

# Rhodium-Catalyzed Synthesis of Isoquinolines and Indenes from Benzyldenehydrazines and Internal Alkynes

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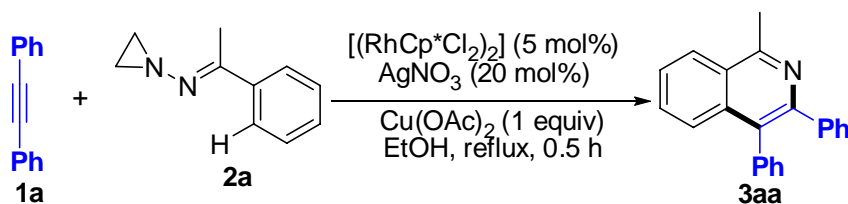
## Supporting Information

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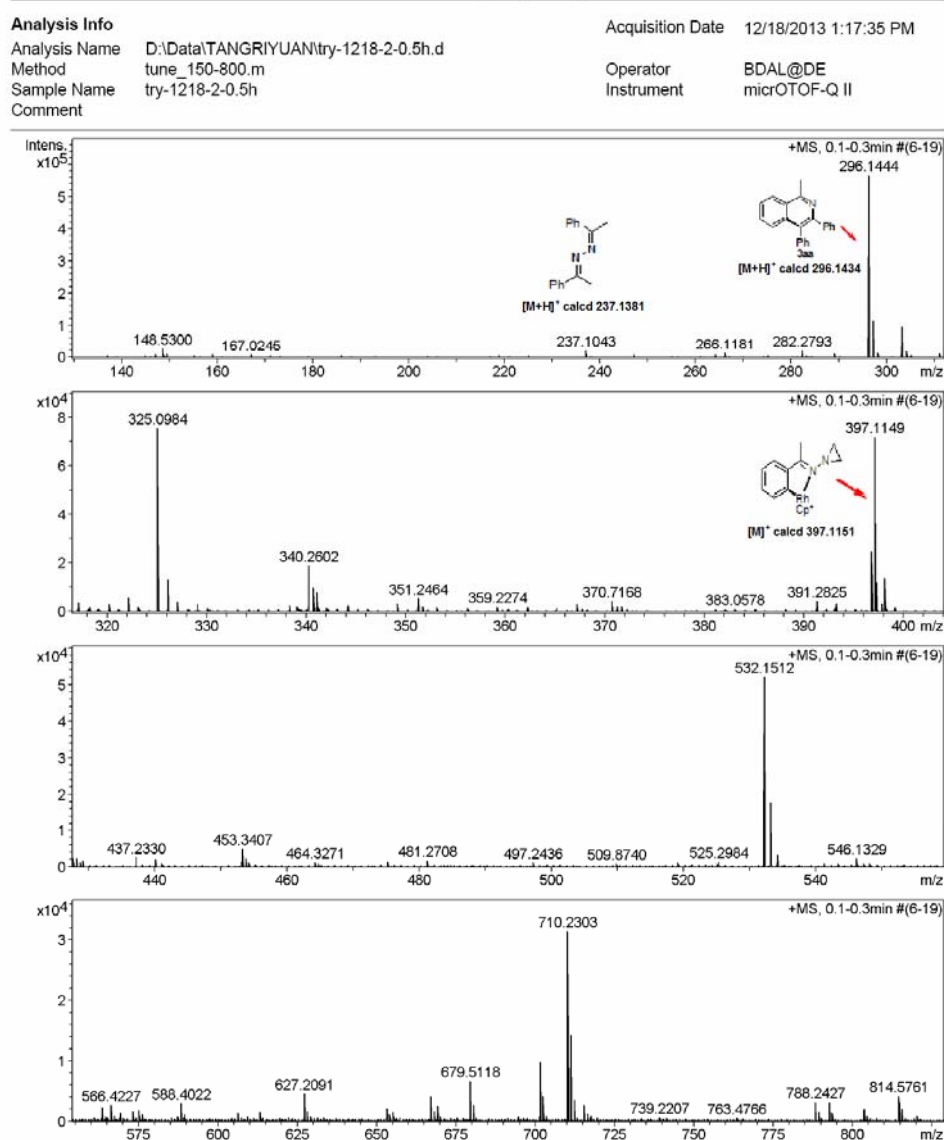
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## (A) Control Experiments

### (a) Figure S1 The Reaction Determined in-situ by HRMS Analysis

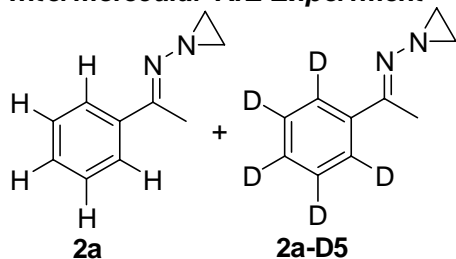


#### Generic Display Report

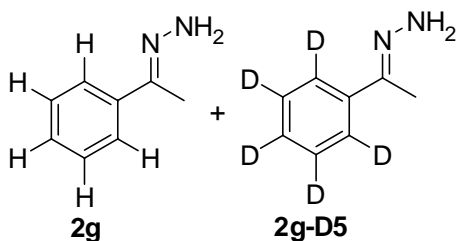


## (b) The Kinetic Isotope Effect Experiments

### Intermolecular KIE Experiment



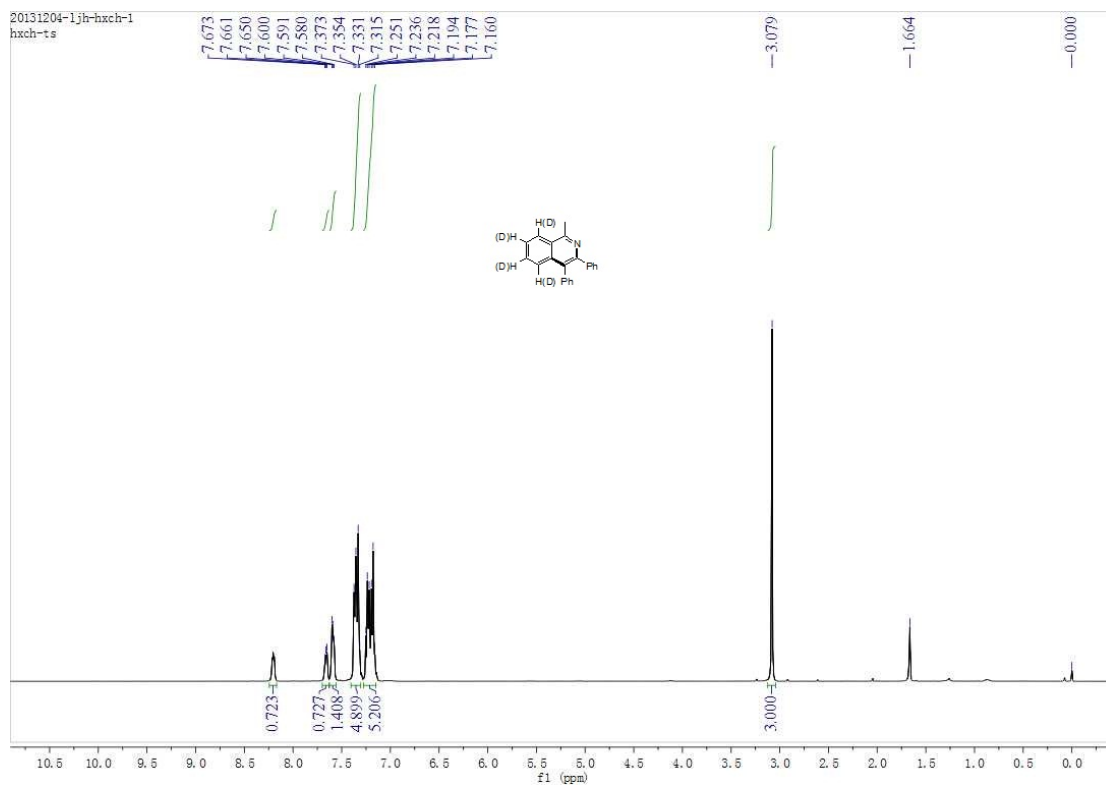
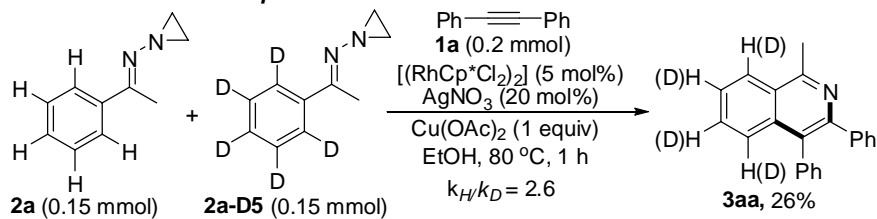
26% yield (1 h),  $k_H/k_D = 2.6$

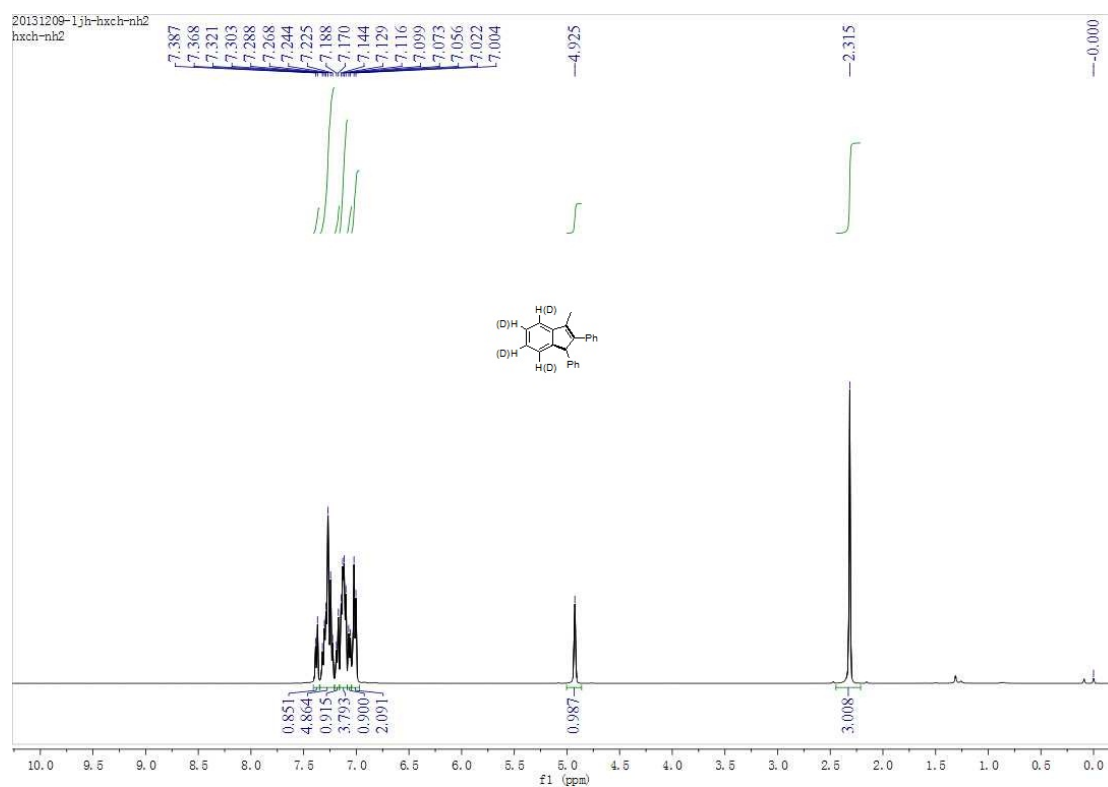
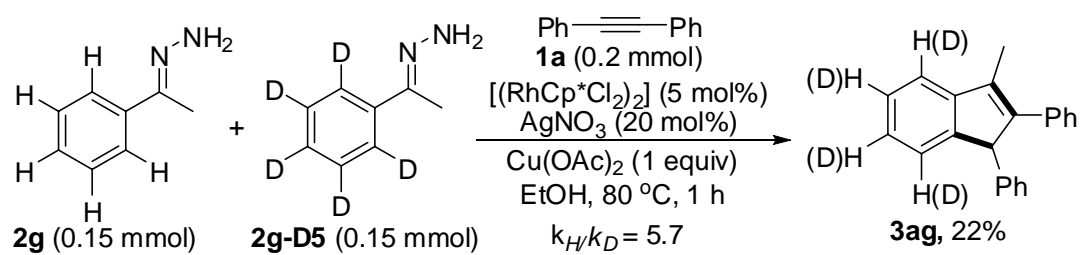


22% yield (1 h),  $k_H/k_D = 5.7$

The intermolecular kinetic isotope effect experiments imply that the C(sp<sup>2</sup>)-H cleavage is not compatible with the SEAr mechanism and the free radical mechanism.

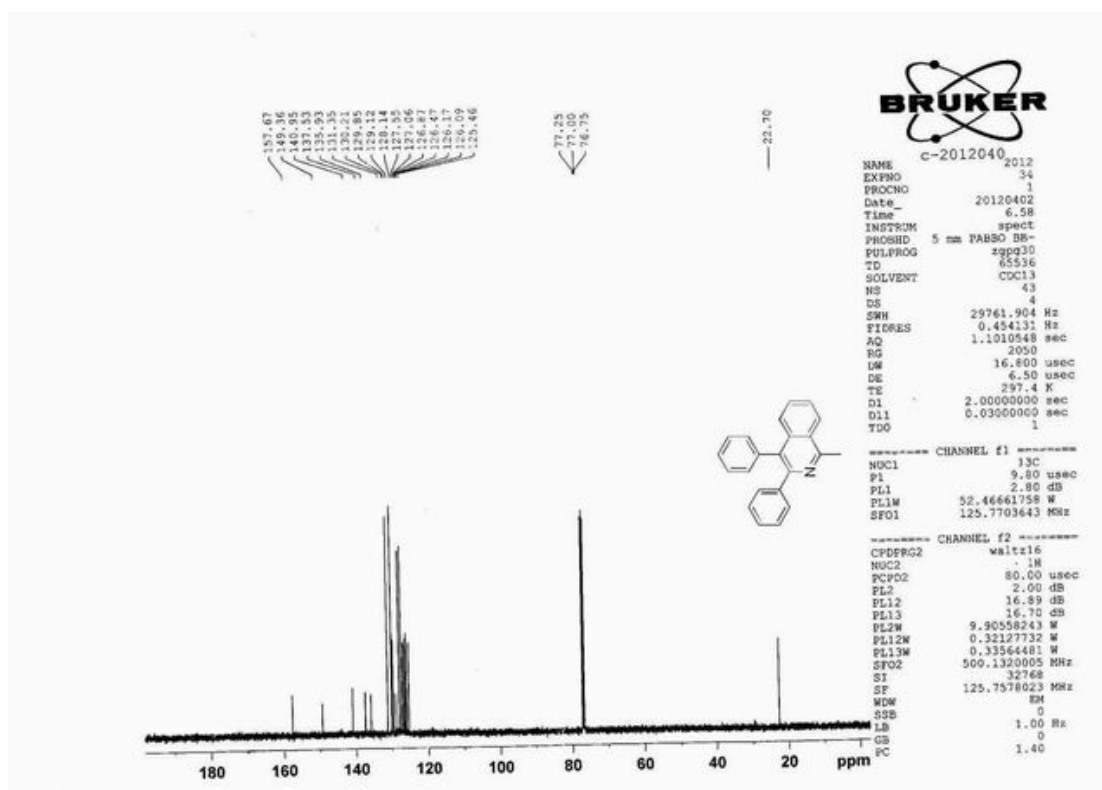
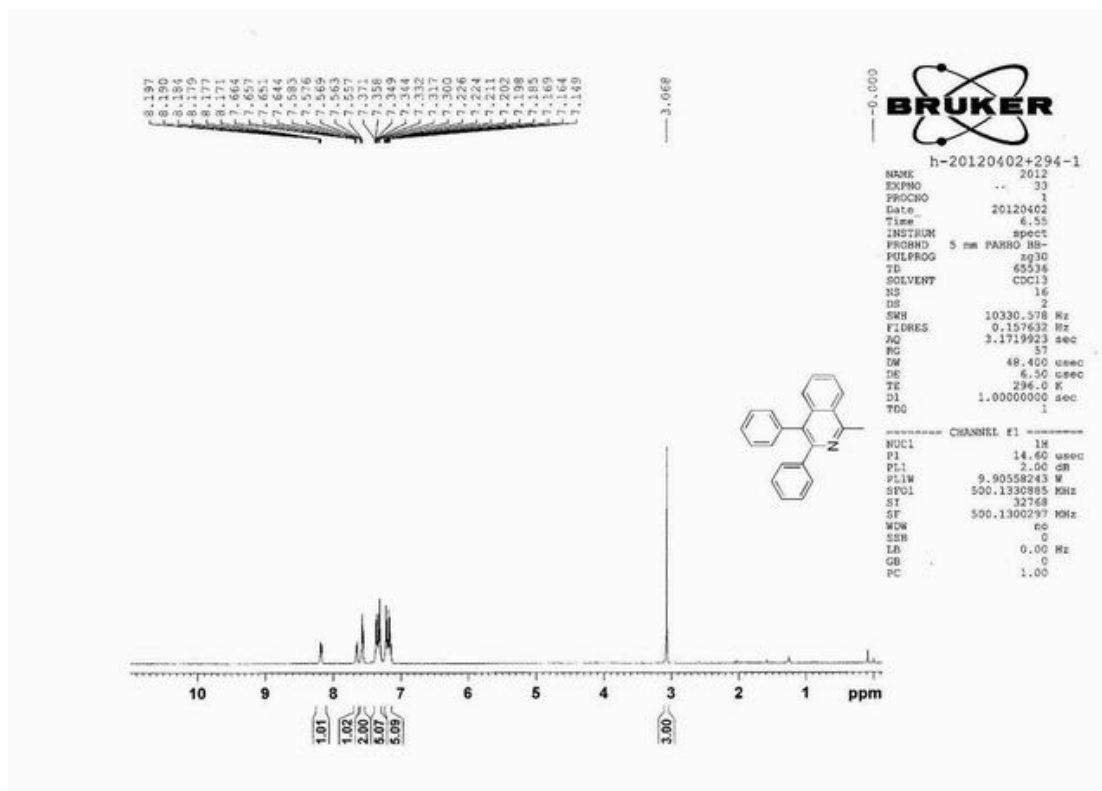
### Intermolecular KIE Experiment



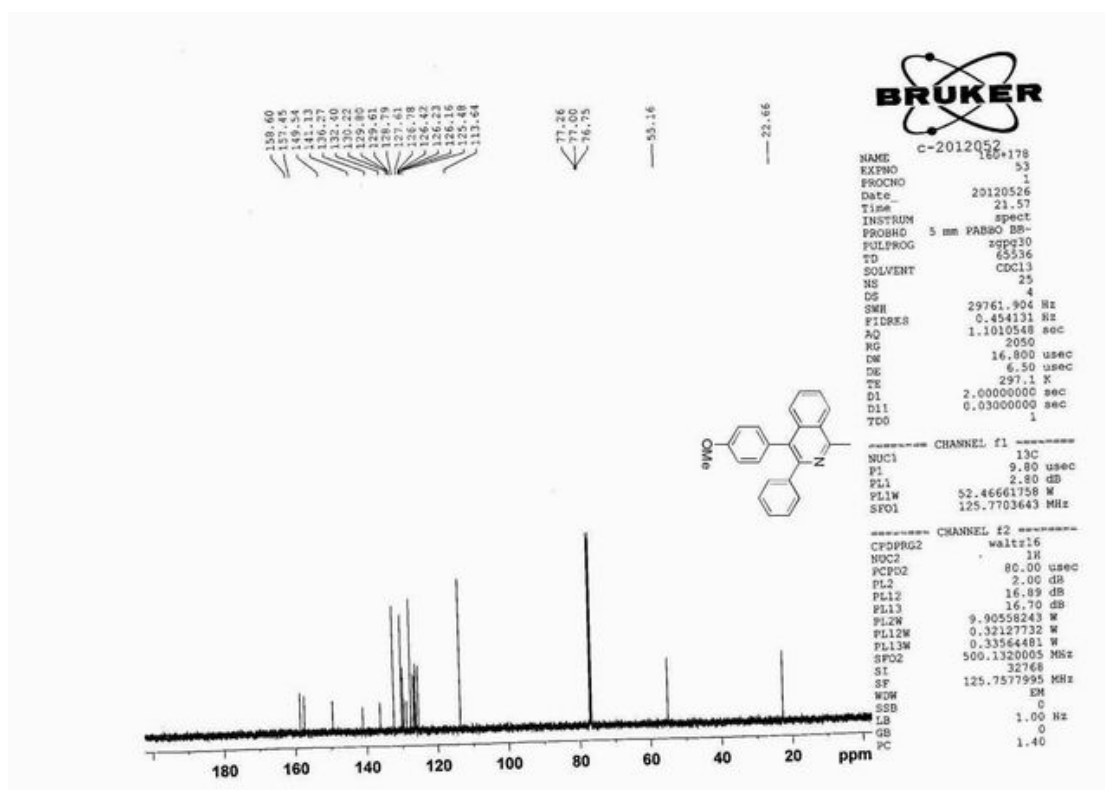
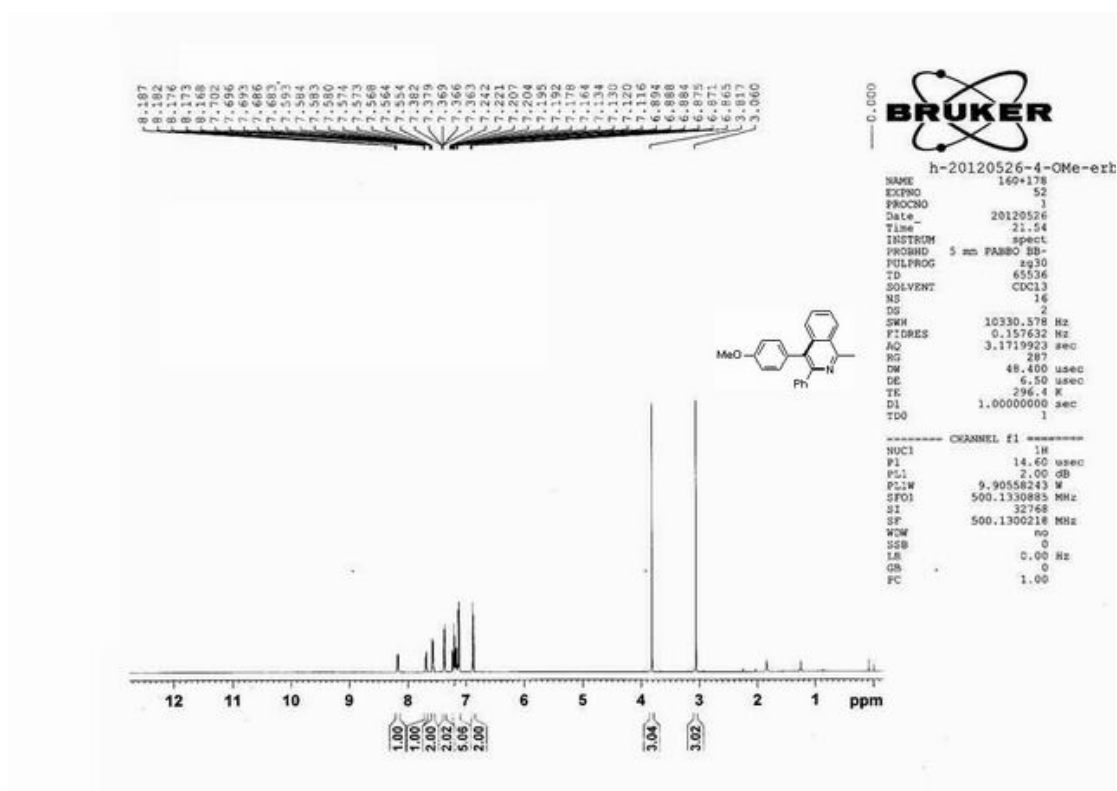


