Supplementary Materials for

Bioinspired Polymer-Bound Organocatalysts for Direct Asymmetric Aldol Reaction: Experimental and Computational Studies

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1. Experimental Section

1.1. Monomer synthesis (Scheme S1)

M2: To a solution of *N*-Boc-6-aminohexanoic acid (**2a**, 0.2 mol) in anhydrous DCM (1 L) 2-chloroethylamine hydrochloride (0.22 mol) was added, followed by TBTU (0.22 mol) and NEt_3 (0.4 mol) at 0 ℃. The resulting mixture was then allowed to stir at r.t. for 24 h. The reaction mixture was in turn washed with saturated aqueous $NaHCO_3$ (3 × 50 mL) and water (3 × 50 mL). The separated organic layer was dried and concentrated under vacuum to give a pale yellow solid (48.7 g, 83% yield). The intermediate product **2b** (27.8 g, 0.1 mol), without further purification, was dissolved in methanol (100 mL) containing NaOH (0.3 mol) and then stirred at r.t. for 24 h. Methanol was removed under vacuum and the residue was mixed with water (~200 mL), followed by extraction with ethyl acetate (3 × 50 mL). The combined organic extract was dried over $MgSO_4$, filtered, and distilled (145 ℃, 4 mbar) in the presence of barium oxide to afford the desired product as a colorless crystal (20.5 g, 80% yield). m.p. 47.7–48.1°C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.22–1.48 (m, $OC(CH_3)_3$, $NCH_2CH_2CH_2$, 13 H), 1.65 (m, $N(CH_2)_3CH_2$, 2 H), 2.27 (t, $N(CH_2)_4CH_2$, 2 H), 3.12 (t, CH_2NHCO, 2 H), 3.82 (t, OCH_2CH_2N, 2 H), 4.22 (t, OCH_2CH_2N, 2H), 4.71 (br, *H*NCO, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 25.4, 26.3, 27.8, 28.4, 29.6, 40.3, 54.2, 67.2, 79.0, 156.0, 168.4. MS (ESI+): *m*/*z* (%) = 279.2 (30.2) $[M + Na]^+$, 535.3 (100) $[2M + Na]^+$.

M3 was synthesized by a procedure similar to that of **M2**, but using *N*-Boc-glycine (**3a**) as the starting material. The product was obtained in a total yield of ~70% as a white solid. m.p. 73.8–74.8°C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.45 (s, OC(C*H*$_3$)$_3$, 9 H), 3.86 (t, NC*H*$_2$CH$_2$O, 2 H), 3.96 (s, OCNHC*H*$_2$, 2 H), 4.32 (t, NCH$_2$C*H*$_2$O, 2 H), 5.15 (s, OCN*H*CH$_2$, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 28.3, 37.9, 54.1, 68.1, 79.8, 155.7, 165.4. MS (ESI+): *m*/*z* (%) = 223.2 (90.5) $[M + Na]^+$, 423.2 (100) $[2M + Na]^+$.

(*R/S*)-**M4** was synthesized according to the reported method [1]. Boc-(*R*)-alanine ((*R*)-**4a**, 0.1 mol), 2-aminoethanol (0.1 mol) and PPh_3 (0.3 mol) were dissolved in anhydrous DCM (800 mL). To the solution DIPEA (0.3 mol) and CCl_4 (0.5 mol) at 0 ℃ was added slowly. The mixture was warmed to room temperature and stirred for 72 h. The solvent was evaporated under vacuum and the residue subjected to distillation (135 ℃, 5 mbar), affording a pale yellow liquid (65% yield). $[\alpha]^{20}_D$ = +49.7° (*c* 0.01 g/mL, MeOH). (*S*)-**M4** was obtained by the same procedure; 60% yield, $[\alpha]^{20}_D$ = –49° (*c* 0.01 g/mL, MeOH). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.39 (d, NHCHC*H*$_3$, 3 H), 1.45 (s, OC(C*H*$_3$)$_3$, 9 H), 3.85 (t, NC*H*$_2$CH$_2$O, 2 H), 4.32 (t, NCH$_2$C*H*$_2$O, 2 H), 4.42 (m, OCNHC*H*, 1 H), 5.21 (s, OCN*H*CH, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 19.6, 28.3, 44.7, 54.1, 68.2, 79.6, 155.0, 168.9, 165.4. MS (ESI+): *m*/*z* (%) = 237.2 (52.1) $[M + Na]^+$, 451.2 (100) $[2M + Na]^+$.

1.2. Catalyst synthesis

P1–P4 were prepared according to the reported method [2].

P5 (Scheme S2): To a stirred solution of poly(allyamine) hydrochloride (1 g) in water (5 mL) DMSO (25 mL) was added slowly, followed by TBTU (3.81 g), Boc-L-proline (2.49 g), and NEt_3 (3.0 mL). After stirring at ambient temperature for 24 h, the solvent was removed under vacuum, the residue was dissolved in a minimal amount of methanol, and an excess amount of ether was added to precipitate out the intermediate product **P5a** (2.2 g, 82% yield). Then, **P5a** (1.0 g) was treated with a 1:1 TFA/DCM mixture (10 mL) for 12 h at room temperature. After evaporation of the solvent and suspending the residue in distilled water, and an appropriate amount of saturated aq. $NaHCO_3$ was added to adjust pH to ~8. Finally, the suspension was dialyzed against distilled water using 1 kDa molecular weight-cutoff dialysis membrane and freeze-

dried to yield the desired catalyst **P5** (1.23 g, 91% yield). Characterization data of polymeric catalysts are listed in Table S1.

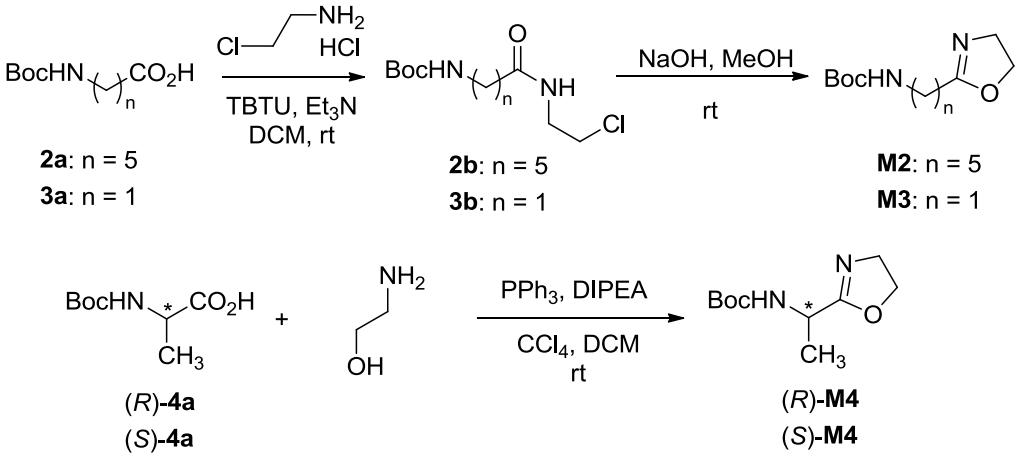
MC1 and **MC2**: the synthesis method is similar to that for **P5**.

MC1: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.42 (s, 1H), 4.26–3.95 (m, 2H), 3.85–3.72 (m, 1H), 3.59–3.20 (m, 4H), 3.16–2.97 (m, 2H), 2.98 (s, 1H), 2.37–2.10 (m, 1H), 1.97–1.87 (m, 1H), 1.82–1.63 (m, 2H), 1.35–0.85 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 175.22, 167.19, 60.43, 47.21, 40.98, 38.59, 30.76, 26.05, 14.01, 12.92. $[\alpha]^{20}_{D}$ = –87° (*c* 0.01 g/mL, MeOH).

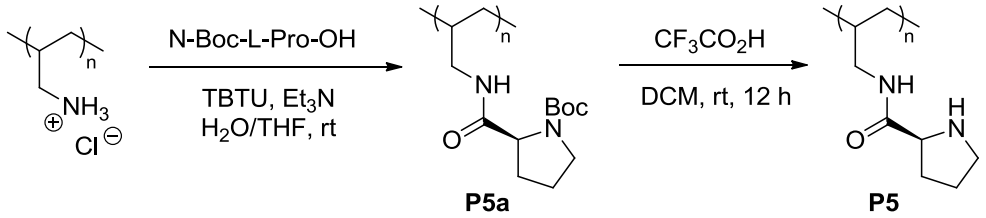
MC2: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.88 (*t*, C*H*$_3$, 3H), 1.21–1.33 (m, C*H*$_2$C*H*$_2$C*H*$_2$CH$_3$, 6H), 1.45 (m, C*H*$_2$(CH$_2$)$_3$CH$_3$, 2H), 1.66 (m, OCCHCH$_2$C*H*$_2$, 2H), 1.87 (m, OCCHC*H*$_2$CH$_2$, 1H), 2.05-2.25 (m, OCCHC*H*$_2$CH$_2$， OCCHN*H*, 2H), 2.84-3.07 (tt, OCCHNHC*H*$_2$, 2H), 3.21 (q, C*H*$_2$(CH$_2$)$_4$CH$_3$, 2H), 3.72 (q, OCC*H*, 1H), 7.63 (s, OCN*H*, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.0, 22.5, 26.2, 26.6, 29.6, 30.8, 31.5, 38.9, 47.8, 60.6 and 174.9, $[\alpha]^{20}_{D}$ = –52° (*c* 0.01 g/mL, MeOH).

1.3. General procedure for organocatalysis

The polymer resin (0.027 mmol of prolinamide units, 0.1 equiv) was added to 0.4 mL of cyclohexanone (3.78 mmol, 14 equiv) containing TFA (0.08 equiv) and water (10 μL). The suspension was stirred for several mins at ambient temperature and then 4-nitrobenzaldehyde (0.27 mmol, 1 equiv) was added. The resulting solution was stirred at a given temperature for a certain period of time and poured into a large amount of ethyl ether. The resin was separated from the solution by filtration, washed with ether, and reused for next catalytic cycle when necessary. A saturated aqueous NH_4Cl solution (~2 mL) was added to the collected filtrate, extracted with DCM (3 × 5 mL). The organic phase was dried over $MgSO_4$. After solvent evaporation, the residue was analyzed to determine *syn/anti* ratio by ^{1}H NMR spectroscopy, then chromatographed on a silica gel column (*n*-hexane/EtOAc, 4:1) to give the pure product a white/pale yellow powder. The *ee* value was determined by chiral-phase HPLC (a Chiralpak AD-H column; 1:9 *i*-PrOH/*n*-hexane, 20 ℃, 1 mL/min, λ = 254 nm, R_t = 23.0 min (minor), 30.3 min (major)).



Scheme S1. Synthesis route of 2-oxazoline monomers.



Scheme S2. Synthesis of the reference catalyst **P5**.

Table S1. Characterization data of prolinamide catalysts and their precursors.

Entry	Precursors	M_n[a] (×10^3)	PDI[a]	Catalysts	d_g[b] (%)	$[\alpha]_D^{20}$ (°)[c]
1	(*R*)-**P1b**			(*R*)-**P1**	97	–30
2	(*S*)-**P1b**			(*S*)-**P1**	98	–25
3	**P2b**	9.62	1.08	**P2**	96	–44
4	**P3b**	8.75	1.05	**P3**	>99	–55
5	(*R*)-**P4b**	10.68	1.17	(*R*)-**P4**	>99	–38
6	(*S*)-**P4b**	7.69	1.18	(*S*)-**P4**	>99	–53
7	P**5a**	9.51	1.29	**P5**	>99	–58

[a] Determined by GPC based on calibration with PS standards in THF. [b] The grafting degree of L-proline was measured by ^{1}H NMR (see Figure S12-S14). [c] c = 0.01 g/mL, MeOH.

Table S2. Aldol reaction of cyclohexanone with 4-nitrobenzaldehye catalyzed by **P3** in the presence of different amounts of water [a]

CH PNBA **1**

(2*S*,1'*R*): *anti*-**1a**
(2*R*,1'*S*): *anti*-**1b**
(2*S*,1'*S*): *syn*-**1a**
(2*R*,1'*R*): *syn*-**1b**

Entry	Water (μl)	TFA (μl)	Yield (%)[b]	*dr* (*syn*/*anti*)[c]	ee (%)[d]
1	0	0	-	-	-
2	0	1.6	-	-	-
3	10	0	45	28:72	42
4	3	1.6	77	26:74	88
5	5	1.6	77	17:83	88
6	10	1.6	86	16:84	88
7	20	1.6	82	21:79	85
8	40	1.6	54	19:81	79

[a] Reaction condition: PNBA 0.27 mmol (1 equiv.), CH 0.4 mL (14 equiv.), TFA 1.6 μL, 12 h. **P3** (0.027 mmol, based on the content of proline moieties in the polymer, 0.1 equiv.). [b] Isolated yield. [c] Determined by ^{1}H NMR analysis of the crude product. [d] Determined by chiral-phase HPLC for *anti*-**1**.

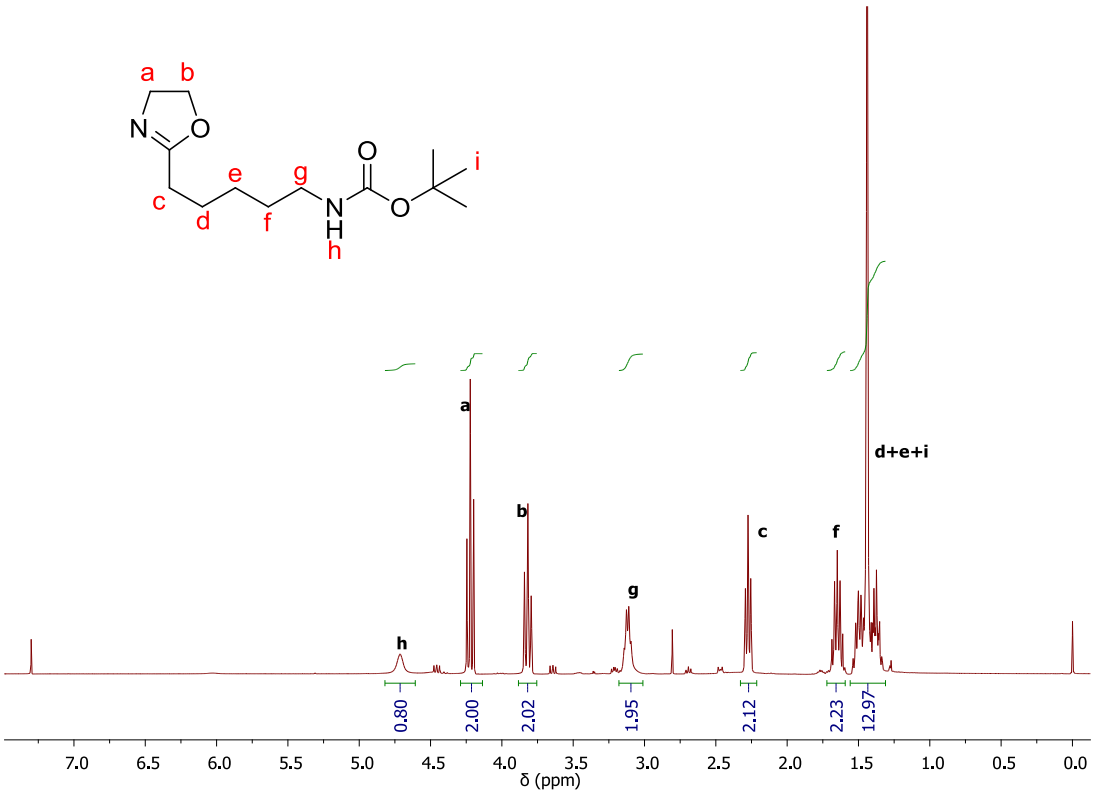


Figure S1. ^{1}H NMR spectrum of **M2** in $CDCl_3$.

