

Support Information

Rhodium(III)-Catalyzed Cascade Oxidative Annulation Reactions of Aryl Imidazolium Salts with Alkynes involving Multiple C–H Bond Activation

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¹H NMR data for imidazolium salts 1

1-Phenyl-3-(2,4,6-trimethylbenzyl)imidazolium chloride (1a)

¹H NMR (CDCl₃) δ 11.79 (s, 1H), 7.78 (d, *J* = 7.7 Hz, 2H), 7.57 (t, *J* = 7.5 Hz, 3H), 7.51 (dd, *J* = 11.1, 3.5 Hz, 1H), 6.94 (s, 2H), 6.90 (s, 1H), 5.86 (s, 2H), 2.33 (s, 6H), 2.30 (s, 3H).

1-(4-Fluorophenyl)-3-(2,4,6-trimethylbenzyl)imidazolium chloride (1b)

¹H NMR (DMSO-*d*₆) δ 9.79 (s, 1H), 8.31 (t, *J* = 1.7 Hz, 1H), 7.86 (dd, *J* = 9.0, 4.6 Hz, 2H), 7.75 (t, *J* = 1.7 Hz, 1H), 7.52 (t, *J* = 8.8 Hz, 2H), 6.98 (s, 2H), 5.48 (s, 2H), 2.32 (s, 6H), 2.26 (s, 3H).

1-(4-Chlorophenyl)-3-(2,4,6-trimethylbenzyl)imidazolium chloride (1c)

¹H NMR (DMSO-*d*₆) δ 9.83 (s, 1H), 8.35 (s, 1H), 7.86 (s, 1H), 7.76 (s, 1H), 7.75 (s, 1H), 7.72 (s, 1H), 6.98 (s, 2H), 5.47 (s, 2H), 2.31 (s, 6H), 2.26 (s, 3H).

1-(4-Bromophenyl)-3-(2,4,6-trimethylbenzyl)imidazolium chloride (1d)

¹H NMR (DMSO-*d*₆) δ 9.84 (s, 1H), 8.35 (d, *J* = 1.7 Hz, 1H), 7.86 (d, *J* = 8.8 Hz, 2H), 7.77 (d, *J* = 14.3 Hz, 3H), 6.98 (s, 2H), 5.48 (s, 2H), 2.31 (s, 6H), 2.26 (s, 3H).

1-p-Tolyl-3-(2,4,6-trimethylbenzyl)imidazolium chloride (1e)

¹H NMR (CDCl₃) δ 11.44 (s, 1H), 7.63 (d, *J* = 8.2 Hz, 3H), 7.31 (d, *J* = 8.2 Hz, 2H), 6.91 (d, *J* = 6.9 Hz, 3H), 5.81 (s, 2H), 2.38 (s, 3H), 2.30 (s, 6H), 2.28 (s, 3H).

1-(4-Methoxyphenyl)-3-(2,4,6-trimethylbenzyl)imidazolium chloride (1f)

¹H NMR (CDCl₃) δ 11.20 (s, 1H), 7.69 (d, *J* = 8.8 Hz, 2H), 6.96 (d, *J* = 8.7 Hz, 2H), 6.88 (s, 3H), 5.73 (s, 2H), 3.77 (s, 3H), 2.26 (d, *J* = 4.7 Hz, 9H).

1-(4-(Dimethylamino)phenyl)-3-(2,4,6-trimethylbenzyl)imidazolium chloride (1g)

¹H NMR (CDCl₃) δ 11.05 (s, 1H), 7.52 (d, *J* = 8.1 Hz, 3H), 6.90 (s, 3H), 6.70 (d, *J* = 8.9 Hz, 2H), 5.77 (s, 2H), 2.96 (s, 6H), 2.28 (s, 6H), 2.27 (s, 3H).

1-(4-*tert*-Butylphenyl)-3-(2,4,6-trimethylbenzyl)imidazolium chloride (1h)

¹H NMR (DMSO-*d*₆) δ 9.79 (s, 1H), 8.30 (s, 1H), 7.70 (d, *J* = 1.7 Hz, 3H), 7.64 (d, *J* = 8.8 Hz, 2H), 6.98 (s, 2H), 5.48 (s, 2H), 2.31 (s, 6H), 2.26 (s, 3H), 1.32 (s, 9H).

1-(4-Nitrophenyl)-3-(2,4,6-trimethylbenzyl)imidazolium chloride (1i)

^1H NMR (DMSO- d_6) δ 10.00 (s, 1H), 8.49 (d, J = 8.7 Hz, 3H), 8.12 (d, J = 9.0 Hz, 2H), 7.82 (s, 1H), 6.99 (s, 2H), 5.50 (s, 2H), 2.32 (s, 6H), 2.26 (s, 3H).

1,3-diphenylimidazolium chloride (1j)

^1H NMR (DMSO- d_6) δ 10.63 (s, 1H), 8.68 (s, 2H), 8.03 (dd, J = 5.5, 3.2 Hz, 4H), 7.69 (t, J = 7.7 Hz, 4H), 7.62 (t, J = 7.4 Hz, 2H).

1-Phenyl-3-(2,4,6-trimethylbenzyl)benzo[d]imidazolium bromide (1k)

^1H NMR (DMSO- d_6) δ 9.76 (s, 1H), 8.18 (d, J = 8.1 Hz, 1H), 7.85 – 7.66 (m, 8H), 7.01 (s, 2H), 5.78 (s, 2H), 2.34 (s, 6H), 2.28 (s, 3H).

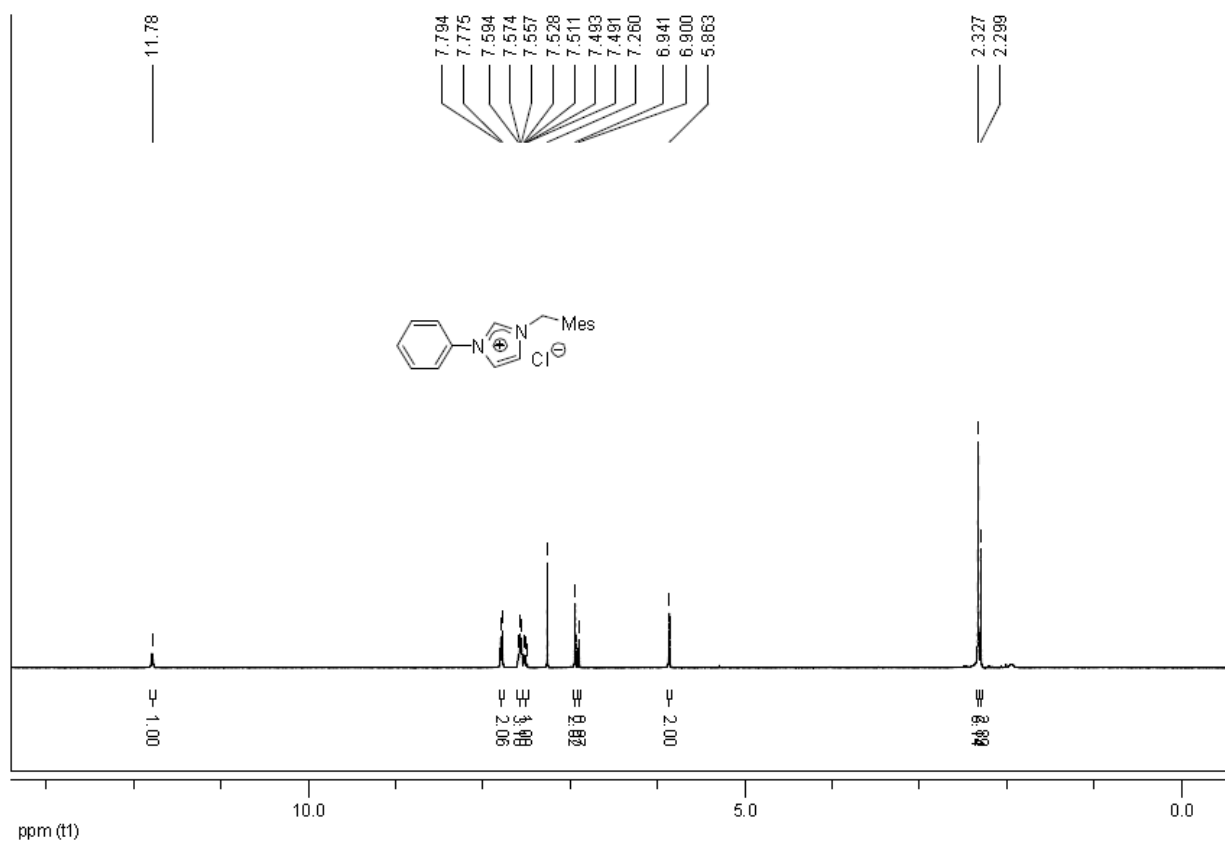
3-methyl-1-phenylimidazolium iodide (1l)

^1H NMR (CDCl₃) δ 10.37 (d, J = 23.3 Hz, 1H), 7.73 (ddd, J = 27.3, 9.5, 2.2 Hz, 4H), 7.59 – 7.48 (m, 3H), 4.25 (d, J = 6.6 Hz, 3H).

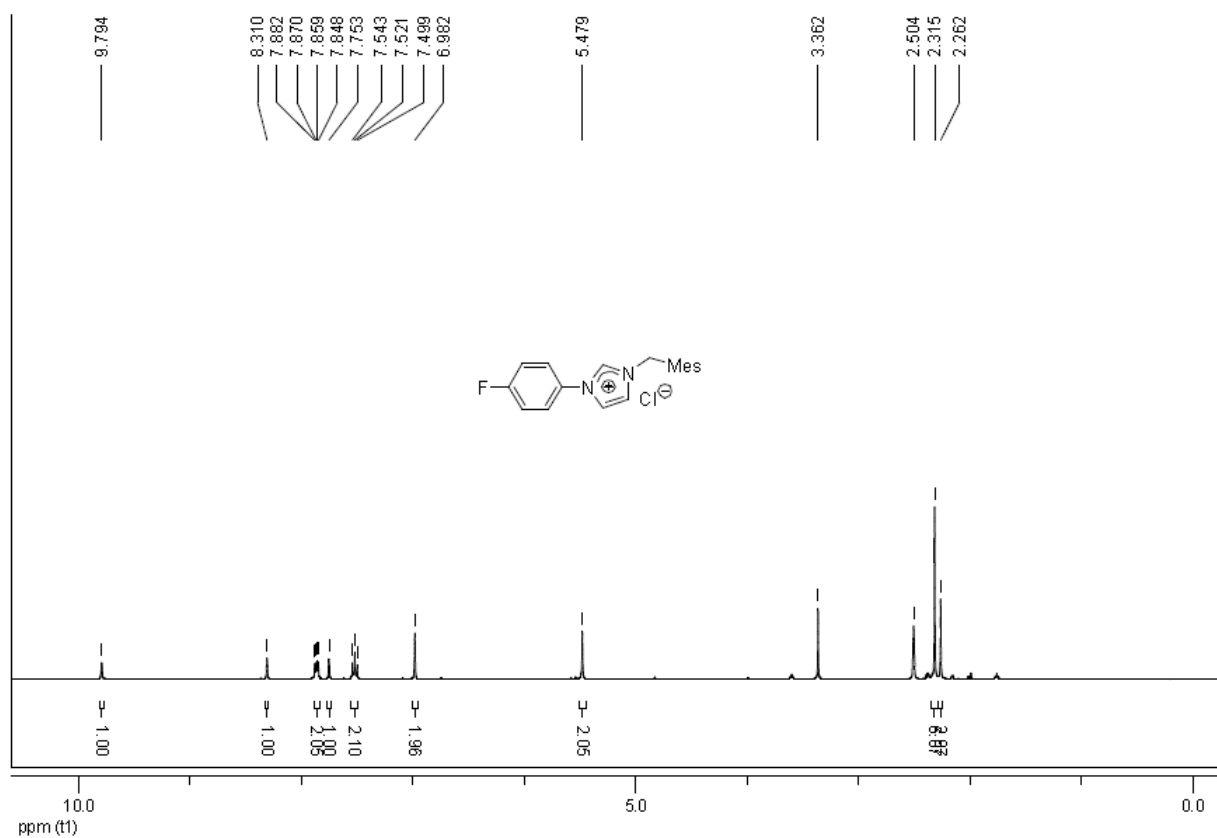
2-methyl-1-phenyl-3-(2,4,6-trimethylbenzyl)imidazolium chloride (1m)

^1H NMR (CDCl₃) δ 7.70 (dd, J = 6.1, 3.2 Hz, 2H), 7.58 – 7.53 (m, 3H), 7.27 (d, J = 2.1 Hz, 1H), 6.94 (s, 2H), 6.66 (d, J = 2.1 Hz, 1H), 5.49 (s, 2H), 2.91 (s, 3H), 2.34 (s, 6H), 2.30 (s, 3H).

