ESI *for*

Base free *N*-alkylation of anilines with $ArCH_2OH$ and transfer hydrogenation of aldehydes/ketones catalyzed with complexes of η^5-Cp*Ir(III) with chalcogenated Schiff bases of anthracene-9-carbaldehyde

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Content

Table S1. Crystal data and structural refinement parameters of **L2**

Compounds	**L2**
Empirical formula	C23 H19 N Se
Formula wt.	388.35
Crystal size [mm]	0.34 x 0.32 x 0.28
Crystal system	Monoclinic
Space group	P 21/c
Unit Cell dimension	a = 18.368(5) b = 5.1780(14) c = 20.341(5) α = 90° β =96.023(6)° γ = 90°
Volume [Å3]	1806.6(8)
Z	4
Density (Calc.) [Mg.m –3]	1.428
Absorption coeff. [mm–1]	2.083
F(000)	792.0
θ range [°]	1.187– 24.982
Index ranges	-21<=h<=16, -6<=k<=6 -24<=l<=19
Reflections collected	7368
Independent reflections (Rint.)	3170 (0.0637)
Max./min. Transmission	0.557/0.498
Data/restraints/parameters	3170/0/226
Goodnessoffit on F2	0.946
Final R indices [I >2σ(I)]	R1 = 0.0610 wR2 = 0.1322
R indices (all data)	R1 = 0.1097 wR2 = 0.1661
Largest diff. peak/hole [e.Å^3]	0.507/-0.368
CCDC No.	1573735

Table S2. Crystal data and structural refinement parameters of **1** and **2**

Compounds	**1**	**2**
Empirical formula	C33 H33 F6 Ir N P S	C33 H33 F6 Ir N P Se
Formula wt.	812.85	859.75
Crystal size [mm]	0.32 x 0.20 x 0.08	0.33 x 0.32 x 0.29
Crystal system	Monoclinic	Monoclinic
Space group	P 21	P 21
Unit Cell dimension	a = 8.9391(4) Å b = 18.8103(8)Å c = 9.2977(4) Å α = 90° β = 105.3090(10)° γ = 90°	a = 9.0129(17)Å b = 18.866(4))Å c = 9.4669(19)Å α = 90° β = 104.644(4)° γ = 90°
Volume [Å3]	1507.91(11)	1557.4(5)
Z	2	2
Density (Calc.) [Mg.m –3]	1.790	1.833
Absorption coeff. [mm–1]	4.612	5.567
F(000)	800.0	836.0
θ range [°]	2.27–28.300	2.16–19.34
Index ranges	-11<=h<=11 -25<=k<=25 -12<=l<=12	-10<=h<=9 -16<=k<=22 -11<=l<=11
Reflections collected	28172	7551
Independent reflections ($R_{int.}$)	7492 (0.0900)	5489 (0.0409)
Max./min. Transmission	0.468/0.345	0.200/0.156
Data/restraints/parameters	7492/1/393	5489/1/393
Goodness of fit on F_2	1.016	1.017
Final R indices [I >2σ(I)]	R1 = 0.0337, wR2 = 0.0917	R_1 = 0.0456, wR_2 = 0.0849
R indices (all data)	R1 = 0.0344, wR2 = 0.0922	R_1 = 0.0554, wR_2 = 0.0886
Largest diff. peak/hole [e.Å–3]	1.365/-1.682	1.392/-0.582
CCDC No.	1816978	1573738

Table S3. Crystal data and structural refinement parameters of **3** and **4**

Compounds	**3**	**4**
Empirical formula	C33 H34 Cl F6 Ir N P S	C33 H34 Cl F6 Ir N P Se
Formula wt.	849.31	896.21
Crystal size [mm]	0.31 x 0.30 x 0.28	0.35 x 0.31 x 0.29

Crystal system	Monoclinic	Monoclinic
Space group	P21/c	P21/c
Unit Cell dimension	a = 12.252(2) Å b = 13.705(2) Å c = 19.940(3) Å α = 90° β = 105.778(4) γ = 90°	a = 12.2212(6) Å b = 13.7085(7) Å c = 20.0843(11) Å α = 90° β = 105.1270(10) γ = 90°
Volume [Å3]	3222.1(9)	3248.2(3)
Z	4	4
Density (Calc.) [Mg.m –3]	1.751	1.833
Absorption coeff. [mm–1]	4.401	5.422
F(000)	1672.0	1744.0
θ range [°]	2.28–18.39	2.28–28.33
Index ranges	-14<=h<=14 -16<=k<= 10 -20<=l<=23	-16<=h<=16 -18<=k<= 18 -26<=l<=26
Reflections collected	13663	90693
Independent reflections (Rint.)	5672 (0.0659)	8133 (0.0460)
Max./min. Transmission	0.292/0.279	0.208/0.164
Data/restraints/parameters	5672 / 0 / 402	8133 /0/402
Goodness of fit on F2	0.938	1.024
Final R indices [I >2σ(I)]	R1 =0.0645, wR2 = 0.1475	R1 = 0.0192, wR2 = 0.0404
R indices (all data)	R1 = 0.0910, wR2 = 0.1636	R1 = 0.0288, wR2 = 0.0431
Largest diff. peak/hole [e.Å–3]	1.207/-2.261	0.435/-0.680
CCDC No.	1573739	1816993

Table S4. Selected bond lengths [Å] and bond angles [°]

	Bond length [Å]	Bond angle [o]
L2	Se(1)—C(18) 1.922(6) Se(1)—C(17) 1.961(6) N(1)—C(15) 1.247(8) N(1)—C(16) 1.464(7)	C(18) — Se(1)— C(17) 96.7(3) C(15)— N(1)— C(16) 117.0(5) N(1)— C(15)—C(14) 124.7(6)
1	Ir(1)—S(1) 2.326(2) Ir (1)—N(1) 2.047(6) Ir (1)—C(12) 2.050(7) S(1)—C(18) 1.775(14) S(1)—C(17) 1.841(18) N(1)—C(15) 1.280(9) N(1)—C(16) 1.475(9) C(24) — Ir(1) 2.212(6) C(26) — Ir(1) 2.173(7) C(28) — Ir(1) 2.244(7) C(30) — Ir(1) 2.165(13) C(32) — Ir(1) 2.186(6)	C(12)—Ir(1)—S(1) 98.1(3) N(1)— Ir(1)—S(1) 82.0(3) C(12)— Ir(1)—N(1) 85.1(2) S(1)— Ir(1)— C(32) 104.23(19) S(1)— Ir(1)— C(30) 155.3(4) S(1)— Ir(1)— C(28) 118.8(2) S(1)— Ir(1)— C(26) 156.82(19) S(1)— Ir(1)— C(24) 140.17(18) C(18)— S(1)— Ir(1) 113.7(3) C(17)— S(1)— Ir(1) 101.5(3) N(1)— Ir(1)— C(32) 162.7(3) N(1)— Ir(1)— C(30) 126.4(3) N(1)— Ir(1)— C(28) 99.4(3) N(1)— Ir(1)— C(26) 104.2(2) N(1)— Ir(1)— C(24) 138.1(2) C(15)— N(1)— Ir(1) 124.9(5) C(16)— N(1)— Ir(1) 114.2(4) C(12)— Ir(1)— C(32) 109.7(3) C(12)— Ir(1)— C(30) 147.5(3) C(12)— Ir(1)— C(28) 143.4(2) C(12)— Ir(1)— C(26) 104.9(3) C(12))— Ir(1)— C(24) 89.0(3) C(11)— C(12)— Ir(1) 122.4(5) C(13)— C(12)— Ir(1) 118.2(5)
2	Ir(1)—Se(1) 2.4474(18) Ir (1)—N(1) 2.057(11) Ir (1)—C(2) 2.064(12) Se(1)—C(18) 1.943(15) Se(1)—C(17) 2.01(2) N(1)—C(15) 1.277(18) N(1)—C(16) 1.465(16) C(24) — Ir(1) 2.240(14) C(26) — Ir(1) 2.178(15) C(28) — Ir(1) 2.200(15) C(30) — Ir(1) 2.192(15)	C(2)—Ir(1)—Se(1) 98.4(3) N(1)— Ir(1)—Se(1) 82.5(3) C(2)— Ir (1)—N(1) 85.7(5) Se(1)— Ir(1)— C(32) 94.3(6) Se(1)— Ir(1)— C(30) 105.2(4) Se(1)— Ir(1)— C(28) 141.4(6) Se(1)— Ir(1)— C(26) 154.3(5) Se(1)— Ir(1)— C(24) 116.4(5) C(18)— Se(1)— Ir(1) 111.3(5) C(17)— Se(1)— Ir(1) 96.6(5) N(1)— Ir(1)— C(32) 127.9(5) N(1)— Ir(1)— C(30) 163.4(5) N(1)— Ir(1)— C(28) 136.0(7)

	C(32) — Ir(1) 2.256(13)	N(1)— Ir(1)— C(26) 102.5(6) N(1)— Ir(1)— C(24) 99.8(6) C(15)— N(1)— Ir(1) 123.5(11) C(16)— N(1)— Ir(1) 115.9(10) C(2)— Ir(1)— C(32) 145.5(6) C(2)— Ir(1)— C(30) 107.2(6) C(2)— Ir(1)— C(28) 88.5(5) C(2)— Ir(1)— C(26) 88.5(4) C(2))— Ir(1)— C(24) 145.1(6) C(1)— C(2)— Ir(1) 117.7(10) C(3)— C(2)— Ir(1) 122.6(10)
3	Ir(1)—S(1) 2.353(2) Ir (1)—Cl(1) 2.398(3) Ir (1)—N(1) 2.085(7) S(1)—C(17) 1.833(10) S(1)—C(18) 1.790(11) N(1)—C(15) 1.272(11) N(1)—C(16) 1.449(12) C(24) — Ir(1) 2.171(9) C(26) — Ir(1) 2.177(9) C(28) — Ir(1) 2.167(9) C(30) — Ir(1) 2.203(9) C(32) — Ir(1) 2.163(9)	Cl(1)—Ir(1)—S(1) 92.41(10) N(1)— Ir (1)—S(1) 82.5(2) Cl(1)— Ir (1)—N(1) 84.5(2) S(1)— Ir(1)— C(32) 159.9(3) S(1)— Ir(1)— C(30) 135.6(3) S(1)— Ir(1)— C(28) 101.0(2) S(1)— Ir(1)— C(26) 96.5(3) S(1)— Ir(1)— C(24) 124.0(2) N(1)— Ir(1)— C(32) 115.1(3) N(1)— Ir(1)— C(30) 131.7(3) N(1)— Ir(1)— C(28) 111.5(3) N(1)— Ir(1)— C(26) 149.1(3) N(1)— Ir(1)— C(24) 153.4(3) Cl(1)— Ir(1)— C(32) 98.7(3) Cl (1)— Ir(1)— C(30) 95.9(3) Cl (1)— Ir(1)— C(28) 160.2(3) Cl (1)— Ir(1)— C(26) 126.4(3) Cl (1)— Ir(1)— C(24) 95.5(3)
4	Ir(1)—Se(1) 2.4614(3) Ir (1)—Cl(1) 2.3932(6) Ir (1)—N(1) 2.1058(17) Se(1)—C(17) 1.959(2) Se(1)—C(18) 1.929(3) N(1)—C(15) 1.271(3) N(1)—C(16) 1.473(3) C(24) — Ir(1) 2.183(2) C(26) — Ir(1) 2.176(2) C(28) — Ir(1) 2.172(2) C(30) — Ir(1) 2.192(2) C(32) — Ir(1) 2.165(2)	Cl(1)—Ir(1)—Se(1) 92.985(19) N(1)— Ir (1)—Se(1) 83.67(6) Cl(1)— Ir (1)—N(1) 84.19(5) Se(1)— Ir(1)— C(32) 99.86(7) Se(1)— Ir(1)— C(30) 134.84(7) Se(1)— Ir(1)— C(28) 158.98(6) Se(1)— Ir(1)— C(26) 122.71(6) Se(1)— Ir(1)— C(24) 94.70(7) N(1)— Ir(1)— C(32) 111.81(9) N(1)— Ir(1)— C(30) 96.27(8) N(1)— Ir(1)— C(28) 114.65(8) N(1)— Ir(1)— C(26) 153.50(8) N(1)— Ir(1)— C(24) 149.91(9) Cl(1)— Ir(1)— C(32) 160.36(7)

		Cl (1)— Ir(1)— C(30) 132.06(7) Cl (1)— Ir(1)— C(28) 98.84(7) Cl (1)— Ir(1)— C(26) 95.80(7) Cl (1)— Ir(1)— C(24) 125.88(7)

