Supporting Information

Optically Active Helical Polyacetylene Bearing Ferrocenyl Amino-Acid Derivative in Pendants. Preparation and Application as Chiral Organocatalyst for Asymmetric Aldol Reaction

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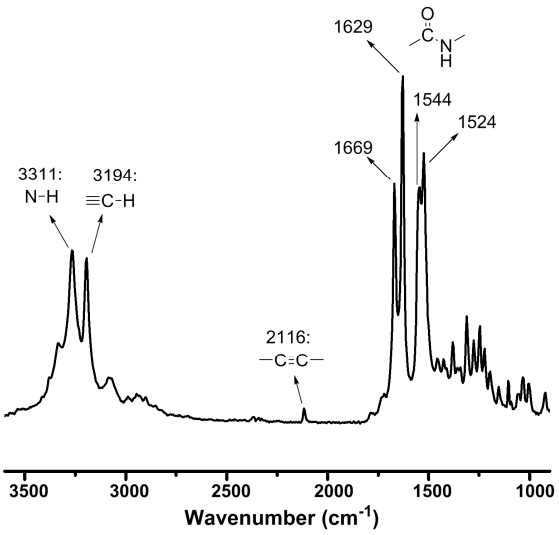

Figure S1. FT-IR spectrum of chiral monomer **L-MAFc** (in KBr tablet).

IR (KBr): 3311 (N-H), 3194 (H-C≡C), 2116 (C≡C), 1669, 1544 (CONH), 1629, 1524 (CONH) cm^{-1}.

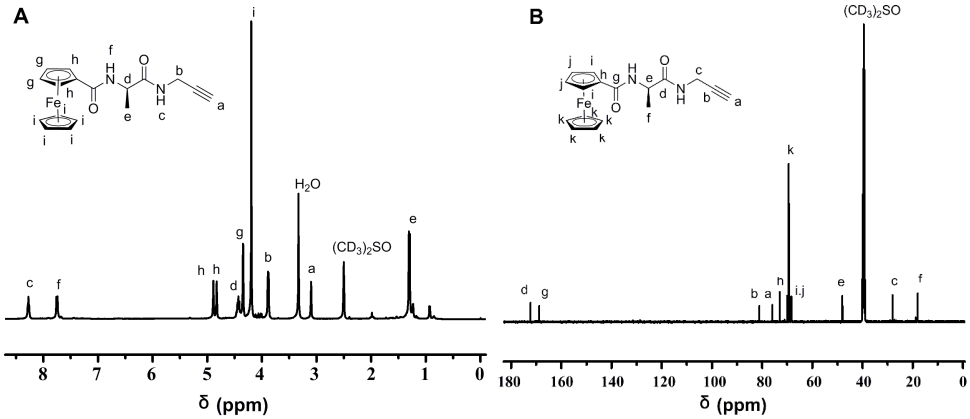

Figure S2. (A) ^{1}H and (B) ^{13}C NMR spectra of **L-MAFc**; measured in DMSO at 25 °C.

^{1}H NMR ([D_6]DMSO) δ=8.28 (d, *J* = 4.9 Hz, 1H; NH), 7.75 (d, *J* = 7.8 Hz, 1H; NH), 4.89 (s, 1H; H-2, Fc), 4.83 (s, 1H; H-5, Fc), 4.43 (dt, *J* = 14.7, 7.2 Hz, 1H; CH), 4.34 (s, 2H; H-3, H-4, Fc), 4.19 (s, 5H, $Cp_{unsubst.}$), 3.88 (dd, *J* = 5.2, 2.2 Hz, 2H; CHCC*H*$_2$-), 3.10 (s, 1H; C*H*CCH$_2$-), 1.30 (d, *J* = 7.2 Hz, 3H; CH_3-). ^{13}C NMR ([D_6]DMSO) δ=172.3 (CONH), 168.8 (COFc), 81.1 (CH*C*-), 75.9 (*C*HC-), 73.0 (C-1, Fc), 69.9 ($Cp_{unsubst.}$), 69.4 (C-2, C-5, Fc), 68.3 (C-3, C-4, Fc), 48.0 (CH_3*C*H), 28.02 (CHC*C*H$_2$-), 18.0 (*C*H_3CH).

