SUPPLEMENTARY INFORMATION (SI)

Convenient hydrogenation of furfural to furfuryl alcohol in metal-catalyzed and organo-catalyzed environments

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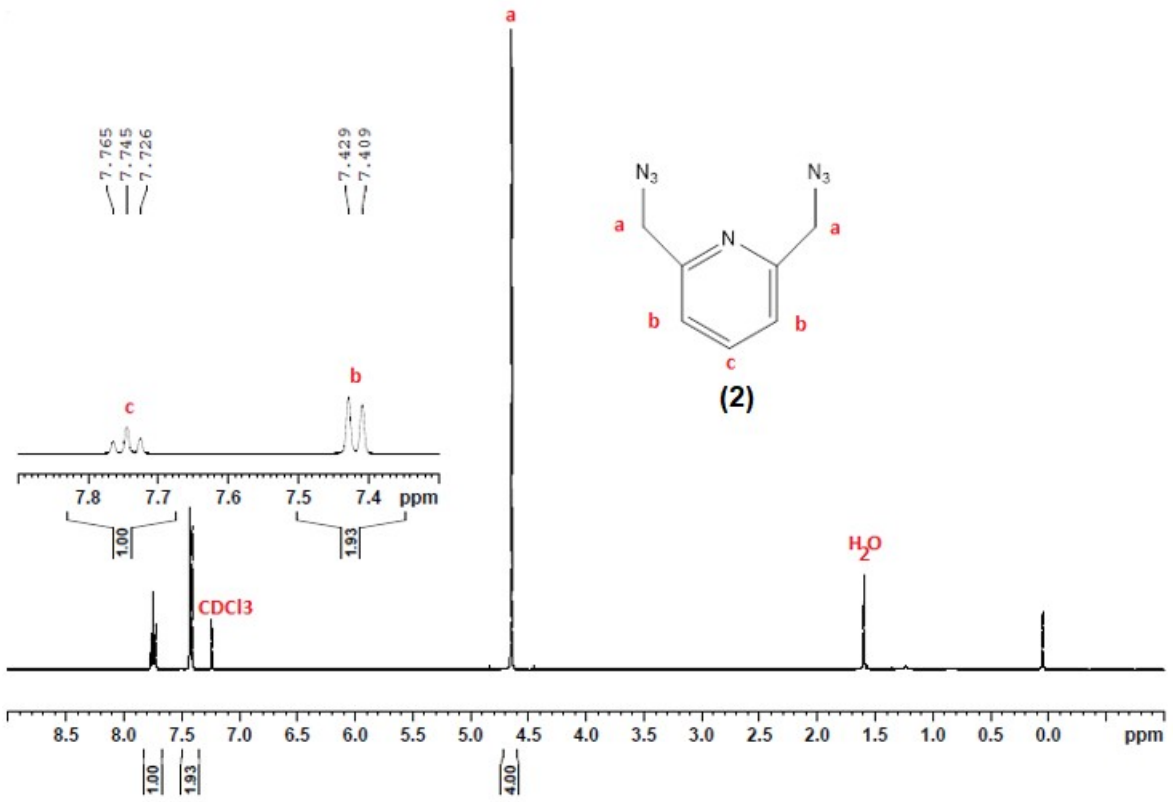
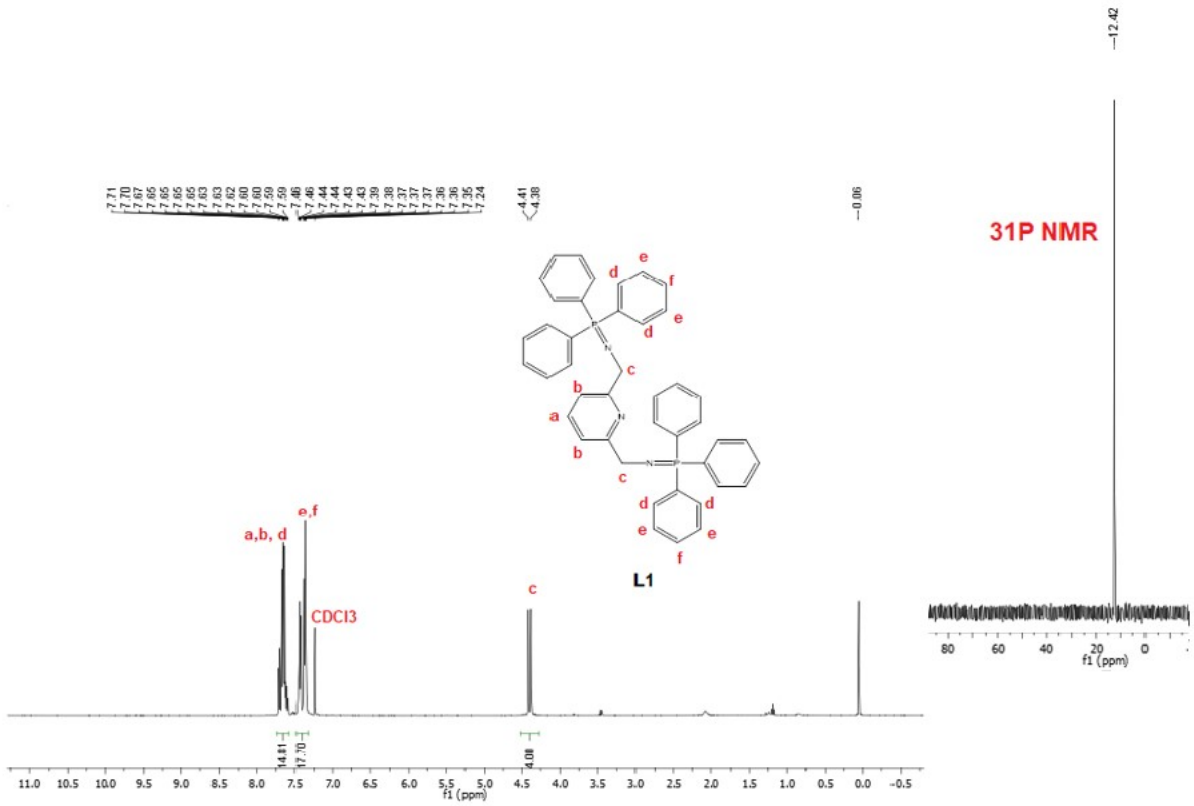
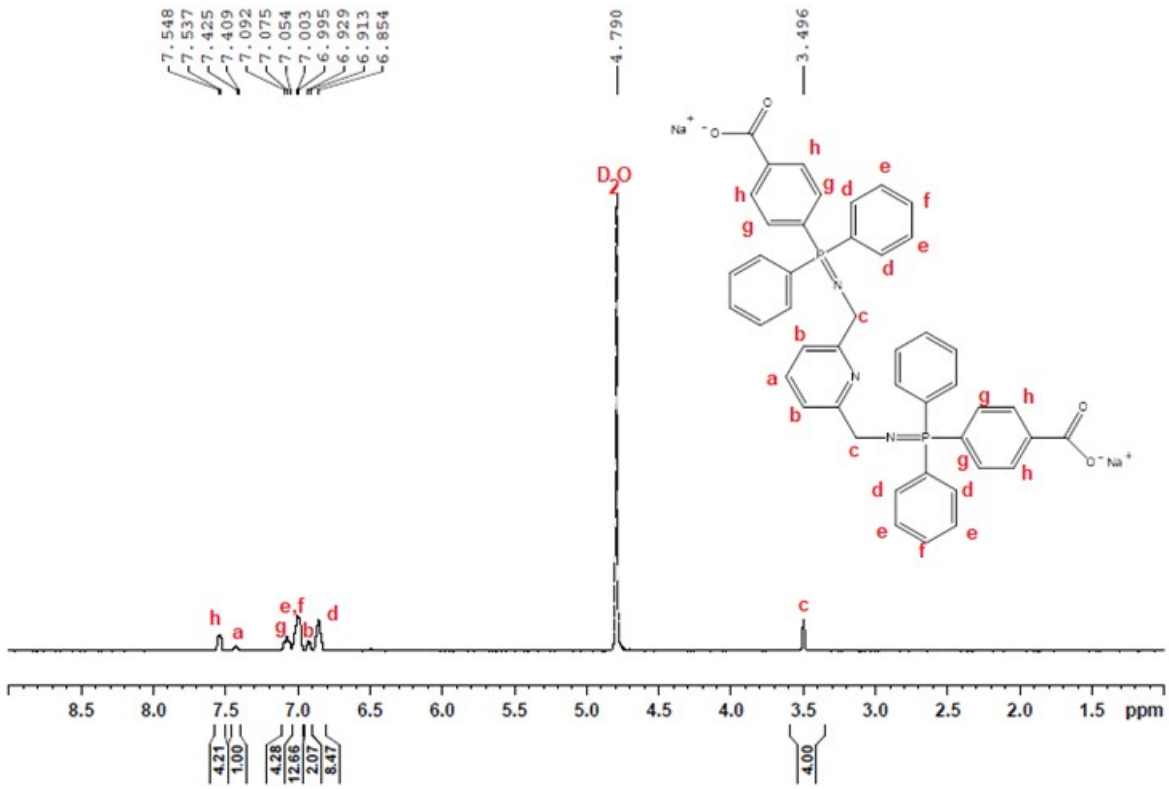


