Electronic Supplementary Material (ESI) for New Journal of Chemistry.
This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2018

Electronic Supplementary Information

Preparation of hydrido [CNC]-pincer cobalt complexes via selective C-H/C-F bond activation and their catalytic performances

Fei Yang,[a] Yangyang Wang,[a,b] Faguan Lu,[a] Shangqing Xie,[a] Xinghao Qi,[a] Hongjian Sun,[a] Xiaoyan Li*,[a], Olaf Fuhr[c] and Dieter Fenske[c]

1. Selected X-ray crystallographic data

	4	**8**	**11**
formula	$C_{23}H_{28}CoF_2NP_2$	$C_{23}H_{26}CoF_4NP_2$	$C_{23}H_{27}CoF_2INP_2$
M_z	477.33	513.34	603.23
crystal system	Monoclinic	Monoclinic	Orthorhombic
space group	P2(1)/c	P2(1)/c	Pbca
a [Å]	14.015(3)	14.433(7)	16.600(2)
b [Å]	12.369(3)	12.378(6)	15.531(2)
c [Å]	13.372(3)	13.442(6)	19.029(3)
α [°]	90.00	90.00	90.00
β [°]	101.86(3)	102.169(8)	90.00
γ [°]	90.00	90.00	90.00
V [Å^3]	2268.6(8)	2347.4(19)	4906.0(12)
T [K]	273(2)	293(2)	293(2)
Z	4	4	8
μ[mm^{-1}]	0.923	0.909	2.114
total reflns	13111	12675	27459
unique reflns	5164	4041	5567
R_{int}	0.0210	0.0297	0.0940
R_1[I>2σ(I)]	0.0295	0.0324	0.0497
wR(F^2)[I>2σ(I)]	0.0843	0.0919	0.1171
R_1(all data)	0.0361	0.0481	0.0961
wR(F^2)(all data)	0.0946	0.1047	0.1345
GOF on F^2	0.613	0.994	1.047