## (B) Spectra

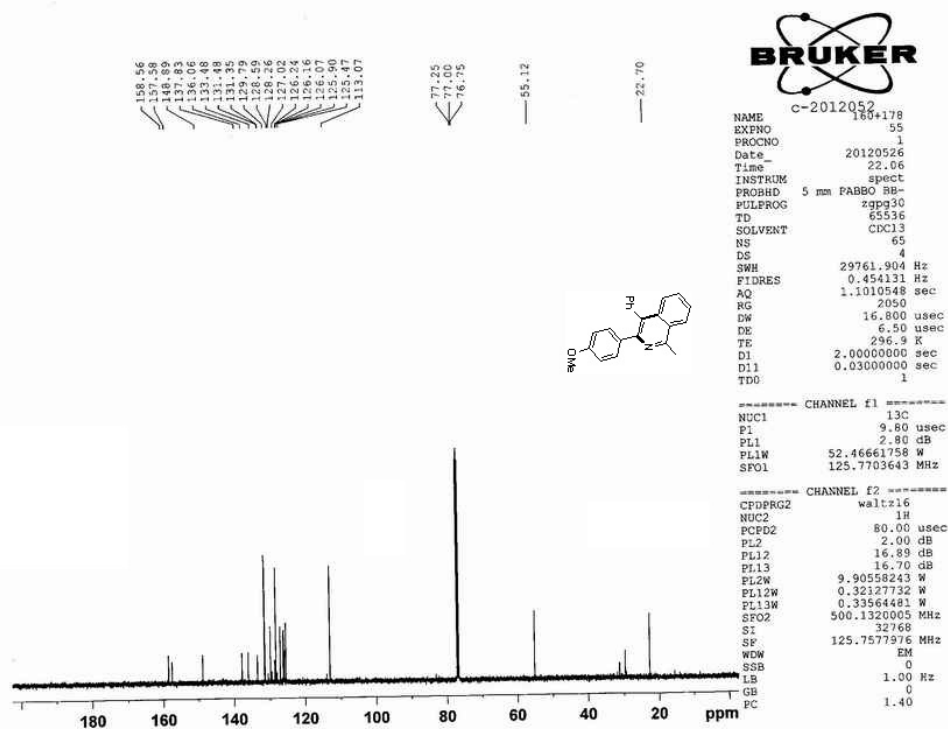
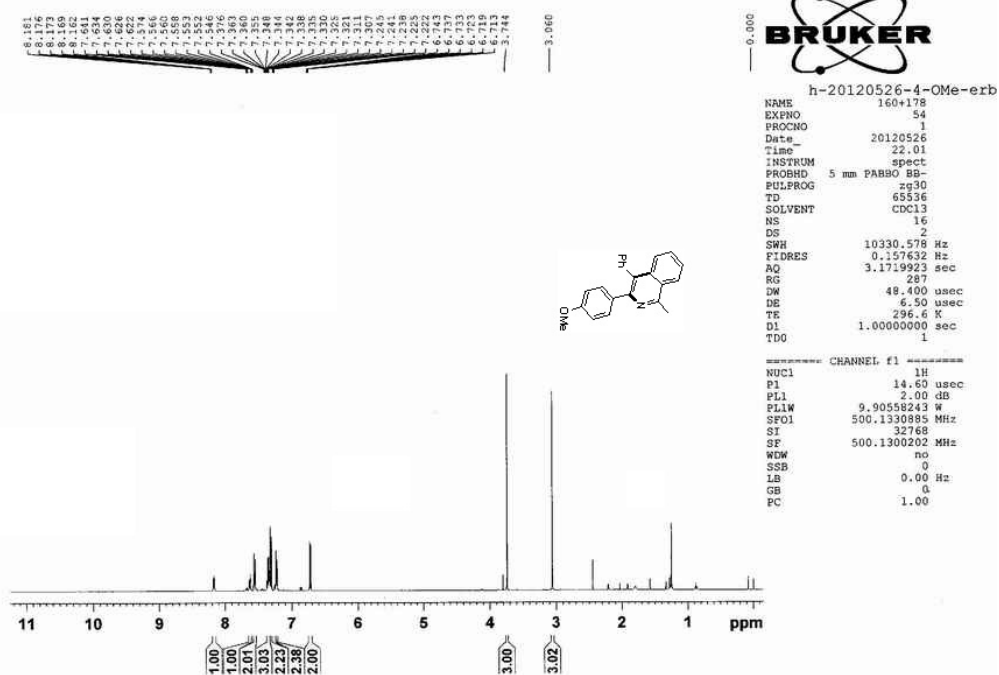
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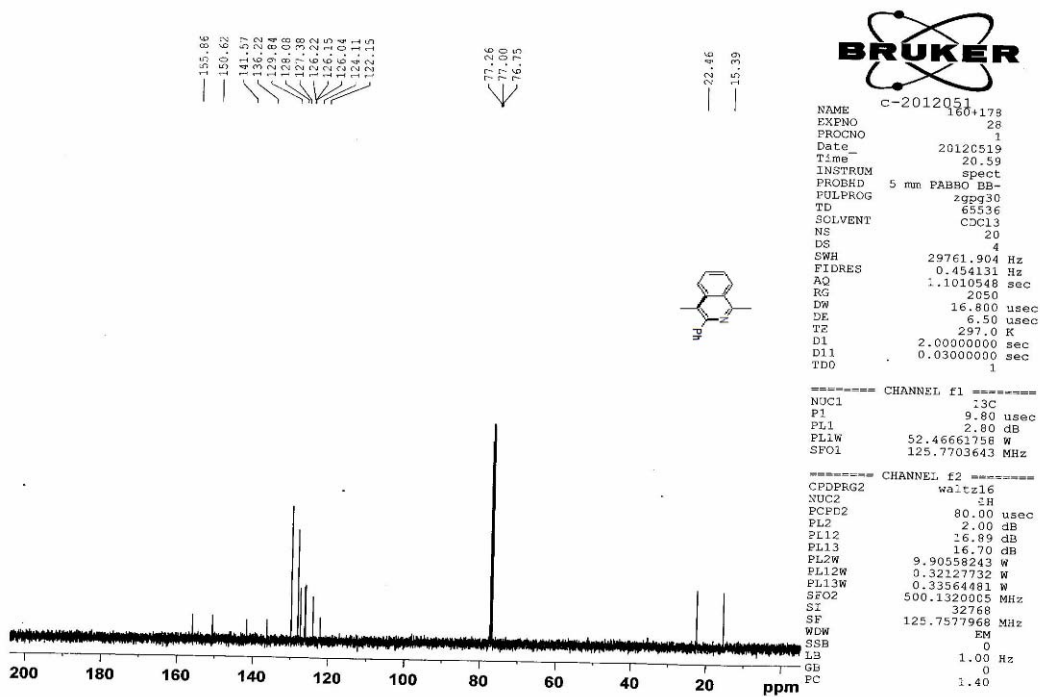
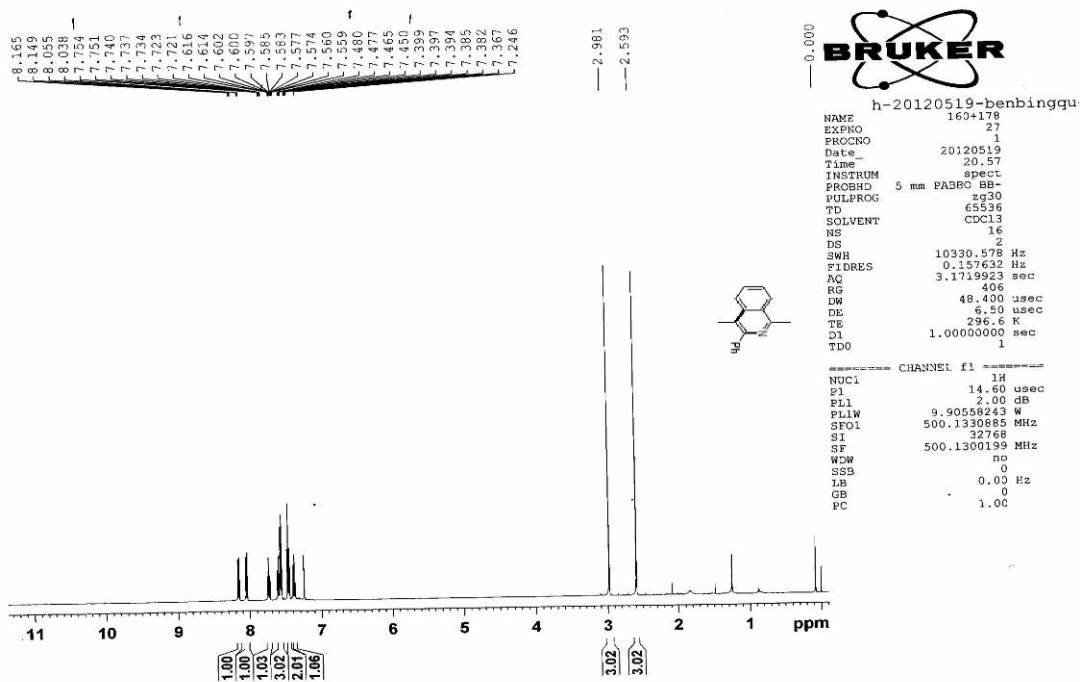
# 4-(4-Methoxyphenyl)-1-methyl-4-phenylisoquinoline (3ba)



### 3-(4-Methoxyphenyl)-1-methyl-3-phenylisoquinoline (3ba')

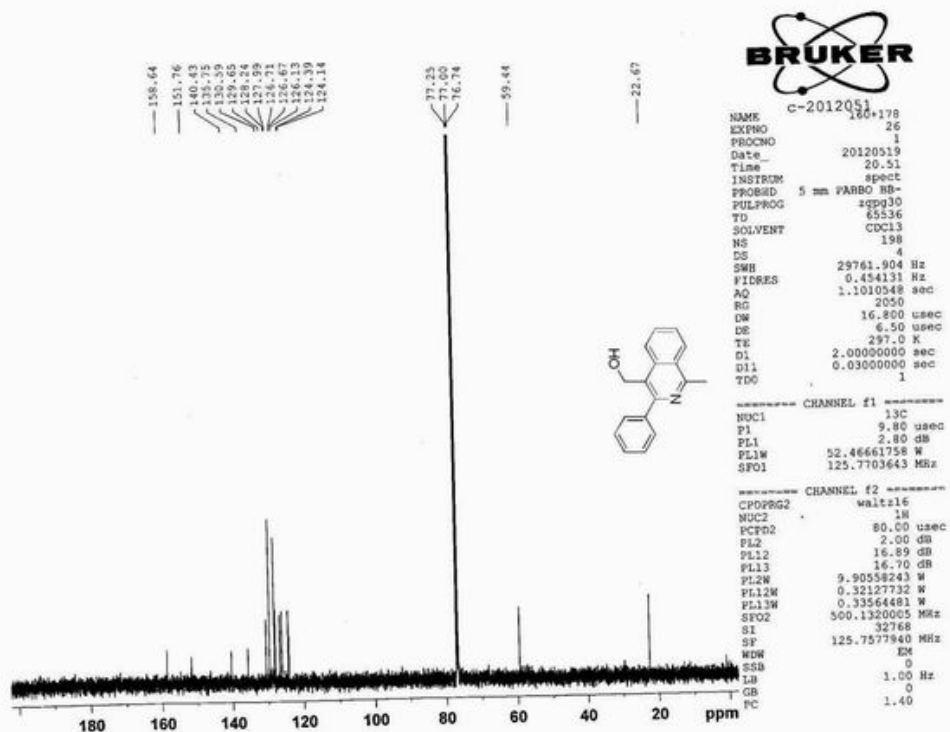
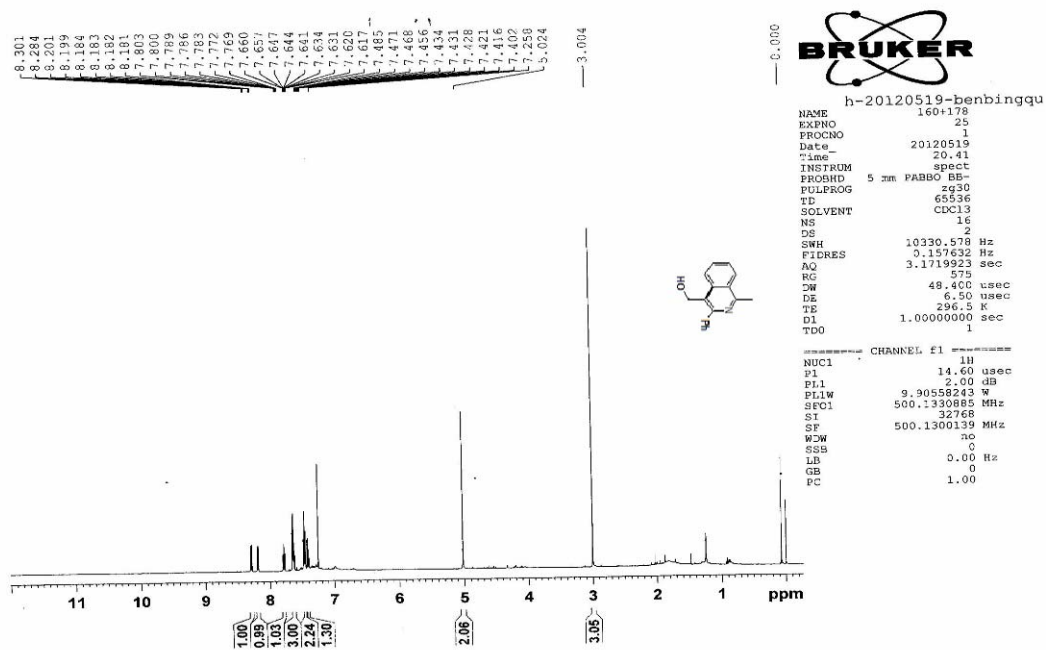


### 1,4-Dimethyl-3-phenylisoquinoline (3ca)

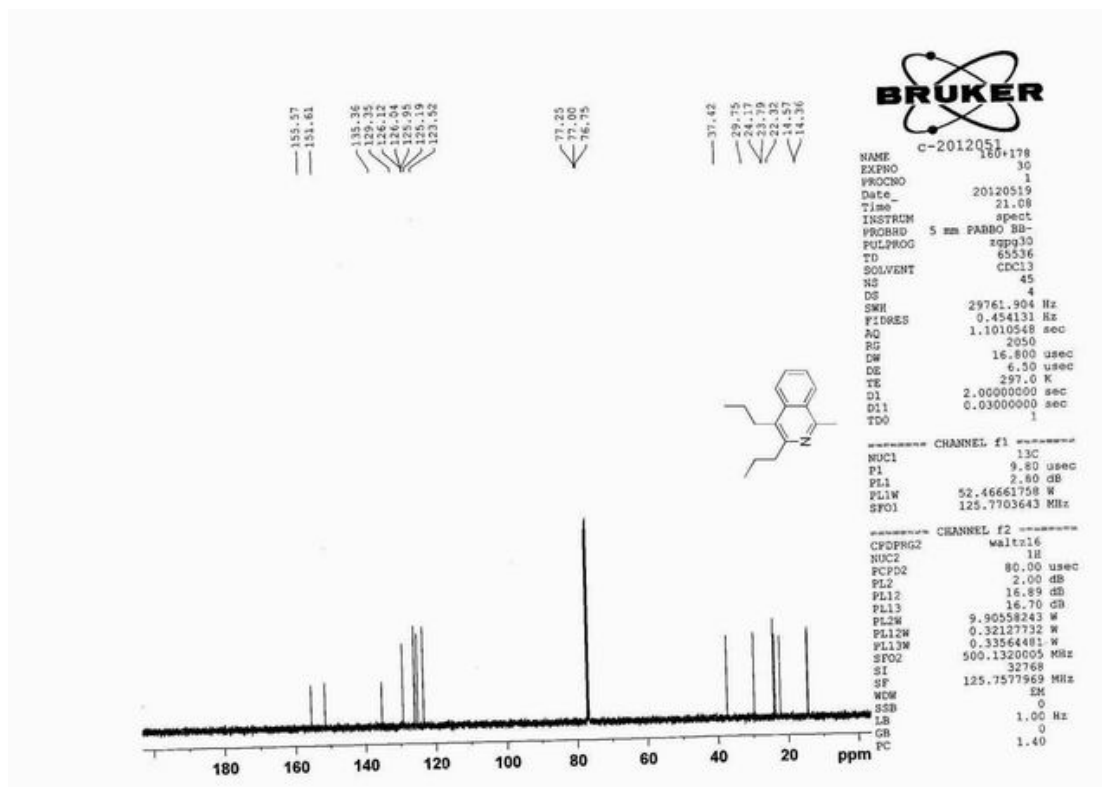
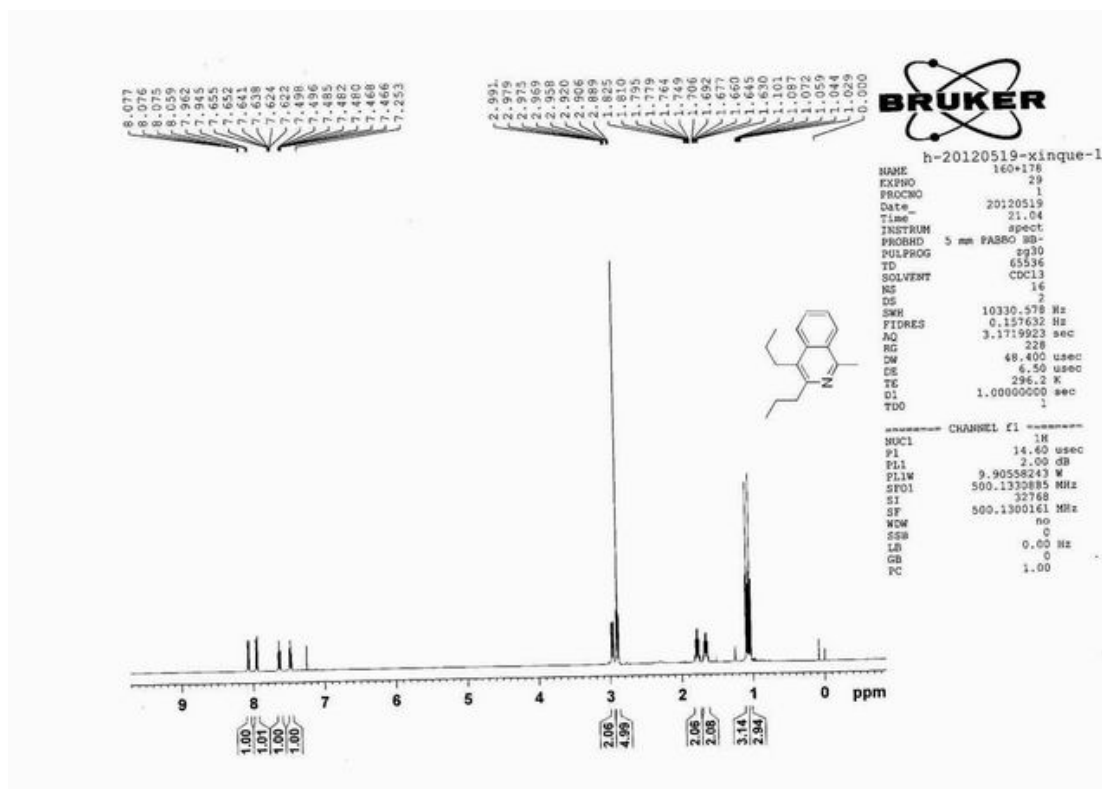




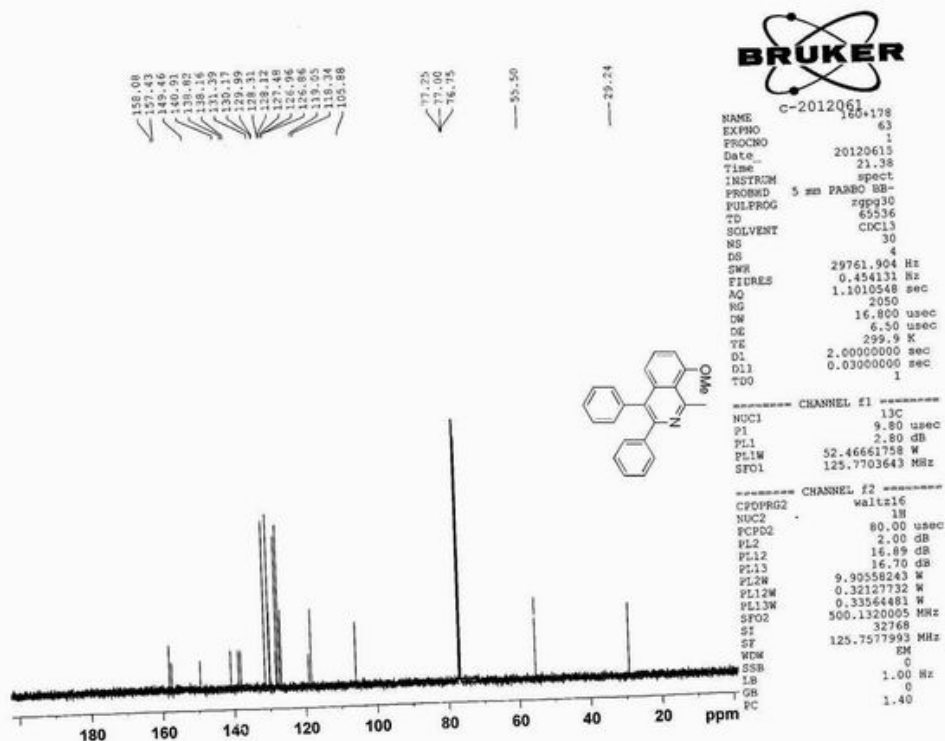
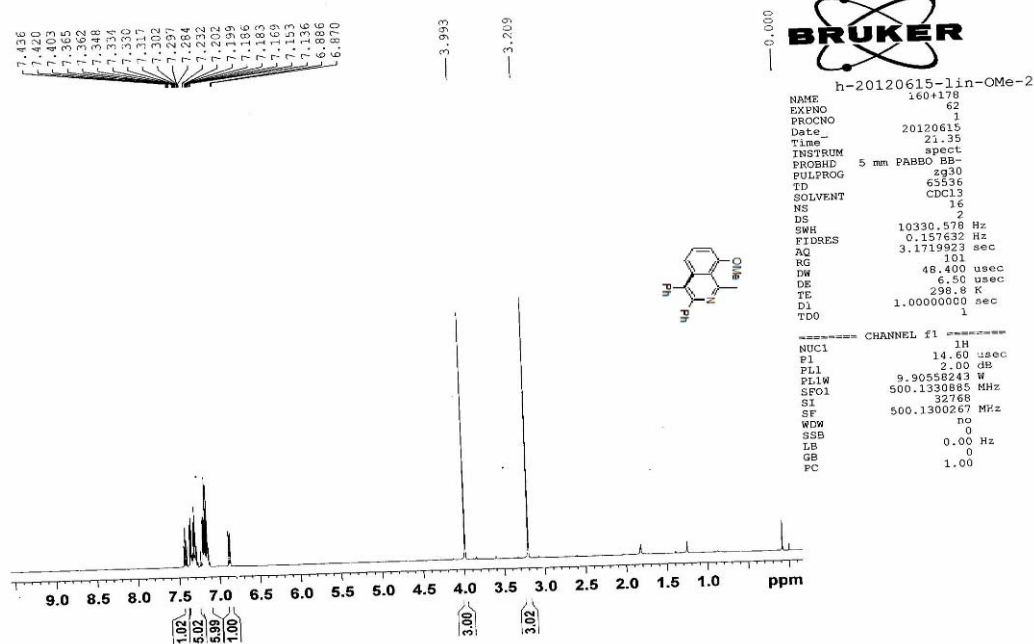
(1-Methyl-3-phenylisoquinolin-4-yl)methanol (3da)



