Supplementary Material (ESI) for Chemical Communications
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Asymmetric core-expanded aza-BODIPY analogues: facile synthesis and optical properties

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I. Experimental section

II. Supplementary Figure

I. Experimental Section

I.1 Materials and instrumentations

All reagents were obtained from commercial suppliers and used without further purification unless otherwise indicated. All air and moisture-sensitive reactions were carried out under nitrogen atmosphere in oven-dried glassware. Glassware was dried in an oven at 120 °C and cooled under a stream of inert gas before use. Both dichloromethane and triethylamine were distilled over calcium hydride. ^{1}H NMR spectra were recorded on a Bruker DRX400 spectrometer and referenced to the residual proton signals of the solvent. HR-MS were recorded on a Bruker Daltonics microTOF-Q II spectrometer. All the solvents employed for the spectroscopic measurements were of UV spectroscopic grade (Aldrich).

I.2 Synthesis and characterisation

Aza-boron-pyridyl-ketoazaphenalene (**4a**)

A solution of imino-ketoazaphenalene (100 mg, 0.51 mmol) and 4-(octyloxy)pyridin-2-amine (124 mg, 0.56 mmol) in n-butanol (6 ml) was heated under reflux for 24h, ammonia was evolved, when the solution was cooled, a orange-yellow solid was precipitated. The crude product was dissolved in dry dichloromethane solution (100 ml) and treated with $BF_3 \cdot OEt_2$ (1.1 ml) in the presence of triethylamine (1 ml) at room temperature for 1 h. The reaction was quenched by adding water, the organic layer was dried over $MgSO_4$, filtered, and evaporated to dryness. The crude product was purified by silica-gel flash column chromatography (80% Hexane/Ethyl acetate) and recrystallized from CH_2Cl_2/hexane to provide **4a** as cyan powder with high yield of 30%. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.09 (d, *J* = 8.0 Hz, 1 H), 8.65 (d, *J* = 8.0 Hz, 1 H), 8.30 (d, *J* = 7.0 Hz, 1 H), 8.20-8.17 (m, 2 H), 7.77–7.72 (m, 2 H), 7.07 (s, 1 H), 6.85 (d, *J* = 8.0 Hz, 1 H), 4.20 (t, *J* = 6.5 Hz, 2 H), 1.91-1.85 (m, 2 H), 1.53-1.46 (m, 2 H), 1.37-1.31 (m, 8 H), 0.90 (t, *J* = 6.6 Hz, 3 H); UV/Vis (CH_2Cl_2), λ_{max} (ε) = 399 nm (39700 dm^3 mol^{-1} cm^{-1}); HRMS-ESI: m/z: calcd $[C_{25}H_{26}BF_2N_3O_2+H]^+$ m/z = 450.2159; found m/z = 472.1978, $[M+Na]^+$; 450.2159, $[M+H]^+$; 430.2097, $[M-F]^+$;

Compound **4b** was obtained as yellow powder in 31% yield by following a procedure similar to that of **4a**. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.92 (d, *J* = 7.6 Hz, 1 H), 8.65 (d, *J* = 7.2 Hz, 1 H), 8.13 (dd, *J* = 8.0 Hz, 2 H), 7.95 (d, *J* = 7.8 Hz, 1 H), 7.76-7.67 (m, 2 H), 7.43-7.32 (m, 3 H), 4.36 (t, *J* = 7.1 Hz, 2 H), 1.93-1.86 (m, 2 H), 1.48-1.39 (m, 2 H), 1.00 (t, *J* = 7.4 Hz, 3H); UV/Vis (CH_2Cl_2), λ_{max} (ε) = 401 nm (26200 dm^3 mol^{-1} cm^{-1}); HRMS-ESI: m/z: calcd $[C_{23}H_{19}BF_2N_4O+Na]^+$ m/z = 439.1512 ; found m/z = 439.1517, $[M+Na]^+$.

Compound **4c** was obtained as a yellow solid in 28% yield by following a procedure similar to that of **4a**. ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 8.94 (d, *J* = 8.0 Hz, 1 H), 8.58 (d, *J* = 7.6 Hz, 1 H), 8.20 (d, *J* = 7.6 Hz, 2 H), 7.99 (d, *J* = 8.8 Hz, 1 H), 7.76-7.69 (m, 3 H), 7.61 (m, 1 H), 1.33 (s, 9 H); UV/Vis (CH_2Cl_2), λ_{max} (ε) = 429 nm (31700 dm^3 mol^{-1} cm^{-1}); HRMS-ESI: m/z: calcd $[C_{23}H_{18}BF_2N_3OS+H]^+$ m/z = 434.1304; found m/z =434.1304 $[M+H]^+$; 414.1242, $[M-F]^+$.

Compound **4d** was obtained as orange-red crystals in 26% yield by following a procedure similar to that of **4a**. ^{1}H NMR (400 MHz, $CDCl_3$): δ= 8.98 (d, *J* = 7.4, 1 H), 8.70 (d, *J* = 7.4, 1 H), 8.23 (d, *J* = 8.1 Hz, 2 H), 8.11 (d, *J* = 9.0 Hz, 1 H), 7.81-7.73 (m, 2 H), 7.21-7.16 (m, 2 H), 4.02 (t, *J* = 6.8 Hz, 2 H), 1.82 (m, 2 H), 1.48 (m, 2H), 1.36-1.30 (m, 8 H), 0.90 (t, *J* = 6.5 Hz, 3 H); UV/Vis (CH_2Cl_2), λ_{max} (ε) = 431 nm (34800 dm^3 mol^{-1} cm^{-1}); HRMS-ESI: m/z: calcd $[C_{27}H_{26}BF_2N_3O_2S+H]^+$ m/z = 506.1880; found m/z = 506.1880, $[M+H]^+$; 486.1817, $[M-F]^+$.

I.3 X-ray structure determination

The X-ray diffraction data were collected on a Bruker Smart Apex CCD diffractometer with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) using the ω–2θ scan mode. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares methods using SHELX-2000.[S1-S2] All calculations and molecular graphics were carried out on a computer using the SHELX-2000 program package and Diamond 3.2.

4c: $C_{23}H_{18}BF_2N_3OS$, CH_2Cl_2; A yellow block-like crystal of the approximate dimensions 0.15 × 0.14 × 0.12 mm^3 was measured. Monoclinic, space group P2(1)/n, *a* = 9.5908(8) Å, *b* = 10.9141(10) Å, *c* = 22.863(2) Å, α = 90, β = 99.059(2), γ = 90, V = 2363.3(4) Å^3, Z = 4, F(000) = 1064, ρ = 1.530 Mgm^{-3}, R_1 = 0.0488, wR_2 = 0.1529, GOF = 1.032, residual electron density between 0.402 and −0.482 eÅ^{-3}.

4d: $C_{27}H_{26}BF_2N_3O_2S$; A orangey-red block-like crystal of the approximate dimensions 0.12 × 0.11 × 0.10 mm^3 was measured. Monoclinic, space group P2(1)/n, a = 14.57220(10) Å, b = 16.04600(10) Å, c = 22.1206(2) Å, α = 90, β = 107.66, γ = 90, V = 4928.66(6) $Å^3$, Z = 8, F(000) = 2112, ρ = 1.511 Mgm^{-3}, R_1 = 0.0715, wR_2 = 0.2230, GOF = 1.081, residual electron density between 0.851 and −0.675 $eÅ^{-3}$.

CCDC No.1020987 for **4c** and No 1020988 for **4d** containing the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB21EZ, UK; fax: (+44)1223–336–033; E-mail: deposit@ccdc.cam.ac.uk).

1.4 Spectroscopic measurements

UV-visible absorption spectra were recorded on a Shimadzu 3000 spectrophotometer. Fluorescence spectra were measured on a Hitachi F-2700 luminescence spectrometer with a 150 W xenon lamp. The fluorescence lifetimes of the samples were determined with a Horiba Jobin Yvon Fluorolog-3 spectrofluorimeter. Absorption and emission measurements were carried out in 1×1 cm quartz cuvettes. Drop casting films were prepared by evaporation of the dye (1 mM) in dichloromethane onto a clean silicon wafer substrates, hose films were stable and no change in emission was observed over an extended period of time. The absolute quantum yields and emission spectra in the solid state were measured in Horiba Jobin Yvon Fluorolog-3 spectrofluorimeter with integrating sphere. For all measurements, the temperature was kept constant at (298±2) K. Dilute solutions with absorbance of less than 0.05 at the excitation wavelength were used for the measurement of fluorescence quantum yields. 9,10-Diphenylanthracene was used as the standard (Φ_F = 0.90 in cyclohexane).[S3] The quantum yield, Φ, was calculated using equation (1):

$$\Phi_{sample}=\Phi_{std}\left[\frac{I\,sample}{I\,std}\;\frac{A\,std}{A\,sample}\right]\left[\frac{n\,sample}{n\,std}\right]^2 \quad (1)$$

where the *sample* and *std* subscripts denote the sample and standard, respectively, I is the integrated emission intensity, A stands for the absorbance, and n is refractive index.

When the fluorescence decays were monoexponential, the rate constants of radiative (k_r) and nonradiative (k_{nr}) deactivation were calculated from the measured fluorescence quantum yield (Φ_F) and fluorescence lifetime (τ) according to equations (2) and (3):

$$k_r = \Phi_F/\tau \qquad (2)$$

$$k_{nr} = (1-\Phi_F)/\tau \qquad (3)$$

I.5 DFT calculations

The G09W software package was used to carry out a DFT geometry optimization using the B3LYP functional with 6-31G(d) basis sets.[S4] The same approach was used to calculate the absorption properties based on time-dependent (TD-DFT) method.

