Supporting Information for:

Phenazasiline/Spiroacridine Donor Combined with Methyl-Substituted Linkers for Efficient Deep Blue Thermally Activated Delayed Fluorescence Emitters

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1. Synthesis and Characterization

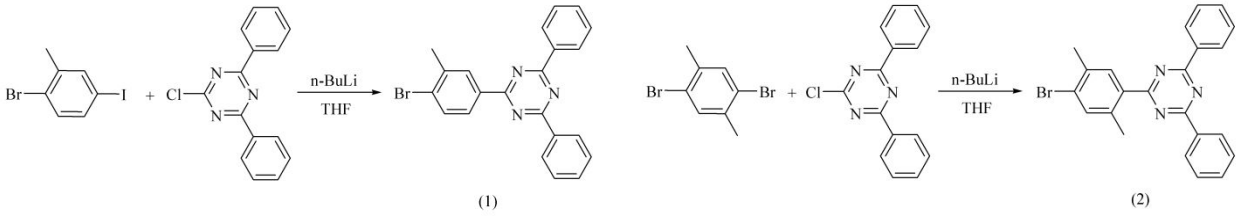
1.1. Materials

All reagents were purchased from Aldrich and TCI. Solvents were dried by using standard procedures.

1.2. Instruments

^{1}H-NMR and ^{13}C-NMR spectra were recorded on a Bruker 300 and Avance 500 spectrometer. Jeol JMS-700 mass spectrometer was used to obtain the mass spectra of the samples.

1.3. Synthesis scheme and procedure

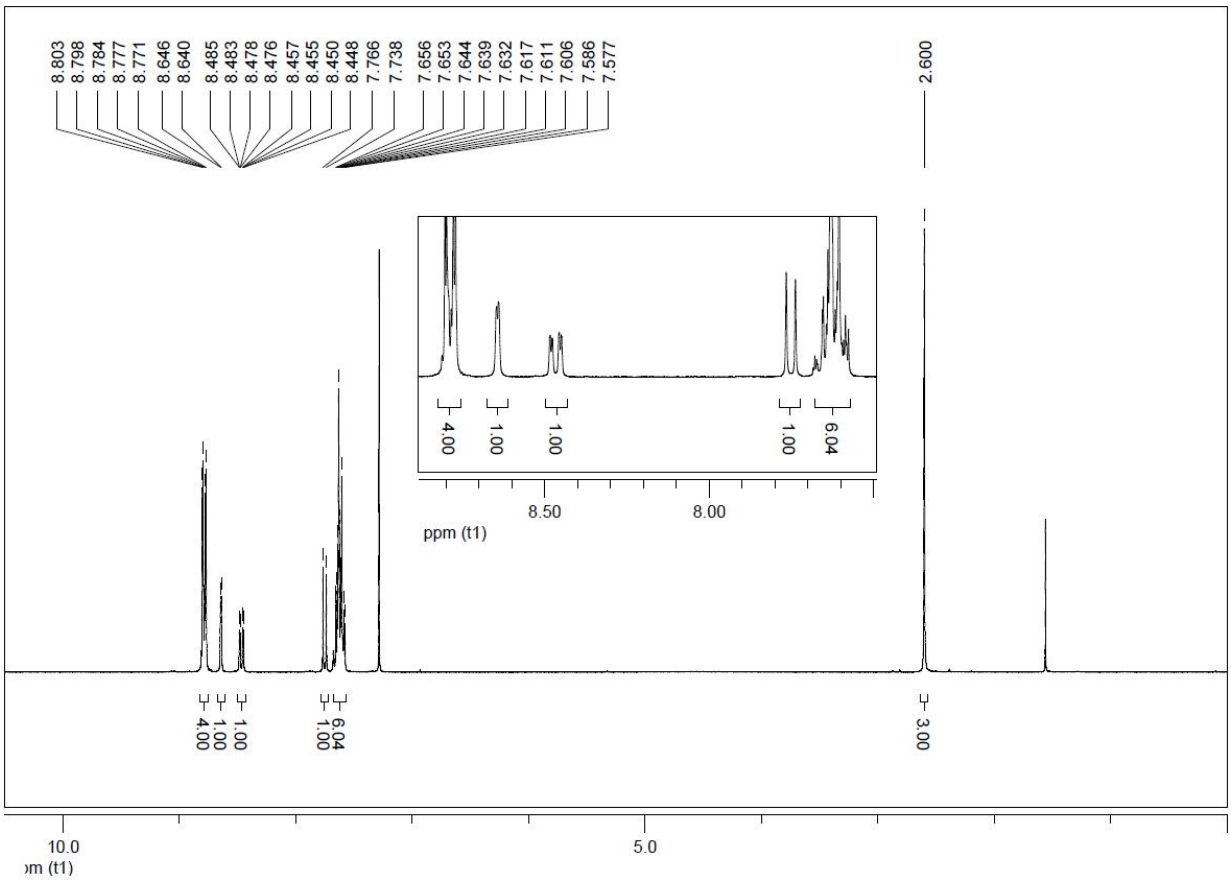


Synthesis Scheme 1.

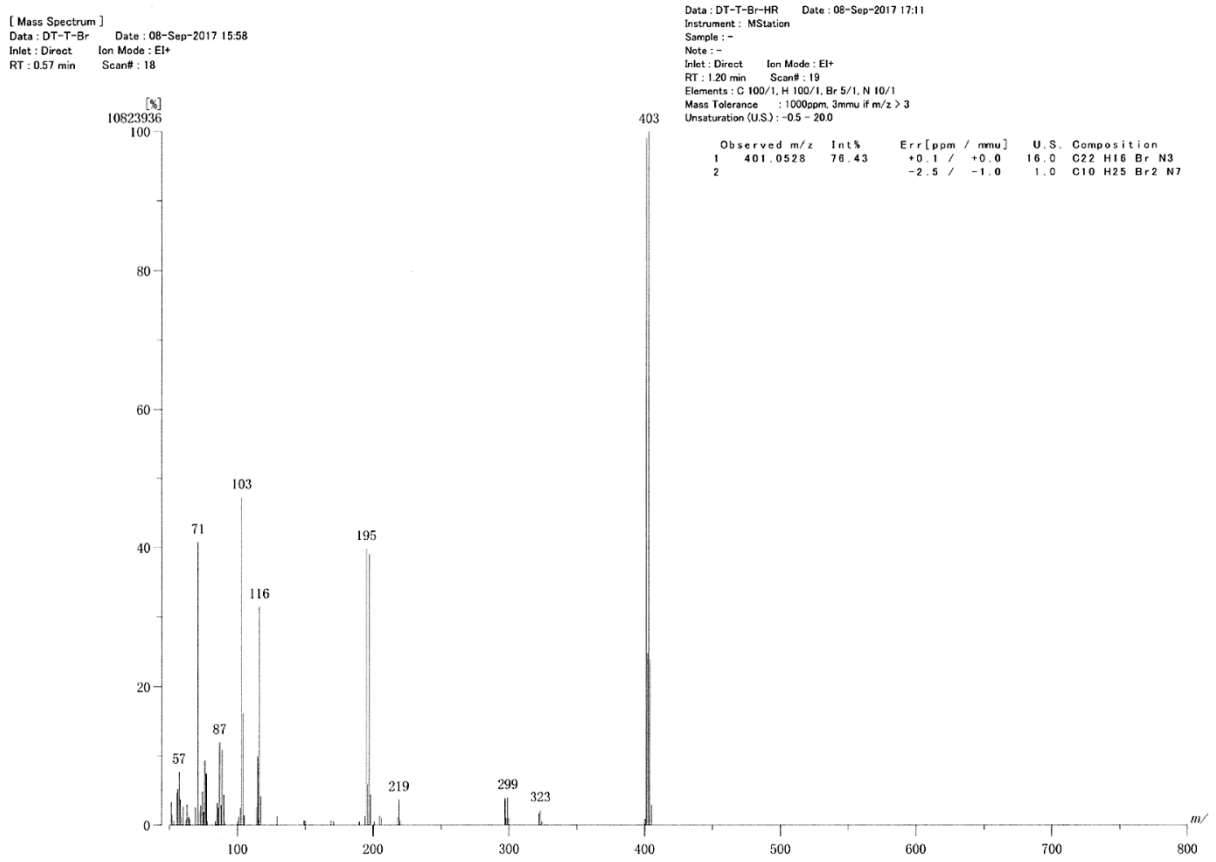
Synthesis of 2-(4-bromo-3-methylphenyl)-4,6-diphenyl-1,3,5-triazine (1).

The reaction was followed by reported method. (Chemistry of Materials, 30, 857−863; 2018, DOI**:** 10.1021/acs.chemmater.7b04437). The product was obtained by column chromatography using toluene/n-hexane (1/9). White solid. Yield : 4.6 g (22.63 %)

^{1}H-NMR (300 MHz, $CDCl_3$) δ = 8.80-8.77 (m, 4H), 8.64 (d, J = 1.8 Hz, 1H), 8.46 (d, J = 8.4 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.65-7.57 (m, 6H), 2.60 (s, 3H). MS EI (m/z): 401.05 (M+, 100%).



Synthesis Figure 1. ^{1}H-NMR Spectra of 2-(4-bromo-3-methylphenyl)-4,6-diphenyl-1,3,5-triazine.

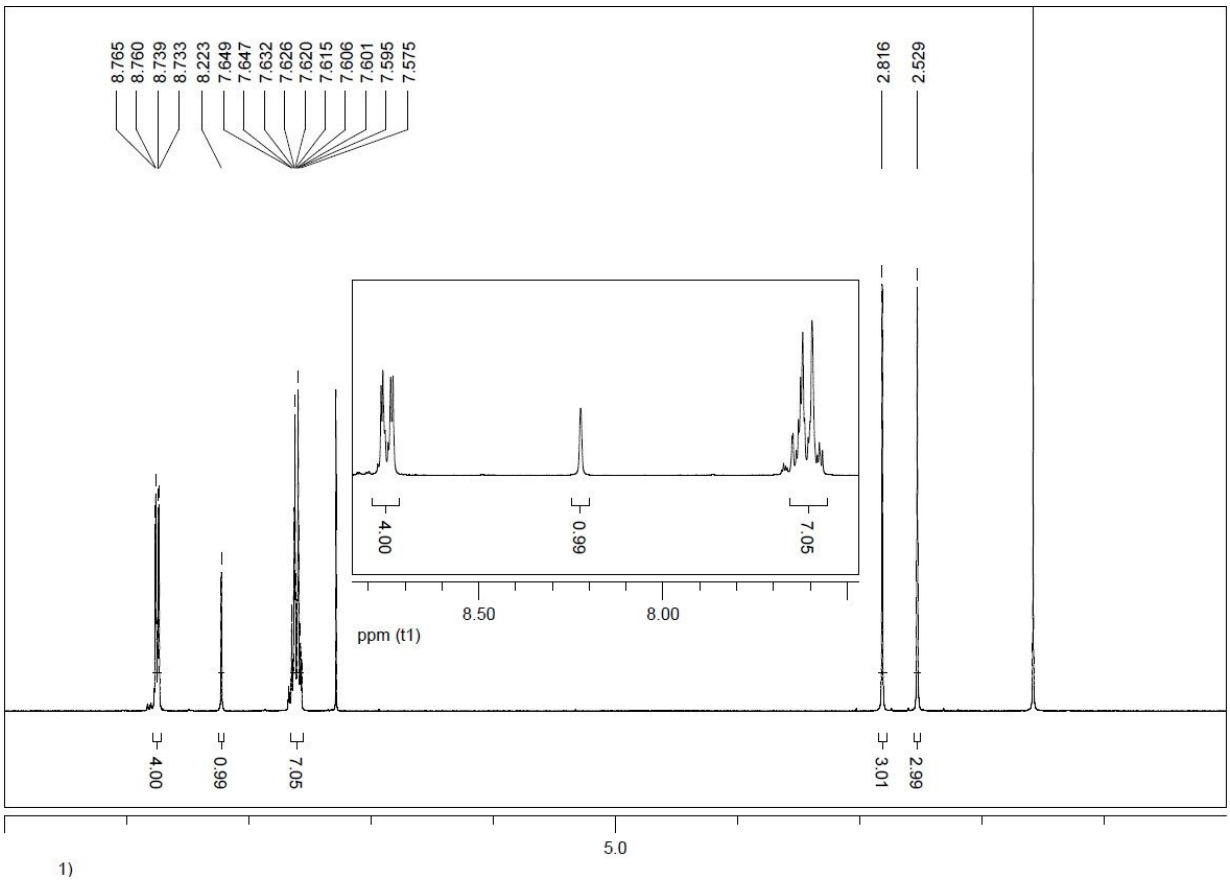


Synthesis Figure 2. EI Mass Spectra of 2-(4-bromo-3-methylphenyl)-4,6-diphenyl-1,3,5-triazine.

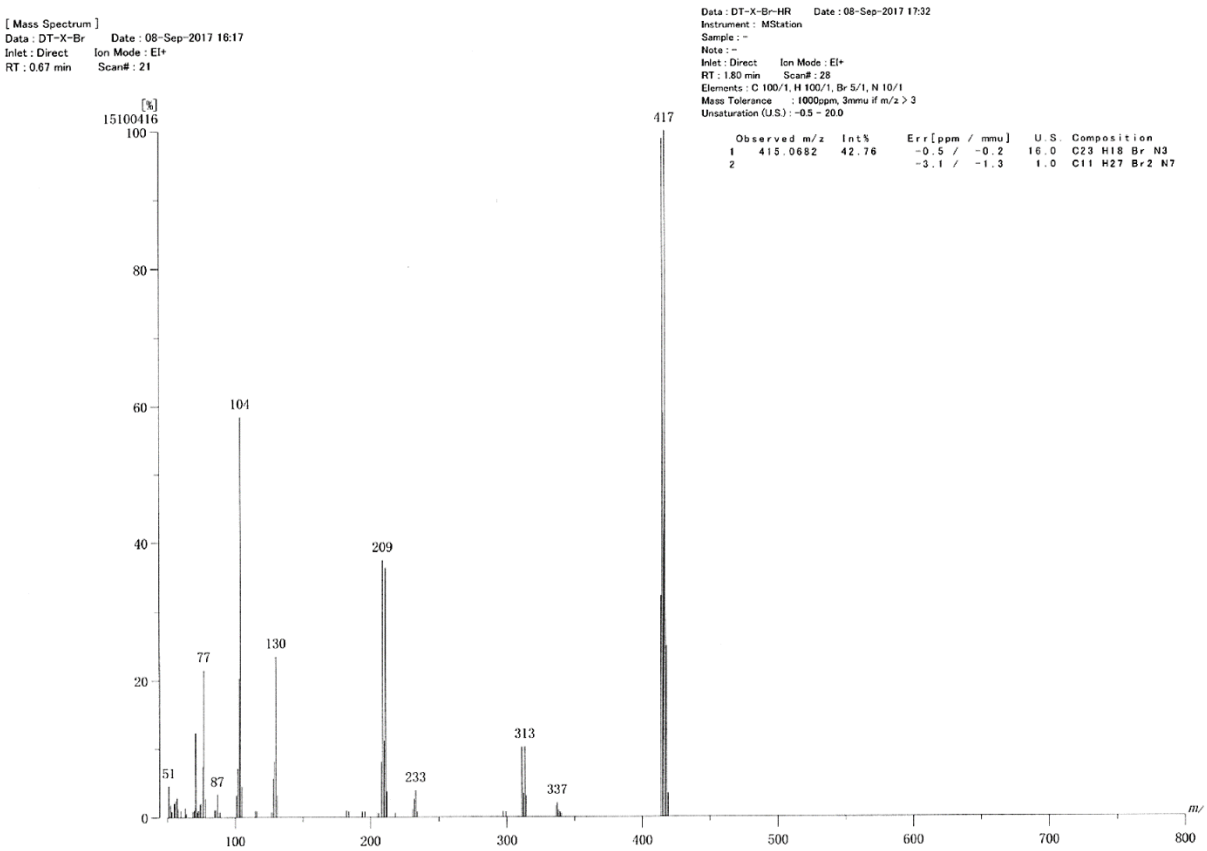
Synthesis of 2-(4-bromo-2,5-dimethylphenyl)-4,6-diphenyl-1,3,5-triazine (2).

