

Supplementary Materials

Facile Synthesis of Electroactive and Electrochromic Triptycene Poly(ether-imide)s Containing Triarylamine Units via Oxidative Electro-coupling

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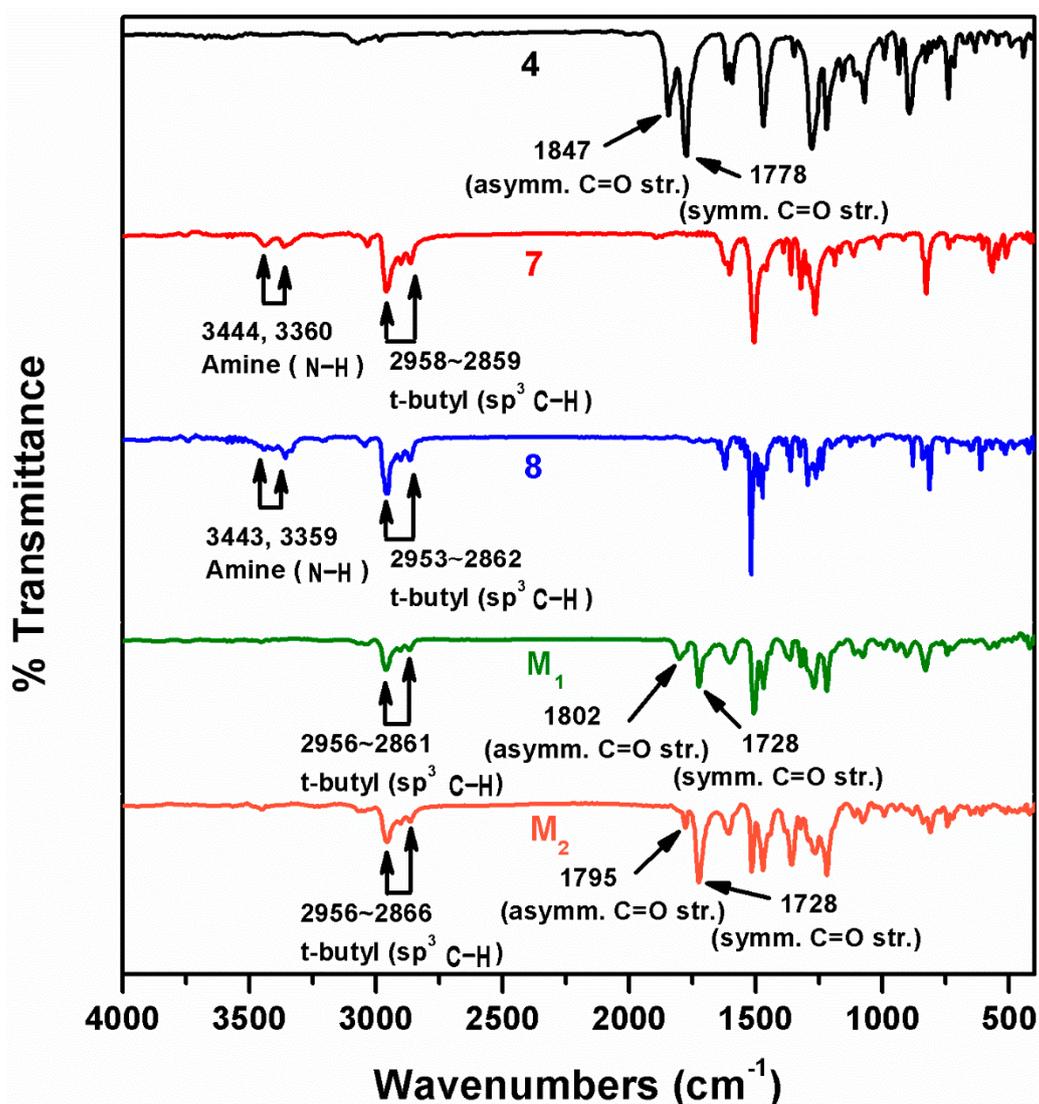


Figure S1. IR spectra of model compounds M₁ and M₂ together with compounds 4, 7 and 8.

