

## Supporting Information

### **Synthesis, Structures, and DNA and Protein Binding of Ruthenium(II)-p-Cymene Complexes of Substituted Pyridylimidazo[1,5-a]pyridine: Enhanced Cytotoxicity of Complexes of Ligands Appended with Carbazole Moiety**

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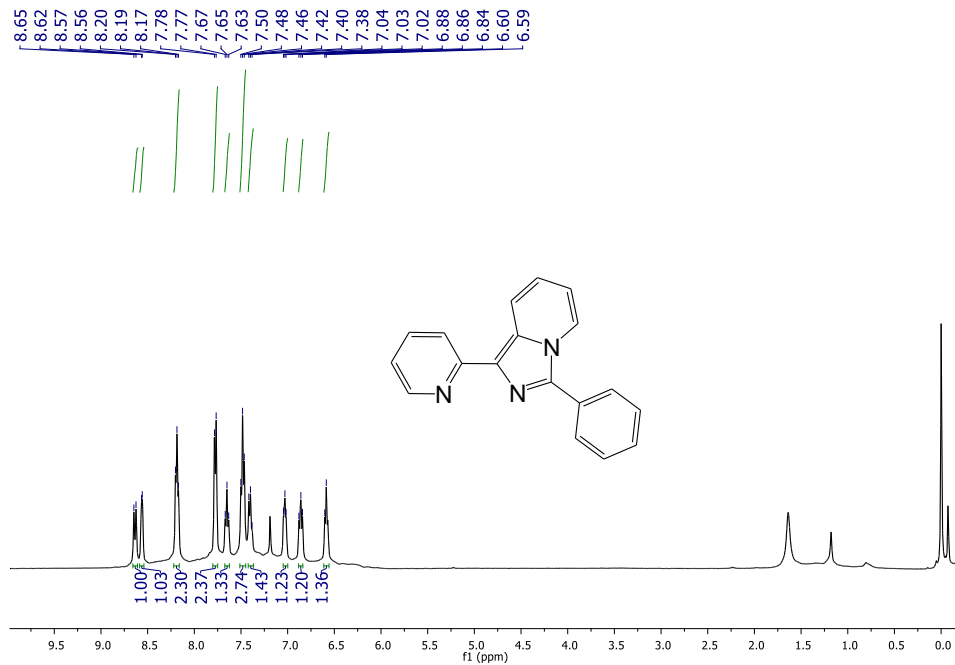
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**Figure S1.**  $^1\text{H}$  NMR spectrum of L1 in  $\text{CDCl}_3$ .

13C TL-1, CDCl3, 09/11/16, SAIF, NEHU

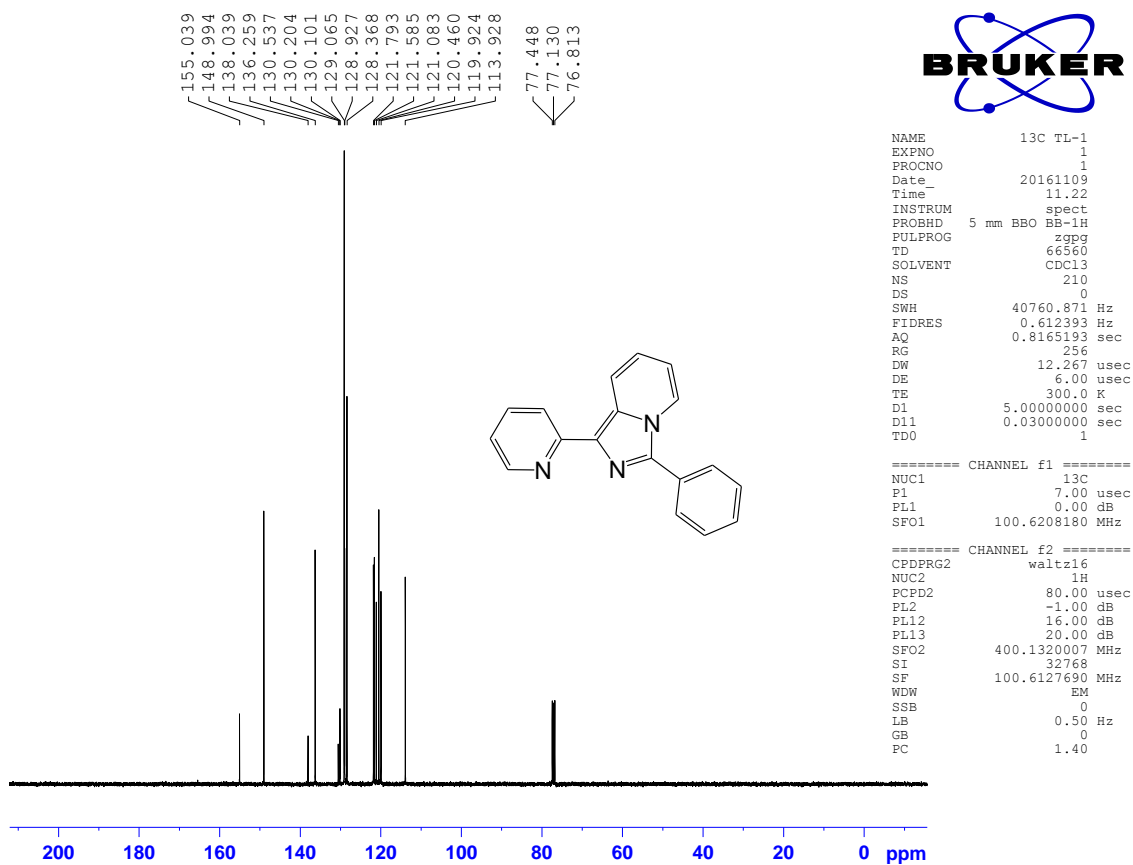
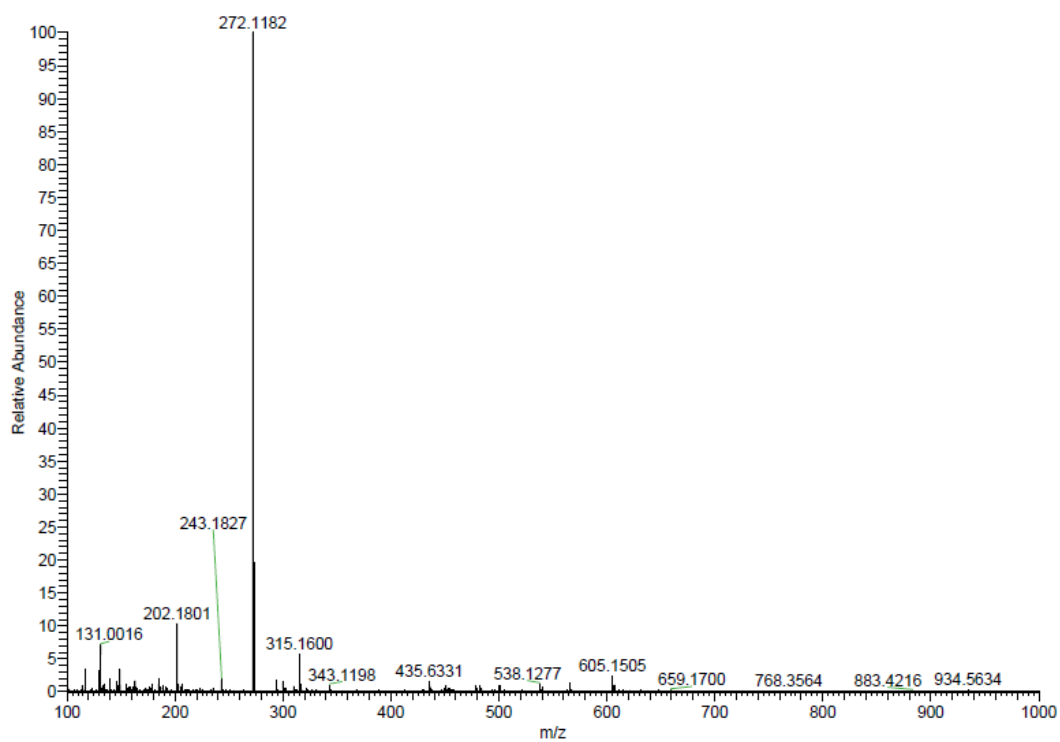
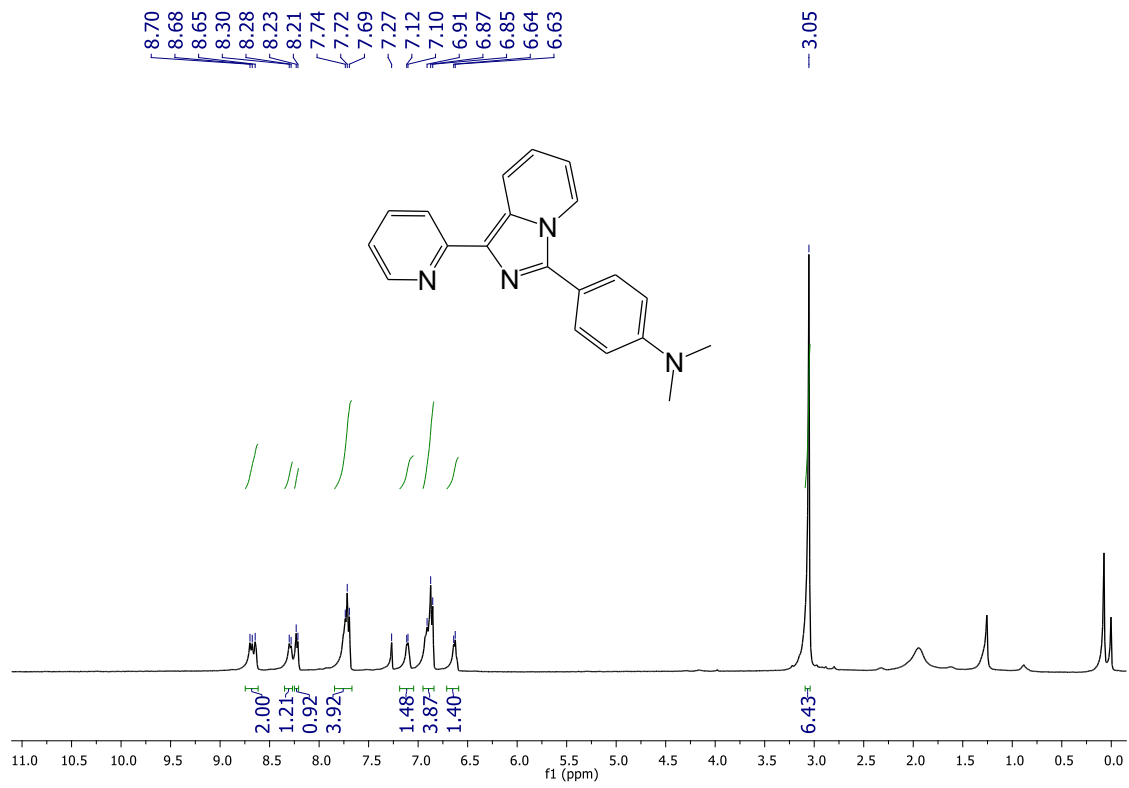


Figure S2.  $^{13}\text{C}$  NMR spectrum of L1 in  $\text{CDCl}_3$ .