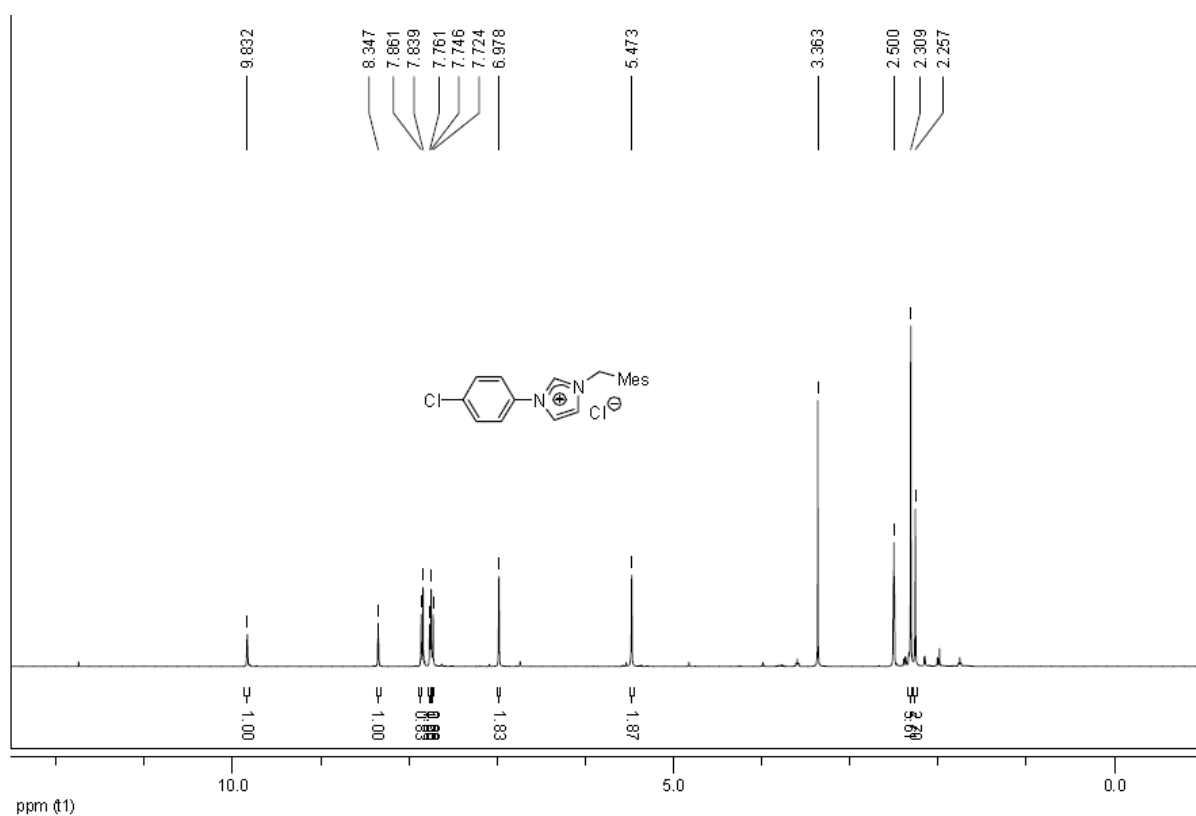
¹H NMR spectrum of 1a



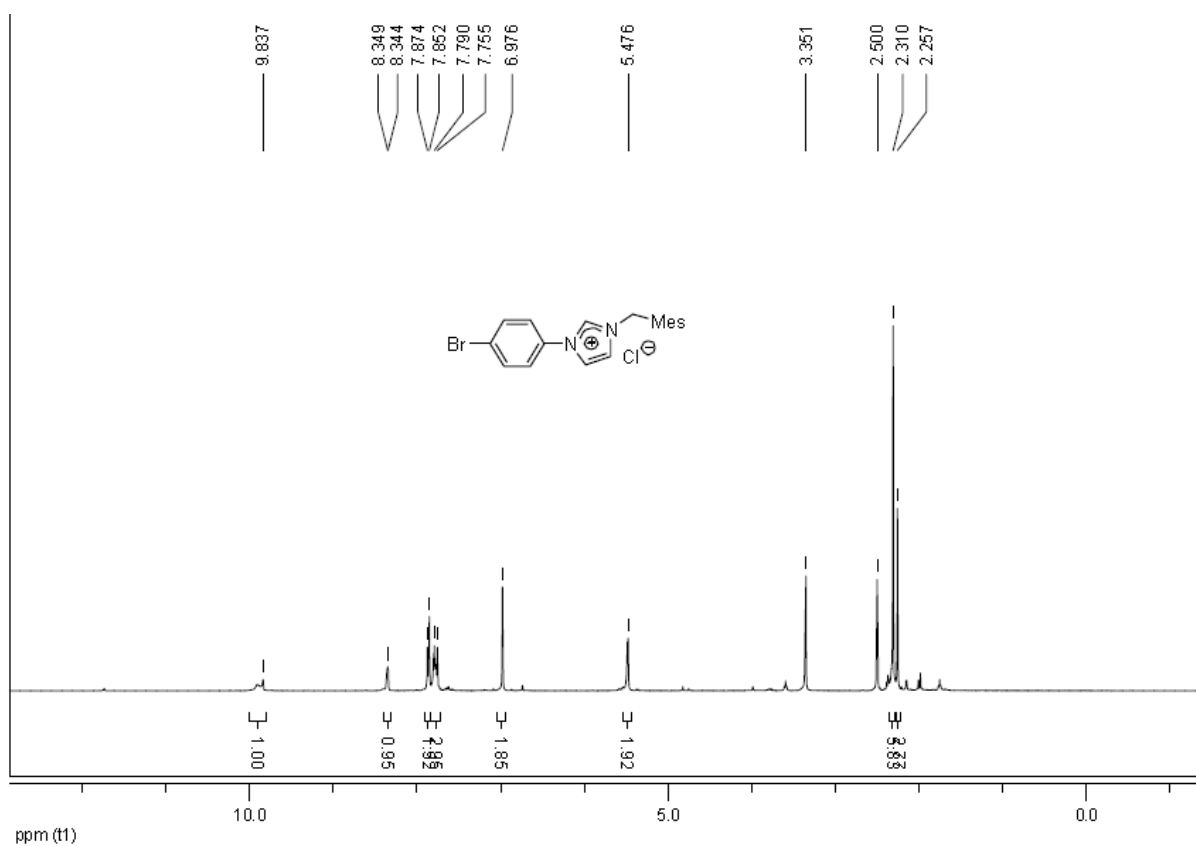
¹H NMR spectrum of 1b



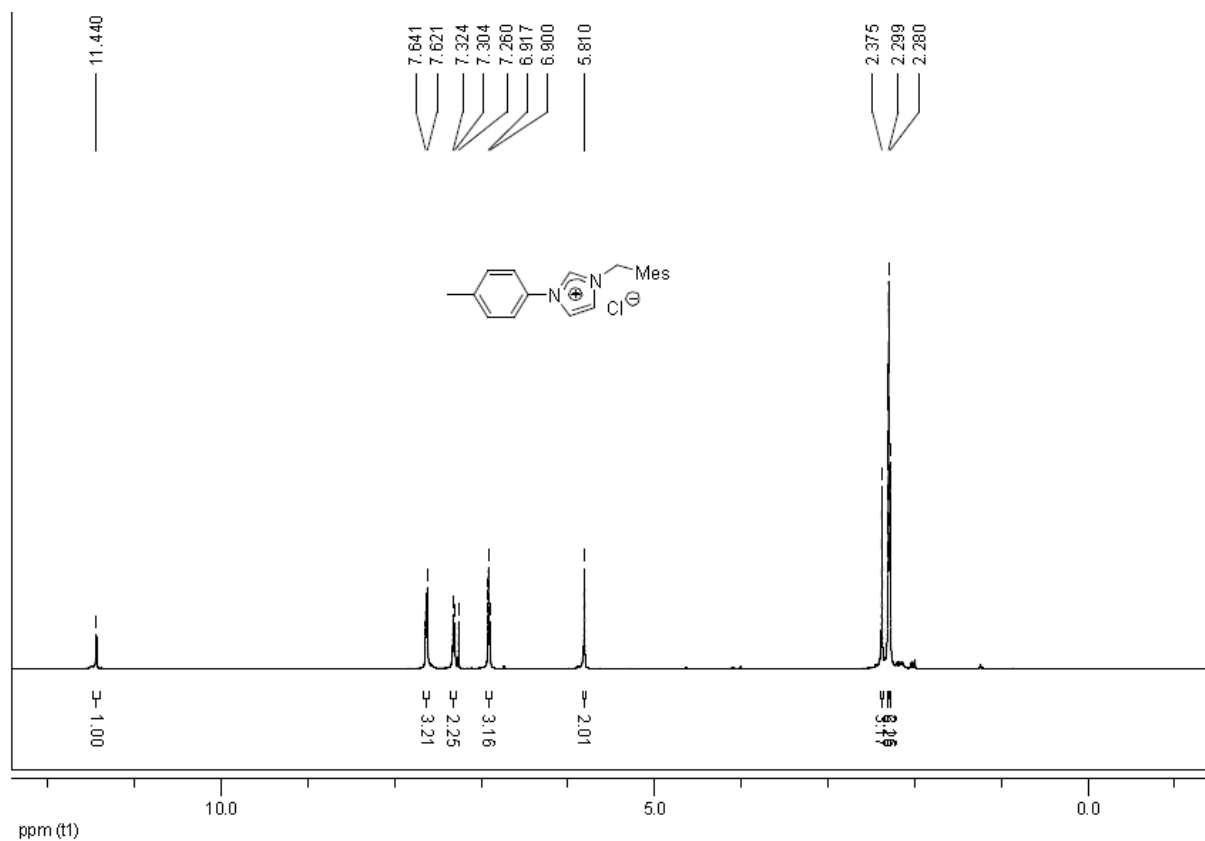
¹H NMR spectrum of 1c



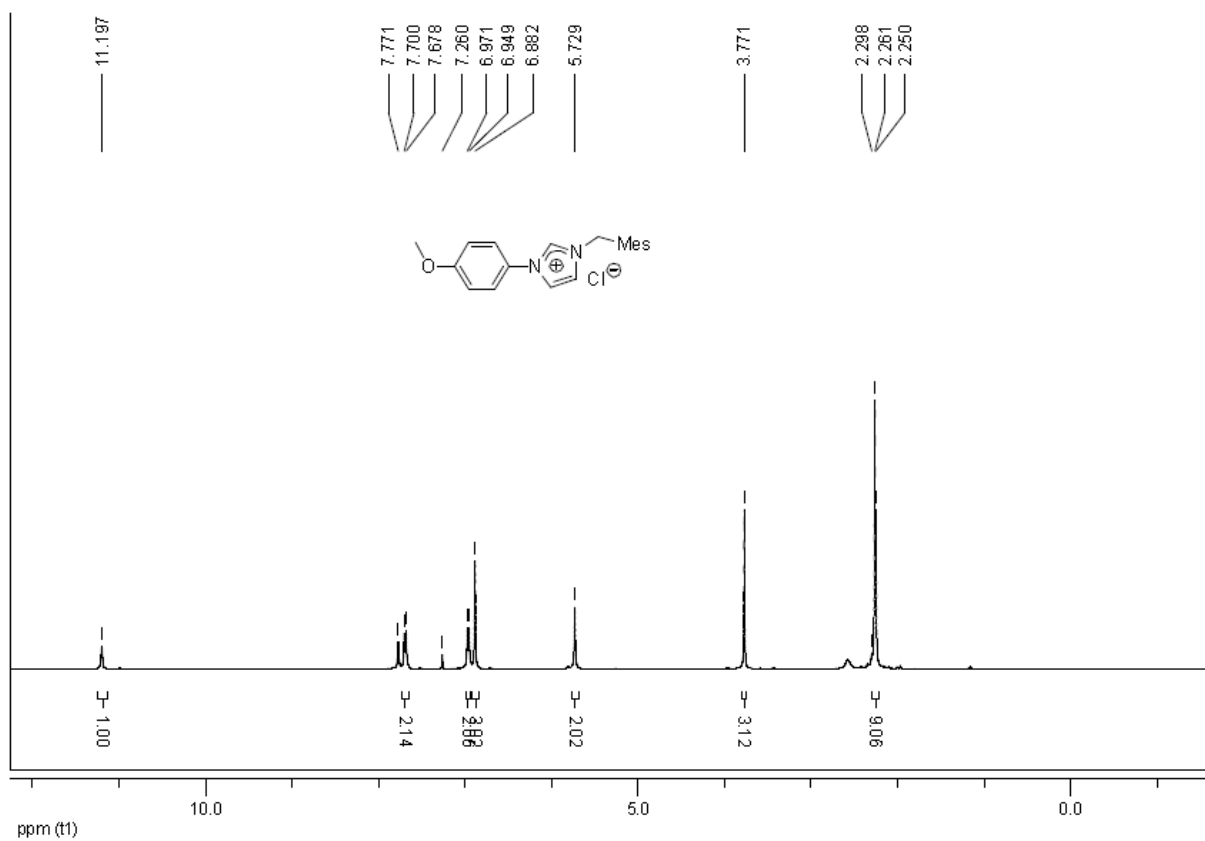
¹H NMR spectrum of 1d



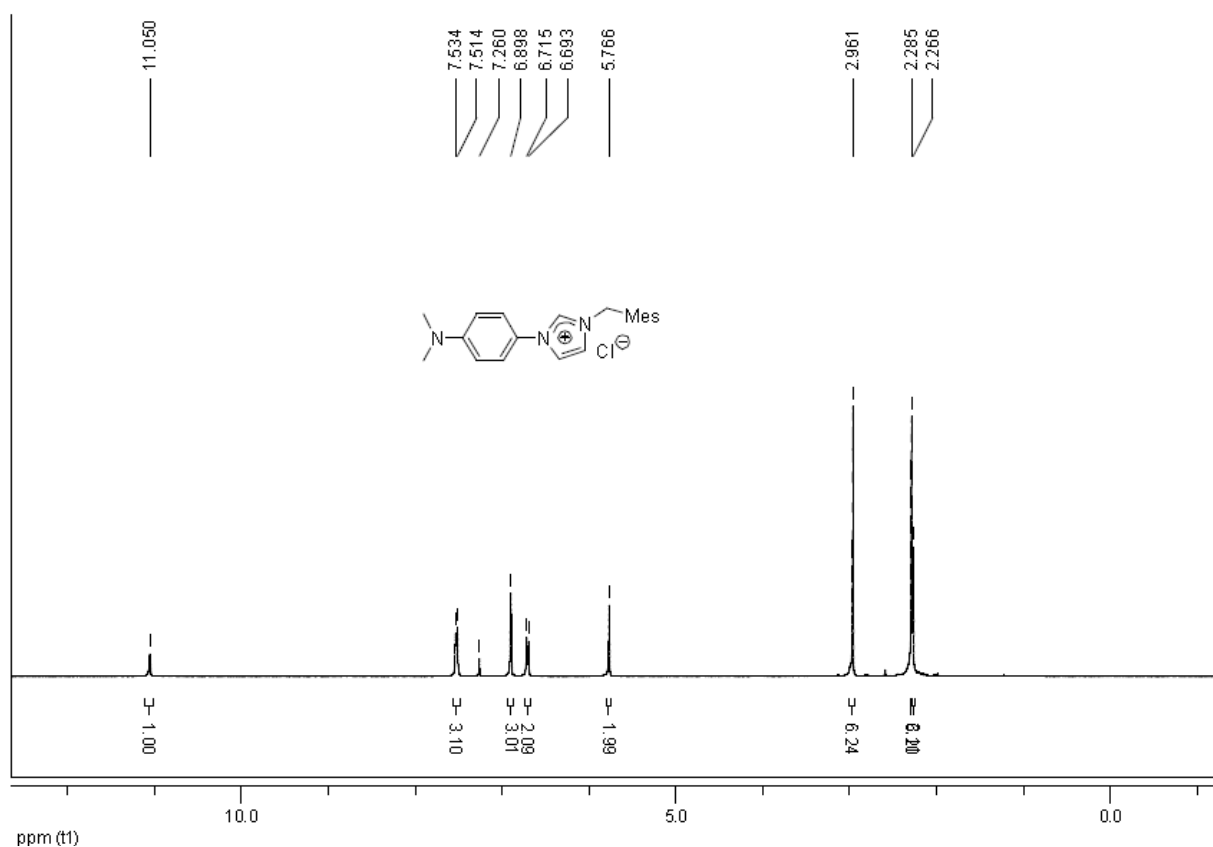
¹H NMR spectrum of 1e



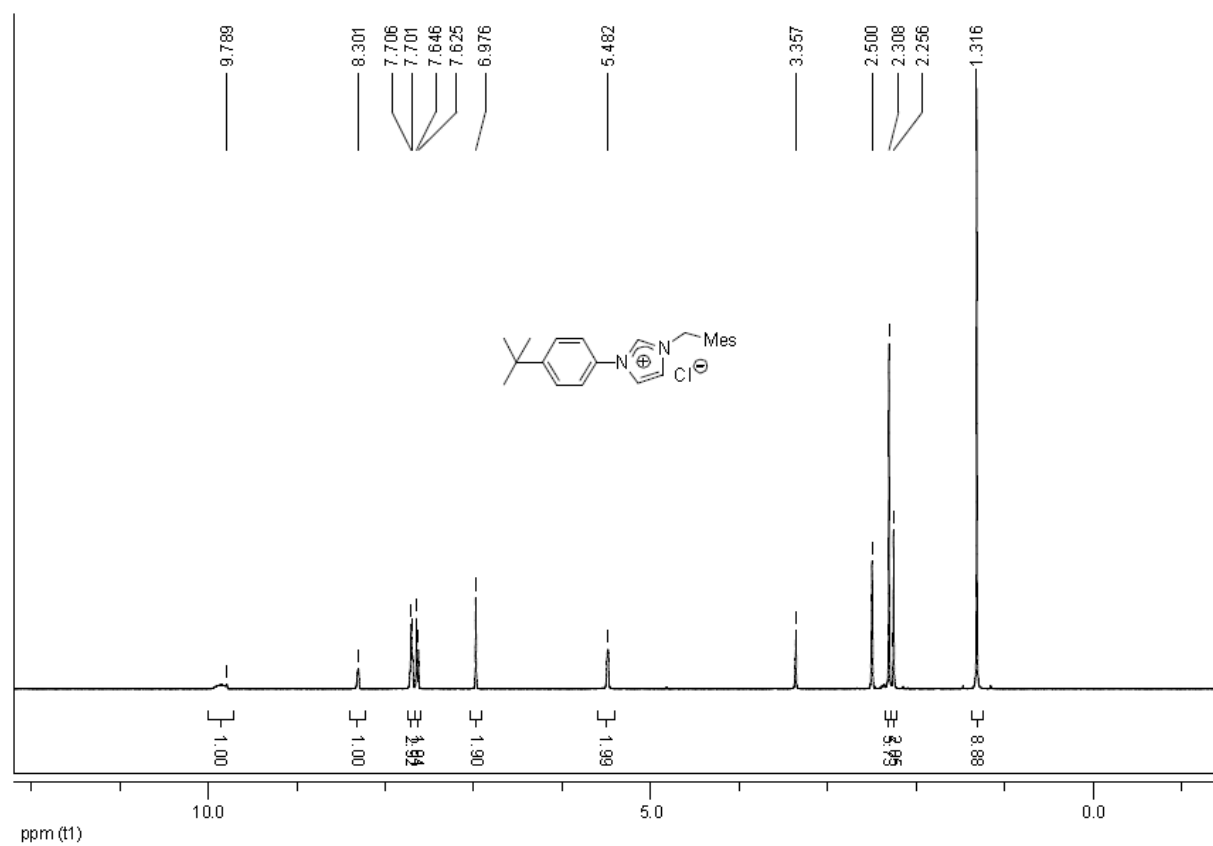
¹H NMR spectrum of 1f



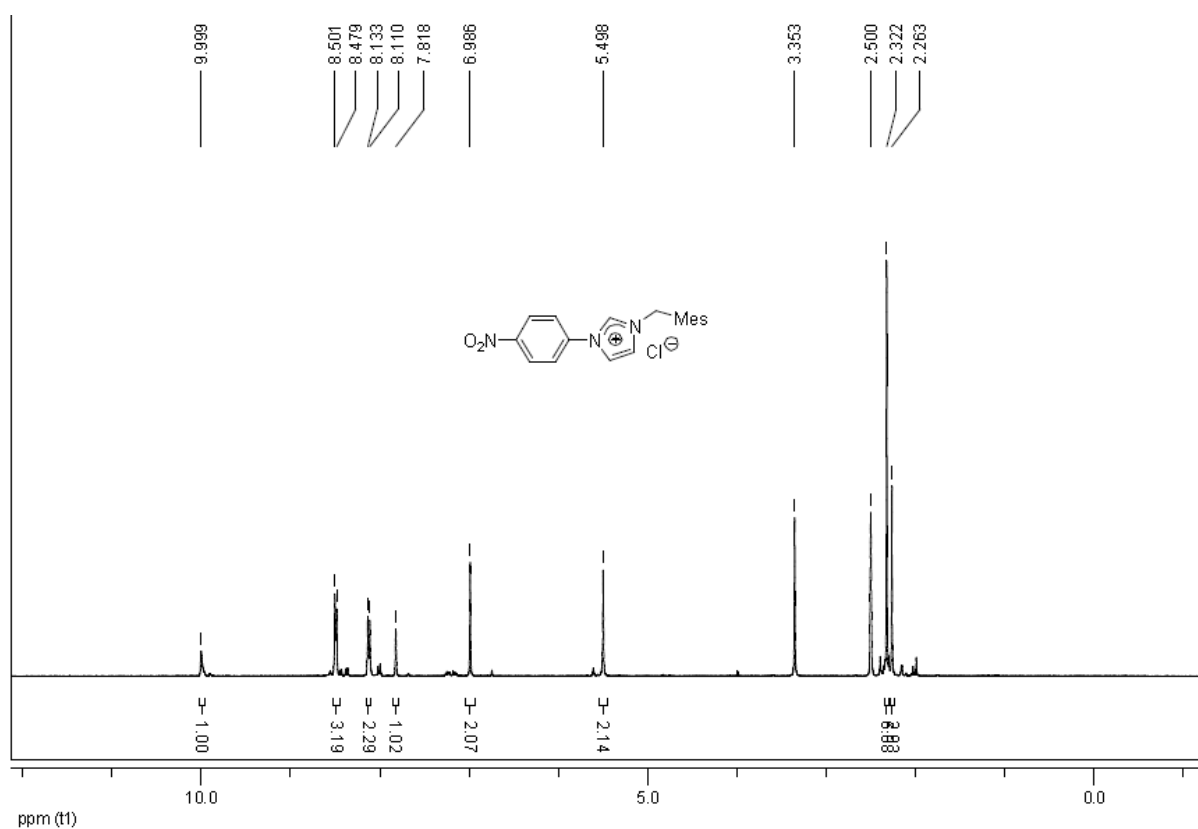
¹H NMR spectrum of 1g



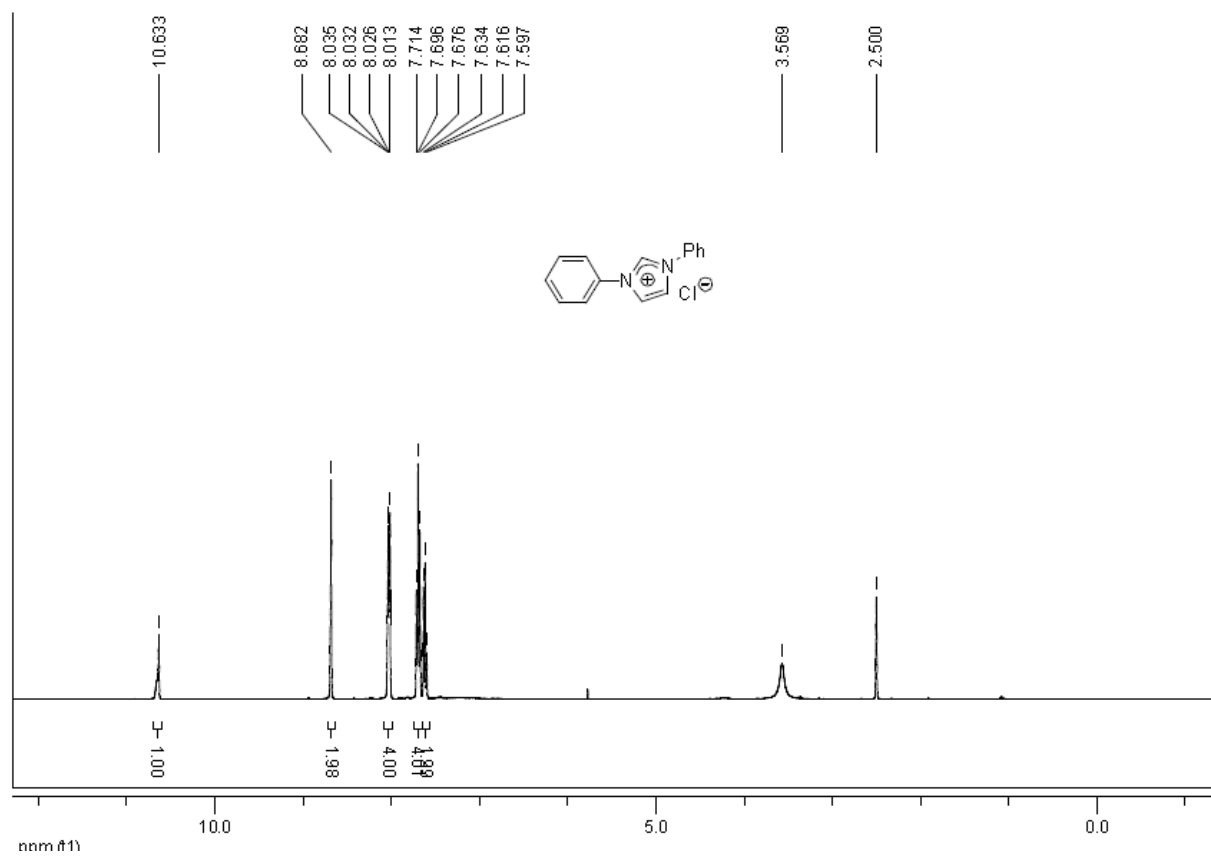
¹H NMR spectrum of 1h



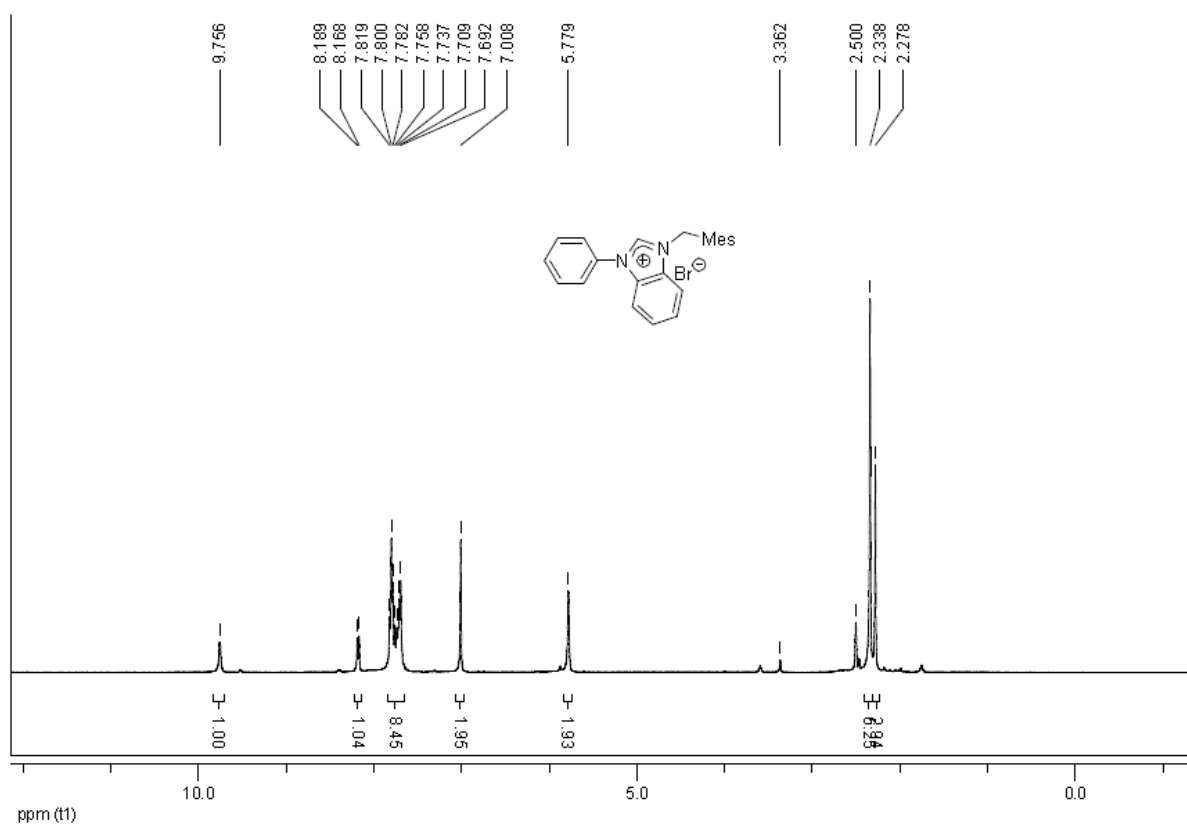
¹H NMR spectrum of 1i



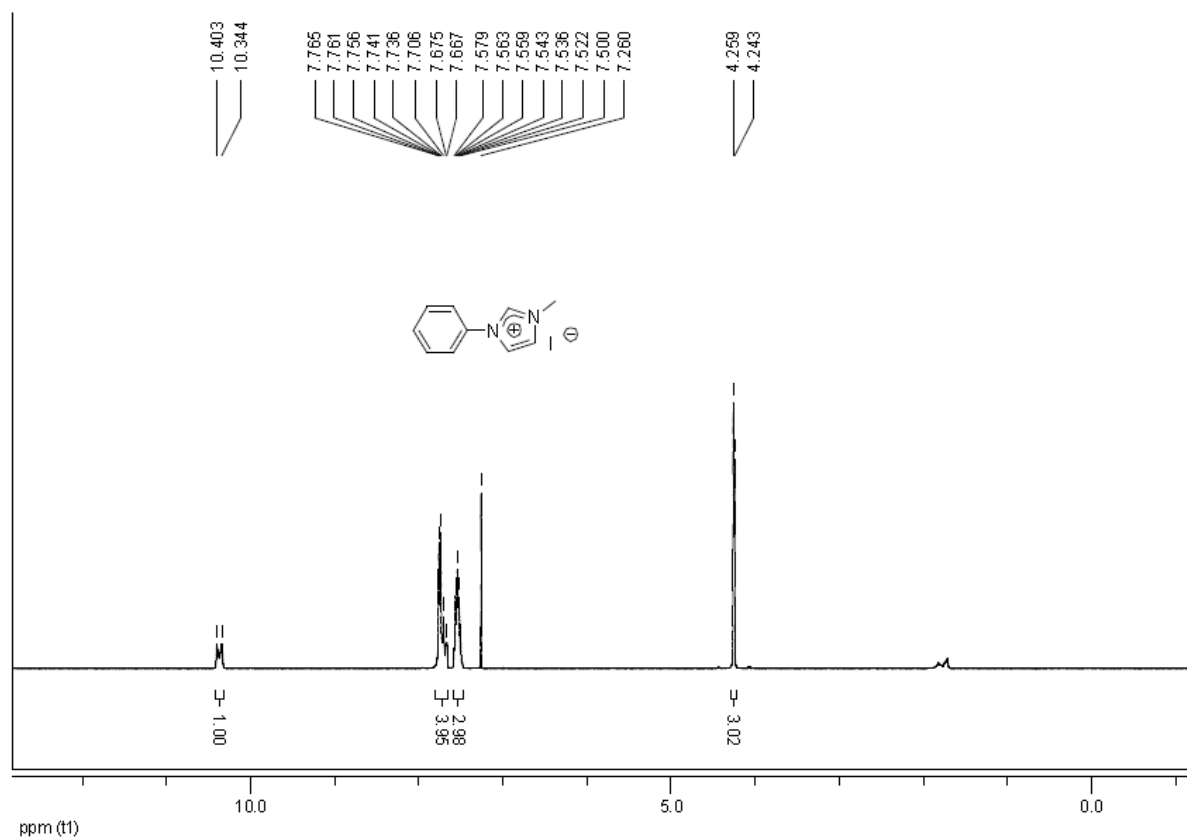
¹H NMR spectrum of 1j



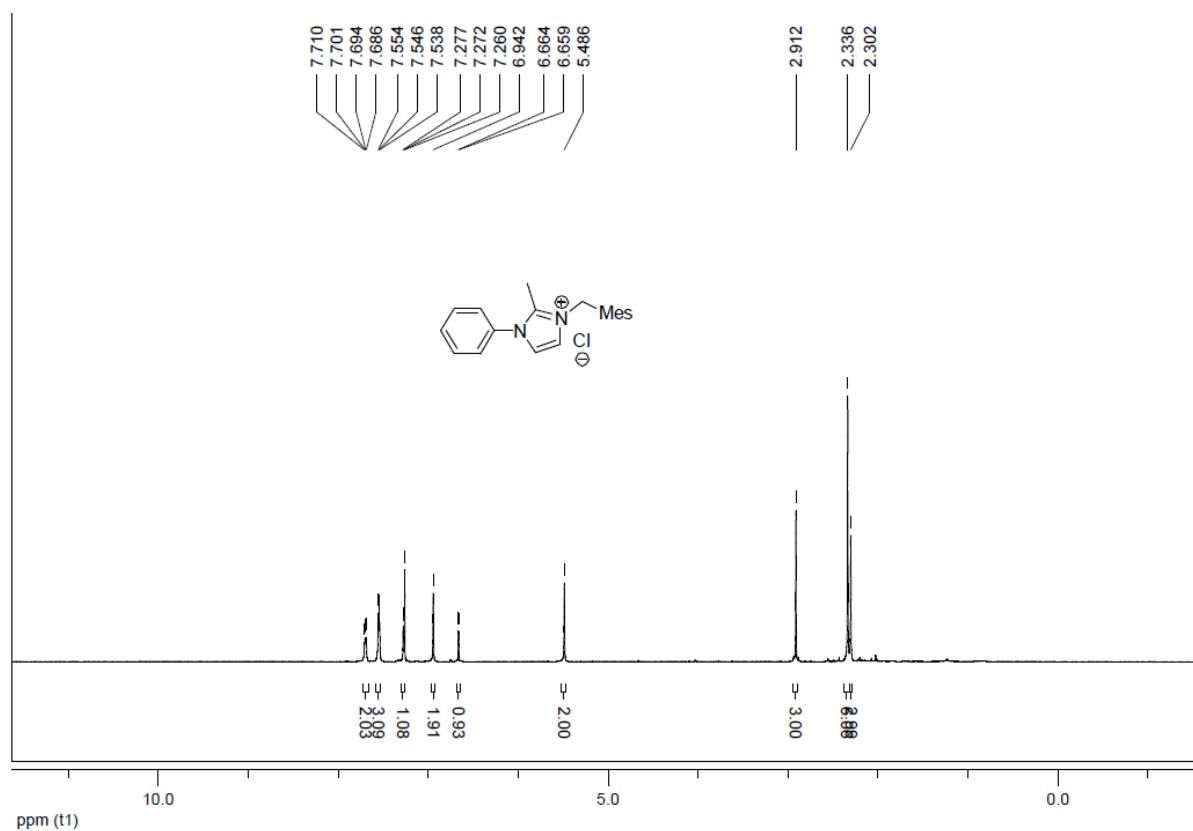
¹H NMR spectrum of 1k



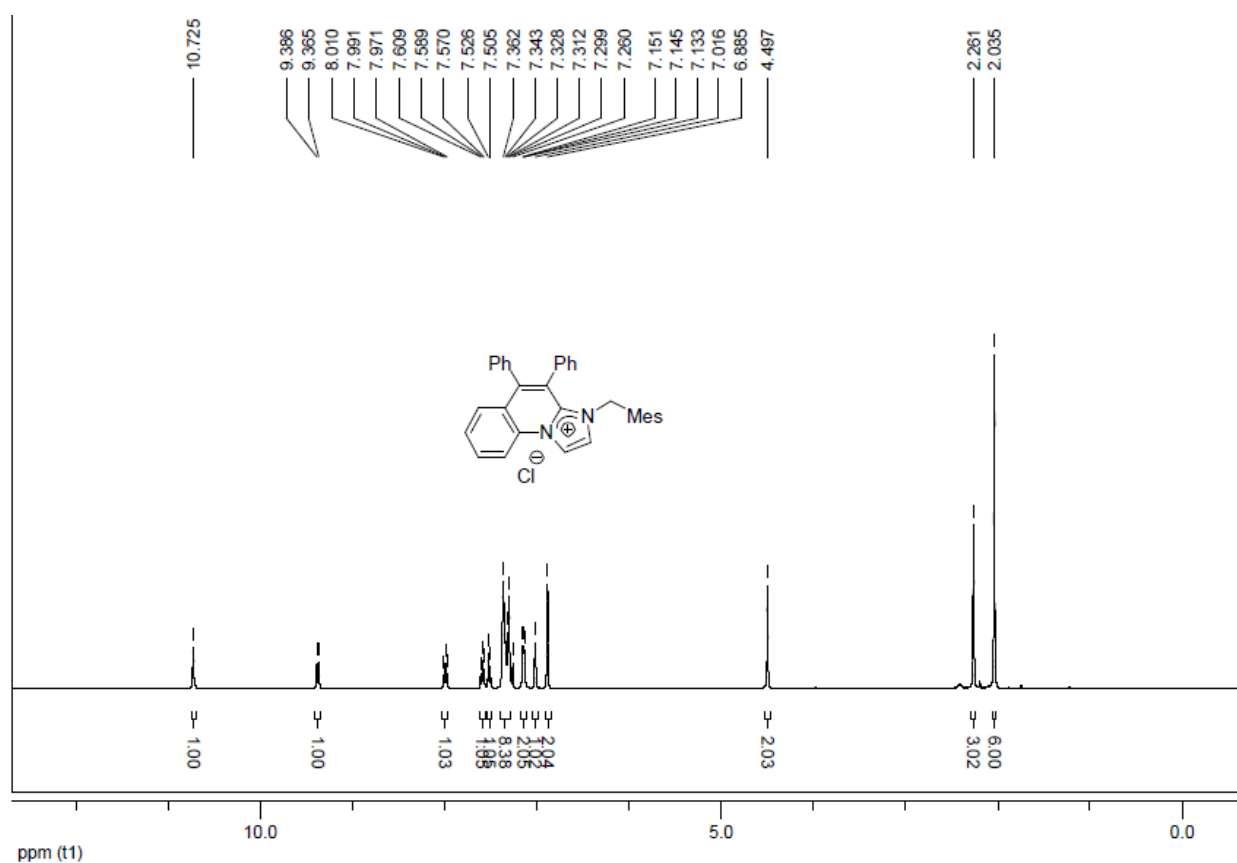
¹H NMR spectrum of 1l



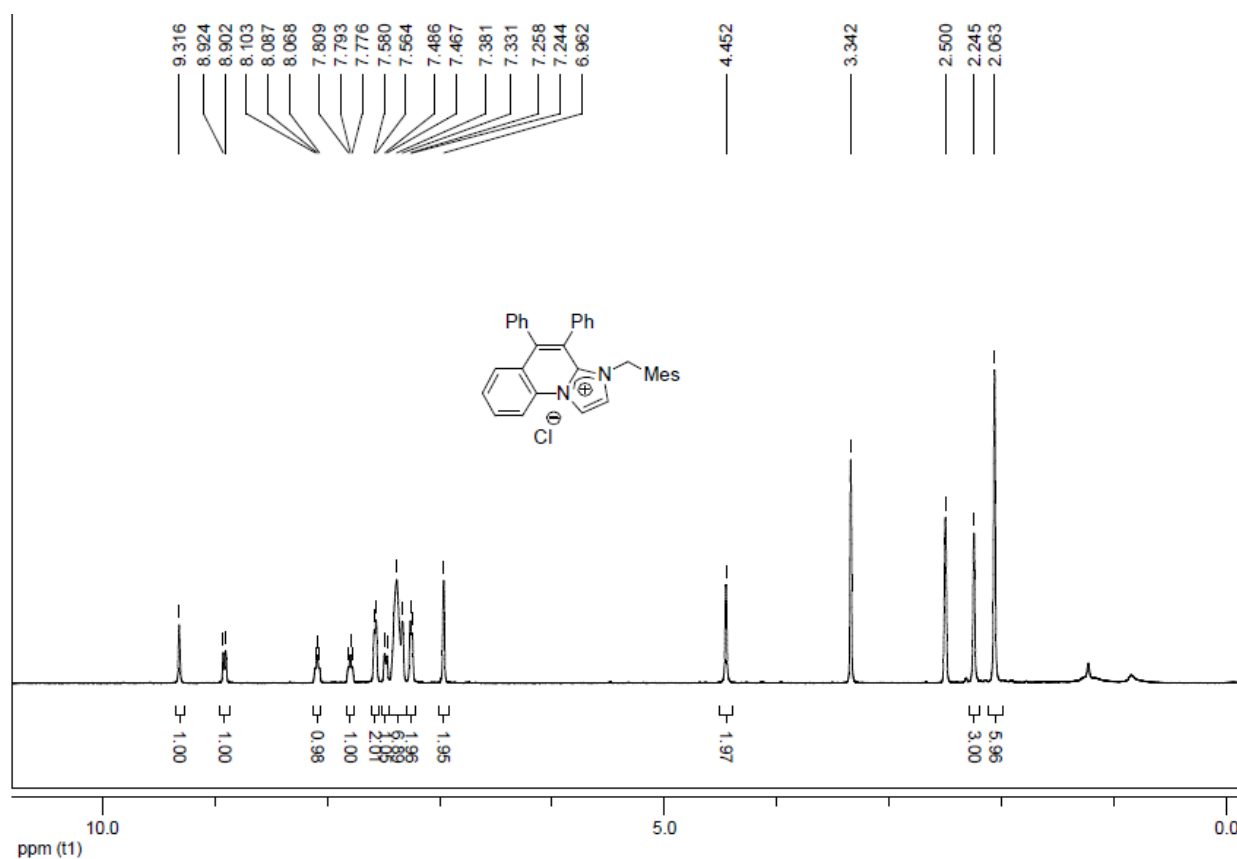
¹H NMR spectrum of 1m



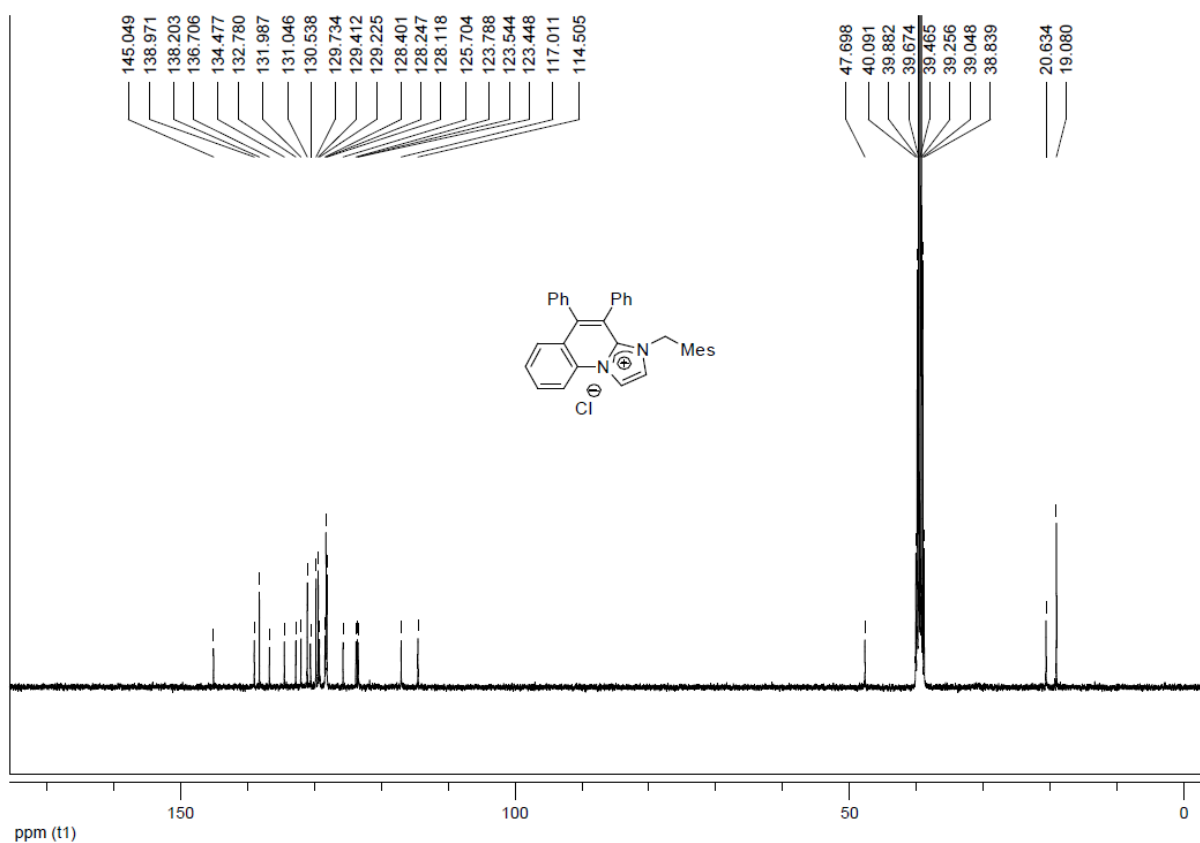
¹H NMR spectrum of 3aa (in CDCl₃)



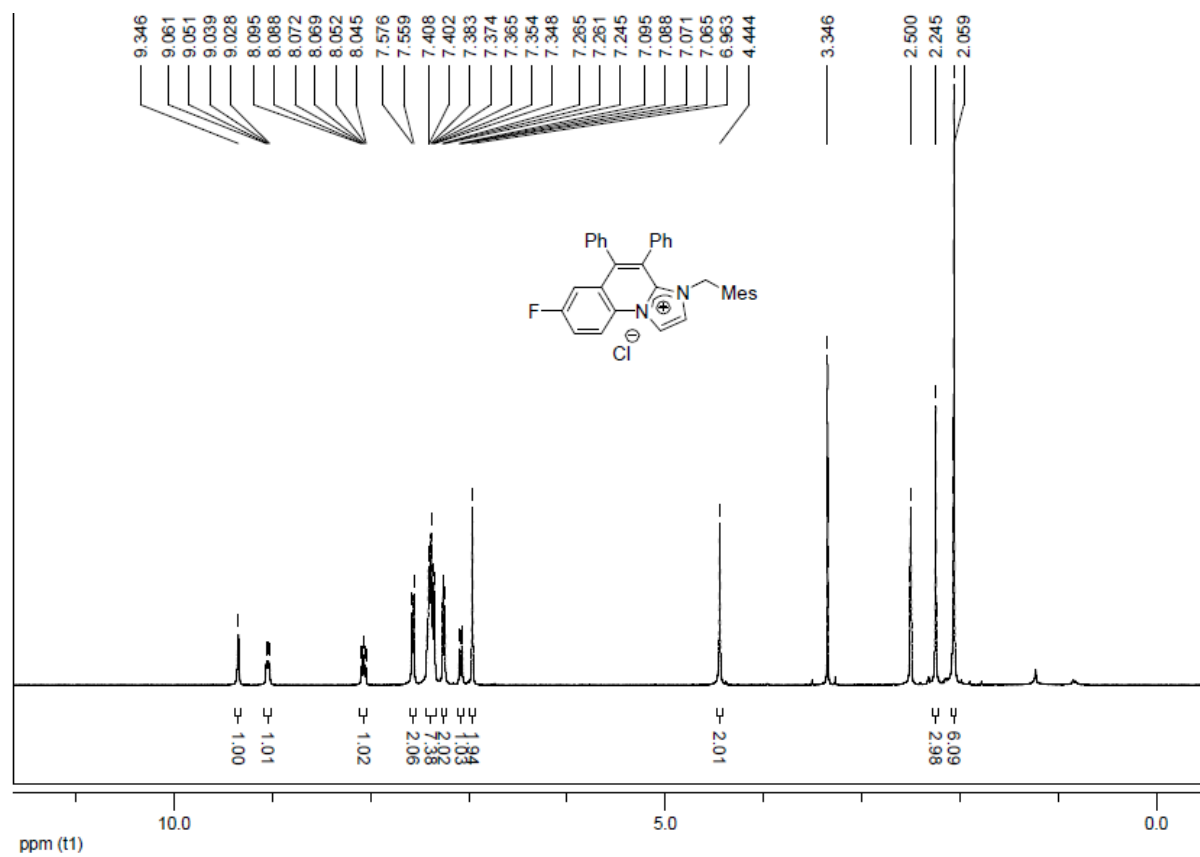
¹H NMR spectrum of 3aa (in DMSO-*d*₆)