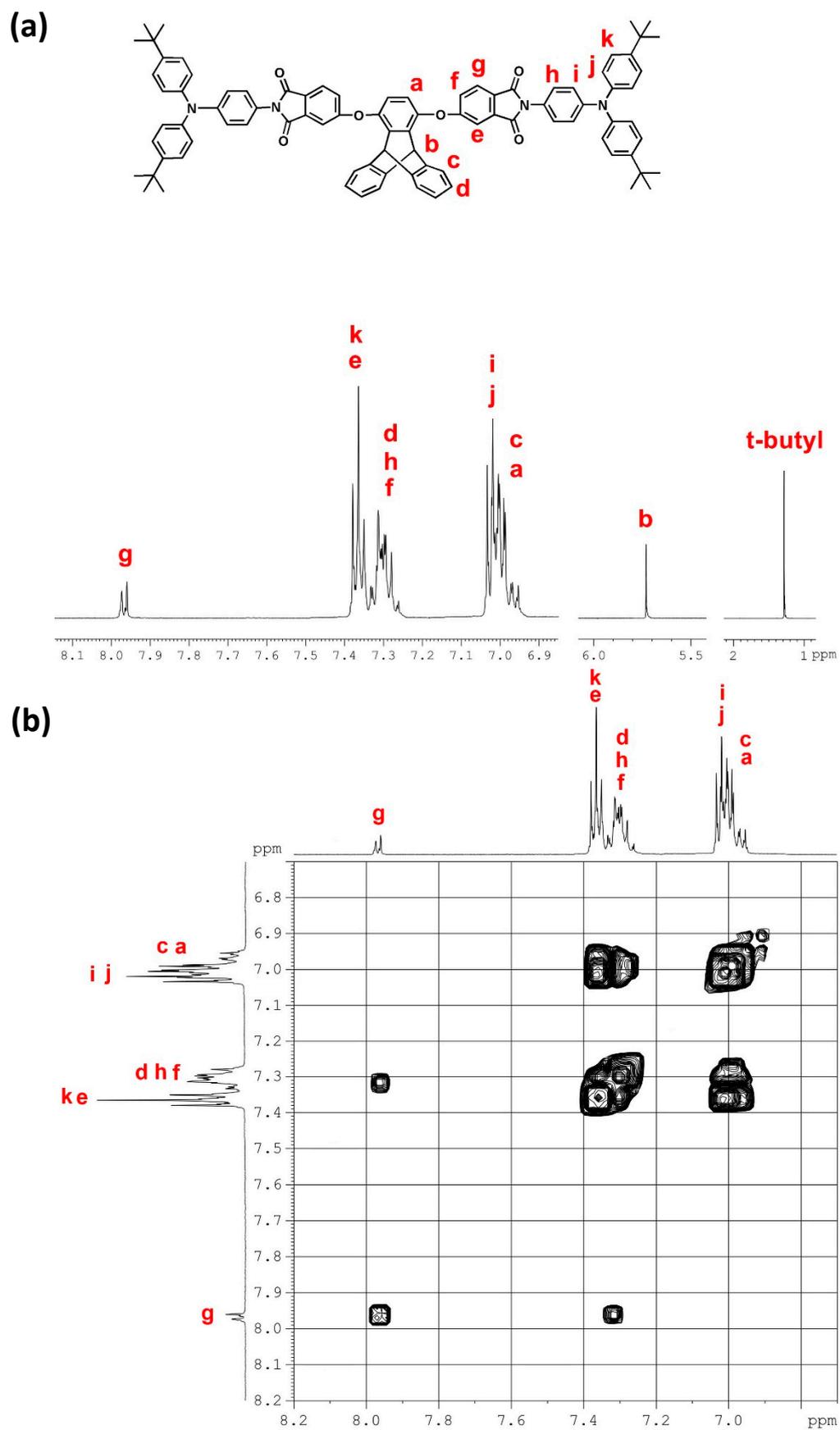


Figure S2. (a) ^1H NMR and (b) H-H COSY spectra of M_1 in $\text{DMSO-}d_6$.

