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ESI *for*

Palladacycles of sulfated and selenated Schiff bases of ferrocene-carboxaldehyde as catalysts for O-arylation and Suzuki–Miyaura coupling

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Table S1. Crystal data and structural refinement parameters for 1- 3

Compounds	**1**	**2**	**3**
Empirical formula	C_{19} H_{18}ClFeNPd S	C_{19} H_{18}ClFeNPdSe	C_{37} H_{33}ClFeNPPd S
Formula wt.	490.10	537.00	752.37
Crystal size [mm]	0.43 × 0.21 × 0.19	0.34×0.25×0.22	0.35×0.27 ×0.15
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	*P 21/c*	*P 2(1)/c*	*P -1*
Unit Cell dimension	a = 9.193(2) b = 11.622(3)) c = 17.081(4) α = 90.00 β = 101.079(4) γ = 90.00	*a* = 9.203(7) *b* = 11.673(8) *c* = 17.075(12) α = 90.00° β = 101.083(13) γ = 90.00°	a = 10.0905(14) b = 10.5555(14) c = 18.524(3) α =100.307(2) β = 93.349(2) γ =116.254(2)
Volume [Å^3]	1790.9(7)	1800(2)	1719.6(4)
Z	4	4	2
Density (Calc.) [Mg·m^{-3}]	1.818	1.982	1.453
Absorption coeff. [mm^{-1}]	2.079	3.975	1.156
F(000)	976.0	1048	764.0
θ range [°]	2.13 – 24.99	2.85–27.26	2.21 - 25.00
Index ranges	-10 ≤ *h* ≤ 10 -13 ≤ *k* ≤ 13 -20 ≤ *l* ≤ 20	-10≤ *h* ≤ 7 -13≤ *k* ≤ 13 -18 ≤ *l* ≤ 18	-11≤ *h* ≤ 11 -12≤ *k* ≤ 12 -22≤ *l* ≤ 22
Reflections collected	16747	7033	16403
Independent reflections ($R_{int.}$)	3151 (0.0489)	3045 (0.0320)	6044(0.0245)
Max./min. Transmission	0.674 /0.598	0.447 / 0.358	0.839/0.696
Data/restraints/parameters	3151 /0/ 217	3045 /0/217	6030/0/388
Goodness-of-fit on F^2	1.170	1.058	1.156
Final R indices [I >2σ(I)]	R_1 = 0.0492 wR_2 = 0.0859	R_1 = 0.0866 wR_2 = 0.1414	R_1 = 0.0725 wR_2 = 0.2261
R indices (all data)	R_1 = 0.0389 wR_2 = 0.0825	R_1 = 0.0477 wR_2 = 0.0.1328	R_1 = 0.0660 wR_2 = 0.2205
Largest diff. peak/hole [e.Å^{-}	0.632/ -0.419	0.936 /-0.606	1.450/-0.383

^{3}]			

Table S2. Selected bond lengths and bond angles of 1- 3

Complex	Bond length [Å]		Bond angle [^{o}]	
1.	Pd1— S1 N1— Pd1 Cl1— Pd1 C11— Pd1 C9 —N1 C6— S1	2.4249(12) 2.012(4) 2.2870(14) 1.973(4)) 1.274(6) 1.785(5)	N1— Pd1— Cl1 C11— Pd1— S1 C11 —Pd1 —Cl1 N1— Pd1— S1 C11 —Pd1 —N1 C7 —Se1— Pd1 C9 —N1 —Pd1 C8— N1 —Pd1	174.00(11) 165.62(14) 93.74(15) 84.68(11) 81.03(18) 93.22(16) 116.9(3) 120.0(3)
2.	Pd1— Se1 N1— Pd1 Cl1— Pd1 C11— Pd1 C9 —N1 C6— Se1	2.5058(14) 2.025(5) 2.286(2) 1.956(6) 1.286(8) 1.912(6)	N1— Pd1— Cl1 C11— Pd1— Se1 C11 —Pd1 —Cl1 N1— Pd1— Se1 C11 —Pd1 —N1 C7 —Se1— Pd1 C9 —N1 —Pd1 C8— N1 —Pd1	174.53(15) 166.61(18) 93.8(2) 85.25(16) 81.6(2) 90.6(2) 115.9(4) 121.5(4)
3	Pd1— P1 N1— Pd1 Cl1— Pd1 C11— Pd1 C9 —N1 C6— Se1	2.2445(17) 2.131(6 2.370(2) 2.003(7 1.272(10) 1.775(9	N1— Pd1— Cl1 C11— Pd1— P1 C11 —Pd1 —Cl1 N1— Pd1— P1 C11 —Pd1 —N1 C25— P1— Pd1 C31— P1 —Pd1 C37— P1— Pd1	92.36(18) 92.00(2) 173.1(2) 172.07(19) 80.90(3) 111.90(2) 114.60(2) 17.00(2)

Table S3. Non-covalent interactions C–H···Cl distances (Å) of complexes 1- 3

Complex 1	Complex 2	Complex 3
H1-Cl1 2.934	H1-Cl1 2.888	Cl1-H22 2.945
H2-Cl 1 2.879	H2-Cl 1 2.924	H9-F6 2.612
H14-Cl1 2.744	H14-Cl1 2.602	
C15-H13 2.899	H7B-H17 2.357	