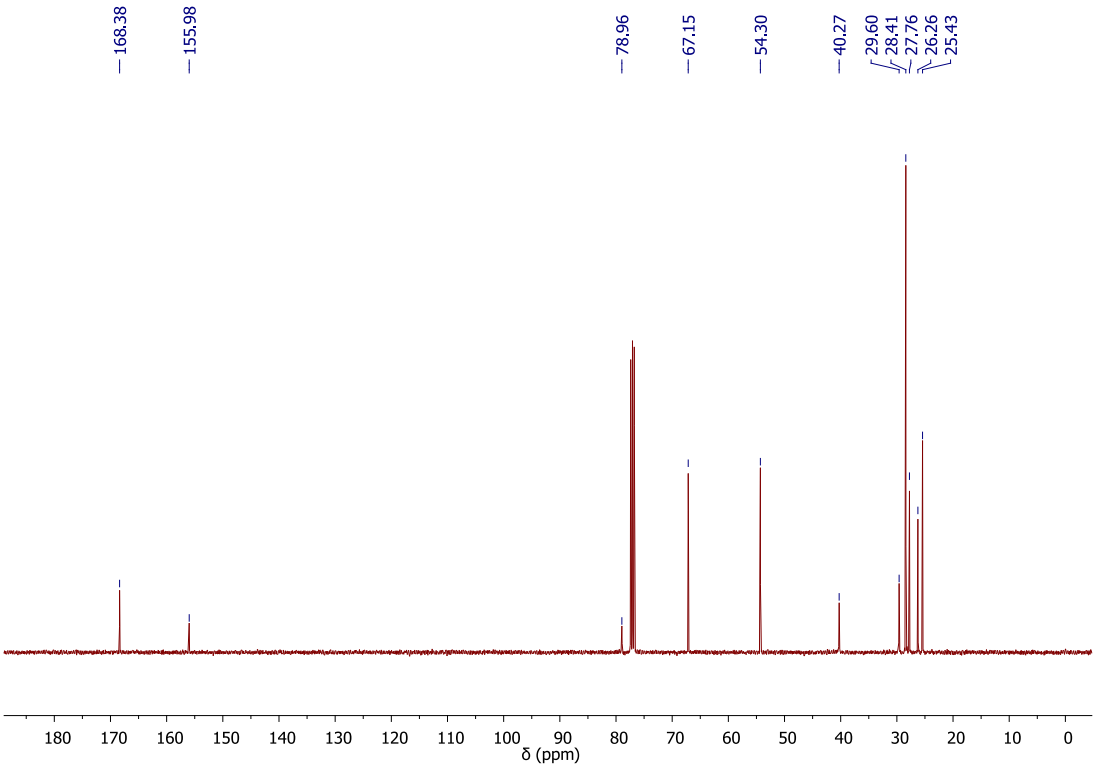


Figure S2. ^{13}C NMR spectrum of **M2** in $CDCl_3$.

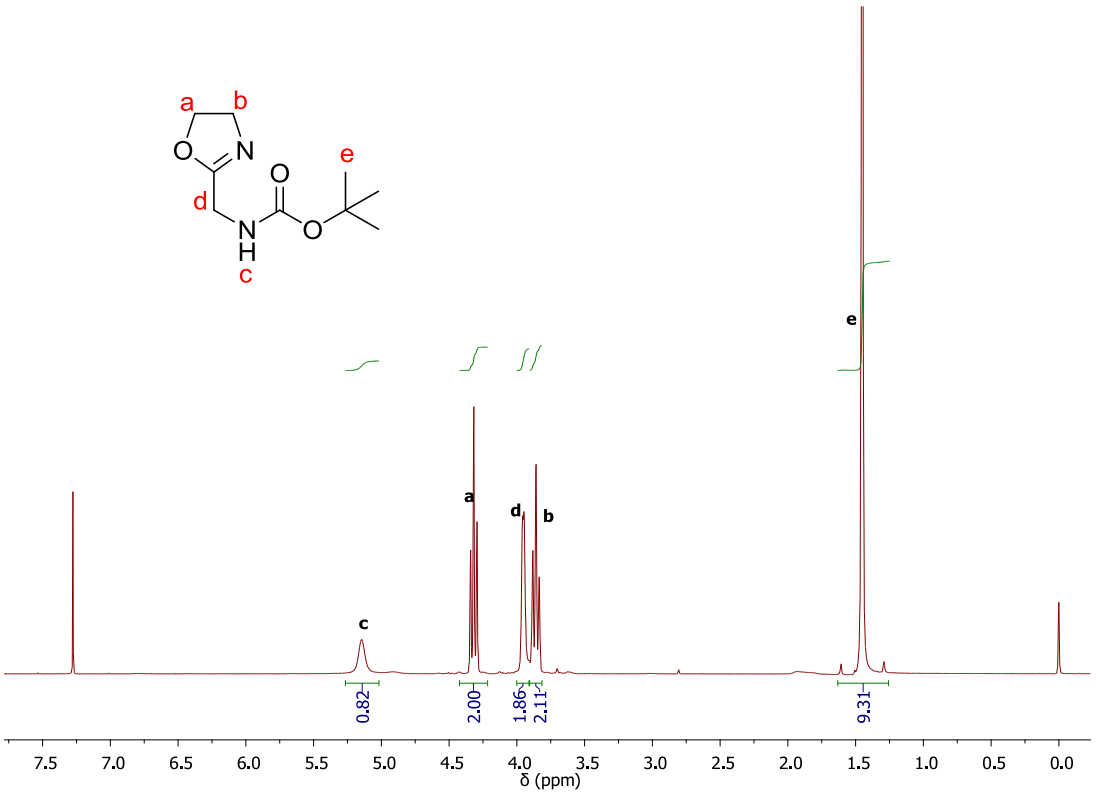


Figure S3. ^{1}H NMR spectrum of **M3** in $CDCl_3$.

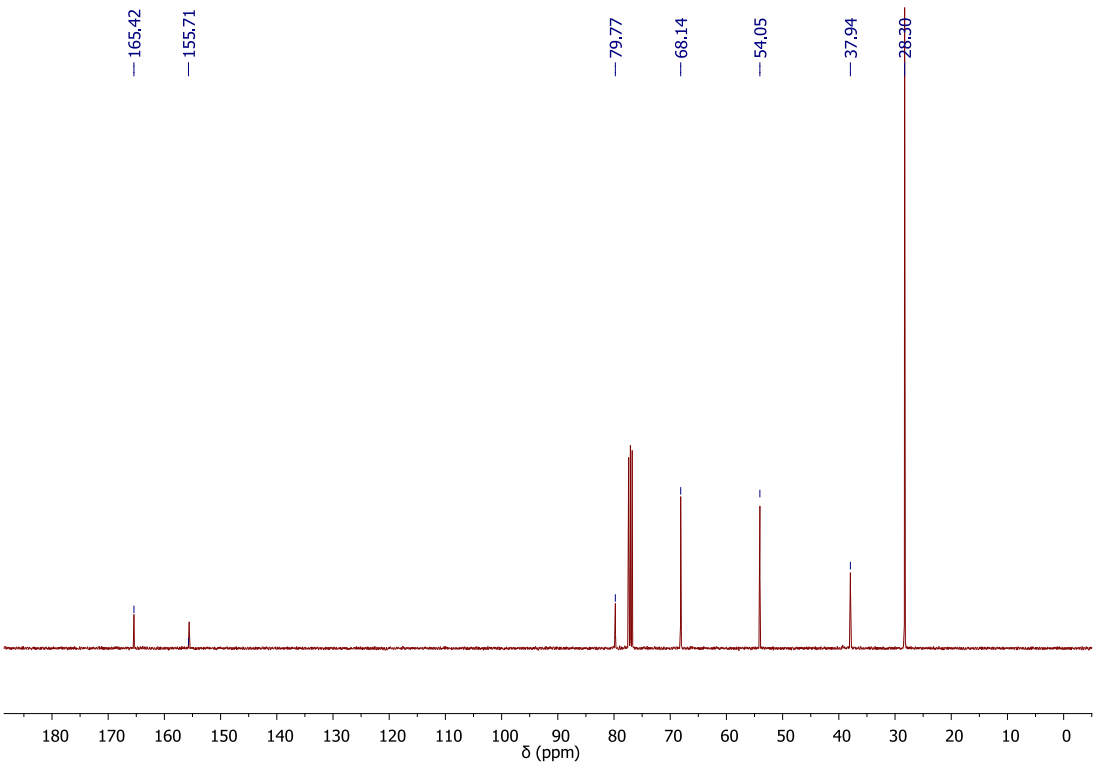


Figure S4. ^{13}C NMR spectrum of **M3** in $CDCl_3$.

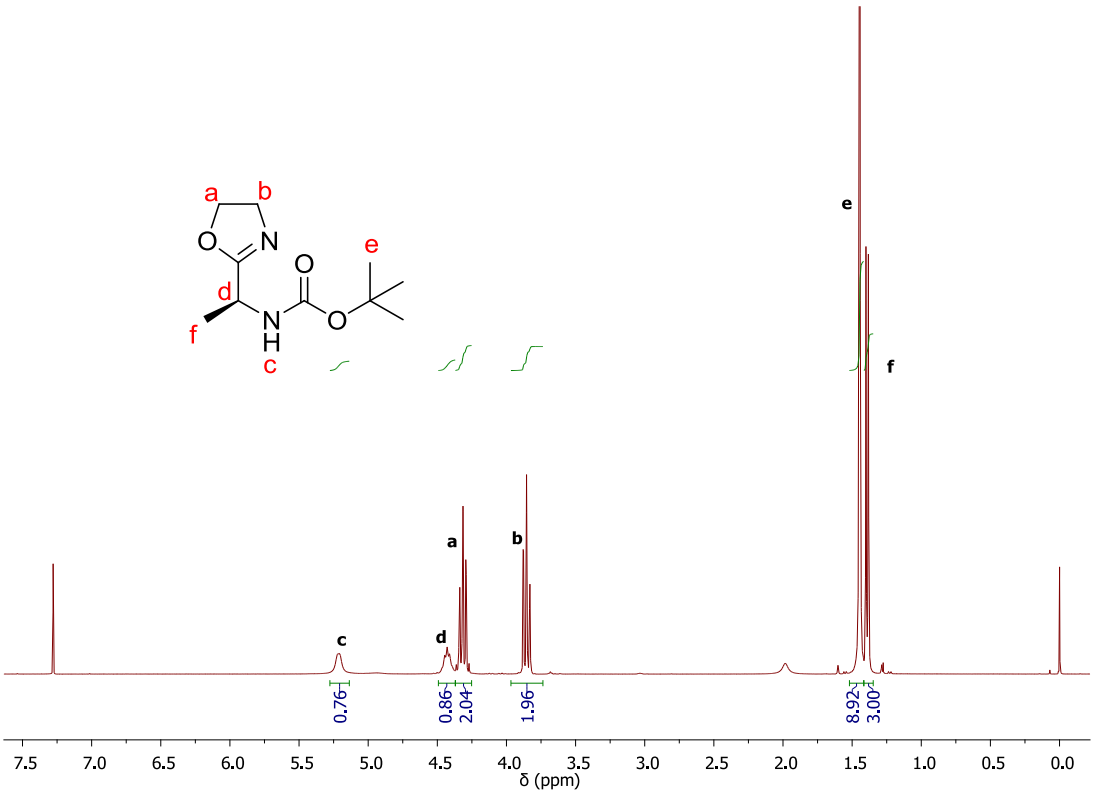


Figure S5. ^{1}H NMR spectrum of (*S*)-**M4** in $CDCl_3$.

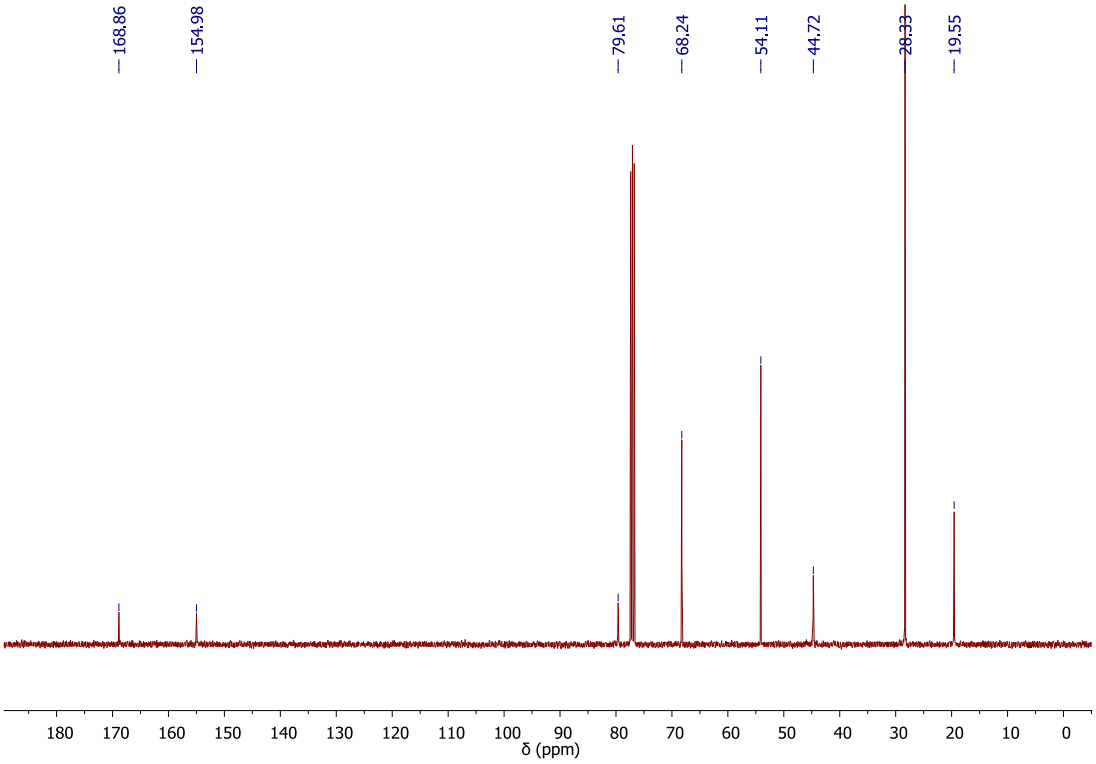


Figure S6. ^{13}C NMR spectrum of (*S*)-**M4** in $CDCl_3$.

