

Supporting information

Regioselective Synthesis of Chromones via Cyclocarbonylative Sonogashira Coupling Catalyzed by Highly Active Bridged-Bis(N- Heterocyclic Carbene)Palladium(II) Complexes

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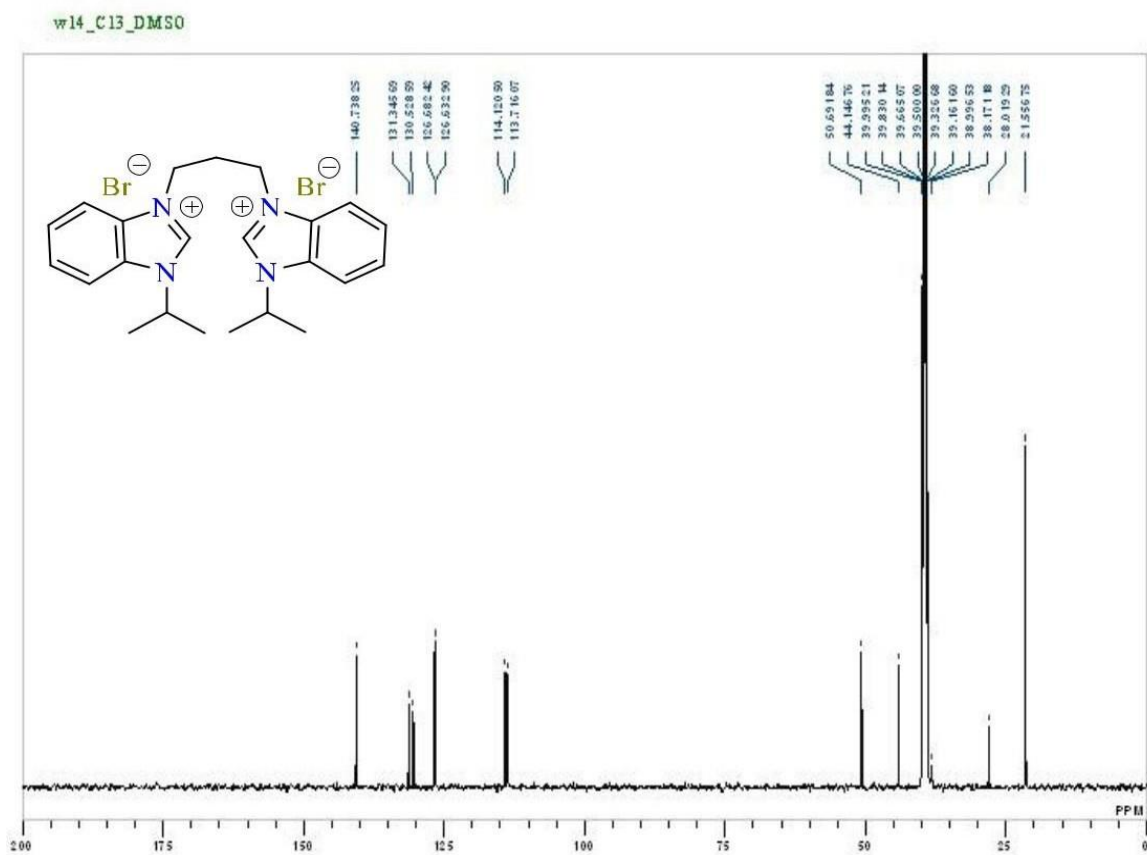
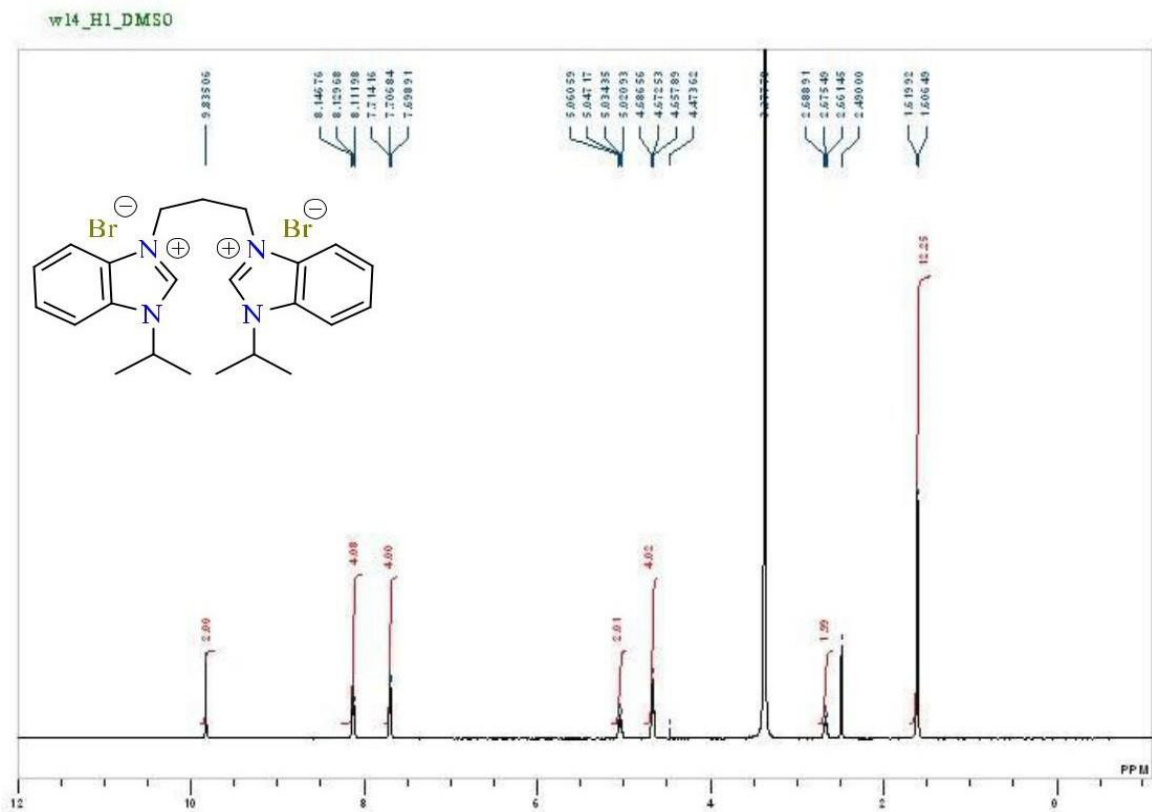


Figure S1. ^1H NMR and ^{13}C NMR spectra of pre-ligand L1

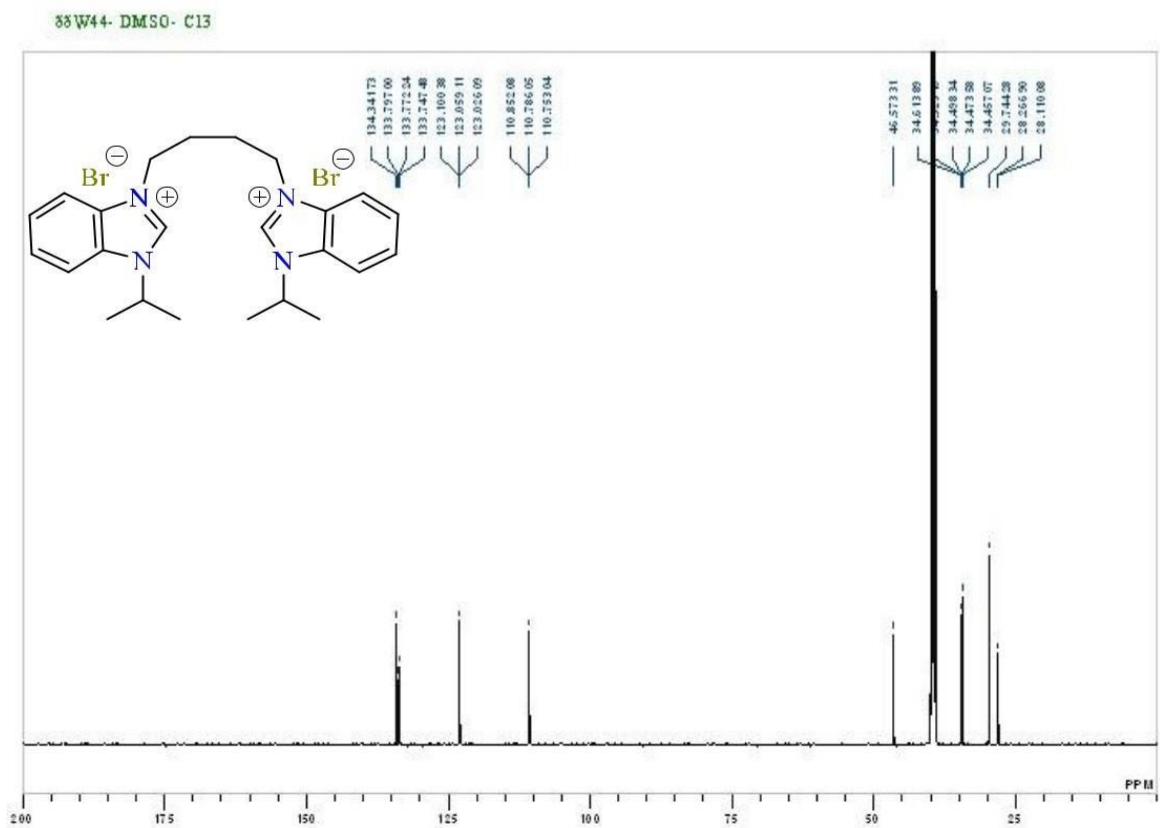
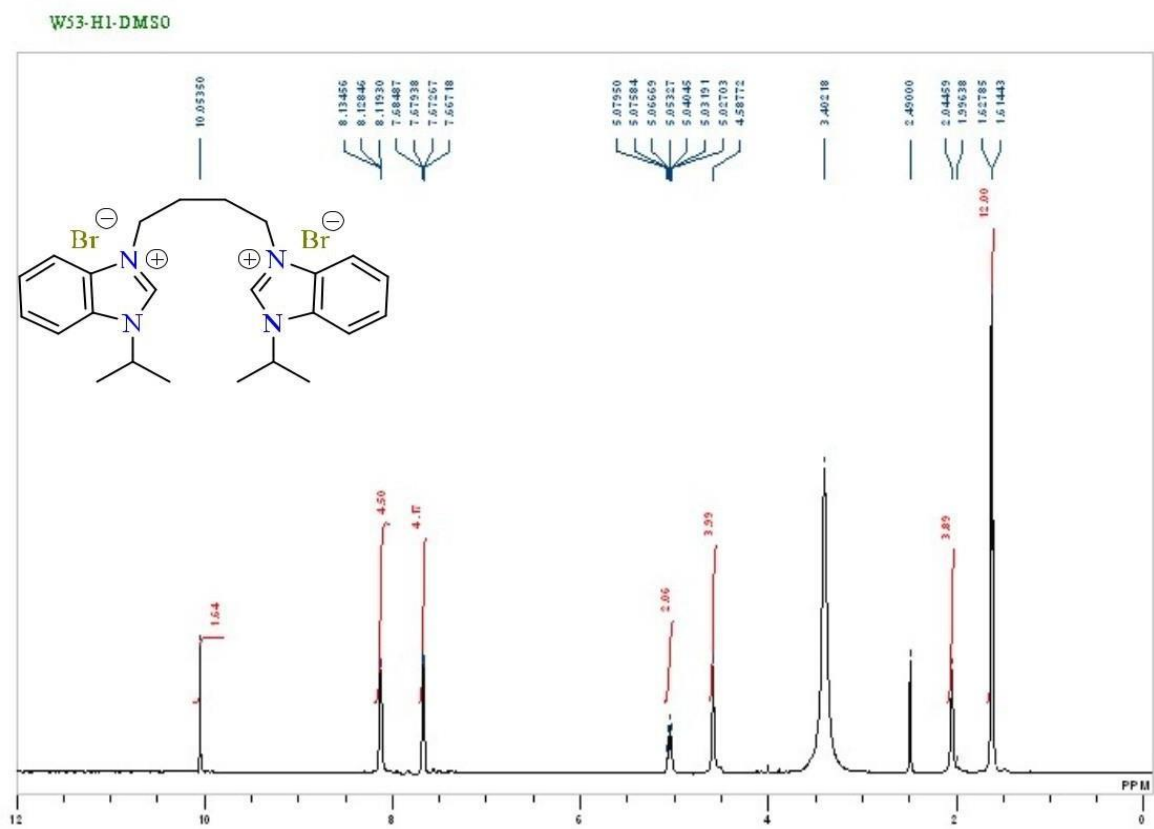


