Supporting Information

for

$BF_3 \cdot Et_2O$ Catalyzed atom-economical approach to highly substituted indole-3-carbinols from nitrosobenzenes and propargylic alcohols

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Crystallographic data for product 3o (1579786)

Molecular formula $C_{48}H_{30}F_5NO_2$

Molecular weight M = 747.73

Temperature T = 150 (2) K

Radiation MoK\a

Size 0.33 × 0.23 × 0.12 mm

Space group Triclinic, C2/c

a = 29.898(3) Å

b = 12.7893(14) Å

c = 24.928(3) Å

α = 90.00

β = 123.131(2)

γ = 90.00

Volume V = 7982.2(15) Å3

R_1 = 0.0364

wR_2 = 0.0452

z = 8

Dcalcd = 1.244 mg cm^{-3}

$F(000)$ = 3088

Absorption coefficient = 0.091 mm^{-1}

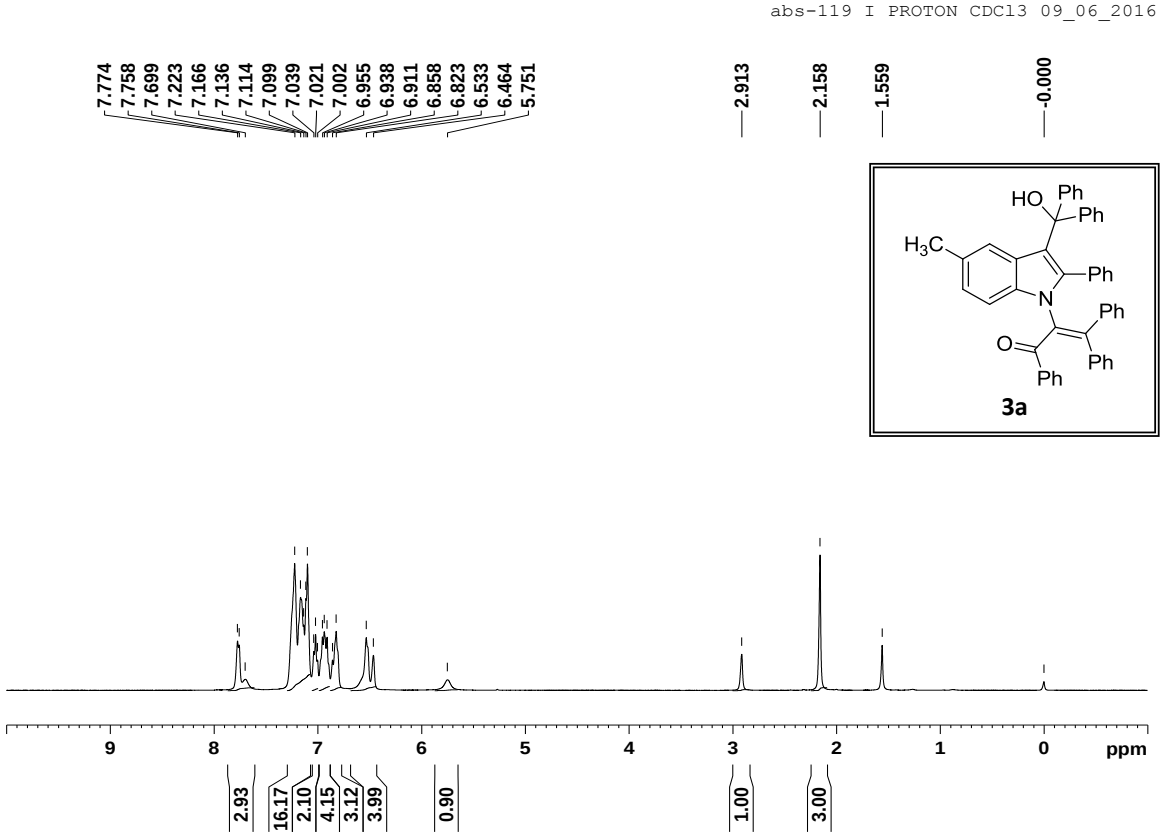
λ = 0.71073 Å,

No of unique reflections 7801

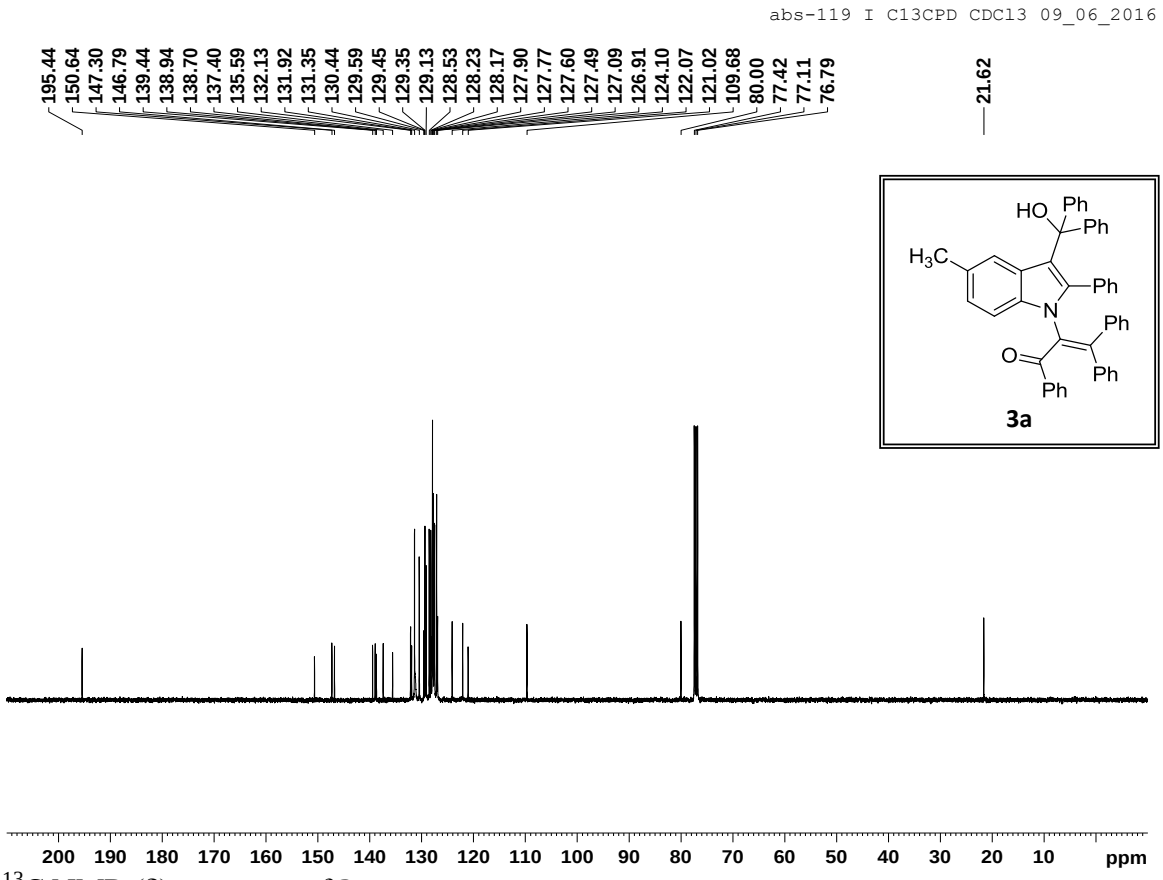
No of parameters 6303

$\Delta\rho_{max}$, $\Delta\rho_{min}$ ($eÅ_3$) 0.290, -0.241

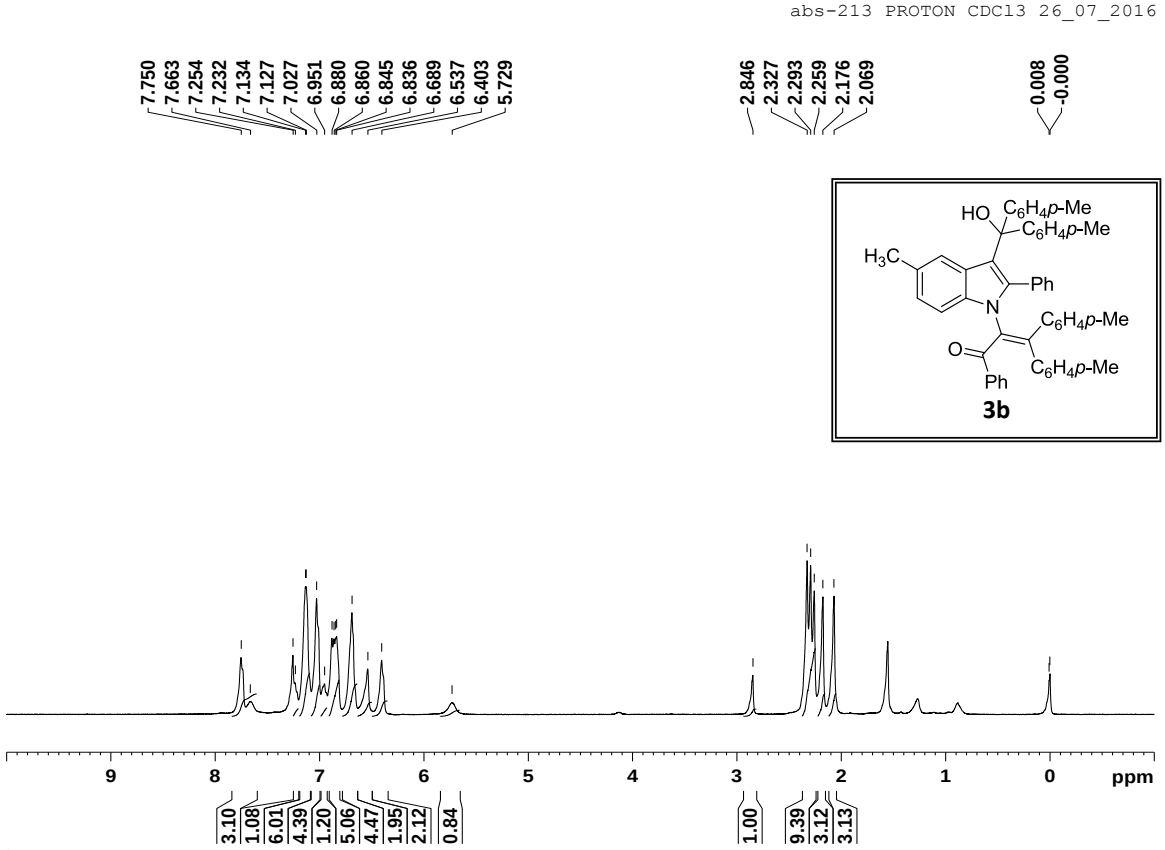
The intermolecular H-bonding interactions are:
C(47)–H(47)···F(3); H(47)···F(3) = 2.657 Å, and < C(47)–H(47)···F(3) = 128.90°
C(32)–H(32)···F(5); H(32)···F(5) = 2.521 Å, and < C(32)–H(32)···F(5) = 121.83°
C(10)–H(10)···O(2); H(10)···O(2) = 2.638 Å, and < C(10)–H(10)···O(2) = 152.59°
C(38)–H(38)···O(1); H(38)···O(1) = 2.497 Å, and < C(38)–H(38)···O(1) = 156.87°
O(2)–H(1)···O(1); H(1)···O(1) = 2.048 Å, and < O(2)–H(1)···O(1) = 172.21°



