Supporting Information

Ruthenium-complex-catalysed De-ammonification Polycondensation of Aromatic Diamines

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Contents

Synthesis of monomers.

Synthesis of APM-d_4. APM (0.70 g, 3.5 mmol) was stirred vigorously in a mixture of CH_2Cl_2 (10 mL) and D_2O (2 mL). The solvents were removed under vacuum, and the resulting solid was dried under vacuum to yield APM-d_4 as a white powder (0.65 g, 91%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.96 (d, J = 6.8 Hz, 4H), 6.62 (d, J = 6.8 Hz, 4H), 3.77 (s, 2H), 3.53 (s, 0.13H). ^{2}H NMR (400 MHz, $CHCl_3$): δ 3.55.

OTL-d_4 and BAS-d_4 were synthesized using the same method as for the synthesis of APM-d_4.

Data of **OTL-d_4.** ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.22 (d, J = 8.0 Hz, 4H), 6.71 (d, J = 8.0 Hz, 4H), 3.57 (s, 0.26H). ^{2}H NMR (400 MHz, $CHCl_3$): δ 3.61.

Data of **BAS-d_4.** ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.67 (d, J = 6.0 Hz, 4H), 6.64 (d, J = 7.5 Hz, 4H), 4.04 (s, 0.20H). ^{2}H NMR (400 MHz, $CHCl_3$): δ 4.11.

^{1}H NMR data of the polymers.

^{1}H NMR data of **poly(OTL)**. δ 6.68-7.32 (8H), 6.24 (0.22H), 5.03 (0.97H), 2.12 (6H).

^{1}H NMR data of **poly(OTL-*d*$_4$)**. δ 6.66-7.29 (8H), 6.21 (0.20H), 5.02 (0.78H), 2.09 (6H).

^{1}H NMR data of **poly(MTL)**. δ 6.43-7.37 (8H), 6.18 (0.17H), 4.02 (0.50H), 1.89 (6H).

^{1}H NMR data of **poly(TMB)**. δ 6.74-7.15 (4H), 6.24 (0.15H), 4.69 (0.58H), 2.13 (12H).

^{1}H NMR data of **poly(APM)**. δ 6.43-7.27 (8H), 6.23 (0.19H), 4.84 (0.55H), 3.74 (2H).

^{1}H NMR data of **poly(APM)'**. δ 6.45-7.23 (8H), 4.82 (0.60H), 3.78 (2H).

^{1}H NMR data of **poly(APM-*d*$_4$)**. δ 6.46-7.43 (8H), 6.23 (0.19H), 4.86 (0.55H), 3.76 (2H).

^{1}H NMR data of **poly(AMM)**. δ 6.49-7.07 (8H), 6.17 (0.36H), 4.62 (0.61H), 3.69 (1.7H), 1.98 (6.0H).

^{1}H NMR data of **poly(APE)**. δ 6.60-7.43 (8H), 6.23 (0.23H), 4.98 (0.47H).

^{1}H NMR data of **poly(BAS)**. δ 6.57-7.43 (8H), 6.30 (0.28H), 5.98-6.17 (1.1H).

^{1}H NMR data of **poly(BAS)'**. δ 6.57-7.56 (8H), 6.18 (1H).

^{1}H NMR data of **poly(BAS-*d*$_4$)**. δ 6.57-7.43 (8H), 6.30 (0.26H), 5.97-6.12 (1H).

^{1}H NMR data of **poly(BAO)**. δ 6.69-8.12 (8H), 6.34 (0.17H), 5.896 (0.55H).

^{1}H NMR data of **poly(DAB)**. δ 6.59-7.51 (8H), 6.33 (0.31H), 5.87-6.16 (0.62H).

^{1}H NMR data of **poly(APM)-BA**. δ 6.54-7.77 (8H), 4.43-4.51 (2.95H), 2.45 (11H including water), 2.45 (3H), 1.61 (4H).

^{1}H NMR data of **poly(APM)-BS(Na$^+$)**. δ 8.64 (0.64H), 7.03-7.26 (8H), 6.03 (0.81H), 3.75 (0.76H), 2.95 (1.1H), 1.25 (4H), 0.84 (3H).

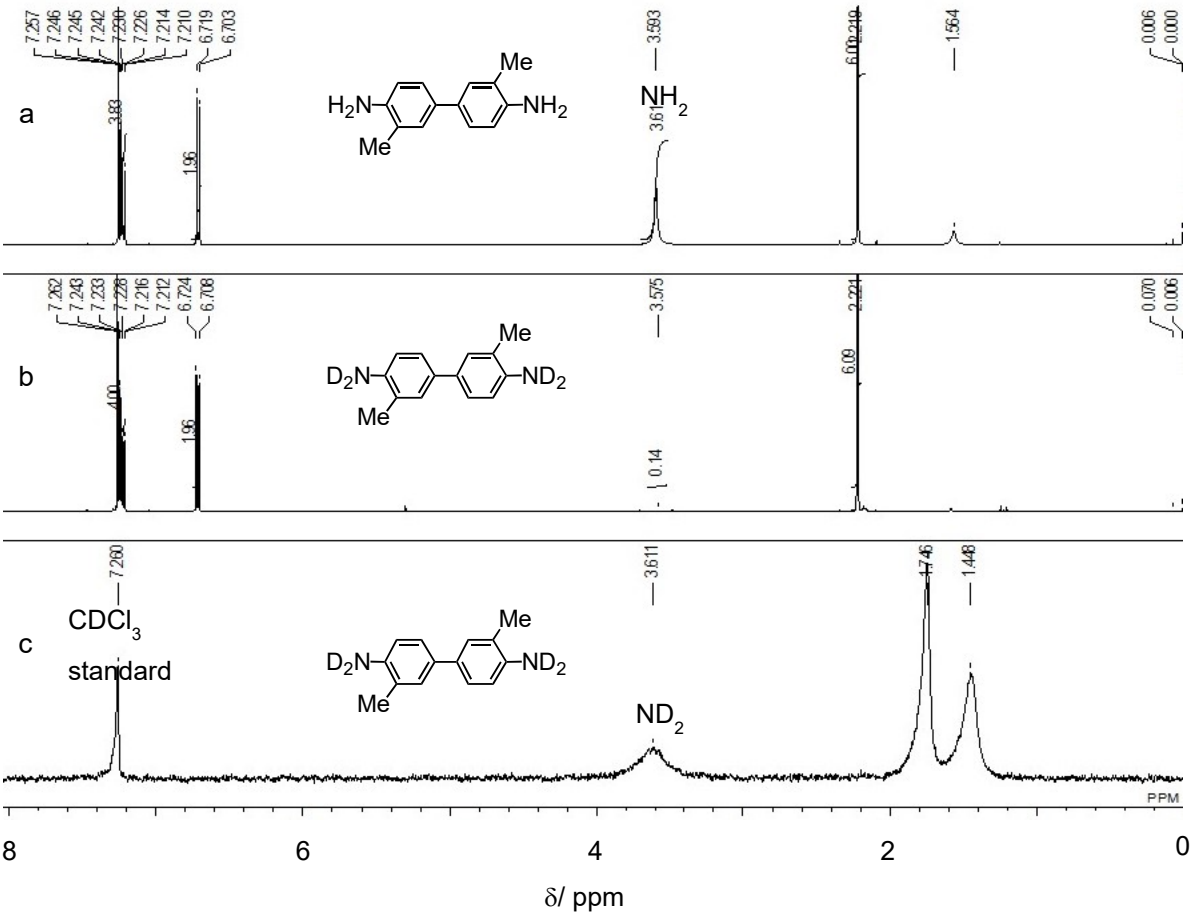

Figure S1a. ^{1}H NMR spectra of (a) OTL and (b) OTL-d_4 in $CDCl_3$ and ^{2}H NMR spectrum of OTL-d_4 in $CHCl_3$.

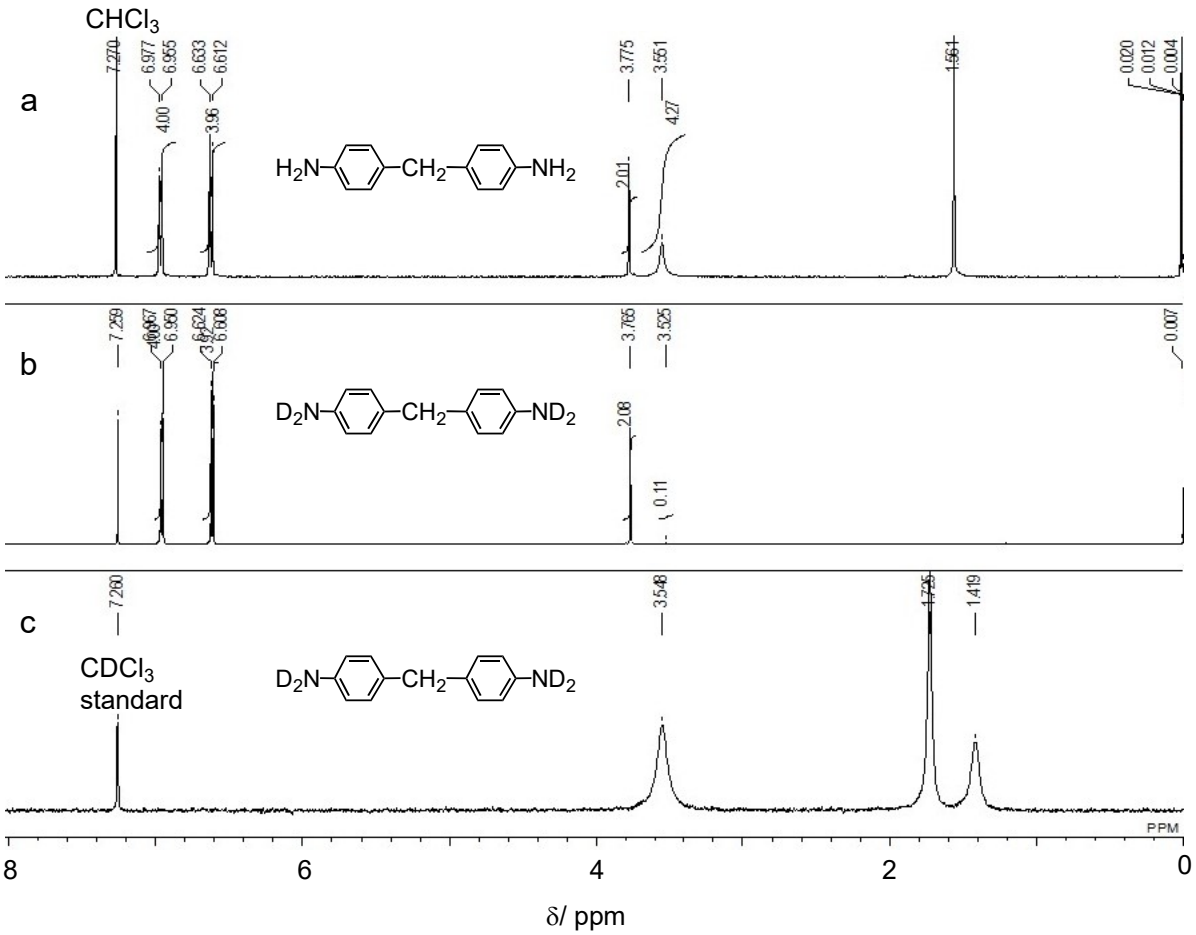

Figure S1b. ^{1}H NMR spectra of (a) APM and (b) APM-d_4 in $CDCl_3$ and ^{2}H NMR spectrum of APM-d_4 in $CHCl_3$.