Figure S2. ¹H NMR and ¹³C NMR spectra of pre-ligand L2

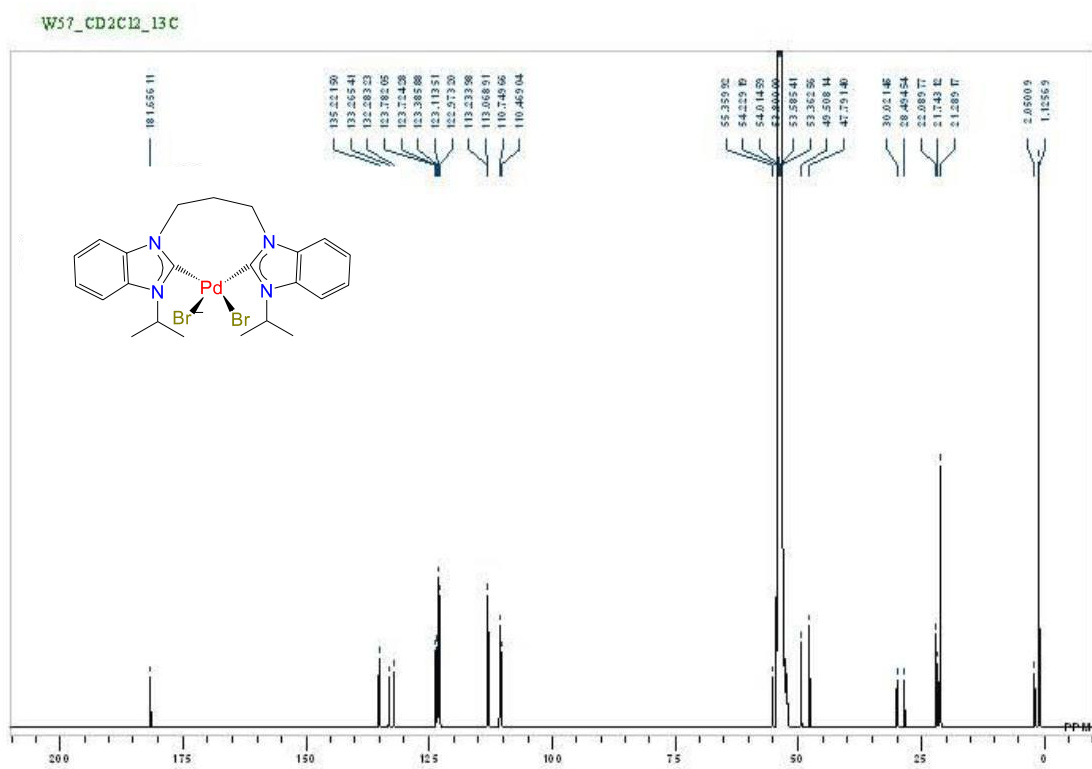
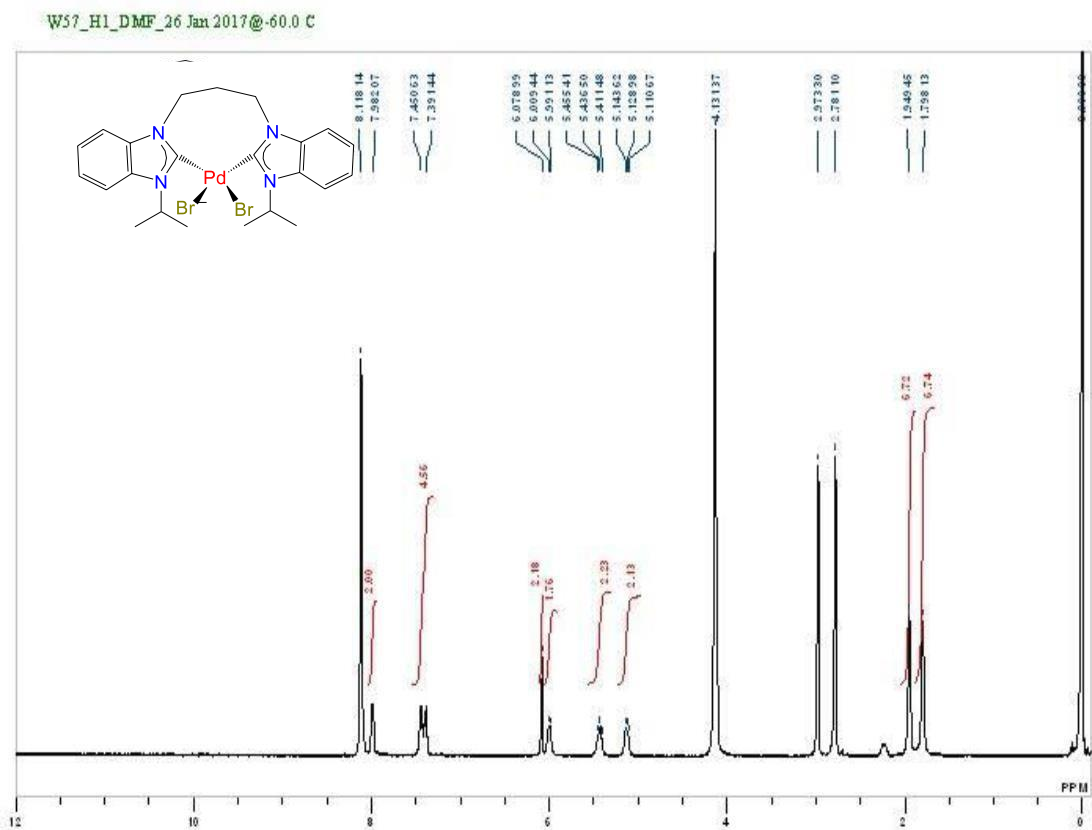


Figure S4. ¹H NMR and ¹³C NMR spectra of complex C1

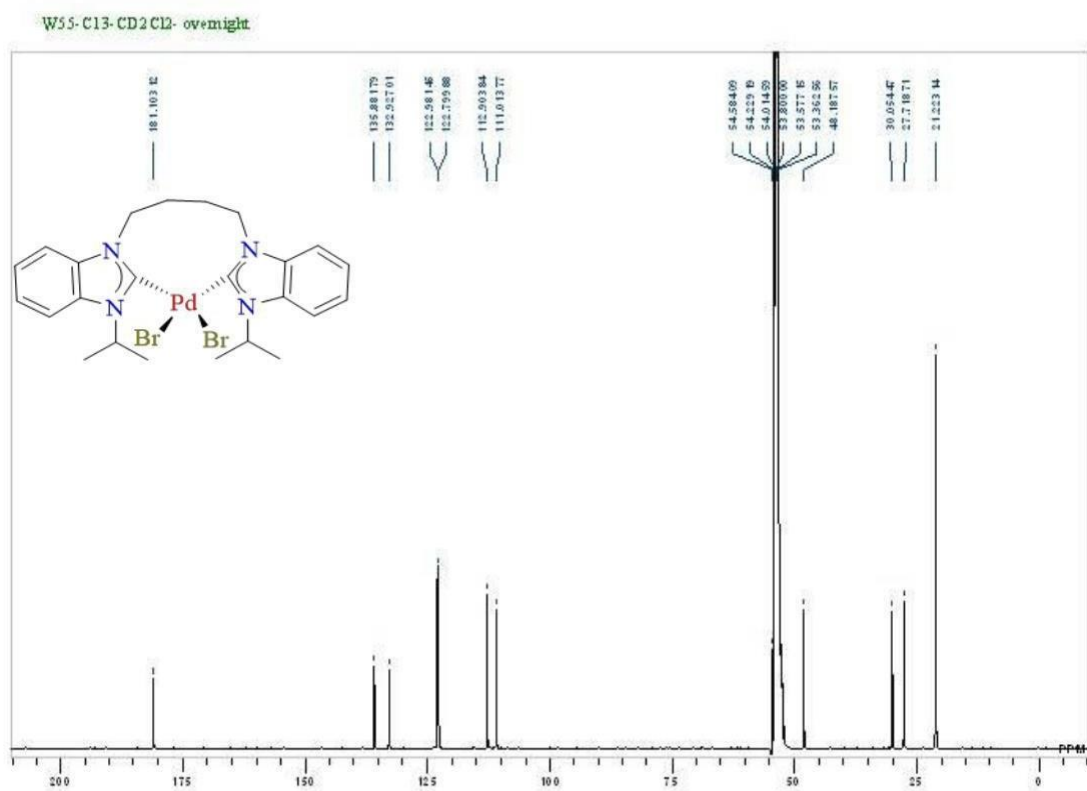
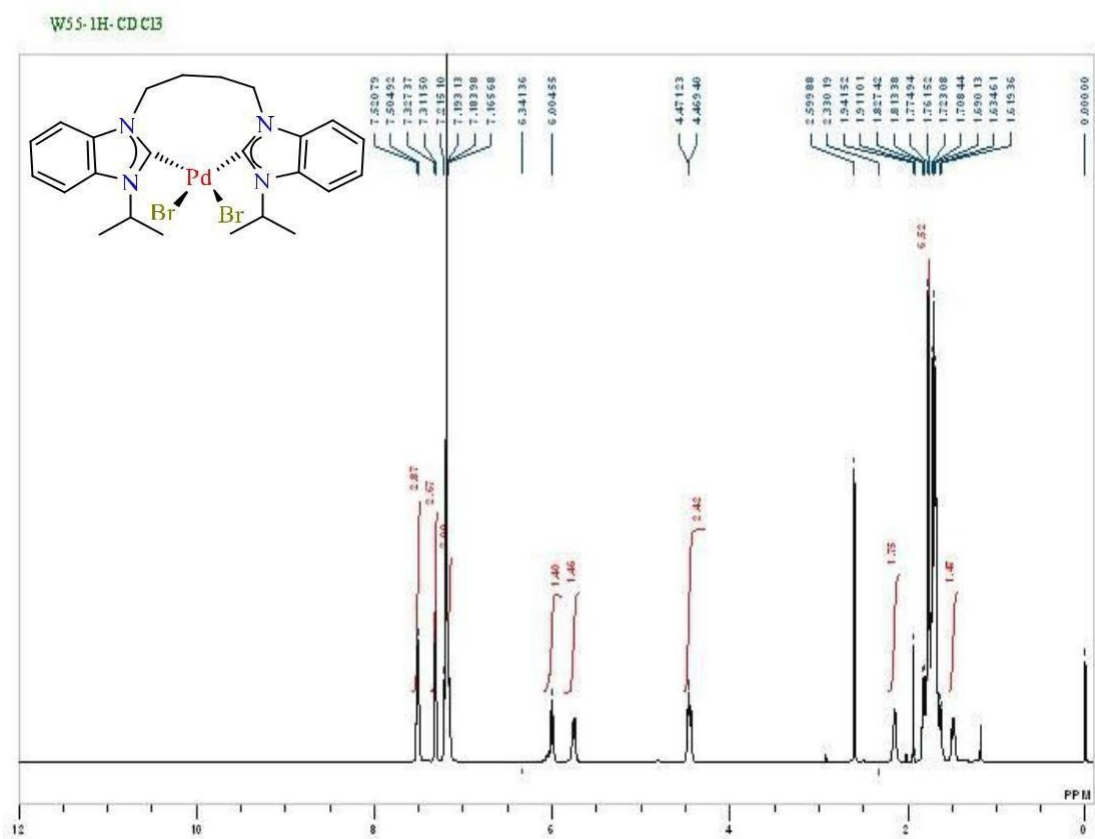


Figure S5. ¹H NMR and ¹³C NMR spectra of complex C2

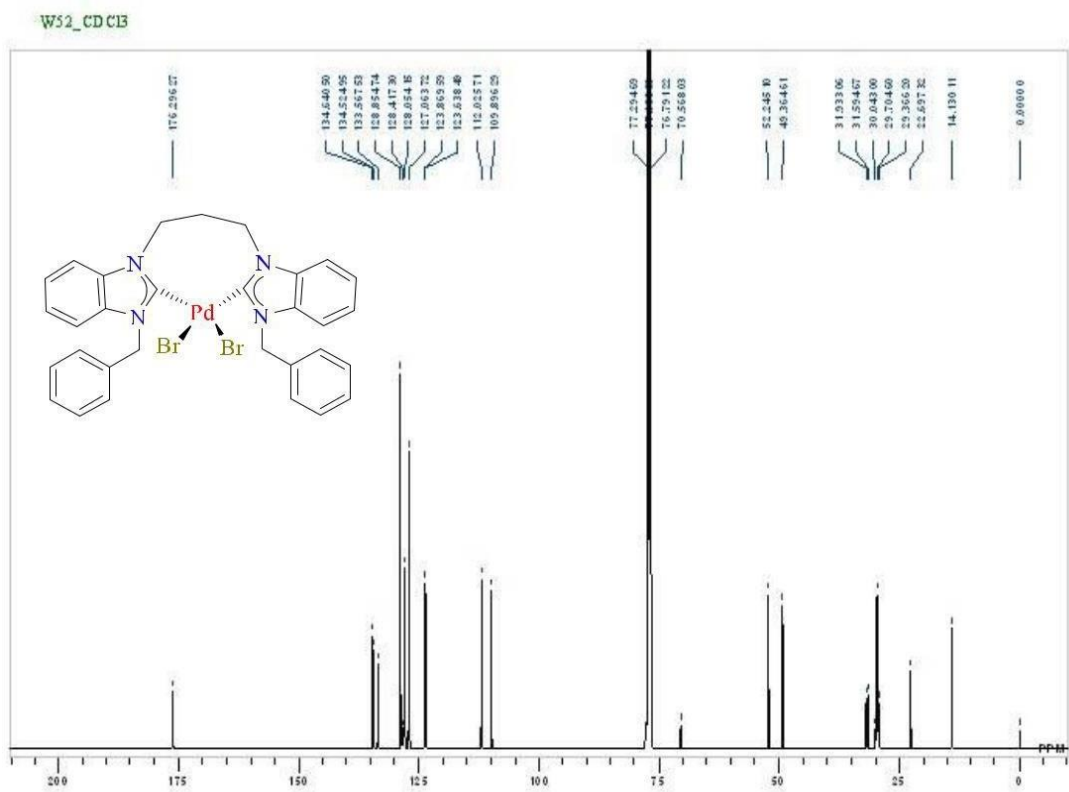
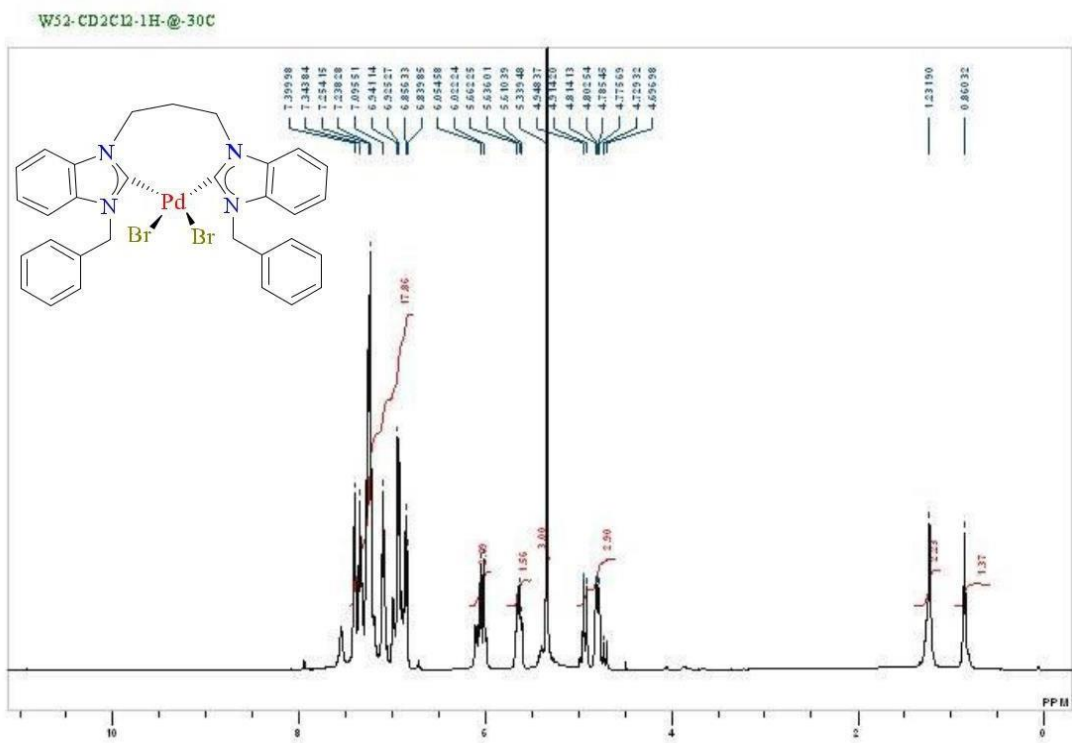