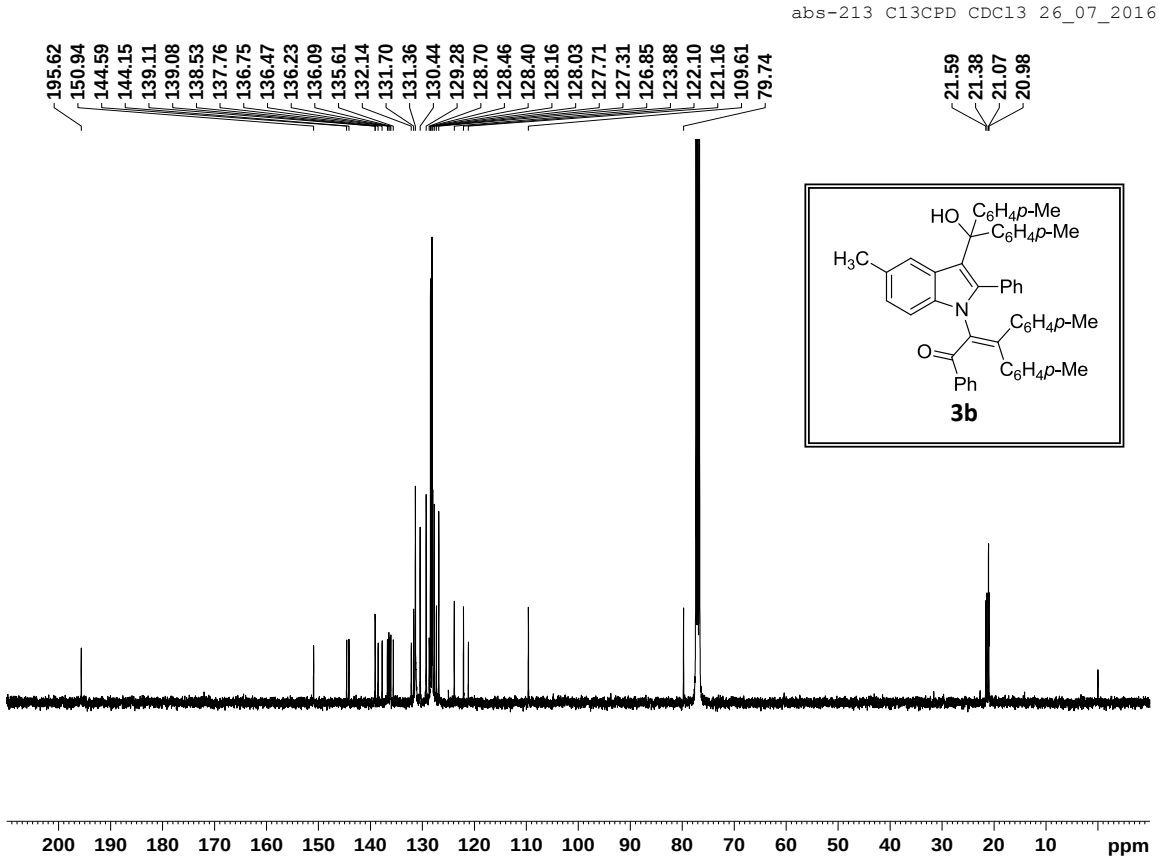
^{1}H NMR (δ) spectrum of **3a**



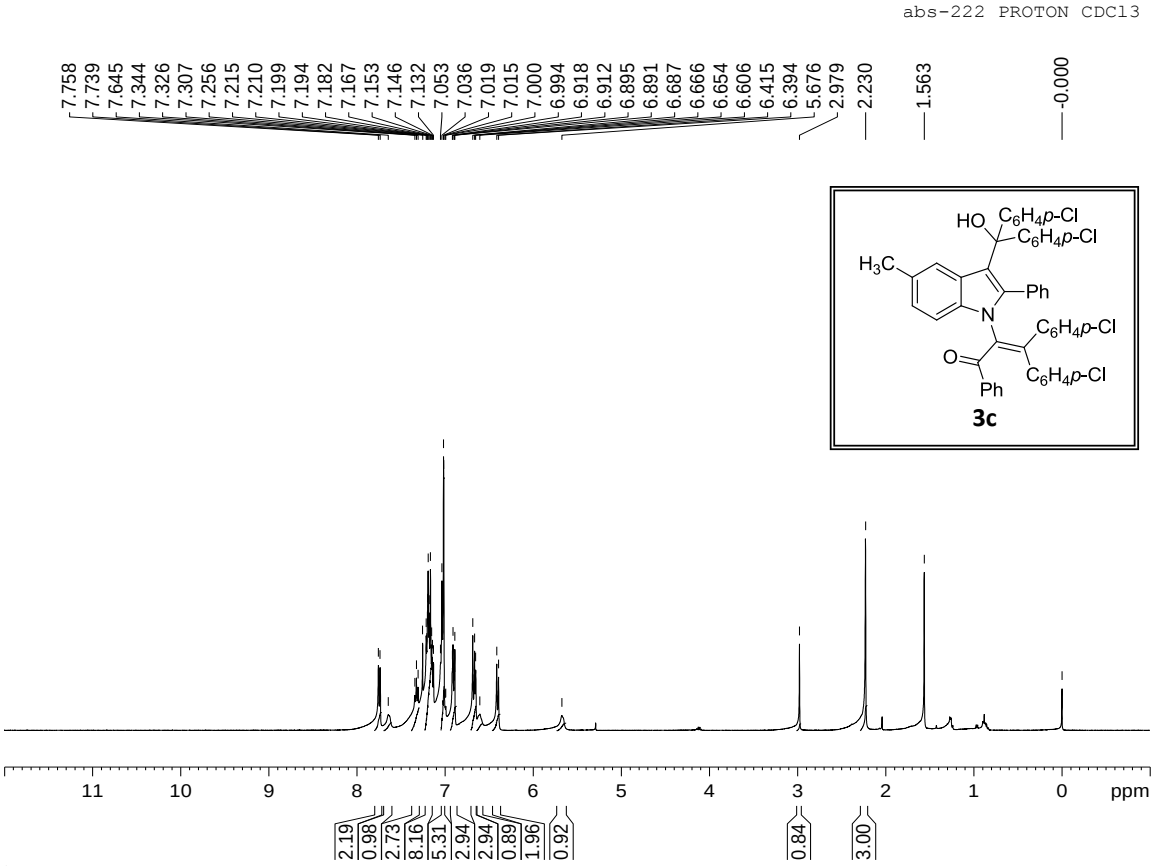
^{13}C NMR (δ) spectrum of **3a**



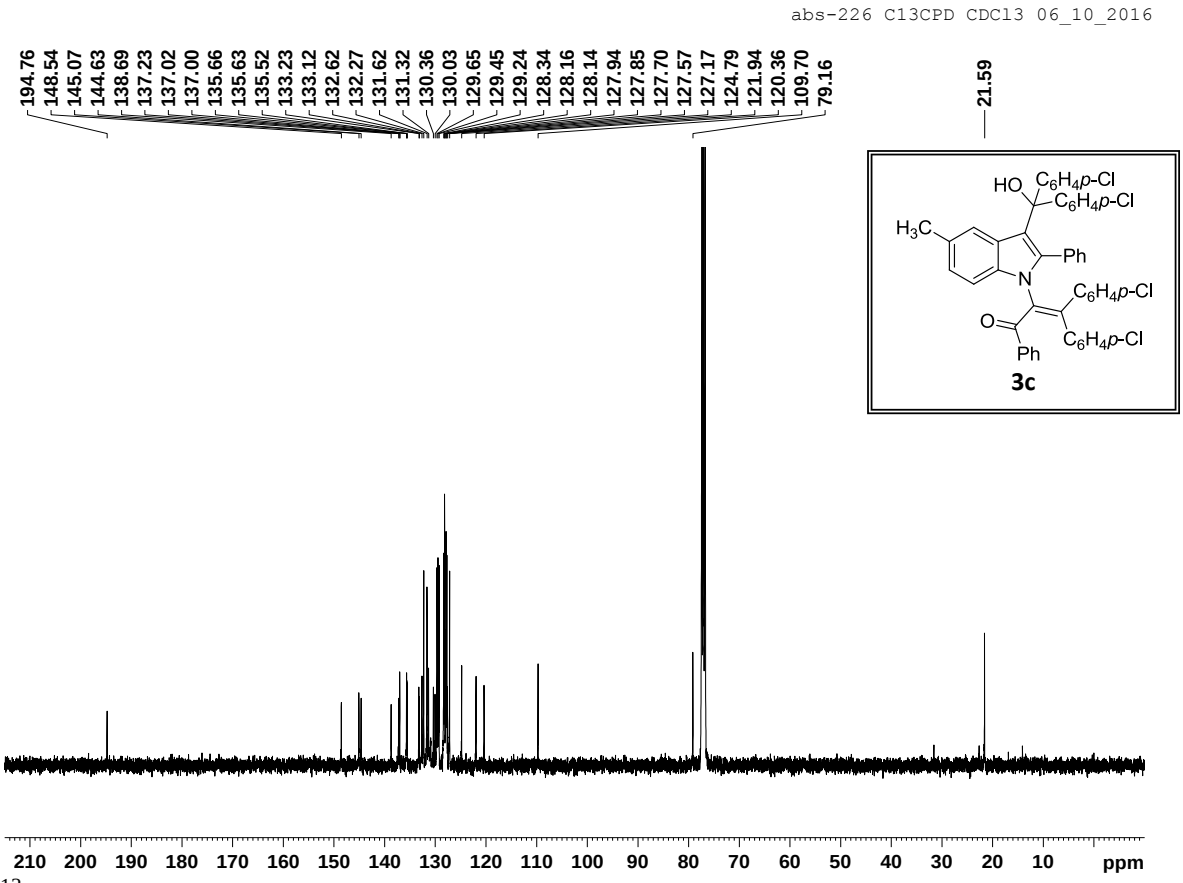
^{1}H NMR (δ) spectrum of **3b**



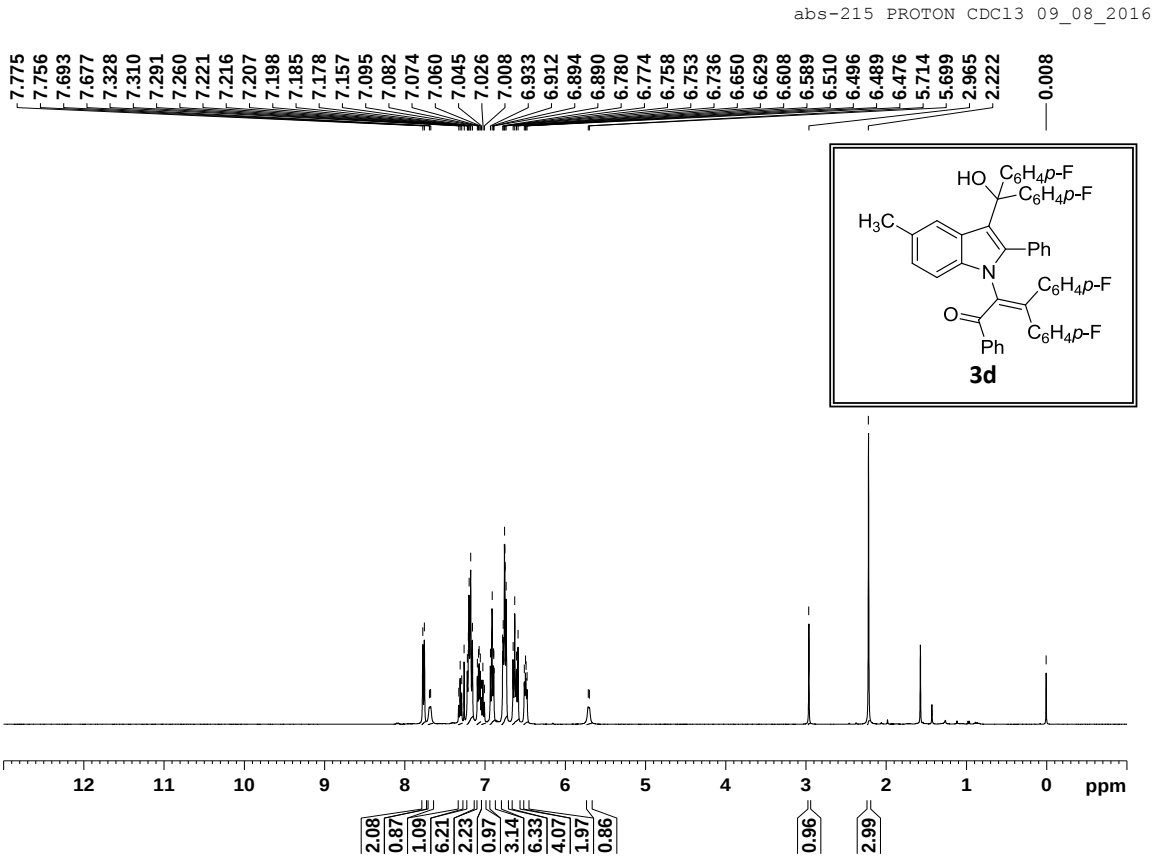
^{13}C NMR (δ) spectrum of **3b**



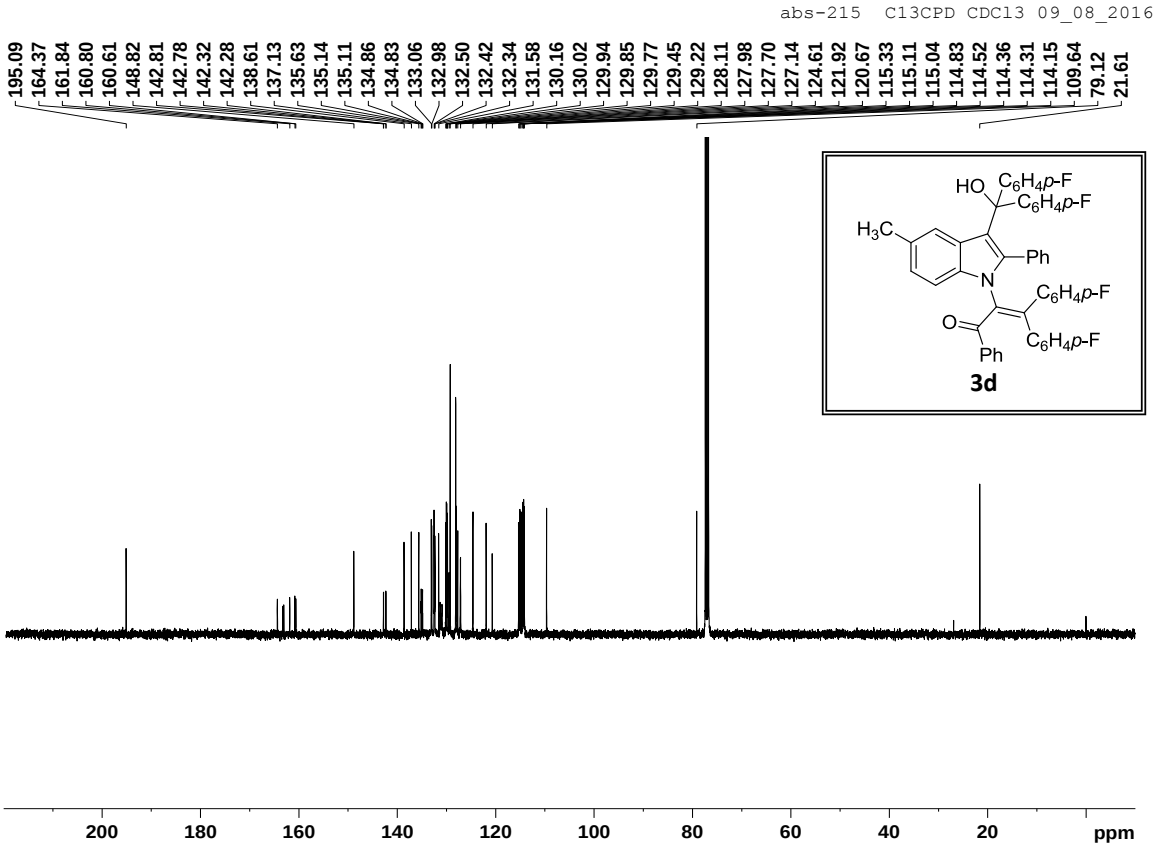
^{1}H NMR (δ) spectrum of **3c**



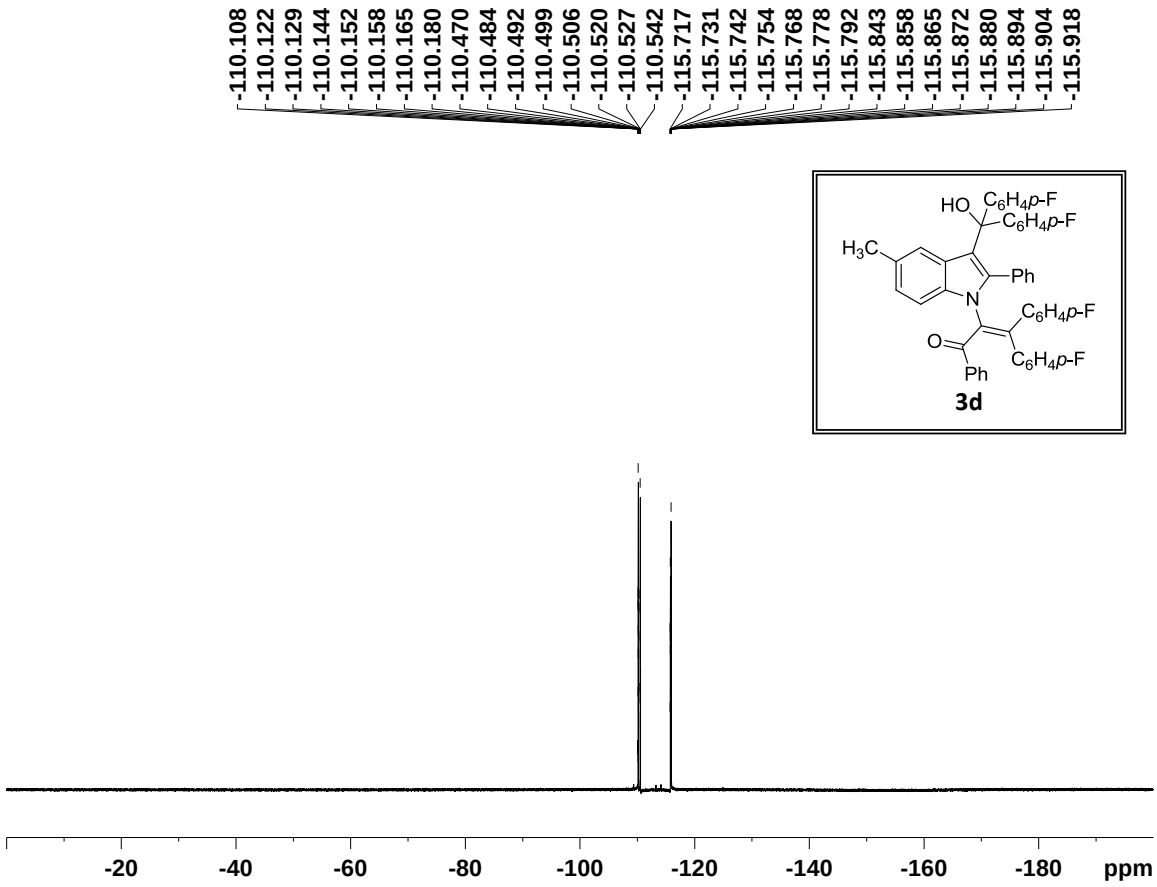