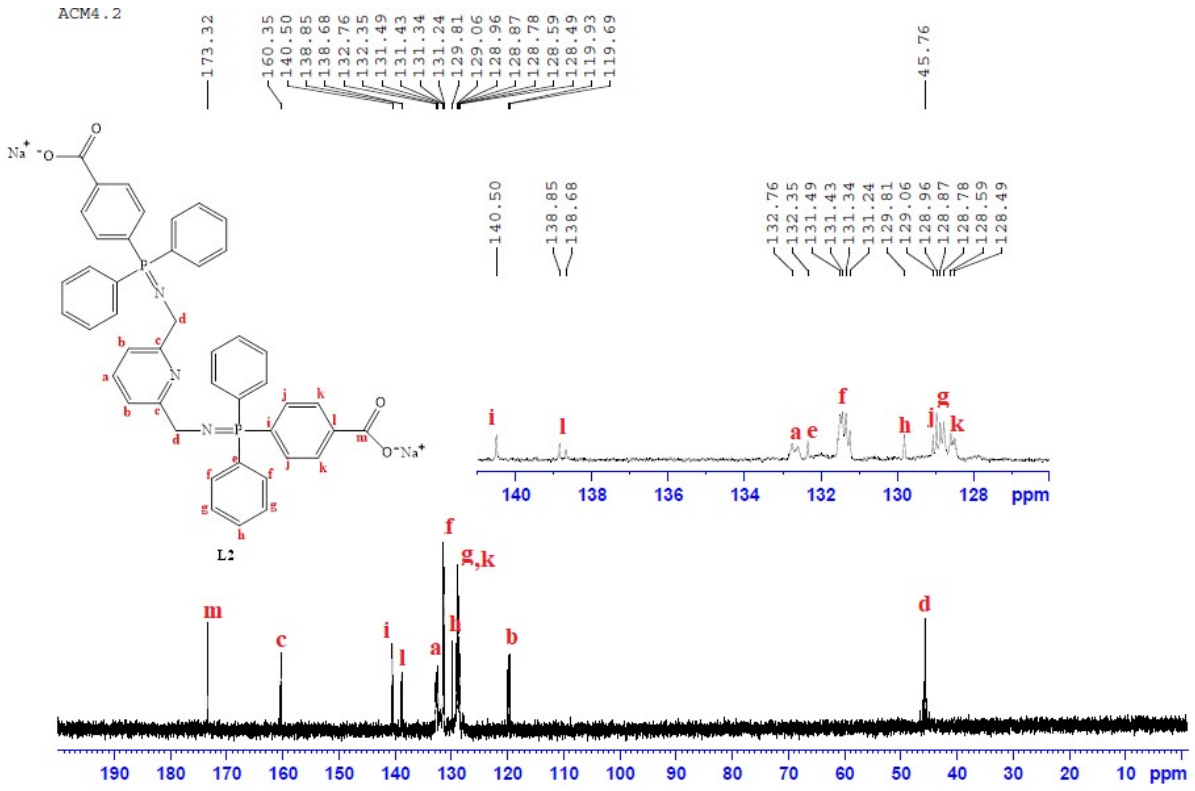
SI-Figure 1: The ^{1}H NMR of **(2)** was recorded in $CDCl_3$ at 25 °C.



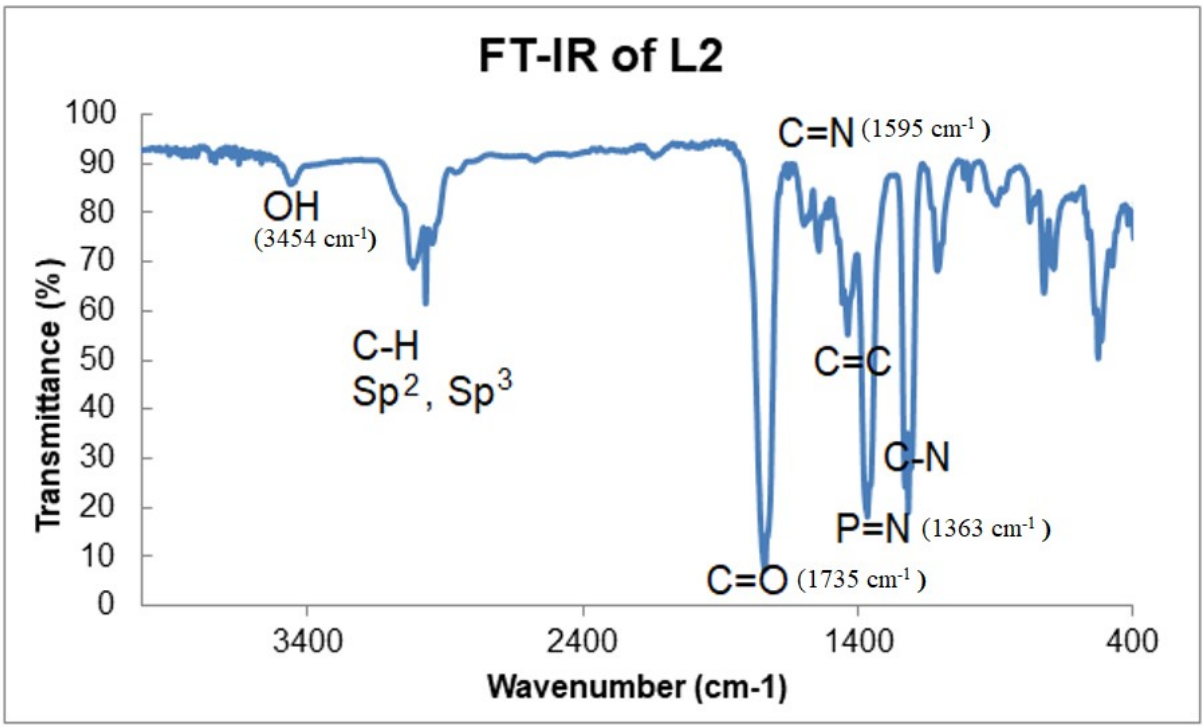
SI-Figure 2: The ^{1}H NMR and ^{31}P NMR for **L1** recorded in $CDCl_3$ at 25 °C.



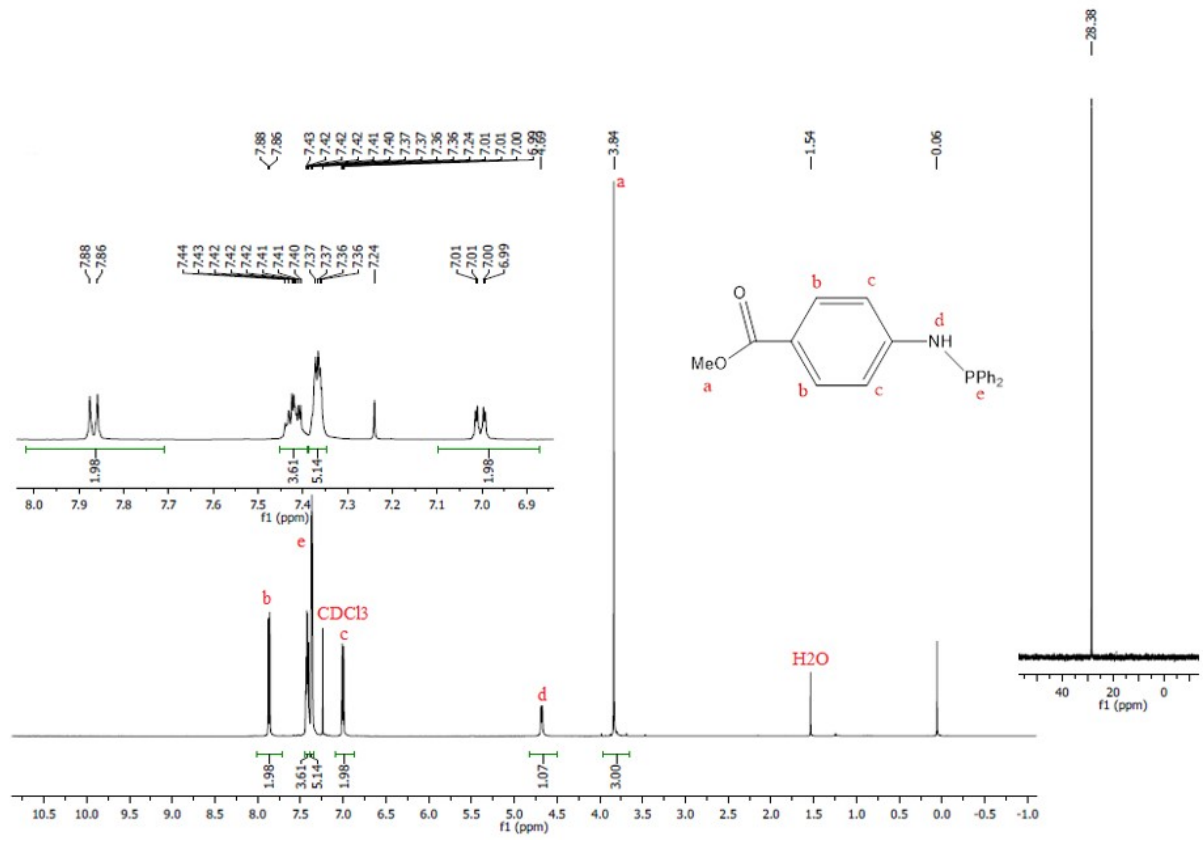
SI-Figure 3: The ^{1}H NMR of **L2** recorded in D_2O and NaOD at 25 °C.



SI-Figure 4: The ^{13}C NMR of **L2** recorded in D_2O and NaOD at 25 °C.