The reaction was followed by reported method (Chemistry of Materials, 30, 857−863; 2018, DOI**:** 10.1021/acs.chemmater.7b04437). The product was obtained by column chromatography using toluene/n-hexane (1/5). White solid. Yield : 14.4 g (45.65 %)

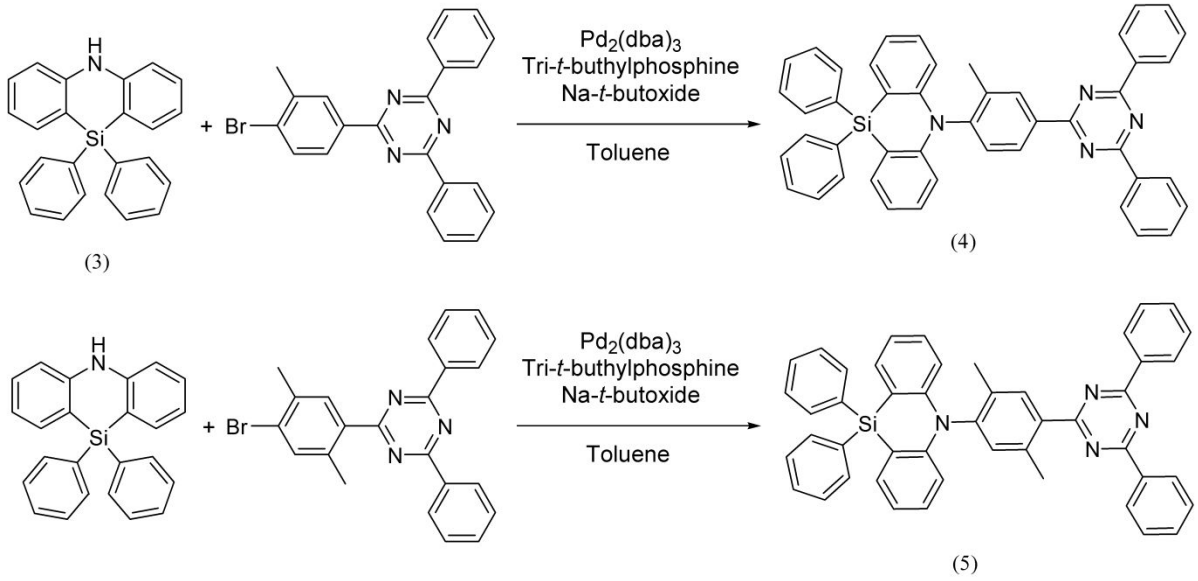
^{1}H-NMR (300 MHz, $CDCl_3$) δ = 8.76-8.73 (m, 4H), 8.22 (s, 1H), 7.65-7.57 (m, 7H), 2.81(s, 3H), 2.52 (s, 3H). MS EI (m/z): 415.06 (M+, 100%).



Synthesis Figure 3. ^{1}H-NMR Spectra of 2-(4-bromo-2,5-dimethylphenyl)-4,6-diphenyl-1,3,5-triazine.



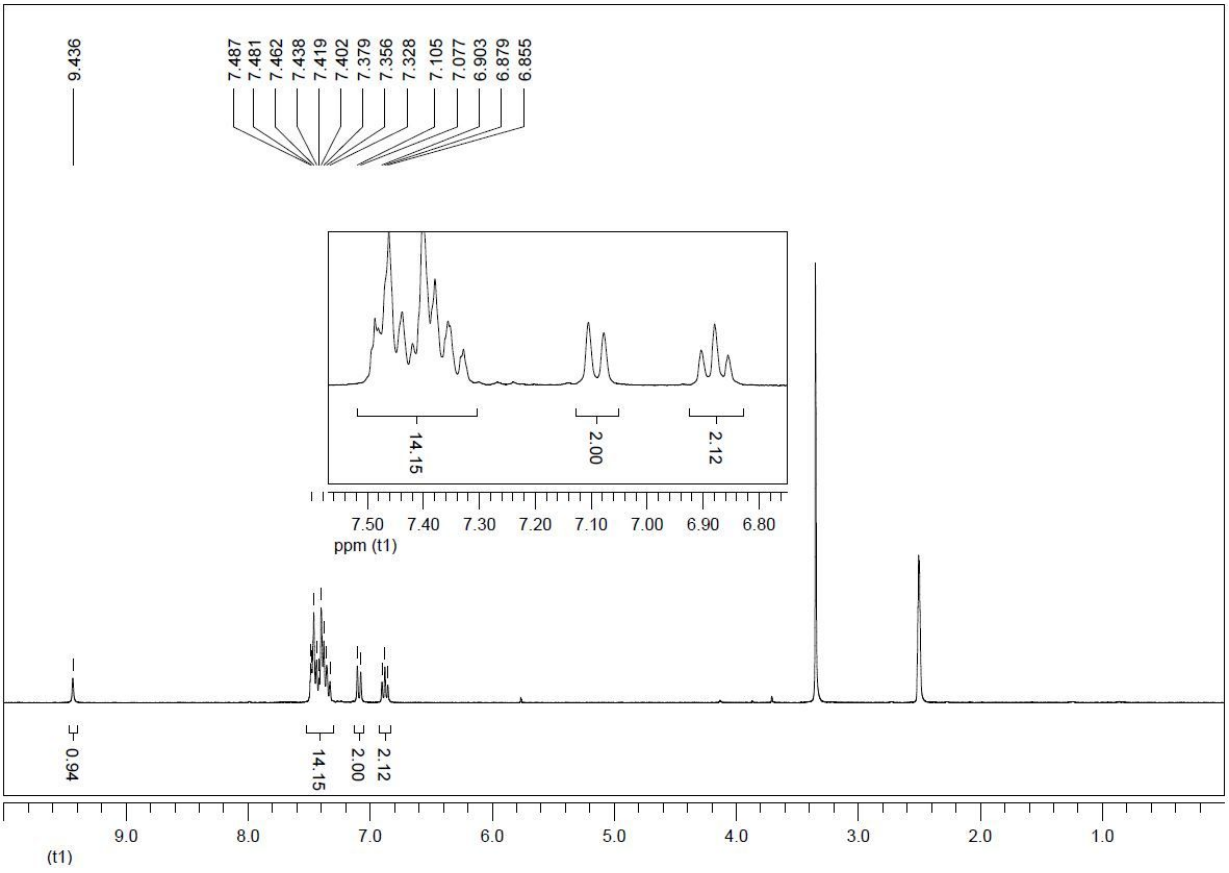
Synthesis Figure 4. EI Mass Spectra of 2-(4-bromo-2,5-dimethylphenyl)-4,6-diphenyl-1,3,5-triazine.



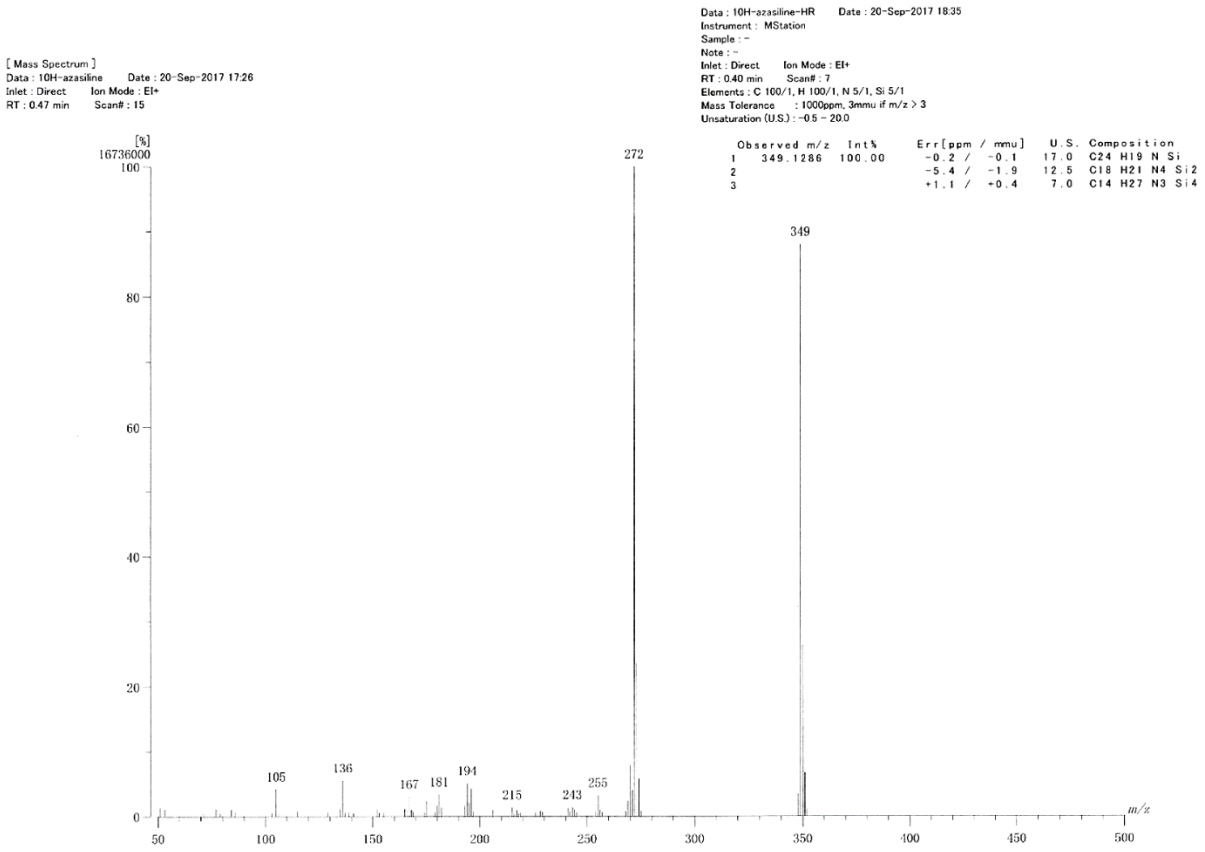
Synthesis Scheme 2.

Synthesis of 10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline (3).

The reaction was followed by reported methods. (Chemistry of Materials, 27, 6675-6681; 2015, **DOI:** 10.1021/acs.chemmater.5b02515) The crude product was purified by column chromatography using hexane/ethyl acetate (5/1). White solid. Yield: 4.25 g (42.30 %). ^{1}H-NMR (300 MHz, DMSO) δ = 9.43 (s, 1H), 7.49-7.33 (m, 14H), 7.09 (d, J = 8.3 Hz, 2H), 6.88 (t, J = 7.2 Hz, 2H). MS (EI) m/z : 349.1286 (M+, 100%).



Synthesis Figure 5. ^{1}H-NMR Spectra of 10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline



Synthesis Figure 6. EI Mass Spectra of 10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline.

Synthesis of 5-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2-methylphenyl)-10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline (4).

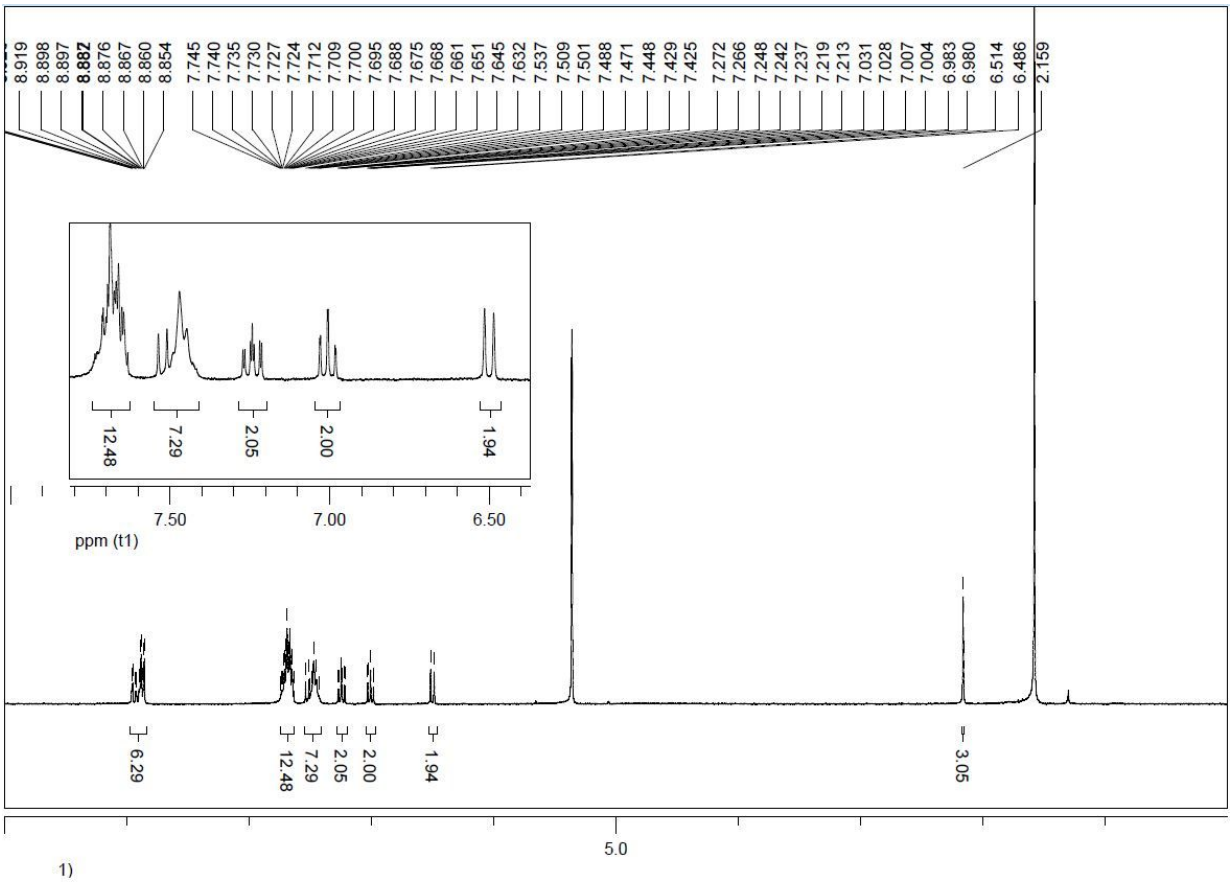
10,10-Diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline (0.9 g, 2.57 mmol) and 2-(4-bromo-3-methylphenyl)-4,6-diphenyl-1,3,5-triazine (1.04 g, 2.57 mmol) were mixed in dry toluene (15 mL). Na-*t*-butoxide (0.74 g, 7.72 8 mmol), tri-*t*-buthylphosphine (0.05 g, 0.257 mmol), and tris(dibenzylideneacetone)dipalladium(0) (0.12 g, 0.128 mmol) were added and stirred for 10 h at 90 °C. The reaction mixture was extracted with dichloromethane and dried over anhydrous $MgSO_4$. The product was purified by a column with hexane and dichloromethane (Hex : MC = 3:1). Pale yellow solid. Yield : 1.02 g, (51.03 %)