Mass spectra-

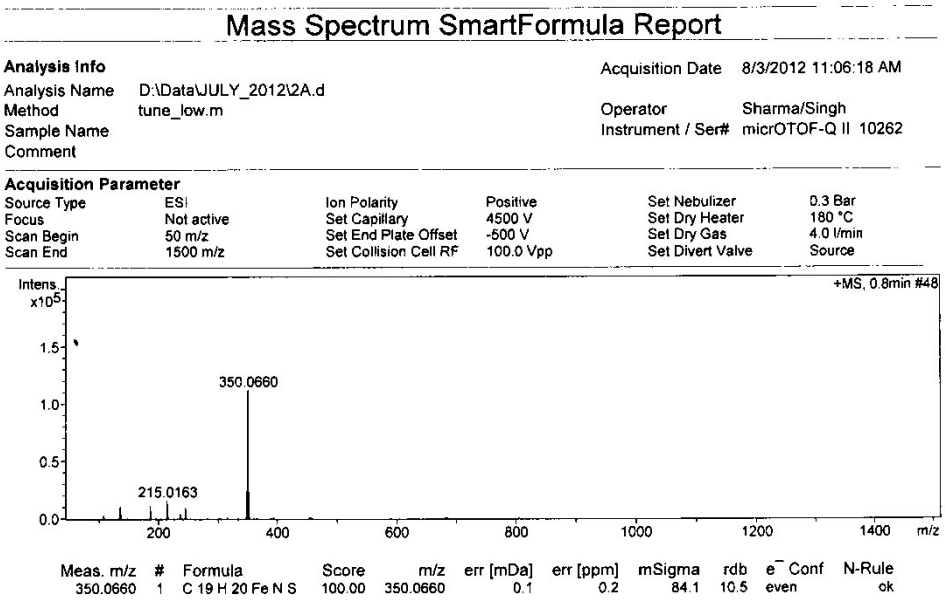


Fig S1 Mass spectrum of ligand **1**

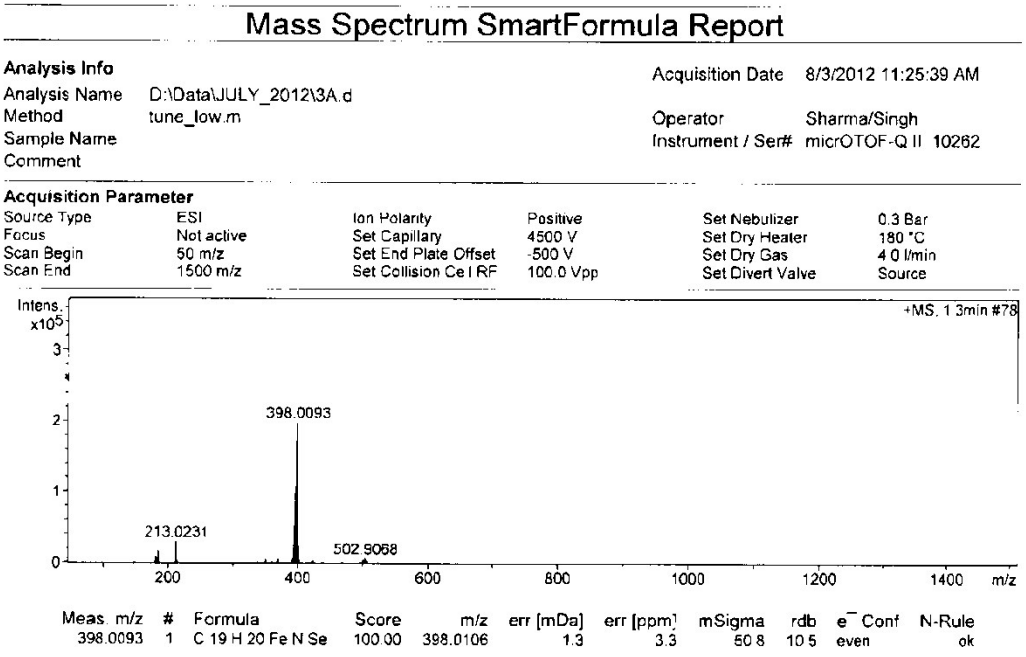


Fig S2 Mass spectrum of ligand **2**

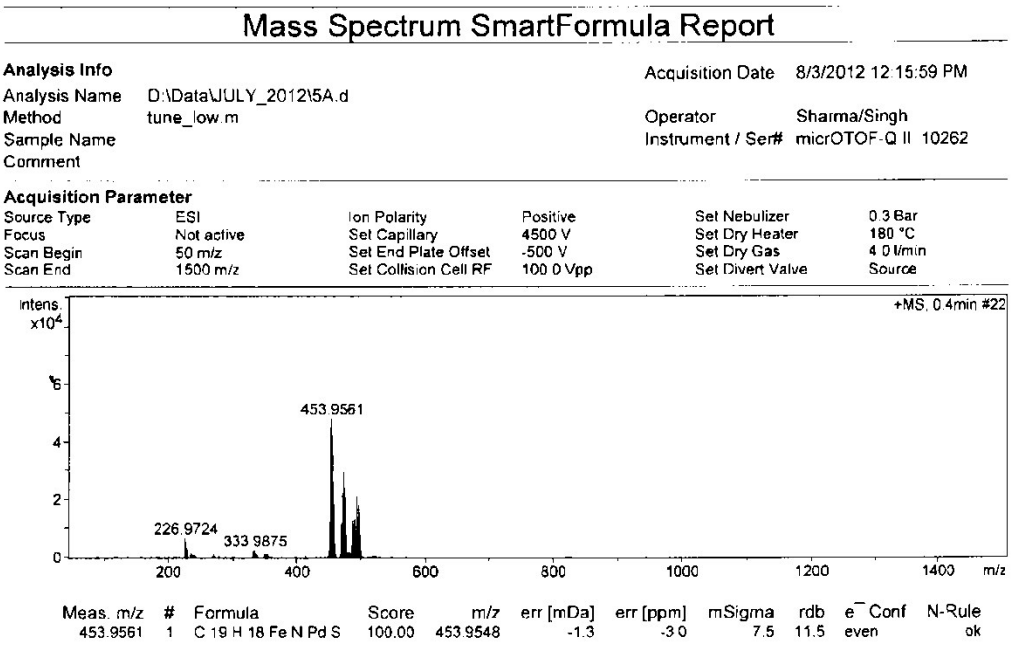