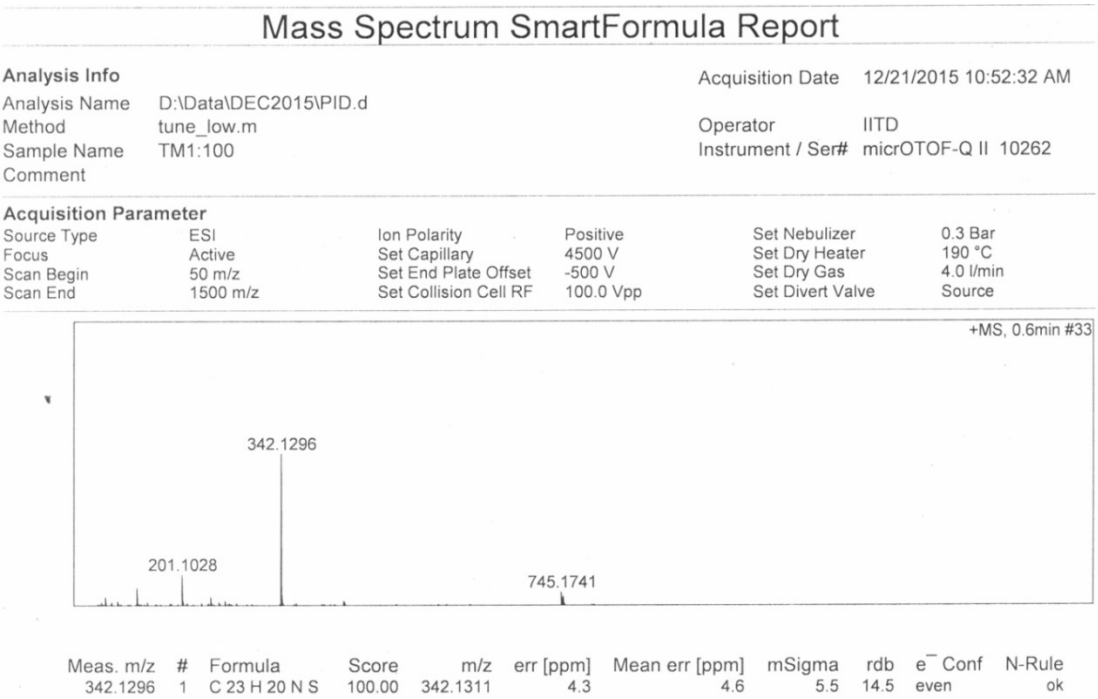

Fig. S1. Mass spectra of Ligand **L1**

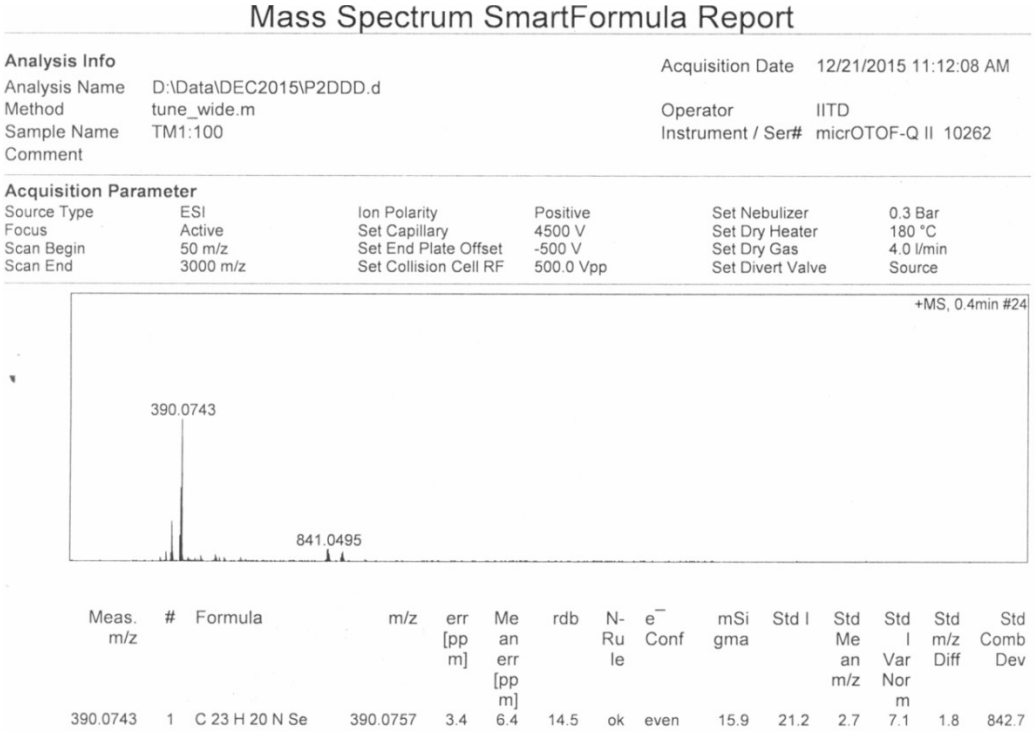

Figure S2. Mass spectra of Ligand L2

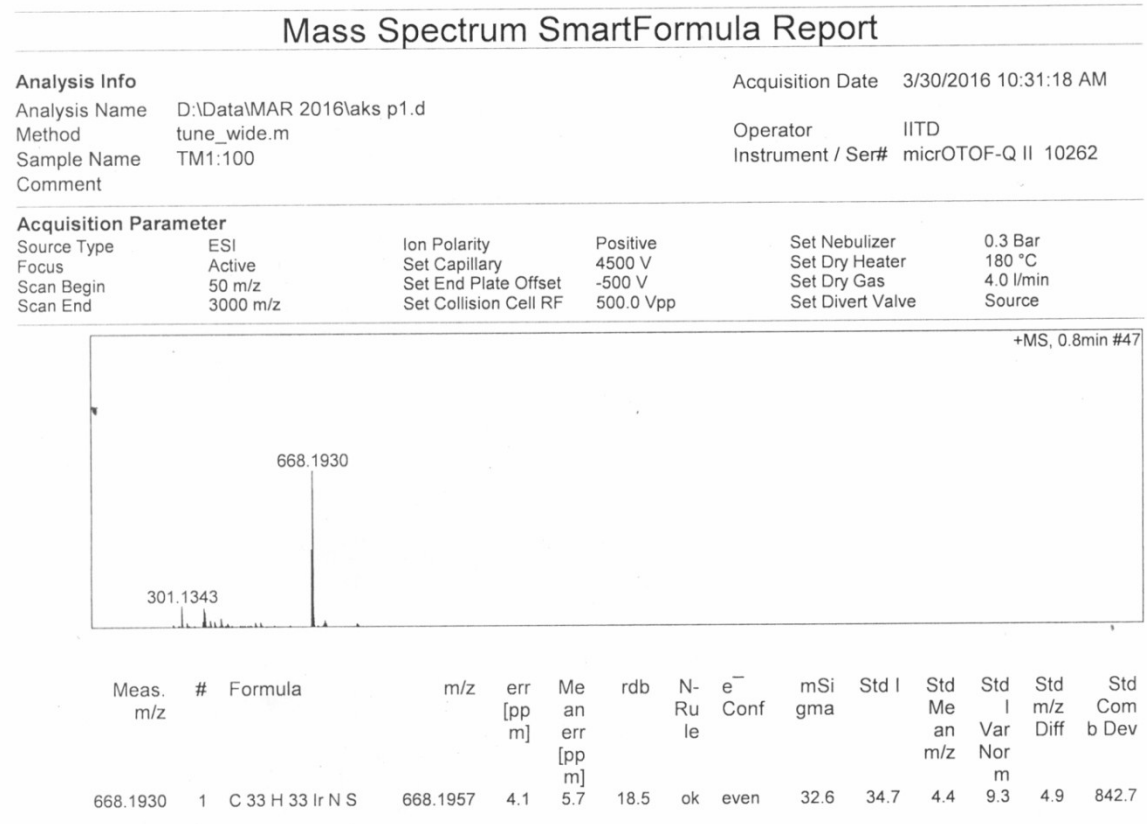

Fig. S3. Mass spectra of Complex **1**

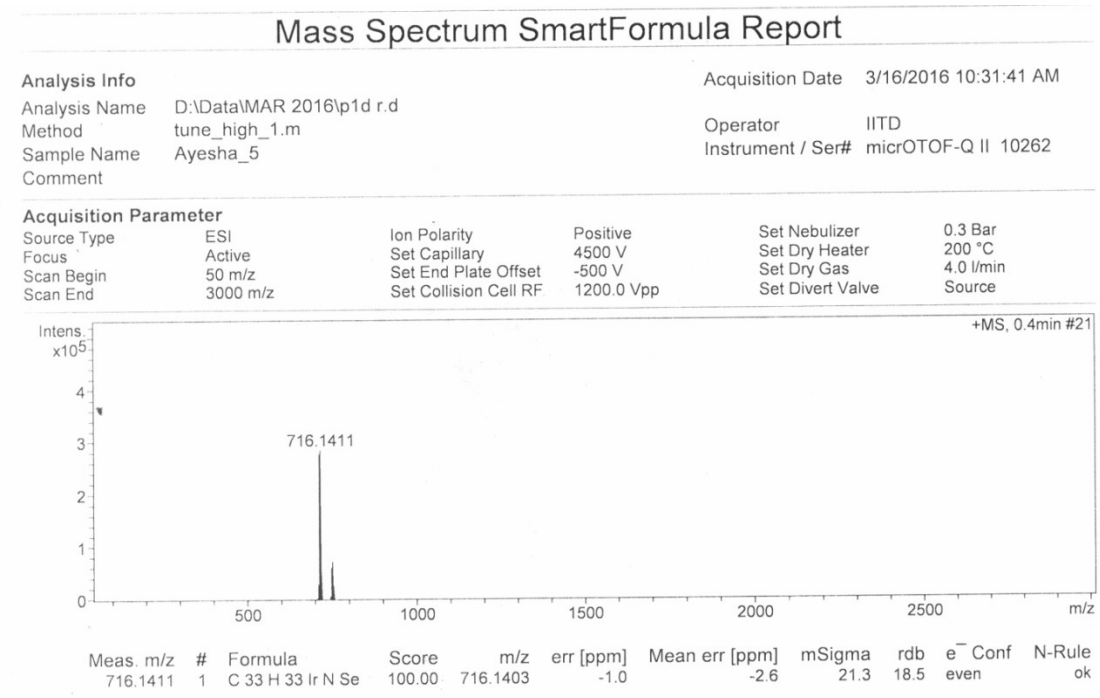

Fig. S4. Mass spectra of Complex **2**

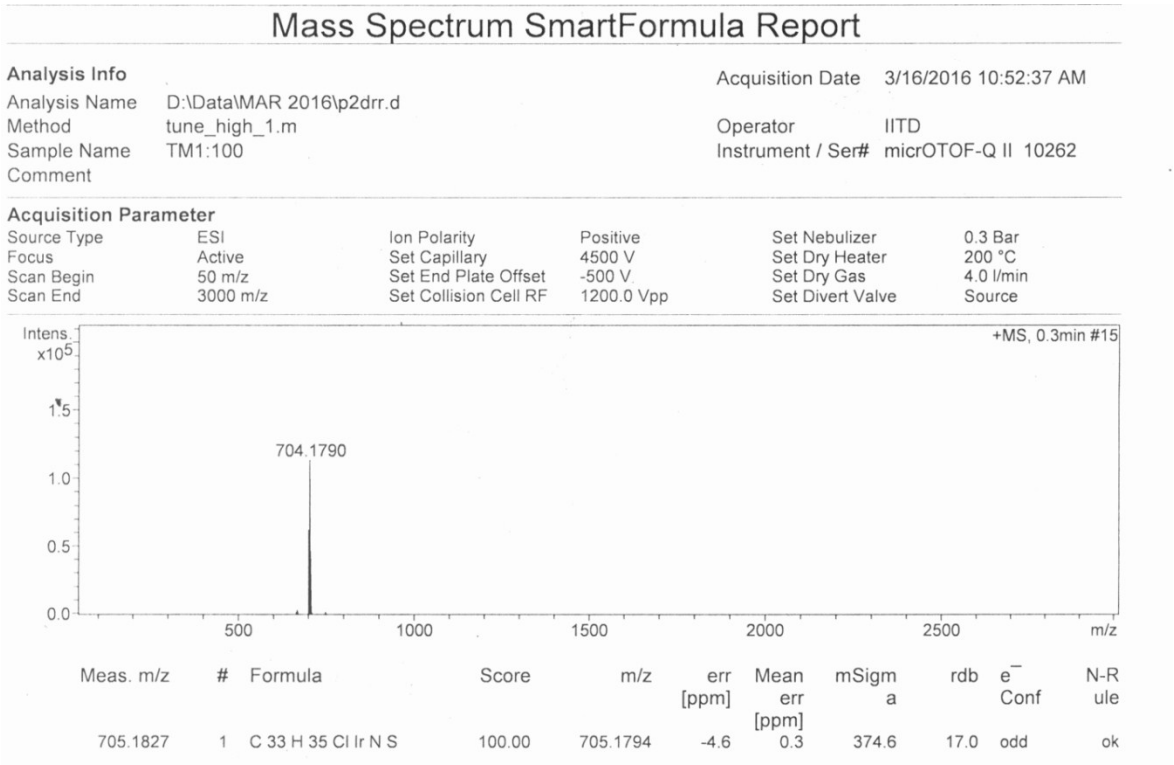

Fig. S5. Mass spectra of Complex **3**

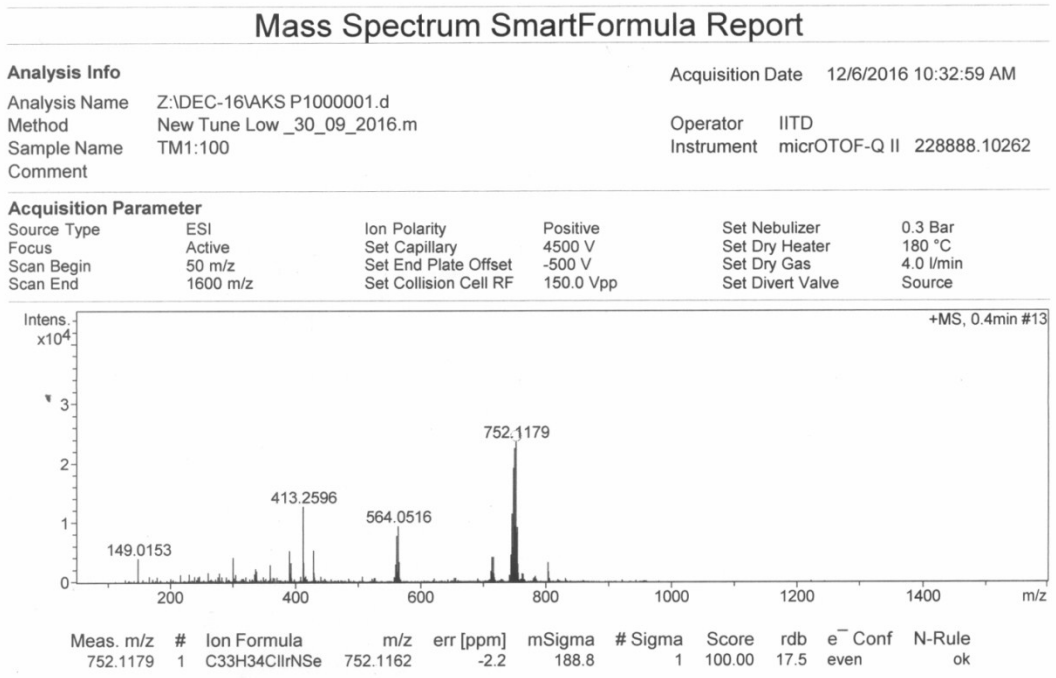

Fig. S6. Mass spectra of Complex **4**

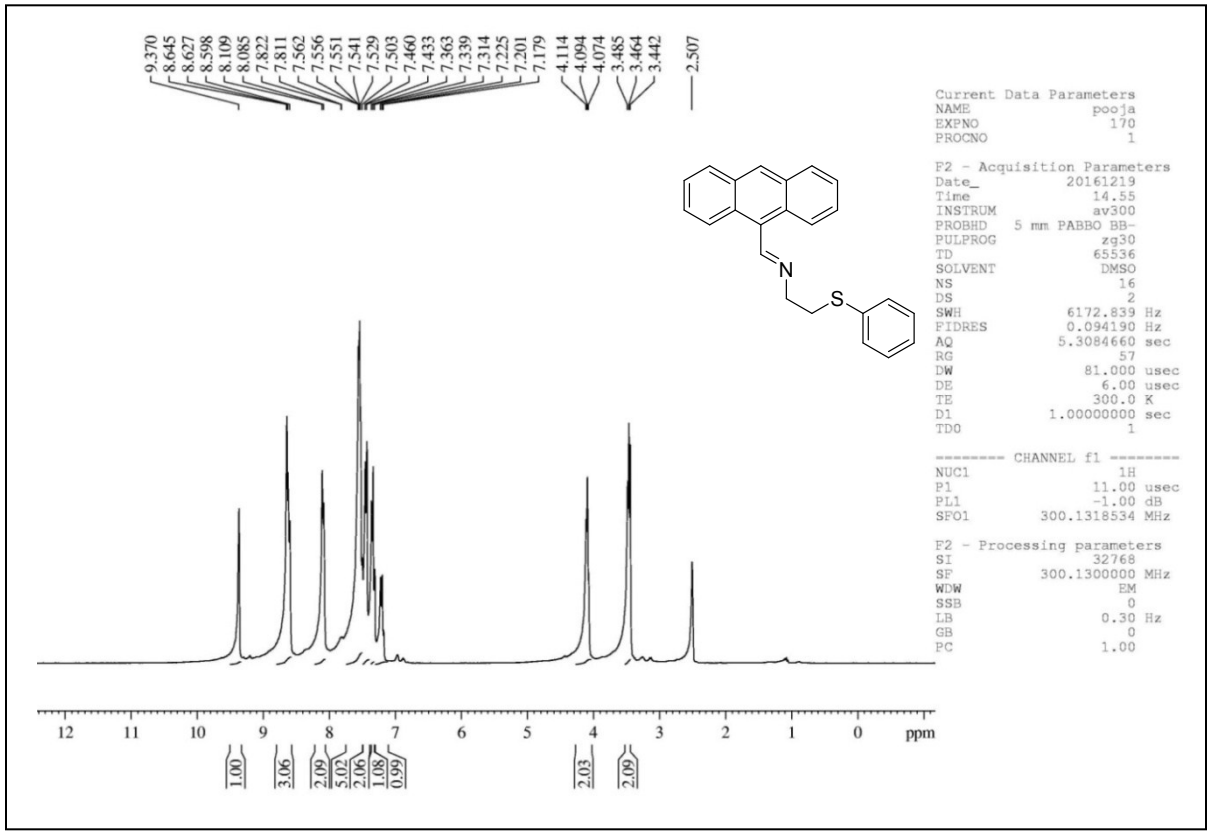

Fig. S7. ^{1}H NMR of Ligand **L1**

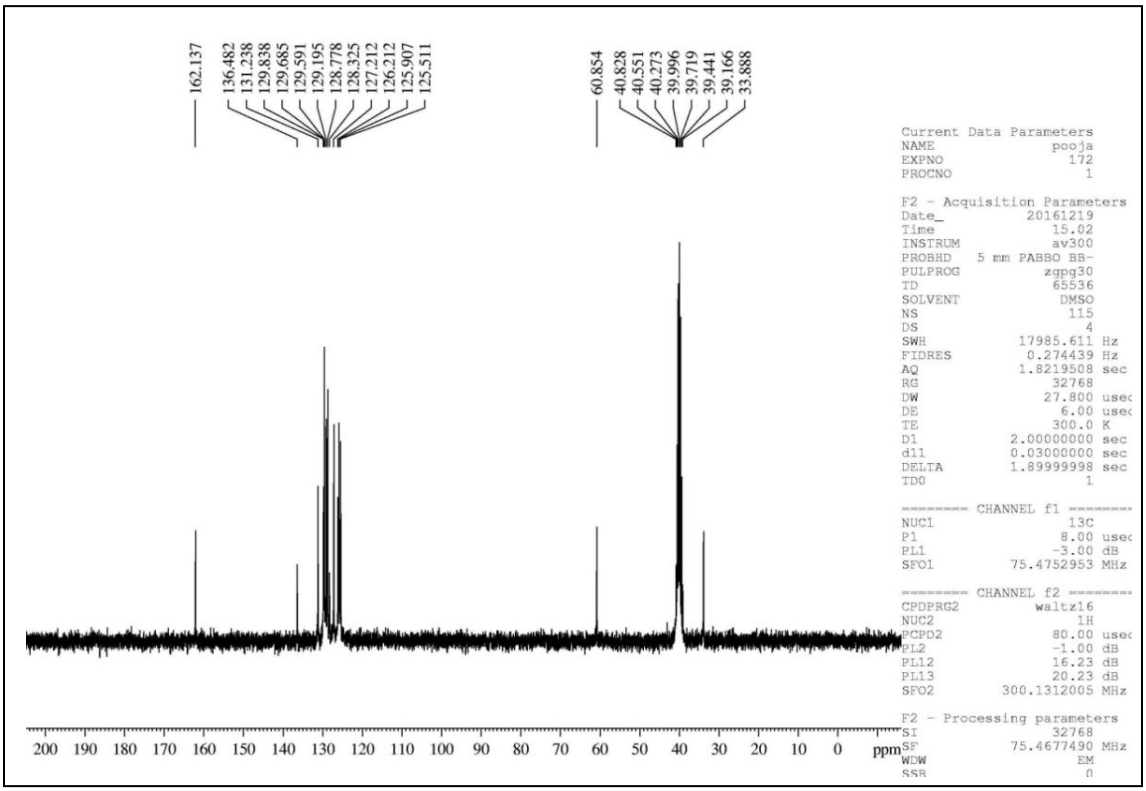

Fig. S8. ^{13}C NMR of Ligand **L1**

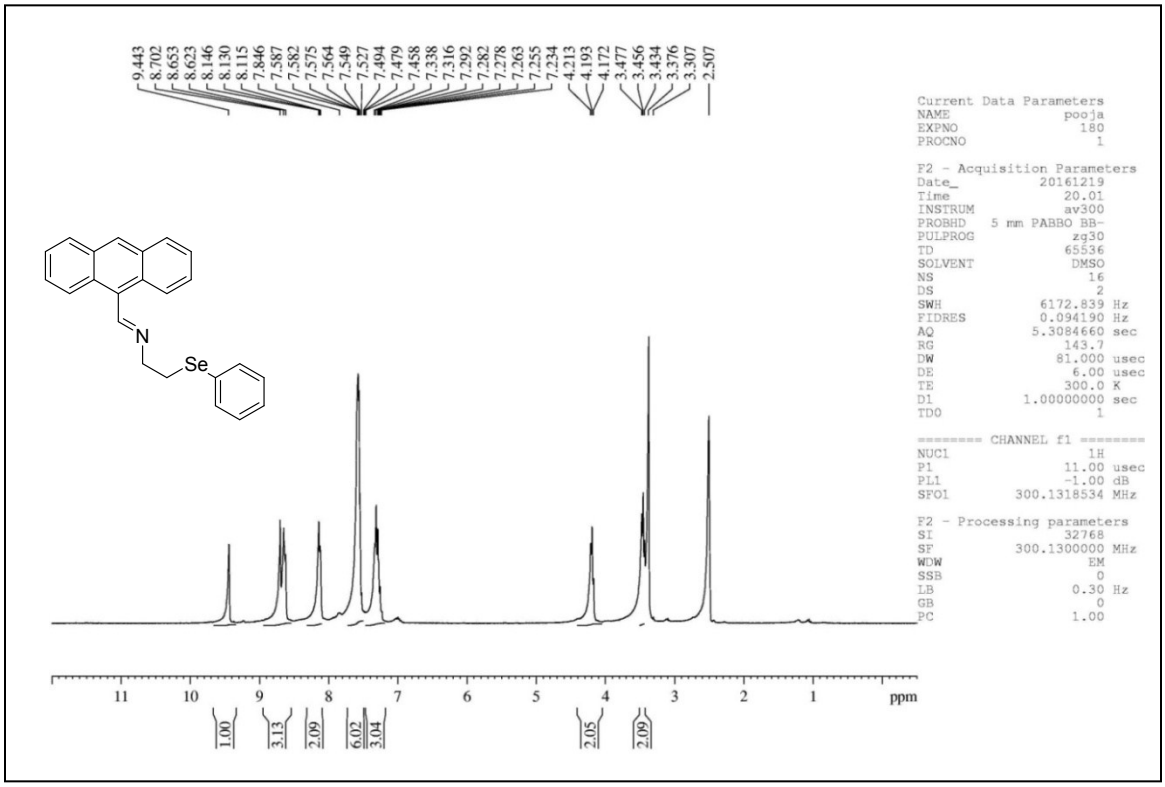

Fig. S9. ^{1}H NMR of Ligand **L2**

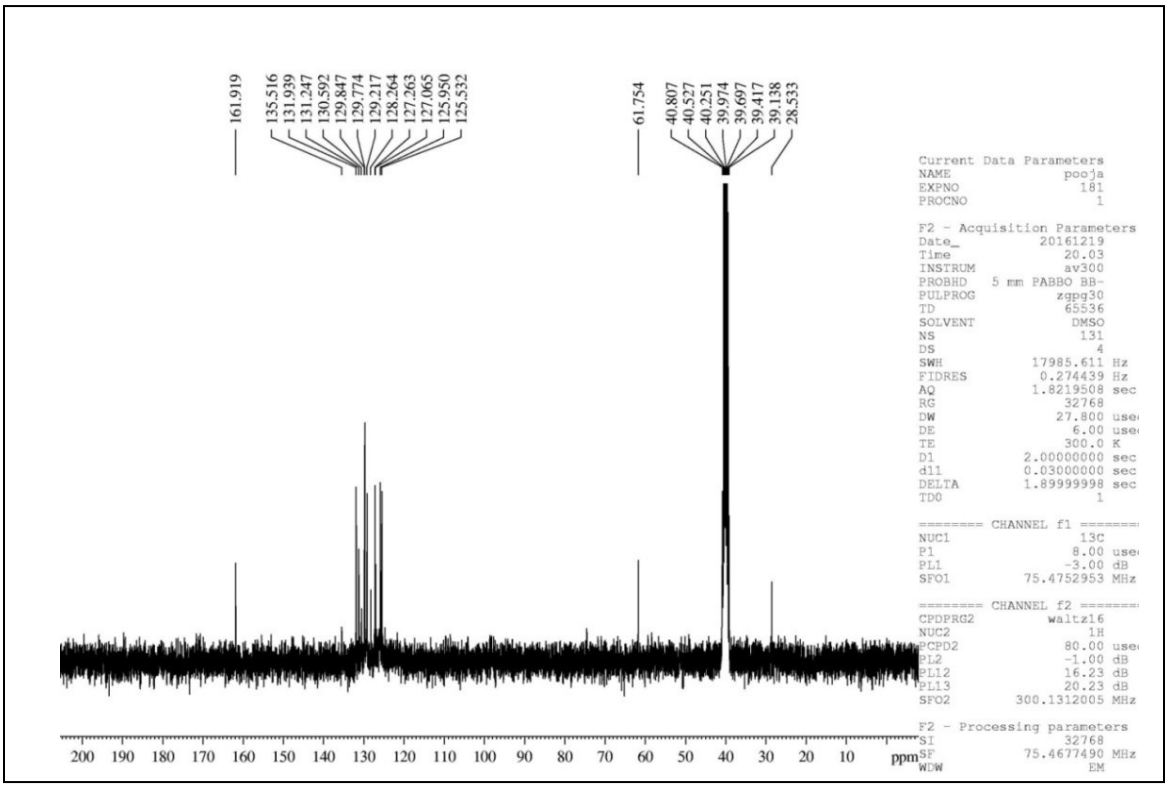

Fig. S10. ^{13}C NMR of Ligand **L2**

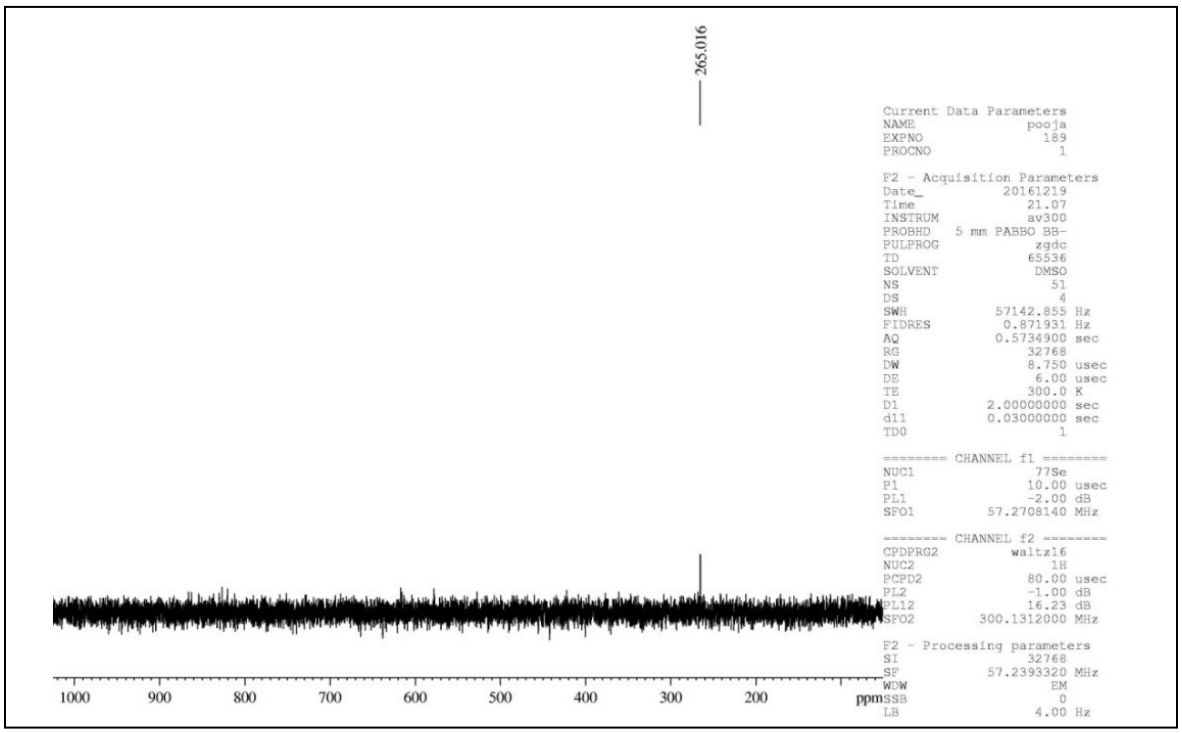

Fig. S11. ^{77}SeNMR of Ligand **L2**

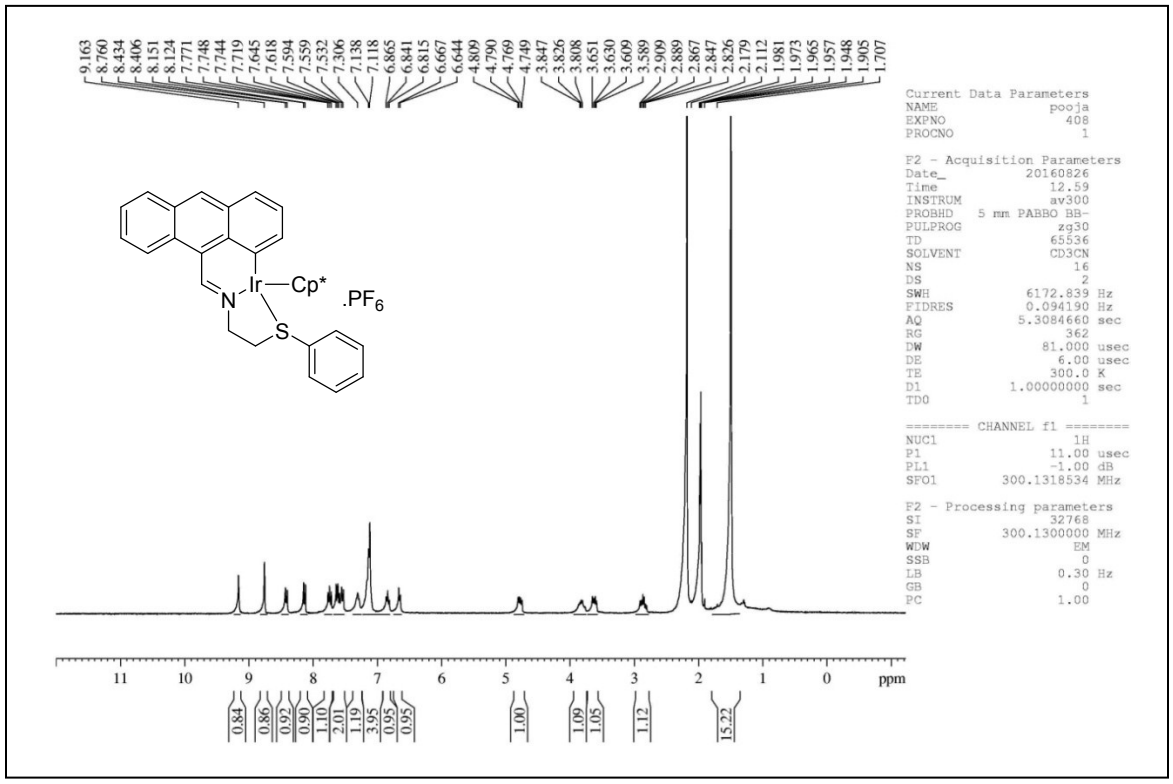

Fig. S12. ^{1}H NMR of complex **1.**

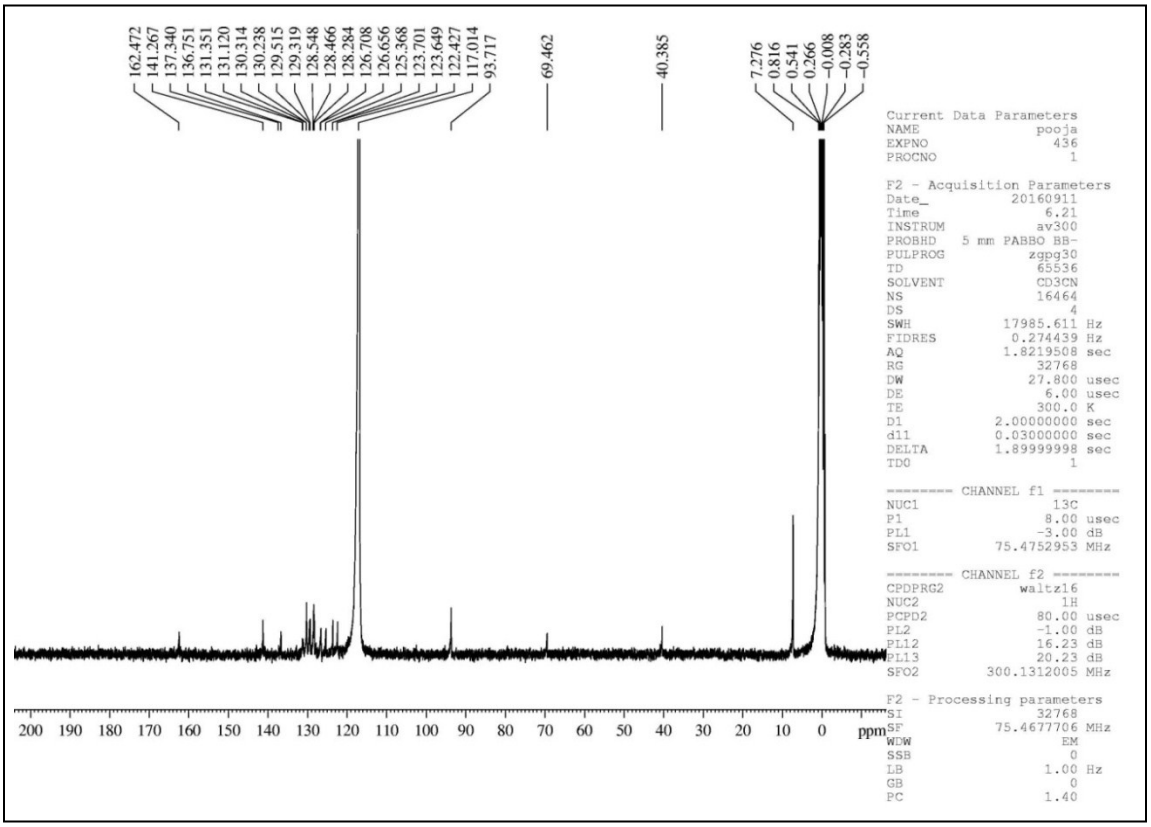

Fig. S13. ^{13}CNMR of complex **1.**

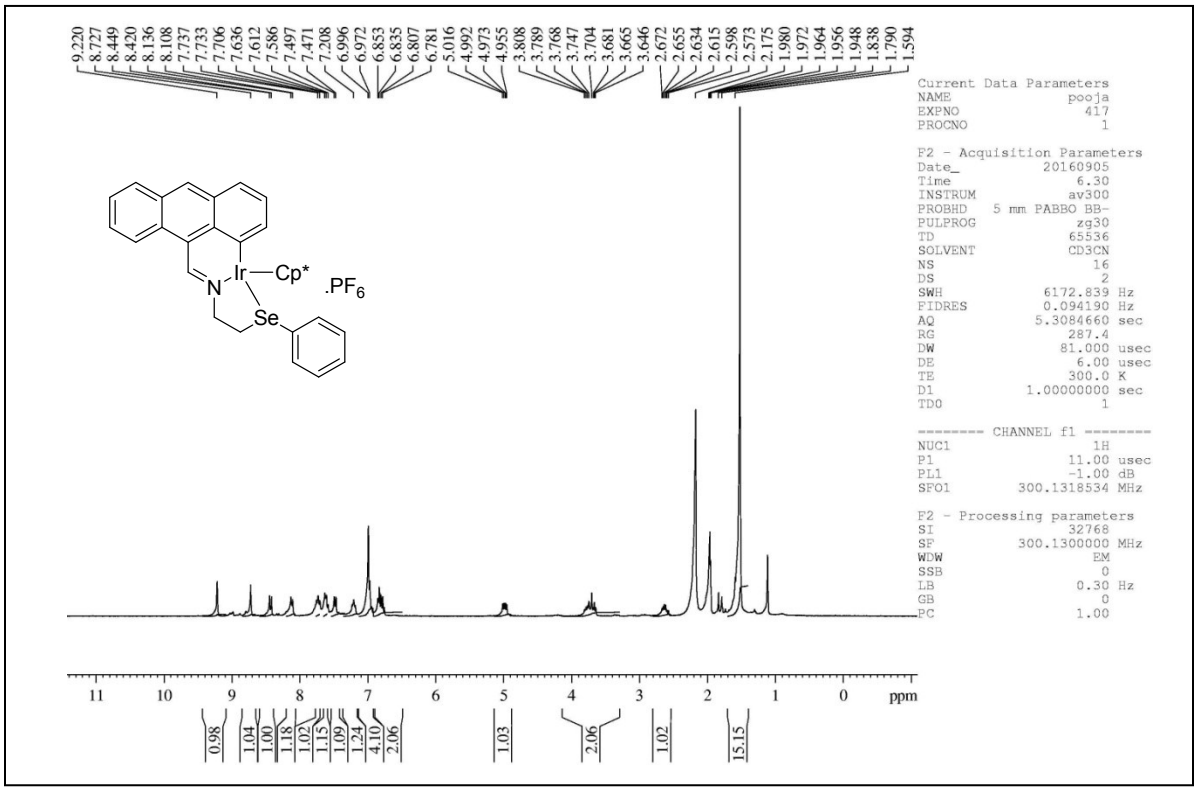