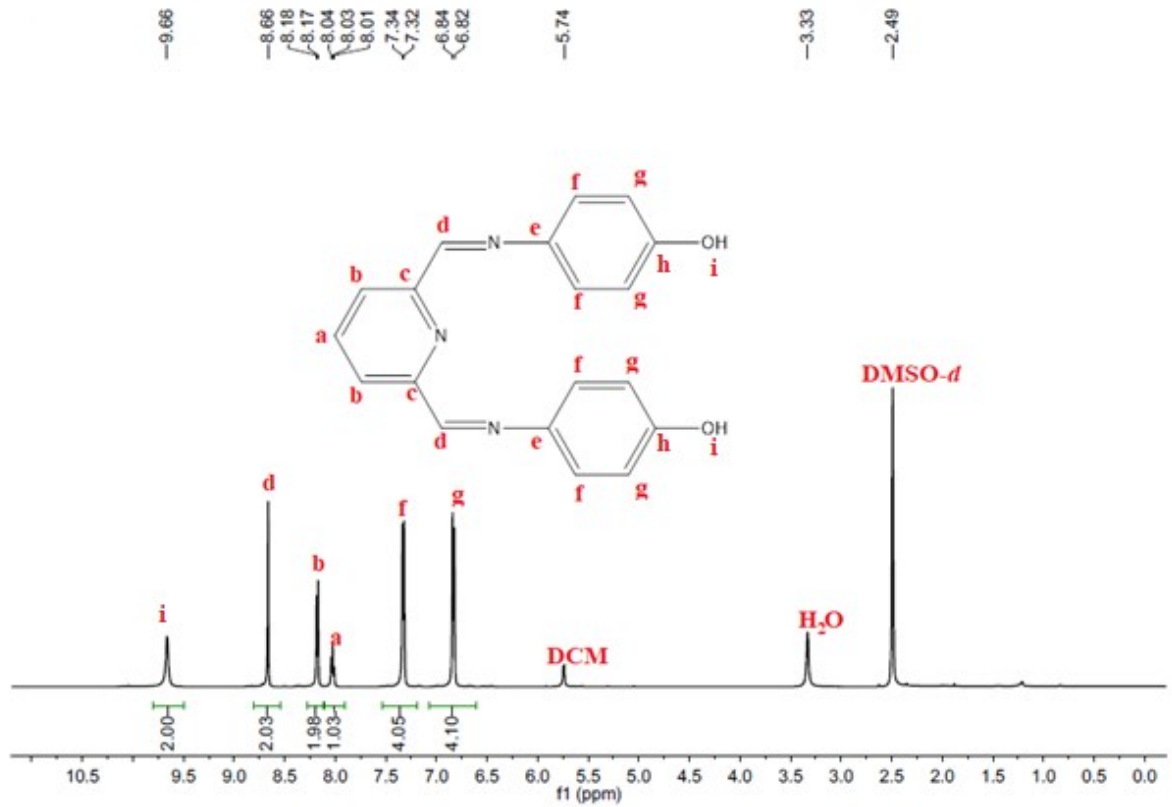


SI-Figure 5: The FT-IR spectroscopy of **L2** recorded.

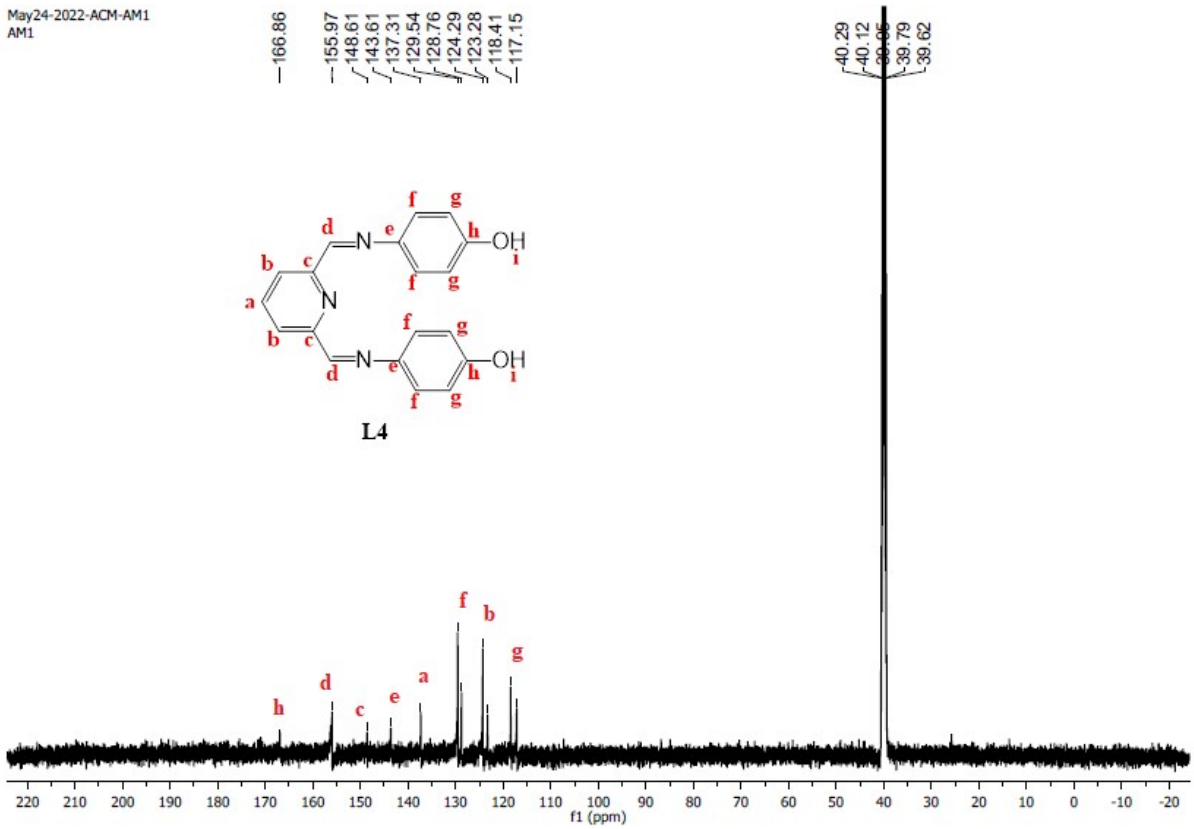


SI-Figure 6, The ^{1}H NMR and ^{31}P NMR for **(4)** were recorded in $CDCl_3$ at 25 °C.

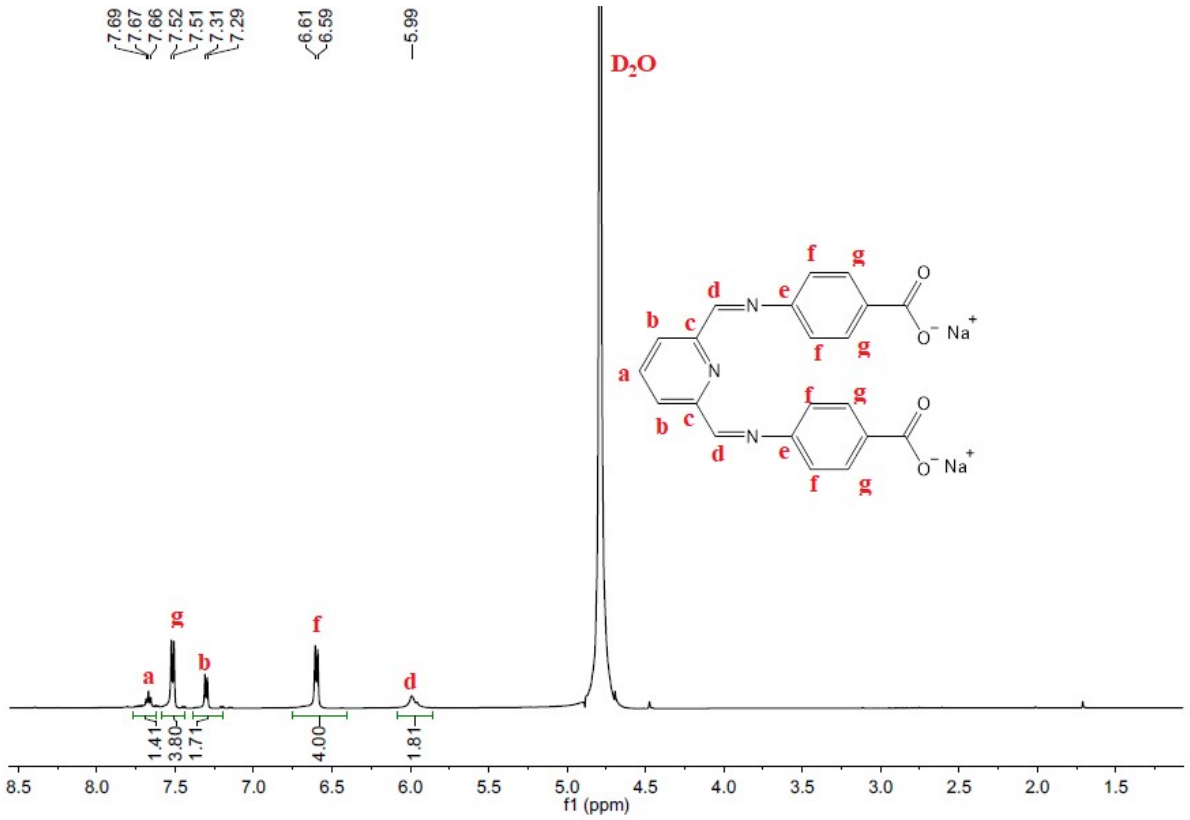
SI-Figure 7. The ^{31}P NMR of **L3** was recorded in $CDCl_3$ at 25 °C.