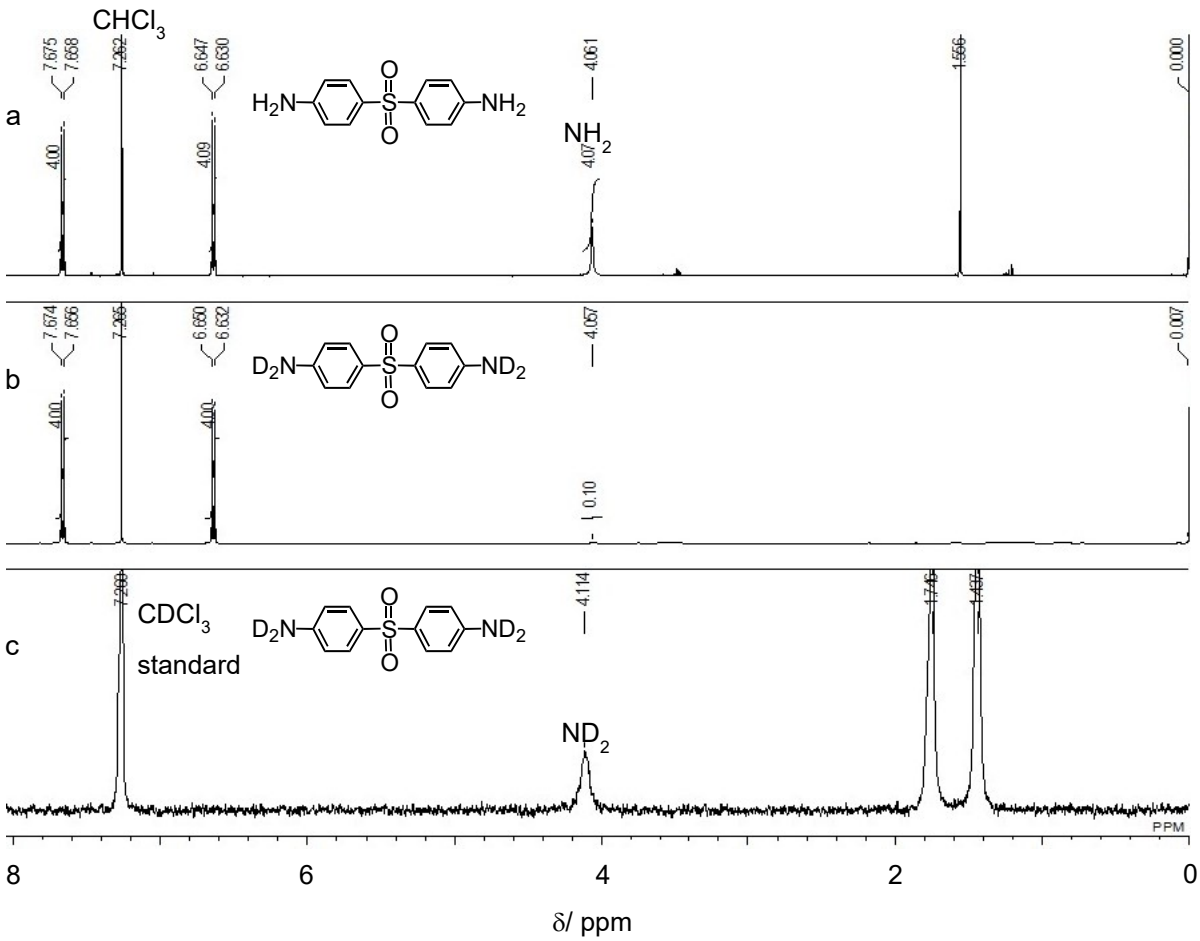

Figure S1c. ^{1}H NMR spectra of (a) BAS and (b) BAS-d_4 in $CDCl_3$ and ^{2}H NMR spectrum of BAS-d_4 in $CHCl_3$.

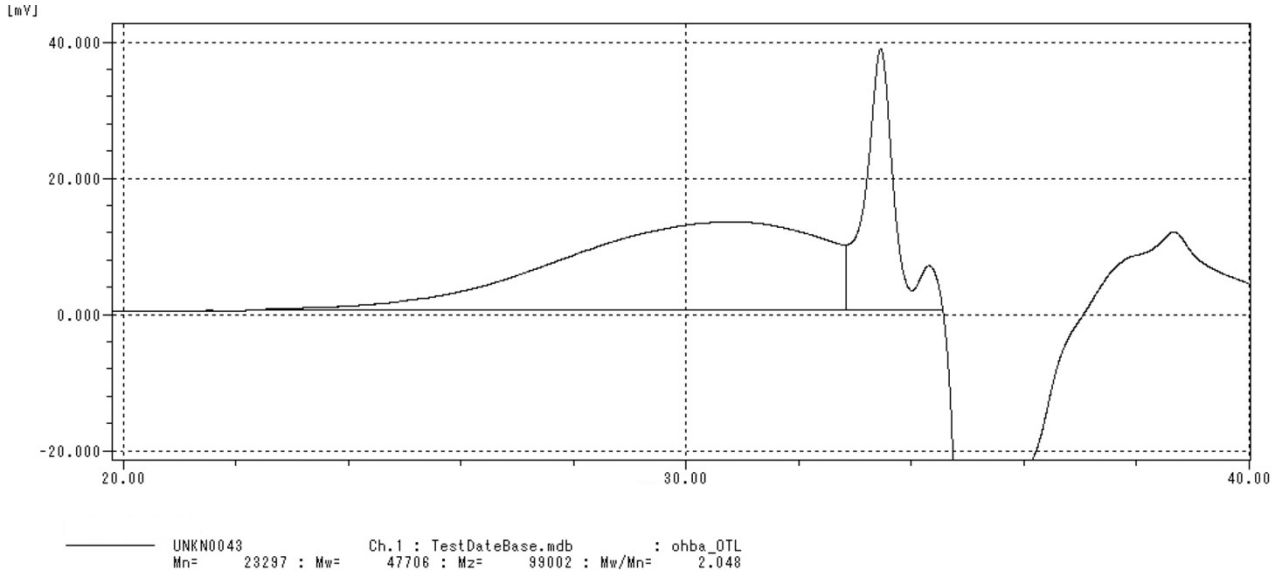

Figure S2a. GPC curve of **poly(OTL)**.

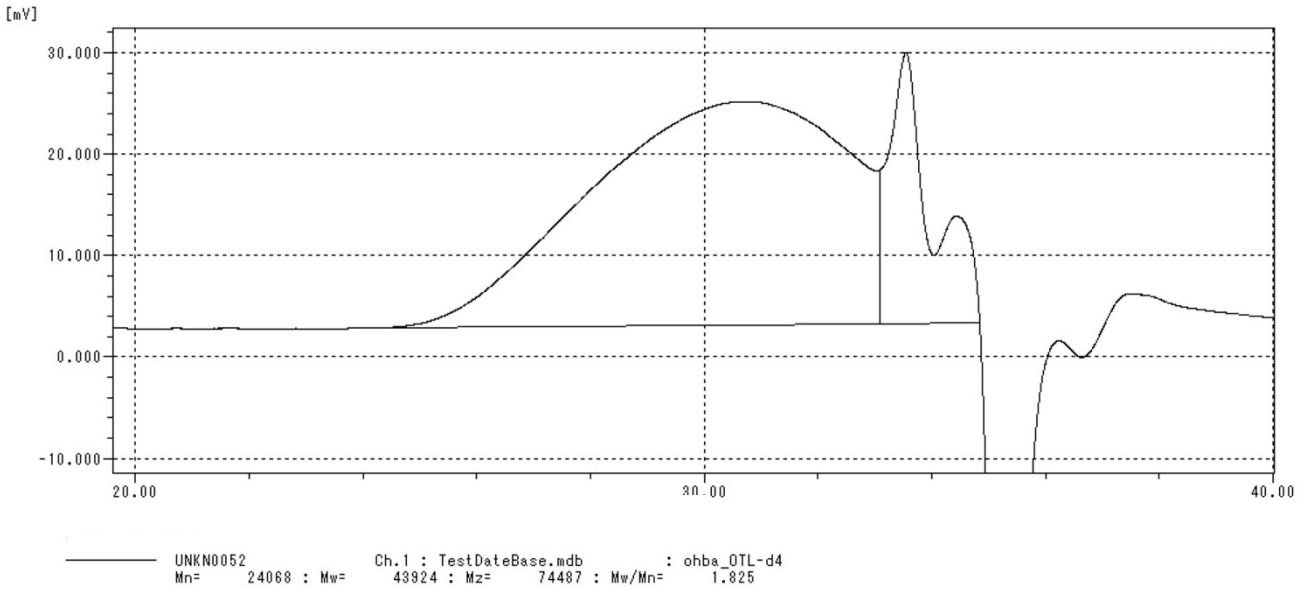

Figure S2b. GPC curve of **poly(OTL-d_4)**.

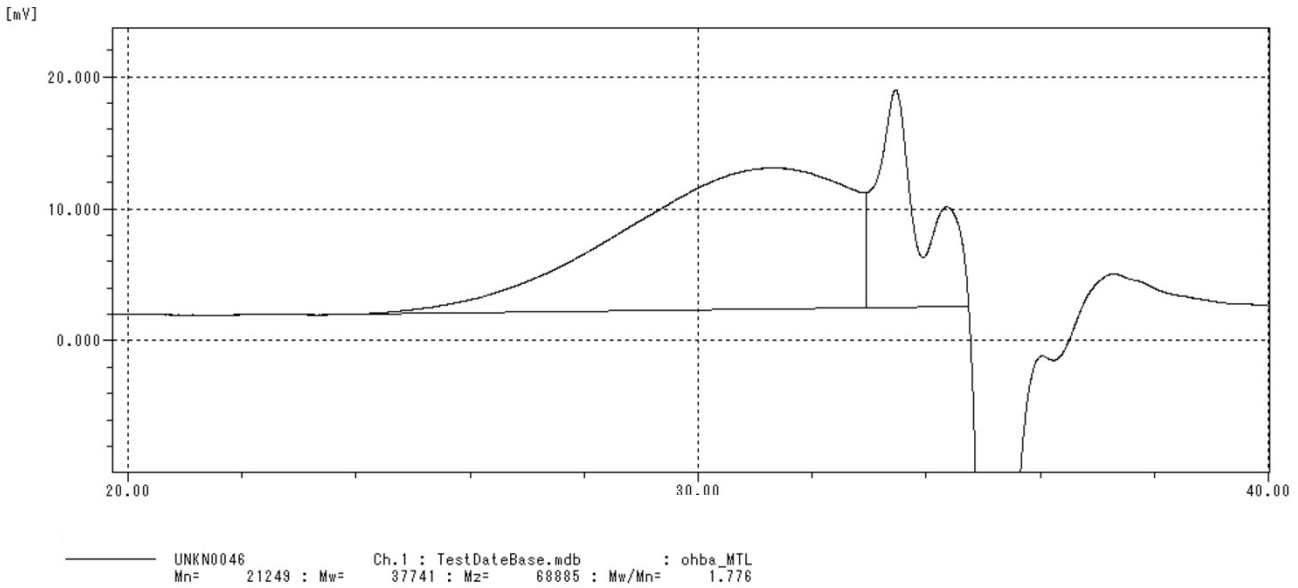

Figure S2c. GPC curve of **poly(MTL)**.

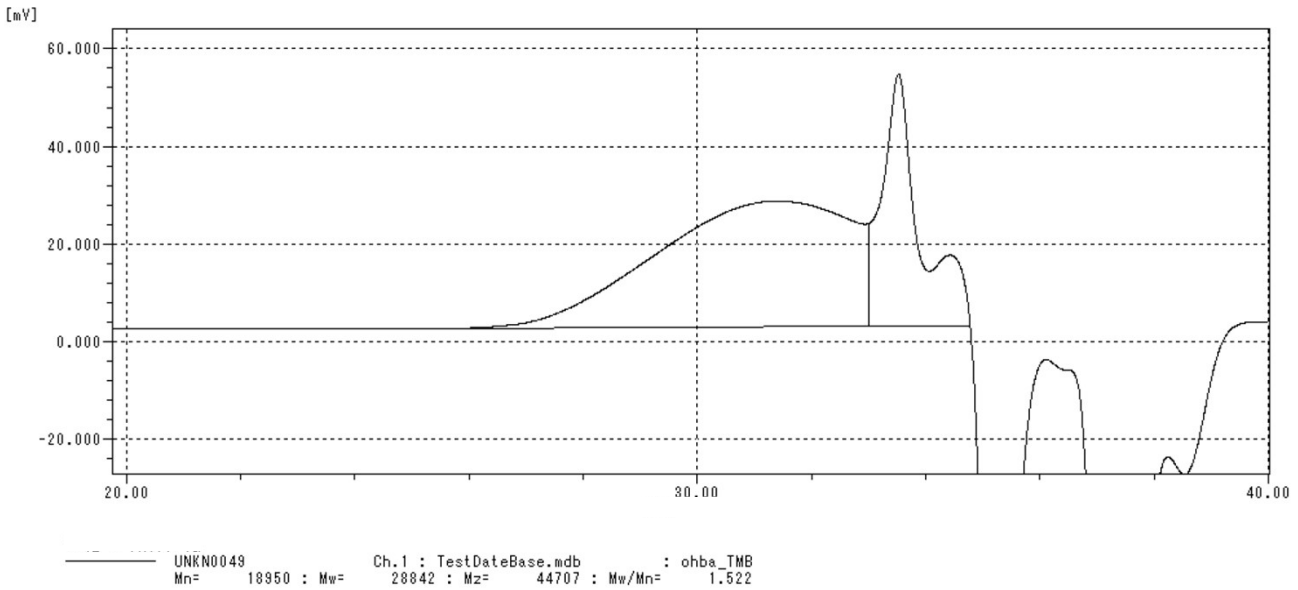

Figure S2d. GPC curve of **poly(TMB)**.