^{1}H-NMR (300 MHz, CD_2Cl_2) δ = 8.95-8.85 (m, 6H), 7.71-7.64(m, 12H), 7.53-7.44 (m, 7H), 7.27-

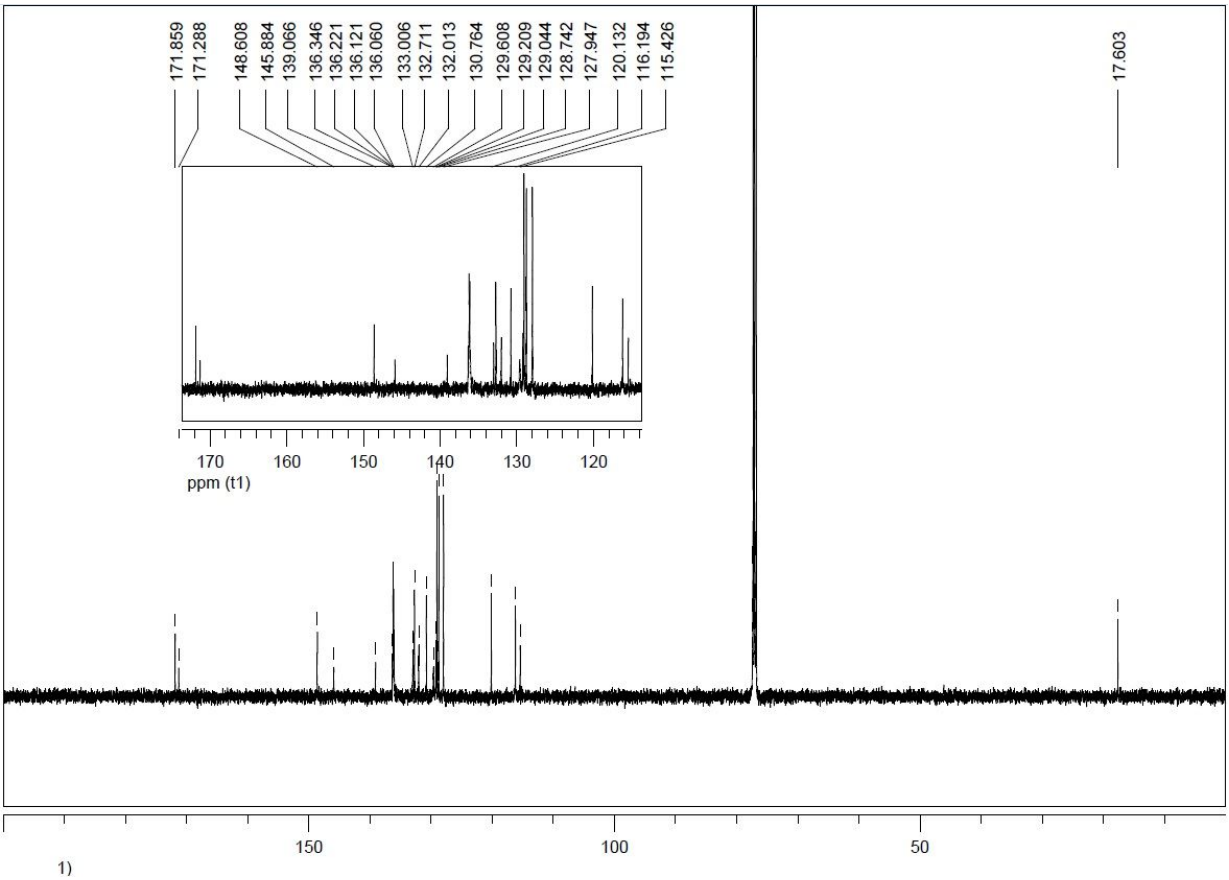
7.21 (m, 2H), 7.03-6.98 (m, 2H), 6.50 (d, J = 8.4 Hz, 2H), 2.15 (s, 3H).

^{13}C-NMR (500 MHz, $CDCl_3$) δ = 171.85, 171.28, 148.60, 145.88, 139.06, 136.34, 136.22, 136.12, 136.06, 133.00, 132.71, 132.01, 130.76, 129.60, 129.20, 129.04, 128.74, 127.94, 120.13, 116.19, 115.42, 17.60.

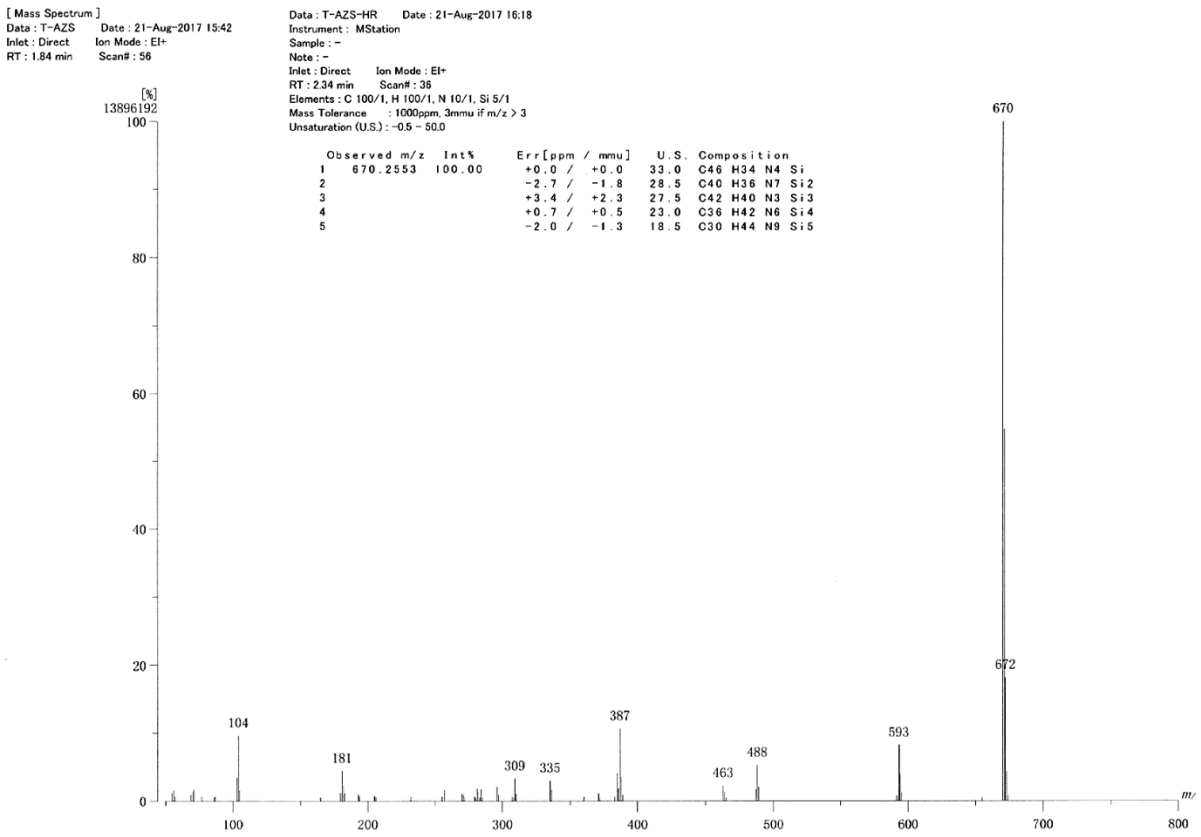
HRMS (EI) m/z $C_{46}H_{34}N_4Si$ Cacld: 670.2553, Found: 670.2553 (M+, 100%).



Synthesis Figure 7. ^{1}H-NMR Spectra of 5-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2-methylphenyl)-10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline.



Synthesis Figure 8. ^{13}C-NMR Spectra of 5-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2-methylphenyl)-10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline.



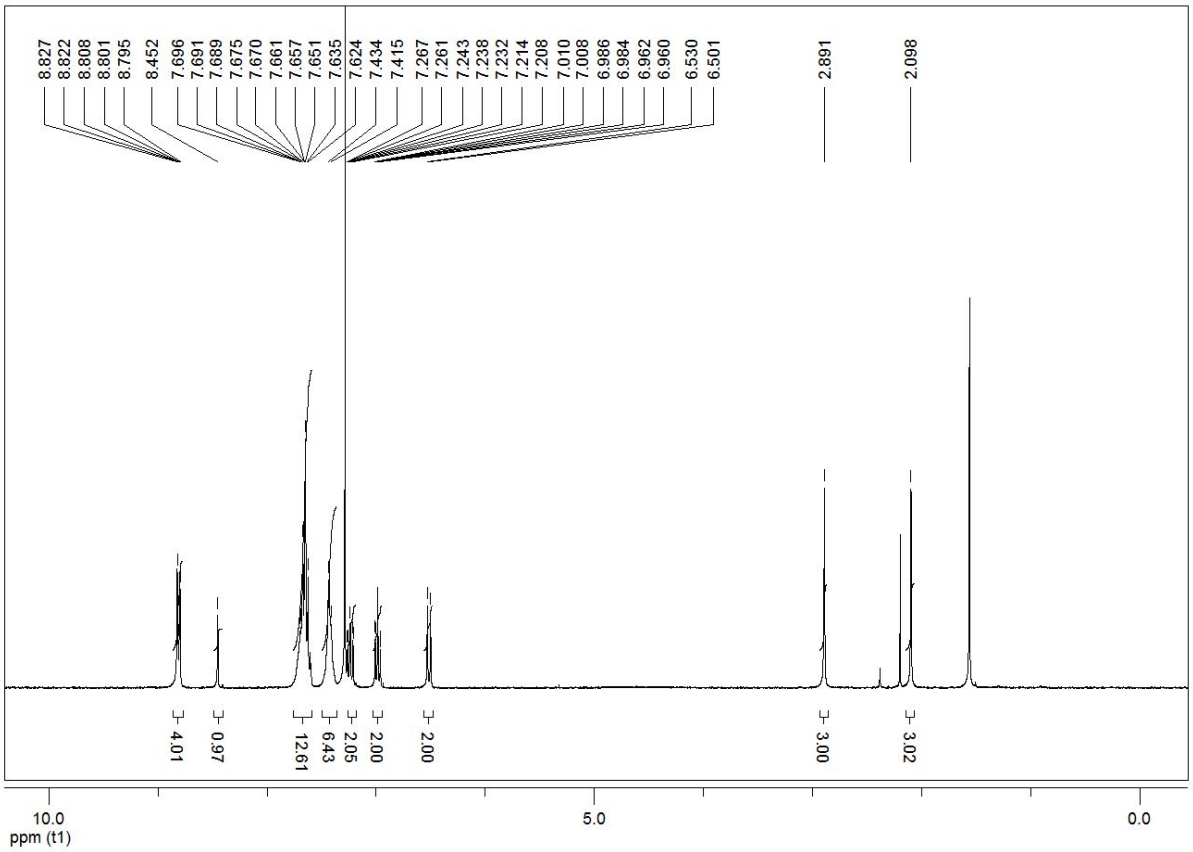
Synthesis Figure 9. EI Mass Spectra of 5-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2-methylphenyl)-10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline.

Synthesis of 5-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2,5-dimethylphenyl)-10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline (5).

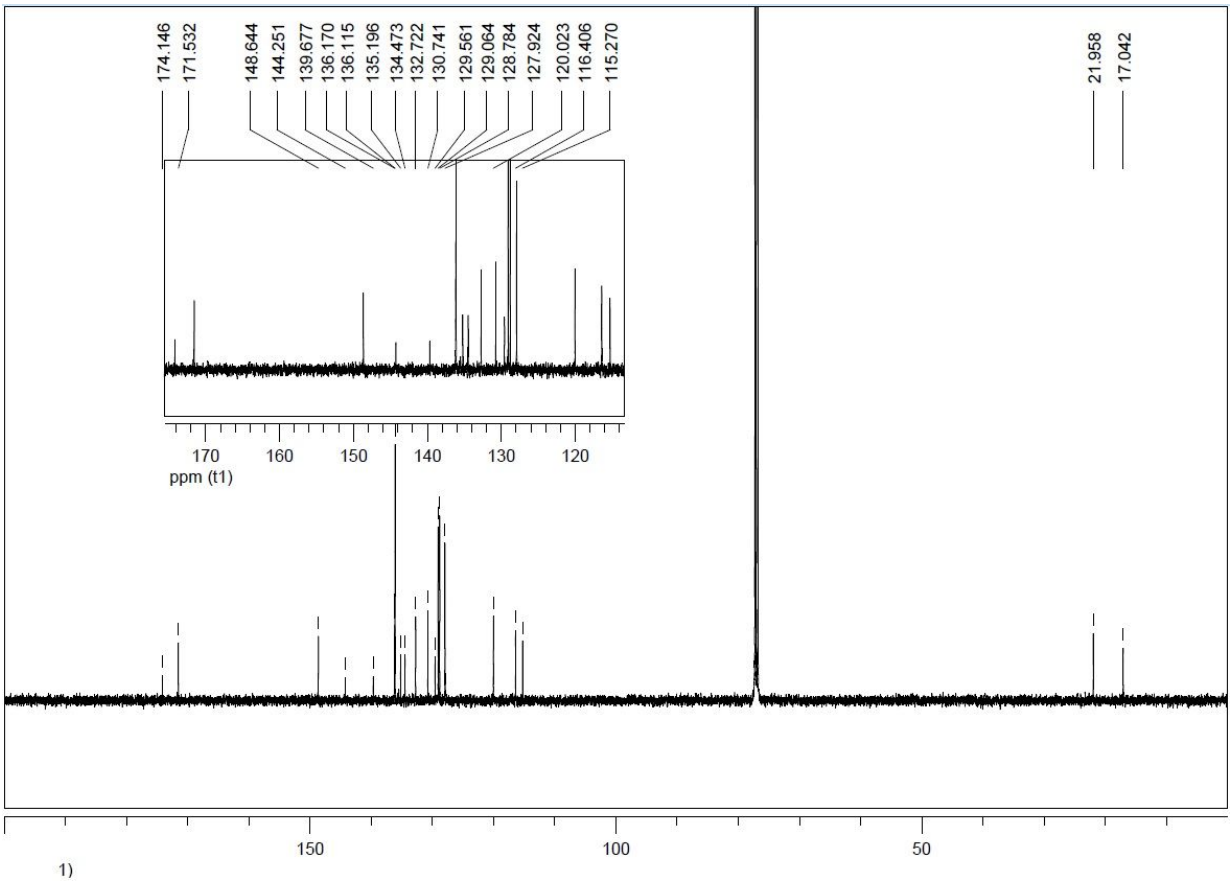
The synthesis was proceeded by similar reaction of synthesis of 5-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2-methylphenyl)-10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline. 10,10-Diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline (1.00 g, 2.86 mmol) and 2-(4-bromo-2,5-dimethylphenyl)-4,6-diphenyl-1,3,5-triazine (1.19 g, 2.86 mmol) were mixed in dry toluene (15 mL). Na-*t*-butoxide (0.82 g, 8.58 mmol), tri-*t*-buthylphosphine (0.06 g, 0.286 mmol), and tris(dibenzylideneacetone)dipalladium(0) (0.13 g, 0.143 mmol) were added and stirred for 10 h at 90 °C. The reaction mixture was extracted with dichloromethane and dried over anhydrous $MgSO_4$.