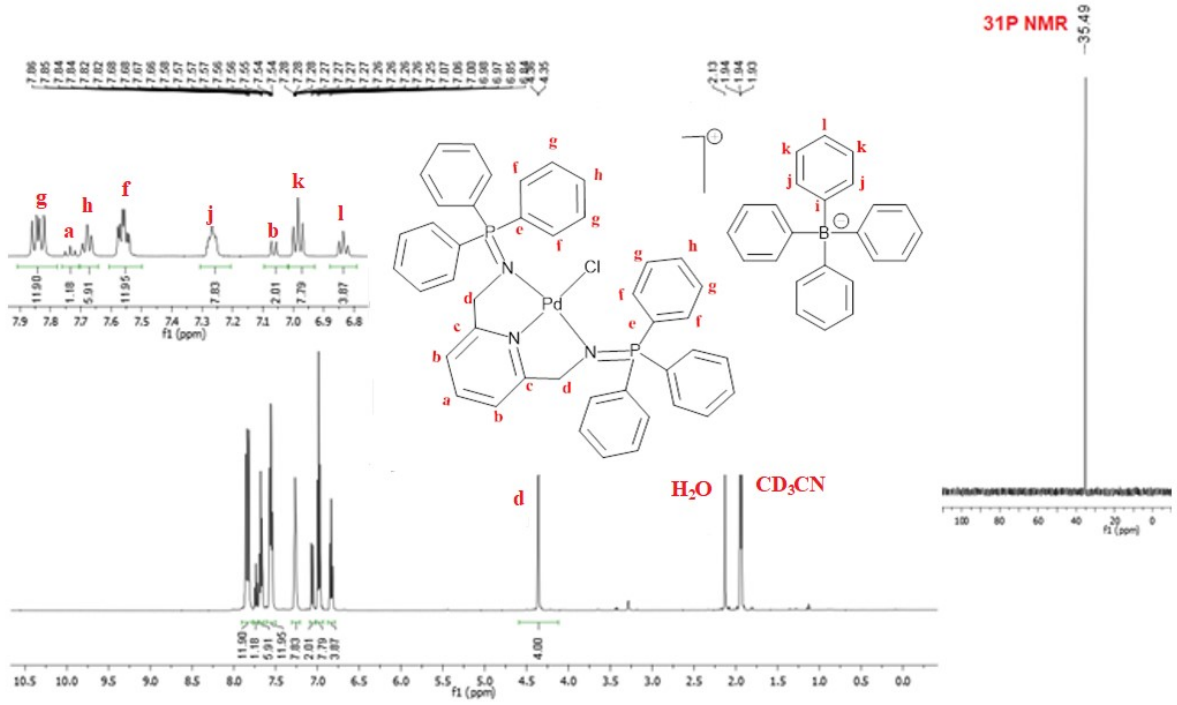
SI-Figure 8: The ^{1}H NMR of **L4** recorded in DMSO-$_{d6}$ at 25 °C.



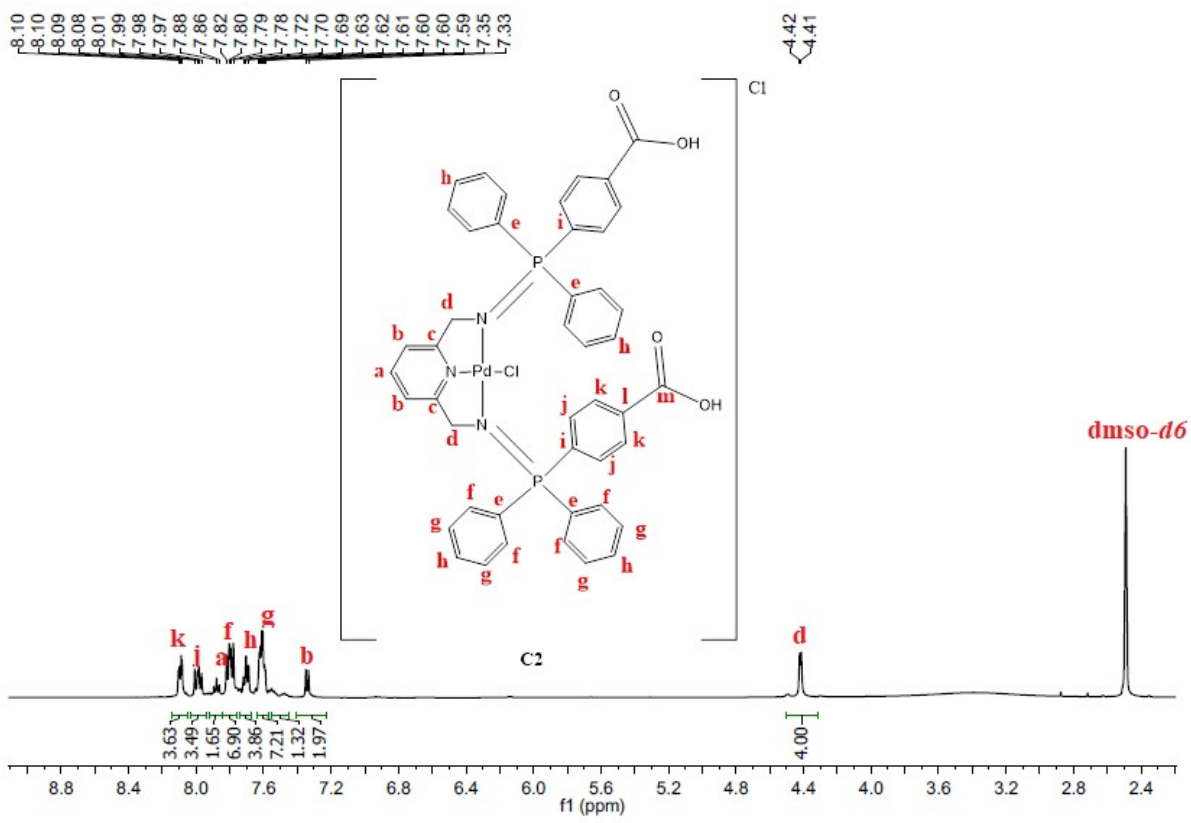
SI-Figure 9: The ^{13}C NMR of **L4** recorded in $DMSO_{-d6}$ at 25 °C.



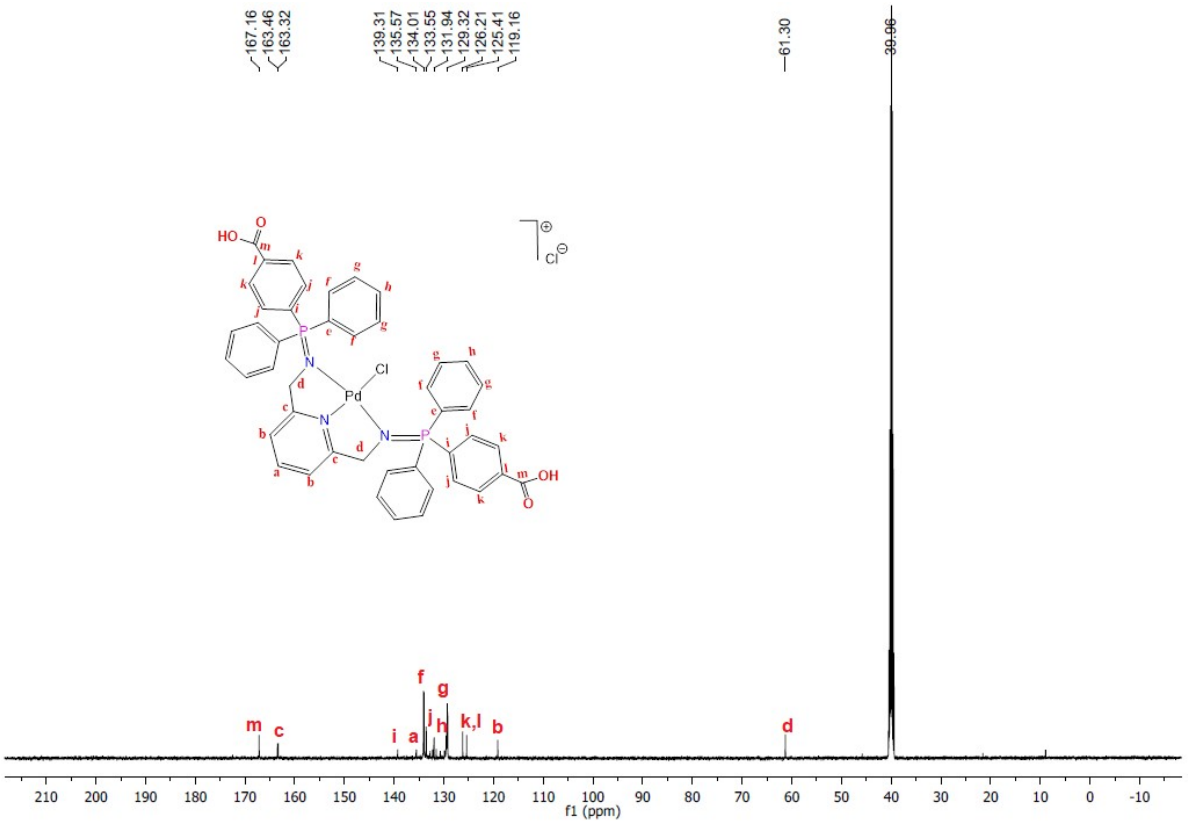
SI-Figure 10: The ^{1}H NMR of **L5** recorded in D_2O and NaOD at 25 °C.



