Earth abundant metal complexes of donor functionalised *N*-heterocyclic carbene ligands: synthesis, characterization and application as amination catalysts

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Supplementary Material

Analyses data for synthesized imidazolium salts and Ag-, Ni- & Co-NHC complexes

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Data for functionalised imidazolium salts with picolyl moiety (1)

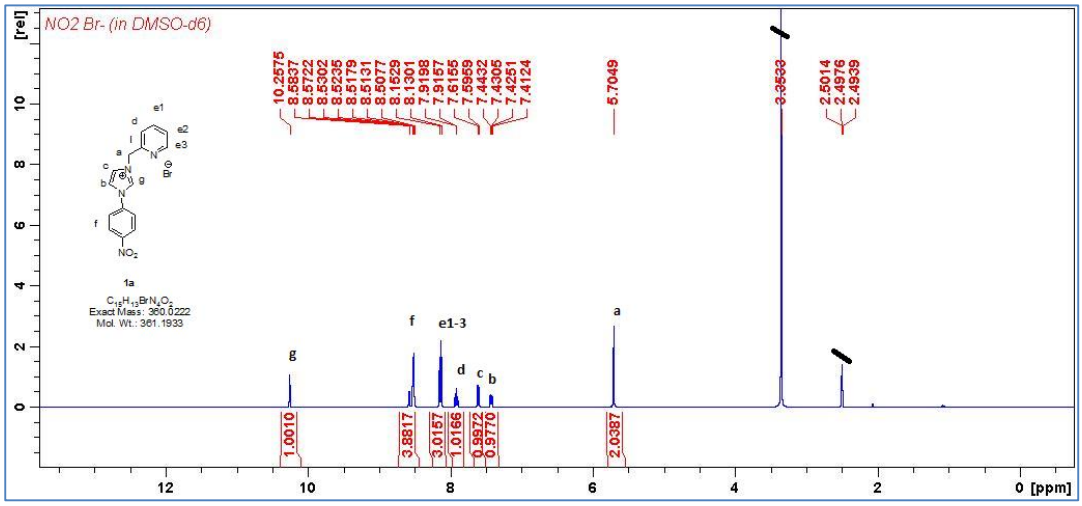


Figure S1: ^{1}H NMR spectrum of 1-(4-nitrophenyl)-3-(pyridine-2-ylmethyl)-1H-imidazol-3-ium bromide (1a).

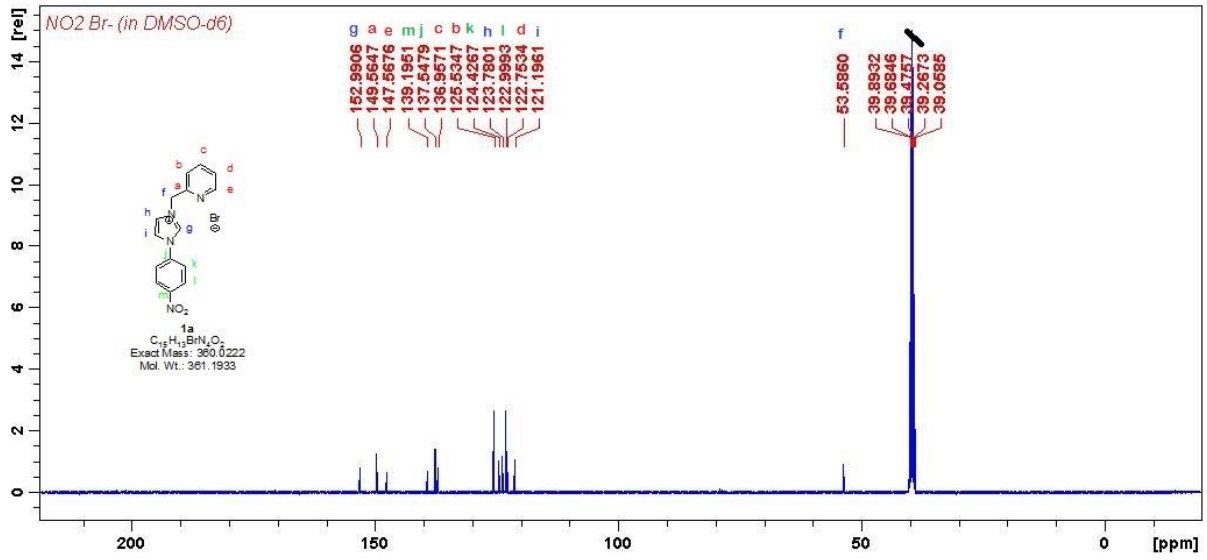


Figure S2: ^{13}C NMR spectrum of 1a.

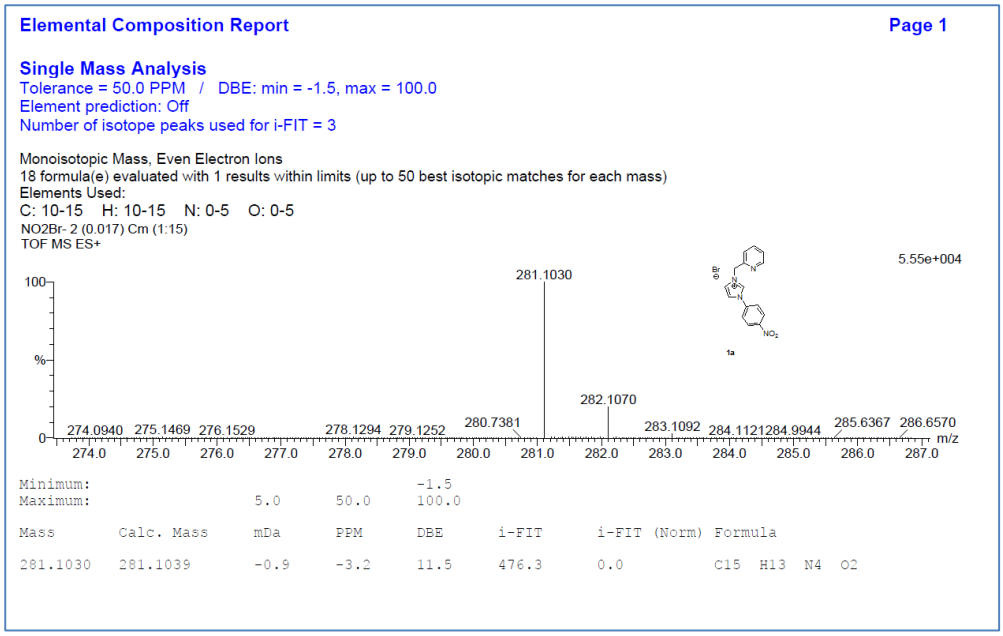


Figure S3: HRMS spectrum of 1a.

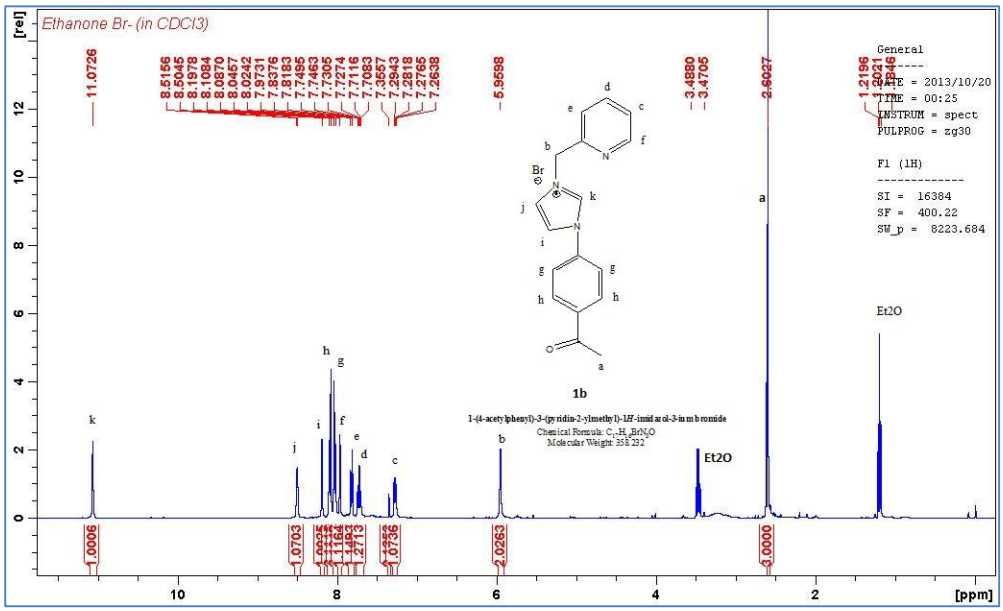


Figure S4: ^{1}H NMR spectrum of 1-(4-acetylphenyl)-3-(pyridine-2-ylmethyl)-1H-imidazol-3-ium bromide (1b).

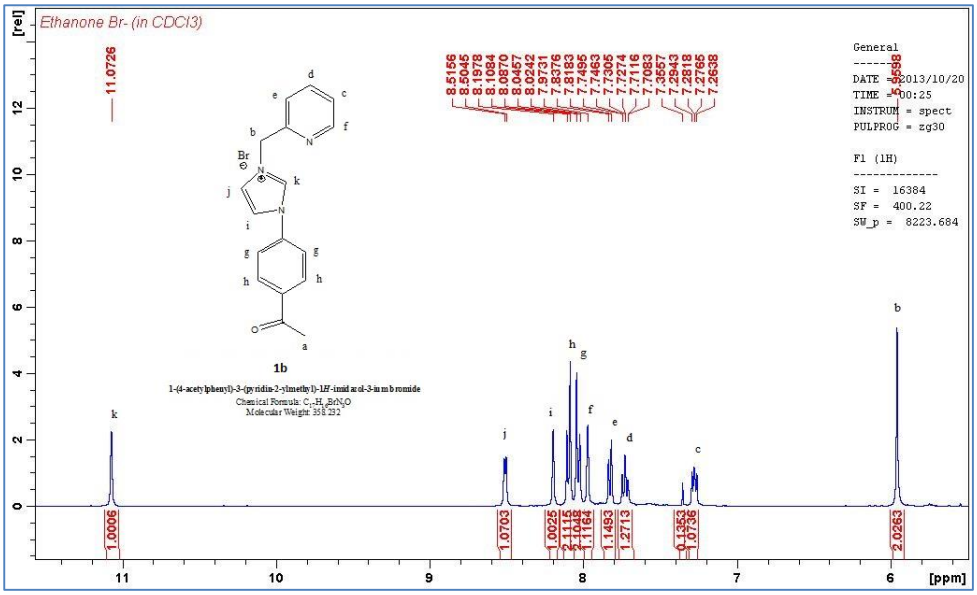


Figure S5: Expanded ^{1}H NMR spectrum of 1b.

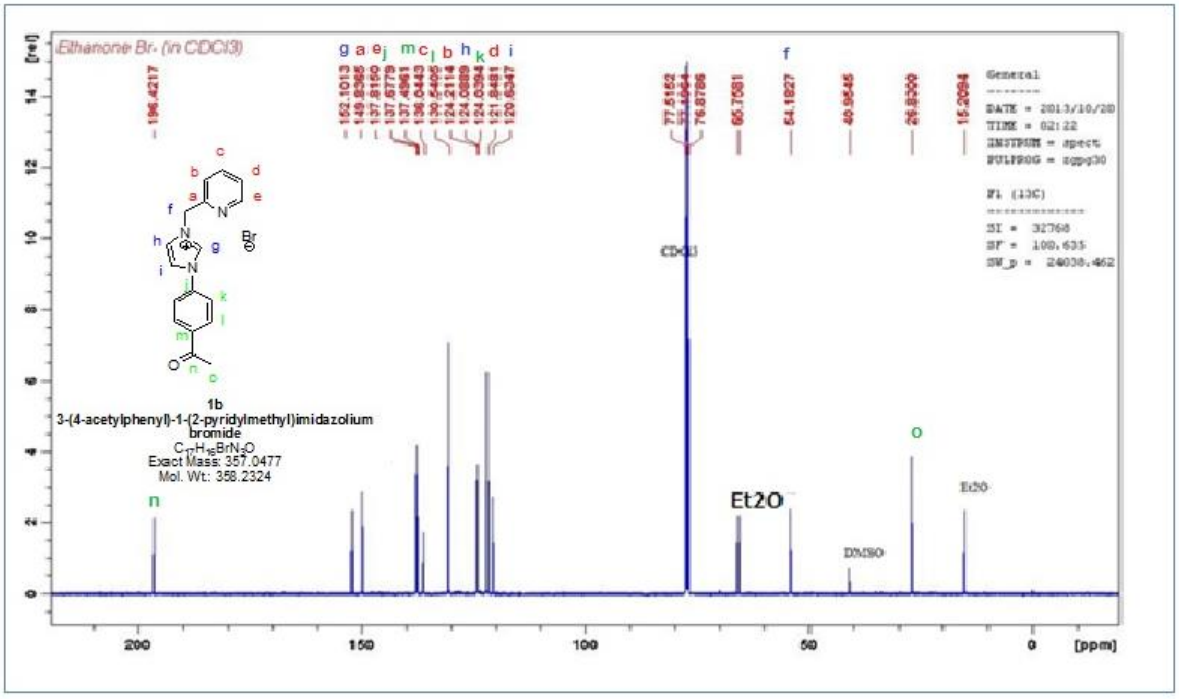


Figure S6: ^{13}C NMR spectrum of 1b.

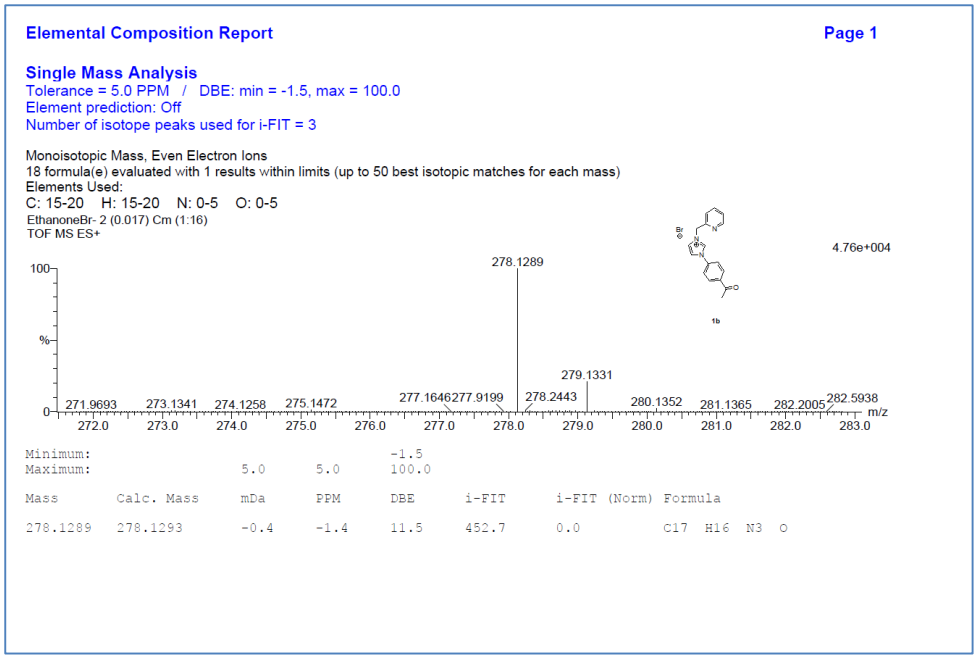


Figure S7: HRMS spectrum of 1b.

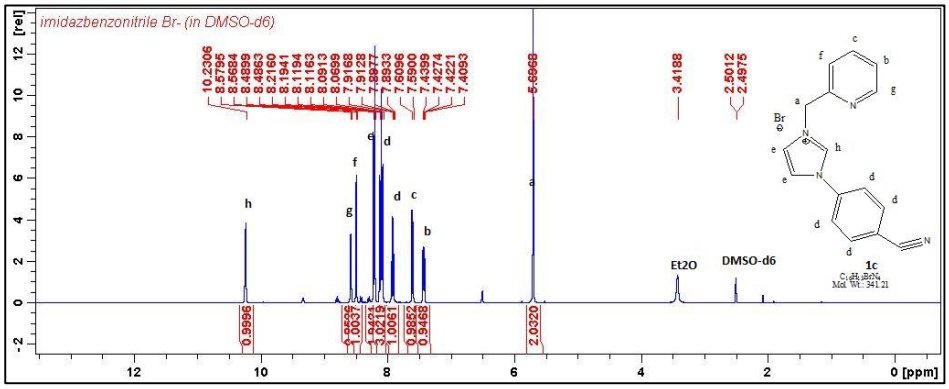


Figure S8: ^{1}H NMR spectrum for 3-(4-cyanophenyl)-1-(2-pyridylmethyl)imidazolium bromide (1c).

