

Aryl-Substituted Acridine Donor Derivatives Modulate the Transition Dipole Moment Orientation and Exciton Harvesting Properties of Donor-Acceptor TADF Emitters

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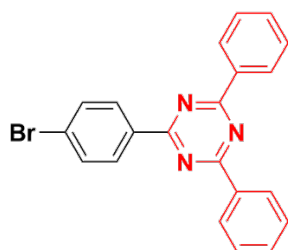
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SUPPORTING INFORMATION

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Experimental Section

2-(4-bromophenyl)-4,6-diphenyl-1,3,5-triazine (BrPh-dPh-TRZ)



BrPh-dPh-TRZ was prepared following a literature procedure.¹⁸ A mixture of 4-bromobenzoyl chloride (5.0 g, 22.78 mmol, 1 equiv.) and benzonitrile (4.699 mL, 45.57 mmol, 2 equiv.), in DCM (30 mL), was cooled to 0°C in an ice bath and stirred for 30 min. Antimony pentachloride (2.924 mL, 22.78 mmol, 1 equiv.) was then added dropwise with a glass pipette. The solution immediately turned from white to canary yellow. The solution was stirred at room temperature over-night. The yellow solid was filtered and washed with dichloromethane. With an ice-bath, the yellow solid was added to a 35% ammonia solution (175 mL) and stirred in the ice bath for 30 min, and then 3h at room temperature. The white solid was then filtered and washed with cold MeOH to yield the desired product. (8.701 g). **Yield:** 98%; **Mp:** 200-210°C ; **R_f:** 0.90 (ethyl acetate/cyclohexane = 1:4); **¹H NMR** (500 MHz, CDCl₃) δ: 8.78 – 8.76 (dt, *J*=6.9, 1.4, 1.1, 4H), 8.67-8.64 (dt, *J*=8.6, 2.4, 1.8, 2H), 7.73-7.70 (dt, *J*= 8.5, 2.5, 1.9, 2H), 7.64-7.57 (m, 6H); **¹³C NMR** (126 MHz, CDCl₃) δ: 171.89, 171.00, 136.15, 135.33, 132.82, 132.06, 130.62, 129.12, 128.84, 127.63; **GC-MS retention time:** 13.529 min; **purity:** >99%; **Mass Theoretical:** (C₂₁H₁₄BrN₃) 387.04; **Mass found:** 387.

Spectral data matches those previously reported in the literature.¹⁹

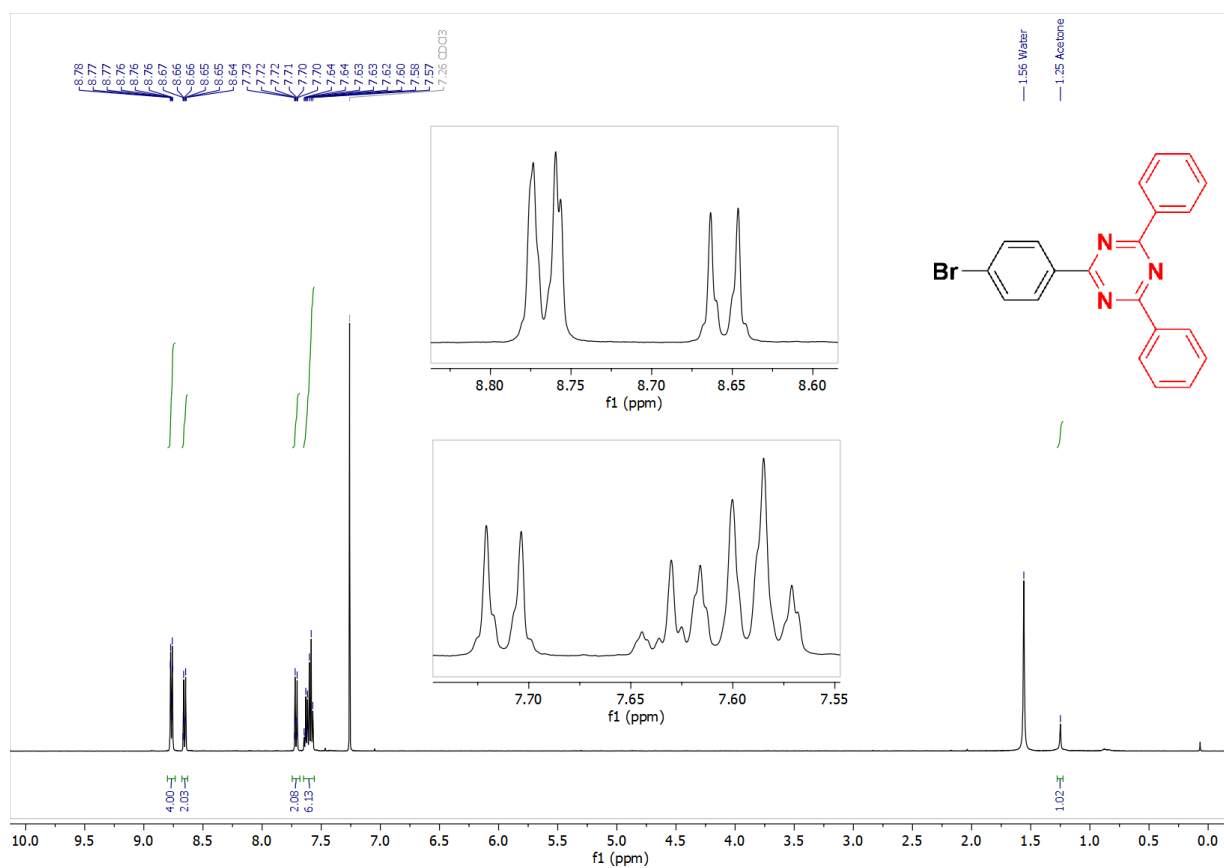


Figure S1. ¹H NMR of BrPh-dPh-TRZ in CDCl₃.

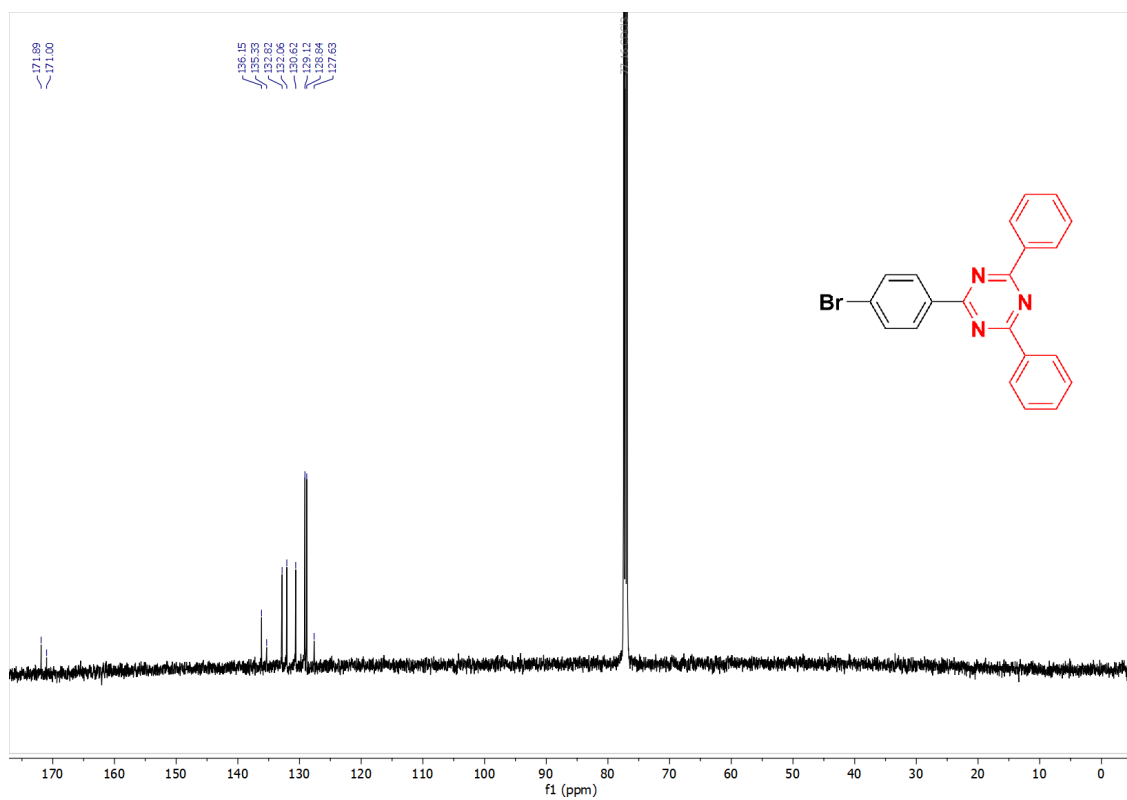
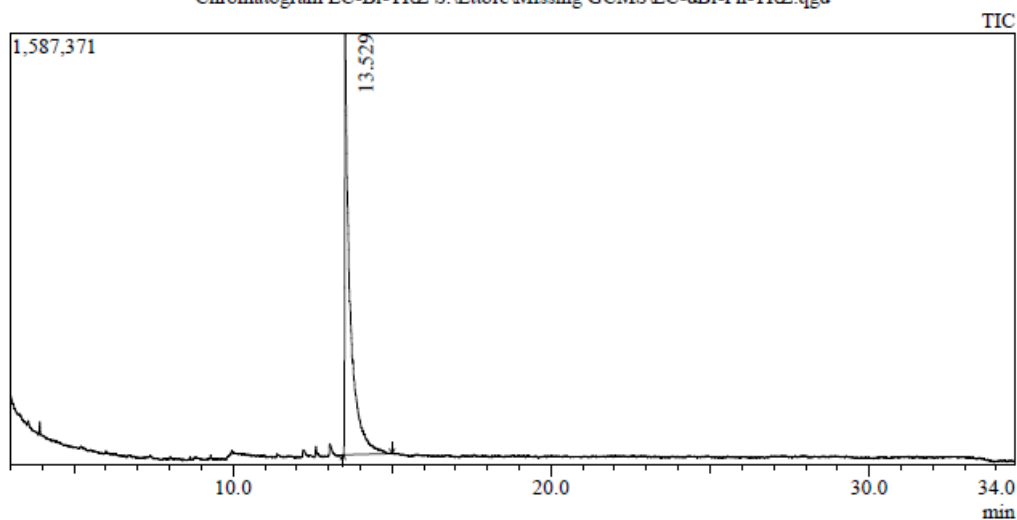


Figure S2. ¹³C NMR of BrPh-dPh-TRZ in CDCl₃.

Sample Information

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 Sample Amount : 1
 Dilution Factor : 1
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 Org Data File : S:\Ettore\Missing GCMS\EC-dBr-Ph-TRZ.qgd
 Method File : S:\standard method 1 for RTX-1 column 330 injection-long.qgm
 Org Method File : S:\standard method 1 for RTX-1 column 330 injection-long.qgm
 Report File :
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 Modified by : Admin
 Modified : 30/05/2022 14:18:08

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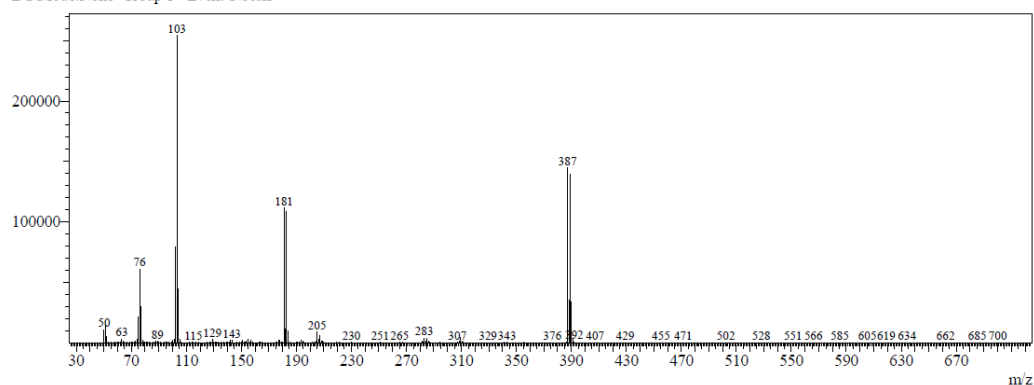
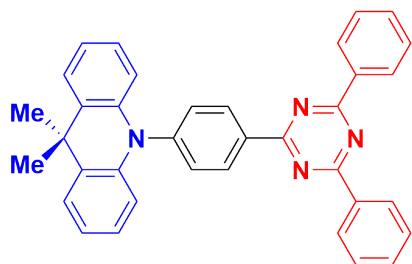


Figure S3. GC-MS trace of BrPh-dPh-TRZ.

10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-9,9-dimethyl-9,10-dihydroacridine (DMAC-TRZ)



To a schlenk flask fitted with a reflux condenser was added DMAC (2.0 g, 9.6 mmol, 1 equiv.), 2-(4-bromophenyl)-4,6-diphenyl-1,3,5-triazine (**BrPh-dPh-TRZ**) (4.1 g, 10.5 mmol, 1.1 equiv.), tribasic potassium carbonate (4.0 g, 28.8 mmol, 3 equiv.) palladium(II) acetate (214.5 mg, 0.96 mmol, 0.1 equiv.), tri-*tert*-butylphosphonium tetrafluoroborate (1.1 g, 3.8 mmol, 0.4 equiv.), and dry toluene (200 mL). The flask was connected to a Schlenk line via a reflux condenser and the mixture was heated to reflux, under N₂ atmosphere. After 48 h, the reaction was diluted with water, and the organic layer was extracted with DCM (50 mL × 3). The combined organic extracts were washed with brine, dried over Mg₂SO₄ and concentrated by rotary evaporation. The crude was then washed with cold pentane (250 mL) and cold diethyl ether (250 mL) to achieve the desired product as a light brown solid (2.1 g). **Yield:** 42%; **Mp:** 250-253°C; **R_f:** 0.76 (ethyl acetate/cyclohexane = 1 :4); **¹H NMR** (500 MHz, CDCl₃) δ: 9.04 – 9.02 (dt, *J*= 8.3, 2.3, 2.1, 2H), 8.83-8.81 (dt, *J*= 6.6, 1.4, 1.4, 4H), 7.66 – 7.56 (m, 8H), 7.50-7.48 (dd, *J*= 7.5, 1.7, 2H), 7.01-6.94 (m, 4H), 6.39-6.37 (dd, *J*= 8.0, 1.3, 2H), 1.73 (s, 6H); **¹³C NMR** (126 MHz, CDCl₃) δ: 172.00, 171.22, 140.74, 136.23, 136.21, 132.86, 131.75, 131.68, 130.36, 129.17, 128.88, 126.60, 125.51, 121.98, 114.33, 36.19, 31.46.

Spectral data match those previously reported in the literature.²⁰

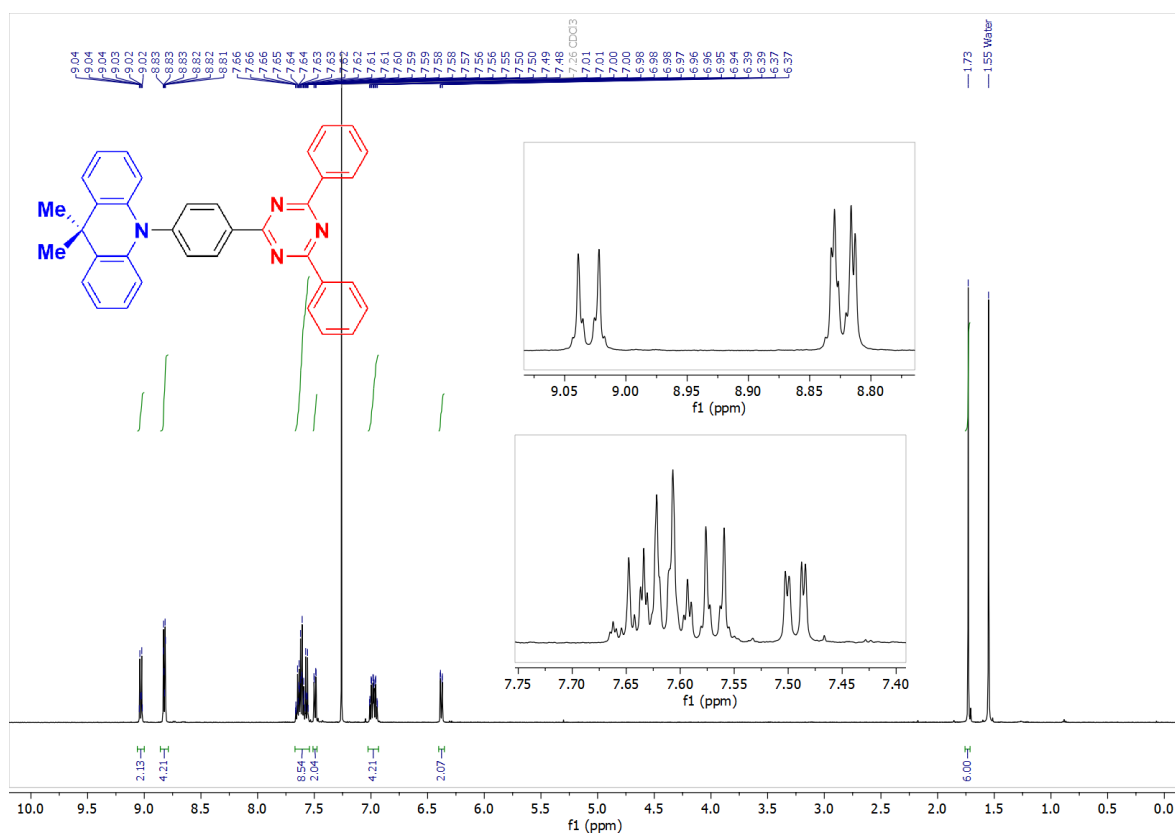


Figure S4. ¹H NMR of **DMAC-TRZ** in CDCl₃.

