Supporting Information for

Studies of cyanomethylcarbamoyl-bridged anthracene and pyrene fluorophores

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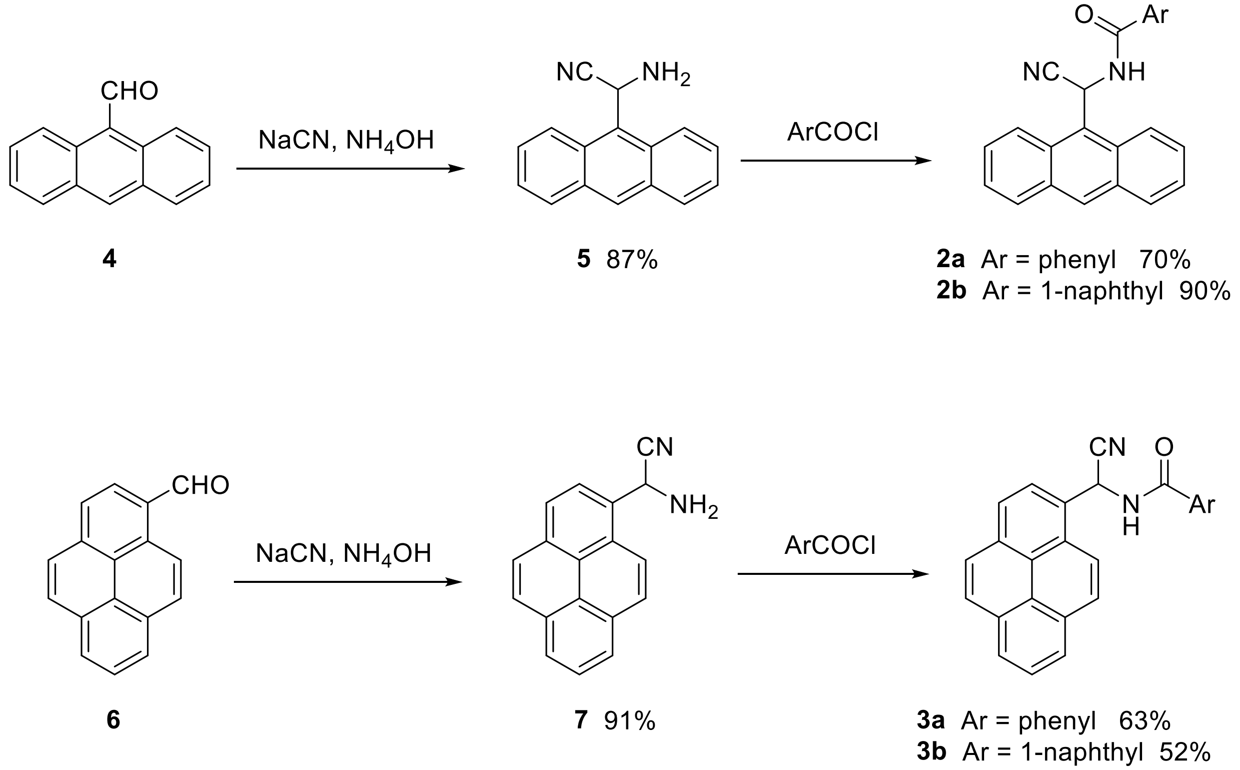
1. Synthetic Procedures for Compounds 2-3



Scheme S-1 Stepwise synthetic procedures for compounds **2-3**.

General Procedure for the synthesis of α-aminonitriles 5 and 7

α-Aminonitriles **5** and **7** were prepared according to the literature procedure.[1] A cooled mixture of the corresponding aldehyde (1.0 mmol) in ammonium hydroxide (20 mL) and ethanol (10 mL) was stirred for 10 min. Sodium cyanide (NaCN) (0.050 g, 1.0 mmol) was added in small portions. Ammonium chloride (0.053 g, 1.0 mmol) was then added to the solution. The flask was securely stoppered and left under continuous stirring for 24 h at rt. The resulting product was extracted with chloroform (2 ×15 mL). The organic layers were combined and dried over anhydrous $MgSO_4$. The organic solvent was removed under reduced pressure to give α-aminonitriles as a solid.

2-Amino-2-(anthracen-9-yl)acetonitrile (5). 9-Anthracenecarboxaldehyde (0.21 g, 1.0 mmol) was reacted according to the general procedure, yielding compound **5** (0.18 g, 87%) as an orange solid. m.p. 143-145 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.57 (1 H, s), 8.50 (2 H, d, J =9.0), 8.10

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[1] Younes, E. A.; Hussein, N.; Shtaiwi, M.; Shahrokhi, F.; Safieh, K. A. A.; Zhao, Y. N-(Cyano(naphthalen-1-yl)methyl)benzamides: Synthesis, Crystal Structures, and Colorimetric Sensing of Fluoride Anions. *New J. Chem.* **2020**, *44*, 16546-16556.

(2 H, d, *J* = 8.5), 7.68 (2 H, ddd, *J* = 9.0, 6.6, 1.4), 7.60 -7.53 (2 H, m), 6.41 (1 H, s), 3.75 (1 H, q, *J* = 7.0), 2.31 (1 H, s) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 131.63, 130.06, 129.81, 128.92, 127.46, 125.32, 122.94, 121.41, 40.93 ppm; HRMS (APPI-TOF, negative mode) *m/z* calcd. for $C_{16}H_{12}N_2$ 232.1000; found 232.0999 $[M]^{+\cdot}$.

2-Amino-2-(pyren-1-yl)acetonitrile (7). 1-Pyrenecarboxaldehyde (0.23g, 1.0 mmol) was reacted according to the general procedure, yielding compound **7** (0.21g, 91%) as yellow solid. m.p. 116-119 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.51 (1 H, d, *J* = 9.3), 8.43- 8.27 (5 H, m), 8.28- 8.18 (2 H, m), 8.13 (1 H, t, *J* = 7.6), 6.09 (1 H, s), 3.13 (2 H, d, *J* = 7.2) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ 131.78, 131.37, 131.22, 130.61, 128.49, 128.25, 127.83, 127.76, 127.00, 126.19, 126.05, 125.41, 125.32, 124.55, 124.21, 123.36, 122.87, 44.70 ppm; HRMS (APPI-TOF, positive mode) m/z calcd. for $C_{18}H_{14}N_2$ 256.1000; found 256.0994 $[M]^{+\cdot}$.

General procedure for acylation reaction

To a solution of (1.0 mmol) acyl chloride in dry THF (15 mL) at 0 °C were added α-aminonitrile (1.0 mmol) and then triethylamine (1.0 mL). The resulting mixture was allowed to be slowly warmed up to room temperature and stirred for 3 h. The white precipitate of triethylammonium chloride was then removed by suction filtration. The solution was subjected to evaporation under reduced pressure, and the resulting crude solid product was purified by recrystallization from ethanol/water to afford pure acylated product.

***N*-(anthracen-9-yl(cyano)methyl)benzamide (2a)**. Benzoyl chloride (0.14 g, 1.0mmol) and 2-amino-2-(anthracen-9-yl)acetonitrile (**5**) (0.23g, 1.0 mmol) were reacted according to the general procedures, yielding compound **2a** (0.10g, 70%) as an orange solid.

***N*-(anthracen-9-yl(cyano)methyl)-2-naphthamide (2b).** 1-Naphthoyl chloride (0.19 g, 1.0mmol) and 2-amino-2-(anthracen-9-yl)acetonitrile (**5**) (0.23 g, 1.0 mmol) were reacted according to the general procedures, yielding compound **2b** (0.42g , 90%) as an white solid.

***N*-(cyano(pyren-1-yl)methyl)benzamide (3a).** Benzoyl chloride (0.14 g, 1.0 mmol) and 2-amino-2-(pyren-1-yl)acetonitrile (**7**) (0.26g, 1.0 mmol) were reacted according to the general procedures, yielding compound **3a** (0.24 , 63%) as a pale yellow solid.

***N*-(cyano(pyren-1-yl)methyl)-2-naphthamide (3b). 1-**Naphthoyl chloride (0.19 g, 1.0 mmol) and 2-amino-2-(pyren-1-yl)acetonitrile (**7**) (0.26g, 1.0 mmol) were reacted according to the general procedures, yielding compound **3b** (0.13 g , 52%) as a white solid.

2. NMR Spectra of Compounds 2-3

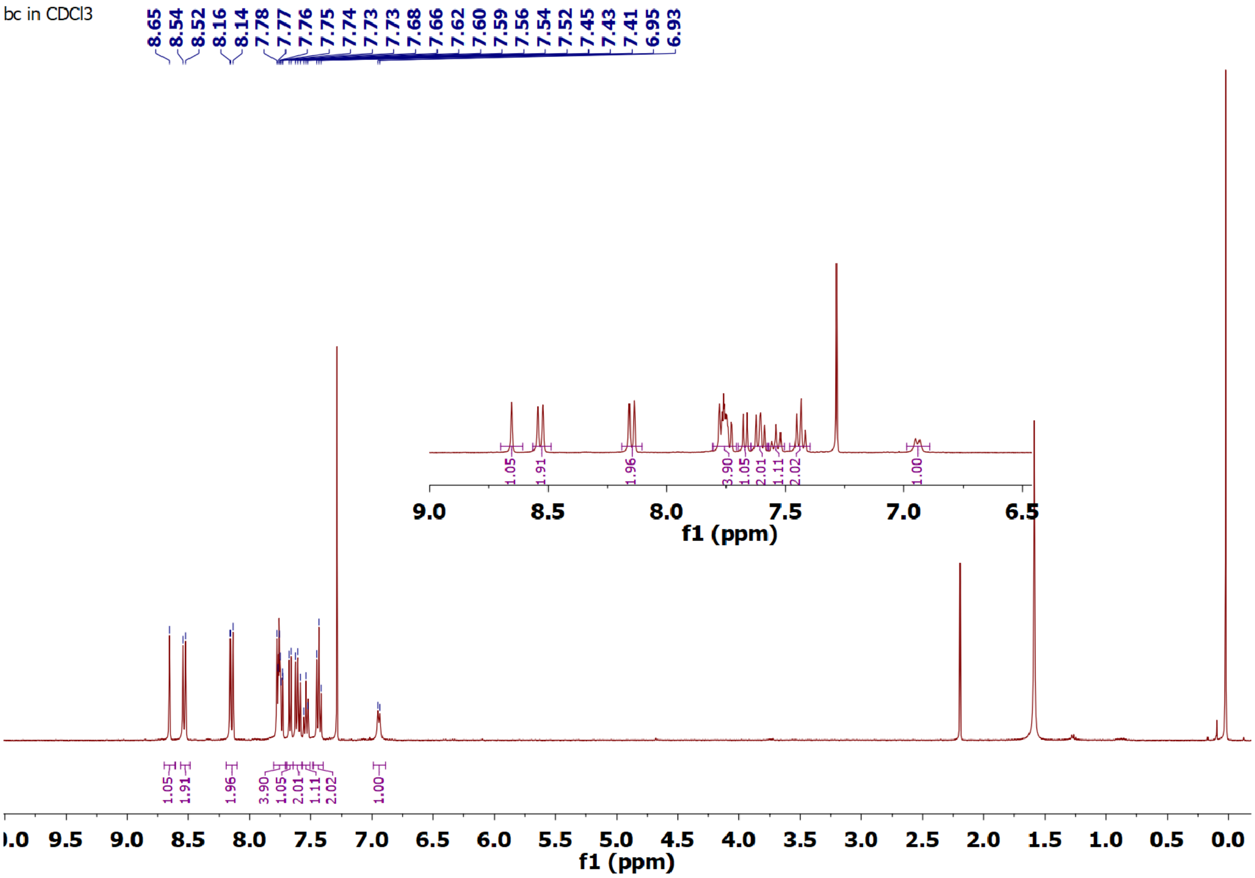


Fig. S-1 ^{1}H NMR (400 MHz, CDCl$_3$) spectrum of compound **2a**.

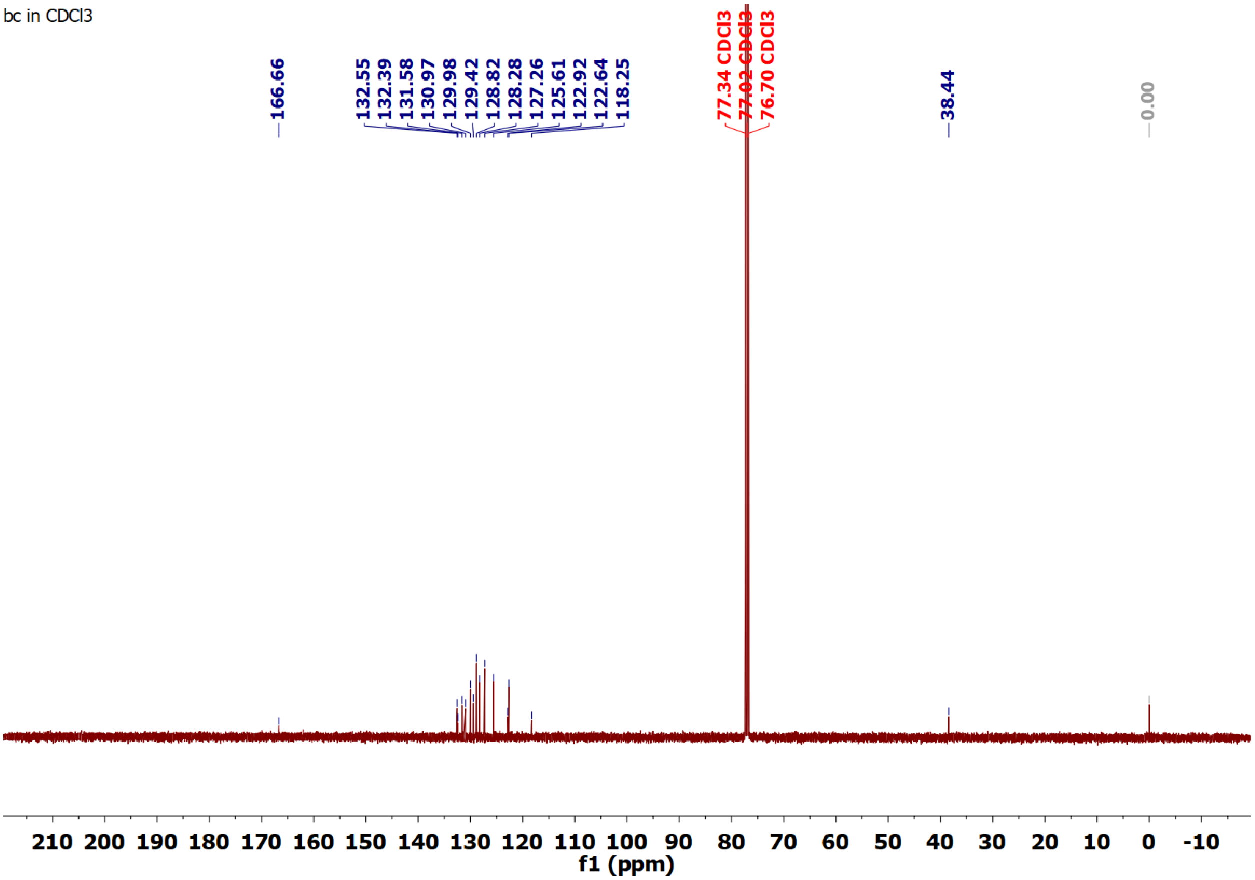


Fig. S-2 ^{13}C NMR (100 MHz, CDCl$_3$) spectrum of compound **2a**.