Fig. S14. ^{1}H NMR of complex **2.**

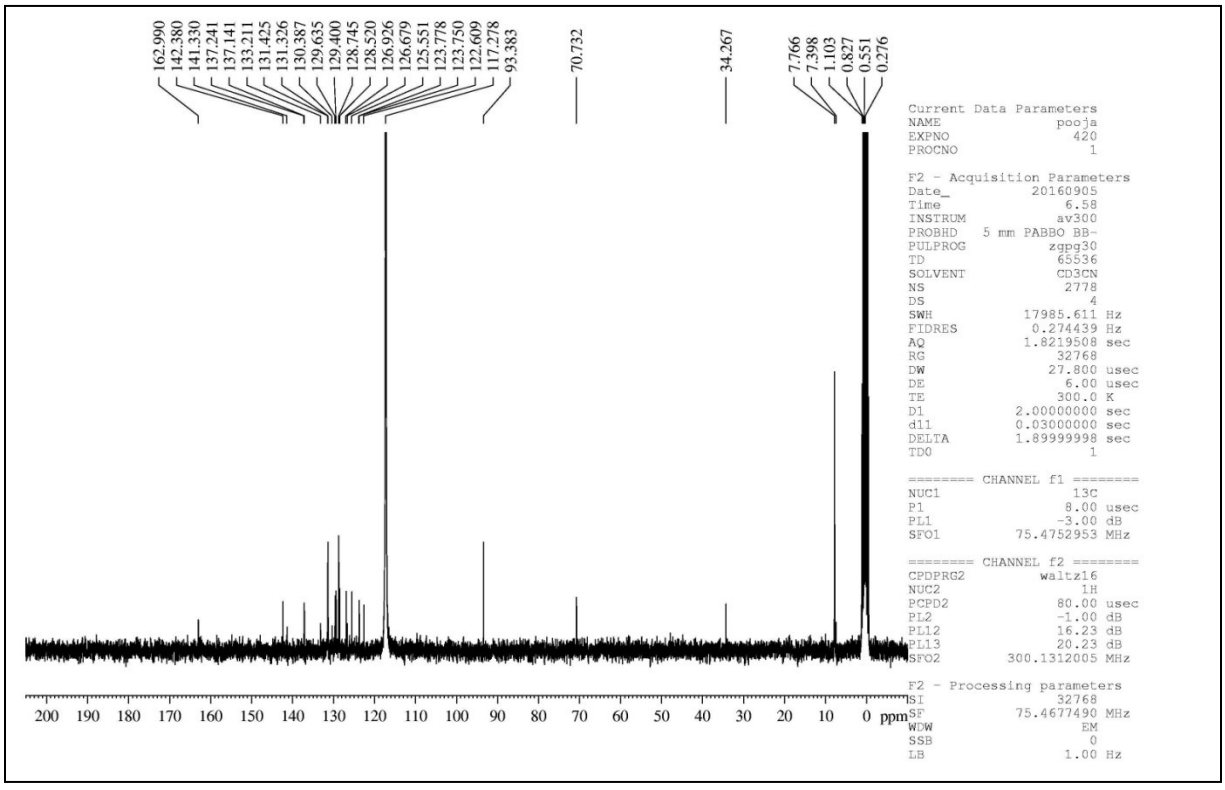

Fig. S15. ^{13}C NMR of complex **2.**

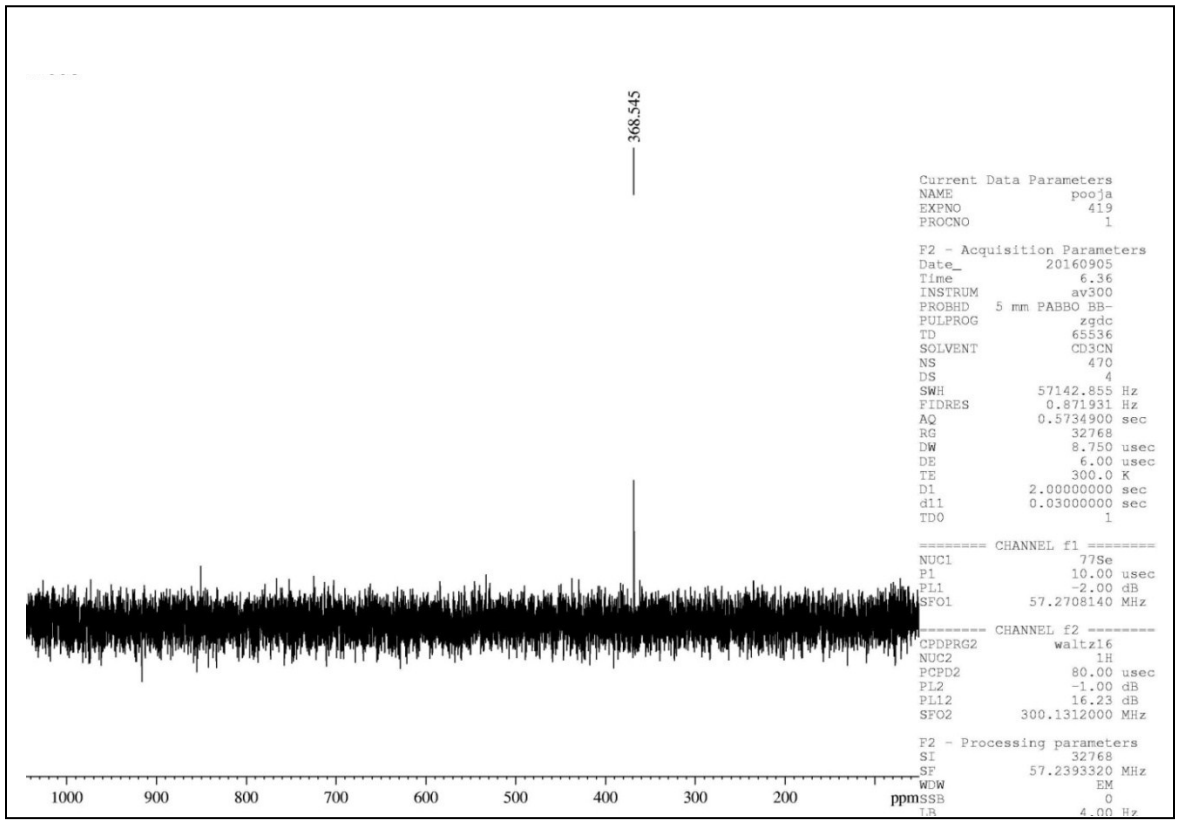

Fig. S16. ^{77}Se NMR of complex **2.**

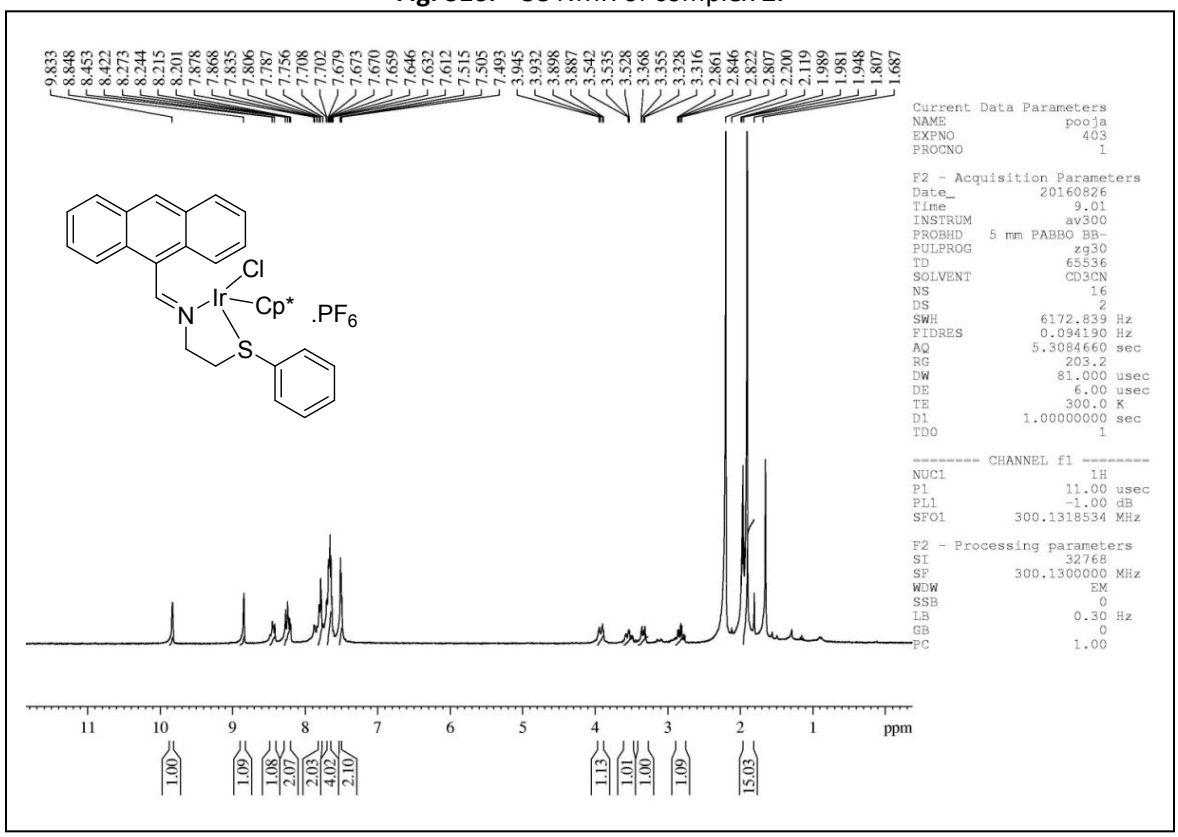

Fig. S17. ^{1}H NMR of complex **3.**

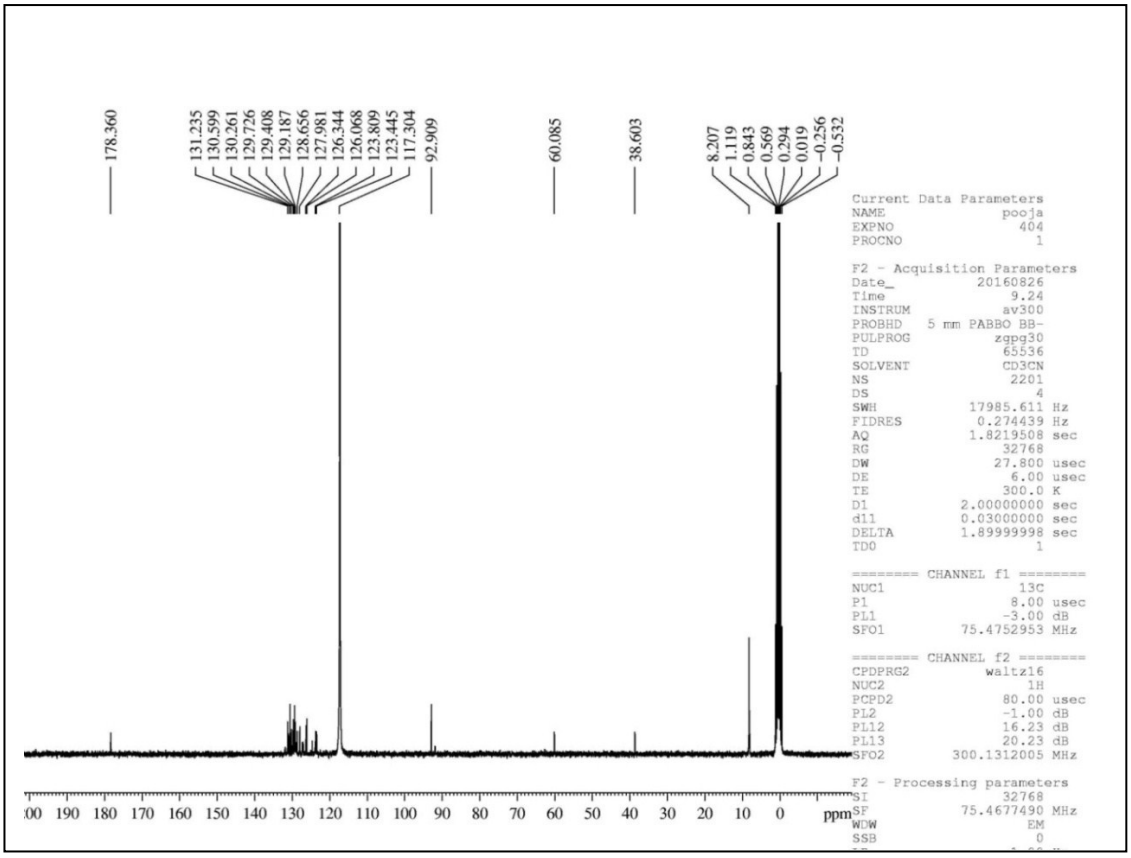

Fig. S18. ^{13}C NMR of complex **3.**

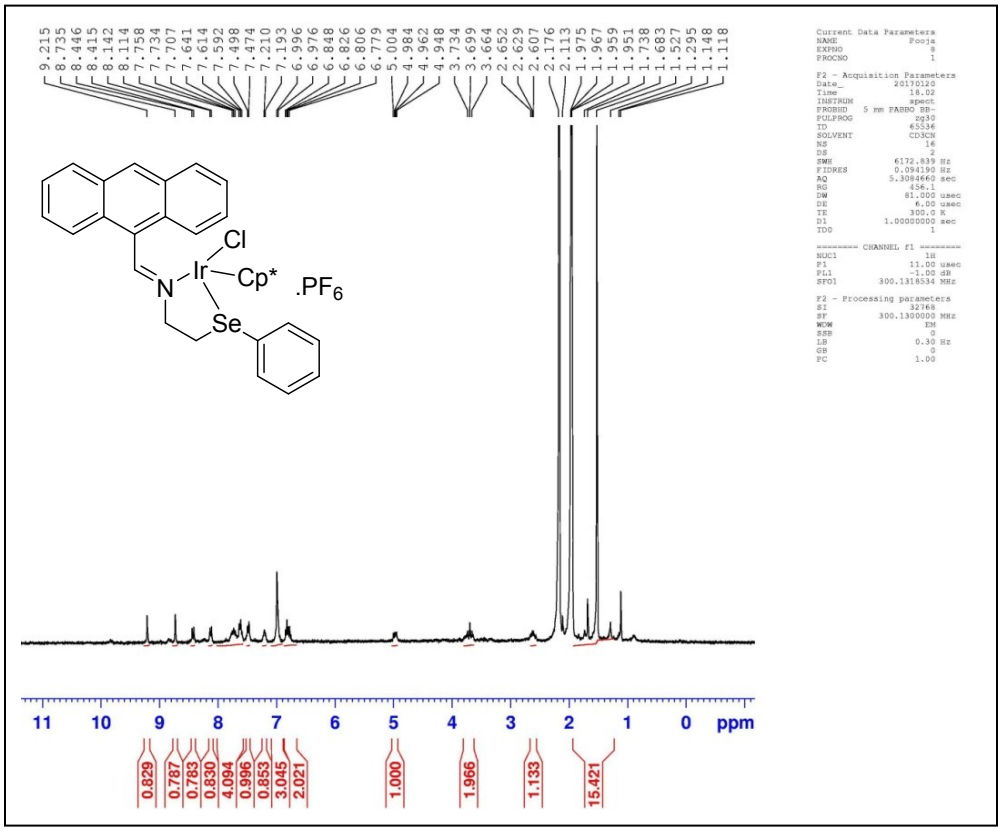

Fig. S19. ^{1}H NMR of complex **4.**

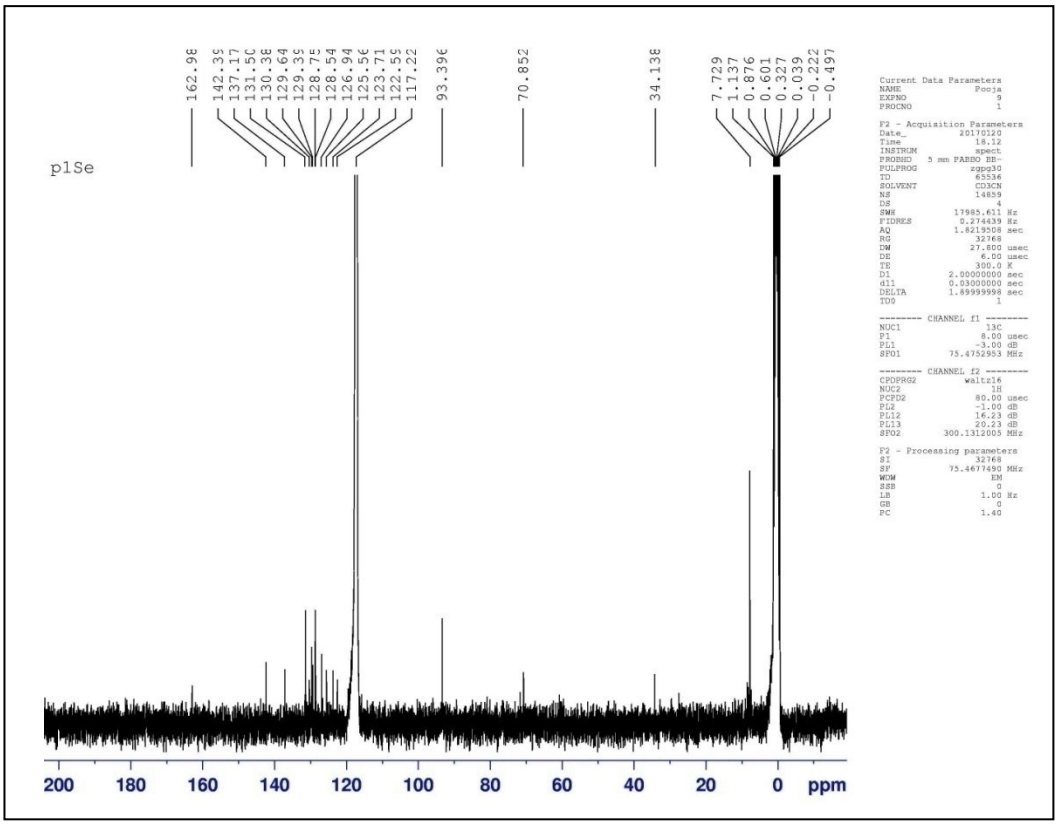

Fig. S20. ^{13}C NMR of complex **4.**

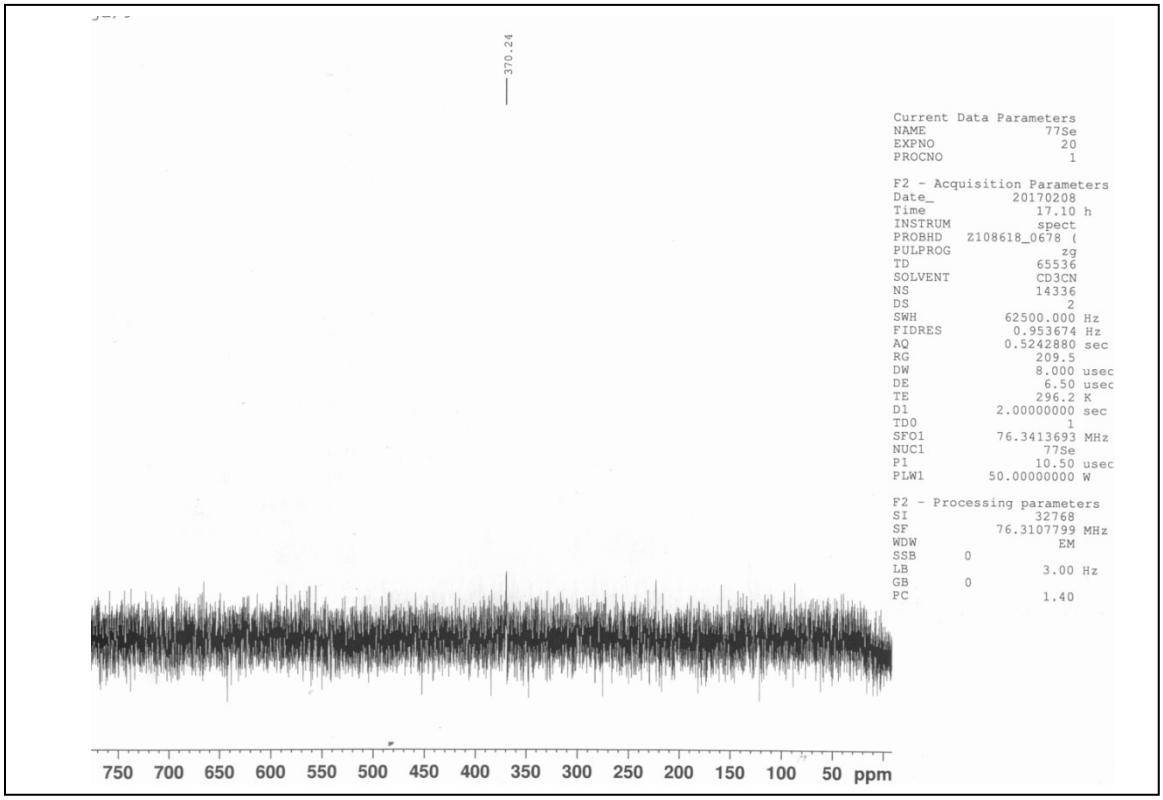

Fig. S21. ^{77}Se NMR of complex **4.**

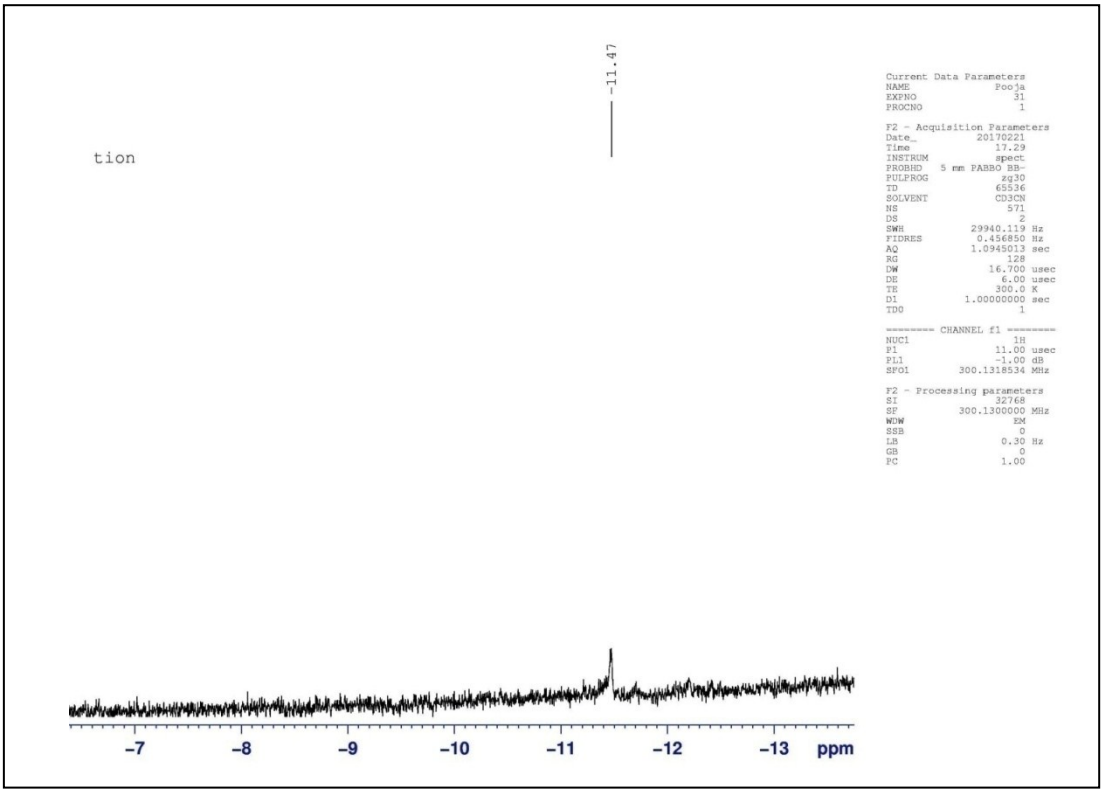

Fig.S22. ^{1}H NMR of Iridium hydride species in transfer hydrogenation reaction after 1h of reaction mixture .

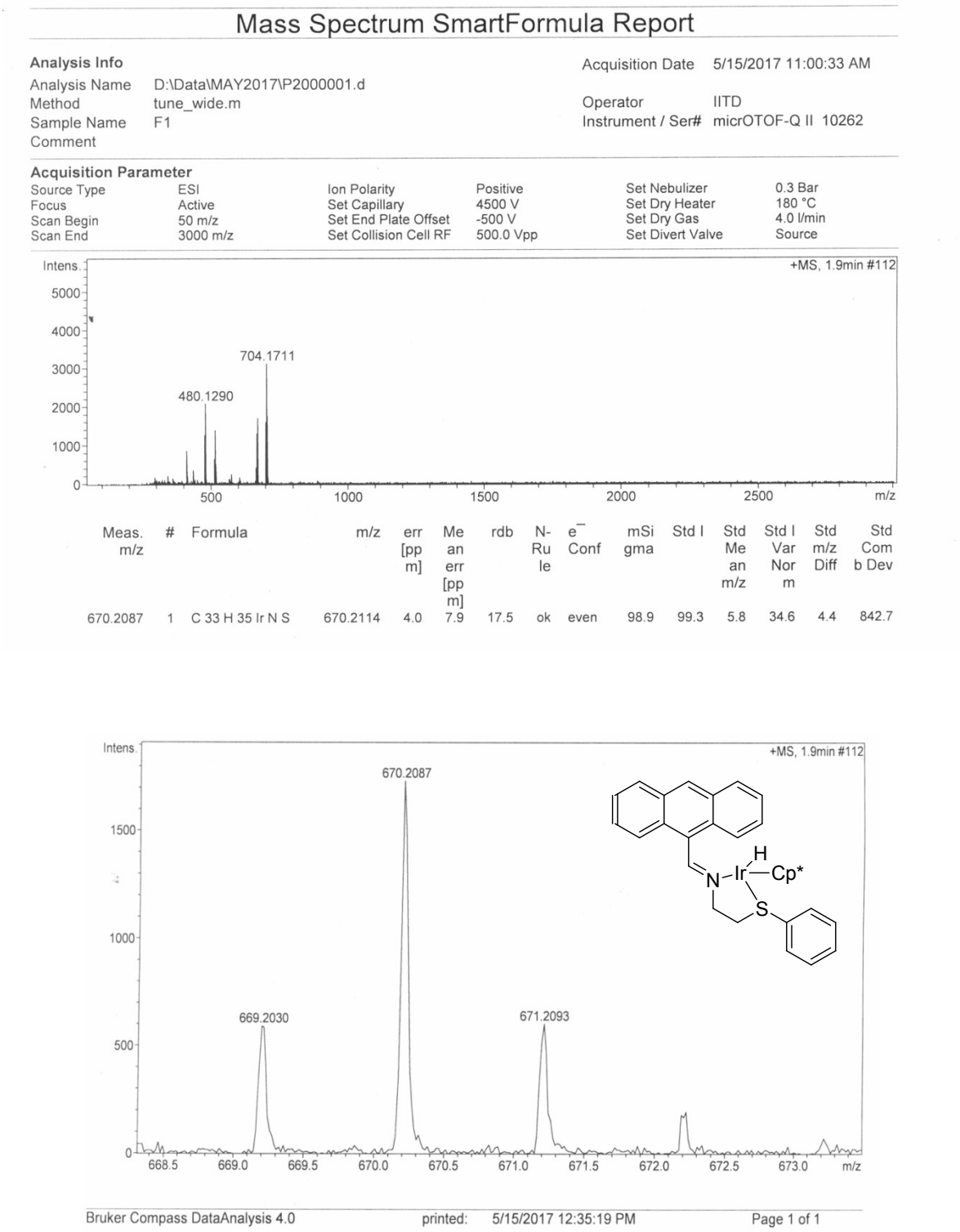

Fig. S23. Mass spectra of Iridium hydride species in transfer hydrogenation reaction with catalyst 3 after 1h of reaction.

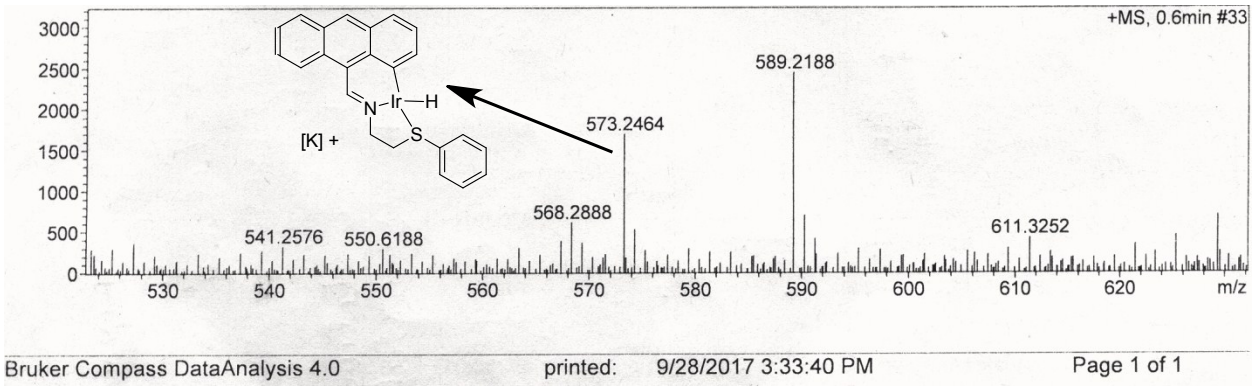

Fig. S24. Mass spectra of Iridium hydride species in transfer hydrogenation reaction with catalyst 1 after 2h of reaction mixture.