^{13}C NMR (δ) spectrum of **3c**



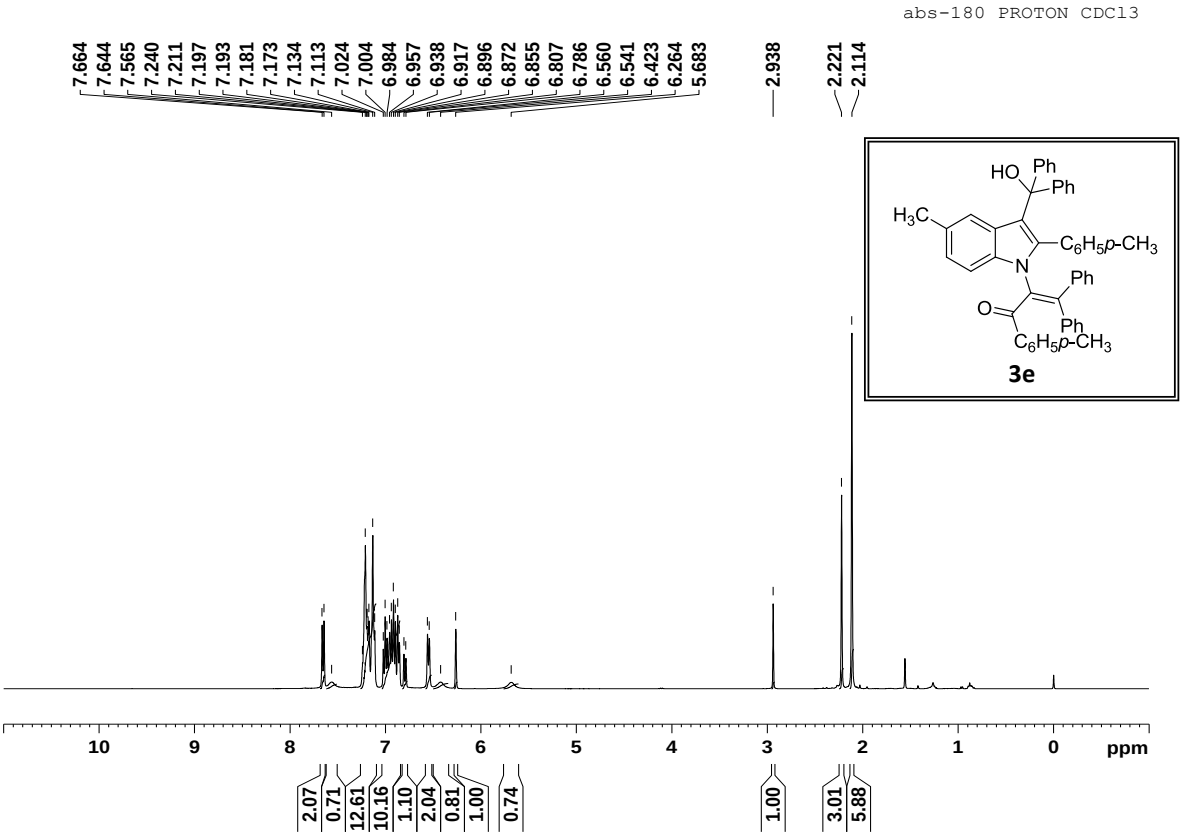
^{1}H NMR (δ) spectrum of **3d**



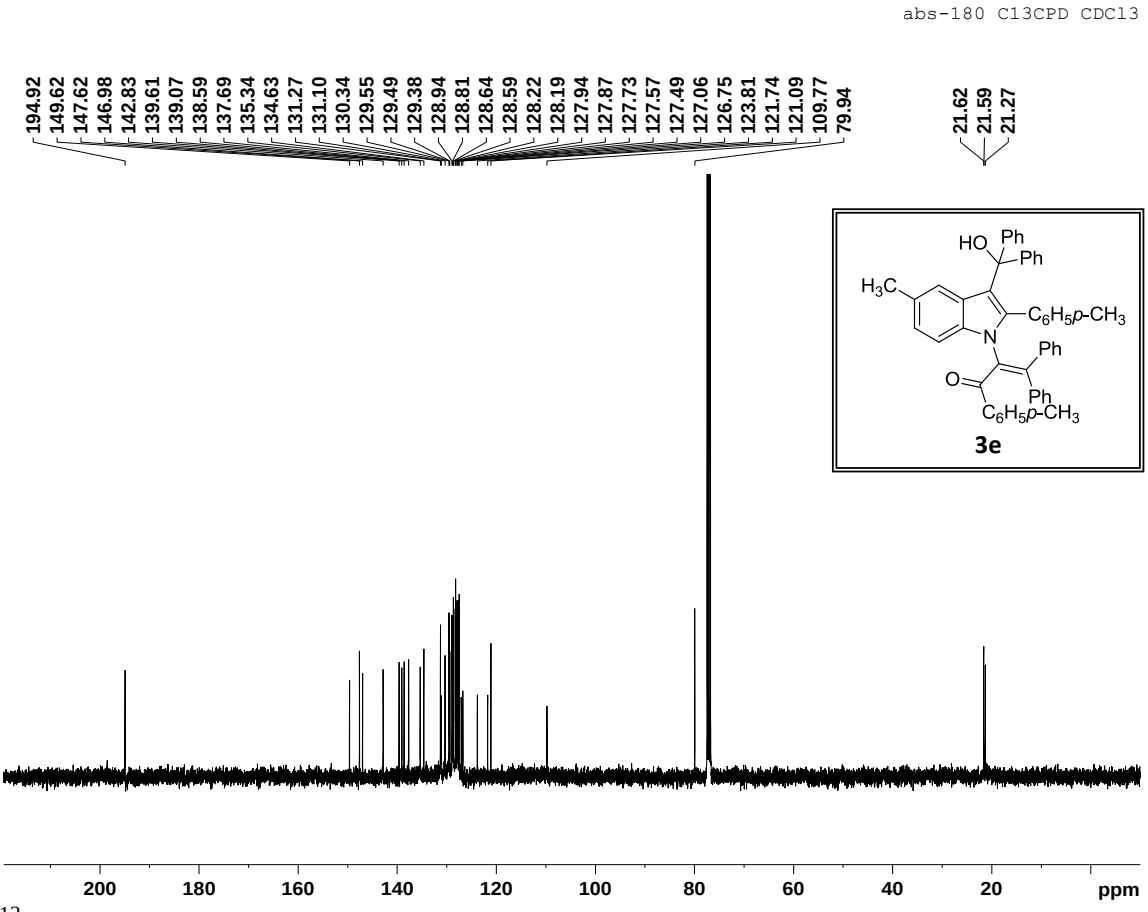
^{13}C NMR (δ) spectrum of **3d**



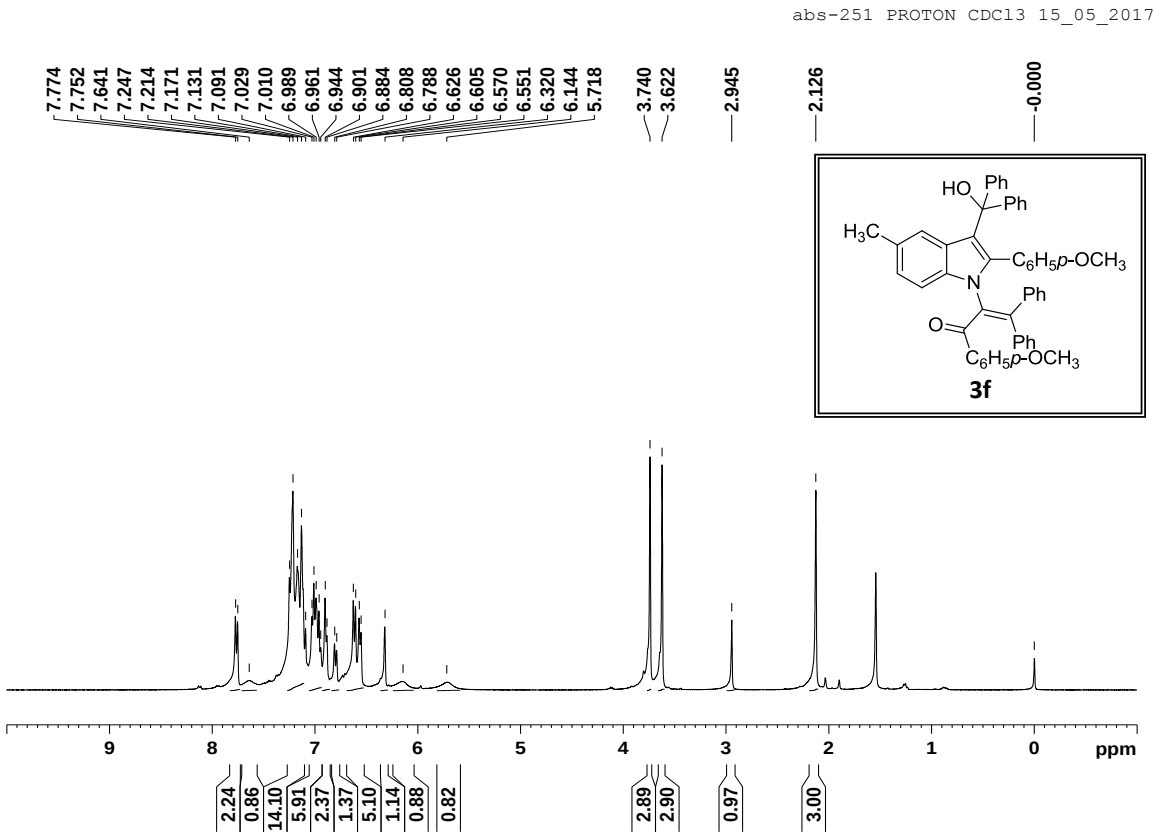
^{19}F NMR (δ) spectrum of **3d**



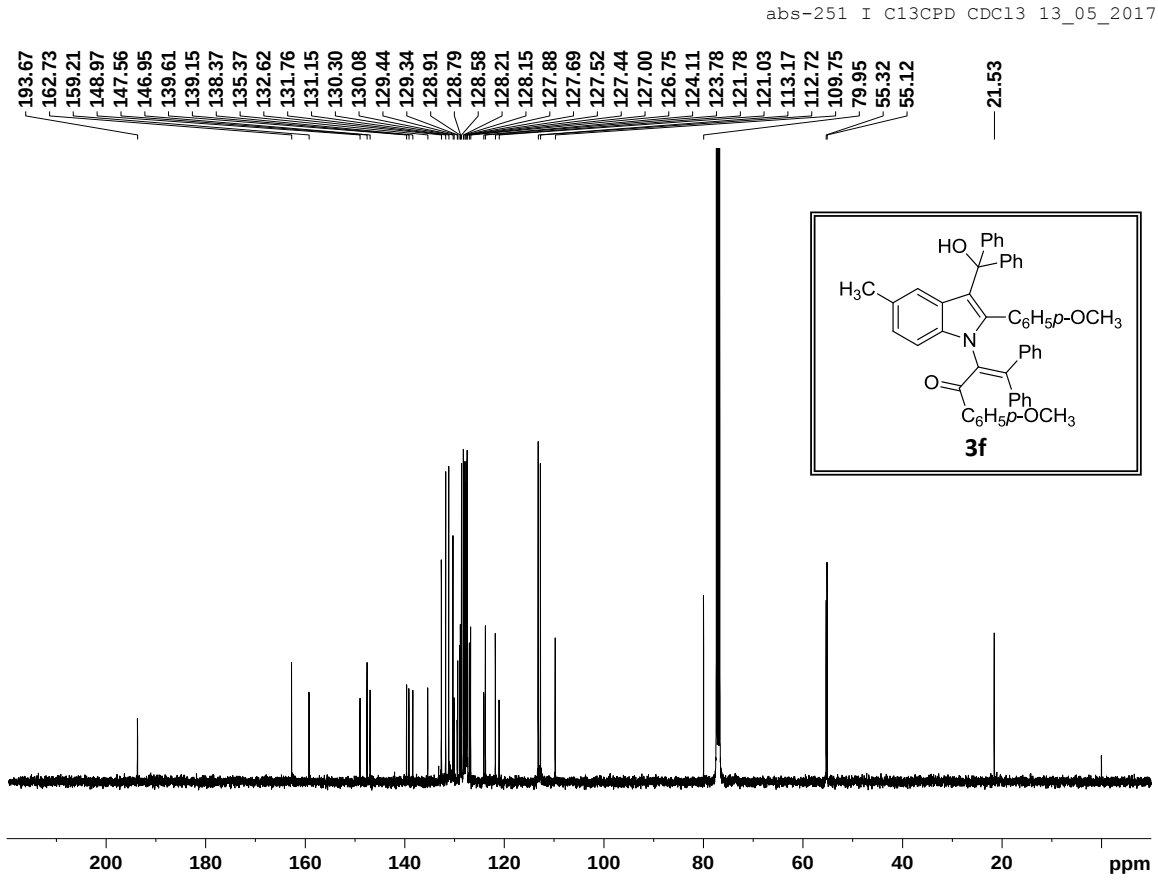
^{1}H NMR (δ) spectrum of **3e**



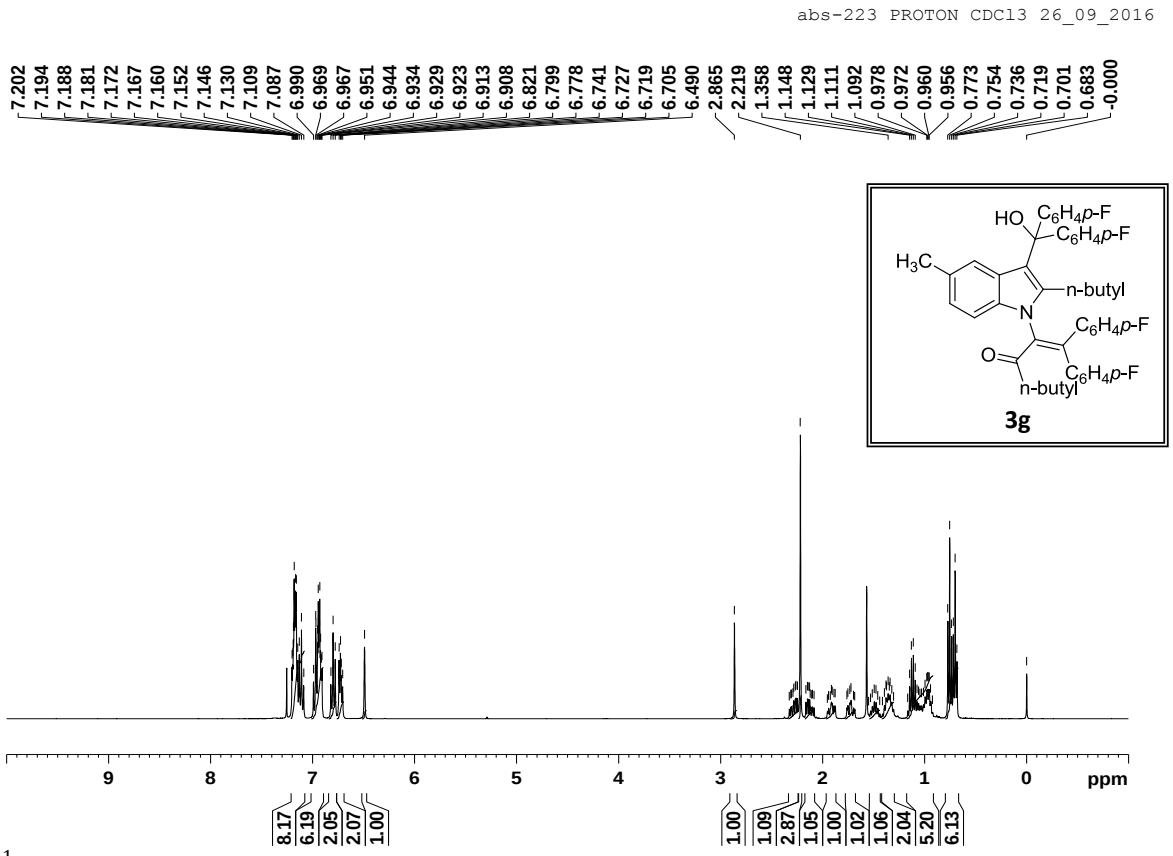