II Supplementary data

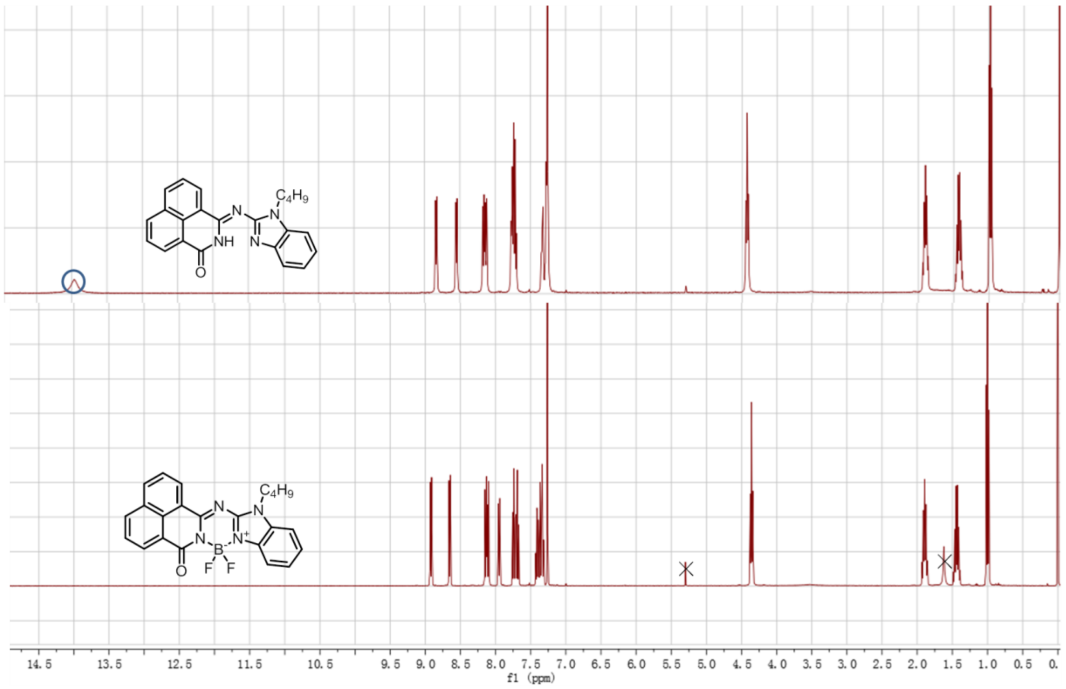

Fig. S1 ^{1}H NMR spectra of **4b** and it's precursor.

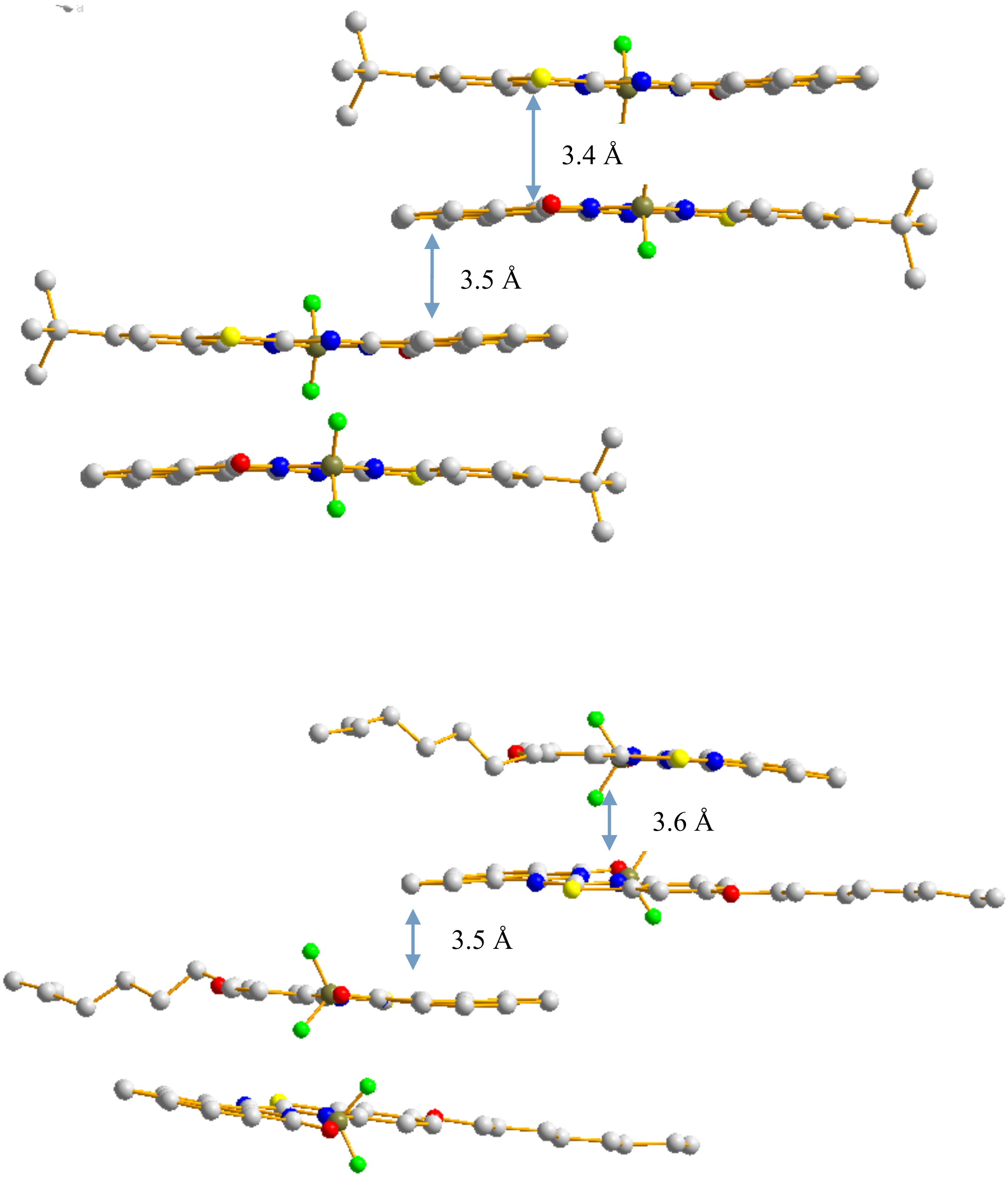

Fig. S2 View of the π–π stacking interactions of **4c** (Top) and **4d** (Bottom).

Table S1. Spectroscopic and photophysical properties of **1-4** in various solvents at 298K.

	Solvent	λ_{abs} [nm]	λ_{em} [nm]	fwhm$_{em}$ [nm]	$\Delta\nu_{em\text{-}ab}$ [cm^{-1}]	Φ_F [c]	τ_f [ns]	k_r [10^8 s^{-1}]	k_{nr} [10^8 s^{-1}]
4a	hexane	378(sh), 396, 415(sh)	424(sh), 451	72	3080	0.10	1.00	1.0	9.0
	Toluene	382(sh), 399, 420(sh)	436(sh), 462	78	3418	0.25	2.23	1.1	3.4
	CH_2Cl_2	382(sh), 399, 418(sh)	437(sh), 463	77	3464	0.43	3.16	1.4	1.8
	THF	381(sh), 398, 417(sh)	461	82	3433	0.14	1.52	0.9	5.7
	CH_3CN	381(sh), 396, 414(sh)	462	85	3608	0.11	1.45	0.8	6.1
4b	hexane	397, 418(sh)	458(sh), 489	83	4739	0.19	2.08	0.9	3.9
	Toluene	402, 420(sh)	474(sh), 504	88	5034	0.13	1.87	0.7	4.7
	CH_2Cl_2	401	512	91	5406	0.10	1.59	0.6	5.7
	THF	400	510	92	5392	0.06	1.43	0.4	6.6
	CH_3CN	399	516	93	5683	0.04	1.01	0.4	9.5
4c	hexane	407, 427	474(sh), 504	81	3578	0.16	1.98	0.8	4.2
	Toluene	414(sh), 432	489(sh), 515	86	3731	0.12	1.61	0.7	5.5
	CH_2Cl_2	429	524	86	4226	0.06	1.18	0.5	8.0
	THF	427	519	89	4151	0.05	0.97	0.5	9.8
	CH_3CN	423	524	89	4557	0.03	0.90	0.3	10.8
4d	hexane	423, 445(sh)	503(sh), 535	81	4949	0.025	0.73	0.3	13..4
	Toluene	429	549	79	5095	0.013	0.45	0.3	21.9
	CH_2Cl_2	431	553	76	5119	0.006	0.23	0.3	43.2
	THF	428	555	77	5346	0.005	0.22	0.2	45.2
	CH_3CN	429	558	77	5389	<0.002[b]	n.d.[d]	n.d.	n.d.

[a] sh=shoulder. [b] Could not be reliably determined. [c] Relative fluorescence quantum yield. [d] Not determined.

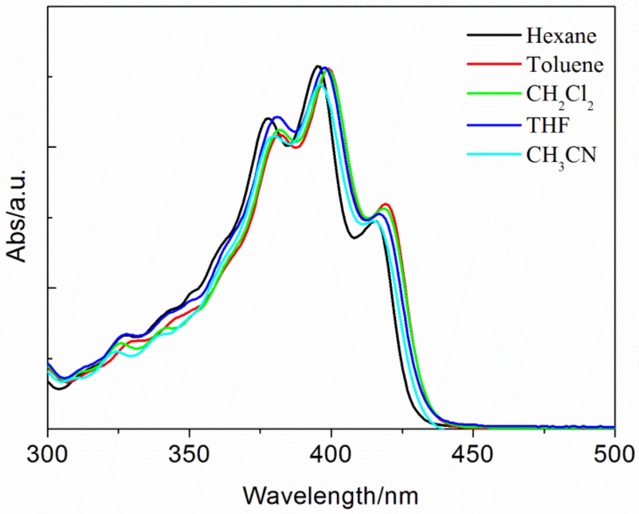

Fig. S3. Absorption spectra of **4a** in a range of different solvents.