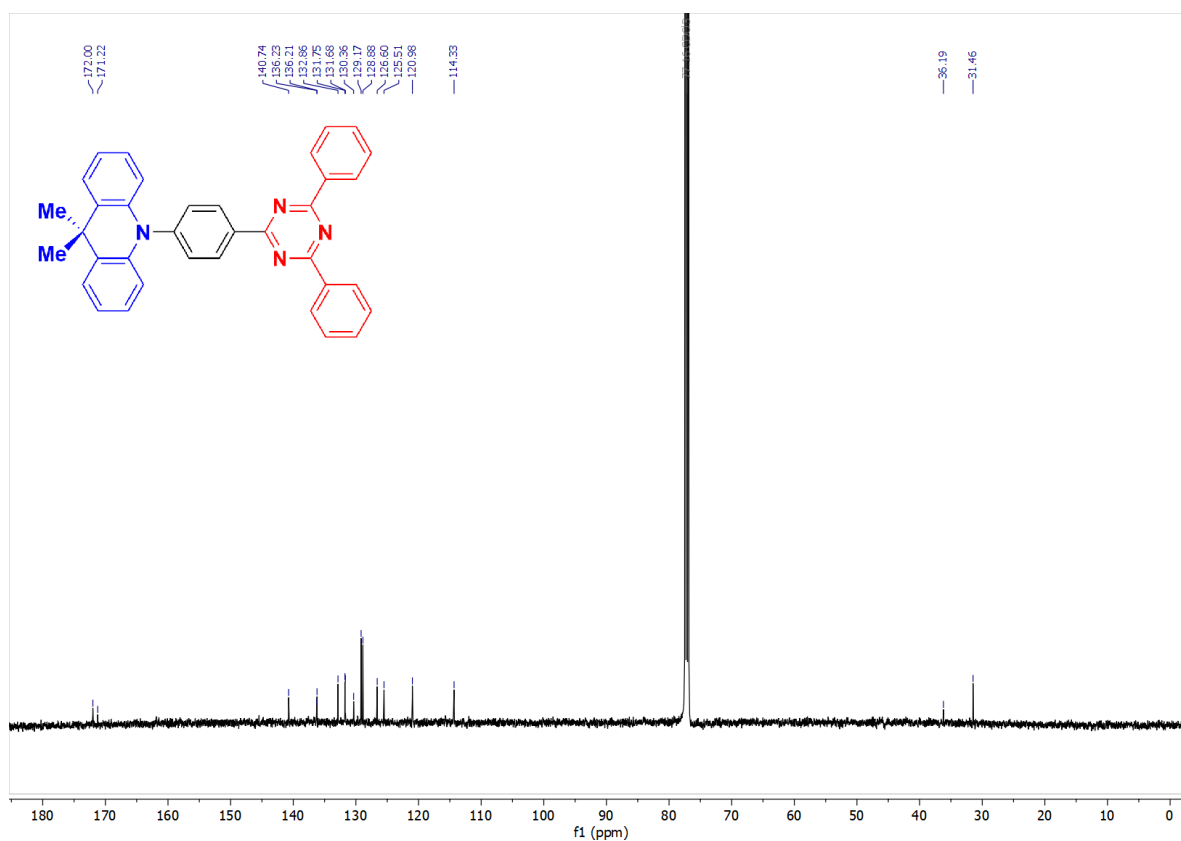
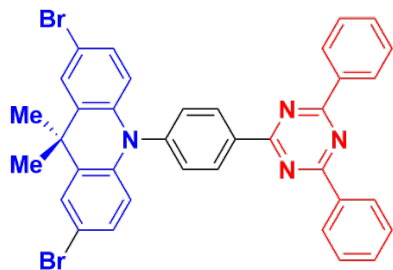


Figure S5. ¹³C NMR of **DMAC-TRZ** in CDCl₃.

2,7-dibromo-10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-9,9-dimethyl-9,10-dihydroacridine (dBr-DMAC-TRZ)



To a round bottom flask **DMAC-TRZ** (2.06 g, 3.99 mmol, 1 equiv.) and THF (90 mL) were added. The solution was cooled in an ice bath and a solution of *N*-bromosuccinimide (NBS, 1.63 g, 9.17 mmol, 2.3 equiv.) in THF (100 mL) was slowly added. The reaction mixture turned red, then yellow and then brown with the continuous addition of the NBS solution. The solution was stirred overnight, at room temperature, in darkness. The reaction was diluted with water, extracted with DCM (3 × 50 mL). The organic phase was washed with brine, dried over MgSO₄ and concentrated under reduced pressure. The crude was then washed with cold pentane (250 mL) and cold diethyl ether (250 mL) to achieve the desired product as a light brown solid (2.22 g). **Yield:** 75%; **Mp:** decomposition at 250 °C; **R_f:** 0.83 (ethyl acetate/cyclohexane= 1:4); **¹H NMR** (300 MHz, CDCl₃) δ: 9.05-9.02 (dt, *J*= 8.7, 2.3, 1.9, 2H), 8.83-8.80 (dt, *J*= 6.3, 1.6, 1.3, 6H), 7.66 – 7.59 (m, 4H), 7.55-7.54 (d, *J*= 2.3, 2H), 7.52-7.49 (dt, *J*= 8.2, 2.8, 1.7, 2H), 7.10-7.06 (dd, *J*= 8.8, 2.3, 2H), 6.25-6.22 (d, *J*= 8.8, 2H), 1.68 (s, 6H). **¹³C NMR** (126 MHz, CDCl₃) δ: 172.06, 170.99, 144.43, 139.58, 136.86, 136.10, 132.95, 131.98, 131.90, 131.31, 128.56, 128.17, 128.90, 128.36, 116.03, 113.77, 36.48, 31.17; **HR-MS** (APCI) [M+H]⁺ **Calculated:** (C₃₆H₂₇⁷⁹Br₂N₄⁺) 673.0579, **Found:** 673.0602.

Spectral data match those previously reported in the literature.²¹

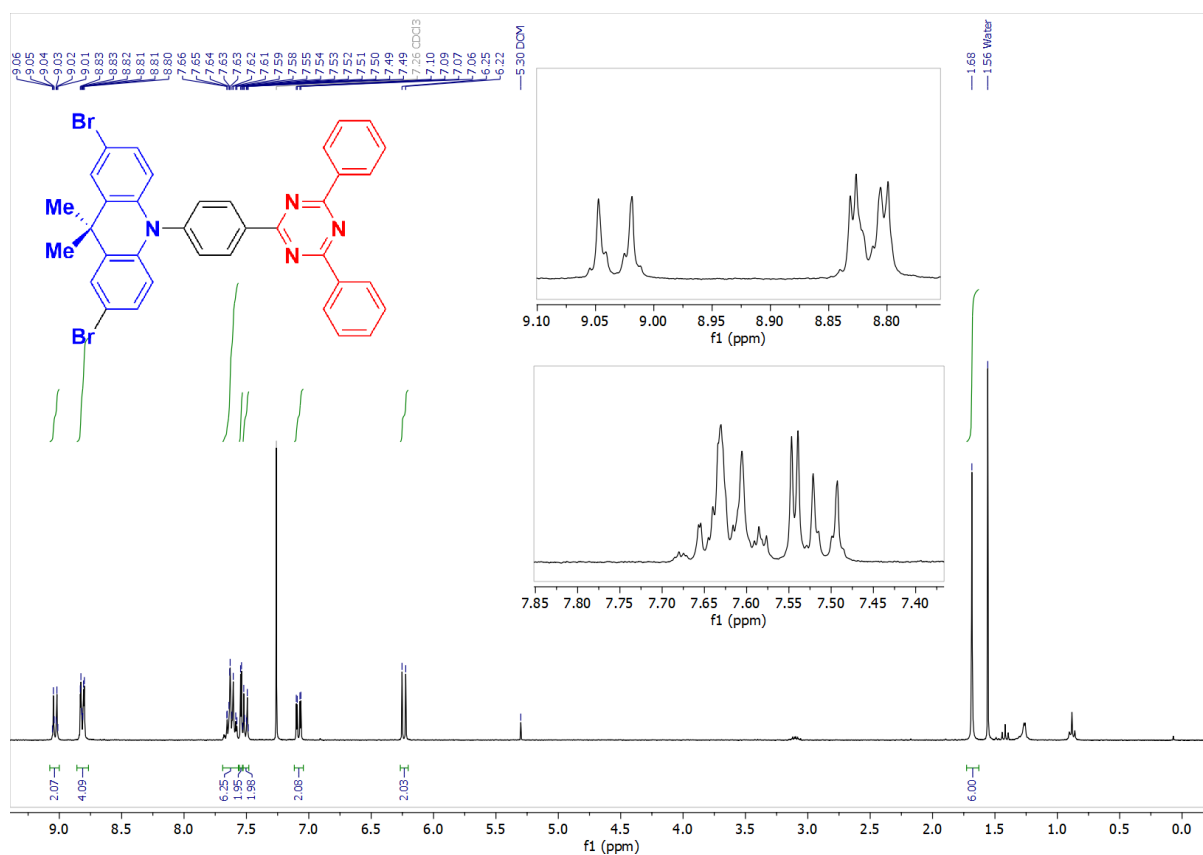


Figure S6. ¹H NMR of dBr-DMAC-TRZ in CDCl₃.

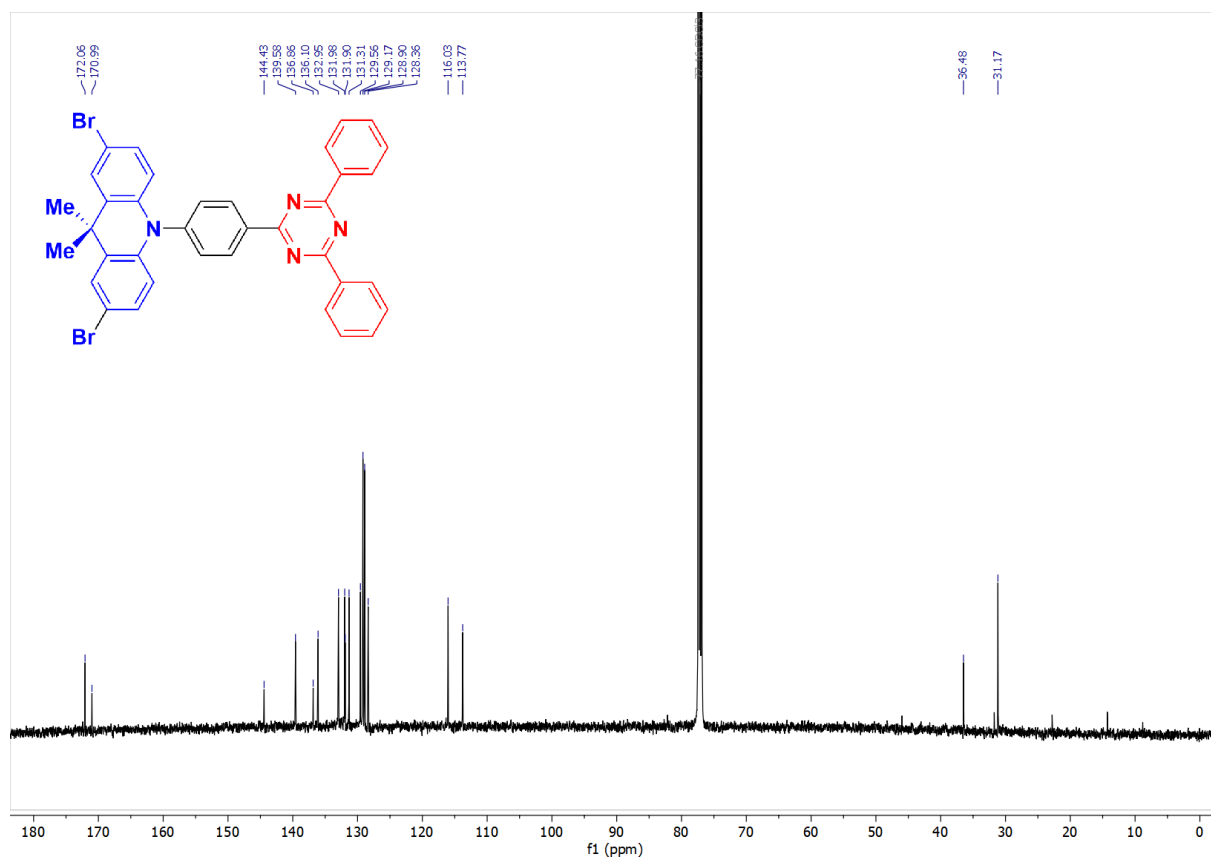


Figure S7. ¹³C NMR of dBr-DMAC-TRZ in CDCl₃.

School of Chemistry Mass Spectrometry Service

SampleID

Sample Description

Analysis Name

Method

Instrument

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maXis impact

Source Type

APCI

Ion Polarity

Positive

Submitter

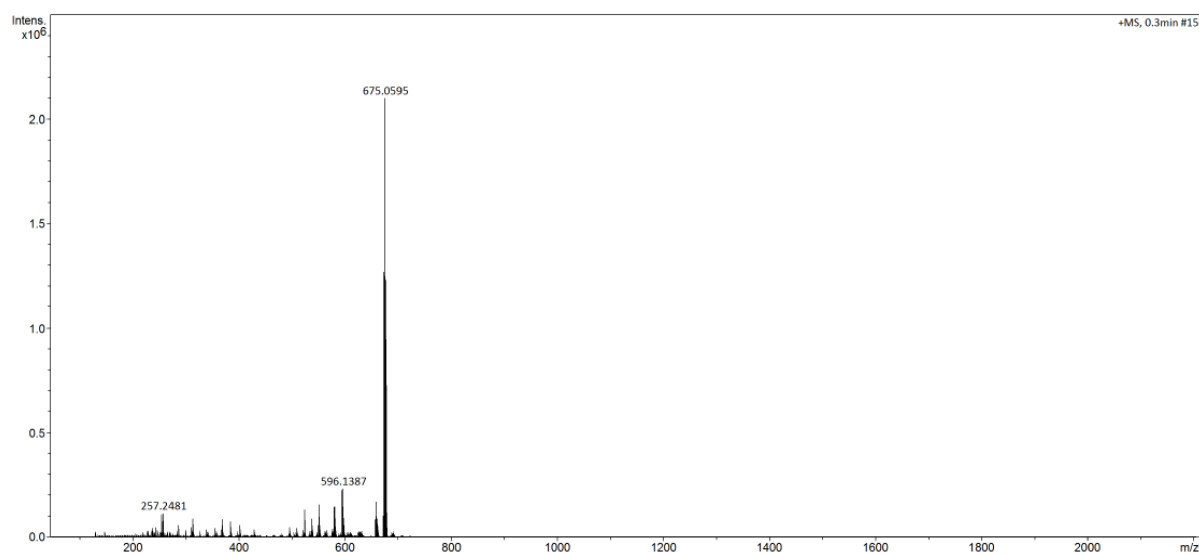
Supervisor

Acquisition Date

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Bruker Compass DataAnalysis 4.3

Analysis Name

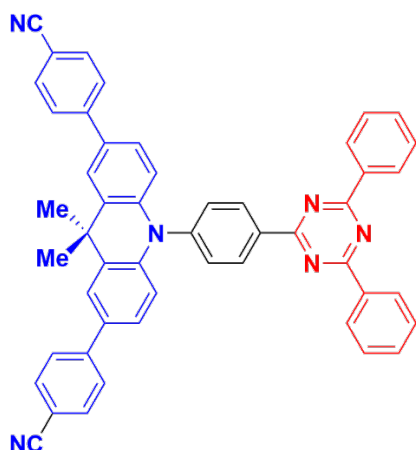
dBrPh_DMAC_TRZ_a.d

12/03/2022 17:46:15

1 of 1

Figure S8. HRMS analysis report for **dBr-DMAC-TRZ**.

4,4'-(10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-9,9-dimethyl-9,10-dihydroacridine-2,7-diyl)dibenzonitrile (CNPh-DMAC-TRZ)



The same reaction procedure as **'BuPh-DMAC-TRZ** was followed but with a different boronic acid, (4-cyanophenyl)boronic acid (0.872 g, 5.931 mmol, 4 equiv.). After 72 h, the reaction was diluted with THF and filtered over celite to remove any unreacted palladium. The solution was diluted with water, and the organic layer was extracted with DCM (3 × 50 mL). The organic phase was washed with brine, dried over MgSO₄ and concentrated under reduced pressure. The target product was isolated as yellow solid after purification by column chromatography on silica gel using 5:1 hexane/EtOAc as eluent. It was then further purified *via* recrystallization in THF/MeOH. (0.448 g). The compound was further purified by gradient temperature sublimation. **Yield:** 42%; **Mp:** 390-395 °C; **R_f:** 0.82 (MeOH/DCM = 1:99); **¹H NMR** (500 MHz, CDCl₃) δ: 9.10-9.08 (d, *J*= 8.3, 2H), 8.84-8.82 (d, *J*= 7.0, 4H), 7.75 – 7.60 (m, 20H), 6.50-6.48 (d, *J*= 8.6, 2H), 1.85 (s, 6H); **¹³C NMR** (126 MHz, CDCl₃) δ: 171.98, 170.89, 145.37, 144.31, 140.62, 136.87, 135.96, 132.87, 132.65, 131.97, 131.91, 131.28, 130.61, 129.05, 128.80, 126.96, 125.62, 124.58, 119.19, 115.05, 110.01, 36.42, 31.94; **HPLC retention time:** 10.365; **purity:** 100.00%; **HR-MS** (APCI) [M+H]⁺ **Calculated:** (C₅₀H₃₅N₆⁺) 719.2918, **Found:** 719.2947; **EA** (C₅₀H₃₄N₆) **Calculated** C: 83.54, H: 4.77, N: 11.69; **Found** C: 82.63, H: 4.78, N: 11.55. The carbon content is not within 0.4% error; however, the remaining characterization is consistent and demonstrates the identity and purity of the compound.

