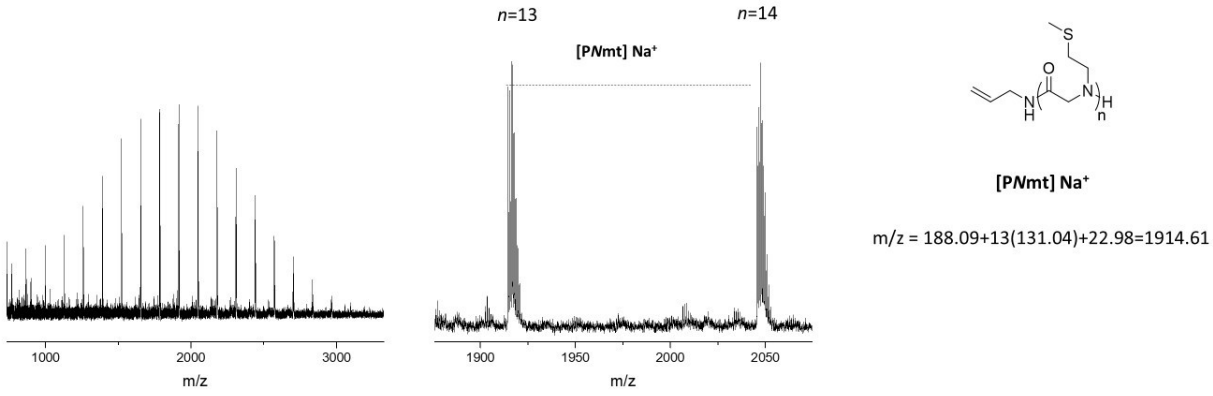


Figure S21. Identification of the P*N*mt **6'** by MALDI TOF using dithranol as matrix agent.

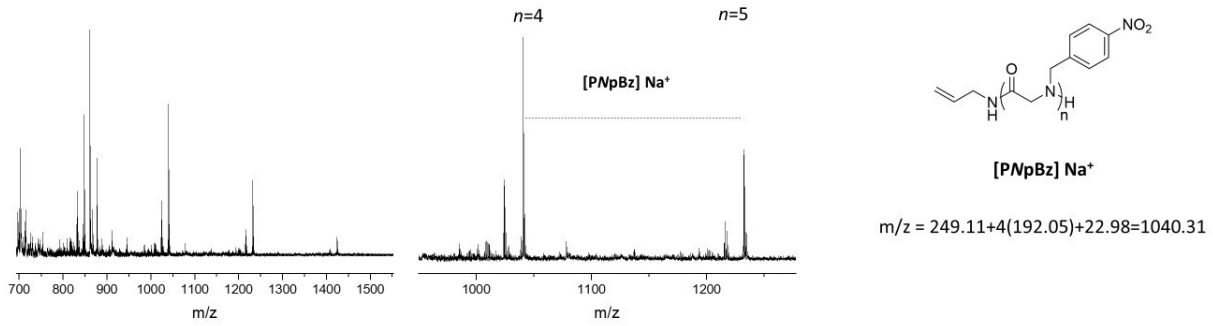


Figure S22. Identification of the P*N*pBz **7'** by MALDI TOF using dithranol as matrix agent.

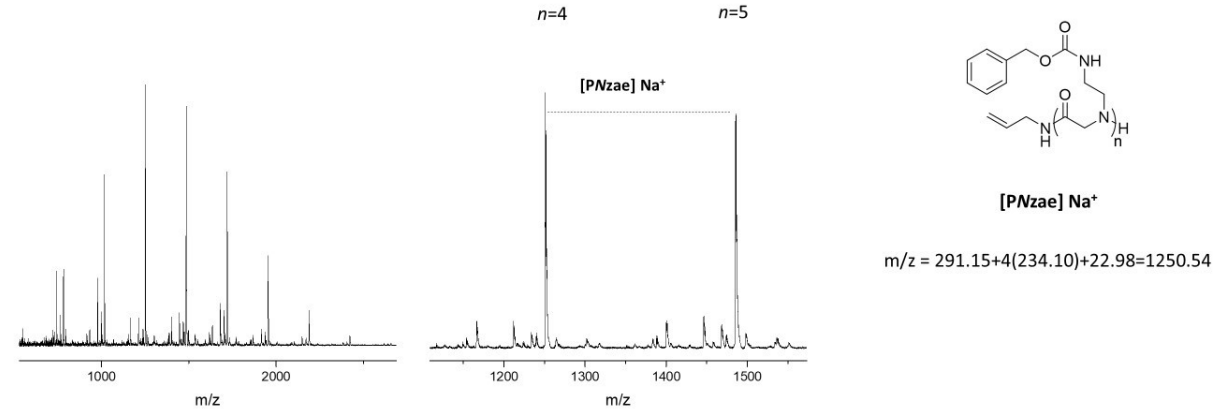


Figure S23. Identification of the P*N*Zae **8'** by MALDI TOF using dithranol as matrix agent.

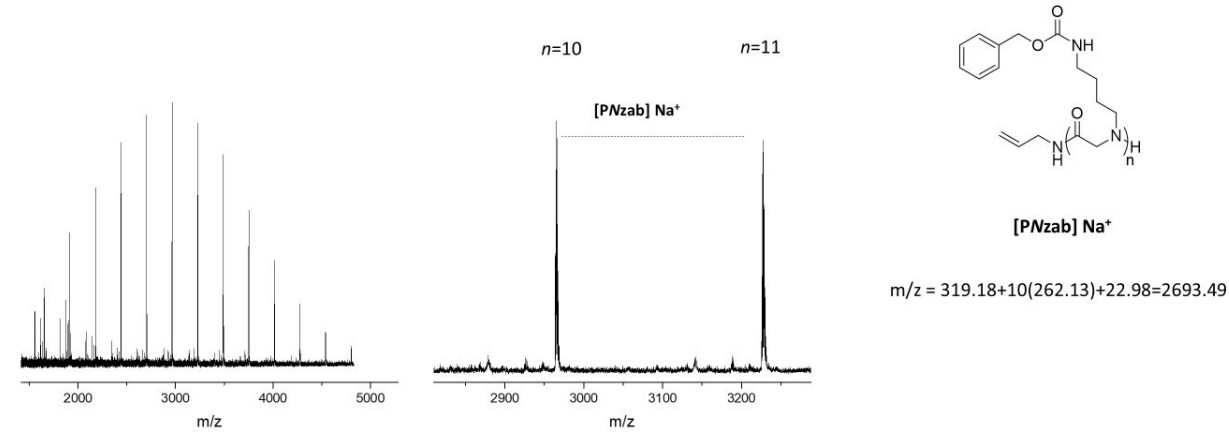


Figure S24. Identification of the P*N*Zab **9'** by MALDI TOF using dithranol as matrix agent.