The product was purified by a column with hexane and dichloromethane (Hex : MC = 3:1). Pale yellow solid. Yield : 1.32 g, (65.67 %)

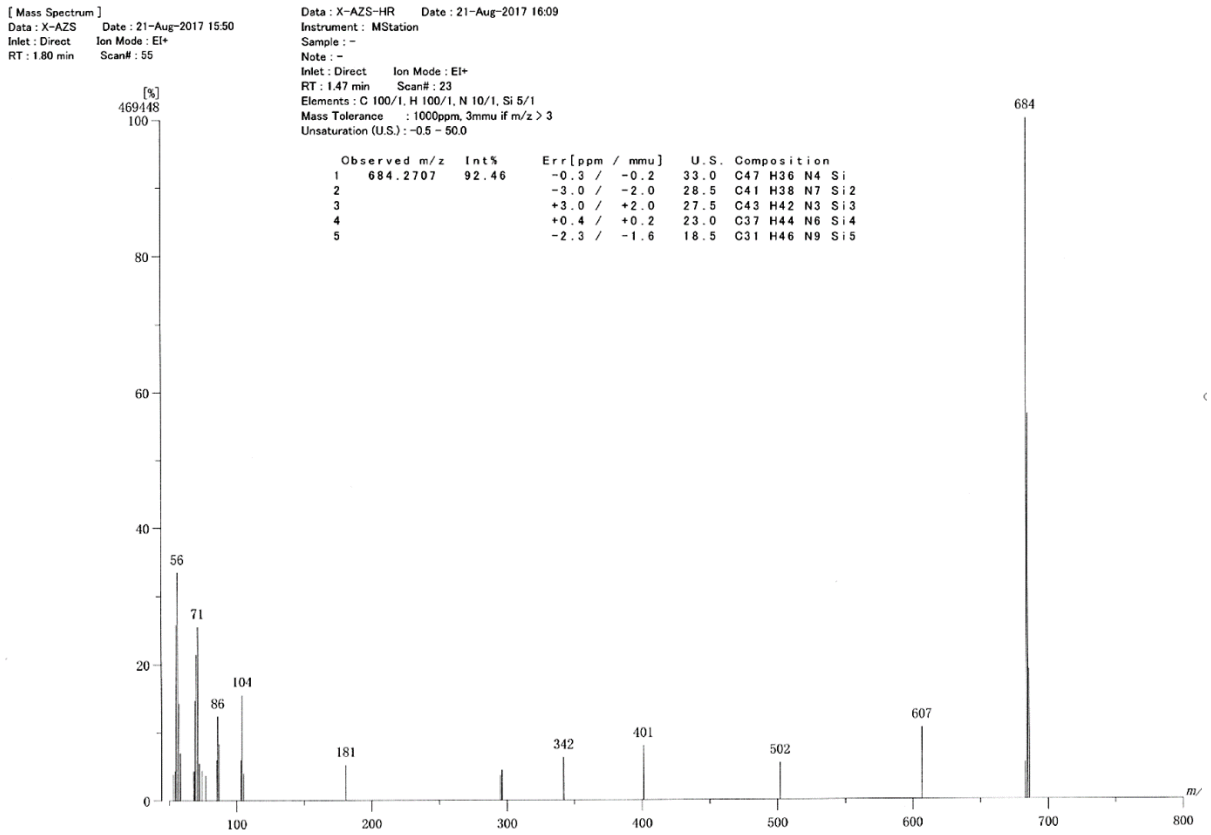
^{1}H-NMR (300 MHz, $CDCl_3$) δ = 8.82-8.79 (m, 4H), 8.42 (s, 1H), 7.69-7.62 (m, 13H), 7.43-7.41 (m, 6H), 7.23 (t, J = 7.2 Hz, 2H), 6.98 (t, J = 7.2 Hz, 2H), 6.51 (d, J = 8.5 Hz, 2H), 2.89 (s, 3H), 2.09 (s, 3H) ^{13}C-NMR (500 MHz, $CDCl_3$) δ = 174.14, 171.53, 148.64, 144.25, 139.67, 136.17, 136.11, 135.19, 134.47, 132.72, 130.74, 129.56, 129.06, 128.78, 127.9, 120.02, 116.40, 115.27, 21.95, 17.04 HRMS (EI) m/z $C_{47}H_{36}N_4Si$ Cacld:684.2709, Found: 684.2707 (M+, 100%).



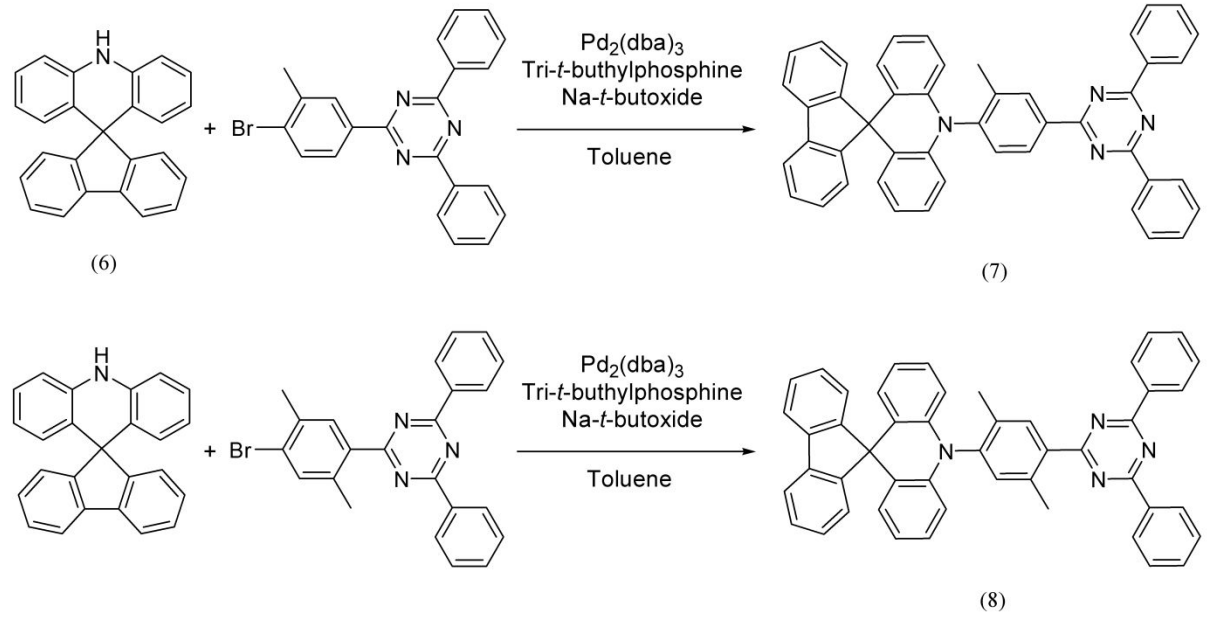
Synthesis Figure 10. ^{1}H-NMR Spectra of 5-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2,5-dimethylphenyl)-10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline.



Synthesis Figure 11. ^{13}C-NMR Spectra of 5-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2,5-dimethylphenyl)-10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline.



Synthesis Figure 12. EI Mass Spectra of 5-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2,5-dimethylphenyl)-10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline.

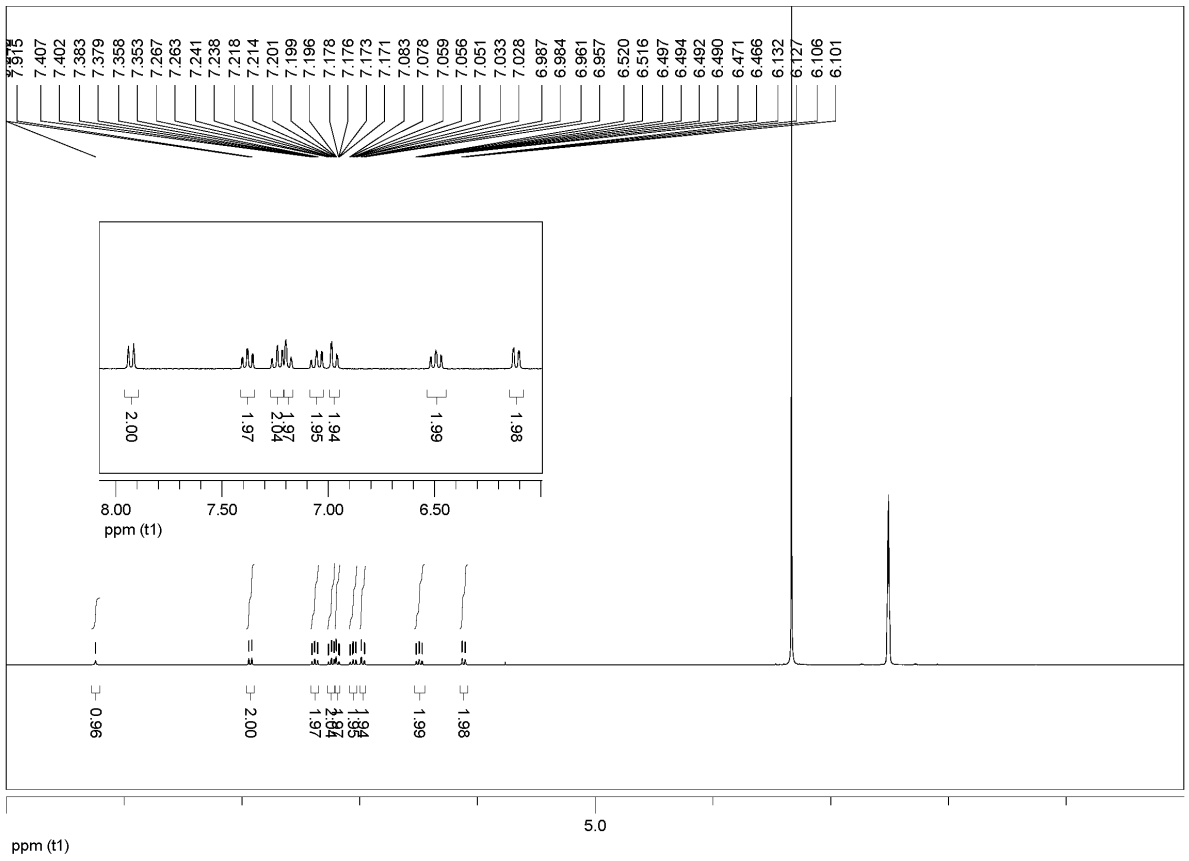


Synthesis Scheme 3.

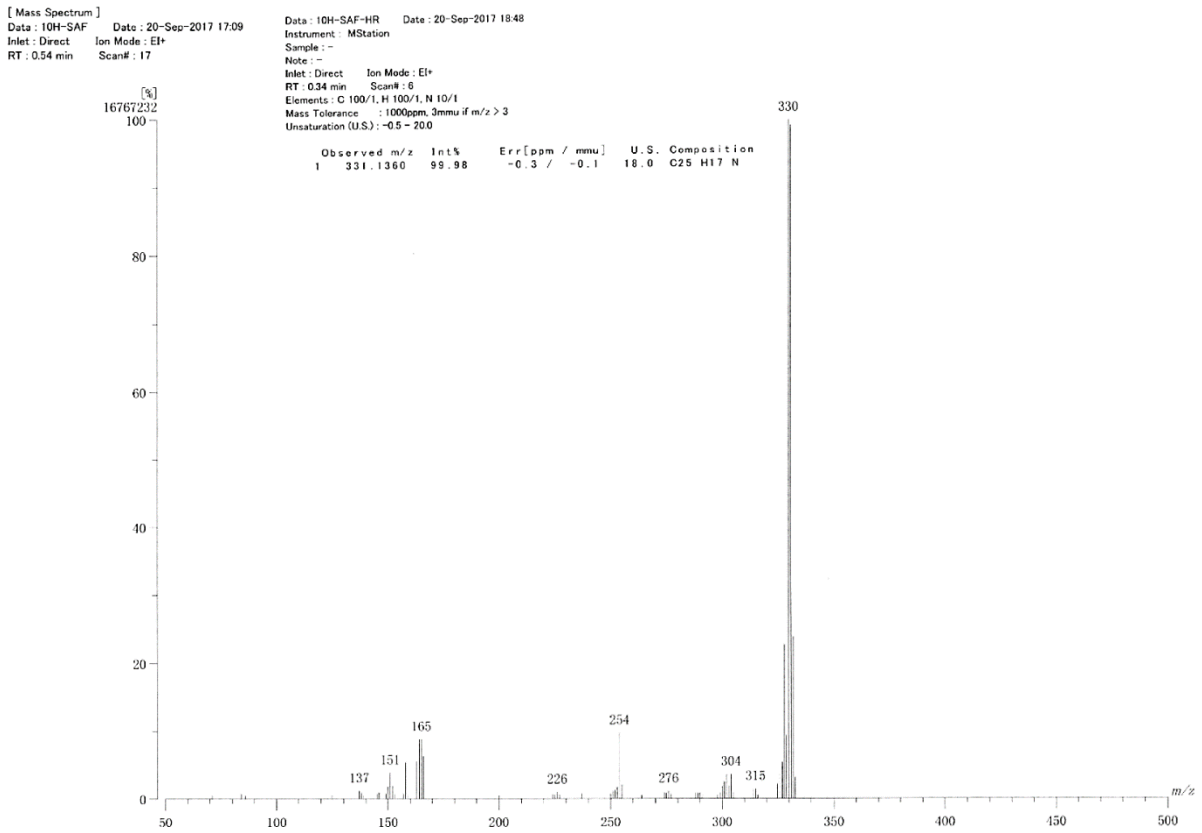
Synthesis of 10H-spiro[acridine-9,9'-fluorene] (6)

Synthetic procedure was followed the reported method. (Advanced Materials, 28, 6976-6983; 2016, DOI: 10.1002/adma.201601675).

The crude product was purified by column chromatography using dichloromethane and hexane (1:5). Pale yellow solid. Yield : 22.6 g (67.68 %) ^{1}H-NMR (300 MHz, DMSO) δ = 9.24 (s, 1H), 7.93 (d, J = 7.5 Hz, 2H), 7.38 (t, J = 7.5 Hz, 2H), 7.24 (t, J = 7.5 Hz, 2H), 7.20-7.17 (m, 2H), 7.08-7.03 (m, 2H), 6.97 (d, J = 7.8 Hz, 2H), 6.52-6.46 (m, 2H), 6.12 (d, J = 7.8 Hz, 2H). MS (EI) m/z 331.1360 (M+, 100%).



Synthesis Figure 13. ^{1}H-NMR Spectra of 10H-spiro[acridine-9,9'-fluorene].



