Supplementary Materials

Steric and electronic effect of Cp-substituents on the structure of the ruthenocene based palladium pincer borohydrides

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Table S1. Crystal data and structure refinement parameters for **3a**, **3b**.

	3a	**3b**
Empirical formula	$C_{33}H_{58}BF_3P_2PdRu$	$C_{33}H_{61}BP_2PdRu$
Formula weight	792.01	738.03
Crystal system	Monoclinic	Orthorhombic
Space group	$P2_1/c$	$P2_12_12_1$
a, Å	18.5494(6)	11.3765(5)
b, Å	12.0953(4)	15.0316(6)
c, Å	15.8197(5)	21.0022(9)
α, °	90	90
β, °	90.2560(10)	90
γ, °	90	90
V, $Å^3$	3549.3(2)	3591.5(3)
Z	4	4
D_{calc} ($g \cdot cm^{-3}$)	1.482	1.365
μ(cm^{-1})	10.59	10.30
F(000)	1632	1536
$2\Theta_{max}$, °	58	58
Reflections measured	72725	36743
Independent reflections	9442	9578
Observed reflections [I > 2σ(I)]	8034	8230
R_1	0.0235	0.0394
wR_2	0.0535	0.0729
GOF	1.023	1.009

Figure S1. ^{1}H NMR spectrum (400.13 MHz) of **2a** in $CDCl_3$.

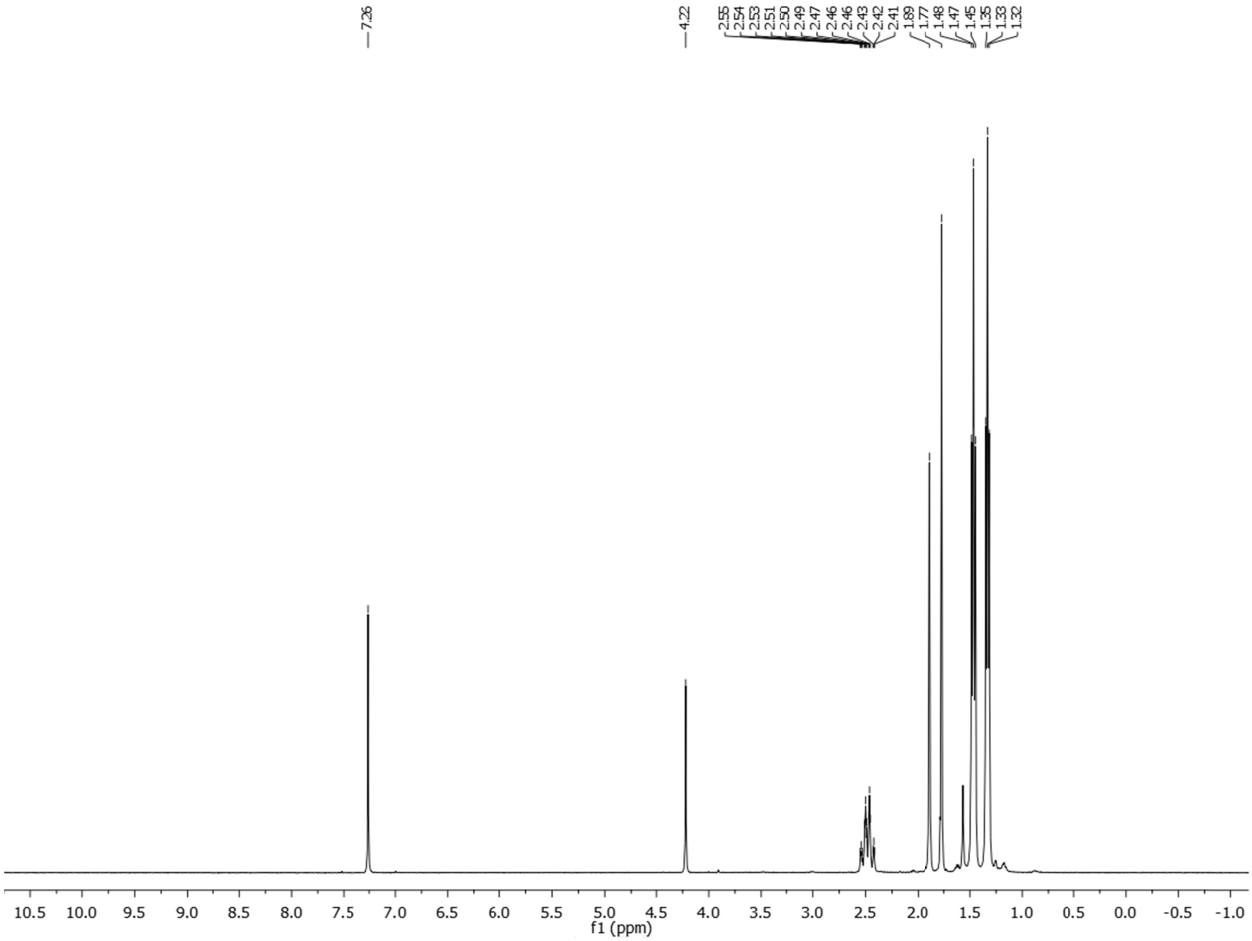

Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum (161.98 MHz) of **2a** in $CDCl_3$.