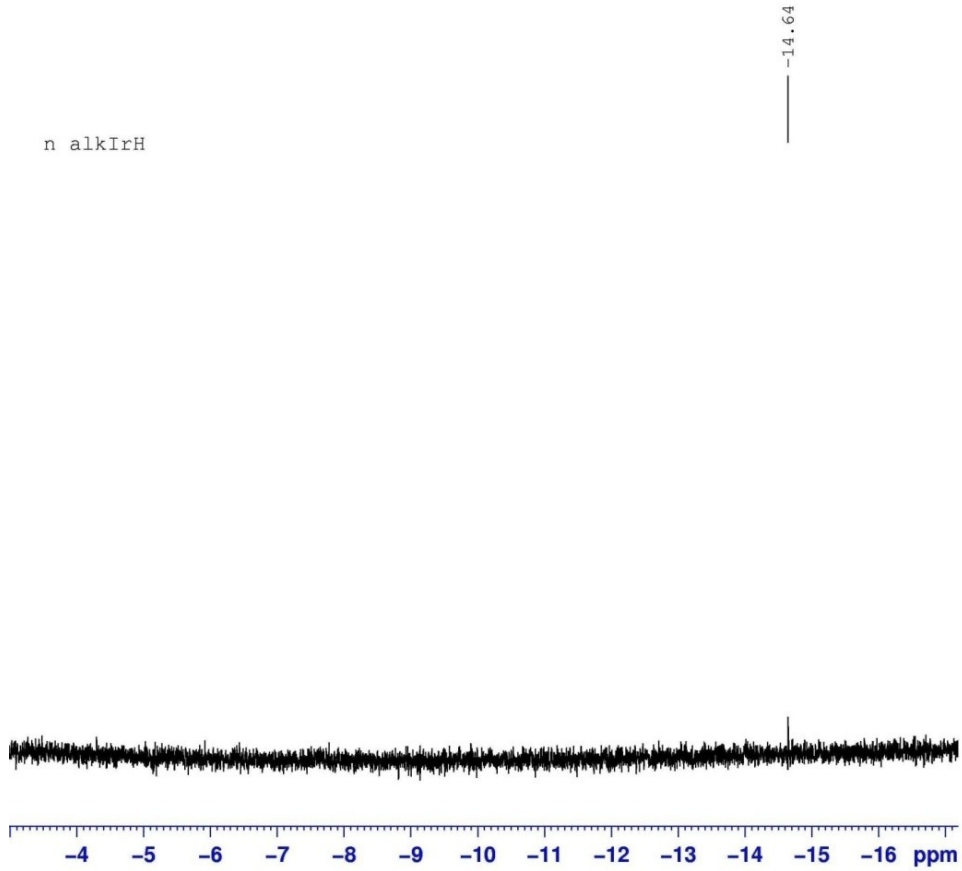

Fig. S25. ^{1}H NMR of Iridium hydride species in N-alkylation of aniline with benzylalcohol after 1h of reaction mixture .

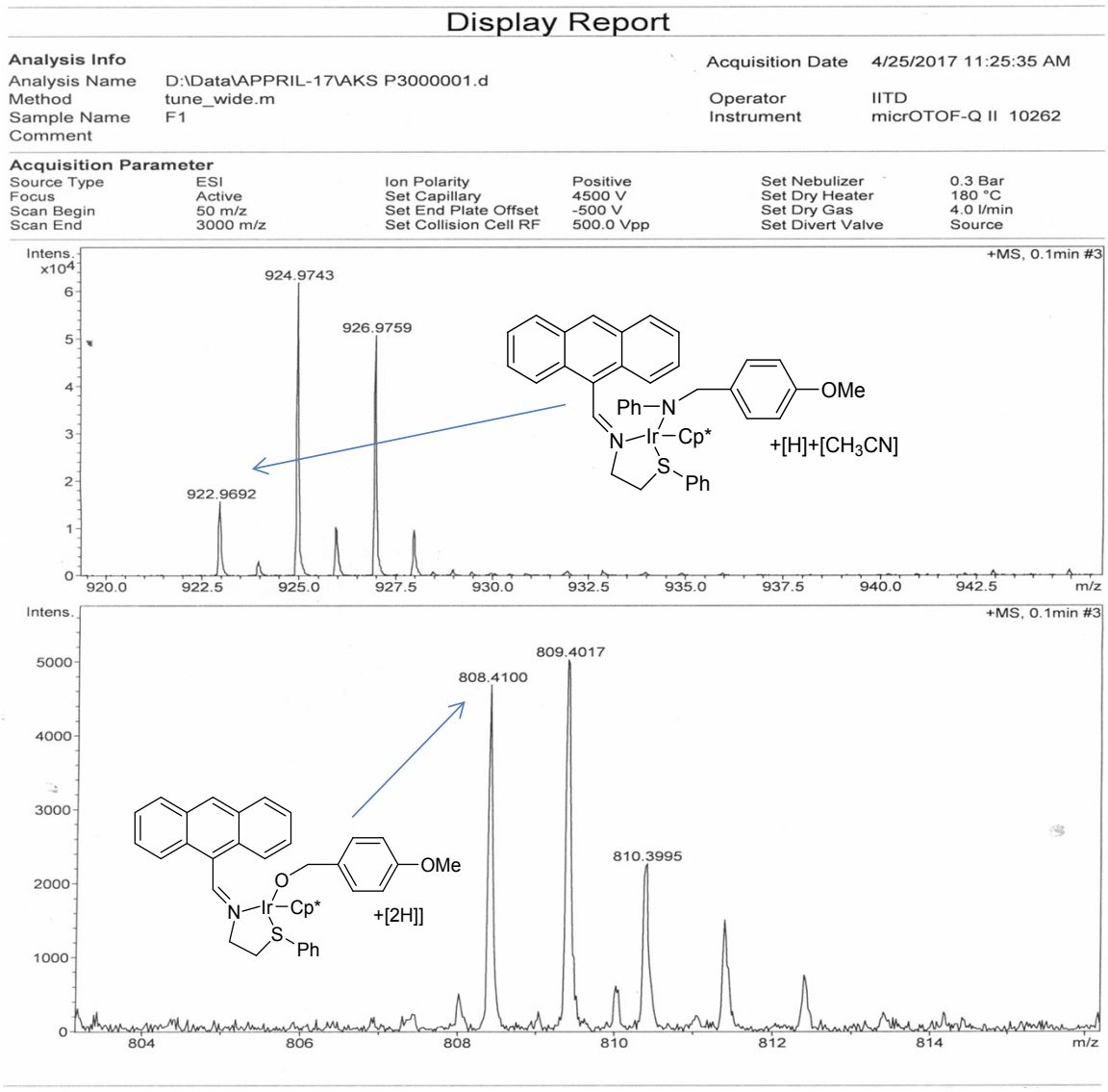

Fig. S26. Mass spectra of amido iridium and alkoxo-iridium species in N-alkylation of aniline with p-methoxybenzylalcohol using catalyst 3 after 1h of reaction mixture.

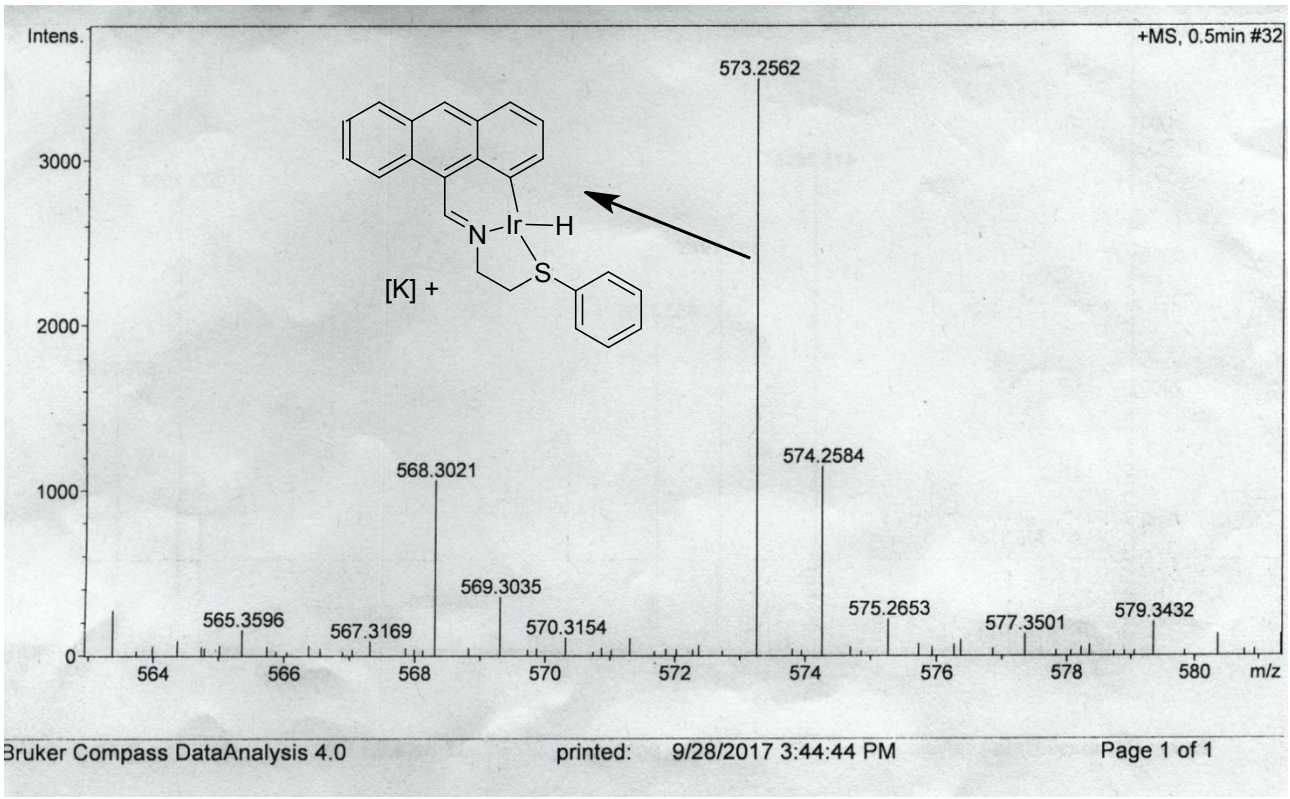

Fig. S27. Mass spectra of Iridium hydride species in N-alkylation of aniline with benzylalcohol with catalyst 1 after 2h of reaction mixture.

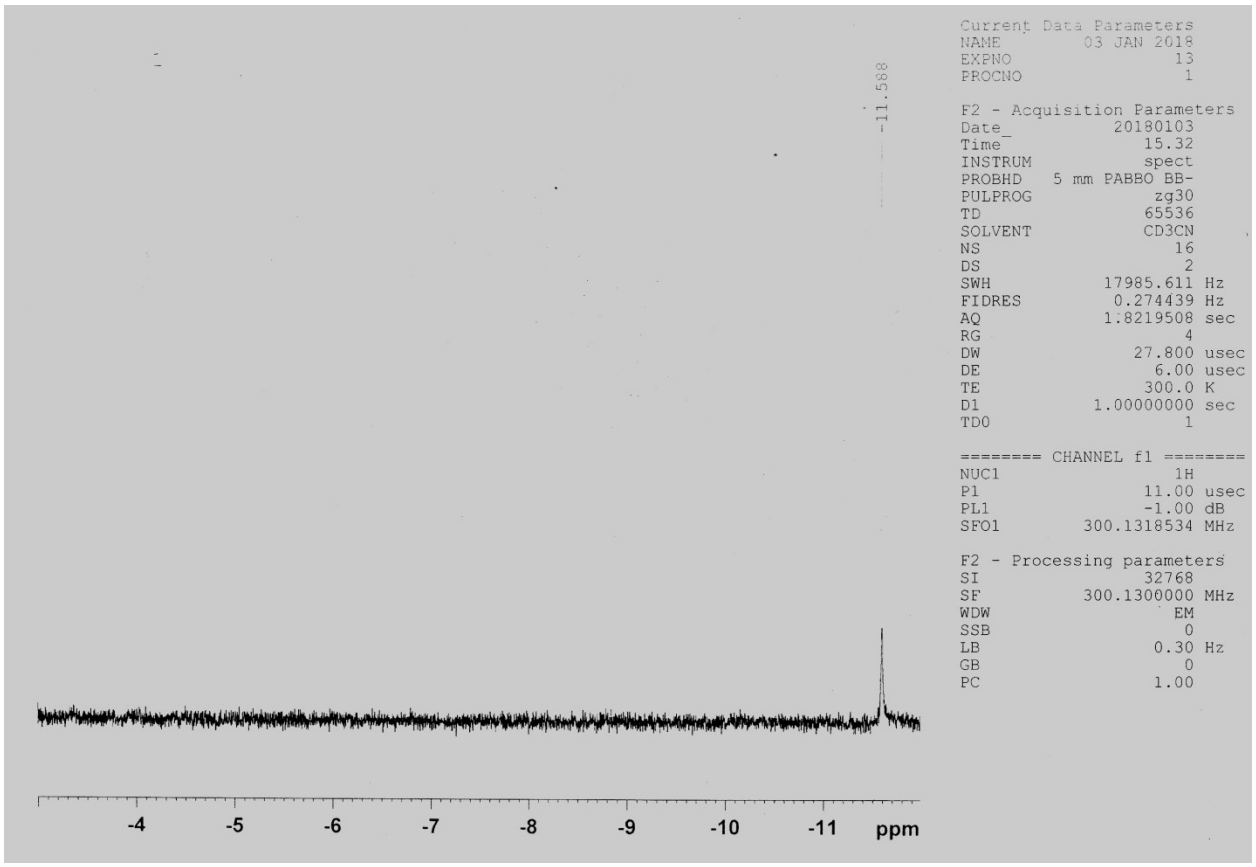

Fig. S28. ^{1}H NMR spectra of Iridium hydride species.

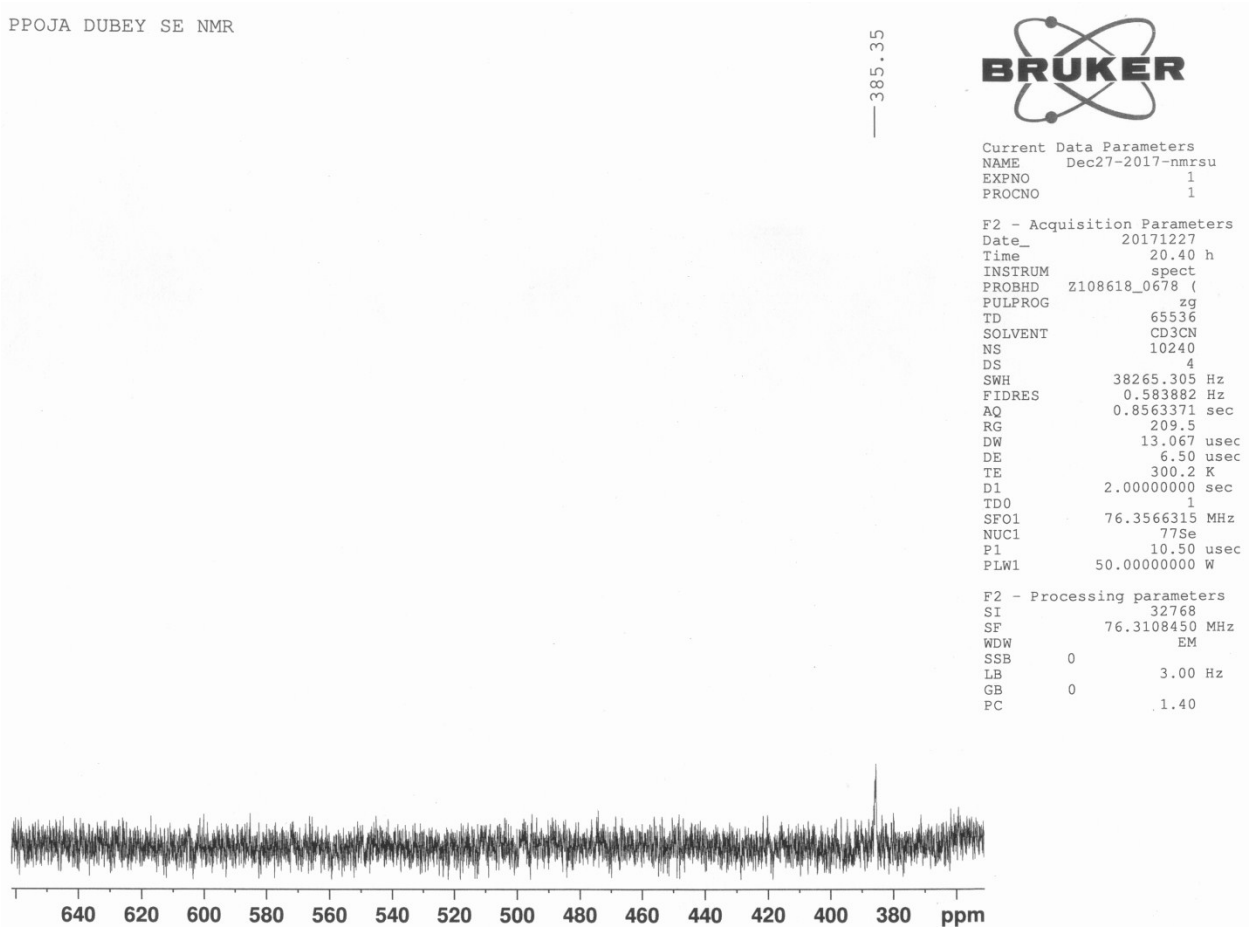

Fig. S29. ^{77}Se NMR spectra of Iridium hydride species.