T1\_1 #71 RT: 0.86 AV: 1 NL: 9.56E8  
T: FTMS + p ESI Full ms [100.00-1000.00]

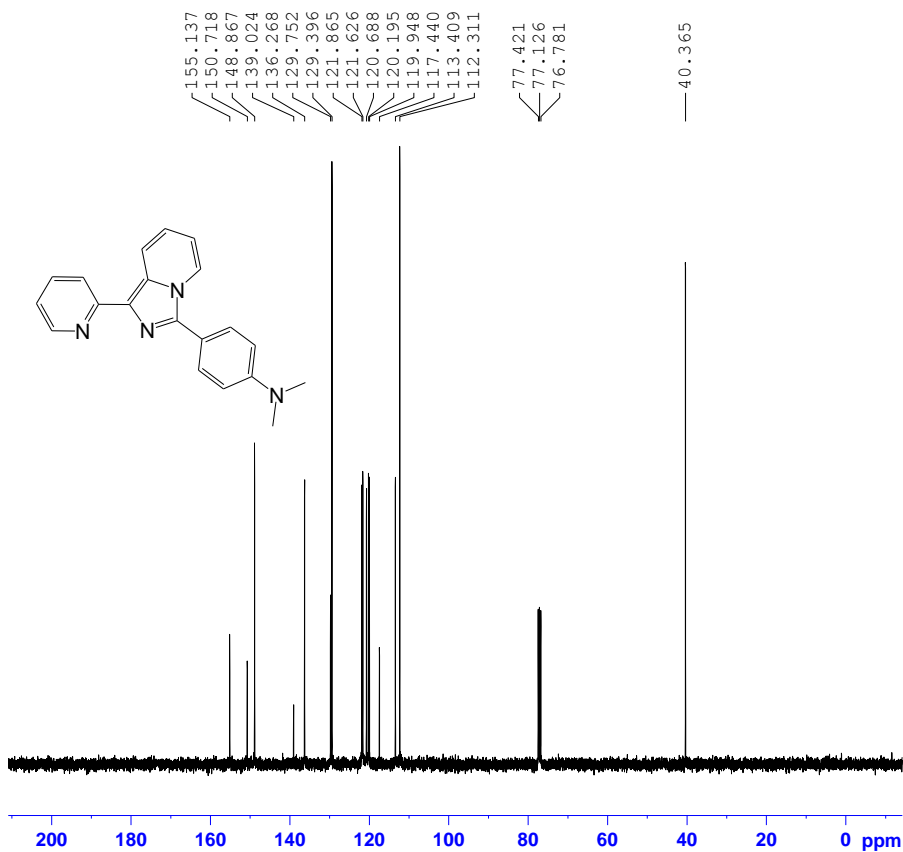


**Figure S3.** HRMS-ESI for **L1**, Calcd for  $C_{18}H_{14}N_3$ : 272.1188  $[M+H]^+$ , Found: 272.1182  $[M+H]^+$ .



**Figure S4.** <sup>1</sup>H NMR spectrum of L2 in CDCl<sub>3</sub>.

13C TL-6, CDCl3, 09/11/16, SAIF, NEHU



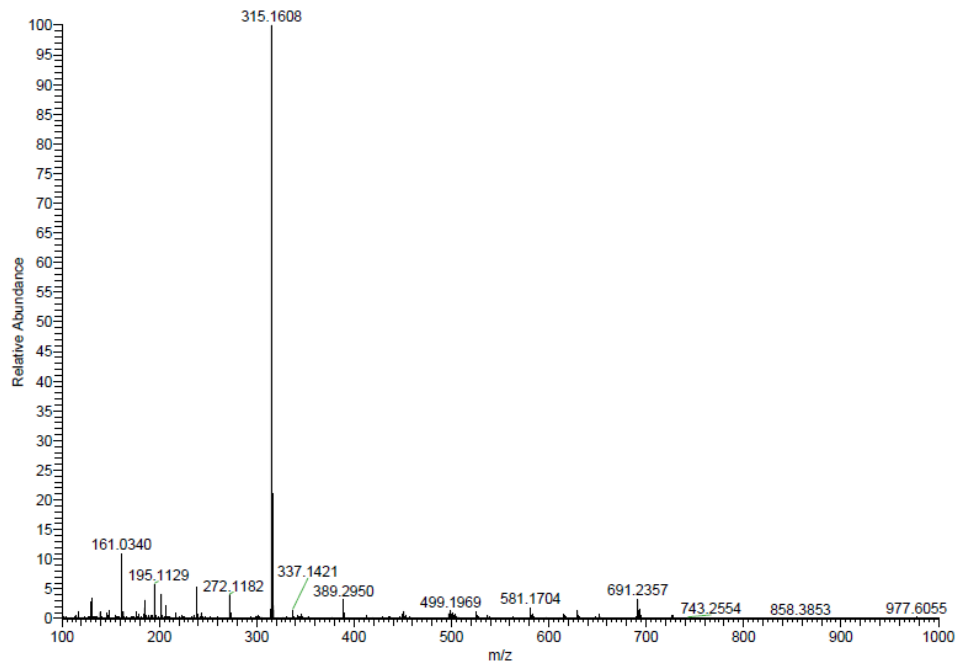
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EXPNO         1
PROCNO        1
Date_         20161109
Time          13.07
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg
TD            66560
SOLVENT       CDCl3
NS            310
DS            0
SWH           40760.871 Hz
FIDRES        0.612393 Hz
AQ            0.8165193 sec
RG            256
DW            12.267 usec
DE            6.00 usec
TE            300.0 K
D1            5.0000000 sec
D11           0.0300000 sec
TDD           1

===== CHANNEL f1 =====
NUC1          13C
P1            7.00 usec
PL1           0.00 dB
SFO1         100.6208180 MHz

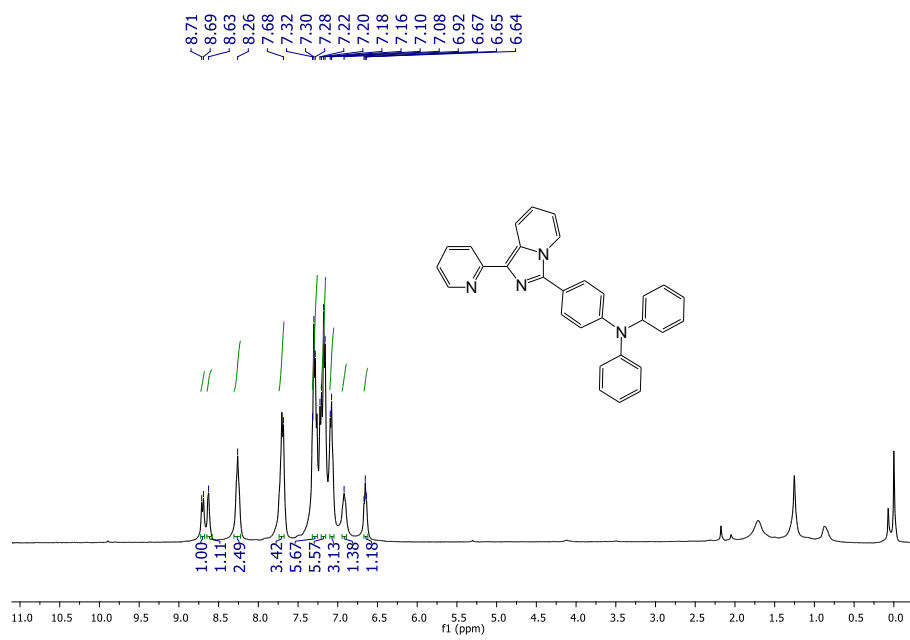
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -1.00 dB
PL12          16.00 dB
PL13          20.00 dB
SFO2         400.1320007 MHz
SI            32768
SF           100.6127690 MHz
WDW           EM
SSB           0
LB            0.50 Hz
GB            0
PC            1.40
```

Figure S5. <sup>13</sup>C NMR spectrum of L2 in CDCl<sub>3</sub>.

T6 #81 RT: 0.84 AV: 1 NL: 9.80E8  
T: FTMS + p ESI Full ms [100.00-1000.00]



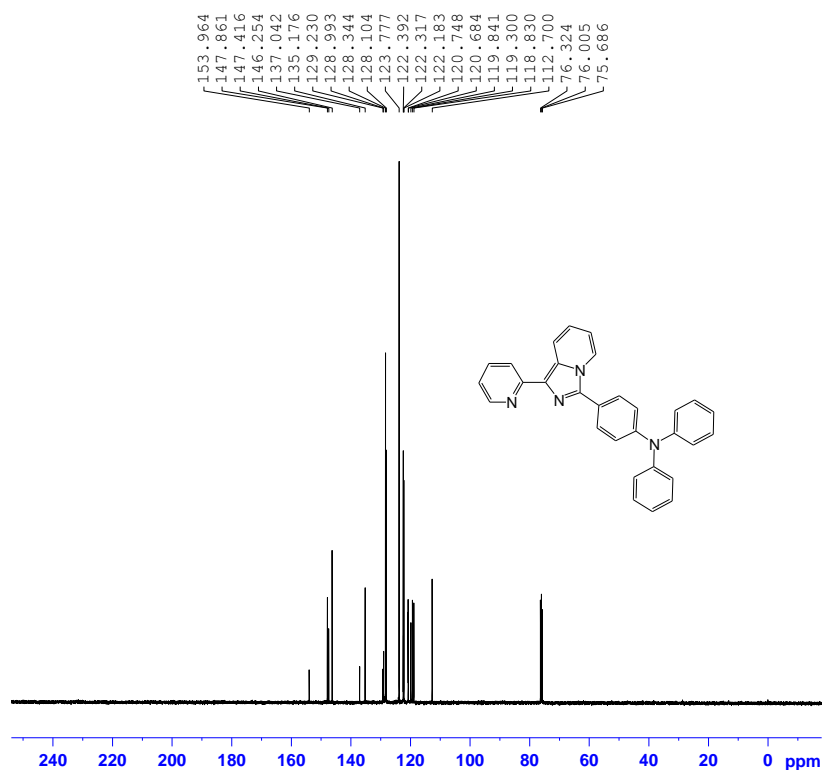
**Figure S6.** HRMS-ESI for **L2**, Calcd for  $C_{20}H_{19}N_4$ : 315.1610  $[M+H]^+$ , Found: 315.1604  $[M+H]^+$ .



