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Supporting Information

Tuning J-aggregate Formation and Emission Efficiency in Cationic Diazapentacenium Dyes

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Experimental Section

Materials

Chemicals were purchased from commercial suppliers and used without further purification, unless described otherwise. For the photophysical studies, all the solutions were prepared with solvents of spectroscopic grade (Uvasol) from Merck.

Photophysical Characterization

Sample preparation

An appropriate amount of powder of each compound was weighted to produce a stock solution of ~ 10^{-4} mol L^{-1} when diluted in 5.0 mL of spectroscopic grade solvent. Then, an aliquot of the stock solution was diluted with the proper amount of solvent to obtain the desired concentration (2.0, 5.0, 10, 25 and 50x10^{-6} mol L^{-1}) in 2.0 mL of final volume. The stock solutions were kept in the dark prior to use.

Steady state and time-resolved fluorescence measurements

The absorption spectra were recorded using Shimadzu UV-2450. Fluorescence spectroscopic studies were performed using Horiba-Jobin-Yvon Fluorolog 3-22 spectrofluorimeter. The fluorescence quantum yields (ϕ_F) of all compounds in solution were measured using the absolute method with a Hamamatsu Quantaurus QY absolute photoluminescence quantum yield spectrometer, model C11347 (integration sphere). The x and y color parameters were determined with the acquisition of the transmittance spectra of the samples in solution using Shimadzu UV-2600 equipped with Color Analysis software. The color parameters were determined according to the CIE (Commission Internationale de l'Eclairage proceedings) 1931 scale diagram[1].

Fluorescence decays were measured using a home-built Time-Correlated Single Photon Counting (TCSPC) apparatus, as described previously[2], using an IBH nanoLED (460 nm, 1.0 kHz) as excitation source. The fluorescence decays and the instrumental response function (IRF) were collected using 1024 channels in a time scale up to 97.1 ps/channel; alternate measurements (500 counts) of the pulse profile at the excitation wavelength and the sample emission were performed until 3kCounts at the maximum were reached. All samples were prepared immediately before the fluorescence decay acquisition and deaerated/purged with nitrogen for 20 min to avoid oxygen quenching. Deconvolution of

the fluorescence decay curves was performed using modulation function method in the SAND program (by G. Striker), as previously reported[3].

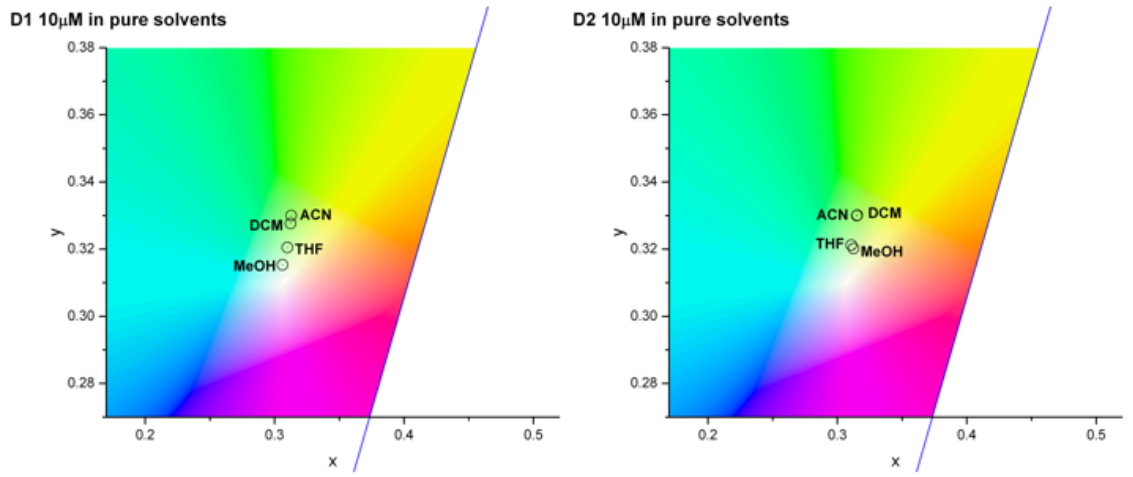


Figure SI1. Positions of the x/y chromaticity parameters of solutions of compounds **D1** and **D2** in acetonitrile (ACN), dichloromethane (DCM), methanol (MeOH) and tetrahydrofuran (THF), concentration: 10μmol L^{-1}, in the Commission Internationale de l'Eclairage (CIE) 1932 chromaticity diagram.

Table SI1. Color coordinates, following the Commission Internationale de l'Eclairage (CIE) 1932 chromaticity diagram scale, of diazapentacenium salt solutions (**D1** and D2) in the pure solvents acetonitrile (ACN), dichloromethane (DCM), methanol (MeOH) and tetrahydrofuran (THF), concentration: 10μmol L^{-1}.

Dyes	Solvent	x	y
D1	THF	0.3100	0.3205
	DCM	0.3124	0.3276
	MeOH	0.3062	0.3153
	MeCN	0.3129	0.3300
D2	THF	0.3109	0.3212
	DCM	0.3153	0.3301
	MeOH	0.3126	0.3202
	MeCN	0.3151	0.3300

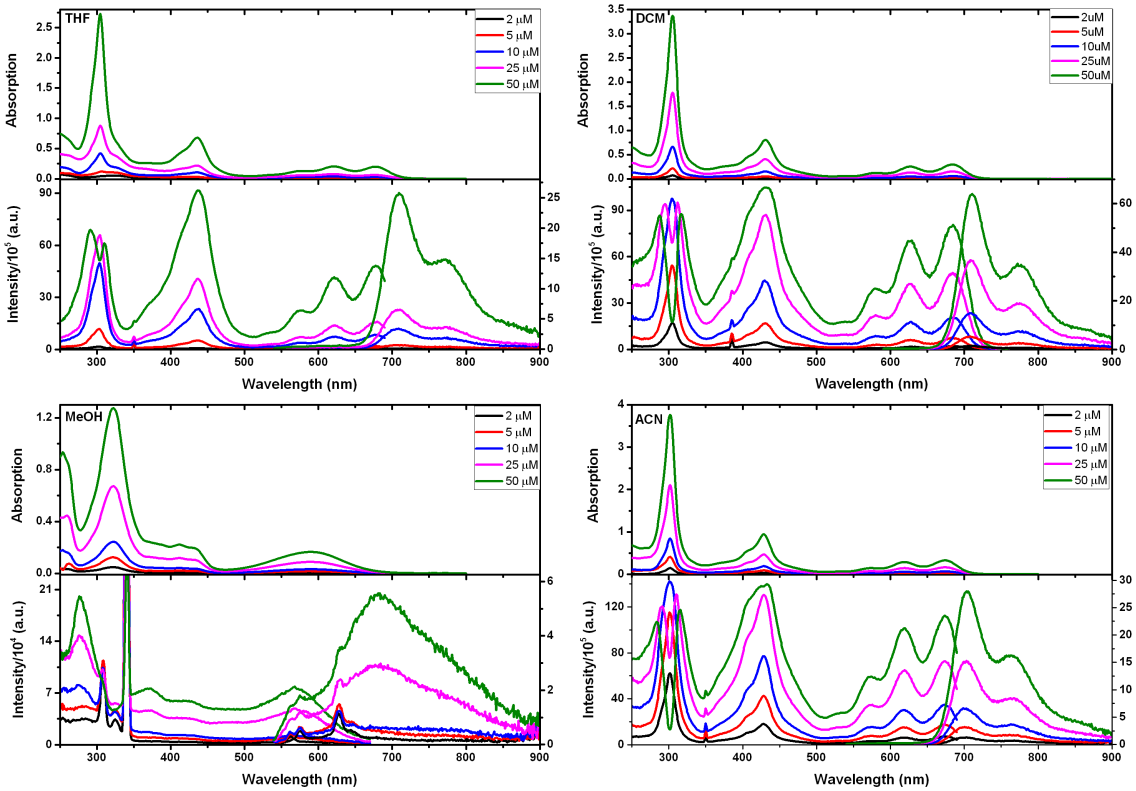


Figure SI2. Absorption, fluorescence excitation and emission spectra of **D1** tetrahydrofuran (THF), dichloromethane (DCM), methanol (MeOH) and acetonitrile (ACN) of increasing concentration, from 2.0×10^{-6} mol L^{-1} to 5.0×10^{-5} mol L^{-1}.

