

Supplementary Information

New β -carboline containing imidazolium derivatives as potential VEGFR2 inhibitors: synthesis, X-ray structure, antiproliferative evaluations, and molecular modeling

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¹H NMR, ¹³C NMR and HRMS data of the target compoundsS2-S57

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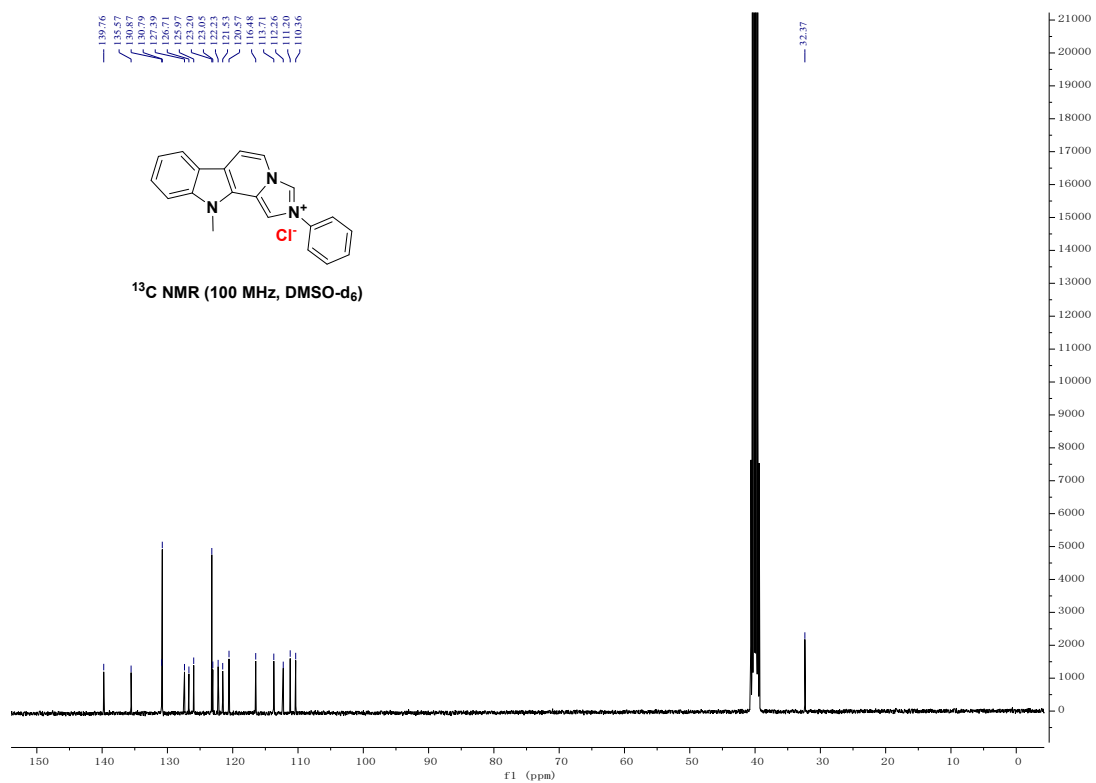
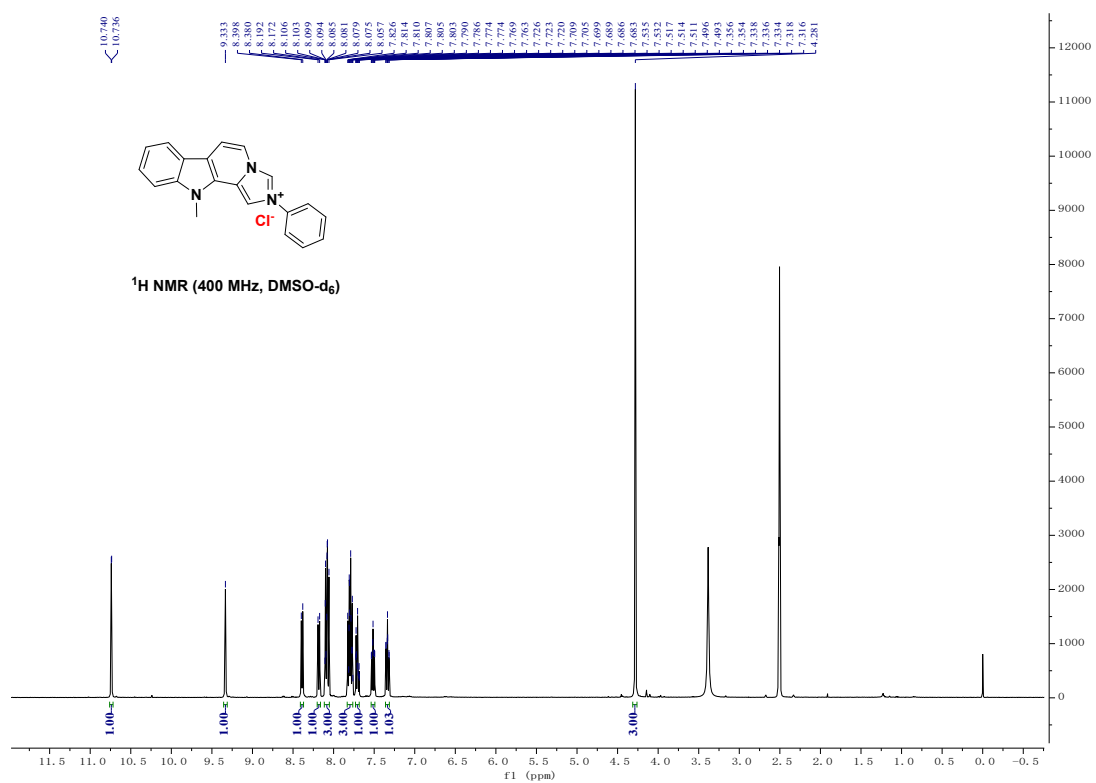


Figure S1-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3a

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T: FTMS + p ESI Full ms [150.00-2000.00]

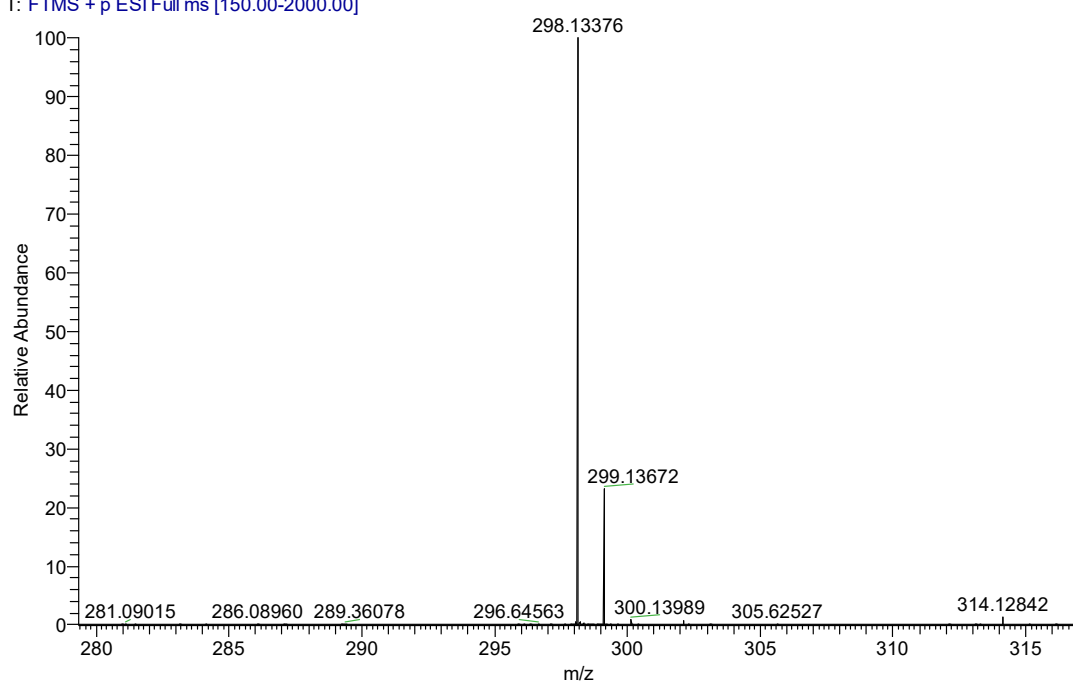


Figure S1-2 the HRMS data of compound 3a

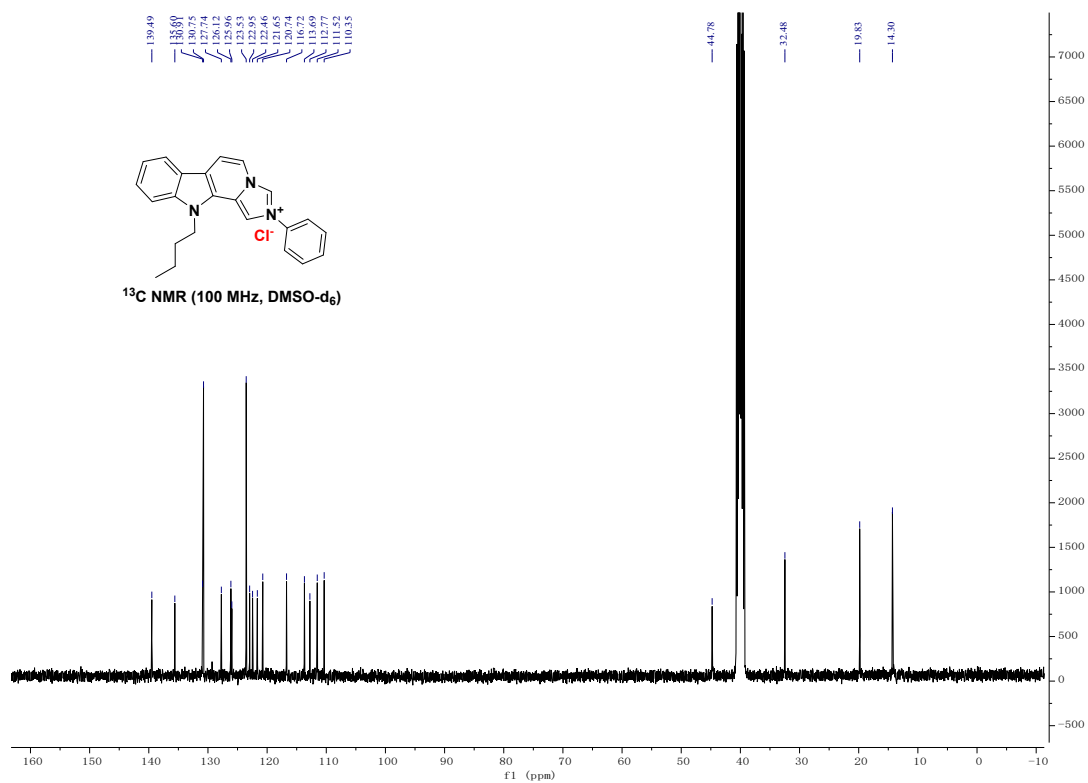
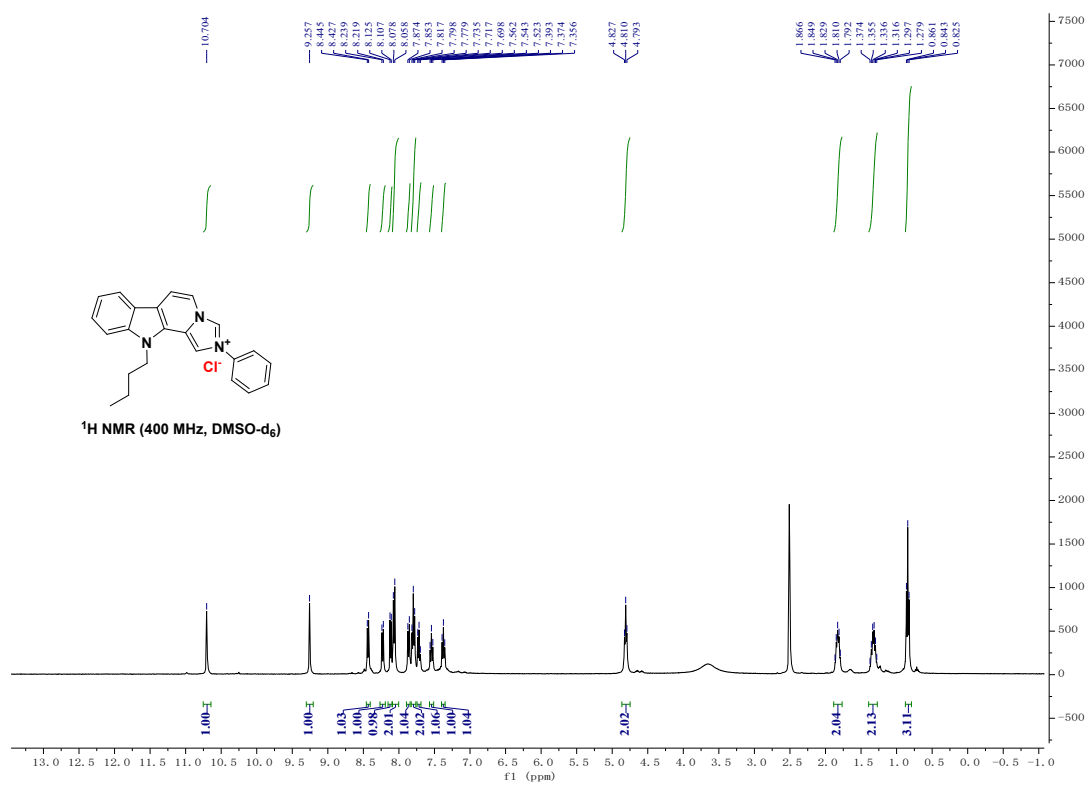


Figure S2-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3b

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T: FTMS + p ESI Full ms [150.00-2000.00]

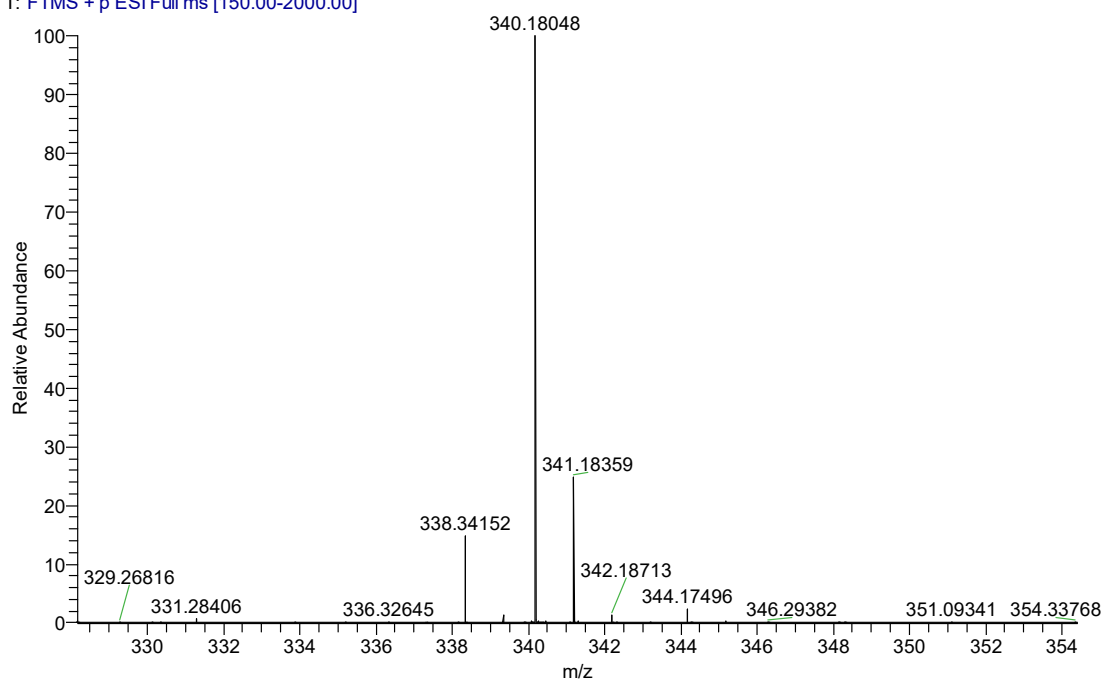


Figure S2-2 the HRMS data of compound 3b

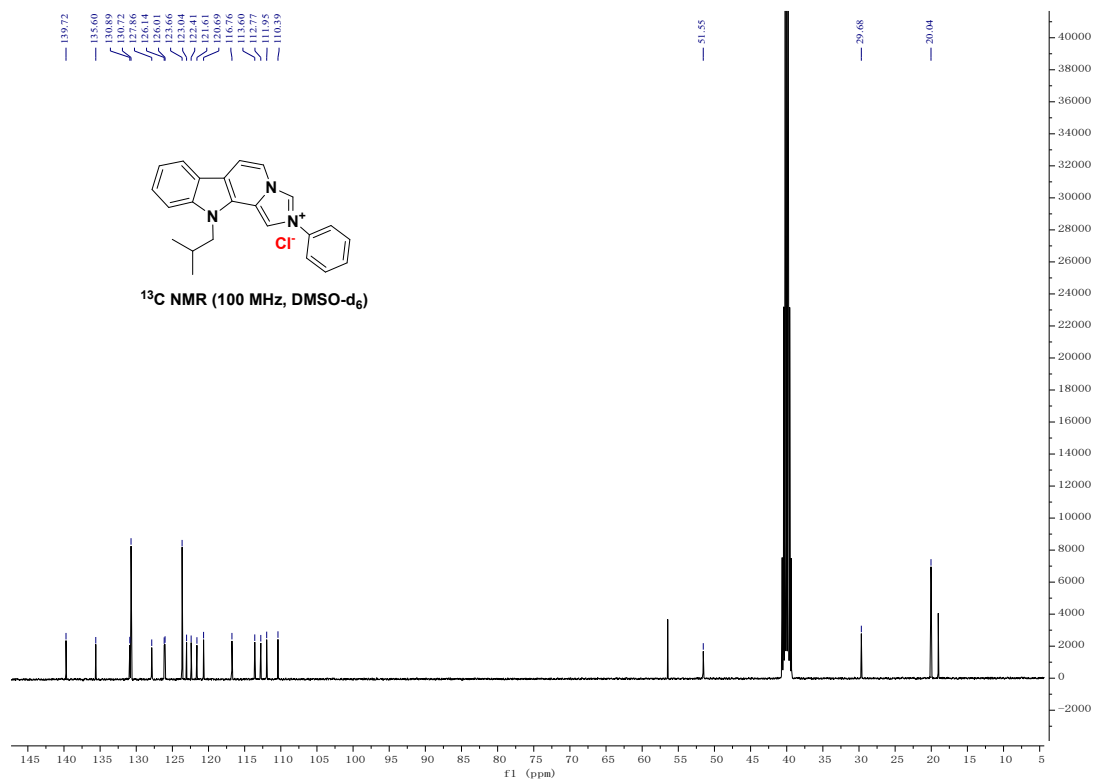
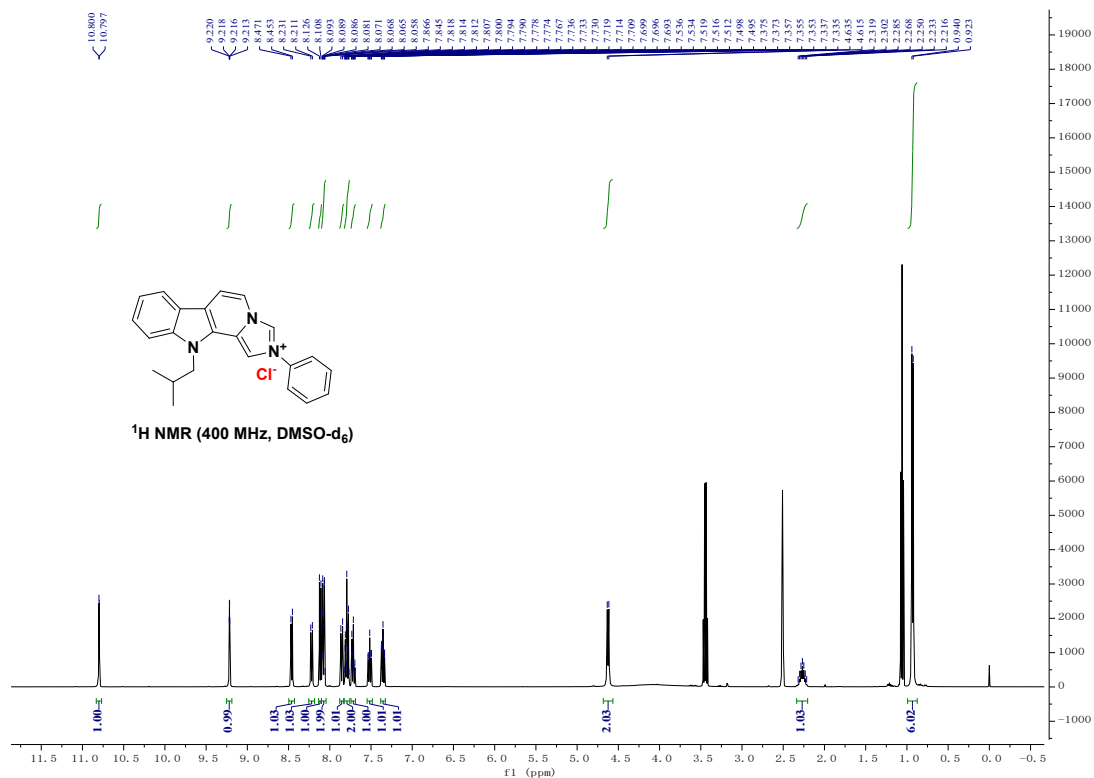


Figure S3-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound **3c**

113 #11 RT: 0.14 AV: 1 NL: 6.61E8
T: FTMS + p ESI Full ms [150.00-2000.00]

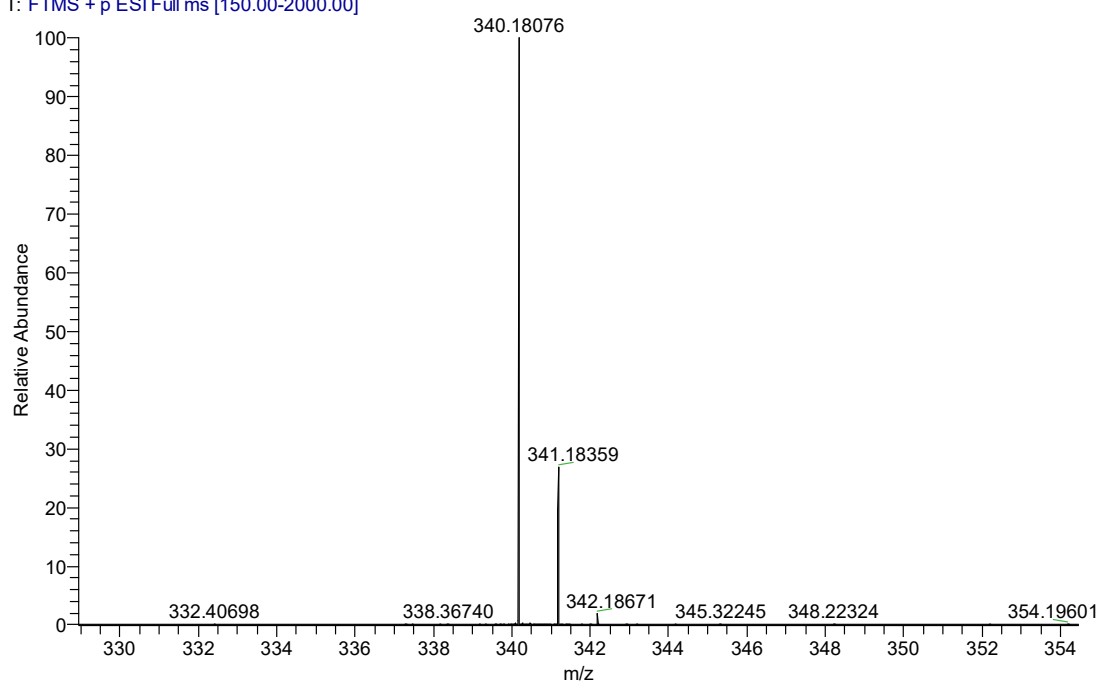


Figure S3-2 the HRMS data of compound 3c

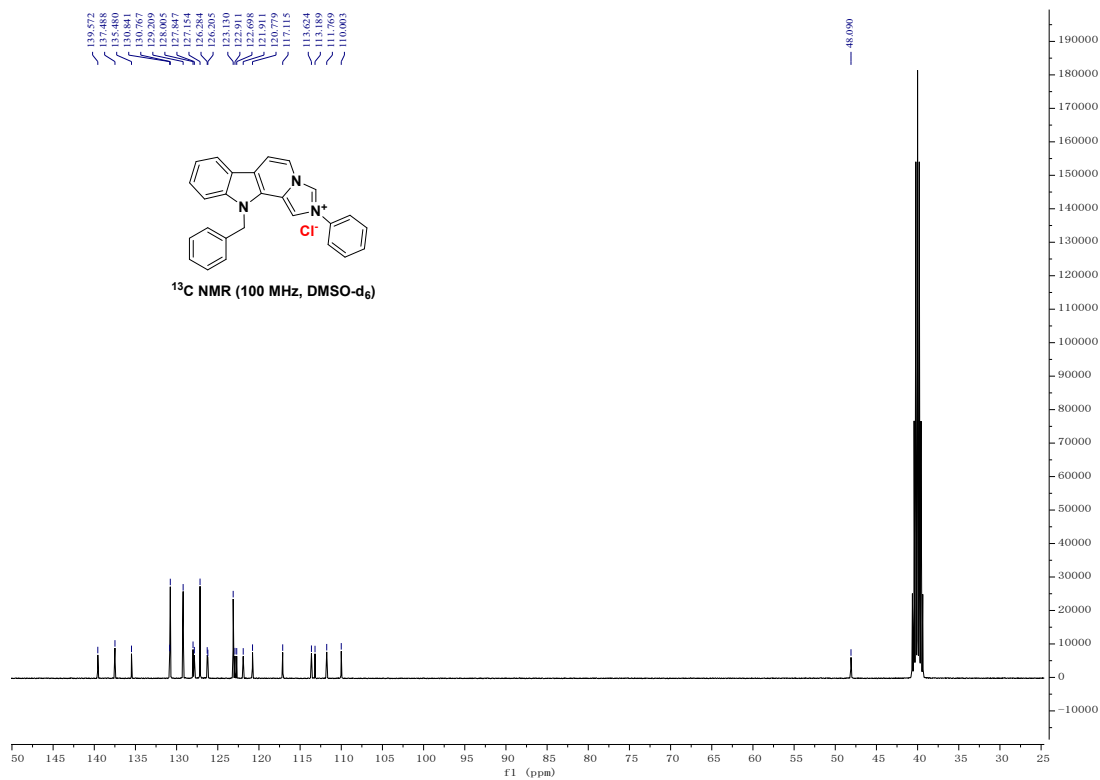
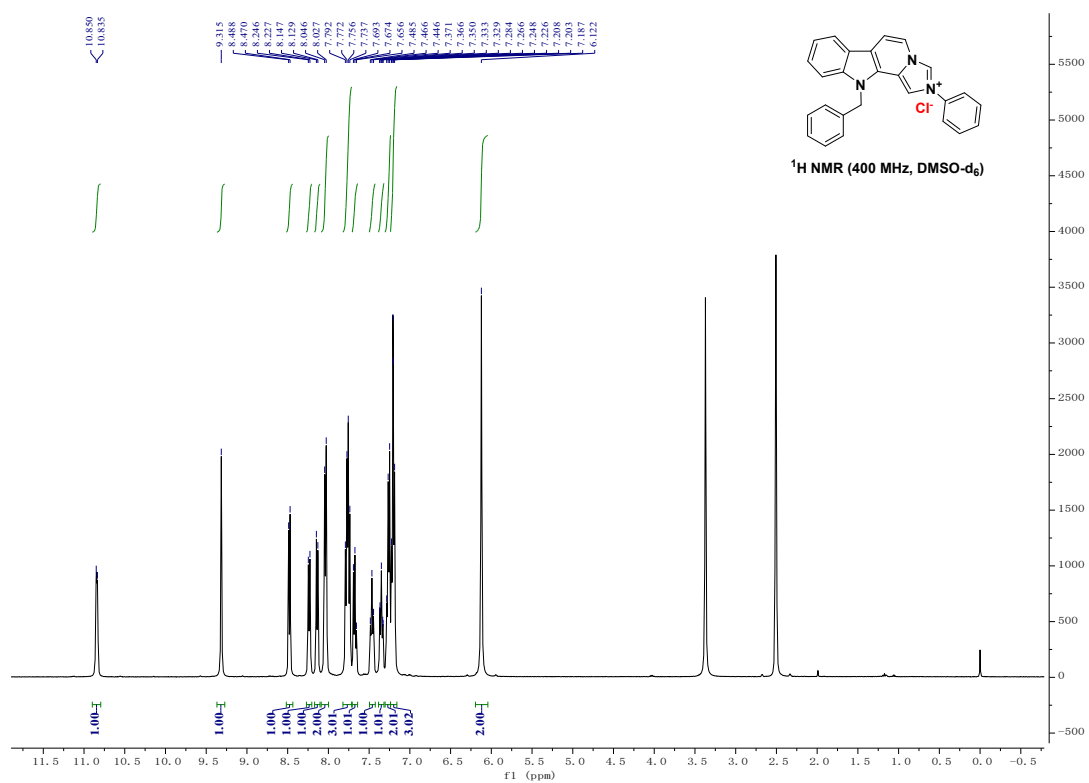