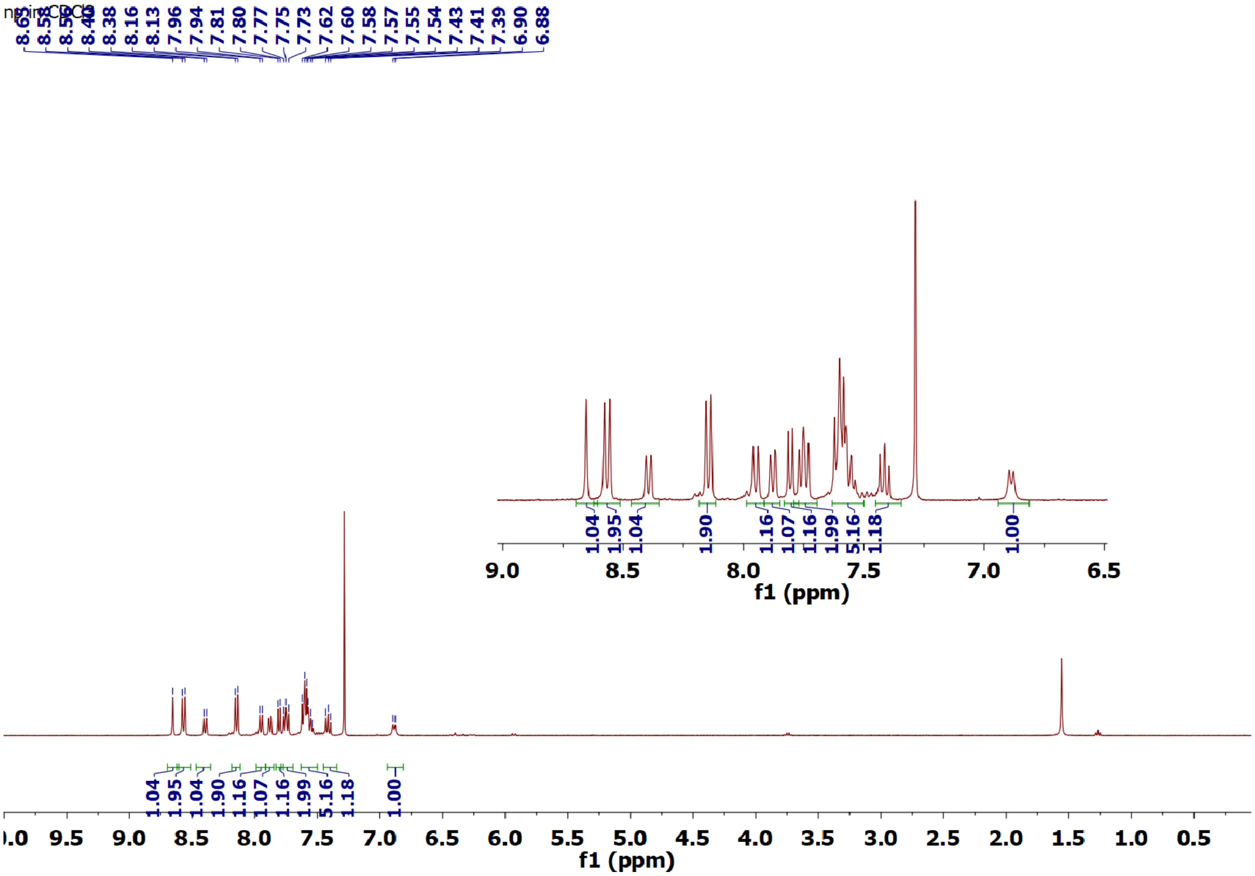


Fig. S-3 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2b**.

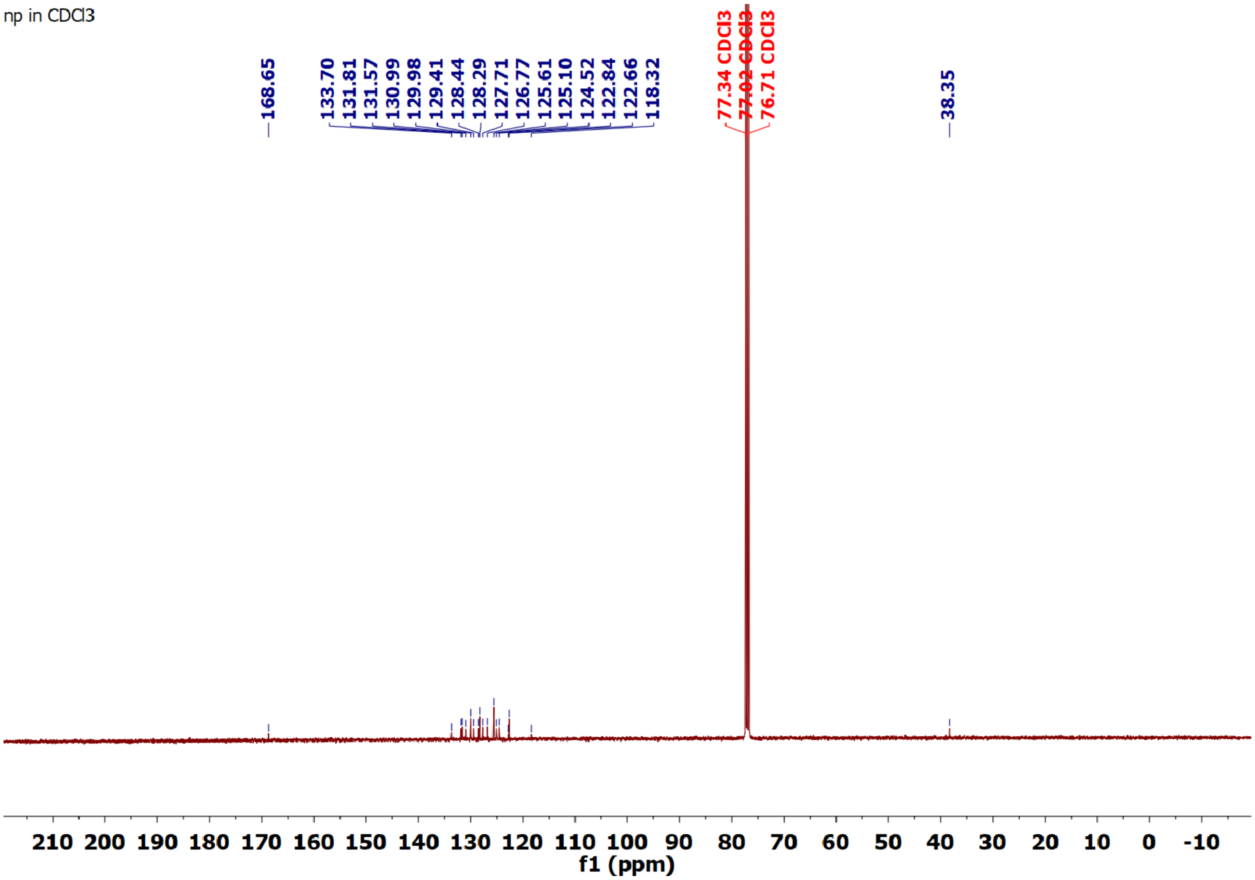


Fig. S-4 ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **2b**.

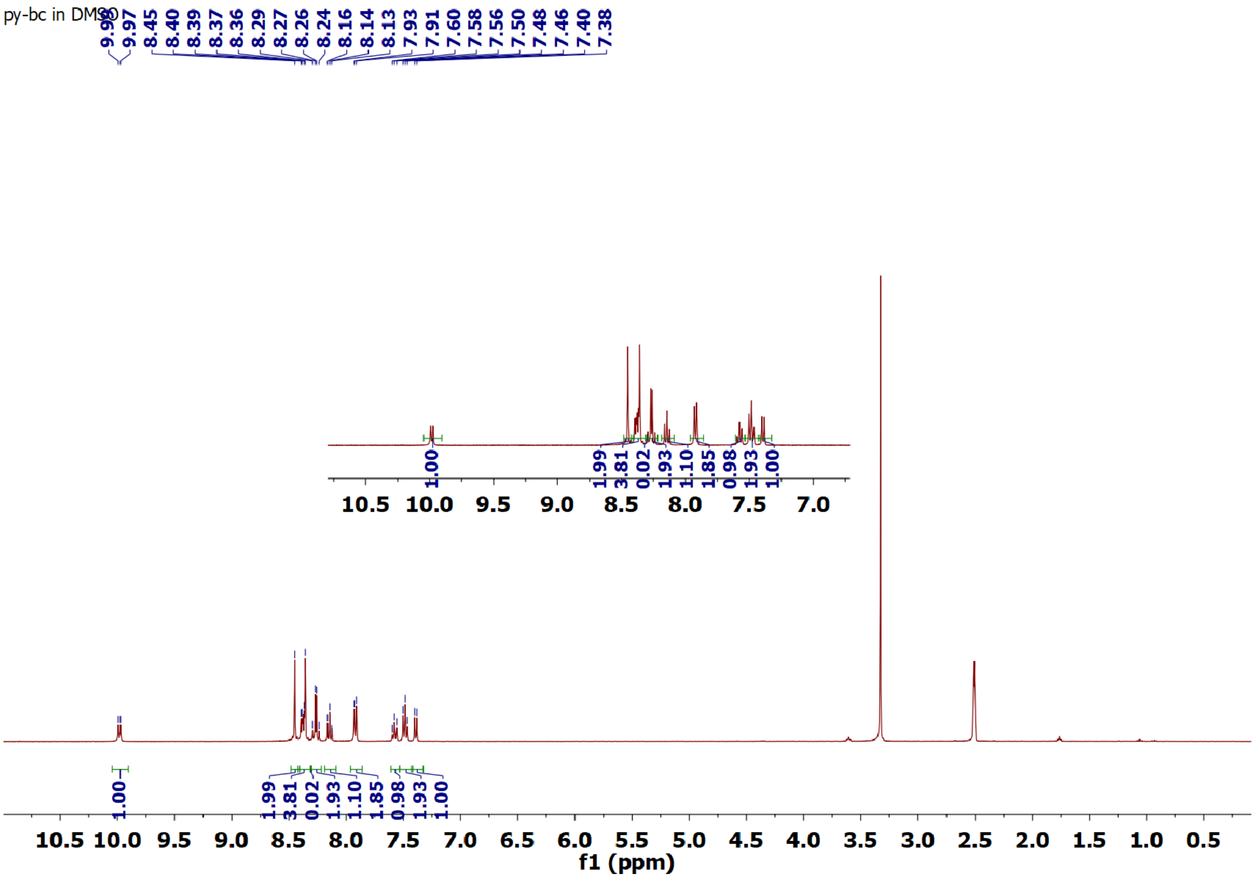


Fig. S-5 ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **3a**.

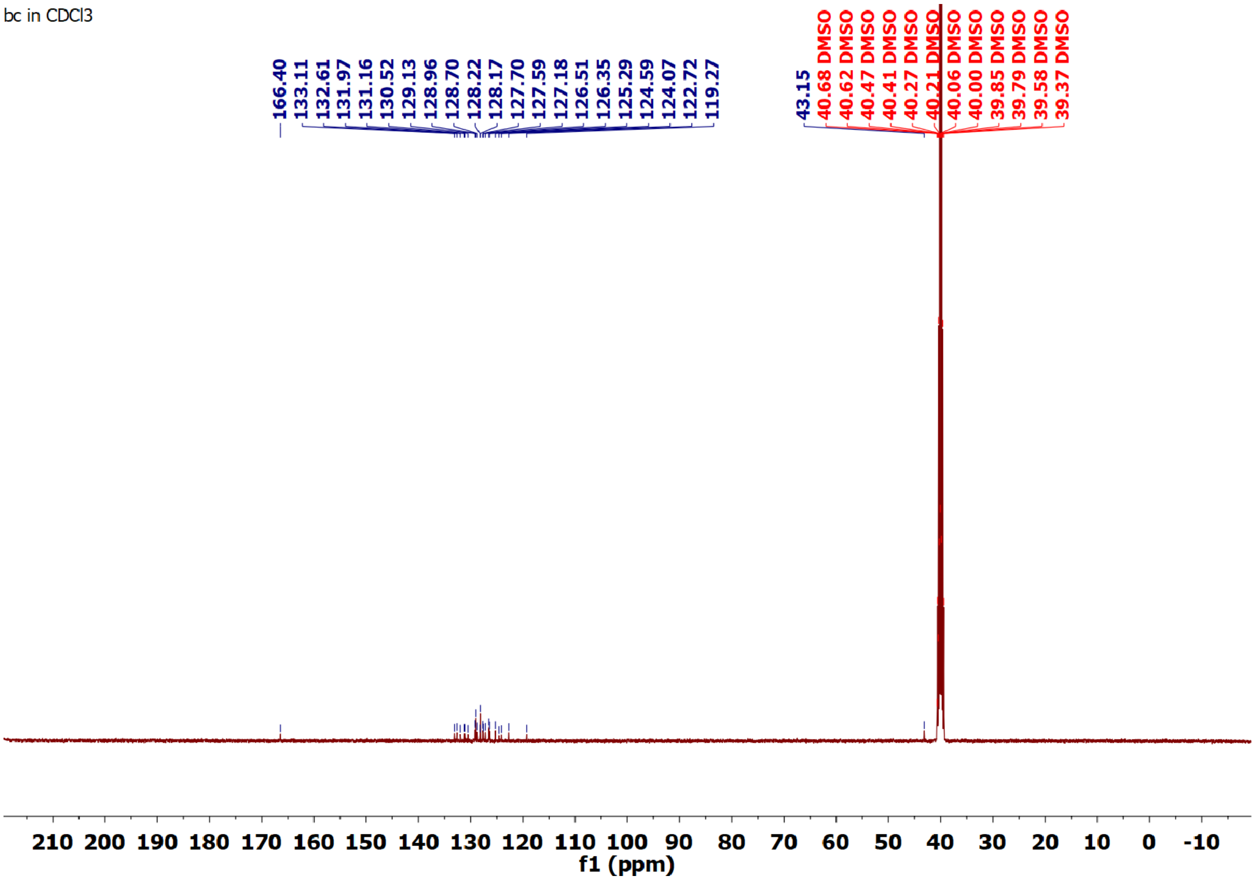


Fig. S-6 ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **3a**.

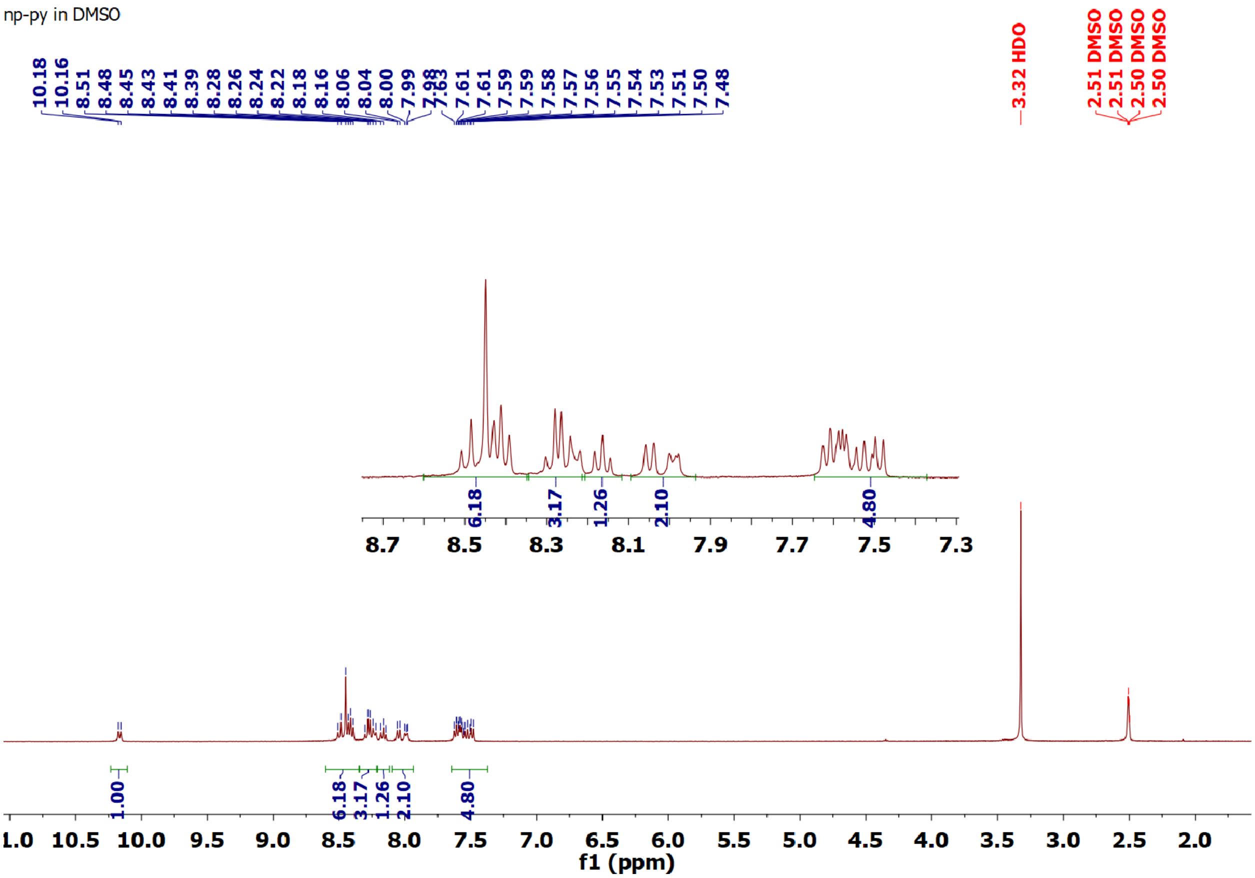


Fig. S-7 ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **3b**.