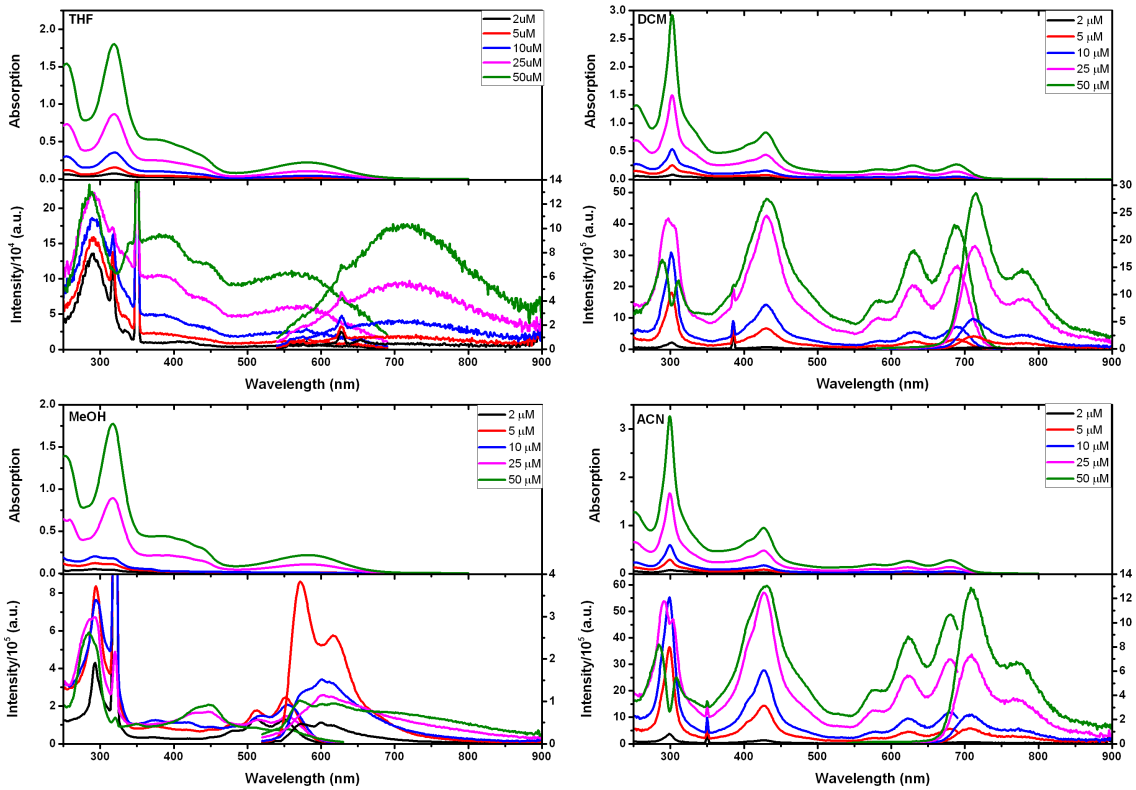


Figure SI3. Absorption, fluorescence excitation and emission spectra of **D2** in tetrahydrofuran (THF), dichloromethane (DCM), methanol (MeOH) and acetonitrile (ACN) of increasing concentration, from 2.0×10^{-6} mol L^{-1} to 5.0×10^{-5} mol L^{-1}.

Synthesis and structural characterization of diazapentacenes dyes

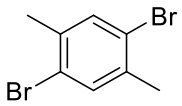
Methods

NMR spectra were recorded on a Bruker AVANCE 400 or AVANCE III 600. APCI (Atmospheric Pressure Chemical Ionization) and ESI (electrospray ionisation) mass spectra were obtained on a Bruker Daltronik micrOTOF system.

The melting points (Mp) of the diazapentacenium salts were measured using a Digital Melting Point (Electrothermal IA900) with a temperature range from 35-400ºC, with a rate of 2ºC per minute.

Synthesis of 1,4-Bis(4-decylbenzoyl)-2,5-dibromobenzene

1,4-Dibromo-2,5-dimethylbenzene[4]



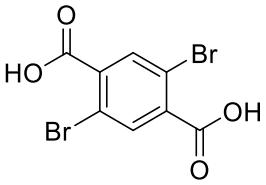
p-Xylene (23.09 mL, 188 mmol, 1.0 eq.) and iodine (0.24 g, 0.94 mmol, 0.005 eq.) are mixed with dichloromethane (DCM) (100 ml) in a two-necked flask and cooled down to 0 °C. Over a period of an hour bromine (20.3 mL, 396 mmol, 2.1 eq.) is added dropwise under exclusion of light. After adding the full amount of bromine, the reaction is stirred for additional 16 h at room temperature. Afterwards the reaction is completed by adding 20 % (w/w) aqueous potassium hydroxide solution (31.7 g, 565 mmol, 3.0 eq.). For workup the organic phase has been separated. The water phase was extracted two times with dichloromethane. The combined organic phases were washed two times with "brine", dried over magnesium sulfate, and concentrated. After recrystallization from methanol 1,4-dibromo-2,5-dimethylbenzene (25.04 g, 95.6 mmol) is obtained as a white crystalline solid in a 51 % yield.

^{1}H-NMR (400 MHz, $CDCl_3$, 300 K): δ [ppm] = 7,39 (s, 2H); 2,33 (s, 6H).

^{13}C^{1}H-NMR (101 MHz, $CDCl_3$, 300 K): δ [ppm] = 137,0; 133,9; 123,3; 22,1.

MS (APCI): m/z $[M]^+$ = 261,8987 $[M^+]$ (calc.: m/z = 261,8993).

2,5-Dibromoterephthalic acid [5]

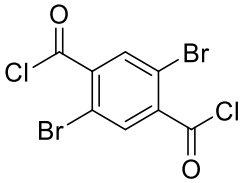


1,4-Dibromo-2,5-dimethylbenzene (20.00 g, 76 mmol, 1.0 eq.) and pyridine (220 ml) were placed into a 1 l-three-necked flask. The mixture is stirred and refluxed. Next, a warm solution of potassium permanganate (53.9 g, 341 mmol, 4.5 eq.) in water (150 ml) is added dropwise over a period of one hour. The reaction mixture is stirred under reflux overnight. After cooling to room temperature, the solid residue is filtered off and washed with water and ethyl acetate. The water phase is washed with ethyl acetate. Diluted, aqueous hydrochloric acid is added to the combined water phases until the mixture reaches a pH value of >3. The resulting white suspension is three times extracted with ethyl acetate. The combined organic phases are concentrated to dryness. The resulting solid is suspended in water with potassium hydroxide (5.14 g, 92 mmol, 1.2 eq.). The mixture is heated up to 90 °C, and potassium permanganate (16.8 g, 106 mmol, 1.4 eq.) in water (220 ml) is added dropwise over a period of one hour. Afterwards the reaction mixture is stirred overnight. After cooling down to room temperature, methanol (ca. 50 ml) is added. The solid precipitate is filtered off and washed with water. Dilute, aqueous hydrochloric acid is again added to the combined water phases until the mixture reaches a pH value of >3. The resulting white suspension is extracted with ethyl acetate, the organic phase washed two times with water, and one time with “brine”, dried over magnesium sulfate, and concentrated to dryness. The product 2,5-dibromoterephthalic acid (13.52 g, 42.0 mmol) is obtained as a white solid in an overall yield of 55%.