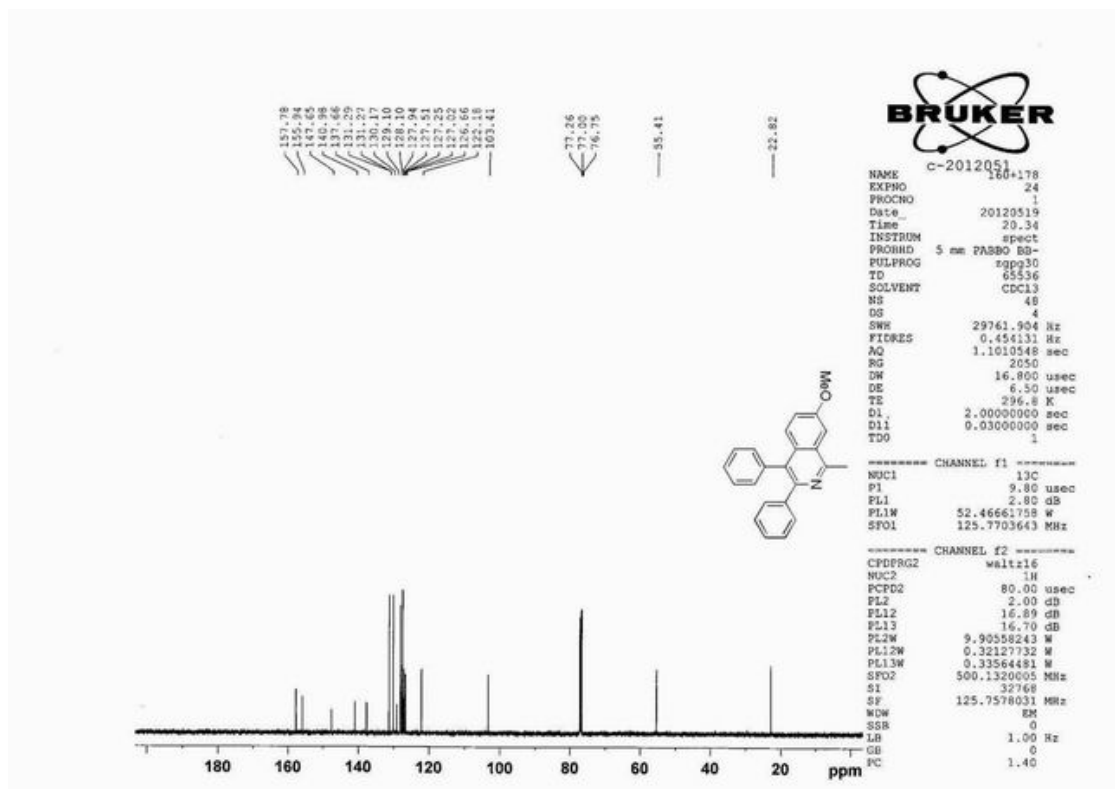
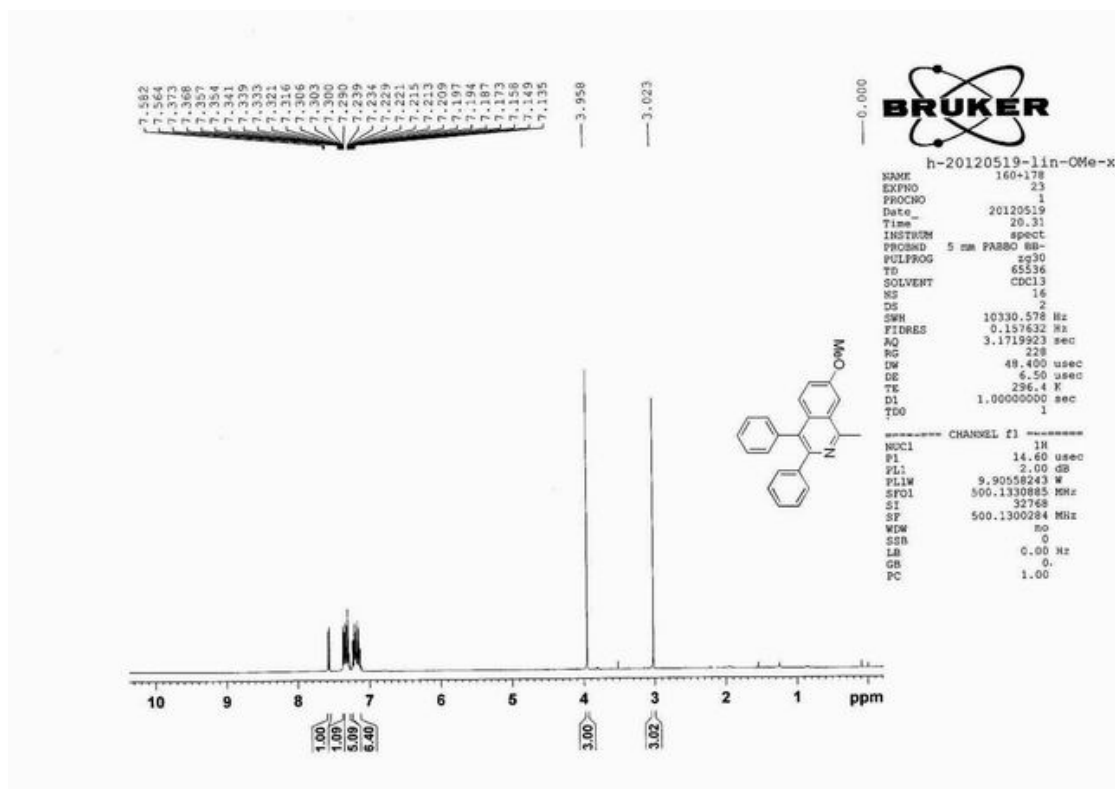
# 1-Methyl-3,4-dipropylisoquinoline (3ea)



# 8-Methoxy-1-methyl-3,4-diphenylisoquinoline (3ah)



# 7-Methoxy-1-methyl-3,4-diphenylisoquinoline (3ai)



Chemical structure: COc1c2ccccc2nc3ccccc13

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) data:

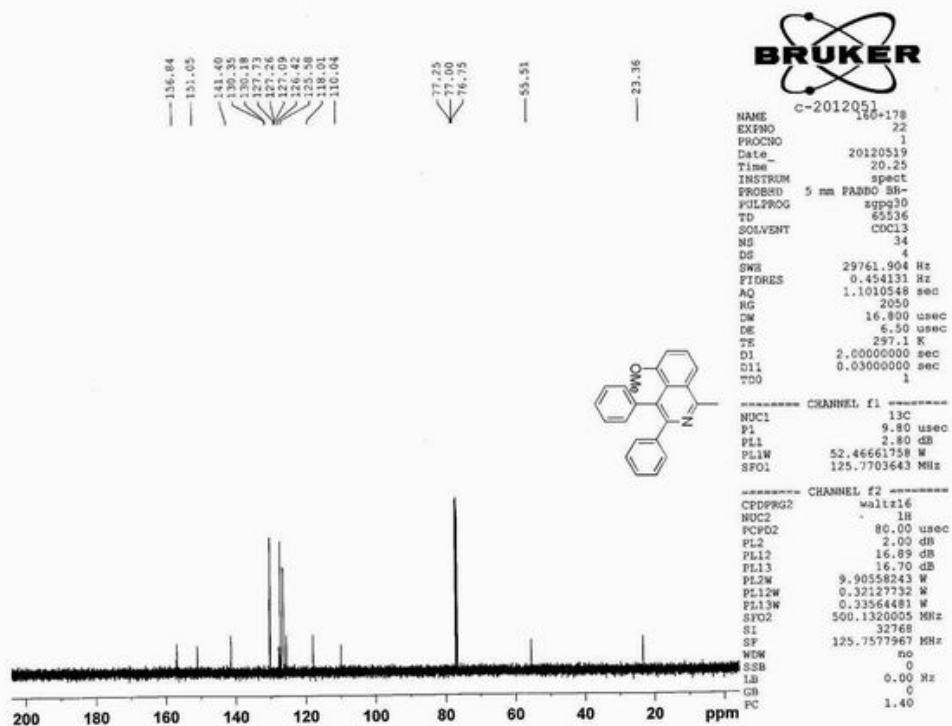
Chemical Shift (ppm)	Integration
7.796, 7.794, 7.779, 7.777, 7.534, 7.518, 7.502, 7.477, 7.230, 7.226, 7.222, 7.213, 7.210, 7.172, 7.161, 7.157, 7.153, 7.150, 7.146, 7.141, 7.139, 7.135, 7.128, 7.115, 7.106, 7.102, 7.091, 7.087, 6.945, 6.940	1.00, 1.02, 2.00, 2.05, 1.03
3.395, 3.034	3.00, 3.00

Acquisition parameters:

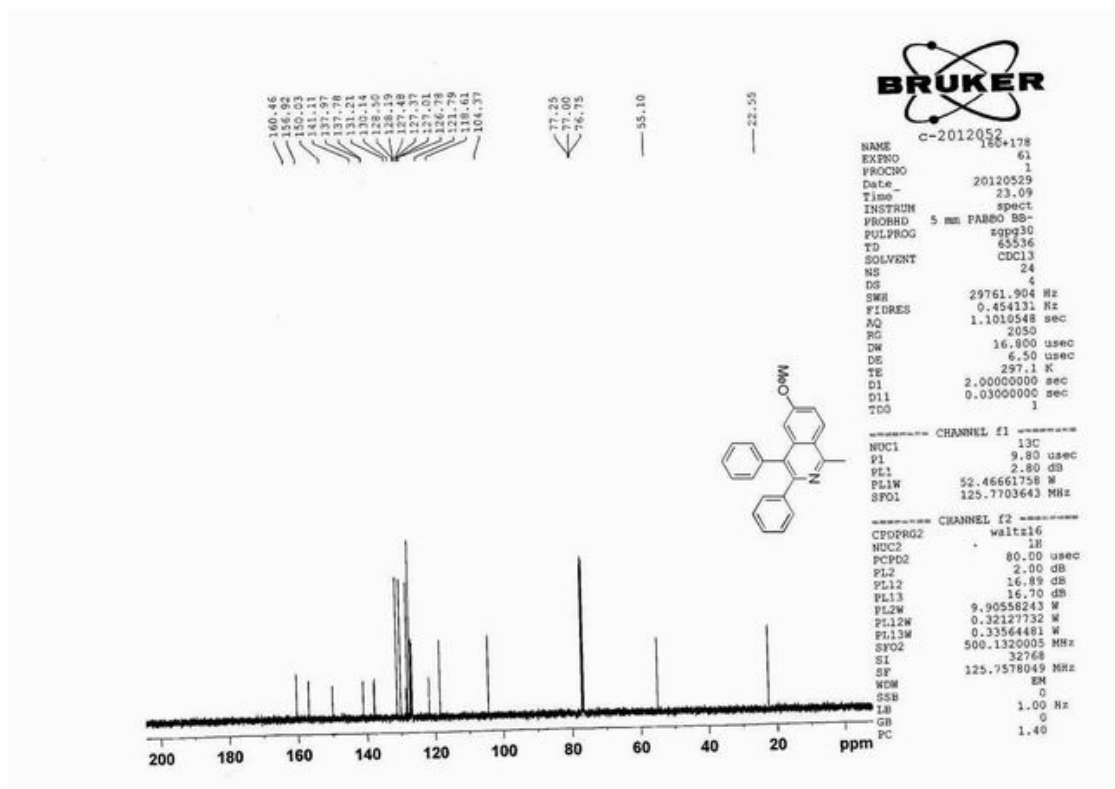
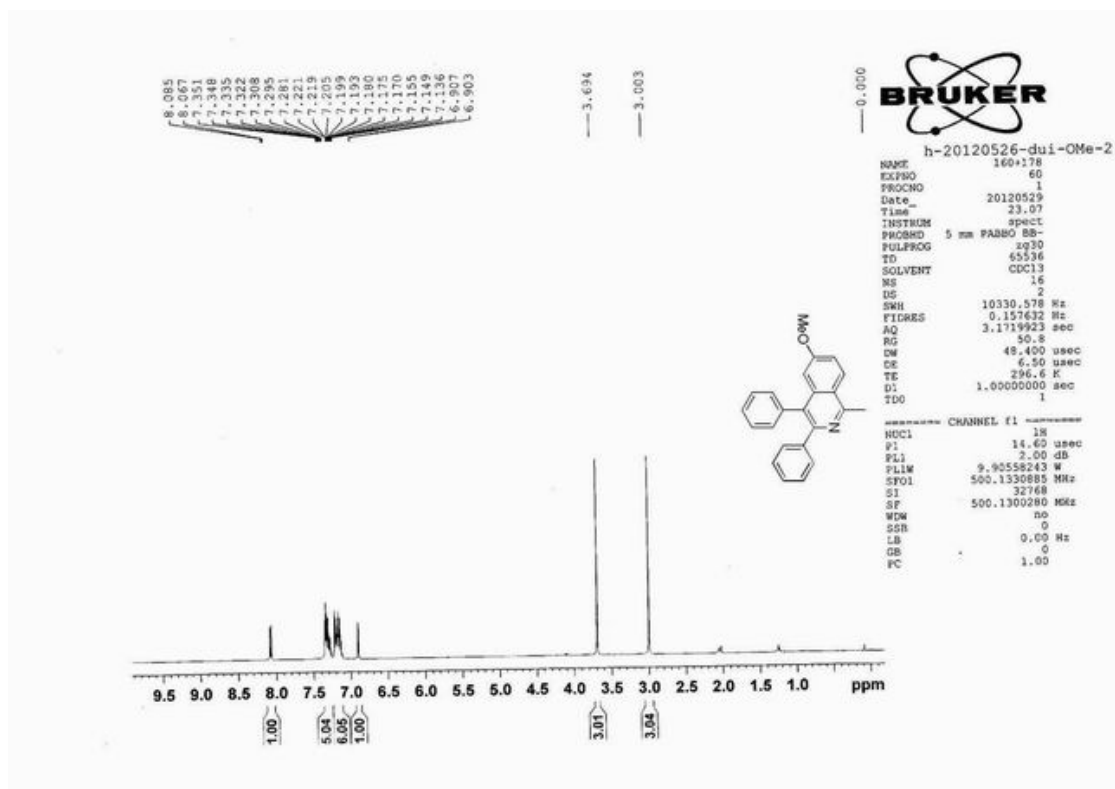
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- EXPNO: 160+178
- PROCNO: 1
- Date\_: 20120519
- Time: 20.22
- INSTRUM: spect
- PROBHD: 5 mm PABBO BB-
- PULPROG: zg30
- TD: 65536
- SOLVENT: CDCl3
- NS: 16
- DS: 2
- SWH: 10330.578 Hz
- FIDRES: 0.157632 Hz
- AQ: 3.1719923 sec
- RG: 456
- DW: 48.400 usec
- DE: 6.50 usec
- TE: 296.4 K
- D1: 1.00000000 sec
- TD0: 1

Channel f1 parameters:

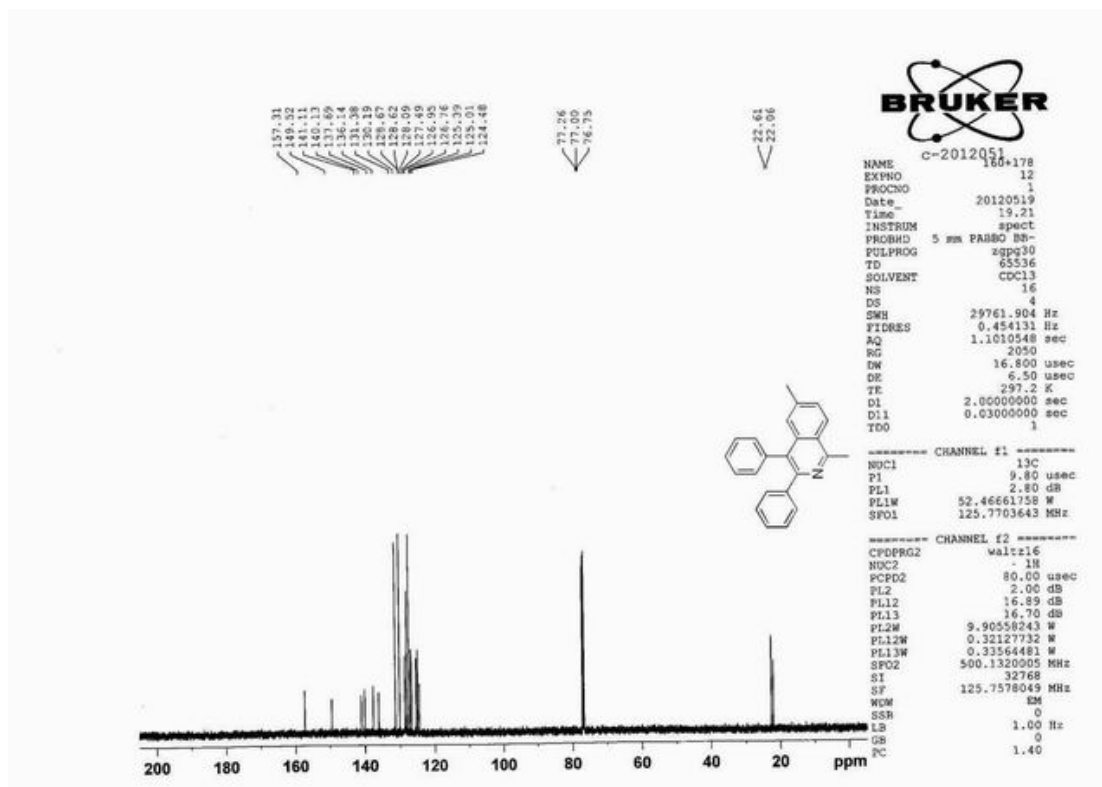
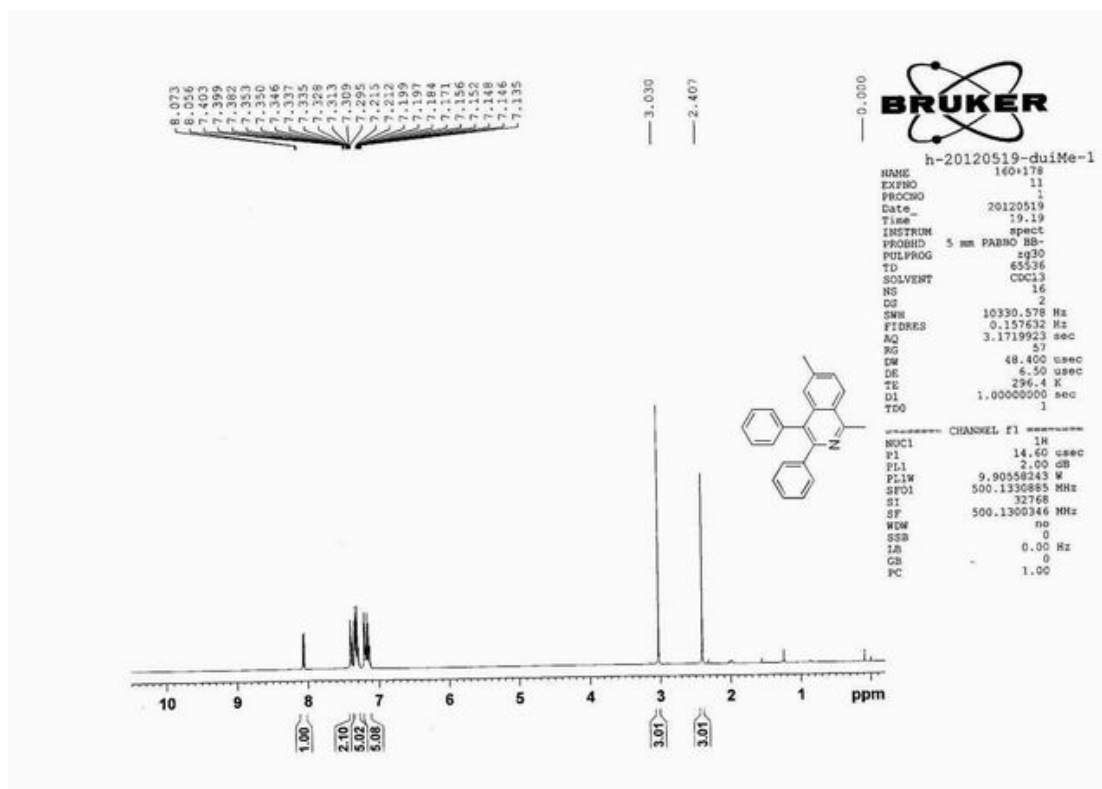
- MUCL: 1H
- PL: 14.40 usec
- PL1: 2.00 dB
- PL1W: 9.90558243 W
- SFO1: 500.1330885 MHz
- SI: 32768
- SF: 500.1300195 MHz
- WDW: no
- SSB: 0
- LB: 0.90 Hz
- GB: 0
- PC: 1.00



