

Supporting Information

Imidazole-Directed Fabrication of Three Polyoxovanadates-based Copper Frameworks as Efficient Catalysts for Constructing of C-N bonds

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Table 1. Crystallographic data for POVCFs 1-3

	POVCFs 1	POVCFs 2	POVCFs 3
Formula	C ₂₄ H ₃₉ CuN ₈ O ₁₁ V	C ₁₂ H ₂₀ CuN ₄ O ₆ V	C ₄₈ H ₈₀ CuN ₁₆ O ₂₈ V ₁
	4	2	0
M_r	882.93	481.74	1902.22
Crystal system	triclinic	Monoclinic	orthorhombic
Space group	<i>P-1</i>	<i>P21/c</i>	<i>Pccn</i>
Temperature	298(2)	298(2) K	293(2)K
a (Å)	11.2508(8)	9.2616(7)	21.7725(7)
b (Å)	11.9199(9)	5.5433(4)	21.9575(9)
c (Å)	15.2277(14)	17.1092(11)	14.8458(6)
α (deg)	105.431(2)	90	90
β (deg)	94.1680(10)	93.4420(10)	90
γ (deg)	108.872(2)	90	90
V (Å ³)	1834.3(3)	876.80(11)	7097.3(5)
Z	2	2	4
D_{calc} (g cm ⁻³)	1.599	1.825	1.780
$F(000)$	896	486	3852
$R_1[I > 2\sigma(I)]$	0.0611	0.0400	0.0650
$wR_2[I > 2\sigma(I)]$	0.1762	0.1054	0.1738
$R_1(\text{all data})$	0.0878	0.0561	0.0890
$wR_2(\text{all data})$	0.1938	0.1136	0.1946
GOOF	1.049	1.043	1.040
CCDC No.	2009806	2009807	2009808