**Figure S7.** <sup>1</sup>H NMR spectrum of L3 in CDCl<sub>3</sub>.



13C TL-14, CDCl3, 09/11/16, SAIF, NEHU



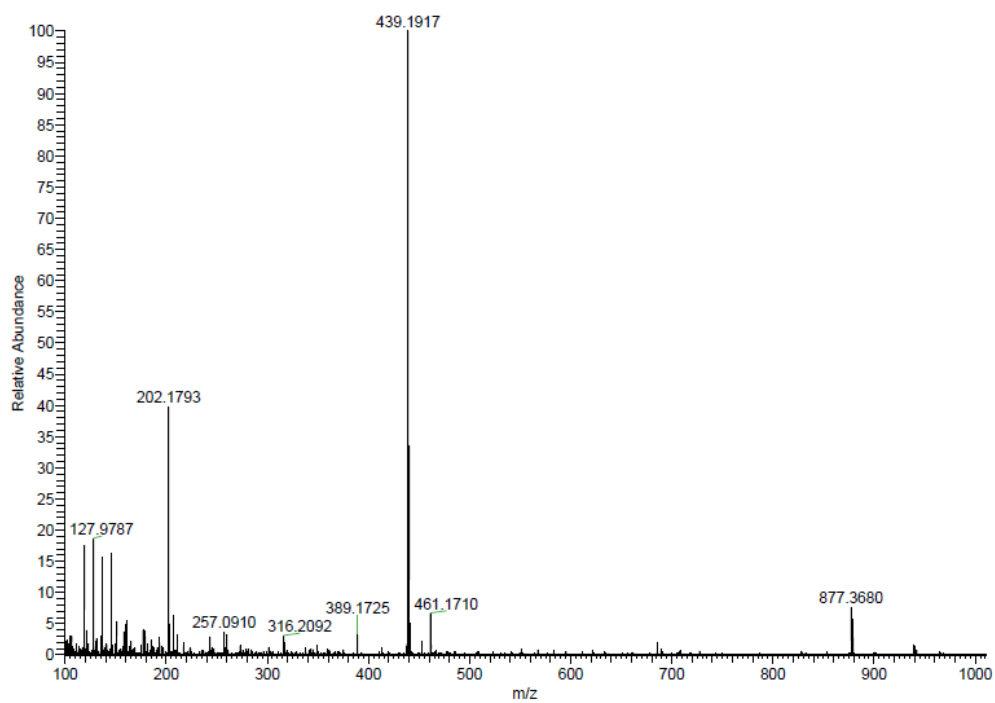
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PROCNO 1
Date_ 20161109
Time 14.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65560
SOLVENT CDCl3
NS 310
DS 0
SWH 40760.871 Hz
FIDRES 0.612393 Hz
AQ 0.8165193 sec
RG 256
DW 12.267 usec
DE 6.00 usec
TE 300.0 K
D1 5.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
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P1 7.00 usec
PL1 0.00 dB
SFO1 100.6208180 MHz

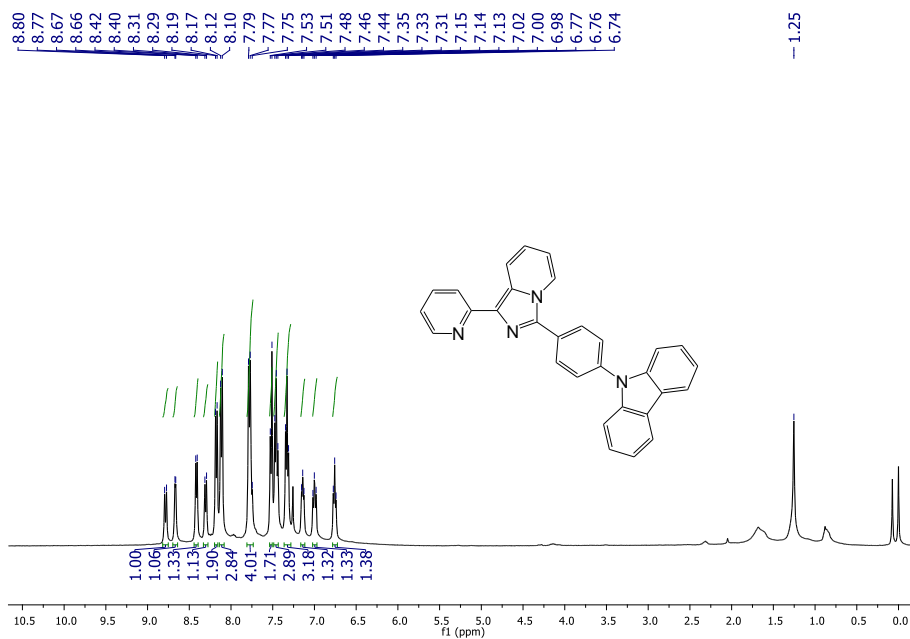
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CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.00 dB
PL13 20.00 dB
SFO2 400.1320007 MHz
SI 32768
SF 100.6128781 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
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Figure S8.  $^{13}\text{C}$  NMR spectrum of L3 in  $\text{CDCl}_3$ .

T14-2 #226-258 RT: 1.00-1.15 AV: 33 SB: 63 0.00-0.28 NL: 1.19E7  
T: FTMS + p ESI Full ms [100.00-1000.00]

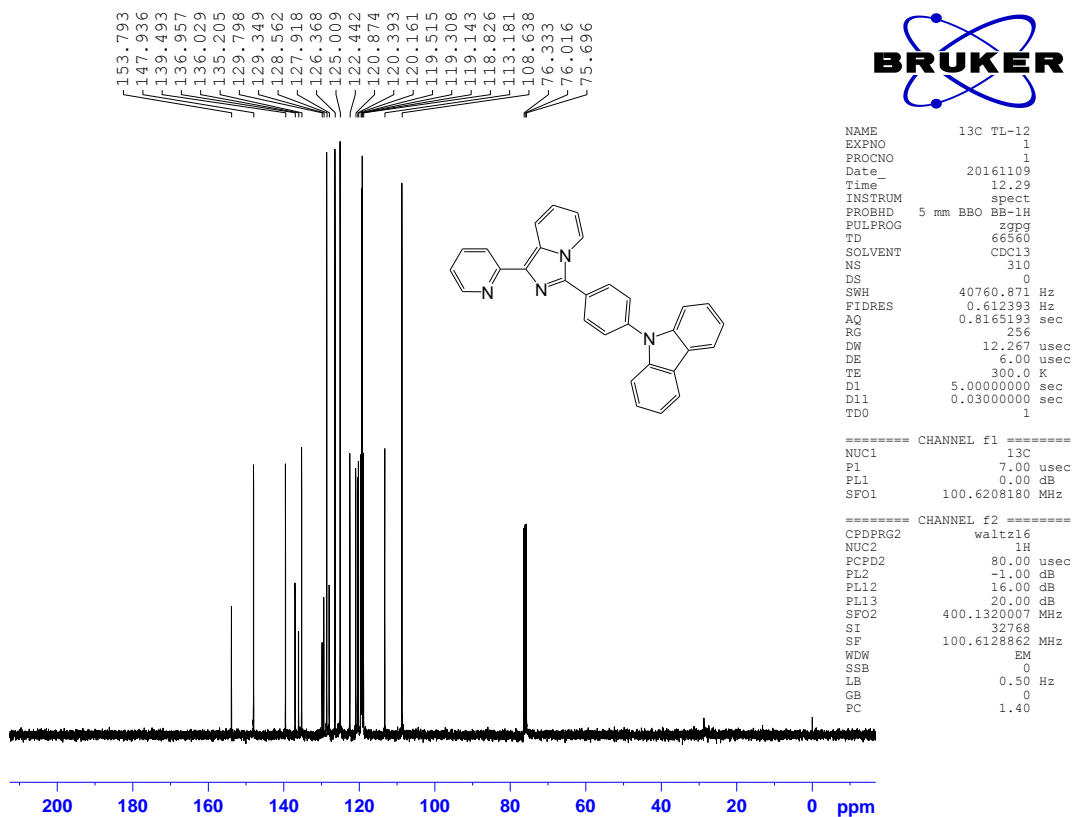


**Figure S9.** HRMS-ESI for L3, Calcd for  $C_{30}H_{23}N_4$ : 439.1923  $[M+H]^+$ , Found: 439.1917  $[M+H]^+$ .

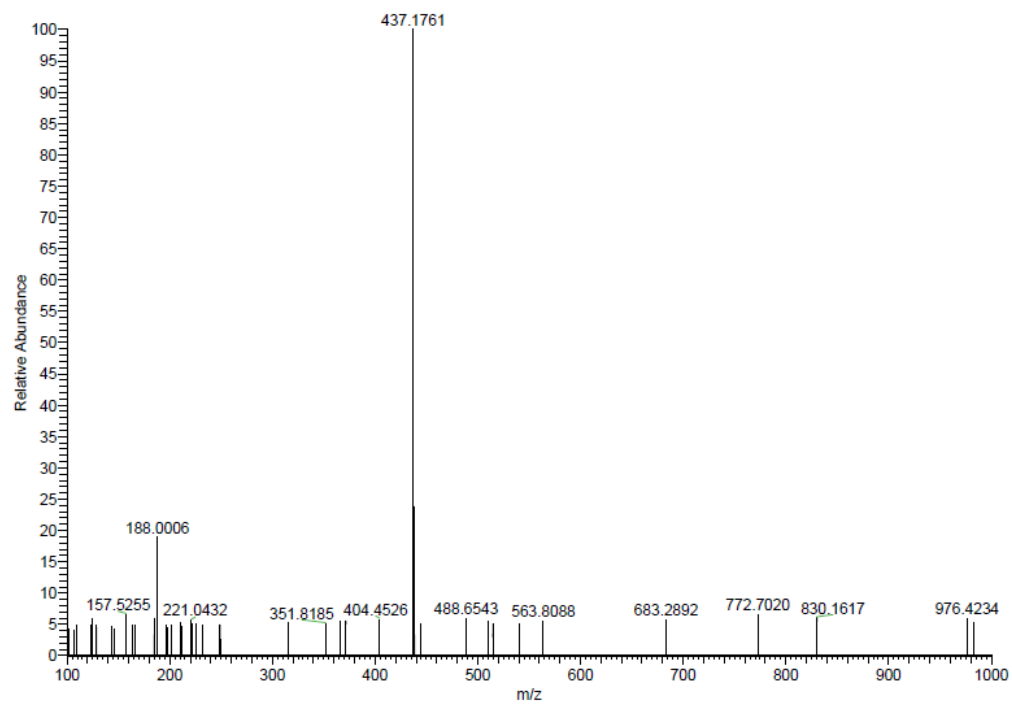