Figure S6. ^1H NMR and ^{13}C NMR spectra of complex C3

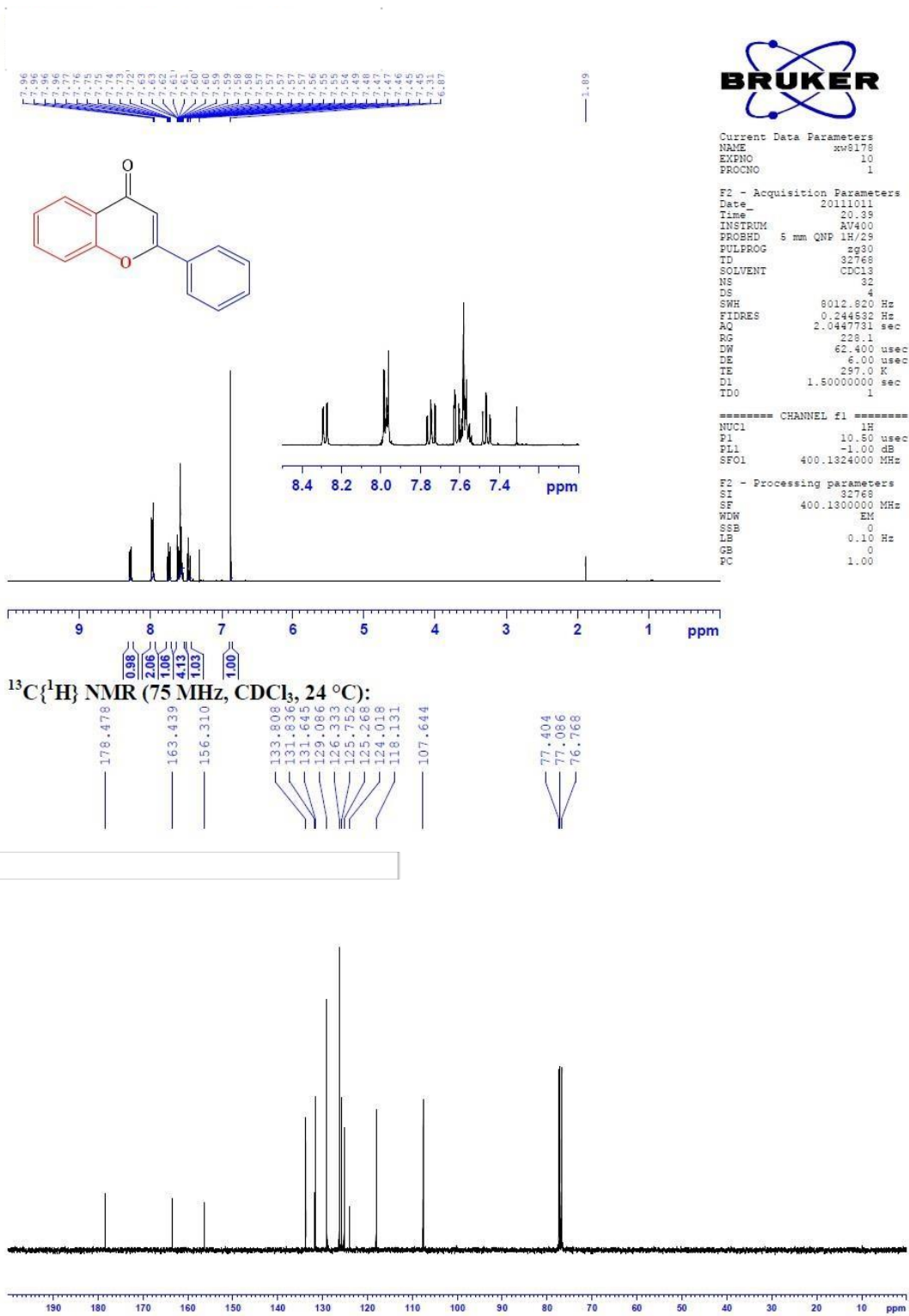
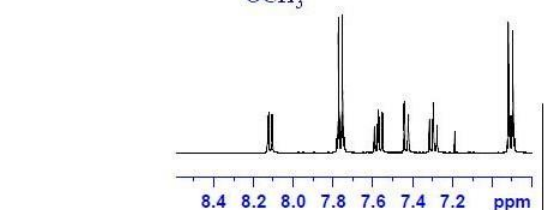
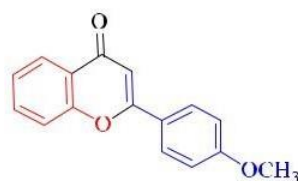


Figure S7. ^1H NMR and ^{13}C NMR spectra of product 3aa

^1H NMR (300 MHz, CDCl_3 , 24 °C):

Wu XW8196

AulH CDC13 /opt/topspin 1110 40



Current Data Parameters
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EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111013
Time 8.08
INSTRUM AV400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 4
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 128
DW 62.400 usec
DE 6.00 usec
TE 297.0 K
D1 1.5000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 -1.00 dB
SF01 400.1324000 MHz

F2 - Processing parameters
SI 32768
SF 400.1300500 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3 , 24 °C):

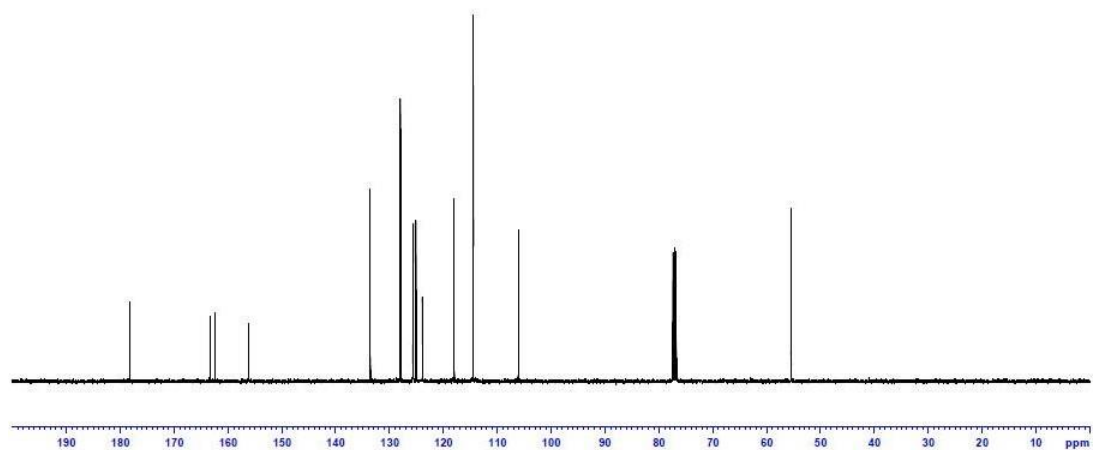
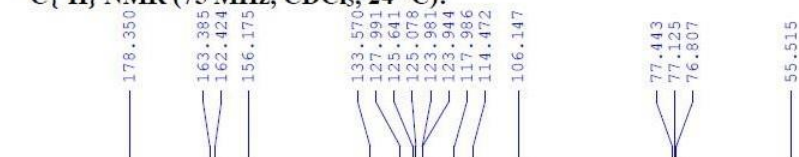


Figure S8. ^1H NMR and ^{13}C NMR spectra of product 3ab

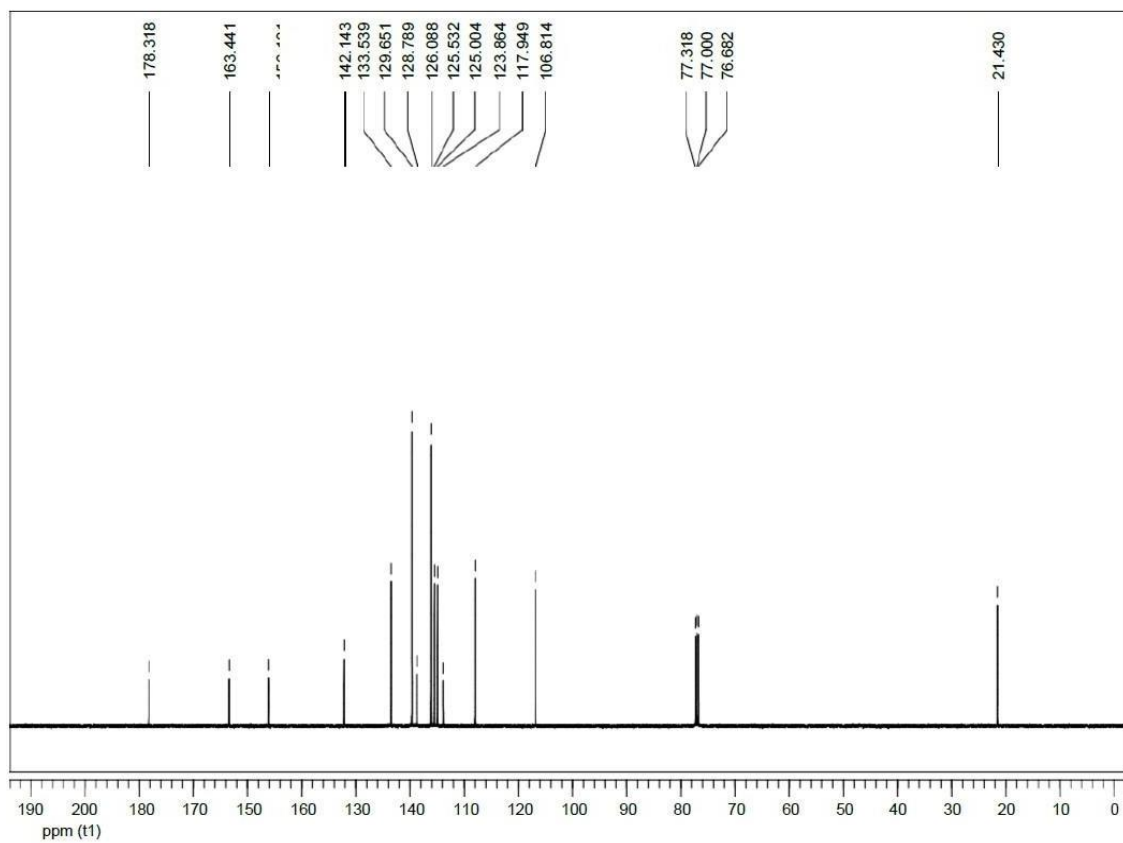
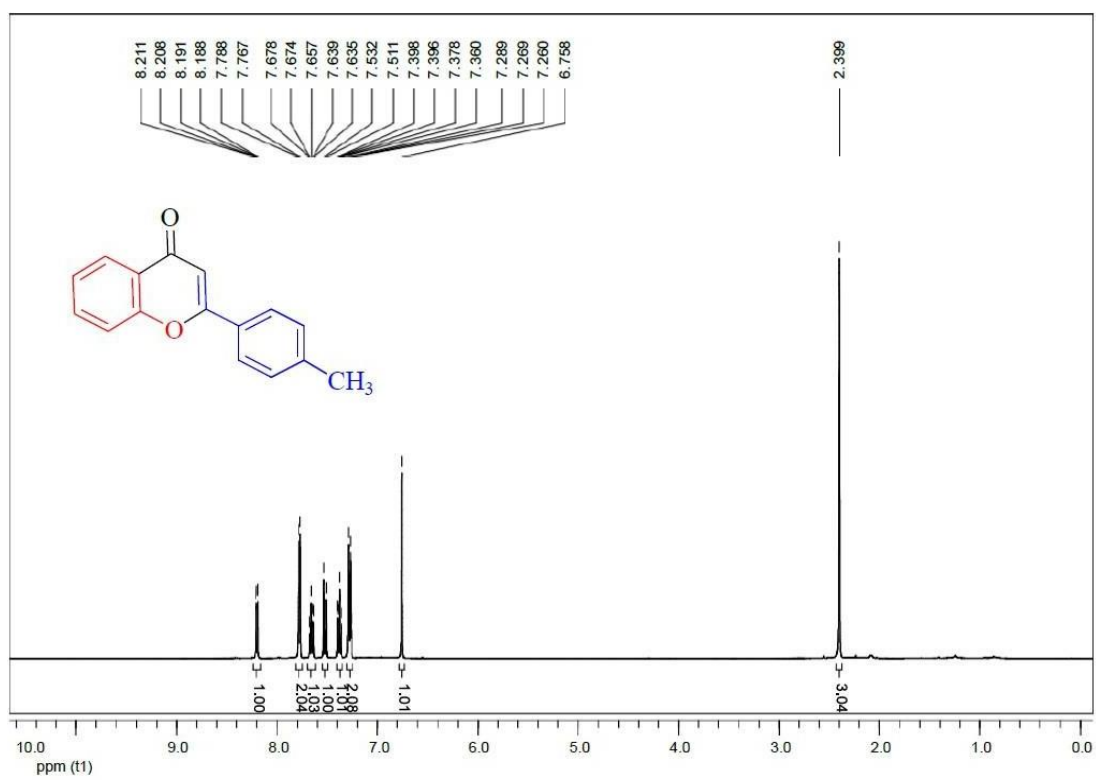