^{1}H-NMR (400 MHz, DMSO-d_6, 300 K): δ [ppm] =13,90 (s, 2H), 8,01 (s, 2H).

^{13}C^{1}H-NMR (101 MHz, DMSO-d_6, 300 K): δ [ppm] = 165,5; 137,0; 134,9; 118,7.

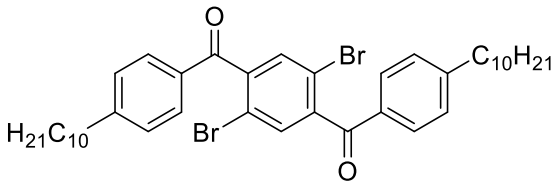
2,5-Dibromoterephthaloyl dichloride[6]



2,5-Dibromoterephthalic acid (6.5 g, 20.1 mmol, 1.0 eq.) is placed in a 50 ml-two-necked flask, together with dry toluene (20.0 ml). Afterwards thionyl chloride (9.1 ml,

125 mmol, 14.8 eq.) and DMF (0.5 ml) are injected into the reaction mixture. The reaction mixture is stirred and refluxed for two hours. The reaction mixture turns into a clear, yellow solution. The solvents and the excess of the thionyl chloride are removed under vacuum. 2,5-Dibromoterephthaloyl dichloride is obtained as a yellow solid and is used directly without further purification.

1,4-Bis(4-decylbenzoyl)-2,5-dibromobenzene[6]



In a heated three-necked flask 2,5-dibromoterephthaloyl dichloride (7.2 g, 19.95 mmol, 1.0 eq.) and aluminum (III) chloride (6.39 g, 47.89 mmol, 2,4 eq.) are suspended in dry dichloromethane (50 ml). Afterwards the mixture is cooled down to 0 °C and stirred.

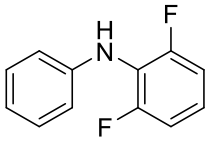
n-Decylbenzene (11.7 ml, 45.9 mmol, 2.3 eq.) is added dropwise to the mixture, and stirred at room temperature for 1 day. For workup a beaker is filled with aqueous hydrochloric acid (2M) and ice before the reaction mixture is poured into the beaker. After dilution with water and dichloromethane the organic phase is isolated. The organic phase is washed once with "brine" and two times with water, dried over magnesium sulfate, and concentrated to dryness. After recrystallization from acetone the product, 1,4-bis(4-decylbenzoyl)-2,5-dibromobenzene (9.51 g, 14.22 mmol), is obtained as a white solid in a 71 % yield.

^{1}H-NMR (400 MHz, $CDCl_3$, 300 K): δ [ppm] = 7,76 (d, *J* = 8,3 Hz, 4H), 7,58 (s, 2H), 7,32 (d, *J* = 8,3 Hz, 4H), 2,75 – 2,65 (m, 4H), 1,64 (q, *J* = 7,4 Hz, 4H), 1,30 (d, *J* = 23,6 Hz, 28H), 0,93 – 0,83 (m, 6H).

^{13}C^{1}H-NMR (101 MHz, $CDCl_3$, 300 K): δ [ppm] = 193,2; 150,2; 143,7; 133,5; 133,5; 130,8; 129,4; 118,2; 36,4; 32,1; 31,5; 29,4; 29,5; 29,4; 24,2; 15,1.

MS (APCI): m/z $[M]^+$ = 725,2428 (calc.: m/z = 725,2391).

2,6-Difluoro-N-phenylaniline[7]



In a heated two-necked flask iodobenzene (0.61 ml, 5.5 mmol, 1.0 eq.), sodium *tert*-butoxide (1.6 g, 16.0 mmol, 3.0 eq.) and palladium (ll) acetate (61 mg, 0.27 mmol, 0.05 eq.) are dissolved in toluene (100.0 ml). Afterwards, tri-*tert*-butylphosphine (0.2 mL, 0.82 mmol, 0.15 eq.) and 2,6-difluoroaniline (0.65 ml, 6.0 mmol, 1.1 eq.) are injected to the reaction mixture. The mixture is heated up under stirring to 120 °C for 16 h. For workup, the mixture is extracted three times with dichloromethane at room temperature, and the organic phase washed two times with water and once with "brine". The organic phase is dried over magnesium sulfate and concentrated to dryness. The raw product is purified by column chromatography (stationary phase: silica gel, eluent: N-hexane/ethyl acetate, 19/1). The combined organic phases are concentrated to dryness and the product dried. After recrystallization from acetone the product, 2,6-difluoro-N-phenylaniline (0.65 g, 3.2 mmol), is obtained as an orange oil in 58 % yield.

^{1}H-NMR (600 MHz, $CDCl_3$, 300 K): δ [ppm] = 7,47 – 7,44 (m, 2H), 7,26 – 7,22 (m, 1H), 7,17 (t, *J* = 7,8 Hz, 2H), 7,13 (t, *J* = 7,4 Hz, 1H), 7,03 (d, *J* = 7,5 Hz, 2H), 5,68 (s, 1H).

^{13}C^{1}H-NMR (151 MHz, $CDCl_3$, 300 K): δ [ppm] = 157,7; 156,1; 156,0; 143,7; 129,2; 123,4; 120,9; 116,0; 112,1; 112,1; 112,0; 111,9; 77,2.

^{19}F-NMR (376 MHz, $CDCl_3$, 300 K): δ [ppm] = -120,44 (t, *J* = 6,9 Hz).

MS (FD): m/z $[M]^+$ = 205,06790 (calc.: m/z = 205,07031).

Synthesis of precursors PCH and PCF

The synthesis of the diazapentacene precursors[8] 1,4-Bis(N,N-diphenylamino) -2,5-bis(4-decylbenzoyl)benzene (**PCH**) and 1,4-bis(N-phenyl-N-2,5-difluorophenylamino)-2,5-bis(4-decylbenzoyl)benzene (**PCF**, Scheme 1) started with the preparation of 1,4-bis(4-decylbenzoyl)-2,5-dibromobenzene, in a four step procedure from *p*-xylene (for further details, see *Support Information*). In a heated two-necked flask the diphenylamine monomer (2.2 eq.), 1,4-bis(4-decylbenzoyl)-2,5-dibromobenzene (1.0 eq.), sodium *tert*-butoxide (3.0 eq.) and palladium (ll) acetate (0.05 eq.) are dissolved in toluene (15.0 ml). Afterwards tri-*tert*-butylphosphine (0.15 eq.) is injected and the reaction mixture heated up to 120 °C and stirred for 16 h. For workup the reaction is extracted three times with DCM at room temperature, two times washed with water and once with "brine". The

isolated organic phase is dried over magnesium sulfate and concentrated to dryness. The raw product is purified by column chromatography (stationary phase: silica gel, eluent: n-hexane/ethyl acetate, 9/1). After column chromatography the product still contains small amounts of impurities, which are removed by washing with hot methanol. The products **PCH** and **PCF** are obtained as yellow neon-colored crystalls in yields of 32 % (0.4 g, 0.44 mmol) and 38 % (0.52 g, 0.53 mmol), respectively.

PCH: **^{1}H-NMR** (400 MHz, $CDCl_3$, 300 K): δ [ppm] = 7,45 (d, *J* = 8,2 Hz, 4H), 7,25 (s, 2H), 7,10 – 7,04 (m, 12H), 6,91 – 6,85 (m, 8H), 6,83 (dt, *J* = 7,2, 1,2 Hz, 4H), 2,58 (t, *J* = 7,6 Hz, 4H), 1,55 (dd, *J* = 15,0, 7,7 Hz, 4H), 1,32 – 1,22 (m, 28H), 0,90 – 0,85 (m, 6H). **^{13}C^{1}H-NMR** (101 MHz, $CDCl_3$, 300 K): δ [ppm] = 191,8; 151,2; 149,0; 143,0; 129,2; 123,9; 122,9; 118,0; 99,9; 77,2; 33,3; 31,2; 29,8; 29,6; 29,5; 29,3; 14,3. **MS** (APCI): m/z $[M+H]^+$ 901,5708 (calc.: m/z = 901,5667).