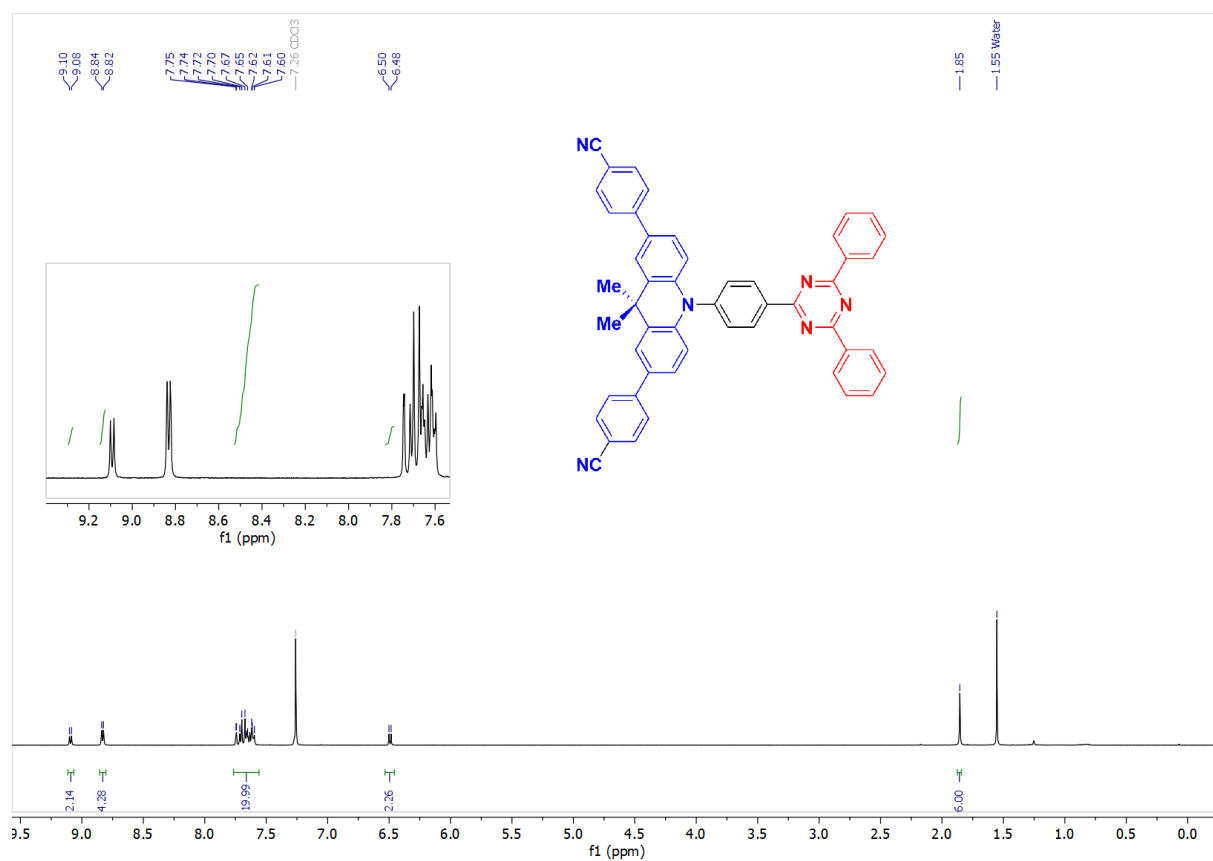


Figure S9. ^1H NMR of CNPh-DMAC-TRZ in CDCl_3 .

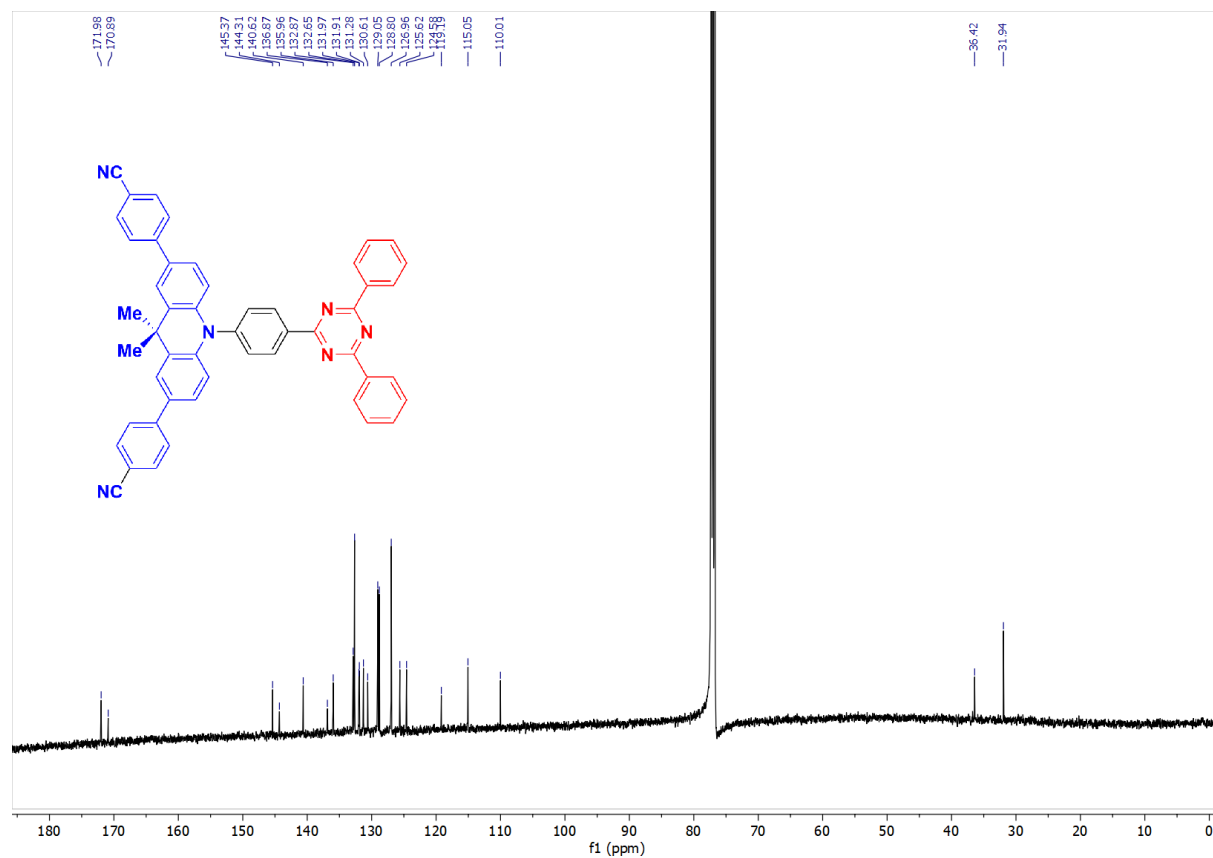


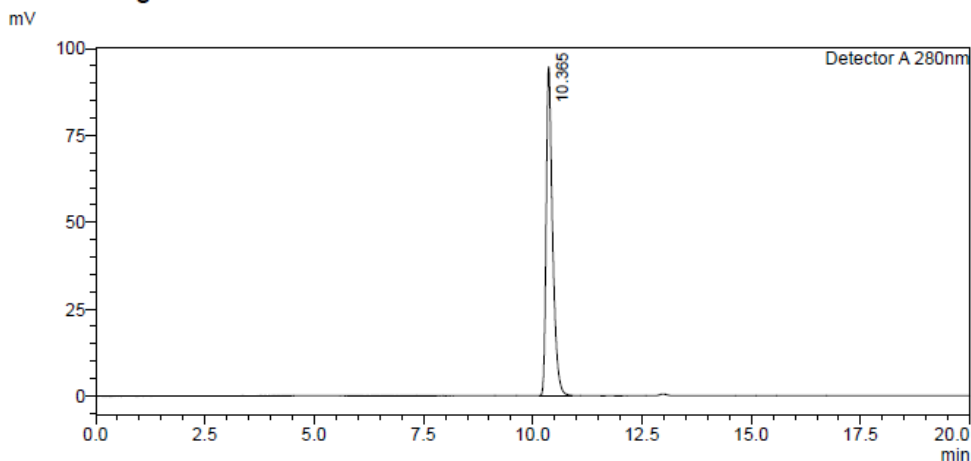
Figure S10. ^{13}C NMR of CNPh-DMAC-TRZ in CDCl_3 .

HPLC Trace Report31May2022

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Figure S11. HPLC analysis report for CNPh-DMAC-TRZ.

School of Chemistry Mass Spectrometry Service

SampleID
Sample Description
Analysis Name
Method
Instrument

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DIP Pos 3.m
maXis impact

Source Type APCI Ion Polarity Positive

Submitter

Supervisor
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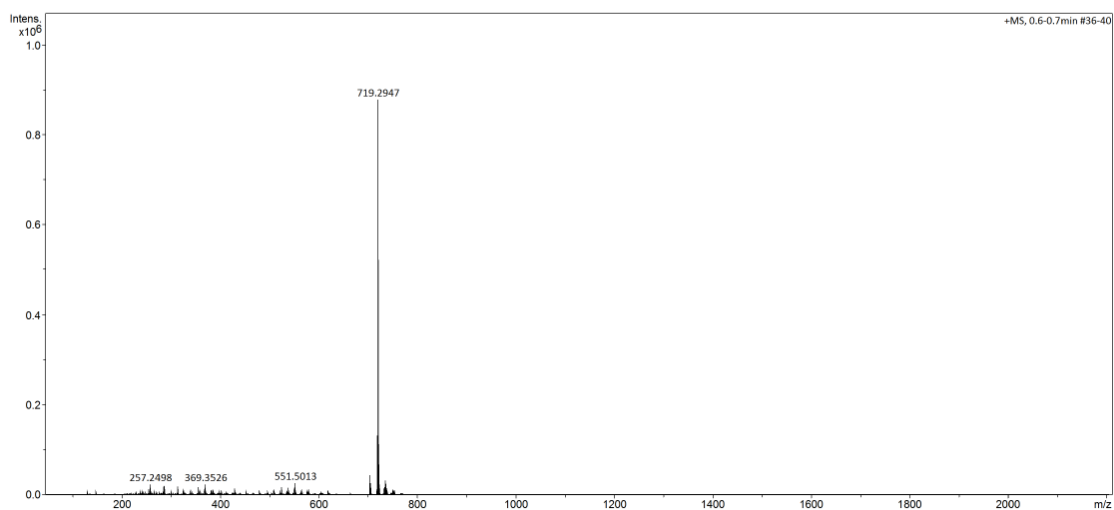


Figure S12. HRMS analysis report for CNPh-DMAC-TRZ.

S12

Elemental Analysis Service Request Form

Researcher name Ettore Crovini

Researcher email ec254@st-andrews.ac.uk

NOTE: Please submit ca. 10 mg of sample

Sample reference number	EC-4046
Name of Compound	dCNPh-DMAC-TRZ
Molecular formula	C ₅₀ H ₃₄ N ₆
Stability	Air stable
Hazards	None
Other Remarks	None

Analysis type: Elemental Analysis

Single ☐ Duplicate ☒ Triplicate ☐

Analysis Result:

Element	Expected %	Found (1)	Found (2)	Found (3)
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Hydrogen	4.77	4.68	4.78	
Nitrogen	11.69	11.51	11.55	

Authorising Signature:


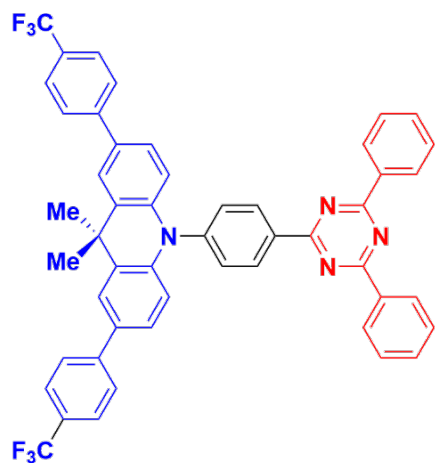
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Signature	
comments	

Figure S13. EA analysis report for CNPh-DMAC-TRZ.

10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-9,9-dimethyl-2,7-bis(4-(trifluoromethyl)phenyl)-9,10-dihydroacridine (CF₃Ph-DMAC-TRZ)



The same reaction procedure as **BuPh-DMAC-TRZ** was followed but with a different boronic acid, 4-trifluoromethyl-phenylboronic acid (1.126 g, 5.931 mmol, 4 equiv.). After 72 h, the reaction was diluted with THF and filtered over celite to remove any unreacted palladium. The solution was diluted with water, and the organic layer was extracted with DCM (3 × 50 mL). The organic phase was washed with brine, dried over MgSO₄ and concentrated under reduced pressure. The target product was isolated as yellow solid after purification by column chromatography on silica gel using 5:1 hexane/EtOAc as eluent. It was then further purified *via* recrystallization in THF/EtOH. (0.6706 g). The compound was further purified by gradient temperature sublimation. **Yield:** 56%; **Mp:** 320-325 °C; **R_f:** 0.49 (ethyl acetate/cyclohexane = 1:9); **¹H NMR** (500 MHz, CDCl₃) δ: 9.10-9.08 (d, *J*=8.5, 2H), 8.85-8.83 (dd, *J*=8.2, 1.4, 4H), 7.76-7.75 (d, *J*=2.1, 2H), 7.68 – 7.61 (m, 16H), 7.28 (d, *J*=2.1, 1H), 6.50-6.49 (d, *J*=8.6, 2H), 1.87 (s, 6H); **¹³C NMR** (126 MHz, CDCl₃) δ: 172.08, 171.08, 144.74, 144.66, 140.50, 136.83, 136.13, 132.96, 132.66, 131.98, 131.51, 130.65, 129.18, 128.92, 126.87, 125.87, 125.84, 125.69, 125.61, 124.74, 115.01, 36.54, 32.04; **HPLC retention time:** 10.185 min; **purity:** 100.00%; **HR-MS** (APCI) [M+H]⁺ **Calculated:** (C₅₀H₃₅F₆N₄⁺) 805.2760, **Found:** 805.2798; **EA** (C₅₀H₃₄F₆N₄) **Calculated** C: 74.62, H: 4.26, N: 6.96; **Found** C: 74.88, H: 4.30, N: 6.89.

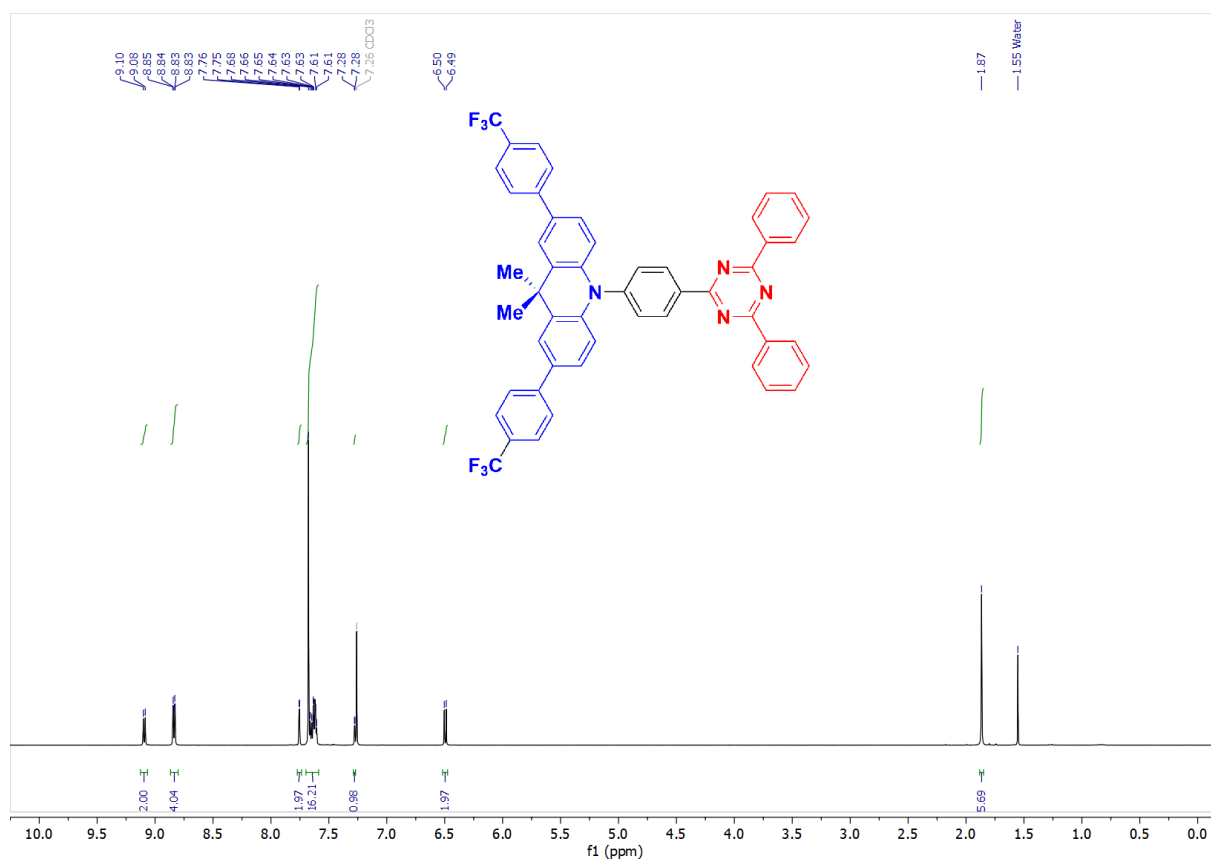


Figure S14. ¹H NMR of CF₃Ph-DMAC-TRZ in CDCl₃.