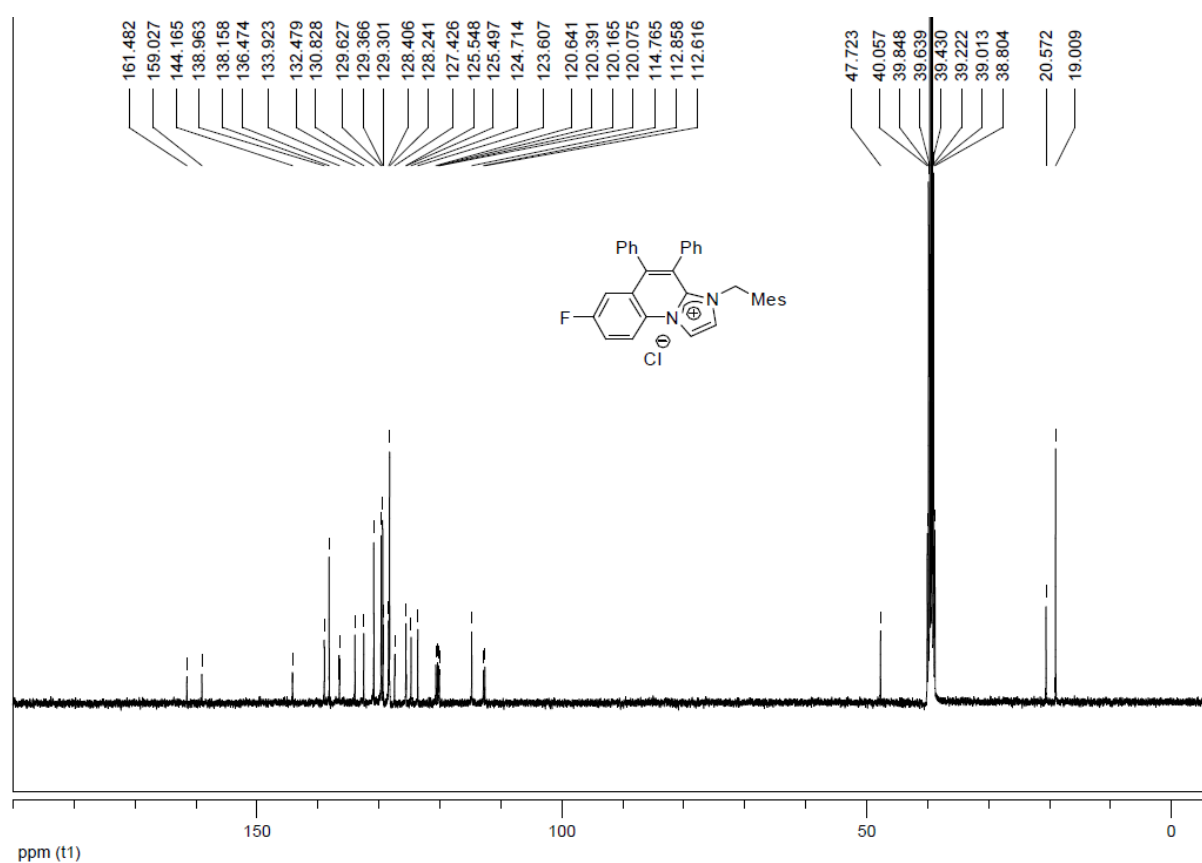
¹³C NMR spectrum of 3aa



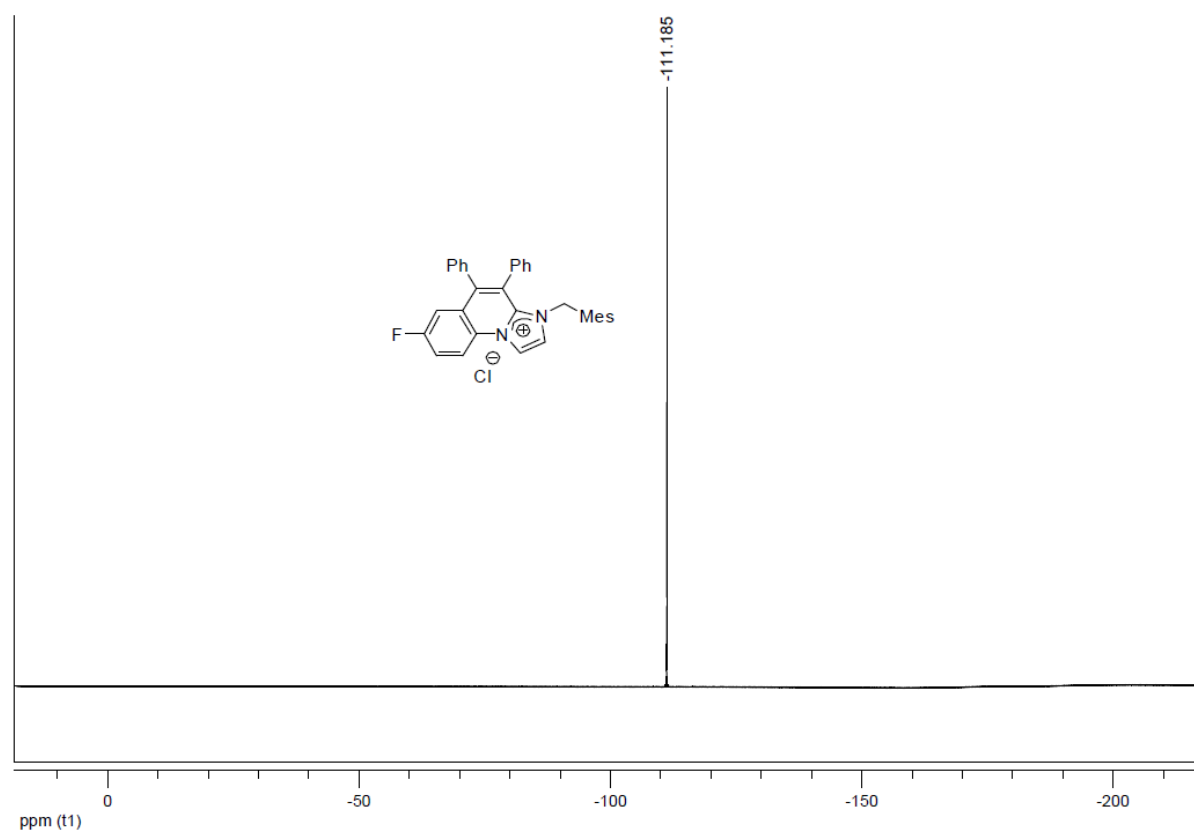
¹H NMR spectrum of 3ba



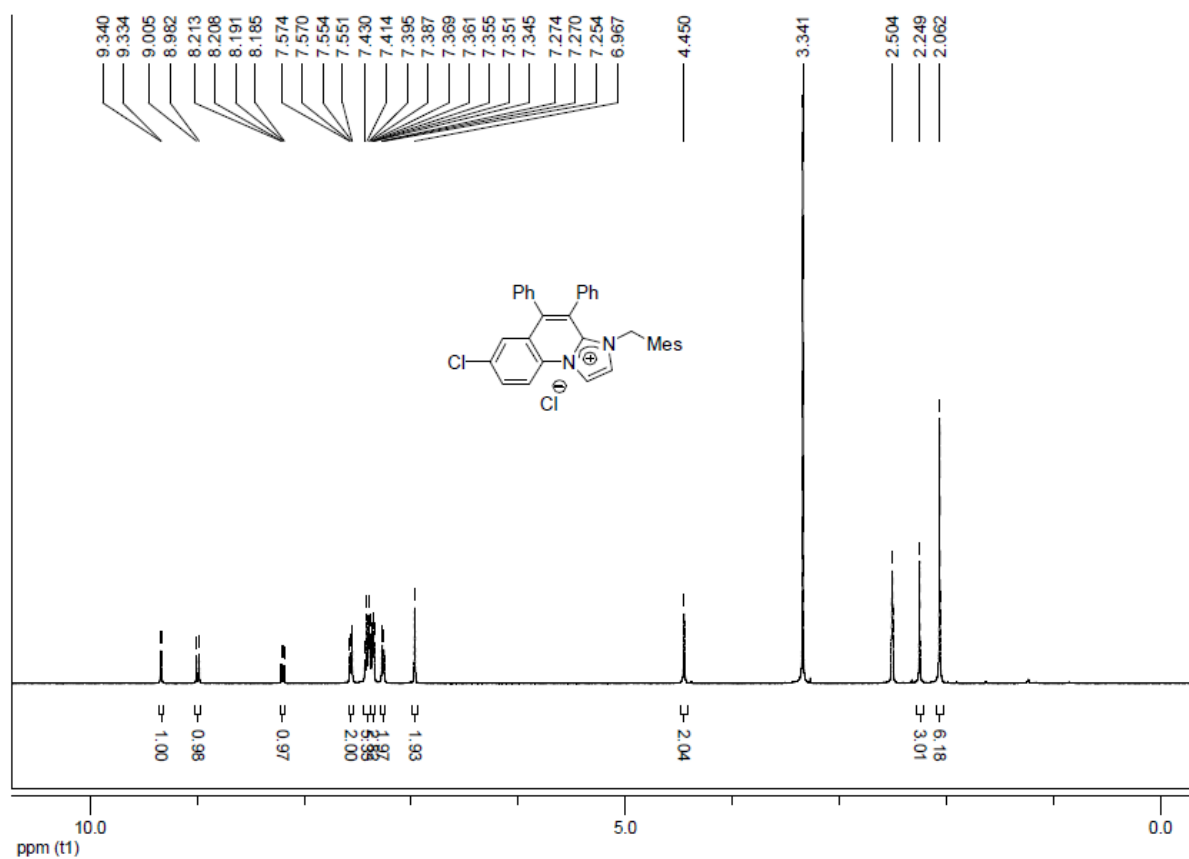
¹³C NMR spectrum of 3ba



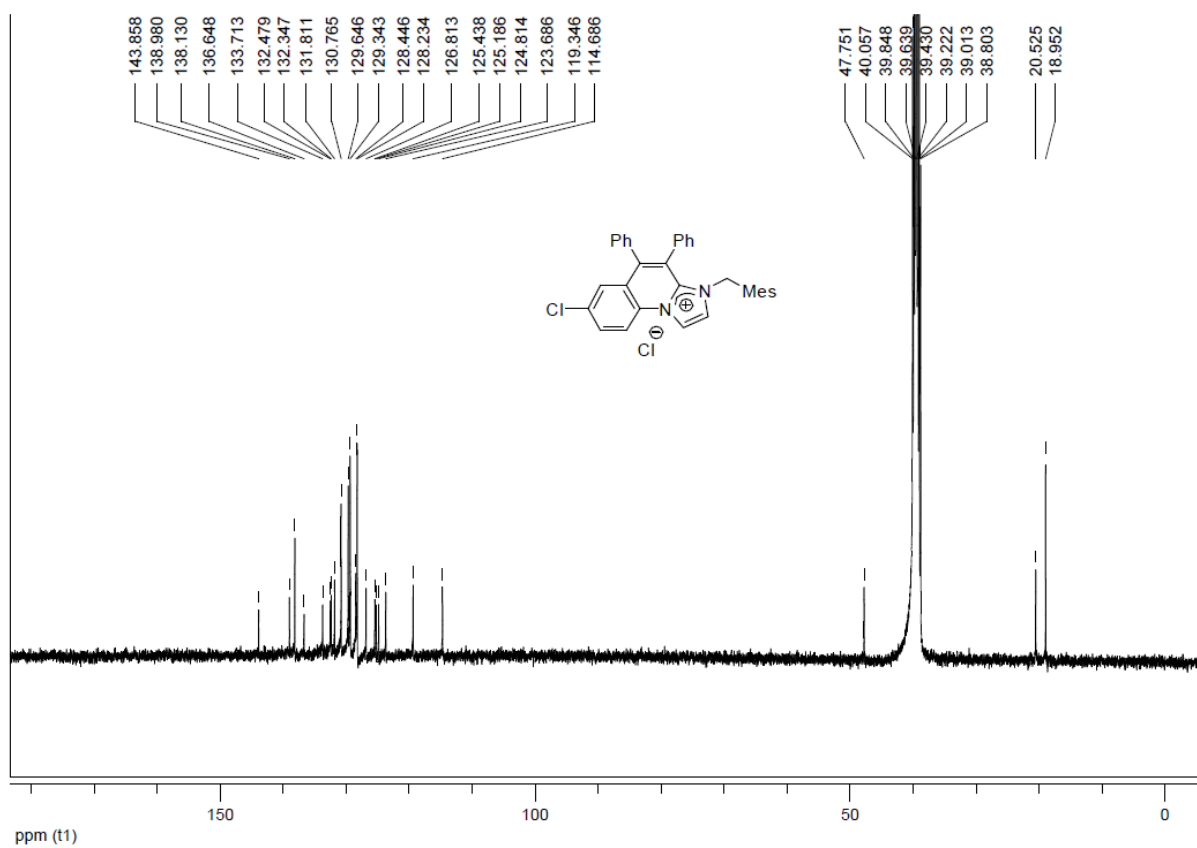
¹⁹F NMR spectrum of 3ba



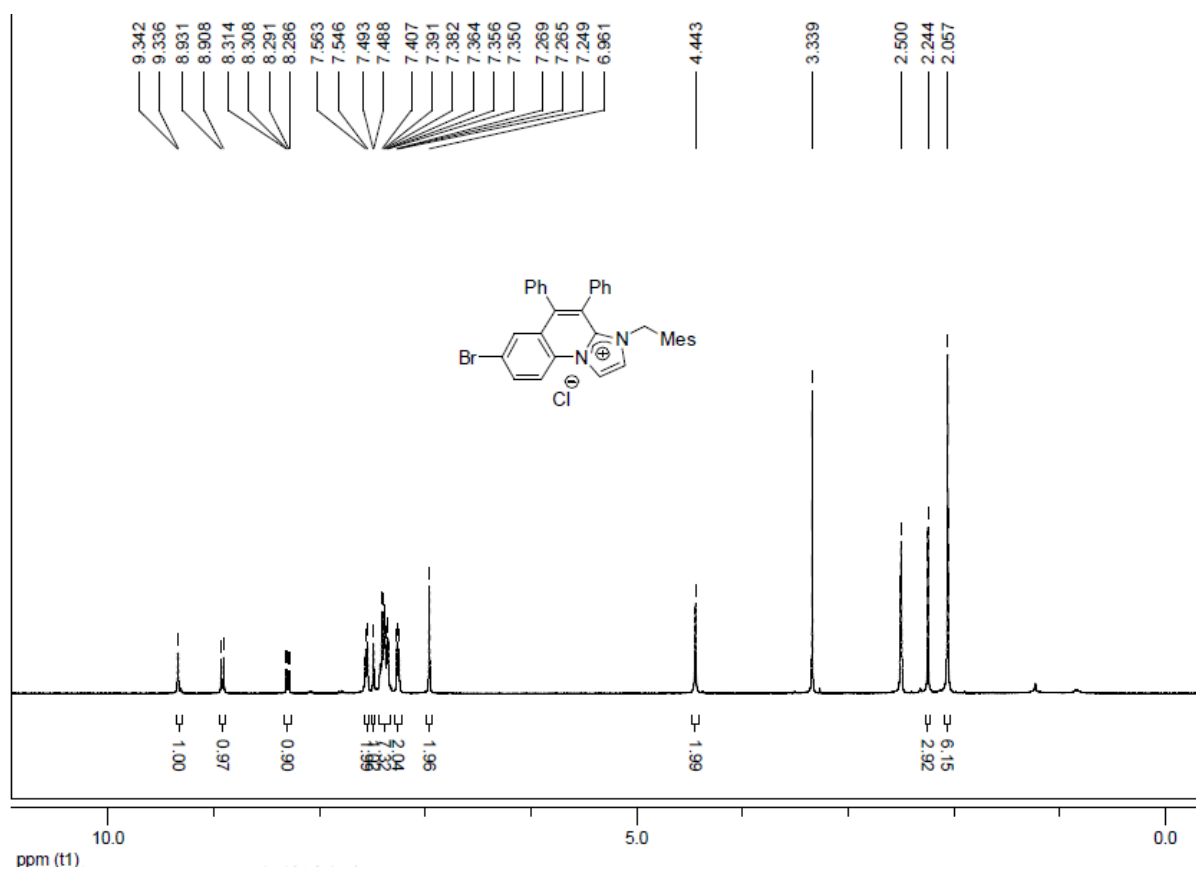
¹H NMR spectrum of 3ca



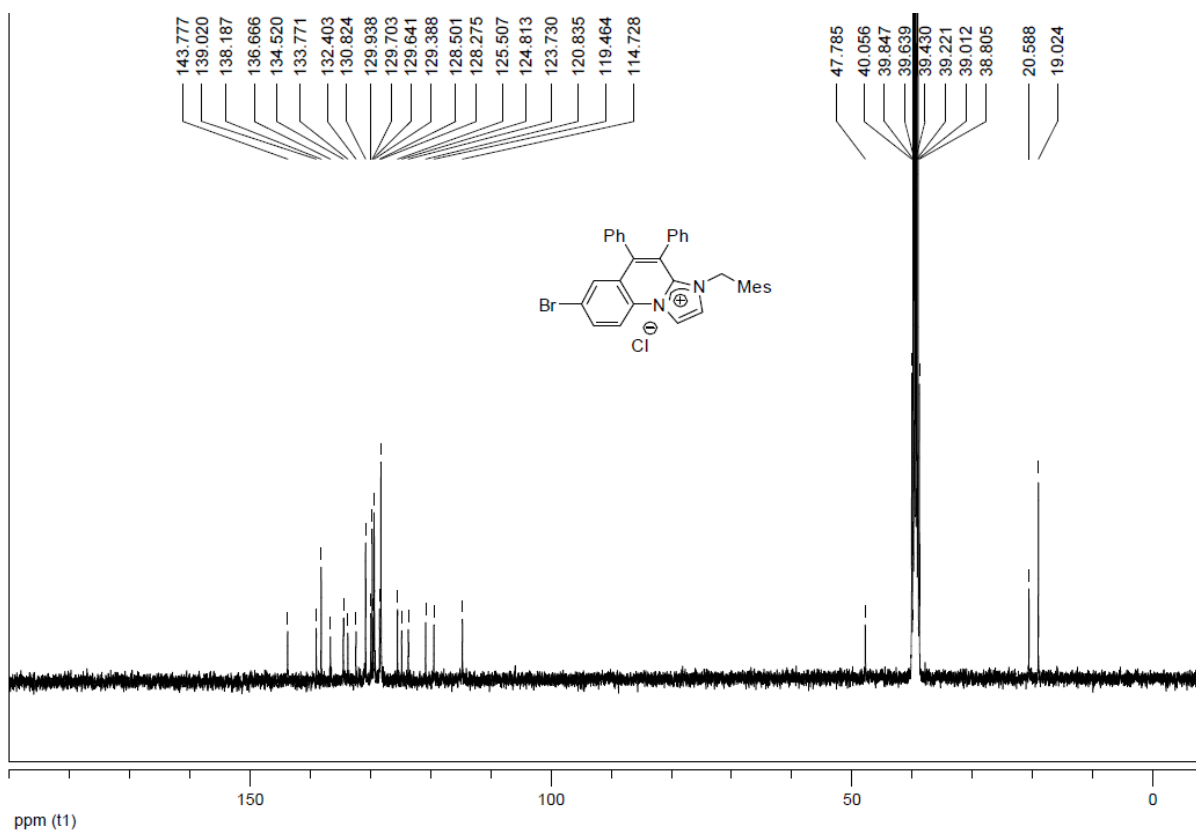
¹³C NMR spectrum of 3ca



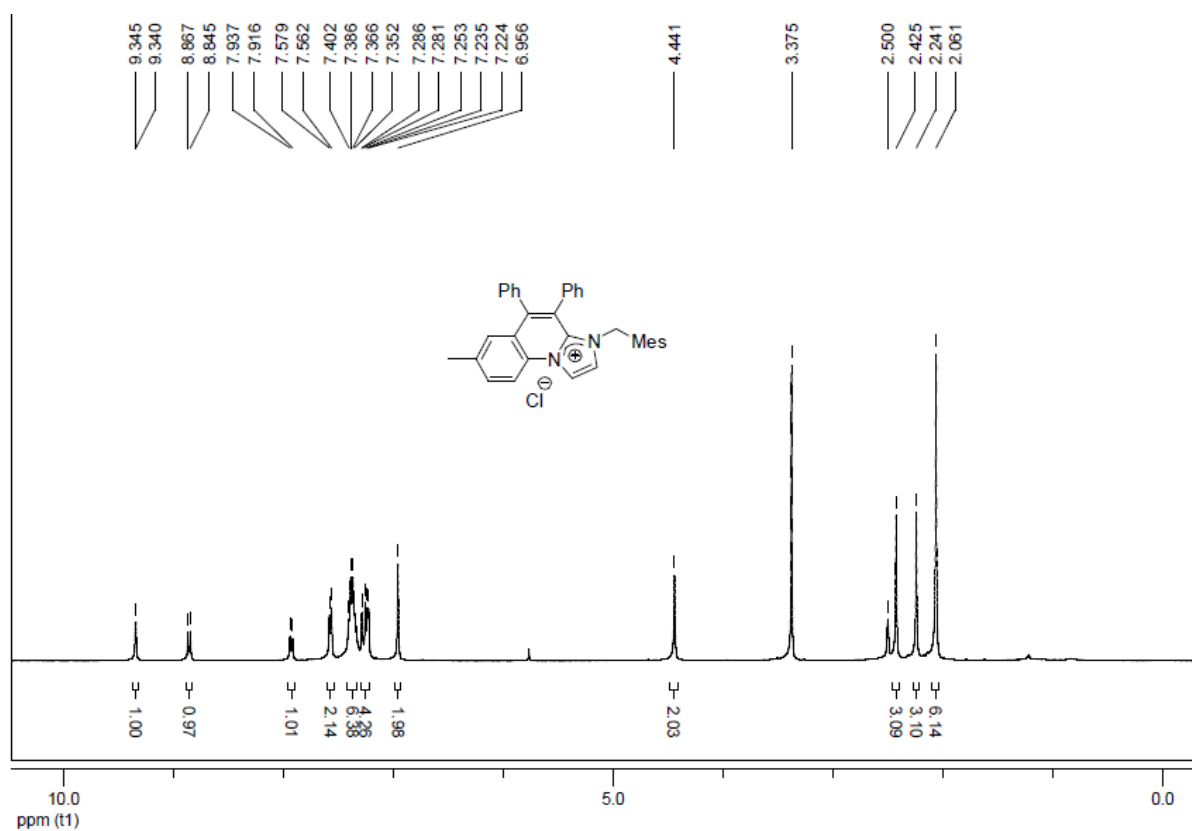
¹H NMR spectrum of 3da



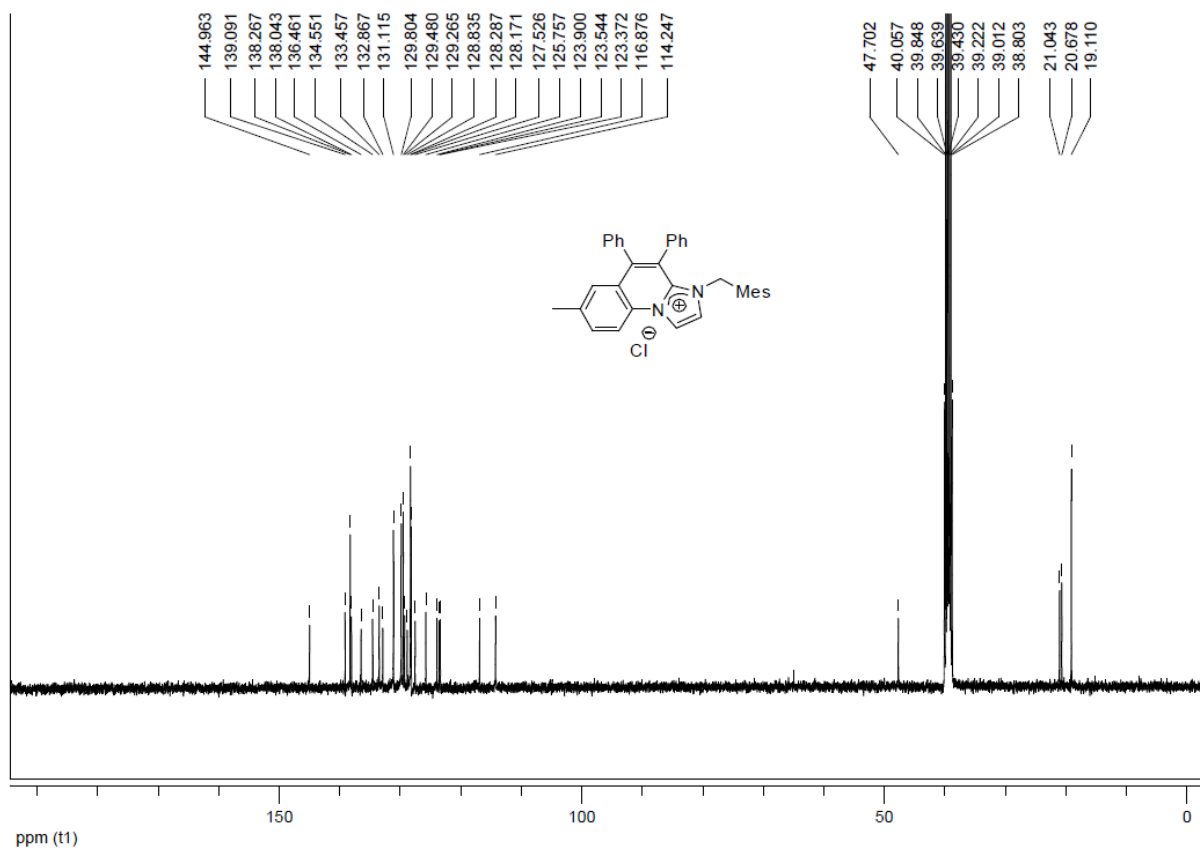
^{13}C NMR spectrum of 3da



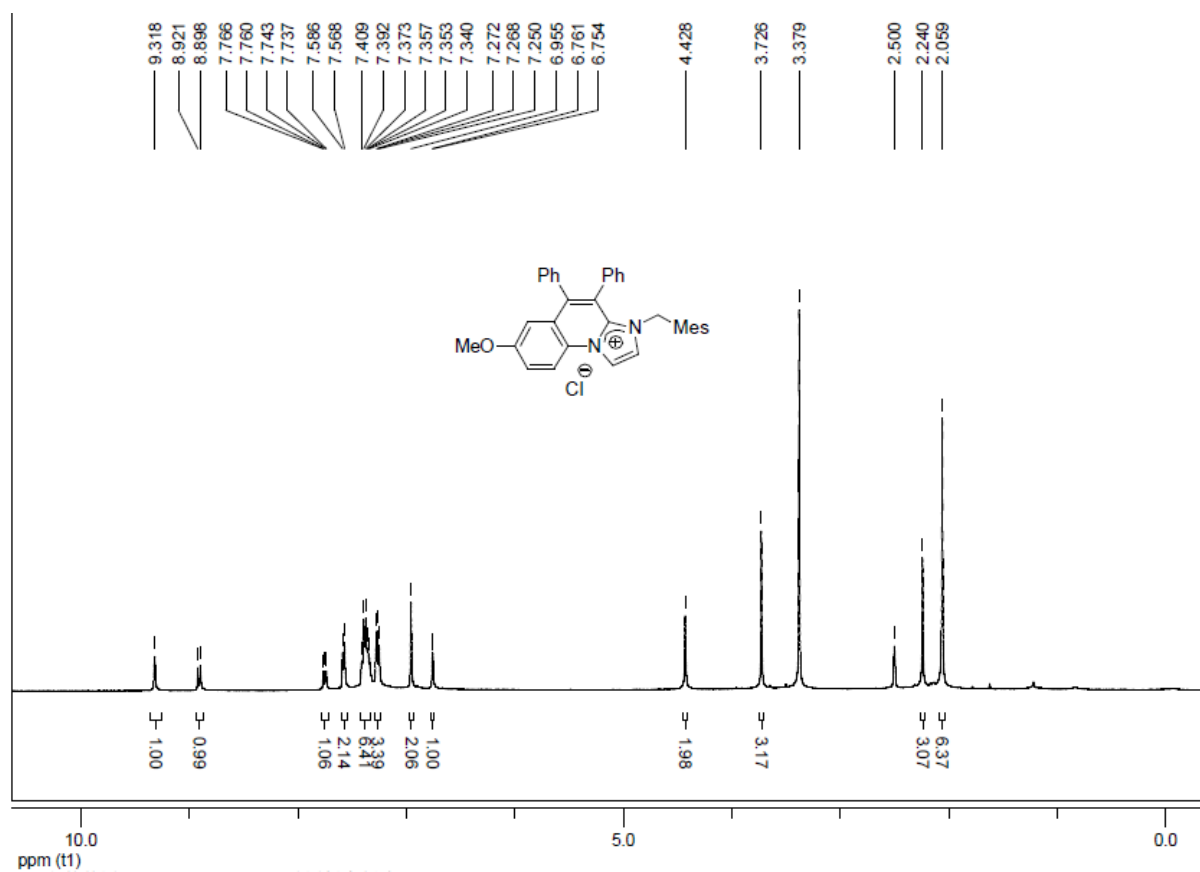
¹H NMR spectrum of 3ea



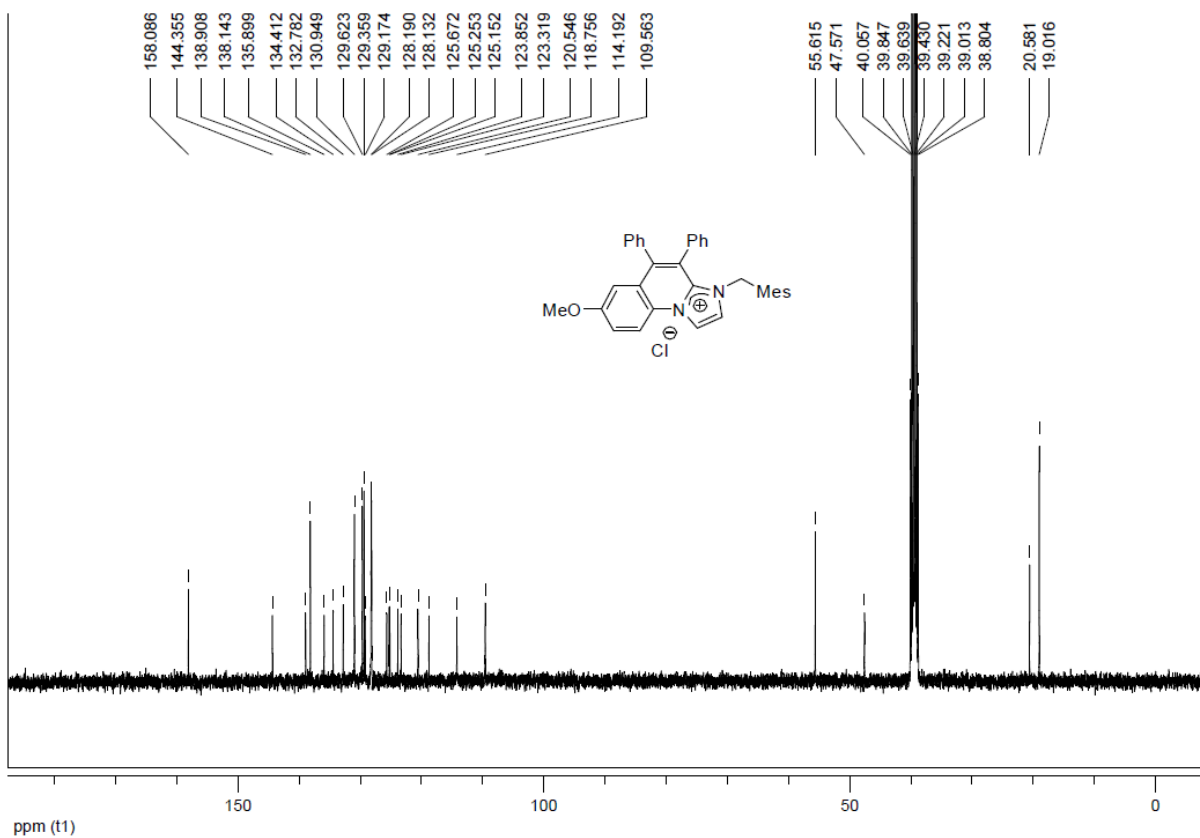
¹³C NMR spectrum of 3ea



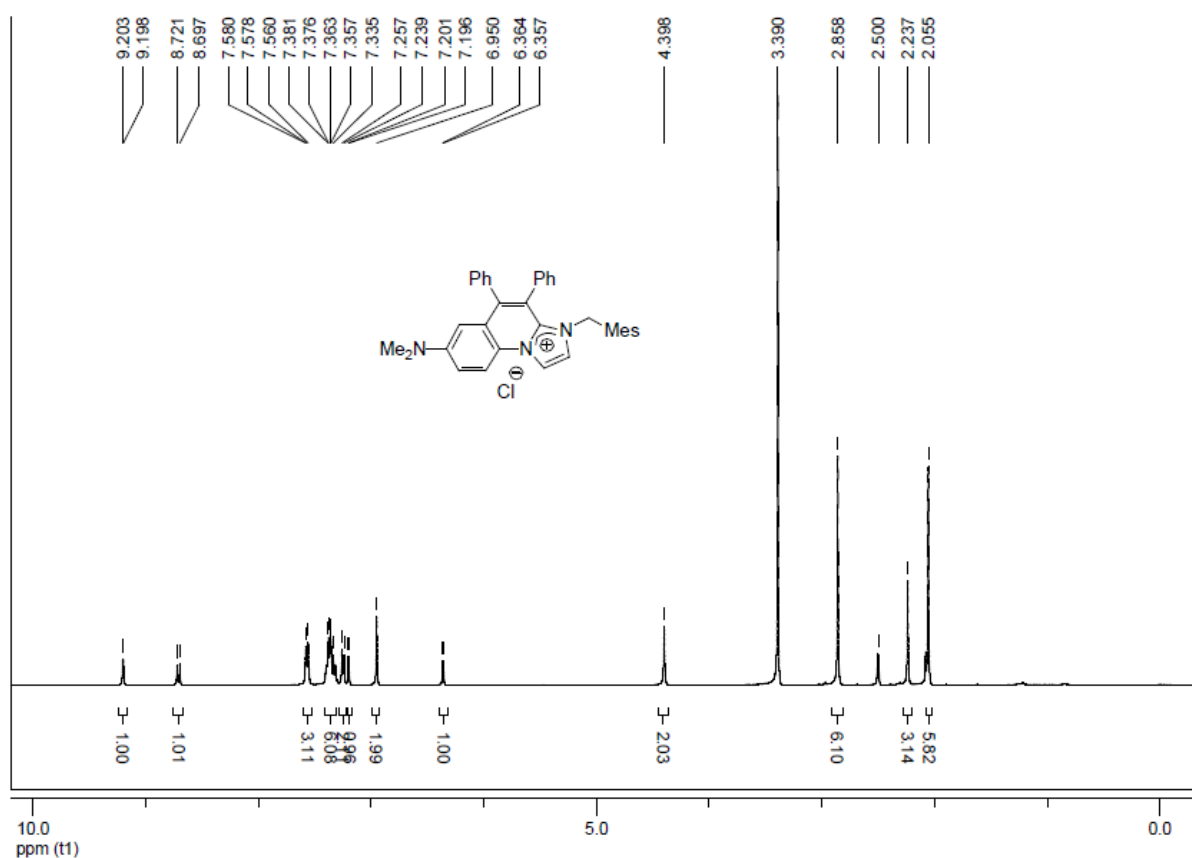
¹H NMR spectrum of 3fa



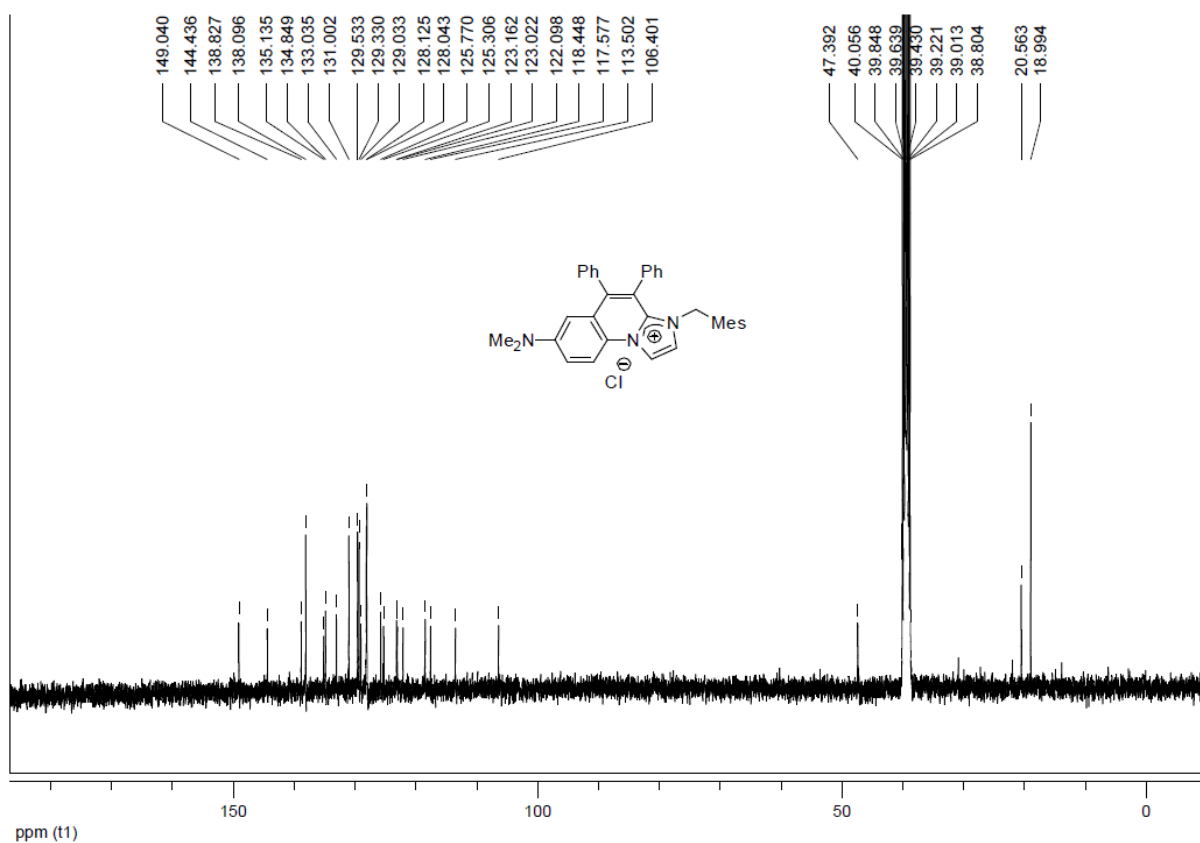
¹³C NMR spectrum of 3fa



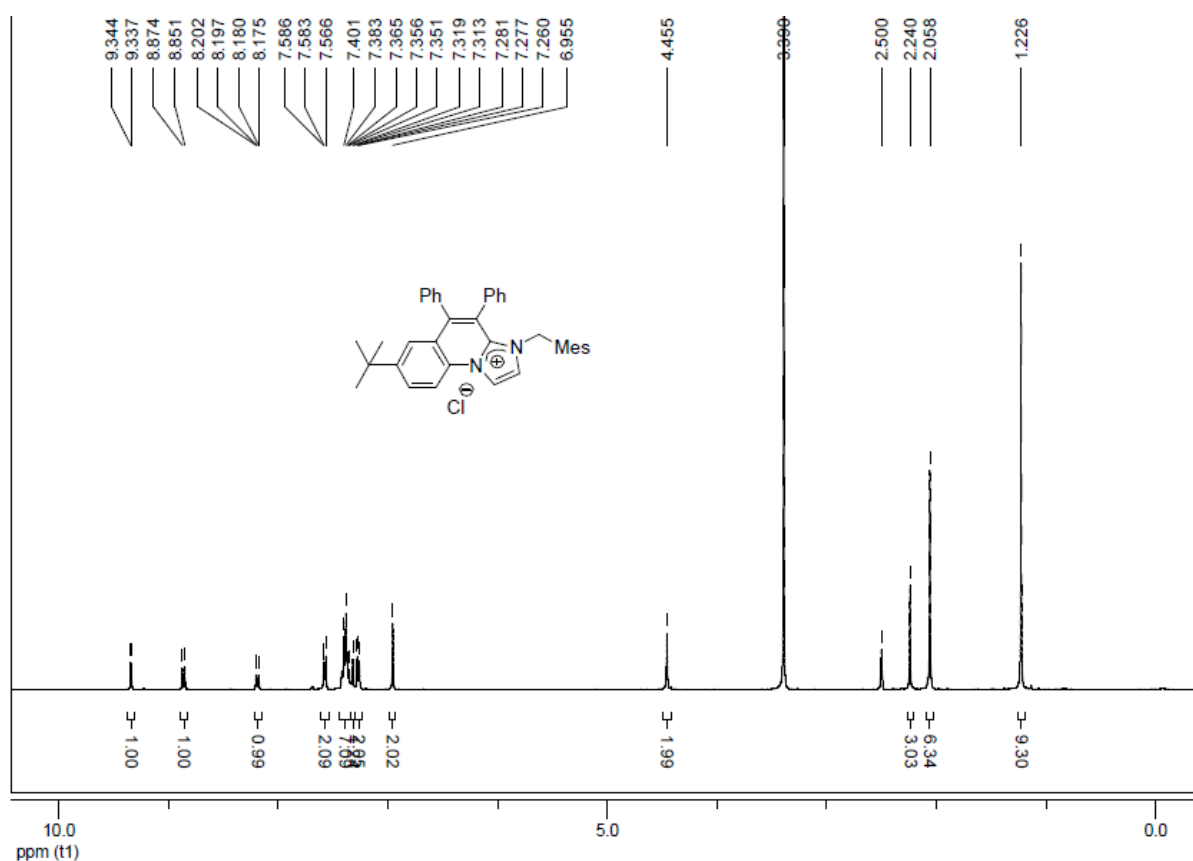
¹H NMR spectrum of 3ga



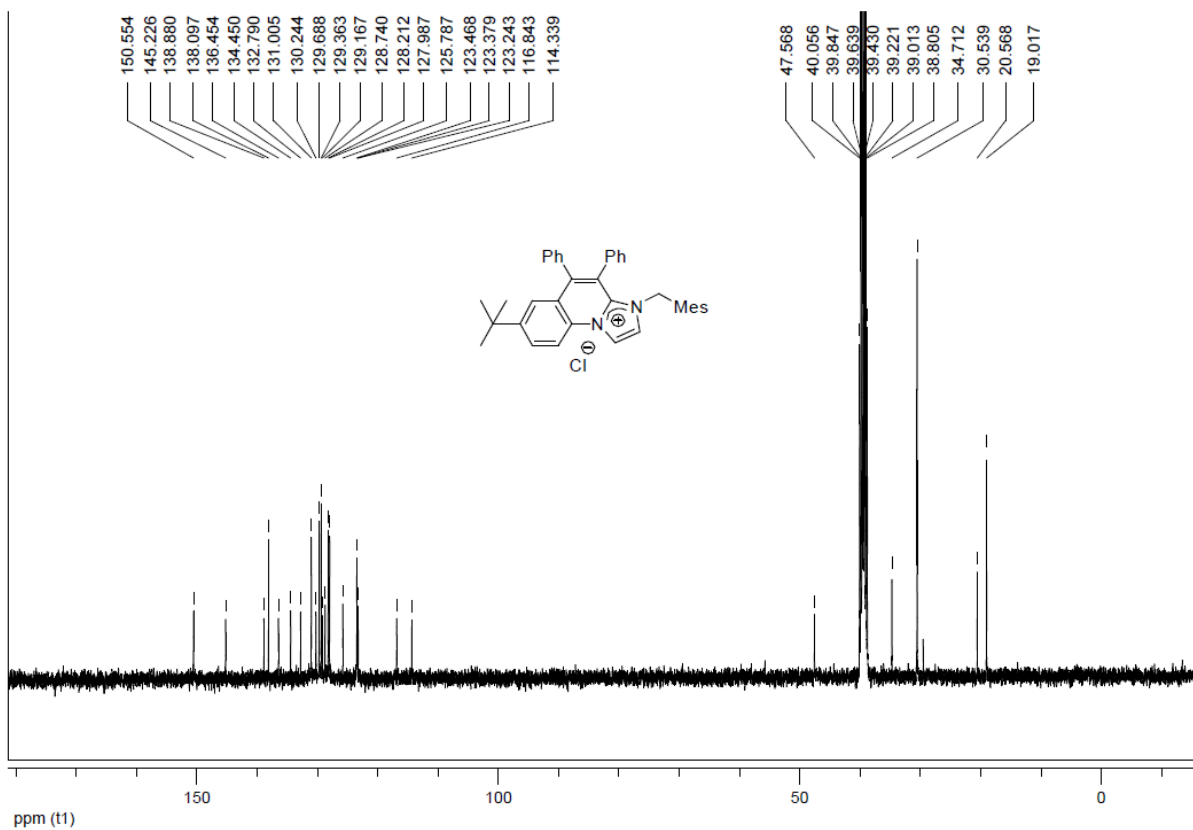
¹³C NMR spectrum of 3ga



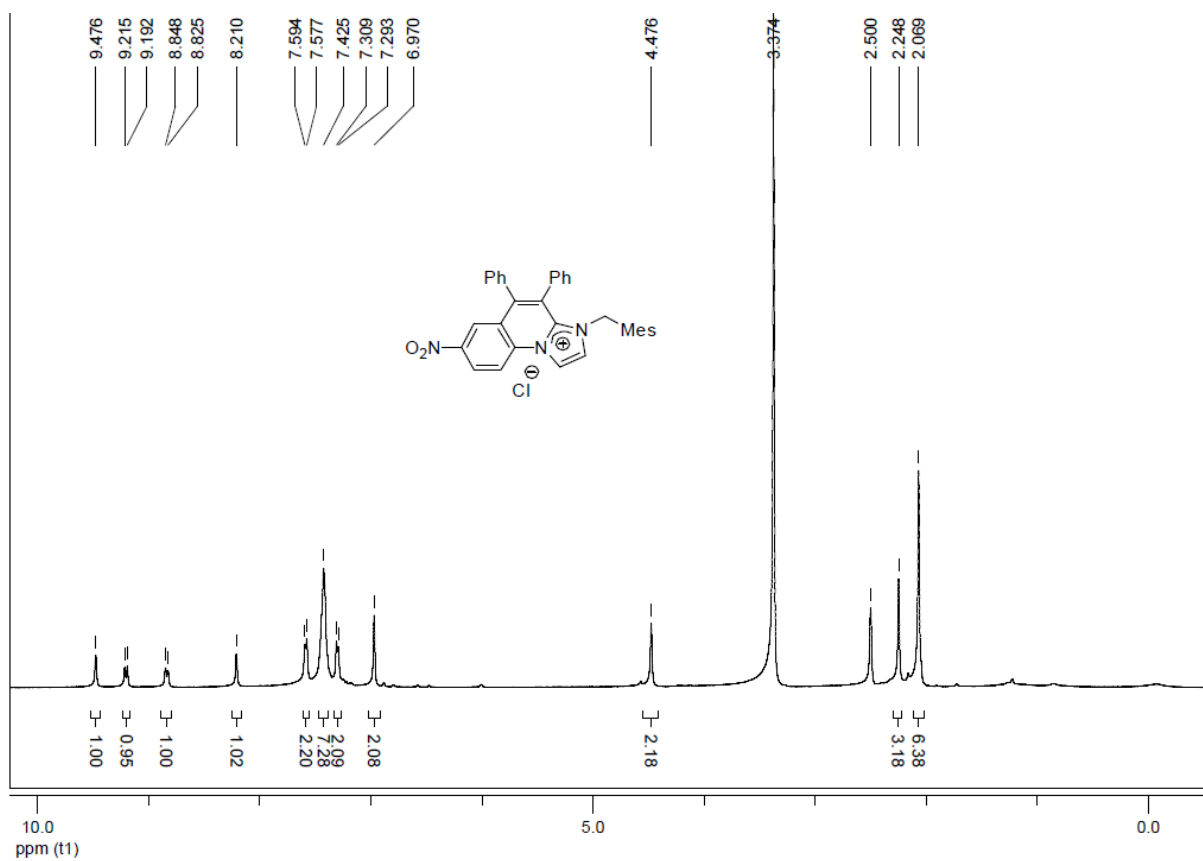
¹H NMR spectrum of 3ha



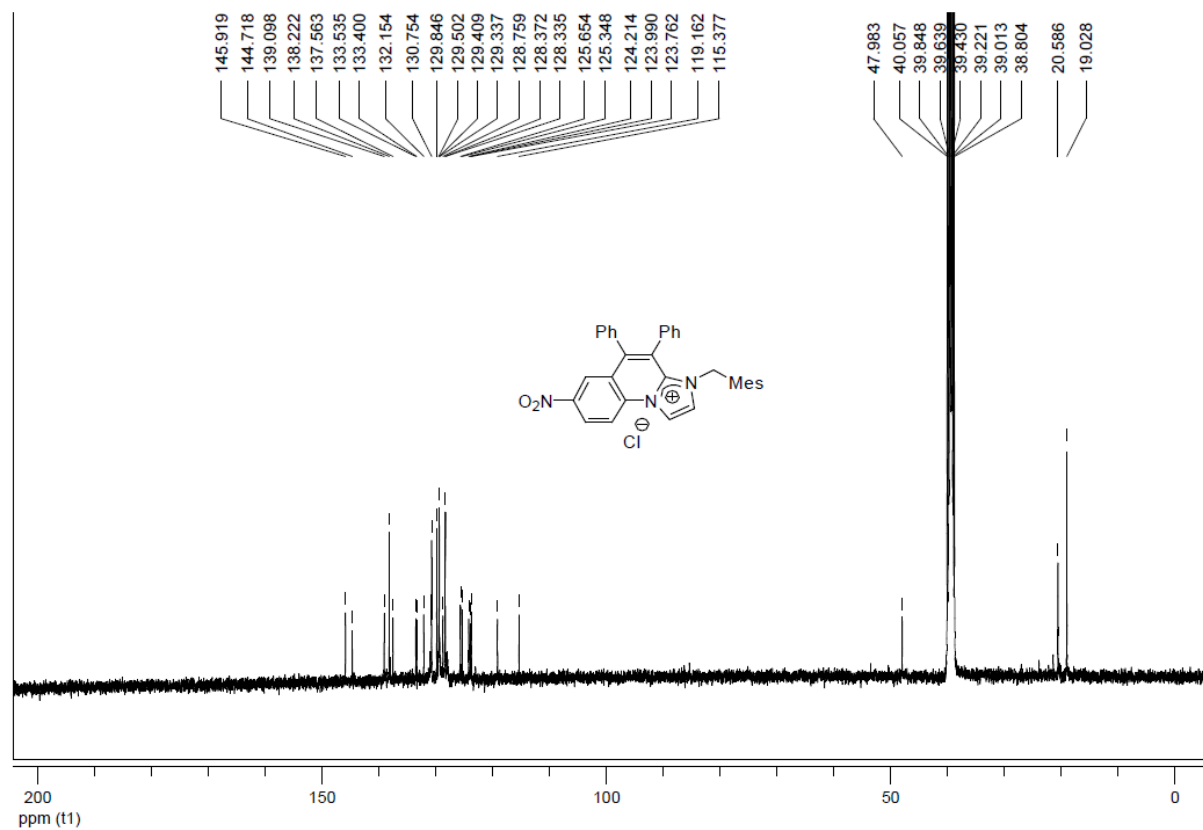
¹³C NMR spectrum of 3ha



¹H NMR spectrum of 3ia



¹³C NMR spectrum of 3ia



[illegible]

Chemical structure of 1-chloro-2,3-diphenyl-1H-benzotriazolium cation:

c1ccc2c(c1)c(c3cc[n+]3c2c4ccccc4)C5=CC=CC=C5.[Cl-]

¹³C NMR spectrum (ppm):

Peak (ppm)
145.688
136.906
135.333
134.412
132.150
131.038
130.865
130.358
129.758
129.249
128.562
128.501
128.361
128.131
128.043
127.581
127.097
126.993
123.971
123.581
116.986
114.229
40.057
39.847
39.639
39.430
39.221
39.013
38.803

Chemical structure of compound 10: Cc1ccc2c3c(c1[n+]2C(=C3C4=CC=CC=C4)C5=CC=CC=C5)C6=CC=CC=C6.[Br-]

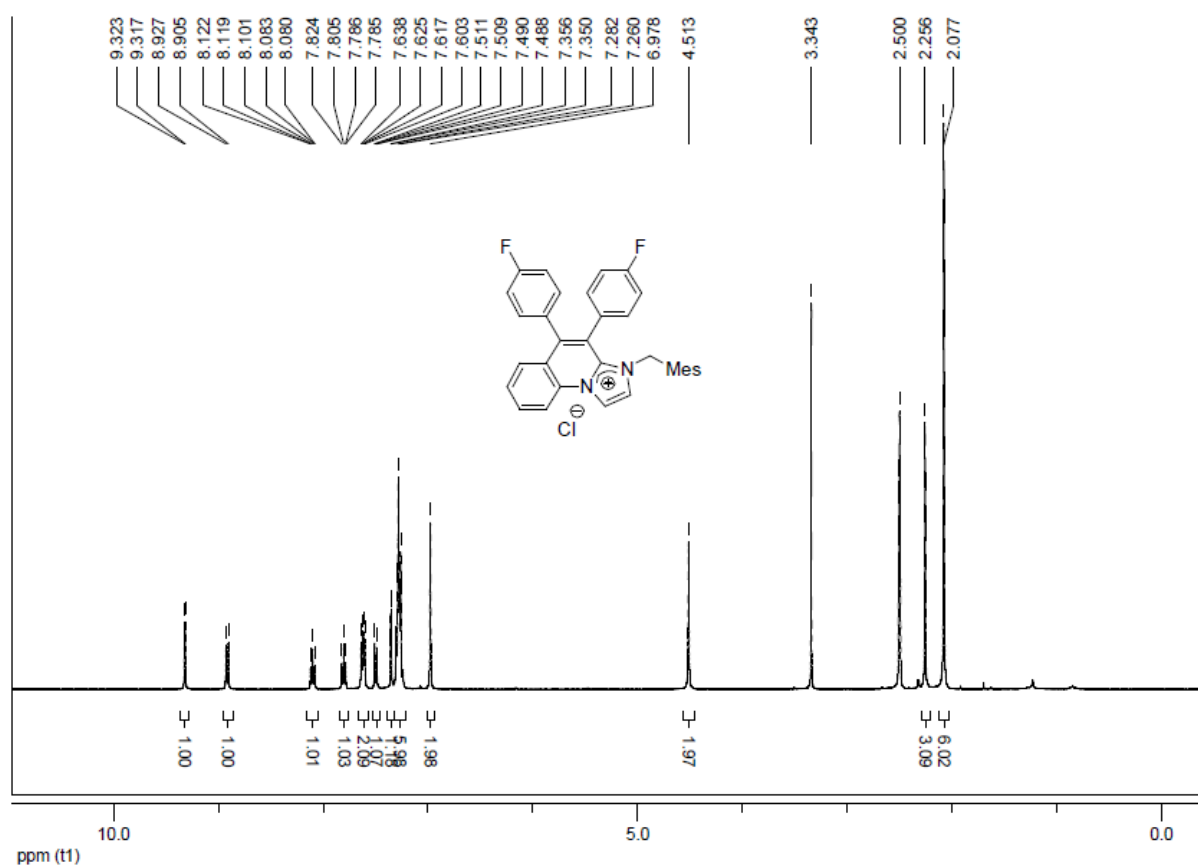
¹H NMR spectrum (CDCl₃):

Chemical Shift (ppm)	Integration
9.426, 9.404, 9.313, 9.291, 8.265, 8.263, 8.244, 8.225, 7.905, 7.887, 7.868, 7.859, 7.839, 7.819, 7.709, 7.689, 7.670, 7.618, 7.598, 7.515, 7.506, 7.497, 7.493, 7.394, 7.375, 7.353, 7.338, 7.329, 7.325, 7.299, 7.280, 7.130, 7.109, 6.841, 5.082, 3.351, 2.500, 2.191, 1.922	0.98, 0.98, 1.00, 2.12, 1.00, 1.00, 1.00, 1.00, 1.99, 1.99, 6.05, 2.98

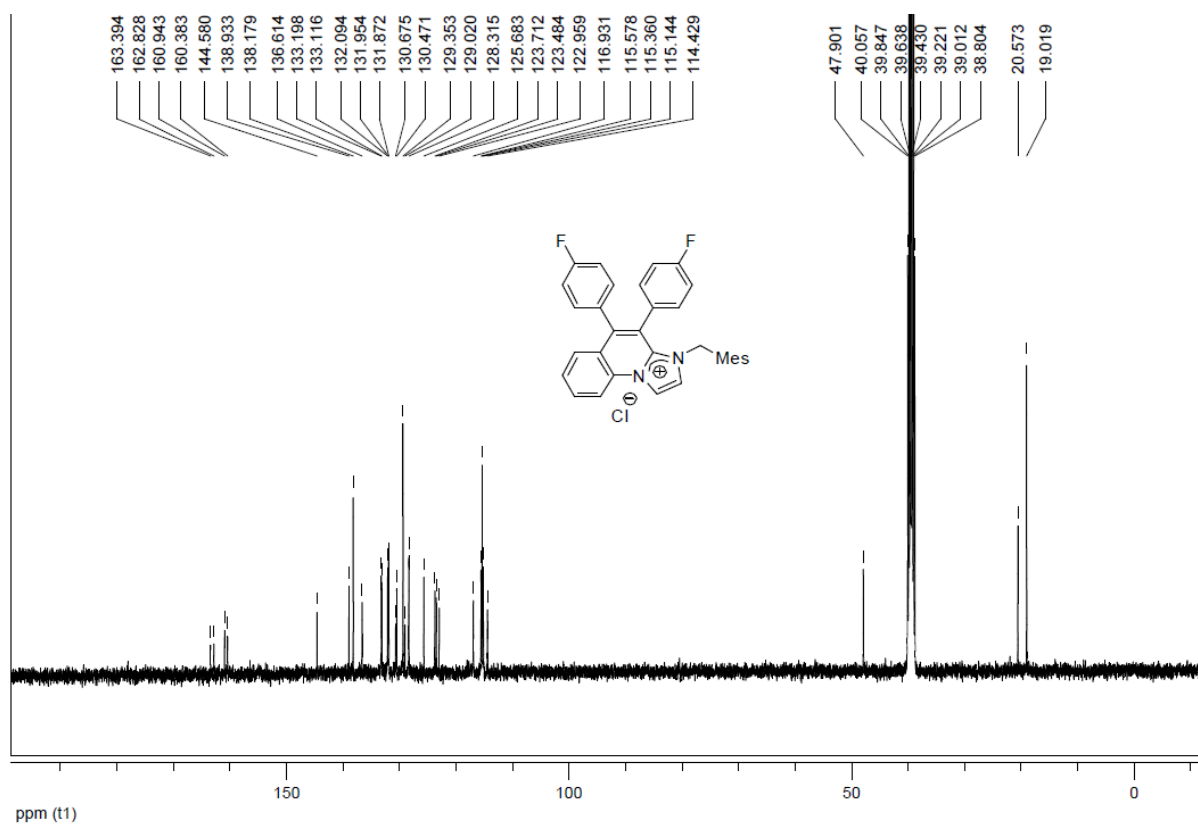
Chemical structure of compound 10 is shown above the spectrum. The structure is a cationic complex consisting of a phenanthrene-like core with a positive charge on the nitrogen atom, a bromide counterion, and a mesityl group attached to the nitrogen.

1H NMR spectrum (CDCl₃) of compound 10. The x-axis is labeled 'ppm (t1)' and ranges from 0 to 15. The spectrum shows several peaks: a multiplet between 7.0 and 8.0 ppm, a sharp singlet at 7.26 ppm, a sharp singlet at 7.80 ppm, a multiplet between 2.5 and 3.0 ppm, and a sharp singlet at 2.82 ppm.