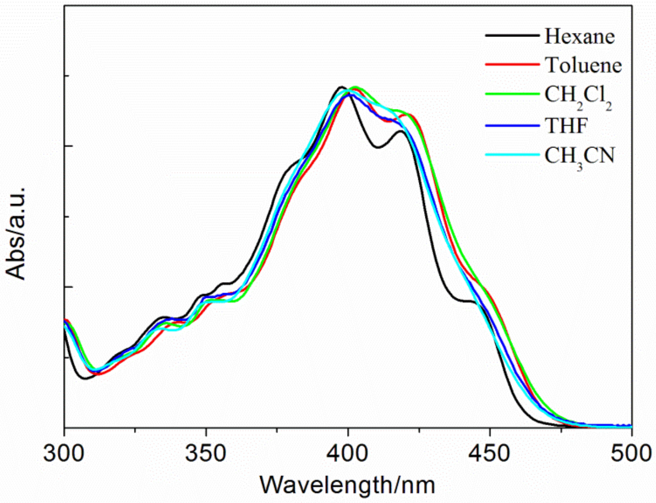

Fig. S4. Absorption spectra of **4b** in a range of different solvents.

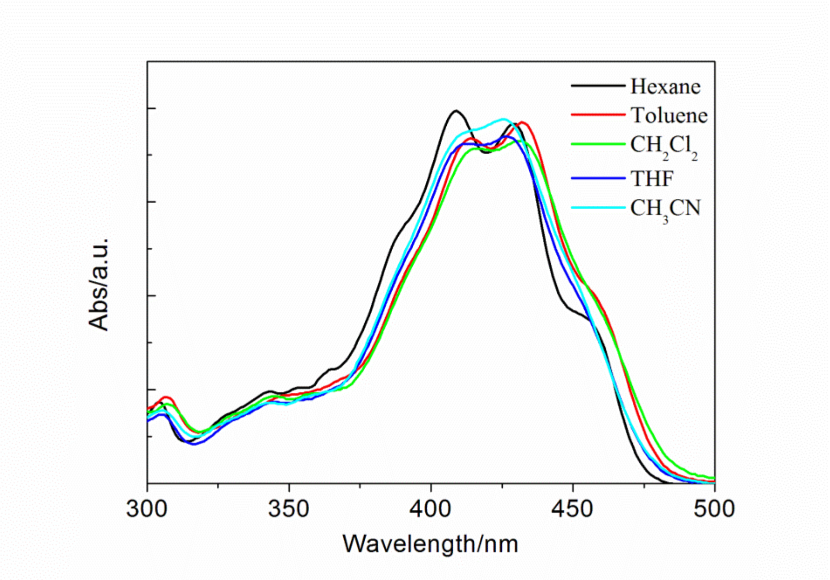

Fig. S5. Absorption spectra of **4c** in a range of different solvents.

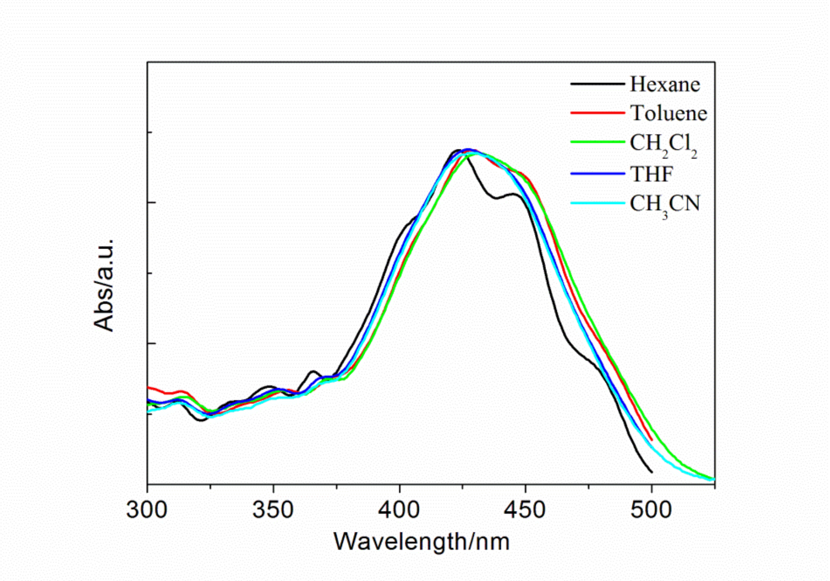

Fig. S6. Absorption spectra of **4d** in a range of different solvents.

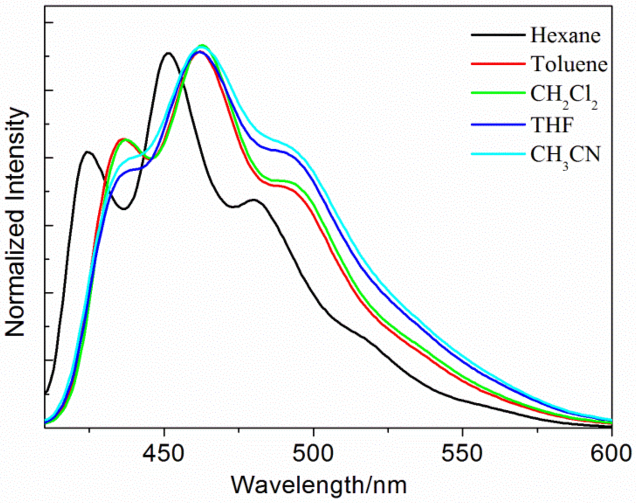

Fig. S7. Emission spectra of **4a** in a range of different solvents.

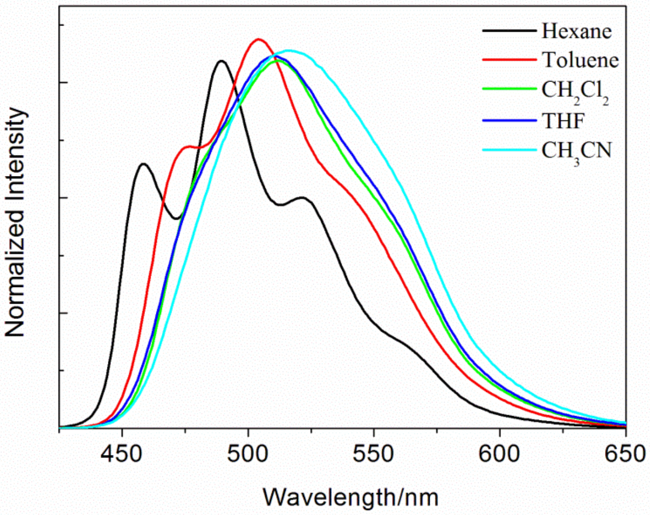

Fig. S8. Emission spectra of **4b** in a range of different solvents.

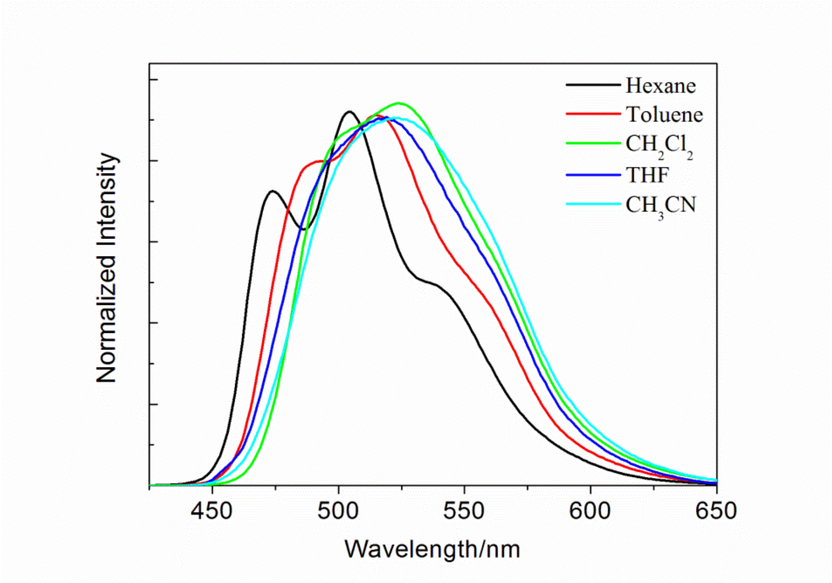

Fig. S9. Emission spectra of **4c** in a range of different solvents.

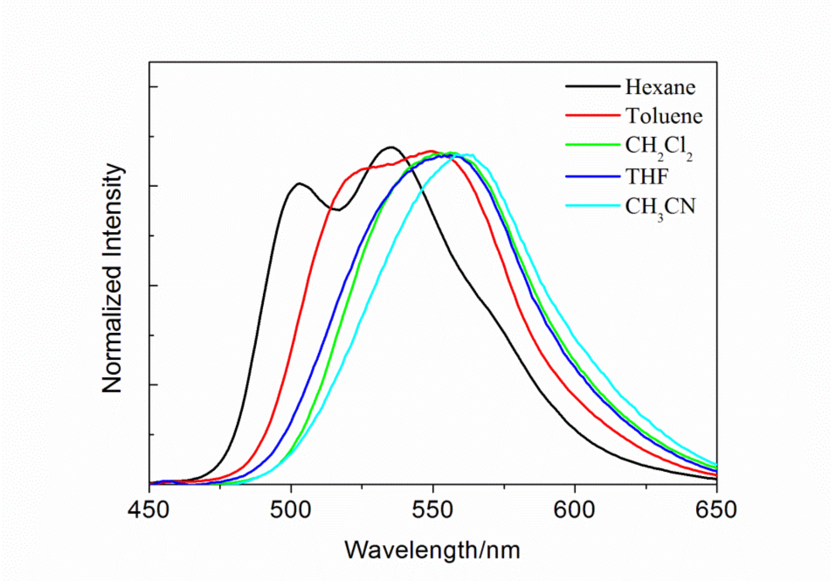

Fig. S10. Emission spectra of **4d** in a range of different solvents.

