Supporting Information for

Tunable anchoring groups@Acridone linked tri-phenylamine based pendant chromophores and their effects on photovoltaic performance as sensitizers for dye-sensitized solar cells

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Experimental Section

Materials

4-bromo-N-phenylaniline (Sigma-Aldrich), 4-bromophenol (Sigma-Aldrich) Acridone (Sigma-Aldrich) malononitrile (Sigma-Aldrich), 2-amino-5-nitrobenzonitrile (Sigma-Aldrich), 5-aminopicolinic acid (Sigma-Aldrich), tetrazol-5-amine (Alfa Aesar), tetrabutylammonium perchlorate (TBAP) (Sigma-Aldrich), methacrylic acid, ammonium acetate, acetic acid, triethylamine (THF), N,N-dimethylformamide (DMF), potassium phosphate, copper powder, , hydrochloric acid, titanium tetrachloride ($TiCl_4$), 1,10-Phenanthroline, 1, 2-diaminocyclohexane, potassium iodide and 2, 2'-Azobisisobutyronitrile (AIBN) (Merck, Germany) were used as received. Dichloromethane (DCM), ethanol, acetic acid, methanol (MeOH) and tetrahydrofuran (THF) (SRL, India) solvents were purified by usual procedures. All column chromatographic separations were carried out using silica gel (60-120 mesh) (SRL, India).

Compound characterization and Methods

Characterization of products was achieved by the following instruments: ^{1}H and ^{13}C NMR was measured in $CDCl_3$ or DMSO-d_6 on a Bruker Avance 500 MHz spectrometer.Chemical shifts (δ values) were recorded in units of ppm relative to tetramethylsilane (TMS) as an internal standard. FT-IR spectra were recorded in the 4000-400 cm^{-1} range on a Shimadzu FTIR 8400s using KBr pellets. Gas chromatography-mass spectrometry (GC-MS) was used to record GC-MS spectra by JEOL GCMATE II GC-MS. Molecular weight and molecular weight distribution (M_w/M_n) were determined by gel permeation chromatography (GPC). All reactions were monitored by using TLC plates.

Synthetic procedures and characterization data

4-((4-bromophenyl) (phenyl)amino)phenol (TPA)

A mixture of 4-bromo-N-phenylaniline (1) (8.06 mmol), 4-bromophenol (2) (8.84 mmol), CuI (1.08 mmol), K_3CO_3 (5.07 mmol), and 1, 10-phenanthroline (1.0 mmol) in toluene (30 ml) was degassed with N_2 for 5 mins and then stirred at reflux under N_2 atmosphere for 24 hrs. After the mixture was cooled, water (50 mL) was added, and the mixture was extracted with CH_2Cl_2 (50 mL × 2). The combined organic phase was washed with water (100 mL × 2) and brine solution (100 ml), dried over anhydrous Na_2SO_4, and filtered. The solvent was removed from dryness, and the residue was purified by silica gel column chromatography using a mixture of

$CHCl_3$ and methanol as eluent followed by recrystallization with a mixture of $CHCl_3$ and methanol (1.60 g, yield 80 %).

^{1}H NMR ($CDCl_3$, 500 MHz, δ ppm): 4.15 (s, 1H), 6.92 (d, *J* = 7.6 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 7.29-7.11 (m, *J* = 7.2 Hz, 1H), 7.38 (d, *J* = 8.5 Hz, 2H), 7.66 (d, *J* = 6.7 Hz, 2H), 7.81 (d, *J* = 7.0 Hz, 2H) 8.07 (d, *J* = 15.7 Hz, 2H). ^{13}C NMR ($CDCl_3$, 126 MHz, δ ppm): 115.4, 119.1, 121.3, 123.1, 127.8, 131.0, 135.2, 137.5, 139.8, 142.6, 147.6, 156.1. FT-IR (KBr pellet, cm^{-1}): 3352, 3041, 2840, 2218, 1930, 1663, 1428, 1319, 1232, 1081, 963, 820, 716.

10-(4-((4-hydroxyphenyl)(phenyl)amino)phenyl)acridin-9(10H)-one (ATPA)

A mixture of compound TPA (2.94 mmol), acridone (3) (6.67 mmol), CuI (1.08 mmol), K_3PO_4 (5.07 mmol), and (±)-trans-1, 2-diaminocyclohexane (1.00 mmol) in DMF (30 ml) was degassed with N_2 for 5 mins and then stirred at reflux under N_2 atmosphere for 24 hrs. After the mixture was cooled, water (50 mL) was added, and the mixture was extracted with CH_2Cl_2 (50 mL × 2). The combined organic phase was washed with water (100 mL × 2) and brine solution (100 ml), dried over anhydrous Na_2SO_4, and filtered. The solvent was removed from dryness, and the residue was purified by silica gel column chromatography using a mixture of $CHCl_3$ and methanol as eluent followed by recrystallization with a mixture of $CHCl_3$ and methanol. Pale yellow solids (yield 73%). ^{1}H NMR ($CDCl_3$, 500 MHz, δ ppm): 5.10 (s, 3H), 6.81 (d, *J* = 7.6 Hz, 2H), 6.99 (d, *J* = 8.4 Hz, 2H), 7.19-7.08 (m, *J* = 6.6 Hz, 1H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.29-7.18 (m, *J* = 14.6 Hz, 2H), 7.34 (d, *J* = 5.5 Hz, 2H), 7.61 (d, *J* = 9.0 Hz, 2H), 7.73-7.68 (m, *J* = 6.5 Hz, 2H), 8.21 (d, *J* = 15.5 Hz, 2H). ^{13}C NMR ($CDCl_3$, 126 MHz, δ ppm): 109.1, 117.4, 115.1, 119.5, 121.1, 125.1, 127.8, 131.2, 133.7, 135.8, 138.8, 140.2, 145.1, 147.6, 158.1, 160.1, 179.2. FT-IR (KBr pellet, cm^{-1}): 3350, 3035, 2922, 2861, 1740, 1665, 1320, 1248, 1140, 1060, 955, 817, 720. GC-MS Anal. Calcd. for $C_{31}H_{22}N_2O_2$: 454.52. Found (m/z): 456.77.

2-(10-(4-((4-hydroxyphenyl)(phenyl)amino)phenyl)acridin-9(10H)-ylidene)malononitrile (AT1)

Compound ATPA (1 g, 2.20 mmol) was first dissolved in dry pyridine (10 mL) under nitrogen and the mixture was allowed to stir for 30 mins at room temperature. $TiCl_4$ (0.21 mL, 1.45 mmol) was then added dropwise into the mixture. The mixture was heated to 80 °C and malononitrile (0.34 g, 5.15 mmol) in dry pyridine (10 mL) was added dropwise. The resulting mixture was continuously heated and refluxed at 120 °C for 24 hrs. A brownish slurry was obtained after cooling down to room temperature. The reaction mixture was filtered through a short silica column eluting with CH_2Cl_2 to remove black impurities and the red effluent was

collected and subjected to column chromatography using $CHCl_3$/MeOH (4:1, v/v) as the eluent. Yellow solids (yield 70%). ^{1}H NMR ($CDCl_3$, 500 MHz, δ ppm): 4.82 (s, 3H), 6.74 (d, *J* = 8.0 Hz, 2H), 6.87 (d, *J* = 5.4 Hz, 2H), 6.98 (d, *J* = 6.5 Hz, 2H), 7.06 (d, *J* = 9.0 Hz, 2H), 7.23-7.01 (m, *J* = 8.2 Hz, 1H), 7.39-7.28 (m, *J* = 7.5 Hz, 2H), 7.42 (d, *J* = 15.0 Hz, 2H), 7.55 (d, *J* = 8.5 Hz, 2H), 7.83-7.71 (m, *J* = 14.5 Hz, 2H). ^{13}C NMR ($CDCl_3$, 126 MHz, δ ppm): 85.1, 115.5, 119.2, 120.3, 123.1, 127.8, 129.3, 131.7, 134.2, 138.8, 140.8, 144.1, 158.1, 167.2. FT-IR (KBr pellet, cm^{-1}): 3338, 3051, 3020, 2851, 2254, 1670, 1610, 1448, 1319, 1232, 1140, 1055, 960, 882, 820, 714. Anal. Calcd. for $C_{34}H_{22}N_4O$: C, 81.26; H, 4.41; N, 11.15; O, 3.18. Found: C, 82.58; H, 5.34; N, 12.68; O, 4.49. GC-MS Anal. Calcd. for $C_{34}H_{22}N_4O$: 502.56. Found (m/z): 503.89.