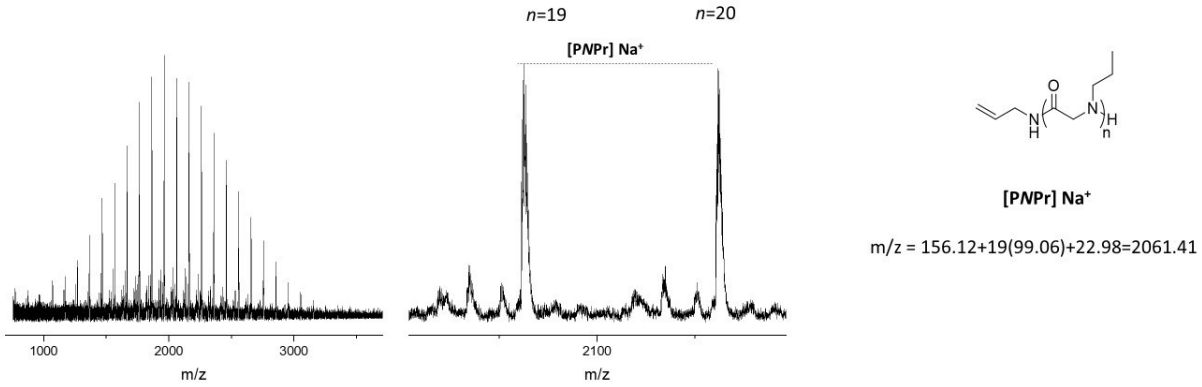
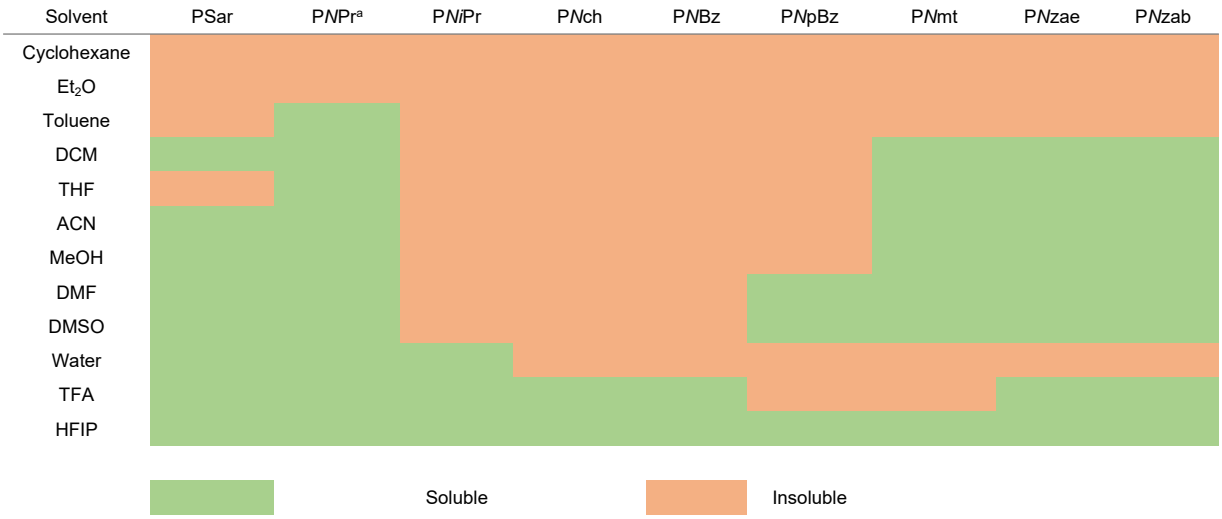


Figure S25. Identification of the P*N*Pr **10'** by MALDI TOF using dithranol as matrix agent.

Table S1. Solubility test of the poly(*N*-substituted)glycines initiated with allylamine at M/I=20 (1 mg/mL).



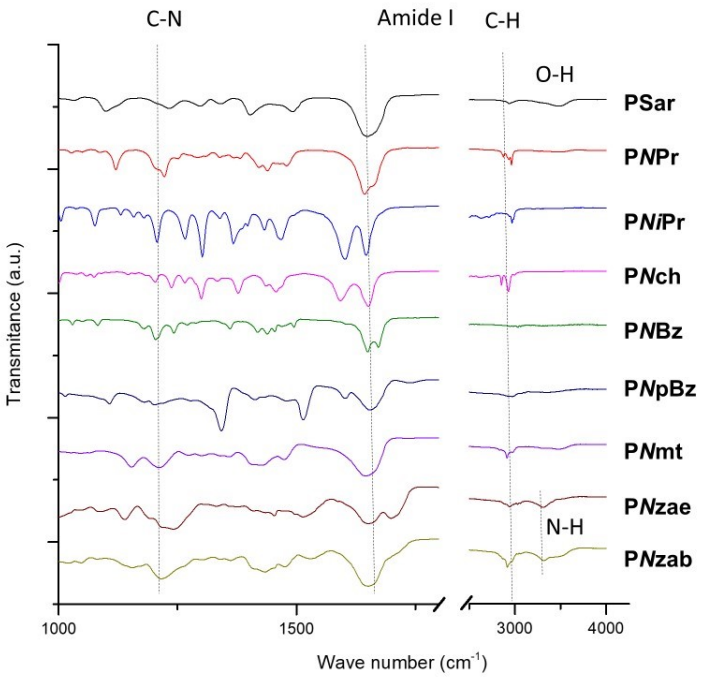
[a] Solubility in water was afforded upon evaporation of its solution in MeOH

Table S2. Characterization of the polypeptides and polypeptoids bearing different *N*-alkylated group.

