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SUPPORTING INFORMATION

Cu^{I}/Cu^{III} prototypical organometallic mechanism for the deactivation of an active pincer-like Cu^{I} catalyst in Ullmann-type couplings

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1. Supplementary methods

1.1 Materials and Methods

The reagents and solvents used were commercially available unless indicated otherwise. Solvents were purchased from SDS and were purified and dried by passing them through an activated alumina purification system (MBraun SPS-800). The preparation and handling of air-sensitive materials were performed in a N_2 drybox (Jacomex-GP-Concept-II-P) with O_2 and H_2O concentrations of <1 ppm. Ligand **L_3** was synthesized following published procedures.[1]

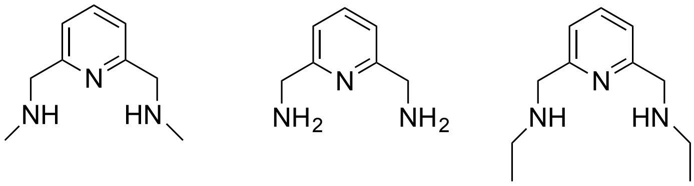
1.2 Instrumentation

^{1}H and ^{13}C NMR spectra were recorded with a Bruker 400 MHz or Bruker 300 MHz NMR spectrometer. Chemical shifts (δ) are reported in ppm and were directly referenced to the solvent signal. GC product analyses were performed with an Agilent 7820A gas chromatograph equipped with an HP-5 capillary column (30 m × 0.32 mm × 0.25 µm) and a flame ionization detector. GC–MS analyses were performed with an Agilent 7890A gas chromatograph equipped with an HP-5 capillary column interfaced with an Agilent 5975C mass spectrometer. The electron ionization (EI) source was set at 70 eV.

High resolution mass spectra (HRMS) were recorded with a Bruker MicrOTOF-Q IITM instrument with ESI or Cryospray ionization sources at the Serveis Tècnics de Recerca of the University of Girona. Samples were introduced into the mass spectrometer ion source by direct injection through a syringe pump and were externally calibrated by using sodium formate.

All analyses were carried out on gas chromatography instrument Agilent 7820A GC-System (Agilent) equipped with a fused silica capillary column Agilent HP-5 19091J-102 (25m x 200µm x 0.33µm). The stationary phase used is 5%-phenylmethylpolysiloxane. Temperatures range, in which the column is working, cannot be higher than 325ºC. The injection was carried out on a split/splitless automatic injector Agilent G4513A at 275ºC, in split mode with ratio 100:1 and volume injected was 1µL. Helium was the carrier gas at a rate of 2ml/min in inlet. The detection was conducted by a FID (Agilent 7820A GC-System), which temperature was 300ºC, and the hydrogen flow rate was 40mL/min and air flow rate was 350 mL/min, respectively, with a makeup flow of 20 mL/min. The temperature program was as follows: starting at 75ºC for 0.5 min and then raised to 190ºC at 10ºC/min. A ramp to 300ºC at 20ºC/min and 1 min hold was needed to purge the system. The analysis time was 18.5 min.

Scheme S1. Tridentate pincer-like triamines used as auxiliary ligands in this work.



L_3 L_4 L_5

1.3 General Procedure for Catalytic Experiments

A vial was loaded with the base (1.8 mmol), the solid nucleophile (1.8 mmol), the corresponding auxiliary ligand (10 mol%). Then, in an inert-atmosphere glovebox, copper(I) (10 mol%) in DMSO and the aryl iodide (0.9 mmol) were added. Liquid nucleophiles were added after the aryl iodide. The vial was sealed, and the reaction mixture was kept under an inert atmosphere and placed in a preheated oil bath at the required temperature. After the reaction mixture was stirred for 24 h, 1,3,5-trimethoxybenzene (200 μL, 1.5 M in DMSO) as internal standard was added. Subsequently, the reaction was quenched by the addition of AcOEt (5 mL). The workup consisted of the filtration of 400 μL of the crude product through silica gel using AcOEt as eluent. All samples were analyzed by gas chromatography. The GC yields were obtained through calibration curves obtained with authentic sample of all products with 1,3,5-trimethoxybenzene as an internal standard.