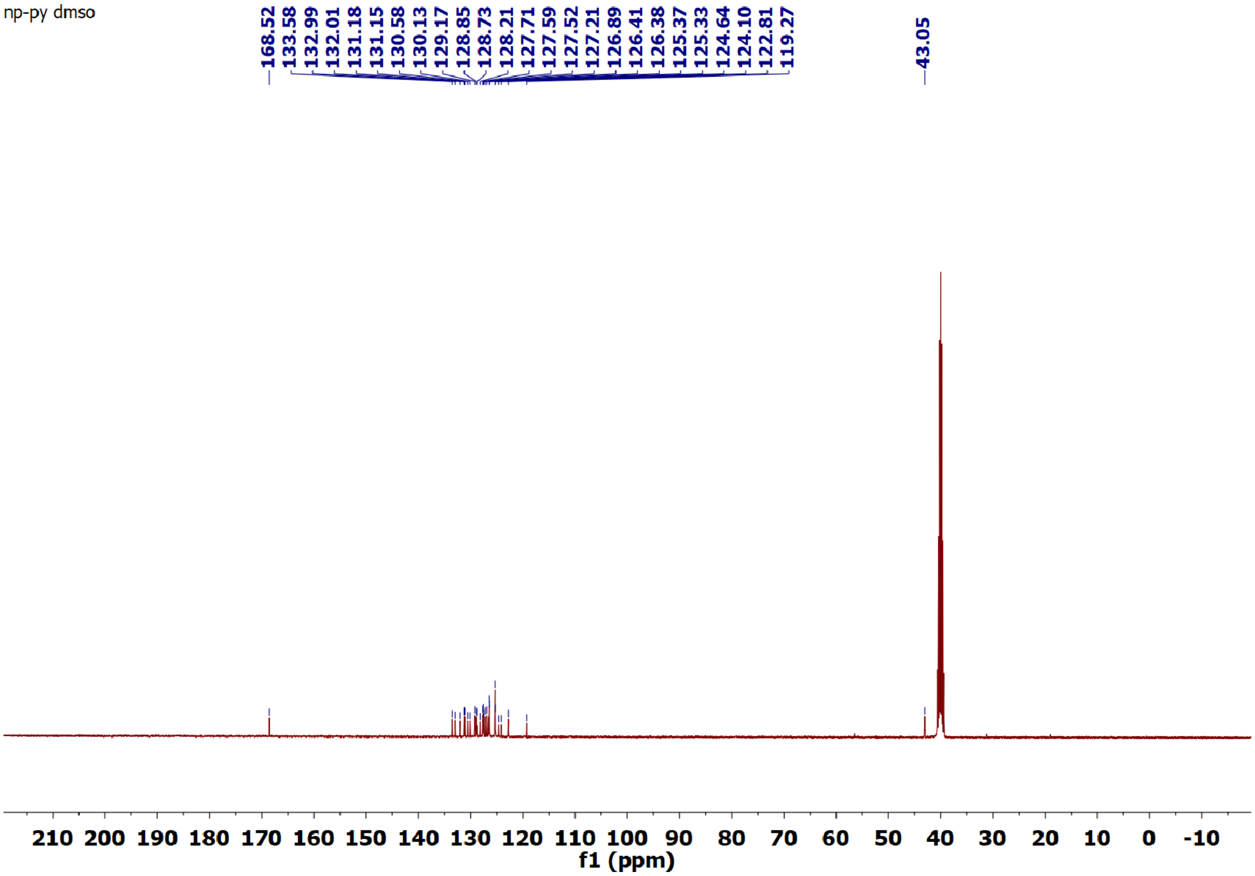


Fig. S-8 ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **3b**.

3. UV-Vis Titrations of Compounds 2-3 with TBAF

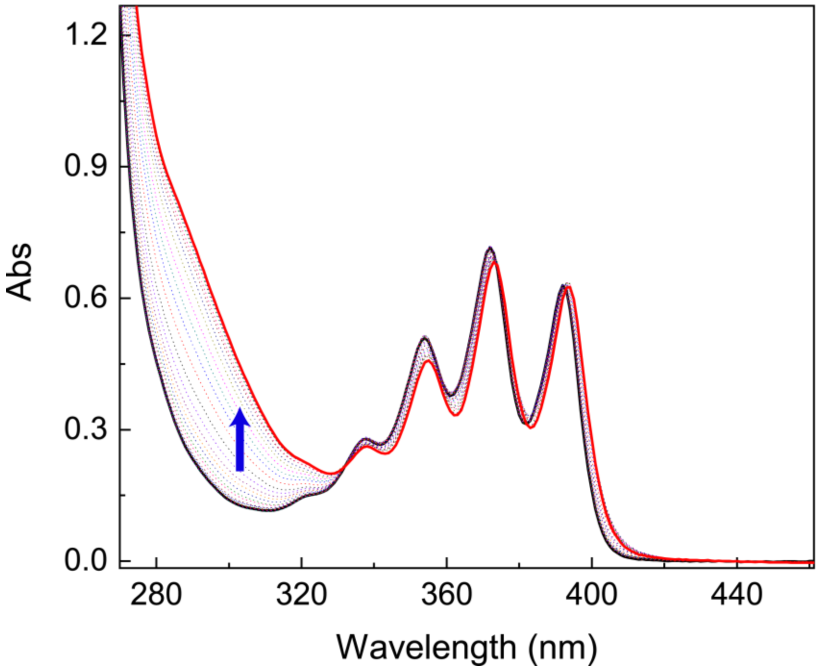


Fig. S-9 UV-Vis absorption spectra monitoring the titration of **2a** (5.55×10^{-5} M) with TBAF (from 0 to 65.1 equivalents) in DMSO. The arrow indicates the trend of increasing titration.

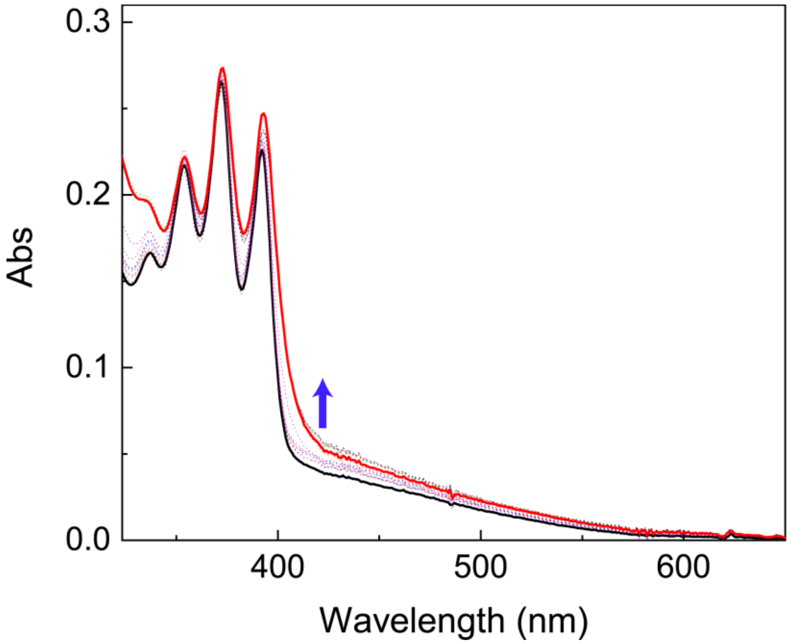


Fig. S-10 UV-Vis absorption spectra monitoring the titration of **2b** (2.42×10^{-5} M) with TBAF (from 0 to 211 equivalents) in DMSO. The arrow indicates the trend of increasing titration.

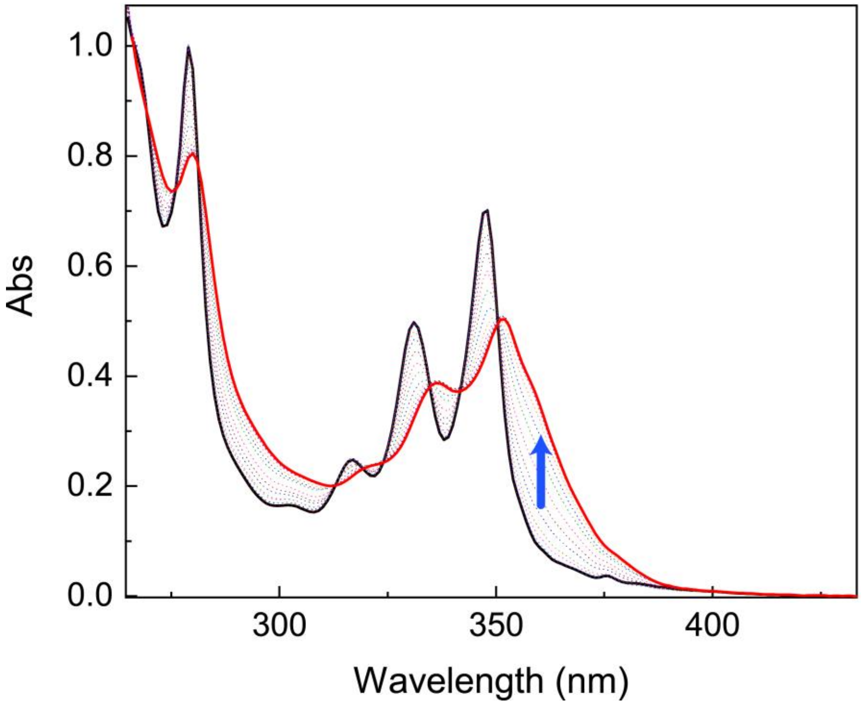


Fig. S-11 UV-Vis absorption spectra monitoring the titration of **3a** (1.66×10^{-5} M) with TBAF (from 0 to 120 equivalents) in DMSO. The arrow indicates the trend of increasing titration.

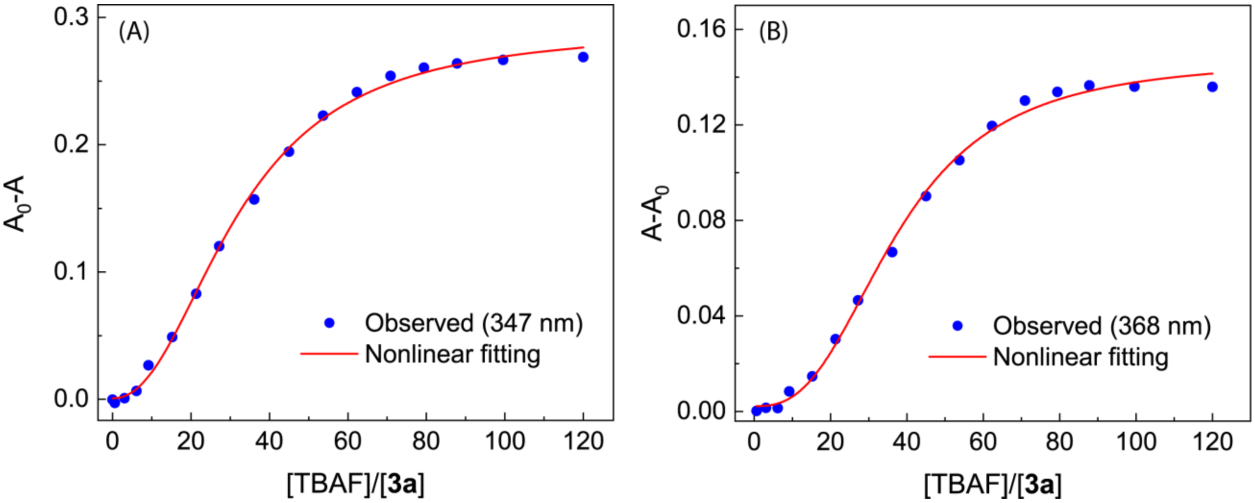


Fig. S-12 Plots of absorbance change against molar equivalent of TBAF during the titration of **3a** (1.66×10^{-5} M) with TBAF (from 0 to 120 equivalents) in DMSO. (A) at 347 nm, (B) at 368 nm. A_0 is the absorbance measured before titration, and A is the absorbance measured during the titration.

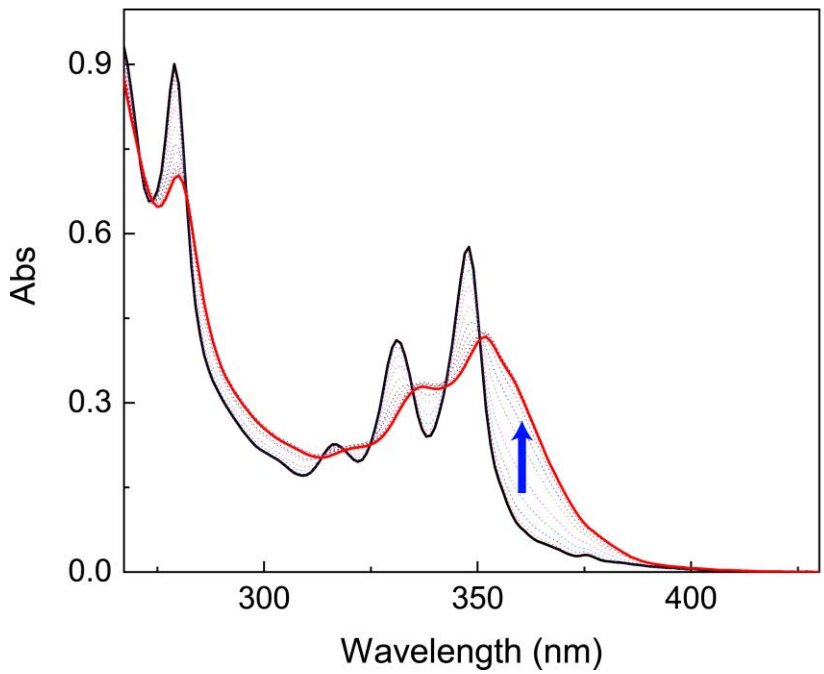


Fig. S-13 UV-Vis absorption spectra monitoring the titration of **3b** (1.45×10^{-5} M) with TBAF (from 0 to 123 equivalents) in DMSO. The arrow indicates the trend of increasing titration.

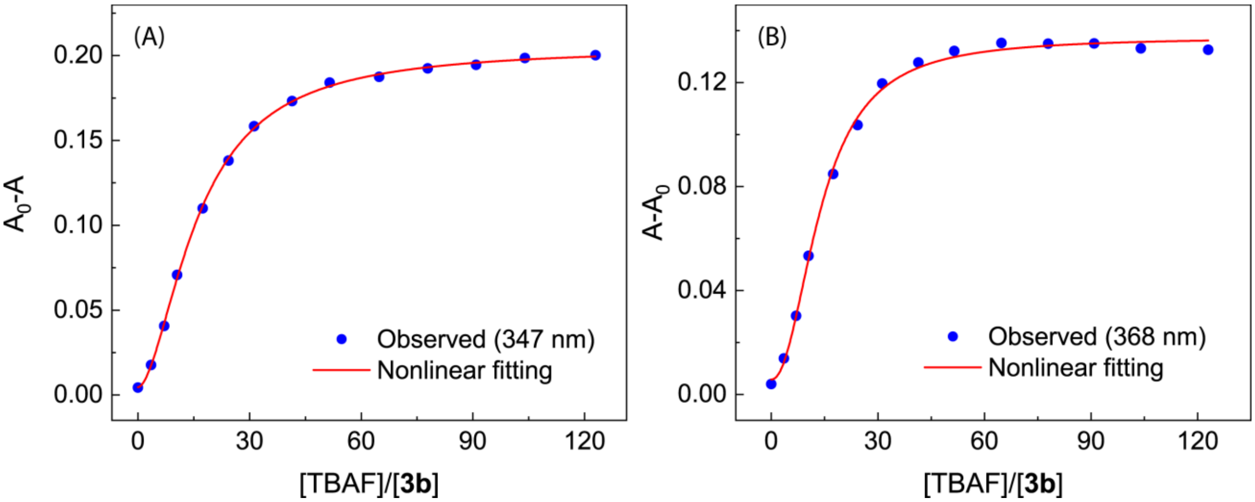


Fig. S-14 Plots of absorbance change against molar equivalent of TBAF during the titration of **3b** (1.45×10^{-5} M) with TBAF (from 0 to 123 equivalents) in DMSO. (A) at 347 nm, (B) at 368 nm. A_0 is the absorbance measured before titration, and A is the absorbance measured during the titration.