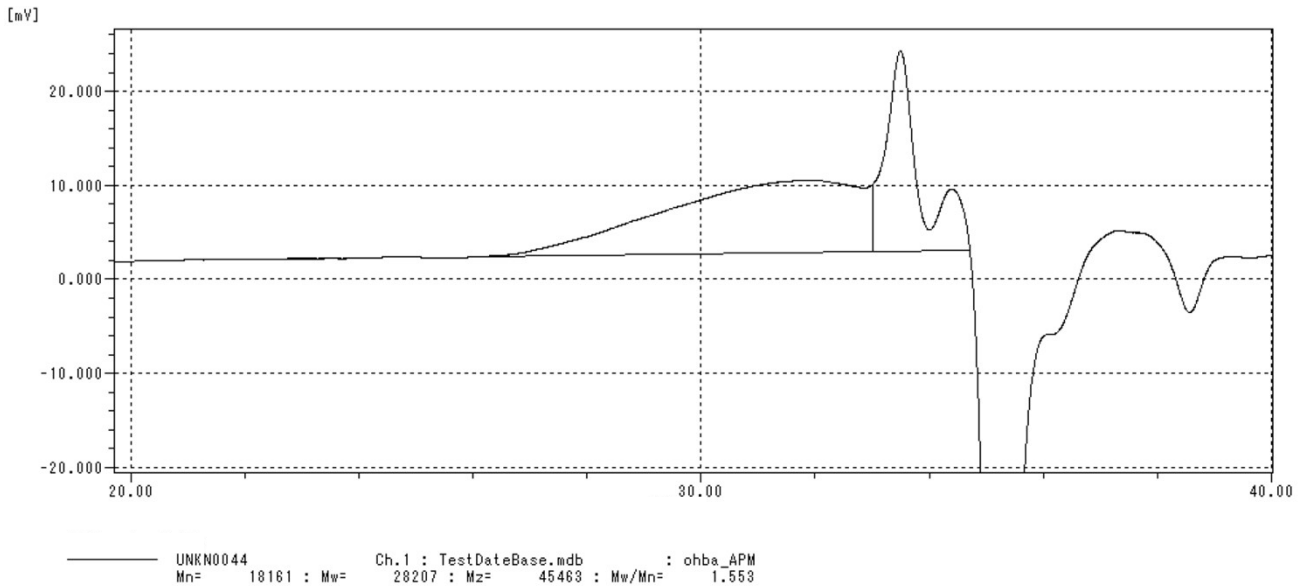

Figure S2e. GPC curve of **poly(APM)**.

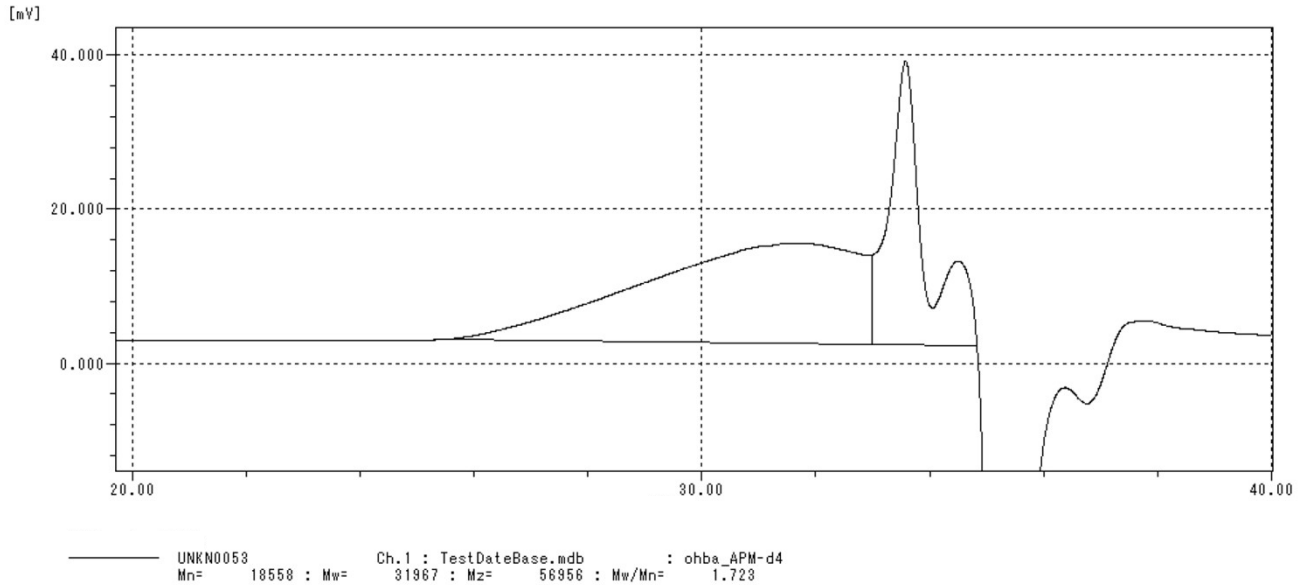

Figure S2f. GPC curve of **poly(APM-d_4)**.

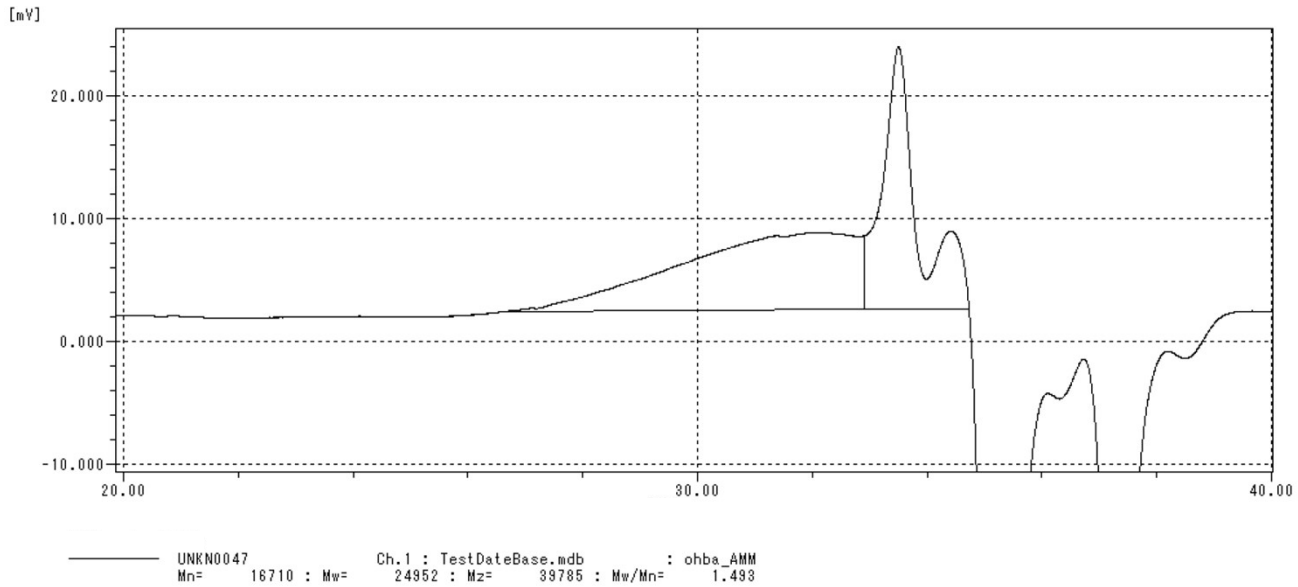

Figure S2g. GPC curve of **poly(AMM)**.

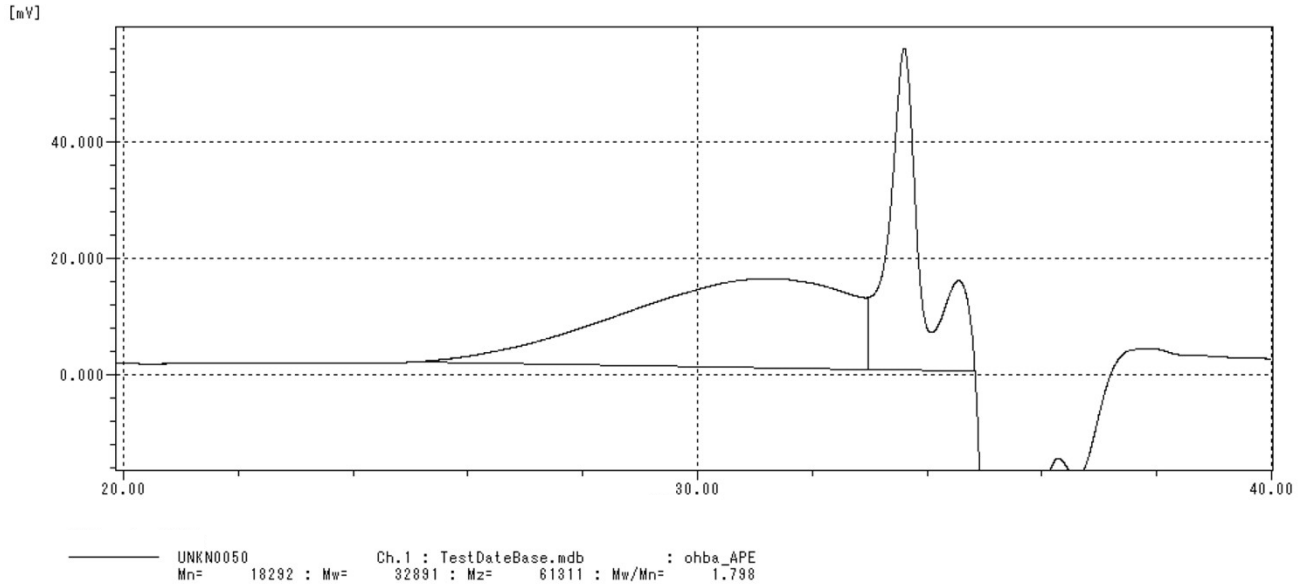

Figure S2h. GPC curve of **poly(APE)**.

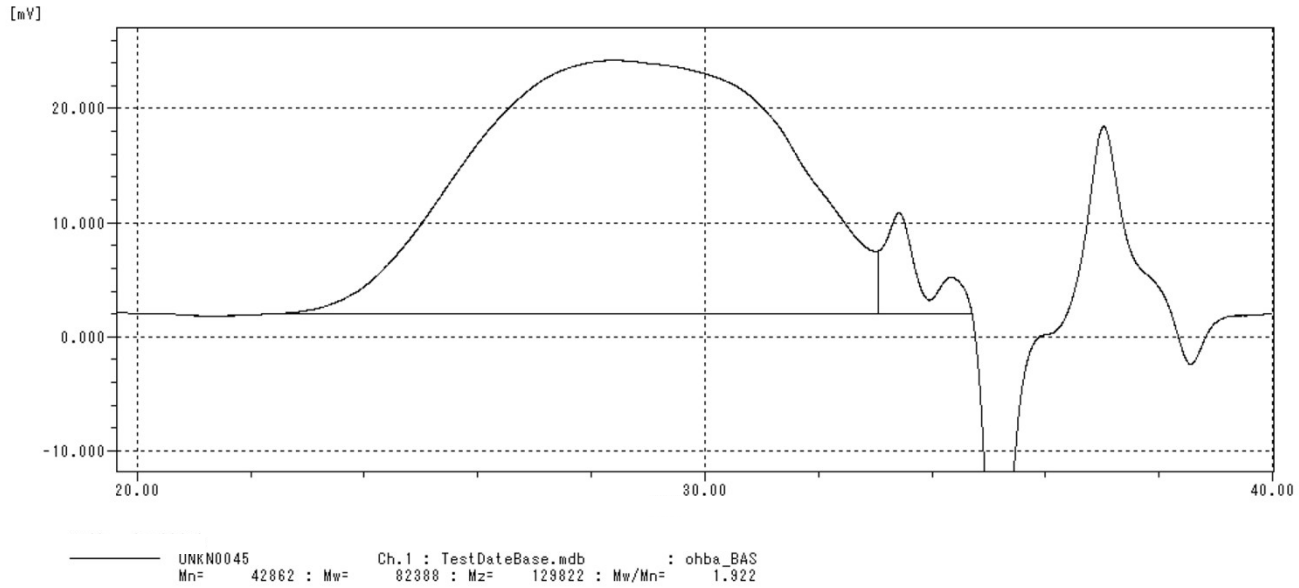

Figure S2i. GPC curve of **poly(BAS)**.

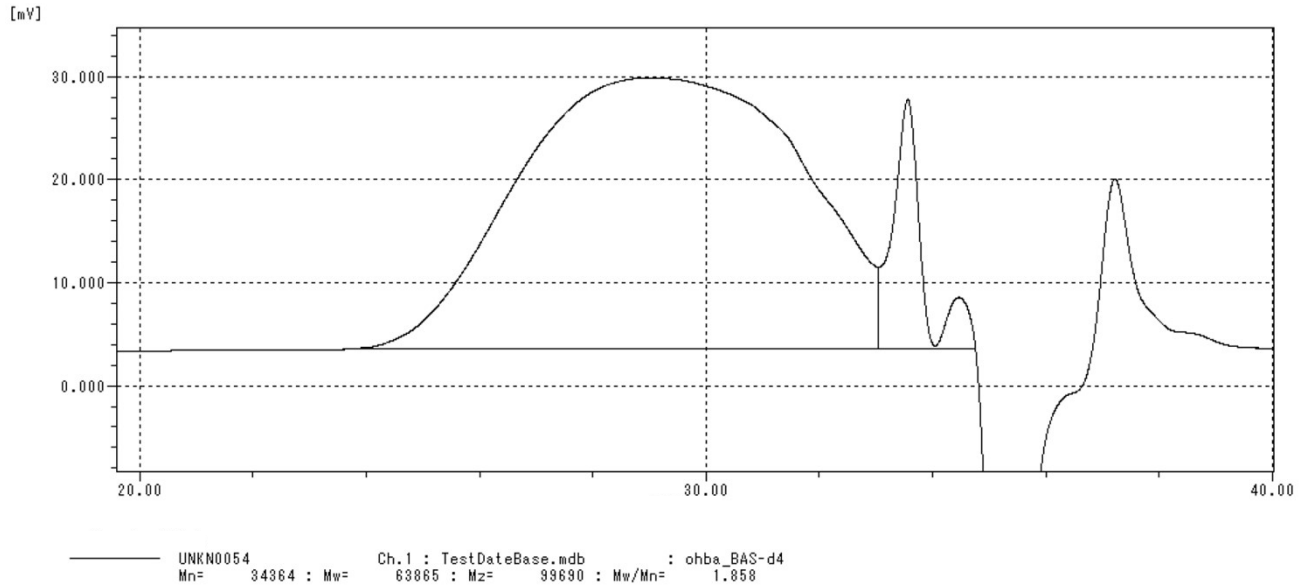

Figure S2j. GPC curve of **poly(BAS-d_4)**.

