Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
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Synthesis and Spectroscopic Properties of Novel *Meso*-cyano Boron-pyridyl-isoindoline Dyes

Hui Liu, Hua Lu* Fan Wu, Zhifang Li, Nagao Kobayashi and Zhen Shen,

I. Supplementary Figure

II. Supplementary data

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I. Supplementary Figure

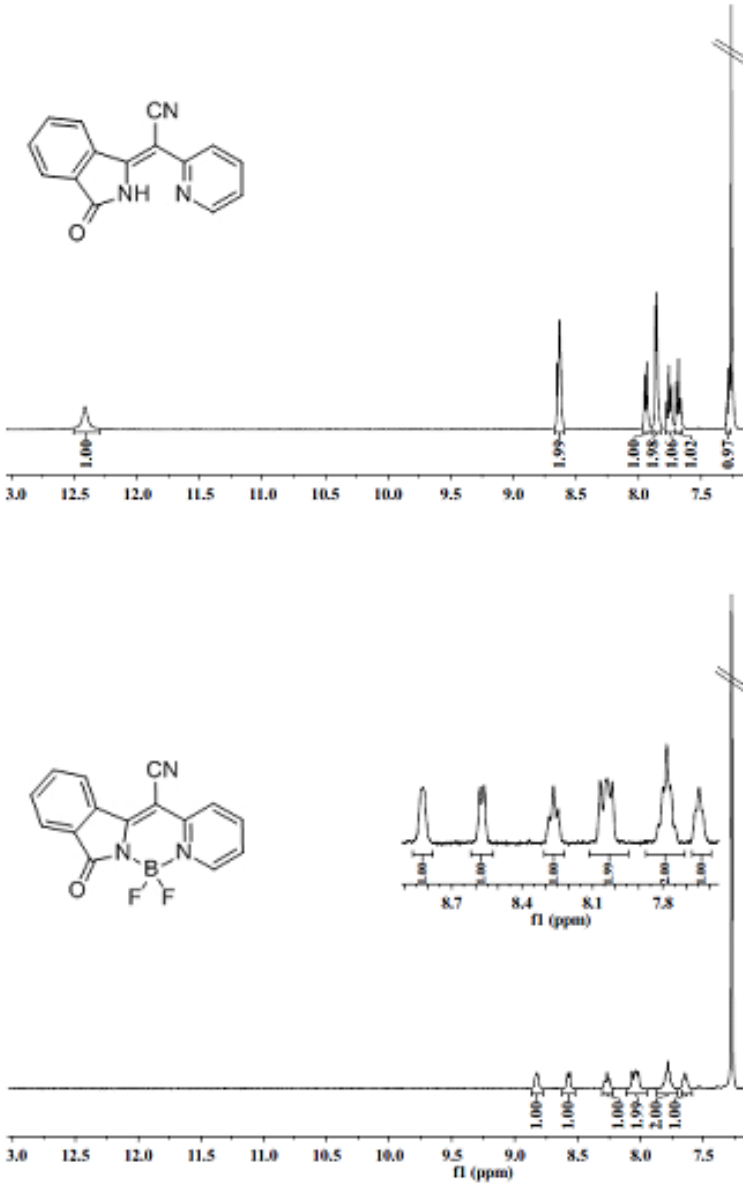


Figure S1. ^{1}H NMR spectra of **1** and its precursor.