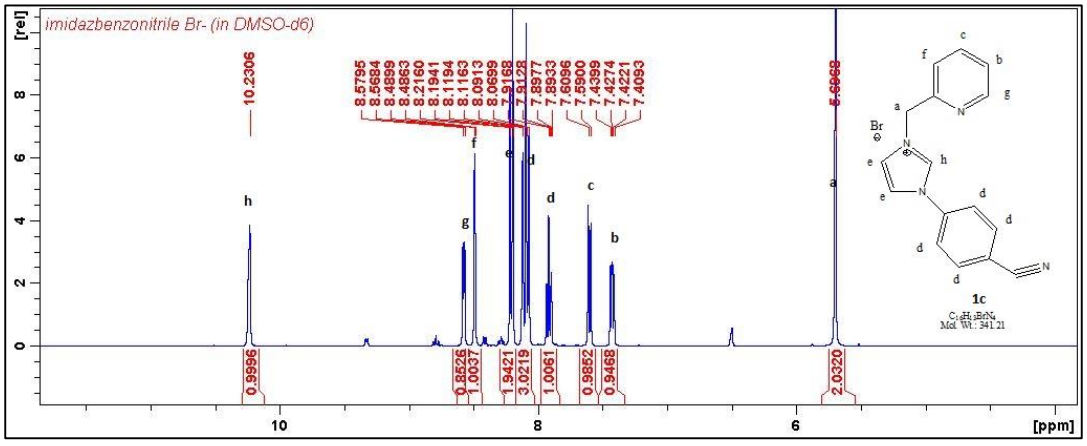


Figure S9: Expanded ^{1}H NMR spectrum of 1c.

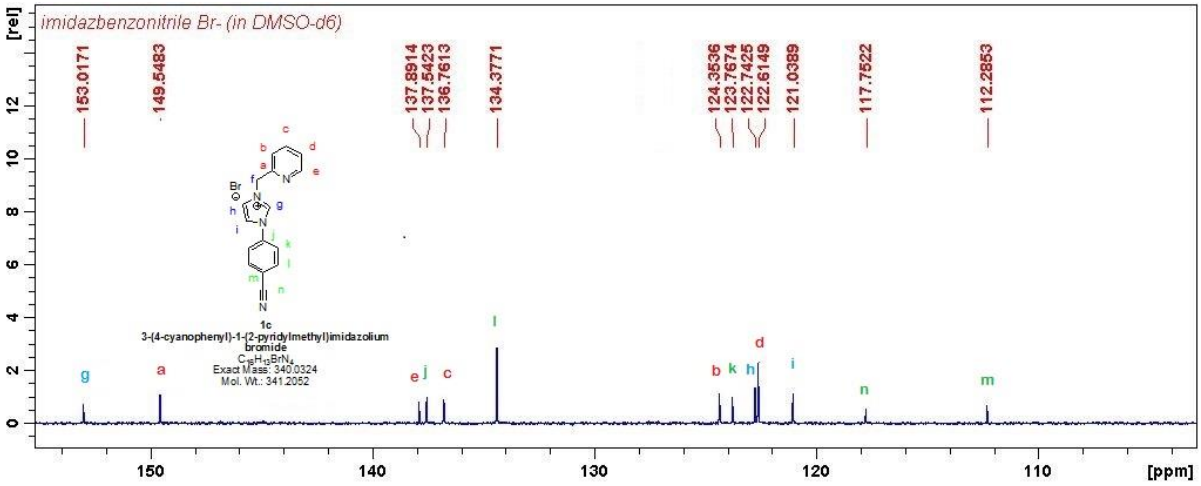


Figure S10: Expanded ^{13}C NMR spectrum of 1c.

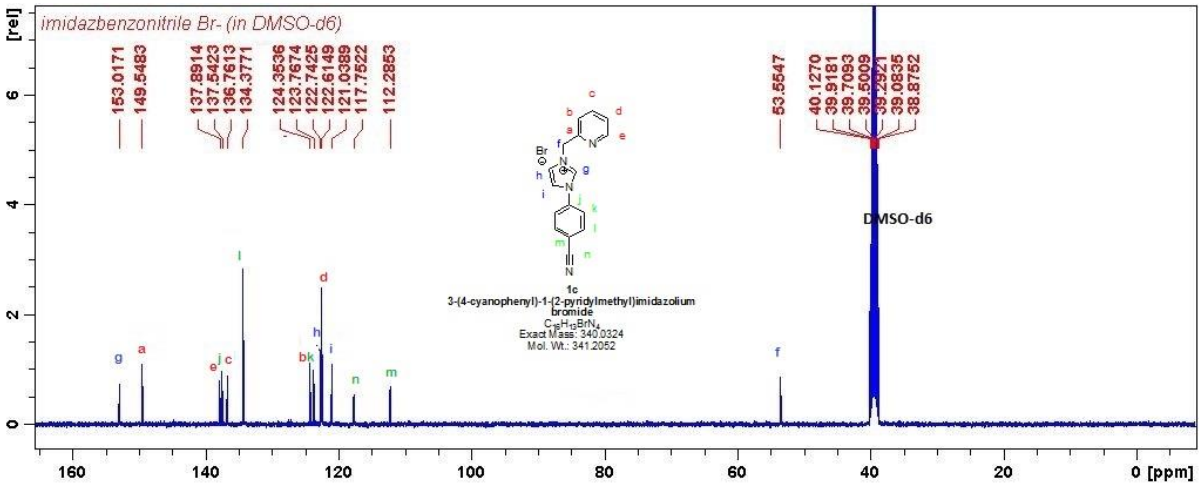


Figure S11: ^{13}C NMR spectrum of 1c.

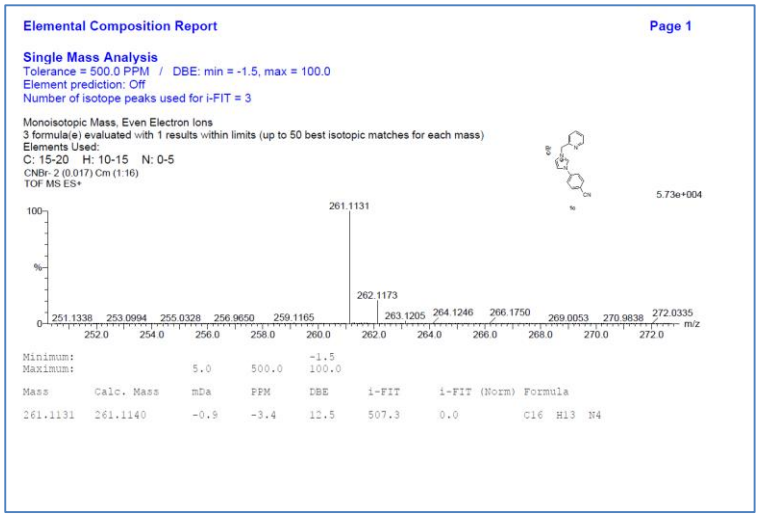


Figure S12: HRMS spectrum of 1c.

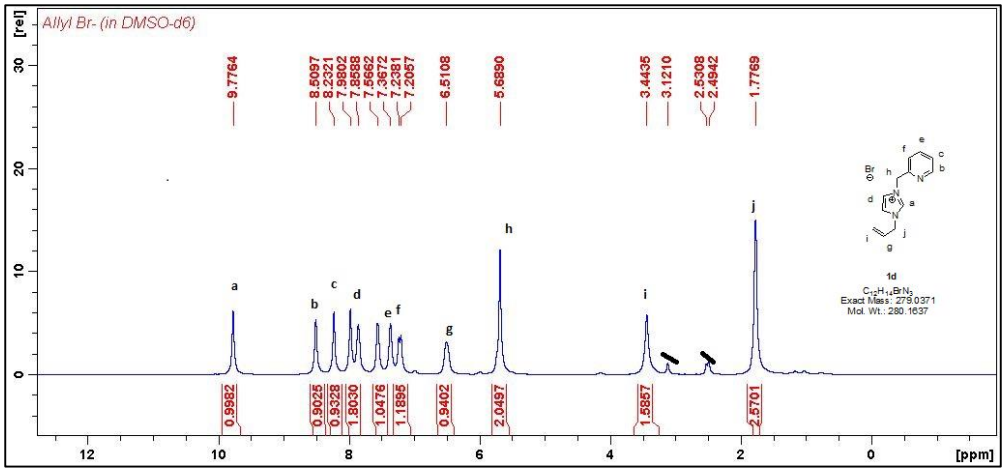


Figure S13: 1H NMR spectrum for 3-allyl-1-(2-pyridylmethyl)imidazolium bromide (1d).

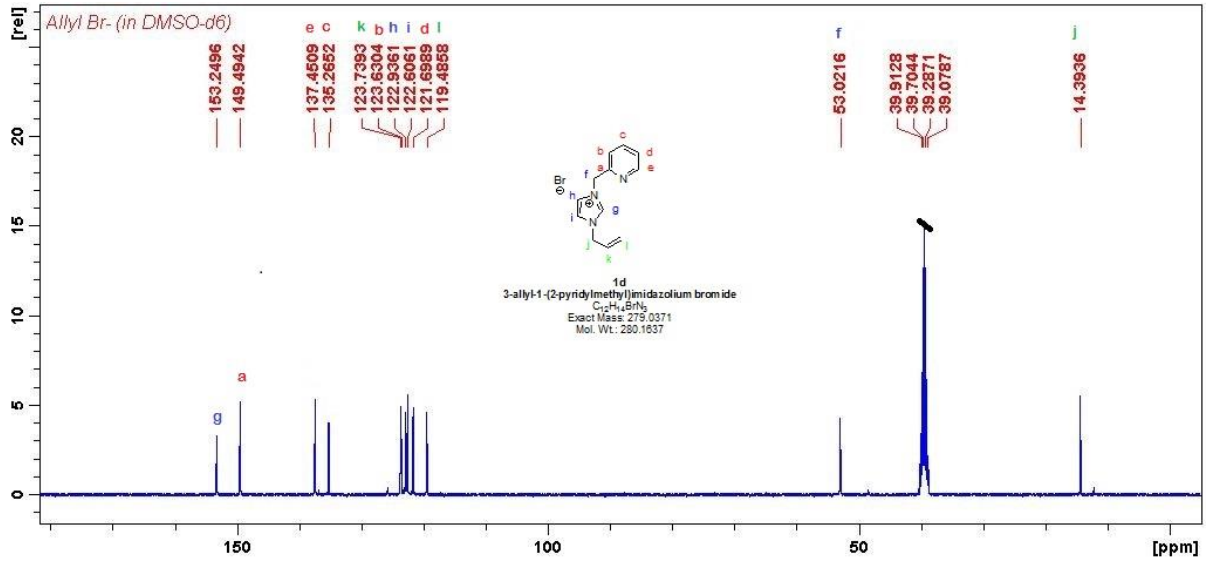


Figure S14: ^{13}C NMR spectrum of 1d.

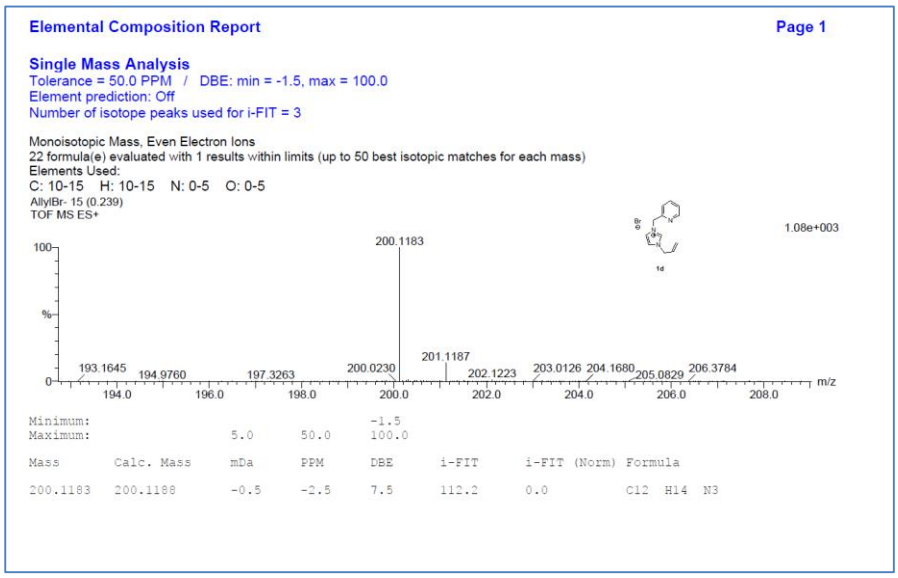


Figure S15: HRMS spectrum of 1d.

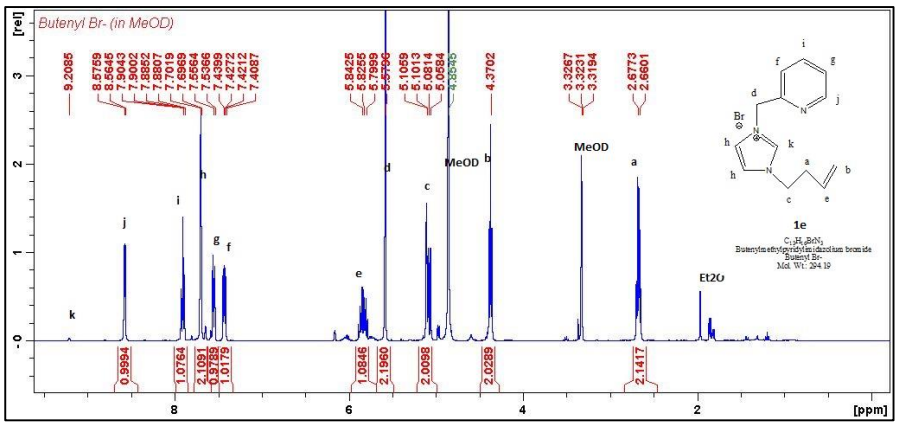


Figure S16: ^{1}H NMR spectrum of 3-butenyl-1-(2-pyridylmethyl)imidazolium bromide (1e).

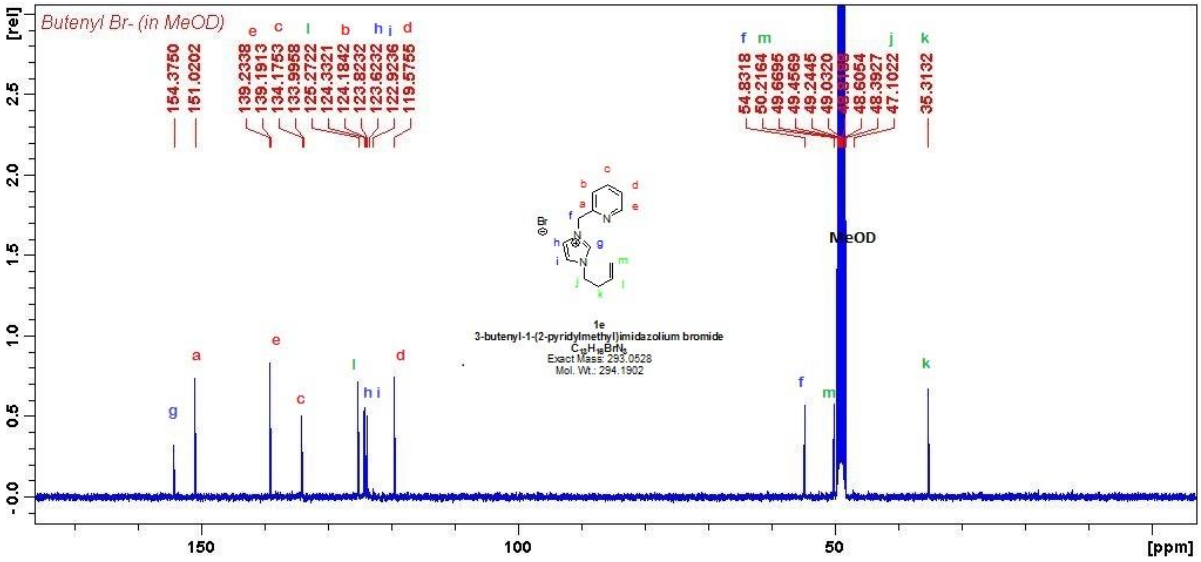


Figure S17: ^{13}C NMR spectrum of 1e.