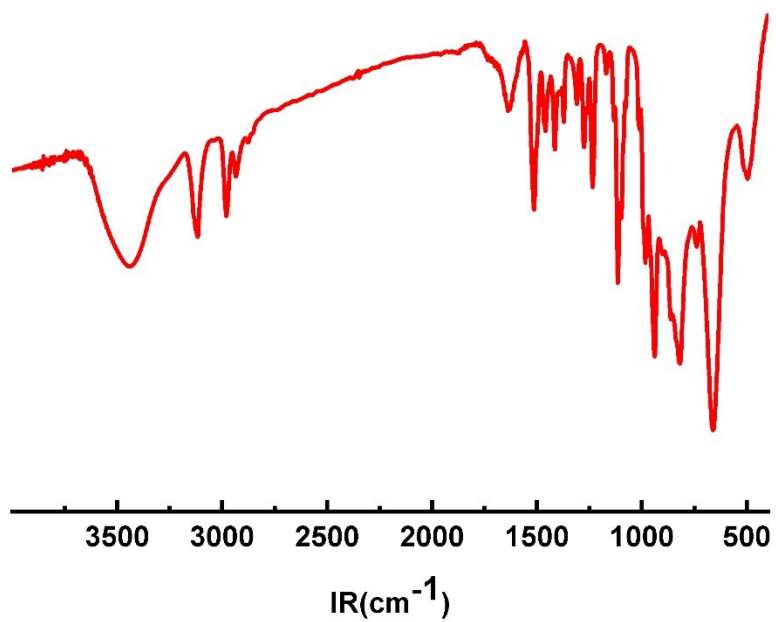


Figure S1. The IR spectrum of POVCFs 1

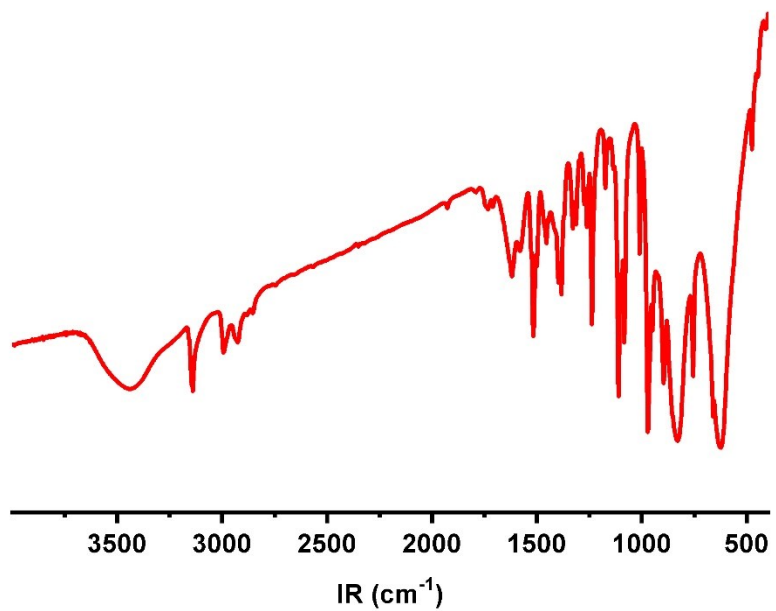


Figure S2. The IR spectrum of POVCFs 2

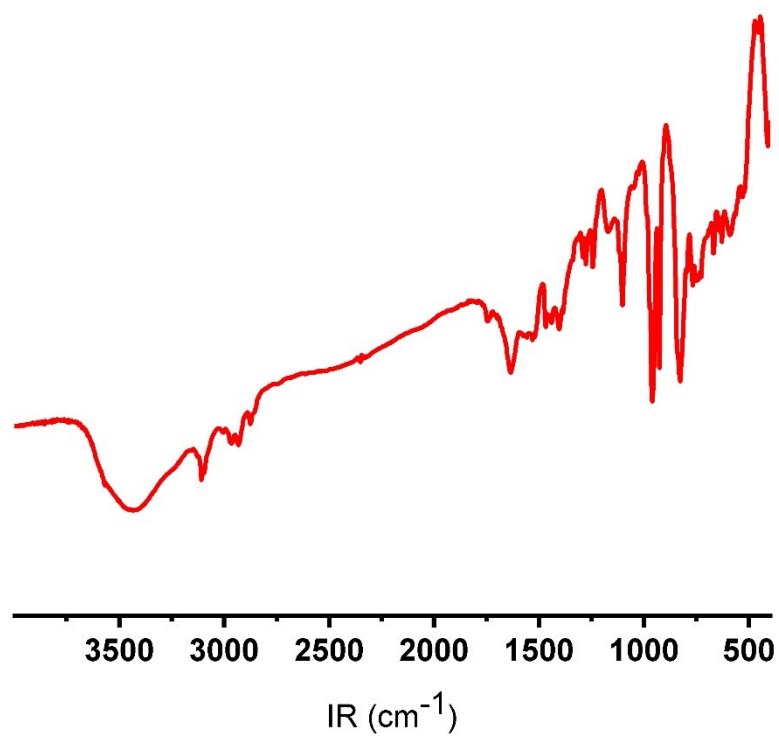


Figure S3. The IR spectrum of POVCFs 3

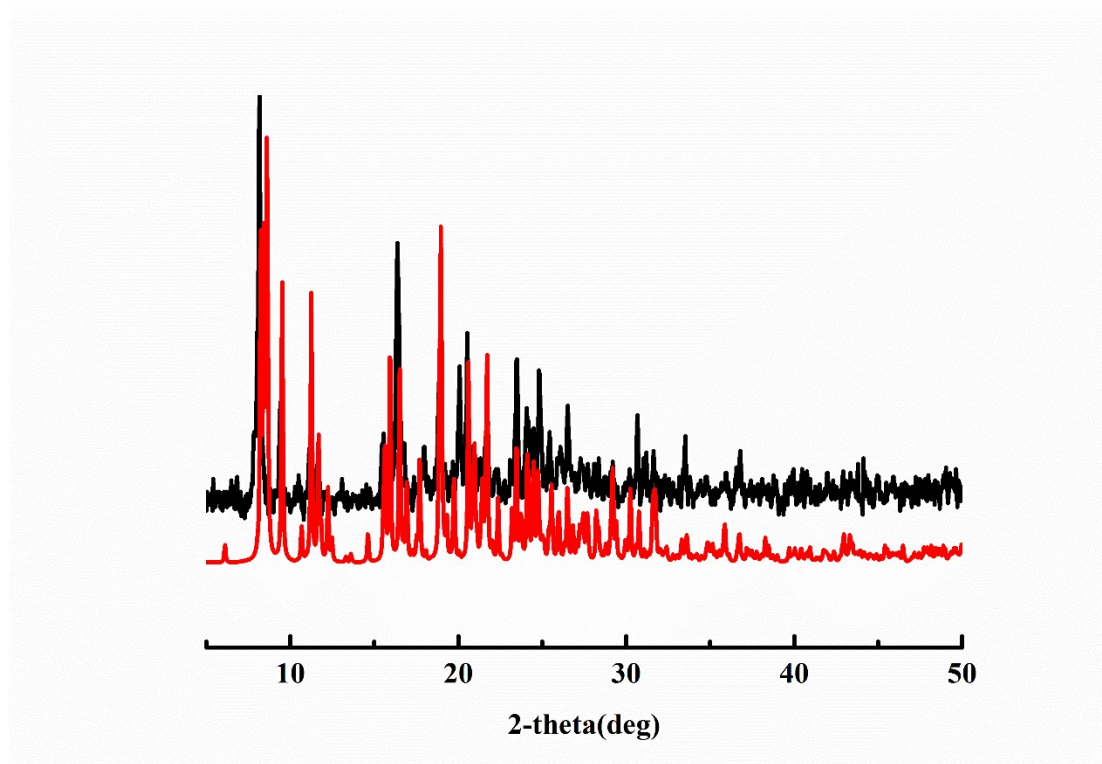


Figure S4. The PXRD spectrum of POVCFs 1

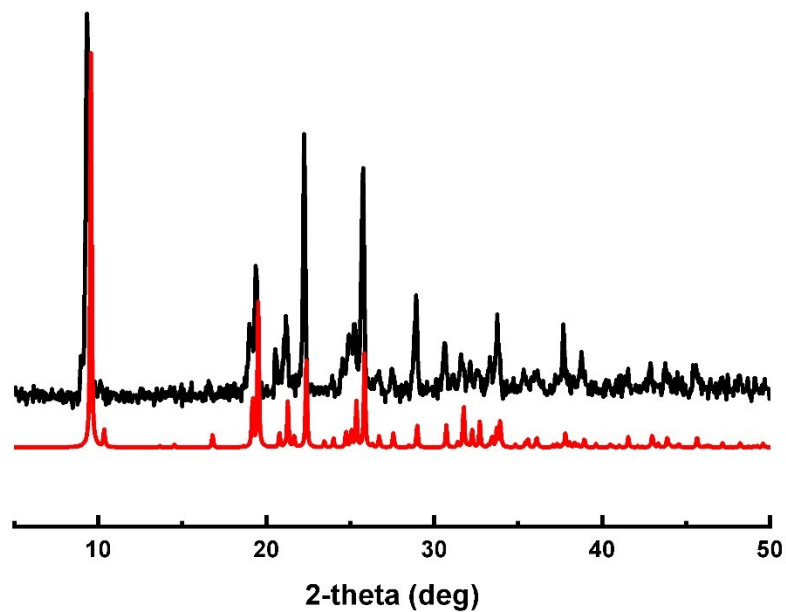