2. IR, ^{1}H NMR, ^{31}P NMR and ^{19}F NMR spectra of new complexes

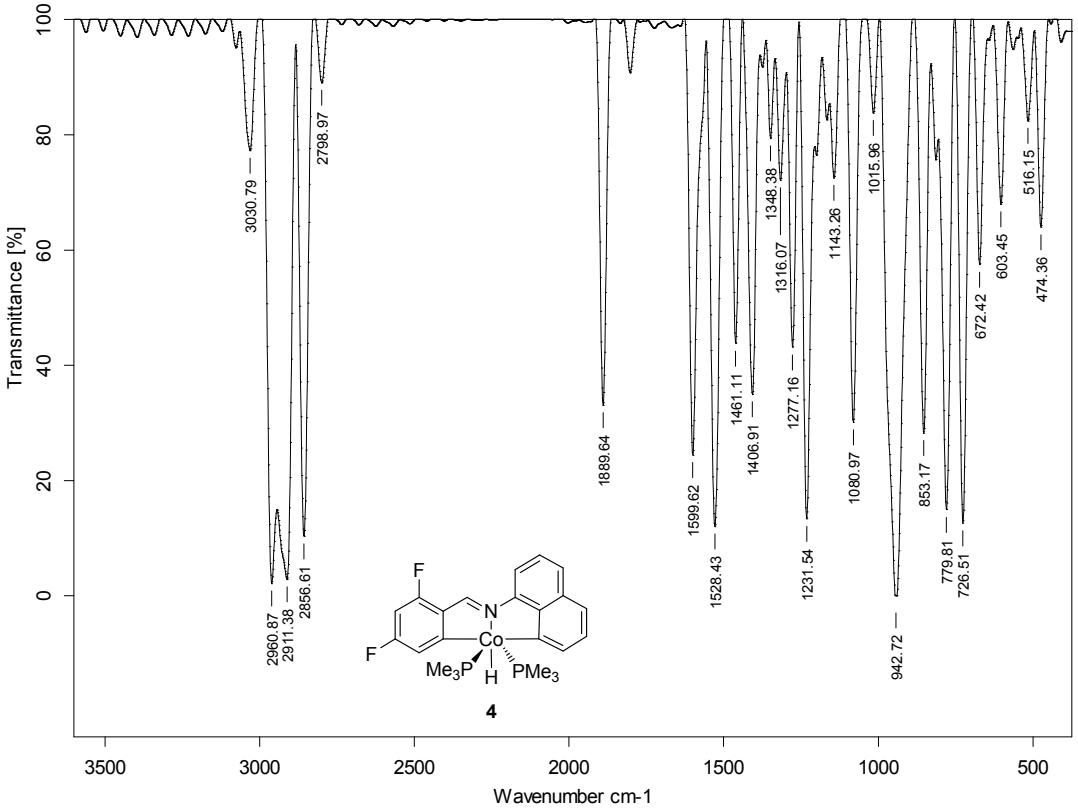


Fig S1 IR spectrum of **4**

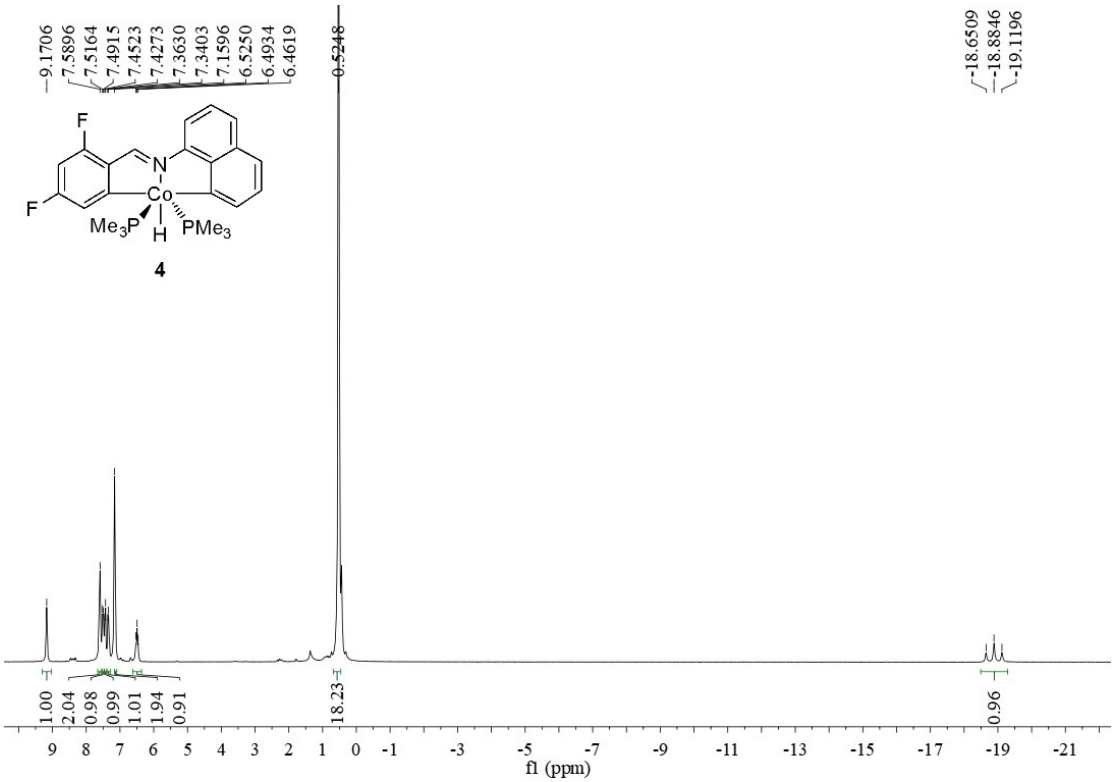


Fig S2 ^{1}H NMR spectrum of **4**

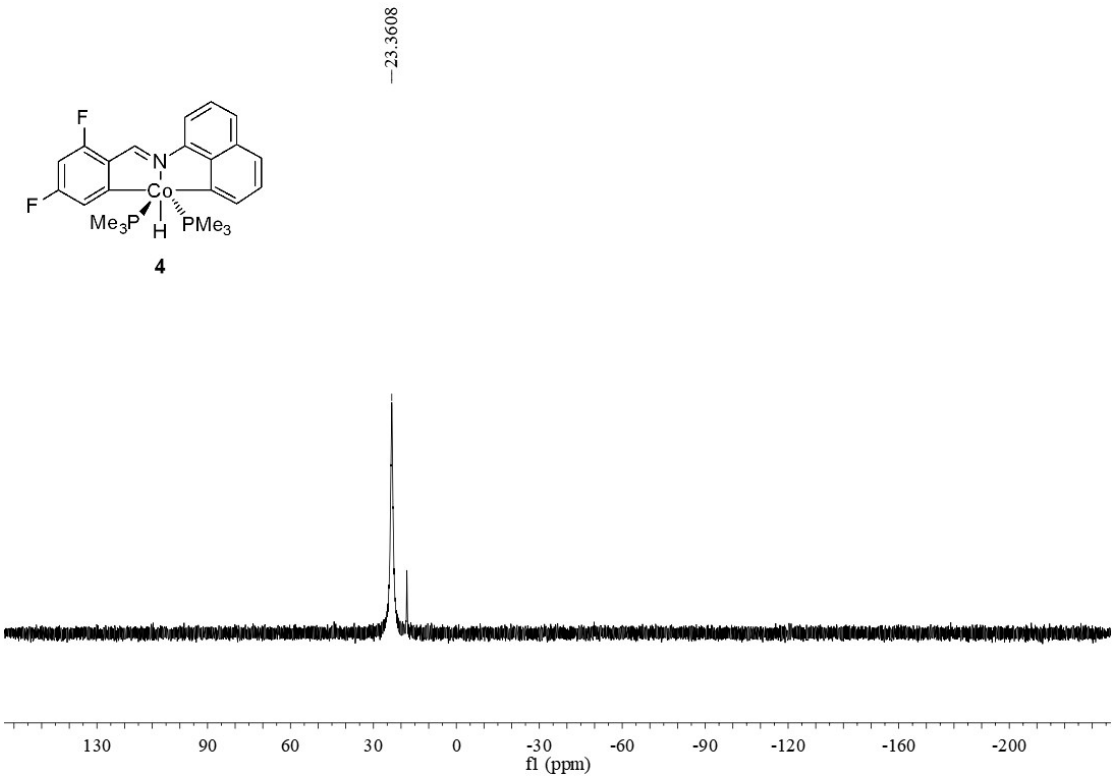


Fig S3 ^{31}P NMR spectrum of **4**

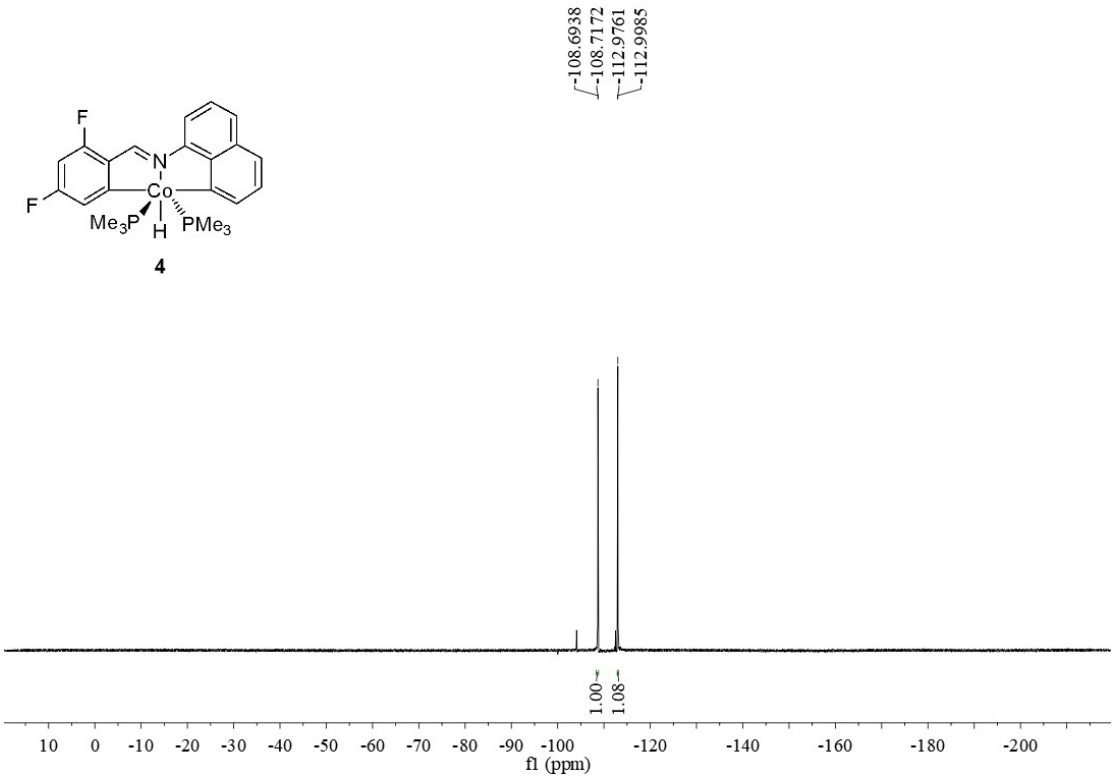


Fig S4 ^{19}F NMR spectrum of **4**

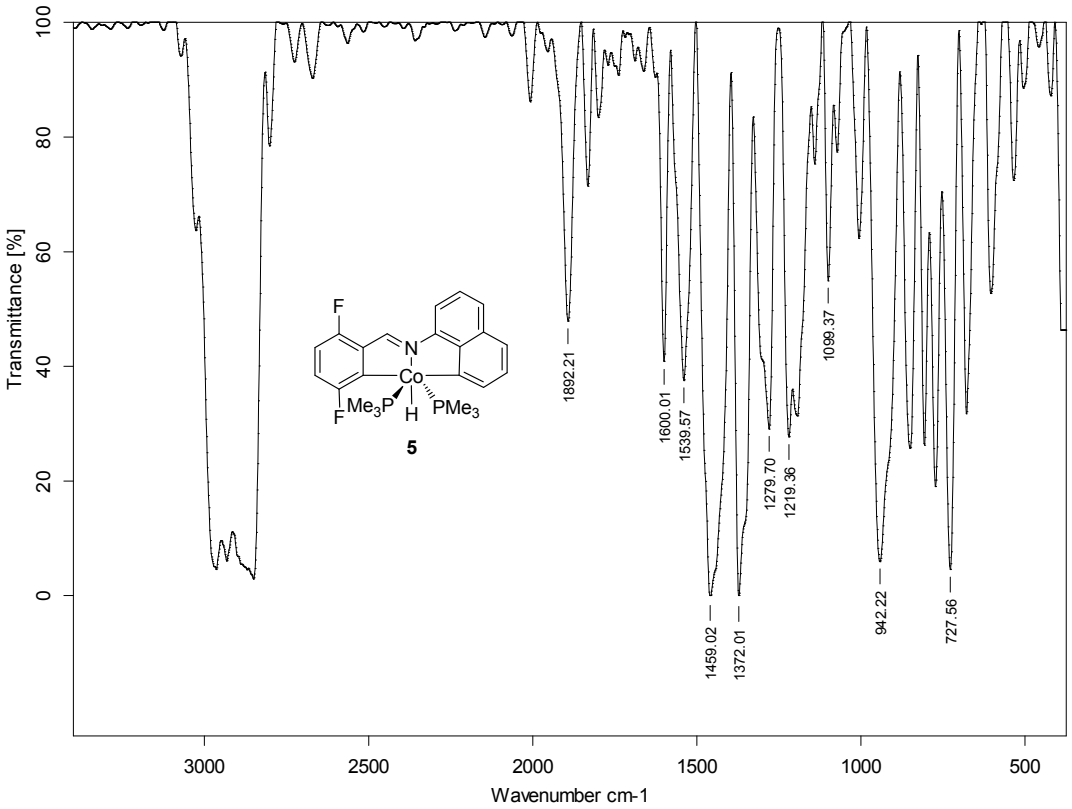


Fig S5 IR spectrum of **5**

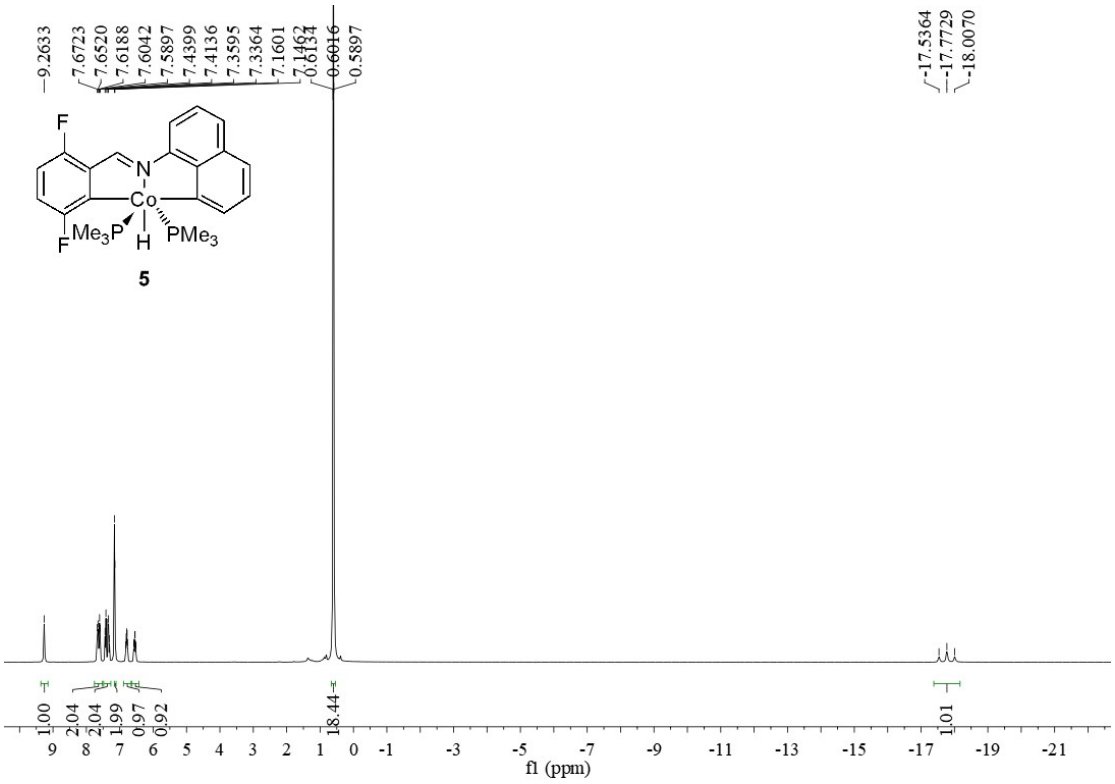


Fig S6 ^{1}H NMR spectrum of **5**

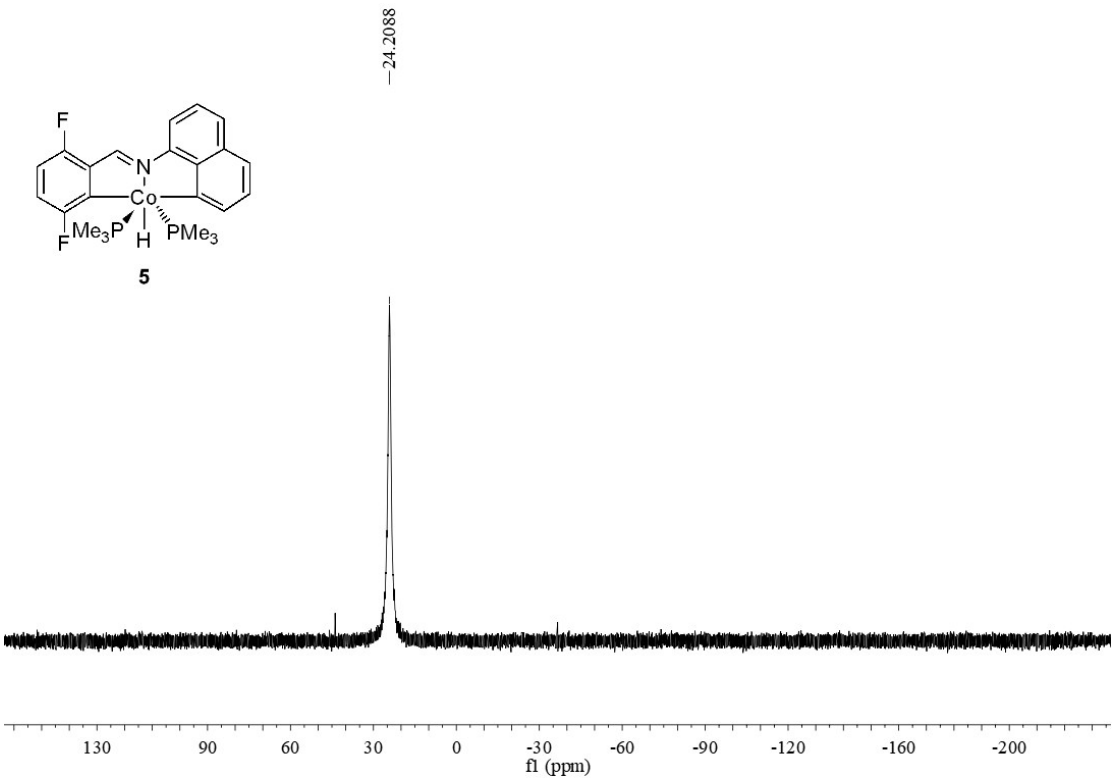


Fig S7 ^{31}P NMR spectrum of **5**

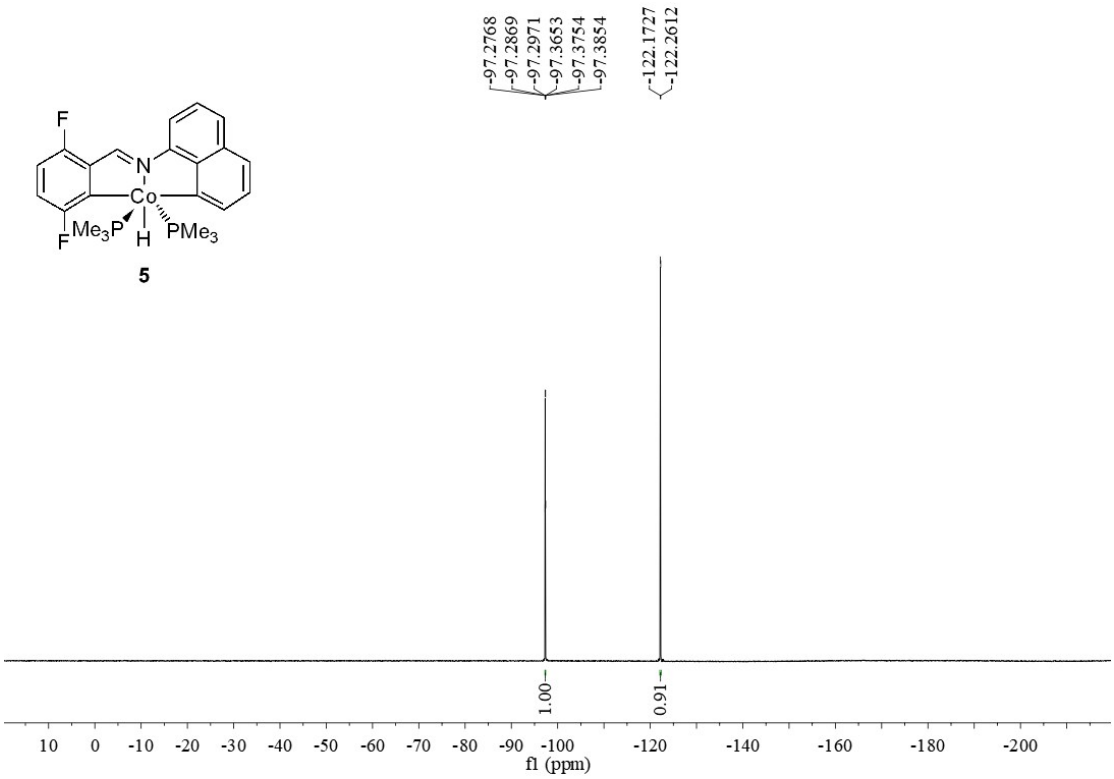


Fig S8 ^{19}F NMR spectrum of **5**

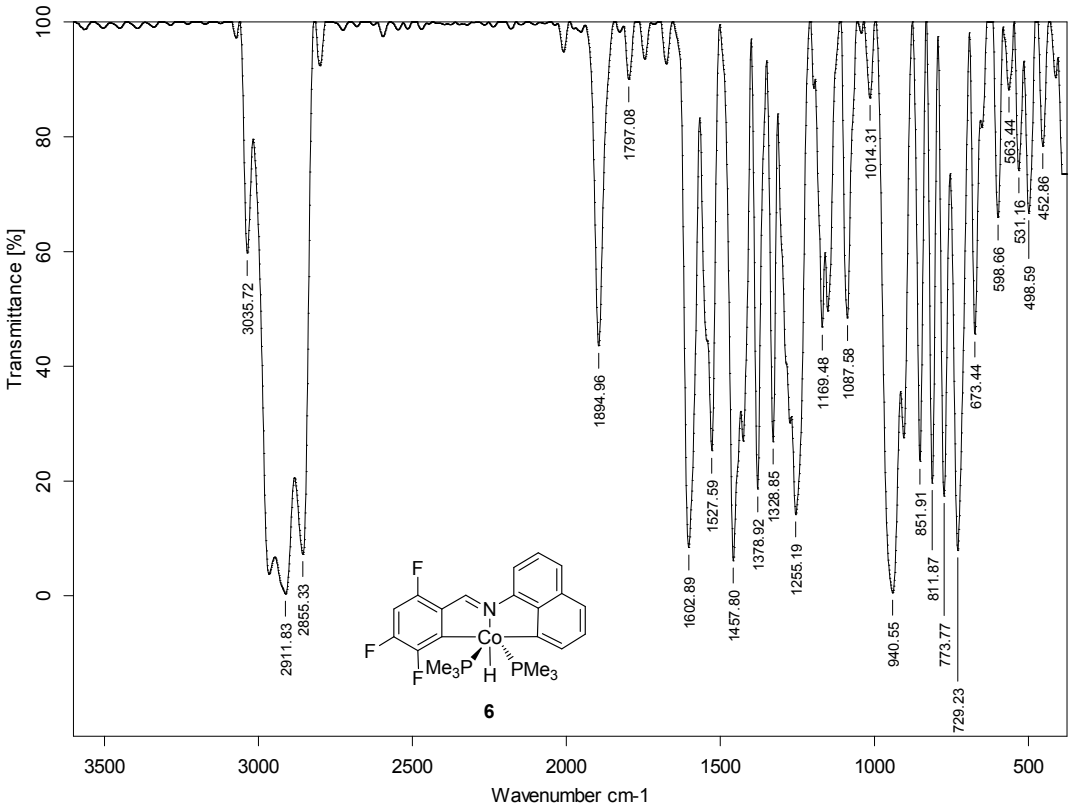


Fig S9 IR spectrum of **6**

