

Mechanofluorochromic properties of 1,4-diphenylanthracene derivatives with hypsochromic shift

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1. Supplementary figures and tables

1.1 Fluorescence spectra of the pristine, ground and stored (5 min. after grinding) samples of 1,4-diphenylanthracene derivatives

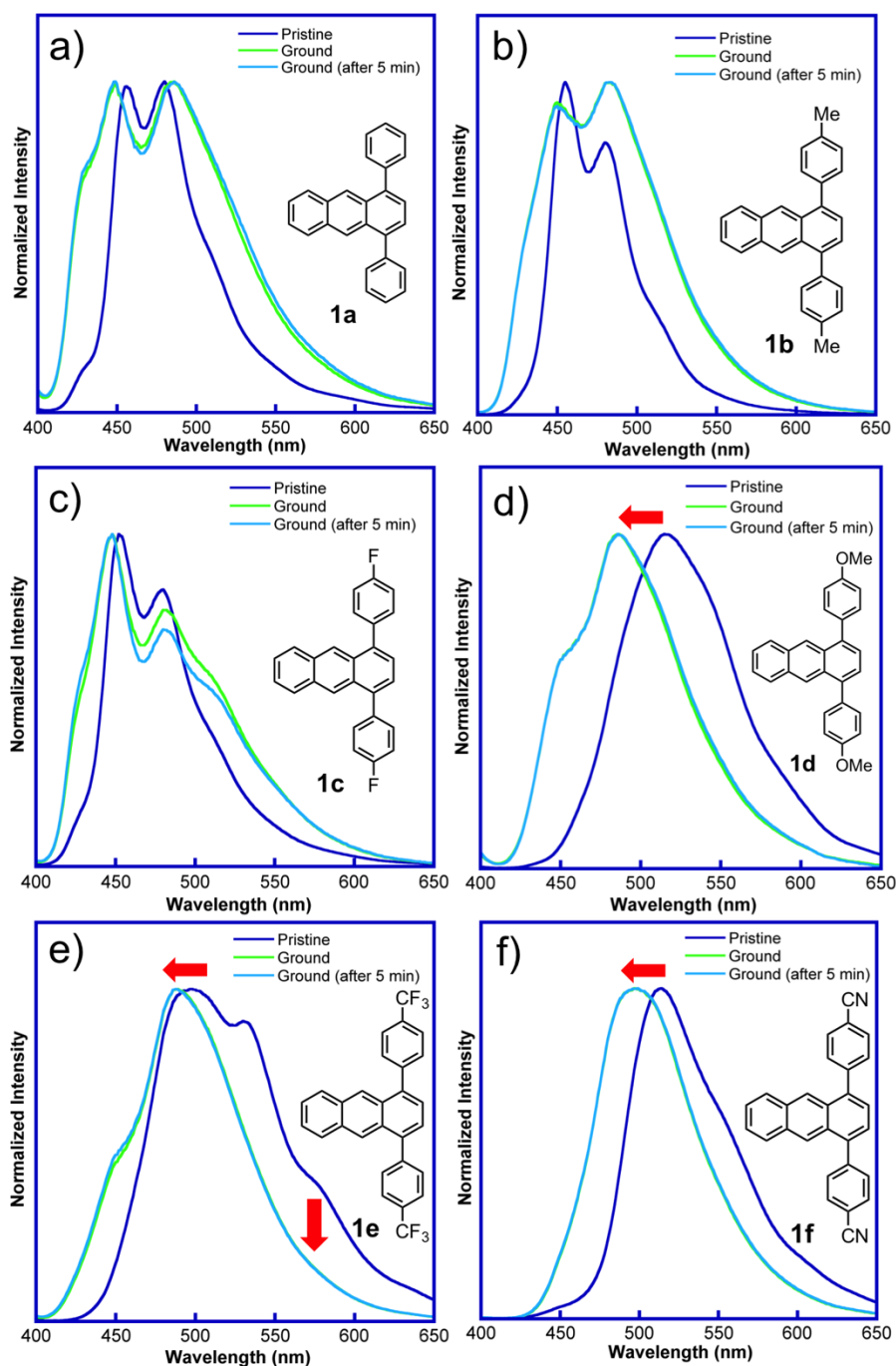


Figure S1. Normalized fluorescence spectra of pristine, ground and stored (5 min. after grinding) samples ($\lambda_{\text{ex}} = 365$ nm), a) **1a** (R=H), b) **1b** (R=Me), c) **1c** (R=F), d) **1d** (R=OMe), e) **1e** (R=CF₃), f) **1f** (R=CN).

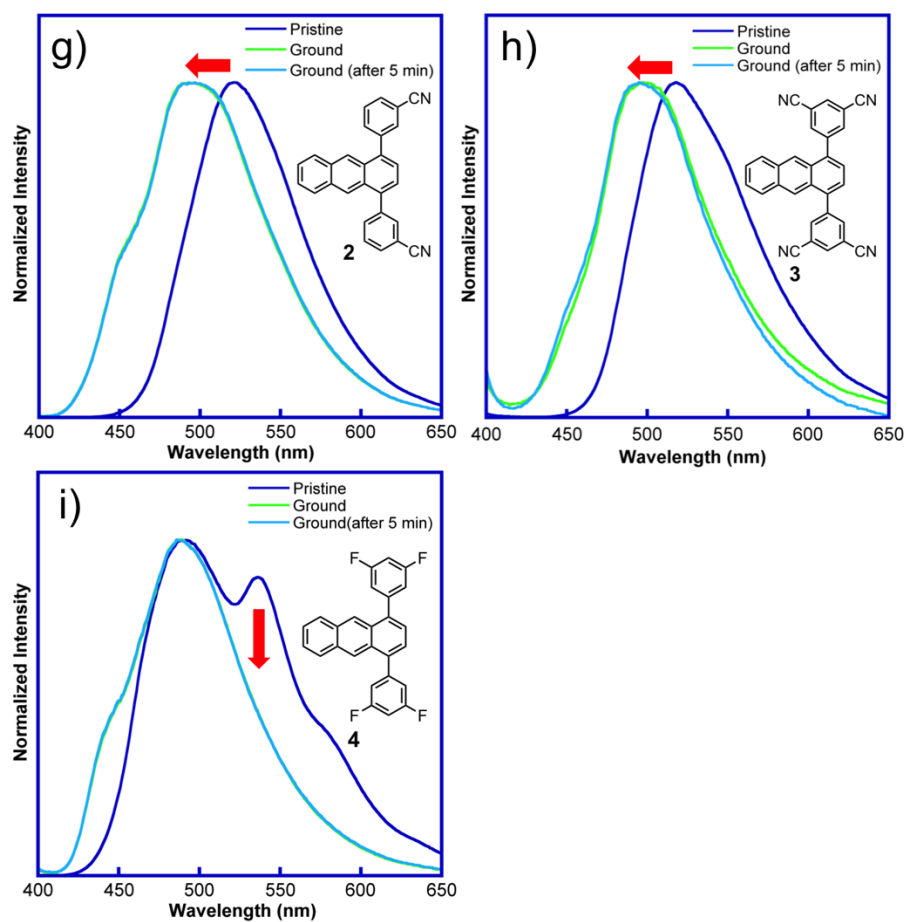


Figure S1 (contd.). Normalized fluorescence spectra of pristine, ground and stored (5 min. after grinding) samples ($\lambda_{\text{ex}} = 365$ nm), g) **2** (3-CN), h) **3** (3,5-CN₂, R'=CN), i) **4** (3,5-F₂, R'=F).

1.2 Fluorescence images of the pristine, ground, stored (5 min after grinding) samples, heated and fumed samples of 1,4-diphenylanthracene derivatives

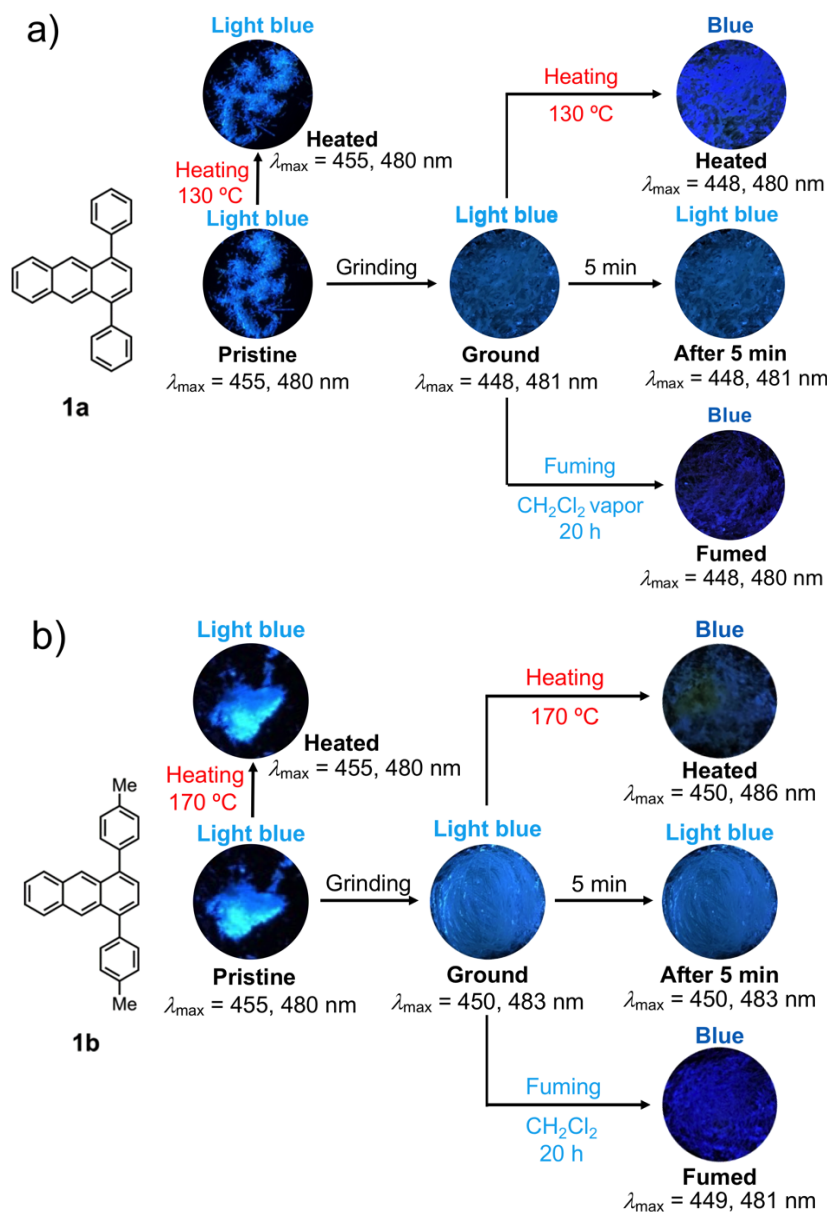


Figure S2. Fluorescence images of 1,4-diphenylanthracene derivatives pristine, ground, stored (5 min after grinding), heated and fumed samples during a 365 nm UV irradiation, a) **1a** (R=H), b) **1b** (R=Me).

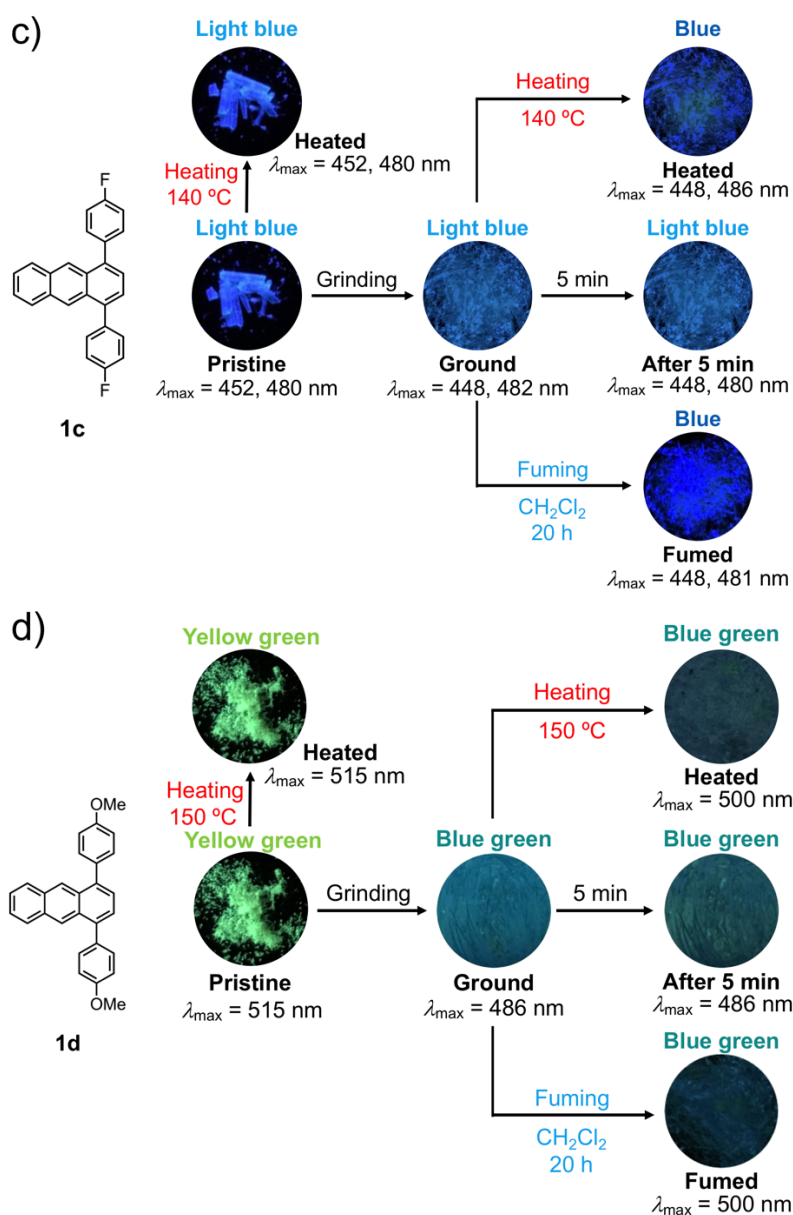


Figure S2 (contd.). Fluorescence images of 1,4-diphenylanthracene derivatives pristine, ground, stored (5 min after grinding), heated and fumed samples during a 365 nm UV irradiation, c) **1c** (R=F), b) **1d** (R=OMe).

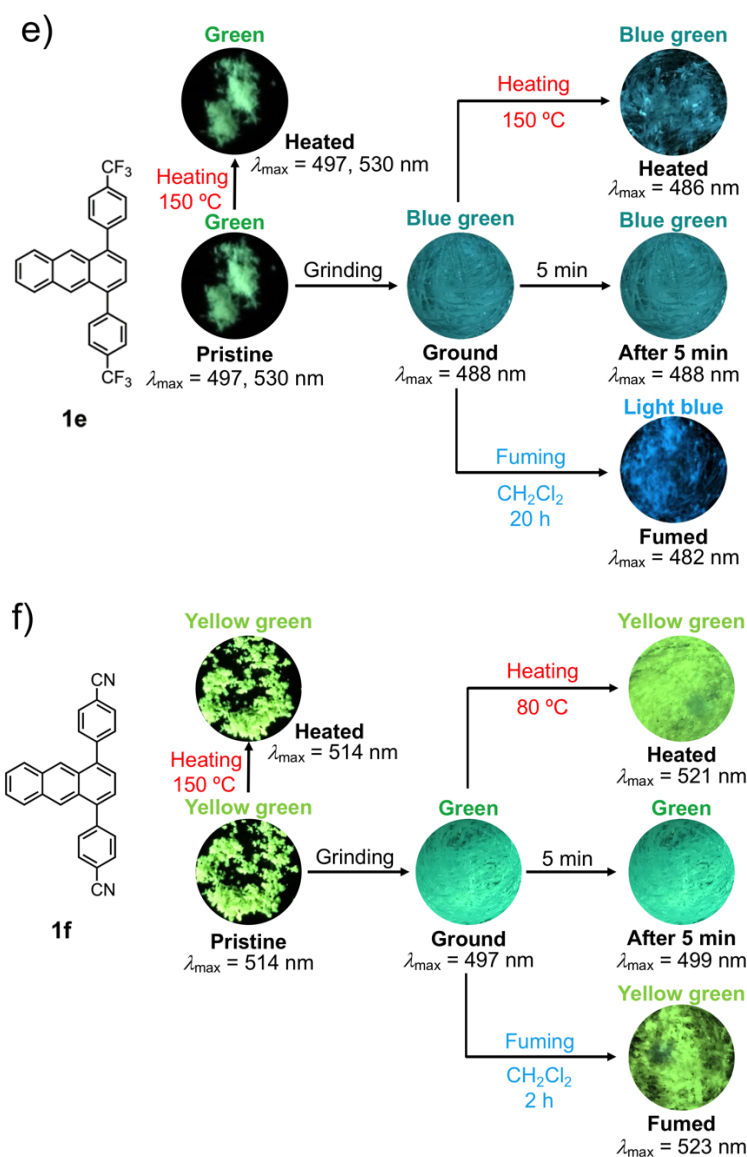


Figure S2 (contd.). Fluorescence images of 1,4-diphenylanthracene derivatives pristine, ground, stored (5 min after grinding), heated and fumed samples during a 365 nm UV irradiation, e) **1e** (R=CF₃), f) **1f** (R=CN).

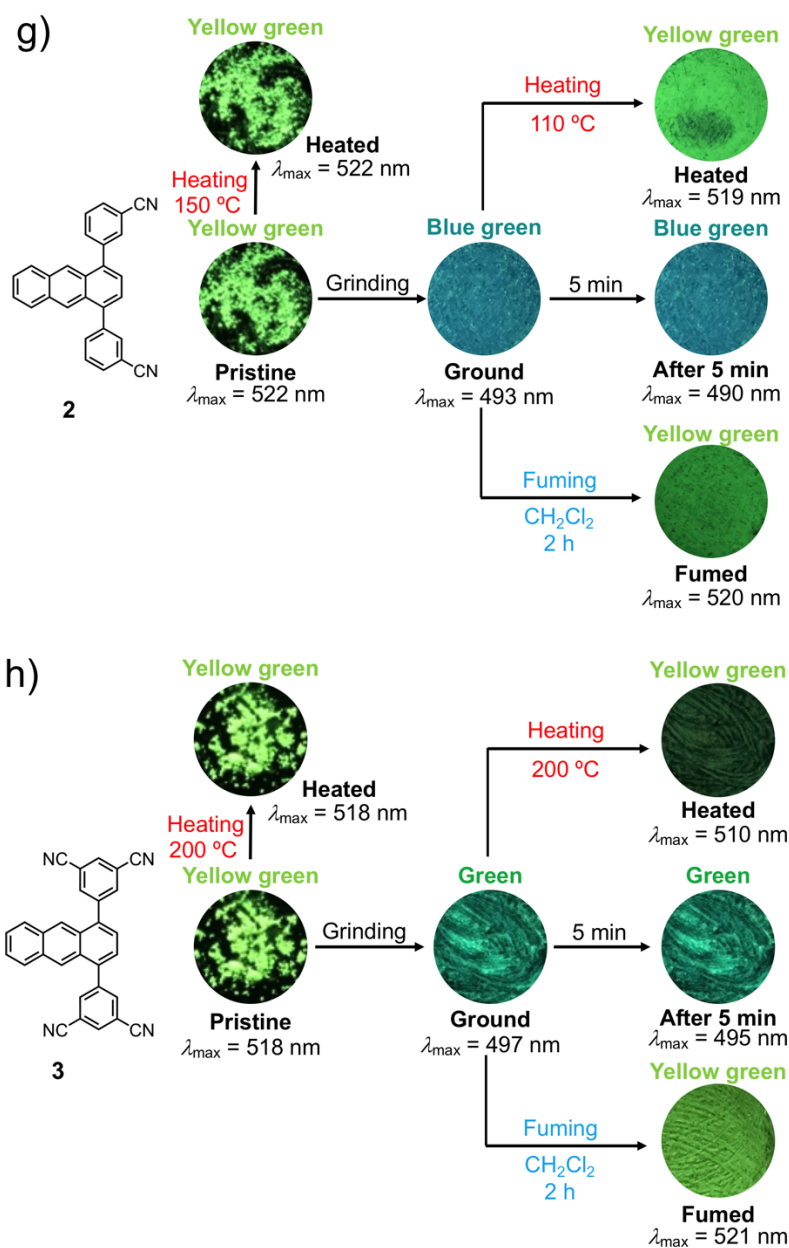


Figure S2 (contd.). Fluorescence images of 1,4-diphenylanthracene derivatives pristine, ground, stored (5 min after grinding), heated and fumed samples during a 365 nm UV irradiation, g) **2** (3-CN), h) **3** (3,5-CN₂, R'=CN).

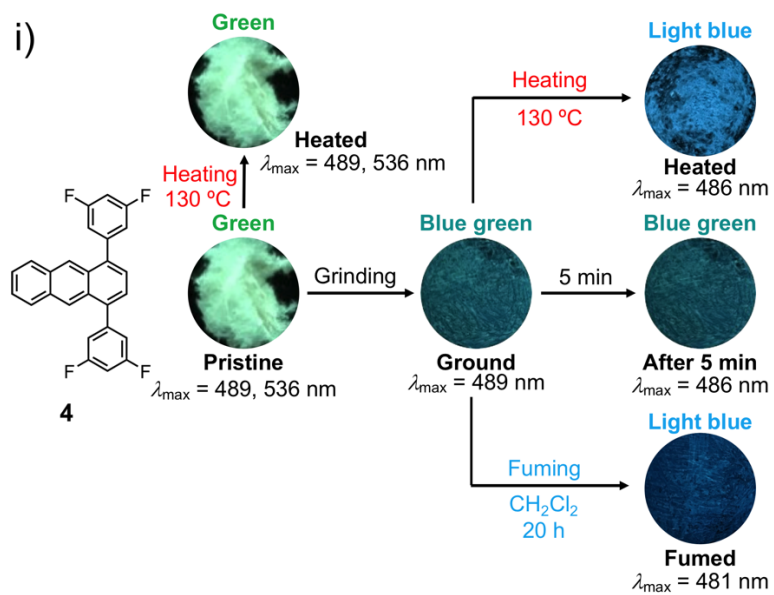


Figure S2 (contd.). Fluorescence images of 1,4-diphenylanthracene derivatives pristine, ground, stored (5 min after grinding), heated and fumed samples during a 365 nm UV irradiation, i) **4** (3,5-F₂, R'=F).

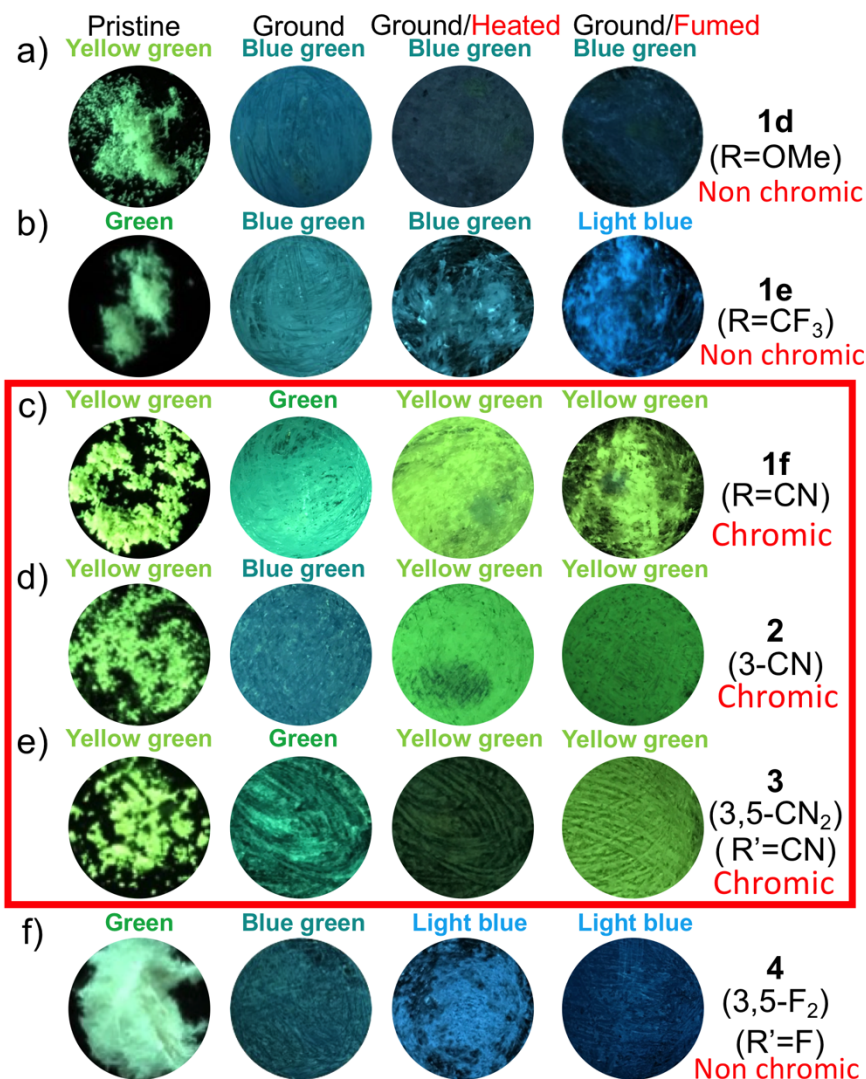


Figure S3. Fluorescent images of the pristine, ground, heated and fumed (CH₂Cl₂ vapor) samples of 1,4-diphenylanthracene derivatives **1d-1f**, and **2-4** during a 365 nm UV irradiation, a) **1d** (R=OMe, heated at 150 °C for 5 min., fumed with CH₂Cl₂ vapor for 20 h), b) **1e** (R=CF₃, heated at 150 °C for 5 min., fumed with CH₂Cl₂ vapor for 20 h), c) **1f** (R=CN, heated at 80 °C for 5 min., fumed with CH₂Cl₂ vapor for 2 h), d) **2** (3-CN, heated at 110 °C for 5 min., fumed with CH₂Cl₂ vapor for 2 h), e) **3** (3,5-CN₂, R'=CN, heated at 200 °C for 5 min., fumed with CH₂Cl₂ vapor for 2 h), f) **4** (3,5-F₂, R'=F, heated at 130 °C for 5 min., fumed with CH₂Cl₂ vapor for 20 h).

1.3 Fluorescence spectra of the pristine, ground, ground-fumed and ground-heated samples of 1,4-diphenylanthracene derivatives

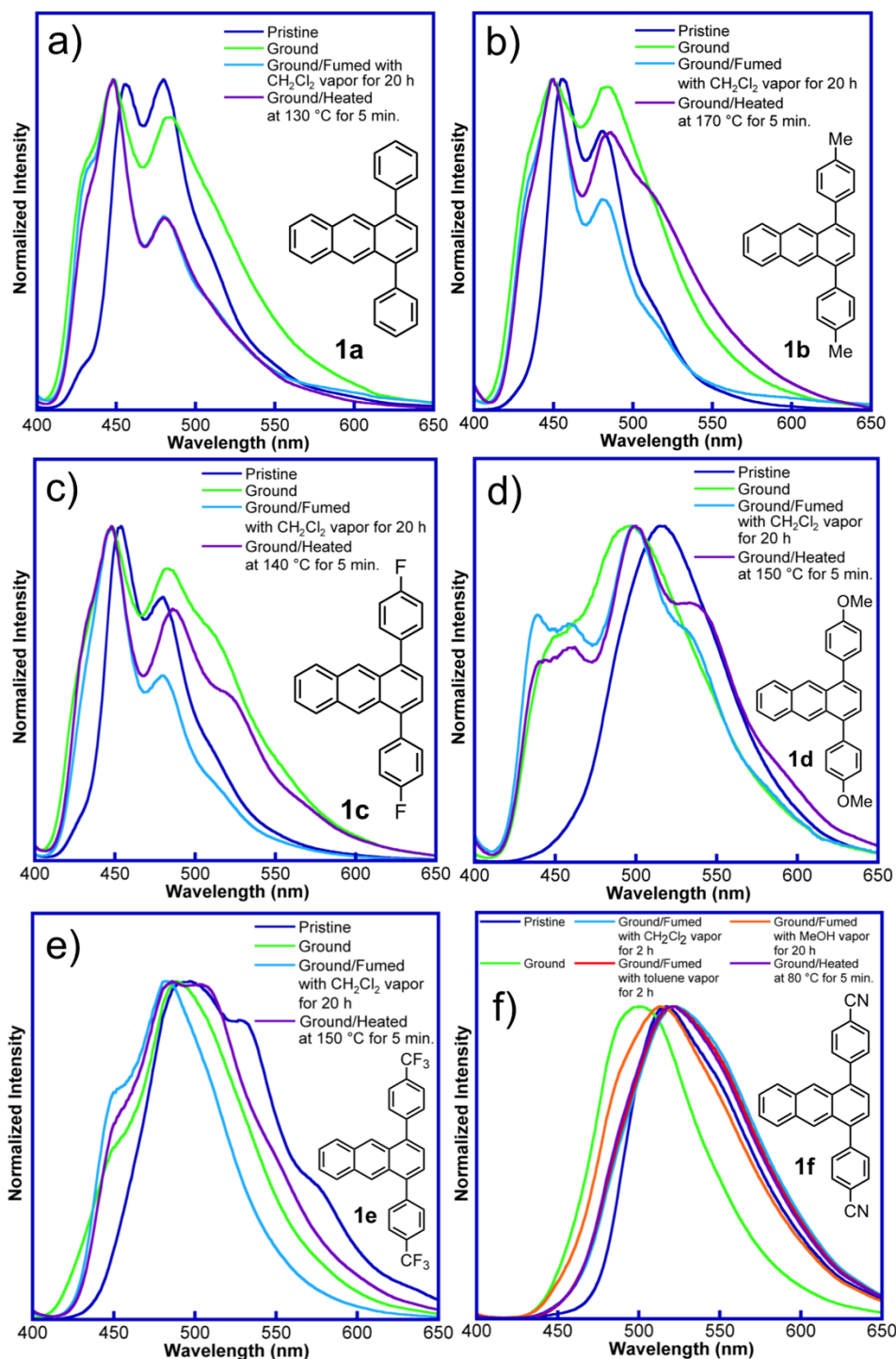


Figure S4. Normalized fluorescence spectra of the pristine, ground, ground-fumed and ground-heated samples ($\lambda_{\text{ex}}=365$ nm), a) **1a** (R=H), b) **1b** (R=Me), c) **1c** (R=F), d) **1d** (R=OMe), e) **1e** (R=CF₃), f) **1f** (R=CN).

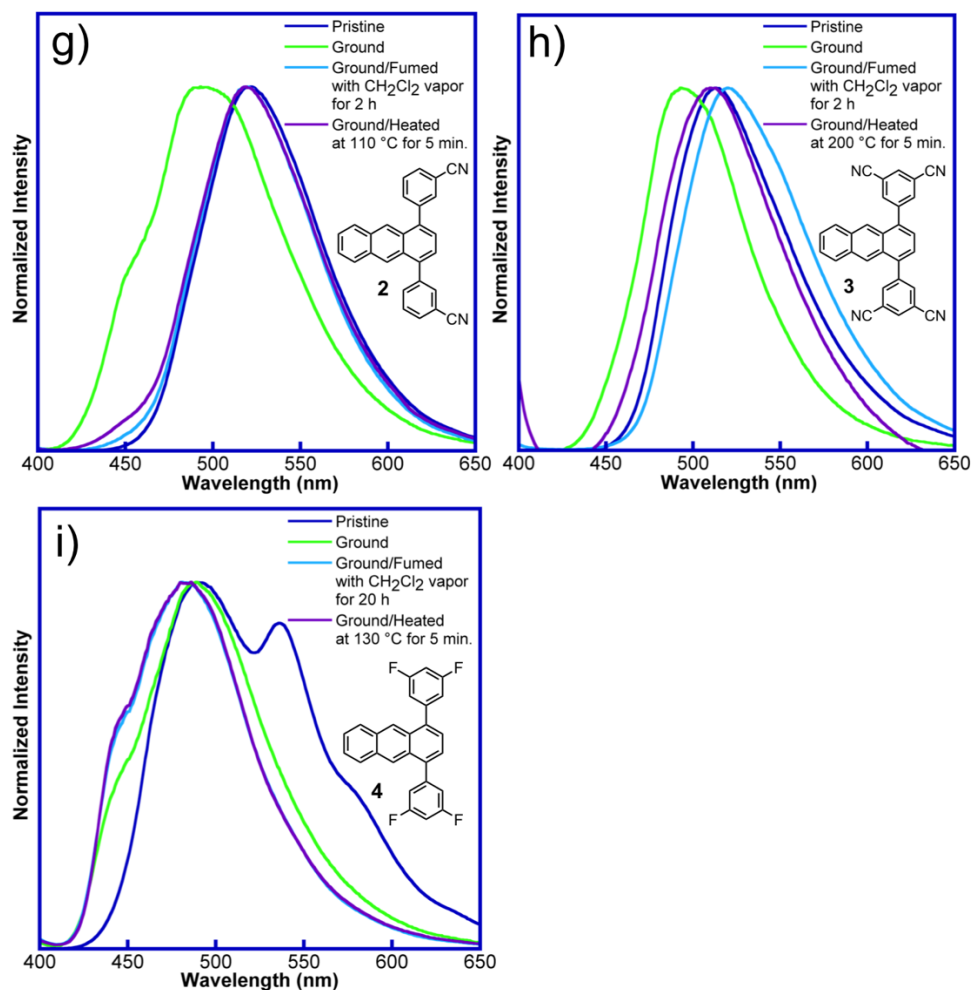


Figure S4 (contd.). Normalized fluorescence spectra of the pristine, ground, ground-fumed and ground-heated samples ($\lambda_{\text{ex}}=365$ nm), g) **2** (3-CN), h) **3** (3,5-CN₂, R'=CN), i) **4** (3,5-F₂, R'=F).

1.4 Vapochromic properties of 1,4-diphenylanthracene derivatives

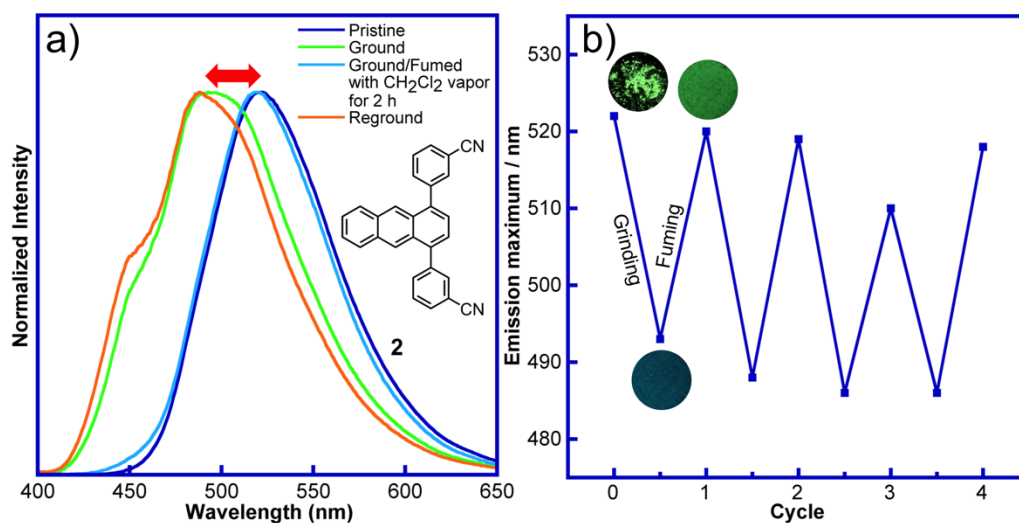


Figure S5. Vapochromic properties of 1,4-diphenylanthracene derivative **2** (3-CN), a) fluorescence spectra of pristine, ground, ground-fumed (CH₂Cl₂ vapor, 2 h) and reground samples, b) repeated grinding-fuming cycles.

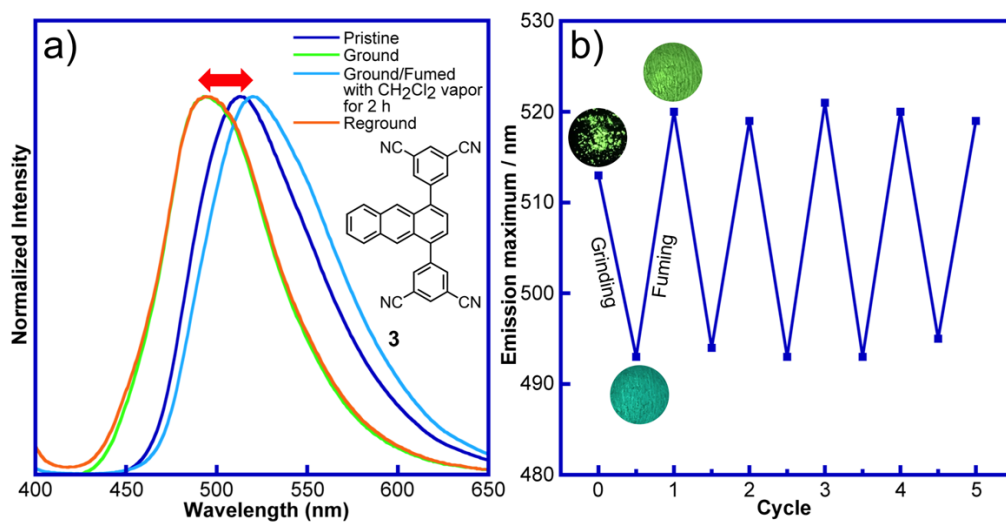


Figure S6. Vapochromic properties of 1,4-diphenylanthracene derivative **3** (3,5-CN₂, R'=CN), a) fluorescence spectra of pristine, ground, ground-fumed (CH₂Cl₂ vapor, 2 h) and reground samples, b) repeated grinding-fuming cycles.

1.5 Thermochromic properties of 1,4-diphenylanthracene derivatives

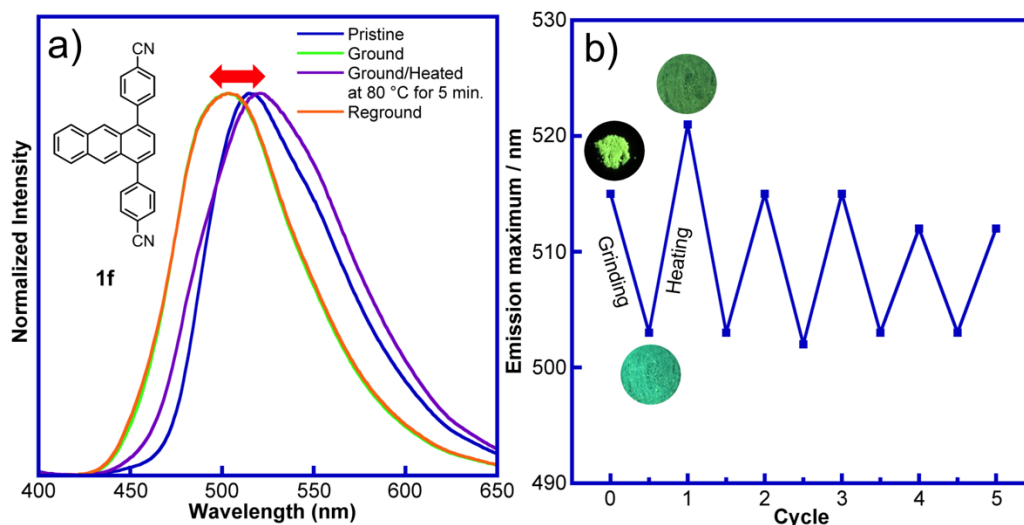


Figure S7. Thermochromic properties of 1,4-diphenylanthracene derivative **1f** (R=CN), a) fluorescence spectra of pristine, ground, ground-heated (80 °C for 5 min.) and reground samples, b) repeated grinding-heating cycles.

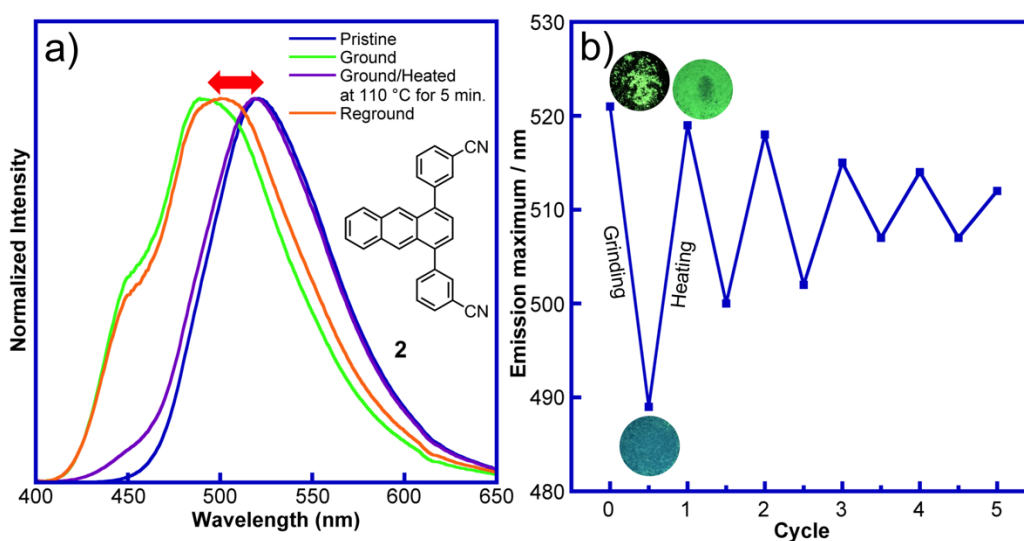


Figure S8. Thermochromic properties of 1,4-diphenylanthracene derivative **2** (3-CN), a) fluorescence spectra of pristine, ground, ground-heated (110 °C for 5 min.) and reground samples, b) repeated grinding-heating cycles.