2-((10-(4-((4-hydroxyphenyl)(phenyl)amino)phenyl)acridin-9(10H)-ylidene)amino)-5-nitrobenzonitrile (AT2)

A mixture of compound ATPA (1 g, 1.98 mmol) and 2-amino-5-nitrobenzonitrile (0.389 g, 2.38 mmol) was refluxed in 10 mL of acetic acid (AcOH) for 24 hrs. After that the reaction mixture was poured into cold water (100 mL) and the resulting precipitate was collected and purified by column chromatography (SiO_2, 4:1, $CHCl_3$/MeOH). Yellow solids (yield 70%). ^{1}H NMR ($CDCl_3$, 500 MHz, δ ppm): 4.78 (s, 3H), 6.88 (d, *J* = 16.5 Hz, 2H), 6.93 (d, *J* = 8.0 Hz, 2H), 7.01 (d, *J* = 7.7 Hz, 2H), 7.19-7.05 (m, *J* = 9.5 Hz, 1H), 7.26 (d, *J* = 7.9 Hz, 2H), 7.37-7.29 (m, *J* = 15.6 Hz, 2H), 7.43 (d, *J* = 8.5 Hz, 2H), 7.66 (d, *J* = 16.4 Hz, 2H), 7.79-7.69 (m, *J* = 5.0 Hz, 2H), 8.11 (s, 1H), 8.28 (d, *J* = 6.5 Hz, 2H), 8.37 (d, *J* = 9.1 Hz, 1H). ^{13}C NMR ($CDCl_3$, 126 MHz, δ ppm): 105.2, 113.4, 118.7, 120.3, 121.1, 123.6, 125.8, 127.3, 128.1, 129.0, 131.2, 133.8, 135.3, 138.9, 144.4, 148.6, 149.3, 153.1, 162.8, 169.2. FT-IR (KBr pellet, cm^{-1}): 3353, 3220, 3011, 2851, 2254, 1680, 1669, 1540, 1329, 1222, 1059, 970, 885, 818, 724. Anal. Calcd. for $C_{38}H_{25}N_5O_3$: C, 76.11; H, 4.20; N, 11.68; O, 8.00. Found: C, 77.81; H, 5.69; N, 12.91; O, 9.09. GC-MS Anal. Calcd. for $C_{38}H_{25}N_5O_3$: 599.64. Found (m/z): 600.92. Similarly, compound **AT3-4** was prepared from compound ATPA using the same procedure described above.

5-((10-(4-((4-hydroxyphenyl)(phenyl)amino)phenyl)acridin-9(10H)ylidene)amino) picolinic acid (AT3) (yield 75 %). ^{1}H NMR ($CDCl_3$, 500 MHz, δ ppm): 4.98 (s, 3H), 6.69 (d, *J* = 5.5 Hz, 2H), 6.89 (d, *J* = 14.8 Hz, 2H), 7.01-6.92 (m, *J* = 6.5 Hz, 1H), 7.11 (d, *J* = 9.0 Hz, 2H), 7.23-7.15 (m, *J* = 6.0 Hz, 2H), 7.38 (d, *J* = 7.5 Hz, 2H), 7.47 (d, *J* = 8.5 Hz, 1H), 7.56 (d, *J* = 9.4 Hz, 2H), 7.75-7.62 (m, *J* = 15.2 Hz, 2H), 8.01(s, *J* = 7.2 Hz, 1H), 8.18 (d, *J* = 8.8 Hz, 2H), 8.49 (d, *J* = 15.0 Hz, 1H), 10.93 (s, 1H). ^{13}C NMR ($CDCl_3$, 126 MHz, δ ppm): 108.3, 115.4, 119.8, 121.5, 124.2, 126.8, 127.3, 129.5, 131.2, 133.6, 137.9, 139.8, 142.1, 144.6, 147.3,

149.5, 158.1, 161.4, 165.7, 171.2. FT-IR (KBr pellet, cm^{-1}): 3355, 3280, 3038, 2987, 2258, 1710, 1690, 1665, 1530, 1329, 1280, 1180, 1049, 965, 879, 821, 720. Anal. Calcd. for $C_{37}H_{26}N_4O_3$: C, 77.34; H, 4.56; N, 9.75; O, 8.35. Found: C, 78.58; H, 5.64; N, 10.99; O, 9.49. GC-MS Anal. Calcd. for $C_{37}H_{26}N_4O_3$: 574.63. Found (m/z): 575.89.

4-((4-(9-((2H-tetrazol-5-yl)imino)acridin-10(9H)-yl)phenyl)(phenyl)amino)phenol (AT4) (yield 72 %). ^{1}H NMR ($CDCl_3$, 500 MHz, δ ppm): 5.05 (s, 3H), 6.77 (d, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 7.7 Hz, 2H), 7.26 (d, *J* = 9.5 Hz, 2H), 7.41-7.33 (m, *J* = 15.4 Hz, 1H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.79-7.64 (m, *J* = 6.5 Hz, 2H), 7.83 (d, *J* = 13.9 Hz, 2H), 8.15-8.01 (m, *J* = 16.0 Hz, 2H), 8.31 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR ($CDCl_3$, 126 MHz, δ ppm): 110.7, 115.1, 119.5, 121.4, 125.6, 127.8, 129.6, 130.2, 132.7, 137.7, 139.8, 144.2, 148.6, 155.7, 159.4, 163.7, 168.2. FT-IR (KBr pellet, cm^{-1}): 3364, 3288, 3035, 2851, 2214, 1673, 1630, 1520, 1319, 1277, 1169, 1039, 973, 875, 818, 724. Anal. Calcd. for $C_{32}H_{23}N_7O$: C, 73.69; H, 4.44; N, 18.80; O, 3.07. Found: C, 74.58; H, 5.49; N, 19.18; O, 4.81. GC-MS Anal. Calcd. for $C_{32}H_{23}N_7O$: 521.57. Found (m/z): 522.28.

Synthesis of monomers AT-M(1-4)

A double-necked flask was charged with a mixture of a compound AT1 (1 g, 1.98 mmol) dissolved in dry DCM and treated with freshly distilled methacryloyl chloride (0.3 mL, 3.0 mmol) in the presence of triethylamine (TEA), at 0-5 ˚C. The above mixture was stirred at room temperature in presence of nitrogen atmosphere for 6 hrs. The quaternary ammonium salt was filtered and the reaction mixture separated using excess of DCM. The crude monomer was purified by column chromatography using $CHCl_3$/methanol (SiO_2; 4:1 v/v) as eluent. The obtained monomer AT-M1 was pale yellow coloured solid (yield 70%).

^{1}H NMR ($CDCl_3$, 500 MHz, δ ppm): 1.89 (s, 3H), 6.67 (d, *J* = 6.5 Hz, 1H), 7.05 (d, *J* = 9.0 Hz, 1H), 7.21 (d, *J* = 14.6 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.73-7.64 (m, *J* = 9.5 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 2H), 8.18-8.02 (m, *J* = 5.8 Hz, 1H), 8.30-8.22 (m, *J* = 8.6 Hz, 2H), 8.41 (d, *J* = 7.1 Hz, 2H), 8.55 (d, *J* = 15.2 Hz, 2H) (Fig. S5). ^{13}C NMR ($CDCl_3$, 126 MHz, δ ppm): 26.8, 89.2, 110.8, 115.7, 119.5, 120.7, 122.4, 124.3, 125.6, 127.8, 129.5, 131.6, 133.8, 135.9, 138.6, 139.2, 142.5, 145.7, 148.6, 166.3, 169.1 (Fig. S5). FT-IR (KBr pellet, cm^{-1}): 3274, 3060, 2962, 2849, 2253, 1714, 1634, 1556, 1342, 1261, 1097, 934, 860, 803, 750 (Fig. S4). Anal. Calcd. for $C_{39}H_{26}N_4O_2$: C, 82.37; H, 4.59; N, 9.85; O, 5.61. Found: C, 83.58; H, 5.39; N, 10.78; O, 6.19. GC-MS Anal. Calcd. for $C_{39}H_{26}N_4O_2$: 570.64. Found (m/z): 571.89.