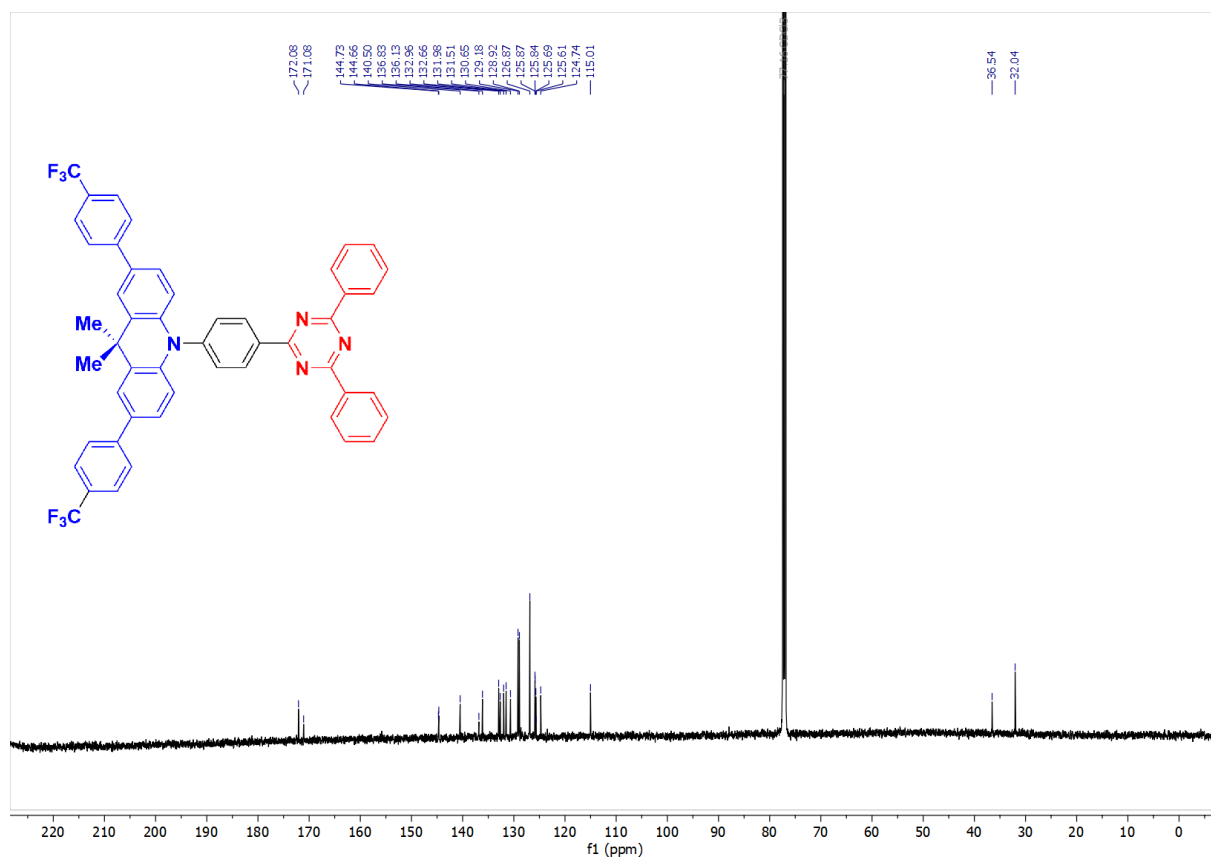


Figure S15. ¹³C NMR of CF₃Ph-DMAC-TRZ in CDCl₃.

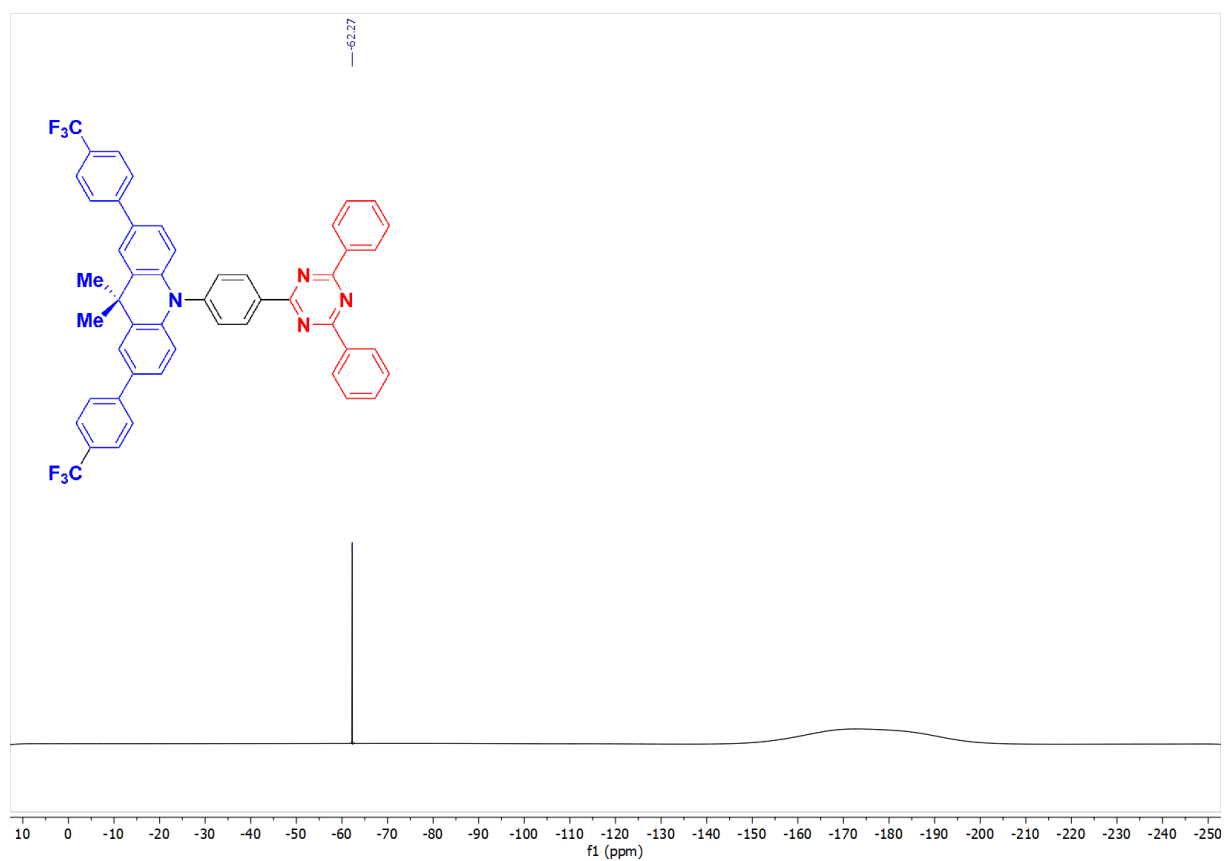


Figure S16. ^{19}F NMR of **CF₃Ph-DMAC-TRZ** in CDCl_3 .

HPLC Trace Report24Mar2022

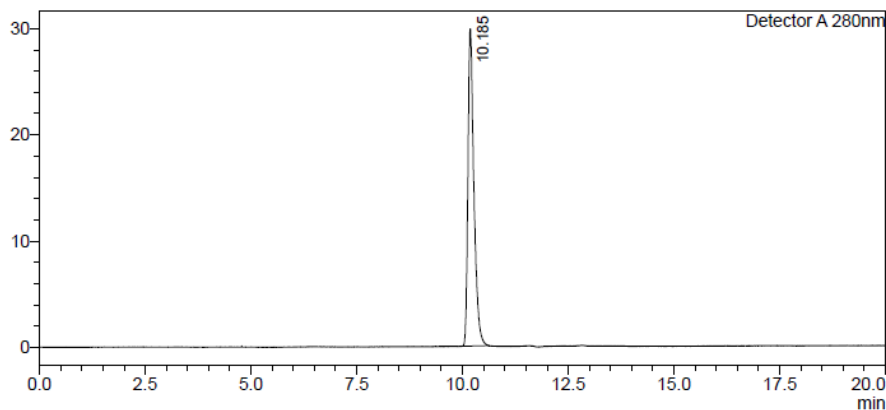
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 Injection Volume : 1 uL
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Figure S17. HPLC analysis report for CF₃Ph-DMAC-TRZ.

School of Chemistry Mass Spectrometry Service

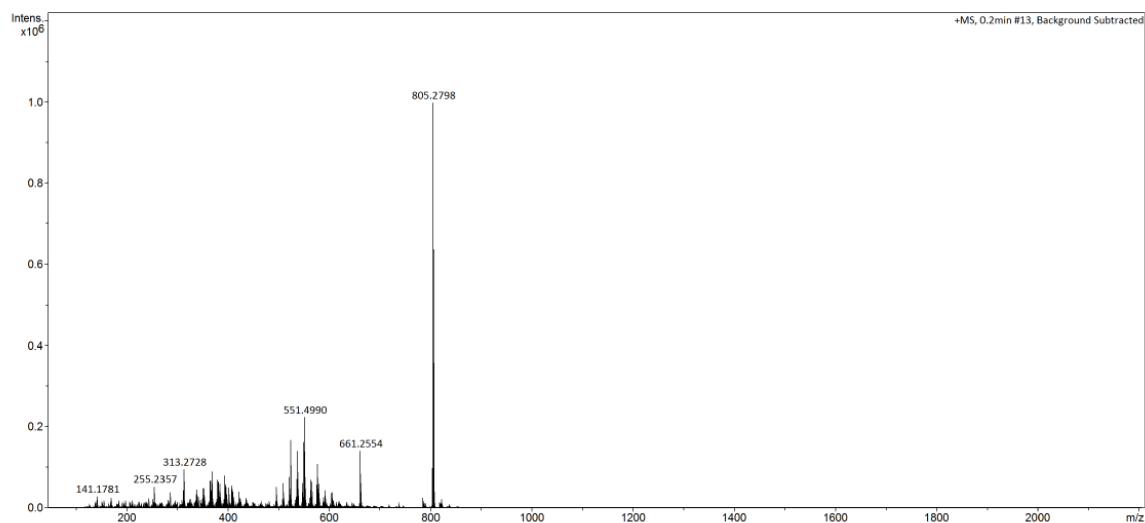
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 Analysis Name
 Method
 Instrument

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 maXis impact

Source Type APCI Ion Polarity Positive

Submitter

Supervisor
 Acquisition Date
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 Scan End 2200 m/z



Bruker Compass DataAnalysis 4.3

Analysis Name EC_3620_a.d

18/05/2022 14:10:37

1 of 1

Figure S18. HRMS analysis report for CF₃Ph-DMAC-TRZ.

Elemental Analysis Service Request Form

Researcher name Ettore Crovini

Researcher email ec254@st-andrews.ac.uk

NOTE: Please submit ca. 10 mg of sample

Sample reference number	EC-3620
Name of Compound	dCF ₃ Ph-DMAC-TRZ
Molecular formula	C ₅₀ H ₃₄ F ₅ N ₄
Stability	Air stable
Hazards	None
Other Remarks	None

Analysis type: Elemental Analysis

Single ☐ Duplicate ☒ Triplicate ☐

Analysis Result:

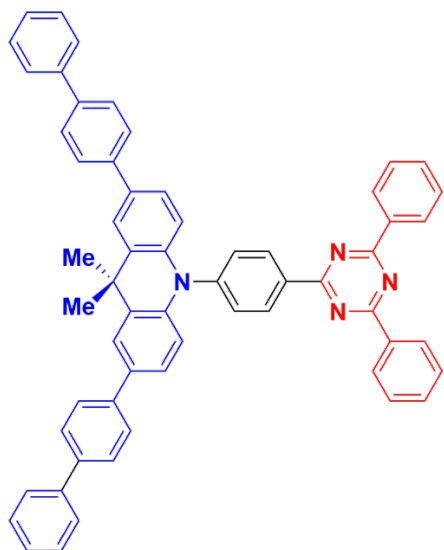
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Hydrogen	4.26	4.30	4.31	
Nitrogen	6.96	6.90	6.88	
Fluorine	14.16			

Authorising Signature:

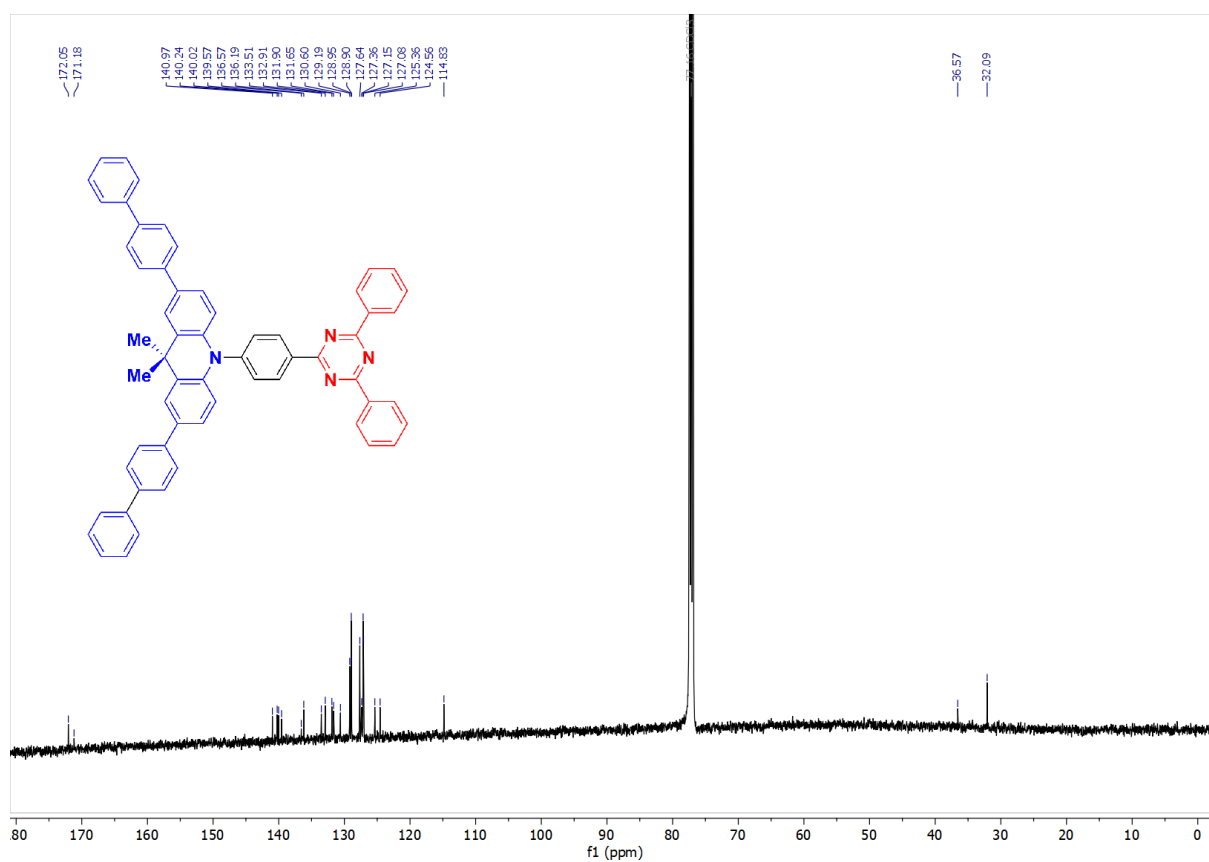
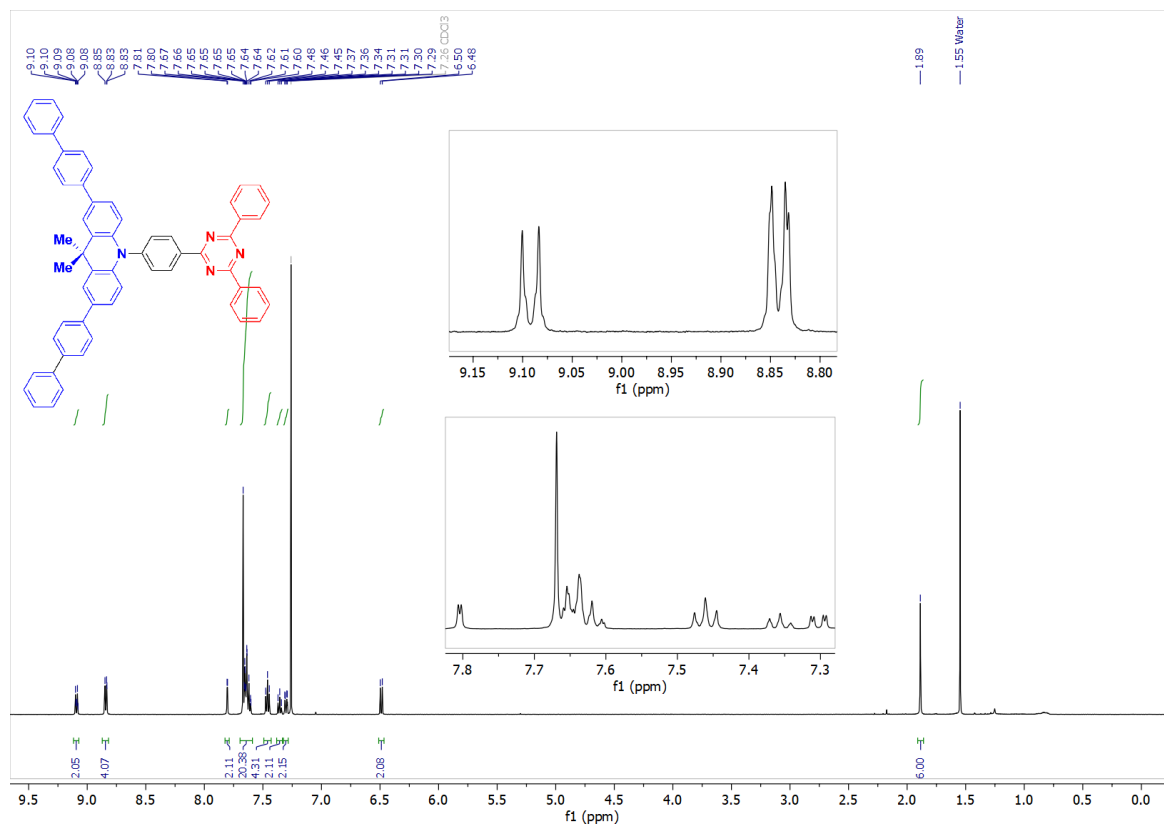
Date completed	29.04.22
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comments	

Figure S19. EA analysis report for CF₃Ph-DMAC-TRZ.

2,7-di([1,1'-biphenyl]-4-yl)-10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-9,9-dimethyl-9,10-dihydroacridine (dPh-DMAC-TRZ)



The same reaction procedure as **BuPh-DMAC-TRZ** was followed but with a different boronic acid, [1,1'-biphenyl]-4-ylboronic acid (1.174 g, 5.931 mmol, 4 equiv.). After 72 h, the reaction was diluted with THF and filtered over celite to remove any unreacted palladium. The solution was diluted with water, and the organic layer was extracted with DCM (3 × 50 mL). The organic phase was washed with brine, dried over MgSO₄ and concentrated under reduced pressure. The target product was isolated as yellow solid after purification by column chromatography on silica gel using 5:1 hexane/EtOAc as eluent. It was then further purified *via* recrystallization in THF/MeOH. (0.650 g). The compound was further purified by gradient temperature sublimation. **Yield:** 53%; **Mp:** 330-335 °C ; **R_f:** 0.67 (ethyl acetate/cyclohexane = 1:4); **¹H NMR** (500 MHz, CDCl₃) δ: 9.10-9.08 (dt, *J* = 8.4, 2.1, 1.4, 2H), 8.85-8.83 (dt, *J* = 6.7, 1.6, 1.0, 2H), 7.81-7.80 (d, *J* = 2.1, 4H), 7.67-7.70 (m, 20H), 7.48 – 7.45 (t, *J* = 7.7, 7.7, 4H), 7.37-7.34 (t, *J* = 7.4, 7.4, 2H), 7.31-7.29 (dd, *J* = 8.6, 2.1, 2H), 6.50-6.48 (d, *J* = 8.6, 2H), 1.89 (s, 6H); **¹³C NMR** (126 MHz, CDCl₃) δ: 172.05, 171.18, 140.97, 140.24, 140.02, 139.57, 136.57, 136.19, 133.51, 132.91, 131.90, 131.65, 130.60, 129.19, 128.95, 128.90, 127.64, 127.36, 127.15, 127.08, 125.36, 124.56, 114.83, 36.57, 32.09; **HPLC retention time:** 10.326; **purity:** 100.00%; **HR-MS (APCI) [M+H]⁺ Calculated:** (C₆₀H₄₅N₄⁺) 821.3639, **Found:** 821.3653; **EA** (C₆₀H₄₄N₄) **Calculated** C: 87.77, H: 5.40, N: 6.82; **Found** C: 87.36, H: 5.41, N: 6.79.