Figure S4-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3d

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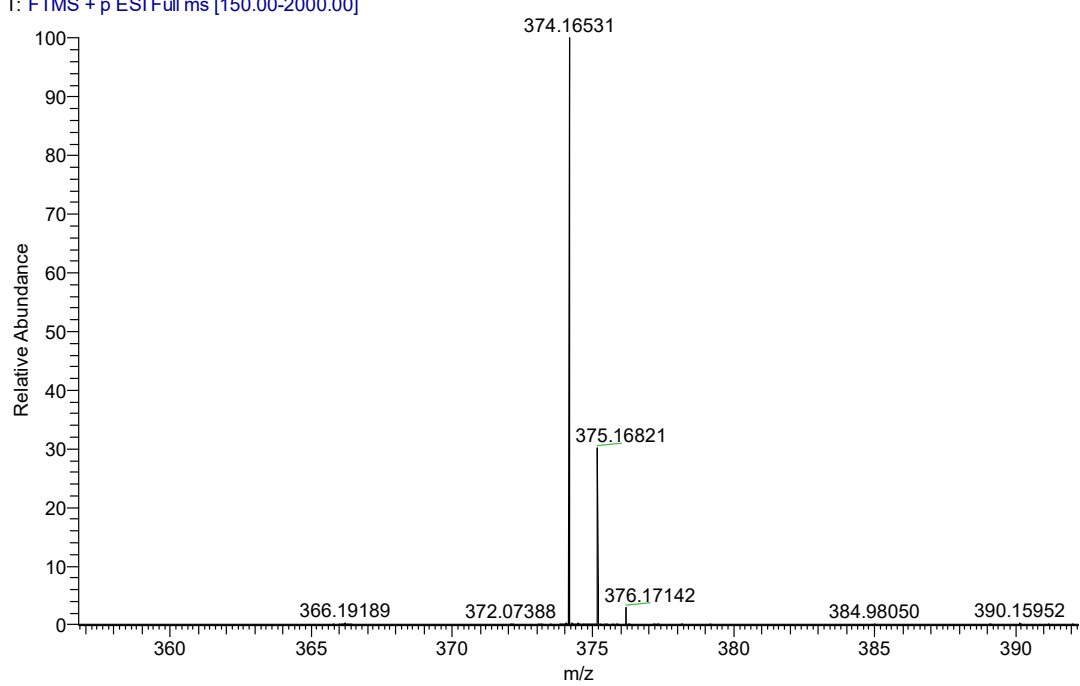


Figure S4-2 the HRMS data of compound **3d**

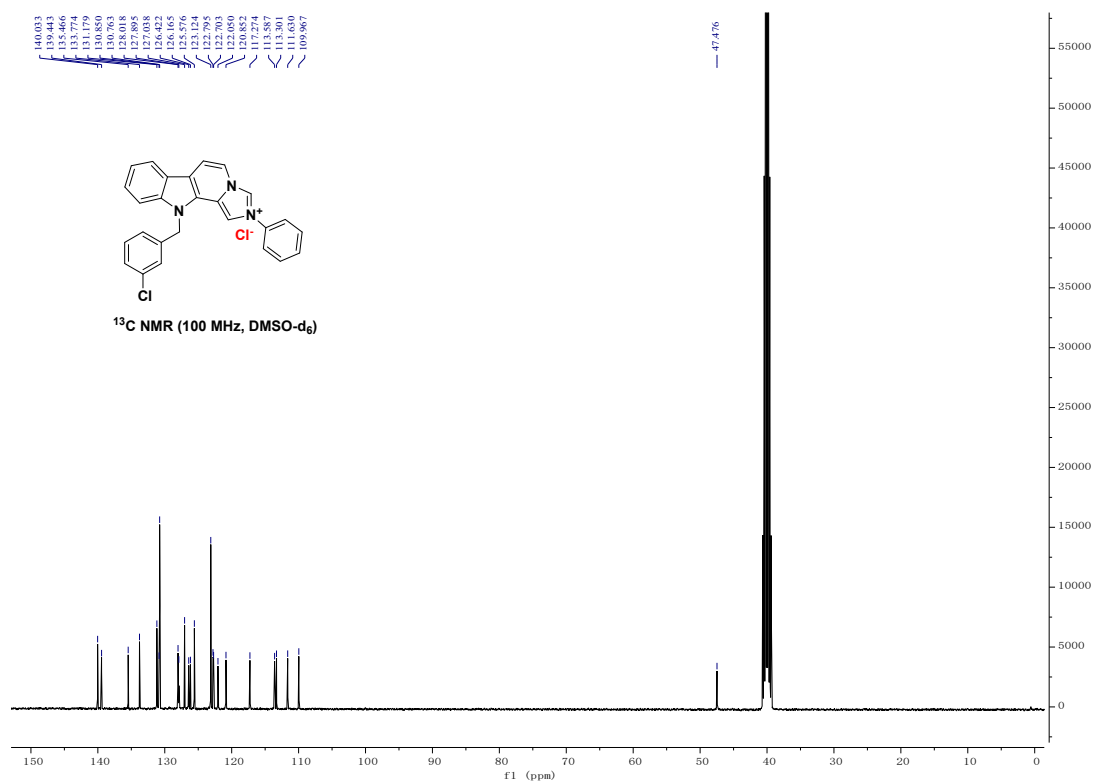
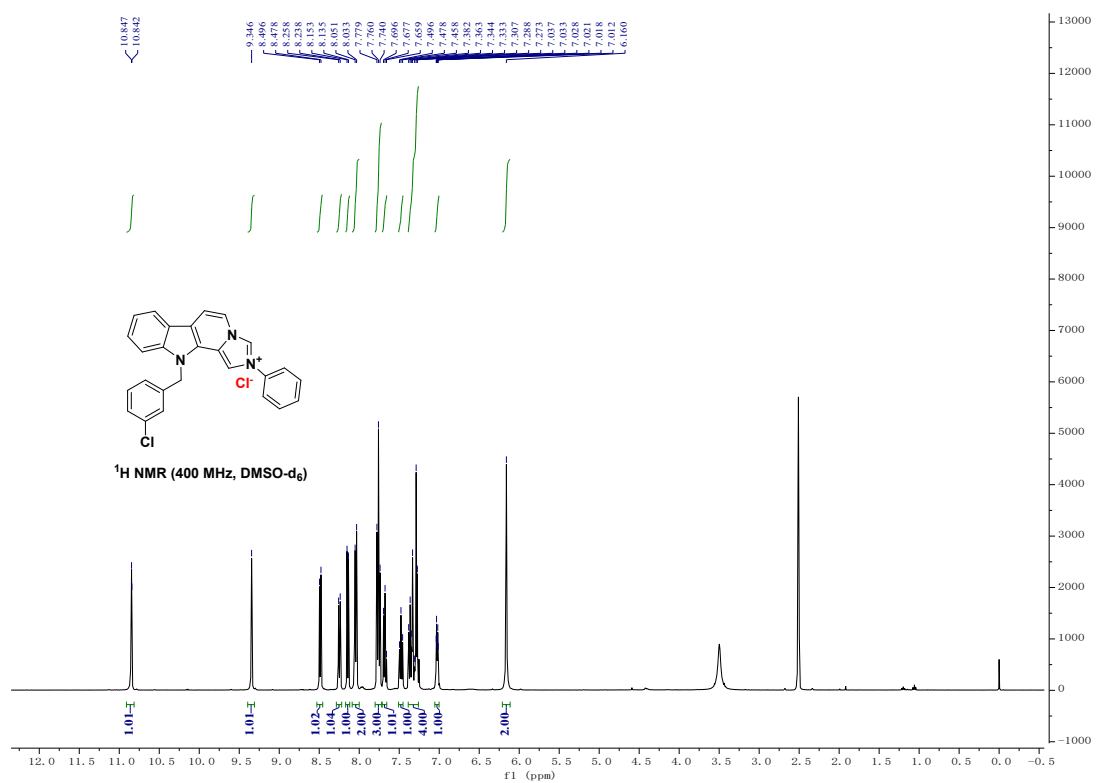


Figure S5-1 the ^1H NMR spectrum and ^{13}C NMR spectrum of compound **3e**

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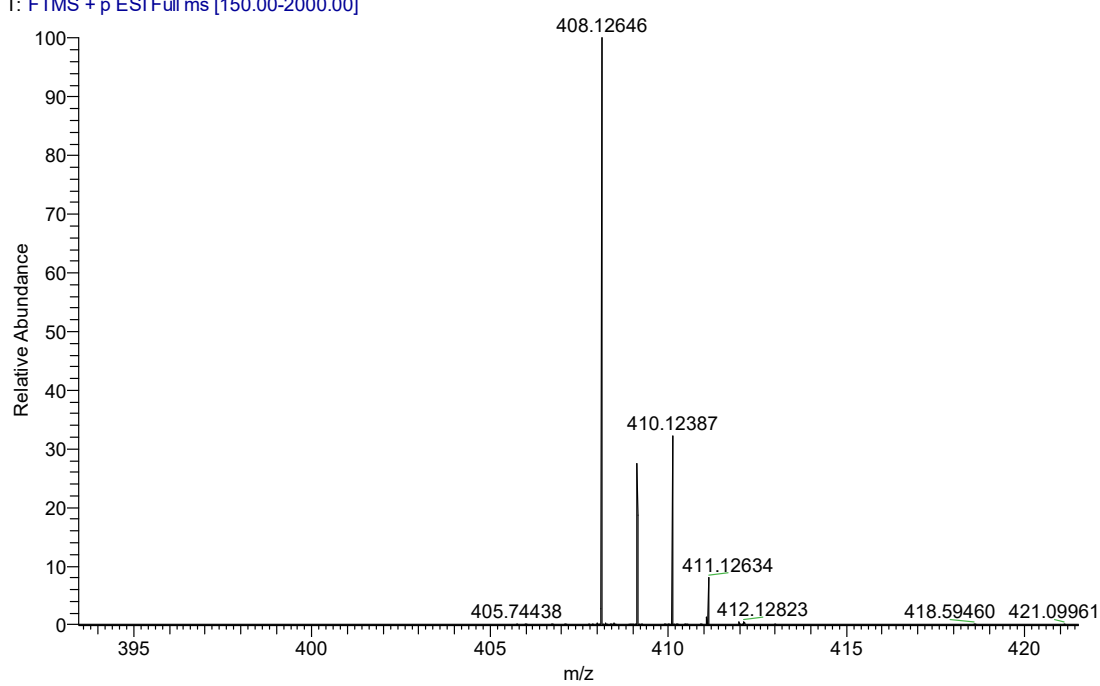


Figure S5-2 the HRMS data of compound 3e

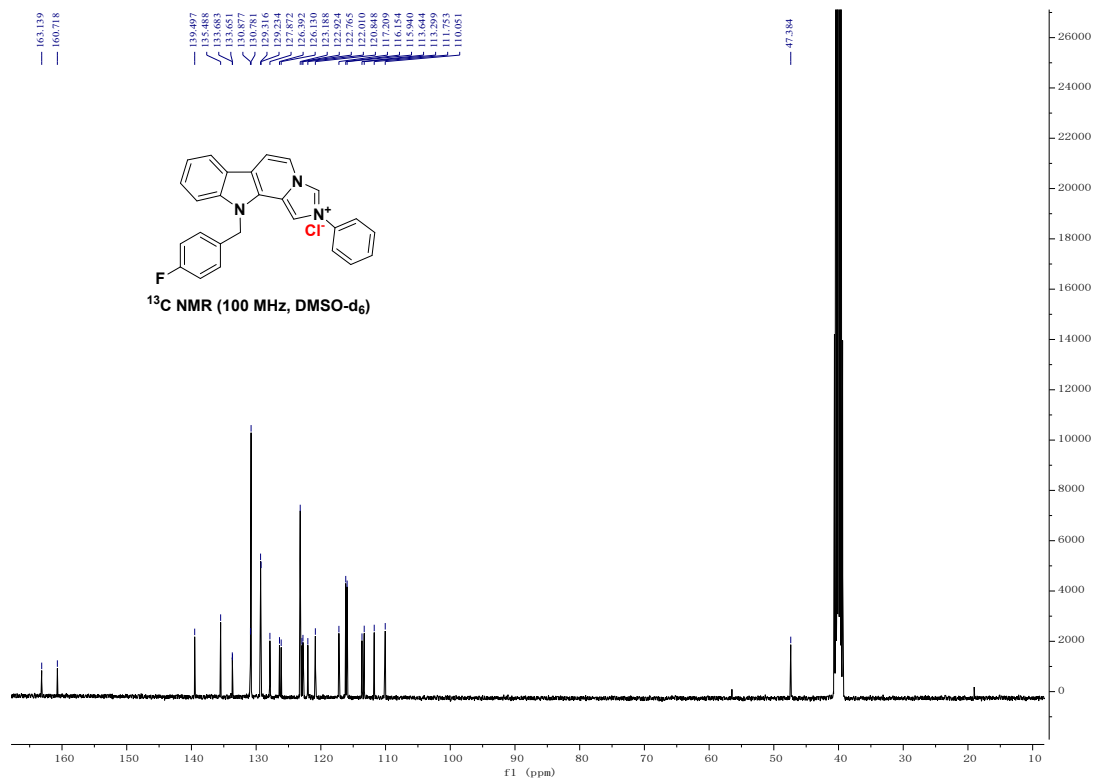
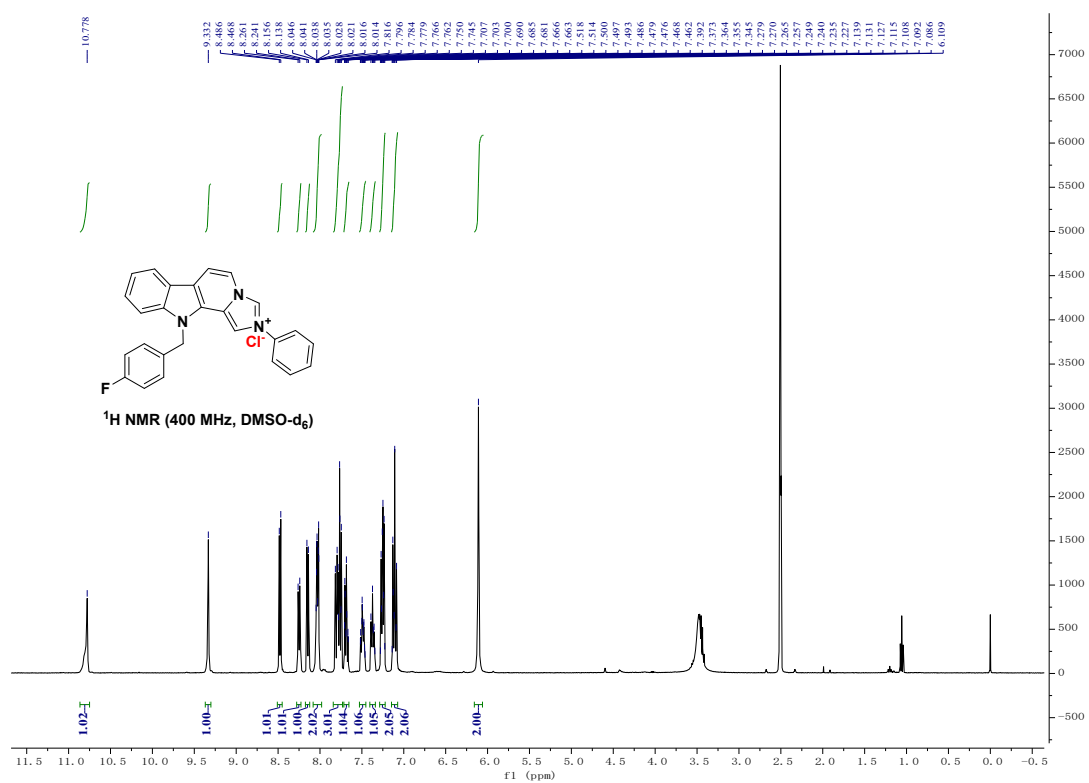


Figure S6-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3f

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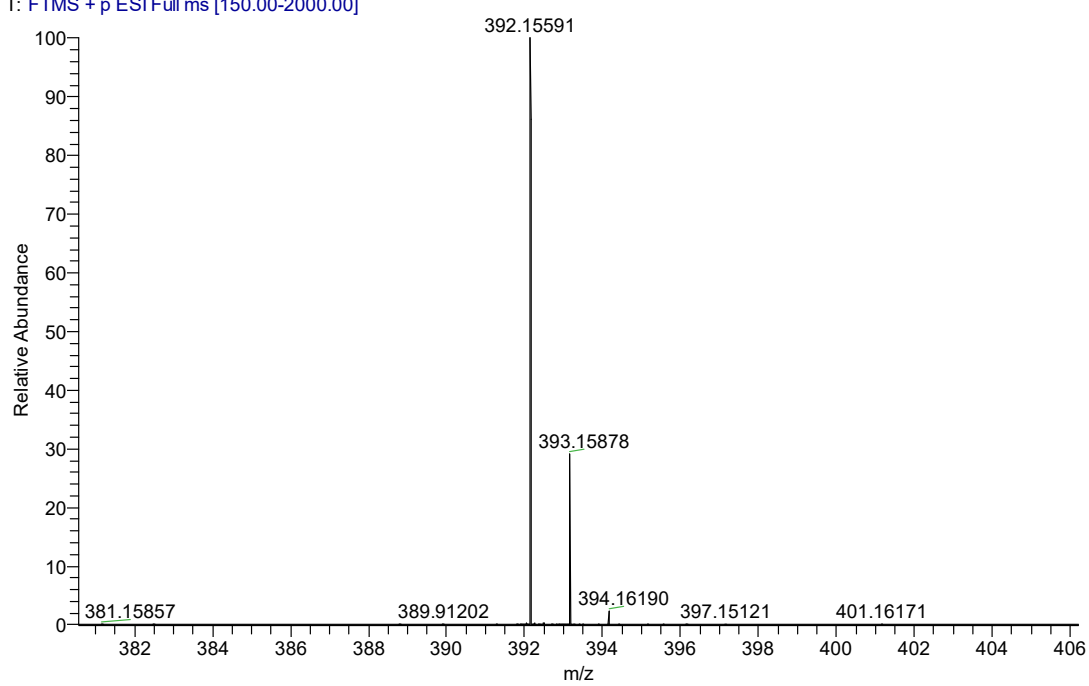


Figure S6-2 the HRMS data of compound 3f

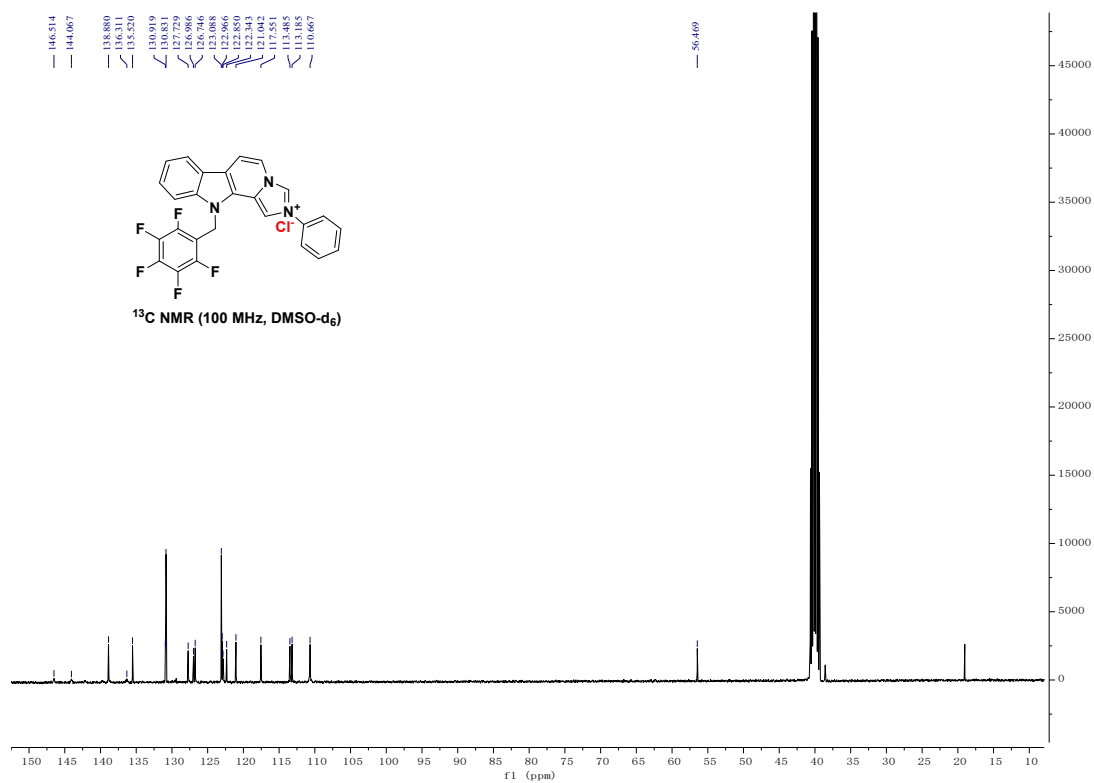
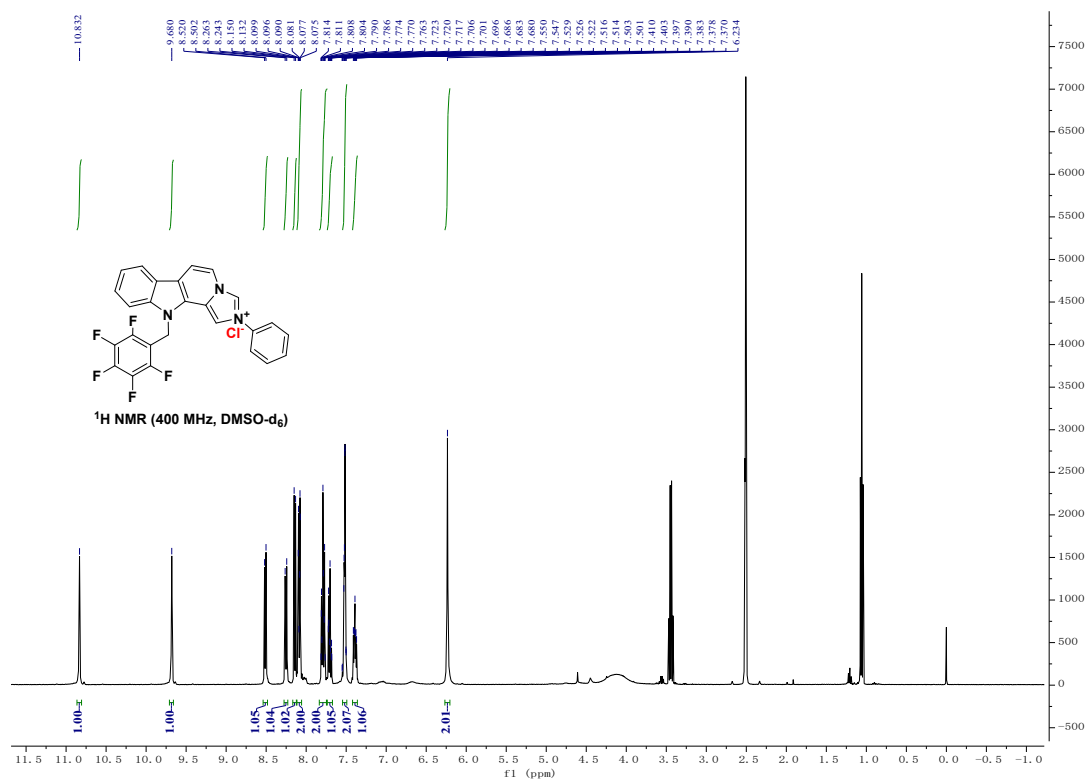


Figure S7-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3g

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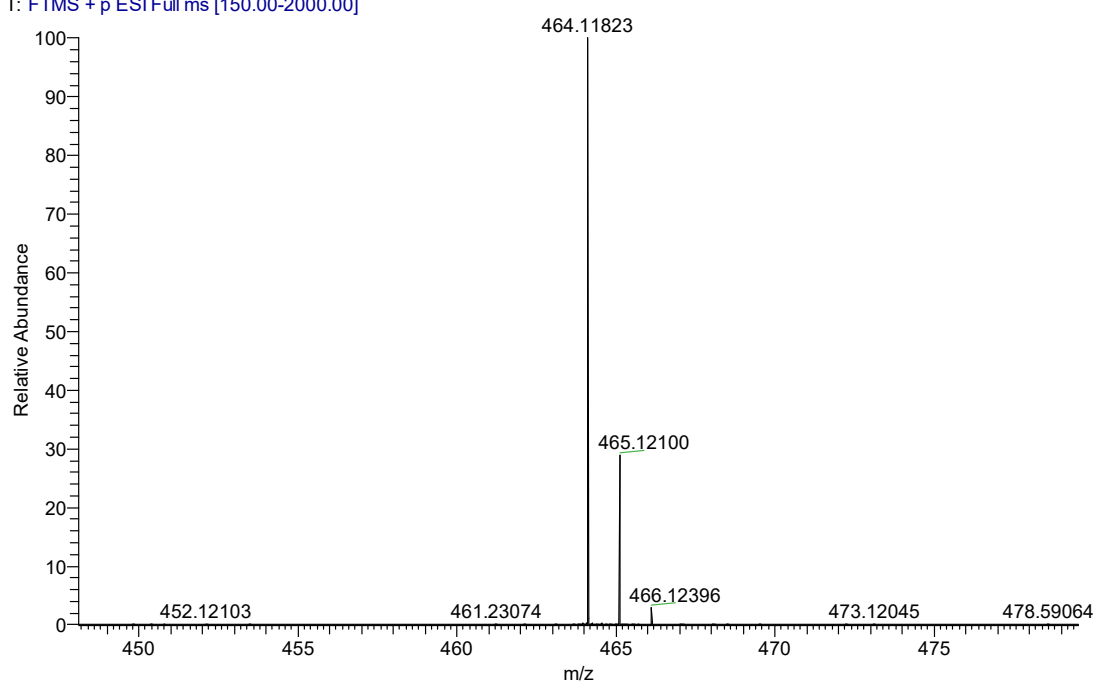