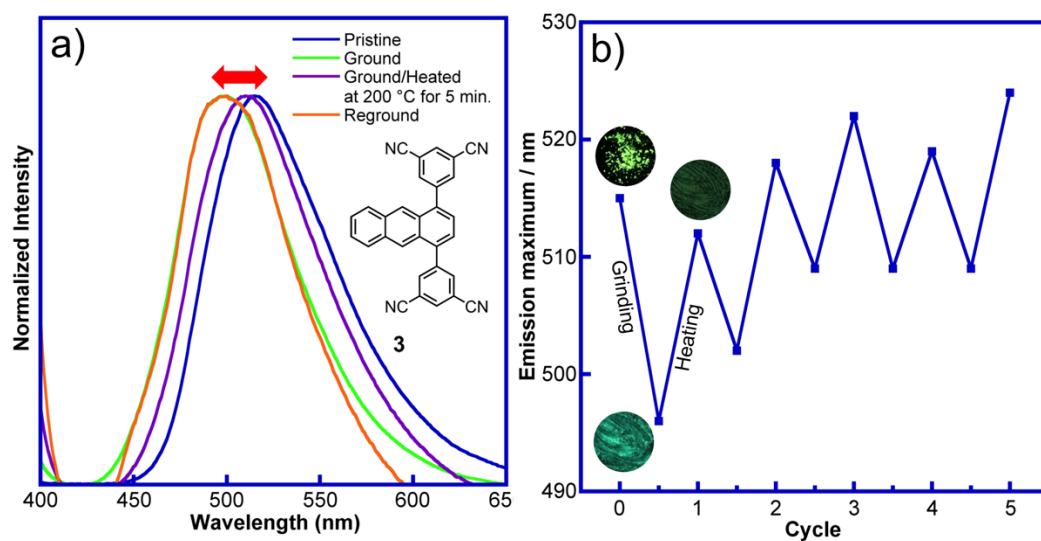


Figure S9. Thermochromic properties of 1,4-diphenylanthracene derivative **3** (3,5-CN₂, R'=CN), a) fluorescence spectra of pristine, ground, ground-heated (200 °C for 5 min.) and reground samples, b) repeated grinding-heating cycles.

1.6 IR spectra of the CN-substituted 1,4-diphenylanthracene derivatives 1f, 2

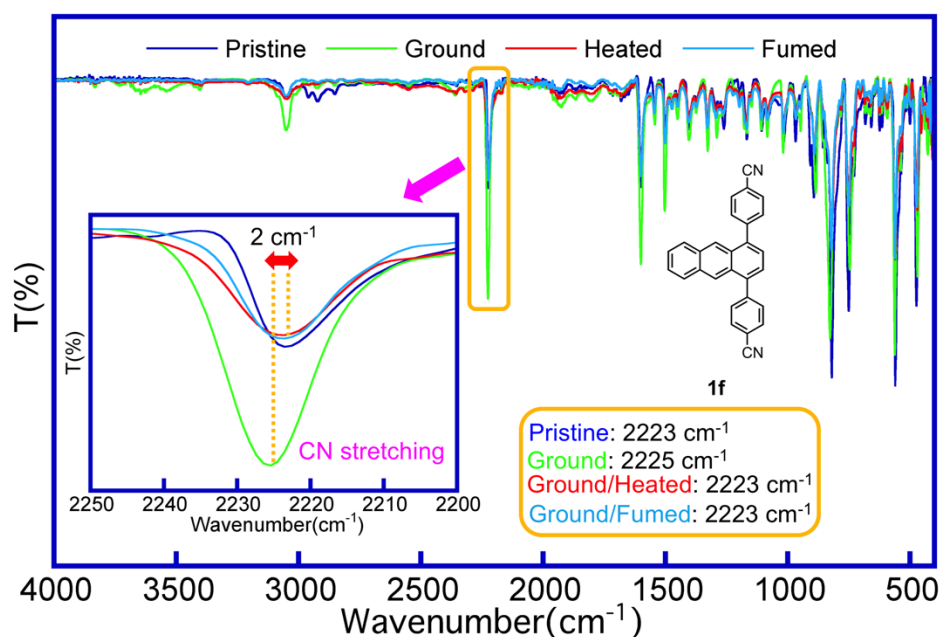


Figure S10. IR spectra of the CN-substituted 1,4-diphenylanthracene derivative **1f** before grinding (pristine), after grinding (ground), ground-heated (80 °C for 5 min) and ground-fumed (with CH₂Cl₂ vapor for 2 h) samples in the CN stretching region.

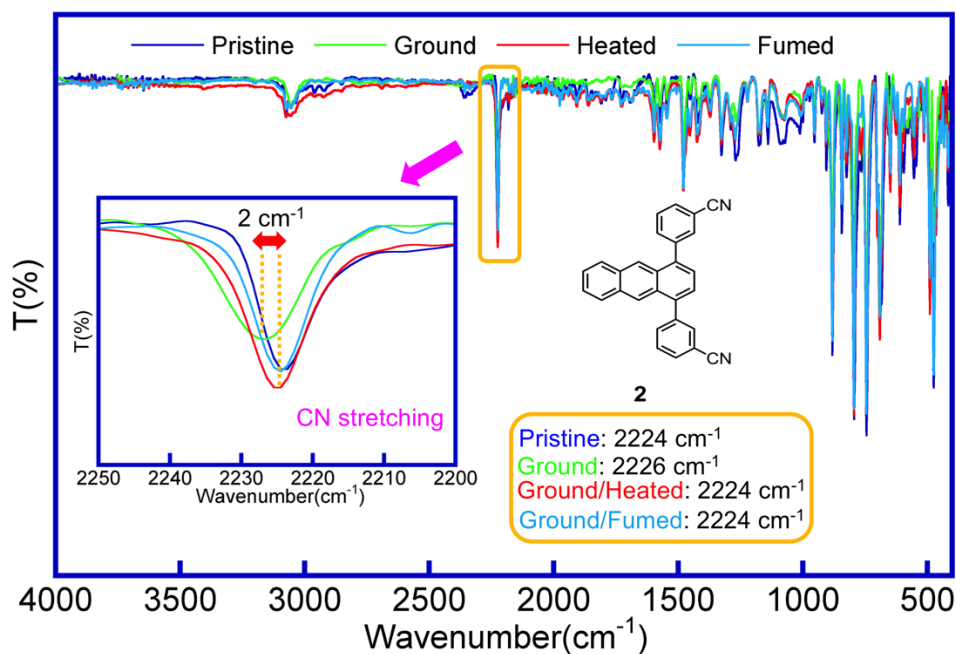


Figure S11. IR spectra of the CN-substituted 1,4-diphenylanthracene derivative **2** before grinding (pristine), after grinding (ground), ground-heated (110 °C for 5 min) and ground-fumed (with CH₂Cl₂ vapor for 2 h) samples in the CN stretching region.

1.7 DSC profiles of 1,4-diphenylanthracene derivatives

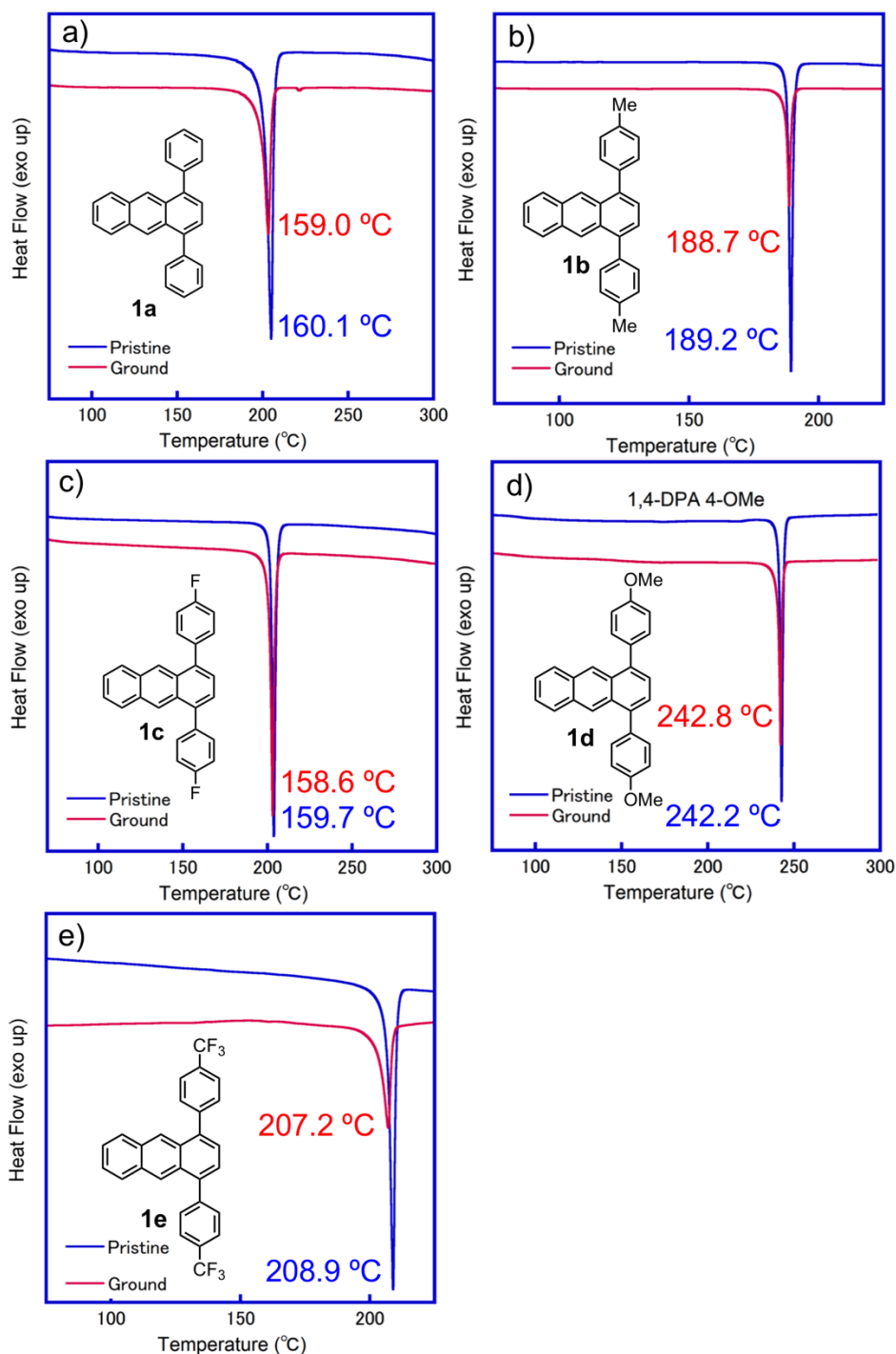


Figure S12. DSC profiles of 1,4-diphenylanthracene derivatives before grinding (pristine) and after grinding (ground), a) **1a** (R=H), b) **1b** (R=Me), c) **1c** (R=F), d) **1d** (R=OMe), e) **1e** (R=CF₃).

1.8 UV-vis absorption spectra of the pristine and ground samples

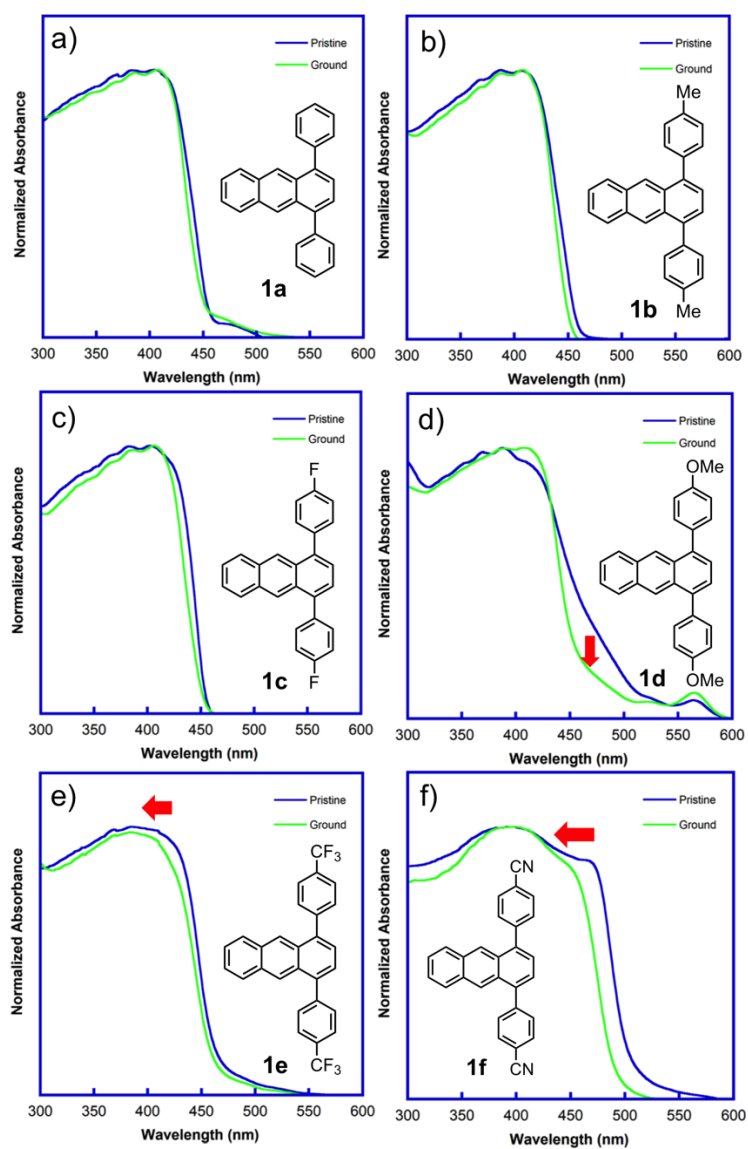


Figure S13. UV-vis absorption spectra of the pristine and ground samples of the 1,4-diphenylanthracene derivatives, a) **1a** (R=H), b) **1b** (R=Me), c) **1c** (R=F), d) **1d** (R=OMe), e) **1e** (R=CF₃), f) **1f** (R=CN).

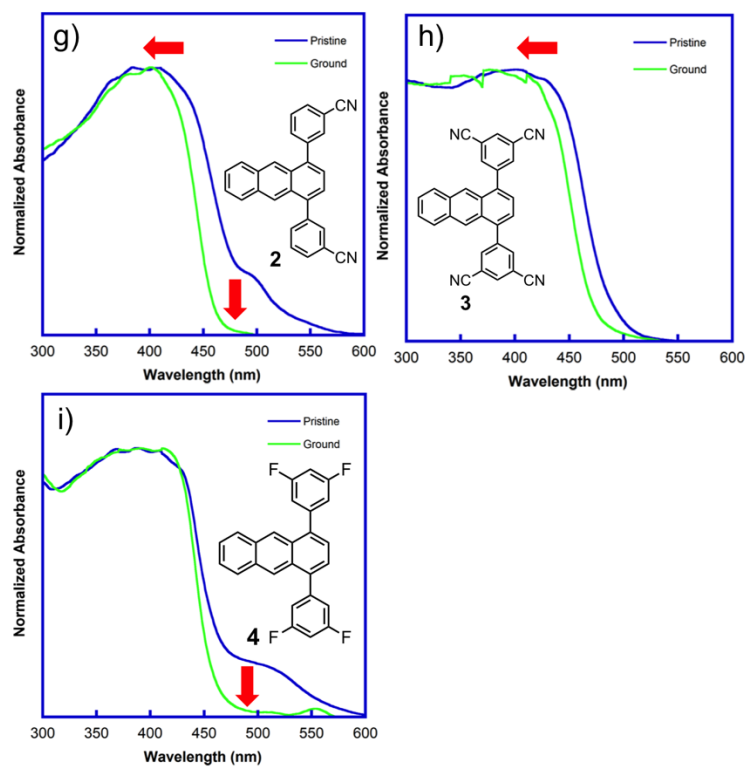


Figure S13 (contd.). UV-vis absorption spectra of the pristine and ground samples of the 1,4-diphenylanthracene derivatives, g) **2** (3-CN), h) **3** (3,5-CN₂, R'=CN), i) **4** (3,5-F₂, R'=F).

1.9 UV-vis absorption spectra of 1,4-diphenylanthracene derivatives (in CHCl₃)

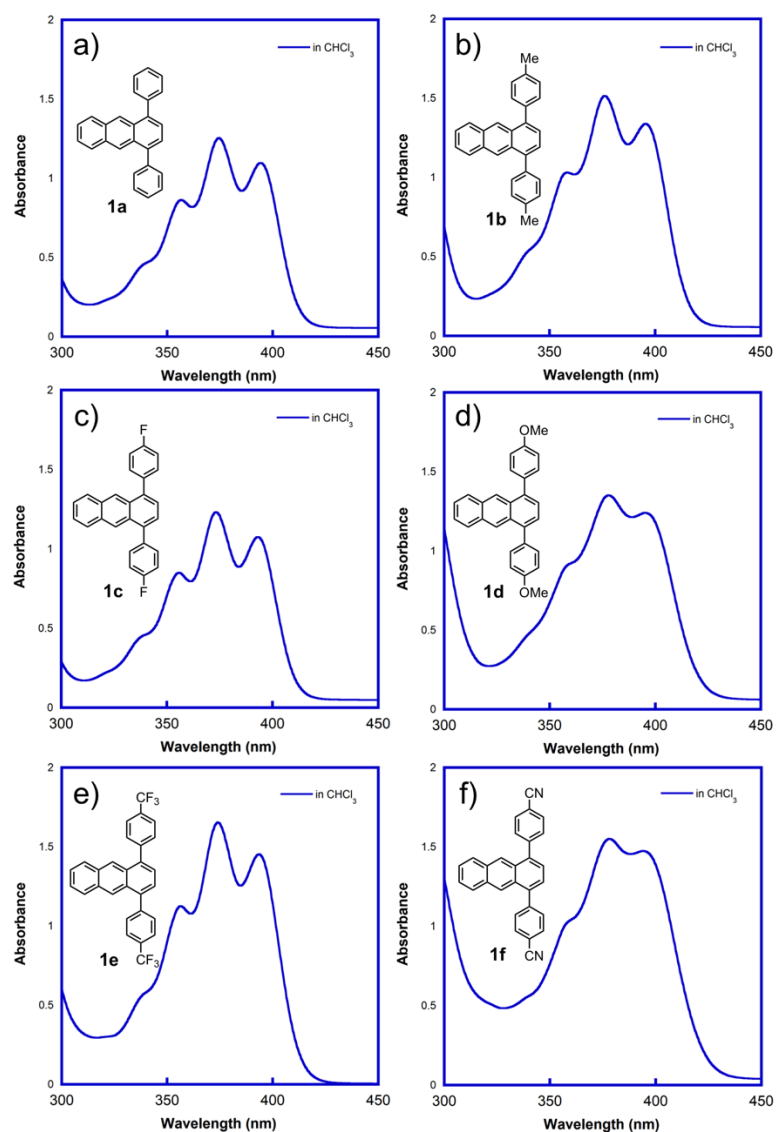


Figure S14. UV-vis absorption spectra of 1,4-diphenylanthracene derivatives (0.1 mM in CHCl₃), a) **1a** (R=H), b) **1b** (R=Me), c) **1c** (R=F), d) **1d** (R=OMe), e) **1e** (R=CF₃), f) **1f** (R=CN).

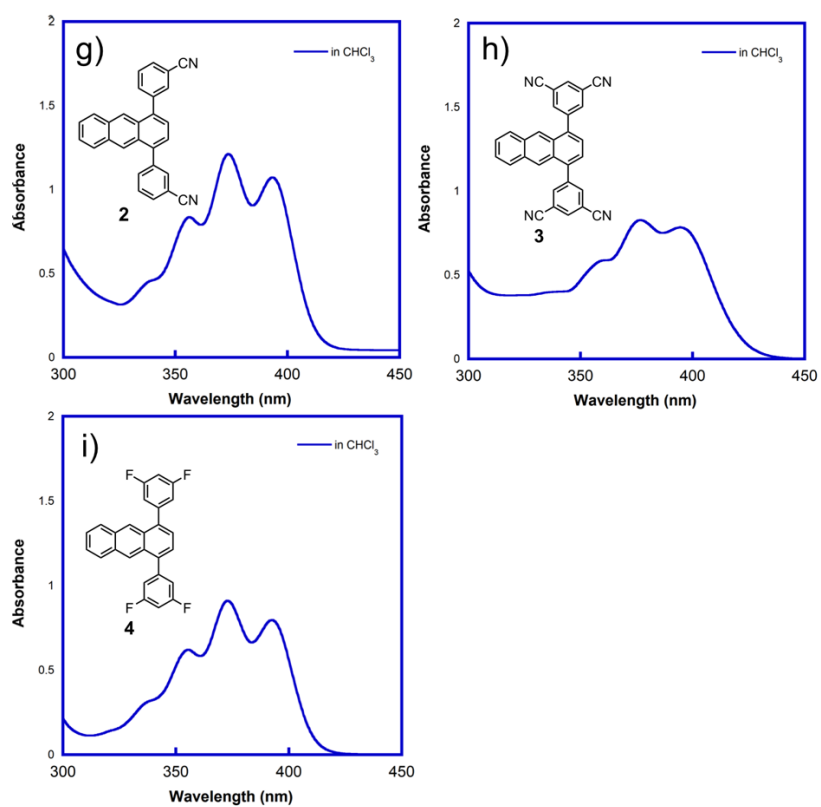


Figure S14 (contd.). UV-vis absorption spectra of 1,4-diphenylanthracene derivatives (0.1 mM in CHCl_3), g) **2** (3-CN), h) **3** (3,5-CN₂, R'=CN), i) **4** (3,5-F₂, R'=F).

1.10 Fluorescence spectra of 1,4-diphenylanthracene derivatives (in CHCl_3)

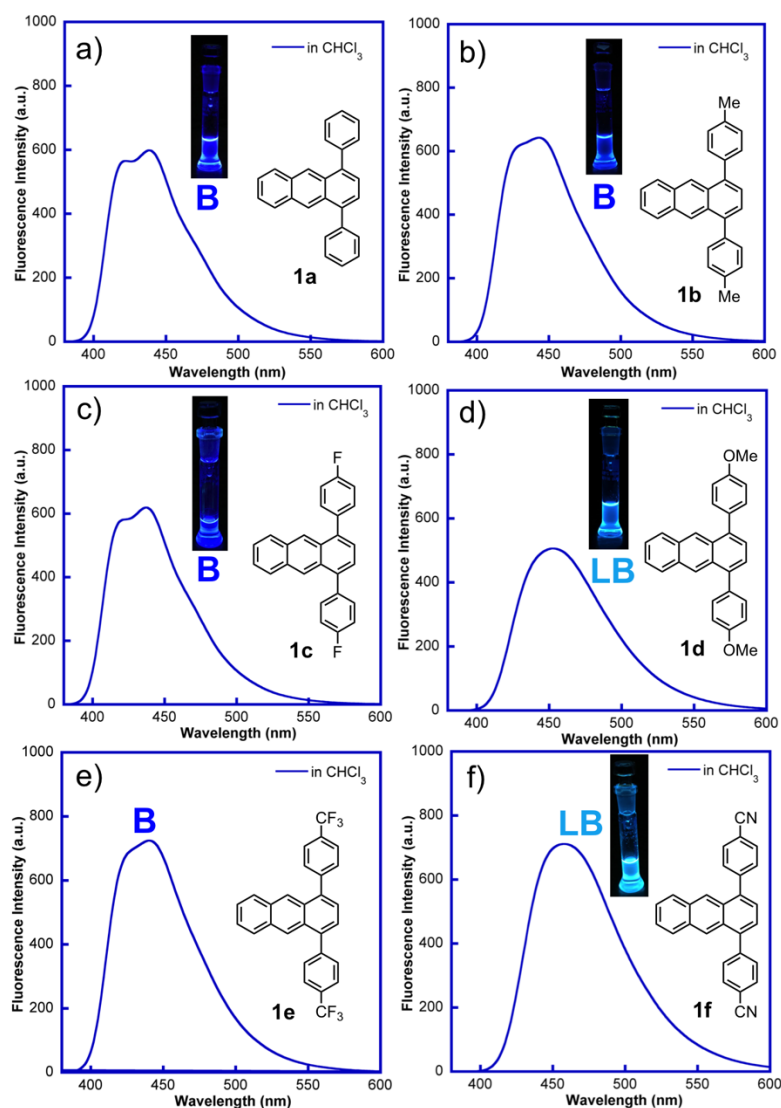


Figure S15. Fluorescence spectra of 1,4-diphenylanthracene derivatives (25 μM in CHCl_3 , $\lambda_{\text{ex}} = 365$ nm): a) **1a** (R=H), b) **1b** (R=Me), c) **1c** (R=F), d) **1d** (R=OMe), e) **1e** (R=CF₃), f) **1f** (R=CN).

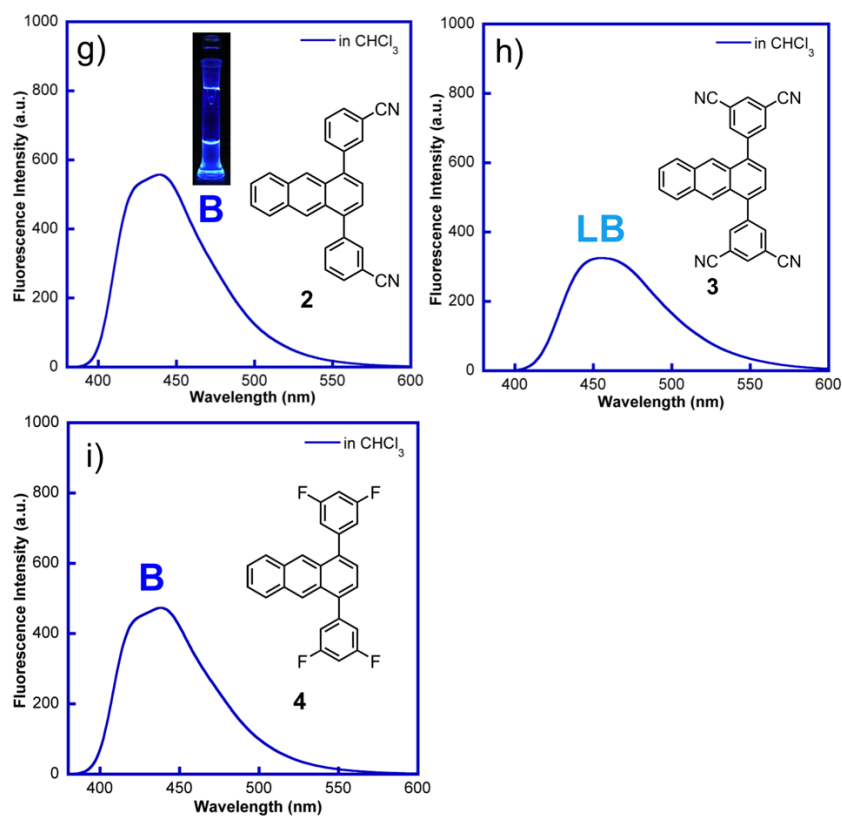


Figure S15 (contd.). Fluorescence spectra of 1,4-diphenylanthracene derivatives (25 μ M in CHCl_3 , $\lambda_{\text{ex}} = 365$ nm): g) **2** (3- CN), h) **3** (3,5- CN_2 , $\text{R}'=\text{CN}$), i) **4** (3,5- F_2 , $\text{R}'=\text{F}$).

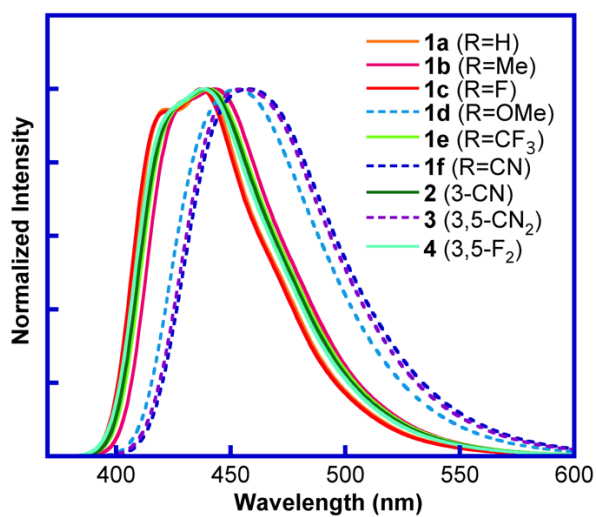


Figure S16. Fluorescence spectra of 1,4-diphenylanthracene derivatives (25 μ M in CHCl_3 , $\lambda_{\text{ex}} = 365$ nm).

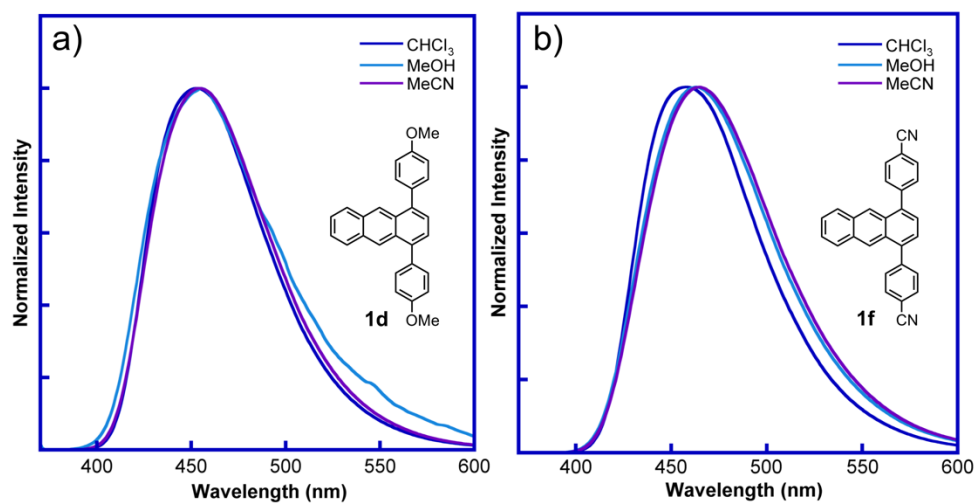


Figure S17. Fluorescence spectra of 1,4-diphenylanthracene derivatives (25 μM in different solvents, $\lambda_{\text{ex}} = 365 \text{ nm}$): a) **1d** (R=OMe), b) **1f** (R=CN).

1.11 Fluorescence spectra of 1,4-diphenylanthracene derivatives in PMMA film

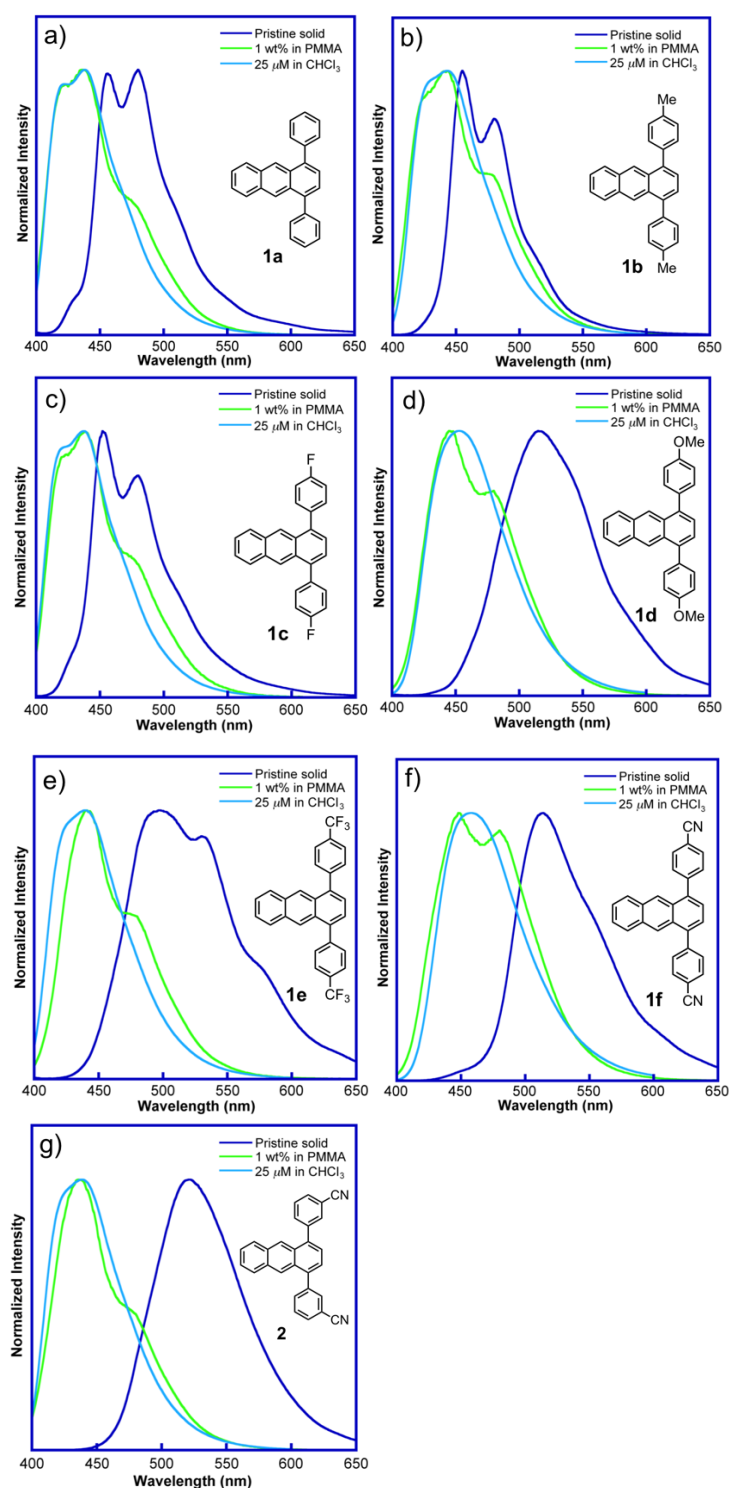


Figure S18. Fluorescence spectra of 1,4-diphenylanthracene derivatives in pristine solid, 25 μM in CHCl_3 solution, 1 wt% in PMMA film ($\lambda_{\text{ex}} = 365 \text{ nm}$), a) **1a** ($\text{R}=\text{H}$), b) **1b** ($\text{R}=\text{Me}$), c) **1c** ($\text{R}=\text{F}$), d) **1d** ($\text{R}=\text{OMe}$), e) **1e** ($\text{R}=\text{CF}_3$), f) **1f** ($\text{R}=\text{CN}$), g) **2** (3-CN).

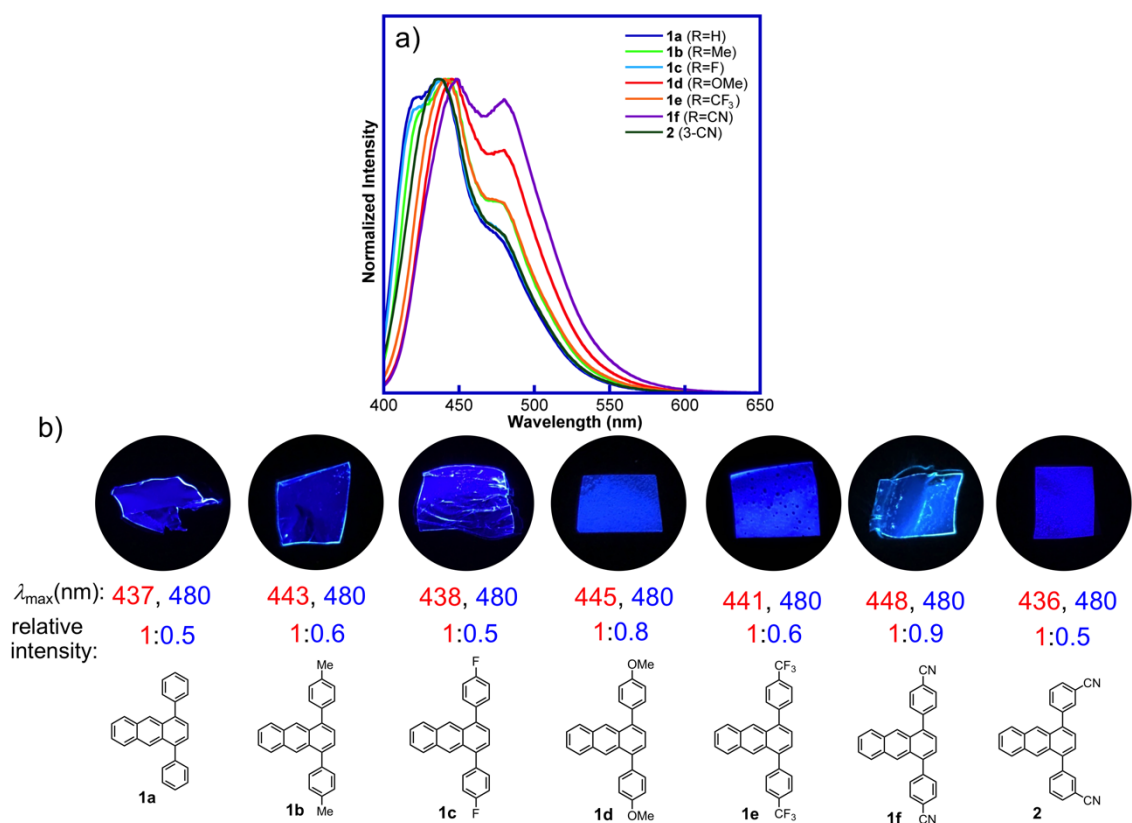


Figure S19. Fluorescence spectra and photographs of 1,4-diphenylanthracene derivatives in PMMA film (1 wt%), a) comparison of normalized fluorescence spectra ($\lambda_{\text{ex}} = 365 \text{ nm}$), b) photographs in PMMA film (under 365 nm UV light) and relative intensities of fluorescence spectra.