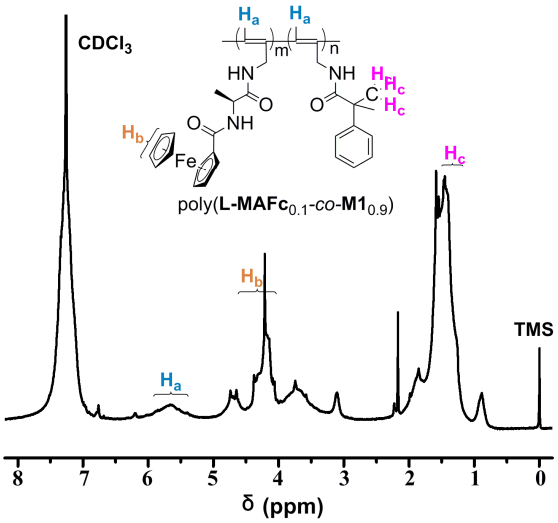

Figure S3. ^{1}H NMR spectrum of poly(**L-MAFc**$_{0.1}$-*co*-**M1**$_{0.9}$); measured in $CDCl_3$ at 25 °C.

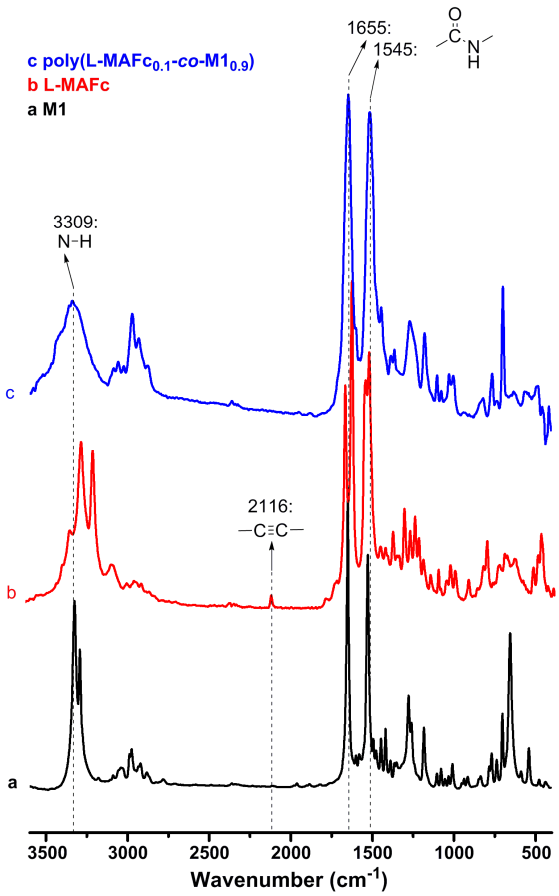

Figure S4. Typical FT-IR spectra of (a) **M1**, (b) **L-MAFc** and (c) poly(**L-MAFc**$_{0.1}$-*co*-**M1**$_{0.9}$) (in KBr tablet).

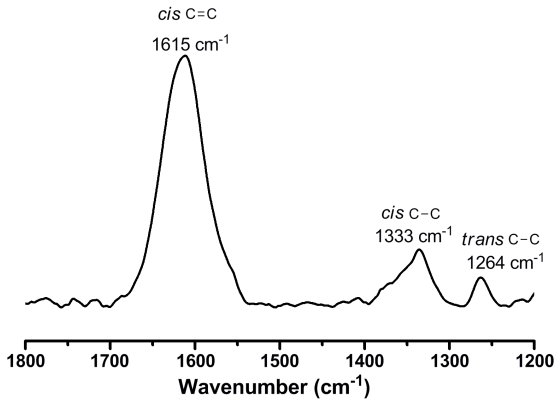

Figure S5. Typical Raman spectrum of poly(**L-MAFc**$_{0.1}$-*co*-**M1**$_{0.9}$).