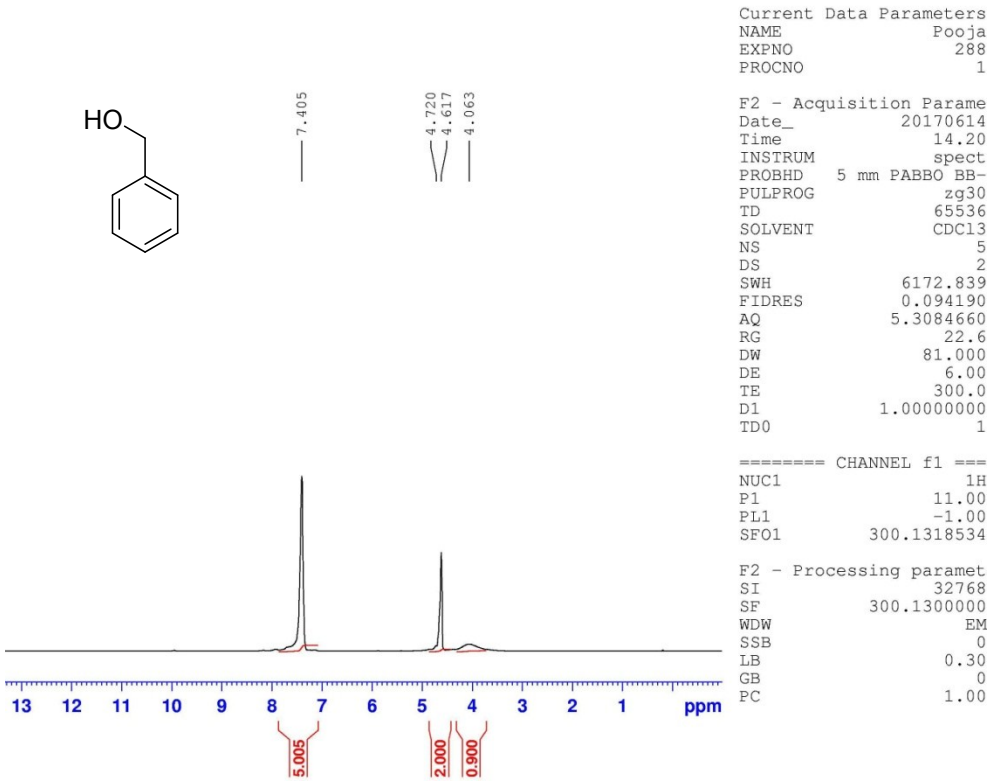

Fig. S30. ^{1}H NMR of Phenylmethanol

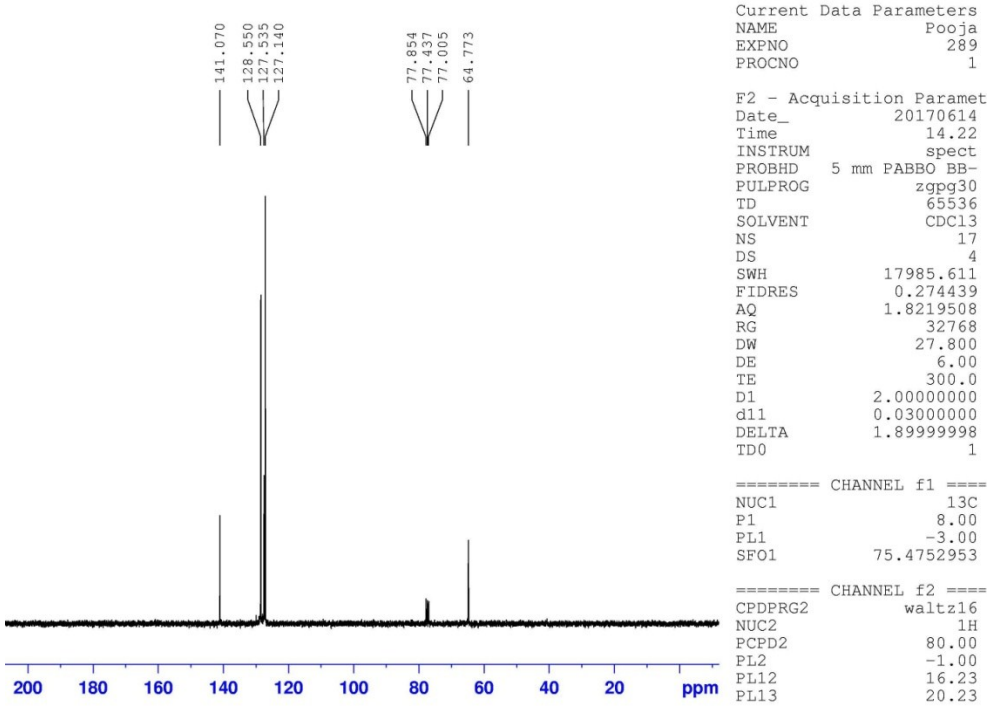

Fig. S31. ^{13}C{^{1}H} NMR of Phenylmethanol

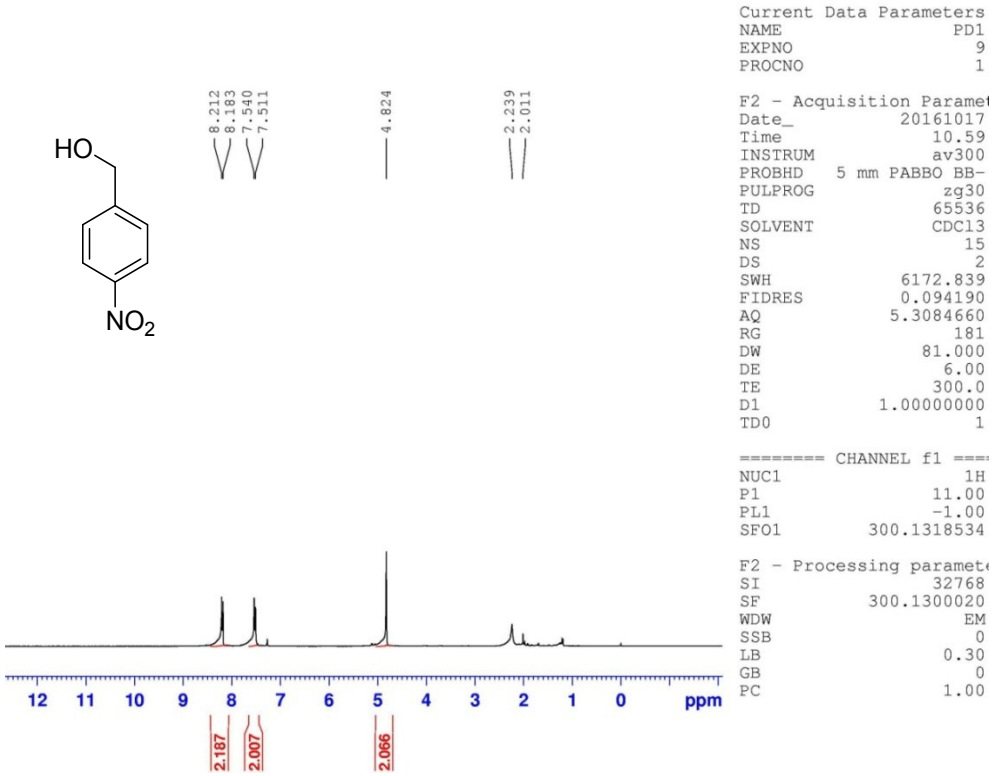

Fig. S32. ^{1}H NMR of (4-Nitrophenyl)methanol

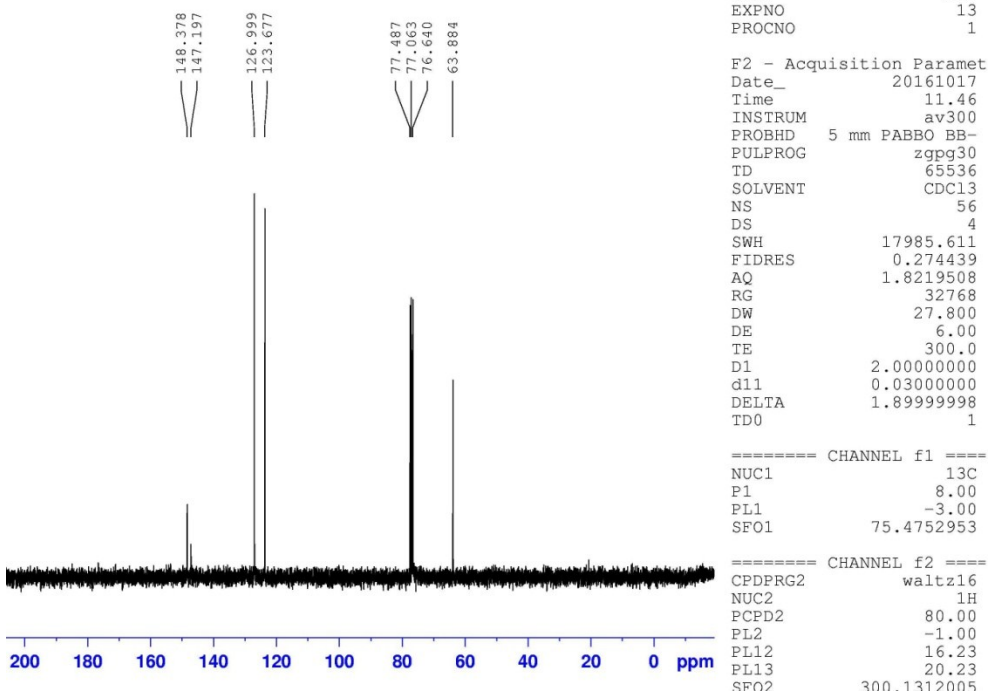

Fig. S33. ^{13}C NMR of (4-Nitrophenyl)methanol

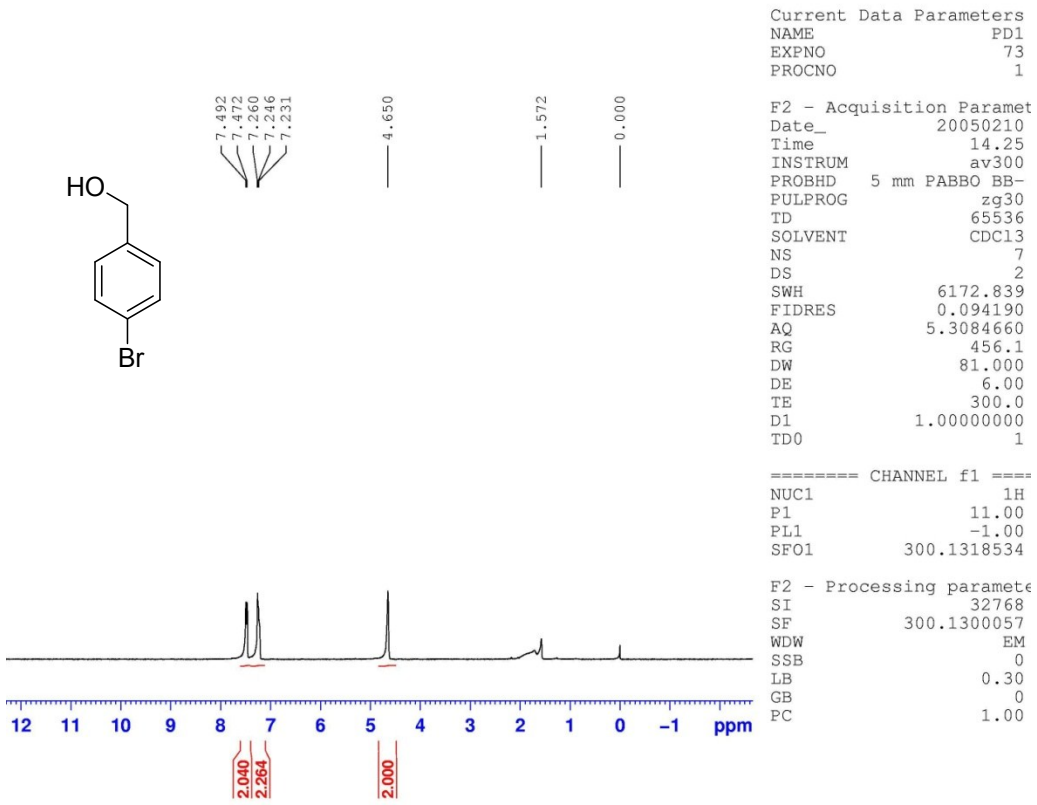

Fig. S34. ^{1}H NMR of (4-bromophenyl)methanol

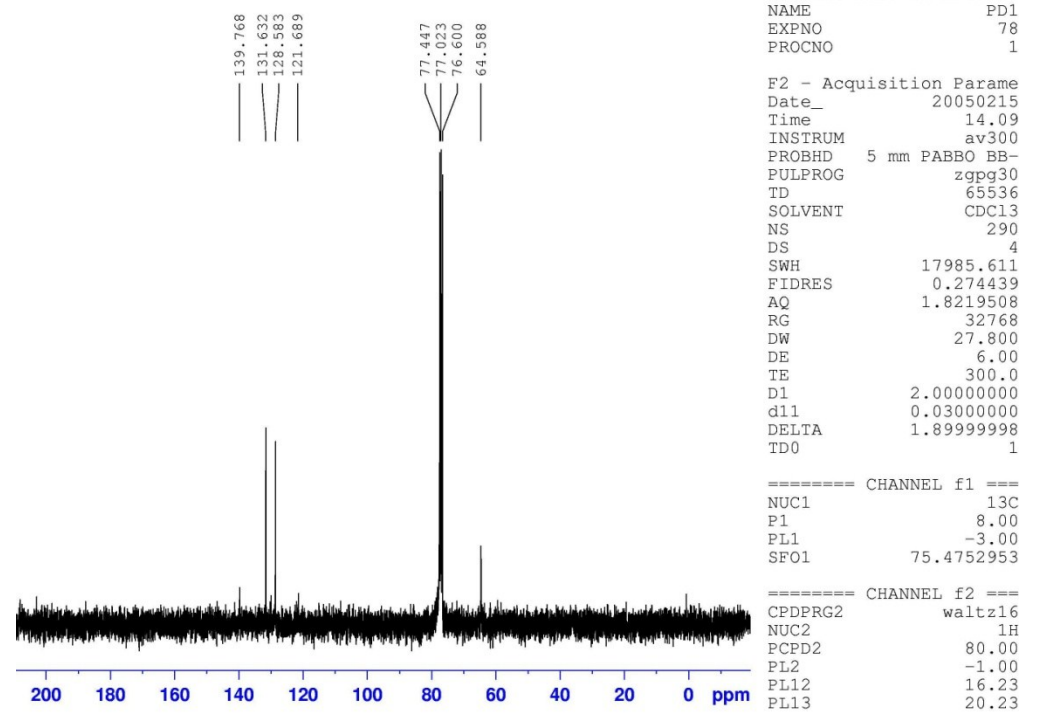

Fig. S35. ^{13}C NMR of (4-bromophenyl)methanol

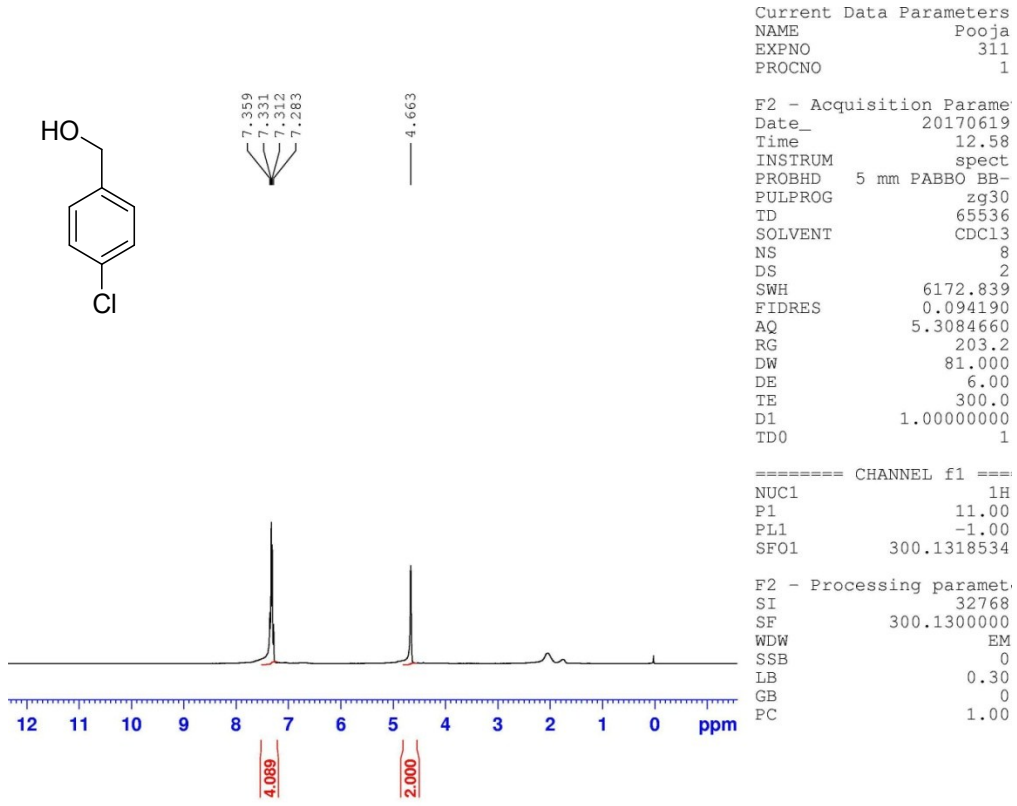

Fig. S36. ^{1}H NMR of (4-chlorophenyl)methanol

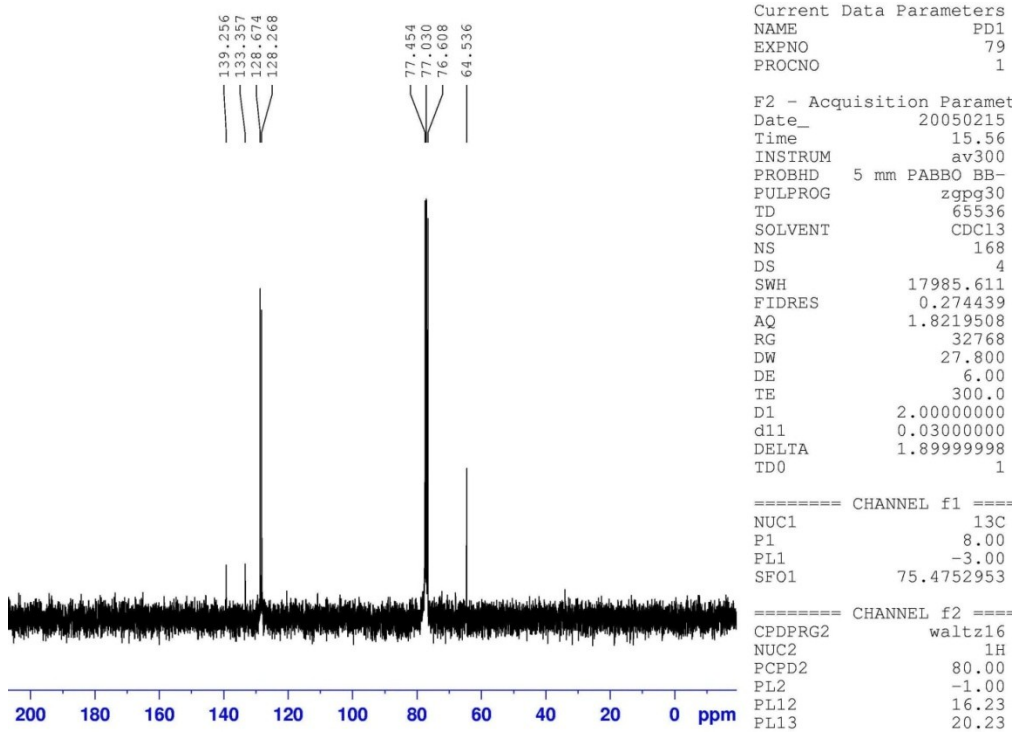

Fig. S37. ^{13}C NMR of (4-chlorophenyl)methanol

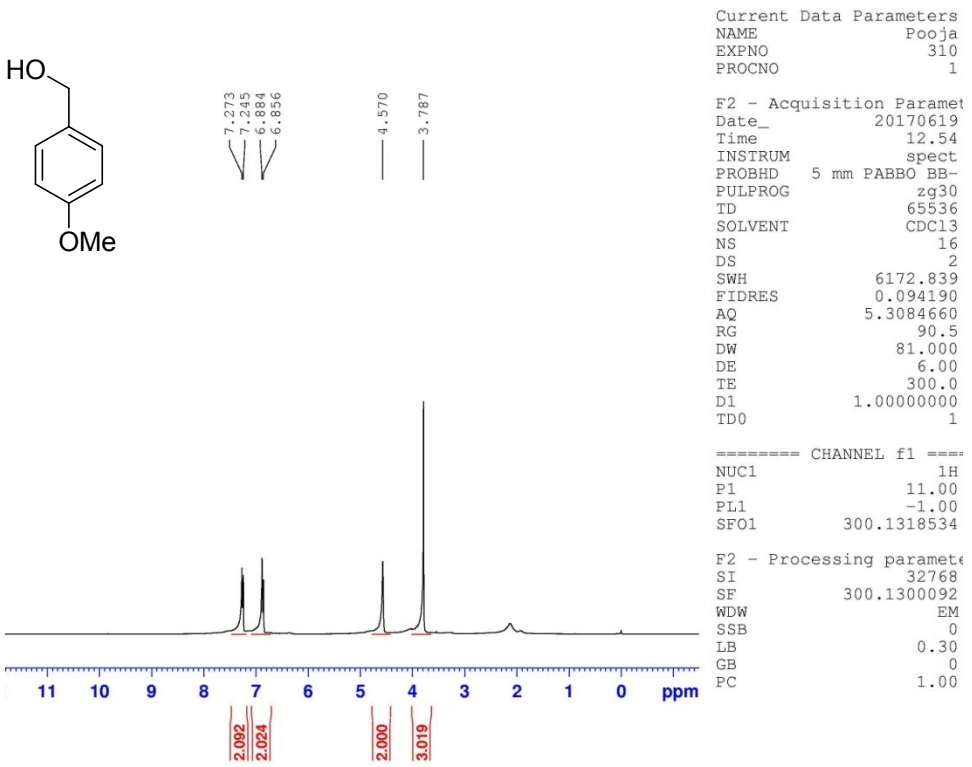

Fig. S38. ^{1}H NMR of (4-methoxyphenyl)methanol

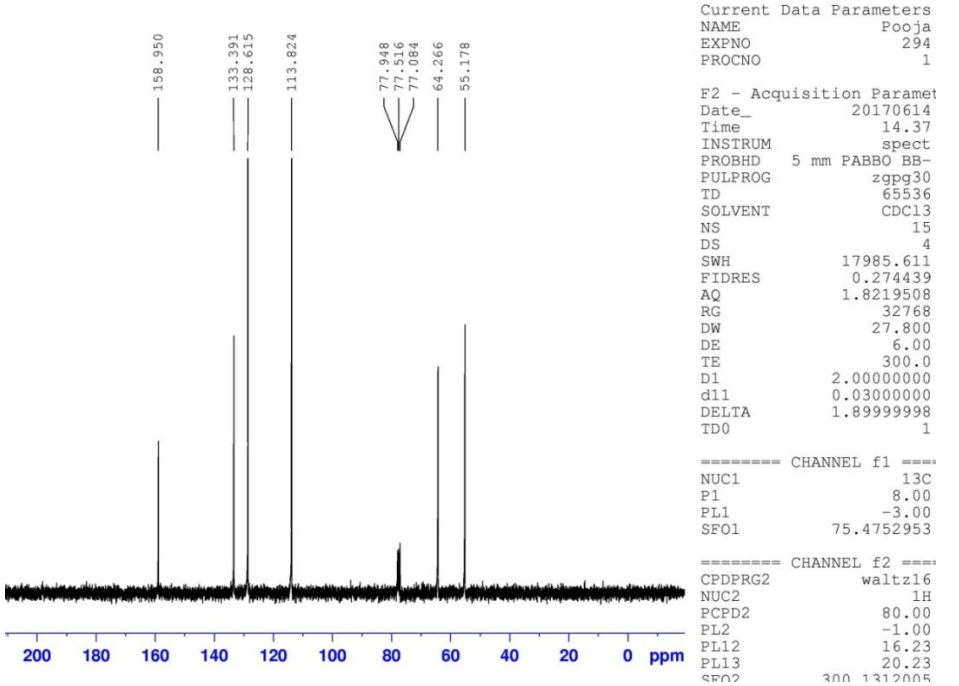

Fig. S39. ^{13}C{^{1}H} NMR of (4-methoxyphenyl)methanol

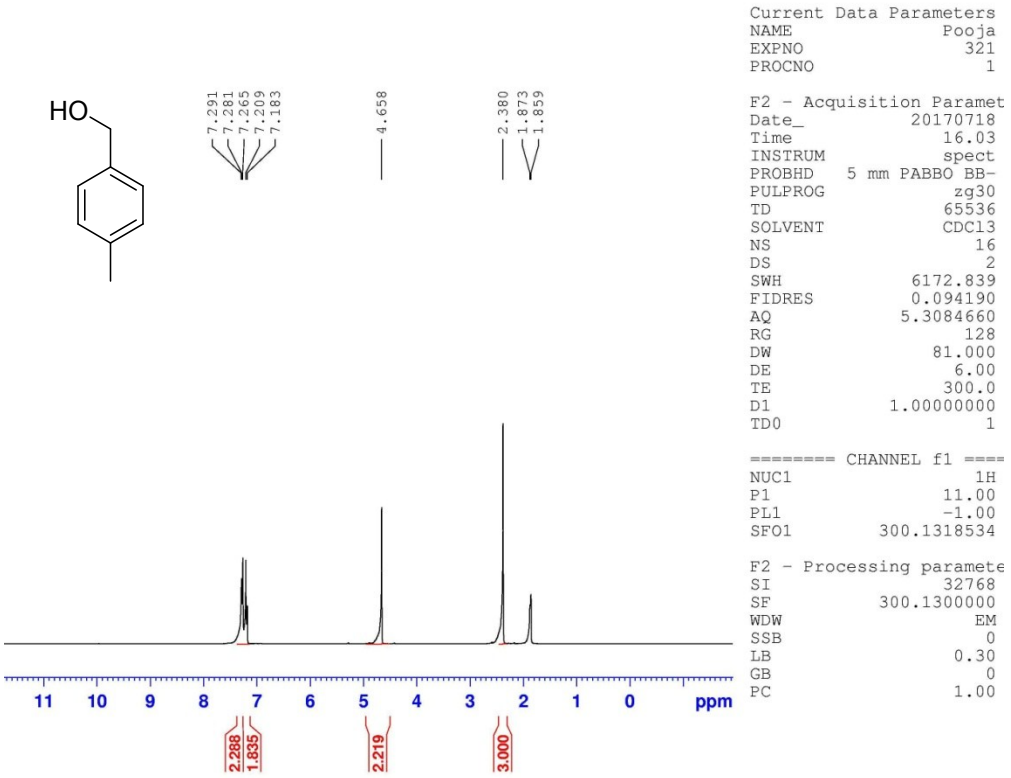

Fig. S40. ^{1}H NMR of *p*-Tolylmethanol

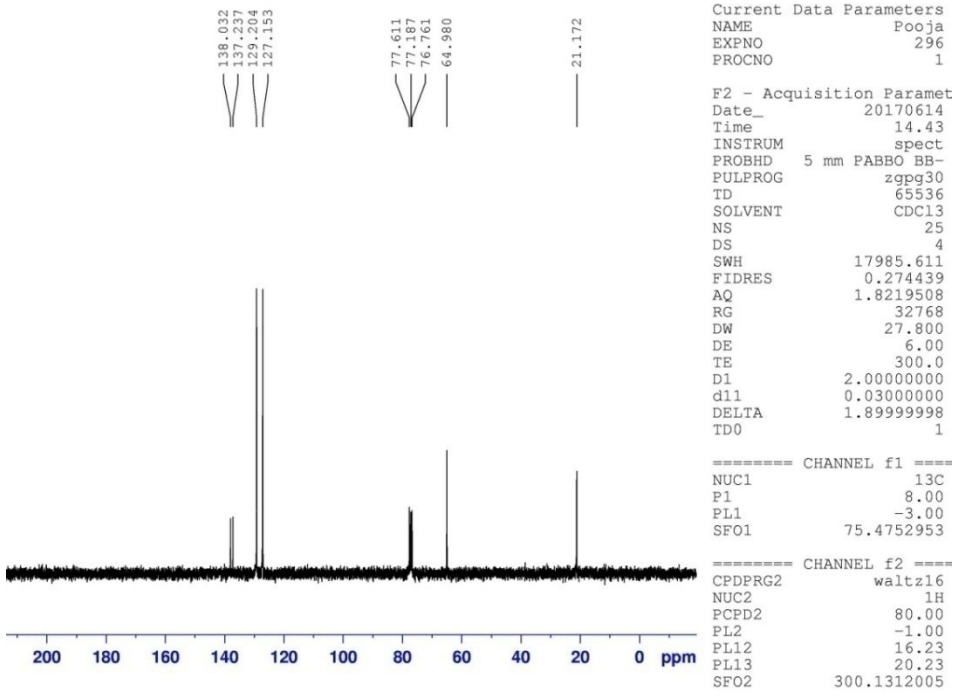

Fig. S41. ^{13}C{^{1}H} NMR of *p*-Tolylmethanol

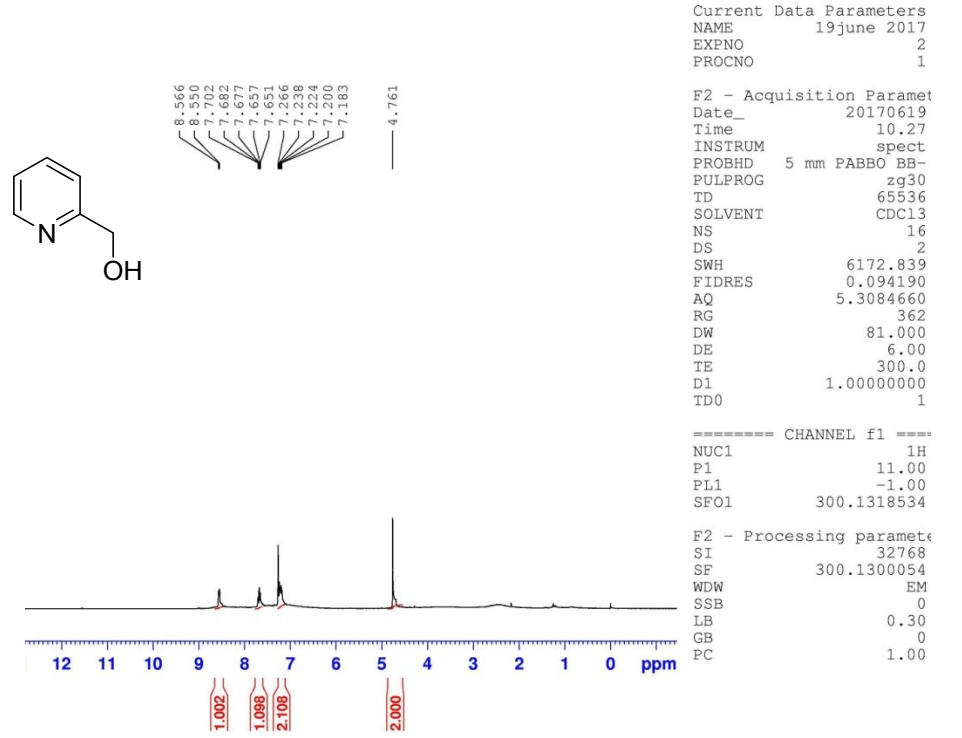

Fig. S42. ^{1}H NMR of *pyridine-2-ylmethanol*

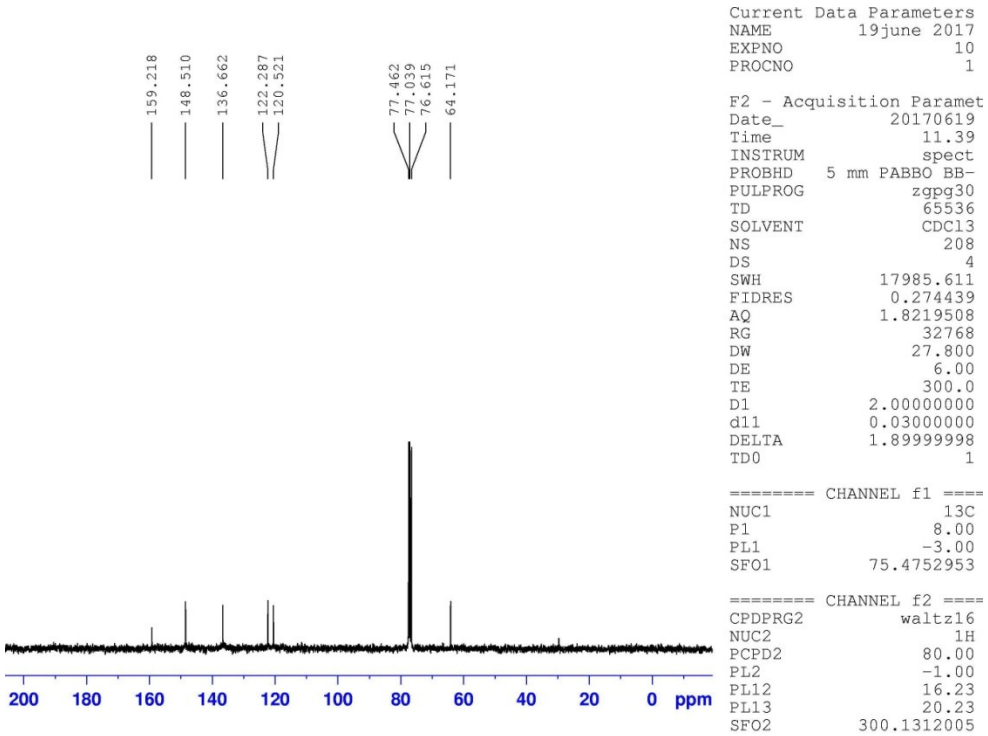

Fig. S43. ^{13}C{^{1}H} NMR of *pyridine-2-ylmethanol*

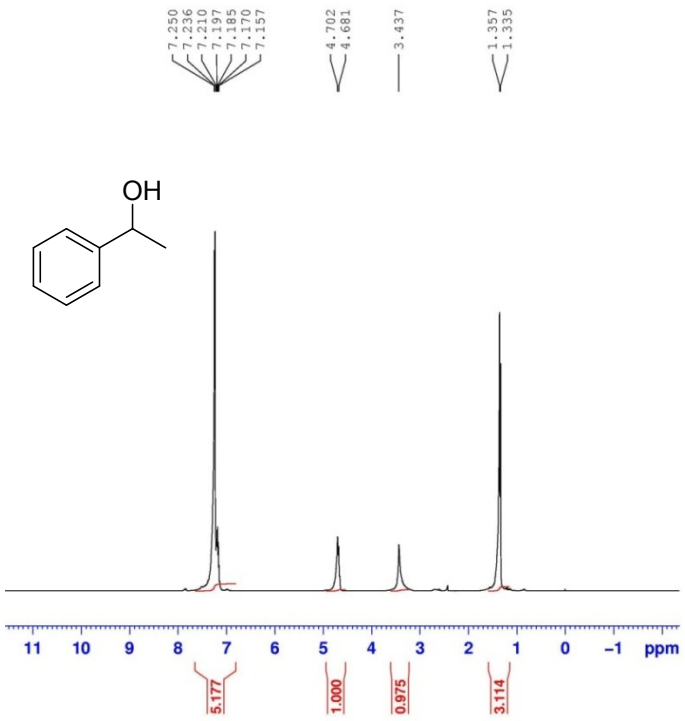


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Fig. S44. ^{1}H NMR of 1-phenylethanol

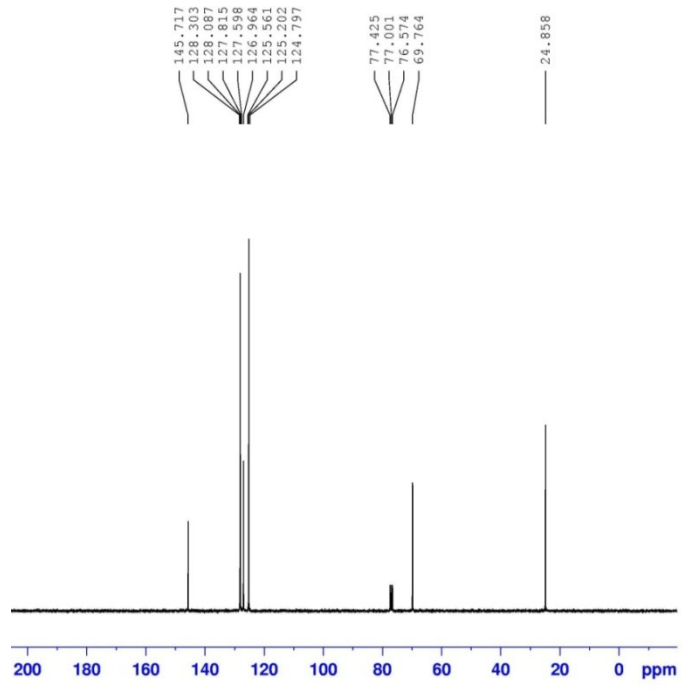


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Fig. S45. ^{13}C{^{1}H} NMR of 1-phenylethanol