Figure S7-2 the HRMS data of compound 3g

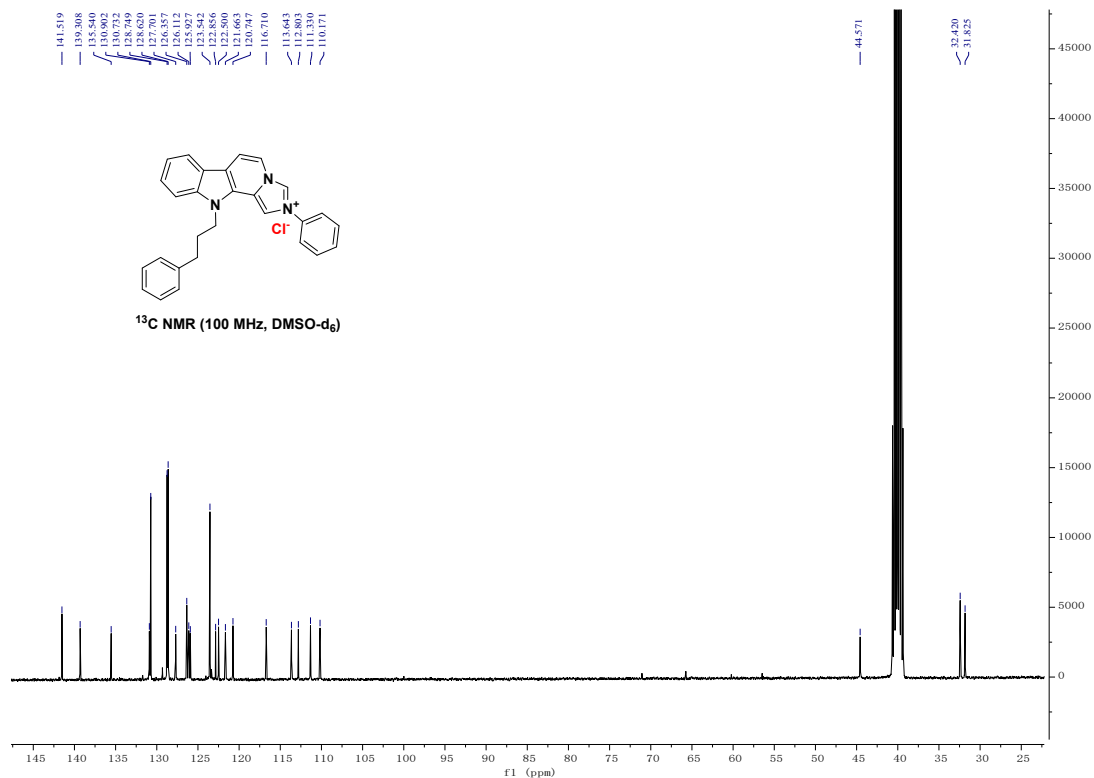
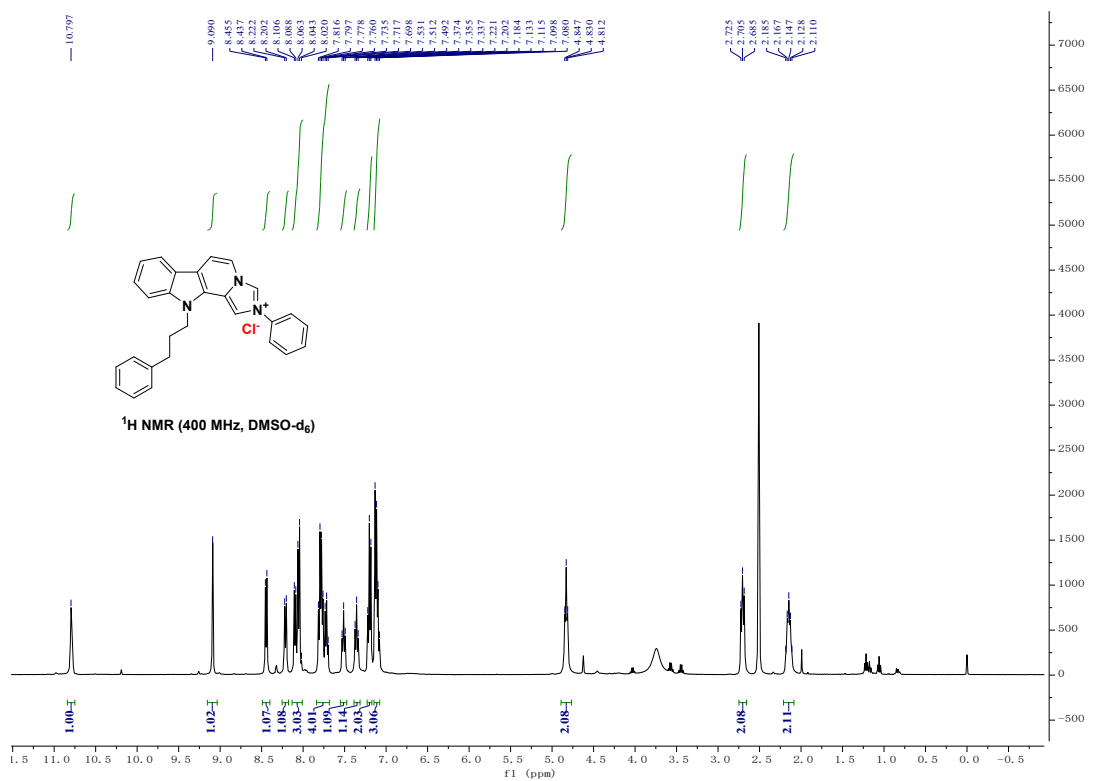


Figure S8-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3h

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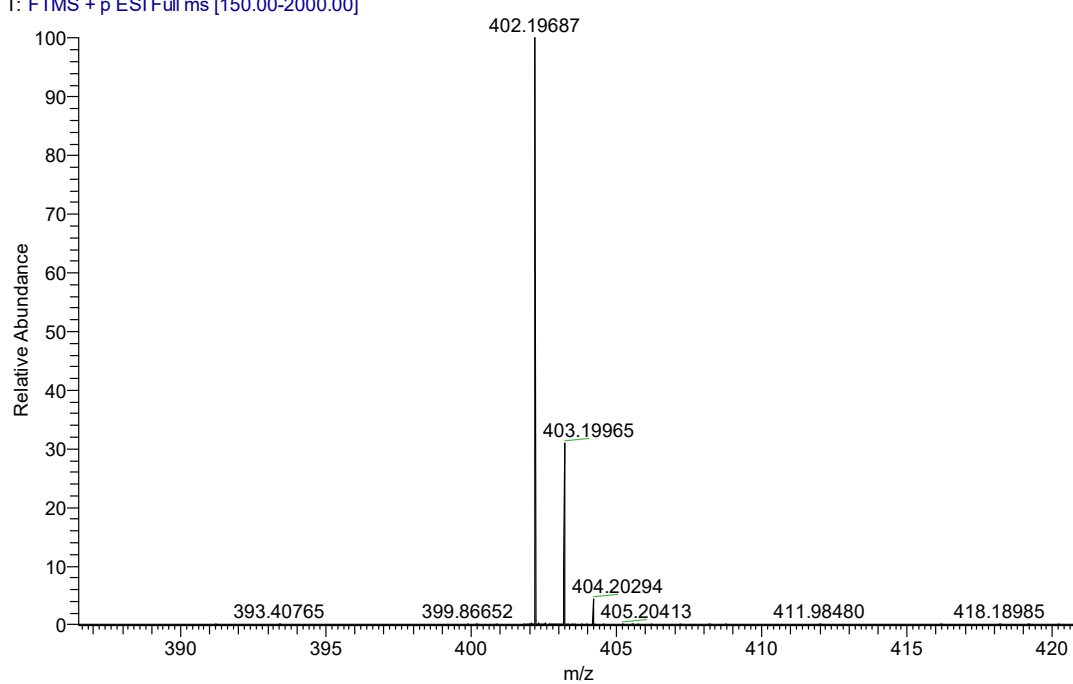


Figure S8-2 the HRMS data of compound **3h**

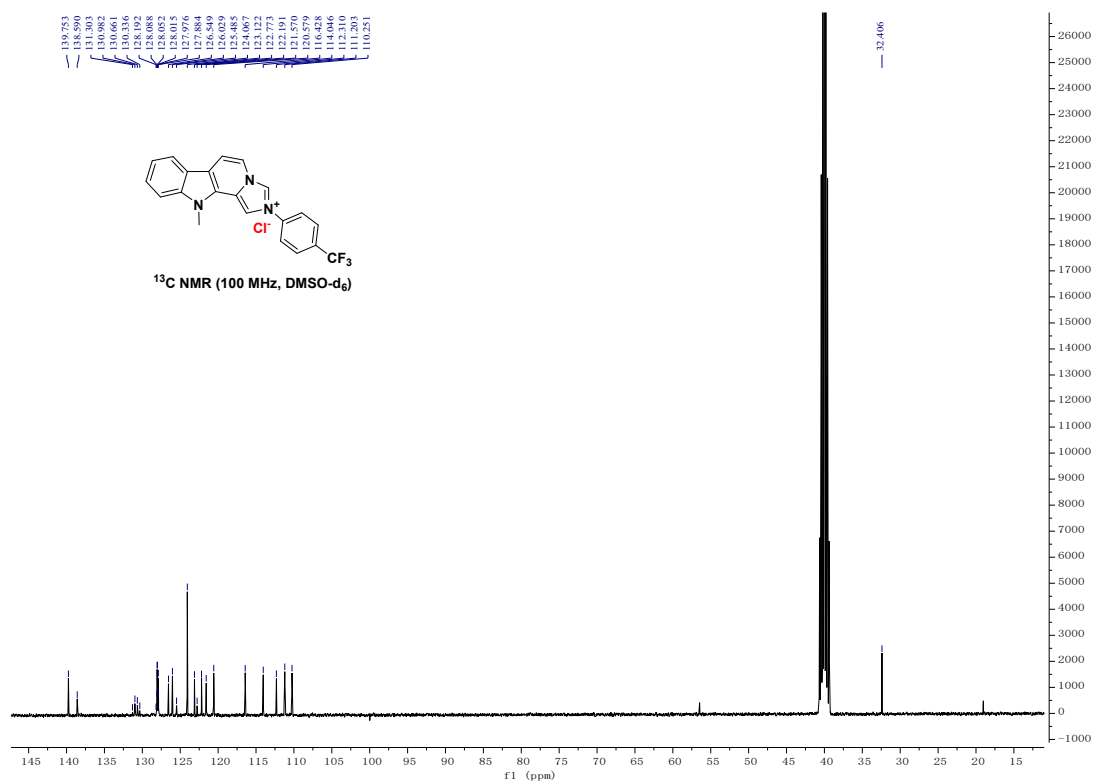
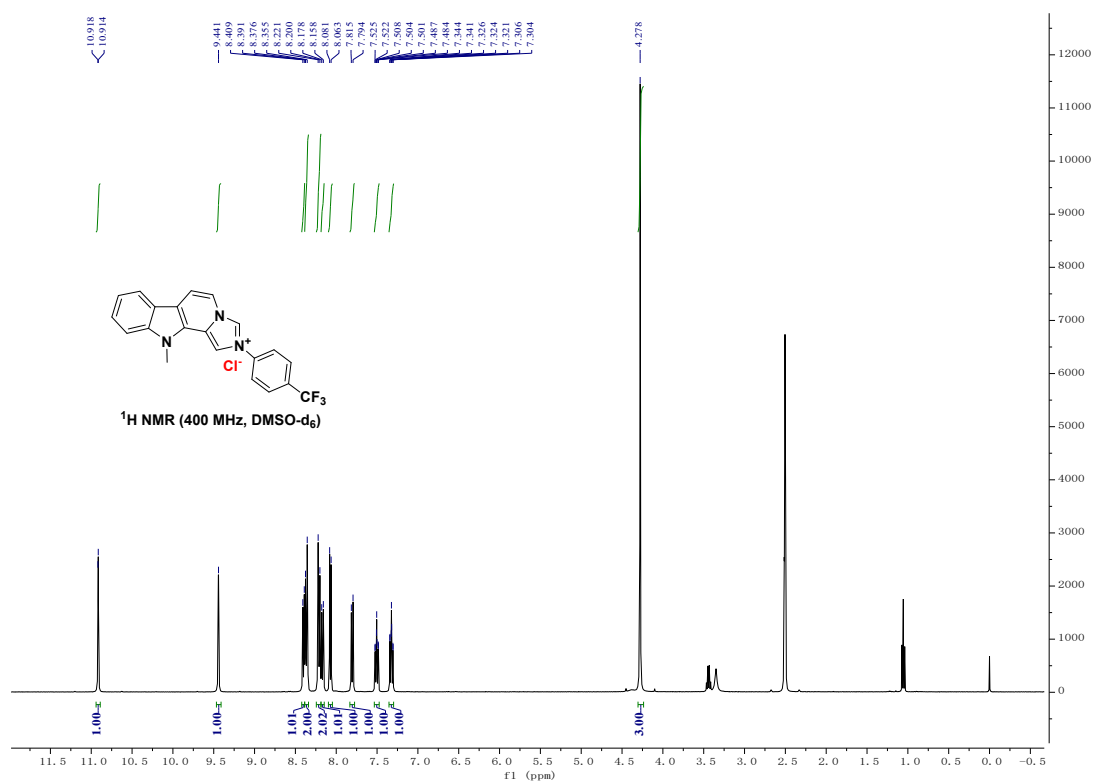


Figure S9-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound **3i**

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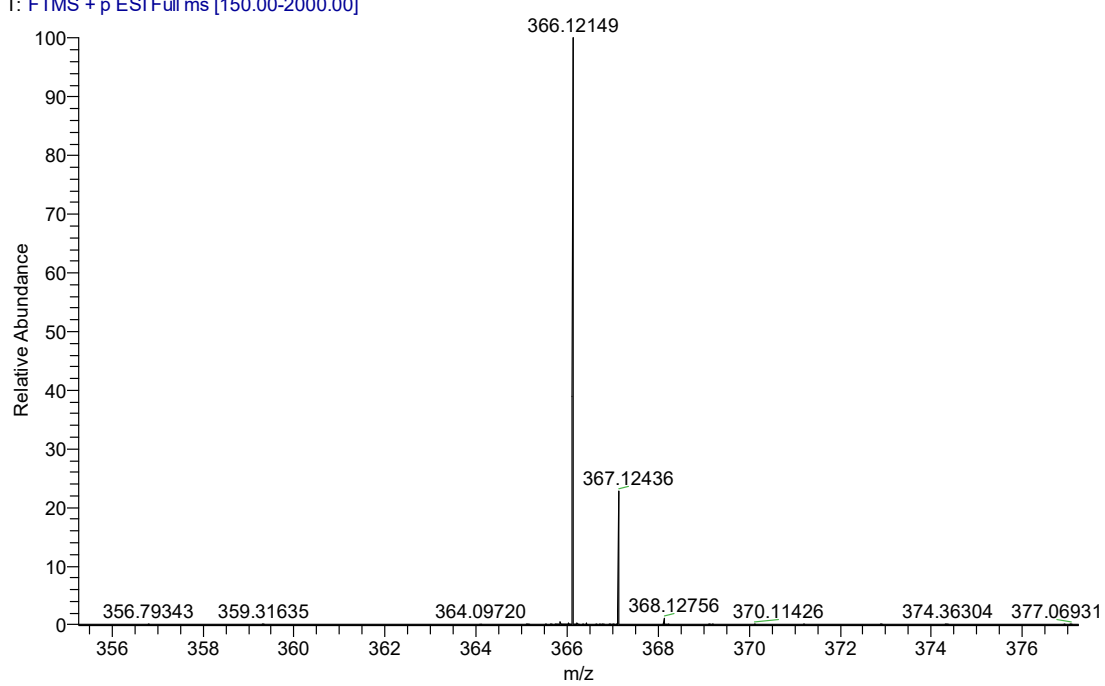


Figure S9-2 the HRMS data of compound **3i**

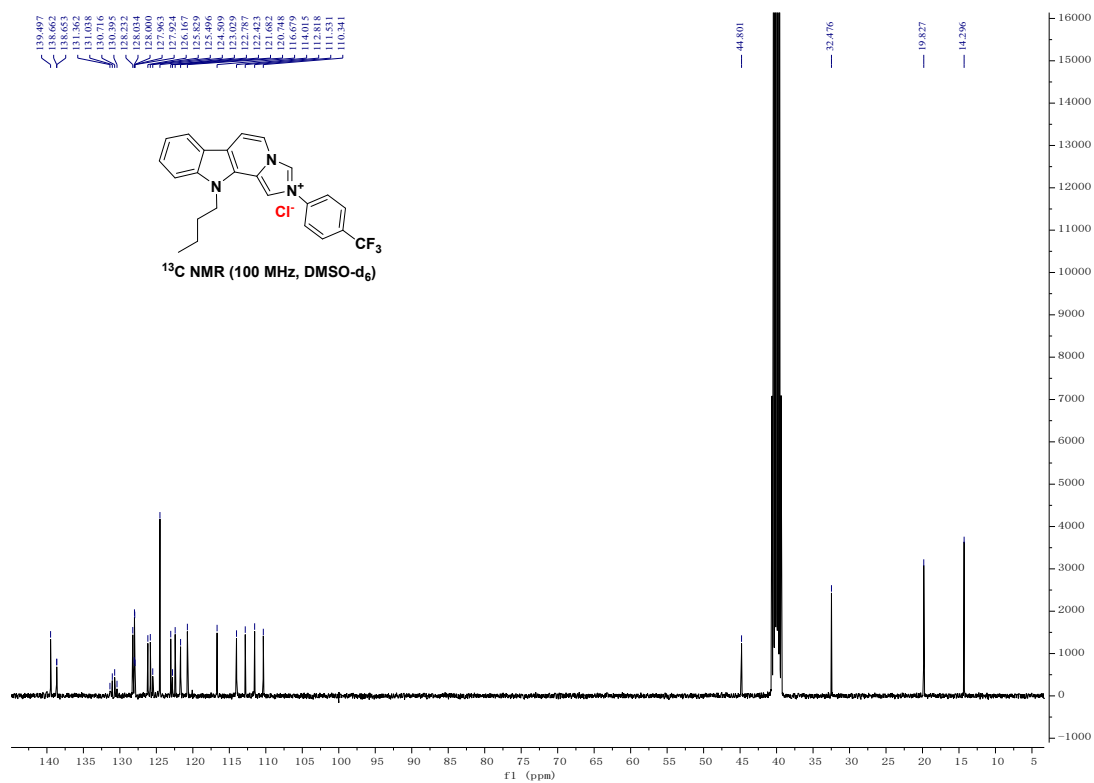
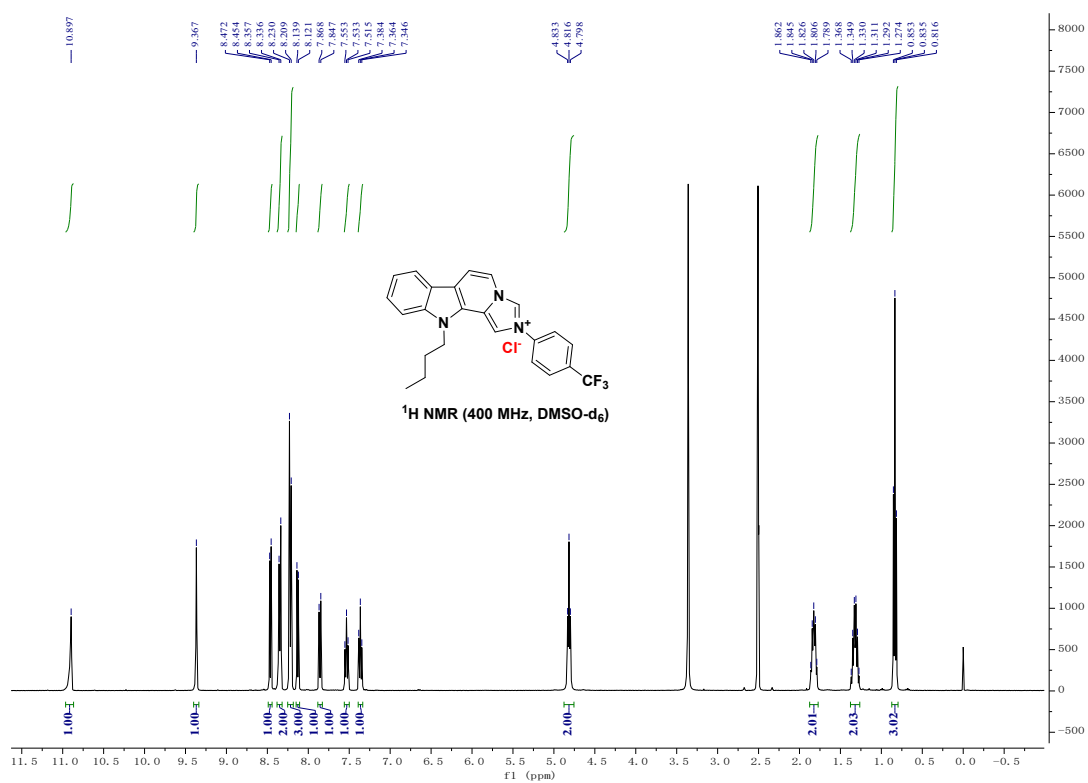


Figure S10-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound **3j**

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T: FTMS + p ESI Full ms [150.00-2000.00]

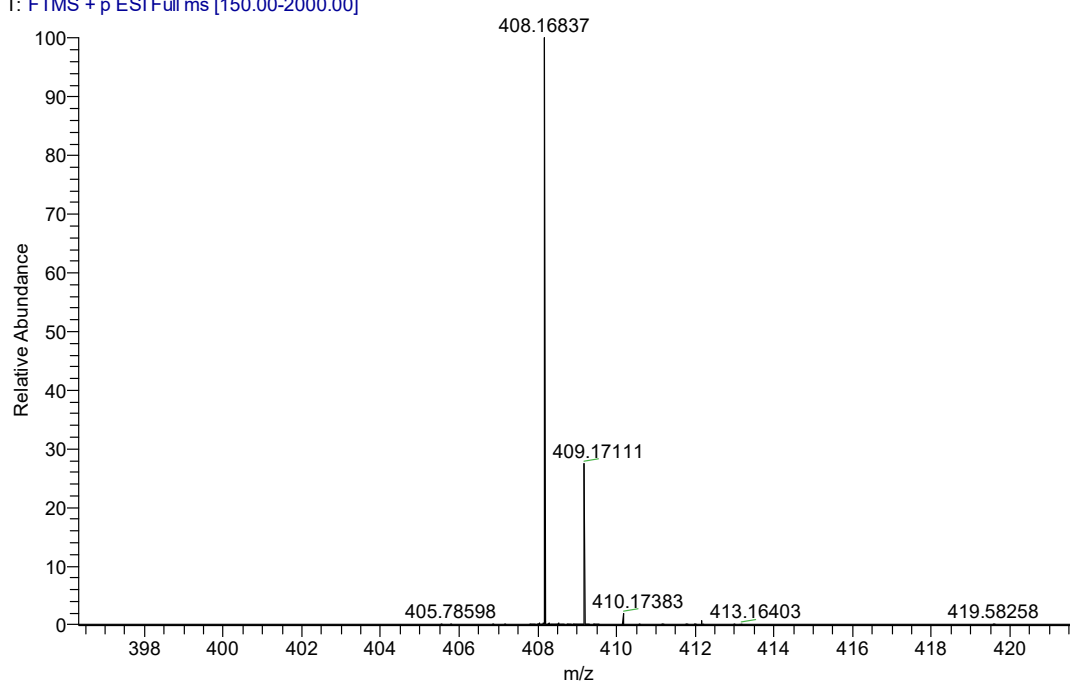


Figure S10-2 the HRMS data of compound **3j**

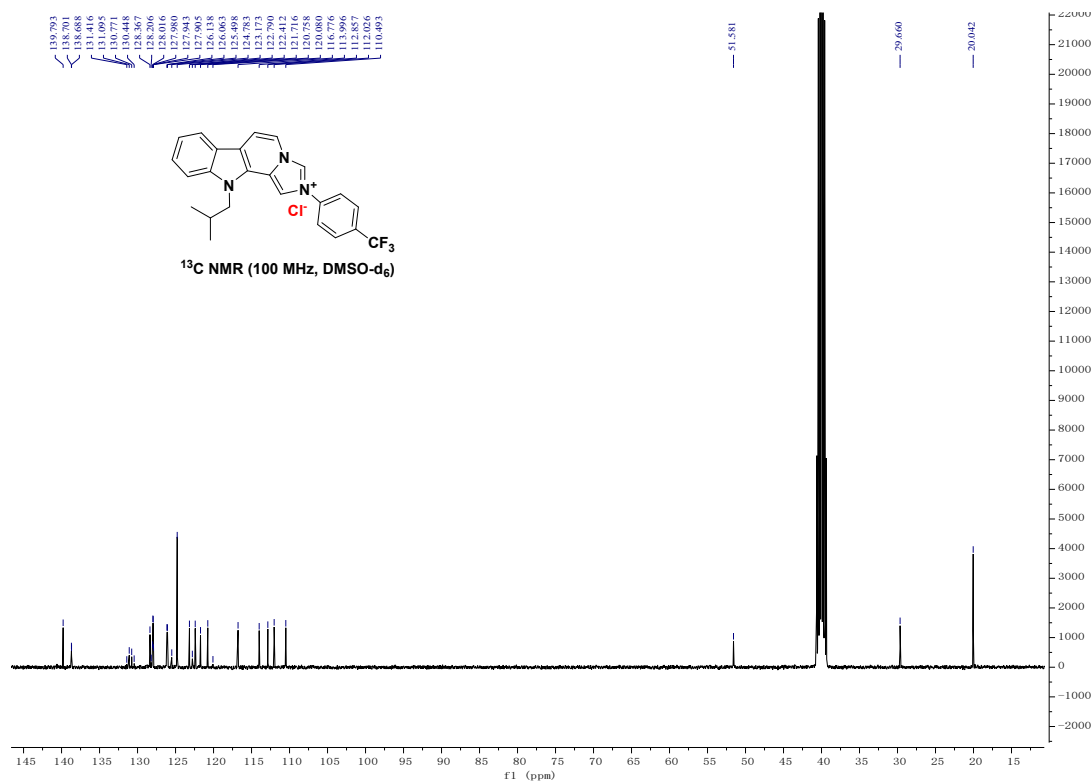
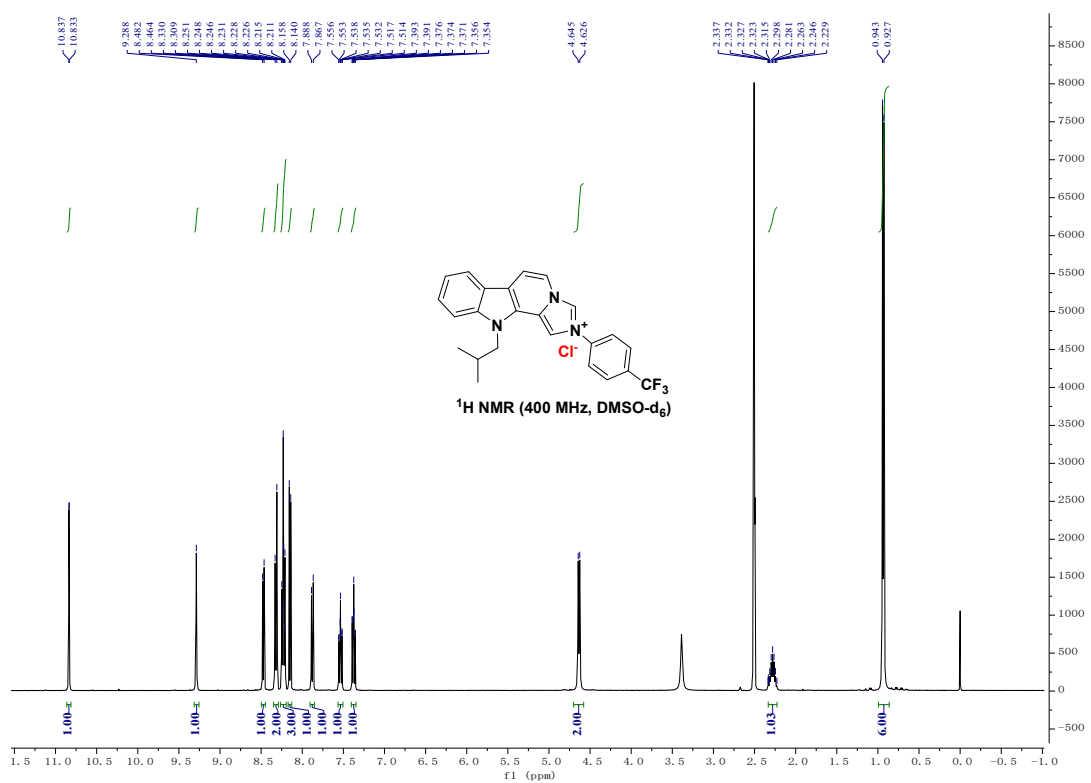