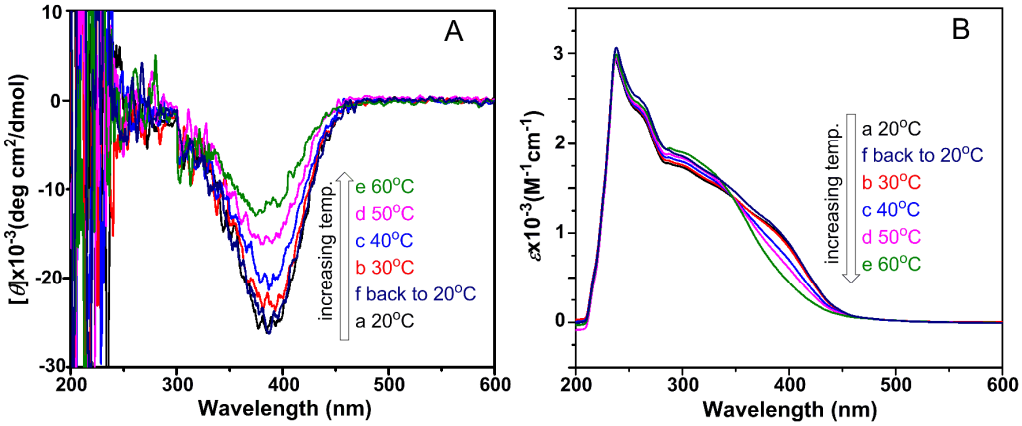

Figure S6. (A) CD and (B) UV-vis spectra of poly(**D-MAFc**$_{0.1}$-*co*-**M1**$_{0.9}$) at increasing temperatures (from 20 to 60 ^{o}C) in THF (c = 1 x 10^{-3} mol/L).

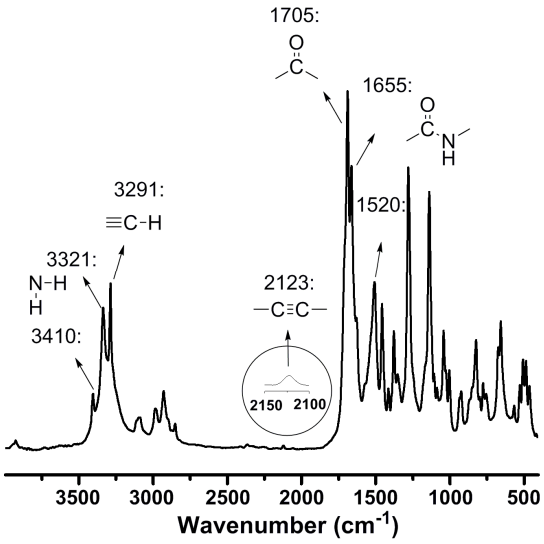

Figure S7. FT-IR spectrum of chiral monomer **L-MTFc** (in KBr tablet).

IR (KBr): 3410 (N-H free), 3321 (N-H assoc.), 3291 (H-C≡C), 2123 (C≡C), 1705 (C=O), 1655, 1520 (CONH) cm^{-1}.

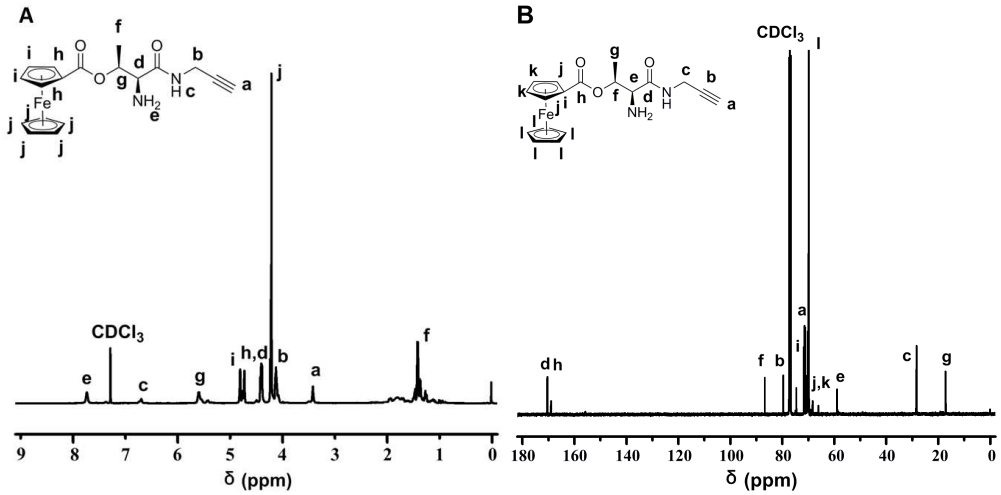

Figure S8. (A) ^{1}H and (B) ^{13}C NMR spectra of **L-MTFc**; measured in $CDCl_3$ at 25 °C.