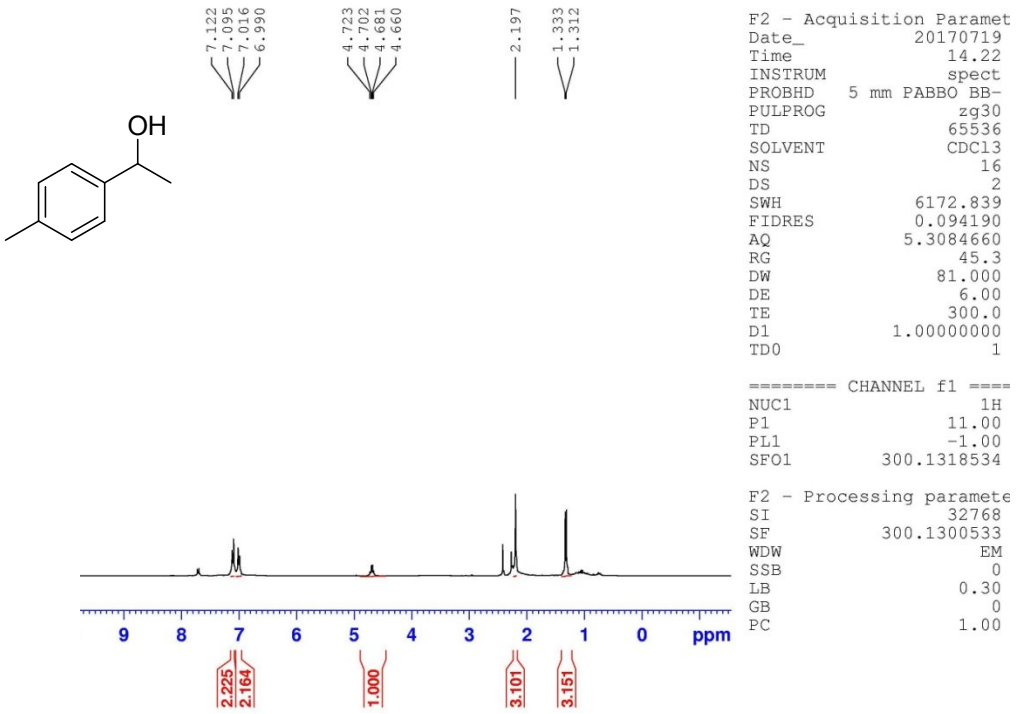

Fig. S46. ^{1}H NMR of 1-(*p-tolyl*)ethanol

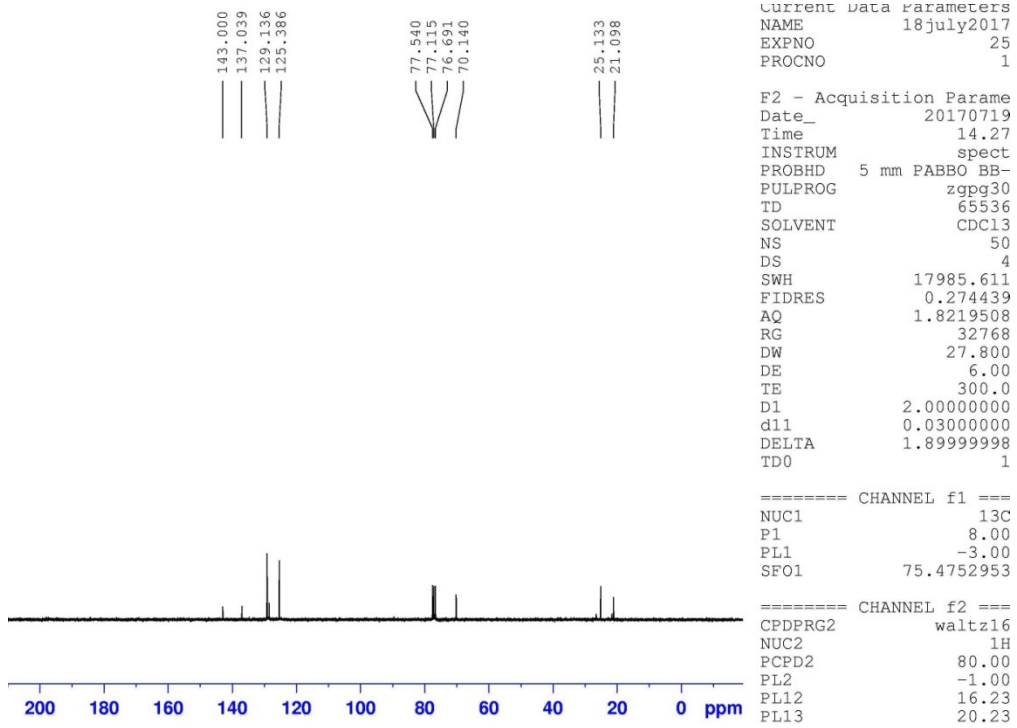

Fig. S47. ^{13}C{^{1}H} NMR of 1-(*p-tolyl*)ethanol

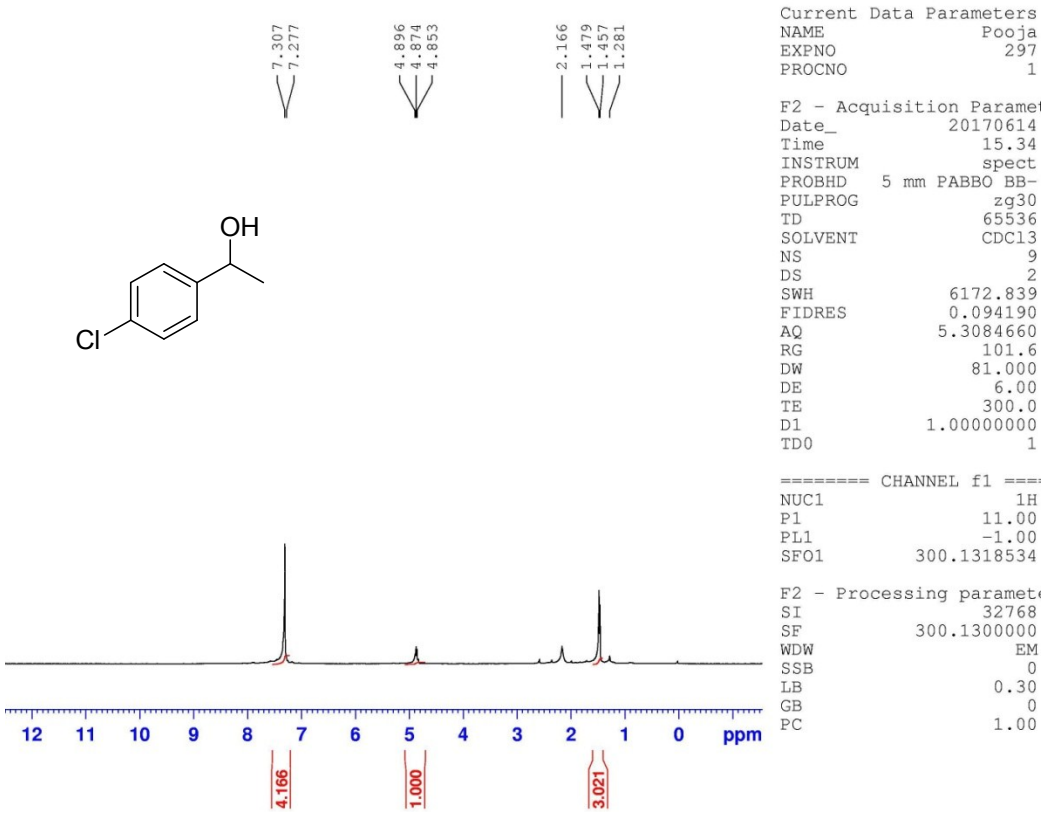

Fig. S48. ^{1}H NMR of 1-(*p*-chloro)ethanol

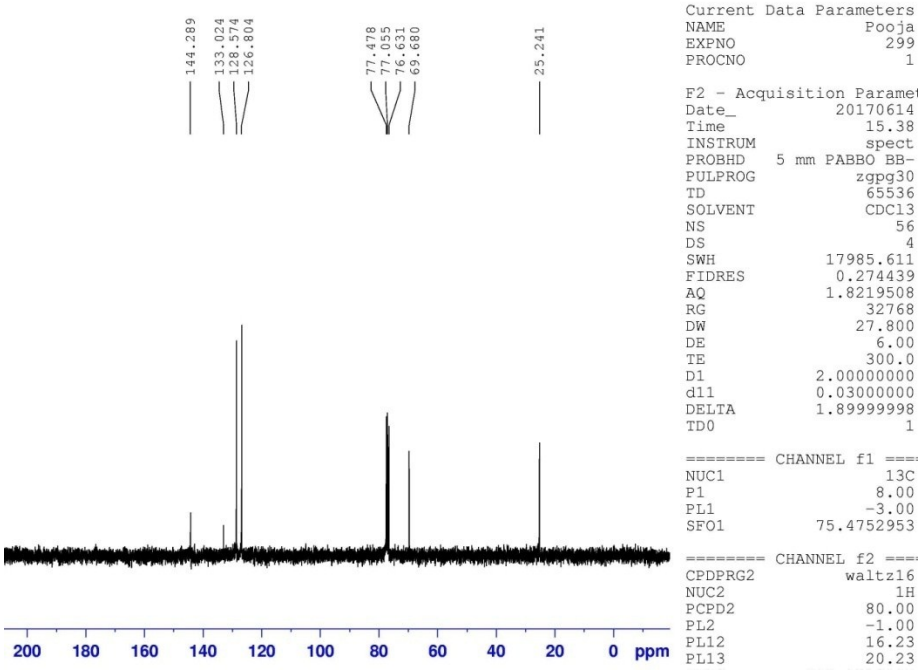

Fig. S49. ^{13}C NMR of 1-(*p*-chloro)ethanol

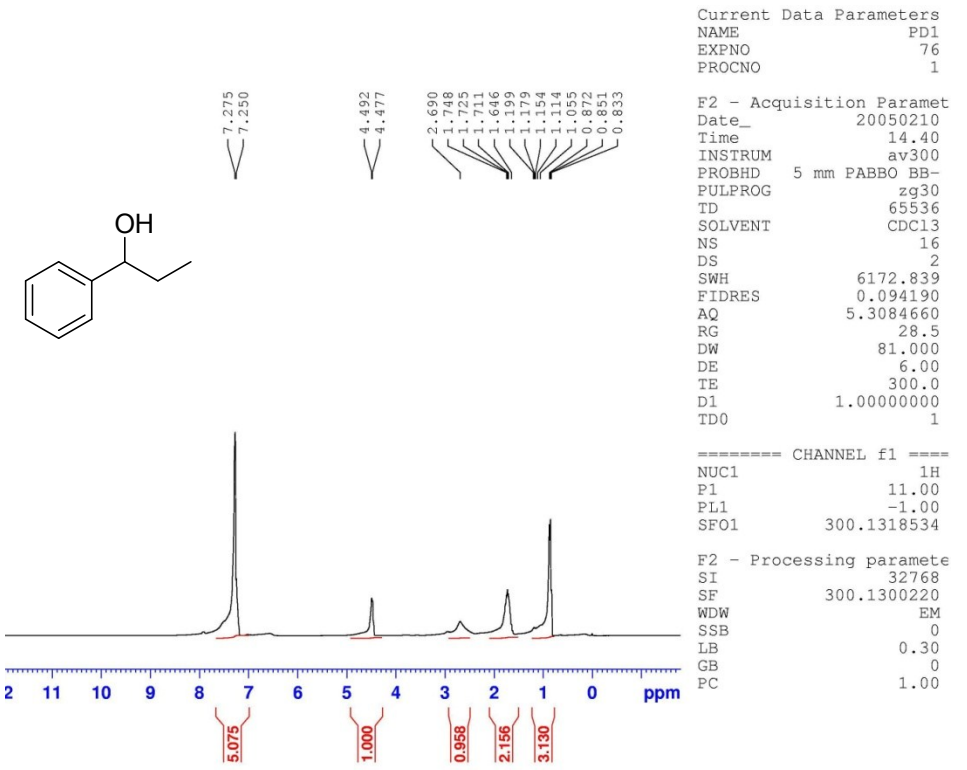

Fig. S50. ^{1}H NMR of 1-phenylpropan-1-ol

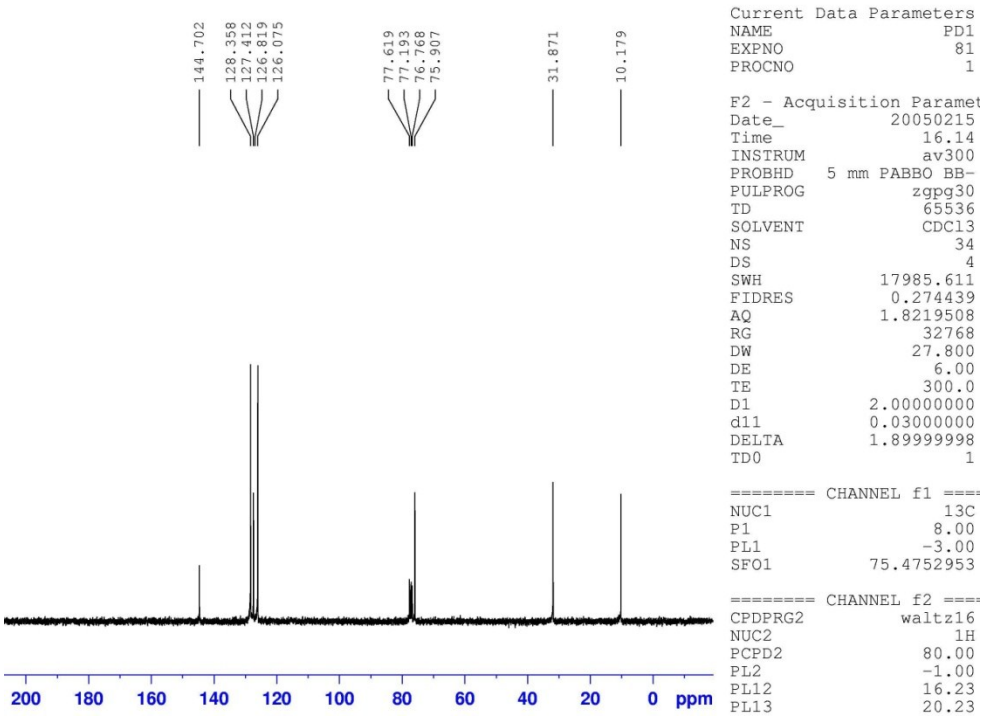

Fig. S51. ^{13}C NMR of 1-phenylpropan-1-ol

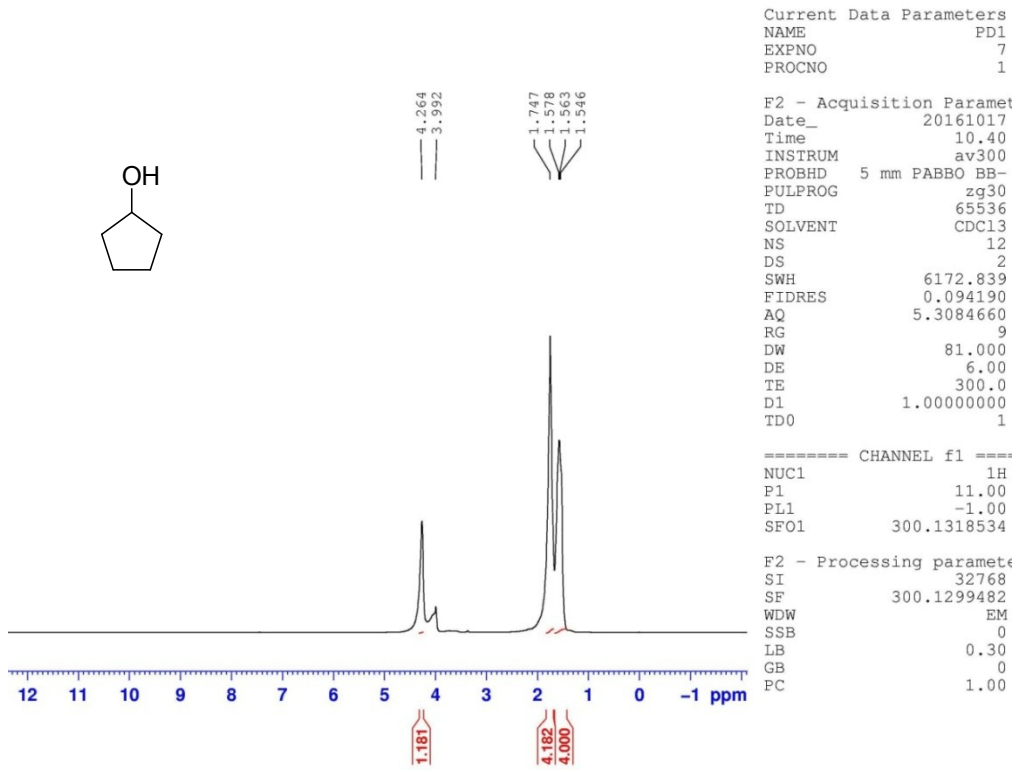

Fig. S52. ^{1}H NMR of cyclopentanol

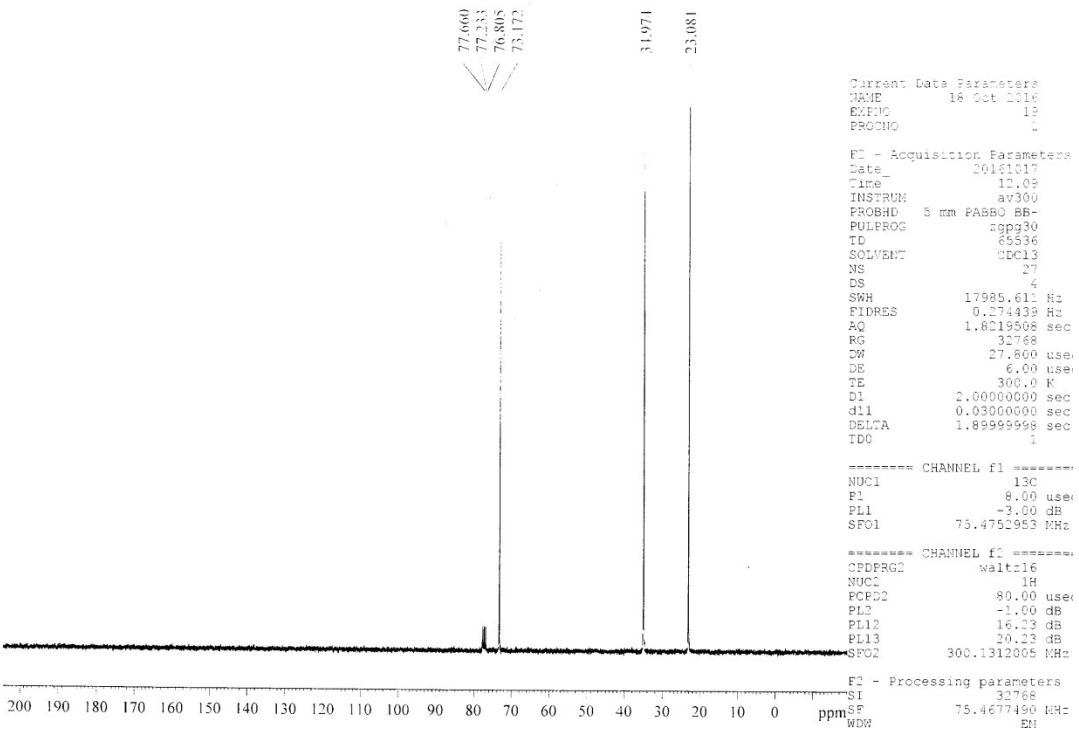

Fig. S53. ^{13}C NMR of cyclopentanol

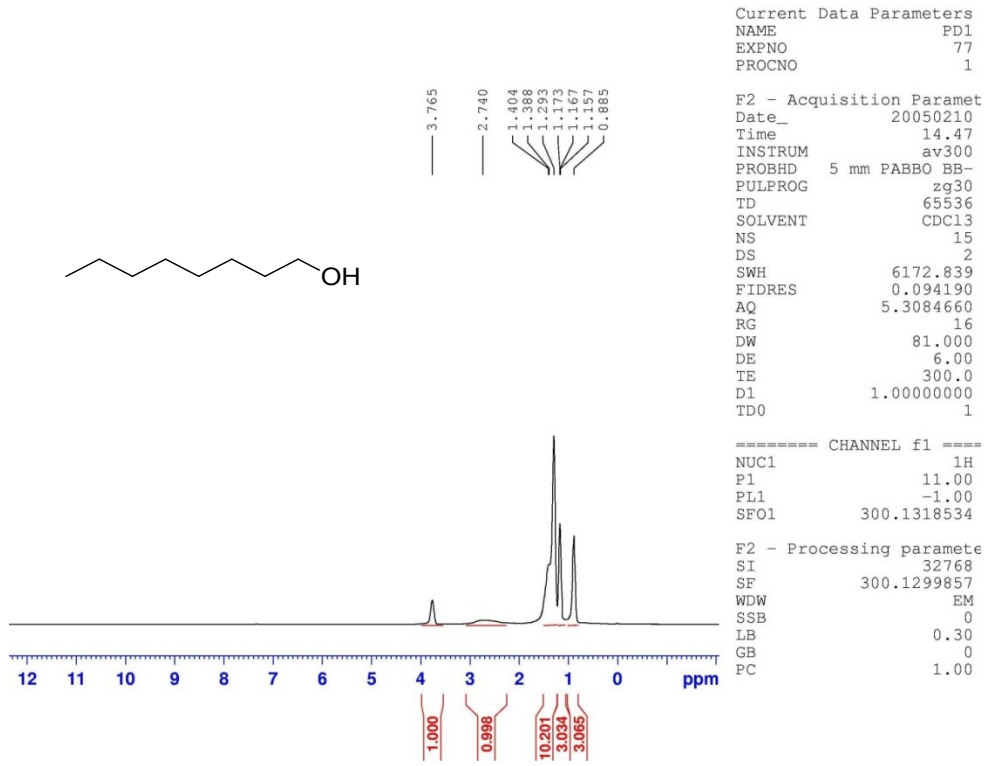

Fig. S54. ^{1}H NMR of octan-2-ol

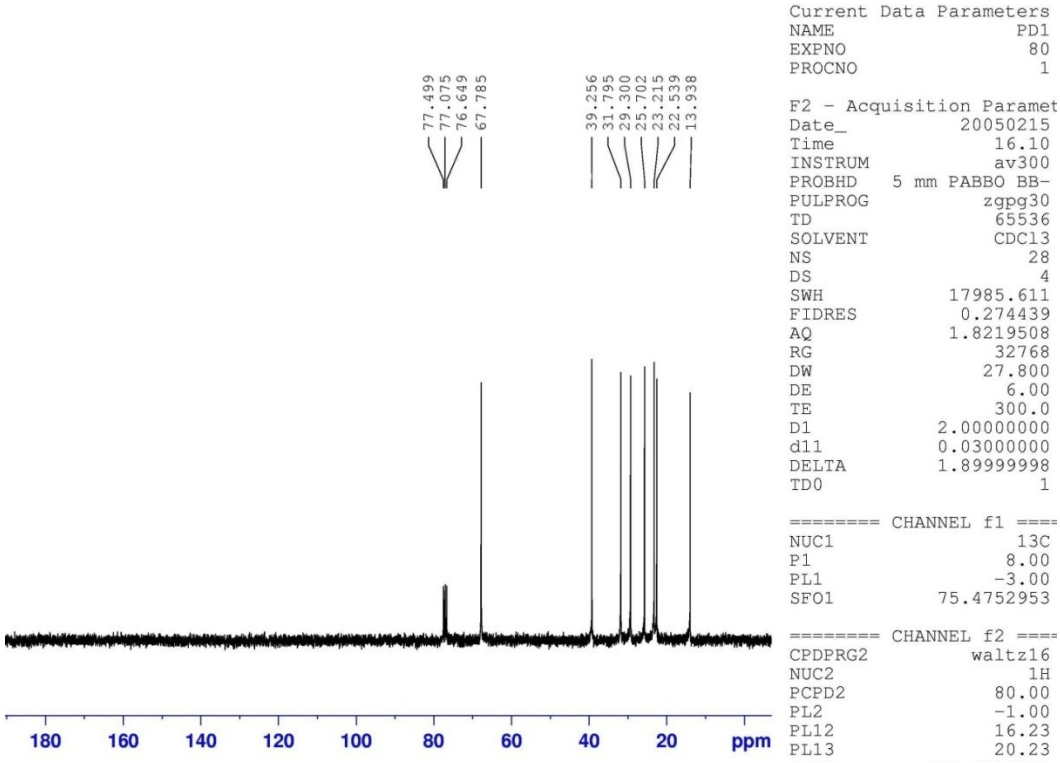

Fig. S55. ^{13}C NMR of octan-2-ol

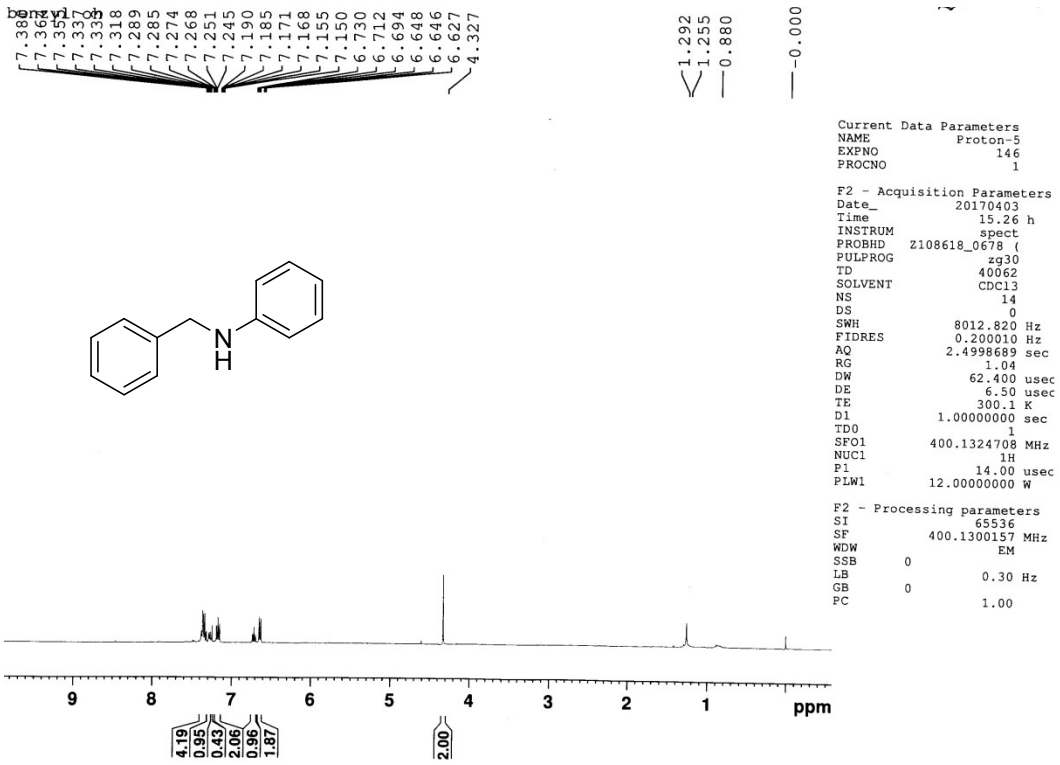

Fig. S56. ^{1}H NMR of N-Benzylaniline

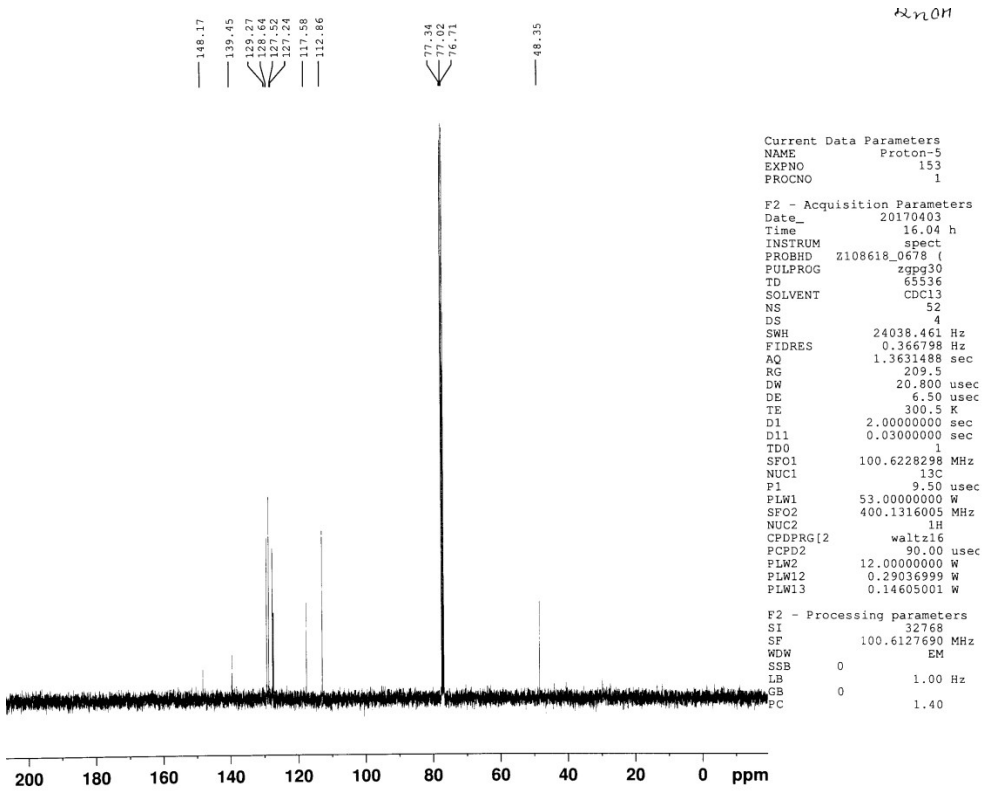

Fig. S57. ^{13}C NMR of N-Benzylaniline

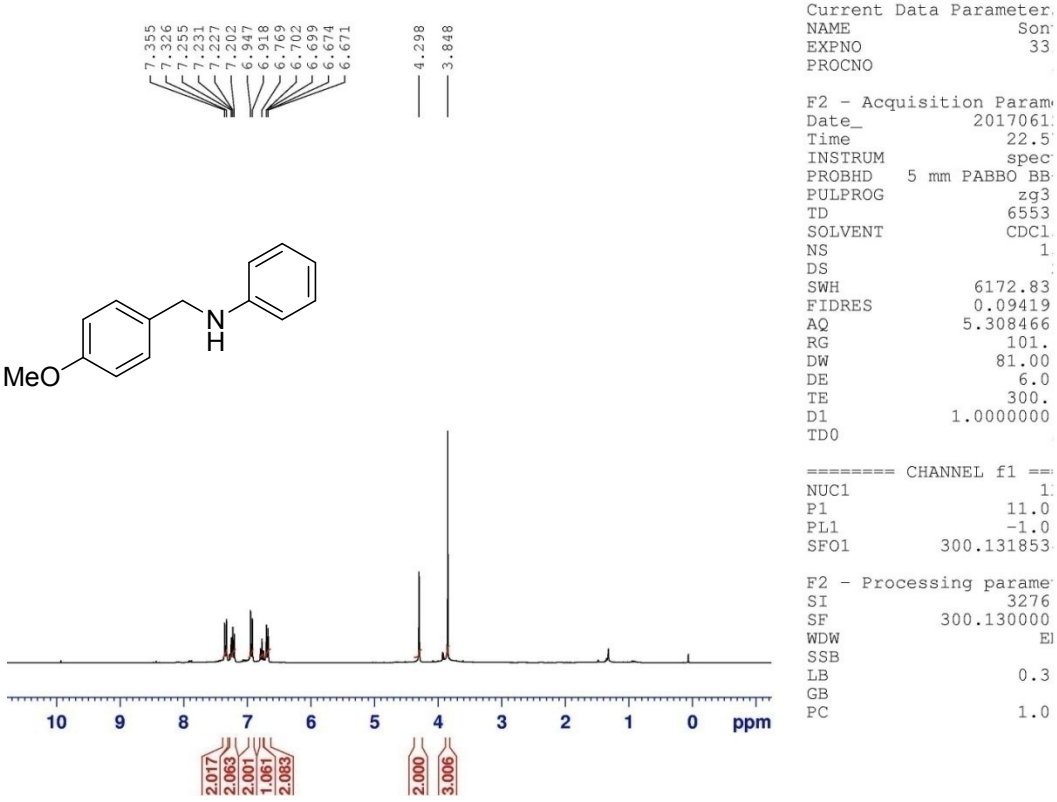

Fig. S58. ^{1}H NMR of N-(4-Methoxybenzyl)aniline

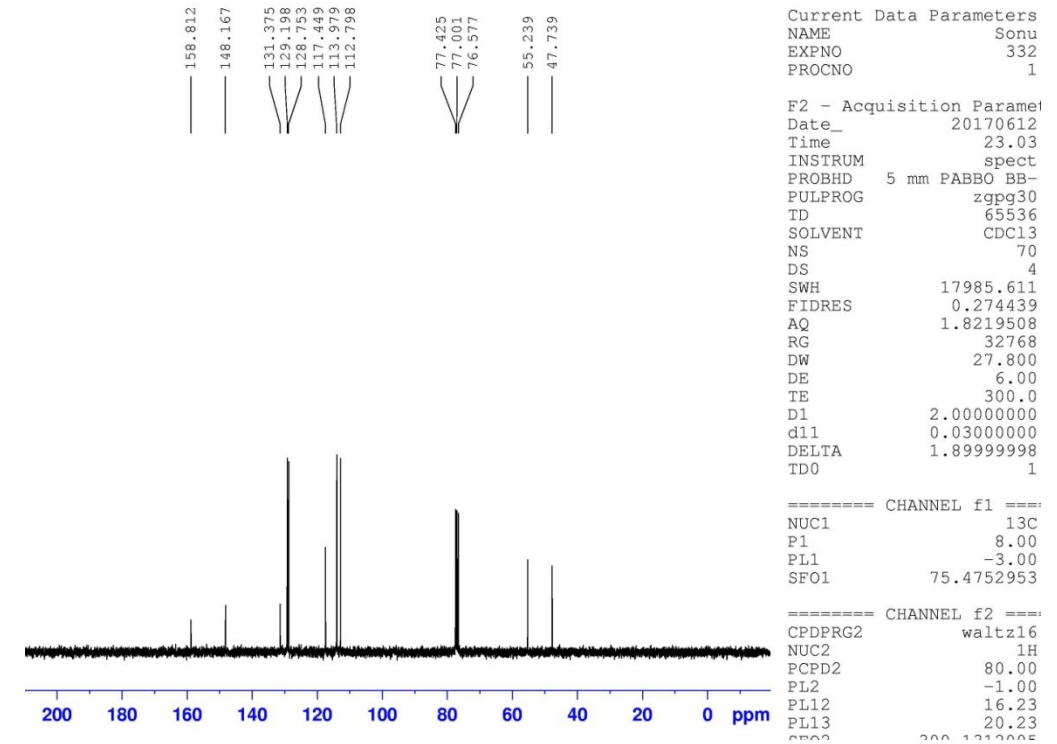

Fig. S59. ^{13}C NMR of N-(4-Methoxybenzyl)aniline

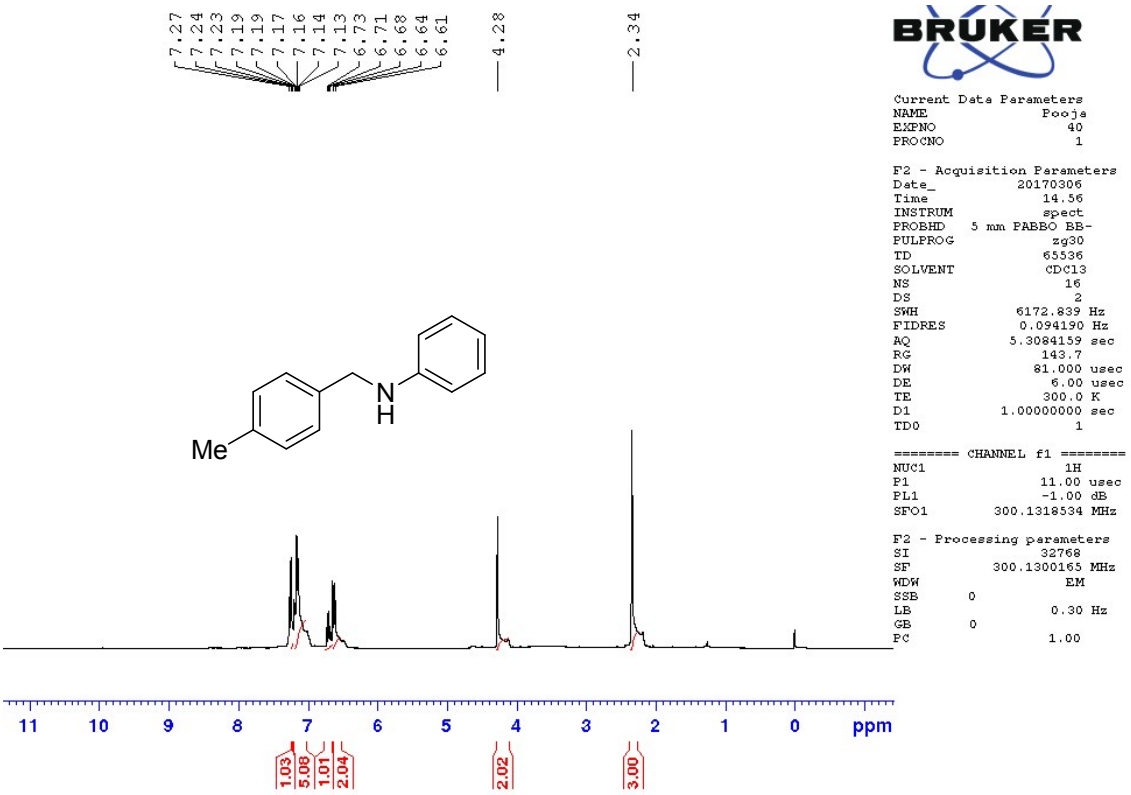

Fig. S60. ^{1}H NMR of N-(4-Methylbenzyl)aniline

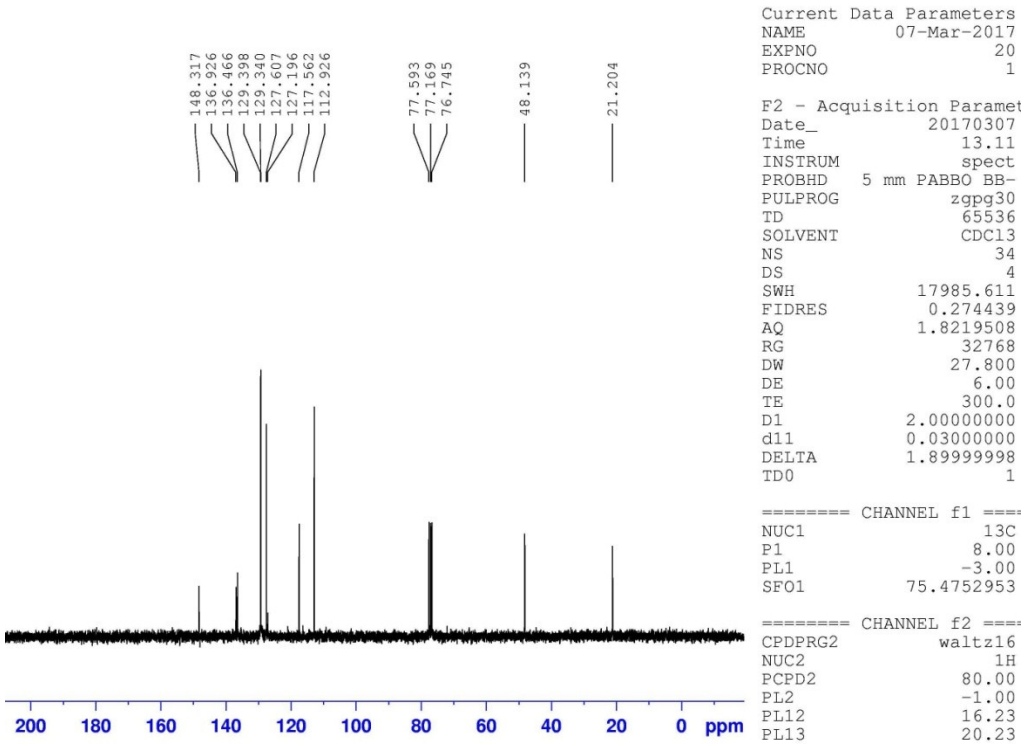

Fig. S61. ^{13}C NMR of N-(4-Methylbenzyl)aniline

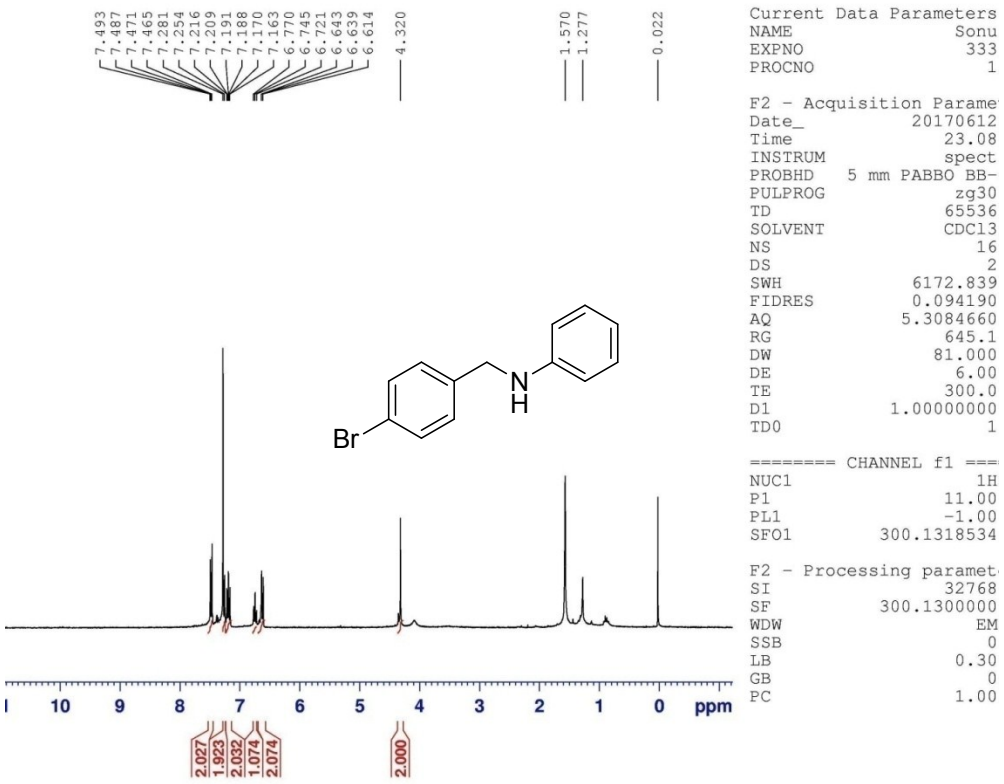

Fig. S62. ^{1}H NMR of N-(4-Bromobenzyl)aniline

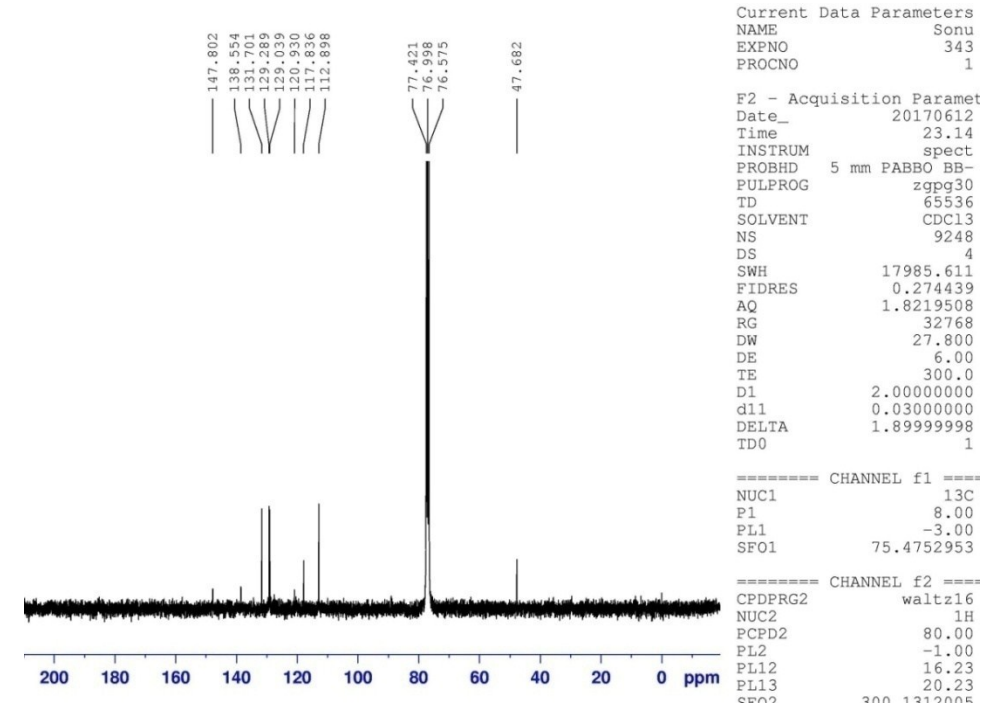

Fig. S63. ^{1}H NMR of N-(4-Bromobenzyl)aniline

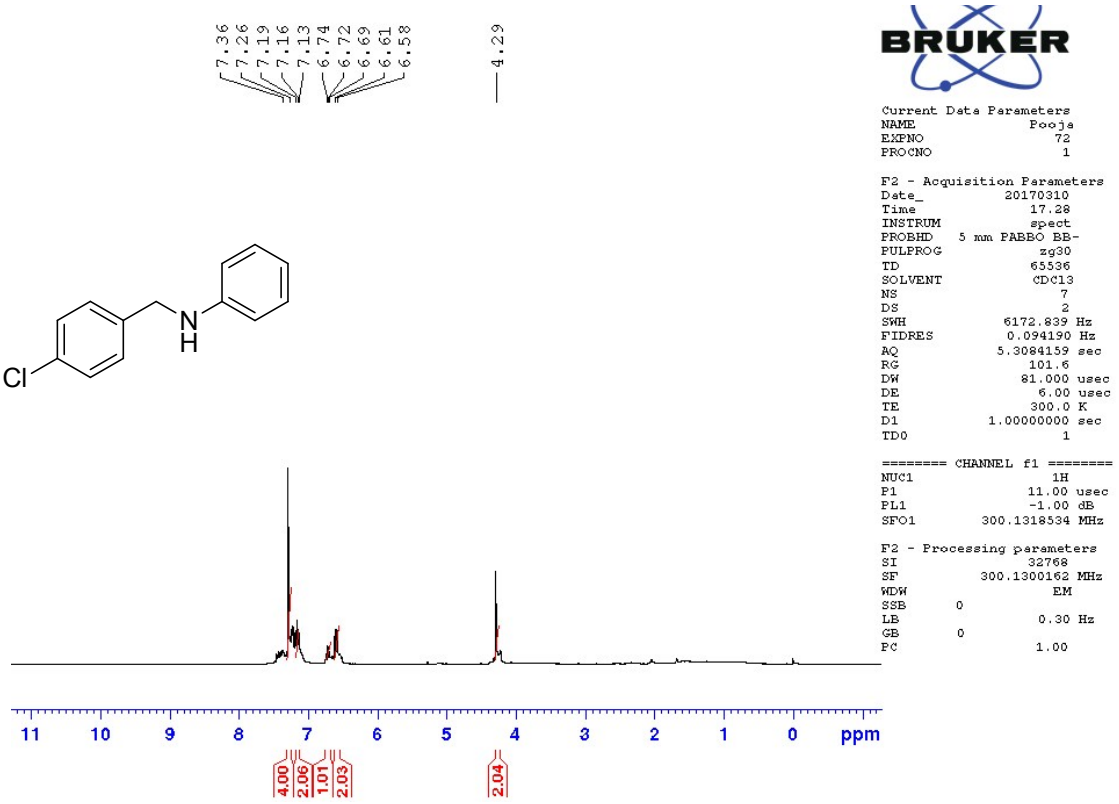

Fig. S63. ^{1}H NMR of N-(4-Chlorobenzyl)aniline

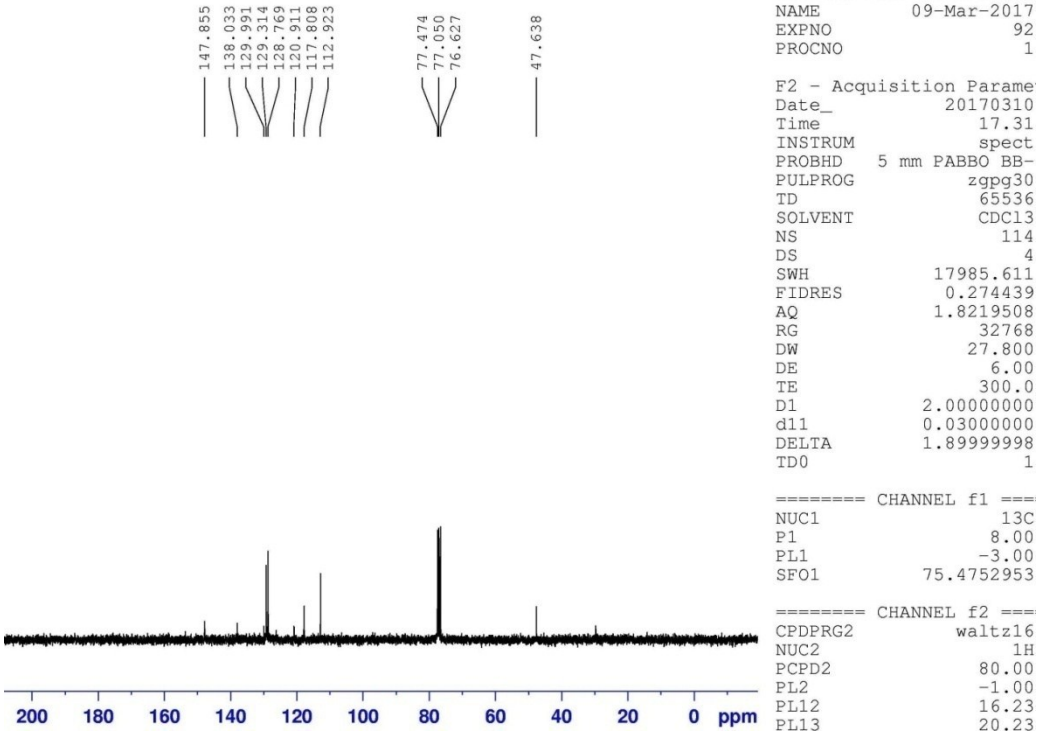

Fig. S64. ^{1}H NMR of N-(4-Chlorobenzyl)aniline

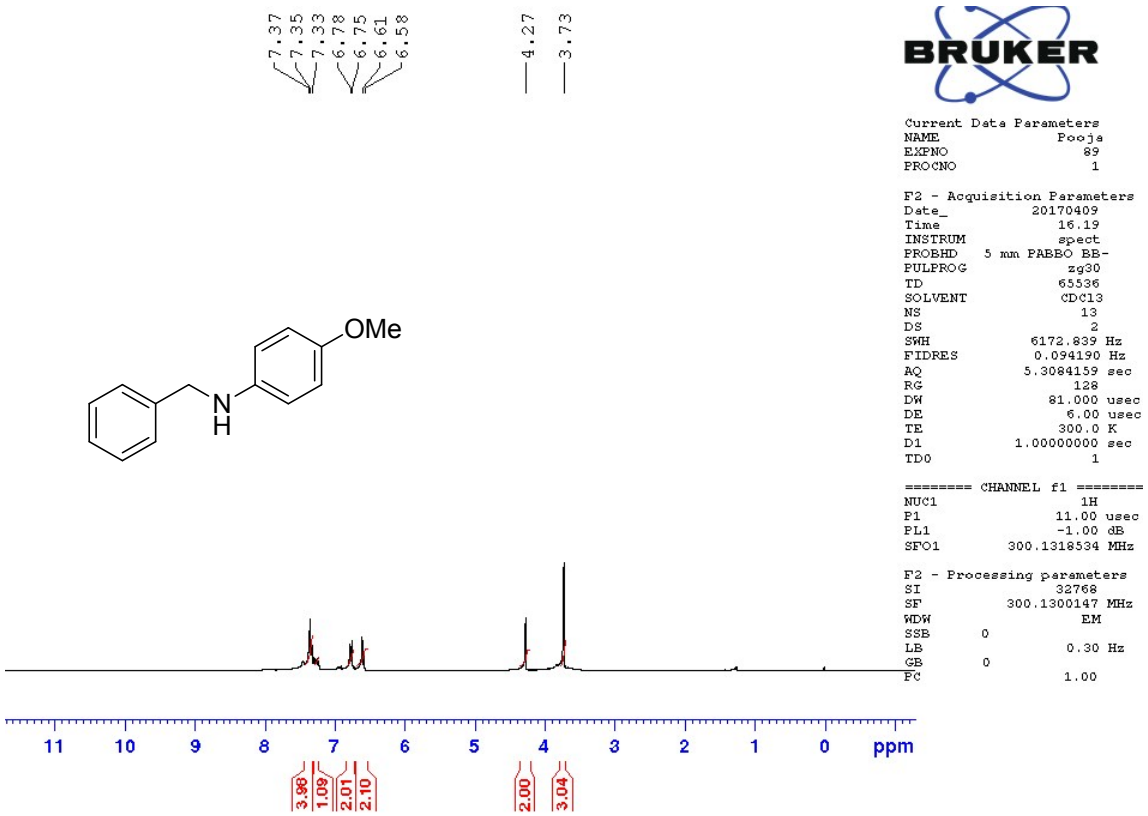

Fig. S65. ^{1}H NMR of N-Benzyl-4-methoxyaniline

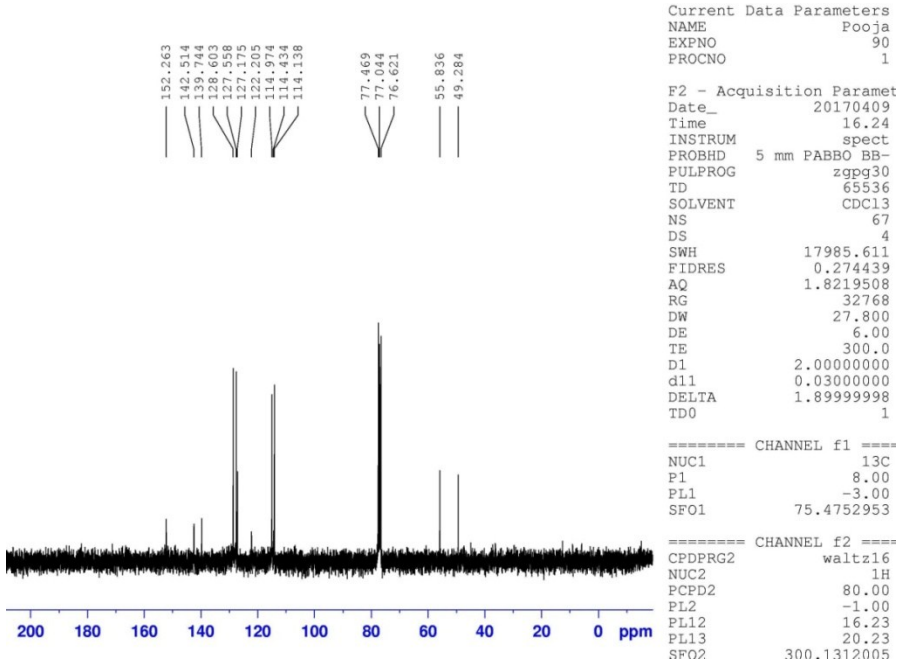

Fig. S66. ^{13}C NMR of N-Benzyl-4-methoxyaniline

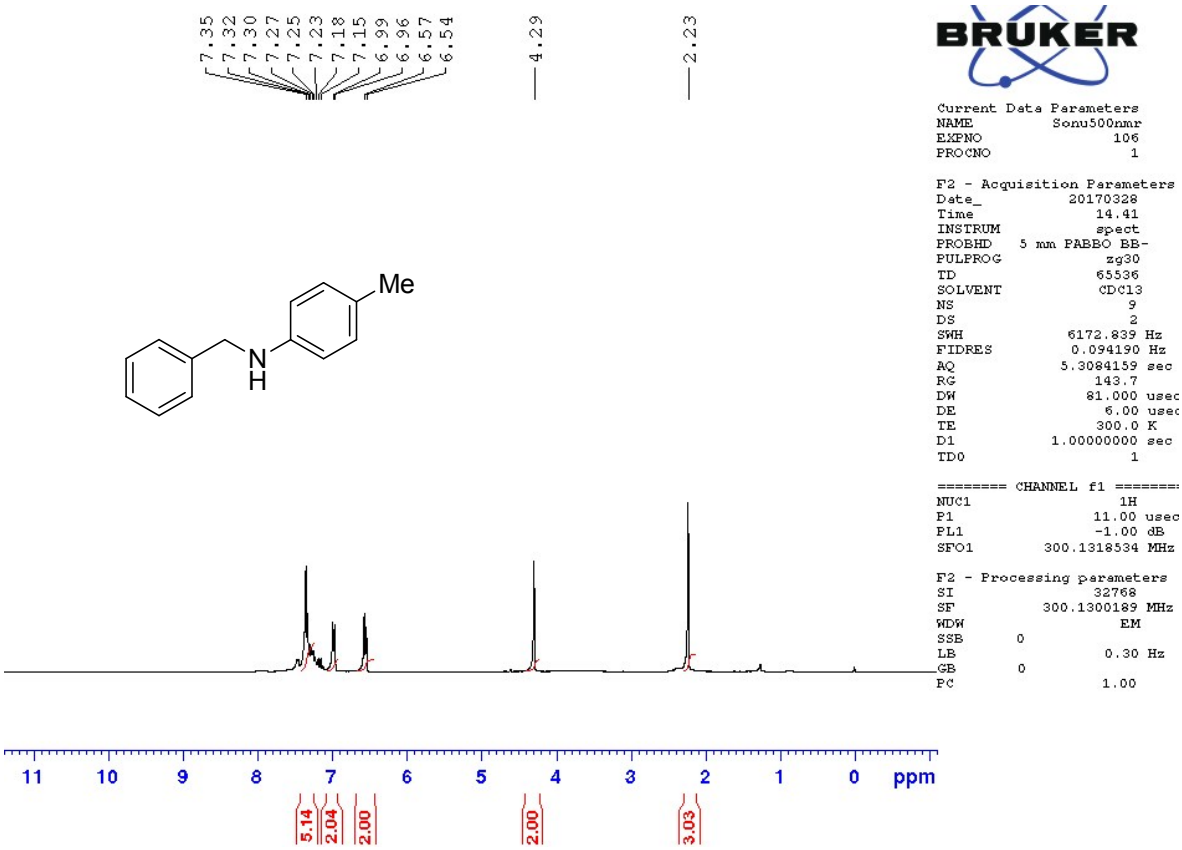

Fig. S67. ^{13}C NMR of N-Benzyl-4-methylaniline

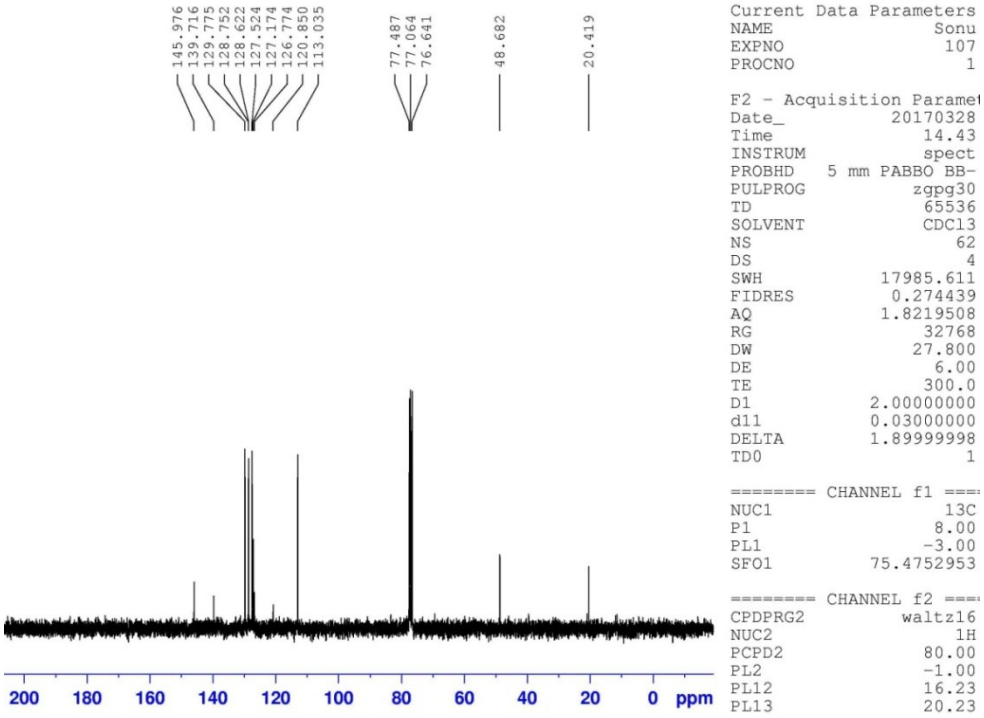

Fig. S68. ^{13}C NMR of N-Benzyl-4-methylaniline

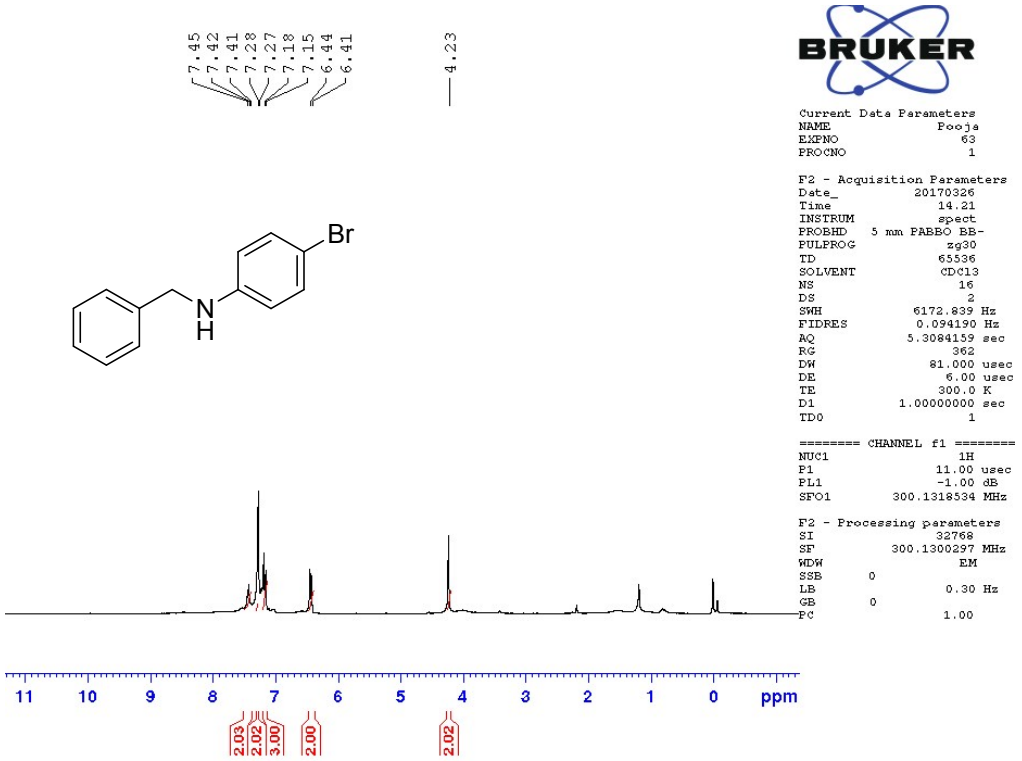

Fig. S69. ^{13}C NMR of N-Benzyl-4-bromoaniline

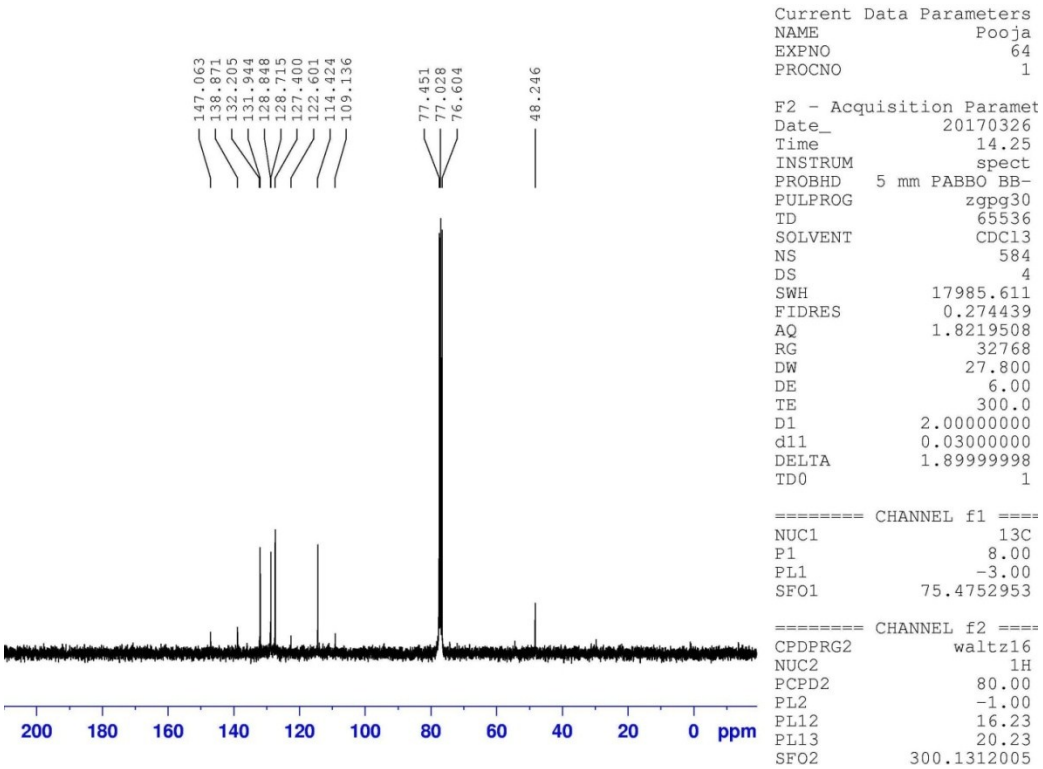

Fig. S70. ^{13}C NMR of N-Benzyl-4-bromoaniline

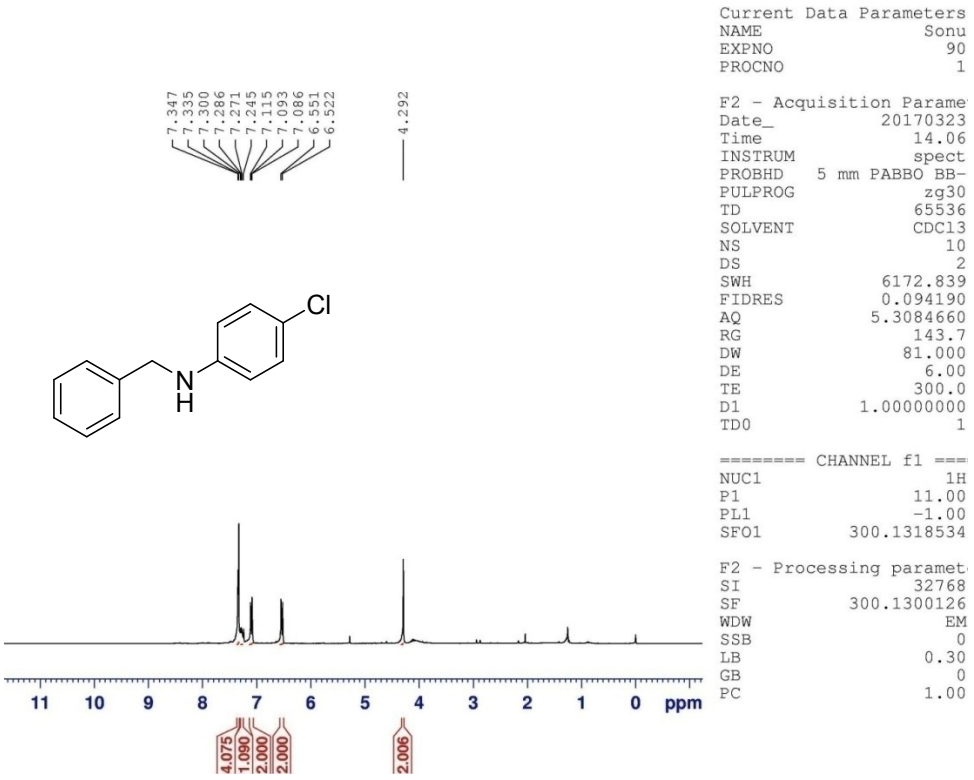

Fig. S71. ^{13}C NMR of N-Benzyl-4-Chloroaniline

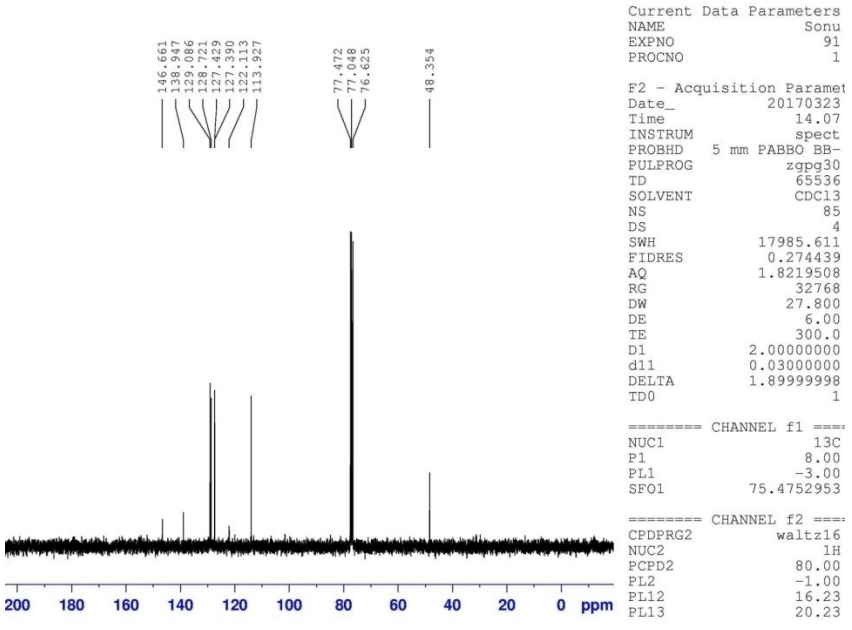

Fig. S72. ^{13}C NMR of N-Benzyl-4-Chloroaniline

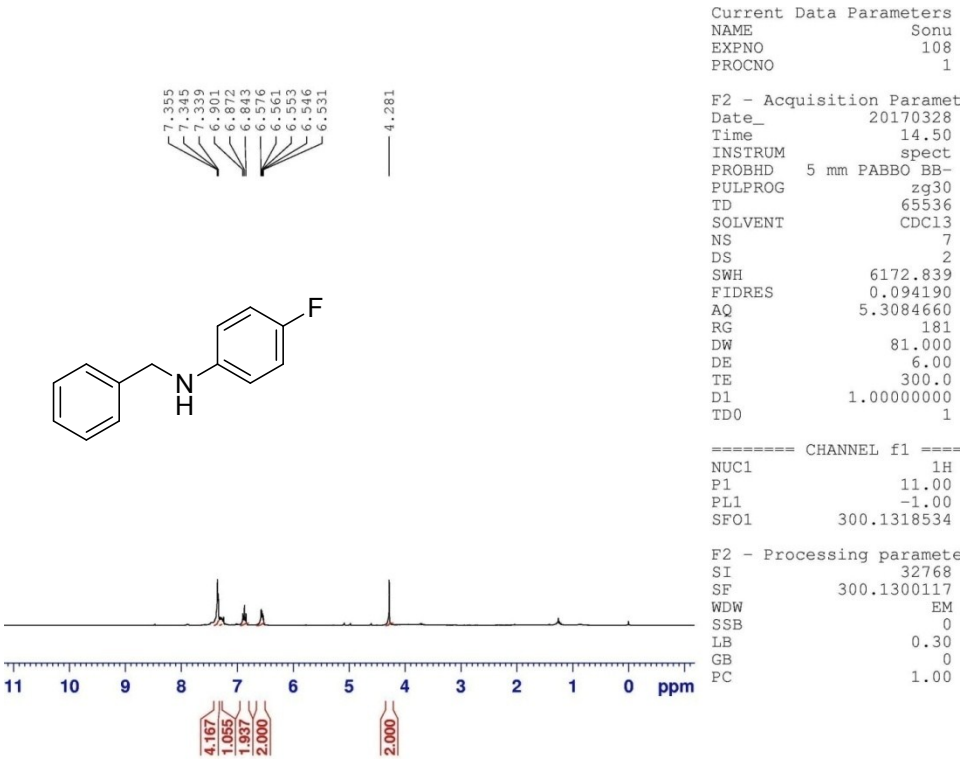

Fig. S73. ^{13}C NMR of N-Benzyl-4-Fluoroaniline

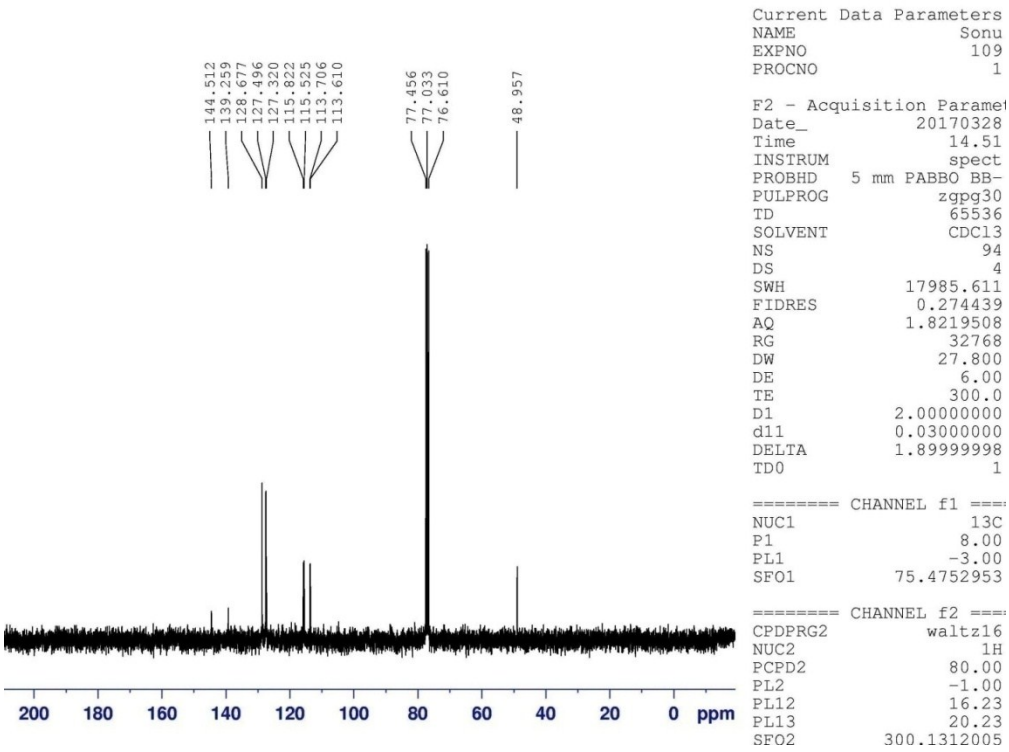

Fig. S74. ^{13}C NMR of N-Benzyl-4-Fluoroaniline

The NMR spectral data of compounds found as reported in literature.

Phenylmethanol[1]: ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm): 4.61 (s, 2H), 7.46 (m,5H). $^{13}C\{^{1}H\}$ NMR (75 MHz, CDCl3, 25 ºC, TMS): δ (ppm) 64.7, 127.1, 127.5, 128.5, 141.0.