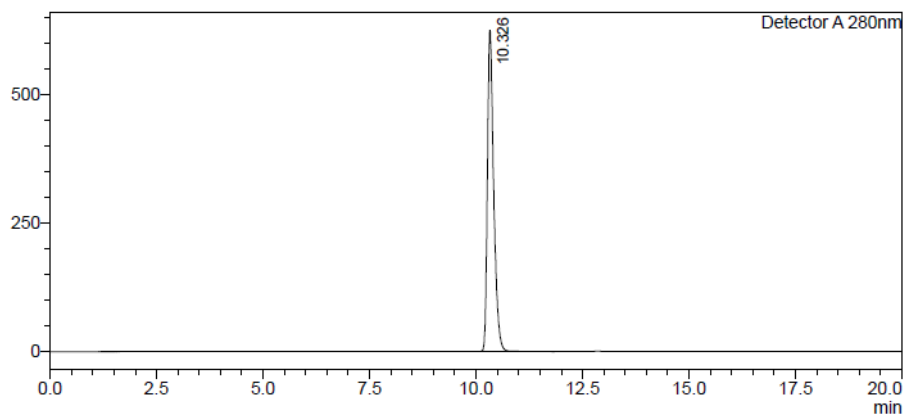
HPLC Trace Report06Apr2022

<Sample Information>

Sample Name : EC-4044-dP-DMAC-TRZ
 Sample ID :
 Method Filename : 100% THF 20 mins 280nm - DH.lcm
 Batch Filename : 06-04-22.lcb
 Vial # : 1-47
 Injection Volume : 10 uL
 Date Acquired : 06/04/2022 11:55:36
 Date Processed : 06/04/2022 12:15:39
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

mV



<Peak Table>

Detector A 280nm

Peak#	Ret. Time	Area	Height	Area%	Area/Height	Width at 5% Height
1	10.326	6401268	622597	100.000	10.282	0.364
Total		6401268	622597	100.000		

Figure S22. HPLC analysis report for dPh-DMAC-TRZ.

School of Chemistry Mass Spectrometry Service

SampleID

Sample Description

Analysis Name

Method

Instrument

D:\Data\stuartwarriner\manual\EC_4044_a.d

DIP Pos 3.m

maXis impact

Source Type

APCI

Ion Polarity

Positive

Submitter

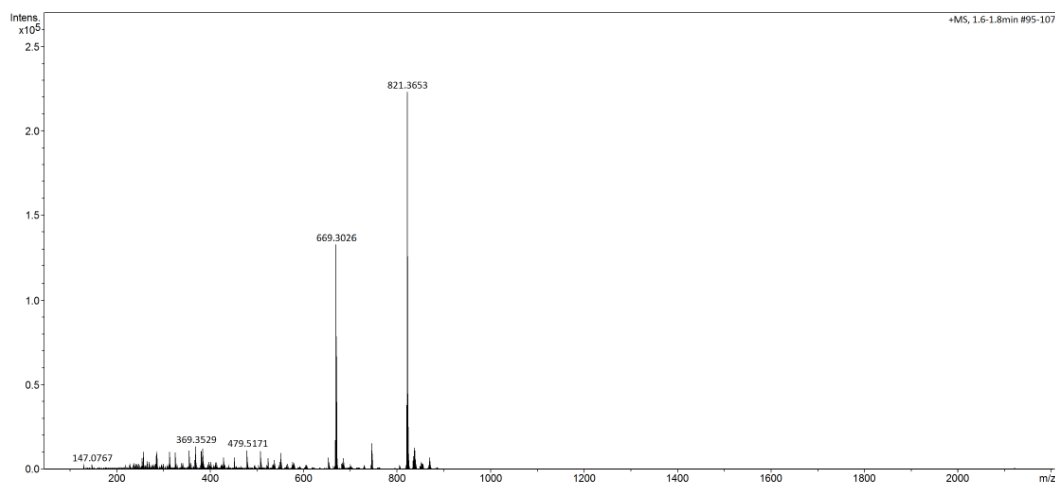
Supervisor

Acquisition Date

Scan Begin

18/05/2022 15:08:34

Scan End



Bruker Compass DataAnalysis 4.3

Analysis Name

EC_4044_a.d

18/05/2022 15:13:45

1 of 1

Figure S23. HRMS analysis report for dPh-DMAC-TRZ.

Elemental Analysis Service Request Form

Researcher name Ettore Crovini

Researcher email ec254@st-andrews.ac.uk

NOTE: Please submit ca. 10 mg of sample

Sample reference number	EC-4044
Name of Compound	dPh-DMAC-TRZ
Molecular formula	C ₅₀ H ₄₄ N ₄
Stability	Air stable
Hazards	None
Other Remarks	None

Analysis type: Elemental analysis

Single ☐ Duplicate ☒ Triplicate ☐

Analysis Result:

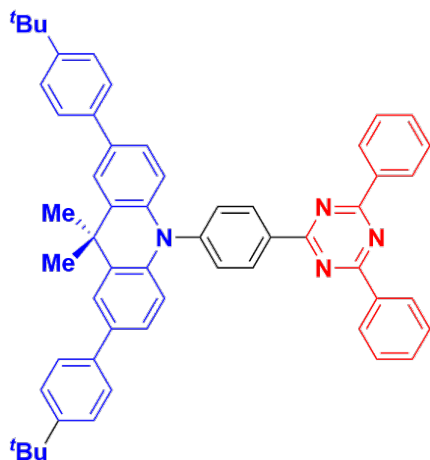
Element	Expected %	Found (1)	Found (2)	Found (3)
Carbon	87.77	87.93	86.79	
Hydrogen	5.40	5.47	5.35	
Nitrogen	6.82	6.84	6.74	

Authorising Signature:

Date completed	29.04.22
Signature	S-P C.
comments	

Figure S24. EA analysis report for dPh-DMAC-TRZ.

2,7-bis(4-(tert-butyl)phenyl)-10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-9,9-dimethyl-9,10-dihydroacridine (tBuPh-DMAC-TRZ)



To a pressure vessel were added 2,7-dibromo-10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-9,9-dimethyl-9,10-dihydroacridine (**dBr-DMAC-TRZ**) (1.0 g, 1.48 mmol, 1 equiv.) and 4-*tert*-butylphenyl-boronic acid (1.1 g, 5.93 mmol, 4 equiv.) and the vessel was degassed by alternating vacuum and nitrogen 3 times. THF (22 mL), and 16.5 mL of a 2 M Cs₂CO₃ solution in water were added and the bi-phasic solution was degassed by bubbling N₂ trough for 30 min. Pd(PPh₃)₄ was then added and the reaction was left to stir under pressure at 110°C for 72h. A yellow crystalline solid crashed out of the solution. The mixture was left to cool, and the yellow solid was filtered and washed with water (250 mL) and MeOH (250 mL) to achieve the desired product (0.73 g). The compound was further purified by gradient temperature sublimation **Yield:** 63%; **Mp:** 325-330 °C; **R_f:** 0.50 (ethyl acetate/cyclohexane = 1 :9); **¹H NMR** (300 MHz, CDCl₃) δ: 9.08-9.06 (d, *J*= 7.1, 2H),, 8.84-8.82 (d, *J*= 4.2, 4H), 7.73 (d, *J*= 2.0, 2H), 7.67-, 7.60 (m, 8H), 7.53-7.45 (dd, *J*= 22.3, 8.84, 8H), 7.24-7.22 (dd, *J*= 8.55, 2.05, 2H), 6.46-6.44 (d, *J*= 8.5, 2H), 1.83 (s, 6H), 1.36 (s, 18H); **¹³C NMR** (126 MHz, CDCl₃) δ = 172.02, 171.20, 149.65, 145.33, 139.81, 138.54, 136.41, 136.20, 133.92, 132.88, 131.83, 131.67, 130.47, 129.18, 128.89, 126.44, 125.81, 125.28, 124.55, 114.67, 36.52, 34.63, 31.91, 31.54; **HPLC retention time:** 10.239 min; **purity:** >99%; **HR-MS** (APCI) [M+H]⁺ **Calculated:** (C₅₆H₅₃N₄⁺) 781.4268, **Found:** 781.4268; **EA** (C₅₆H₅₂N₄) **Calculated** C: 86.12, H: 6.71, N: 7.17; **Found** C: 86.51, H: 6.76, N: 7.15.

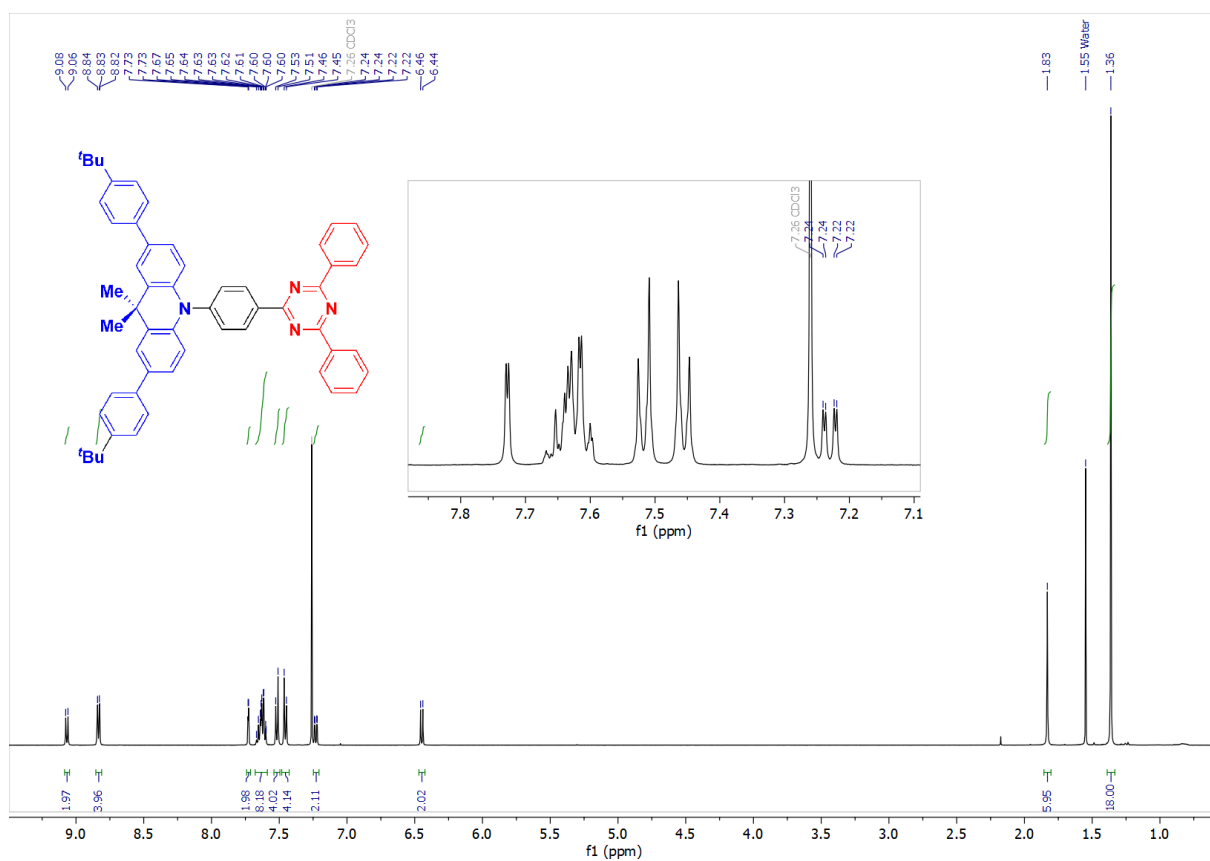


Figure S25. ¹H NMR of 'BuPh-DMAC-TRZ in CDCl₃.

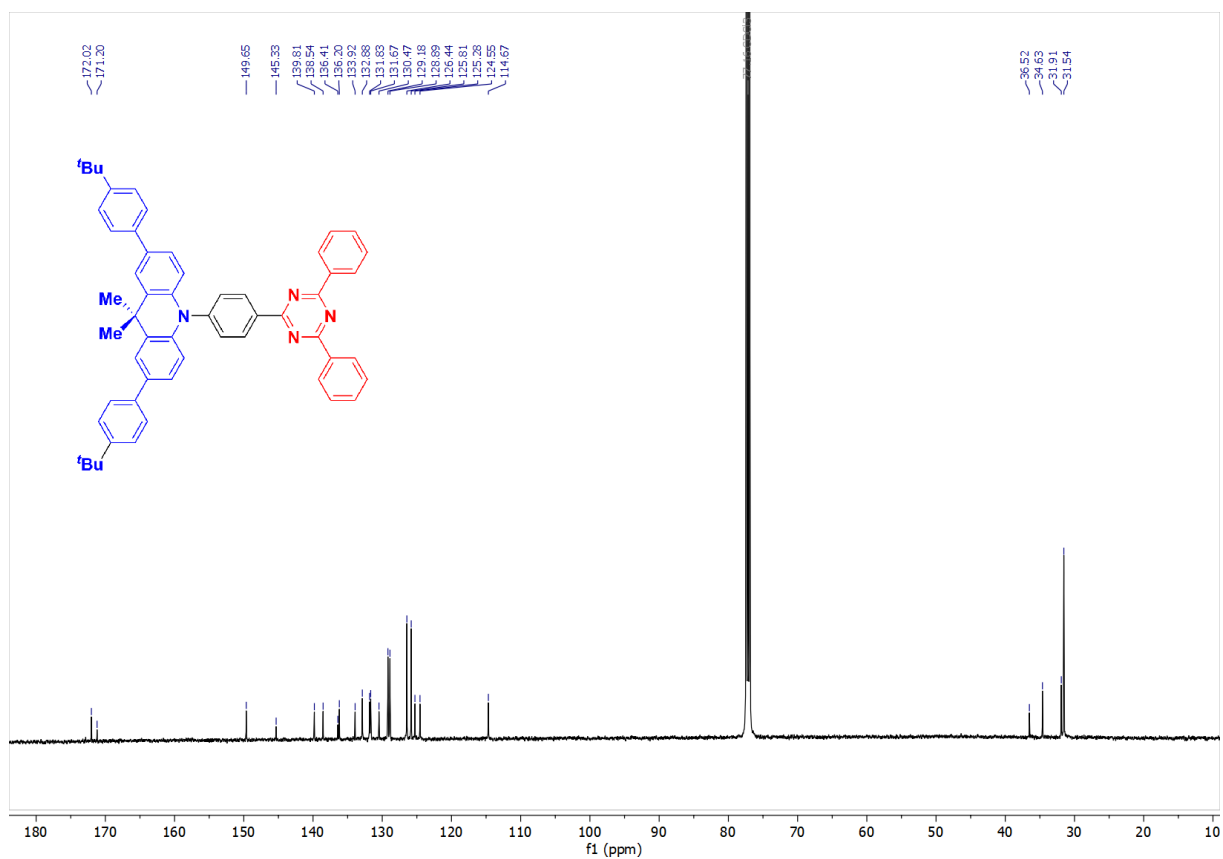


Figure S26. ¹³C NMR of 'BuPh-DMAC-TRZ in CDCl₃.

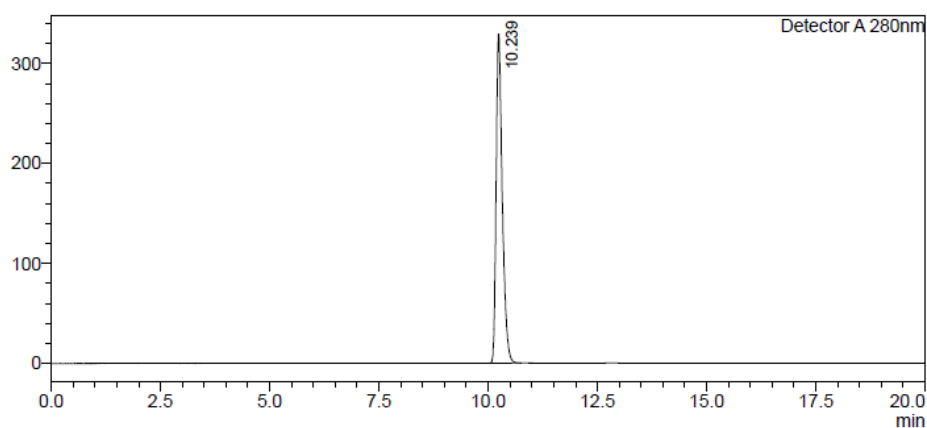
HPLC Trace Report24Mar2022

<Sample Information>

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 Sample ID :
 Method Filename : 100% THF 20 mins 280nm - DH.lcm
 Batch Filename : 23-03-22.lcb
 Vial # : 1-2
 Injection Volume : 10 uL
 Date Acquired : 23/03/2022 17:18:29
 Date Processed : 23/03/2022 17:38:33
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

mV



<Peak Table>

Detector A 280nm

Peak#	Ret. Time	Area	Height	Area%	Area/Height	Width at 5% Height
1	10.239	3232827	328784	100.000	9.833	0.349
Total		3232827	328784	100.000		

Figure S27. HPLC analysis report for 'BuPh-DMAC-TRZ.