PCF: **^{1}H-NMR** (400 MHz, $CDCl_3$, 300 K): δ [ppm] = 7,52 (d, *J* = 8,3 Hz, 4H), 7,19 (s, 2H), 7,15 – 7,10 (m, 2H), 7,12 – 7,07 (m, 4H), 6,92 – 6,88 (m, 8H), 6,88 – 6,80 (m, 2H), 6,64 (t, *J* = 8,4 Hz, 4H), 2,59 (t, *J* = 7,6 Hz, 4H), 1,56 (d, *J* = 12,6 Hz, 4H), 1,36 – 1,19 (m, 28H), 1,02 – 0,78 (m, 6H). **^{13}C^{1}H-NMR** (101 MHz, $CDCl_3$, 300 K): δ [ppm] = 194,3; 149,2; 146,7; 140,4; 136,1; 133,9; 129,9; 129,2; 128,3; 126,2; 122,8; 120,9; 112,6; 112,4; 36,2; 32,1; 31,2; 29,8; 29,7; 29,6; 29,5; 29,3; 22,8; 14,3. **^{19}F-NMR** (376 MHz, $CDCl_3$, 300 K): δ [ppm] = -115,7. **MS** (FD): m/z $[M]^+$ = 972,52420 (calc.: m/z = 972,52169).

Synthesis of the diazapentacenium salts D1 and D2

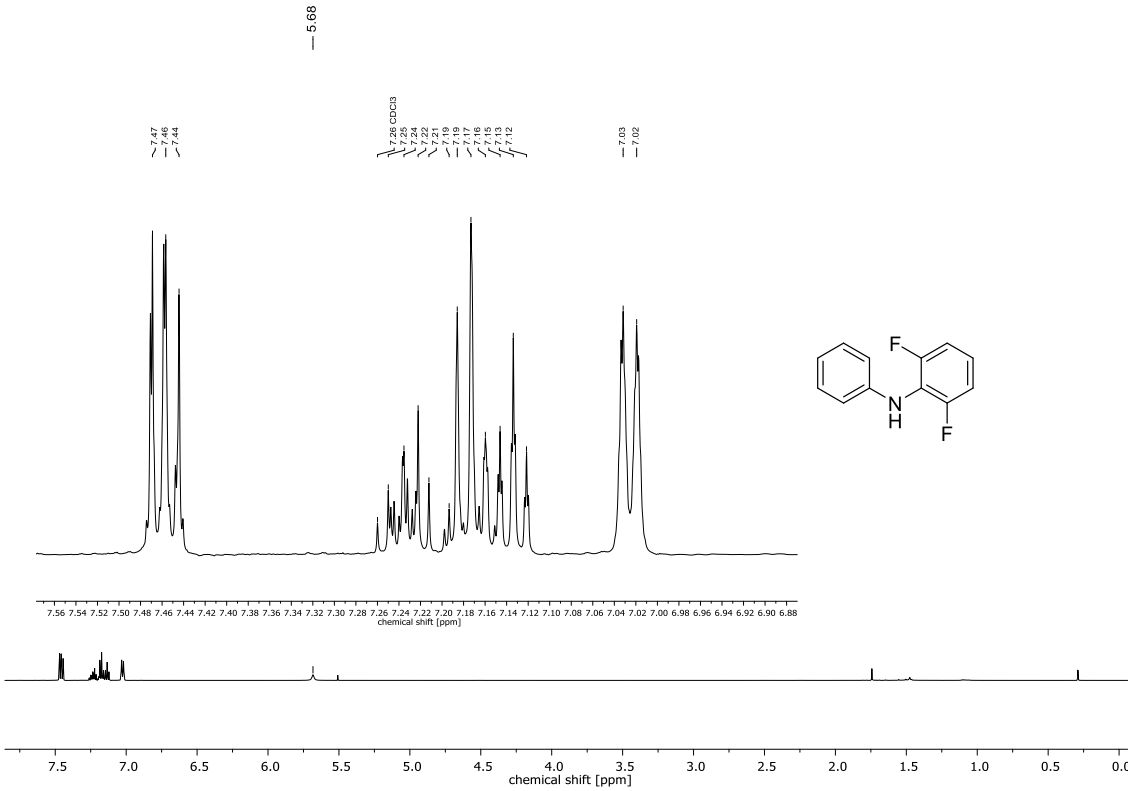
The precursors **PCH** (0.11 g, 0.12 mmol. 1.0 eq.) or **PCF** (0.21 g, 0.22 mmol. 1.0 eq.) were dissolved in dry toluene (5.0 ml) in a microwave vessel under argon. Afterwards trifluoromethanesulfonic acid (TFMSA) (10.0 eq.) is injected dropwise. The reaction mixture was stirred at 50 °C for 3 h. For workup the organic phase was extracted three times with DCM, filtrated over silica gel and the silica gel washed with DCM (1.00 l). The organic phase is concentrated to dryness. The products **7**,14-Bis(4-decylphenyl)-5,12-diphenyl-5,12-diazapentacenium bistriflate, **D1**, (0.10 g, 0.12 mmol) and **7,14-**bis(4-decylphenyl)-5,12-bis(2,6-difluorophenyl)-5,12-diazapentacenium bistriflate, **D2**, (0.20 g, 0.22 mmol) are obtained in quantitative yields as dark green solids.

D1: **^{1}H-NMR** (400 MHz, $CDCl_3$/TFA-d_1, 300 K): δ [ppm] = 8,46 (s, 2H), 8,25 (t, *J* = 10,3 Hz, 4H), 7,81 (m, 8H), 7,64 (d, *J* = 9,0 Hz, 2H), 7,59 – 7,52 (m, 4H), 7,44 (d, *J* = 7,6 Hz, 4H), 7,38 (d, *J* = 7,8 Hz, 4H), 2,82 (t, 4H), 1,80 (dt, *J* = 15,8, 7,4 Hz, 4H), 1,59 – 1,23 (m, 28H), 0,93 (t, 6H). **^{13}C^{1}H-NMR** (101 MHz, $CDCl_3$/TFA-d_1, 300 K): δ [ppm] = 132,5;

132,0; 131,0; 129,5; 128,0; 77,2; 32,2; 31,8; 29,9; 29,8; 29,6; 22,9; 14,0. **^{19}F-NMR** (376 MHz, $CDCl_3$, 300 K): δ [ppm] = -76,16. **MS** (FD): m/z [M-TfO-TfO^-] = 866,5525 (calc.: m/z = 866,5534). Mp > 400ºC (decomposition).

D2: **^{1}H-NMR** (400 MHz, $CDCl_3$, 300 K): δ [ppm] = 8,48 (s, 2H, H_1), 8,39 (d, *J* = 5,8 Hz, 2H), 8,34 (d, *J* = 9,0 Hz, 2H), 7,89 (t, *J* = 8,9, 6,6 Hz, 2H), 7,81 (dddd, *J* = 15,1, 9,2, 6,5, 3,0 Hz, 2H), 7,71 (d, *J* = 9,2 Hz, 2H), 7,55 (d, *J* = 8,1 Hz, 4H), 7,49 (d, *J* = 8,1 Hz, 4H), 7,41 (dd, *J* = 8,7, 7,2 Hz, 3H), 2,81 (dd, *J* = 9,2, 6,6 Hz, 4H), 1,75 (m, 4H), 1,58 – 1,17 (m, 28H), 1,00 – 0,81 (t, 8H). **^{13}C^{1}H-NMR** (101 MHz, $CDCl_3$, 300 K): δ [ppm] = 148,4; 146,1; 145,3; 131,4; 129,6; 129,4; 127,8; 123,1; 120,4; 117,3; 114,1; 36,2; 32,1; 31,8; 29,8; 29,7; 29,5; 22,8; 14,2. **^{19}F-NMR** (376 MHz, $CDCl_3$, 300 K): δ [ppm] = -78,64; -115,22. **MS** (FD): m/z [M-TfO-TfO^-] = 938,52272 (calc.: m/z = 938,51621). Mp > 400ºC (decomposition).