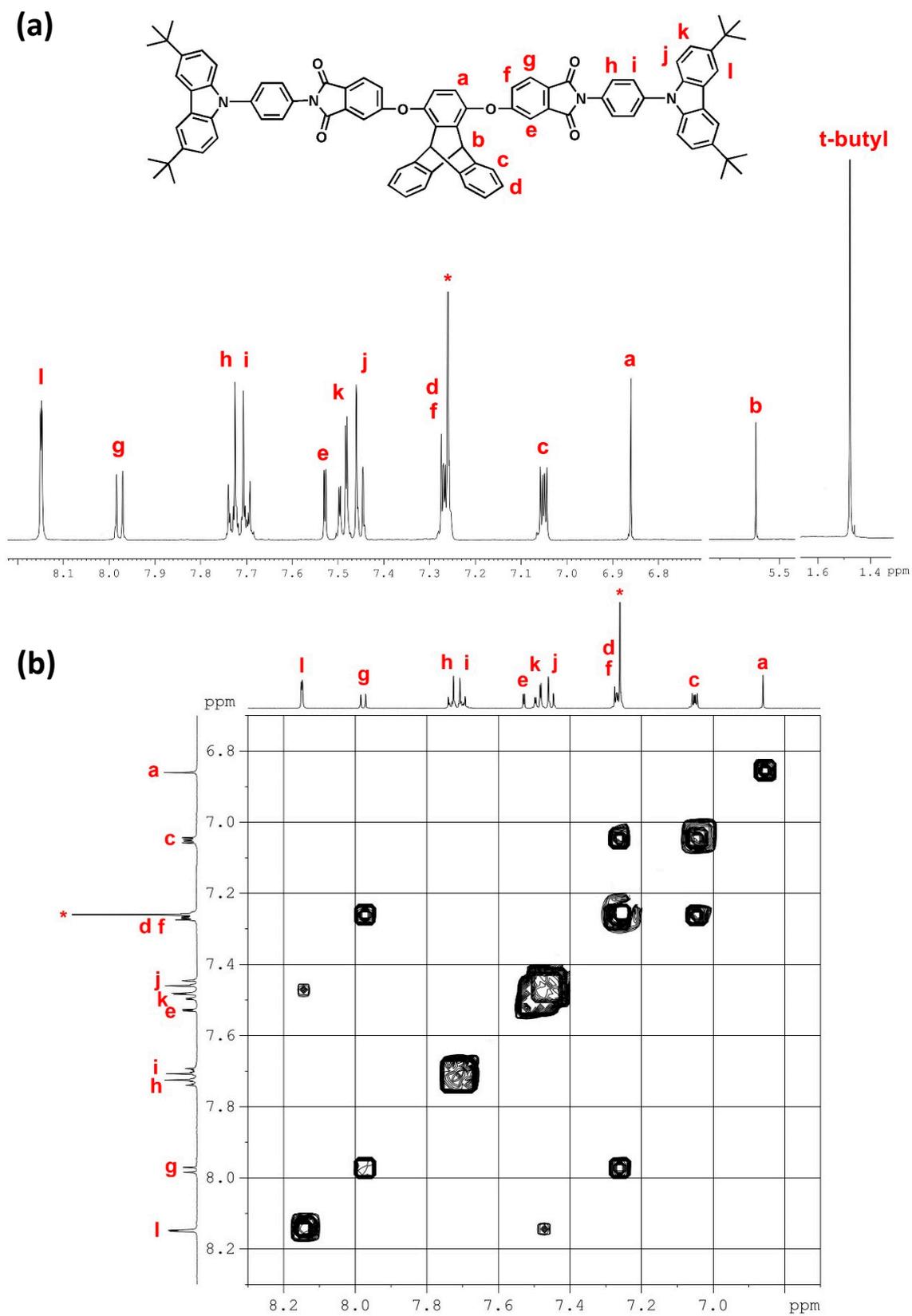


Figure S3. (a) ^1H NMR and (b) H-H COSY spectra of M_2 in CDCl_3 (* solvent peak).

Elemental Composition Report

Single Mass Analysis

Tolerance = 200.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

172 formula(e) evaluated with 41 results within limits (all results (up to 1000) for each mass)

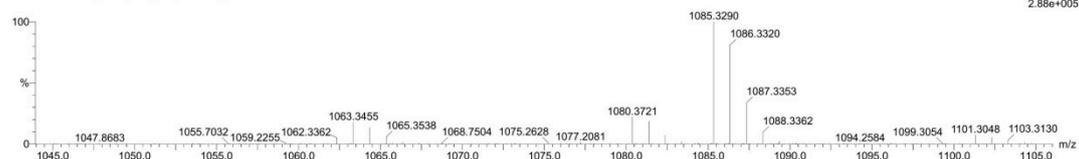
Elements Used:

C: 70-80 H: 40-100 N: 1-5 O: 1-10 Na: 1-1

TPA

170421esi06 592 (5.746) Cm (592-(569+616))