^{1}H NMR ($CDCl_3$) δ=7.74 (s, 2H; NH_2), 6.70 (s, 1H; CONH), 5.58 (t, *J* = 11.3 Hz, 1H; CH_3CH-), 4.81 (s, 2H; H-2, H-5, Fc), 4.73 (s, 2H; H-3, H-4, Fc), 4.41 (dt, *J* = 7.2, 3.8 Hz, 1H; CH), 4.21 (s, 5H; $Cp_{unsubst.}$), 4.10 (dd, *J* = 5.2, 2.2 Hz, 2H; $CHCC\underline{H_2}$-), 3.42 (s, 1H; $C\underline{H}CCH_2$-), 1.14 (d, *J* = 6.1 Hz, 3H; CH_3-). ^{13}C NMR ($CDCl_3$) δ=173.1 (CONH), 170.4 (COFc), 87.1 ($CHCH_3$), 79.61 ($CHCCH_2$-), 76.9 (C-1, Fc),), 72.1 (CHC-), 70.2 (C-2, C-5, Fc), 69.9 ($Cp_{unsubst.}$), 68.3 (C-3, C-4, Fc), 60.0 (CH), 29.4 ($CHCCH_2$-), 17.2 (CH_3-).

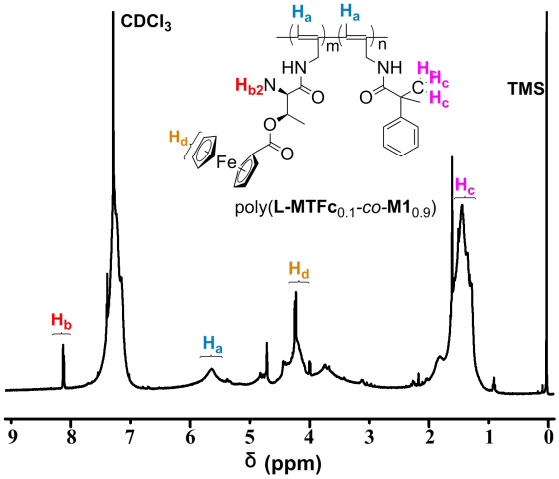

Figure S9. ^{1}H NMR spectrum of poly(**L-MTFc**$_{0.1}$-*co*-**M1**$_{0.9}$); measured in $CDCl_3$ at 25 °C.

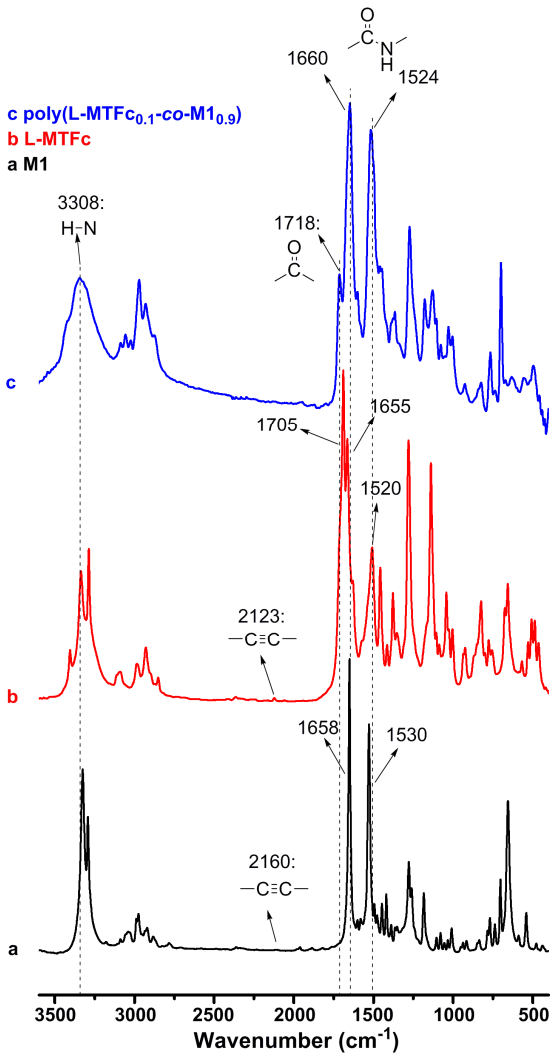

Figure S10. Typical FT-IR spectra of (a) **M1**, (b) **L-MTFc** and (c) poly(**L-MTFc**$_{0.1}$-*co*-**M1**$_{0.9}$) (in KBr tablet).