NMR Data



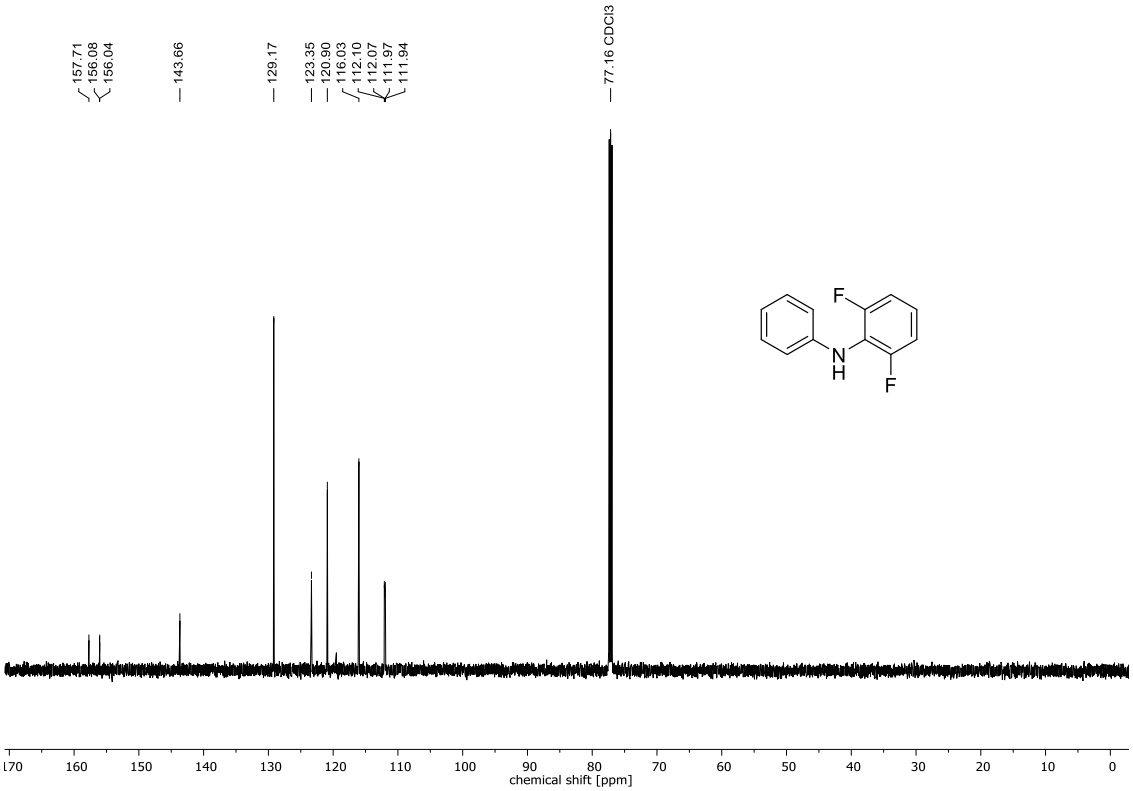


Figure SI4. ^{1}H NMR (top) and $^{13}C\{1H\}$ NMR spectra (bottom) of 2,6-difluoro-N-phenylaniline in $CDCl_3$.

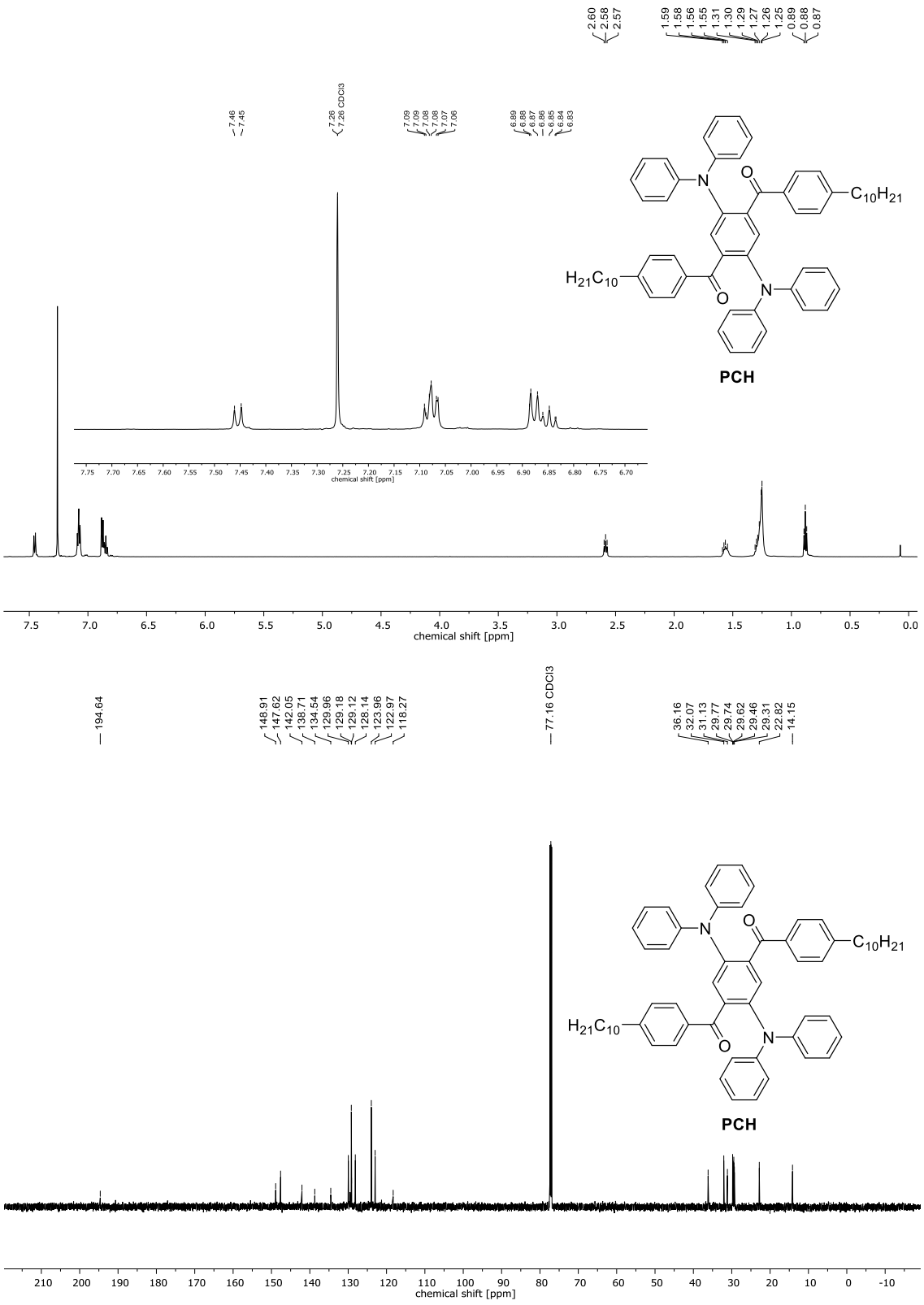


Figure SI5. ^{1}H NMR (top) and $^{13}C\{1H\}$ NMR spectra (bottom) of **PCH** in $CDCl_3$.