School of Chemistry Mass Spectrometry Service

SampleID

Sample Description

Analysis Name

Method

Instrument

D:\Data\stuart\wanner\manual\dtBuPh_DMALC_TRZ_b.d

DIP Pos 3.m

maXis impact

Source Type

APCI

Ion Polarity

Positive

Submitter

Supervisor

Acquisition Date

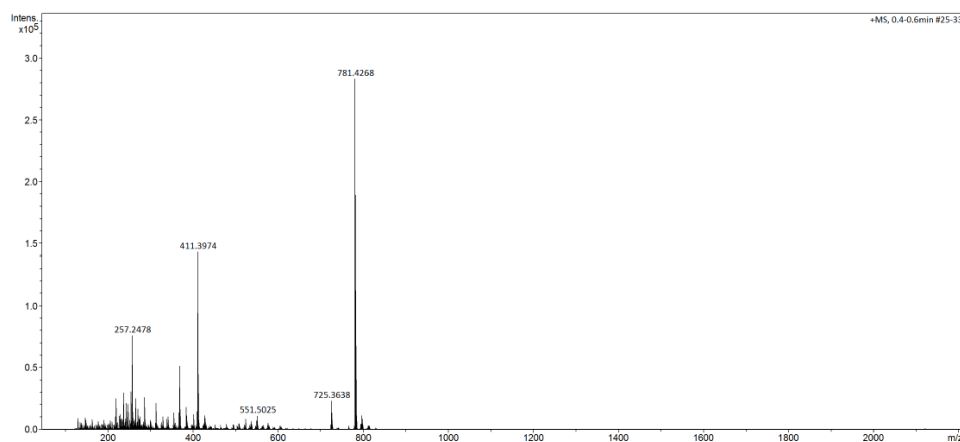
Scan Begin

50 m/z

12/03/2022 17:48:23

Scan End

2200 m/z



Bruker Compass DataAnalysis 4.3

Analysis Name

dtBuPh_DMALC_TRZ_b.d

12/03/2022 17:50:34

1 of 1

Figure S28. HRMS analysis report for 'BuPh-DMAC-TRZ.

Elemental Analysis Service Request Form

Researcher name Ettore Crovini

Researcher email ec254@st-andrews.ac.uk

NOTE: Please submit ca. 10 mg of sample

Sample reference number	EC-3621
Name of Compound	d'BuPh-DMAC-TRZ
Molecular formula	C ₅₆ H ₅₂ N ₄
Stability	Air stable
Hazards	No hazards
Other Remarks	None

Analysis type: Elemental analysis

Single ☐ Duplicate ☒ Triplicate ☐

Analysis Result:

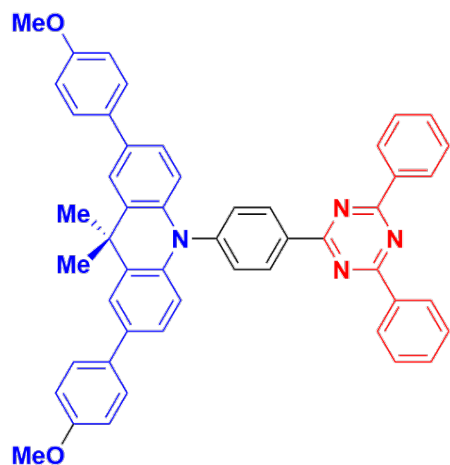
Element	Expected %	Found (1)	Found (2)	Found (3)
Carbon	86.12	86.77	86.25	
Hydrogen	6.71	6.75	6.77	
Nitrogen	7.17	7.15	7.16	

Authorising Signature:

Date completed	29.04.22
Signature	S-P C
comments	

Figure S29. EA analysis report for d'BuPh-DMAC-TRZ.

10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-2,7-bis(4-methoxyphenyl)-9,9-dimethyl-9,10-dihydroacridine (OMePh-DMAC-TRZ)



The same reaction procedure as **BuPh-DMAC-TRZ** was followed, but with a different boronic acid, 4-methoxy-phenyl-boronic acid (0.901 g, 5.931 mmol, 4 equiv.). After 72 h, the reaction was diluted with THF and filtered over celite to remove any unreacted palladium. The solution was diluted with water, and the organic layer was extracted with DCM (3 × 50 mL). The organic phase was washed with brine, dried over MgSO₄ and concentrated under reduced pressure. The target product was isolated as yellow solid after purification by column chromatography on silica gel using 5:1 hexane/EtOAc as eluent. It was then further purified *via* recrystallization in THF/Ether. (0.502 g). The compound was furtherly purified by gradient temperature sublimation. **Yield:** 47%; **Mp:** 300-305 °C; **R_f:** 0.39 (ethyl acetate/cyclohexane= 1:9); **¹H NMR** (500 MHz, CDCl₃) δ: 9.08-9.05 (dt, *J*= 8.4, 2.3, 1.7, 2H), 8.84 – 8.82 (dt, *J*= 7.0, 1.6, 1.6 4H), 7.69 (d, *J*= 2.1, 2H), 7.67-7.60 (m, 8H) 7.52-7.49 (dt, *J*= 8.5, 2.6, 2.0, 4H), 7.20-7.18 (dd, *J*= 8.56, 2.08, 2H), 6.99-6.96 (dt, *J*= 8.7, 3.0, 1.5, 4H), 6.45-6.43 (d, *J*= 8.5, 2H), 3.85 (s, 6H), 1.84 (s, 6H); **¹³C NMR** (126 MHz, CDCl₃) δ: 172.02, 171.20, 158.77, 145.37, 139.56, 136.38, 136.19, 134.02, 133.68, 132.88, 131.83, 131.62, 130.53, 129.18, 128.89, 127.77, 125.02, 124.22, 114.71, 114.32, 55.52, 36.52, 31.98; **HPLC retention time:** 10.444 min; **purity:** 100.00%; **HR-MS** (APCI) [M+H]⁺ **Calculated:** (C₅₀H₄₁N₄O₂⁺) 729.3224, **Found:** 729.3253; **EA** (C₅₀H₄₀N₄O₂) **Calculated** C: 82.39, H: 5.53, N: 7.69; **Found** C: 82.59, H: 5.57, N: 7.62.

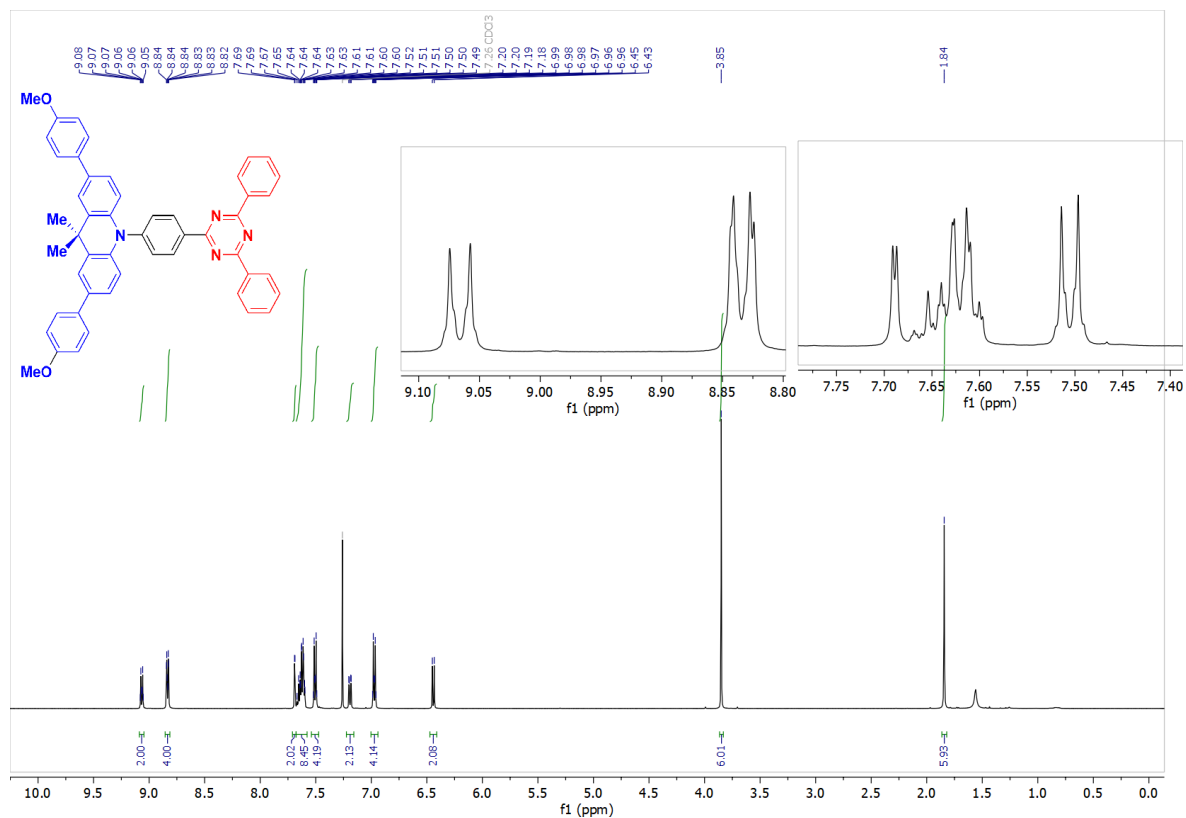


Figure S30. ^1H NMR of OMePh-DMAC-TRZ in CDCl₃.

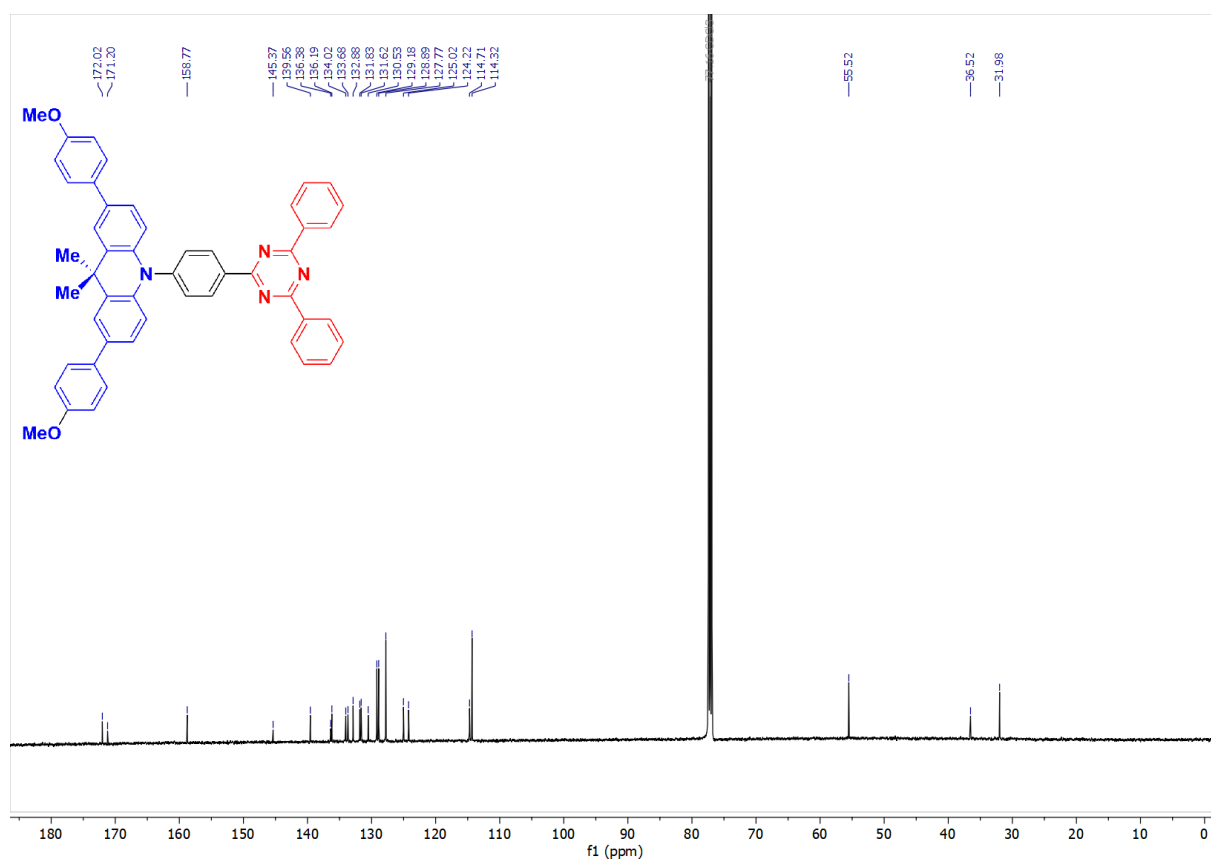


Figure S31. ^{13}C NMR of OMePh-DMAC-TRZ in CDCl₃.

HPLC Trace Report24Mar2022

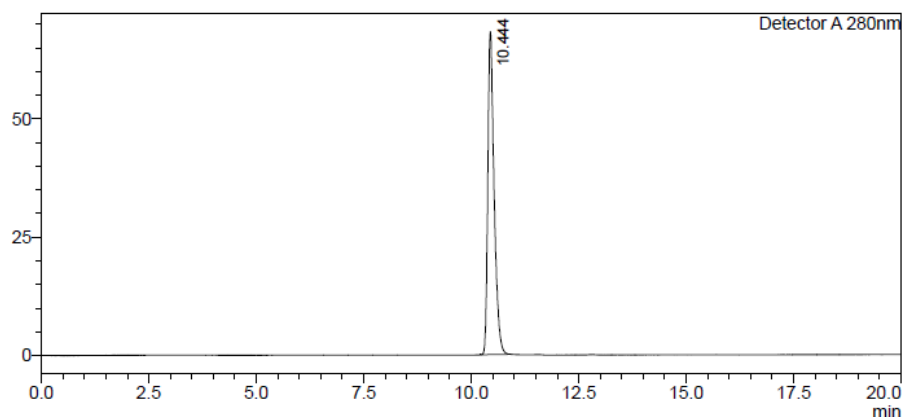
<Sample Information>

Sample Name : dOMePhDMAC-TRZ-S1
 Sample ID :
 Method Filename : 100% THF 20 mins 280nm - DH.lcm
 Batch Filename : 23-03-22.lcb
 Vial # : 1-4
 Injection Volume : 1 uL
 Date Acquired : 23/03/2022 18:40:01
 Date Processed : 23/03/2022 19:00:04

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

mV



<Peak Table>

Detector A 280nm

Peak#	Ret. Time	Area	Height	Area%	Area/Height	Width at 5% Height
1	10.444	693776	68194	100.000	10.174	0.362
Total		693776	68194	100.000		

Figure S32. HPLC analysis report for OMePh-DMAC-TRZ.

School of Chemistry Mass Spectrometry Service

SampleID
 Sample Description
 Analysis Name
 Method
 Instrument

D:\Data\stuartwarriner\manual\EC_4043_a.d
 DIP Pos 3.m
 maXis impact

Source Type
 APCI

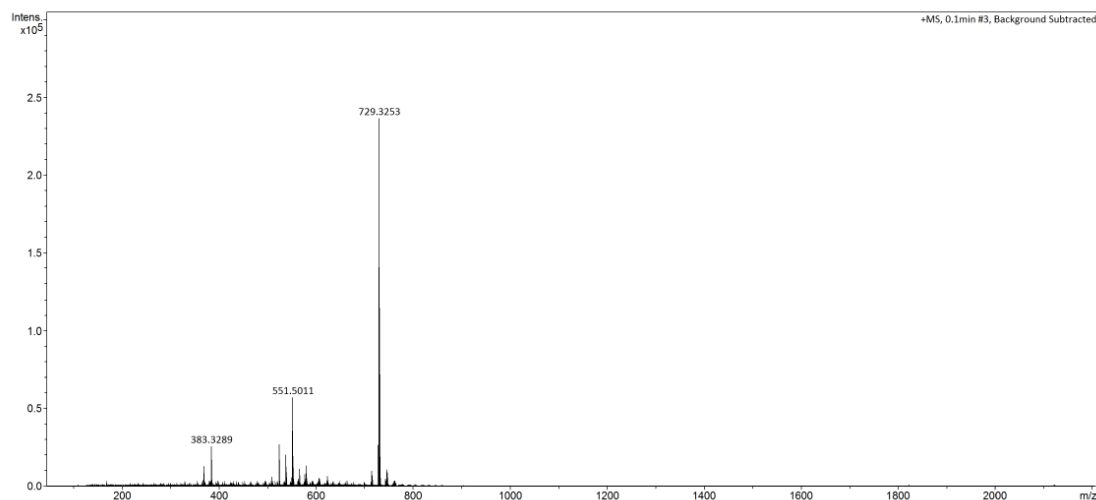
Ion Polarity
 Positive

Submitter

Supervisor
 Acquisition Date
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18/05/2022 14:32:15
 50 m/z

Scan End
 2200 m/z



Bruker Compass DataAnalysis 4.3

Analysis Name

EC_4043_a.d

18/05/2022 14:38:57

1 of 1

Figure S33. HRMS analysis report for OMePh-DMAC-TRZ.

Elemental Analysis Service Request Form

Researcher name Ettore Crovini

Researcher email ec254@st-andrews.ac.uk

NOTE: Please submit ca. 10 mg of sample

Sample reference number	EC-4043
Name of Compound	dOMePh-DMAC-TRZ
Molecular formula	C ₅₀ H ₄₀ N ₄ O ₂
Stability	Air stable
Hazards	None
Other Remarks	None

Analysis type: Elemental Analysis

Single ☐ Duplicate ☒ Triplicate ☐

Analysis Result:

Element	Expected %	Found (1)	Found (2)	Found (3)
Carbon	82.39	82.71	82.46	
Hydrogen	5.53	5.57	5.57	
Nitrogen	7.69	7.62	7.61	
Oxygen	4.39			

Authorising Signature:

Date completed	29.04.22
Signature	J - P L
comments	

Figure S34. EA analysis report for OMePh-DMAC-TRZ.

DFT Calculations

Table S1. Excited states properties of **DMAC-TRZ** and its derivatives.