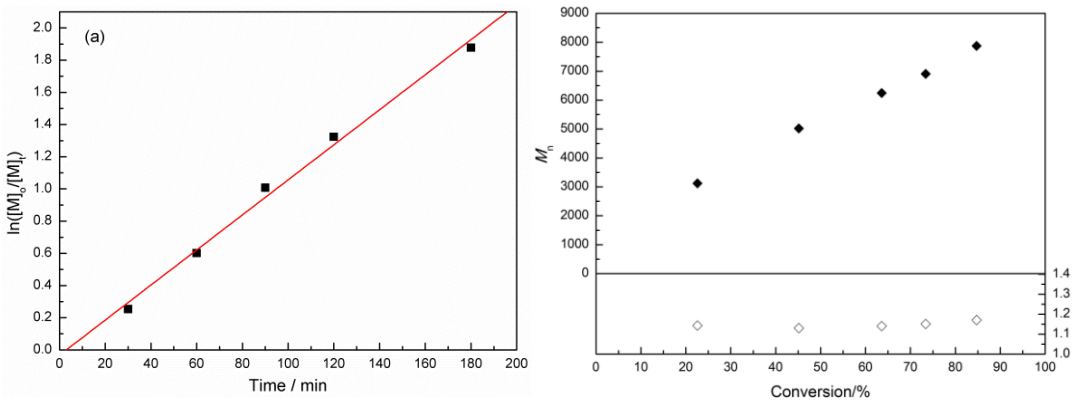


Figure S7. (a) Kinetics plots for polymerizations of **M2** initiated with $Sc(OTf)_3$ ($[M]_0/[I]_0 = 100$) in acetonitrile ($[M]_0 = 2.0$ M) at 90°C. (b) Evolution of the molar mass (M_n) and the PDI value with monomer conversion (determined by SEC, RI detection, PS calibration, using THF as eluent).

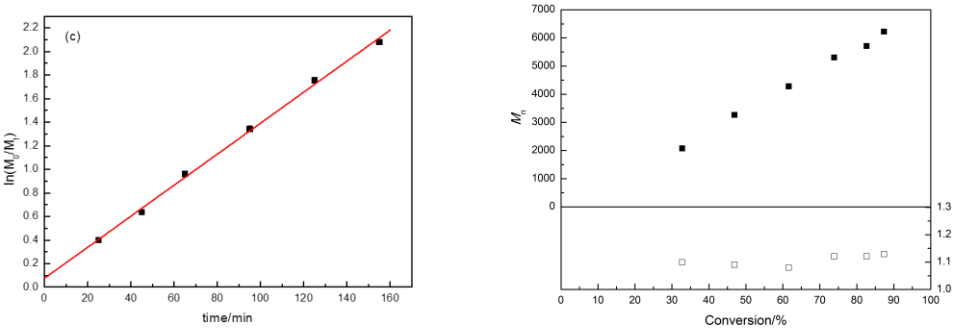


Figure S8. (a) Kinetics plots for polymerizations of (*S*)-**M4** initiated with $Sc(OTf)_3$ ($[M]_0/[I]_0 = 100$) in acetonitrile ($[M]_0 = 2.0$ M) at 90°C. (b) Evolution of the molar mass (M_n) and the PDI value with monomer conversion (determined by SEC, RI detection, PS calibration, using THF as eluent).

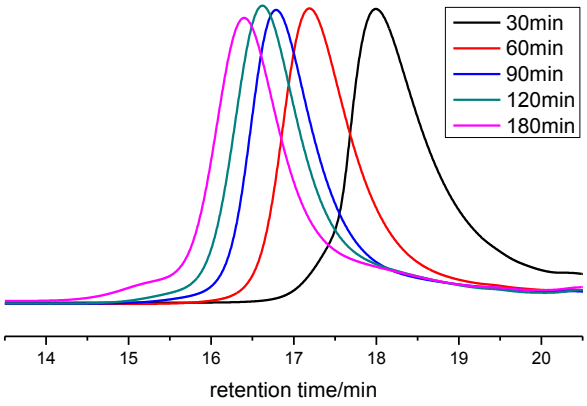


Figure S9. GPC traces of **P2a** samples collected periodically from the polymerization kinetic experiments, PS standard, with THF as the eluent.

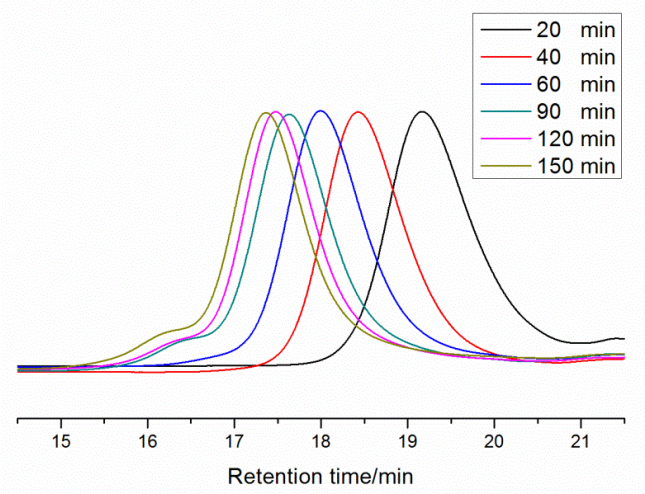


Figure S10. GPC traces of (*S*)-**P4a** samples collected periodically from the polymerization kinetic experiments, PS standard, THF as the eluent.

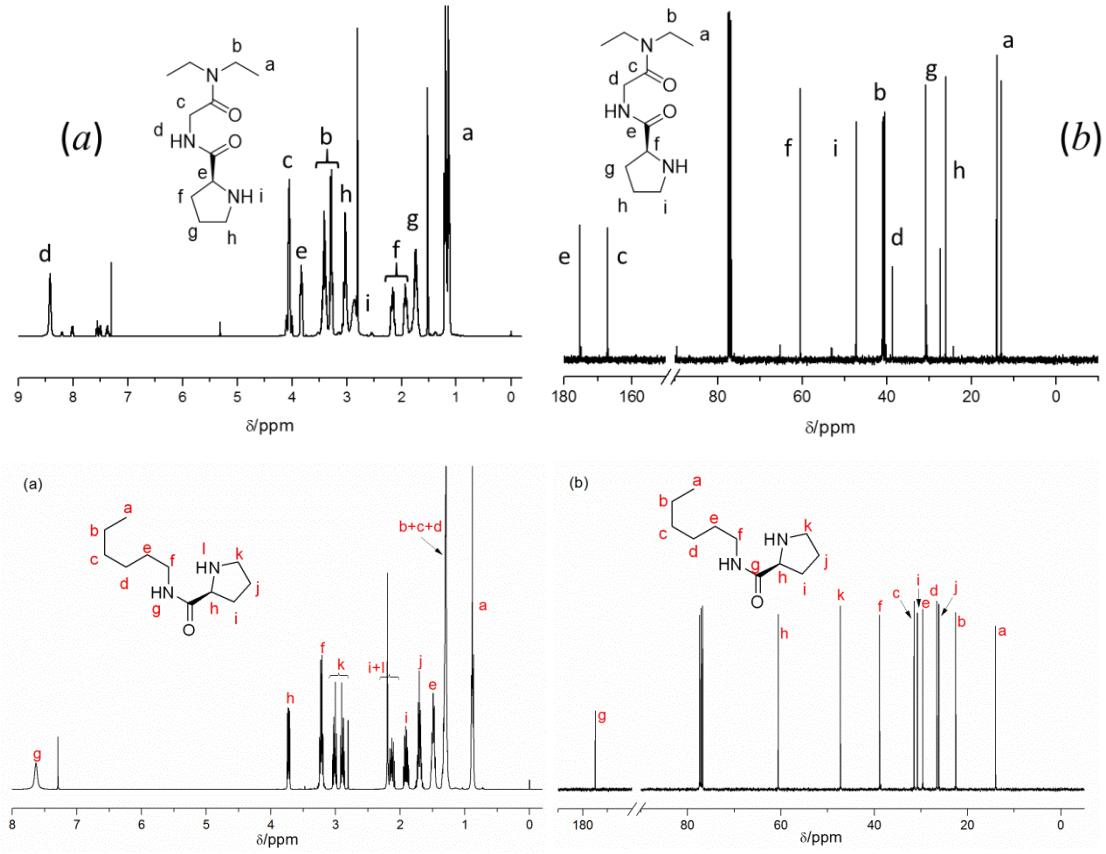


Figure S11. ^{1}H- and ^{13}C NMR spectra of **MC1** (top) and **MC2** (bottom) in $CDCl_3$.

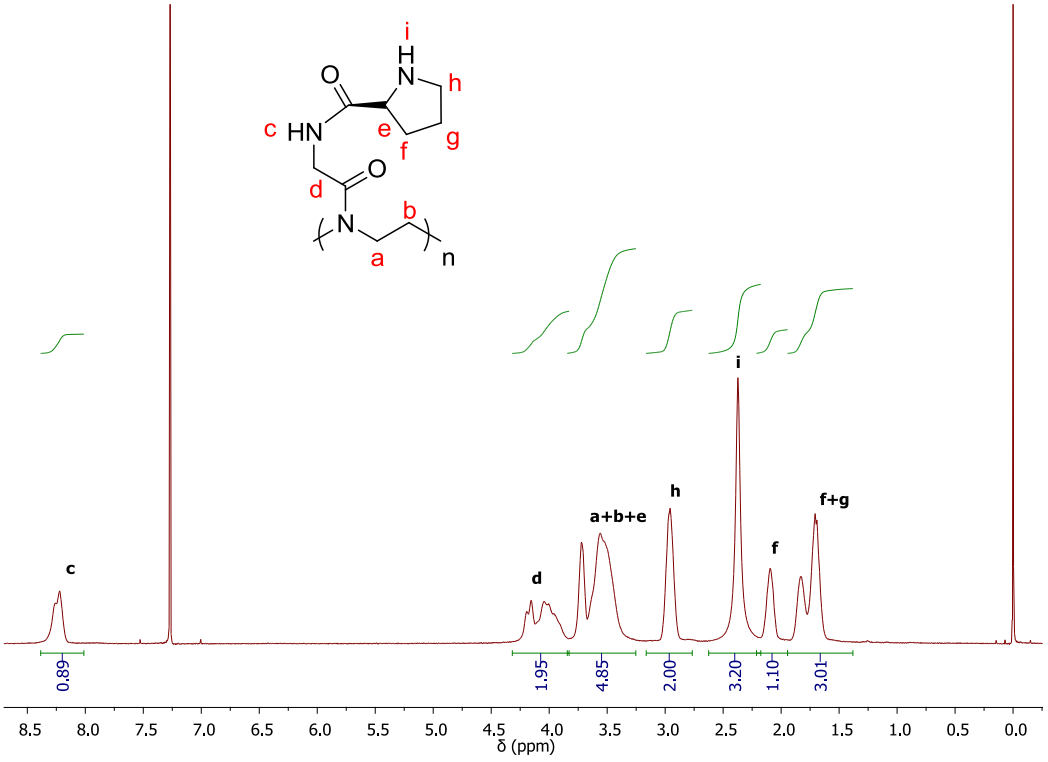


Figure S12. ^{1}H NMR spectrum of **P3** in $CDCl_3$ (the grafting degree: h/d X 100%).

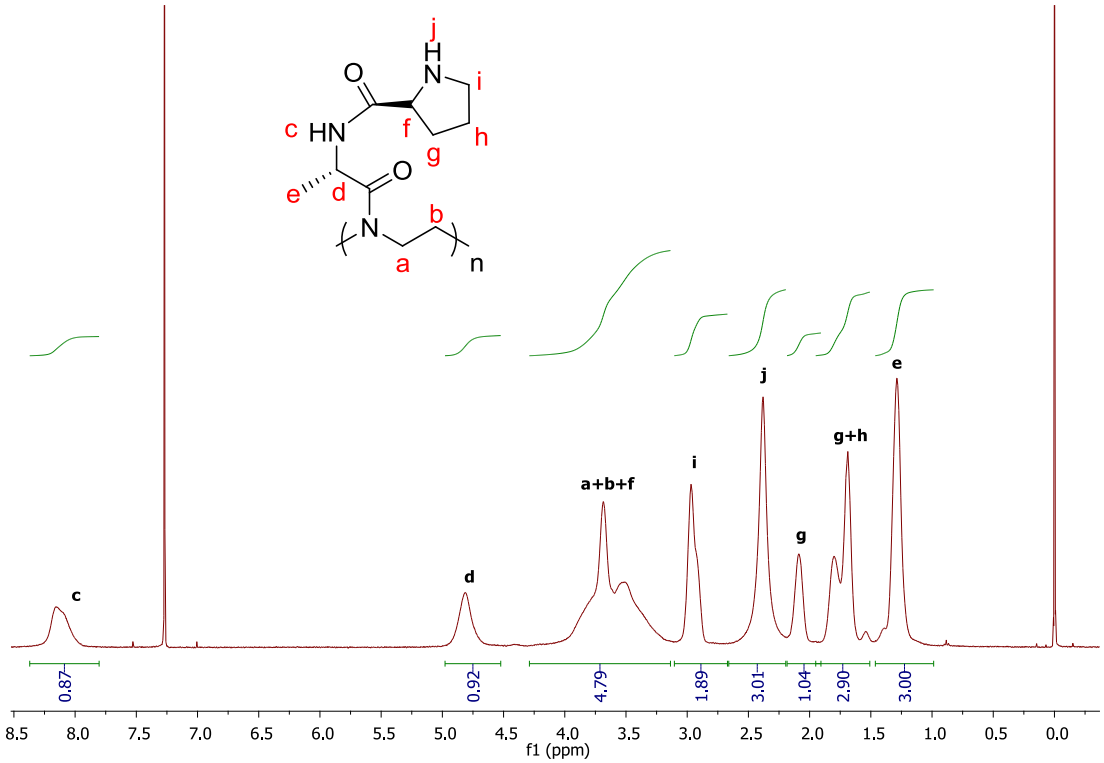


Figure S13. ^{1}H NMR spectrum of (*S*)-**P4** in $CDCl_3$ (the grafting degree: i/2d X 100%)

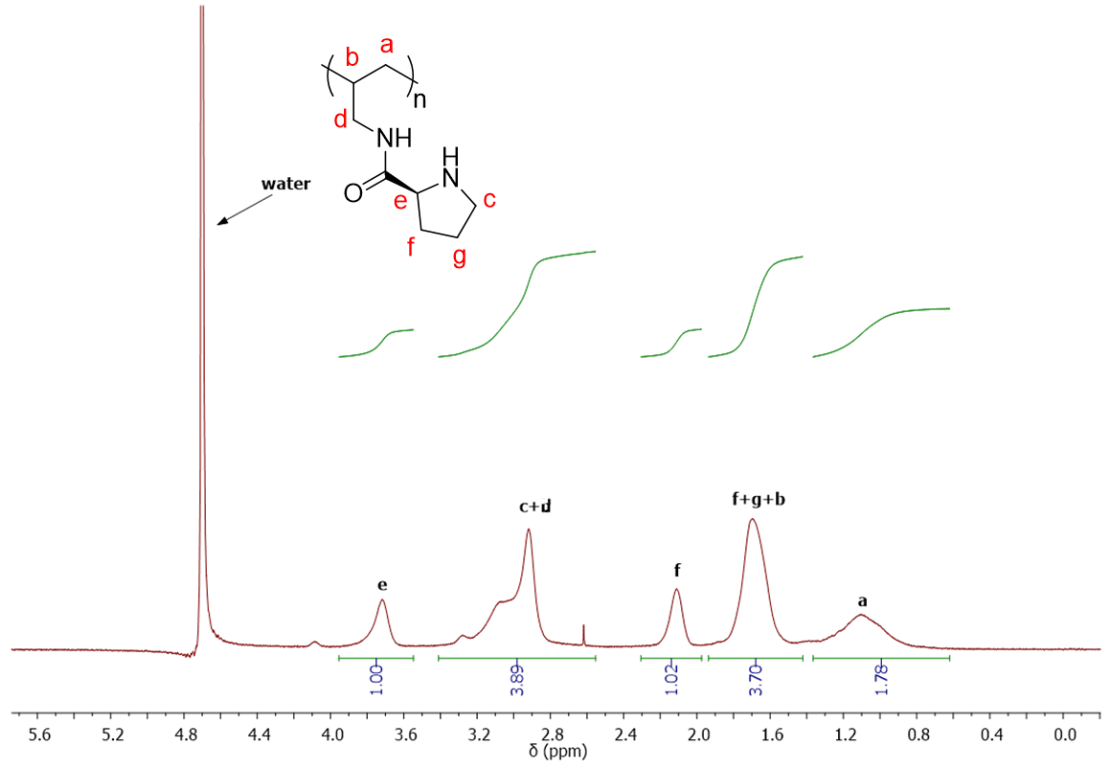


Figure S14. ^{1}H NMR spectrum of **P5** in D_2O (the grafting degree: 2e/(c+d-2e) X 100%)