1.4 General Procedure for determining $[L_x\text{-}N(C_6H_5)\text{-}Cu^I]^+$ species using the Cryospray device in the MicrOTOF-Q II TM

The general procedure for determining copper intermediate species after 0.5 h reaction consists on the filtration of 0.1 mL of the crude mixture through a N_2 purged 0.45 µm Acrodisc® syringe filter. Afterwards, the filtrate was diluted with CH_3CN to a 1 mM concentration under an inert atmosphere. Samples were introduced into the mass spectrometer ion source by direct injection through a syringe pump. The temperature of the nebulizing and drying gases was set at 50ºC and the capillary voltage was set to 4500 V.

1.5 Measurements of the He tagging IRPD spectra

The He tagging infrared photodissociation IRPD spectra were measured with the ISORI instrument.[2] The ions were generated in electrospray ion source, mass selected by the first quadrupole and transferred with an octopole to a cryo-cooled wire quadrupole ion trap operated at 3 K and 1 Hz. The ions were trapped with 200 ms of helium buffer gas pulse. After a 400 ms time delay, about 1 % of the trapped ions were transformed to helium tagged complexes (*m/z* four units higher than the parent ions). After a 530 ms time delay, the ion cloud was irradiated by 5 photon pulses generated in an optical parametric oscillator (OPO) operating at 10 Hz frequency. At 995 ms, the exit electrode of the trap was opened, the ions were mass-analyzed by the second quadrupole, and their number (N) was determined by a Daly type detector operated in ion-counting mode. In the following cycle the light from the OPO was blocked by a mechanical shutter, giving the number of non-irradiated ions (N_0). The He@IRPD spectra are constructed as the wavenumber dependence of $(1 - N/N_0)$.

1.5.1 Generation of the *m/z* 332 ions from the reaction mixture

All solid reagents were put into respective reaction vessels and flushed with N_2 for 30 minutes before use. Solvents were also flushed with nitrogen for the same time to purge dissolved oxygen. 17 mg of **L₃**.$(HCl)_2$ (0.07 mmol), 301 mg of K_3PO_4 (1.4 mmol), 170 mg of *p*-methoxyphenol (1.4 mmol), 100 µL of 1-iodo-3,5-dimethylbenzene and a small stir bar were put in a 25 ml flask equipped with a rubber septum. To a small vial with

13.5 mg of CuI (0.07 mmol), 1 ml of DMSO was added and the mixture was stirred until dissolution of CuI. Then, the solution was transferred to a 25 ml flask. The reaction mixture was heated for 30 minutes to 50 °C on water bath. The resulting solution was taken into a syringe and through a 30-μm pore size PTFE filter introduced to 10 ml of acetonitrile. The resulting solution was used in the experiments. The unused portion was stored in liquid nitrogen and melted before use. Ionization conditions: Capillary temperature 200°C, capillary voltage 30V, tube lens voltage 80 V, sheath gas (N_2) pressure 5 psi.

1.5.2 Generation of the *m/z* 304 ions from the reaction mixture

The preparation procedure was carried in an analogous manner to *m/z* 332 (cf. 1.5.1). 13.5 mg of CuI was dissolved in 1 ml DMSO, that had been degassed by bubbling Ar through it for 30 minutes. This solution was added to 170 mg of *p*-methoxyphenol, 17 mg of **L3**.$(HCl)_2$, 301 mg K_3PO_4 and 141 mg PhI that had been previously put to 5 ml flask with a stir bar. Reaction mixture was heated and stirred for 30 minutes at 50 °C, transferred to 10 ml of degassed acetonitrile, stored in liquid nitrogen and melted before measurement. Ionization conditions: capillary temperature 200 °C, cap. voltage 10 V, tube lens voltage 80 V, sheath gas (N_2) pressure 2 psi.