21-Apr-2017
1: TOF MS ES+
2.88e+005



Minimum: -1.5
Maximum: 100.0

| Mass | Calc. Mass | mDa | PPM | DBE | Formula |
|-----------|------------|--------|--------|------|------------------|
| 1085.3290 | 1085.3315 | -2.5 | -2.3 | 51.5 | C72 H46 N4 O6 Na |
| | 1085.3326 | 3.4 | 3.1 | 60.5 | C79 H42 N4 O Na |
| | 1085.3355 | -6.5 | -6.0 | 55.5 | C77 H46 N2 O4 Na |
| | 1085.3203 | 8.7 | 8.0 | 51.5 | C73 H46 N2 O7 Na |
| | 1085.3414 | -12.4 | -11.4 | 46.5 | C70 H50 N2 O9 Na |
| | 1085.3144 | 14.6 | 13.5 | 60.5 | C80 H42 N2 O2 Na |
| | 1085.3468 | -17.8 | -16.4 | 55.5 | C76 H46 N4 O3 Na |
| | 1085.3104 | 18.6 | 17.1 | 56.5 | C75 H42 N4 O4 Na |
| | 1085.3567 | -27.7 | -25.5 | 50.5 | C74 H50 N2 O6 Na |
| | 1085.2991 | 29.9 | 27.5 | 56.5 | C76 H42 N2 O5 Na |
| | 1085.2951 | 33.9 | 31.2 | 52.5 | C71 H42 N4 O7 Na |
| | 1085.3679 | -38.9 | -35.8 | 50.5 | C73 H50 N4 O5 Na |
| | 1085.3719 | -42.9 | -39.5 | 54.5 | C78 H50 N2 O3 Na |
| | 1085.2839 | 45.1 | 41.6 | 52.5 | C72 H42 N2 O8 Na |
| | 1085.3778 | -48.8 | -45.0 | 45.5 | C71 H54 N2 O8 Na |
| | 1085.3831 | -54.1 | -49.8 | 54.5 | C77 H50 N4 O2 Na |
| | 1085.3890 | -60.0 | -55.3 | 45.5 | C70 H54 N4 O7 Na |
| | 1085.3930 | -64.0 | -59.0 | 49.5 | C75 H54 N2 O5 Na |
| | 1085.4043 | -75.3 | -69.4 | 49.5 | C74 H54 N4 O4 Na |
| | 1085.4083 | -79.3 | -73.1 | 53.5 | C79 H54 N2 O2 Na |
| | 1085.4142 | -85.2 | -78.5 | 44.5 | C72 H58 N2 O7 Na |
| | 1085.4195 | -90.5 | -83.4 | 53.5 | C78 H54 N4 O Na |
| | 1085.4254 | -96.4 | -88.8 | 44.5 | C71 H58 N4 O6 Na |
| | 1085.4294 | -100.4 | -92.5 | 48.5 | C76 H58 N2 O4 Na |
| | 1085.4407 | -111.7 | -102.9 | 48.5 | C75 H58 N4 O3 Na |
| | 1085.4447 | -115.7 | -106.6 | 52.5 | C80 H58 N2 O Na |
| | 1085.4506 | -121.6 | -112.0 | 43.5 | C73 H62 N2 O6 Na |

| Sample name ^o | 分子式 ^o | 結構式 ^o | Exact mass ^o |
|--------------------------|--|------------------|-------------------------|
| TPA ^o | C ₇₂ H ₄₆ N ₄ O ₆ ^o | | 1062.34 ^o |

Elemental Composition Report

Single Mass Analysis

Tolerance = 200.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

166 formula(e) evaluated with 35 results within limits (all results (up to 1000) for each mass)

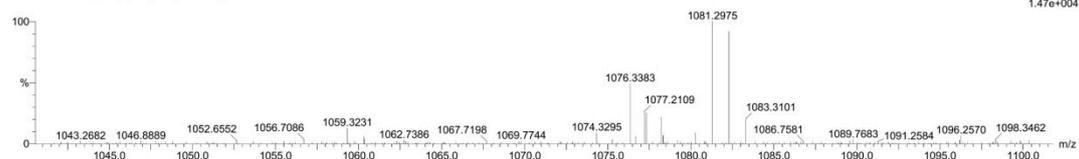
Elements Used:

C: 70-80 H: 40-100 N: 1-5 O: 1-10 Na: 1-1

NPC

170421esi07 588 (5.712) Cm (588-(576+597))