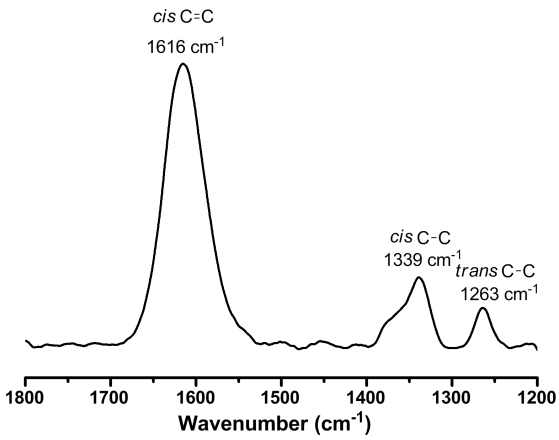

Figure S11. Raman spectrum of poly(**L-MTFc**$_{0.1}$-*co*-**M1**$_{0.9}$).

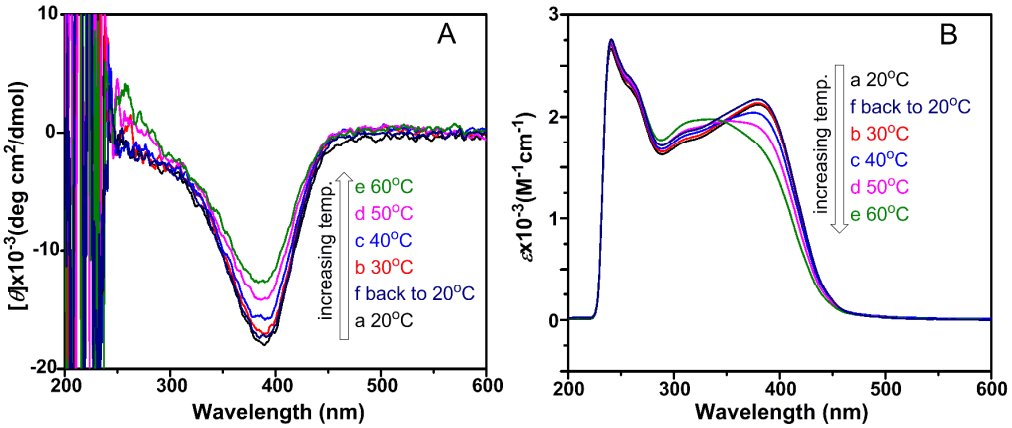

Figure S12. (A) CD and (B) UV-vis spectra of poly(**D-MTFc**$_{0.1}$-*co*-**M1**$_{0.9}$) at increasing temperatures (from 20 to 60 °C) in THF (c = 1 x 10^{-3} mol/L).

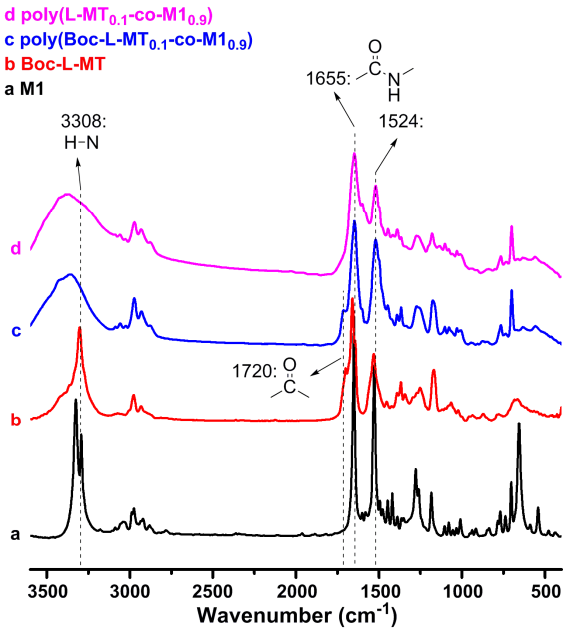

Figure S13. Typical FT-IR spectra of (a) **M1**, (b) **Boc-L-MT** and (c) poly(**Boc-L-MT**$_{0.1}$-*co*-**M1**$_{0.9}$) (d) poly(**L-MT**$_{0.1}$-*co*-**M1**$_{0.9}$) (in KBr tablet).

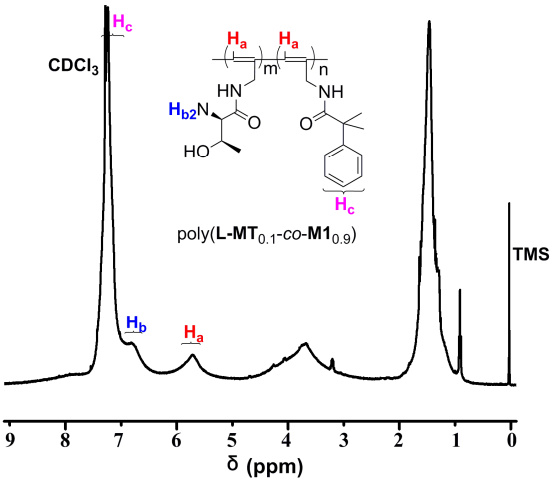

Figure S14. ^{1}H NMR spectrum of poly(**L-MT**$_{0.1}$-*co*-**M1**$_{0.9}$); measured in $CDCl_3$ at 25 °C.