Figure S5. The PXRD spectrum of POVCFs 2

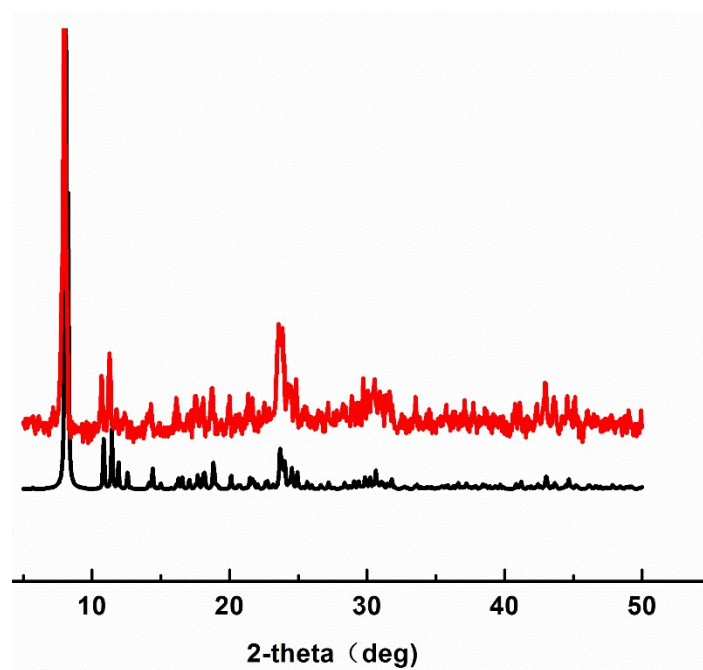


Figure S6. The PXRD spectrum of POVCFs 3

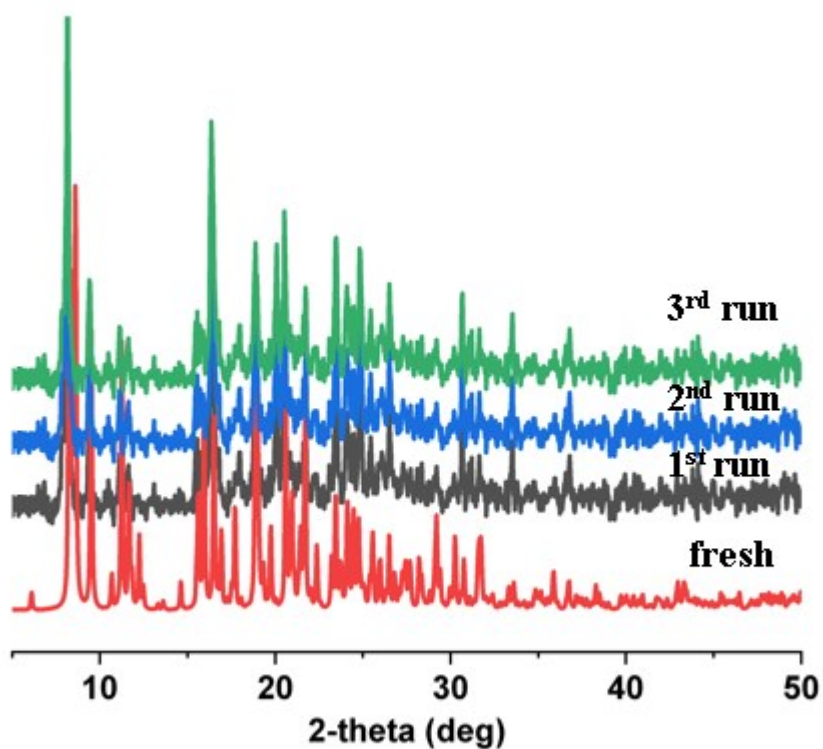


Figure S7. The powder XRD patterns of POVCFs 1 before and after three runs of reaction

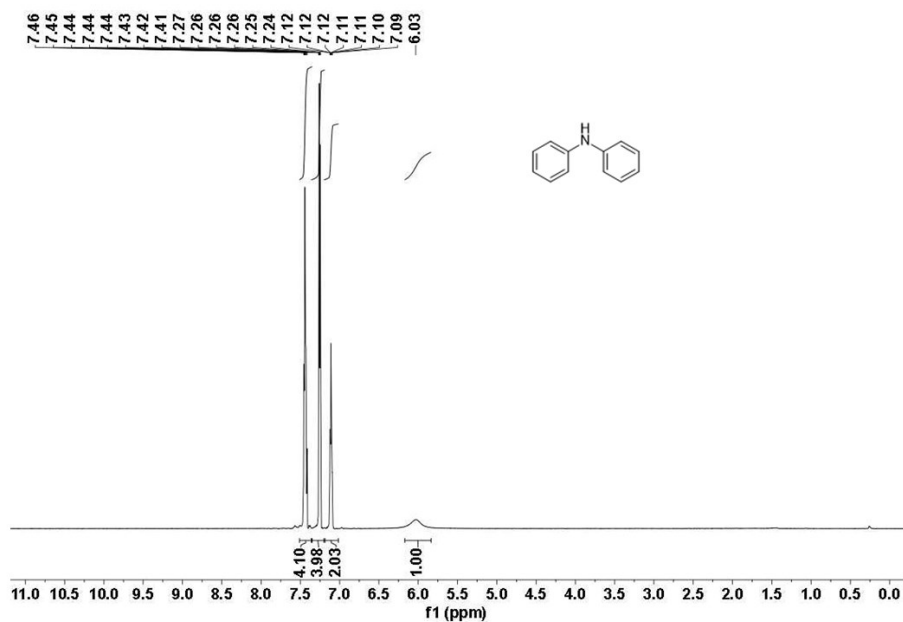


Figure S8 ^1H NMR spectrum of product 3a (entry 1) in CDCl_3 .