1.12 Fluorescence lifetime decay profiles of pristine, ground, ground-heated and ground-fumed samples of 1,4-diphenylanthracene derivatives

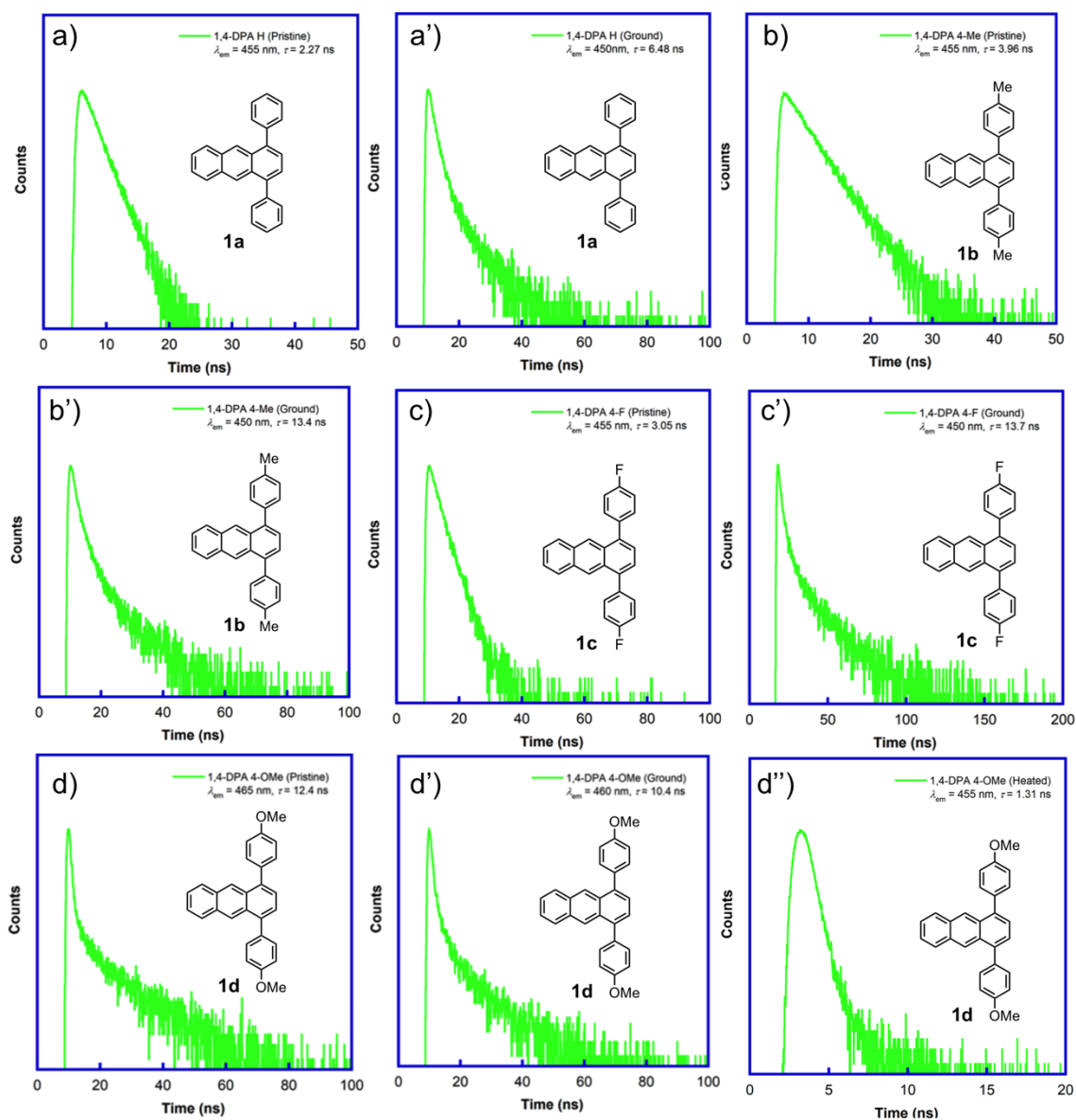


Figure S20. Fluorescence lifetime decay profile of pristine, ground, ground-heated and ground-fumed samples of 1,4-diphenylanthracene derivatives ($\lambda_{ex} = 365 \text{ nm}$): a) **1a** (R=H, pristine), a') **1a** (R=H, ground), b) **1b** (R=Me, pristine), b') **1b** (R=Me, ground), c) **1c** (R=F, pristine), c') **1c** (R=F, ground), d) **1d** (R=OMe, pristine), d') **1c** (R=OMe, ground), d'') **1d** (R=OMe, ground-heated, 150 °C for 5 min.).

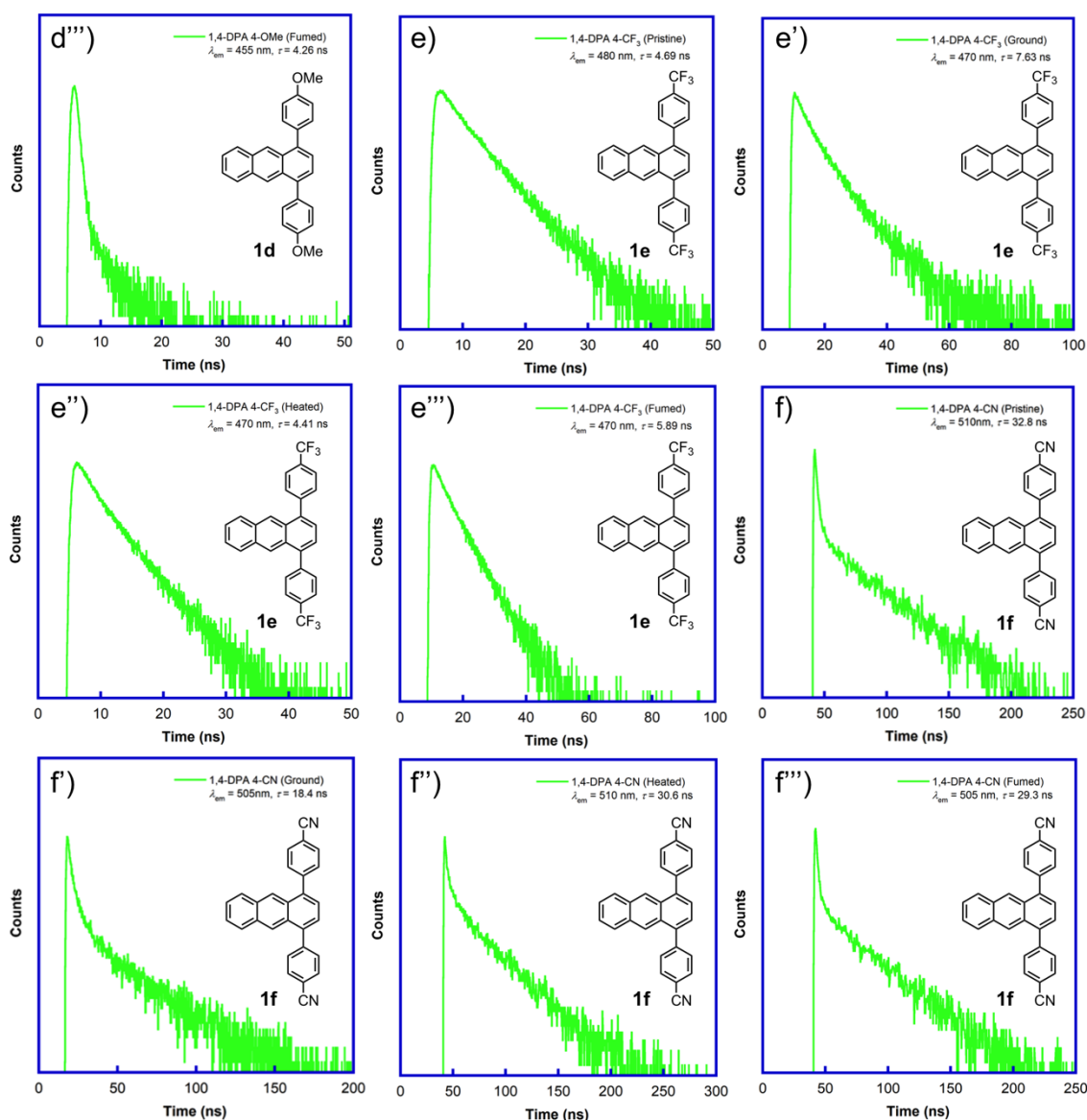


Figure S20 (contd.). Fluorescence lifetime decay profile of pristine, ground, ground-heated and ground-fumed samples of 1,4-diphenylanthracene derivatives ($\lambda_{ex} = 365$ nm): d''') **1c** (R=OMe, ground-fumed, CH₂Cl₂ vapor for 20 h), e) **1e** (R=CF₃, pristine), e') **1e** (R=CF₃, ground), e'') **1e** (R=CF₃, ground-heated, 150 °C, 5 min.), e''') **1e** (R=CF₃, ground-fumed, CH₂Cl₂ vapor for 20 h), f) **1f** (R=CN, pristine), f') **1f** (R=CN, ground), f'') **1f** (R=CN, ground-heated, 80 °C, 5 min.), f''') **1f** (4-CN, ground-fumed, CH₂Cl₂ vapor for 2 h).

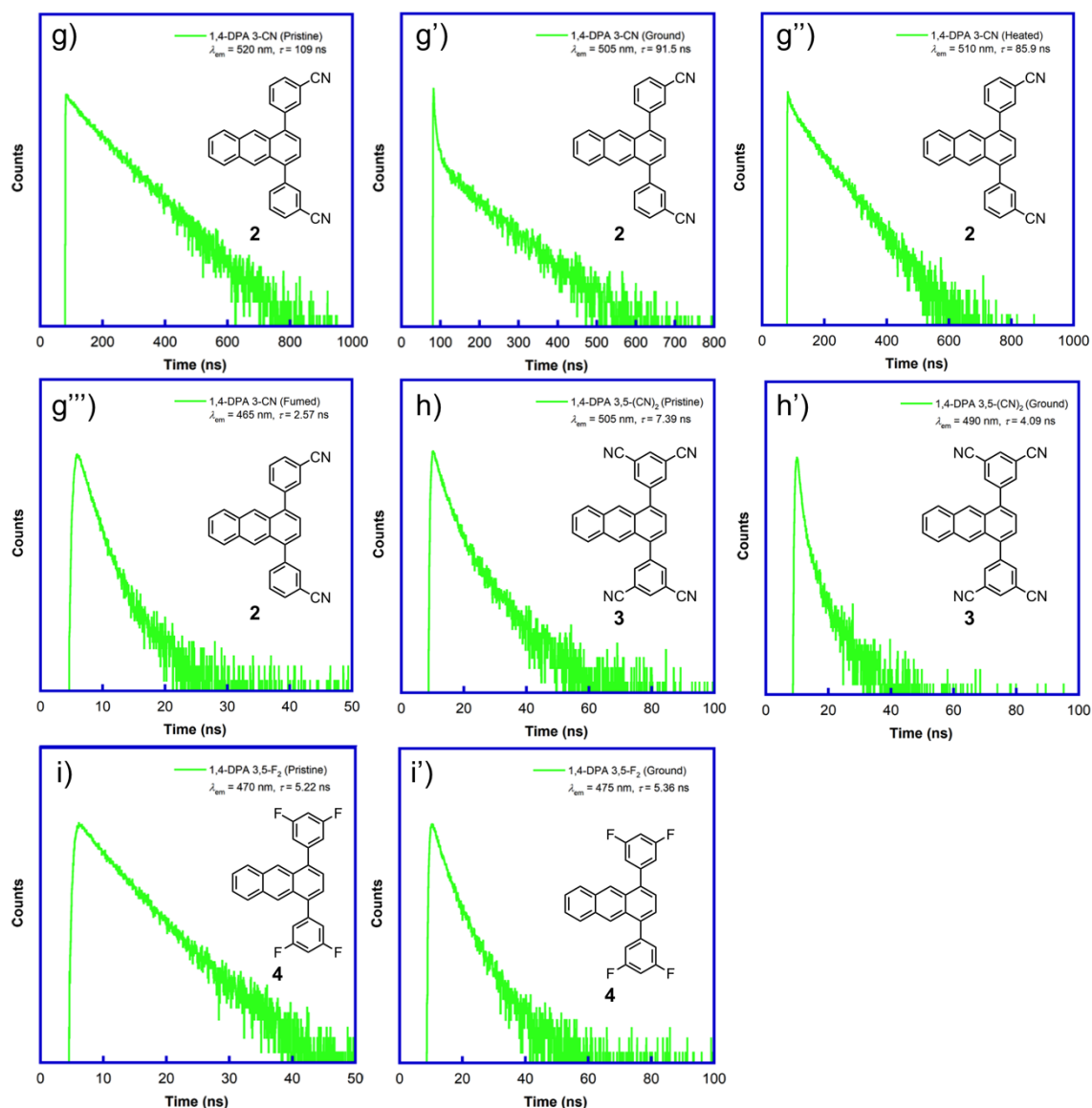


Figure S20 (cont.). Fluorescence lifetime decay profile of pristine, ground, ground-heated and ground-fumed samples of 1,4-diphenylanthracene derivatives ($\lambda_{ex} = 365$ nm): g) **2** (3-CN, pristine), g') **2** (3-CN, ground), g'') **2** (3-CN, ground-heated, 110 °C, 5 min.), g''') **2** (3-CN, ground-fumed, CH₂Cl₂ vapor for 2h), h) **3** (3,5-CN₂, R'=CN, pristine), h') **3** (3,5-CN₂, R'=CN, ground), i) **4** (3,5-F₂, R'=F, pristine), i') **4** (3,5-F₂, R'=F, ground).

1.13 Fluorescence lifetime decay profiles of 1,4-diphenylanthracene derivatives in CHCl_3 solution

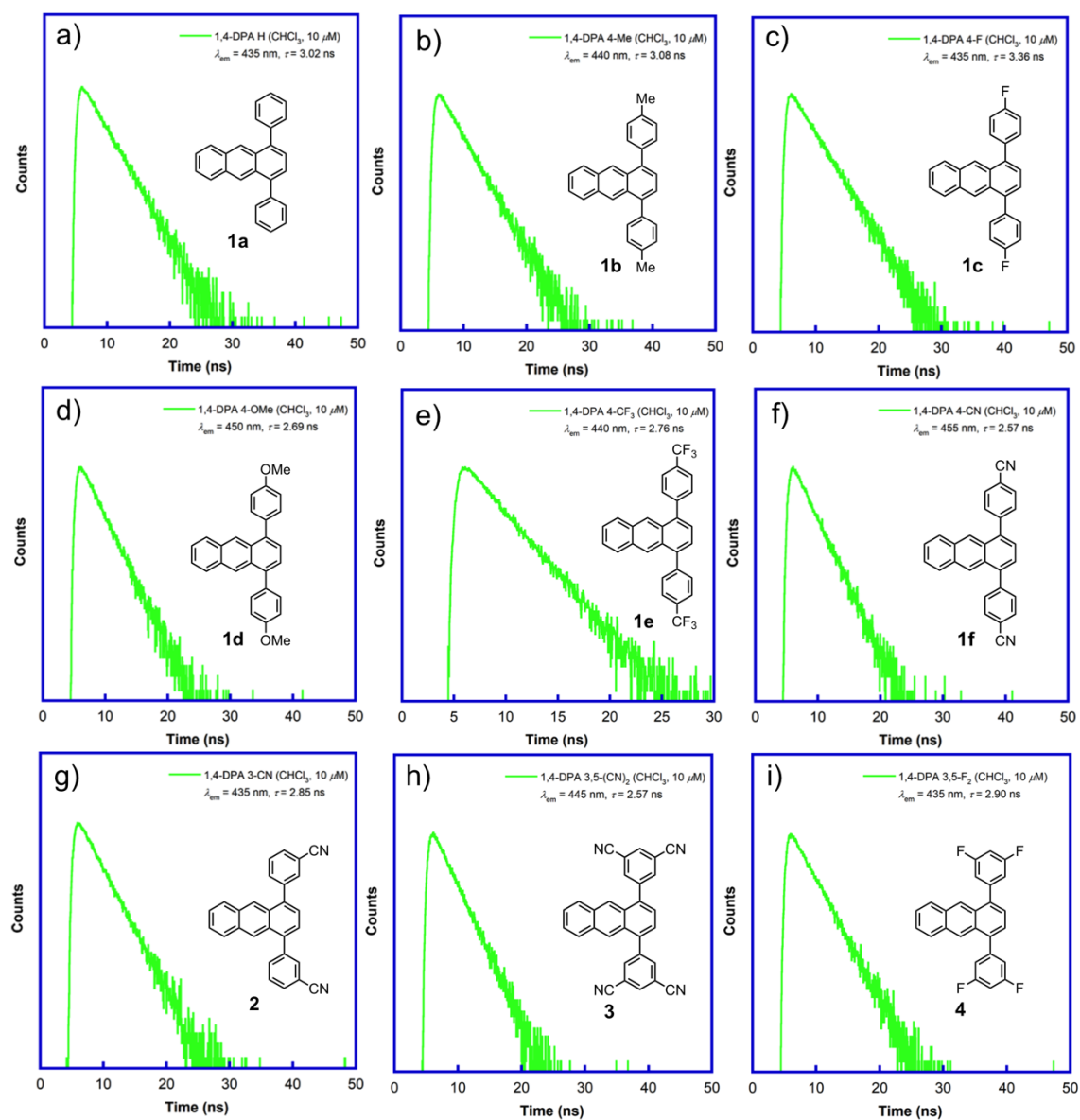


Figure S21. Fluorescence lifetime decay profile of 1,4-diphenylanthracene derivatives in CHCl_3 (10 μM , $\lambda_{\text{ex}} = 365 \text{ nm}$) after Ar bubbling: a) **1a** (R=H), b) **1b** (R=Me), c) **1c** (R=F), d) **1d** (R=OMe), e) **1e** (R=CF₃), f) **1f** (R=CN), g) **2** (3-CN), h) **3** (3,5-CN₂, R'=CN), i) **4** (3,5-F₂, R'=F).

1.14 Fluorescence lifetime decay profiles of 1,4-diphenylanthracene derivatives in PMMA film

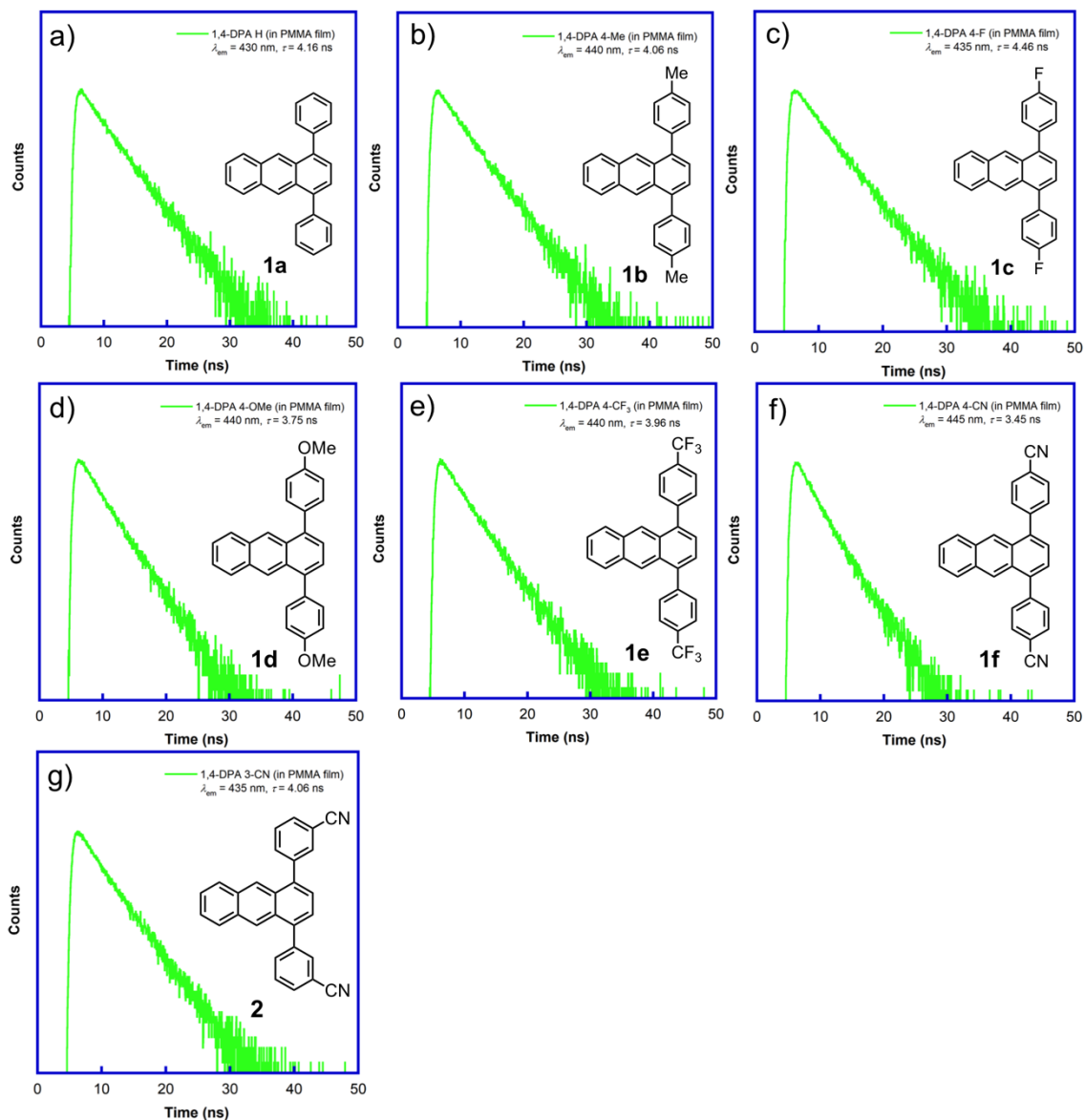


Figure S22. Fluorescence lifetime decay profiles of 1,4-diphenylanthracene derivatives in PMMA film (1 wt%, $\lambda_{\text{ex}} = 365$ nm): a) **1a** (R=H), b) **1b** (R=Me), c) **1c** (R=F), d) **1d** (R=OMe), e) **1e** (R=CF₃), f) **1f** (R=CN), g) **2** (3-CN).

1.15 Photophysical properties of 1,4-diphenylanthracene derivatives

Table S1. Photophysical properties of 1,4-diphenylanthracene derivatives

compds.	ϕ_f^a		τ^b / ns		k_f / ns ⁻¹		k_{nr} / ns ⁻¹	
	soln. ^c	pristine (ground)	soln. ^c	pristine (ground)	soln.	pristine (ground)	soln.	pristine (ground)
1a (R=H)	0.47	0.20 (0.23)	3.02	2.27 (6.48)	0.156	0.088 (0.035)	0.175	0.352 (0.119)
1b (R=Me)	0.49	0.31 (0.21)	3.08	3.96 (13.4)	0.159	0.078 (0.016)	0.166	0.174 (0.059)
1c (R=F)	0.49	0.24 (0.25)	3.36	3.05 (13.7)	0.146	0.079 (0.018)	0.152	0.249 (0.055)
1d (R=OMe)	0.40	0.15 (0.18)	2.69	12.4 (10.4)	0.149	0.012 (0.017)	0.223	0.069 (0.079)
1e (R=CF ₃)	0.51	0.37 (0.33)	2.76	4.69 (7.63)	0.185	0.079 (0.043)	0.178	0.134 (0.088)
1f (R=CN)	0.55	0.26 (0.33)	2.57	32.8 (18.4)	0.214	0.008 (0.018)	0.175	0.023 (0.036)
2 (3-CN)	0.46	0.71 (0.37)	2.85	109 (91.5)	0.161	0.007 (0.004)	0.189	0.003 (0.007)
3 (3,5-CN ₂)	0.41	0.15 (0.05)	2.57	7.39 (4.09)	0.160	0.020 (0.012)	0.230	0.115 (0.232)
4 (3,5-F ₂)	0.50	0.44 (0.22)	2.90	5.22 (5.36)	0.172	0.084 (0.041)	0.172	0.107 (0.146)

^a Fluorescence quantum yield determined by a calibrated integrating sphere, ^b Averaged fluorescence lifetimes, ^c CHCl₃ solution (10 μ M) after Ar bubbling.

Table S2. Photophysical properties of 1,4-diphenylanthracene derivatives in PMMA film

PMMA films	$\lambda_{\max}/\text{nm}^a$ Luminous color ^b	ϕ_f^c	τ^d / ns	k_f^e / ns ⁻¹	k_{nr}^f / ns ⁻¹
1a (R=H)	437 B	0.64	4.16	0.154	0.087
1b (R=Me)	443 B	0.66	4.06	0.163	0.084
1c (R=F)	438 B	0.63	4.42	0.143	0.084
1d (R=OMe)	445 B	0.67	3.75	0.179	0.088
1e (R=CF ₃)	441 B	0.64	3.96	0.162	0.091
1f (R=CN)	448 LB	0.71	3.45	0.206	0.084
2 (3-CN)	436 B	0.62	4.06	0.153	0.094

^aSolid-state (1wt% in PMMA film) emission (λ_{ex} =365 nm), ^bLuminous color under 365 nm UV irradiation, B: blue, LB: light blue, ^cFluorescence quantum yield determined by a calibrated integrating sphere at λ_{ex} =365 nm, ^dAveraged fluorescence lifetime at λ_{ex} =365 nm, ^eRate constant for fluorescence, ^fRate constant for nonradiative decay.

2. X-ray analysis of 1,4-diphenylanthracene derivatives

2.1. Single crystal X-ray analysis

Table S3. Crystallographic data for **1a-1d**

Compounds	1a (R=H)	1b (R=Me)	1c (R=F)	1d (R=OMe)
Chemical formula	C ₂₆ H ₁₈	C ₂₈ H ₂₂	C ₂₆ H ₁₆ F ₂	C ₂₈ H ₂₂ O ₂
Temperature /K	293	100	100	100
Crystal system	orthorhombic	orthorhombic	triclinic	orthorhombic
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> -1	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> /Å	5.8982(11)	5.9154(2)	5.8772(2)	5.9797(3)
<i>b</i> /Å	14.477(4)	13.6349(3)	11.5283(6)	13.9553(7)
<i>c</i> /Å	20.400(4)	23.8451(6)	14.1198(7)	23.2841(10)
α /°			113.856(2)	
β /°			95.664(2)	
γ /°			90.875(2)	
<i>V</i> /Å ³	1741.9(7)	1923.25(9)	869.07(7)	1943.02(16)
<i>Z</i>	4	4	2	4
Radiation type	MoK α	MoK α	MoK α	MoK α
<i>D</i> _{calcd.} /Mgm ⁻³	1.260	1.238	1.400	1.335
Collected reflections	5485	19998	11351	23611
Unique reflections	3191	3916	3032	3959
<i>R</i> _{int}	0.0488	0.0485	0.0369	0.0794
<i>R</i> _I (<i>I</i> > 2σ(<i>I</i>))	0.0712	0.0395	0.0393	0.0476
<i>R</i> _I (all data)	0.1368	0.0425	0.0452	0.0585
<i>R</i> _w (all data)	0.2276	0.1045	0.1067	0.1186
Goodness-of fit	1.007	1.018	1.029	1.046

Table S4. Crystallographic data for **1f** and **2**

Compounds	1f (R=CN)	2 (3-CN)
Chemical formula	C ₂₈ H ₁₆ N ₂	C ₂₈ H ₁₆ N ₂
Temperature /K	100	293
Crystal system	triclinic	triclinic
Space group	<i>P</i> -1	<i>P</i> -1
<i>a</i> /Å	11.0734(2)	8.2867(7)
<i>b</i> /Å	12.9373(2)	10.2528(8)
<i>c</i> /Å	14.2271(2)	12.4967(11)
α /°	80.5840(10)	75.726(7)
β /°	86.7280(10)	78.035(7)
γ /°	75.6040(10)	82.179(7)
<i>V</i> /Å ³	1974.29(5)	1002.56(15)
<i>Z</i>	4	2
Radiation type	CuK α	MoK α
<i>D</i> _{calcd.} /Mgm ⁻³	1.298	1.260
Collected reflections	18220	6102
Unique reflections	6871	4100
<i>R</i> _{int}	0.0513	0.0254
<i>R</i> _{<i>I</i>} (<i>I</i> > 2σ(<i>I</i>))	0.0470	0.0579
<i>R</i> _{<i>I</i>} (all data)	0.0633	0.1105
<i>R</i> _{<i>w</i>} (all data)	0.1327	0.1691
Goodness-of fit	1.016	1.031

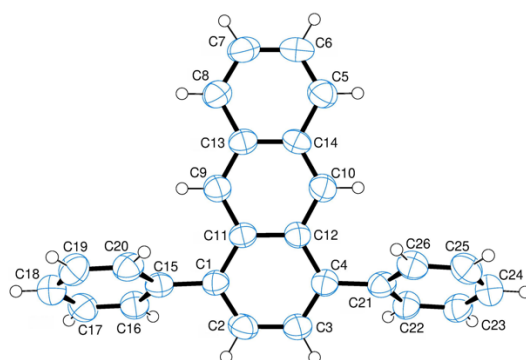


Figure S23. ORTEP drawing of **1a** (R=H).

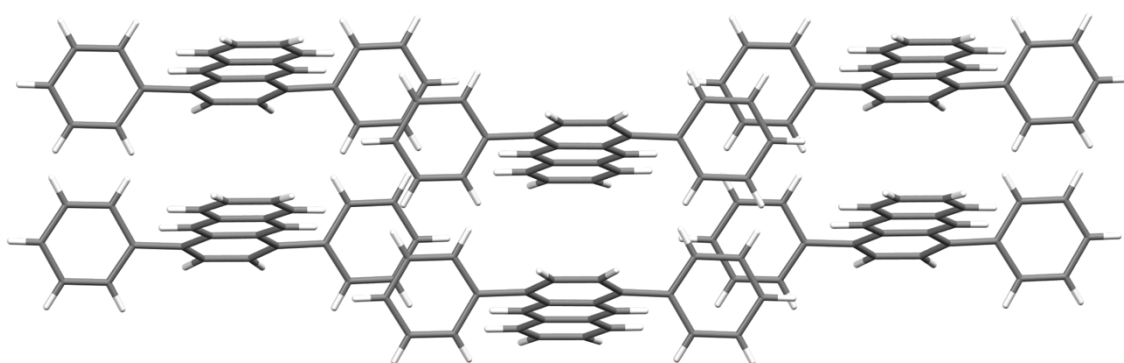


Figure S24. Crystal packing of **1a** (R=H).

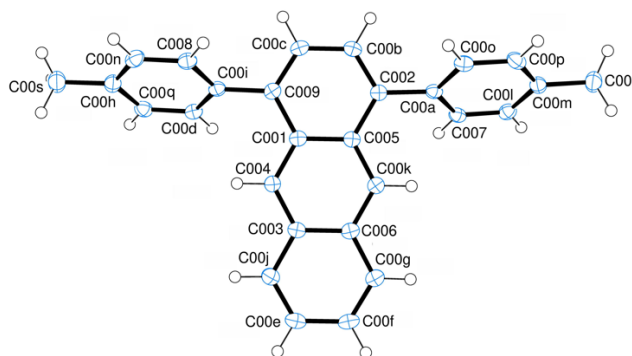


Figure S25. ORTEP drawing of **1b** (R=Me).

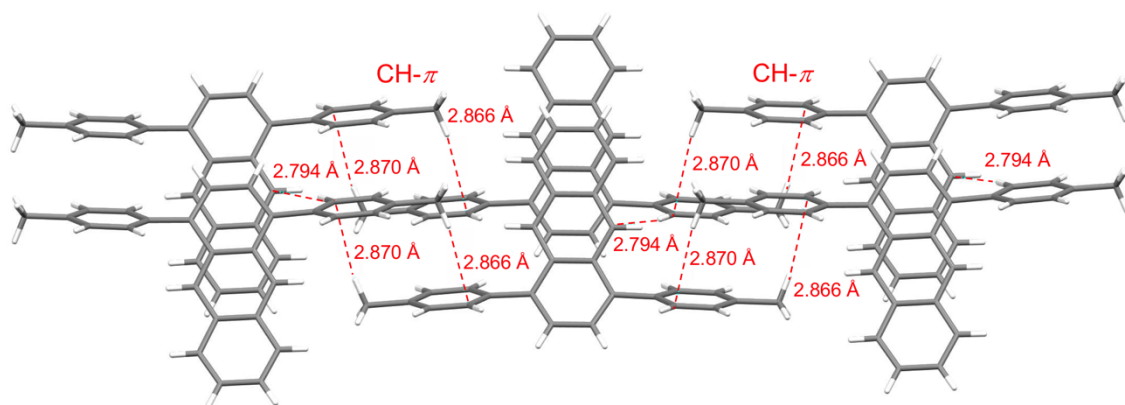


Figure S26. Crystal packing of **1b** (R=Me).

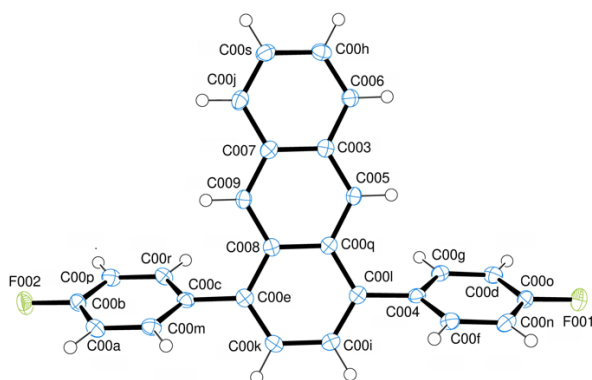


Figure S27. ORTEP drawing of **1c** (R=F).

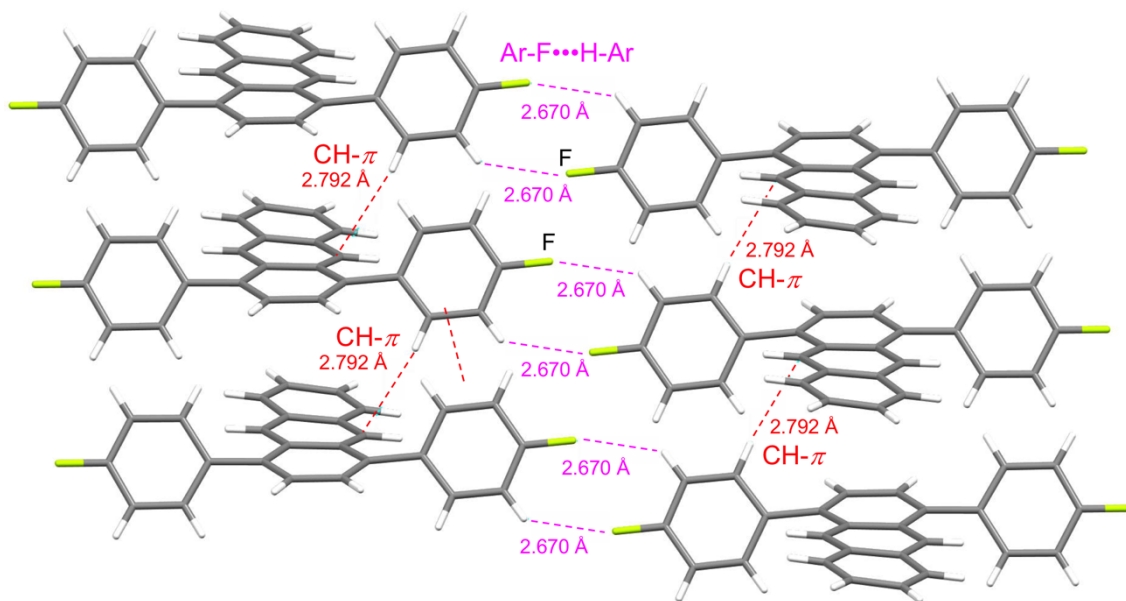


Figure S28. Crystal packing of **1c** (R=F).

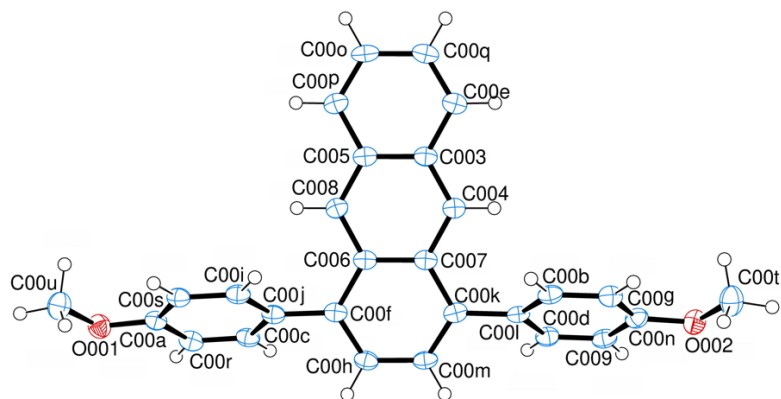


Figure S29. ORTEP drawing of **1d** (R=OMe).

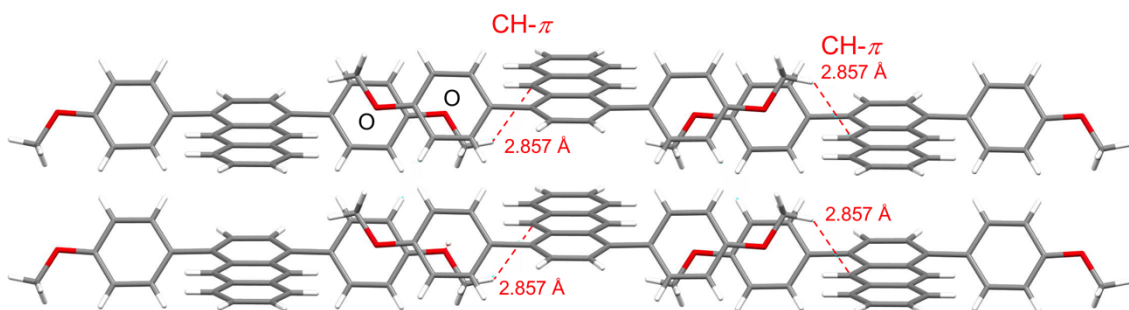


Figure S30. Crystal packing of **1d** (R=OMe).

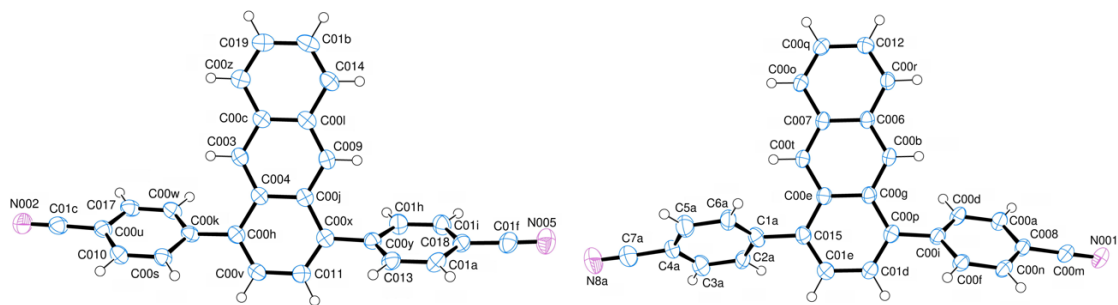


Figure S31. ORTEP drawing of **1f** (R=CN).

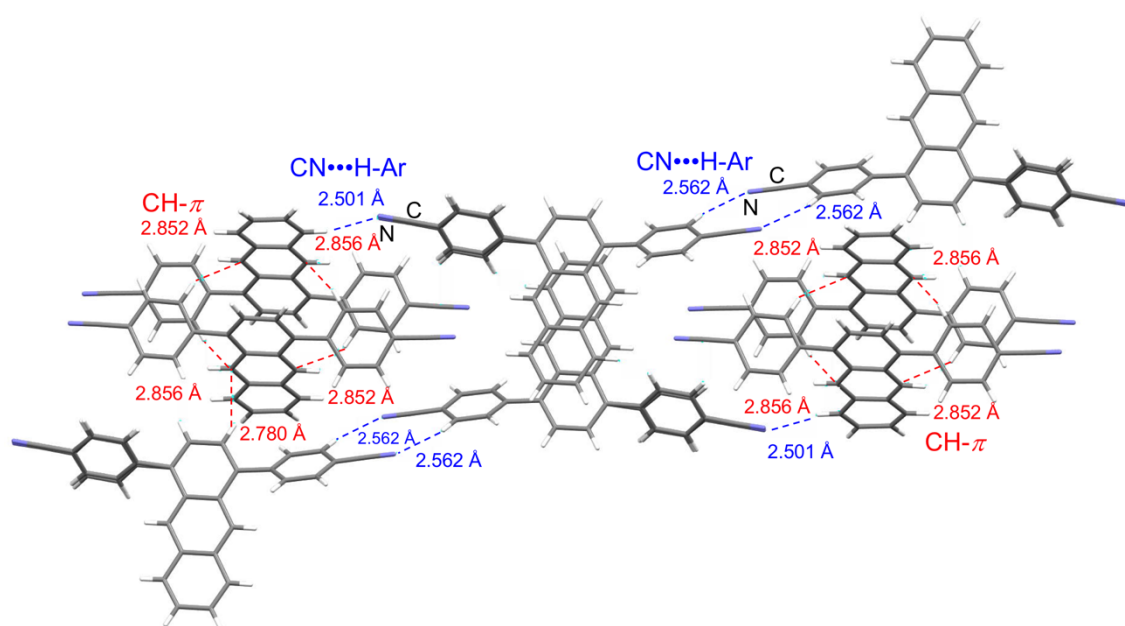


Figure S32. Crystal packing of **1f** (R=CN).

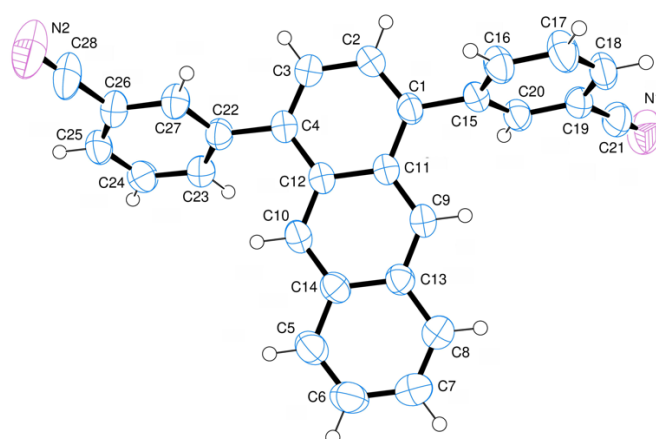


Figure S33. ORTEP drawing of **2** (3-CN).