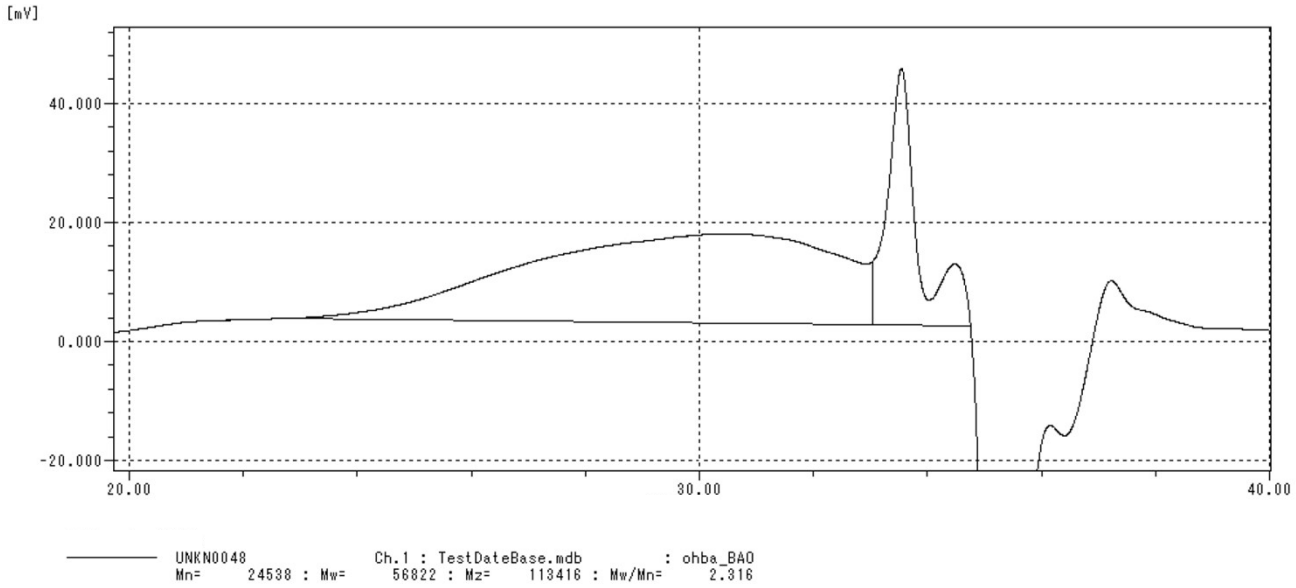

Figure S2k. GPC curve of **poly(BAO)**.

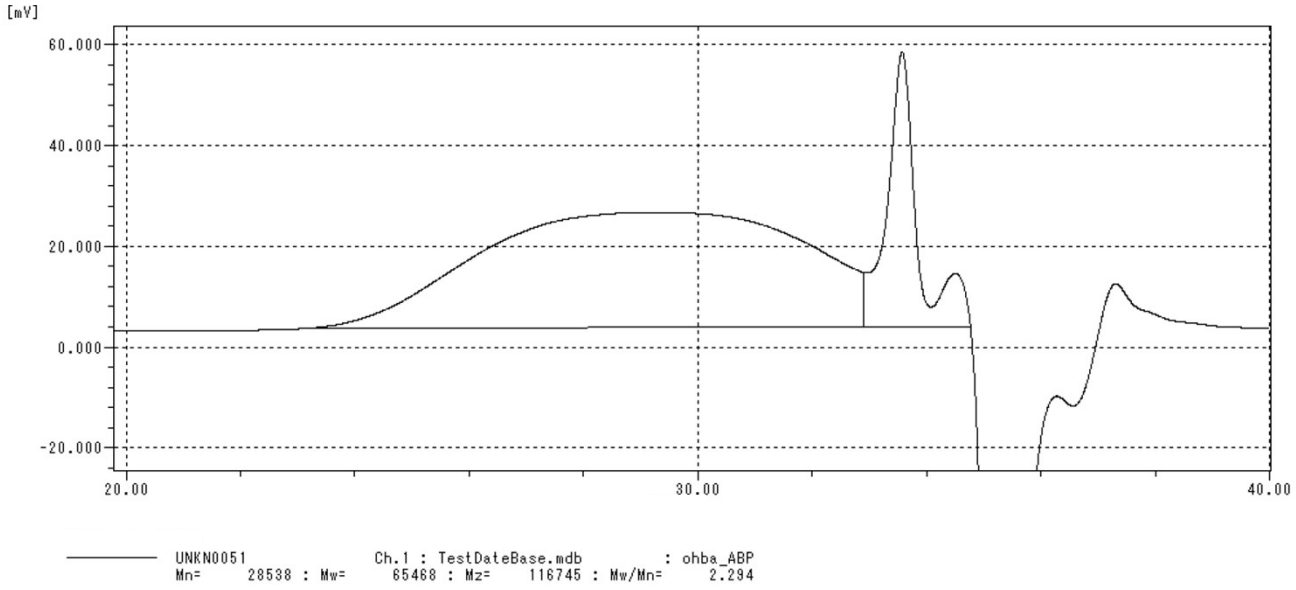

Figure S2l. GPC curve of **poly(DAB)**.

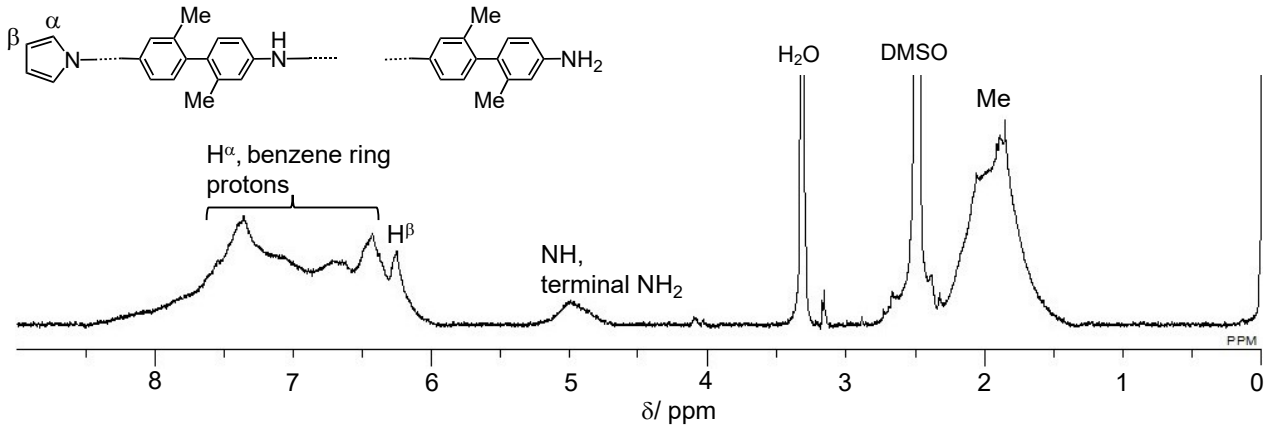

Figure S3a. ^{1}H NMR spectrum of **poly(MTL)** in DMSO-d_6.

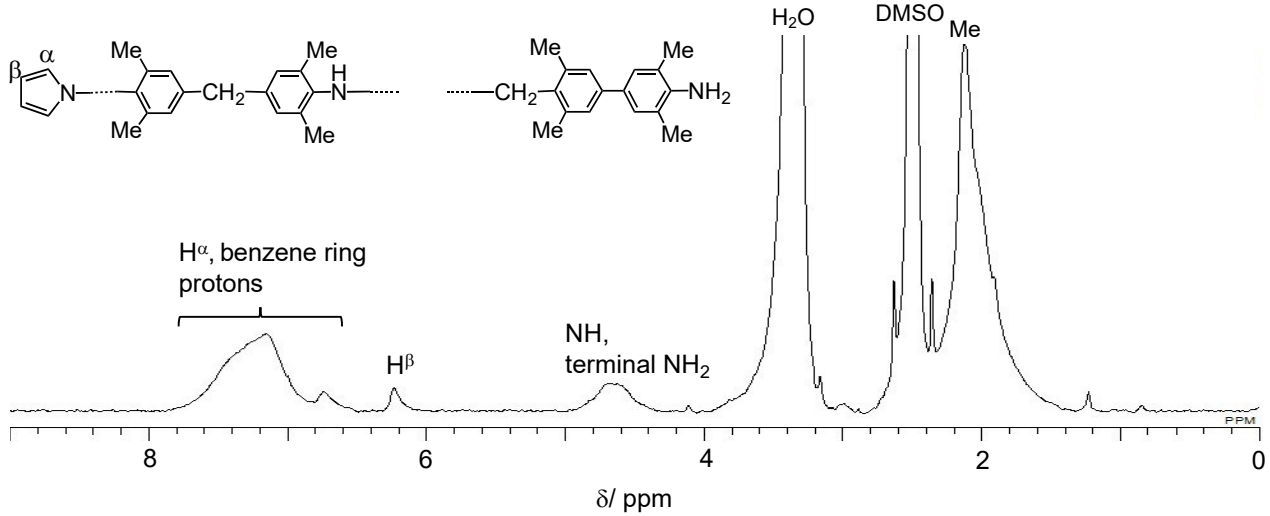

Figure S3b. ^{1}H NMR spectrum of **poly(TMB)** in DMSO-d_6.

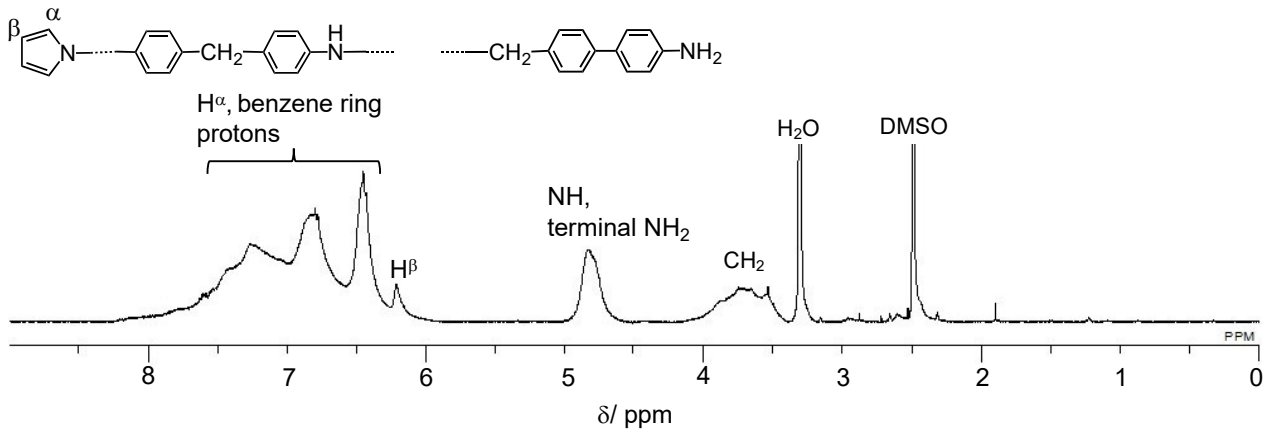

Figure S3c. ^{1}H NMR spectrum of **poly(APM)** in DMSO-d_6.

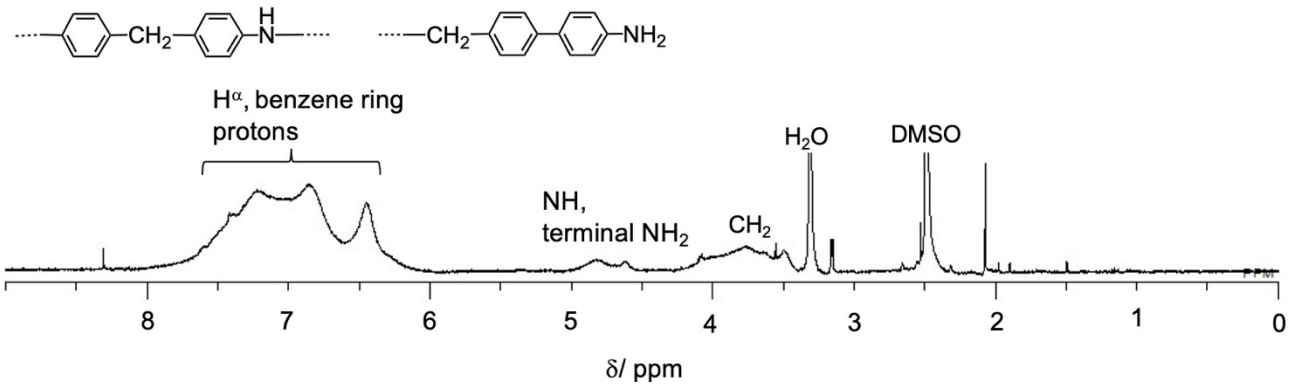

Figure S3d. ^{1}H NMR spectrum of **poly(APM)'** in DMSO-d_6.