Fig S3 Mass spectrum of complex **1**

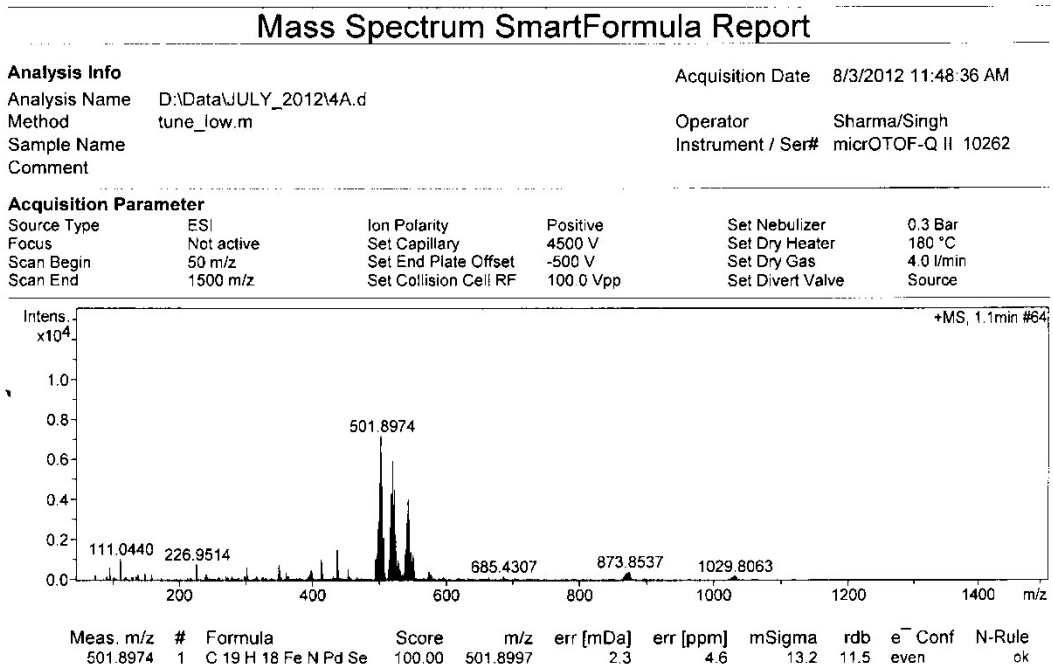


Fig S4 Mass spectrum of complex **2**

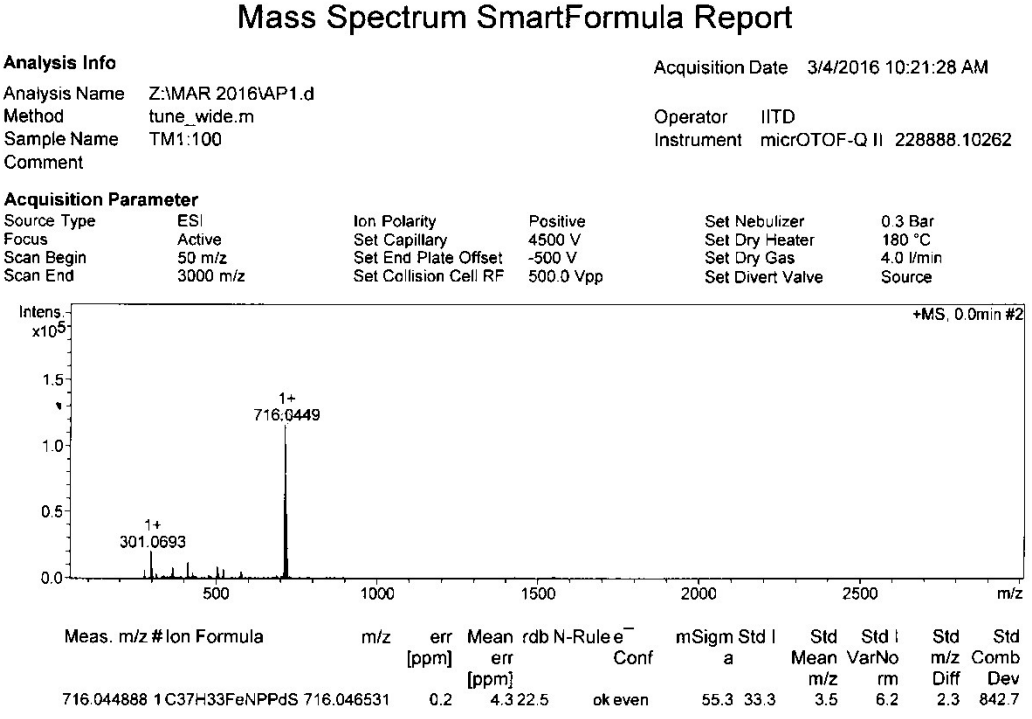
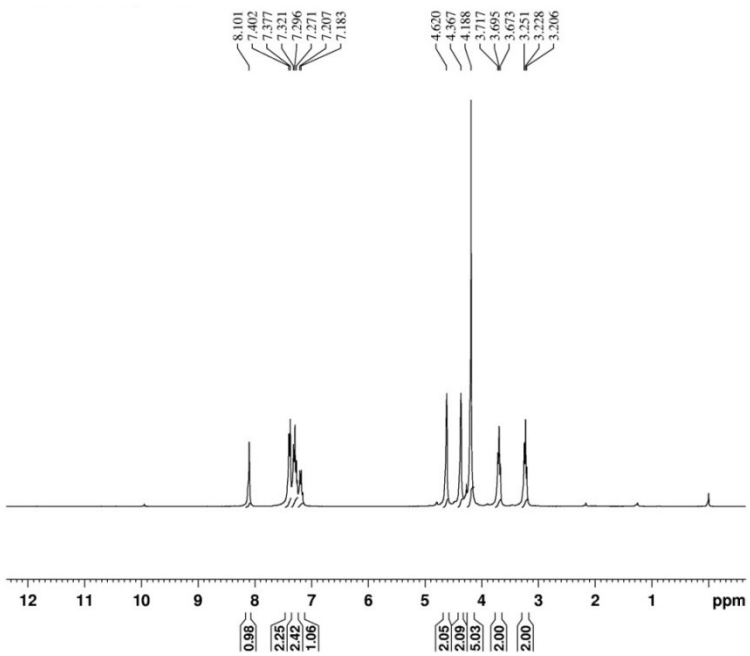
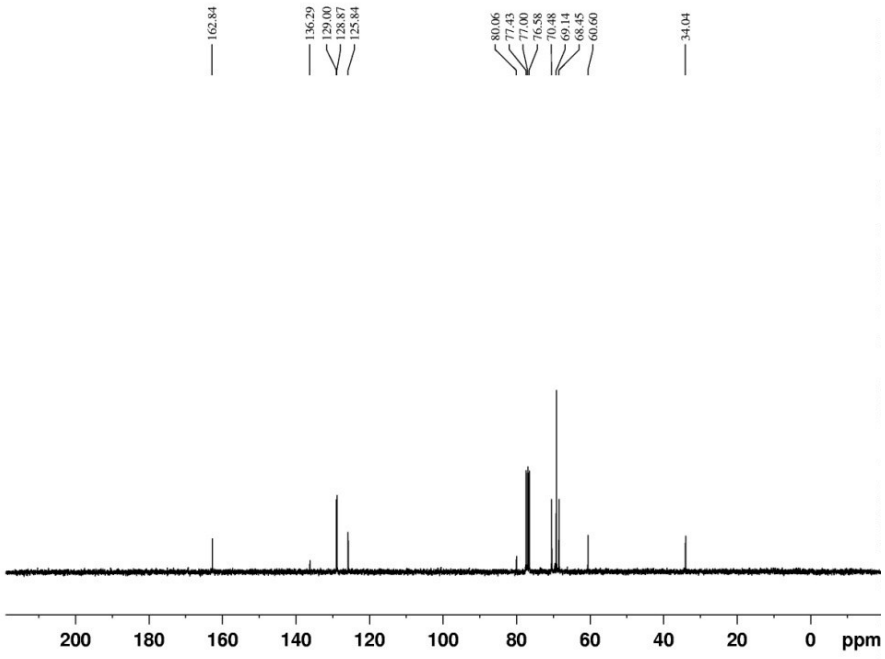