4. ^{1}H NMR Titrations of Compounds 2a with TBAF

To understand the interactions of compounds **2** and **3** with fluoride anion in the solution phase, ^{1}H NMR titration experiment of **2a** with TBAF in acetone-d_6 was conducted. As shown in Fig. S-15, the aromatic region of **2a** was monitored during the titration process. Assignments of the amido N-H and various aromatic (phenyl and anthryl) protons in **2a** are given in Scheme S-2.

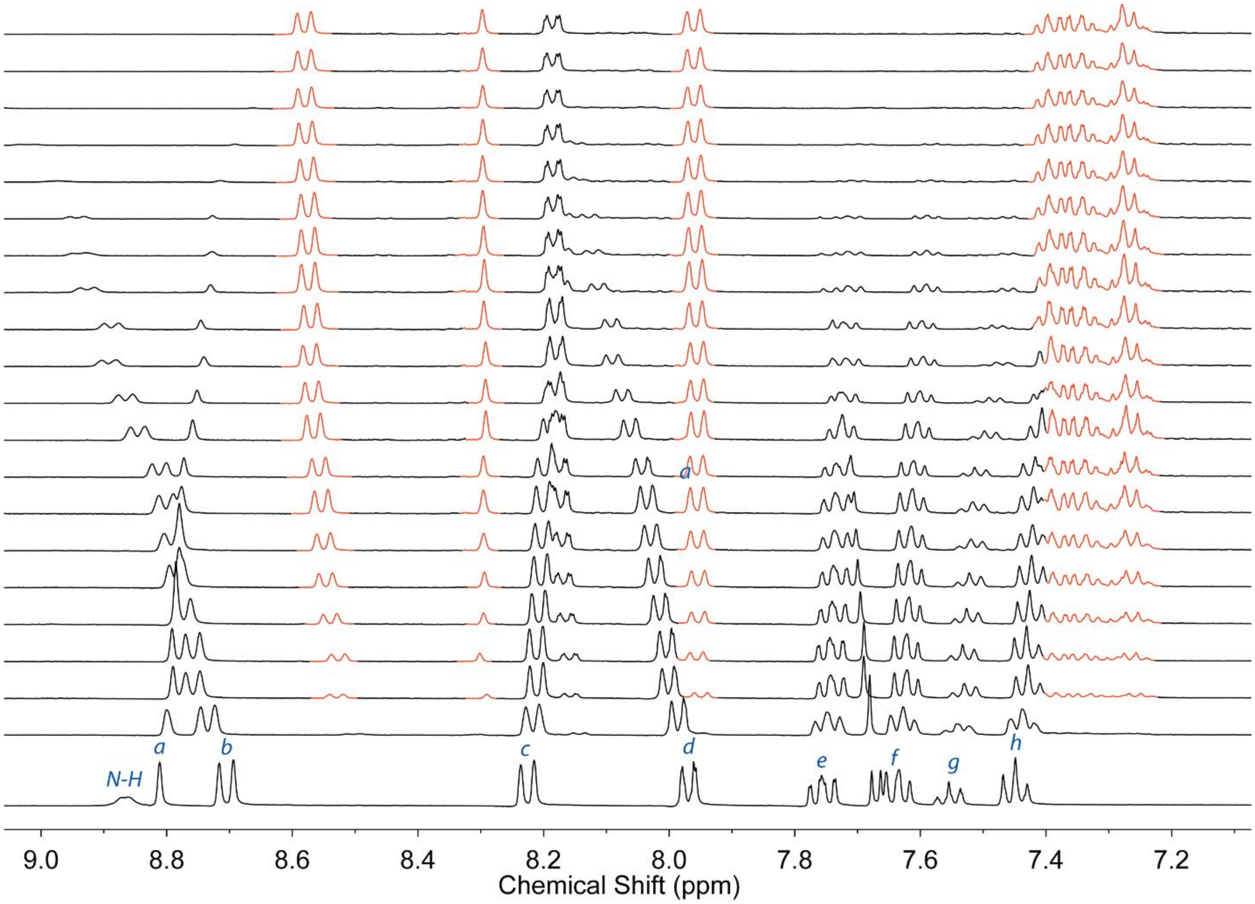
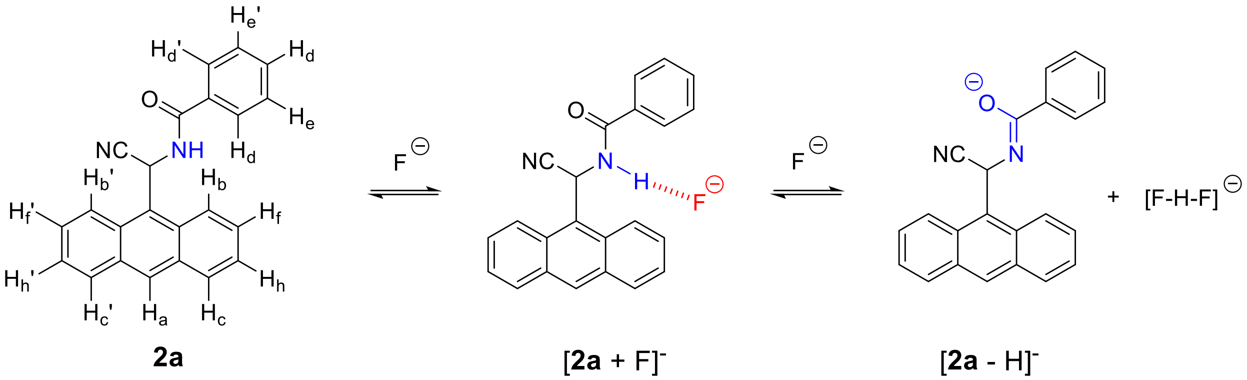


Fig. S-15 ^{1}H NMR (400 MHz, acetone-d_6) spectra monitoring the titration of **2a** (1.7×10^{-3} M) with TBAF. TBAF was added from 0.00 to 2.50 molar equiv (from bottom to top), and 0.125 molar equiv of TBAF was added in each step.



Scheme S-2 Stepwise interactions of **2a** with fluoride anion in the solution phase.

The ^{1}H NMR titration results are in agreement with the two steps shown in Scheme S-2. In the first step, a hydrogen-bonded complex [**2a** + F]$^{-}$ is formed, resulting in immediate dissapearance of the amido NH signal and significant shifts of other aromatic proton signals. The NMR patterns confirm that this step is a rapid equilibrium process. With increasing addition of TBAF, a new set of proton signals (highlighted by red color in Fig. S-15) emerge with increasing intensity, but no significant shifts in their resonance frequencies. These signals can be assigned to the deprotonation step illustrated in Scheme S-2, resulting in a deprotonated anion of **2a**. This assignment is further evidenced by the ^{1}H NMR titration experiment of **2a** with NaOH carried out in DMSO-d_6. Herein, DMSO-d_6 was chosen as the solvent in consideration of the solubility of NaOH. As shown in Fig. S-16, after addition of more than 3.50 molar equiv of base (NaOH) into the solution of **2a**, the ^{1}H NMR spectrum is significantly changed into a new spectral pattern that bears resemblance to the pattern observed at the end stage of the fluoride titiration (see Fig. S-15). Overall, our NMR titration results concur with the UV-Vis and fluorescence titration data, confirming that two steps take place when the cyanomethylcarbamoyl bridge of **2a** is interacting with fluroide anion. This mechaism should be operative in the cases of **2b**, and **3a**/**b** as well, given that they contain the same cyanomethylcarbamoyl bridge in their molecular structures.

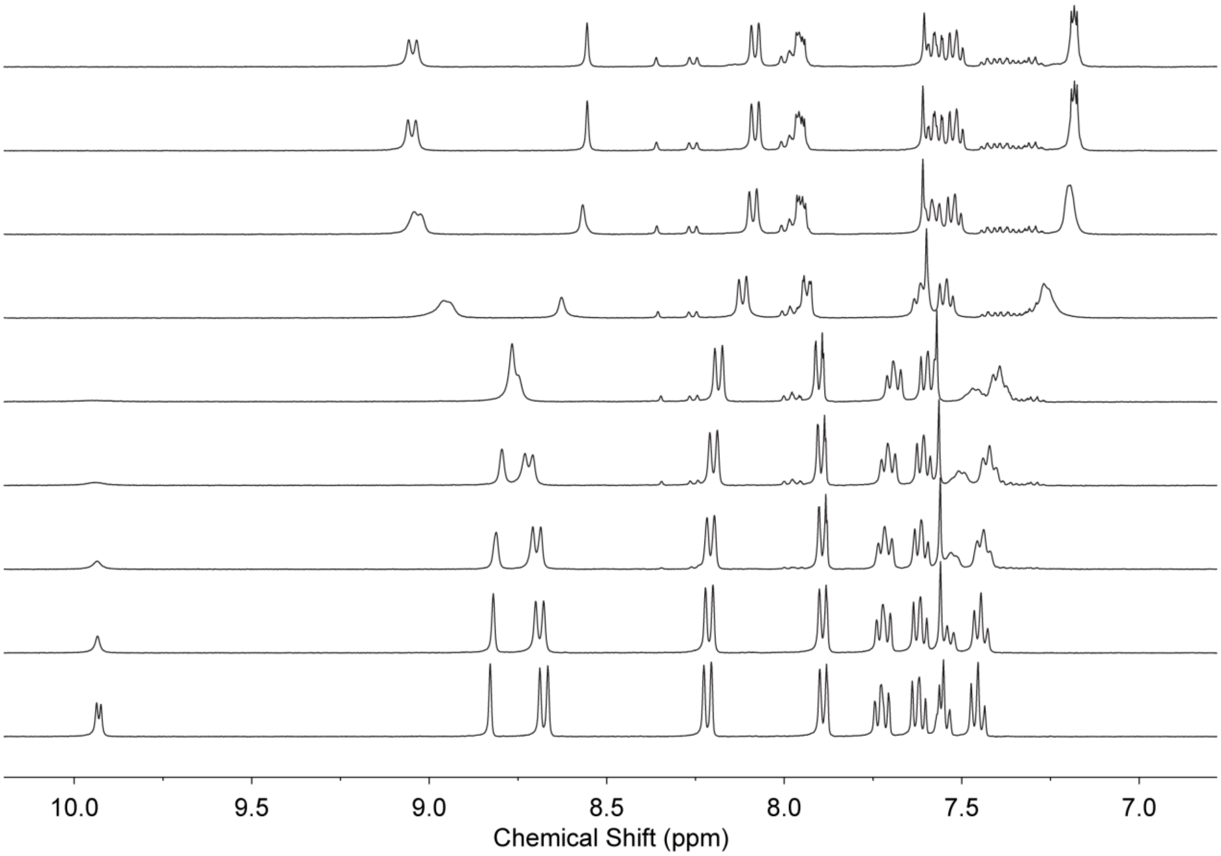
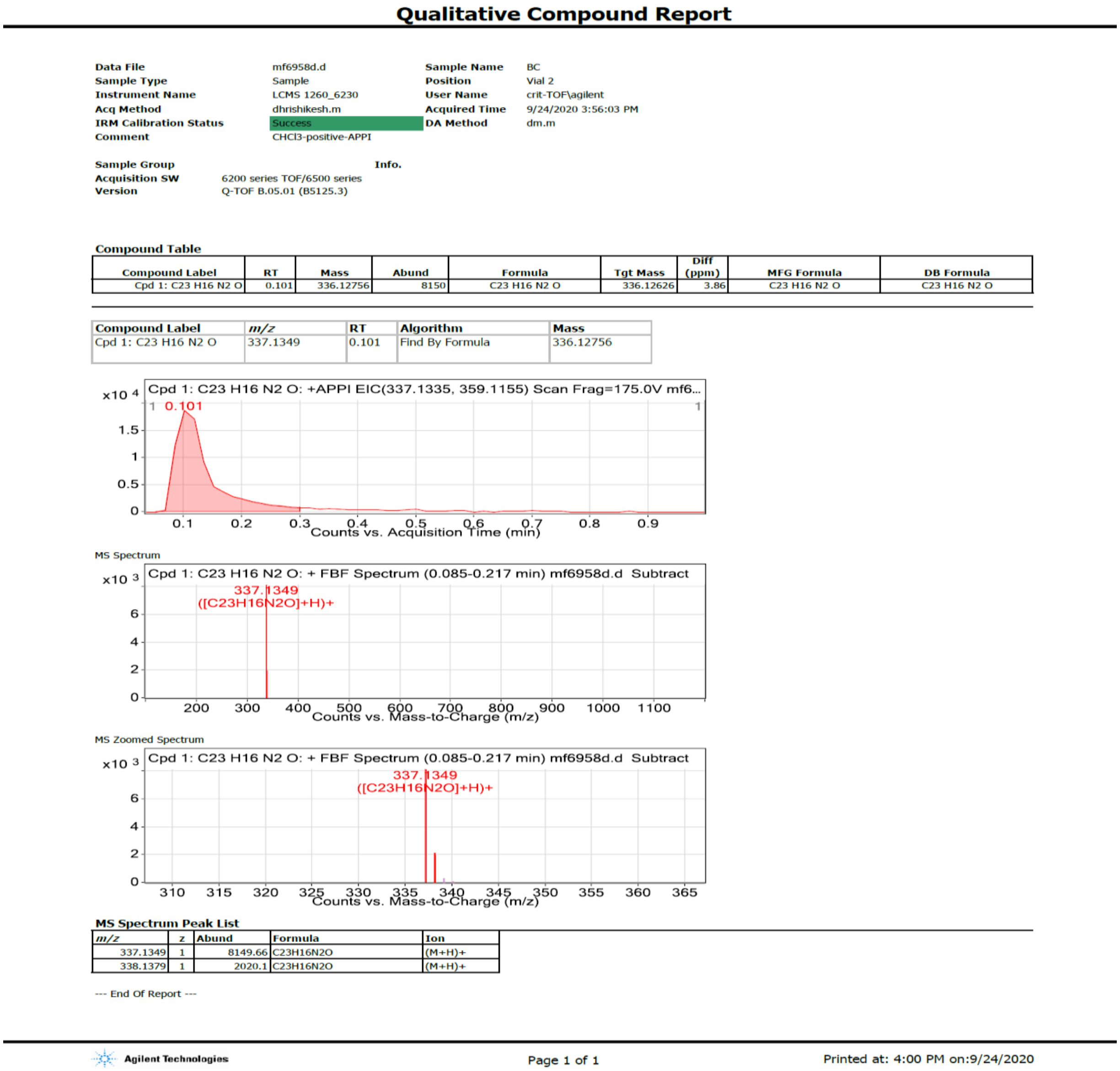


Fig. S-16 ^{1}H NMR (400 MHz, DMSO-d_6) spectra monitoring the titration of **2a** (1.7×10^{-3} M) with NaOH. NaOH was added from 0.00 to 4.00 molar equiv (from bottom to top), and 0.50 molar equiv of NaOH was added in each step.