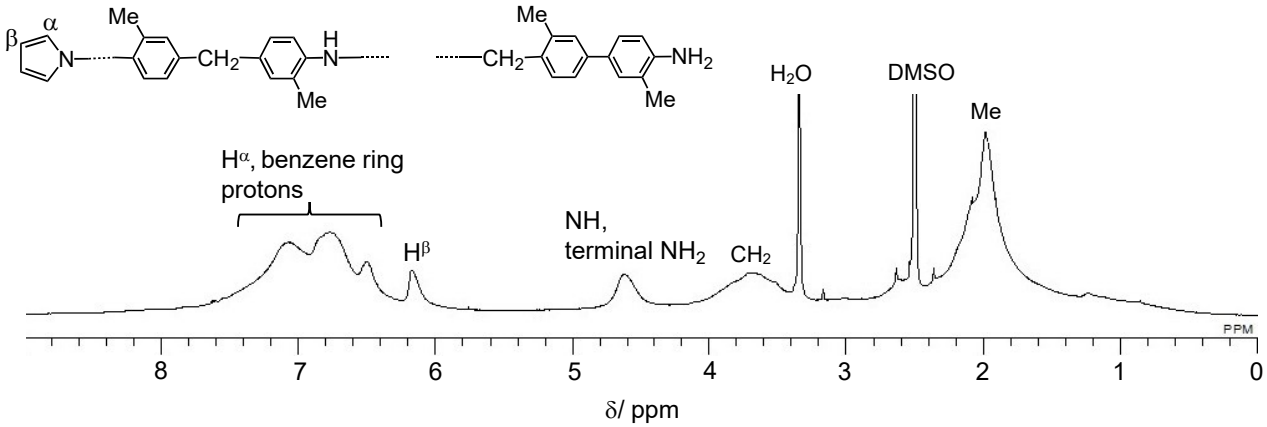

Figure S3e. ^{1}H NMR spectrum of **poly(AMM)** in DMSO-d_6.

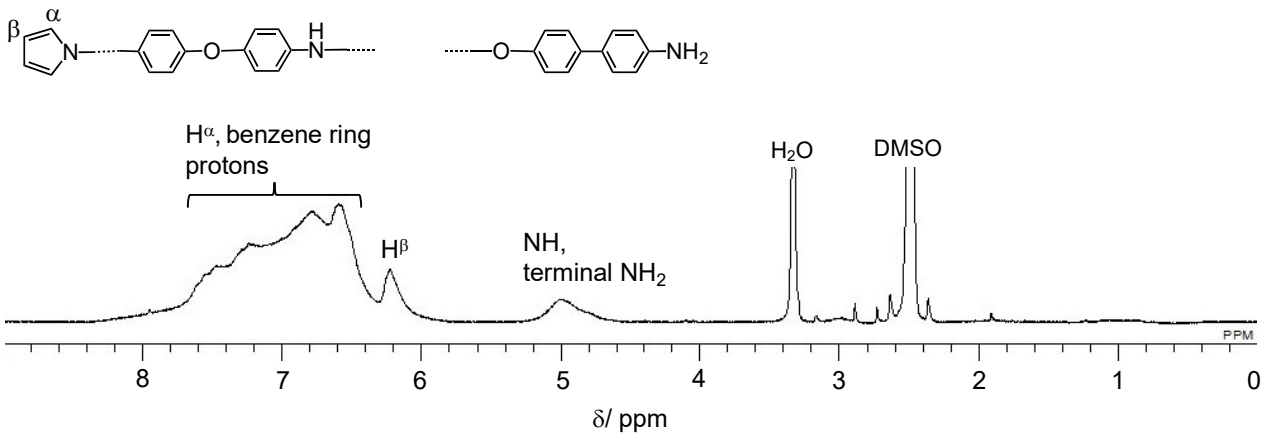

Figure S3f. ^{1}H NMR spectrum of **poly(APE)** in DMSO-d_6.

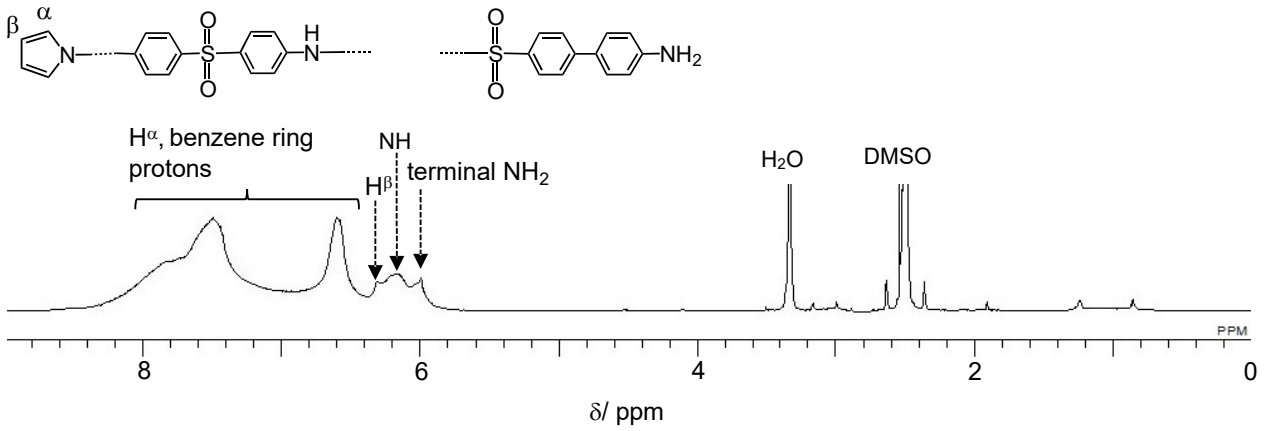

Figure S3g. ^{1}H NMR spectrum of **poly(BAS)** in DMSO-d_6.

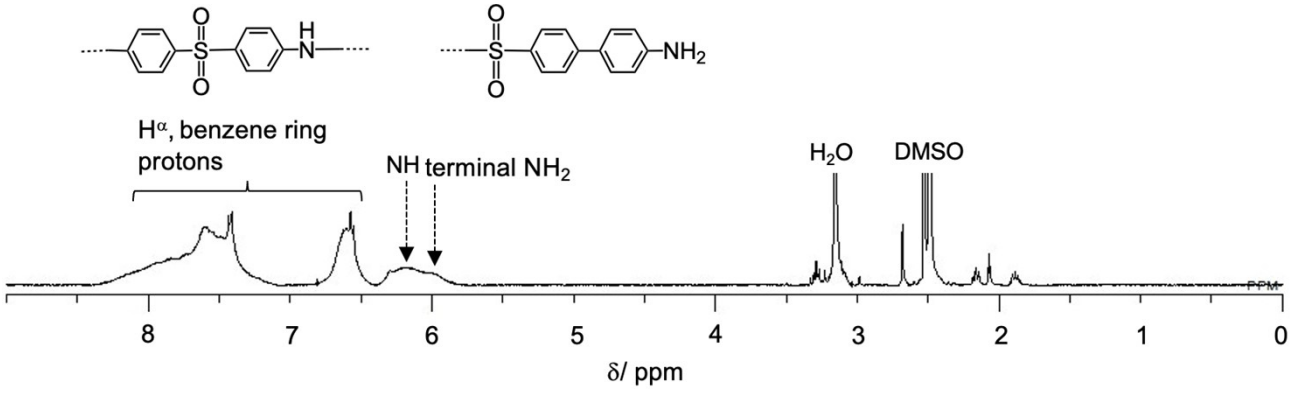

Figure S3h. [1]H NMR spectrum of **poly(BAS)'** in DMSO-d_6.

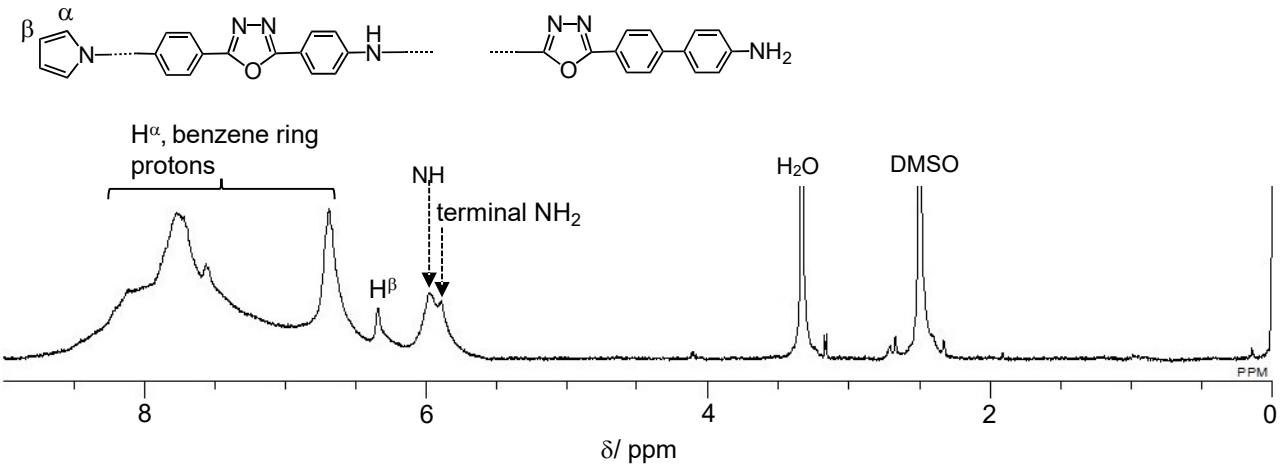

Figure S3i. [1]H NMR spectrum of **poly(BAO)** in DMSO-d_6.

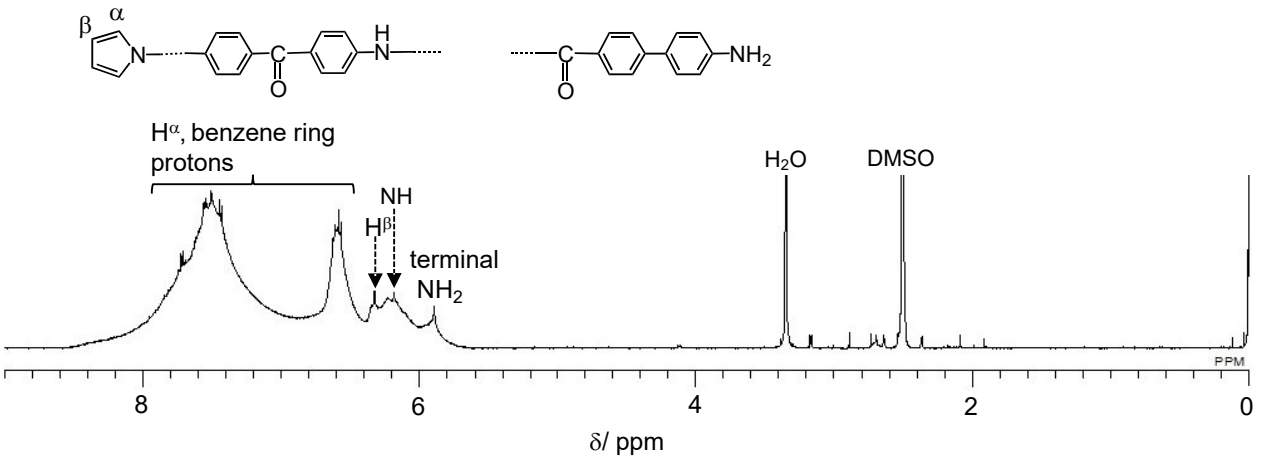

Figure S3j. [1]H NMR spectrum of **poly(DAB)** in DMSO-d_6.

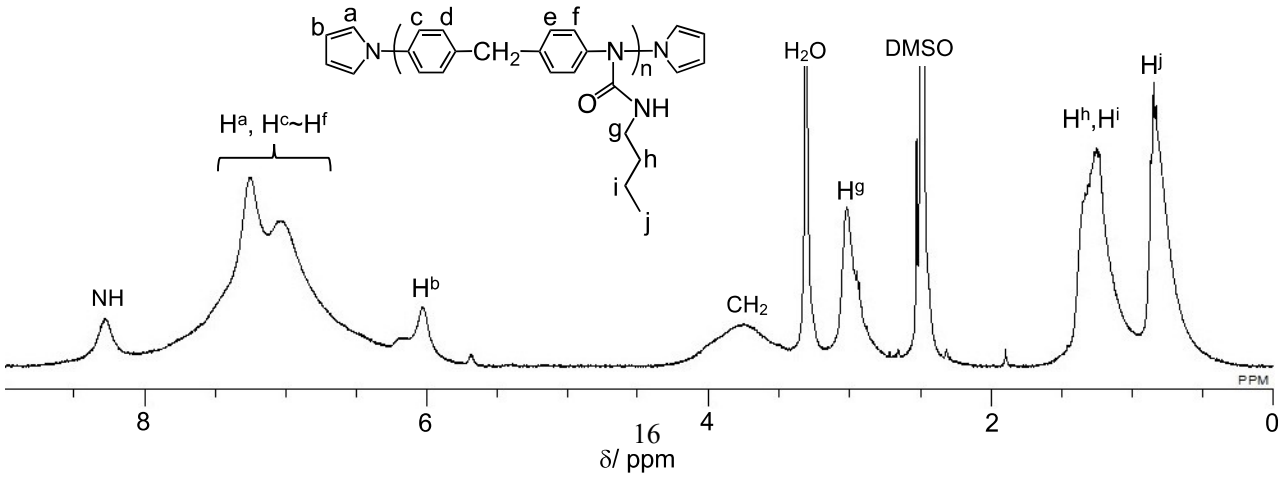

Figure S3k. ^{1}H NMR spectrum of **poly(APM)-BA** in DMSO-d_6.

