

## Supporting Information

### Copper(II) Catalyzed Synthesis of Novel Helical Luminescent Benzo[4,5]imidazo[1,2-*a*][1,10]phenanthrolines via an Intramolecular C–H Amination Reaction

Ramon Borges da Silva,<sup>a</sup> Rodolfo Inêz Teixeira,<sup>a</sup> James L. Wardell,<sup>b,c</sup> Solange M. S. V. Wardell,<sup>d</sup> and Simon J. Garden<sup>a\*</sup>

<sup>a</sup> Instituto de Química, Universidade Federal do Rio de Janeiro, Centro Tecnológica, Bloco A, Cidade Universitária, Ilha do Fundão, 21949-909 Rio de Janeiro, RJ, Brazil.

<sup>b</sup> Instituto de Tecnologia em Fármacos – Farmanguinhos, Fiocruz. R. Sizenando Nabuco, 100, Manguinhos, 21041-250, Rio de Janeiro, RJ, Brazil.

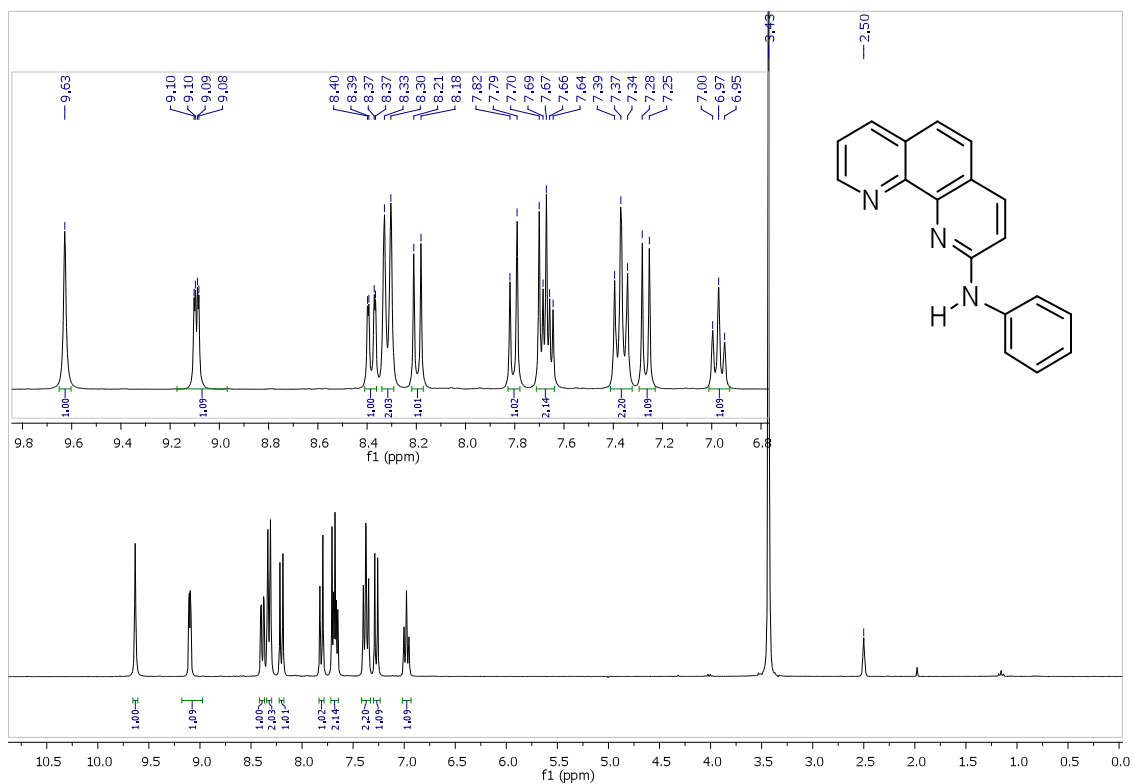
<sup>c</sup> Department of Chemistry, University of Aberdeen, Old Aberdeen, AB24 3UE, Scotland

<sup>d</sup> CHEMSOL, 1 Harcourt Road, Aberdeen AB15 5NY, Scotland.

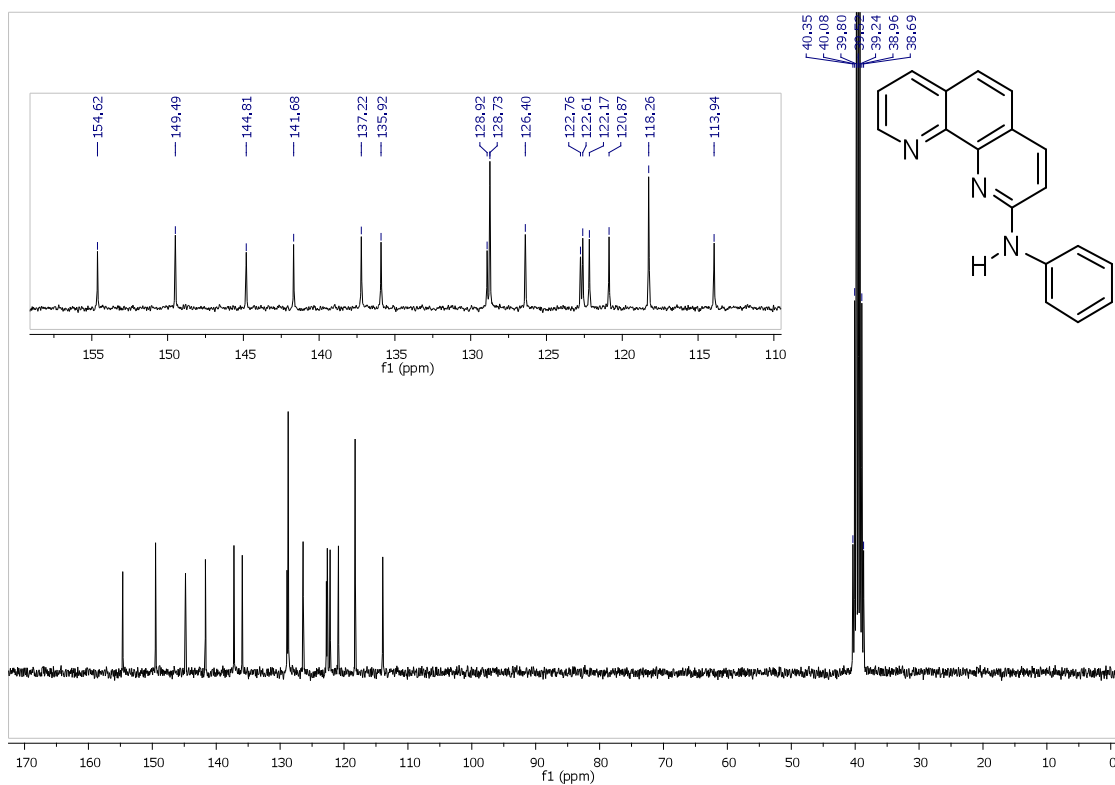
\*E-mail: garden@iq.ufrj.br; Tel: +55-21-3938-7135

#### Contents

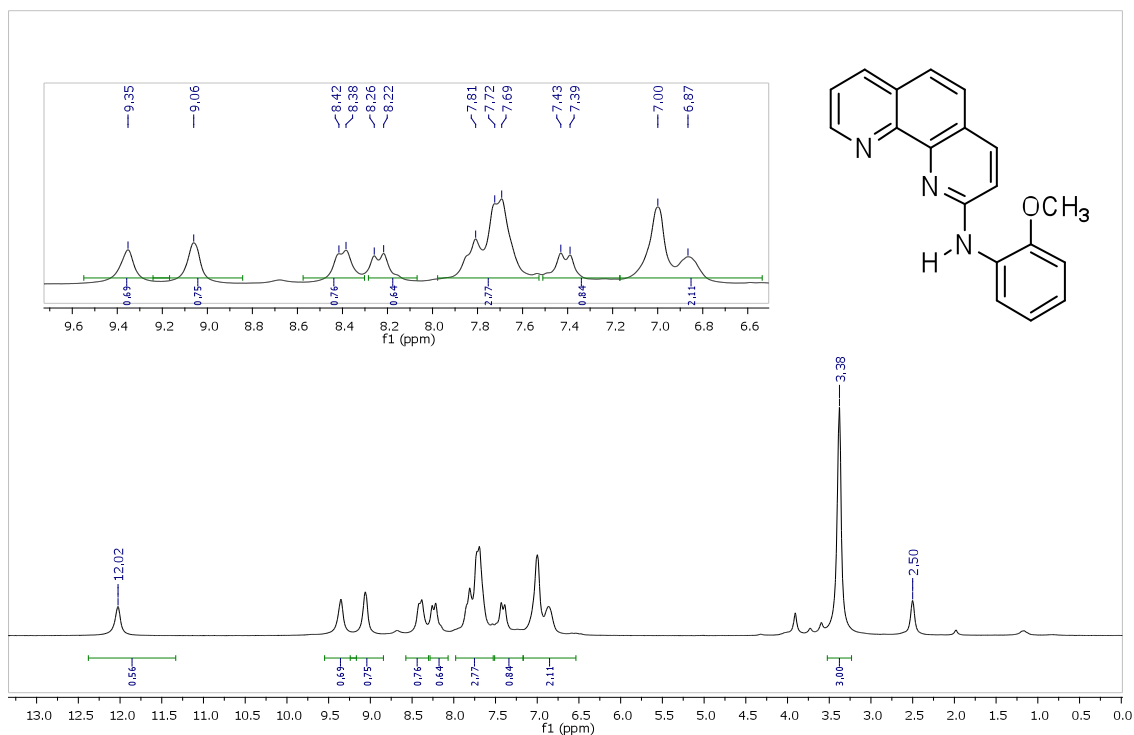
	Pages
<sup>1</sup> H, <sup>13</sup> C spectra of compounds <b>3</b>	2 - 21
<sup>1</sup> H, <sup>13</sup> C spectra of compound <b>5</b>	22
<sup>1</sup> H, <sup>13</sup> C spectra of compounds <b>6</b>	23 - 34
HRMS of compounds <b>3</b> , <b>5</b> and <b>6</b>	35 - 50
2D NMR of compound <b>3a</b> and of compound <b>6a</b>	51 - 53
Theoretical calculations of <b>6a</b> and <b>6aTS</b>	55 - 56
Absorption, emission and excitation spectra of <b>6a</b> in different solvents.	56 - 58
Crystallography Experimental and details	59 - 66



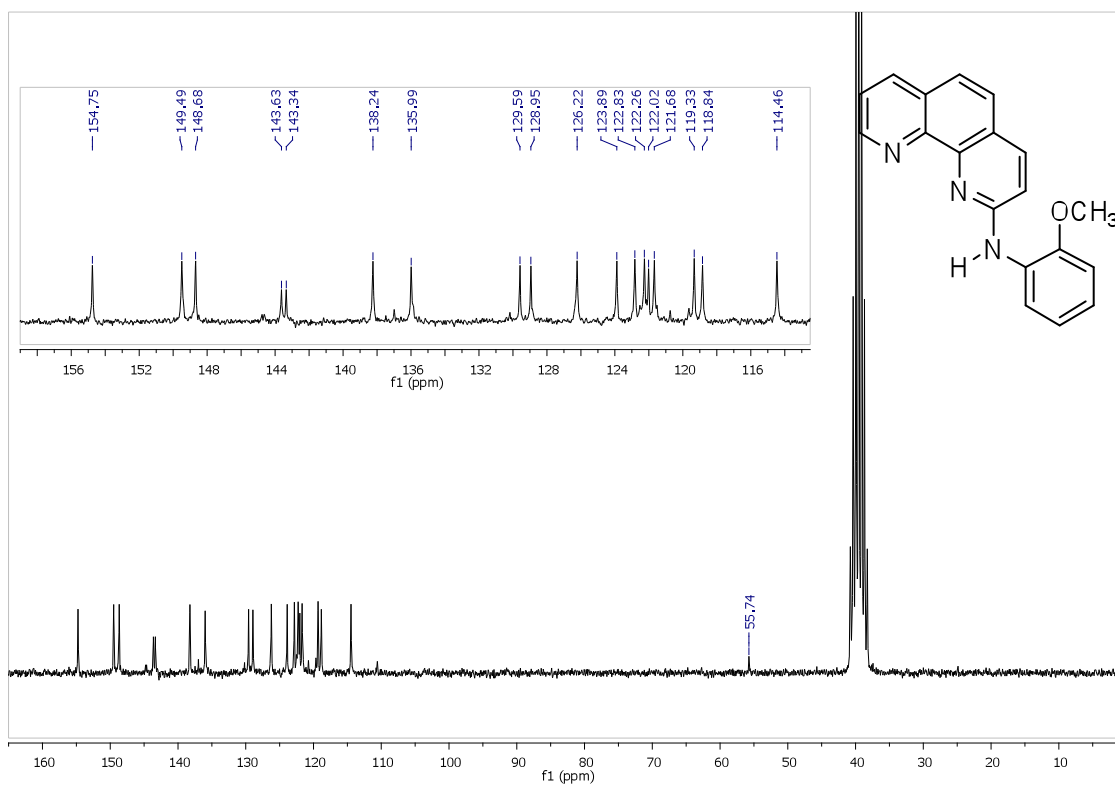
SI Figure 1: <sup>1</sup>H NMR: *N*-phenyl-1,10-phenanthroline (**3a**), (300 MHz, DMSO-d<sub>6</sub>).



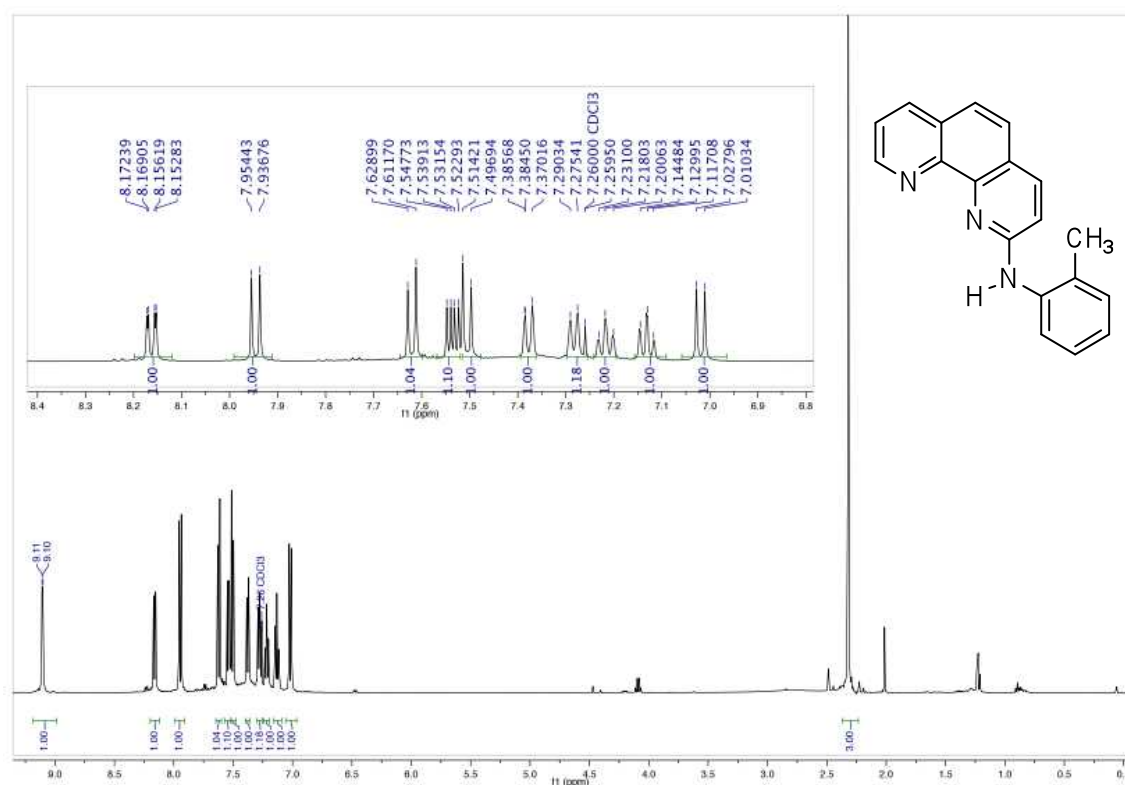
SI Figure 2: <sup>13</sup>C NMR: *N*-phenyl-1,10-phenanthroline (**3a**), (75 MHz, DMSO-d<sub>6</sub>).



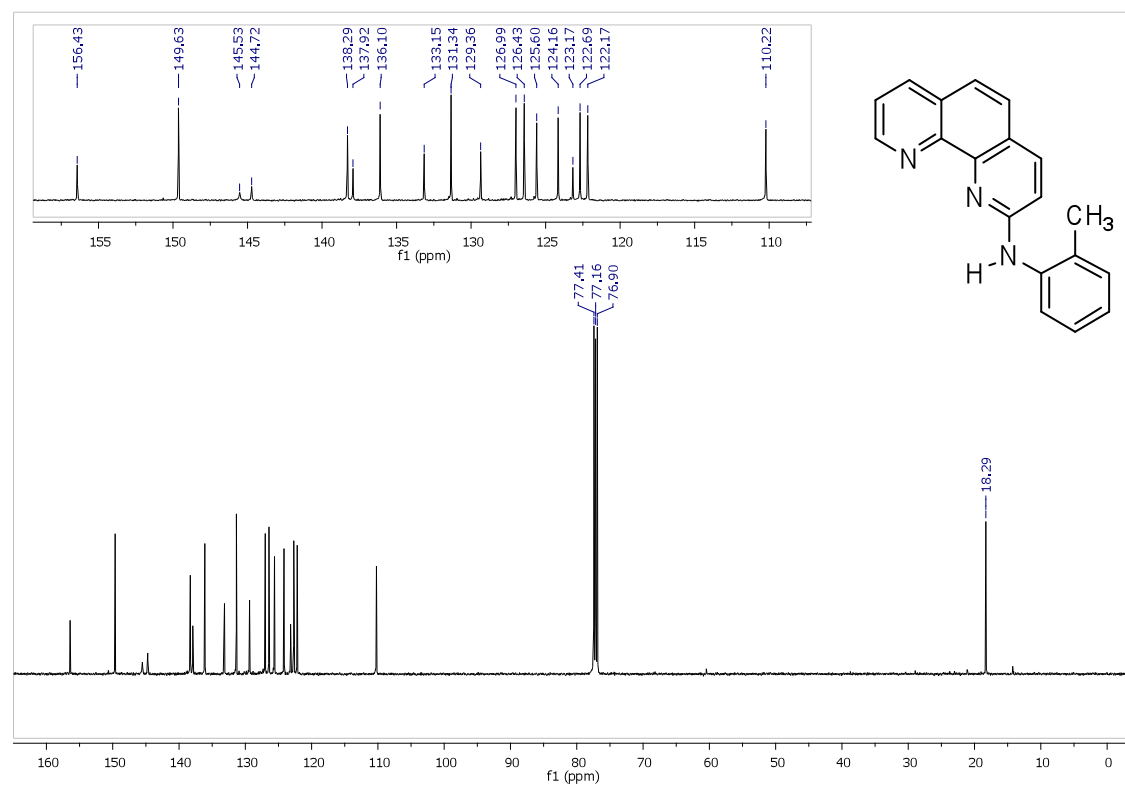
SI Figure 3: <sup>1</sup>H NMR: *N*-(2-methoxyphenyl)-1,10-phenanthroline-2-amine (3b), (200 MHz, DMSO-d<sub>6</sub>).



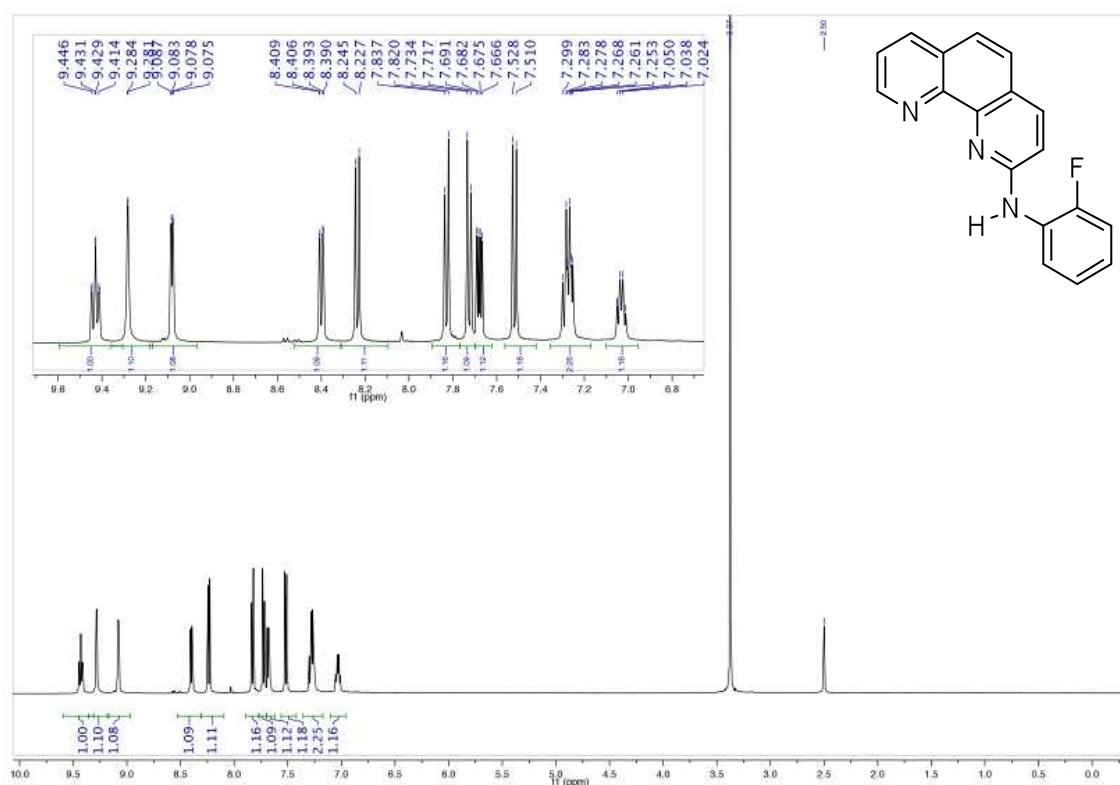
SI Figure 4: <sup>13</sup>C NMR: *N*-(2-methoxyphenyl)-1,10-phenanthroline-2-amine (3b), (50 MHz, DMSO-d<sub>6</sub>).



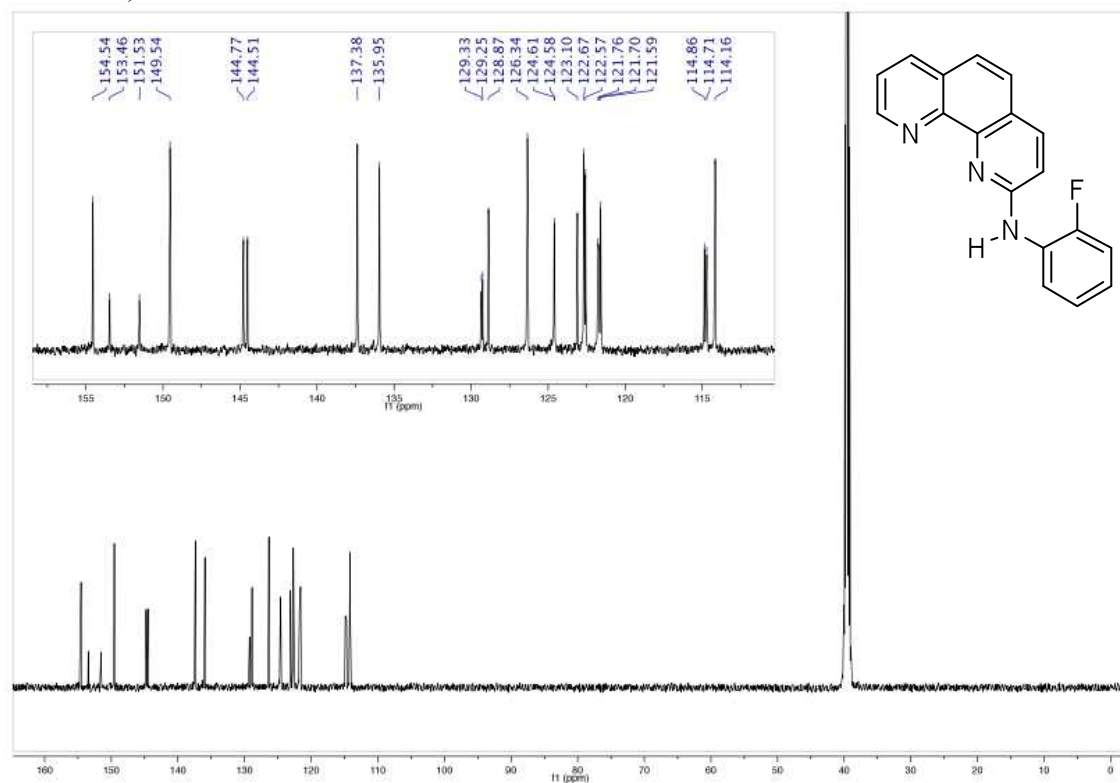
SI Figure 5: <sup>1</sup>H NMR *N*-*o*-tolyl-1,10-phenanthroline-2-amine (**3c**), (500 MHz, CDCl<sub>3</sub>).



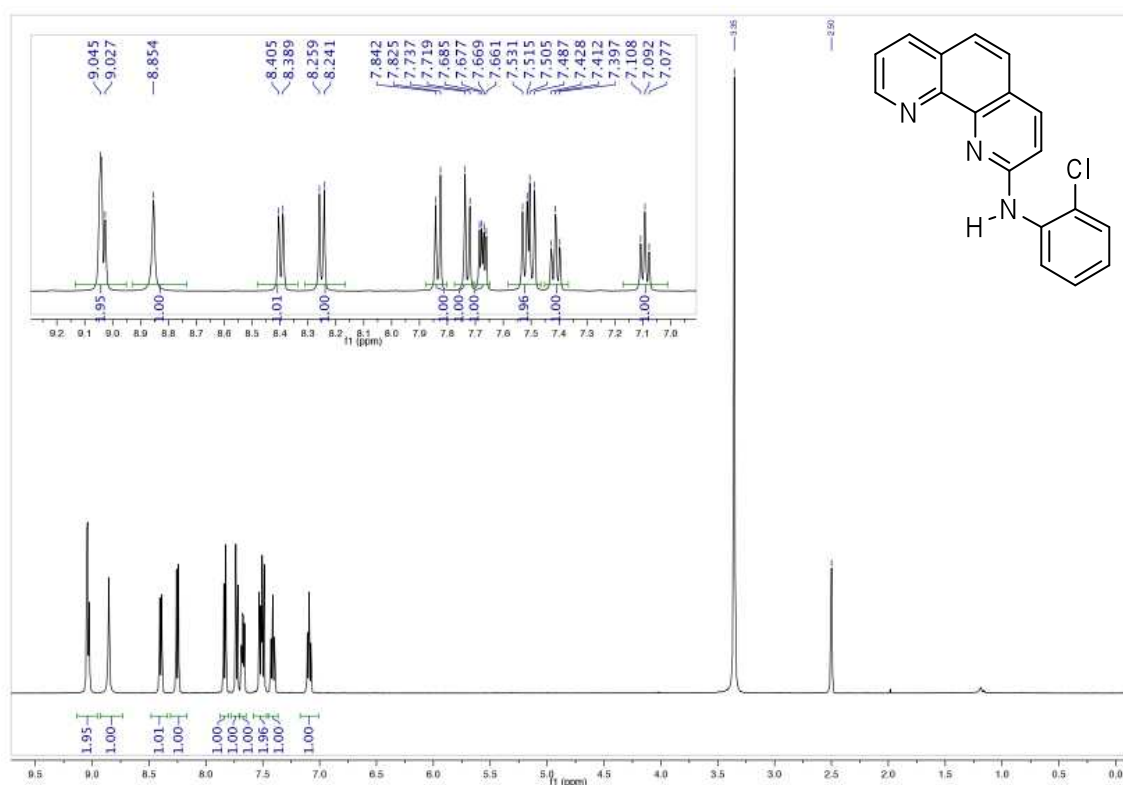
SI Figure 6: <sup>13</sup>C NMR: *N*-*o*-tolyl-1,10-phenanthroline-2-amine (**3c**), (125 MHz, CDCl<sub>3</sub>).



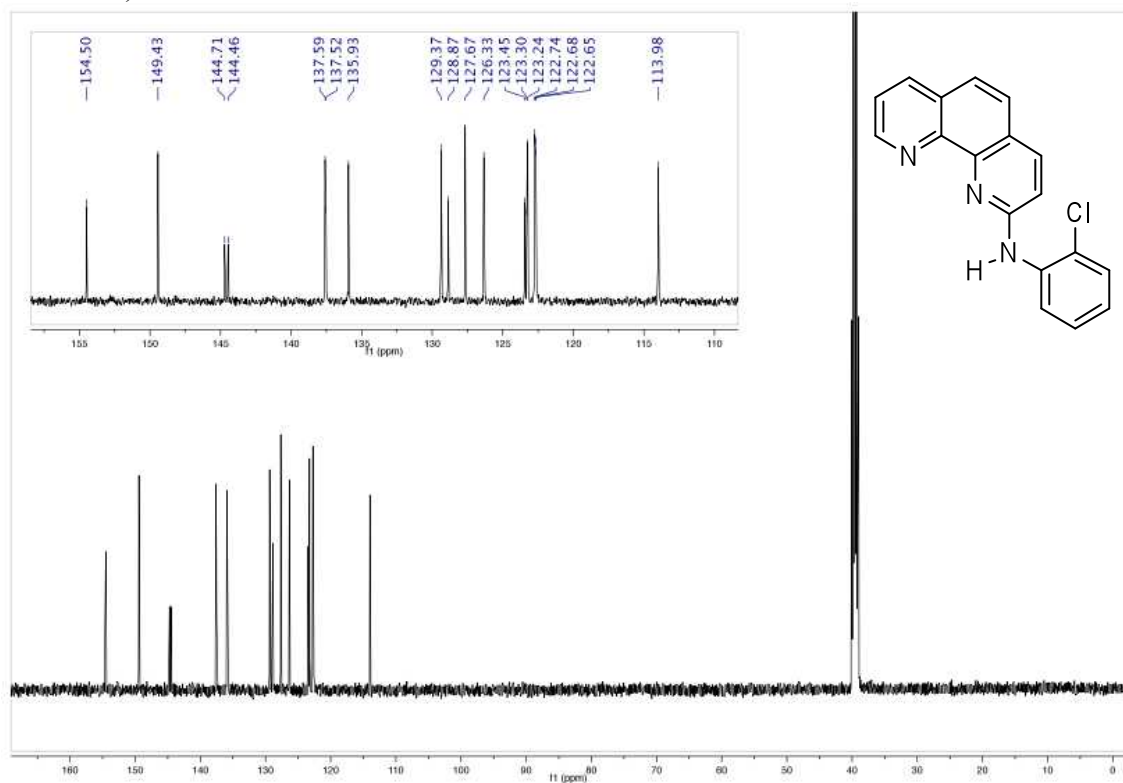
SI Figure 7: <sup>1</sup>H NMR: *N*-(2-fluorophenyl)-1,10-phenanthroline-2-amine (**3d**), (500 MHz, DMSO-d<sub>6</sub>)



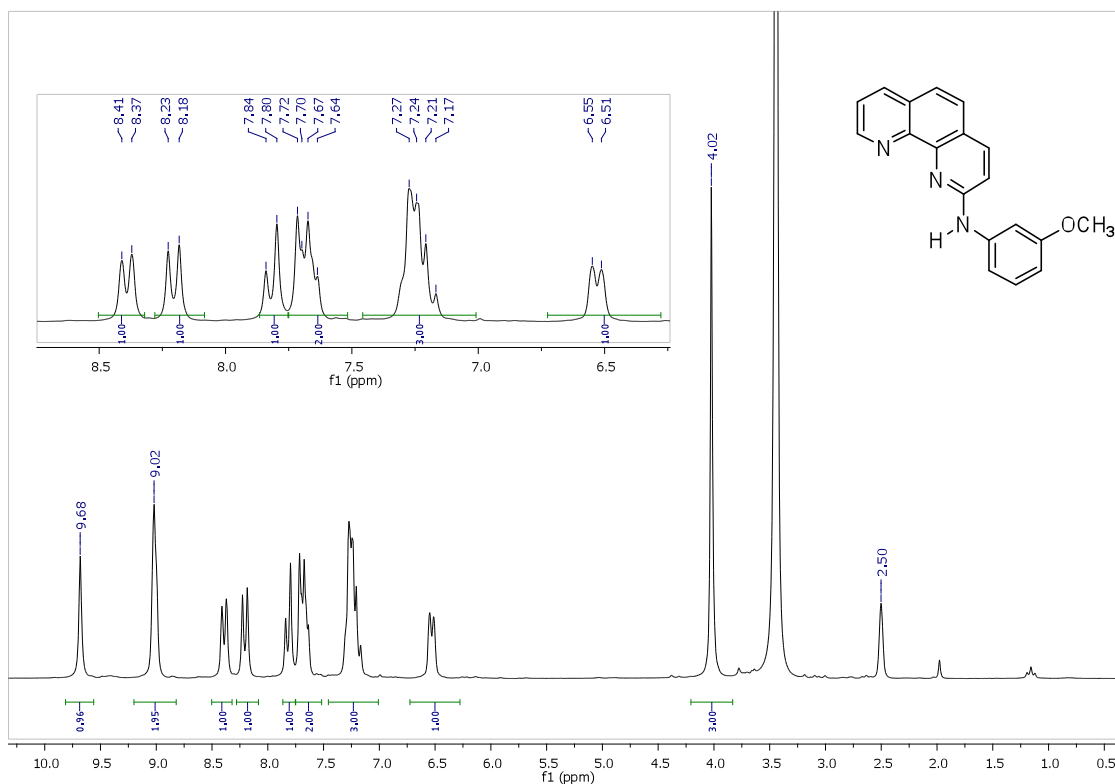
SI Figure 8: <sup>13</sup>C NMR: *N*-(2-fluorophenyl)-1,10-phenanthroline-2-amine (**3d**), (125 MHz, DMSO-d<sub>6</sub>)



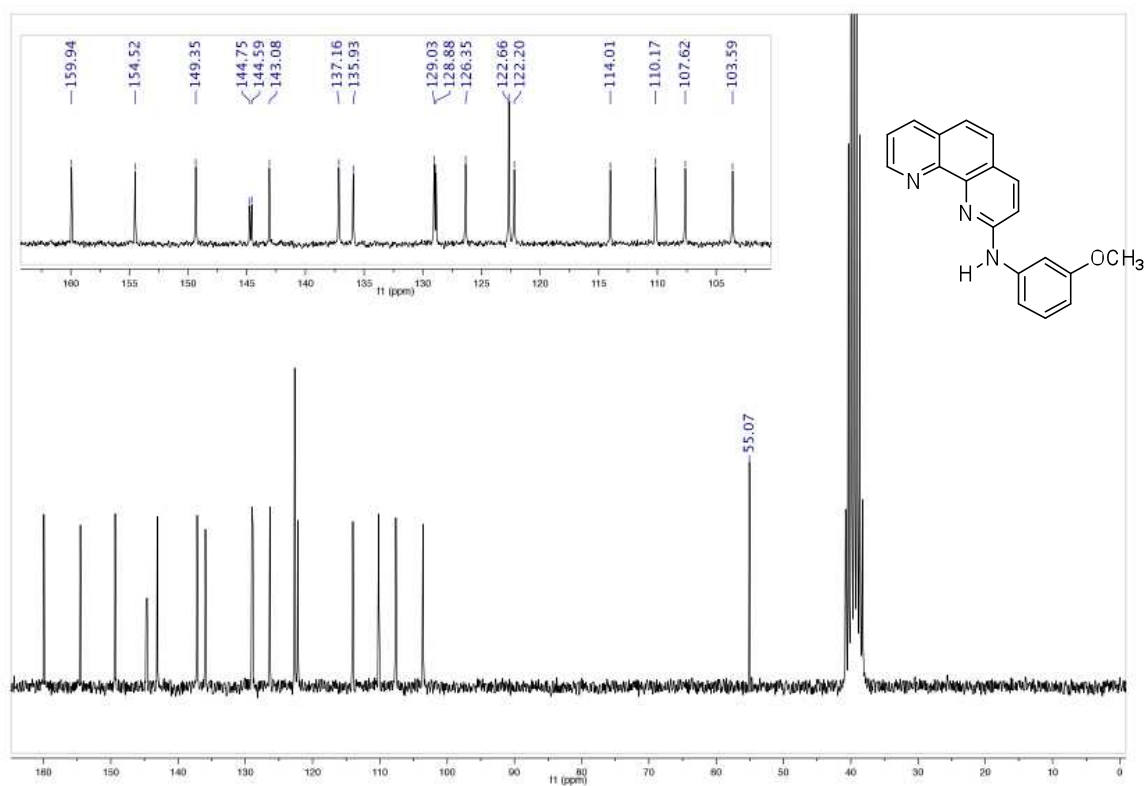
SI Figure 9: <sup>1</sup>H NMR: *N*-(2-chlorophenyl)-1,10-phenanthroline-2-amine (**3e**), (500 MHz, DMSO-d<sub>6</sub>).



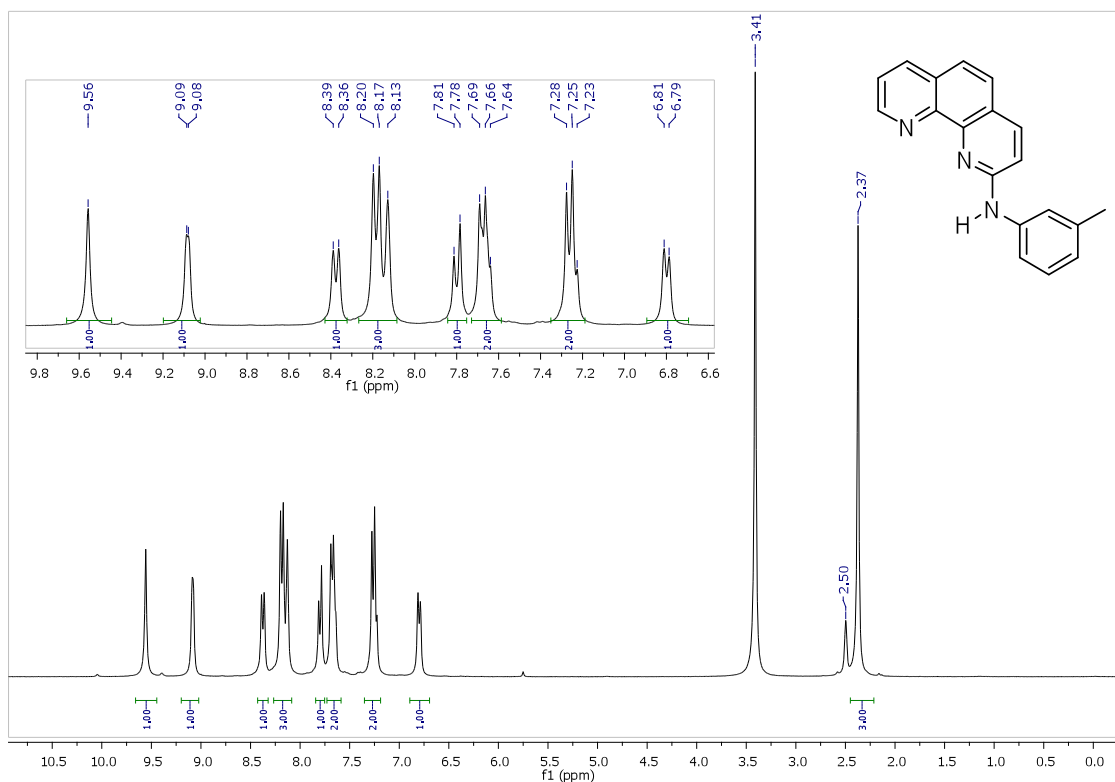
SI Figure 10: <sup>13</sup>C NMR: *N*-(2-chlorophenyl)-1,10-phenanthroline-2-amine (**3e**), (125 MHz, DMSO-d<sub>6</sub>).