The above synthesis procedure was followed for preparation of monomers **AT-M2, AT-M3** and **AT-M4**.

Monomer **AT-M2*:*** Yield 65%. ^{1}H NMR ($CDCl_3$, 500 MHz, δ ppm): 1.99 (s, 3H), 6.87 (d, *J* = 6.5 Hz, 1H), 6.98 (d, *J* = 5.0 Hz, 1H), 7.28 (s, *J* = 9.6 Hz, 1H), 7.35 (d, *J* = 14.3 Hz, 2H), 7.51 (d, *J* = 7.5 Hz, 2H), 7.69-7.58 (m, *J* = 8.1 Hz, 1H), 7.73 (d, *J* = 16.4 Hz, 2H), 7.91 (d, *J* = 7.0 Hz, 2H), 8.08-7.99 (m, *J* = 8.8 Hz, 2H), 8.29-8.13 (m, *J* = 9.6 Hz, 2H), 8.31 (d, *J* = 8.0 Hz, 2H), 8.45 (d, *J* = 15.4 Hz,, 2H), 8.57 (d, *J* = 9.1 Hz, 1H) (Fig. S7). ^{13}C NMR ($CDCl_3$, 126 MHz, δ ppm): 29.8, 95.46, 111.7, 118.1, 120.5, 122.4, 124.7, 125.6, 128.9, 129.3, 131.6, 134.8, 136.4, 137.6, 139.2, 140.5, 144.7, 146.2, 149.6, 161.2, 165.3, 171.6 (Fig. S7). FT-IR (KBr pellet, cm^{-1}): 3301, 3247, 2917, 2849, 1954, 1724, 1632, 1598, 1560, 1470, 1249, 1181, 1066, 967, 876, 807, 730 (Fig. S6). Anal. Calcd. for $C_{42}H_{29}N_5O_4$: C, 75.55; H, 4.38; N, 10.49; O, 9.58. Found: C, 76.83; H, 5.39; N, 11.87; O, 10.81. GC-MS Anal. Calcd. for $C_{42}H_{29}N_5O_4$: 667.71. Found (m/z): 668.92.

Monomer **AT-M3*:*** Yield 75%. ^{1}H NMR ($CDCl_3$, 500 MHz, δ ppm): 2.01 (s, 3H), 6.45 (s, 1H), 6.92 (d, *J* = 7.8 Hz, 1H), 7.15 (d, *J* = 9.5 Hz, 2H), 7.23 (s, *J* = 14.4 Hz, 1H), 7.33 (d, *J* = 8.6 Hz, 2H), 7.48-7.32 (m, *J* = 6.6 Hz, 1H), 7.61-7.50 (m, *J* = 8.5 Hz, 2H), 7.79 (d, *J* = 8.1 Hz, 2H), 7.85 (d, *J* = 15.8 Hz, 1H), 7.91 (d, *J* = 9.5 Hz, 2H), 8.18 (d, *J* = 7.0 Hz, 2H), 8.37-8.22 (m, *J* = 8.4 Hz, 2H), 8.51(d, *J* = 6.3 Hz, 1H), 10.90 (s, 1H) (Fig. S9). ^{13}C NMR ($CDCl_3$, 126 MHz, δ ppm): 28.4, 109.7, 115.6, 119.5, 121.7, 123.7, 124.6, 126.8, 127.3, 129.6, 130.5, 135.2, 137.6, 142.9, 145.6, 148.6, 149.2, 151.6, 164.8, 166.6, 168.3, 169.7 (Fig. S9). FT-IR (KBr pellet, cm^{-1}): 3422, 3053, 2960, 2924, 1925, 1710, 1656, 1625, 1599, 1455, 1353, 1230, 1182, 1024, 967, 897, 816, 748 (Fig. S8). Anal. Calcd for $C_{41}H_{30}N_4O_4$: C, 76.62; H, 4.70; N, 8.72; O, 9.96. Found: C, 77.58; H, 5.43; N, 9.18; O, 10.59. GC-MS Anal. Calcd. for $C_{41}H_{30}N_4O_4$: 642.70. Found (m/z): 643.55.

Monomer **AT-M4*:*** Yield 68%. ^{1}H NMR ($CDCl_3$, 500 MHz, δ ppm): 1.85 (s, 3H), 4.12 (s, 1H), 6.32 (d, *J* = 7.7 Hz, 1H), 7.15 (d, *J* = 15.2 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.45-7.38 (m, *J* = 6.5 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 2H), 7.79-7.63 (m, *J* = 8.6 Hz, 2H), 8.02 (d, *J* = 14.1 Hz, 2H), 8.21-8.11 (m, *J* = 9.5 Hz, 2H), 8.35 (d, *J* = 6.4 Hz, 2H), 8.61-8.49 (m, *J* = 8.0 Hz, 2H) (Fig. S11). ^{13}C NMR ($CDCl_3$, 126 MHz, δ ppm): 28.8, 105.7, 110.4, 118.9, 120.5, 122.4, 125.7, 127.2, 128.3, 130.4, 133.8, 135.2, 137.6, 142.5, 144.6, 147.3, 158.4, 161.7, 165.2, 169.3 (Fig. S11). FT-IR (KBr pellet, cm^{-1}): 3255, 3062, 2925, 2582, 1725, 1673, 1614, 1525, 1465, 1261, 1173, 1031, 977, 879, 813, 750 (Fig. S10). Anal. Calcd. for $C_{36}H_{27}N_7O_2$: C, 73.33; H, 4.62; N,

16.63; O, 5.43. Found: C, 74.58; H, 5.39; N, 17.78; O, 6.67. GC-MS Anal. Calcd. for $C_{36}H_{27}N_7O_2$: 589.65. Found (m/z): 590.12.

Synthesis of polymers AT-P(1-4)