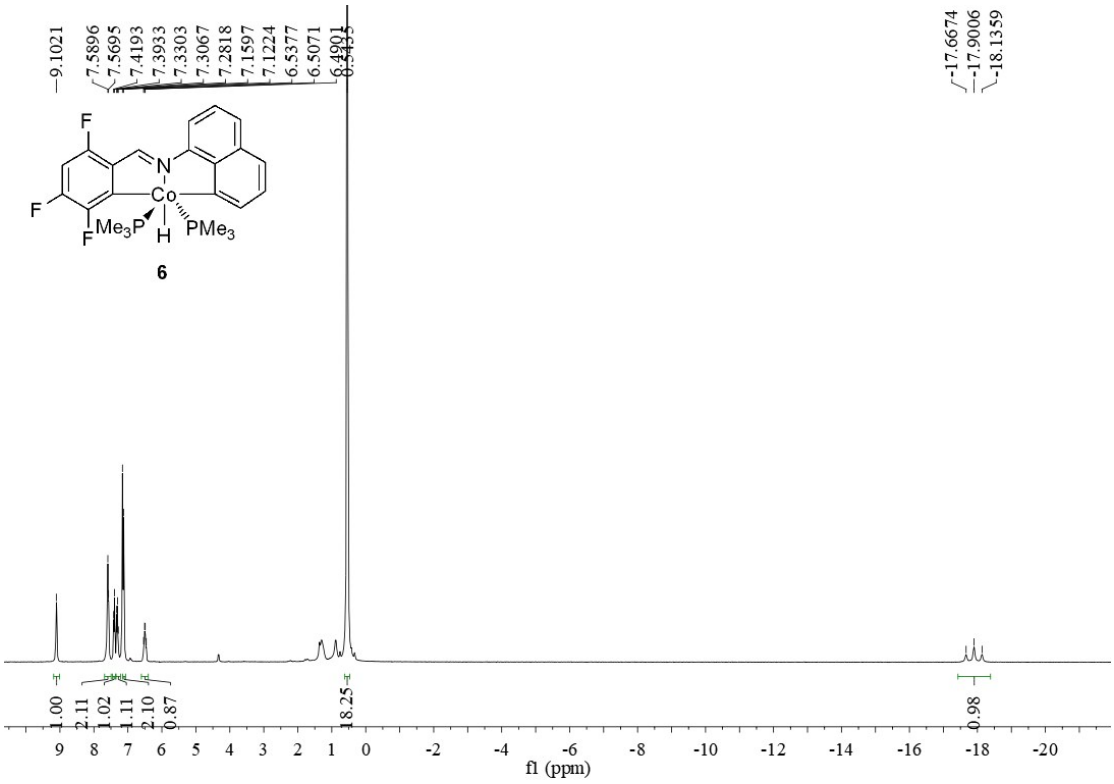


Fig S10 ^{1}H NMR spectrum of **6**

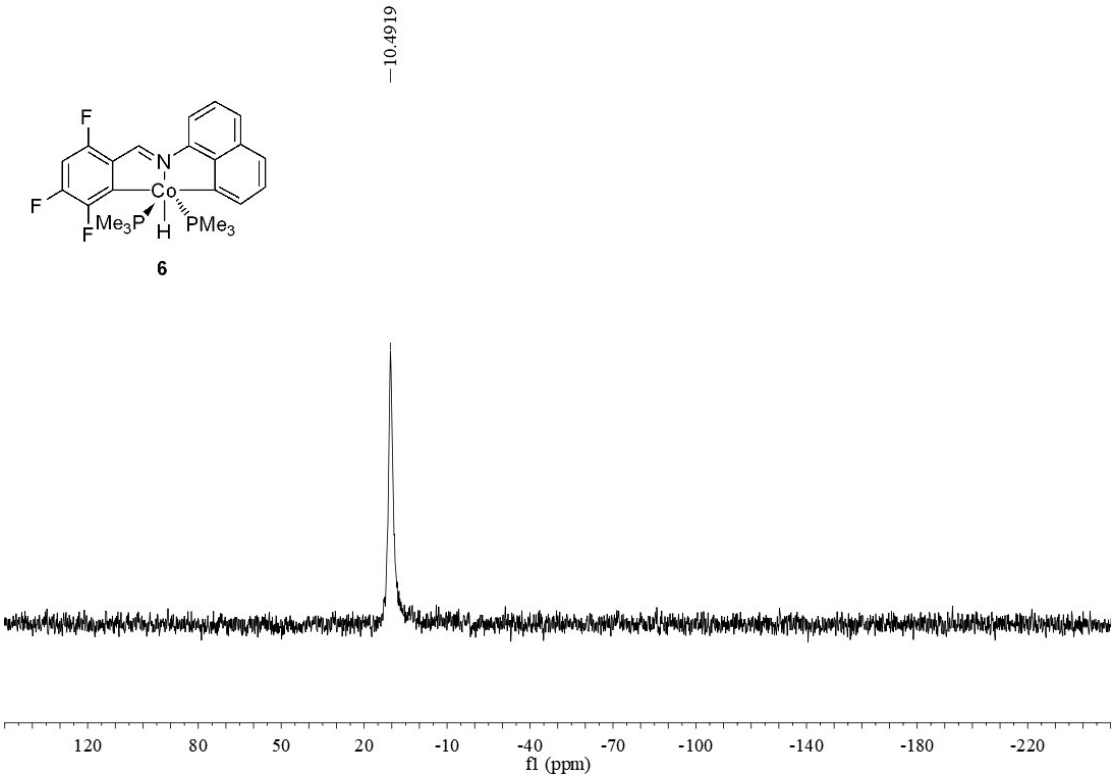


Fig S11 ^{31}P NMR spectrum of **6**

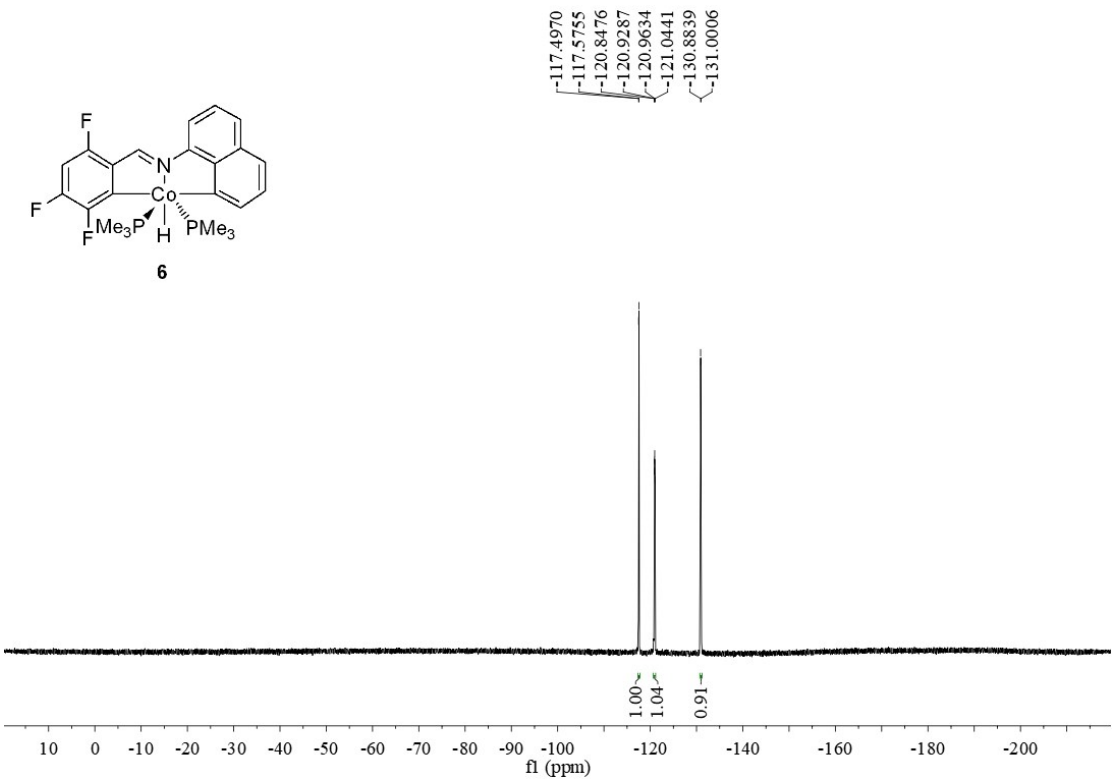


Fig S12 ^{19}F NMR spectrum of **6**

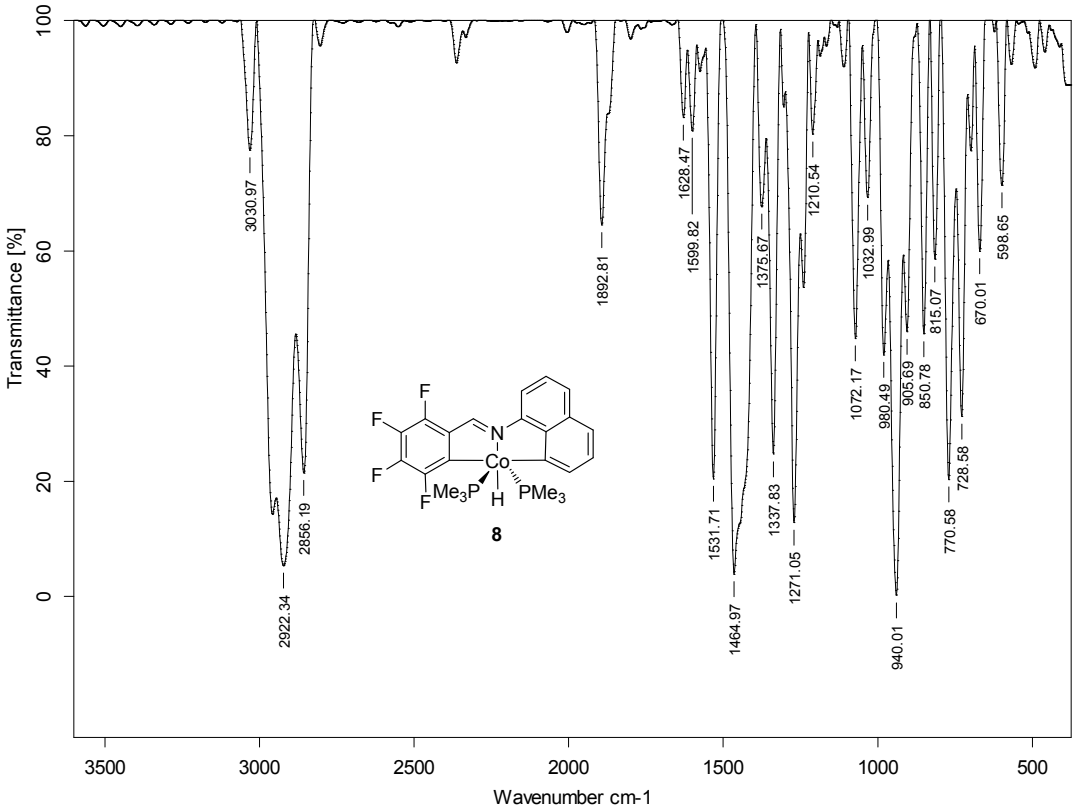


Fig S13 IR spectrum of **8**

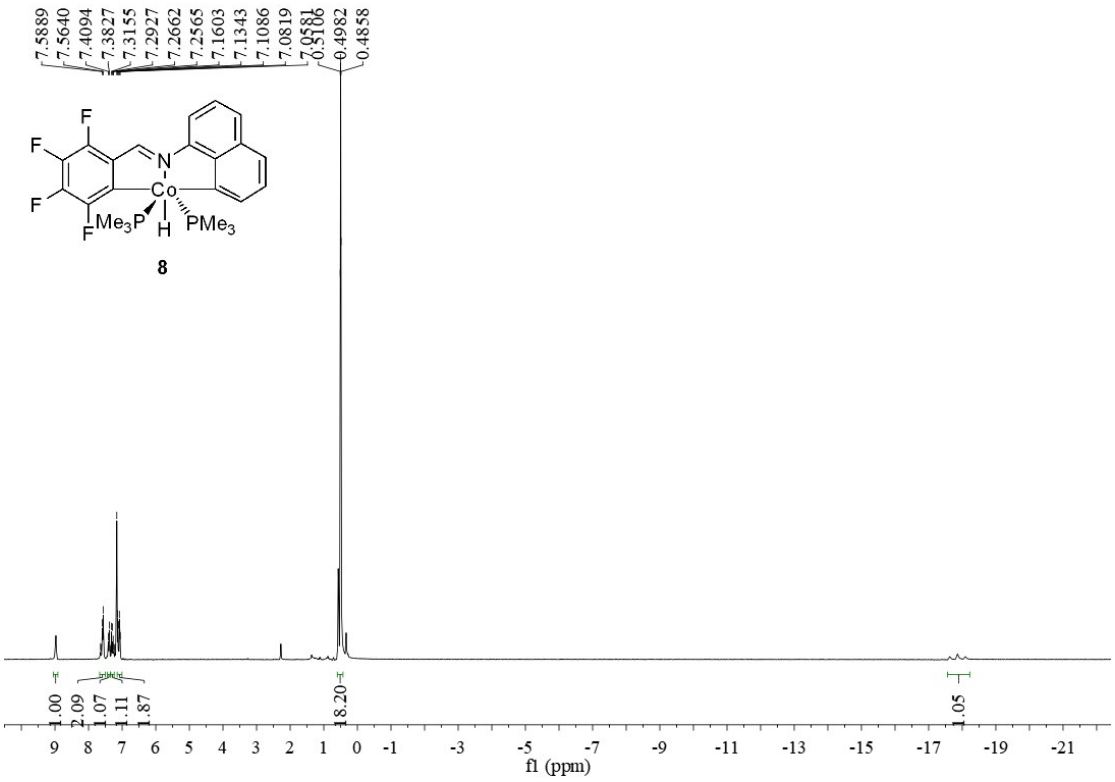


Fig S14 ^{1}H NMR spectrum of **8**

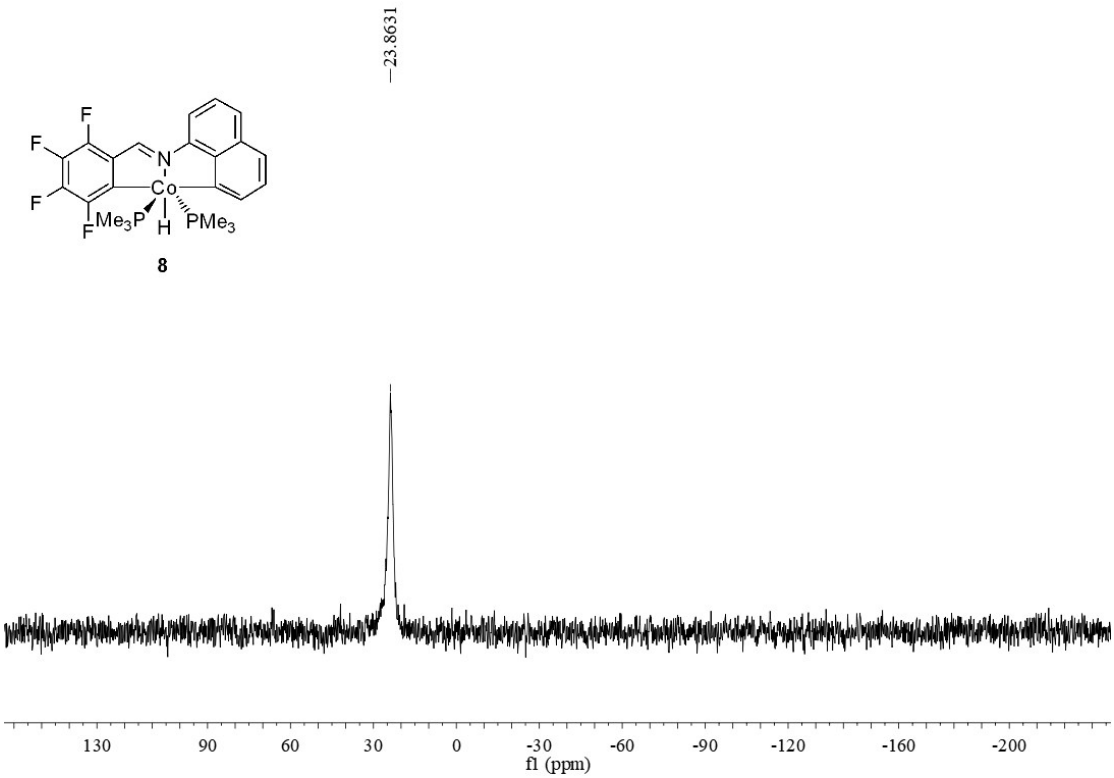


Fig S15 ^{31}P NMR spectrum of **8**

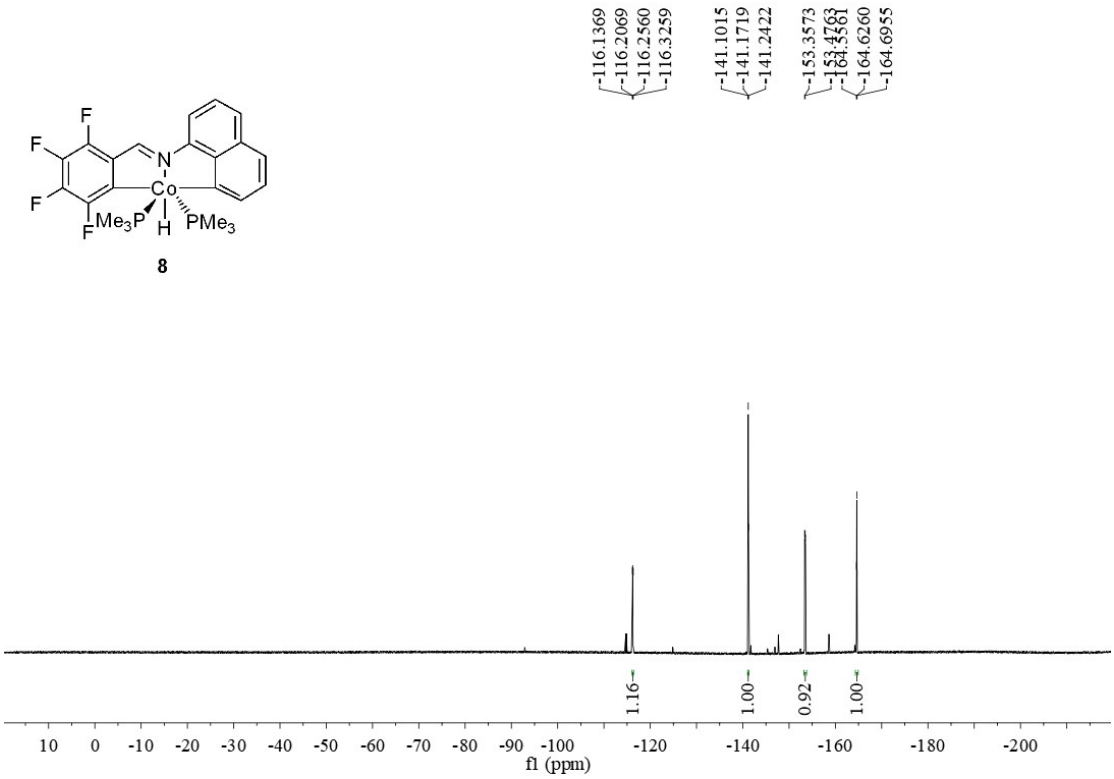


Fig S16 ^{19}F NMR spectrum of **8**

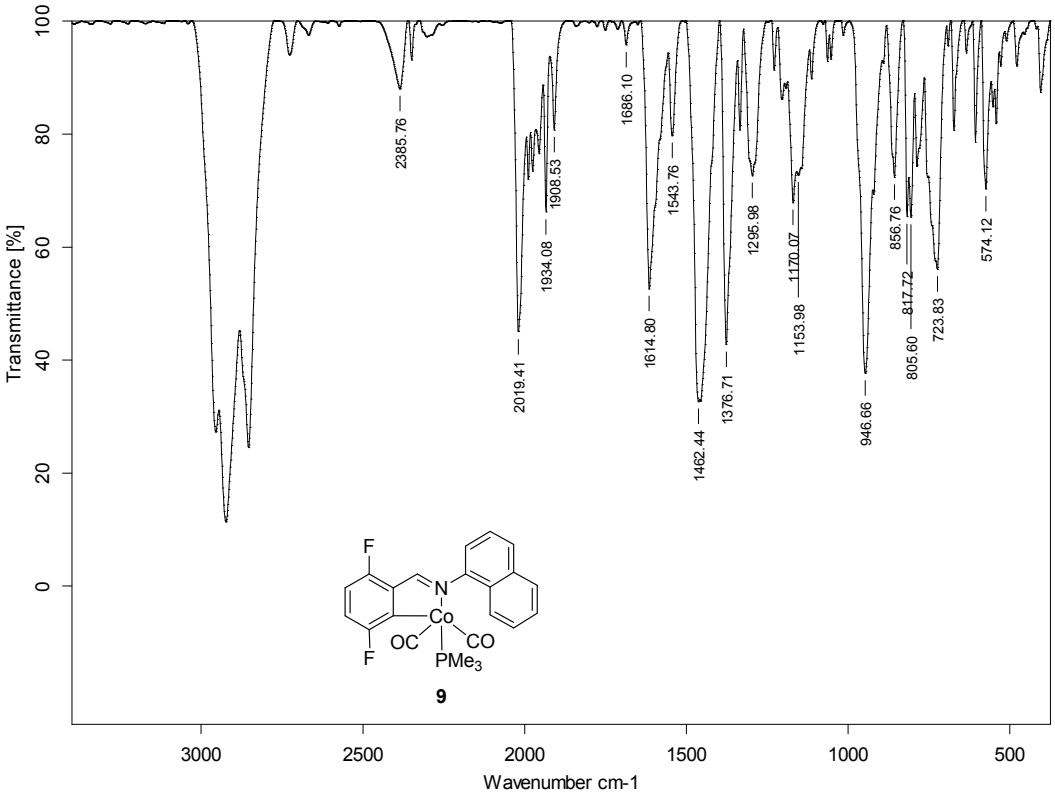


Fig S17 IR spectrum of **9**

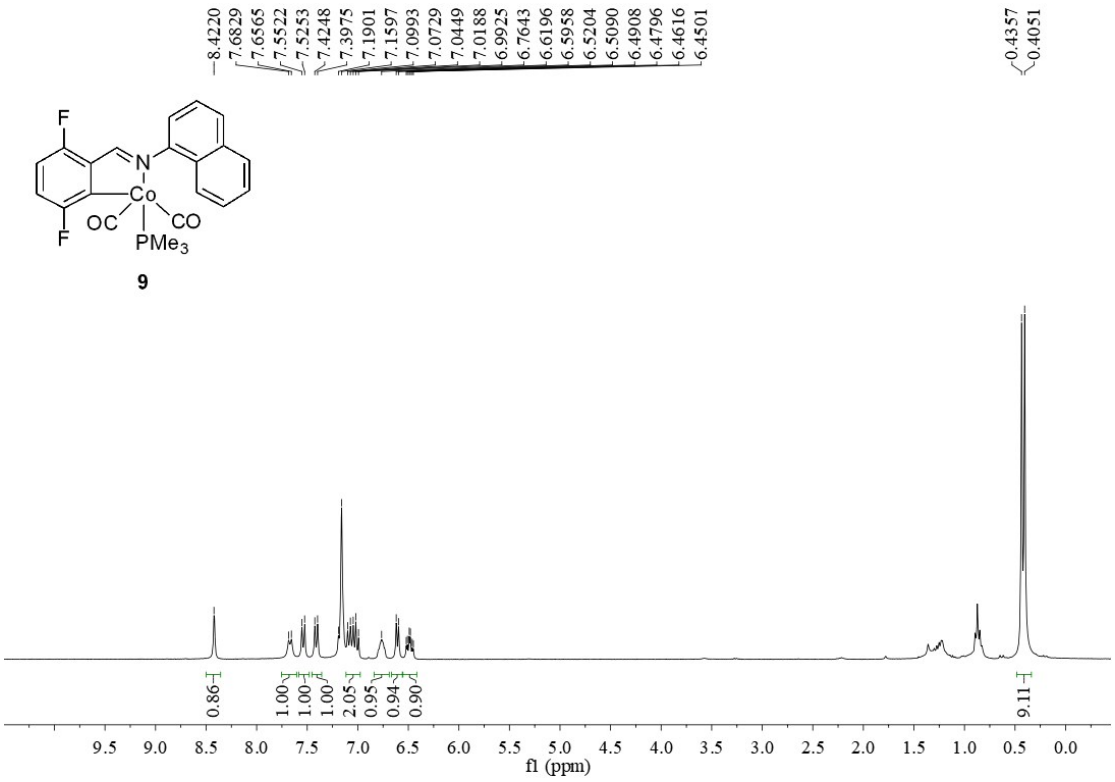


Fig S18 ^{1}H NMR spectrum of **9**

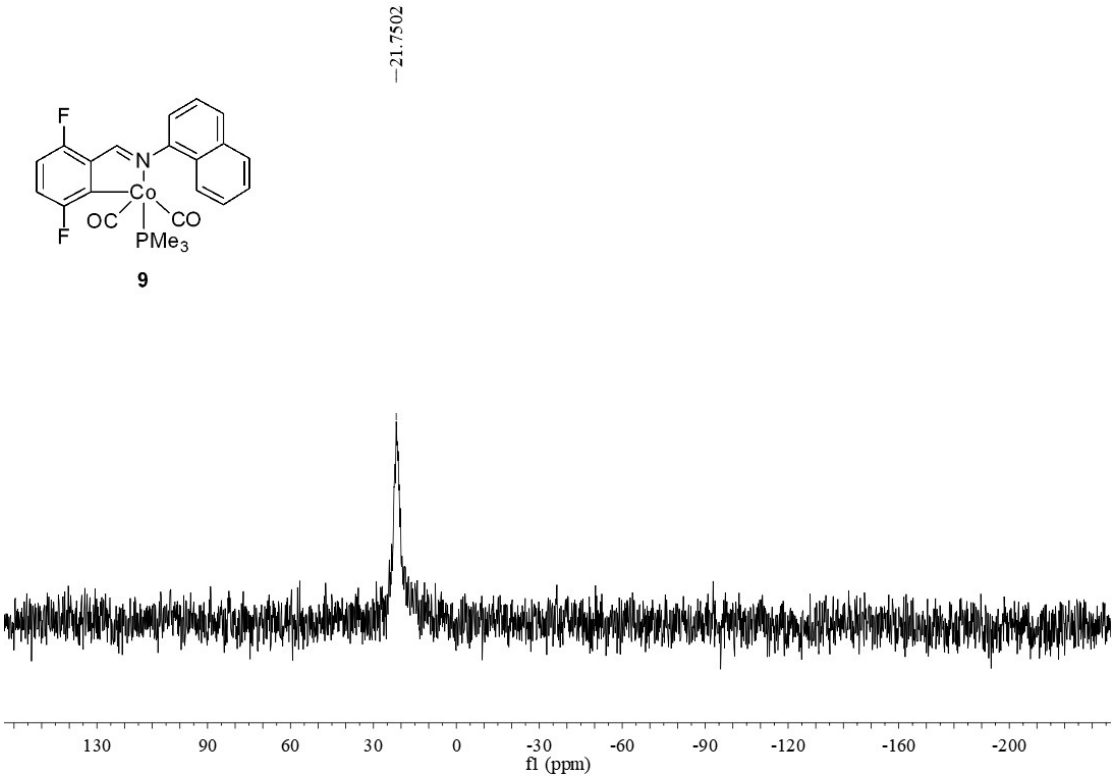


Fig S19 ^{31}P NMR spectrum of **9**

