

Supplementary Material

β -Pinene and camphor based, pyrazole-tethered triarylphosphines as chiral P,N ligands for palladium

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Table of Contents

X-ray crystal structure.....	S2
Spectrum of all compounds.....	S3

Crystallographic information

X-ray crystal structure of ligand (C3) (Figure 1).

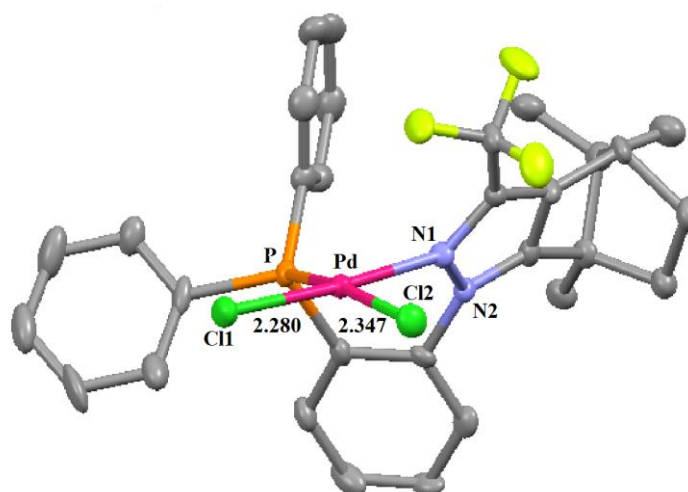


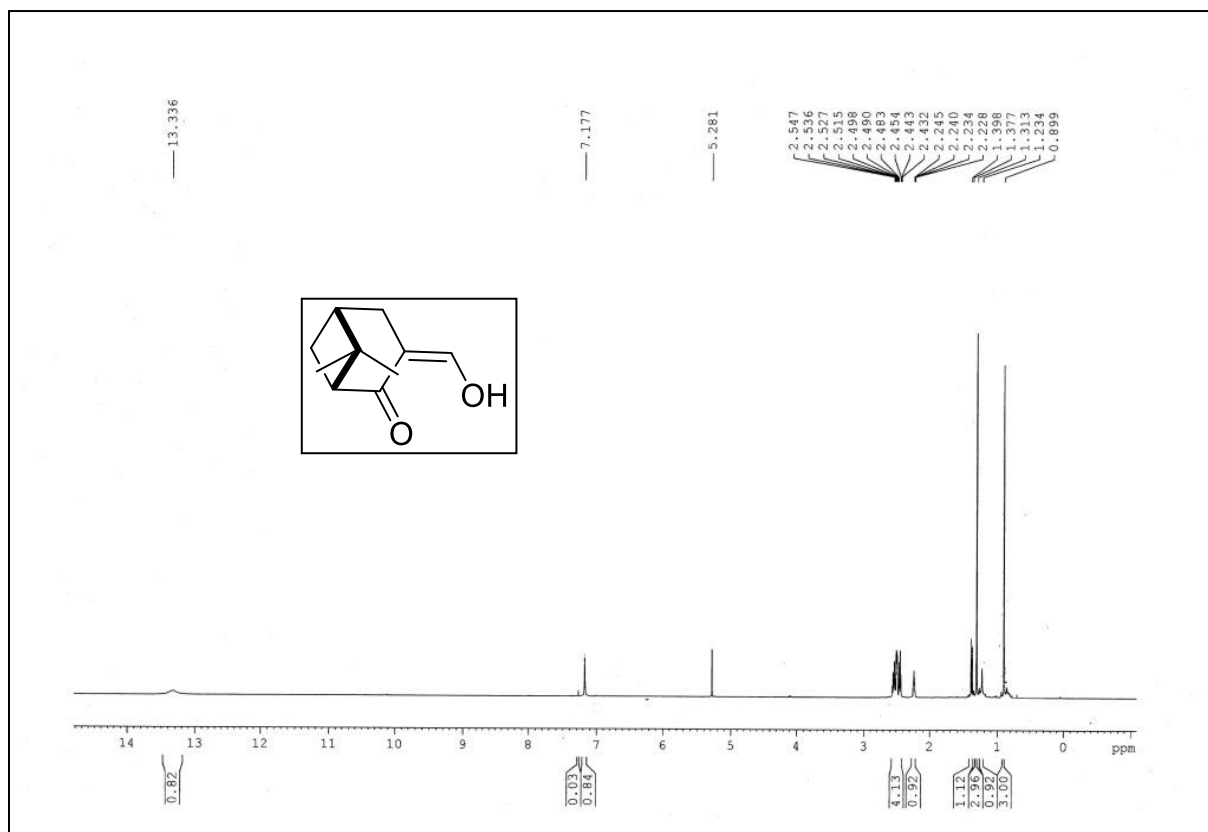
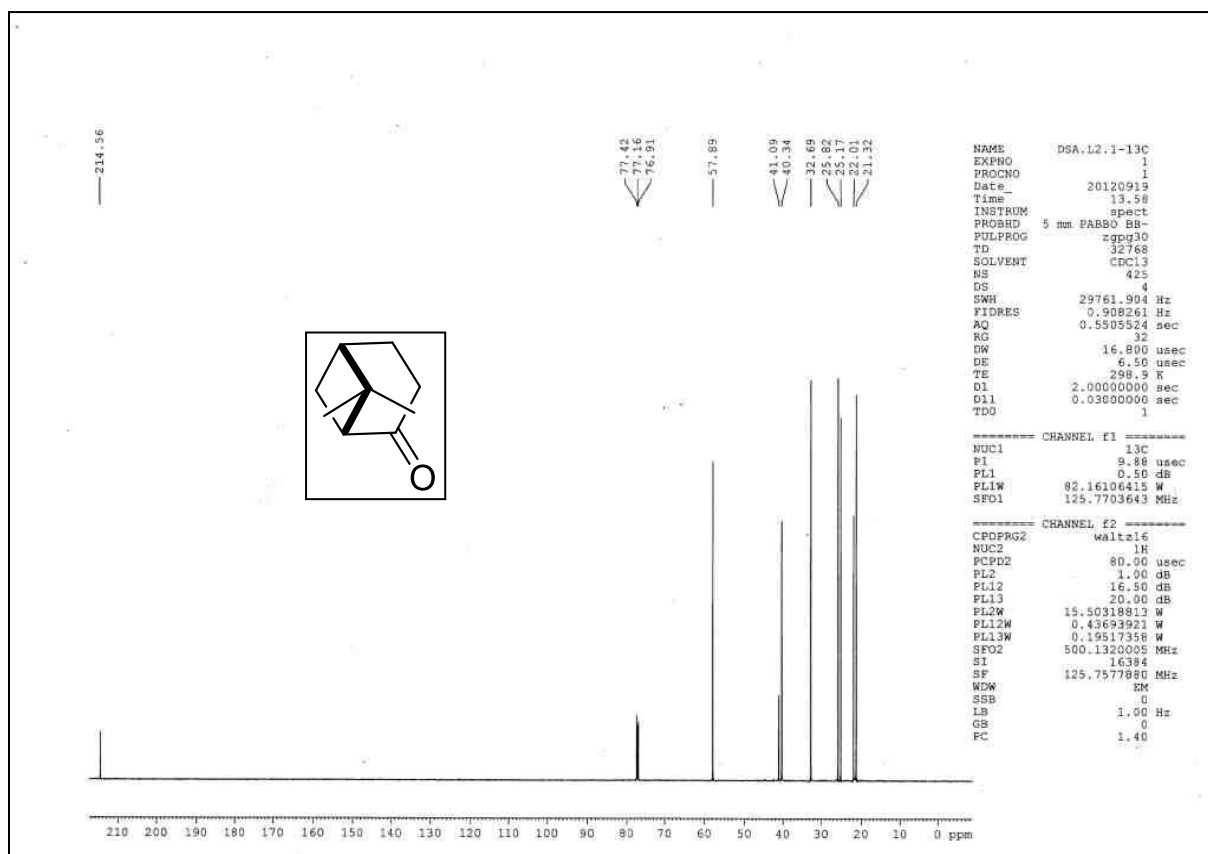
Figure 1: Thermal ellipsoid plot of Pd-L3 (C3) complex drawn at 50 % probability level.