Figure S9. ^1H NMR and ^{13}C NMR spectra of product 3ac

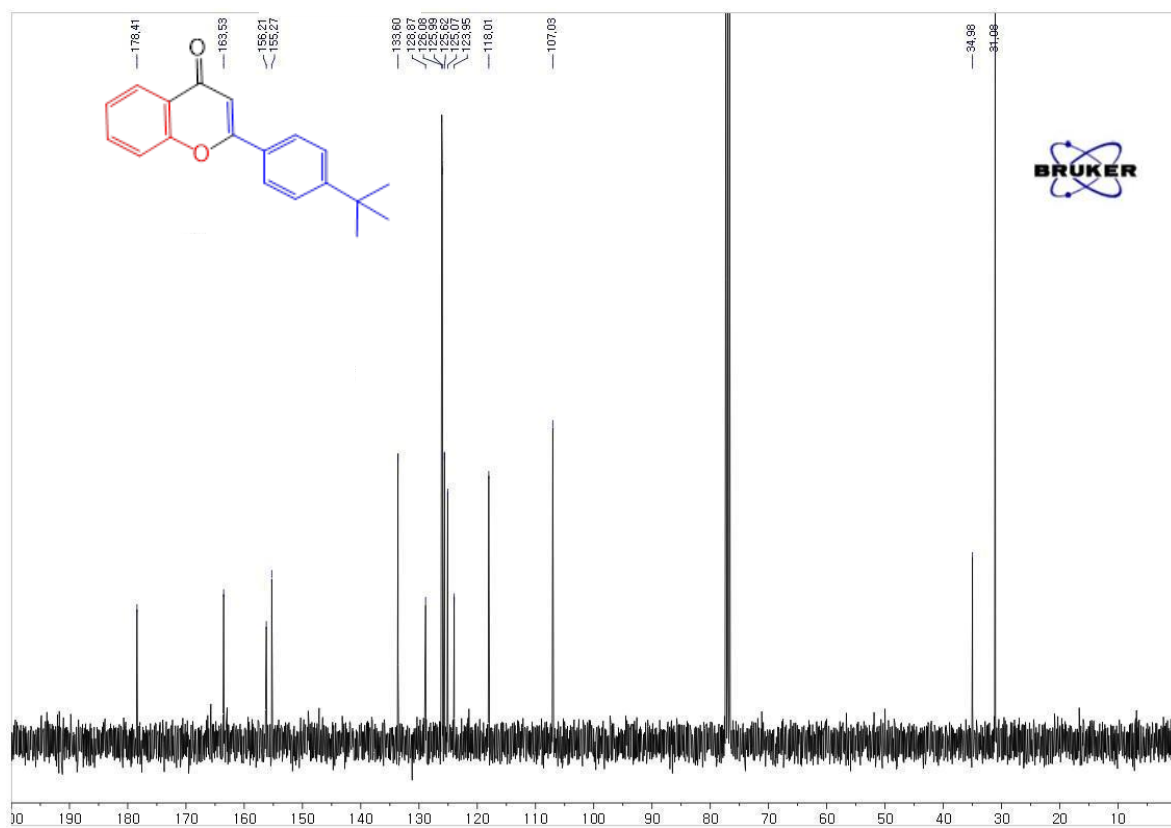
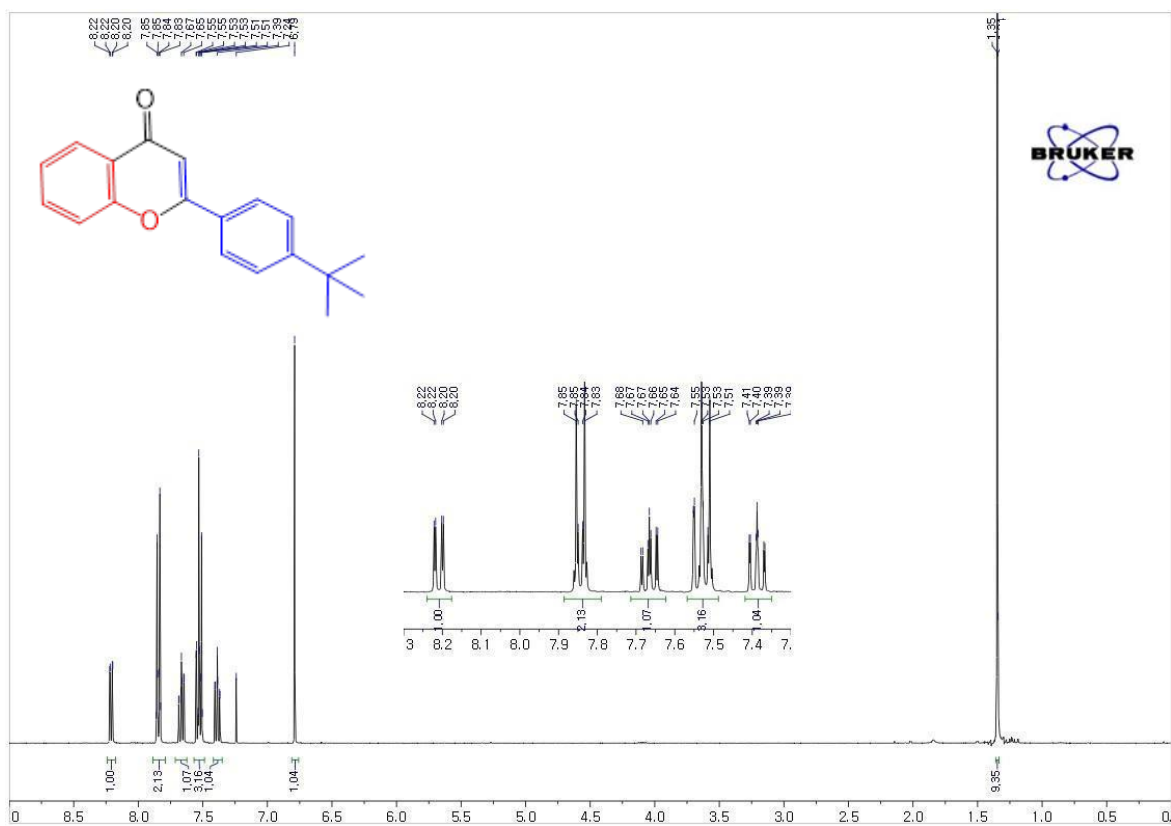


Figure S10. ¹H NMR and ¹³C NMR spectra of product 3ad

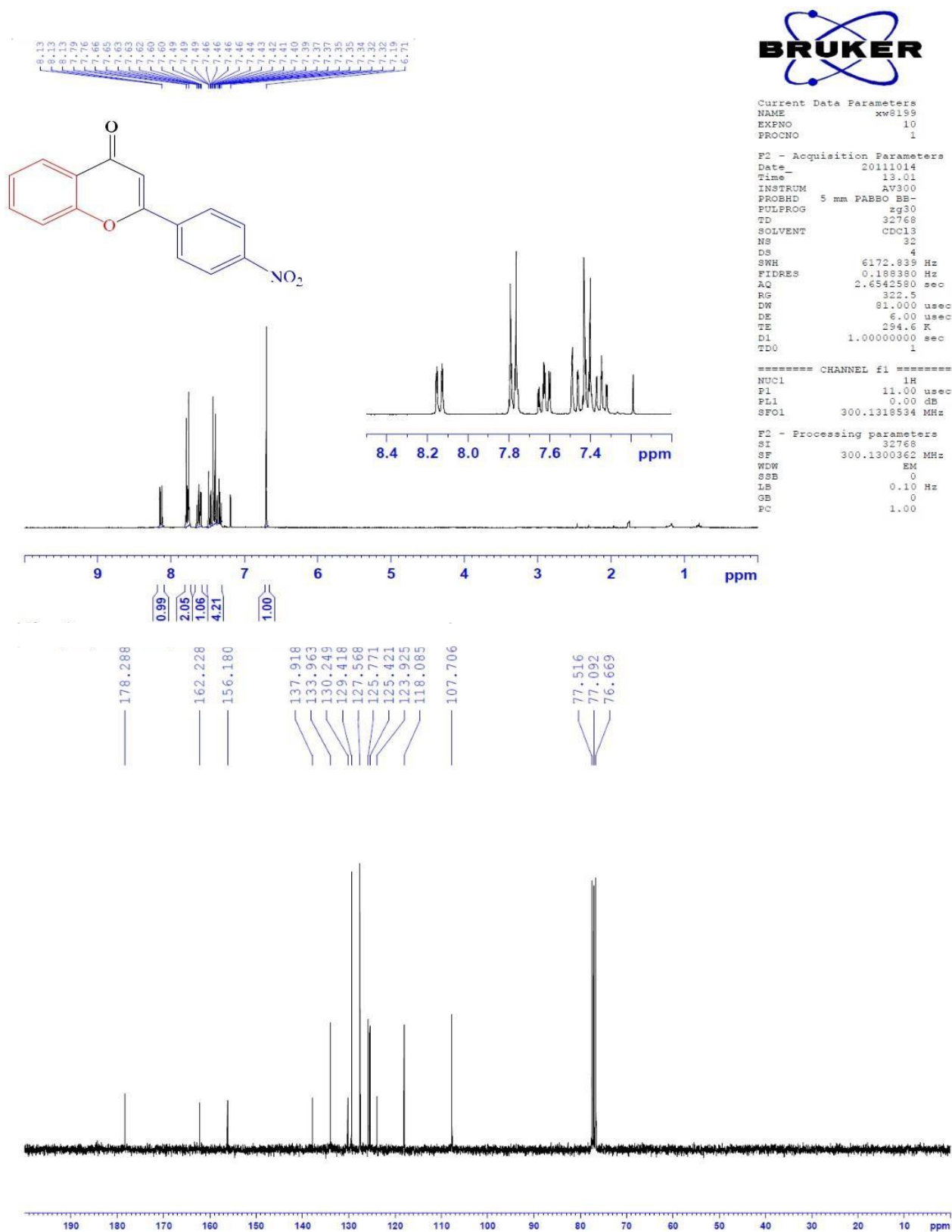
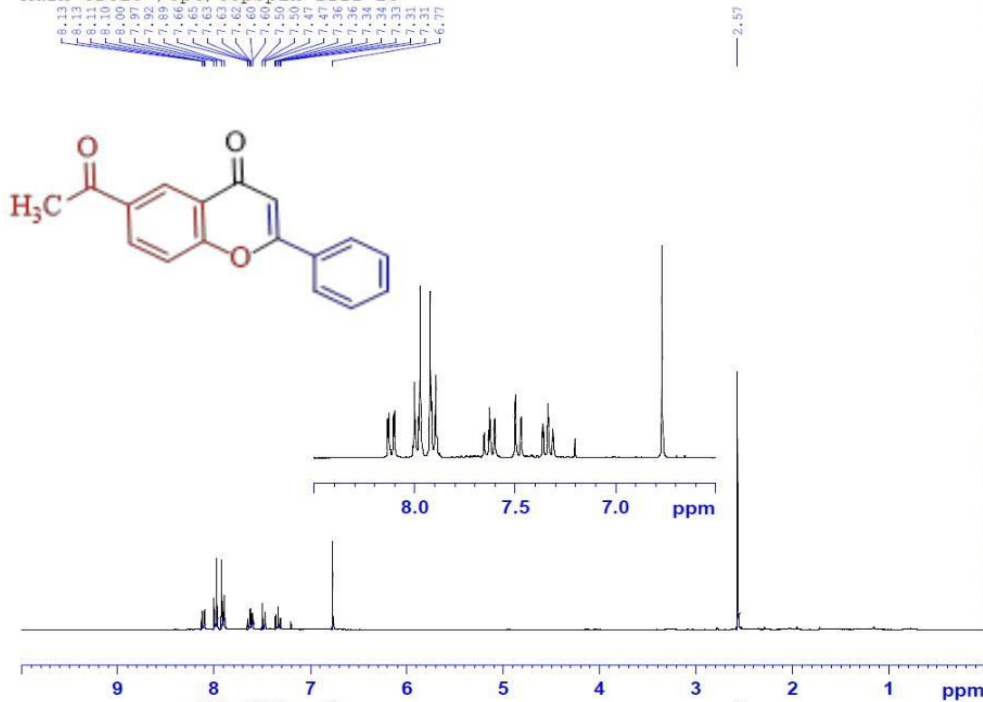


Figure S11. ¹H NMR and ¹³C NMR spectra of product 3ae

^1H NMR (300 MHz, CDCl_3 , 24 °C):

Wu XW8216

AulH CDCl_3 /opt/topspin 1111 25



$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3 , 24 °C):