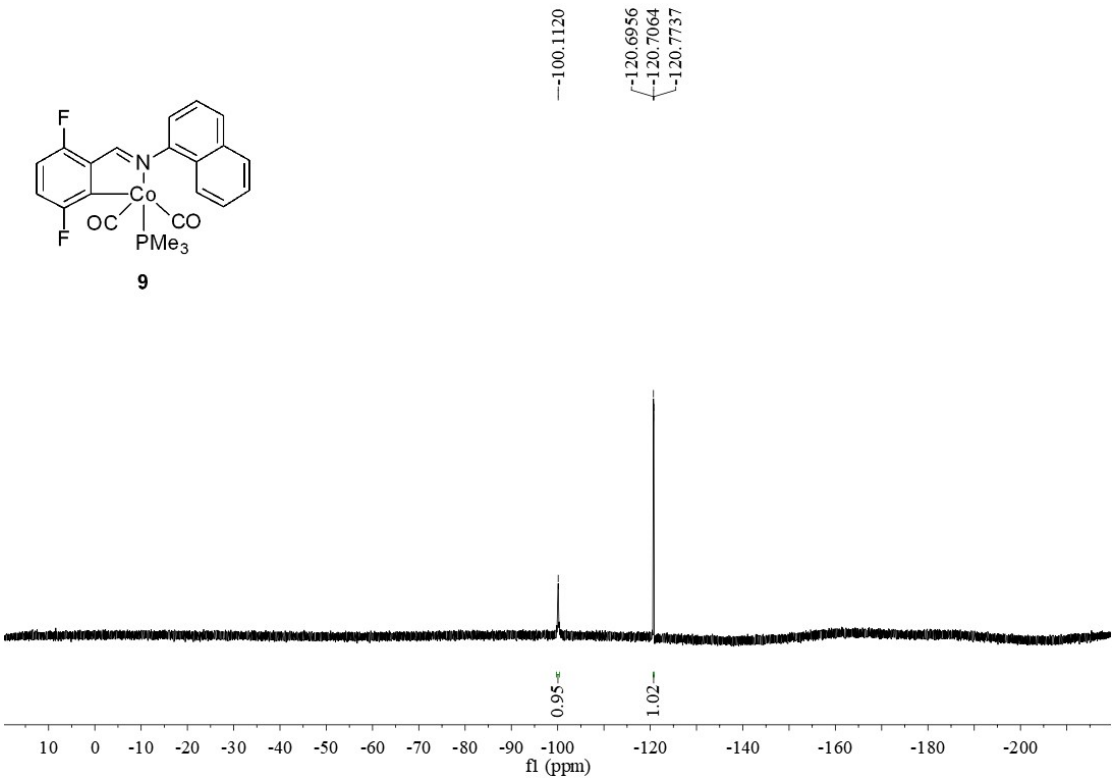


Fig S20 ^{19}F NMR spectrum of **9**

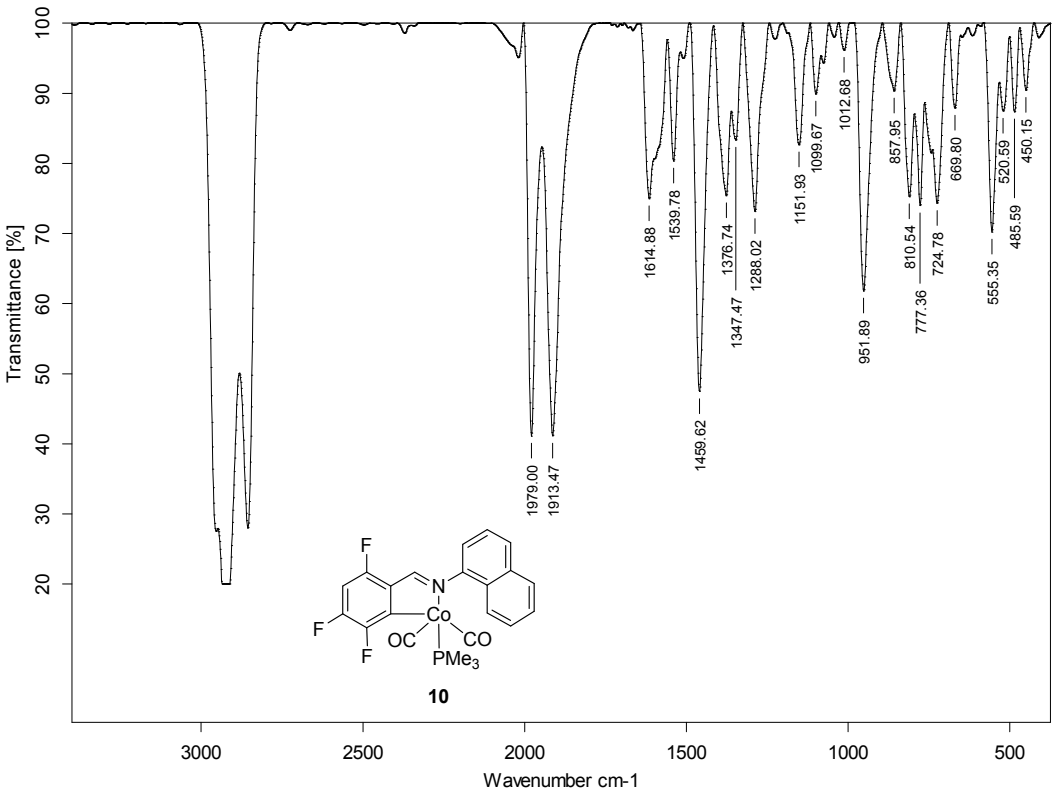


Fig S21 IR spectrum of **10**

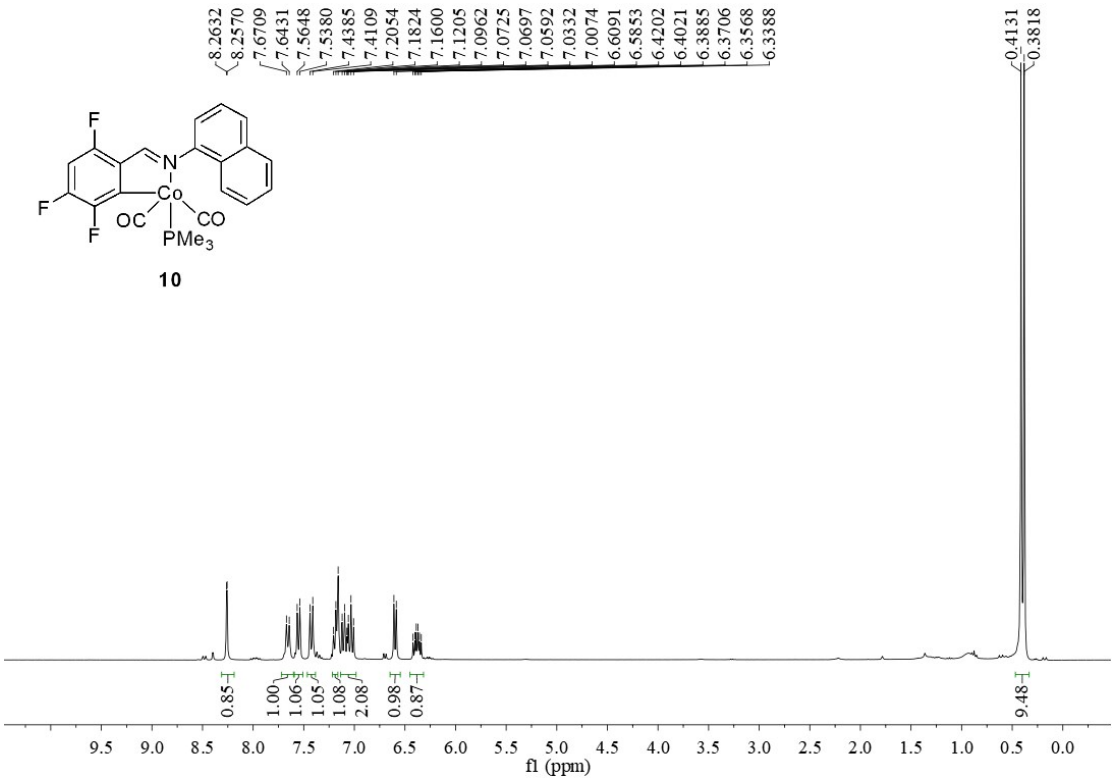


Fig S22 ^{1}H NMR spectrum of **10**

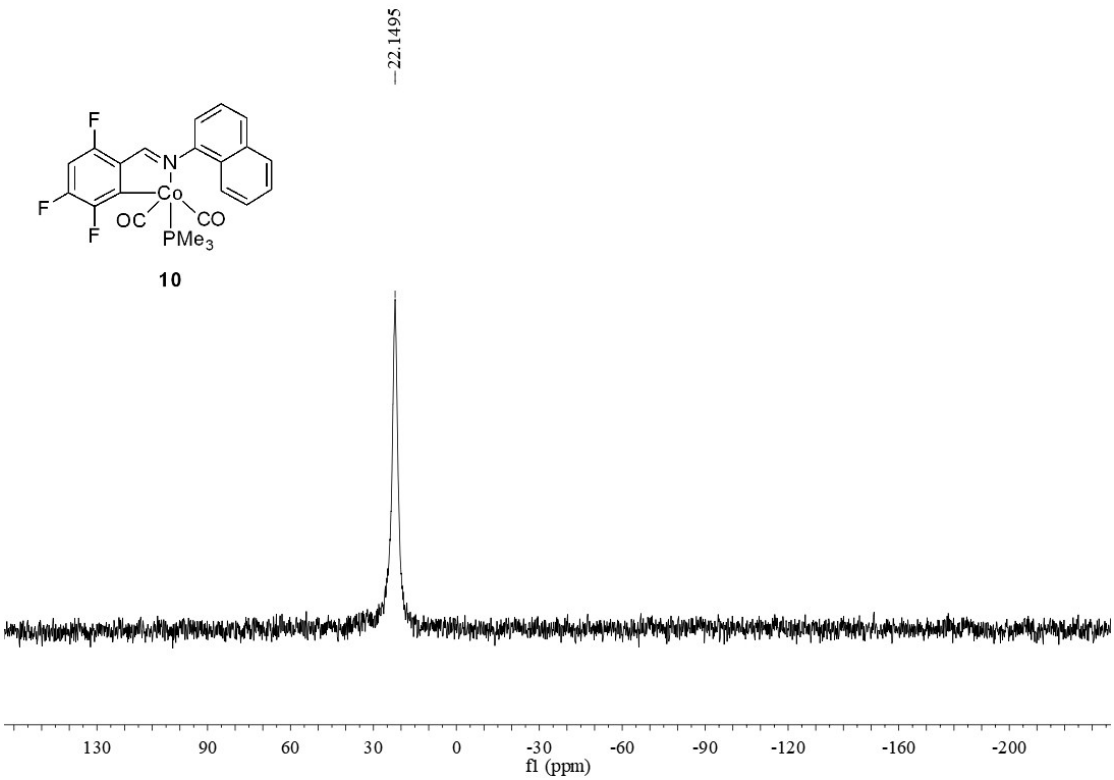


Fig S23 ^{31}P NMR spectrum of **10**

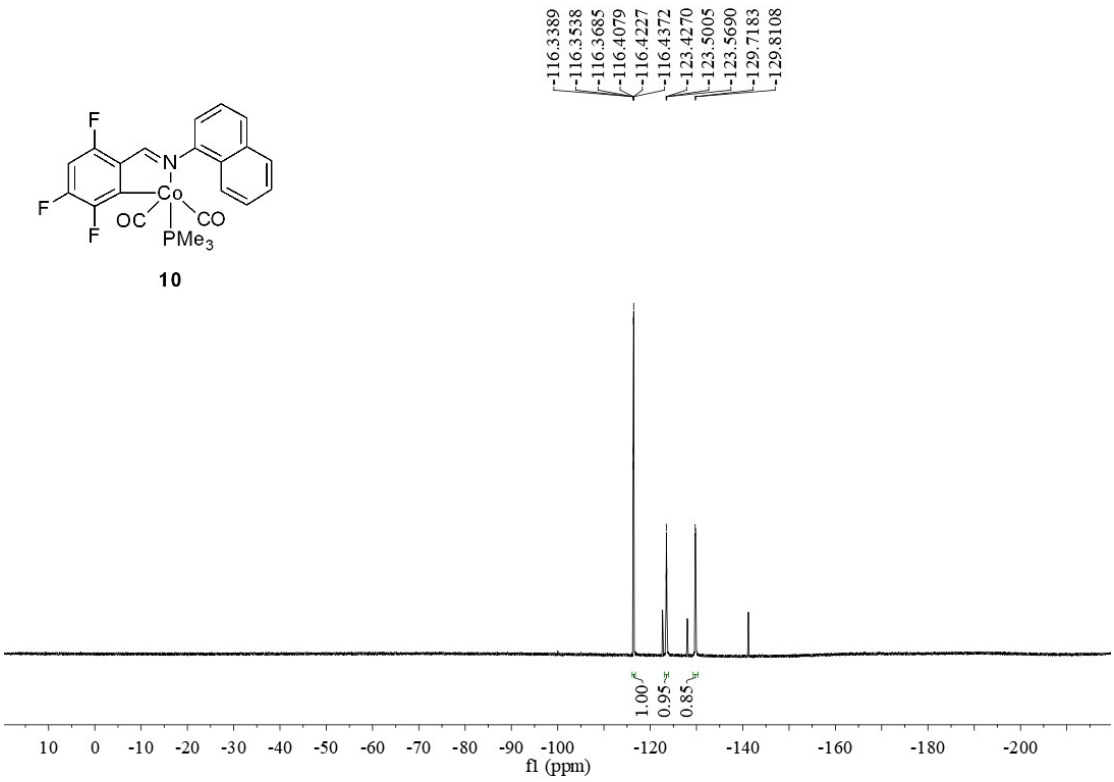


Fig S24 ^{19}F NMR spectrum of **10**

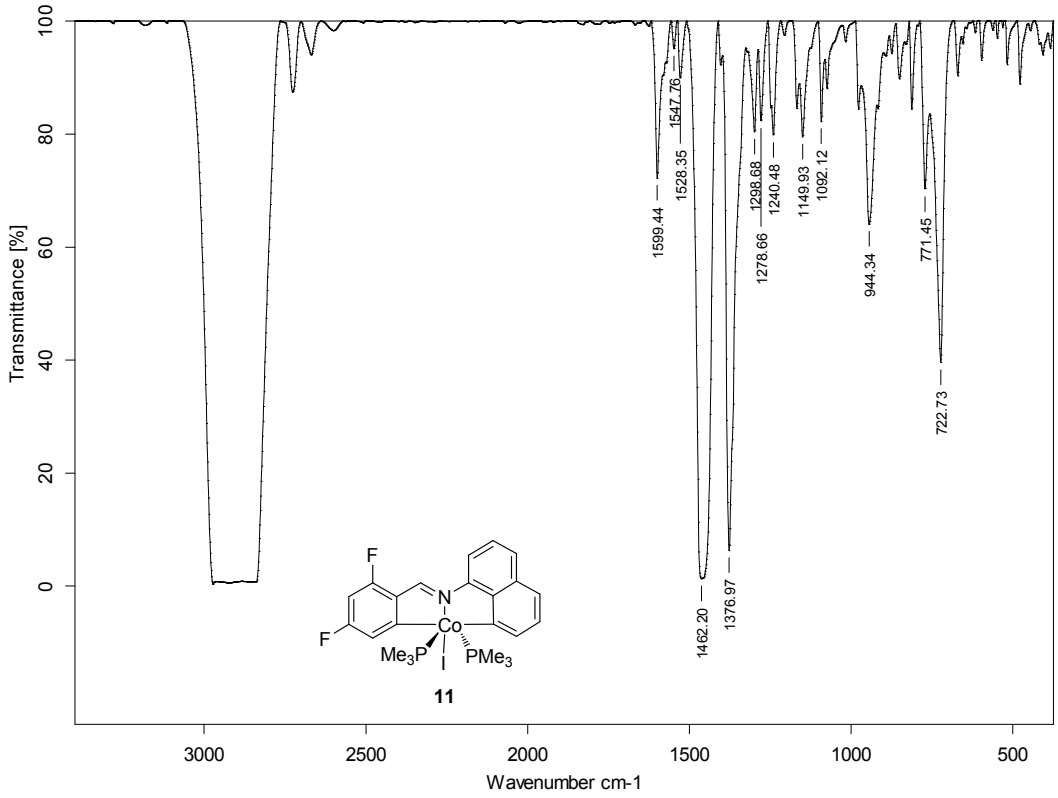


Fig S25 IR spectrum of **11**

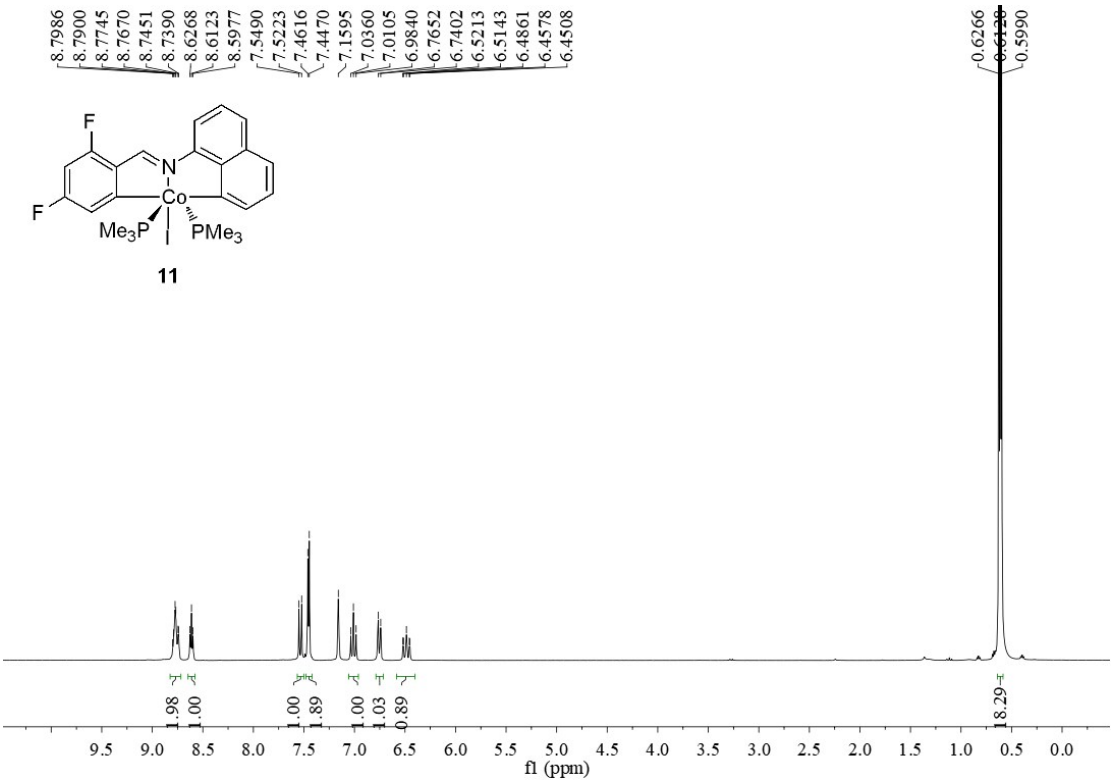


Fig S6 ^{1}H NMR spectrum of **11**

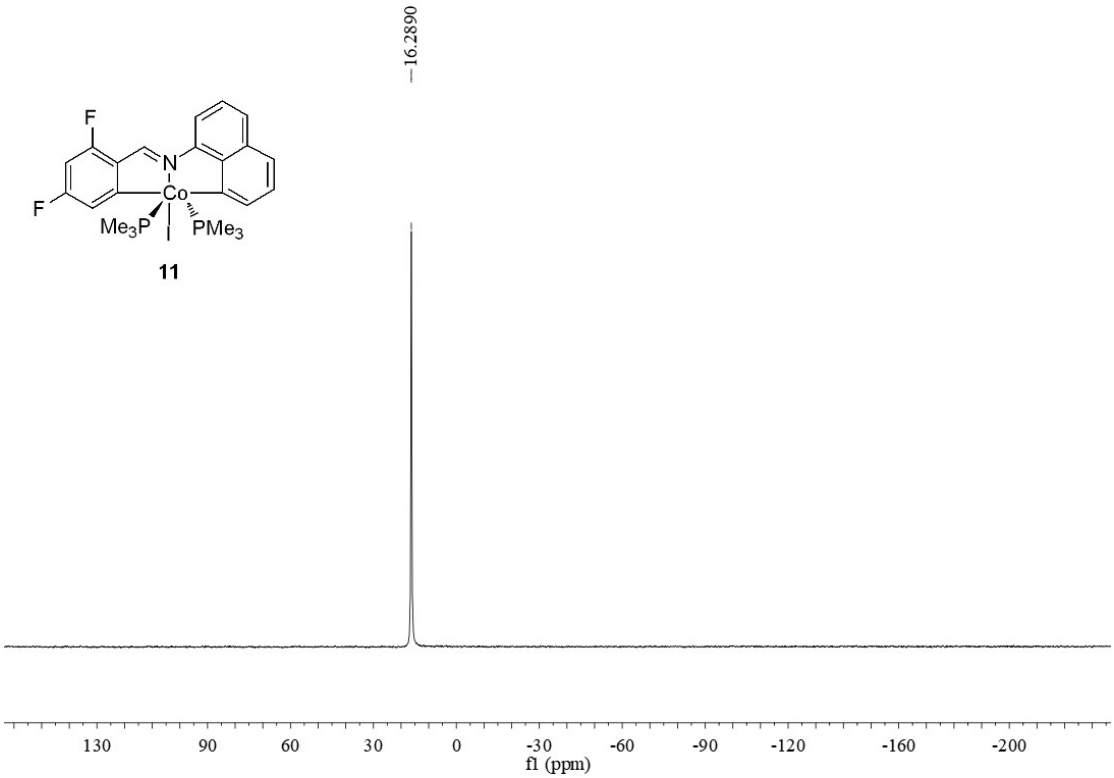


Fig S27 ^{31}P NMR spectrum of **11**

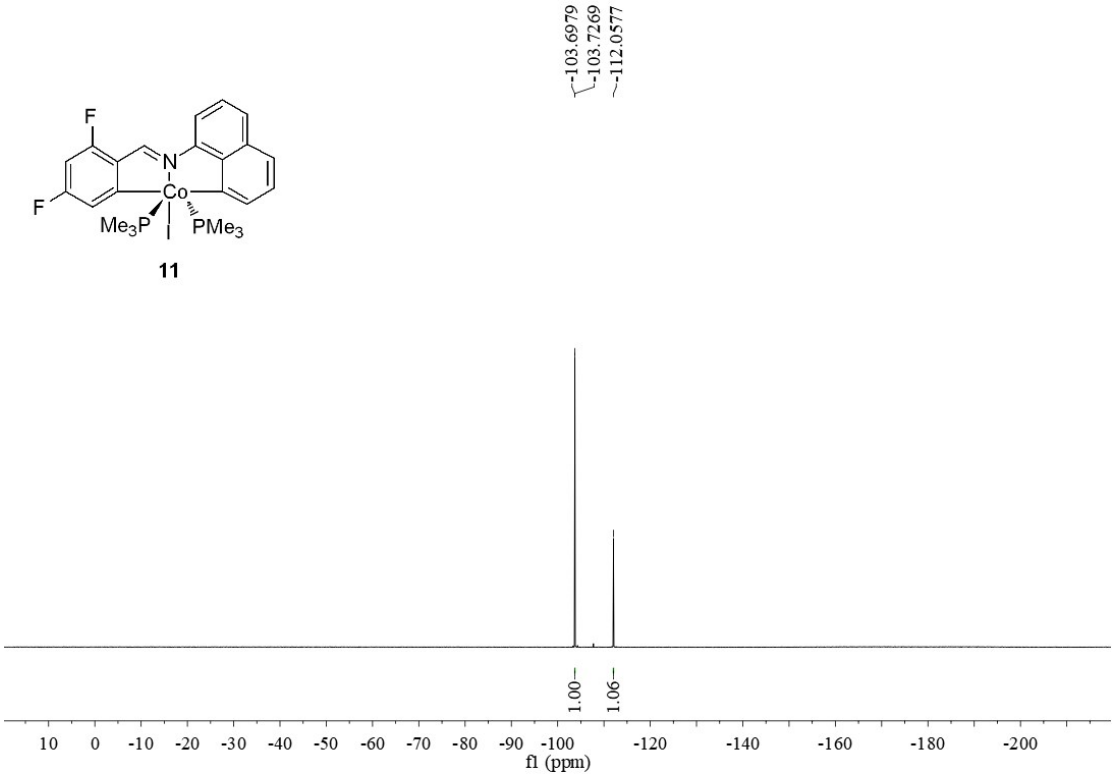


Fig S28 ^{19}F NMR spectrum of **11**

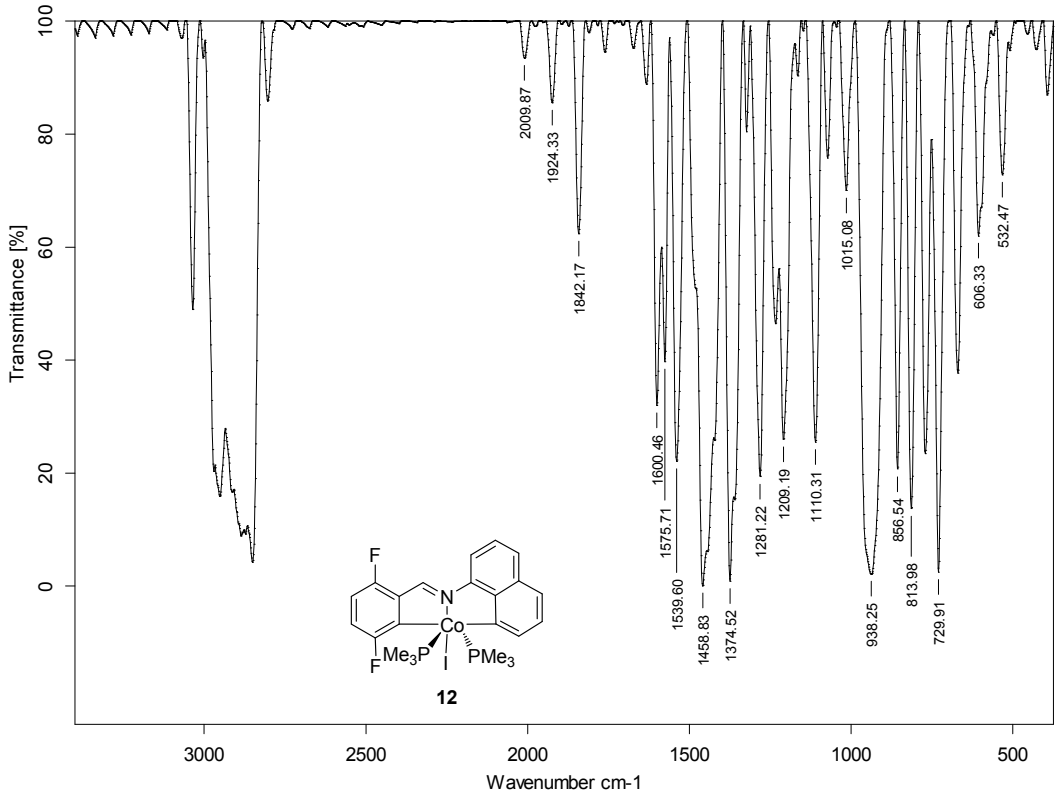


Fig S29 IR spectrum of **12**