21-Apr-2017
1: TOF MS ES+
1.47e+004

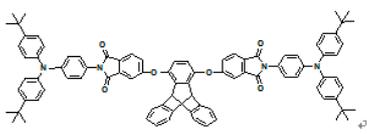


Minimum: -1.5
Maximum: 100.0

| Mass | Calc. Mass | mDa | PPM | DBE | Formula |
|-----------|------------|--------|--------|------|------------------|
| 1081.2975 | 1081.3002 | -2.7 | -2.5 | 53.5 | C72 H42 N4 O6 Na |
| | 1081.3042 | -6.7 | -6.2 | 57.5 | C77 H42 N2 O4 Na |
| | 1081.2890 | 8.5 | 7.9 | 53.5 | C73 H42 N2 O7 Na |
| | 1081.3101 | -12.6 | -11.7 | 48.5 | C70 H46 N2 O9 Na |
| | 1081.3155 | -18.0 | -16.6 | 57.5 | C76 H42 N4 O3 Na |
| | 1081.3254 | -27.9 | -25.8 | 52.5 | C74 H46 N2 O6 Na |
| | 1081.3366 | -39.1 | -36.2 | 52.5 | C73 H46 N4 O5 Na |
| | 1081.3406 | -43.1 | -39.9 | 56.5 | C78 H46 N2 O3 Na |
| | 1081.3465 | -49.0 | -45.3 | 47.5 | C71 H50 N2 O8 Na |
| | 1081.3518 | -54.3 | -50.2 | 56.5 | C77 H46 N4 O2 Na |
| | 1081.3577 | -60.2 | -55.7 | 47.5 | C70 H50 N4 O7 Na |
| | 1081.3617 | -64.2 | -59.4 | 51.5 | C75 H50 N2 O5 Na |
| | 1081.3730 | -75.5 | -69.8 | 51.5 | C74 H50 N4 O4 Na |
| | 1081.3770 | -79.5 | -73.5 | 55.5 | C79 H50 N2 O2 Na |
| | 1081.3829 | -85.4 | -79.0 | 46.5 | C72 H54 N2 O7 Na |
| | 1081.3882 | -90.7 | -83.9 | 55.5 | C78 H50 N4 O Na |
| | 1081.3941 | -96.6 | -89.3 | 46.5 | C71 H54 N4 O6 Na |
| | 1081.3981 | -100.6 | -93.0 | 50.5 | C76 H54 N2 O4 Na |
| | 1081.4094 | -111.9 | -103.5 | 50.5 | C75 H54 N4 O3 Na |
| | 1081.4134 | -115.9 | -107.2 | 54.5 | C80 H54 N2 O Na |
| | 1081.4193 | -121.8 | -112.6 | 45.5 | C73 H58 N2 O6 Na |
| | 1081.4305 | -133.0 | -123.0 | 45.5 | C72 H58 N4 O5 Na |
| | 1081.4345 | -137.0 | -126.7 | 49.5 | C77 H58 N2 O3 Na |
| | 1081.4404 | -142.9 | -132.2 | 40.5 | C70 H62 N2 O8 Na |
| | 1081.4457 | -148.2 | -137.1 | 49.5 | C76 H58 N4 O2 Na |
| | 1081.4556 | -158.1 | -146.2 | 44.5 | C74 H62 N2 O5 Na |
| | 1081.4669 | -169.4 | -156.7 | 44.5 | C73 H62 N4 O4 Na |

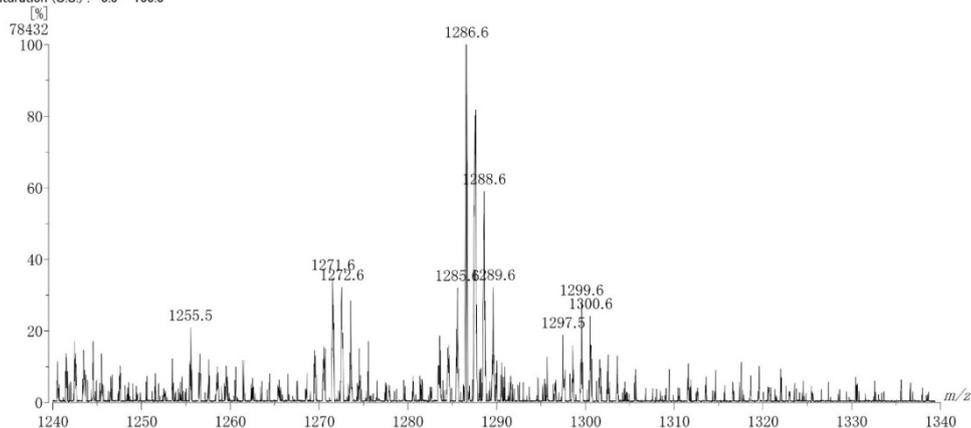
| Sample name ^o | 分子式 ^o | 結構式 ^o | Exact mass ^o |
|--------------------------|--|------------------|-------------------------|
| NPC ^o | C ₇₂ H ₄₂ N ₄ O ₆ ^o | | 1058.31 ^o |

Figure S4. Mass spectra of monomers TPA-TPDI and NPC-TPDI.

| Sample name ^o | 分子式 ^o | 結構式 ^o | Exact mass ^o |
|--------------------------|--|--|-------------------------|
| TPA-tBu ^o | C ₈₈ H ₇₈ N ₄ O ₆ ^o |  | 1286.59 ^o |

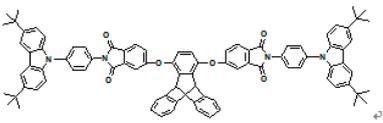
[Mass Spectrum]