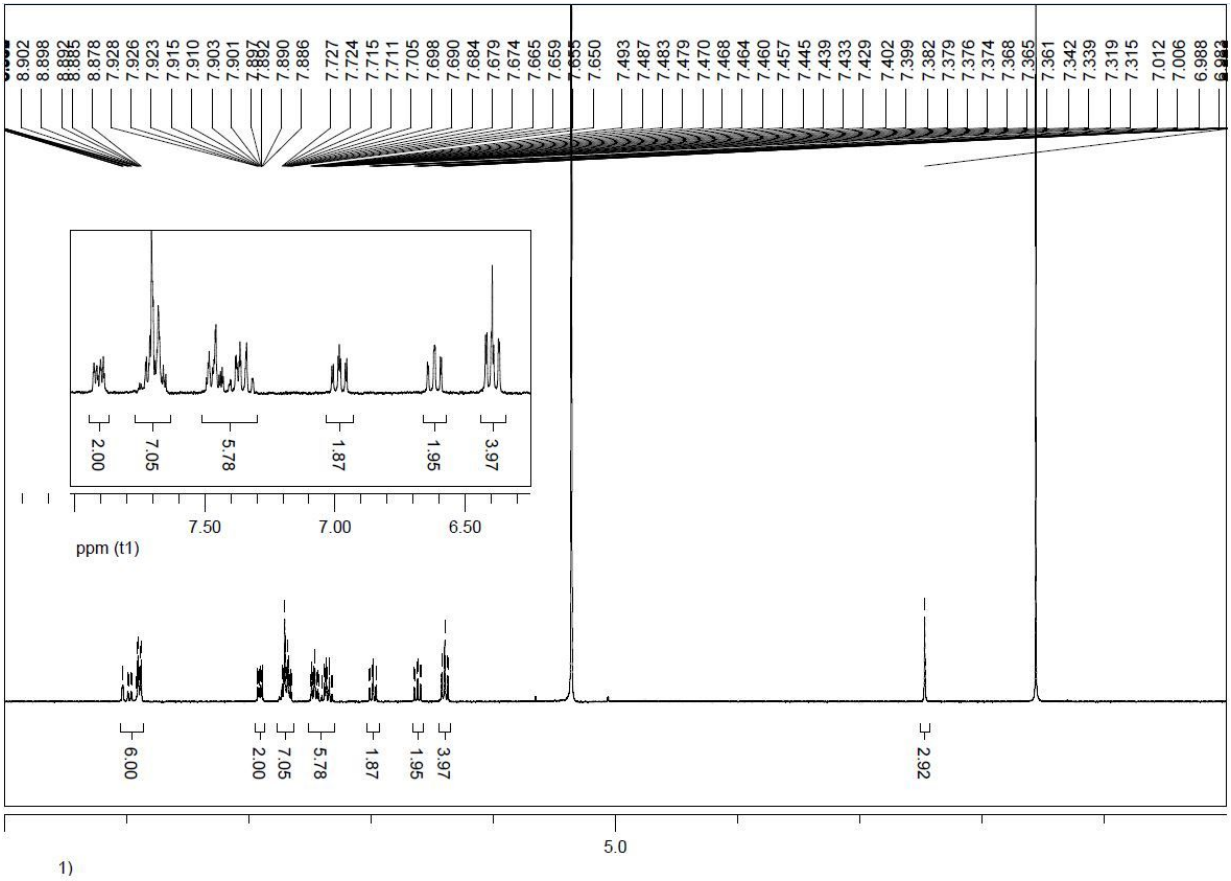
Synthesis Figure 14. EI Mass Spectra of 10H-spiro[acridine-9,9'-fluorene].

Synthesis of 10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2-methylphenyl)-10H-spiro[acridine-9,9'-fluorene] (7).

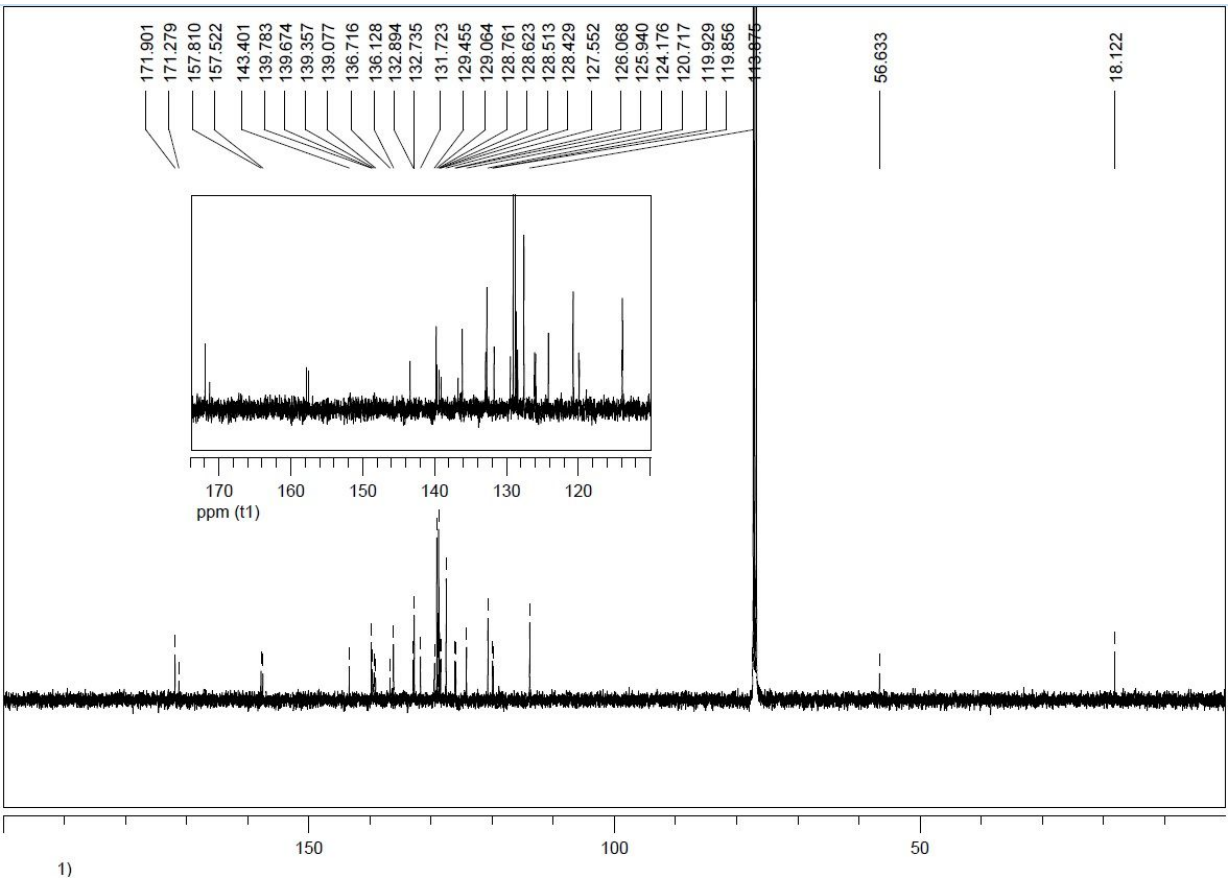
10*H*-spiro[acridine-9,9'-fluorene] (1.00 g, 3.02 mmol) and 2-(4-bromo-3-methylphenyl)-4,6-diphenyl-1,3,5-triazine (1.38 g, 3.32 mmol) were mixed in dry toluene (20 mL). Na-*t*-butoxide (0.87 g, 9.05 mmol), tri-*t*-buthylphosphine (0.06 g, 0.302 mmol) and tris(dibenzylideneacetone)dipalladium(0) (0.14 g, 0.151 mmol) were added and stirred for 10 h at 90 °C. The reaction mixture was extracted with dichloromethane and dried over anhydrous $MgSO_4$. The product was purified by a column with hexane and dichloromethane (Hex : MC = 3:1). Pale yellow solid. Yield : 1.32 g, (65.67 %)

^{1}H-NMR (300 MHz, CD_2Cl_2) δ = 9.03-9.02 (m, 1H), 8.99-8.95 (m, 1H), 8.92-8.87 (m, 4H), 7.93-

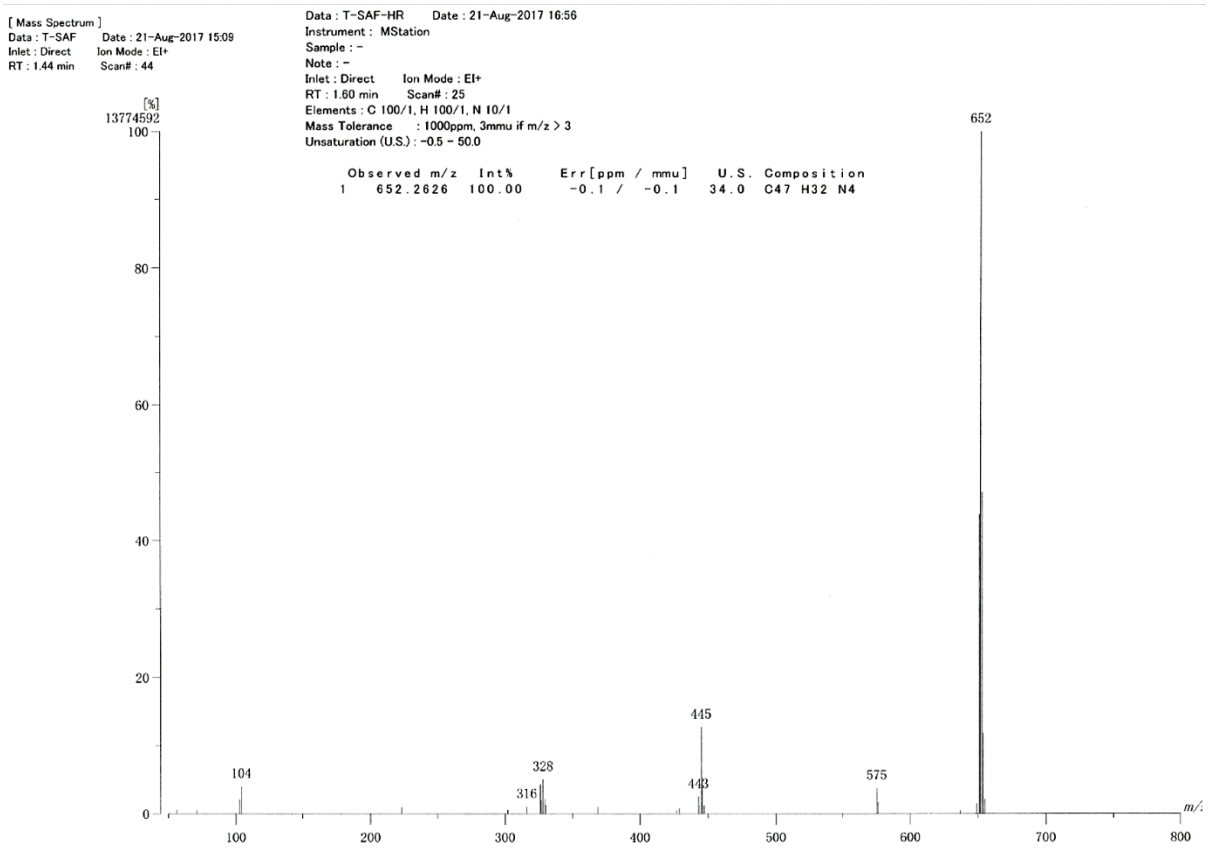
7.88 (m, 2H), 7.72-7.65 (m, 7H), 7.49-7.43 (m, 3H), 7.40-7.31 (m, 3H), 6.98 (t, J = 7.2 Hz, 2H), 6.62 (t, J = 7.2 Hz, 2H), 6.39 (t, J = 7.2 Hz, 4H), 2.46 (s, 3H). ^{13}C-NMR (500 MHz, $CDCl_3$) δ = 171.90, 171.27, 157.81, 157.52, 143.40, 139.78, 139.67, 139.35, 139.07, 136.12, 132.73, 131.72, 129.45, 129.06, 128.76, 128.62, 128.51, 128.42, 127.55, 126.06, 125.94, 124.17, 120.71, 119.92, 119.85, 113.87, 56.63, 18.12 HR-MS (EI) m/z $C_{47}H_{32}N_4$ Cacld:652.2627, Found:652.2626 (M+, 100%).



Synthesis Figure 15. ^{1}H-NMR Spectra of 10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2-methylphenyl)-10H-spiro[acridine-9,9'-fluorene].



Synthesis Figure 16. ^{13}C-NMR Spectra of 10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2-methylphenyl)-10H-spiro[acridine-9,9'-fluorene].

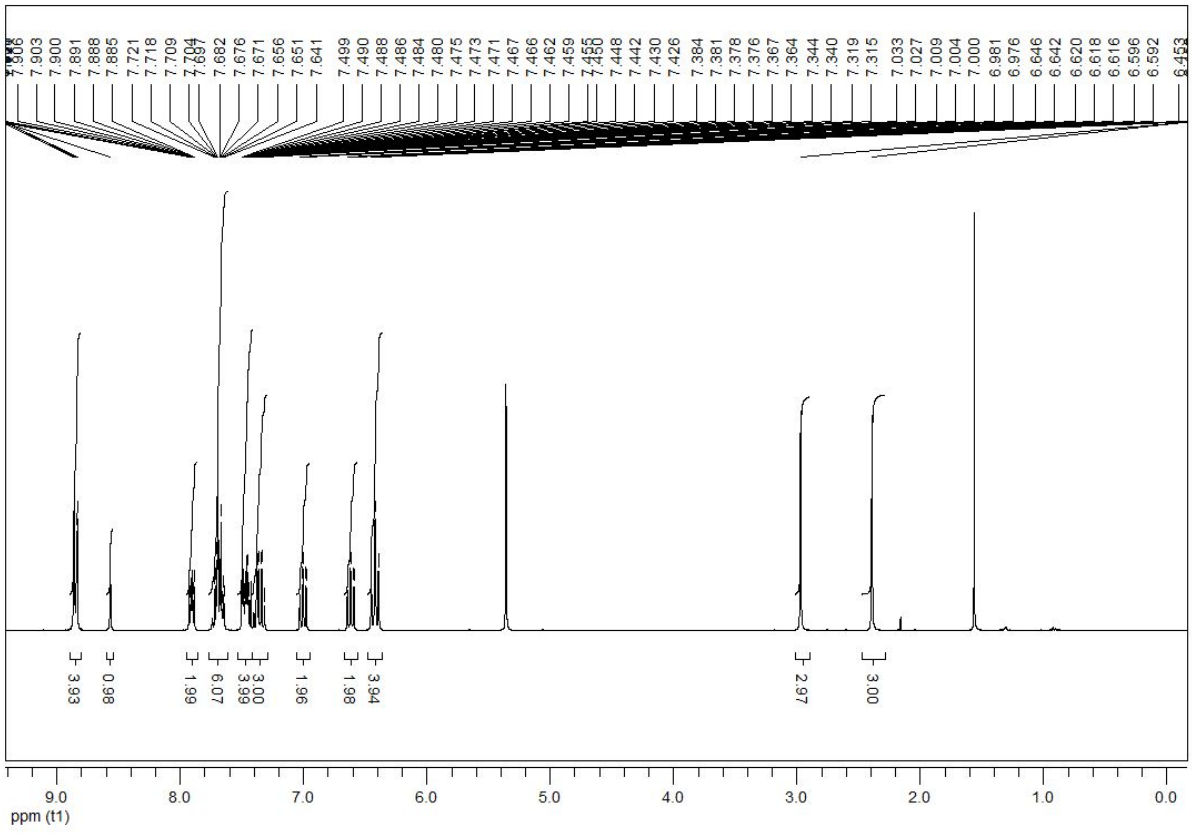


Synthesis Figure 17. EI Mass Spectra of 10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2-methylphenyl)-10H-spiro[acridine-9,9'-fluorene].