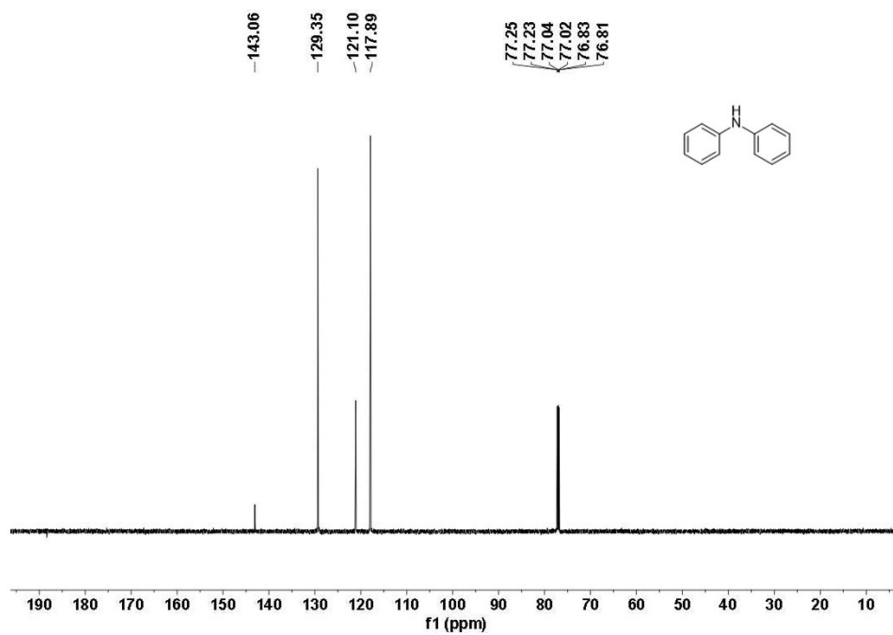


Figure S9 ^{13}C NMR spectrum of product 3a (entry 1) in CDCl_3 .

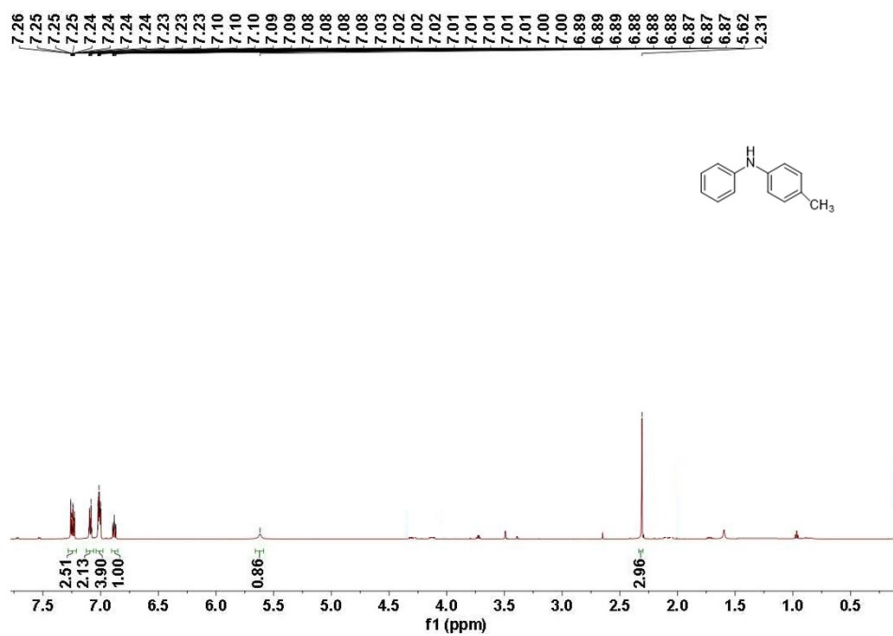


Figure S10 ^1H NMR spectrum of product 3b (entry 2) in CDCl_3 .

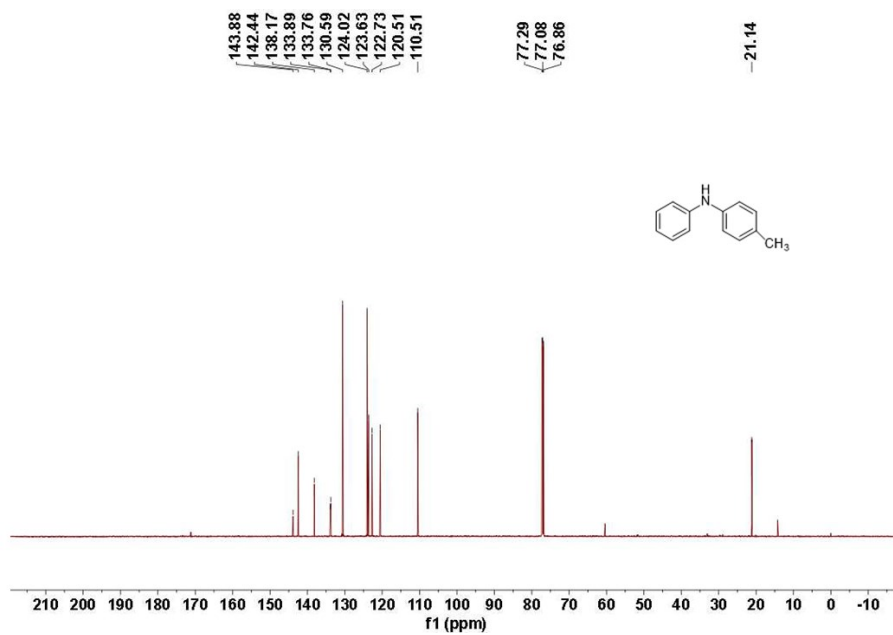


Figure S11 ¹³C NMR spectrum of product 3b (entry 2) in CDCl₃.