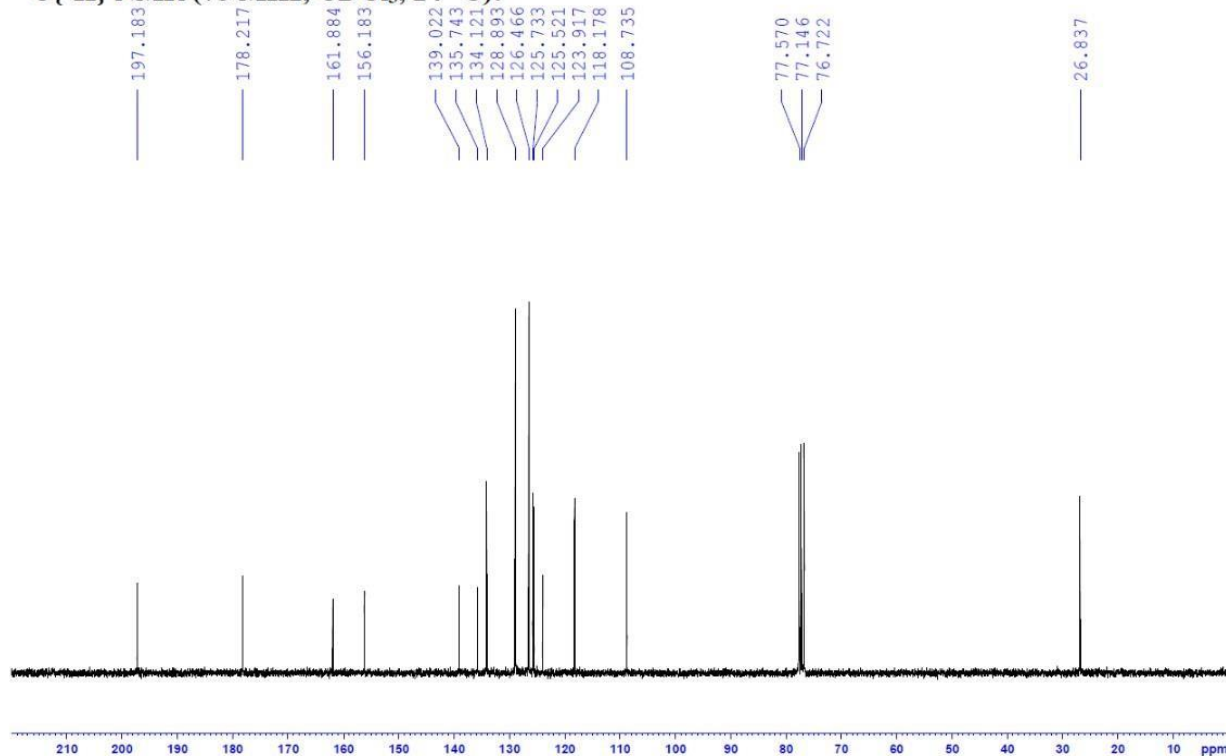


Figure S12. ^1H NMR and ^{13}C NMR spectra of product 3ba

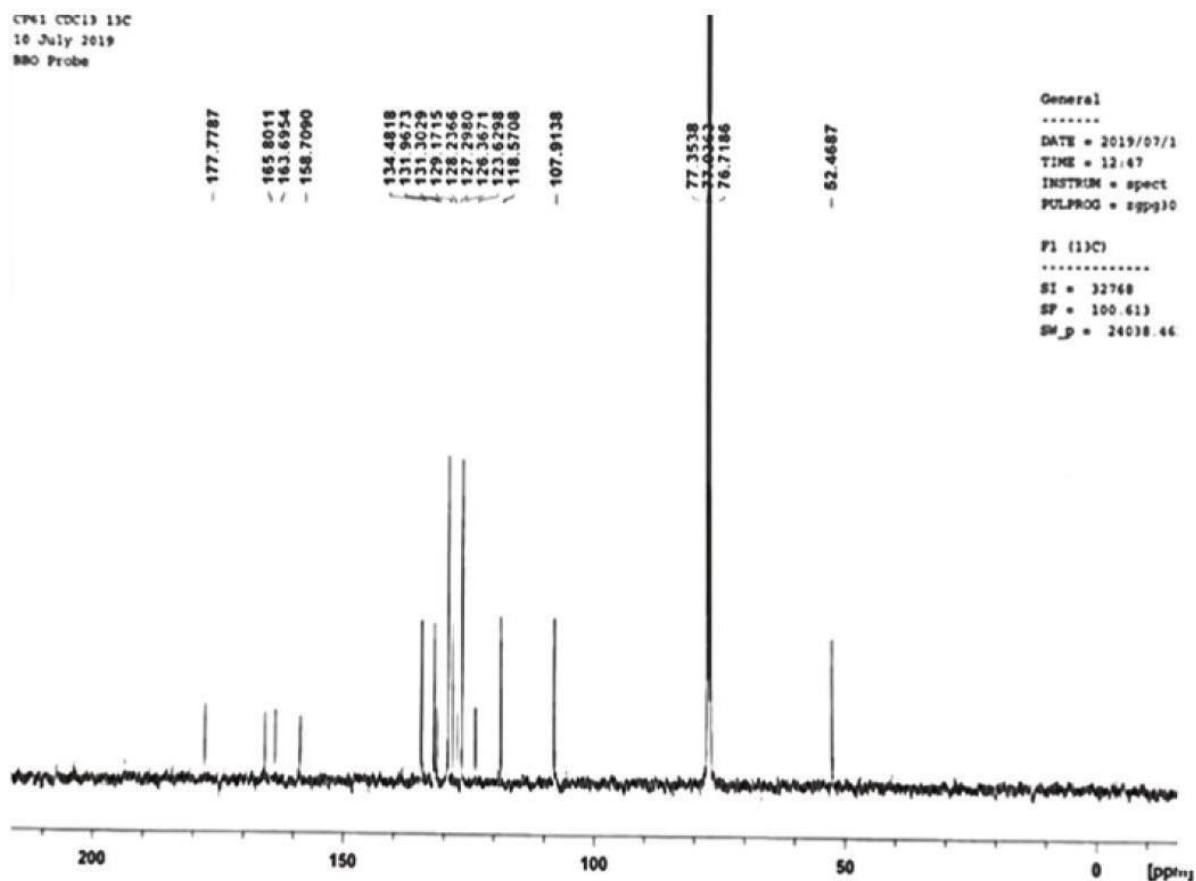
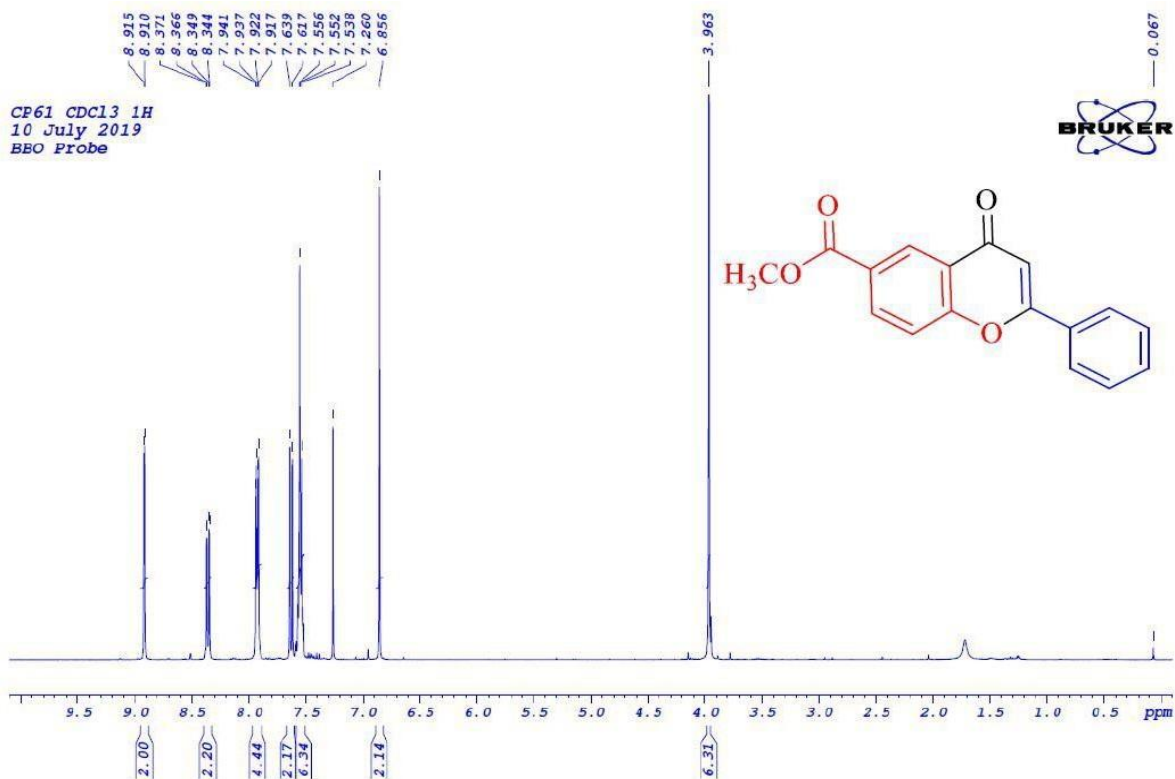


Figure S13. ^1H NMR and ^{13}C NMR spectra of product 3ca

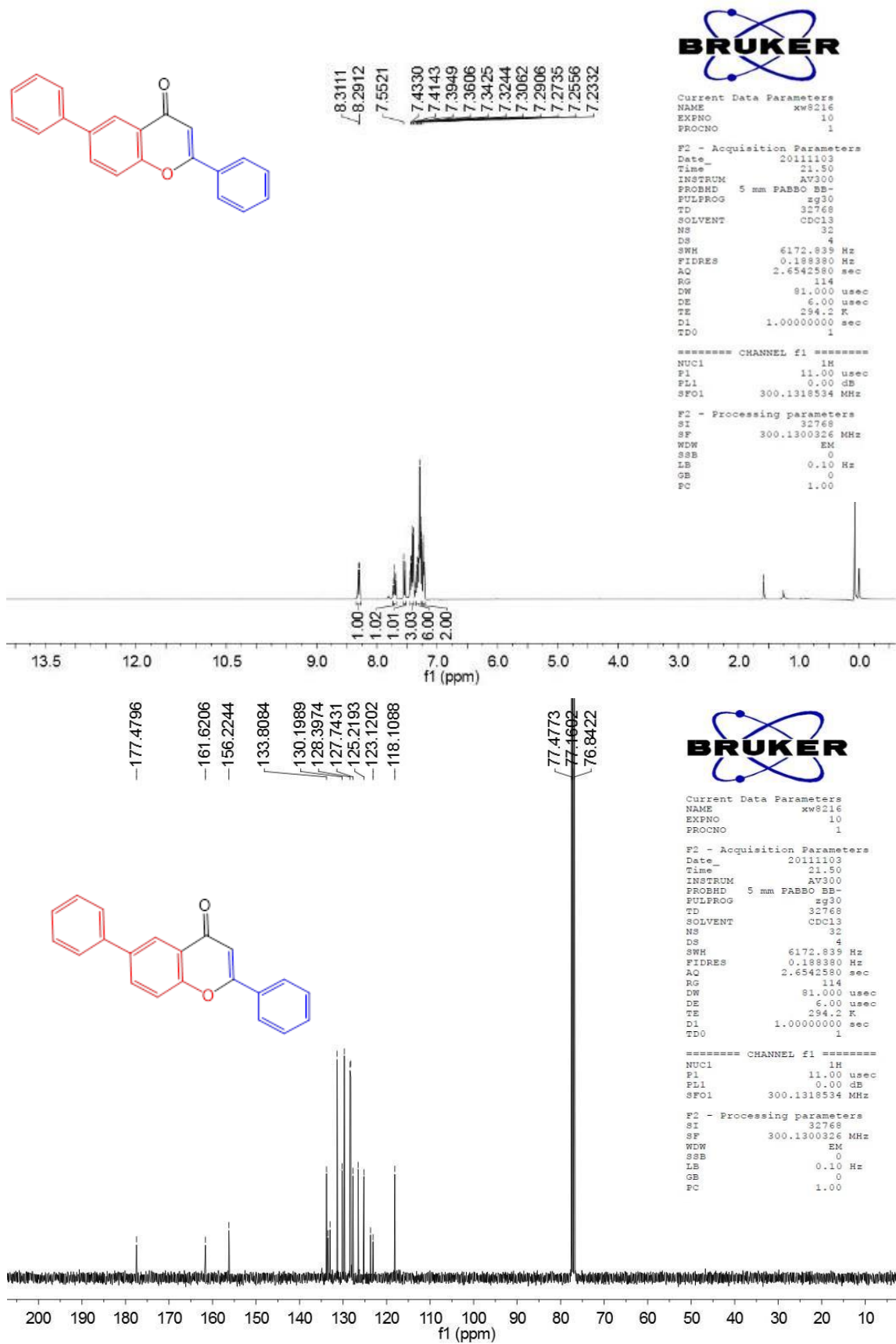
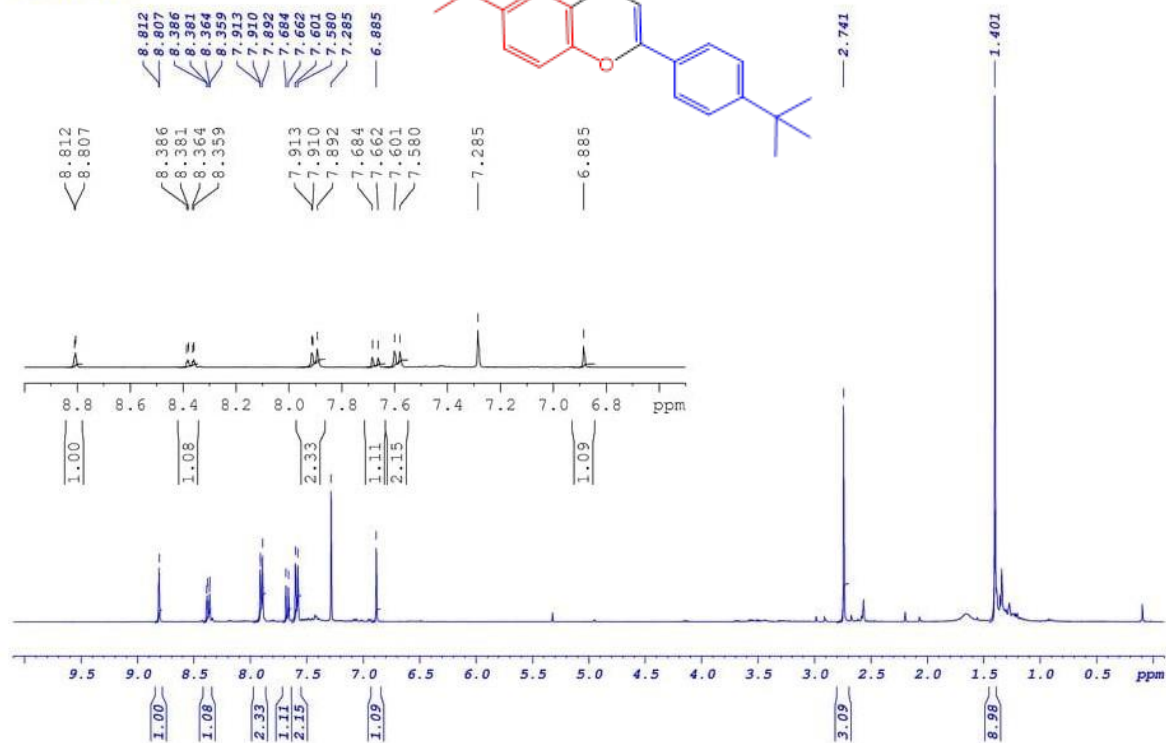