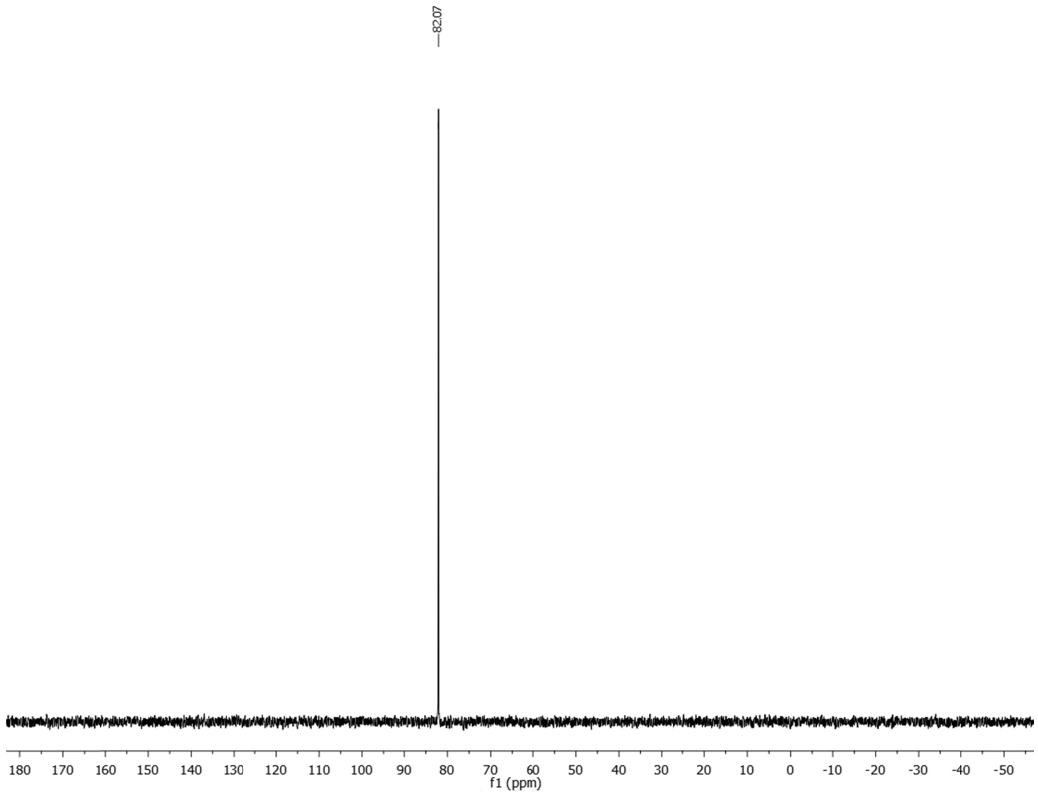

Figure S3. ^{19}F NMR spectrum (376.50 MHz) of **2a** in $CDCl_3$.

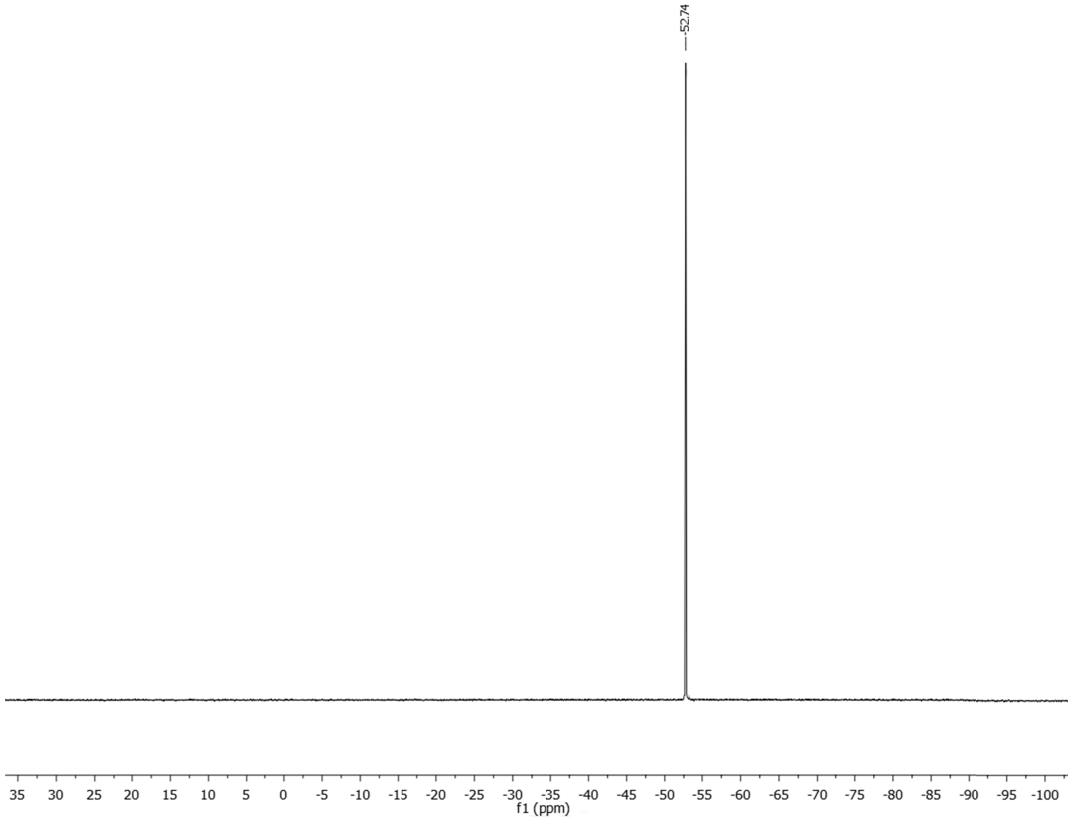

Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum (150.93 MHz) of **2a** in $CDCl_3$.