Figure S11-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3k

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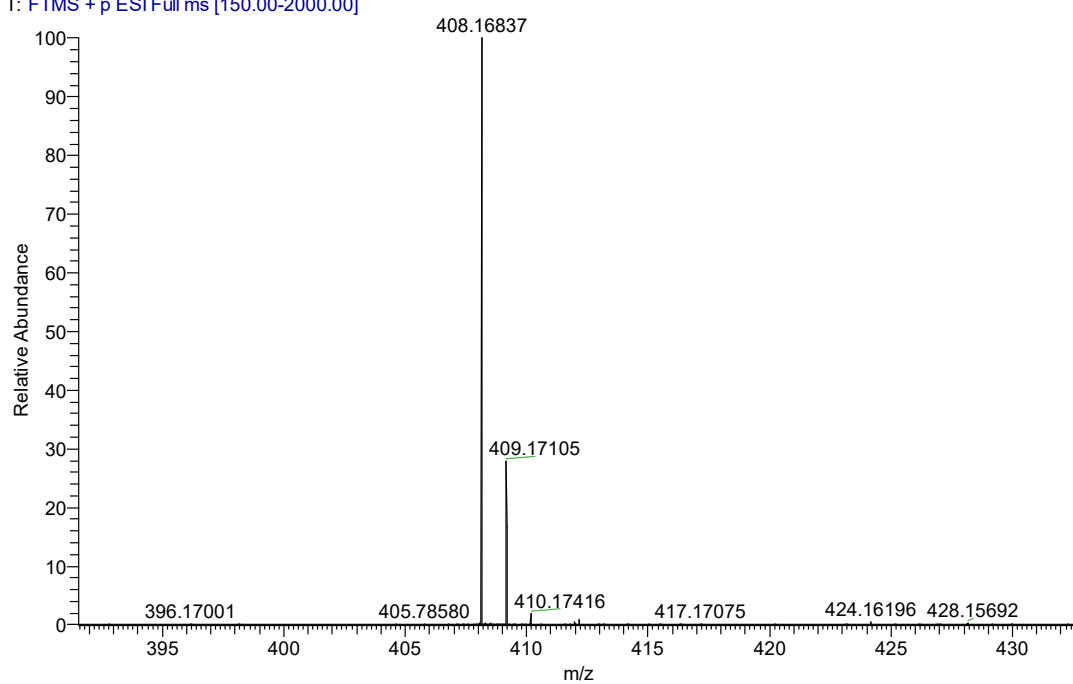


Figure S11-2 the HRMS data of compound **3k**

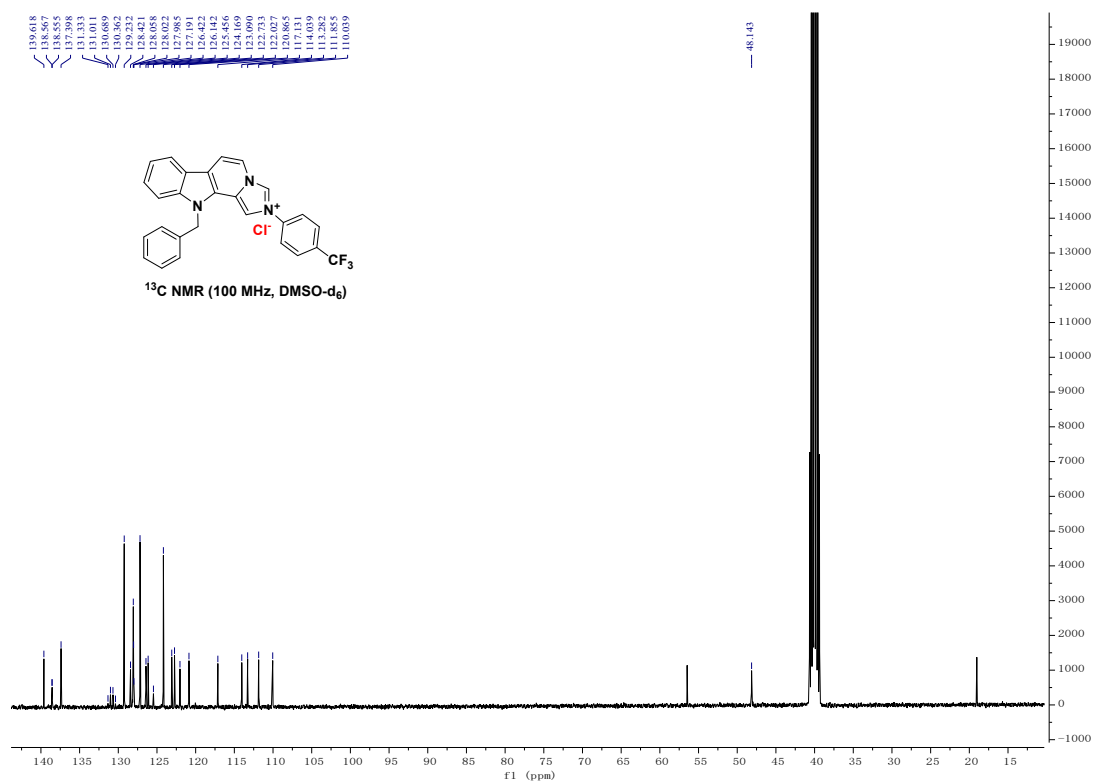
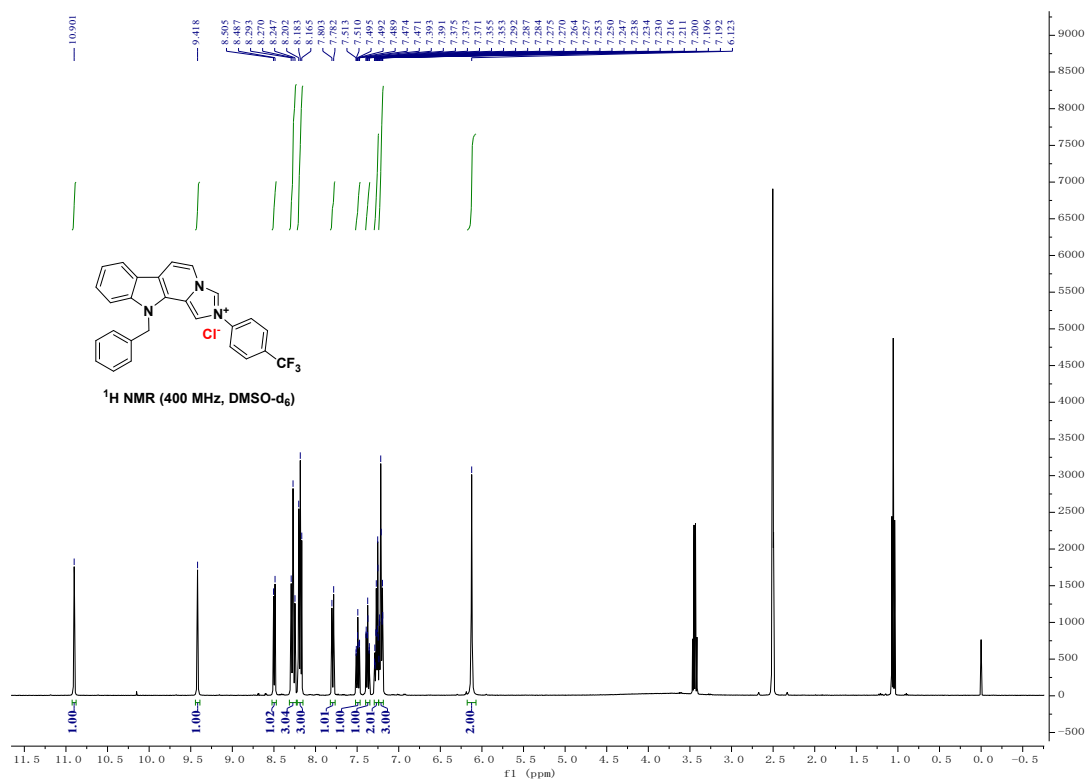


Figure S12-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 31

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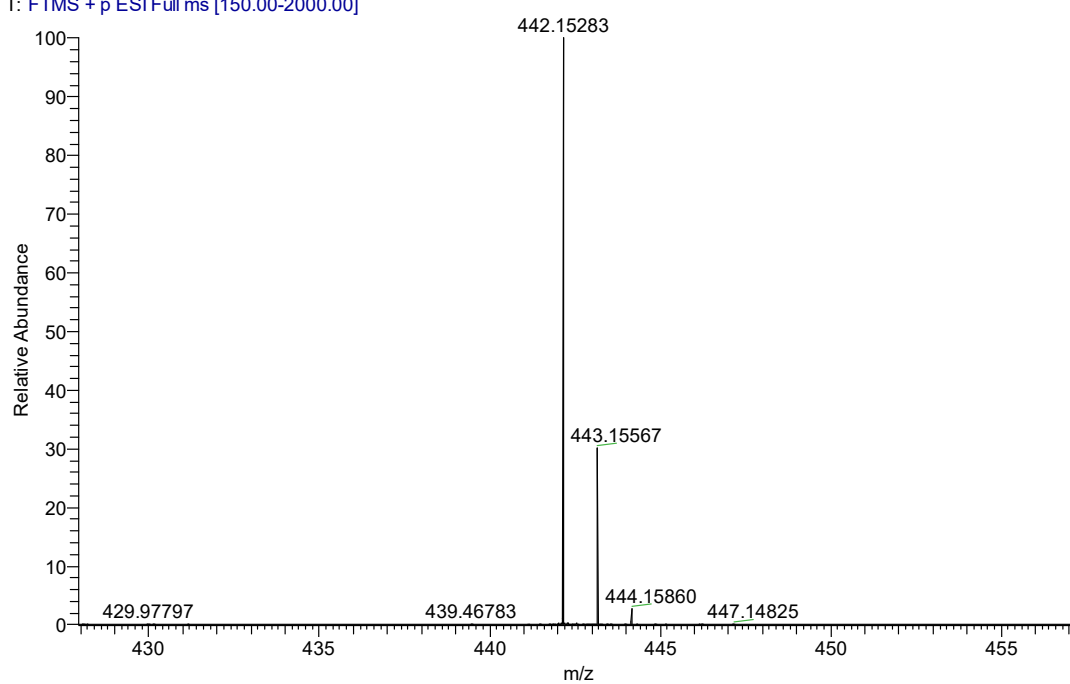


Figure S12-2 the HRMS data of compound **31**

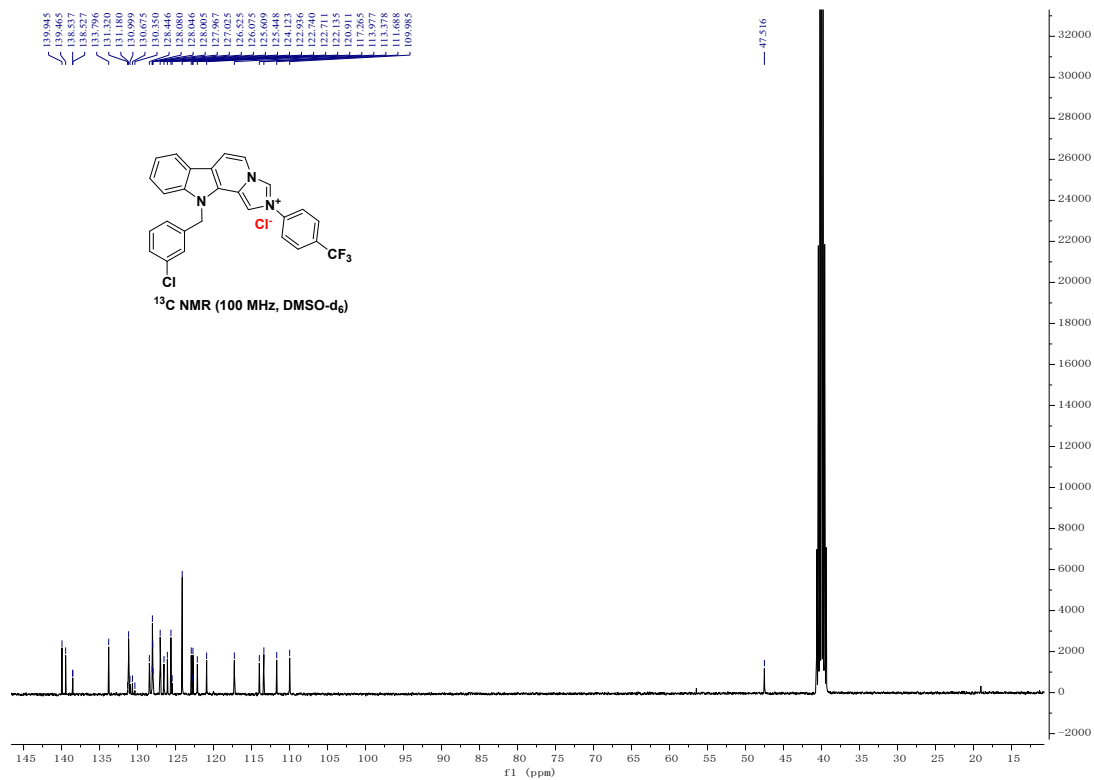
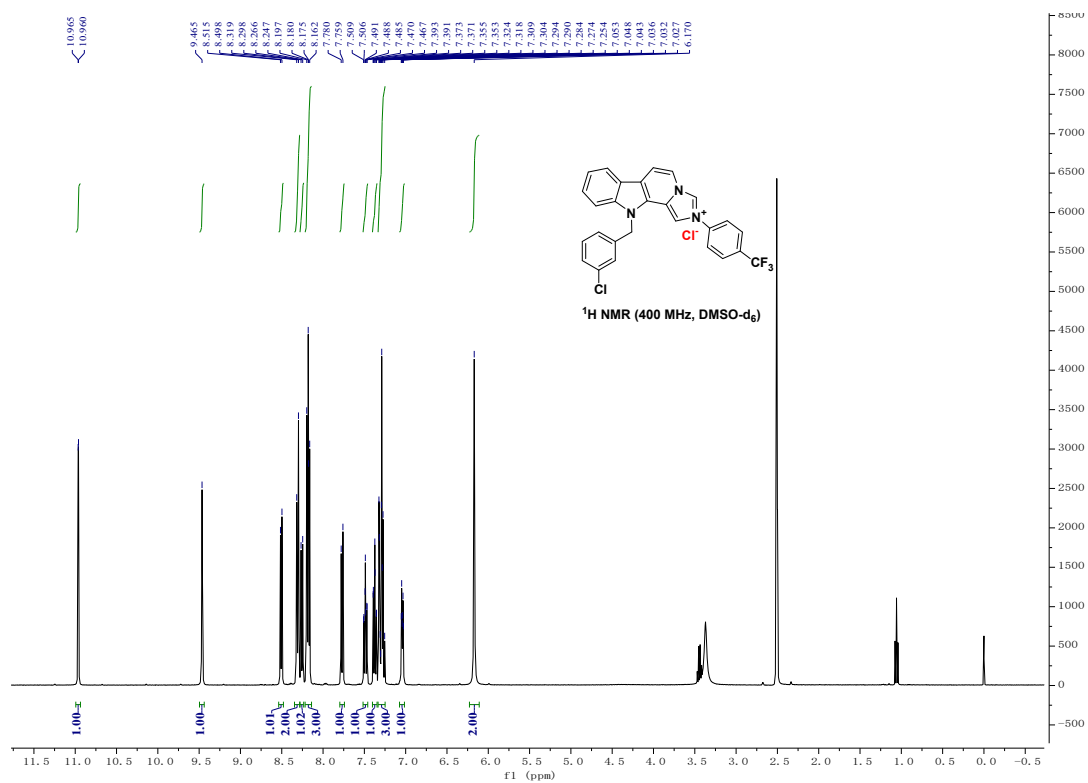


Figure S13-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound **3m**

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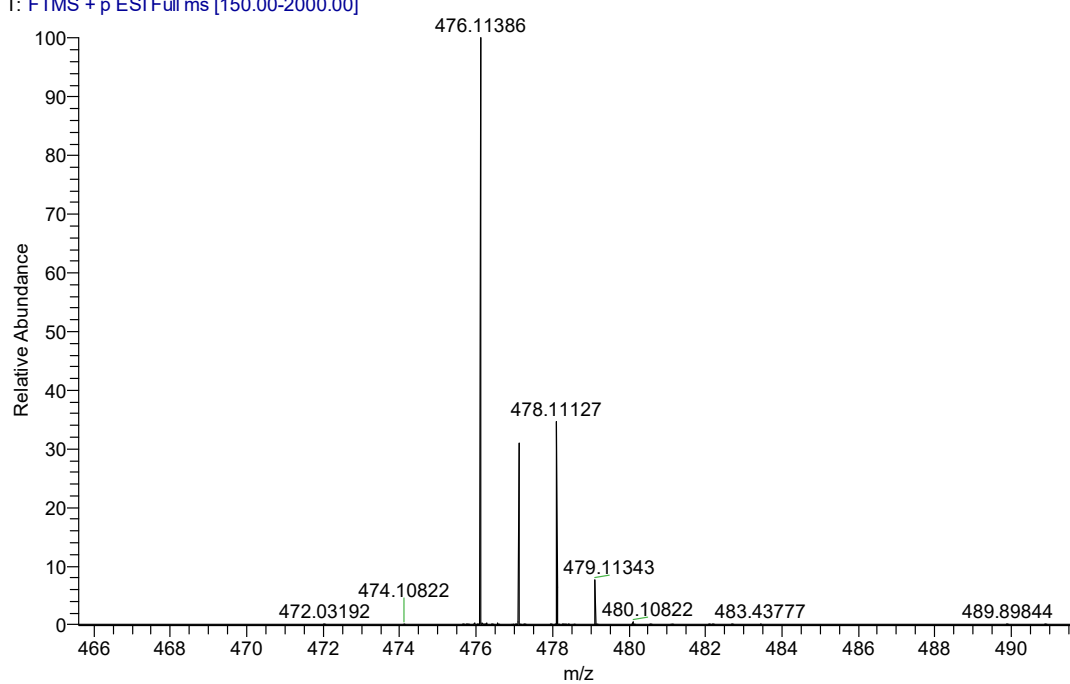


Figure S13-2 the HRMS data of compound **3m**

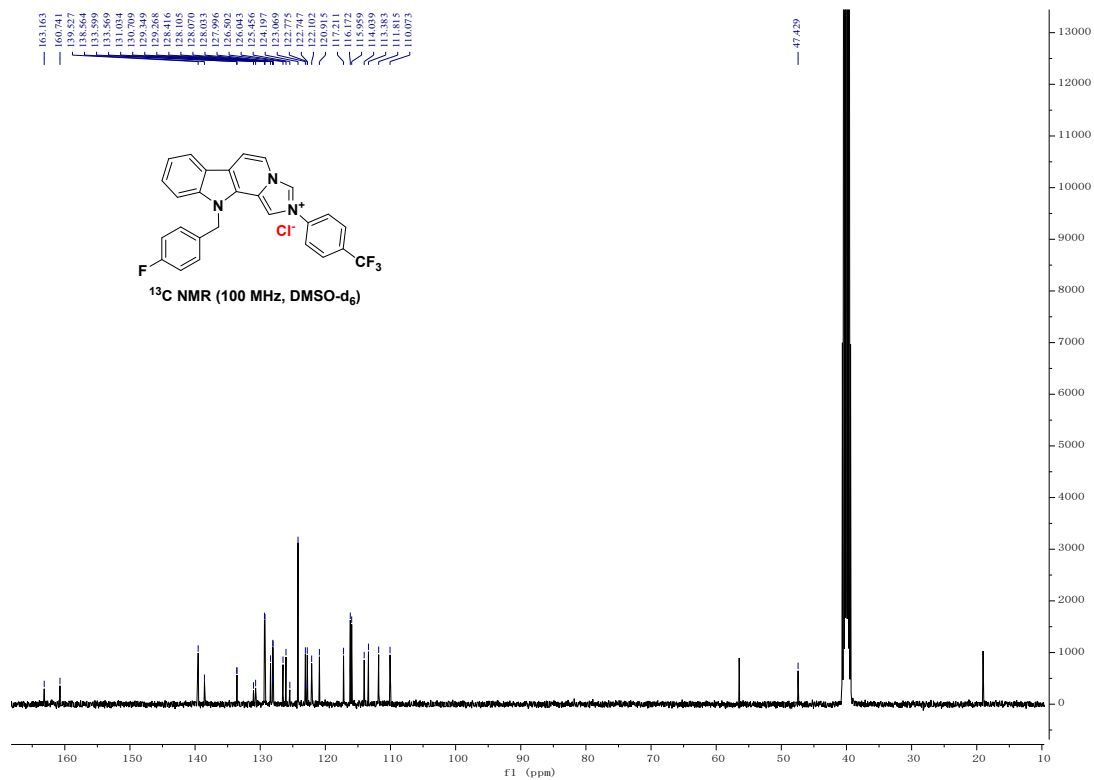
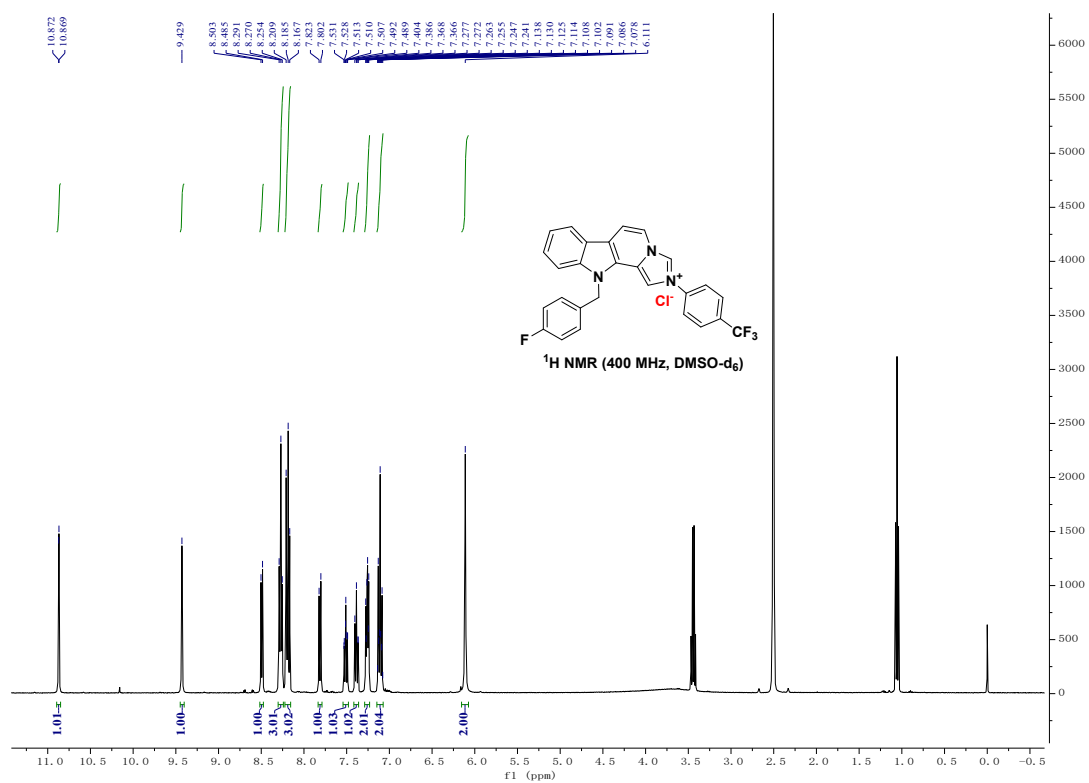


Figure S14-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3n

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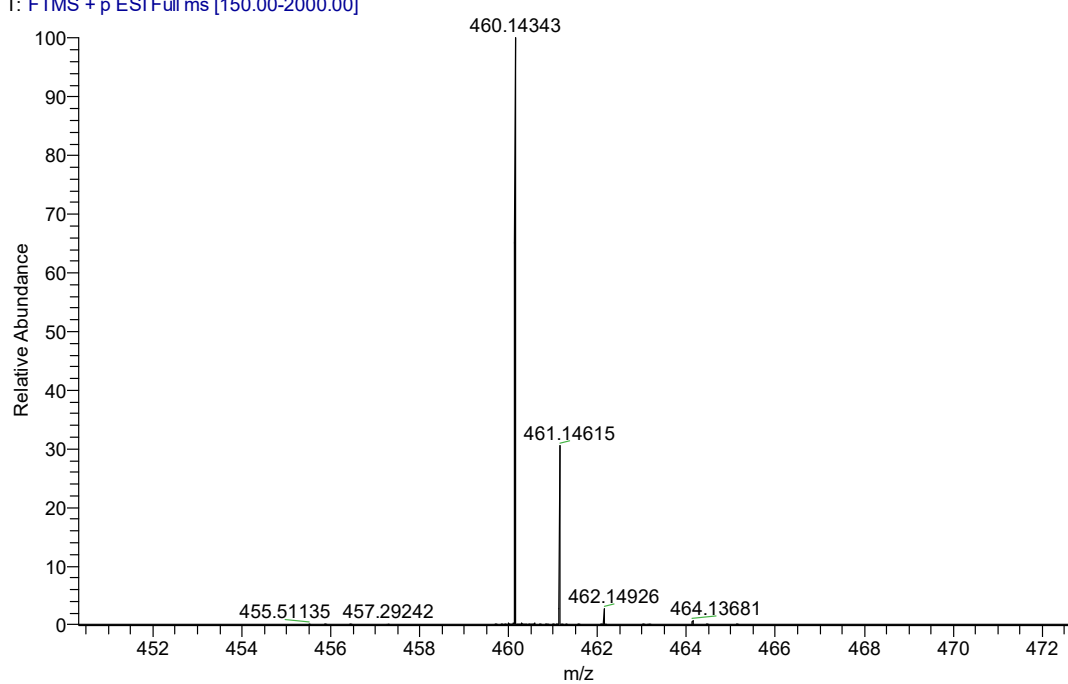