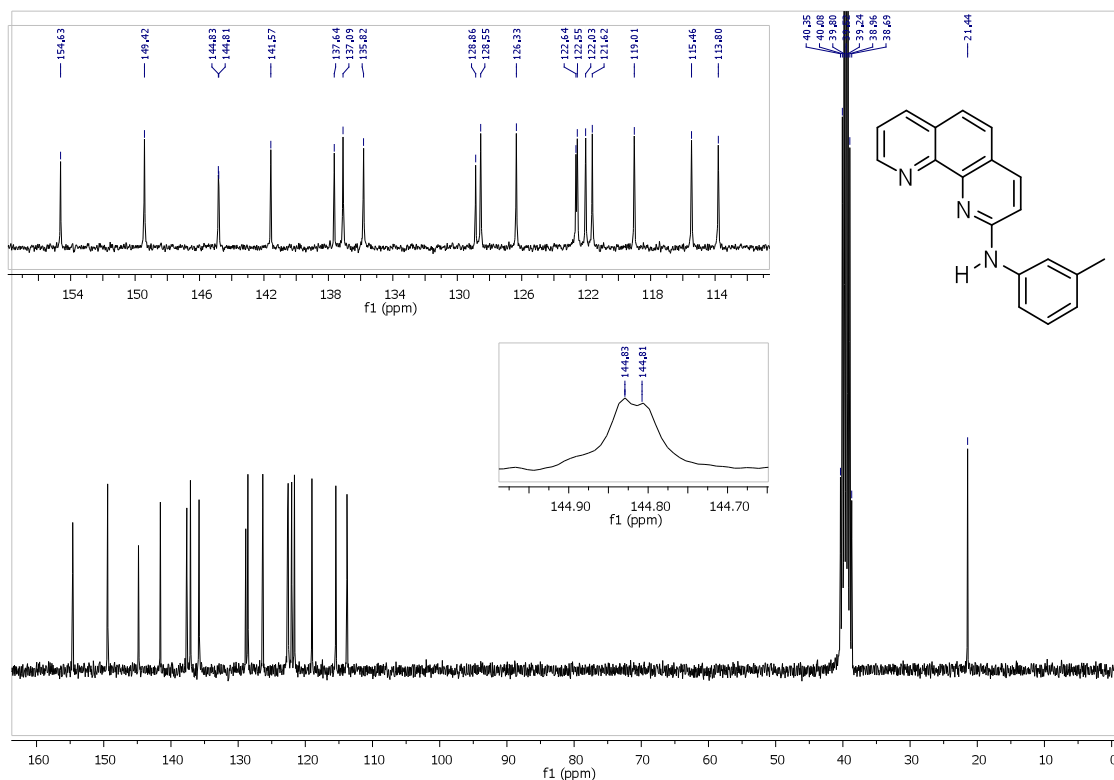
SI Figure 11: <sup>1</sup>H NMR: *N*-(3-methoxyphenyl)-1,10-phenanthroline-2-amine (**3f**), (200 MHz, DMSO-d<sub>6</sub>).



SI Figure 12: <sup>13</sup>C NMR: *N*-(3-methoxyphenyl)-1,10-phenanthroline-2-amine (**3f**), (50 MHz, DMSO-d<sub>6</sub>).

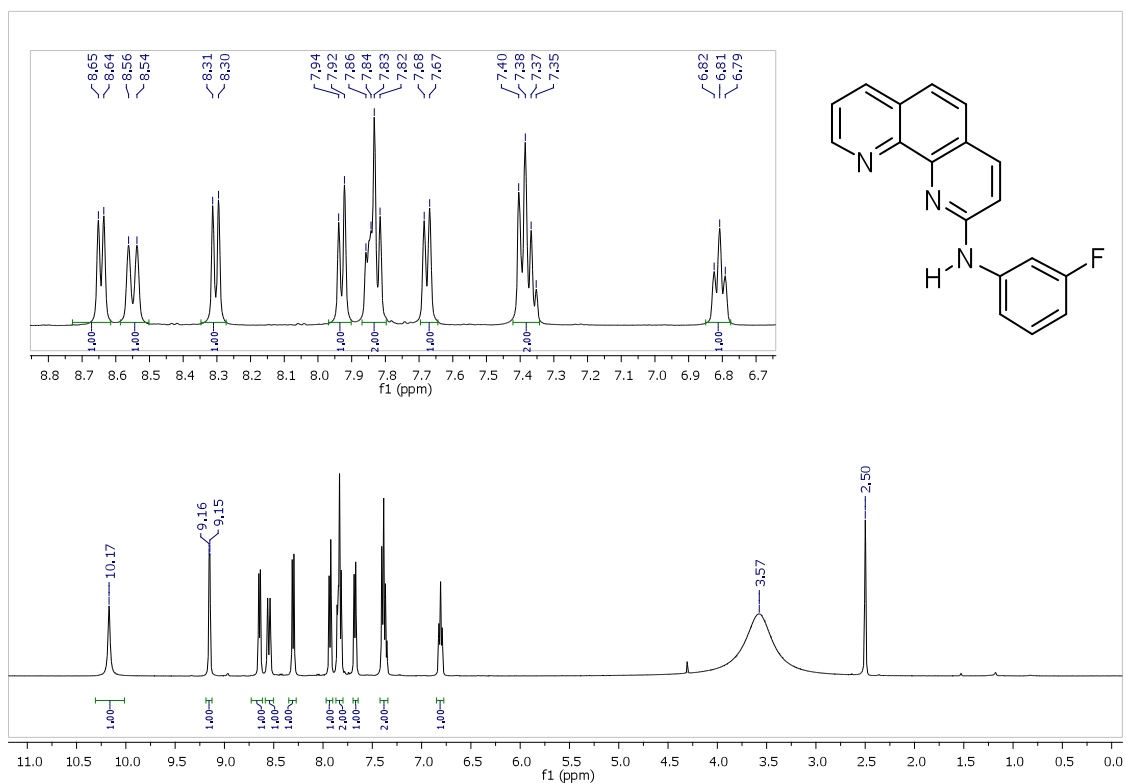


SI Figure 13: <sup>1</sup>H NMR: *N*-m-tolyl-1,10-phenanthroline-2-amine (**3g**), (300 MHz, DMSO-d<sub>6</sub>).

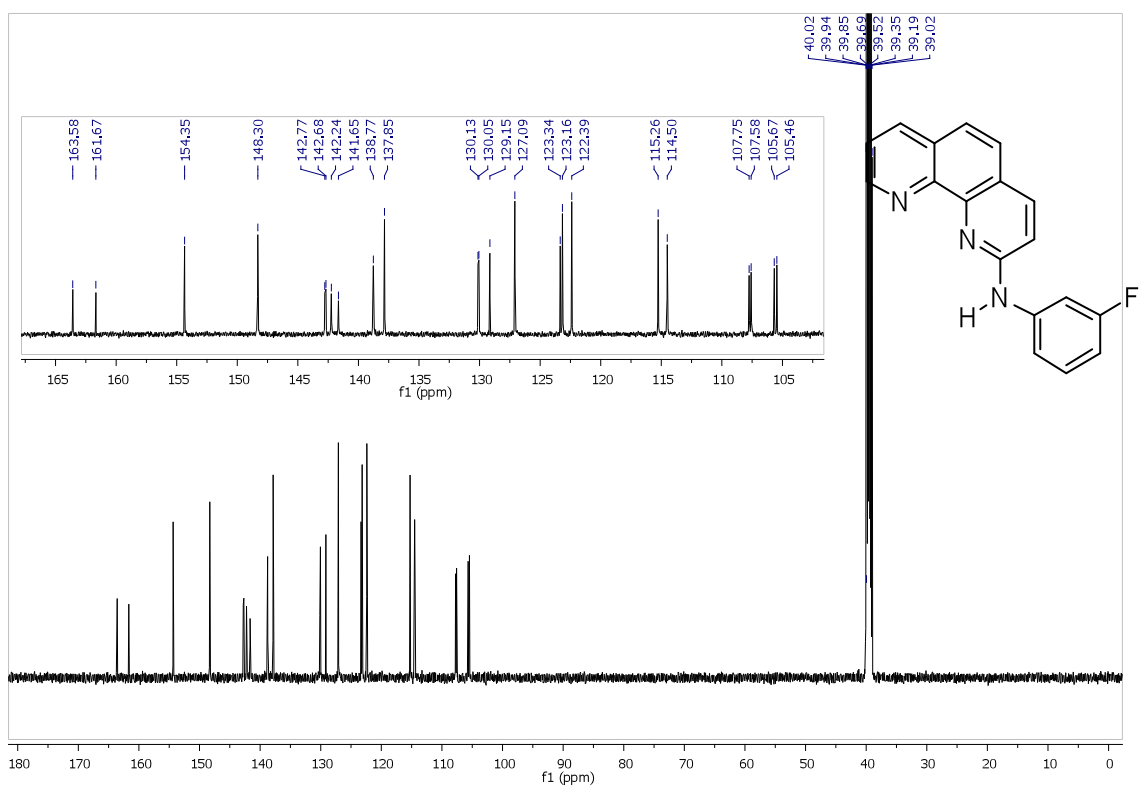


SI Figure 14: <sup>13</sup>C NMR: *N*-m-tolyl-1,10-phenanthroline-2-amine (**3g**), (75 MHz, DMSO-d<sub>6</sub>).

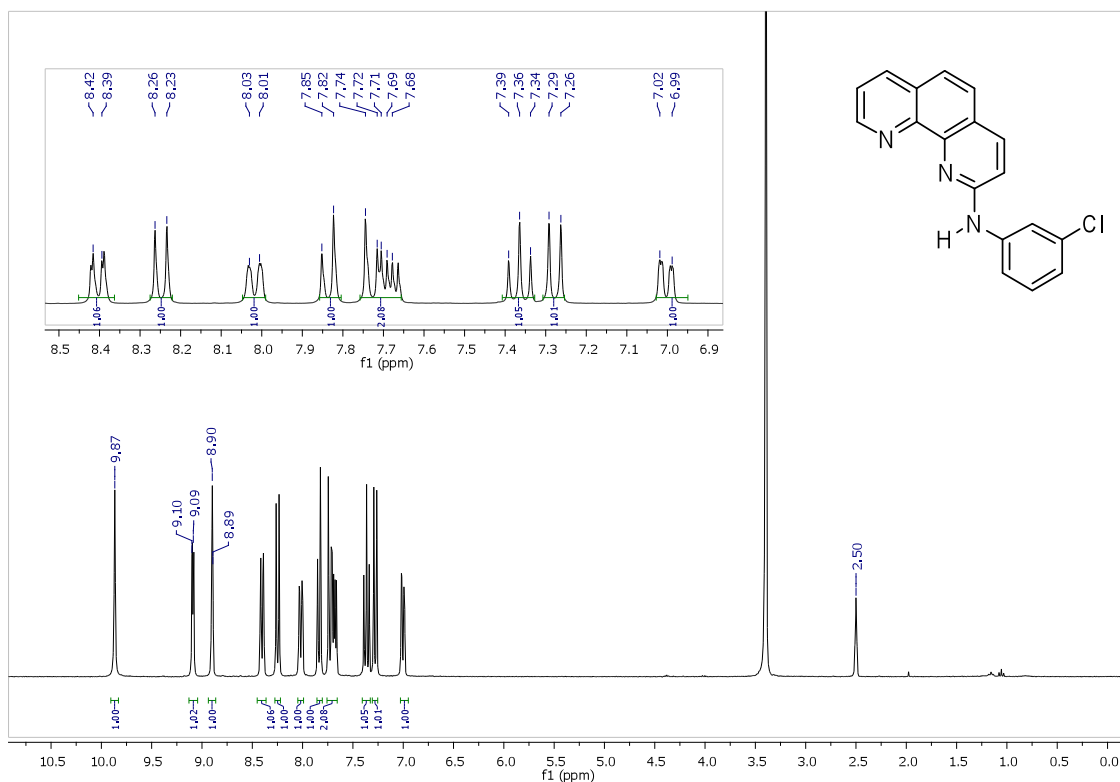




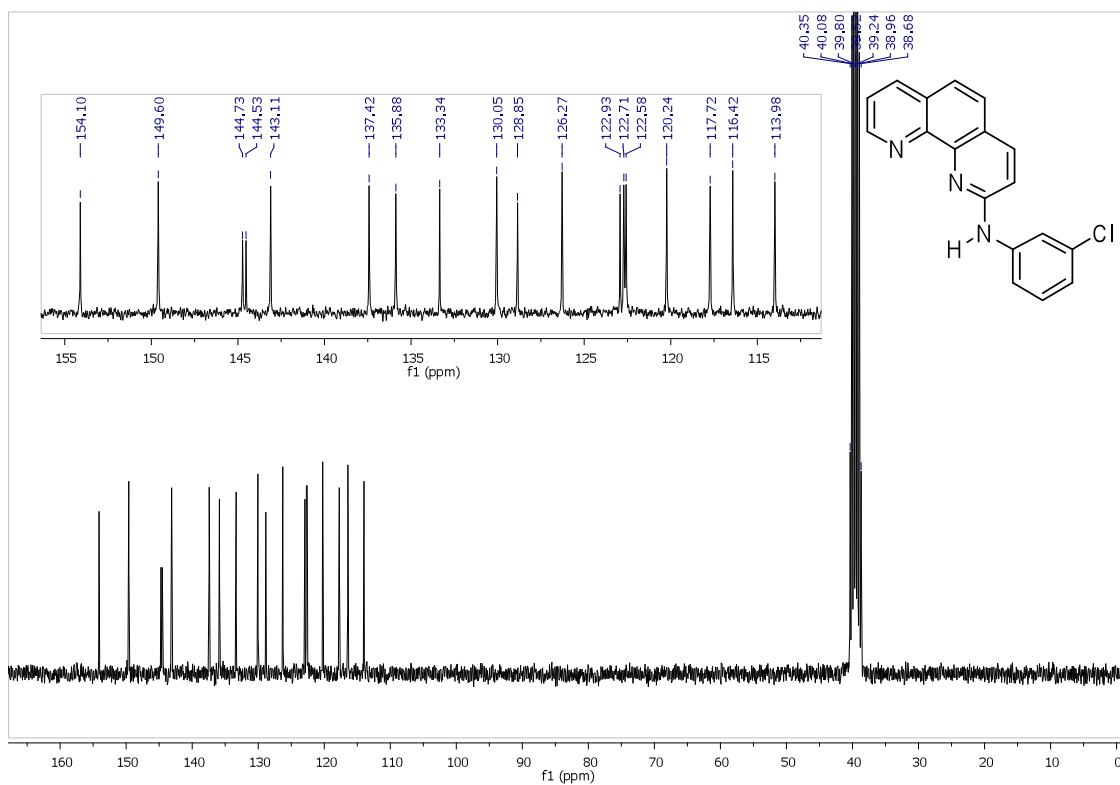
SI Figure 15: <sup>1</sup>H NMR: *N*-(3-fluorophenyl)-1,10-phenanthroline-2-amine (**3h**), (500 MHz, DMSO-*d*<sub>6</sub>).



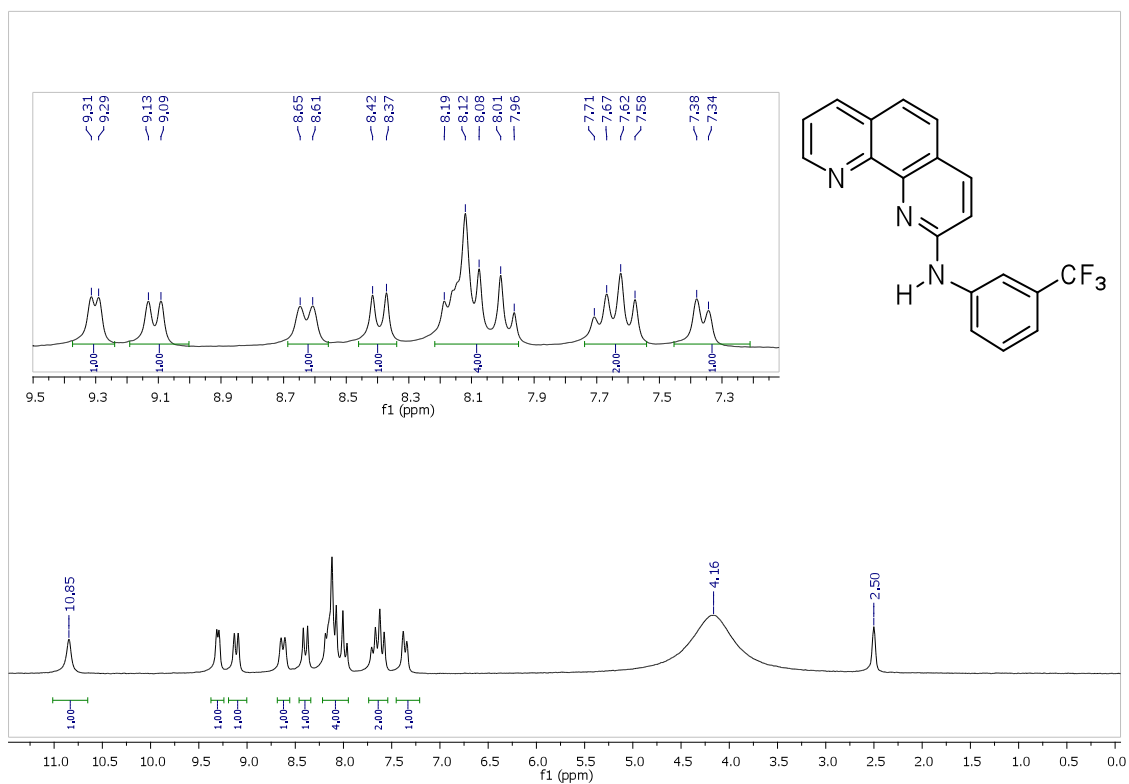
SI Figure 16: <sup>13</sup>C NMR: *N*-(3-fluorophenyl)-1,10-phenanthroline-2-amine (**3h**), (125 MHz, DMSO-*d*<sub>6</sub>).



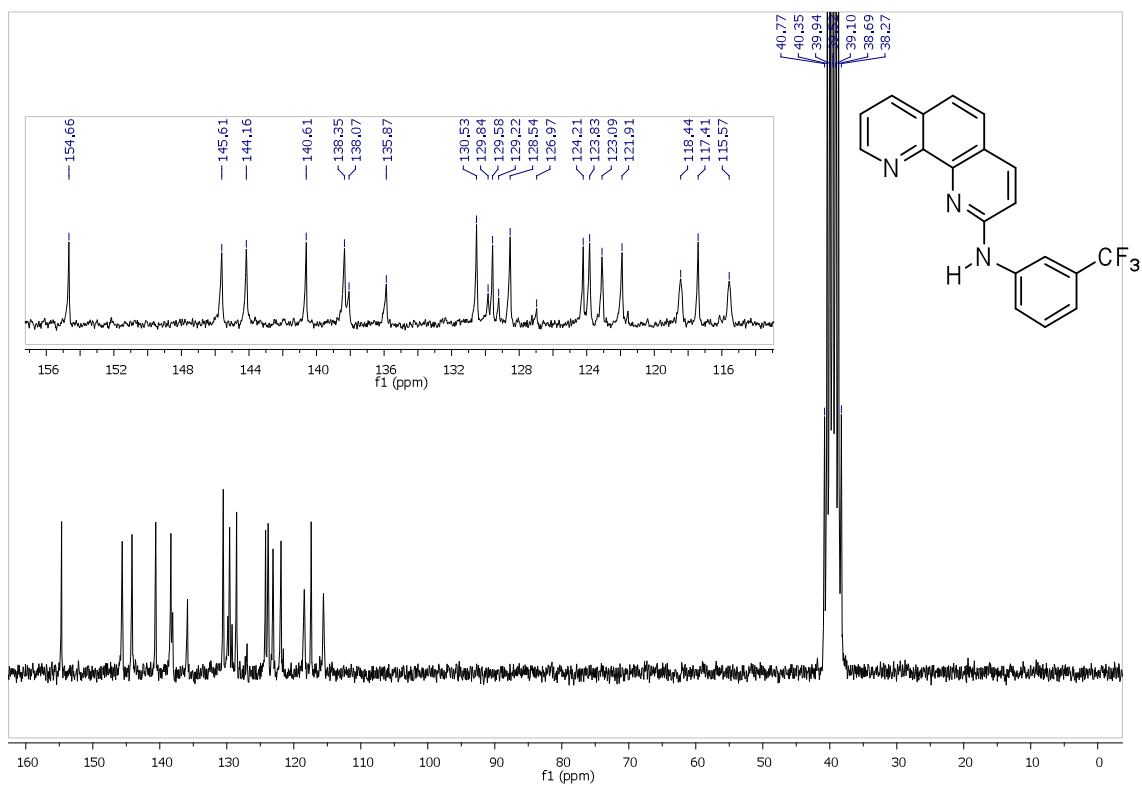
SI Figure 17: <sup>1</sup>H NMR: *N*-(3-chlorophenyl)-1,10-phenanthroline-2-amine (**3i**), (300 MHz, DMSO-*d*<sub>6</sub>).



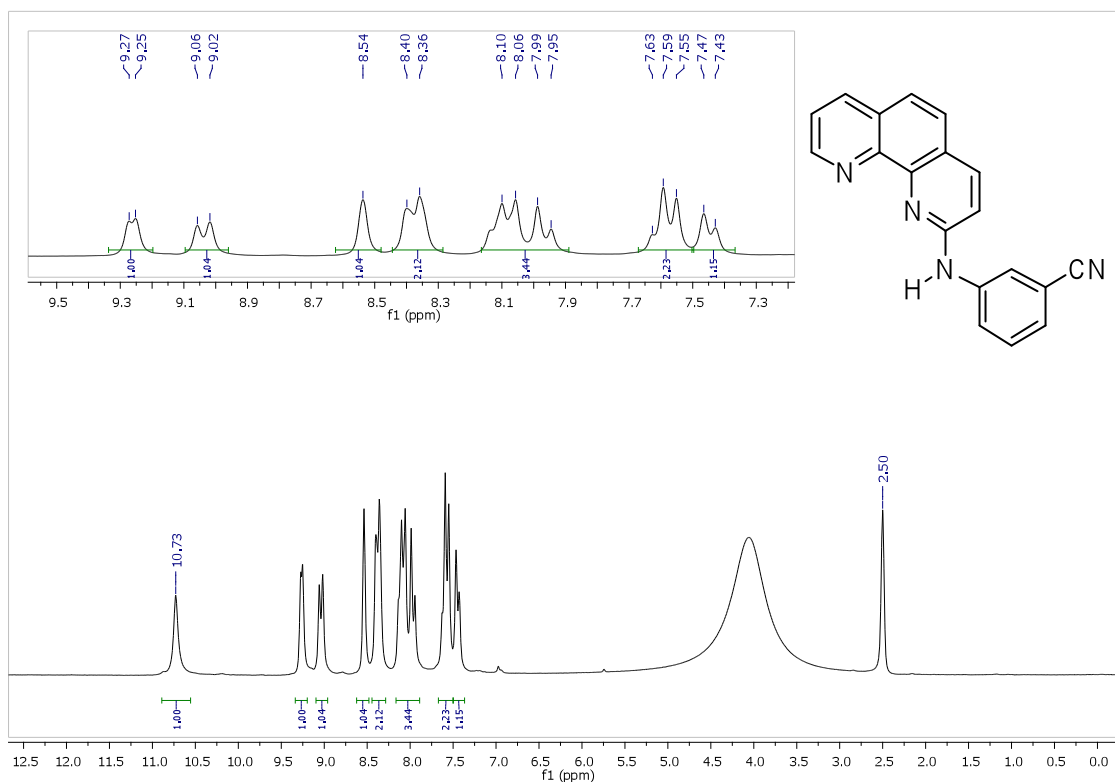
SI Figure 18: <sup>13</sup>C NMR: *N*-(3-chlorophenyl)-1,10-phenanthroline-2-amine (**3i**), (75 MHz, DMSO-*d*<sub>6</sub>).



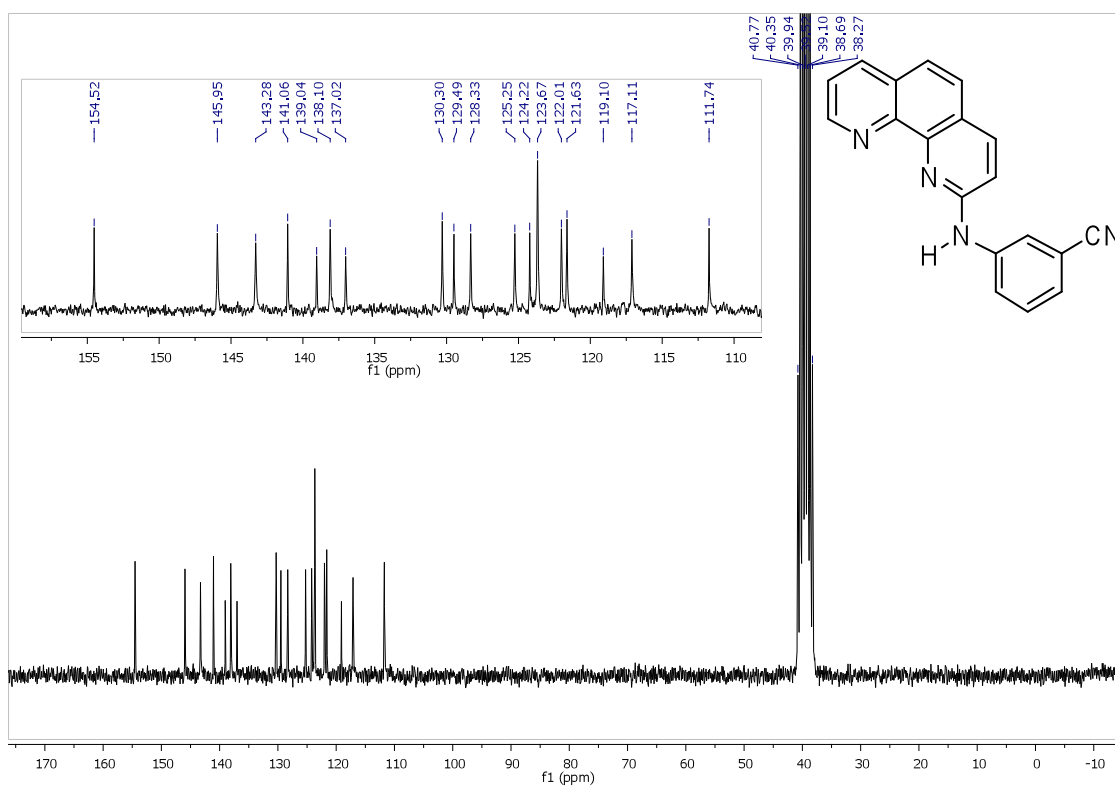
SI Figure 19: <sup>1</sup>H NMR: *N*-(3-(trifluoromethyl)phenyl)-1,10-phenanthroline-2-amine (**3j**) (200 MHz, DMSO-d<sub>6</sub>).



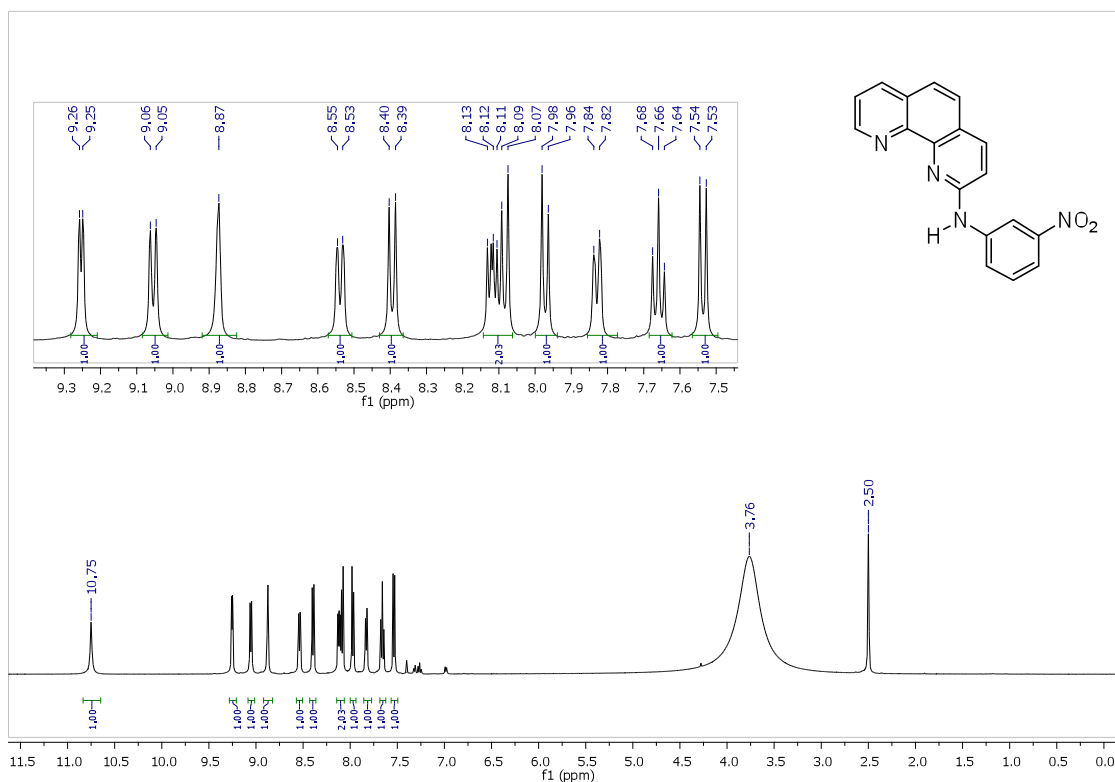
SI Figure 20: <sup>13</sup>C NMR: *N*-(3-(trifluoromethyl)phenyl)-1,10-phenanthroline-2-amine (**3j**), (50 MHz, DMSO-d<sub>6</sub>)



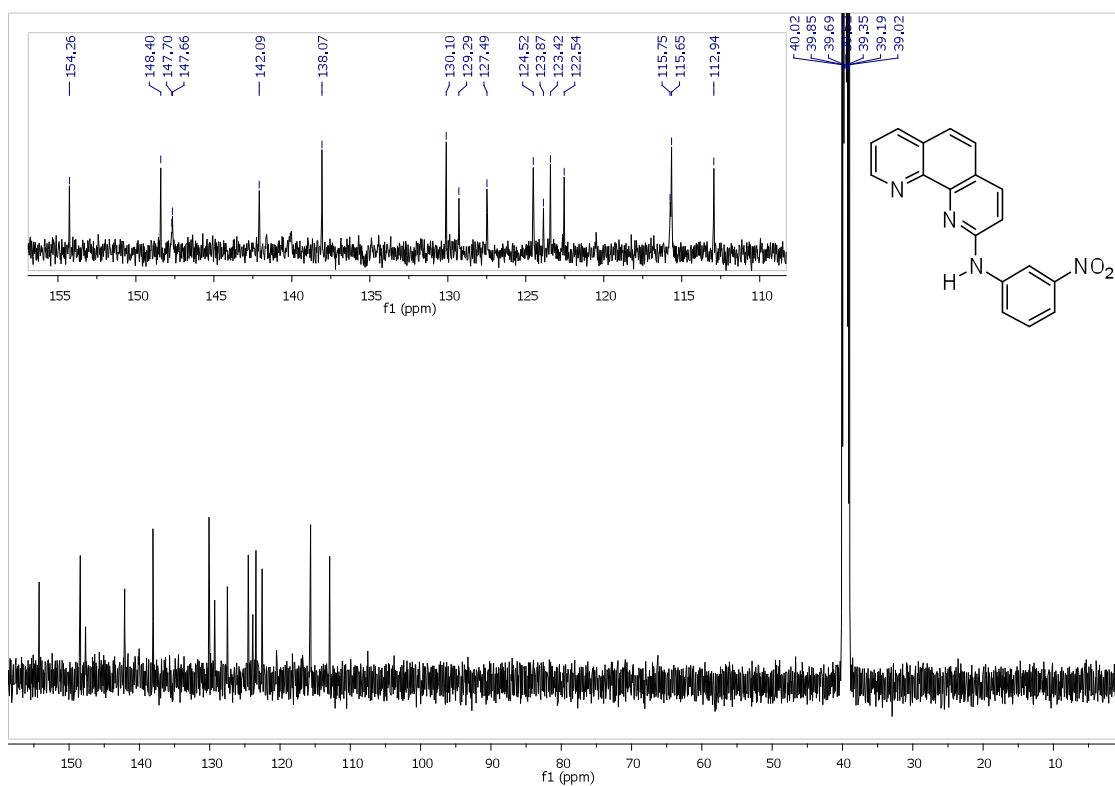
SI Figure 21: <sup>1</sup>H NMR: 3-(1,10-phenanthrolin-2-ylamino)benzonitrile (**3k**), (200 MHz, DMSO-d<sub>6</sub>).



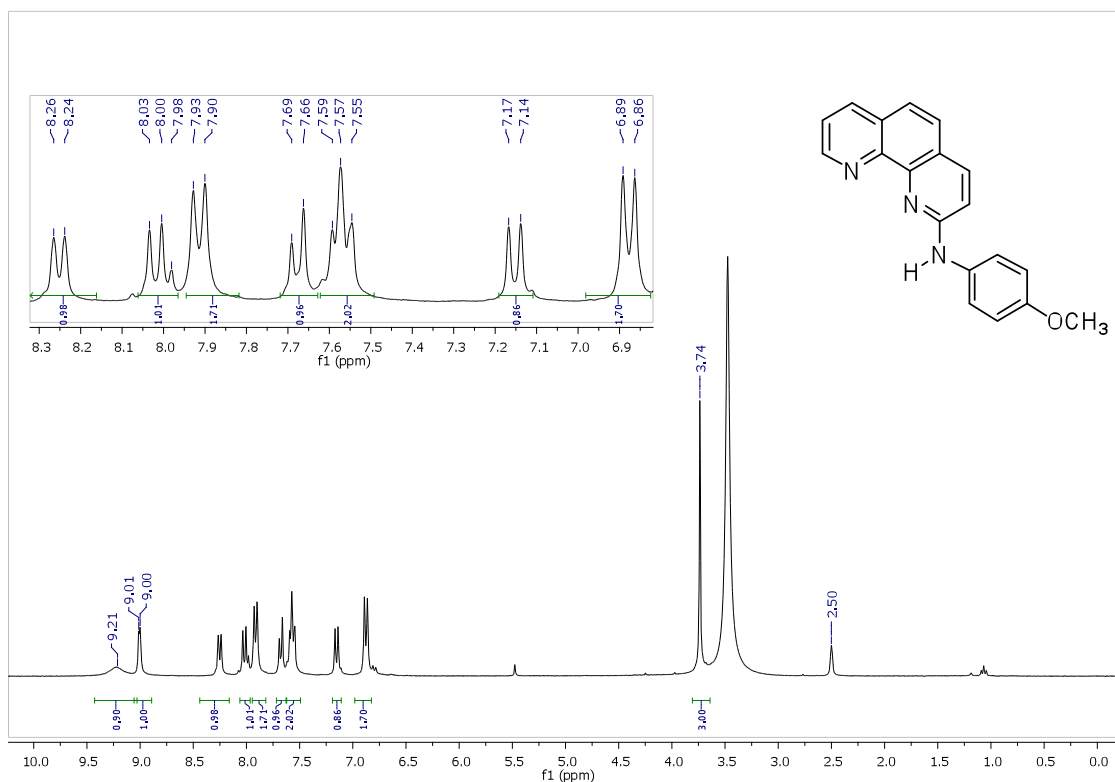
SI Figure 22: <sup>13</sup>C NMR: 3-(1,10-phenanthrolin-2-ylamino)benzonitrile (**3k**), (50 MHz, DMSO-d<sub>6</sub>).



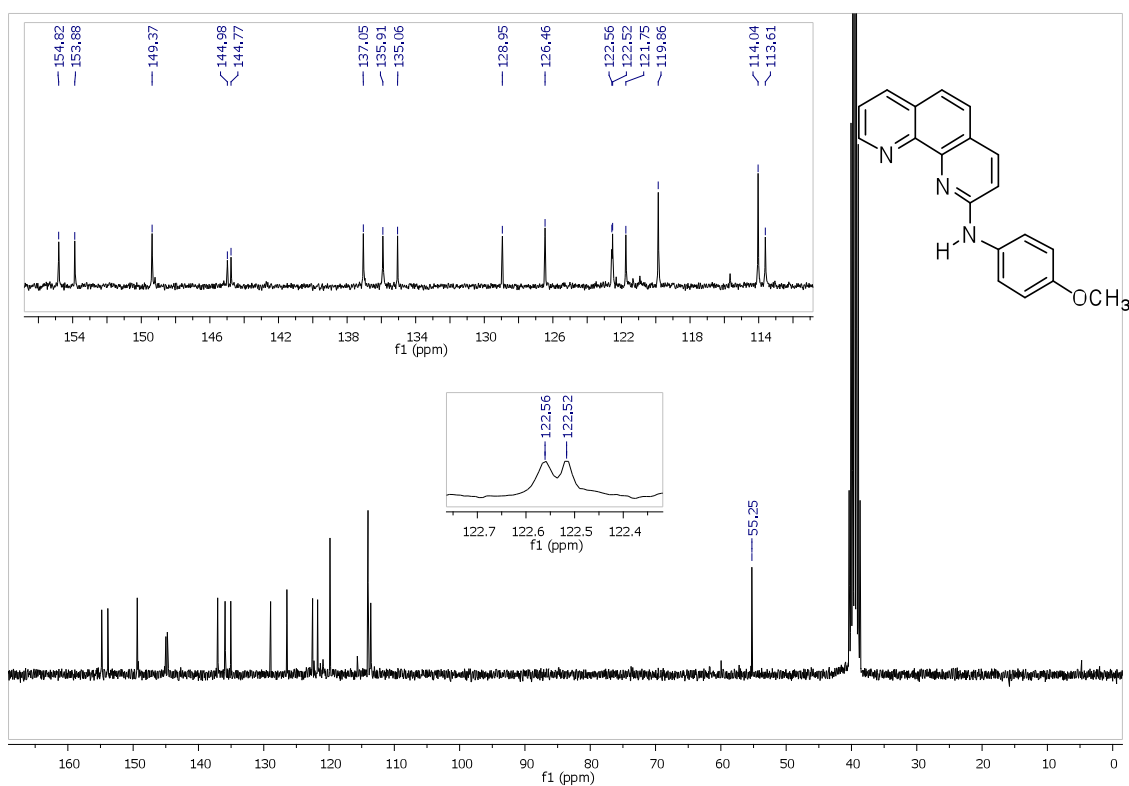
SI Figure 23: <sup>1</sup>H NMR: *N*-(3-nitrophenyl)-1,10-phenanthroline-2-amine (**31**), (500 MHz, DMSO-*d*<sub>6</sub>).