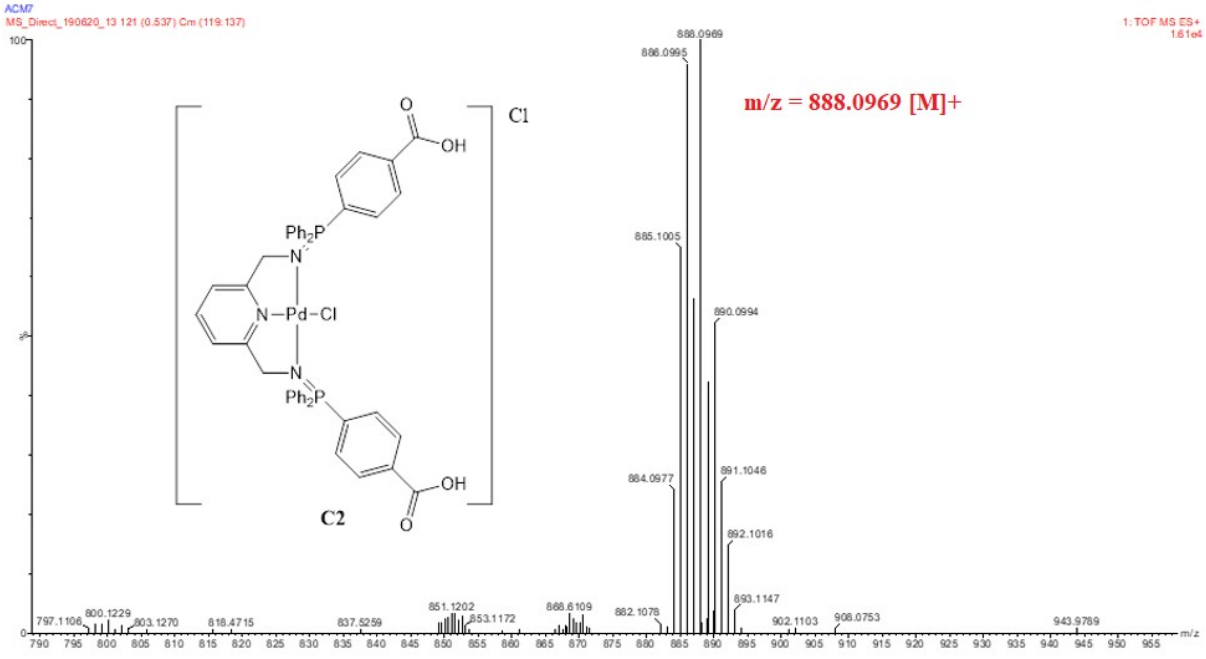
SI-Figure 11: The ^{1}H NMR and the ^{31}P NMR of **C1** were recorded in CD_3CN at 25 °C.



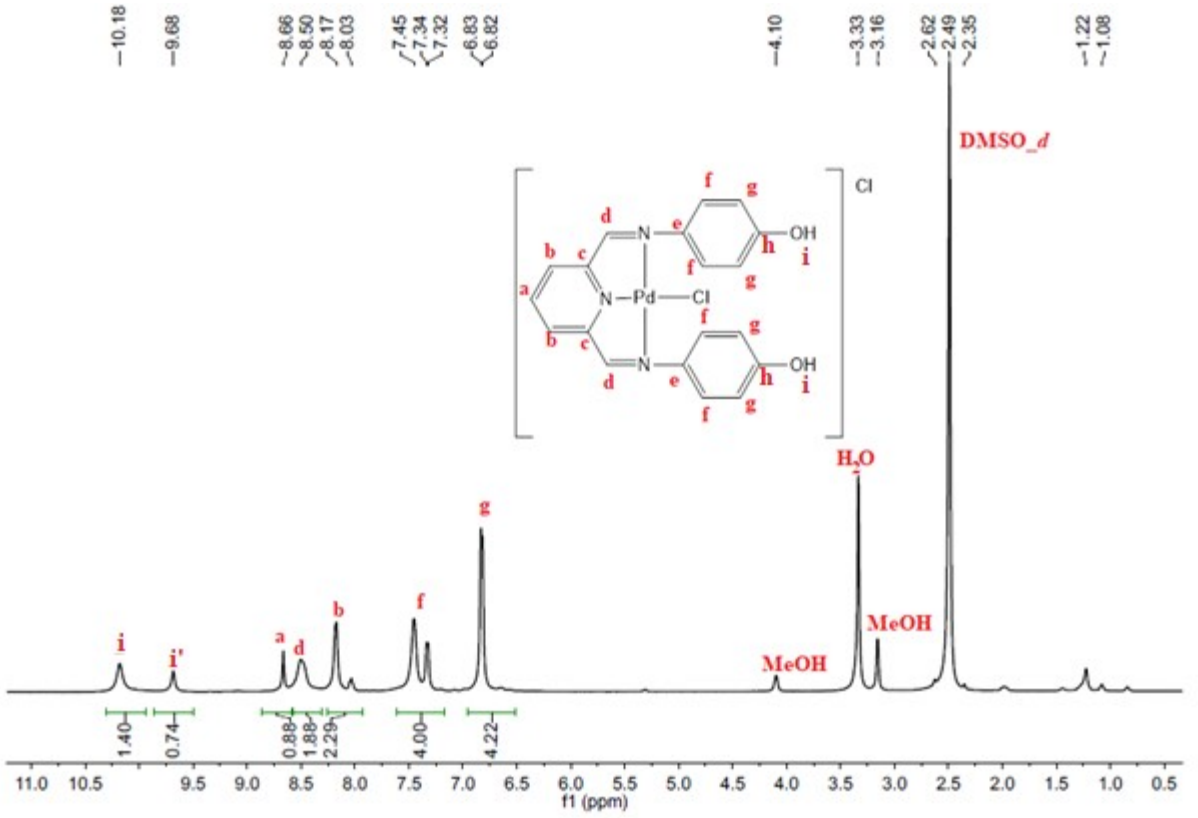
SI-Figure 12a: The ^{1}H NMR of **C2** recorded in $DMSO_{-d6}$ at 25 °C.



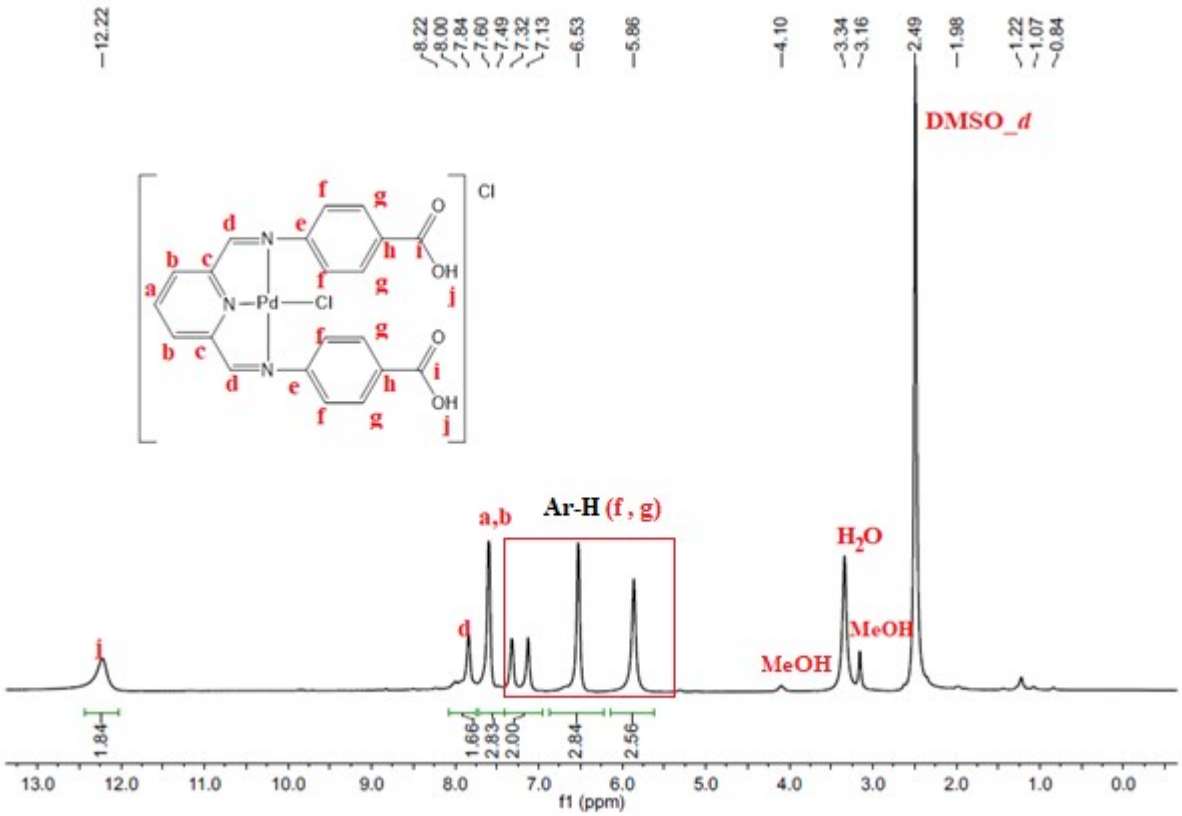
SI-Figure 12b: The $^{13}C\{H\}$ NMR of **C2** recorded in DMSO$_{-d6}$ at 25 °C.