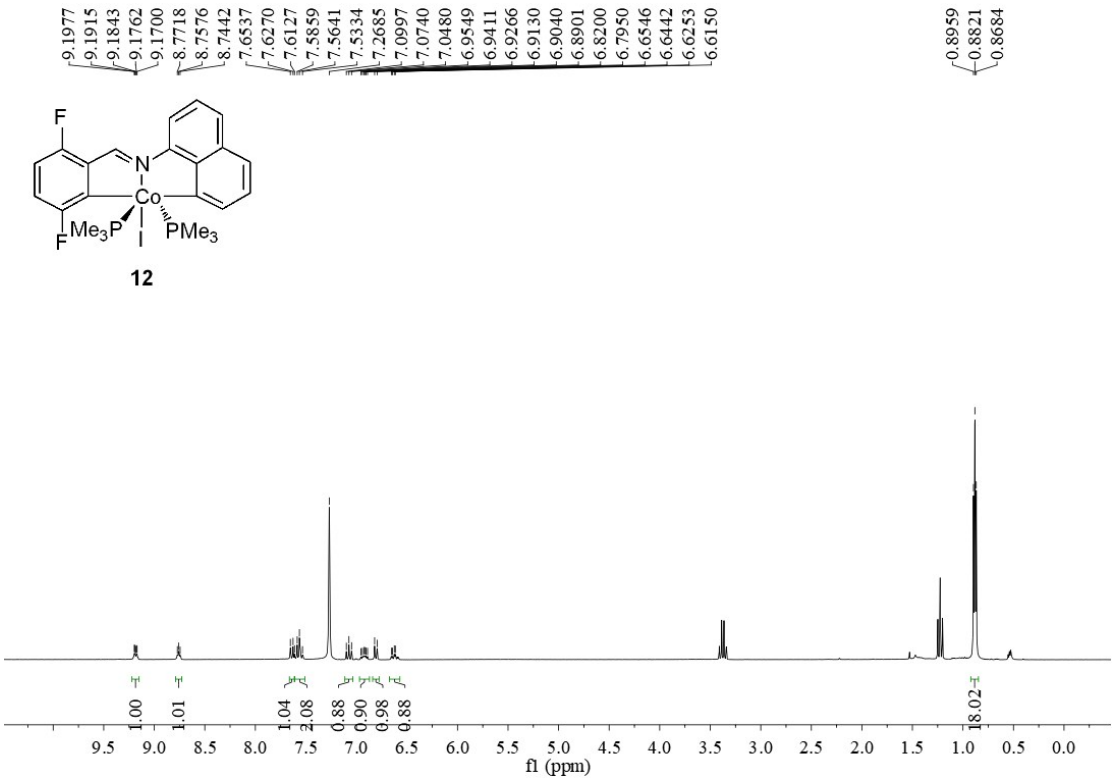


Fig S30 ^{1}H NMR spectrum of **12**

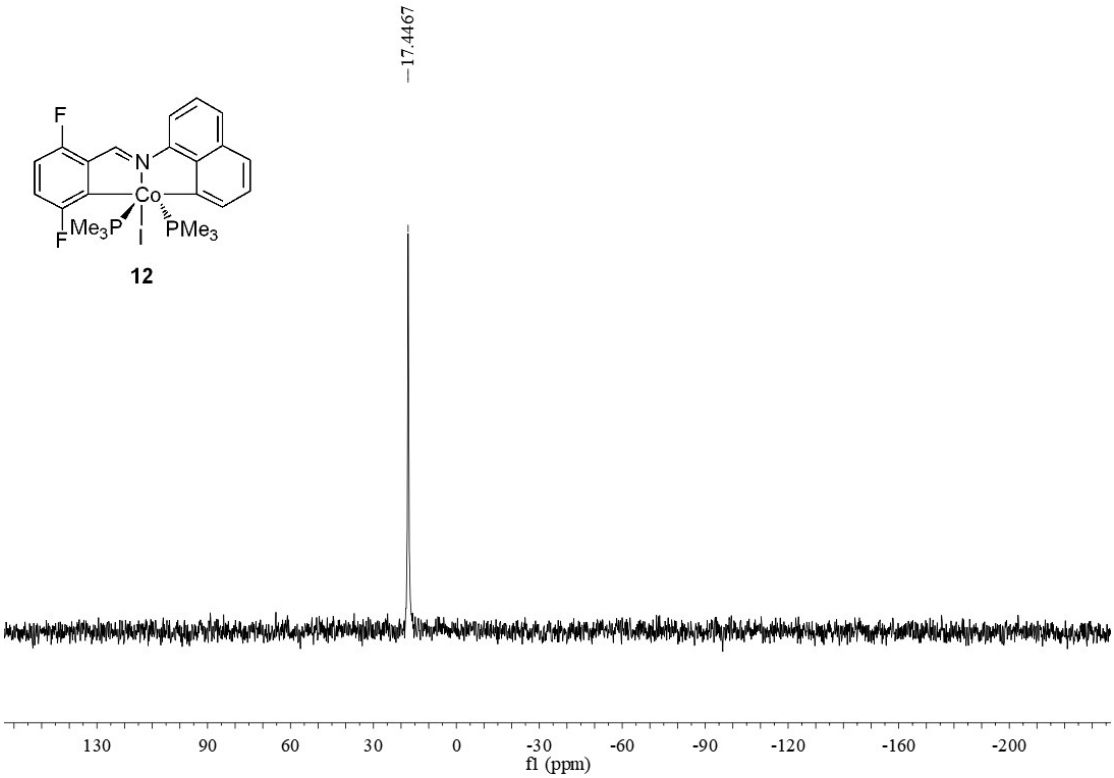


Fig S31 ^{31}P NMR spectrum of **12**

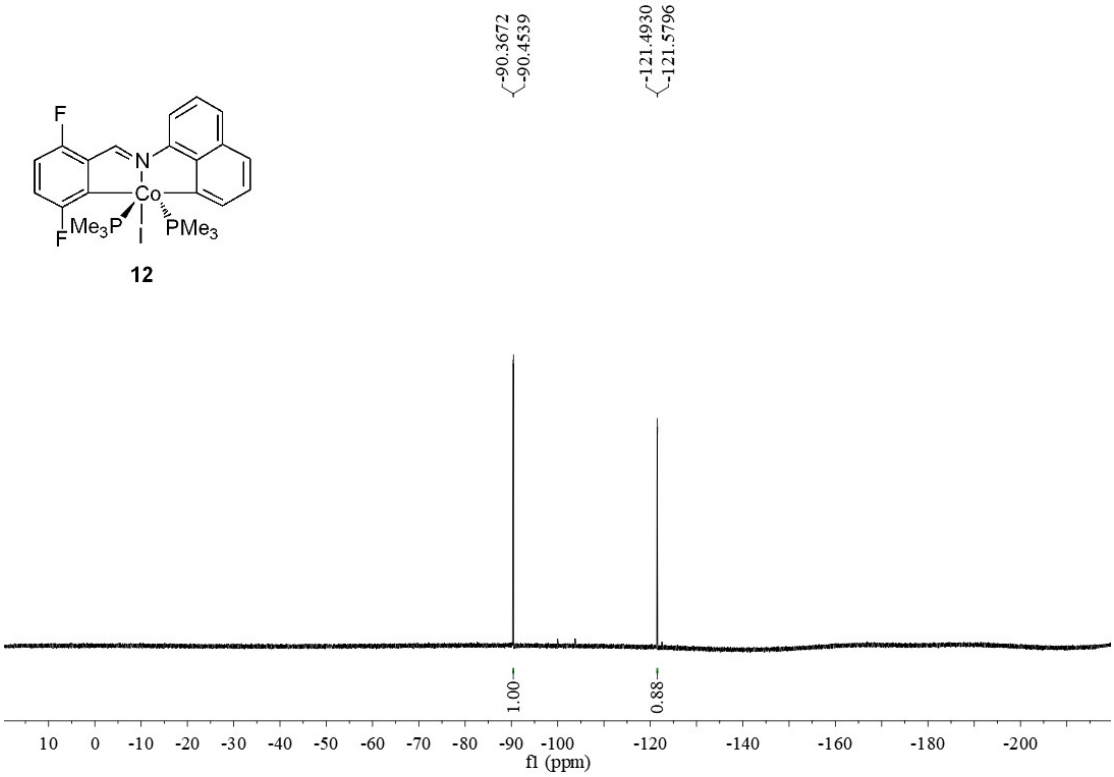


Fig S32 ^{19}F NMR spectrum of **12**

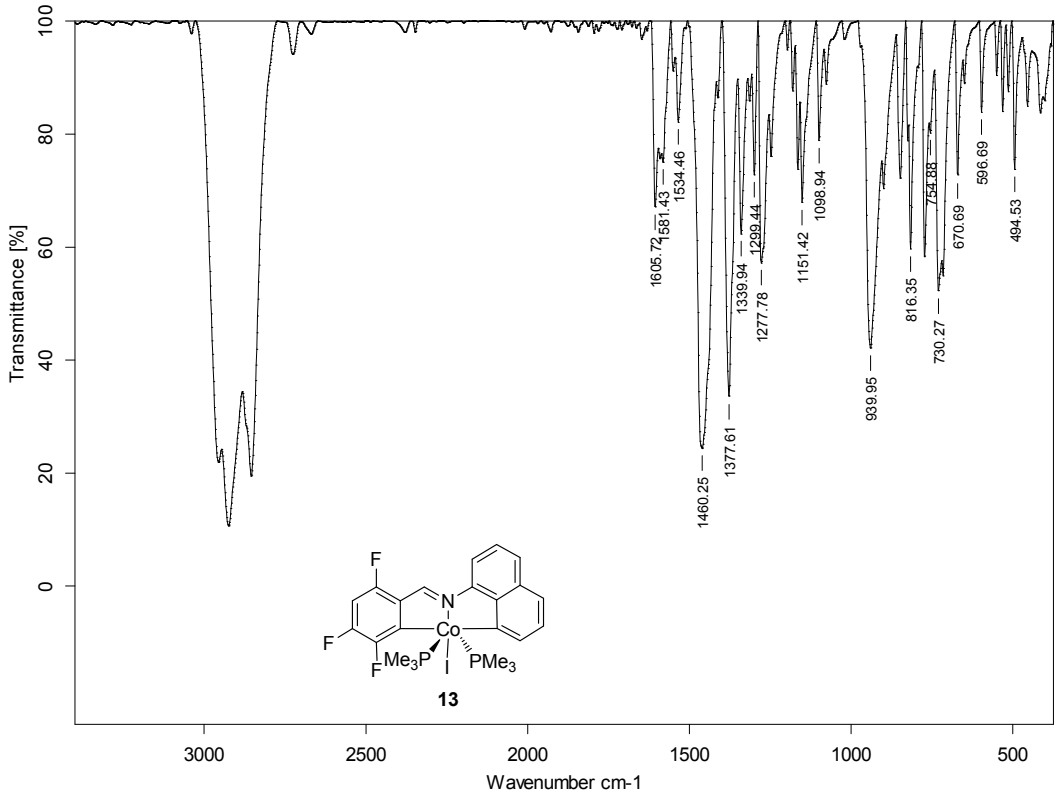


Fig S33 IR spectrum of **13**

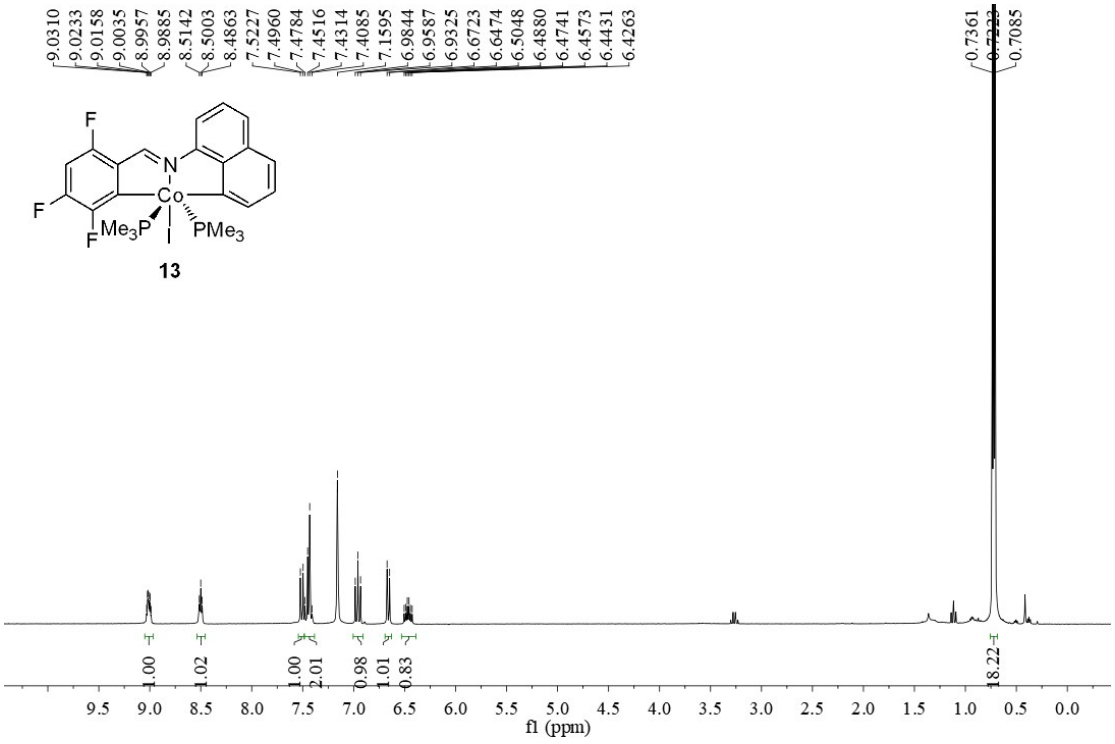


Fig S34 ^{1}H NMR spectrum of **13**

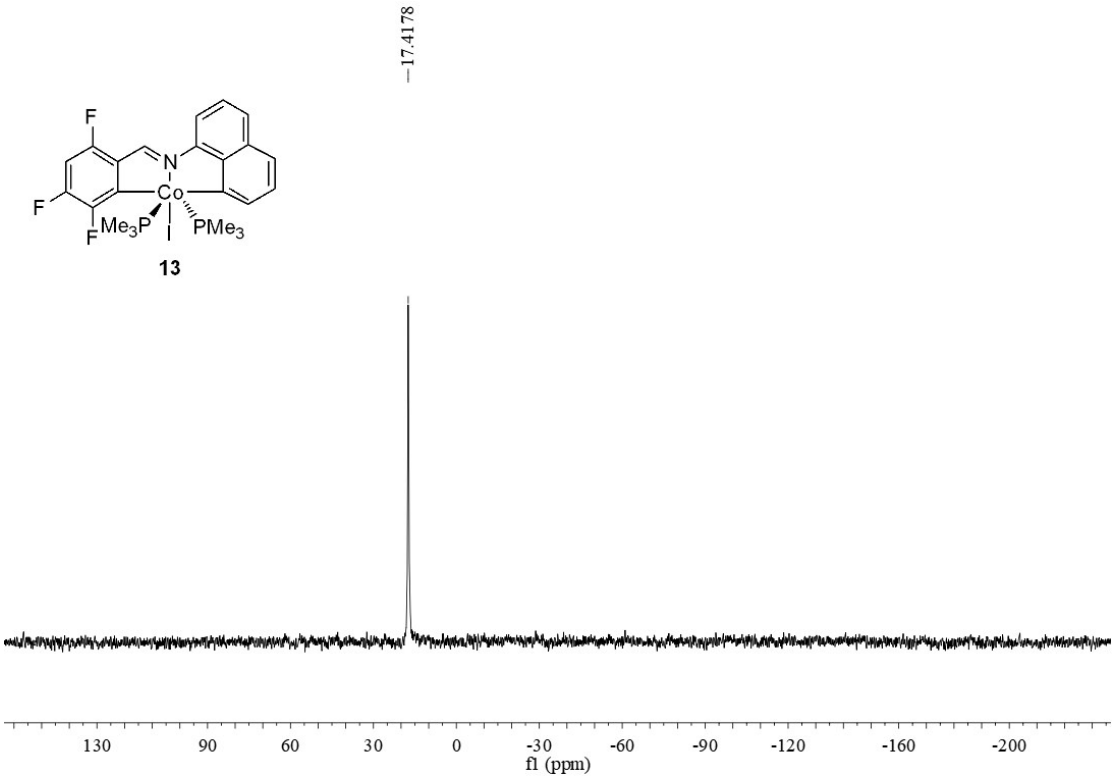


Fig S35 ^{31}P NMR spectrum of **13**

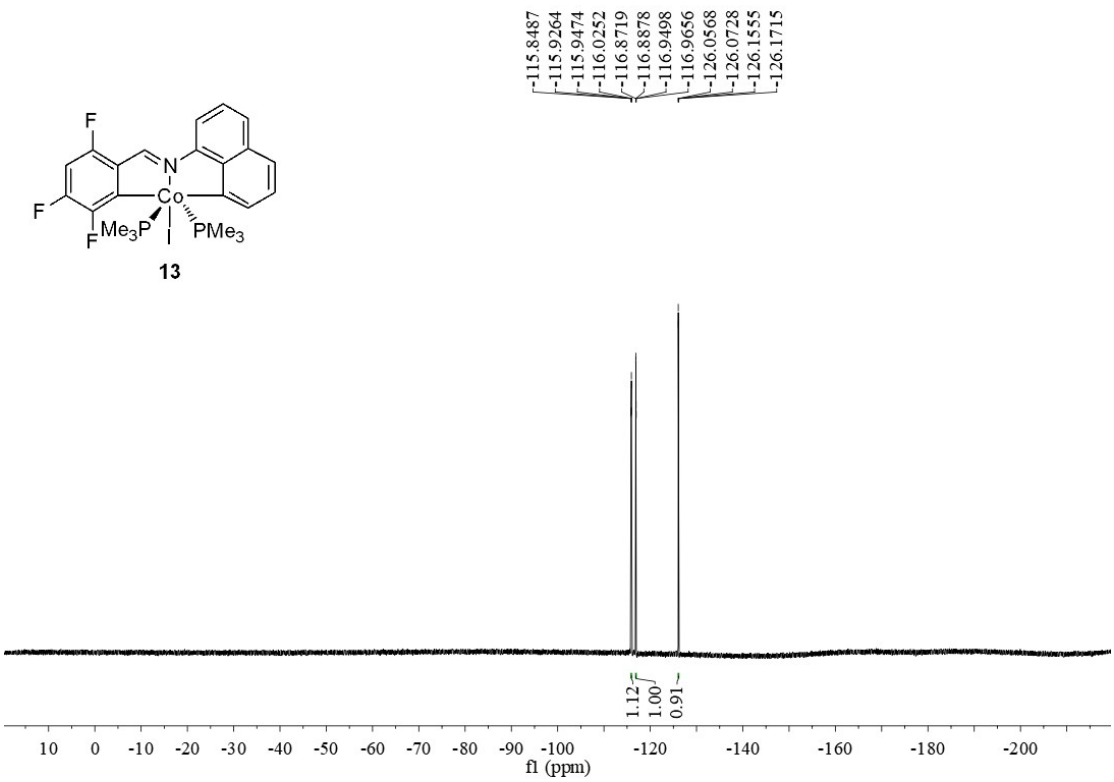


Fig S36 ^{19}F NMR spectrum of **13**

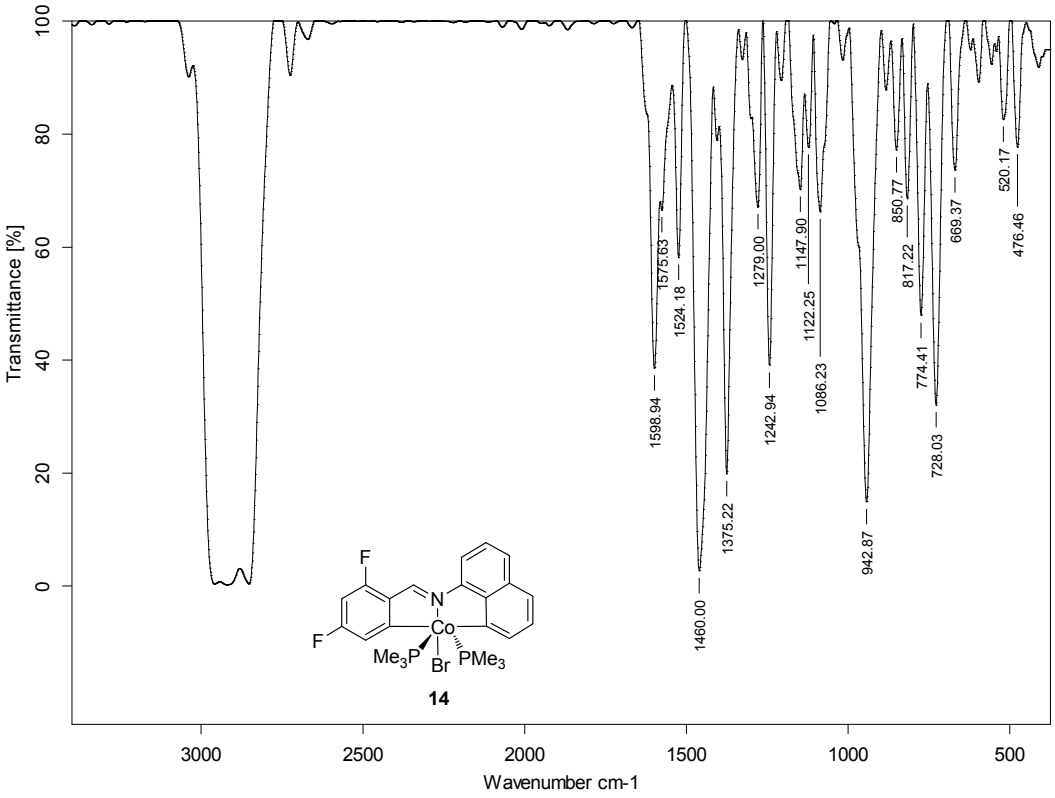


Fig S37 IR spectrum of **14**

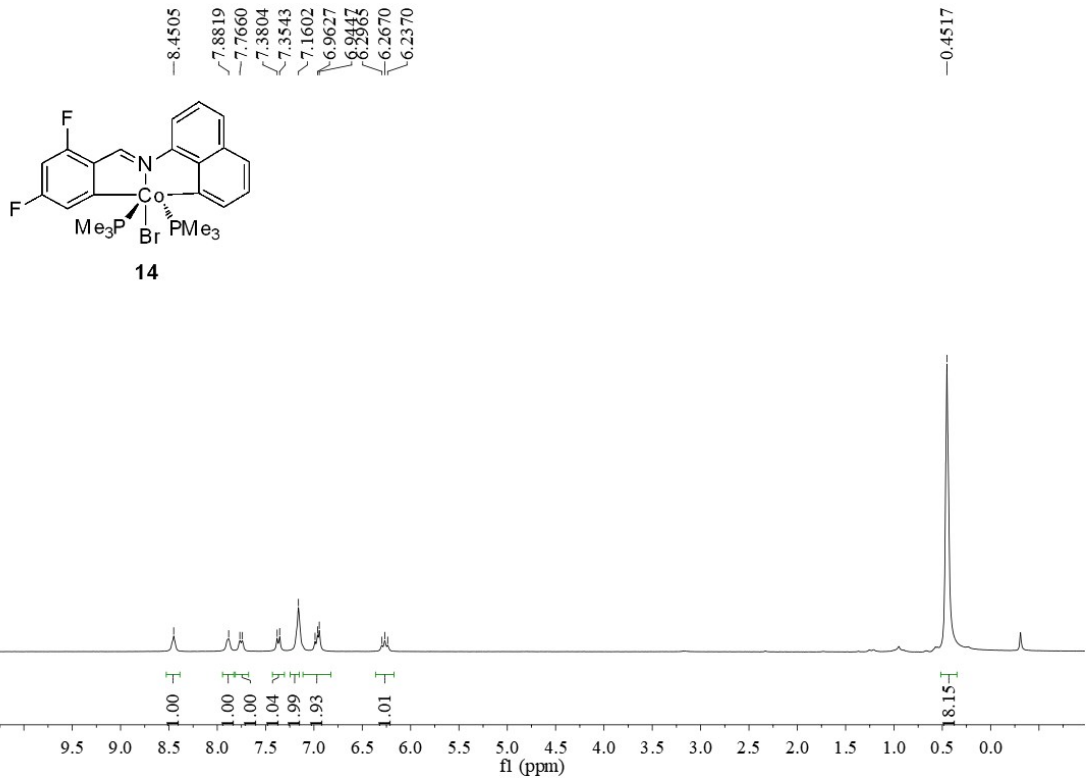


Fig S38 ^{1}H NMR spectrum of 1**4**

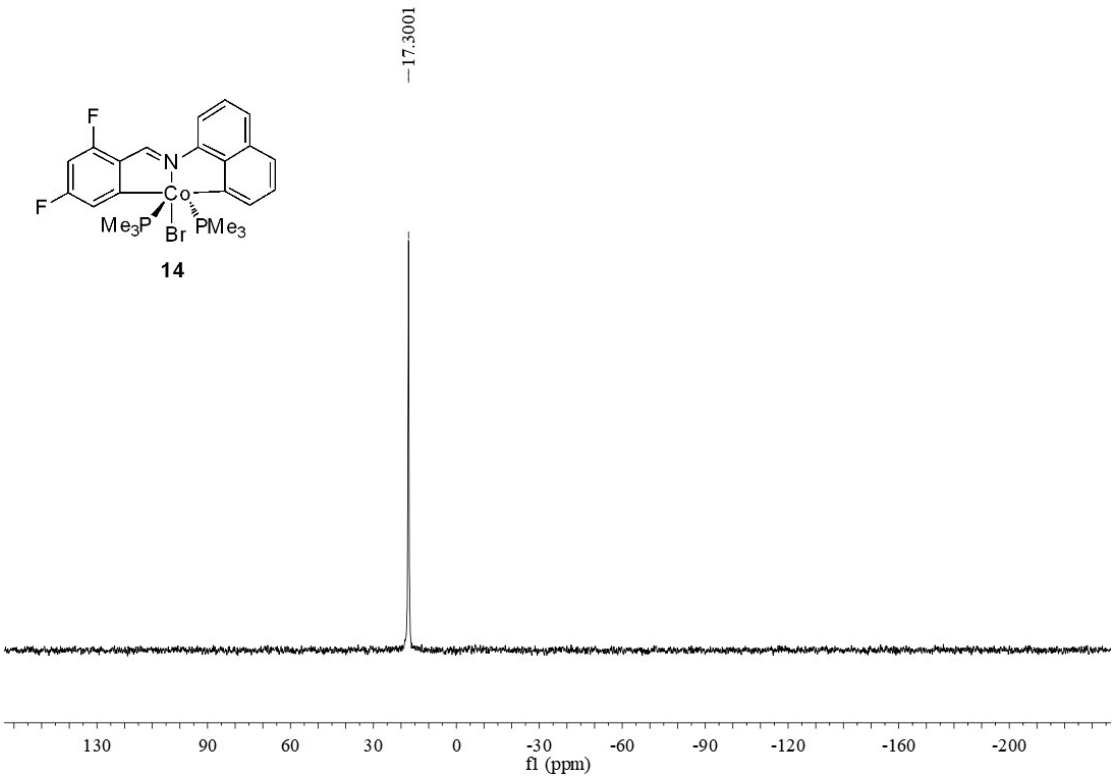