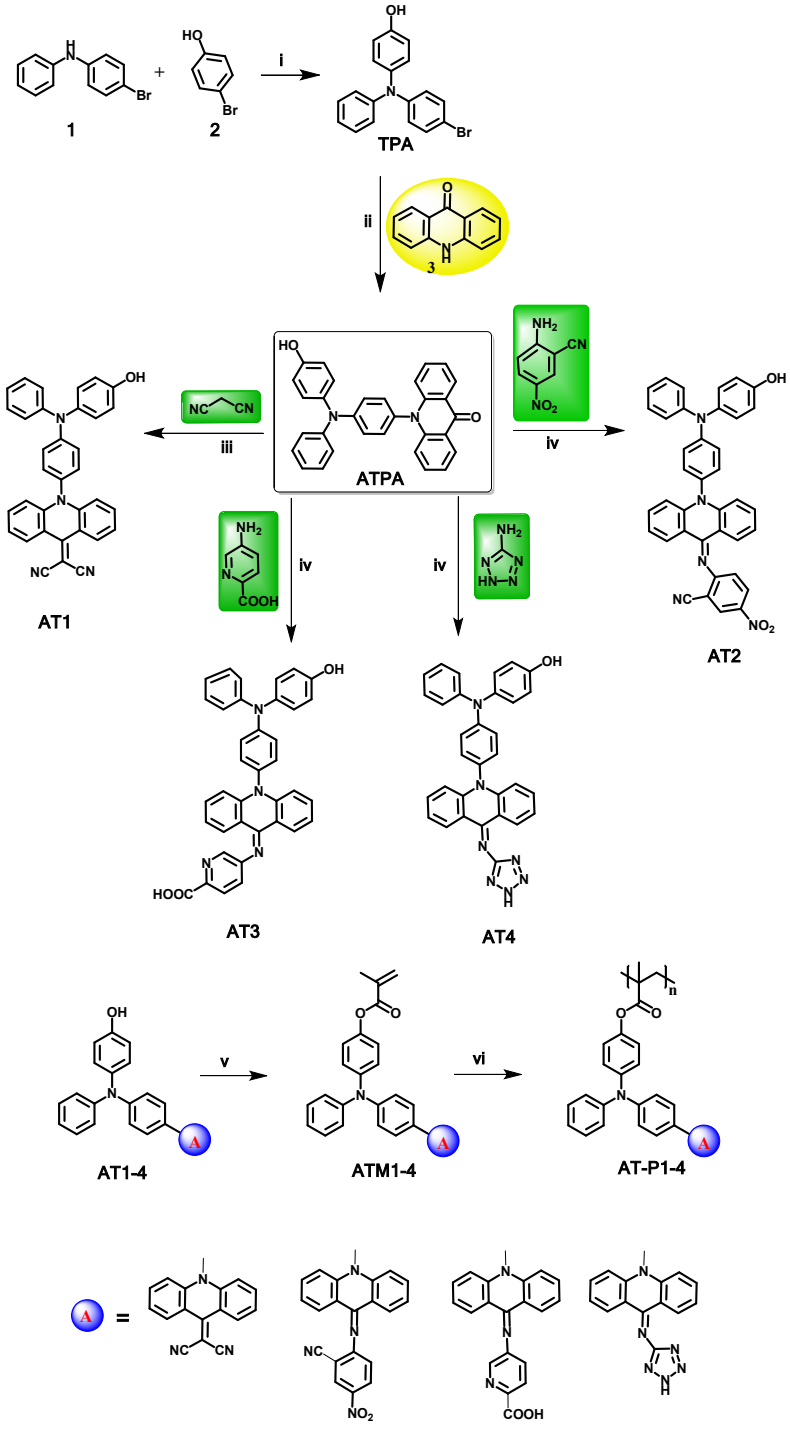
The methacrylate polymers **AT-P(1-4)** were synthesized by solution free radical polymerization using AIBN as initiator. To a Schlenk flask were added monomer (**AT-M1**) and AIBN (0.5% wt. of monomer) in 10 mL THF solution, and the flask was tightly sealed with rubber septum. The reaction mixture was then degassed by purging with nitrogen gas for 30 min, and the flask was sealed and kept at 75±5 °C oil bath with constant stirring. After 48 hours, the polymer is exposed to the air and cooled to room temperature, and then poured into methanol to precipitate the polymer. The polymer obtained was separated by filtration and purified by repeated precipitation from chloroform into methanol and then dried in vacuum. The yield obtained was 70%. By the similar procedure, polymers **AT-P2**, **AT-P3** and **AT-P4** were prepared (Scheme 1). The characterization data of **AT-P1, AT-P2, AT-P3** and **AT-P4** are given below.

Polymer **AT-P1**: ^{1}H NMR (DMSO-d_6, 500 MHz, δ ppm): 1.19-1.01 (m, *J* = 6.5 Hz, 2H), 1.51 (s, 3H), 2.05-2.22 (m, *J* = 9.2 Hz, 2H), 7.27 (d, *J* = 5.5 Hz, 2H), 7.39-7.28 (m, *J* = 7.1 Hz, 1H), 7.48 (d, *J* = 8.5 Hz, 2H), 7.60 (d, *J* = 7.0 Hz, 2H), 7.77-7.68 (m, *J* = 15.8 Hz, 2H), 7.81 (d, *J* = 14.5 Hz, 2H), 7.90 (d, *J* = 8.2 Hz, 1H), 8.05-7.90 (m, *J* = 6.4 Hz, 2H), 8.28 (d, *J* = 7.8 Hz, 2H), 8.37 (d, *J* = 8.0 Hz, 2H) (Fig. S5). ^{13}C NMR ($CDCl_3$, 126 MHz, δ ppm): 27.6, 38.1, 41.5, 89.3, 104.2, 114.2, 117.6, 119.3, 122.7, 125.3, 126.1, 128.6, 133.7, 135.2, 138.9, 139.3, 142.2, 145.6, 148.4, 158.5, 165.1, 173.3 (Fig. S5). FTIR (KBr pellet, cm^{-1}): 3274, 3027, 2961, 2849, 2325, 1728, 1634, 1597, 1343, 1261, 1023, 935, 860, 802, 751 (Fig. S4). GPC: M_w = 23500 g·mol^{-1}, M_w/M_n = 1.52.

Polymer **AT-P2**: ^{1}H NMR (DMSO-d_6, 500 MHz, δ ppm): 1.23-1.39 (m, *J* = 7.1 Hz, 2H), 1.78 (s, 3H), 2.05 (m, *J* = 5.5 Hz, 2H), 6.29 (s, 1H), 6.49 (d, *J* = 16.8 Hz, 2H), 6.88 (d, *J* = 15.1 Hz, 2H), 7.00-6.92 (m, *J* = 9.0 Hz, 1H), 7.10 (d, *J* = 8.5 Hz, 2H), 7.28-7.11 (m, *J* = 7.8 Hz, 2H), 7.29 (d, *J* = 9.4 Hz, 2H), 7.38 (d, *J* = 14.2 Hz, 2H), 7.65-7.50 (m, *J* = 8.1 Hz, 2H), 7.88 (d, *J* = 7.8 Hz, 2H), 8.02-7.90 (m, *J* = 5.5 Hz, 1H), 8.30 (d, *J* = 16.4 Hz, 2H) (Fig. S7). ^{13}C NMR (DMSO-d_6, 126 MHz, δ ppm): 23.6, 31.7, 39.5, 97.4, 108.2, 113.2, 118.3, 120.6, 121.4, 123.7, 125.5, 126.3, 127.5, 129.1, 130.2, 132.3, 134.7, 137.2, 140.3, 144.8, 148.6, 151.5, 159.3, 164.9, 169.3, 178.3 (Fig. S7). FTIR (KBr pellet, cm^{-1}): 3360, 3234, 3061, 2948, 2852, 1727, 1634, 1598, 1531, 1473, 1346, 1159, 1022, 1022, 937, 816, 752 (Fig. S6). GPC: M_w = 27900 g·mol^{-1}, M_w/M_n = 1.87.

Polymer **AT-P3**: ^{1}H NMR (DMSO-d_6, 500 MHz, δ ppm): 1.13-1.08 (m, J = 9.0 Hz, 2H), 1.82 (s, 3H), 2.18-2.05 (m, J = 6.6 Hz, 2H), 6.93 (d, J = 9.8 Hz, 2H), 7.13 (s, 1H), 7.08-6.99 (m, J = 14.1 Hz, 2H), 7.24 (d, J = 8.5 Hz, 2H), 7.38 (d, J = 6.8 Hz, 2H), 7.50 (d, J = 8.4 Hz, 2H), 7.62 (d, J = 8.5 Hz, 2H), 7.75-7.68 (m, J = 15.6 Hz, 2H), 7.86-7.79 (m, J = 9.4 Hz, 2H), 8.05 (d, J = 7.7 Hz, 2H), 8.22 (d, J = 8.5 Hz, 1H) 11.56 (s, 1H) (Fig. S9). ^{13}C NMR ($CDCl_3$, 126 MHz, δ ppm): 25.6, 35.7, 49.1, 98.6, 107.2, 113.5, 118.7, 119.6, 121.7, 123.5, 124.7, 126.5, 127.6, 129.1, 131.6, 133.4, 135.8, 137.9, 139.2, 141.2, 144.8, 145.3, 148.4, 149.6, 154.4, 165.9, 168.3, 169.5, 174.7 (Fig. S9). FTIR (KBr pellet, cm^{-1}): 3412, 3054, 3018, 2851, 1713, 1659, 1626, 1505, 1353, 1232, 1179, 1023, 968, 859, 816, 748 (Fig. S8). GPC: M_w = 33400 g·mol^{-1}, M_w/M_n = 1.90.