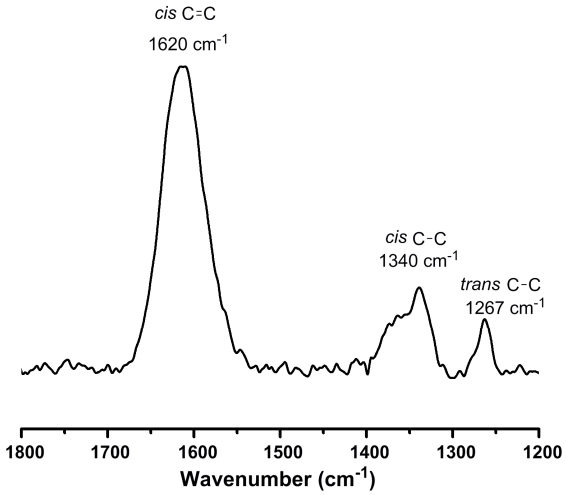

Figure S15. Raman spectrum of poly(**L-MT**$_{0.1}$-*co*-**M1**$_{0.9}$).

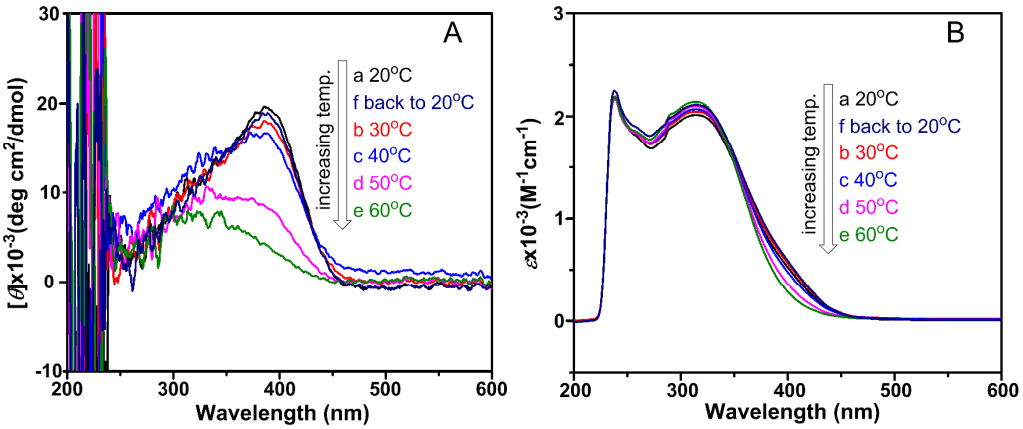

Figure S16. (A) CD and (B) UV-vis spectra of poly(**L-MT**$_{0.1}$-*co*-**M1**$_{0.9}$) at increasing temperatures (from 20 to 60 °C) in THF (c = 1 x 10^{-3} mol/L).

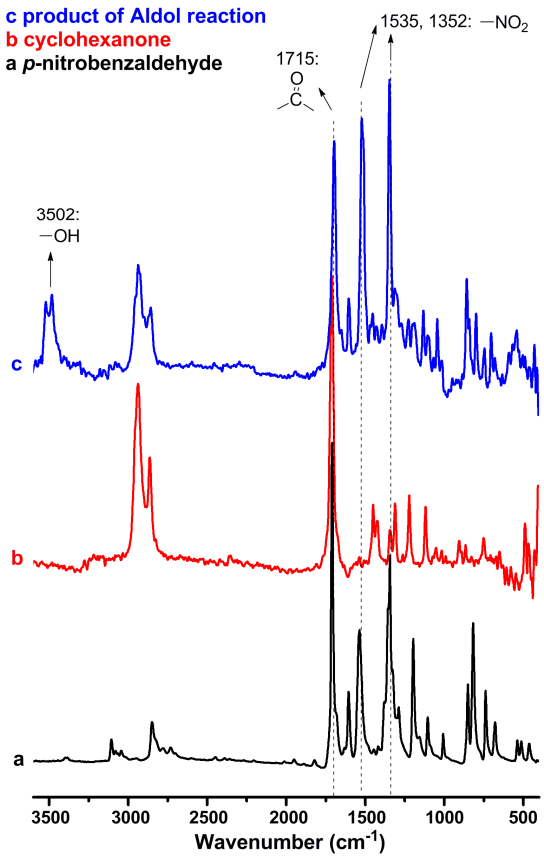

Figure S17. FT-IR spectra of the Aldol reaction product (in KBr tablet).