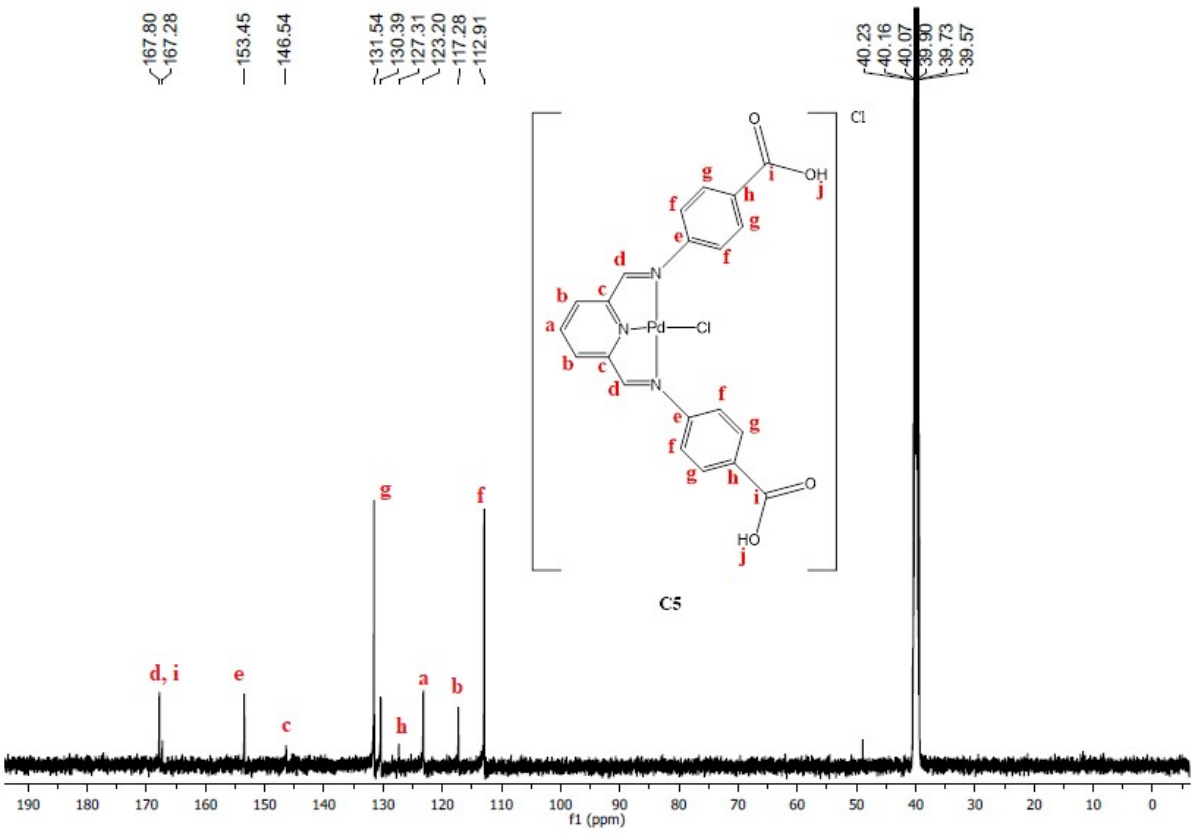
SI-Figure 13. HR-ESI-MS spectrum of **C2.**



SI-Figure 14: The ^{1}H NMR of **C4** recorded in DMSO$_{-d6}$ at 25 °C.



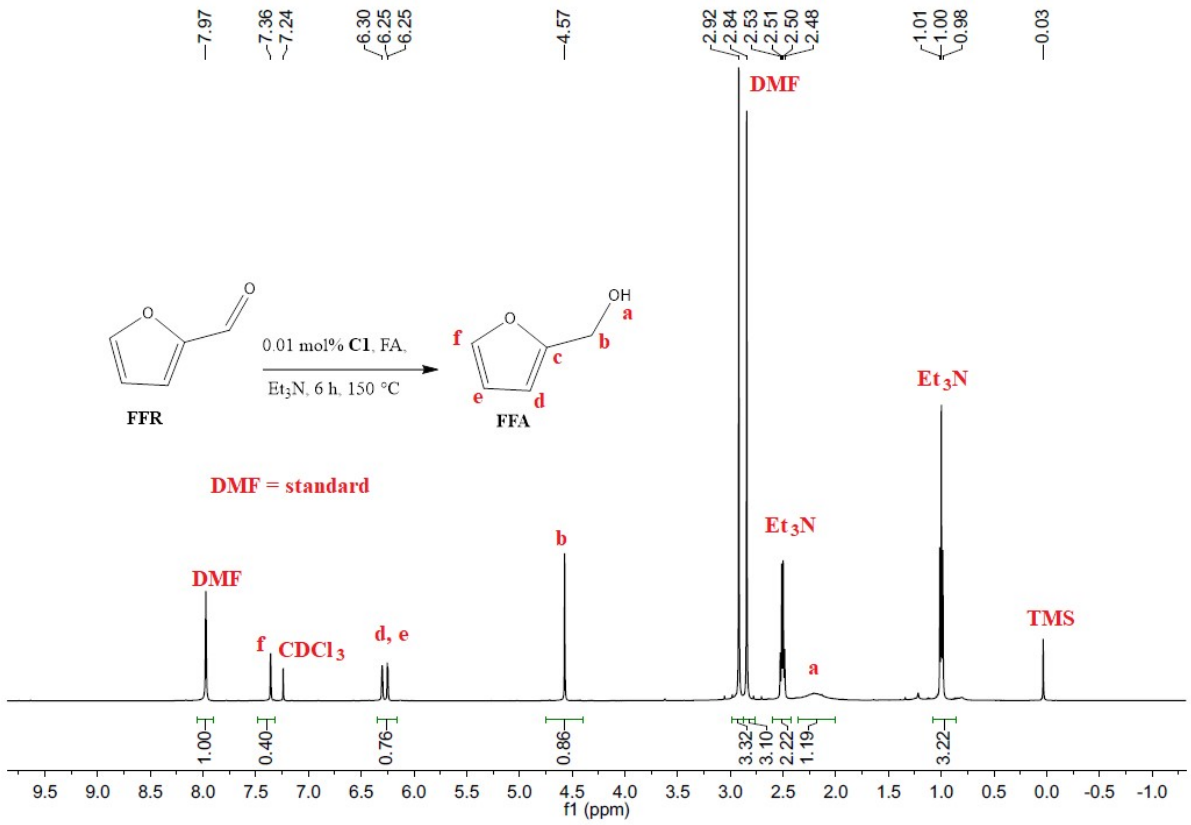
SI-Figure 15: The ^{1}H NMR of **C5** recorded in DMSO-$_{d6}$ at 25 °C.



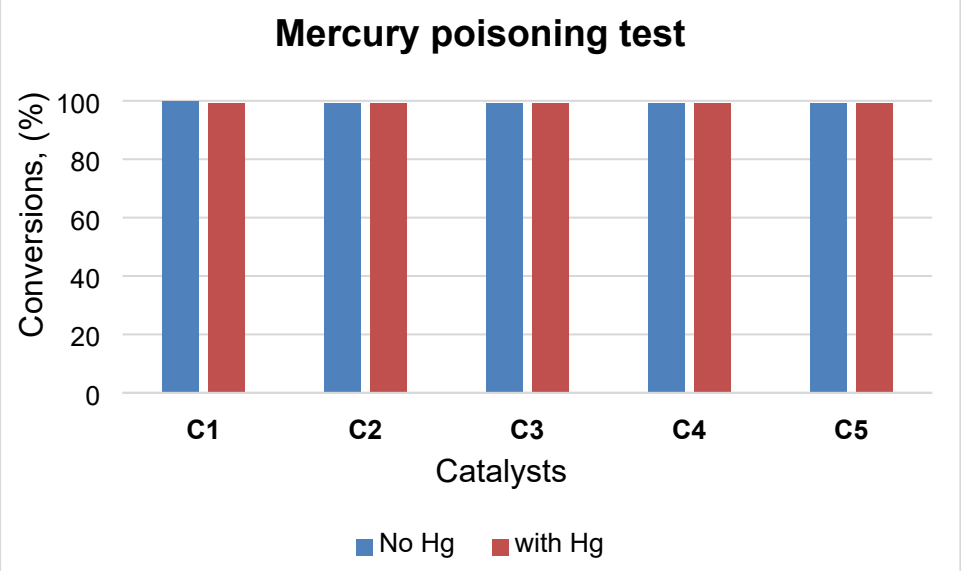
SI-Figure 16: The ^{13}C NMR of **C5** recorded in DMSO-*d6* at 25 °C.