Polymer **AT-P4**: ^{1}H NMR (DMSO-d_6, 500 MHz δ ppm): 1.29-1.18 (m, J = 9.5 Hz, 2H), 1.91 (s, 3H), 2.09 (m, J = 16.1 Hz, 2H), 6.71 (d, J = 14.8 Hz, 2H), 6.87-6.75 (m, J = 5.7 Hz, 2H), 7.02-6.95 (m, J = 8.5 Hz, 1H), 7.18 (d, J = 8.0 Hz, 2H), 7.39-7.23 (m, J = 7.4 Hz, 2H), 7.68 (d, J = 14.5 Hz, 2H), 7.81 (d, J = 8.6 Hz, 2H), 7.95 (d, J = 9.1 Hz, 2H), 8.11 (d, J = 15.5 Hz, 2H), 8.32 (d, J = 6.0 Hz, 2H) (Fig. S11). ^{13}C NMR (DMSO-d_6, 126 MHz, δ ppm): 28.6, 38.7, 44.5, 88.6, 102.5, 113.8, 118.2, 120.6, 121.7, 123.5, 124.1, 126.4, 127.6, 129.5, 131.7, 133.2, 134.2, 137.9, 139.1, 141.5, 143.9, 146.5, 149.4, 157.7, 161.9, 167.7, 169.3, 175.8 (Fig. S11). FTIR (KBr pellet, cm^{-1}): 3338, 3060, 2924, 2869, 2234, 1741, 1673, 1594, 1368, 1261, 1145, 1031, 981, 879, 815, 754 (Fig. S10). GPC: M_w = 31900 g·mol^{-1}, M_w/M_n = 1.43.



Scheme 1. Synthetic pathway for the polymers **AT-P1-4**
Reagents and Conditions: i) K_2CO_3, CuI/1,10-phenanthroline in toluene at 100-115 °C ii) K_3PO_4/CuI/1, 2-diaminocycloheane/DMF at 110°c iii) $TiCl_4$, pyridine at 120 °C iv) AcOH/reflux v) Methacryloyl chloride/DCM at 0°c vi) ACBN/THF at 70-75°c