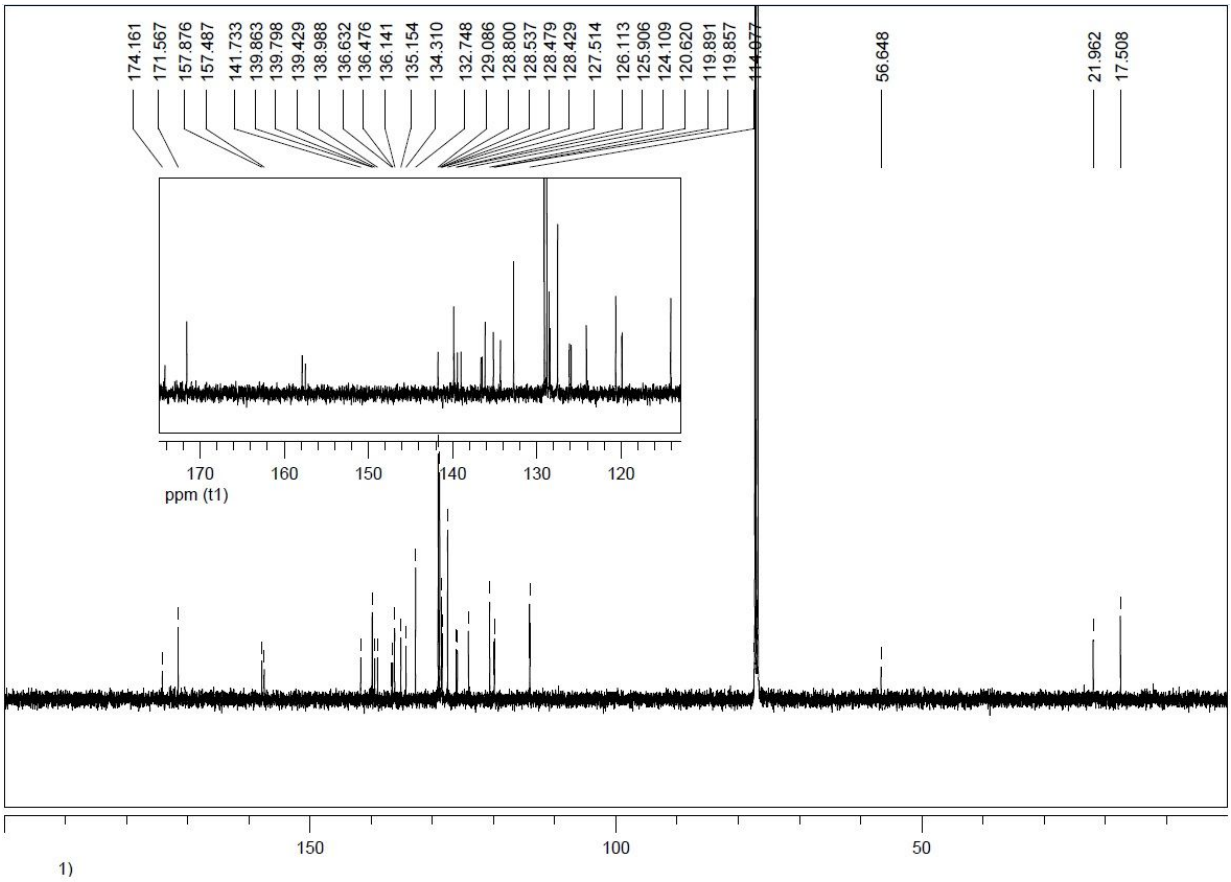
Synthesis of 10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2,5-dimethylphenyl)-10H-spiro[acridine-9,9'-fluorene] (8).

10*H*-spiro[acridine-9,9'-fluorene] (0.9 g, 2.72 mmol) and 2-(4-bromo-2,5-dimethylphenyl)-4,6-diphenyl-1,3,5-triazine (1.20 g, 2.99 mmol) were mixed in dry toluene (20 mL). Na-*t*-butoxide (0.78 g, 8.15 mmol), tri-*t*-buthylphosphine (0.05 g, 0.272 mmol) and tris(dibenzylideneacetone)dipalladium(0) (0.12 g, 0.136 mmol) was added and stirred for 10 h at 90 °C. The reaction mixture was extracted with dichloromethane and dried over anhydrous $MgSO_4$. The product was purified by a column with hexane and dichloromethane (Hex : MC = 3:1). Pale yellow solid. Yield : 1.21 g, (68.25 %)

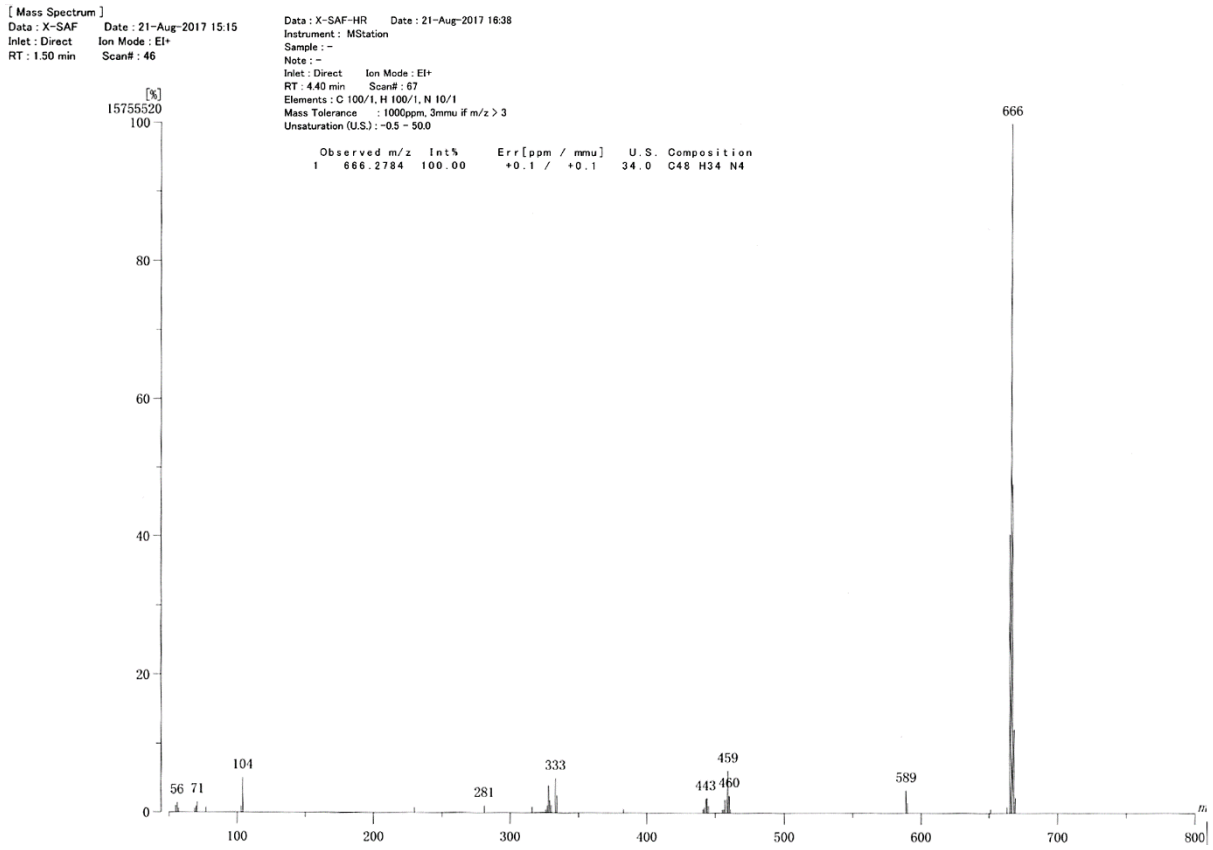
^{1}H-NMR (300 MHz, CD_2Cl_2) δ = 8.86-8.83 (m, 4H), 8.56 (s, 1H), 7.93-7.88 (m, 2H), 7.72-7.64 (m, 6H), 7.49-7.42 (m, 4H), 7.39 (d, J = 7.5 Hz, 1H), 7.34 (t, J = 7.5 Hz, 2H), 7.03-6.97 (m, 2H), 6.64-6.59 (m, 2H), 6.45-6.38 (m, 4H), 2.97 (s, 3H), 2.39 (s, 3H). ^{13}C-NMR (500 MHz, $CDCl_3$) δ = 174.16, 171.56, 157.87, 157.48, 141.73, 139.86, 139.79, 139.42, 138.98, 136.63, 136.47, 136.14, 135.15, 134.31, 132.74, 129.08, 128.80, 128.53, 128.47, 128.42, 127.51, 126.11, 125.90, 124.10, 120.62, 119.89, 119.85, 114.07, 56.65, 21.96, 17.50. HR-MS (EI) m/z $C_{48}H_{34}N_4$ Cacld:666.2783, Found:666.2784 (M+, 100%).



Synthesis Figure 18. ^{1}H-NMR Spectra of 10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2,5-dimethylphenyl)-10H-spiro[acridine-9,9'-fluorene].



Synthesis Figure 19. ^{13}C-NMR Spectra of 10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2,5-dimethylphenyl)-10H-spiro[acridine-9,9'-fluorene].



Synthesis Figure 20. EI Mass Spectra of 10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)-2,5-dimethylphenyl)-10H-spiro[acridine-9,9'-fluorene].

2. Experimental Methods

2.1. TGA, DSC, CV

The thermal analysis were performed by a TA TGA 2100 thermogravimetric analyzer in a nitrogen atmosphere at a rate of 10 ^{o}C/min. Differential scanning calorimeter (DSC) was performed using a TA DSC 2010 device at a heating rate of 10 ^{o}C/min. Cyclic voltammetry (CV) was performed using a CH instruments electrochemical analyzer. A three-electrode system composed of a glassy carbon working electrode, a platinum wire counter electrode and Ag/AgCl reference electrode was used. The 0.1 M of tetrabutylammonium hexafluorophosphate (TBAP) in choloroform was used as the electrolyte. The ferrocenium/ferrocene(4.43 eV) couple was used as internal standard. The cyclic voltammograms were obtained at a scan rate of 50 mV/s. HOMO level was obtained by oxidation onset and LUMO level was obtained by adding optical bandgap to HOMO level.

2.2. Fabrication of organic thin film

Organic films for photoluminescence measurements were fabricated by thermal deposition onto pre-cleaned fused-silica substrates at a base pressure of $<5\times10^{-7}$ torr. OLEDs were fabricated by thermal deposition onto 75-nm-thick patterned ITO glass substrates at a base pressure of $<5\times10^{-7}$ torr. Before deposition of the organic layers, the ITO substrates were pre-cleaned with isopropyl alcohol and then exposed to a UV-ozone for 10 minutes.

2.3. Photoluminescence and Electroluminescence Measurement

Absorbance of 10^{-5} M toluene solution was measured with Varian Cary 5000 UV-Vis-NIR spectrometer. The PLQY was measured using a monochromator-attached photomultiplier tube (PMT) with a PL sample in an integrating sphere (Labsphere) using a continuous wave 325 nm He/Cd laser (Kimmon Koha) for excitation. PL spectra and angle-dependent PL measurements

were measured with a CCD spectrometer (Ocean Optics Maya2000) using a He/Cd laser (325 nm) for excitation. The p-polarized light emitted from PL samples was measured by attaching the film substrate to a half-cylinder lens with index-matching oil and changing the angle between the sample and the detector from -90° to 90° using a motorized rotational stage. Transient PL was measured with a streak camera (Hamamatsu Photonics) using a nitrogen laser (337 nm, Usho Optical Systems) as the excitation source. The current densities, luminance, and EL spectra of OLEDs were measured using a programmable source meter (Keithley 2400) and spectrophotometer (Spectrascan PR650, Photo Research).

3. Supporting Tables and Figures

Table S1. Device performance of Blue (CIEy < 0.16) TADF OLEDs.

Dopant Name	Maximum EQE	CIE Coordinate	Reference
TTAZ	23.7	(0.148, 0.158)	This Work
CzoB	22.6	(0.139, 0.150)	Ref. 21
PX-SBA	20.8	(0.16, 0.13)	Ref. 33
DABNA-2	20.2	(0.12, 0.13)	Ref. 24
3	20.1	(0.14, 0.16)	Ref. 27
DMTDAc	19.8	(0.15, 0.13)	Ref. 31
ICzDAc	19.5	(0.15, 0.16)	Ref. 17
Cz-TRZ3	19.2	(0.148, 0.098)	Ref. 8
4	18.4	(0.138, 0.140)	Ref. 22
Cz-TRZ4	18.3	(0.150, 0.097)	Ref. 8
B2	18.3	(0.13, 0.11)	Ref. 35
Ac-3MHPM	17.8	(0.16, 0.15)	Ref. 20
DCzTrz	17.8	(0.15, 0.16)	Ref. 28
5	17.3	(0.150, 0.086)	Ref. 22
CNICtCz	16.0	(0.14, 0.13)	Ref. 29
TXAZ	16.0	(0.148, 0.131)	This Work
DtDCzTrz	14.7	(0.15, 0.11)	Ref. 34
tDCzTrz	14.5	(0.15, 0.12)	Ref. 34
DMOC-DPS	14.5	(0.16, 0.16)	Ref. 26
CNBPCz	14.0	(0.14, 0.12)	Ref. 23
ICzAc	13.7	(0.15, 0.09)	Ref. 17
DABNA-1	13.5	(0.13, 0.09)	Ref. 24
4	13.3	(0.14, 0.16)	Ref. 27
CNICCz	12.4	(0.15, 0.08)	Ref. 29
5	11.4	(0.15, 0.15)	Ref. 18
FA-TA	11.2	(0.15, 0.13)	Ref. 37
DCzBN3	10.3	(0.16, 0.06)	Ref. 36
3	9.9	(0.15, 0.07)	Ref. 16
Cz2BP	8.1	(0.16, 0.14)	Ref. 30
DCzBN2	7.7	(0.15, 0.07)	Ref. 36
2CzdOXDPh	6.8	(0.161, 0.150)	Ref. 19
PA-TA	6.7	(0.15, 0.10)	Ref. 37
2CzdOXD4MeOPh	6.6	(0.147, 0.108)	Ref. 19
SPXZPO	6.3	(0.16, 0.12)	Ref. 32

Table S2. DFT calculation results of the TADF emitters.

(eV)	$S_{1,VA}$	$T_{1,VA}$	$\Delta E_{ST,VA}$	$S_{1,VE}$	HOMO	LUMO
SpiroAC-TRZ	3.19	3.18	0.012	2.83	-5.74	-1.42
TTSA	3.24	3.23	0.011	2.88	-5.74	-1.39
TXSA	3.36	3.35	0.010	2.91	-5.74	-1.32
DTPDDA	3.39	3.38	0.011	3.01	-5.93	-1.41
TTAZ	3.46	3.44	0.012	3.03	-5.95	-1.38
TXAZ	3.54	3.53	0.010	3.08	-5.91	-1.31

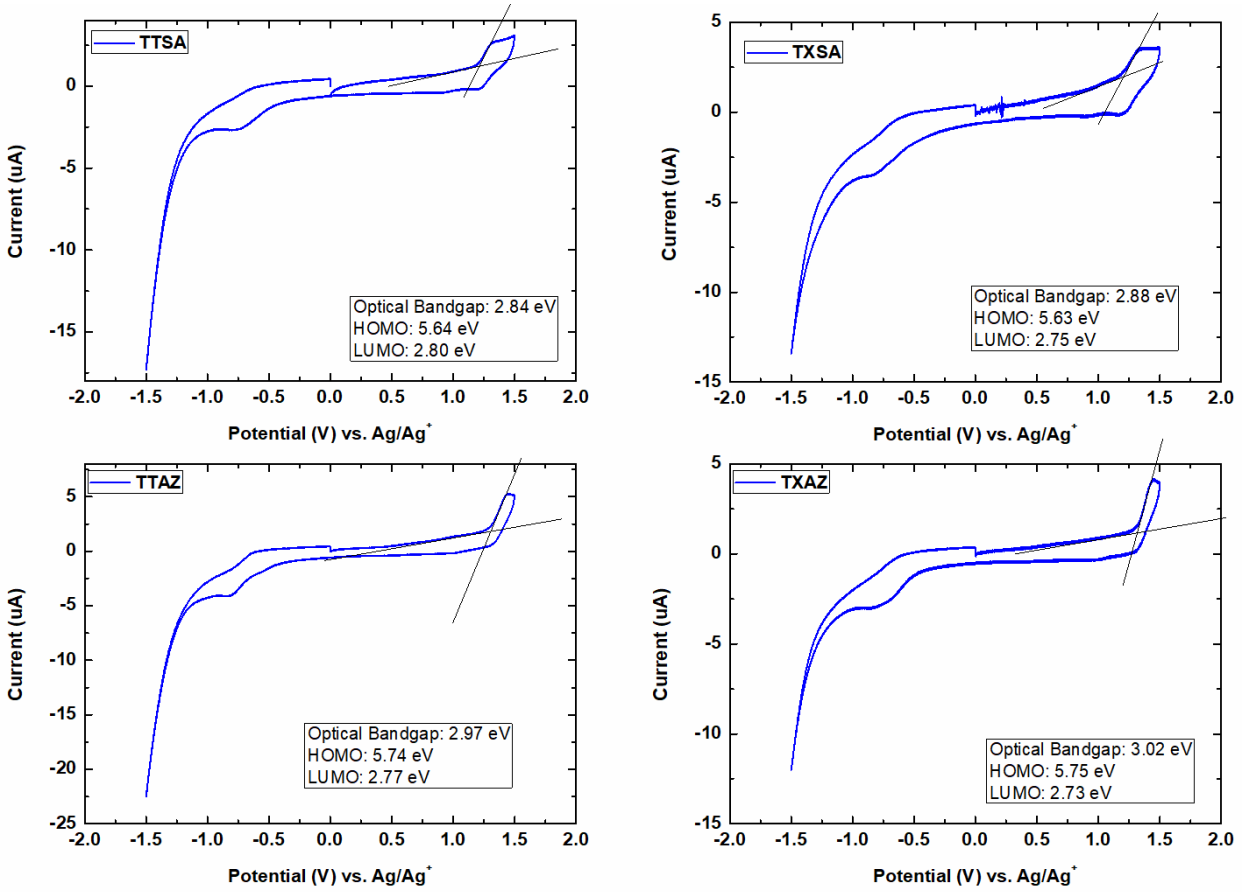


Figure S1. Cyclic Voltammetry curve of the molecules.