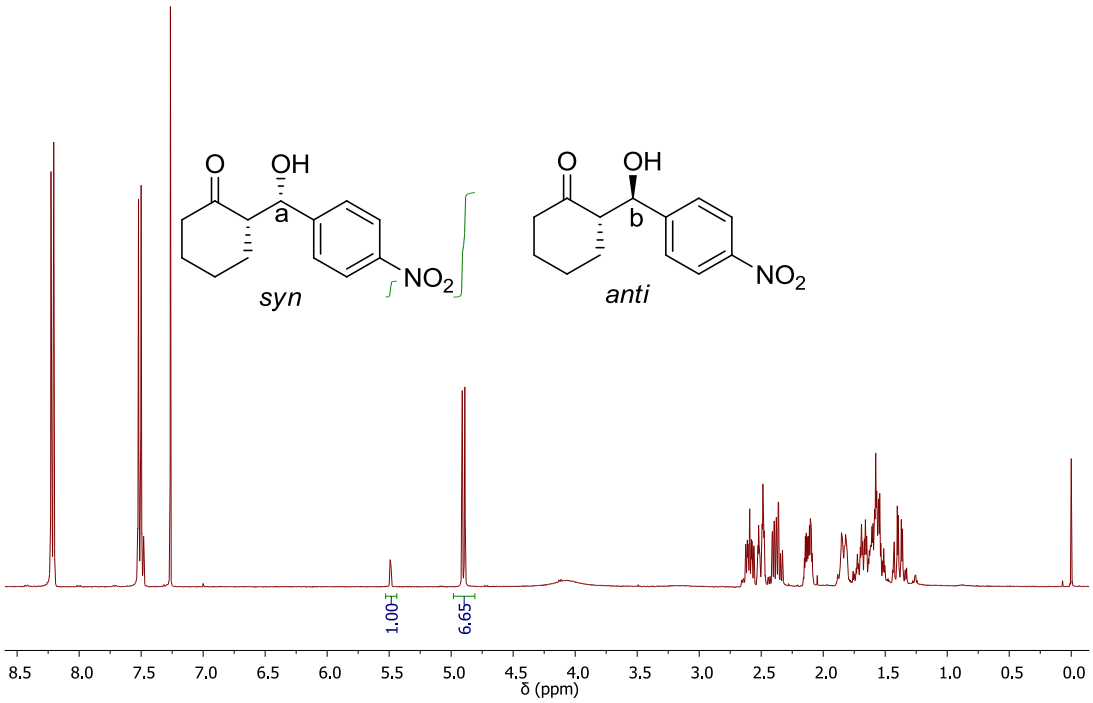
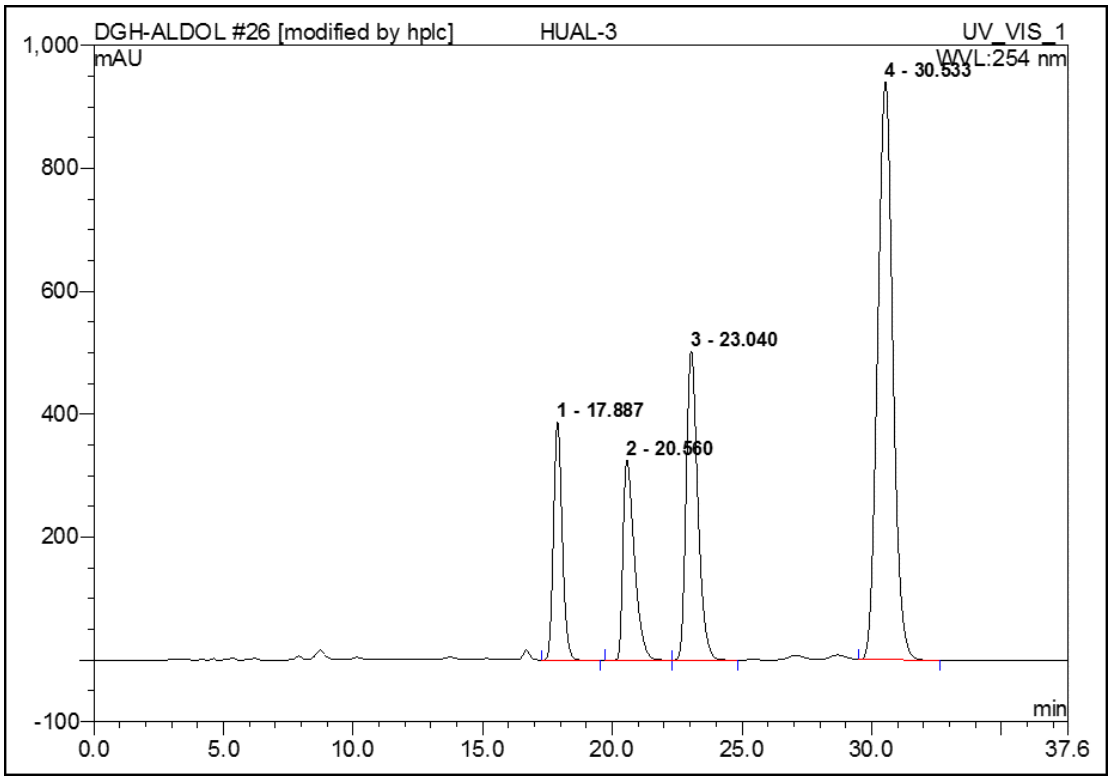
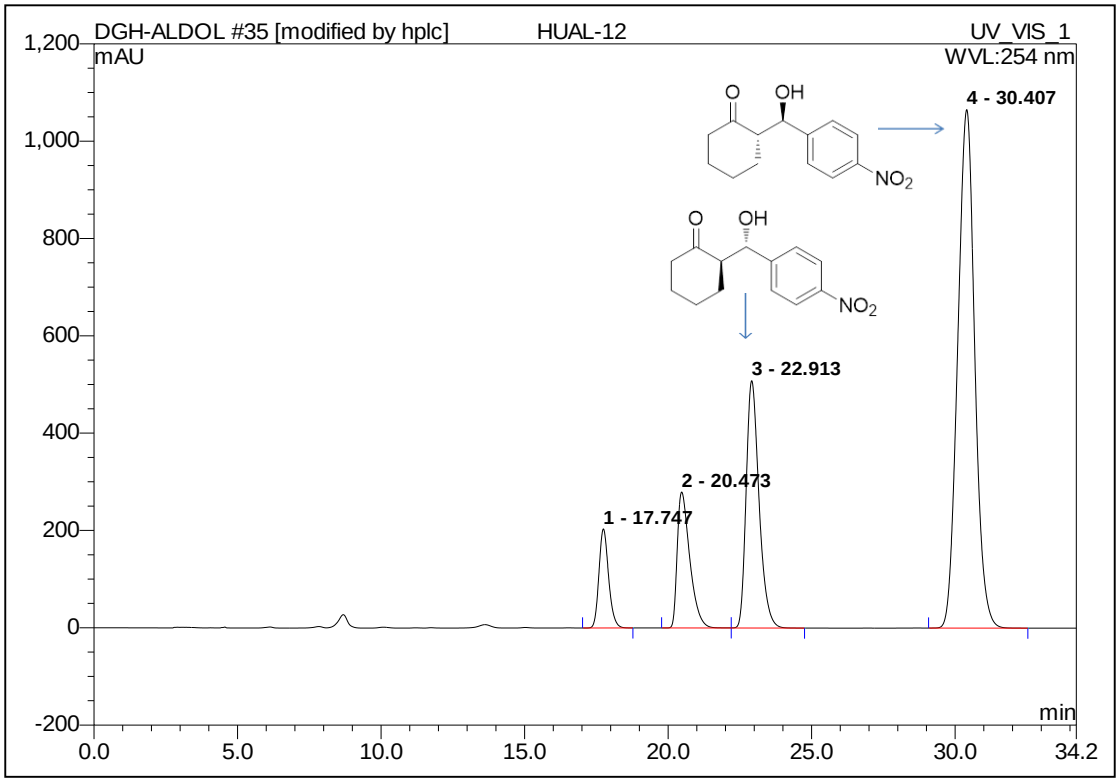


Figure S15. Determination of the *anti*/*syn* ratio (*dr*) of the aldol products by ^{1}H NMR.



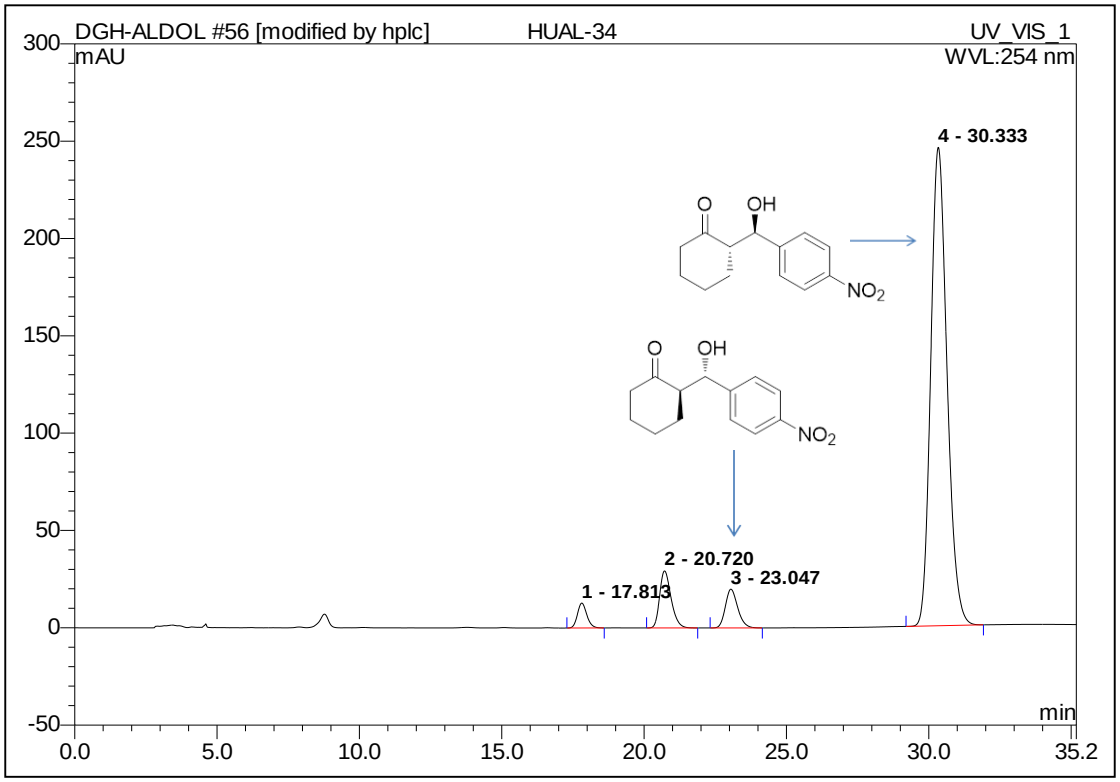
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	17.89	n.a.	386.844	151.165	12.38	n.a.	BMB
2	20.56	n.a.	324.814	165.999	13.60	n.a.	BM *
3	23.04	n.a.	502.610	261.364	21.41	n.a.	MB*
4	30.53	n.a.	940.123	642.026	52.60	n.a.	BMB*
Total:			2154.391	1220.555	100.00	0.000	

Figure S16. HPLC chart for the aldol products (Table 2 entry 1). Peaks 1# and 2# are assignable to *syn*-**1**, peaks 3# and 4# to *anti*-**1**, Chiralpak AD-H, *n*-hexane/*i*PrOH 1:9, 1.0 mL/min. The absolute configuration of the products was deduced by comparing the HPLC retention times with reported values (ref. 3 and 4).



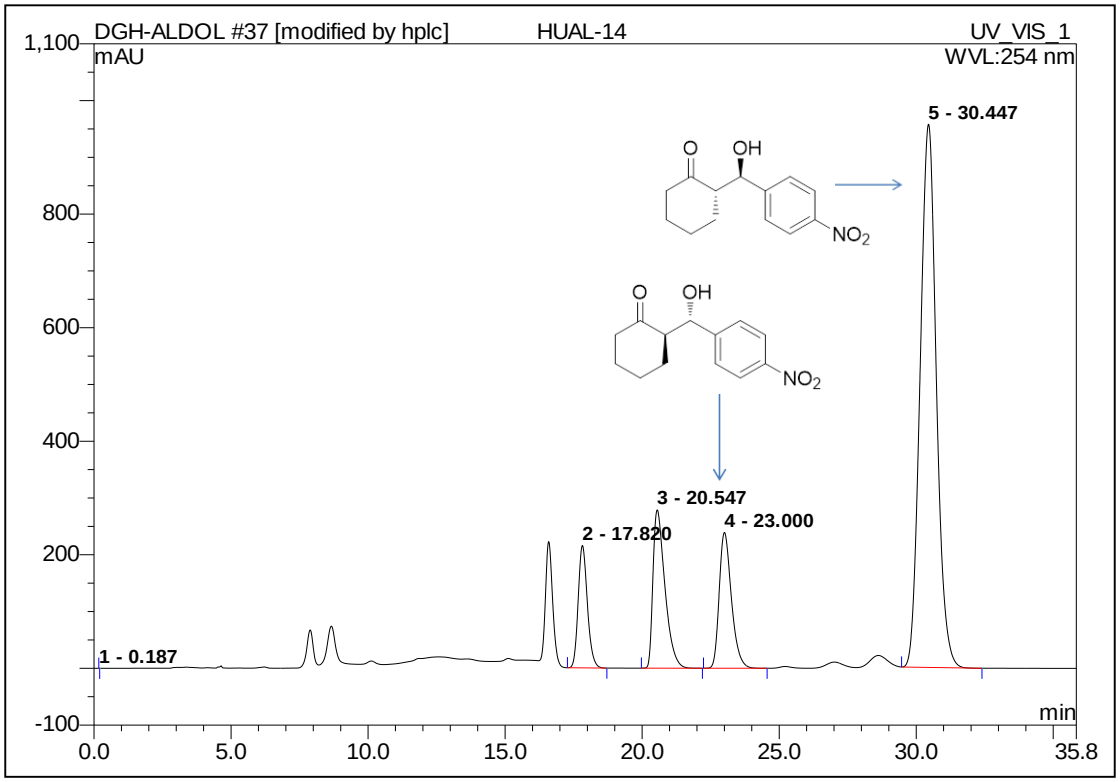
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	17.75	n.a.	203.423	79.115	6.51	n.a.	BMB*
2	20.47	n.a.	279.308	141.224	11.62	n.a.	BM *
3	22.91	n.a.	508.274	264.318	21.74	n.a.	MB
4	30.41	n.a.	1065.477	731.118	60.14	n.a.	BMB*
Total:			2056.482	1215.774	100.00	0.000	

Figure S17. HPLC chart for the aldol products (Table 2 entry 9), Peaks 1# and 2# are assignable to *syn*-**1**, peaks 3# and 4# to *anti*-**1**, Chiralpak AD-H, *n*-hexane/*i*PrOH 1:9, 1.0 mL/min.