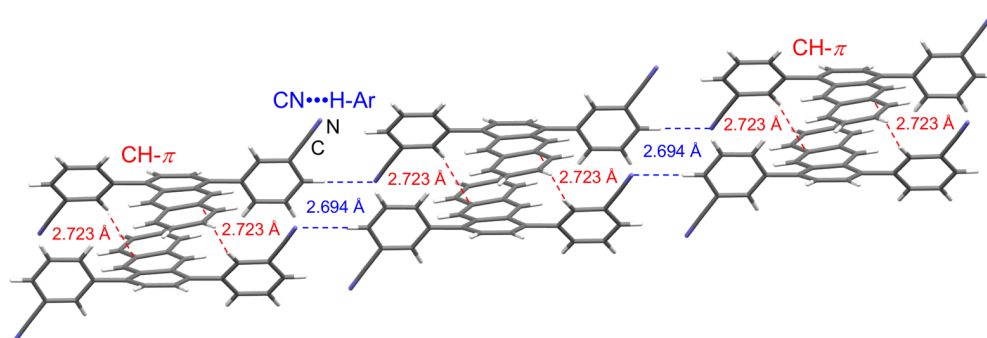


Figure S34. Crystal packing of **2** (3-CN).

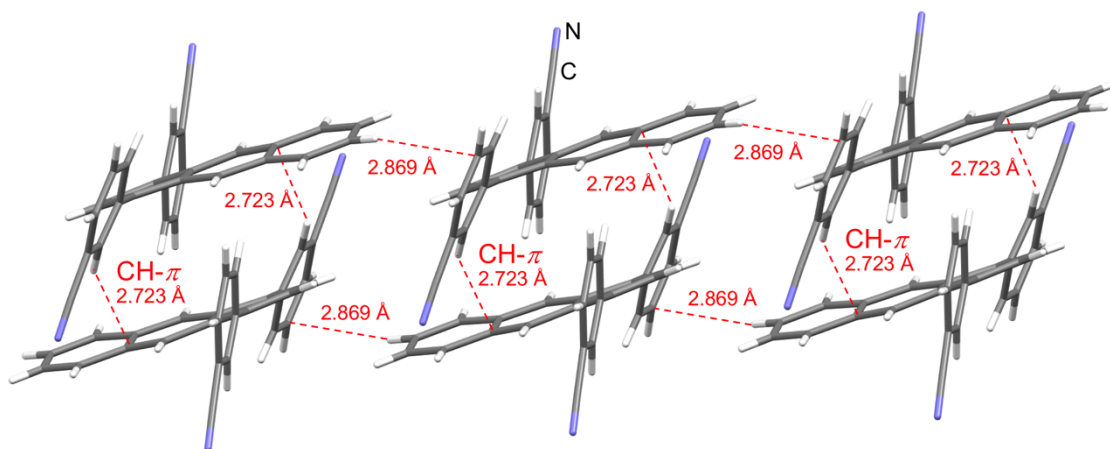


Figure S35. Crystal packing of **2** (3-CN).

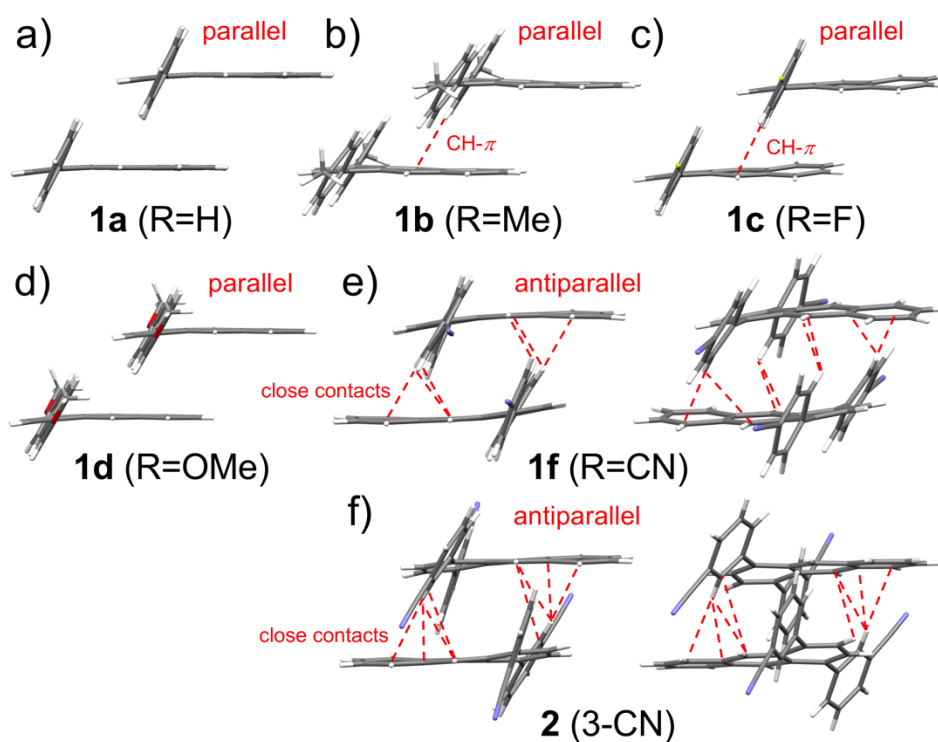


Figure S36. Crystal packing of 1,4-diphenylanthracene derivatives showing bimolecular interactions, a) **1a** (R=H), b) **1b** (R=Me), c) **1c** (R=F), d) **1d** (R=OMe), e) **1f** (R=CN), f) **2** (3-CN).

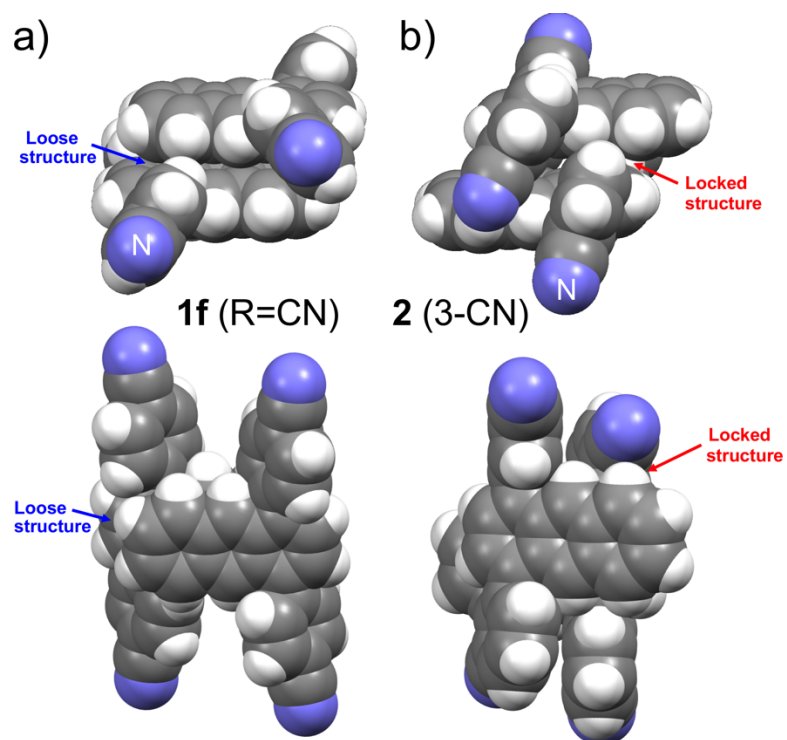


Figure S37. Crystal packing structure of 1,4-diphenylanthracene derivatives showing bimolecular interactions, a) **1f** (R=CN), b) **2** (3-CN).

2.2. Powder X-ray diffraction (PXRD) pattern of 1,4-diphenylanthracene derivatives

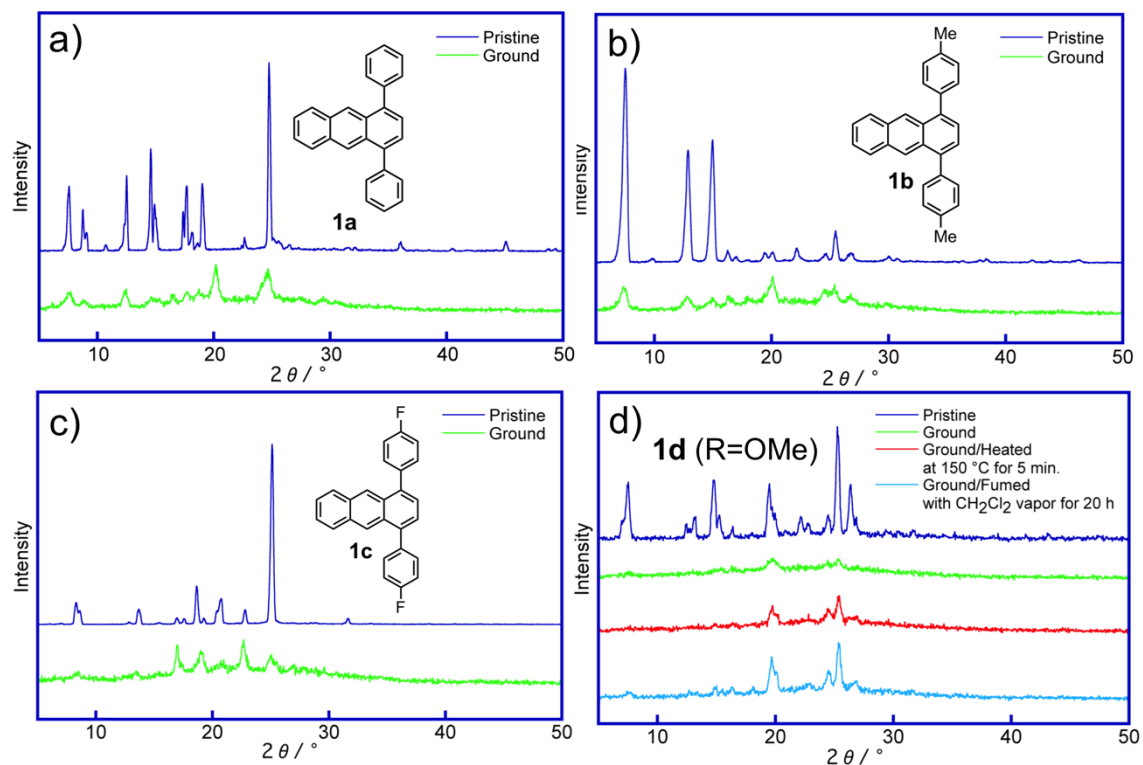


Figure S38. Powder X-ray diffraction (PXRD) patterns of 1,4-diphenylanthracene derivatives in pristine, ground, ground-fumed and ground-heated state, a) **1a** (R=H), b) **1b** (R=Me), c) **1c** (R=F), d) **1d** (R=OMe).

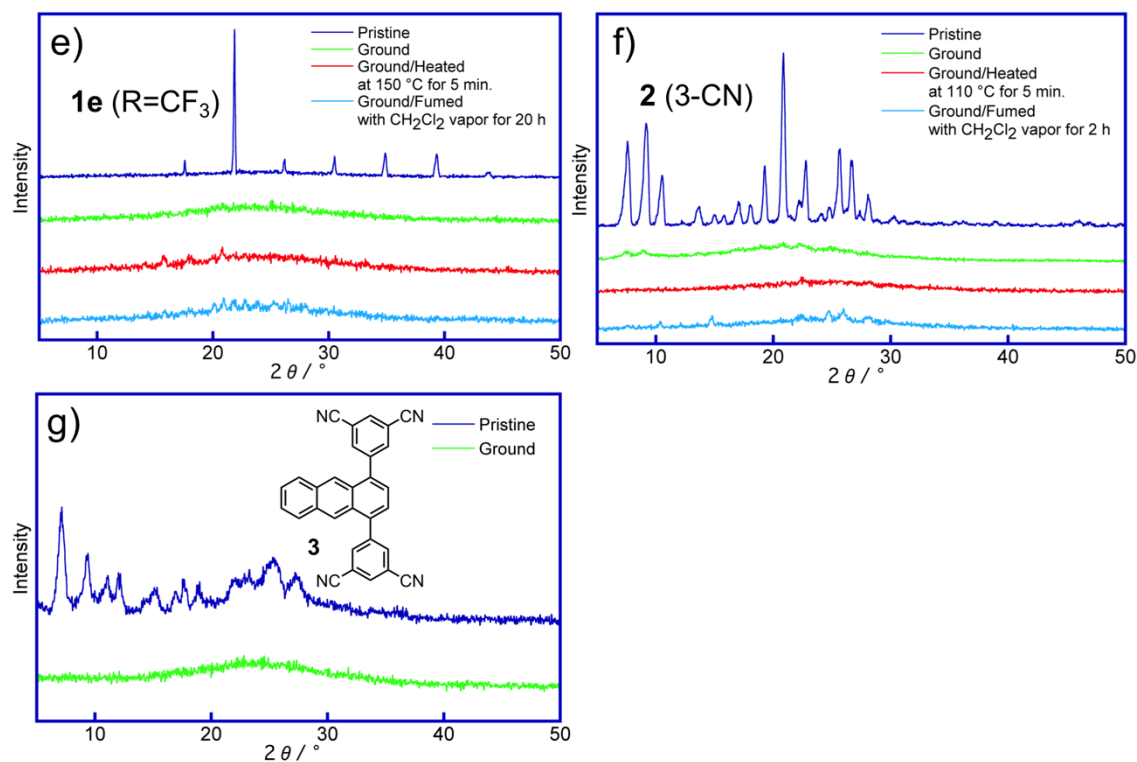


Figure S38 (contd.). Powder X-ray diffraction (PXRD) patterns of 1,4-diphenylanthracene derivatives in pristine, ground, ground-fumed and ground-heated state, e) **1e** (R= CF₃), f) **2** (3-CN), g) **3** (3,5-CN₂, R'=CN).

3. DFT calculation of the obtained crystal structures

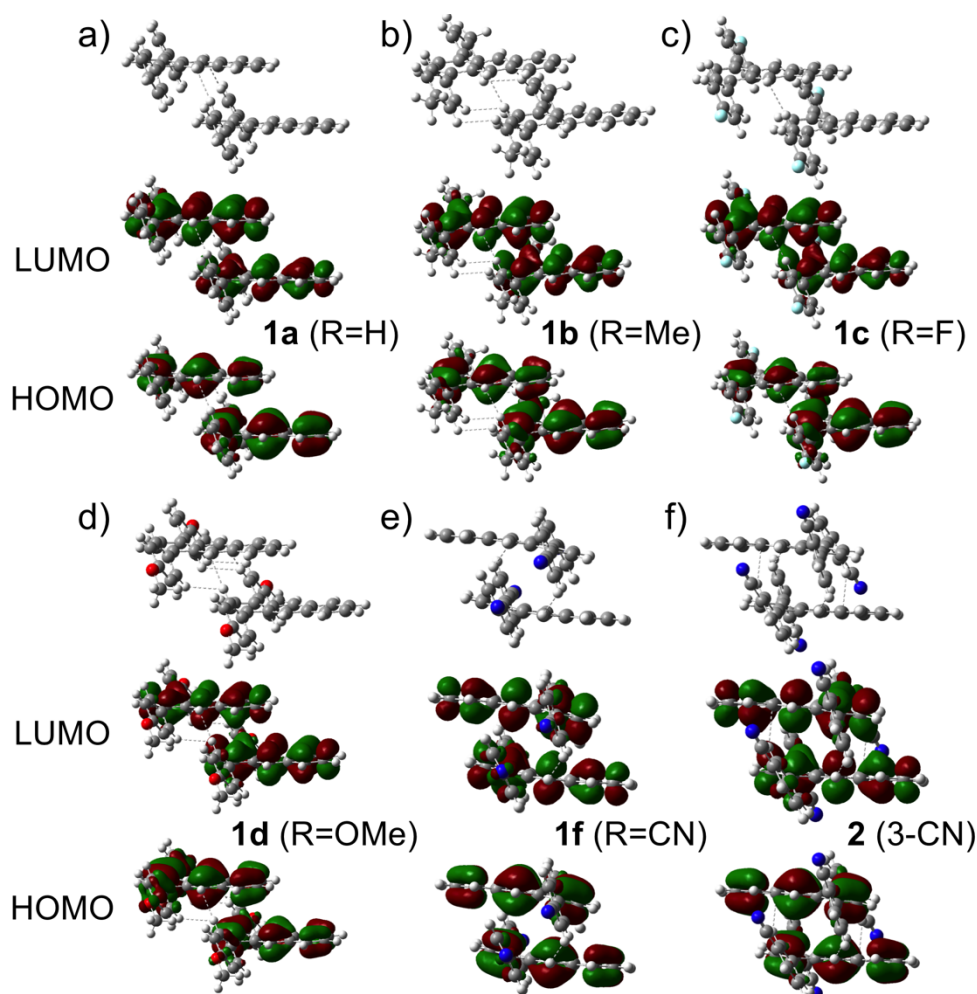


Figure S39. Electron cloud distribution of HOMO and LUMO from crystal structures (2 molecules) of 1,4-diphenylanthracene derivatives calculated by B3LYP-D3/6-31G*, a) **1a** (R=H), b) **1b** (R=Me), c) **1c** (R=F), d) **1d** (R=OMe), e) **1f** (R=CN), f) **2** (3-CN).

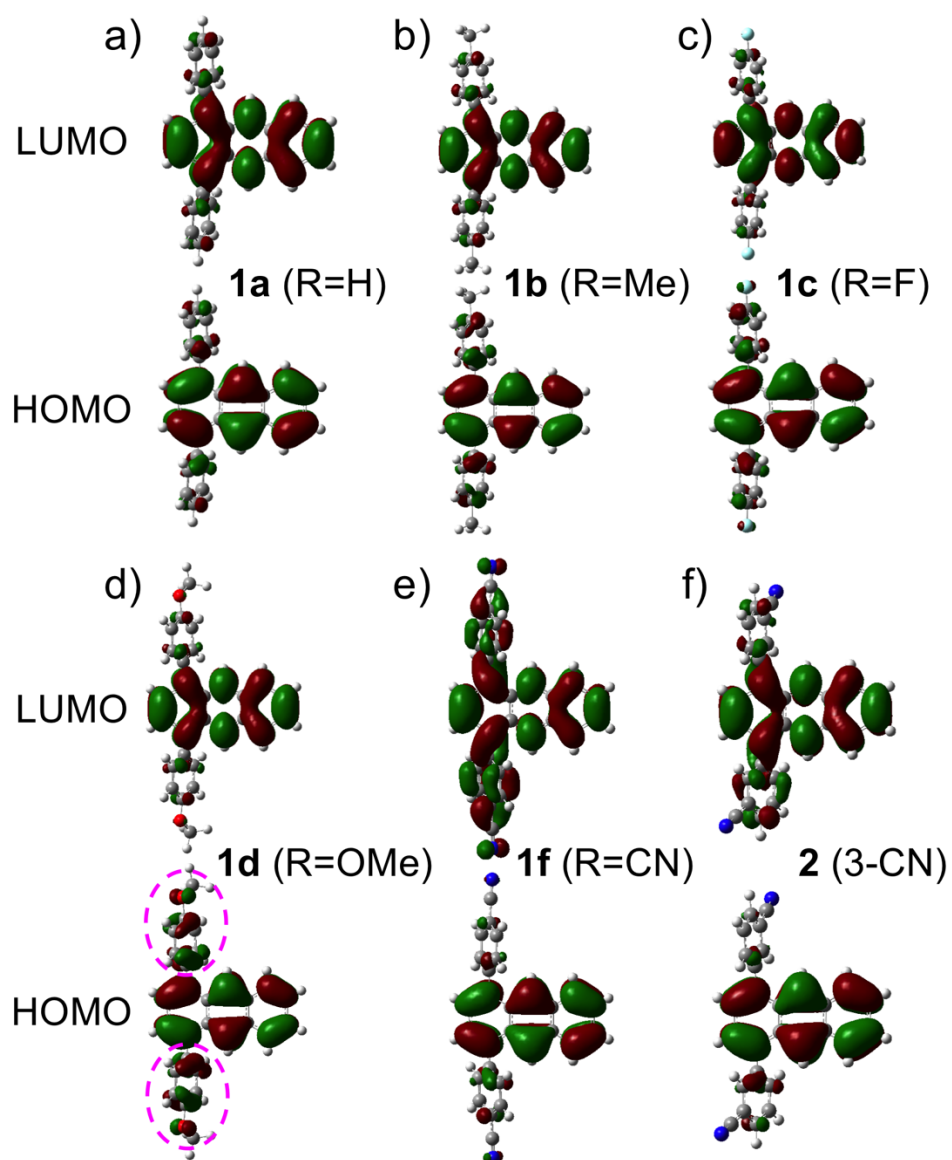


Figure S40. Electron cloud distribution of HOMO and LUMO from crystal structures (1 molecule) of 1,4-diphenylanthracene derivatives calculated by B3LYP-D3/6-31G*, a) **1a** (R=H), b) **1b** (R=Me), c) **1c** (R=F), d) **1d** (R=OMe), e) **1f** (R=CN), f) **2** (3-CN).

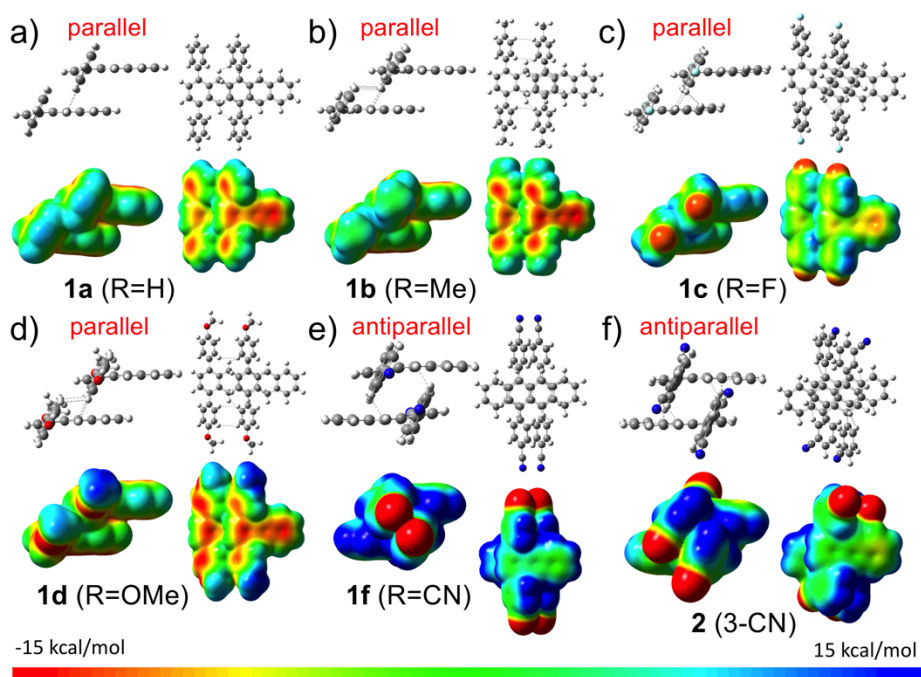


Figure S41. Electrostatic potential maps of 1,4-diphenylanthracene derivatives (bimolecular packing structures) calculated using B3LYP-D3/6-31G* from the obtained crystal data, a) **1a** (R=H), b) **1b** (R=Me), c) **1c** (R=F), d) **1d** (R=OMe), e) **1f** (R=CN), f) **2** (3-CN).

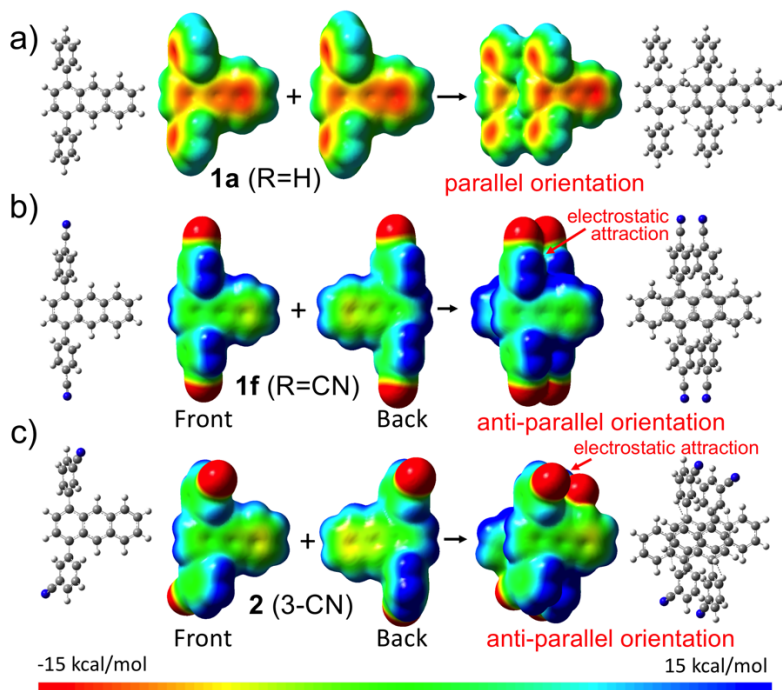


Figure S42. Schematic representation of the electrostatic potential maps for the bimolecular packing structure formation of 1,4-diphenylanthracene derivatives calculated using B3LYP-D3/6-31G* from the obtained crystal data, a) **1a** (R=H), b) **1f** (R=CN), c) **2** (3-CN).

4. UV irradiation experiments for 1,4-diphenylanthracene derivatives

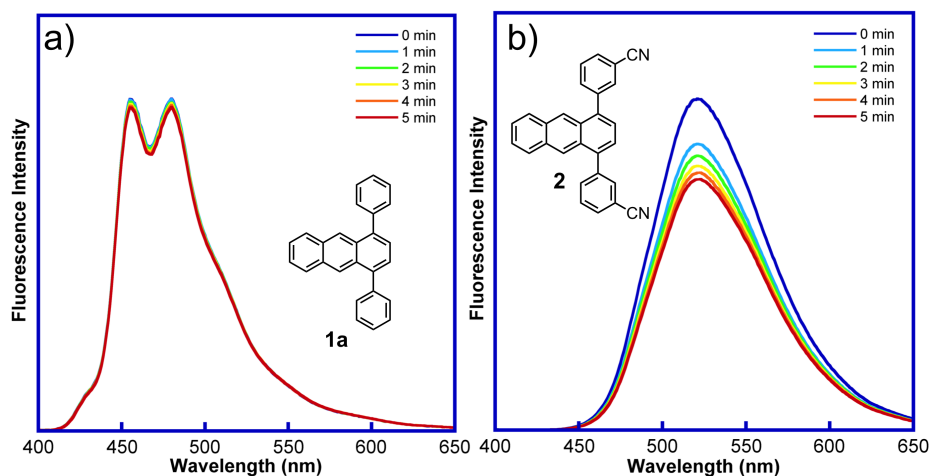


Figure S43. Fluorescence spectra of 1,4-diphenylanthracene derivatives after 365 nm UV irradiation in the solid state ($\lambda_{\text{ex}} = 365$ nm), a) **1a** (R=H), b) **2** (3-CN).

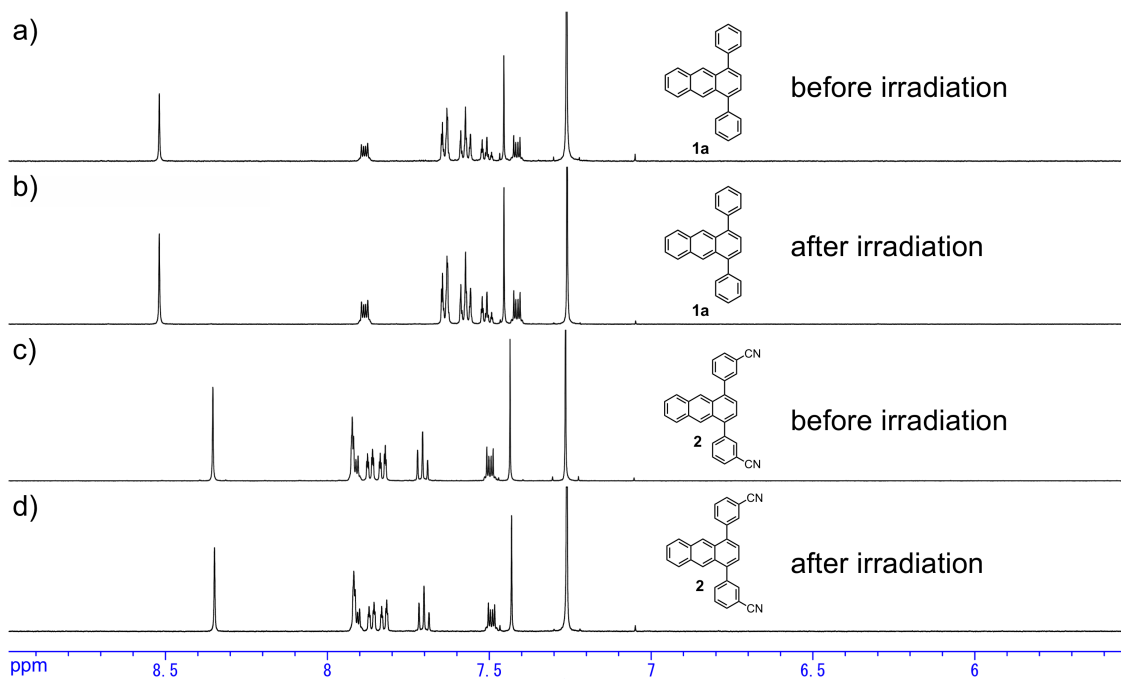
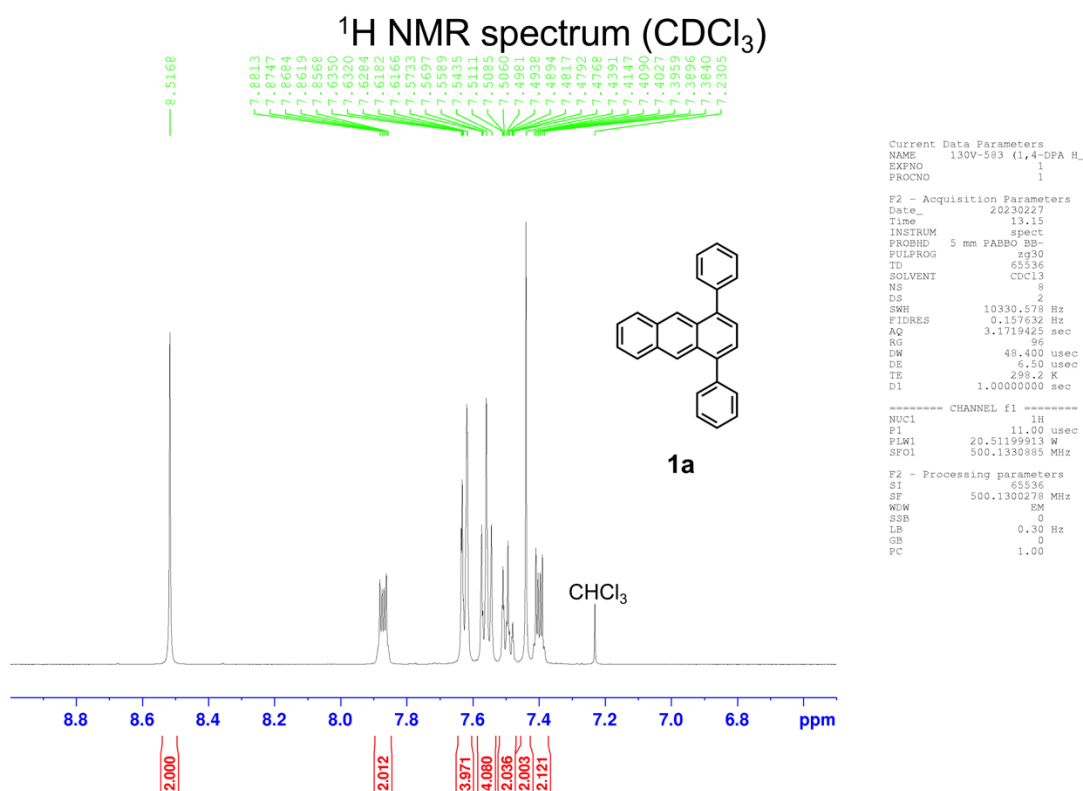
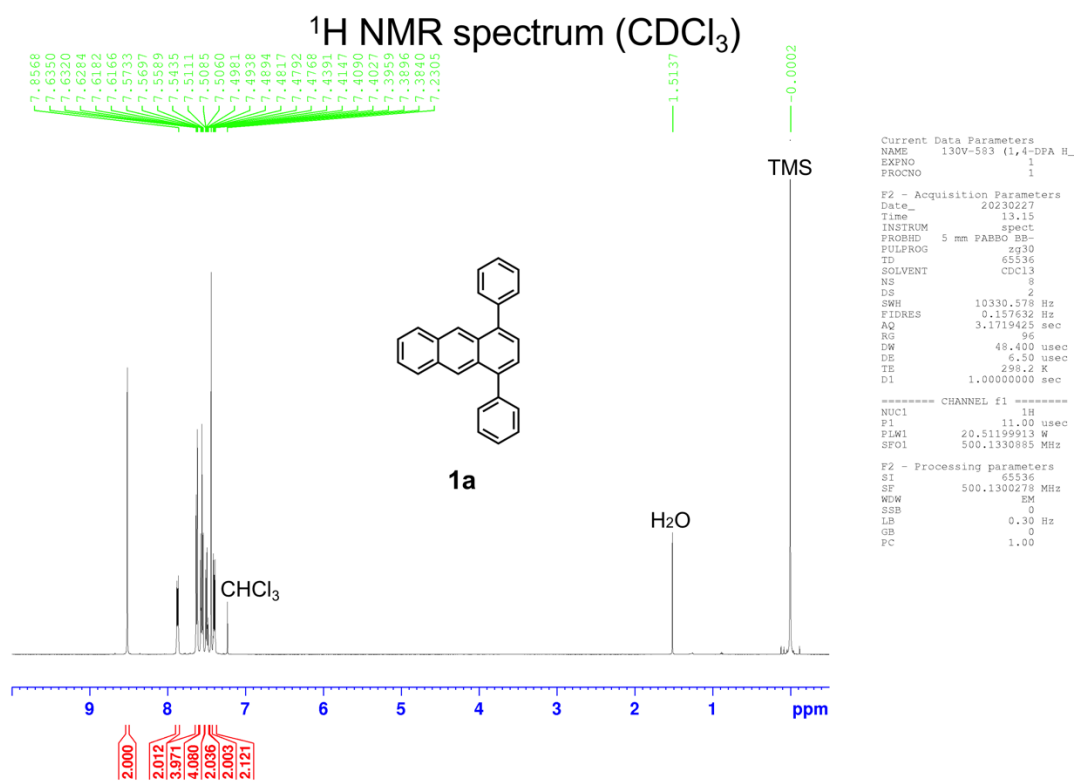
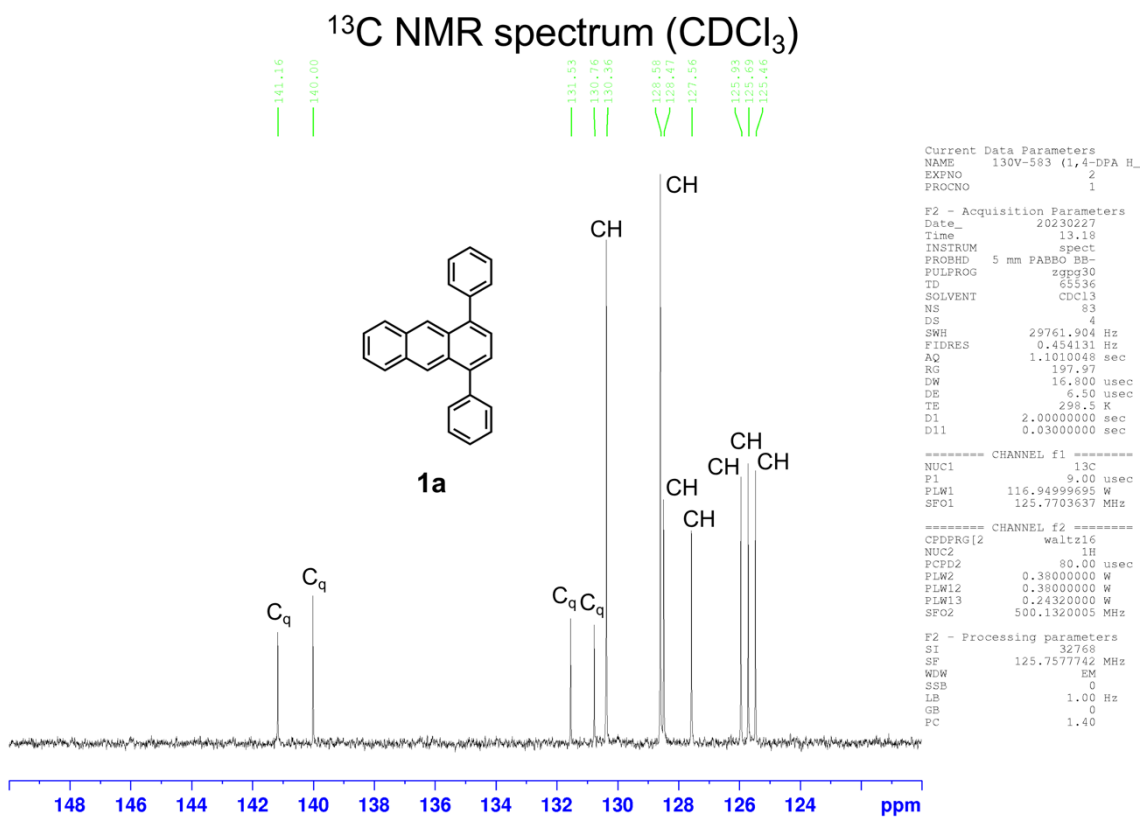
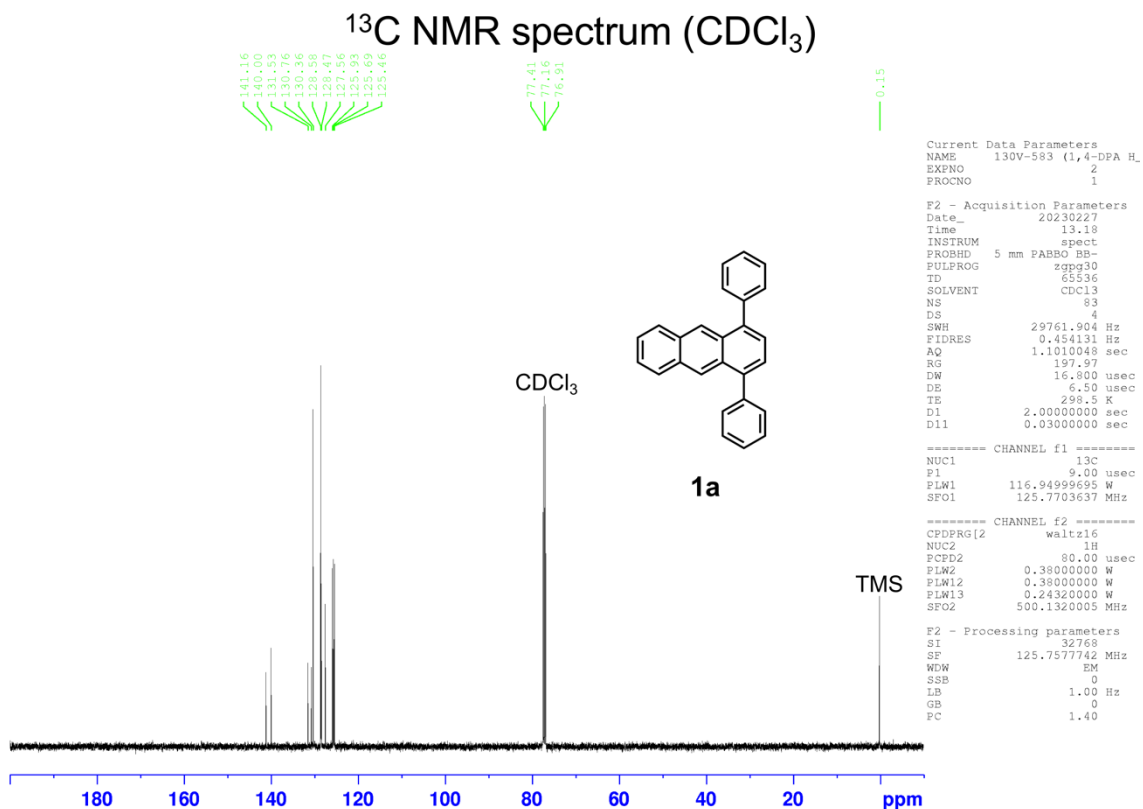


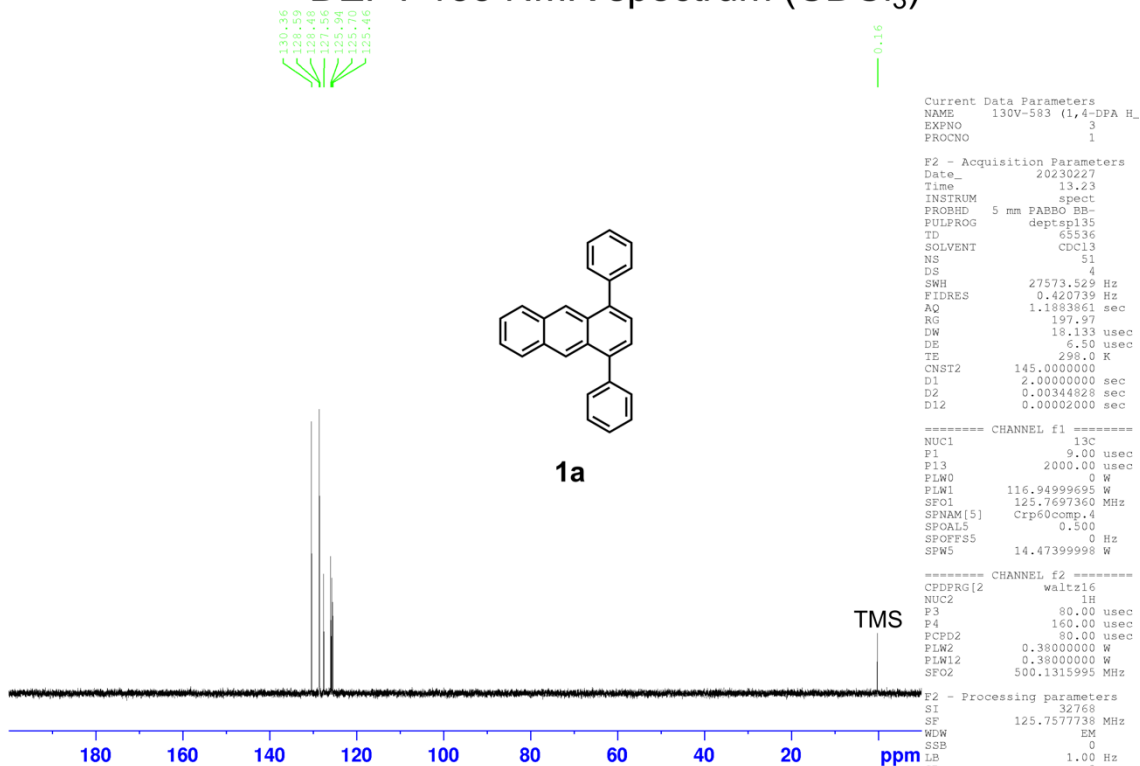
Figure S44. ^1H NMR spectra (CDCl_3) of 1,4-diphenylanthracene derivatives before and after 365 nm UV irradiation (5 min) in the solid state ($\lambda_{\text{ex}} = 365$ nm), a) **1a** (R=H, before irradiation), b) **1a** (R=H, after irradiation of 365 nm UV light, 5 min), c) **2** (3-CN, before irradiation), d) **2** (3-CN, after irradiation of 365 nm UV light, 5 min).