Polymer	MW theoretical (g mol^{-1})	MW from ^{1}H-NMR (g mol^{-1})	M_n from SEC (g mol^{-1})	$Đ_M$	Yield (%)
PGly[a]	1198	1100	-	-	90
P*N*MeAla	1759	1600	-	-	79
PSar (1')	1477	1600	1000	1.03	60
P*Ni*Pr (2')	2037	2400	1500[b]	1.16	63
P*N*ch (3')	2837	3800	800[b]	1.29	79
P*N*Bz (4')	2997	2600	1600[b]	1.19	68
P*N*tfg (5')[c]	-	-	-	-	-
P*N*mt (6')	2677	2900	5400	1.22	41
P*N*pBz (7')	3897	3900	4000[d]	1.91	69

P*N*zae (8')	4737	5200	4000	1.29	64
P*N*zab (9')	5297	6100	5600	1.08	52
P*N*Pr (10')	2037	2200	2400	1.09	58

[a] The polymer was not soluble even in HFIP. [b] Determined in HFIP. [c] The polymer was not obtained due to very low conversion. [d] Calculated for a multiple peak distribution.



Amide I, C=O (cm^{-1})	C-N (cm^{-1})	C-H (cm^{-1})
1650	1230	2935
1643	1222	2965
1647, 1602	1205	2970
1650, 1593	1207	2931
1649, 1672	1203	-
1652	1205	-
1649	1215	2914
1650	1238	2939
1650	1217	2918

Figure S26. Characteristic peaks indicating the presence of poly(*N*-substituted)glycines by FTIR-ATR.

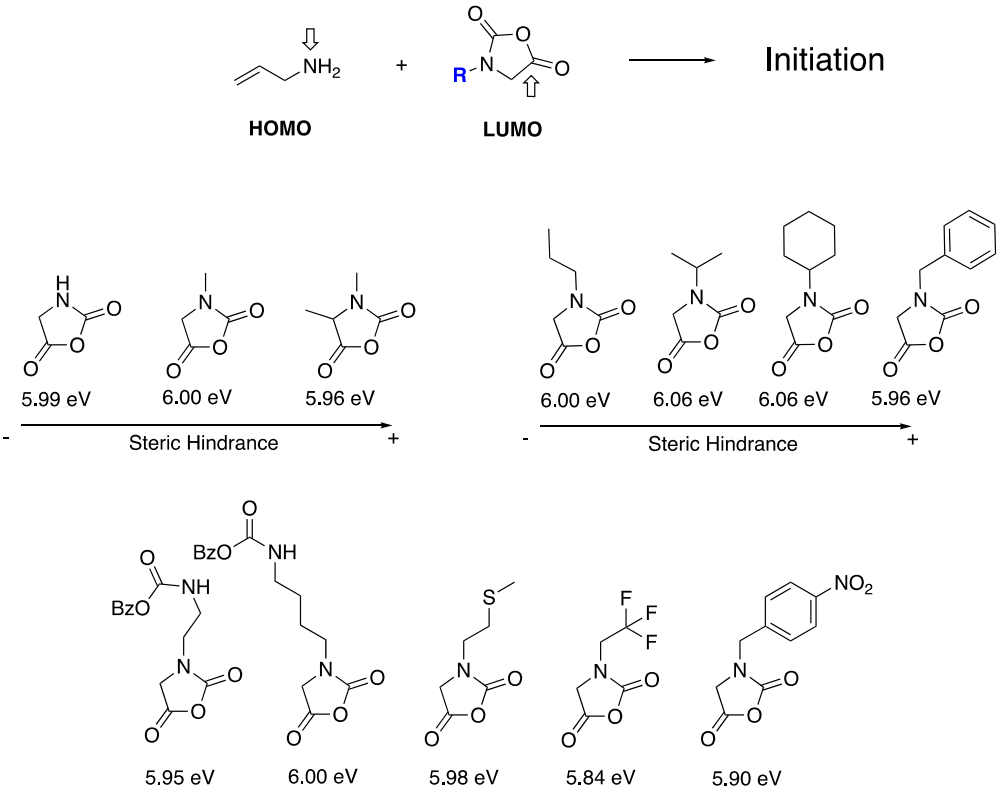


Figure S27. Comparing allylamine HOMO energy to LUMO energies of NNCA monomers affords an evaluation of the electronic effect of the N-alkylation during the initiation step.

Table S3. Cartesian coordinates of the optimized structure

Gly NCA

6	0.628460000	0.436848000	0.966490000
6	-0.829877000	0.047696000	1.053564000
7	-1.278748000	0.333461000	-0.293879000
6	-0.304375000	0.803620000	-1.084226000
8	0.877614000	0.873950000	-0.311240000
8	1.478740000	0.401268000	1.807946000
1	-1.335573000	0.653457000	1.809541000
8	-0.305428000	1.138664000	-2.242187000
1	-2.218187000	0.184676000	-0.633236000
1	-0.920449000	-1.008852000	1.318397000

Methyl ester-Glycine

6	1.083490000	0.861987000	0.273913000
6	0.285719000	-0.252556000	-0.368399000
7	0.313868000	-0.160788000	-1.825686000
1	1.267621000	-0.258703000	-2.163396000
8	1.886919000	1.567211000	-0.300516000
8	0.820666000	0.950563000	1.584892000
1	-0.745555000	-0.188113000	-0.013594000
1	-0.211115000	-0.937712000	-2.216613000
1	0.699177000	-1.189094000	0.036735000
6	1.573895000	1.927575000	2.344102000
1	1.206106000	1.843605000	3.363619000
1	2.638690000	1.696093000	2.300352000
1	1.391835000	2.928926000	1.953270000