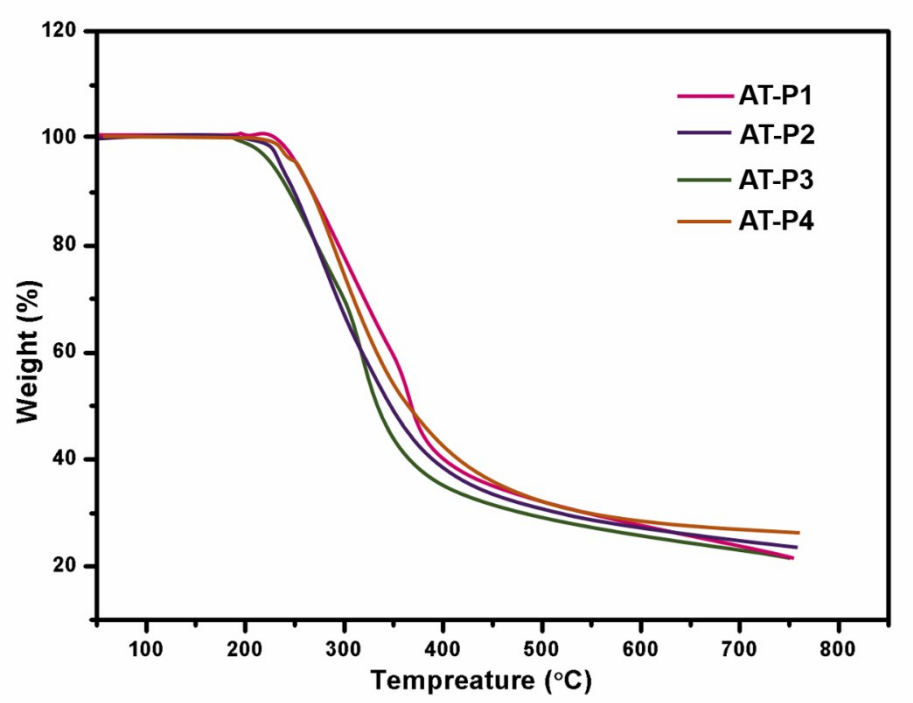


Figure S1. TGA curves of polymers **AT-P1, AT-P2, AT-P3 and AT-P4**

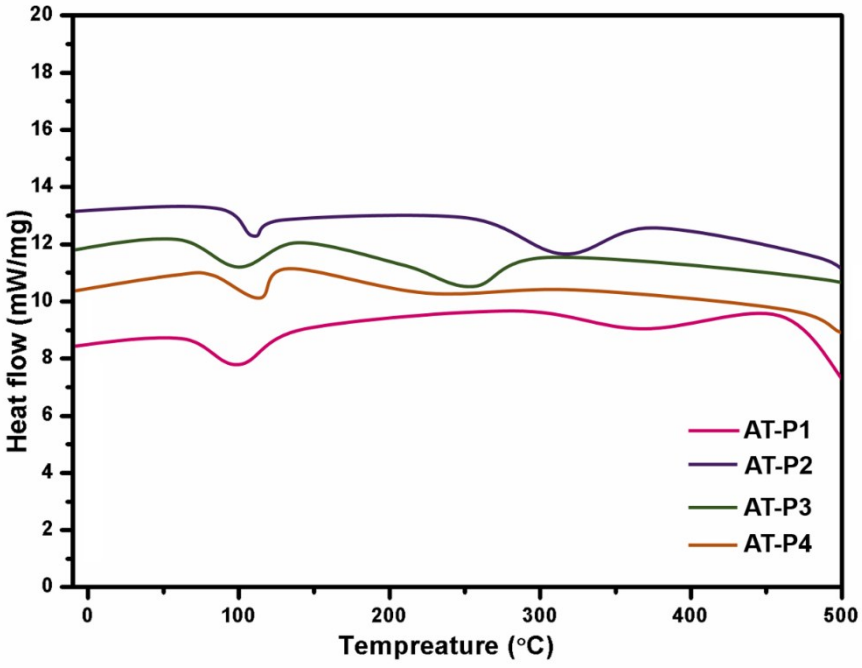


Figure S2. DSC curves of polymers **AT-P1, AT-P2, AT-P3 and AT-P4**

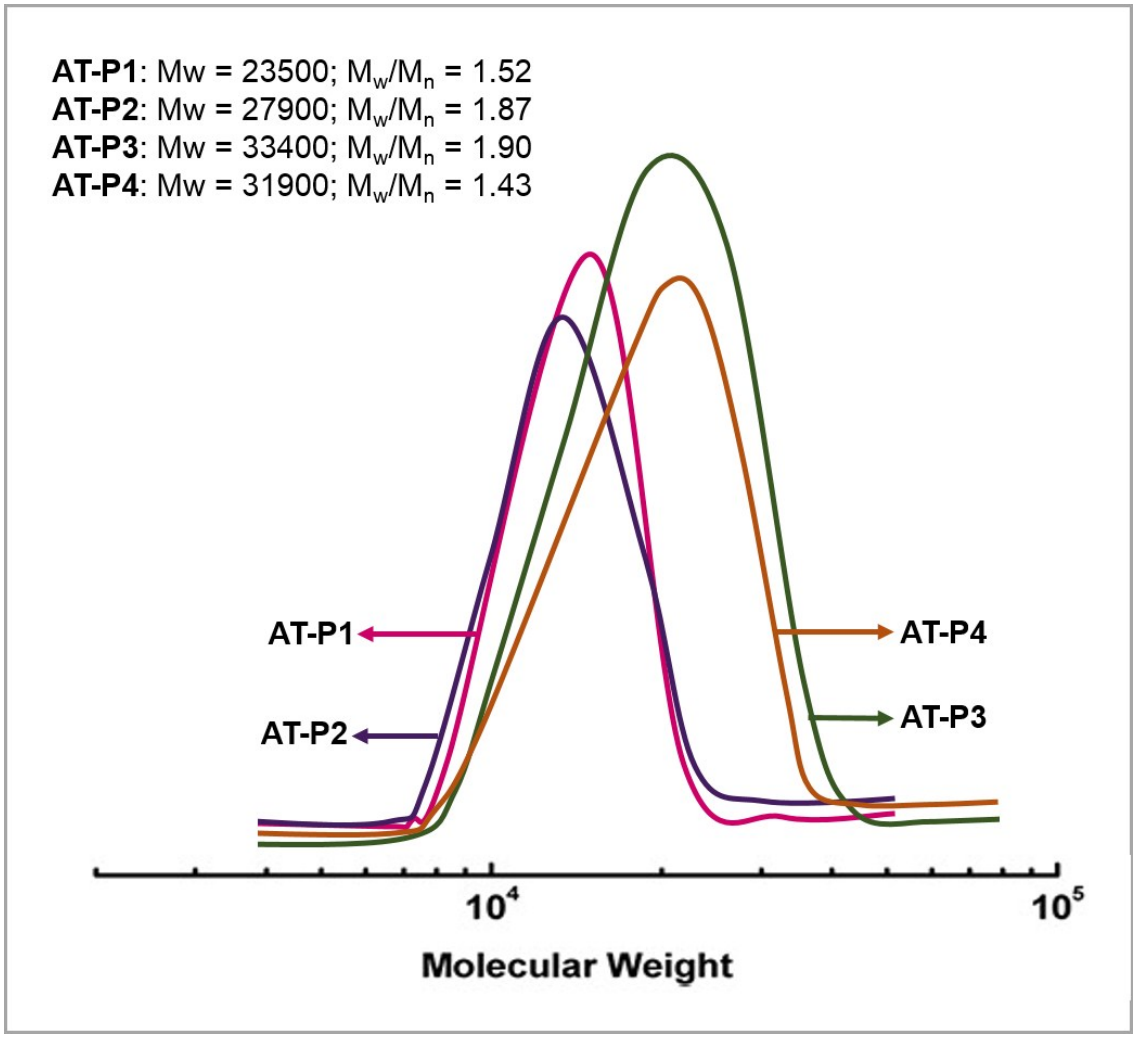


Figure S3. GPC curves of polymers **AT-P1, AT-P2, AT-P3 and AT-P4**

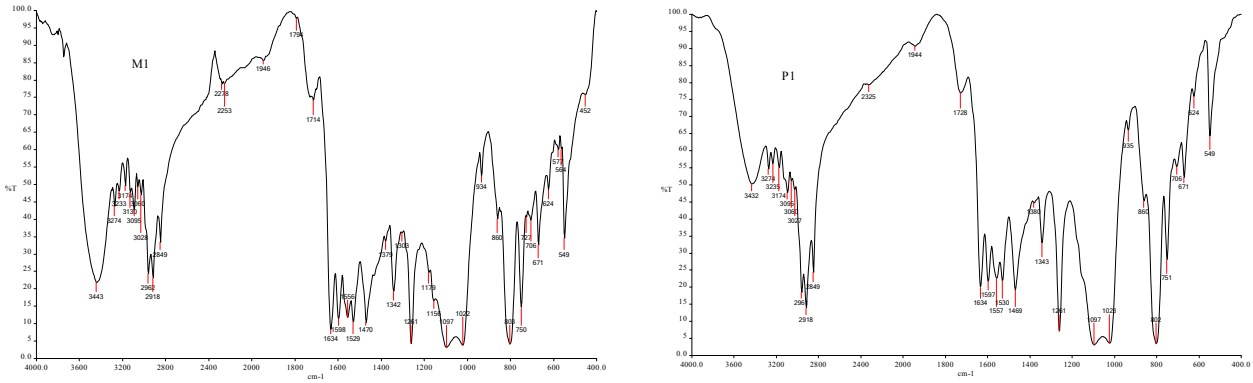


Figure S4. FT-IR spectra of monomers **AT-M1** and polymers **AT-P1**