Excited State ^a	Energy / eV	Nature ^b	Character of the transition
DMAC-TRZ			
T₁	2.56	H→L (97%) H→(L+2) 2%	³ CT
S₁ (f=0.00)	2.57	H→L (97%) H→(L+2) 2%	¹ CT
CNPh-DMAC-TRZ			
T₁	2.76	H→L (97%)	³ CT
S₁ (f=0.00)	2.77	H→L (97%)	¹ CT
CF₃Ph-DMAC-TRZ			
T₁	2.66	H→L (97%)	³ CT
S₁ (f=0.05)	2.67	H→L (97%)	¹ CT
dPh-DMAC-TRZ			
T₁	2.47	H→L (97%)	³ CT
S₁ (f=0.00)	2.48	H→L (97%)	¹ CT
OMePh-DMAC-TRZ			
T₁	2.36	H→L (97%)	³ CT
S₁ (f=0.00)	2.37	H→L (97%)	¹ CT
^tBuPh-DMAC-TRZ			
T₁	2.43	H→L (97%)	³ CT
S₁ (f=0.00)	2.43	H→L (97%)	¹ CT

^a PBE0/6-31G(d,p); ^b the transitions highlighted in red are the main ones contributing to the excited state character.

Table S2. Properties of the excited states involved in the UV-vis absorption transitions of CNPh-DMAC-TRZ, CF₃Ph-DMAC-TRZ, dPh-DMAC-TRZ, ^tBuPh-DMAC-TRZ, OMePh-DMAC-TRZ.

Excited State ^a	Energy / eV; nm	Nature	Character of the transition
CNPh-DMAC-TRZ			
S ₃ (f=1.15)	3.39; 366	H→(L+2) (98%)	¹ LE (DMAC)
S ₄ (f=0.23)	3.78; 328	H→(L+3) (95%)	¹ LE (DMAC)
CF₃Ph-DMAC-TRZ			
S ₃ (f=1.00)	3.64; 341	H→(L+2) (97%)	¹ LE (DMAC)
S ₅ (f=0.15)	4.09; 303	H→(L+3) (82%) H→(L+6) (9%)	¹ LE (DMAC)
dPh-DMAC-TRZ			
S ₃ (f=1.41)	3.53; 351	H→(L+2) (96%)	¹ LE (DMAC)
S ₅ (f=0.25)	3.93; 315	H→(L+3) (89%) H→(L+4) (4%)	
^tBuPh-DMAC-TRZ			
S ₄ (f=0.57)	3.74; 331	H→(L+2) (80%) H→(L+4) (16%)	¹ LE (DMAC)
OMePh-DMAC-TRZ			
S ₅ (f=0.25)	3.72; 333	H→(L+3) (77%) H→(L+4) (21%)	¹ LE (DMAC)

^a PBE0/6-31G(d,p); ^b the transitions highlighted in red are those involved in the UV transitions.

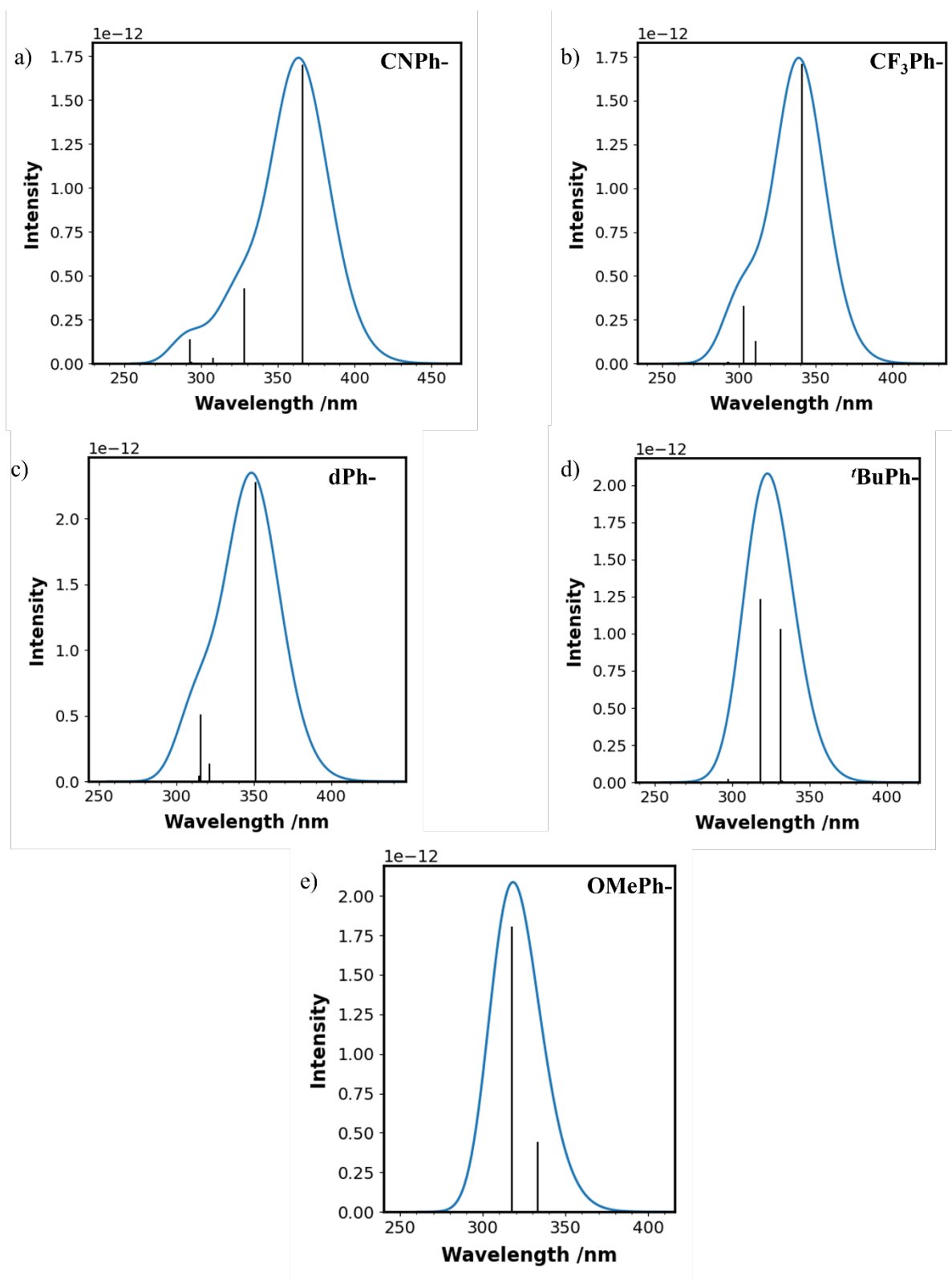


Figure S35. Simulated absorption spectra of **DMAC-TRZ** and derivatives (Obtained at the TDA-DFT-PBE0/6-31G(d,p) level, Isovalue for new surfaces: MO=0.02, Density=0.0004).

Table S3. Calculated optoelectronic properties of **DMAC-TRZ** and derivatives.

R-DMAC- TRZ	S₁ / eV	T₁ / eV	HOMO / eV	LUMO / eV
DMAC-TRZ	2.57	2.56	-5.13	-1.91
CNPh-	2.77	2.76	-5.57	-2.17
CF₃Ph-	2.67	2.66	-5.38	-2.08
dPh-	2.48	2.47	-5.05	-1.97
^tBuPh-	2.37	2.36	-4.97	-1.93
OMePh-	2.43	2.43	-4.87	-1.91

Optoelectronic characterization

Table S4. Electrochemical properties of **DMAC-TRZ** and derivatives.

R-DMAC-TRZ	E_{ox} / V^a	E_{red} / V^a	HOMO / eV^b	LUMO / eV^b
DMAC-TRZ	0.97	-1.72	-5.31	-2.62
CNPh-	1.04	-1.68	-5.38	-2.66
CF₃Ph-	0.80	-1.68	-5.35	-2.66
dPh-	0.86	-1.69	-5.21	-2.65
^tBuPh-	0.81	-1.71	-5.15	-2.63
OMePh-	0.79	-1.69	-5.13	-2.65

^a obtained from DPV; ^b obtained from the redox potentials from the DPV, E_{HOMO/LUMO} = -(E_{ox/red} + 4.8), where E_{ox/red} was obtained from the DPV corrected vs Fc/Fc⁺.

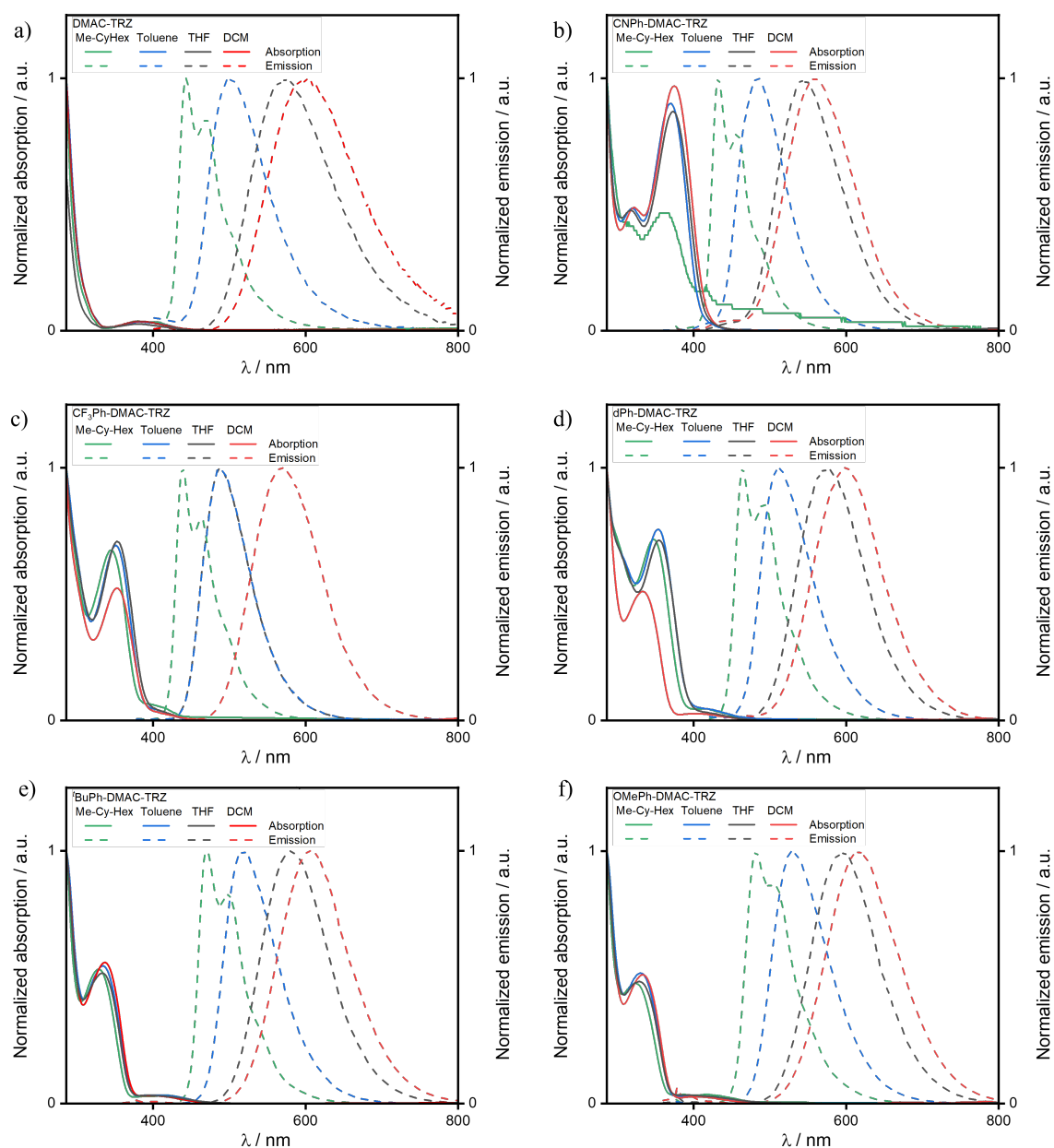


Figure S36. Absorption and emission spectra of **DMAC-TRZ** and derivatives in different solvents ($\lambda_{\text{exc}} = 340 \text{ nm}$).

Table S5. Emission wavelength of **DMAC-TRZ** and derivatives in different solvents.

R-DMAC-TRZ	λ_{PL} / nm	λ_{PL} / nm	λ_{PL} / nm	λ_{PL} / nm
	Me-Cyhex	Toluene	THF	DCM
DMAC-TRZ	443/ 470 ^a	500	573	602
CNPh-	433/ 457 ^a	484	544	561
CF₃Ph-	439/ 498 ^a	487	560	567
dPh-	465/ 491 ^a	511	576	598
^tBuPh-	470/ 498 ^a	518	580	604
OMePh-	482/ 504 ^a	528	594	620

^a peak maxima of the two bands in the Me-Cyhex solution.

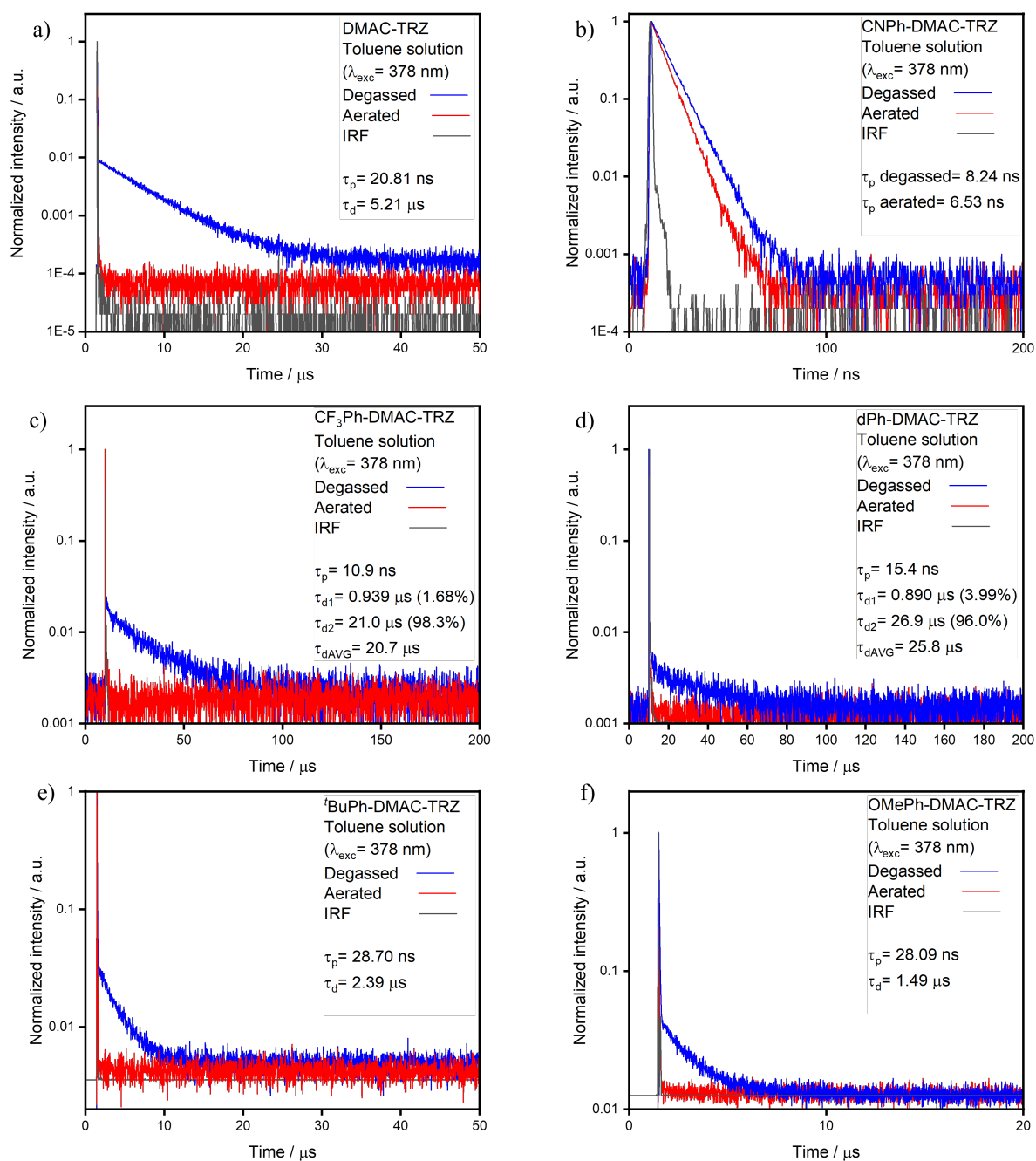


Figure S37. Time-resolved fluorescence decay of degassed and aerated solutions of **DMAC-TRZ** and derivatives (Toluene, 10^{-5} M solutions, $\lambda_{\text{exc}} = 378 \text{ nm}$).

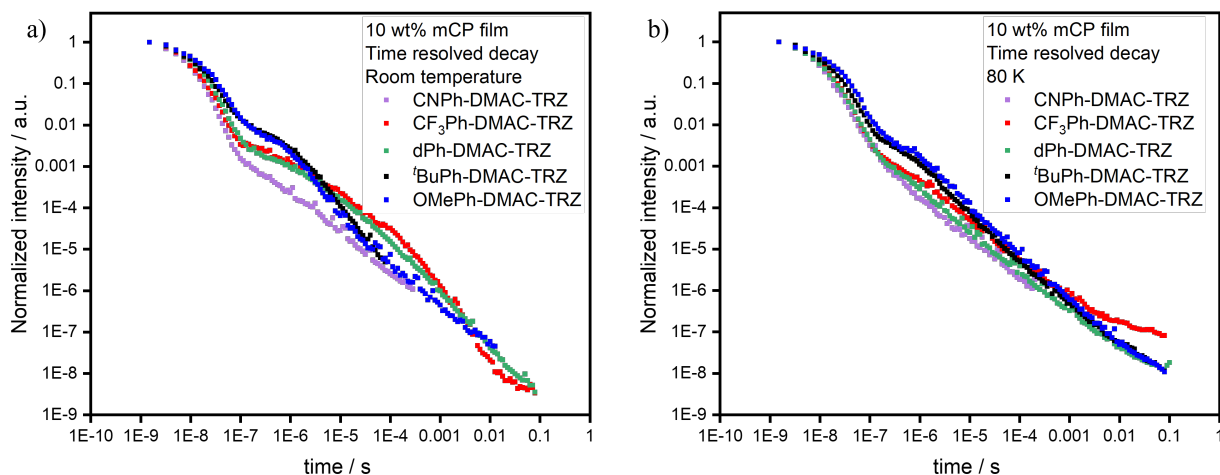


Figure S38. Time-resolved fluorescence decay at a) room temperature; b) 80 K of the extended derivatives in 10 wt% doped films in mCP ($\lambda_{\text{exc}} = 355$ nm).