Fig S39 ^{31}P NMR spectrum of **14**

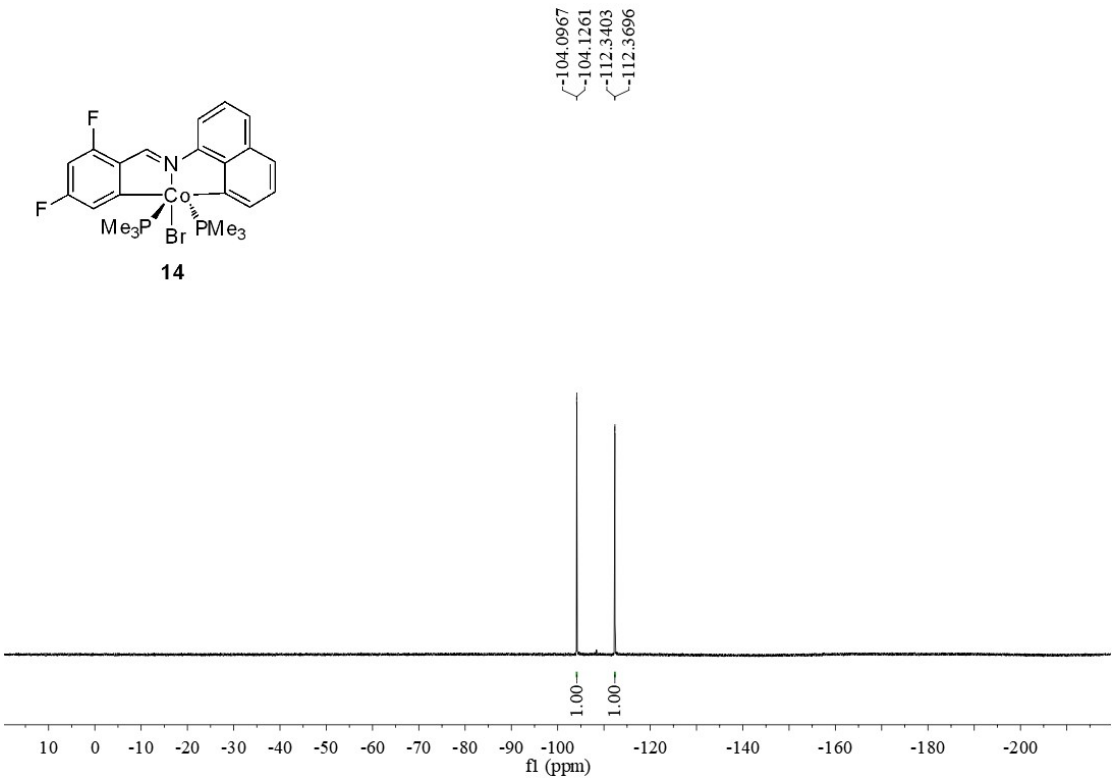


Fig S40 ^{19}F NMR spectrum of **14**

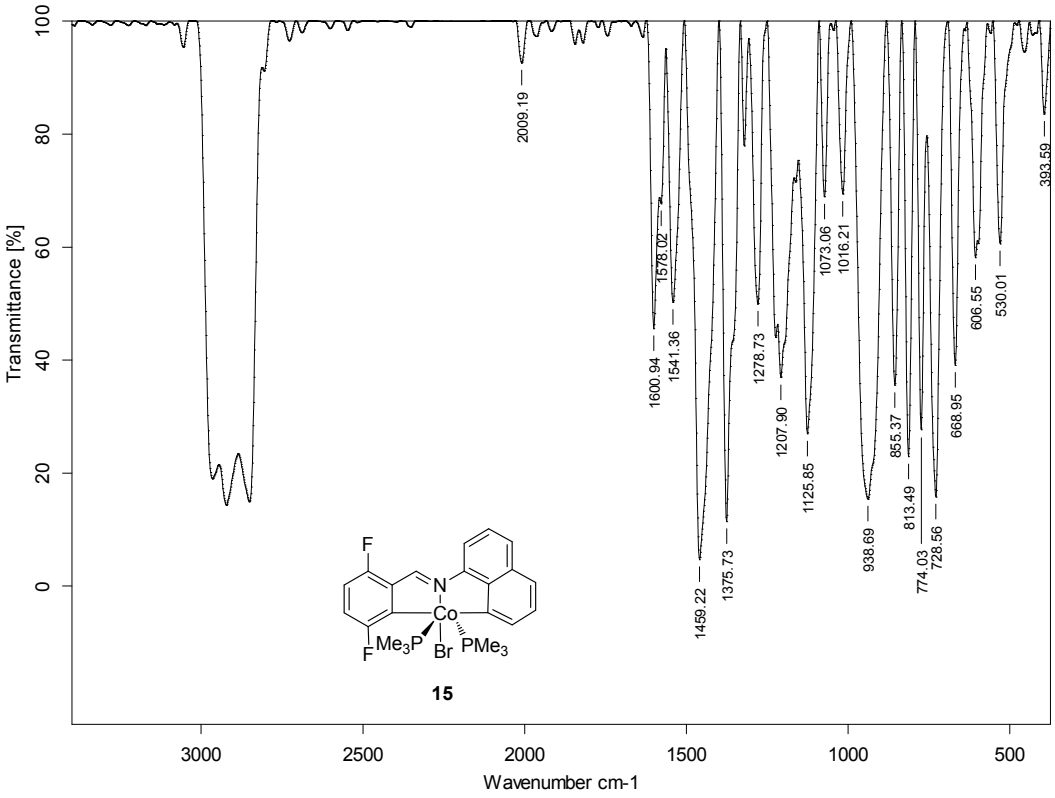


Fig S41 IR spectrum of 1**5**

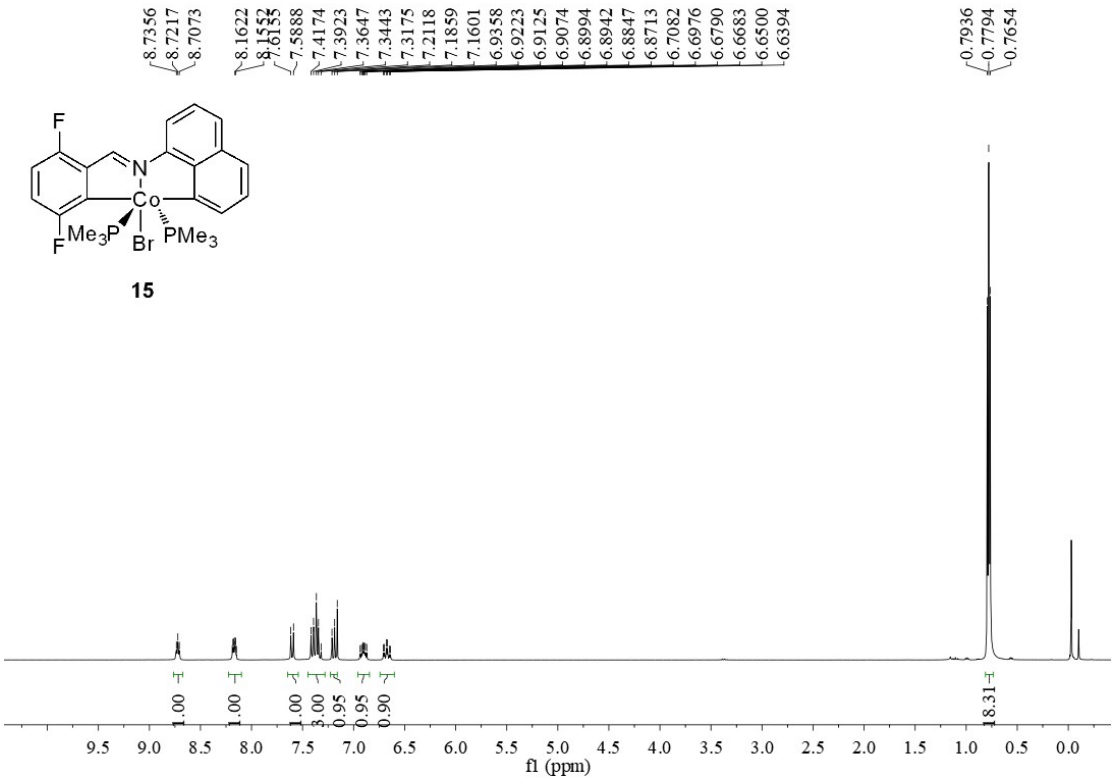


Fig S42 [1]H NMR spectrum of **15**

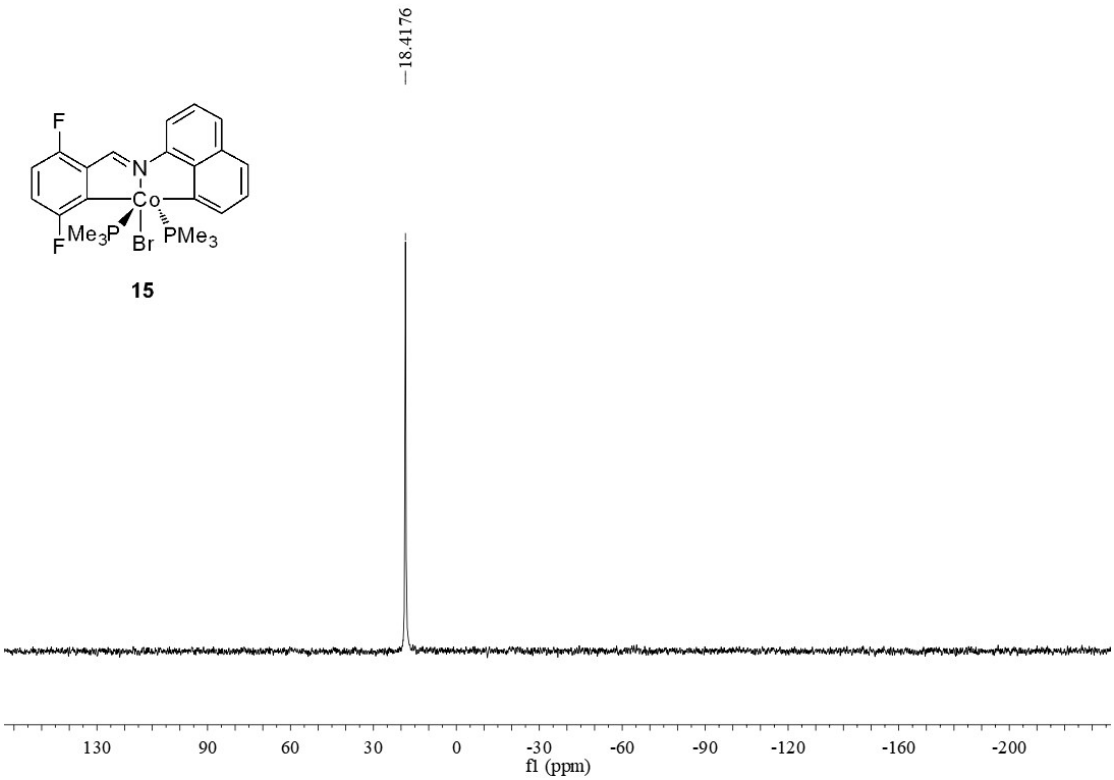


Fig S43 ^{31}P NMR spectrum of 1**5**

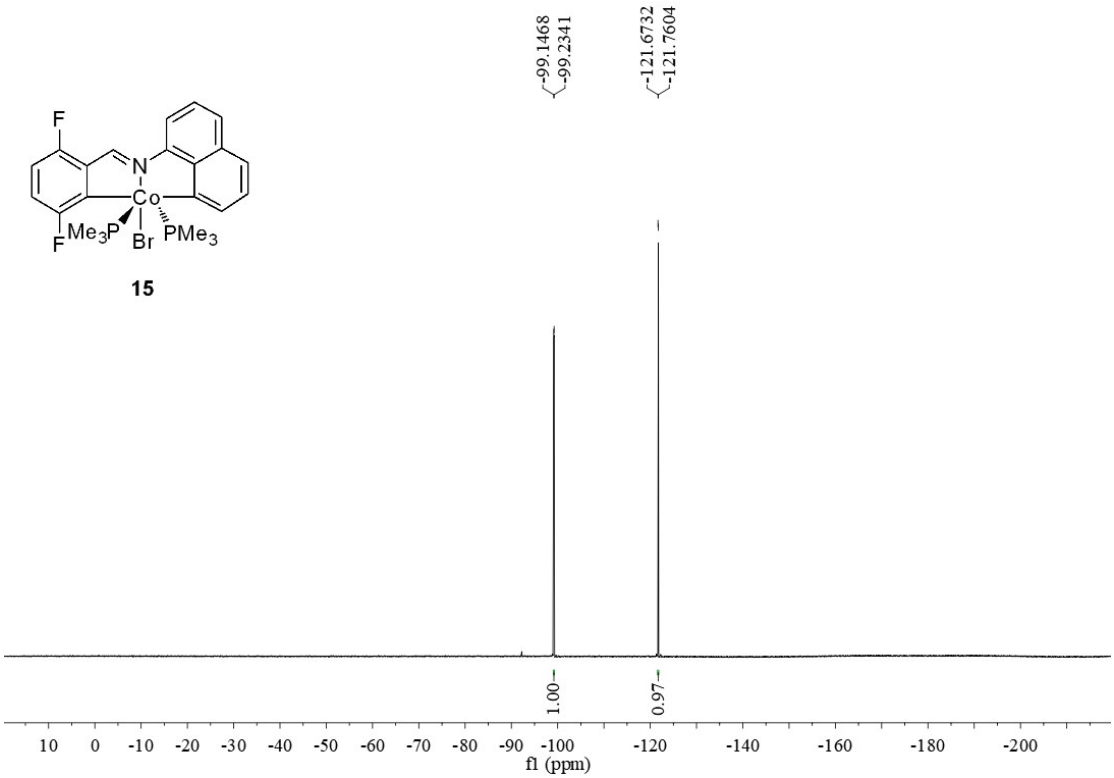


Fig S44 ^{19}F NMR spectrum of 1**5**

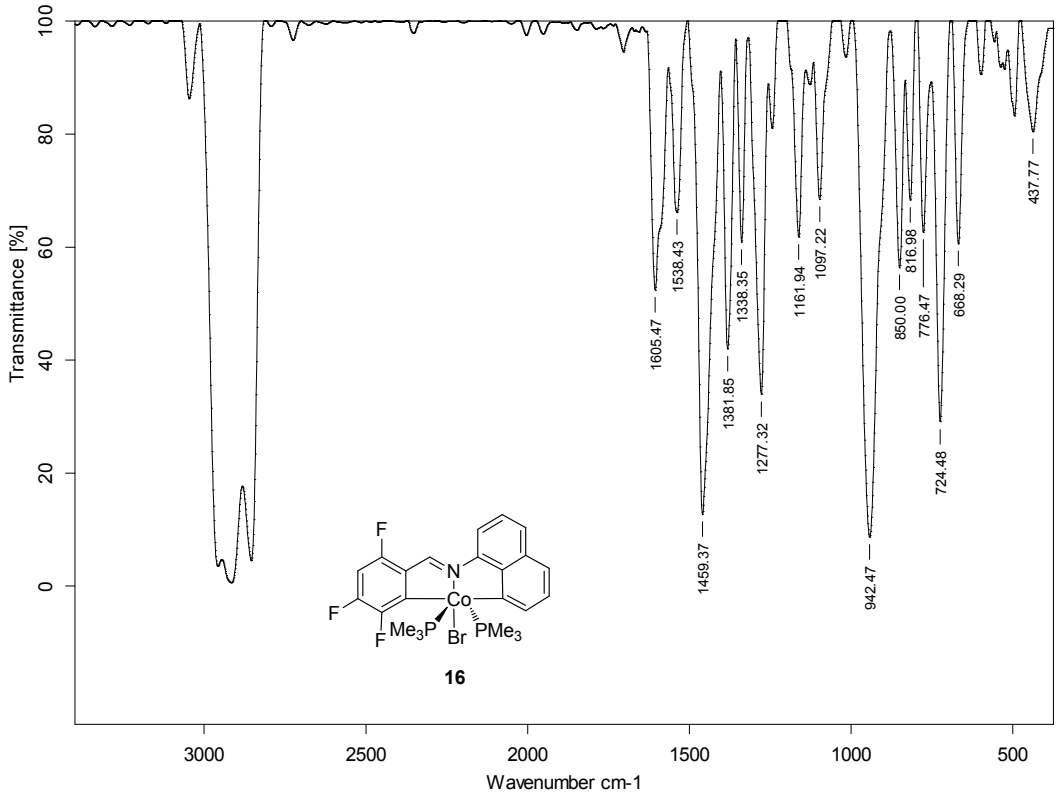


Fig S45 IR spectrum of **16**

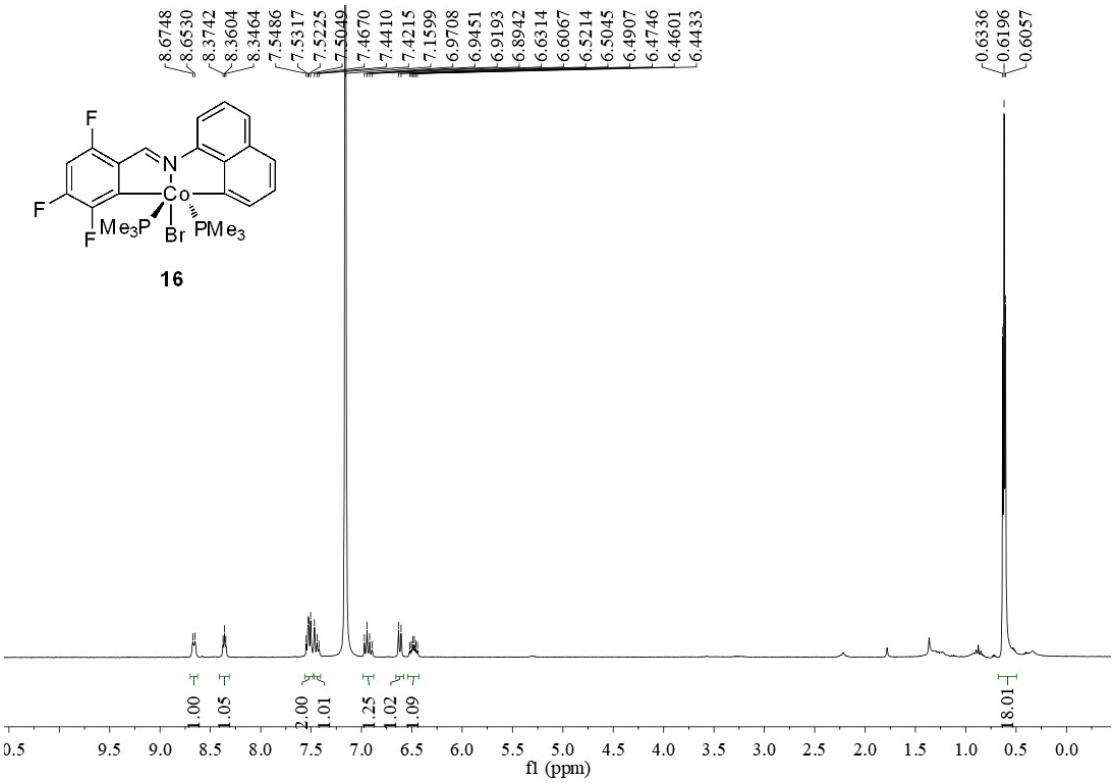


Fig S46 ^{1}H NMR spectrum of **16**

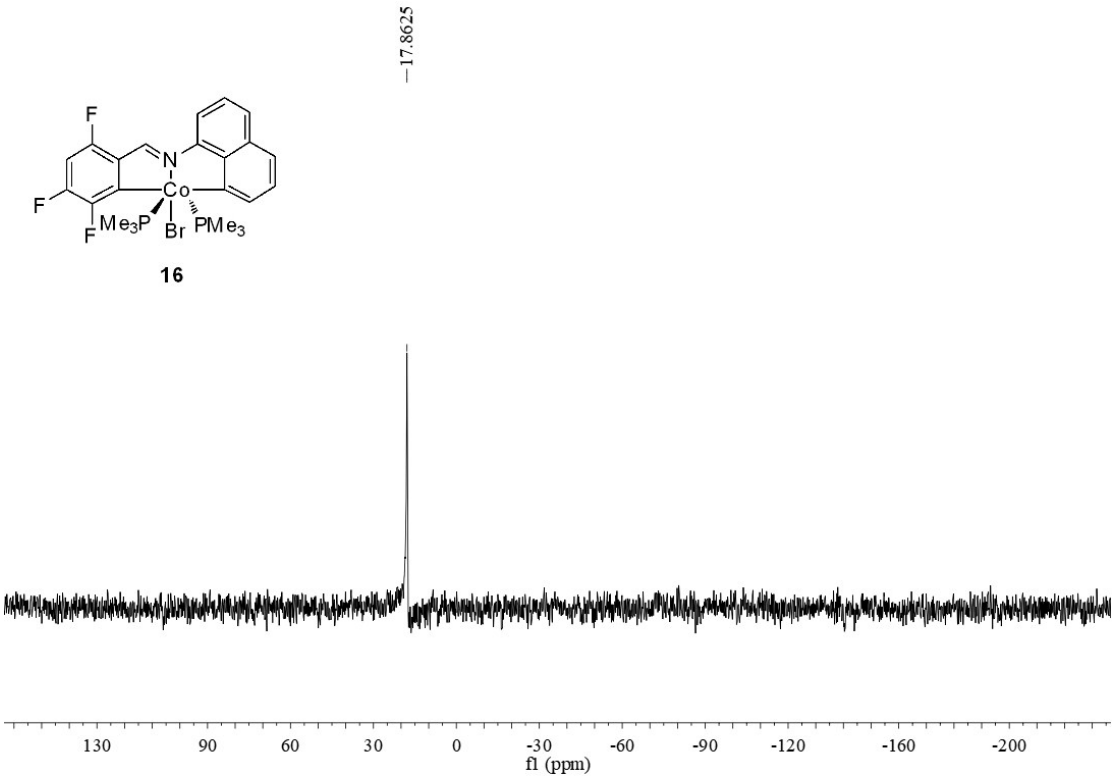


Fig S47 ^{31}P NMR spectrum of **16**

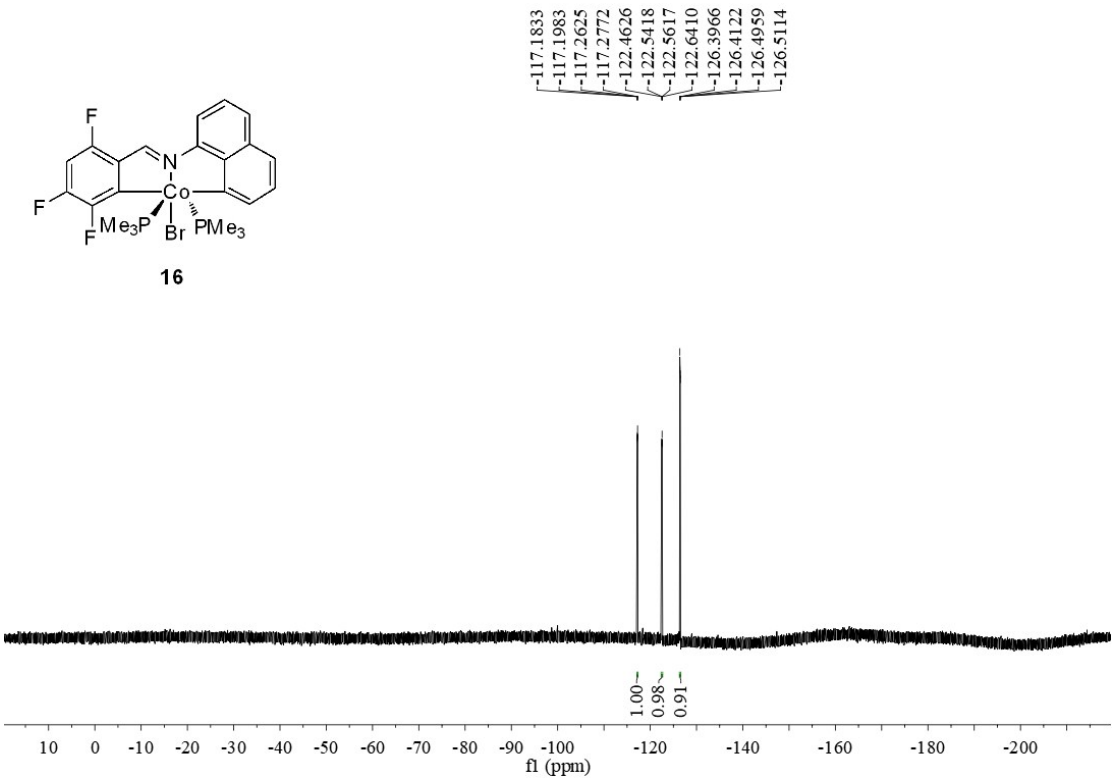
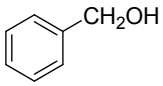
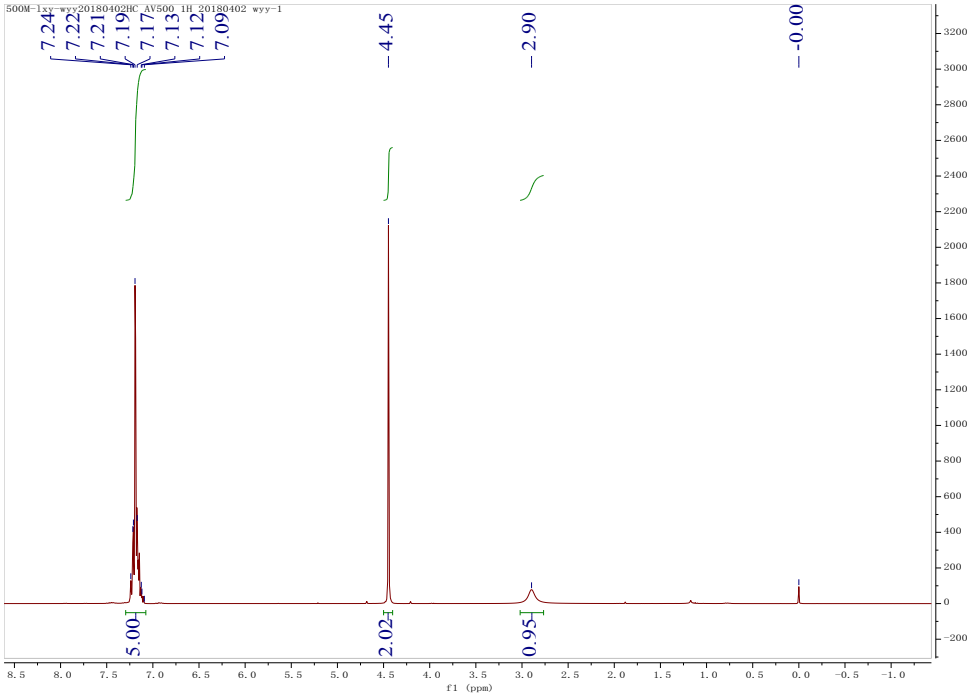