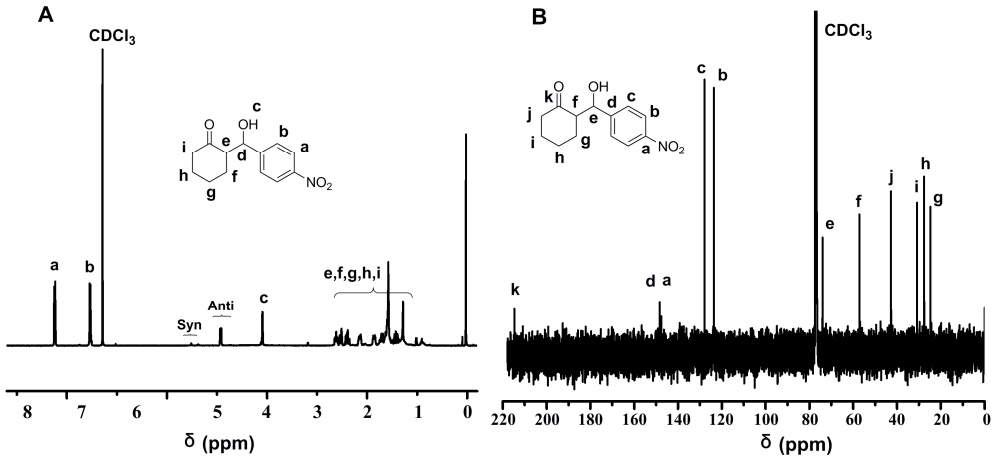

Figure S18. (A) ^{1}H and (B) ^{13}C NMR spectra of the Aldol reaction product; measured in $CDCl_3$ at 25 °C.

(2*S*, 1'*R*)-2-(hydroxyl-(p-nitrophenyl) methyl) cyclohexan-1-one: ^{1}H NMR ($CDCl_3$), δ (ppm): 8.20–8.21 (d, 2H, J = 8.6), 7.50–7.51(d, 2H, J = 8.6), 4.89–4.91(dd, 1H, J = 8.3, J = 3.2), 4.05–4.06 (d, 1H, J = 3.2), 2.57–2.61 (m, 1H), 2.48–2.52 (m, 1H),. 2.34–2.39 (m, 1H), 2.09–2.14 (m, 1H), 1.82–1.84 (m, 1H), 1.63–1.71(m, 1H), 1.52–1.61(m, 2H), 1.35–1.42 (m, 1H). ^{13}C NMR ($CDCl_3$), δ (ppm): 214.8, 148.4, 147.6, 127.9, 123.6, 74.0, 57.2, 42.7, 30.8, 27.7, 24.7.

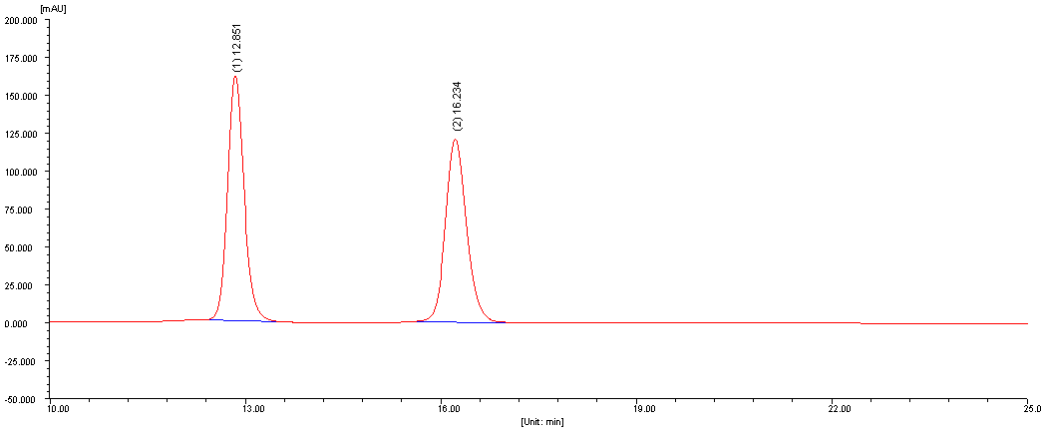

Figure S19. Typical HPLC spectrum of the racemic Aldol reaction product.