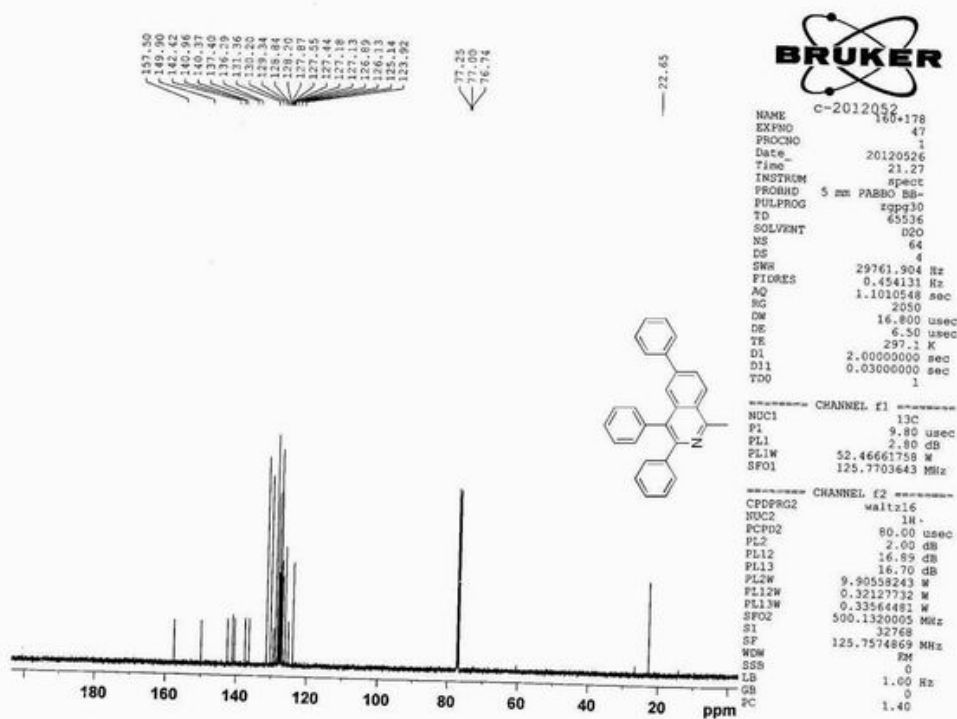
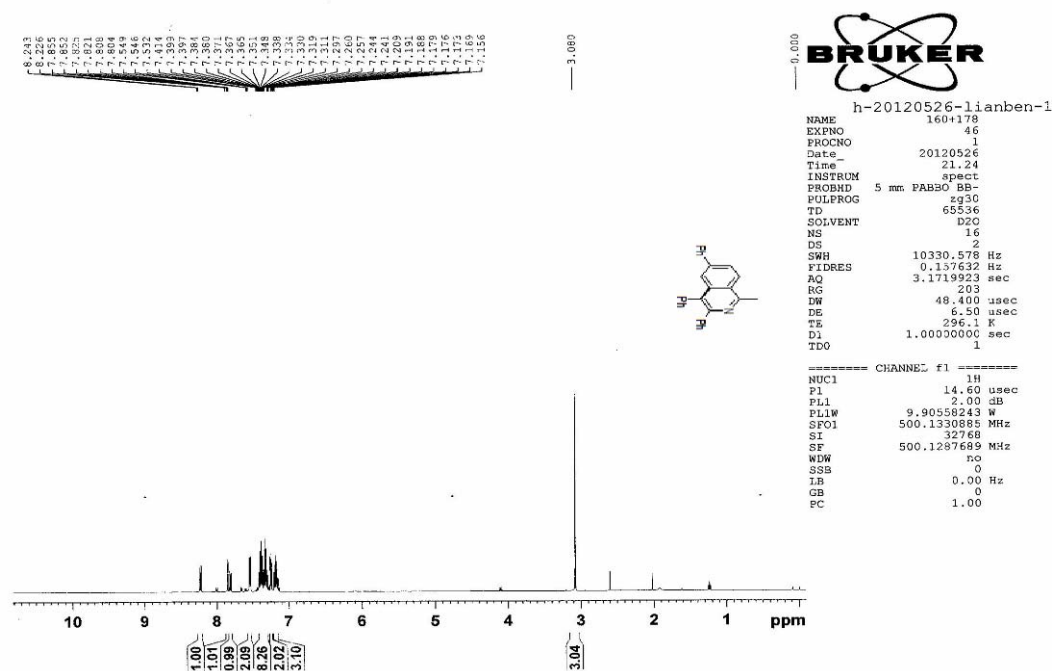
### 6-Methoxy-1-methyl-3,4-diphenylisoquinoline (3aj)



# 1,6-Dimethyl-3,4-diphenylisoquinoline (3ak)

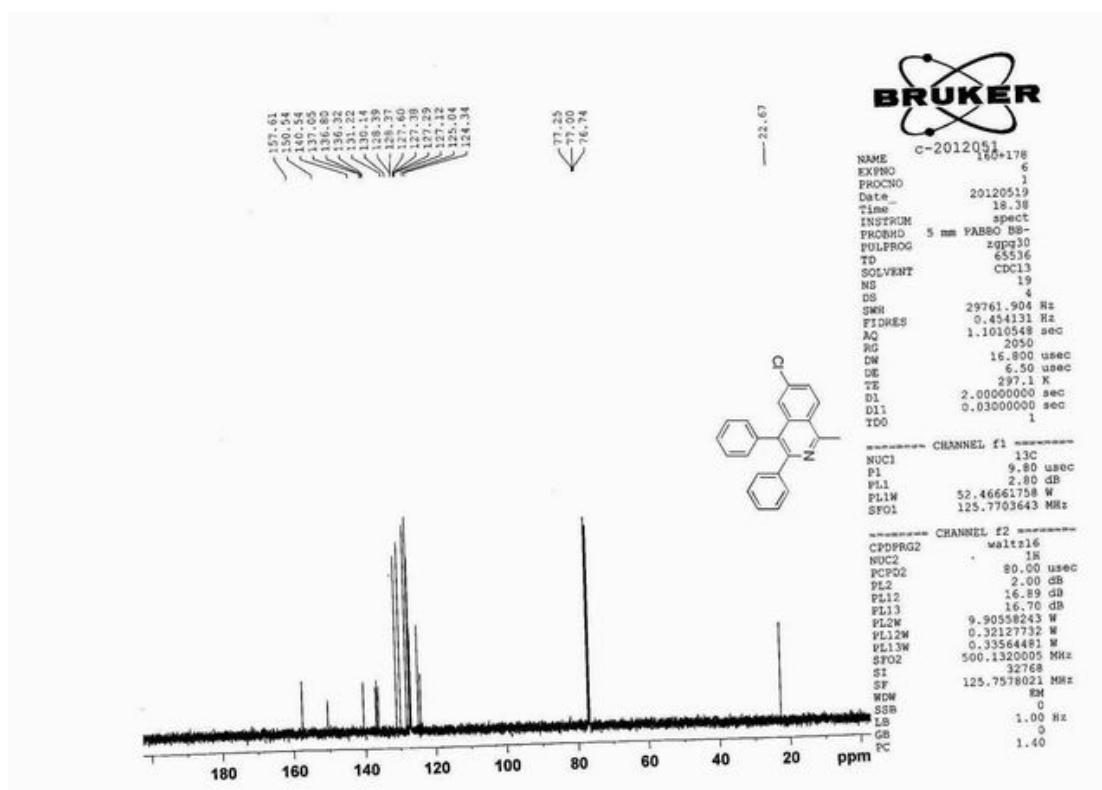
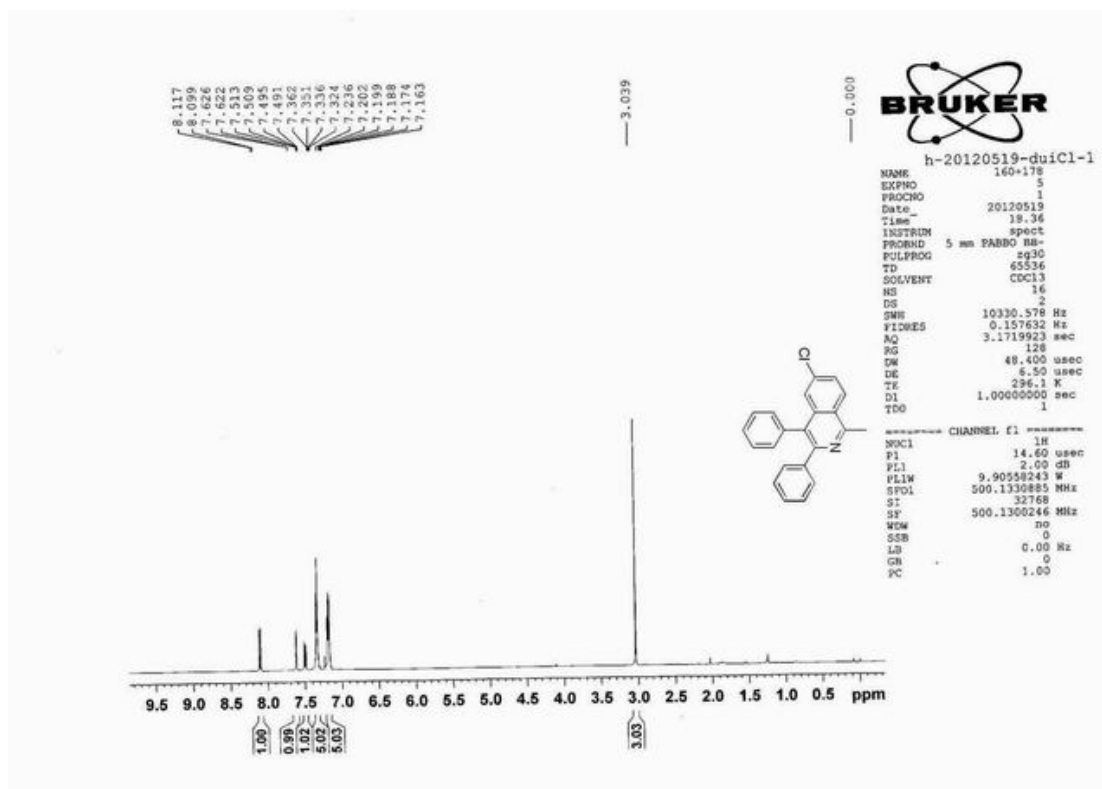


# 1-Methyl-3,4,6-triphenylisoquinoline (3al)

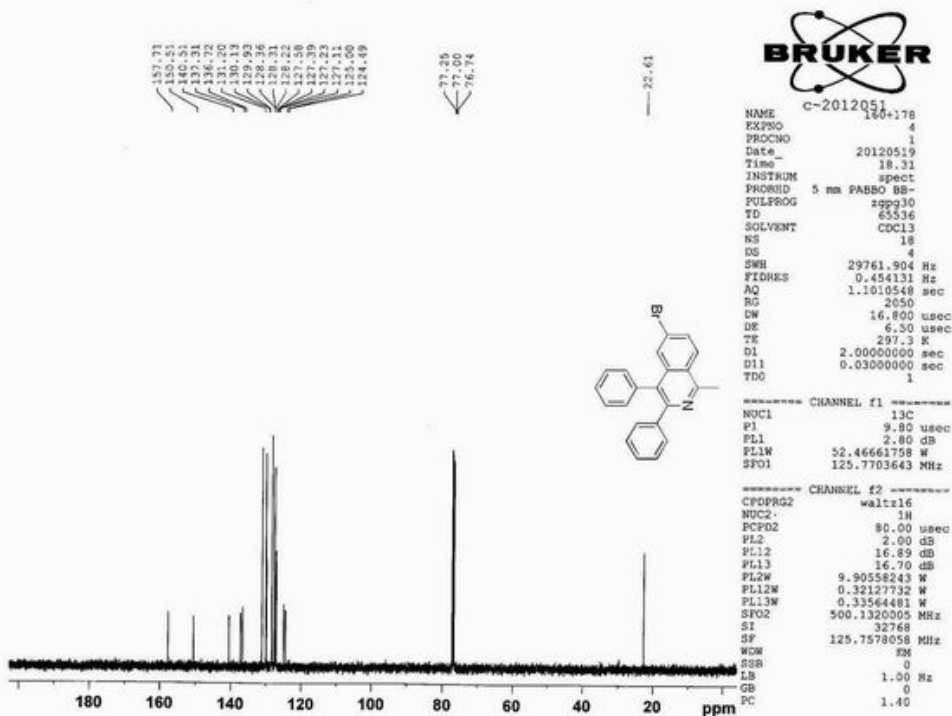
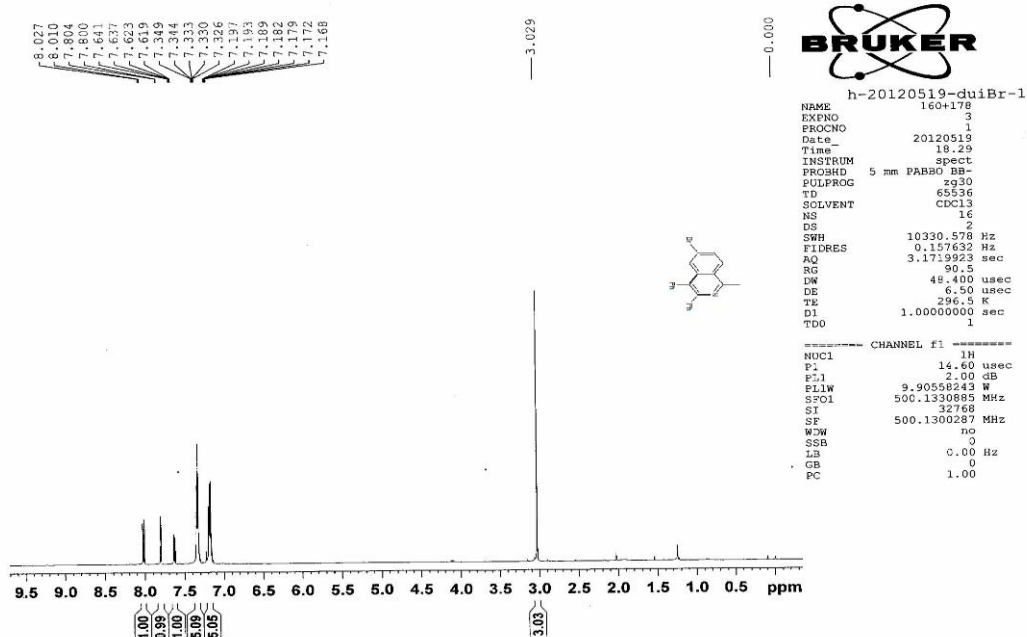




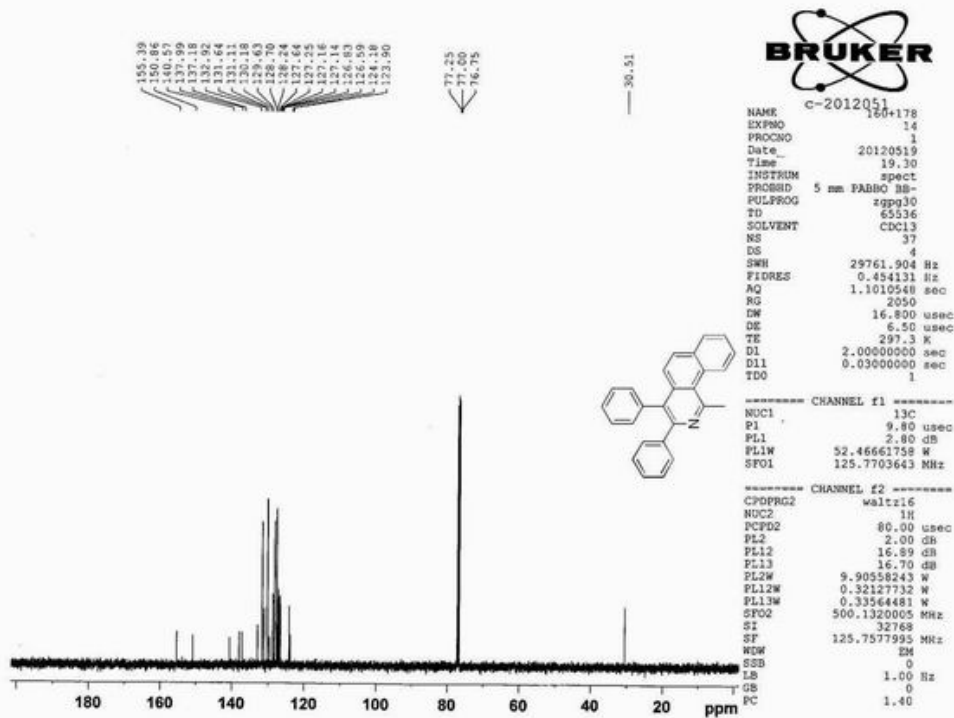
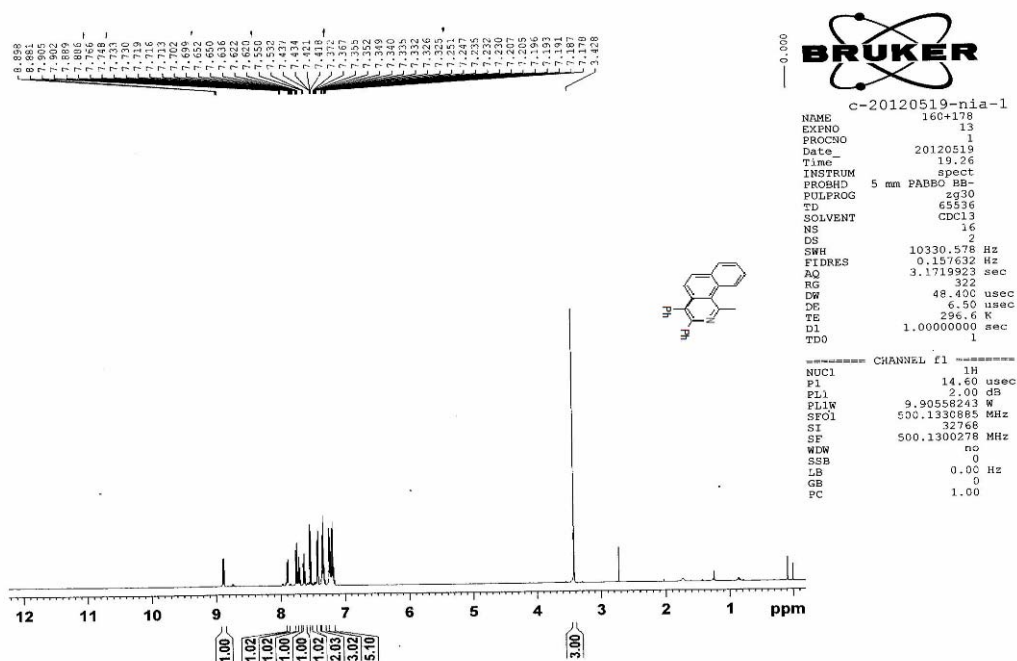
# 6-Chloro-1-methyl-3,4-diphenylisoquinoline (3am)



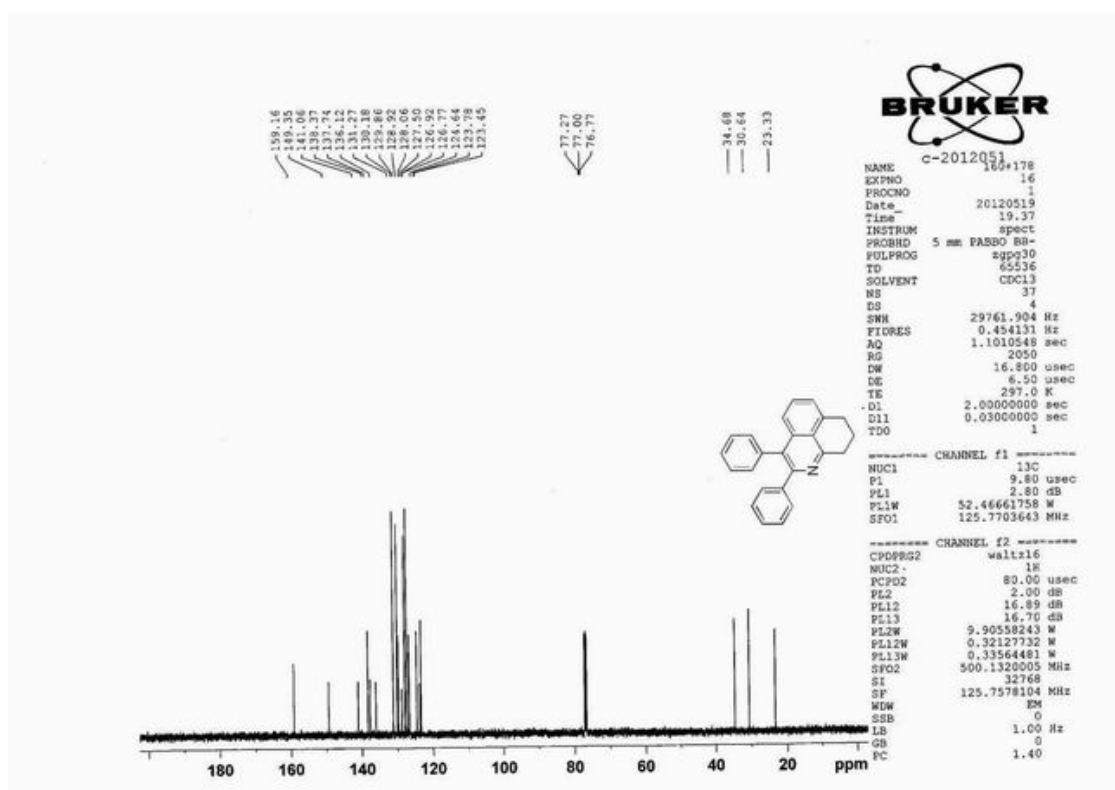
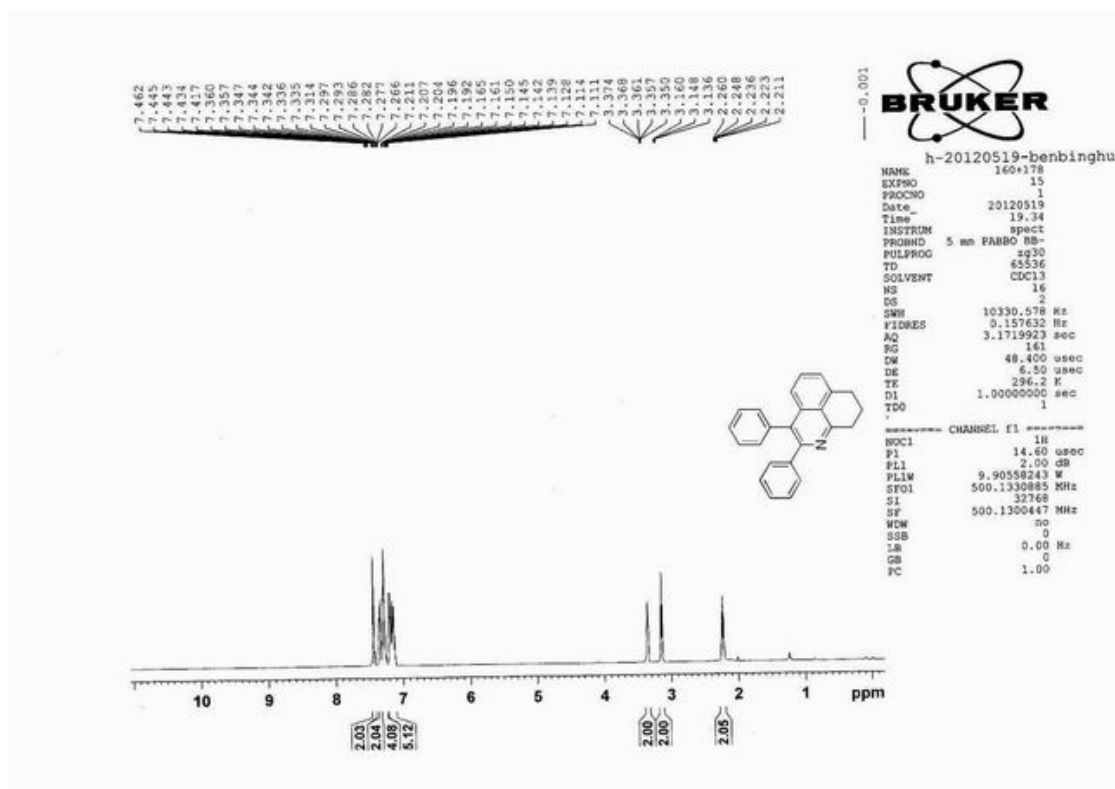
# 6-Bromo-1-methyl-3,4-diphenylisoquinoline (3an)