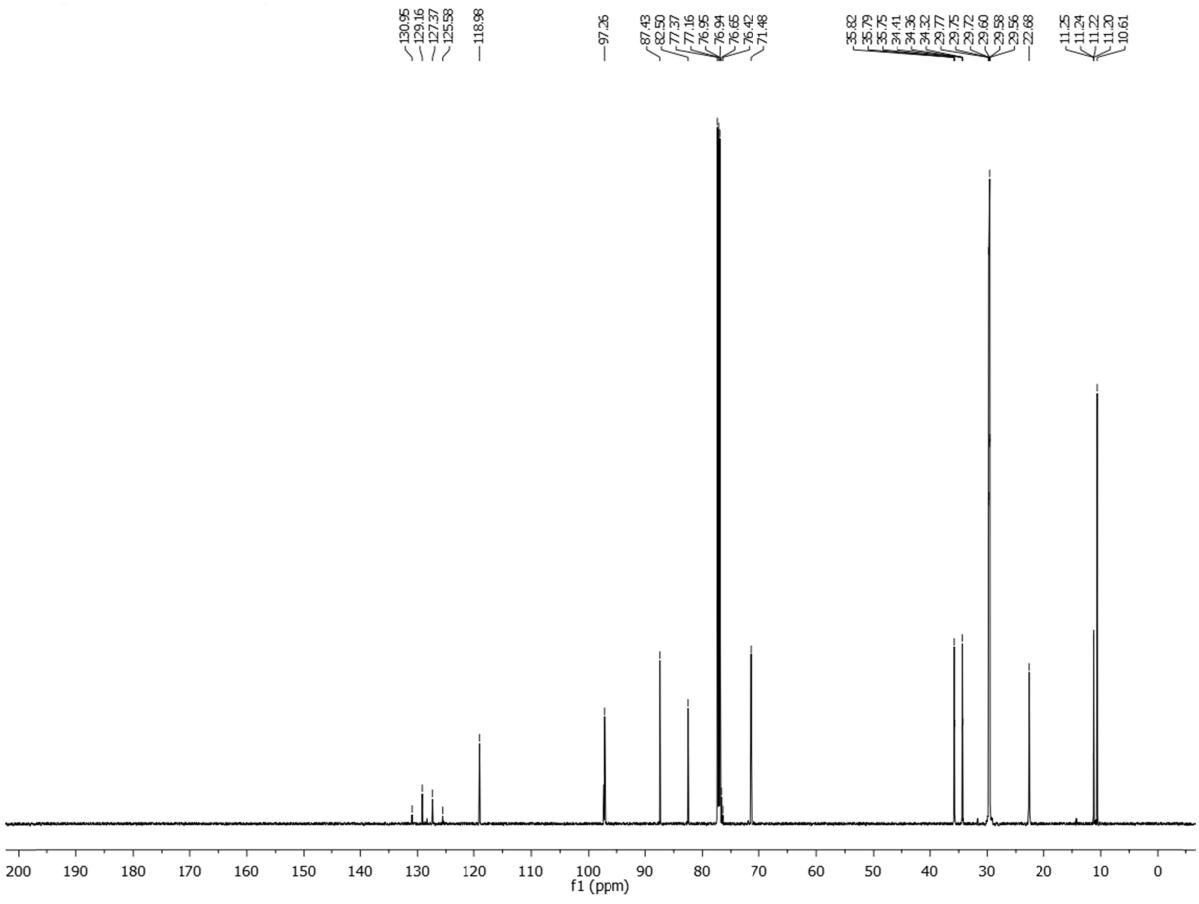

Figure S5. ^{1}H NMR spectrum (400.13 MHz) of **3a** in C_6D_6.

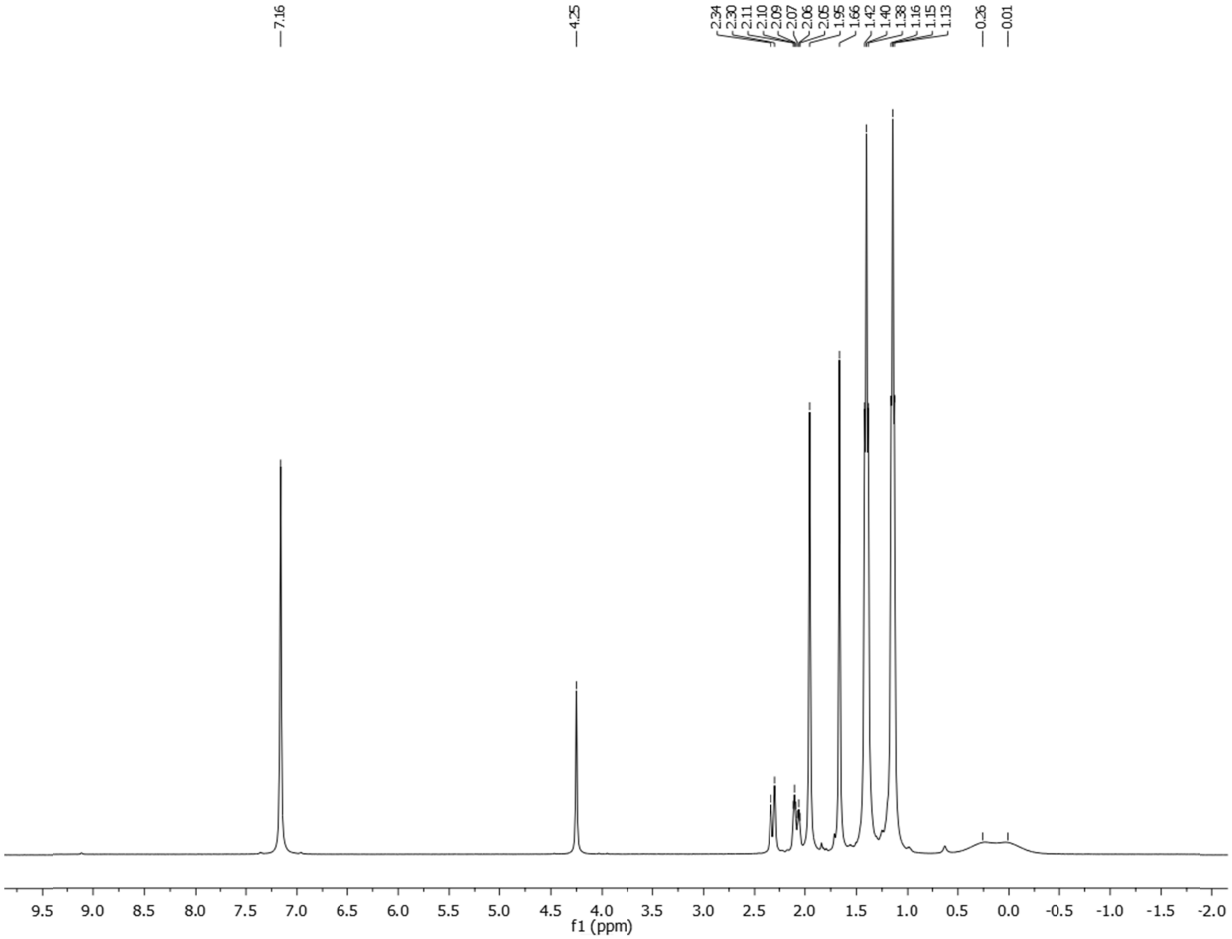

Figure S6. $^{11}B\{^{1}H\}$ NMR spectrum (128.38 MHz) of **3a** in C_6D_6.