^{13}C NMR (δ) spectrum of **3e**



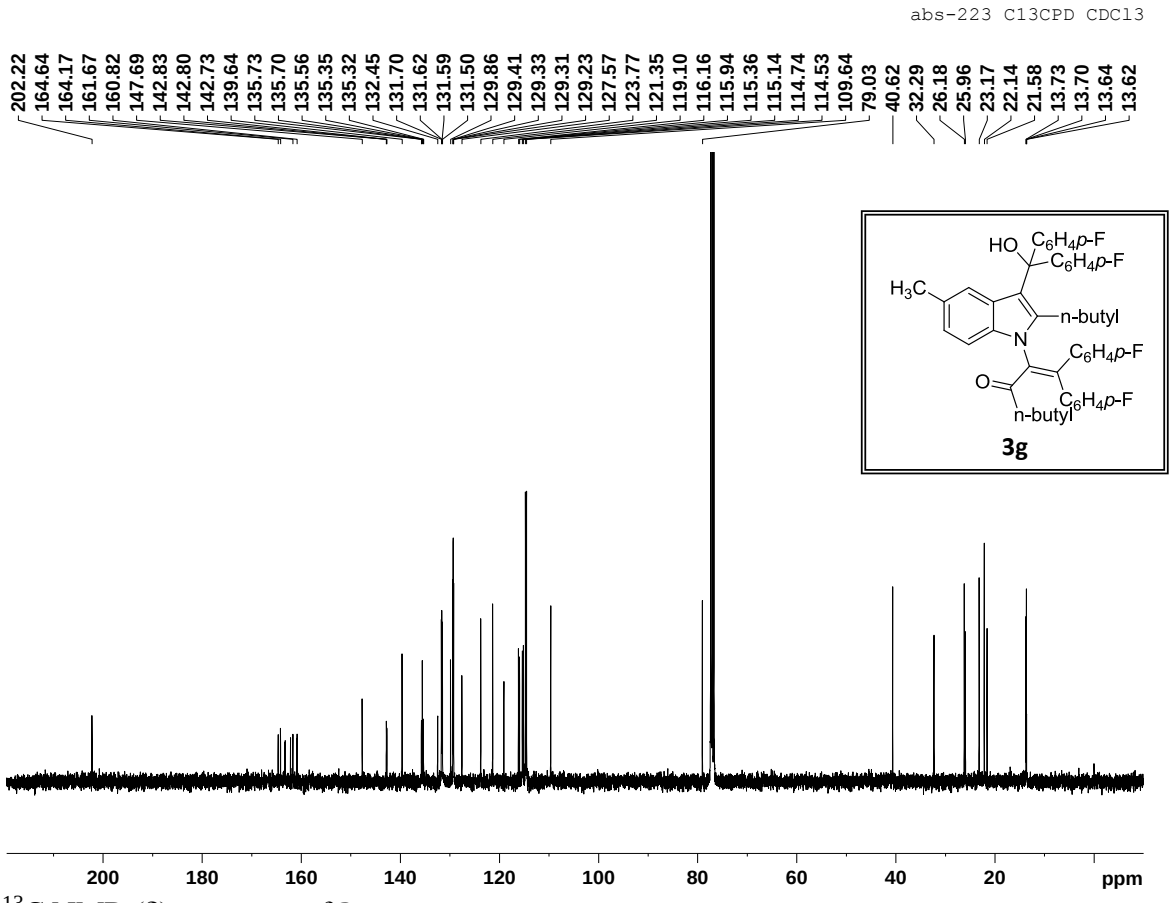
^{1}H NMR (δ) spectrum of **3f**



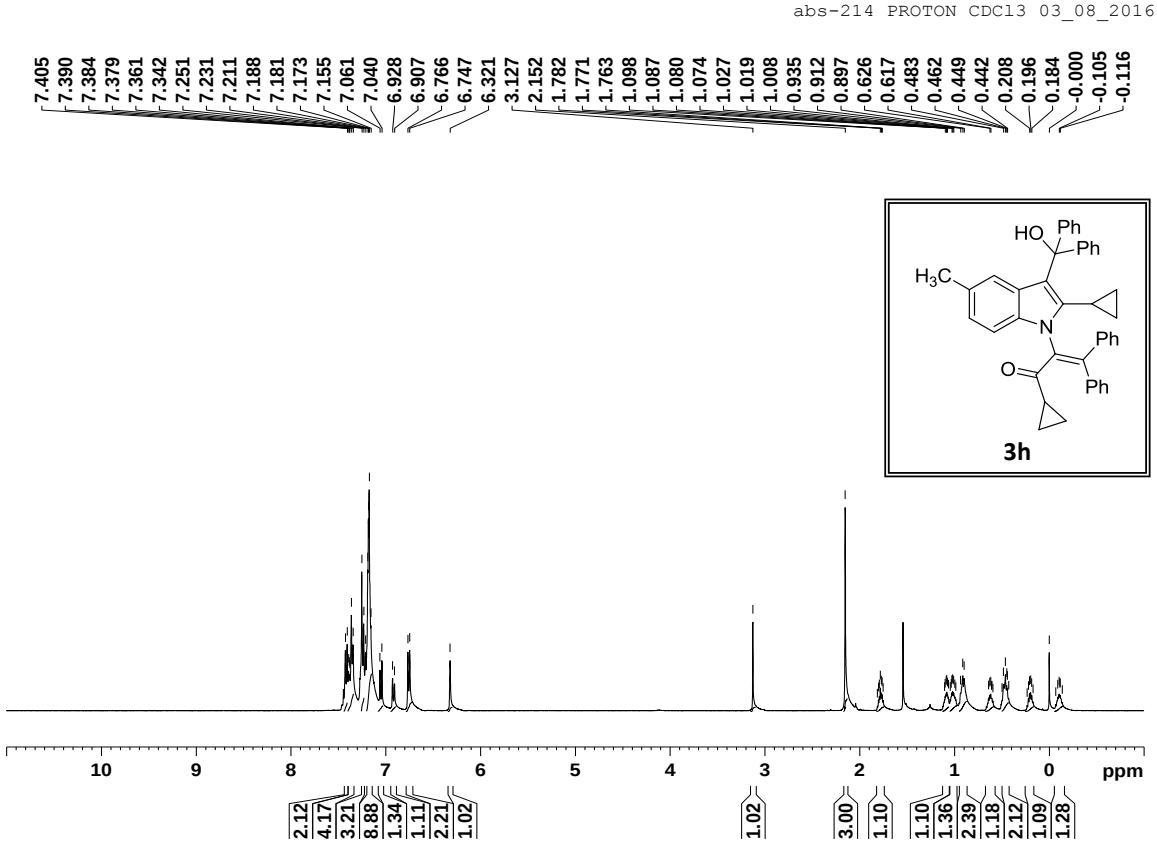
^{13}C NMR (δ) spectrum of **3f**



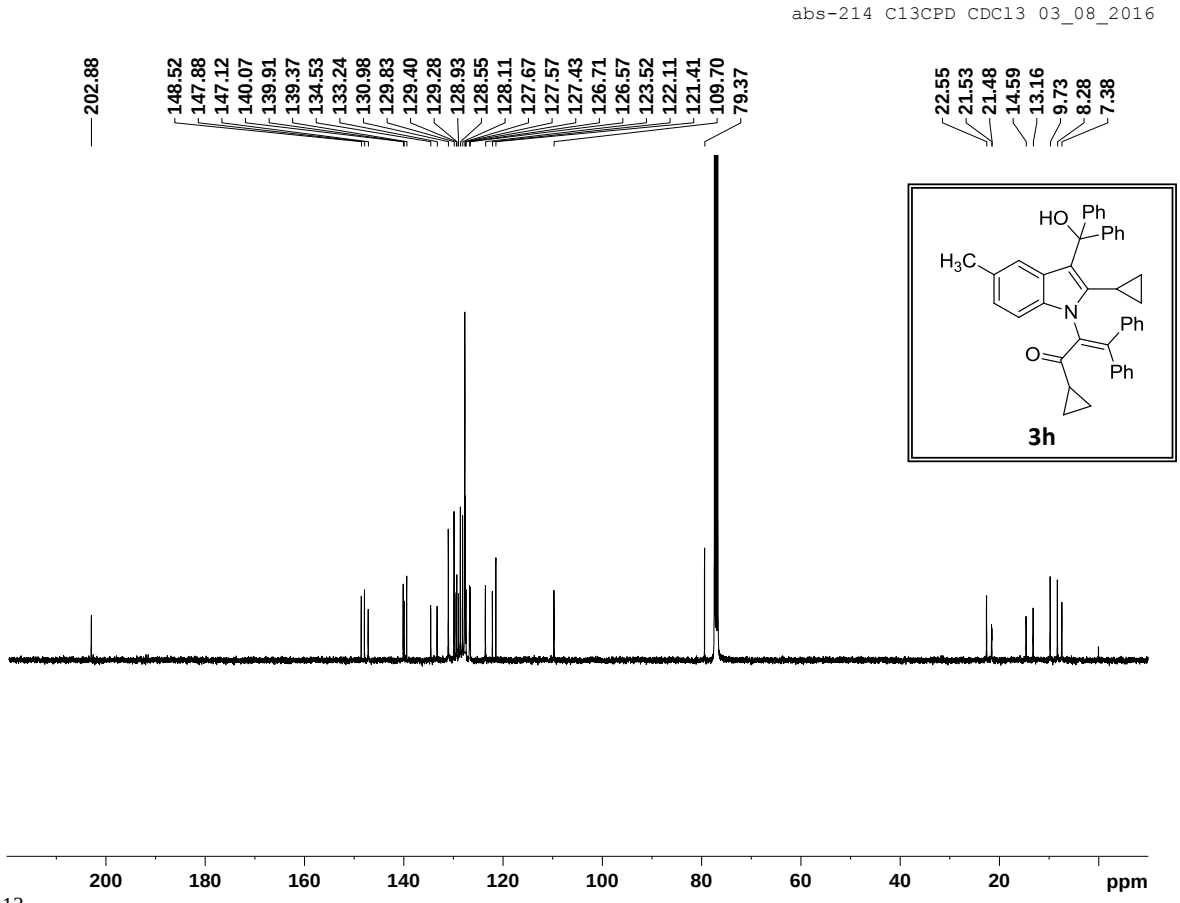
^{1}H NMR (δ) spectrum of **3g**



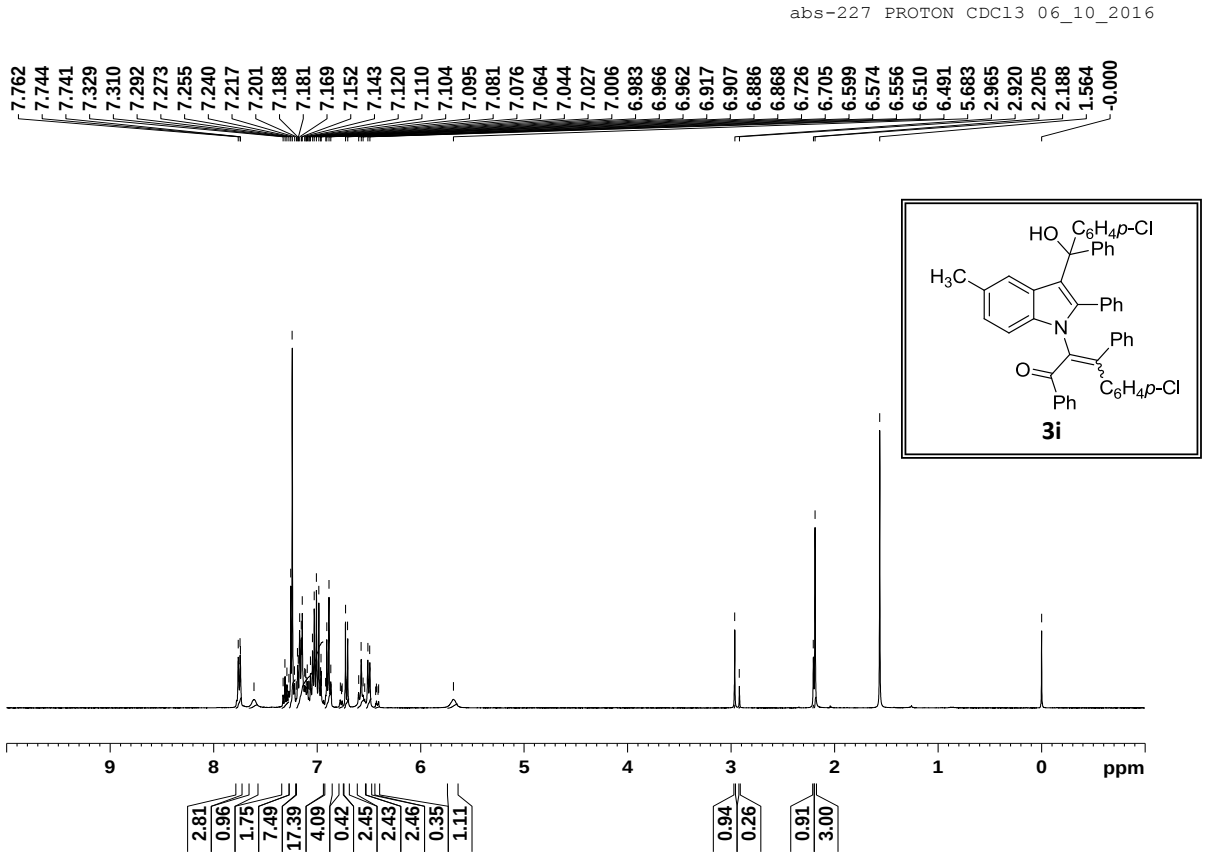
^{13}C NMR (δ) spectrum of **3g**



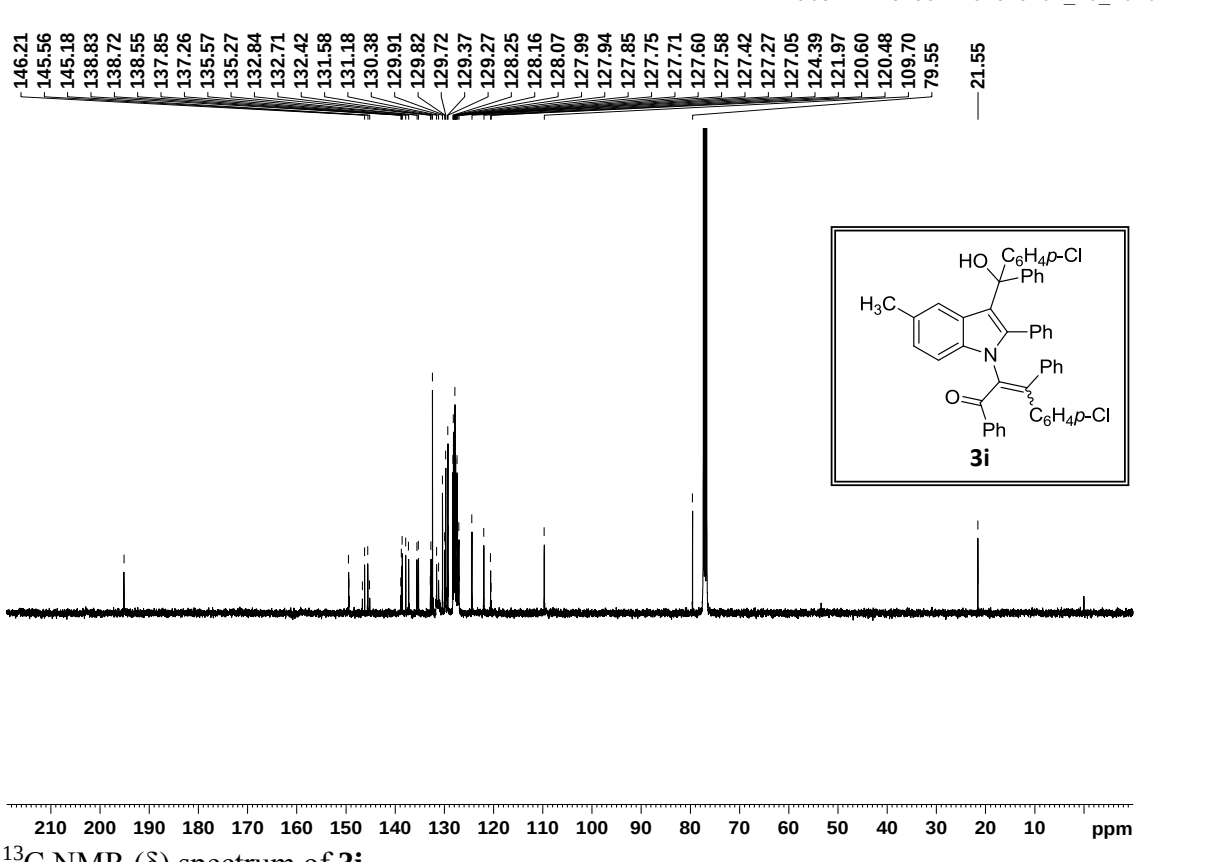
^{1}H NMR (δ) spectrum of **3h**