1.5.3 Generation of the m/z 304 ions from the pre-synthesized complex

19 mg of CuI was dissolved in 1 ml degassed DMSO under argon and transferred to a vial with phenylated ligand. Half of the resulting DMSO solution was diluted in 5 ml ACN and measured. Ionization conditions: capillary temperature 150 °C, cap. voltage 0 V, tube lens voltage 100 V, sheath gas pressure 5 psi.

1.5.4 Wavenumber dependence of the laser power

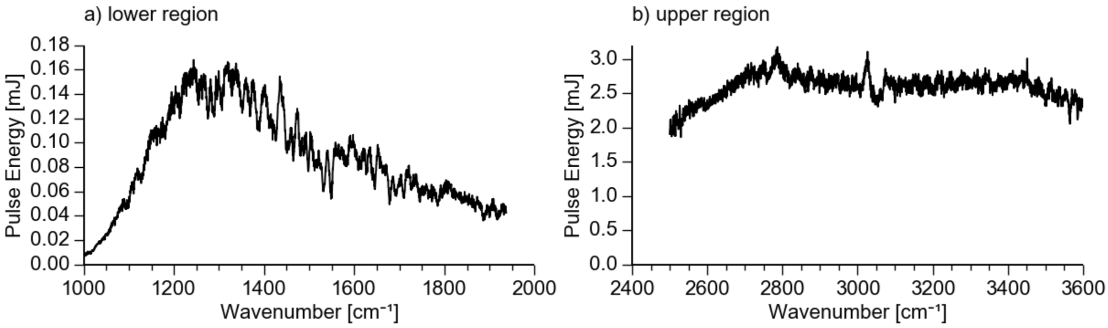


Figure S1. Typical dependence of pulse energy of the OPO laser on the wavenumber in (a) lower region and (b) upper region. The laser power was measured after the ion trap.

1.5.5 DFT calculations of the IR spectra.

Geometry optimizations and frequency calculations have been performed using the B3LYP method with Grimme's D3 dispersion correction[3] employing 6-31G(d,p) basis set on C, H and N atoms and 6-311G(d) on Cu atom as implemented in the Gaussian 09 revision D.01.[4] All optimized structures were confirmed as minima on the potential energy surface by the frequency calculations. When comparing the theoretical spectra to the experimental ones a scaling factor of 0.98 was used. Reported relative energies in Figure 2 (main text) include unscaled zero-point energy corrections.

1.5.6 Coordinates of structures listed in Figure 2 of the main text.

Structure 2b)

Cu	0.462542	-0.437976	0.012008
N	1.251831	-2.065374	0.910322
C	0.278988	-3.168752	0.677271
H	0.615470	-4.101027	1.141048
H	0.163431	-3.308217	-0.398180
H	-0.684945	-2.883256	1.104963
N	0.095847	0.069494	1.804532
C	1.461459	-1.786561	2.369862
H	2.482142	-1.409432	2.496786
H	1.370861	-2.701849	2.963973
N	-0.725418	0.914250	-0.484381
C	0.491848	-0.711895	2.819826
C	0.065028	-0.431220	4.110838
H	0.367830	-1.051137	4.947483
C	-0.766643	0.682957	4.298652
H	-1.120675	0.921080	5.296723
C	-1.143433	1.491113	3.222151
H	-1.779020	2.357281	3.367599
C	-0.683639	1.149198	1.951391
C	-0.864778	1.860011	0.638116
H	-1.850988	2.340886	0.566832
H	-0.124403	2.683106	0.613209
C	-0.619550	1.653312	-1.737256
H	-1.500636	2.304620	-1.830648
H	-0.611712	0.964375	-2.579390
H	0.272857	2.296571	-1.802462
C	1.045796	-0.907390	-1.717596
C	2.391191	-0.736562	-2.032365
C	0.171765	-1.560102	-2.581692
C	2.887112	-1.232777	-3.251139
H	3.067725	-0.214321	-1.358547
C	0.648653	-2.069071	-3.800890
H	-0.881612	-1.658983	-2.329079
C	2.004102	-1.898000	-4.109035
C	4.333216	-1.031604	-3.636536
C	-0.282660	-2.756152	-4.770515
H	2.382239	-2.290389	-5.050327
H	2.139023	-2.328127	0.481900
H	4.959143	-0.813074	-2.766756
H	4.433886	-0.191499	-4.333737
H	4.739004	-1.916732	-4.135365
H	-1.196531	-3.101052	-4.279234
H	0.199162	-3.618248	-5.241419
H	-0.578107	-2.071130	-5.573917