Fig S5 Mass spectrum of complex **3**

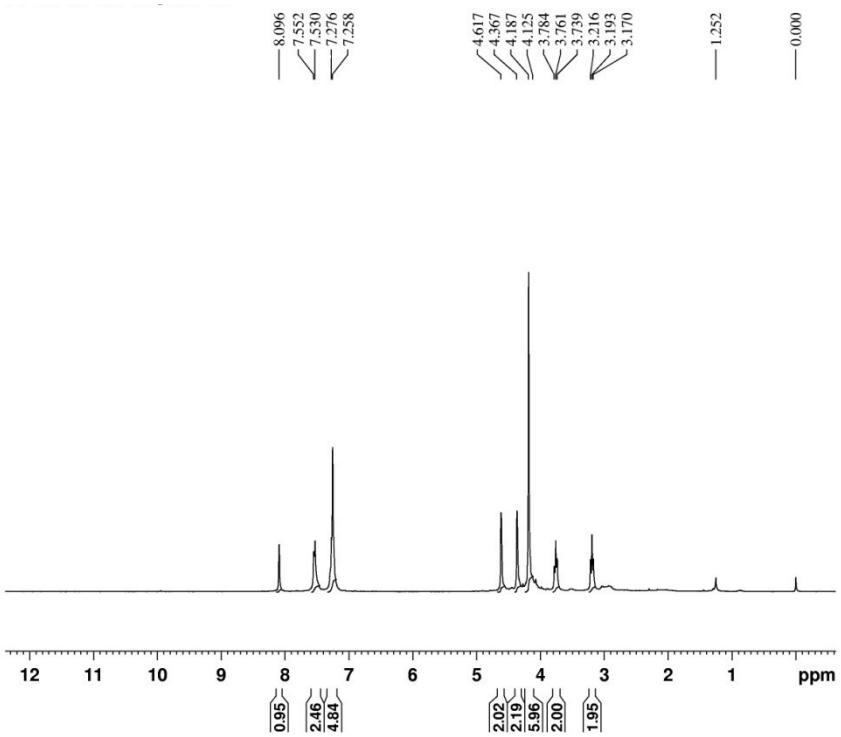
NMR spectra-



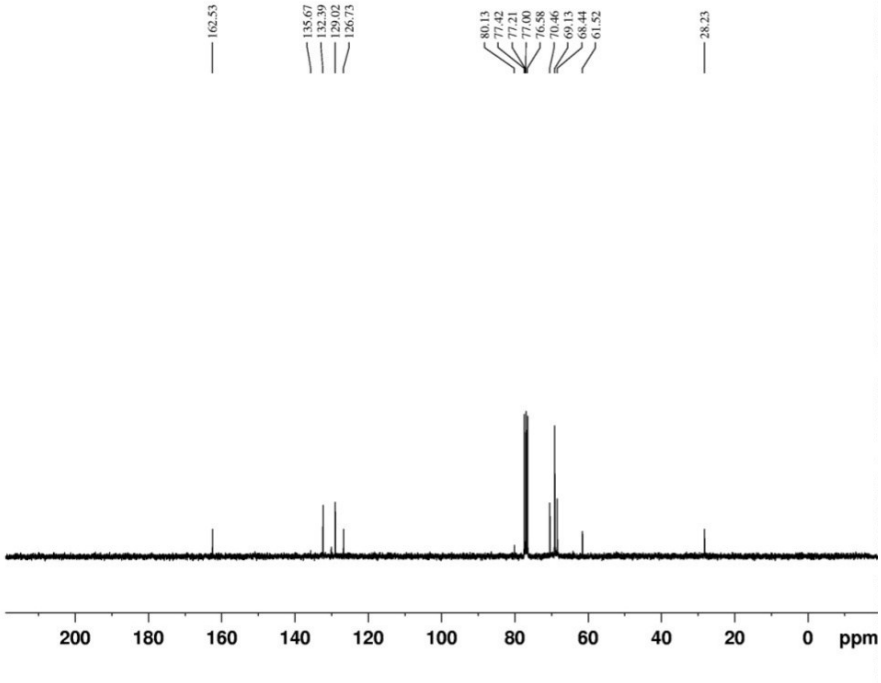
FigureS6 ^{1}H NMR spectrum of ligand **L1**



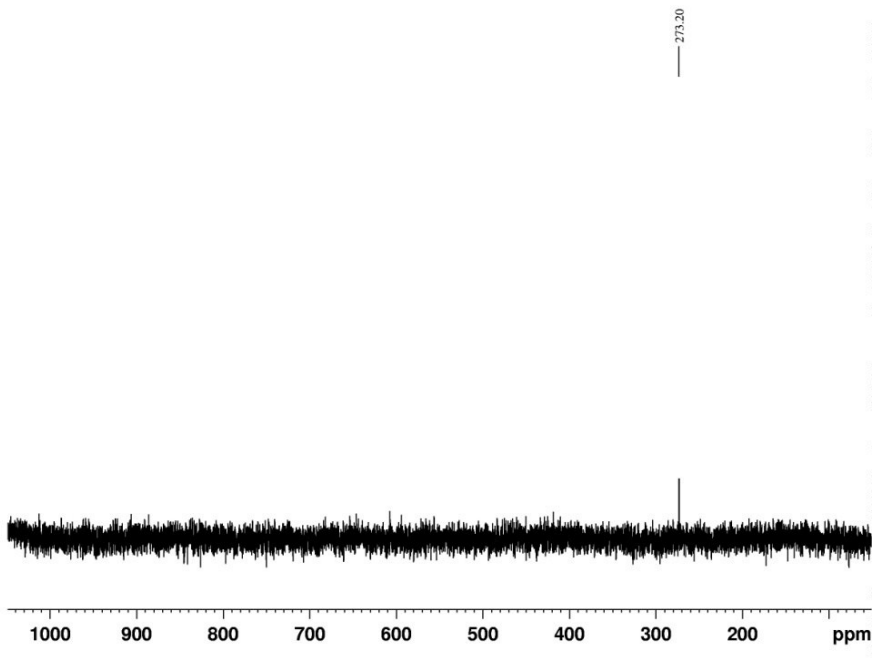
FigureS7 ^{13}C{^{1}H} NMR spectrum of ligand **L1**



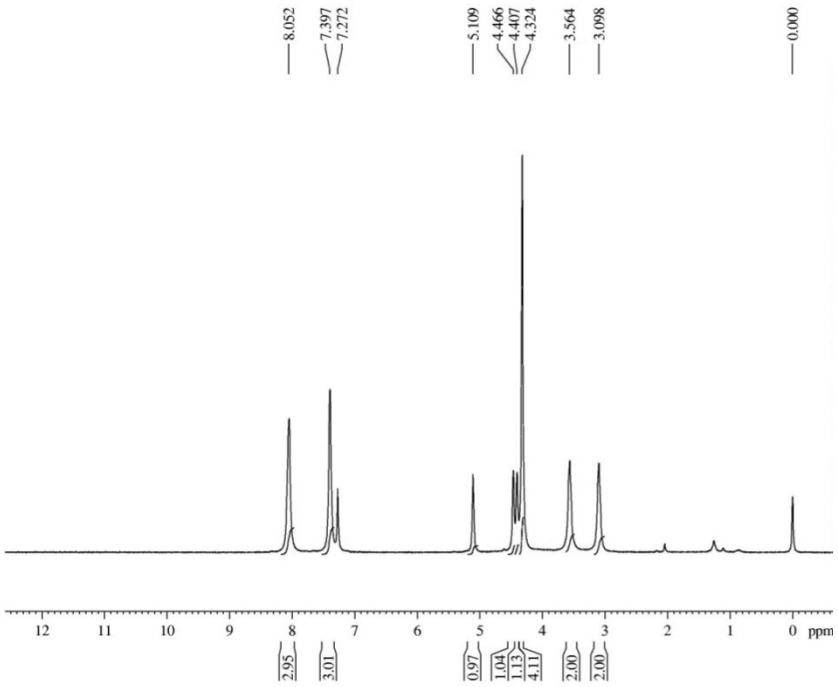
FigureS8 ^{1}H NMR spectrum of ligand **L2**