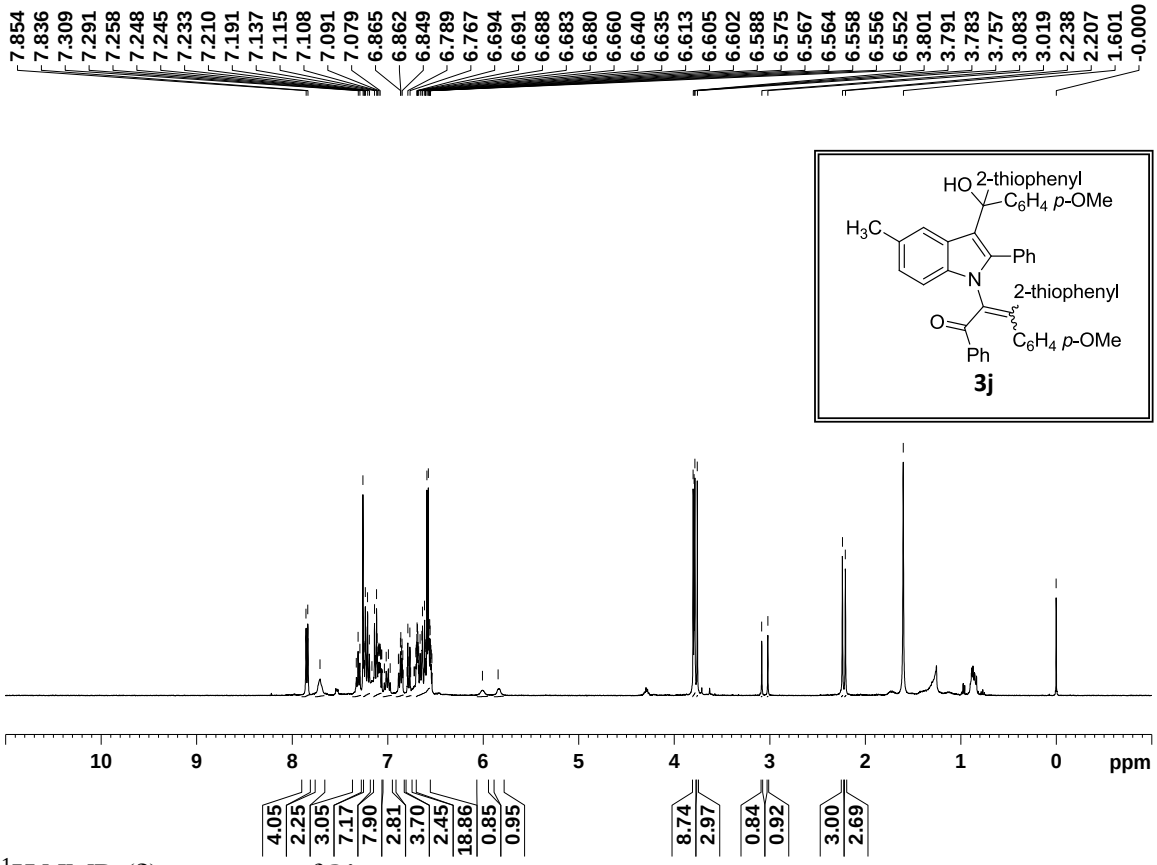
^{13}C NMR (δ) spectrum of **3h**



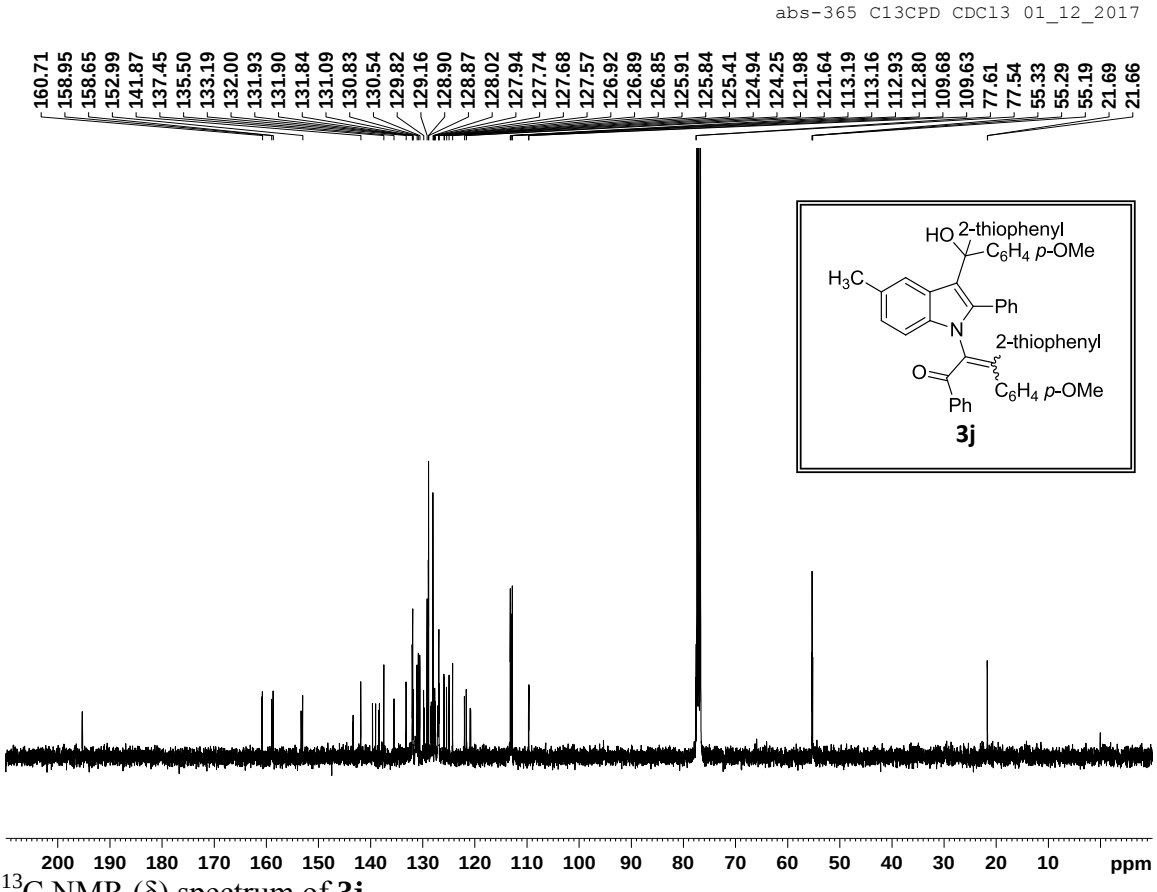
^{1}H NMR (δ) spectrum of **3i**



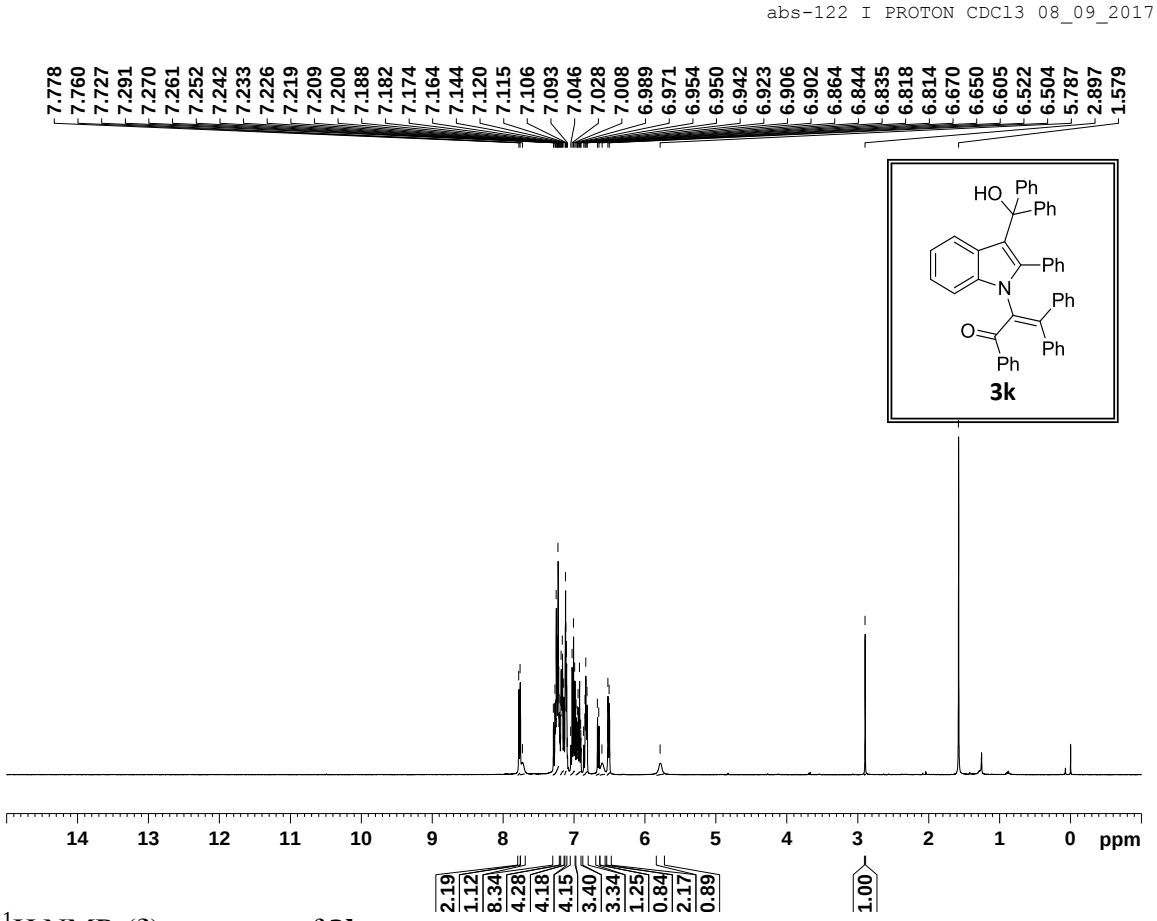
^{13}C NMR (δ) spectrum of **3i**



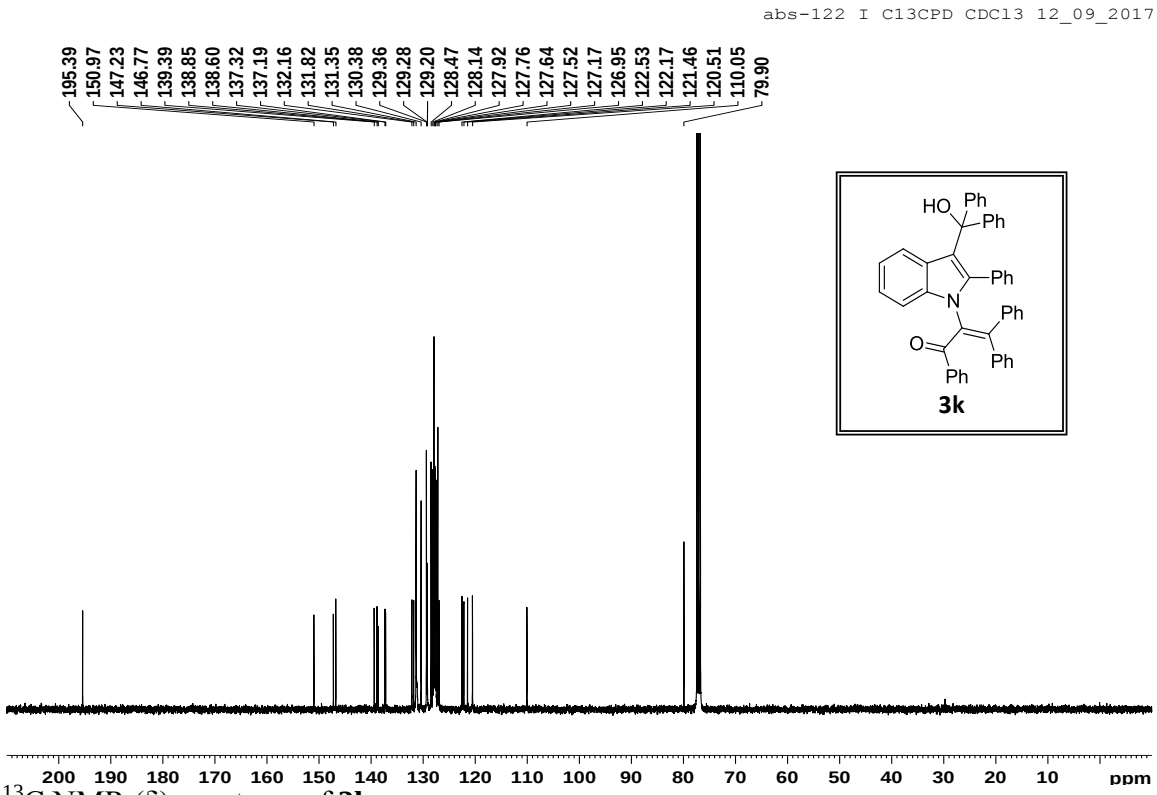
^{1}H NMR (δ) spectrum of **3j**



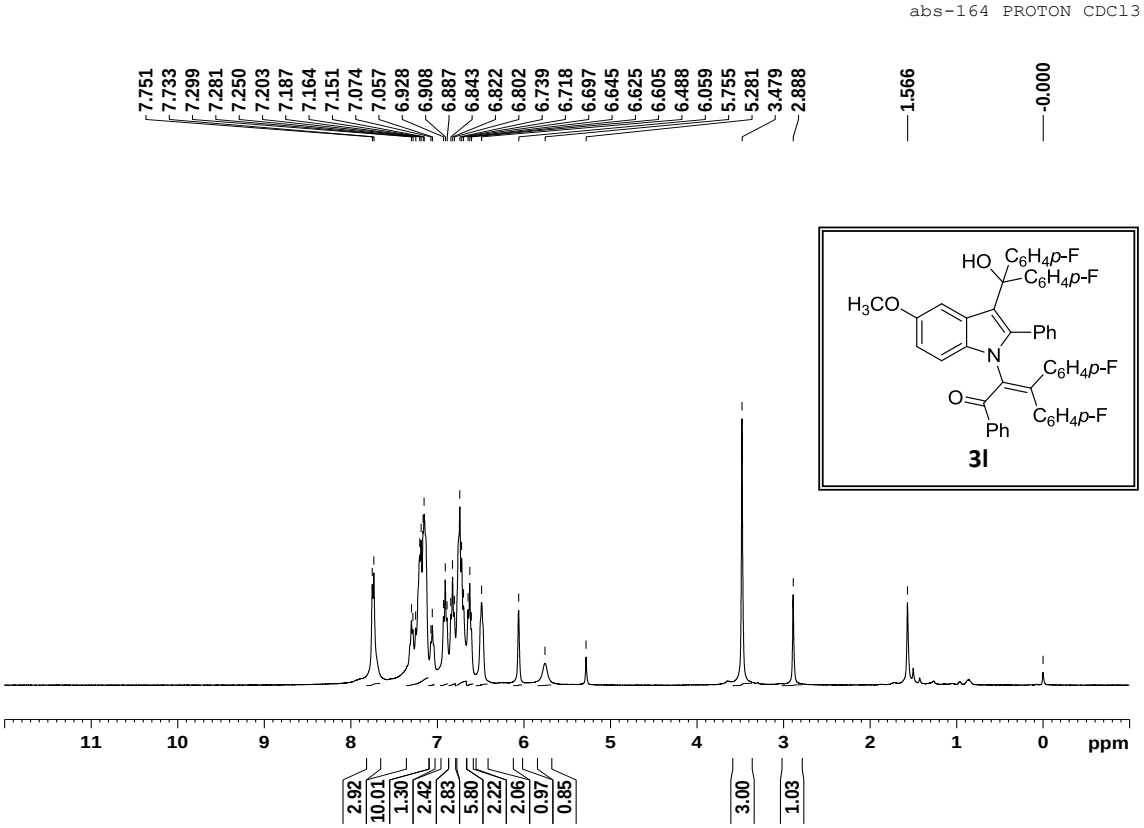
^{13}C NMR (δ) spectrum of **3j**



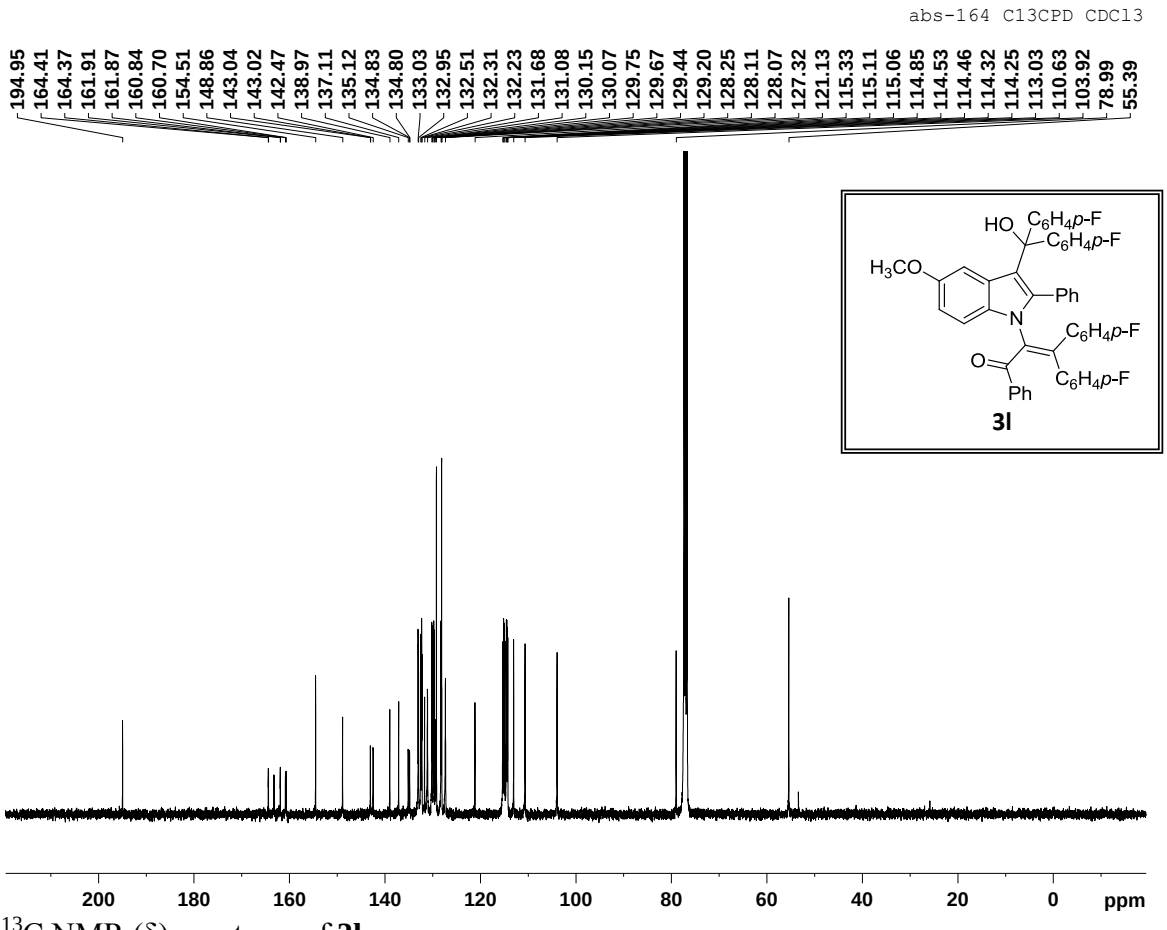