Structure 2c)

Cu	1.070354	0.477986	0.012476
N	1.709130	-2.671738	1.099729
C	0.940164	-3.892498	1.319034
H	1.225536	-4.322309	2.281751
H	1.180203	-4.624875	0.545147
H	-0.148287	-3.726409	1.320357
N	0.356028	0.106956	1.898566
C	1.830748	-1.808230	2.286928
H	2.655257	-1.107360	2.153372
H	2.093101	-2.445978	3.134210
N	-0.395174	1.859580	-0.100308
C	0.572262	-1.017086	2.616222
C	-0.337848	-1.426360	3.594535
H	-0.150014	-2.331970	4.161338
C	-1.473421	-0.654853	3.836701
H	-2.190102	-0.956118	4.594132
C	-1.678711	0.513086	3.098444
H	-2.548228	1.139147	3.268379
C	-0.737656	0.858611	2.134264
C	-0.814029	2.127391	1.303875
H	-1.809804	2.581224	1.353689
H	-0.103202	2.852353	1.717211
C	-0.014362	3.085772	-0.841867
H	-0.809138	3.839958	-0.844917
H	0.224843	2.806946	-1.869681
H	0.879143	3.513837	-0.381701
C	1.637136	-2.064815	-0.157512
C	0.814998	-2.532537	-1.181484
C	2.433917	-0.887946	-0.405269
C	0.721929	-1.863137	-2.427327
H	0.201218	-3.412294	-1.031968
C	2.269124	-0.154983	-1.613579
H	3.305565	-0.696509	0.217036
C	1.410660	-0.677546	-2.623333
C	-0.158964	-2.445847	-3.504614
C	3.236513	0.957237	-1.964185
H	1.324794	-0.143975	-3.565449
H	-1.192794	1.443222	-0.583339
H	-1.181599	-2.598758	-3.141530
H	0.216739	-3.424943	-3.821966
H	-0.203394	-1.800932	-4.385423
H	3.703538	1.387024	-1.073647
H	2.733975	1.762355	-2.508795
H	4.034887	0.575088	-2.608720

Structure 2d)

Cu	0.471578	-0.302111	-0.755693
N	1.483287	-2.123694	0.096193
C	0.510250	-3.225760	0.149737
H	0.890234	-4.114279	0.671795
H	0.234071	-3.502287	-0.869861
H	-0.391357	-2.881309	0.665263
N	0.268747	-0.013412	1.234556
C	1.967908	-1.706455	1.419800
H	2.898499	-1.144705	1.273006
H	2.195606	-2.553412	2.082190
N	-1.256724	1.252178	-0.571174
C	0.956073	-0.784830	2.082349
C	0.755826	-0.705204	3.463338
H	1.323758	-1.341505	4.134195
C	-0.182105	0.203032	3.954071
H	-0.357770	0.284736	5.021842
C	-0.906821	0.994958	3.059251
H	-1.655926	1.697856	3.408982
C	-0.659109	0.848689	1.695129
C	-1.395528	1.592363	0.652093
H	-2.048965	2.410407	0.976372
H	1.319533	1.580324	-2.354836
C	-1.972407	1.984653	-1.601668
H	-2.579227	2.814128	-1.216770
H	-2.621132	1.288820	-2.144816
H	-1.248787	2.380152	-2.323103
C	1.548961	0.520921	-2.441104
C	2.888083	0.095752	-2.335925
C	0.547442	-0.398158	-2.837567
C	3.252183	-1.208727	-2.670160
H	3.649548	0.808331	-2.033228
C	0.909989	-1.724996	-3.195030
H	-0.439325	-0.037029	-3.121788
C	2.245810	-2.103605	-3.095832
C	4.692134	-1.658988	-2.618623
C	-0.146145	-2.674835	-3.701109
H	2.528943	-3.115499	-3.377333
H	2.269029	-2.392437	-0.487636
H	5.321564	-0.943641	-2.083514
H	5.098120	-1.766074	-3.631014
H	4.792329	-2.635367	-2.132360
H	-1.021555	-2.688884	-3.042701
H	0.233973	-3.696010	-3.784936
H	-0.498269	-2.369761	-4.693339