Figure S14-2 the HRMS data of compound **3n**

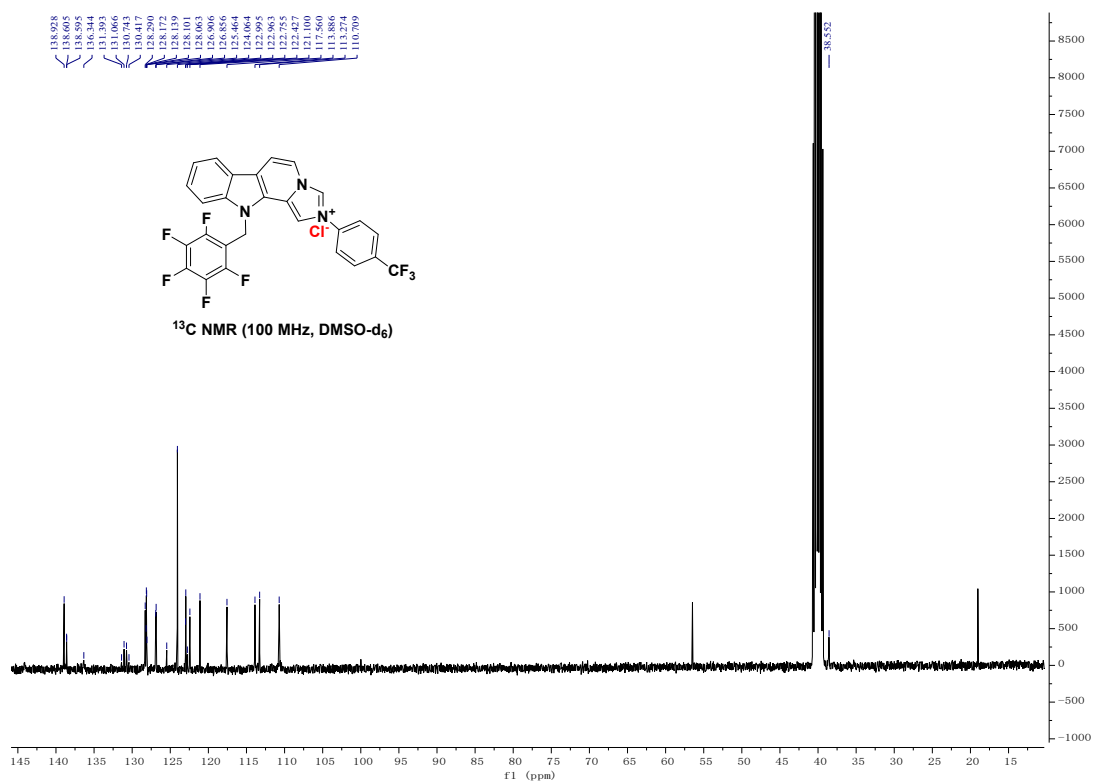
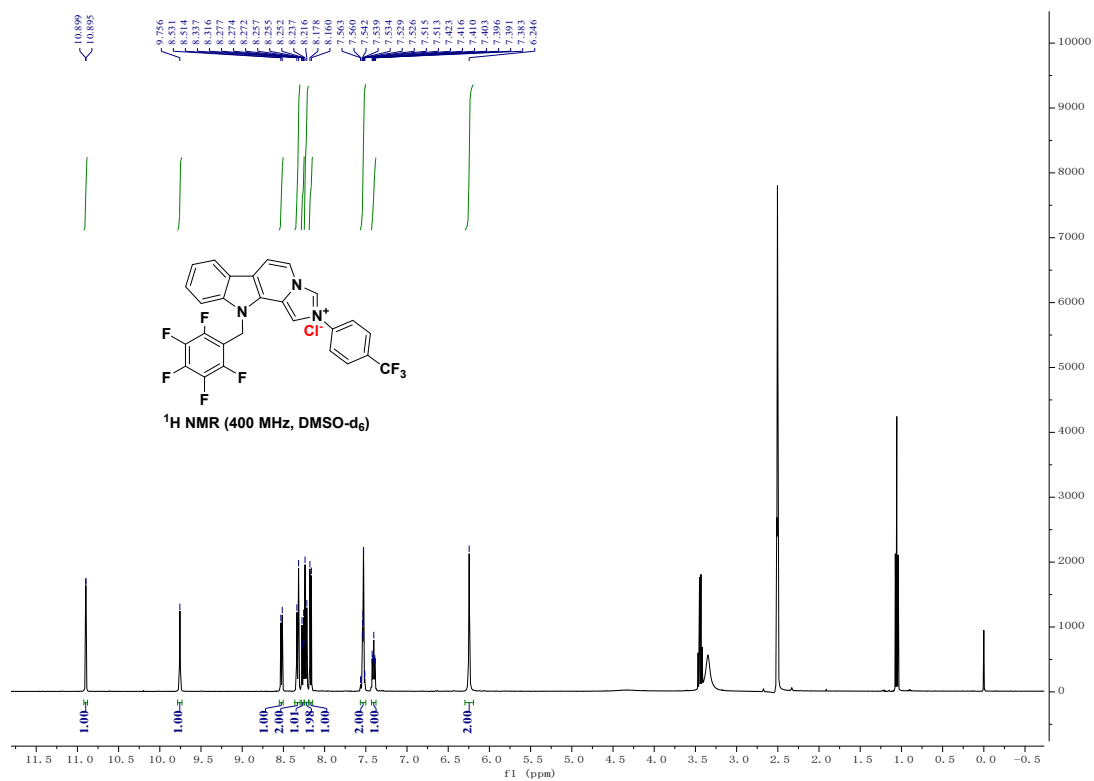


Figure S15-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound **30**

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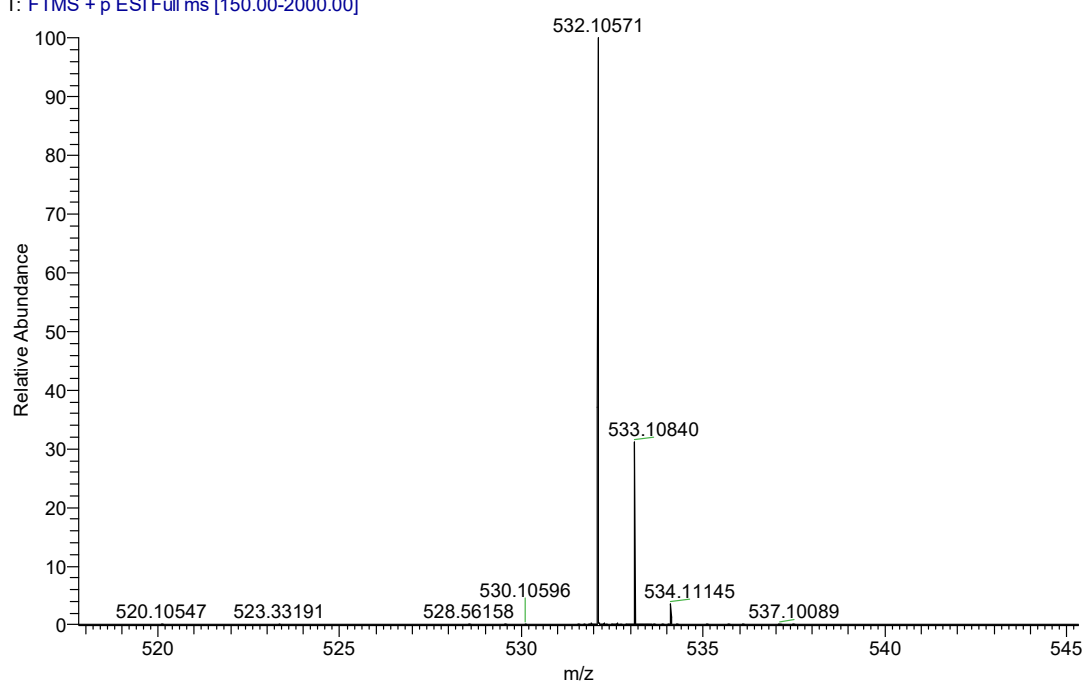


Figure S15-2 the HRMS data of compound **3o**

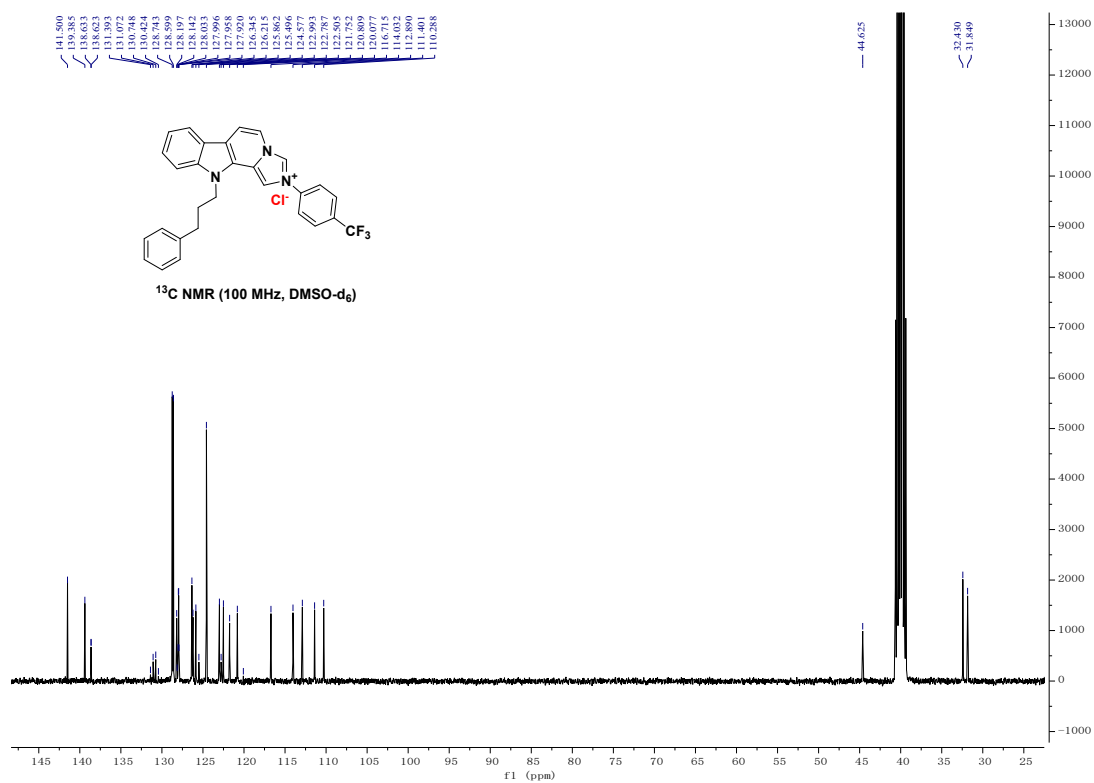
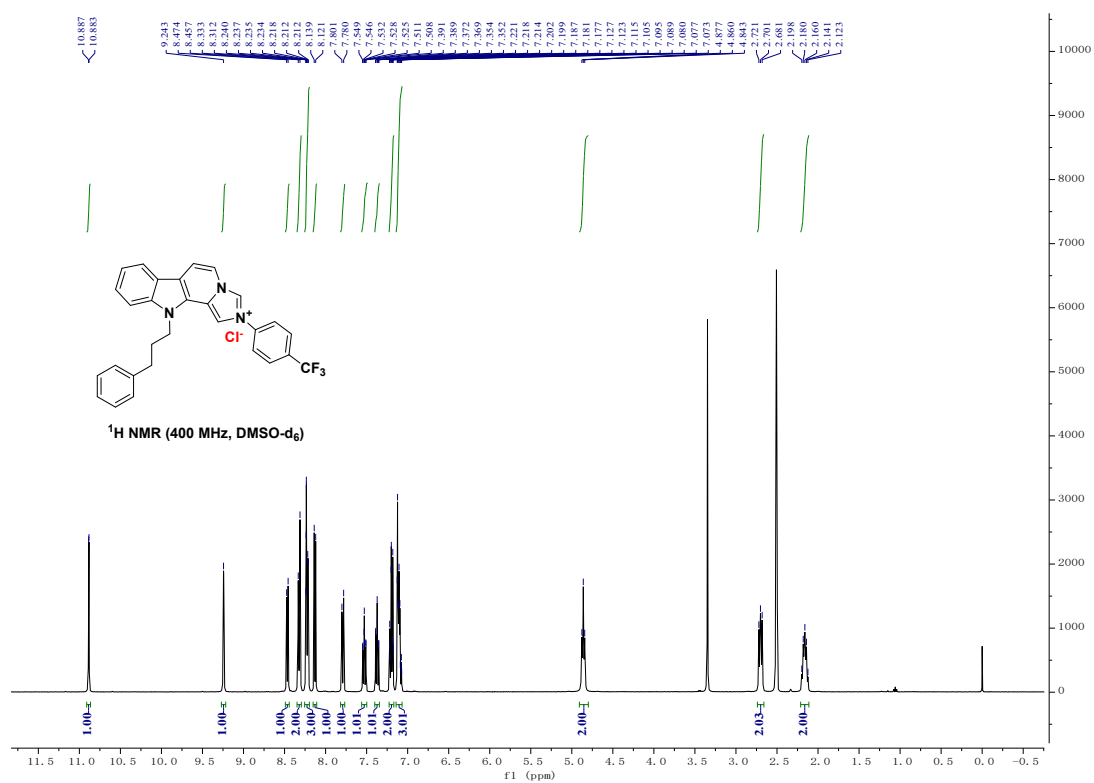


Figure S16-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3p

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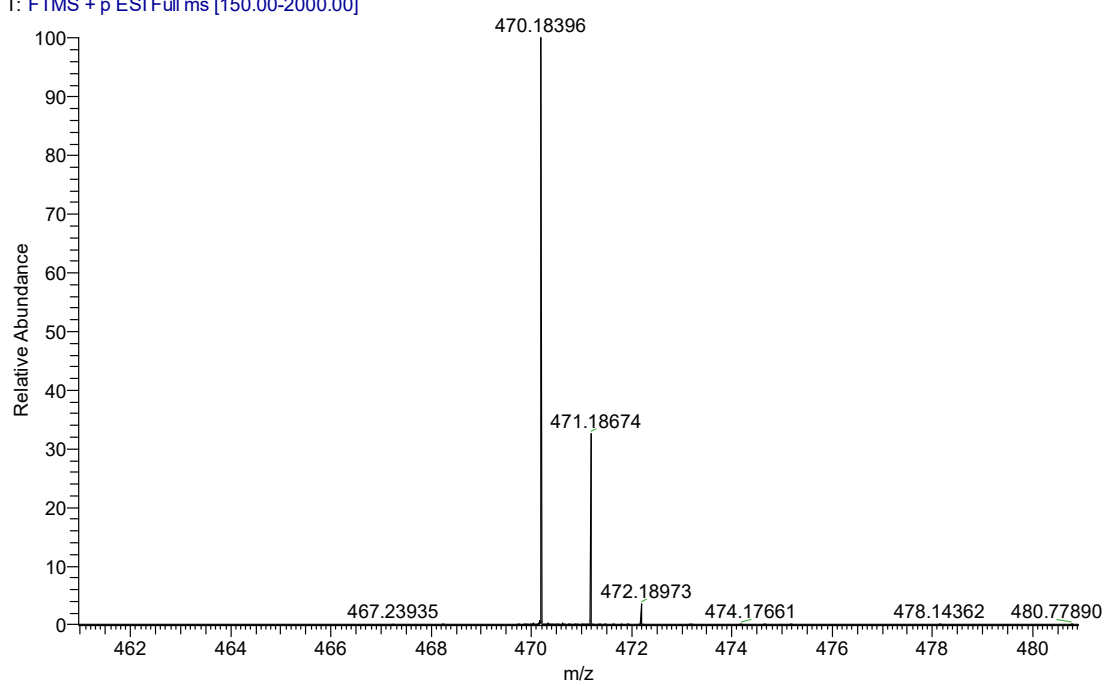


Figure S16-2 the HRMS data of compound **3p**

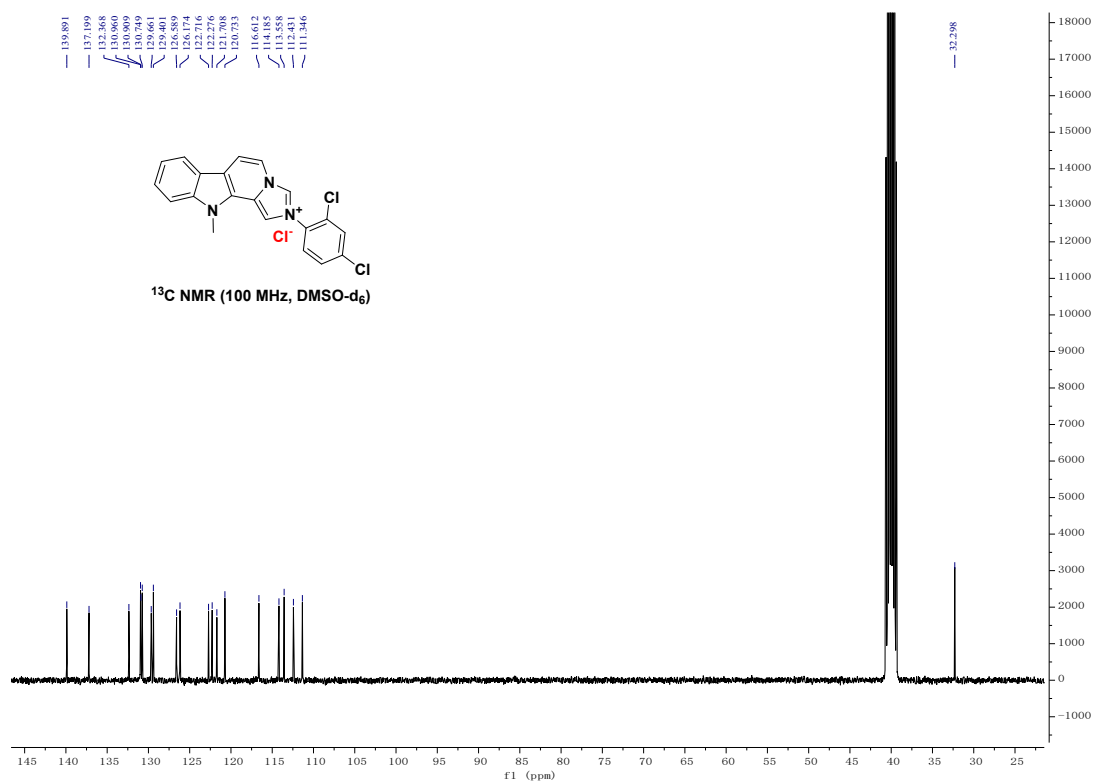
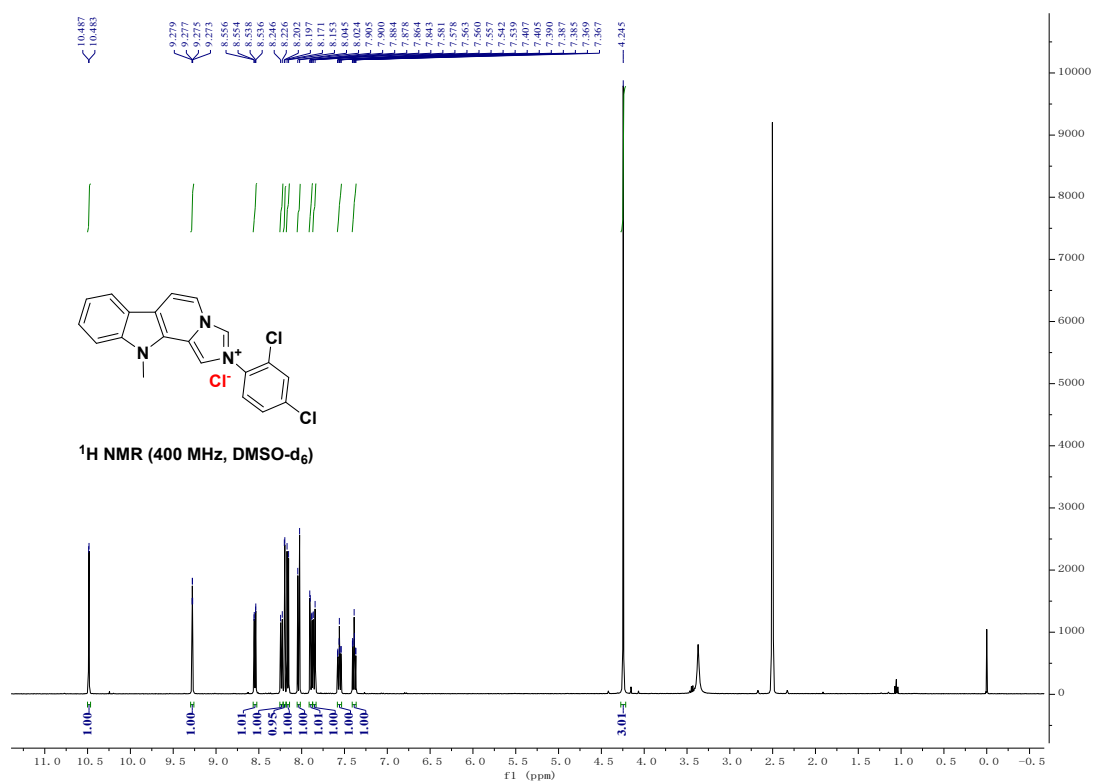


Figure S17-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3q

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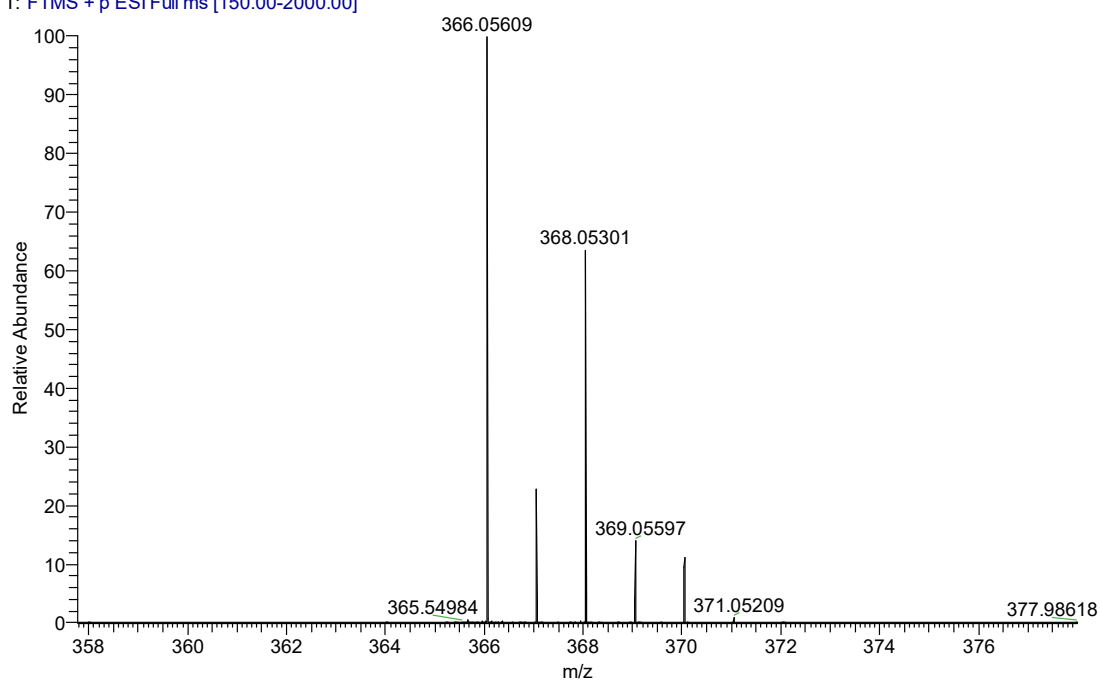


Figure S17-2 the HRMS data of compound **3q**

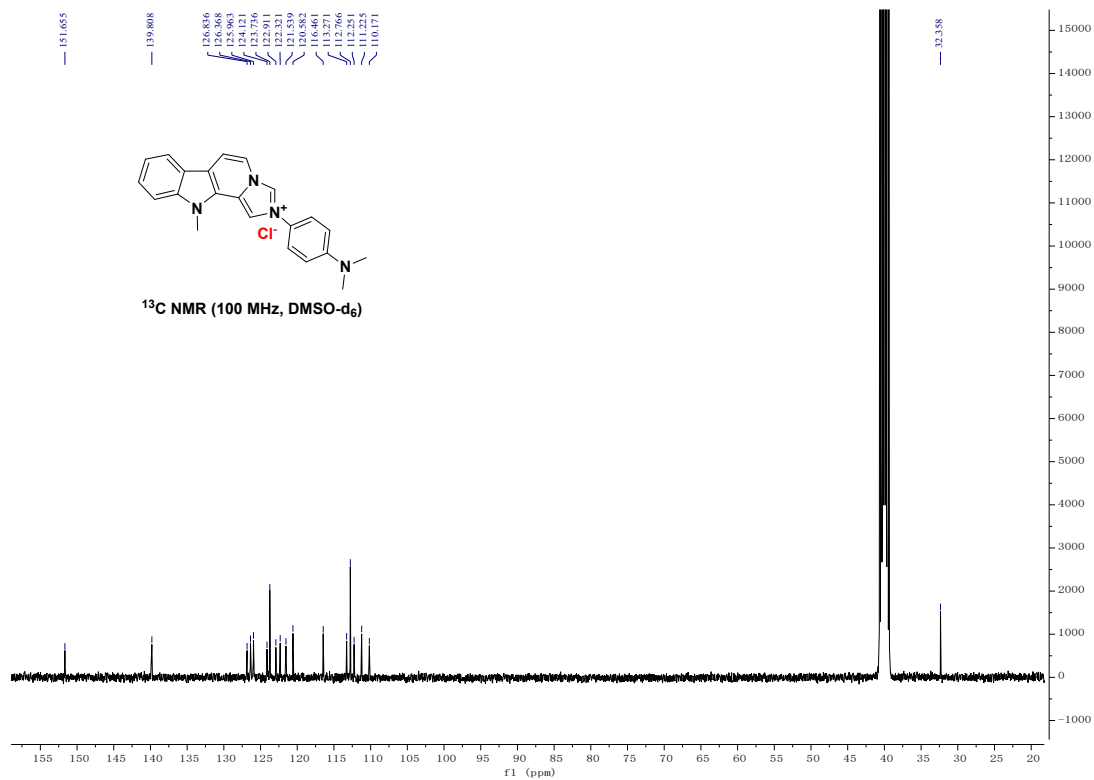
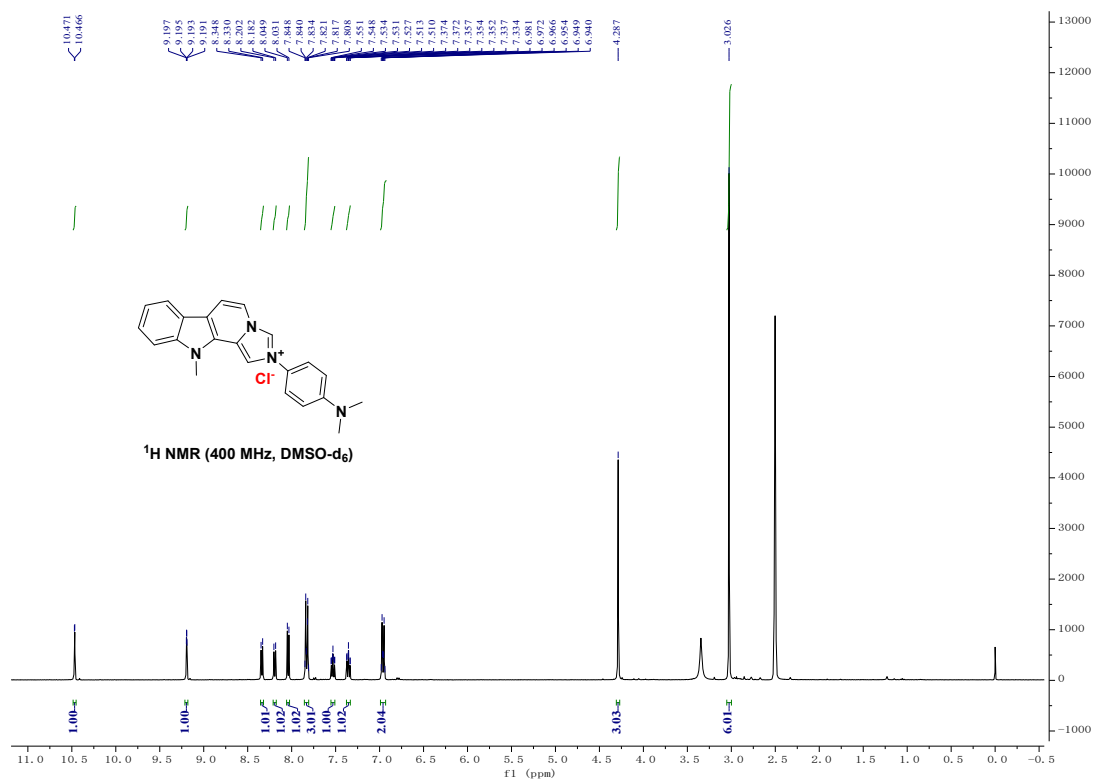