5. High-Resolution Mass Spectra for Compounds 2-3



Qualitative Compound Report

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IRM Calibration Status	Success	**DA Method**	dm.m
Comment	CHCl3-positive-APPI		

Sample Group		**Info.**
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125.3)	

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C23 H16 N2 O	0.101	336.12756	8150	C23 H16 N2 O	336.12626	3.86	C23 H16 N2 O	C23 H16 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C23 H16 N2 O	337.1349	0.101	Find By Formula	336.12756

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MS Spectrum

Cpd 1: C23 H16 N2 O: + FBF Spectrum (0.085-0.217 min) mf6958d.d Subtract

MS Zoomed Spectrum

Cpd 1: C23 H16 N2 O: + FBF Spectrum (0.085-0.217 min) mf6958d.d Subtract

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
337.1349	1	8149.66	C23H16N2O	(M+H)+
338.1379	1	2020.1	C23H16N2O	(M+H)+

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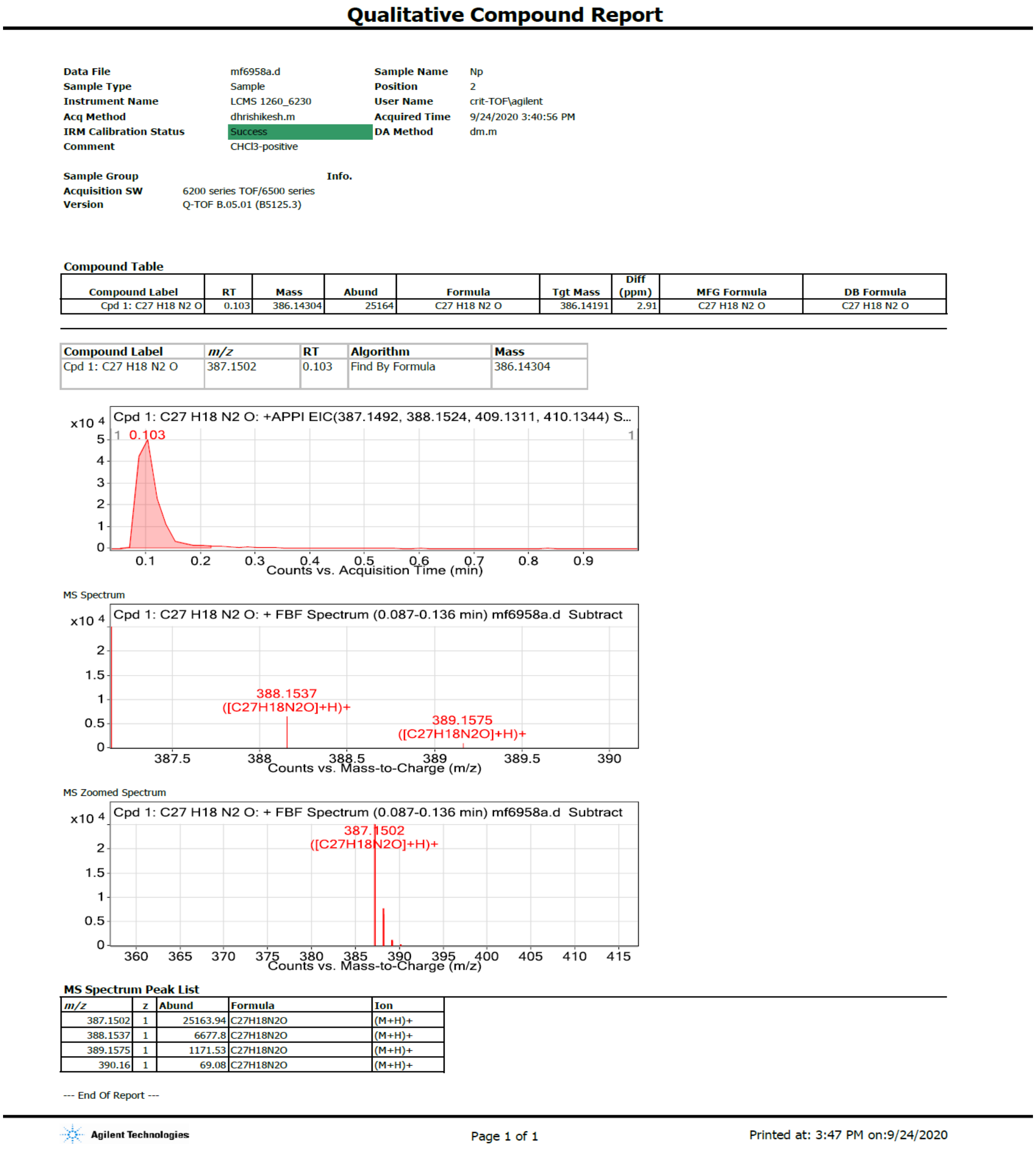
Fig. S-17 High-resolution mass spectrum (APPI-TOF, positive mode) of compound **2a.**



Qualitative Compound Report

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IRM Calibration Status	Success	**DA Method**	dm.m
Comment	CHCl3-positive		

Sample Group		**Info.**
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125.3)	

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C27 H18 N2 O	0.103	386.14304	25164	C27 H18 N2 O	386.14191	2.91	C27 H18 N2 O	C27 H18 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C27 H18 N2 O	387.1502	0.103	Find By Formula	386.14304

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
387.1502	1	25163.94	C27H18N2O	(M+H)+
388.1537	1	6677.8	C27H18N2O	(M+H)+
389.1575	1	1171.53	C27H18N2O	(M+H)+
390.16	1	69.08	C27H18N2O	(M+H)+

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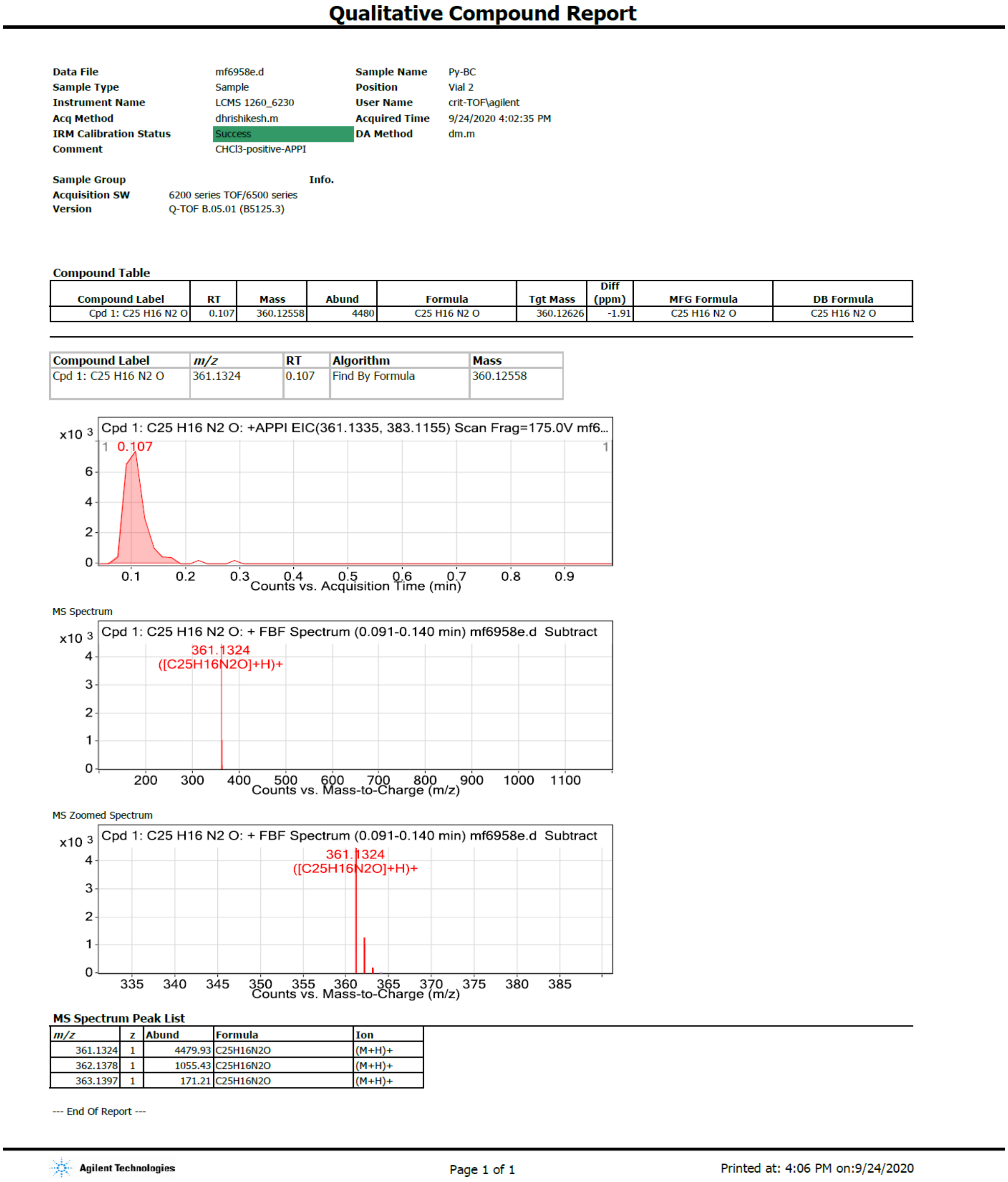
Fig. S-18 High-resolution mass spectrum (APPI-TOF, positive mode) of compound **2b.**



Qualitative Compound Report

Data File	mf6958e.d	**Sample Name**	Py-BC
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IRM Calibration Status	🟩 Success	**DA Method**	dm.m
Comment	CHCl3-positive-APPI		

Sample Group		**Info.**
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125.3)	

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C25 H16 N2 O	0.107	360.12558	4480	C25 H16 N2 O	360.12626	-1.91	C25 H16 N2 O	C25 H16 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C25 H16 N2 O	361.1324	0.107	Find By Formula	360.12558

Cpd 1: C25 H16 N2 O: +APPI EIC(361.1335, 383.1155) Scan Frag=175.0V mf6...

MS Spectrum

Cpd 1: C25 H16 N2 O: + FBF Spectrum (0.091-0.140 min) mf6958e.d Subtract

MS Zoomed Spectrum

Cpd 1: C25 H16 N2 O: + FBF Spectrum (0.091-0.140 min) mf6958e.d Subtract

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
361.1324	1	4479.93	C25H16N2O	(M+H)+
362.1378	1	1055.43	C25H16N2O	(M+H)+
363.1397	1	171.21	C25H16N2O	(M+H)+

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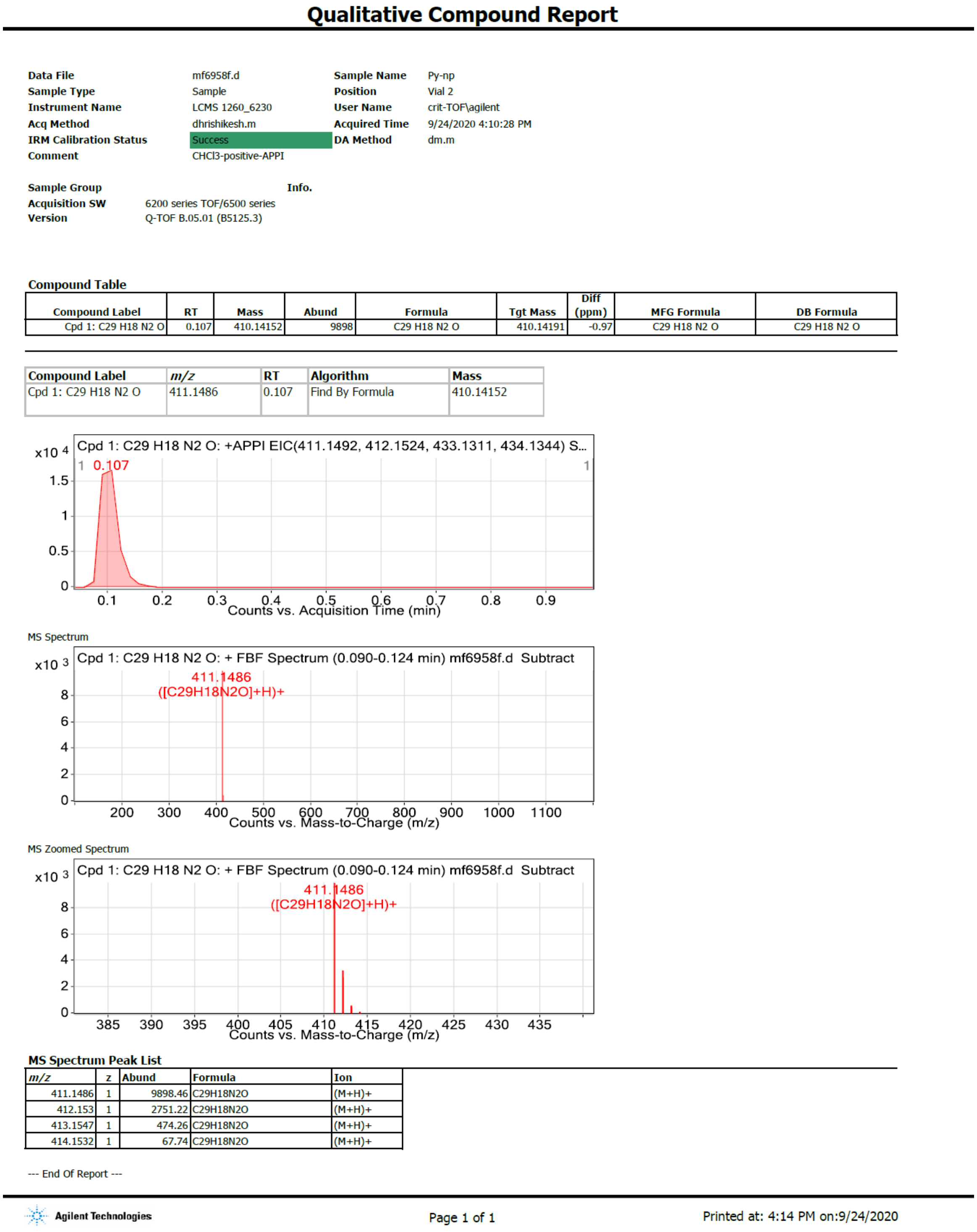
Fig. S-19 High-resolution mass spectrum (APPI-TOF, positive mode) of compound **3a.**



Qualitative Compound Report

Data File	mf6958f.d	**Sample Name**	Py-np
Sample Type	Sample	**Position**	Vial 2
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Acq Method	dhrishikesh.m	**Acquired Time**	9/24/2020 4:10:28 PM
IRM Calibration Status	Success	**DA Method**	dm.m
Comment	CHCl3-positive-APPI		

Sample Group		**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.3)	

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C29 H18 N2 O	0.107	410.14152	9898	C29 H18 N2 O	410.14191	-0.97	C29 H18 N2 O	C29 H18 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C29 H18 N2 O	411.1486	0.107	Find By Formula	410.14152

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
411.1486	1	9898.46	C29H18N2O	(M+H)+
412.153	1	2751.22	C29H18N2O	(M+H)+
413.1547	1	474.26	C29H18N2O	(M+H)+
414.1532	1	67.74	C29H18N2O	(M+H)+

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Fig. S-20 High-resolution mass spectrum (APPI-TOF, positive mode) of compound **3b.**

6. Concentration-Dependent Fluorescence Behavior of 2 and 3

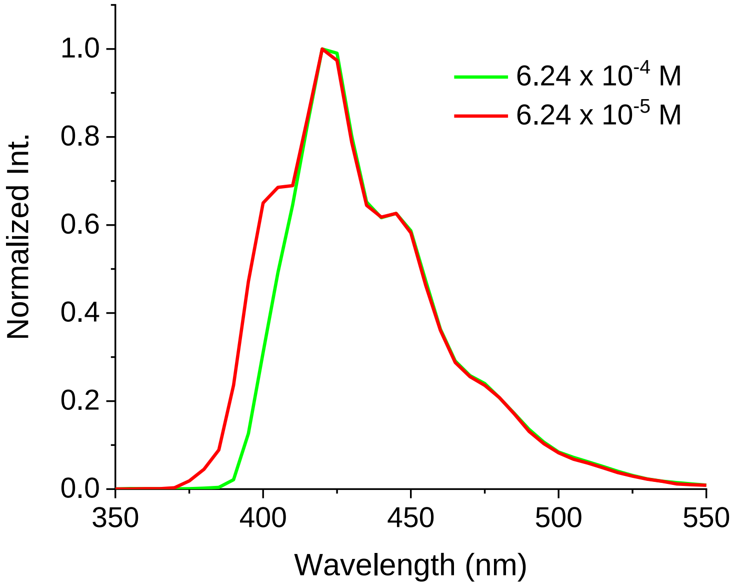


Fig. S-21 Normalized fluorescence spectra of **2a** measured in CH_2Cl_2 at different concentrations (λ_{ex} = 345 nm).