Sarcosine NCA

6	0.635234000	0.469808000	0.959146000
6	-0.775423000	-0.060419000	1.038889000

7	-1.278409000	0.224370000	-0.292618000
6	-0.358656000	0.823638000	-1.061898000
8	0.823896000	0.977533000	-0.298901000
8	1.495246000	0.484535000	1.792602000
1	-1.334988000	0.464219000	1.819041000
1	-0.767169000	-1.131107000	1.263643000
8	-0.403648000	1.208974000	-2.205679000
6	-2.630083000	-0.104381000	-0.726592000
1	-2.749991000	0.212753000	-1.760643000
1	-3.359359000	0.415225000	-0.101780000
1	-2.792251000	-1.182451000	-0.656909000

Methyl ester-Sarcosine

6	0.415820000	-0.866111000	0.248633000
6	-0.658040000	-1.758500000	0.830444000
7	-1.800833000	-1.882999000	-0.061110000
8	1.566403000	-0.990793000	0.923323000
8	0.261261000	-0.105157000	-0.684149000
1	-0.915393000	-1.329575000	1.815676000
1	-0.227427000	-2.744342000	1.028539000
6	-2.920875000	-2.588909000	0.569197000
1	-3.772078000	-2.595736000	-0.114927000
1	-3.240139000	-2.134731000	1.520419000
1	-2.636865000	-3.626002000	0.769337000
1	-2.101860000	-0.954898000	-0.342776000
6	2.662042000	-0.132039000	0.520850000
1	2.935835000	-0.332999000	-0.515037000
1	2.379717000	0.914817000	0.637388000
1	3.482685000	-0.383034000	1.188081000

N-Me-Ala-NCA

6	0.666357000	0.418180000	0.985766000
6	-0.773768000	-0.045815000	1.088487000
7	-1.300972000	0.396865000	-0.200873000

6	-0.384381000	1.044908000	-0.933122000
8	0.835440000	1.047235000	-0.218011000
8	1.561922000	0.289095000	1.771132000
1	-1.252453000	0.512314000	1.902092000
8	-0.457467000	1.573049000	-2.017441000
6	-2.705698000	0.283342000	-0.574784000
1	-3.007965000	-0.764887000	-0.590866000
1	-2.835342000	0.707228000	-1.568483000
1	-3.327666000	0.831151000	0.137483000
6	-0.894725000	-1.549731000	1.345190000
1	-1.946274000	-1.834534000	1.404716000
1	-0.412588000	-2.122483000	0.550049000
1	-0.421069000	-1.791846000	2.298285000

Methyl ester N-Me-Ala-Glycine

6	0.556716000	0.824490000	2.023196000
6	-0.928815000	0.676622000	1.714404000
7	-1.324633000	1.700008000	0.745872000
8	0.990605000	-0.135161000	2.847365000
8	1.265891000	1.717874000	1.605367000
1	-1.435915000	0.830040000	2.684157000
6	-2.748847000	2.043987000	0.804224000
1	-2.937253000	2.887208000	0.136422000
1	-3.085592000	2.317994000	1.816558000
1	-3.360287000	1.205628000	0.461143000
6	-1.271413000	-0.737456000	1.218141000
1	-2.338831000	-0.803585000	0.997244000
1	-0.715189000	-0.966162000	0.305114000
1	-1.034883000	-1.485874000	1.975684000
1	-0.771594000	2.534760000	0.913033000
6	2.381120000	-0.077851000	3.250644000
1	2.577825000	0.851304000	3.786520000
1	2.524494000	-0.934177000	3.905074000
1	3.028789000	-0.150667000	2.376874000

N-Pr-NCA

6	2.508644000	2.525843000	-1.008646000
6	1.519591000	1.800470000	-0.129551000
7	0.529108000	1.353931000	-1.093883000
6	0.846872000	1.720513000	-2.344290000
8	2.064104000	2.442799000	-2.301411000
8	3.520517000	3.094442000	-0.712845000
1	1.099475000	2.483753000	0.615011000
1	2.016275000	0.974463000	0.387131000
8	0.281171000	1.536542000	-3.395446000
6	-1.667258000	-1.664860000	-0.155344000
1	-2.108748000	-1.276326000	0.767977000
1	-2.418777000	-1.582849000	-0.947340000
6	-0.670196000	0.587969000	-0.745003000
1	-1.096965000	1.040637000	0.154659000
1	-1.386088000	0.726957000	-1.557218000
6	-0.390914000	-0.902154000	-0.521701000
1	0.351047000	-1.019904000	0.275382000
1	0.049348000	-1.320433000	-1.432899000
1	-1.454303000	-2.726005000	-0.002883000

Methyl ester N-Pr-Glycine

6	2.865980000	2.672320000	-0.917918000
6	2.231460000	1.749286000	0.100788000
7	1.586542000	0.613384000	-0.537524000
8	3.364257000	3.844852000	-0.483884000
8	2.978991000	2.403431000	-2.095912000
1	1.483652000	2.307974000	0.673460000
1	3.026413000	1.482188000	0.816562000
6	1.179779000	-2.111925000	2.212480000
1	0.435781000	-1.612018000	2.842085000
1	0.655122000	-2.856664000	1.604727000
6	0.970094000	-0.337626000	0.398231000

1	0.234616000	0.213529000	0.997017000
1	0.407225000	-1.059686000	-0.203666000
6	1.923133000	-1.103067000	1.331320000
1	2.470115000	-0.400117000	1.969297000
1	2.671499000	-1.623646000	0.720557000
1	1.868848000	-2.645947000	2.873058000
1	2.251614000	0.132629000	-1.136517000
6	3.275469000	4.242089000	0.907262000
1	3.766303000	5.210892000	0.955761000
1	2.233644000	4.339532000	1.213673000
1	3.799341000	3.529413000	1.545273000