Figure S18-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3r

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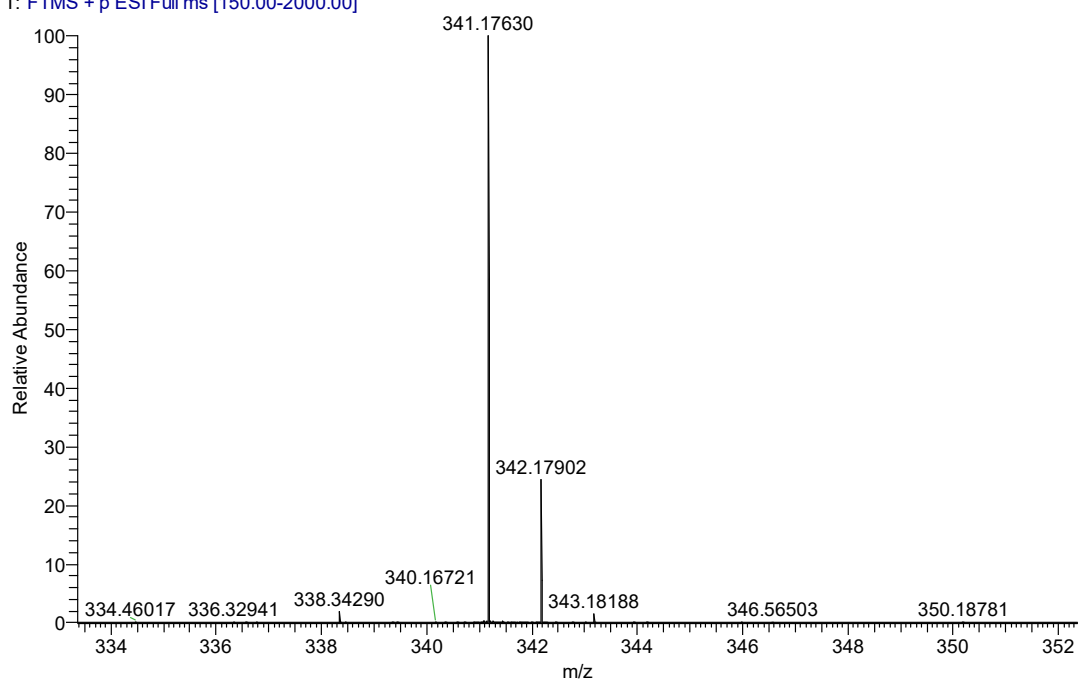


Figure S18-2 the HRMS data of compound **3r**

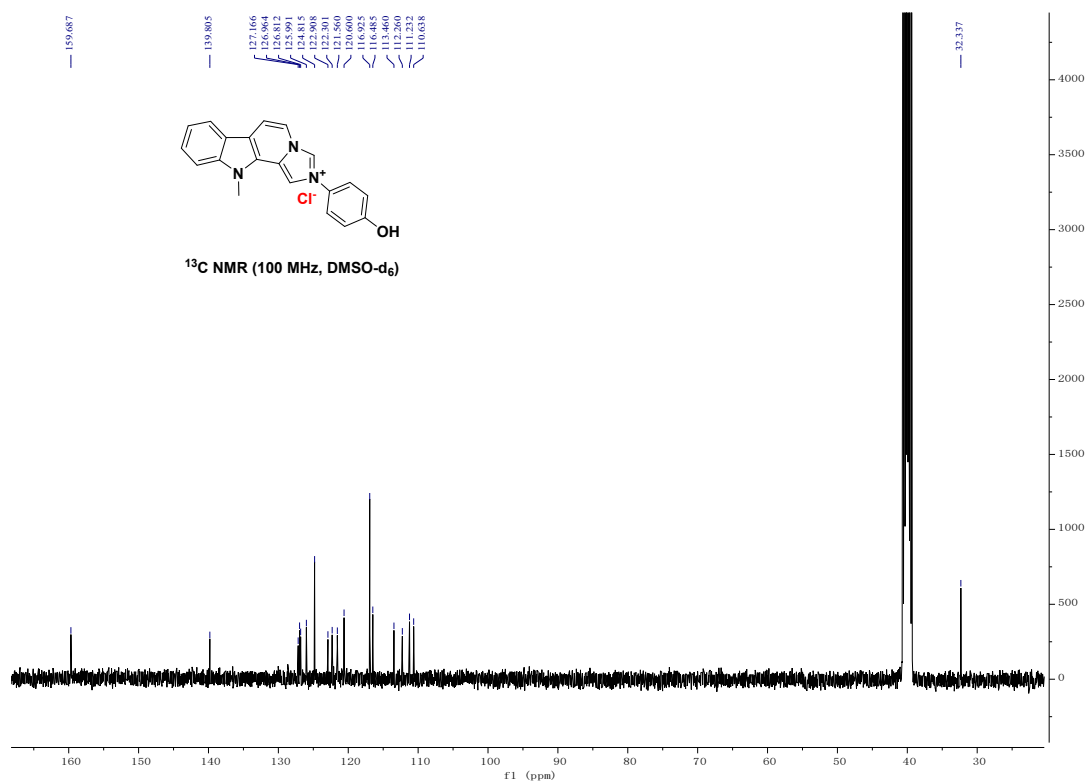
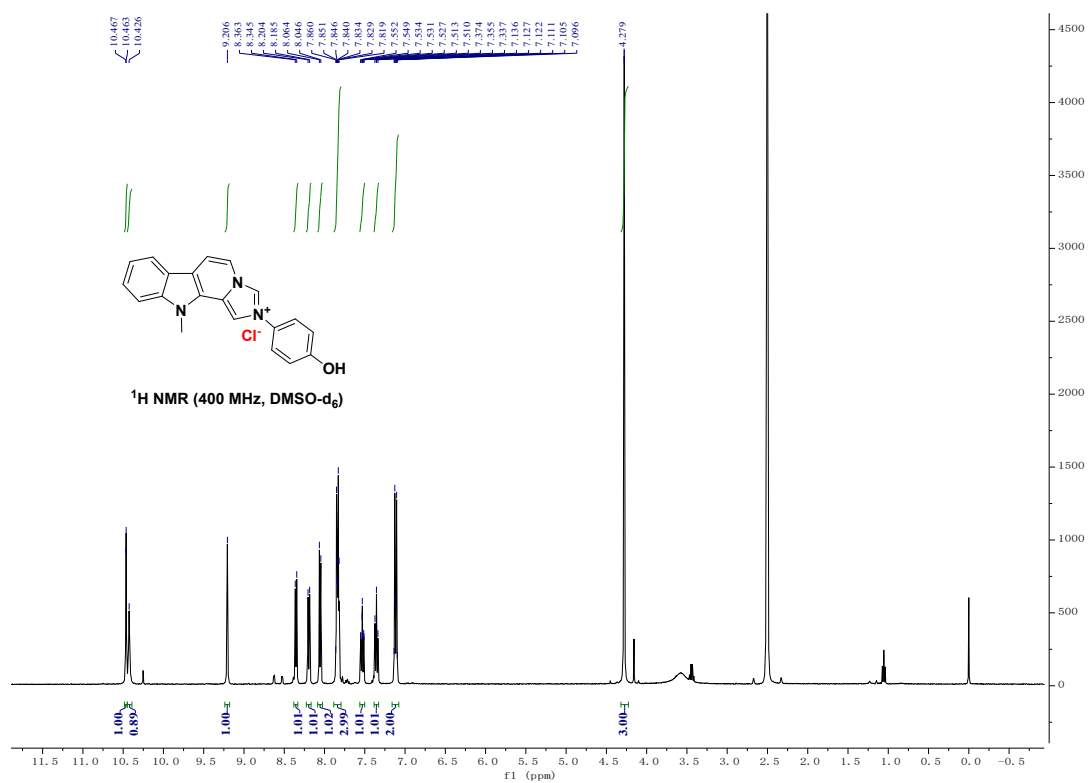


Figure S19-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3s

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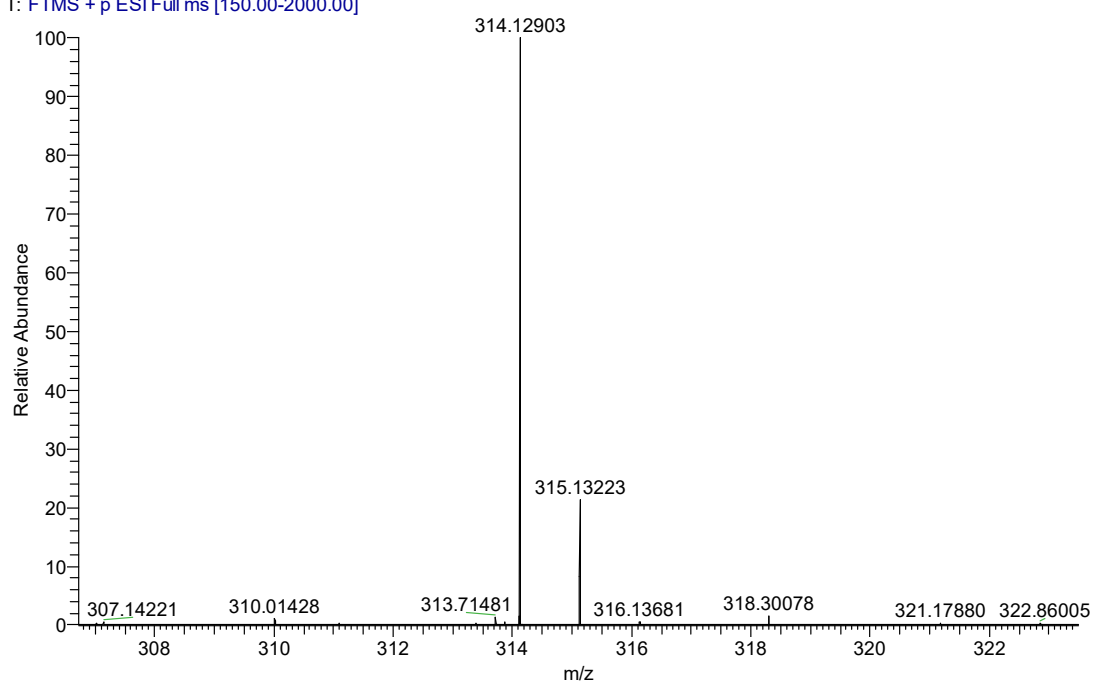


Figure S19-2 the HRMS data of compound **3s**

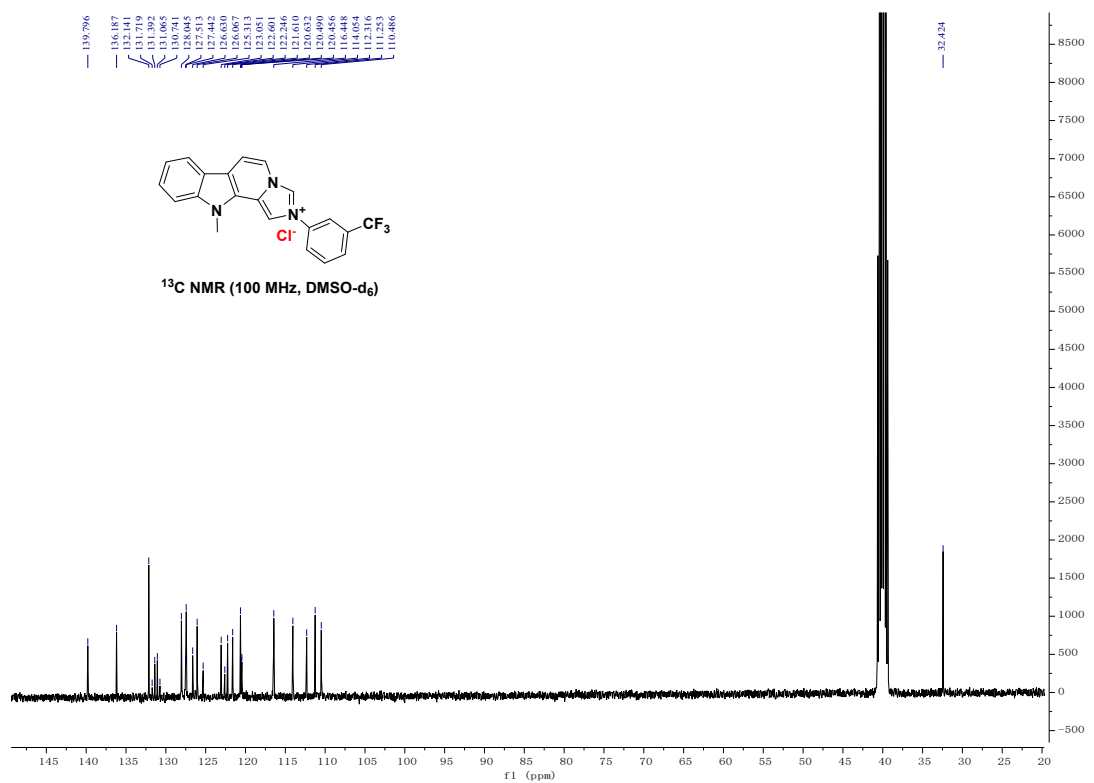
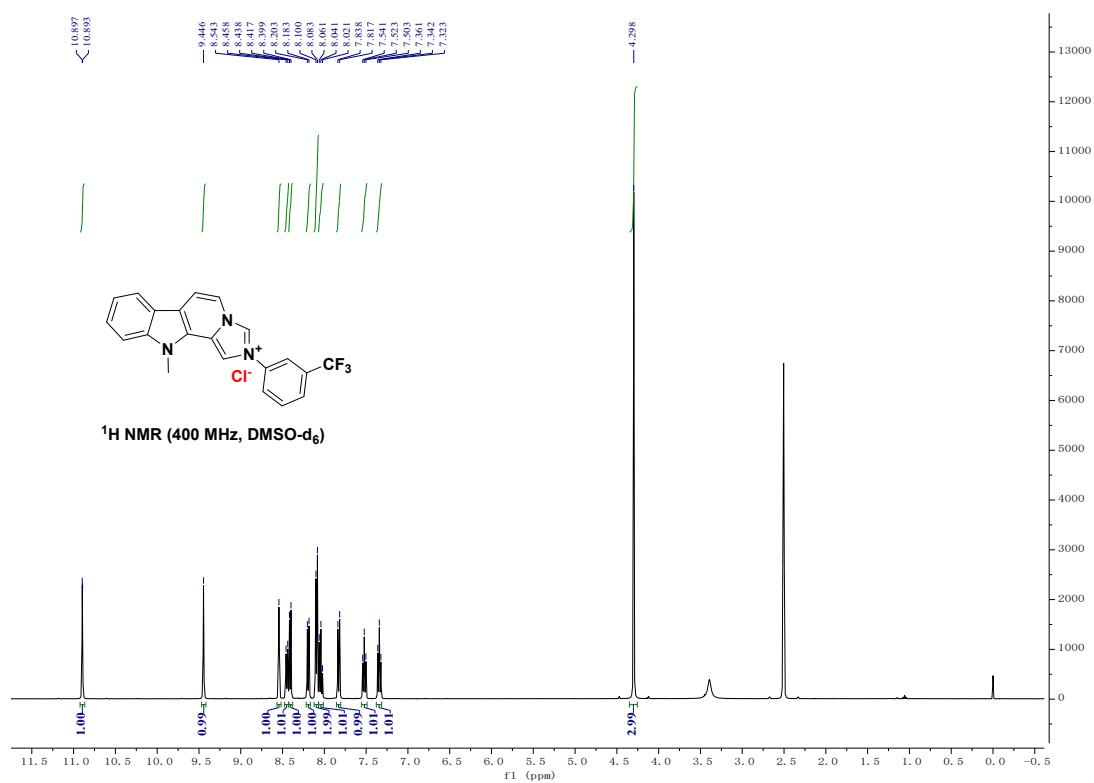


Figure S20-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3t

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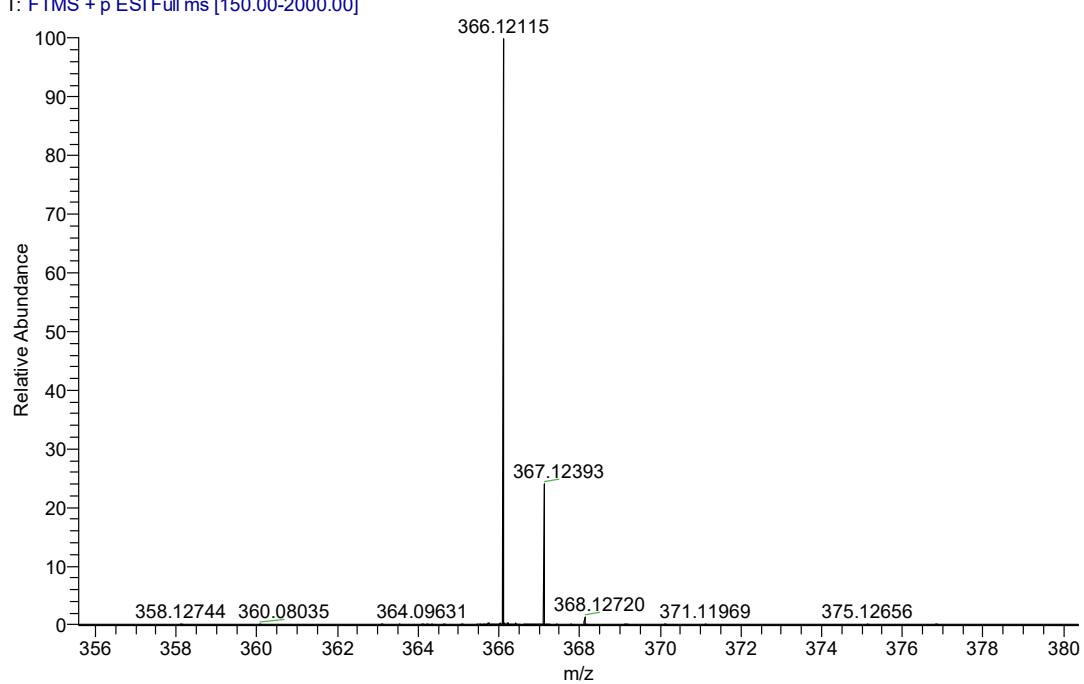


Figure S20-2 the HRMS data of compound **3t**

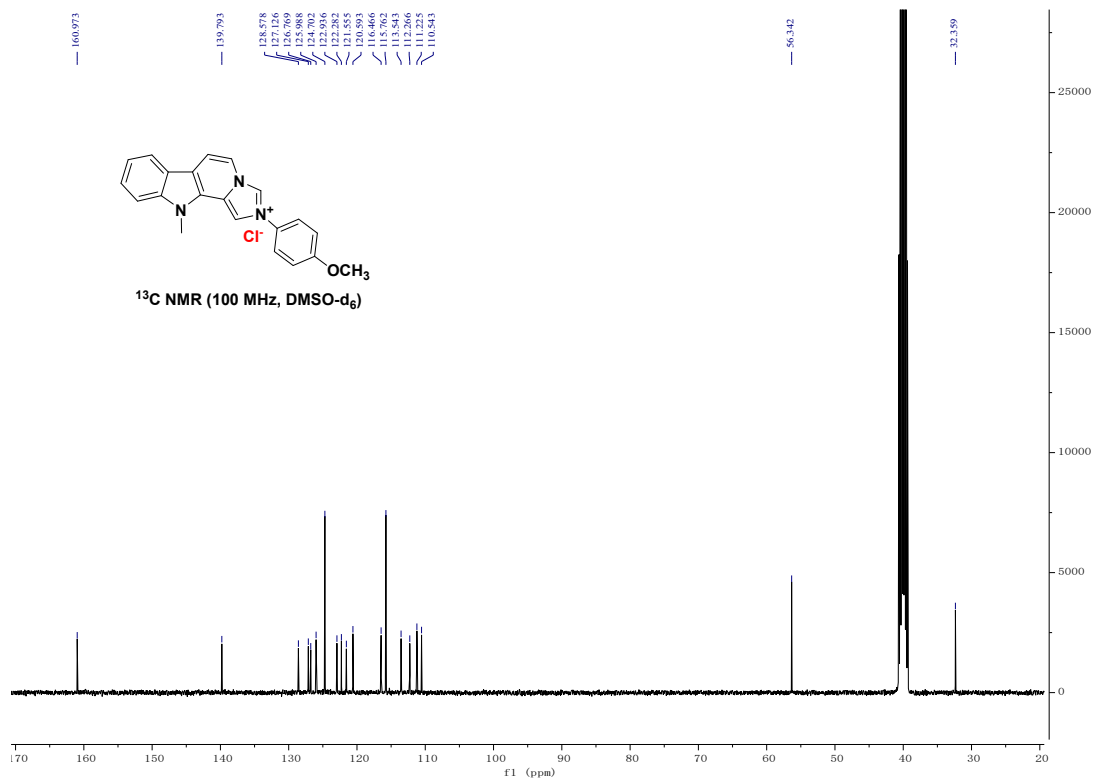
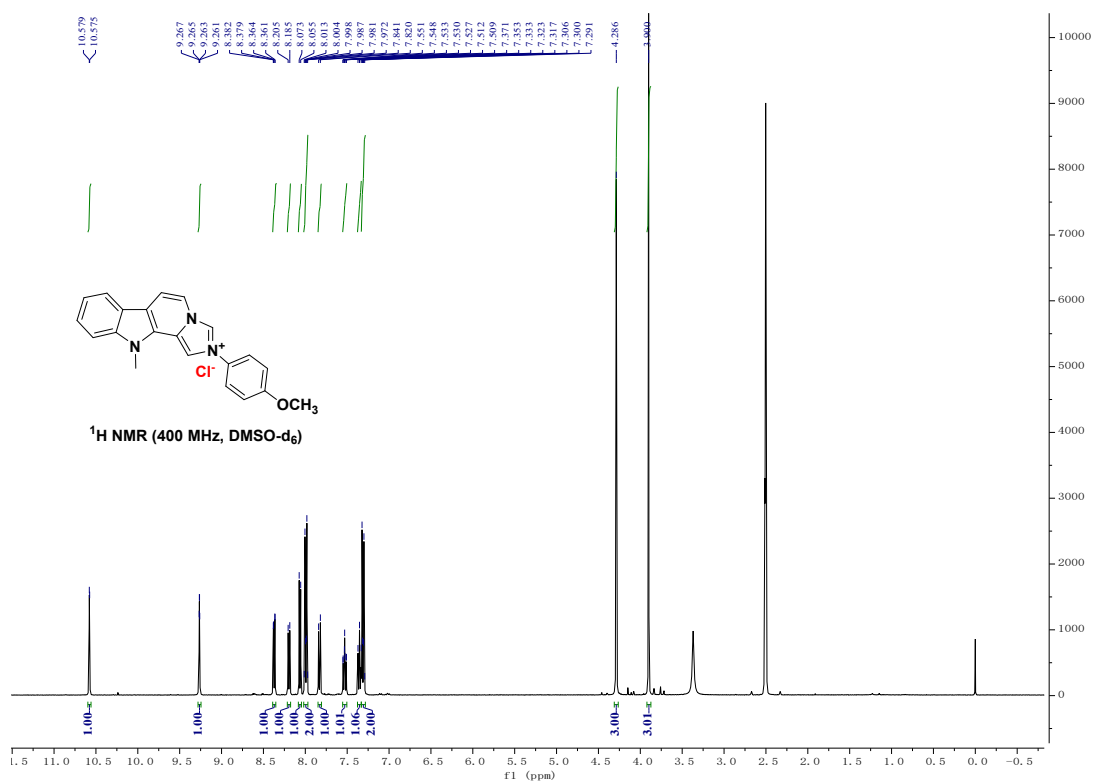


Figure S21-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound **3u**

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T: FTMS + p ESI Full ms [150.00-2000.00]