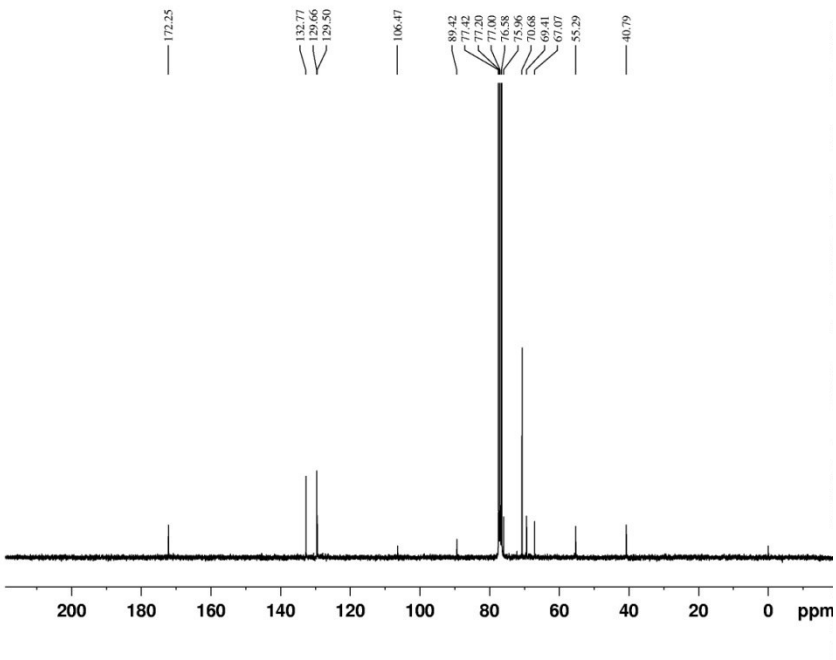
FigureS9 ^{13}C{^{1}H} NMR spectrum of ligand **L2**