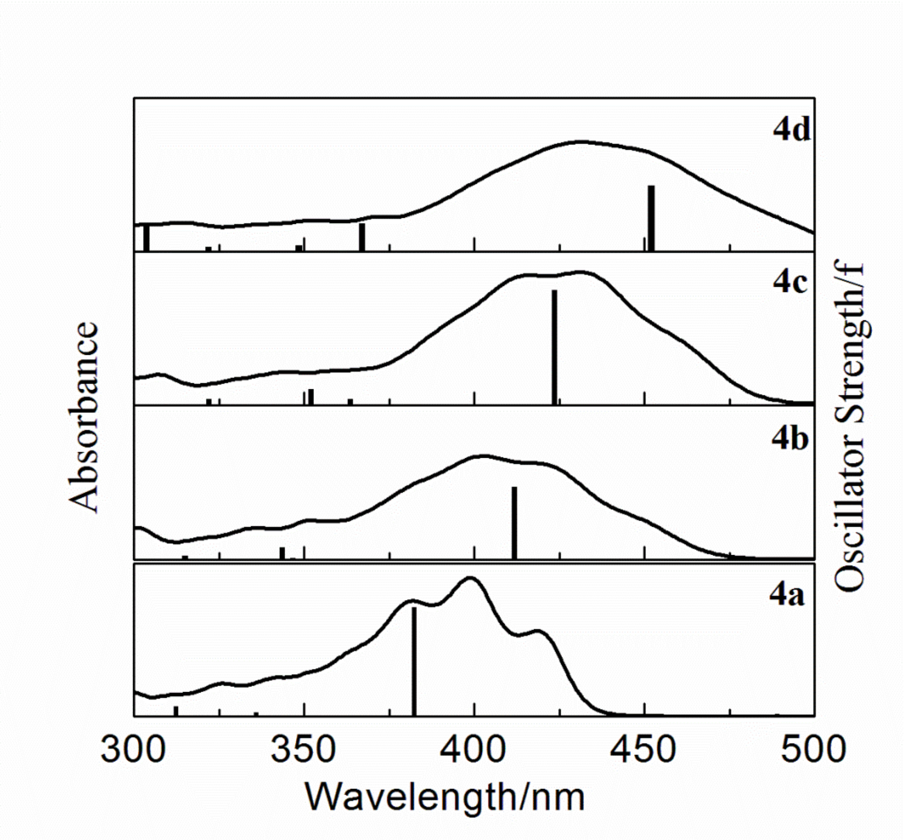

Fig. S11 The experimental spectra and TD-DFT spectra of **4a–4d** calculated using the B3LYP functional with 6-31G(d) basis sets.

Table S2. Calculated electronic excitation energies, oscillator strengths, and eigenvectors for the TD-DFT spectra of **4a–4d** carried out using the B3LYP functional with 6-31G(d) basis sets.

	State [a]	Energy [eV]	λ [nm]	*f* [b]	Orbitals (coefficient) [c]
4a	S_1	3.24	382	0.5351	H >L (+98%)
	S_3	3.69	336	0.0199	H-1>L(+92%)
	S_3	3.97	312	0.0487	H-3>L(+79%)
4b	S_1	3.01	412	0.5223	H >L (+99%)
	S_3	3.58	346	0.0100	H-2->L (+93%)
	S_4	3.61	344	0.0844	H-1>L (+89%)
4c	S_1	2.93	424	0.6264	H >L (+99%)
	S_3	3.41	364	0.0292	H-1>L (+80%) H-2->L(18%)
	S_4	3.52	352	0.0747	H-2>L(+78%)
4d	S_1	2.74	452	0.4695	H>L(+100%)
	S_3	3.38	367	0.1990	H-1>L(+91%)
	S_4	3.56	348	0.0397	H-2>L(+89%)

[a] Excited state. [b] Oscillator strength. [c] MOs involved in the transitions with H and L denoting the HOMO and LUMO, respectively. [d] Type of excited state.

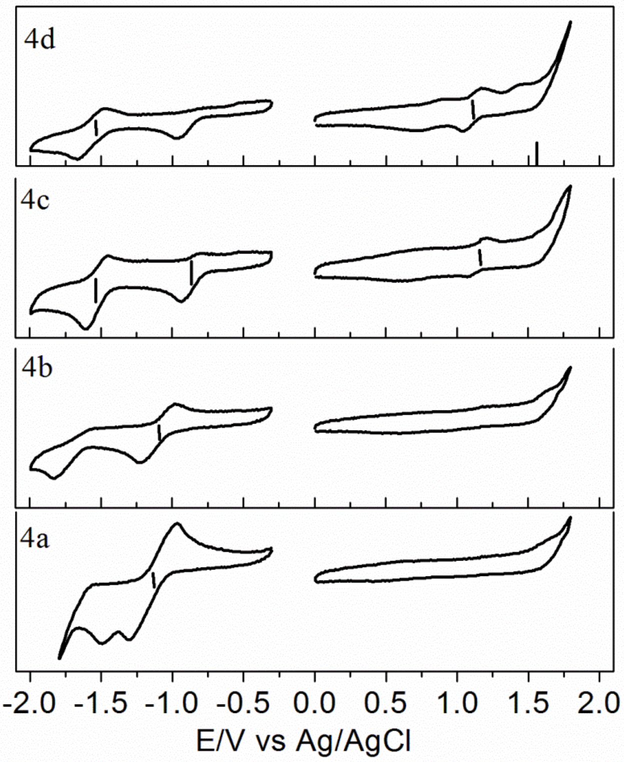

Fig. S12 Cyclic voltammograms of **4a–4d** in *ortho*-dichlorobezene. Scan rates: 100 mv/s.

Table S3. Redox potentials and electronics states of compounds **4a–4d** (in *ortho*-dichlorobezene, 0.1 M TBAP, scan rate 100 mV s^{-1}).[a]

	E_g[b]	$E^{ox}_{1/2}$	$E^{red}_{1/2}$ 1 st	$E^{red}_{1/2}$ 2 nd	LUMO[c]	HOMO
4a	2.92	n.d	-1140	n.d	-3.26	-6.18
4b	2.71	n.d	-1100	n.d	-3.30	-6.01
4c	2.62	1160	-870	-1530	-3.53	-6.15
4d	2.48	1110	-950 [d]	-1590	-	-

[a] Referenced against Fc^+/Fc. [b] Energy band gap, determined from wavelength of intersection point of UV-vis and PL; [c] $E_{LUMO} = -e(E^{red}_{1/2} + 4.4)$, $E_{HOMO} = E_{LUMO} - E_g$; [d] The value of E_p

III. References

S1 C. L. Picou, E. D. Stevens, M. Shah and J. H. Boyer, *Acta Crystallogr. Sect. C* 1990, **46**, 1148.

S2 SMART, SAINT, SADABS and SHELXTL, Bruker AXS Inc., Madison, 2000.

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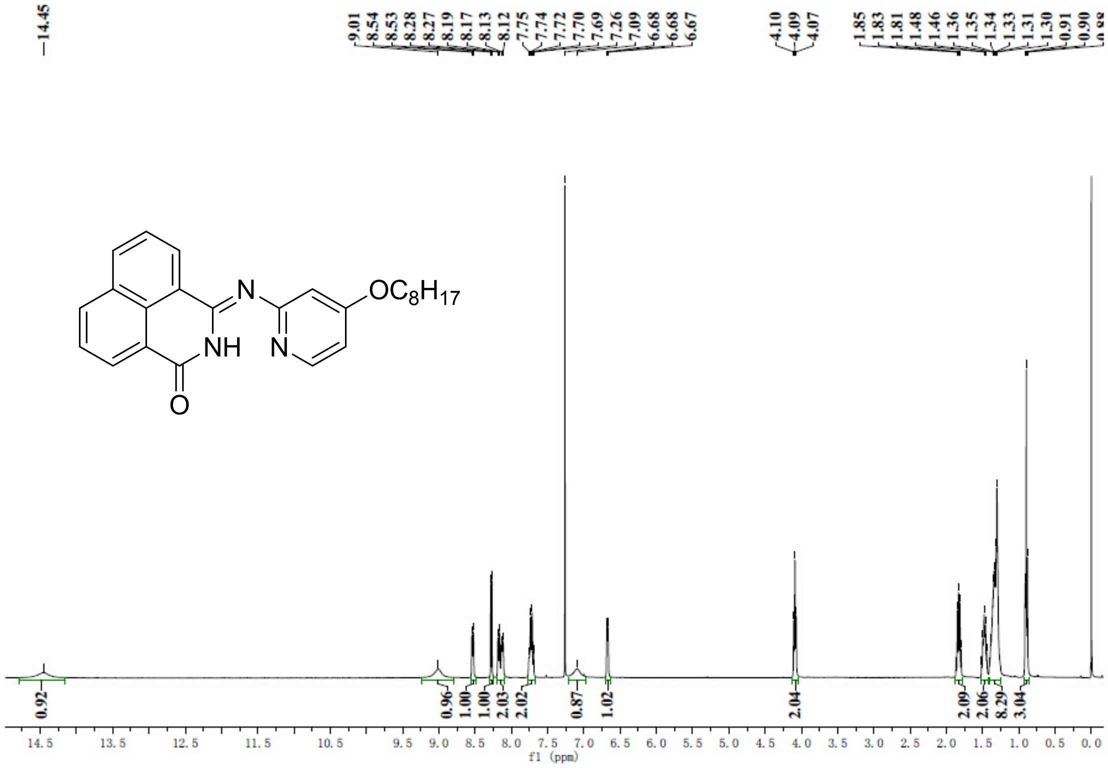
S4 Gaussian 09, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