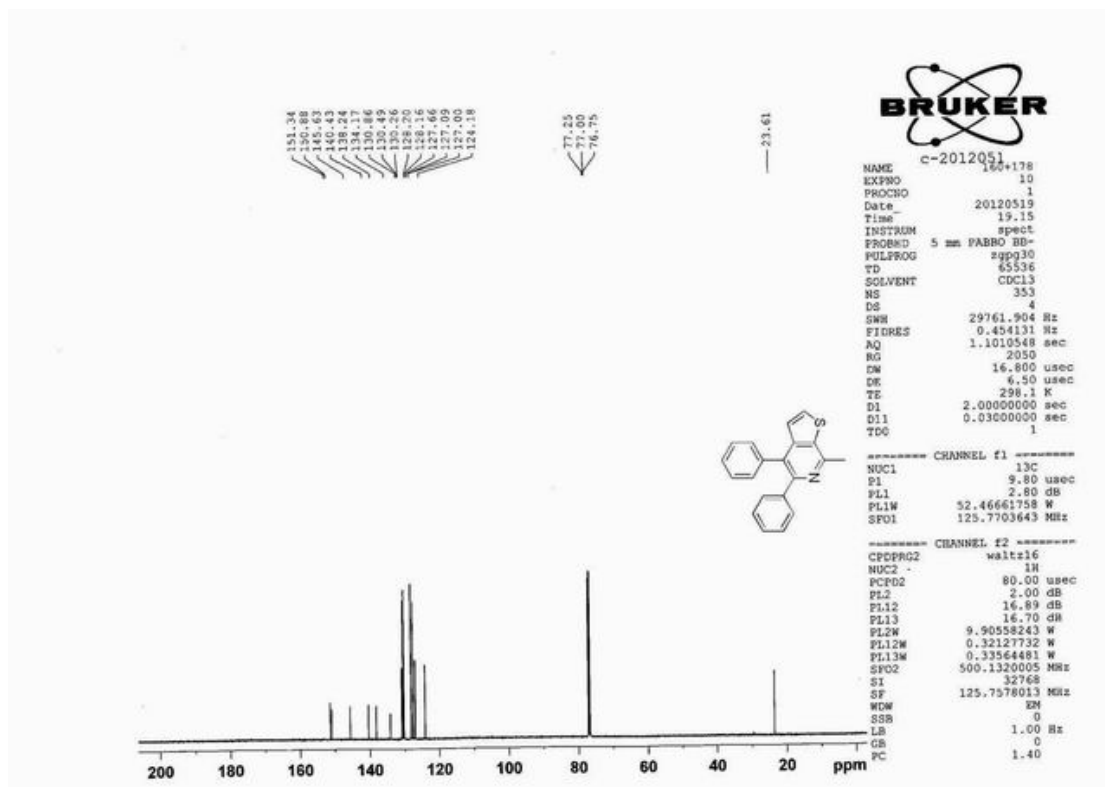
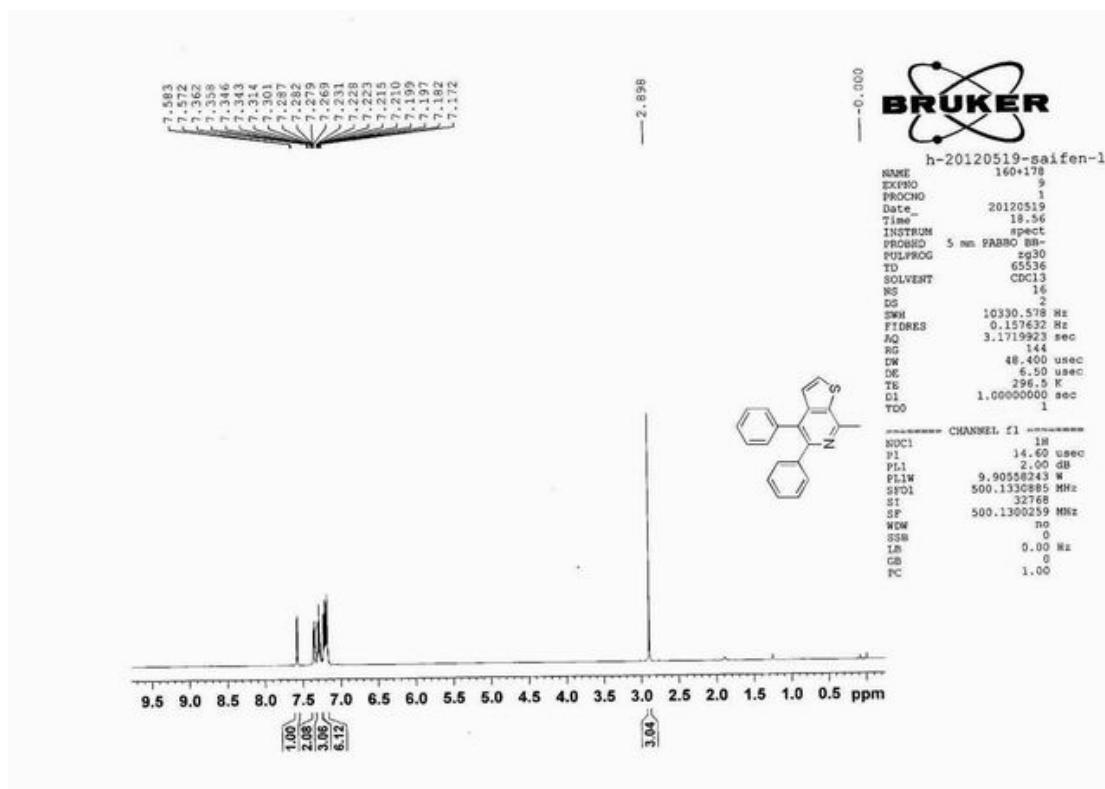
# 1-Methyl-3,4-diphenylbenzo[h]isoquinoline (3ao)



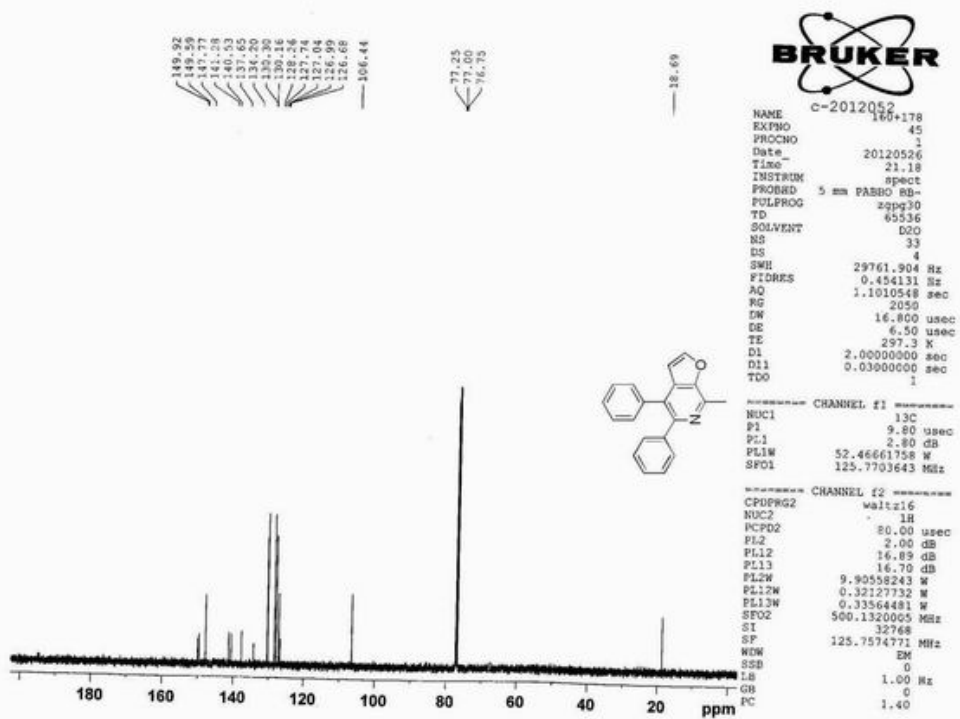
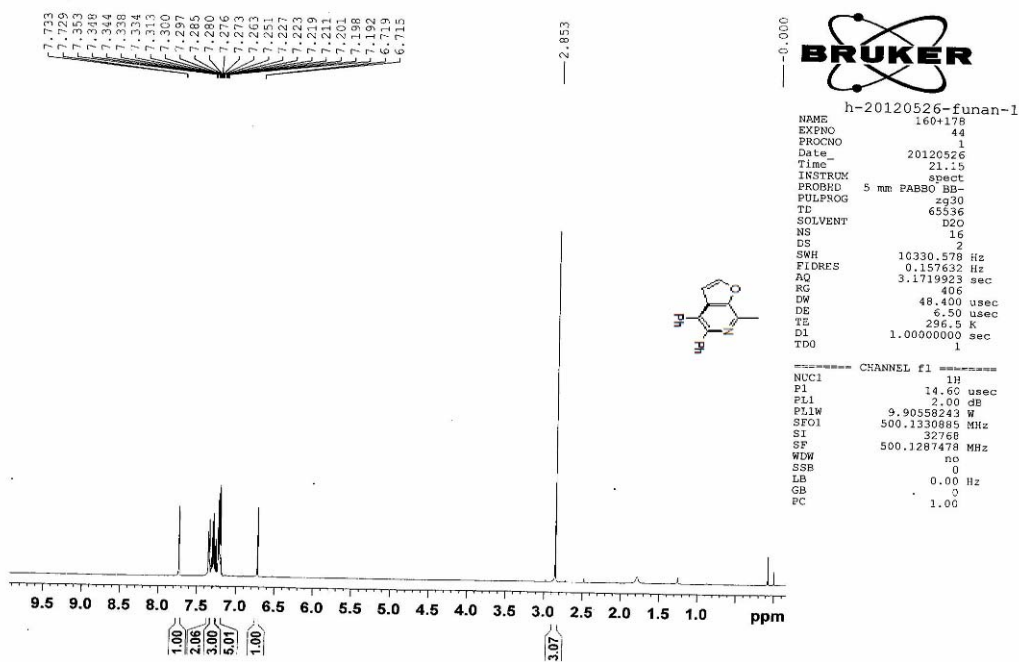
## 2,3-Diphenyl-8,9-dihydro-7H-benzo[de]quinoline (3ap)



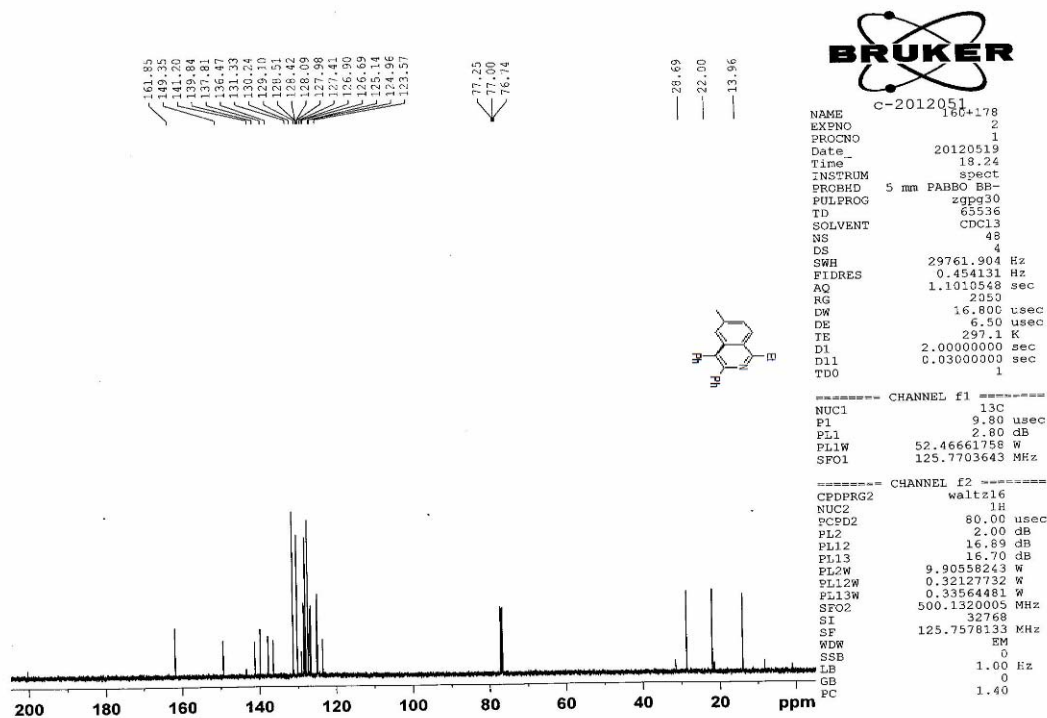
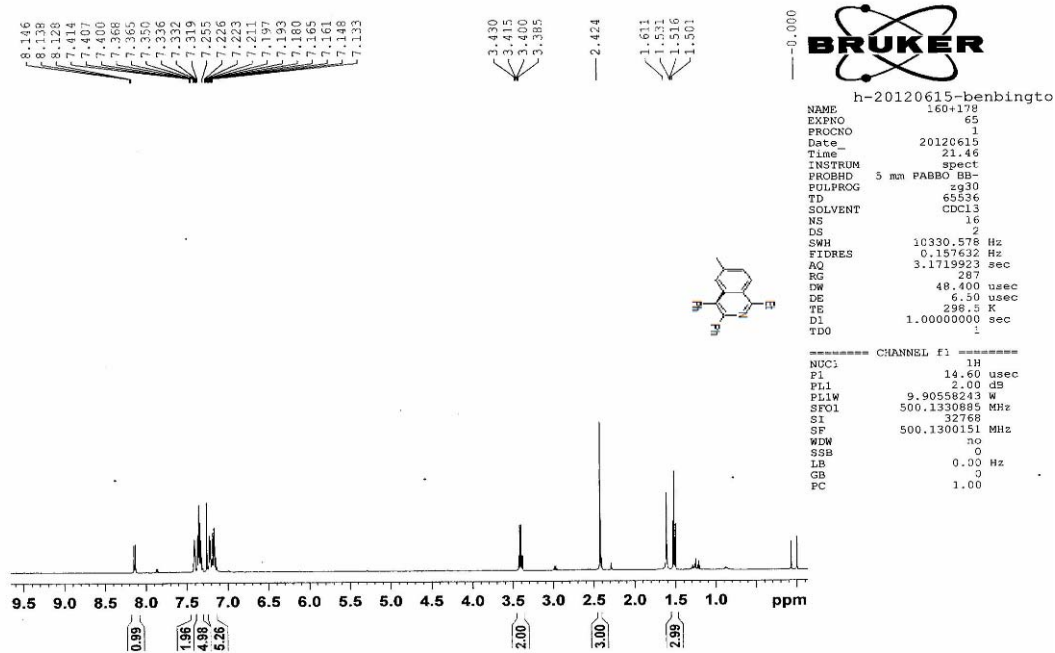
# 7-Methyl-4,5-diphenylthieno[2,3-c]pyridine (3aq)



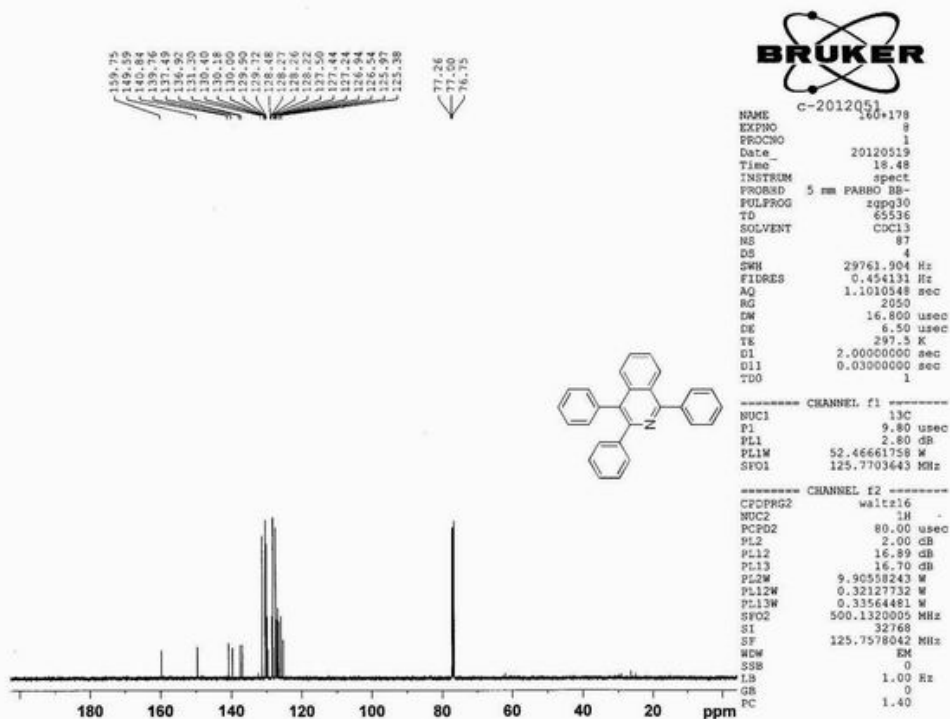
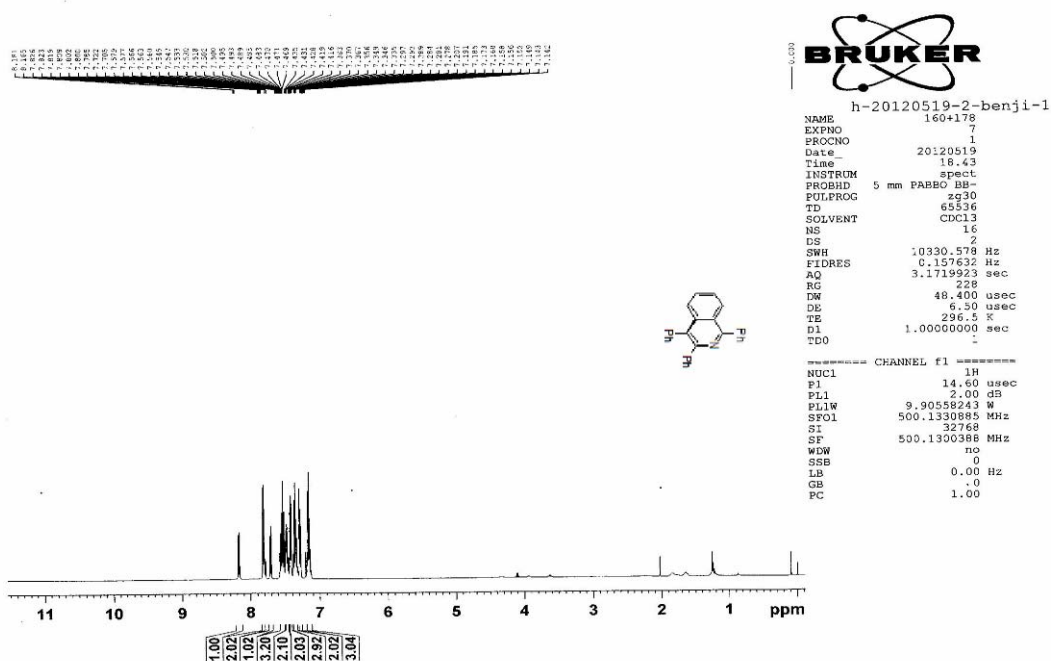
### 7-Methyl-4,5-diphenylfuro[2,3-c]pyridine (3ar)



# 1-Ethyl-6-methyl-3,4-diphenylisoquinoline (3as)

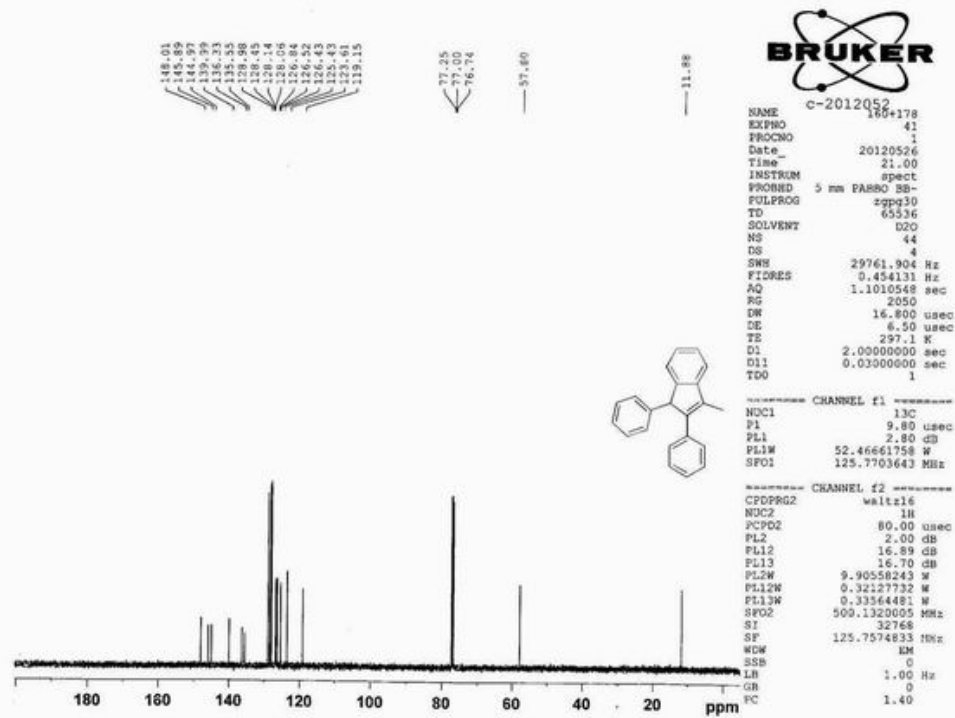
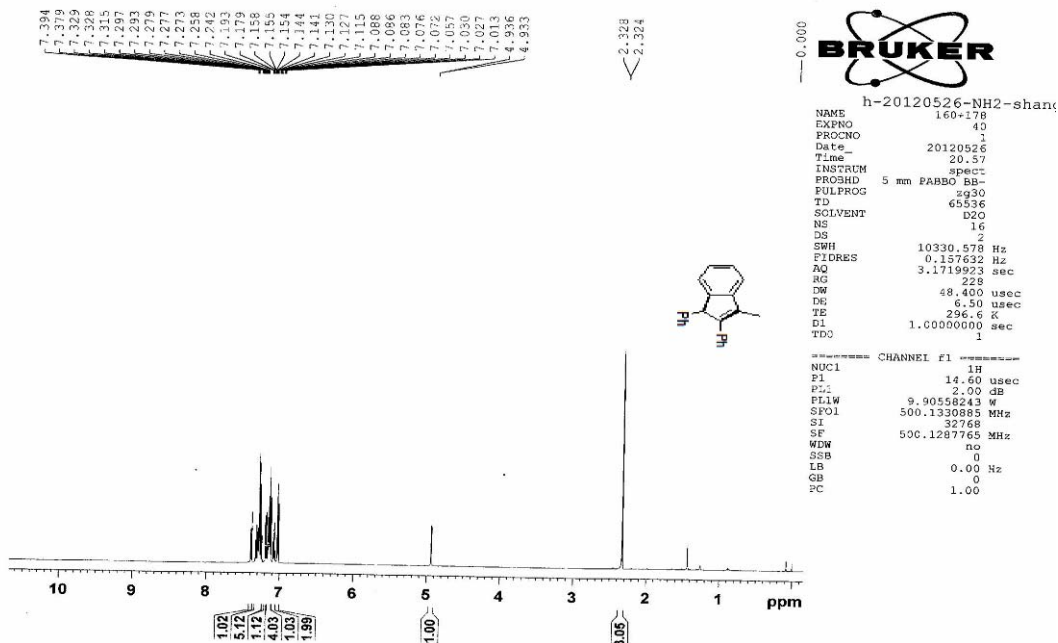