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	17.81	n.a.	12.753	4.861	2.54	n.a.	BMB*
2	20.72	n.a.	29.274	13.620	7.12	n.a.	BMB
3	23.05	n.a.	19.885	9.988	5.22	n.a.	BMB
4	30.33	n.a.	245.805	162.792	85.12	n.a.	BMB*
Total:			307.717	191.261	100.00	0.000	

Figure S18. HPLC chart for the aldol products (Table 2 entry 5). Peaks 1# and 2# are assignable to *syn*-**1**, peaks 3# and 4# to *anti*-**1**. Chiralpak AD-H, *n*-hexane/*i*PrOH 1:9, 1.0 mL/min.



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	0.19	n.a.	0.001	0.000	0.00	n.a.	BMB
2	17.82	n.a.	215.527	83.637	8.35	n.a.	BMB*
3	20.55	n.a.	278.668	140.925	14.07	n.a.	BMB*
4	23.00	n.a.	239.102	123.600	12.34	n.a.	BMB
5	30.45	n.a.	956.948	653.405	65.24	n.a.	BMB*
Total:			1690.246	1001.567	100.00	0.000	

Figure S19. HPLC chart for the aldol products (Table 2 entry 10). Peaks 1# and 2# are assignable to *syn*-**1**, peaks 3# and 4# to *anti*-**1**. Chiralpak AD-H, *n*-hexane/*i*PrOH 1:9, 1.0 mL/min.

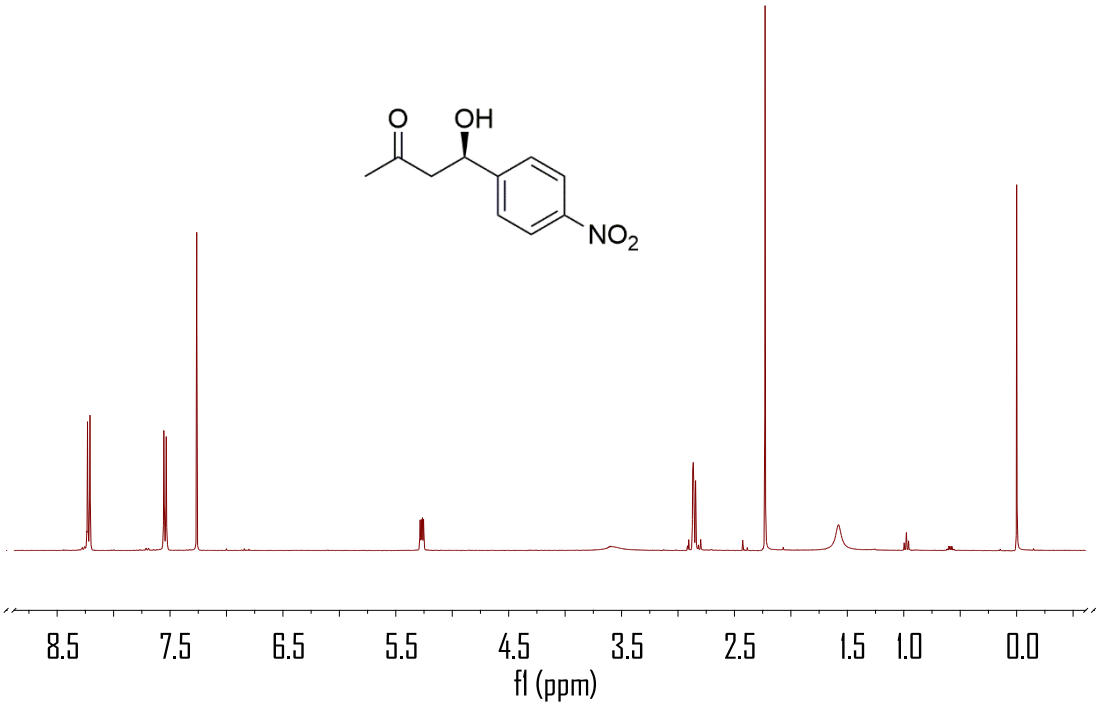
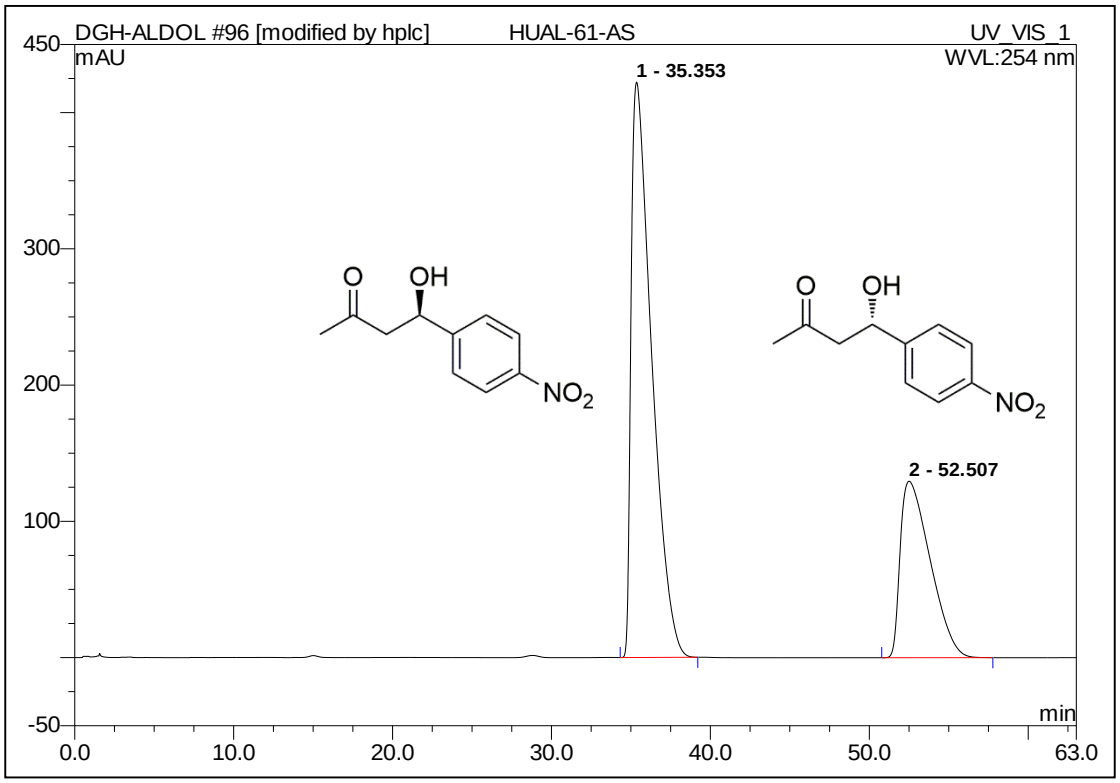


Figure S20. ^{1}H NMR spectrum of the aldol adduct of acetone to 4-nitrobenzaldehye.



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	35.35	n.a.	422.279	633.710	69.17	n.a.	BMB*
2	52.51	n.a.	129.516	282.400	30.83	n.a.	BMB
Total:			551.795	916.110	100.00	0.000	

Figure S21. A representative HPLC chart for the aldol adducts of acetone to 4-nitrobenzaldehye, Chiralpak AS-H, *n*-hexane/*i*PrOH 1:9, 1 mL/min.

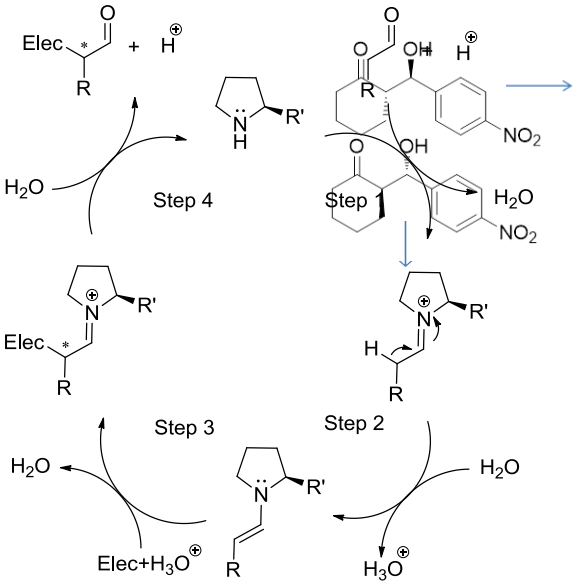


Figure S22. Pyrrolidine-catalyzed α-functionalization of aldehydes (Elec = electrophile) [5].

References:

1. Miller, J.J.; Rajaram, S.; Pfaffenroth, C.; Sigman, M. Synthesis of amine functionalized oxazolines with applications in asymmetric catalysis. *Tetrahedron* **2009**, *65*, 3110–3119.

2. Wang, Y.; Shen, H.; Zhou, L.; Hu, F.; Xie, S.; Jiang, L. Novel poly(2-oxazoline)s with pendant L-prolinamide moieties as efficient organocatalysts for direct asymmetric aldol reaction. *Catal. Sci. Technol*. **2016**, *6*, 6739–6749.

3.Mase, N.; Nakai, Y.; Ohara, N.; Yoda, H.; Takabe, K.; Tanaka, F.; Barbas, C. Organocatalytic direct asymmetric aldol reactions in water. *J. Am. Chem. Soc.* **2006**, *128*, 734–735.

4.Pearson, A.; Panda, S. *N*-Prolinylanthranilic acid derivatives as bifunctional organocatalysts for asymmetric aldol reactions. *Tetrahedron* **2011**. 67, 3969–3975.

5. Bertelsen, S.; Jorgensen, K.A. Organocatalysis–after the gold rush. *Chem. Soc. Rev*. **2009**, *38*, 2178–2189.

2. Cartesian Coordinates of transition states

TS_{a1}

N	1.90318900	-1.64468600	0.41530100
C	1.68682800	-2.26165000	-0.93790200
C	3.21044600	-0.94573300	0.45065700
H	0.75446700	-1.88663800	-1.35096400
H	1.63833500	-3.34746400	-0.79521200
C	2.91647100	-1.83287900	-1.74920100
C	3.99899300	-1.60726800	-0.68450400
H	3.68775100	-1.07064800	1.42362400
C	3.06000800	0.58983700	0.17992300
H	2.70507300	-0.89185800	-2.26512400
H	3.18797300	-2.59072700	-2.48806700
H	4.80348900	-0.94669400	-1.00860100
H	4.43257700	-2.55640700	-0.34720200
O	4.12578300	1.21907000	0.17215700
N	1.82075100	1.04465900	-0.02444400
H	0.67352500	0.39030900	-0.23234000
C	1.03353000	-1.61002300	1.38555300
C	1.43716000	-0.99561500	2.70584900
H	1.70060000	0.05260300	2.51925200
H	2.36005600	-1.48845200	3.03770700
C	-0.38597200	-1.97748700	1.15887400
H	-0.47969800	-2.63924900	0.29766000
C	-2.84059400	-1.30279600	-0.98071700
C	-2.50348200	-0.78351600	0.27801400
C	-3.53101300	-0.45849500	1.17356300
C	-4.86759300	-0.66908000	0.84173100
C	-5.16535200	-1.20785200	-0.40691500
C	-4.16735900	-1.52366800	-1.32969900

H	-2.04699600	-1.49874400	-1.69278000
H	-3.28723100	-0.01833400	2.13650000
H	-5.67292300	-0.42029800	1.52114400
H	-4.44560300	-1.92365400	-2.29661800
C	-1.03697900	-0.55032500	0.62190300
O	-0.35682000	-0.09778400	-0.46655900
H	-0.99579100	0.13274700	1.49222400
C	1.76022900	2.41518400	-0.48066200
H	2.48674300	3.03838700	0.05501800
H	0.75515400	2.80718200	-0.28448100
C	2.04780000	2.51496300	-1.99784000
O	2.29724200	1.51881200	-2.67019500
N	2.00264200	3.76936600	-2.55987600
C	2.25023000	3.91915500	-3.98553900
H	3.10799900	4.58145500	-4.15986400
H	2.45886200	2.93572100	-4.40231000
H	1.37502900	4.35213200	-4.48762200
C	1.70875600	5.00019100	-1.84830400
H	2.52696900	5.72124200	-1.97644200
H	0.79017700	5.46430800	-2.23336000
H	1.58110700	4.82495500	-0.78265300
N	-6.57134700	-1.43935900	-0.76657300
O	-6.80783400	-1.91731300	-1.87647100
O	-7.43202100	-1.14523800	0.06405300
C	-1.09526700	-2.60714600	2.38748800
H	-2.07100300	-2.12917300	2.51265700
H	-1.30690800	-3.65952800	2.17309700
C	-0.30967800	-2.49432700	3.70423600
H	0.45842400	-3.27845200	3.75722000
H	-0.98248300	-2.66133300	4.55155000

C 0.36926000 -1.12752900 3.80181900

H -0.38054200 -0.33370100 3.70236400

H 0.84468800 -0.98496200 4.77719800

Sum of electronic and thermal Enthalpies= -1450.924737

Sum of electronic and thermal Free Energies= -1451.015533

TS_{a2}

C 0.61801400 -0.40829000 -0.06557400

H -3.68862900 -1.28526100 3.37533000

H -3.66301600 0.10830200 2.27875000

C -4.25385300 -1.72511900 1.28795100

H -5.23979800 -1.29950400 1.10414200

H -4.35392900 -2.78597600 1.54209600

C 0.41188500 -1.96681900 0.45511300

H 0.40277700 -1.96143900 1.54781700

N -2.00441500 -1.72738500 0.59683100

C 2.09297900 -0.01333600 -0.00089300

C -0.97224200 -2.16632800 -0.07469900

O 0.04832400 -0.25181400 -1.27930100

C 1.47431100 -2.97609100 -0.05528900

H -3.57306700 -2.31991300 -0.71441400

C -3.37331300 -1.56683700 0.04808800

C -1.98002400 -1.21684700 2.00630800

C -3.56237100 -0.13527000 -0.55862500

H 0.12261000 0.18160600 0.73656400

O -4.69033700 0.35501100 -0.52257000

H -1.46397000 0.07605900 -1.09748800

H -1.52257900 -1.98764400 2.63243300

C -3.45709500 -0.96148400 2.35805100

H -1.39270600 -0.30125900 2.05732500

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H 2.28556200 -2.41213700 -0.52462000

C 4.75490600 0.78370300 0.04816700

C 2.79645700 0.04668700 1.21195100

C 2.74696000 0.34353900 -1.18568700

C 4.08035500 0.74357100 -1.17146200

C 4.12859900 0.44168100 1.24828900

H 2.29424300 -0.21059900 2.14166700

H 2.16547000 0.31230300 -2.10069900

H 4.60447400 1.02535800 -2.07632400

H 4.68781900 0.49524500 2.17383400

N 6.16096500 1.20197300 0.07478000

O 6.73446500 1.22630800 1.16594300

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N -2.47080100 0.46352500 -1.07121300