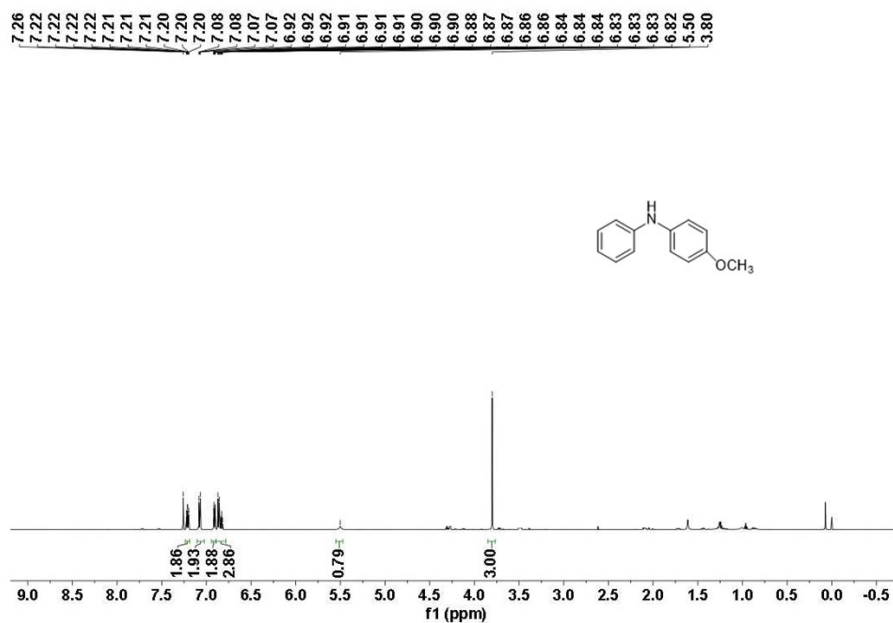


Figure S12 ¹H NMR spectrum of product 3c (entry 3) in CDCl₃.

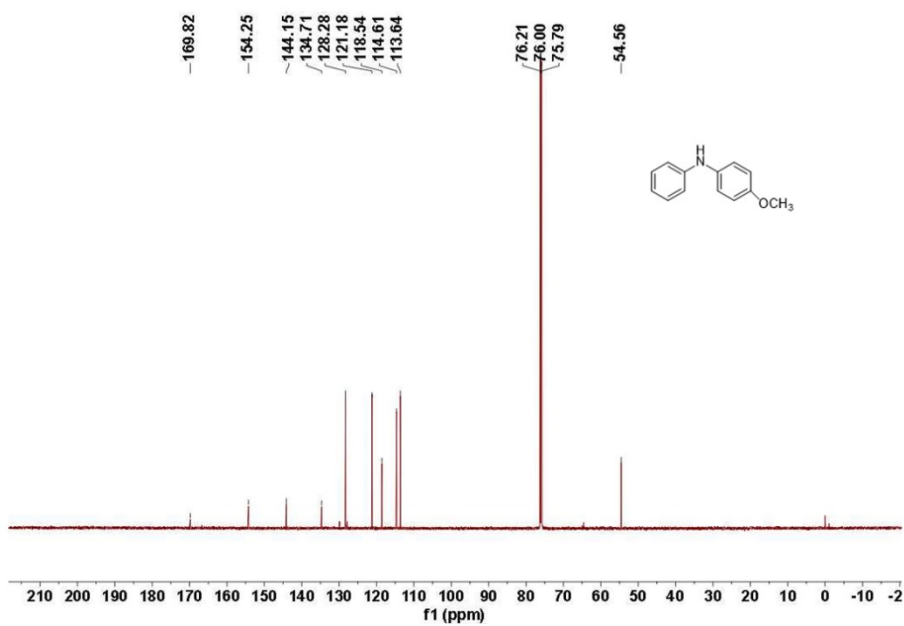


Figure S13 ^{13}C NMR spectrum of product 3c (entry 3) in CDCl_3 .

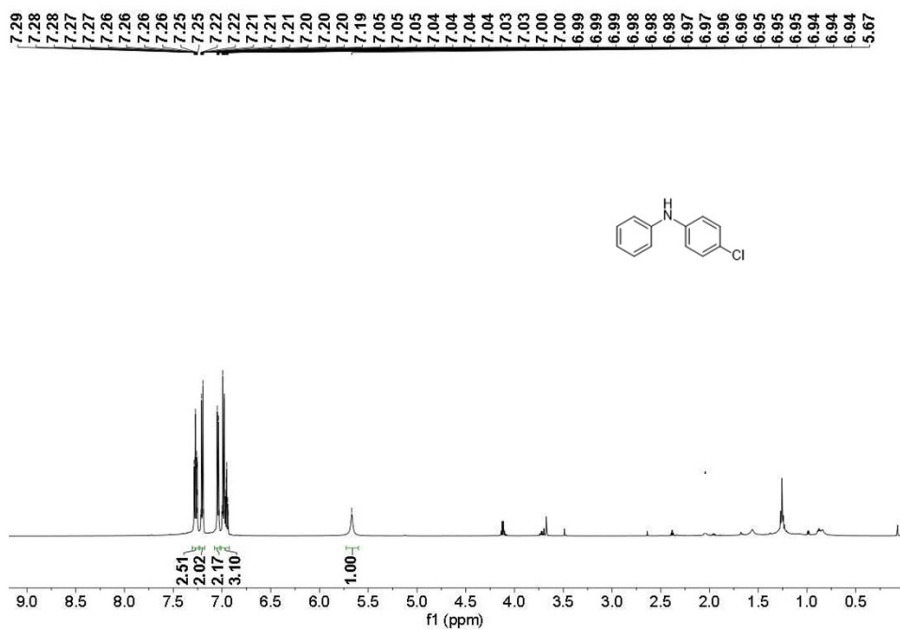


Figure S14 ^1H NMR spectrum of product 3d (entry 4) in CDCl_3 .