(4-Nitrophenyl)methanol[1]: ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm): 4.85 (s, 2H), 7.54 (d, 2H, J = 9 Hz), 8.21 (d, 2H, J = 9 Hz). $^{13}C\{^{1}H\}$ NMR (75 MHz, CDCl3, 25 ºC, TMS): δ (ppm) 63.8, 123.6, 126.9, 147.1, 148.3.

(4-bromophenyl)methanol[1]: ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ(ppm): 4.65 (s, 2H), 7.24 (d, 2H, J = 9 Hz), 7.49 (d, 2H, J = 9 Hz). $^{13}C\{^{1}H\}$ NMR (75 MHz, CDCl3, 25 ºC, TMS): δ (ppm) 64.5, 121.6, 128.5, 131.6, 139.7.

(4-chlorophenyl)methanol[1]: ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm): 4.66 (s, 2H), 7.28-7.35 (m, 4H). : $^{13}C\{^{1}H\}$ NMR (75 MHz, CDCl3, 25 ºC, TMS): δ (ppm) 64.5, 128.2, 128.6, 133.3, 139.2.

(4-methoxyphenyl)methanol[1]: ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm): 3.78 (s, 3H), 4.56 (s, 2H), 6.88 (d, 2H, J = 8.4 Hz), 7.24 (d, 2H, J = 9 Hz). $^{13}C\{^{1}H\}$ NMR (75 MHz, CDCl3, 25 ºC, TMS): δ (ppm) 55.1, 64.2, 113.8, 128.6, 133.2, 159.9

p-Tolylmethanol[1]: ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm): 2.38 (s, 3H), 4.64 (s, 2H), 7.20 (m, 2H), 7.29 (m, 2H). $^{13}C\{1H\}$ NMR (75 MHz, CDCl3, 25 ºC, TMS): δ (ppm) 21.1, 64.9, 127.1, 129.2, 137.2, 138.0.

pyridine-2-ylmethanol[1]: ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm): 4.76 (s, 2H), 7.18-7.26 (m, 2H), 7.65-7.70 (m, 1H), 8.55-8,56 (d, 1H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 64.1, 120.5, 122.2, 136.6, 148.5, 159.2.

phenylethanol[1]: ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 1.35 (d, 3H, J = 6.3 Hz), 3.43 (s, 1H), 4.68-4.70 (m, 1H), 7.15-7.25 (m, 5H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 24.8, 69.7, 124.7, 125.2, 128.48, 145.92.

1-(p-tolyl)ethanol[1]: ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 1.33 (d, 3H, J = 6 Hz), 2.19 (s, 3H), 4.72-4.66 (m, 1H), 6.99-7.01 (d, 2H), 7.09-7.12 (d, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 21.0, 25.1, 70.1, 125.3, 129.1, 137.0, 143.0.

1-phenylpropan-1-ol[1]: ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 0.83 (t, 3H, J = 6), 1.11-1.19 (m, 2H), 2.69 (br, 1H), 4.47 (m, 1H), 7.25-7.27 (m, 5H). $^{13}C\{1H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 10.1, 31.8, 75.9, 126.0, 126.8, 127.4, 128.3, 144.7.

Cyclopentanol[1]: ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 1.54-1.56 (m, 4H) 1.75-1.78 (m, 4H), 4.26 (m, 1H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 23.26, 35.52, 73.96.

octan-2-ol[1] :^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 0.89 (t, 3H, J = 6 Hz), 1.183 (d, 3H, J = 6.3 H Z), 1.30-1.43(m, 10H), 3.76-3.82 (m, 1H).). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 23.0, 34.9, 73.9.

N-Benzylaniline[2]. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ 7.38−7.31 (m, 4H), 7.28−7.26 (m, 1H), 7.19-7.15 (m, 2H), 6.71 (t, J = 8 Hz, 1H), 6.64 (d, J = 8 Hz, 2H), 4.32 (s, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ 148.1, 139.4, 129.2, 128.6, 127.5, 127.2, 117.5, 112.8, 48.3.