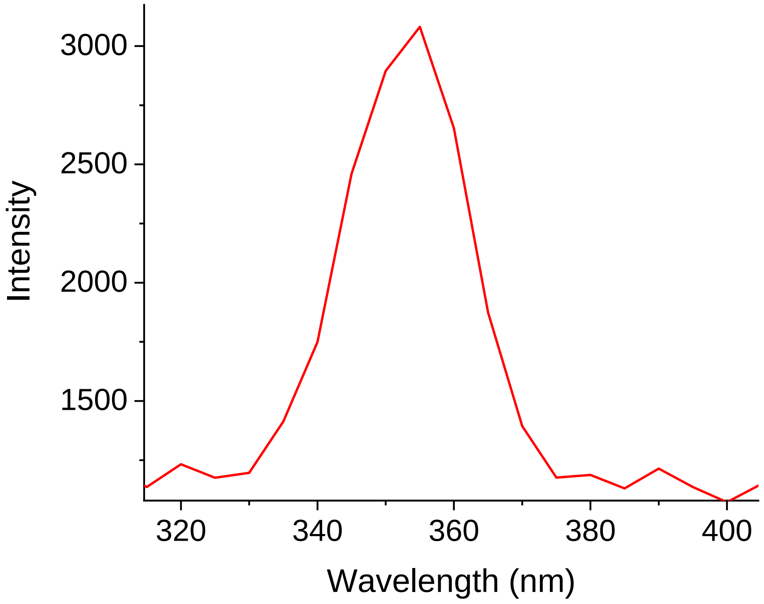


Fig. S-22 Excitation spectrum of **2a** (6.24 × 10^{-5} M in CH_2Cl_2) monitoring the emission at 350 nm.

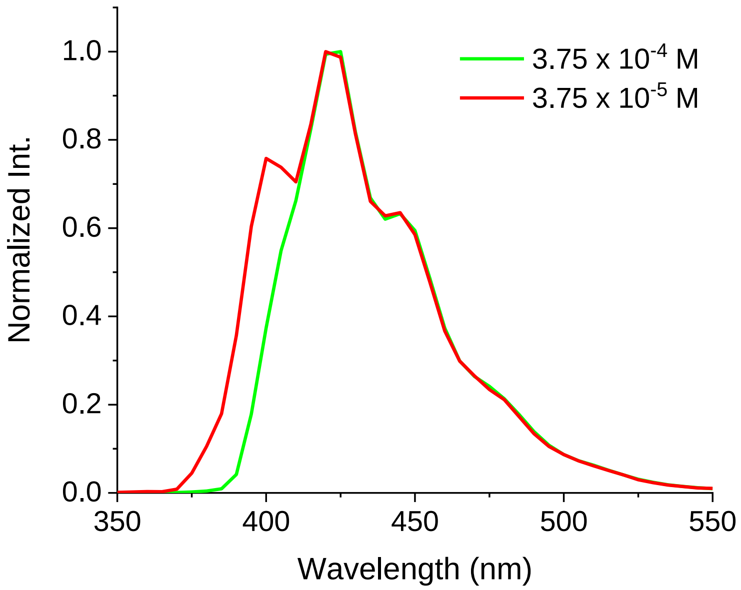


Fig. S-23 Normalized fluorescence spectra of **2b** measured in CH_2Cl_2 at different concentrations (λ_{ex} = 345 nm).

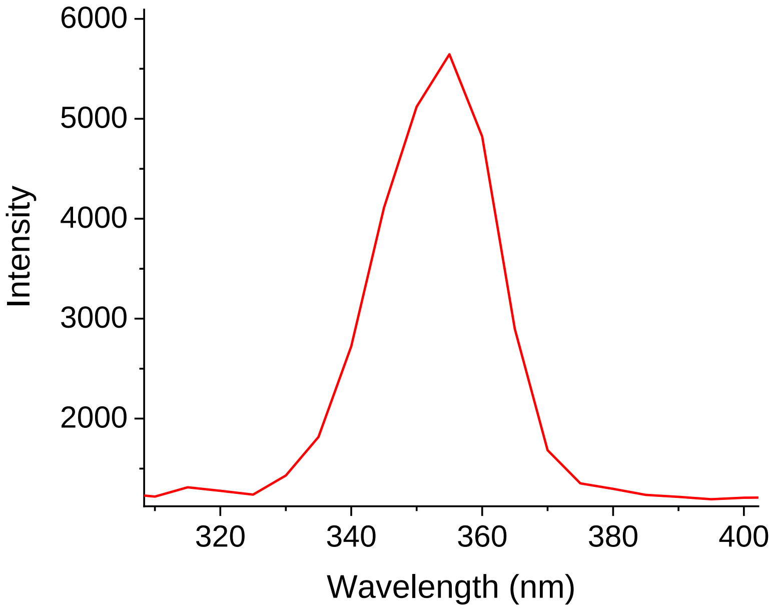


Fig. S-24 Excitation spectrum of **2b** (3.75×10^{-5} M in CH_2Cl_2) monitoring the emission at 350 nm.

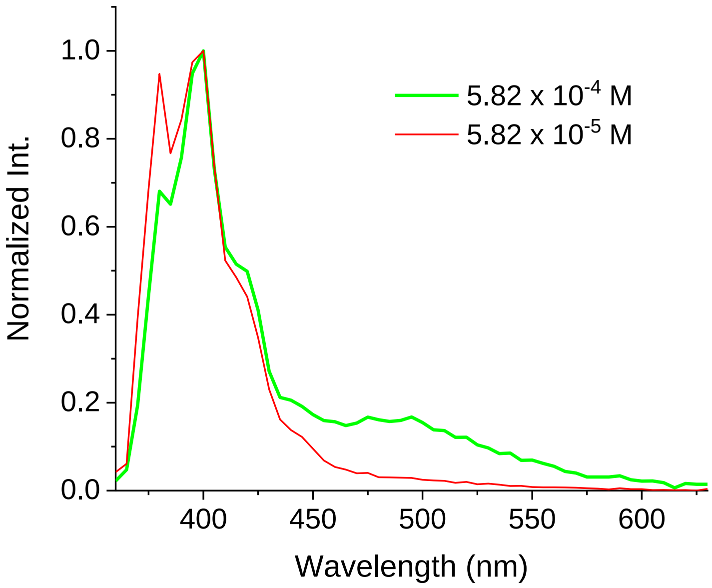


Fig. S-25 Normalized fluorescence spectra of **3a** measured in CH_2Cl_2 at different concentrations (λ_{ex} = 345 nm).

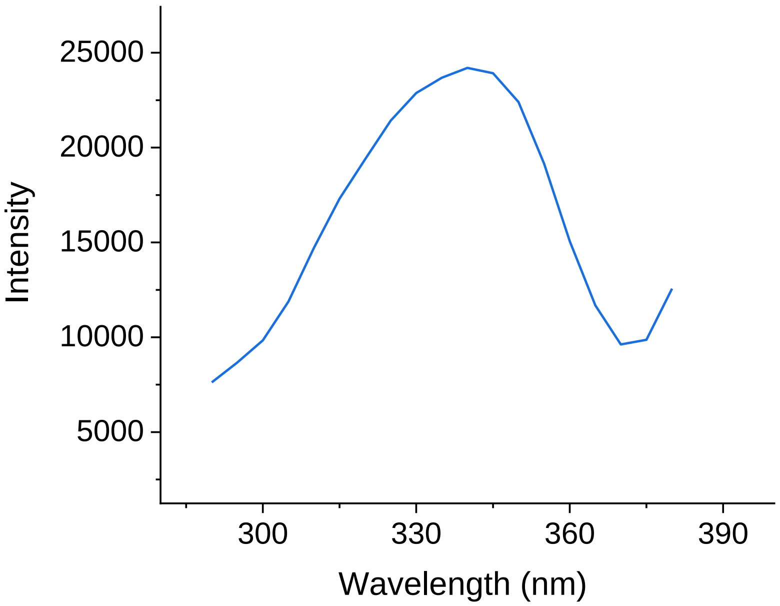


Fig. S-26 Excitation spectrum of **3a** (5.82×10^{-5} M in CH_2Cl_2) monitoring the emission at 380 nm.

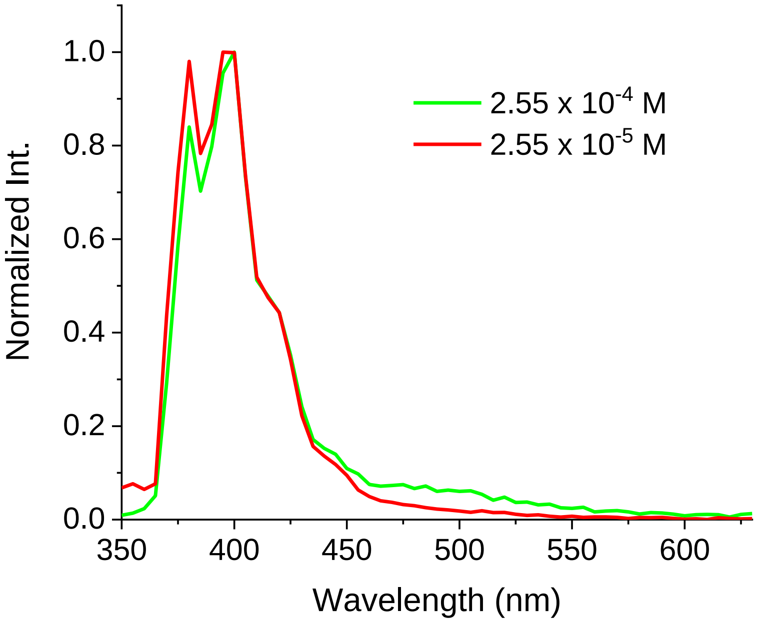


Fig. S-27 Normalized fluorescence spectra of **3b** measured in CH_2Cl_2 at different concentrations (λ_{ex} = 345 nm).

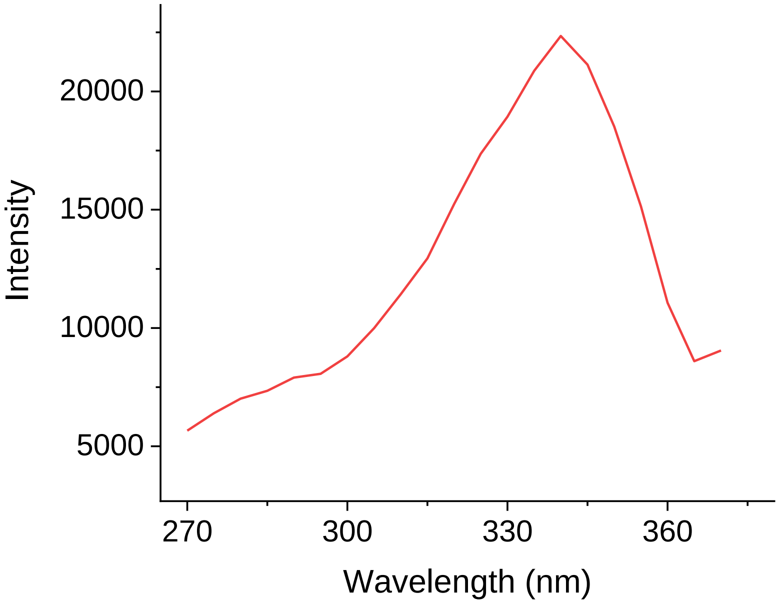


Fig. S-28 Excitation spectrum of **3b** (2.55×10^{-5} M in CH_2Cl_2) monitoring the emission at 380 nm.

7. Detailed Results of DFT and TD-DFT Calculations

Cartesian coordinates and optimized **2a** in gas phase: *E*(RB3LYP) = -1071.090425 hartees; Dipole Moment = 5.911315 Debye; Basis Set = 6-311+G(d,p).

O	-2.12340	-1.79460	1.25280
N	-1.19620	0.22790	0.78700
H	-1.20810	1.01790	0.16100
N	0.36160	1.25680	3.68820
C	-2.20880	-0.70150	0.71240
C	-3.41900	-0.29240	-0.07370
C	-3.78490	1.04400	-0.27390
H	-3.20440	1.84740	0.16560
C	-4.93060	1.35630	-1.00190
H	-5.21370	2.39330	-1.14160
C	-5.71660	0.33790	-1.53780
H	-6.60700	0.58230	-2.10590
C	-5.36180	-0.99570	-1.33280
H	-5.97530	-1.78990	-1.74260
C	-4.22390	-1.31000	-0.59770
H	-3.94220	-2.33950	-0.41540
C	0.06260	-0.10020	1.45440
H	-0.07600	-1.12460	1.79550
C	0.23590	0.68240	2.69610
C	1.27300	-0.02610	0.52330
C	1.90220	-1.22540	0.11160
C	1.47290	-2.53650	0.50400
H	0.59570	-2.66570	1.12340
C	2.13190	-3.66010	0.08590
H	1.77470	-4.63420	0.40000
C	3.27130	-3.57210	-0.75910
H	3.78030	-4.47590	-1.07340
C	3.70890	-2.34840	-1.17580
H	4.57020	-2.26150	-1.82960
C	3.04670	-1.14890	-0.76930
C	3.48790	0.09420	-1.22040
H	4.34390	0.14000	-1.88640
C	2.85540	1.27970	-0.84690
C	3.30850	2.54140	-1.34020
H	4.15970	2.55310	-2.01280
C	2.69080	3.70480	-0.97980
H	3.04270	4.65650	-1.36060
C	1.58250	3.66600	-0.09160
H	1.10360	4.59220	0.20520
C	1.12010	2.47750	0.40580
H	0.29500	2.50410	1.10490
C	1.72680	1.22800	0.05140

Cartesian coordinates and optimized **2b** in gas phase: *E*(RB3LYP) = -1224.764192 hartees; Dipole Moment = 5.797833 Debye; Basis Set = 6-311+G(d,p).

O	-1.48850	0.89940	1.93780
N	-0.31560	-0.79490	0.97800
H	-0.30460	-1.47700	0.23550
N	1.78120	-2.05330	3.40630
C	-1.47090	-0.08290	1.21050
C	-2.68800	-0.62970	0.52040
C	-2.92050	-1.99130	0.55630
H	-2.22640	-2.64030	1.07810
C	-4.07190	-2.55360	-0.03470
H	-4.23580	-3.62320	0.02550
C	-4.97690	-1.74450	-0.67390
H	-5.86330	-2.16810	-1.13450
C	-4.77860	-0.34100	-0.74260
C	-5.70800	0.49790	-1.41200
H	-6.57820	0.04380	-1.87420
C	-5.51240	1.85520	-1.47710
H	-6.22870	2.48630	-1.99070
C	-4.37420	2.43250	-0.87070
H	-4.22700	3.50540	-0.92200
C	-3.45430	1.65160	-0.21150
H	-2.60070	2.10890	0.26810
C	-3.62380	0.24300	-0.12610
C	0.95560	-0.36990	1.56110
H	0.70050	0.52590	2.12450
C	1.42760	-1.32940	2.58110
C	2.01770	-0.03440	0.51350
C	2.39070	1.31660	0.31540
C	1.83570	2.42180	1.04210
H	1.05710	2.26260	1.77550
C	2.24780	3.70660	0.81630
H	1.80260	4.51570	1.38410
C	3.24450	3.99890	-0.15380
H	3.55800	5.02410	-0.31250
C	3.79260	2.98430	-0.88360
H	4.54800	3.18830	-1.63500
C	3.38850	1.62810	-0.68440
C	3.94130	0.60250	-1.44990
H	4.68400	0.84800	-2.20260
C	3.56230	-0.72890	-1.28040
C	4.12650	-1.76210	-2.08960
H	4.85860	-1.48330	-2.84000
C	3.75800	-3.06710	-1.92830
H	4.19200	-3.84300	-2.54810
C	2.80350	-3.40990	-0.93320
H	2.52460	-4.44840	-0.79630
C	2.24170	-2.44940	-0.13610
H	1.54600	-2.76600	0.62940
C	2.58590	-1.06460	-0.27190

Cartesian coordinates and optimized **3a** in gas phase: *E*(RB3LYP) = -1147.353813 hartees; Dipole Moment = 5.707460 Debye; Basis Set = 6-311+G(d,p).