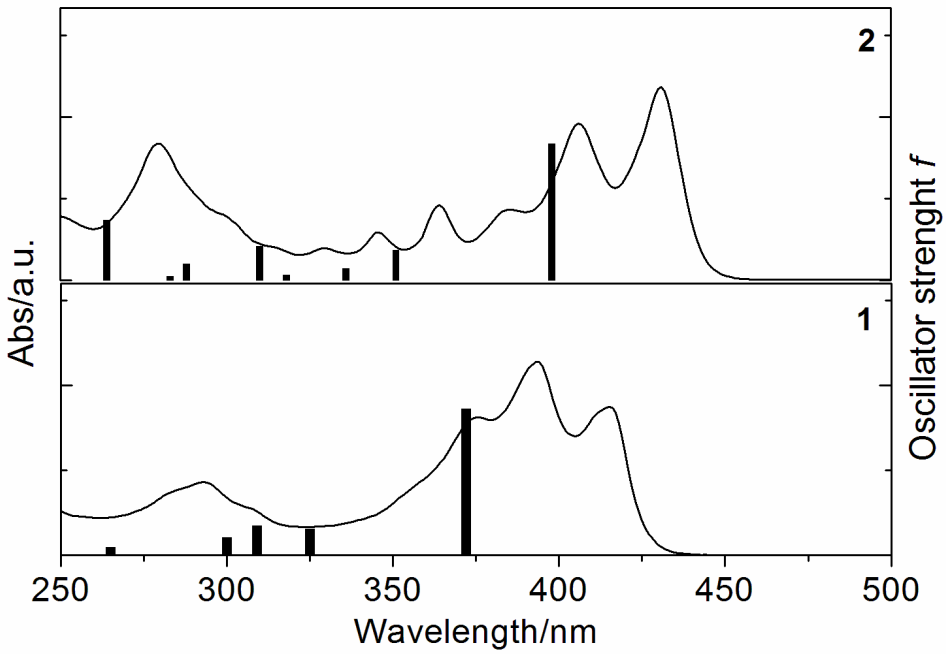
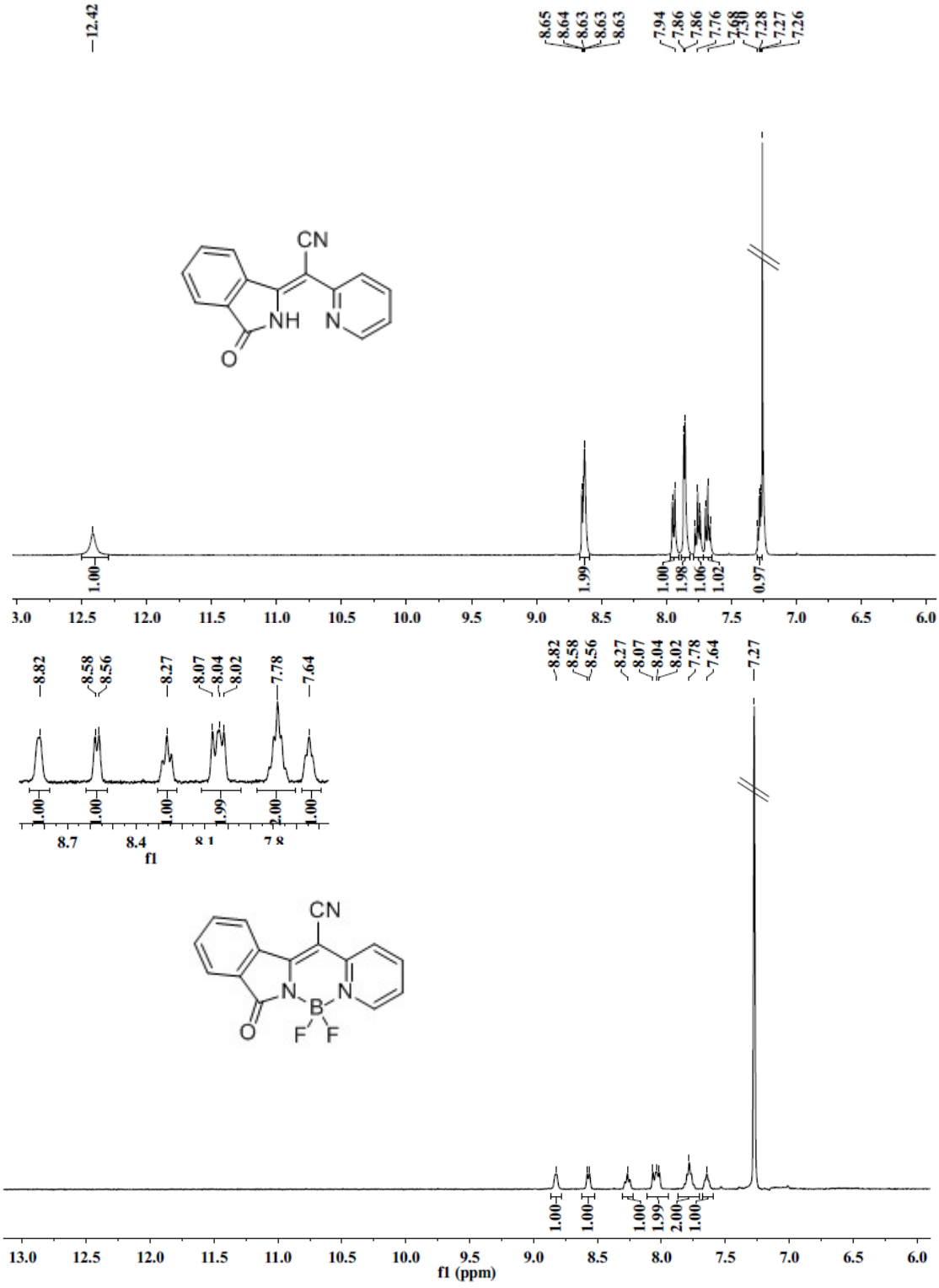