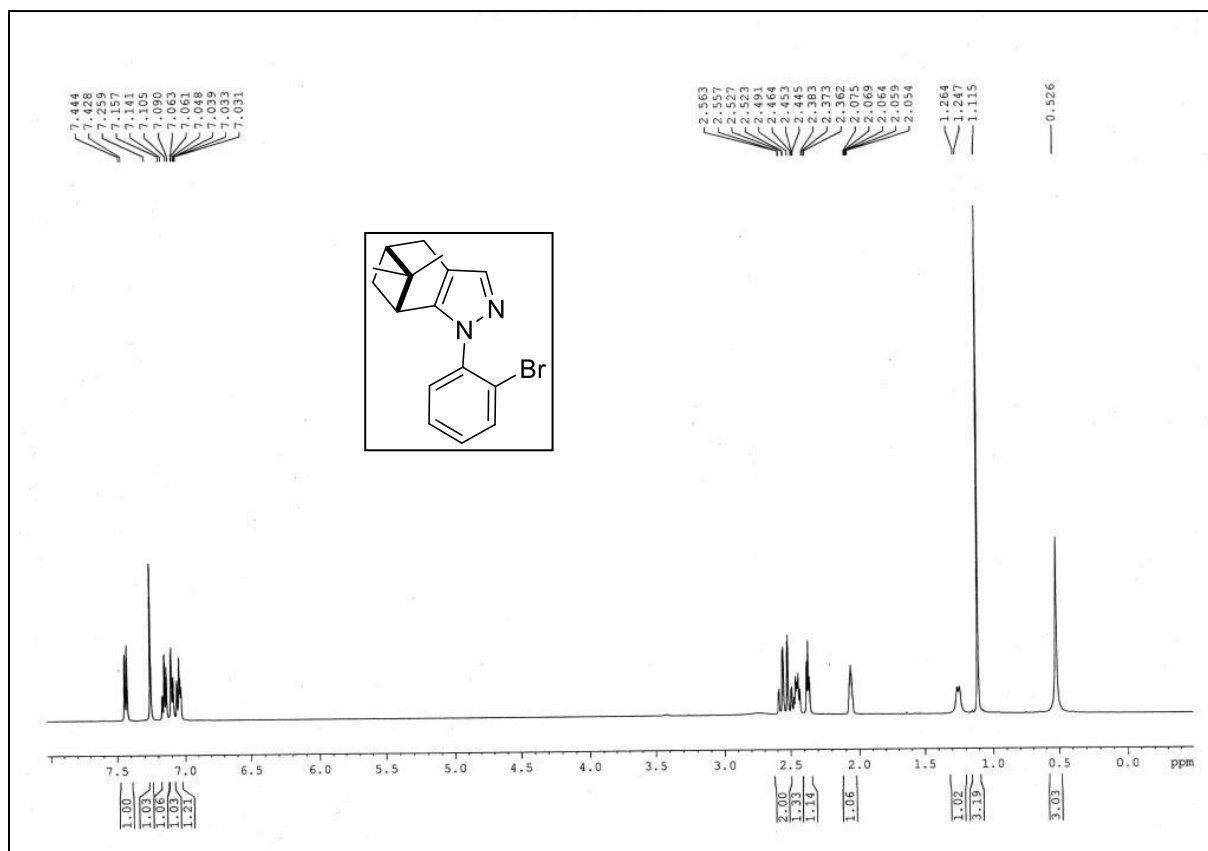
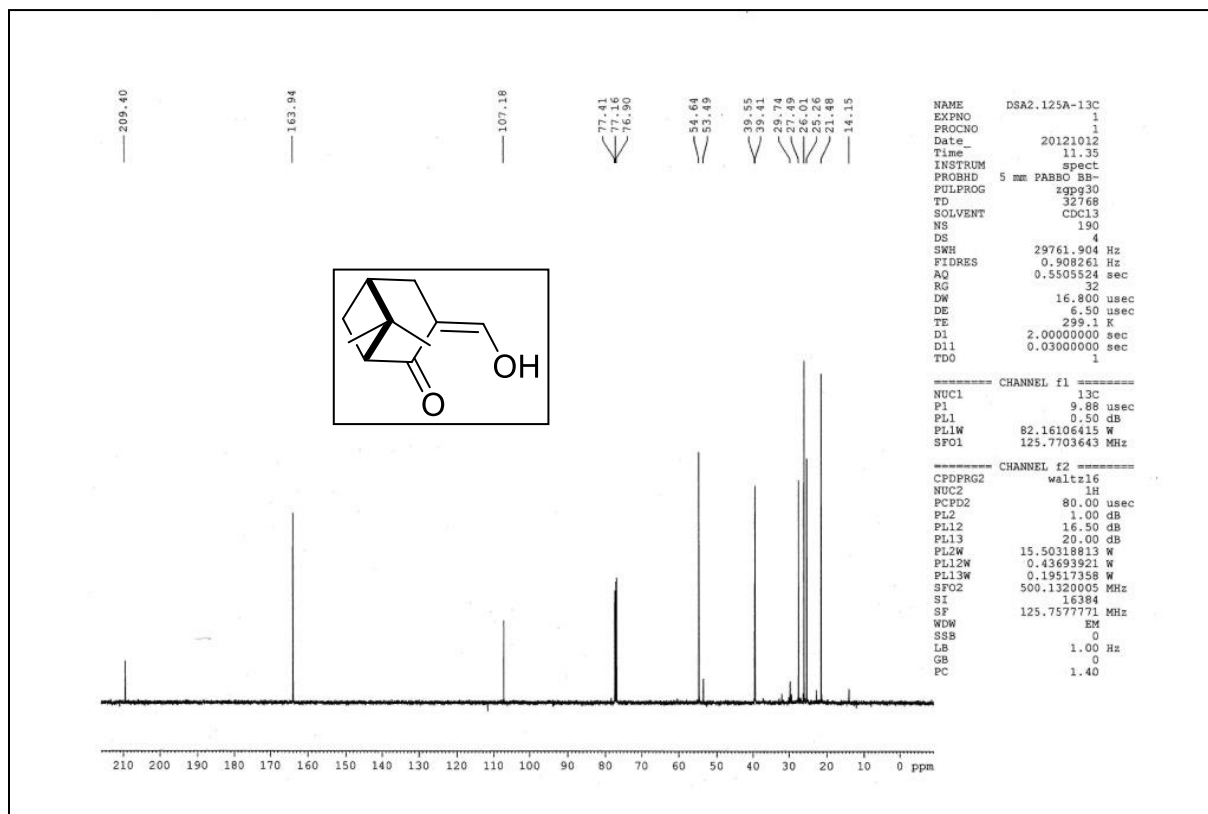
Crystal data of Pd-L1 complex (C3): A colorless block shaped crystal (0.28 X 0.19 X 0.08 mm) was analyzed. Empirical formula $C_{30}H_{28}Cl_2F_3N_2PPd$, $FW = 681.81$, monoclinic space group $P2_1$, $a = 8.8797(7) \text{ \AA}$, $b = 15.9122(12) \text{ \AA}$, $c = 11.4502(9) \text{ \AA}$, $\beta = 102.348(2)^\circ$, $V = 1580.4(2) \text{ \AA}^3$, $T = 150 \text{ K}$, $Z = 2$. $\rho_{\text{calcd}} = 1.433 \text{ g cm}^{-3}$. $F(000) = 688$, $\lambda (\text{Mo-K}\alpha) = 0.71073 \text{ \AA}$, $\mu_{\text{MoK}\alpha} / \text{mm}^{-1} = 0.846$, $2\theta_{\text{max}} = 50.0^\circ$, 15013 total reflections, 5237 unique reflections, 5001 observed ($I > 2\sigma(I)$) 355 parameters; $R_{\text{int}} = 0.0327$, $R_1 = 0.0322$; $wR_2 = 0.0762$ ($I > 2\sigma(I)$), $R_1 = 0.0338$; $wR_2 = 0.0771$ (all data) with GOF = 1.016.