Data : 20170425fab(+)_011_TPA-tBu Date : 25-Apr-2017 15:15
 RT : 3.00 min Scan#: (106,115)
 Elements : C 100/0, H 100/0, N 4/0, O 6/0
 Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
 Unsaturation (U.S.) : -0.5 - 100.0



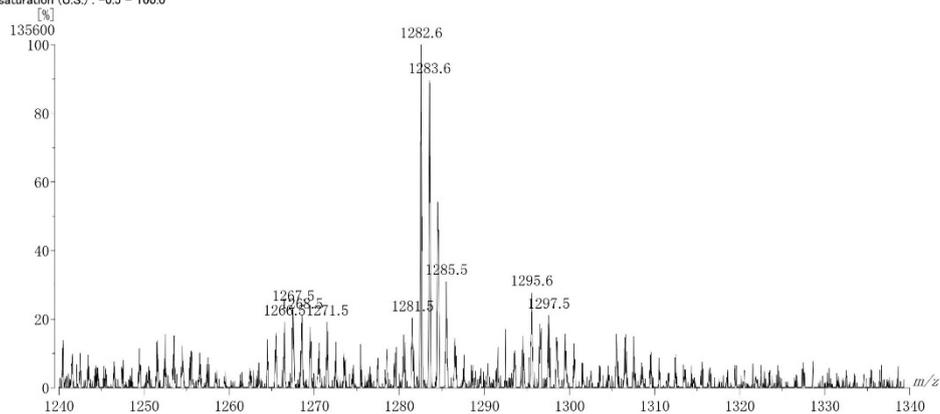
| | Observed m/z | Int% | Err [ppm / mmu] | U. S. | Composition |
|----|--------------|--------|-----------------|-------|---------------|
| 1 | 1286.5910 | 100.00 | +19.1 / +24.5 | 65.5 | C100 H72 N |
| 2 | | | +28.8 / +37.1 | 66.0 | C99 H70 N2 |
| 3 | | | +38.6 / +49.7 | 66.5 | C98 H68 N3 |
| 4 | | | -34.4 / -44.2 | 59.5 | C97 H80 N3 |
| 5 | | | -24.6 / -31.6 | 60.0 | C96 H78 N4 |
| 6 | | | +37.6 / +48.3 | 66.0 | C100 H70 O |
| 7 | | | -35.4 / -45.6 | 59.0 | C99 H82 O |
| 8 | | | -25.6 / -33.0 | 59.5 | C98 H80 N O |
| 9 | | | -15.9 / -20.4 | 60.0 | C97 H78 N2 O |
| 10 | | | -6.1 / -7.8 | 60.5 | C96 H76 N3 O |
| 11 | | | +3.7 / +4.7 | 61.0 | C95 H74 N4 O |
| 12 | | | -7.1 / -9.2 | 60.0 | C98 H78 O2 |
| 13 | | | +2.6 / +3.4 | 60.5 | C97 H76 N O2 |
| 14 | | | +12.4 / +16.0 | 61.0 | C96 H74 N2 O2 |
| 15 | | | +22.2 / +28.5 | 61.5 | C95 H72 N3 O2 |
| 16 | | | +32.0 / +41.1 | 62.0 | C94 H70 N4 O2 |
| 17 | | | +21.1 / +27.2 | 61.0 | C97 H74 O3 |
| 18 | | | +30.9 / +39.8 | 61.5 | C96 H72 N O3 |
| 19 | | | -32.3 / -41.5 | 55.0 | C94 H82 N2 O3 |
| 20 | | | -22.5 / -29.0 | 55.5 | C93 H80 N3 O3 |
| 21 | | | -12.7 / -16.4 | 56.0 | C92 H78 N4 O3 |
| 22 | | | -23.6 / -30.3 | 55.0 | C95 H82 O4 |
| 23 | | | -13.8 / -17.7 | 55.5 | C94 H80 N O4 |
| 24 | | | -4.0 / -5.2 | 56.0 | C93 H78 N2 O4 |
| 25 | | | +5.8 / +7.4 | 56.5 | C92 H76 N3 O4 |
| 26 | | | +15.5 / +20.0 | 57.0 | C91 H74 N4 O4 |
| 27 | | | +4.7 / +6.1 | 56.0 | C94 H78 O5 |
| 28 | | | +14.5 / +18.6 | 56.5 | C93 H76 N O5 |
| 29 | | | +24.3 / +31.2 | 57.0 | C92 H74 N2 O5 |
| 30 | | | +34.0 / +43.8 | 57.5 | C91 H72 N3 O5 |
| 31 | | | -29.2 / -37.5 | 51.0 | C89 H82 N4 O5 |
| 32 | | | +33.0 / +42.5 | 57.0 | C93 H74 O6 |
| 33 | | | -30.2 / -38.9 | 50.5 | C91 H84 N O6 |
| 34 | | | -20.4 / -26.3 | 51.0 | C90 H82 N2 O6 |
| 35 | | | -10.7 / -13.7 | 51.5 | C89 H80 N3 O6 |
| 36 | | | -0.9 / -1.1 | 52.0 | C88 H78 N4 O6 |