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H 1.81177800 -4.49300400 -1.55784500

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H -1.72989400 -2.09357200 -2.06374500

H -1.88778400 -3.65673200 -1.25287800

C 0.07088800 -3.30474200 -2.10033400

H 0.59197300 -2.43950700 -2.52007000

H -0.20137800 -3.97501000 -2.92232500

C -2.28708900 2.65286100 0.02069200

O -2.12711800 2.04766100 1.08046100

N -2.25845200 4.01911100 -0.04657300

C -1.98309700 4.78769100 1.15969900

H -1.05024600 5.35543500 1.05126000

H -2.79742600 5.49601200 1.35450100

H -1.89201800 4.09662300 1.99515400

C -2.40241800 4.79978900 -1.26478400

H -2.73213900 4.18400700 -2.09866300

H -3.14864900 5.58914500 -1.11449600

H -1.45397700 5.27988700 -1.54151800

Sum of electronic and thermal Enthalpies= -1450.920069

Sum of electronic and thermal Free Energies= -1451.011018

TS_{a3}

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O -3.62039500 1.54781100 -2.40281400

C 0.41718800 0.10859100 -0.24278100

H 1.68450400 -2.69379600 -0.33171700

H -3.98581000 -0.25153500 1.12260400

C 0.72032300 -2.75352600 0.17976500

O -0.12228200 0.77047300 0.73911300

H -4.50879200 -0.61329600 -2.85122200

H -4.02585100 -2.03658800 0.99878500

C -3.91614300 -1.10462800 0.44275900

H -1.85907400 -3.10883600 1.76049800

C -2.75027100 -0.53946000 -1.58338000

H -5.38892900 0.00334800 -0.69982500

C -2.89266600 1.01773100 -1.56401300

C -1.53306100 -2.05625700 1.74703200

C -1.48203500 -1.60077400 0.30615600

C -0.19848900 -1.65197400 -0.36873200

C -4.09142100 -1.15017200 -2.00023800

N	-2.57598200	-1.08969500	-0.22078400
C	-0.16337100	-1.90210600	2.42371800
H	-0.29947700	-1.75218700	-1.45066000
H	-1.91552400	-0.82639400	-2.22467100
H	-5.72296300	-1.73462700	-0.63484600
C	-4.93046100	-0.98735000	-0.71813600
H	-3.95387400	-2.20492800	-2.26091000
C	1.93260700	0.01485100	-0.25738000
H	-2.28268900	-1.48378300	2.29721200
H	0.29576900	-3.72596600	-0.10568500
H	1.90402500	-2.29330700	1.95608600
H	0.07859600	0.39371800	-1.26441400
H	0.93408000	-3.74828400	2.09375300
H	-0.24923700	-2.19633900	3.47480100
H	0.08251900	-0.83680600	2.39085500
C	0.92605500	-2.71959800	1.71479000
C	4.71202500	-0.04587900	-0.26050300
C	2.63506600	-0.42663200	-1.38934300
C	2.65320900	0.44561300	0.86455700
C	4.04393900	0.41481400	0.87403000
C	4.02505200	-0.46415100	-1.40084500
H	2.08700600	-0.73587800	-2.27604200
H	2.08972800	0.82726400	1.70874500
H	4.61887100	0.74559400	1.73005400
H	4.58411400	-0.80054400	-2.26482600
N	6.17934700	-0.08227900	-0.26098800
O	6.74438400	-0.49276400	-1.27656400
O	6.76474600	0.29696600	0.75464500
N	-2.22355300	1.67655600	-0.60188100
C	-2.52335600	3.06572500	-0.37319100

H -1.65510700 3.52662100 0.10782300

H -2.70472700 3.56817500 -1.32839800

C -3.77206600 3.21217100 0.53035800

O -4.37685400 2.22258600 0.93859200

N -4.16182700 4.48533400 0.85061500

C -5.34232900 4.68126700 1.68072600

H -5.08682700 5.25721800 2.57868000

H -6.11527800 5.22996700 1.12777600

H -5.72694100 3.70517500 1.96933200

C -3.52212300 5.70395400 0.38226600

H -4.21116800 6.28795100 -0.24203500

H -3.22614200 6.32964200 1.23381700

H -2.63183700 5.49083100 -0.20491300

Sum of electronic and thermal Enthalpies= -1450.916118

Sum of electronic and thermal Free Energies= -1451.008721

TS_{a4}

H -0.80067900 -0.52788600 -0.46301700

O -2.28383500 -1.22277000 2.33132000

C 1.15030300 0.87317800 -1.28415200

H 2.78229400 2.87785400 -0.00828800

H -3.28575100 1.20469000 -0.73766400

C 1.75216100 3.24780900 0.01200200

O 0.12707000 0.11369200 -1.55535100

H -2.94899300 0.83543300 3.26713300

H -3.23904600 2.92704800 -0.26719400

C -3.04586200 1.90759000 0.06346700

H 3.41911000 -2.54204100 1.02300000

C -1.51262600 0.94696800 1.64896800

H -4.28429100 0.60075400 1.27130000

C -1.74125100 -0.58136200 1.43121700

C 3.47226100 -1.65578200 0.40300100

C -0.59952700 2.36366800 -0.21225000

C 0.79691200 2.04280500 0.03498800

C -2.69926300 1.50341100 2.44386500

N -1.59502500 1.75312400 0.39904300

H 3.77874300 1.48472100 -1.85452500

H 0.94636100 1.45056700 0.93689500

H -0.55213000 1.11076800 2.13787600

H -4.56318200 2.32082300 1.59504500

C -3.79857400 1.57355300 1.37003200

H -2.45289400 2.49640400 2.83496600

H 1.43310400 1.59428000 -2.08406100

C 4.72147400 -1.17404200 0.00610100

H 1.65065200 3.80448100 0.95428600

C 2.33182300 -0.98425000 -0.01913200

C 2.42444800 0.16831200 -0.81472800

C -0.86325100 3.30347200 -1.36093200

H 1.34819800 -1.35015700 0.25515200

C 1.50591800 4.20502800 -1.16285400

H 5.83685500 0.28540300 -1.09924300

C 3.69413700 0.61712000 -1.20550600

C 4.85020600 -0.04577400 -0.80053500

H -0.63428900 2.72840200 -2.26939000

C 0.02249800 4.56332800 -1.28123300

H -1.91211600 3.58780200 -1.43409100

H 1.83773800 3.74311600 -2.10000500

H -0.28660600 5.16267700 -0.41454400

H -0.16006200 5.17964300 -2.16801000

H 2.10562300 5.11287400 -1.03315800

N	-1.33424600	-1.09158000	0.25893500
C	-1.77937100	-2.40564400	-0.12334500
H	-1.09545400	-2.78978200	-0.88638400
H	-1.75281000	-3.07388700	0.74324700
N	5.93188500	-1.88025300	0.44176400
O	7.02167500	-1.43218200	0.08026900
O	5.79164300	-2.88096200	1.14698900
C	-3.22207900	-2.35174400	-0.68413400
O	-3.83827900	-1.28962600	-0.74199700
N	-3.76871900	-3.53363300	-1.10773500
C	-3.11674500	-4.83171200	-1.04949500
H	-3.66636100	-5.51144200	-0.38509800
H	-3.08618800	-5.28714100	-2.04743200
H	-2.09575400	-4.75318500	-0.68332400
C	-5.12955600	-3.54384000	-1.62611600
H	-5.77381100	-4.17696600	-1.00298100
H	-5.50834800	-2.52379200	-1.62075700
H	-5.14600600	-3.93754300	-2.64987500

Sum of electronic and thermal Enthalpies= -1450.921730

Sum of electronic and thermal Free Energies= -1451.013171

TS_{b1}

N	1.94214200	-1.75377300	0.42639300
C	1.70691500	-2.44655600	-0.88316600
C	3.26643000	-1.08930500	0.42102200
H	0.78848700	-2.06825100	-1.32346600
H	1.62178100	-3.51931400	-0.67636900
C	2.95276100	-2.11684800	-1.71617200
C	4.03933500	-1.83488900	-0.66915800
H	3.74003600	-1.17509000	1.40015000

C	3.16651800	0.44989900	0.09955900
H	2.76679600	-1.21875000	-2.31157300
H	3.20538300	-2.93229900	-2.39783600
H	4.85511700	-1.20940800	-1.03283700
H	4.45852200	-2.76920000	-0.27784400
O	4.26800200	1.01832200	0.04687300
N	1.94338700	0.95185800	-0.05404200
H	0.76176400	0.30804200	-0.29884000
C	1.07081100	-1.63609200	1.38995700
C	1.49421400	-0.97614100	2.68099500
H	1.79436300	0.05156600	2.44493800
H	2.39871300	-1.48697900	3.03626300
C	-0.36074000	-1.96473600	1.17072800
H	-0.47050900	-2.67642700	0.35202300
C	-2.75651400	-1.35282300	-1.04416300
C	-2.42262600	-0.76142200	0.18314900
C	-3.45330100	-0.34658500	1.03695300
C	-4.79044000	-0.53858100	0.69635100
C	-5.08555600	-1.14997700	-0.51884600
C	-4.08400100	-1.55579400	-1.40138900
H	-1.96027600	-1.62207000	-1.72886100
H	-3.21110800	0.14978700	1.97242300
H	-5.59777800	-0.22071200	1.34383200
H	-4.35984800	-2.01046900	-2.34450600
C	-0.95745200	-0.55368400	0.54299600
O	-0.24061900	-0.17878500	-0.55617000
H	-0.90820100	0.17630800	1.37182700
N	-6.49256000	-1.36394200	-0.88675200
O	-6.72578100	-1.90706800	-1.96687200
O	-7.35603000	-0.99111100	-0.09180800

C	-1.10630300	-2.48943600	2.42721000
H	-2.05020500	-1.94635900	2.52880600
H	-1.38330100	-3.53570800	2.26385700
C	-0.31386000	-2.35961900	3.73749700
H	0.41954400	-3.17374800	3.82178000
H	-0.99223900	-2.46359200	4.59039900
C	0.42170200	-1.01976600	3.77962800
H	-0.29469800	-0.20010700	3.64741200
H	0.90302800	-0.85700200	4.74883400
C	1.88247400	2.38787600	-0.33621300
H	2.63568800	2.91908900	0.25947800
H	0.89263300	2.74649300	-0.02453700
C	2.09396100	2.72117600	-1.82053700
H	1.35936300	2.16308900	-2.41529400
H	3.08714600	2.36250500	-2.11310000
C	1.97180600	4.21960500	-2.11115800
H	2.12303300	4.43521100	-3.17398700
H	0.98124100	4.59997400	-1.83437600
H	2.71556500	4.79442600	-1.54762100

Sum of electronic and thermal Enthalpies= -1282.265845

Sum of electronic and thermal Free Energies= -1282.348298

TS_{b2}

C	0.69804400	-0.42713800	0.13772300
H	-3.42370500	-1.41751600	3.65570900
H	-3.29281000	-0.00051100	2.60718900
C	-4.12029400	-1.72060800	1.58095600
H	-5.08377800	-1.22141700	1.48096100
H	-4.28547000	-2.78334200	1.78915000

C	0.48512700	-2.04758500	0.42294000
H	0.53546000	-2.22147000	1.50099700
N	-1.91321700	-1.78293400	0.73580600
C	2.18152500	-0.06050500	0.19790600
C	-0.92881400	-2.13633700	-0.05306700
O	0.07907800	-0.08350600	-1.00474700
C	1.49742300	-2.97164000	-0.30466900
H	-3.58915800	-2.28803100	-0.46514800
C	-3.31190900	-1.55286900	0.29183900
C	-1.79303900	-1.51613500	2.20466600
C	-3.55154300	-0.13411200	-0.32647000
H	0.25056200	0.03347800	1.05266200
O	-4.72599200	0.23363800	-0.39453600
H	-1.47106800	0.23222300	-0.76800400
H	-1.48131300	-2.44863400	2.68634000
C	-3.20253600	-1.09041000	2.63732800
H	-1.03845200	-0.75438300	2.39456800
H	1.98169800	-3.61981100	0.43298500
H	2.28949600	-2.34620400	-0.72590400
C	4.85525600	0.69152300	0.24365300
C	2.93858800	-0.19506900	1.37140700
C	2.78738800	0.46681700	-0.94786600
C	4.12698400	0.84618500	-0.93496600
C	4.27770000	0.17642000	1.40550500
H	2.47497000	-0.58806600	2.27350600
H	2.16485600	0.58339700	-1.82827600
H	4.61466600	1.25850000	-1.80960300
H	4.87883100	0.08240400	2.30104200
N	6.26907800	1.08601700	0.26872600
O	6.88828800	0.94083000	1.32473300

O 6.75940100 1.53829200 -0.76695500

N -2.48795200 0.56374100 -0.75570700

C 0.90826600 -3.81951500 -1.44119700

H 1.72258500 -4.22718500 -2.04927500

H 0.35815200 -4.68249700 -1.03814800

C -1.25786200 -2.57458700 -1.45828200

H -1.82695400 -1.78218000 -1.94994700

H -1.92708600 -3.44511300 -1.36388900

C -0.03194800 -2.96192800 -2.28677500

H 0.47246300 -2.04224200 -2.59602000

H -0.36453600 -3.49238800 -3.18495400

C -2.69867500 1.87341300 -1.37433400

H -3.58301700 1.82529900 -2.01881000

H -1.82224200 2.06552800 -2.00105700

C -2.87208700 3.00413400 -0.35141700

H -1.99301100 3.02690200 0.30478100

H -3.73949400 2.77231600 0.27650500

C -3.06064000 4.36710600 -1.02299400

H -3.18292200 5.16217200 -0.28085300

H -2.19833200 4.62641600 -1.64787700

H -3.94891700 4.37297400 -1.66461800

Sum of electronic and thermal Enthalpies= -1282.260190

Sum of electronic and thermal Free Energies= -1282.342473

TS_{b3}

H -1.73754300 1.08646600 0.18743600

O -3.77902700 1.38856000 -2.31197500

C 0.23325200 0.07530400 -0.16126900

H 1.71141100 -2.58880200 -0.39424300

H -4.12643900 -0.81483800 1.24731700

C	0.75928300	-2.73098200	0.12303100
O	-0.34727700	0.64026300	0.86546400
H	-4.61302700	-0.77008600	-2.80234400
H	-4.02541600	-2.54139000	0.84889900
C	-3.99077800	-1.53247500	0.43400700
H	-1.73593900	-3.43325900	1.61336500
C	-2.86796000	-0.68217300	-1.52362900
H	-5.51614400	-0.37520900	-0.60849200
C	-3.07937100	0.86977100	-1.44029300
C	-1.54029900	-2.35147800	1.69274400
C	-1.52708200	-1.77659800	0.29528100
C	-0.23785200	-1.67219200	-0.37589200
C	-4.16457600	-1.34555800	-1.99343700
N	-2.65705400	-1.31873000	-0.20293400
C	-0.20134100	-2.09194800	2.40179200
H	-0.33962700	-1.74233000	-1.46102900
H	-2.01704100	-0.87912400	-2.17772600
H	-5.77525700	-2.12028800	-0.69595100
C	-5.01185000	-1.33930000	-0.70859400
H	-3.96279000	-2.36653100	-2.33426500
C	1.75376900	0.12035400	-0.19186000
H	-2.35780900	-1.92305900	2.27630200
H	0.39540400	-3.71870300	-0.19165800
H	1.89419700	-2.19259500	1.90652700
H	-0.12913200	0.41305900	-1.15945600
H	1.12469700	-3.76773400	1.98907000
H	-0.26456400	-2.46333600	3.42955300
H	-0.07382000	-1.00610700	2.43767500
C	0.97810500	-2.73401700	1.65507200
C	4.52634500	0.31779800	-0.21862500