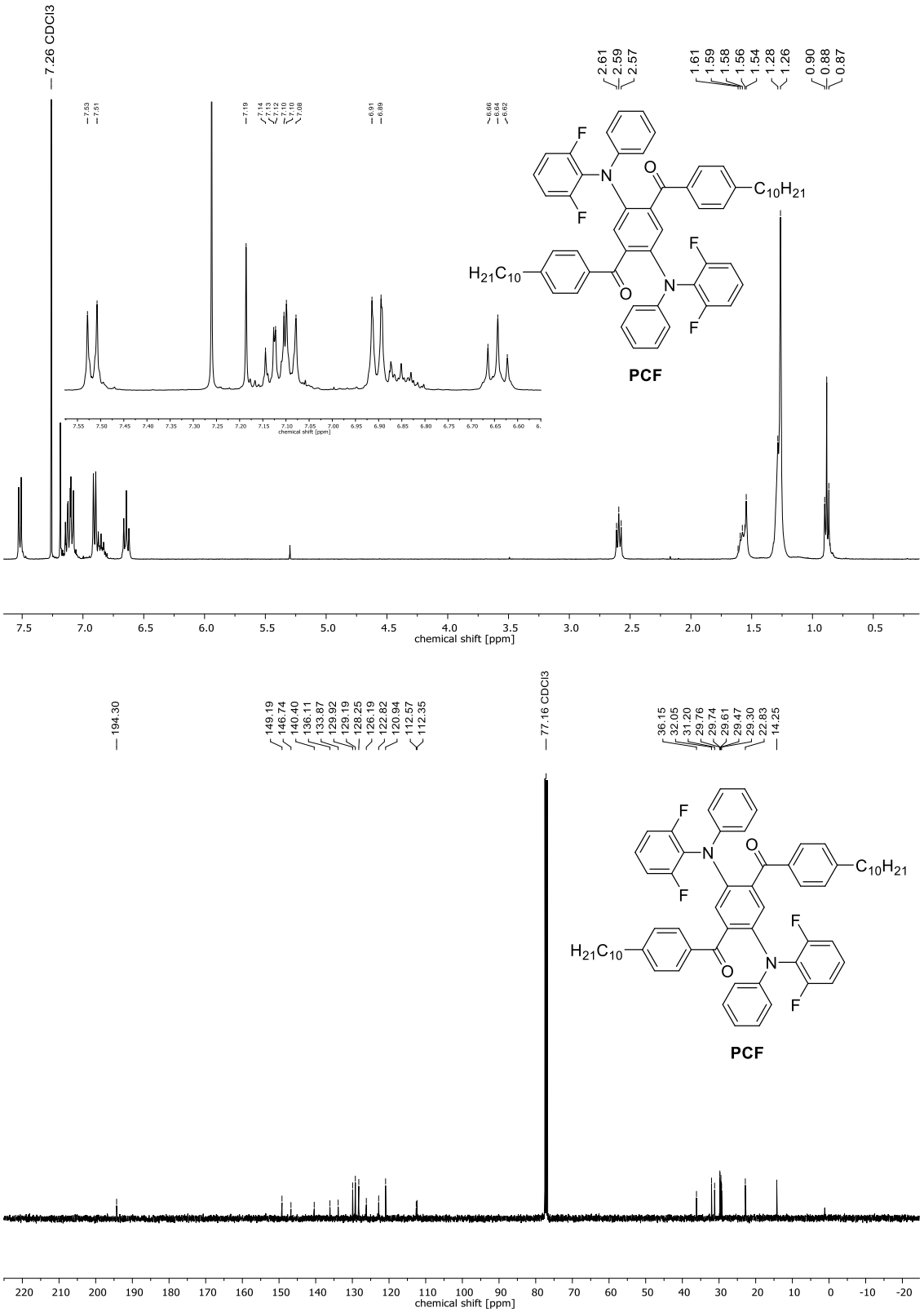


Figure SI6. ^{1}H NMR (top) and $^{13}C\{1H\}$ NMR spectra (bottom) of **PCF** in $CDCl_3$.

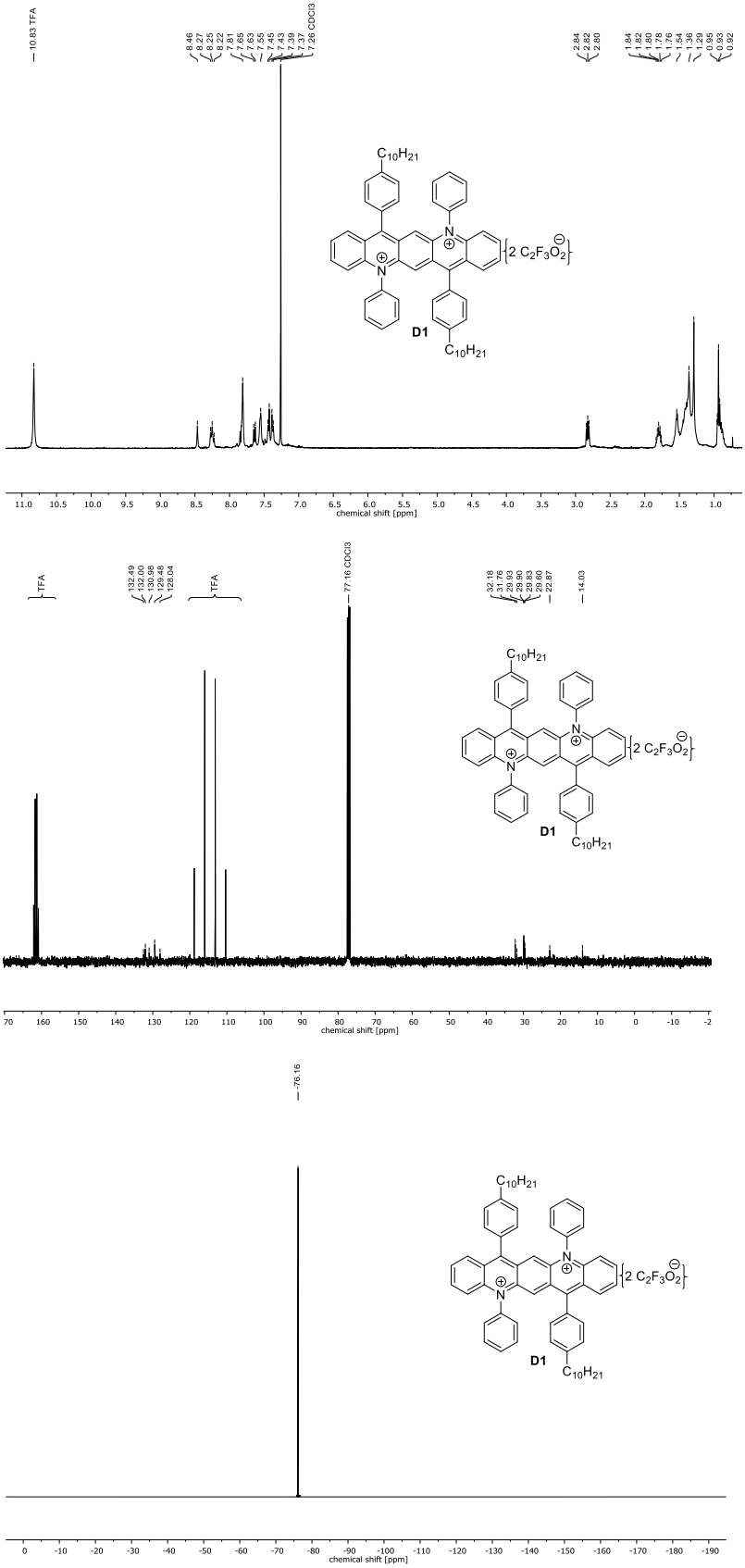


Figure SI7. ^{1}H NMR (top), ^{13}C{1H} NMR (center), ^{19}F NMR spectra (bottom) of **D1** in $CDCl_3$. (Please note: the solubility in $CDCl_3$/TFA is not sufficiently high for recording

better resolved $^{13}C\{1H\}$ NMR spectra, signal overlap may further reduce the number of observed carbons).