Figure S14. ^1H NMR and ^{13}C NMR spectra of product 3da

CP64_CDC13_H1
9 july 2019



CP64_CDC13_13C1
10 July 2019
BBO Probe

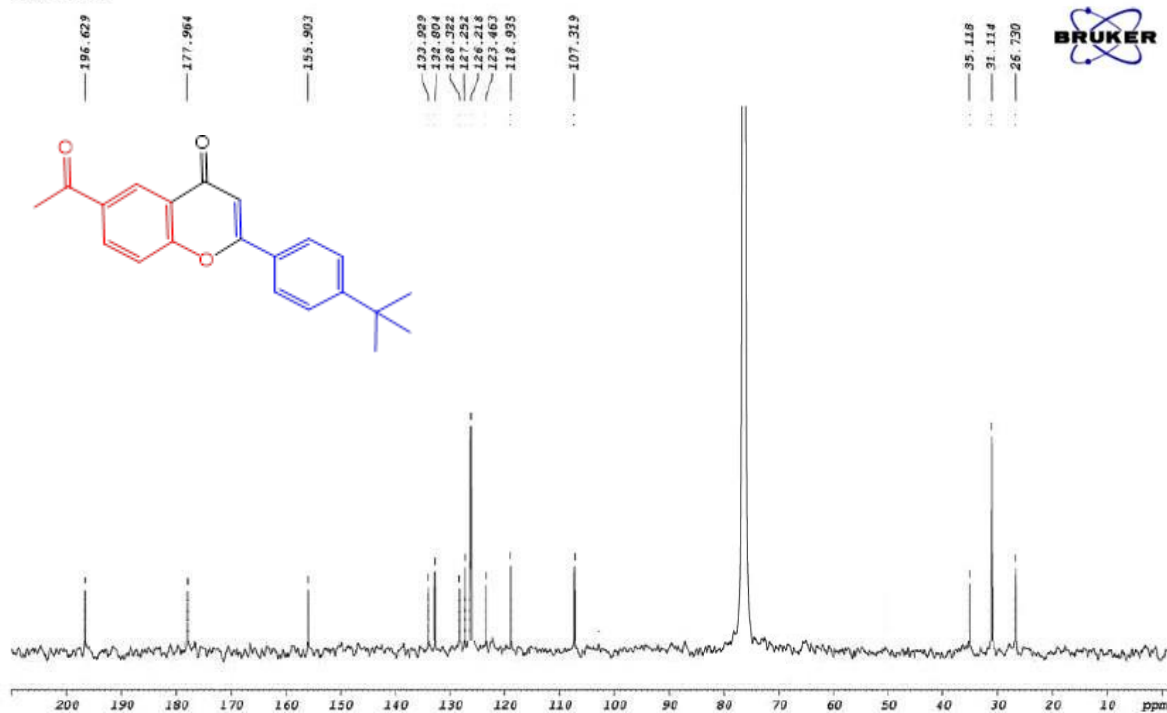


Figure S15. ¹H NMR and ¹³C NMR spectra of product 3bd

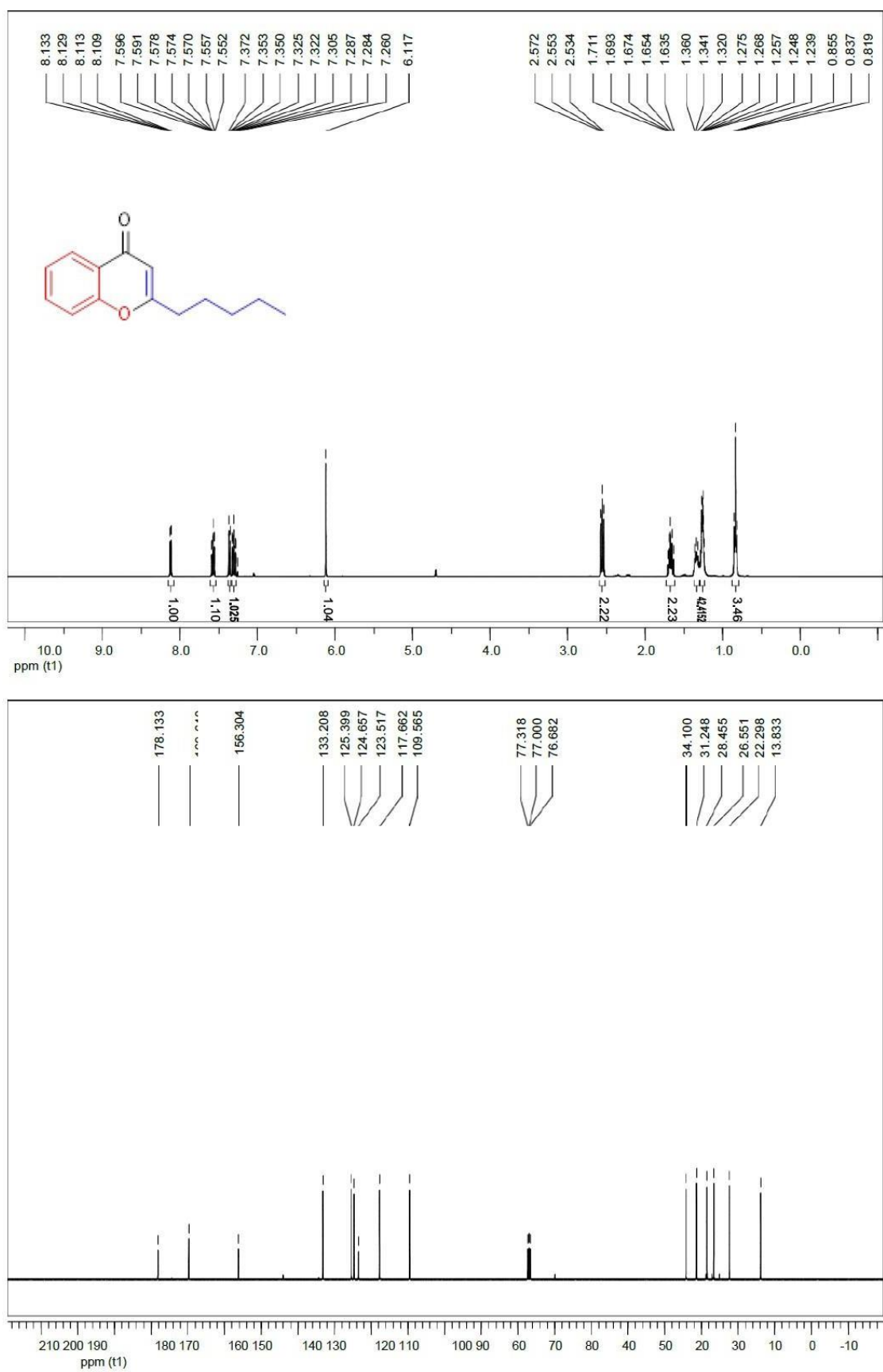


Figure S16. ¹H NMR and ¹³C NMR spectra of product 6aa

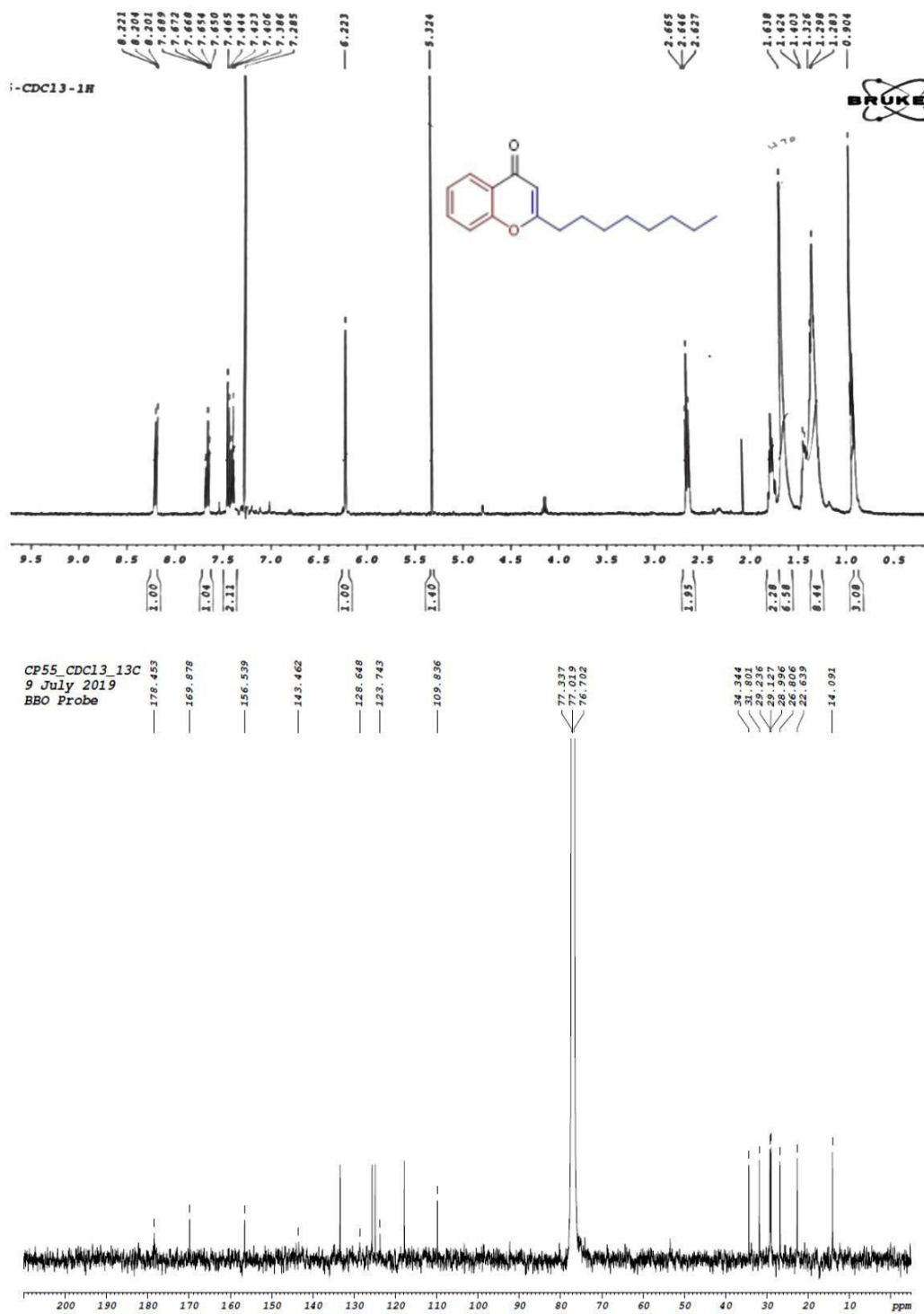


Figure S17. ¹H NMR and ¹³C NMR spectra of product 6ab

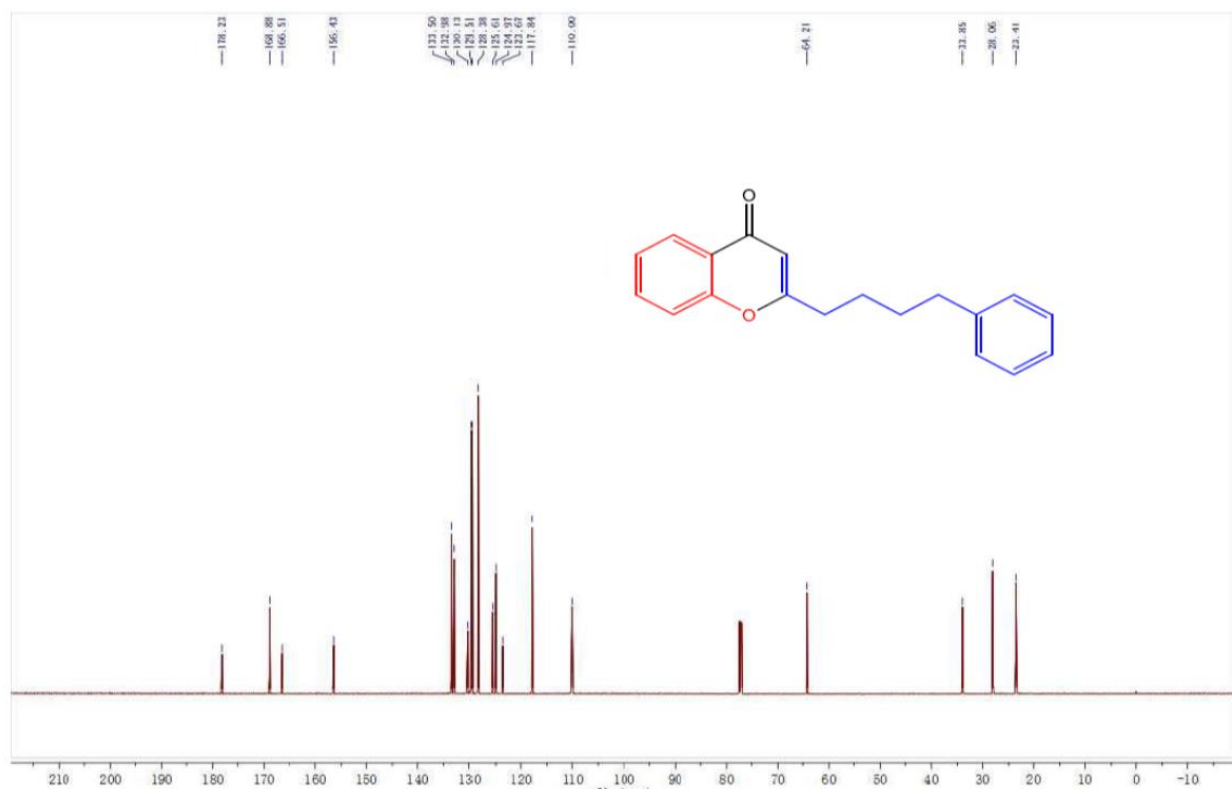
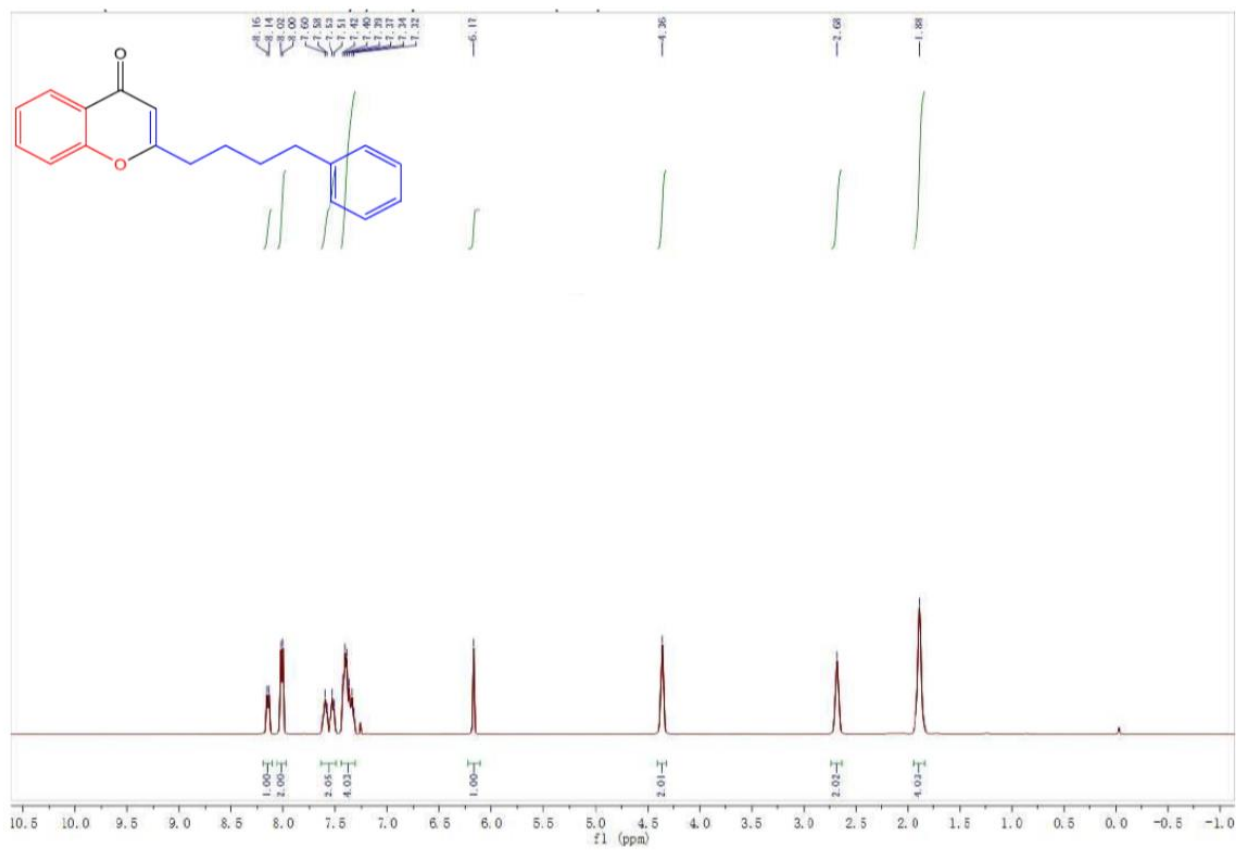
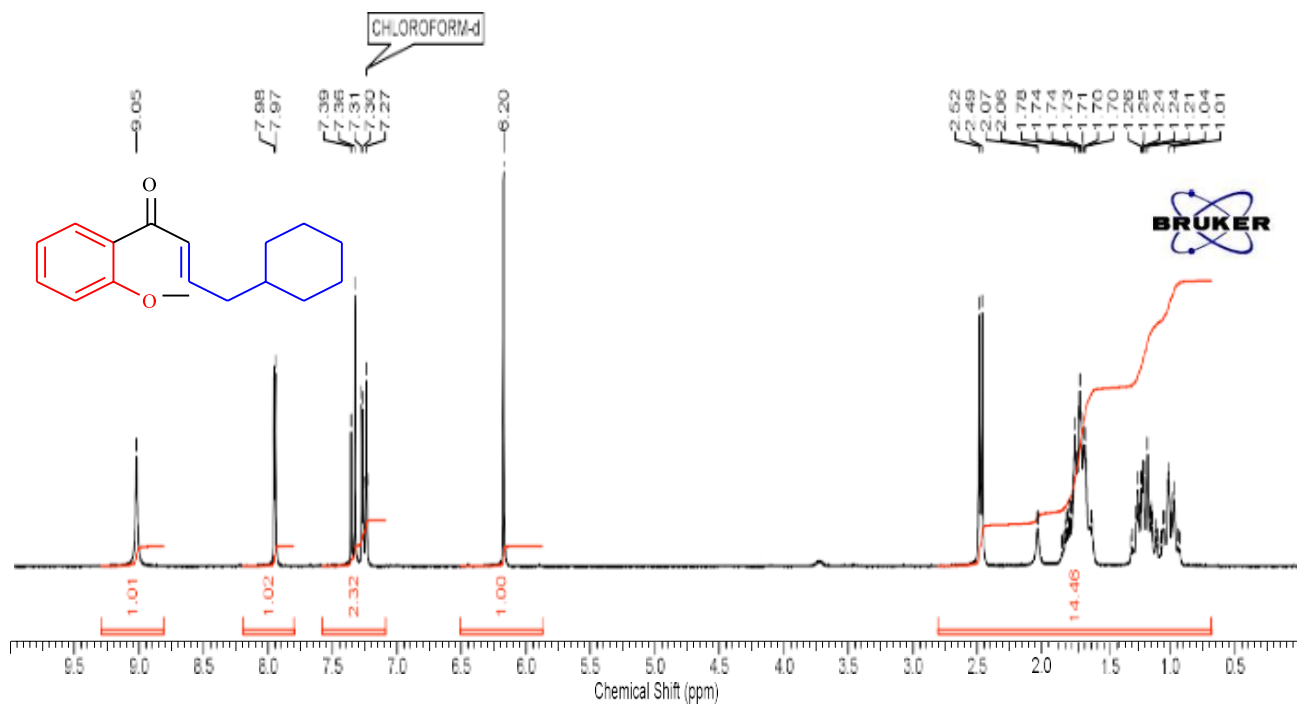