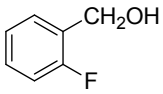
Fig S48 ^{19}F NMR spectrum of **16**

3 ^{1}H NMR spectra of alcohols

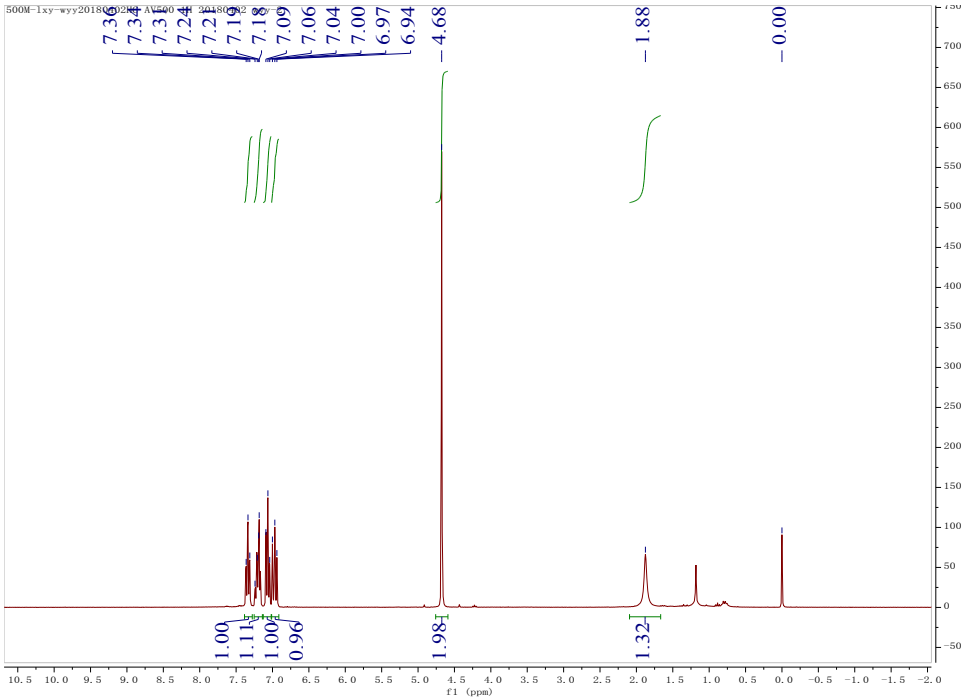


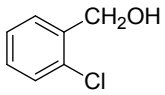
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.24–7.09 (m, *Ar*, 5H), 4.45 (s, CH_2, 2H), 2.90 (s, O*H*, 1H).



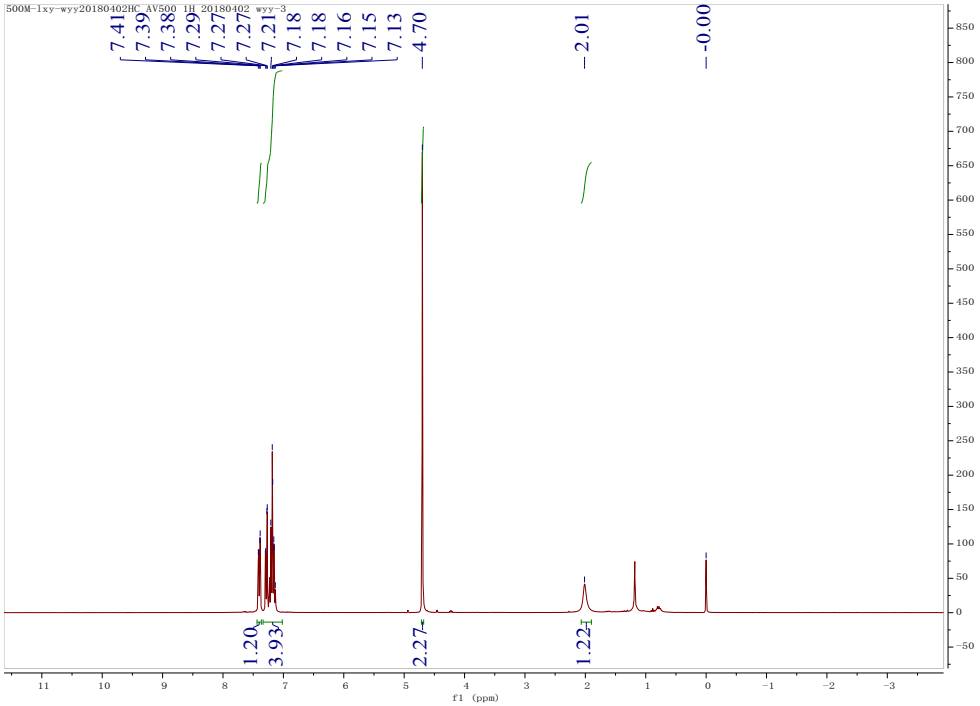


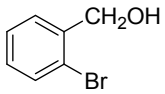
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.36–6.94 (m, *Ar*, 4H), 4.68 (s, CH_2, 2H), 1.88(s, O*H*, 1H).



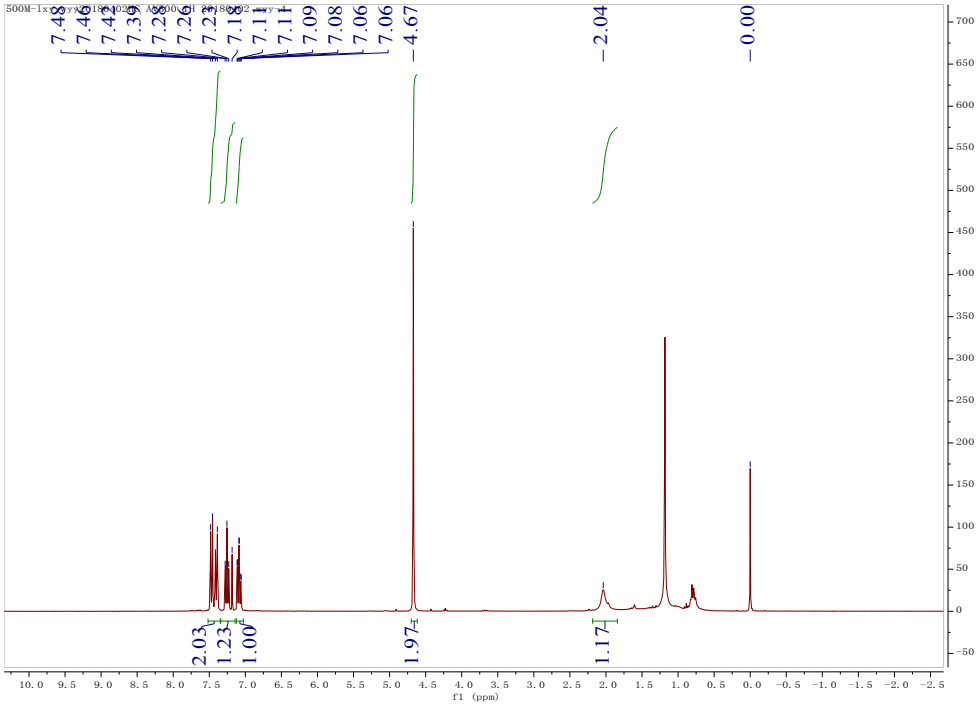


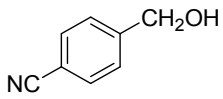
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.41–7.13 (m, *Ar*, 4H), 4.70 (s, CH_2, 2H), 2.01 (s, O*H*, 1H).



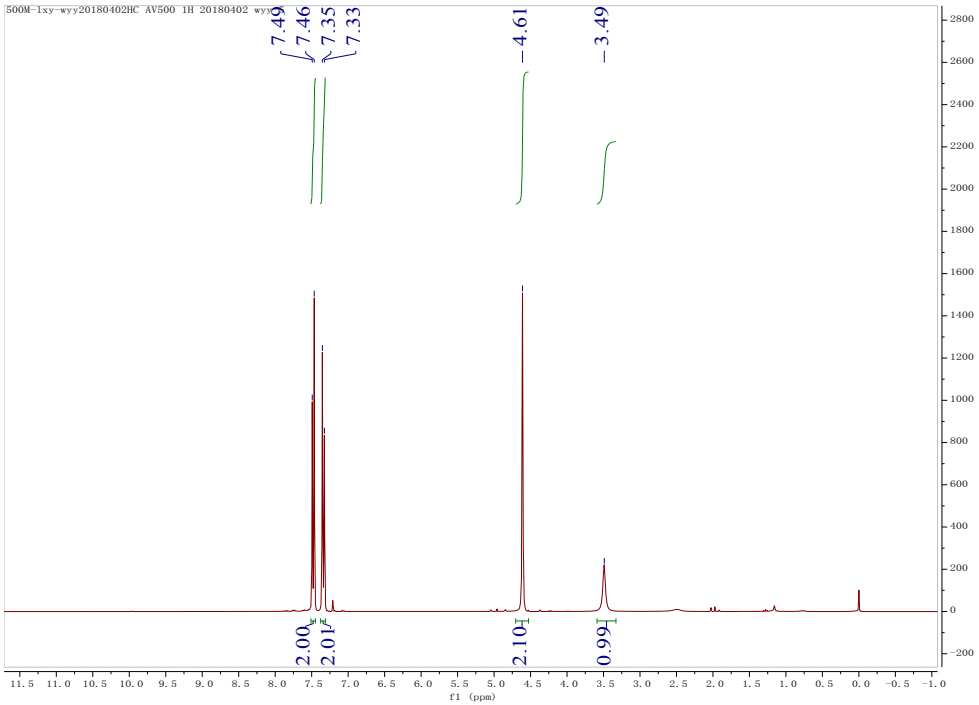


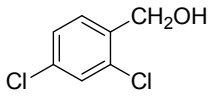
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.48–7.06 (m, *Ar*, 4H), 4.67 (s, CH_2, 2H), 2.04 (s, O*H*, 1H).



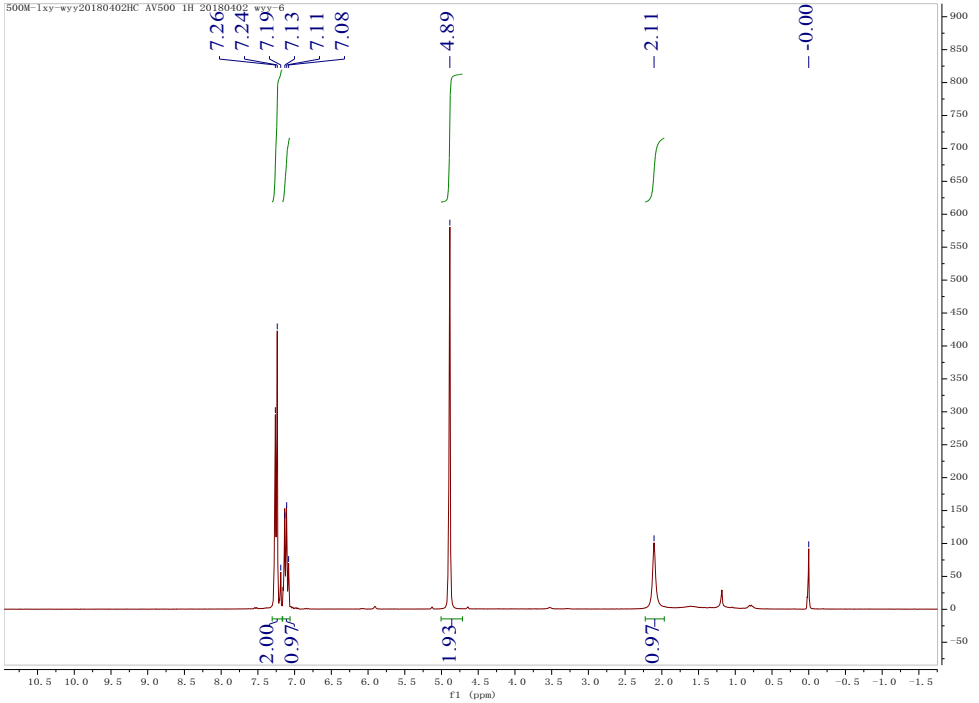


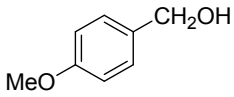
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.49–7.33 (m, *Ar*, 4H), 4.61 (q, CH_2, 2H), 3.49 (s, O*H*, 1H).



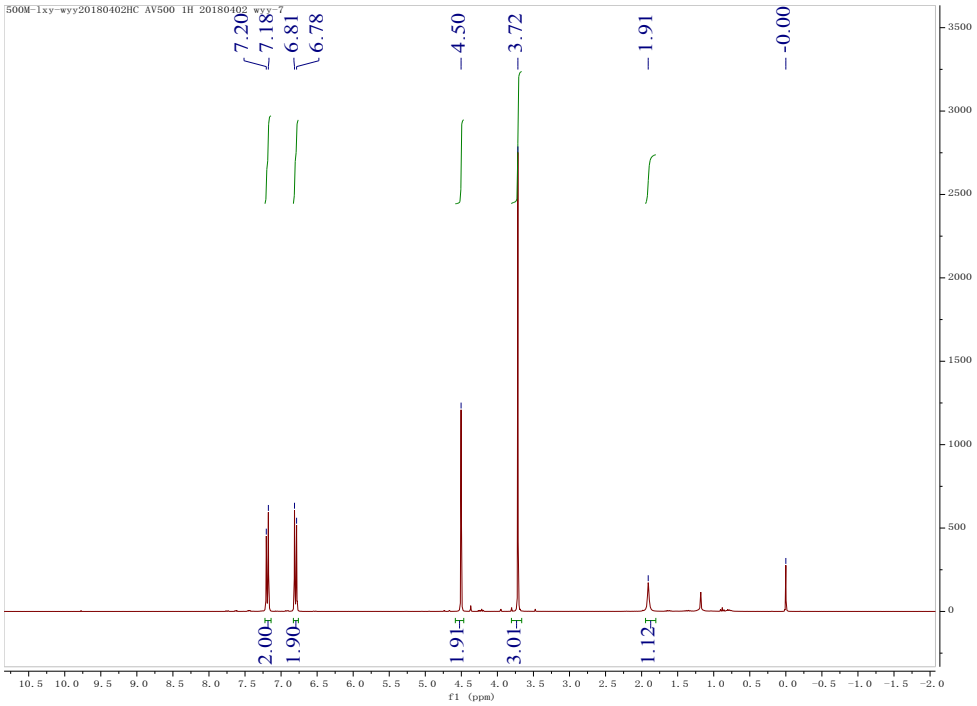


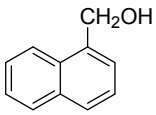
^{1}H NMR (300 MHz, $CDCl_3$, δ): 7.26–7.08 (m, *Ar*, 3H), 4.89 (d, CH_2, 2H), 2.11 (s, O*H*, 1H).



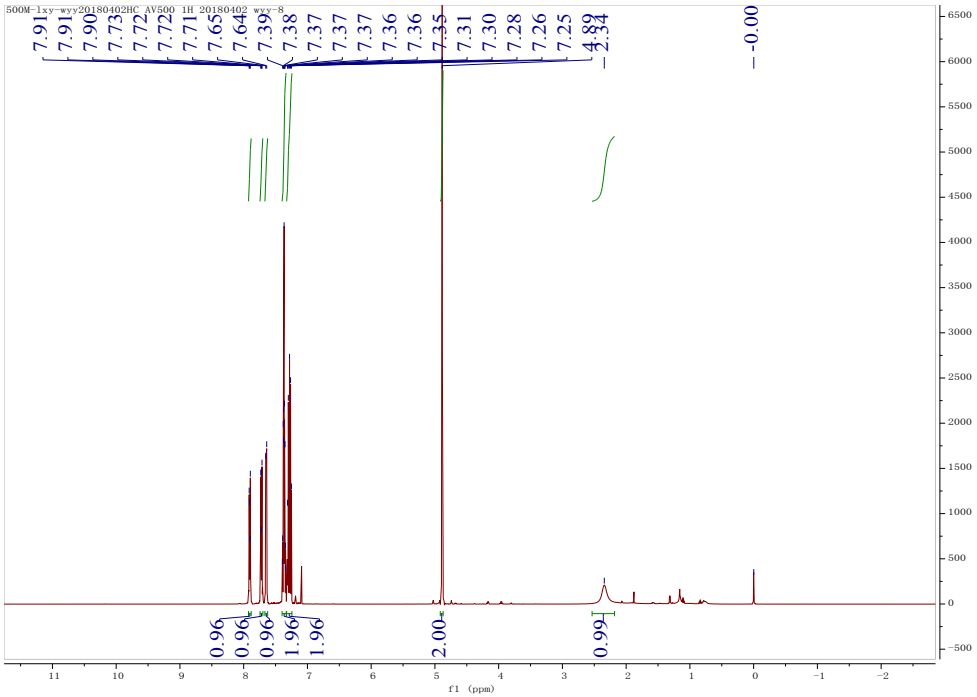


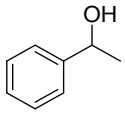
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.20–6.78 (m, *Ar*, 4H), 4.50 (s, CH_2, 2H), 3.72 (s, OCH_3, 3H), 1.91 (s, O*H*, 1H).



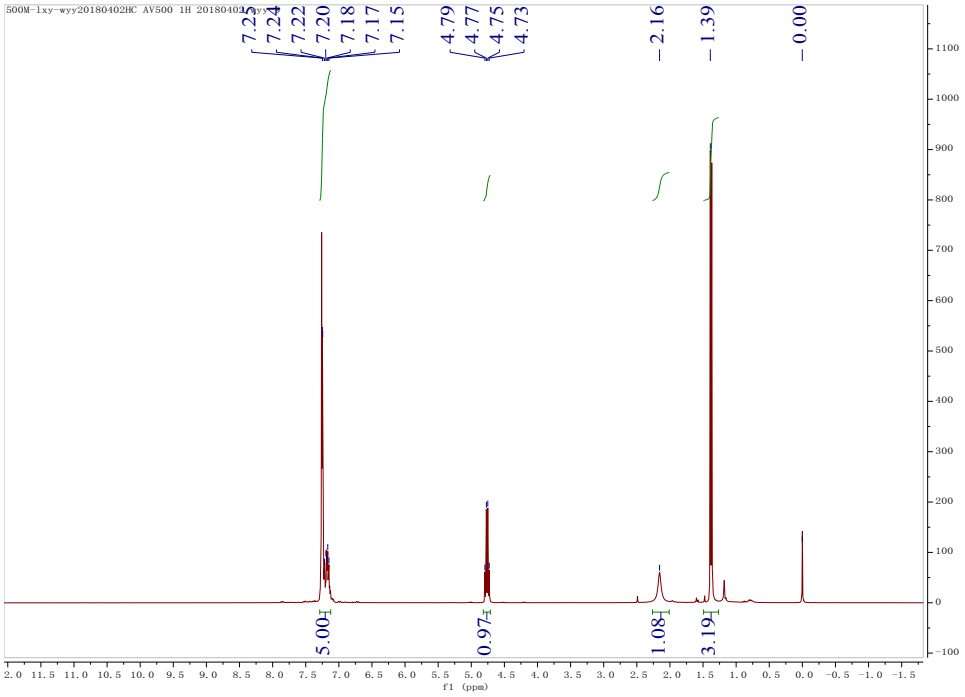


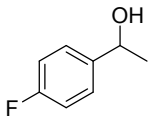
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.91–7.25 (m, *Ar*, 7H), 4.89 (s, CH_2, 2H), 2.34 (s, O*H*, 1H).