# 1,3,4-Triphenylisoquinoline (3at)

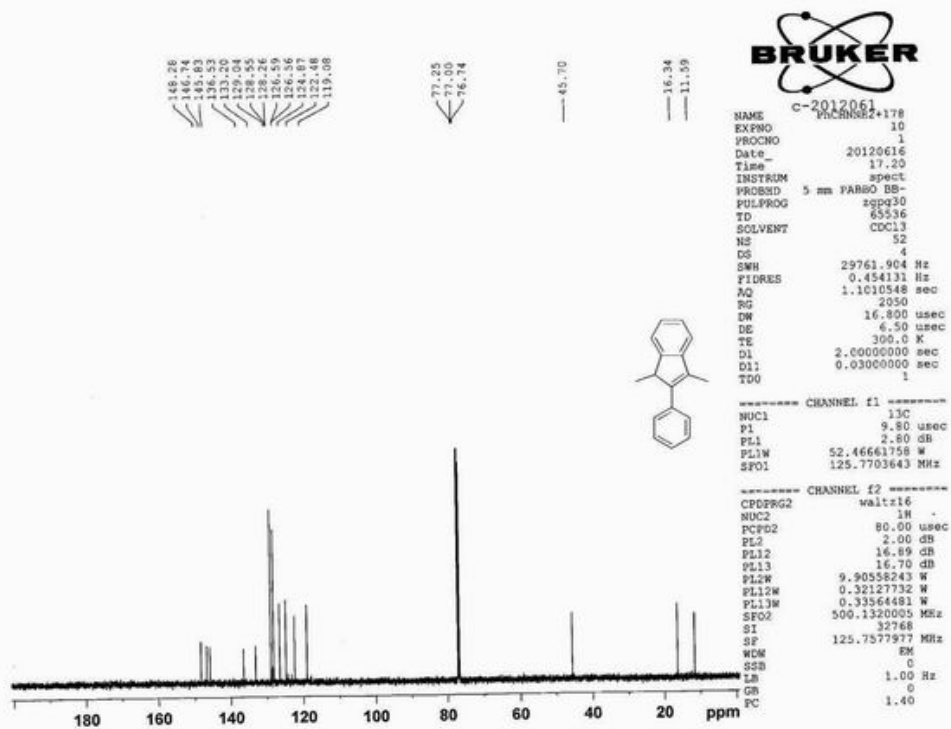
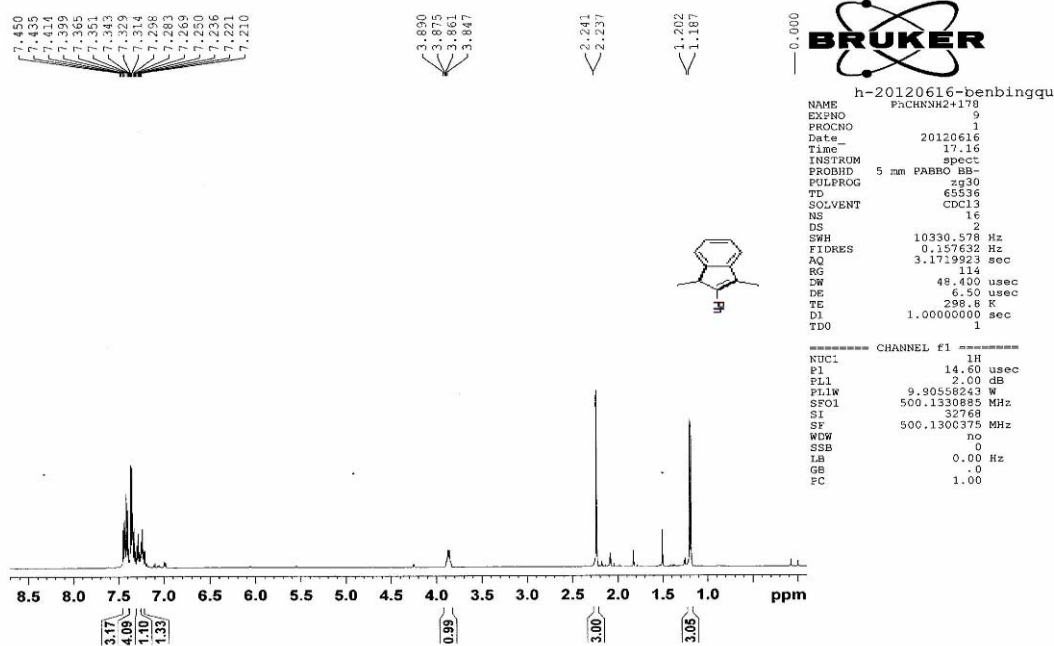




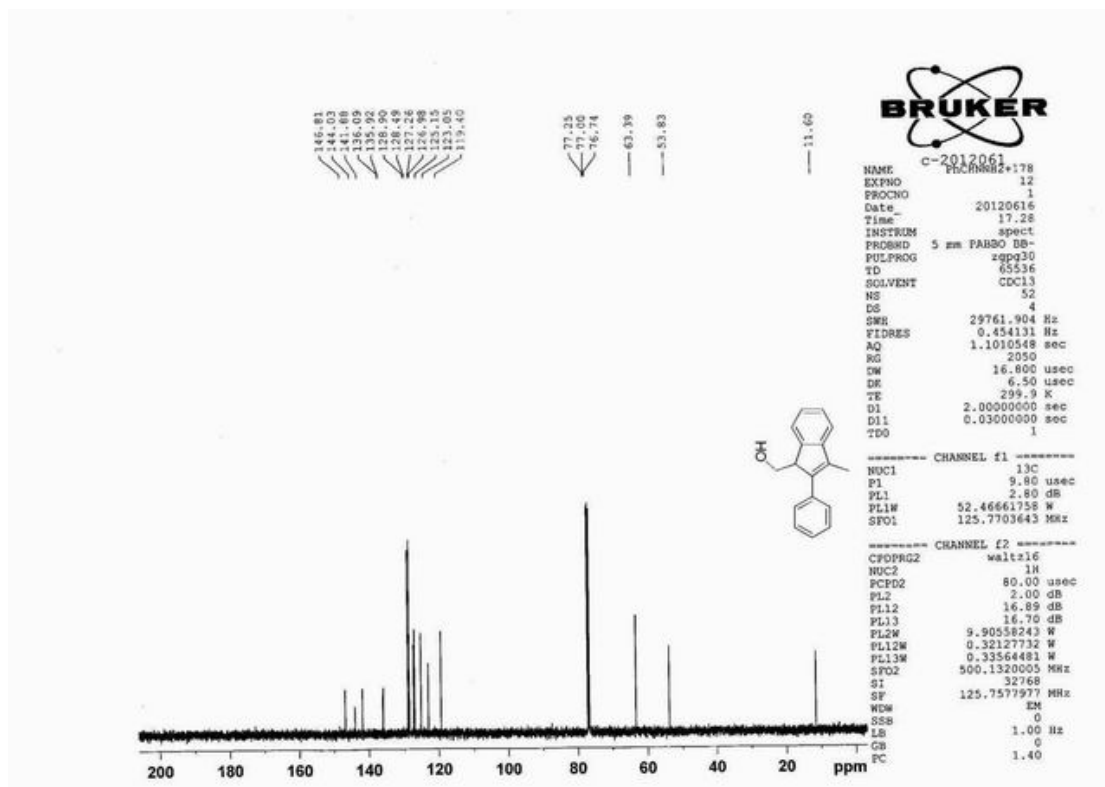
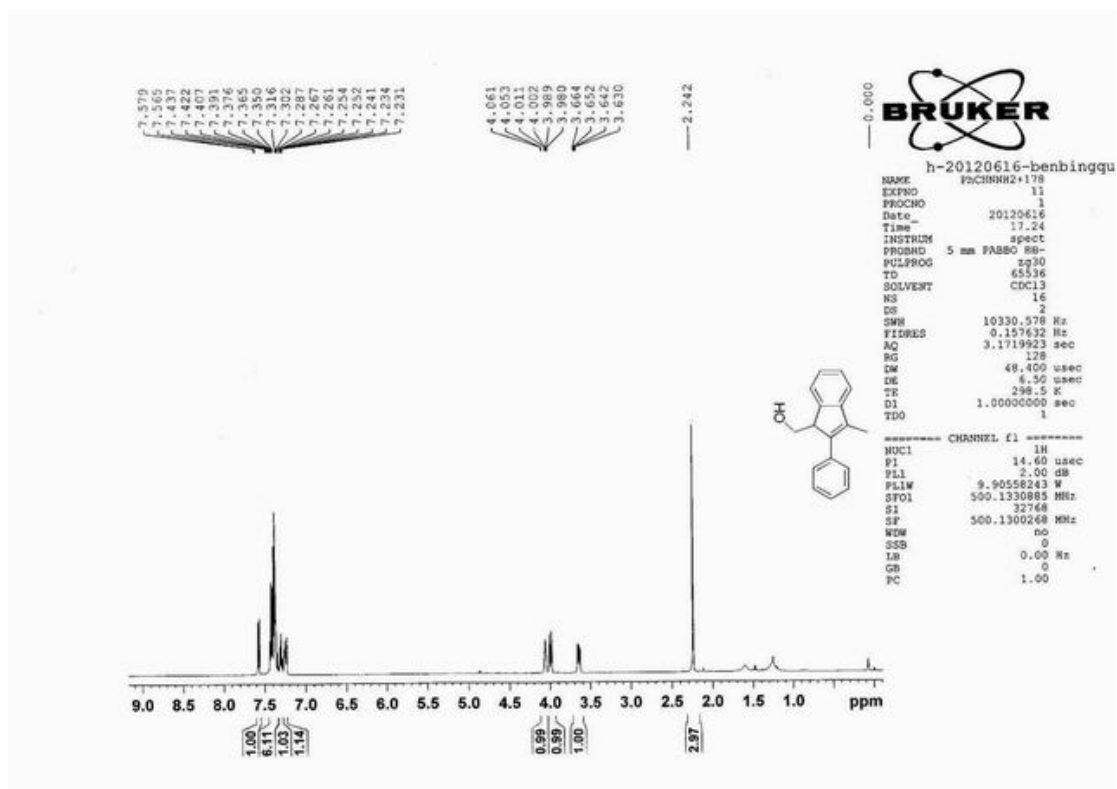
### 3-Methyl-1,2-diphenyl-1H-indene (4ag)



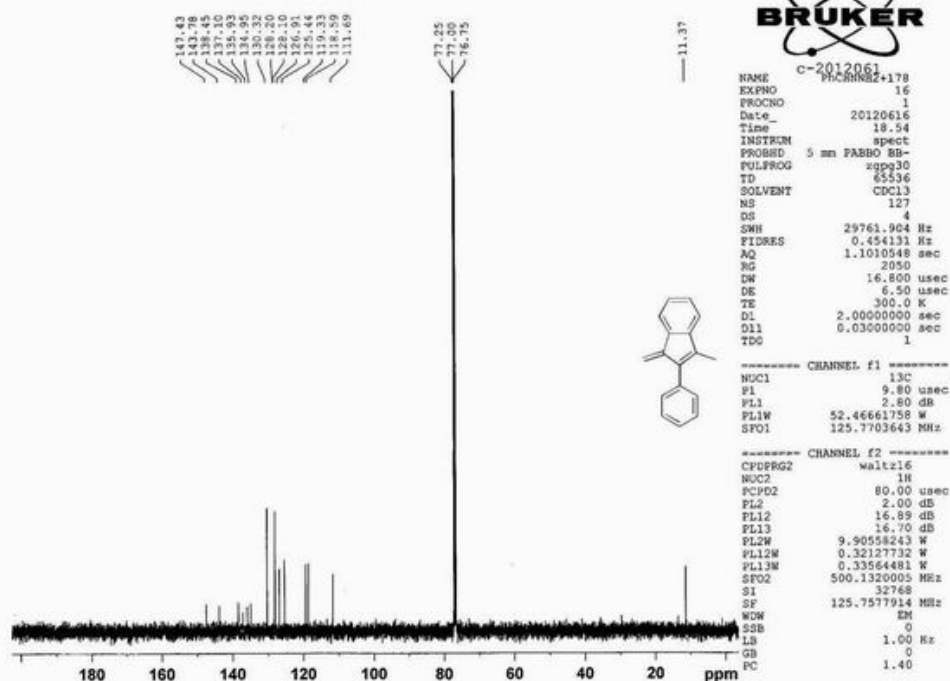
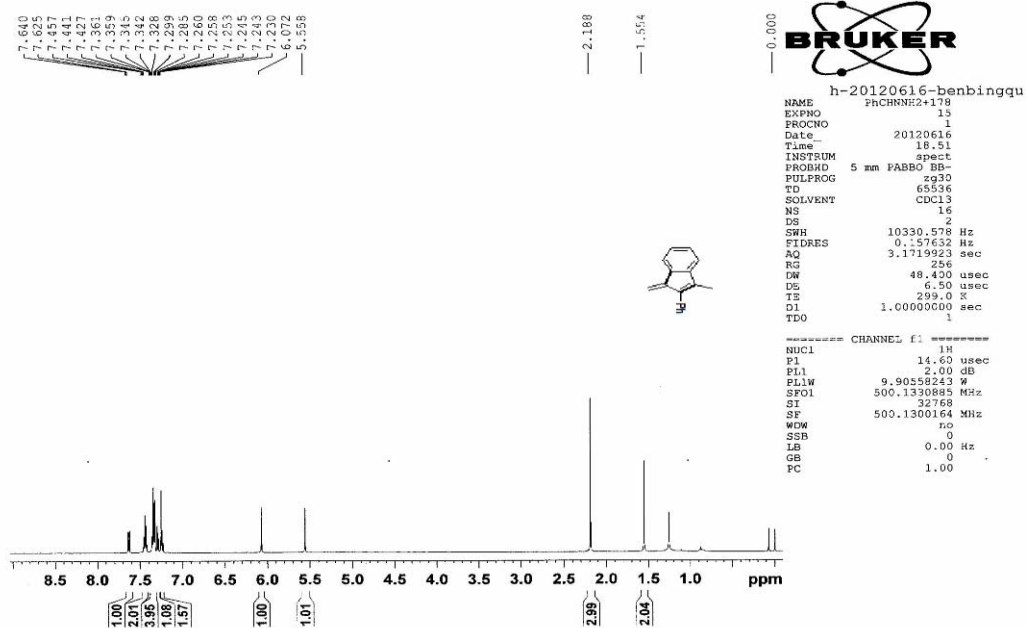
# 1,3-Dimethyl-2-phenyl-1H-indene (4cg)



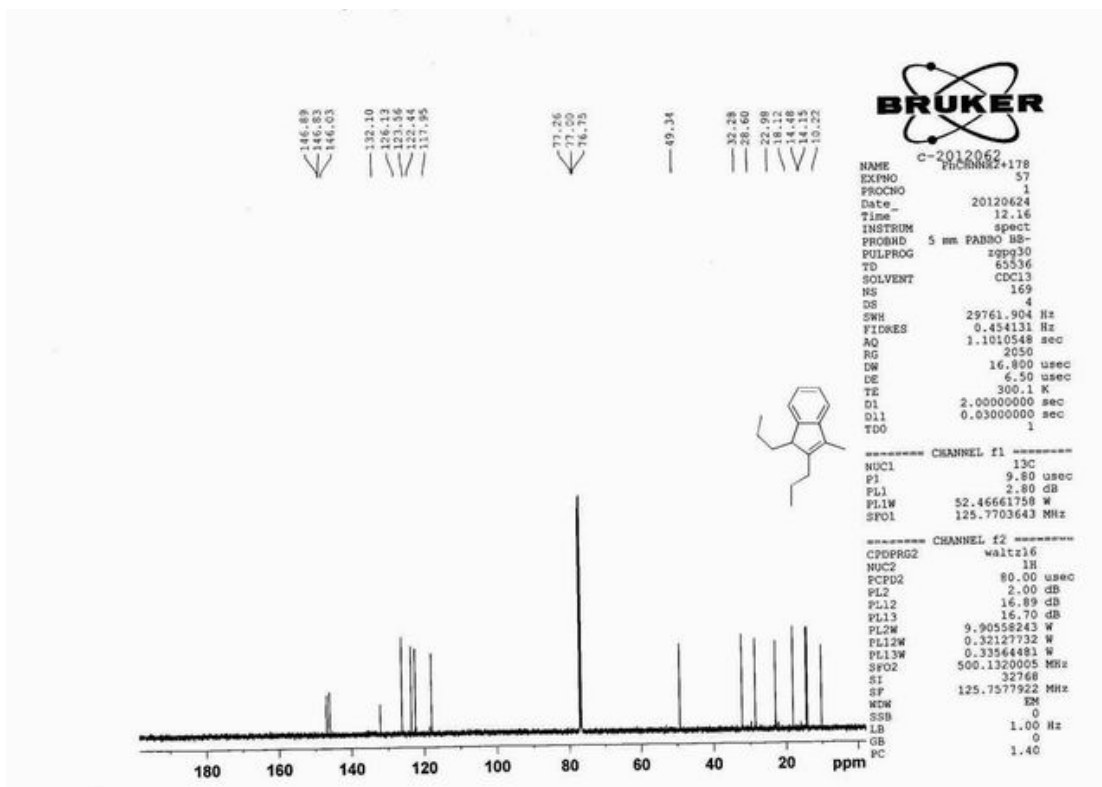
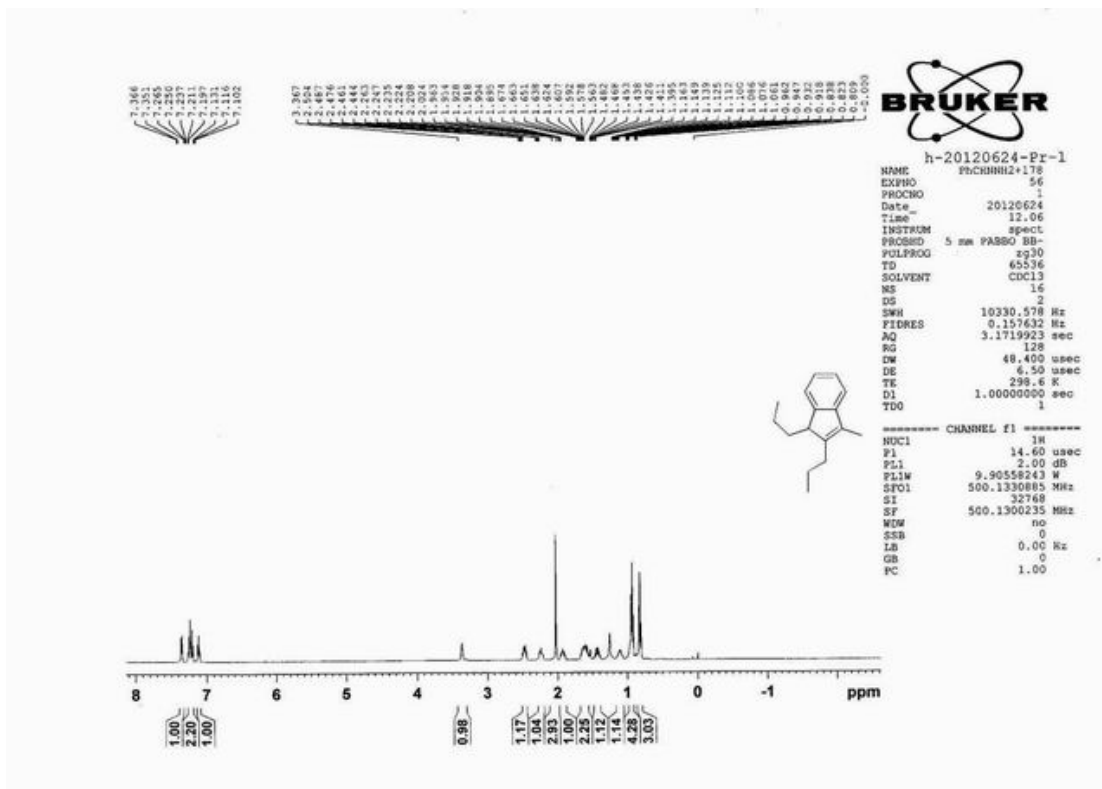
(3-methyl-2-phenyl-1H-inden-1-yl)methanol (4dg)



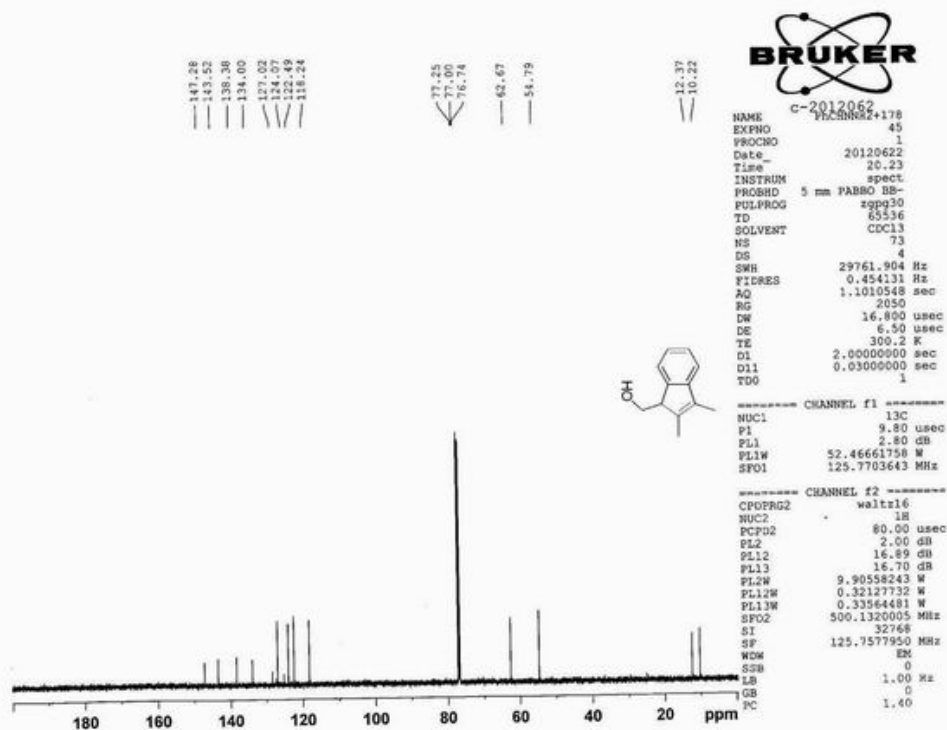
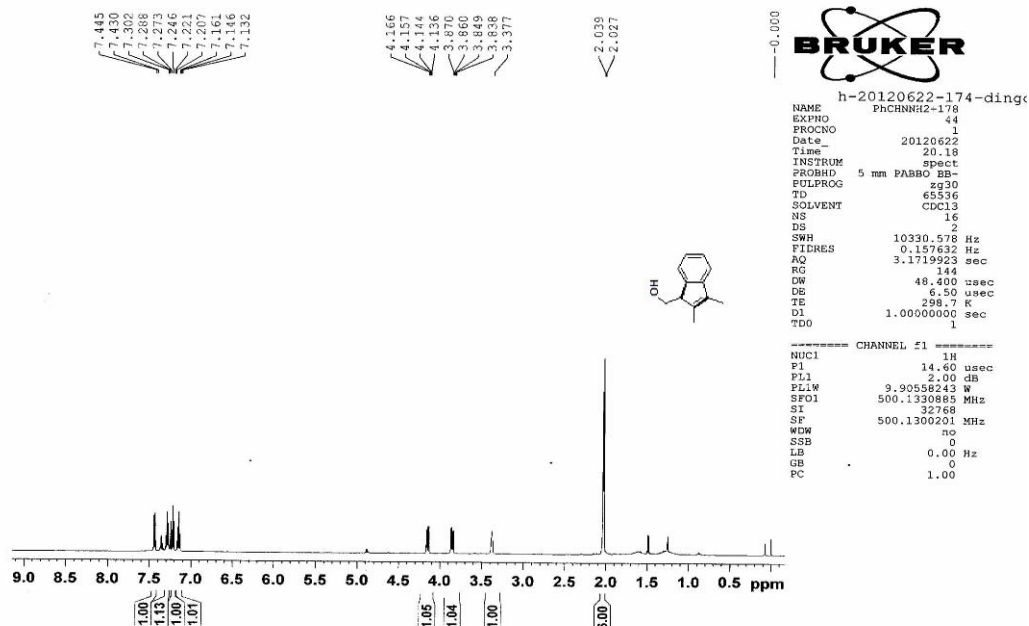
### 3-Methyl-1-methylene-2-phenyl-1H-indene (5dg)