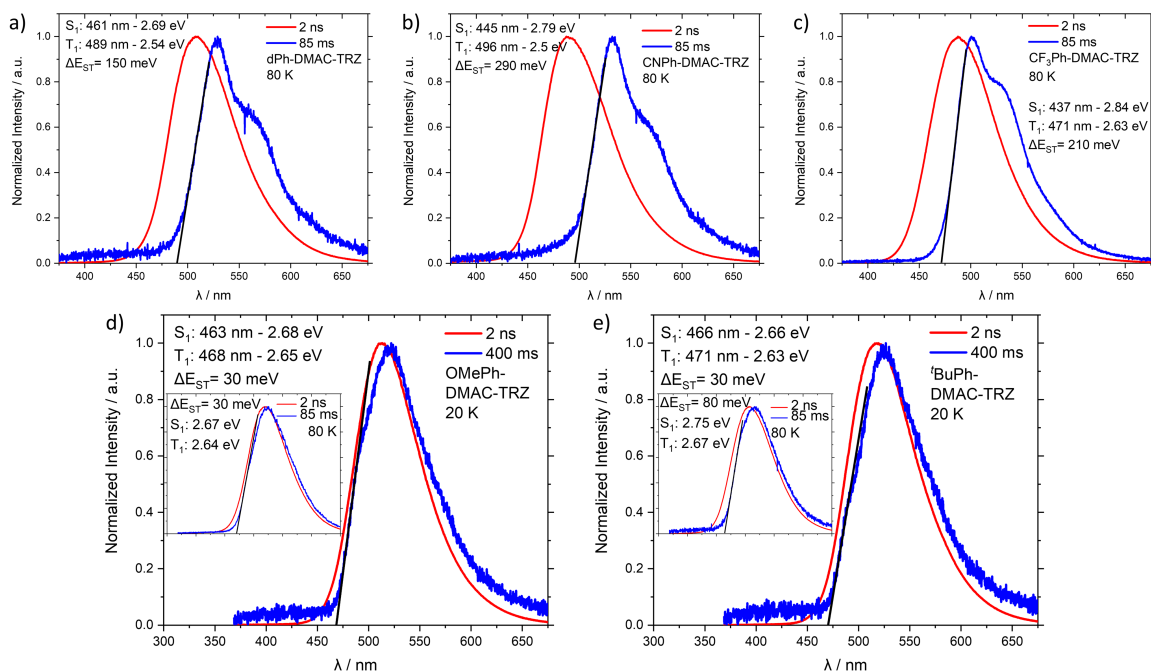


Figure S39. Prompt fluorescence (time delay 2 ns) and phosphorescence (time delay 85 ms) spectra of the extended derivatives, in 10 wt% doped films in mCP, at 80 K (a-c). d) OMePh-DMAC-TRZ and e) tBuPh-DMAC-TRZ measured at 20 K because of their small ΔE_{ST} . Inset: the 80 K spectra.

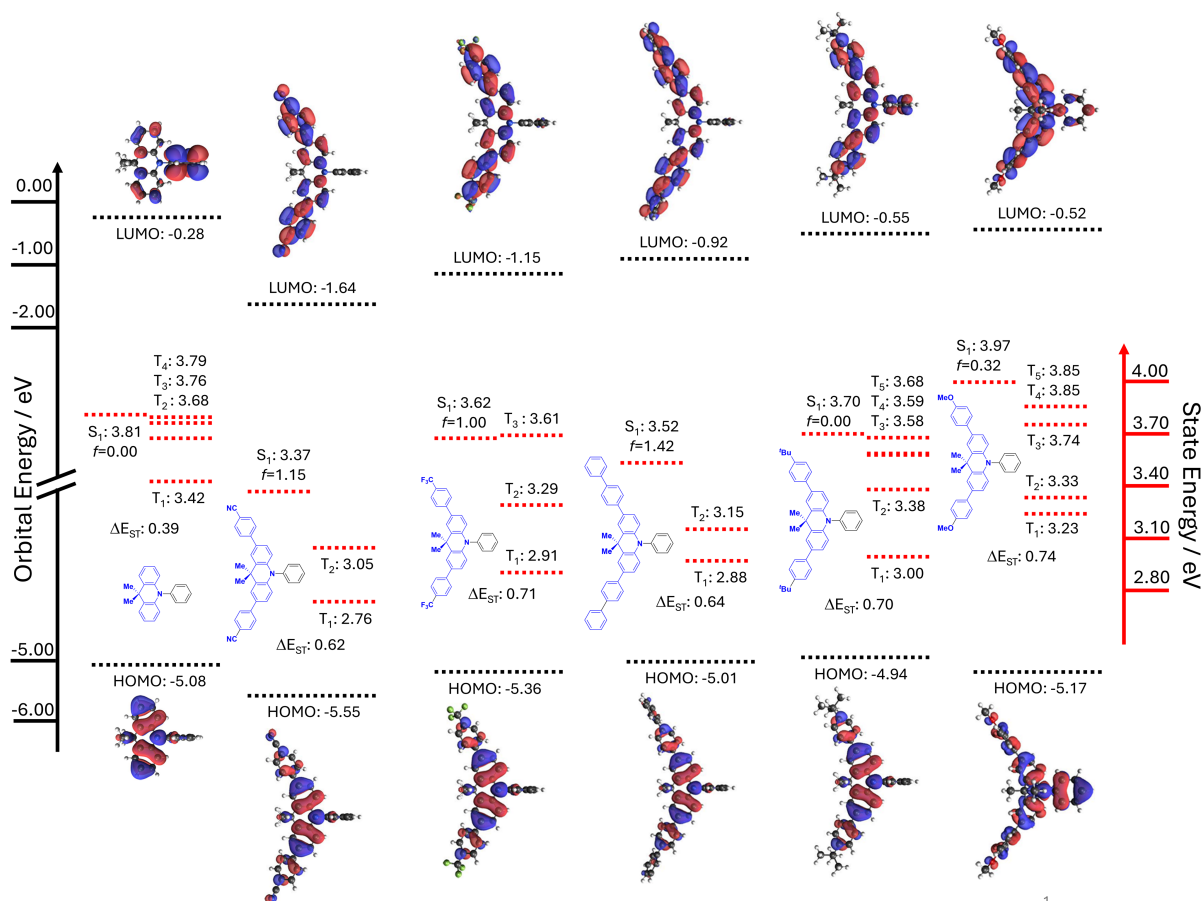


Figure S40. HOMO and LUMO electron density distributions and energy levels, excited-state energy levels of DMAC and its five aryl decorated derivatives (Obtained via DFT and TD-DFT at the PBE0/6-31G(d,p) level, Isovalues: MO=0.02).

Table S6. Photophysical properties of **DMAC-TRZ** and extended derivatives in toluene solution (10^{-5} M), 10 wt% doped films in mCP and 10 wt% doped films in mCBPCN.

R-DMAC-TRZ	Environment	$\lambda_{\text{PL}} / \text{nm}^a$	PLQY N ₂ ; Air ^b / %
H-	Toluene (10^{-5} M)	500	67; 21 ^c
	mCP 10 wt%	499	47; 45 ^d
	mCBPCN 10 wt%	503	87; 62 ^d
CNPh-	Toluene (10^{-5} M)	481	41; 32 ^c
	mCP 10 wt%	499	44; 19 ^d
	mCBPCN 10 wt%	498	34; 19 ^d

CF₃Ph-	Toluene (10 ⁻⁵ M)	532	72; 28 ^c
	mCP 10 wt%	498	51; 38 ^d
	mCBPCN 10 wt%	500	70; 44 ^d
dPh-	Toluene (10 ⁻⁵ M)	514	70; 35 ^c
	mCP 10 wt%	516	66; 50 ^d
	mCBPCN 10 wt%	527	70; 43 ^d
^tBuPh-	Toluene (10 ⁻⁵ M)	524	74; 24 ^c
	mCP 10 wt%	515	66; 64 ^d
	mCBPCN 10 wt%	531	72; 61 ^d
OMePh-	Toluene (10 ⁻⁵ M)	539	75; 23 ^c
	mCP 10 wt%	529	55; 51 ^d
	mCBPCN 10 wt%	539	72; 56 ^d

^a measured at room temperature; ^b $\lambda_{\text{exc}} = 340$ nm; ^c obtained *via* the optically dilute method,³ quinine sulfate (0.5 M) in H₂SO₄ (aq) was used as the reference, $\Phi_{\text{PL}}: 54.6\%$, $\lambda_{\text{exc}} = 360$ nm;²² ^d obtained *via* integrating sphere, for this method we need to consider an average error of $\pm 5\%$.

Table S7. Host and concentration screen of **^tBuPh-DMAC-TRZ** in mCP, mCBPCN and DPEPO.

Host	Doping concentration / wt%	PLQY N ₂ ; Air/ %
mCP	3	65; 61
	5	66; 63
	10	66; 64
	15	62; 60
	20	62; 61
mCBPCN^a	3	62; 57
	5	65; 60
	10	72; 61
	15	79; 64
	20	70; 60
DPEPO^b	3	63; 51

5	67; 49
10	75; 50
15	80; 54
20	73; 55

^a λ_{exc} =340 nm; ^b λ_{exc} =310 nm

Table S8. Emitter properties that might influence the orientation in evaporated films.

10 wt% emitter in mCBPCN host	a^a	MW (g/mol)	x_E/x_H	z_E (Å)
CNPh-DMAC-TRZ	0.16	718.84	1.08	11.53
CF ₃ Ph-DMAC-TRZ	0.26	804.82	1.09	11.53
dPh-DMAC-TRZ	0.15	821.02	1.35	11.53
^t BuPh-DMAC-TRZ	0.25	780.04	1.21	11.53
OMe-DMAC-TRZ	0.20	728.88	1.10	11.53
DMAC-TRZ	0.21	516.63	0.91	11.53

^aanisotropy factor.

OLEDs

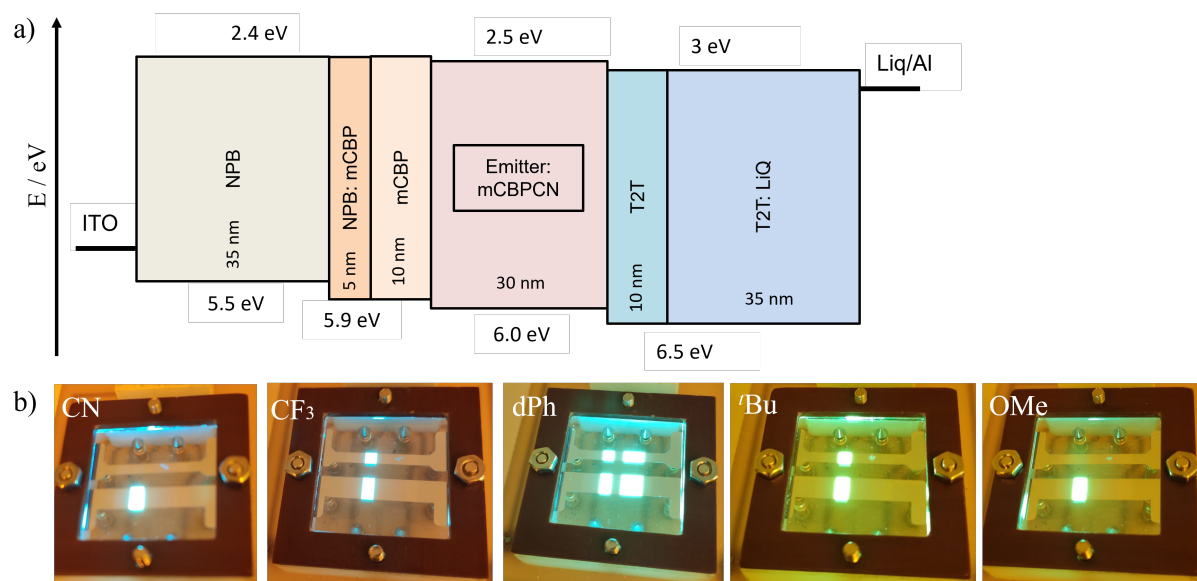


Figure S41. a) OLED stack; b) pictures of the operating OLEDs.

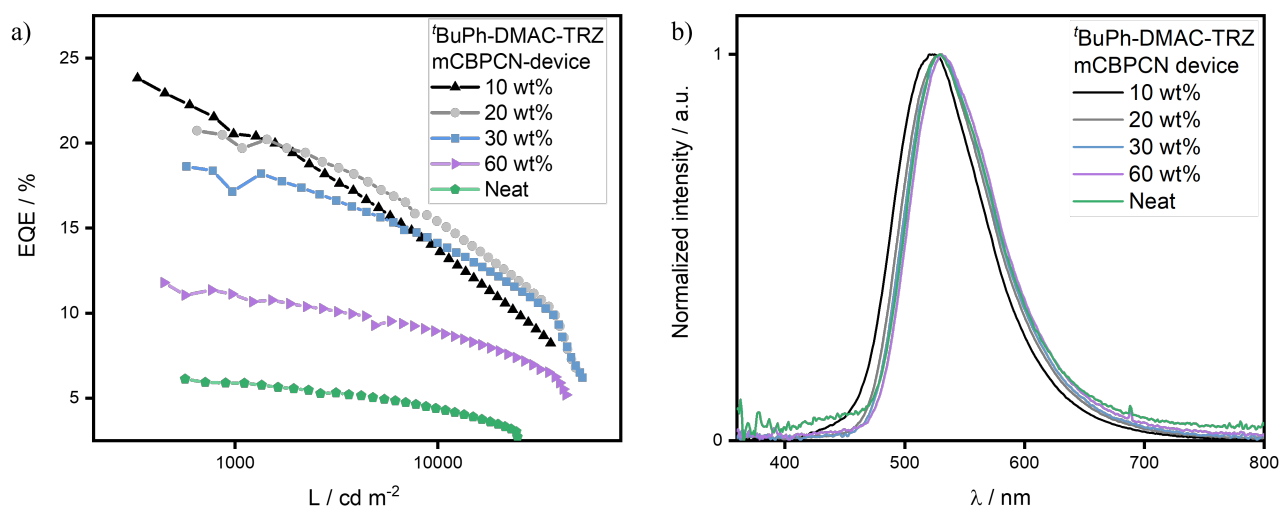


Figure S42. a) EQE vs Luminance curves taken above 500 cd m^{-2} and b) Electroluminescence spectra (at 1000 cd m^{-2}) of the **'BuPh-DMAC-TRZ** OLEDs doped at different concentrations.

Light outcoupling efficiency simulations

The light outcoupling for the device stack reported in the manuscript has been simulated using the commercial software SETFOS from Fluxim.²³ A mode analysis for the six OLEDs (with their individual PL emission spectra considered) was performed while sweeping the transition dipole orientation a from horizontal ($a=0$ to vertical $a=1$). The experimentally measured orientation is marked by a black square for each emitter and is given together with the simulated light outcoupling in the table below.

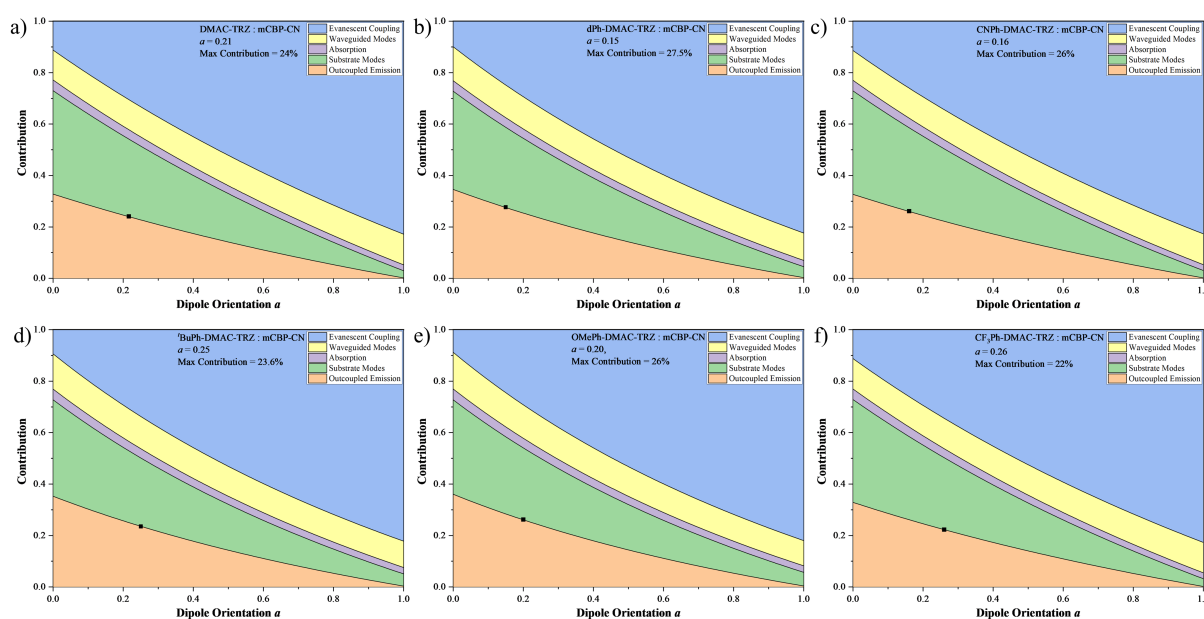


Figure S43. OLED light outcoupling simulation. Emitters at 10 wt% concentration in mCBPCN host of a) DMAC-TRZ, b) dPh-DMAC-TRZ, c) CNPh-DMAC-TRZ, d) 'BuPh-DMAC-TRZ, e) OMePh-DMAC-TRZ, and f) CF₃Ph-DMAC-TRZ.

Table S9. Simulated light outcoupling efficiency.

10 wt% emitter in mCBPCN host	a	Outcoupling Efficiency
dPh-DMAC-TRZ	0.15	28%
CNPh-DMAC-TRZ	0.16	26%
OMe-DMAC-TRZ	0.20	26%
DMAC-TRZ	0.21	24%
'BuPh-DMAC-TRZ	0.25	24%
CF ₃ Ph-DMAC-TRZ	0.26	22%

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