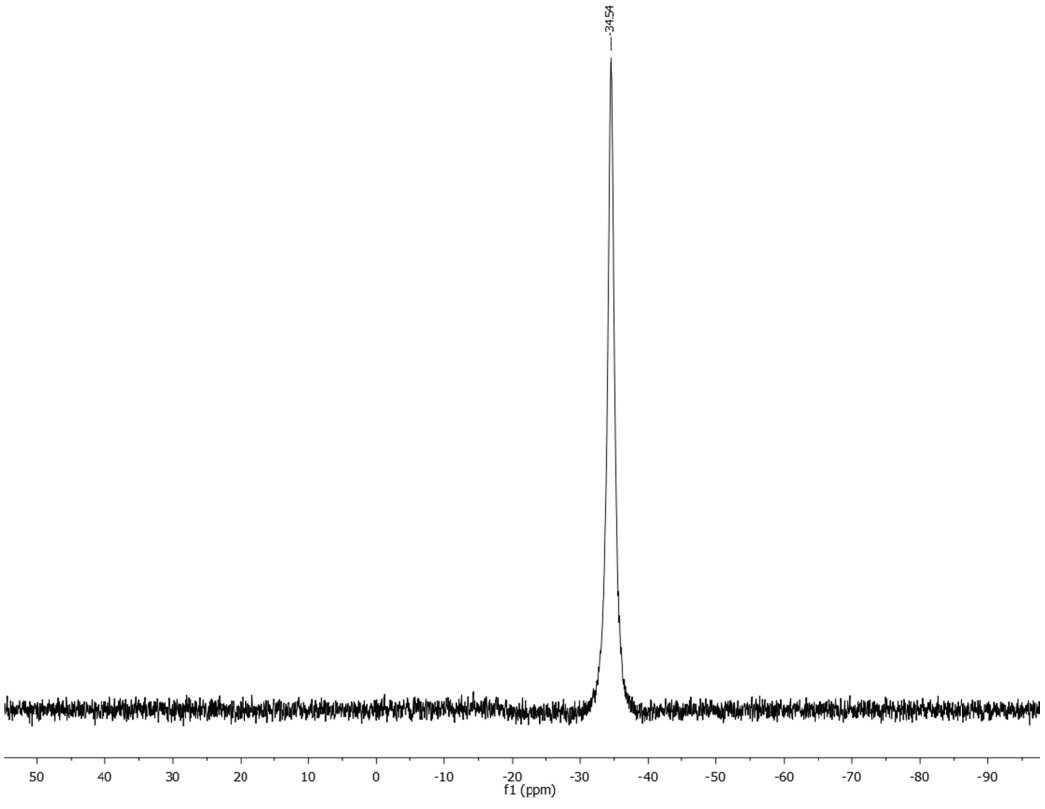

Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum (121.49 MHz) of **3a** in C_6D_6.

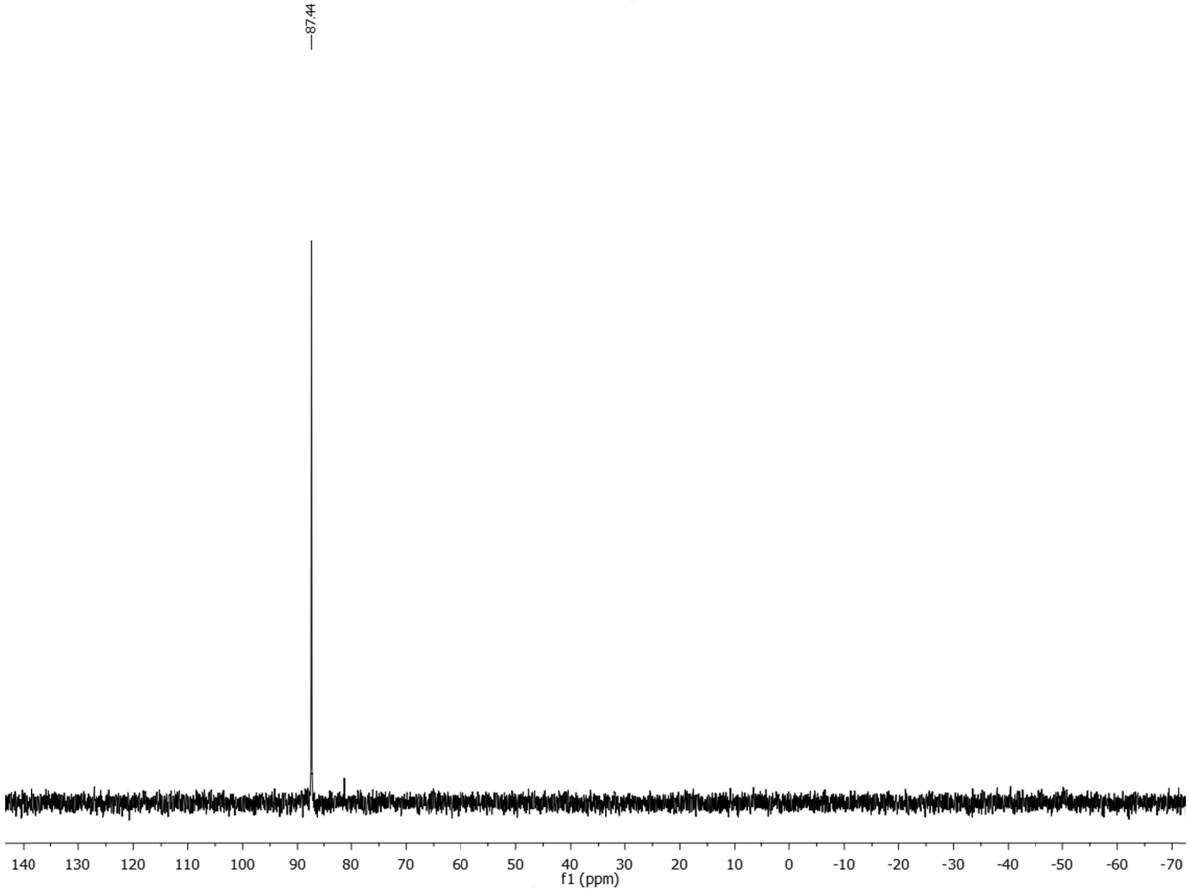

Figure S8. ^{19}F NMR spectrum (376.50 MHz) of **3a** in C_6D_6.