Figure S5. Mass spectra of model compound M1.

| Sample name ^o | 分子式 ^o | 結構式 ^o | Exact mass ^o |
|--------------------------|--|--|-------------------------|
| NPC-tBu ^o | C ₈₈ H ₇₄ N ₄ O ₆ ^o |  | 1282.56 ^o |

[Mass Spectrum]

Data : 20170425fab(+)_013_NPC-tBu Date : 25-Apr-2017 15:43
 RT : 3.46 min Scan# : (122,127)
 Elements : C 100/0, H 100/0, N 4/0, O 6/0
 Mass Tolerance : 30ppm, 5mmu if m/z < 167, 50mmu if m/z > 1667
 Unsaturation (U.S.) : -0.5 - 100.0



| Observed m/z | Int% | Err [ppm / mmu] | U.S. | Composition |
|--------------|--------|-----------------|------|---------------|
| 1 1282.5611 | 100.00 | +20.2 / +25.9 | 67.5 | C100 H68 N |
| 2 | | -23.6 / -30.2 | 62.0 | C96 H74 N4 |
| 3 | | -24.6 / -31.6 | 61.5 | C98 H76 N O |
| 4 | | -14.8 / -19.0 | 62.0 | C97 H74 N2 O |
| 5 | | -5.0 / -6.4 | 62.5 | C96 H72 N3 O |
| 6 | | +4.8 / +6.1 | 63.0 | C95 H70 N4 O |
| 7 | | -6.1 / -7.8 | 62.0 | C98 H74 O2 |
| 8 | | +3.7 / +4.8 | 62.5 | C97 H72 N O2 |
| 9 | | +13.5 / +17.4 | 63.0 | C96 H70 N2 O2 |
| 10 | | +23.3 / +29.9 | 63.5 | C95 H68 N3 O2 |
| 11 | | +22.3 / +28.6 | 63.0 | C97 H70 O3 |
| 12 | | -21.5 / -27.6 | 57.5 | C93 H76 N3 O3 |
| 13 | | -11.7 / -15.0 | 58.0 | C92 H74 N4 O3 |
| 14 | | -22.5 / -28.9 | 57.0 | C95 H78 O4 |
| 15 | | -12.7 / -16.3 | 57.5 | C94 H76 N O4 |
| 16 | | -2.9 / -3.8 | 58.0 | C93 H74 N2 O4 |
| 17 | | +6.9 / +8.8 | 58.5 | C92 H72 N3 O4 |
| 18 | | +16.7 / +21.4 | 59.0 | C91 H70 N4 O4 |
| 19 | | +5.8 / +7.5 | 58.0 | C94 H74 O5 |
| 20 | | +15.6 / +20.1 | 58.5 | C93 H72 N O5 |
| 21 | | +25.4 / +32.6 | 59.0 | C92 H70 N2 O5 |
| 22 | | -28.2 / -36.1 | 53.0 | C89 H78 N4 O5 |
| 23 | | -29.2 / -37.5 | 52.5 | C91 H80 N O6 |
| 24 | | -19.4 / -24.9 | 53.0 | C90 H78 N2 O6 |
| 25 | | -9.6 / -12.3 | 53.5 | C89 H76 N3 O6 |
| 26 | | +0.2 / +0.3 | 54.0 | C88 H74 N4 O6 |
| 27 1283.5663 | 89.64 | +18.2 / +23.3 | 67.0 | C100 H69 N |
| 28 | | +27.9 / +35.9 | 67.5 | C99 H67 N2 |
| 29 | | -25.6 / -32.9 | 61.5 | C96 H75 N4 |
| 30 | | -26.7 / -34.2 | 61.0 | C98 H77 N O |
| 31 | | -16.9 / -21.6 | 61.5 | C97 H75 N2 O |
| 32 | | -7.1 / -9.1 | 62.0 | C96 H73 N3 O |
| 33 | | +2.7 / +3.5 | 62.5 | C95 H71 N4 O |
| 34 | | -8.1 / -10.4 | 61.5 | C98 H75 O2 |
| 35 | | +1.7 / +2.2 | 62.0 | C97 H73 N O2 |
| 36 | | +11.5 / +14.7 | 62.5 | C96 H71 N2 O2 |
| 37 | | +21.3 / +27.3 | 63.0 | C95 H69 N3 O2 |
| 38 | | +20.2 / +26.0 | 62.5 | C97 H71 O3 |
| 39 | | -23.5 / -30.2 | 57.0 | C93 H77 N3 O3 |
| 40 | | -13.7 / -17.6 | 57.5 | C92 H75 N4 O3 |
| 41 | | -24.6 / -31.5 | 56.5 | C95 H79 O4 |
| 42 | | -14.8 / -19.0 | 57.0 | C94 H77 N O4 |
| 43 | | -5.0 / -6.4 | 57.5 | C93 H75 N2 O4 |
| 44 | | +4.8 / +6.2 | 58.0 | C92 H73 N3 O4 |
| 45 | | +14.6 / +18.8 | 58.5 | C91 H71 N4 O4 |
| 46 | | +3.8 / +4.8 | 57.5 | C94 H75 O5 |
| 47 | | +13.6 / +17.4 | 58.0 | C93 H73 N O5 |
| 48 | | +23.4 / +30.0 | 58.5 | C92 H71 N2 O5 |
| 49 | | -21.4 / -27.5 | 52.5 | C90 H79 N2 O6 |
| 50 | | -11.6 / -14.9 | 53.0 | C89 H77 N3 O6 |
| 51 | | -1.8 / -2.4 | 53.5 | C88 H75 N4 O6 |