N-iPr-NCA

6	-1.543502000	3.129790000	-1.802858000
6	-1.597023000	1.910049000	-0.917130000
7	-2.439966000	1.008163000	-1.685748000
6	-2.836722000	1.561993000	-2.840261000
8	-2.287030000	2.870566000	-2.920119000
8	-0.977316000	4.172760000	-1.633709000
1	-2.030926000	2.166510000	0.053703000
1	-0.589638000	1.512926000	-0.761165000
8	-3.529784000	1.143657000	-3.736139000
6	-2.795965000	-0.357074000	-1.222425000
6	-2.228468000	-1.426572000	-2.159823000
6	-4.304832000	-0.490537000	-0.997757000
1	-2.294636000	-0.445090000	-0.256189000
1	-1.148289000	-1.309500000	-2.276762000
1	-2.696650000	-1.377054000	-3.145034000
1	-4.665939000	0.278841000	-0.310604000
1	-4.852420000	-0.407740000	-1.938921000
1	-4.520820000	-1.468974000	-0.561038000
1	-2.422890000	-2.416384000	-1.738352000

Methyl ester N-iPr-Glycine

6	-1.344525000	2.188490000	-2.402826000
6	-1.605825000	1.107785000	-1.376403000
7	-1.373852000	1.599592000	-0.024910000
8	-1.842599000	1.847816000	-3.599307000
8	-0.736730000	3.218600000	-2.196525000
1	-0.967448000	0.257755000	-1.670833000
1	-2.638764000	0.772092000	-1.492583000
6	-1.434307000	0.588371000	1.055986000
6	-0.398167000	-0.541829000	0.926716000
6	-2.854608000	0.035174000	1.211991000
1	-1.196489000	1.150176000	1.965934000
1	0.611370000	-0.134410000	0.812382000
1	-0.606456000	-1.190424000	0.070361000
1	-3.579225000	0.848635000	1.307066000
1	-3.144475000	-0.586584000	0.359064000
1	-2.918069000	-0.588189000	2.108297000
1	-0.408894000	-1.167729000	1.824661000
1	-0.467245000	2.057258000	0.004088000
6	-1.599400000	2.761260000	-4.698282000
1	-2.051201000	3.730572000	-4.487444000
1	-0.527473000	2.875080000	-4.860896000
1	-2.071214000	2.300476000	-5.562363000

N-ch-NCA

6	-1.196807000	2.987407000	-1.841828000
6	-1.232490000	1.653440000	-1.139297000
7	-2.536593000	1.136416000	-1.524243000
6	-3.191323000	1.989401000	-2.326030000
8	-2.371081000	3.133010000	-2.525496000
8	-0.337272000	3.823019000	-1.852703000
1	-1.138369000	1.792678000	-0.058394000
1	-0.410882000	1.021011000	-1.488572000
8	-4.276513000	1.928491000	-2.851796000

6	-3.044951000	-0.176171000	-1.064021000
6	-3.241739000	-1.159656000	-2.227801000
6	-3.705172000	-2.528514000	-1.703980000
6	-4.971649000	-2.406549000	-0.844469000
6	-4.770459000	-1.410040000	0.306063000
6	-4.313211000	-0.035748000	-0.208428000
1	-2.244368000	-0.561754000	-0.424681000
1	-2.304587000	-1.258909000	-2.784965000
1	-3.991393000	-0.756398000	-2.917645000
1	-3.879348000	-3.201794000	-2.548991000
1	-2.902393000	-2.976979000	-1.103783000
1	-5.252631000	-3.387667000	-0.447867000
1	-5.805697000	-2.069622000	-1.473975000
1	-5.696063000	-1.295526000	0.879105000
1	-4.017770000	-1.805501000	1.001414000
1	-4.117106000	0.641786000	0.628434000
1	-5.107511000	0.413008000	-0.814594000

Methyl ester N-ch-Glycine

6	-1.664293000	2.956009000	-1.072987000
6	-2.312656000	2.321498000	0.137724000
7	-3.718975000	2.031438000	-0.112498000
8	-0.486381000	3.509790000	-0.754978000
8	-2.119310000	2.943481000	-2.198263000
1	-2.203323000	3.005508000	0.981974000
1	-1.697135000	1.437370000	0.373033000
6	-4.423870000	1.241456000	0.920854000
6	-4.561948000	2.024461000	2.235154000
6	-5.407553000	1.252259000	3.261213000
6	-4.849507000	-0.156855000	3.512592000
6	-4.694969000	-0.939019000	2.200221000
6	-3.842629000	-0.164028000	1.181221000
1	-5.435047000	1.103611000	0.516889000
1	-5.009708000	3.002609000	2.029296000

1	-3.568000000	2.211321000	2.660900000
1	-5.456642000	1.813843000	4.200108000
1	-6.437709000	1.171165000	2.890302000
1	-5.501446000	-0.702959000	4.203231000
1	-3.869829000	-0.075642000	4.002150000
1	-4.247956000	-1.920433000	2.391613000
1	-5.688892000	-1.127061000	1.772712000
1	-3.785643000	-0.714548000	0.235001000
1	-2.818566000	-0.080579000	1.565891000
6	0.285388000	4.086082000	-1.838209000
1	0.508523000	3.325017000	-2.586107000
1	-0.265685000	4.909142000	-2.293556000
1	1.200078000	4.448696000	-1.376450000
1	-3.798179000	1.551933000	-1.004800000

N-Bz-NCA

6	-1.589998000	3.277865000	-2.077676000
6	-1.528629000	2.345097000	-0.893245000
7	-2.198149000	1.162965000	-1.408604000
6	-2.588764000	1.321390000	-2.684786000
8	-2.227821000	2.622726000	-3.099488000
8	-1.183119000	4.398026000	-2.190531000
1	-2.047444000	2.787120000	-0.037985000
1	-0.488599000	2.148450000	-0.616359000
8	-3.152311000	0.569092000	-3.441674000
6	-2.351713000	-0.079146000	-0.649805000
1	-2.715063000	-0.829936000	-1.354007000
1	-1.364029000	-0.397127000	-0.306925000
6	-3.297709000	0.051879000	0.529661000
6	-4.594607000	0.551336000	0.357249000
6	-2.892650000	-0.361831000	1.801638000
6	-5.469487000	0.634264000	1.438783000
6	-3.769998000	-0.285470000	2.885797000