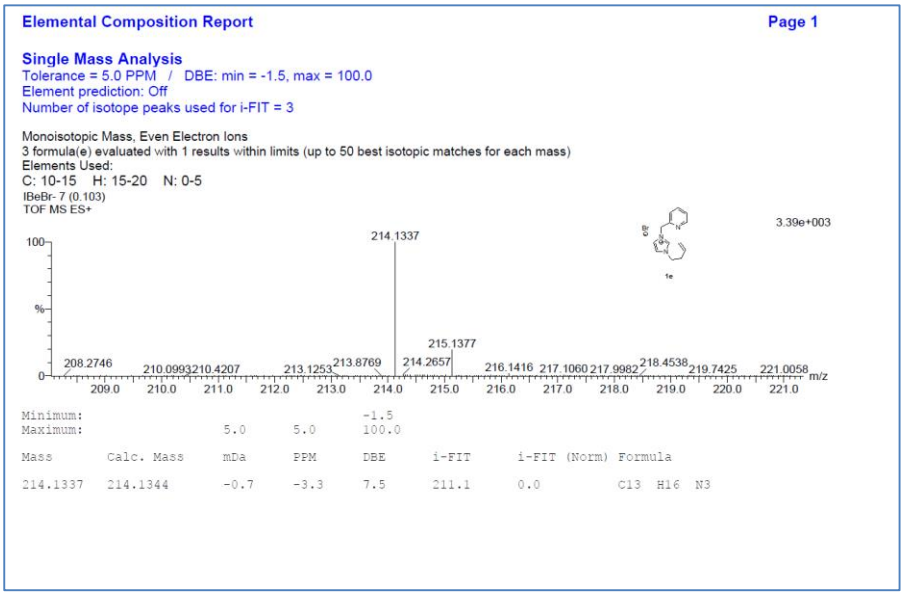


Figure S18: HRMS spectrum of 1e.

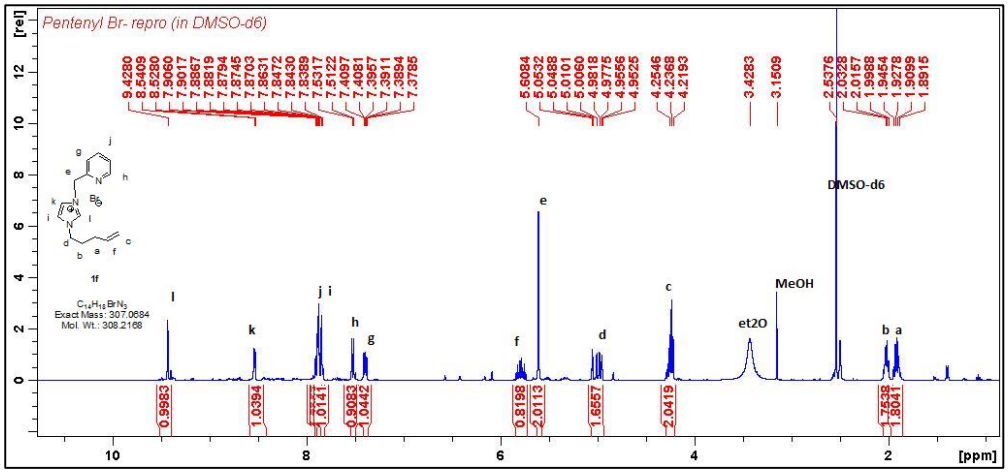


Figure S19: ^{1}H NMR spectrum of 3-pentenyl-1-(2-pyridylmethyl)imidazolium bromide (1f).

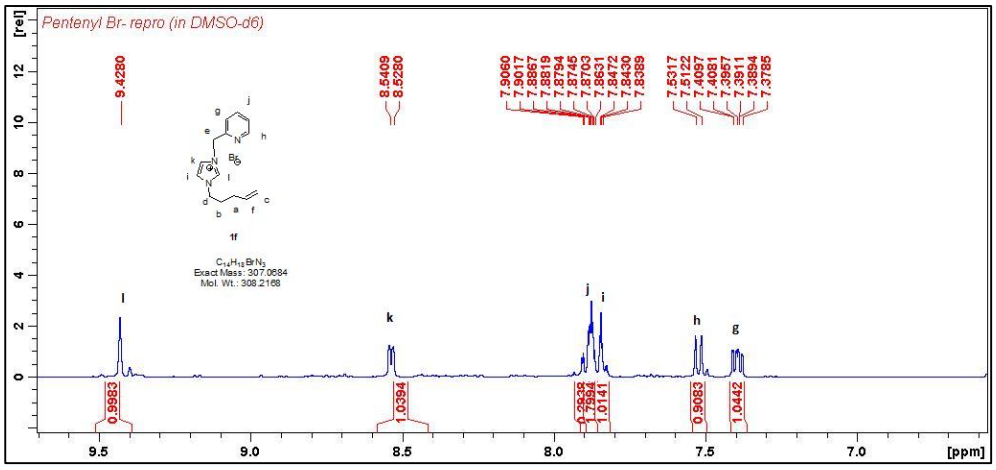


Figure S20: Expanded ^{1}H NMR spectrum of 1f showing the aromatic region.

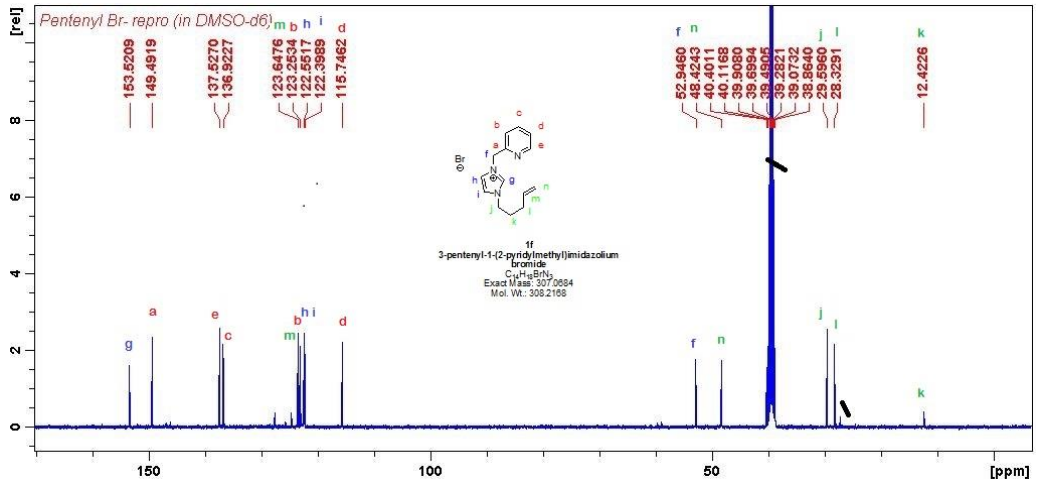


Figure S21: ^{13}C NMR spectrum of 1f.

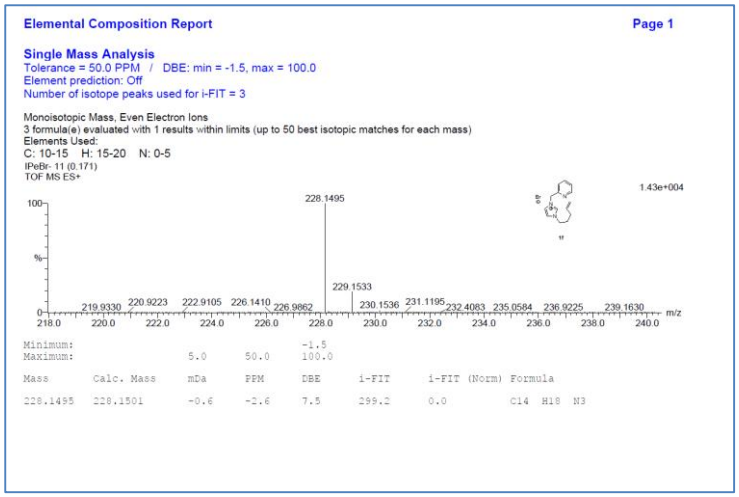


Figure S22: HRMS spectrum of 1f.

Data for picolyl functionalised imidazol-2-ylidene(NHC)-Ag(I) complexes (2)

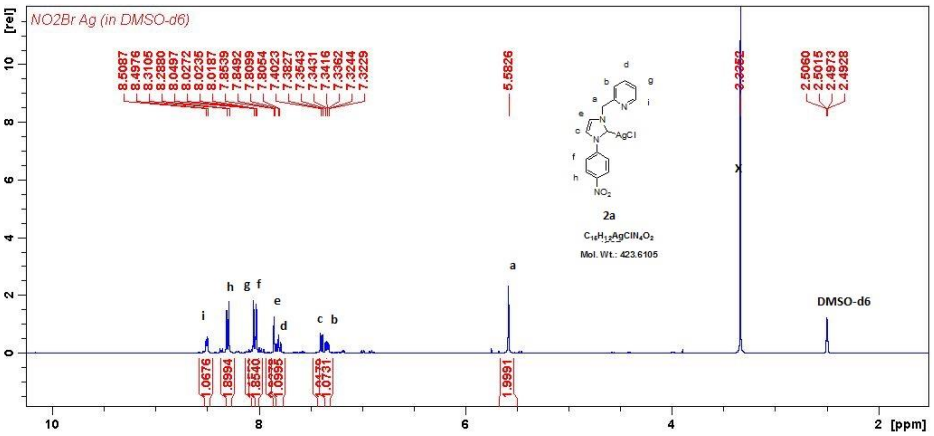


Figure S23: ^{1}H NMR spectrum for [1-(4-nitrophenyl)-3-(2-pyridyl)imidazol-2-ylidene]silver chloride (2a).

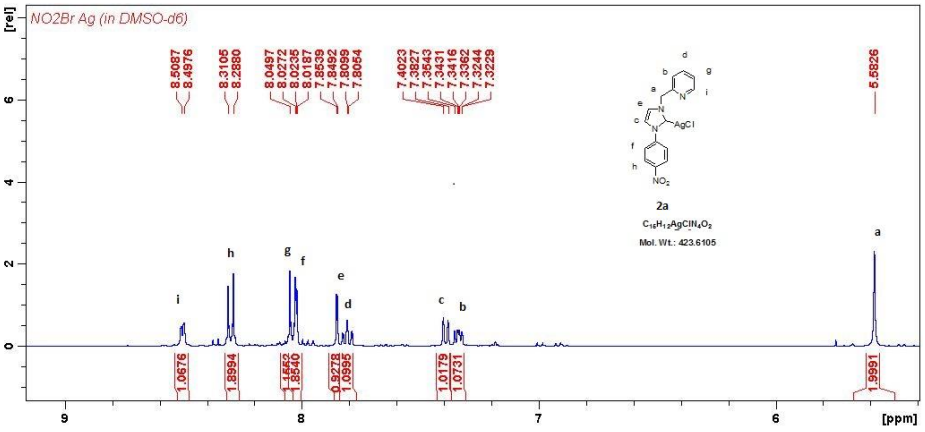


Figure S24: Expanded ^{1}H NMR spectrum of 2a.

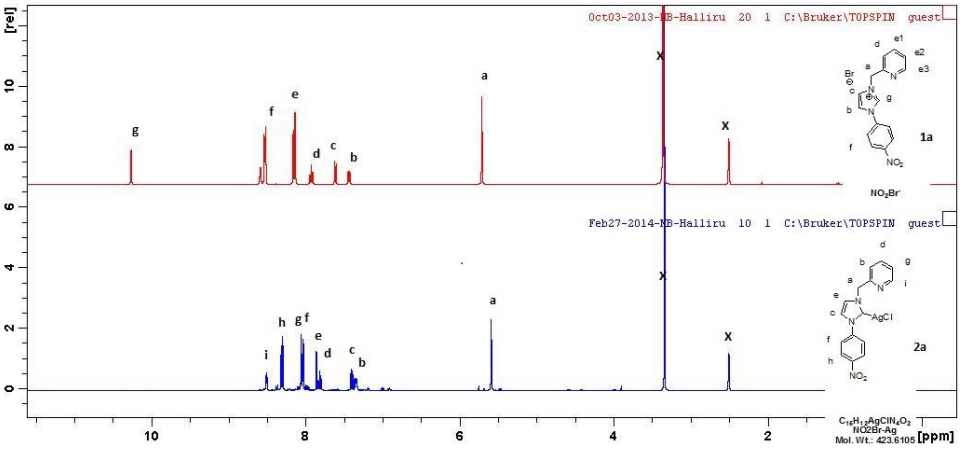


Figure S25: Comparative ^{1}H NMR spectra of 1a (top) and 2a (bottom).

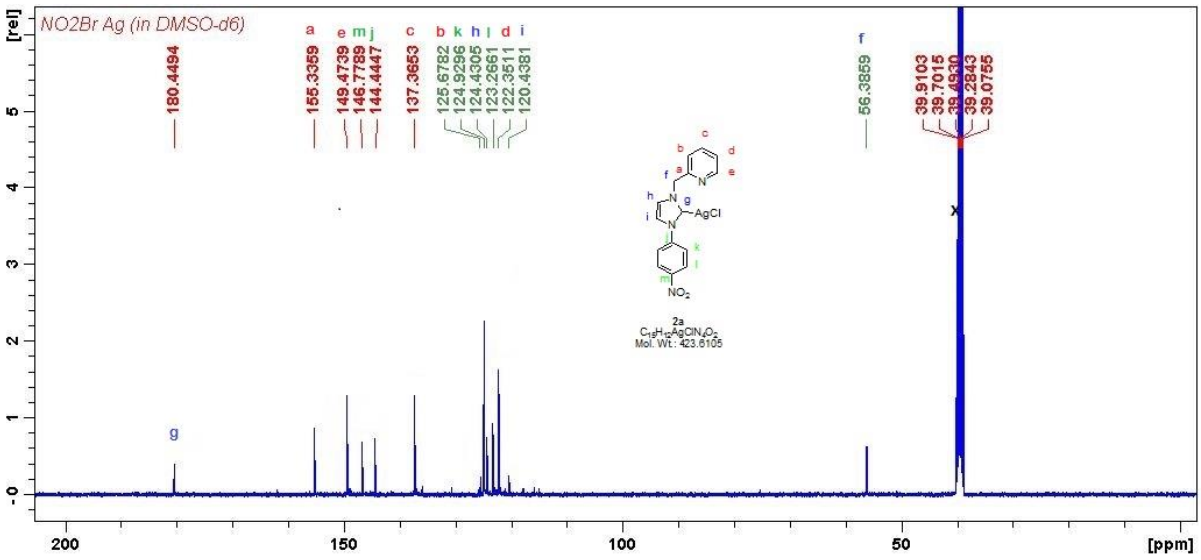


Figure S26: ^{13}C NMR spectrum of 2a.

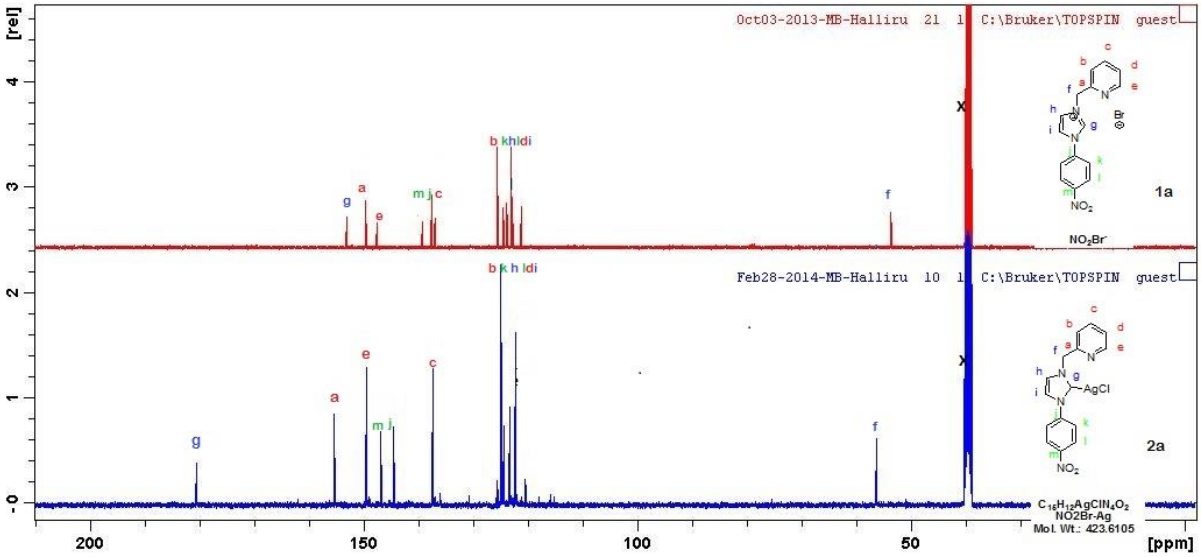


Figure S27: Comparative ^{13}C NMR spectra of 1a and 2a.