1.6 Computational details of the mechanistic study

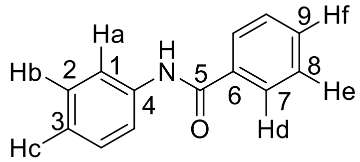
All density functional theory (DFT) calculations on copper systems depicted in Figure 5 of the main text were carried out with the Gaussian09 software rev. D.01,[4] using the Becke hybrid B3LYP exchange-correlation functional.[5] The geometries were optimized using for C, N, H, S, O and Cu atoms the 6-31G* basis set, and for iodine the Stuttgart-Dresden relativistic effective core potential (SDD) and its associated basis set,[6] augmented with *d* and *f* functions (orbital exponents of $\alpha_d(I) = 0.73$ and $\alpha_f(I) = 0.55$).[7] The numerical computation of two electron-integrals made use of a pruned grid having 99 radial shells and 590 angular points per shell (integral=ultrafine keyword in Gaussian09). The effect of DMSO solvent was introduced through the SMD model.[8] Dispersion effects were also introduced employing the Grimme‘s D3 correction with Becke-Johnson damping (D3BJ). Analytical Hessians were computed at the same level of theory of the geometry optimizations to evaluate the thermal and entropy corrections ($G_{corr.}$) at T = 298.15 K. The nature of the located stationary points was characterized by frequency calculations in solvent phase, where minima have no imaginary frequencies and transition states only one. Single point calculations on the equilibrium geometries, including also the solvent and dispersion effects, with the cc-pVTZ dunning basis set on C, H, N, S, O and Cu atoms and Stuttgart-Dresden relativistic effective core potential (SDD) and its associated basis set,[6] augmented with *d* and *f* functions (orbital exponents of $\alpha_d(I) = 0.73$ and $\alpha_f(I) = 0.55$)[7] on iode ($E_{cc\text{-}pvtz}$), were used to refine the free energies values (G). Then, the final Gibbs energies were evaluated as:

$$G = E_{cc\text{-}pvtz} + G_{corr.} \quad (1)$$

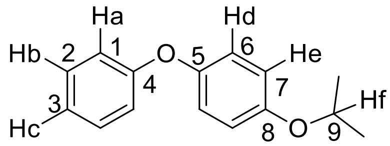
In the free energy balances, the effect of the change associated with moving from a standard state gas phase pressure of 1 atm to a standard state gas-phase concentration of 1M (14.1 M for DMSO molecules) was also included ($\Delta G^{\circ/*}$).[9] Thus, the final energy differences use the standard state of an ideal gas at a gas phase concentration of 1 $mol{\cdot}L^{-1}$ (14.1 $mol{\cdot}L^{-1}$) dissolved as an ideal dilute solution at a liquid phase concentration of 1 $mol{\cdot}L^{-1}$((14.1 $mol{\cdot}L^{-1}$). The value of $\Delta G^{\circ/*}$ at 298 K is 1.89 kcal mol^{-1} for 1M standard state solutes and 3.46 $kcal{\cdot}mol^{-1}$ for 14.1 M explicit solvent DMSO molecules. The X-ray diffraction structure of [$\mathbf{L_3}$-Cu(II)$(OTf)_2$] (see Figure S19) has been chosen as starting point for geometry optimizations. The geometry visualizations have been edited with the Chemcraft program (www.chemcraft.org).