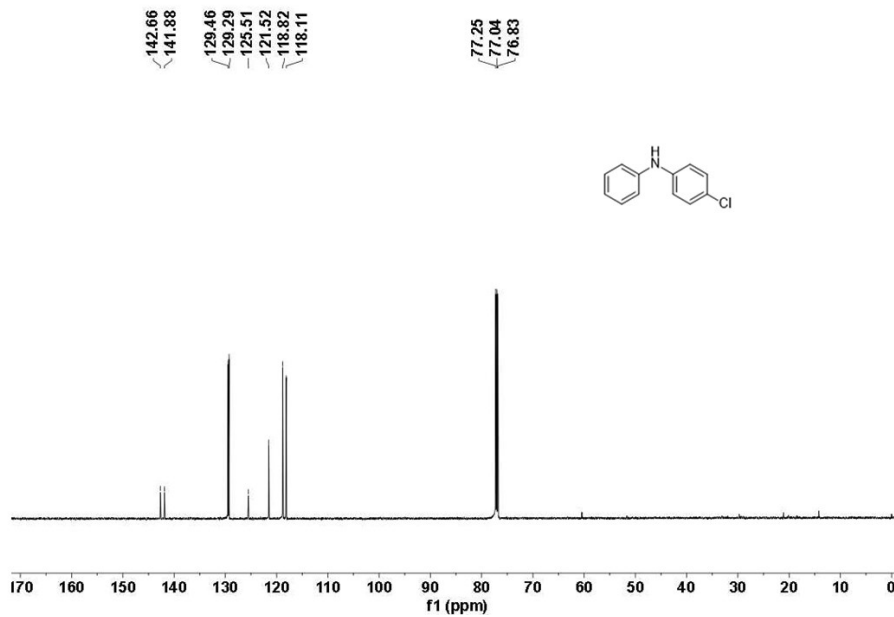


Figure S15 ¹³C NMR spectrum of product 3d (entry 4) in CDCl₃.

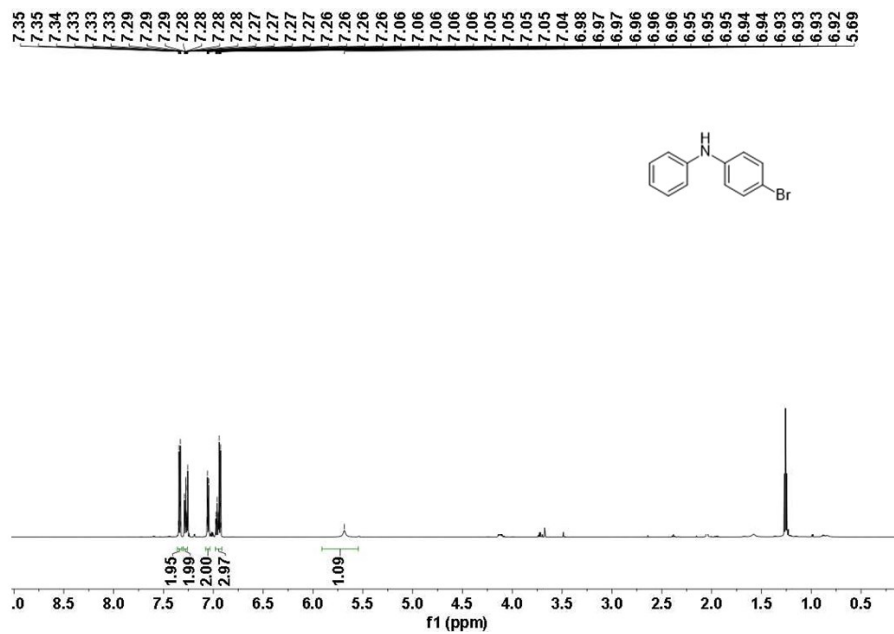


Figure S16 ¹H NMR spectrum of product 3e (entry 5) in CDCl₃.

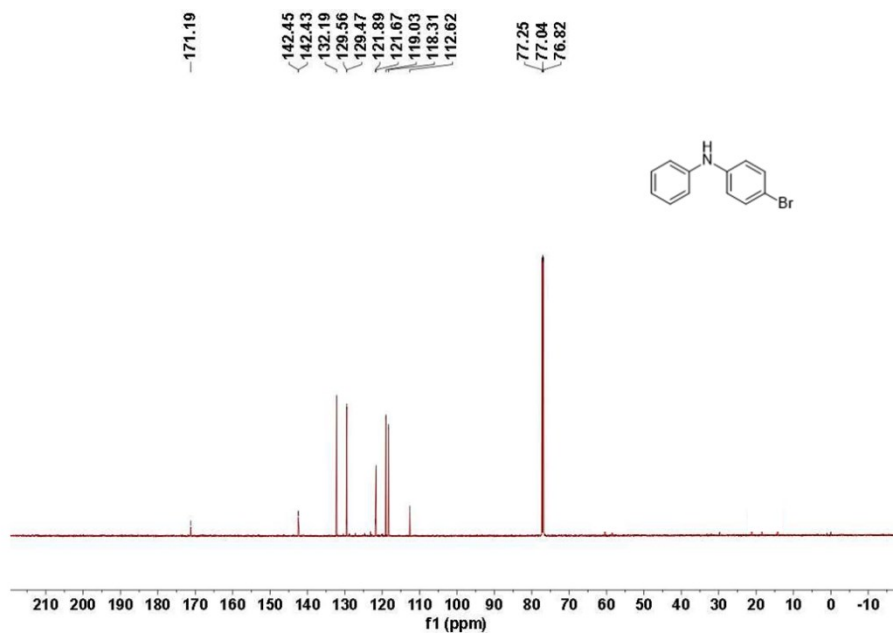


Figure S17 ¹³C NMR spectrum of product 3e (entry 5) in CDCl₃.