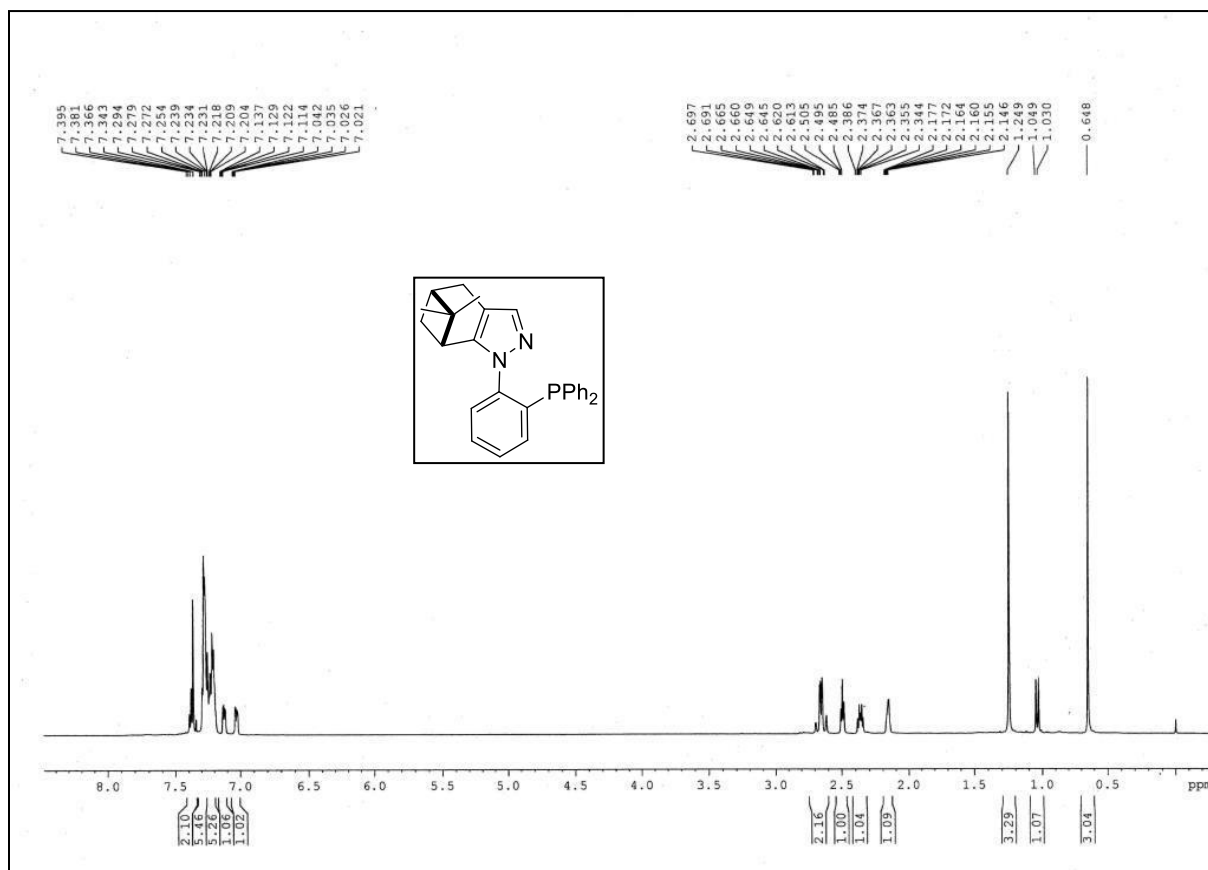
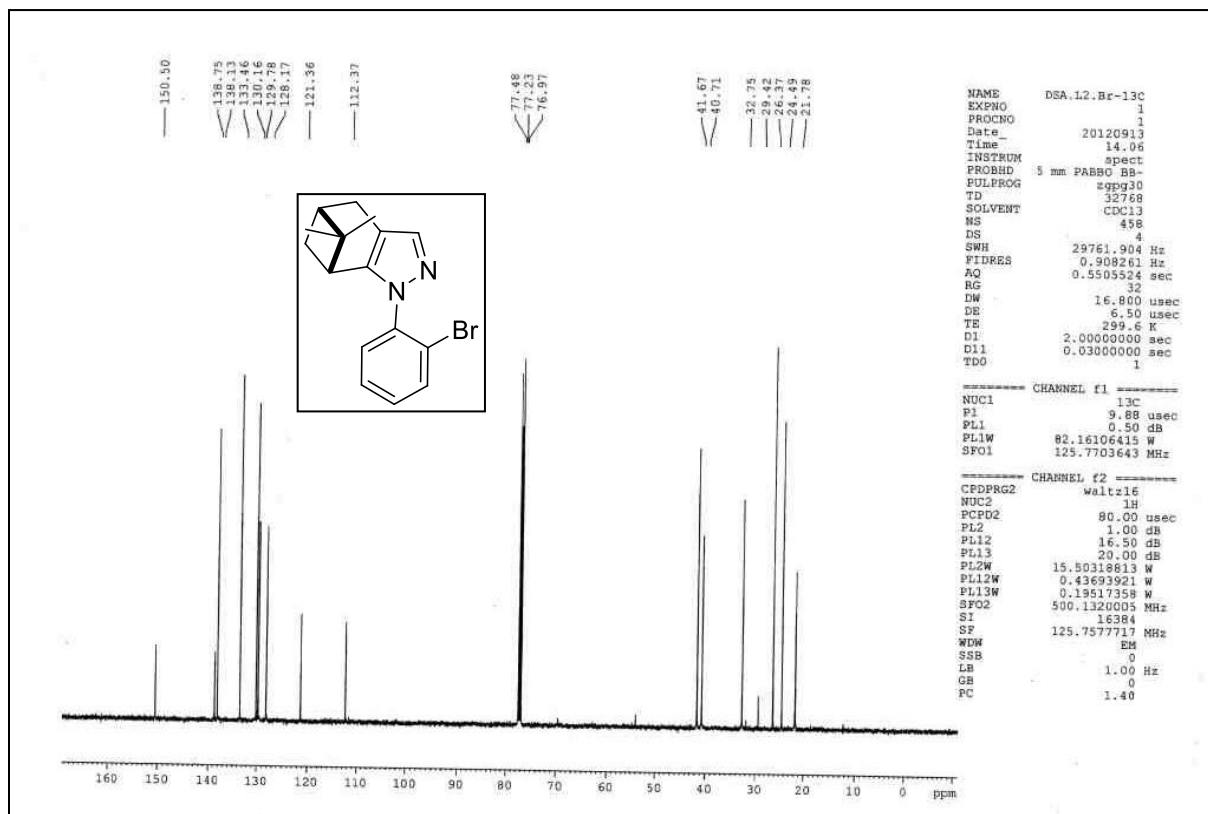
Chemical structure of bicyclo[2.2.1]heptan-2-one is shown in a box above the spectrum.