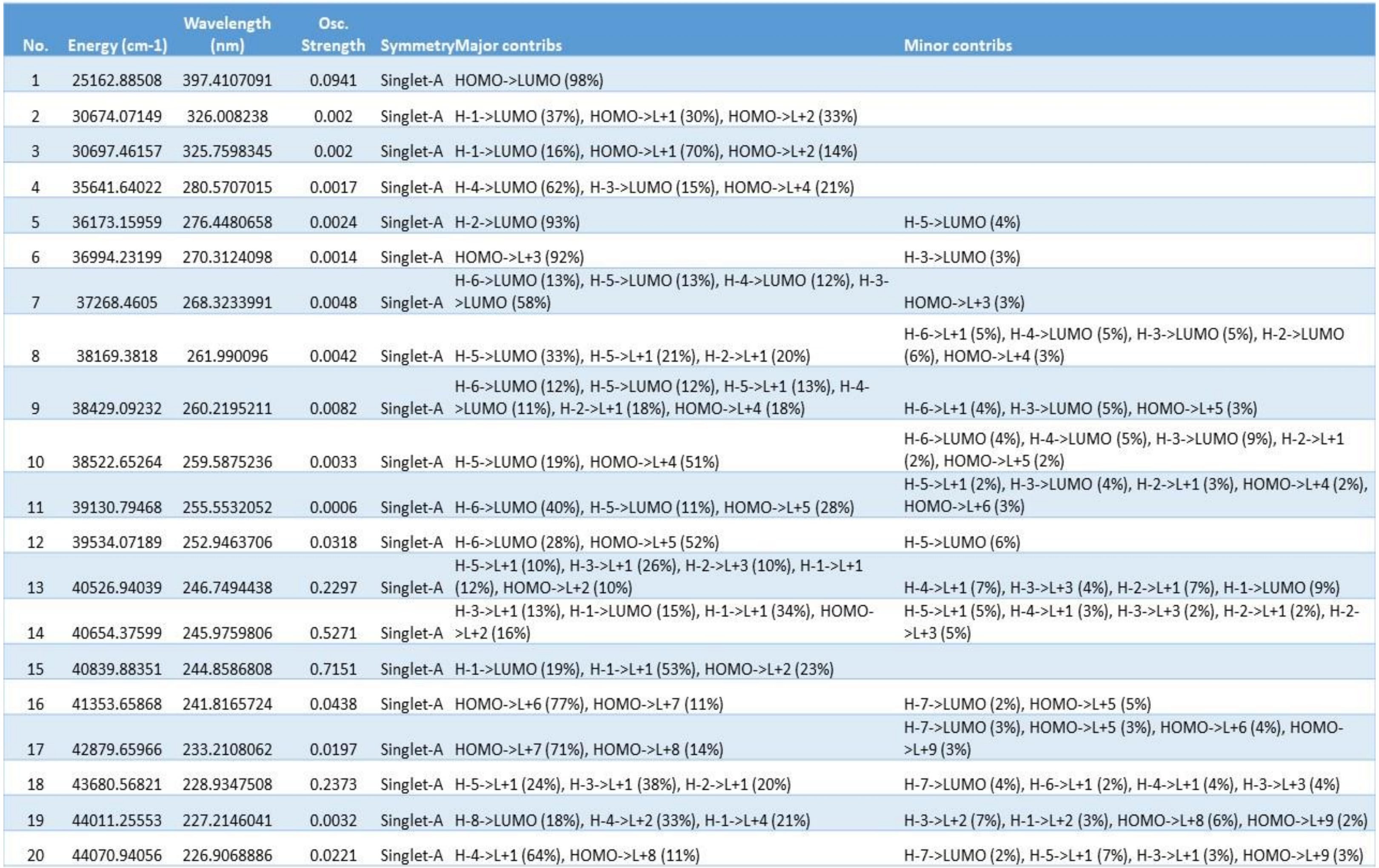
O	-2.89720	-0.11380	-1.97140
N	-2.13640	0.99280	-0.14230
H	-2.28550	1.22080	0.82850
N	-2.04040	4.26040	-1.09760
C	-2.95570	0.08440	-0.76570
C	-3.91620	-0.65350	0.11910
C	-3.69100	-0.86840	1.48410
H	-2.77790	-0.52280	1.95620
C	-4.61910	-1.57460	2.24560
H	-4.43120	-1.74740	3.29900
C	-5.78000	-2.06640	1.65170
H	-6.50340	-2.61280	2.24630
C	-6.00490	-1.86260	0.29010
H	-6.90450	-2.24860	-0.17560
C	-5.07410	-1.16770	-0.47470
H	-5.22570	-1.01250	-1.53560
C	-1.16280	1.79220	-0.88610
H	-1.16530	1.37800	-1.89750
C	-1.64310	3.18160	-1.01180
C	0.23550	1.70890	-0.27650
C	0.71880	2.74670	0.52050
H	0.11430	3.63500	0.66440
C	1.96990	2.67640	1.12080
H	2.32150	3.50050	1.73170
C	2.78720	1.55530	0.94020
C	4.08590	1.45470	1.54530
H	4.43090	2.27890	2.16050
C	4.86930	0.36170	1.35680
H	5.84840	0.30110	1.82020
C	4.42900	-0.73710	0.54390
C	5.22180	-1.87450	0.33550
H	6.19960	-1.92890	0.80210
C	4.76890	-2.92480	-0.45840
H	5.39690	-3.79560	-0.60810
C	3.51680	-2.86380	-1.06070
H	3.16860	-3.68450	-1.67870
C	2.68880	-1.74530	-0.88020
C	1.39400	-1.64450	-1.48470
H	1.04690	-2.46530	-2.10350
C	0.60120	-0.55490	-1.30080
H	-0.37050	-0.53460	-1.77790
C	1.02720	0.55530	-0.49030
C	2.31540	0.48180	0.12620
C	3.14270	-0.66470	-0.07010

Cartesian coordinates and optimized **3a** in gas phase: *E*(RB3LYP) = -1301.027717 hartees; Dipole Moment = 5.369467 Debye; Basis Set = 6-311+G(d,p).

O	-2.11390	0.25260	-1.79050
N	-1.22220	1.23370	0.05110
H	-1.30820	1.39800	1.04280
N	-0.93410	4.53110	-0.75350
C	-2.11010	0.39310	-0.57520
C	-3.03040	-0.34920	0.35120
C	-2.50800	-0.93510	1.48850
H	-1.44710	-0.85390	1.69690
C	-3.32180	-1.68080	2.36770
H	-2.88010	-2.14250	3.24300
C	-4.66140	-1.82080	2.10630
H	-5.29580	-2.38870	2.77880
C	-5.24490	-1.23270	0.95420
C	-4.42320	-0.49130	0.04310
C	-0.22350	2.00190	-0.69250
H	-0.29300	1.64030	-1.72160
C	-0.61040	3.42490	-0.73220
C	1.18810	1.79330	-0.14670
C	1.77130	2.75320	0.68070
H	1.23450	3.67050	0.89470
C	3.03680	2.56880	1.22340
H	3.46700	3.33440	1.85980
C	3.76850	1.40750	0.95240
C	5.08010	1.18990	1.49590
H	5.50400	1.95600	2.13640
C	5.77970	0.05930	1.21960
H	6.76980	-0.08970	1.63730
C	5.23440	-0.96360	0.37210
C	5.93950	-2.13810	0.07360
H	6.92890	-2.28110	0.49460
C	5.38560	-3.11310	-0.75180
H	5.94690	-4.01420	-0.97150
C	4.11780	-2.93840	-1.29630
H	3.69090	-3.70070	-1.93910
C	3.37540	-1.77890	-1.02500
C	2.06800	-1.56130	-1.56860
H	1.64200	-2.32350	-2.21250
C	1.35890	-0.43290	-1.29720
H	0.37350	-0.32350	-1.73210
C	1.89040	0.60270	-0.45090
C	3.19370	0.41190	0.10630
C	3.93290	-0.77470	-0.18200
C	-5.03690	0.08600	-1.10160
C	-6.63280	-1.36630	0.68670
C	-6.38530	-0.06170	-1.32630
C	-7.19350	-0.79380	-0.42790
H	-8.25470	-0.90130	-0.62200
H	-7.24420	-1.92960	1.38380

H	-6.83330	0.38630	-2.20610
H	-4.42700	0.63010	-1.80860

Table S-1 TD-DFT calculated electronic transitions, oscillator strength (*f*), and MO composition for compounds **2a**.



No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	25162.88508	397.4107091	0.0941	Singlet-A	HOMO->LUMO (98%)	
2	30674.07149	326.008238	0.002	Singlet-A	H-1->LUMO (37%), HOMO->L+1 (30%), HOMO->L+2 (33%)	
3	30697.46157	325.7598345	0.002	Singlet-A	H-1->LUMO (16%), HOMO->L+1 (70%), HOMO->L+2 (14%)	
4	35641.64022	280.5707015	0.0017	Singlet-A	H-4->LUMO (62%), H-3->LUMO (15%), HOMO->L+4 (21%)	
5	36173.15959	276.4480658	0.0024	Singlet-A	H-2->LUMO (93%)	H-5->LUMO (4%)
6	36994.23199	270.3124098	0.0014	Singlet-A	HOMO->L+3 (92%)	H-3->LUMO (3%)
7	37268.4605	268.3233991	0.0048	Singlet-A	H-6->LUMO (13%), H-5->LUMO (13%), H-4->LUMO (12%), H-3->LUMO (58%)	HOMO->L+3 (3%)
8	38169.3818	261.990096	0.0042	Singlet-A	H-5->LUMO (33%), H-5->L+1 (21%), H-2->L+1 (20%)	H-6->L+1 (5%), H-4->LUMO (5%), H-3->LUMO (5%), H-2->LUMO (6%), HOMO->L+4 (3%)
9	38429.09232	260.2195211	0.0082	Singlet-A	H-6->LUMO (12%), H-5->LUMO (12%), H-5->L+1 (13%), H-4->LUMO (11%), H-2->L+1 (18%), HOMO->L+4 (18%)	H-6->L+1 (4%), H-3->LUMO (5%), HOMO->L+5 (3%)
10	38522.65264	259.5875236	0.0033	Singlet-A	H-5->LUMO (19%), HOMO->L+4 (51%)	H-6->LUMO (4%), H-4->LUMO (5%), H-3->LUMO (9%), H-2->L+1 (2%), HOMO->L+5 (2%)
11	39130.79468	255.5532052	0.0006	Singlet-A	H-6->LUMO (40%), H-5->LUMO (11%), HOMO->L+5 (28%)	H-5->L+1 (2%), H-3->LUMO (4%), H-2->L+1 (3%), HOMO->L+4 (2%), HOMO->L+6 (3%)
12	39534.07189	252.9463706	0.0318	Singlet-A	H-6->LUMO (28%), HOMO->L+5 (52%)	H-5->LUMO (6%)
13	40526.94039	246.7494438	0.2297	Singlet-A	H-5->L+1 (10%), H-3->L+1 (26%), H-2->L+3 (10%), H-1->L+1 (12%), HOMO->L+2 (10%)	H-4->L+1 (7%), H-3->L+3 (4%), H-2->L+1 (7%), H-1->LUMO (9%)
14	40654.37599	245.9759806	0.5271	Singlet-A	H-3->L+1 (13%), H-1->LUMO (15%), H-1->L+1 (34%), HOMO->L+2 (16%)	H-5->L+1 (5%), H-4->L+1 (3%), H-3->L+3 (2%), H-2->L+1 (2%), H-2->L+3 (5%)
15	40839.88351	244.8586808	0.7151	Singlet-A	H-1->LUMO (19%), H-1->L+1 (53%), HOMO->L+2 (23%)	
16	41353.65868	241.8165724	0.0438	Singlet-A	HOMO->L+6 (77%), HOMO->L+7 (11%)	H-7->LUMO (2%), HOMO->L+5 (5%)
17	42879.65966	233.2108062	0.0197	Singlet-A	HOMO->L+7 (71%), HOMO->L+8 (14%)	H-7->LUMO (3%), HOMO->L+5 (3%), HOMO->L+6 (4%), HOMO->L+9 (3%)
18	43680.56821	228.9347508	0.2373	Singlet-A	H-5->L+1 (24%), H-3->L+1 (38%), H-2->L+1 (20%)	H-7->LUMO (4%), H-6->L+1 (2%), H-4->L+1 (4%), H-3->L+3 (4%)
19	44011.25553	227.2146041	0.0032	Singlet-A	H-8->LUMO (18%), H-4->L+2 (33%), H-1->L+4 (21%)	H-3->L+2 (7%), H-1->L+2 (3%), HOMO->L+8 (6%), HOMO->L+9 (2%)
20	44070.94056	226.9068886	0.0221	Singlet-A	H-4->L+1 (64%), HOMO->L+8 (11%)	H-7->LUMO (2%), H-5->L+1 (7%), H-3->L+1 (3%), HOMO->L+9 (3%)

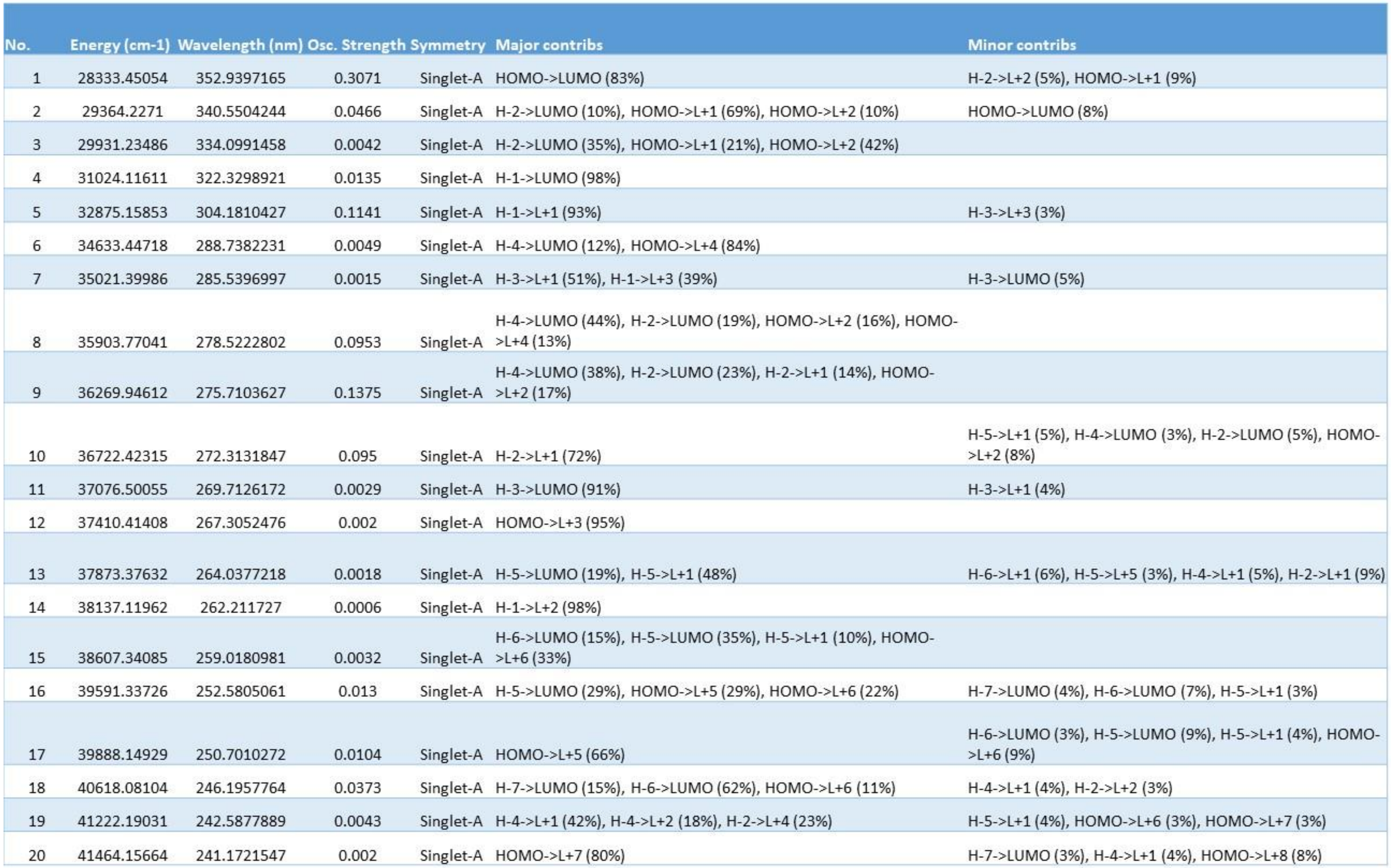
Table S-2 TD-DFT calculated electronic transitions, oscillator strength (*f*), and MO composition for compounds **2b**.