Figure S6. Mass spectra of model compound M2.

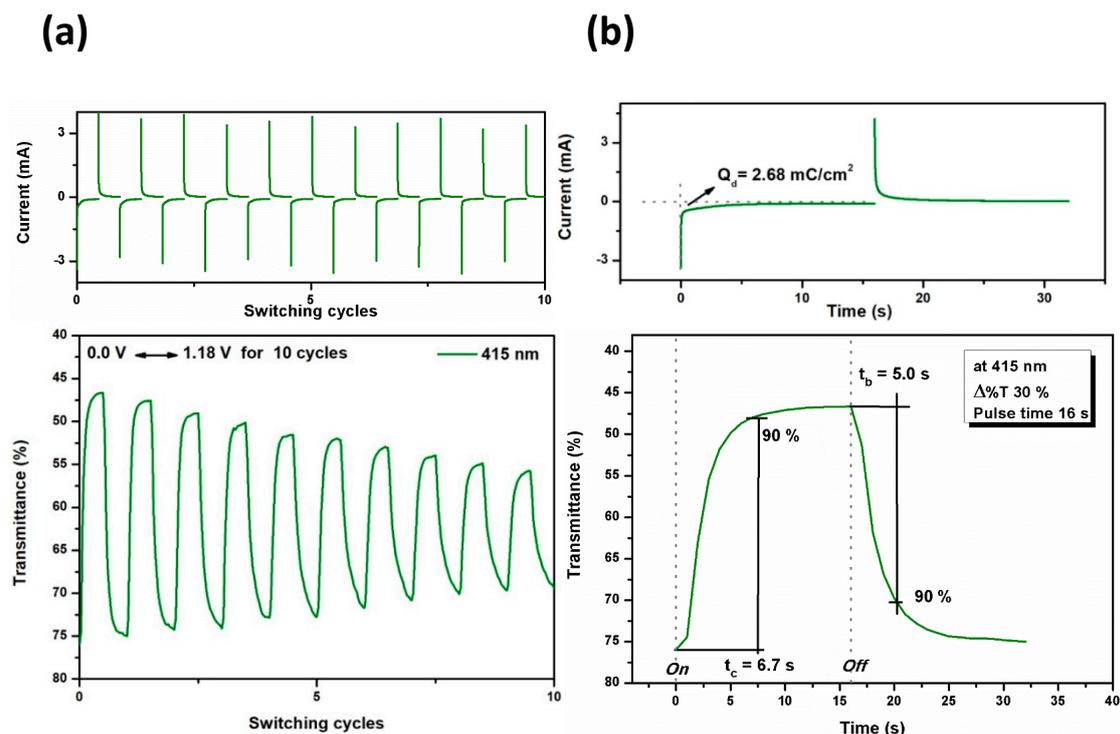


Figure S7. Potential step absorptiometry of the cast film of NPC-TPPI on the ITO-glass slide (coated area $\sim 1 \text{ cm}^2$) (in CH_2Cl_2 with $0.1 \text{ M Bu}_4\text{NClO}_4$ as the supporting electrolyte) by applying a potential step; (a) optical switching at potential $0.00 \text{ V} \leftrightarrow 1.18 \text{ V}$ (10 cycles) with a pulse width of 16 s, monitored at $\lambda_{\text{max}} = 415 \text{ nm}$; (b) the 1st cycle transmittance change for the NPC-TPPI thin film.