^{1}H NMR (δ) spectrum of **3k**



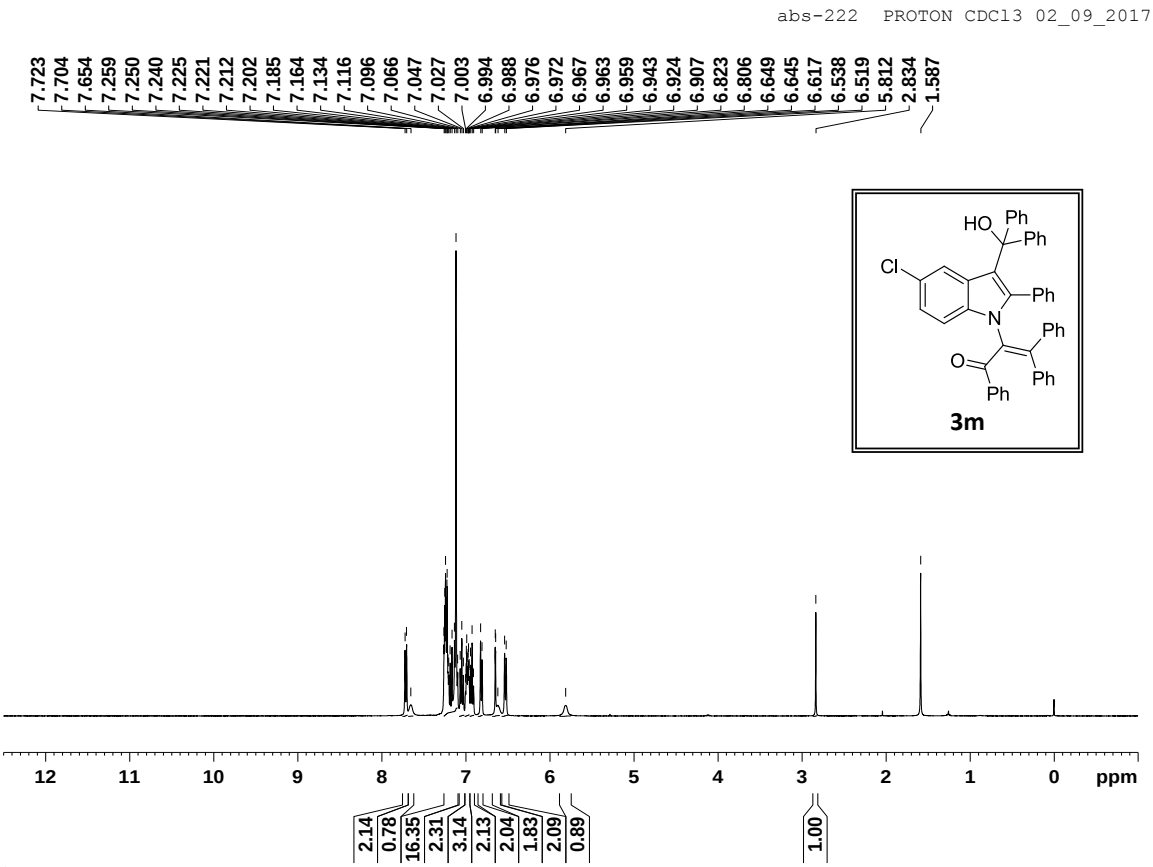
^{13}C NMR (δ) spectrum of **3k**



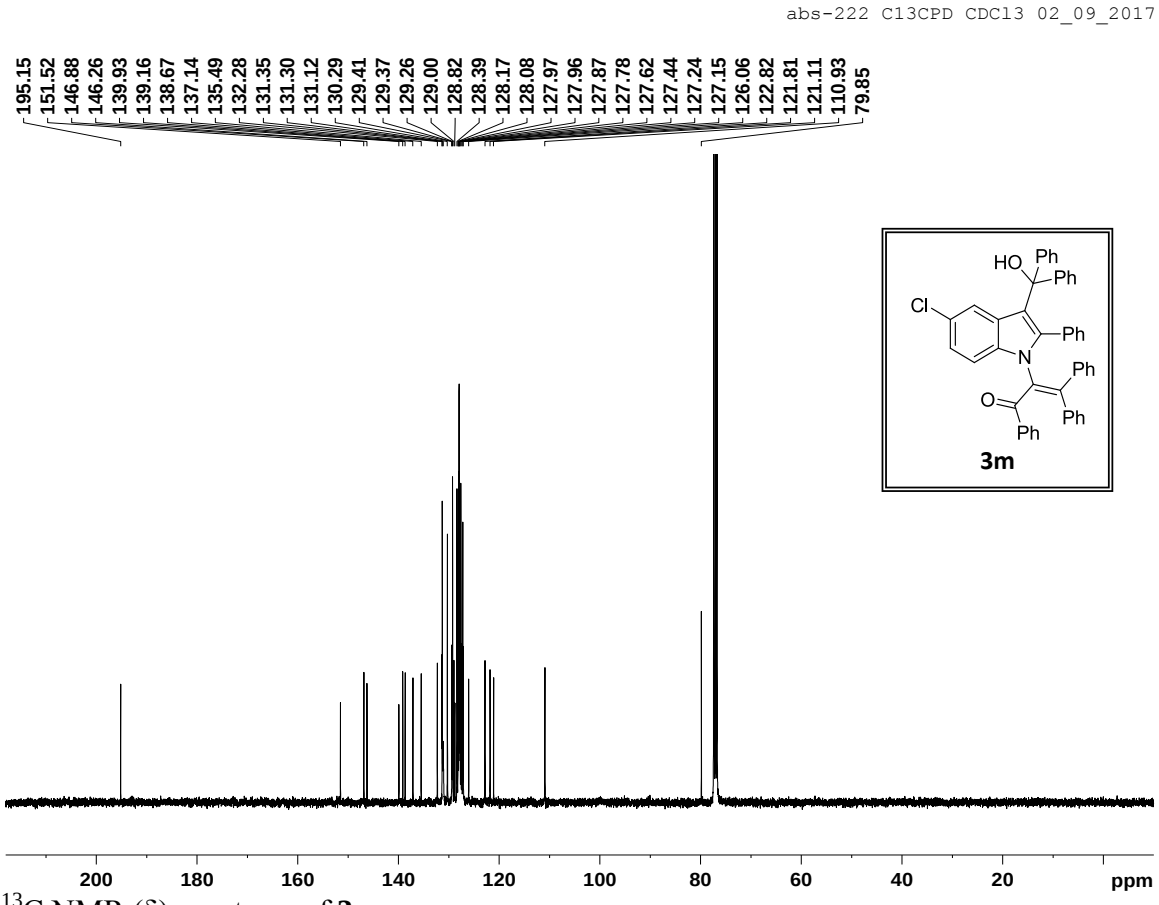
^{1}H NMR (δ) spectrum of **3l**



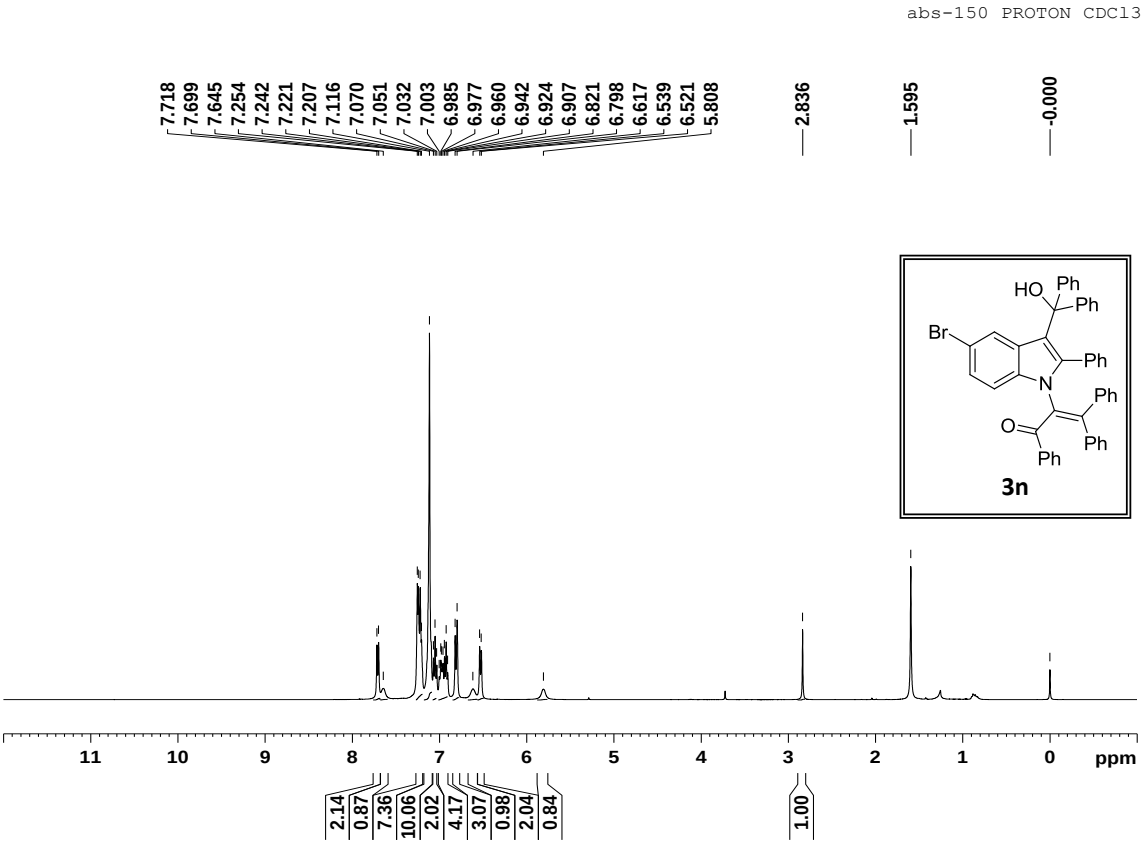
^{13}C NMR (δ) spectrum of **3l**



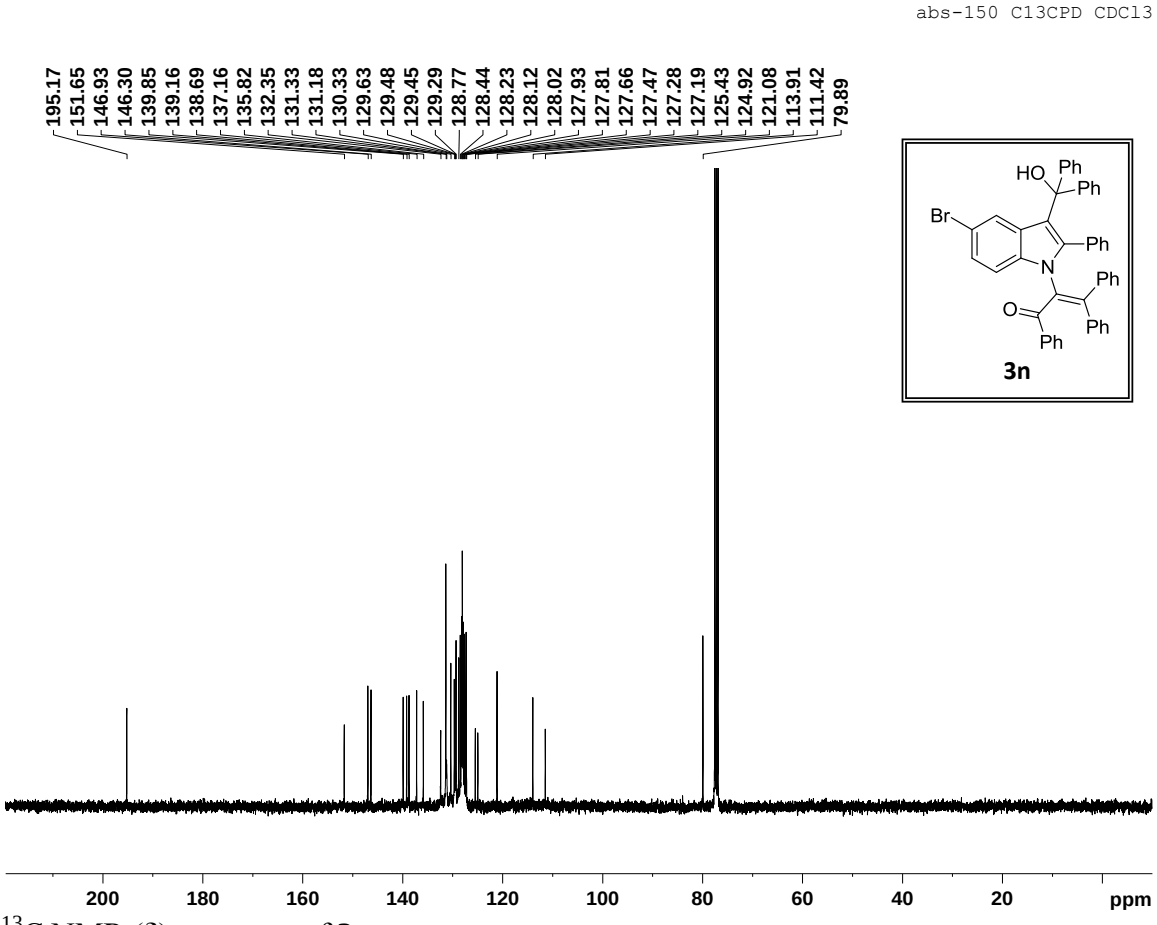
^{1}H NMR (δ) spectrum of **3m**



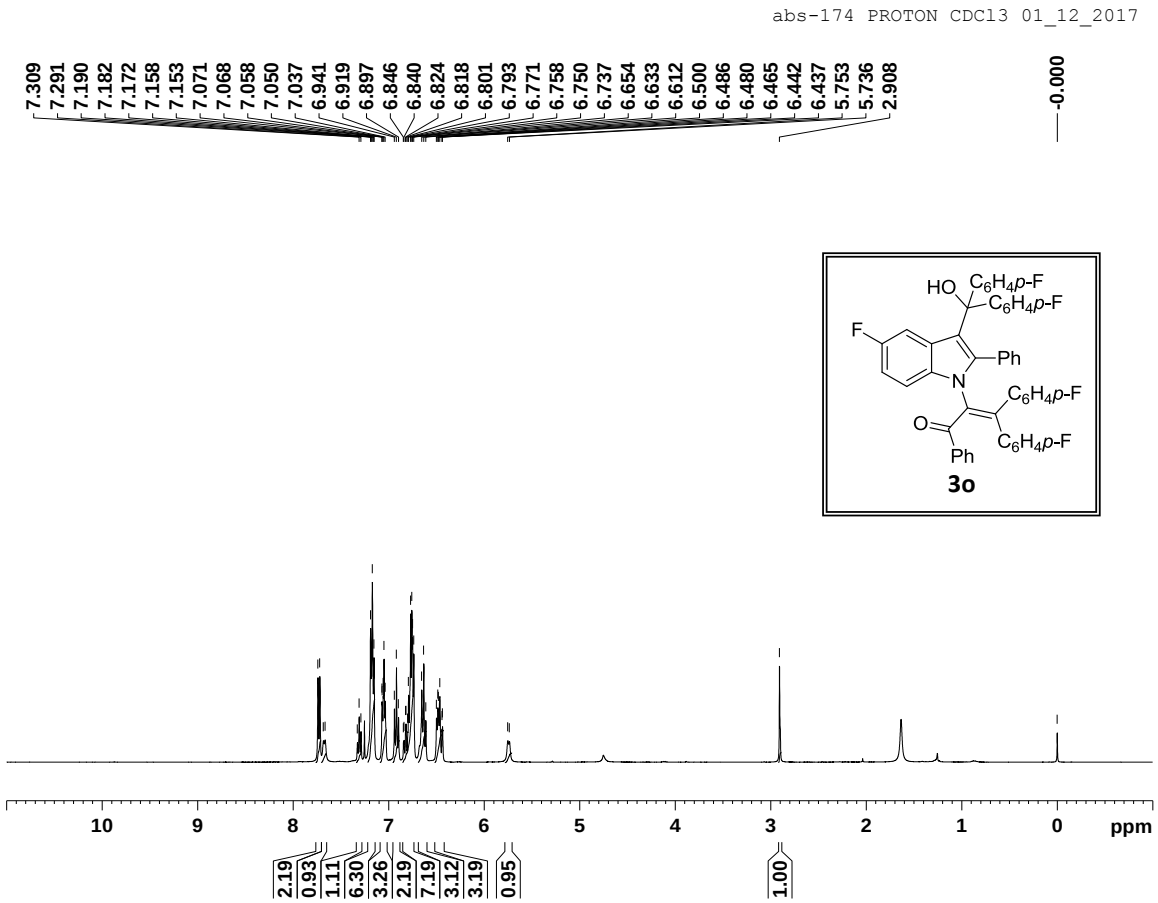
^{13}C NMR (δ) spectrum of **3m**