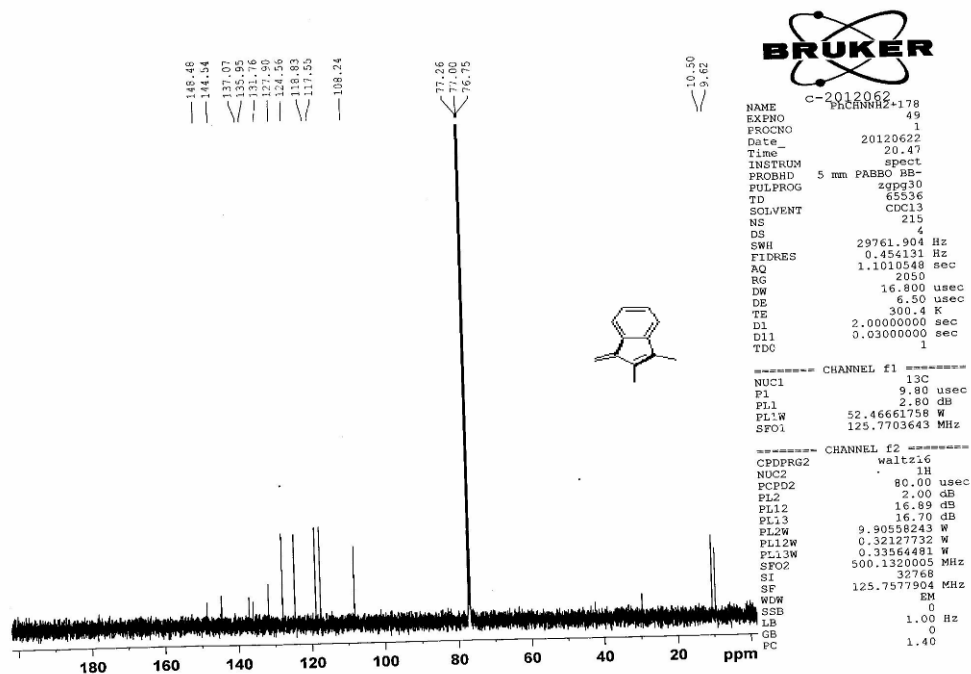
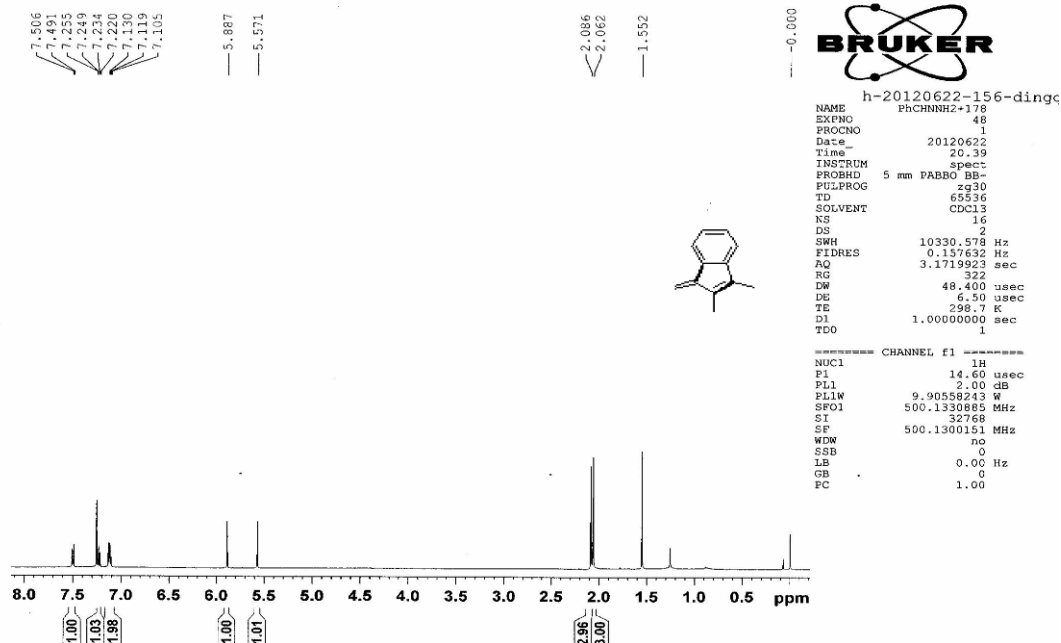
### 3-Methyl-1,2-dipropyl-1H-indene (4eg)



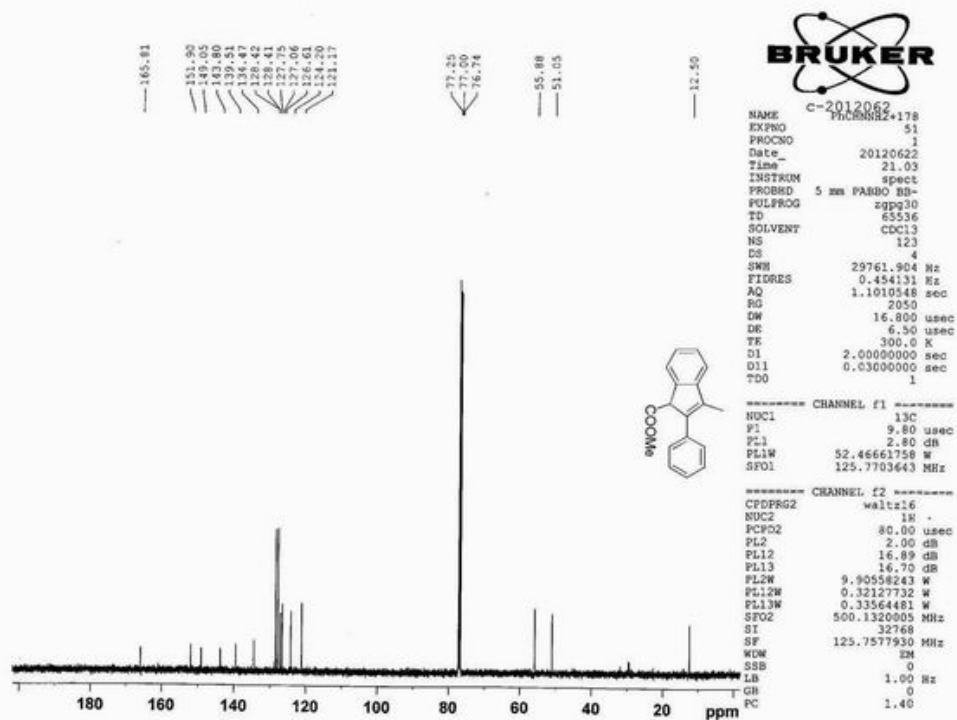
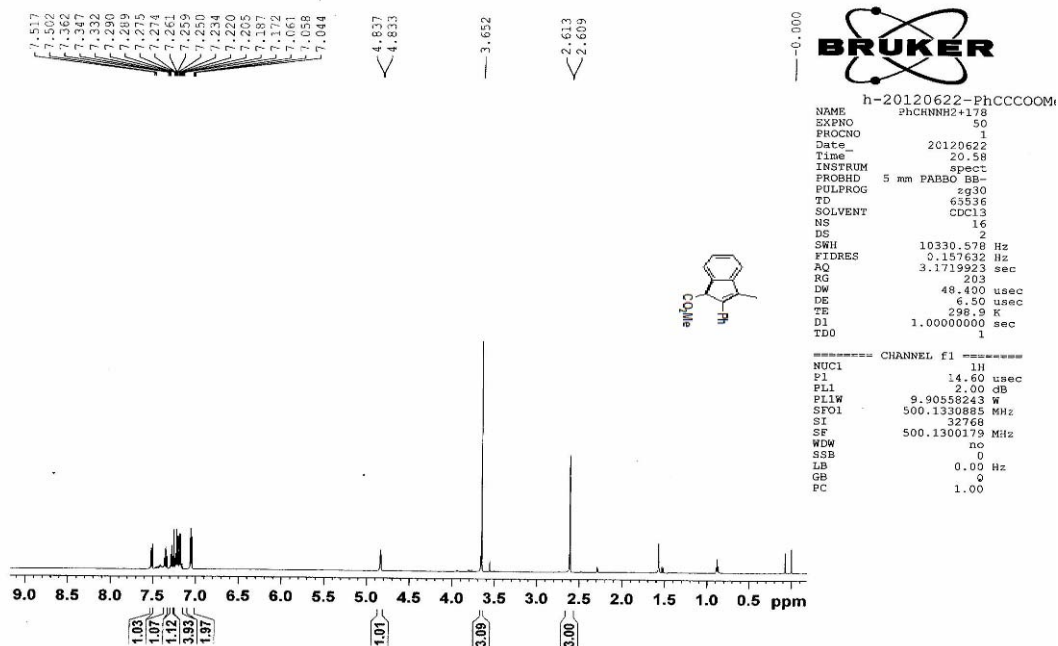
(2,3-Dimethyl-1H-inden-1-yl)methanol (4fg)



# 2,3-Dimethyl-1-methylene-1H-indene (5fg)

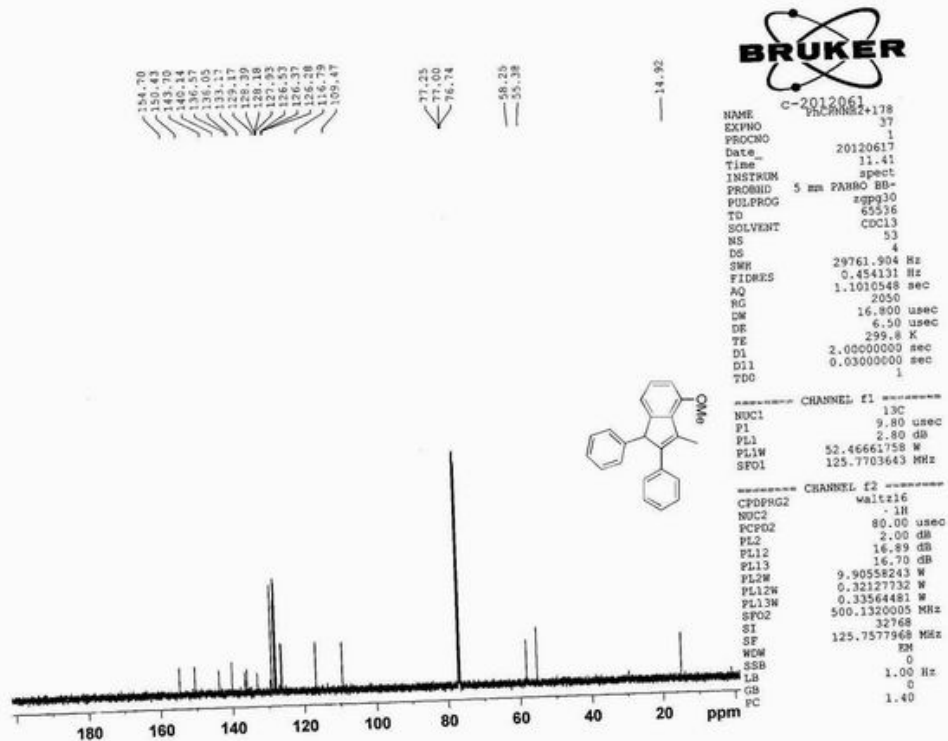
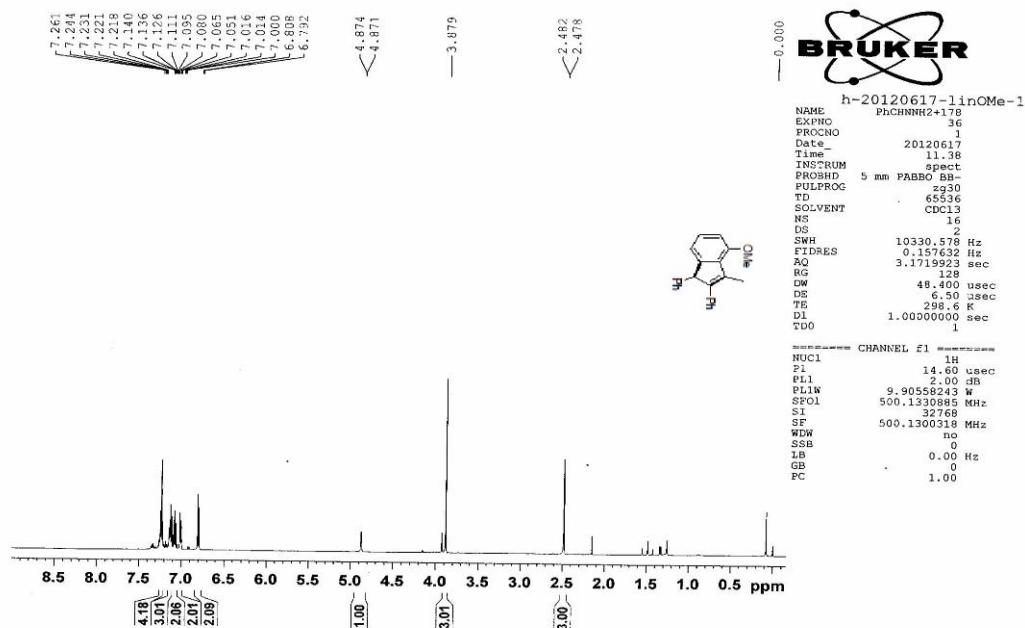


# Methyl 3-methyl-2-phenyl-1H-indene-1-carboxylate (4gg)

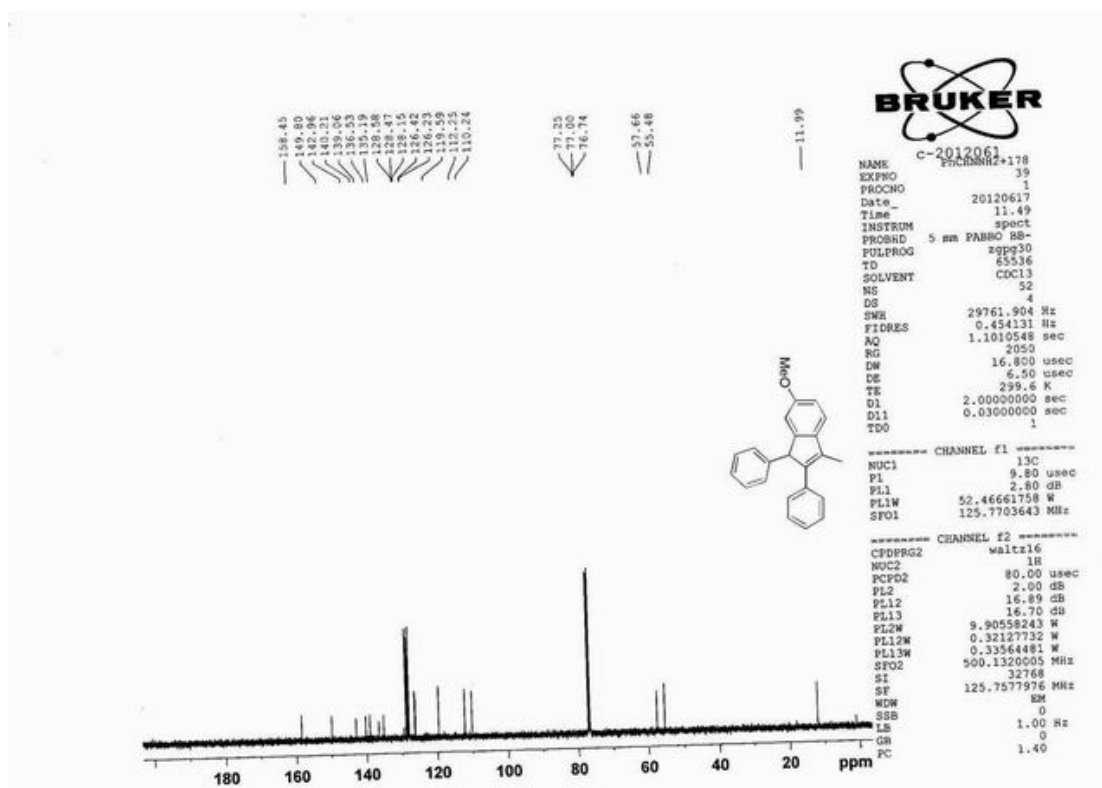




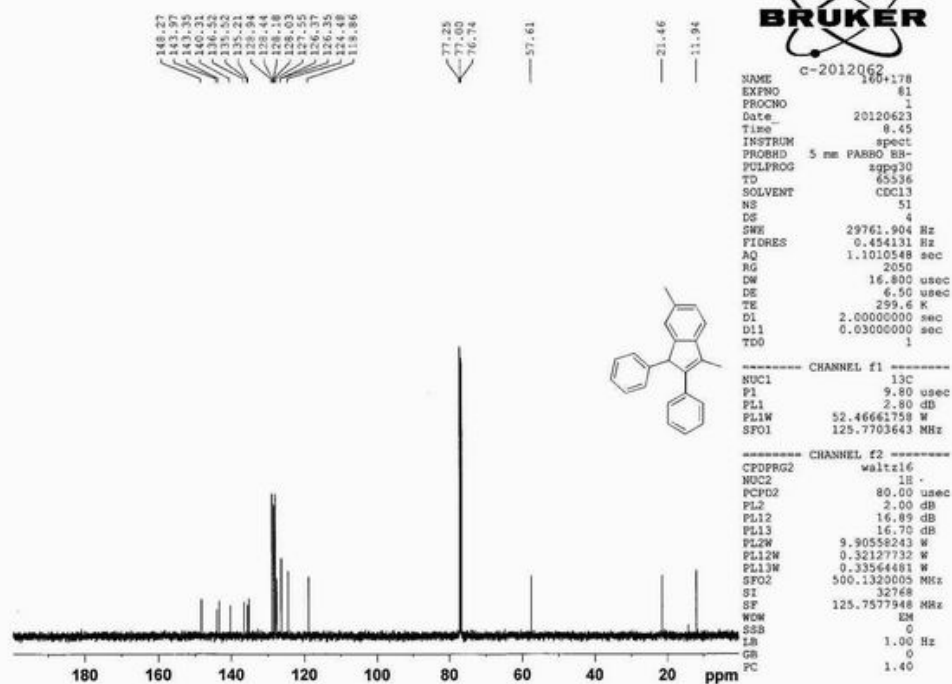
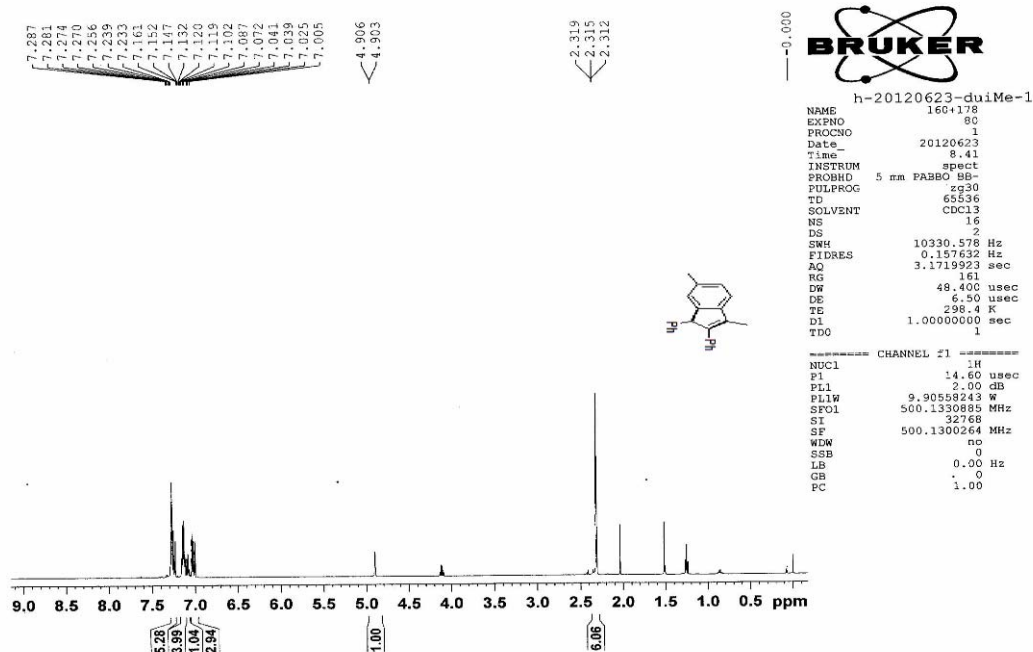
# 4-Methoxy-3-methyl-1,2-diphenyl-1H-indene (4au)