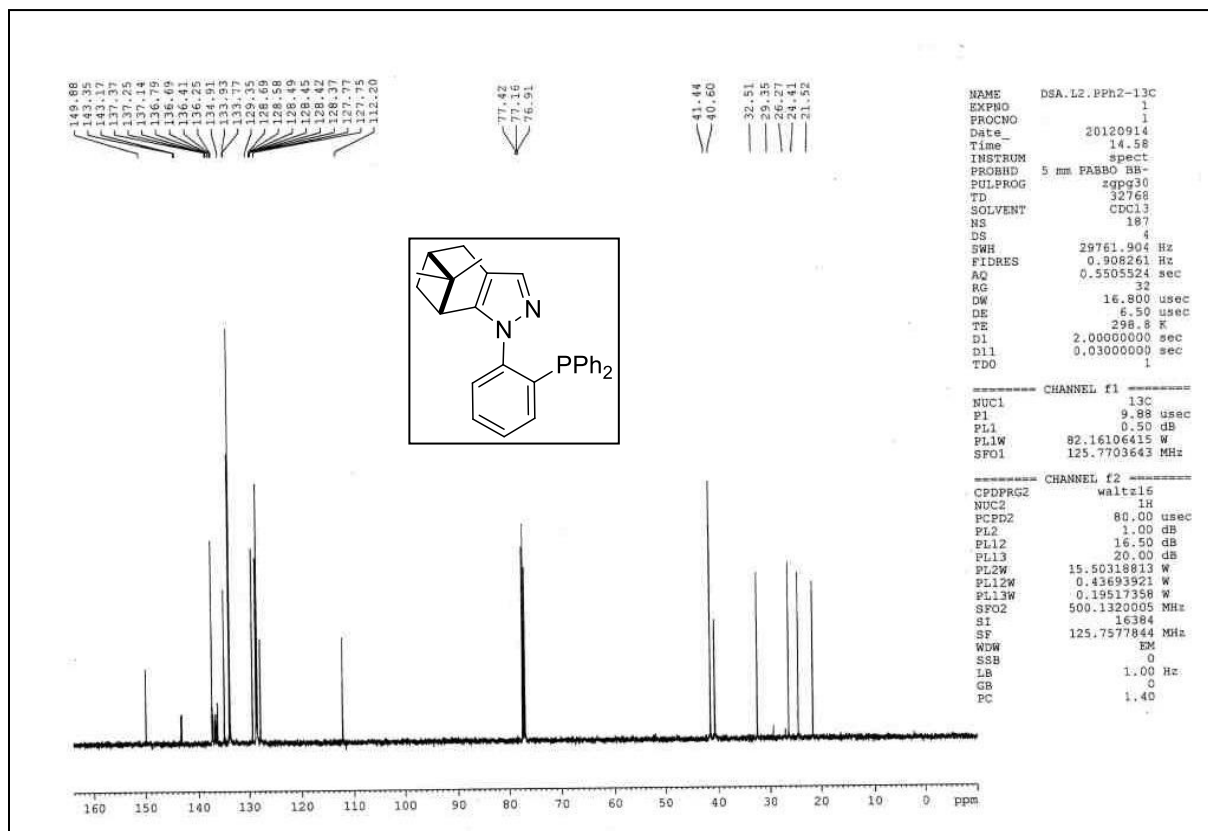
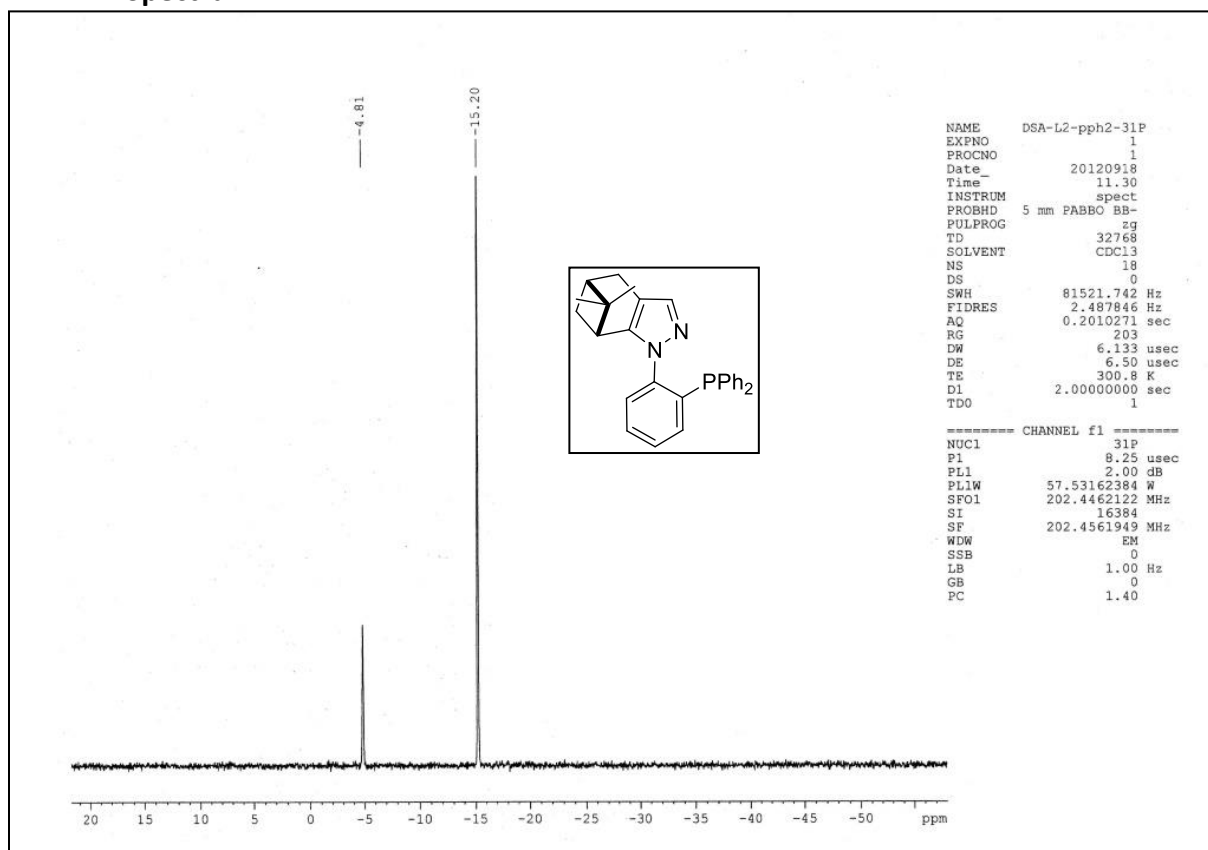
¹H NMR spectrum (ppm) with integration values:

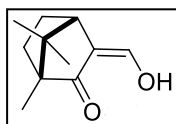
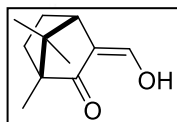
Chemical Shift (ppm)	Integration
2.486	3.15
2.476	1.14
2.461	1.00
2.447	1.11
2.443	1.09
2.436	1.08
2.432	3.28
2.422	3.25
2.415	
2.407	
2.395	
2.383	
2.242	
2.239	
2.224	
2.220	
2.205	
2.201	
2.199	
2.182	
2.181	
2.179	
2.175	
2.170	
2.112	
1.987	
1.953	
1.959	
1.956	
1.940	
1.936	
1.932	
1.929	
1.917	
1.914	
1.910	
1.906	
1.860	
1.845	
1.838	
1.833	
1.829	
1.825	
1.819	
1.802	
1.788	
1.769	
1.754	
0.734	