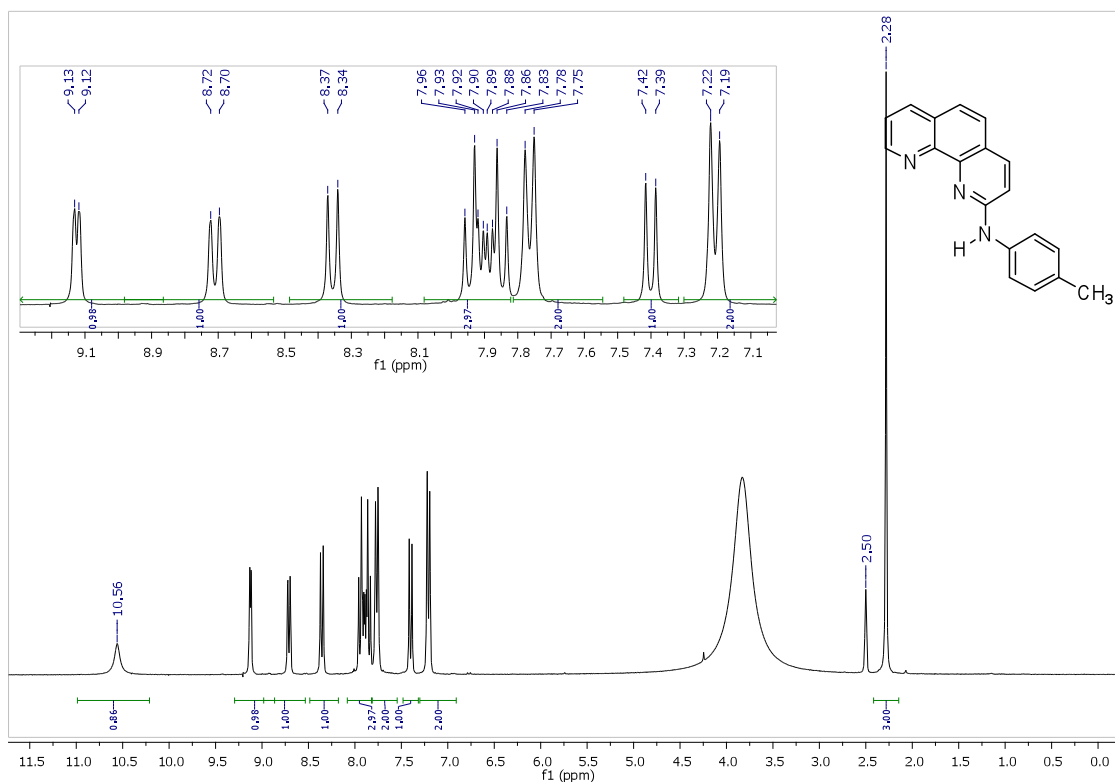
SI Figure 24: <sup>13</sup>C NMR: *N*-(3-nitrophenyl)-1,10-phenanthroline-2-amine (**31**), (125 MHz, DMSO-*d*<sub>6</sub>).



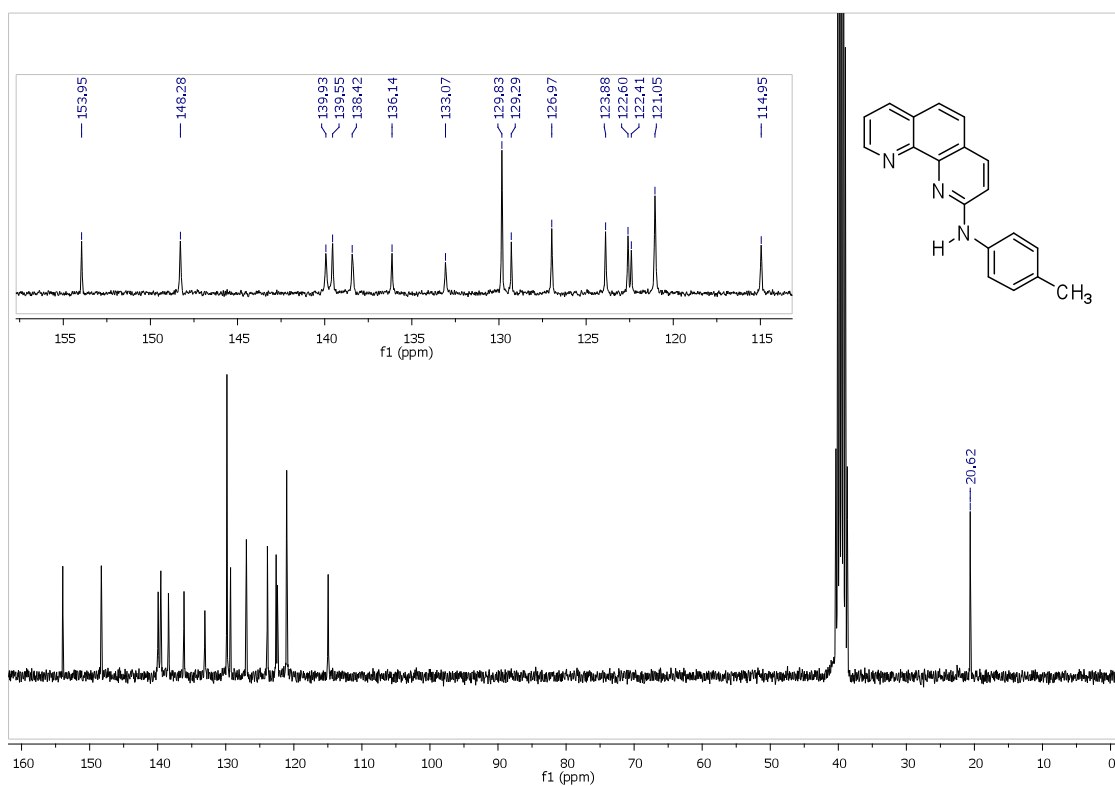
SI Figure 25:  $^1\text{H}$  NMR: *N*-(4-methoxyphenyl)-1,10-phenanthroline-2-amine (**3m**), (300 MHz,  $\text{DMSO-d}_6$ ).



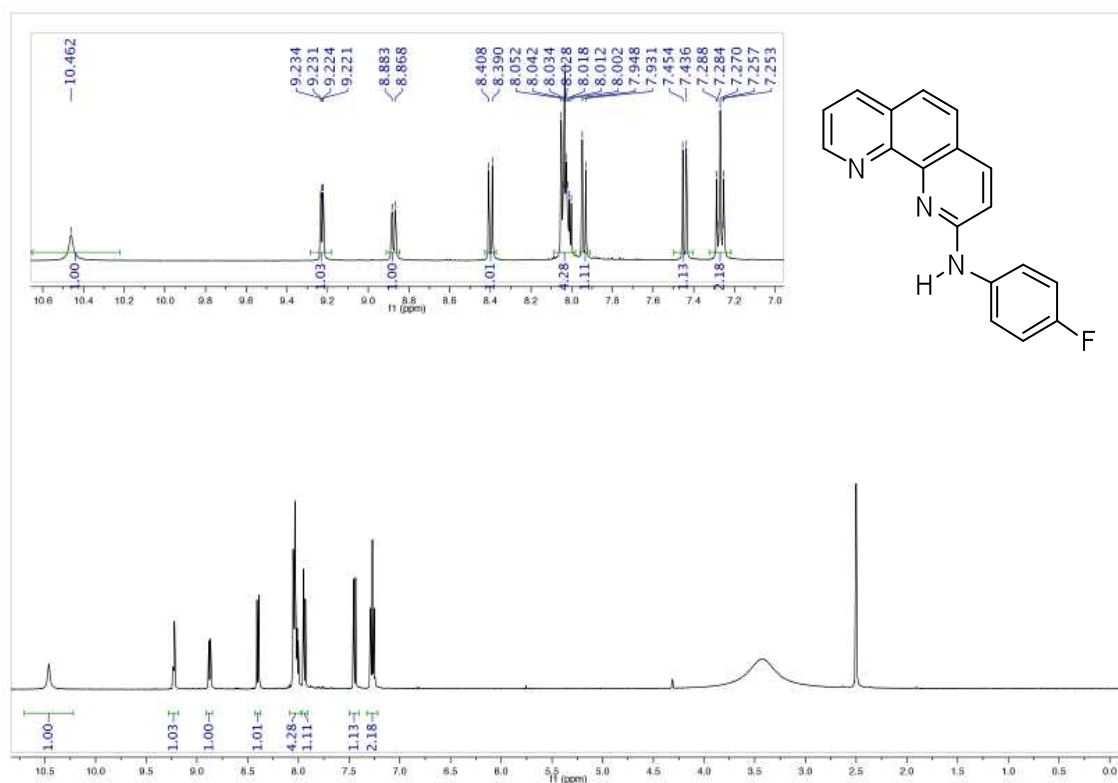
SI Figure 26:  $^{13}\text{C}$  NMR: *N*-(4-methoxyphenyl)-1,10-phenanthroline-2-amine (**3m**), (75 MHz,  $\text{DMSO-d}_6$ ).



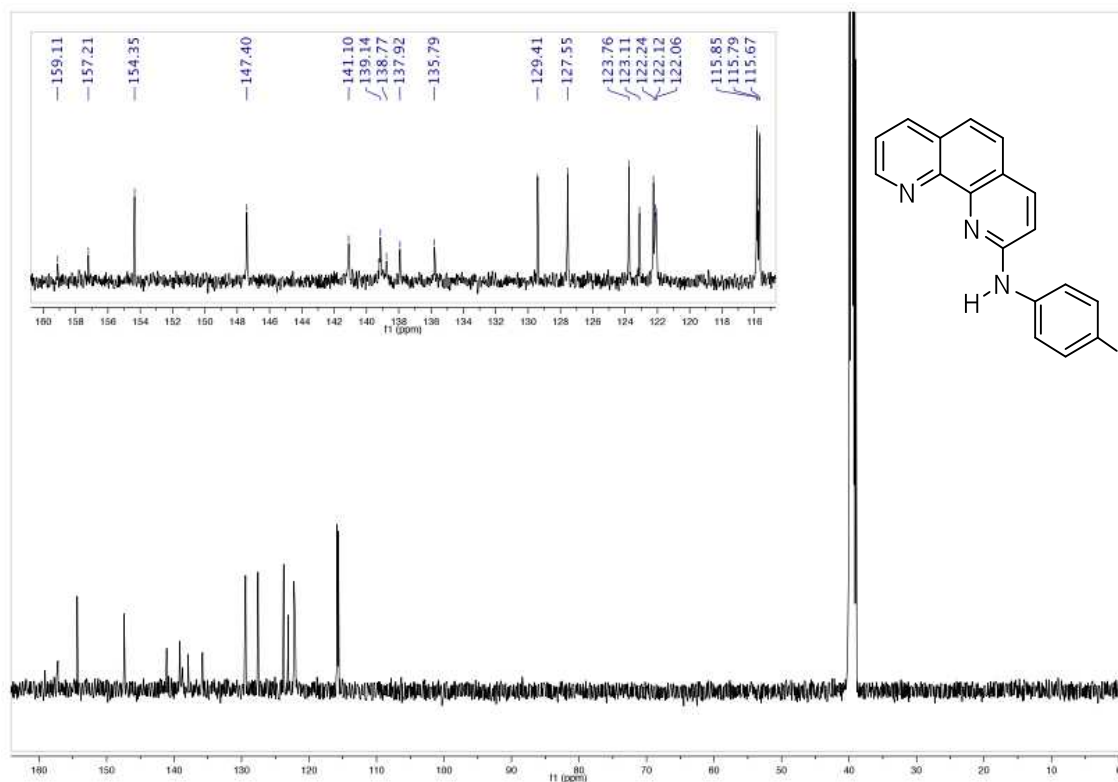
SI Figure 27: <sup>1</sup>H NMR: *N*-p-tolyl-1,10-phenanthroline-2-amine (**3n**), (300 MHz, DMSO-d<sub>6</sub>).



SI Figure 28: <sup>13</sup>C NMR: *N*-p-tolyl-1,10-phenanthroline-2-amine (**3n**), (75 MHz, DMSO-d<sub>6</sub>).

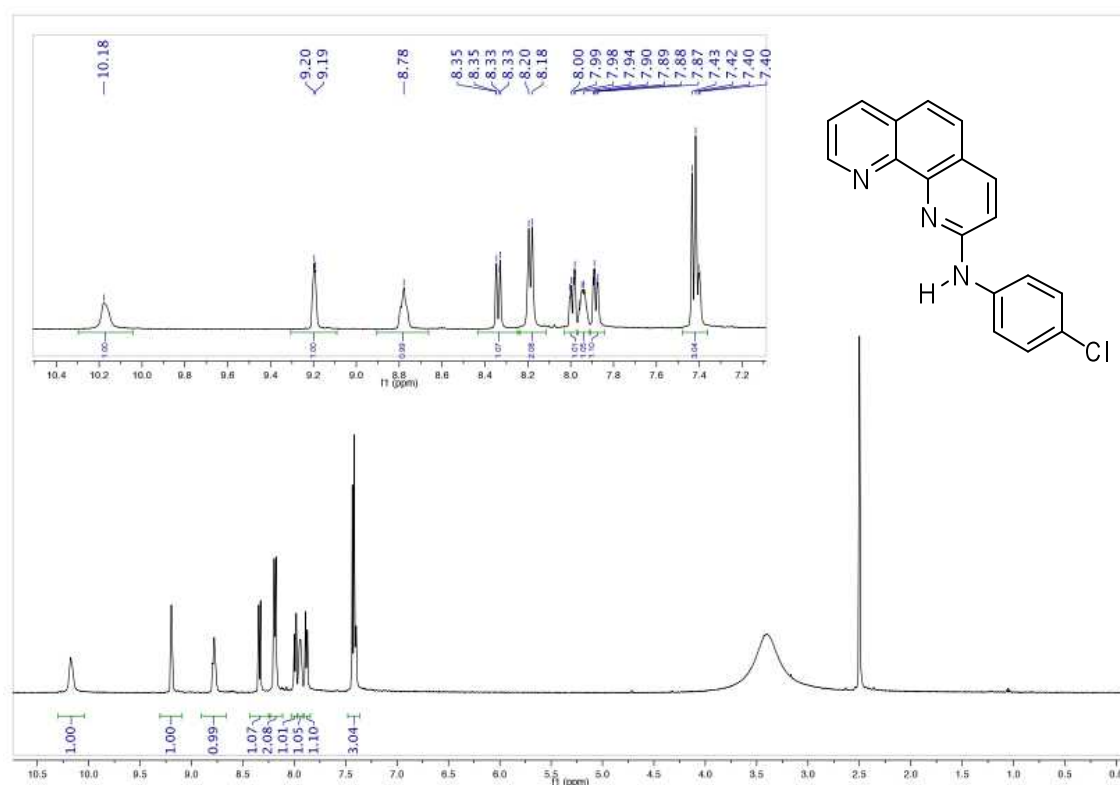


SI Figure 29: <sup>1</sup>H NMR: *N*-(4-fluorophenyl)-1,10-phenanthroline-2-amine (**30**), (200 MHz, DMSO-d<sub>6</sub>).

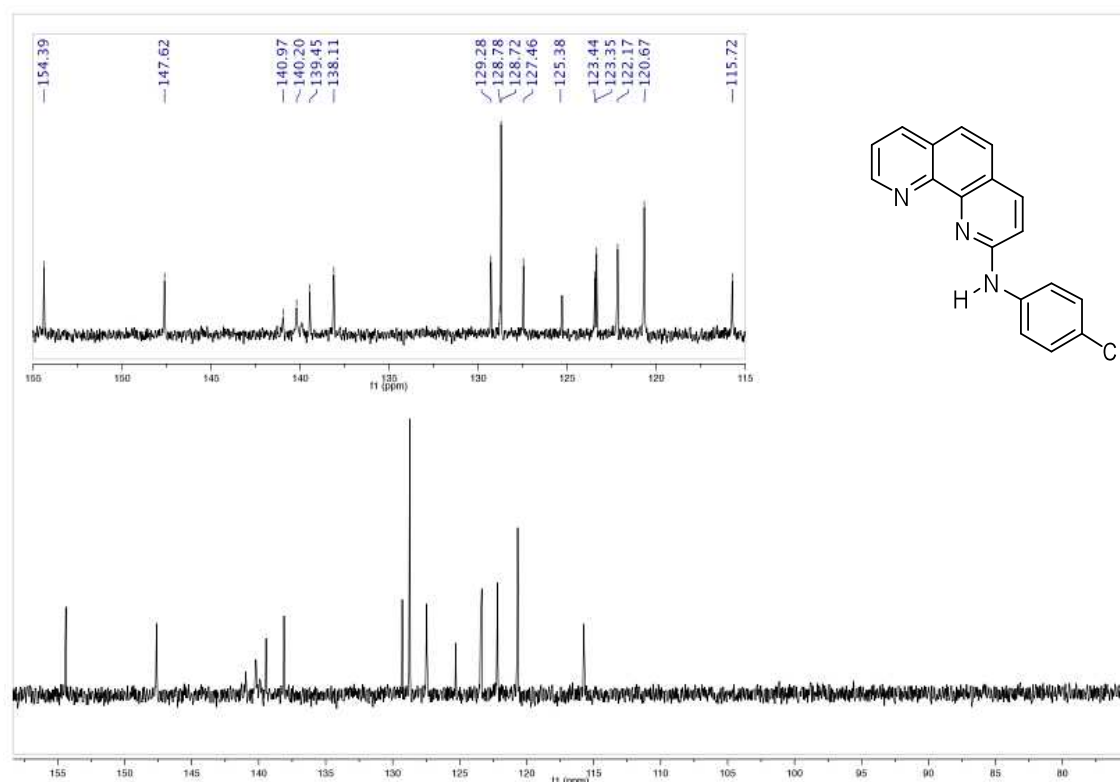


SI Figure 30: <sup>13</sup>C NMR: *N*-(4-fluorophenyl)-1,10-phenanthroline-2-amine (**30**), (50 MHz, DMSO-d<sub>6</sub>).

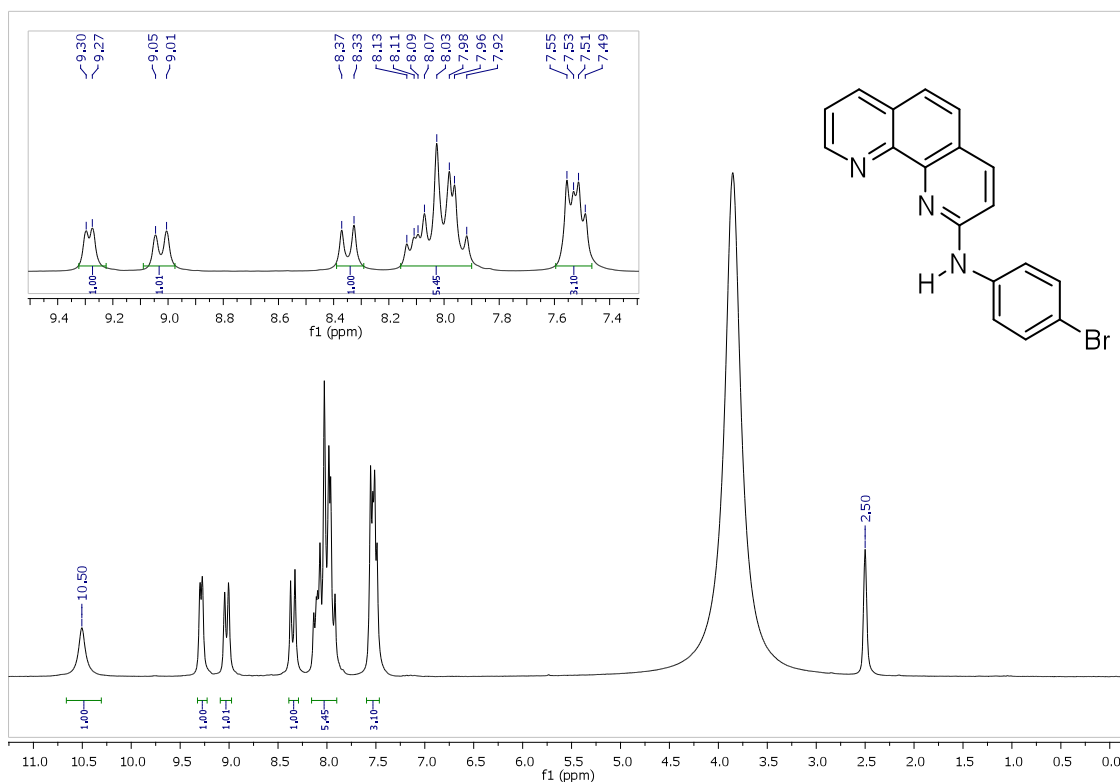




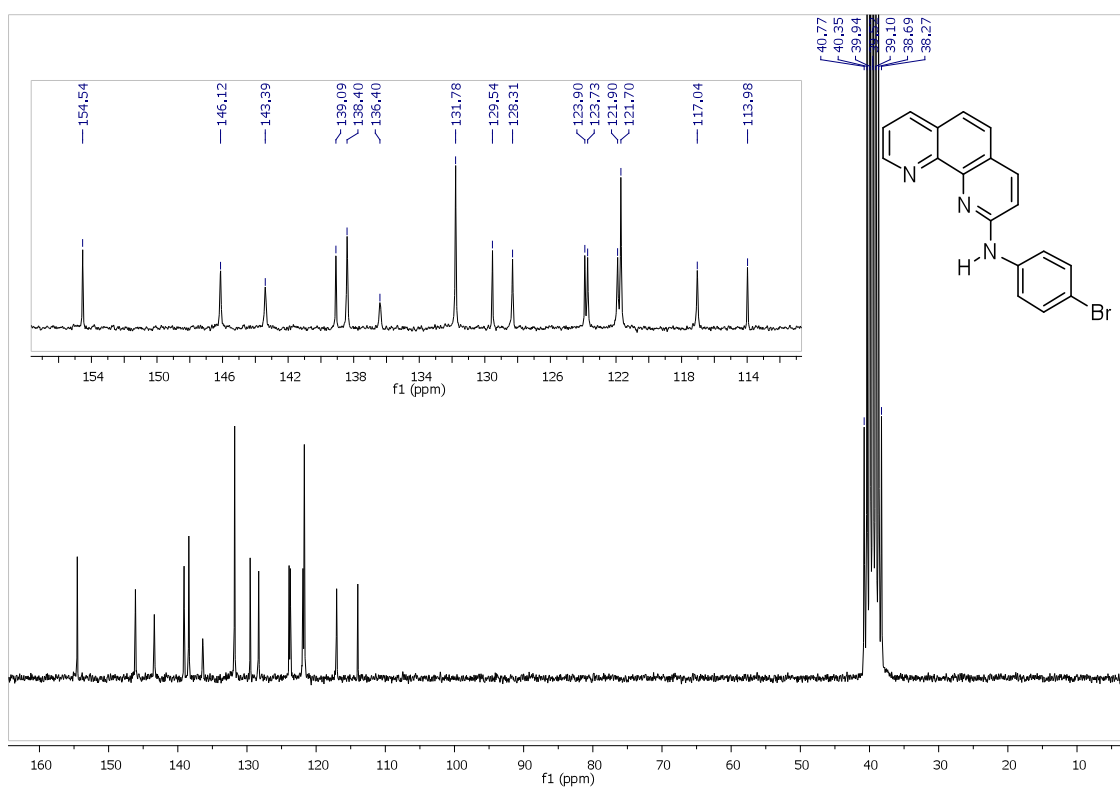
SI Figure 31: <sup>1</sup>H NMR: *N*-(4-chlorophenyl)-1,10-phenanthroline-2-amine (**3p**), (300 MHz, DMSO-d<sub>6</sub>).



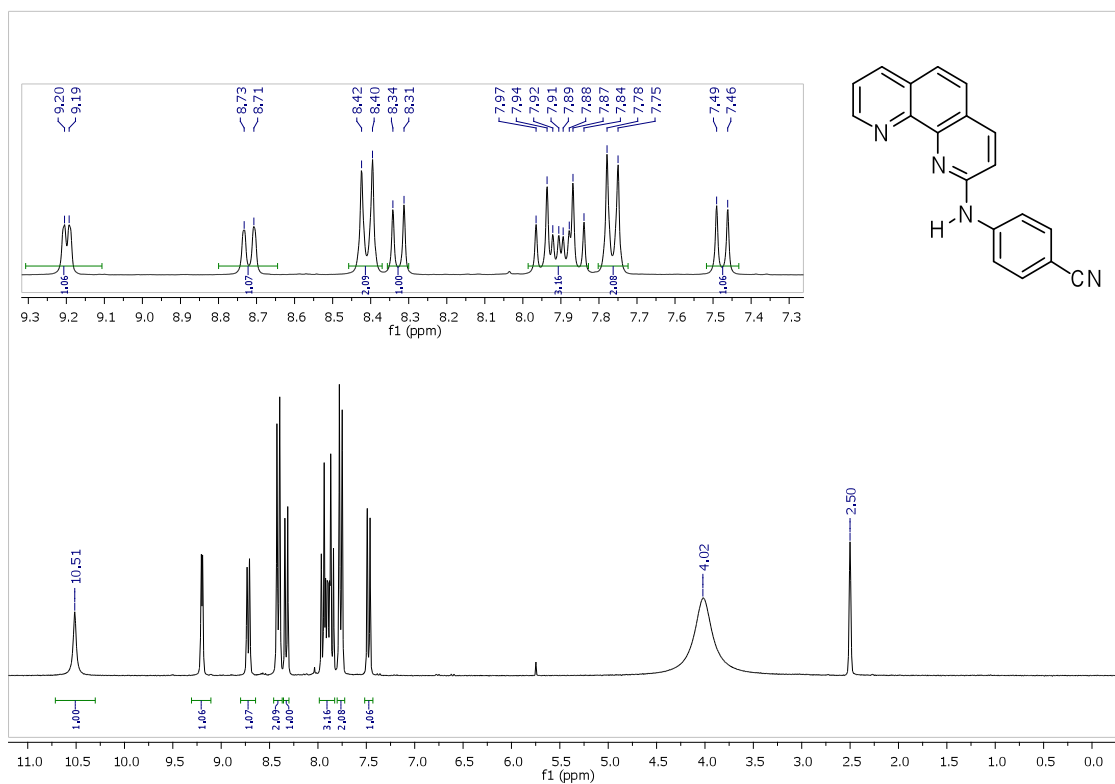
SI Figure 32: <sup>13</sup>C NMR: *N*-(4-chlorophenyl)-1,10-phenanthroline-2-amine (**3p**), (75 MHz, DMSO-d<sub>6</sub>).



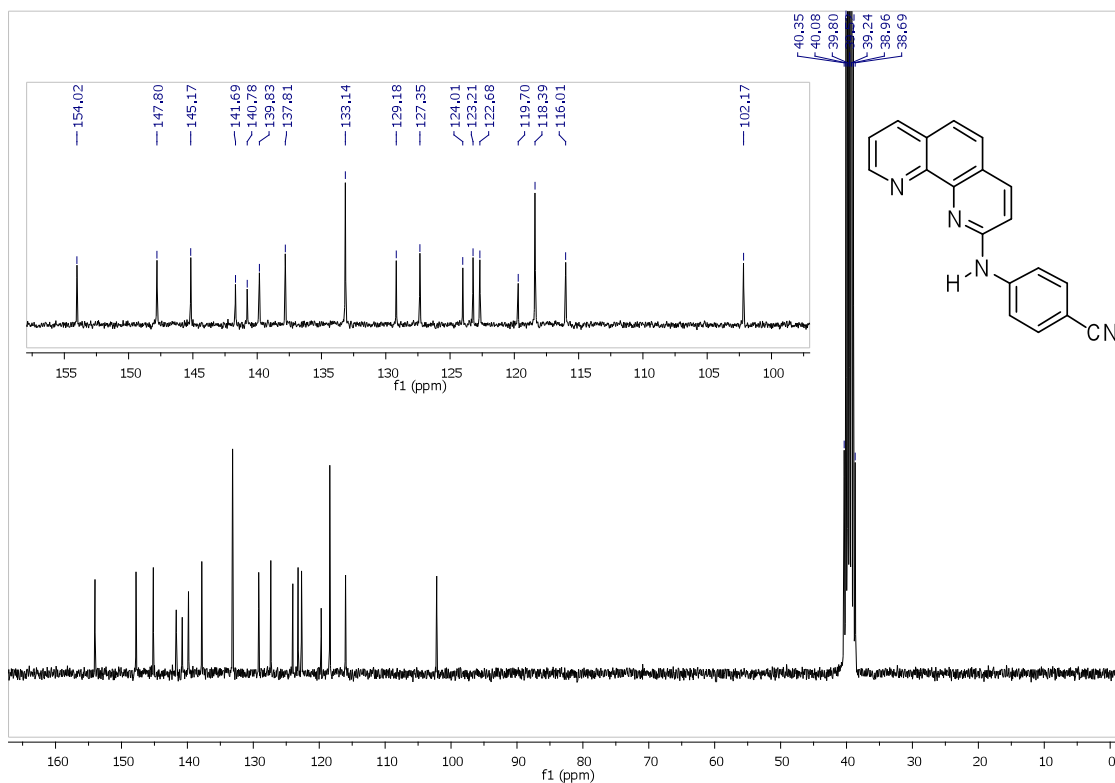
SI Figure 33: <sup>1</sup>H NMR: *N*-(4-bromophenyl)-1,10-phenanthroline-2-amine (**3q**), (200 MHz, DMSO-d<sub>6</sub>).



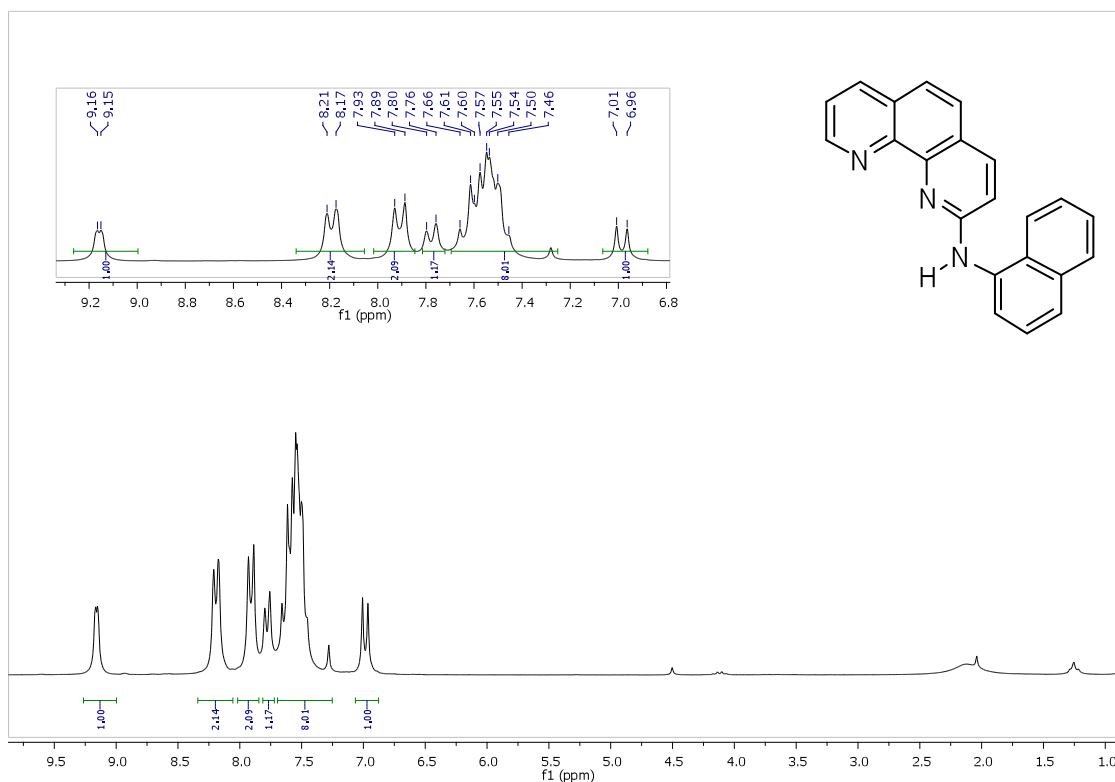
SI Figure 34: <sup>13</sup>C NMR: *N*-(4-bromophenyl)-1,10-phenanthroline-2-amine (**3q**) (50 MHz, DMSO-d<sub>6</sub>).



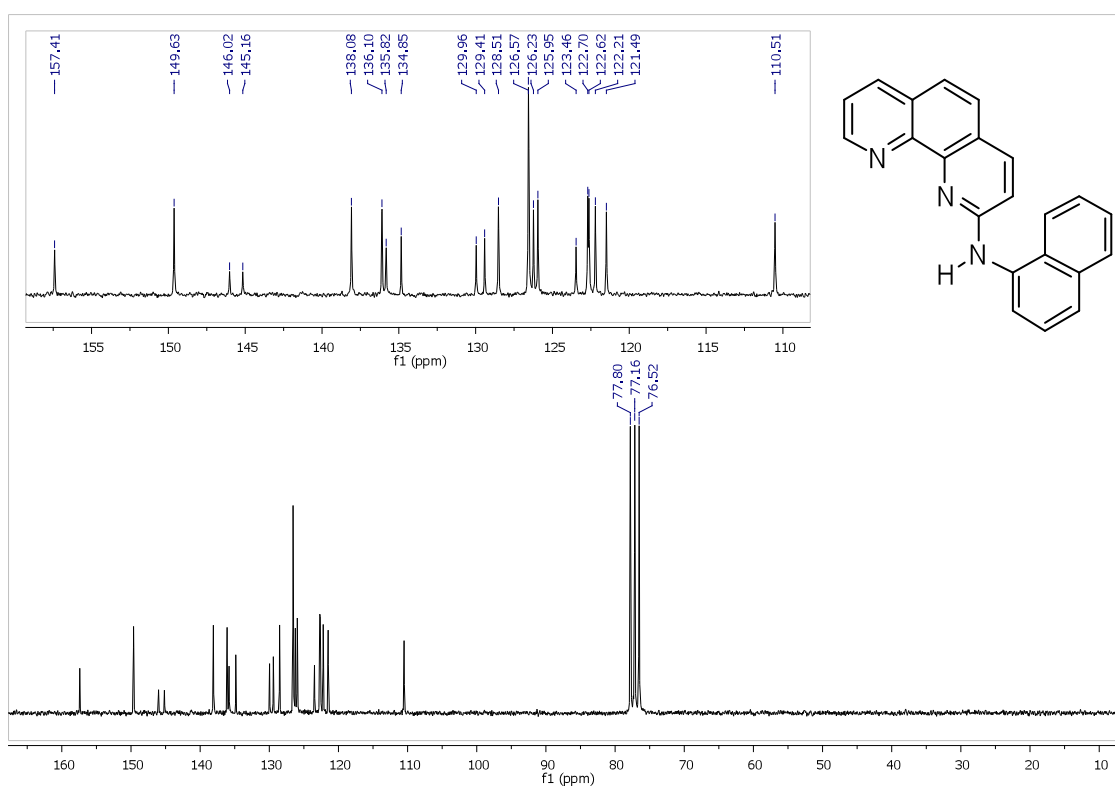
SI Figure 35: <sup>1</sup>H NMR: 4-(1,10-phenanthrolin-2-ylamino)benzonitrile (**3r**), (300 MHz, DMSO-d<sub>6</sub>).



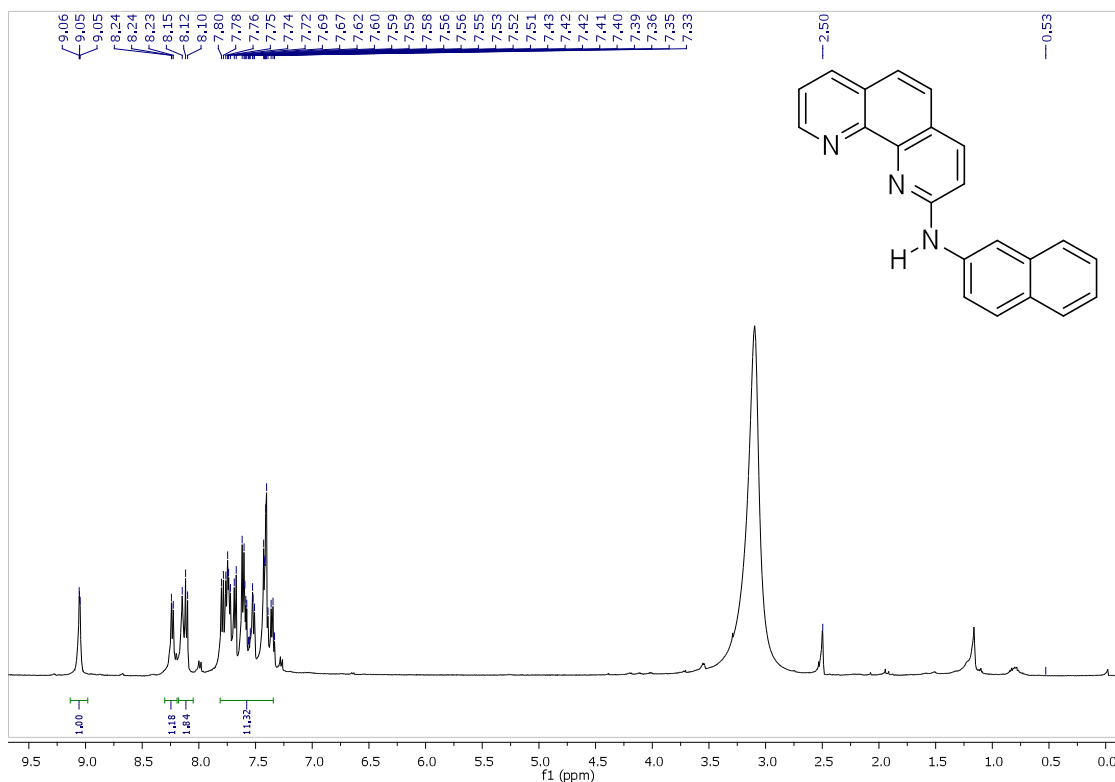
SI Figure 36: <sup>13</sup>C NMR: 4-(1,10-phenanthrolin-2-ylamino)benzonitrile (**3r**), (75 MHz, DMSO-d<sub>6</sub>).