SI-Table 1 Crystal data and structure refinement for C1

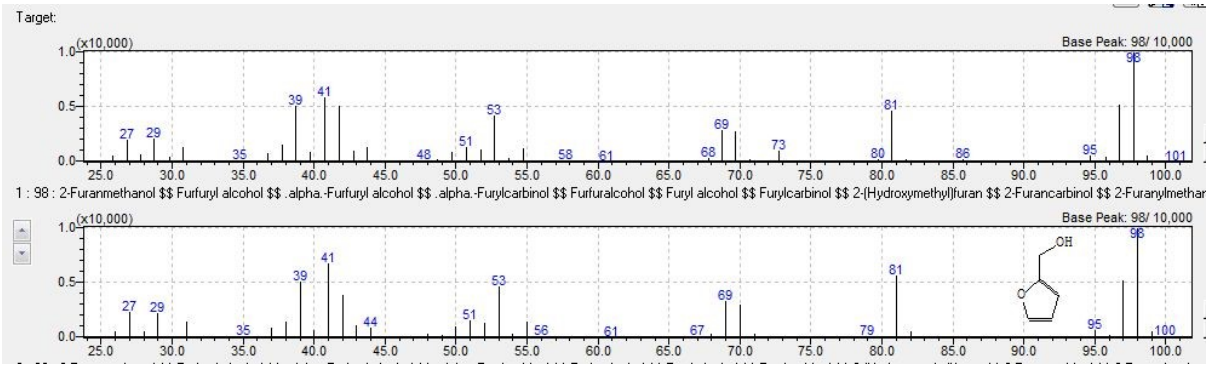
Empirical formula	C_{67} $H_{57}B$ ClN_3P_2Pd
Formula weight	1117.28 g/mol
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.9953(5)
b/Å	16.9291(8)
c/Å	27.3479(12)
α/°	90
β/°	103.019(1)
γ/°	90
Volume/Å^3	5861.9(4)
Z	96
ρ_{calc}g/cm^3	1.2965
μ/mm^{-1}	0.550
F(000)	2243.4
Crystal size/mm^3	0.3 × 0.2 × 0.2
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.02 to 52.84
Index ranges	$-15 \leq h \leq 16$, $-21 \leq k \leq 21$, $-34 \leq l \leq 34$
Reflections collected	152571
Independent reflections	12018 [R_{int} = 0.0670, R_{sigma} = 0.0275]
Data/restraints/parameters	12018/0/702
Goodness-of-fit on F^2	1.820
Final R indexes [I>=2σ (I)]	R_1 = 0.0702, wR_2 = 0.2216
Final R indexes [all data]	R_1 = 0.0824, wR_2 = 0.2327
Largest diff. peak/hole / e Å^{-3}	2.72/-2.90



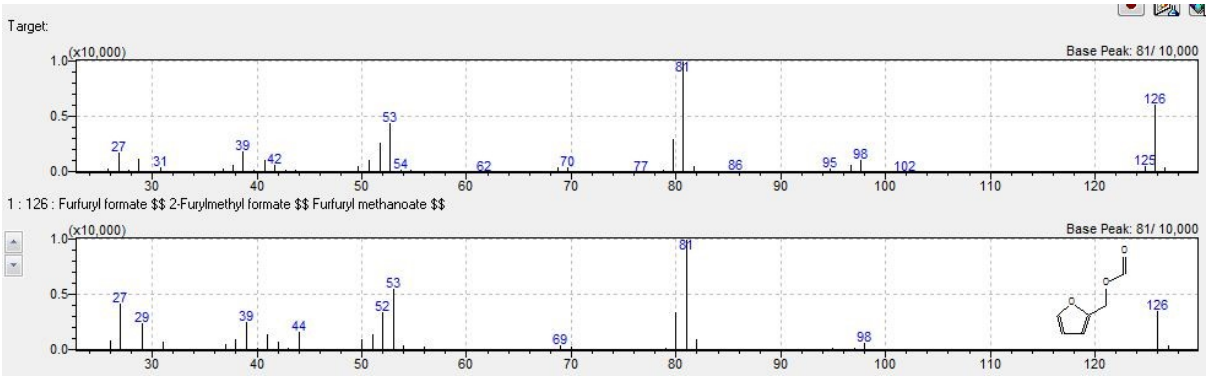
SI-Figure 17. The ^{1}H NMR of the hydrogenation of FFR to FFA using **C1** after the reaction was recorded in $CDCl_3$ at 25 °C.



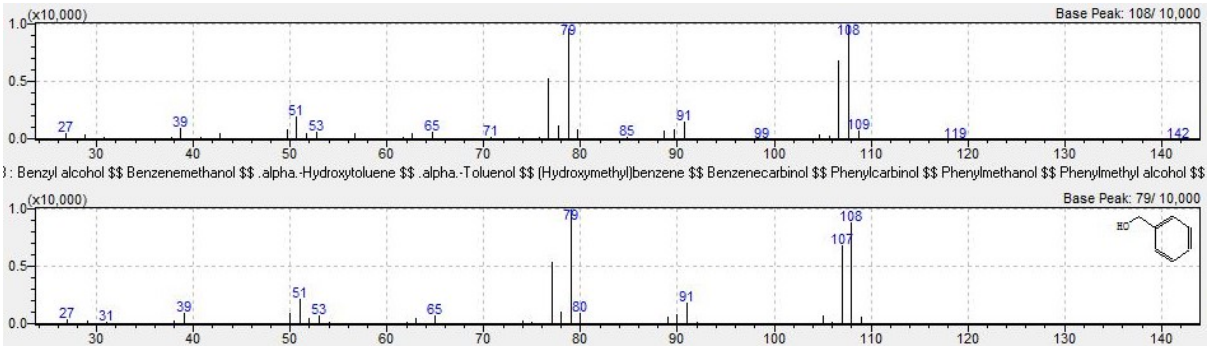
SI-Figure 18. **Reaction conditions**: Reactions were carried out using catalysts **C1 – C5**, in formic acid (5 mmol) with 5 mmol of FFR and 5 mmol of amine. The reaction was allowed to run for 6 hours at 150 °C in the presence of 5 mg of mercury (Hg). Thereafter, DMF was used as an internal standard, mmol product was determined by ^{1}H NMR spectroscopy.



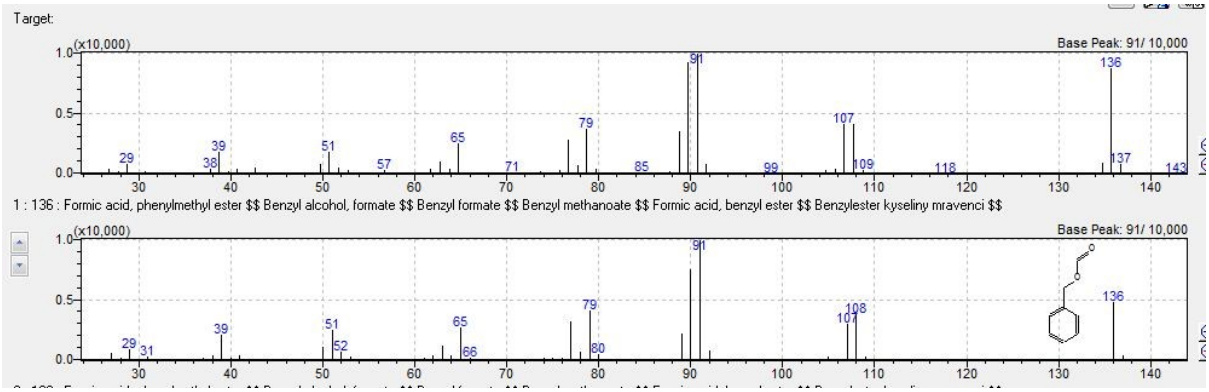
SI-Figure 19. GC-MS of furfuryl alcohol as a product of the organo-catalyzed furfural.



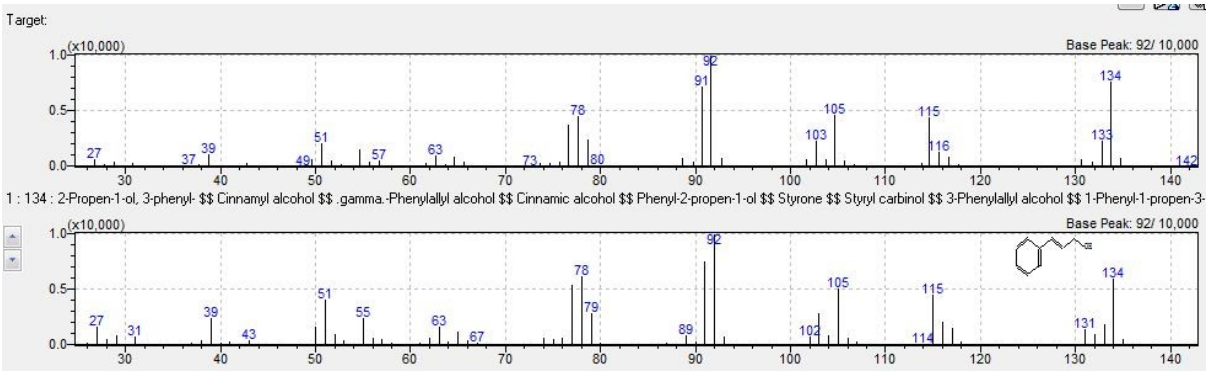
SI-Figure 20. GC-MS of furfuryl formate as a product of the organo-catalyzed furfural.