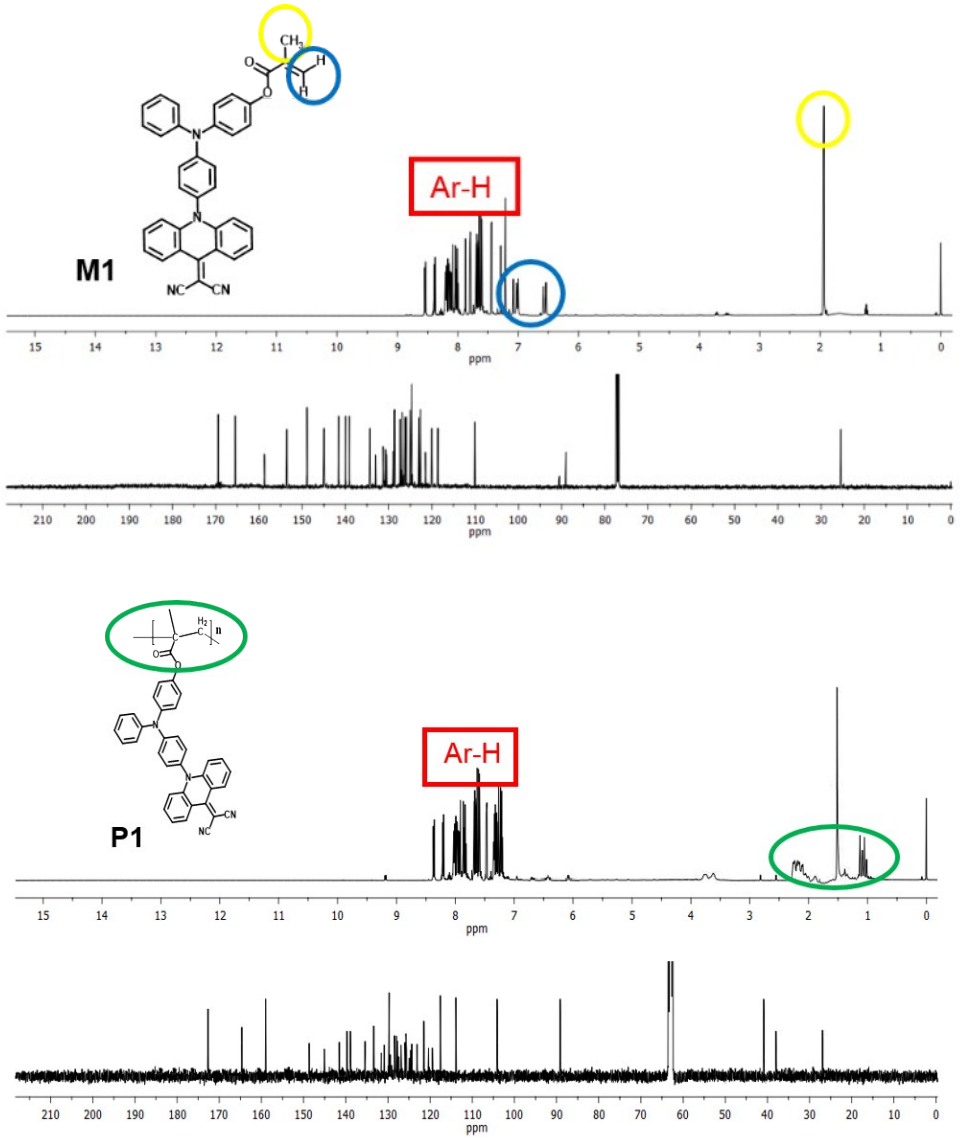


Figure S5. ^{1}H-NMR, ^{13}C-NMR Monomer **AT-M1** and Polymer **AT-P1**

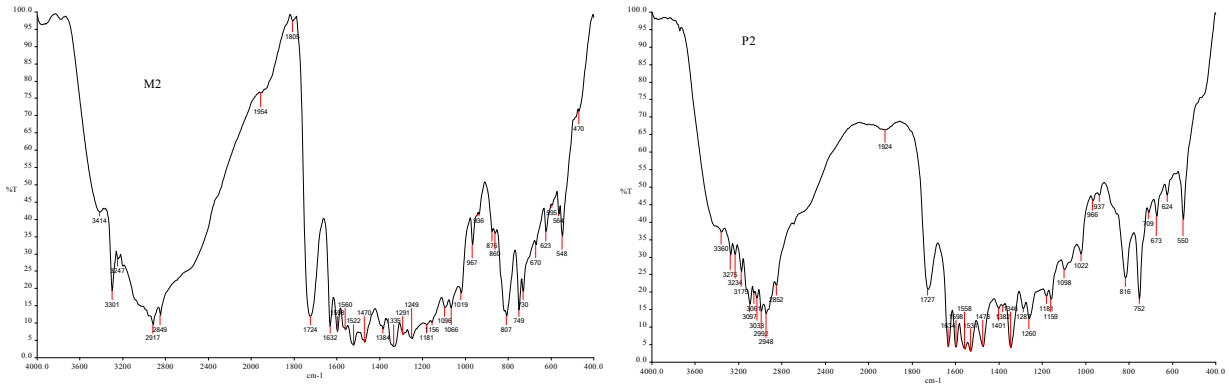


Figure S6. FT-IR spectra of monomers **AT-M2** and polymers **AT-P2**

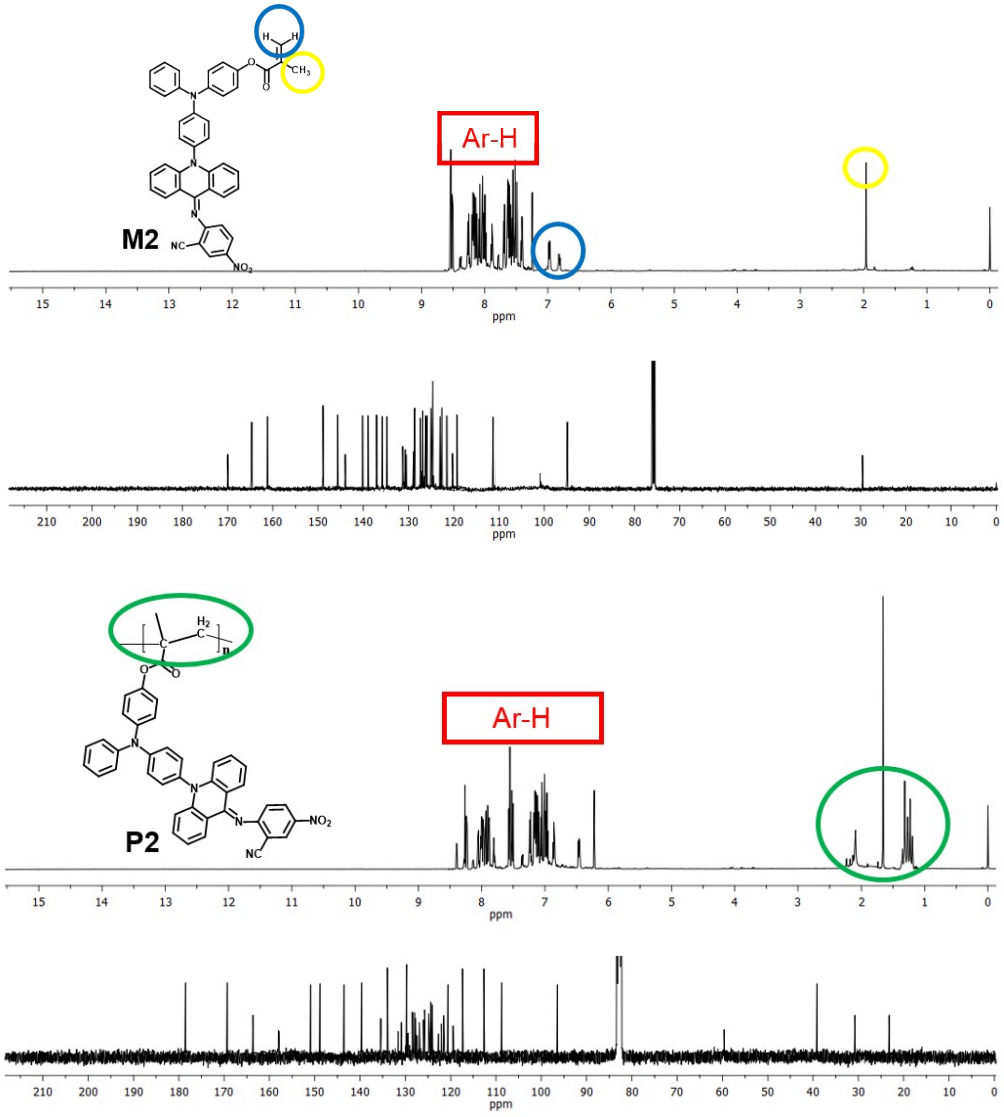


Figure S7. ^{1}H-NMR, ^{13}C-NMR Monomer **AT-M2** and Polymer **AT-P2**

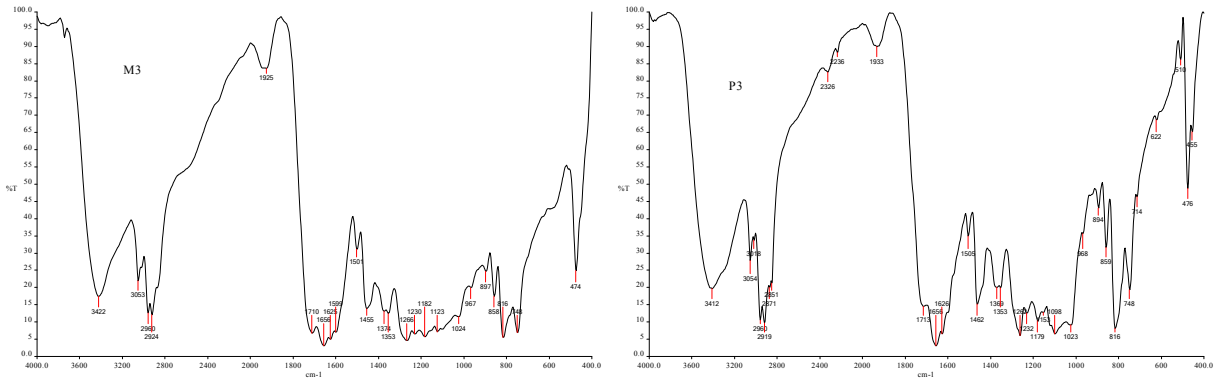