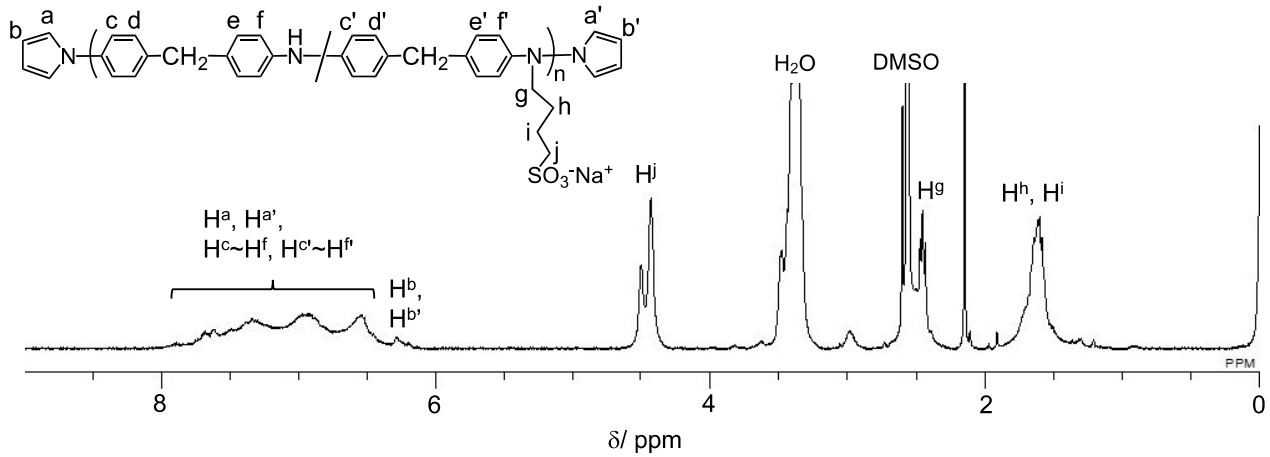

Figure S3l. ^{1}H NMR spectrum of **poly(APM)-BS(Na^{+})** in DMSO-d_6.

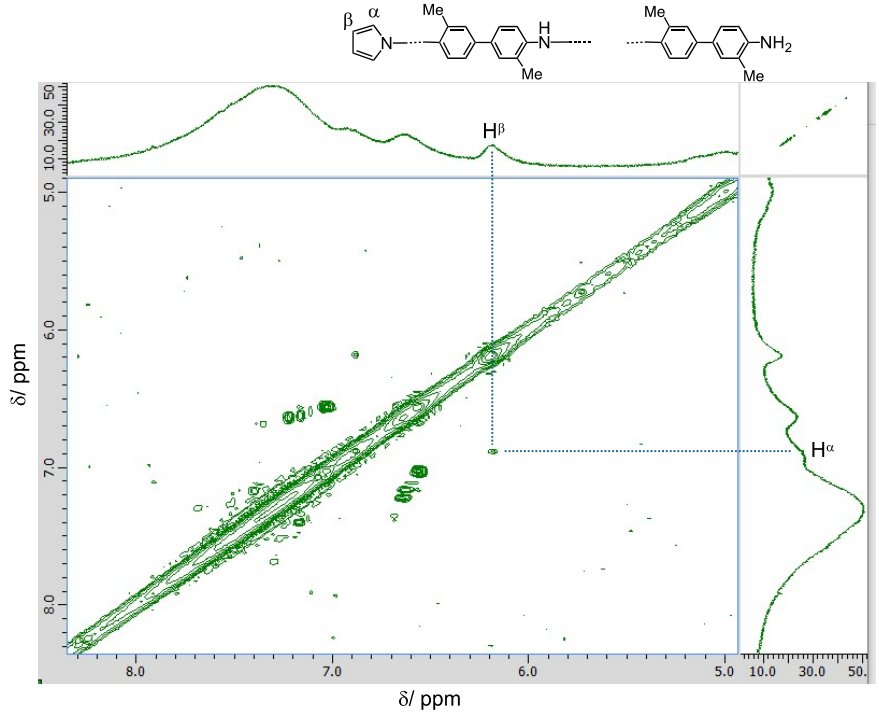

Figure S3m. ^{1}H-^{1}H COSY NMR spectrum of **poly(OTL)** in DMSO-d_6.

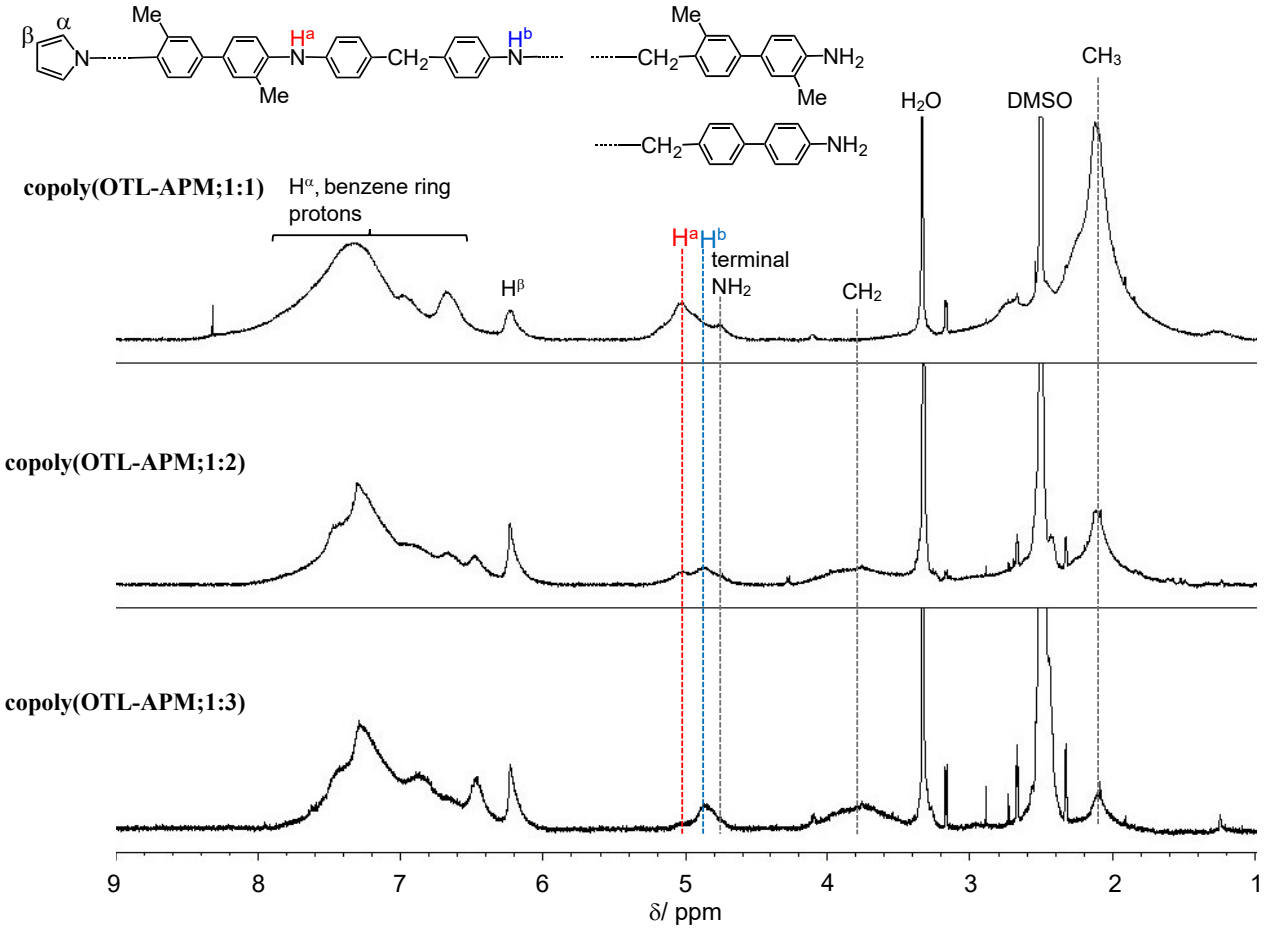

Figure S4. ^{1}H NMR spectra of **copoly(OTL-APM;1:1)**, **copoly(OTL-APM;1:2)** and **copoly(OTL-APM;1:3)** in DMSO-d_6.

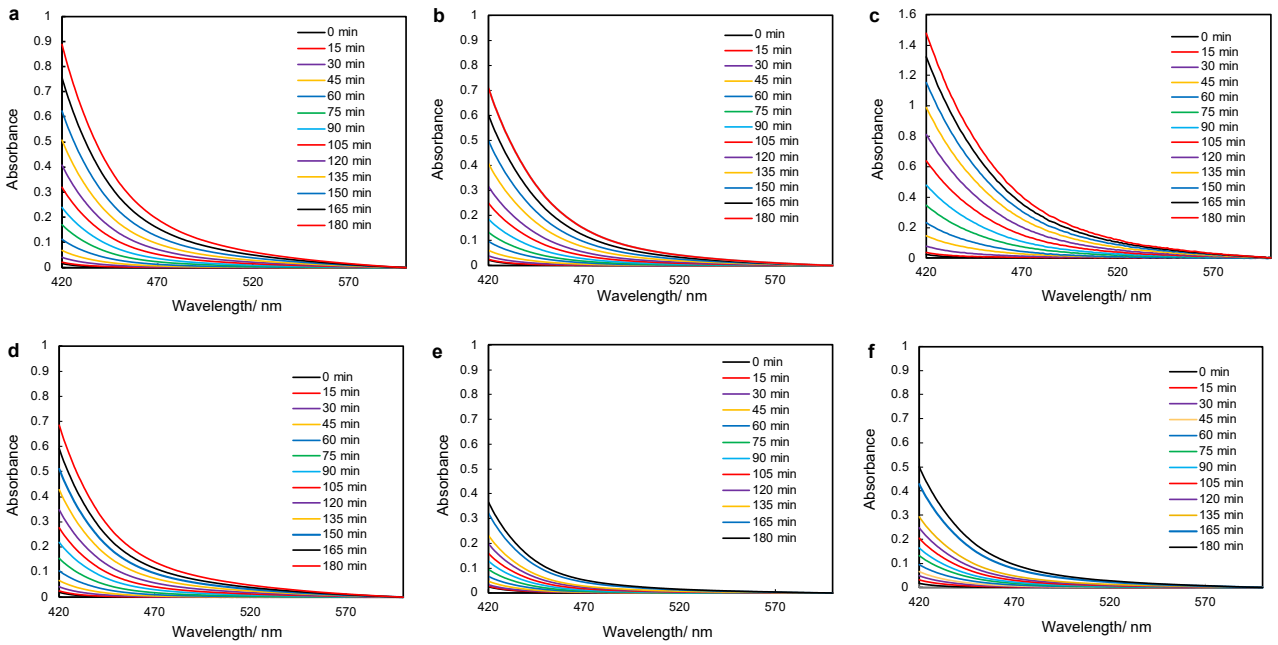

Figure S5. UV-vis spectral changes of the cold aqueous solution of Nessler's reagent containing ammonia generated from the $RuCl_2(PPh_3)_2$-catalyzed polycondensation of (a) OTL, (b) APM, (c) BSA, (d) OTL-d_4, (e) APM-d_4 and (e) BAS-d_4 in the presence BD were monitored at 15-minute intervals.

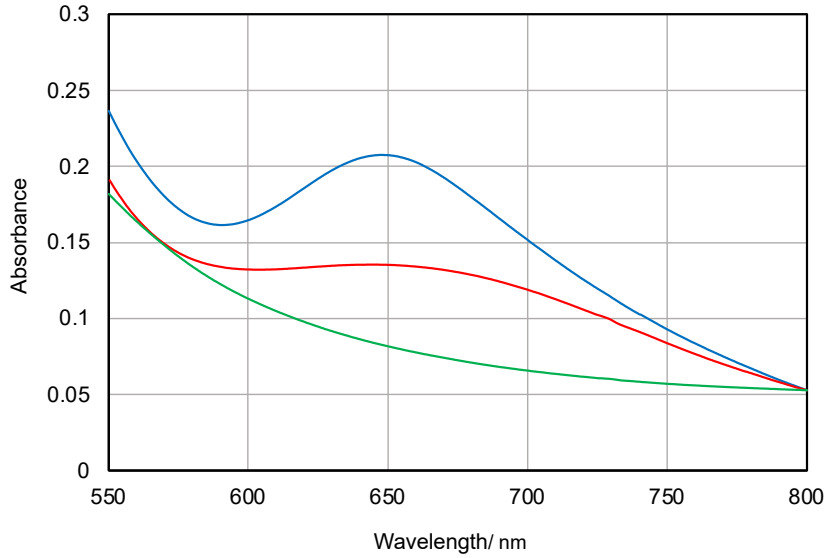

Figure S6. UV-vis spectra of the NMP solution of $RuCl_2(PPh_3)_3$ and BD measured before heating (blue curve) and 5 min (red curve), and 30 min (green curve) after heating at 180 ˚C.