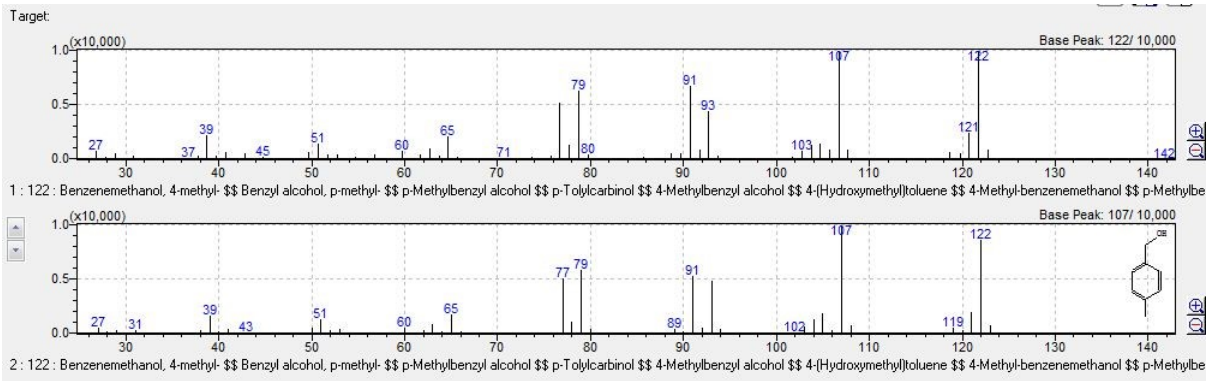
SI-Figure 21. GC-MS of benzyl alcohol as a product of the organo-catalyzed benzyaldehyde.



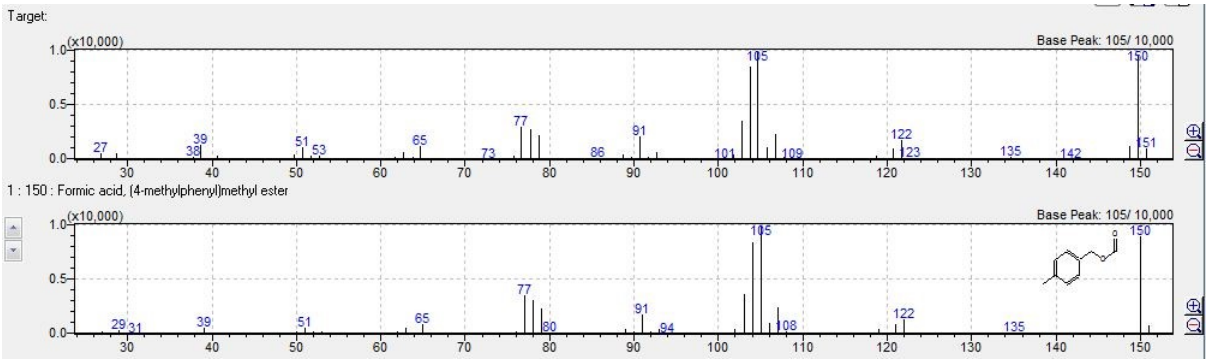
SI-Figure 22. GC-MS of benzyl formate as a product of the organo-catalyzed benzaldehyde.



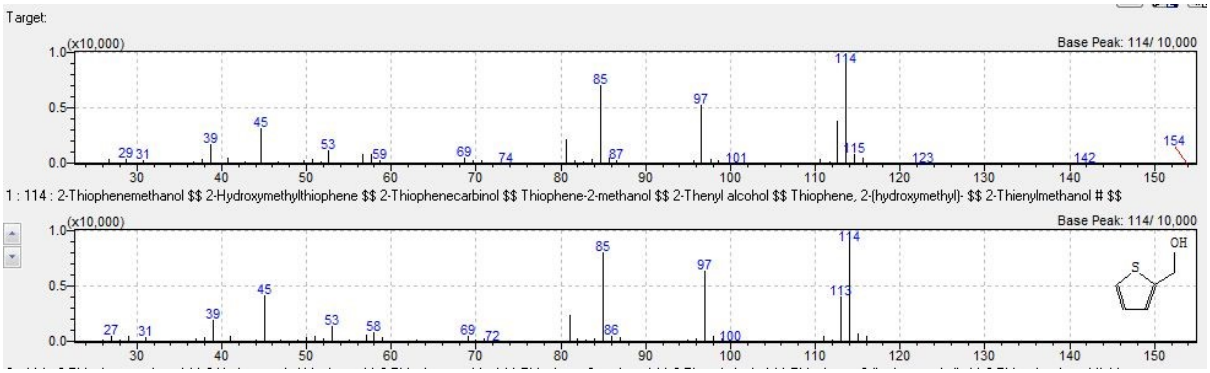
SI-Figure 23. GC-MS of cinnamyl alcohol as a product of the organo-catalyzed cinnamaldehyde.



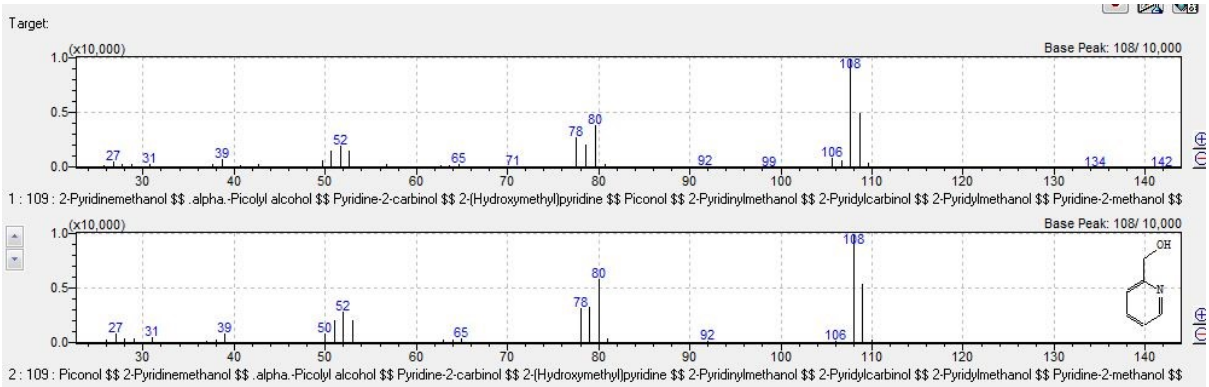
SI-Figure 24. GC-MS of 4-Methylbenzyl ethanol, a product of the organo-catalyzed 4-methyl benzyl aldehyde.



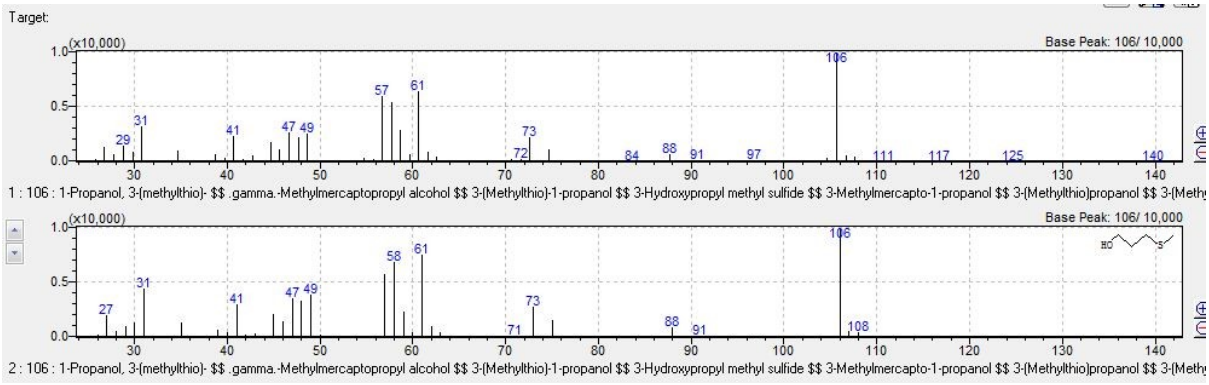
SI-Figure 25. GC-MS of 4-Methylbenzyl formate, a product of the organo-catalyzed 4-methyl benzyl aldehyde.



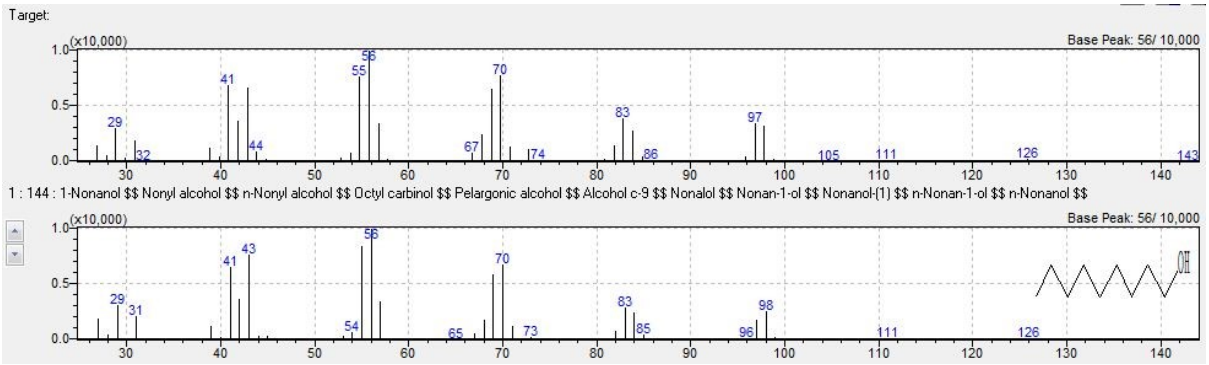
SI-Figure 26. GC-MS of 2-thiophene ethanol, a product of the organo-catalyzed thiophene-2-carboxaldehyde.



SI-Figure 27. GC-MS of 2-pyridyl ethanol, a product of the organo-catalyzed 2-pyridyl carboxaldehyde.



SI-Figure 28. GC-MS of 3-(Methylthio) propanol, a product of the organo-catalyzed 3-(methyltio) propionaldehyde.



SI-Figure 29. GC-MS of Nonanol a product of the organo-catalyzed nonanal.