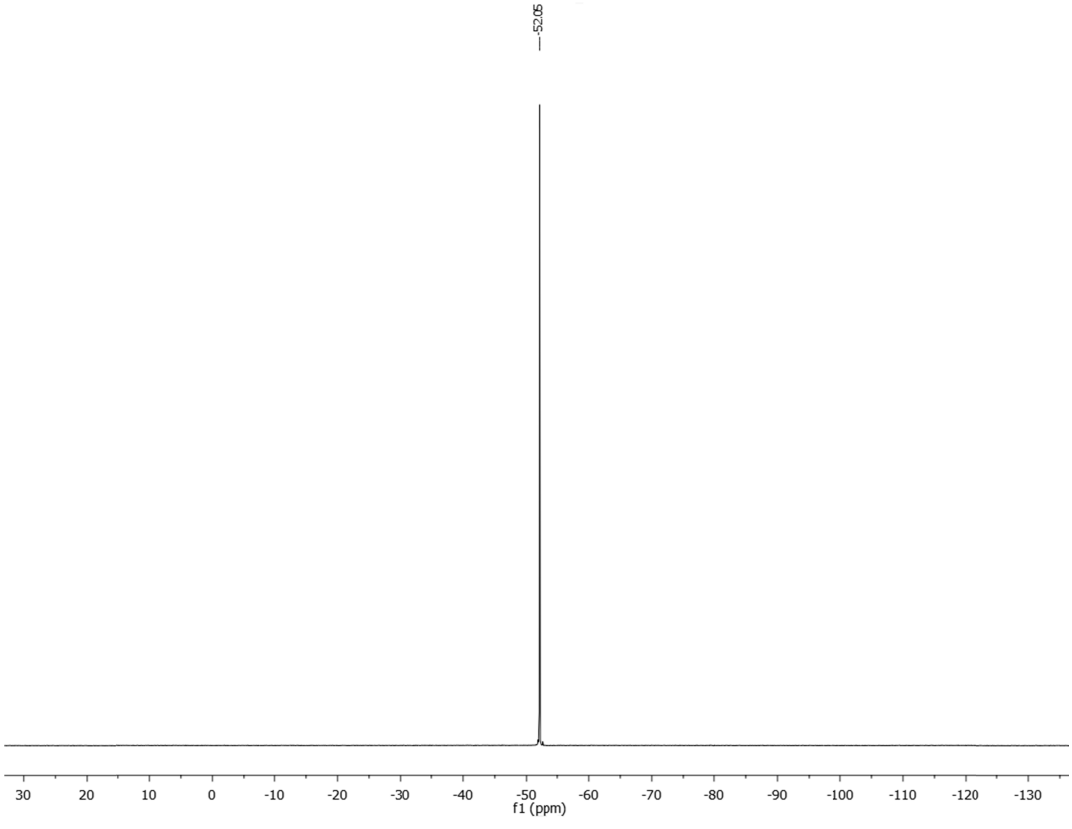

Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum (150.93 MHz) of **3a** in C_6D_6.

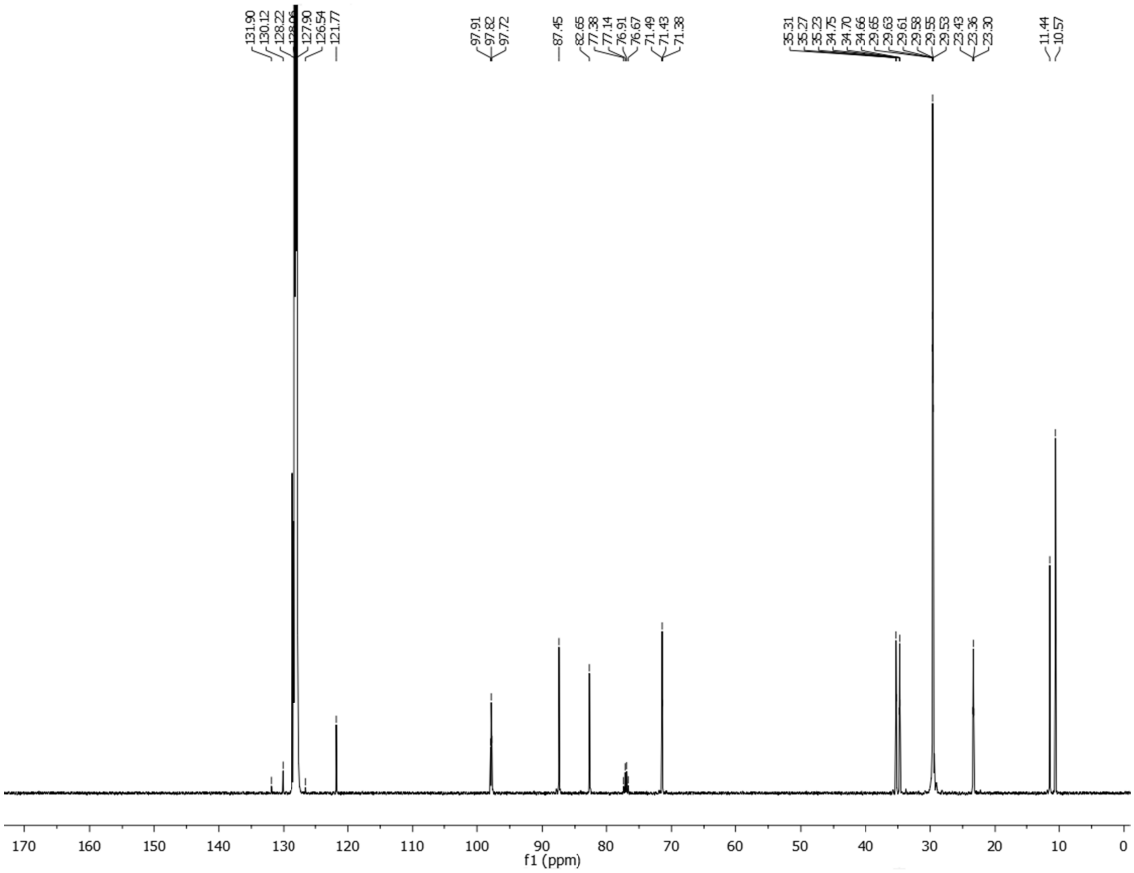

Figure S10. ^{1}H NMR spectrum (400.13 MHz) of **3b** in C_6D_6.