Figure S18. ¹H NMR and ¹³C NMR spectra of product 6ac



CP5CDCl13C1
9 July 2019
BBO Probe

178.453
169.878
156.539
143.462
128.648
123.743
109.836
77.337
77.019
76.702
34.344
31.801
29.236
29.127
28.996
26.806
22.639
14.091

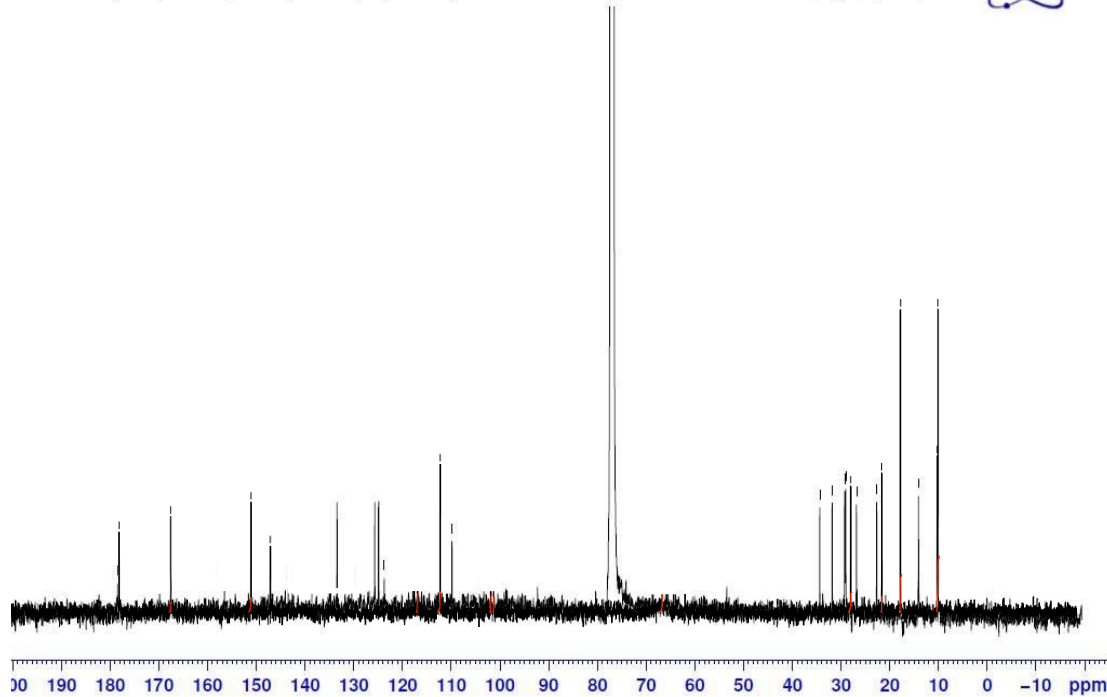


Figure S19. ¹H NMR and ¹³C NMR spectra of product 6ad

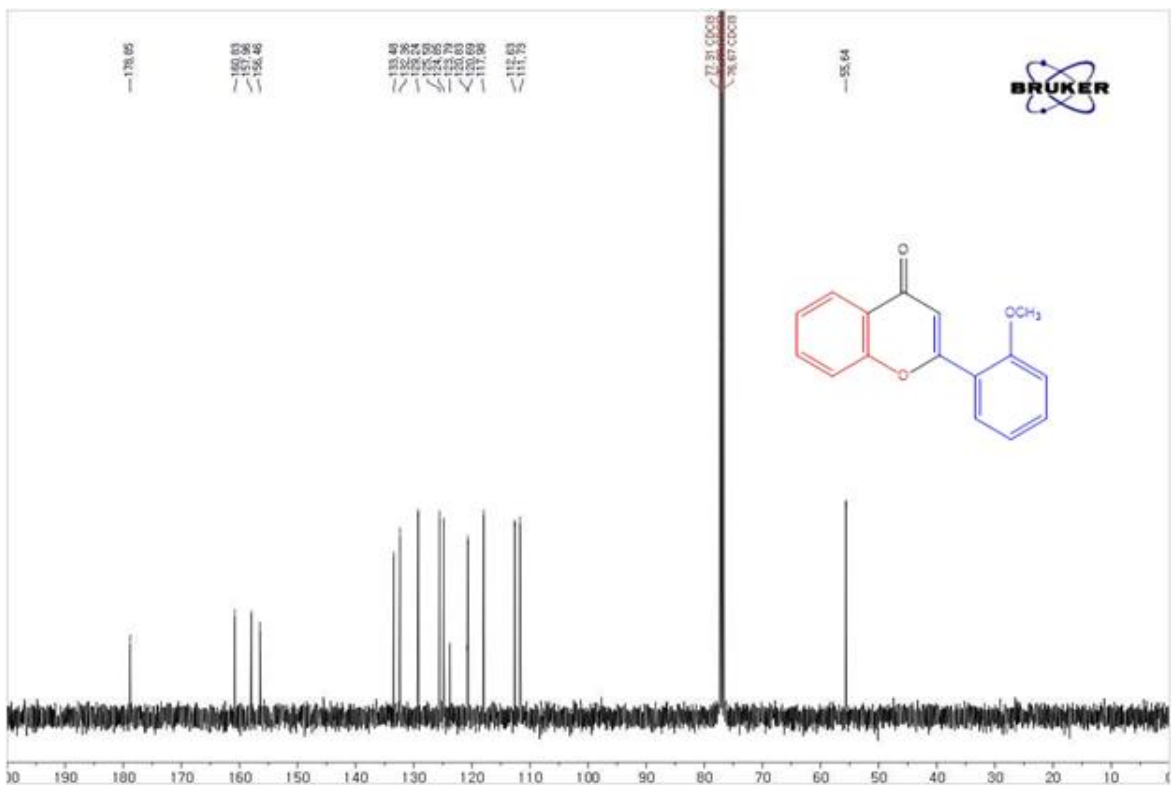
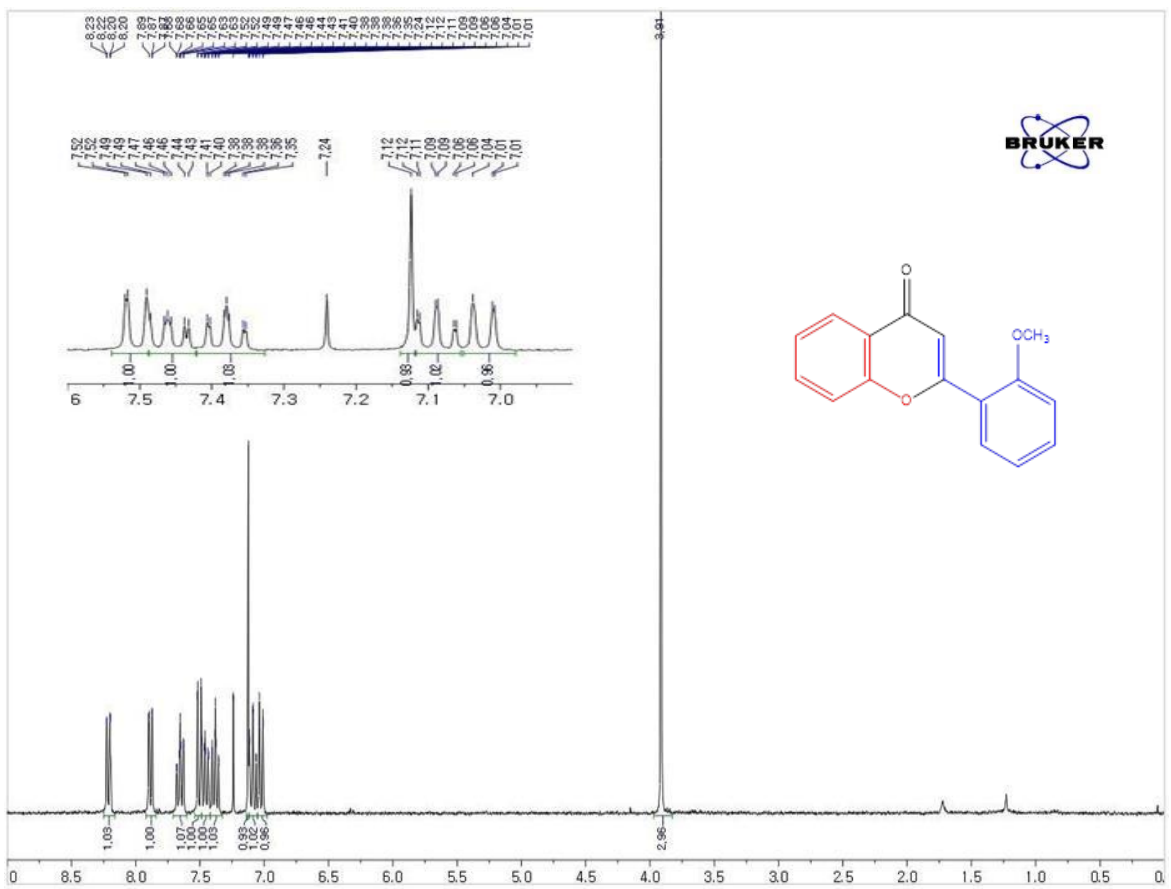