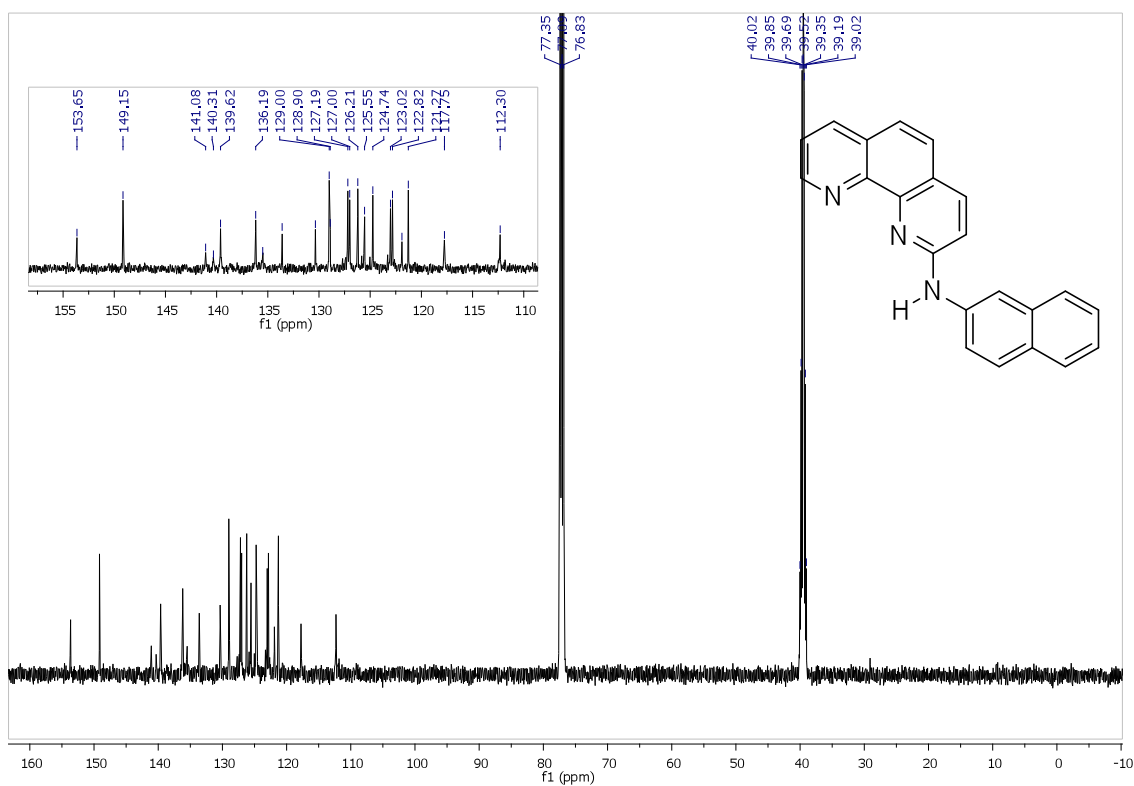
SI Figure 37: <sup>1</sup>H NMR: *N*-(naphthalen-1-yl)-1,10-phenanthroline-2-amine (**3s**) (200 MHz, CDCl<sub>3</sub>).



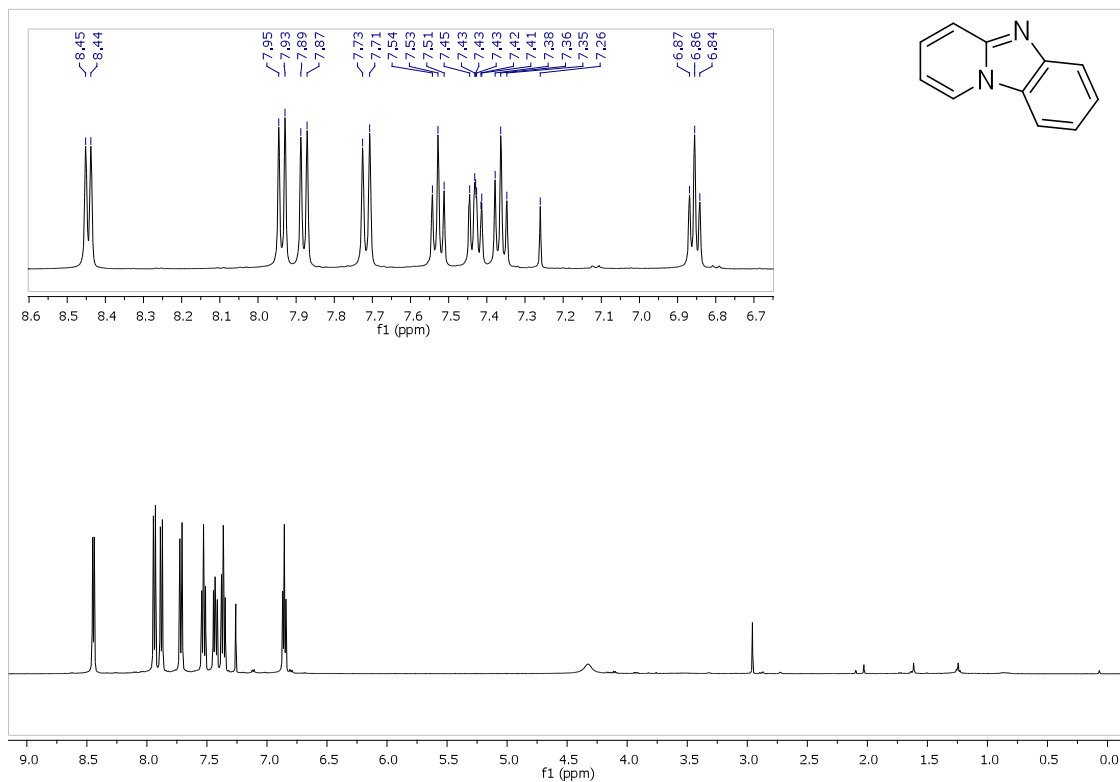
SI Figure 38: <sup>13</sup>C NMR: *N*-(naphthalen-1-yl)-1,10-phenanthroline-2-amine (**3s**), (50 MHz, CDCl<sub>3</sub>).



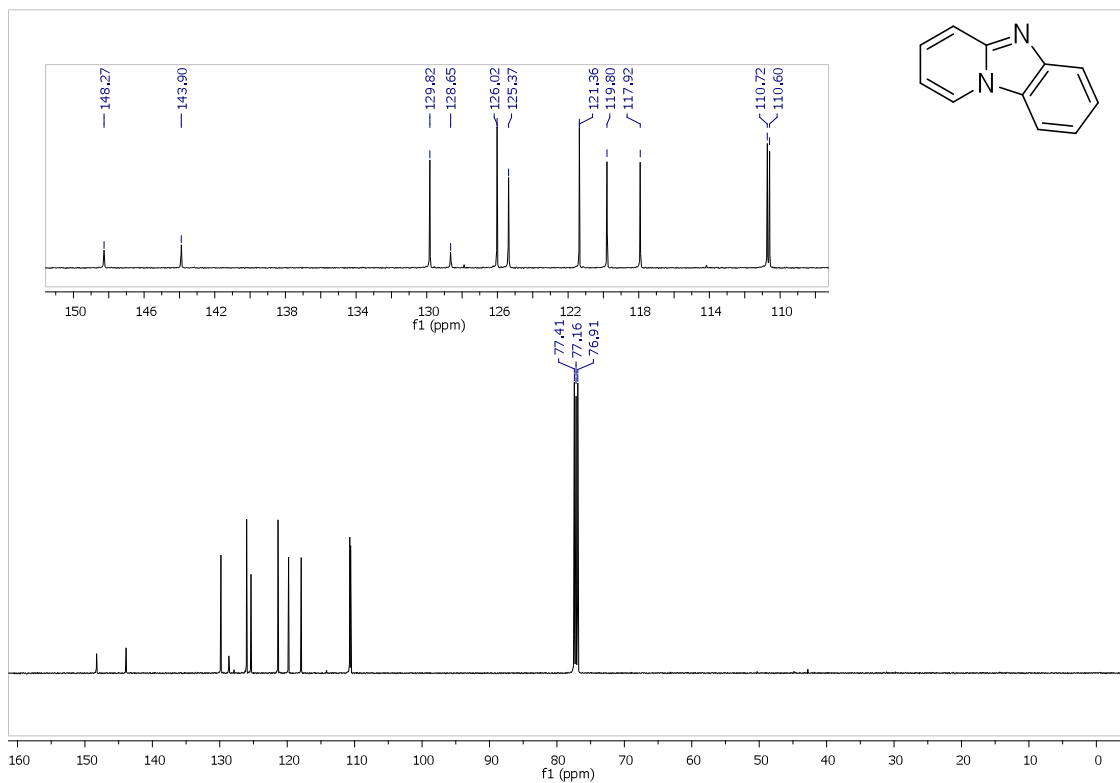
SI Figure 39: <sup>1</sup>H NMR: *N*-(naphthalen-2-yl)-1,10-phenanthroline-2-amine (**3t**), (500 MHz, DMSO-d<sub>6</sub>, CDCl<sub>3</sub>).



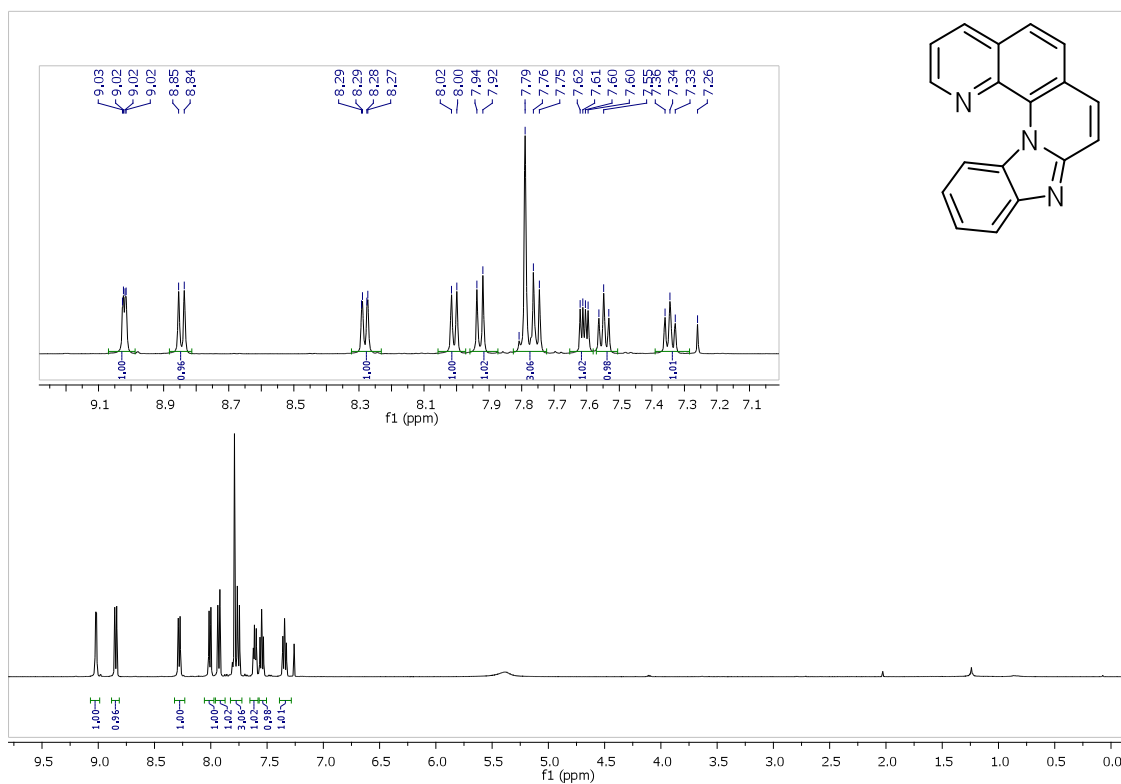
SI Figure 40: <sup>13</sup>C NMR: *N*-(naphthalen-2-yl)-1,10-phenanthroline-2-amine (**3t**), (125 MHz, DMSO-d<sub>6</sub>, CDCl<sub>3</sub>).



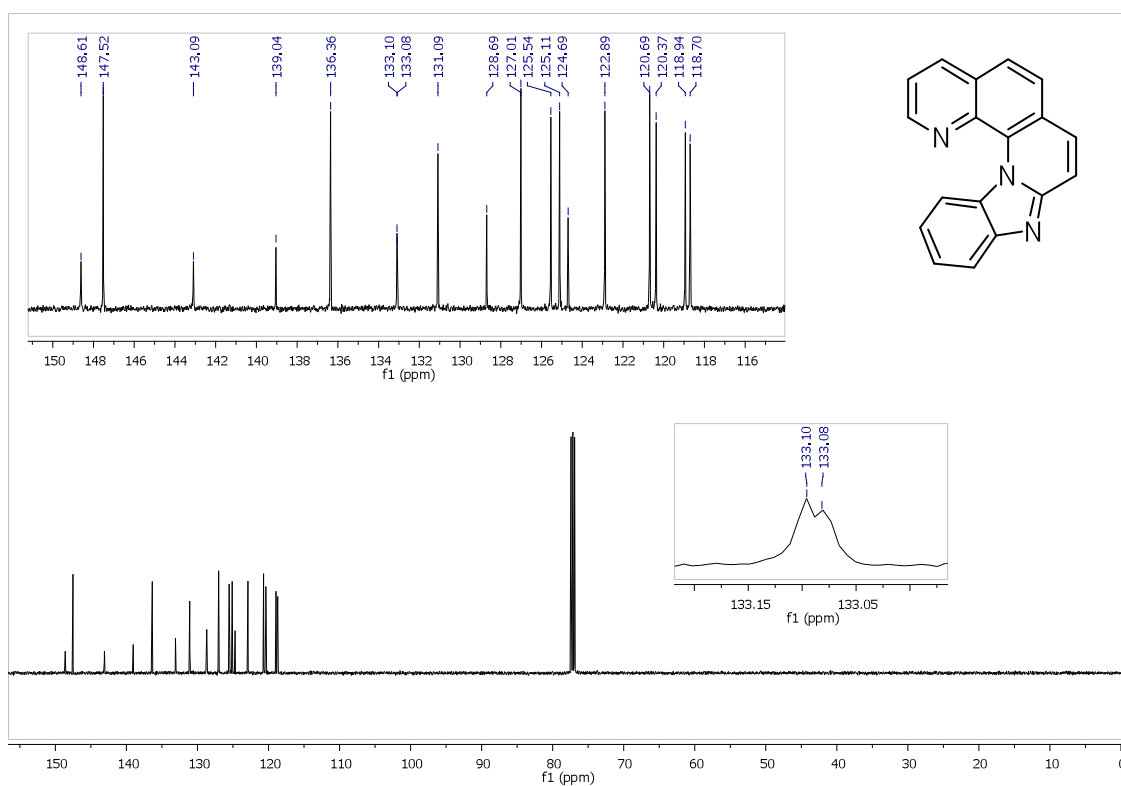
SI Figure 41: <sup>1</sup>H NMR: benzo[4,5]imidazo[1,2-*a*]pyridine (**5**), (500 MHz, CDCl<sub>3</sub>).



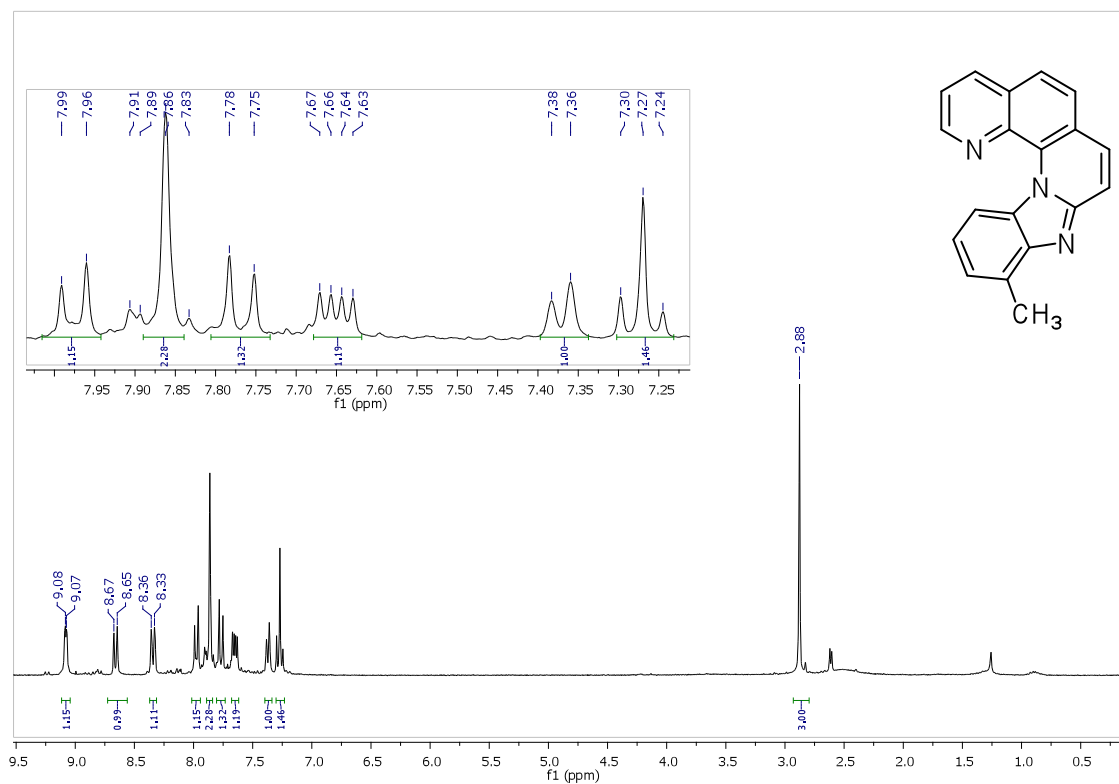
SI Figure 42: <sup>13</sup>C NMR: benzo[4,5]imidazo[1,2-*a*]pyridine (**5**), (125 MHz, CDCl<sub>3</sub>).



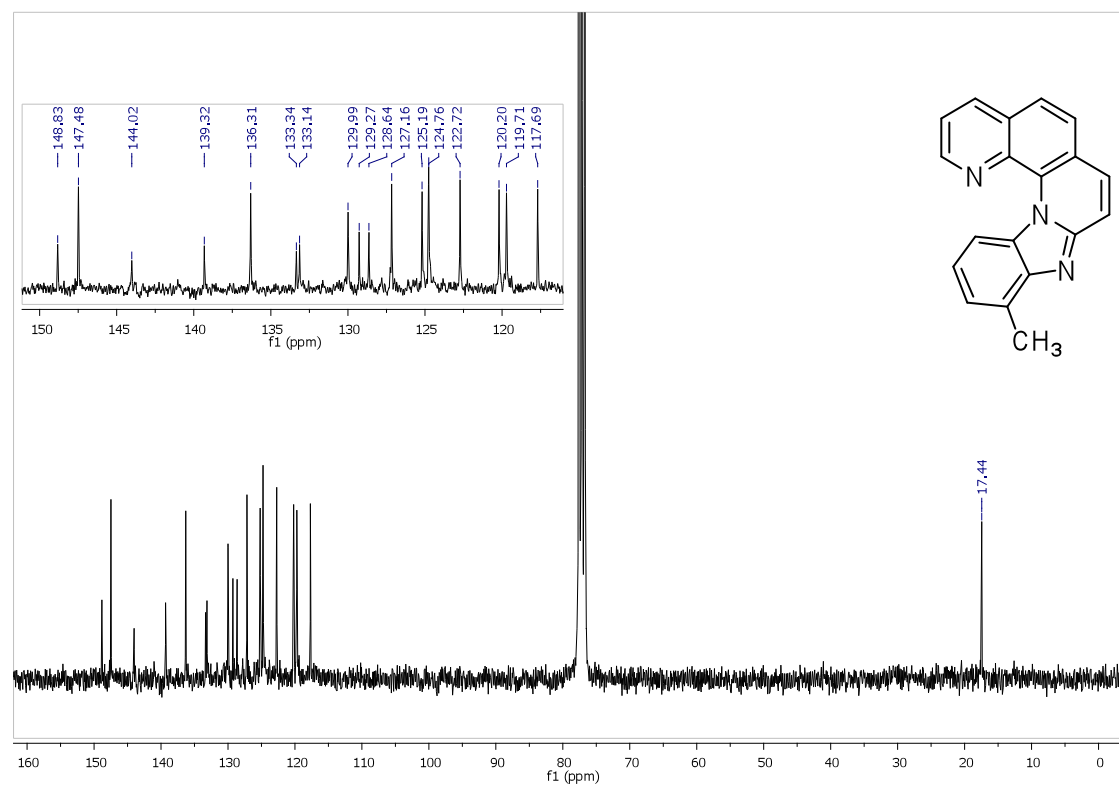
SI Figure 43: <sup>1</sup>H NMR: benzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**6a**), (500 MHz, CDCl<sub>3</sub>).



SI Figure 44: <sup>13</sup>C NMR: benzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**6a**), (125 MHz, CDCl<sub>3</sub>).

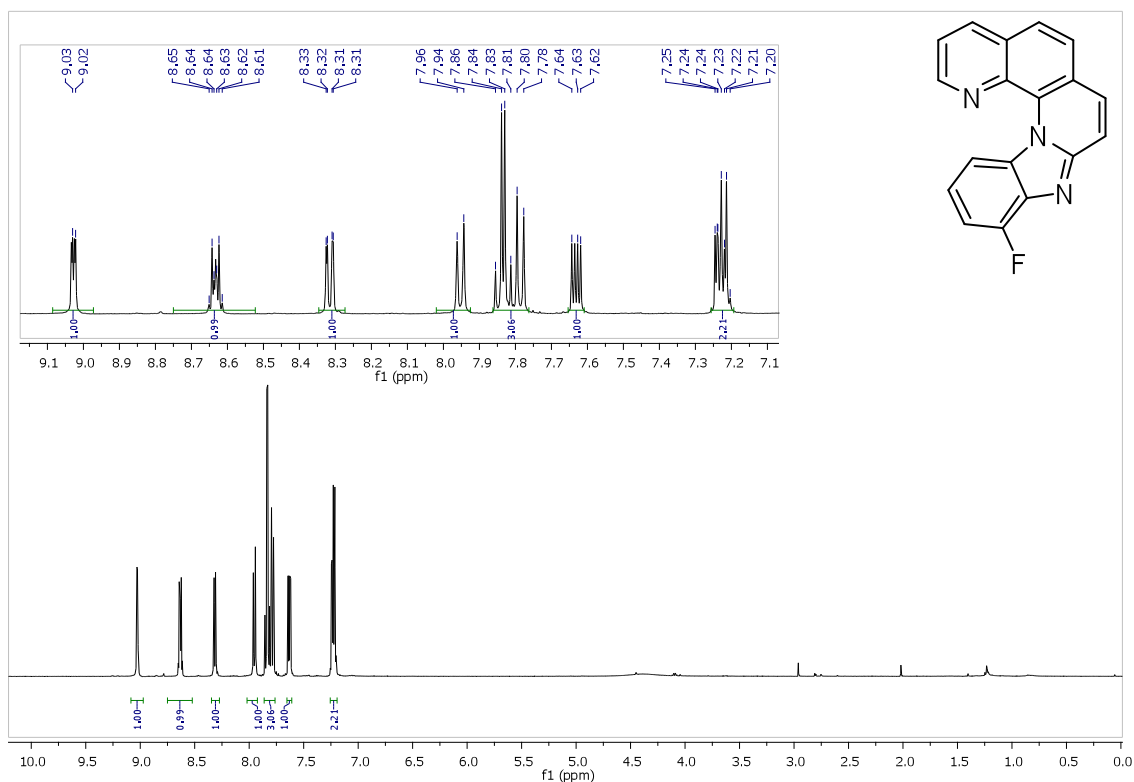


SI Figure 45: <sup>1</sup>H NMR: 12-methylbenzo[4,5]imidazo[1,2-*a*][1,10]phenanthroline (**6c**), (300 MHz, CDCl<sub>3</sub>).

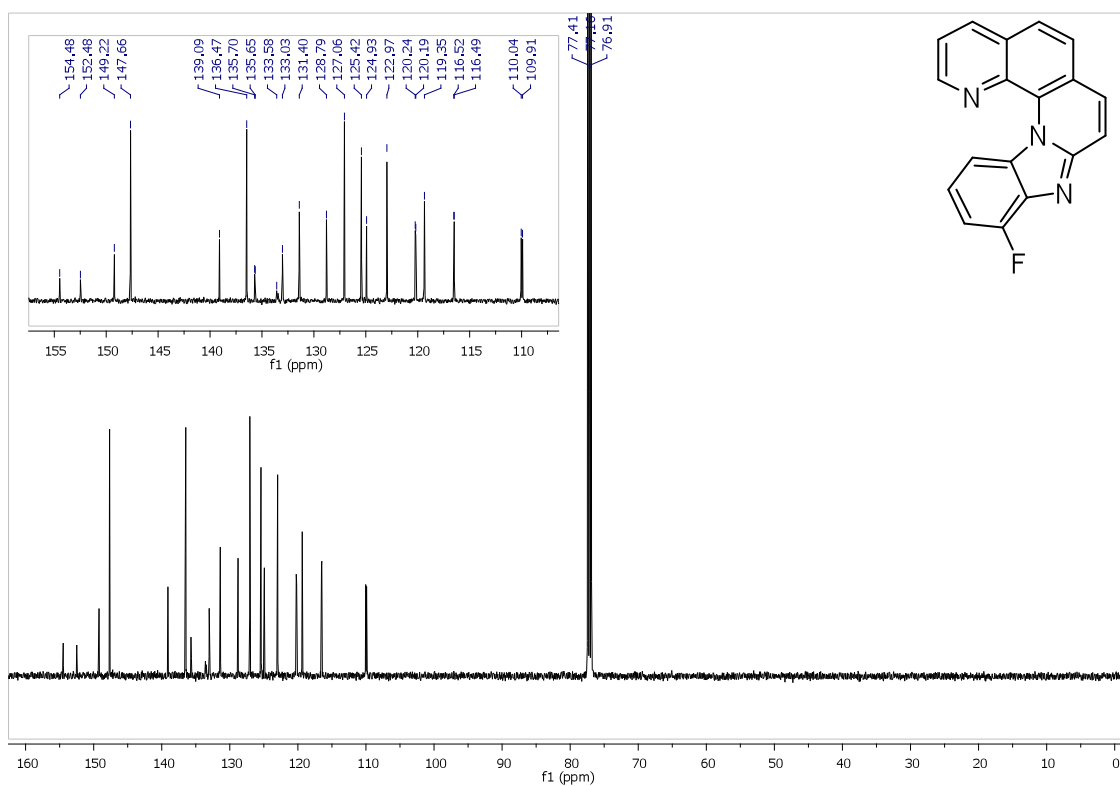


SI Figure 46: <sup>13</sup>C NMR: 12-methylbenzo[4,5]imidazo[1,2-*a*][1,10]phenanthroline (**6c**), (75 MHz, CDCl<sub>3</sub>).

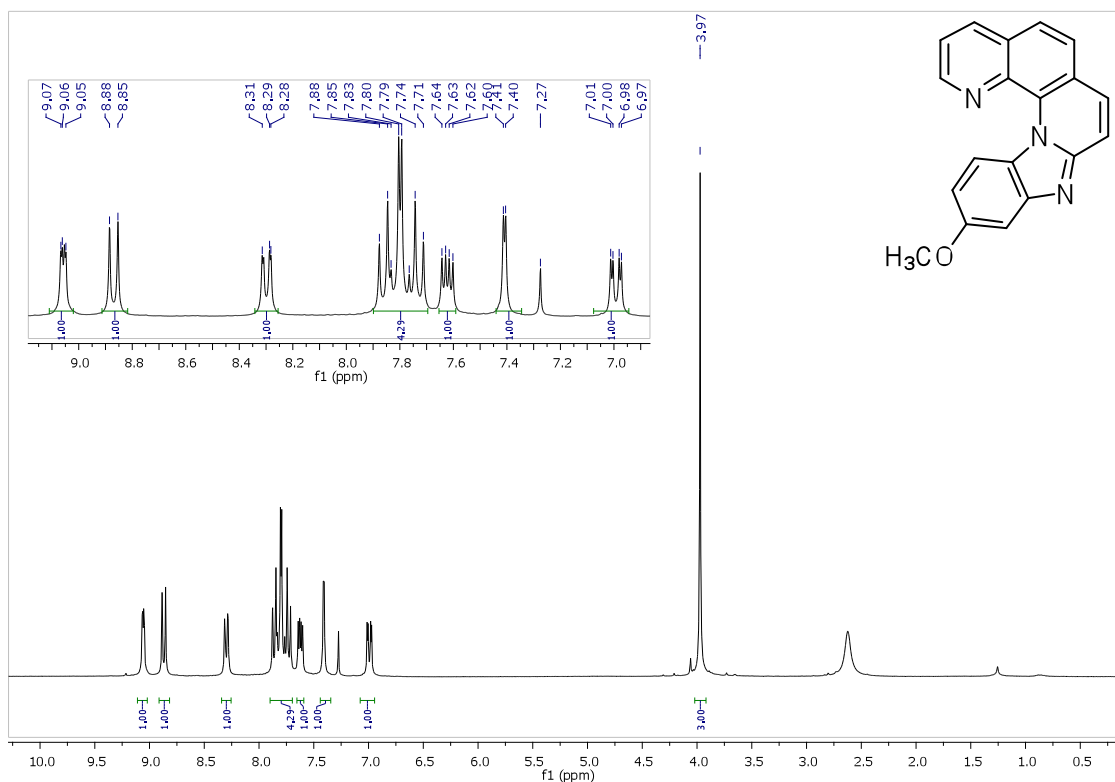




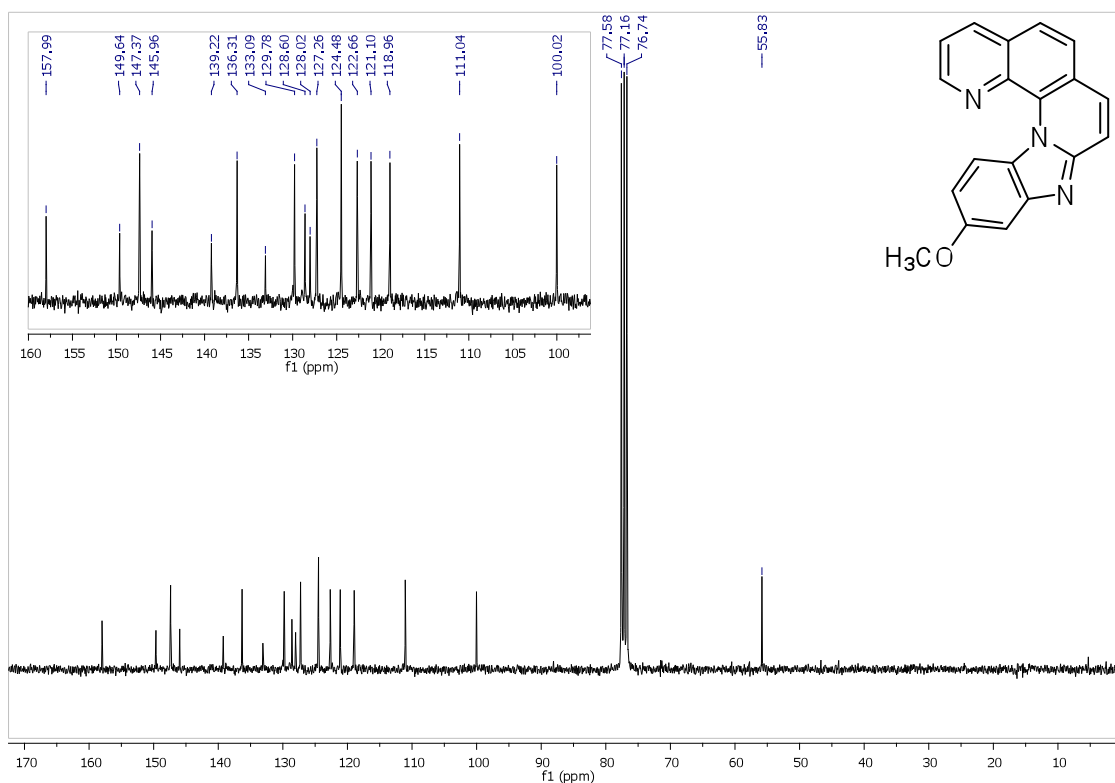
SI Figure 47: <sup>1</sup>H NMR: 12-fluorobenzo[4,5]imidazo[1,2-*a*][1,10]phenanthroline (**6d**), (500 MHz, CDCl<sub>3</sub>).



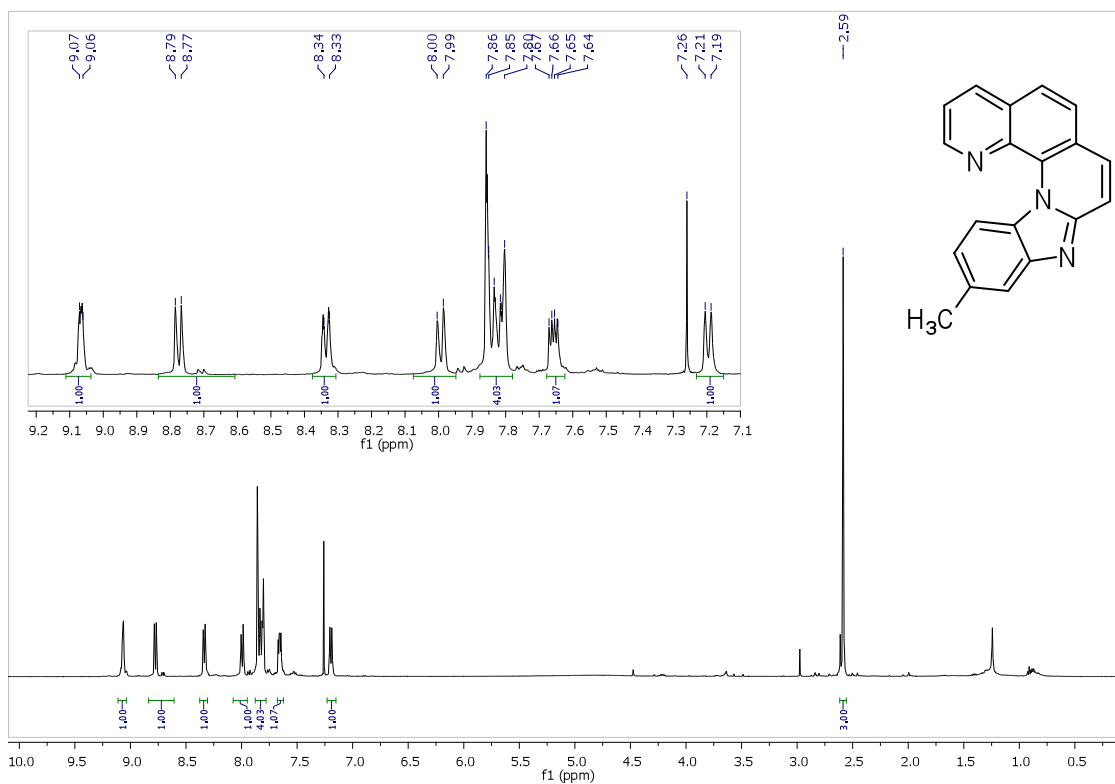
SI Figure 48: <sup>13</sup>C NMR: 12-fluorobenzo[4,5]imidazo[1,2-*a*][1,10]phenanthroline (**6d**), (125 MHz, CDCl<sub>3</sub>).



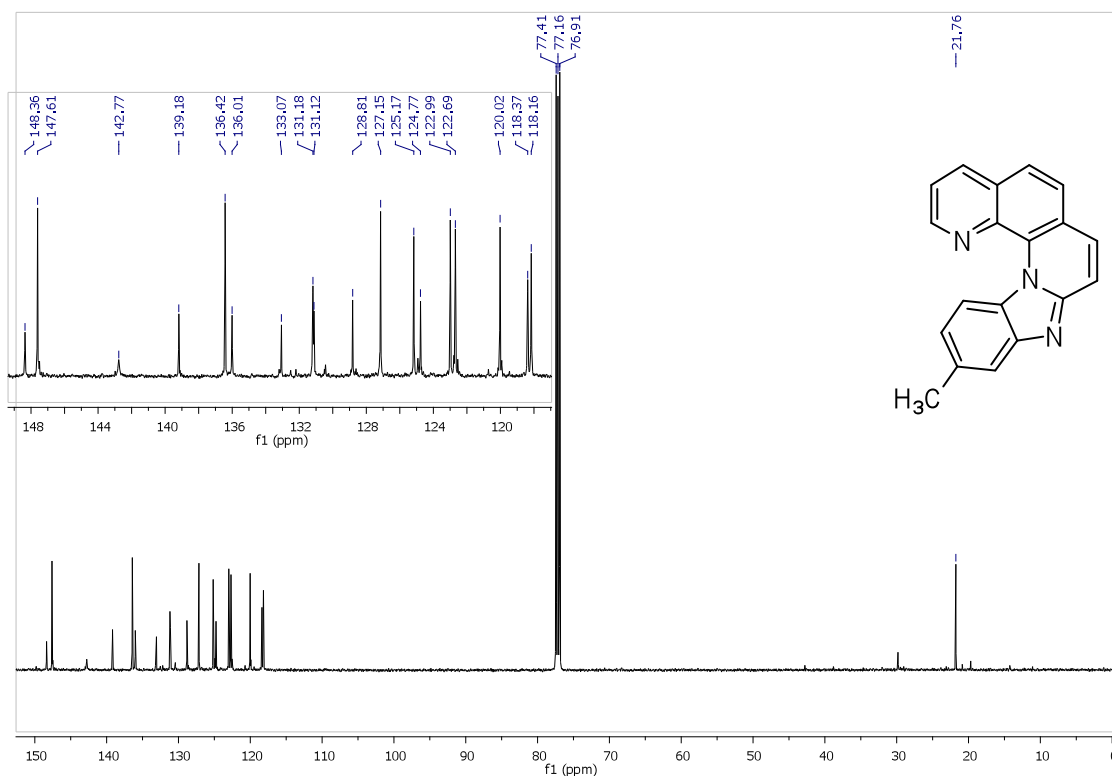
SI Figure 49: <sup>1</sup>H NMR: 13-methoxybenzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**6f**), (300 MHz, CDCl<sub>3</sub>).