IV ^{1}H NMR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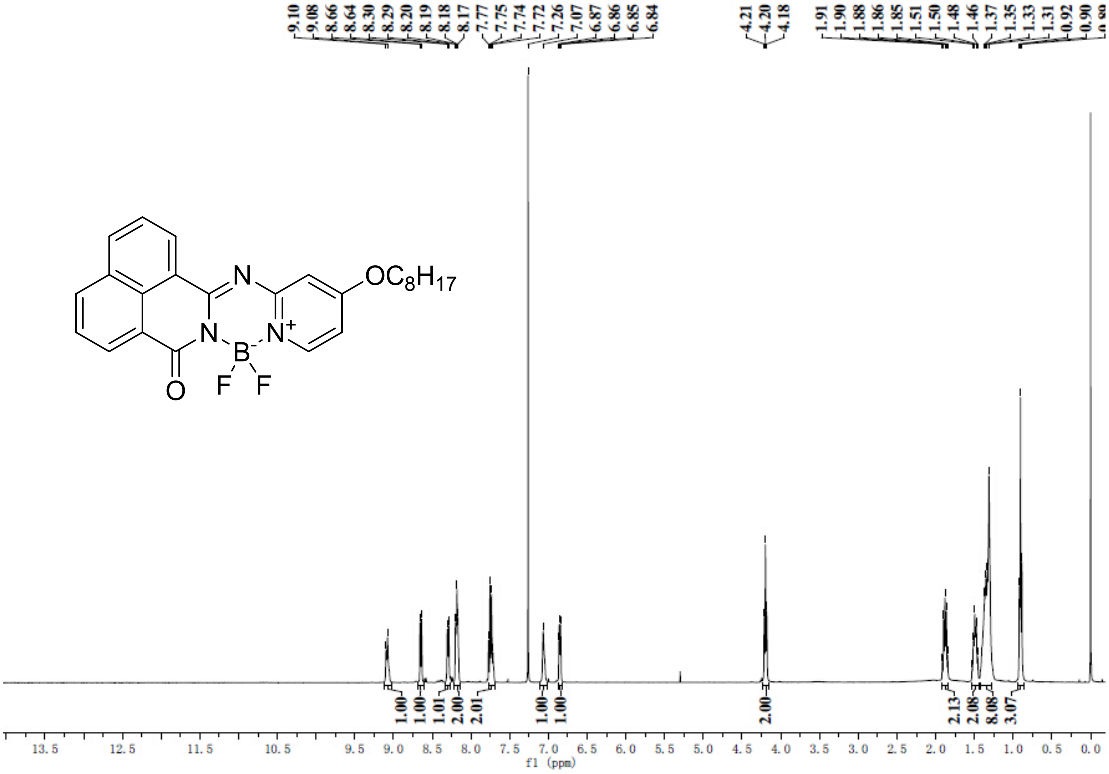
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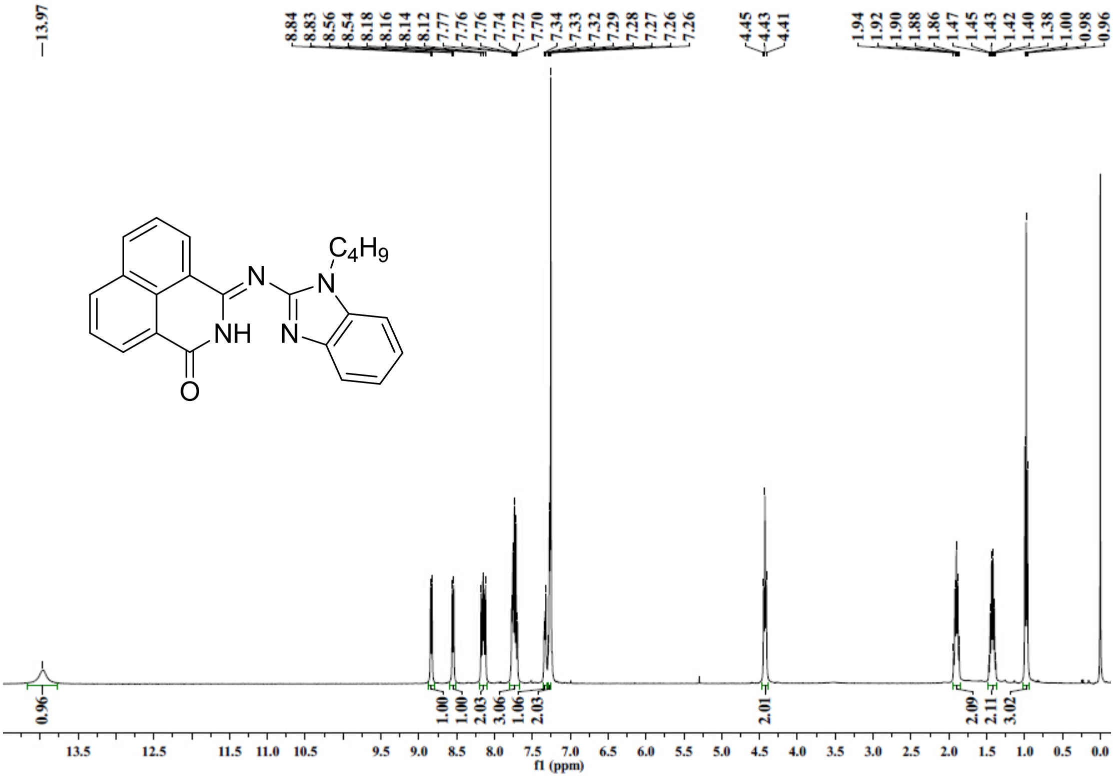
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1.5
1.0