Figure S20. ¹H NMR and ¹³C NMR spectra of product 3af

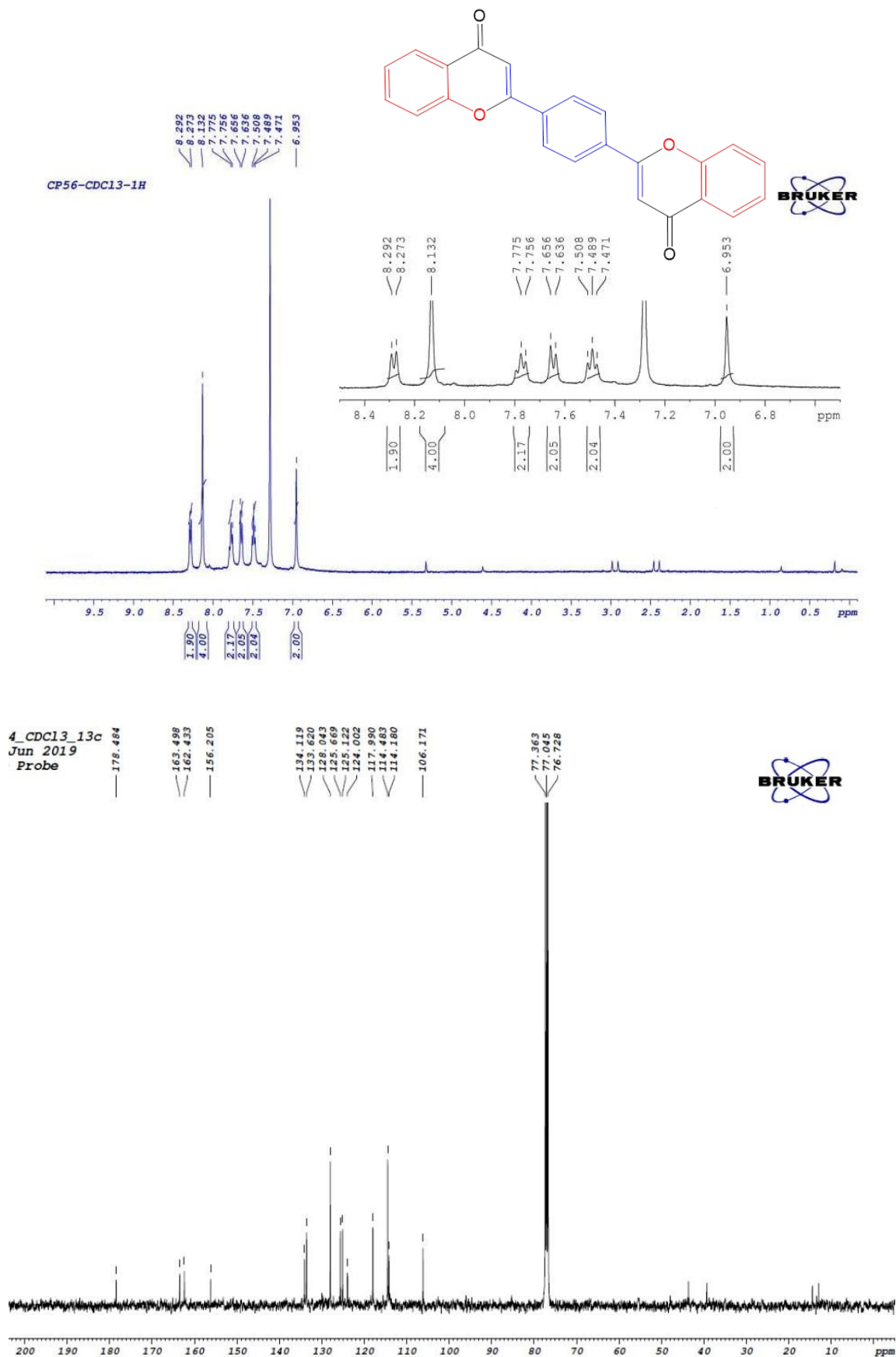


Figure S21. ^1H NMR and ^{13}C NMR spectra of product 8a

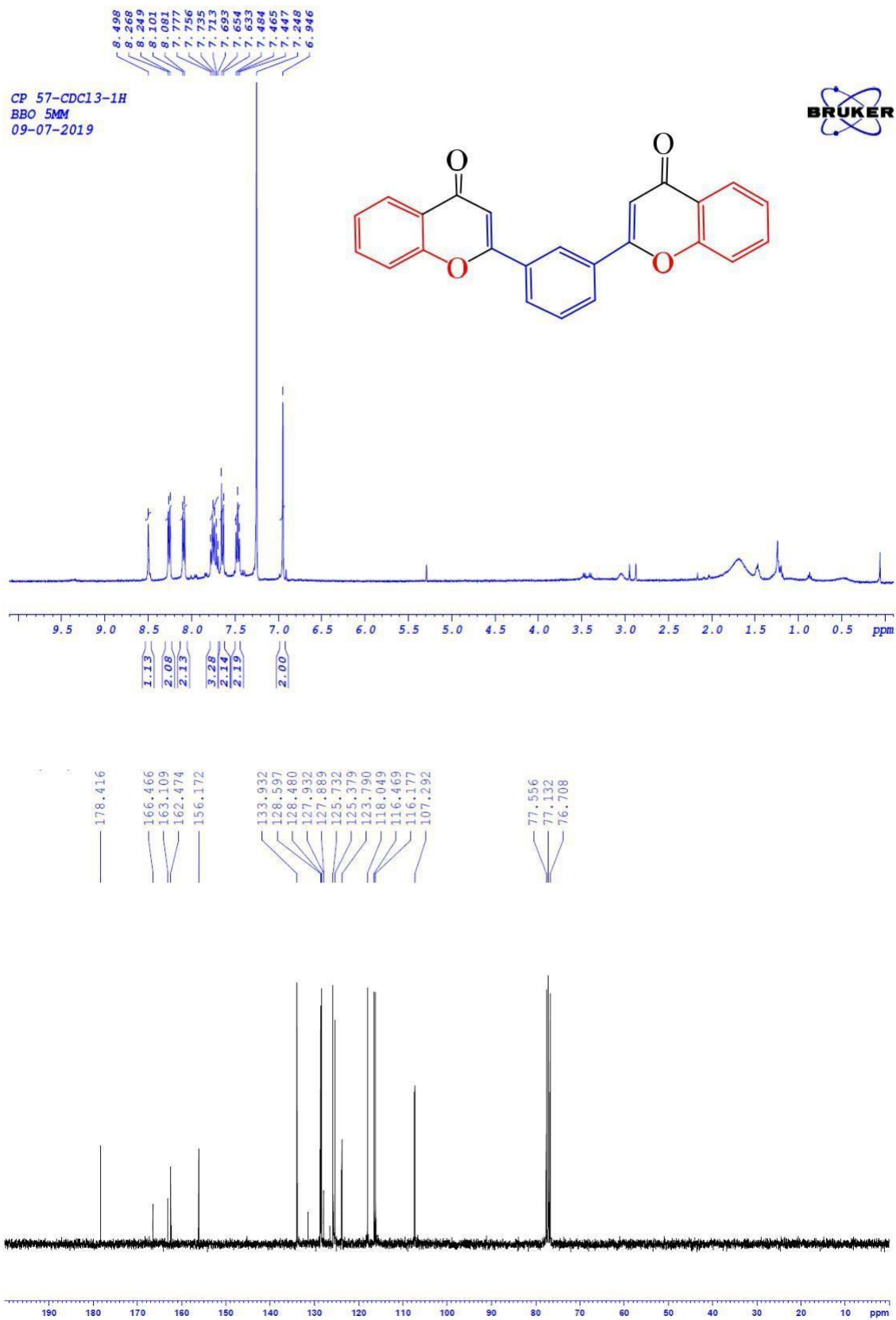


Figure S22. ^1H NMR and ^{13}C NMR spectra of product 8b

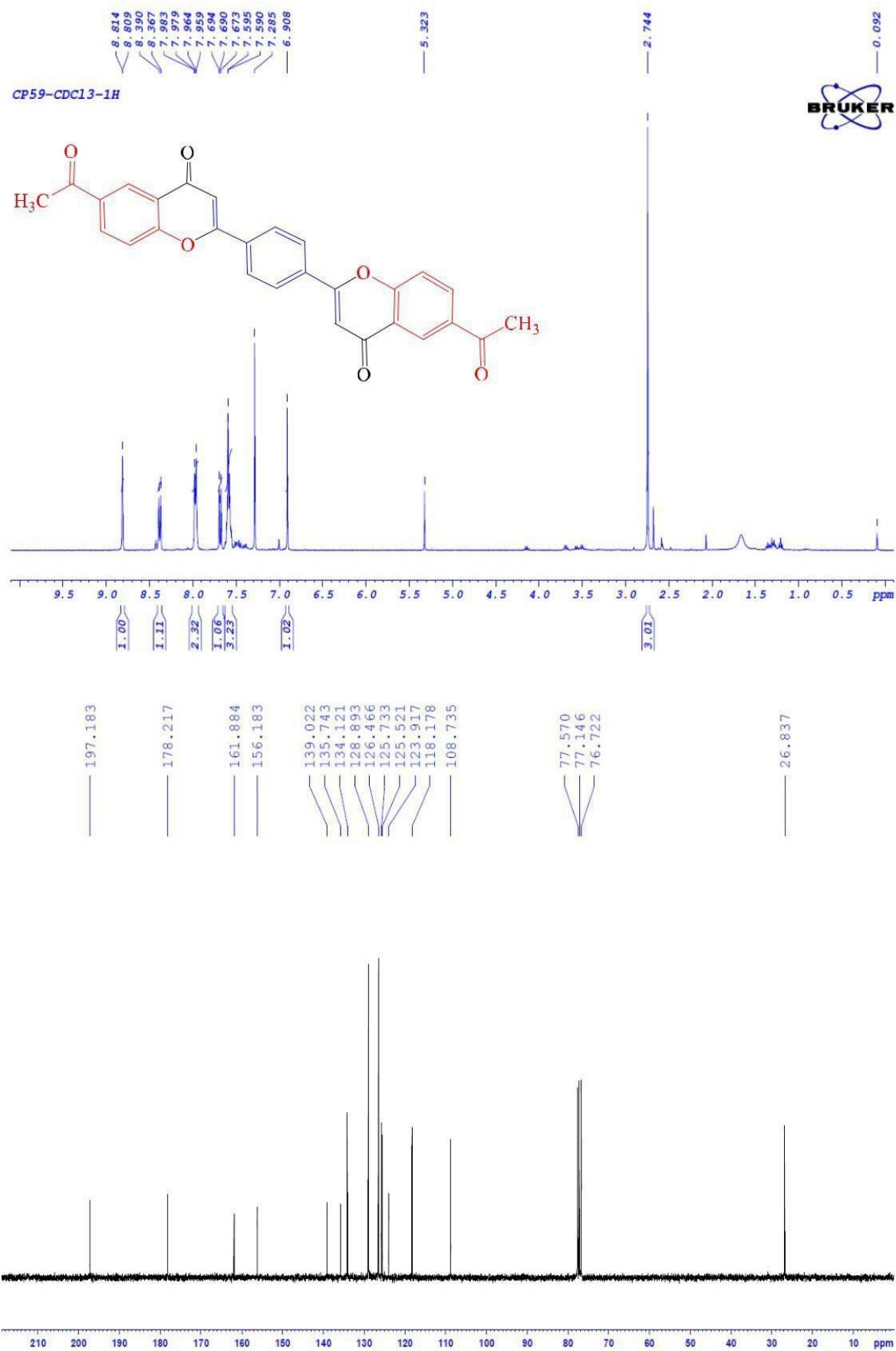


Figure S23. ¹H NMR and ¹³C NMR spectra of product 8c

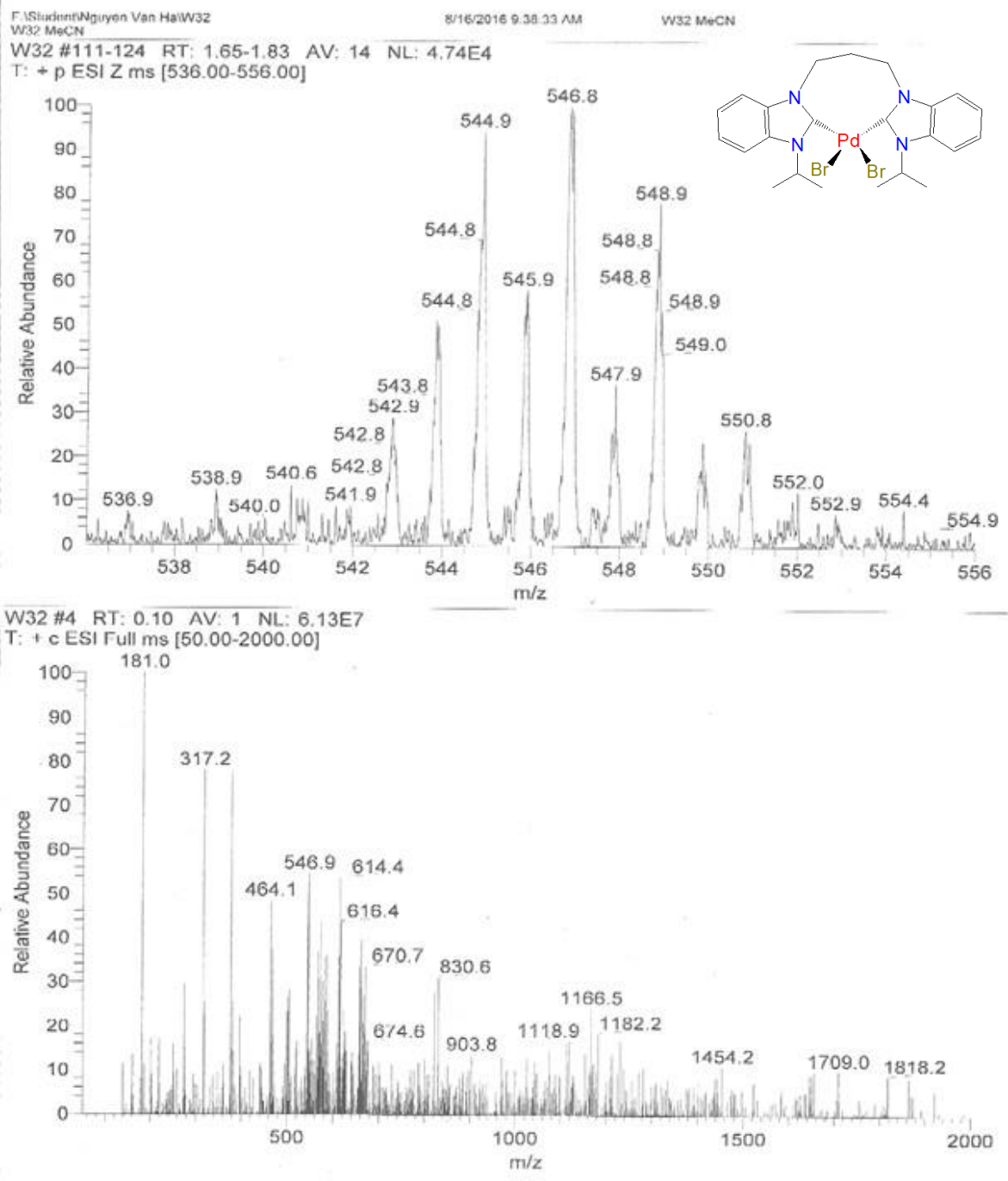


Figure S24. ESI spectra of complex C1

Instrument Name ESI TOF/MS
Acq Method HRMS Full MS
DA Method HRMS MS
User Name Fischer
Data Filename D:\MassHunter\Data\1611\16111709.d
Sample Name W52D
Position Val 42
Comment MeOH/0.1%HOAc in H2O 90:10



User Spectra

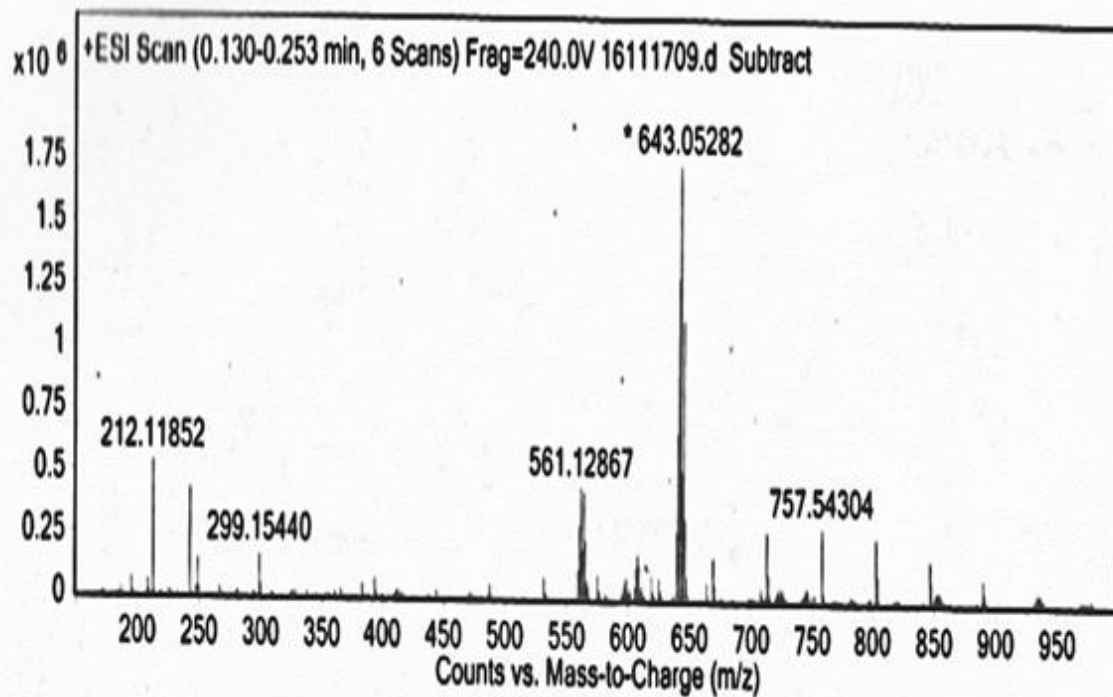


Figure S25. ESI spectra of complex C2

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T: ITMS + c ESI Full ms [66.00-2000.00]

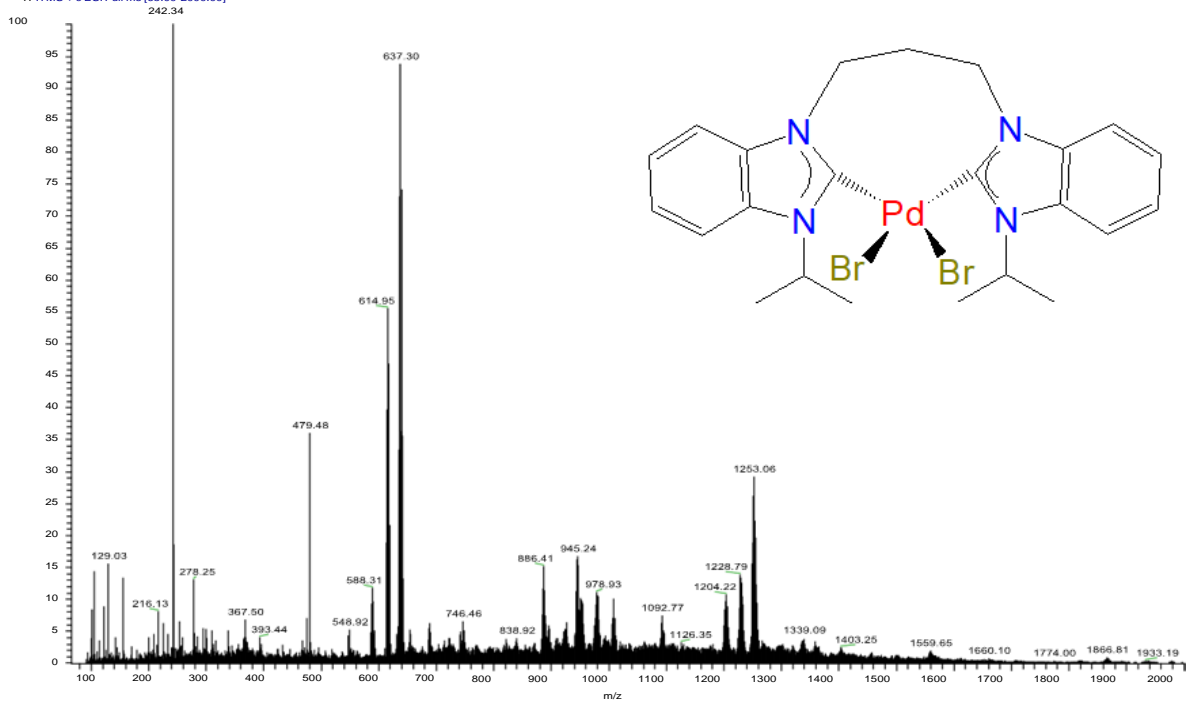


Figure S26. ESI spectra of complex C3