**Figure S10.**  $^1\text{H}$  NMR spectrum of **L4** in  $\text{CDCl}_3$ .

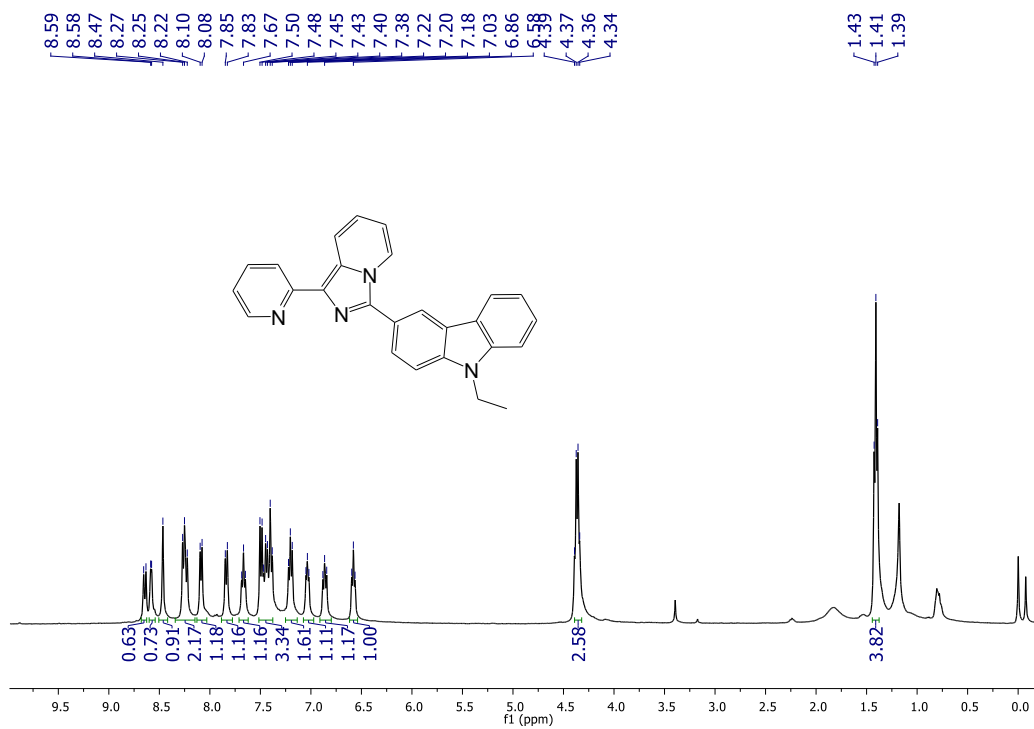
13C TL-12, CDC13, 09/11/16, SAIF, NEHU



T12\_1 #67 RT: 0.67 AV: 1 NL: 1.07E6  
T: FTMS + p ESI Full ms [100.00-1000.00]



**Figure S12.** HRMS-ESI for **L4**, Calcd for  $C_{30}H_{21}N_4$ : 437.1766  $[M+H]^+$ , Found: 437.1761  $[M+H]^+$ .



**Figure S13.**  $^1\text{H}$  NMR spectrum of L5 in  $\text{CDCl}_3$ .

13C TL-13, CDCl3, 09/11/16, SAIF, NEHU

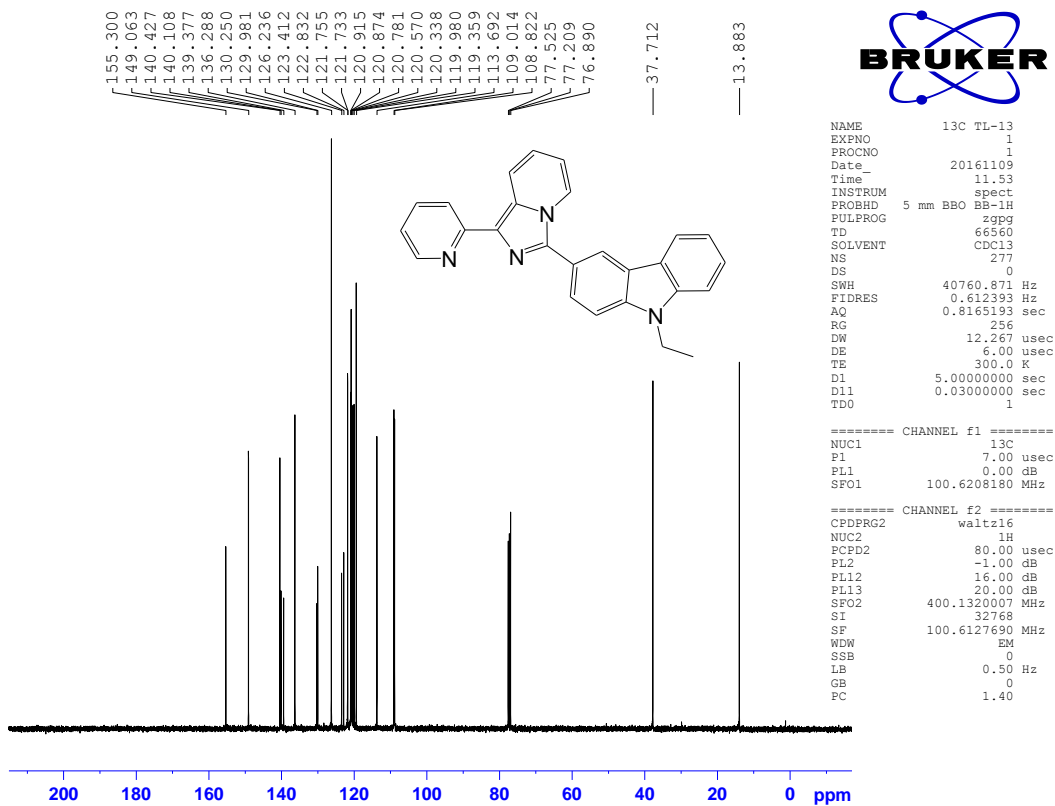
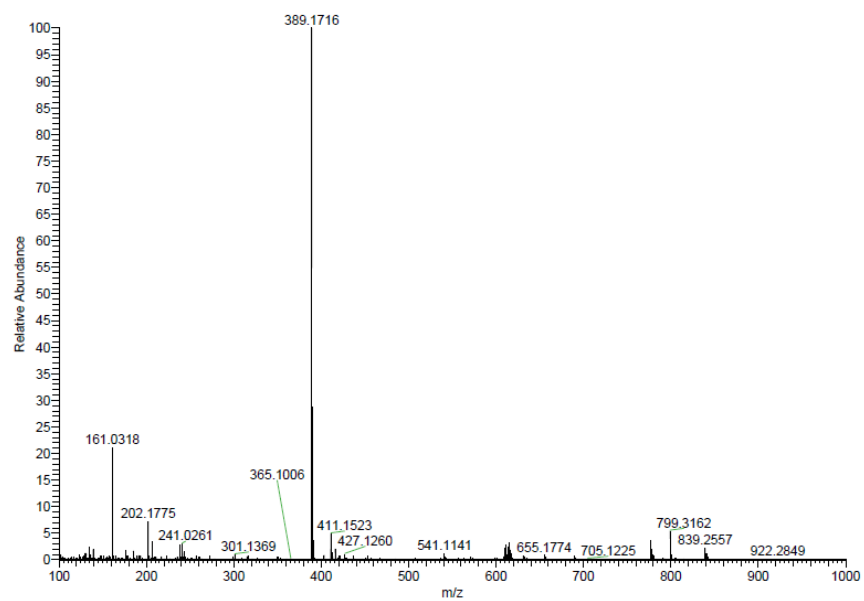


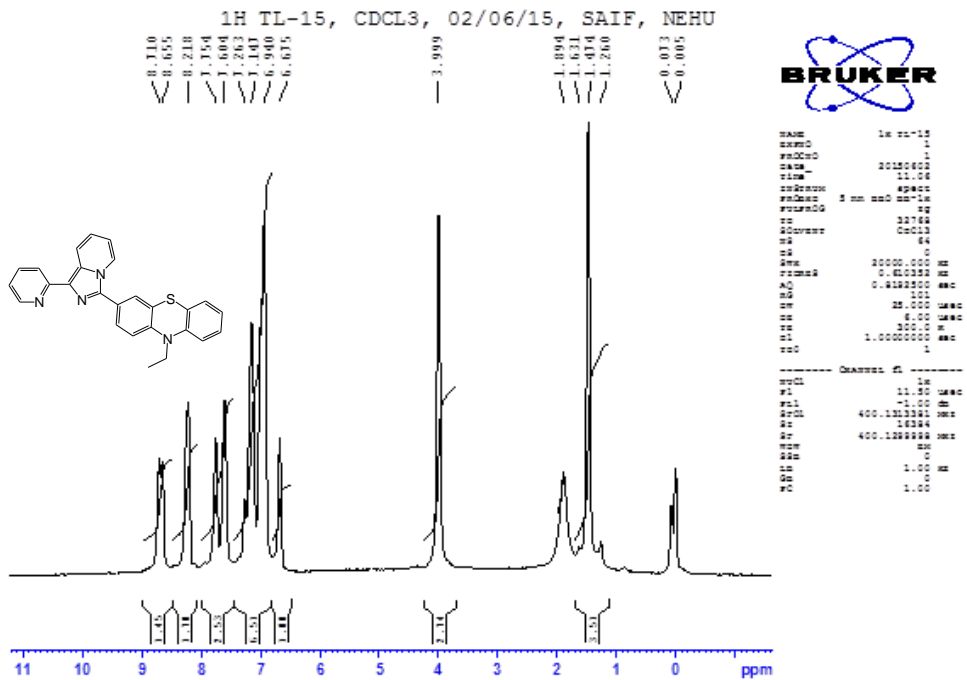
Figure S14. <sup>13</sup>C NMR spectrum of L5 in CDCl<sub>3</sub>.

T13 #131 RT: 1.25 AV: 1 NL: 5.11E8  
T: FTMS + p ESI Full ms [100.00-1000.00]



**Figure S15.** HRMS-ESI for **L5**, Calcd for  $C_{26}H_{21}N_4$ : 389.1766  $[M+H]^+$ , Found: 389.1716  $[M+H]^+$ .