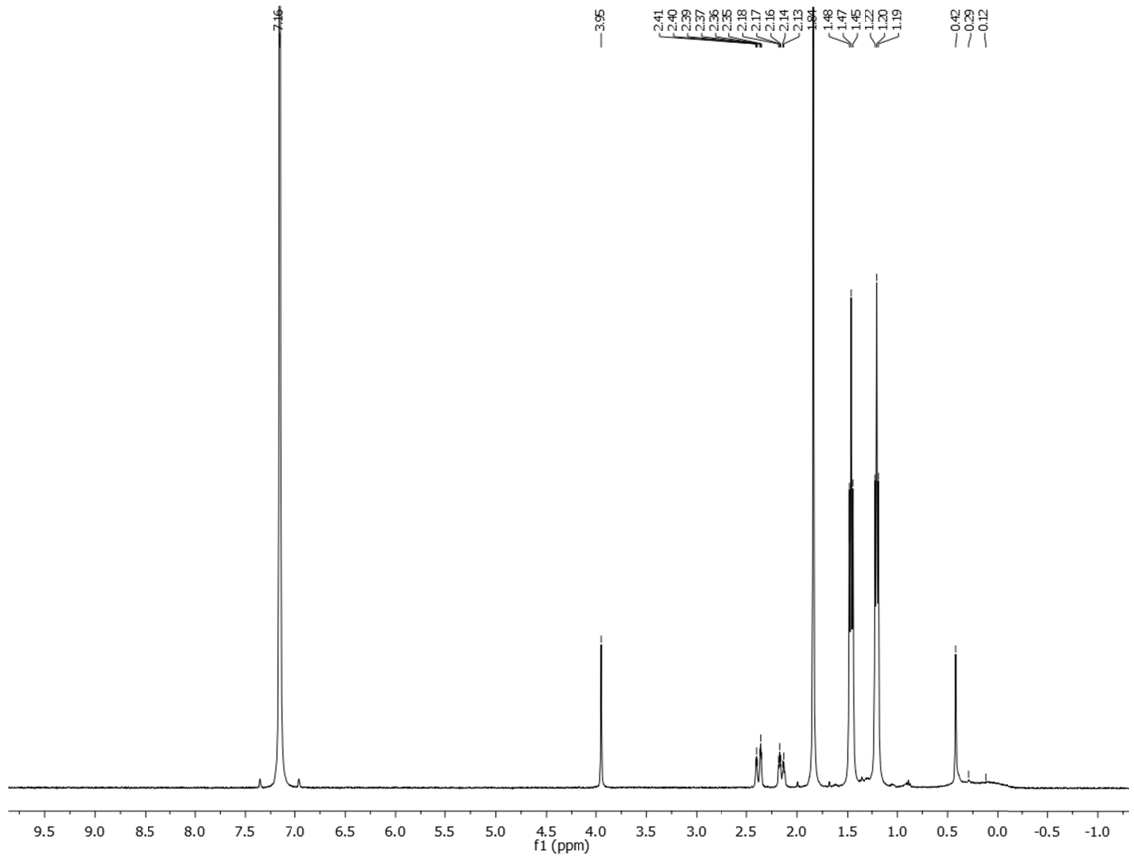

Figure S11. $^{11}B\{^{1}H\}$ NMR spectrum (128.38 MHz) of **3b** in C_6D_6.

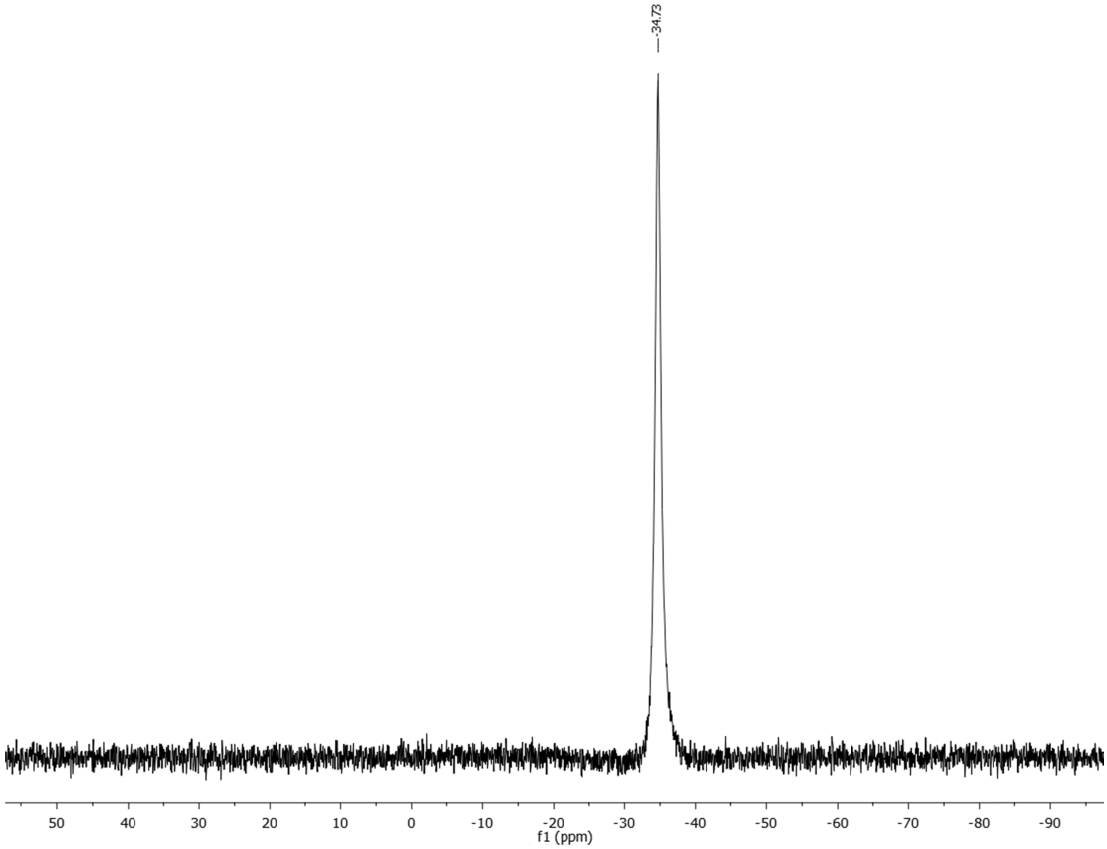

Figure S12. $^{31}P\{^{1}H\}$ NMR spectrum (161.98 MHz) of **3b** in C_6D_6.