5. NMR spectra of new compounds

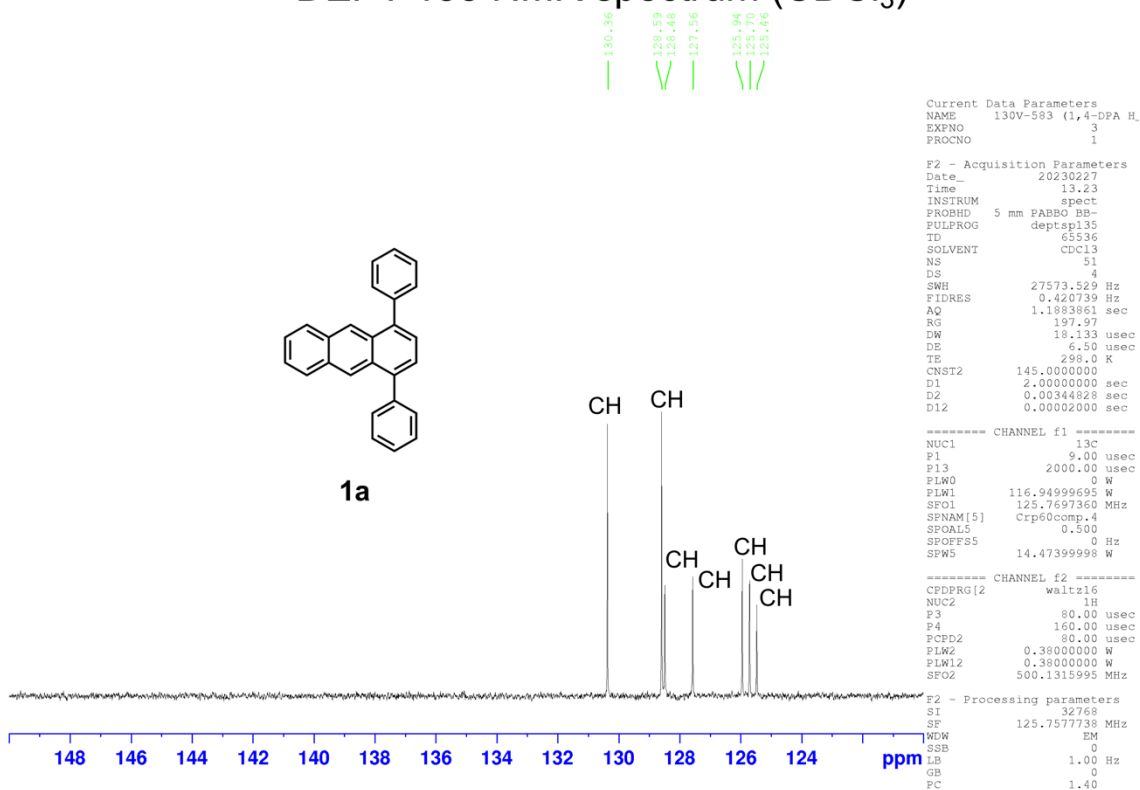


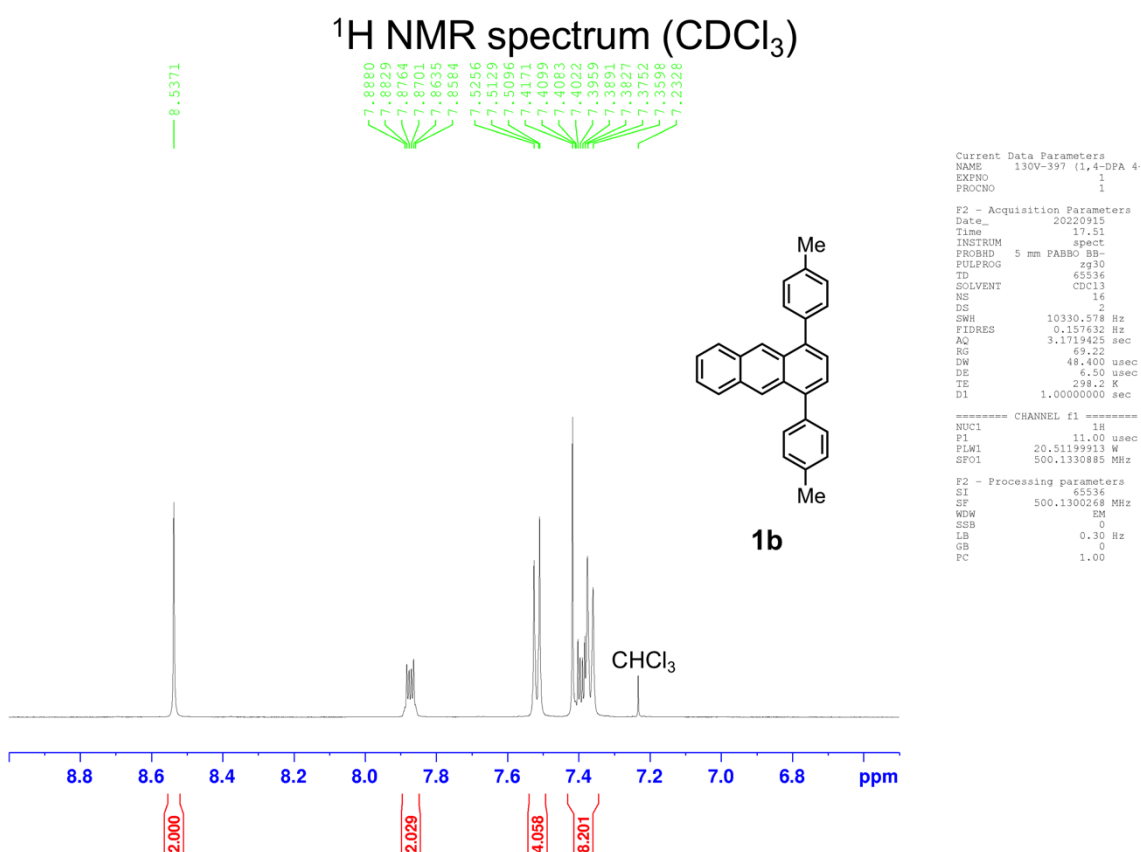
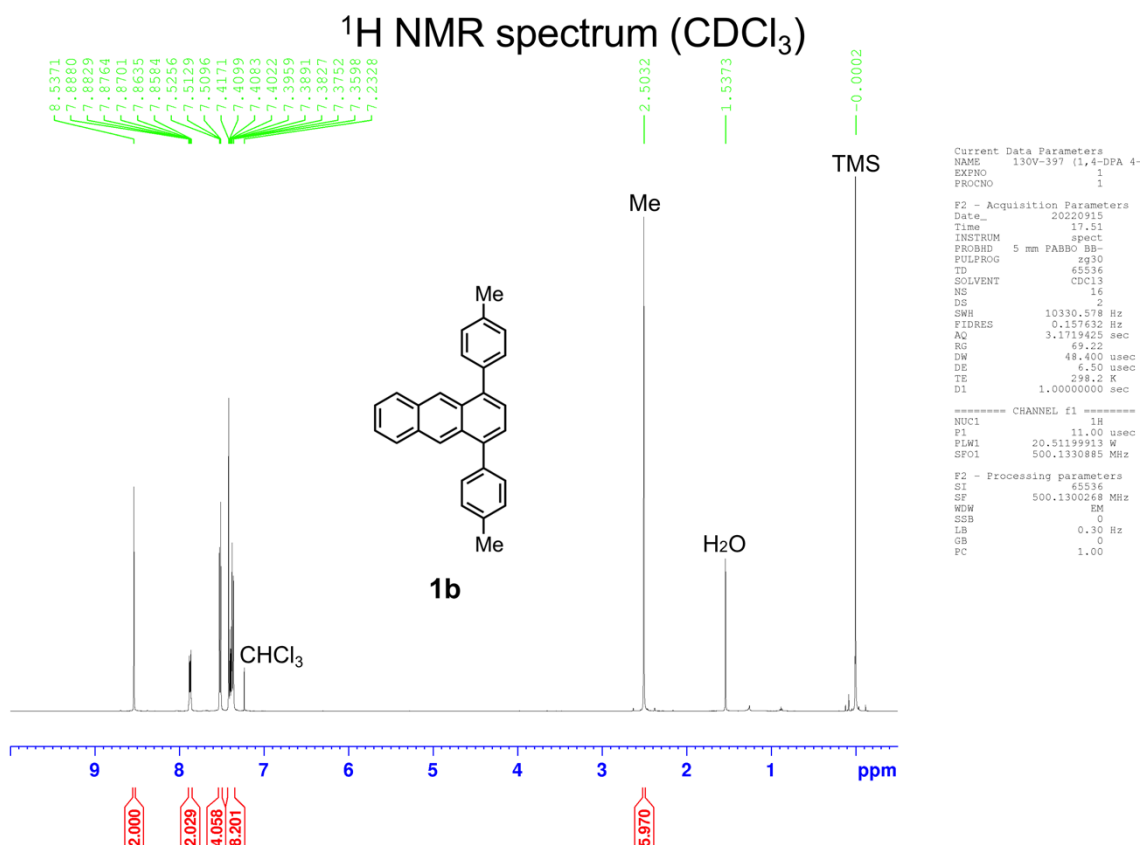


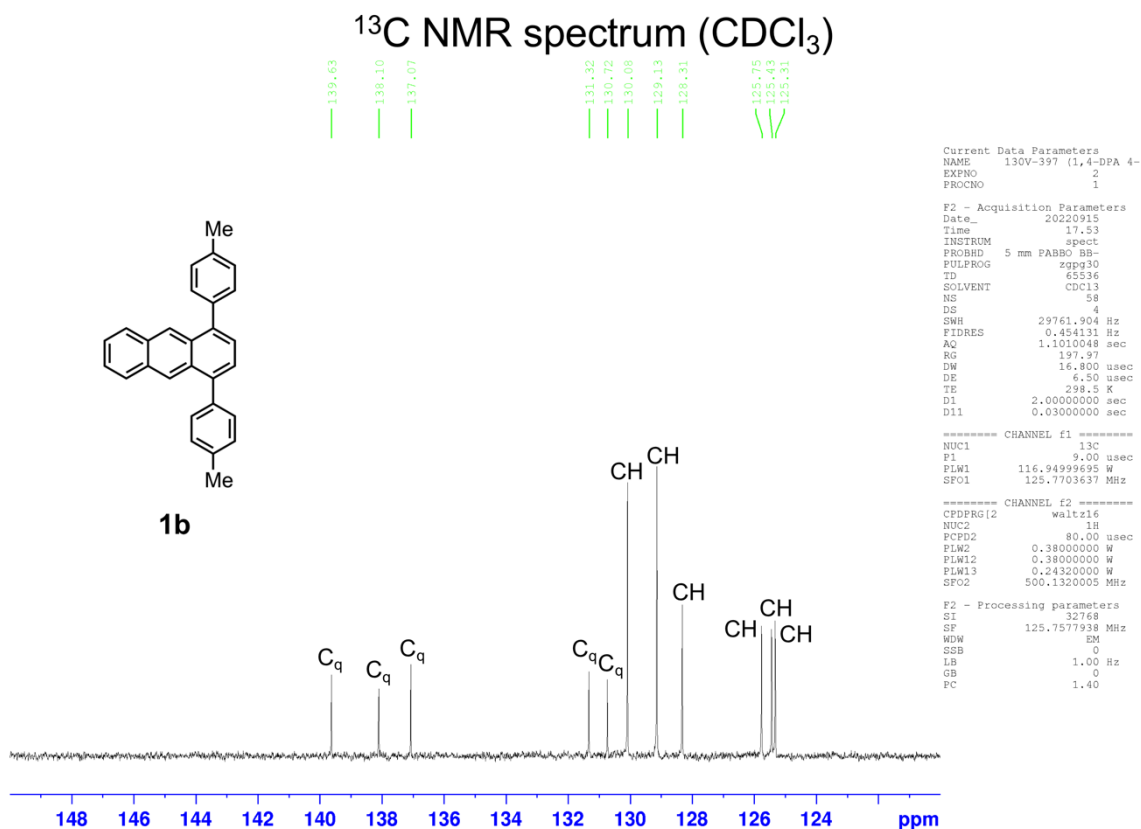
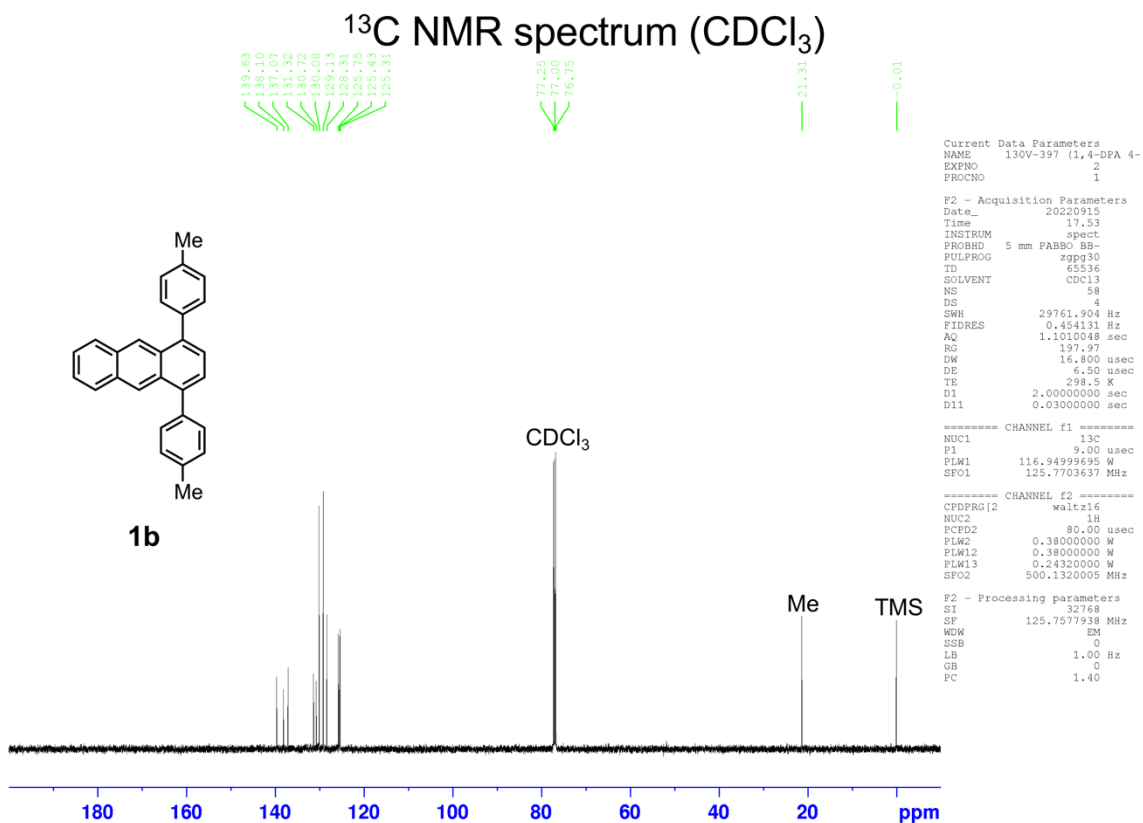
DEPT 135 NMR spectrum (CDCl₃)



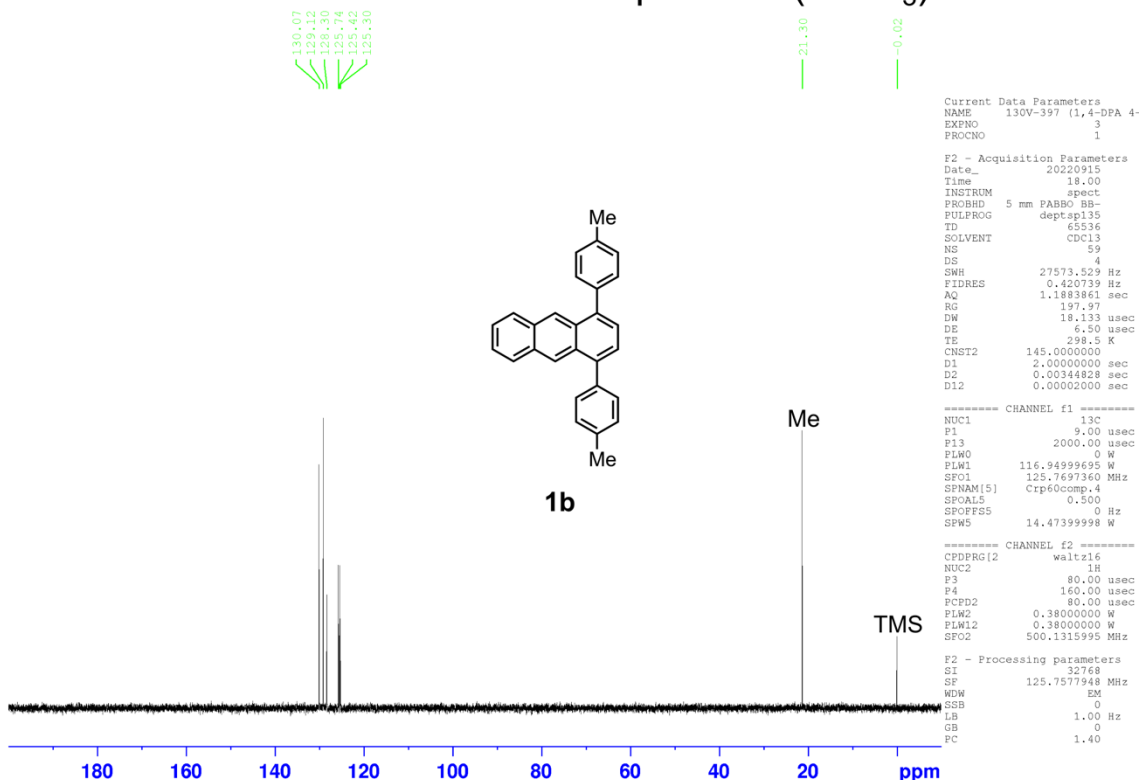
DEPT 135 NMR spectrum (CDCl₃)



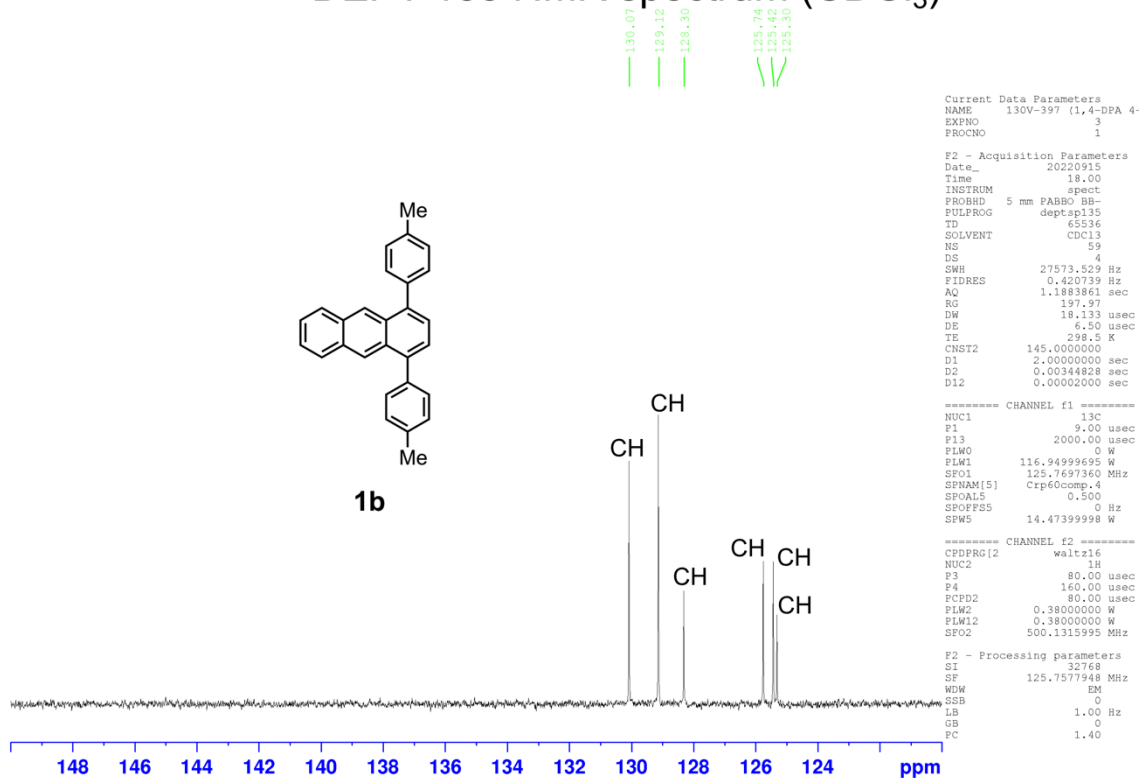


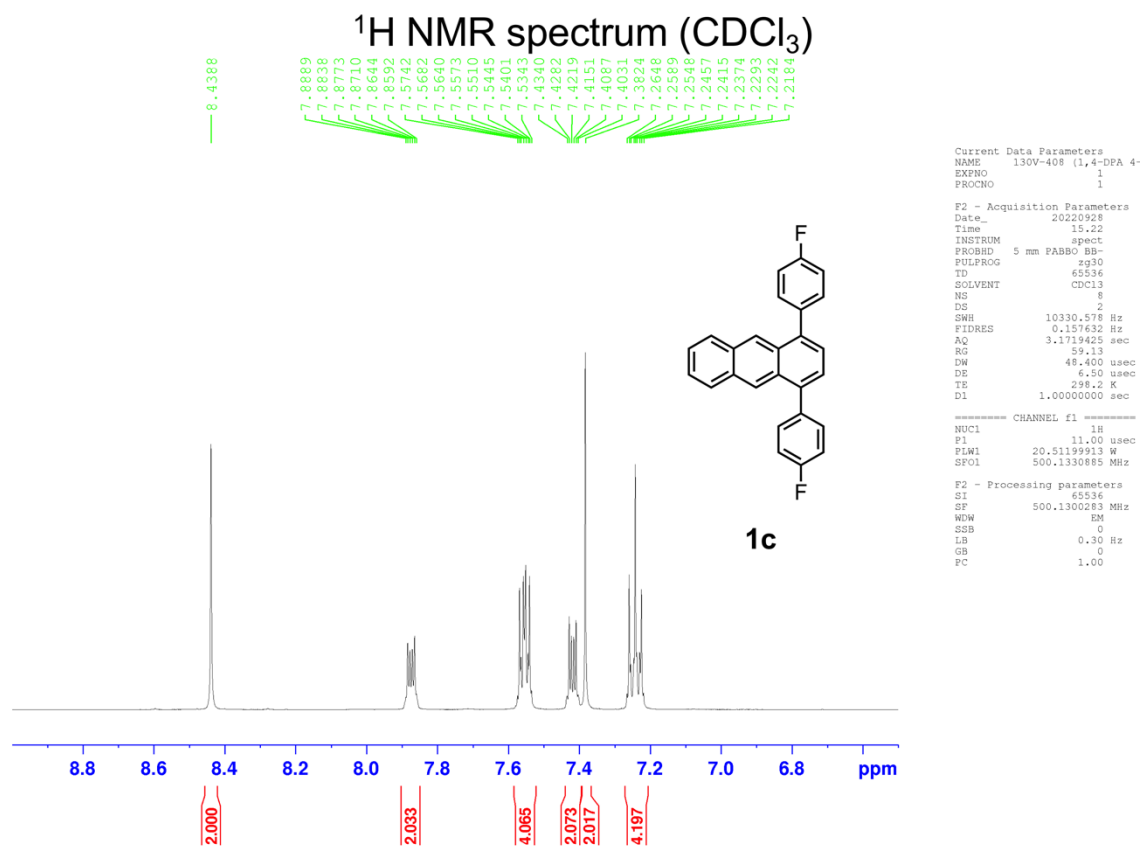
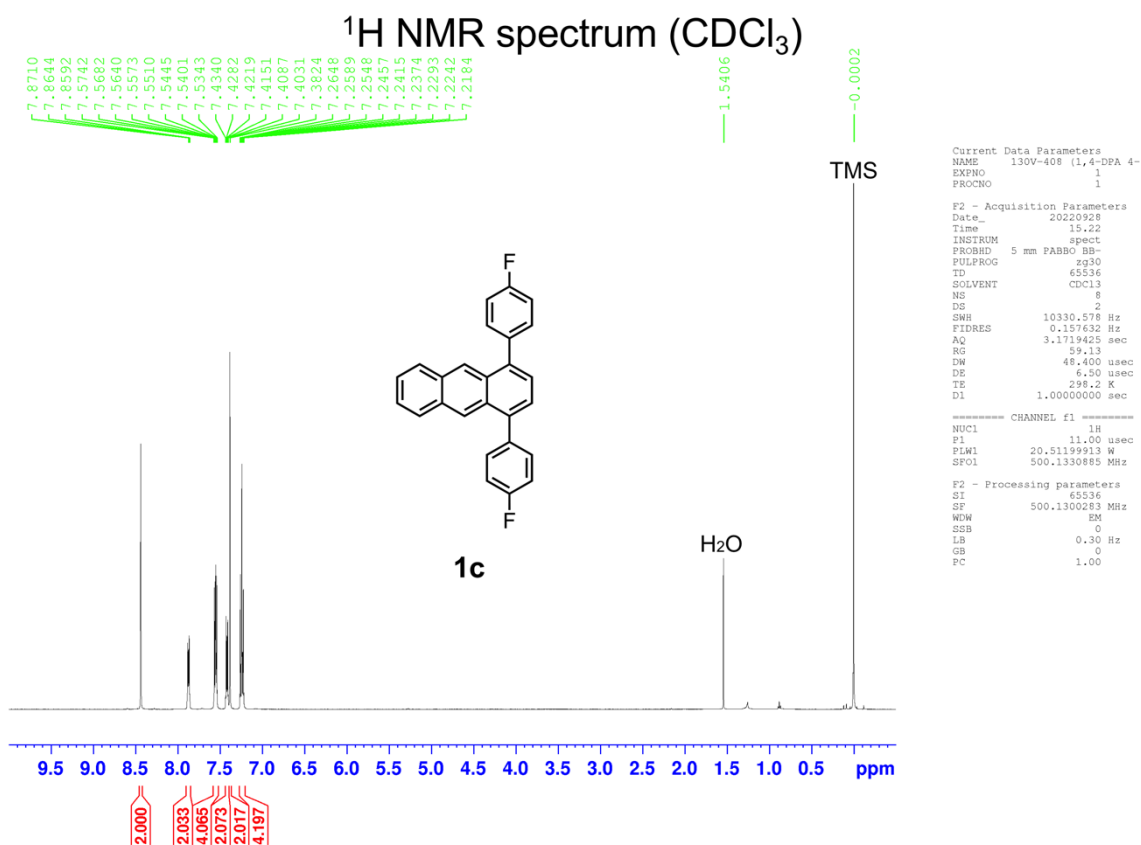


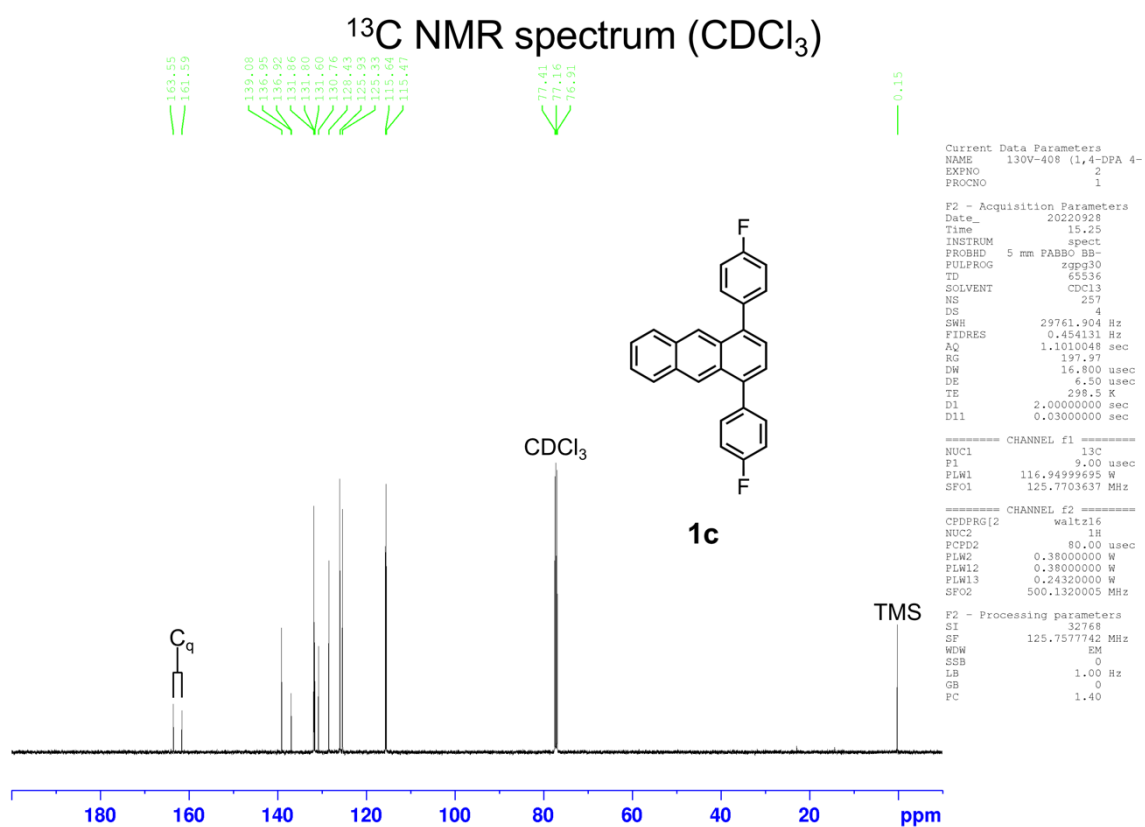
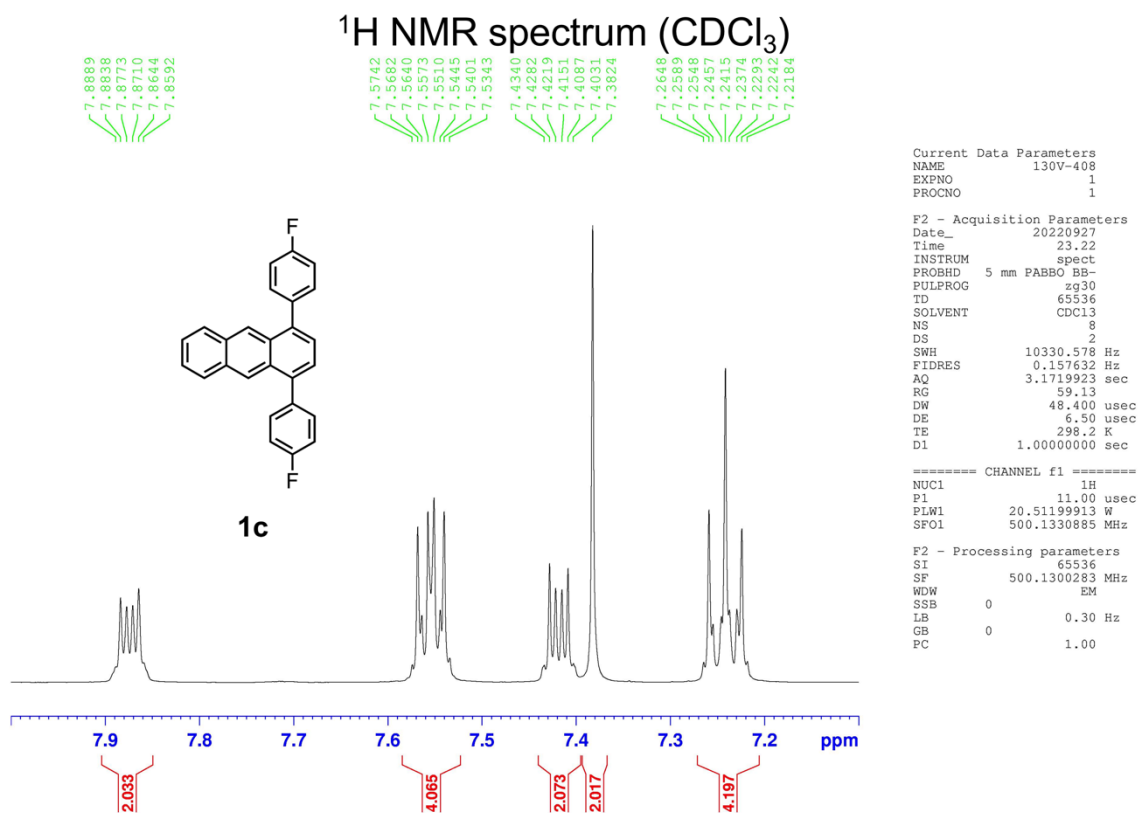
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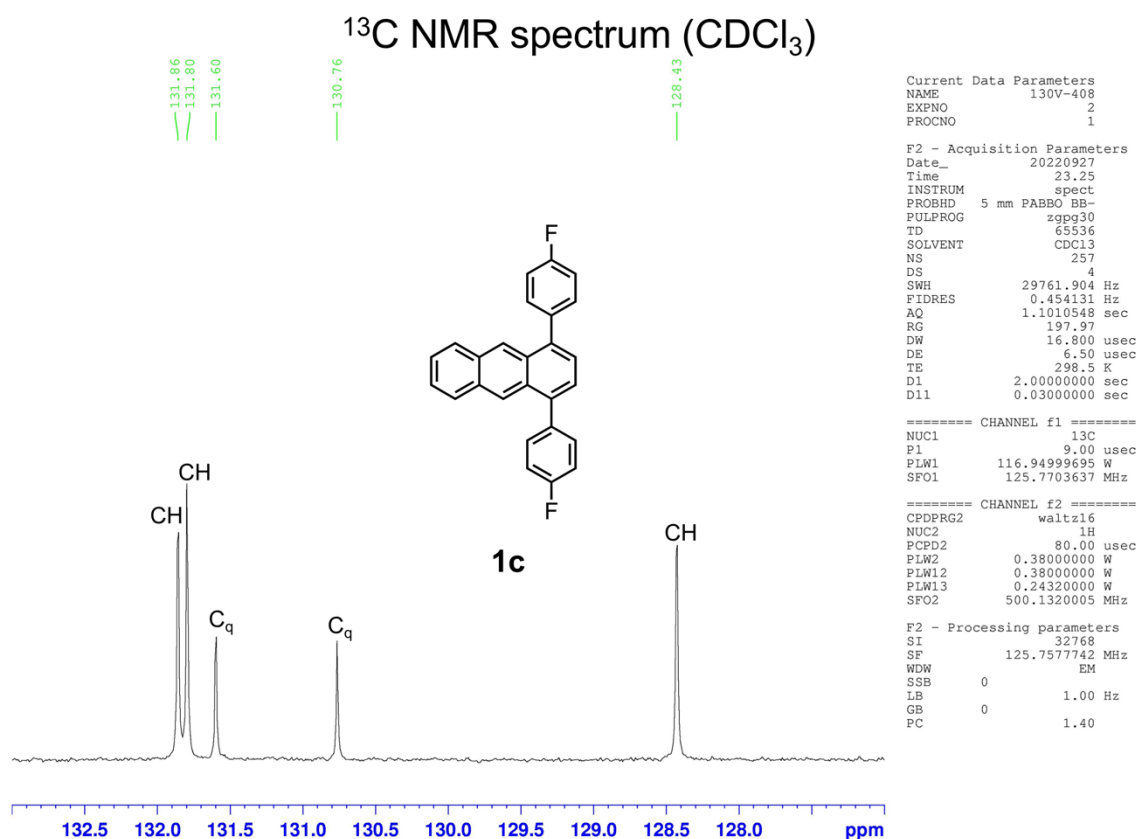
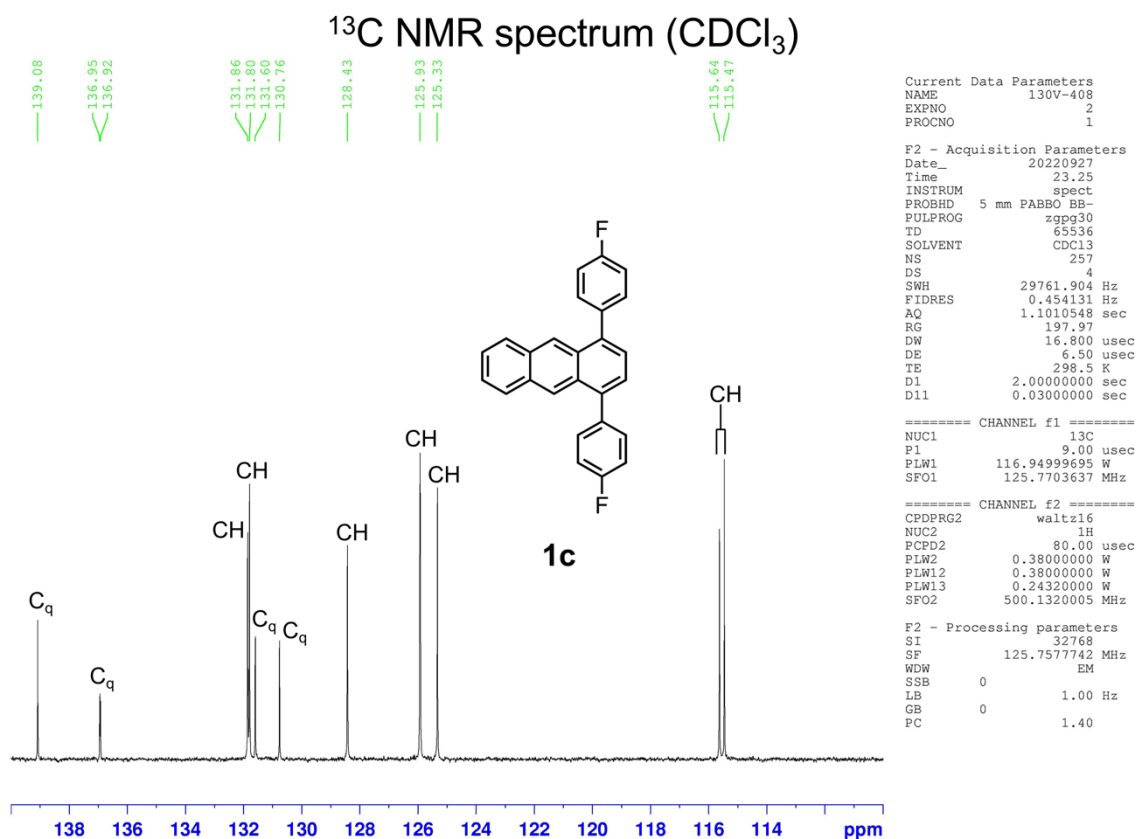