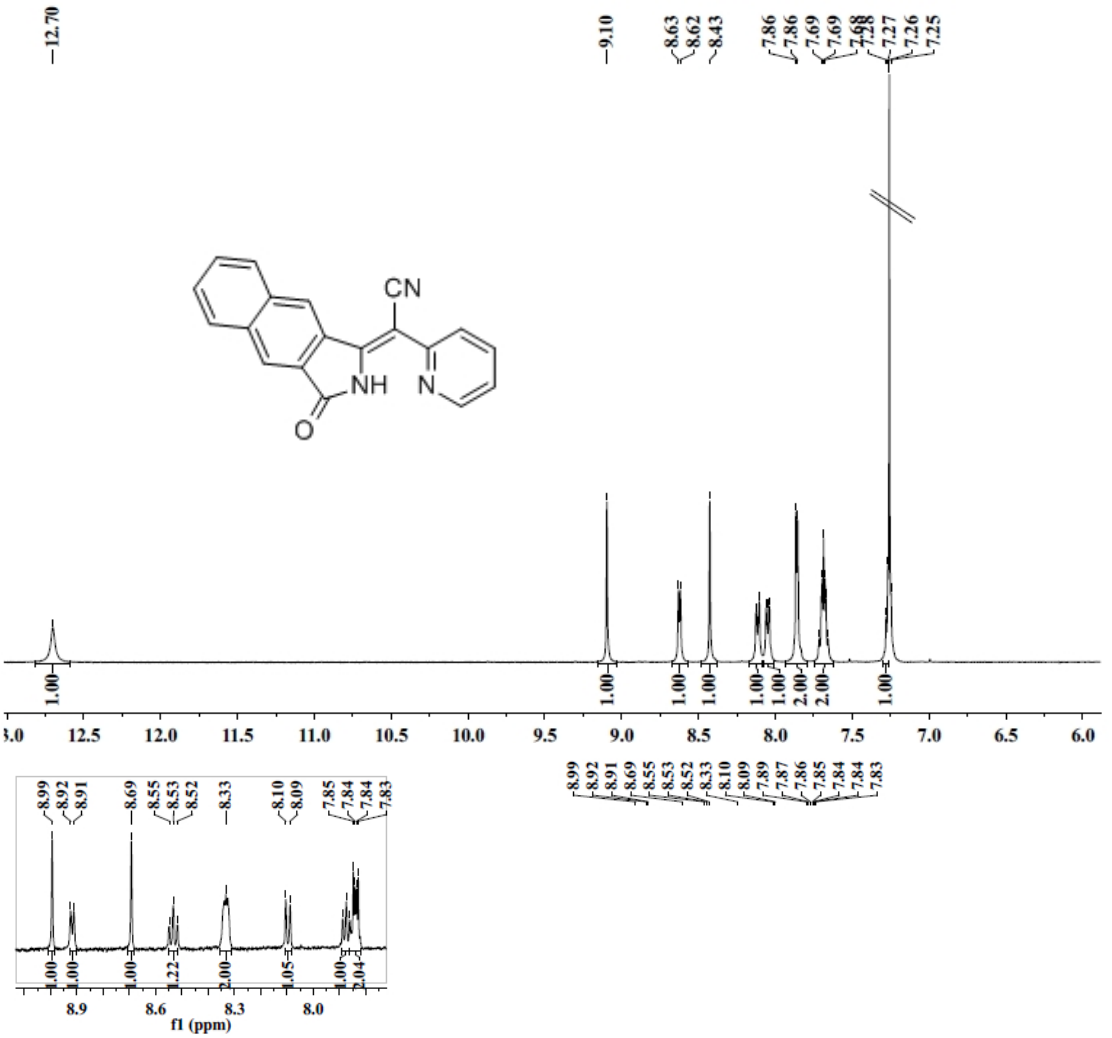