FigureS10 $^{77}Se\{^{1}H\}$ NMR spectrum of ligand **L2**

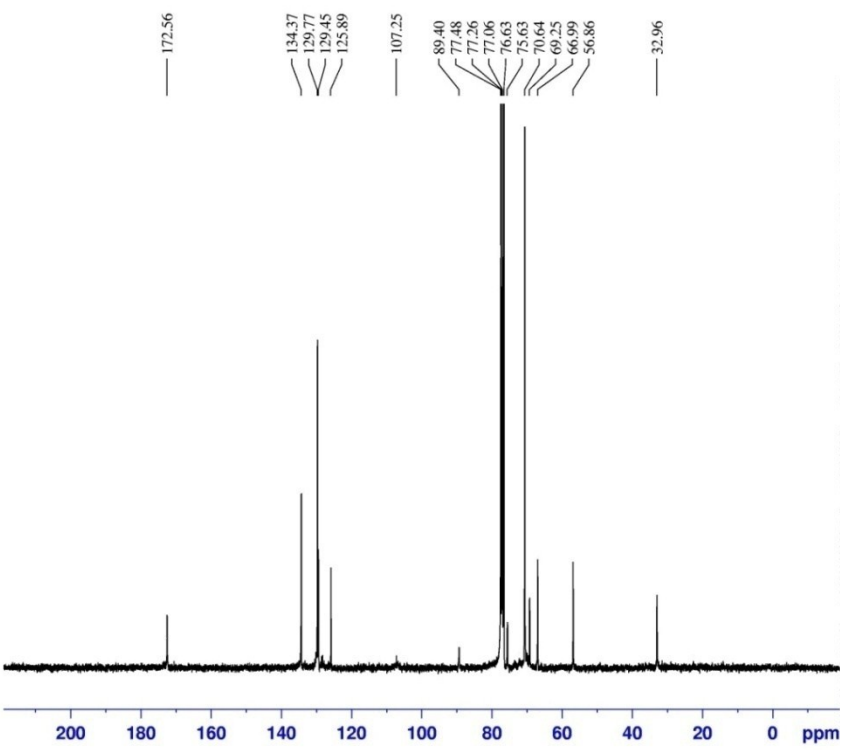


FigureS11 ^{1}H NMR spectrum of **1**

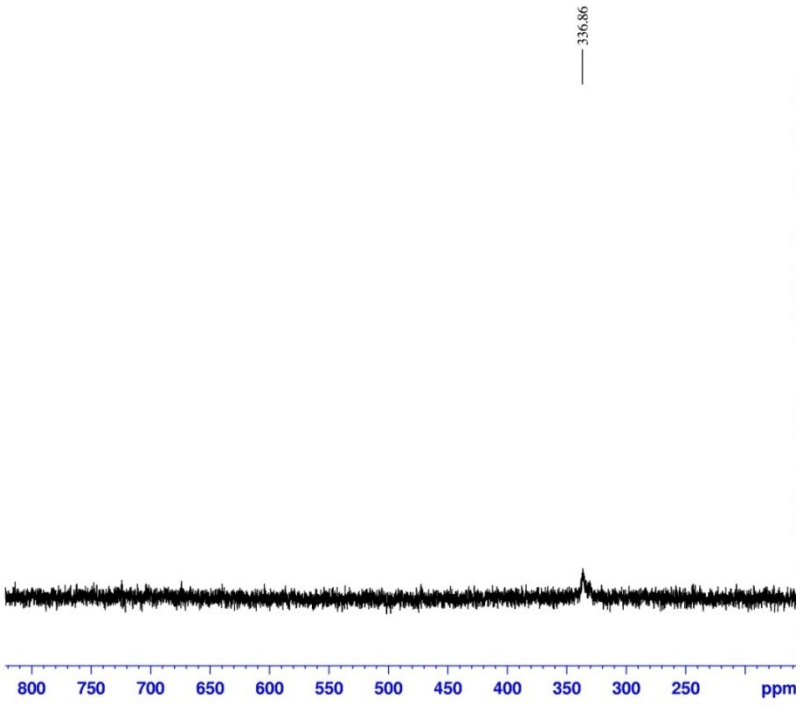


FigureS12 $^{13}C\{^{1}H\}$ NMR spectrum of **1**

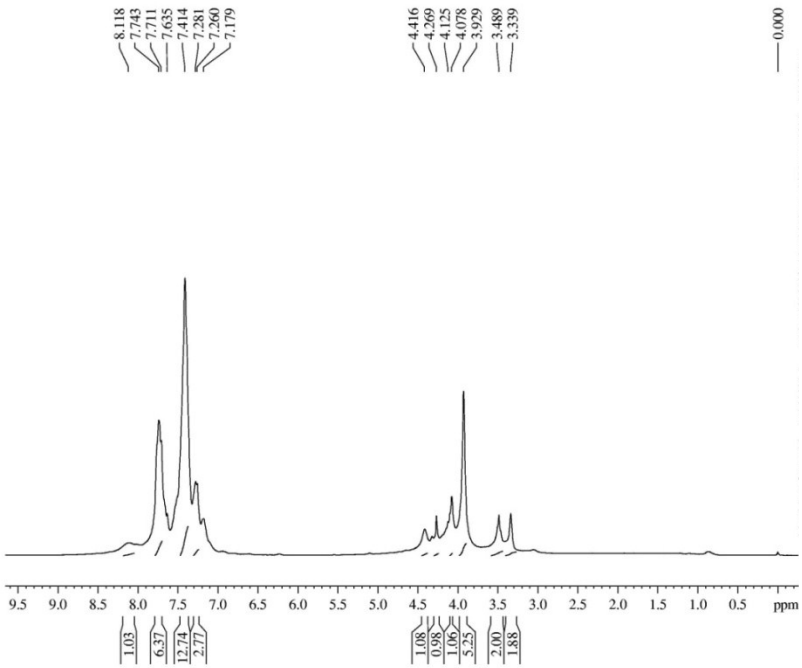
FigureS13 ^{1}H NMR spectrum of **2**



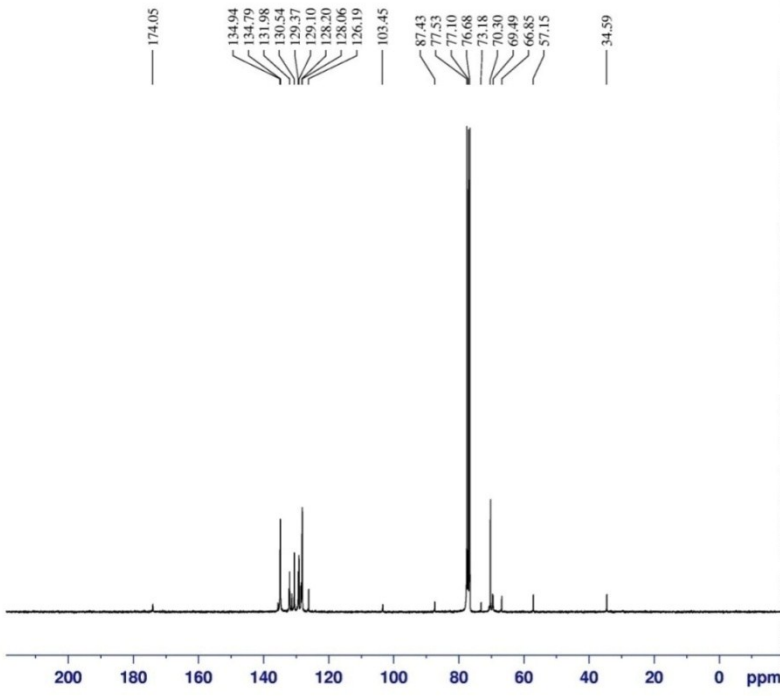
FigureS14 $^{13}C\{^{1}H\}$ NMR spectrum of **2**



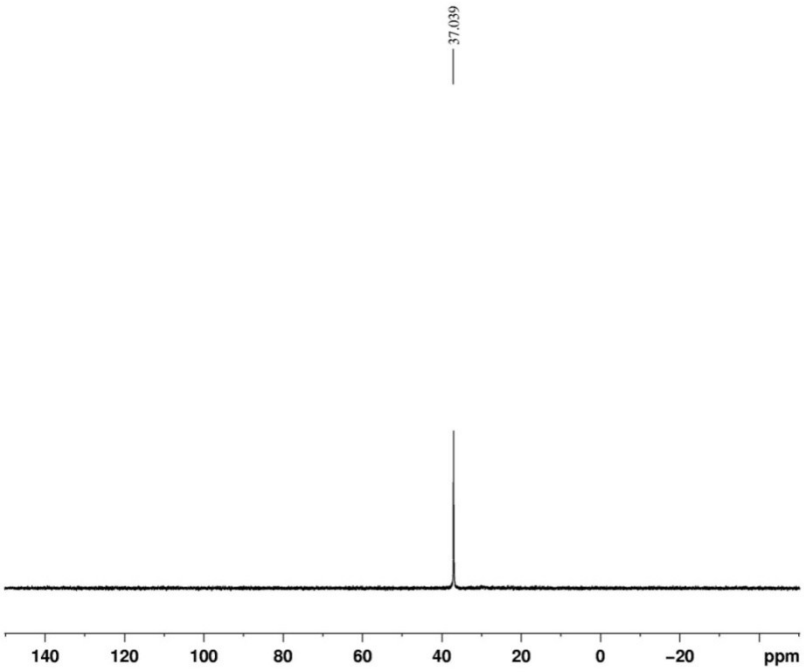
FigureS15 $^{77}Se\{^{1}H\}$ NMR spectrum of **2**



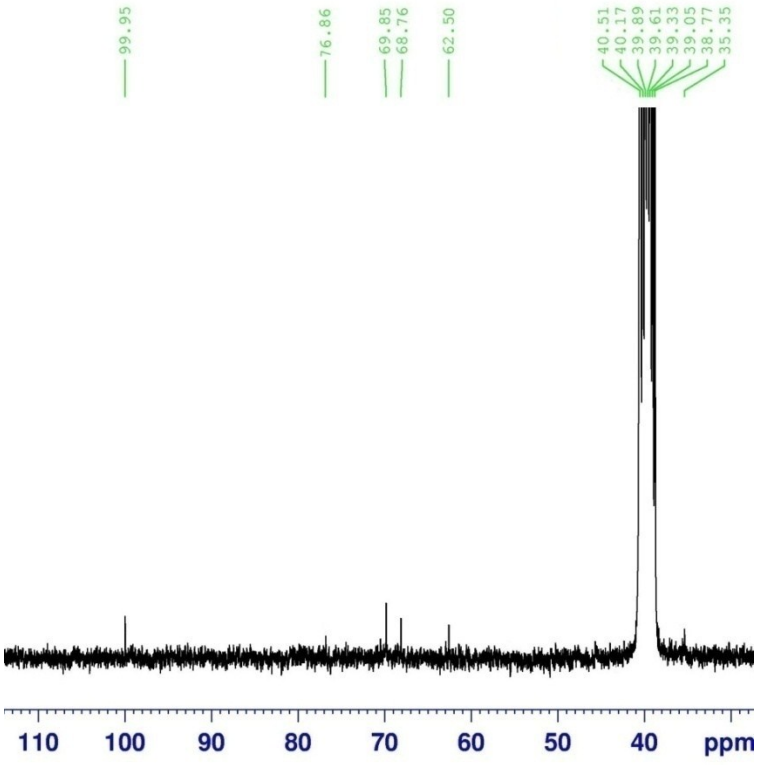
FigureS16 ^{1}H NMR spectrum of **3**



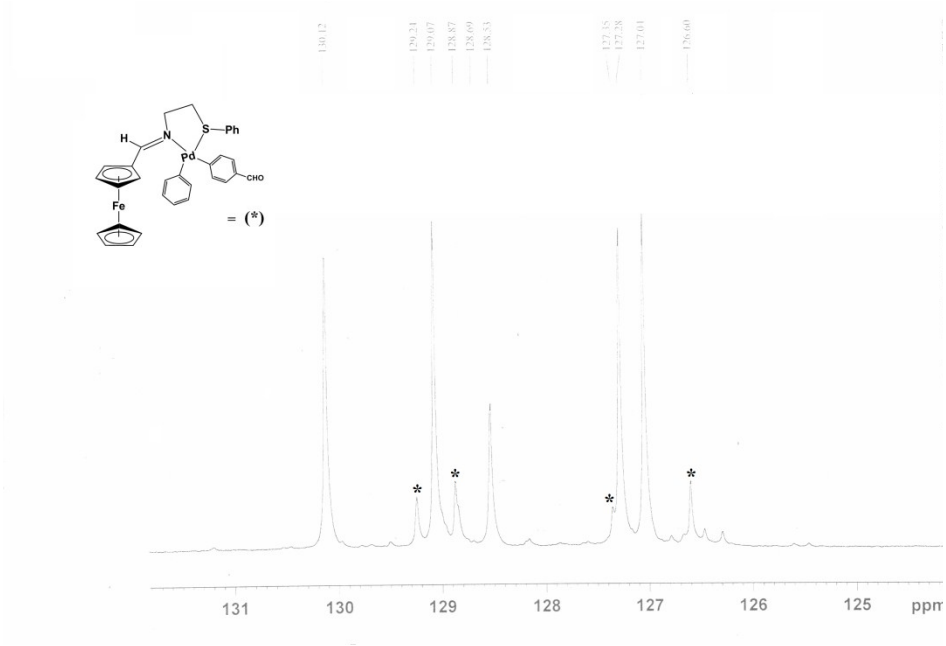
FigureS17 ^{13}C{^{1}H} NMR spectrum of **3**