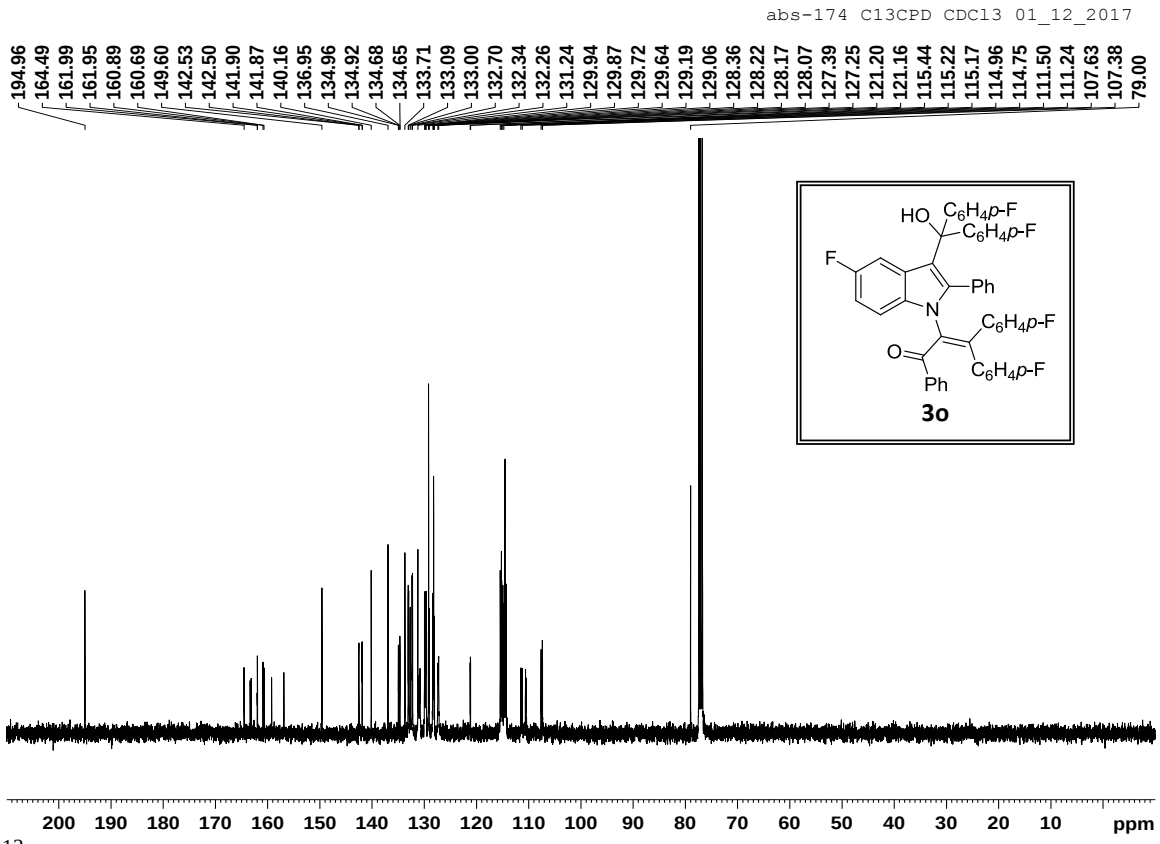
^{1}H NMR (δ) spectrum of **3n**



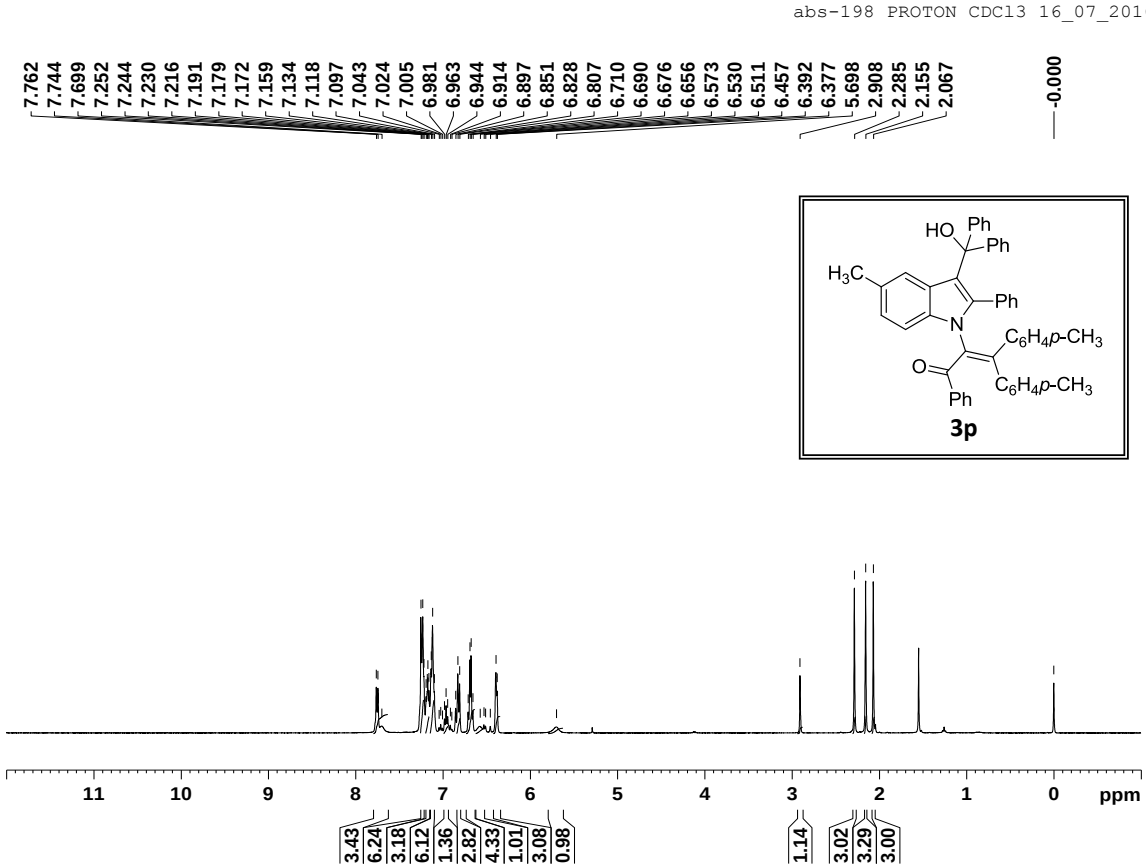
^{13}C NMR (δ) spectrum of **3n**



^{1}H NMR (δ) spectrum of **3o**



^{13}C NMR (δ) spectrum of **3o**



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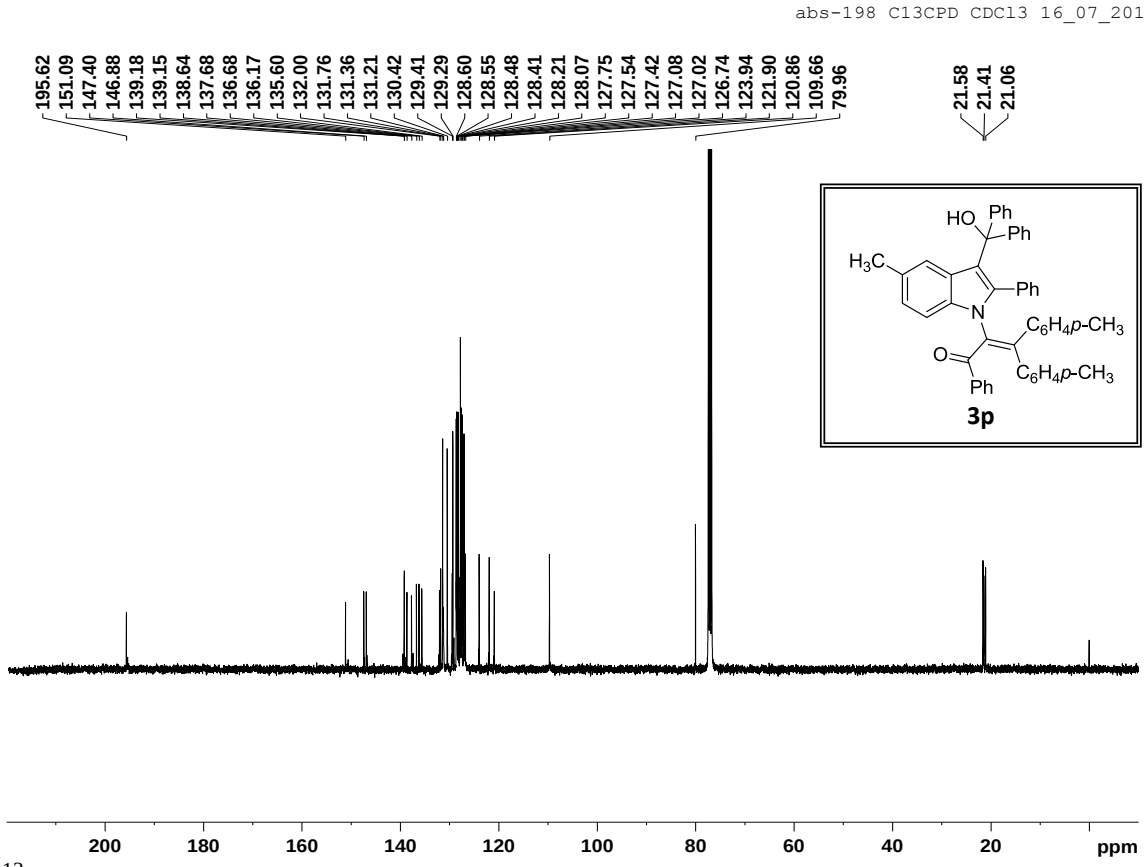
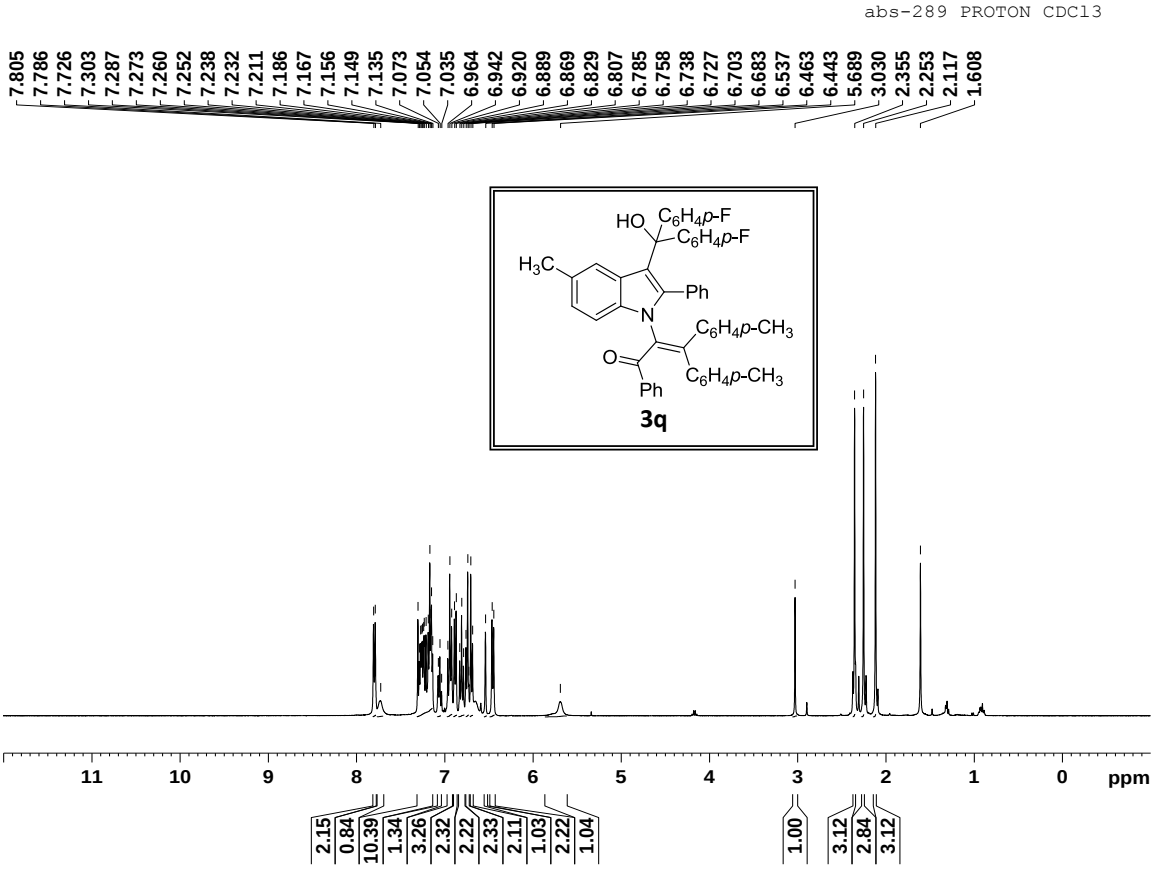
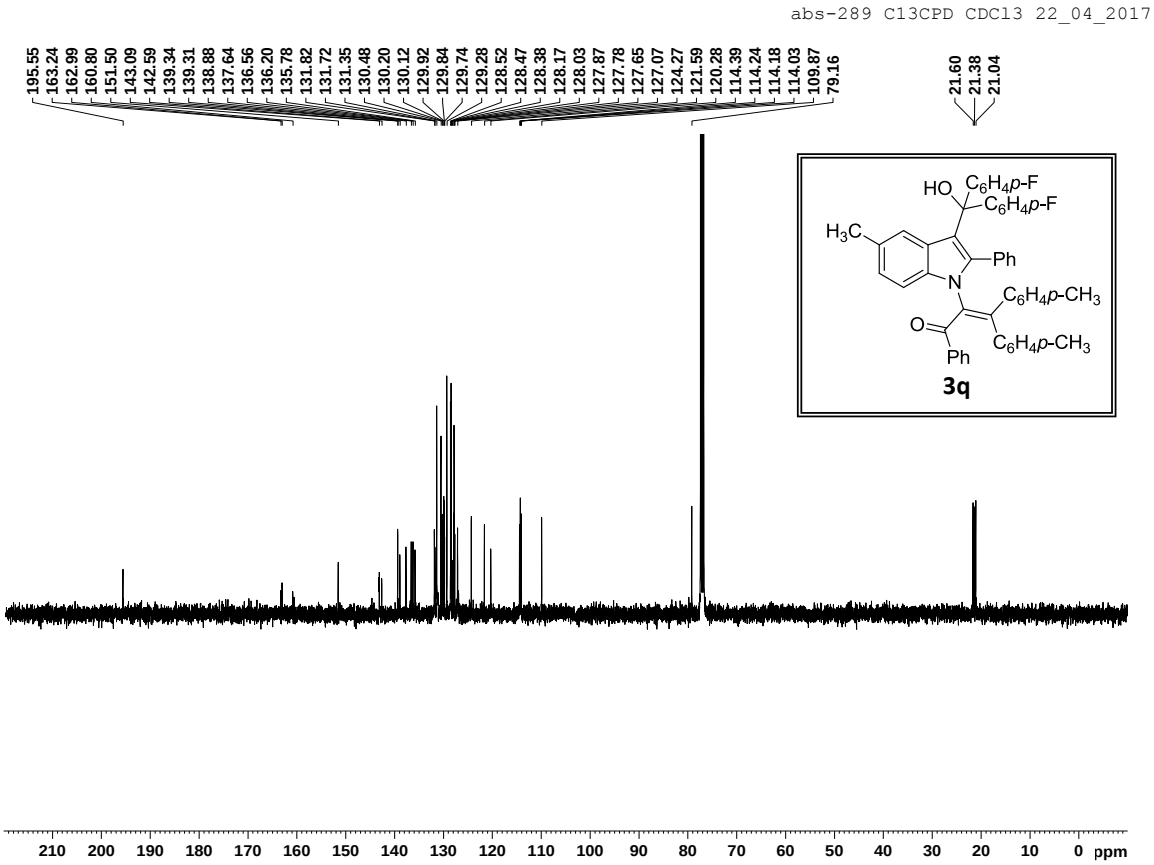