**Figure S16.**  $^1\text{H}$  NMR spectrum of **L6** in  $\text{CDCl}_3$ .

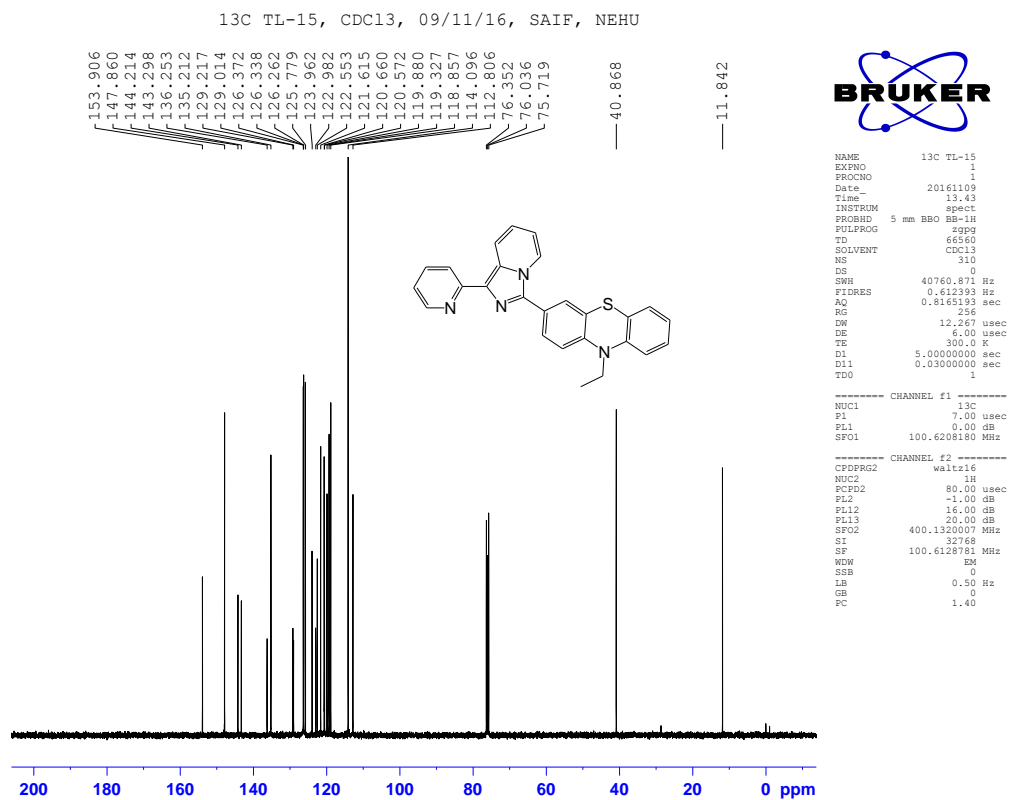
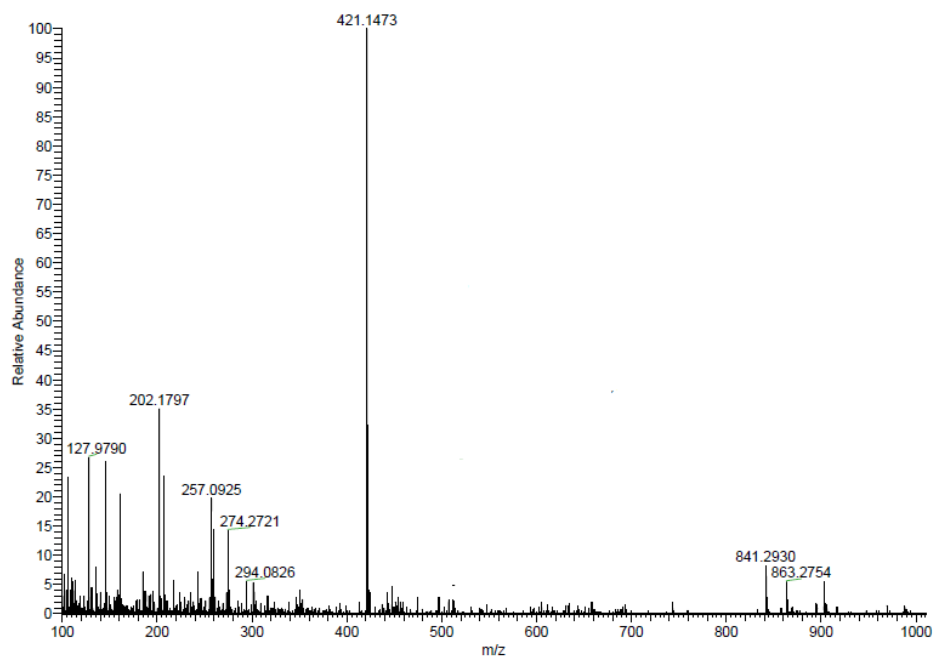
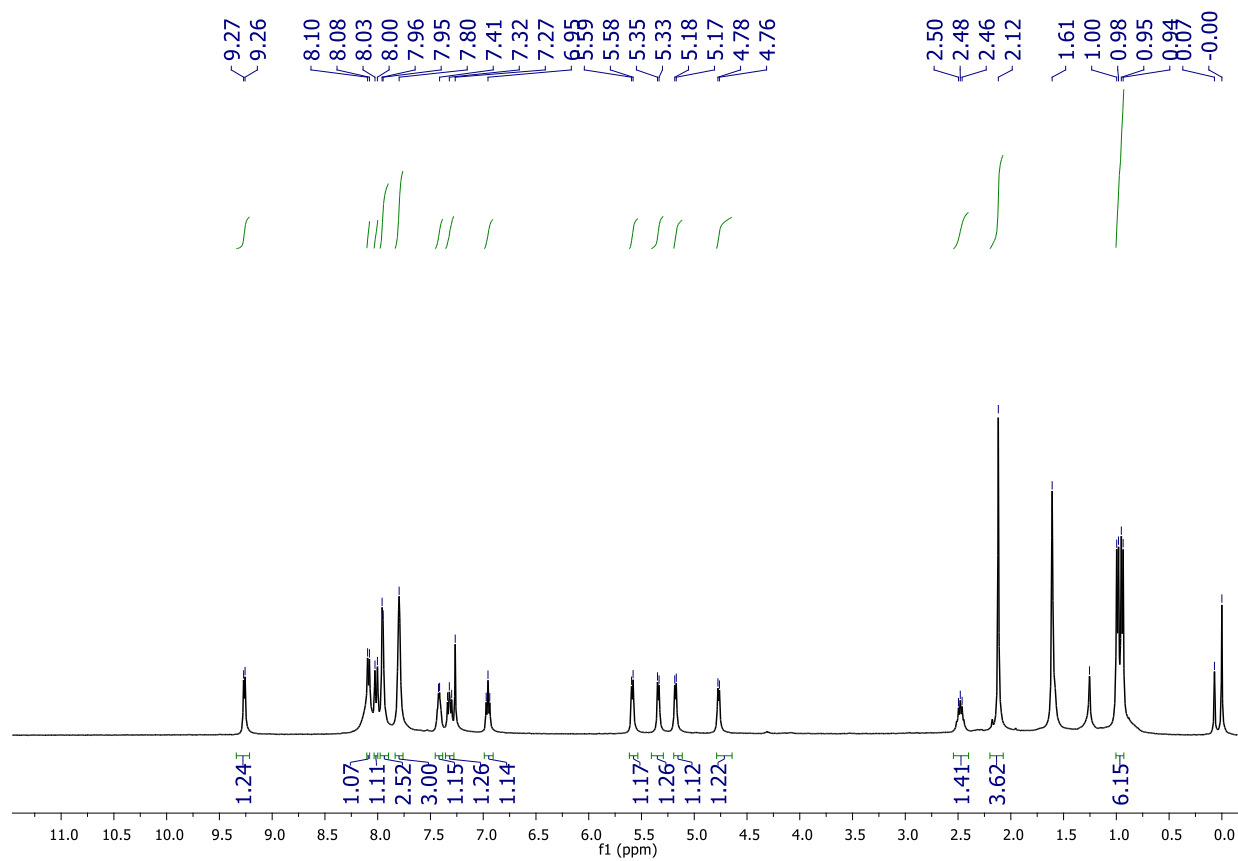


Figure S17. <sup>13</sup>C NMR spectrum of L6 in CDCl<sub>3</sub>.

T15 #88-89 RT: 0.39-0.40 AV: 2 SB: 17 1.83-1.90 NL: 1.53E7  
T: FTMS + p ESI Full ms [100.00-1000.00]



**Figure S18.** HRMS-ESI for **L6**, Calcd for  $C_{26}H_{21}N_4S$ : 421.1487  $[M+H]^+$ , Found: 421.1473  $[M+H]^+$ .



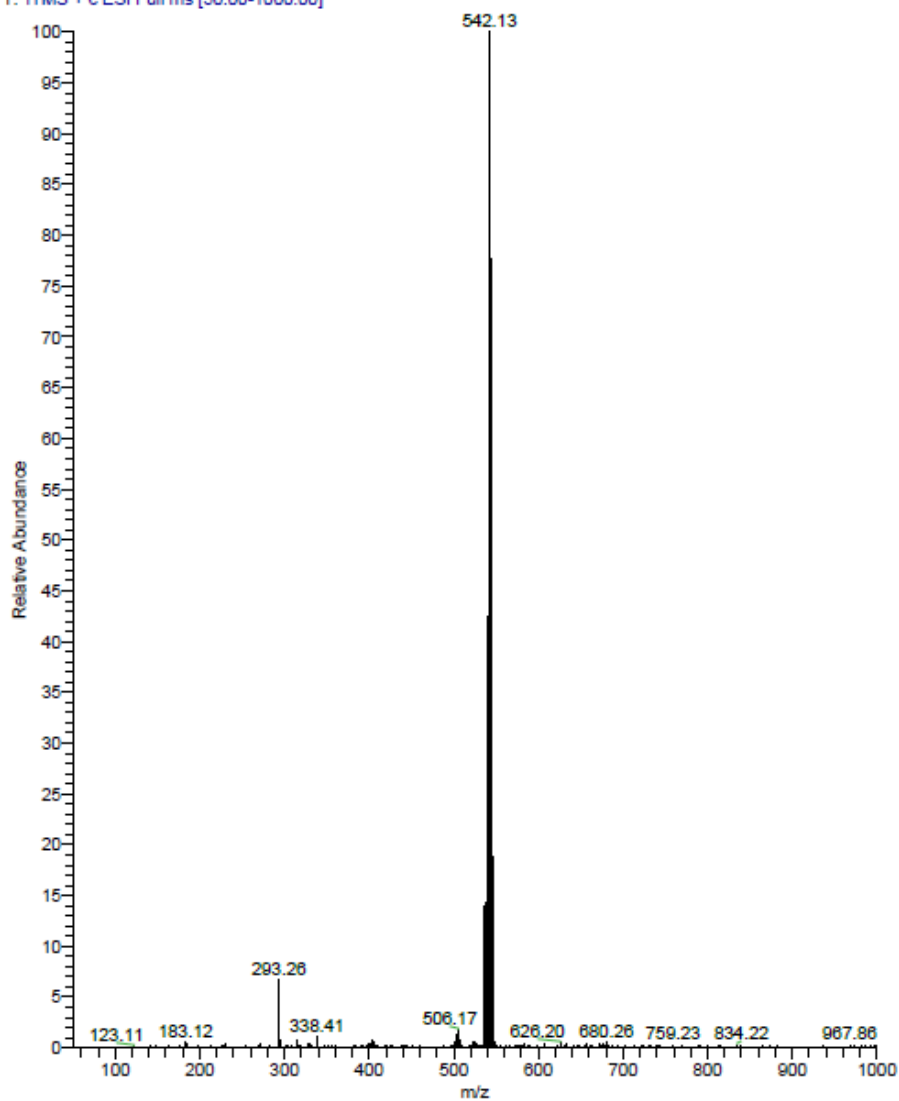
**Figure S19.**  $^1\text{H}$  NMR spectrum of  $[\text{Ru}(\eta^6\text{-cymene})(\text{L1})\text{Cl}]\text{BF}_4$  (**1**) in  $\text{CDCl}_3$ .