6	-5.059581000	0.213733000	2.706709000
1	-4.923737000	0.877495000	-0.624174000
1	-1.888450000	-0.747299000	1.945696000
1	-6.471062000	1.023690000	1.292884000
1	-3.442776000	-0.611100000	3.867212000
1	-5.741442000	0.276907000	3.547839000

Methyl ester N-Bz-Glycine

6	-2.504315000	3.391296000	-1.830394000
6	-2.803424000	3.158941000	-0.366264000
7	-3.853042000	2.167492000	-0.184067000
8	-1.766447000	4.495594000	-2.003028000
8	-2.850971000	2.664031000	-2.738184000
1	-3.097674000	4.110620000	0.084205000
1	-1.845590000	2.874211000	0.105849000
6	-4.037339000	1.773787000	1.219550000
1	-4.656910000	0.871578000	1.215719000
1	-3.083967000	1.507700000	1.702385000
6	-4.720919000	2.845021000	2.050945000
6	-5.950938000	3.385085000	1.651443000
6	-4.149526000	3.291535000	3.246433000
6	-6.592732000	4.346600000	2.430370000
6	-4.790670000	4.252655000	4.032250000
6	-6.014294000	4.783360000	3.625692000
1	-6.401586000	3.049826000	0.723451000
1	-3.194541000	2.885752000	3.565364000
1	-7.545294000	4.753987000	2.108901000
1	-4.331919000	4.587603000	4.956339000
1	-6.513947000	5.531163000	4.232368000
6	-1.342513000	4.799561000	-3.355241000
1	-0.729228000	3.987511000	-3.746819000
1	-2.211581000	4.954994000	-3.994552000
1	-0.760062000	5.713876000	-3.273459000
1	-3.632173000	1.342949000	-0.733875000

N-pnBz-NCA

6	-1.820145000	3.125618000	-2.588410000
6	-1.804039000	2.573195000	-1.184142000
7	-2.291518000	1.219011000	-1.391063000
6	-2.529259000	0.962426000	-2.692016000
8	-2.258727000	2.132288000	-3.429268000
8	-1.523068000	4.214221000	-2.985273000
1	-2.455695000	3.166741000	-0.536931000
1	-0.787035000	2.592138000	-0.780868000
8	-2.908211000	-0.042473000	-3.240248000
6	-2.355634000	0.211406000	-0.339219000
1	-2.505731000	-0.753094000	-0.829934000
1	-1.389455000	0.174695000	0.169333000
6	-3.465169000	0.449171000	0.667590000
6	-4.738226000	0.863904000	0.257582000
6	-3.227073000	0.205462000	2.024834000
6	-5.761903000	1.029567000	1.181363000
6	-4.239866000	0.360537000	2.963711000
6	-5.496841000	0.771471000	2.525571000
1	-4.937335000	1.061902000	-0.789236000
1	-2.242576000	-0.107917000	2.353050000
1	-6.746595000	1.348615000	0.869522000
1	-4.059841000	0.173004000	4.013248000
7	-6.572731000	0.939473000	3.508026000
8	-7.678130000	1.299059000	3.108286000
8	-6.324999000	0.712725000	4.690451000

Methyl ester N-pnBz-Glycine

6	-1.674032000	2.749143000	-3.448983000
6	-2.777565000	1.992709000	-2.742331000
7	-2.586001000	0.553453000	-2.853696000
8	-1.666077000	4.038028000	-3.088377000
8	-0.911412000	2.270885000	-4.262827000

1	-3.723688000	2.360465000	-3.173466000
1	-2.783461000	2.282393000	-1.687799000
6	-3.649857000	-0.248812000	-2.233784000
1	-3.362925000	-1.298977000	-2.338319000
1	-3.669270000	-0.021434000	-1.164351000
6	-5.043464000	-0.055465000	-2.813385000
6	-5.339565000	-0.512407000	-4.106489000
6	-6.045929000	0.589549000	-2.078360000
6	-6.599848000	-0.331741000	-4.658935000
6	-7.315763000	0.782719000	-2.611702000
6	-7.574096000	0.318002000	-3.899396000
1	-4.577525000	-1.021146000	-4.687482000
1	-5.834642000	0.942374000	-1.075194000
1	-6.830688000	-0.687745000	-5.653153000
1	-8.089754000	1.280576000	-2.043877000
7	-8.908165000	0.514921000	-4.472093000
8	-9.123965000	0.097212000	-5.608744000
8	-9.758156000	1.090451000	-3.794642000
6	-0.703196000	4.899572000	-3.744959000
1	-0.869131000	5.887640000	-3.323430000
1	0.310382000	4.558498000	-3.532827000
1	-0.879364000	4.906450000	-4.820950000
1	-2.462888000	0.292991000	-3.827699000

N-MeSEt-NCA

6	-1.856706000	3.347279000	-1.895866000
6	-2.284666000	2.406494000	-0.795724000
7	-2.471053000	1.162036000	-1.521457000
6	-2.192230000	1.294564000	-2.827462000
8	-1.817728000	2.637687000	-3.067401000
8	-1.582613000	4.511629000	-1.841657000
1	-3.209069000	2.761405000	-0.330641000
1	-1.503735000	2.343071000	-0.031655000

8	-2.223913000	0.494209000	-3.730743000
6	-2.891923000	-0.097768000	-0.902644000
1	-3.630609000	0.158891000	-0.133184000
1	-3.401120000	-0.685740000	-1.665831000
6	-1.749937000	-0.885360000	-0.280807000
1	-0.999835000	-0.231419000	0.167762000
1	-1.265016000	-1.571221000	-0.978631000
16	-2.414245000	-2.021496000	1.103643000
1	-1.237566000	-2.822082000	0.857564000
1	-3.161449000	-0.857896000	1.559910000
6	-2.225653000	-2.468230000	2.909491000
1	-1.448664000	-1.853021000	3.364354000
1	-3.187484000	-2.276623000	3.392679000
1	-1.943609000	-3.523393000	2.953764000