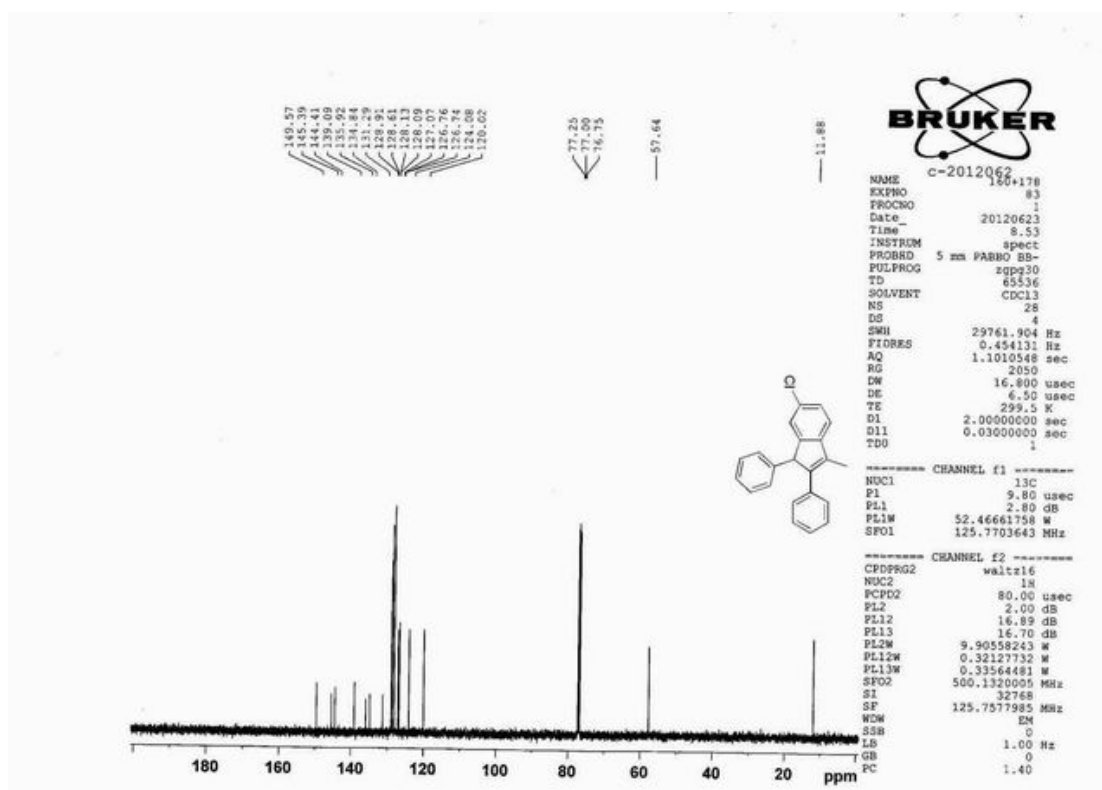
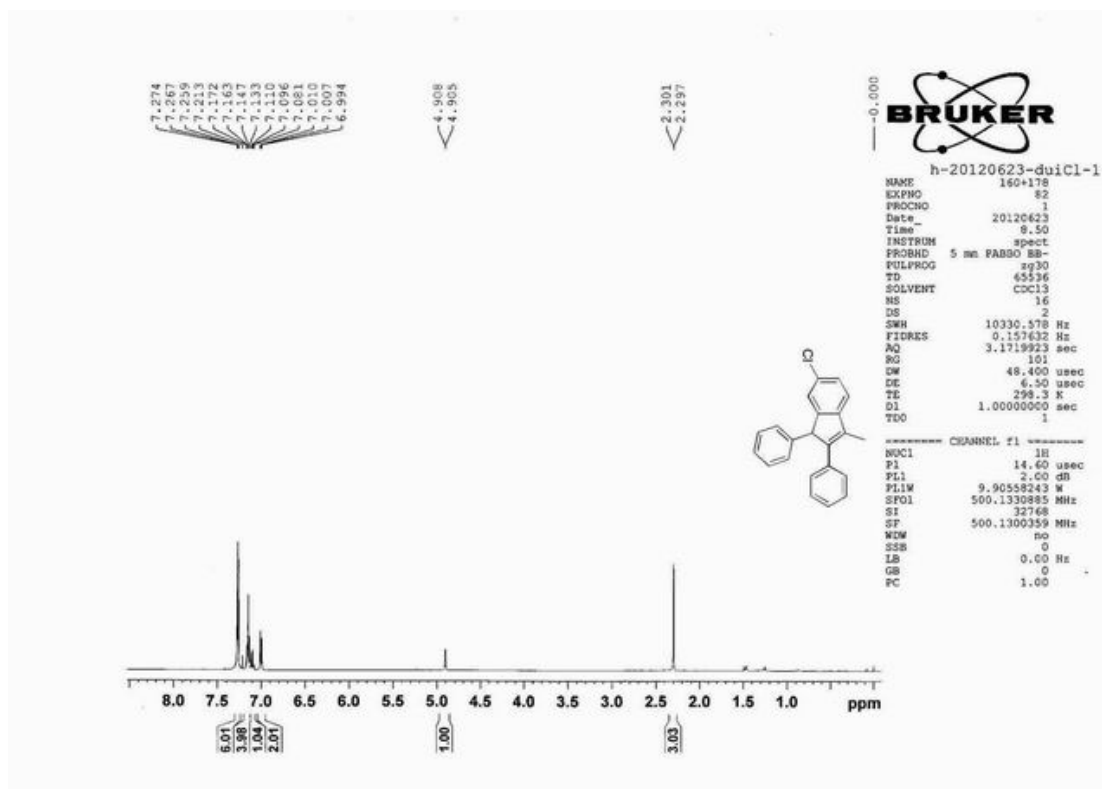
Chemical structure: COc1ccc2c(c1)c(c3ccccc23)C=C4C(=C5C(=C4)C(=C6C(=C5)C(=C7C(=C6)C(=C8C(=C7)C(=C9C(=C8)C(=C10C(=C9)C(=C11C(=C10)C(=C12C(=C11)C(=C13C(=C12)C(=C14C(=C13)C(=C15C(=C14)C(=C16C(=C15)C(=C17C(=C16)C(=C18C(=C17)C(=C19C(=C18)C(=C20C(=C19)C(=C21C(=C20)C(=C22C(=C21)C(=C23C(=C22)C(=C24C(=C23)C(=C25C(=C24)C(=C26C(=C25)C(=C27C(=C26)C(=C28C(=C27)C(=C29C(=C28)C(=C30C(=C29)C(=C31C(=C30)C(=C32C(=C31)C(=C33C(=C32)C(=C34C(=C33)C(=C35C(=C34)C(=C36C(=C35)C(=C37C(=C36)C(=C38C(=C37)C(=C39C(=C38)C(=C40C(=C39)C(=C41C(=C40)C(=C42C(=C41)C(=C43C(=C42)C(=C44C(=C43)C(=C45C(=C44)C(=C46C(=C45)C(=C47C(=C46)C(=C48C(=C47)C(=C49C(=C48)C(=C50C(=C49)C(=C51C(=C50)C(=C52C(=C51)C(=C53C(=C52)C(=C54C(=C53)C(=C55C(=C54)C(=C56C(=C55)C(=C57C(=C56)C(=C58C(=C57)C(=C59C(=C58)C(=C60C(=C59)C(=C61C(=C60)C(=C62C(=C61)C(=C63C(=C62)C(=C64C(=C63)C(=C65C(=C64)C(=C66C(=C65)C(=C67C(=C66)C(=C68C(=C67)C(=C69C(=C68)C(=C70C(=C69)C(=C71C(=C70)C(=C72C(=C71)C(=C73C(=C72)C(=C74C(=C73)C(=C75C(=C74)C(=C76C(=C75)C(=C77C(=C76)C(=C78C(=C77)C(=C79C(=C78)C(=C80C(=C79)C(=C81C(=C80)C(=C82C(=C81)C(=C83C(=C82)C(=C84C(=C83)C(=C85C(=C84)C(=C86C(=C85)C(=C87C(=C86)C(=C88C(=C87)C(=C89C(=C88)C(=C90C(=C89)C(=C91C(=C90)C(=C92C(=C91)C(=C93C(=C92)C(=C94C(=C93)C(=C95C(=C94)C(=C96C(=C95)C(=C97C(=C96)C(=C98C(=C97)C(=C99C(=C98)C(=C100C(=C99)C(=C101C(=C100)C(=C102C(=C101)C(=C103C(=C102)C(=C104C(=C103)C(=C105C(=C104)C(=C106C(=C105)C(=C107C(=C106)C(=C108C(=C107)C(=C109C(=C108)C(=C110C(=C109)C(=C111C(=C110)C(=C112C(=C111)C(=C113C(=C112)C(=C114C(=C113)C(=C115C(=C114)C(=C116C(=C115)C(=C117C(=C116)C(=C118C(=C117)C(=C119C(=C118)C(=C120C(=C119)C(=C121C(=C120)C(=C122C(=C121)C(=C123C(=C122)C(=C124C(=C123)C(=C125C(=C124)C(=C126C(=C125)C(=C127C(=C126)C(=C128C(=C127)C(=C129C(=C128)C(=C130C(=C129)C(=C131C(=C130)C(=C132C(=C131)C(=C133C(=C132)C(=C134C(=C133)C(=C135C(=C134)C(=C136C(=C135)C(=C137C(=C136)C(=C138C(=C137)C(=C139C(=C138)C(=C140C(=C139)C(=C141C(=C140)C(=C142C(=C141)C(=C143C(=C142)C(=C144C(=C143)C(=C145C(=C144)C(=C146C(=C145)C(=C147C(=C146)C(=C148C(=C147)C(=C149C(=C148)C(=C150C(=C149)C(=C151C(=C150)C(=C152C(=C151)C(=C153C(=C152)C(=C154C(=C153)C(=C155C(=C154)C(=C156C(=C155)C(=C157C(=C156)C(=C158C(=C157)C(=C159C(=C158)C(=C160C(=C159)C(=C161C(=C160)C(=C162C(=C161)C(=C163C(=C162)C(=C164C(=C163)C(=C165C(=C164)C(=C166C(=C165)C(=C167C(=C166)C(=C168C(=C167)C(=C169C(=C168)C(=C170C(=C169)C(=C171C(=C170)C(=C172C(=C171)C(=C173C(=C172)C(=C174C(=C173)C(=C175C(=C174)C(=C176C(=C175)C(=C177C(=C176)C(=C178C(=C177)C(=C179C(=C178)C(=C180C(=C179)C(=C181C(=C180)C(=C182C(=C181)C(=C183C(=C182)C(=C184C(=C183)C(=C185C(=C184)C(=C186C(=C185)C(=C187C(=C186)C(=C188C(=C187)C(=C189C(=C188)C(=C190C(=C189)C(=C191C(=C190)C(=C192C(=C191)C(=C193C(=C192)C(=C194C(=C193)C(=C195C(=C194)C(=C196C(=C195)C(=C197C(=C196)C(=C198C(=C197)C(=C199C(=C198)C(=C200C(=C199)C(=C201C(=C200)C(=C202C(=C201)C(=C203C(=C202)C(=C204C(=C203)C(=C205C(=C204)C(=C206C(=C205)C(=C207C(=C206)C(=C208C(=C207)C(=C209C(=C208)C(=C210C(=C209)C(=C211C(=C210)C(=C212C(=C211)C(=C213C(=C212)C(=C214C(=C213)C(=C215C(=C214)C(=C216C(=C215)C(=C217C(=C216)C(=C218C(=C217)C(=C219C(=C218)C(=C220C(=C219)C(=C221C(=C220)C(=C222C(=C221)C(=C223C(=C222)C(=C224C(=C223)C(=C225C(=C224)C(=C226C(=C225)C(=C227C(=C226)C(=C228C(=C227)C(=C229C(=C228)C(=C230C(=C229)C(=C231C(=C230)C(=C232C(=C231)C(=C233C(=C232)C(=C234C(=C233)C(=C235C(=C234)C(=C236C(=C235)C(=C237C(=C236)C(=C238C(=C237)C(=C239C(=C238)C(=C240C(=C239)C(=C241C(=C240)C(=C242C(=C241)C(=C243C(=C242)C(=C244C(=C243)C(=C245C(=C244)C(=C246C(=C245)C(=C247C(=C246)C(=C248C(=C247)C(=C249C(=C248)C(=C250C(=C249)C(=C251C(=C250)C(=C252C(=C251)C(=C253C(=C252)C(=C254C(=C253)C(=C255C(=C254)C(=C256C(=C255)C(=C257C(=C256)C(=C258C(=C257)C(=C259C(=C258)C(=C260C(=C259)C(=C261C(=C260)C(=C262C(=C261)C(=C263C(=C262)C(=C264C(=C263)C(=C265C(=C264)C(=C266C(=C265)C(=C267C(=C266)C(=C268C(=C267)C(=C269C(=C268)C(=C270C(=C269)C(=C271C(=C270)C(=C272C(=C271)C(=C273C(=C272)C(=C274C(=C273)C(=C275C(=C274)C(=C276C(=C275)C(=C277C(=C276)C(=C278C(=C277)C(=C279C(=C278)C(=C280C(=C27



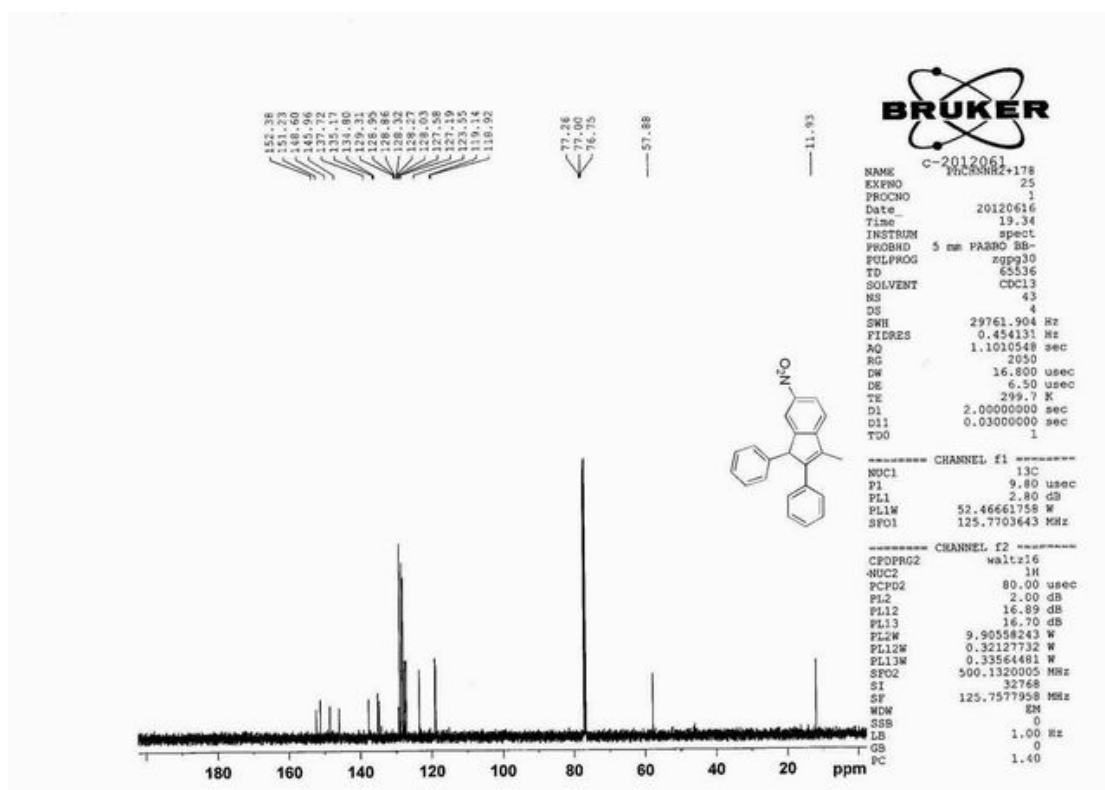
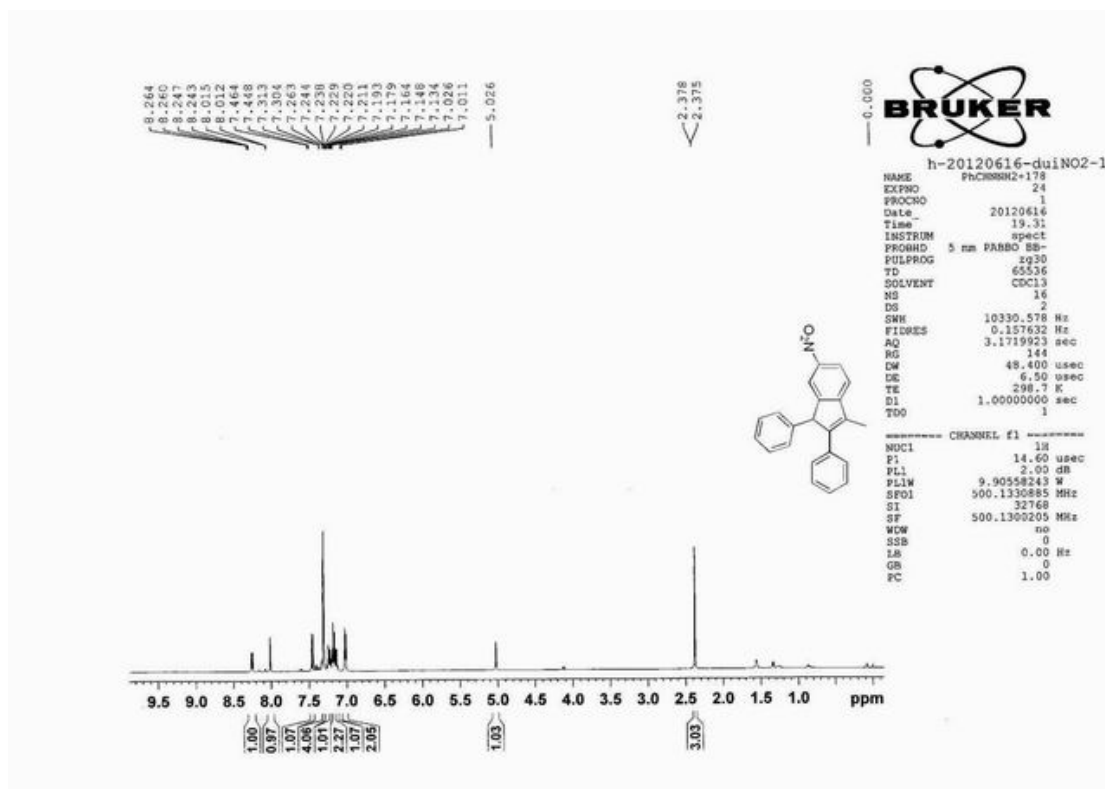
# 3,6-dimethyl-1,2-diphenyl-1H-indene (4aw)



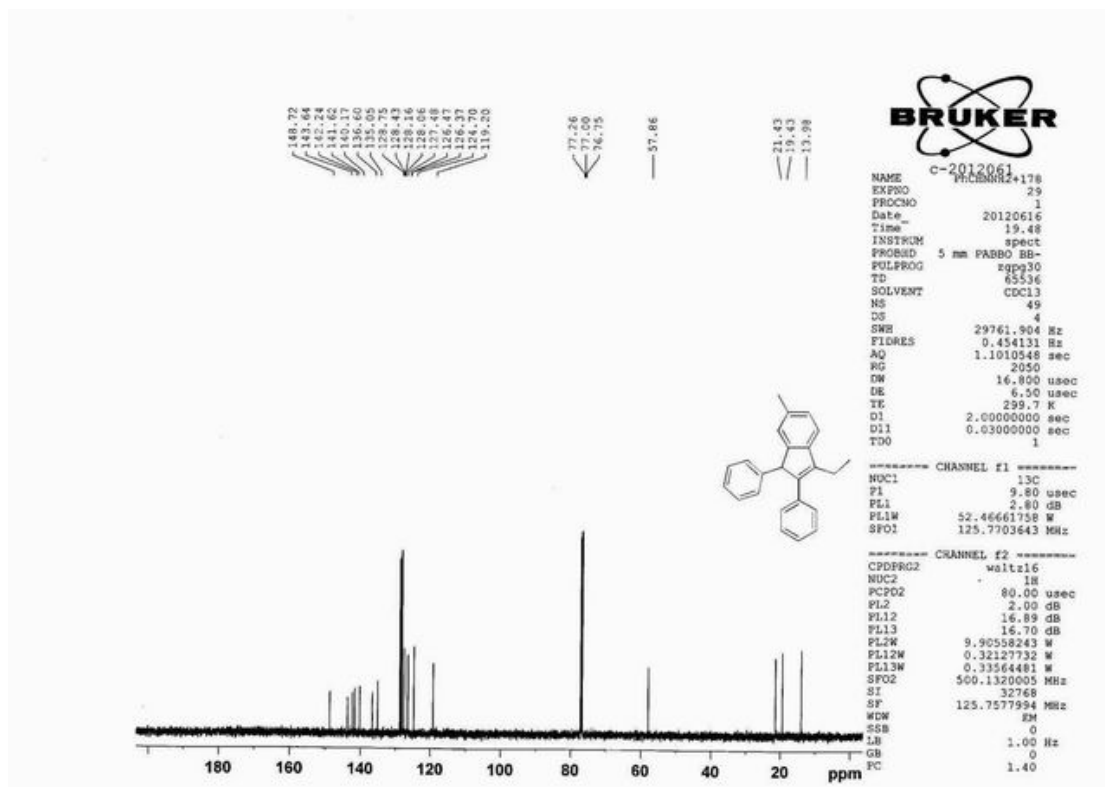
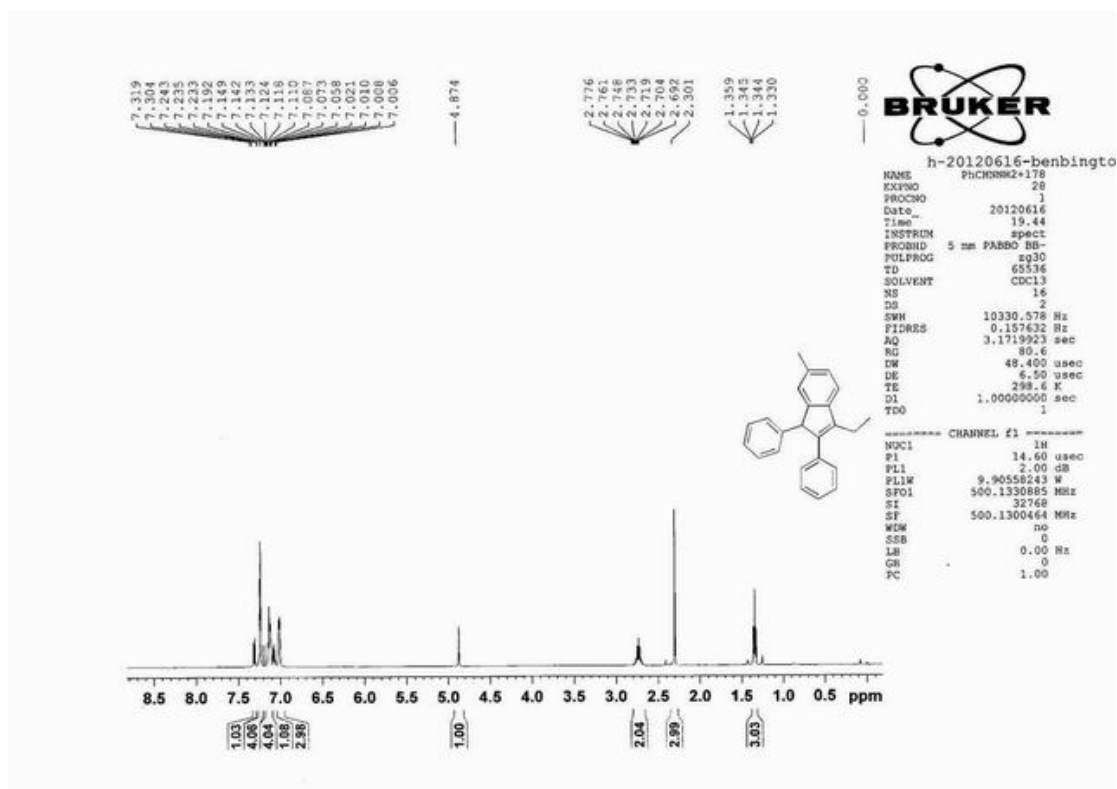
# 6-Chloro-3-methyl-1,2-diphenyl-1H-indene (4ax)



### 3-Methyl-6-nitro-1,2-diphenyl-1H-indene (4ay)



### 3-Ethyl-6-methyl-1,2-diphenyl-1H-indene (4az)



# 1,2-bis(1-phenylethylidene)hydrazine (6aa)