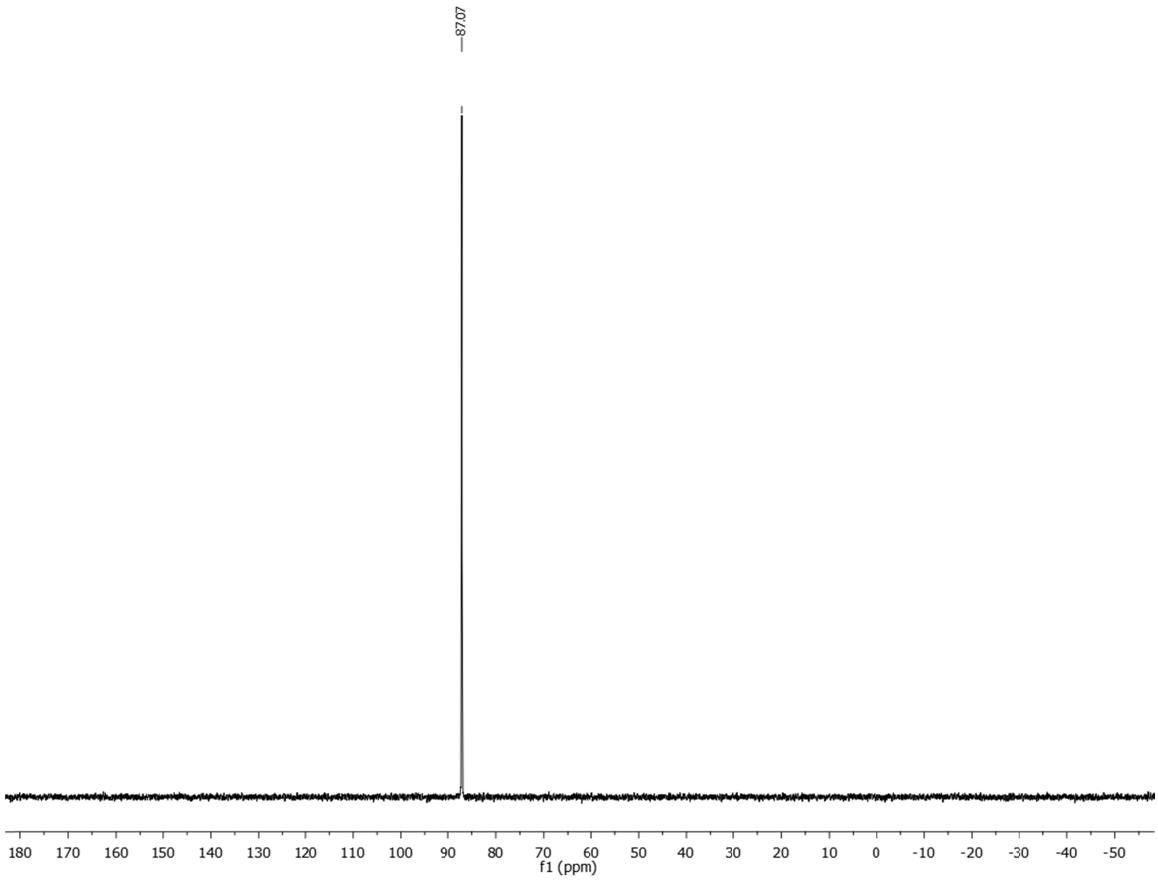

Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum (150.93 MHz) of **3b** in C_6D_6.

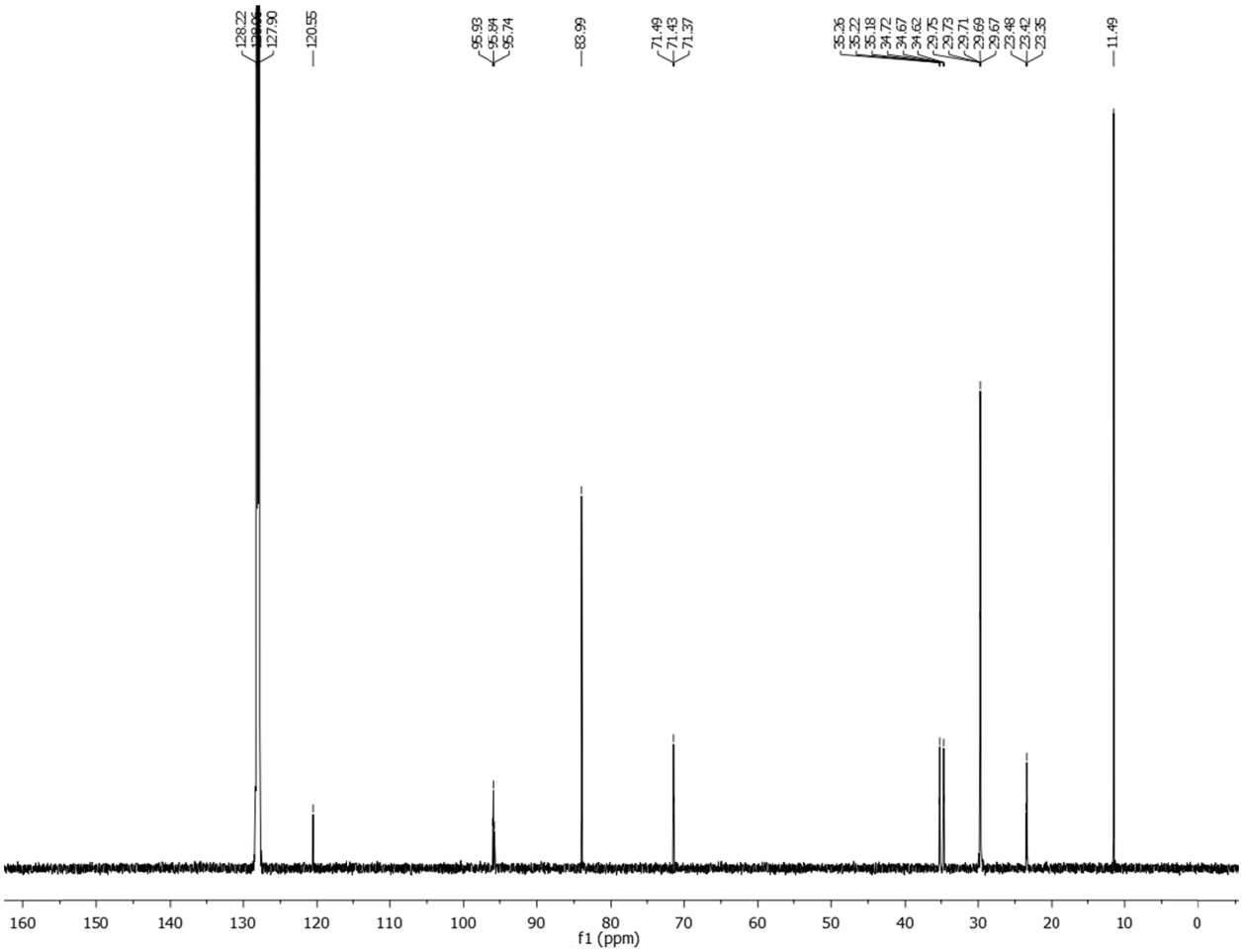

Figure S14. FTIR spectra of **3a** in KBr pellet.