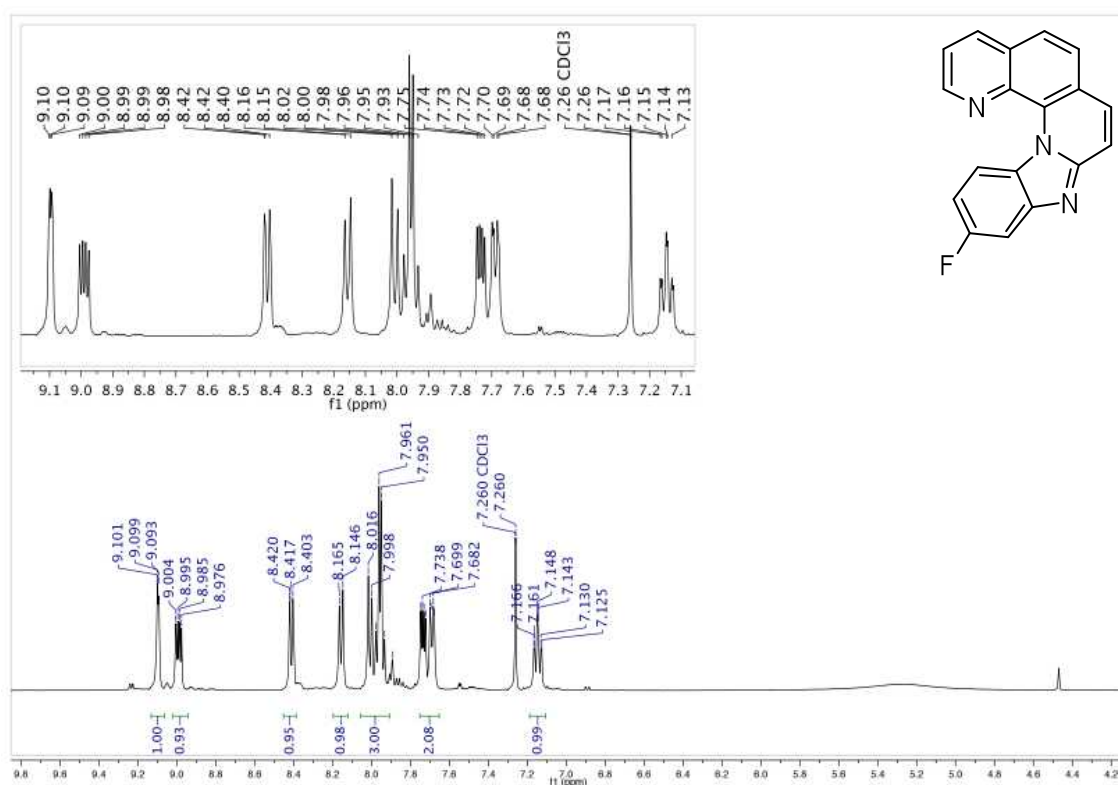
SI Figure 50: <sup>13</sup>C NMR: 13-methoxybenzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**6f**), (75 MHz, CDCl<sub>3</sub>).



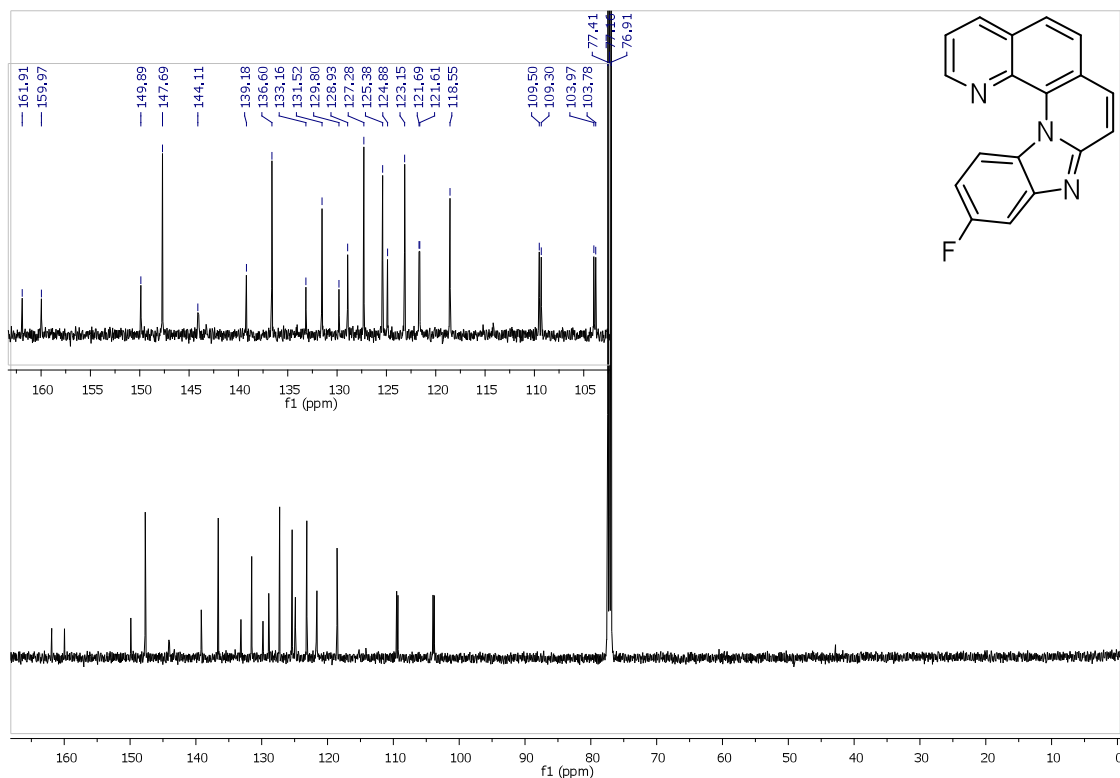
SI Figure 51: <sup>1</sup>H NMR: 13-methylbenzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**6g**), (500 MHz, CDCl<sub>3</sub>).



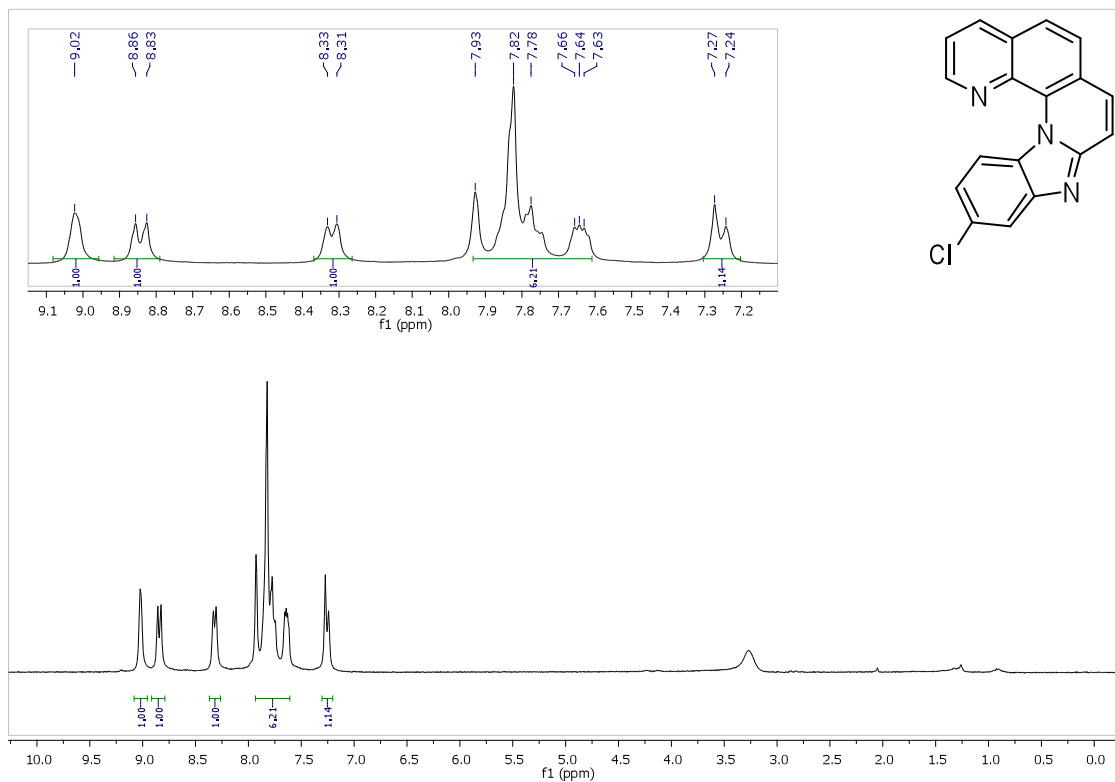
SI Figure 52: <sup>13</sup>C NMR: 13-methylbenzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**6g**), (75 MHz, CDCl<sub>3</sub>).



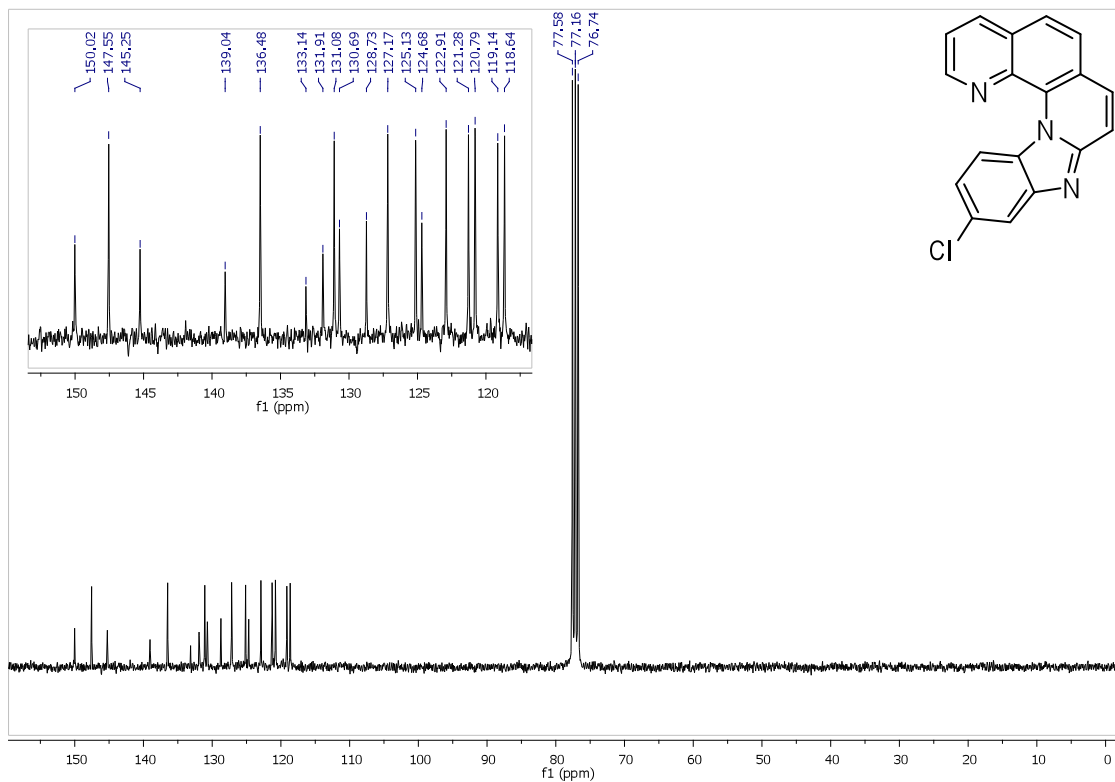
SI Figure 53: <sup>1</sup>H NMR: 13-fluorobenzo[4,5]imidazo[1,2-*a*][1,10]phenanthroline (**6h**), (500 MHz, CDCl<sub>3</sub>).



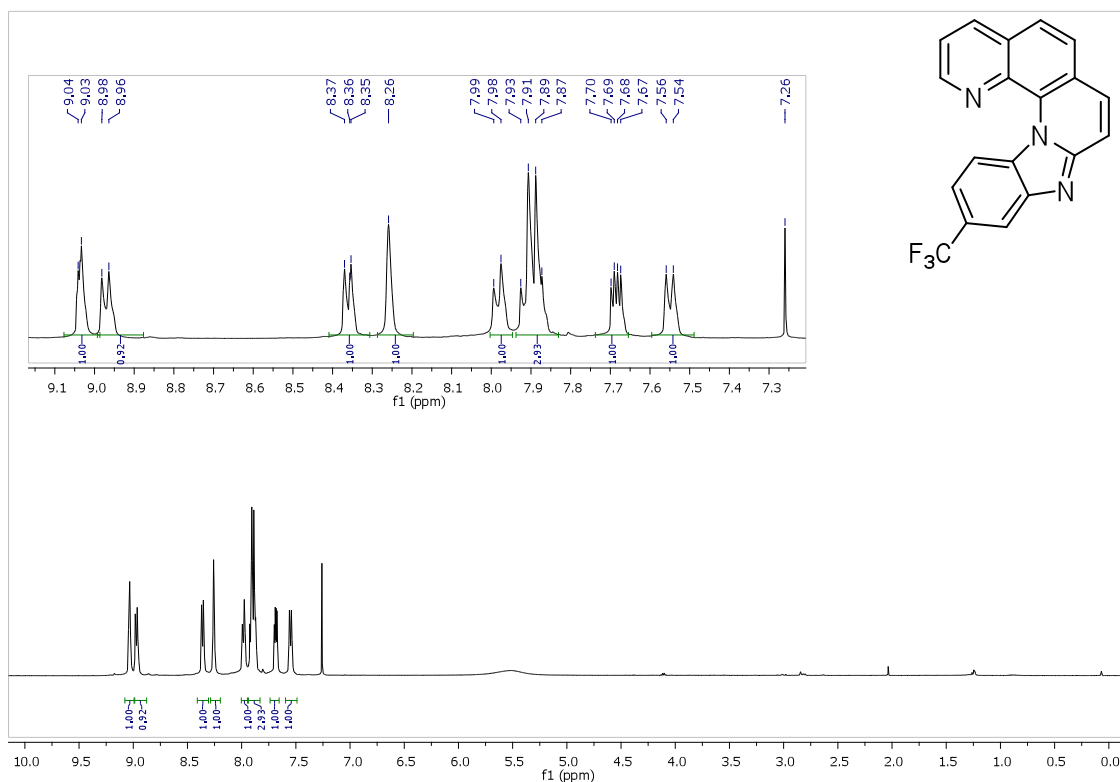
SI Figure 54: <sup>13</sup>C NMR: 13-fluorobenzo[4,5]imidazo[1,2-*a*][1,10]phenanthroline (**6h**), (125 MHz, CDCl<sub>3</sub>).



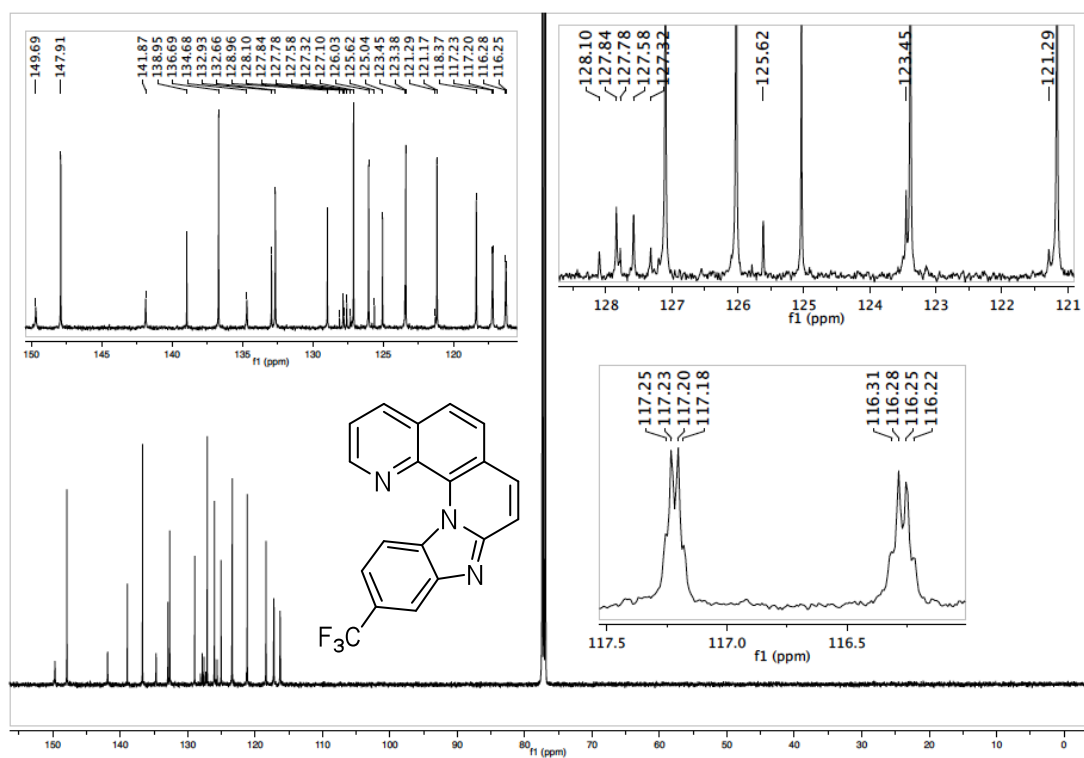
SI Figure 55: <sup>1</sup>H NMR: 13-chlorobenzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**6i**), (300 MHz, CDCl<sub>3</sub>)



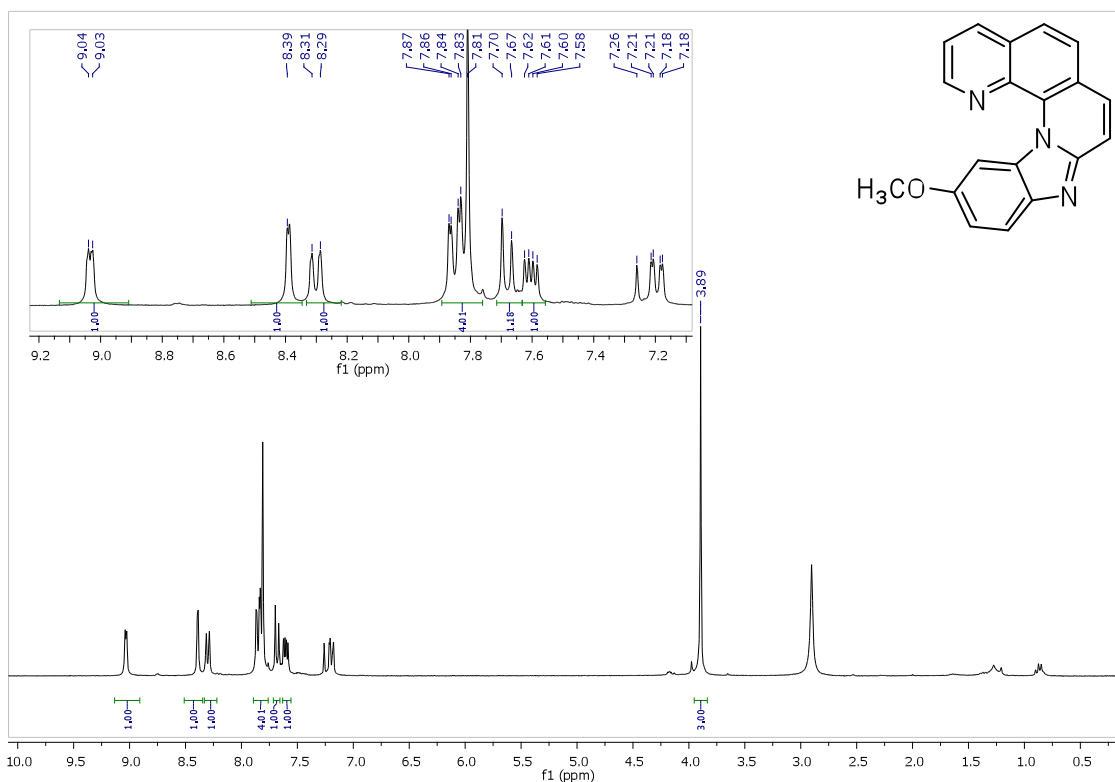
SI Figure 56: <sup>13</sup>C NMR: 13-chlorobenzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**6i**), (75 MHz, CDCl<sub>3</sub>).



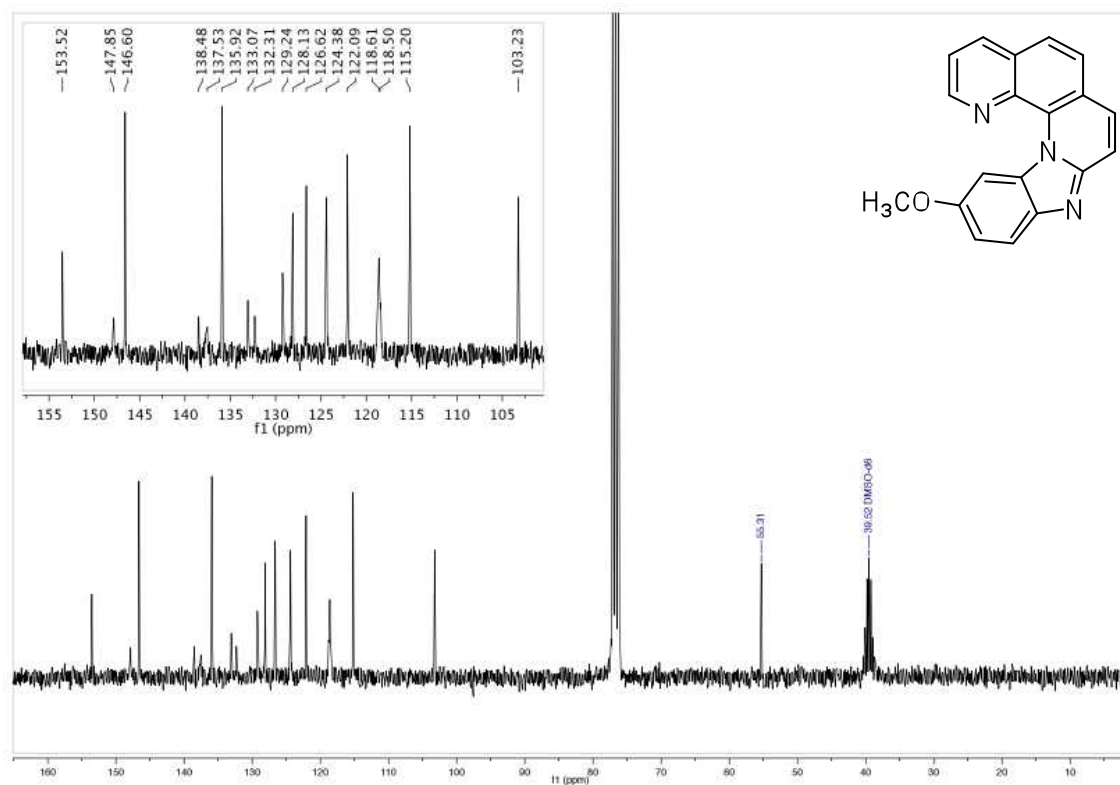
SI Figure 57: <sup>1</sup>H NMR: 13-(trifluoromethyl)benzo[4,5]imidazo[1,2-*a*][1,10]phenanthroline (**6j**), (500 MHz, CDCl<sub>3</sub>).



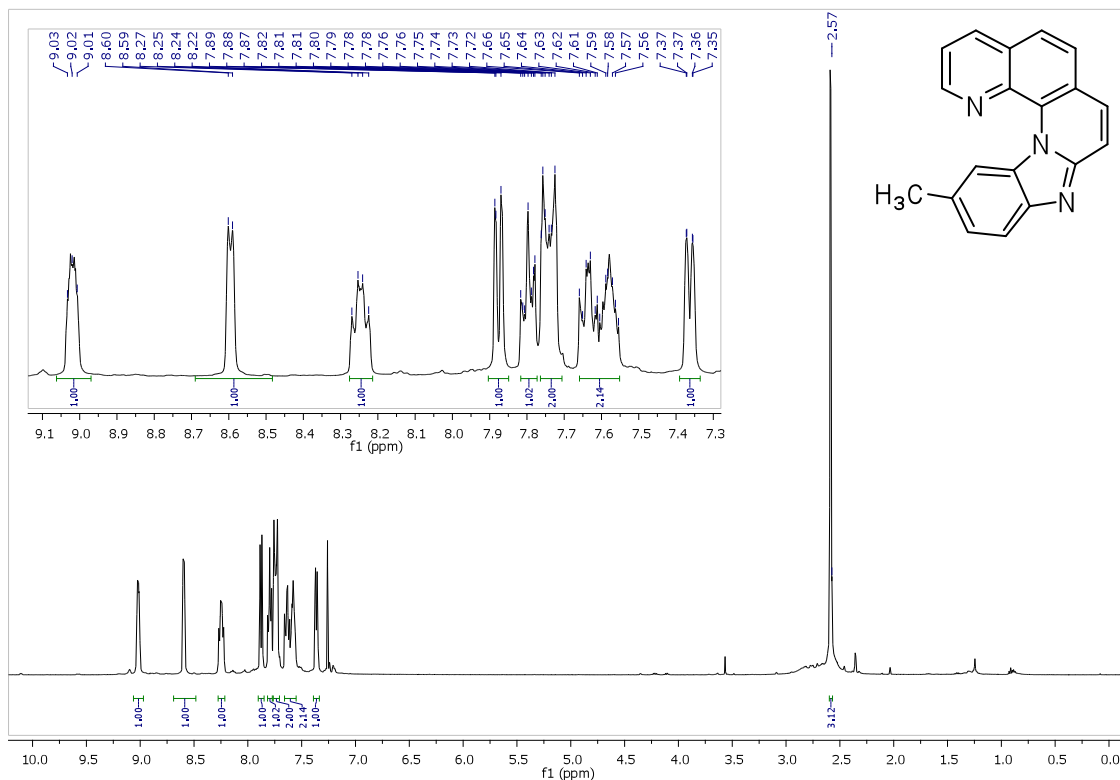
SI Figure 58: <sup>13</sup>C NMR: 13-(trifluoromethyl)benzo[4,5]imidazo[1,2-*a*][1,10]phenanthroline (**6j**), (125 MHz, CDCl<sub>3</sub>)



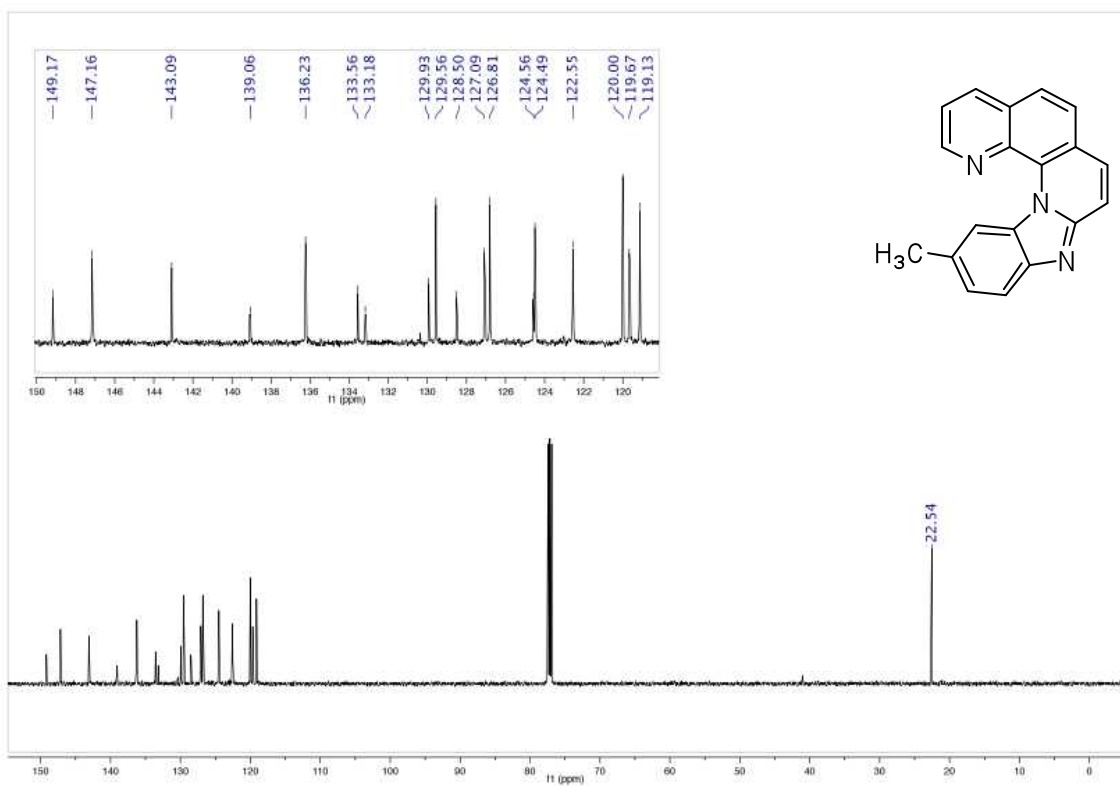
SI Figure 59: <sup>1</sup>H NMR: 14-methoxybenzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**6m**), (300 MHz, CDCl<sub>3</sub>, DMSO-d<sub>6</sub>).



SI Figure 60: <sup>13</sup>C NMR: 14-methoxybenzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**6m**), (75 MHz, CDCl<sub>3</sub>, DMSO-d<sub>6</sub>).

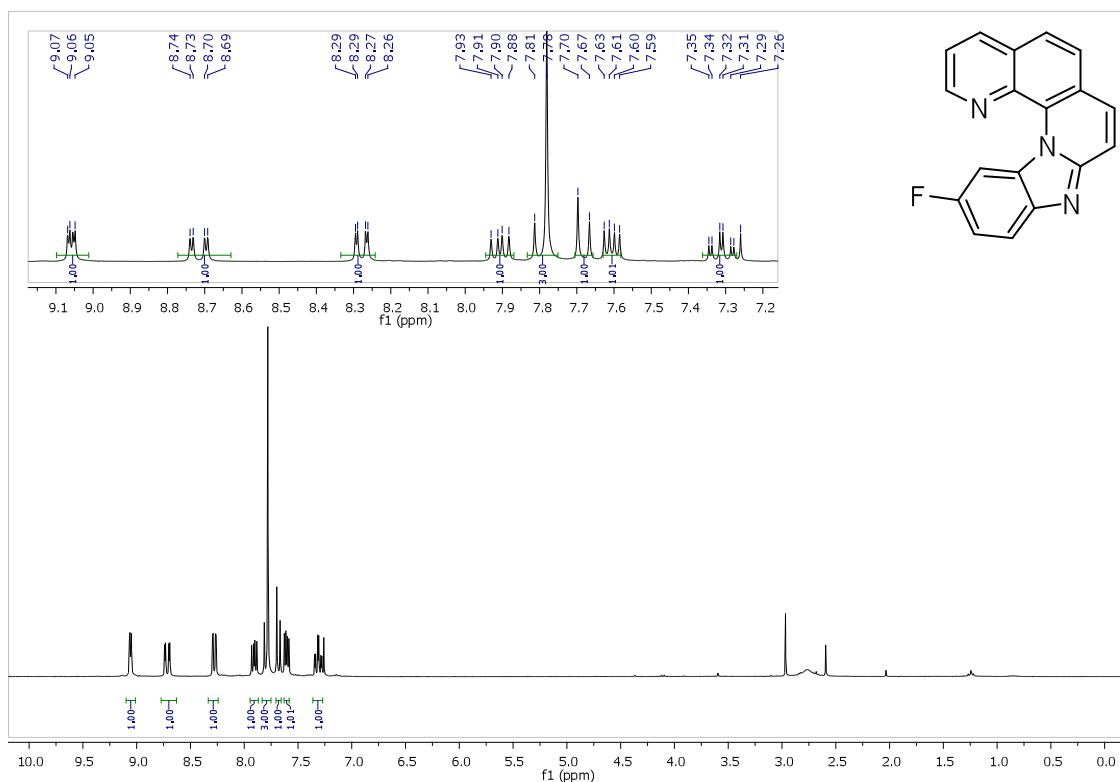


SI Figure 61:  $^1\text{H NMR}$ : 14-methylbenzo[4,5]imidazo[1,2-*a*][1,10]phenanthroline (**6n**), (500 MHz,  $\text{CDCl}_3$ ).

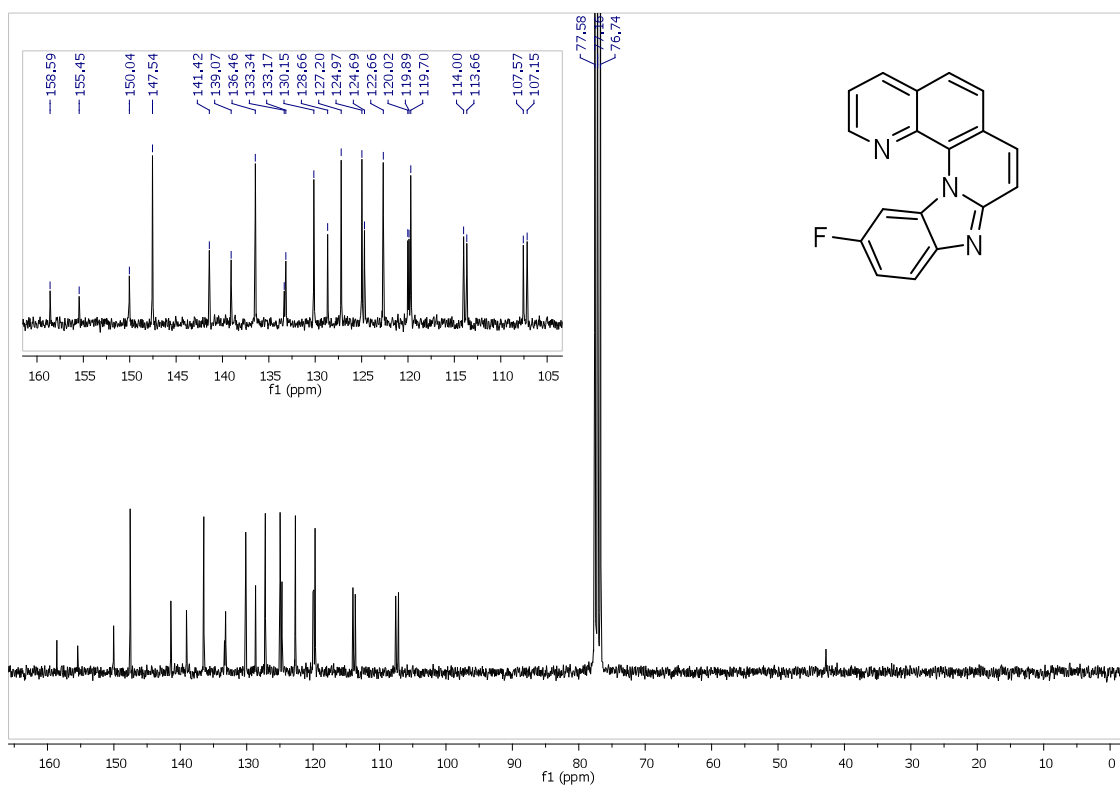


SI Figure 62:  $^{13}\text{C NMR}$ : 14-methylbenzo[4,5]imidazo[1,2-*a*][1,10]phenanthroline (**6n**), (125 MHz,  $\text{CDCl}_3$ ).

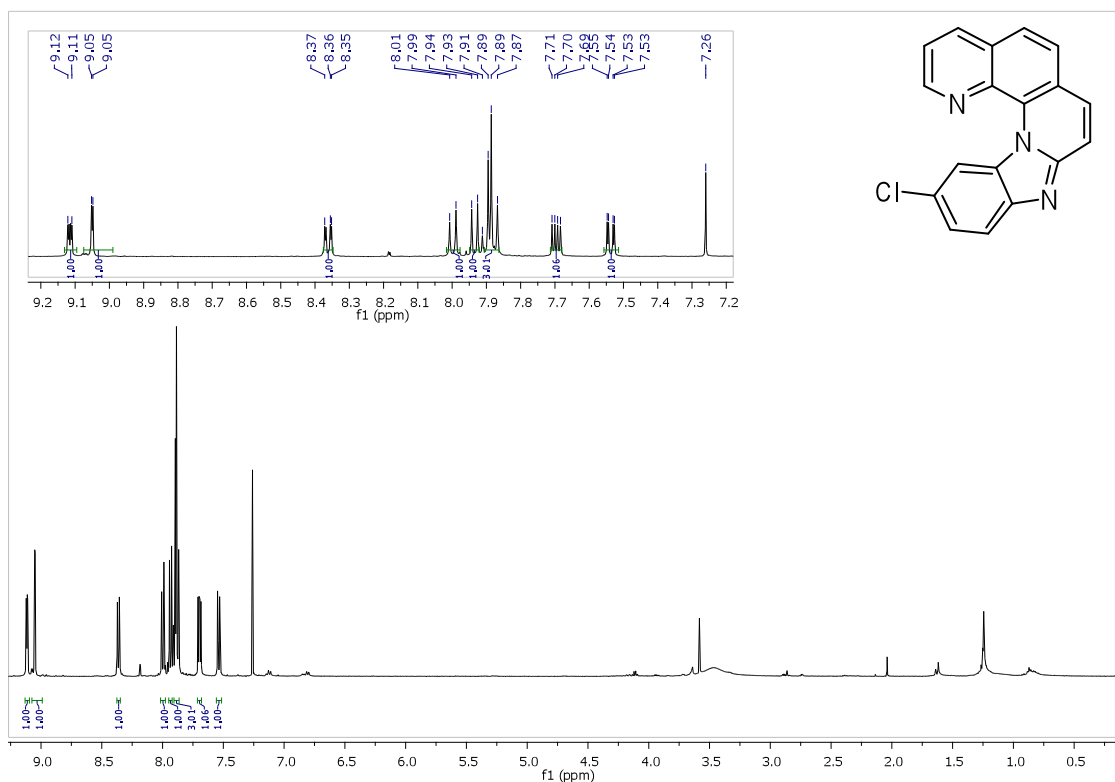




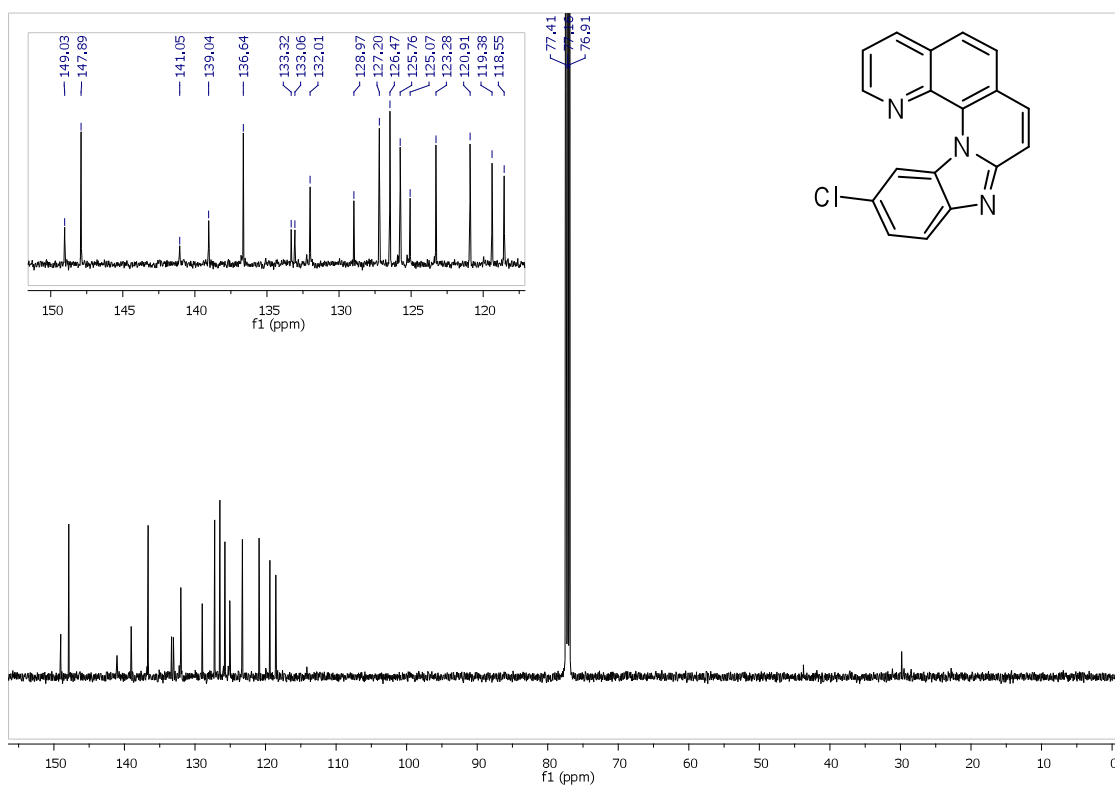
SI Figure 63: <sup>1</sup>H NMR: 14-fluorobenzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**60**), (300 MHz, CDCl<sub>3</sub>).