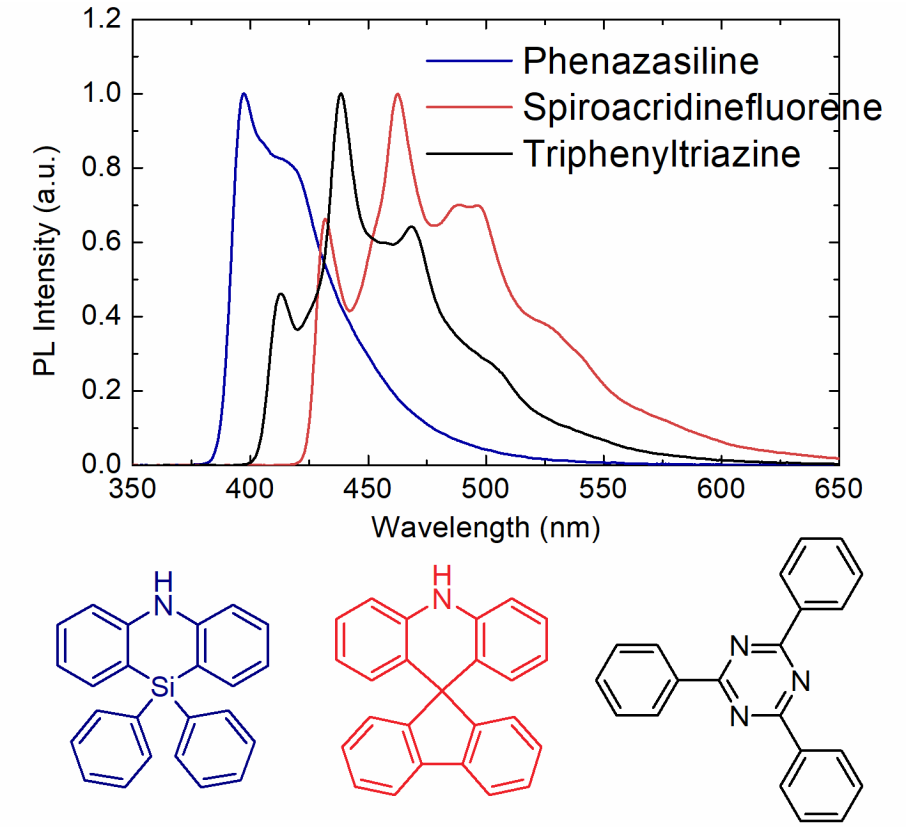


Figure S2. Phosphorescence of phenazasiline, Spiroacridinefluorene and Triphenyltriazine. Frozen 10^{-5} M toluene solution at 77 K, 200 ms delayed after UV-excitation off. Phenazasiline T_1=3.12 eV, Sprioacridinefluorene T_1= 2.86 eV, Triphenyltriazine T_1 = 3.00 eV .

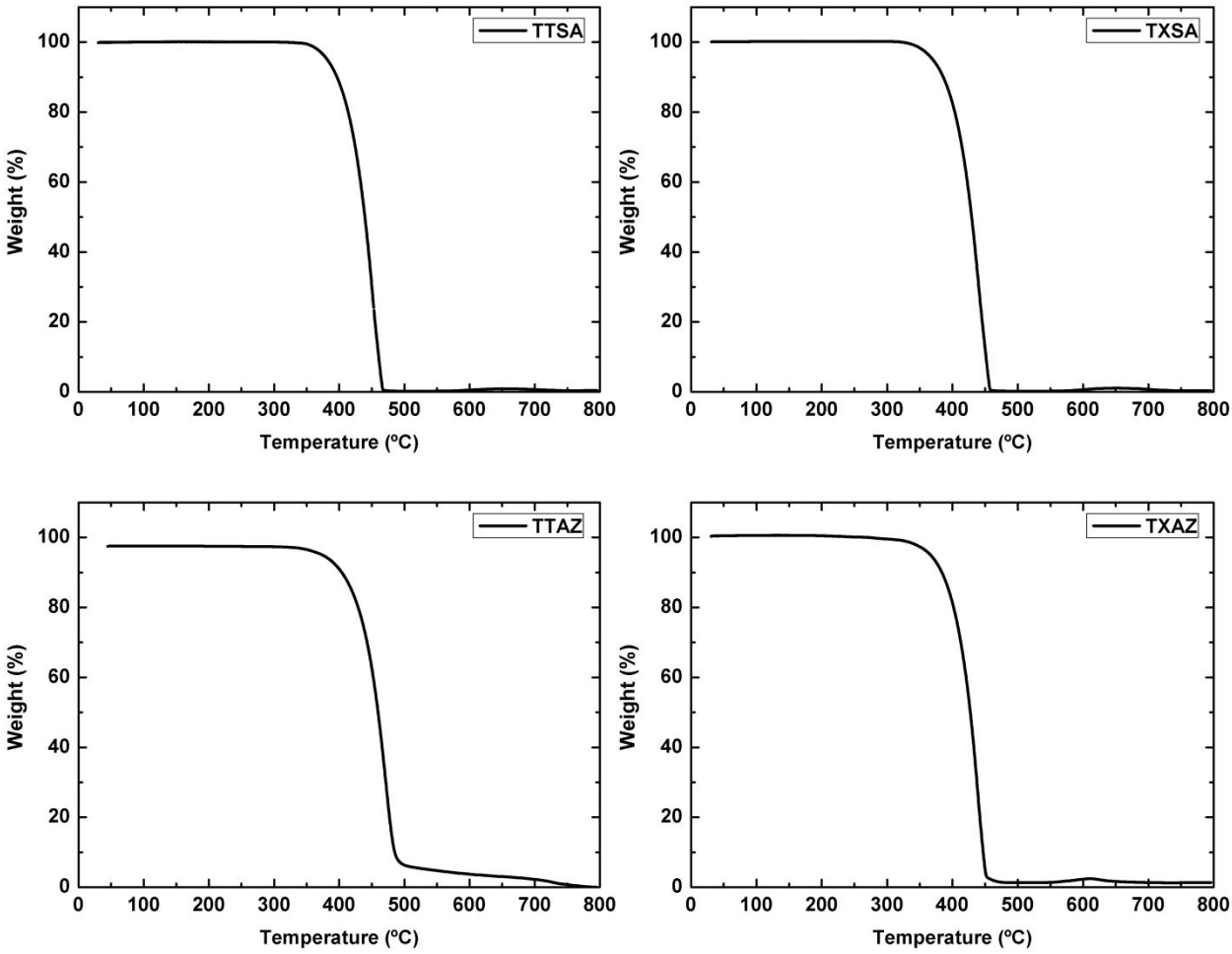


Figure S3. Thermogravimetric analysis (TGA) of the compounds

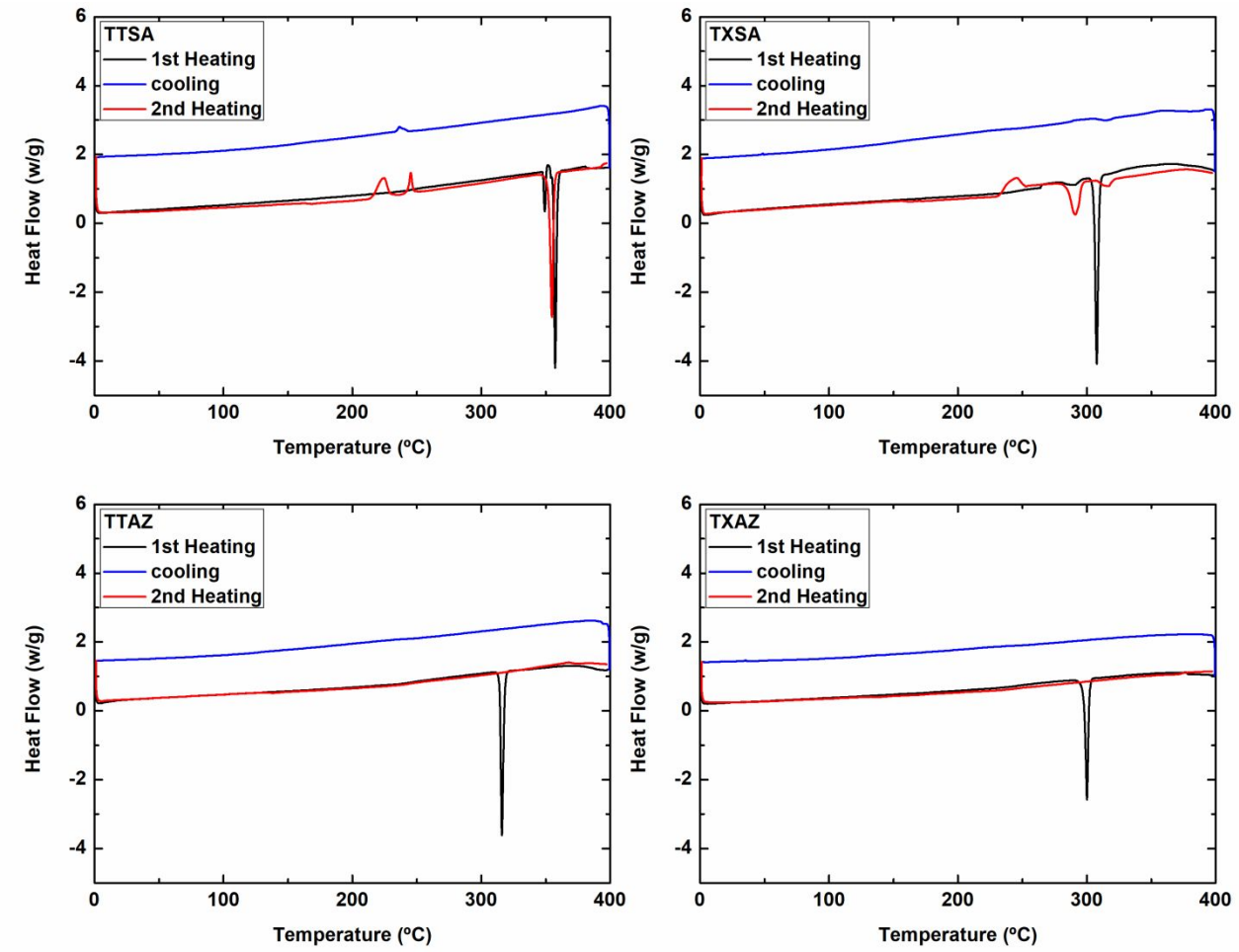


Figure S4. Differential scanning calorimetry (DSC) of the compounds

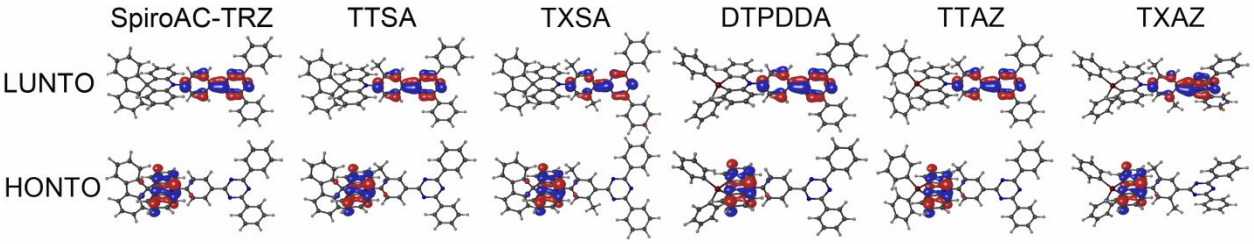


Figure S5. Optimized S_0 state geometries and natural transition orbitals of $S_0 \rightarrow T_1$ vertical excitation of the molecules.

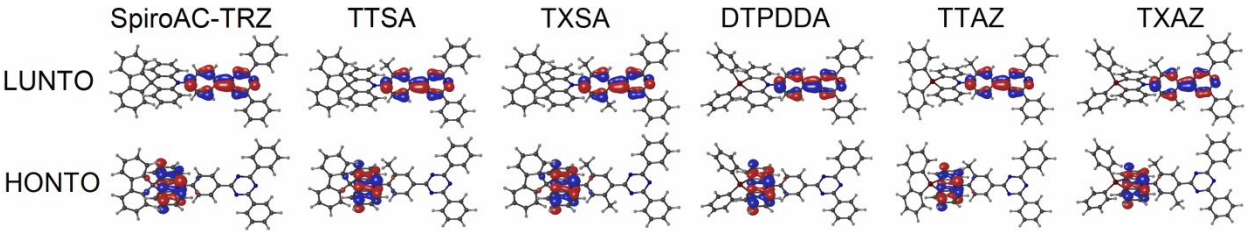


Figure S6. Optimized S_1 state geometries and natural transition orbitals of $S_1 \rightarrow S_0$ vertical emission of the molecules.