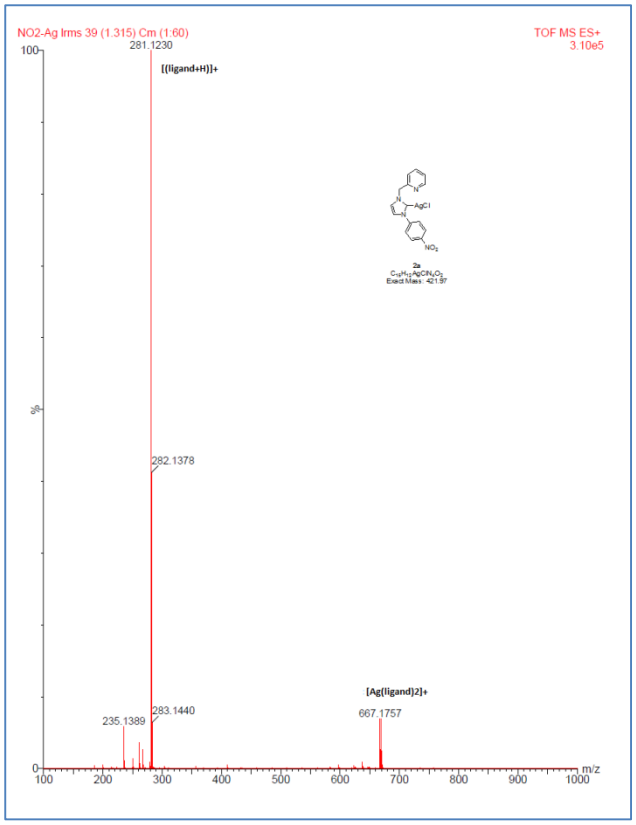


Figure S28: TOF MS-ES$^+$ spectrum of 2a.

Data for picolyl functionalised imidazol-2-ylidene(NHC)-Ni(II) and Co(II) complexes (3)

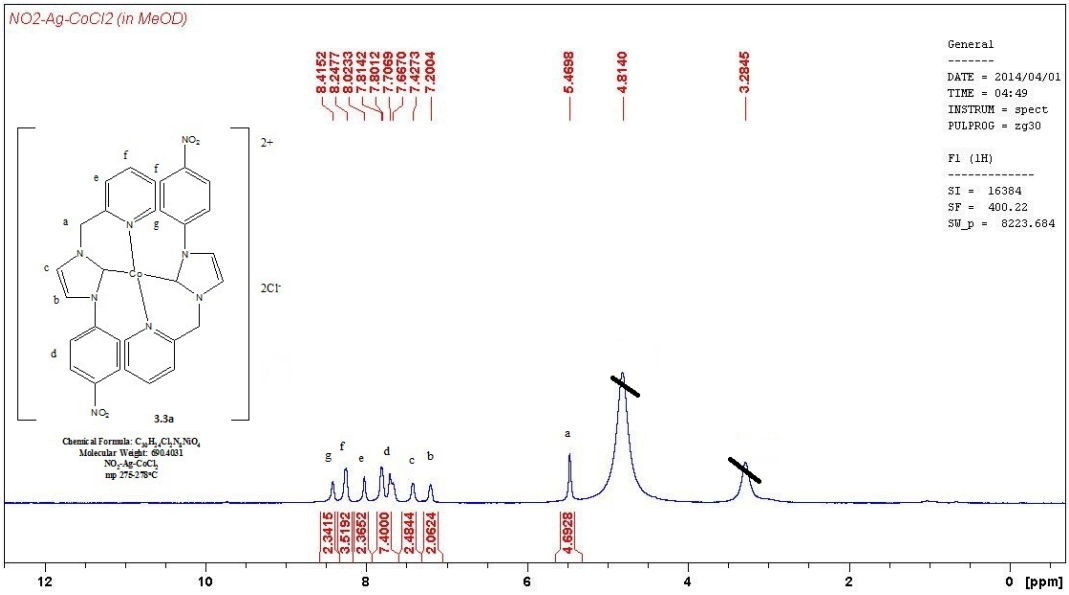


Figure S29: ^{1}H NMR spectrum of Co[3-(4-nitrophenyl)-1-picolyimidazolin-2-ylidene]$_2$Cl$_2$ (3a).

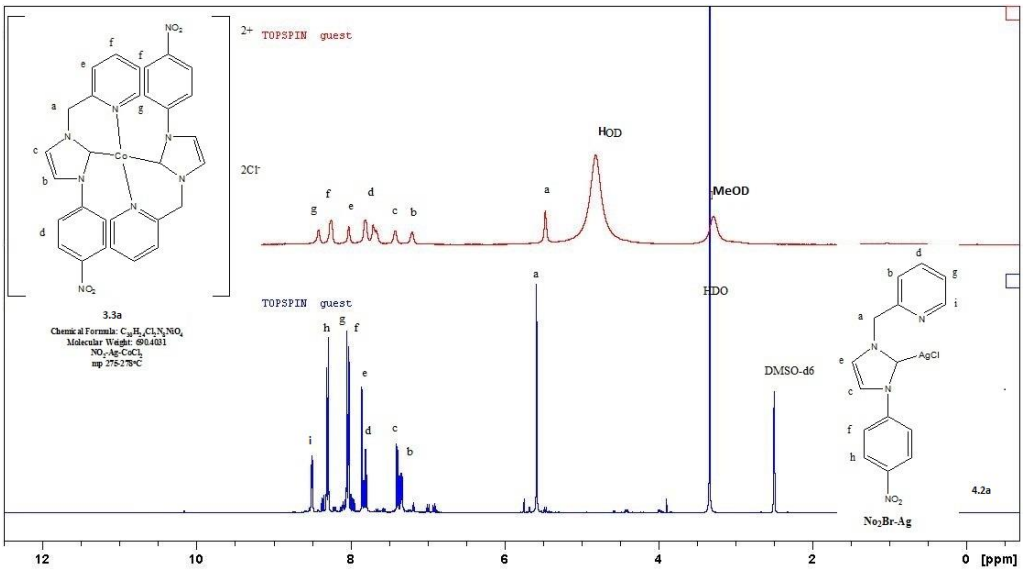


Figure S30: Comparative ^{1}H NMR spectra of 3a (top) and 2a (bottom).

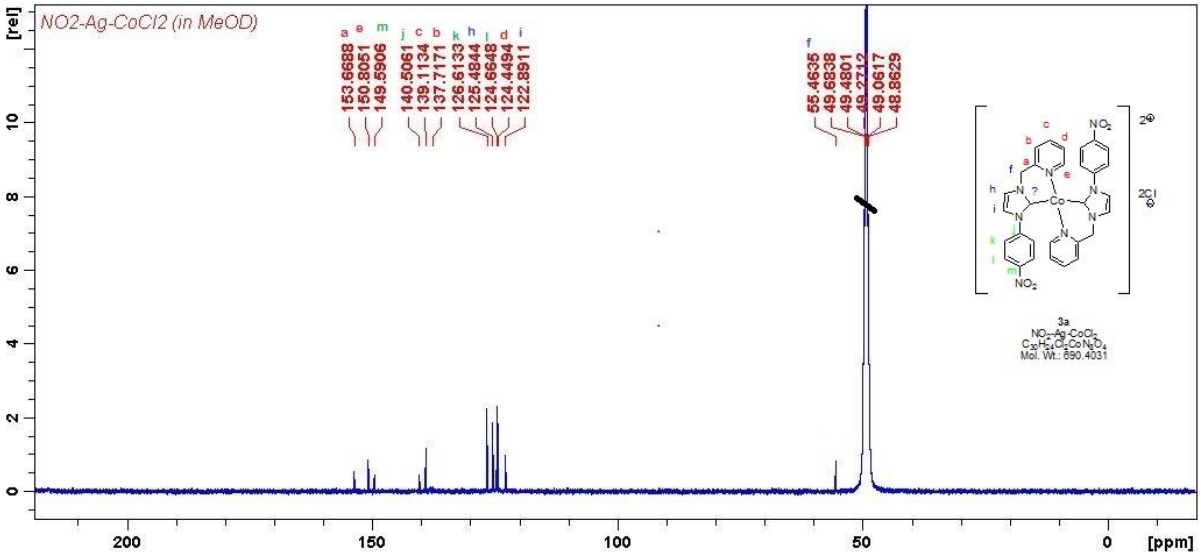


Figure S31: ^{13}C NMR spectrum of 3a.

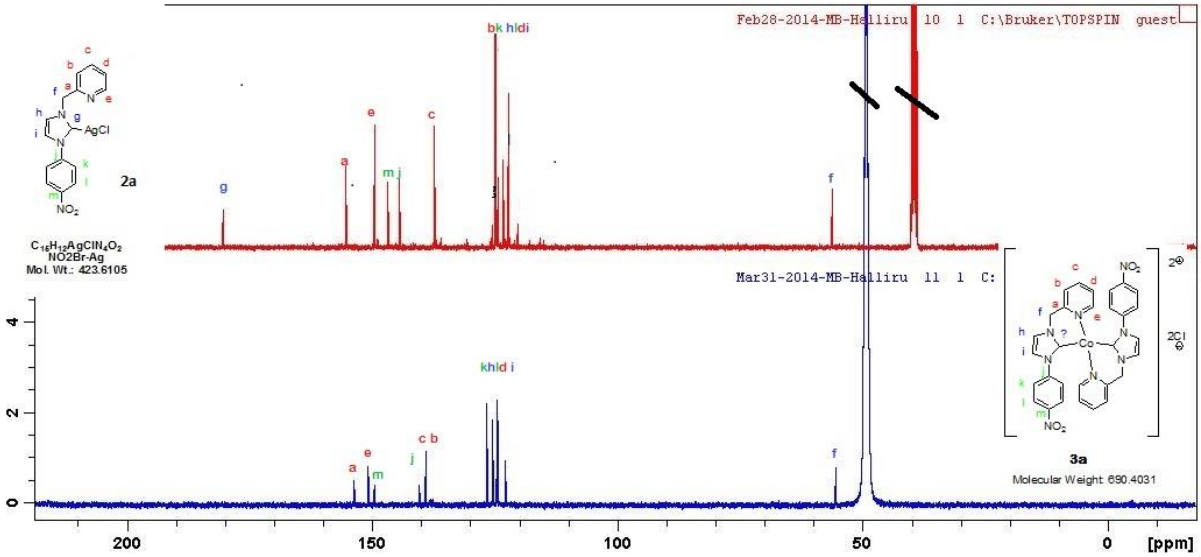


Figure S32: comparative ^{13}C NMR spectra of 2a (top) and 3a (bottom).

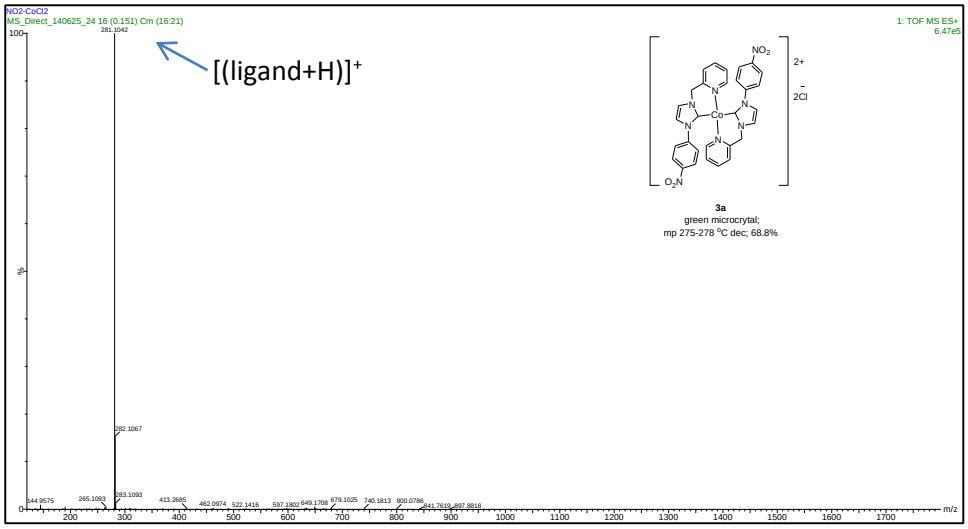


Figure S33: MS-ES$^+$ spectrum (1) of 3a.

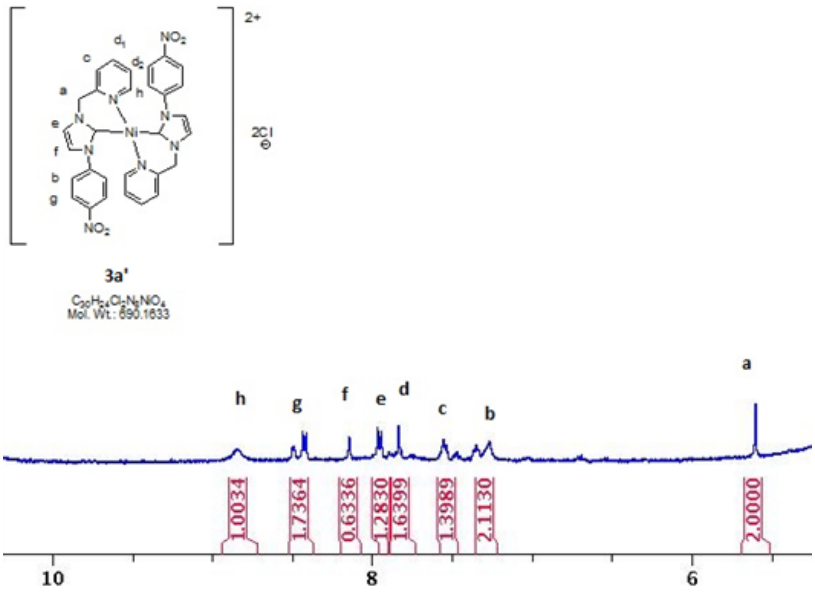


Figure S34: ^{1}H NMR spectrum of Ni[3-(4-nitrophenyl)-1-picolyimidazolin-2-ylidene]$_2$Cl$_2$ (3a').

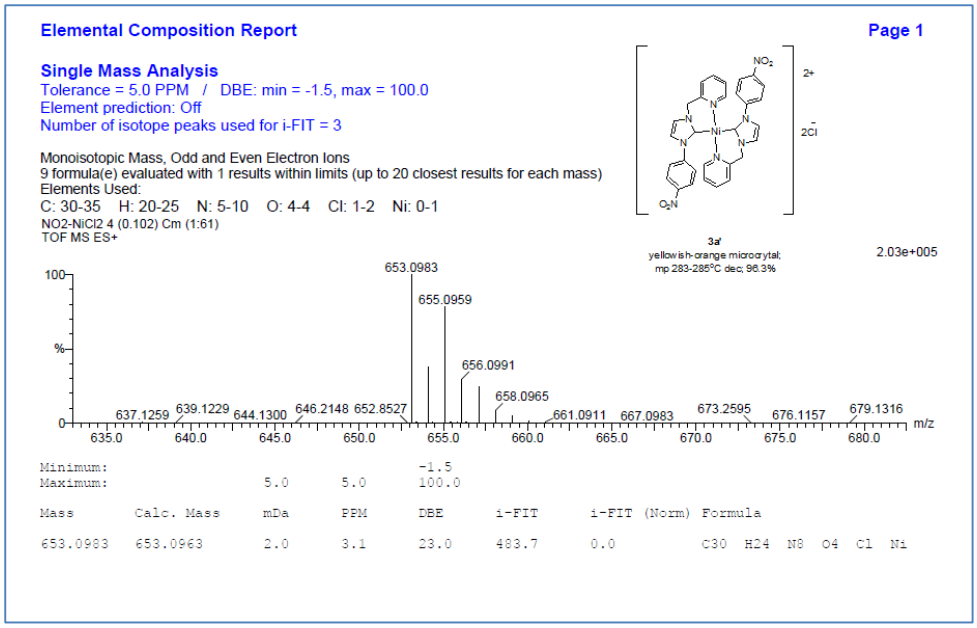


Figure S35: HRMS spectrum of 3a'.

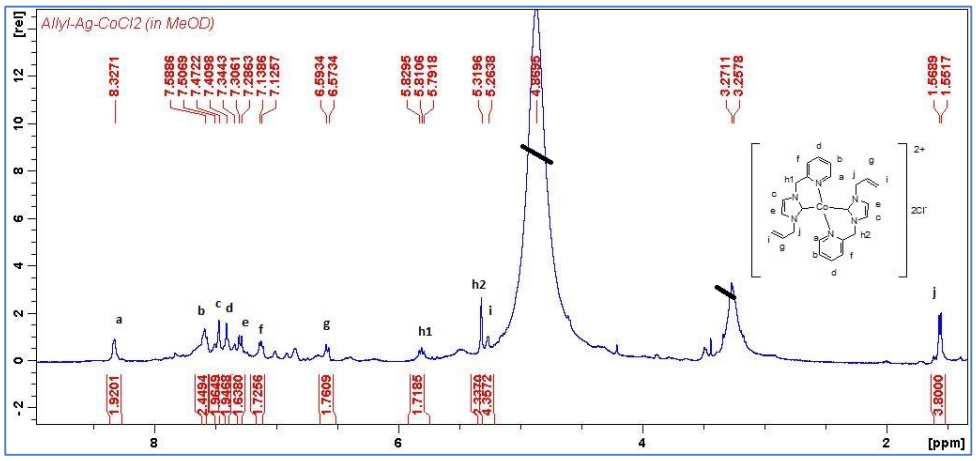


Figure S36: ^{1}H NMR spectrum of Co(3-allyl-1-picolyimidazolin-2-ylidene)$_2$Cl$_2$ (3d).