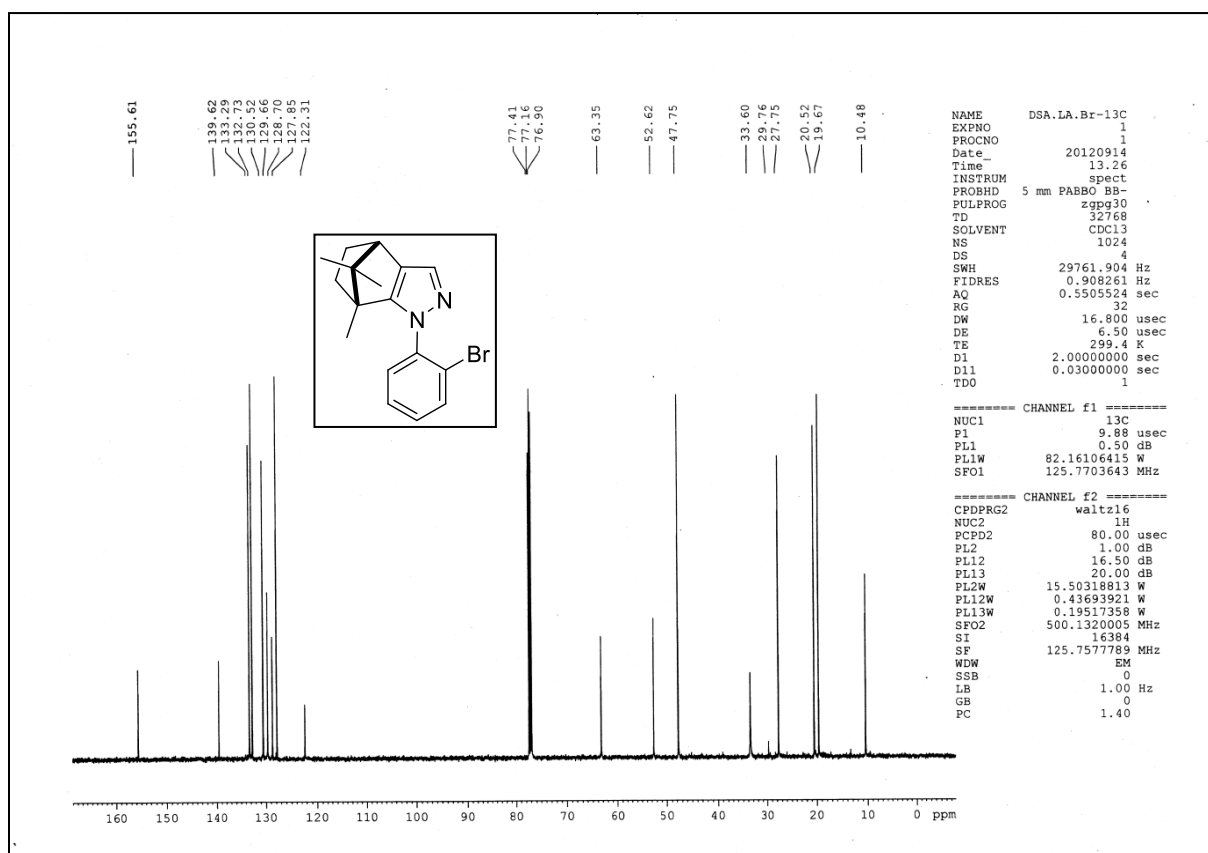
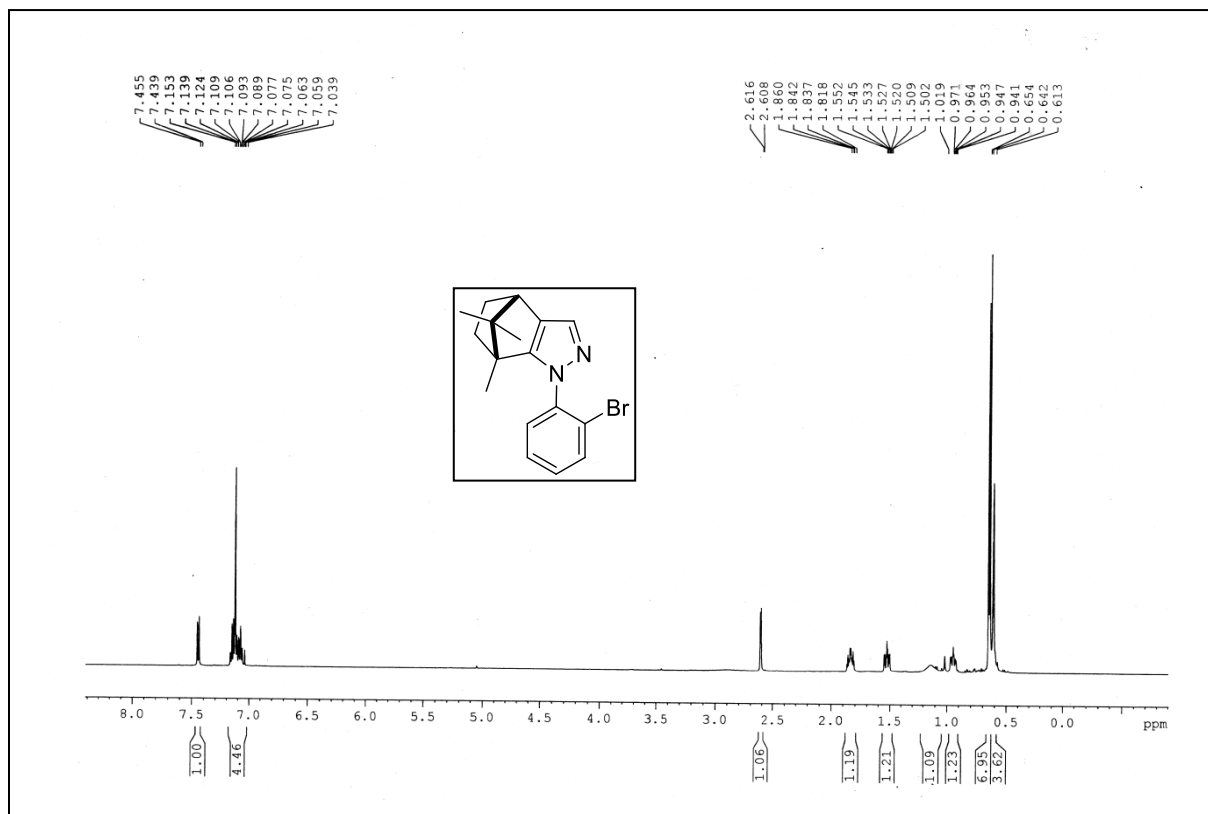


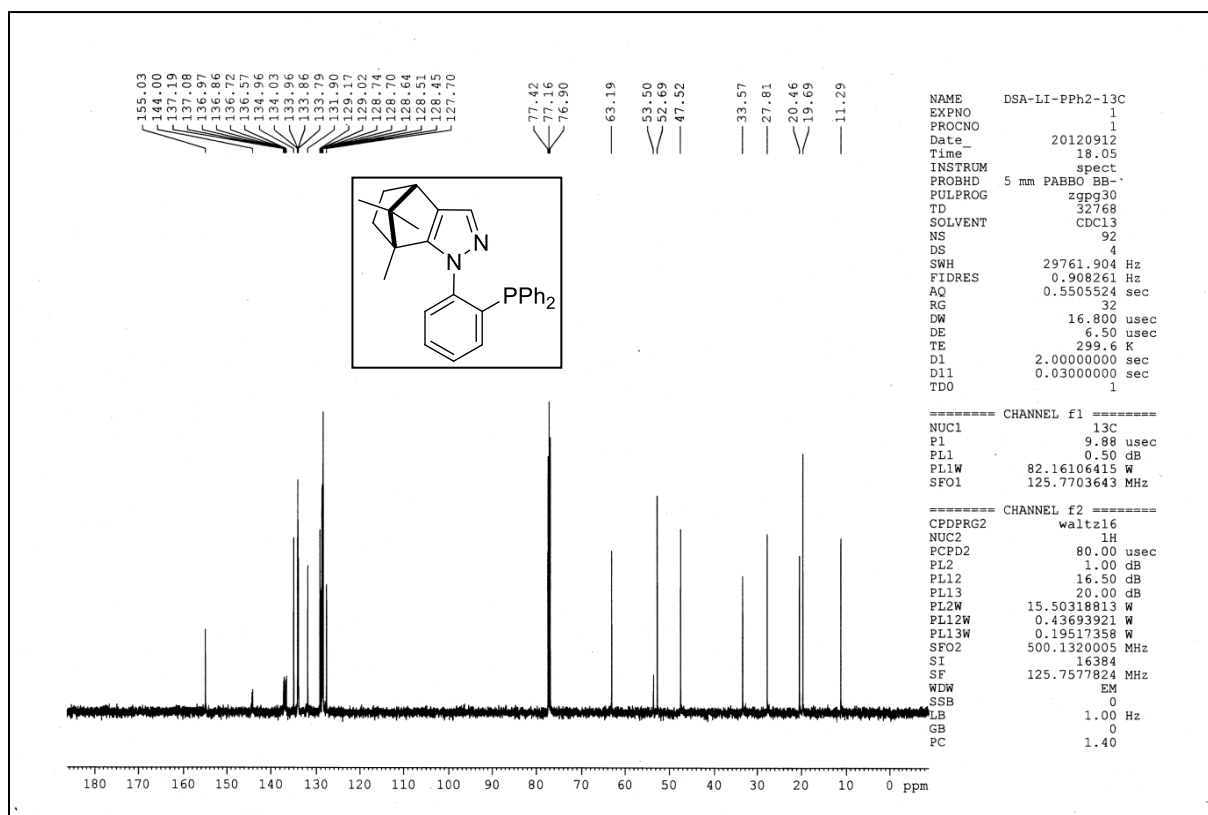
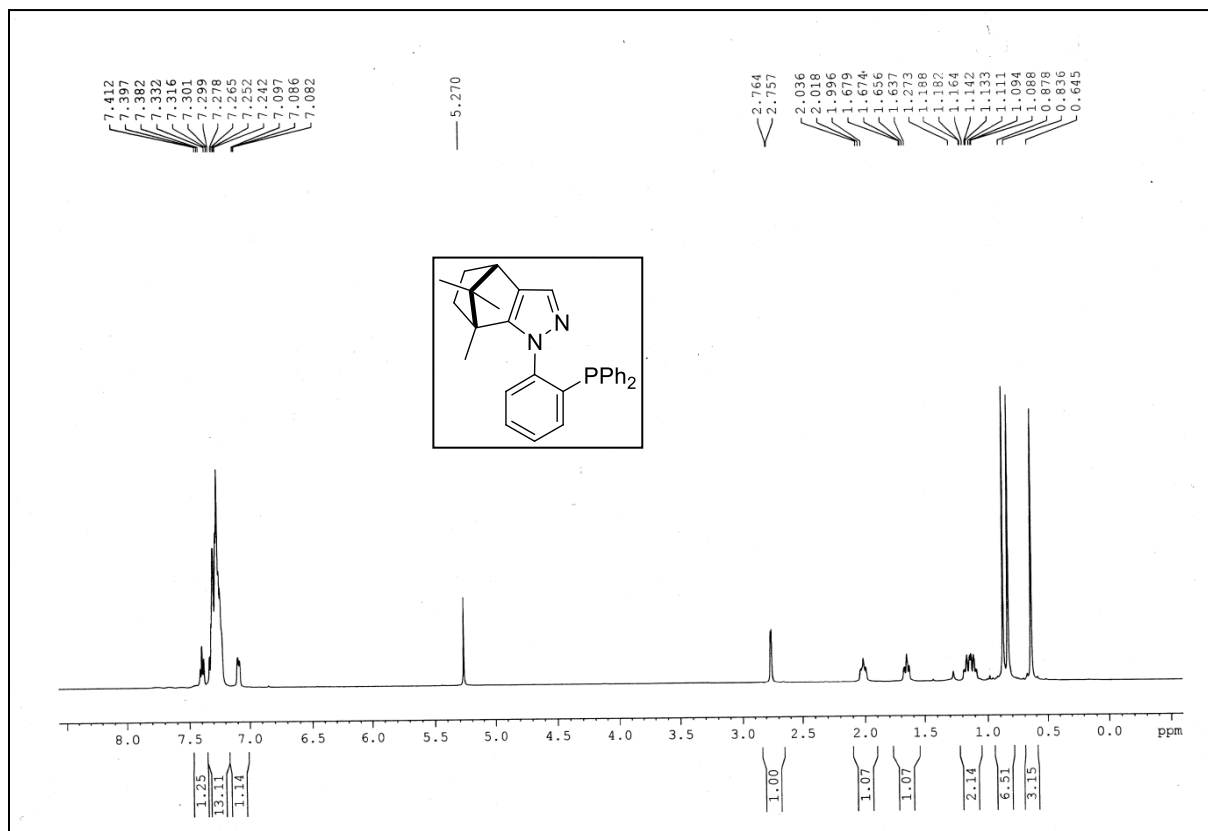