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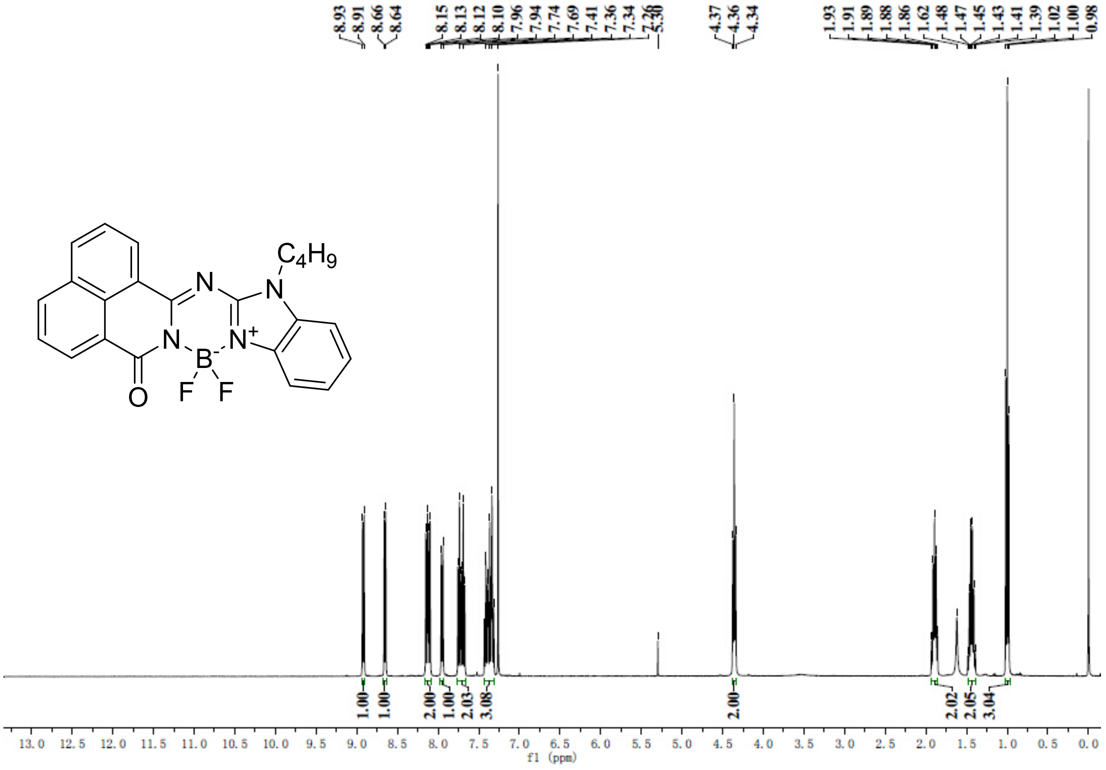
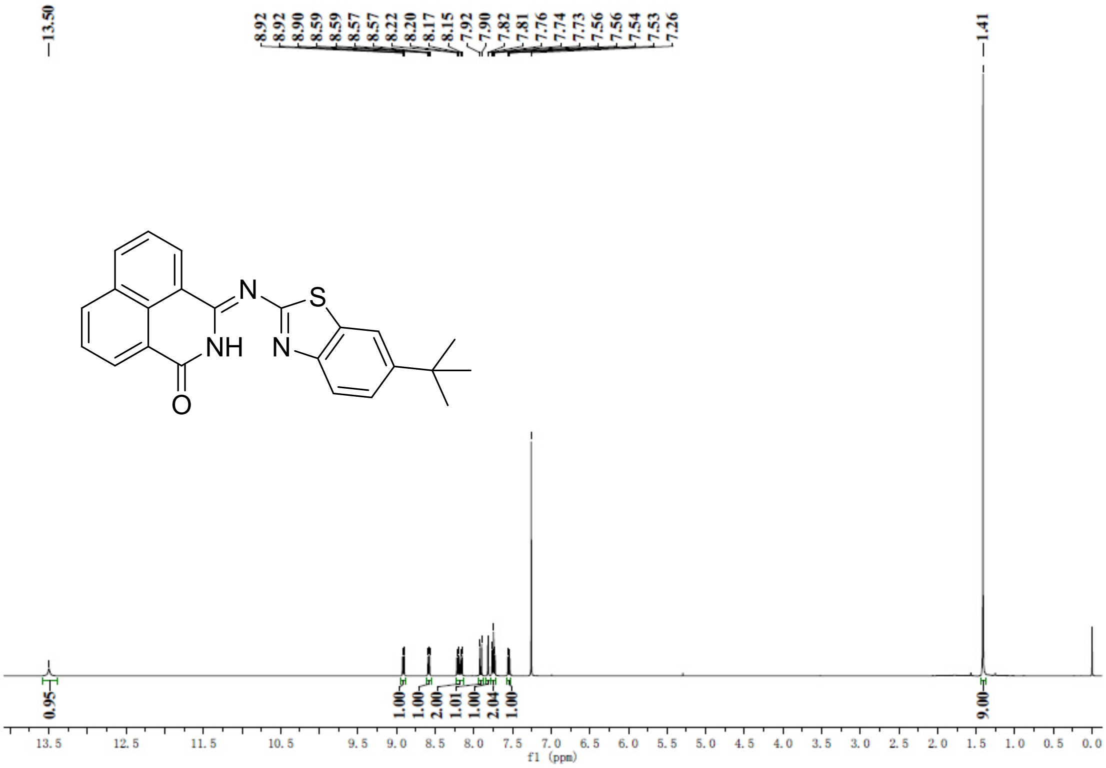
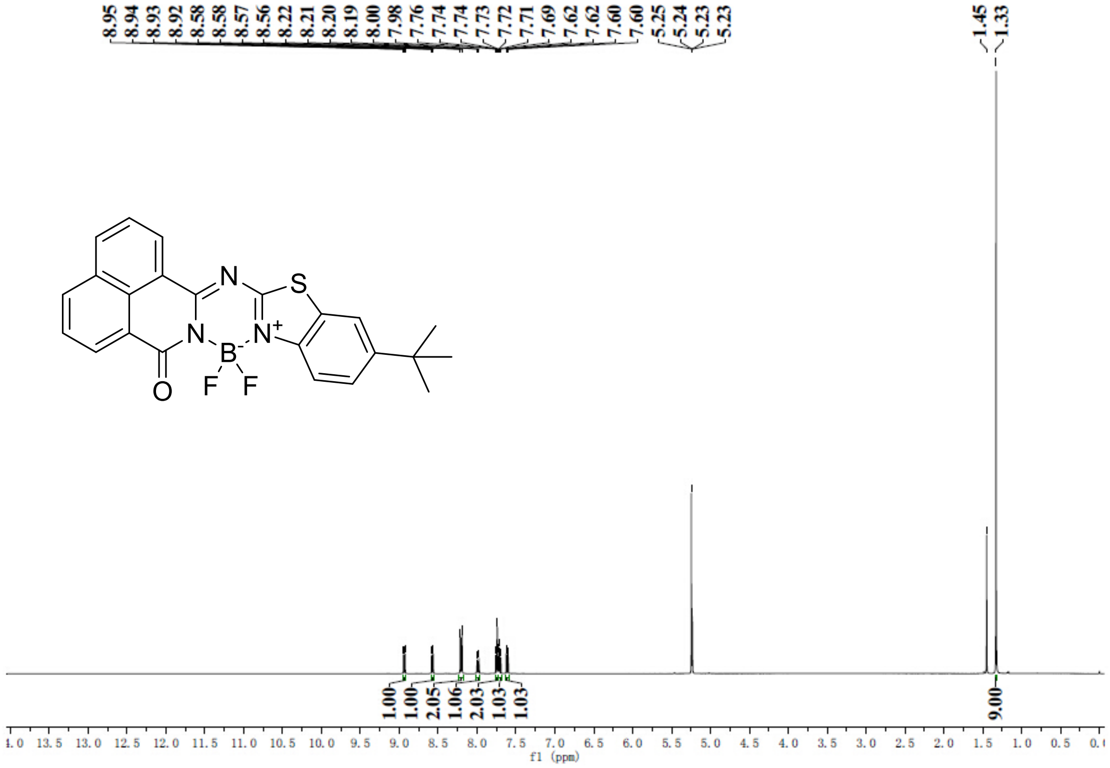
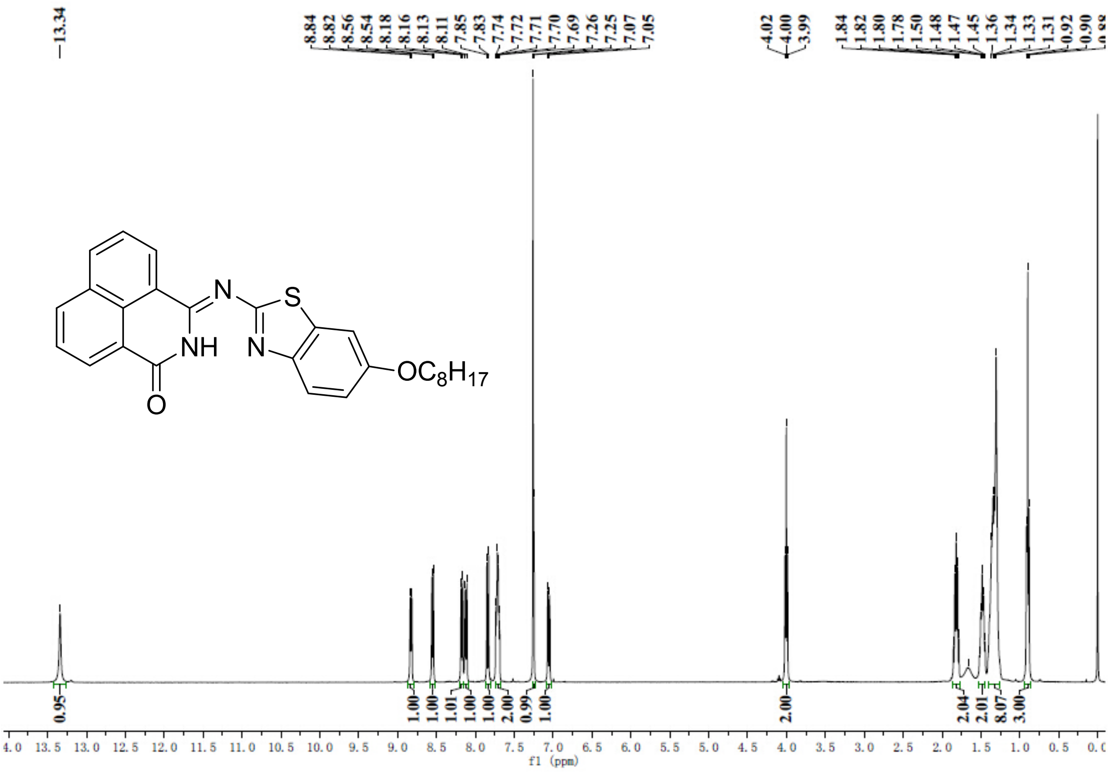
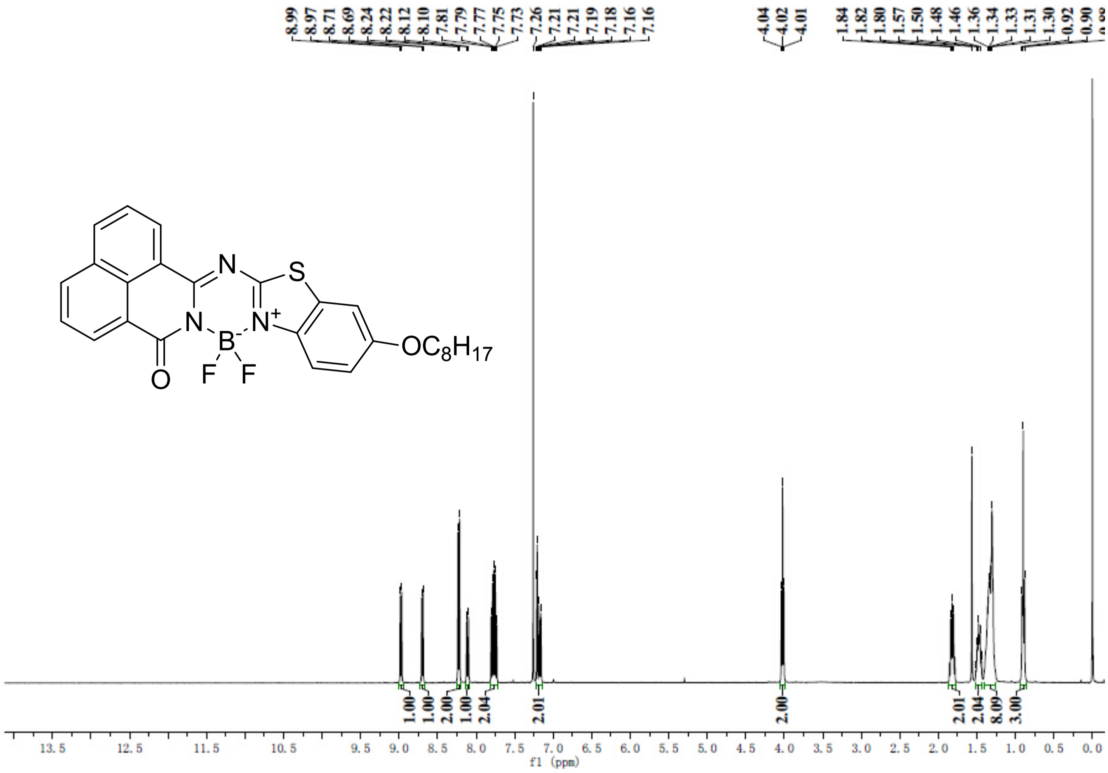
0.0
f1 (ppm)