DEPT 135 NMR spectrum (CDCl₃)

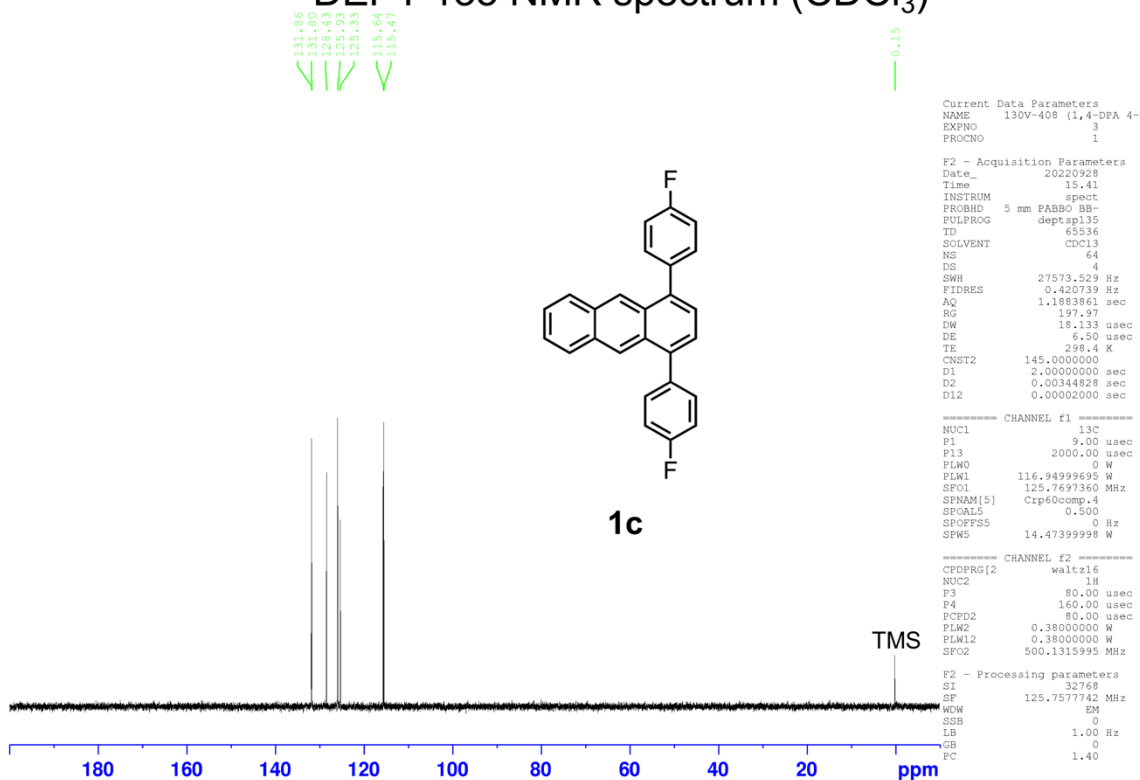




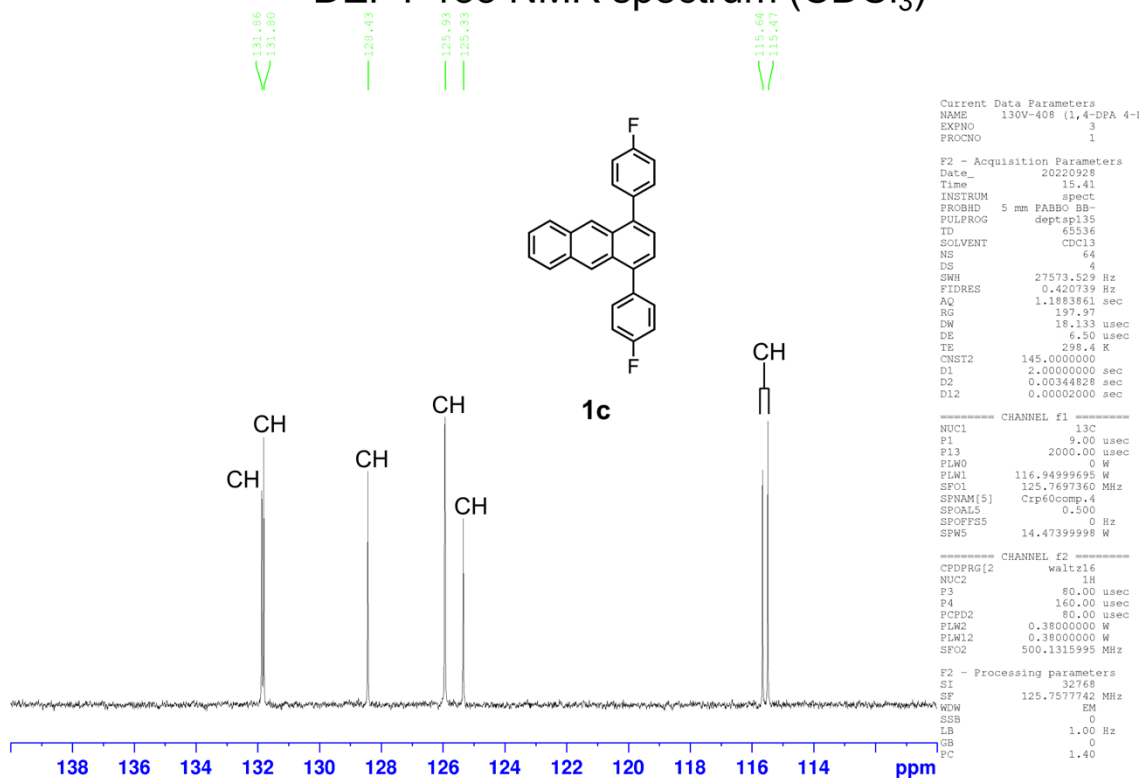




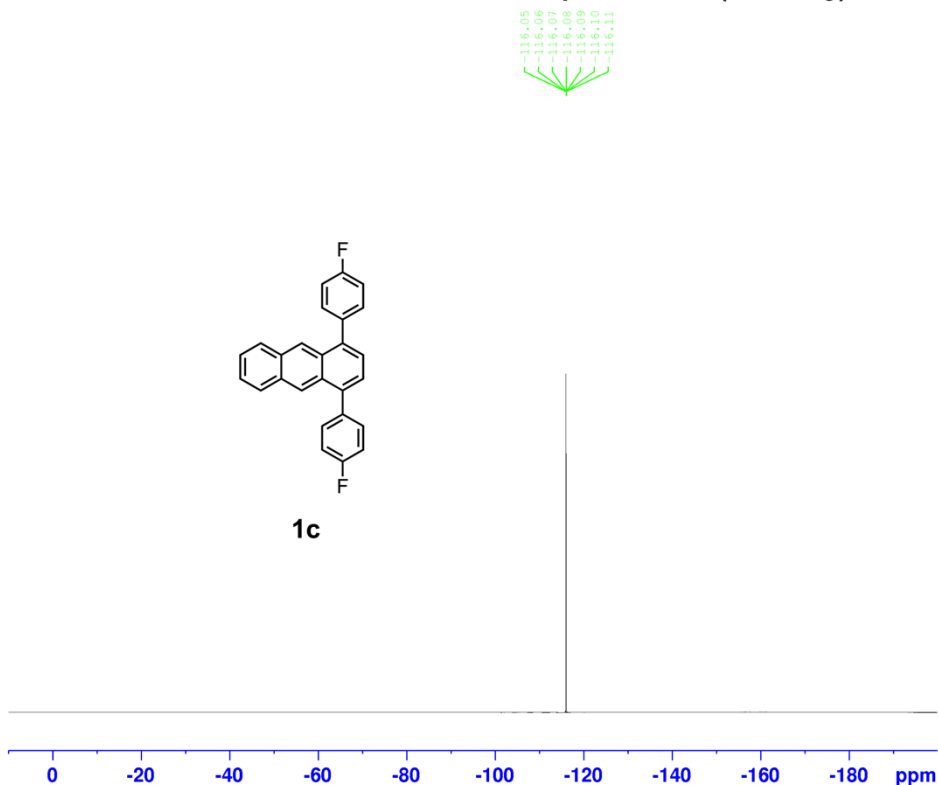
DEPT 135 NMR spectrum (CDCl₃)



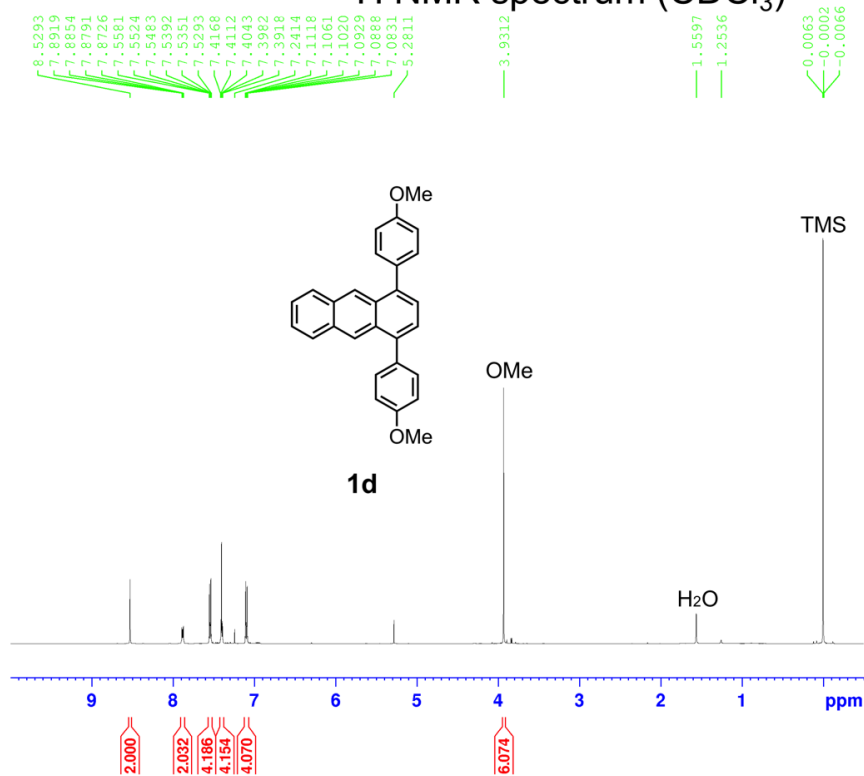
DEPT 135 NMR spectrum (CDCl₃)

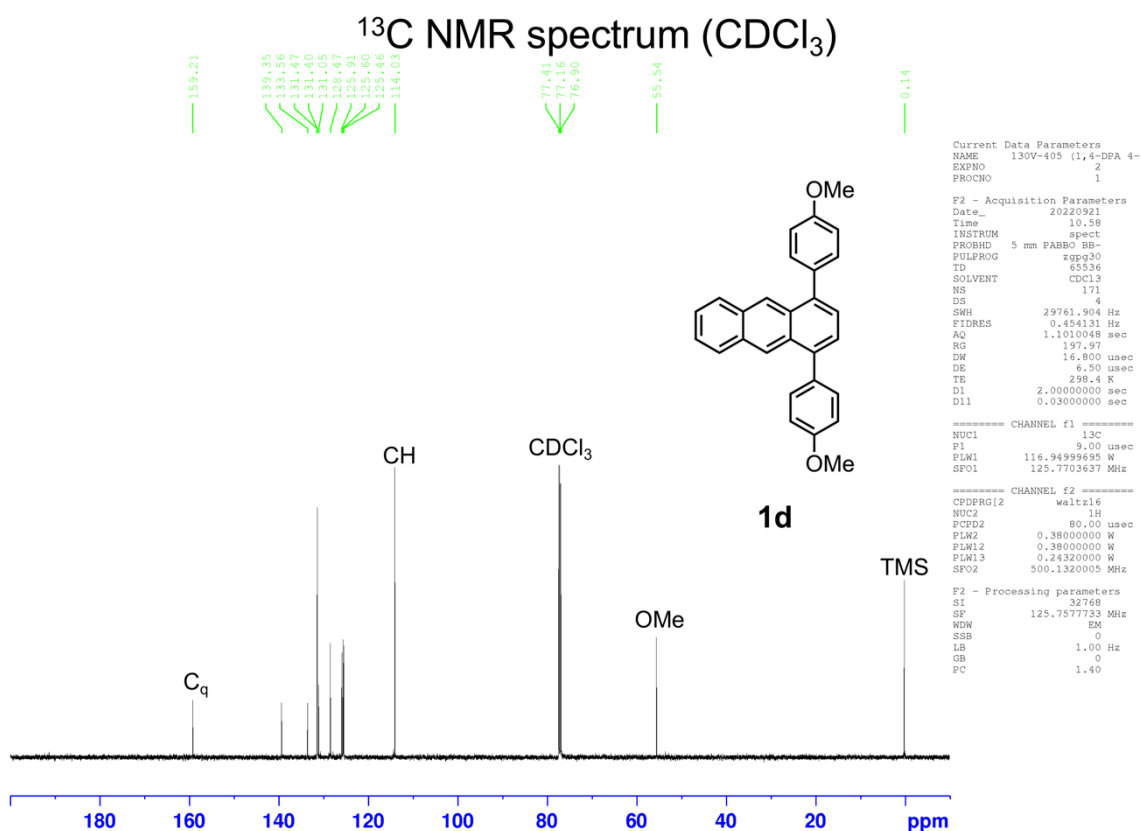
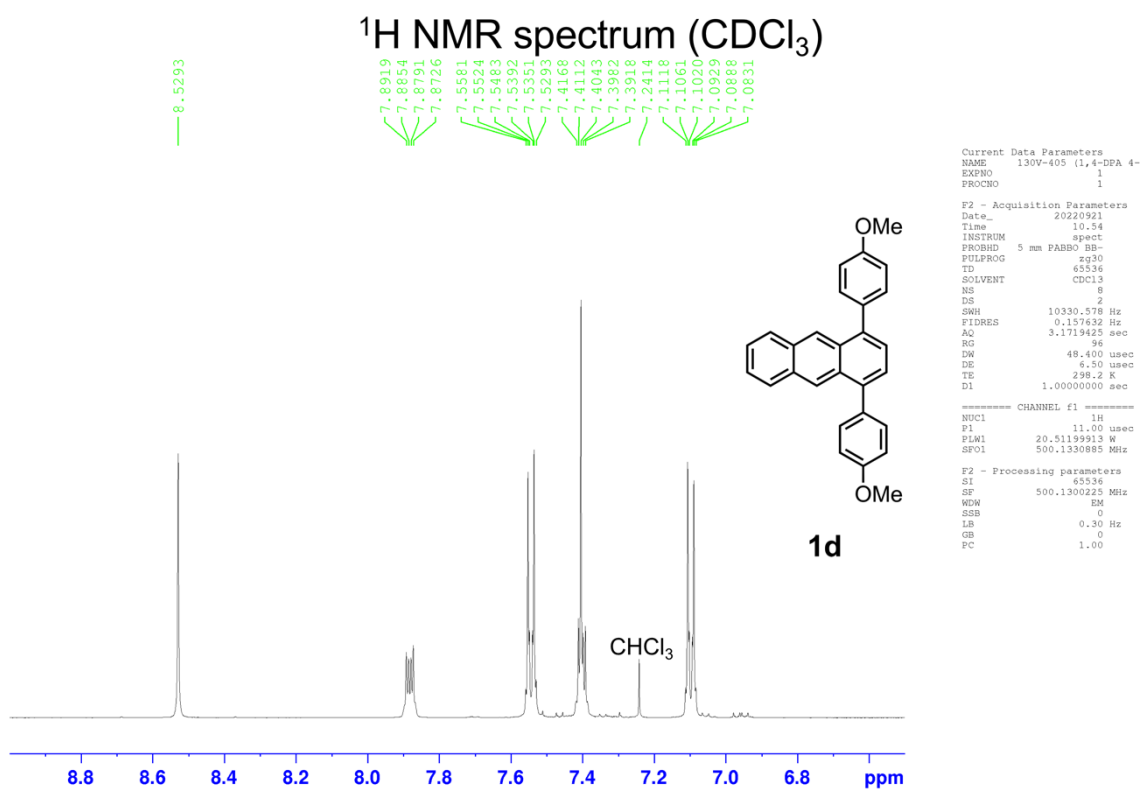


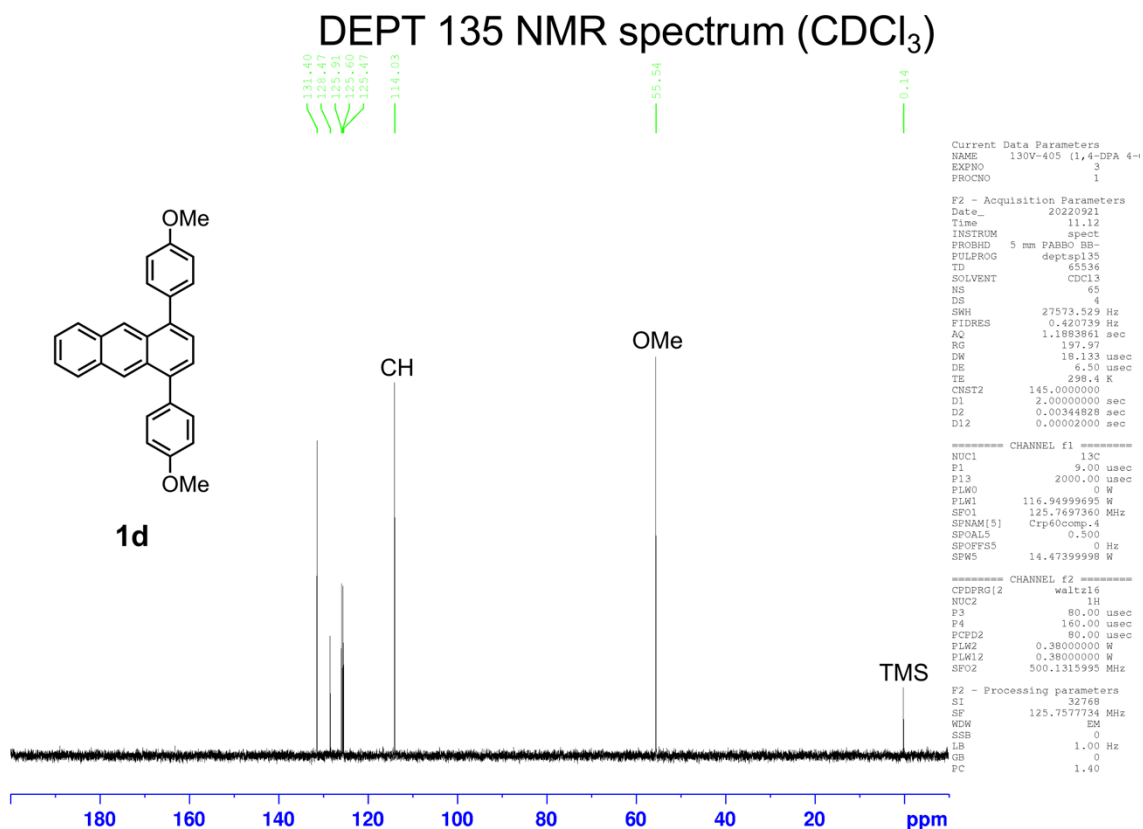
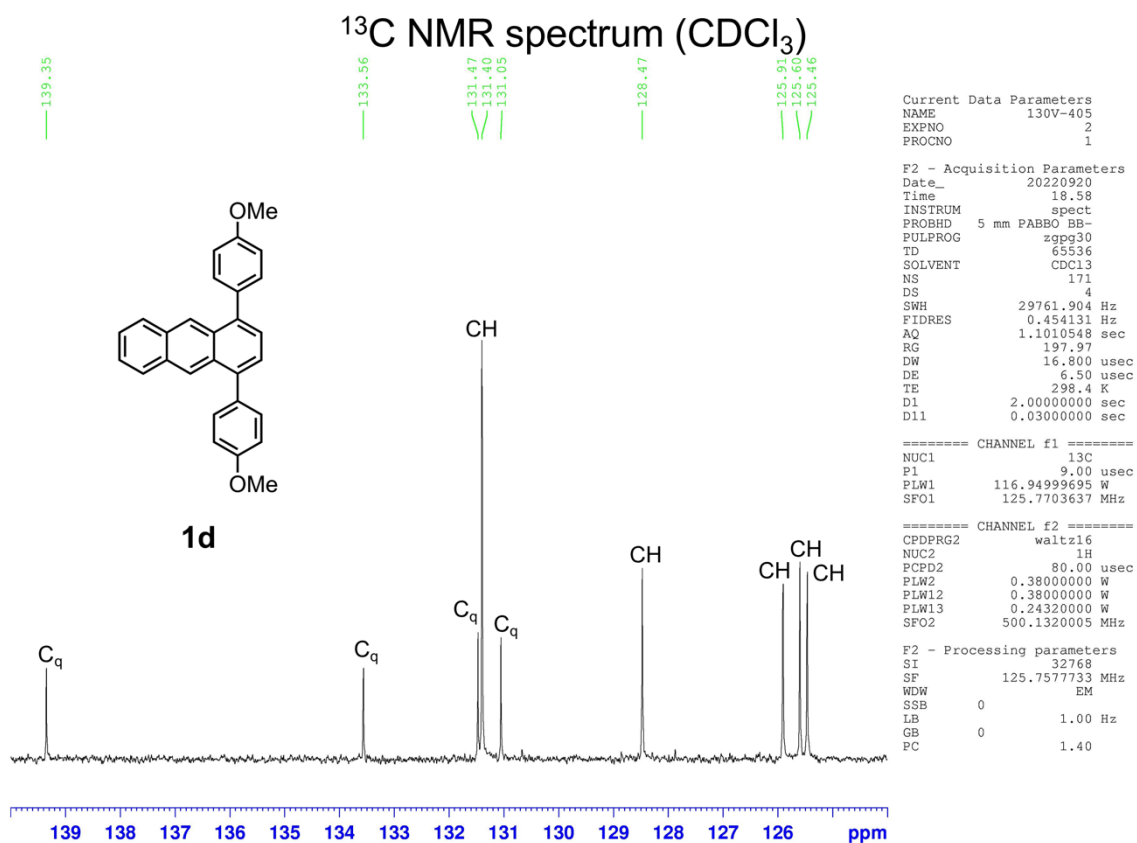
¹⁹F NMR spectrum (CDCl₃)



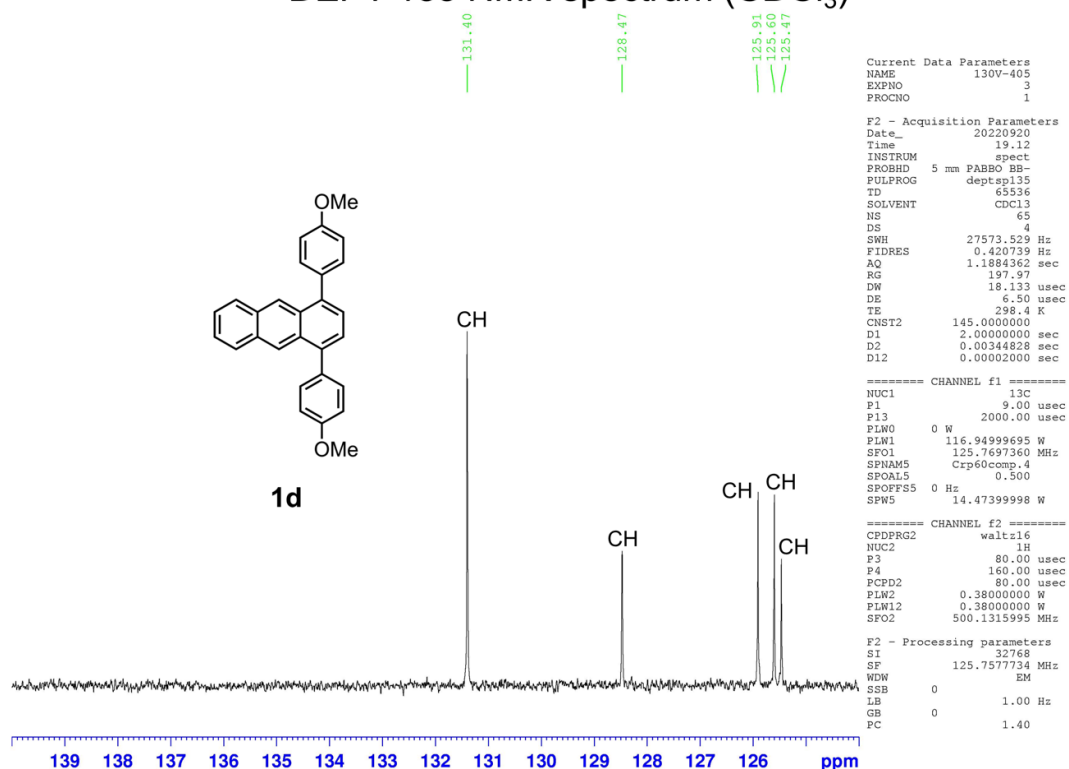
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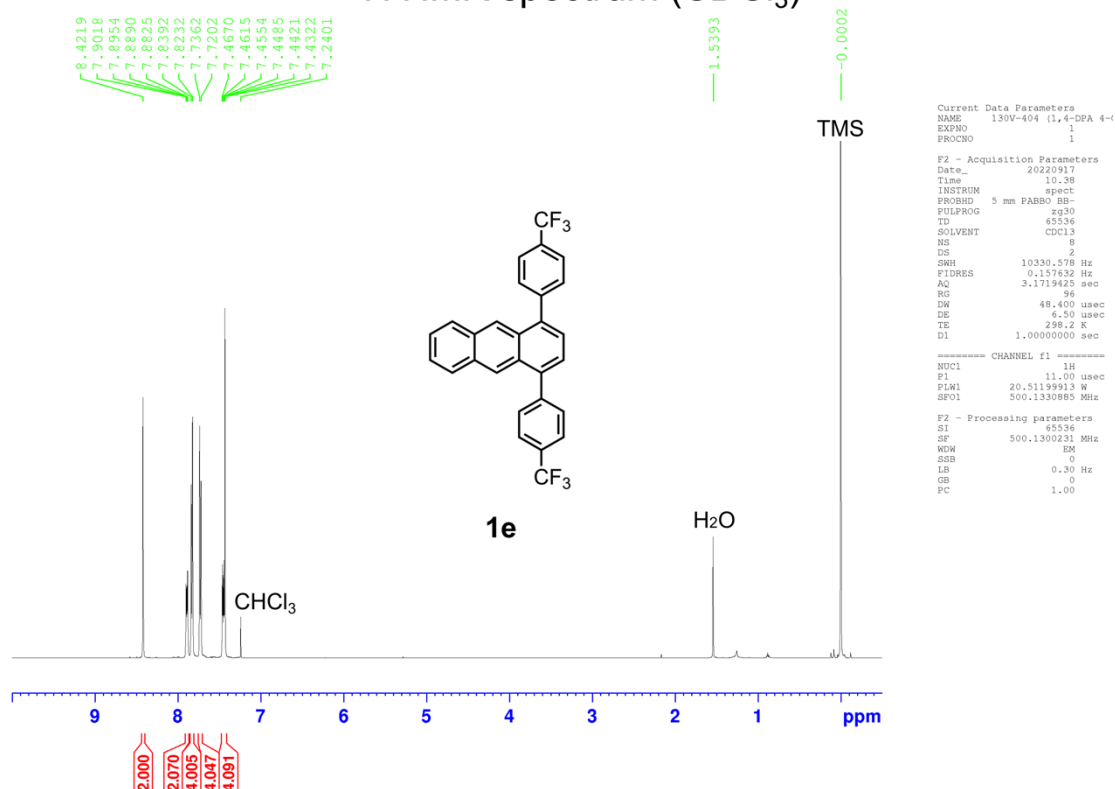


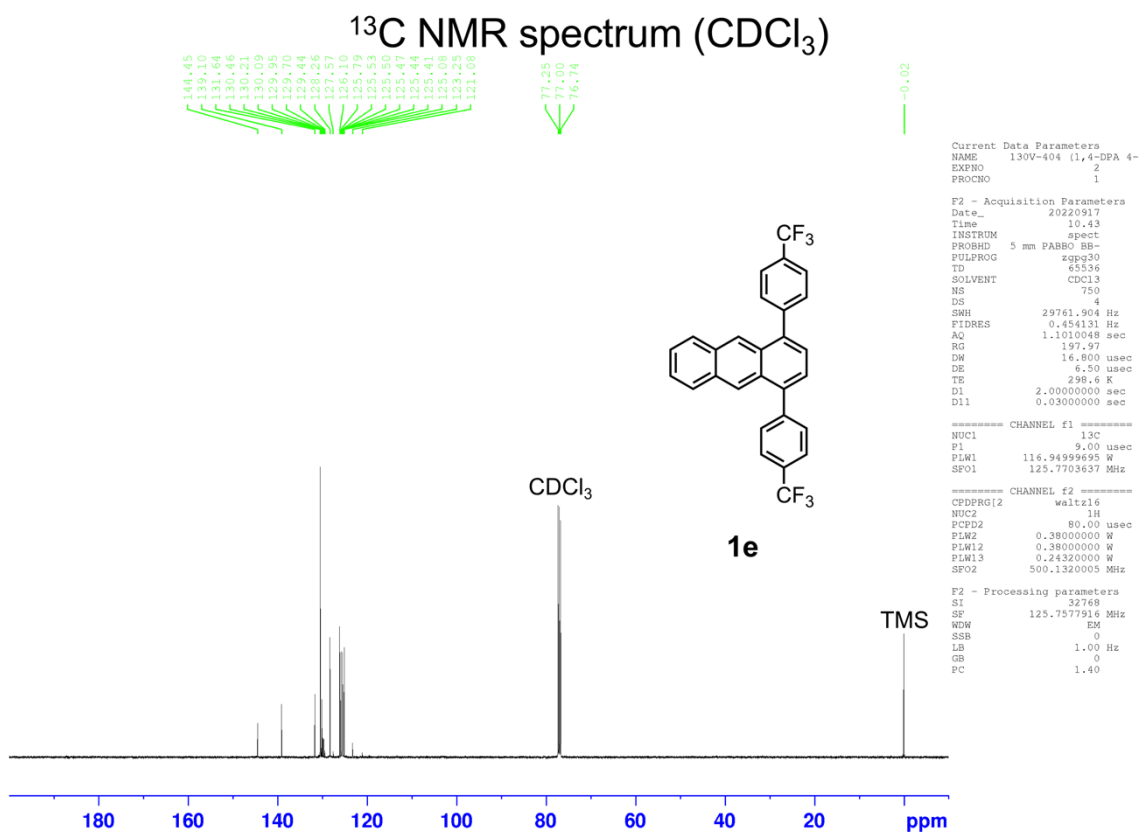
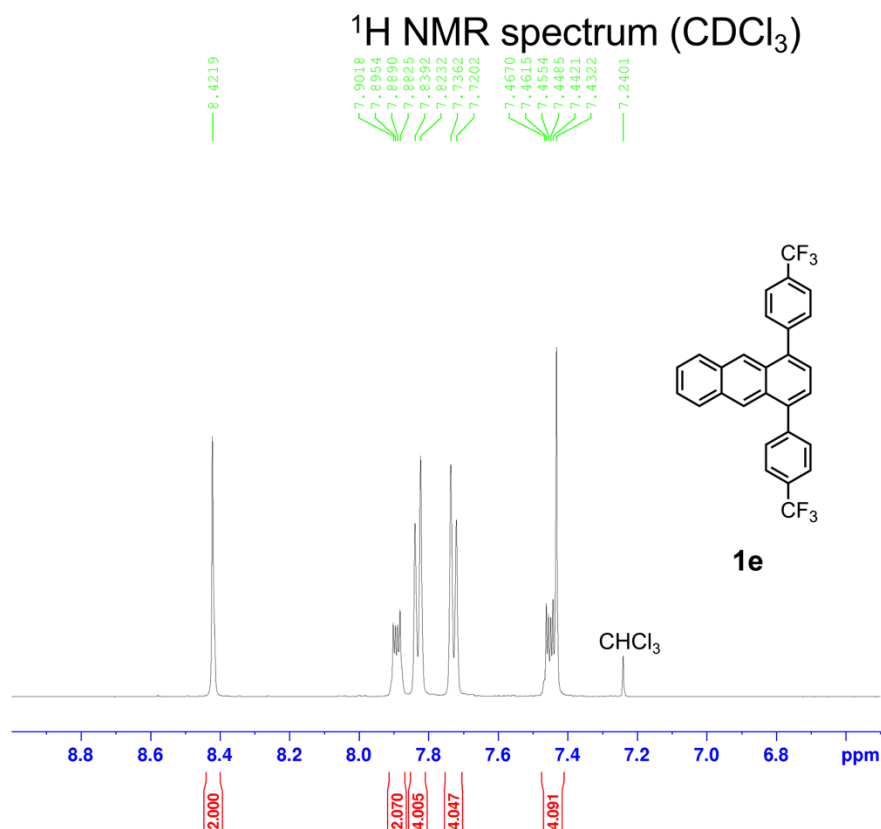


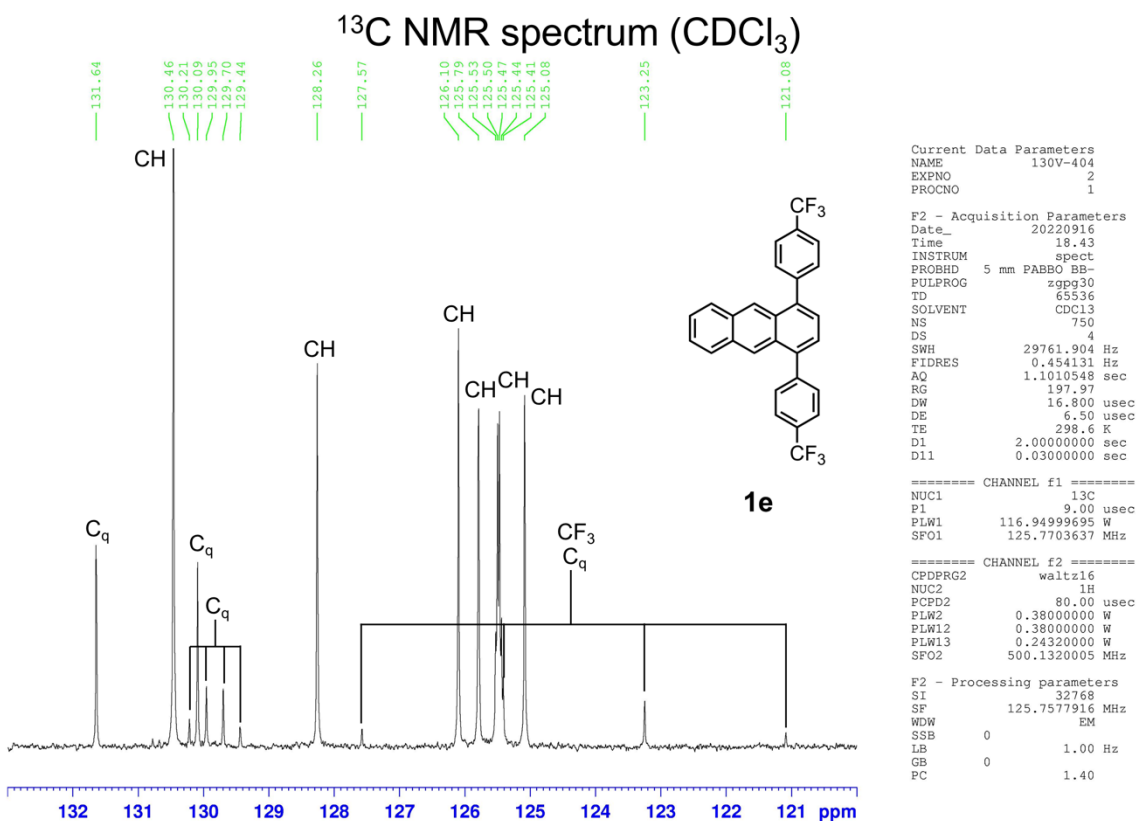
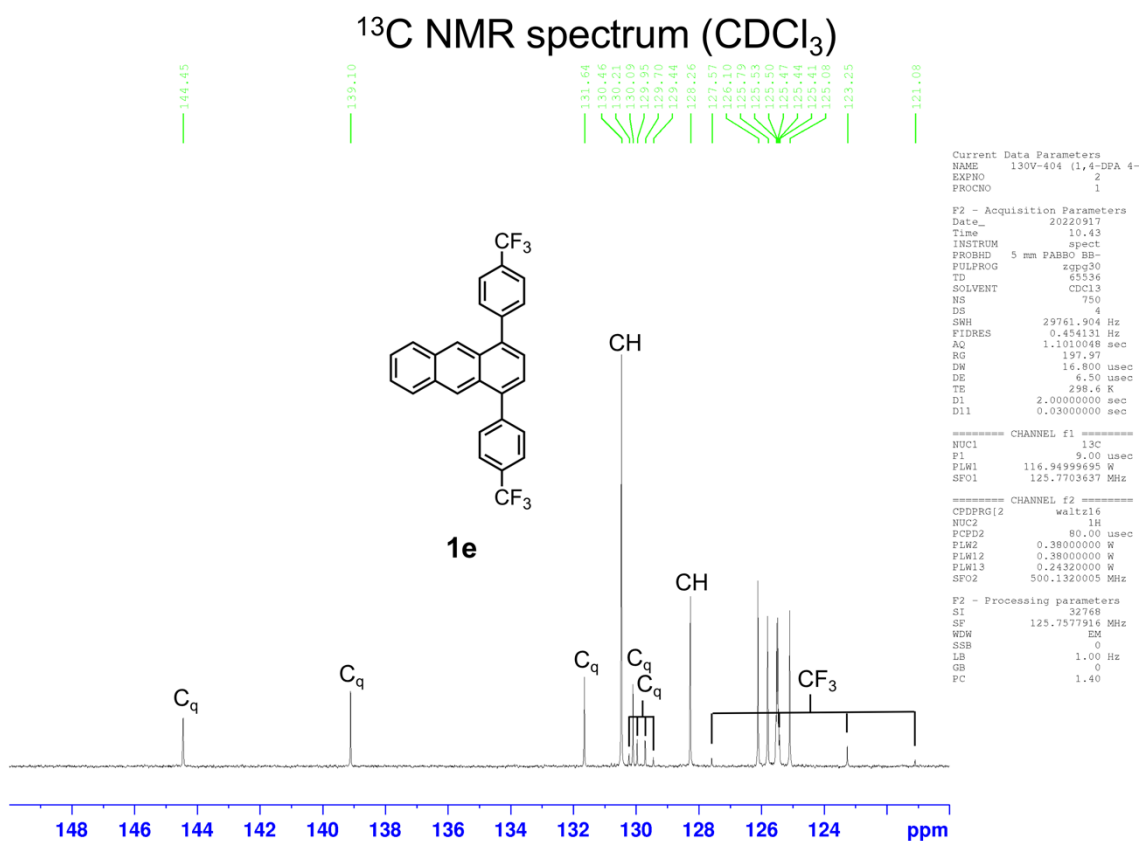
DEPT 135 NMR spectrum (CDCl₃)