SI Figure 64: <sup>13</sup>C NMR: 14-fluorobenzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**60**), (75 MHz, CDCl<sub>3</sub>).



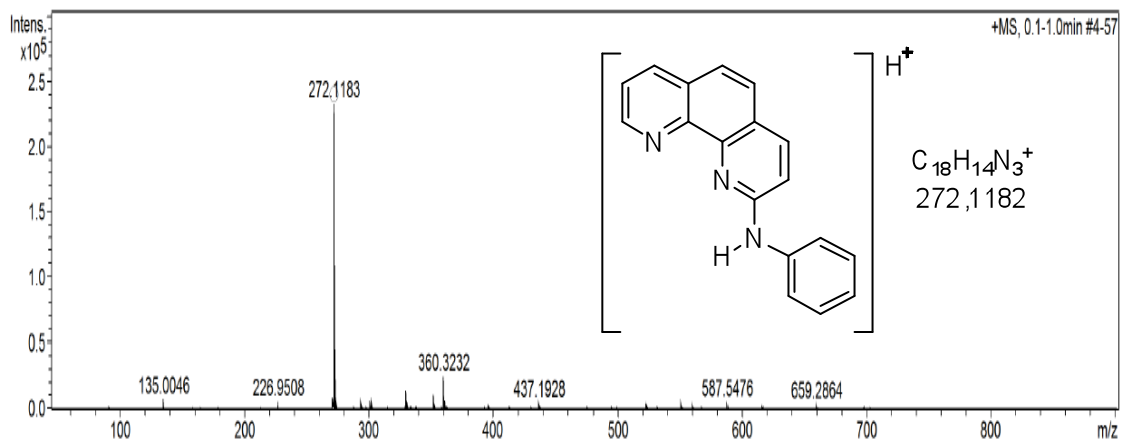
SI Figure 65: <sup>1</sup>H NMR: 14-chlorobenzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**6p**), (500 MHz, CDCl<sub>3</sub>).



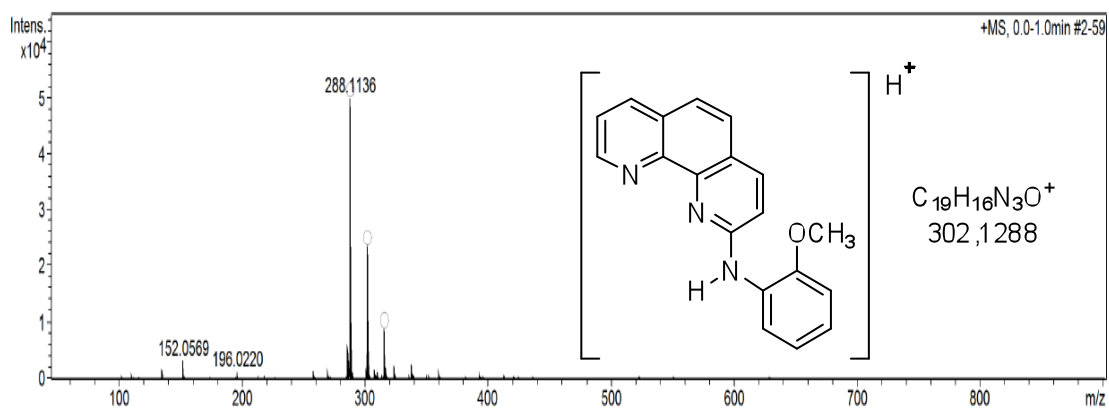
SI Figure 66: <sup>13</sup>C NMR: 14-chlorobenzo[4,5]imidazo[1,2-a][1,10]phenanthroline (**6p**), (125 MHz, CDCl<sub>3</sub>).

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	5.0 l/min
Scan End	896 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste


 SI Figure 67: HRMS of compound **3a**
**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	5.0 l/min
Scan End	896 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

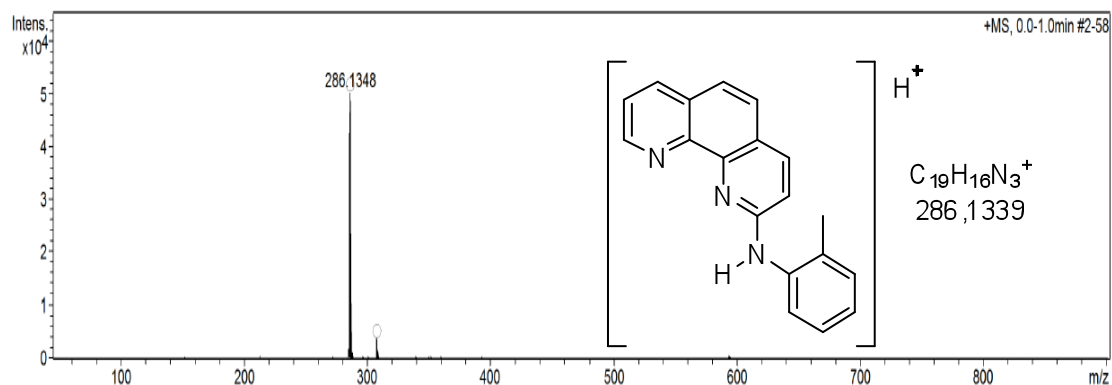


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
288.1136	1	C18H14N3O	288.1131	-1.6	0.2	1	100.00	13.5	even	ok
302.1289	1	C19H16N3O	302.1288	-0.5	3.7	1	100.00	13.5	even	ok
316.1442	1	C20H18N3O	316.1444	0.7	16.1	1	100.00	13.5	even	ok

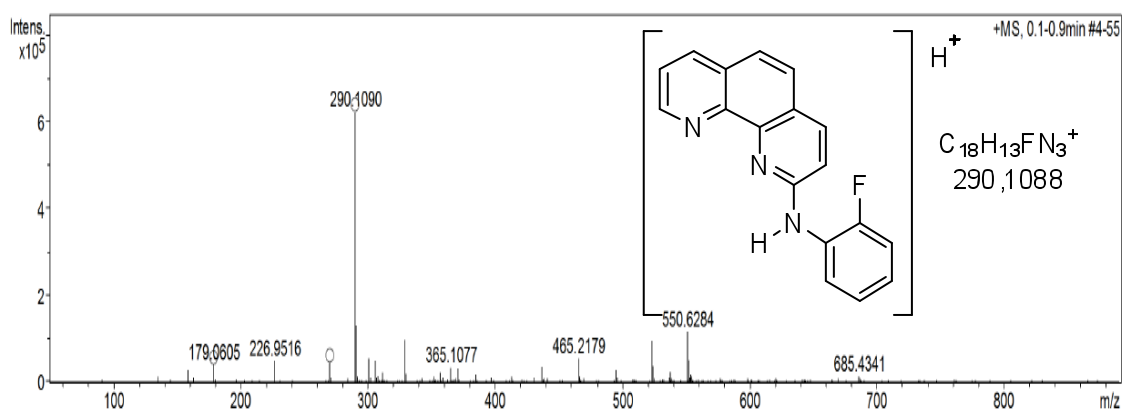
 SI Figure 68: HRMS of compound **3b**.

**Acquisition Parameter**

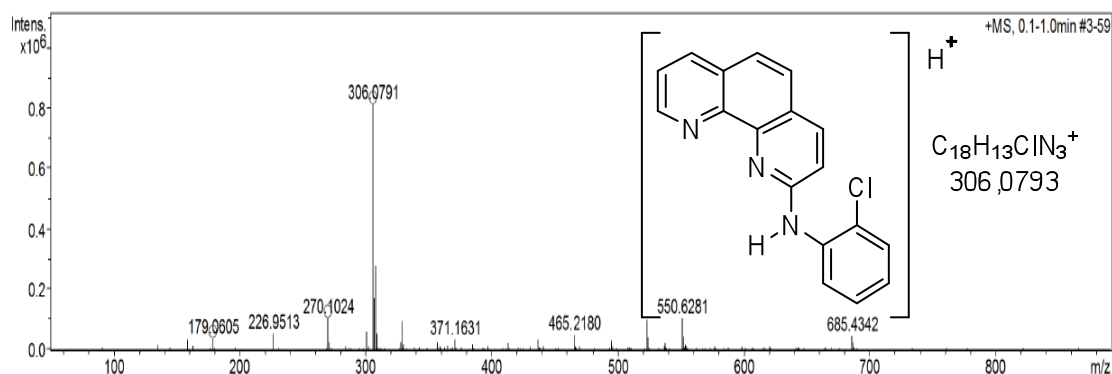
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	5.0 l/min
Scan End	896 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

SI Figure 69: HRMS of compound **3c****Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3800 V	Set Dry Gas	5.0 l/min
Scan End	890 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

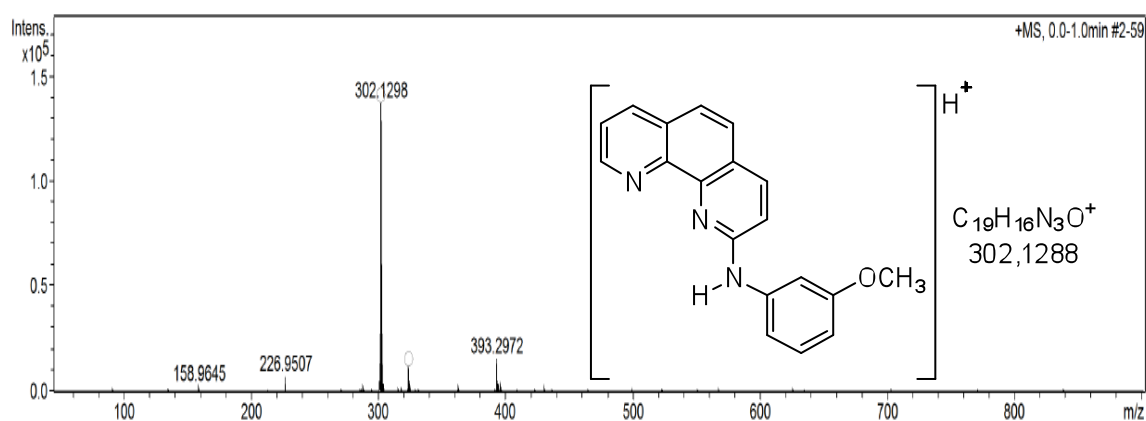
SI Figure 70: HRMS of compound **3d**

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3800 V	Set Dry Gas	5.0 l/min
Scan End	890 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



SI Figure 71: HRMS of compound **3e**

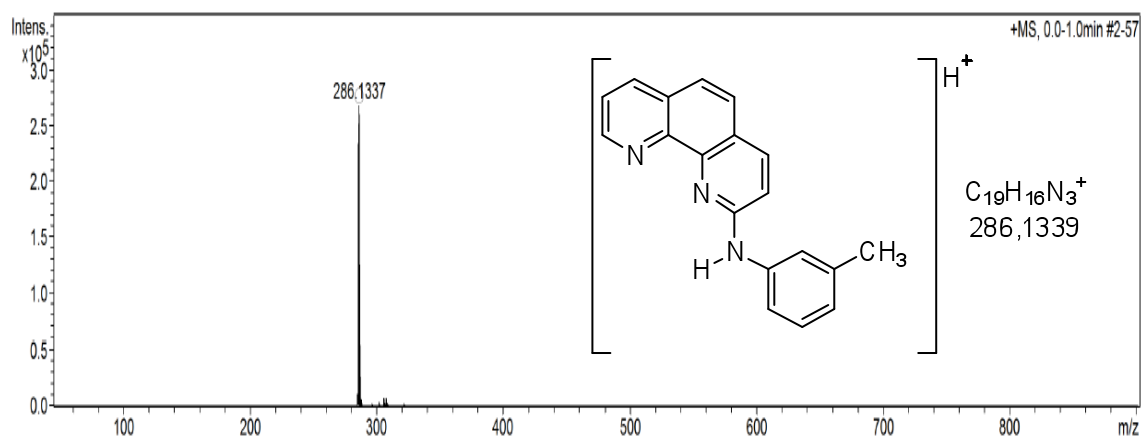
Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	5.0 l/min
Scan End	896 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



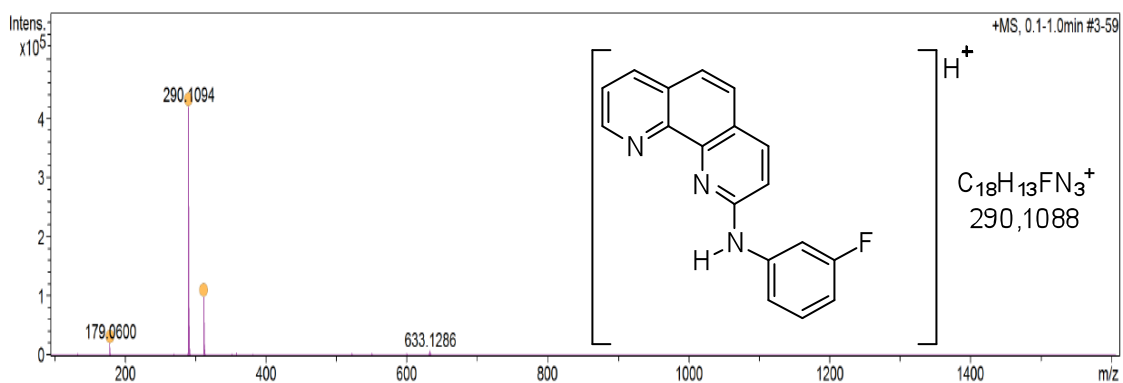
SI Figure 72: HRMS of compound **3f**

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	5.0 l/min
Scan End	896 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

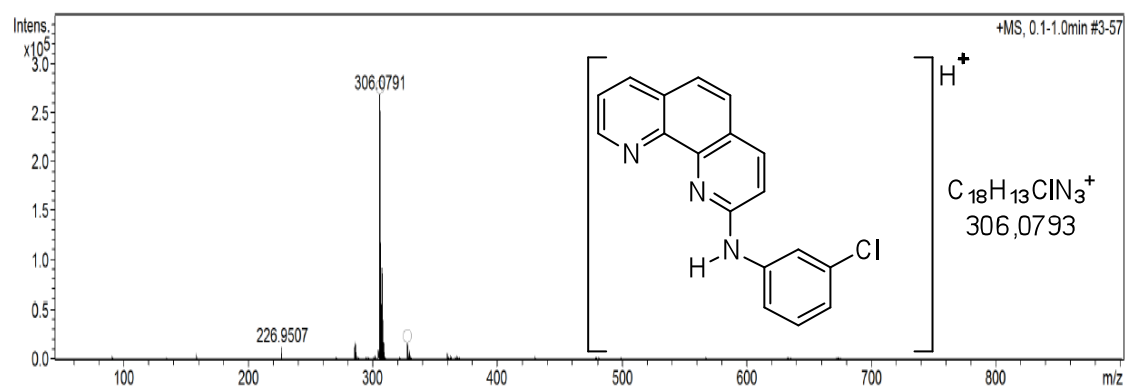
SI Figure 73: HRMS of compound **3g****Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	3500 V	Set Dry Gas	5.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

SI Figure 74: HRMS of compound **3h**

**Acquisition Parameter**

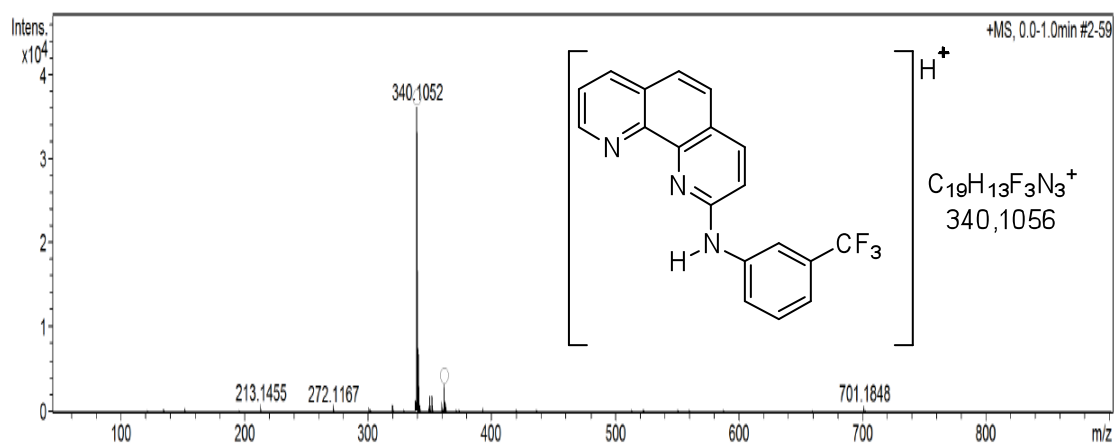
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	5.0 l/min
Scan End	896 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



SI Figure 75: HRMS of compound 3i

**Acquisition Parameter**

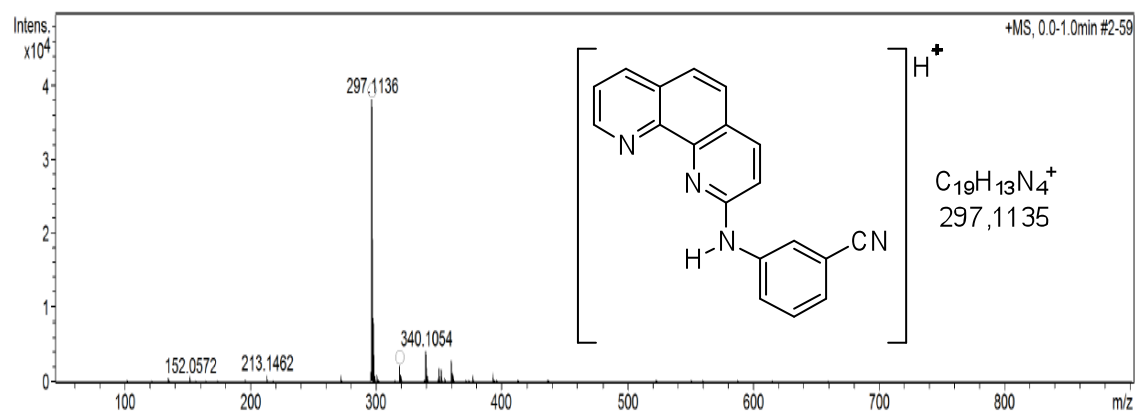
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	5.0 l/min
Scan End	896 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



SI Figure 76: HRMS of compound 3j

**Acquisition Parameter**

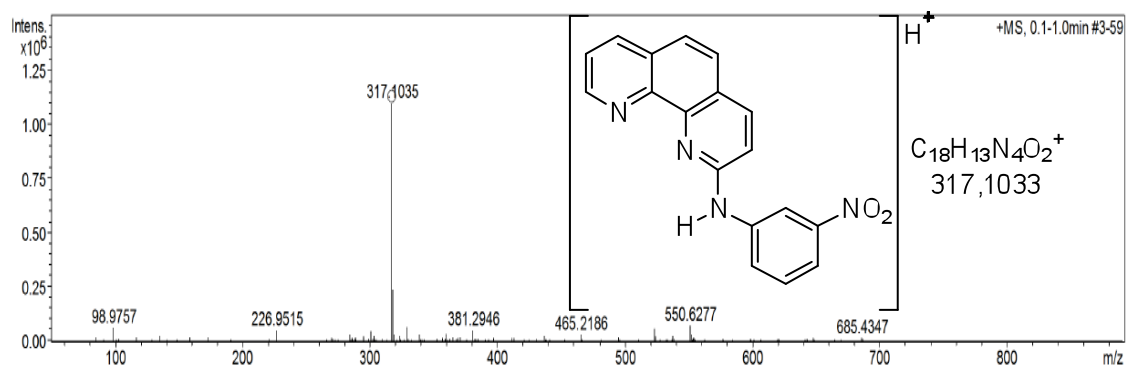
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	5.0 l/min
Scan End	896 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



SI Figure 77: HRMS of compound 3k

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3500 V	Set Dry Gas	5.0 l/min
Scan End	890 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

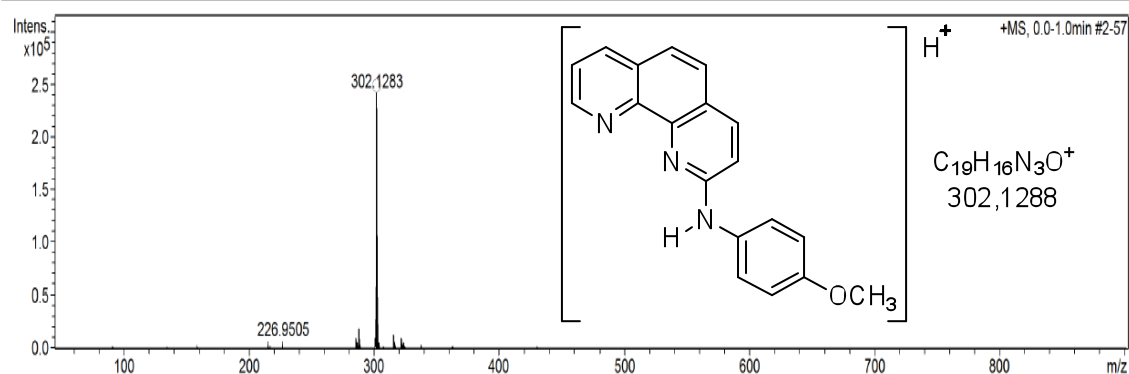


SI Figure 78: HRMS of compound 3l

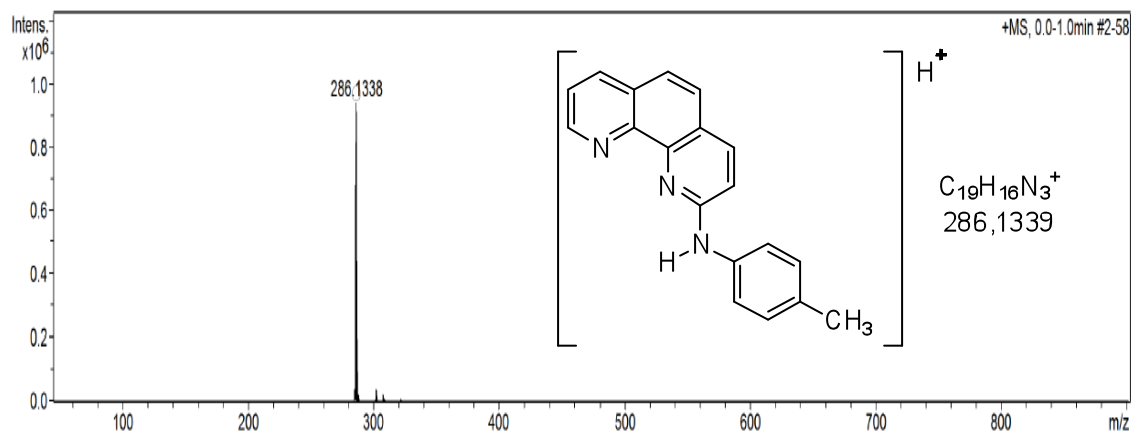


**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	5.0 l/min
Scan End	896 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

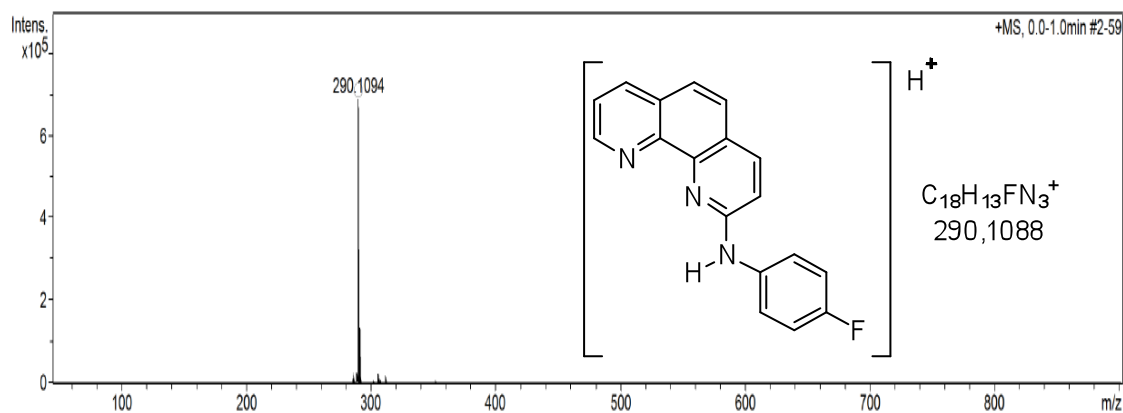
SI Figure 79: HRMS of compound **3m****Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	5.0 l/min
Scan End	896 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

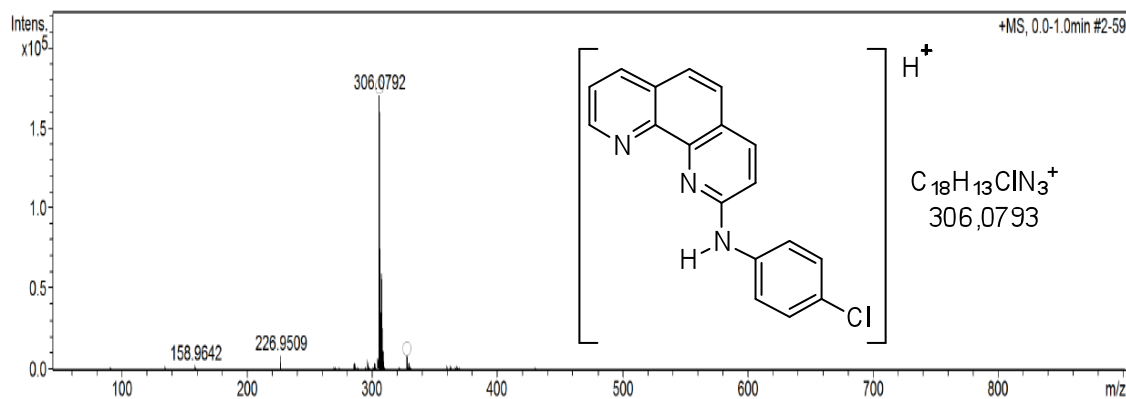
SI Figure 80: HRMS of compound **3n**

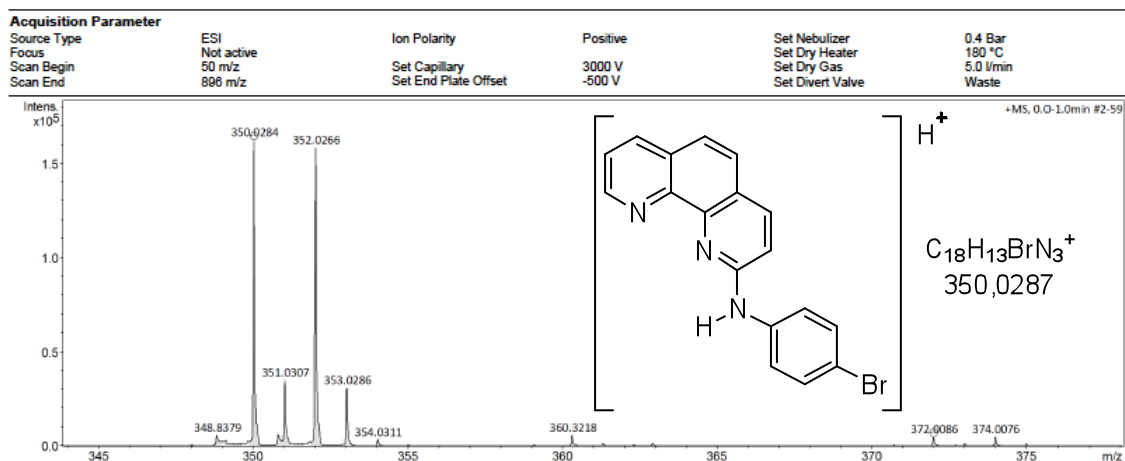
**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	5.0 l/min
Scan End	896 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

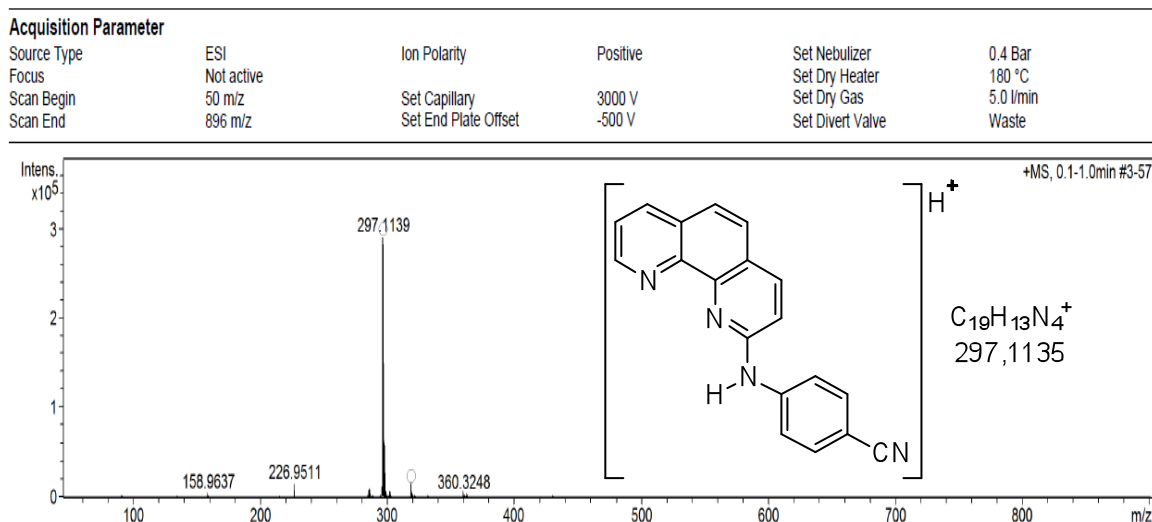
SI Figure 81: HRMS of compound **3o****Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3000 V	Set Dry Gas	5.0 l/min
Scan End	896 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

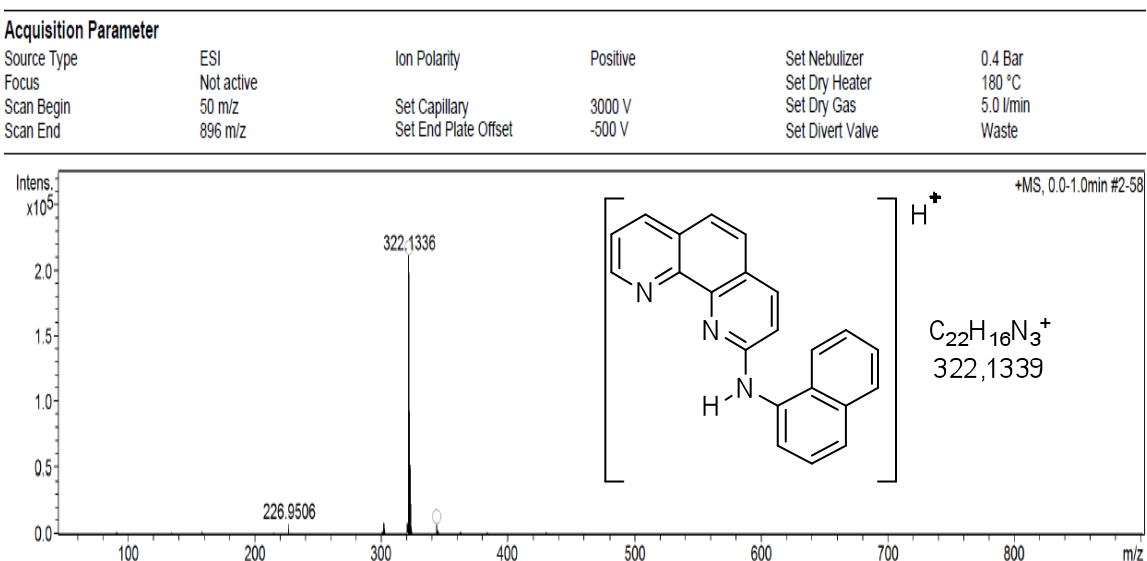
SI Figure 82: HRMS of compound **3p**



SI Figure 83: HRMS of compound **3q**



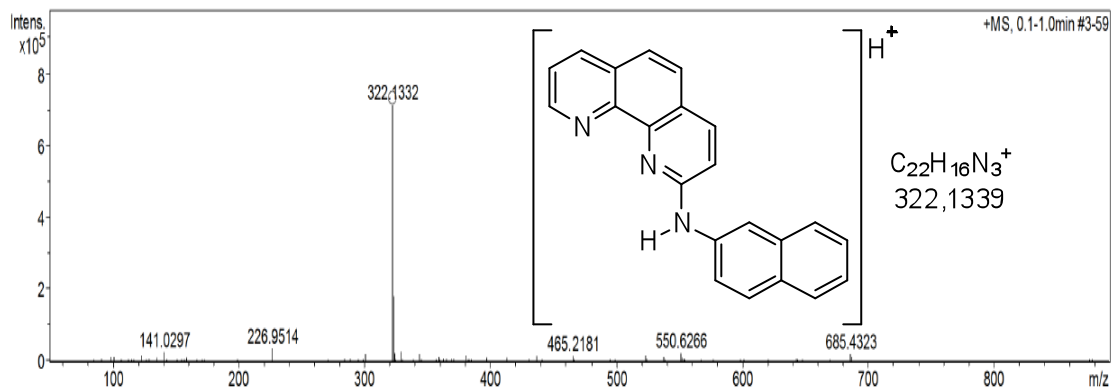
SI Figure 84: HRMS of compound **3r**



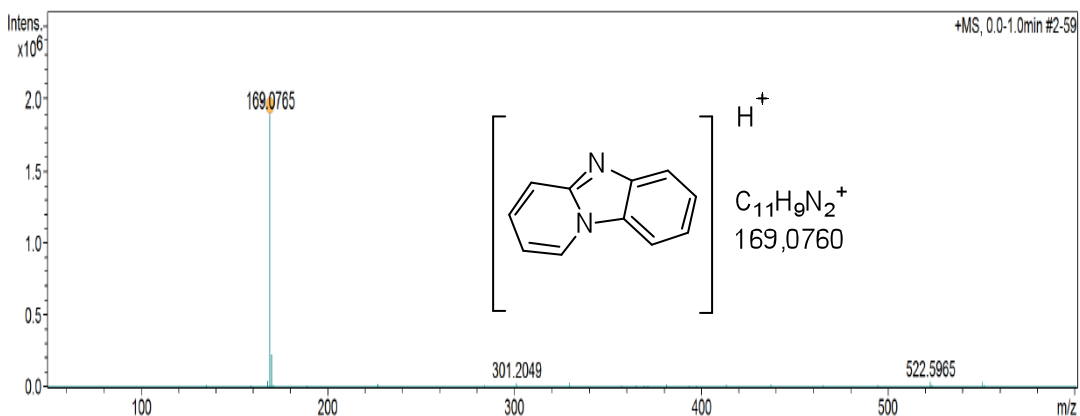
SI Figure 85: HRMS of compound **3s**

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3500 V	Set Dry Gas	5.0 l/min
Scan End	890 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

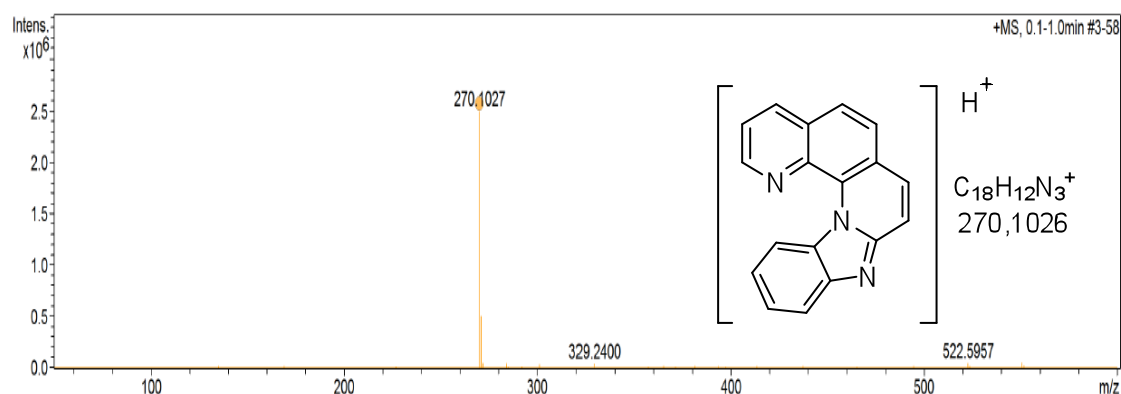
SI Figure 86: HRMS of compound **3t****Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