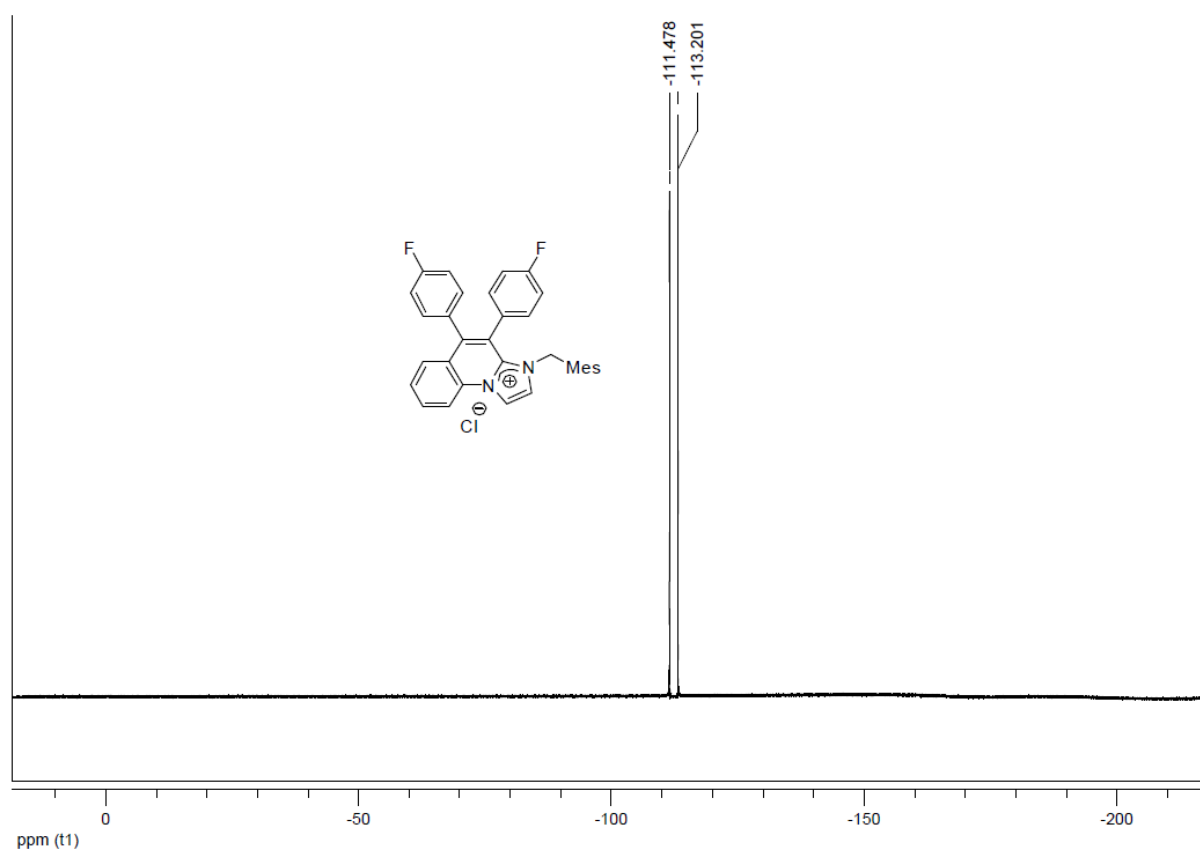
¹H NMR spectrum of 3ab



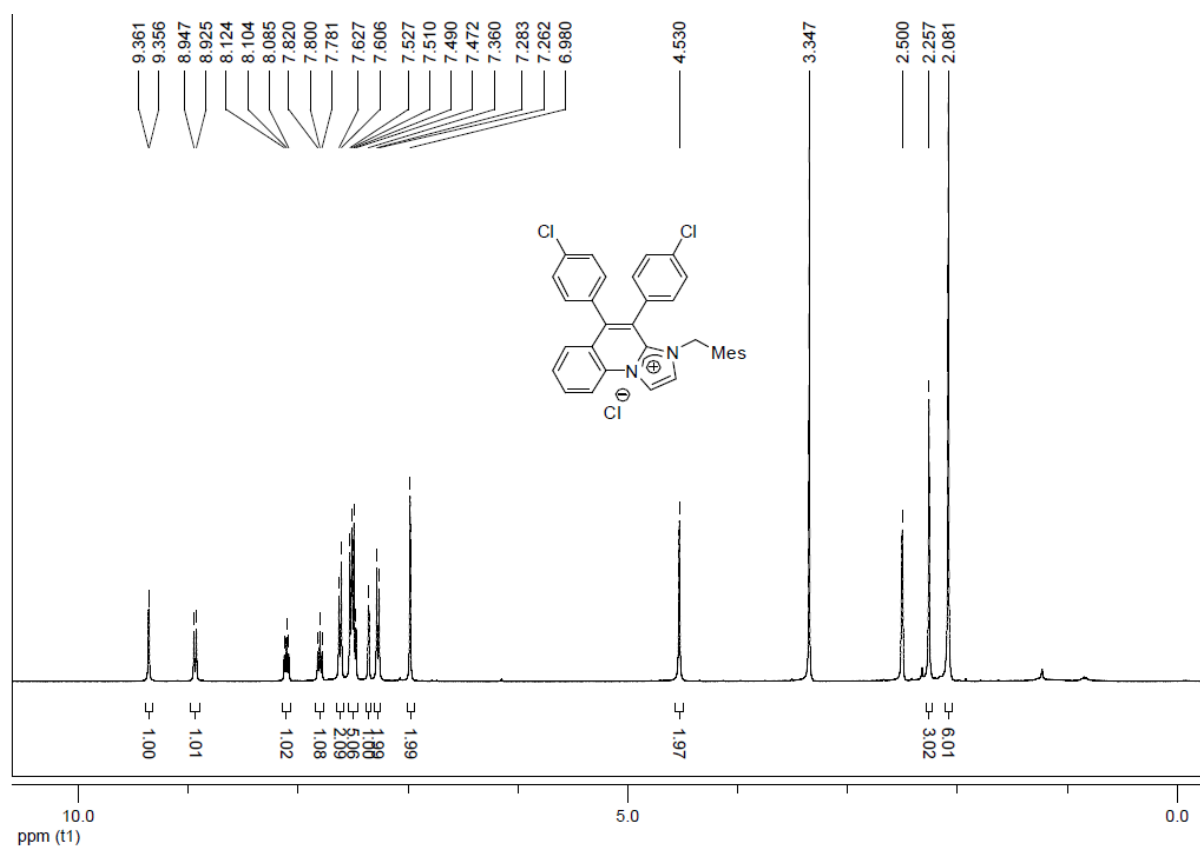
¹³C NMR spectrum of 3ab



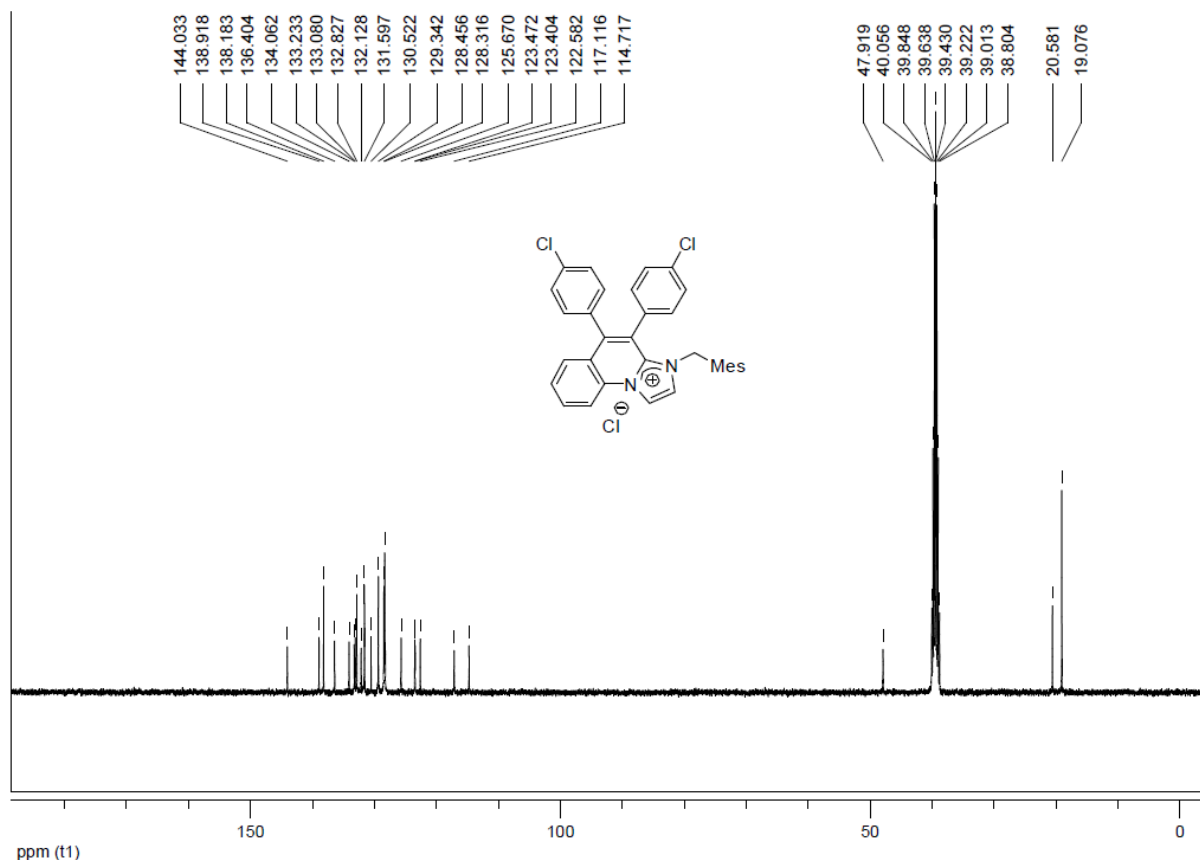
¹⁹F NMR spectrum of 3ab



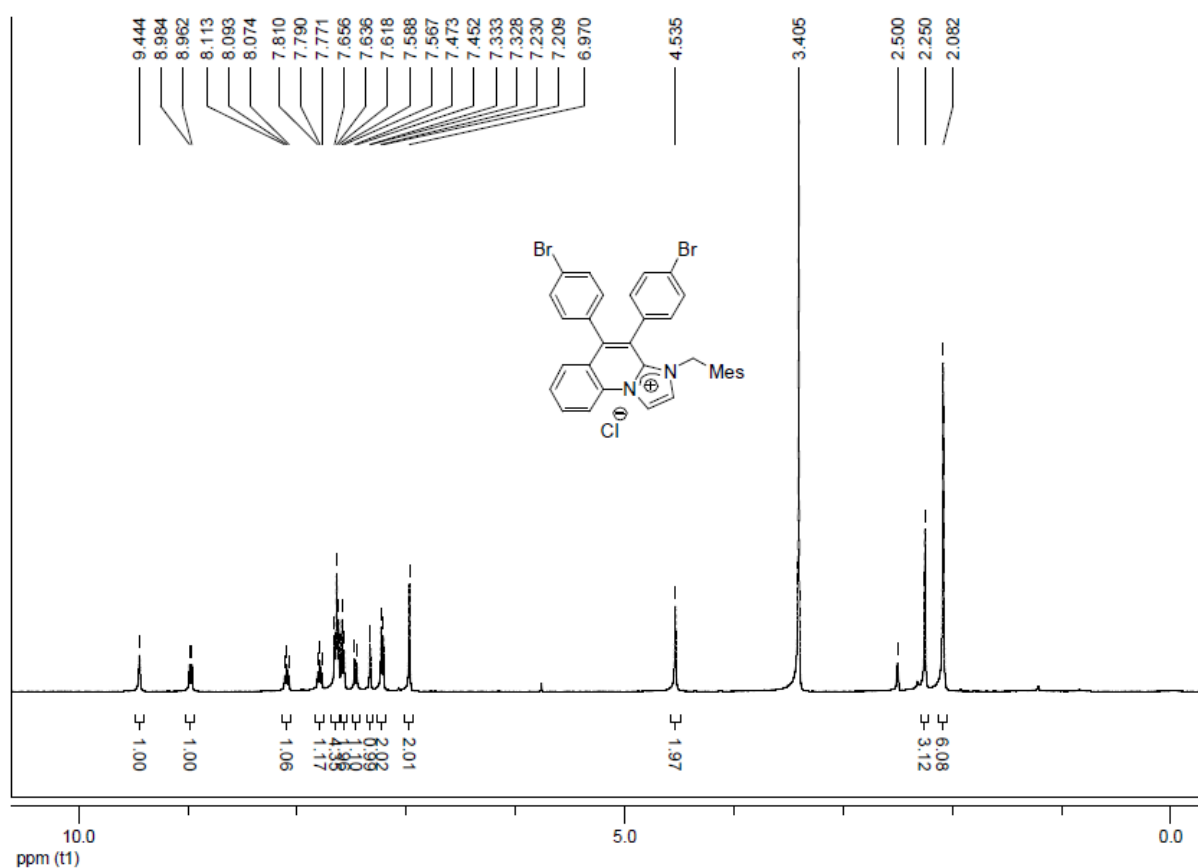
¹H NMR spectrum of 3ac



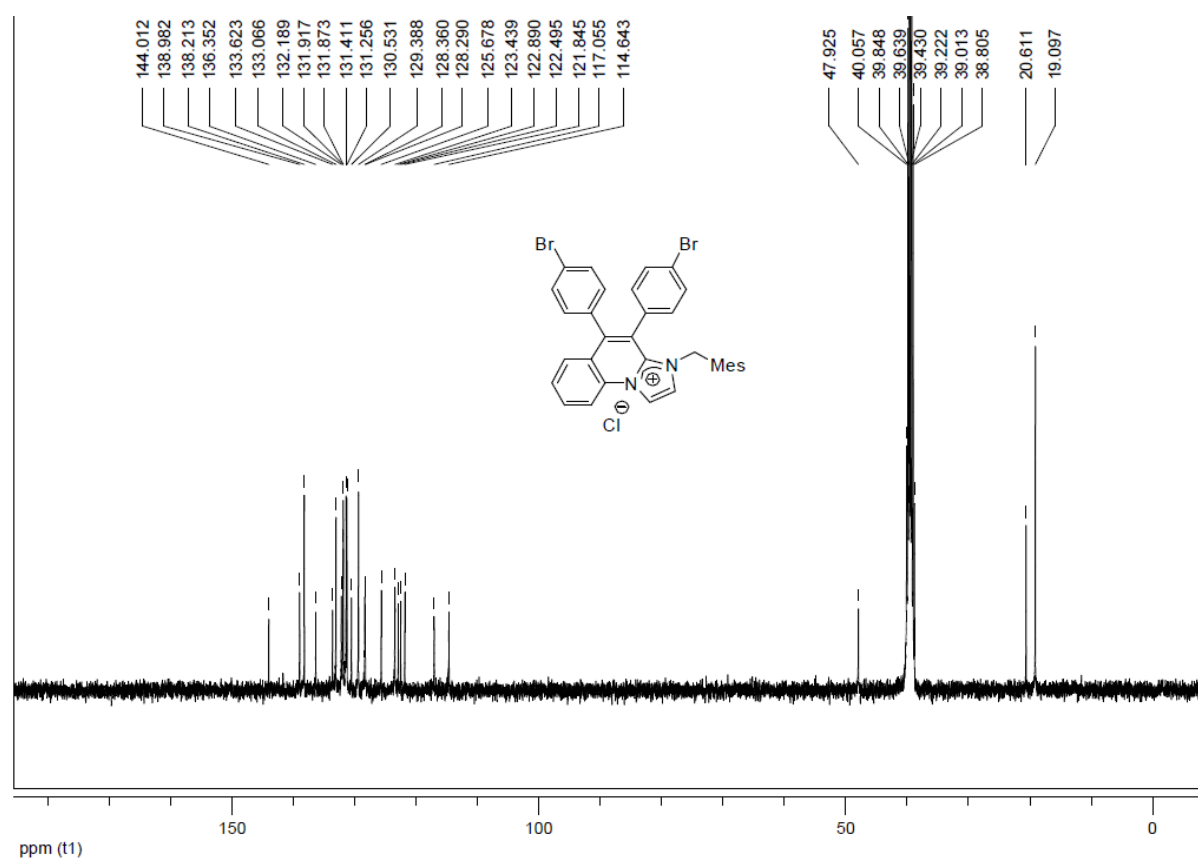
¹³C NMR spectrum of 3ac



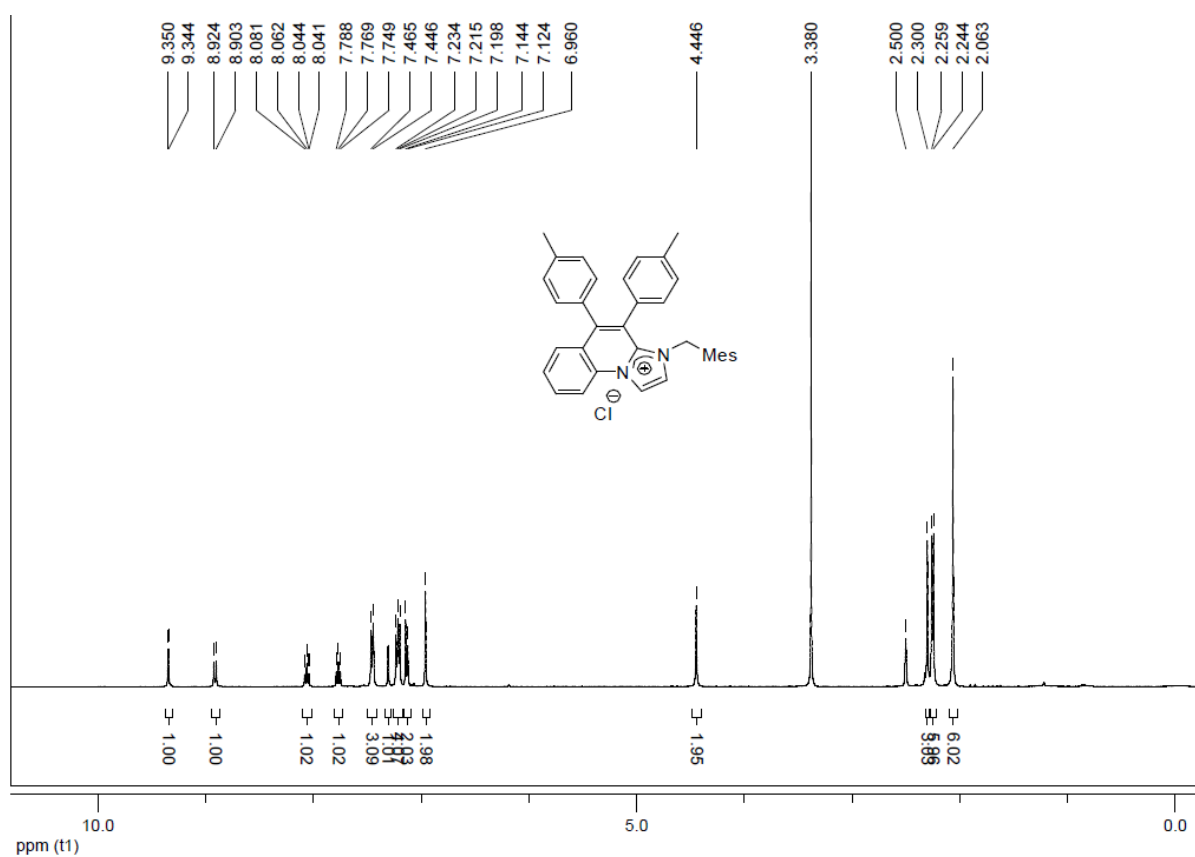
¹H NMR spectrum of 3ad



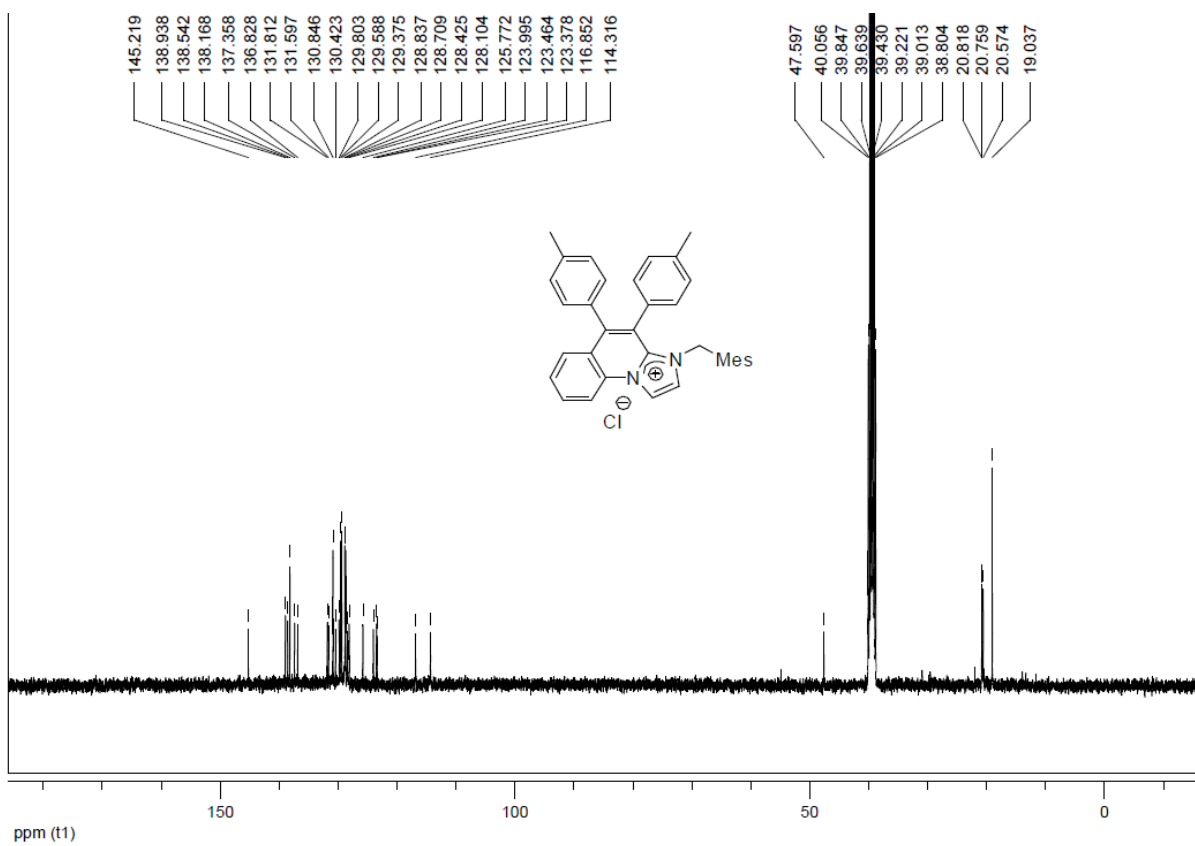
¹³C NMR spectrum of 3ad



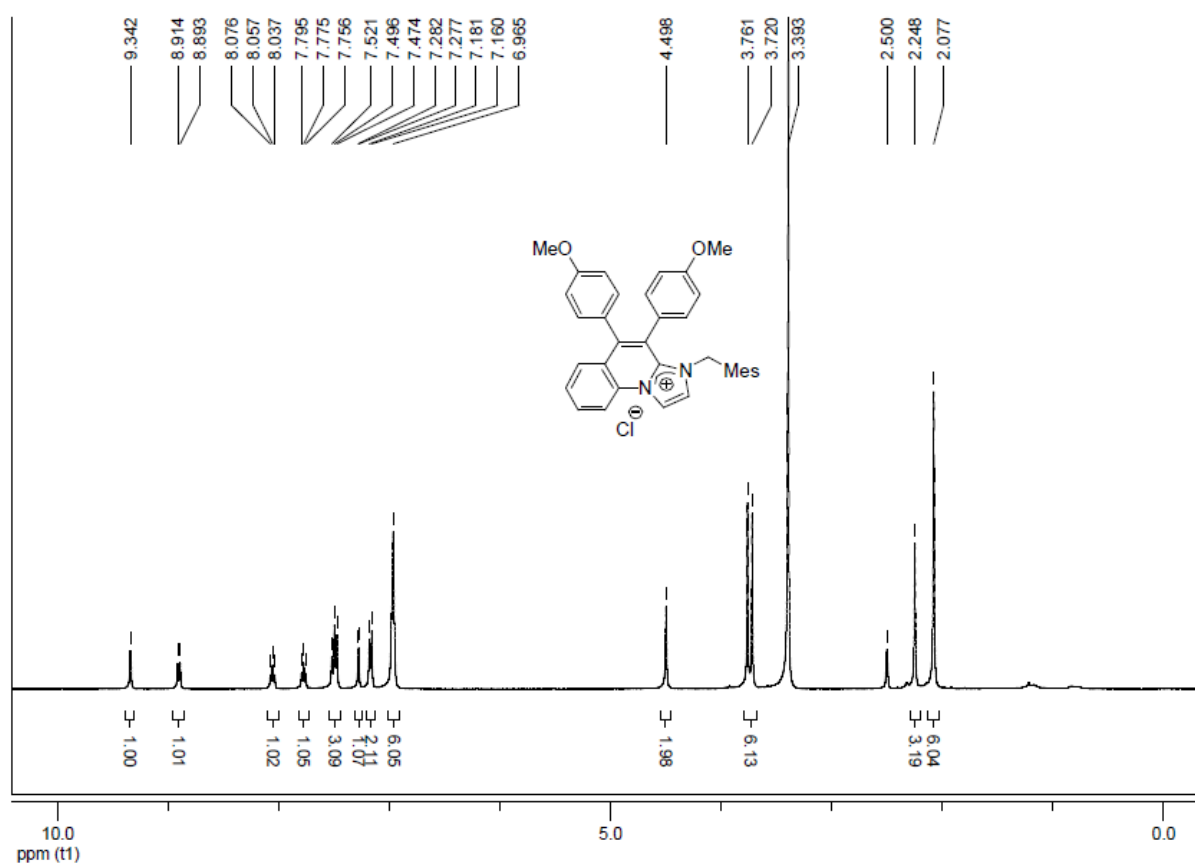
¹H NMR spectrum of 3ae



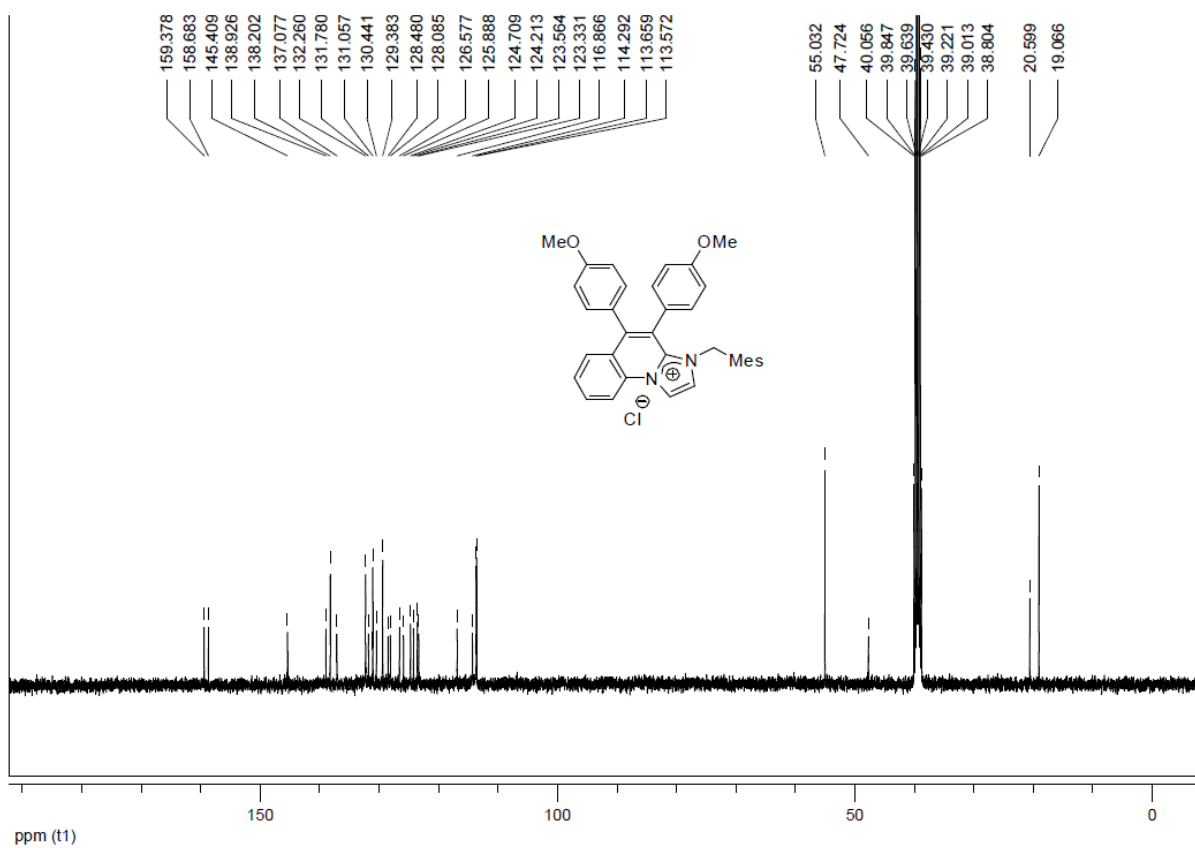
¹³C NMR spectrum of 3ae



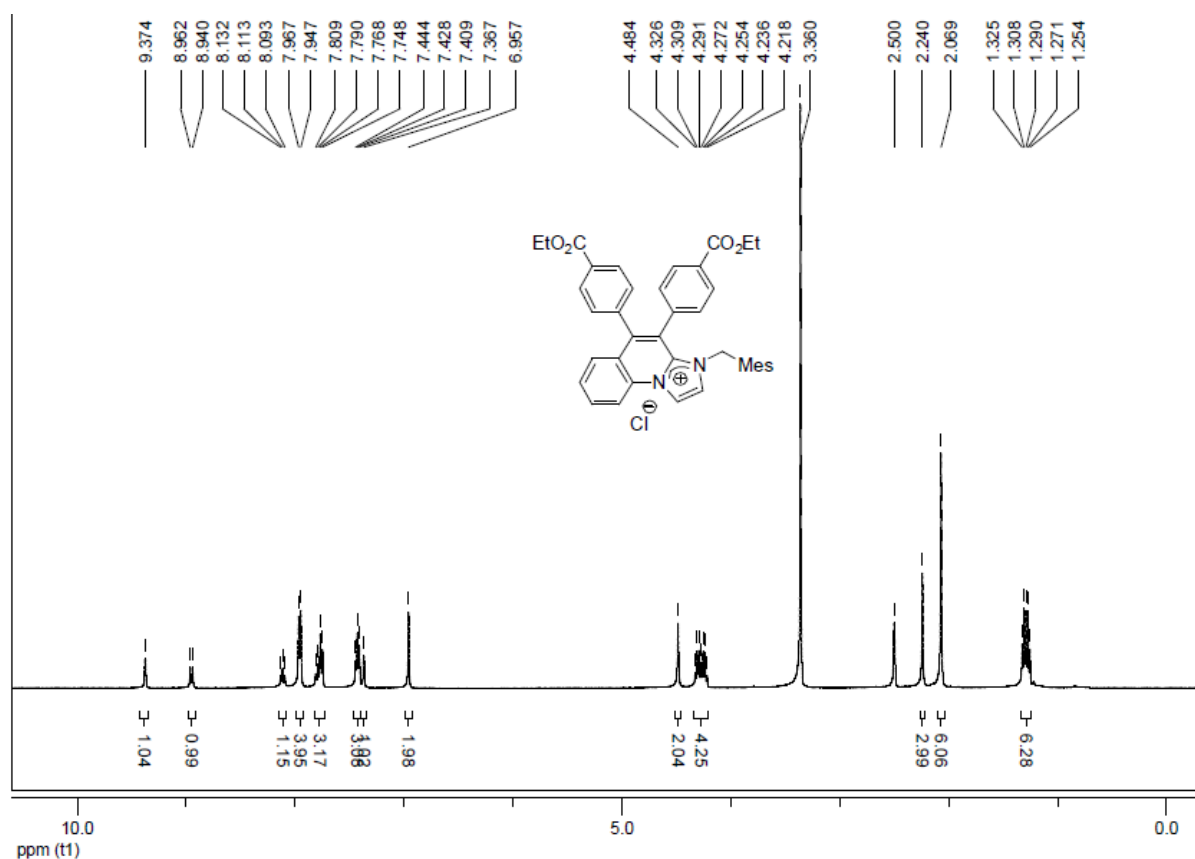
¹H NMR spectrum of 3af



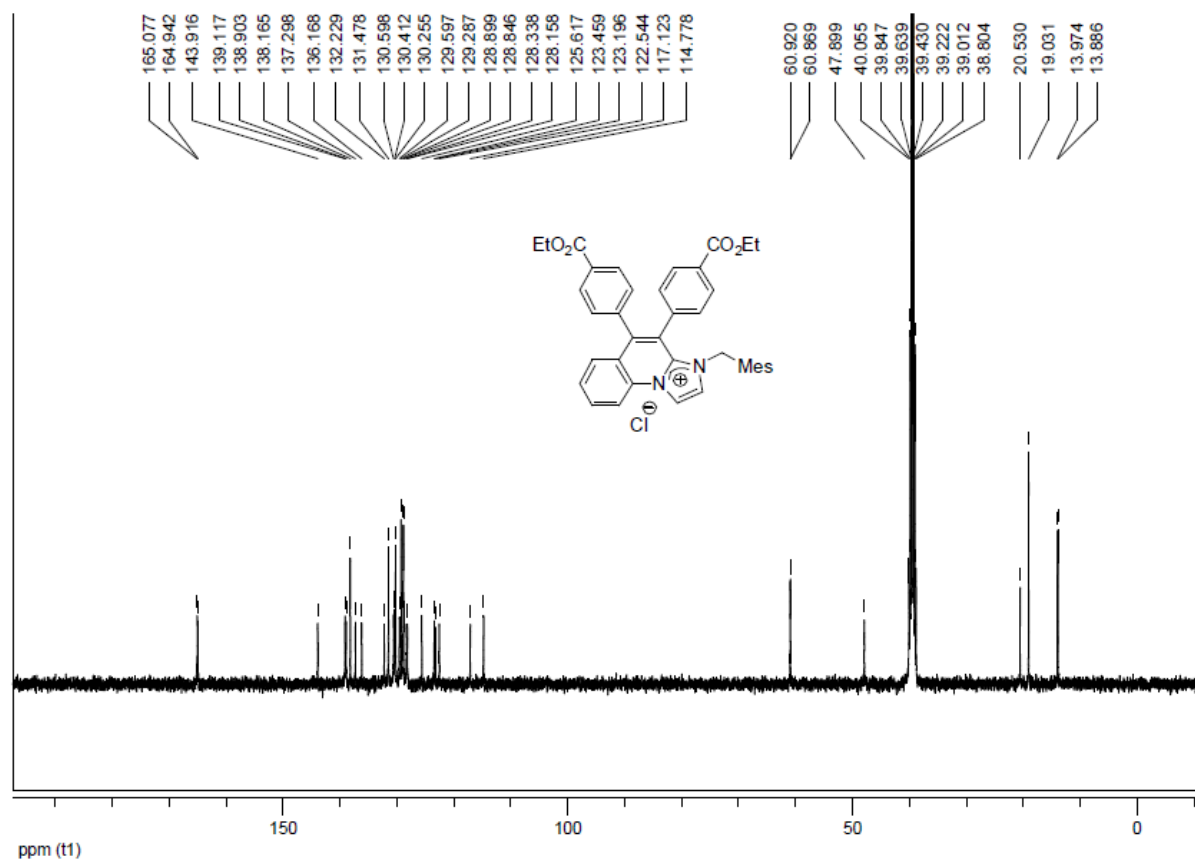
¹³C NMR spectrum of 3af



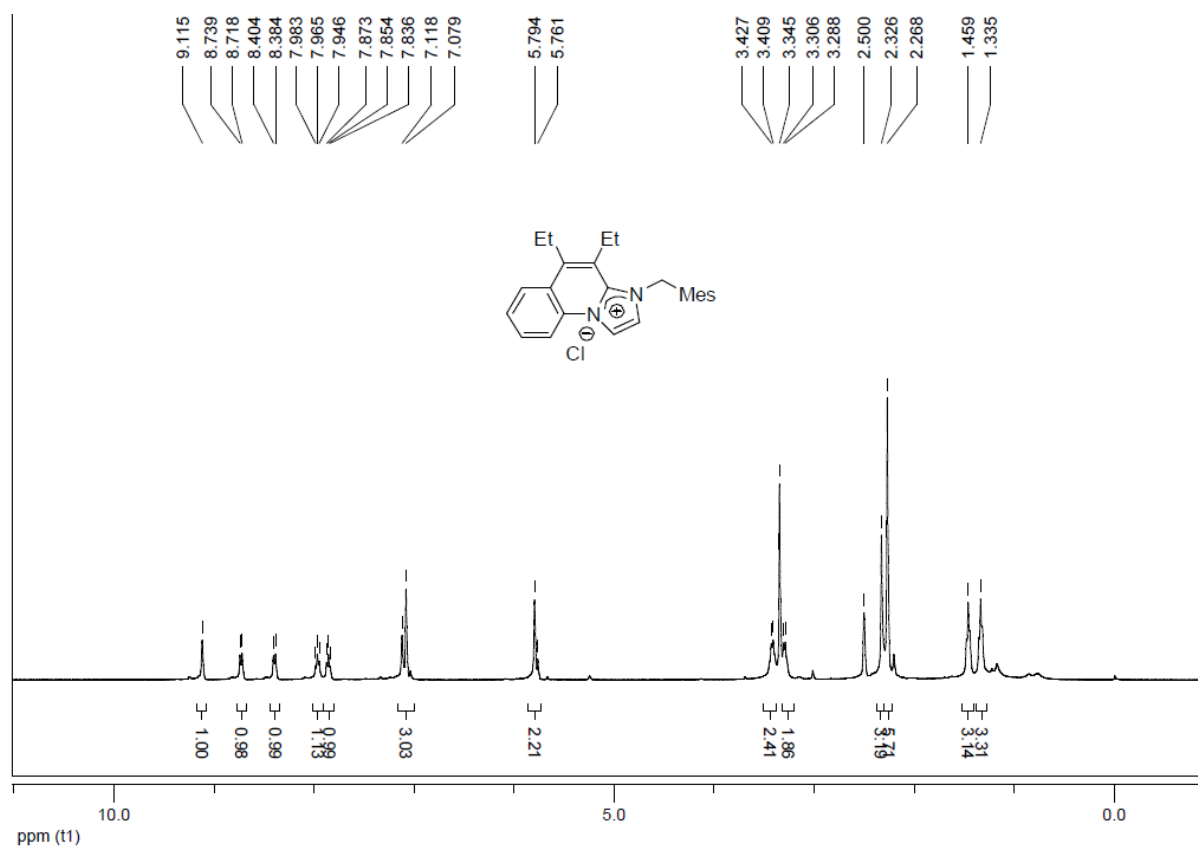
¹H NMR spectrum of 3ag



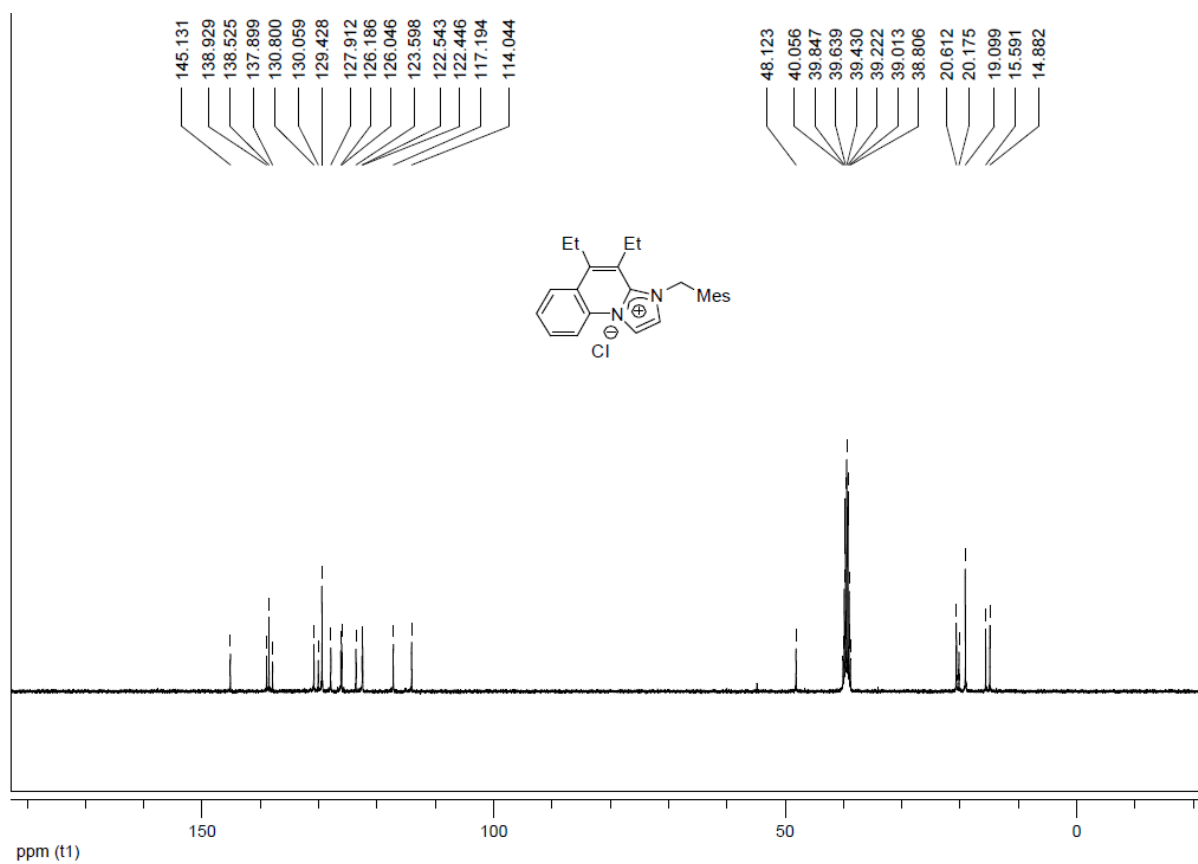
¹³C NMR spectrum of 3ag



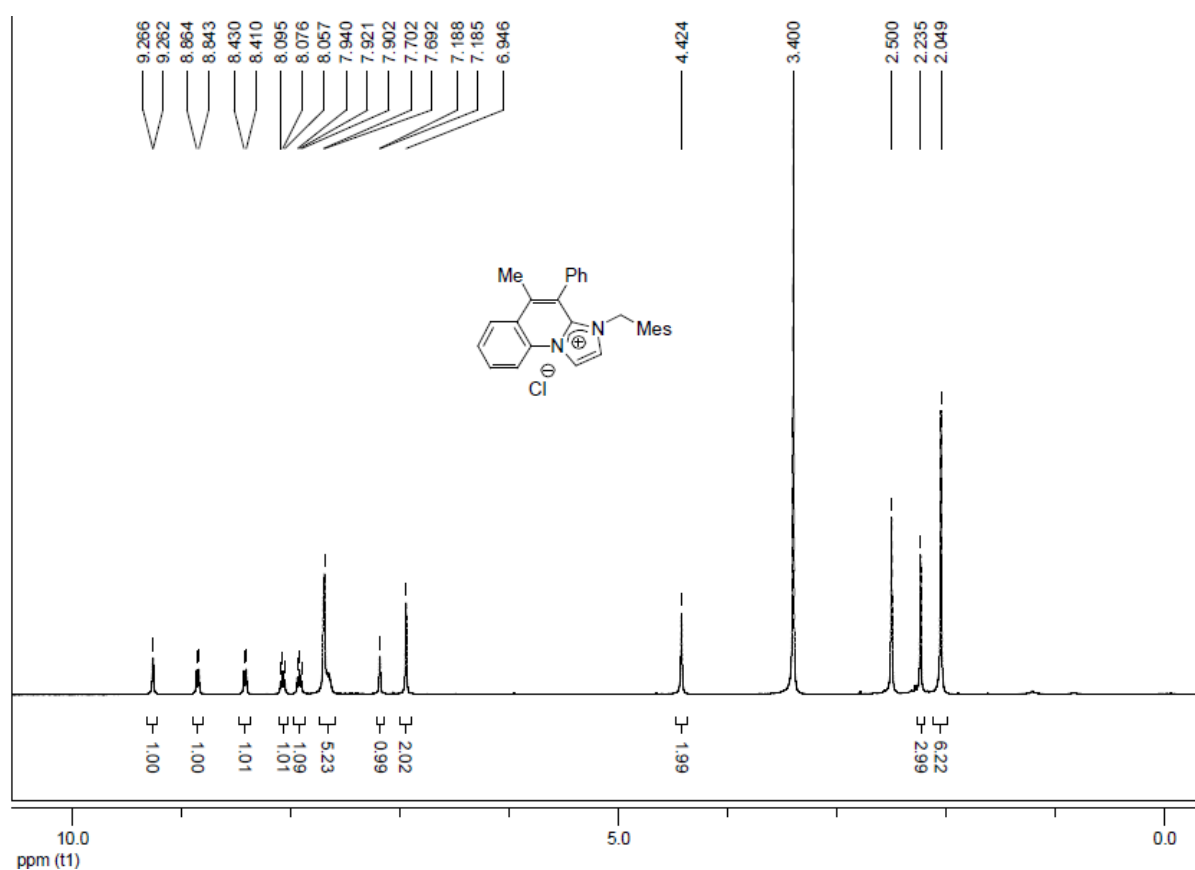
¹H NMR spectrum of 3ah



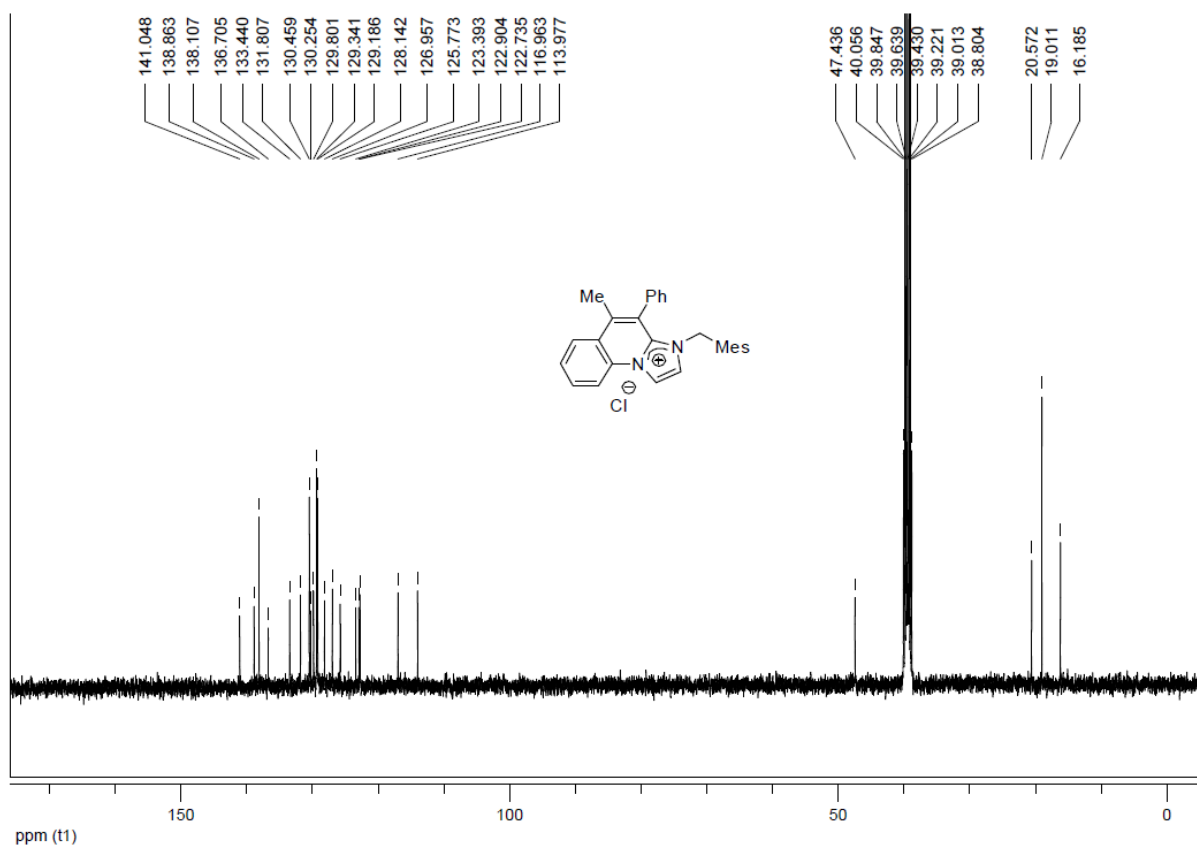
¹³C NMR spectrum of 3ah



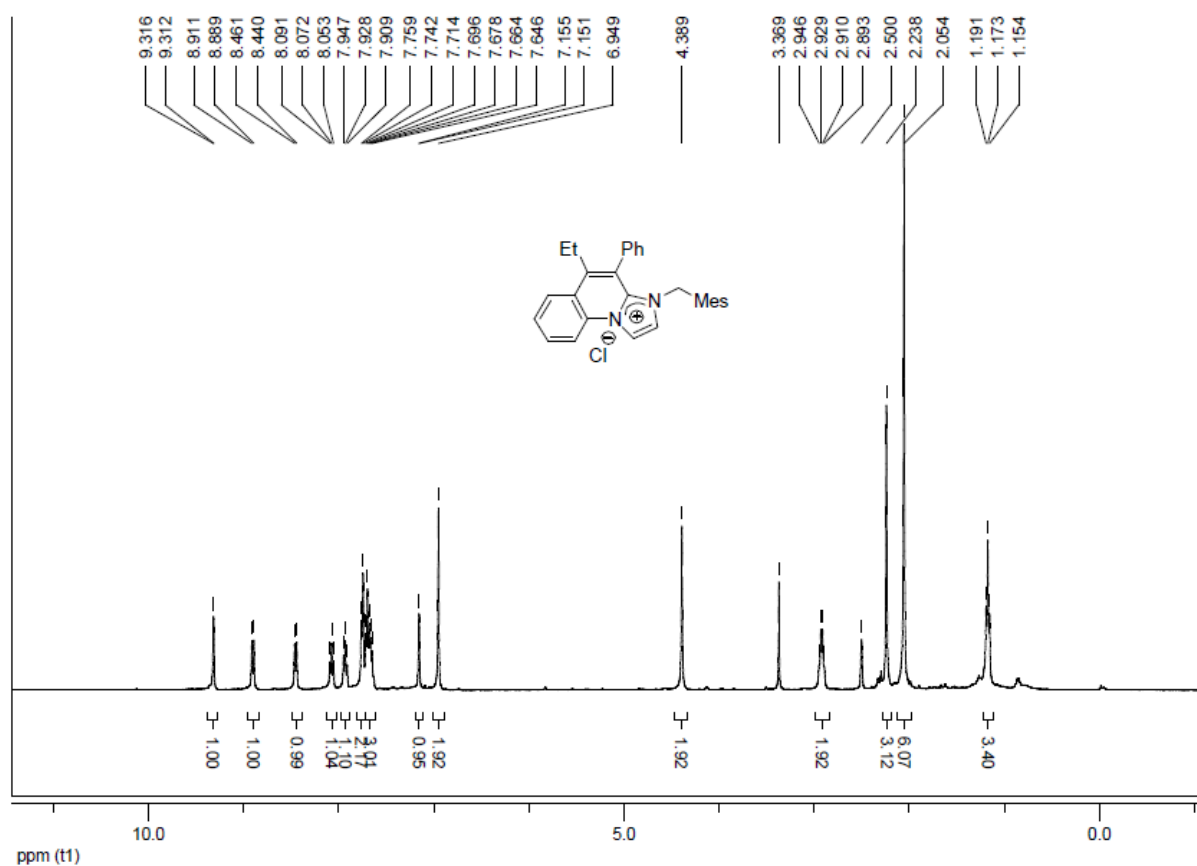
¹H NMR spectrum of 3ai



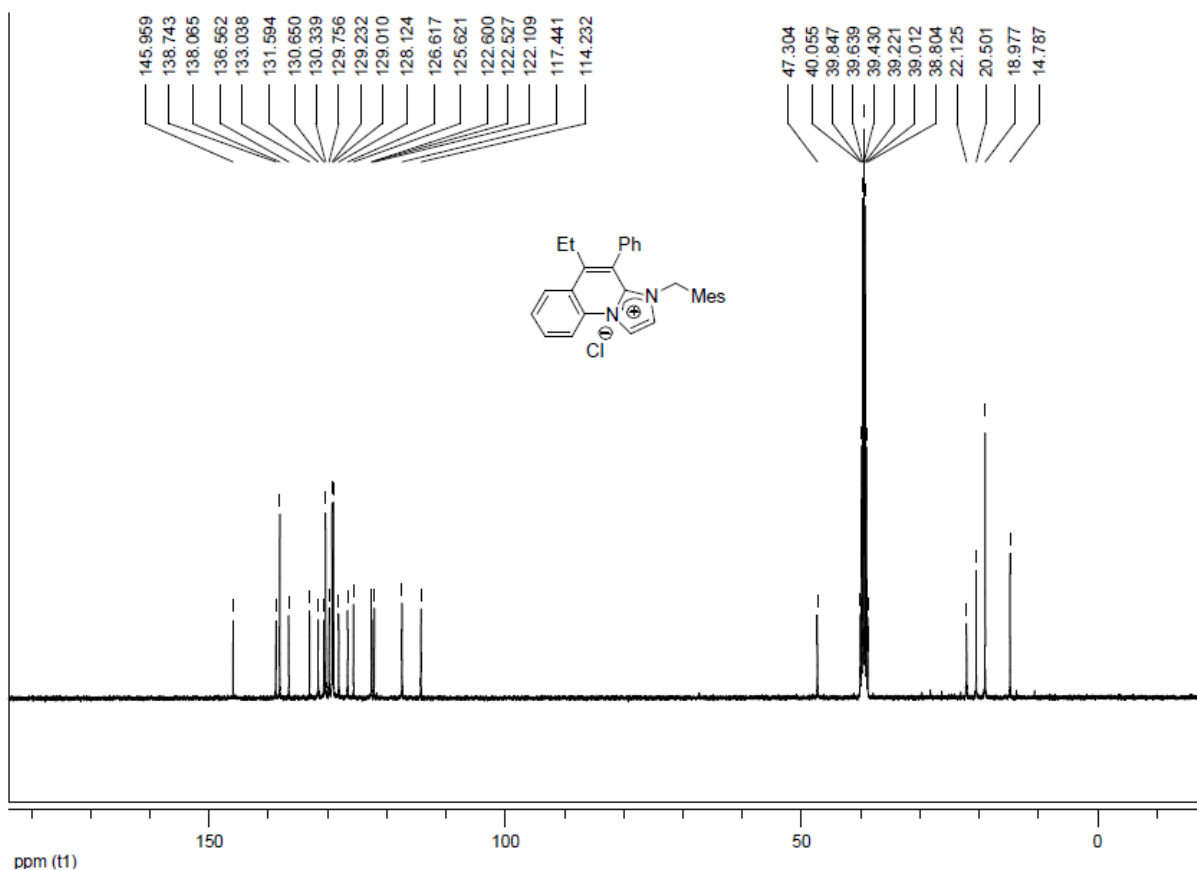
¹³C NMR spectrum of 3ai



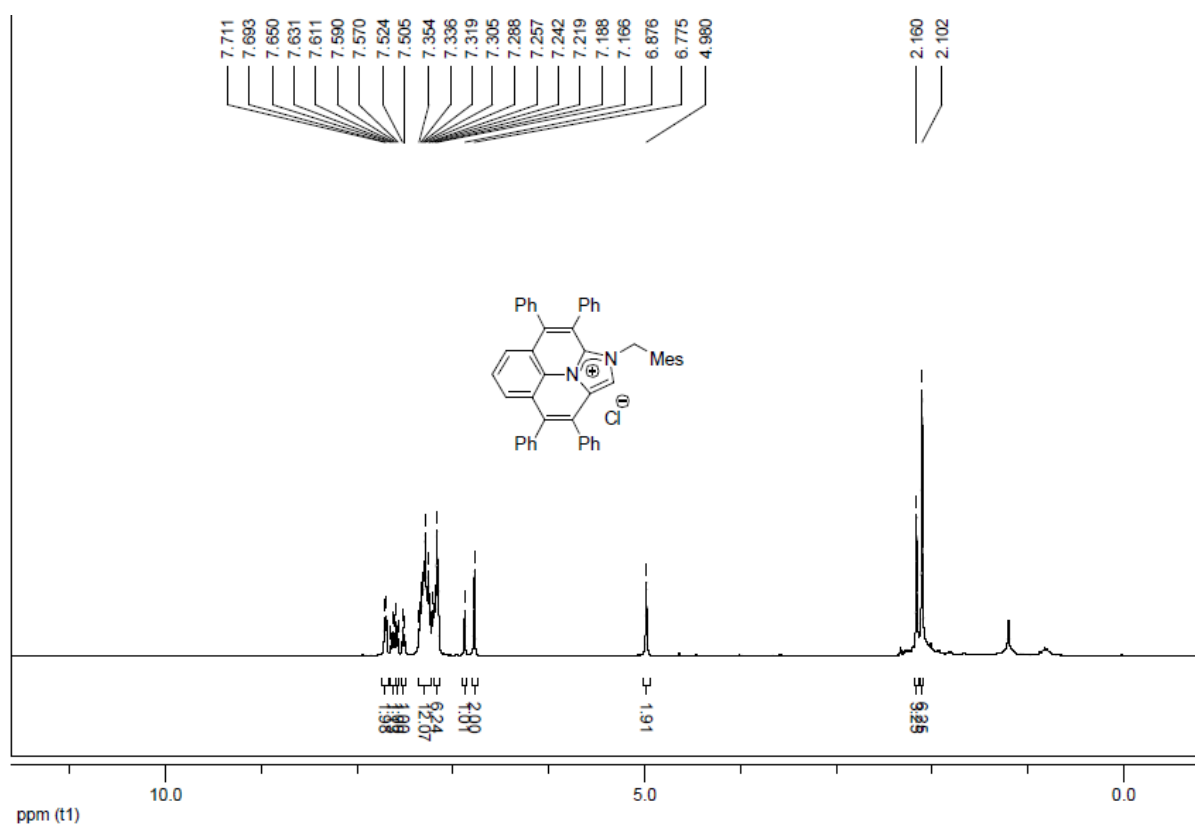
¹H NMR spectrum of 3aj



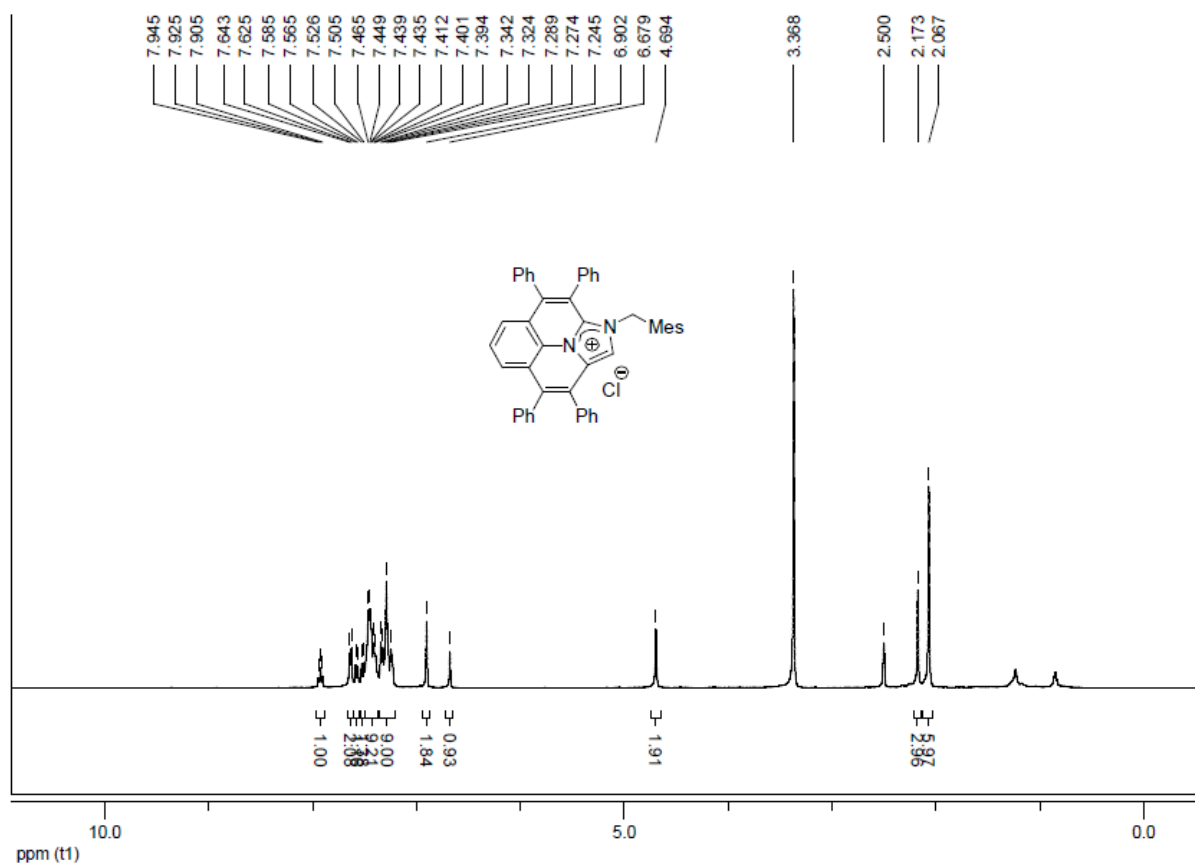
¹³C NMR spectrum of 3aj



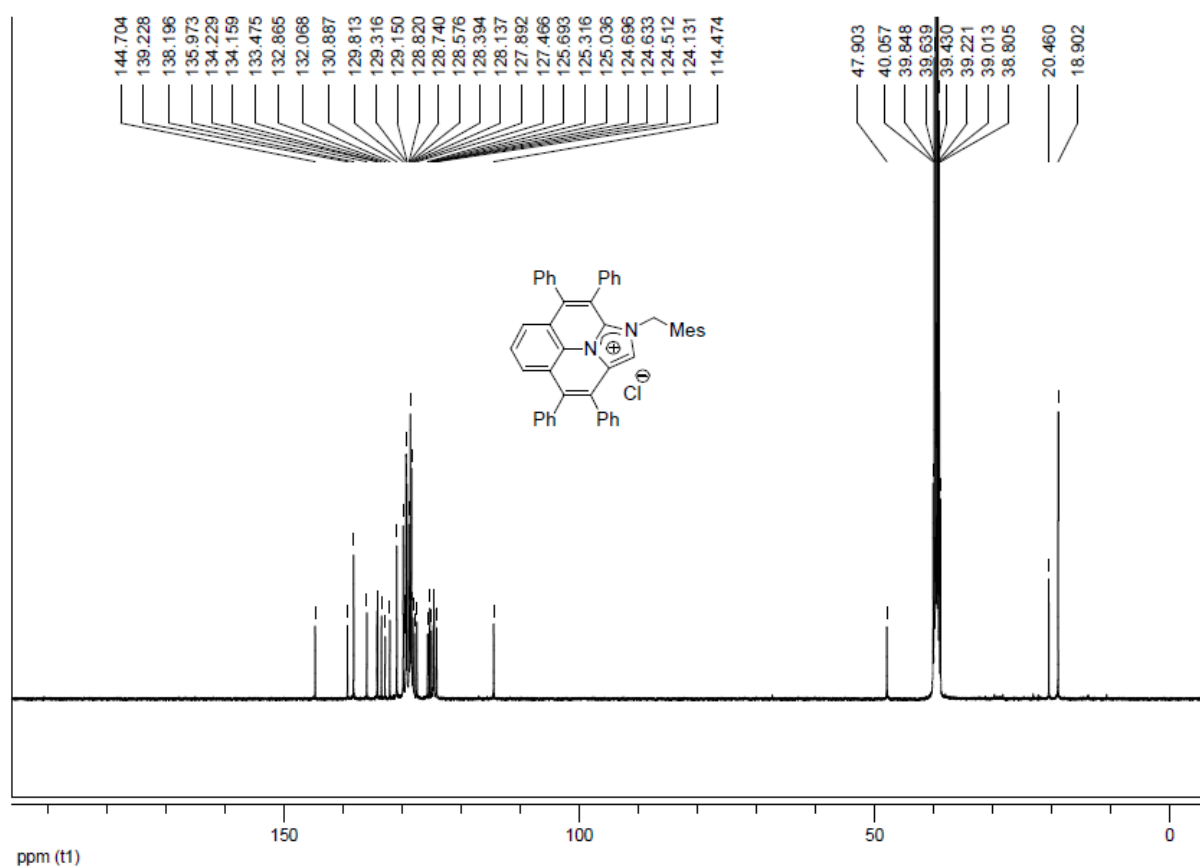
¹H NMR spectrum of 4aa (in CDCl₃)



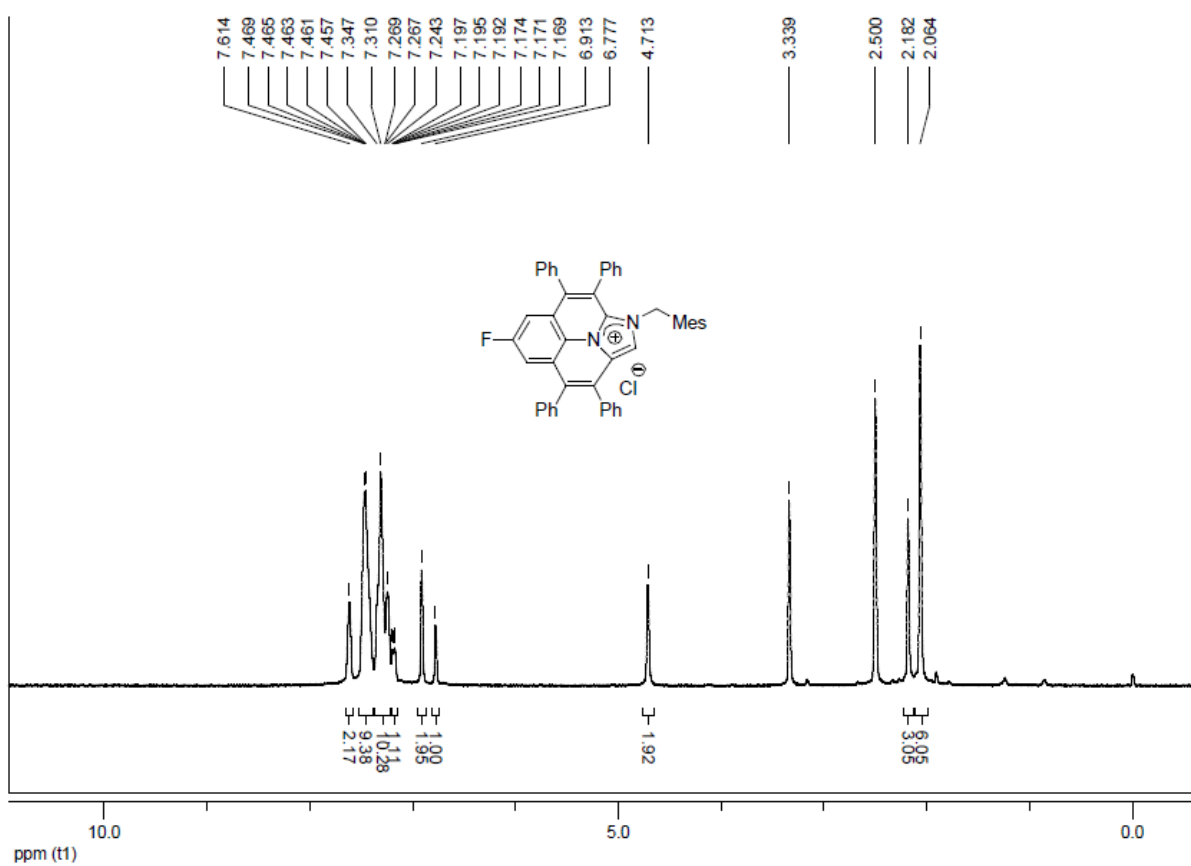
¹H NMR spectrum of 4aa (in DMSO-*d*₆)



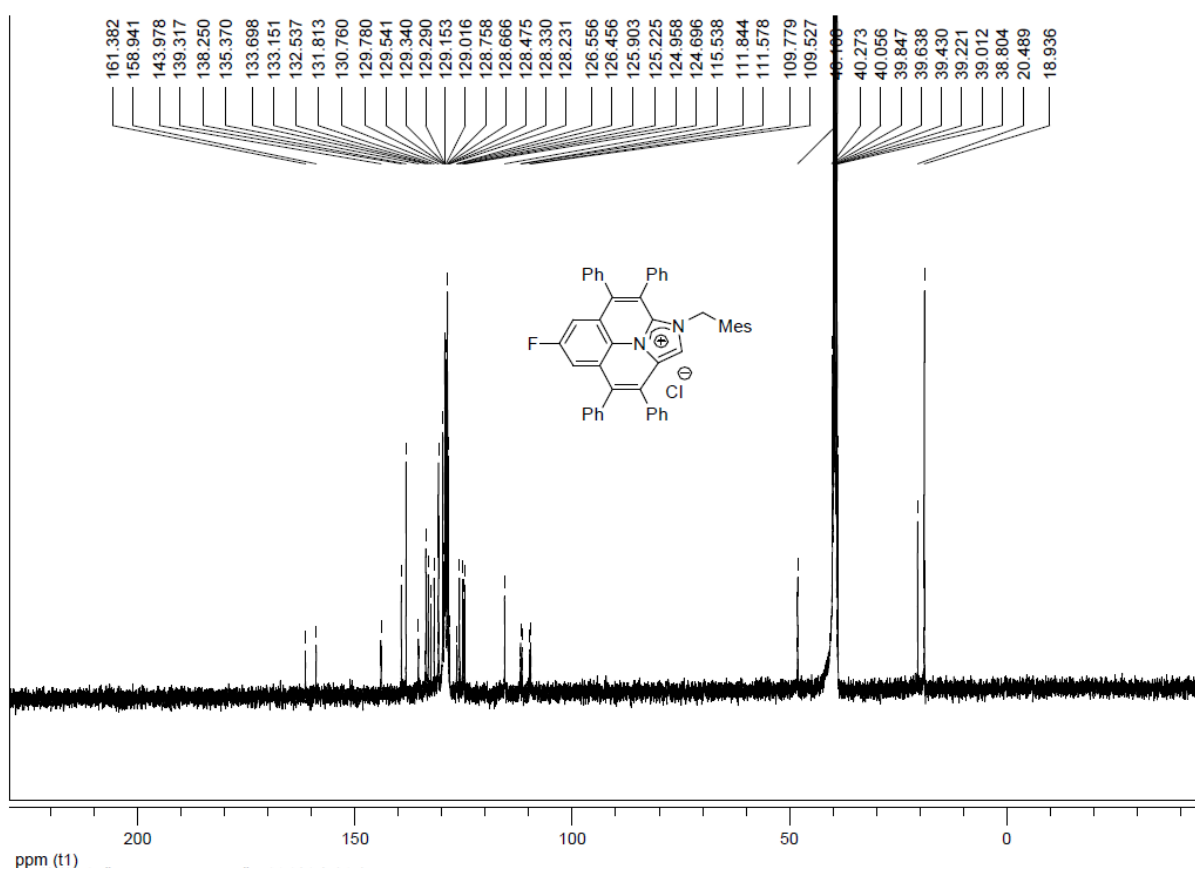
¹³C NMR spectrum of 4aa



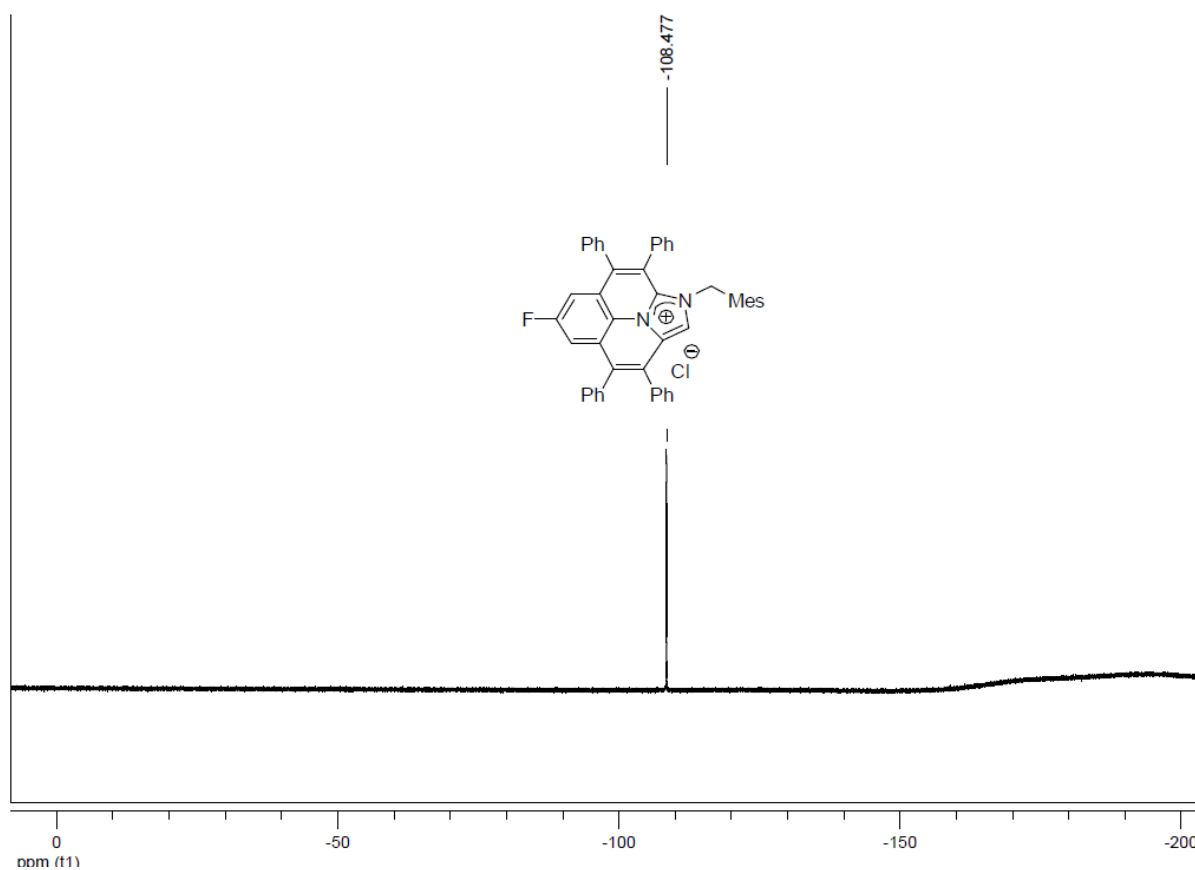
¹H NMR spectrum of 4ba



¹³C NMR spectrum of 4ba



¹⁹F NMR spectrum of 4ba

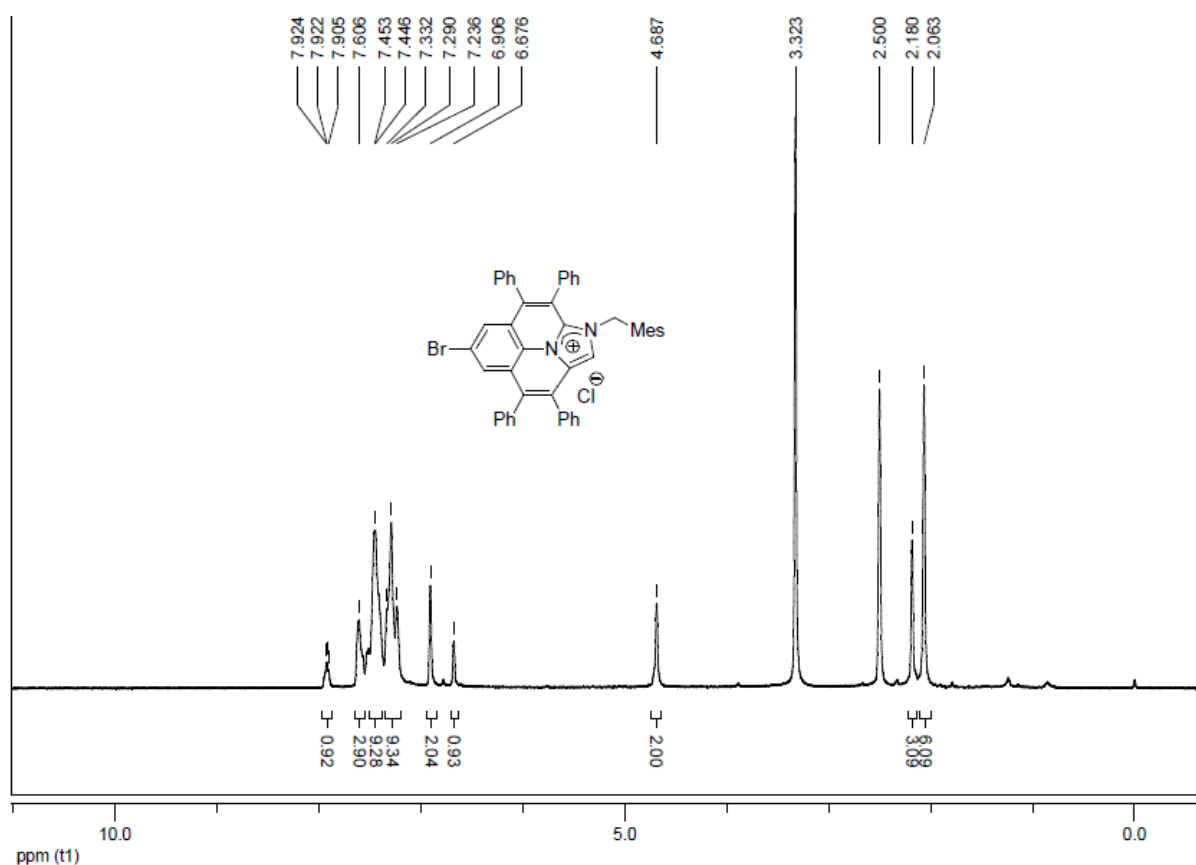


Chemical Structure of Compound 10:

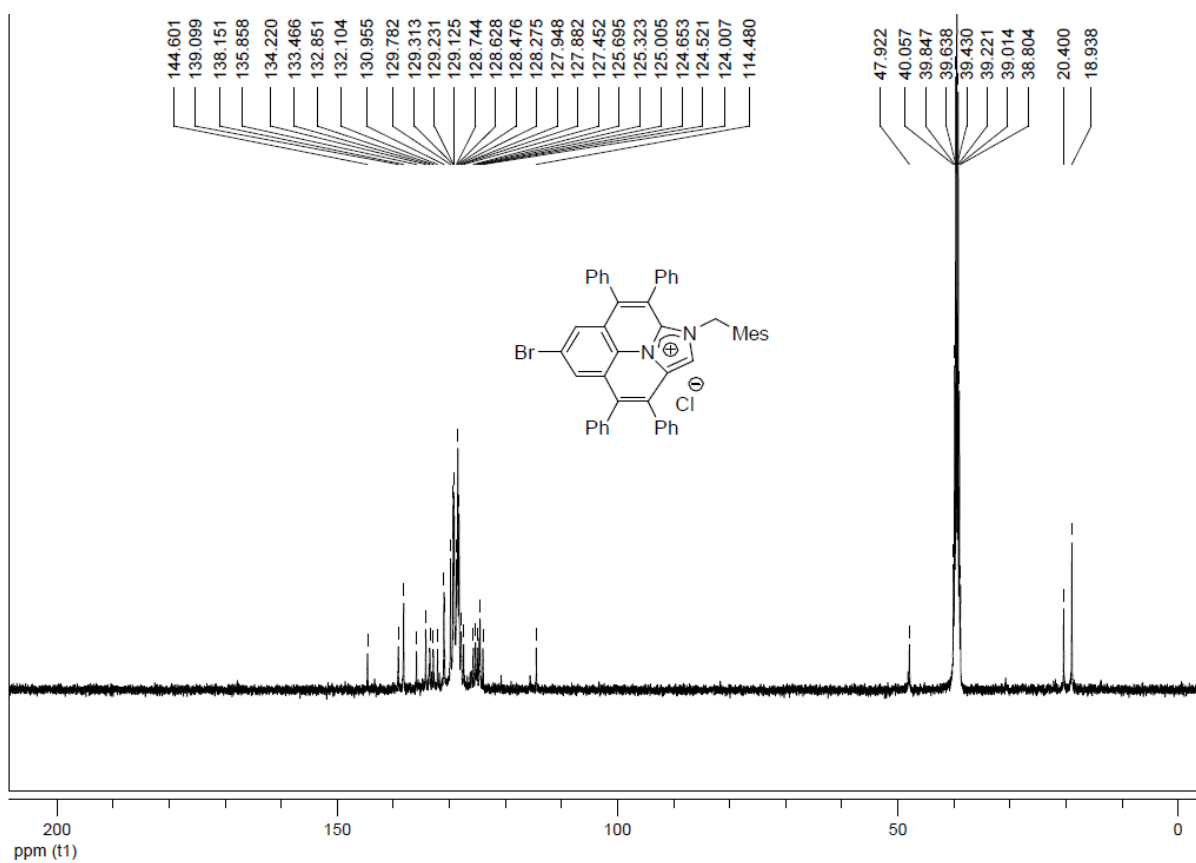
Cc1cn2c(c3cc(Cl)ccc3c2n1C4=CC=CC=C4)C(=C5C=CC=C5)C(=C6C=CC=C6)C(=C7C=CC=C7)C(=C8C=CC=C8)C(=C9C=CC=C9)C(=C10C=CC=C10)C(=C11C=CC=C11)C(=C12C=CC=C12)C(=C13C=CC=C13)C(=C14C=CC=C14)C(=C15C=CC=C15)C(=C16C=CC=C16)C(=C17C=CC=C17)C(=C18C=CC=C18)C(=C19C=CC=C19)C(=C20C=CC=C20)C(=C21C=CC=C21)C(=C22C=CC=C22)C(=C23C=CC=C23)C(=C24C=CC=C24)C(=C25C=CC=C25)C(=C26C=CC=C26)C(=C27C=CC=C27)C(=C28C=CC=C28)C(=C29C=CC=C29)C(=C30C=CC=C30)C(=C31C=CC=C31)C(=C32C=CC=C32)C(=C33C=CC=C33)C(=C34C=CC=C34)C(=C35C=CC=C35)C(=C36C=CC=C36)C(=C37C=CC=C37)C(=C38C=CC=C38)C(=C39C=CC=C39)C(=C40C=CC=C40)C(=C41C=CC=C41)C(=C42C=CC=C42)C(=C43C=CC=C43)C(=C44C=CC=C44)C(=C45C=CC=C45)C(=C46C=CC=C46)C(=C47C=CC=C47)C(=C48C=CC=C48)C(=C49C=CC=C49)C(=C50C=CC=C50)C(=C51C=CC=C51)C(=C52C=CC=C52)C(=C53C=CC=C53)C(=C54C=CC=C54)C(=C55C=CC=C55)C(=C56C=CC=C56)C(=C57C=CC=C57)C(=C58C=CC=C58)C(=C59C=CC=C59)C(=C60C=CC=C60)C(=C61C=CC=C61)C(=C62C=CC=C62)C(=C63C=CC=C63)C(=C64C=CC=C64)C(=C65C=CC=C65)C(=C66C=CC=C66)C(=C67C=CC=C67)C(=C68C=CC=C68)C(=C69C=CC=C69)C(=C70C=CC=C70)C(=C71C=CC=C71)C(=C72C=CC=C72)C(=C73C=CC=C73)C(=C74C=CC=C74)C(=C75C=CC=C75)C(=C76C=CC=C76)C(=C77C=CC=C77)C(=C78C=CC=C78)C(=C79C=CC=C79)C(=C80C=CC=C80)C(=C81C=CC=C81)C(=C82C=CC=C82)C(=C83C=CC=C83)C(=C84C=CC=C84)C(=C85C=CC=C85)C(=C86C=CC=C86)C(=C87C=CC=C87)C(=C88C=CC=C88)C(=C89C=CC=C89)C(=C90C=CC=C90)C(=C91C=CC=C91)C(=C92C=CC=C92)C(=C93C=CC=C93)C(=C94C=CC=C94)C(=C95C=CC=C95)C(=C96C=CC=C96)C(=C97C=CC=C97)C(=C98C=CC=C98)C(=C99C=CC=C99)C(=C100C=CC=C100)C(=C101C=CC=C101)C(=C102C=CC=C102)C(=C103C=CC=C103)C(=C104C=CC=C104)C(=C105C=CC=C105)C(=C106C=CC=C106)C(=C107C=CC=C107)C(=C108C=CC=C108)C(=C109C=CC=C109)C(=C110C=CC=C110)C(=C111C=CC=C111)C(=C112C=CC=C112)C(=C113C=CC=C113)C(=C114C=CC=C114)C(=C115