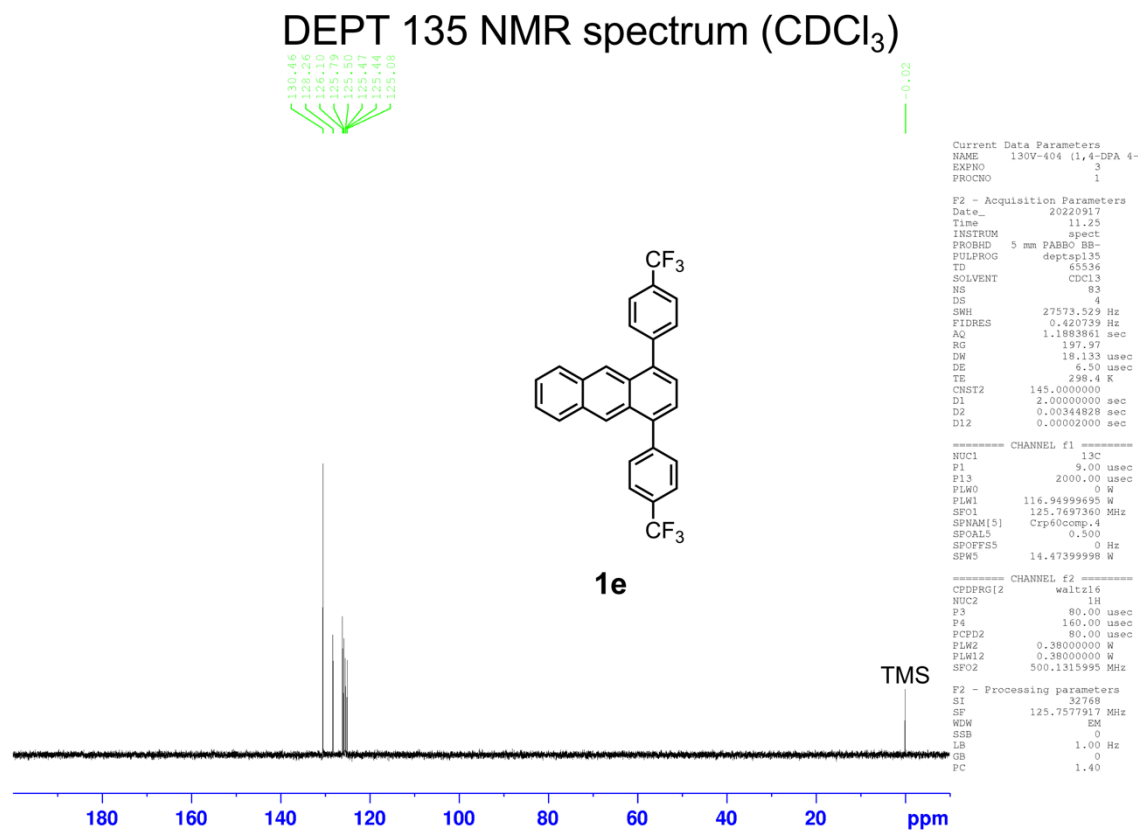
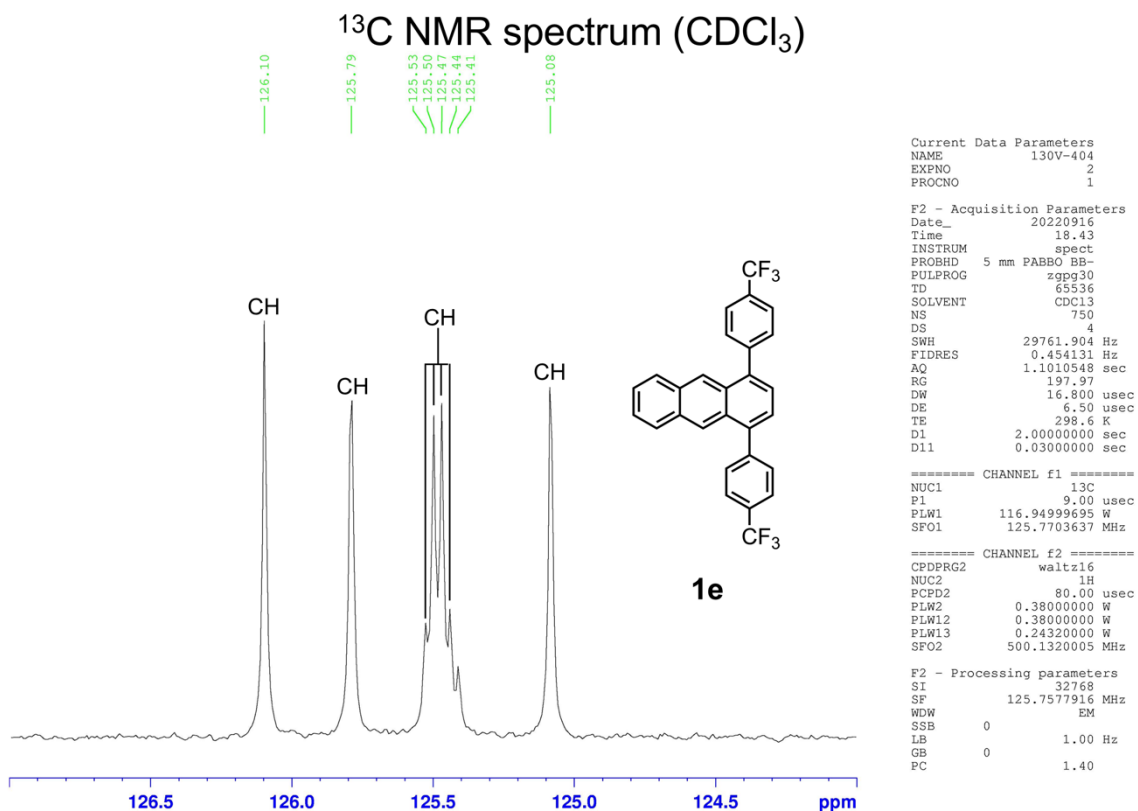


¹H NMR spectrum (CDCl₃)

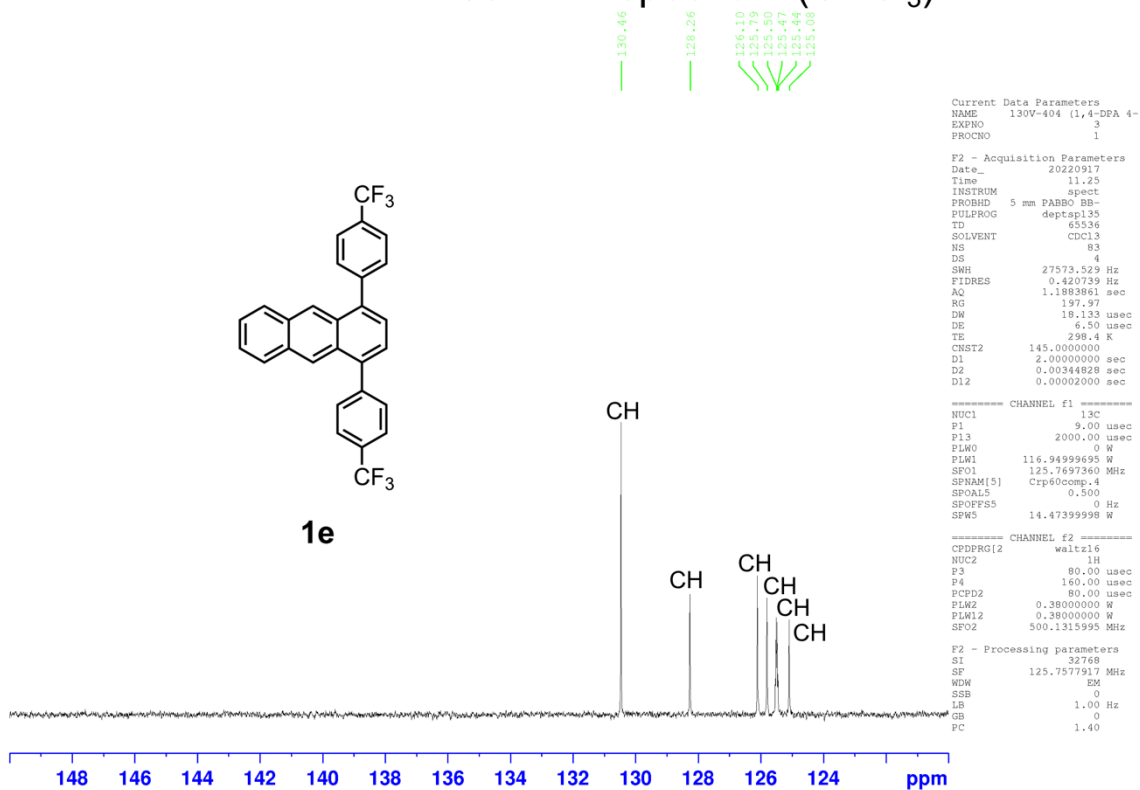




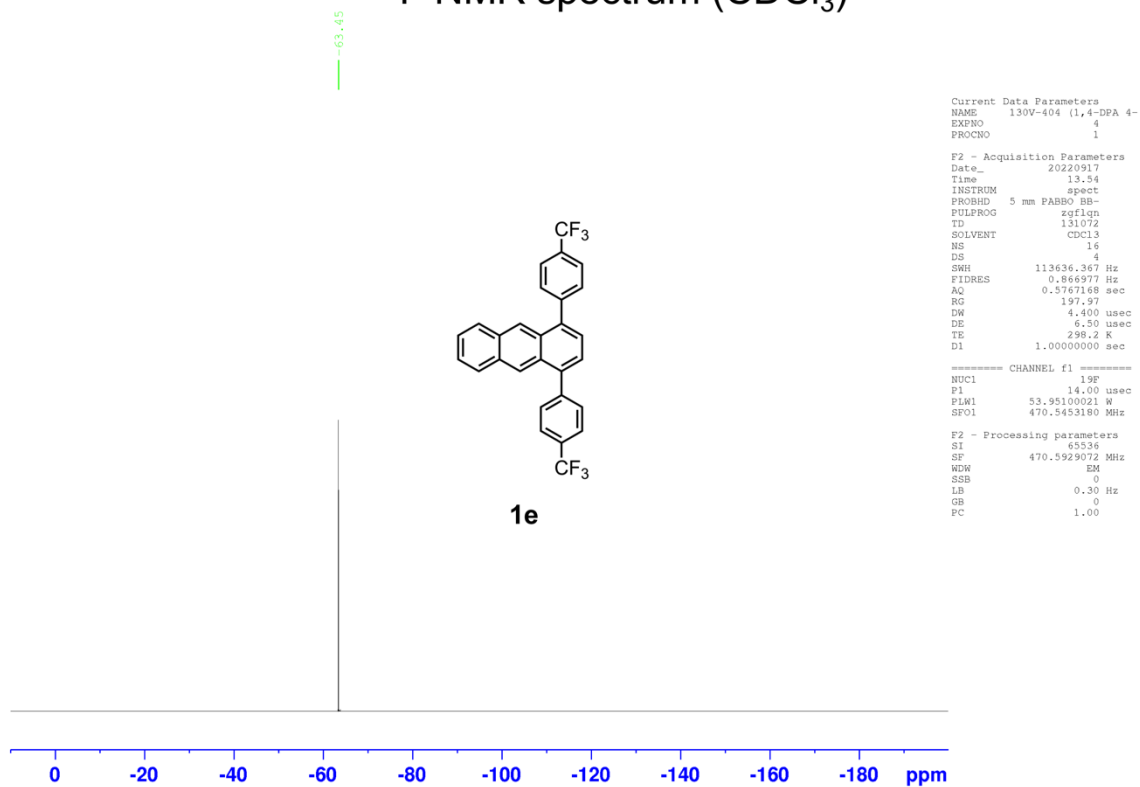




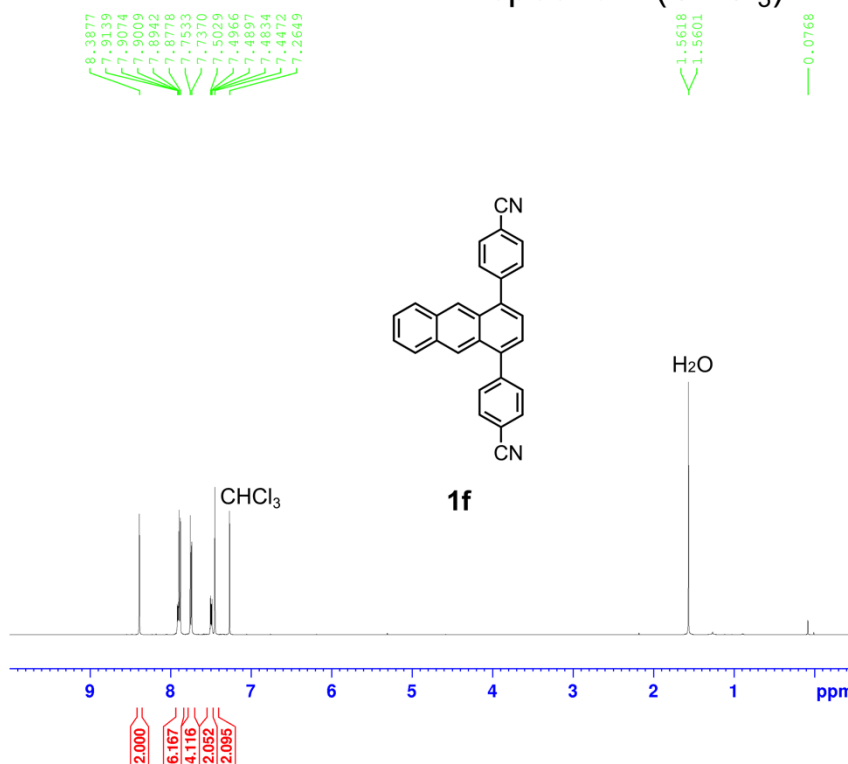
DEPT 135 NMR spectrum (CDCl₃)



¹⁹F NMR spectrum (CDCl₃)



¹H NMR spectrum (CDCl₃)



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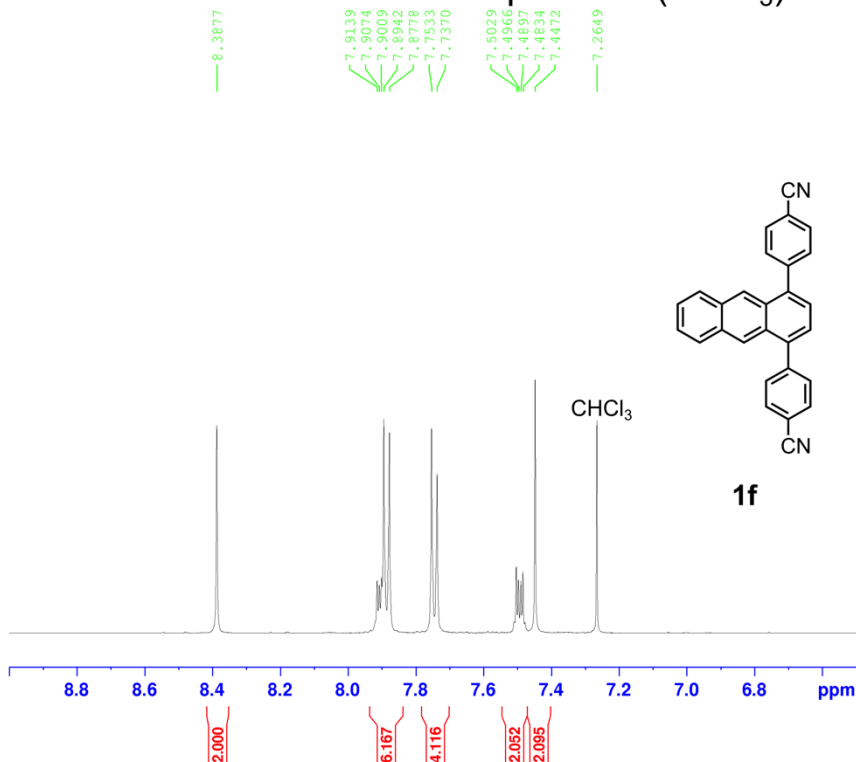
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RG         197.97
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DE         6.50 usec
TE         298.2 K
D1         1.00000000 sec

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SFO1       500.1330885 MHz

F2 - Processing parameters
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```

¹H NMR spectrum (CDCl₃)



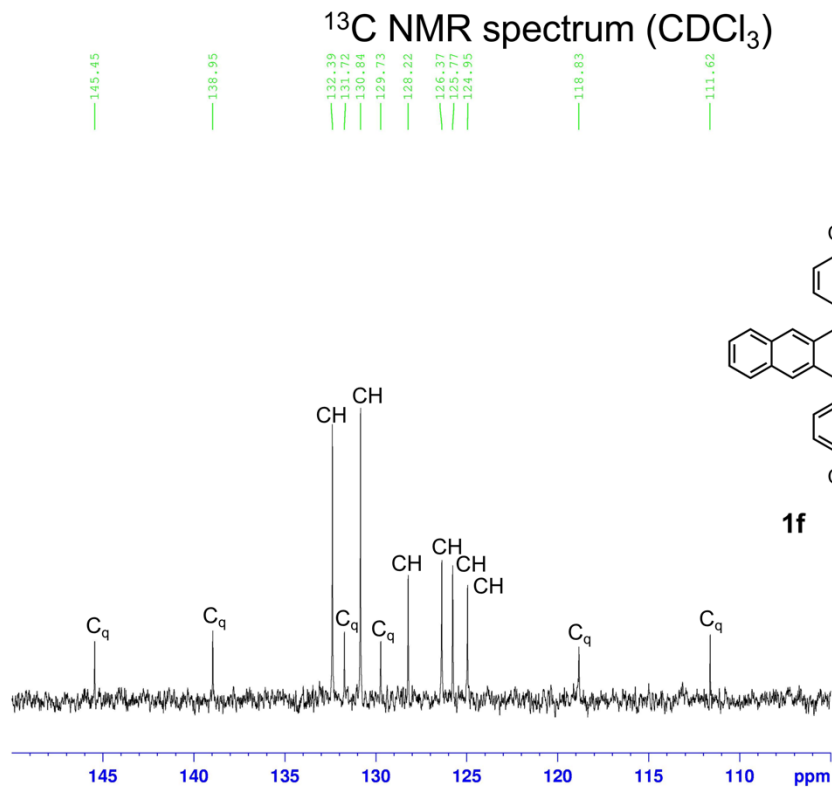
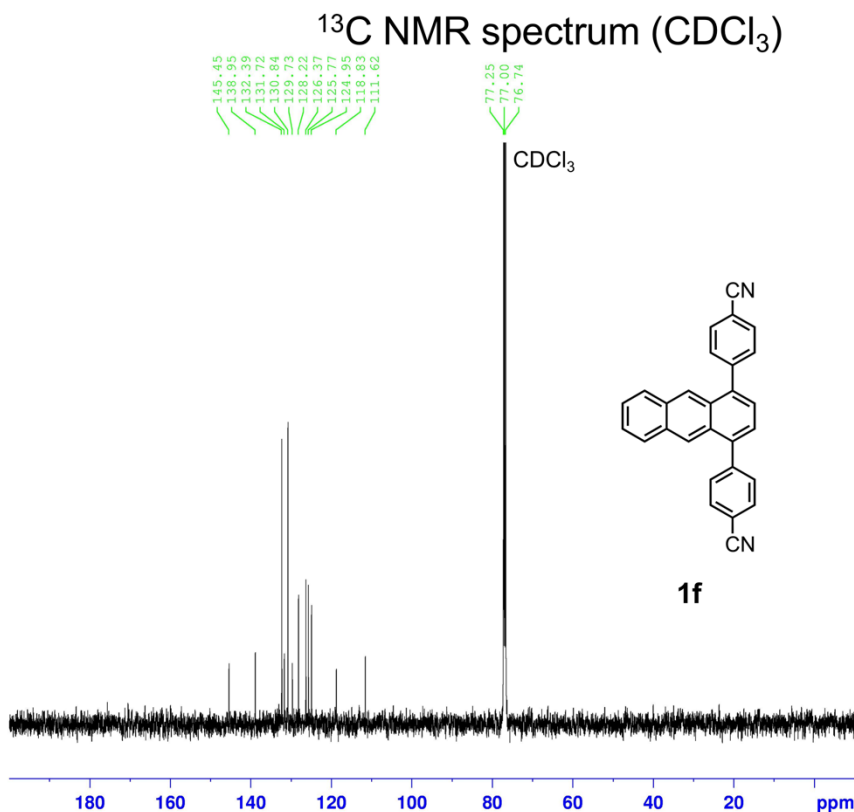
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Current Data Parameters
NAME      13C 14-DPA 4-CN
EXPNO     1
PROCNO    1

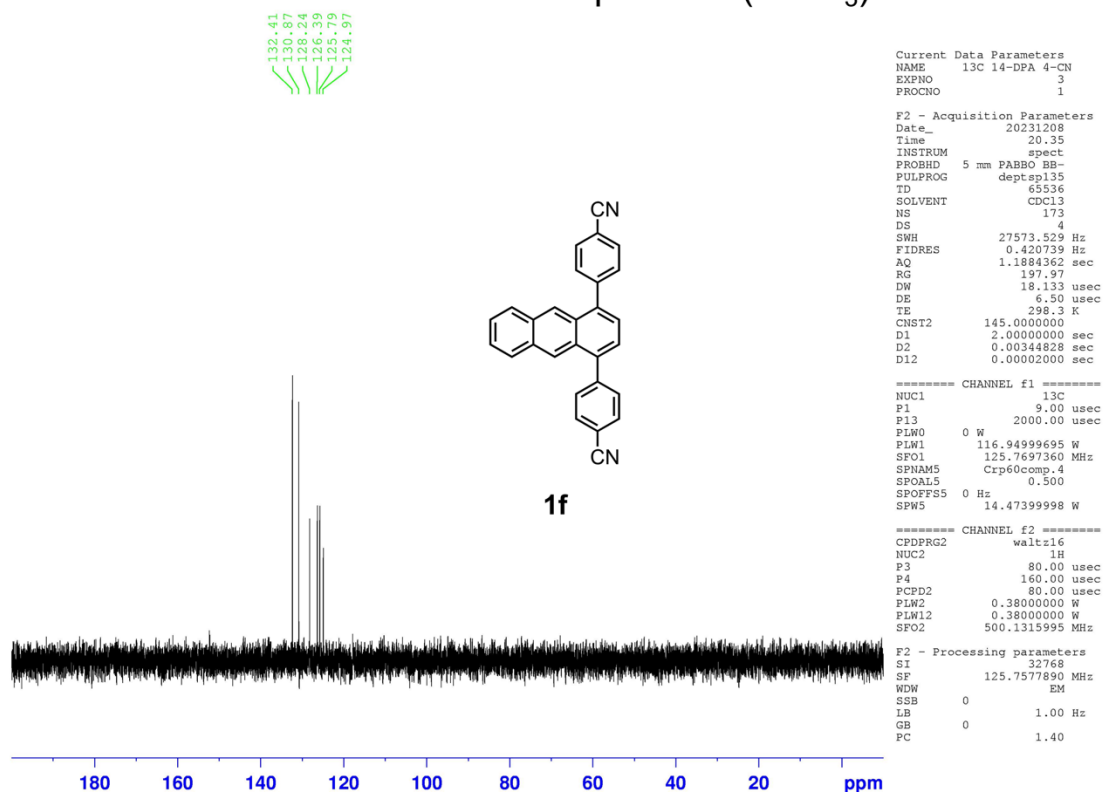
F2 - Acquisition Parameters
Date_     20231209
Time      13.05
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1719425 sec
RG         197.97
DW         48.400 usec
DE         6.50 usec
TE         298.2 K
D1         1.00000000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         11.00 usec
PLW1       20.51199913 W
SFO1       500.1330885 MHz

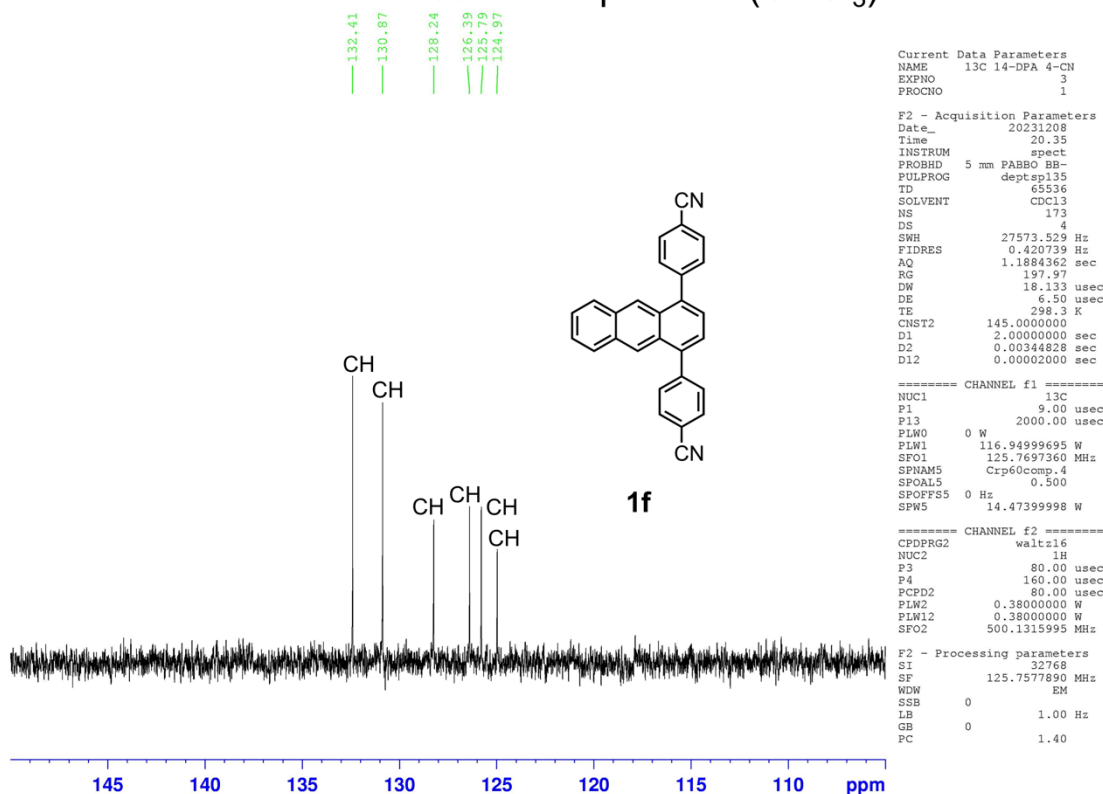
F2 - Processing parameters
SI         65536
SF         500.1300107 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
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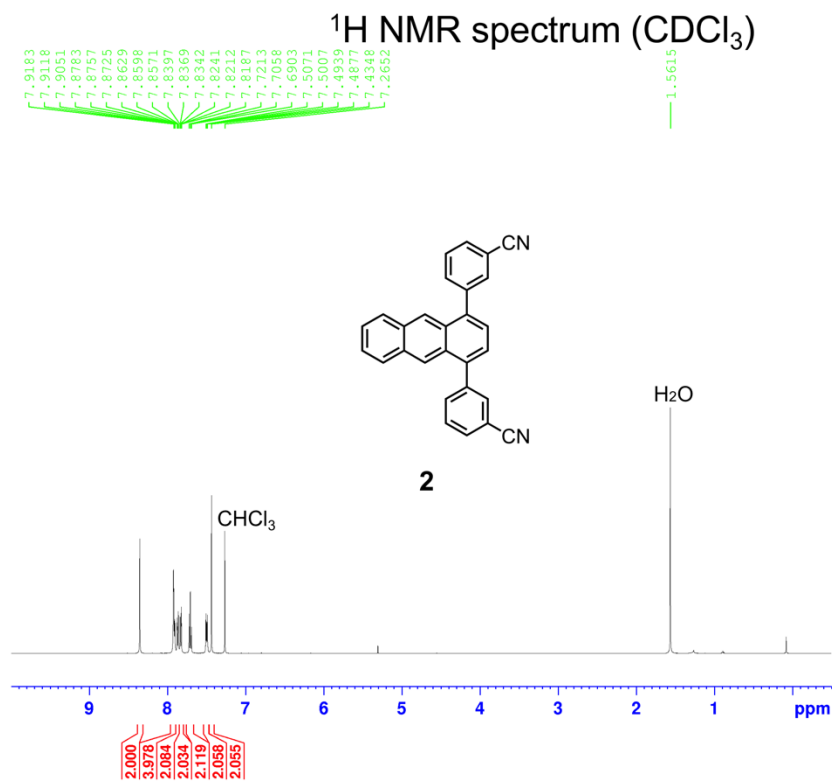


DEPT 135 NMR spectrum (CDCl₃)



DEPT 135 NMR spectrum (CDCl₃)



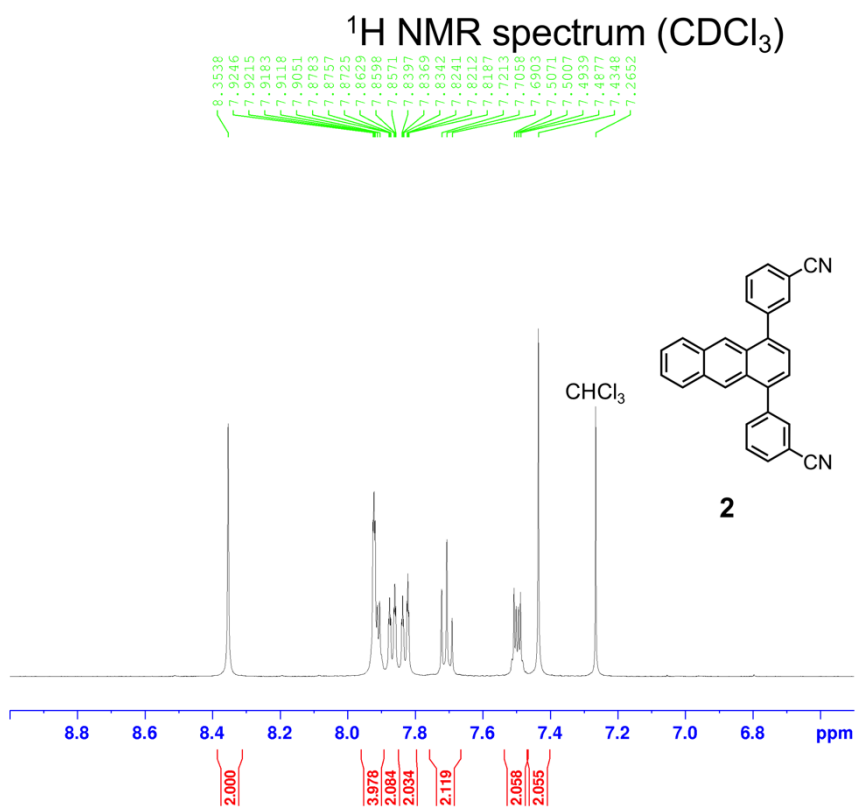


Current Data Parameters
NAME 13C 14-DPA 3-CN
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231209
Time 15.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 197.97
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PLW1 20.51199913 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 65536
SF 500.1330107 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

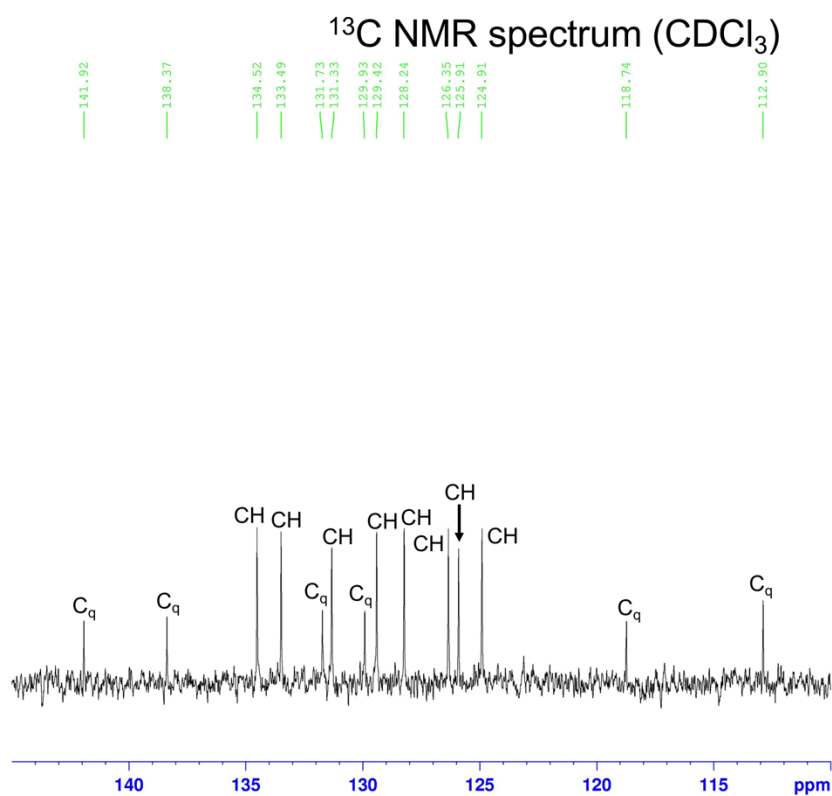
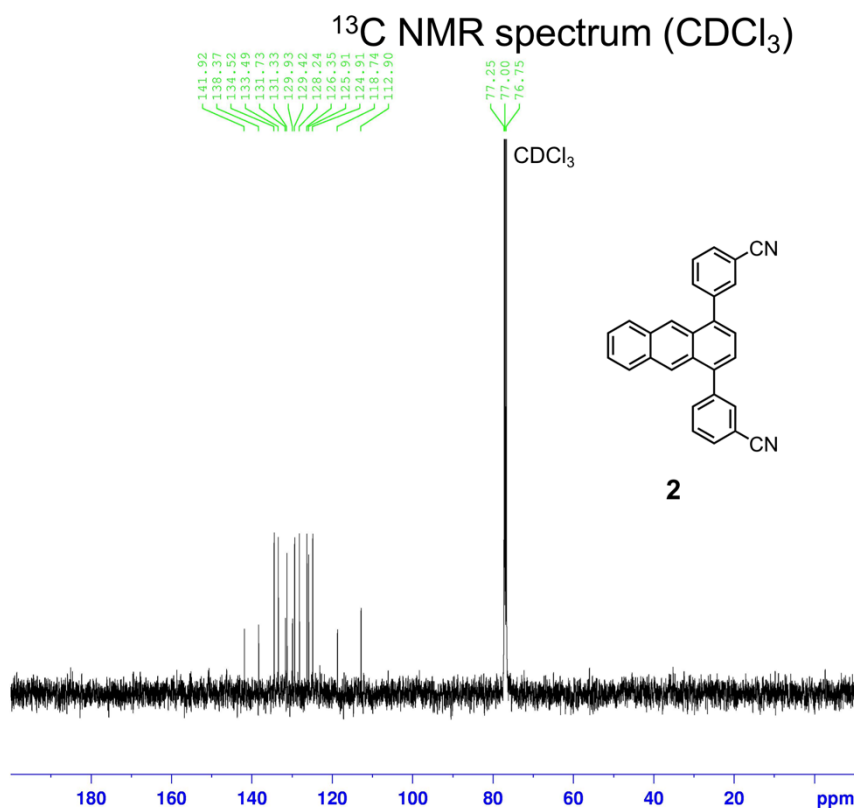


Current Data Parameters
NAME 13C 14-DPA 3-CN
EXPNO 1
PROCNO 1

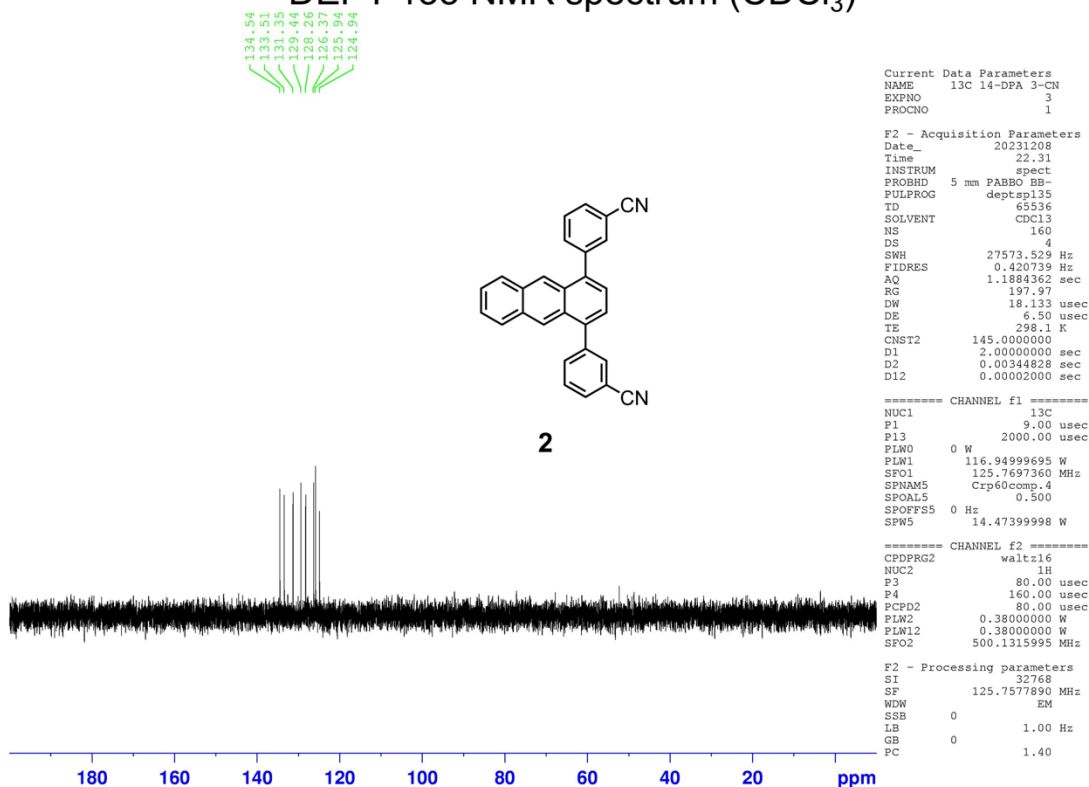
F2 - Acquisition Parameters
Date_ 20231209
Time 15.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 197.97
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PLW1 20.51199913 W
SFO1 500.1330885 MHz

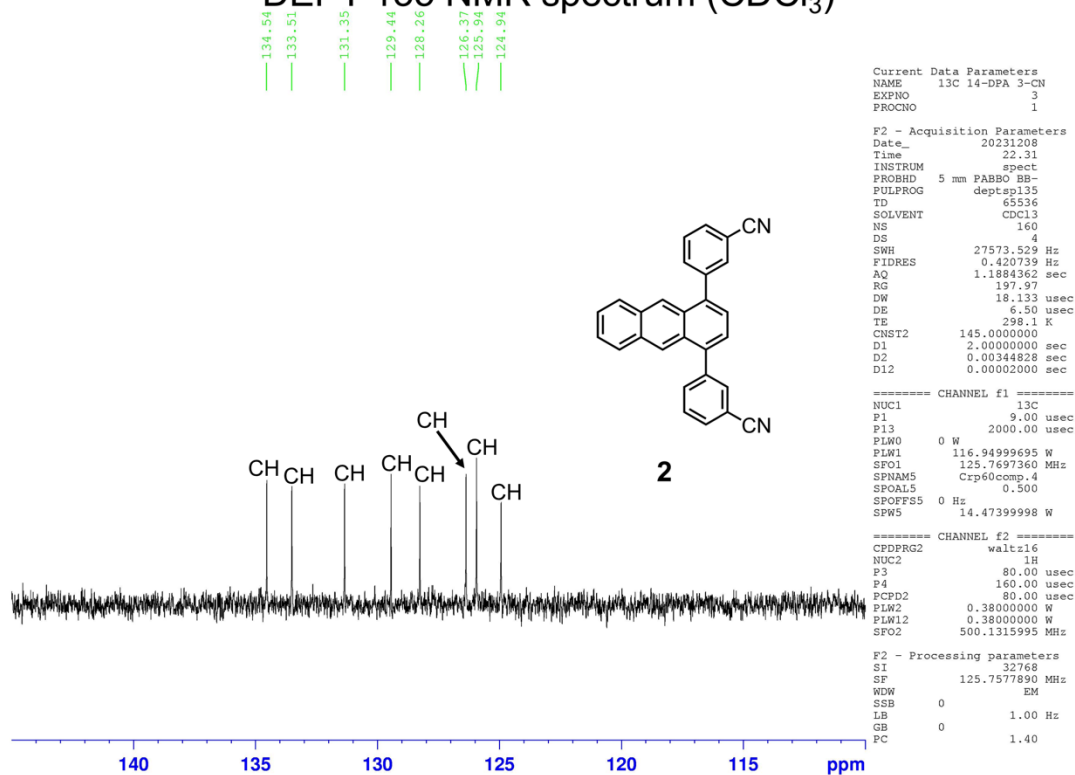
F2 - Processing parameters
SI 65536
SF 500.1330107 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