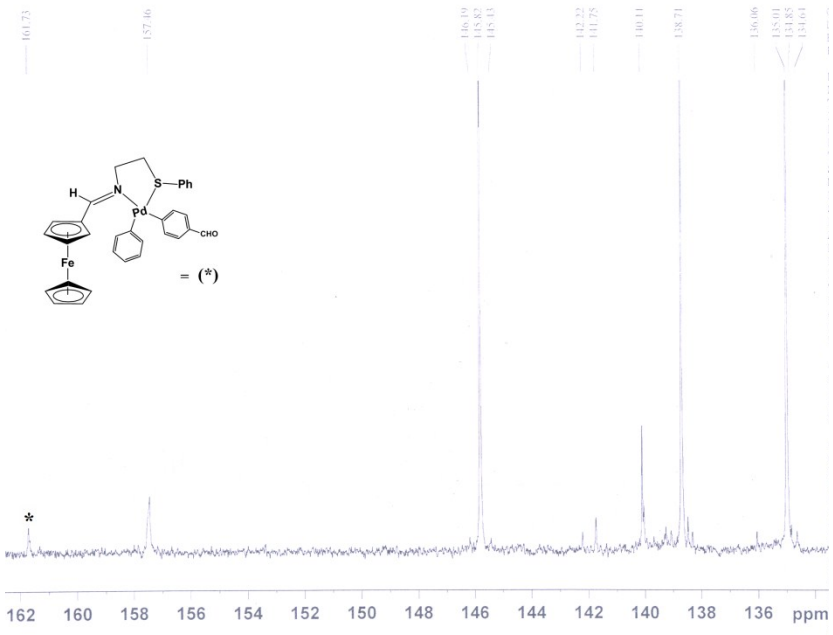
FigureS18 $^{31}P\{^{1}H\}$ NMR spectrum of **3**



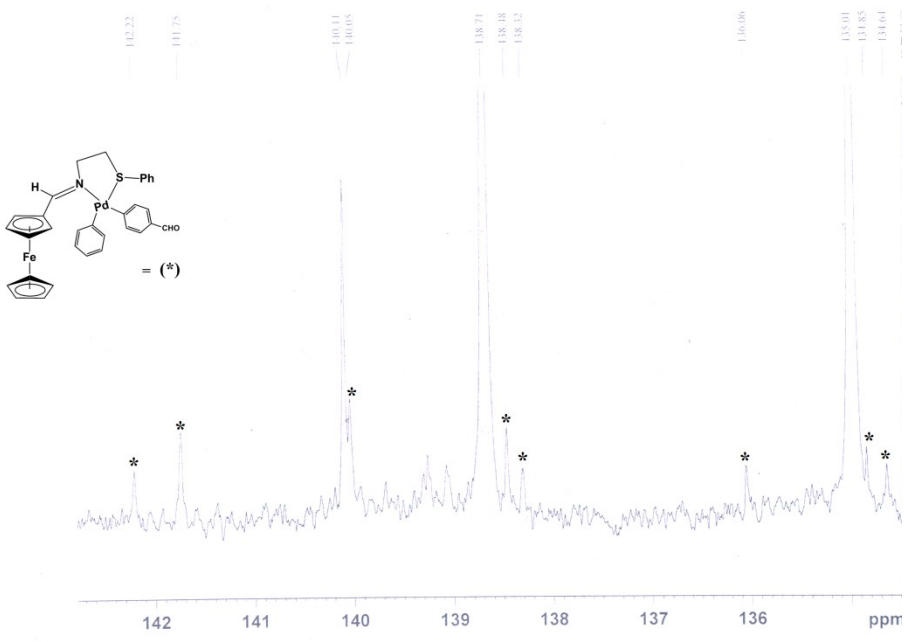
FigureS19 $^{13}C\{^{1}H\}$ NMR spectrum of catalysis reaction mixture (C-O coupling)



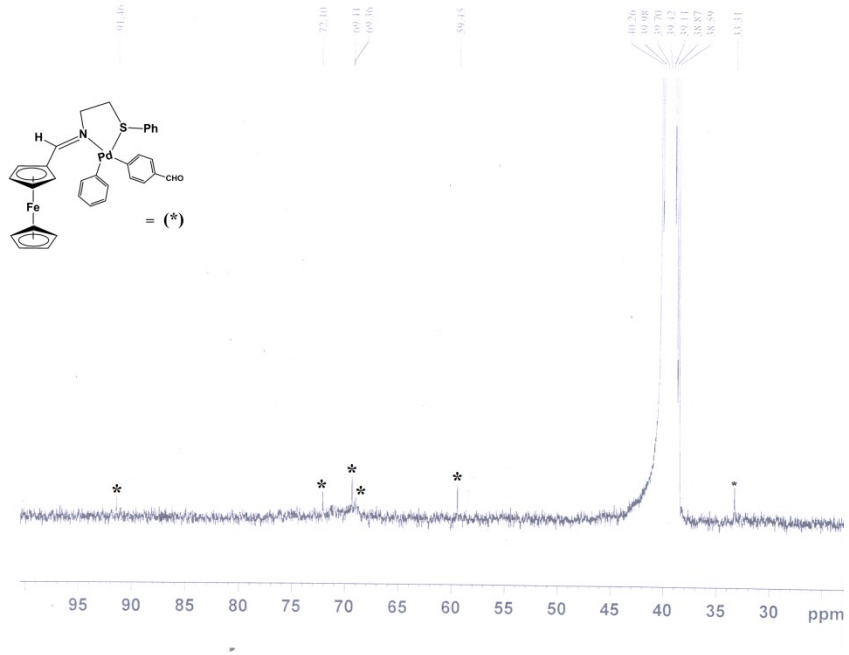
FigureS20 $^{13}C\{^{1}H\}$ NMR spectrum of catalysis reaction mixture (C-C coupling)