N-(4-Methoxybenzyl)aniline[2]. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ 7.33-7.30 (d, J = 9 Hz, 2H), 7.20 (t, J = 6 Hz, 2H), 6.89 (d, J = 9 Hz, 2H), 6.74 (m, 1H), 6.65 (d, J = 6 Hz, 2H), 4.27 (s, 2H), 3.82 (s, 3H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ 158.8, 148.2, 131.4, 129.2, 128.8, 117.5, 114.0, 112.8, 55.3, 47.8.

N-(4-Methylbenzyl)aniline[2]. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ7.27- 7.24 (m, 1H), 7.23-7.16 (m, 5H), 6.73-6.68 (m, 1H), 6.64-6.61 (m, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ 148.3, 136.9, 136.4, 129.3, 129.3, 127.6, 117.5, 112.9, 48.1, 21.1.

N-(4-Bromobenzyl)aniline[2]. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ 7.49-7.46 (m, 2H), 7.28-7.20 (m, 2H), 7.19-7.16 (m, 2H), 6.77-6.72 (m, 1H), 6.64-6.61 (m, 2H), 4.32 (s, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ 147.8, 138.5, 131.7, 129.2, 129.0, 120.9, 117.8, 112.8, 47.6.

N-(4-Chlorobenzyl)aniline[2]. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ 7.36-7.26 (s, 4H), 7.19-7.23 (m, 2H), 6.74-6.69 (m, 1H), 6.61-6.58 (m, 1H), 6.60-6.57 (m, 1H), 4.30 (s, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ 147.8, 138.0, 129.9, 129.3, 128.7, 120.9, 117.8, 112.9, 47.6.

N-Benzyl-4-methoxyaniline[2]. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ 7.37−7.32 (m, 5H), 6.75 (d, J = 9 Hz, 2H), 6.60 (d, J = 9 Hz, 2H), 4.27 (s, 2H), 3.81 (s, 3H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ 152.2, 142.5, 139.7, 128.6, 127.5, 127.1, 114.9, 114.3, 55.8, 49.2.

N-Benzyl-4-methylaniline[2]. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ 7.34−7.15 (m, 5H), 6.98 (d, J = 6 Hz, 2H), 6.56 (d, J = 9 Hz, 2H), 4.29 (s, 2H), 2.22 (s, 3H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ 145.9, 139.7, 129.7, 128.7, 127.5, 127.1, 126.7, 113.0, 48.6, 20.4.

N-Benzyl-4-bromoroaniline[2]**.** ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ 7.44−7.42 (m, 2H), 7.27-7.20 (m, 2H), 7.17-7.14 (m, 3H), 6.44-6.41 (d, J = 9 Hz, 2H), 4.22 (s, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ 147.0, 138.8, 132.2, 131.9, 128.8, 128.7, 122.6, 114.2, 109.1, 48.6

N-Benzyl-4-chloroaniline[2]. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ 7.34−7.30 (m, 4H), 7.28-7.24 (m, 1H), 7.11-7.08 (m, 2H), 6.55 (d, J = 9 Hz, 2H), 4.29 (s, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ 146.5, 138.8, 129.0, 128.7, 127.4, 127.3, 122.1, 113.9, 48.3.

N-Benzyl-4-fluoroaniline[2]. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ 7.35−7.33 (m, 5H), 6.90-6.84 (d, J = 9 Hz, 2H), 6.57-6.53 (m, 2H), 4.29 (s, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ 144.5, 139.2, 128.6, 127.4, 127.3, 115.8, 115.5,113.7, 113.6, 48.9.

Reference

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