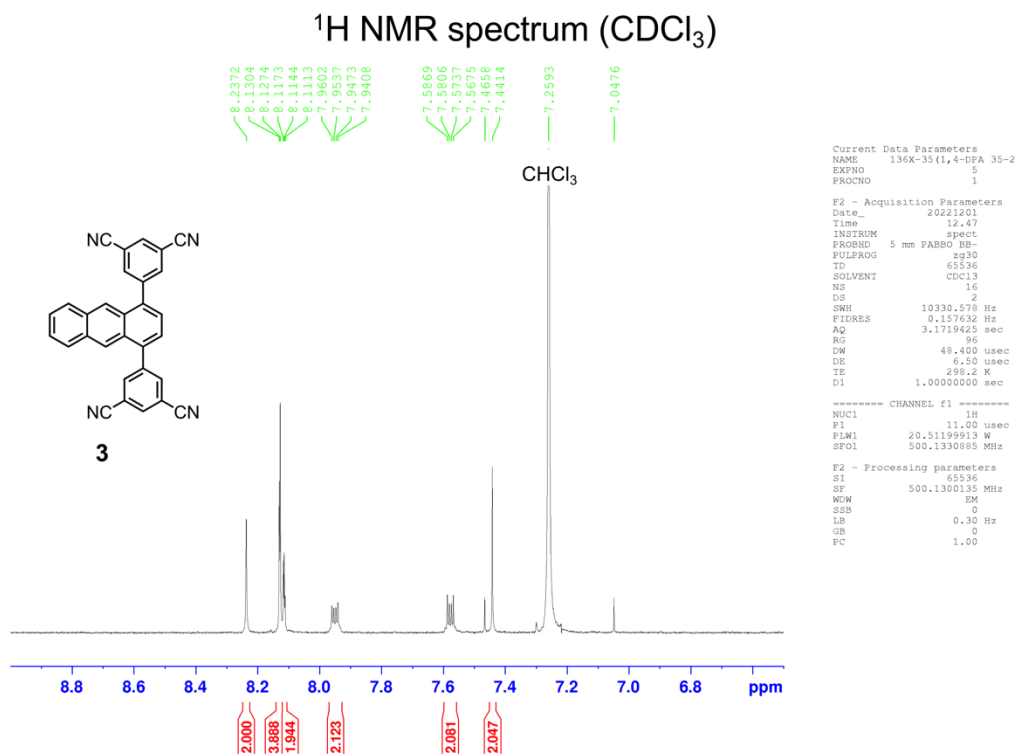
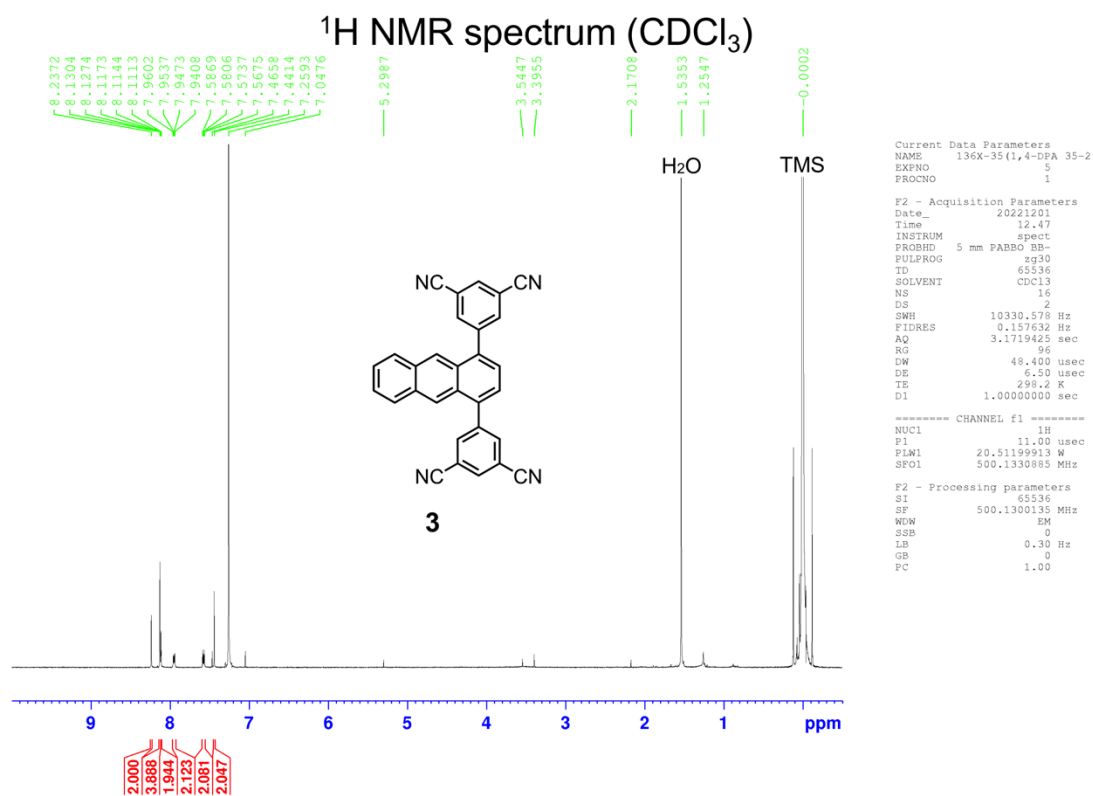


DEPT 135 NMR spectrum (CDCl₃)

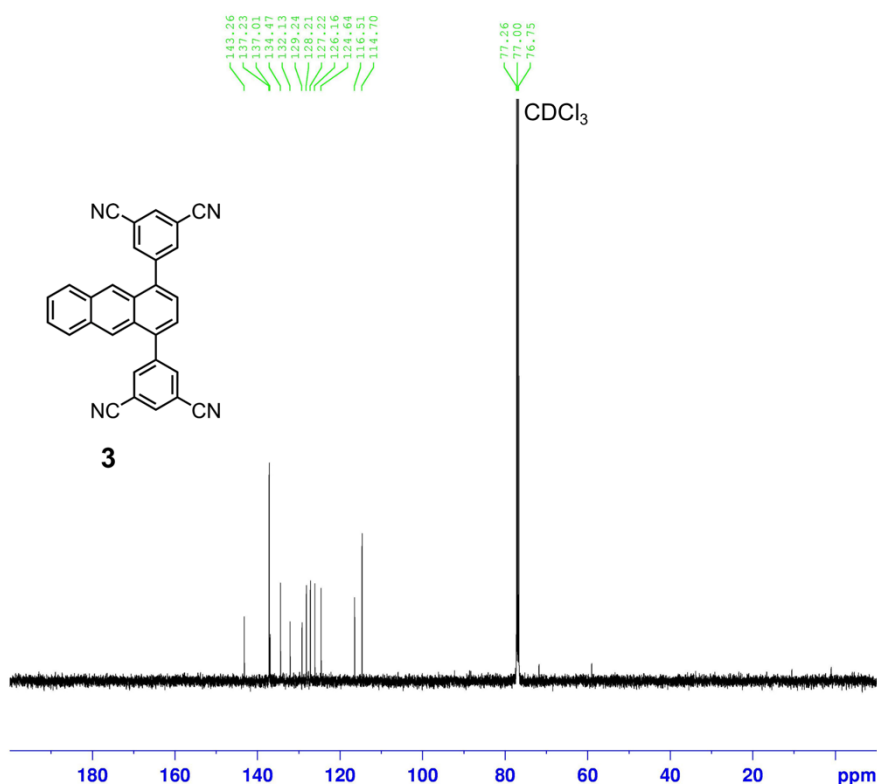


DEPT 135 NMR spectrum (CDCl₃)





¹³C NMR spectrum (CDCl₃)



```

Current Data Parameters
NAME      kannen231123
EXPNO     2
PROCNO    1

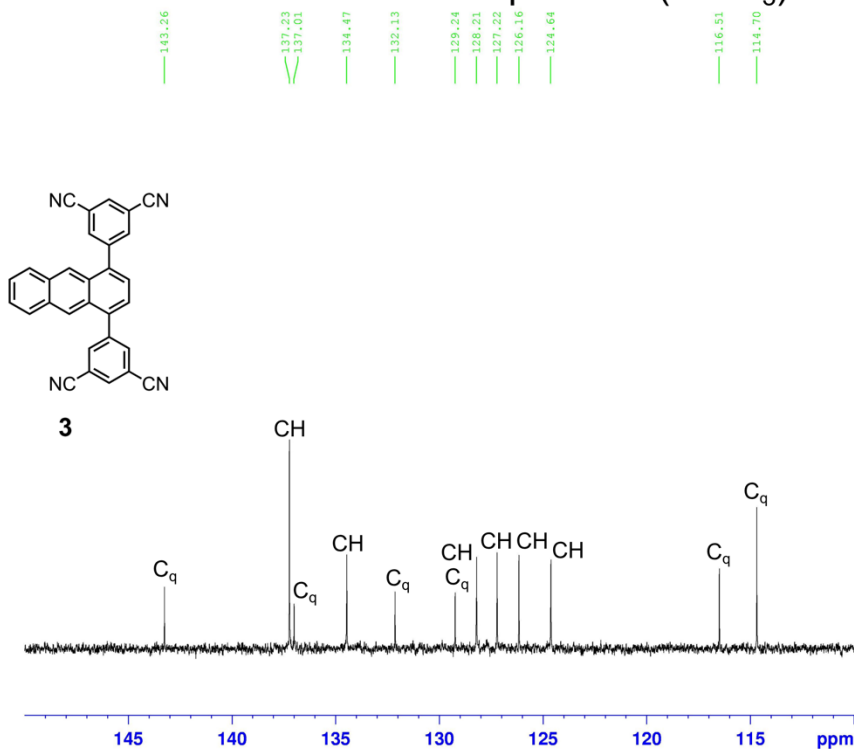
F2 - Acquisition Parameters
Date_     20231123
Time      20.30
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS         1121
DS         4
SWH        29761.904 Hz
FIDRES     0.454131 Hz
AQ         1.1010548 sec
RG         197.97
DW         16.800 usec
DE         6.50 usec
TE         298.2 K
D1         2.00000000 sec
D11        0.03000000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         9.00 usec
PLW1       116.94999695 W
SFO1       125.7703637 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       80.00 usec
PLW2        0.38000000 W
PLW12       0.38000000 W
PLW13       0.24320000 W
SFO2        500.1320005 MHz

F2 - Processing parameters
SI          32768
SF          125.7577909 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
    
```

¹³C NMR spectrum (CDCl₃)



```

Current Data Parameters
NAME      kannen231123
EXPNO     2
PROCNO    1

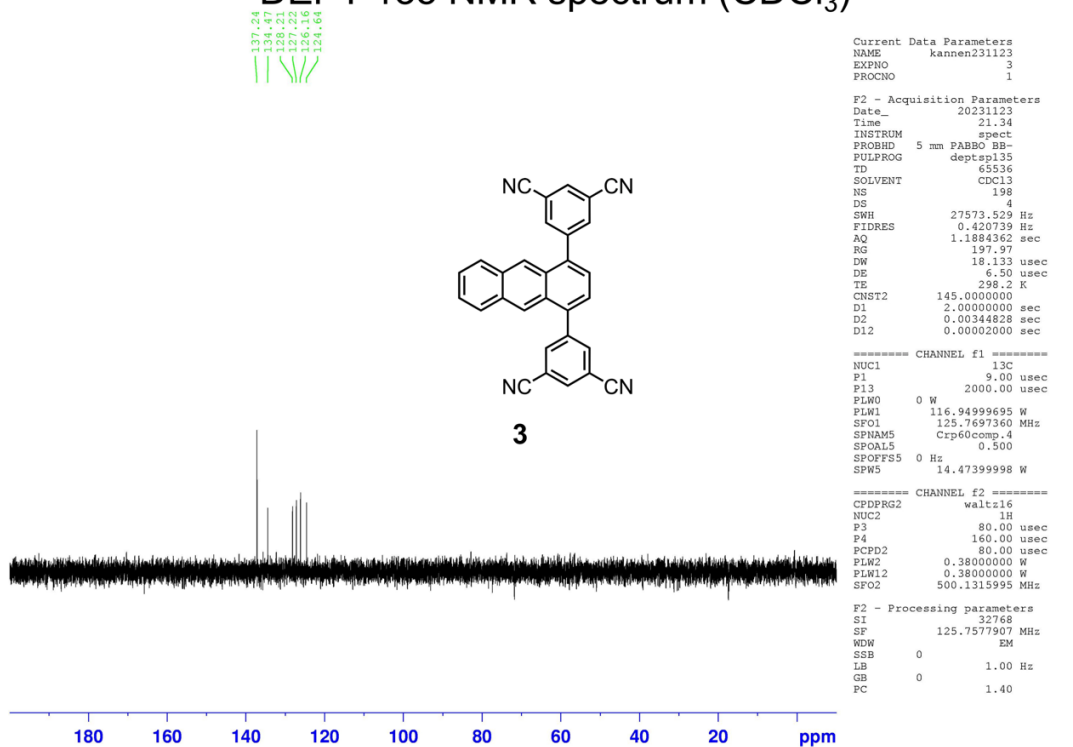
F2 - Acquisition Parameters
Date_     20231123
Time      20.30
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS         1121
DS         4
SWH        29761.904 Hz
FIDRES     0.454131 Hz
AQ         1.1010548 sec
RG         197.97
DW         16.800 usec
DE         6.50 usec
TE         298.2 K
D1         2.00000000 sec
D11        0.03000000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         9.00 usec
PLW1       116.94999695 W
SFO1       125.7703637 MHz

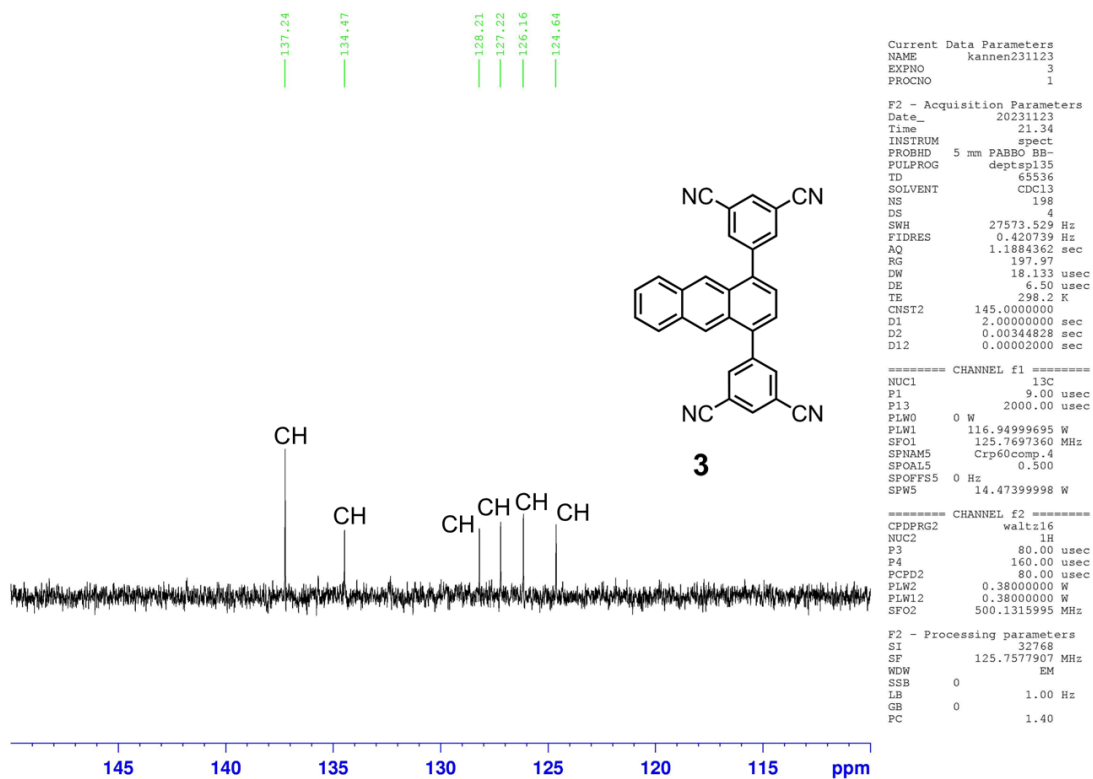
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       80.00 usec
PLW2        0.38000000 W
PLW12       0.38000000 W
PLW13       0.24320000 W
SFO2        500.1320005 MHz

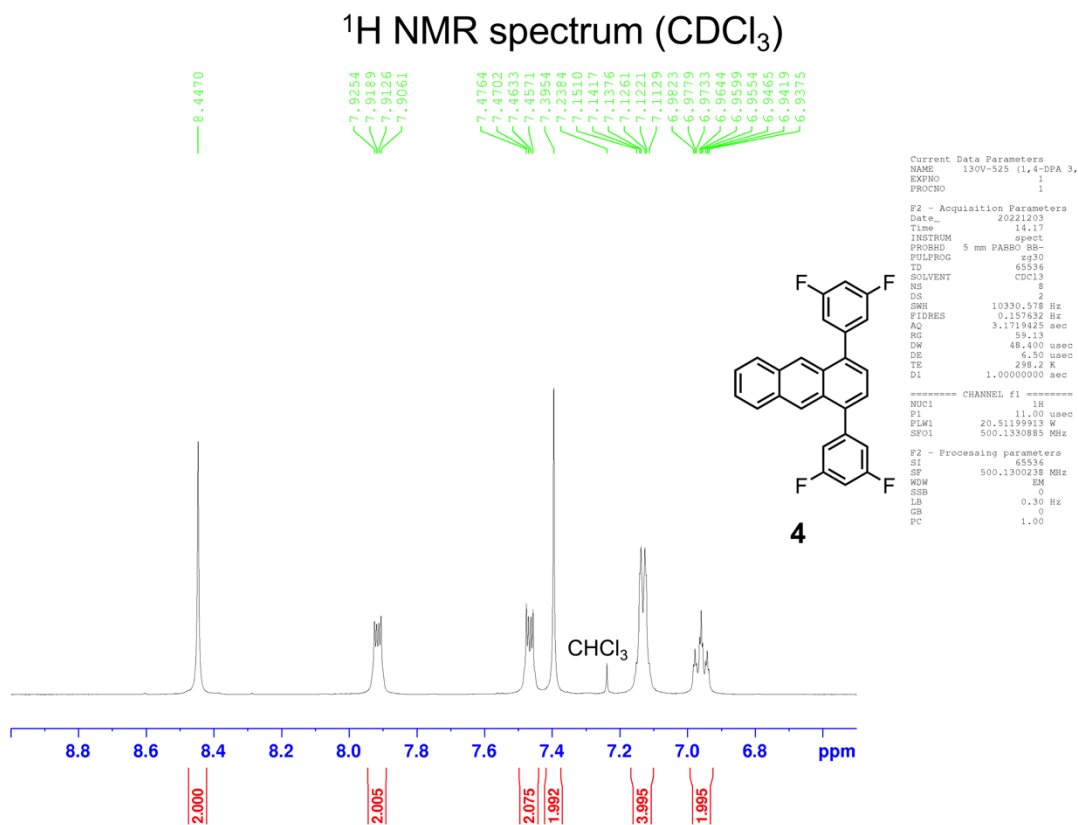
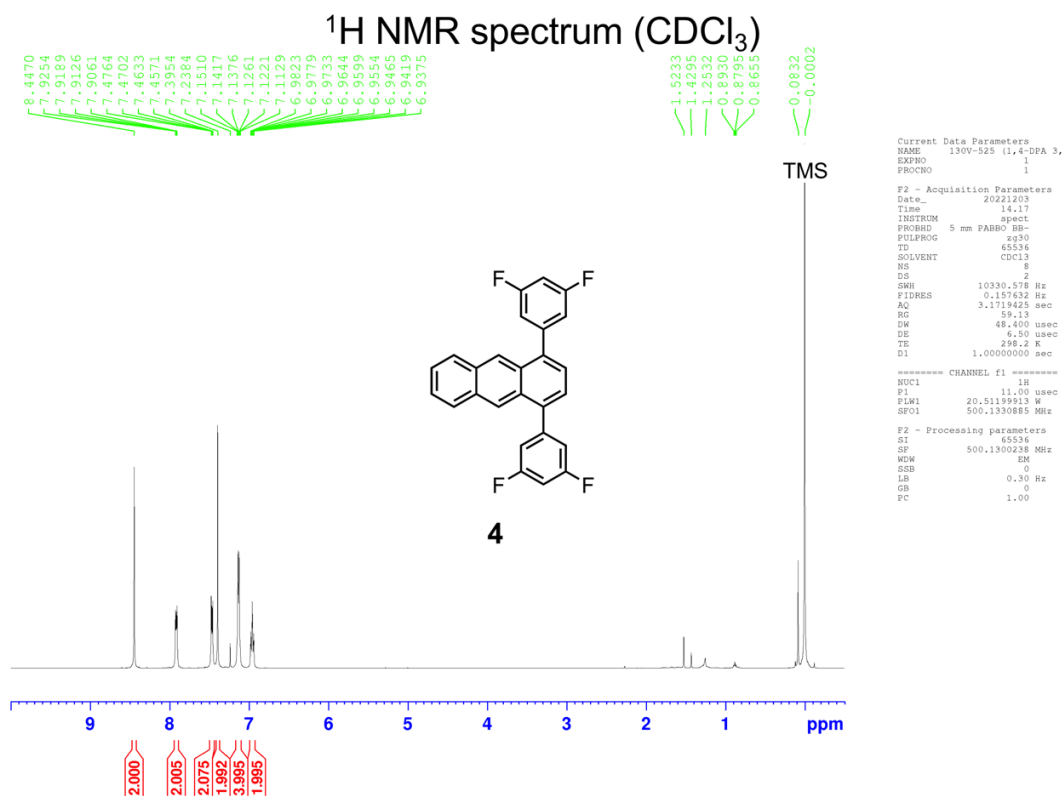
F2 - Processing parameters
SI          32768
SF          125.7577909 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
    
```

DEPT 135 NMR spectrum (CDCl₃)

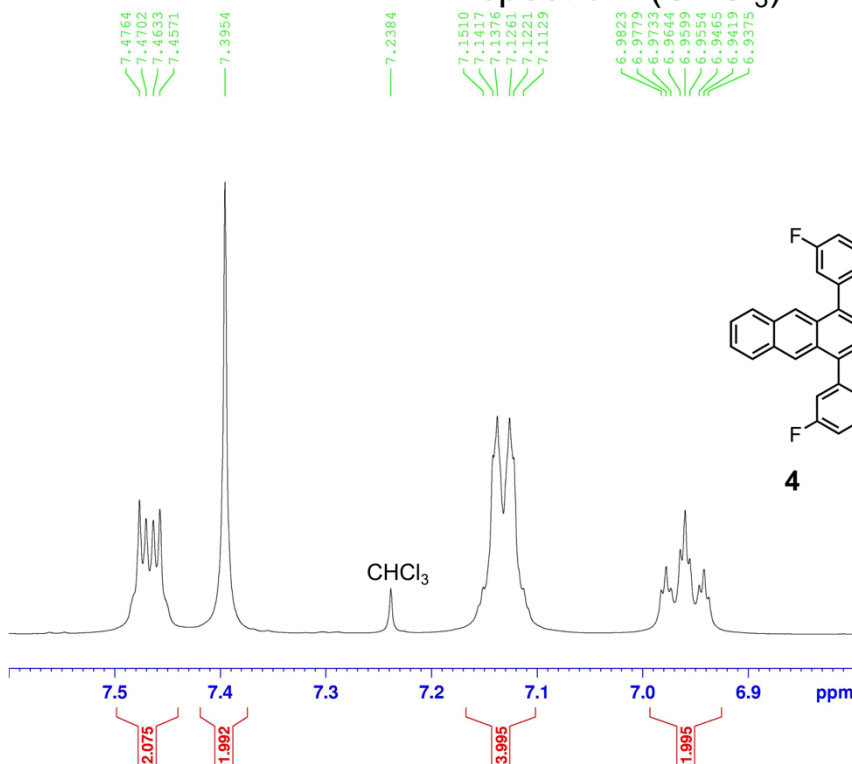


DEPT 135 NMR spectrum (CDCl₃)





¹H NMR spectrum (CDCl₃)



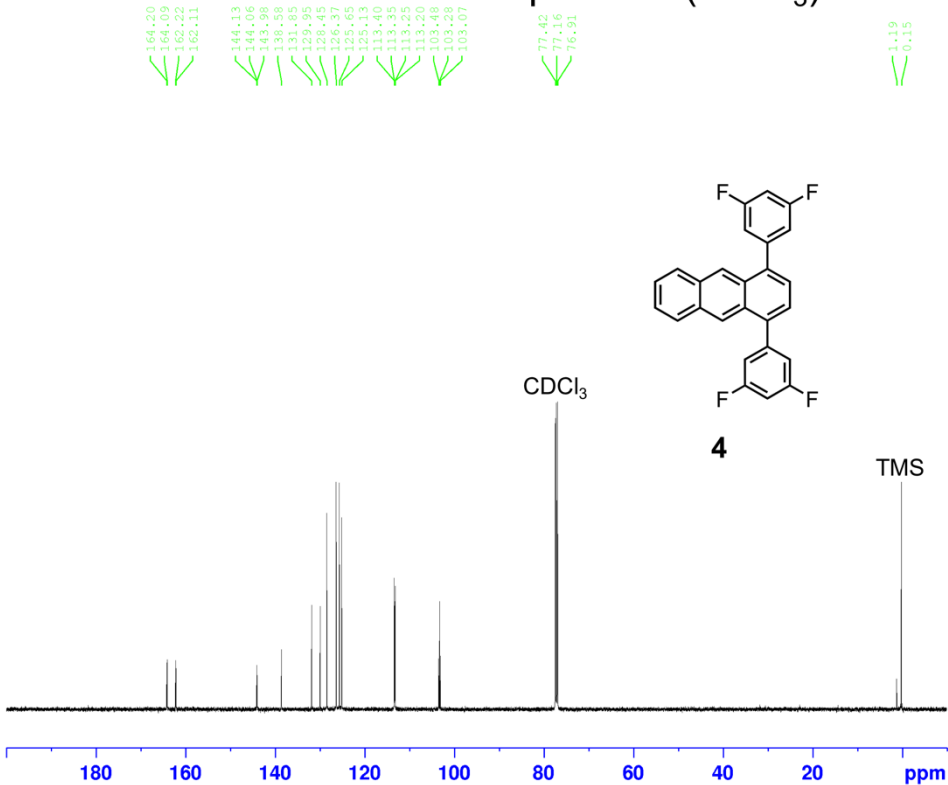
Current Data Parameters
 NAME 130V-525
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20221202
 Time 21.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 59.13
 DW 48.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PLW1 20.51199913 W
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300238 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR spectrum (CDCl₃)



Current Data Parameters
 NAME 130V-525 (1,4-DFA 3,
 EXPNO 2
 PROCNO 1

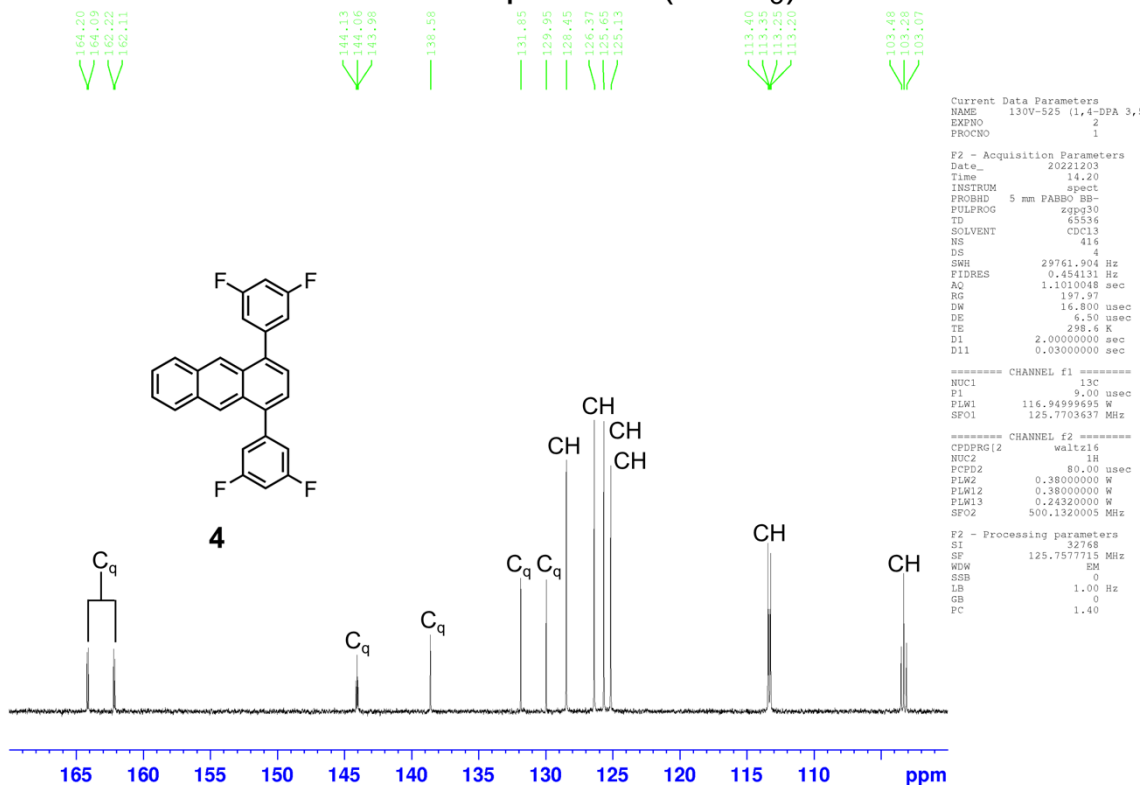
F2 - Acquisition Parameters
 Date_ 20221203
 Time 14.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 416
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 197.57
 DW 16.800 usec
 DE 6.50 usec
 TE 298.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PLW1 116.94999695 W
 SFO1 125.7703637 MHz

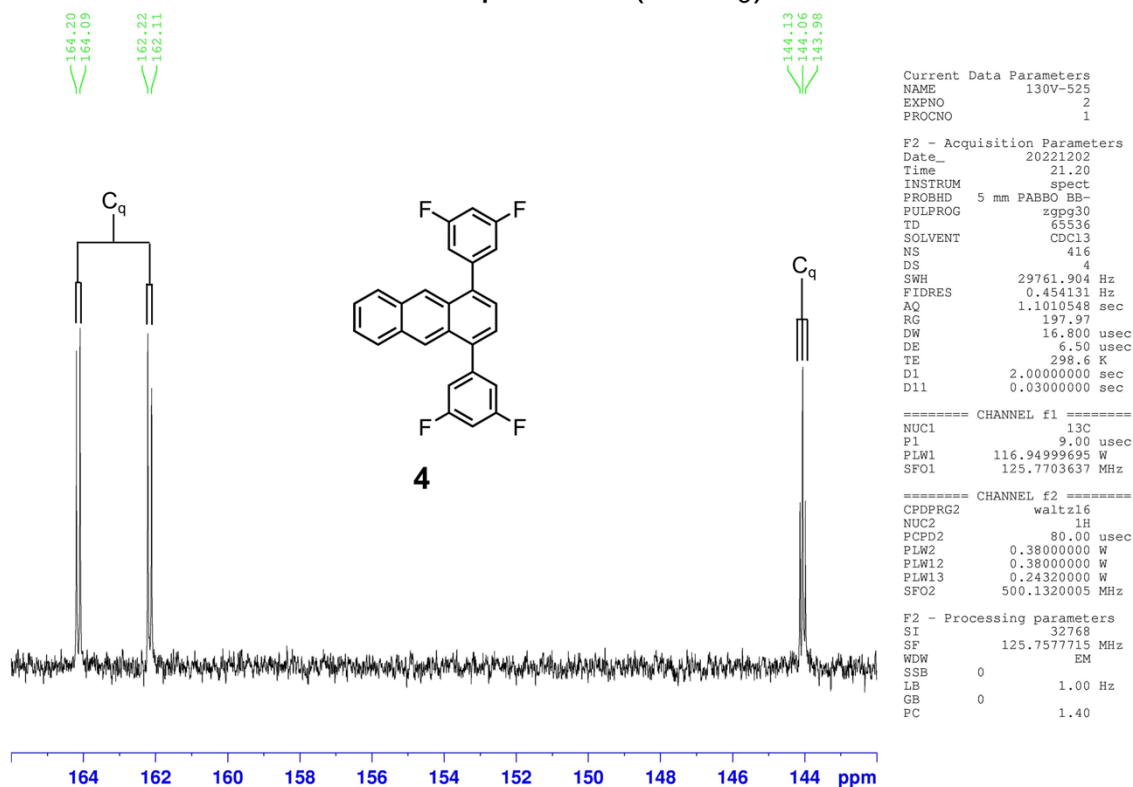
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PLW2 0.38000000 W
 PLW12 0.38000000 W
 PLW13 0.24320000 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577715 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

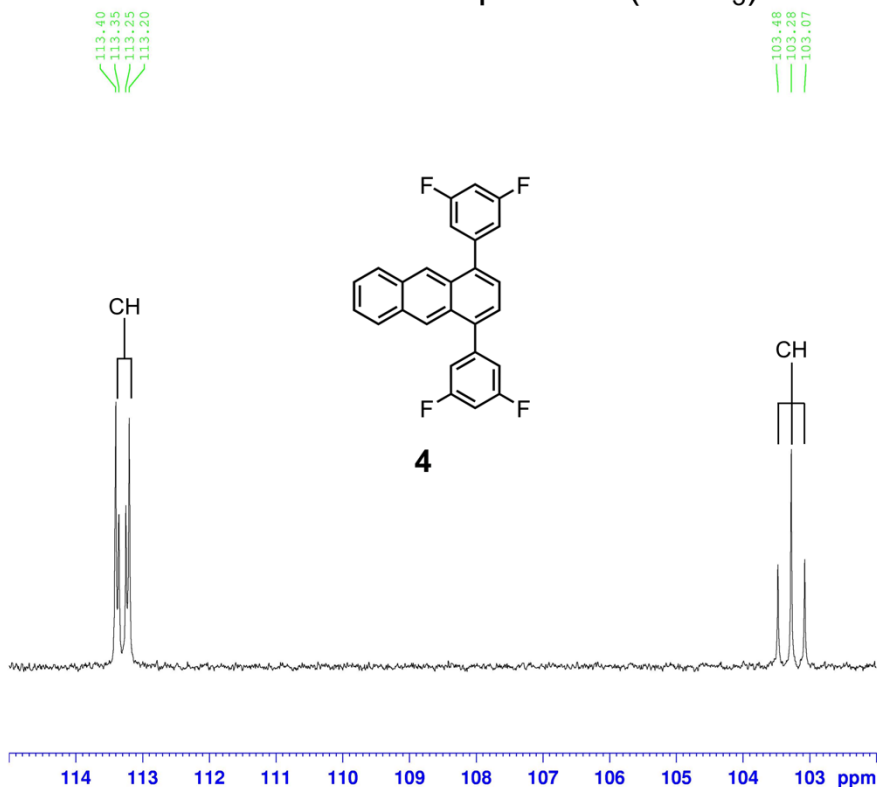
¹³C NMR spectrum (CDCl₃)



¹³C NMR spectrum (CDCl₃)



¹³C NMR spectrum (CDCl₃)



Current Data Parameters
NAME 130V-525
EXPNO 2
PROCNO 1

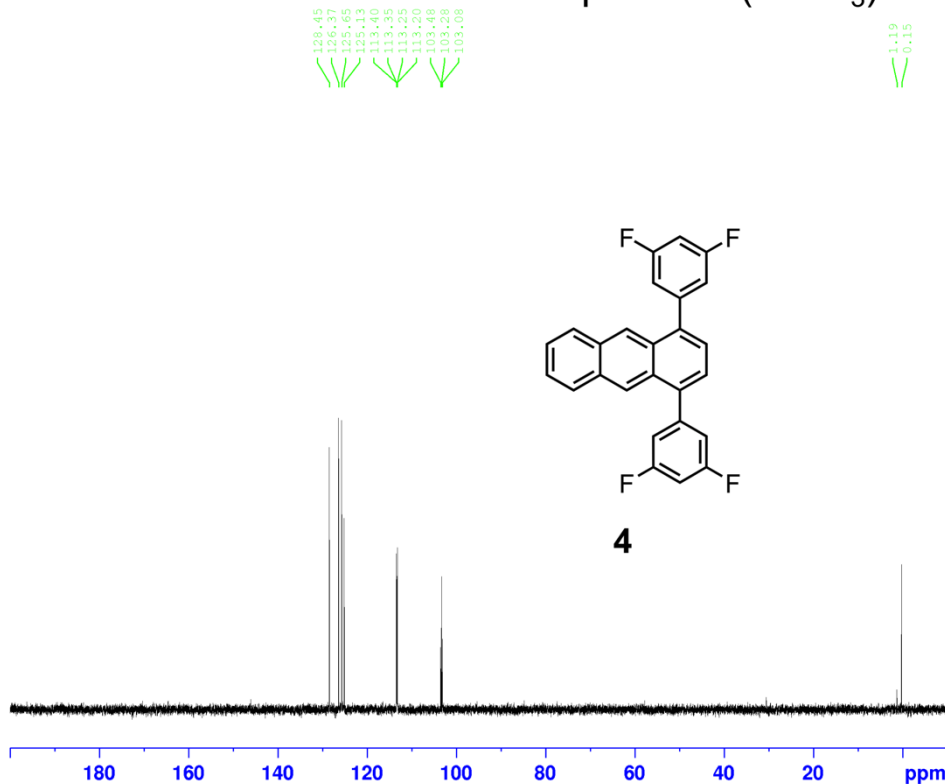
F2 - Acquisition Parameters
Date_ 20221202
Time 21.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 416
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 197.97
DW 16.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PLW1 116.94999695 W
SFO1 125.7703637 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 0.38000000 W
PLW12 0.38000000 W
PLW13 0.24320000 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577715 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

DEPT 135 NMR spectrum (CDCl₃)



Current Data Parameters
NAME 130V-525 (1,4-DFA 3,1
EXPNO 3
PROCNO 1

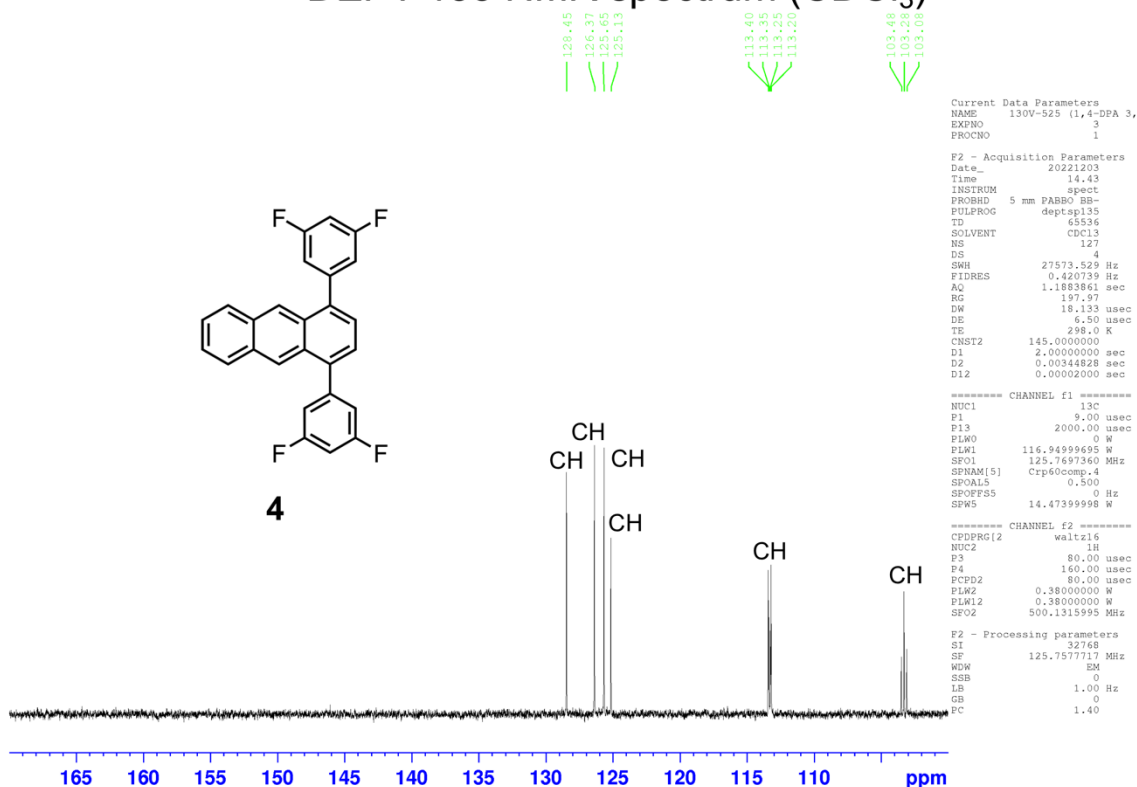
F2 - Acquisition Parameters
Date_ 20221203
Time 14.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 127
DS 4
SWH 27573.529 Hz
FIDRES 0.420739 Hz
AQ 1.1583861 sec
RG 197.97
DW 18.133 usec
DE 6.50 usec
TE 298.6 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 2000.00 usec
PLW0 0 W
PLW1 116.94999695 W
SFO1 125.7697360 MHz
SPNAM(5) Crp60comp.4
SFOAL5 0.500
SFOFF55 0 Hz
SPW5 14.47399998 W

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 80.00 usec
P4 160.00 usec
PCPD2 80.00 usec
PLW2 0.38000000 W
PLW12 0.38000000 W
SFO2 500.1315995 MHz

F2 - Processing parameters
SI 32768
SF 125.7577715 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

DEPT 135 NMR spectrum (CDCl₃)



¹⁹F NMR spectrum (CDCl₃)