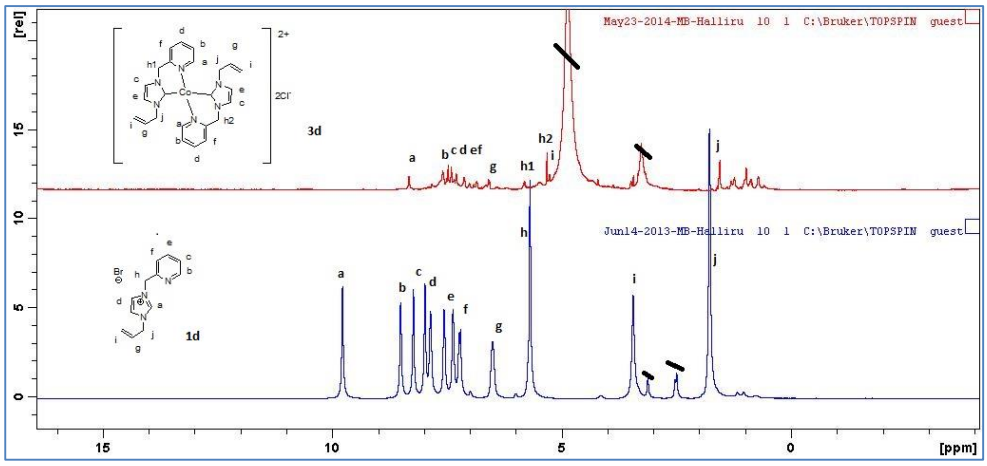


Figure S37: Comparative ^{1}H NMR spectra of 3d (top) and 1d (bottom).

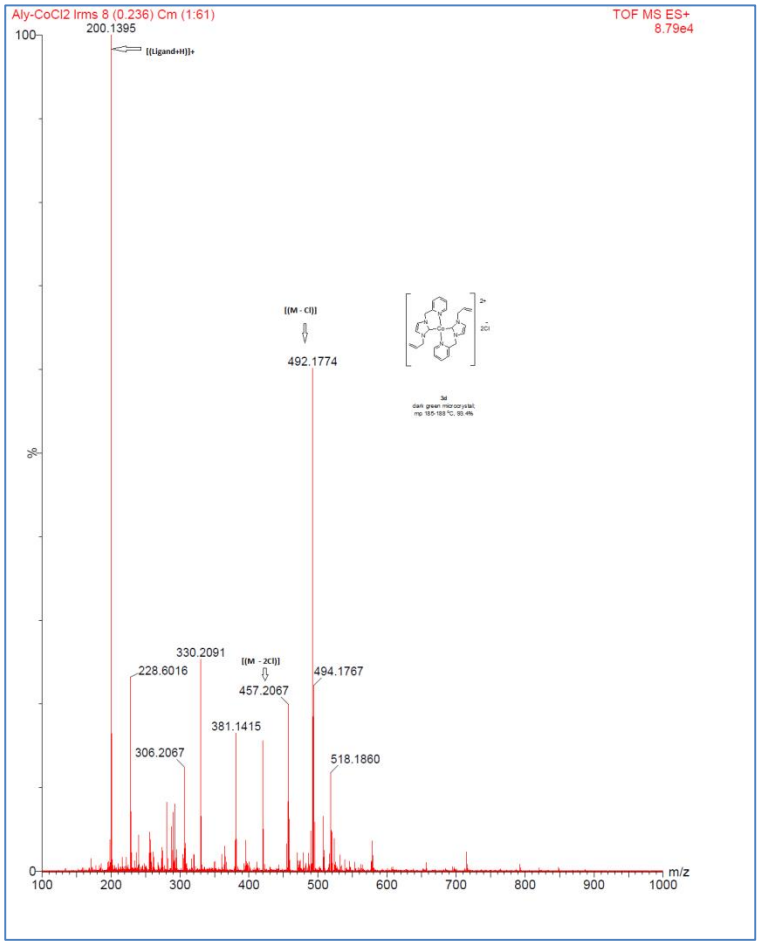


Figure S38: TOF MS-ES^{+} spectrum of 3d.

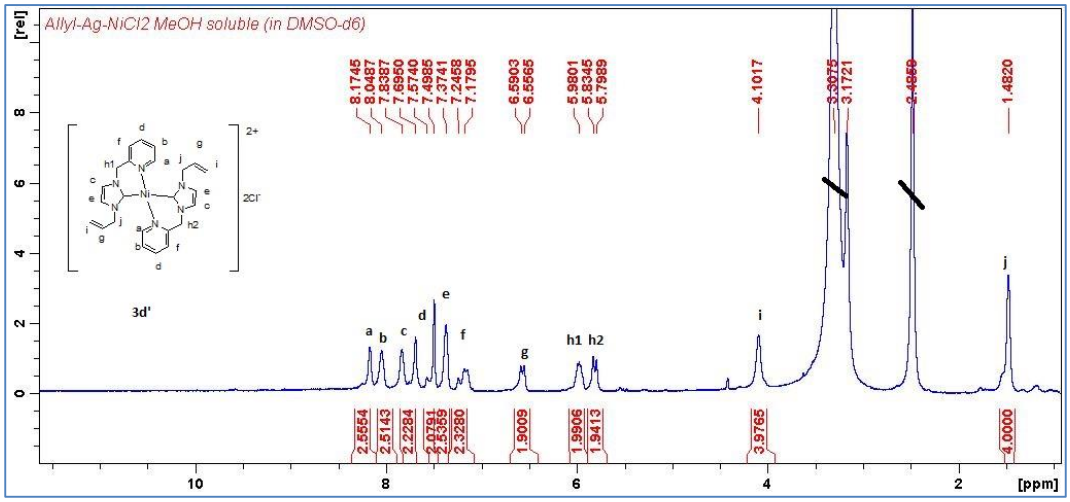


Figure S39: ^{1}H NMR spectrum of Ni(3-allyl-1-picolyimidazolin-2-ylidene)$_2$Cl$_2$ (3d').

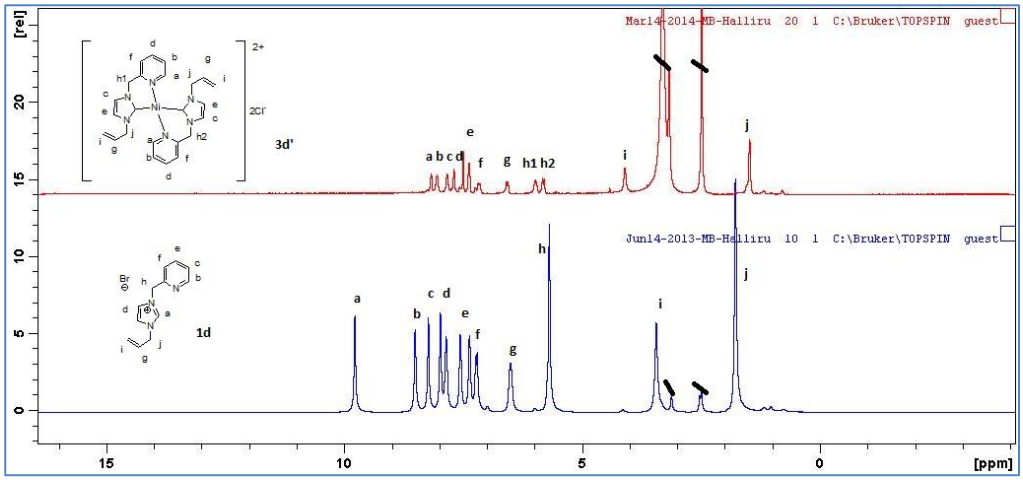


Figure S40: Comparative ^{1}H NMR spectra of 3d' (top) and 1d (bottom).

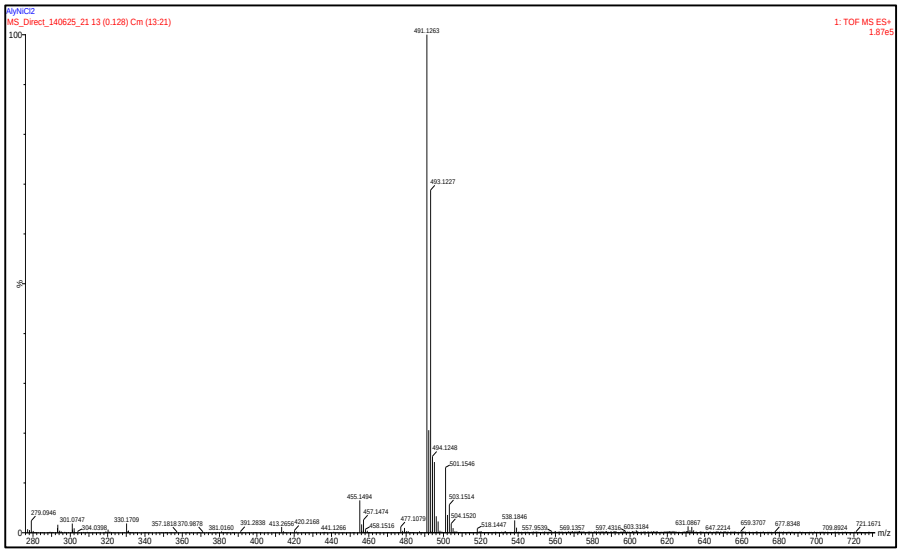


Figure S41: TOF MS-ES+ spectrum of 3d'.

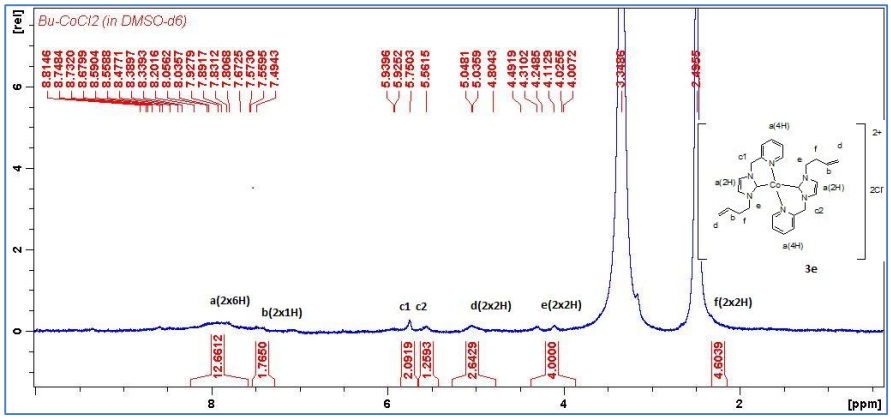


Figure S42: ^{1}H NMR spectrum of Co(3-butenyl-1-picolyimidazolin-2-ylidene)$_2$Cl$_2$ (3e).

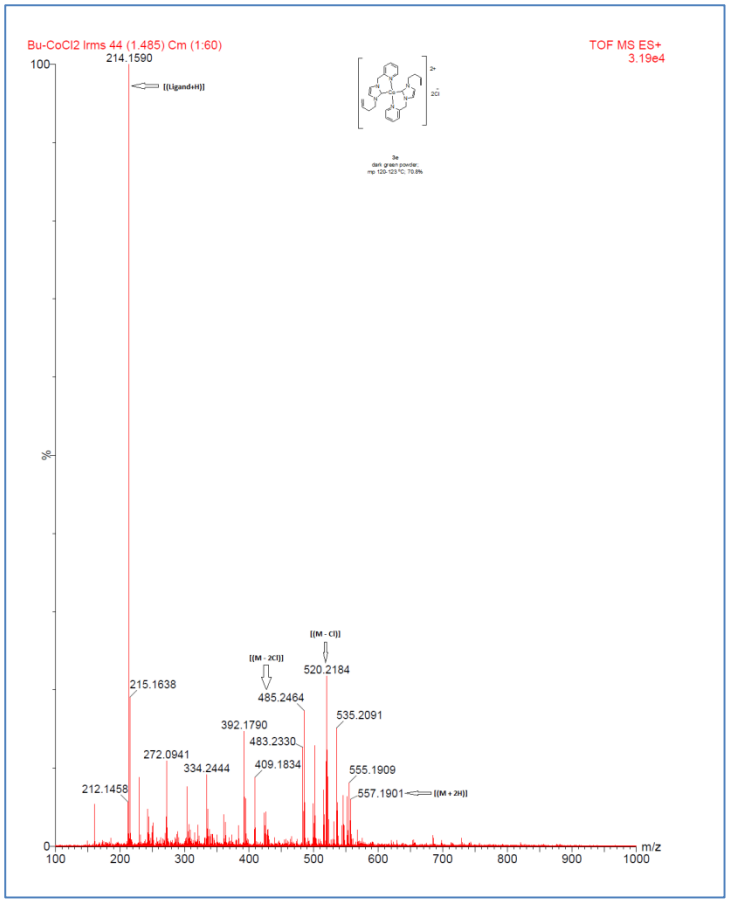


Figure S43: TOF MS-ES$^+$ spectrum of 3e.

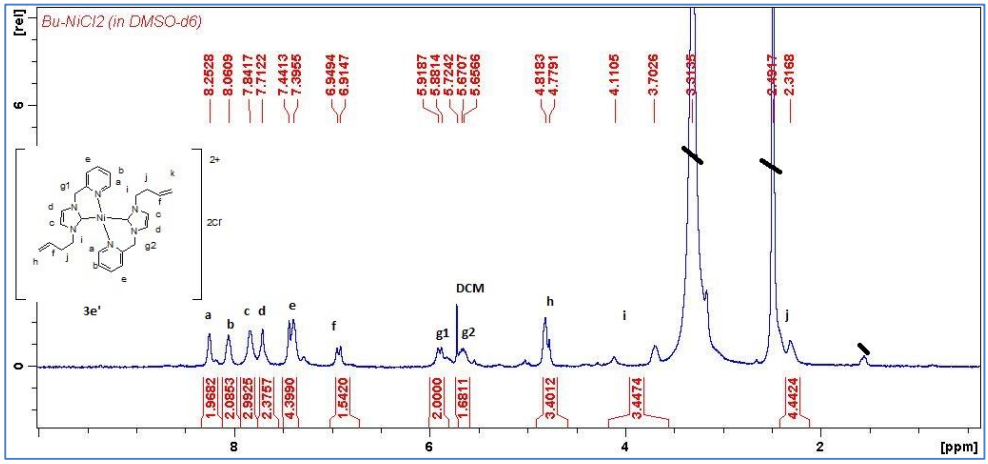


Figure S44: ^{1}H NMR spectrum of Ni(3-butenyl-1-picolyimidazolin-2-ylidene)$_2$Cl$_2$ (3e′).

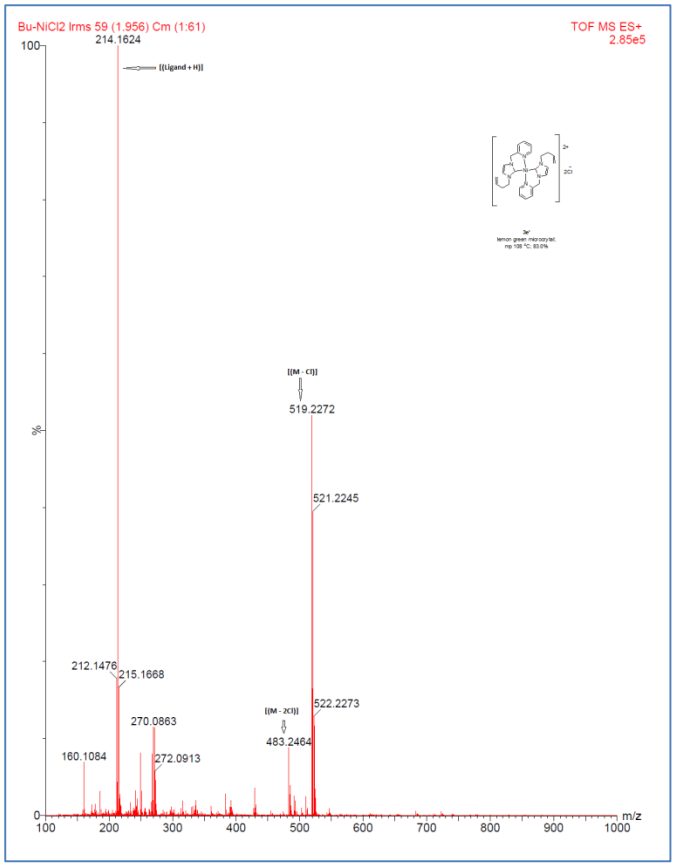
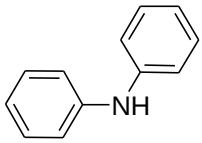


Figure S45: TOF MS-ES$^+$ spectrum of 3e′.