Methyl ester N-MeSEt-Glycine

6	-1.939222000	3.761402000	-1.603203000
6	-2.557841000	3.061844000	-0.412561000
7	-3.728376000	2.288491000	-0.803219000
8	-1.058795000	4.690987000	-1.210962000
8	-2.172260000	3.500539000	-2.765150000
1	-2.844528000	3.814731000	0.326560000
1	-1.746060000	2.470560000	0.042745000
6	-4.363870000	1.541667000	0.286168000
1	-4.602606000	2.246472000	1.088519000
1	-5.309040000	1.144531000	-0.093794000
6	-3.521413000	0.384849000	0.844758000
1	-2.570100000	0.716709000	1.256375000
1	-3.358697000	-0.390245000	0.095251000
16	-4.453217000	-0.400947000	2.237628000
1	-4.855640000	-1.523658000	1.234998000
1	-3.737024000	0.654763000	3.160476000
6	-3.473195000	-1.673907000	3.102344000
1	-2.510091000	-1.783975000	2.606335000

1	-3.329453000	-1.332473000	4.127867000
1	-4.033178000	-2.607653000	3.039718000
1	-3.496217000	1.666714000	-1.571949000
6	-0.333885000	5.390591000	-2.253236000
1	-1.029627000	5.934380000	-2.892602000
1	0.322851000	6.080839000	-1.729600000
1	0.246691000	4.683204000	-2.845991000

N-gtfEt-NCA

6	-1.513732000	3.275320000	-1.960890000
6	-1.622356000	2.357357000	-0.768265000
7	-2.334524000	1.220376000	-1.336860000
6	-2.585571000	1.389162000	-2.656219000
8	-2.104679000	2.650828000	-3.034872000
8	-1.023888000	4.361904000	-2.045774000
1	-2.175707000	2.849937000	0.034619000
1	-0.626971000	2.084311000	-0.406543000
8	-3.111468000	0.653121000	-3.449571000
6	-2.590032000	-0.021391000	-0.641661000
1	-2.723120000	-0.822919000	-1.368132000
1	-1.748626000	-0.267099000	0.008720000
6	-3.844131000	0.043506000	0.217736000
9	-4.953806000	0.301245000	-0.508548000
9	-4.040408000	-1.129621000	0.855763000
9	-3.765156000	1.009245000	1.165446000

Methyl ester N-gtfEt-Glycine

6	-0.779031000	3.500535000	-1.985961000
6	-1.764674000	2.371531000	-1.689622000
7	-1.559560000	1.161214000	-2.461935000
8	-0.913659000	4.499986000	-1.107053000
8	0.008227000	3.511047000	-2.908946000
1	-2.765886000	2.765892000	-1.891808000
1	-1.731626000	2.152768000	-0.620030000

6	-0.365453000	0.391193000	-2.148232000
1	0.071084000	-0.021788000	-3.058927000
1	0.414629000	0.969215000	-1.639437000
6	-0.689012000	-0.791606000	-1.252923000
9	-1.535868000	-1.675790000	-1.832819000
9	0.435955000	-1.481817000	-0.932471000
9	-1.265494000	-0.421213000	-0.080490000
1	-1.602261000	1.354730000	-3.454237000
6	-0.074638000	5.667051000	-1.299199000
1	-0.337405000	6.345210000	-0.491091000
1	0.976866000	5.385659000	-1.237915000
1	-0.285115000	6.123613000	-2.266872000

N-ZNEt-NCA

6	-0.946662000	2.453875000	-1.829509000
6	-1.526735000	1.876190000	-0.561246000
7	-1.053093000	0.502630000	-0.614186000
6	-0.313308000	0.268167000	-1.711807000
8	-0.240736000	1.462758000	-2.461396000
8	-1.035845000	3.561189000	-2.275228000
1	-2.618839000	1.941213000	-0.577390000
1	-1.149194000	2.426382000	0.305314000
8	0.233187000	-0.736294000	-2.096906000
6	-1.374445000	-0.516338000	0.380568000
1	-2.415824000	-0.380233000	0.680580000
1	-1.284259000	-1.491865000	-0.099192000
6	-0.448460000	-0.439545000	1.608333000
1	-0.516128000	0.544437000	2.074983000
1	0.587000000	-0.598133000	1.301648000
7	-0.790148000	-1.443994000	2.600869000
1	-0.411863000	-2.375727000	2.508313000
6	-1.669884000	-1.214123000	3.602822000
8	-2.237158000	-0.149910000	3.815055000

8	-1.839721000	-2.324269000	4.360779000
6	-2.775025000	-2.205132000	5.476020000
1	-2.392668000	-1.456446000	6.170983000
1	-3.736625000	-1.870602000	5.084375000
6	-2.886421000	-3.555292000	6.127611000
6	-2.107885000	-3.870551000	7.246417000
6	-3.767297000	-4.517398000	5.618323000
6	-2.205767000	-5.126760000	7.846812000
6	-3.863533000	-5.774931000	6.213224000
6	-3.082409000	-6.081469000	7.329549000
1	-1.428189000	-3.128069000	7.652584000
1	-4.381508000	-4.279429000	4.755422000
1	-1.602344000	-5.357240000	8.718066000
1	-4.550046000	-6.512157000	5.811135000
1	-3.160982000	-7.057147000	7.796731000

Methyl ester N-ZNEt-Glycine

6	1.023928000	3.239111000	-0.361255000
6	0.891387000	1.841867000	0.206156000
7	1.316316000	0.833568000	-0.754174000
8	0.379333000	4.130314000	0.403266000
8	1.654261000	3.534650000	-1.354864000
1	-0.156869000	1.675017000	0.471049000
1	1.455770000	1.848193000	1.152698000
6	1.205563000	-0.547780000	-0.281861000
1	0.177731000	-0.715529000	0.057016000
1	1.374399000	-1.209953000	-1.136648000
6	2.184954000	-0.941891000	0.842768000
1	2.037924000	-0.324847000	1.728403000
1	3.212857000	-0.792828000	0.500159000
7	2.050022000	-2.344702000	1.230167000
1	2.498250000	-3.042921000	0.654255000
6	1.238623000	-2.843527000	2.190226000
8	1.101149000	-4.042779000	2.422307000