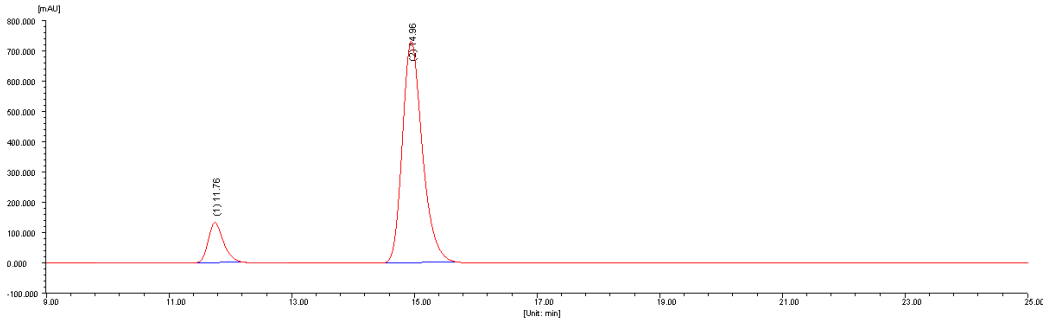

Figure S20. Typical HPLC spectrum of the Aldol reaction product catalyzed by poly(**L-MT**$_{0.1}$-*co*-**M1**$_{0.9}$).

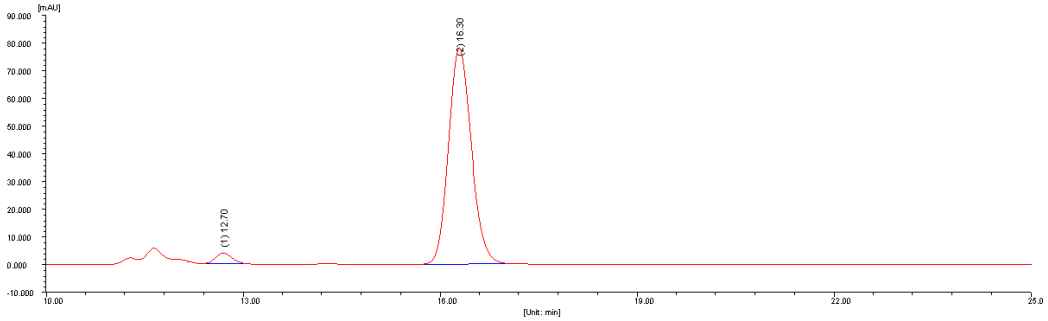

Figure S21. Typical HPLC spectrum of the Aldol reaction product catalyzed by poly(**L-MTFc**$_{0.1}$-*co*-**M1**$_{0.9}$) in the presence of PhCOOH (0.1 equiv.) and H_2O (10 equiv.).

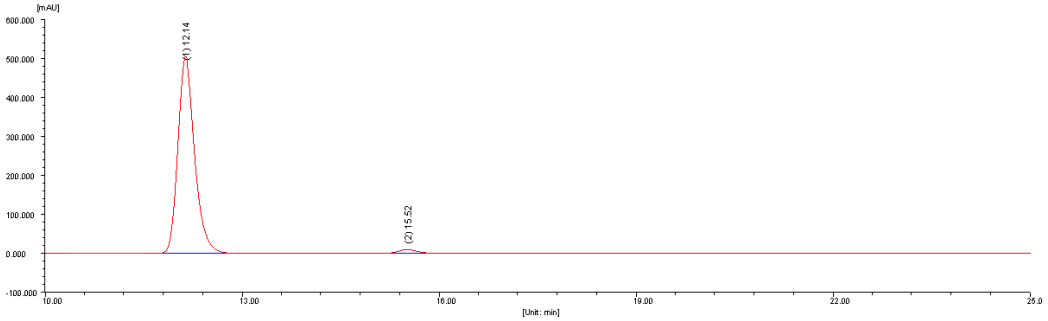

Figure S22. Typical HPLC spectrum of the Aldol reaction product catalyzed by poly(**D-MTFc**$_{0.1}$-*co*-**M1**$_{0.9}$) in the presence of PhCOOH (0.1 equiv.) and H_2O (10 equiv.).