No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	25178.20961	397.1688279	0.0948	Singlet-A	HOMO->LUMO (98%)	
2	28892.39276	346.111867	0	Singlet-A	H-1->LUMO (100%)	
3	29055.31675	344.1710888	0.0003	Singlet-A	HOMO->L+1 (99%)	
4	30688.58947	325.854012	0.0017	Singlet-A	H-2->LUMO (53%), HOMO->L+2 (47%)	
5	32888.86995	304.0542291	0.1203	Singlet-A	H-1->L+1 (94%)	H-3->L+3 (3%)
6	34893.96426	286.582514	0.0002	Singlet-A	H-3->LUMO (99%)	
7	35074.63245	285.1063376	0.0019	Singlet-A	H-3->L+1 (57%), H-1->L+3 (41%)	
8	35670.67618	280.3423168	0.0013	Singlet-A	H-5->LUMO (21%), H-4->LUMO (56%), HOMO->L+4 (21%)	
9	36813.5638	271.6390093	0.0011	Singlet-A	H-5->LUMO (64%), H-4->LUMO (28%)	H-5->L+1 (2%)
10	37028.91384	270.0592311	0.0013	Singlet-A	HOMO->L+3 (96%)	
11	37681.41637	265.3828057	0.0076	Singlet-A	H-5->L+1 (50%), H-4->L+1 (30%)	H-6->LUMO (5%), H-5->LUMO (2%), H-5->L+5 (2%)
12	38080.66081	262.6004851	0.0056	Singlet-A	H-6->LUMO (89%)	H-5->L+1 (2%), HOMO->L+6 (2%)
13	38538.78373	259.4788686	0.0012	Singlet-A	H-4->LUMO (12%), HOMO->L+4 (73%)	H-5->LUMO (7%)
14	39046.10646	256.1074818	0	Singlet-A	H-2->L+1 (99%)	
15	39415.50839	253.7072439	0.0189	Singlet-A	HOMO->L+5 (88%)	HOMO->L+6 (8%)
16	39538.10466	252.9205708	0.0141	Singlet-A	HOMO->L+6 (75%)	H-8->LUMO (4%), H-6->LUMO (2%), HOMO->L+5 (8%), HOMO->L+7 (4%)
17	39787.32998	251.3362923	0.0006	Singlet-A	H-1->L+2 (99%)	
18	40677.76607	245.8345422	1.2792	Singlet-A	H-2->LUMO (43%), HOMO->L+2 (48%)	
19	41445.60589	241.2801016	0.0155	Singlet-A	HOMO->L+7 (79%), HOMO->L+8 (11%)	HOMO->L+6 (4%)
20	41724.67372	239.6663439	0.0287	Singlet-A	H-1->L+5 (83%)	H-7->L+1 (5%), H-3->L+3 (4%), H-1->L+4 (4%)

Table S-3 TD-DFT calculated electronic transitions, oscillator strength (*f*), and MO composition for compounds **3a**.

Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
350.8225376	0.3312	Singlet-A	HOMO->LUMO (90%)	H-1->L+2 (6%)
337.0143059	0.0064	Singlet-A	H-1->LUMO (40%), HOMO->L+1 (19%), HOMO->L+2 (39%)	
321.7109759	0.0117	Singlet-A	HOMO->L+1 (78%), HOMO->L+2 (14%)	H-1->LUMO (7%)
288.3822785	0.0033	Singlet-A	HOMO->L+4 (84%)	H-3->LUMO (6%), H-2->LUMO (6%)
278.3534485	0.0635	Singlet-A	H-3->LUMO (30%), H-2->LUMO (27%), H-1->LUMO (13%), HOMO->L+2 (12%), HOMO->L+4 (14%)	
274.7085126	0.2392	Singlet-A	H-3->LUMO (12%), H-2->LUMO (16%), H-1->LUMO (35%), HOMO->L+2 (30%)	
268.7945909	0.0004	Singlet-A	HOMO->L+3 (99%)	
264.2346725	0.0234	Singlet-A	H-6->L+1 (12%), H-2->L+1 (14%), H-1->L+1 (46%)	H-5->LUMO (2%), H-5->L+1 (8%), H-3->LUMO (4%), H-3->L+1 (5%), H-2->LUMO (3%)
260.6352596	0.0094	Singlet-A	H-5->LUMO (15%), H-3->LUMO (20%), H-2->LUMO (25%), H-1->L+1 (22%), HOMO->L+5 (11%)	H-4->LUMO (4%)
257.8867088	0.003	Singlet-A	H-5->LUMO (14%), H-4->LUMO (15%), H-3->LUMO (10%), HOMO->L+5 (27%)	H-6->LUMO (6%), H-5->L+1 (2%), H-2->LUMO (6%), H-2->L+1 (3%), H-1->L+1 (8%)
256.5207891	0.0056	Singlet-A	H-3->LUMO (14%), H-2->LUMO (12%), H-2->L+1 (19%), H-1->L+1 (21%)	H-6->L+1 (9%), H-5->L+1 (9%), H-4->LUMO (3%), H-3->L+1 (6%)
251.6679042	0.0138	Singlet-A	H-4->LUMO (60%), HOMO->L+5 (21%)	H-7->LUMO (7%), H-4->L+1 (2%)
248.0279127	0.0596	Singlet-A	H-5->LUMO (39%), HOMO->L+5 (16%)	H-7->LUMO (7%), H-5->L+1 (6%), H-4->L+1 (8%), H-4->L+3 (3%), H-3->L+1 (3%), H-3->L+3 (3%), H-2->L+1 (3%), H-1->L+2 (3%)
244.5399361	0.006	Singlet-A	H-5->LUMO (15%), H-5->L+1 (14%), H-4->LUMO (11%), H-4->L+1 (27%)	H-4->L+3 (5%), H-3->L+3 (6%), H-2->L+1 (3%), H-2->L+3 (3%), HOMO->L+5 (3%), HOMO->L+6 (4%)
243.0109624	0.0021	Singlet-A	HOMO->L+6 (68%)	H-7->LUMO (4%), H-5->LUMO (4%), H-1->L+4 (4%), HOMO->L+5 (3%), HOMO->L+7 (7%)
241.4069453	0.0008	Singlet-A	H-3->L+2 (17%), H-2->L+2 (15%), H-1->L+4 (44%)	H-3->L+1 (7%), H-2->L+1 (4%), HOMO->L+6 (8%)
238.7065711	0.0087	Singlet-A	H-6->LUMO (85%)	H-7->LUMO (7%), H-4->LUMO (2%)
234.7029739	0.5305	Singlet-A	H-3->L+1 (15%), H-1->L+2 (45%)	H-7->LUMO (8%), H-5->L+1 (6%), H-4->L+1 (5%), HOMO->LUMO (3%), HOMO->L+7 (4%)
232.9303994	0.0114	Singlet-A	HOMO->L+7 (74%)	H-3->L+1 (7%), HOMO->L+6 (4%), HOMO->L+8 (5%)
232.4325916	0.2148	Singlet-A	H-3->L+1 (38%), H-2->L+1 (16%), H-1->L+2 (25%)	H-1->L+4 (3%), HOMO->L+7 (5%)

Table S-4 TD-DFT calculated electronic transitions, oscillator strength (*f*), and MO composition for compounds **3b**.



No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	28333.45054	352.9397165	0.3071	Singlet-A	HOMO->LUMO (83%)	H-2->L+2 (5%), HOMO->L+1 (9%)
2	29364.2271	340.5504244	0.0466	Singlet-A	H-2->LUMO (10%), HOMO->L+1 (69%), HOMO->L+2 (10%)	HOMO->LUMO (8%)
3	29931.23486	334.0991458	0.0042	Singlet-A	H-2->LUMO (35%), HOMO->L+1 (21%), HOMO->L+2 (42%)	
4	31024.11611	322.3298921	0.0135	Singlet-A	H-1->LUMO (98%)	
5	32875.15853	304.1810427	0.1141	Singlet-A	H-1->L+1 (93%)	H-3->L+3 (3%)
6	34633.44718	288.7382231	0.0049	Singlet-A	H-4->LUMO (12%), HOMO->L+4 (84%)	
7	35021.39986	285.5396997	0.0015	Singlet-A	H-3->L+1 (51%), H-1->L+3 (39%)	H-3->LUMO (5%)
8	35903.77041	278.5222802	0.0953	Singlet-A	H-4->LUMO (44%), H-2->LUMO (19%), HOMO->L+2 (16%), HOMO->L+4 (13%)	
9	36269.94612	275.7103627	0.1375	Singlet-A	H-4->LUMO (38%), H-2->LUMO (23%), H-2->L+1 (14%), HOMO->L+2 (17%)	
10	36722.42315	272.3131847	0.095	Singlet-A	H-2->L+1 (72%)	H-5->L+1 (5%), H-4->LUMO (3%), H-2->LUMO (5%), HOMO->L+2 (8%)
11	37076.50055	269.7126172	0.0029	Singlet-A	H-3->LUMO (91%)	H-3->L+1 (4%)
12	37410.41408	267.3052476	0.002	Singlet-A	HOMO->L+3 (95%)	
13	37873.37632	264.0377218	0.0018	Singlet-A	H-5->LUMO (19%), H-5->L+1 (48%)	H-6->L+1 (6%), H-5->L+5 (3%), H-4->L+1 (5%), H-2->L+1 (9%)
14	38137.11962	262.211727	0.0006	Singlet-A	H-1->L+2 (98%)	
15	38607.34085	259.0180981	0.0032	Singlet-A	H-6->LUMO (15%), H-5->LUMO (35%), H-5->L+1 (10%), HOMO->L+6 (33%)	
16	39591.33726	252.5805061	0.013	Singlet-A	H-5->LUMO (29%), HOMO->L+5 (29%), HOMO->L+6 (22%)	H-7->LUMO (4%), H-6->LUMO (7%), H-5->L+1 (3%)
17	39888.14929	250.7010272	0.0104	Singlet-A	HOMO->L+5 (66%)	H-6->LUMO (3%), H-5->LUMO (9%), H-5->L+1 (4%), HOMO->L+6 (9%)
18	40618.08104	246.1957764	0.0373	Singlet-A	H-7->LUMO (15%), H-6->LUMO (62%), HOMO->L+6 (11%)	H-4->L+1 (4%), H-2->L+2 (3%)
19	41222.19031	242.5877889	0.0043	Singlet-A	H-4->L+1 (42%), H-4->L+2 (18%), H-2->L+4 (23%)	H-5->L+1 (4%), HOMO->L+6 (3%), HOMO->L+7 (3%)
20	41464.15664	241.1721547	0.002	Singlet-A	HOMO->L+7 (80%)	H-7->LUMO (3%), H-4->L+1 (4%), HOMO->L+8 (8%)

8. Crystallographic Data and Detailed Refinements for 2-3

Table S-5 Crystal data and structure refinement of 2a

Empirical formula	$C_{23}H_{16}N_2O$
Formula weight	336.38
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.8120(2)
b/Å	12.8630(3)
c/Å	15.4670(3)
α/°	110.229(2)
β/°	96.599(2)
γ/°	106.447(2)
Volume/Å^3	1706.94(8)
Z	4
ρ_{calc}g/cm^3	1.309
μ/mm^{-1}	0.639
F(000)	704.0
Crystal size/mm^3	0.24 × 0.1 × 0.06
Radiation	Cu $K\alpha$ (λ = 1.54184)
2θ range for data collection/°	6.268 to 154.68
Index ranges	$-12 \leq h \leq 11$, $-15 \leq k \leq 16$, $-19 \leq l \leq 15$
Reflections collected	42515
Independent reflections	7152 [R_{int} = 0.0533, R_{sigma} = 0.0330]
Data/restraints/parameters	7152/0/476
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0430, wR_2 = 0.1102
Final R indexes [all data]	R_1 = 0.0496, wR_2 = 0.1145
Largest diff. peak/hole / e Å^{-3}	0.25/-0.23

Table S-6 Crystal data and structure refinement of **2b**

Empirical formula	$C_{57}H_{39}Cl_9N_4O_2$
Formula weight	1130.97
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.3742(2)
b/Å	11.1000(2)
c/Å	11.2768(2)

α/°	92.4379(16)
β/°	94.2137(15)
γ/°	91.8446(16)
Volume/Å^3	1293.07(4)
Z	1
ρ_{calc}g/cm^3	1.452
μ/mm^{-1}	4.842
F(000)	578.0
Crystal size/mm^3	0.208 × 0.137 × 0.07
Radiation	Cu $K\alpha$ (λ = 1.54184)
2θ range for data collection/°	7.87 to 154.746
Index ranges	$-12 \leq h \leq 13$, $-14 \leq k \leq 13$, $-13 \leq l \leq 14$
Reflections collected	32585
Independent reflections	5420 [R_{int} = 0.0665, R_{sigma} = 0.0381]
Data/restraints/parameters	5420/42/405
Goodness-of-fit on F^2	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0437, wR_2 = 0.1124
Final R indexes [all data]	R_1 = 0.0485, wR_2 = 0.1165
Largest diff. peak/hole / e Å^{-3}	0.97/-0.57

Table S-7 Crystal data and structure refinement of **3a**

Empirical formula	$C_{25}H_{16}N_2O$
Formula weight	360.40
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.04500(10)
b/Å	20.4122(2)
c/Å	17.8760(2)
β/°	103.3480(10)
Volume/Å^3	3566.29(7)
Z	8
ρ_{calc}g/cm^3	1.342
μ/mm^{-1}	0.652
F(000)	1504.0
Crystal size/mm^3	0.194 × 0.115 × 0.059
Radiation	Cu $K\alpha$ (λ = 1.54184)
2θ range for data collection/°	6.676 to 159.572
Index ranges	$-12 \leq h \leq 12$, $-26 \leq k \leq 25$, $-19 \leq l \leq 22$
Reflections collected	88647

Independent reflections	7713 [R_{int} = 0.0699, R_{sigma} = 0.0315]
Data/restraints/parameters	7713/0/513
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0663, wR_2 = 0.1790
Final R indexes [all data]	R_1 = 0.0770, wR_2 = 0.1918
Largest diff. peak/hole / e Å^{-3}	0.59/-0.23

Table S-8 Crystal data and structure refinement of **3b**

Empirical formula	$C_{30}H_{19}Cl_3N_2O$
Formula weight	529.82
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	4.8515(2)
b/Å	21.8040(12)
c/Å	11.5794(5)
β/°	91.942(4)
Volume/Å^3	1224.19(10)
Z	2
ρ_{calc}g/cm^3	1.437
μ/mm^{-1}	3.607
F(000)	544.0
Crystal size/mm^3	0.2 × 0.05 × 0.04
Radiation	Cu $K\alpha$ (λ = 1.54184)
2θ range for data collection/°	7.64 to 149.936
Index ranges	$-6 \le h \le 6$, $-27 \le k \le 23$, $-14 \le l \le 14$
Reflections collected	23474
Independent reflections	4748 [R_{int} = 0.0808, R_{sigma} = 0.0523]
Data/restraints/parameters	4748/17/367
Goodness-of-fit on F^2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0694, wR_2 = 0.1904
Final R indexes [all data]	R_1 = 0.0840, wR_2 = 0.2025
Largest diff. peak/hole / e Å^{-3}	0.37/-0.51
Flack parameter	0.03(4)