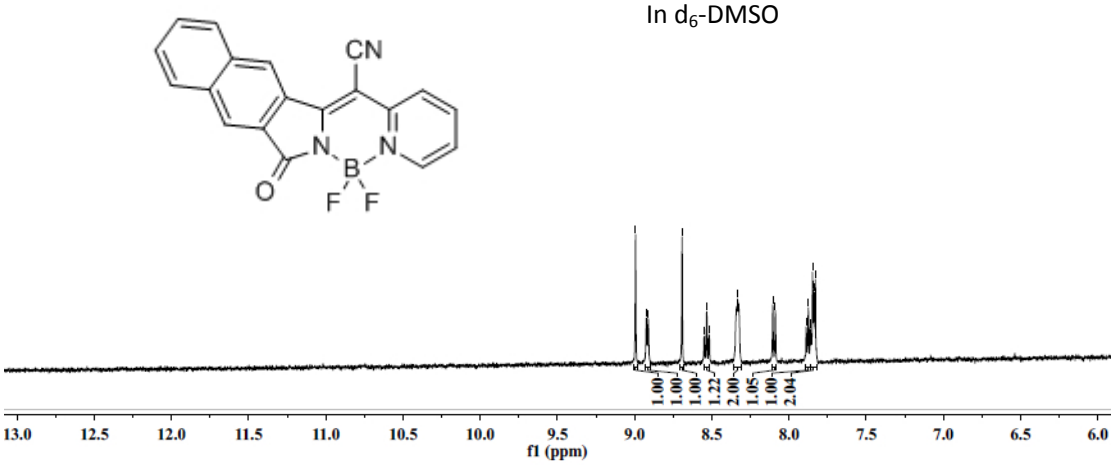
Figure S2 TD-DFT spectra of **1** and **2** calculated using the B3LYP functional with 6-31G(d) basis sets. The experimental spectraof **1** and **2** are plotted against a secondary axis.