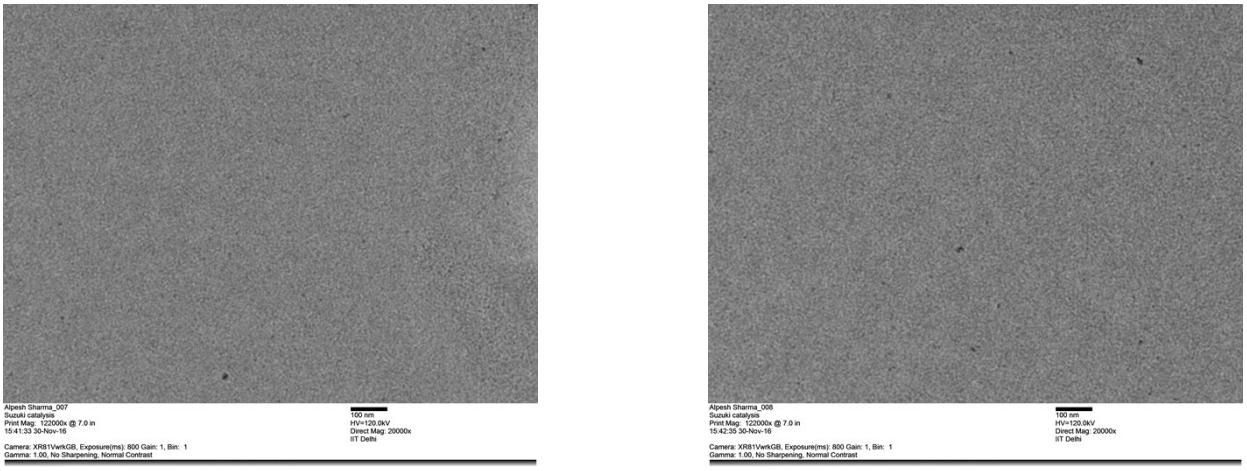
FigureS21 $^{13}C\{^{1}H\}$ NMR spectrum of catalysis reaction mixture (C-C coupling)



FigureS22 $^{13}C\{^{1}H\}$ NMR spectrum of catalysis reaction mixture (C-C coupling)



FigureS23 $^{13}C\{^{1}H\}$ NMR spectrum of catalysis reaction mixture (C-C coupling)



FigureS24 TEM images of catalysis reaction mixture (a) C-O coupling, (b) Suzuki-Miyaura coupling

NMR Data of products of C-O coupling reaction (3a-3j)-

4-phenoxybenzaldehyde (**3a**):[1] Yellow liquid. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): δ (ppm): 9.92 (s, 1H), 7.84-7.86 (d, 2H), 7.40-7.45 (t, 2H), 7.20-7.26 (m, 1H), 7.05-7.11 (t, 4H).

1-(4-phenoxyphenyl)ethanone (**3b**)**:**[1] White Solid. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): 7.91-7.96 (d, 2H), 7.36-7.42 (t, 2H), 7.19-7.22 (t, 1H), 7.06-7.08 (d, 2H), 6.97-7.02 (d, 2H), 2.57 (s, 3H).

1-Nitro-4-phenoxybenzene (**3c**):[2]Yellow Solid. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): 8.11-8.14 (d, 2H), 7.34-7.40 (t, 2H), 7.16-7.21 (t, 1H), 7.01-7.03 (d, 2H), 6.92-6.95 (d, 2H).

4-phenoxybenzonitrile (**3d**):[1]White Solid. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si):7.49-7.55 (m, 2H), 7.30-7.35 (t, 2H), 7.11-7.17 (t, 1H), 6.96-6.98 (d, 2H), 6.90-6.93(d, 2H).

2-phenoxybenzaldehyde (**3e**):[1]Yellow liquid. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): 10.45 (s, 1H), 7.85-7.88 (d, 1H), 7.41-7.47 (t, 1H), 7.30-7.35 (t, 2H), 7.10-7.14 (t, 2H), 6.98-7.01 (d, 2H), 6.81-6.84 (d, 1H).

1-(2-phenoxyphenyl)ethanone (**3f**):[2]Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): 7.83-7.86 (d, 1H), 7.35-7.45 (m, 3H), 7.15-7.20 (m, 2H), 7.01-7.03 (d, 2H) 6.90-6.92 (d, 2H) 2.64 (s, 3H).

Diphenyl ether (**3g**):[2]Colorless liquid. ^{1}H NMR(300 MHz, $CDCl_3$, 25°C vs Me_4Si): 7.24-7.28 (t, 4H), 7.02-7.05 (t, 2H), 6.93- 6.95 (d, 4H).

1-Methyl-4-phenoxybenzene(3h):[2]Colorless liquid. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): 7.46-7.48 (m, 2H), 7.23-7.26 (t, 2H), 7.06- 7.07 (m, 1H), 6.98-7.04 (m, 2H), 6.89-6.91 (m, 2H), 2.26 (s, 3H).

1-Methoxy-4-phenoxybenzene(3i):[1]Colorless liquid. 1H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): 7.25-7.32 (m, 2H), 7.01-7.06 (t, 1H), 6.93- 7.01 (m, 4H), 6.86-6.90 (m, 2H), 3.81 (s, 3H).

2-phenoxypyridine(3j):[3] Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): 8.12-8.13 (m, 1H), 7.58-7.62 (t, 1H), 7.31-7.35 (t, 2H), 7.05-7.18 (m, 3H), 6.90-6.93 (t, 1H), 6.81-6.84 (d, 1H).

NMR Data of products of Suzuki-Miyaura coupling reaction (6a-6i)-

4−Phenylbenzaldehyde(6a):[4] Light yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): δ 10.06 (s, 1H),7.95 (d, J = 8.4 Hz, 2H),7.75 (d, J = 8.4 Hz, 2H),7.63−7.65 (m, 2H),7.39−7.51 (m, 3H).

4-Nitrobiphenyl(6b):[5] Pale yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): δ 8.27 (d, J = 9.0 Hz, 2H), 7.71 (d, J = 9.0 Hz, 2H), 7.61 (d, J = 8.4 Hz, 2H), 7.41−7.51 (m, 3H).

4-Phenylbenzonitrile(6c):[5] Pale yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): δ 7.54−7.61 (m, 4H), 7.49−7.52 (m, 2H), 7.34−7.45 (m, 3H).

4−Acetylbiphenyl(6d):[5] White solid. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): 8.02 (d, J = 8.4 Hz, 2H), 7.60−7.68 (m, 4H), 7.38−7.48 (m, 3H), δ 2.62 (s, 3H).

Biphenyl(6e): [5] White solid: ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): 7.58 (d, J = 6.9 Hz, 4H),7.42 (t, J = 7.5 Hz, 4H),δ 7.33 (t, J = 7.5 Hz, 2H).

Biphenyl-4-carboxylic acid(6f):[6] White solid. ^{1}H NMR (300 MHz, DMSO, 25°C vs Me_4Si): δ, 8.03 (d, J = 8.4 Hz, 2H), 7.79 (d, J = 8.4 Hz, 2H),7.73 (d, J = 6.9 Hz, 2H), 7.39−7.52 (m, 3H).

4−Phenylpyridine (6g):[7]Brown solid. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): 8.65 (d, J = 5.4 Hz, 2H),7.62 (d, J = 8.1 Hz, 2 H),δ 7.40−7.50 (m, 5H).

4-Methylbiphenyl (6h):[5] Colorless solid. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): 7.55−7.58 (m, 2H),7.48 (d, J = 8.1 Hz, 2H),7.38−7.42 (m, 2H),7.27−7.32 (m, 1H),7.23 (d, J = 7.8 Hz, 2H),δ 2.37 (s, 3H).

4-Methoxybiphenyl (6i):[5] White solid. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C vs Me_4Si): 7.50−7.55 (m, 4H), 7.40 (t, J = 7.2 Hz, 2H),7.28−7.31 (m, 1H),6.96 (d, J = 8.4 Hz, 2H),δ 3.82 (s, 3H).

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