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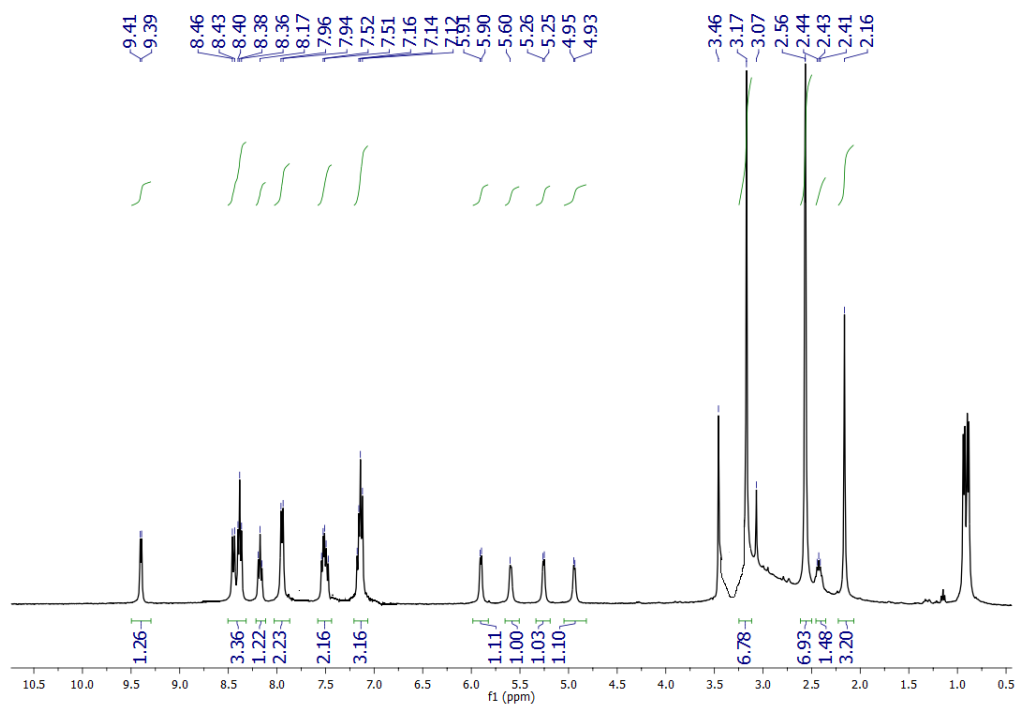
9/23/2014 4:54:22 PM

T-1

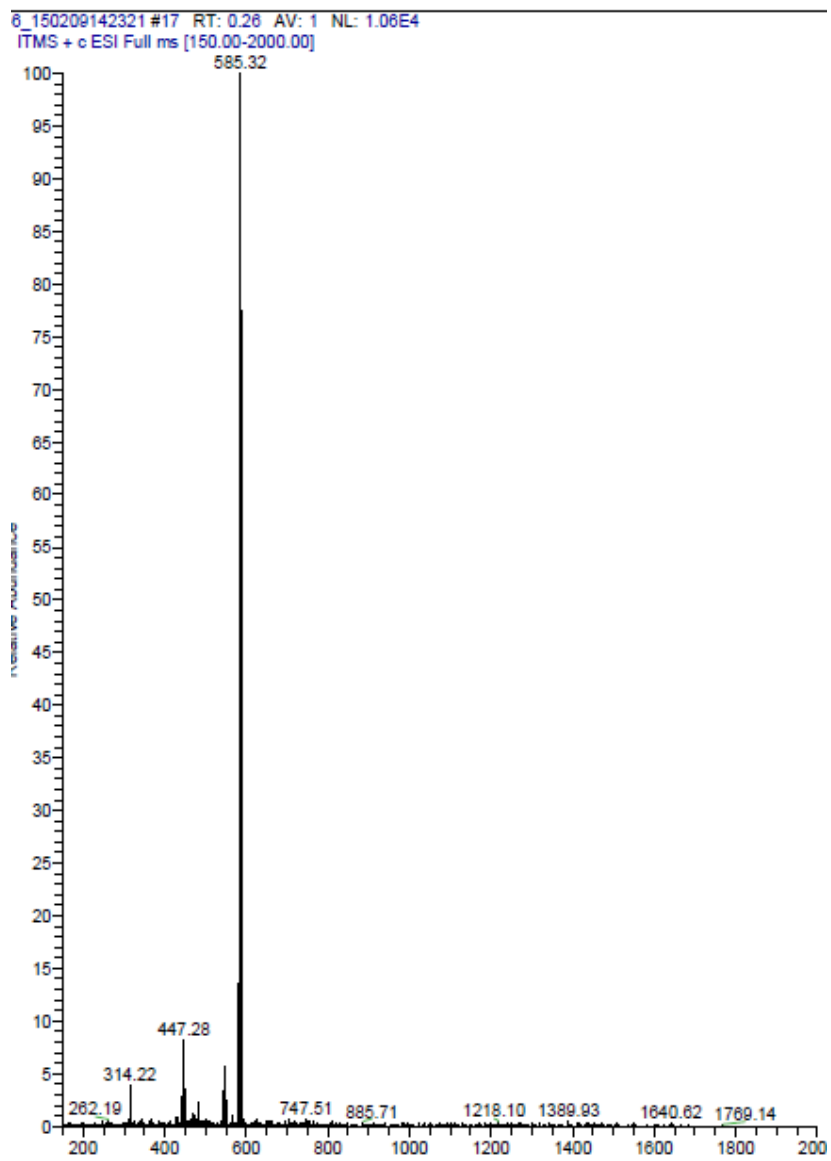
T-1 #32 RT: 0.40 AV: 1 NL: 3.59E3  
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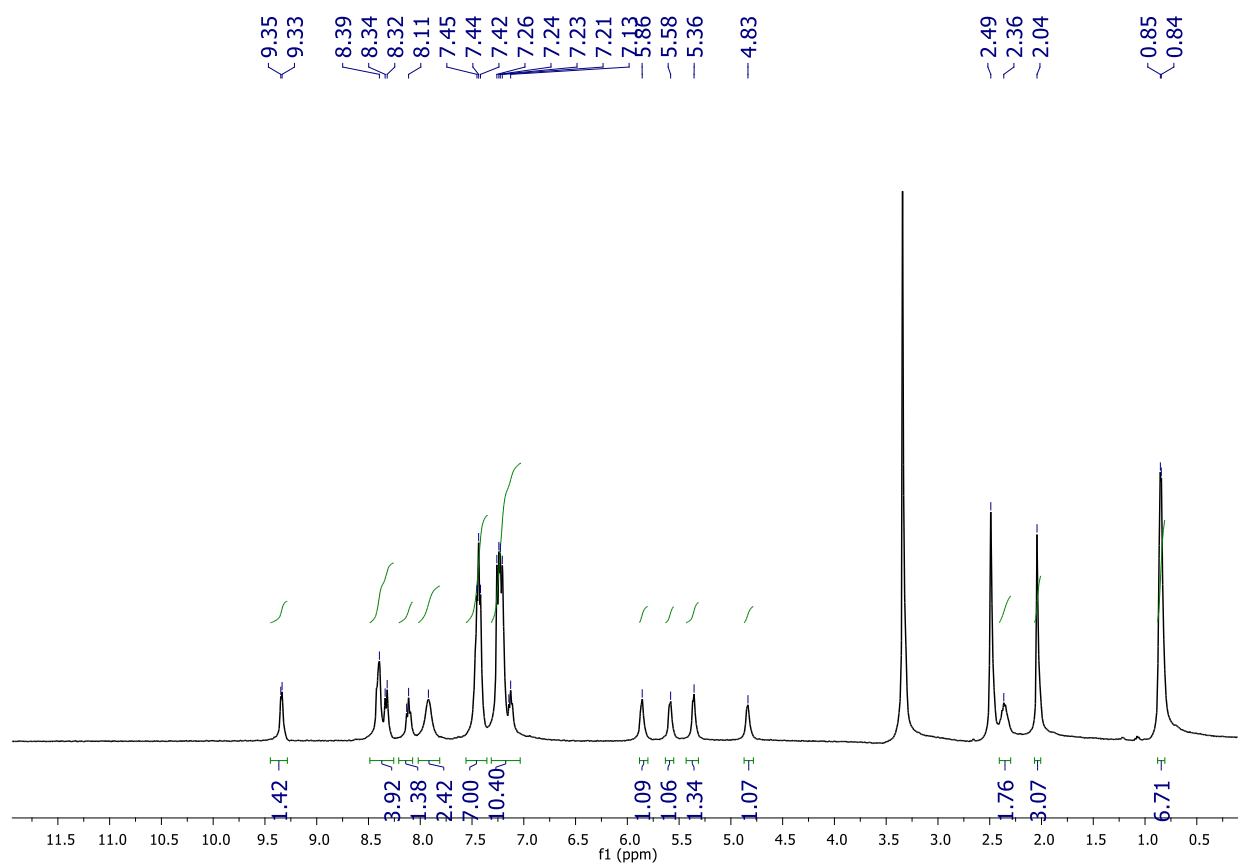
**Figure S20.** ESI-MASS Spectrum of  $[\text{Ru}(\eta^6\text{-cymene})(\text{L1})\text{Cl}]\text{BF}_4$ . (1)



**Figure S21.** <sup>1</sup>H NMR spectrum of [Ru(η<sup>6</sup>-cymene)(L2)Cl]BF<sub>4</sub> in DMSO-D<sub>6</sub>. (2)

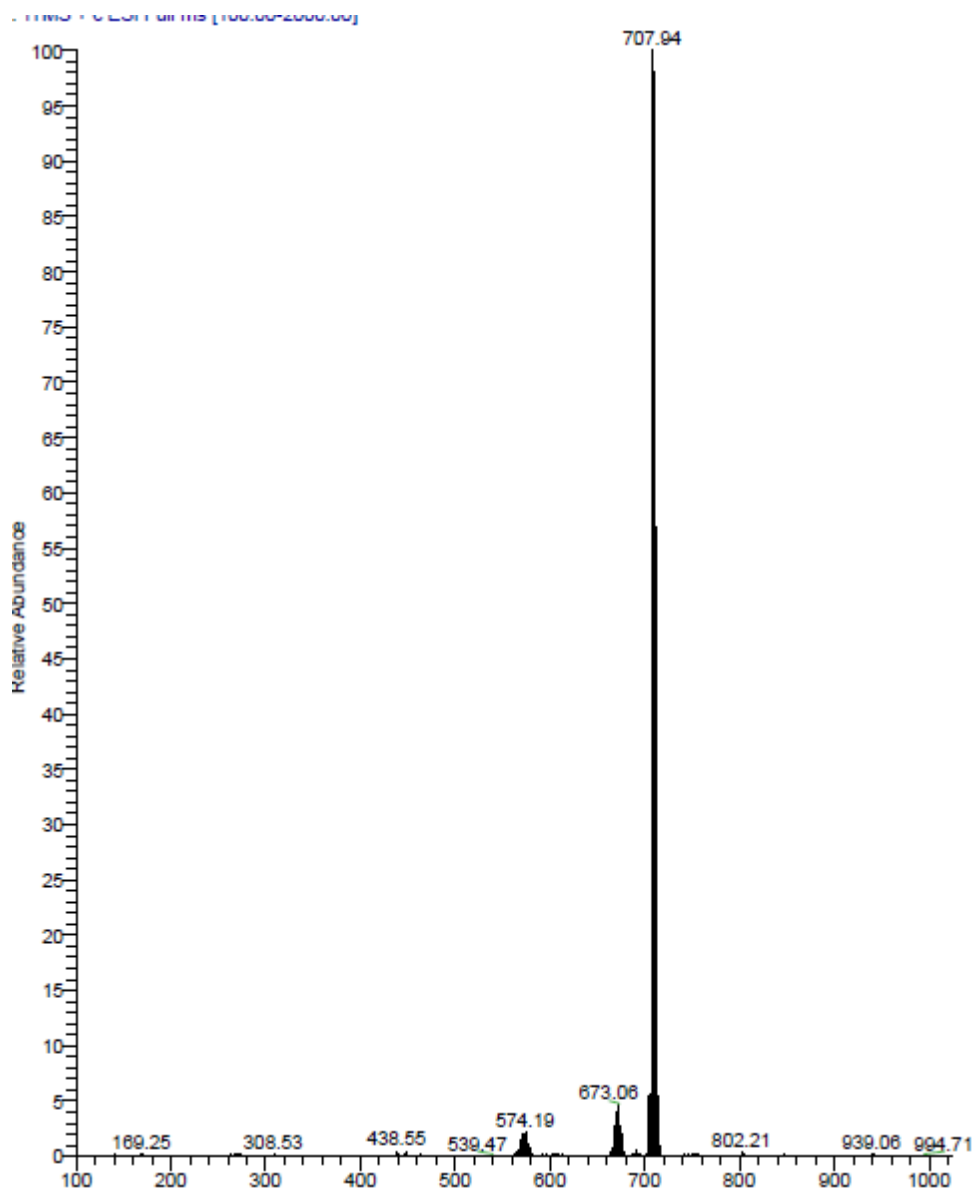