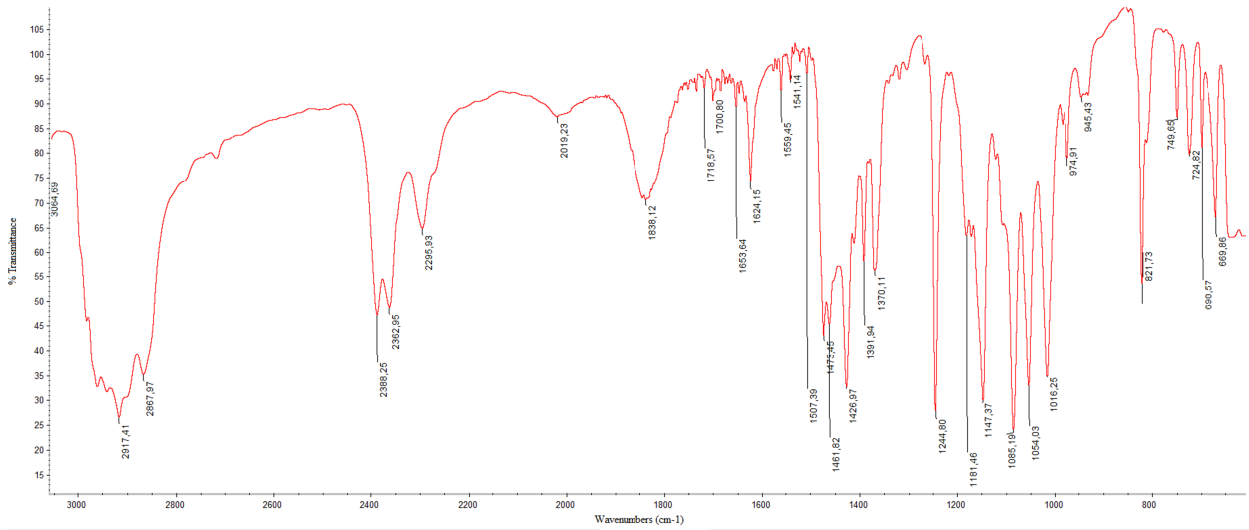

Figure S15. FTIR spectra of **3b** in KBr pellet.

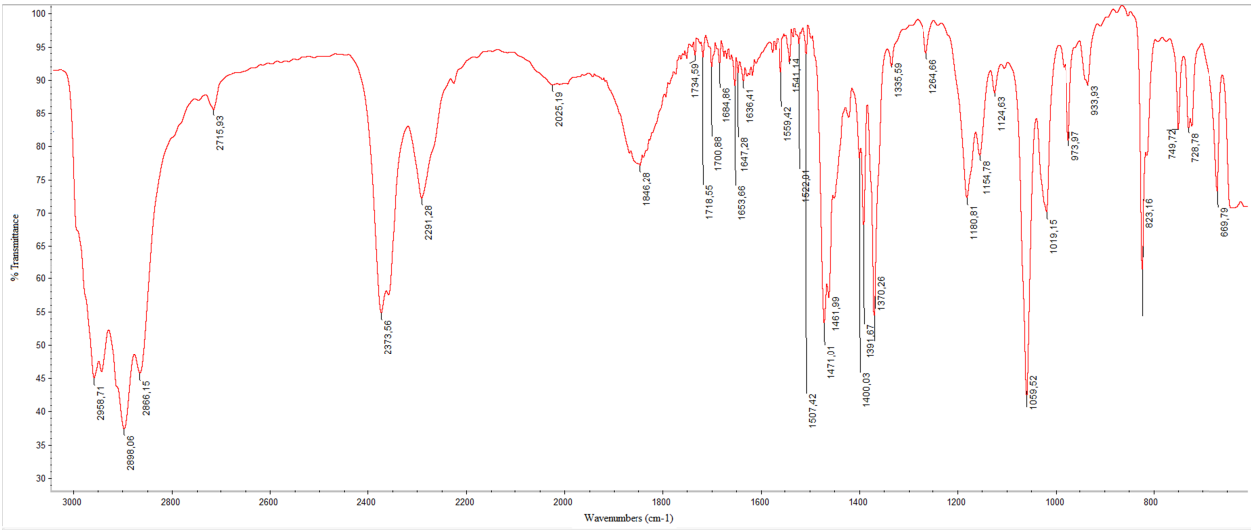

Figure S16. FTIR spectra of **3a** solution in CH_2Cl_2 (c = 0.01 M).

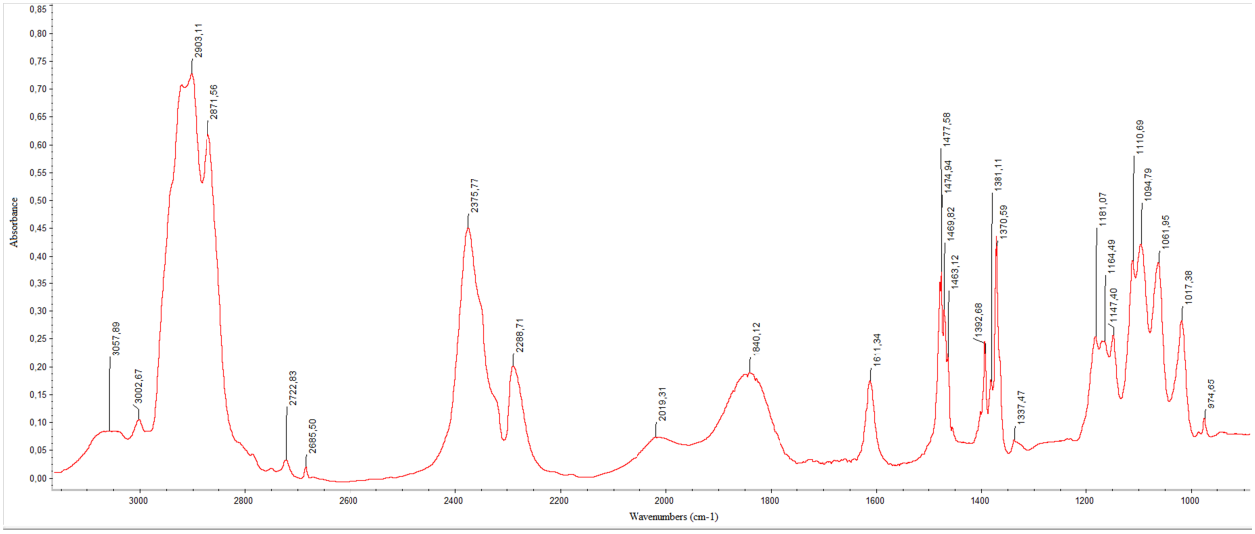

Figure S17. FTIR spectra of **3b** solution in CH_2Cl_2 (c = 0.01 M).