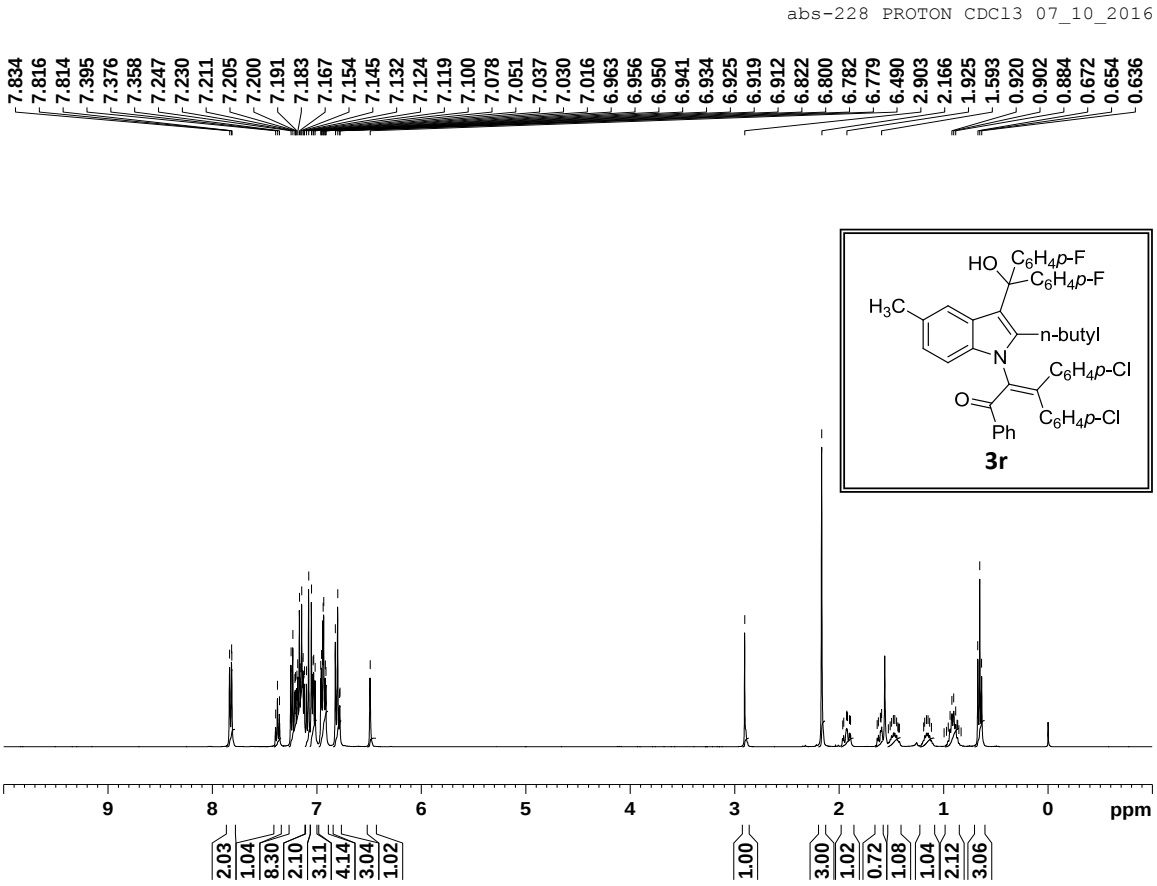
^{13}C NMR (δ) spectrum of **3p**



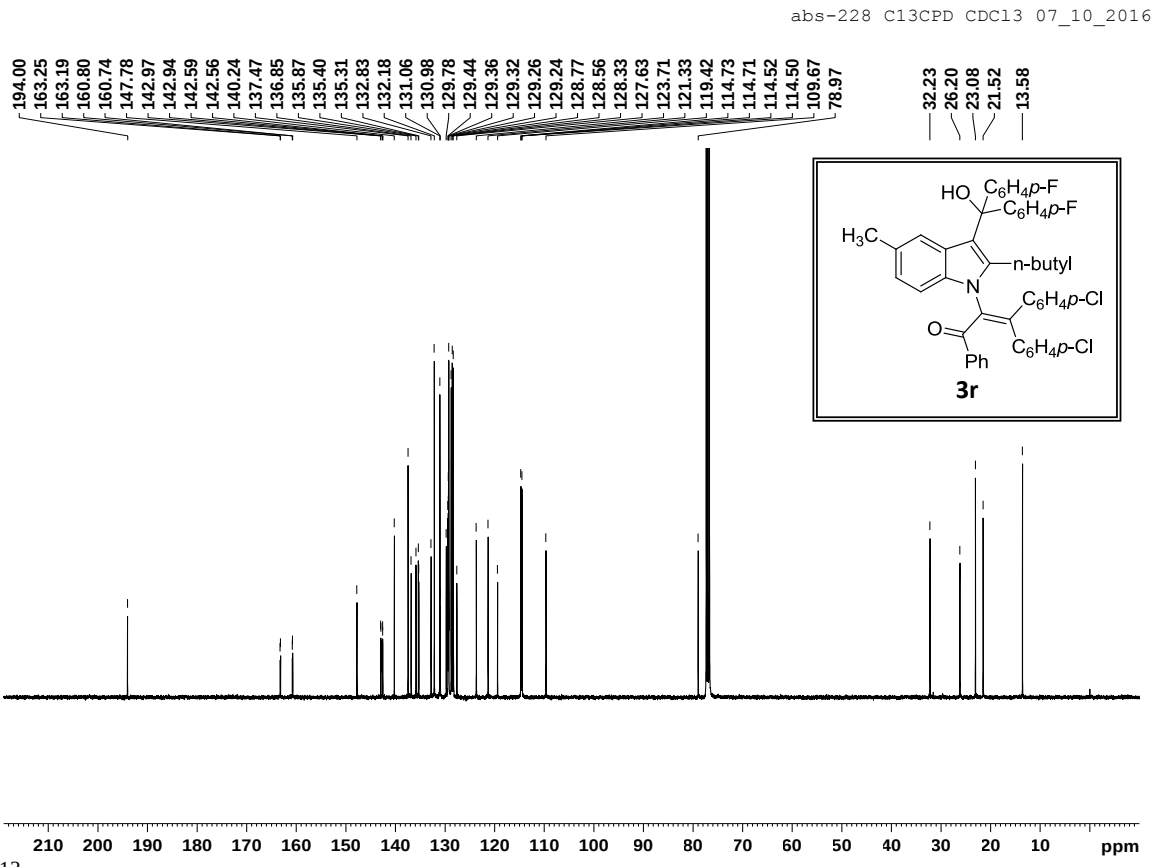
^{1}H NMR (δ) spectrum of **3q**



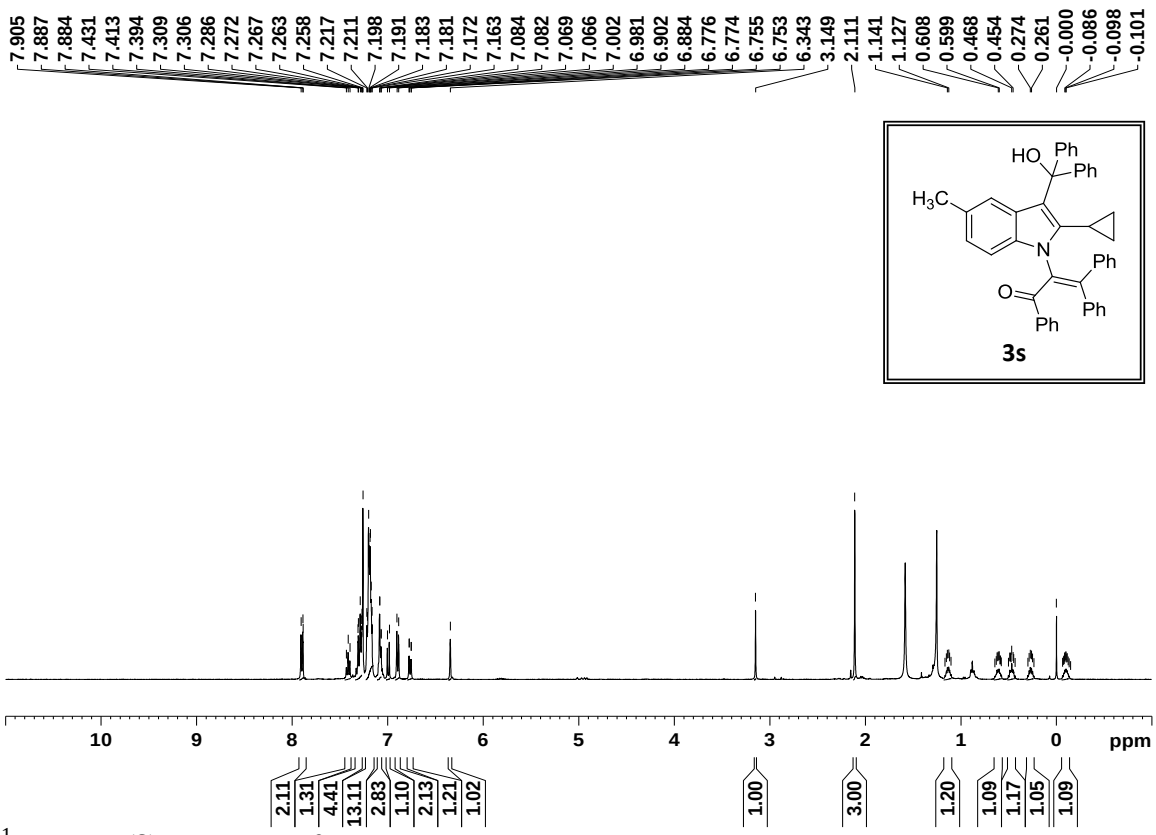
^{13}C NMR (δ) spectrum of **3q**



^{1}H NMR (δ) spectrum of **3r**



^{13}C NMR (δ) spectrum of **3r**



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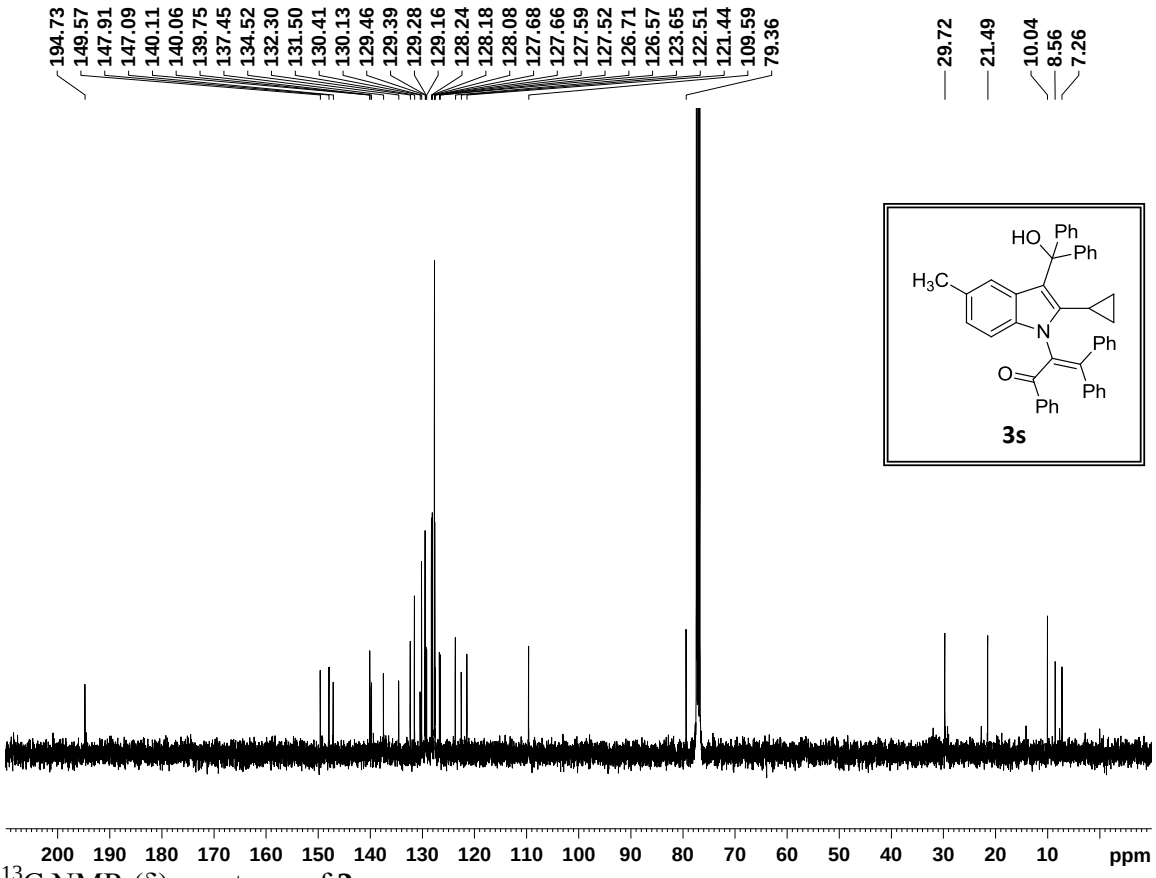
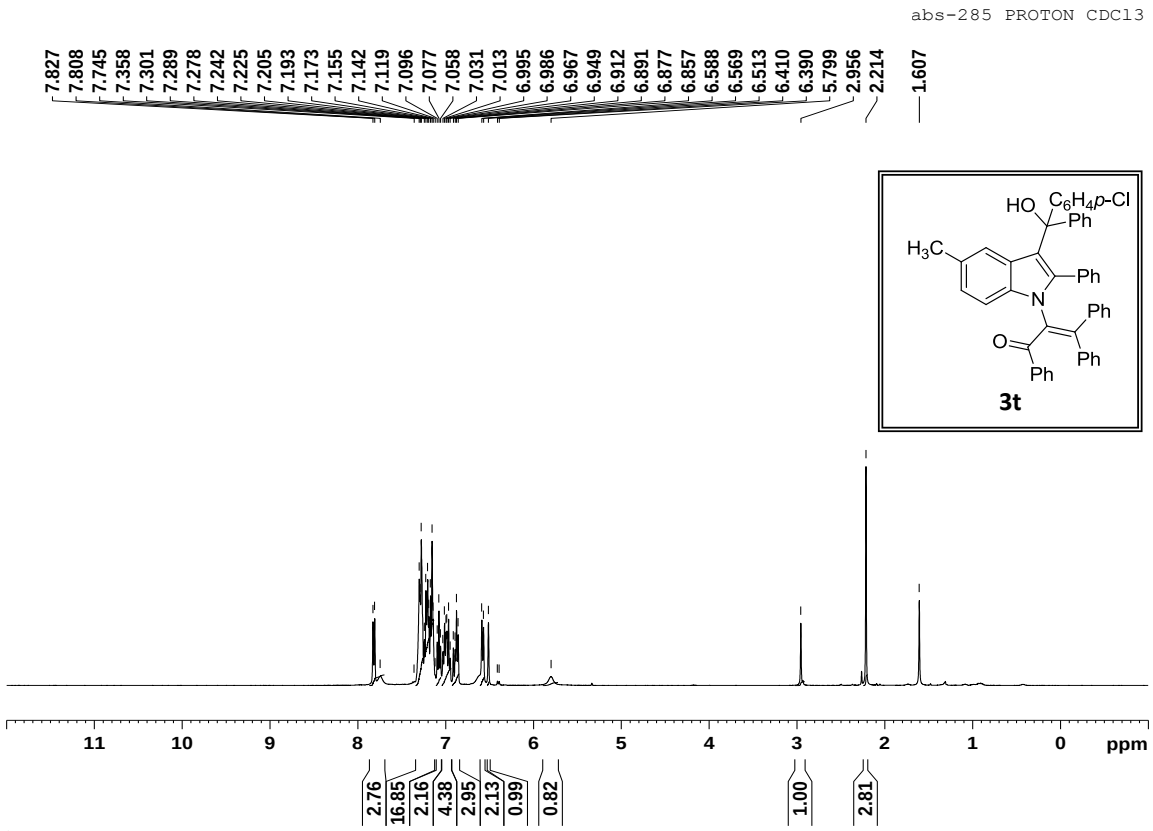
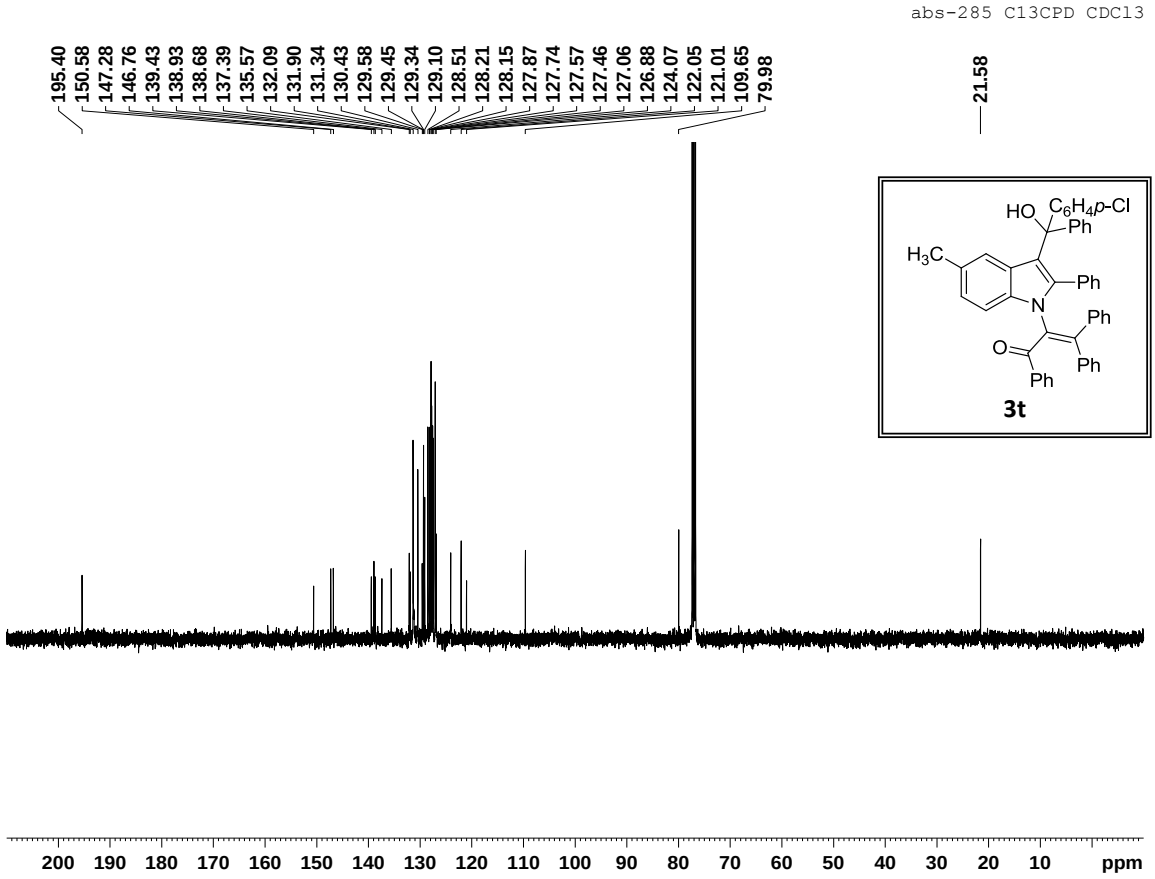


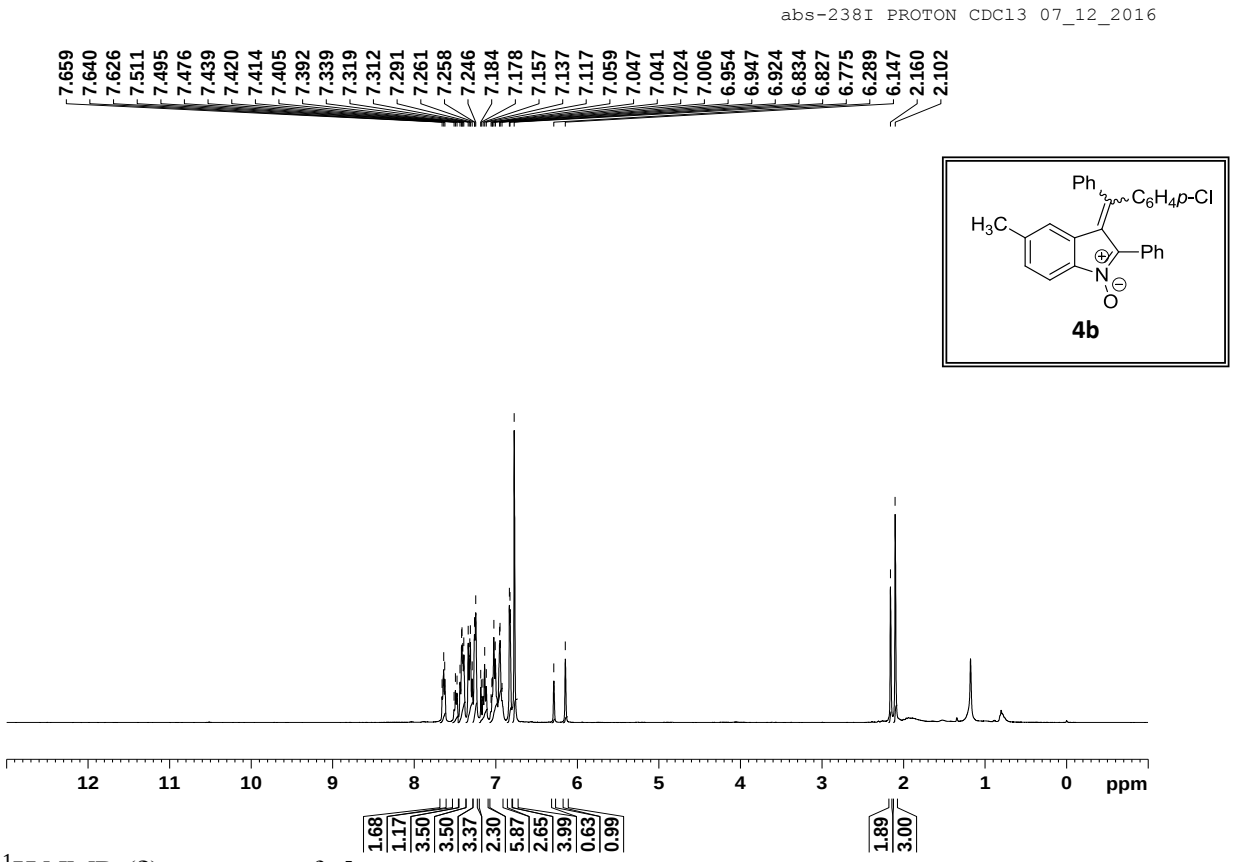
^{13}C NMR (δ) spectrum of **3s**



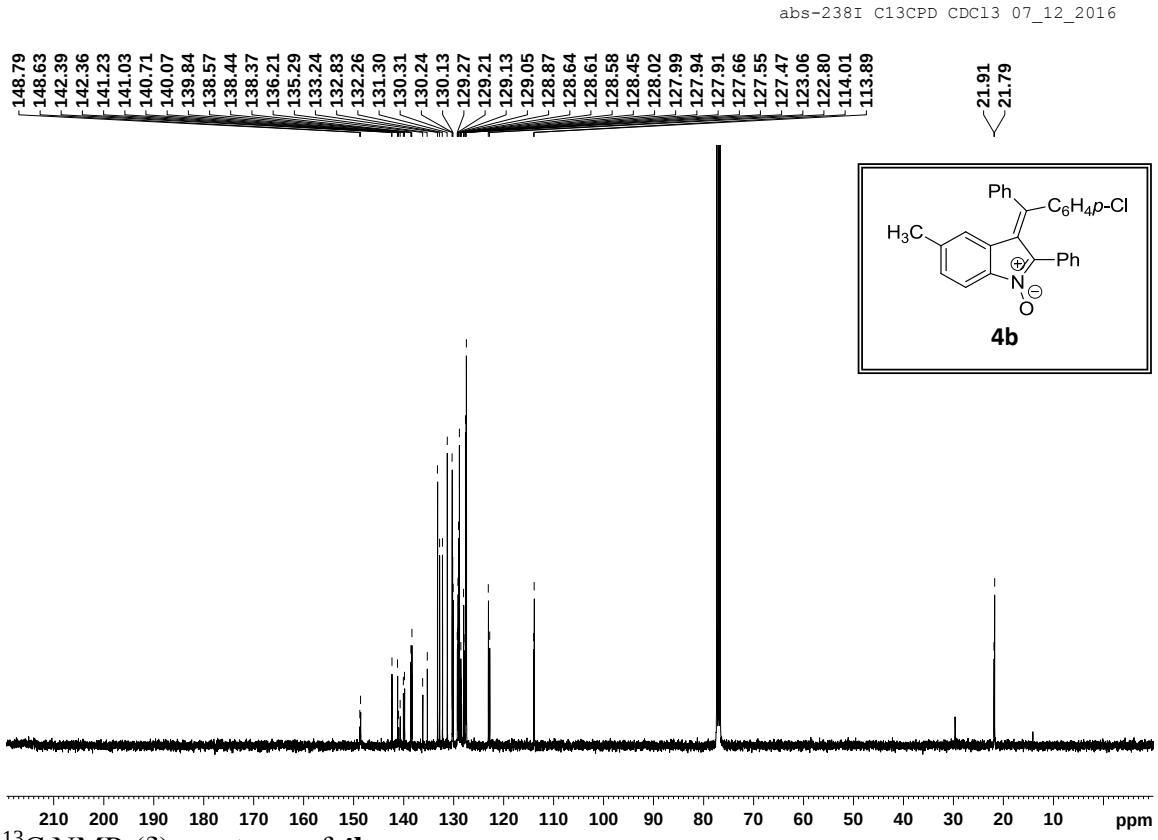
^{1}H NMR (δ) spectrum of **3t**



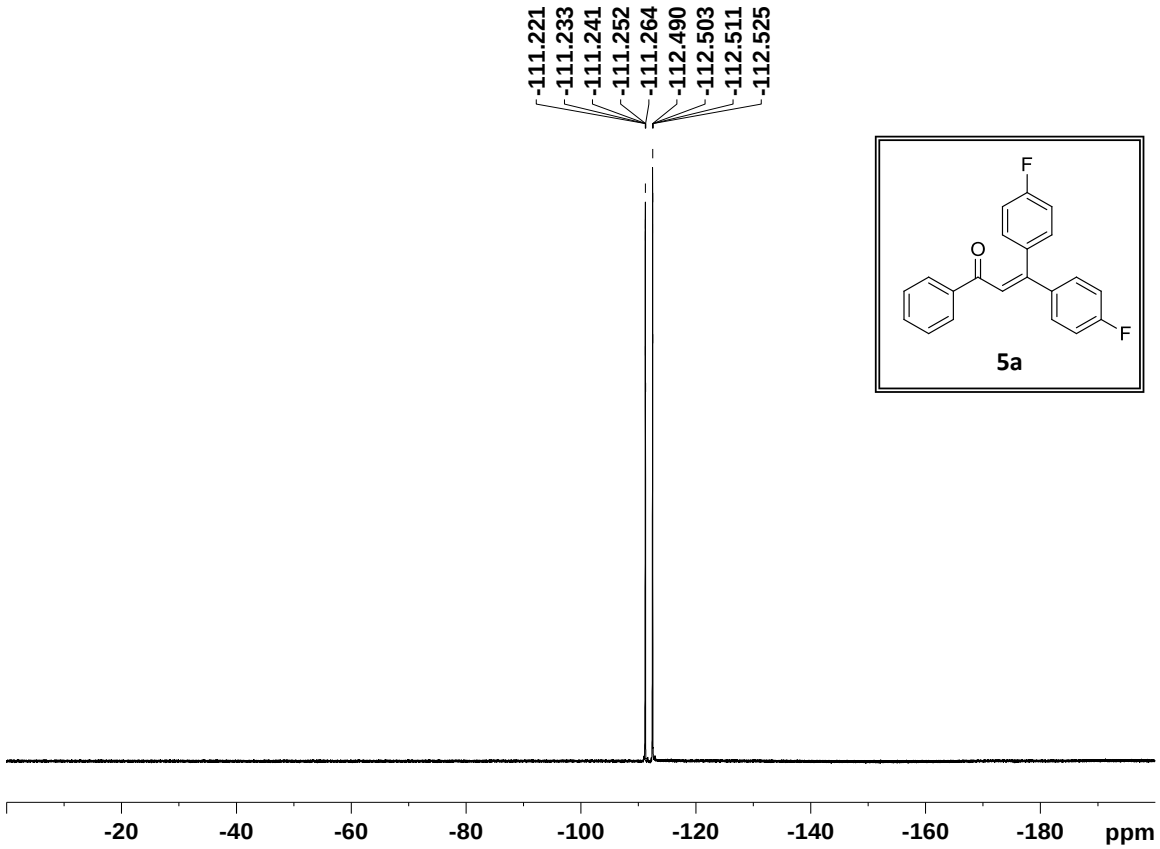
^{13}C NMR (δ) spectrum of **3t.**



^{1}H NMR (δ) spectrum of **4b**



^{13}C NMR (δ) spectrum of **4b**



^{19}F NMR (δ) spectrum of **5a**