C 2.48131300 -0.21225900 -1.34497900

C 2.44329200 0.57616500 0.93919100

C 3.83121800 0.67452100 0.93667400

C 3.86868000 -0.12065900 -1.36855100

H 1.95478500 -0.53721900 -2.23917000

H 1.85477100 0.87362500 1.80003700

H 4.38242300 1.02713000 1.79956800

H 4.44697200 -0.37221400 -2.24859100

N 5.99111200 0.41587000 -0.23148500

O 6.57994700 0.09387800 -1.26521000

O 6.55033500 0.81117700 0.79254800

N -2.48543000 1.52100300 -0.42838900

C -2.58654800 2.97778100 -0.34943700

H -1.69114600 3.32366200 0.17731200

H -2.57205200 3.39341200 -1.36290100

C -3.84947900 3.45313100 0.38037700

H -3.87447600 3.00166000 1.38039600

H -4.72442600 3.07866200 -0.16323800

C -3.91647900 4.97853100 0.49274100

H -3.91979700 5.44936700 -0.49662600

H -4.82341900 5.29894800 1.01496600

H -3.05731900 5.37533100 1.04563600

Sum of electronic and thermal Enthalpies= -1282.256100

Sum of electronic and thermal Free Energies= -1282.339713

TS_{b4}

H -0.95756900 -0.40204900 -0.42539500

O -2.37882100 -1.02279300 2.42396500

C 1.02641300 0.90053300 -1.26263800

H 2.76169000 2.74260600 0.09441500

H -3.38760400 1.84709300 -0.83320500

C 1.75332400 3.16796700 0.09494200

O -0.03623800 0.17708900 -1.52832800

H -3.16377800 1.01944700 3.22667900

H -3.16914500 3.40251100 -0.00446100

C -3.09828900 2.31912700 0.10857200

H 3.23200900 -2.66564800 0.87378200

C -1.66894900 1.12960900 1.66909600

H -4.36697100 0.86513800 1.12233900

C -1.88735800 -0.40833000 1.47293300

C 3.30154700 -1.76655300 0.27427000

C -0.63741300 2.45059500 -0.20367400

C 0.73497500 2.00979300 0.04386900

C -2.86623200 1.70417400 2.43375300

N -1.68106800 1.95554300 0.42606600

H 3.66122000 1.41624300 -1.91542900

H 0.81782100 1.39049900 0.93727600

H -0.72321900 1.27820700 2.19198300

H -4.71688700 2.54103900 1.56264000

C -3.91459600 1.84018400 1.32105900

H -2.61223000 2.67984300 2.86232300

H 1.31893300 1.61123700 -2.07051600

C 4.55504300 -1.32584300 -0.15458500

H 1.64695300 3.69746400 1.05185900

C 2.17654200 -1.03765900 -0.09112800

C 2.28900700 0.12936000 -0.86172600

C -0.81617900 3.42086500 -1.34067800

H 1.18922000 -1.37074500 0.20838600

C 1.59601900 4.17286300 -1.05473100

H 5.69187000 0.11448900 -1.26301400

C 3.56224300 0.53579200 -1.28579400

C 4.70301400 -0.18370600 -0.93803300

H -0.58357700 2.85272400 -2.25185600

C 0.14106200 4.62529300 -1.20397400

H -1.84491900 3.76427800 -1.44260800

H 1.92844500 3.72108100 -1.99624200

H -0.15624800 5.22145700 -0.33095800

H 0.02116600 5.27202100 -2.07955900

H 2.24323000 5.03938300 -0.87925500

N -1.51922600 -0.94102600 0.30396000

N 5.75004600 -2.09049200 0.22247500

O 6.84386700 -1.67870200 -0.16875200

O 5.59330300 -3.09950600 0.91170400

C -1.66524500 -2.37740300 0.07992000

H -1.42052400 -2.91299700 1.00417300

H -0.93091500 -2.65215600 -0.68464600

C -3.07439600 -2.77359200 -0.38098400

H -3.32406700 -2.20631600 -1.28636700

H -3.78848300 -2.47483000 0.39484300

C -3.19534900 -4.27547800 -0.65282900

H -4.20569000 -4.53927900 -0.98088000

H -2.49816800 -4.59628400 -1.43535300

H -2.97576200 -4.86074000 0.24708300

Sum of electronic and thermal Enthalpies= -1282.260190

Sum of electronic and thermal Free Energies= -1282.342473

TS_{c1}

C -0.96787300 -0.55631500 0.34706500

H 3.53095900 -2.93953200 -2.15353400

C 3.28176600 -0.98440000 0.59819700

H 1.01562300 -2.53556700 -1.14882400

H 2.10349800 -3.67937800 -0.33398000

C 3.13629700 -2.14663000 -1.51536000

C 4.16099200 -1.64044100 -0.49284900

H 3.76227100 -1.06387600 1.57802400

C 3.01381000 0.51560600 0.33690400

H 2.80421200 -1.32897800 -2.16350900

C 1.97583000 -2.63474300 -0.64485200

H 4.89111900 -0.94676700 -0.91410000

H 4.70947700 -2.47695500 -0.04951100

O 1.88797400 0.96018500 0.02308800

N 4.06379300 1.31655800 0.48251100

H 4.99509100 0.98996500 0.75198800

C 1.14641500 -1.82883200 1.57985300

C 1.48948700 -1.10333700 2.86654700

H 1.79369200 -0.07399900 2.64611000

H 2.37041000 -1.59534200 3.30329700

C -0.07255400 -2.48614300 1.44335400

H -0.24033000 -3.06236500 0.54077300

C -2.55305000 -1.72614900 -1.18274500

C -2.28711100 -1.10116500 0.05207400

C -3.32136100 -0.95121100 0.99515100

C -4.59891600 -1.43020700 0.72162100

C -4.82390000 -2.05596600 -0.50035500

C -3.82333100 -2.20784400 -1.46182100

H -1.76220600 -1.81658900 -1.91864000

H -3.13374000 -0.43396500 1.93090800

H -5.41507500 -1.32306700 1.42476900

H -4.05944600 -2.69127700 -2.40139500

N 2.03770200 -1.76382300 0.55870500

H -0.85391700 0.03920200 1.25208100

N	-6.17890500	-2.57219100	-0.79595200
O	-6.34639200	-3.11459100	-1.88438900
O	-7.03670200	-2.42338200	0.06948100
C	-0.92291900	-2.87315500	2.63444500
H	-1.92332400	-2.42710800	2.54383400
H	-1.09572400	-3.95534500	2.59623400
C	-0.29722300	-2.48703000	3.98263800
H	0.46773300	-3.22278200	4.26132700
H	-1.05652000	-2.51194600	4.76964600
C	0.34758500	-1.10336800	3.89376100
H	-0.40877300	-0.35792700	3.61387900
H	0.74379600	-0.78744200	4.86323700
C	4.03806300	2.75137700	0.25965600
H	3.70907100	2.97220900	-0.76141200
H	3.32975000	3.23210000	0.94337000
O	-0.14451500	-0.34852200	-0.63530000
H	0.70958100	0.16120100	-0.34792500
C	5.48219400	3.23726700	0.50988200
O	6.32888600	2.39843000	0.83368700
N	5.74536900	4.55445900	0.36327600
C	4.76993400	5.56852800	-0.01887100
H	4.68921800	6.32924700	0.76561800
H	5.08416000	6.06396700	-0.94422800
H	3.78246400	5.14009600	-0.18093700
C	7.10524300	5.04232800	0.59507300
H	7.49505600	5.51040300	-0.31503600
H	7.10386000	5.78605000	1.39894800
H	7.73813600	4.20299600	0.87429400

Sum of electronic and thermal Enthalpies= -1451.338446

Sum of electronic and thermal Free Energies= -1451.430893

TS_{c2}

C	0.76024900	0.23729600	0.02171100
H	-3.62963500	-1.46877500	3.35623500
H	-3.36087100	0.00367400	2.41963300
H	-4.31733700	-2.70600400	1.34554600
H	-5.08845300	-1.13585500	1.10206600
C	-4.12577200	-1.63642500	1.21751700
C	-3.18624400	-1.44026400	0.00637800
H	0.57159000	-2.00142800	1.53857700
H	0.19152200	0.33505000	0.94340100
C	4.22618400	0.33269800	1.43429200
H	-1.61610100	-2.49974400	2.50404900
N	-1.85641700	-1.66595800	0.58035500
C	2.20760200	0.29584200	0.08701300
C	1.23697100	-3.64978700	-1.46128600
C	4.96038000	0.48193800	0.25809800
O	0.16337300	0.54153900	-1.09140500
C	1.63263000	-2.94196400	-0.15794100
H	2.25423300	0.12203300	2.24654300
H	-3.40087300	-2.17496300	-0.77508200
C	-1.86892300	-1.53169300	2.05428300
C	-3.30373600	-0.03659000	-0.64408000
H	-1.12633600	-0.80431500	2.39636900
H	1.99780900	-3.67315400	0.57338400
H	2.48379200	-2.27272500	-0.34684300
O	-2.33201300	0.73407100	-0.78448400
H	-0.85115500	0.59672400	-0.95993600
H	0.68452300	-4.57009700	-1.23263700
C	-0.95007000	-2.40274400	-1.58336300
H	-1.45246200	-1.56583000	-2.08182000