8.93
8.91
8.66
8.64
8.15
8.13
8.12
8.10
7.96
7.94
7.74
7.69
7.41
7.36
7.34
7.26
5.30
4.37
4.36
4.34
1.93
1.91
1.89
1.88
1.86
1.62
1.48
1.47
1.45
1.43
1.41
1.39
1.02
1.00
0.98
C4H9
N
N
N
N+
B-
F
F
O
1.00
1.00
2.00
1.00
2.03
3.08
2.00
2.02
2.05
3.04
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

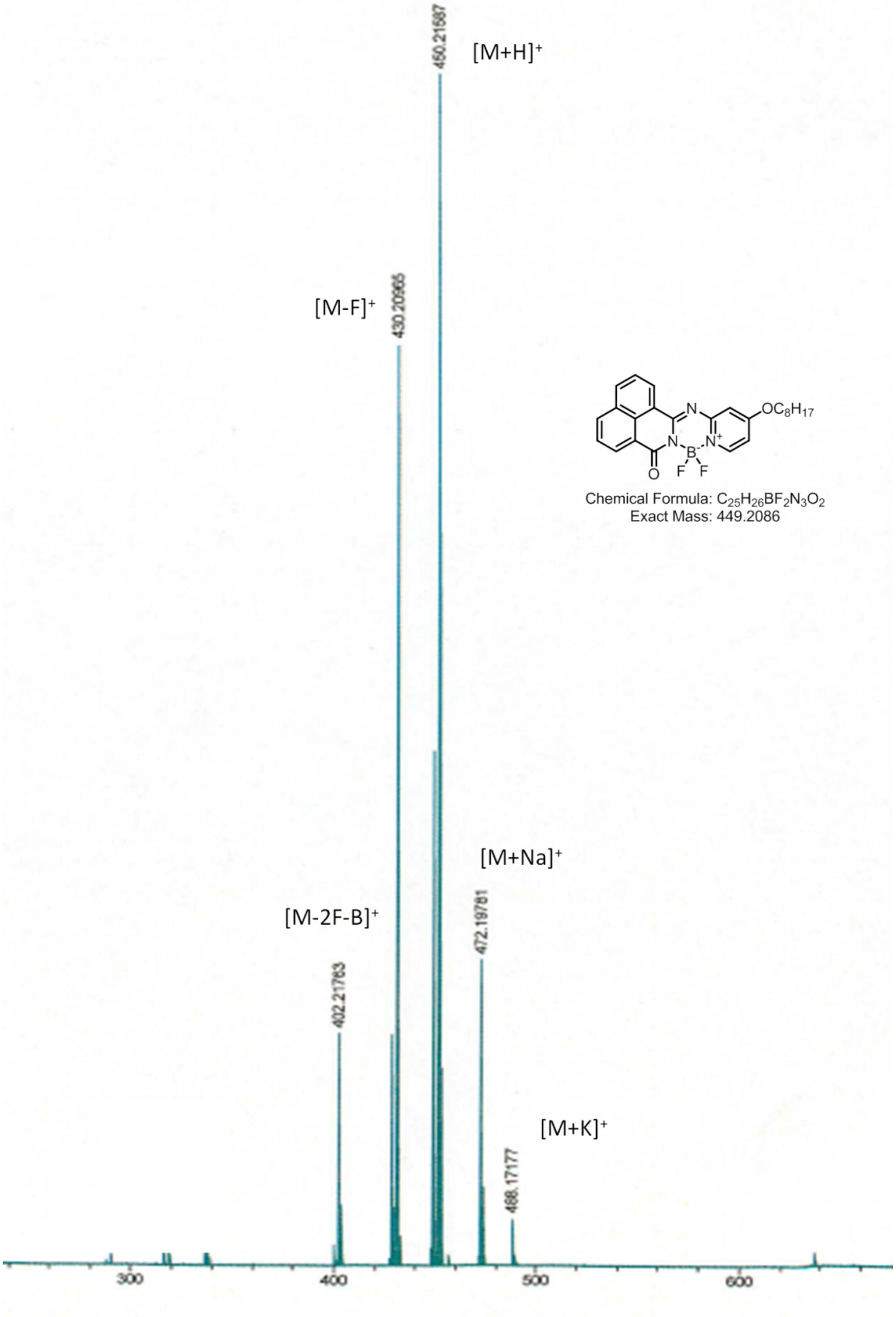

13.50
8.92
8.92
8.90
8.59
8.59
8.57
8.57
8.22
8.20
8.17
8.15
7.92
7.90
7.82
7.81
7.76
7.74
7.73
7.56
7.54
7.53
7.26
1.41
N
S
NH
N
O
0.95
1.00
1.00
2.00
1.01
1.00
2.04
1.00
9.00
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

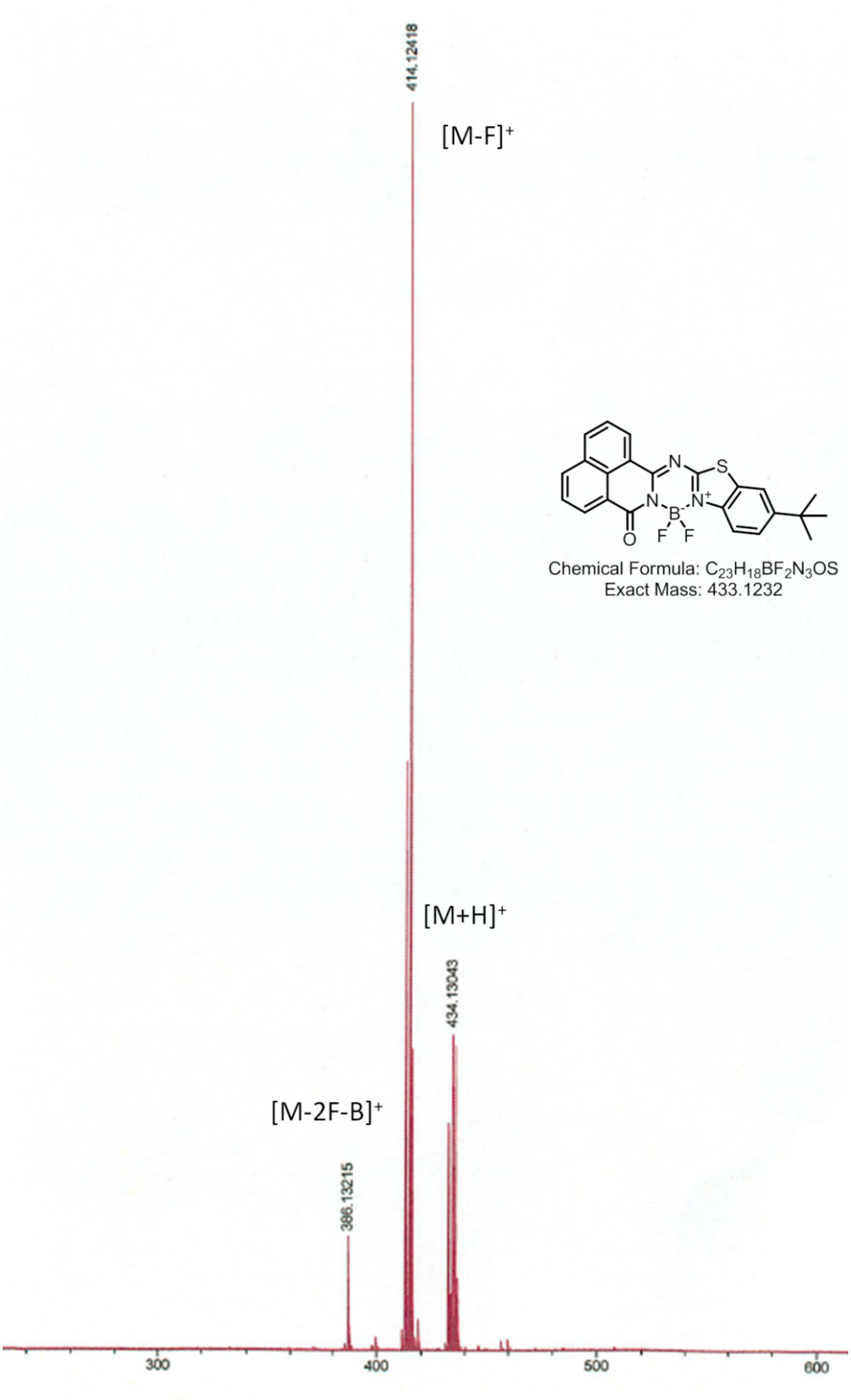

8.95
8.94
8.93
8.92
8.58
8.58
8.57
8.56
8.22
8.21
8.20
8.19
8.00
7.98
7.76
7.74
7.74
7.73
7.72
7.71
7.69
7.62
7.62
7.60
7.60
5.25
5.24
5.23
5.23
1.45
1.33
N
S
N
B⁻
N⁺
O
F
F
1.00
1.00
2.05
1.06
2.03
1.03
1.03
9.00
14.0
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