SI Figure 87: HRMS of compound **5**

**Acquisition Parameter**

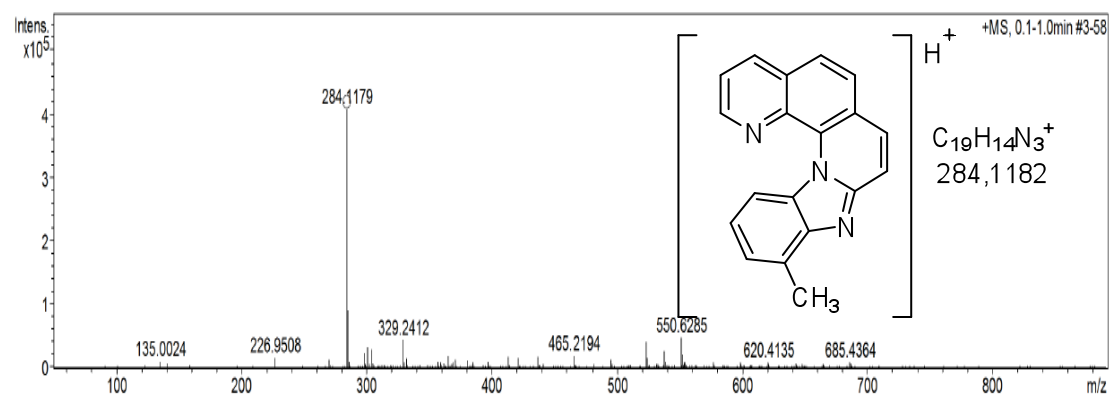
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



SI Figure 88: HRMS of compound 6a

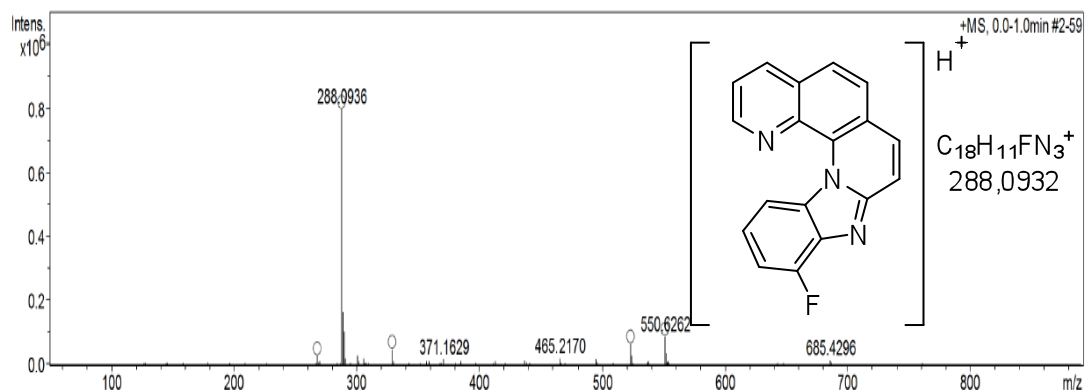
**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3500 V	Set Dry Gas	5.0 l/min
Scan End	890 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



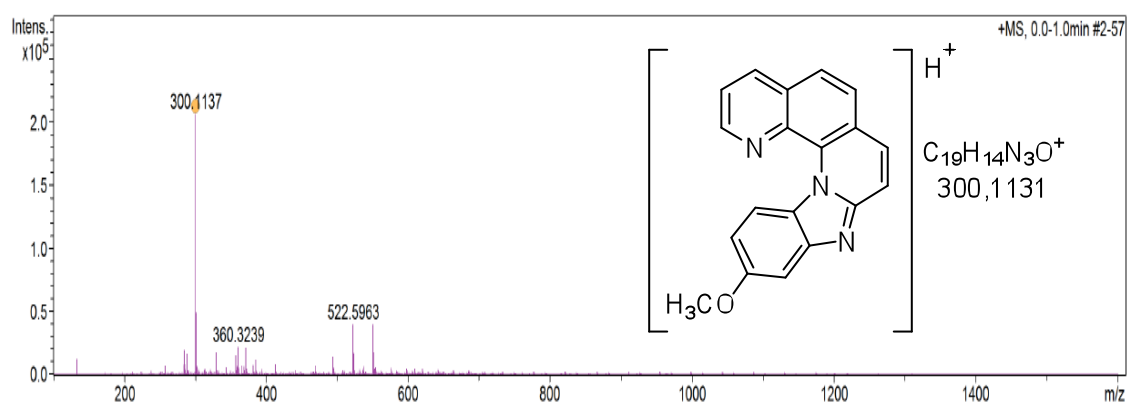
SI Figure 89: HRMS of compound 6c

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3800 V	Set Dry Gas	5.0 l/min
Scan End	890 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



SI Figure 90: HRMS of compound **6d**

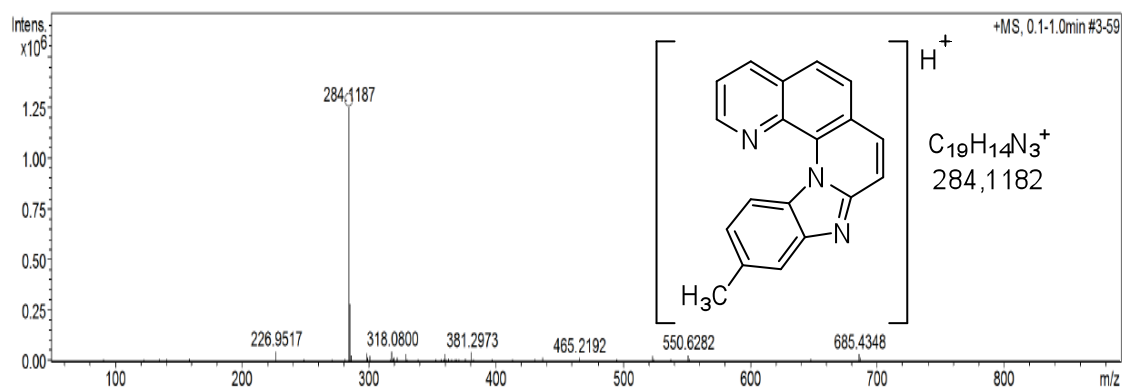
Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	3500 V	Set Dry Gas	5.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



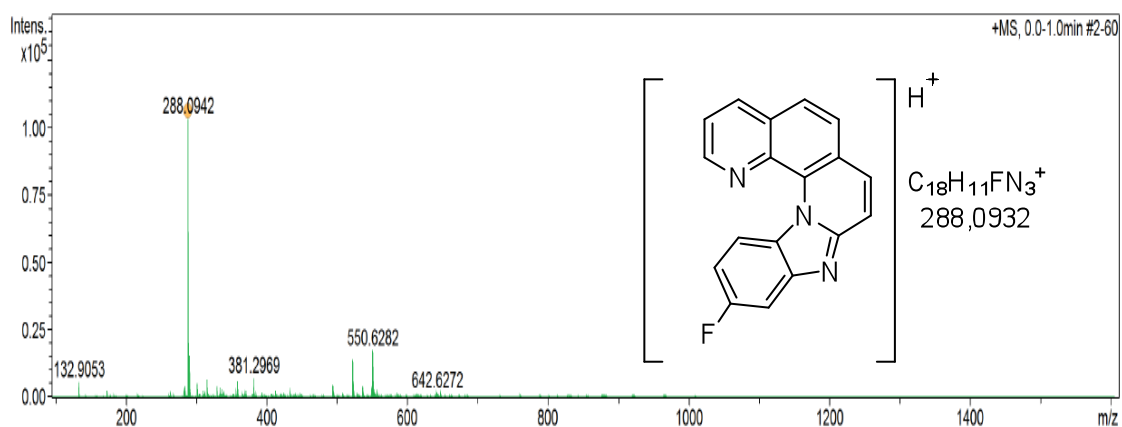
SI Figure 91: HRMS of compound **6f**

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3500 V	Set Dry Gas	5.0 l/min
Scan End	890 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

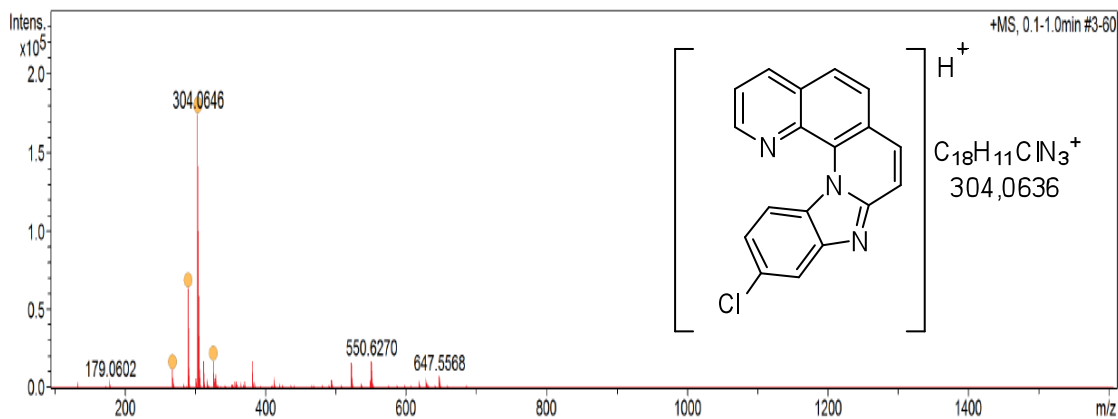
SI Figure 92: HRMS of compound **6g****Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	3500 V	Set Dry Gas	5.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

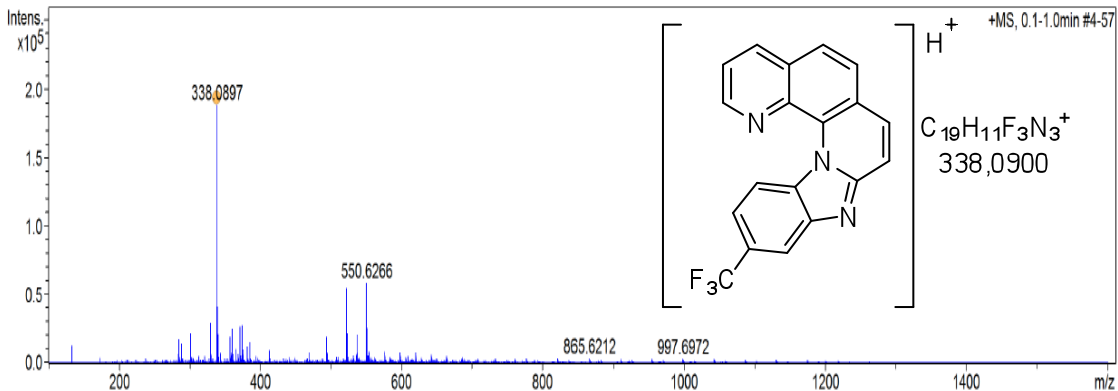
SI Figure 93: HRMS of compound **6h**

**Acquisition Parameter**

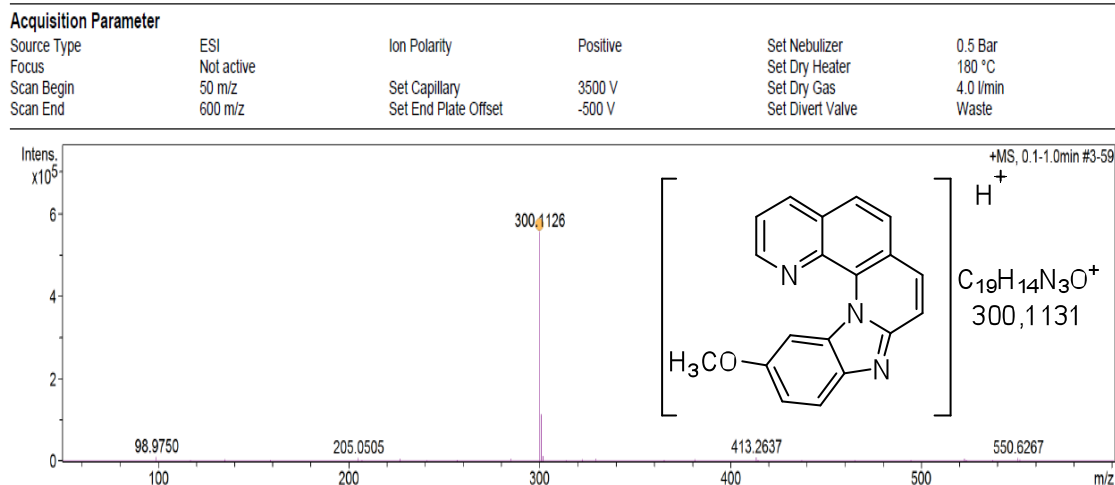
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	3500 V	Set Dry Gas	5.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

SI Figure 94: HRMS of compound **6i****Acquisition Parameter**

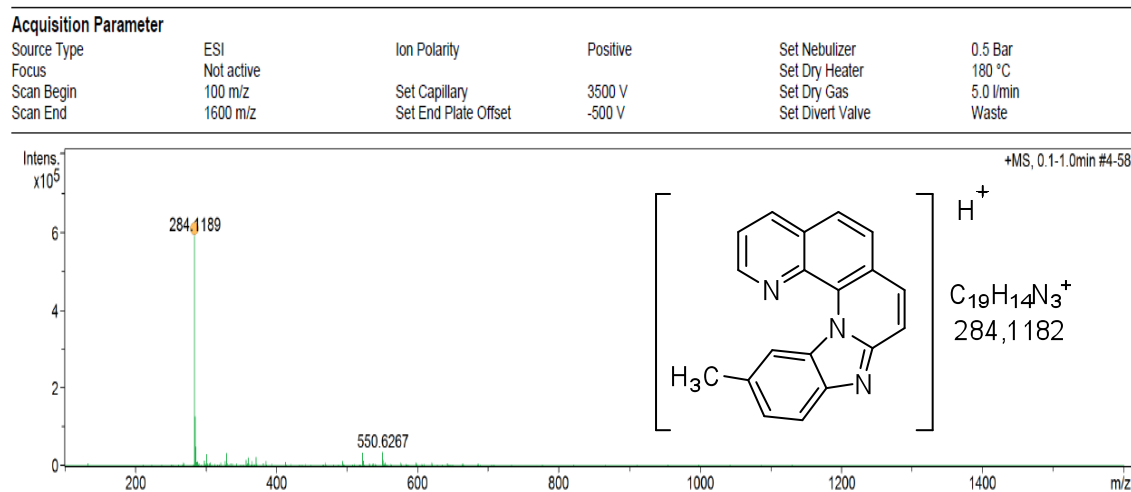
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	3500 V	Set Dry Gas	5.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

SI Figure 95: HRMS of compound **6j**





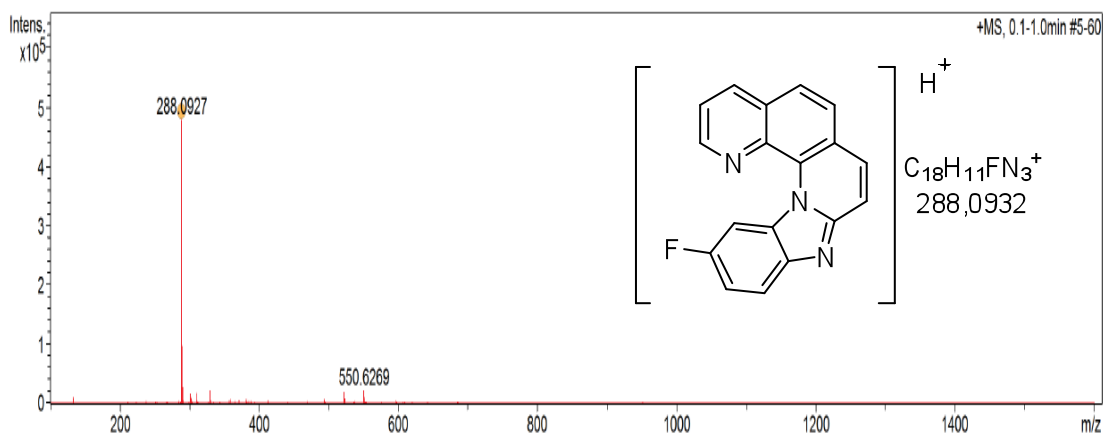
SI Figure 96: HRMS of compound **6m**



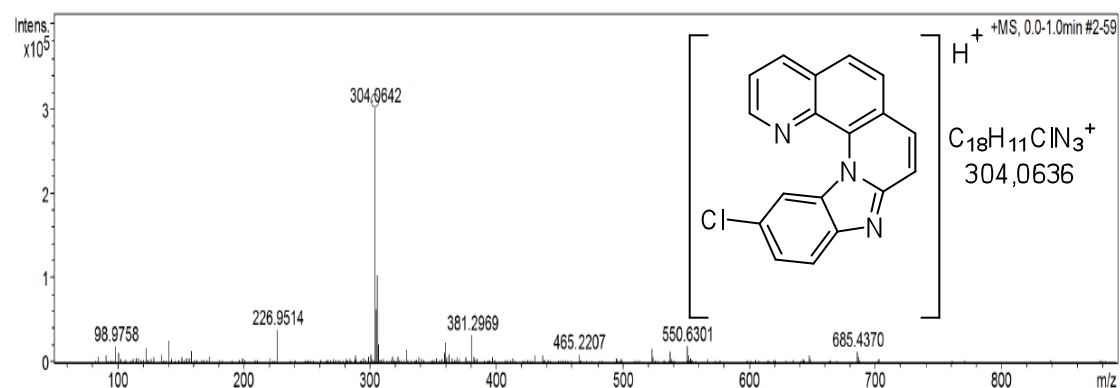
SI Figure 97: HRMS of compound **6n**

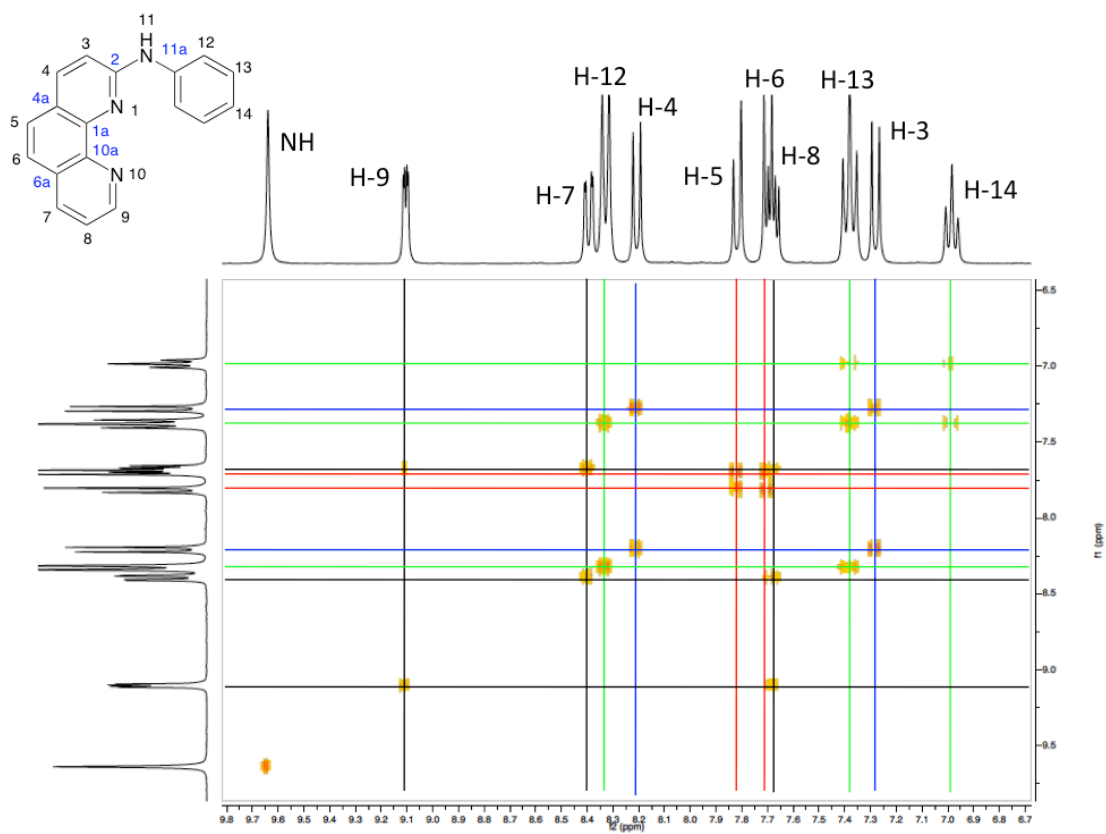
**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	3500 V	Set Dry Gas	5.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

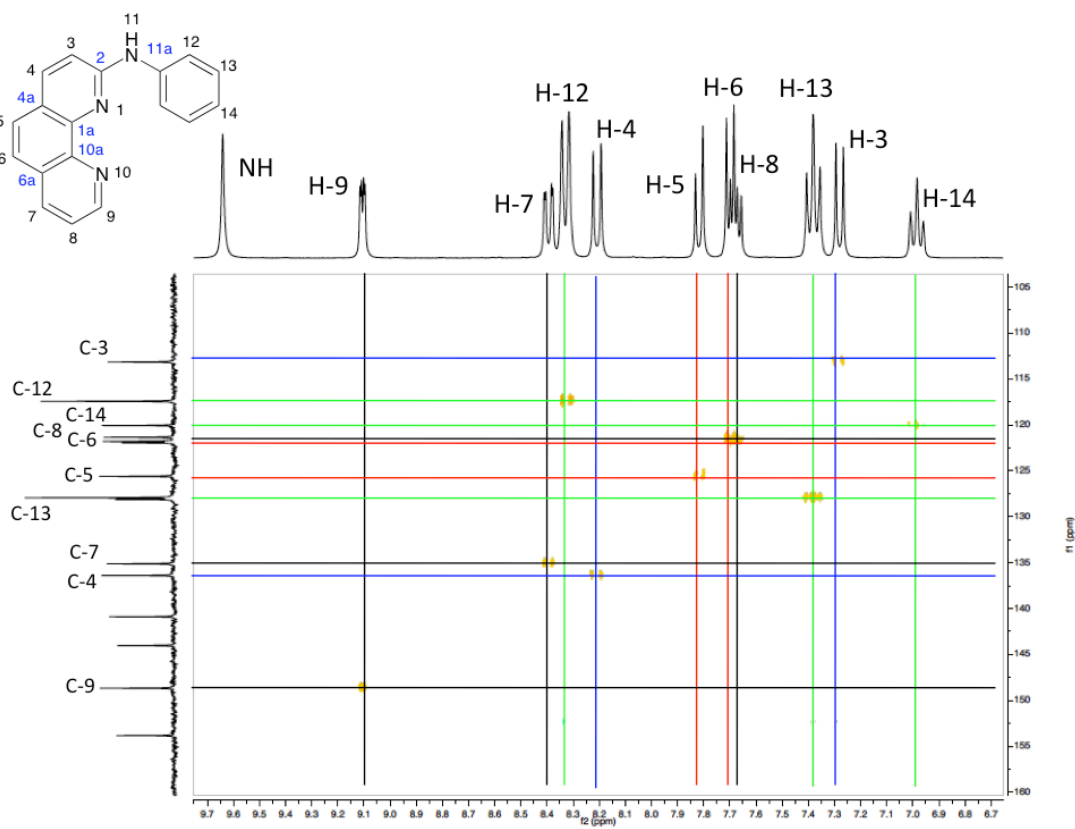
SI Figure 98: HRMS of compound **6o****Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	3500 V	Set Dry Gas	5.0 l/min
Scan End	890 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

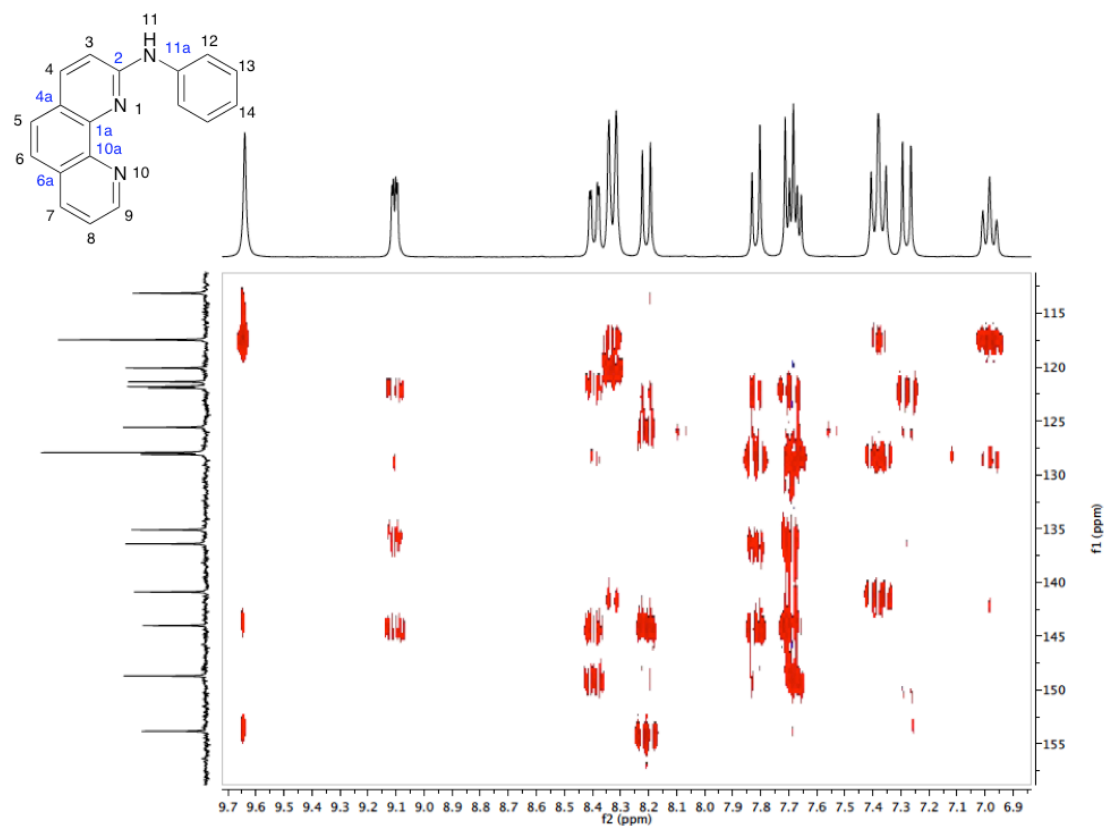
SI Figure 99: HRMS of compound **6p**



SI Figure 100: COSY spectrum of *N*-phenyl-1,10-phenanthroline (**3a**)



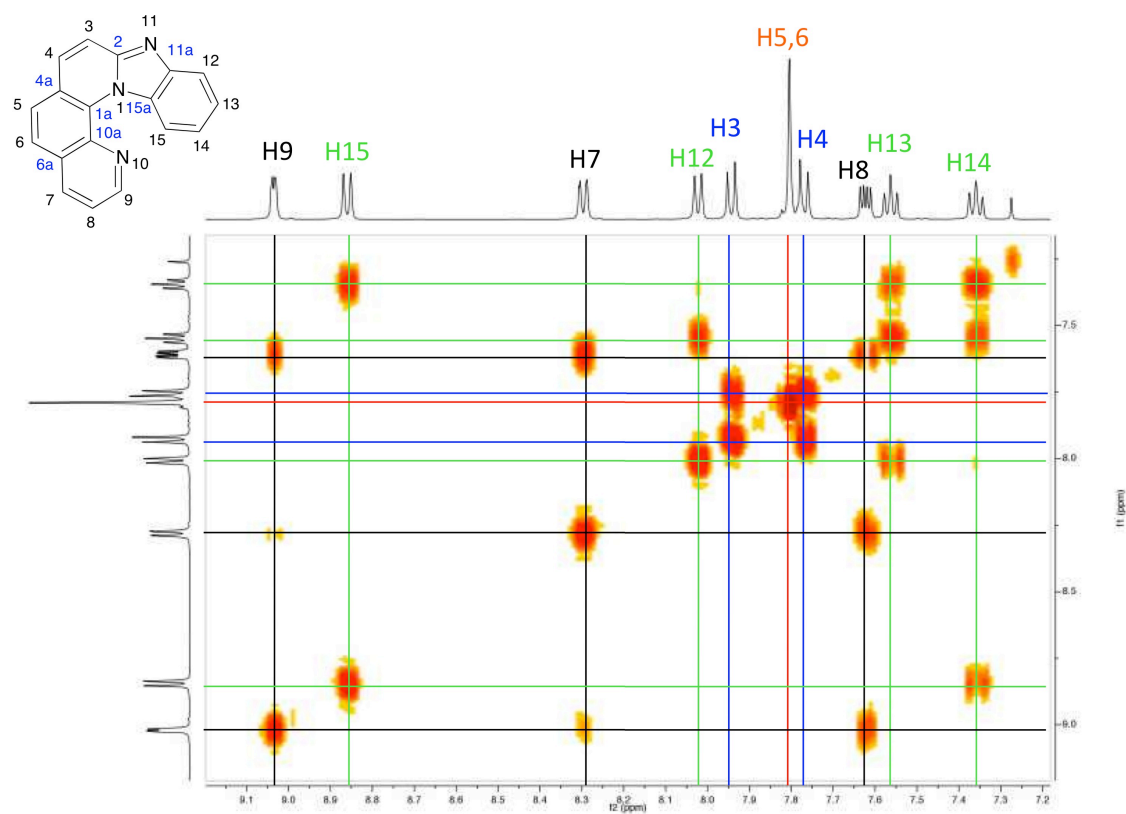
SI Figure 101: HMBC spectrum of *N*-phenyl-1,10-phenanthroline (**3a**)



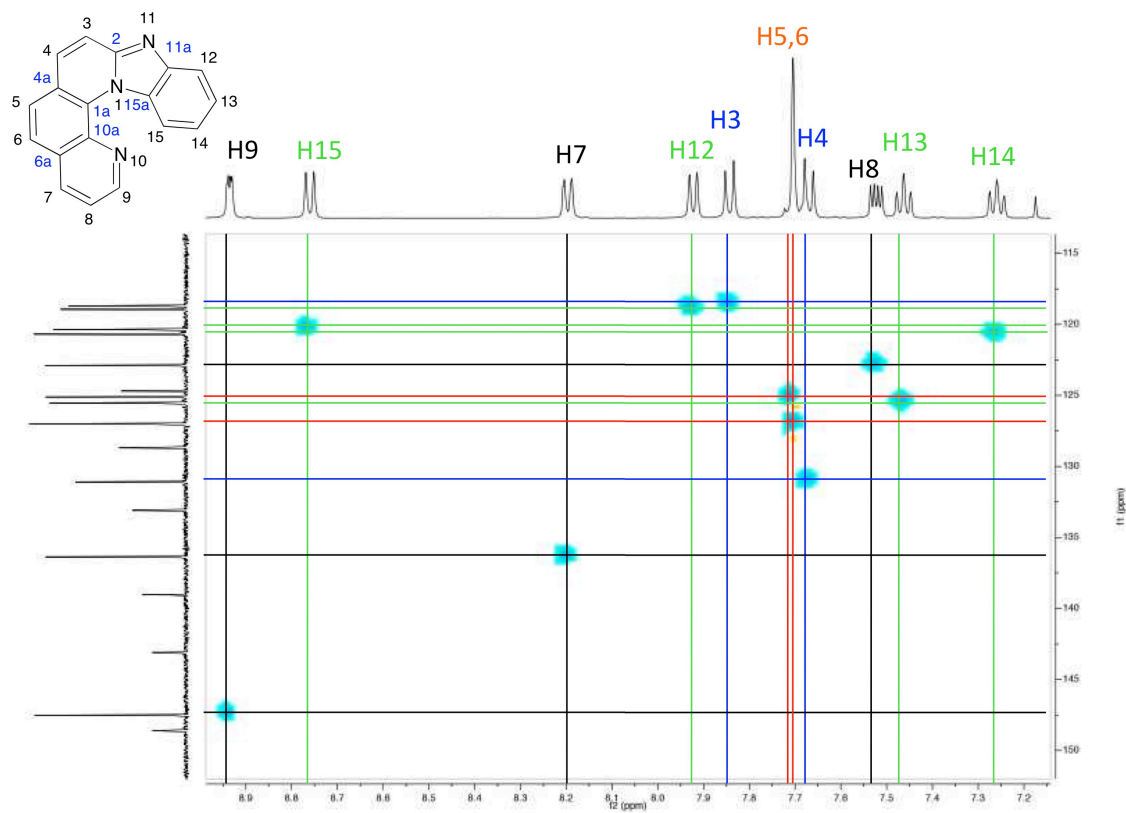
SI Figure 102: HMBC spectrum of *N*-phenyl-1,10-phenanthroline (**3a**)

SI Table 1. Heteronuclear multiple bond correlations (HMBC)

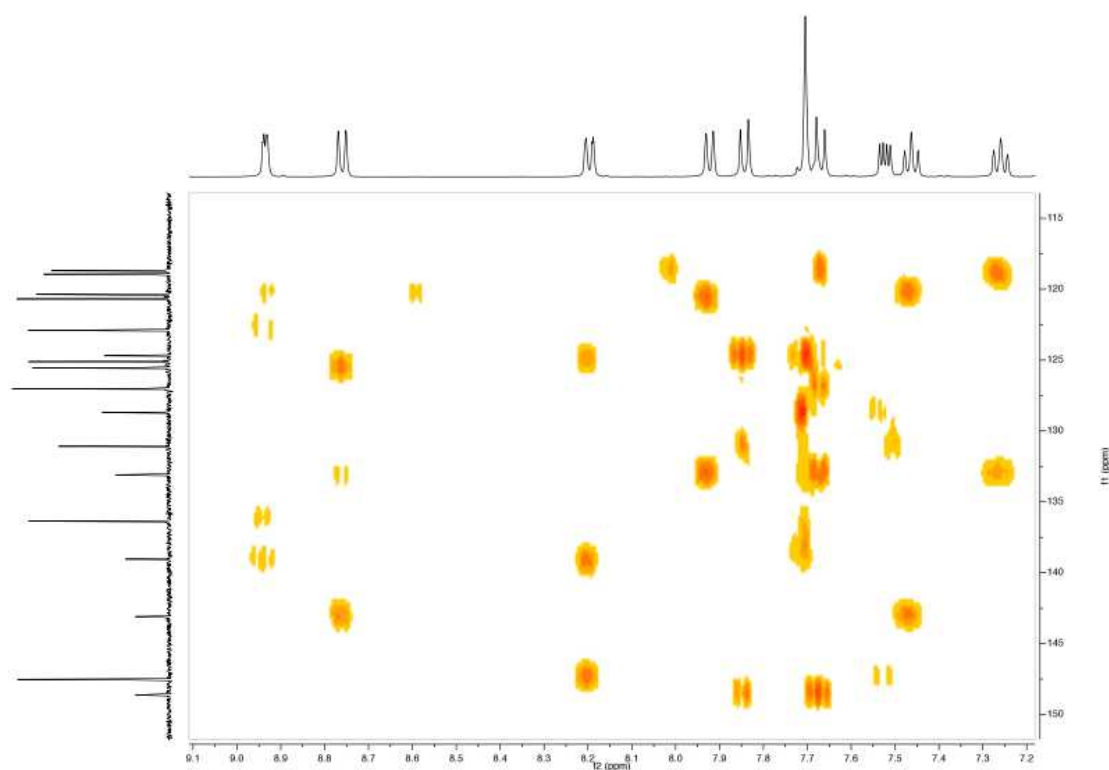
	<sup>1</sup> H NMR	NH	H9	H7	H12	H4	H5	H6	H8	H13	H3	H14
<sup>13</sup> C NMR	δ	9.63	9.09	8.38	8.32	8.20	7.81	7.70	7.68	7.37	7.27	6.97
C3	113.94	<sup>3</sup> J										
C12	118.26	<sup>3</sup> J								<sup>2</sup> J		<sup>3</sup> J
C14	120.87				<sup>3</sup> J							
C8	122.17		<sup>2</sup> J									
C6	122.61			<sup>3</sup> J								
C4a	122.76						<sup>2</sup> J	<sup>3</sup> J				<sup>3</sup> J
C5	126.40					<sup>3</sup> J						
C13	128.83											<sup>2</sup> J
C6a	128.92		<sup>4</sup> J	<sup>2</sup> J			<sup>3</sup> J		<sup>3</sup> J			
C7	135.92		<sup>3</sup> J									
C4	137.22						<sup>3</sup> J	<sup>4</sup> J W				
C11a	141.68				<sup>2</sup> J					<sup>3</sup> J		
C10a/C1a	144.81	<sup>4</sup> J W	<sup>3</sup> J	<sup>3</sup> J		<sup>3</sup> J	<sup>3</sup> J	<sup>3</sup> J				
C9	149.49			<sup>3</sup> J					<sup>2</sup> J			
C2	154.62	<sup>3</sup> J				<sup>3</sup> J						



SI Figure 103: COSY spectrum of benzo[4,5]imidazo[1,2-*a*][1,10]phenanthroline (**6a**).



SI Figure 104: HMBC spectrum of benzo[4,5]imidazo[1,2-*a*][1,10]phenanthroline (**6a**).



SI Figure 105: HMBC spectrum of benzo[4,5]imidazo[1,2-*a*][1,10]phenanthroline (**6a**).

SI Table 2. Heteronuclear multiple bond correlations (HMBC).

	<sup>1</sup> H	H9	H15	H7	H12	H3	H5,6	H4	H8	H13	H14
<sup>13</sup> C	δ	9.02	8.85	8.28	8.01	7.93	7.79	7.75	7.61	7.55	7.34
C3	118.70							<sup>2</sup> J			
C12	118.94										<sup>3</sup> J
C15	120.37									<sup>3</sup> J	
C14	120.69				<sup>3</sup> J						
C8	122.89	<sup>2</sup> J									
C4a	124.69					<sup>3</sup> J	<sup>3</sup> J				
C6	125.11			<sup>3</sup> J							
C13	125.54		<sup>3</sup> J								
C5	127.01							<sup>3</sup> J			
C6a	128.69						<sup>3</sup> J		<sup>3</sup> J		
C4	131.09					<sup>2</sup> J	<sup>3</sup> J				
*C1a,	133.08		<sup>4</sup> JU1a				<sup>3</sup> J1a	<sup>3</sup> J1a			
C15a	133.10				<sup>3</sup> J15a						<sup>3</sup> J15a
C7	136.36	<sup>3</sup> J									
C10a	139.04	<sup>3</sup> J		<sup>3</sup> J			<sup>3</sup> J				
C11a	143.09		<sup>3</sup> J							<sup>3</sup> J	
C9	147.52			<sup>3</sup> J					<sup>2</sup> J		
C2	148.61					<sup>2</sup> J		<sup>3</sup> J			

\* Not possible to distinguish between C1a and C15a. The <sup>13</sup>C resonances are arbitrarily assigned.