2. Characterization of coupling products

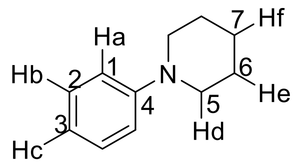
Amides



Benzanilide,[10, 11] *^{1}H-NMR*: (*300MHz, DMSO-d^6, 25ºC)* δ (ppm): 7.17-7.23 (m, 1H, H^c), 7.43-7.48 (m, 2H, H^b), 7.60-7.72 (m, 3H, H^f, H^e), 7.86-7.89 (m, 2H, H^a), 8.03-8.07 (m, 2H, H^d), 10.34 (s, 1H, NH). *^{13}C-NMR*: (*75MHz, DMSO-d^6, 25ºC)* δ (ppm): 120.3 (C_1), 123.7 (C_3), 127.6 (C_7), 128.4 (C_8), 128.6 (C_2), 131.6 (C_9), 134.9 (C_6), 139.2 (C_4), 165.5 (C_5). *HRMS (ESI-TOF (m/z))*: calcd. for $C_{13}H_{11}NONa$ 220.0733; found 220.0725 and calcd. for $(C_{13}H_{11}NO)_2Na$ 417.1573; found 417.1571.



1-methoxyl-4-phenoxybenzene (characterization compared to commercial compound)**:** *^{1}H-NMR*: (4*00MHz, CDCl$_3$, 25ºC)* δ (ppm): 3.81 (s, 3H, H^f), 6.87-6.91 (m, 2H, H^e), 6.93-7.01 (m, 4H, H^a, H^d), 7.05 (t, 1H, *J*=7.4Hz, H^c), 7.28-7.33 (m, 2H, H^d). *^{13}C-NMR*: (*100MHz, CDCl$_3$, 25ºC)* δ (ppm): 55.9 (C_9), 115.1 (C_7), 117.8 (C_1), 121.0 (C_6), 122.6 (C_3), 129.8 (C_2), 150.3 (C_5), 156.1 (C_8), 158.7 (C_4). *GCMS*: t_R: 12.359; MS ($C_{13}H_{12}O_2$): 200.1.

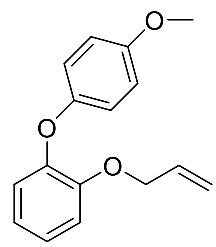


1-phenylpiperidine,[12] *^{1}H-NMR*: (*300MHz, CDCl$_3$, 25ºC)* δ (ppm): 1.55-1.62 (m, 2H^f), 1.68-1.75 (m, 4H^e), 3.14-3.17 (m, 4 H^d), 6.79-6.85 (m, 1H, H^c), 6.92-6.97 (m, 2H, H^a), 7.21-7.28 (m, 2H, H^b). *^{13}C-NMR*: (7*5MHz, CDCl$_3$, 25ºC)* δ (ppm): 24.3 (C_7), 25.9 (C_6), 50.7 (C_5), 116.5 (C_1), 119.2 (C_3), 129.0 (C_2), 152.3 (C_4). *HRMS (ESI-TOF (m/z))*: calcd. for $C_{11}H_{16}N$ 162.1277; found 162.1265.

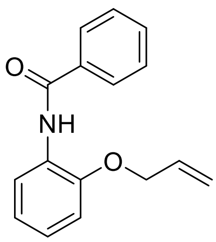
1-(allyloly)-2-iodobenzene (rc)

rc was synthesized following published procedures.[13] The characterization of **rc-H** was performed by comparison to a commercially available sample.