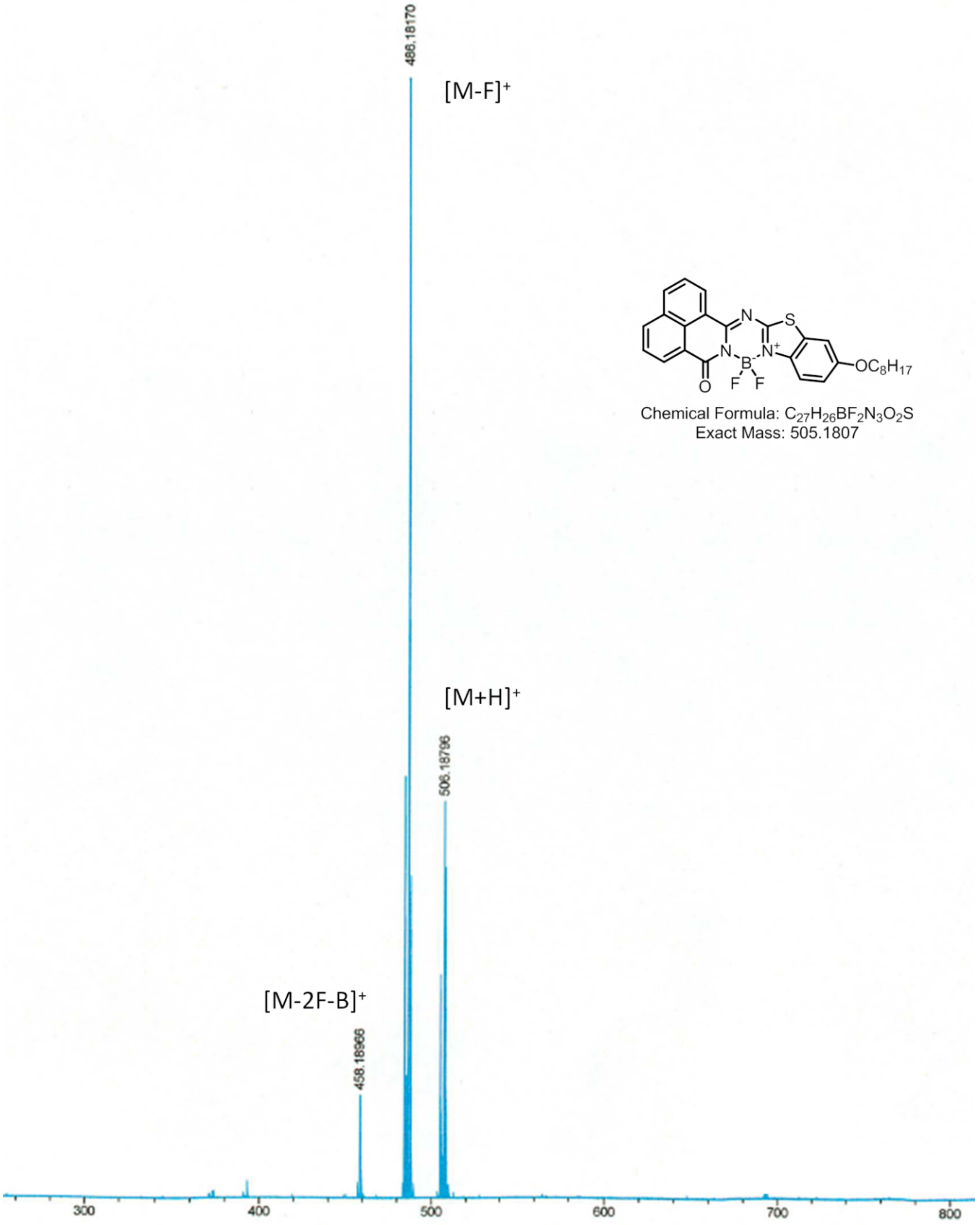

13.34
8.84
8.82
8.56
8.54
8.18
8.16
8.13
8.11
7.85
7.83
7.74
7.72
7.71
7.70
7.69
7.26
7.25
7.07
7.05
4.02
4.00
3.99
1.84
1.82
1.80
1.78
1.50
1.48
1.47
1.45
1.36
1.34
1.33
1.31
0.92
0.90
N
S
NH
N
O
OC_8H_{17}
0.95
1.00
1.00
1.01
1.00
1.00
2.00
0.99
1.00
2.00
2.04
2.01
8.07
3.00
f1 (ppm)

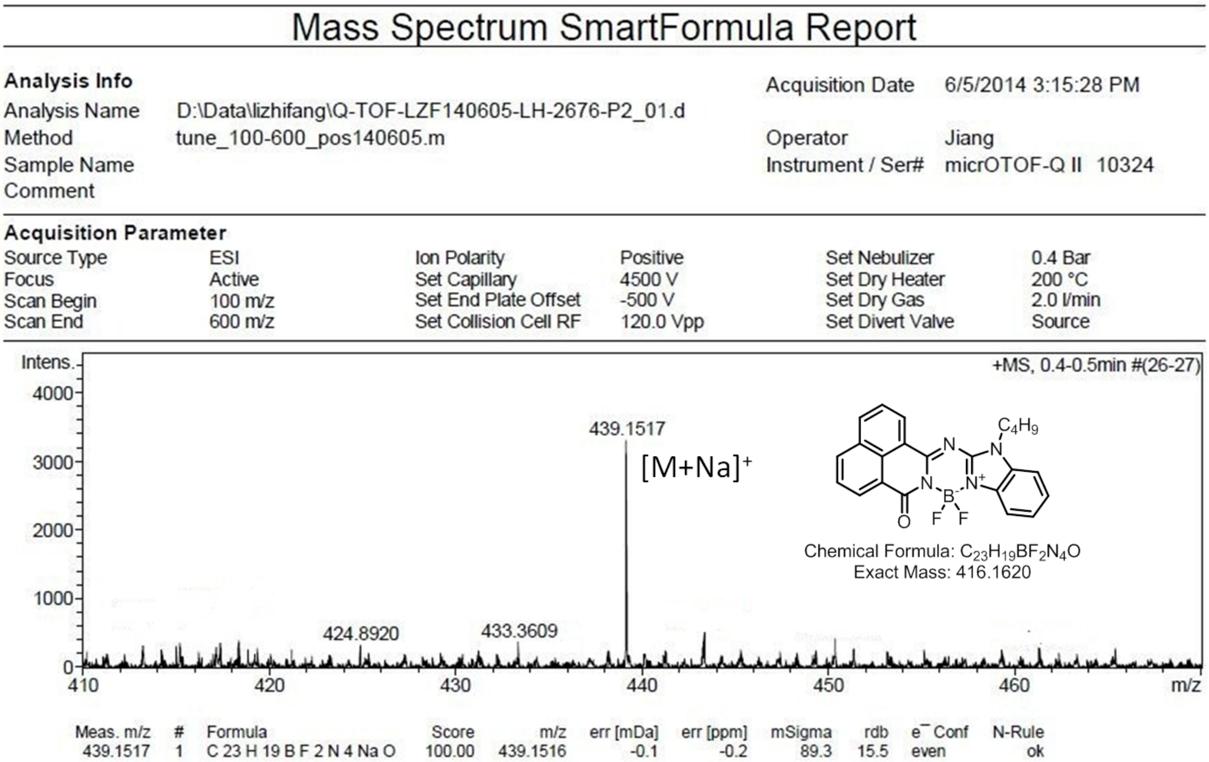

8.99
8.97
8.71
8.69
8.24
8.22
8.12
8.10
7.81
7.79
7.77
7.75
7.73
7.26
7.21
7.21
7.19
7.18
7.16
7.16
4.04
4.02
4.01
1.84
1.82
1.80
1.57
1.50
1.48
1.46
1.36
1.34
1.33
1.31
1.30
0.92
0.90
N
S
N
B^-
N^+
O
F
F
OC_8H_{17}
1.00
1.00
2.00
1.00
2.04
2.01
2.00
2.01
2.04
8.09
3.00
f1 (ppm)

V HR-MS


450.21587
$[M+H]^+$
430.20965
$[M-F]^+$
OC_8H_{17}
N
N
N^+
B^-
F
F
O
Chemical Formula: $C_{25}H_{26}BF_2N_3O_2$
Exact Mass: 449.2086
$[M+Na]^+$
472.19781
$[M-2F-B]^+$
402.21763
$[M+K]^+$
488.17177
300
400
500
600


414.12418
[M-F]+
[M+H]+
434.13043
[M-2F-B]+
386.13215
300
400
500
600
N
S
N
B
N+
O
F
F
Chemical Formula: C23H18BF2N3OS
Exact Mass: 433.1232


486.18170
[M-F]⁺
[M+H]⁺
506.18796
[M-2F-B]⁺
458.18966
N
S
N
B
N⁺
O
F
F
OC8H17
Chemical Formula: C27H26BF2N3O2S
Exact Mass: 505.1807
300
400
500
600
700
800



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\lizhifang\Q-TOF-LZF140605-LH-2676-P2_01.d	Acquisition Date	6/5/2014 3:15:28 PM
Method	tune_100-600_pos140605.m	Operator	Jiang
Sample Name		Instrument / Ser#	micrOTOF-Q II 10324
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	600 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source

Chemical Formula: $C_{23}H_{19}BF_2N_4O$
Exact Mass: 416.1620

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
439.1517	1	C 23 H 19 B F 2 N 4 Na O	100.00	439.1516	-0.1	-0.2	89.3	15.5	even	ok