*Theoretical calculations*

SI Table 3. Calculated energies of **6a** (energy minimum) and **6aTS**, the transition state leading to chirality inversion. [B3LYP/6-31+G(d)]

	<b>6a</b>	<b>6aTS</b> (-45 cm <sup>-1</sup> )*
Total Electronic Energy=	-856.8458656	-856.843579
Zero-point correction=	0.246505	0.246395
Thermal correction to Energy=	0.260234	0.259354
Thermal correction to Enthalpy=	0.261178	0.260299
Thermal correction to Gibbs Free Energy=	0.206062	0.207156
Sum of electronic and zero-point Energies=	-856.599361	-856.597184
Sum of electronic and thermal Energies=	-856.585632	-856.584225
Sum of electronic and thermal Enthalpies=	-856.584688	-856.58328
Sum of electronic and thermal Free Energies=	-856.639804	-856.636423

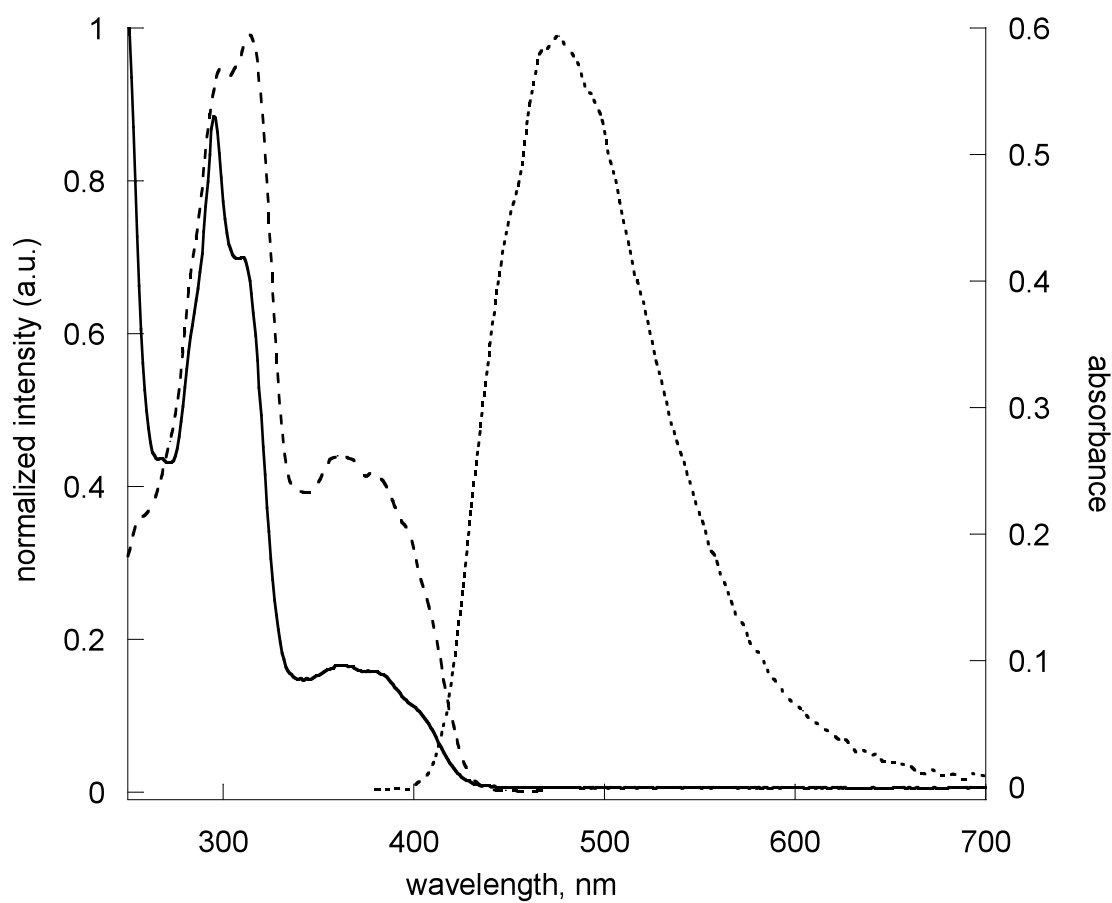
\* imaginary vibration (an in and out of molecular plane wagging motion of the “arms” of the structure giving rise to either of the enantiomers).

*Coordinates for the structures 6a and 6aTS*

	Compound <b>6a</b>			Compound <b>6aTS</b>		
C	-3.195973	-2.669596	-0.350474	3.286087	-2.686682	0.000004
C	-3.757723	-1.476002	0.046343	3.839769	-1.426553	-0.000258
C	-2.949392	-0.32014	0.171633	3.008977	-0.280178	-0.000256
C	-1.54167	-0.46402	-0.066438	1.583439	-0.474693	0.000103
C	-1.810074	-2.68994	-0.625109	1.878869	-2.776793	0.00048
C	-3.504531	0.958625	0.453152	3.567055	1.024235	-0.000389
C	-0.687384	0.693912	0.053065	0.698803	0.675386	-0.0002
C	-1.295702	1.963499	0.182511	1.310181	1.956929	-0.000245
C	-2.700062	2.062617	0.416106	2.729949	2.099143	-0.00038
C	-0.523155	3.164629	0.015293	0.536506	3.165402	0.000096
H	-1.032516	4.121026	0.096076	1.063507	4.11525	0.000023
C	0.798503	3.10252	-0.290965	-0.815128	3.114069	0.00043
C	1.454626	1.839941	-0.309697	-1.465253	1.852501	0.000432
H	-4.571621	1.047411	0.640558	4.647069	1.146375	-0.000708
H	-3.792326	-3.569572	-0.468232	3.898613	-3.583322	-0.000121
H	-4.824419	-1.396347	0.244114	4.918613	-1.287809	-0.000605
H	-1.335428	-3.605372	-0.977281	1.392976	-3.752804	0.0009
H	-3.12037	3.054994	0.558987	3.130744	3.109396	-0.000527
H	1.406968	3.982003	-0.470132	-1.448991	3.993641	0.000712
C	2.924765	0.297054	-0.186832	-2.963392	0.339435	-0.000182
C	4.14192	-0.403361	-0.120839	-4.207019	-0.31498	-0.000601
C	1.677205	-1.686206	0.529632	-1.773091	-1.784924	0.000311
C	4.114757	-1.732036	0.273007	-4.225266	-1.699027	-0.000538
H	5.069353	0.112321	-0.351618	-5.116058	0.279094	-0.000883
C	2.894056	-2.355691	0.612601	-3.012594	-2.417445	0.000014

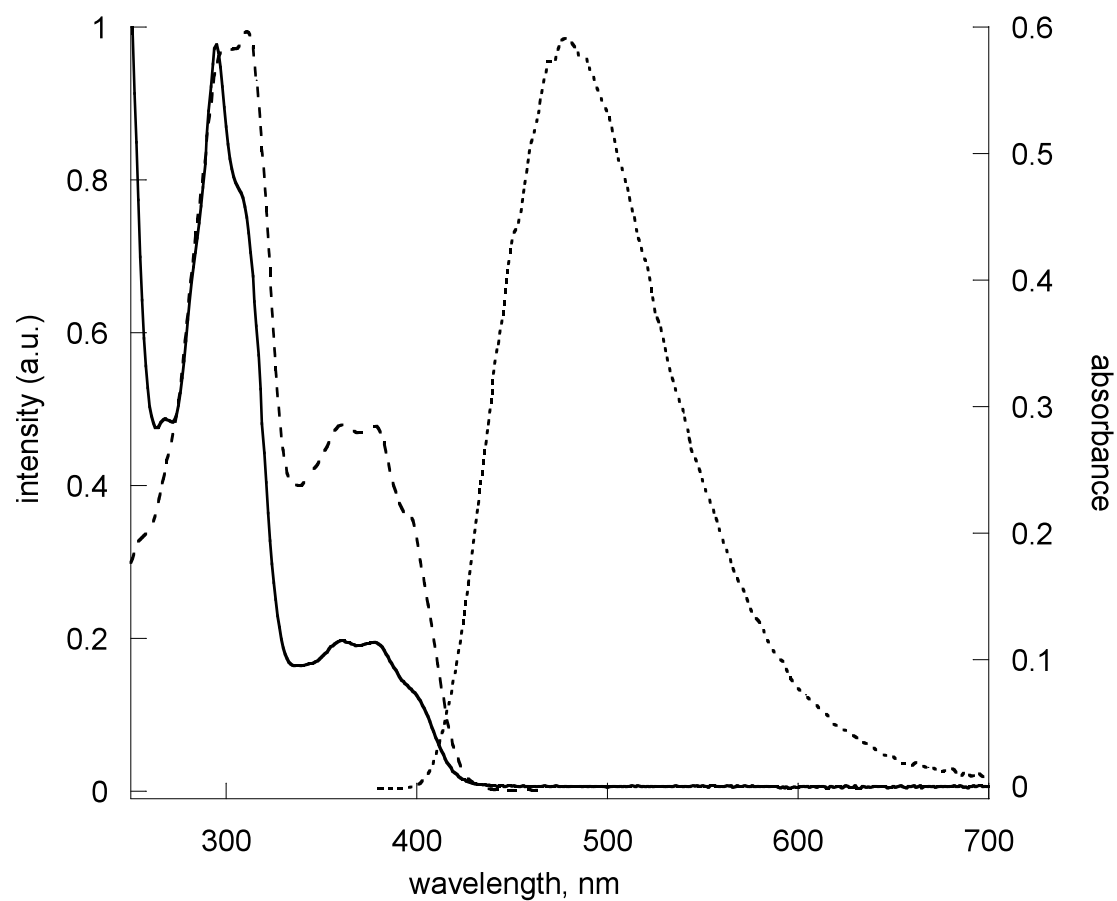
H	0.75909	-2.187768	0.791355	-0.865794	-2.360235	0.000474
H	5.040964	-2.296737	0.342265	-5.171224	-2.23452	-0.000826
H	2.899461	-3.388639	0.950866	-3.035729	-3.504344	0.000075
N	2.748953	1.637408	-0.430735	-2.767643	1.693537	-0.000073
N	-1.016853	-1.644312	-0.480993	1.076703	-1.729212	0.000525
N	0.712971	0.654227	-0.048028	-0.721136	0.62894	0.000576
C	1.690724	-0.353235	0.090567	-1.732756	-0.378088	0.000227

*Absorption, emission and excitation spectra of 6a in different solvents.*

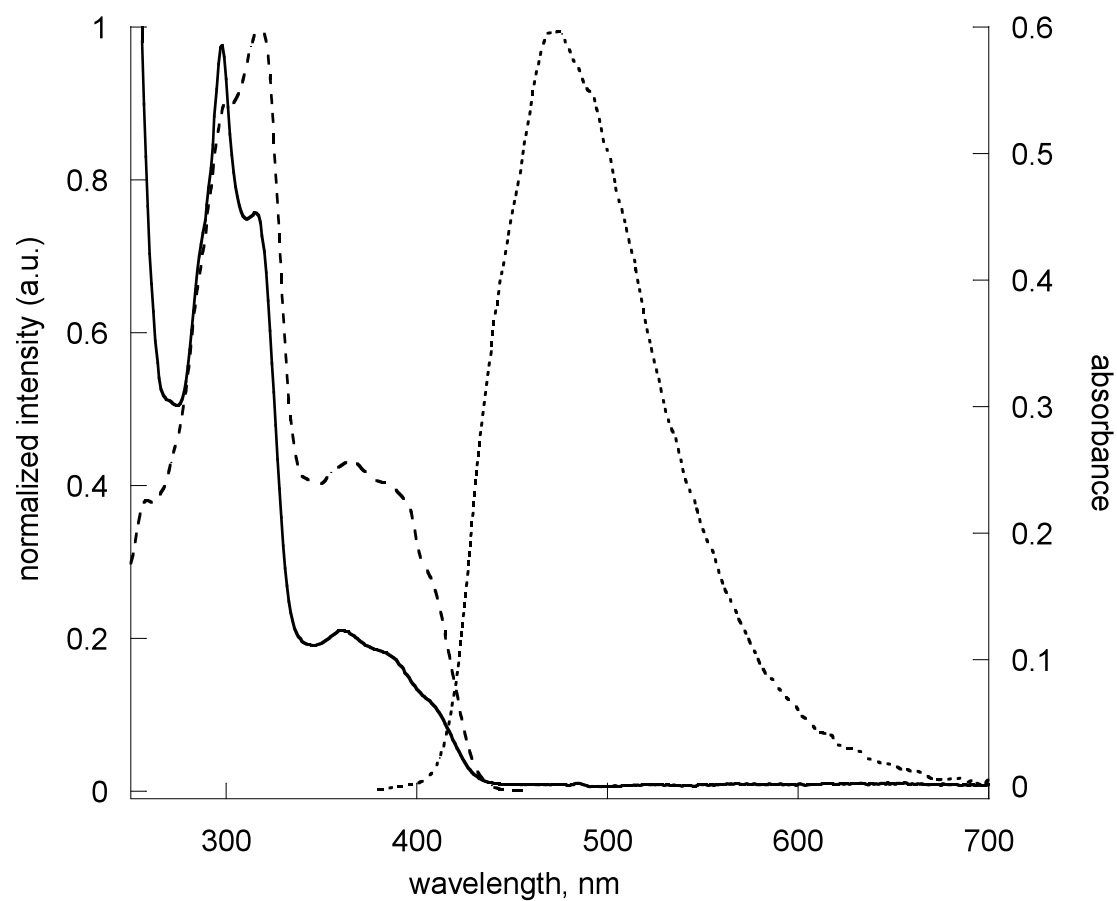


SI Figure 106: Normalized absorption spectra (—), excitation (---) and emission (···) of **6a** in acetonitrile.





SI Figure 107: Normalized Absorption (—), excitation (---) and emission spectra (···) of **6a** in methanol.



SI Figure 108: Normalized absorption (—), excitation (---) and emission spectra (···) of **6a** in dichloromethane.

## Crystallography experimental and details

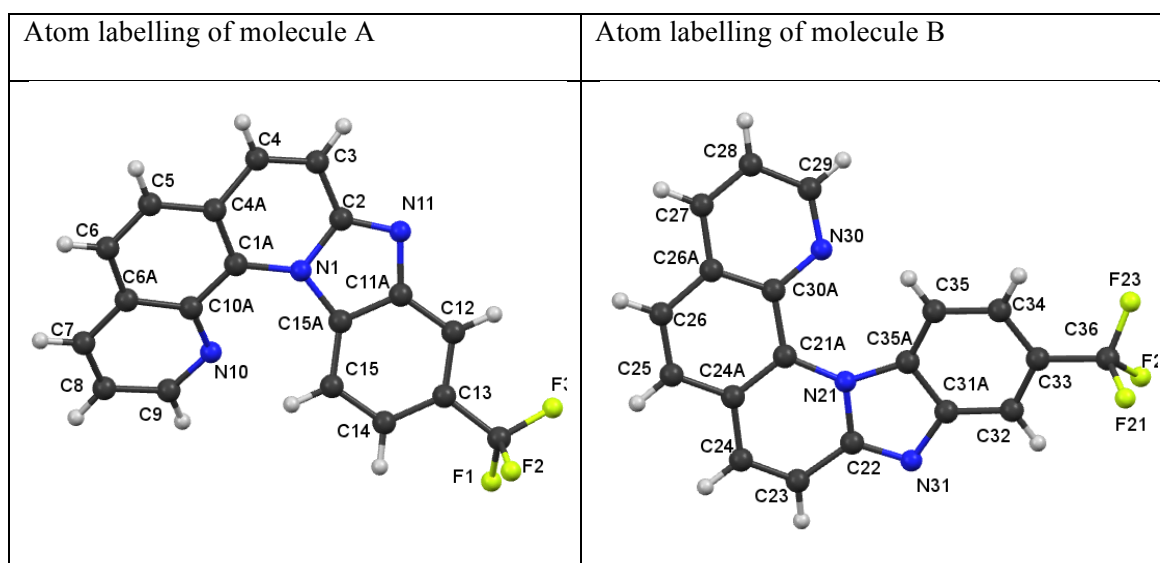
Data for compound **6j** were obtained with Mo-K $\alpha$  radiation at 100(2) K by means of a XtaLAB AFC12 (RCD3): Kappa single diffractometer by the NCS crystallographic service, based at the University of Southampton. Data collection, data reduction and unit cell refinement were achieved with CrysAlisPro 1.171.39.9g.<sup>(1)</sup> Correction for absorption was achieved by CrysAlisPro 1.171.39.9g<sup>(1)</sup> Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The program MERCURY<sup>(2)</sup> were used in the preparation of the Figures. SHELXL97<sup>(3)</sup> and PLATON<sup>(4)</sup> were used in the calculation of molecular geometry. The structures were solved by direct methods using SHELXS-97<sup>(3)</sup> and fully refined by means of the program SHELXL-97.<sup>(3)</sup> All hydrogen atoms were placed in calculated positions.

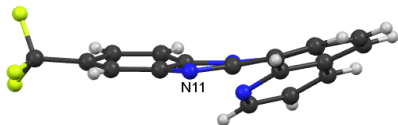
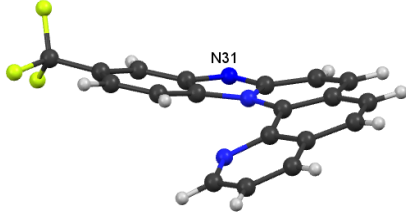
## References

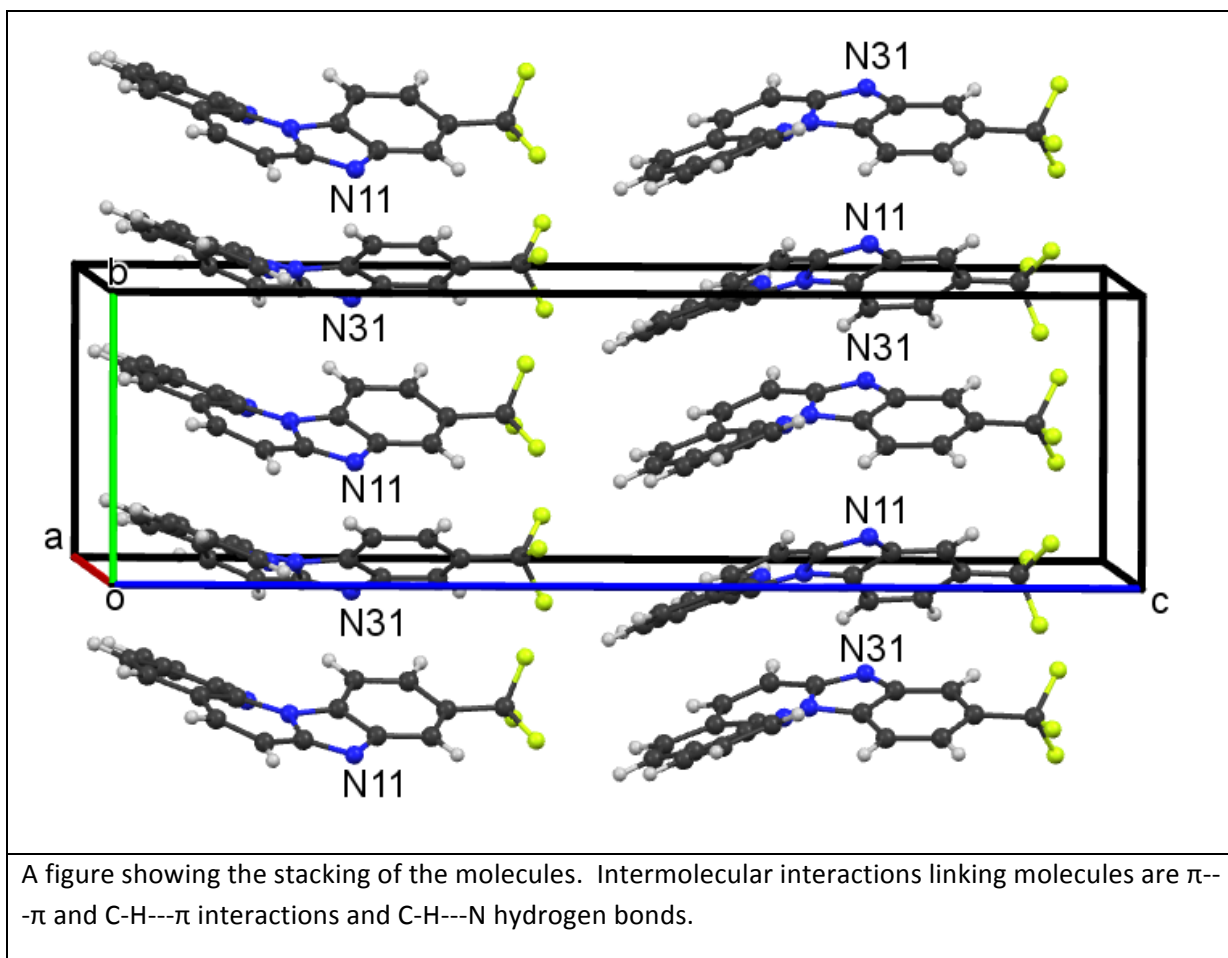
1. CrysAlisPro 1.171.39.9g Rigaku Oxford Diffraction, 2015.
2. MERCURY 3.9 Cambridge Crystallographic Data Centre: Cambridge, UK.
3. Sheldrick, G.M. A short history of SHELX. *Acta Crystallogr. Sect. A Found. Crystallogr.* **2008**, *64*, 112–122.
4. Spek, A.L. Single-crystal structure validation with the program PLATON. *J. Appl. Crystallogr.* **2003**, *36*, 7–13.

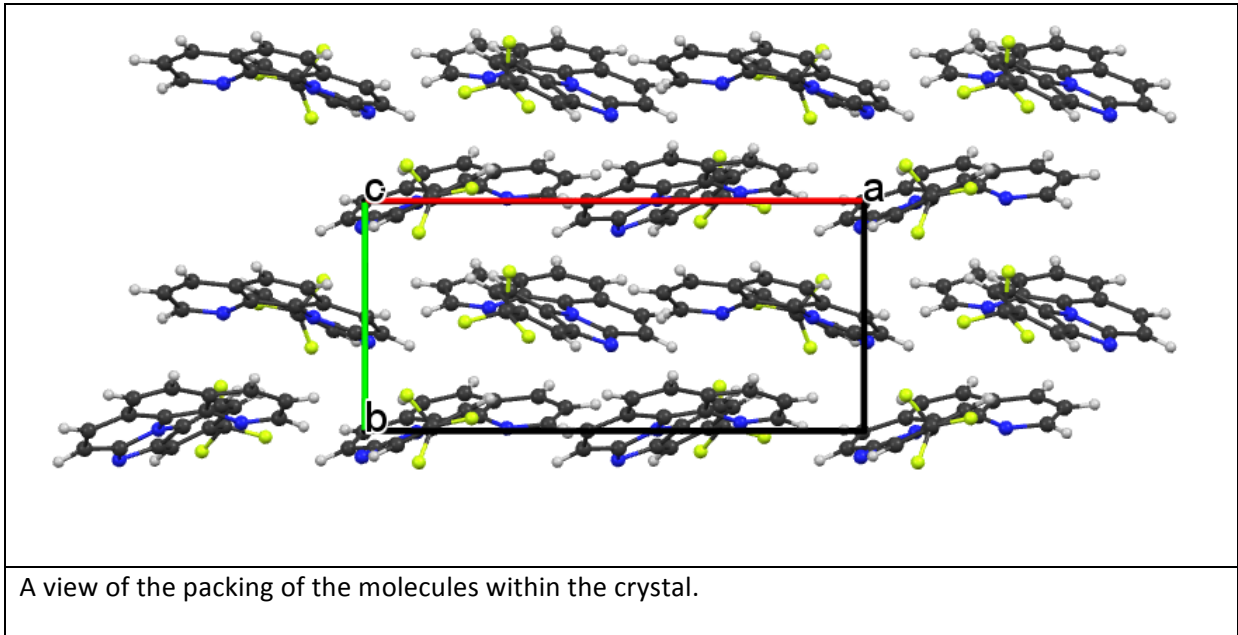
SI Table 4. Crystal data and structure refinement for **6j**.

Identification code	Compound <b>6j</b> , CCDC 1520619
Empirical formula	C <sub>38</sub> H <sub>20</sub> F <sub>6</sub> N <sub>6</sub> (pair of enantiomers)
Formula weight	674.60
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 15.7235(4) Å alpha = 90 deg b = 7.2386(2) Å beta = 96.401(3) deg c = 25.4616(7) Å gamma = 90 deg
Volume	2879.87(14) Å <sup>3</sup>
Z	4
Density (calculated)	1.556 Mg/m <sup>3</sup>
Absorption coefficient	0.122 mm <sup>-1</sup>
F(000)	1376
Crystal size	0.070 x 0.050 x 0.020 mm
Theta range for data collection	2.927 to 27.484 deg.
Index ranges	-18 ≤ h ≤ 20; -9 ≤ k ≤ 9; -33 ≤ l ≤ 23
Reflections collected	22616
Independent reflections	6501 [R(int) = 0.0329]
Reflections observed (>2σ)	5111
Data Completeness	0.983
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.66434
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	6501 / 0 / 451
Goodness-of-fit on F <sup>2</sup>	1.062
Final R indices [I > 2σ(I)]	R <sub>1</sub> = 0.0532 wR <sub>2</sub> = 0.1128
R indices (all data)	R <sub>1</sub> = 0.0738 wR <sub>2</sub> = 0.1223
Largest diff. peak and hole	0.382 and -0.252 e.Å <sup>-3</sup>



Molecule A	Molecule B
	
View of Molecule A	View of molecule B





SI Table 5. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **6j**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

Atom	x	y	z	$U(\text{eq})$
F(1)	8000(1)	10266(2)	9195(1)	32(1)
F(23)	7865(1)	4454(2)	9432(1)	31(1)
F(21)	9163(1)	3450(2)	9509(1)	36(1)
F(2)	7108(1)	8079(2)	9274(1)	37(1)
F(22)	8922(1)	6375(2)	9524(1)	35(1)
F(3)	6725(1)	10899(2)	9368(1)	39(1)
N(21)	8966(1)	5057(2)	7105(1)	18(1)
N(1)	5859(1)	9939(2)	6938(1)	18(1)
N(31)	10064(1)	6129(2)	7693(1)	21(1)
N(10)	7518(1)	9649(2)	6588(1)	20(1)
N(30)	7158(1)	4881(2)	6792(1)	21(1)
N(11)	5072(1)	11257(2)	7539(1)	22(1)
C(10A)	6819(1)	9121(3)	6258(1)	18(1)
C(15A)	6350(1)	9805(3)	7431(1)	18(1)
C(35)	7987(1)	4112(3)	7815(1)	19(1)
C(35A)	8695(1)	4903(3)	7613(1)	17(1)
C(15)	7110(1)	8897(3)	7614(1)	18(1)
C(21A)	8610(1)	4568(3)	6592(1)	17(1)
C(22)	9812(1)	5733(3)	7194(1)	19(1)
C(1A)	5987(1)	9401(3)	6423(1)	18(1)
C(33)	8653(1)	4869(3)	8698(1)	20(1)
C(34)	7976(1)	4129(3)	8358(1)	20(1)
C(30A)	7706(1)	4342(3)	6445(1)	18(1)
C(14)	7369(1)	8958(3)	8149(1)	19(1)
C(13)	6884(1)	9877(3)	8502(1)	19(1)
C(32)	9364(1)	5609(3)	8504(1)	20(1)
C(26A)	7420(1)	3701(3)	5929(1)	21(1)
C(24A)	9163(1)	4438(3)	6200(1)	20(1)
C(31A)	9385(1)	5609(3)	7958(1)	18(1)
C(23)	10333(1)	5768(3)	6773(1)	22(1)
C(6A)	6884(1)	8454(3)	5738(1)	20(1)
C(11A)	5850(1)	10674(3)	7786(1)	20(1)
C(12)	6117(1)	10719(3)	8326(1)	21(1)
C(5)	5355(1)	8590(3)	5535(1)	24(1)
C(4A)	5264(1)	9285(3)	6048(1)	21(1)
C(16)	7176(1)	9796(3)	9077(1)	24(1)
C(6)	6130(1)	8138(3)	5388(1)	23(1)
C(2)	5082(1)	10754(3)	7043(1)	20(1)
C(9)	8277(1)	9446(3)	6422(1)	22(1)
C(3)	4377(1)	10781(3)	6640(1)	22(1)
C(28)	5983(1)	3994(3)	6152(1)	25(1)
C(27)	6528(1)	3498(3)	5796(1)	24(1)
C(29)	6327(1)	4713(3)	6643(1)	23(1)
C(7)	7712(1)	8223(3)	5586(1)	22(1)
C(8)	8408(1)	8713(3)	5925(1)	23(1)
C(25)	8852(1)	3784(3)	5689(1)	23(1)
C(26)	8012(1)	3368(3)	5559(1)	24(1)
C(4)	4454(1)	9992(3)	6171(1)	23(1)
C(36)	8646(1)	4787(3)	9284(1)	25(1)
C(24)	10034(1)	5057(3)	6303(1)	22(1)

SI Table 6. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **6j**.

Bond	Length [ $\text{\AA}$ ]	Angle	[ $^\circ$ ]
F(1)-C(16)	1.341(2)	C(21A)-N(21)-C(35A)	134.51(17)
F(23)-C(36)	1.346(3)	C(21A)-N(21)-C(22)	120.40(16)
F(21)-C(36)	1.349(3)	C(35A)-N(21)-C(22)	104.86(16)
F(2)-C(16)	1.349(3)	C(15A)-N(1)-C(1A)	134.14(17)
F(22)-C(36)	1.350(3)	C(15A)-N(1)-C(2)	105.08(16)
F(3)-C(16)	1.344(2)	C(1A)-N(1)-C(2)	120.74(16)
N(21)-C(21A)	1.408(2)	C(22)-N(31)-C(31A)	104.25(16)
N(21)-C(35A)	1.409(3)	C(9)-N(10)-C(10A)	117.89(18)
N(21)-C(22)	1.411(2)	C(29)-N(30)-C(30A)	117.77(18)
N(1)-C(15A)	1.402(2)	C(2)-N(11)-C(11A)	104.43(17)
N(1)-C(1A)	1.403(3)	N(10)-C(10A)-C(6A)	122.20(18)
N(1)-C(2)	1.410(3)	N(10)-C(10A)-C(1A)	118.64(18)
N(31)-C(22)	1.318(3)	C(6A)-C(10A)-C(1A)	118.93(18)
N(31)-C(31A)	1.378(3)	C(15)-C(15A)-N(1)	134.07(18)
N(10)-C(9)	1.319(3)	C(15)-C(15A)-C(11A)	120.83(18)
N(10)-C(10A)	1.361(3)	N(1)-C(15A)-C(11A)	104.70(17)
N(30)-C(29)	1.325(3)	C(34)-C(35)-C(35A)	117.57(19)
N(30)-C(30A)	1.357(3)	C(34)-C(35)-H(35)	121.2
N(11)-C(2)	1.315(3)	C(35A)-C(35)-H(35)	121.2
N(11)-C(11A)	1.378(3)	C(35)-C(35A)-N(21)	134.76(19)
C(10A)-C(6A)	1.422(3)	C(35)-C(35A)-C(31A)	120.37(18)
C(10A)-C(1A)	1.434(3)	N(21)-C(35A)-C(31A)	104.56(16)
C(15A)-C(15)	1.398(3)	C(14)-C(15)-C(15A)	117.51(18)
C(15A)-C(11A)	1.410(3)	C(14)-C(15)-H(15)	121.2
C(35)-C(34)	1.384(3)	C(15A)-C(15)-H(15)	121.2
C(35)-C(35A)	1.400(3)	C(24A)-C(21A)-N(21)	117.75(17)
C(35)-H(35)	0.9500	C(24A)-C(21A)-C(30A)	118.75(18)
C(35A)-C(31A)	1.414(3)	N(21)-C(21A)-C(30A)	123.31(17)
C(15)-C(14)	1.378(3)	N(31)-C(22)-N(21)	114.03(17)
C(15)-H(15)	0.9500	N(31)-C(22)-C(23)	125.88(18)
C(21A)-C(24A)	1.399(3)	N(21)-C(22)-C(23)	119.79(18)
C(21A)-C(30A)	1.439(3)	C(4A)-C(1A)-N(1)	117.57(18)
C(22)-C(23)	1.422(3)	C(4A)-C(1A)-C(10A)	119.27(18)
C(1A)-C(4A)	1.403(3)	N(1)-C(1A)-C(10A)	122.95(17)
C(33)-C(32)	1.381(3)	C(32)-C(33)-C(34)	121.04(19)
C(33)-C(34)	1.402(3)	C(32)-C(33)-C(36)	117.99(19)
C(33)-C(36)	1.495(3)	C(34)-C(33)-C(36)	120.89(18)
C(34)-H(34)	0.9500	C(35)-C(34)-C(33)	121.86(19)
C(30A)-C(26A)	1.419(3)	C(35)-C(34)-H(34)	119.1
C(14)-C(13)	1.408(3)	C(33)-C(34)-H(34)	119.1
C(14)-H(14)	0.9500	N(30)-C(30A)-C(26A)	122.50(18)
C(13)-C(12)	1.380(3)	N(30)-C(30A)-C(21A)	118.61(18)
C(13)-C(16)	1.486(3)	C(26A)-C(30A)-C(21A)	118.70(18)
C(32)-C(31A)	1.393(3)	C(15)-C(14)-C(13)	121.57(19)
C(32)-H(32)	0.9500	C(15)-C(14)-H(14)	119.2
C(26A)-C(27)	1.413(3)	C(13)-C(14)-H(14)	119.2
C(26A)-C(26)	1.415(3)	C(12)-C(13)-C(14)	121.27(19)
C(24A)-C(25)	1.419(3)	C(12)-C(13)-C(16)	119.90(18)
C(24A)-C(24)	1.436(3)	C(14)-C(13)-C(16)	118.64(18)



C(23)-C(24)	1.338(3)	C(33)-C(32)-C(31A)	117.89(18)
C(23)-H(23)	0.9500	C(33)-C(32)-H(32)	121.1
C(6A)-C(7)	1.410(3)	C(31A)-C(32)-H(32)	121.1
C(6A)-C(6)	1.422(3)	C(27)-C(26A)-C(26)	122.08(19)
C(11A)-C(12)	1.393(3)	C(27)-C(26A)-C(30A)	117.36(19)
C(12)-H(12)	0.9500	C(26)-C(26A)-C(30A)	120.49(19)
C(5)-C(6)	1.354(3)	C(21A)-C(24A)-C(25)	119.92(19)
C(5)-C(4A)	1.422(3)	C(21A)-C(24A)-C(24)	120.20(19)
C(5)-H(5)	0.9500	C(25)-C(24A)-C(24)	119.79(18)
C(4A)-C(4)	1.439(3)	N(31)-C(31A)-C(32)	126.49(18)
C(6)-H(6)	0.9500	N(31)-C(31A)-C(35A)	112.13(17)
C(2)-C(3)	1.425(3)	C(32)-C(31A)-C(35A)	121.20(18)
C(9)-C(8)	1.407(3)	C(24)-C(23)-C(22)	119.53(19)
C(9)-H(9)	0.9500	C(24)-C(23)-H(23)	120.2
C(3)-C(4)	1.341(3)	C(22)-C(23)-H(23)	120.2
C(3)-H(3)	0.9500	C(7)-C(6A)-C(6)	122.68(19)
C(28)-C(27)	1.363(3)	C(7)-C(6A)-C(10A)	117.42(18)
C(28)-C(29)	1.407(3)	C(6)-C(6A)-C(10A)	119.81(18)
C(28)-H(28)	0.9500	N(11)-C(11A)-C(12)	126.77(19)
C(27)-H(27)	0.9500	N(11)-C(11A)-C(15A)	111.88(18)
C(29)-H(29)	0.9500	C(12)-C(11A)-C(15A)	121.04(18)
C(7)-C(8)	1.363(3)	C(13)-C(12)-C(11A)	117.69(19)
C(7)-H(7)	0.9500	C(13)-C(12)-H(12)	121.2
C(8)-H(8)	0.9500	C(11A)-C(12)-H(12)	121.2
C(25)-C(26)	1.359(3)	C(6)-C(5)-C(4A)	121.75(19)
C(25)-H(25)	0.9500	C(6)-C(5)-H(5)	119.1
C(26)-H(26)	0.9500	C(4A)-C(5)-H(5)	119.1
C(4)-H(4)	0.9500	C(1A)-C(4A)-C(5)	119.28(19)
C(24)-H(24)	0.9500	C(1A)-C(4A)-C(4)	120.04(19)
		C(5)-C(4A)-C(4)	120.51(19)
		F(1)-C(16)-F(3)	106.36(17)
		F(1)-C(16)-F(2)	105.35(17)
		F(3)-C(16)-F(2)	105.83(17)
		F(1)-C(16)-C(13)	113.30(17)
		F(3)-C(16)-C(13)	113.32(18)
		F(2)-C(16)-C(13)	112.04(17)
		C(5)-C(6)-C(6A)	120.0(2)
		C(5)-C(6)-H(6)	120.0
		C(6A)-C(6)-H(6)	120.0
		N(11)-C(2)-N(1)	113.69(17)
		N(11)-C(2)-C(3)	126.63(19)
		N(1)-C(2)-C(3)	119.32(18)
		N(10)-C(9)-C(8)	123.94(19)
		N(10)-C(9)-H(9)	118.0
		C(8)-C(9)-H(9)	118.0
		C(4)-C(3)-C(2)	119.72(19)
		C(4)-C(3)-H(3)	120.1
		C(2)-C(3)-H(3)	120.1
		C(27)-C(28)-C(29)	118.73(19)
		C(27)-C(28)-H(28)	120.6
		C(29)-C(28)-H(28)	120.6
		C(28)-C(27)-C(26A)	119.6(2)

		C(28)-C(27)-H(27)	120.2
		C(26A)-C(27)-H(27)	120.2
		N(30)-C(29)-C(28)	123.8(2)
		N(30)-C(29)-H(29)	118.1
		C(28)-C(29)-H(29)	118.1
		C(8)-C(7)-C(6A)	119.67(19)
		C(8)-C(7)-H(7)	120.2
		C(6A)-C(7)-H(7)	120.2
		C(7)-C(8)-C(9)	118.73(19)
		C(7)-C(8)-H(8)	120.6
		C(9)-C(8)-H(8)	120.6
		C(26)-C(25)-C(24A)	121.55(19)
		C(26)-C(25)-H(25)	119.2
		C(24A)-C(25)-H(25)	119.2
		C(25)-C(26)-C(26A)	119.60(19)
		C(25)-C(26)-H(26)	120.2
		C(26A)-C(26)-H(26)	120.2
		C(3)-C(4)-C(4A)	120.99(19)
		C(3)-C(4)-H(4)	119.5
		C(4A)-C(4)-H(4)	119.5
		F(23)-C(36)-F(21)	106.19(17)
		F(23)-C(36)-F(22)	106.49(17)
		F(21)-C(36)-F(22)	105.76(17)
		F(23)-C(36)-C(33)	113.13(18)
		F(21)-C(36)-C(33)	112.40(18)
		F(22)-C(36)-C(33)	112.32(18)
		C(23)-C(24)-C(24A)	121.14(19)
		C(23)-C(24)-H(24)	119.4
		C(24A)-C(24)-H(24)	119.4