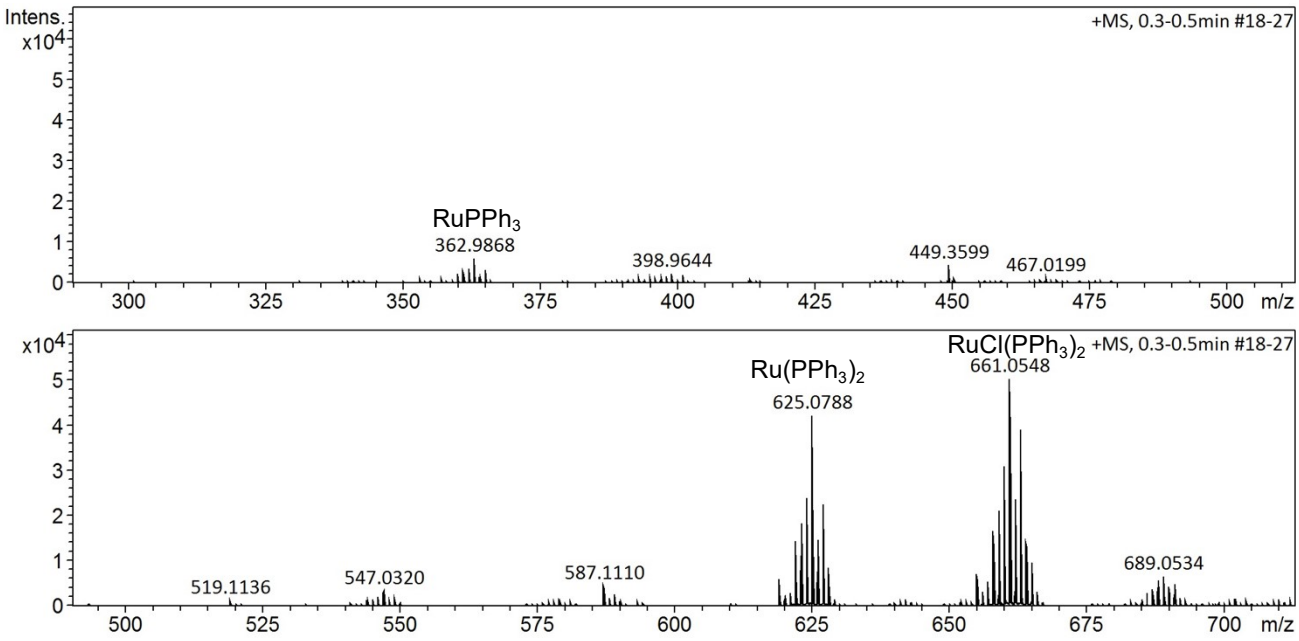

Figure S7. MALDI TOF-MS spectra of the sample obtained from the reaction solution containing OTL, BD, and $RuCl_2(PPh_3)_3$, after heating for 15 min at 180 ˚C.

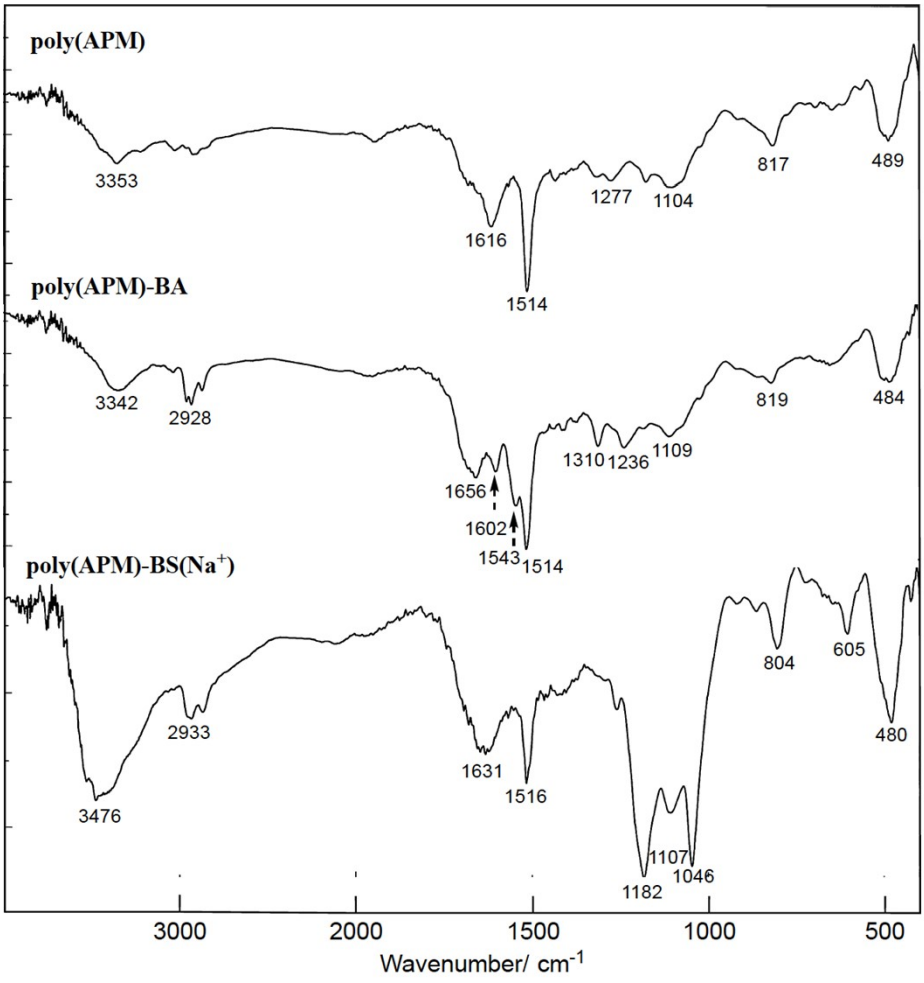

Figure S8. IR spectra of **poly(APM)**, **poly(APM)-BA** and **poly(APM)-BS(Na^+)**.

Calculation of ion conductivity and activation energy.

The ion conductivity (σ) of **poly(APM)-BS(Na^+)** was calculated using the following equation:

$\sigma = d/ (R \bullet S)$

where d is the thickness, R is the bulk resistance obtained from the Nyquist plot of complex impedance measurements, and S is the contact area.

The activation energy for sodium ion conduction (E_a) was calculated using a Arrhenius expression:

$\sigma = \sigma_0 e^{-Ea/RT}$

σ_0 is a constant, R is the gas constant, and T is the temperature.

Table S1. Thermodynamic data.

Structure	*ZPE*	*TCH*	*TCG*	*E*	*H*	*G*
$Ru(PMe_3)_2$	144.283	165.720	94.596	-637508.217	-637342.497	-637413.621
Benzidine	135.587	153.125	93.246	-360060.923	-359907.798	-359967.677
TS1	278.826	318.264	207.875	-997575.443	-997257.179	-997367.568
TS2	276.517	313.337	211.238	-997583.480	-997270.143	-997372.242
3	278.861	319.187	206.442	-997604.799	-997285.612	-997398.357
4	277.987	316.742	207.841	-997615.388	-997298.646	-997407.547

ZPE: Zero-Point Energy Corrections, TCH: Thermal Corrections to Enthalpies, TCG: Thermal Corrections to Gibbs Free Energy, E: Electronic Energies, H: Enthalpies (H), and G: Gibbs Free Energies in NMP at 453 K. All Energies Are Given in Hartree.

Table S2a. Cartesian coordinates of $Ru(PMe_3)_2$.

Ru	44.0	-1.0495584677	-0.2051424884	0.2573052399
P	15.0	0.9222115018	-1.0758435480	0.4552695551
P	15.0	-0.4288012416	1.7009331972	-0.5643108823
C	6.0	0.8137929826	-2.9114308560	0.7360246872
C	6.0	2.1872552311	-1.0298311169	-0.9003802683
C	6.0	1.9918396795	-0.5902897496	1.8944512299
C	6.0	-1.8348729154	2.9180201319	-0.5441375016
C	6.0	0.9103431254	2.7301496993	0.2034196146
C	6.0	0.0685752573	1.8114485300	-2.3510804343
H	1.0	0.1639857636	-3.1189989494	1.5933029418
H	1.0	0.3819788526	-3.3924006680	-0.1471095355
H	1.0	1.8006862169	-3.3481160946	0.9338238493
H	1.0	1.7425063888	-1.3978568261	-1.8293139623
H	1.0	2.5216342501	-0.0004457081	-1.0655400498
H	1.0	3.0629049904	-1.6410359614	-0.6489038591
H	1.0	2.2283112597	0.4759933544	1.8346087737
H	1.0	1.4356131419	-0.7542637024	2.8221176311
H	1.0	2.9279450088	-1.1633324887	1.9262966442
H	1.0	-2.7001405923	2.4926879130	-1.0643379498
H	1.0	-2.1240260650	3.1275995054	0.4904196280
H	1.0	-1.5613808483	3.8595164703	-1.0363233553
H	1.0	0.6914948145	2.8746339256	1.2652332449
H	1.0	1.8721340509	2.2131120976	0.1219516516
H	1.0	1.0001473489	3.7077669013	-0.2865381879
H	1.0	0.9592007894	1.2013570484	-2.5274976067
H	1.0	-0.7385283715	1.4053174027	-2.9679841595
H	1.0	0.2765034195	2.8445351913	-2.6594783423

Table S2b. Cartesian coordinates of benzidine.

C	6.0	0.0011849090	0.0023784350	-0.0006938065
C	6.0	1.4741528805	0.0044592136	0.0033976418
C	6.0	-0.7321358890	1.1979665858	0.0290275471
C	6.0	-0.7184281119	-1.1989975360	-0.0368844252
C	6.0	-2.1059100098	-1.2103265120	-0.0224026492

C	6.0	-2.1198071207	1.1970880721	0.0398169920
C	6.0	-2.8302000560	-0.0127487310	0.0311704988
H	1.0	-0.1797862326	-2.1434314191	-0.0274963076
H	1.0	-2.6388683311	-2.1595171751	-0.0186359131
H	1.0	-0.2002896147	2.1466091573	0.0113160317
H	1.0	-2.6649372802	2.1384382111	0.0311357569
N	7.0	-4.2301855127	-0.0153871503	0.0371727712
C	6.0	2.2027347482	0.9363291060	0.7582479122
C	6.0	2.1973409838	-0.9307142336	-0.7476014799
C	6.0	3.5851101390	-0.9241781105	-0.7626009562
C	6.0	3.5908224747	0.9462597843	0.7529251052
C	6.0	4.3048706201	0.0220393441	-0.0237289109
H	1.0	1.6620063180	-1.6433726875	-1.3701895032
H	1.0	4.1219682401	-1.6384627145	-1.3844763066
H	1.0	1.6664433560	1.6421157653	1.3887819909
H	1.0	4.1341930832	1.6537438589	1.3751164259
N	7.0	5.7110213668	0.0327783365	-0.0271552395
H	1.0	6.0897059206	-0.6990835147	-0.6222203337
H	1.0	6.0924094393	0.9290618197	-0.3148985232
H	1.0	-4.6171181943	-0.9446524291	0.1403929213
H	1.0	-4.6290981262	0.6028009802	0.7354403179

Table S2c. Cartesian coordinates of TS1.

Ru	44.0	-0.4567132686	-0.4437324768	-0.5987908704
C	6.0	1.4208068615	-1.1991384390	-0.6790738144
P	15.0	-0.1809409742	1.7729218023	-0.1098933008
P	15.0	-1.2993787092	-1.0576738797	1.3385208600
N	7.0	-0.0247798731	-2.3604635372	-1.2601957087
H	1.0	0.1453726366	-2.5795005972	-2.2389289359
H	1.0	0.1307397488	-3.1916364754	-0.7026564327
C	6.0	2.0712685516	-0.6760119414	-1.8309660247
C	6.0	2.2654841596	-1.6623541526	0.3589549757
C	6.0	3.6446438263	-1.5411215605	0.2736484061
C	6.0	3.4527808145	-0.5358198981	-1.8912917447
C	6.0	4.2829646897	-0.9649681118	-0.8420779586
H	1.0	1.8283340019	-2.0799823462	1.2641138501
H	1.0	4.2503373905	-1.8601488270	1.1203934878
H	1.0	1.4765390554	-0.3908075417	-2.7027614917

H	1.0	3.9018993547	-0.1297059654	-2.7959882470
C	6.0	5.7501083596	-0.8277120950	-0.9081699697
C	6.0	6.6089836213	-1.7802759656	-0.3351904080
C	6.0	6.3602384286	0.2660363234	-1.5445835818
C	6.0	7.7409218361	0.4017919426	-1.6117079741
C	6.0	7.9910291307	-1.6508280195	-0.3889940358
C	6.0	8.5855816313	-0.5557572557	-1.0319240817
H	1.0	5.7367430355	1.0442345408	-1.9785336439
H	1.0	8.1743447475	1.2719003382	-2.1021811918
H	1.0	6.1846013877	-2.6613316575	0.1403031837
H	1.0	8.6219647017	-2.4135615745	0.0646087709
N	7.0	9.9736319578	-0.3916764356	-1.0415961167
H	1.0	10.3227669357	0.1585028573	-1.8158804190
H	1.0	10.4950009626	-1.2539621884	-0.9487307215
C	6.0	-3.1110834082	-0.7203114179	1.5359628249
C	6.0	-1.2601837546	-2.8665939871	1.7277007325
C	6.0	-0.6342585550	-0.3683345693	2.9193433497
H	1.0	0.4426998237	-0.5545333452	2.9714099704
H	1.0	-0.7960818196	0.7130888359	2.9555692087
H	1.0	-1.1216460553	-0.8247172779	3.7892201820
H	1.0	-1.7622241550	-3.4184905229	0.9281279977
H	1.0	-0.2253473451	-3.2166891154	1.7919219871
H	1.0	-1.7597452427	-3.0756511639	2.6807970603
H	1.0	-3.2990952295	0.3537667932	1.4490006063
H	1.0	-3.6587509883	-1.2270665691	0.7354546717
H	1.0	-3.4858907613	-1.0729240518	2.5048002059
C	6.0	-1.4701225581	2.8880410248	0.6317607950
C	6.0	1.2860714431	2.2170739440	0.9252629397
C	6.0	0.2037803163	2.7313544310	-1.6519174600
H	1.0	-2.3699397554	2.8714305380	0.0078015661
H	1.0	-1.7466300405	2.5329612007	1.6302626955
H	1.0	-1.1180439698	3.9228094108	0.7178427779
H	1.0	1.0718600968	2.2831741128	-2.1452422702
H	1.0	-0.6466018983	2.6904630583	-2.3406629109
H	1.0	0.4280404470	3.7810451161	-1.4283621283
H	1.0	1.1484791864	1.8541717233	1.9478907602
H	1.0	2.1631657299	1.7123843471	0.5090876769
H	1.0	1.4597494914	3.2996796222	0.9525009001

Table S2d. Cartesian coordinates of TS2.