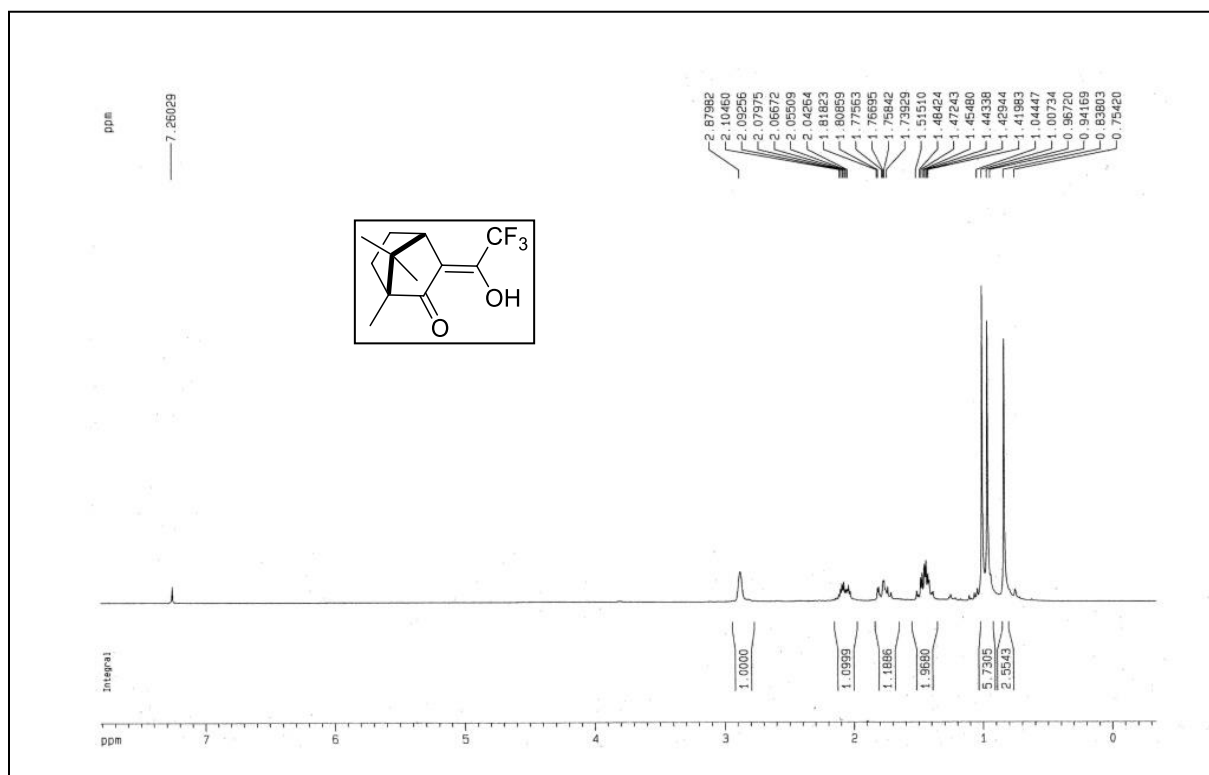
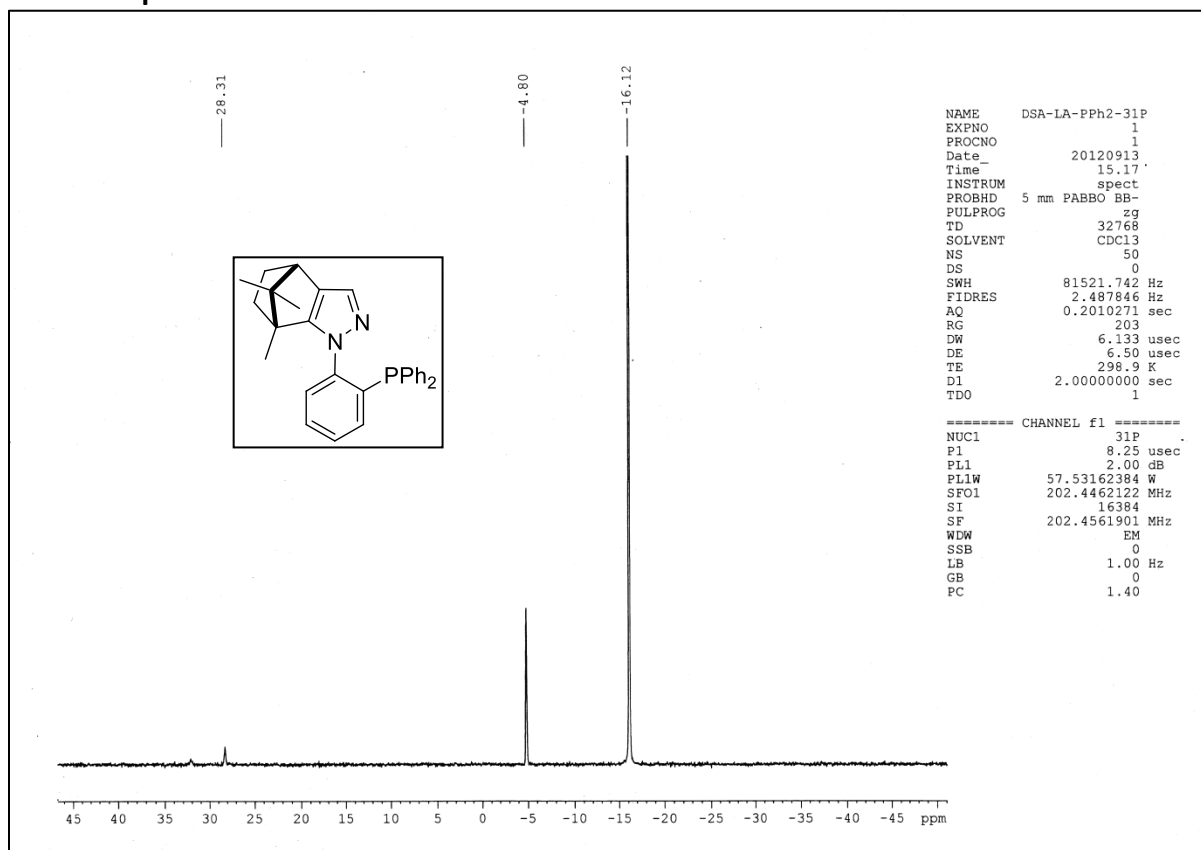