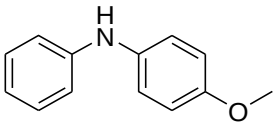
Analysis data for substrates and isolated products

Diphenyl amine:



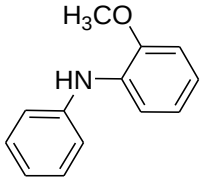
^{1}H NMR (400 MHz, DMSO-d_6): δ 8.12 (bs, 1H, NH), 7.21 (d, *J*=7.4 Hz, 2x2H), 7.06 (d, *J*=7.6 Hz, 2X2H), 6.81 (t, *J*=7.3 Hz, 2x1H). ^{13}C NMR (400 MHz, DMSO-d_6): δ 143.4, 129.1, 119.6, 116.7. FTIR $_{(neat)}$ cm^{-1}: $_{\nu N\text{-}H}$ 3380 (bs, 2^{o} amine), $_{\nu C\text{-}H}$ 3041, $_{\nu C\text{-}N}$ 1307, $_{\nu Ar}$ 741.

4-methoxy-*N*-phenylbenzenamine:



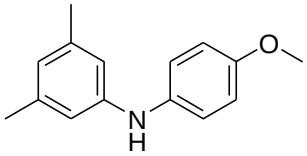
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, *J*=8.8 Hz, 2H), 7.21 (t, *J*=15.8 Hz, 1H), 7.07 (d, *J*=8.8 Hz, 2H), 6.99 (d, *J*=8.9 Hz, 2H), 6.90 (dd, *J*=7.8 Hz, 2H), 3.89 (bs, 1H, N-H), 3.87 (s, 3H, O-CH_3). ^{13}C NMR (400 MHz, $CDCl_3$): δ 161.6, 147.1, 129.3, 124.3, 122.2, 119.6, 115.6, 114.2, 55.6. FTIR$_{(neat)}$ cm^{-1}: $\nu_{N\text{-}H}$ 3343 (bs, 2^{o} amine), ν_{CH} 2935, $\nu_{C\text{-}O}$ 1146, $\nu_{C\text{-}N}$ 1220, ν_{Ar} 827.

2-methoxy-*N*-phenylbenzenamine:



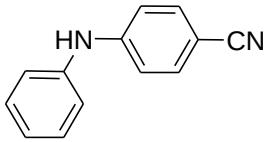
^{1}H NMR (400 MHz, DMSO-d_6): δ 8.14 (bs, 1H, N-H), 7.23 (t, *J*=15.6 Hz, 2x1H), 7.10 (m, 3x1H), 6.82 (t, *J*=7.3 Hz, 1H), 6.65 (d, *J*=4.6 Hz, 1H), 6.59 (d, *J*=1.8 Hz, 1H), 6.39 (d, *J*=4.9 Hz, 1H), 3.70 (s, 3H, O-CH_3). ^{13}C NMR (400 MHz, DMSO-d_6): δ 160.2, 144.8, 143.1, 129.9, 129.1, 119.8, 117.1, 108.9, 104.9, 102.1, 54.8. FTIR$_{(neat)}$cm^{-1}: $\nu_{N\text{-}H}$ 3386 (bs, 2^{o} amine), ν_{CH} 2916, $\nu_{C=C}$ 1591, $\nu_{C\text{-}N}$ 1259, $\nu_{C\text{-}O}$ 1156, ν_{Ar} 688.

4-methoxy-*N*-(3,5-dimethylphenyl)benzenamine:



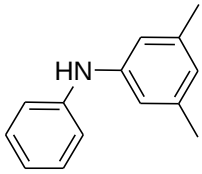
^{1}H NMR (400 MHz, DMSO-d_6): δ 7.82 (d, *J*=8.9 Hz, 2x1H), 7.11 (d, *J*=8.9 Hz, 2x1H), 6.62 (d, *J*=8.9 Hz, 1H), 6.54 (s, 2x1H), 3.85 (s, 2x3H), 3.85 (s, 3H, O-CH_3), 3.72 (bs, 1H, N-H). ^{13}C NMR (400 MHz, DMSO-d_6): δ 161.4, 146.2, 132.7, 124.1, 123.7, 114.5, 107.5, 101.4, 55.7, 55.6. $FTIR_{(neat)}$ cm^{-1}. ν_{N-H} 3320 (bs, 2º amine), ν_{C-H} 2925, $\nu_{C=C}$ 1591, ν_{C-N} 1494, ν_{C-O} 1156, ν_{Ar} 755.

4-(phenylamino)benzonitrile:



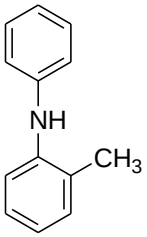
^{1}H NMR (400 MHz, DMSO-d_6): δ 7.89 (d, *J*=7.8 Hz, 4H), 7.61 (m, 4H), 7.29 (t, *J*=7.7 Hz, 1H), 6.84 (bs, 1H, N-H). ^{13}C NMR (400 MHz, DMSO-d6): δ 153.6, 151.9, 131.5, 129.5, 128.8, 127.1, 122.5, 119.8. $FTIR_{(neat)}$ cm^{-1}: ν_{N-H} 3389 (bs, 2º amine), ν_{CN} 2260, $\nu_{C=C}$ 1516, ν_{C-N} 1310, ν_{Ar} 743.

3,5-dimethyl-*N*-phenylbenzenamine:



^{1}H NMR (400 MHz, DMSO-d_6): δ 7.90—7.88 (m, 4x1H), 7.59 (d, *J*=7.6 Hz, 2x1H), 7.17 (s, 1H), 7.15 (s, 1H), 6.98 (bs, 1H, N-H), 2.24 (s, 2x3H, CH_3). ^{13}C NMR (400 MHz, DMSO-d_6): δ 151.9, 139.9, 131.5, 129.4, 128.8, 128.6, 122.5, 119.8, 20.5. FTIR $_{(neat)}$ cm^{-1}: ν_{N-H} 3395 (bs, 2º amine), ν_{C-H} 2921, ν_{Ar} 744, 690.

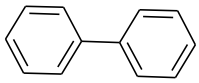
2-methyl-*N*-phenylbenzenamine:



^{1}H NMR (400 MHz, DMSO-d_6): δ 7.28-7.26 (m, 2x1H), 7.14 (t, J=8.0 Hz, 1H), 7.07-7.05 (m, 2x1H), 6.93-6.87 (m, 3x1H), 6.75 (d, J=7.4 Hz, 1H), 5.65 (bs, 1H, NH), 2.31 (s, 1H, CH3). 13C NMR (400

MHz, CDCl3): δ 154.9, 143.1, 139.2, 129.3, 129.2, 121.9, 120.9, 118.5, 117.8, 114.9, 21.5. FTIR $_{(neat)}$ cm^{-1}: ν_{N-H} 3390 (bs, 2º amine), ν_{C-H} 3037, 2922, $\nu_{C=C}$ 1589, ν_{Ar} 744.

Biphenyl:



^{1}H NMR (400 MHz, DMSO-d_6): δ 8.33 (dd, 2x2H), 8.05 (m, 2x3H). FTIR $_{(neat)}$ cm^{-1}: ν_{C-H} 3062, ν_{Ar} 772.

NMR Spectra for aryl amine substrates and isolated arylated products

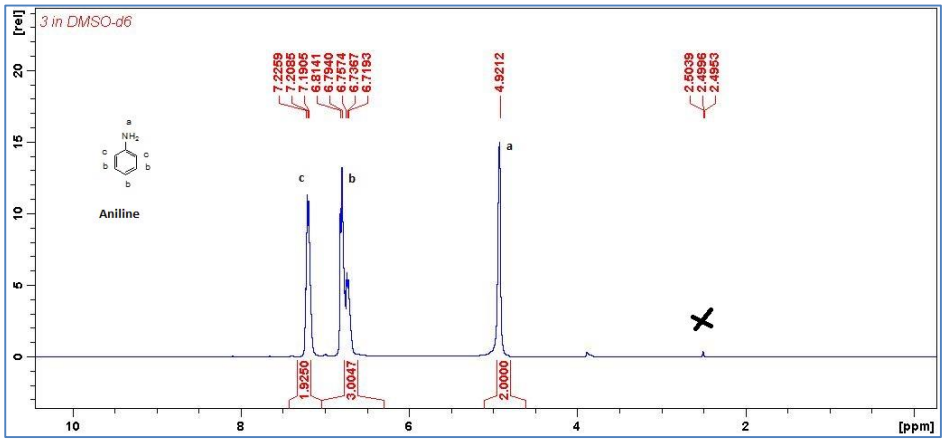


Figure S46: ^{1}H NMR spectrum of aniline.

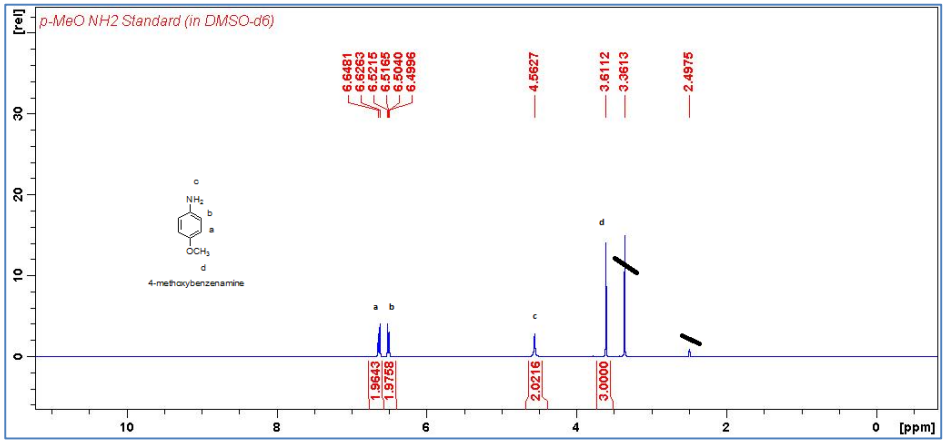


Figure S47: ^{1}H NMR spectrum of 4-methoxybenzenamine.

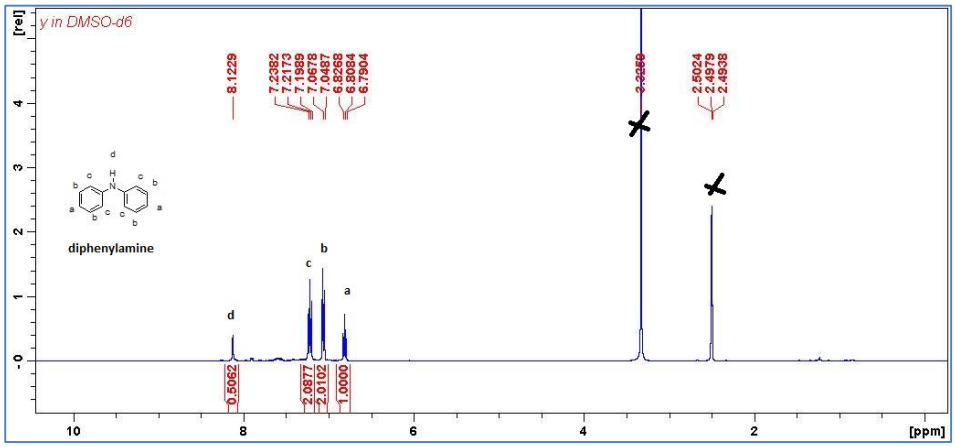


Figure S48: ^{1}H NMR spectrum for diphenylamine.

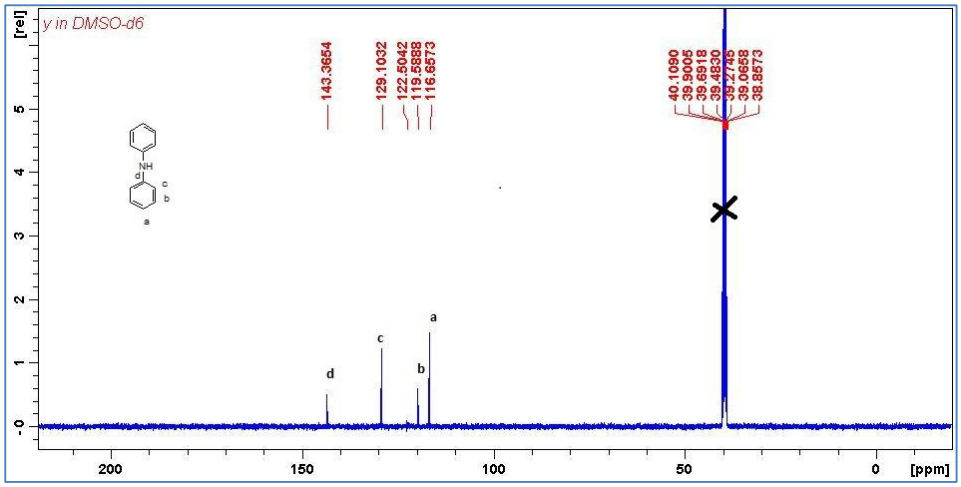


Figure S49: ^{13}C NMR for diphenylamine.

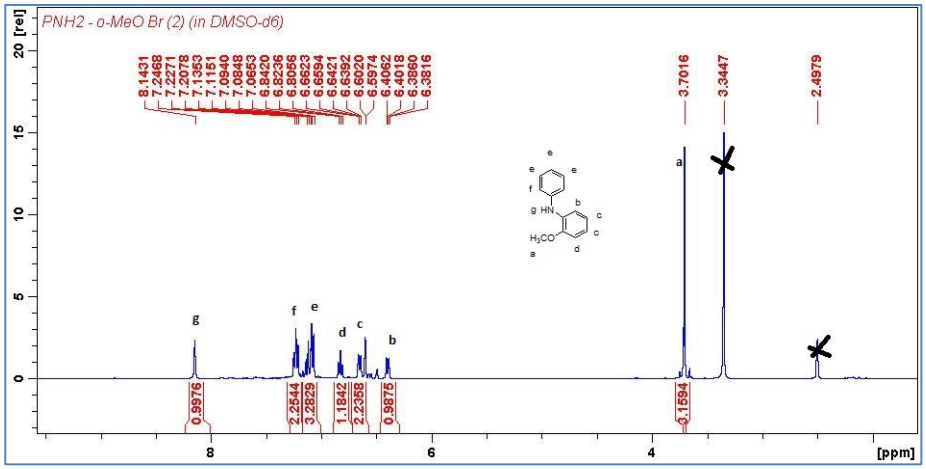


Figure S50: ^{1}H NMR spectrum for 2-methoxy-N-phenylbenzenamine.

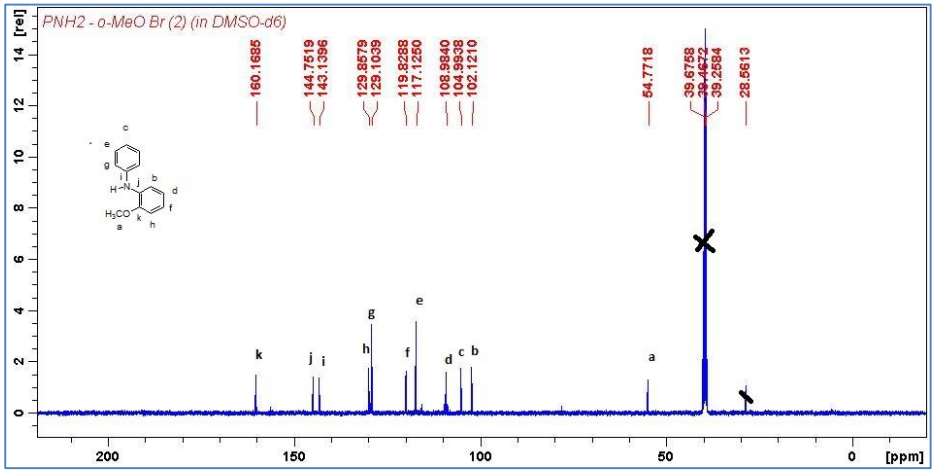


Figure S51: ^{13}C NMR spectrum for 2-methoxy-N-phenylbenzenamine.