**Figure S22.** ESI-MASS Spectrum of  $[\text{Ru}(\eta^6\text{-cymene})(\text{L}2)\text{Cl}]\text{BF}_4$ . (2)

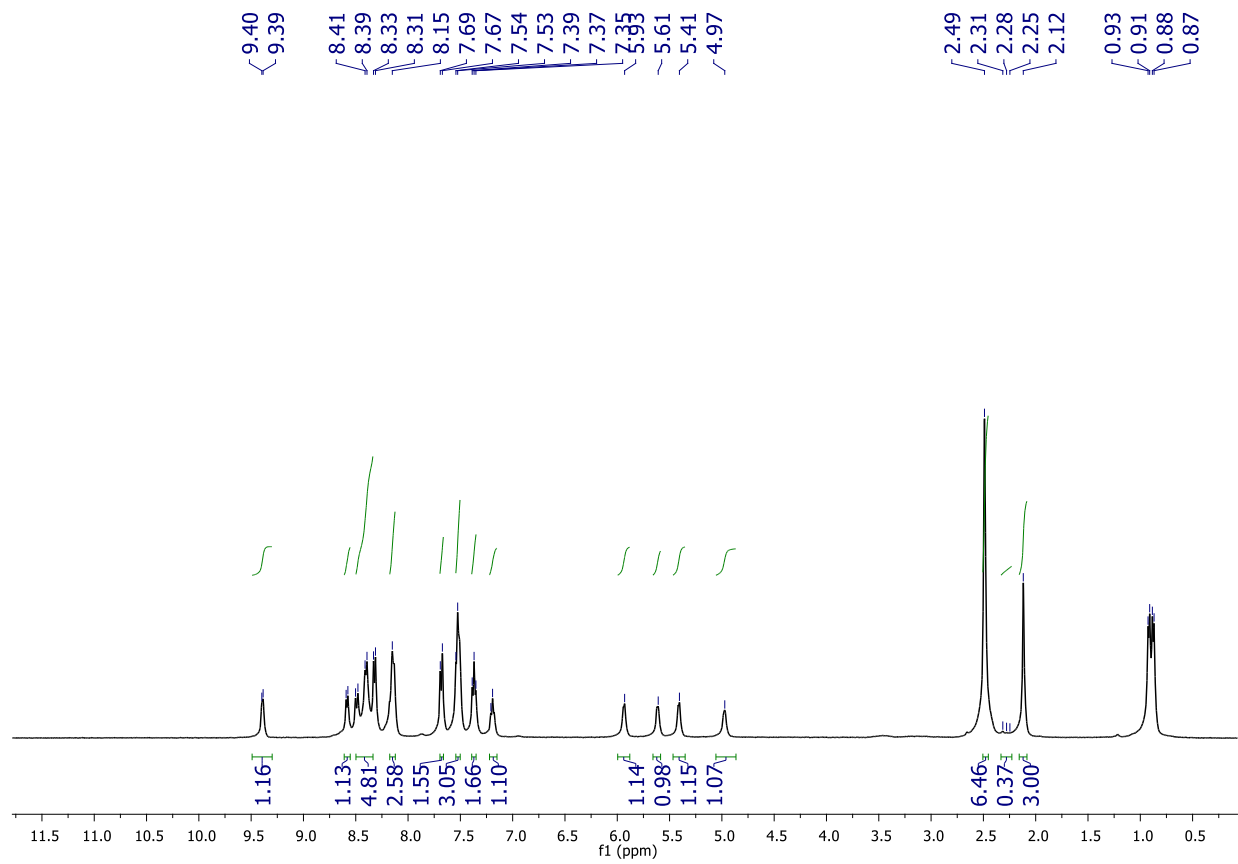


**Figure S23.**  $^1\text{H}$  NMR spectrum of  $[\text{Ru}(\eta^6\text{-cymene})(\text{L}3)\text{Cl}]\text{BF}_4$  in  $\text{DMSO-D}_6$ . (3)

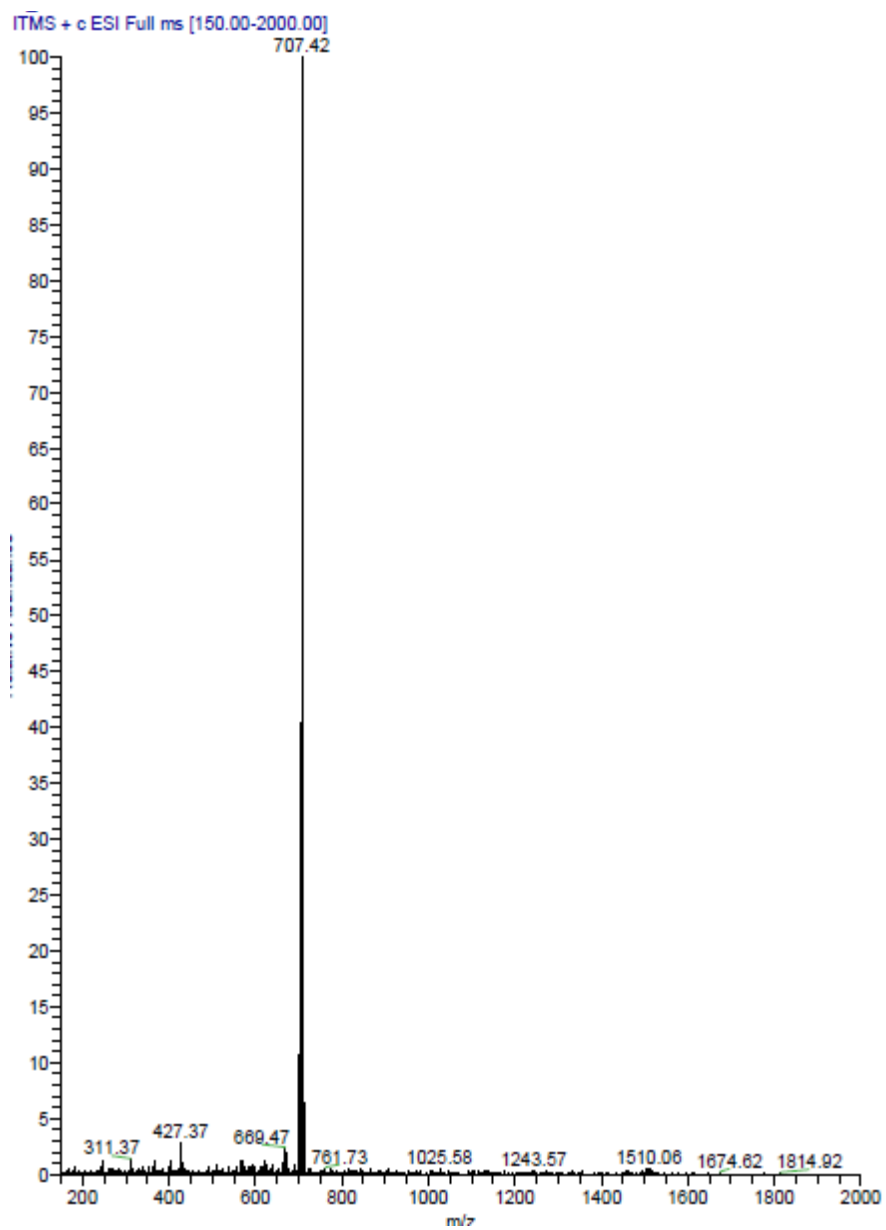




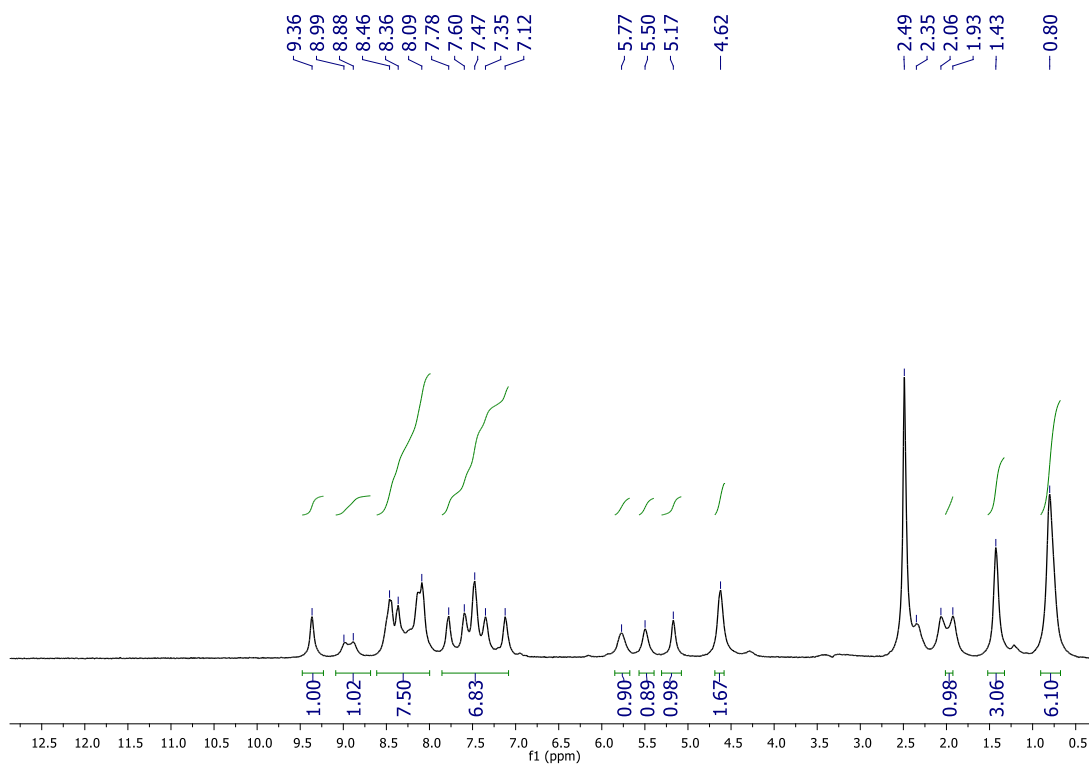
**Figure S24.** ESI-MASS Spectrum of [Ru( $\eta^6$ -cymene)(L3)Cl]BF<sub>4</sub>. (3)



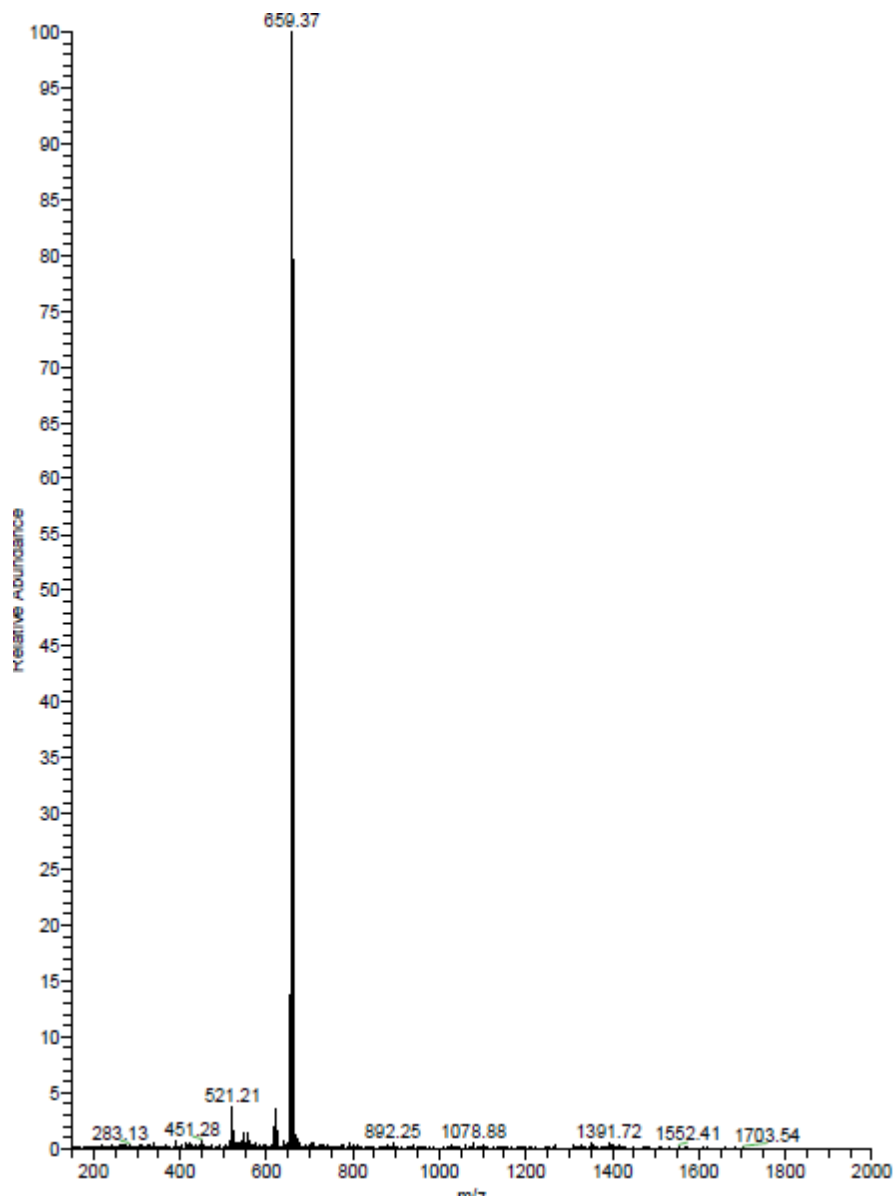
**Figure S25.**  $^1\text{H}$  NMR spectrum of  $[\text{Ru}(\eta^6\text{-cymene})(\text{L4})\text{Cl}]\text{BF}_4$  in  $\text{CDCl}_3$ . (4)



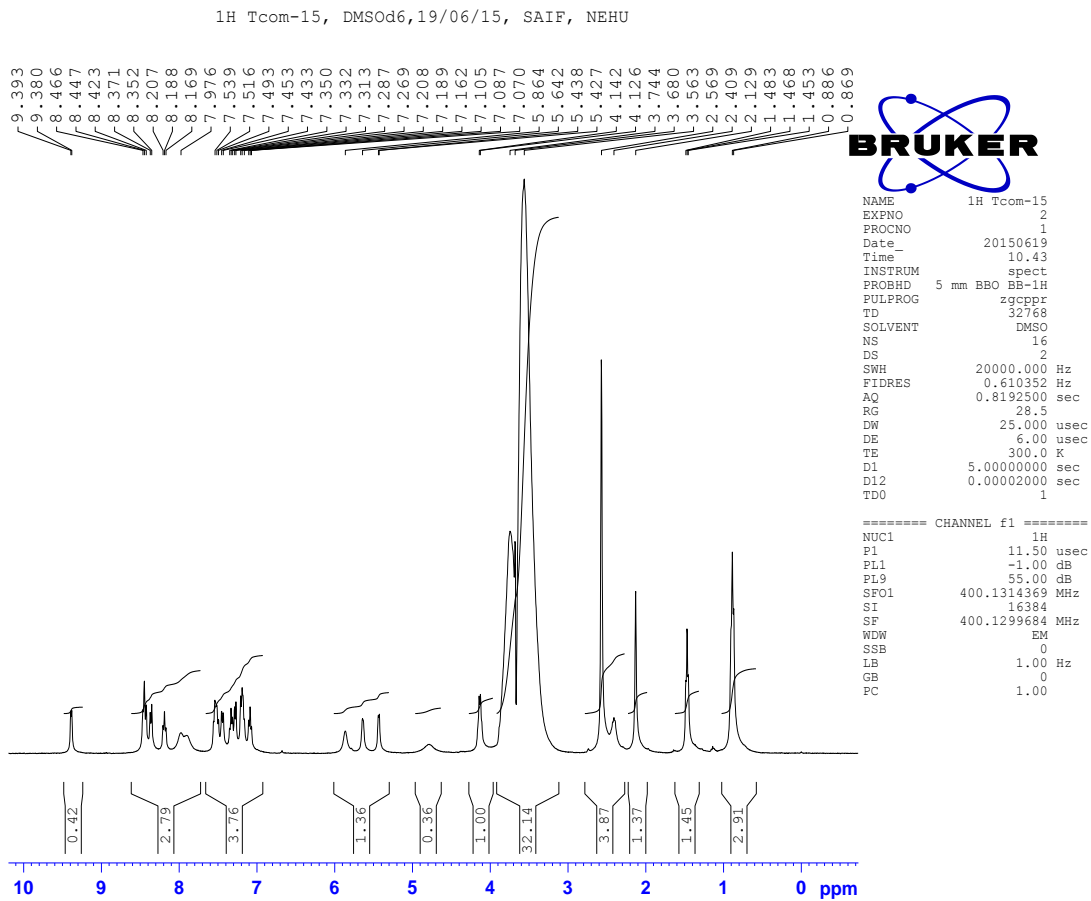