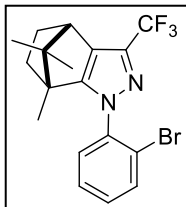
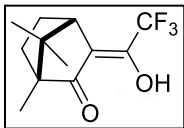
**³¹P NMR Spectrum**

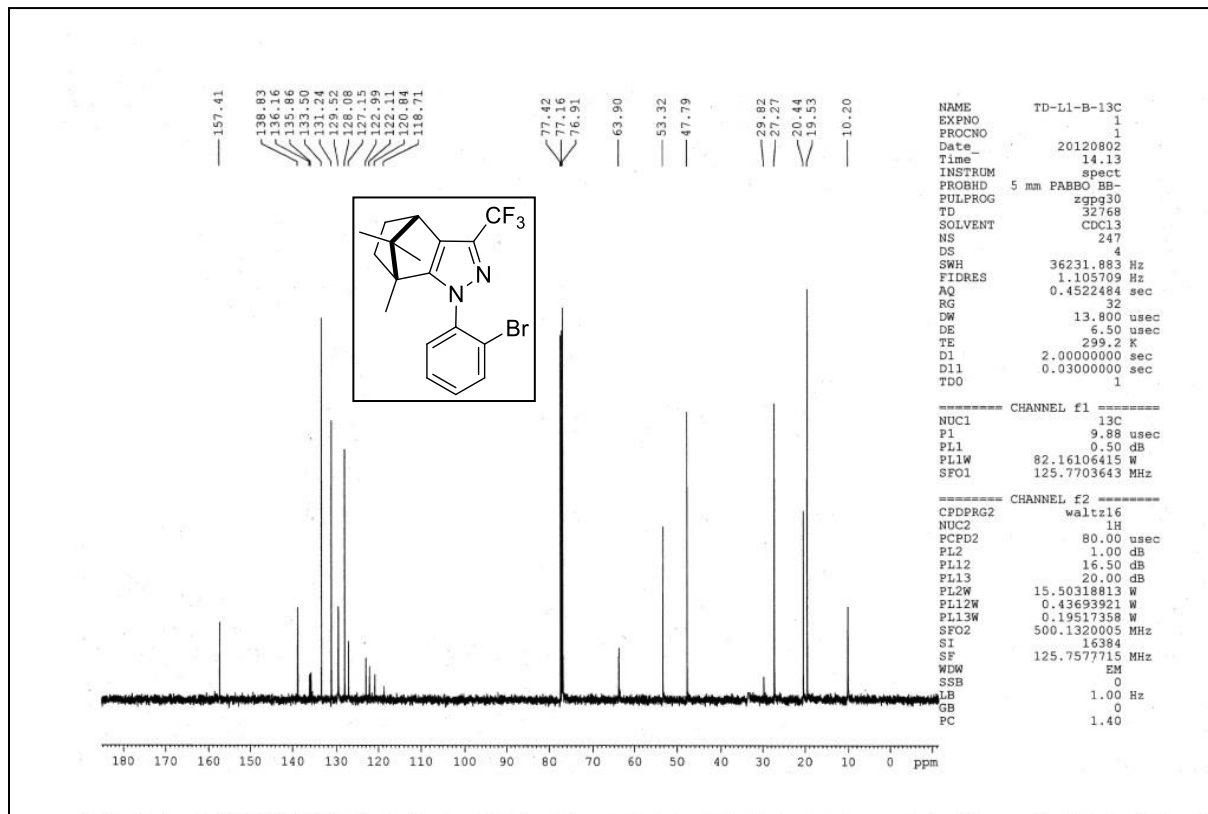
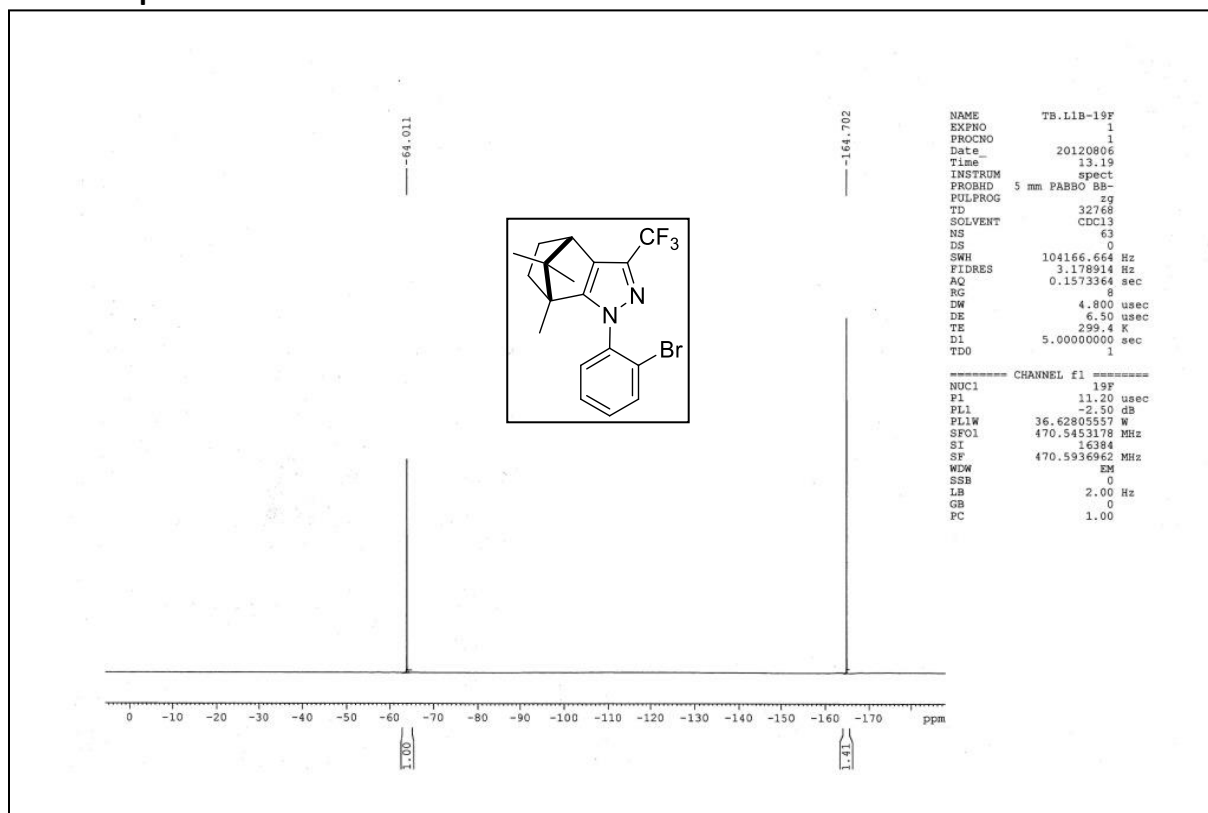