C=CC=C115)C(=C116C=CC=C116)C(=C117C=CC=C117)C(=C118C=CC=C118)C(=C119C=CC=C119)C(=C120C=CC=C120)C(=C121C=CC=C121)C(=C122C=CC=C122)C(=C123C=CC=C123)C(=C124C=CC=C124)C(=C125C=CC=C125)C(=C126C=CC=C126)C(=C127C=CC=C127)C(=C128C=CC=C128)C(=C129C=CC=C129)C(=C130C=CC=C130)C(=C131C=CC=C131)C(=C132C=CC=C132)C(=C133C=CC=C133)C(=C134C=CC=C134)C(=C135C=CC=C135)C(=C136C=CC=C136)C(=C137C=CC=C137)C(=C138C=CC=C138)C(=C139C=CC=C139)C(=C140C=CC=C140)C(=C141C=CC=C141)C(=C142C=CC=C142)C(=C143C=CC=C143)C(=C144C=CC=C144)C(=C145C=CC=C145)C(=C146C=CC=C146)C(=C147C=CC=C147)C(=C148C=CC=C148)C(=C149C=CC=C149)C(=C150C=CC=C150)C(=C151C=CC=C151)C(=C152C=CC=C152)C(=C153C=CC=C153)C(=C154C=CC=C154)C(=C155C=CC=C155)C(=C156C=CC=C156)C(=C157C=CC=C157)C(=C158C=CC=C158)C(=C159C=CC=C159)C(=C160C=CC=C160)C(=C161C=CC=C161)C(=C162C=CC=C162)C(=C163C=CC=C163)C(=C164C=CC=C164)C(=C165C=CC=C165)C(=C166C=CC=C166)C(=C167C=CC=C167)C(=C168C=CC=C168)C(=C169C=CC=C169)C(=C170C=CC=C170)C(=C171C=CC=C171)C(=C172C=CC=C172)C(=C173C=CC=C173)C(=C174C=CC=C174)C(=C175C=CC=C175)C(=C176C=CC=C176)C(=C177C=CC=C177)C(=C178C=CC=C178)C(=C179C=CC=C179)C(=C180C=CC=C180)C(=C181C=CC=C181)C(=C182C=CC=C182)C(=C183C=CC=C183)C(=C184C=CC=C184)C(=C185C=CC=C185)C(=C186C=CC=C186)C(=C187C=CC=C187)C(=C188C=CC=C188)C(=C189C=CC=C189)C(=C190C=CC=C190)C(=C191C=CC=C191)C(=C192C=CC=C192)C(=C193C=CC=C193)C(=C194C=CC=C194)C(=C195C=CC=C195)C(=C196C=CC=C196)C(=C197C=CC=C197)C(=C198C=CC=C198)C(=C199C=CC=C199)C(=C200C=CC=C200)C(=C201C=CC=C201)C(=C202C=CC=C202)C(=C203C=CC=C203)C(=C204C=CC=C204)C(=C205C=CC=C205)C(=C206C=CC=C206)C(=C207C=CC=C207)C(=C208C=CC=C208)C(=C209C=CC=C209)C(=C210C=CC=C210)C(=C211C=CC=C211)C(=C212C=CC=C212)C(=C213C=CC=C213)C(=C214C=CC=C214)C(=C215C=CC=C215)C(=C216C=CC=C216)C(=C217C=CC=C217)C(=C218C=CC=C218)C(=C219C=CC=C219)C(=C220C=CC=C220)C(=C221C=CC=C221)C(=C222C=CC=C222)C(=C223C=CC=C223)C(=C224C=CC=C224)C(=C225C=CC=C225)C(=C226C=CC=C226)C(=C227C=CC=C227)C(=C228C=CC=C228)C(=C229C=CC=C229)C(=C230C=CC=C230)C(=C231C=CC=C231)C(=C232C=CC=C232)C(=C233C=CC=C233)C(=C234C=CC=C234)C(=C235C=CC=C235)C(=C236C=CC=C236)C(=C237C=CC=C237)C(=C238C=CC=C238)C(=C239C=CC=C239)C(=C240C=CC=C240)C(=C241C=CC=C241)C(=C242C=CC=C242)C(=C243C=CC=C243)C(=C244C=CC=C244)C(=C245C=CC=C245)C(=C246C=CC=C246)C(=C247C=CC=C247)C(=C248C=CC=C248)C(=C249C=CC=C249)C(=C250C=CC=C250)C(=C251C=CC=C251)C(=C252C=CC=C252)C(=C253C=CC=C253)C(=C254C=CC=C254)C(=C255C=CC=C255)C(=C256C=CC=C256)C(=C257C=CC=C257)C(=C258C=CC=C258)C(=C259C=CC=C259)C(=C260C=CC=C260)C(=C261C=CC=C261)C(=C262C=CC=C262)C(=C263C=CC=C263)C(=C264C=CC=C264)C(=C265C=CC=C265)C(=C266C=CC=C266)C(=C267C=CC=C267)C(=C268C=CC=C268)C(=C269C=CC=C269)C(=C270C=CC=C270)C(=C271C=CC=C271)C(=C272C=CC=C272)C(=C273C=CC=C273)C(=C274C=CC=C274)C(=C275C=CC=C275)C(=C276C=CC=C276)C(=C277C=CC=C277)C(=C278C=CC=C278)C(=C279C=CC=C279)C(=C280C=CC=C280)C(=C281

Chemical structure of compound 10 is shown as an inset. The structure is a benzimidazole derivative with a 4-chlorophenyl group, two phenyl groups, and a 2-methylimidazol-5-yl group.

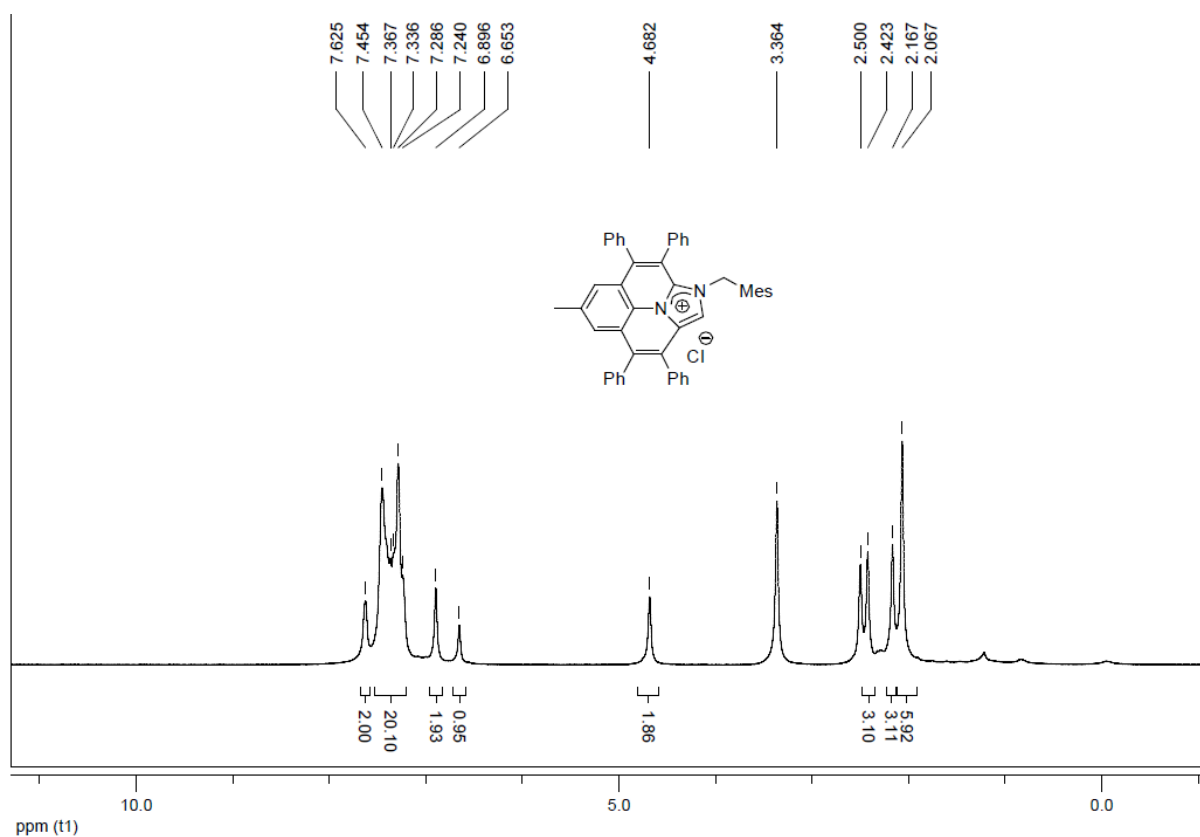
¹H NMR spectrum of 4da



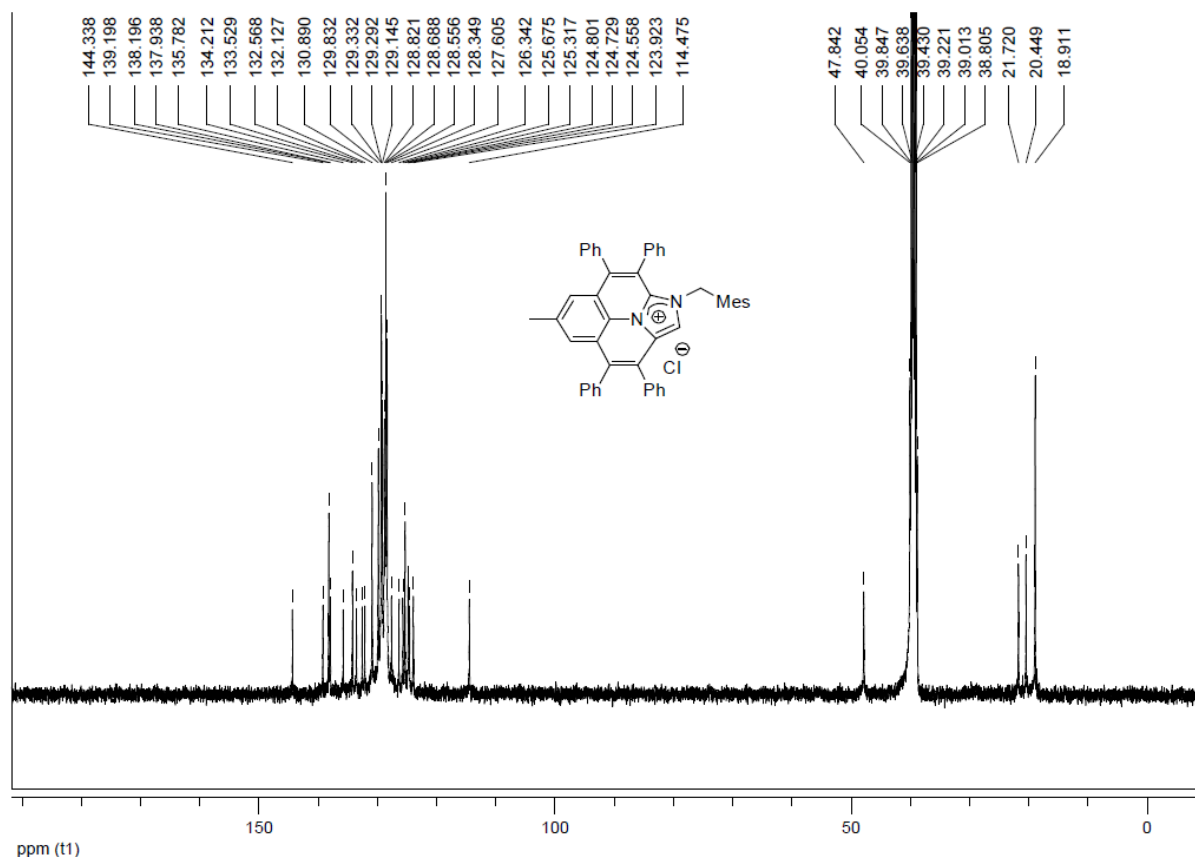
¹³C NMR spectrum of 4da



¹H NMR spectrum of 4ea



¹³C NMR spectrum of 4ea



Chemical structure of compound 10 is shown above the spectrum. The structure is a cationic porphyrin derivative with a central nitrogen atom bonded to a methyl group and a chloride ion. The porphyrin ring is substituted with four phenyl groups and a methoxy group.

¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm (t1), ranging from 0.0 to 10.0. The spectrum shows several peaks corresponding to the protons in the molecule.

Peak assignments and integrations:

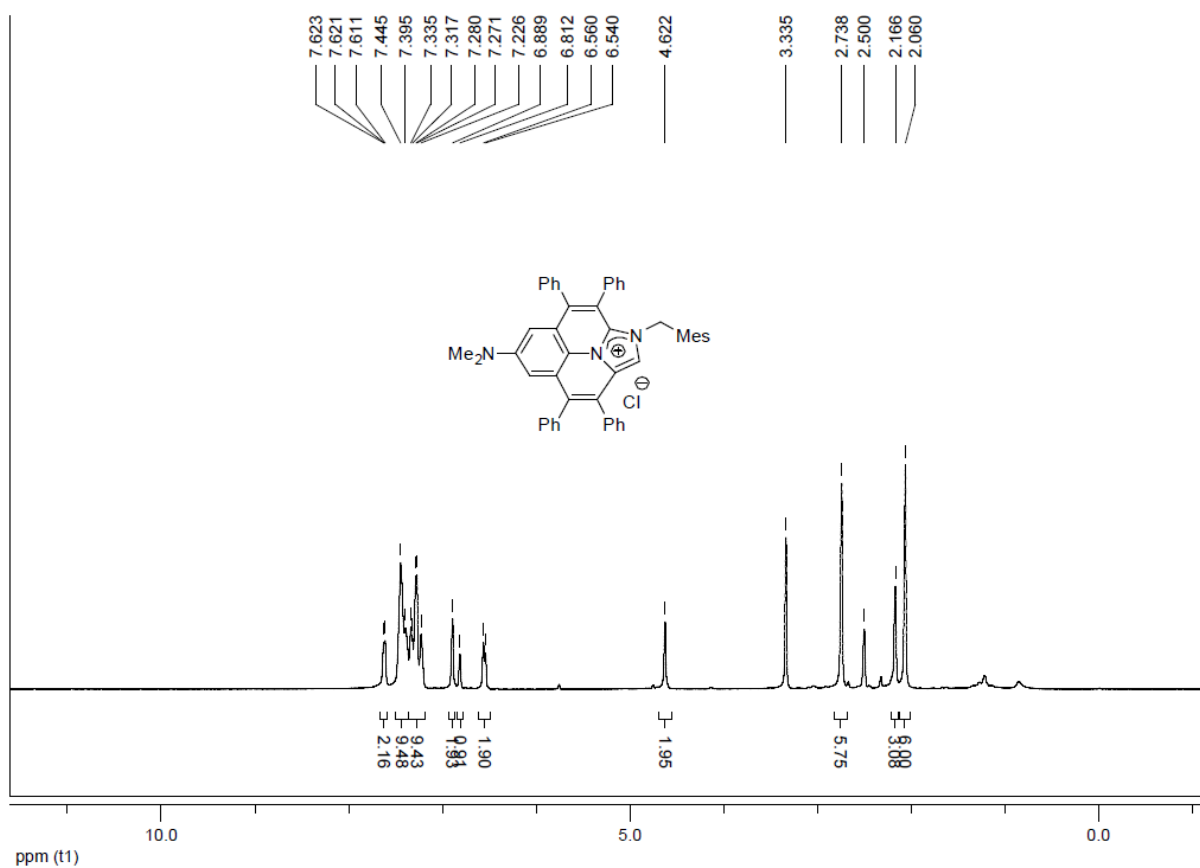
- 7.658, 7.642, 7.468, 7.452, 7.415, 7.402, 7.363, 7.346, 7.288, 7.250, 7.022, 6.895, 6.683 (Aromatic protons, integration: 2.16, 7.13, 9.17, 2.94, 1.03, 0.98)
- 4.692 (Methoxy protons, integration: 1.96)
- 3.646, 3.350 (Methyl protons, integration: 3.00)
- 2.500, 2.168, 2.072 (Methyl protons, integration: 6.06)

Chemical structure of compound 10 is shown above the spectrum. The structure is a cationic porphyrin derivative with a central nitrogen atom bonded to a mesityl group (Mes) and a chloride ion (Cl⁻). The porphyrin ring is substituted with four phenyl groups (Ph) and a methoxy group (MeO).

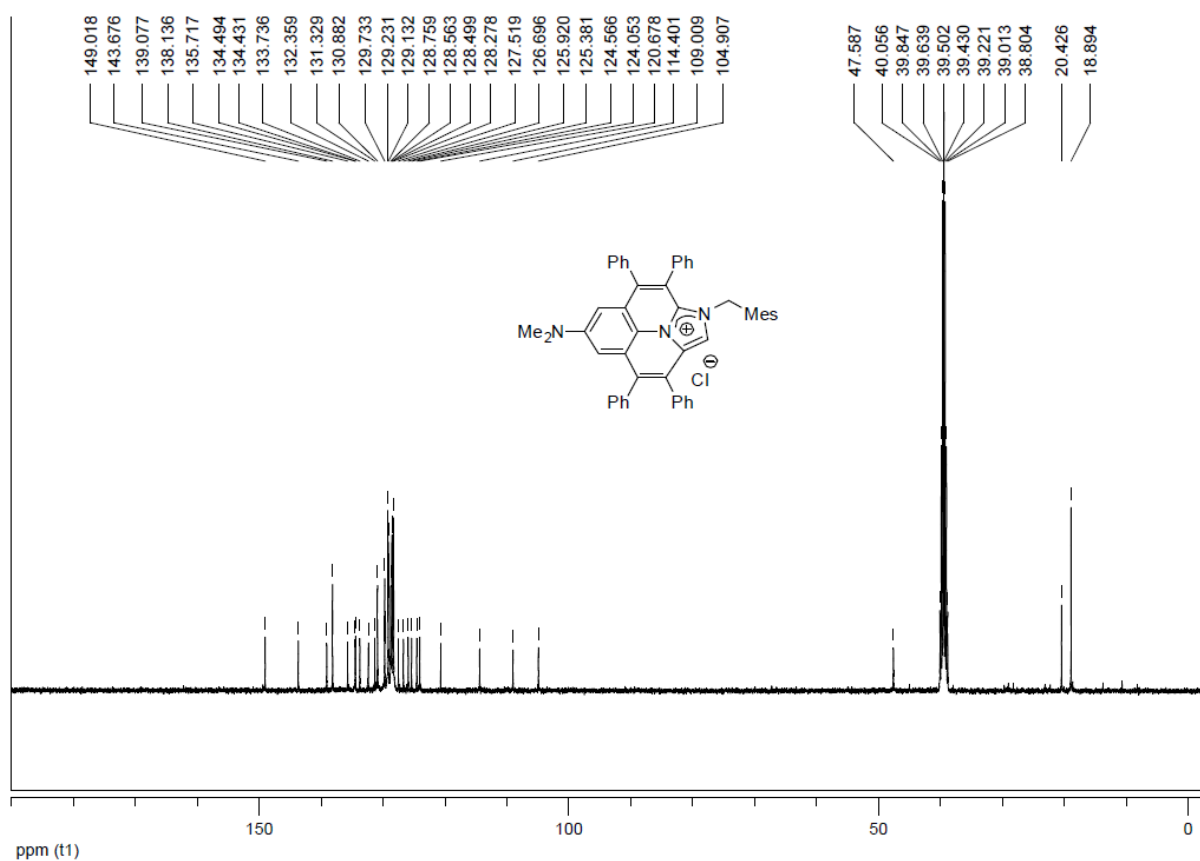
¹³C NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm (f1), ranging from 0 to 150. The spectrum shows peaks corresponding to the porphyrin core, the phenyl groups, the methoxy group, and the mesityl group.

Peak list (ppm): 158.078, 143.889, 139.148, 138.177, 135.411, 134.096, 133.433, 132.084, 130.861, 129.744, 129.265, 129.124, 128.840, 128.727, 128.608, 128.541, 128.447, 128.387, 128.325, 128.148, 127.386, 126.062, 125.298, 125.146, 124.387, 123.183, 114.938, 111.777, 107.061, 55.510, 47.843, 40.056, 39.847, 39.638, 39.430, 39.221, 39.012, 38.803, 20.429, 18.914.

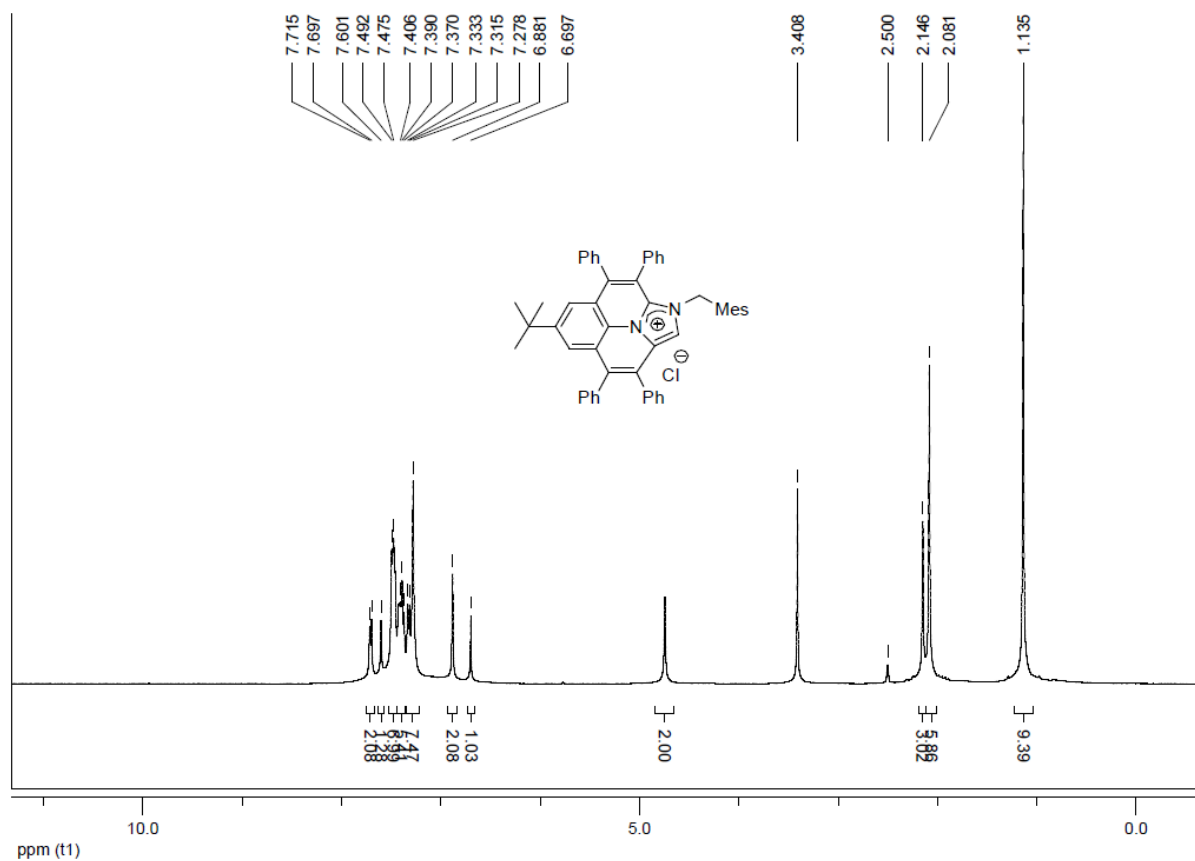
¹H NMR spectrum of 4ga



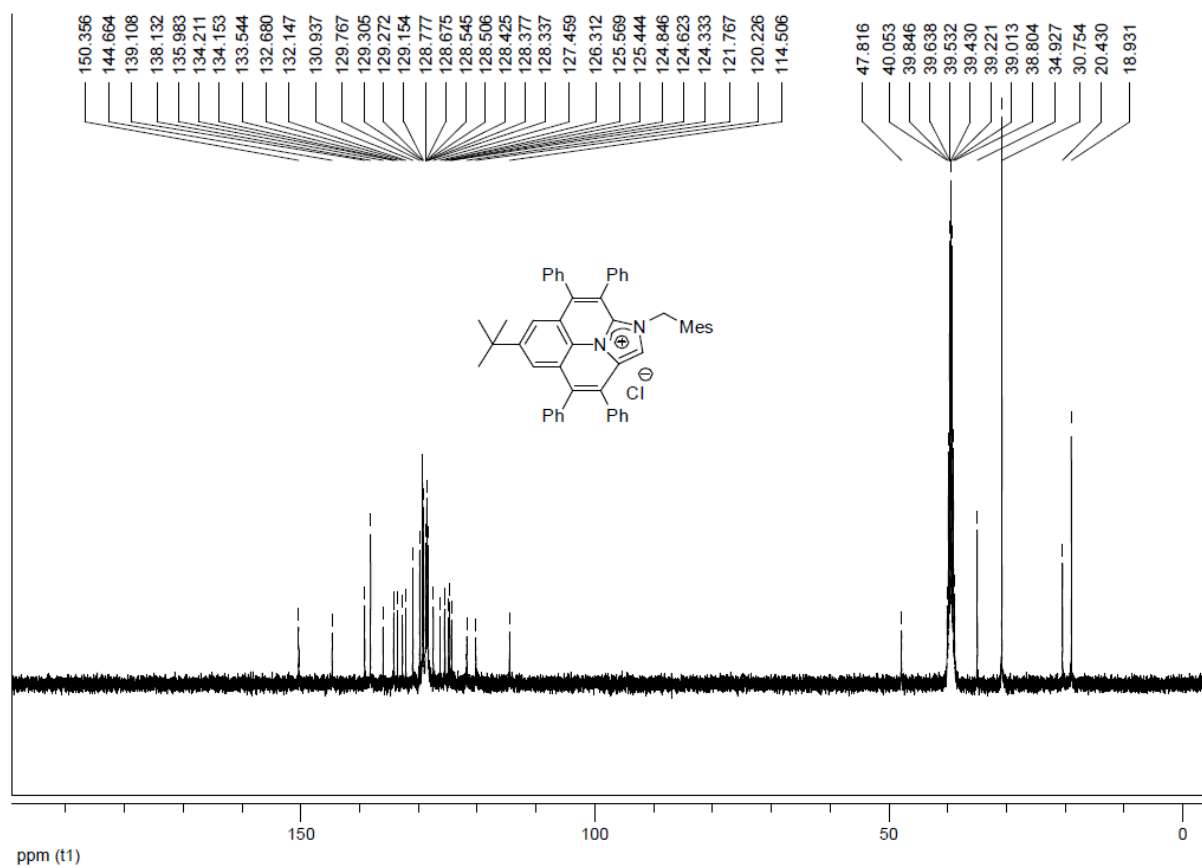
¹³C NMR spectrum of 4ga



¹H NMR spectrum of 4ha



¹³C NMR spectrum of 4ha



Chemical Structure of Compound 10:

CN1C=C(C2=CC=CC=C2)N3C(=C(C4=CC=CC=C4)C(=C(C5=CC=CC=C5)C(=C(C6=CC=CC=C6)C(=C(C7=CC=CC=C7)[N+](=O)[O-])C=C8C=CC(=C(C9=CC=CC=C9)N1)C=C8)C=C6)C=C5)C=C4)C=C3

¹H NMR Spectrum (CDCl₃):

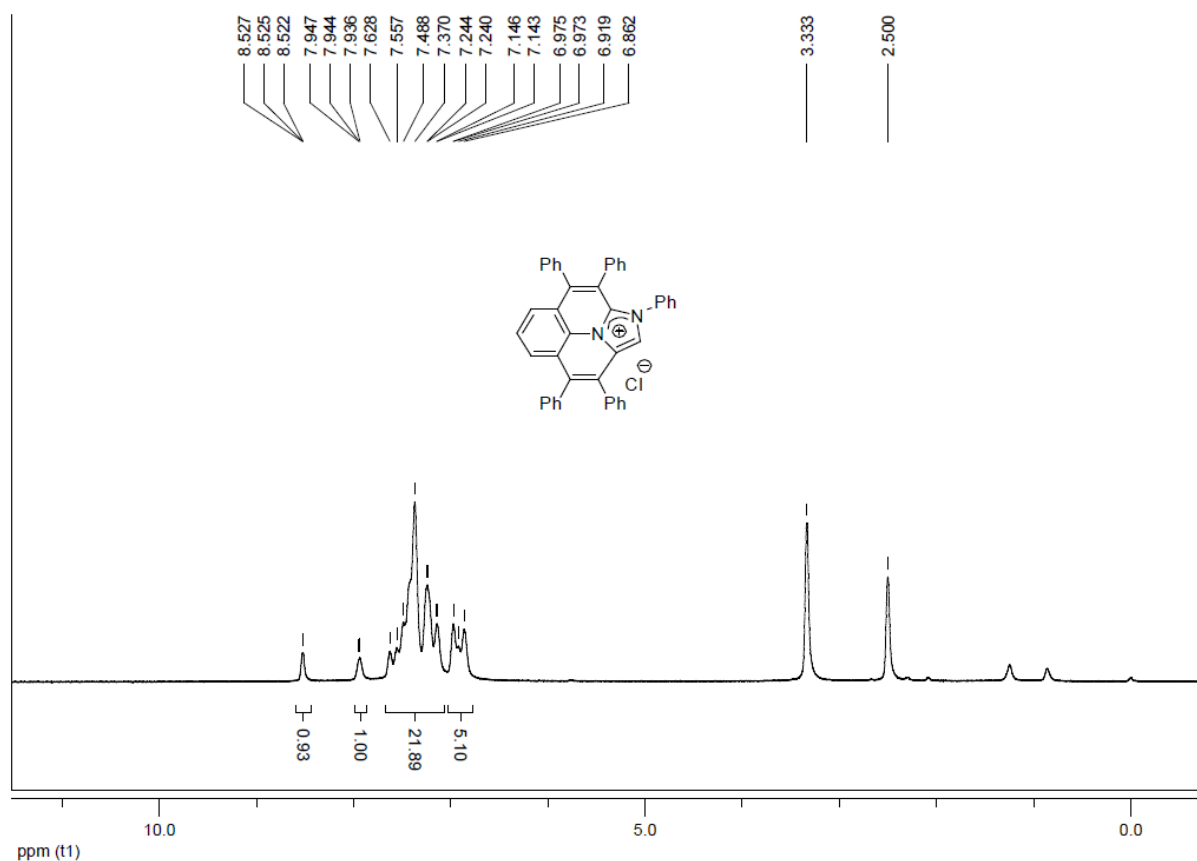
Chemical Shift (ppm)	Integration
8.220, 8.208, 7.688, 7.670, 7.648, 7.521, 7.514, 7.504, 7.485, 7.469, 7.462, 7.454, 7.412, 7.394, 7.366, 7.349, 7.339, 7.329, 7.324, 7.284, 7.276, 7.268, 6.916, 6.873, 4.780	1.88, 9.42, 9.36, 2.13, 2.87
3.361, 3.348	2.00
2.500, 2.177, 2.083	5.98, 3.38

Chemical structure of compound 10 is shown in the center of the spectrum. The structure is a benzimidazole cation with a 4-nitrophenyl group at position 2, a 4-methylphenyl group at position 3, and a 4-chlorophenyl group at position 4. The nitrogen at position 1 is substituted with a methyl group (Mes).

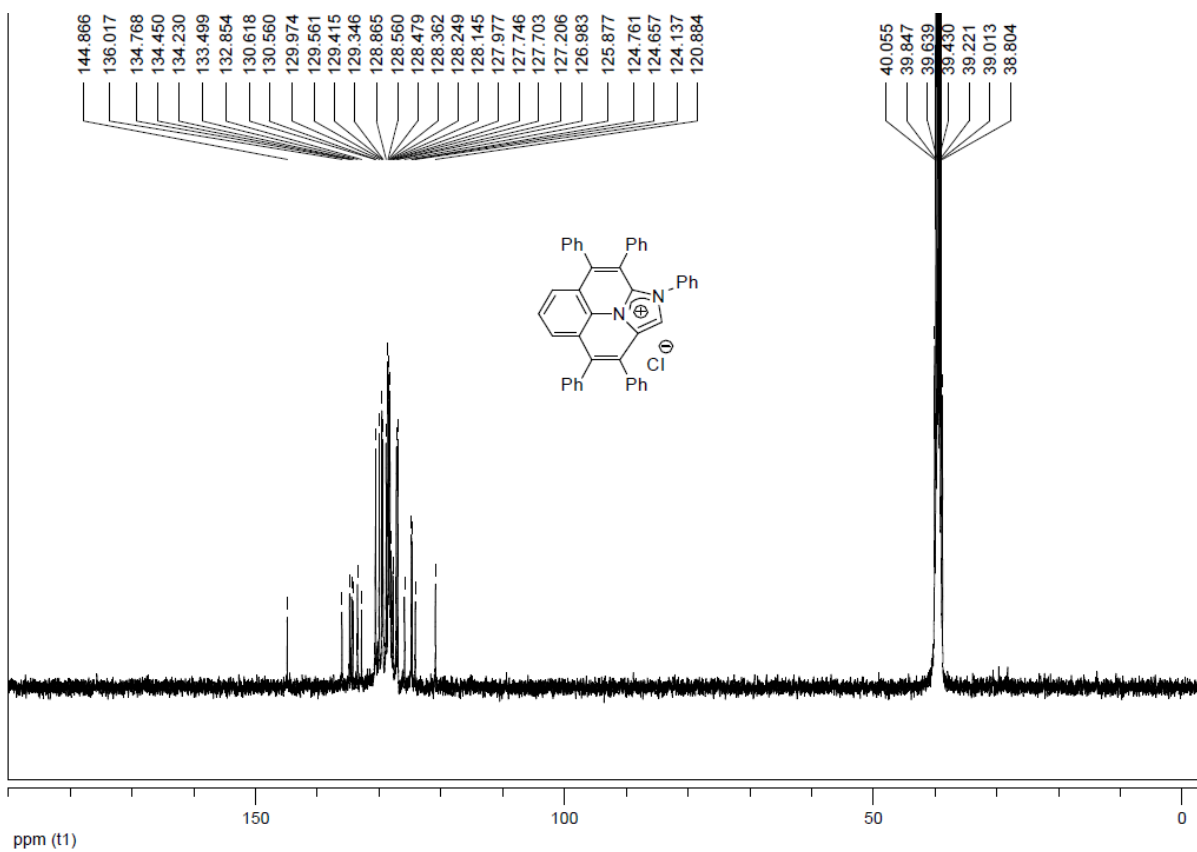
The ^{13}C NMR spectrum shows the following chemical shifts (ppm):

- 145.816
- 144.655
- 139.362
- 138.294
- 135.475
- 133.611
- 133.385
- 133.292
- 132.894
- 131.557
- 130.767
- 130.126
- 129.904
- 129.653
- 129.596
- 129.473
- 129.324
- 129.130
- 129.070
- 128.936
- 128.855
- 128.770
- 128.673
- 128.486
- 127.004
- 126.665
- 125.167
- 125.055
- 118.372
- 117.953
- 116.195
- 48.406
- 40.056
- 39.847
- 39.639
- 39.430
- 39.221
- 39.013
- 38.804
- 20.455
- 18.971

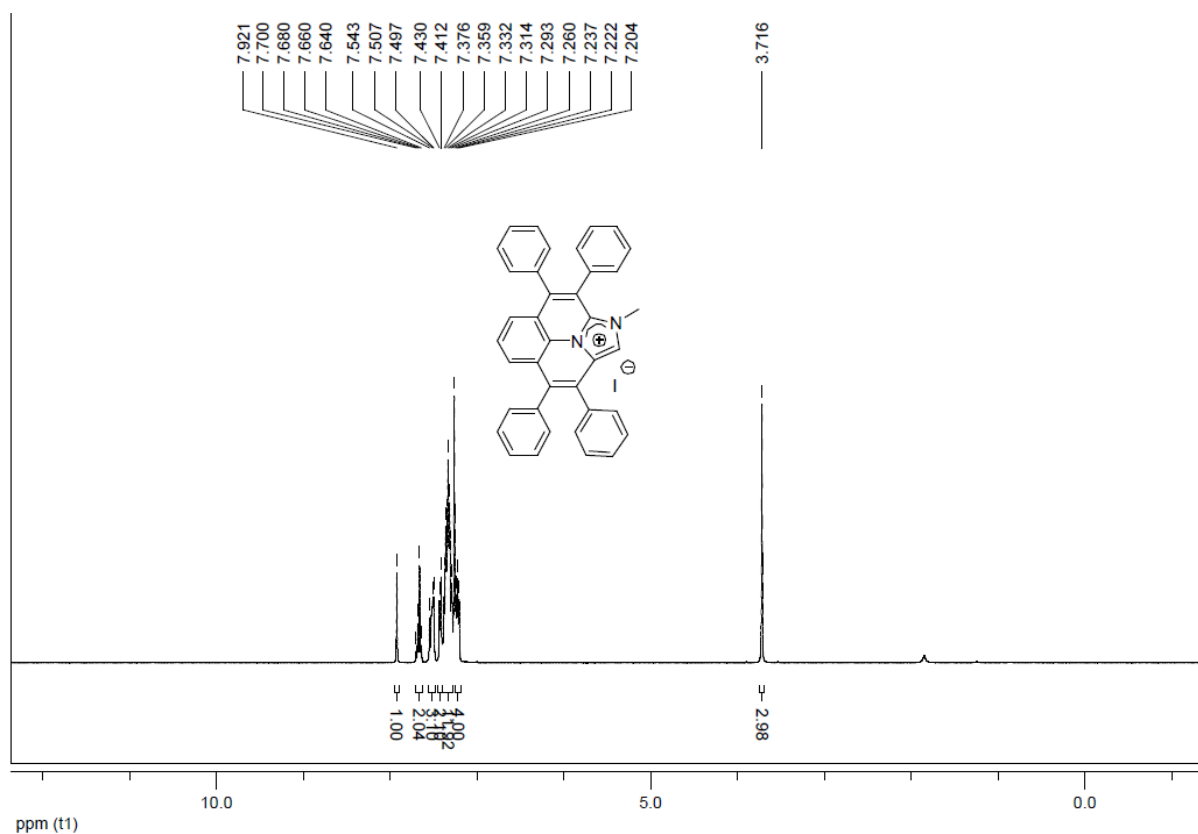
¹H NMR spectrum of 4ja



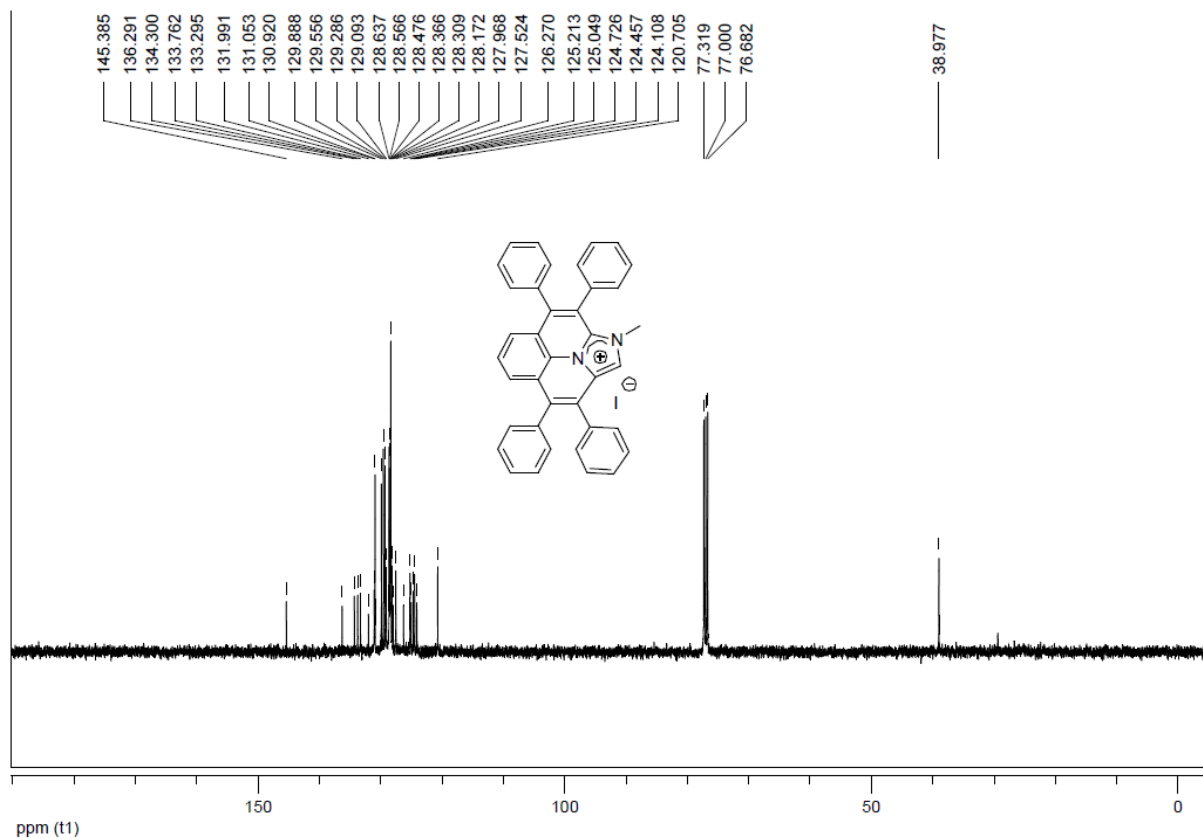
¹³C NMR spectrum of 4ja



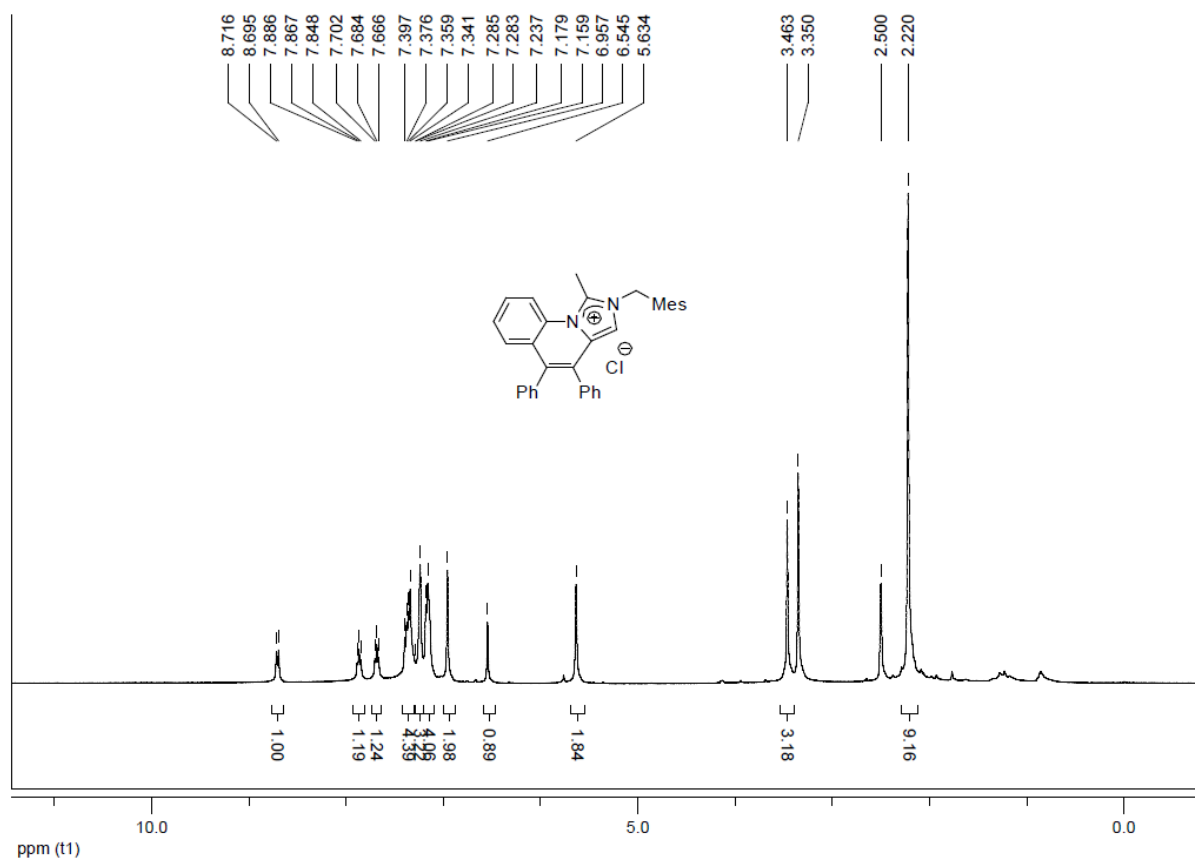
¹H NMR spectrum of 4la



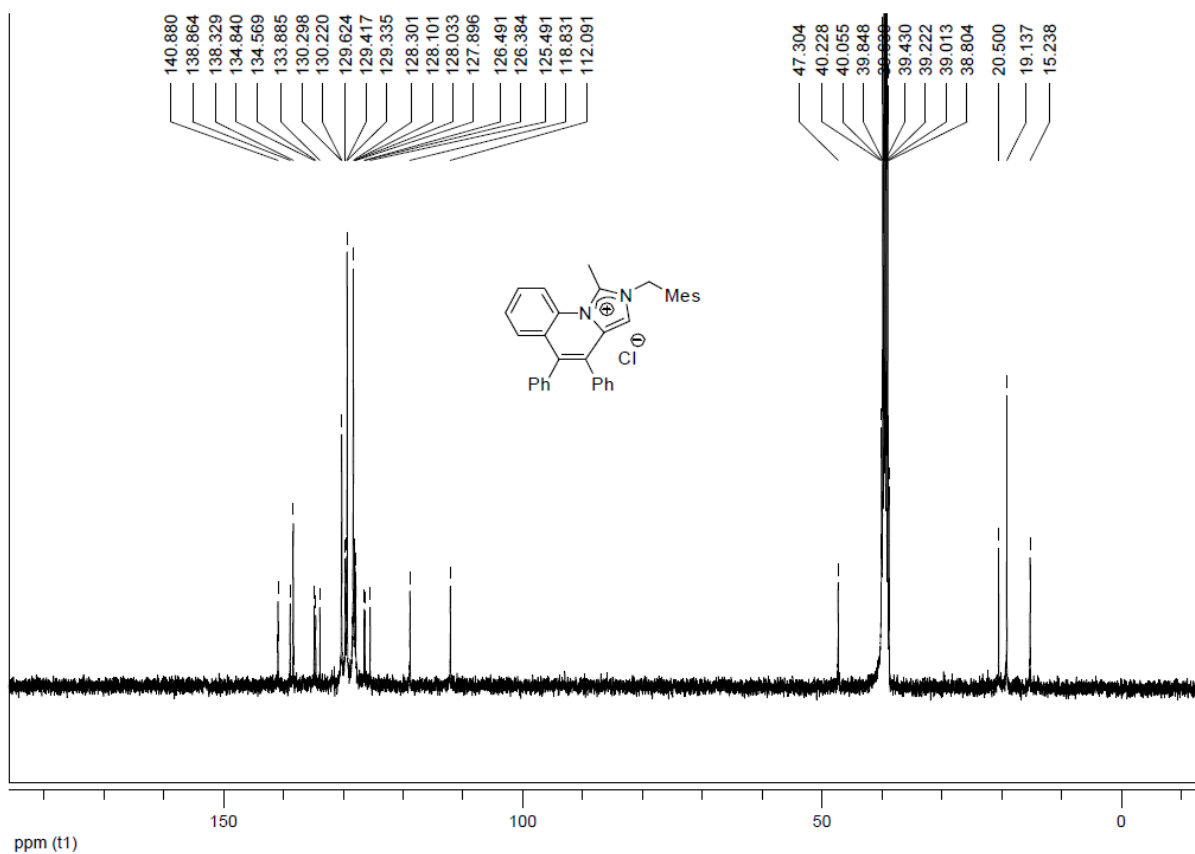
¹³C NMR spectrum of 4la



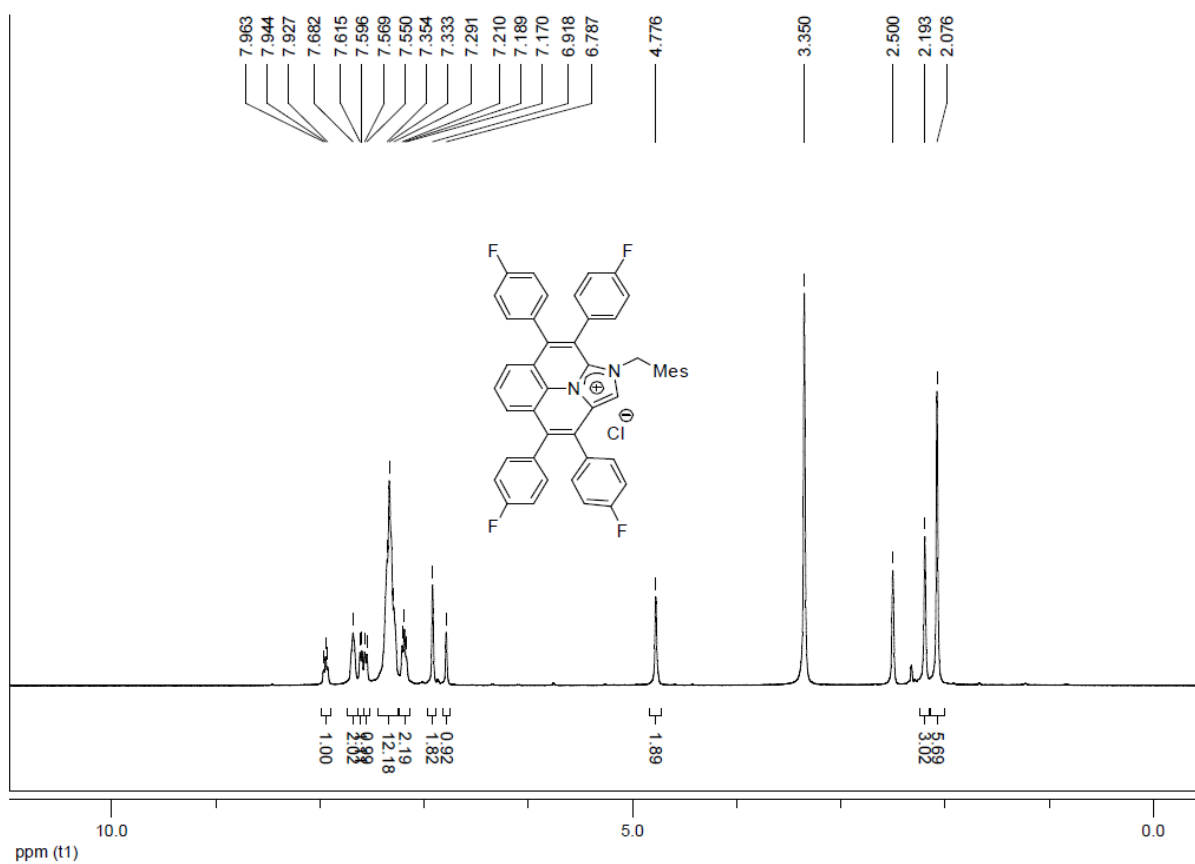
¹H NMR spectrum of 4ma



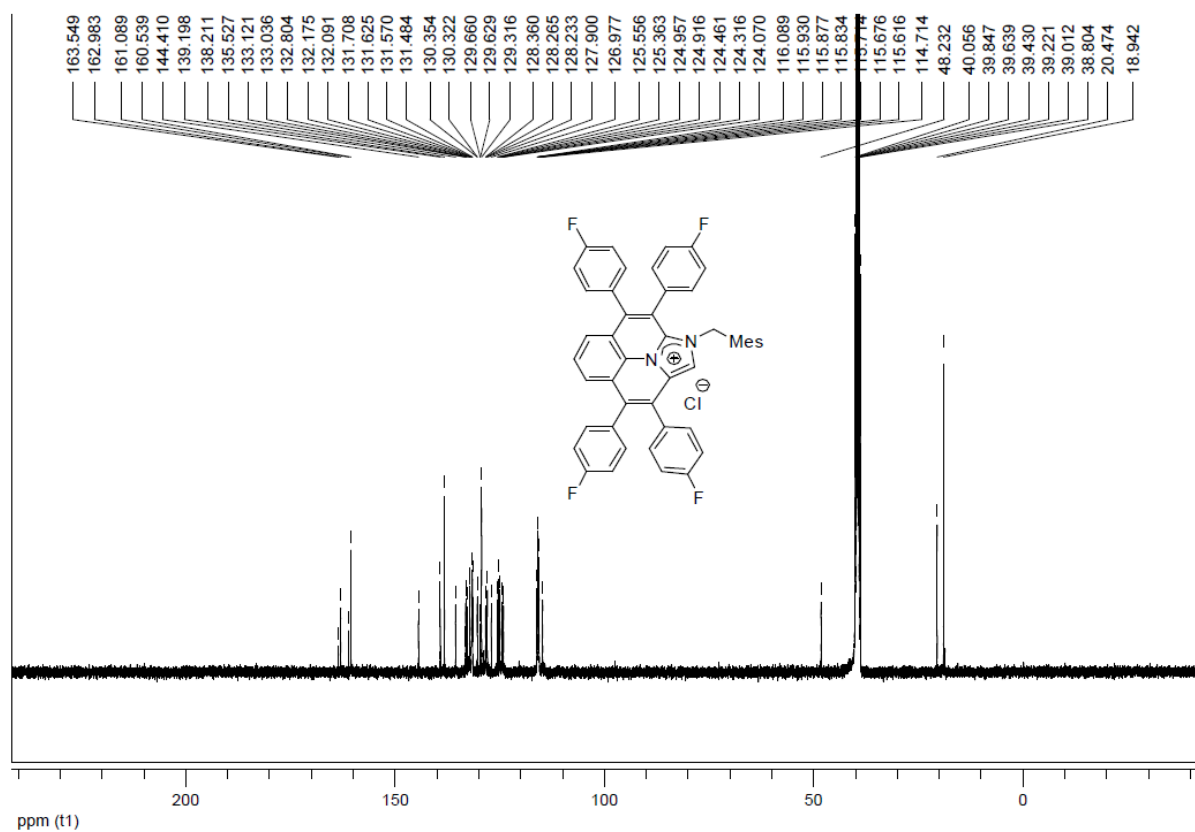
¹³C NMR spectrum of 4ma



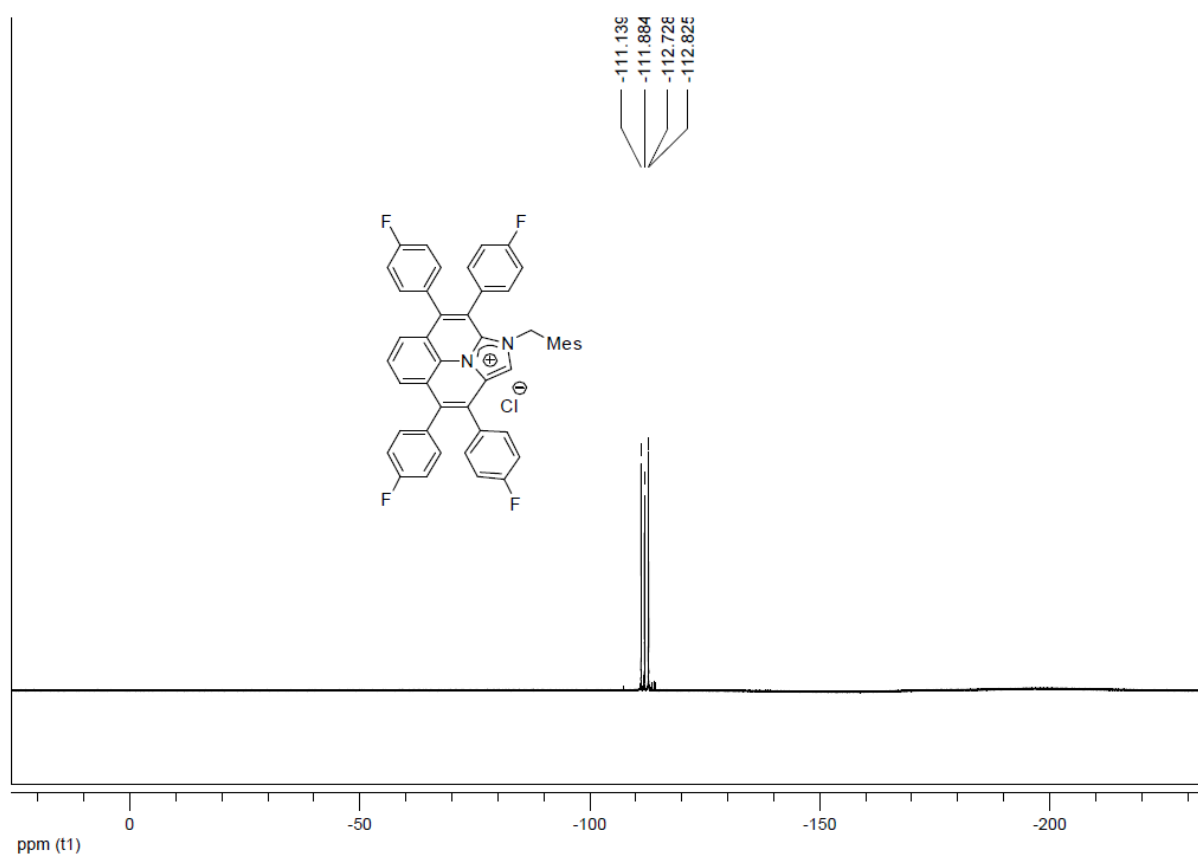
¹H NMR spectrum of 4ab



¹³C NMR spectrum of 4ab



¹⁹F NMR spectrum of 4ab



Chemical Structure of Compound 10:

CN1C(=C2C(=C(C=C2)N1+)C3=CC=C(C=C3)C4=CC=C(C=C4)C5=CC=C(C=C5)C6=CC=C(C=C6)Cl)C7=CC=C(C=C7)Cl

¹H NMR Spectrum (CDCl₃):

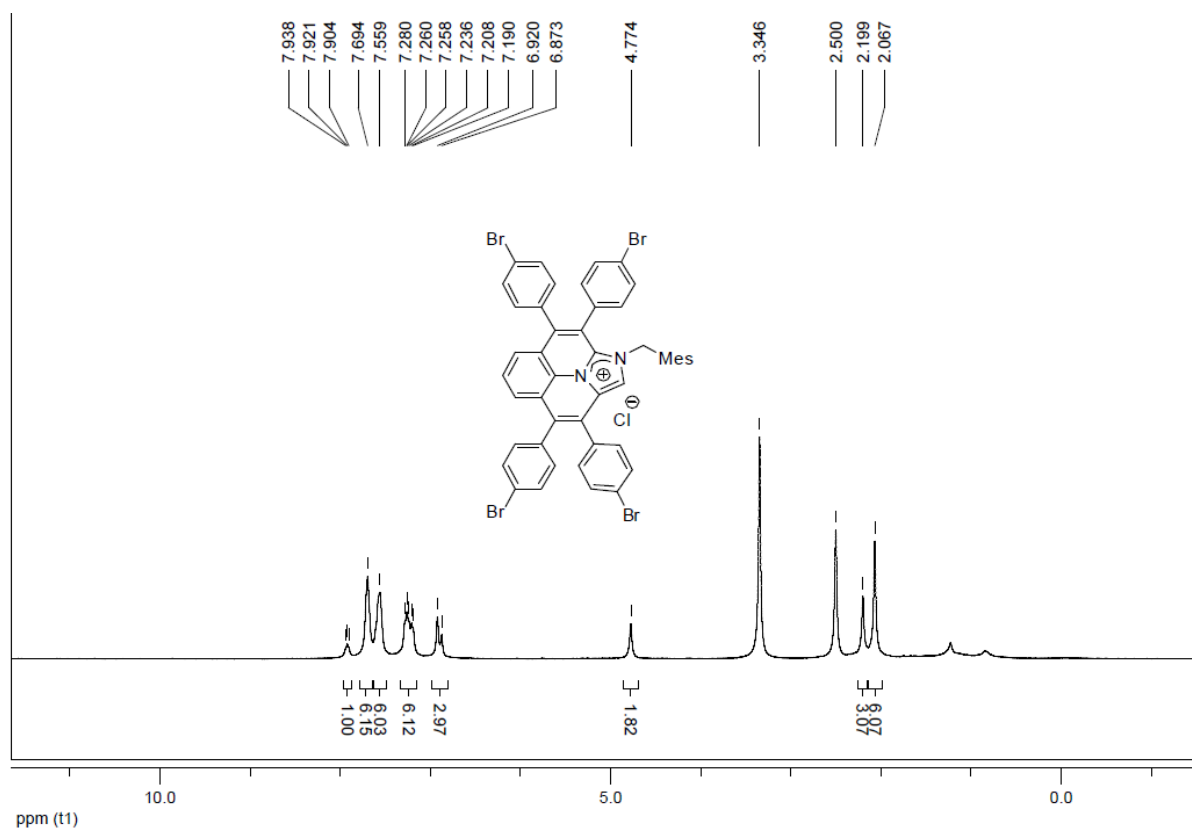
Chemical Shift (ppm)	Integration
7.934, 7.922, 7.905, 7.695, 7.561, 7.282, 7.259, 7.241, 7.209, 7.195, 6.921, 6.874	1.00, 6.11, 6.02, 6.12, 2.80
4.777	1.77
3.340	-
2.500, 2.200, 2.068	5.96, 3.10

Chemical structure of the compound (a chlorinated porphyrin derivative) is shown above the spectrum.

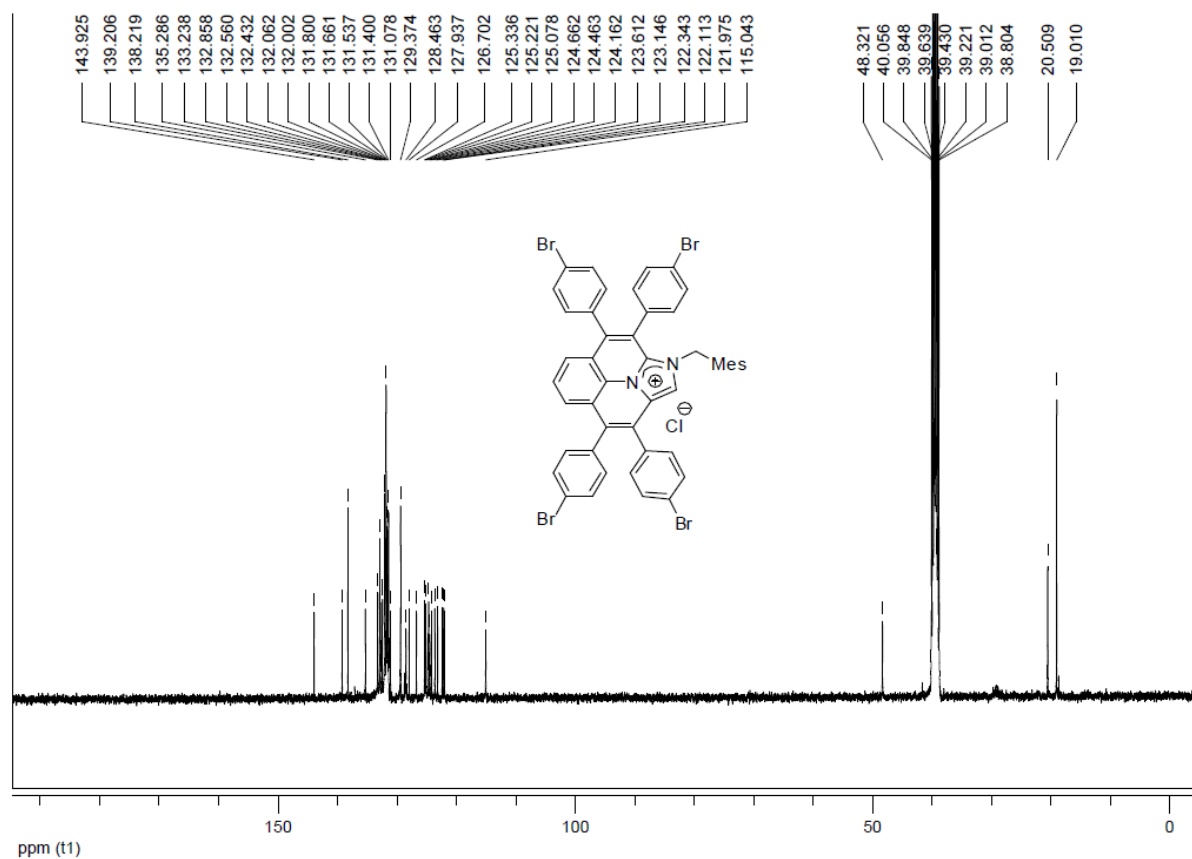
¹³C NMR peaks (ppm):

- 143.984, 139.185, 138.219, 135.327, 134.355, 133.559, 133.380, 133.268, 132.838, 132.644, 132.061, 131.811, 131.301, 131.152, 130.724, 129.345, 129.078, 128.880, 128.731, 128.443, 127.946, 126.746, 125.336, 125.286, 125.039, 124.731, 124.432, 124.230, 123.714, 114.983
- 48.325, 40.056, 39.847, 39.639, 39.430, 39.221, 39.013, 38.804
- 20.492, 19.004

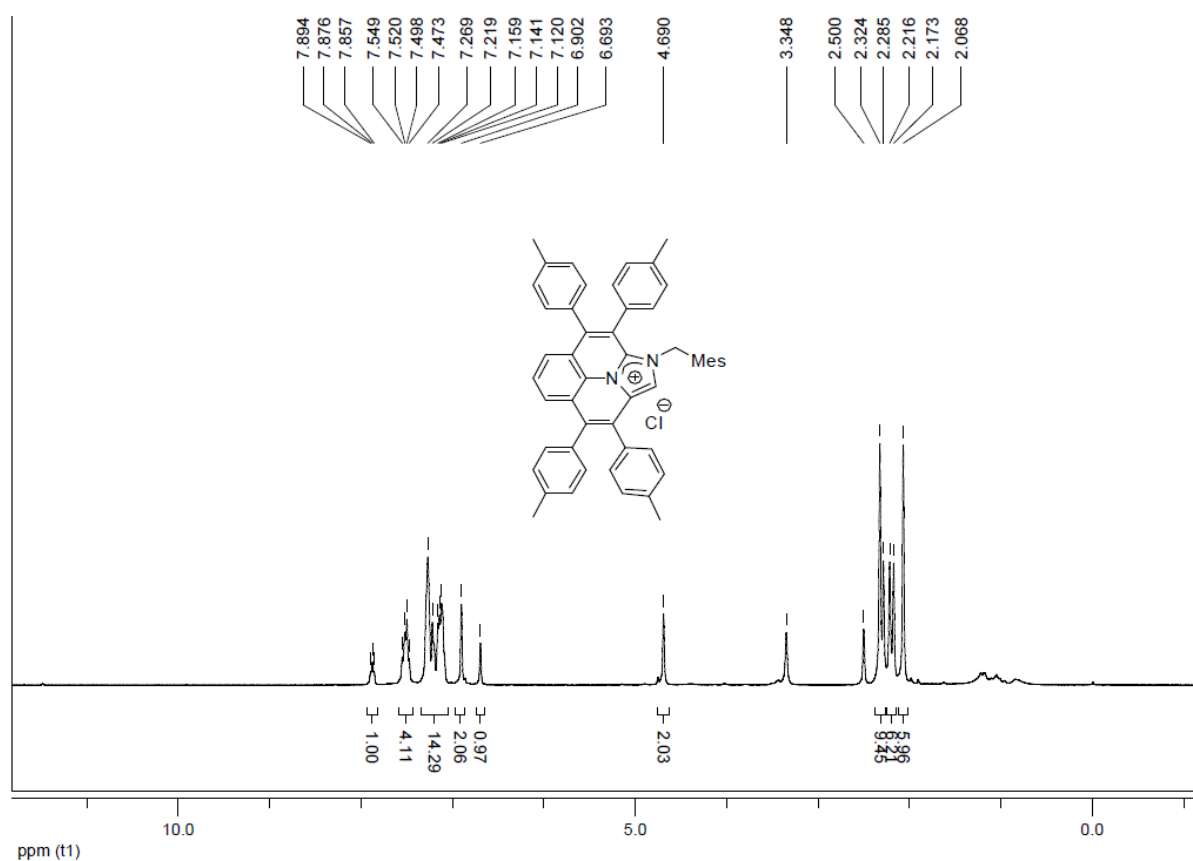
¹H NMR spectrum of 4ad



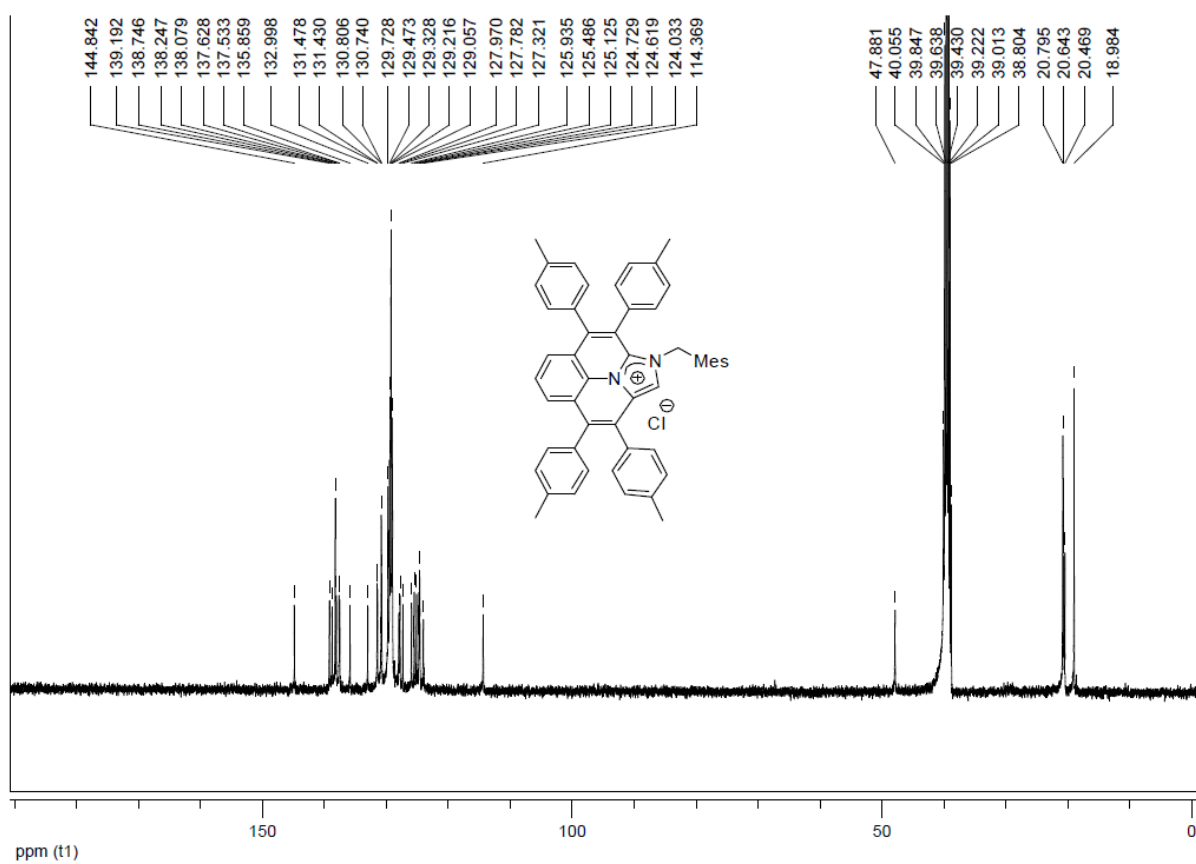
¹³C NMR spectrum of 4ad



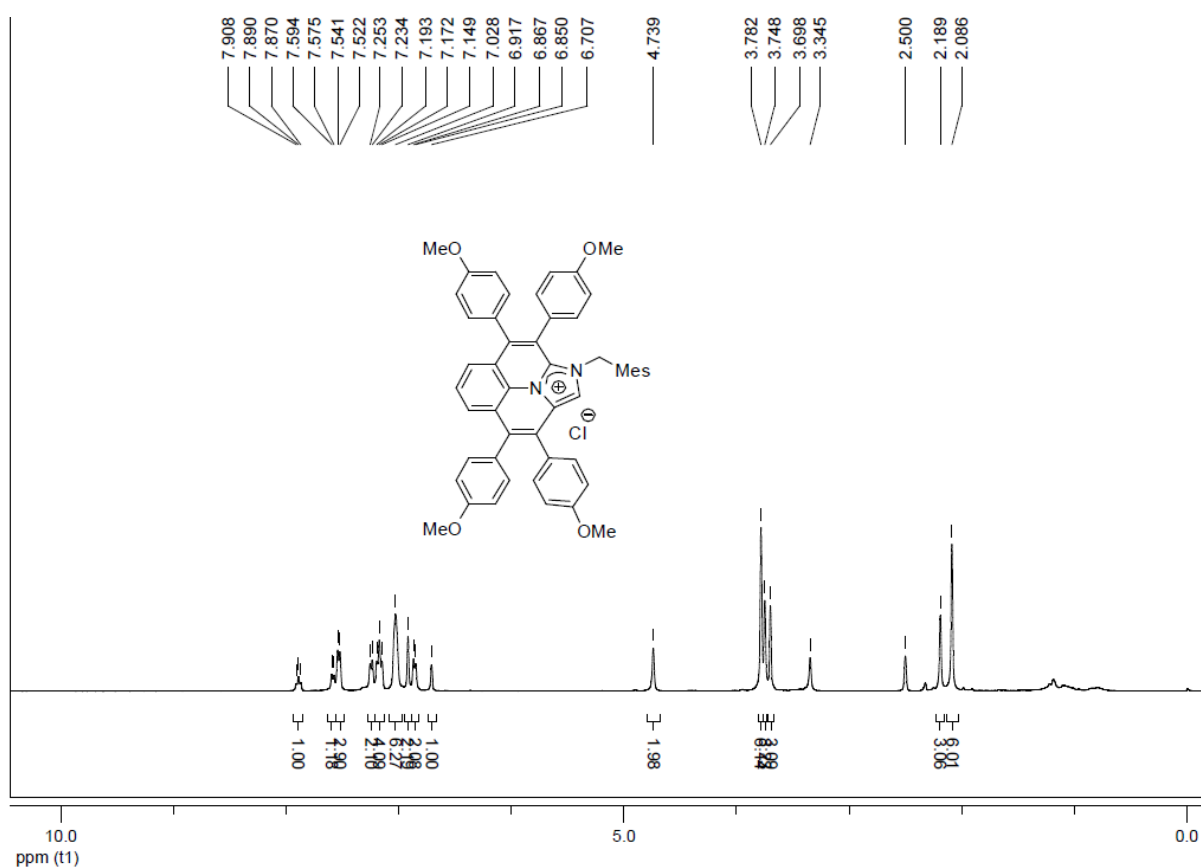
¹H NMR spectrum of 4ae



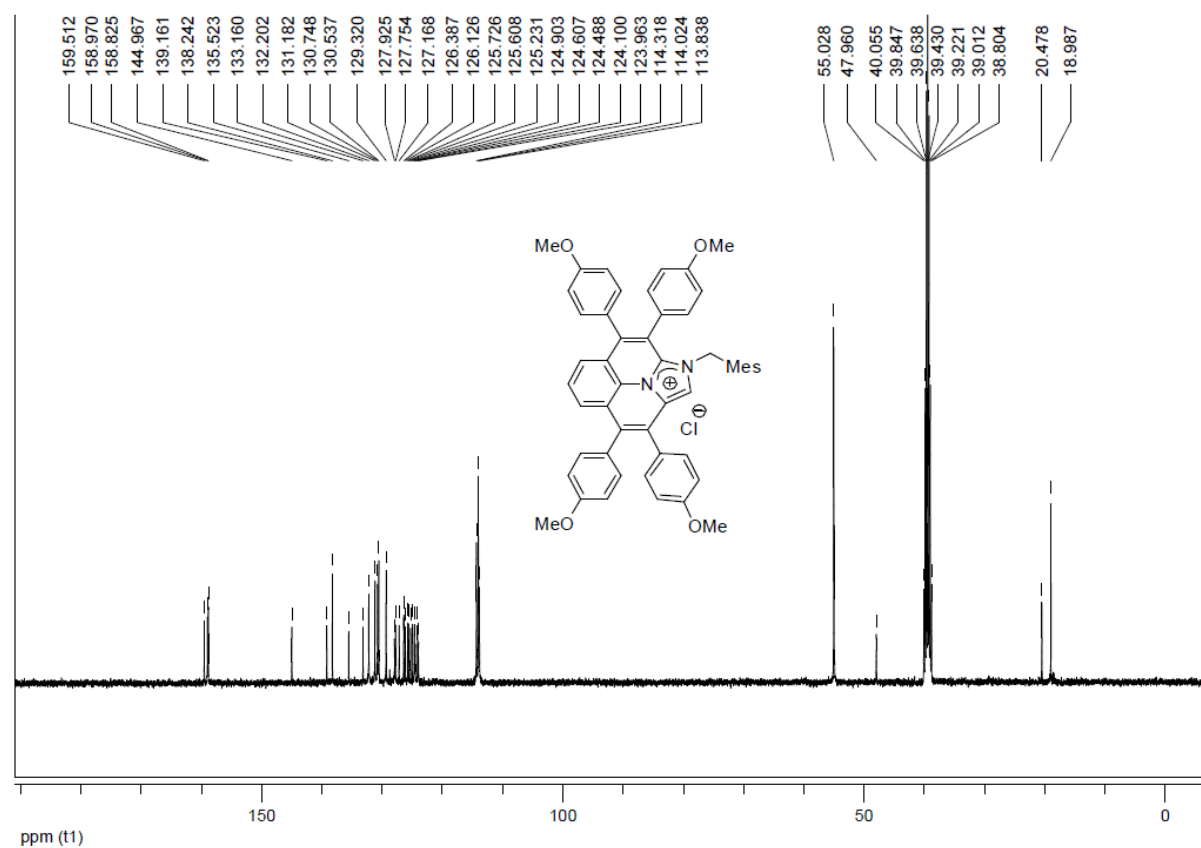
¹³C NMR spectrum of 4ae



¹H NMR spectrum of 4af



¹³C NMR spectrum of 4af



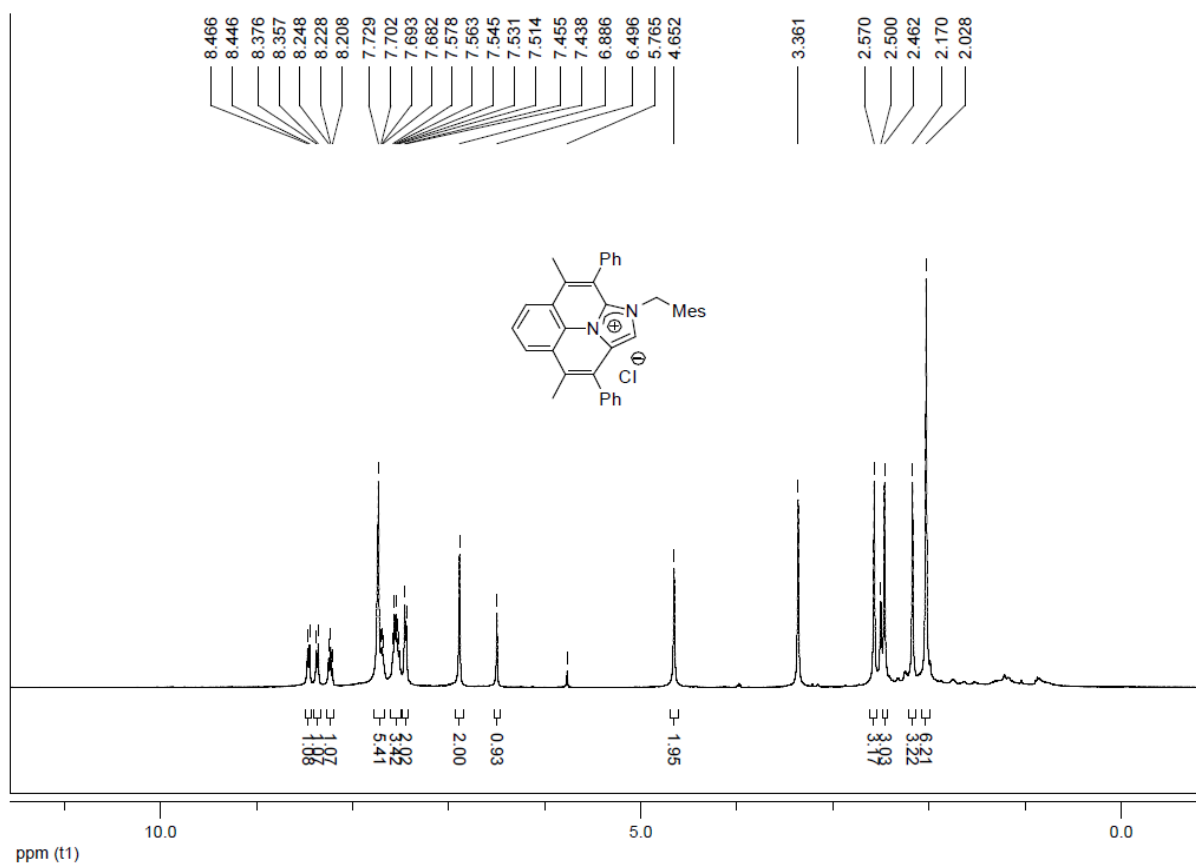
[illegible]

Chemical structure of compound 10: A cationic porphyrin derivative with four phenyl rings, each substituted with an ethyl ester group (EtO₂C), a mesityl group (Mes) on the nitrogen, and a chloride counterion (Cl⁻).

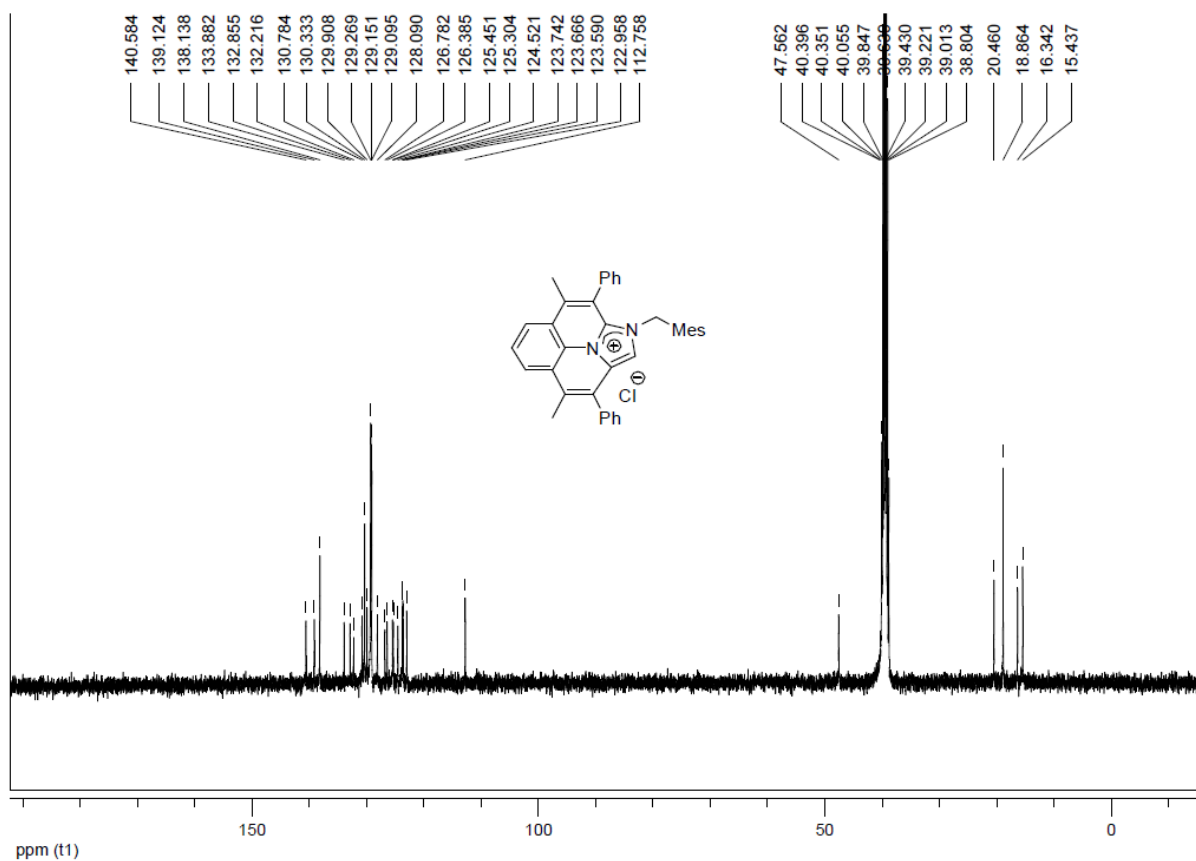
¹³C NMR peaks (ppm): 165.726, 144.551, 139.725, 138.891, 138.623, 138.550, 137.802, 136.593, 135.973, 132.747, 131.642, 131.402, 130.634, 130.565, 130.502, 130.067, 129.759, 129.617, 128.818, 127.728, 127.428, 125.891, 125.346, 125.260, 125.019, 124.731, 124.442, 116.188, 77.317, 77.000, 76.680, 61.239, 61.151, 49.510.

¹H NMR peaks (ppm): 8.874, 8.842, 8.135, 8.074, 7.942, 7.135, 7.074, 6.942, 6.135, 6.074, 5.942, 4.9510, 4.874, 4.842, 4.135, 4.074, 3.942, 2.500, 2.474, 2.442, 2.135, 2.074, 1.942, 1.4135, 1.3874, 1.3613.

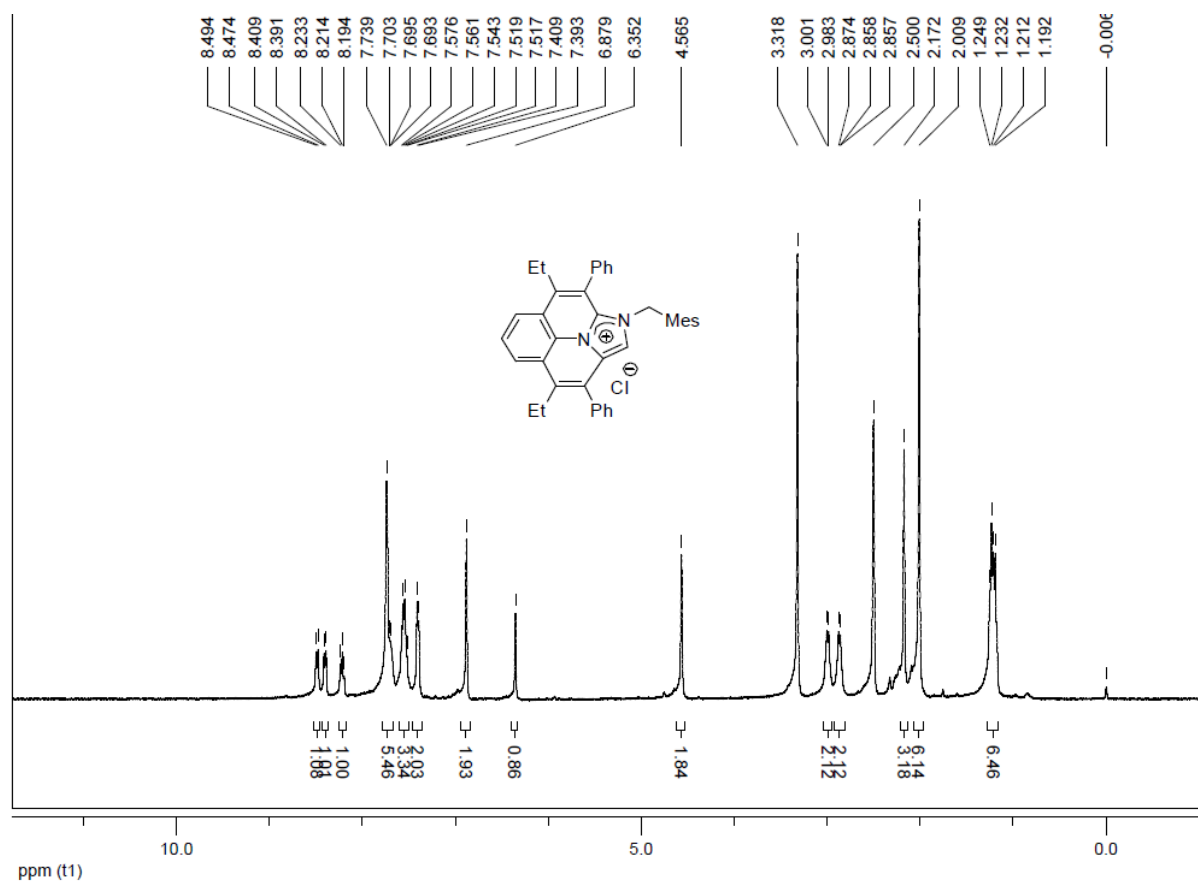
¹H NMR spectrum of 4ai



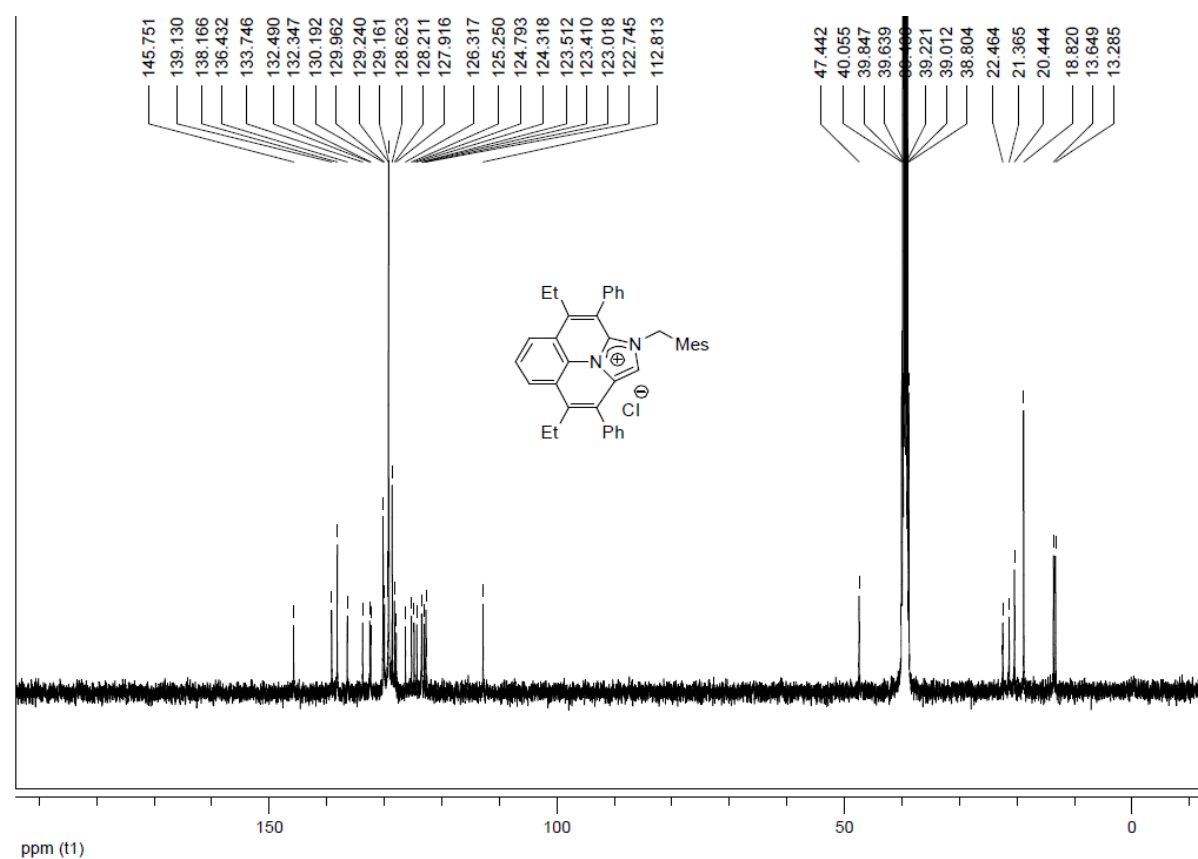
¹³C NMR spectrum of 4ai



¹H NMR spectrum of 4aj



^{13}C NMR spectrum of 4aj



Chemical structure of compound 10 is shown above the spectrum. The structure is a complex polycyclic aromatic cation with a central nitrogen atom bearing a positive charge and a methyl group (Mes). The structure includes several phenyl rings and a chlorine atom (Cl) attached to the central nitrogen atom.

¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm (t1), ranging from 0.0 to 10.0. The spectrum shows several peaks corresponding to the protons in the molecule.

Peak assignments (ppm):

- 7.752, 7.733, 7.672, 7.653, 7.632, 7.612, 7.536, 7.518, 7.390, 7.371, 7.353, 7.333, 7.318, 7.302, 7.281, 7.260, 7.159, 7.141, 7.116, 7.098, 7.074, 7.056, 7.001, 6.982, 6.933, 6.821, 5.030
- 2.346, 2.253, 2.208, 2.144

Integration values (from left to right):

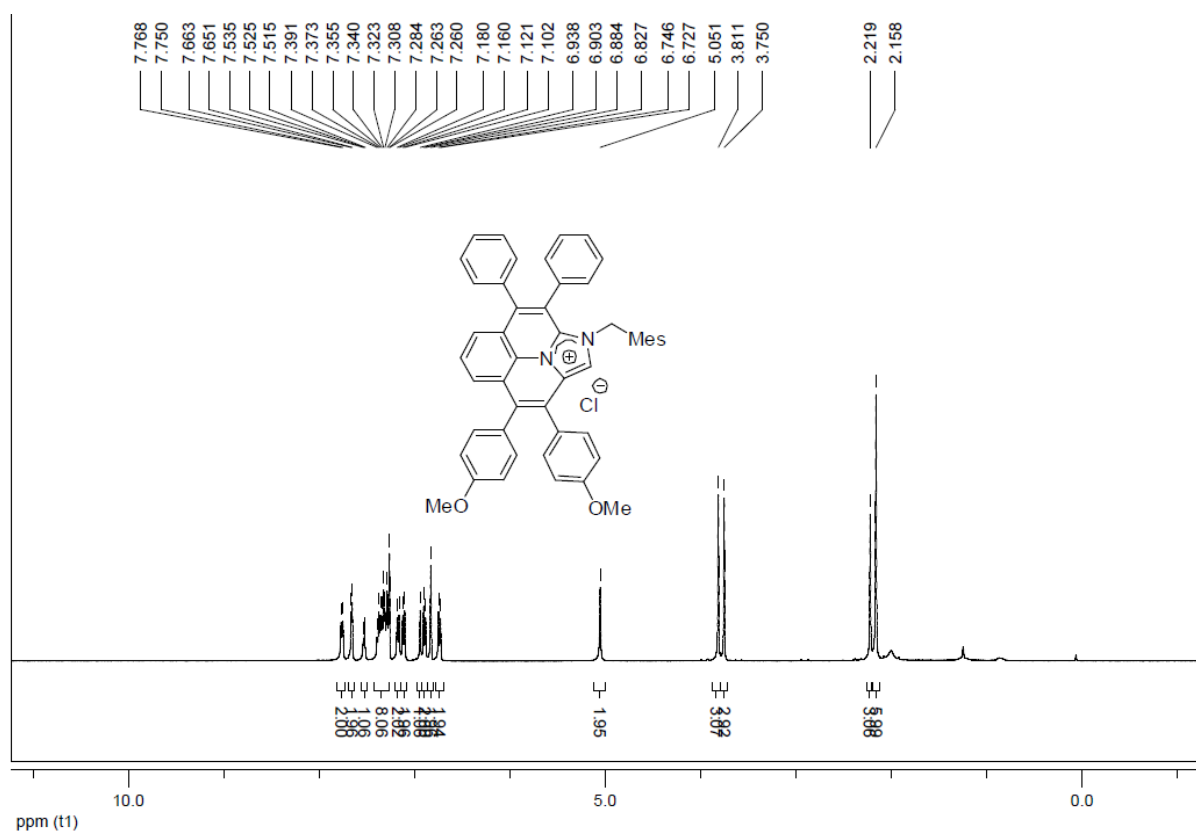
- 3.09, 3.09, 2.16, 8.13, 6.48, 3.09, 2.00, 3.09, 3.09, 3.09

Chemical structure of compound 10 is shown above the spectrum. The structure is a macrocyclic ligand with a central nickel(II) ion coordinated by two nitrogen atoms and two oxygen atoms. The ligand has four phenyl groups and a methyl group. The nickel ion is coordinated by a chloride ion. The chemical structure is shown with a positive charge on the nickel atom and a negative charge on the chloride ion.