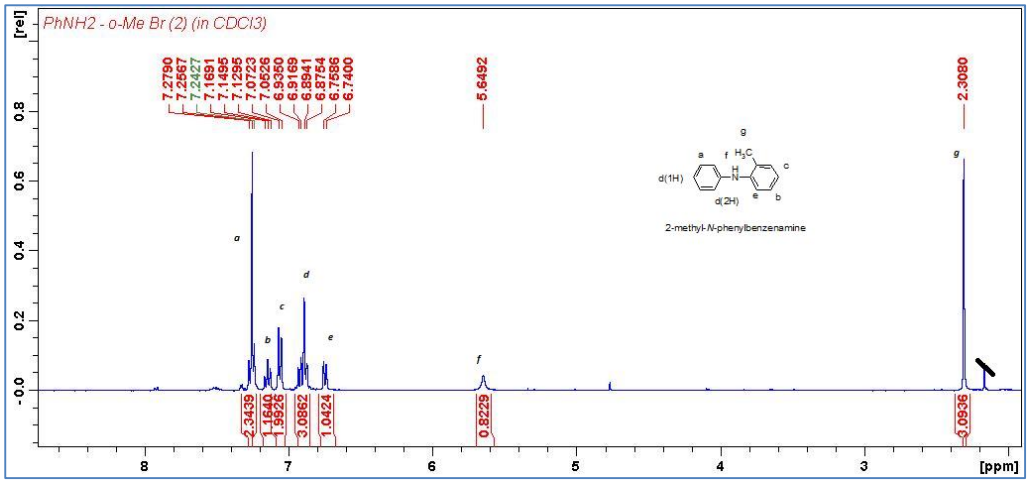


Figure S52: ^{1}H NMR spectrum for 2-methyl-N-phenylbenzenamine.

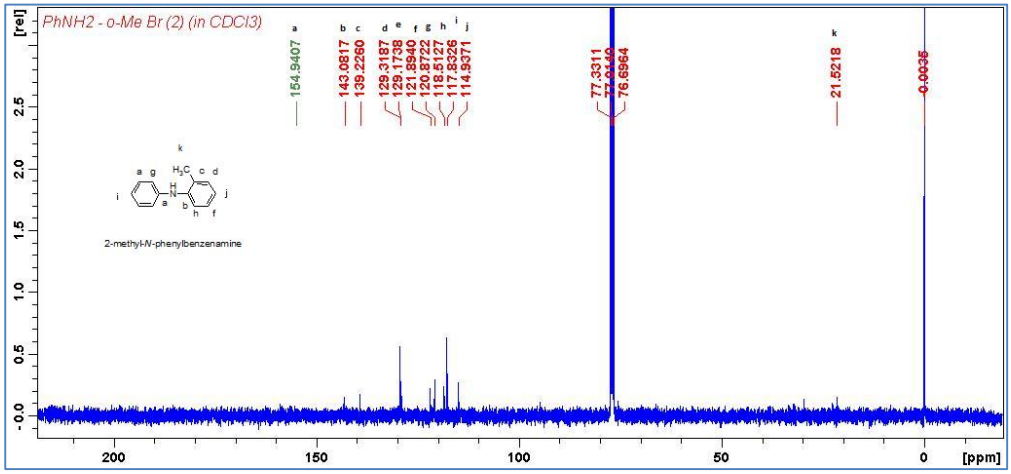


Figure S53: ^{13}C NMR spectrum for 2-methyl-N-phenylbenzenamine.

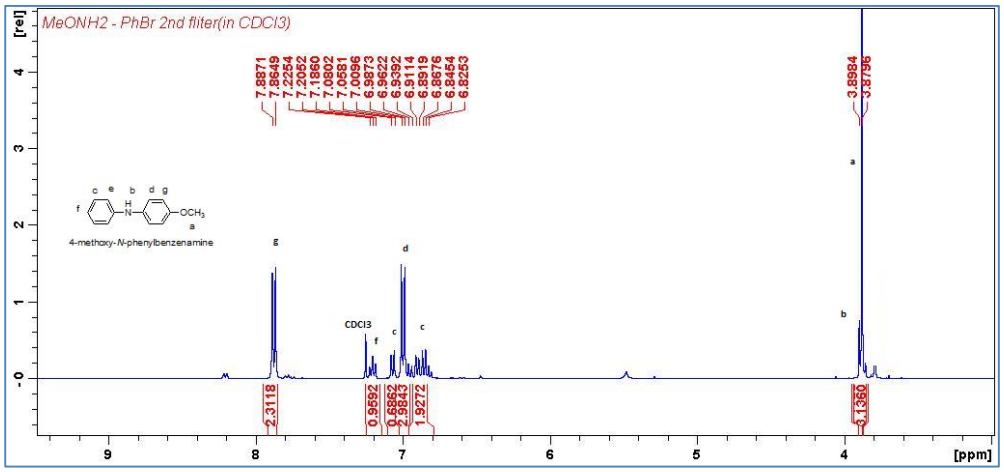


Figure S54: ^{1}H NMR spectrum for 4-methoxy-N-phenylbenzenamine.

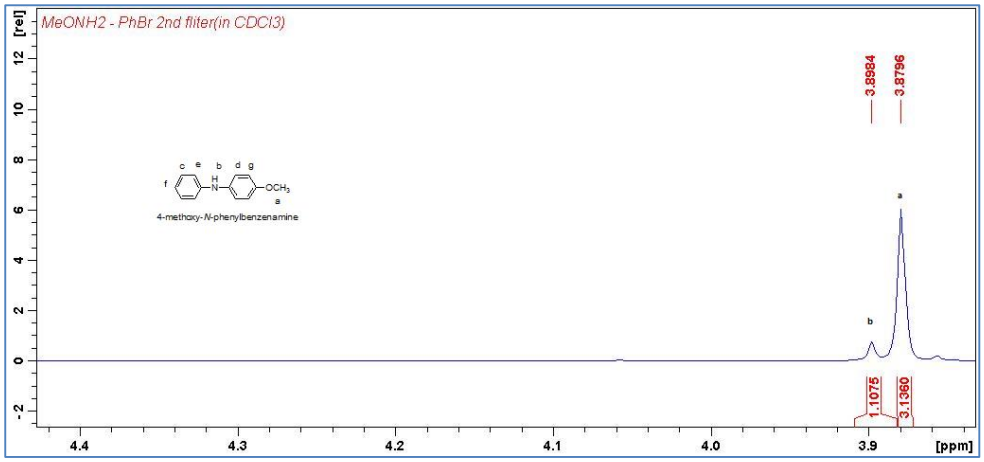


Figure S55: ^{1}H NMR (expanded) spectrum for 4-methoxy-N-phenylbenzenamine.

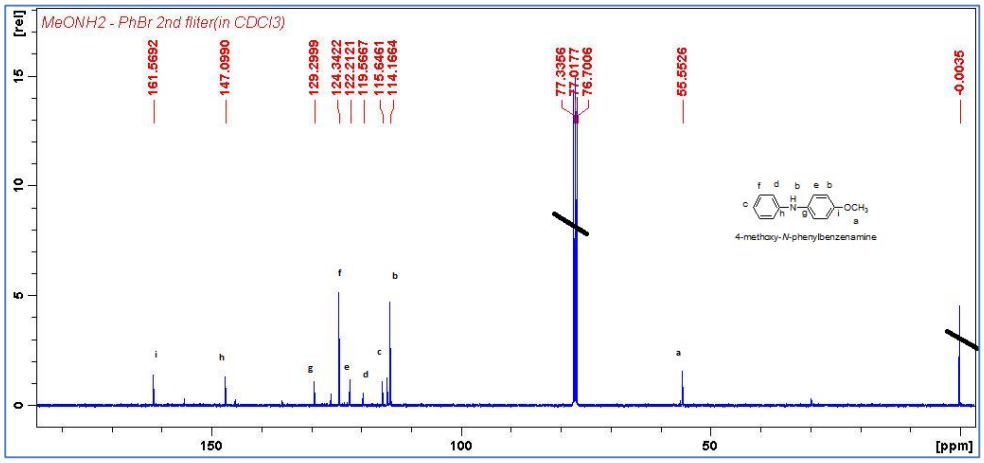


Figure S56: ^{13}C NMR spectrum for 4-methoxy-N-phenylbenzenamine.

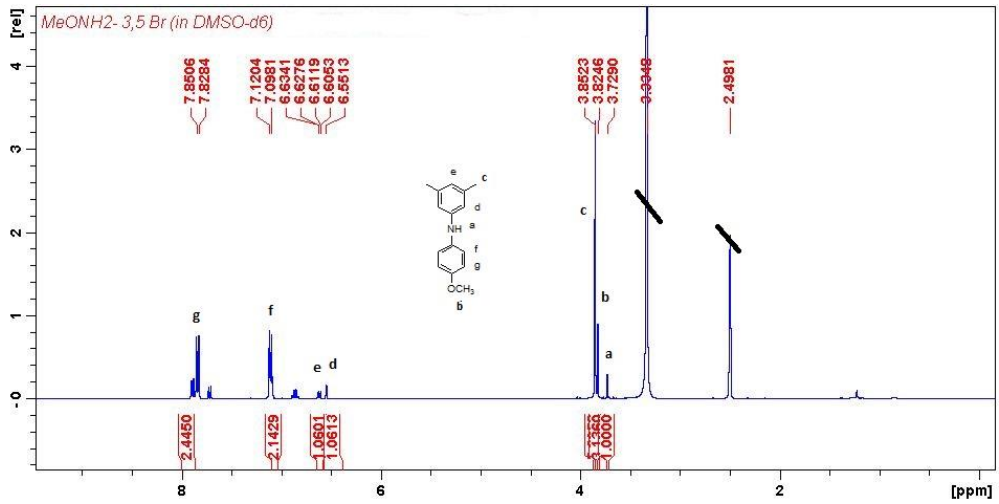


Figure S57: ^{1}H NMR spectrum for 4-methoxy-N-(3,5-dimethylphenyl)benzenamine.

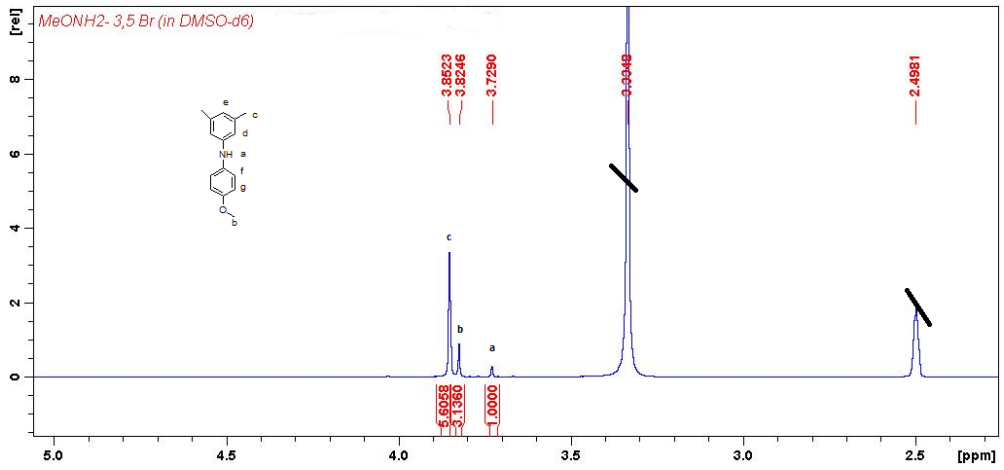


Figure S58: Expanded ^{1}H NMR spectrum for 4-methoxy-N-(3,5-dimethylphenyl)benzenamine.

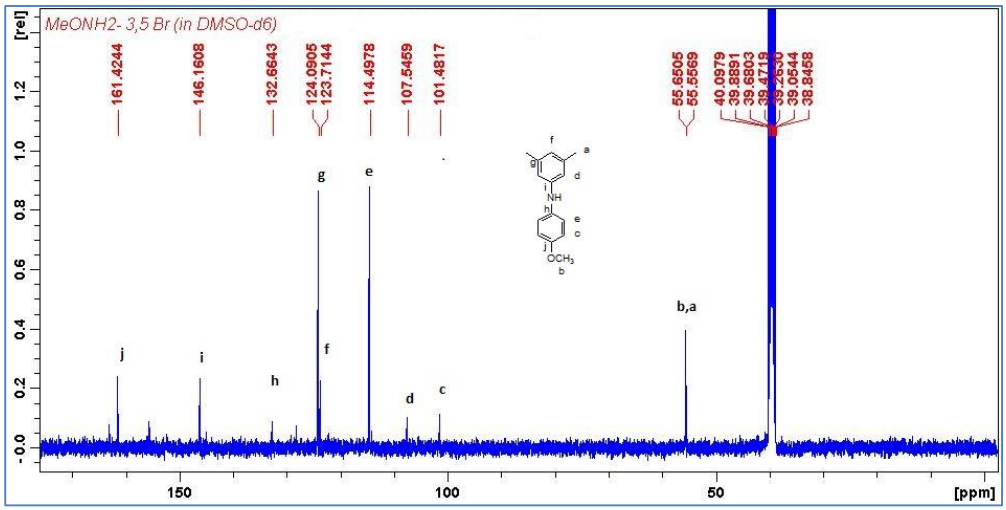


Figure S59: ^{13}C NMR spectrum for 4-methoxy-N-(3,5-dimethylphenyl)benzenamine.

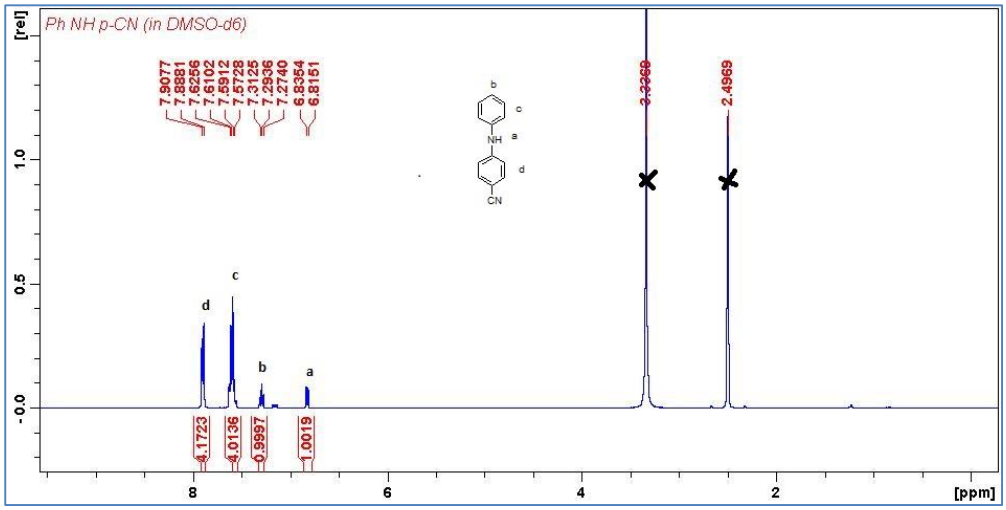


Figure S60: ^{1}H NMR spectrum for 4-(phenylamino)benzonitrile.

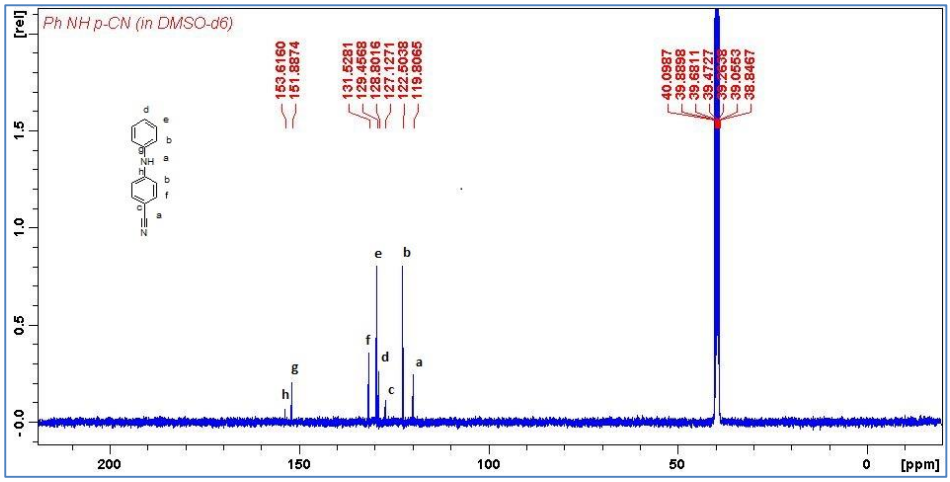


Figure S61: ^{13}C NMR spectrum for 4-(phenylamino)benzonitrile.

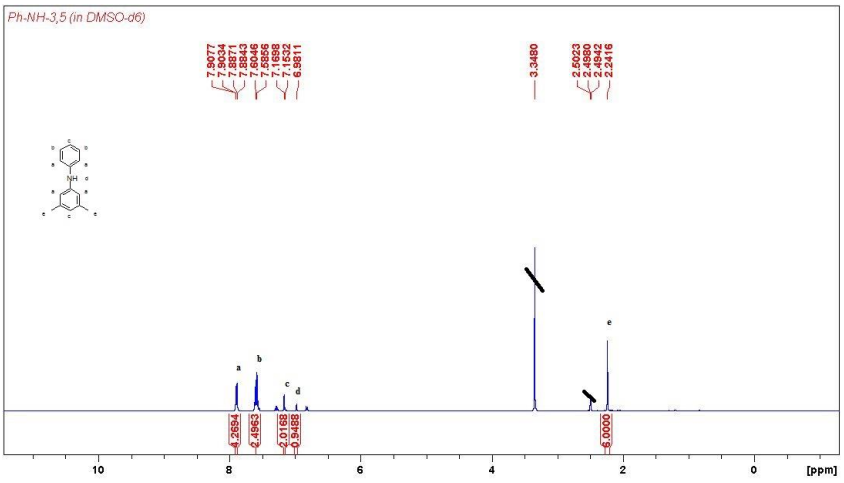


Figure S62: ^{1}H NMR spectrum for 3,5-dimethyl-N-phenylbenzenamine.