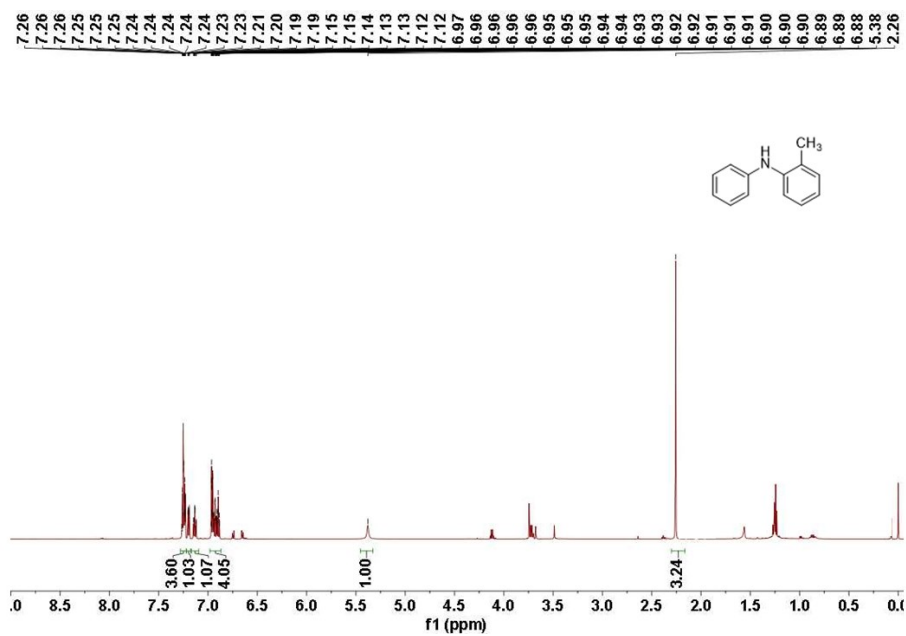


Figure S18 ¹H NMR spectrum of product 3f (entry 6) in CDCl₃.

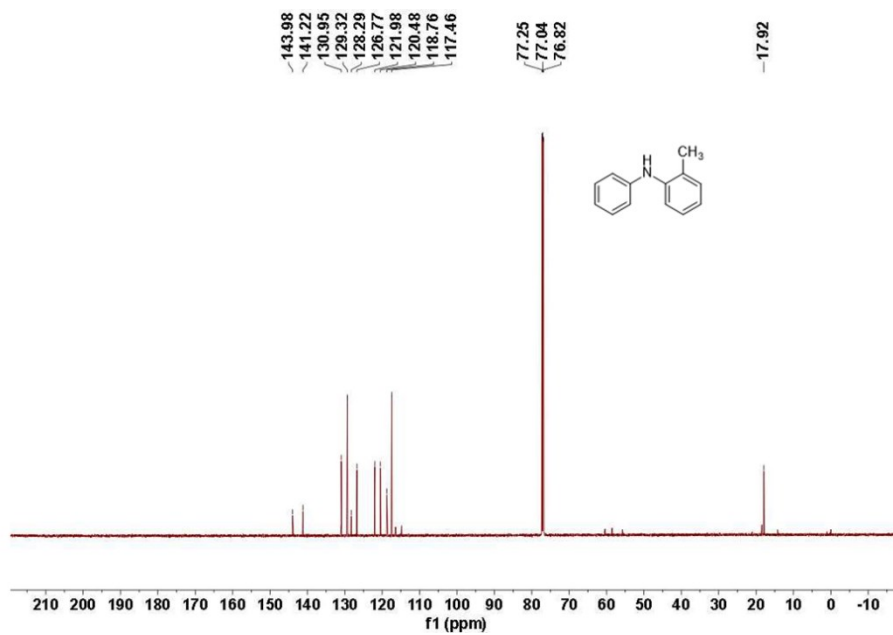


Figure S19 ^{13}C NMR spectrum of product 3f (entry 6) in CDCl_3 .

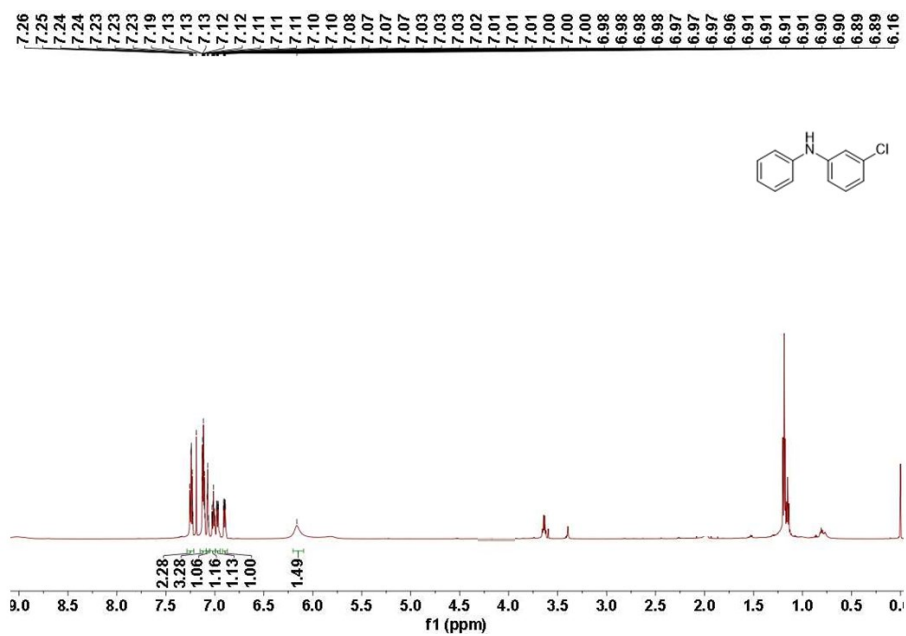


Figure S20 ^1H NMR spectrum of product 3g (entry 7) in CDCl_3 .