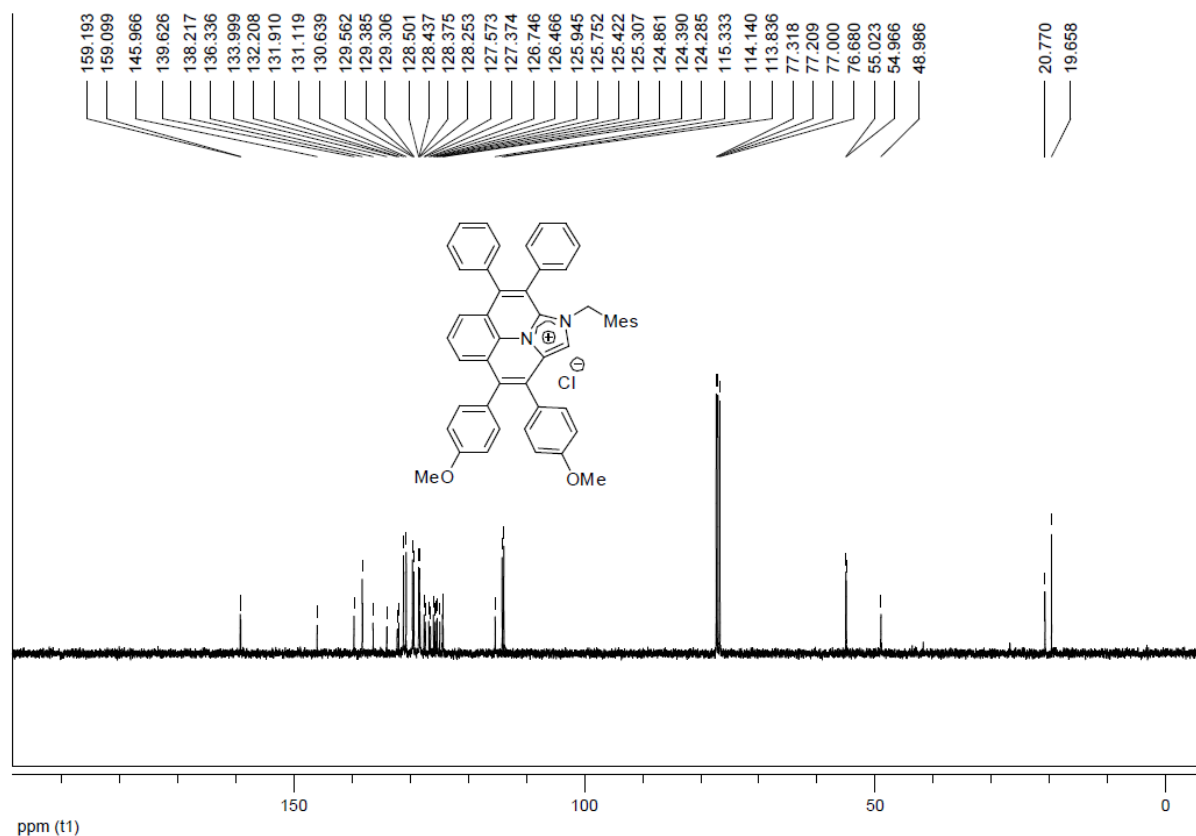
1H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm (t1), ranging from 0 to 10. The spectrum shows several peaks, with the following chemical shifts (ppm) labeled above the peaks:

- 146.035
- 139.642
- 138.299
- 137.885
- 136.774
- 134.034
- 132.290
- 131.943
- 131.392
- 131.138
- 130.590
- 129.712
- 129.570
- 129.426
- 129.378
- 129.191
- 129.108
- 128.538
- 128.413
- 128.291
- 127.596
- 126.656
- 125.863
- 125.458
- 124.894
- 124.500
- 124.368
- 115.419
- 77.318
- 77.209
- 77.000
- 76.882
- 49.052
- 21.125
- 21.058
- 20.791
- 19.693

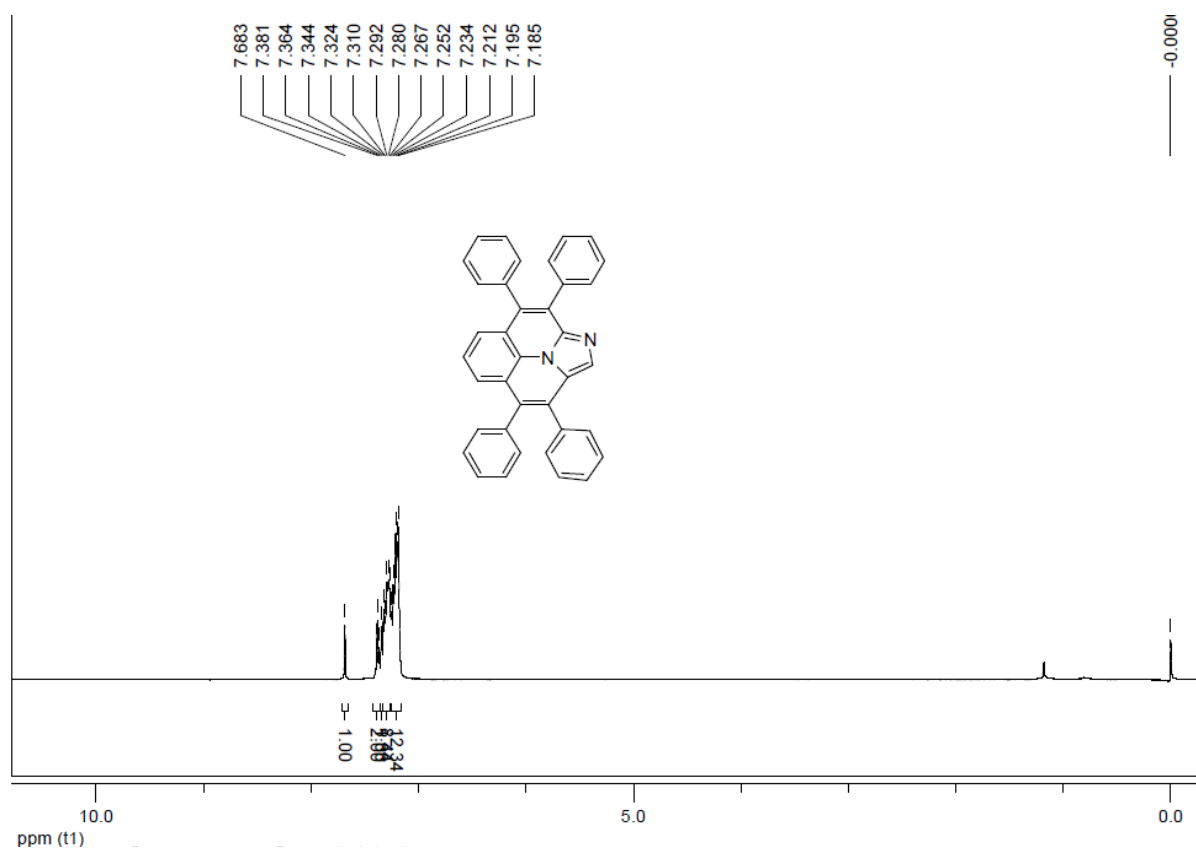
¹H NMR spectrum of 4af'



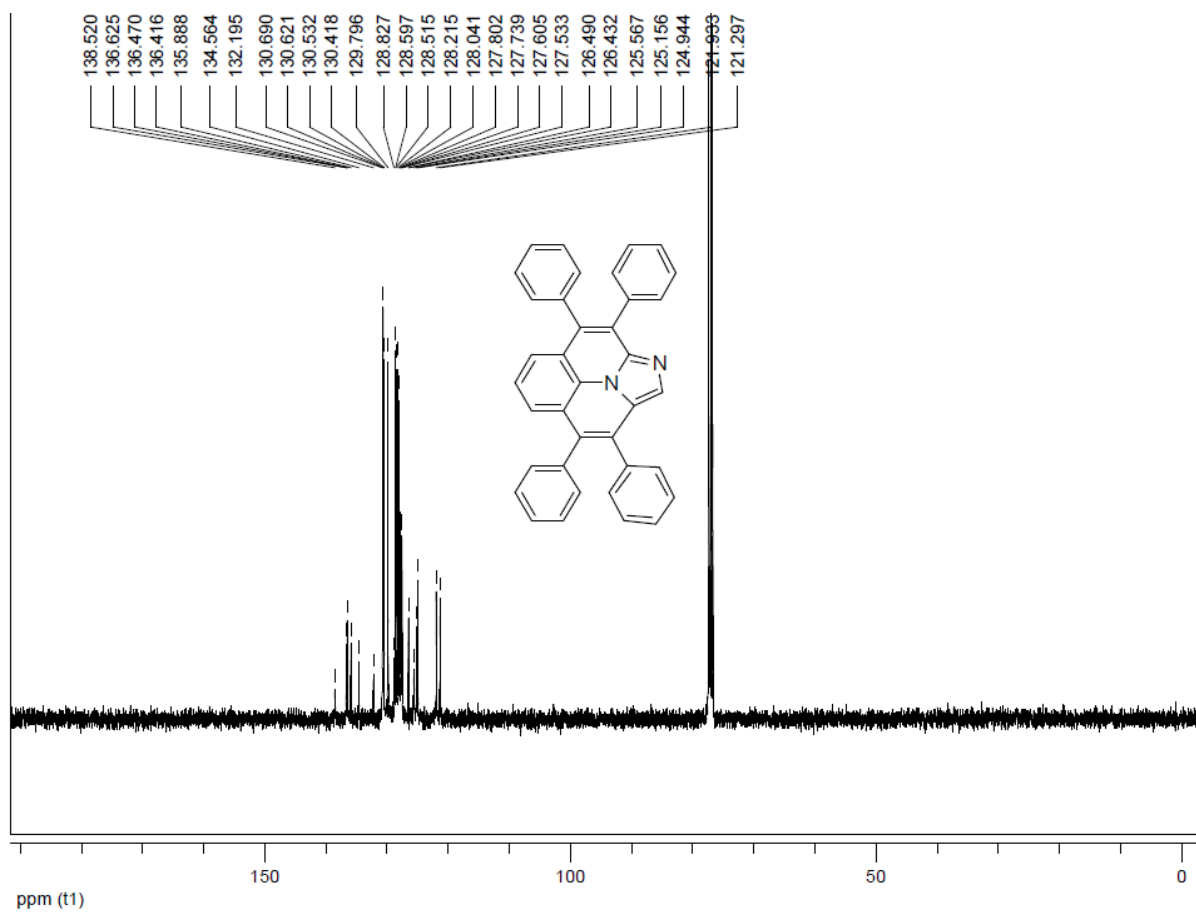
^{13}C NMR spectrum of 4af'



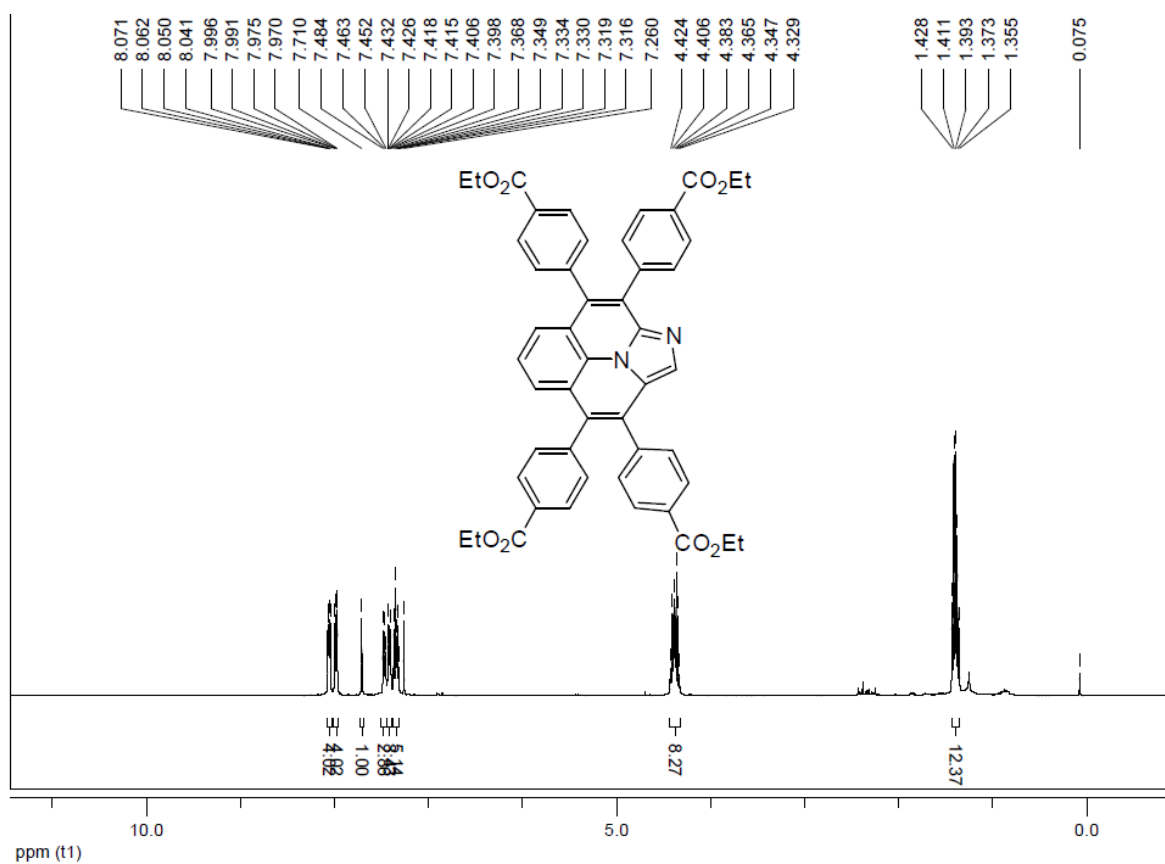
¹H NMR spectrum of 5aa



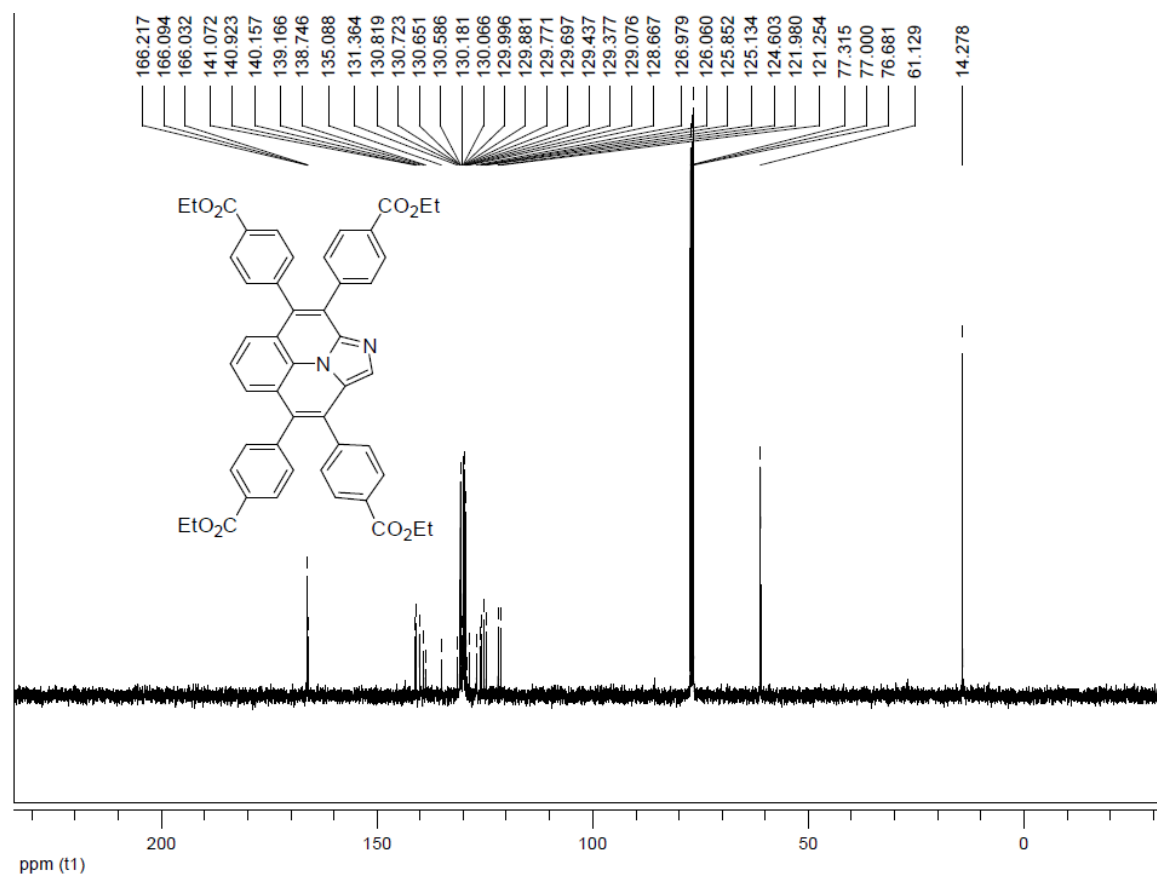
^{13}C NMR spectrum of 5aa



¹H NMR spectrum of 5ag



¹³C NMR spectrum of 5ag



Chemical structure: Cc1c(C)c2ccccc2n1-c3ccccc3

¹H NMR spectrum (CDCl₃) data:

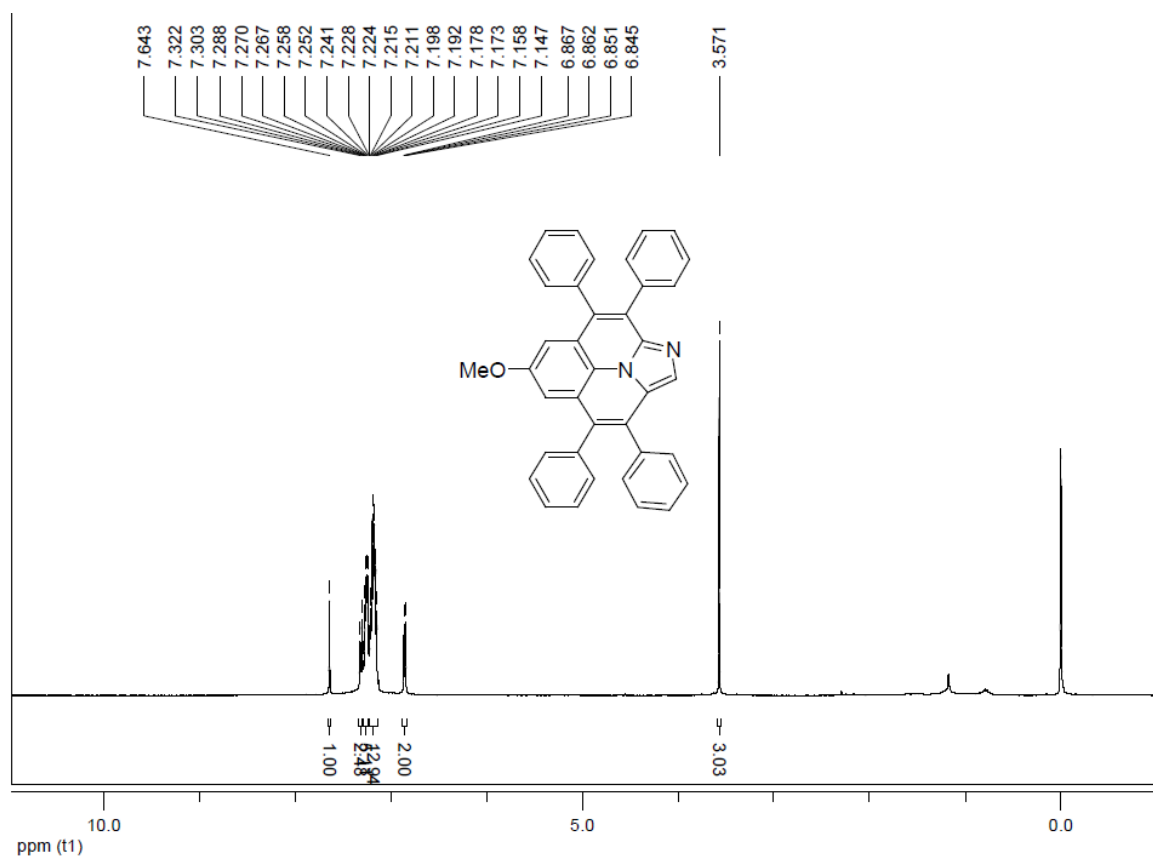
Chemical Shift (ppm)	Integration
7.869, 7.858, 7.847, 7.767, 7.756, 7.570, 7.561, 7.558, 7.548, 7.530, 7.524, 7.512, 7.508, 7.505, 7.501, 7.498, 7.491, 7.484, 7.476, 7.467, 7.462, 7.260	1.00, 1.00
2.536, 2.408	3.01, 2.97

Chemical structure: Cc1c(C2=CC=CC=C2)c3cc(C4=CC=CC=C4)nc5ccccc135

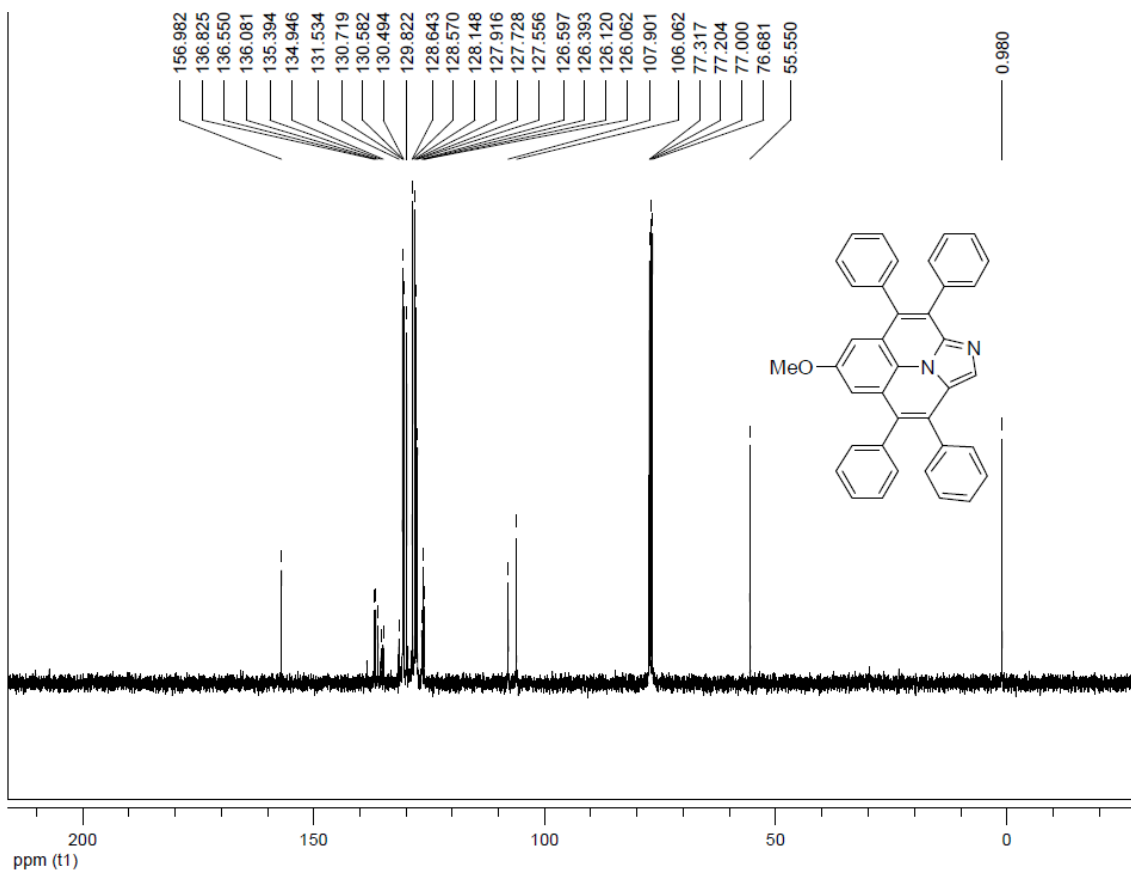
¹³C NMR peaks (ppm):

- 138.494
- 136.574
- 135.535
- 130.317
- 129.618
- 129.425
- 129.119
- 128.811
- 128.635
- 128.512
- 128.119
- 128.055
- 126.102
- 125.988
- 125.165
- 124.899
- 124.767
- 119.429
- 118.733
- 77.317
- 77.204
- 77.000
- 76.683
- 16.155
- 15.486

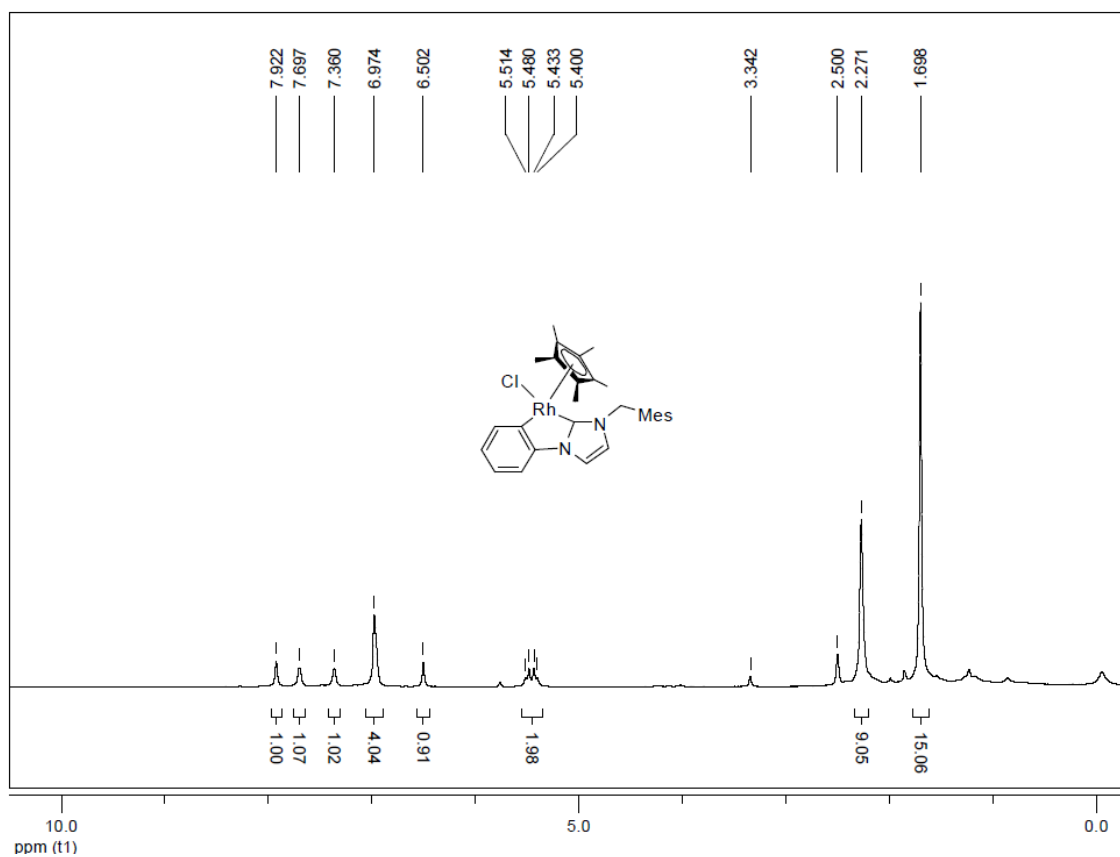
¹H NMR spectrum of 5fa



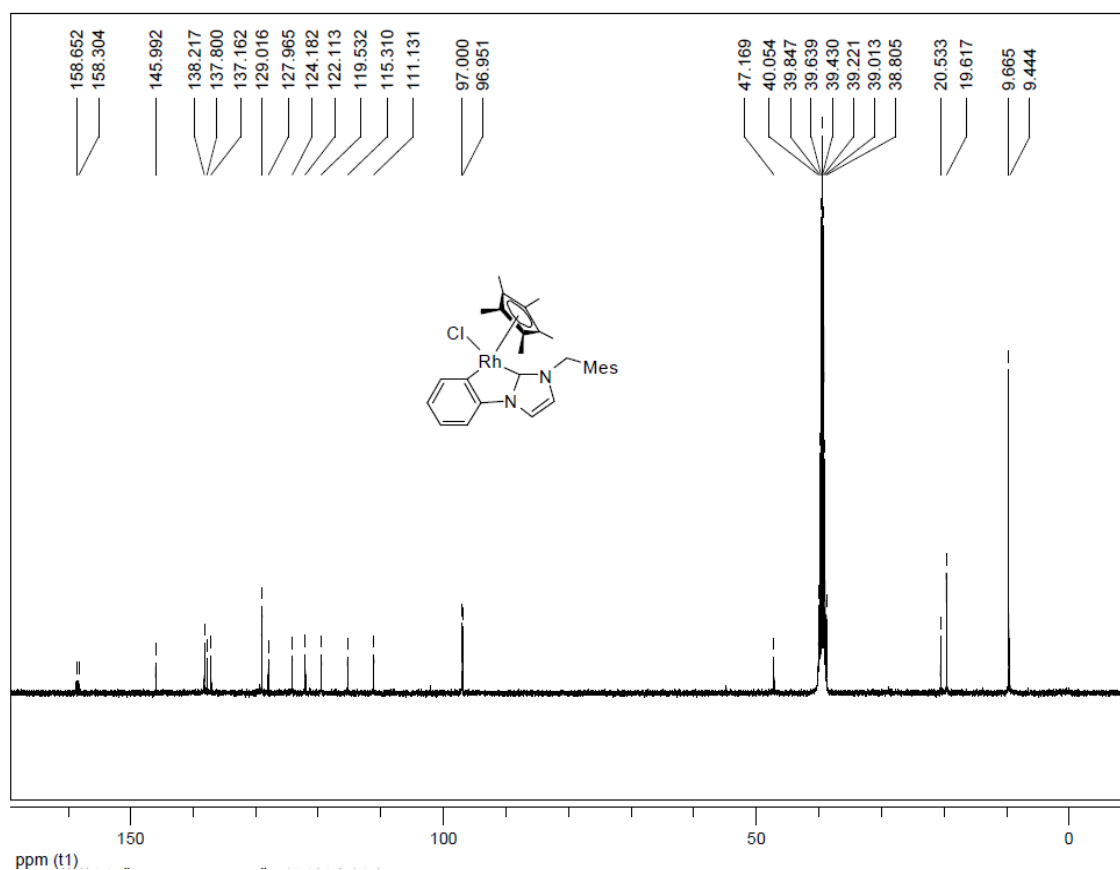
¹³C NMR spectrum of 5fa



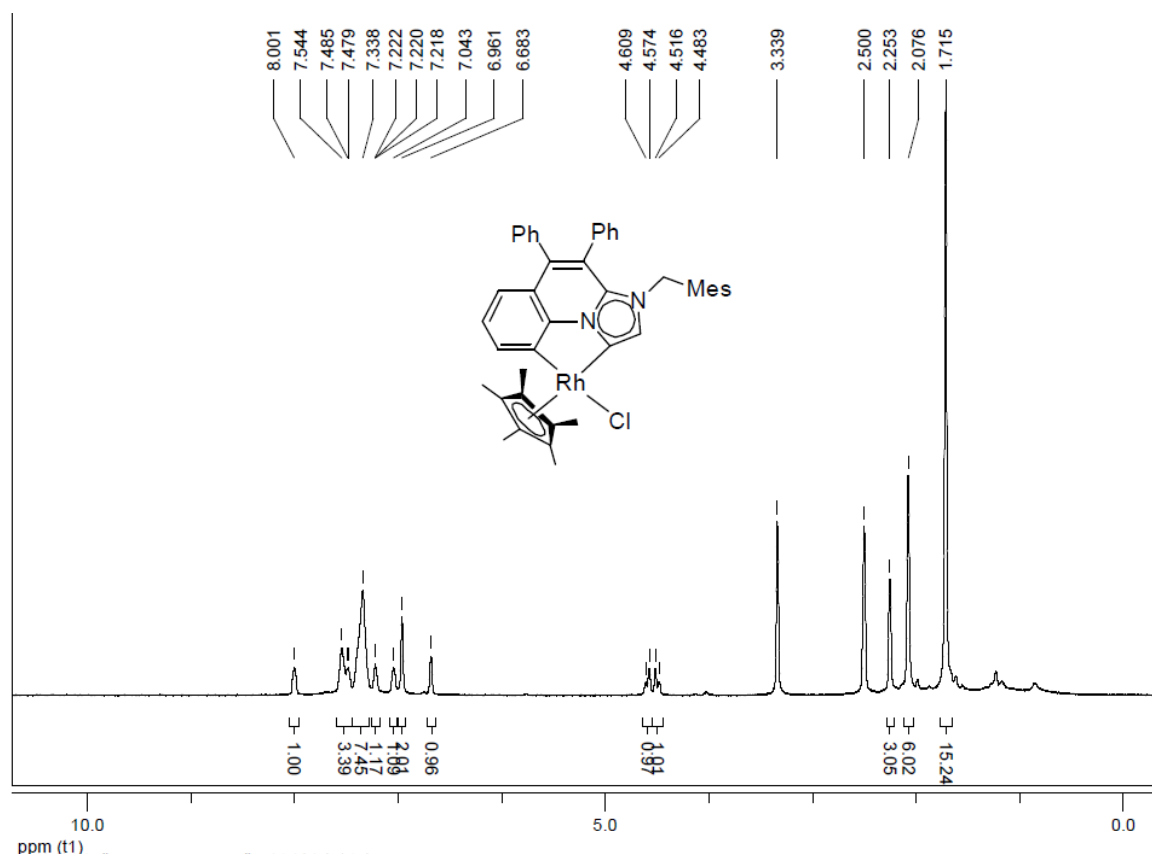
¹H NMR spectrum of intermediate A



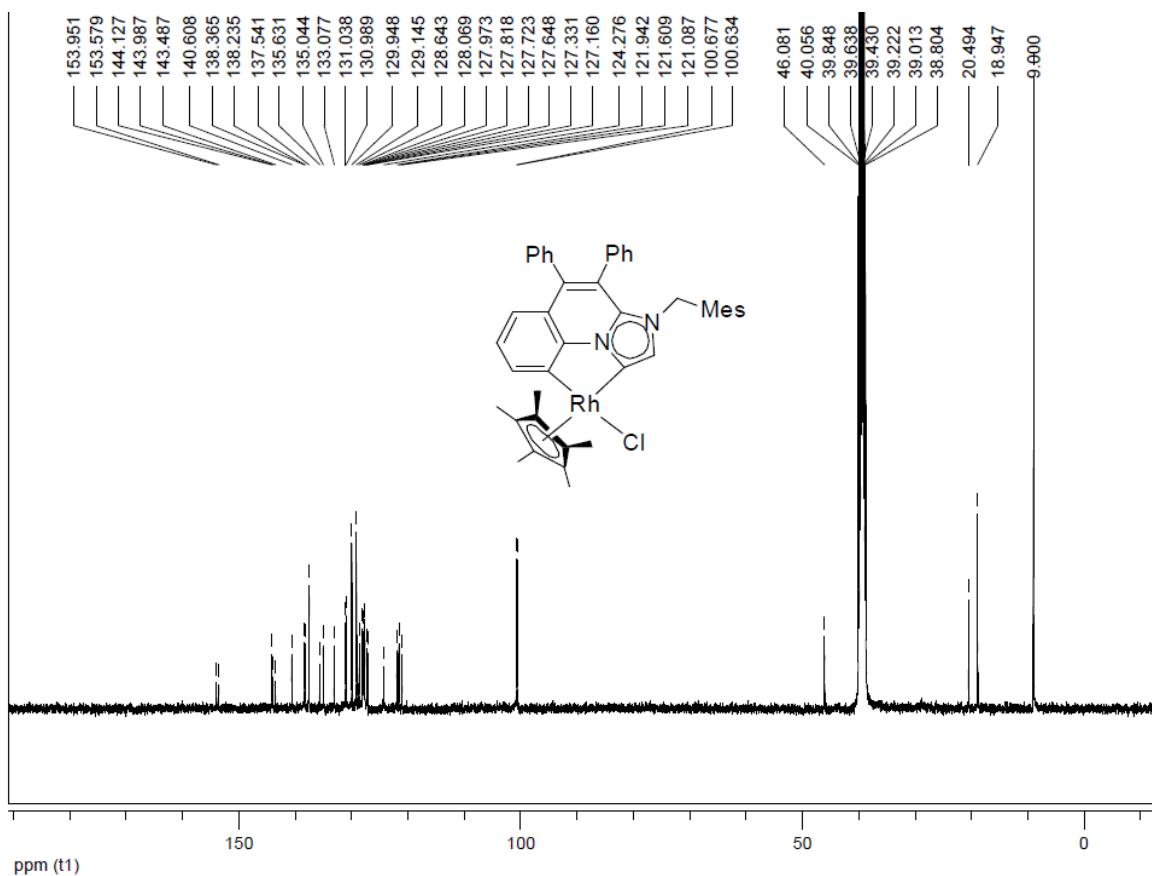
¹³C NMR spectrum of intermediate A



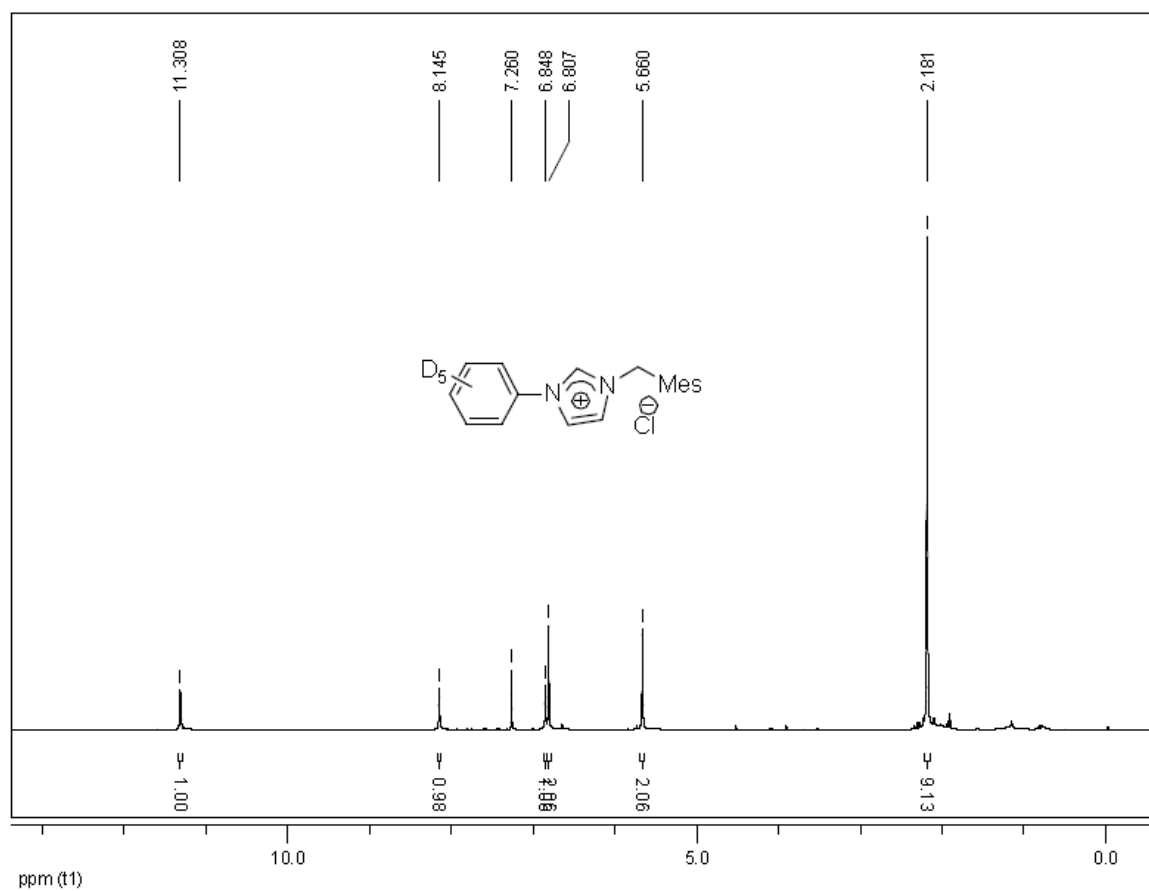
¹H NMR spectrum of intermediate B



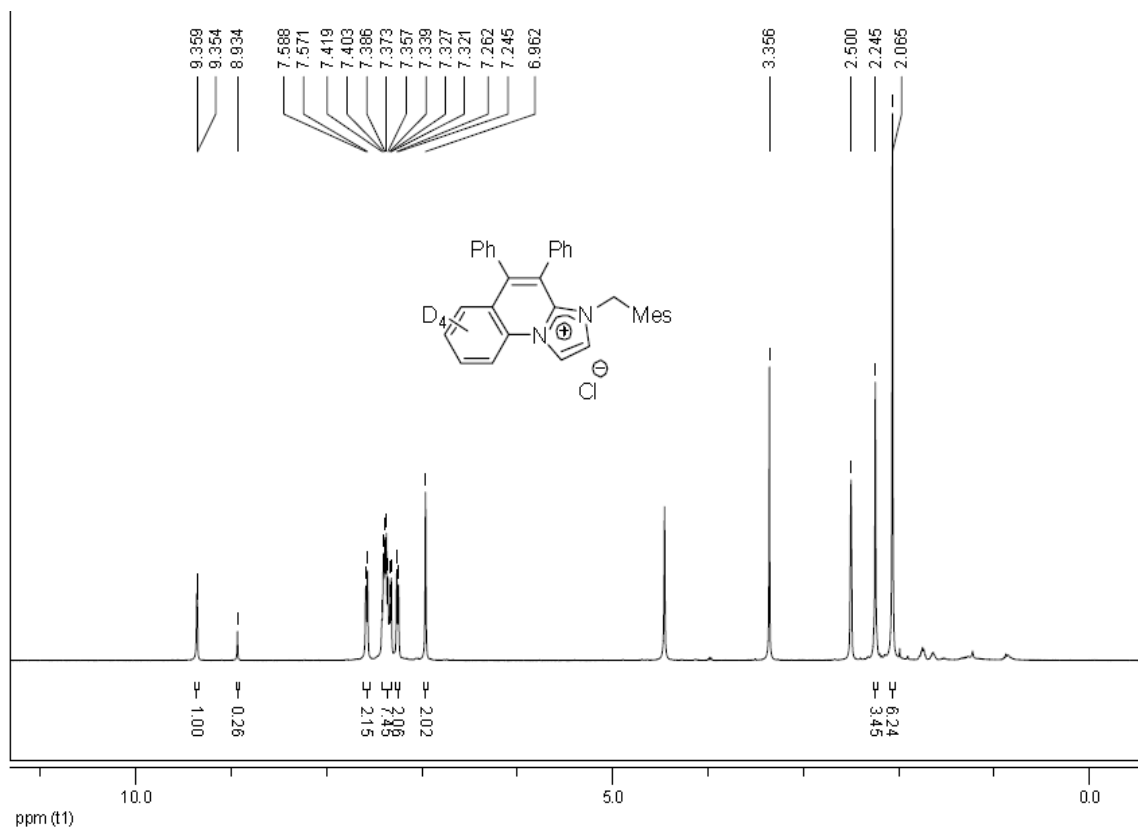
¹³C NMR spectrum of intermediate B



¹H NMR spectrum of 1a-d₅



¹H NMR spectrum of 3aa-d₄



KIE experiments.