**Figure S26.** ESI-MASS Spectrum of  $[\text{Ru}(\eta^6\text{-cymene})(\text{L4})\text{Cl}]\text{BF}_4$ . (4)



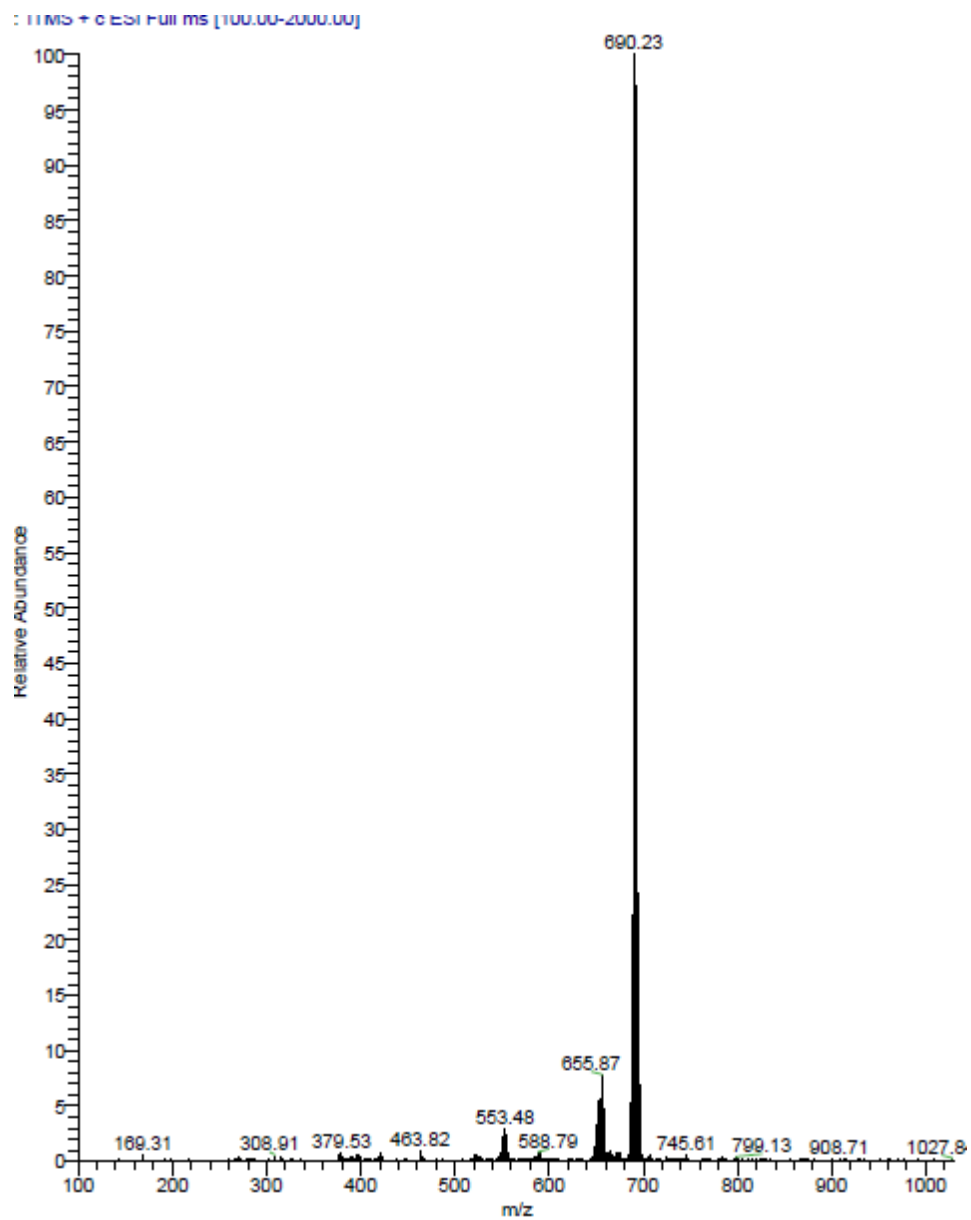
**Figure S27.** <sup>1</sup>H NMR spectrum of [Ru(η<sup>6</sup>-cymene)(L5)Cl]BF<sub>4</sub> in DMSO-D<sub>6</sub>. (5)



**Figure S28.** ESI-MASS Spectrum of  $[\text{Ru}(\eta^6\text{-cymene})(\text{L5})\text{Cl}]\text{BF}_4$ . (5)



**Figure S29.**  $^1\text{H}$  NMR spectrum of  $[\text{Ru}(\eta^6\text{-cymene})(\text{L}6)\text{Cl}]\text{BF}_4$  in  $\text{DMSO-D}_6$ . (6)



**Figure S30.** ESI-MASS Spectrum of  $[\text{Ru}(\eta^6\text{-cymene})(\text{L6})\text{Cl}]\text{BF}_4$ . (6)