8	0.604035000	-1.872883000	2.882703000
6	-0.266726000	-2.313524000	3.967309000
1	-1.051800000	-2.944047000	3.547706000
1	0.325671000	-2.901776000	4.669519000
6	-0.836775000	-1.086448000	4.622385000
6	-2.050982000	-0.546311000	4.184592000
6	-0.153107000	-0.461570000	5.672157000
6	-2.572276000	0.601985000	4.781693000
6	-0.670820000	0.687327000	6.270303000
6	-1.881643000	1.221546000	5.824898000
1	-2.590971000	-1.028099000	3.375673000
1	0.785535000	-0.878034000	6.023298000
1	-3.515944000	1.009652000	4.436651000
1	-0.133700000	1.161469000	7.084589000
1	-2.286532000	2.112957000	6.291242000
1	2.262240000	1.027819000	-1.069422000
6	0.481576000	5.523966000	0.018564000
1	0.057769000	5.670639000	-0.975084000
1	-0.093143000	6.069369000	0.762669000
1	1.524719000	5.840633000	0.031493000

N-ZNBu-NCA

6	0.373962000	2.961027000	-2.722444000
6	-0.452542000	2.355281000	-1.614458000
7	-0.309745000	0.933100000	-1.875315000
6	0.473874000	0.694552000	-2.937750000
8	0.897552000	1.937246000	-3.466576000
8	0.588018000	4.112130000	-2.974498000
1	-1.491507000	2.690261000	-1.686268000
1	-0.049132000	2.654228000	-0.642752000
8	0.822982000	-0.341118000	-3.451566000
6	-0.881852000	-1.524778000	1.030452000
1	-1.894772000	-1.201629000	1.295153000

1	-0.983972000	-2.431219000	0.422173000
6	-0.113244000	-1.866437000	2.313061000
1	-0.023527000	-0.983936000	2.948856000
1	0.898193000	-2.200151000	2.067178000
7	-0.745760000	-2.920489000	3.098329000
1	-0.622939000	-3.880204000	2.810835000
6	-1.621524000	-2.676703000	4.096212000
8	-1.925938000	-1.570179000	4.526167000
8	-2.127489000	-3.837870000	4.588720000
6	-3.054545000	-3.714053000	5.707788000
1	-2.522960000	-3.263878000	6.548015000
1	-3.873930000	-3.058056000	5.412106000
6	-3.548446000	-5.093453000	6.046193000
6	-2.856118000	-5.889780000	6.965406000
6	-4.701117000	-5.603313000	5.437194000
6	-3.304102000	-7.175932000	7.267558000
6	-5.151931000	-6.888722000	5.737950000
6	-4.452741000	-7.677698000	6.653061000
1	-1.966041000	-5.499367000	7.448689000
1	-5.249884000	-4.989422000	4.729585000
1	-2.761212000	-7.782863000	7.984213000
1	-6.049038000	-7.271307000	5.263783000
1	-4.803852000	-8.675892000	6.890310000
6	-0.943699000	-0.117412000	-1.075070000
1	-1.962895000	0.210874000	-0.854583000
1	-1.010984000	-1.004963000	-1.706336000
6	-0.181514000	-0.431120000	0.216307000
1	-0.091393000	0.478014000	0.821522000
1	0.835680000	-0.748407000	-0.038900000

Methyl ester N-ZNBu-Glycine

6	1.568247000	3.386737000	-0.213725000
6	0.423503000	2.828671000	0.604099000
7	0.132844000	1.448538000	0.246038000

8	1.649508000	4.718223000	-0.081135000
8	2.340349000	2.729393000	-0.880182000
1	-0.461327000	3.447793000	0.428146000
1	0.702922000	2.982958000	1.659571000
6	-1.907097000	-0.072335000	3.192816000
1	-2.808013000	0.542220000	3.085470000
1	-2.113973000	-1.031561000	2.703104000
6	-1.647463000	-0.321855000	4.683594000
1	-1.449910000	0.619765000	5.198080000
1	-0.764040000	-0.953683000	4.807887000
7	-2.750510000	-1.001509000	5.366327000
1	-2.783022000	-2.010399000	5.330504000
6	-3.847158000	-0.422444000	5.902726000
8	-4.786609000	-1.043490000	6.396080000
8	-3.792375000	0.927442000	5.852293000
6	-4.919152000	1.643874000	6.440277000
1	-5.832359000	1.328872000	5.933602000
1	-4.987187000	1.378294000	7.496020000
6	-4.666404000	3.115005000	6.257692000
6	-5.084103000	3.767007000	5.091644000
6	-3.997600000	3.848191000	7.244584000
6	-4.832093000	5.127072000	4.911344000
6	-3.744750000	5.208703000	7.067383000
6	-4.160304000	5.850079000	5.899087000
1	-5.610201000	3.208043000	4.324103000
1	-3.676904000	3.353034000	8.155581000
1	-5.162635000	5.622149000	4.004633000
1	-3.228782000	5.767337000	7.841008000
1	-3.965268000	6.908093000	5.760749000
6	-0.969076000	0.841082000	1.005003000
1	-1.855506000	1.471194000	0.866692000
1	-1.191909000	-0.122616000	0.534927000
6	-0.722234000	0.616666000	2.506099000

1	-0.524191000	1.573450000	3.002461000
1	0.180102000	0.003202000	2.626153000
1	0.973745000	0.886527000	0.344287000
6	2.745609000	5.381586000	-0.757822000
1	2.638748000	6.435056000	-0.510704000
1	3.698642000	4.997690000	-0.393296000
1	2.668259000	5.230819000	-1.835117000

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