II. Supplementary data



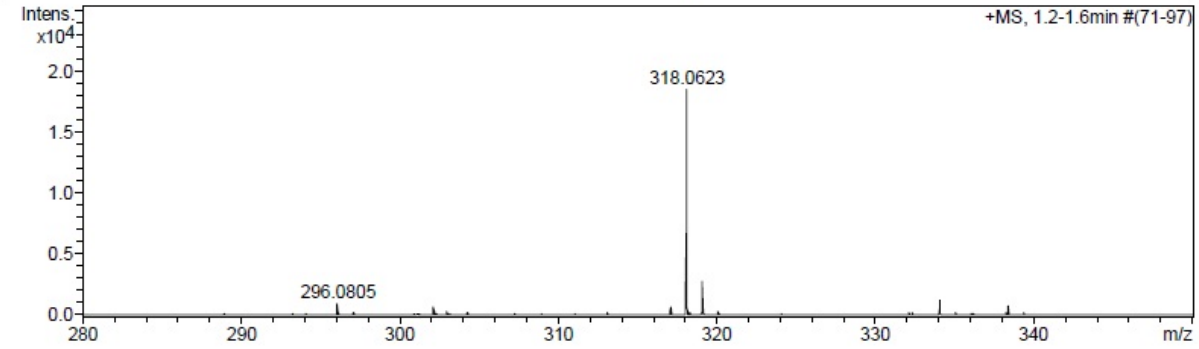

12.70
9.10
8.63
8.62
8.43
7.86
7.86
7.69
7.69
7.28
7.27
7.26
7.25
CN
NH
N
O
1.00
1.00
1.00
1.00
1.00
1.00
2.00
2.00
1.00
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
8.99
8.92
8.91
8.69
8.55
8.53
8.52
8.33
8.10
8.09
7.89
7.87
7.86
7.85
7.84
7.84
7.83
8.99
8.92
8.91
8.69
8.55
8.53
8.52
8.33
8.10
8.09
7.85
7.84
7.84
7.83
1.00
1.00
1.00
1.22
2.00
1.05
1.00
2.04
8.9
8.6
8.3
8.0
f1 (ppm)

In d_6-DMSO


CN
N
B
N
O
F
F
1.00
1.00
1.00
1.22
2.00
1.05
1.00
2.04
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
f1 (ppm)

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
296.0805	1	C 15 H 9 B F 2 N 3 O	100.00	296.0804	-0.1	-0.2	634.3	12.5	even	ok
318.0623	1	C 15 H 8 B F 2 N 3 Na O	100.00	318.0623	0.0	0.1	102.6	12.5	even	ok
334.0373	1	C 15 H 8 B F 2 K N 3 O	100.00	334.0363	-1.0	-3.0	569.7	12.5	even	ok

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
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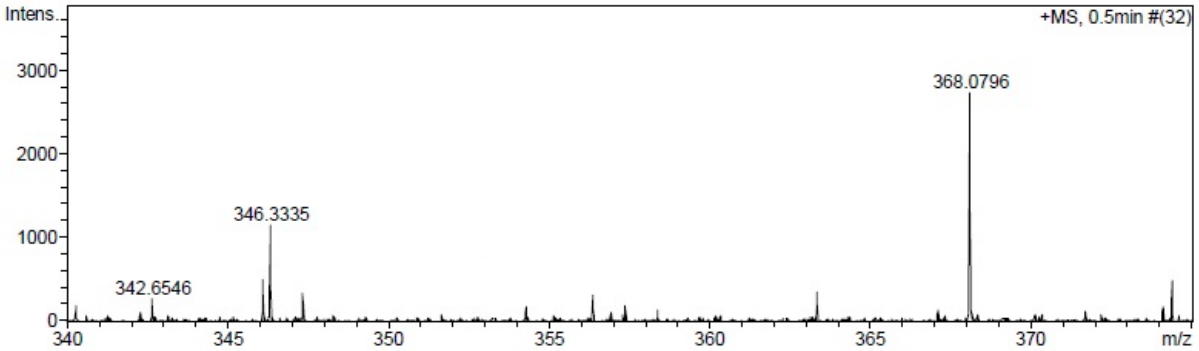

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
346.0976	1	C 19 H 11 B F 2 N 3 O	100.00	346.0961	-1.5	-4.3	638.2	15.5	even	ok
368.0796	1	C 19 H 10 B F 2 N 3 Na O	100.00	368.0781	-1.5	-4.2	94.2	15.5	even	ok

Maldi-Tof High Mass spectra of **1-2**