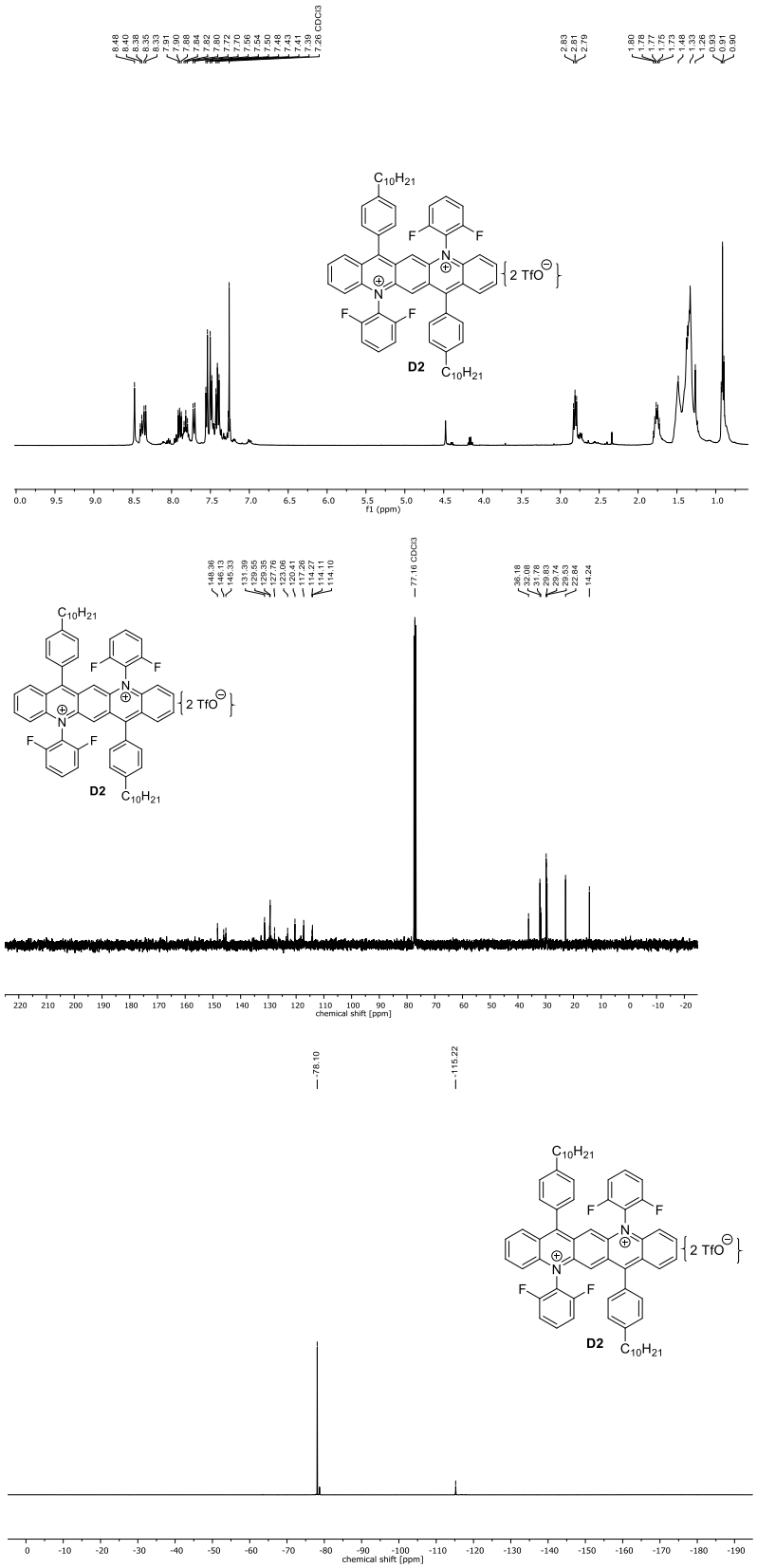
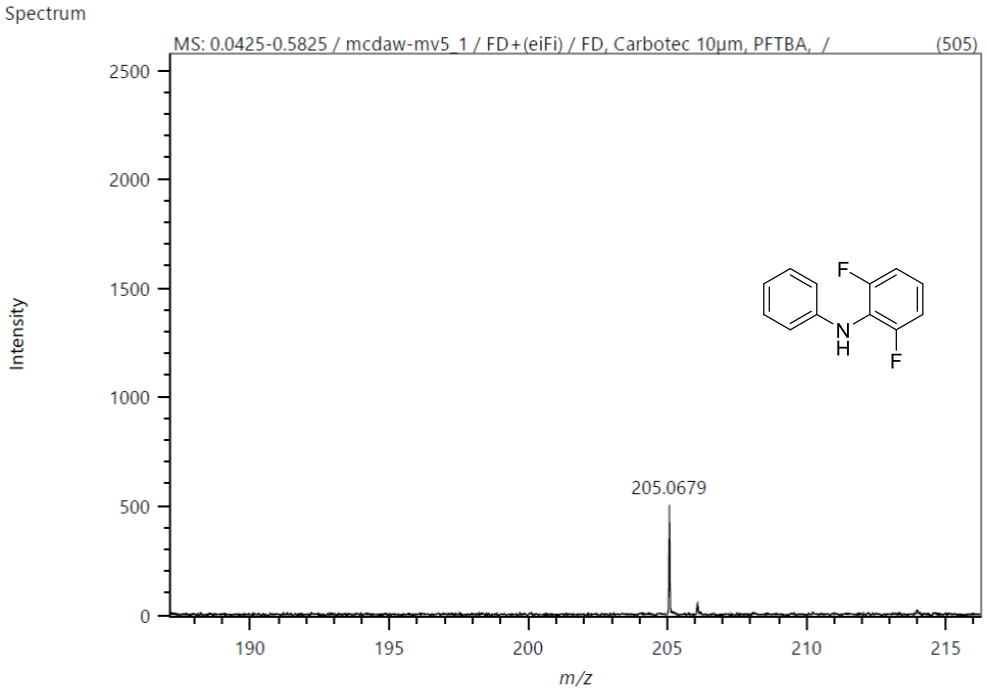


Figure SI8. ^{1}H NMR (top), $^{13}C\{1H\}$ NMR (center), ^{19}F NMR spectra (bottom) of **D2** in $CDCl_3$. (Please note: the solubility in $CDCl_3$ is not sufficiently high for recording better

resolved $^{13}C\{1H\}$ NMR spectra, signal overlap may further reduce the number of observed carbons).

Mass Data



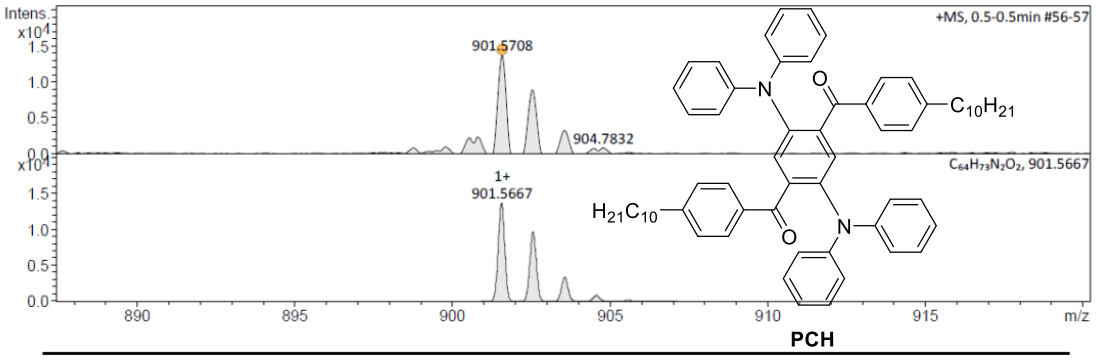
Elemental Composition

Parameters		Elements Set 4:				
Tolerance:	2.50 mDa	Symbol	C	H	N	F
Electron:	Odd/Even	Min	0	0	0	0
Charge:	0	Max	15	10	2	5
DBE:	0.0 - 100.0					