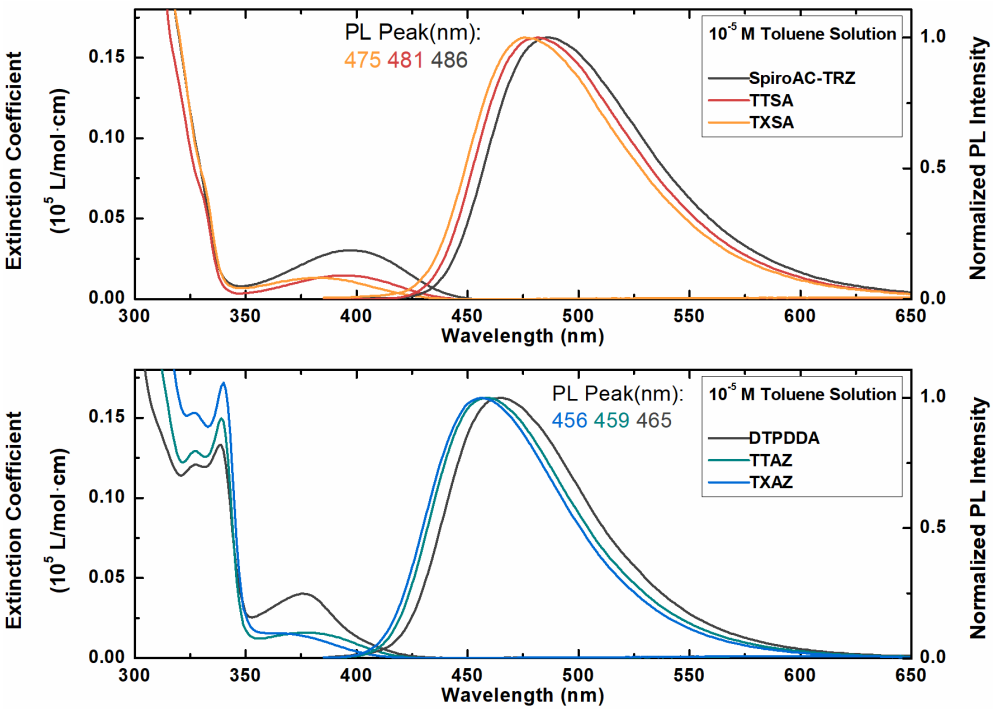


Figure S7. Molar Extinction Coefficient and PL spectrum of emitters in Toluene.

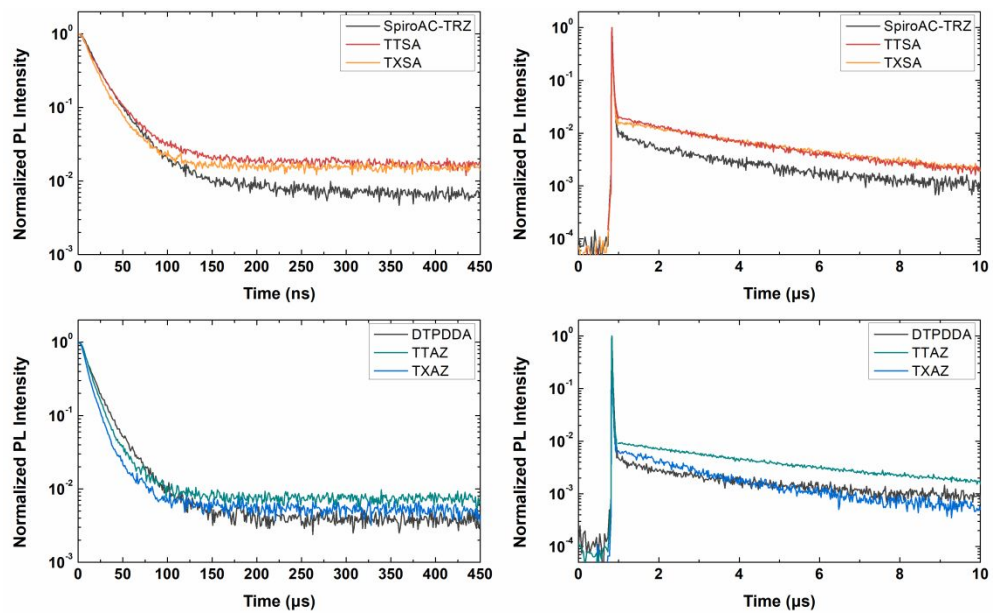


Figure S8. Transient PL decays of emitters 10 wt% doped in mCP:TSPO1 host. (500 ns and 10 μs scale)

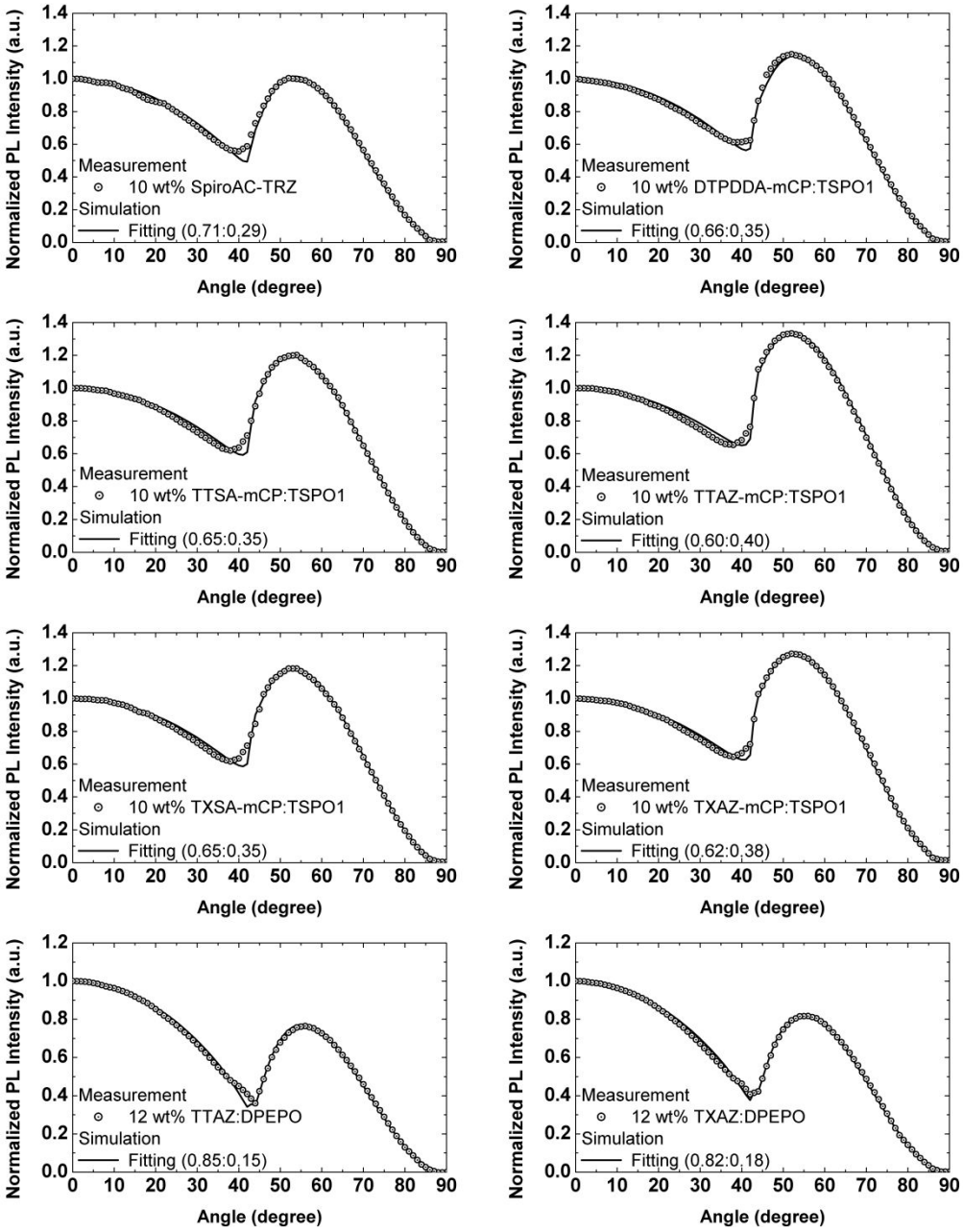


Figure S9. Angle-Dependent PL intensity of p-polarized light from 10 wt% emitter: mCP:TSPO1 and 12 wt% emitter:DPEPO 30 nm films at the wavelength of PL peak of each film.

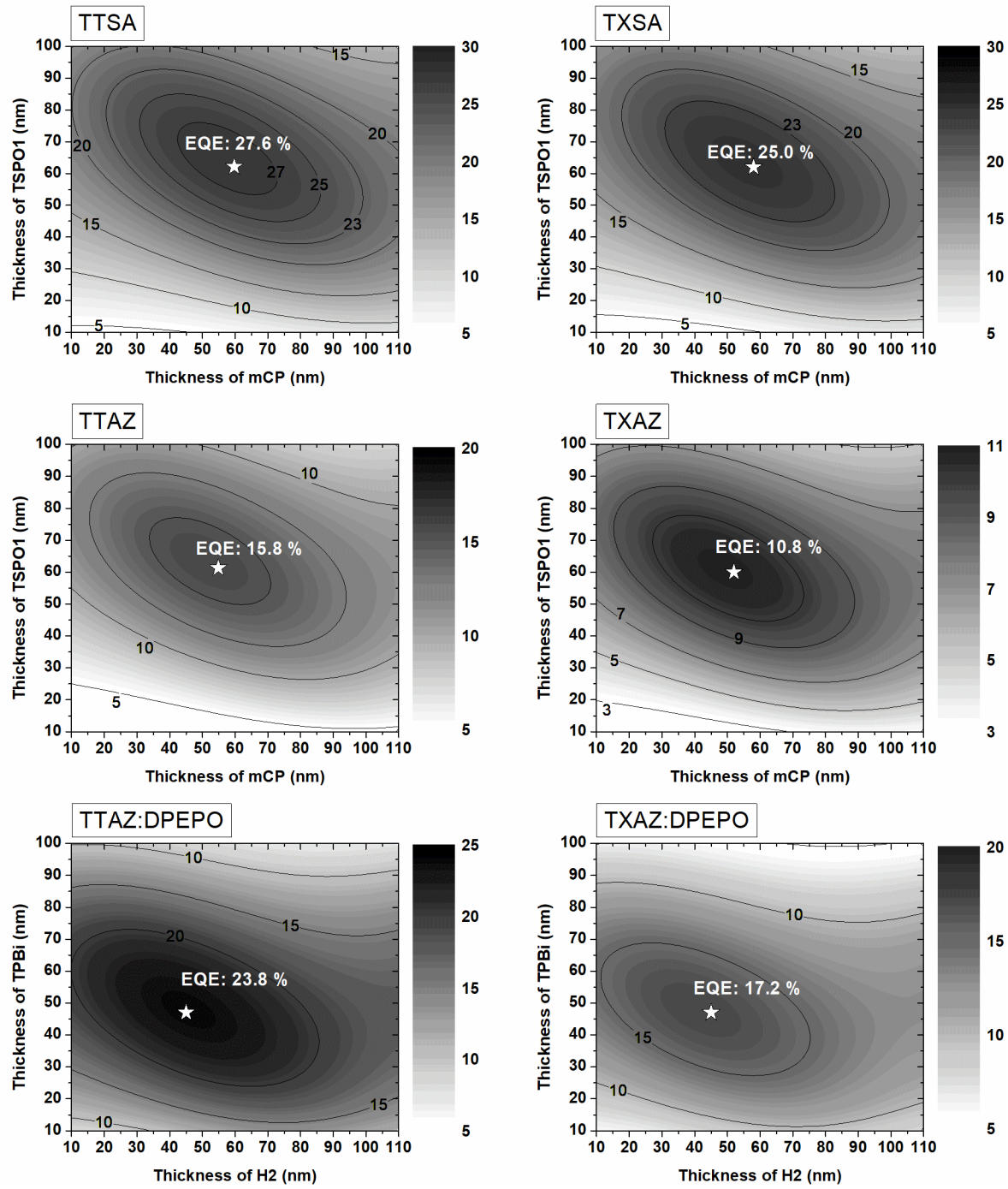


Figure S10. EQE simulation contour plot.

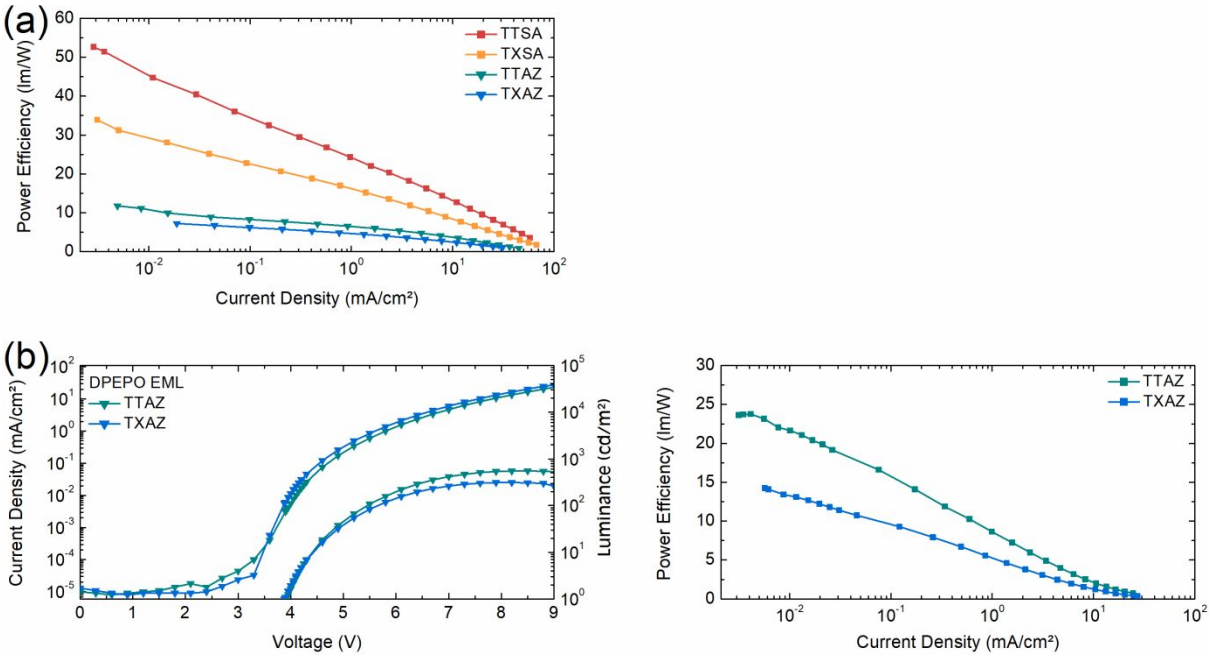
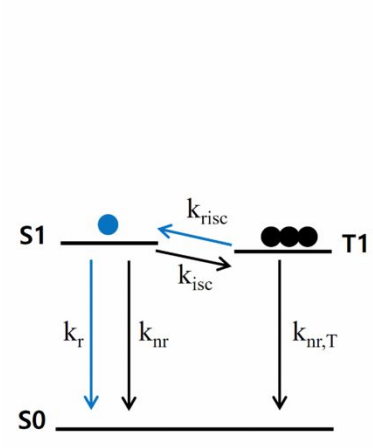


Figure S11 (a) Power Efficiency curve of mCP:TSPO1 device. (b) J-V-L curve and power efficiency of OLEDs based on TTAZ/TXAZ emitters and DPEPO host.



$$\Phi_F = \frac{k_r}{k_r + k_{nr} + k_{isc}},\ \Phi_{ISC} = \frac{k_{isc}}{k_r + k_{nr} + k_{risc}},\ \Phi_{RISC} = \frac{k_{risc}}{k_{risc} + k_{nr,T}}$$

$$\Phi_{PLQY} = \frac{\Phi_F}{1 - \Phi_{ISC}\Phi_{RISC}}$$

$$IQE = \frac{\Phi_F (0.25 + 0.75 \times \Phi_{RISC})}{(1 - \Phi_{ISC}\Phi_{RISC})}$$

$$EQE = \eta_{outcoupling} \cdot IQE$$

$$EQE_{max,cal} = \eta_{outcoupling} \cdot \Phi_{PLQY} (\Phi_{RISC} = 1)$$

$$\frac{EQE}{EQE_{max,cal}} = (0.25 + 0.75 \times \Phi_{RISC}), \Phi_{RISC} = \frac{1}{0.75} \times \left(\frac{EQE}{EQE_{max,cal}} - 0.25 \right)$$

Figure S12. Excited-sate dynamics diagram of TADF molecules and theorectical calculation of EQE and Φ_{RISC}.