Figure S8. FT-IR spectra of monomers **AT-M3** and polymers **AT-P3**

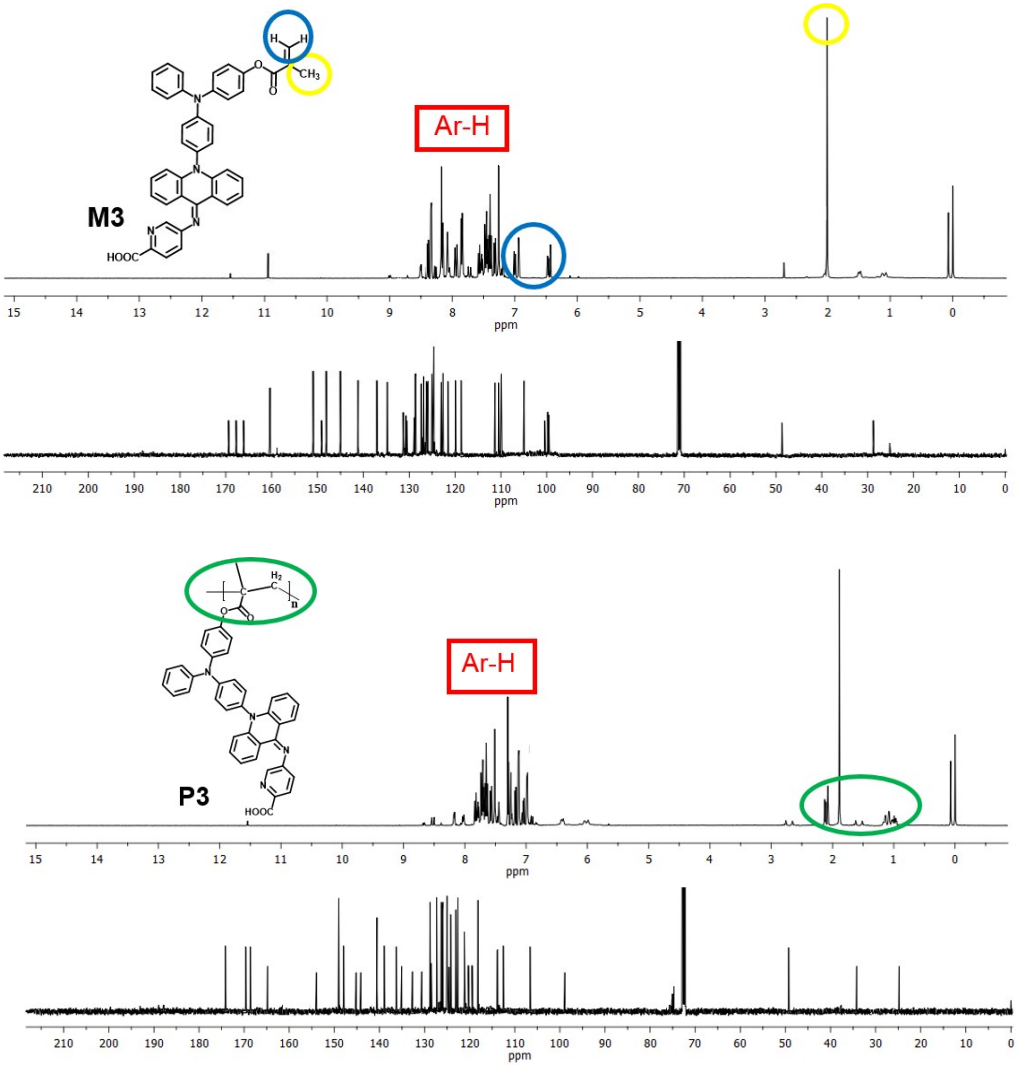


Figure S9. ^{1}H-NMR, ^{13}C-NMR Monomer **AT-M3** and Polymer **AT-P3**

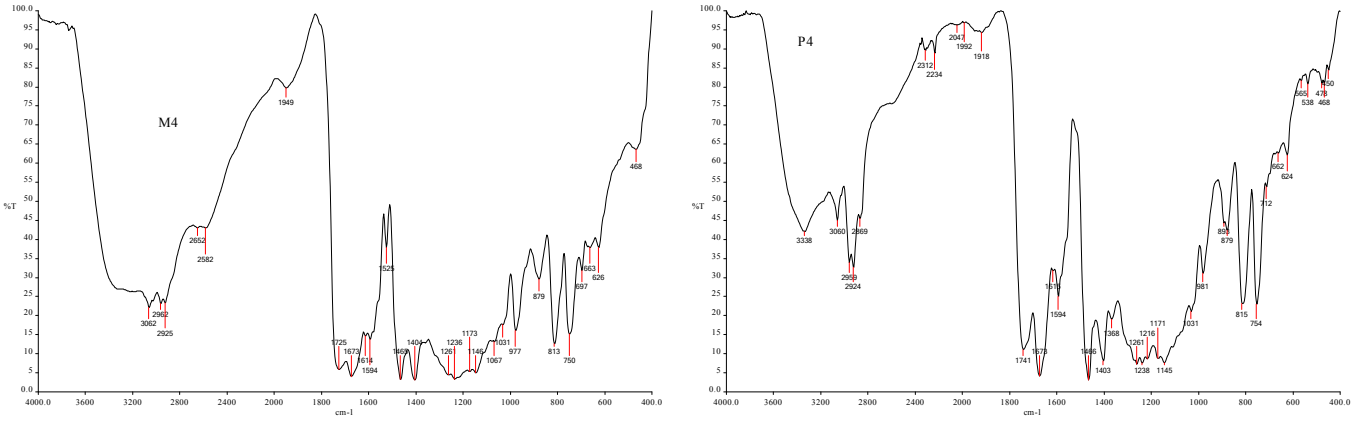


Figure S10. FT-IR spectra of monomers **AT-M4** and polymers **AT-P4**

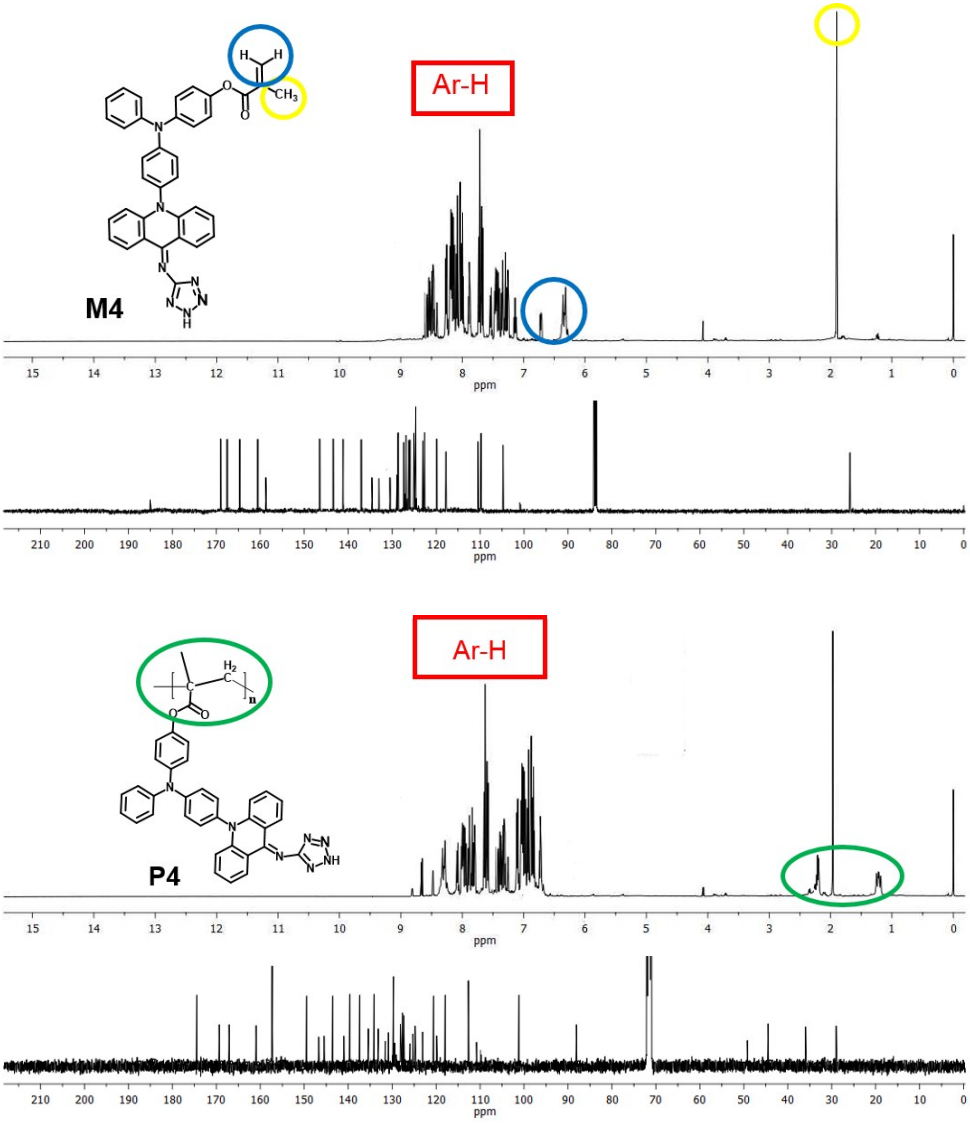


Figure S11. ^{1}H-NMR, ^{13}C-NMR Monomer **AT-M4** and Polymer **AT-P4**