Results

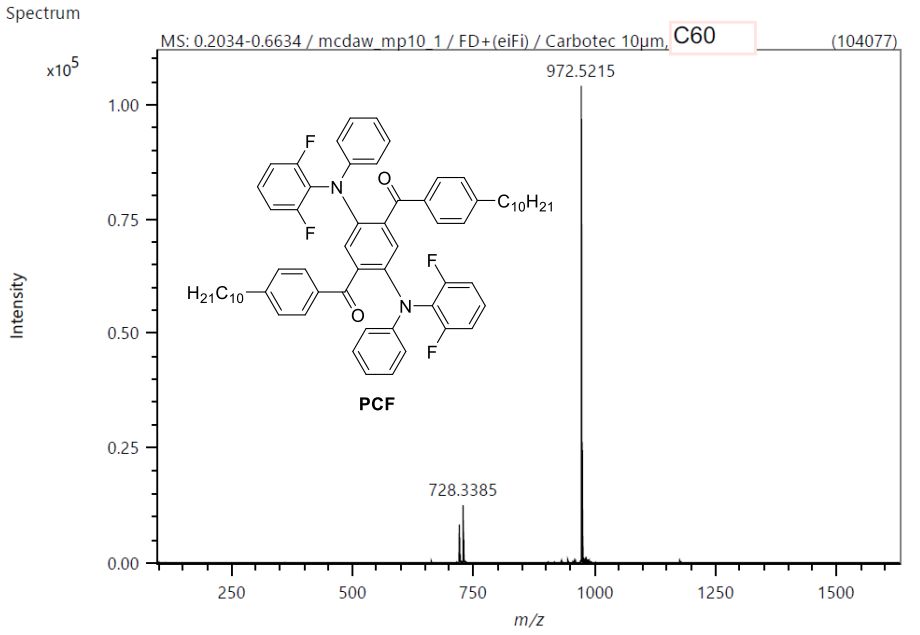
Mass	Intensity	Intensity [%]	Formula	Calculated Mass	Mass Difference [mDa]	DBE
205.06790	504.88	3.91	C12 H9 N F2	205.07031	-2.41	8.0

Figure SI9. FD-mass spectrum spectrum of 2,6-difluoro-N-phenylaniline.



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
901.5708	1	C64H73N2O2	901.5667	-4.6	37.9	1	100.00	29.5	even	ok

Figure SI10. APLCI mass spectrum of **PCH**.



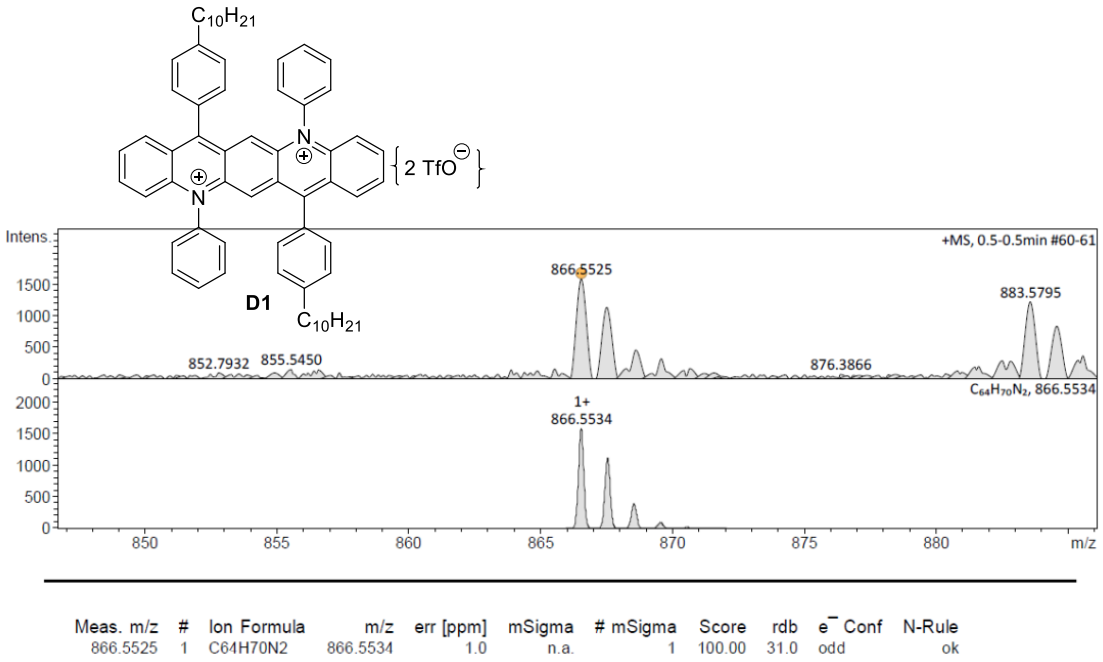
Elemental Composition

Parameters		Elements Set 4:					
Tolerance:	1.00 mDa	Symbol	C	H	O	N	F
Electron:	Odd/Even	Min	0	0	0	0	4
Charge:	0	Max	65	70	5	5	4
DBE:	1.0 - 80.0						

Results

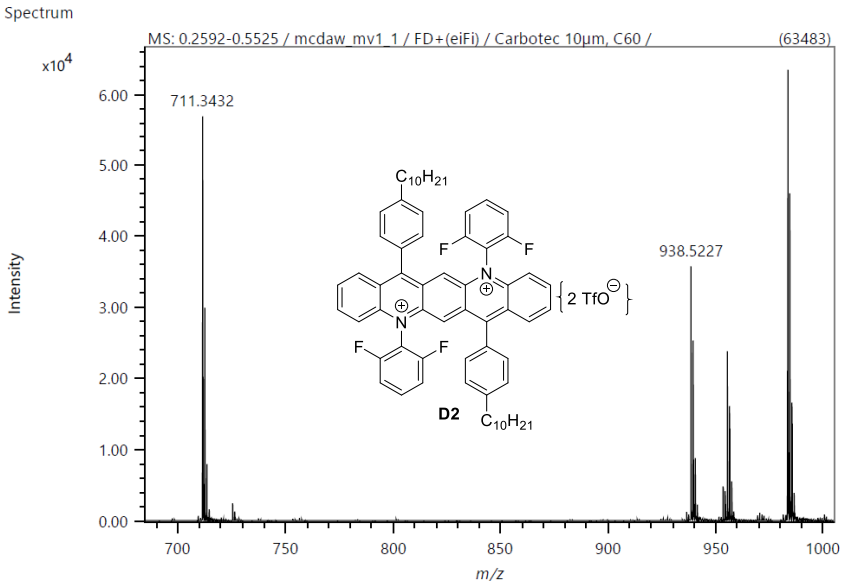
Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	DBE
972.52152	104077.31	C64 H68 N2 O2 F4	972.52169	-0.17	30.0

Figure SI11. FD mass spectrum of **PCF**.



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
866.5525	1	C64H70N2	866.5534	1.0	n.a.	1	100.00	31.0	odd	ok

Figure SI12. FD mass spectrum of **D1**.



Elemental Composition

Parameters		Elements Set 4:				
Tolerance:	6.60 mDa	Symbol	C	H	N	F
Electron:	Odd/Even	Min	0	0	0	0
Charge:	0	Max	65	70	5	5
DBE:	0.0 - 80.0					

Results

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	DBE
938.52272	35803.93	C60 H67 N4 F5	938.52859	-5.87	27.0
		C65 H68 N F4	938.52879	-6.07	30.5
		C64 H66 N2 F4	938.51621	6.51	31.0

Figure SI13. FD mass spectrum of **D2**.

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