H 2.48314700 0.51065100 -2.04497700

C -3.29874700 -1.08894100 2.38787500

H 4.74357500 0.29877400 2.38461900

C 0.36091400 -2.73014500 -2.31203500

C -0.76510800 -2.08192500 -0.11542300

C 2.84488800 0.23629200 1.34227900

C 0.49251400 -2.16848200 0.46921600

C 2.97806800 0.44730700 -1.08284700

C 4.36197900 0.54122400 -0.99890500

H -4.58463000 2.39442900 -1.09418800

H -4.27347700 1.64289500 -2.66143100

H 0.89831100 -1.79953700 -2.52792500

H 2.13370400 -3.94981500 -2.01135300

N -4.52005600 0.29432300 -1.06738100

H -5.34213000 -0.30409700 -0.96248500

C -4.84537200 1.54323800 -1.73224500

H -1.63570000 -3.25952500 -1.65423700

H 0.12439300 -3.18812200 -3.27701600

H 4.98179200 0.66407600 -1.87810000

N 6.43483400 0.58223400 0.35011300

O 7.05363100 0.71317900 -0.70153500

O 6.93024700 0.52510300 1.47169500

C -6.36379100 1.48472400 -2.00627800

O -6.98096000 0.47781200 -1.64430500

N -6.94053800 2.53650900 -2.62866500

C -8.37670500 2.50370800 -2.90595500

H -8.87512700 3.33816700 -2.40130100

H -8.55151000 2.59070600 -3.98352800

H -8.78387400 1.56217000 -2.54434900

C -6.24200000 3.73818200 -3.06875600

H -6.33593300 3.85421600 -4.15435400

H -6.67815100 4.62269000 -2.59144400

H -5.18285500 3.70508000 -2.81956600

Sum of electronic and thermal Enthalpies= -1451.332764

Sum of electronic and thermal Free Energies= -1451.425915

TS_{c3}

O -2.49447600 -2.11469900 -0.54745500

H -1.18703000 -1.62076700 -1.11567400

C 0.44357600 -1.45586200 -0.14546500

H 1.31117700 -0.22193300 2.62150500

H -1.73703400 1.16548900 -2.38352800

C 0.73520700 0.63005100 2.24256900

O -0.22065900 -1.33098600 -1.26786100

H -5.25085900 -0.06028800 -0.37051000

H -2.51188000 2.46809800 -1.45586500

C -2.45526100 1.38169100 -1.59043000

C 3.89083700 -0.55970300 -1.36474900

C -3.16734100 0.07318800 0.35217500

H -3.77137400 -0.16243100 -2.35867500

C -3.14568600 -1.46530700 0.29718100

C 4.06754200 -1.61965100 0.83011900

C -0.83120600 0.95348300 0.26485700

C -0.35453300 0.14644800 1.30566100

C -4.39457100 0.61447600 -0.42643200

N -2.02674000 0.73218600 -0.32215000

H -1.06284800 -0.54253400 1.76122300

H -3.18749800 0.38149700 1.40223500

H -4.46004800 1.46631800 -2.45598800

C -3.84596200 0.80114700 -1.84593100

H -4.69447600 1.57558700 0.00282300

C 1.89148600 -1.27557100 -0.19131400

H 2.21839200 -2.24361300 1.71785000

H 0.24262300 1.05965600 3.12722500

H 1.90100200 -0.38094700 -2.15699200

H 0.05000900 -2.15231500 0.59253000

H 4.39458400 -0.12117500 -2.21701500

C 0.06768400 2.02757300 -0.30145600

H 4.70202700 -1.97875100 1.63047800

C 1.67826800 1.67181200 1.62387500

C 4.64515800 -1.01567100 -0.28411500

C 2.68418300 -1.75157300 0.86973600

C 2.50946200 -0.69556100 -1.31709400

H 0.73367700 1.56479600 -1.04420500

C 0.90515000 2.70371300 0.80088900

H -0.51775300 2.77678500 -0.83773000

H 2.41114300 1.17607900 0.97986200

H 0.23884500 3.28370200 1.45141400

H 1.59012600 3.41907400 0.33595400

H 2.24481300 2.16705200 2.41843600

N -3.93052200 -2.06381900 1.19061400

H -4.49075500 -1.56240500 1.88436800

C -4.15212600 -3.49754400 1.25211600

H -4.53328500 -3.86694300 0.29396300

H -3.21160700 -4.02234700 1.45320000

N 6.11672600 -0.86712400 -0.32957600

O 6.75204700 -1.28271300 0.63517700

O 6.59572600 -0.33478400 -1.32663600

C -5.17153900 -3.71345700 2.39188900

O -5.58292500 -2.71942200 2.99853100

N -5.55831700 -4.97805200 2.66953300

C -5.10158100 -6.17009700 1.96478900

H -4.37256300 -5.92980200 1.19300800

H -4.63618700 -6.86793100 2.66961200

H -5.94896200 -6.67783600 1.49054600

C -6.52666000 -5.21067200 3.74159300

H -7.42617700 -5.68713800 3.33757000

H -6.09215500 -5.86915500 4.50107100

H -6.79008200 -4.25627100 4.19185800

Sum of electronic and thermal Enthalpies= -1451.333425

Sum of electronic and thermal Free Energies= -1451.425156

TS_{c4}

H -3.30820400 -0.96667100 1.16651600

O -0.16521300 -0.56174600 1.59792600

C 0.65431700 0.70192800 -1.62172400

H 2.88800400 2.29094500 0.05000100

H -3.02513500 2.41255400 -1.35070500

C 2.06472000 2.98789600 0.24727500

H -3.70327900 0.68364000 2.48195800

H -3.02876000 3.52600000 0.02816700

C -2.93534000 2.47517100 -0.26319700

H 3.41174000 -2.67920300 -0.02592300

C -1.79686900 1.21583300 1.51489600

H -4.13805800 0.68330200 0.00504700

C -1.35564500 -0.26899100 1.45140900

C 3.26414100 -1.80446600 -0.64646700

C -0.43670700 2.69004300 -0.03538700

C 0.78103000 2.21126300 0.38494800

C -3.27497400 1.47276900 1.86116900

N -1.60807400 1.93233900 0.17987000

H 2.90437100 1.35480600 -2.89476600

H 0.80214800 1.32089800 1.01069100

H -1.12209600 1.67528300 2.23958700

H -4.92238900 2.15913100 0.56890200

C -3.96205200 1.64443500 0.49880600

H -3.35178400 2.40453500 2.43038900

H 0.60774100 1.59964700 -2.23763400

C 4.32722400 -1.32375600 -1.41249000

H 2.29699500 3.43388600 1.22542400

C 2.04821700 -1.13890900 -0.69787400

C 1.91298700 0.00508200 -1.51494700

C -0.53495400 3.95169400 -0.86982200

H 1.21354000 -1.45671000 -0.08328800

C 2.00313800 4.08129000 -0.82553800

H 5.08712100 0.13414800 -2.79115300

C 3.01216200 0.47799400 -2.26337500

C 4.22767000 -0.19296700 -2.21997000

H -0.67324400 3.67851800 -1.92858100

C 0.69402600 4.86466600 -0.71616100

H -1.43186400 4.51574700 -0.60056500

H 2.07719100 3.63193500 -1.82558300

H 0.64778100 5.36010800 0.26113600

H 0.64472100 5.65502500 -1.47090700

H 2.86121200 4.75265100 -0.72770300

N -2.31430400 -1.17976900 1.22234400

N 5.62337400 -2.04253900 -1.35828100

O 6.54573100 -1.58176600 -2.02318100

O 5.67652900 -3.04468200 -0.65247600

C -2.06550600 -2.60589000 1.18343100

H -1.54890300 -2.92913700 2.09410300

H -1.42087100 -2.86299400 0.33444700

O -0.45514800 0.08740400 -1.32663400

H -1.14638400 0.73753000 -0.96087600

C -3.44868200 -3.27468000 1.04577000

O -4.44553600 -2.54850300 0.96890300

N -3.50397300 -4.62596400 1.01040500

C -2.35434700 -5.51597900 1.11467600

H -2.44373600 -6.14959800 2.00451600

H -2.30301400 -6.16786300 0.23547100

H -1.41972700 -4.96247300 1.18314900

C -4.80290200 -5.28654200 0.88767800

H -4.81974600 -5.91612600 -0.00836700

H -4.98734200 -5.91885800 1.76293600

H -5.57846000 -4.52728600 0.81650400

Sum of electronic and thermal Enthalpies= -1451.306996

Sum of electronic and thermal Free Energies= -1451.400175

TS_{d1}

C -0.95220300 -0.59593600 0.23989400

H 3.44366700 -3.16881200 -2.23313500

C 3.29944400 -1.09191400 0.43722800

H 0.96363500 -2.68514400 -1.18270200

H 2.05854200 -3.80227100 -0.34043000

C 3.07722200 -2.34203700 -1.62176400

C 4.13719200 -1.80553900 -0.65172600

H 3.80111700 -1.14858800 1.40870900

C 3.05555900 0.40443600 0.12622200

H 2.73885300 -1.54955100 -2.29703200

C 1.93506200 -2.77252000 -0.69891600

H 4.85920500 -1.13842300 -1.12715000

H 4.69156000 -2.62890800 -0.19131700

O	1.93721900	0.84314100	-0.20431100
N	4.12422900	1.19927700	0.25407900
H	5.00187900	0.77677500	0.52815100
C	1.16260600	-1.83170300	1.49391400
C	1.54302900	-1.04905700	2.73549400
H	1.86115800	-0.03787000	2.45777500
H	2.42276600	-1.53616800	3.18034900
C	-0.07575100	-2.46309800	1.40831700
H	-0.26741600	-3.08527900	0.54181900
C	-2.59428100	-1.81184900	-1.19196300
C	-2.29002900	-1.12257100	-0.00111400
C	-3.30254400	-0.89051300	0.94888500
C	-4.59663300	-1.35119900	0.72594100
C	-4.85966400	-2.04165400	-0.45271700
C	-3.88126800	-2.27573700	-1.42033400
H	-1.82037700	-1.96577100	-1.93530000
H	-3.08525300	-0.32398800	1.84904000
H	-5.39666900	-1.18146800	1.43529700
H	-4.14692300	-2.80689500	-2.32564000
N	2.03881700	-1.84426500	0.45807900
H	-0.80972400	0.05174000	1.10382700
N	-6.23242800	-2.53972700	-0.69422100
O	-6.43293600	-3.13995600	-1.74599000
O	-7.06961900	-2.31931900	0.17590600
C	-0.91090400	-2.77421700	2.63285700
H	-1.90233600	-2.30952000	2.54086600
H	-1.10821300	-3.85265300	2.64845900
C	-0.24924500	-2.34036900	3.94874600
H	0.50624500	-3.07862100	4.24610300
H	-0.99227700	-2.31270500	4.75094700

C 0.42126300 -0.97625400 3.78268700

H -0.32469100 -0.22854300 3.48233300

H 0.84312300 -0.62356500 4.72831800

C 4.13598500 2.63974100 -0.04177100

H 3.09989900 2.93080200 -0.22099300

H 4.48314600 3.16652100 0.85435100

C 5.02130900 2.98443900 -1.24393300

H 4.64573900 2.45248000 -2.12602100

H 6.04065000 2.61786300 -1.06392500

C 5.05491300 4.49243300 -1.50998500

H 5.45471000 5.04118800 -0.65085500

H 5.68787500 4.71876000 -2.37163700

H 4.05356900 4.88186500 -1.72088400

O -0.14800500 -0.45576600 -0.77361500

H 0.71457400 0.04742800 -0.53112600

Sum of electronic and thermal Enthalpies= -1282.672844

Sum of electronic and thermal Free Energies= -1282.757312

TS_{d2}

C 0.59295400 0.25994800 0.06701500

H -3.36697400 -1.49394500 3.84668300

H -3.20661900 -0.01953900 2.88697200

H -4.30534800 -2.72038600 1.93297300

H -5.08698000 -1.14119300 1.78900800

C -4.12212900 -1.65188200 1.78473500

C -3.33778600 -1.45478400 0.46680300

H 0.58494100 -1.97724300 1.51553000

H 0.14939700 0.34923200 1.05561800

H -4.84369000 0.86735200 -3.18686300

C 4.21491500 0.35130000 1.02035800

H -1.48085700 -2.53353800 2.74638300

N -1.94768300 -1.68184200 0.87193700

C 2.03785000 0.33625200 -0.05282600

C 0.89928400 -3.54978000 -1.57884800

C 4.78797900 0.55121600 -0.23491400

O -0.13849800 0.61035600 -0.95464200

C 1.44364700 -2.86415900 -0.31761800

H 2.36790800 0.08780700 2.07440600

H -3.64553400 -2.18750400 -0.28514400

C -1.78005000 -1.56036800 2.33846300

C -3.53103800 -0.04161600 -0.14653600

H -0.99843900 -0.83888600 2.59179500

H 1.89335500 -3.60737000 0.35162300

H 2.26470100 -2.18832400 -0.59261800

O -2.58985100 0.76048300 -0.27698000

H -1.11643500 0.66922800 -0.69135600

H 0.38800700 -4.48195900 -1.30649700

C -1.29887500 -2.32959100 -1.40707500

H -1.86437800 -1.48581500 -1.81965500

H 2.03115500 0.63148600 -2.19288100

C -3.15525000 -1.11209700 2.84634700

H 4.85187400 0.29084600 1.89360600

C -0.08273100 -2.62361100 -2.29683600

C -0.94256600 -2.04483300 0.03611500

C 2.83402200 0.24052800 1.10537700

C 0.38389100 -2.10730700 0.45710300

C 2.64766500 0.53917900 -1.30635200

C 4.03009600 0.64797600 -1.39993000

H -5.98007700 1.96647000 -0.55603800

H -4.31871200 2.17710600 -1.11988200

H 0.41443300 -1.68183800 -2.55577200

H 1.72570200 -3.82665400 -2.23983000

N -4.78253200 0.25532800 -0.51941600

H -5.49863800 -0.44787100 -0.39308800

C -5.18522900 1.51542000 -1.16076500

H -1.98113500 -3.19190500 -1.41772300

H -6.44168200 2.46613100 -4.27190200

C -5.65878500 1.31263000 -2.60399200

H -0.43038000 -3.06429500 -3.23584800

H -6.94128500 3.07799200 -2.69207100

C -6.10861400 2.62950400 -3.24389900

H -6.48701800 0.59181300 -2.61903200

H 4.52881800 0.81052100 -2.34713000

H -5.29203300 3.35843100 -3.26980900

N 6.26111500 0.66706700 -0.33216000

O 6.73630800 0.83826400 -1.45052700

O 6.89888400 0.58108000 0.71302700

Sum of electronic and thermal Enthalpies= -1282.667127

Sum of electronic and thermal Free Energies= -1282.753825

TS_{d3}

O -2.33109800 -2.06545400 -0.64103300

H -1.04168600 -1.51427400 -1.25301600

C 0.60465100 -1.32663100 -0.31945000

H 1.51960600 -0.17956800 2.45177200

H -1.73772500 1.28142600 -2.39057200

C 0.90072700 0.66281400 2.12277600

O -0.09658600 -1.18662600 -1.42084700

H -5.14244800 -0.14068800 -0.32688300

H -2.53114400 2.52666900 -1.40154600

C -2.44032900 1.44772200 -1.57200400

C 3.97846000 -0.27222700 -1.61867400

C -3.04733400 0.05669000 0.34981000

H -3.72057200 -0.12034700 -2.35273700

C -2.96911900 -1.47879100 0.25192800

C 4.26581100 -1.41568800 0.52170600

C -0.74187900 1.00895600 0.21219200

C -0.19741900 0.17258300 1.19744800

C -4.31614700 0.57105100 -0.38011400

N -1.95163500 0.77504400 -0.33757800

H -0.86803800 -0.55574100 1.64930900

H -3.04569700 0.34064600 1.40760700

H -4.47168600 1.48330200 -2.37736700

C -3.81536800 0.82309900 -1.80729600

H -4.64368800 1.50549000 0.08630700

C 2.04496700 -1.09831900 -0.40803000

H 2.46966200 -2.13506400 1.44514400

H 0.41777300 1.03862300 3.03674000

H 1.95752300 -0.12575300 -2.33460000

H 0.26339500 -2.07380100 0.39476600

H 4.43785600 0.21609300 -2.46893900

C 0.09994900 2.13503300 -0.33924300

H 4.93923000 -1.78803500 1.28327000

C 1.78419600 1.76441500 1.51993100

C 4.78437500 -0.74787900 -0.58496300

C 2.88920600 -1.59259500 0.60361300

C 2.60431800 -0.45380700 -1.52916800

H 0.75769200 1.72598400 -1.11985700

C 0.94765400 2.79775300 0.76389900

H -0.52810300 2.88263800 -0.82742900

H 2.51524100 1.32379300 0.83523500

H 0.28180800 3.32547700 1.45788500

H 1.59018800 3.55668000 0.30770300

H 2.35568700 2.24905000 2.31744100

N -3.69352200 -2.13686500 1.16828300

H -4.19260400 -1.59638600 1.86302600

C -3.83129400 -3.59893800 1.23008300

H -4.88951900 -3.85122000 1.09592100

H -3.28334300 -4.00128100 0.37658900

C -3.30642000 -4.17518000 2.54905500

H -2.24606000 -3.91462900 2.65438000

H -3.83065900 -3.70098500 3.38947800

C -3.48773500 -5.69430500 2.61984500

H -2.95052700 -6.19832400 1.80981700

H -3.10681700 -6.08580800 3.56647500

H -4.54379000 -5.97378500 2.54623000

N 6.24849600 -0.55055800 -0.67483500

O 6.93024800 -0.98724200 0.24781500

O 6.67428700 0.04005700 -1.66306300

Sum of electronic and thermal Enthalpies= -1282.667719

Sum of electronic and thermal Free Energies= -1282.752309

TS_{d4}

H -3.62365000 -0.81551300 0.52061500

O -0.55111100 -0.66378500 1.25650100

C 0.71311000 0.80142400 -1.68246500

H 2.80552300 2.07358300 0.32816200

H -2.90404200 2.75042900 -1.64859100

C 2.00151700 2.79769400 0.50505000

H -4.10881300 0.71101300 1.89531000

H -2.99815600 3.71958000 -0.16825300

C -2.93221800 2.69836800 -0.55727300

H 3.02974000 -2.93998500 -0.19505300

C -2.07870100 1.19359500 1.18809800

H -4.25145000 0.97776900 -0.61495800

C -1.70937200 -0.30674000 1.03410600

C 3.01929500 -1.98777000 -0.71012500

C -0.46761800 2.69656000 -0.06719100

C 0.67139500 2.09274200 0.41905700

C -3.56831600 1.52051400 1.40039400

N -1.70102900 2.02221000 -0.03446200

H 3.14851600 1.43165200 -2.56957100

H 0.56890200 1.15635600 0.96389300

H -1.46668800 1.53571100 2.02514000

H -5.01865500 2.43775100 0.01432200

C -4.08577700 1.87081200 -0.00201400

H -3.65377700 2.39743700 2.04981200

H 0.79218700 1.74603600 -2.21872100

C 4.20196800 -1.49891600 -1.26688400

H 2.13937100 3.12782000 1.54503500

C 1.86250200 -1.23133000 -0.82831200

C 1.90455400 0.00795800 -1.50423000

C -0.39359900 4.03059600 -0.78485300

H 0.93502800 -1.55939100 -0.37364900

C 2.12298800 3.99586000 -0.44344600

H 5.22359200 0.05092600 -2.34276800

C 3.11975300 0.48245200 -2.04326100

C 4.27755800 -0.27642400 -1.93077100

H -0.40835700 3.85896100 -1.87350000

C 0.85258200 4.84541100 -0.39803300

H -1.28701000 4.62426500 -0.57616400

H 2.29227200 3.64791000 -1.47177100

H 0.71631400 5.24399000 0.61452300

H 0.93292100 5.70789100 -1.06617100

H 2.99664000 4.59777800 -0.17705600

N -2.68713800 -1.16119200 0.66661300

N 5.43602400 -2.31207700 -1.14037700

O 6.46351900 -1.84545900 -1.62193600

O 5.33714000 -3.38997700 -0.56331200

C -2.48221500 -2.60781600 0.53436500

H -1.58981500 -2.85617800 1.11313000

H -2.27105600 -2.85143600 -0.51533300

C -3.69705300 -3.39519600 1.02958800

H -4.59004400 -3.07935500 0.47183400

H -3.87843600 -3.14778100 2.08234500

C -3.50514300 -4.90608700 0.86977100

H -4.38412100 -5.44842400 1.22712600

H -3.34839000 -5.18023300 -0.17876400

H -2.64116900 -5.25887800 1.44224100

O -0.45790600 0.22397000 -1.60503100

H -1.15855900 0.87490300 -1.30059000

Sum of electronic and thermal Enthalpies = -1282.640673

Sum of electronic and thermal Free Energies = -1282.726292