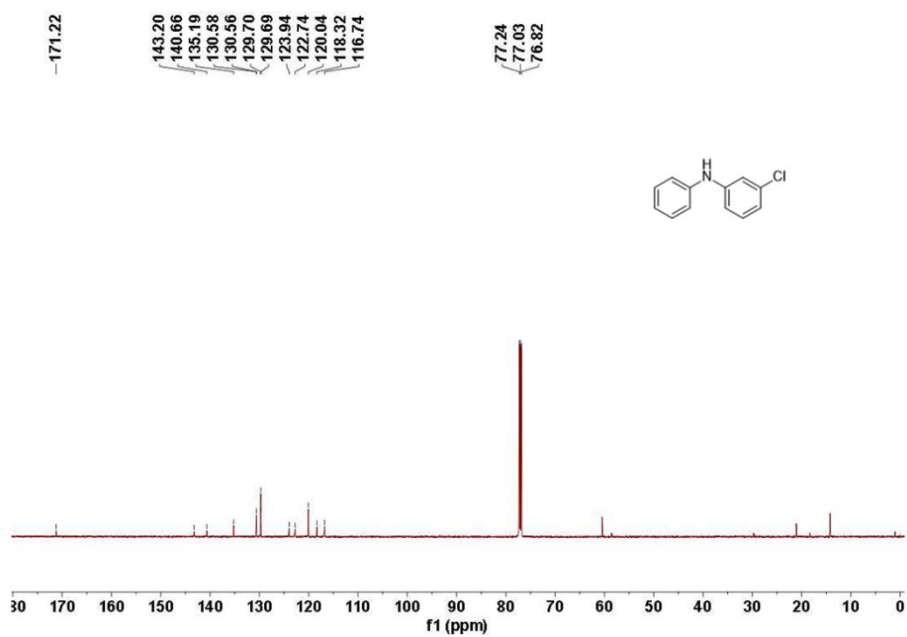


Figure S21 ¹³C NMR spectrum of product 3g (entry 7) in CDCl₃.

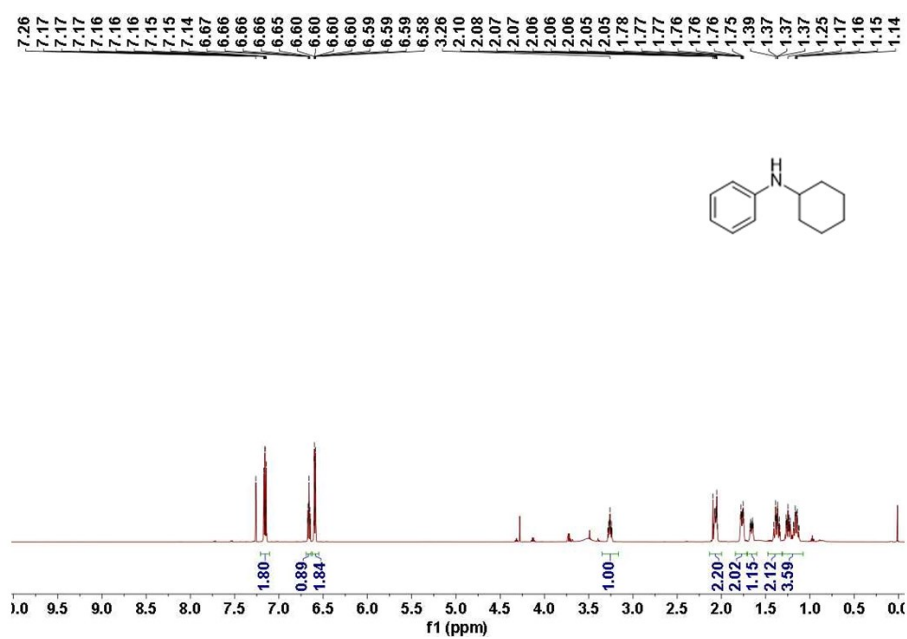


Figure S22 ¹H NMR spectrum of product 3h (entry 8) in CDCl₃.

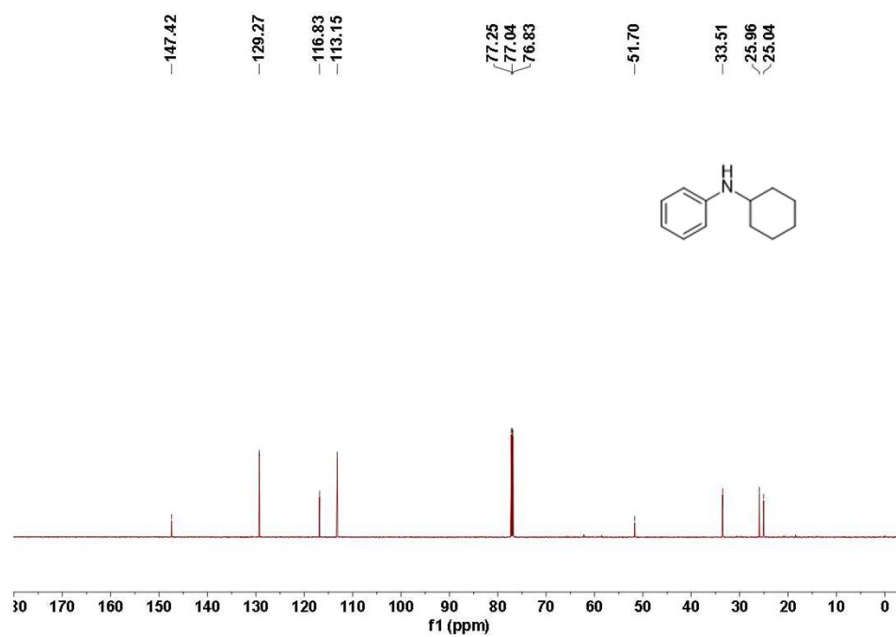


Figure S23 ^{13}C NMR spectrum of product 3h (entry 8) in CDCl_3 .