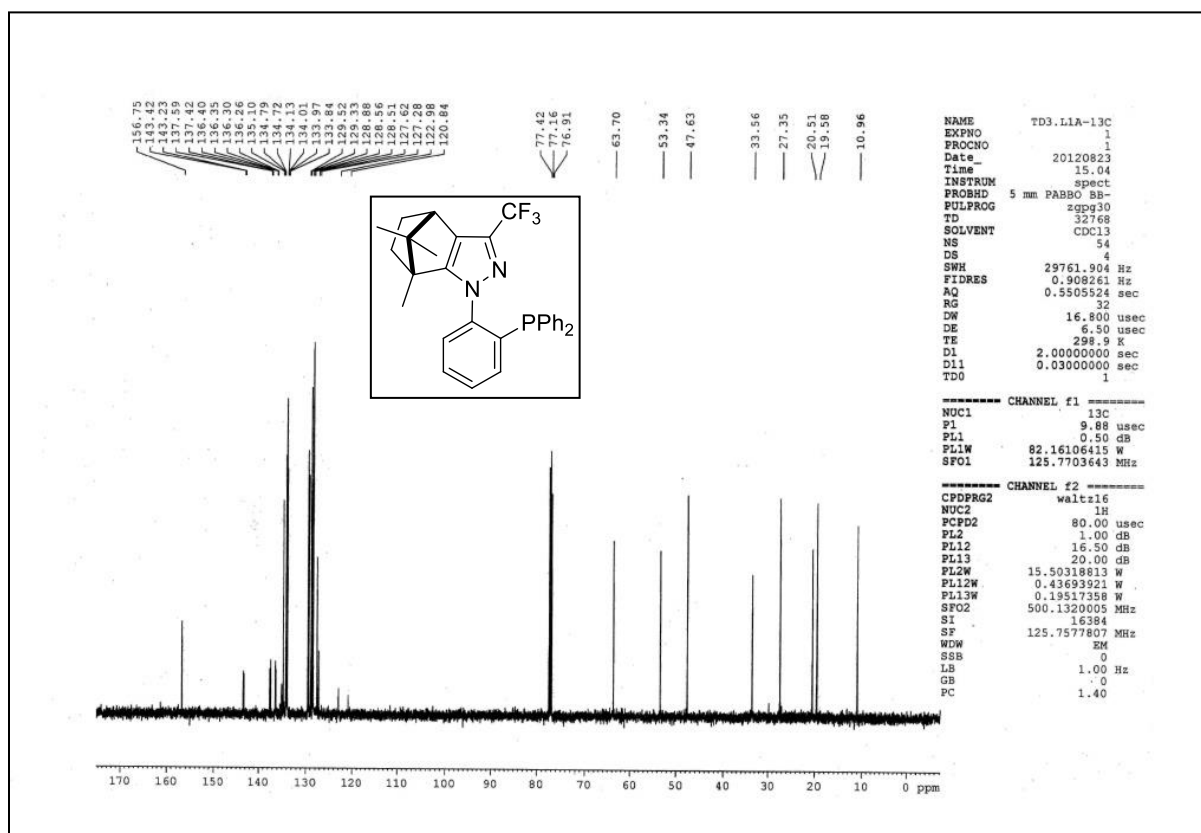
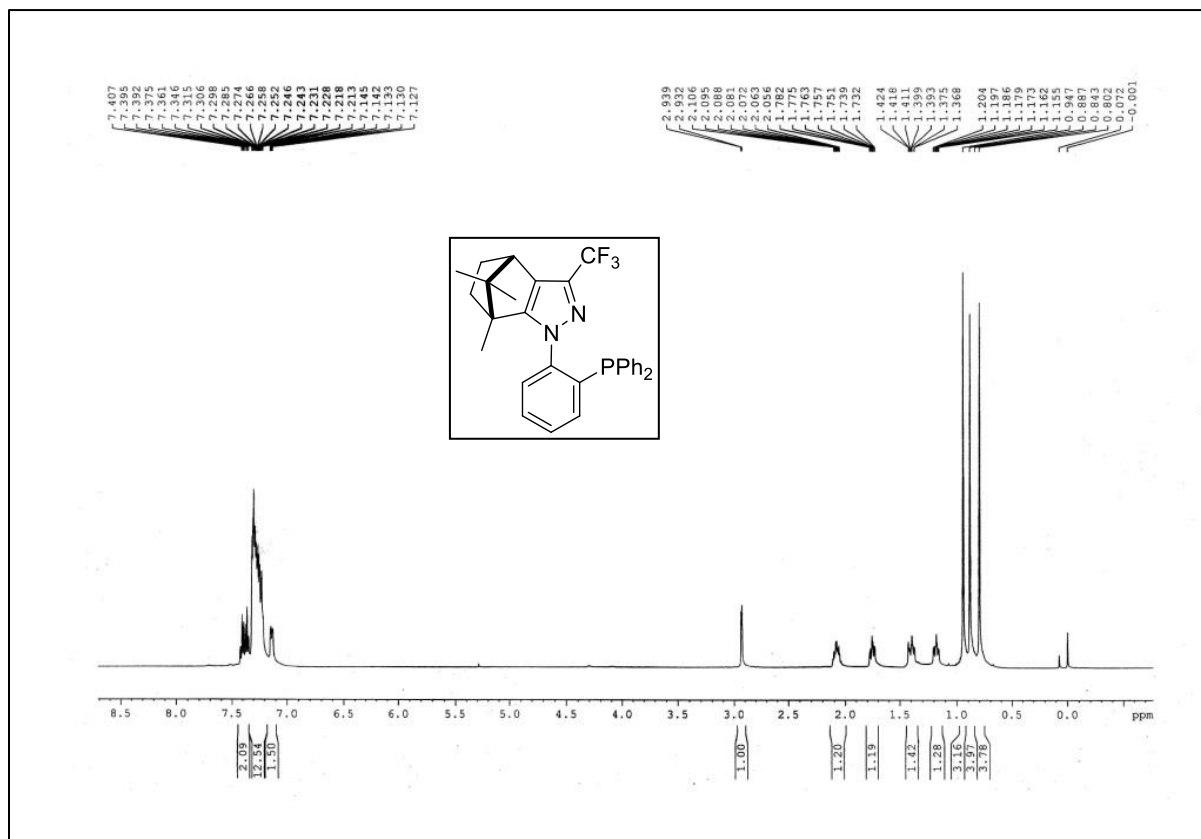


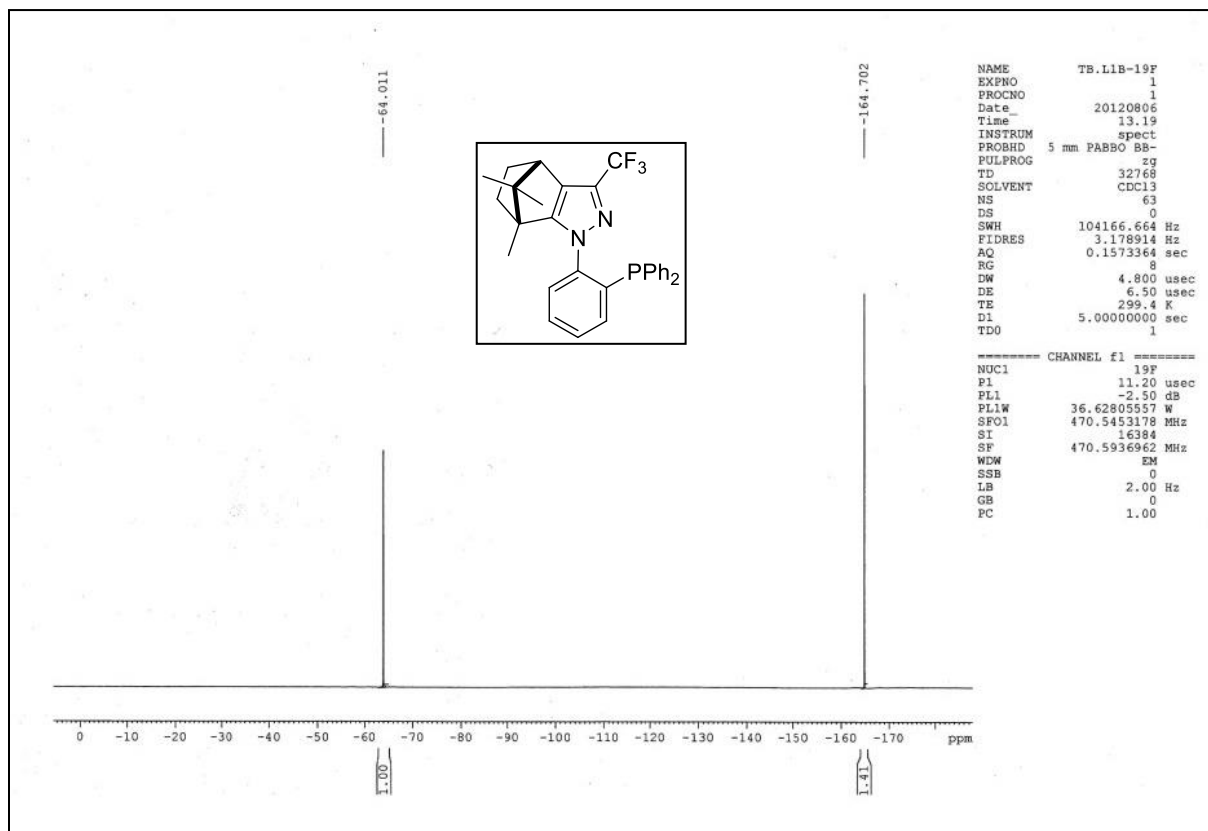


³¹P NMR Spectrum



**¹⁹F NMR Spectrum**

¹⁹F NMR Spectrum :



^{31}P NMR Spectrum