Ru	44.0	-0.8663063172	-0.1539933360	0.3098345025
P	15.0	1.2997693421	-0.6192877362	0.7996732340
P	15.0	-0.4853506296	1.8288861476	-0.5805278803
N	7.0	-2.9725558081	-0.0062377544	0.5543905036
H	1.0	-2.0199437392	0.4777203237	1.3885361245
C	6.0	1.5732934650	-2.3969503165	1.2690110219
C	6.0	2.6820927944	-0.4281447884	-0.4301893295
C	6.0	2.0718460355	0.2046189300	2.2710452899
C	6.0	-1.9724626792	2.9301953235	-0.7122255466
C	6.0	0.7194157238	3.0407854084	0.1360445792
C	6.0	0.0604402825	1.8317484107	-2.3556705328
H	1.0	0.9486820656	-2.6484529856	2.1326471197
H	1.0	1.2798062439	-3.0465983953	0.4381791235
H	1.0	2.6207704144	-2.5966078525	1.5252880711
H	1.0	2.4474396821	-1.0033329779	-1.3318903306
H	1.0	2.7863152142	0.6226910908	-0.7203905333
H	1.0	3.6420551112	-0.7728679566	-0.0275719816
H	1.0	2.0935744609	1.2881726204	2.1254256911
H	1.0	1.4540201872	0.0022292351	3.1513538306
H	1.0	3.0926750610	-0.1531960998	2.4555502899
H	1.0	-2.7490924064	2.4247418782	-1.2956338863
H	1.0	-2.3682376398	3.1356759542	0.2876418303
H	1.0	-1.7319963958	3.8818815615	-1.2005606901
H	1.0	0.4390867891	3.2595532184	1.1708049472
H	1.0	1.7278269369	2.6161341007	0.1393802979
H	1.0	0.7369513912	3.9756666533	-0.4371431672
H	1.0	1.0274283345	1.3286321176	-2.4486884215
H	1.0	-0.6655576230	1.2721078717	-2.9539091777
H	1.0	0.1476265785	2.8487461344	-2.7583723805
H	1.0	-3.6647208695	0.6426716146	0.2037639123
C	6.0	-3.2961740562	-1.3379574602	0.6363507443
C	6.0	-4.4674437005	-1.9373092555	0.1367123225
C	6.0	-2.3056997182	-2.1767879337	1.2001224809
C	6.0	-2.4552714521	-3.5603809337	1.1977171512
C	6.0	-4.6103760171	-3.3157915062	0.1709717081
C	6.0	-3.6106745351	-4.1652935136	0.6857145744

H	1.0	-1.4700567683	-1.7085335479	1.7538868809
H	1.0	-1.6621368136	-4.1819555980	1.6061840360
H	1.0	-5.2528589073	-1.3156591938	-0.2880702373
H	1.0	-5.5350670960	-3.7550814178	-0.1965868908
C	6.0	-3.7871169220	-5.6328672692	0.7029534927
C	6.0	-3.3290637346	-6.4171388498	1.7728250292
C	6.0	-4.4192547093	-6.3071317343	-0.3531638792
C	6.0	-4.5859681482	-7.6858813307	-0.3461827888
C	6.0	-3.4859108157	-7.7970270741	1.7888479746
C	6.0	-4.1198798057	-8.4594445941	0.7271690421
H	1.0	-4.7637786088	-5.7416235985	-1.2157501822
H	1.0	-5.0770850593	-8.1743149848	-1.1859235699
H	1.0	-2.8598431520	-5.9329110992	2.6260517503
H	1.0	-3.1313169988	-8.3706947316	2.6433135392
N	7.0	-4.3343658796	-9.8369621476	0.7665491003
H	1.0	-4.4553142842	-10.2720944550	-0.1384962164
H	1.0	-3.6756948233	-10.3518931662	1.3358254264

Table S2e. Cartesian coordinates of $(PMe_3)_2Ru(NH_2)(C_6H_4\text{-}C_6H_4\text{-}NH_2)$.

Ru	44.0	-0.4625363160	-0.3414711993	-0.6259791051
C	6.0	1.5388702135	-0.4096813449	-0.4120645545
P	15.0	-0.2887290874	1.8901470204	-0.0302119918
P	15.0	-1.0785124198	-1.2155159543	1.2929609582
N	7.0	-1.3537245658	-1.8091601176	-1.6153917836
H	1.0	-1.0781550968	-1.9178408108	-2.5930127702
H	1.0	-1.6521584696	-2.7282151271	-1.2968253553
C	6.0	2.1809864144	-0.3140974404	-1.6693903740
C	6.0	2.3935591120	-0.6193613472	0.6858451242
C	6.0	3.7748030697	-0.7447378303	0.5405881042
C	6.0	3.5579074596	-0.4380100444	-1.8206314660
C	6.0	4.3949419086	-0.6587927495	-0.7138634094
H	1.0	1.9823084227	-0.6711339799	1.6923157518
H	1.0	4.3904702299	-0.8812679692	1.4283000391
H	1.0	1.5837892156	-0.1612700057	-2.5739285506
H	1.0	3.9912541292	-0.3931681382	-2.8182692052
C	6.0	5.8591715305	-0.7881789645	-0.8652319776
C	6.0	6.6050874801	-1.6727688149	-0.0705565176
C	6.0	6.5711797007	-0.0333813763	-1.8106611728

C	6.0	7.9470202590	-0.1530783897	-1.9590963797
C	6.0	7.9817246087	-1.7980339838	-0.2066566536
C	6.0	8.6806374960	-1.0394311596	-1.1569194294
H	1.0	6.0371180362	0.6825163013	-2.4311177767
H	1.0	8.4662446680	0.4603334680	-2.6936204172
H	1.0	6.0901715022	-2.2996796780	0.6536130450
H	1.0	8.5249145060	-2.4989901838	0.4251002408
N	7.0	10.0707938558	-1.1195553089	-1.2605817255
H	1.0	10.4387219565	-0.8667951921	-2.1686000340
H	1.0	10.4650653078	-1.9944507816	-0.9398844259
C	6.0	-2.8926498439	-1.5327395581	1.4335041199
C	6.0	-0.3696064744	-2.8884864407	1.6077478052
C	6.0	-0.7484645137	-0.3650331868	2.8977248863
H	1.0	0.3231954976	-0.1890620282	3.0230345750
H	1.0	-1.2626612420	0.6002750849	2.9189234568
H	1.0	-1.1075142766	-0.9722352124	3.7369664648
H	1.0	-0.6725259334	-3.5618004245	0.8006599591
H	1.0	0.7221881134	-2.8240354626	1.5936277288
H	1.0	-0.7034516304	-3.2997687699	2.5678077798
H	1.0	-3.4282447970	-0.5784141679	1.4480943094
H	1.0	-3.2253250441	-2.0853283784	0.5504039846
H	1.0	-3.1398020640	-2.0986464092	2.3396190678
C	6.0	-1.8571781244	2.7585294145	0.4341145085
C	6.0	0.8732236351	2.5865014280	1.2304308470
C	6.0	0.2197216967	2.8615387863	-1.5221580201
H	1.0	-2.6189991406	2.5534596286	-0.3244877985
H	1.0	-2.2269563937	2.3787719728	1.3926882803
H	1.0	-1.7153908068	3.8427244816	0.5187709006
H	1.0	1.2207327340	2.5418813903	-1.8303099815
H	1.0	-0.4753297138	2.6677424663	-2.3463424157
H	1.0	0.2343486581	3.9388775966	-1.3200179596
H	1.0	0.5858159070	2.2537531109	2.2327089051
H	1.0	1.8821045281	2.2159110827	1.0281850201
H	1.0	0.8757786340	3.6823064343	1.2124717462

Table S2f. Cartesian coordinates of $(PMe_3)_2Ru(H)(NH\text{-}C_6H_4\text{-}C_6H_4\text{-}NH_2)$.

Ru	44.0	-1.1529120362	0.0071916493	0.5551172995
P	15.0	0.8558752276	-1.0342744408	0.6240706203

P	15.0	-0.5329920918	1.9648769860	-0.3057510336
N	7.0	-3.1233834292	0.1841010872	-0.0679281929
H	1.0	-0.6128448281	0.5330794524	1.9546803092
C	6.0	0.7508705291	-2.8118989771	1.1243116801
C	6.0	1.7293330536	-1.1933022196	-1.0016950767
C	6.0	2.2493109517	-0.4806735185	1.7108617335
C	6.0	-1.6537114446	3.3374211435	0.2126753021
C	6.0	1.1159492971	2.7071587851	0.0702994246
C	6.0	-0.5772074304	2.1384932038	-2.1494148132
H	1.0	0.4268685611	-2.8738474459	2.1677547788
H	1.0	0.0033510688	-3.3245617103	0.5119949913
H	1.0	1.7179028560	-3.3182961607	1.0195973026
H	1.0	1.0565306064	-1.6703087791	-1.7213514360
H	1.0	1.9849430425	-0.2005325293	-1.3858726135
H	1.0	2.6468109136	-1.7884870226	-0.9200969399
H	1.0	2.5408079163	0.5434788946	1.4609140567
H	1.0	1.9074863621	-0.4869642830	2.7504471635
H	1.0	3.1251899278	-1.1333234029	1.6153532945
H	1.0	-2.6882204170	3.0519696555	0.0021183615
H	1.0	-1.5646790336	3.4766617029	1.2942434731
H	1.0	-1.4171811169	4.2795488543	-0.2964339655
H	1.0	1.2383299868	2.7744303585	1.1553800254
H	1.0	1.9156389959	2.0747361917	-0.3276963163
H	1.0	1.2120180558	3.7088321928	-0.3645298669
H	1.0	0.1394166335	1.4457287307	-2.6015922464
H	1.0	-1.5745101428	1.8719308438	-2.5135521472
H	1.0	-0.3417365684	3.1599392669	-2.4724573348
H	1.0	-3.4658678236	0.5742436567	-0.9426254742
C	6.0	-3.3236284208	-1.1611372946	0.0495793379
C	6.0	-3.8474801695	-2.0335914555	-0.9453693179
C	6.0	-2.8716667452	-1.7565892773	1.2653983182
C	6.0	-2.8998022661	-3.1461938843	1.4362232998
C	6.0	-3.8986680506	-3.3939488168	-0.7316813606
C	6.0	-3.4113755661	-3.9961059023	0.4556232185
H	1.0	-2.6473324334	-1.1017105719	2.1117565303
H	1.0	-2.5285015162	-3.5667914858	2.3682313676
H	1.0	-4.2215468625	-1.6106309006	-1.8761282661
H	1.0	-4.3434495931	-4.0291367684	-1.4950266583

C	6.0	-3.4763808270	-5.4600395949	0.6480458181
C	6.0	-3.7567454620	-6.0264178292	1.9016319576
C	6.0	-3.2607334366	-6.3509207793	-0.4151711312
C	6.0	-3.3186492555	-7.7277919688	-0.2413972837
C	6.0	-3.8125693070	-7.4013437994	2.0885581929
C	6.0	-3.5953712117	-8.2808660742	1.0175288122
H	1.0	-3.0154014714	-5.9577874519	-1.3991573125
H	1.0	-3.1417831804	-8.3866957190	-1.0897538086
H	1.0	-3.9614459476	-5.3735958698	2.7468062576
H	1.0	-4.0485429052	-7.8029932681	3.0724887112
N	7.0	-3.7132246172	-9.6605795432	1.1865505841
H	1.0	-3.2111071045	-10.2139870078	0.5046511942
H	1.0	-3.5353476387	-9.9882146882	2.1269859470