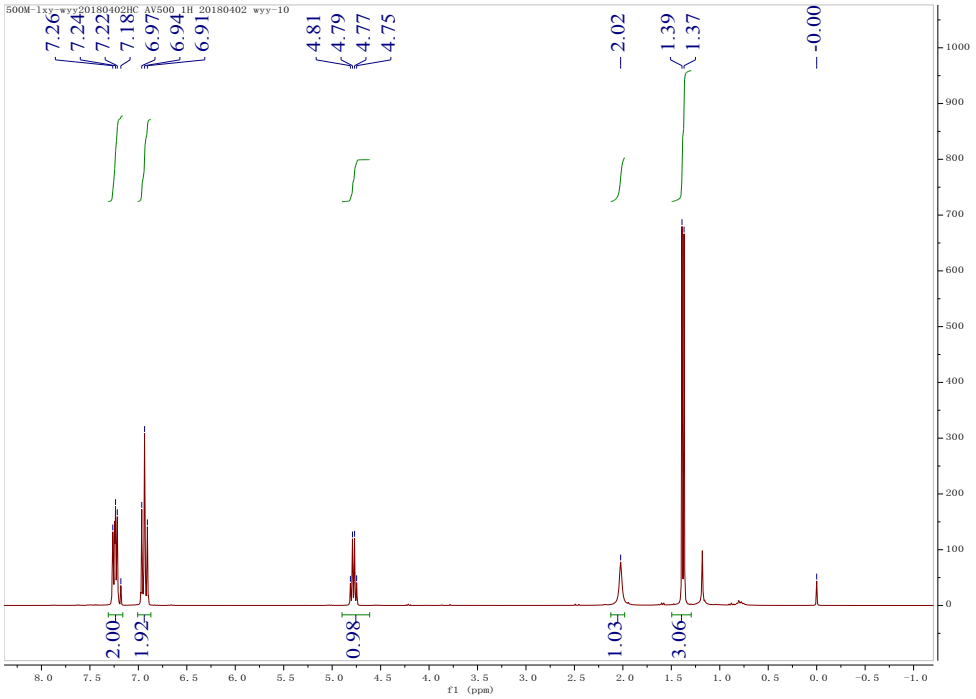


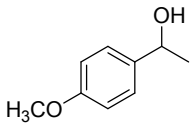
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.25–7.15 (m, *Ar*, 5H), 4.75 (q, C*H*, 1H), 2.16 (s, O*H*, 1H), 1.39 (d, CH_3, 3H).



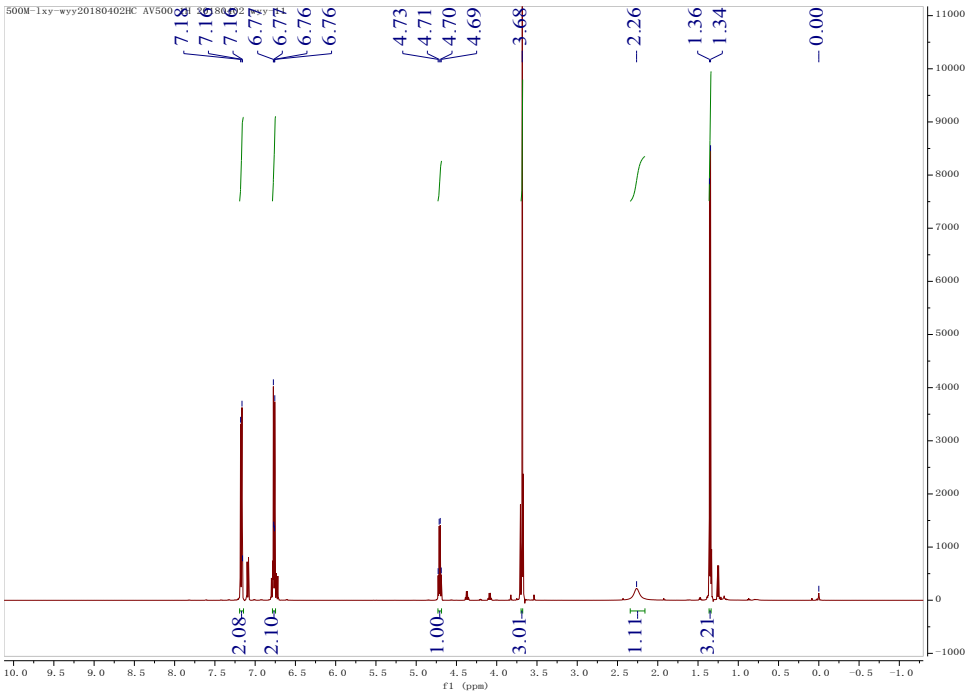


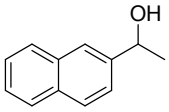
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.26–6.91 (m, *Ar*, 4H), 4.77 (q, C*H*, 1H), 2.02 (s, O*H*, 1H), 1.37 (d, CH_3, 3H).



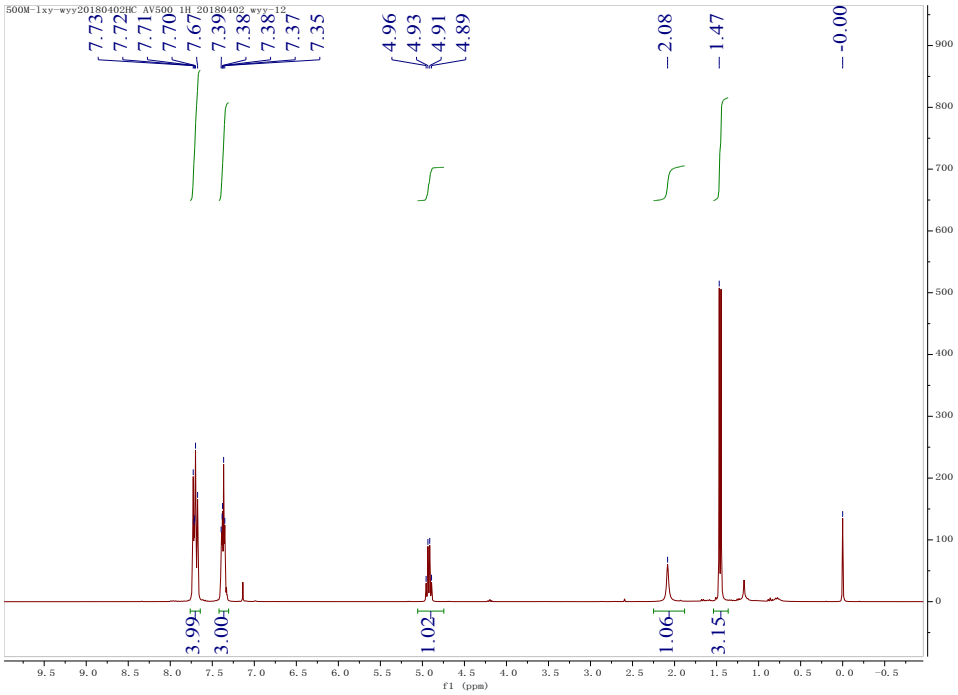


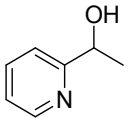
^{1}H NMR (500 MHz, $CDCl_3$, *δ*): 7.18–6.76 (m, *Ar*, 4H), 4.70 (q, C*H*, 1H), 3.68 (s, OCH_3, 3H)，2.26 (s, O*H*, 1H), 1.35 (d, CH_3, 3H).



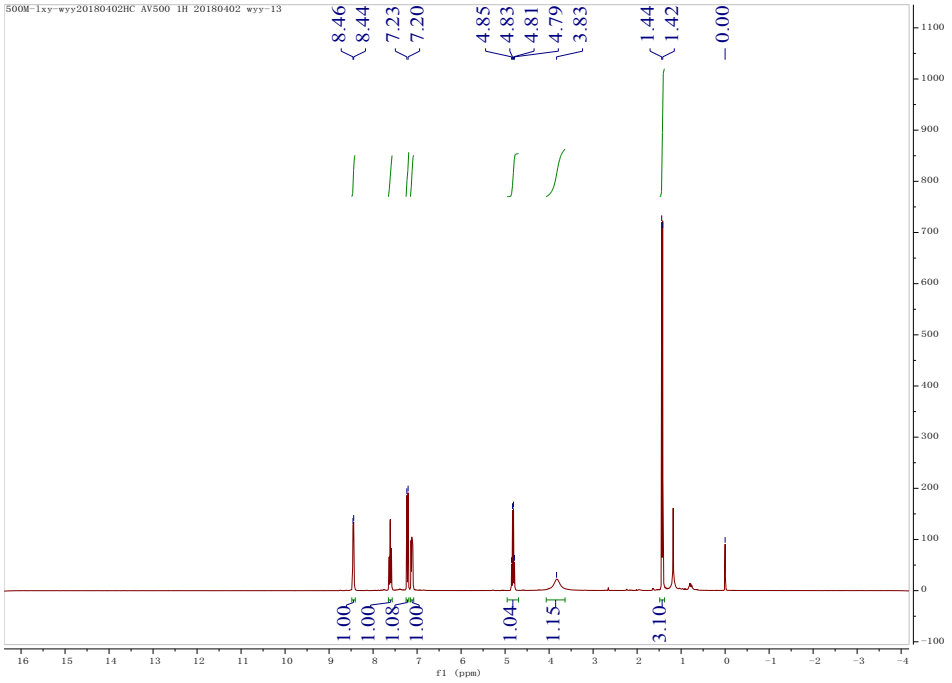


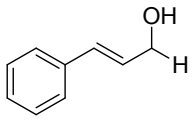
^{1}H NMR (500 MHz, $CDCl_3$, *δ*): 7.73–7.35 (m, *Ar*, 7H), 4.91 (q, C*H*, 1H), 2.06 (s, O*H*, 1H)，1.47 (d, CH_3, 3H).



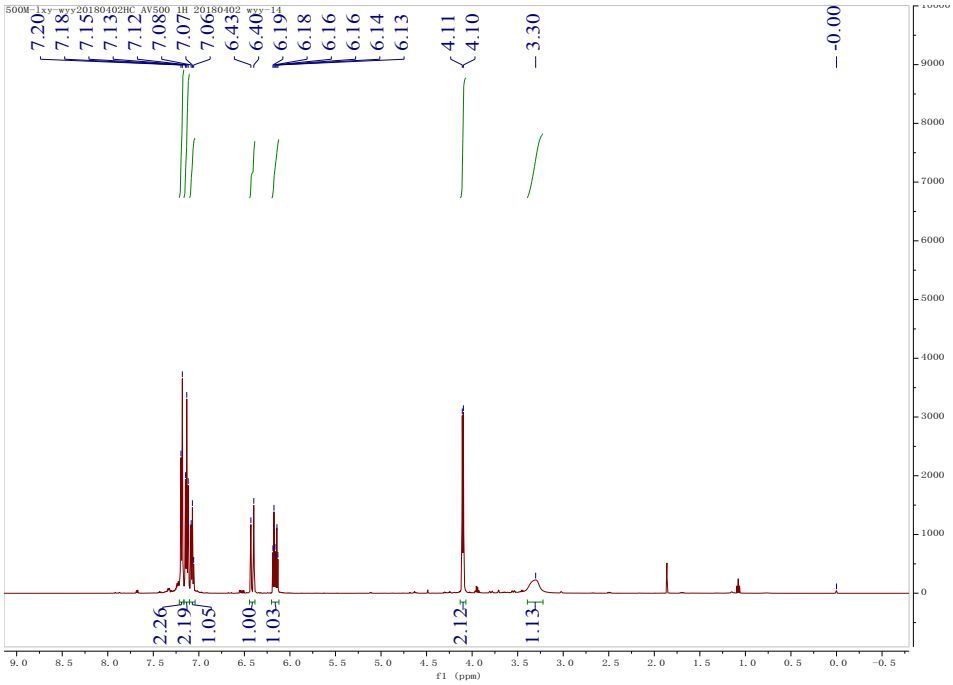


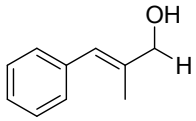
^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.46–7.20 (m, *Ar*, 4H), 4.85-4.79 (q, C*H*, 1H), 3.83 (s, O*H*, 1H) ，1.44-1.42 (d, CH_3, 3H) .



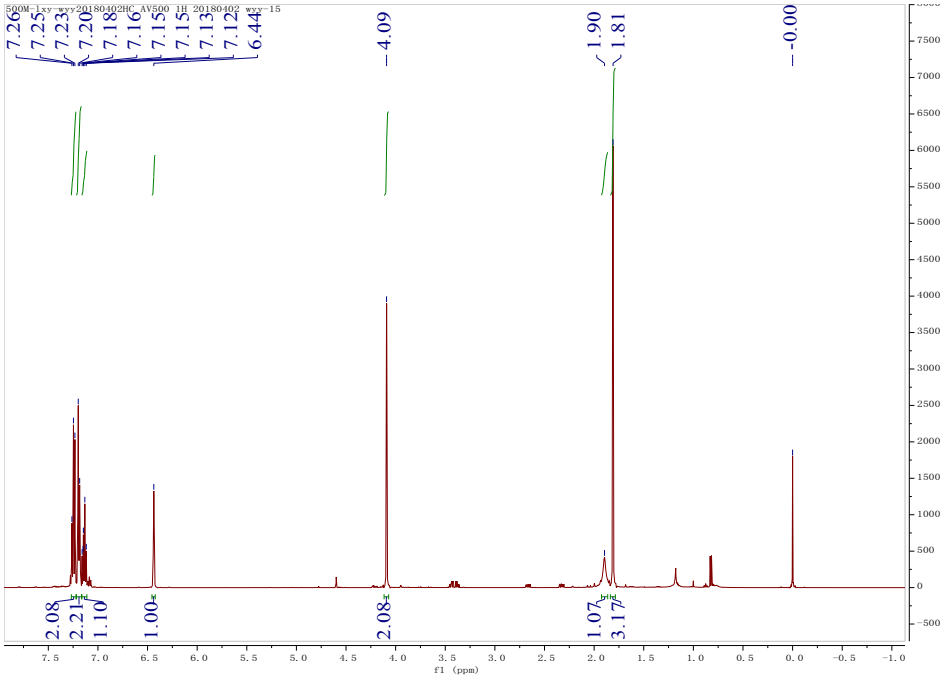


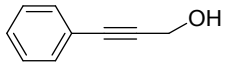
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.20–7.06 (m, *Ar*, 5H), 6.41 (d, *H*C=C, 1H), 6.16 (m, C=C*H*, 1H), 4.10 (dd, CH_2, 2H), 3.30 (s, O*H*, 1H).



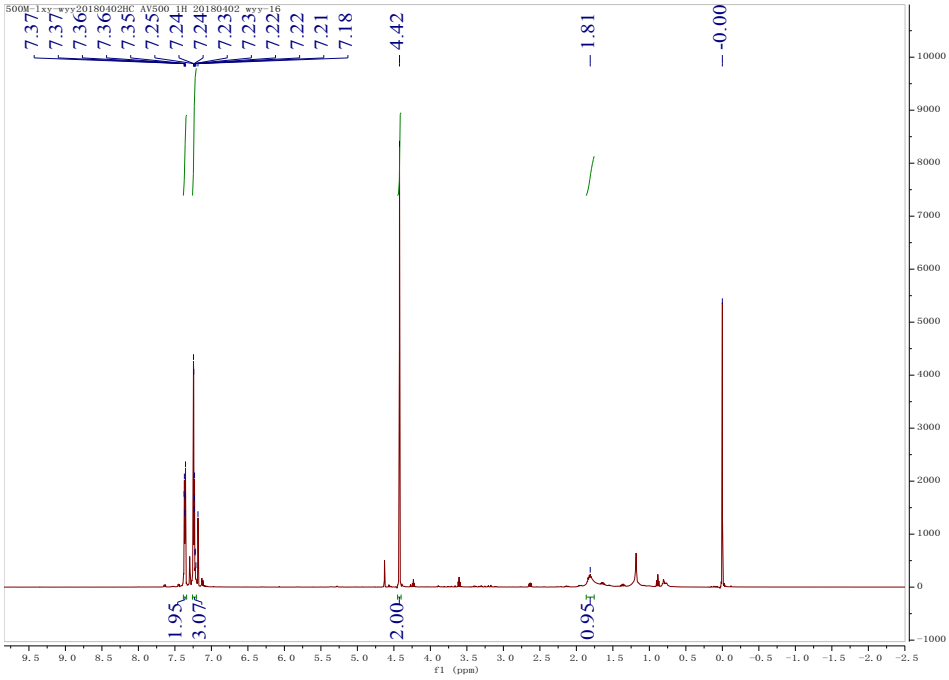


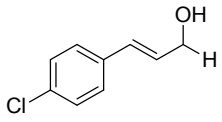
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.26-7.12 (m, *Ar*, 5H), 6.44 (d, *H*C=C, 1H), 4.09 (dd, CH_2, 2H), 1.90 (s, O*H*, 1H) ,1.81 (s, CH_3, 3H).



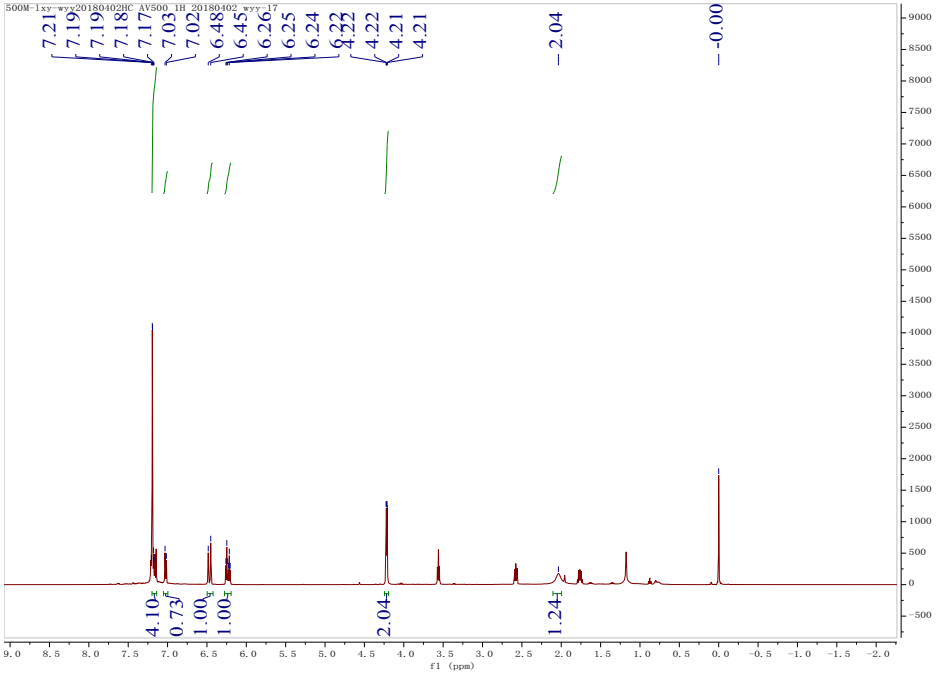


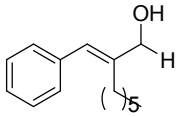
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.37-7.18 (m, *Ar*, 5H), 4.42 (s, CH_2, 2H), 1.81 (s, O*H*, 1H).



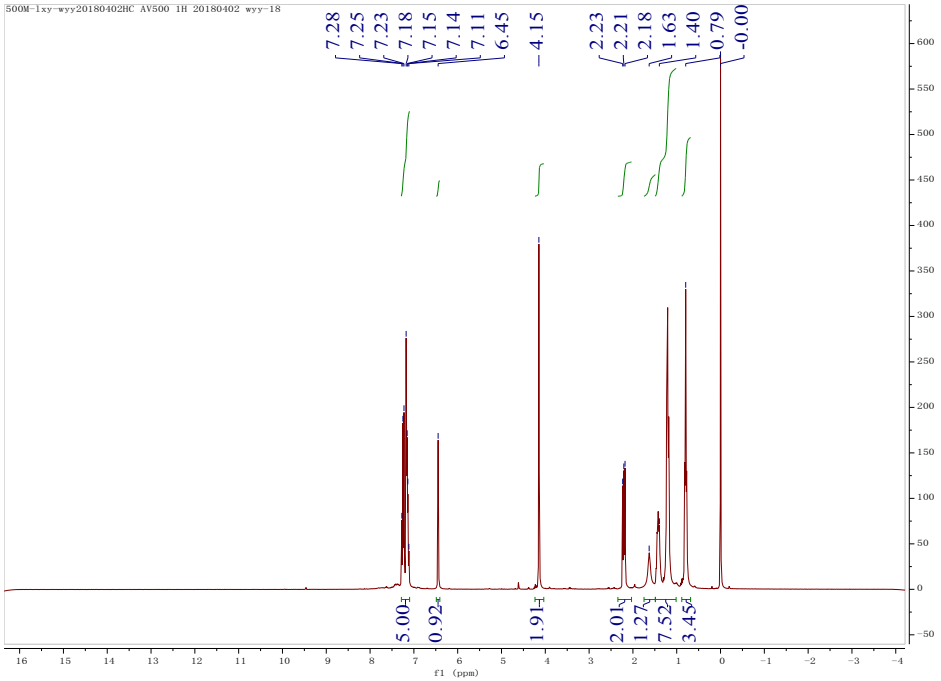


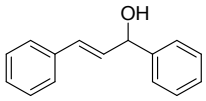
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.21-7.02 (m, *Ar*, 4H), 6.46 (d, *H*C=C, 1H), 6.24 (m, C=C*H*, 1H), 4.21 (dd, CH_2, 2H), 2.04 (s, O*H*, 1H).





^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.28-7.11 (m, *Ar*, 5H), 6.45 (s, *H*C=C, 1H), 4.15 (s, CH_2, 2H), 2.18 (m, CH_2, 2H), 1.63 (s, O*H*, 1H), 1.40 -1.18(m, CH_2, 8H), 0.79 (s, CH_3, 3H).





^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.36-7.10 (m, *Ar*, 5H), 6.50 (dd, *H*C=C, 1H), 6.27 (td, C=CH, 1H), 5.02(t, C*H*, 1H), 1.17 (s, O*H*, 1H).