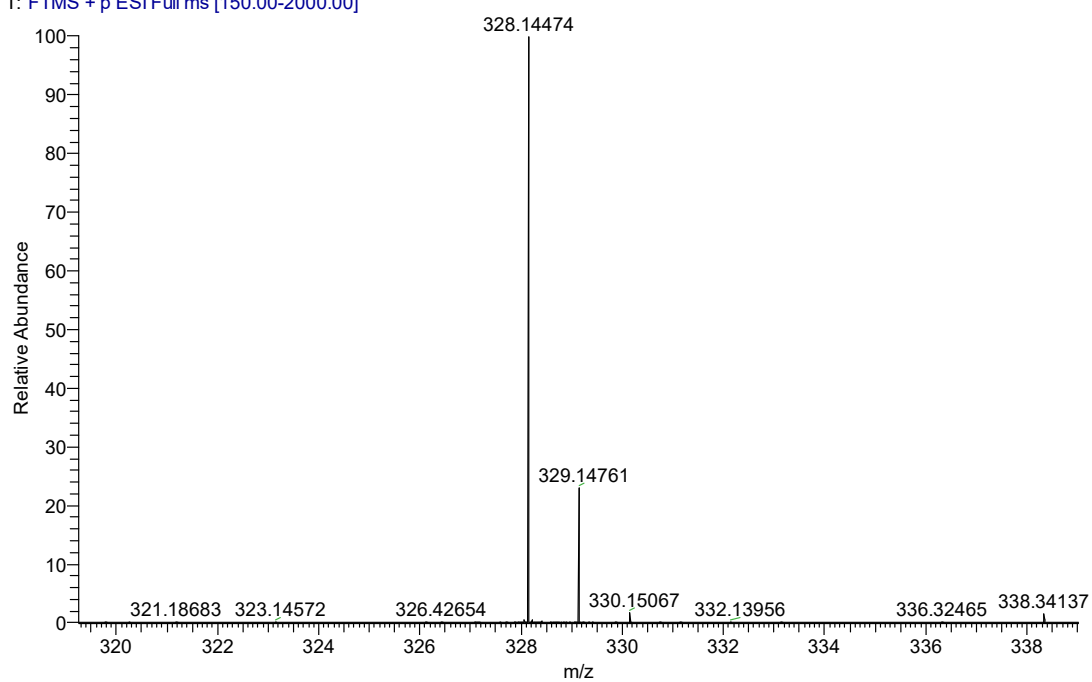


Figure S21-2 the HRMS data of compound **3u**

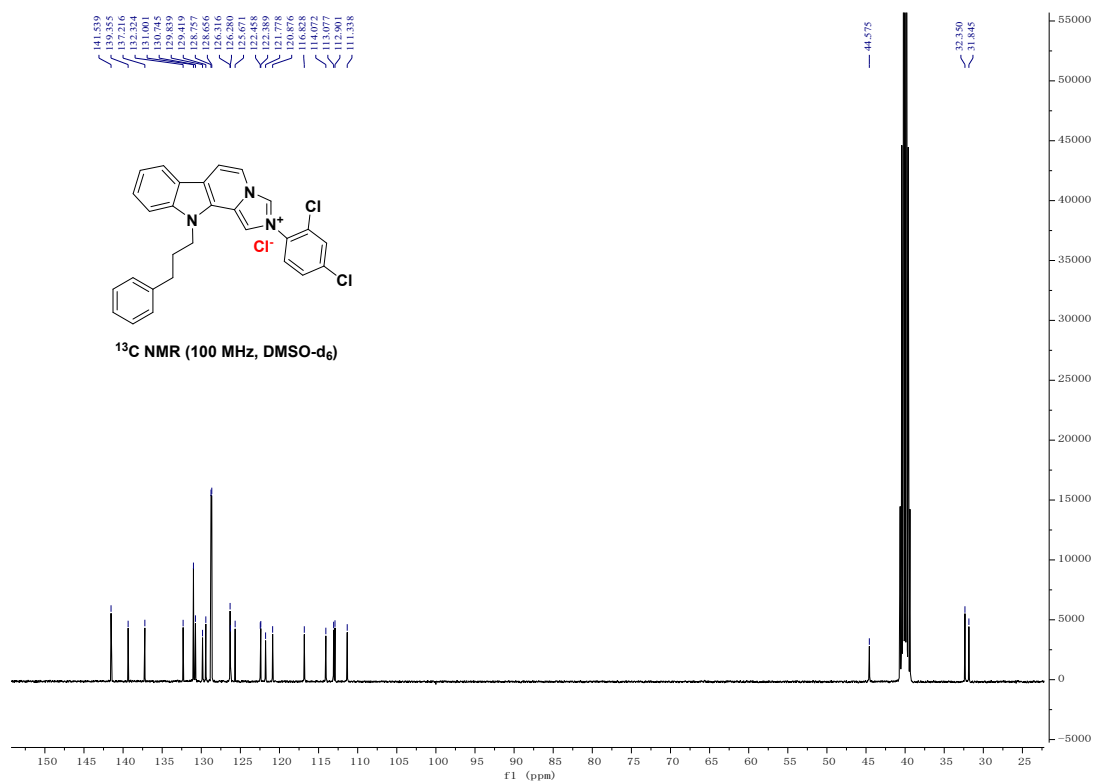
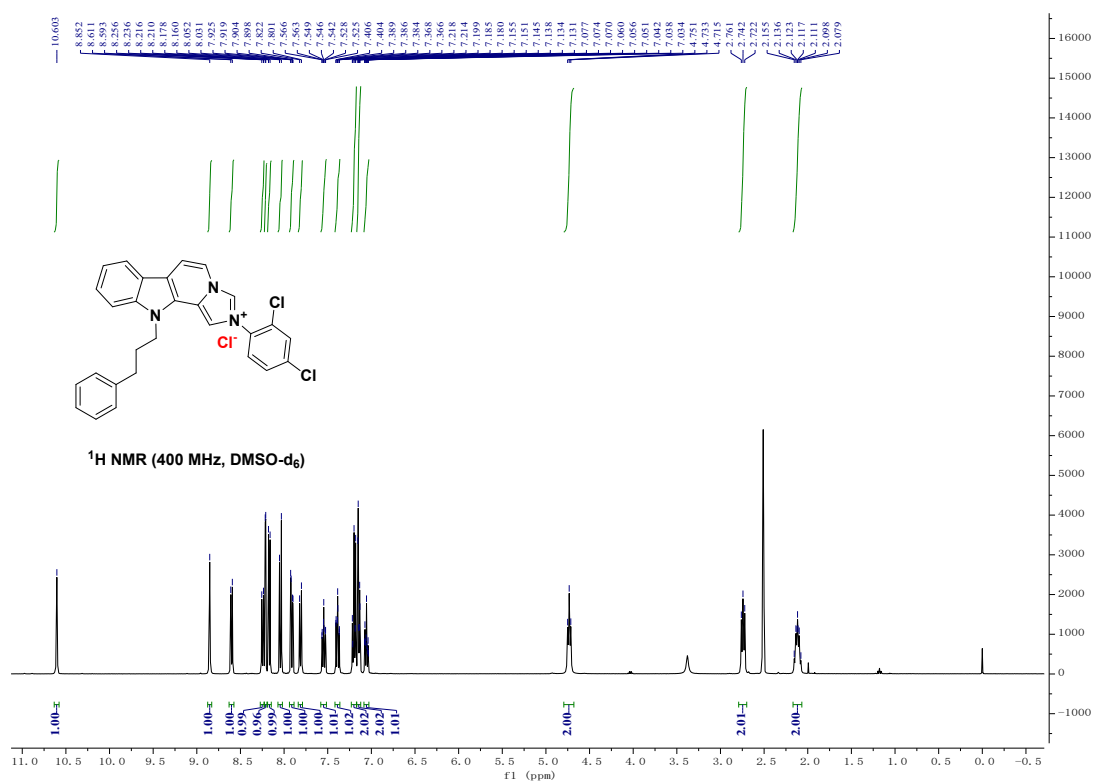


Figure S22-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound **3v**

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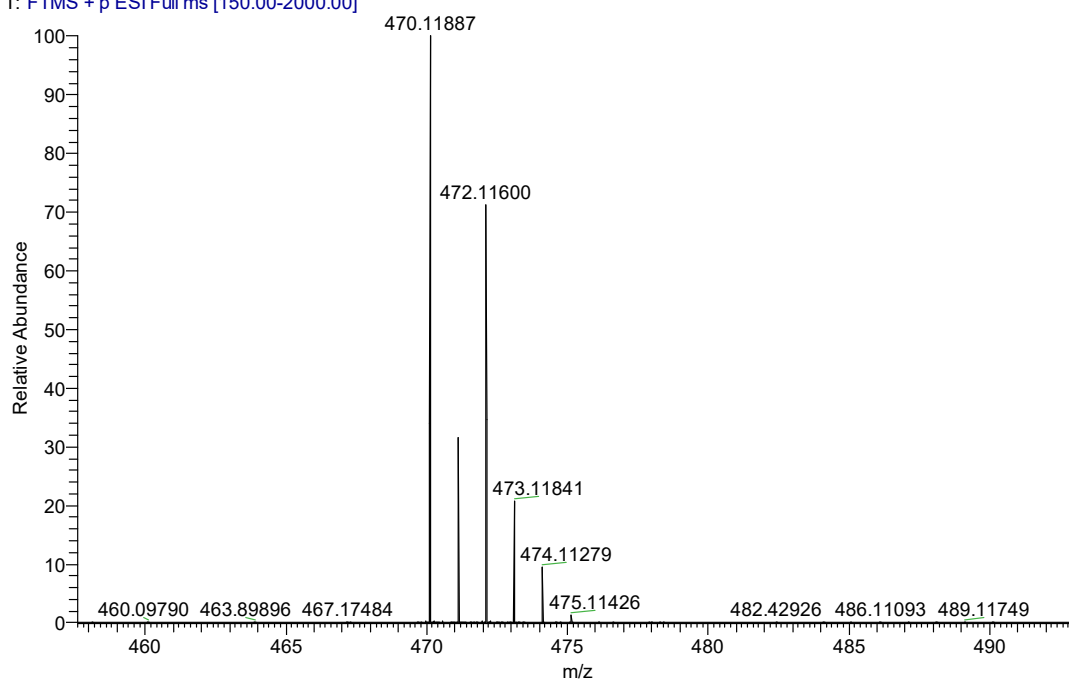


Figure S22-2 the HRMS data of compound **3v**

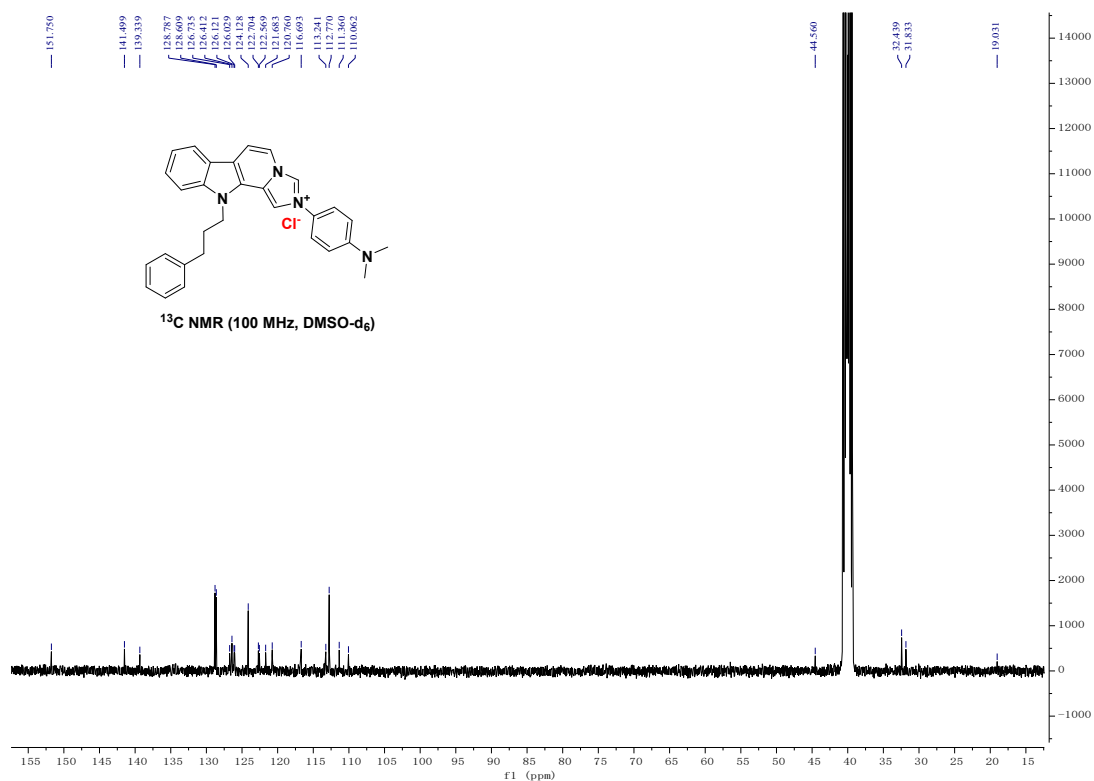
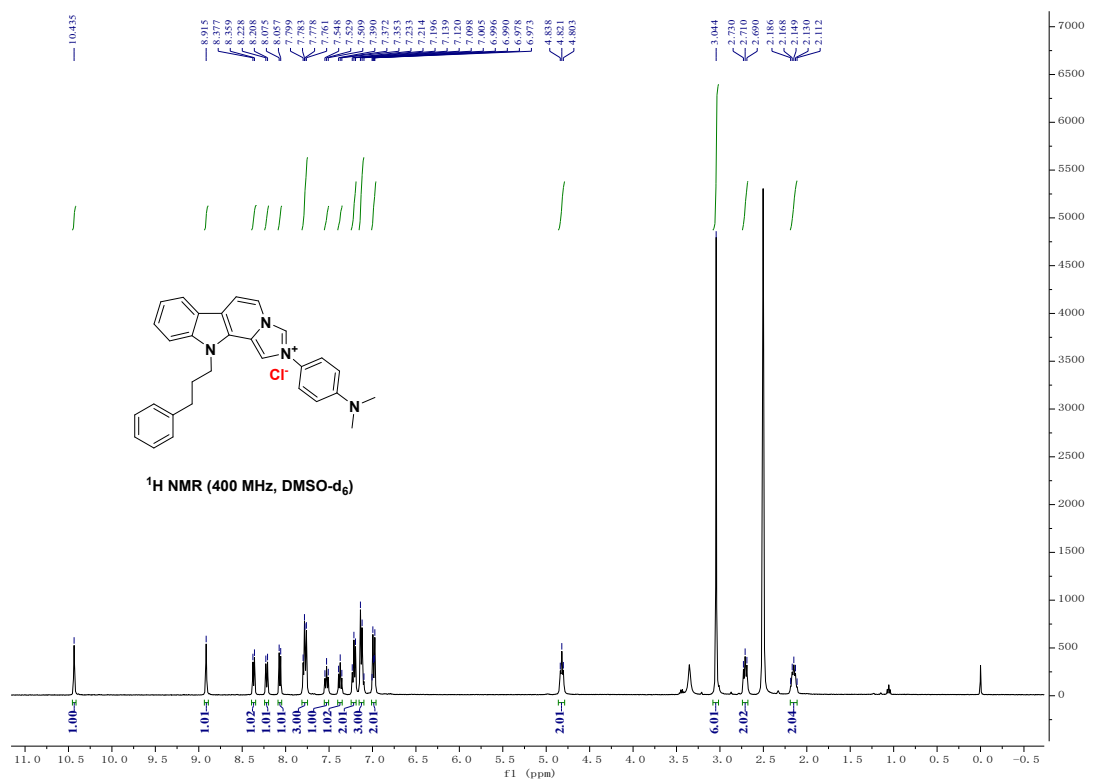


Figure S23-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3w

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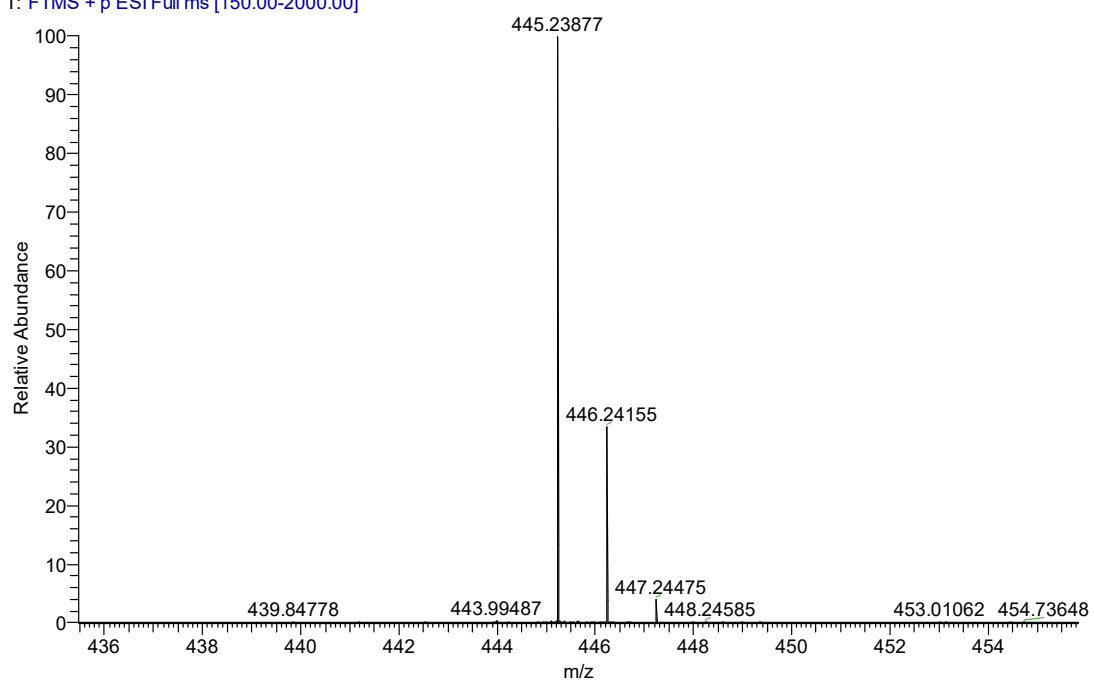


Figure S23-2 the HRMS data of compound **3w**

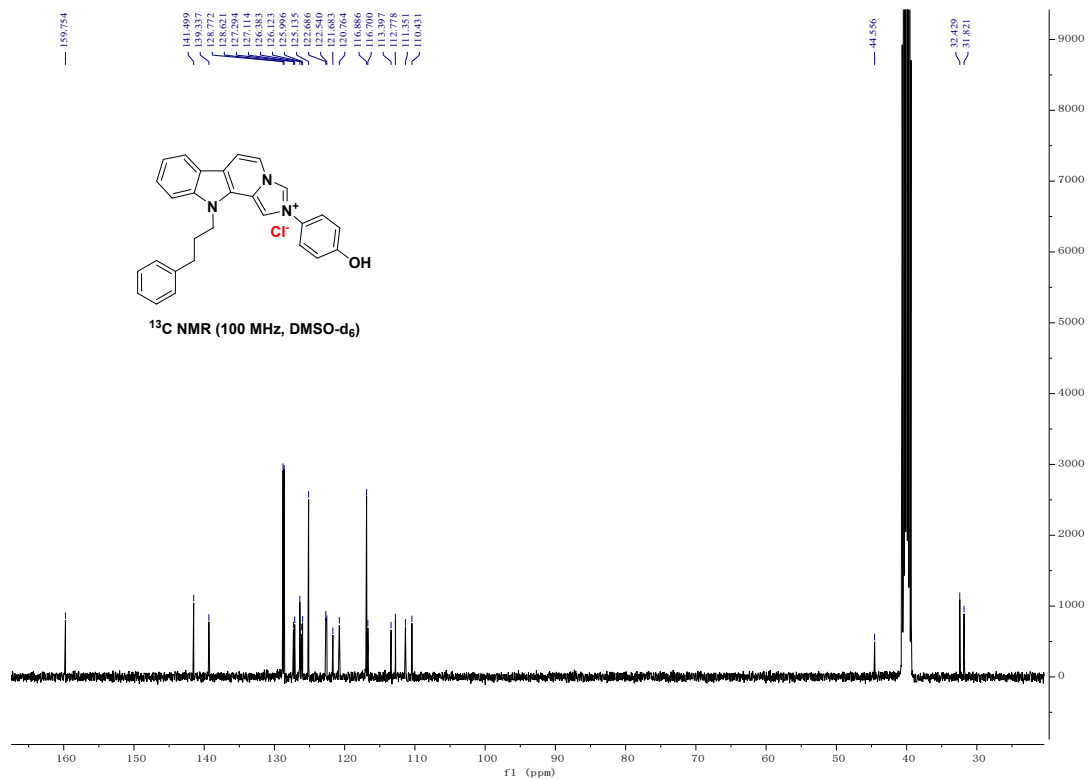
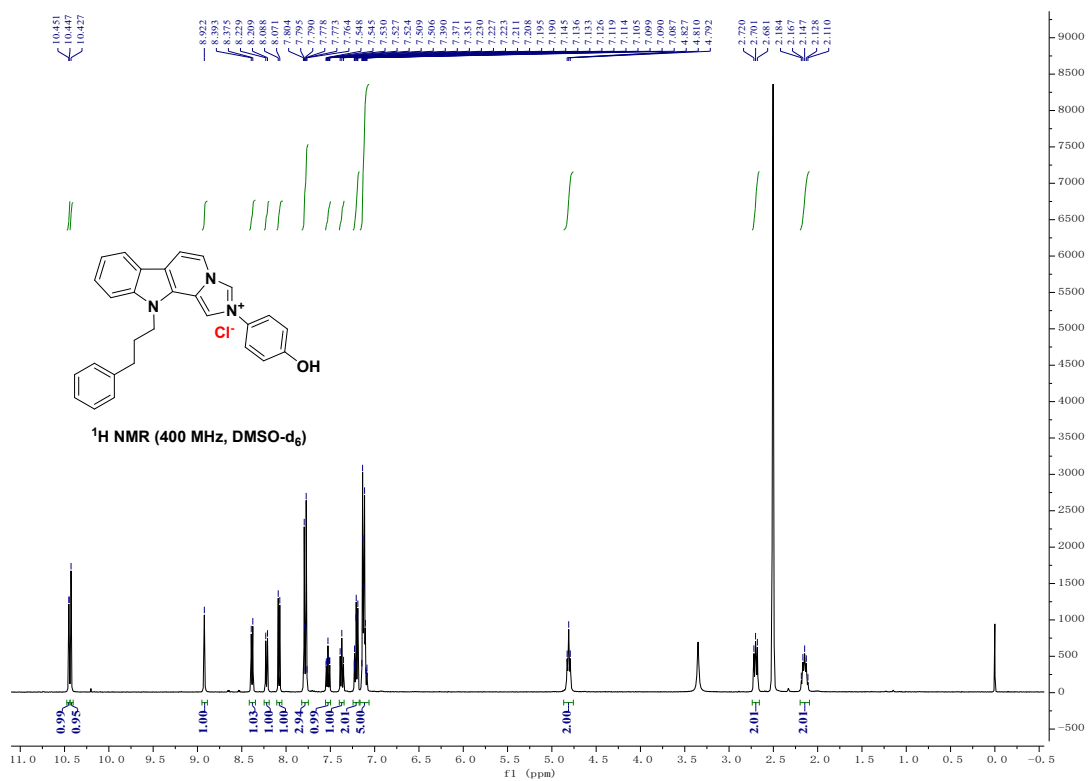


Figure S24-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3x

131 #9 RT: 0.11 AV: 1 NL: 3.54E8
T: FTMS + p ESI Full ms [150.00-2000.00]

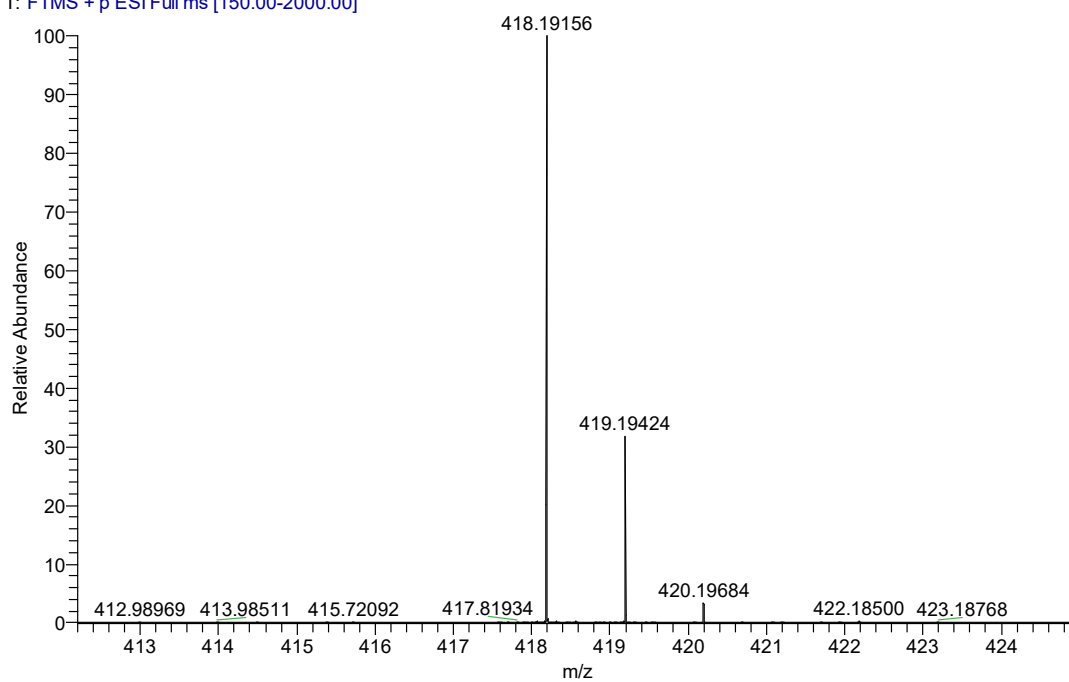


Figure S24-2 the HRMS data of compound **3x**

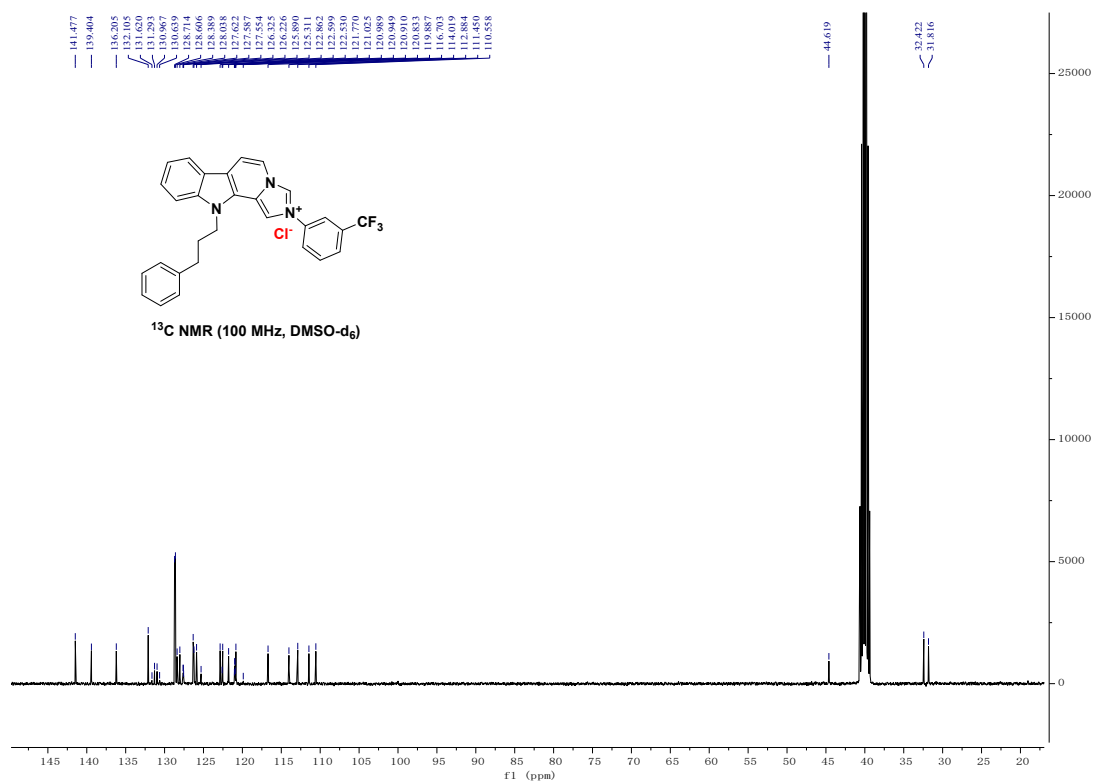
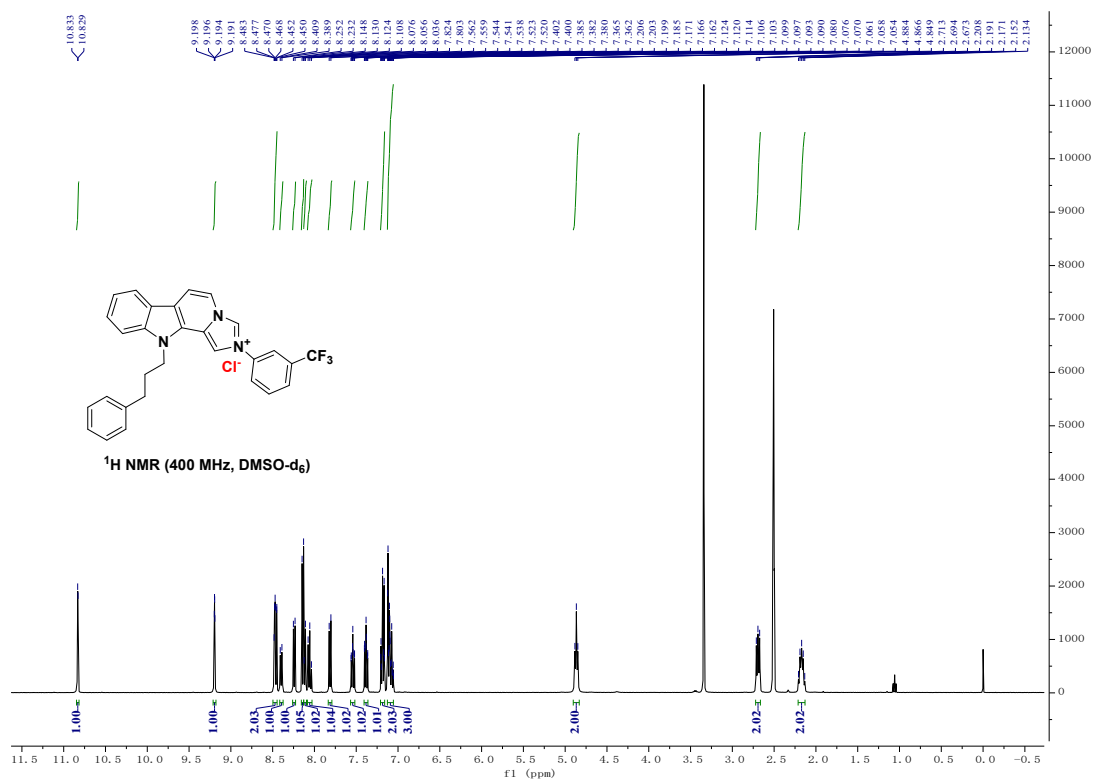