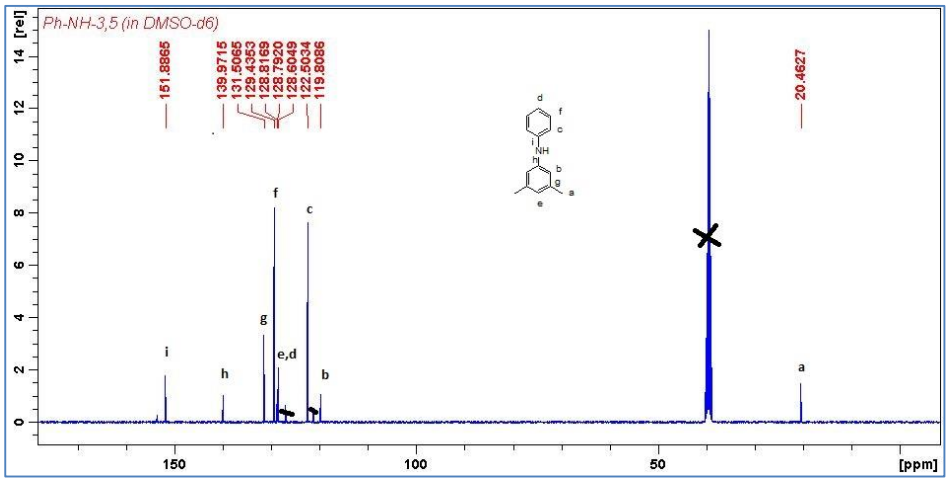


Figure S63: ^{13}C NMR spectrum for 3,5-dimethyl-N-phenylbenzenamine.

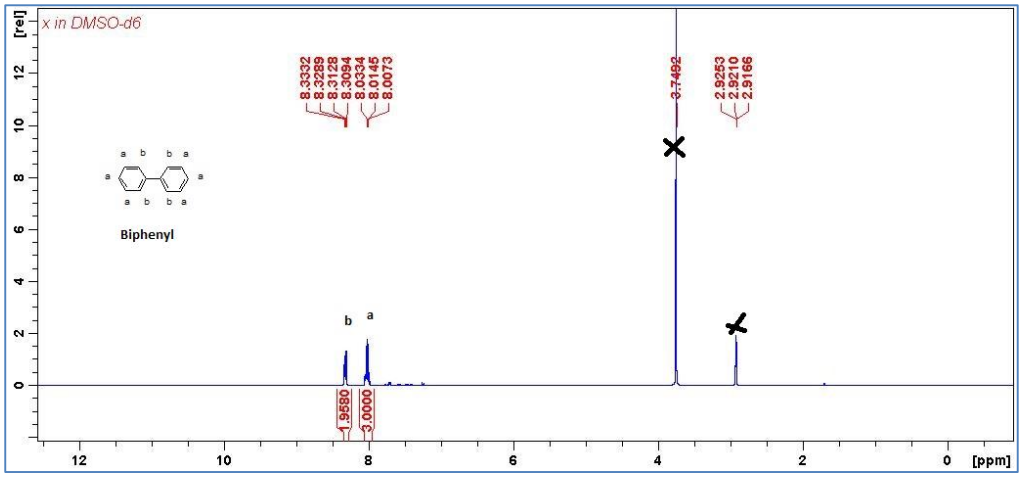


Figure S64: ^{1}H NMR spectrum for biphenyl.

Supplementary material-2

Magnetic susceptibility measurements for the paramagnetic compounds 3d and 3e

Hysteresis loop measurement experiment results for Co(3-allyl-1-picolyimidazolin-2-ylidene)$_2$Cl$_2$ (3d)

Start Time: 9/3/2014 4:09:42 PM Time Completed: 9/3/2014 5:10:24 PM Elapsed Time: 01:00:41
Sample ID: Aly-CoCl2

Experiment: C:\IDEASVSM\Default UserID\Experiments\Hafiz\Hafiz.exp
Data File: C:\IDEASVSM\Default UserID\IbrahimH\Aly-CoCl2.txt
Plot File: C:\IDEASVSM\Default UserID\IbrahimH\Aly-CoCl2.oc2
VSM Exp File: C:\IDEASVSM\Default UserID\Experiments\Hafiz\Hafiz.stp
VSM Data File: C:\IDEASVSM\Default UserID\IbrahimH\Aly-CoCl2.dat

DATA

Coercivity (Hci) 79.265 G

Mr, Negative -0.23028 emu/g

Mr, Positive -0.18188 emu/g

Ms, Negative -1.1903 emu/g

Ms, Positive 0.83096 emu/g

Squareness 2.39E-02

Field(G)	Moment/Mass(emu/g)
57.319	-0.18554
258.55	-0.14491
502.67	-0.11007
753.52	-0.07692
1004.9	-0.05037
1255.2	-0.0345
1505.3	-0.02834
1755	-0.0137
2004.7	0.002502
2254.1	0.009468
2503.1	0.037536
2752.3	0.10101
3001.1	0.21398

3249.9	0.23355
3498.5	0.19827
3747.1	0.19777
3995.2	0.20172
4243.6	0.21627
4491.8	0.23259
4739.7	0.23579
4987.7	0.26097
5235.7	0.27852
5483.9	0.29392
5732	0.3018
5980.1	0.34113
6227.8	0.34604
6475.5	0.36345
6723.2	0.36453
6970.9	0.37486
7218.6	0.38863
7466.3	0.41419
7713.9	0.41223
7961.3	0.43231
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8456	0.46089
8703	0.46085
8950	0.47652
9197.2	0.51552
9443.9	0.50864
9690.7	0.5221
9937.2	0.53235
10184	0.53754
10430	0.55553
10675	0.57044
10921	0.59197
11167	0.62063
11412	0.68687
11657	0.70151
11901	0.73003
12145	0.7514
12388	0.78683
12630	0.80117
12872	0.83094
13113	0.77872
13354	0.73509
13594	0.75189
13822	0.76016
13883	0.75936
13736	0.75448

13517	0.7176
13270	0.73268
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10482	0.55394
10232	0.52379
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9733.7	0.52639
9484.9	0.52705
9236	0.50257
8987.5	0.47954
8738.9	0.45692
8490.5	0.45606
8242.1	0.44061
7993.8	0.41598
7745.3	0.4194
7496.7	0.38654
7248.2	0.36669
6999.6	0.35792
6751.3	0.33471
6502.7	0.32688
6254.2	0.30891
6005.7	0.27623
5757	0.25689
5508.1	0.25289
5259.3	0.25855
5010.6	0.24228
4761.8	0.21933
4512.9	0.21394
4264.1	0.18495
4015.5	0.1804
3766.3	0.17829
3517.3	0.15218
3268.1	0.12664
3019.2	0.095532
2770.3	0.077256
2521.2	0.051604
2272.4	0.02155

2023.6	0.00791
1774.8	-0.00756
1525.9	-0.0215
1277	-0.03906
1028.4	-0.0581
779.02	-0.06783
529.31	-0.09708
280.49	-0.13026
31.625	-0.17449
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-12127	-1.0859
-12370	-1.1
-12613	-1.1031
-12855	-1.111
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3430.2	0.090512
3678.9	0.10193
3927.2	0.13185
4175.7	0.14588
4424.2	0.15706

4672.4	0.17195
4920.7	0.19412
5168.8	0.22277
5417.1	0.25172
5665.2	0.26522
5913.5	0.2569
6161.4	0.28451
6409.3	0.30034
6657.1	0.31439
6904.6	0.31164
7152.5	0.32322
7400.2	0.3438
7647.8	0.37987
7895.5	0.40424
8143	0.39309
8390.2	0.40347
8637.4	0.44981
8884.5	0.4499
9131.5	0.46728
9378.5	0.48248
9625.3	0.49842
9871.9	0.51637
10119	0.52399
10365	0.53216
10611	0.55151
10857	0.55108
11102	0.55982
11347	0.57149
11592	0.59415
11837	0.61497
12081	0.62796
12323	0.64617
12566	0.65506
12808	0.66134
13049	0.68034
13289	0.65891
13529	0.64524
13766	0.65204

Hysteresis loop measurement experiment results for Co(3-butenyl-1-picolyimidazolin-2-ylidene)$_2$Cl$_2$ (3e)

Start Time: 9/3/2014 2:00:04 PM Time Completed: 9/3/2014 3:00:46 PM Elapsed Time: 01:00:41

Sample ID: Bu-CoCl2

Experiment: C:\IDEASVSM\Default UserID\Experiments\Hafiz\Hafiz.exp

Data File: C:\IDEASVSM\Default UserID\IbrahimH\Bu-CoCl2.txt

Plot File: C:\IDEASVSM\Default UserID\IbrahimH\Bu-CoCl2.oc2

VSM Exp File: C:\IDEASVSM\Default UserID\Experiments\Hafiz\Hafiz.stp

VSM Data File: C:\IDEASVSM\Default UserID\IbrahimH\Bu-CoCl2.dat

DATA

Coercivity (Hci)	142.96 G
Mr, Negative	-0.19971 emu/g
Mr, Positive	-0.17298 emu/g
Ms, Negative	-1.0983 emu/g
Ms, Positive	0.68512 emu/g
Squareness	1.50E-02

Field(G)	Moment/Mass(emu/g)
56.45	-0.16726
257.23	-0.12742
501.27	-0.1071
752.1	-0.09127
1003.5	-0.07053
1253.8	-0.04751
1503.8	-0.01835
1753.6	-0.00359
2003.2	0.009746
2252.5	0.029005
2501.8	0.046828
2750.7	0.083359
2999.6	0.19305
3248.5	0.23749
3497.1	0.19736
3745.6	0.18771
3993.9	0.18365

4242.1	0.19256
4490.3	0.21607
4738.3	0.23663
4986.3	0.23887
5234.4	0.2676
5482.4	0.26347
5730.5	0.28513
5978.6	0.28081
6226.4	0.29225
6474.1	0.3207
6721.8	0.32684
6969.5	0.34966
7217.1	0.35396
7464.9	0.36638
7712.4	0.38321
7959.9	0.40905
8207.3	0.41989
8454.5	0.43235
8701.7	0.44488
8948.7	0.44634
9195.7	0.46619
9442.5	0.46908
9689.2	0.47576
9935.8	0.48734
10182	0.50085
10428	0.51208
10674	0.53339
10920	0.54126
11165	0.55478
11410	0.54812
11655	0.57114
11900	0.58306
12144	0.59811
12387	0.62492
12629	0.65937
12871	0.63991
13112	0.63649
13352	0.65968
13592	0.65119
13821	0.67226
13888	0.68512
13745	0.6846
13527	0.66005
13281	0.64839
13025	0.6181
12768	0.60674

12511	0.62113
12256	0.58028
12002	0.57669
11749	0.58354
11497	0.56664
11245	0.52957
10993	0.51158
10743	0.51761
10493	0.48929
10243	0.47418
9993.9	0.46753
9744.7	0.44608
9495.9	0.42737
9247.2	0.42815
8998.5	0.399
8750	0.39295
8501.5	0.37134
8253.2	0.35897
8004.9	0.34439
7756.4	0.33675
7507.7	0.32557
7259.3	0.31678
7010.7	0.29603
6762.3	0.27884
6513.8	0.26262
6265.3	0.25663
6016.7	0.24673
5768	0.24114
5519.2	0.22025
5270.5	0.2006
5021.6	0.18487
4772.9	0.17161
4523.9	0.14201
4275.2	0.13116
4026.6	0.11322
3777.6	0.10169
3528.2	0.081004
3279.3	0.067449
3030.2	0.05002
2781.3	0.037636
2532.4	0.02102
2283.5	-0.00309
2034.7	-0.02096
1785.8	-0.04507
1537	-0.05509
1288.2	-0.05903

1039.5	-0.08707
789.98	-0.11286
540.42	-0.13499
291.55	-0.14309
42.745	-0.16878
-206.04	-0.1932
-454.82	-0.22062
-703.98	-0.25507
-953.41	-0.28188
-1202.3	-0.3082
-1451.1	-0.33908
-1699.5	-0.35444
-1948.3	-0.36307
-2197.5	-0.3842
-2447	-0.41227
-2696.4	-0.42162
-2945.7	-0.43838
-3194.6	-0.45952
-3443.2	-0.46606
-3691.9	-0.47448
-3940.3	-0.48641
-4189.5	-0.49444
-4438.8	-0.49239
-4688.2	-0.52829
-4937.5	-0.54648
-5186.4	-0.57226
-5435.5	-0.57805
-5684.3	-0.60152
-5933.2	-0.61379
-6181.7	-0.61673
-6430.1	-0.63312
-6678.3	-0.64292
-6926.5	-0.66836
-7174.8	-0.67578
-7423.1	-0.6737
-7671.2	-0.69128
-7919.4	-0.72516
-8167.3	-0.71974
-8415.2	-0.74008
-8663.2	-0.76089
-8911	-0.76571
-9158.7	-0.77888
-9406.4	-0.78809
-9654	-0.80072
-9901.3	-0.80918
-10148	-0.81574

-10395	-0.81897
-10642	-0.84365
-10889	-0.84132
-11135	-0.85788
-11381	-0.87336
-11626	-0.89548
-11871	-0.91476
-12116	-0.97355
-12359	-1.0171
-12602	-1.0413
-12844	-1.0618
-13086	-1.0685
-13326	-1.0727
-13567	-1.0934
-13674	-1.0983
-13527	-1.0885
-13307	-1.0815
-13059	-1.036
-12802	-0.95964
-12545	-0.95058
-12288	-0.96384
-12033	-0.97694
-11779	-0.92593
-11525	-0.92361
-11272	-0.8796
-11020	-0.86027
-10769	-0.85523
-10518	-0.84544
-10267	-0.84523
-10017	-0.81486
-9767.4	-0.80523
-9517.7	-0.8036
-9268.4	-0.79088
-9018.9	-0.78408
-8769.7	-0.77158
-8520.5	-0.76206
-8271.6	-0.74891
-8022.8	-0.7283
-7773.5	-0.70708
-7524.2	-0.70748
-7275.2	-0.67384
-7026.1	-0.68143
-6777.3	-0.67176
-6528	-0.65834
-6279.1	-0.63336
-6030	-0.6119

-5780.6	-0.60272
-5531.1	-0.59932
-5281.6	-0.59767
-5032	-0.57142
-4782.3	-0.54798
-4532.3	-0.52454
-4282.5	-0.50451
-4032.9	-0.49159
-3783.6	-0.47392
-3534.3	-0.4666
-3285.3	-0.4545
-3036.2	-0.43146
-2786.8	-0.40915
-2537	-0.40121
-2287.5	-0.38255
-2038	-0.36356
-1788.9	-0.35338
-1540.1	-0.33783
-1291.1	-0.3082
-1042.5	-0.28895
-792.93	-0.27601
-543.41	-0.25081
-294.61	-0.2328
-45.656	-0.20609
203.1	-0.17131
451.98	-0.13824
701.22	-0.11331
950.5	-0.08301
1199.5	-0.07461
1448	-0.04579
1696.8	-0.02759
1945.6	-0.00845
2194.2	0.016621
2443	0.026952
2691.6	0.04036
2940.4	0.048532
3188.9	0.06352
3437.7	0.070753
3686.3	0.084913
3934.7	0.097802
4183.2	0.11018
4431.5	0.11986
4679.9	0.14273
4928.1	0.15927
5176.3	0.18446
5424.6	0.20551

5672.6	0.22414
5921	0.23478
6168.8	0.22763
6416.7	0.23966
6664.4	0.25244
6912.1	0.26871
7159.8	0.29479
7407.7	0.30161
7655.3	0.30237
7902.9	0.30674
8150.4	0.33079
8397.7	0.35741
8644.7	0.3633
8891.9	0.36882
9139	0.39129
9385.9	0.39842
9632.7	0.40632
9879.4	0.42179
10126	0.44703
10372	0.4622
10618	0.52668
10864	0.53816
11110	0.55588
11355	0.52187
11600	0.51019
11844	0.52464
12088	0.52823
12331	0.53997
12573	0.55898
12815	0.56256
13056	0.58123
13296	0.59792
13536	0.31225
13772	-0.41121