Figure S25-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound **3y**

132 #10 RT: 0.13 AV: 1 NL: 1.01E9
T: FTMS + p ESI Full ms [150.00-2000.00]

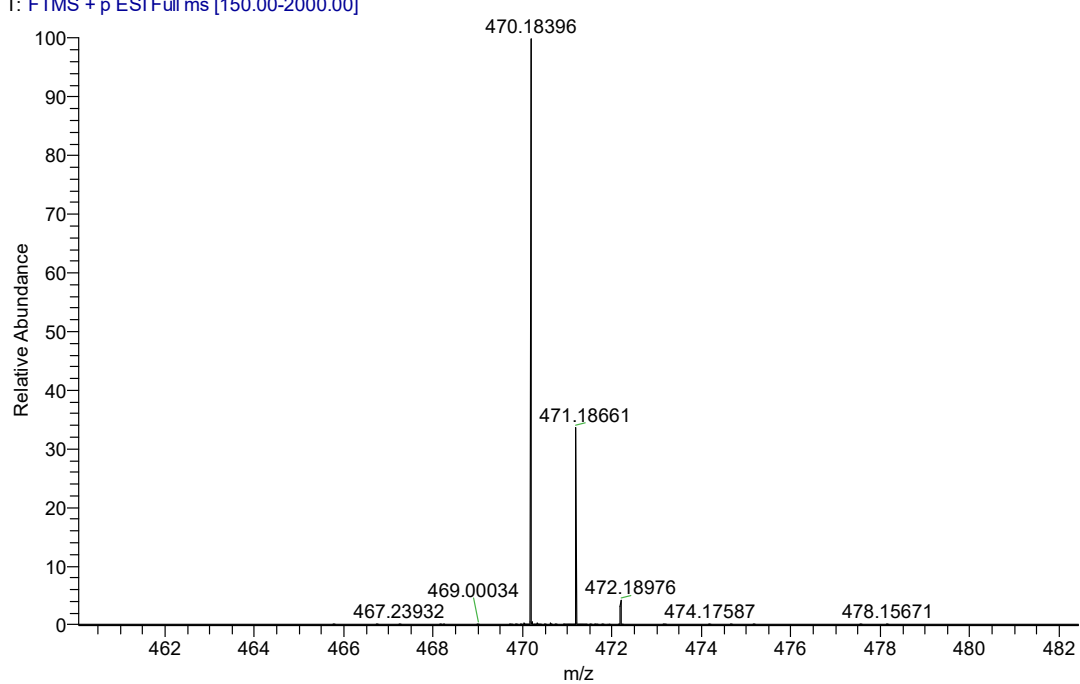


Figure S25-2 the HRMS data of compound **3y**

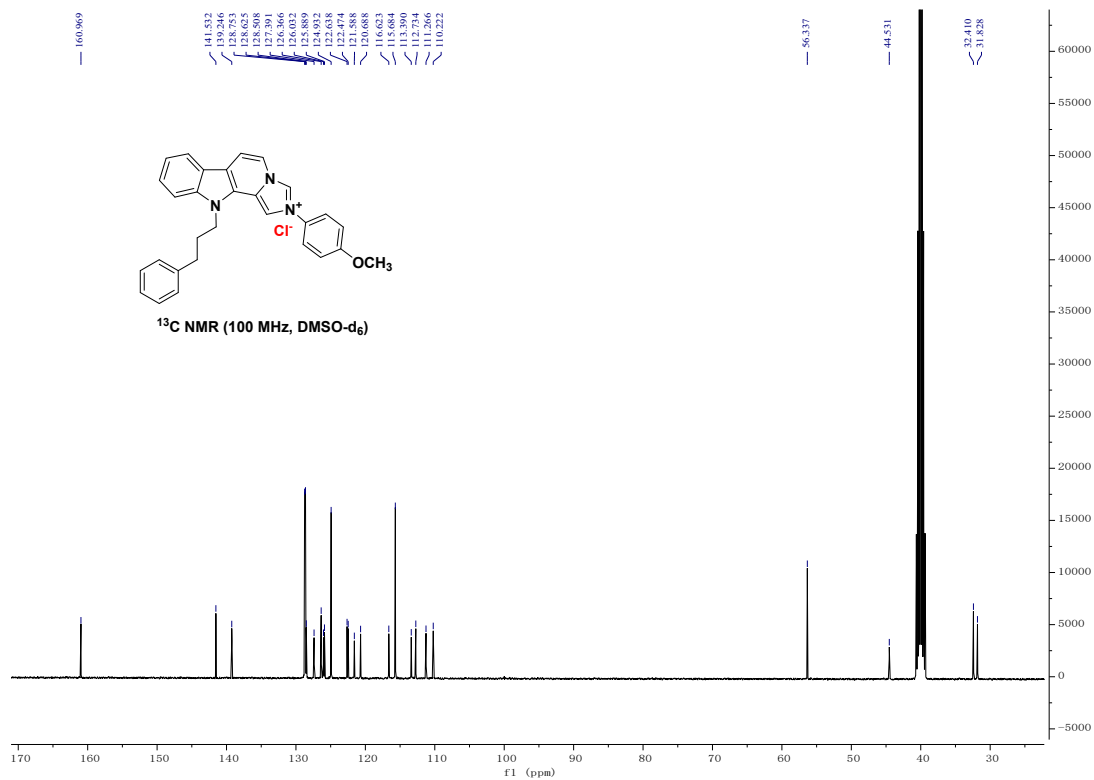
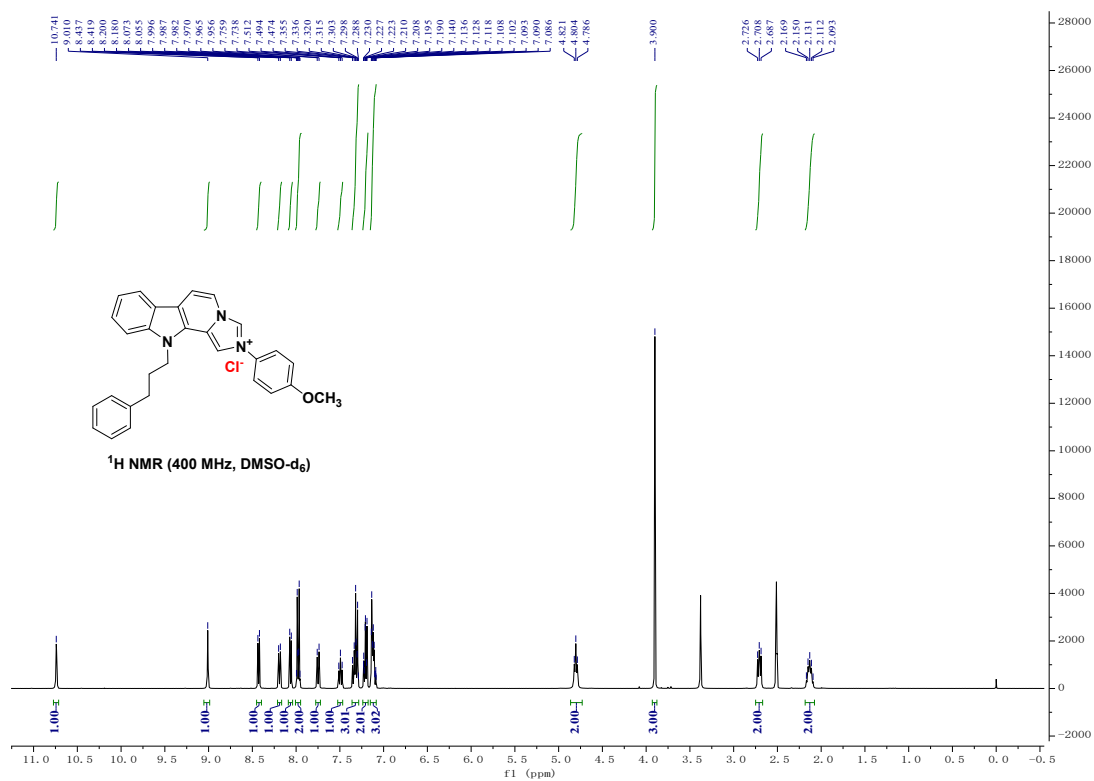


Figure S26-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3z

122 #9 RT: 0.11 AV: 1 NL: 7.93E8
T: FTMS + p ESI Full ms [150.00-2000.00]

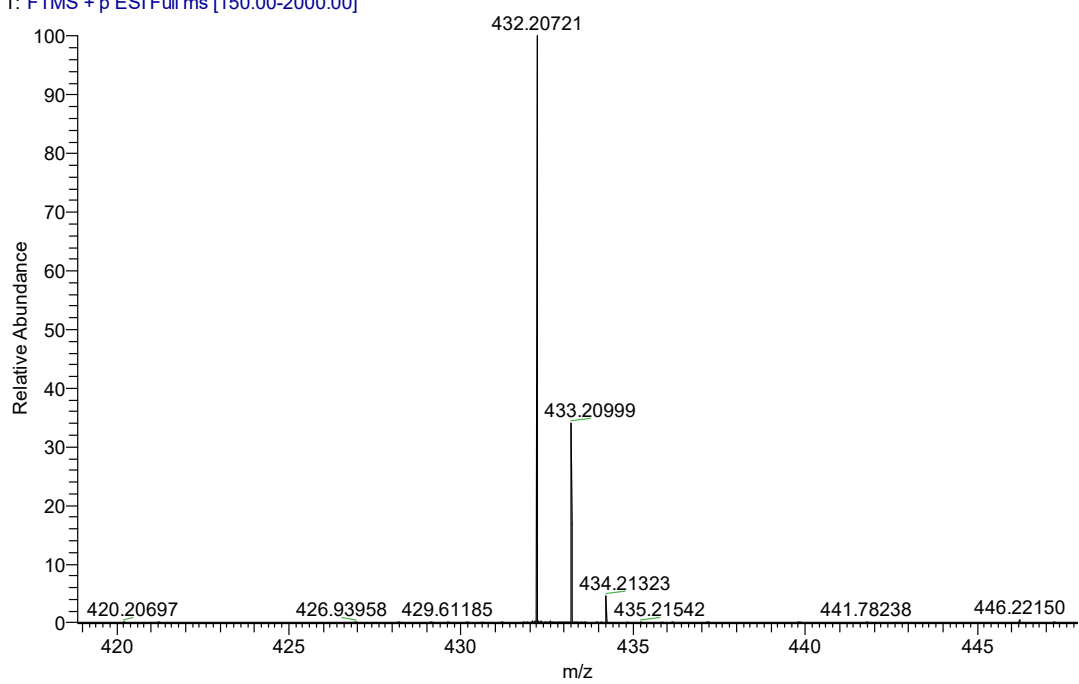


Figure S26-2 the HRMS data of compound **3z**

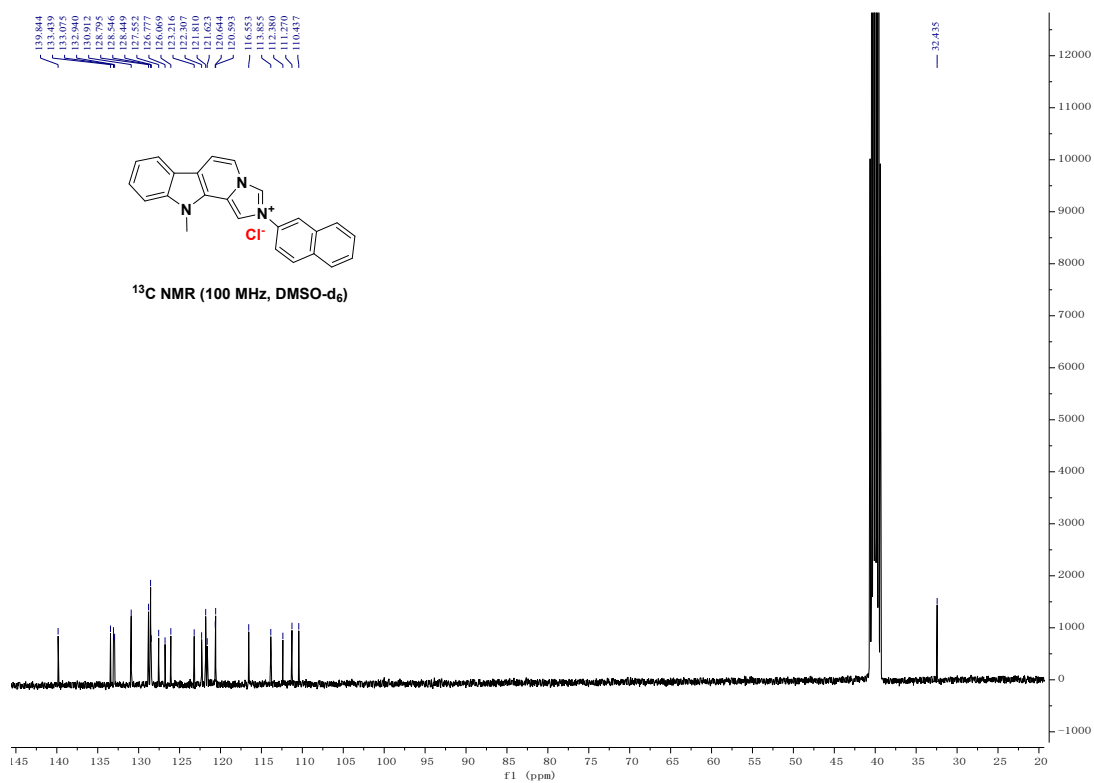
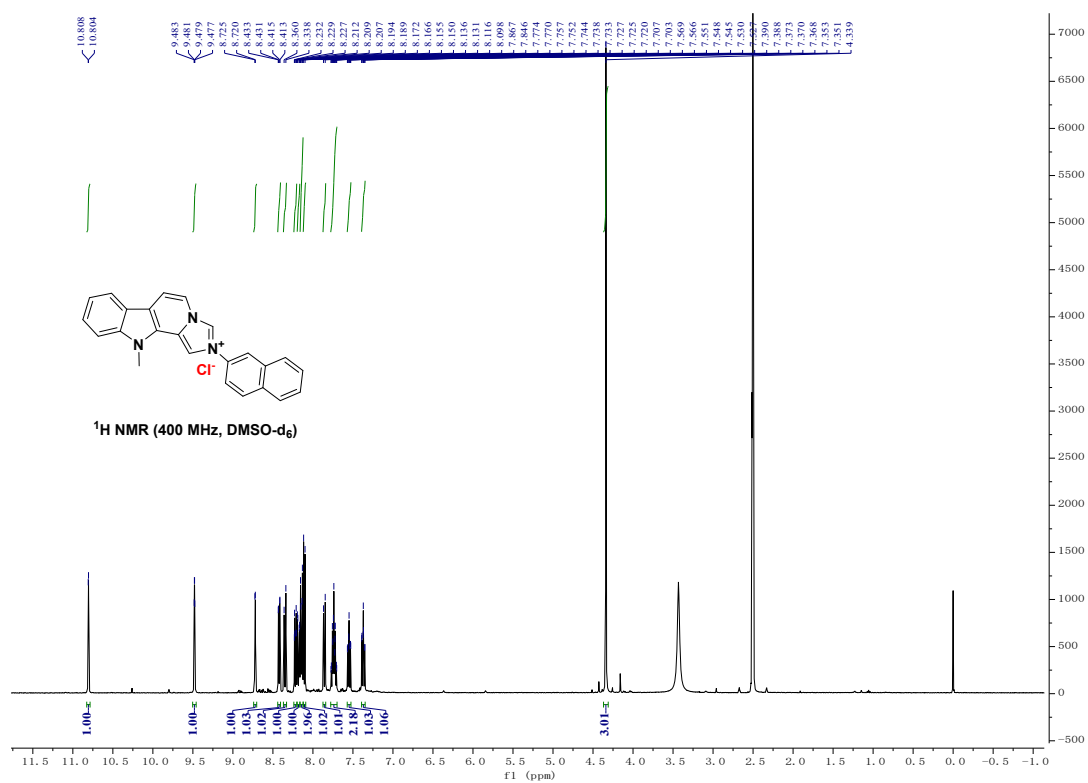


Figure S27-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound 3aa

127 #14 RT: 0.19 AV: 1 NL: 1.41E8
T: FTMS + p ESI Full ms [150.00-2000.00]

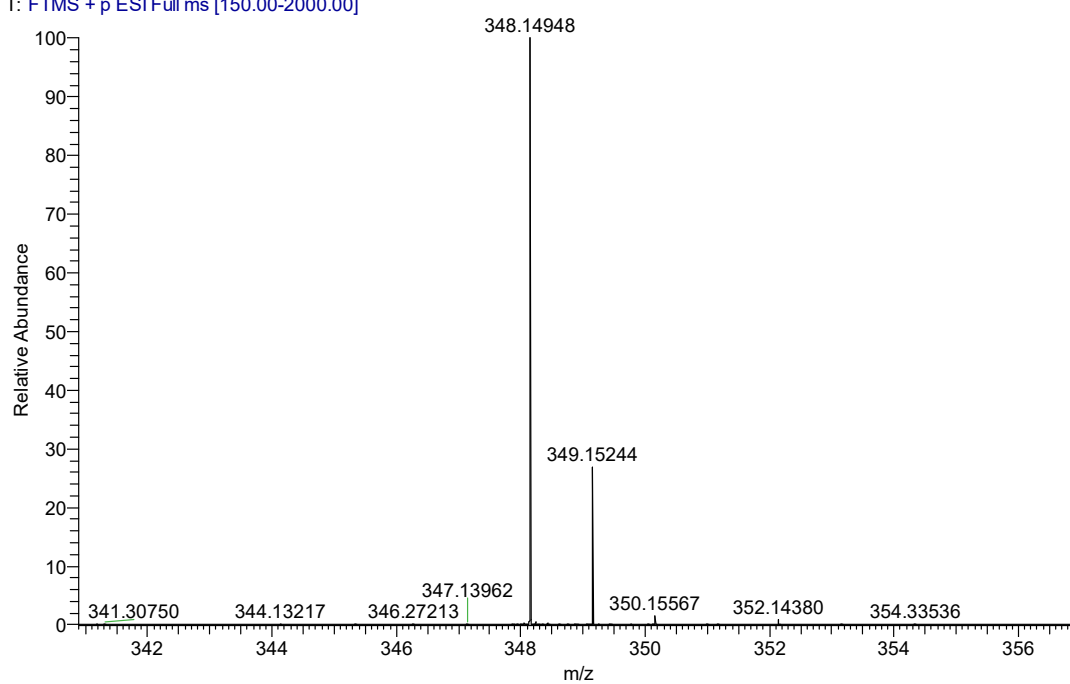


Figure S27-2 the HRMS data of compound **3aa**

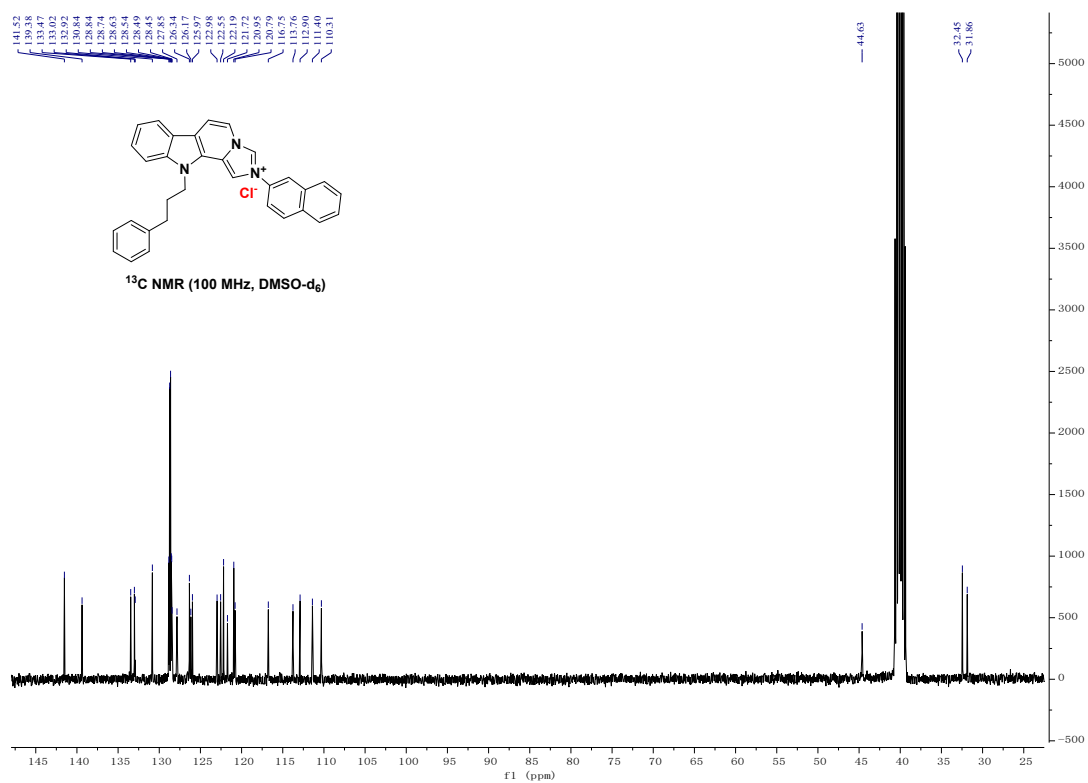
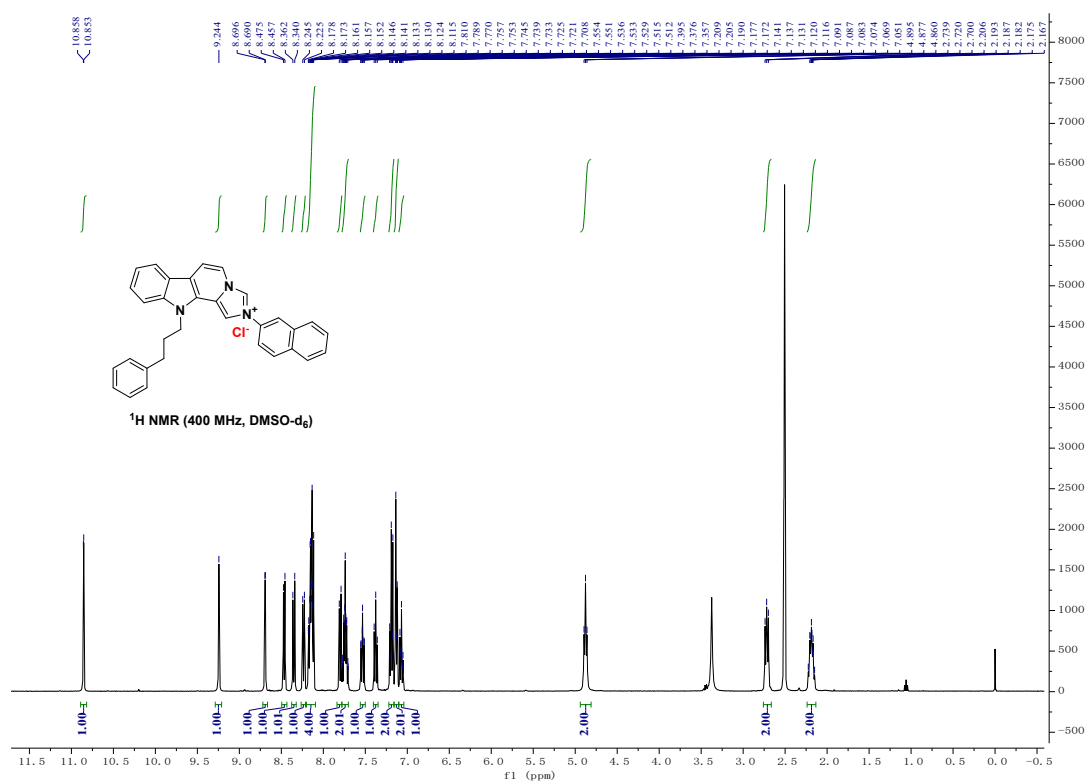


Figure S28-1 the ¹H NMR spectrum and ¹³C NMR spectrum of compound **3ab**

133 #13 RT: 0.17 AV: 1 NL: 2.14E8
T: FTMS + p ESI Full ms [150.00-2000.00]

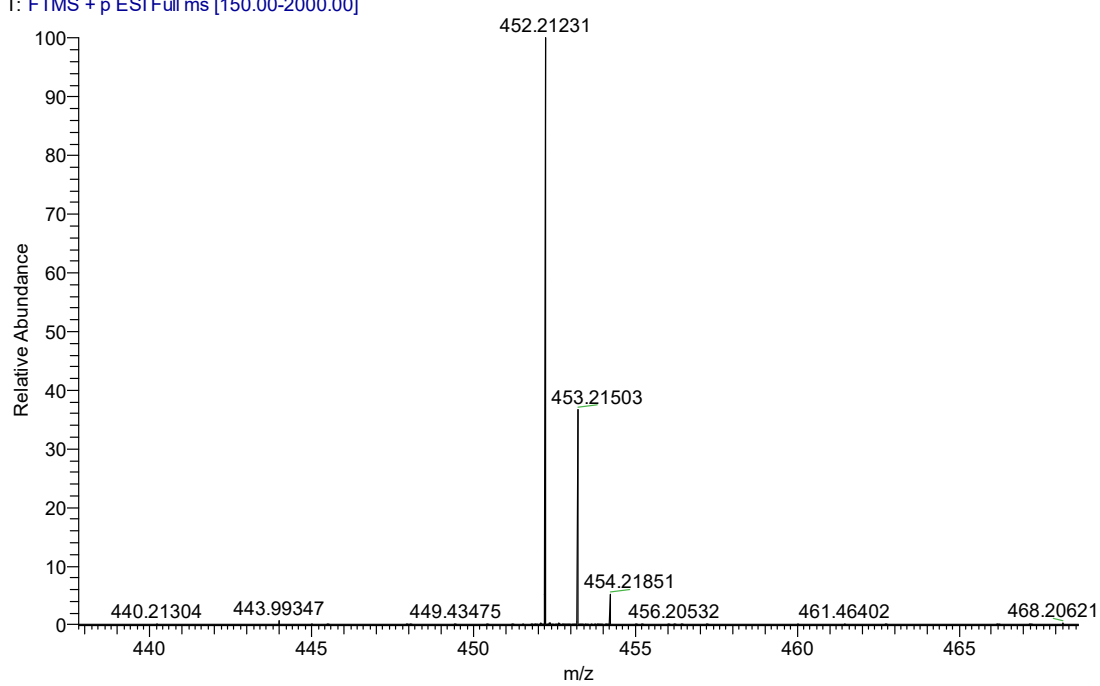


Figure S28-2 the HRMS data of compound **3ab**