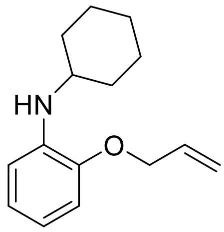
1-(allyloxy)-2-(4-methoxyphenoxy)benzene (rc-2): *^{1}H-NMR*: (*300MHz, $CDCl_3$, 25ºC)* δ (ppm): 3.81 (s, 3H), 4.62 (dt, $^3J_{HH}$=5.23Hz, $^4J_{HH}$=1.55Hz, 2H), 5.24 (ddd, $^2J_{HH}$=10.50 Hz, $^3J_{HH}$=3.21 Hz, $^4J_{HH}$=1.64Hz, 1H), 5.34 (ddd, $^2J_{HH}$=17.25 Hz, $^3J_{HH}$=3.65 Hz, $^4J_{HH}$=1.72Hz, 1H), 5.94- 6.08 (m, 1H), 6.84- 6.97 (m, 6H), 7.01- 7.09 (m, 2H). *^{13}C-NMR*: (*75MHz, $CDCl_3$, 25ºC)* δ (ppm): 55.6, 69.9, 114.6, 114.9, 117.5, 119.1, 119.9, 121.4, 123.8, 133.2, 146.9, 149.8, 151.3, 155.2. *HRMS (ESI-TOF (m/z))*: calcd. for $C_{16}H_{16}O_3Na$ 279.0992; found 279.0999 and calcd. for $(C_{16}H_{16}O_3)_2Na$ 535.2091; found 535.2084.



N-(2-(allyloxy)phenyl)benzamide (rc-3): *^{1}H-NMR*: (*300MHz, $CDCl_3$, 25ºC)* δ (ppm): 4.68 (dt, $^3J_{HH}$=5.28Hz, $^4J_{HH}$=1.44Hz, 2H), 5.37 (ddd, $^2J_{HH}$=10.50 Hz, $^3J_{HH}$=3.17 Hz, $^4J_{HH}$=1.32Hz, 1H), 5.46 (ddd, $^2J_{HH}$=17.29 Hz, $^3J_{HH}$=3.47 Hz, $^4J_{HH}$=1.61Hz, 1H),6.05- 6.12 (m, 1H), 6.95 (dd, $^3J_{HH}$=7.25Hz, $^4J_{HH}$=2.37Hz, 1H), 7.05- 7.09 (m, 2H), 7.50- 7.58 (m, 3H), 7.92 (dd, $^3J_{HH}$=8.28Hz, $^4J_{HH}$=1.76Hz, 1H). *^{13}C-NMR*: (*75MHz, $CDCl_3$, 25ºC)* δ (ppm): 69.6, 111.5, 118.2, 119.9, 121.5, 123.8, 127.0, 128.1, 128.8, 131.7, 132.8, 135.7, 147.1, 165.2. *HRMS (ESI-TOF (m/z))*: calcd. for $C_{16}H_{15}NO_2Na$ 276.0995; found 276.0991 and calcd. for $(C_{16}H_{15}NO_2)_2Na$ 529.2098; found 529.2083.



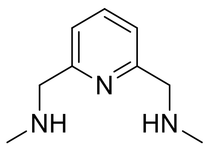
2-(allyloxy)-N-cyclohexylaniline (rc-4): *^{1}H-NMR*: (*400MHz, $CDCl_3$, 25ºC)* δ (ppm): 1.15-1.31 (m, 3H), 1.31- 1.48 (m, 3H), 1.61- 1.73 (m, 1H), 1.73- 1.86 (m, 2H), 2.09 (d, $^3J_{HH}$=12.18 Hz, 2H), 3.22- 3.34 (m, 1H), 4.19 (s, 1H, NH), 4.57 (dt, $^3J_{HH}$=5.23Hz, $^4J_{HH}$=1.51Hz, 2H), 5.30 (ddd, $^2J_{HH}$=10.50 Hz, $^3J_{HH}$=3.21 Hz, $^4J_{HH}$=1.64Hz, 1H), 5.42 (ddd, $^2J_{HH}$=17.23 Hz, $^3J_{HH}$=3.55 Hz, $^4J_{HH}$=1.58Hz, 1H), 6.04- 6.18 (m, 1H), 6.63 (dd, $^2J_{HH}$=10.50 Hz, $^3J_{HH}$=8.17Hz, $^4J_{HH}$=1.44Hz, 2H), 6.79 (dd, $^3J_{HH}$=8.04Hz, $^4J_{HH}$=1.41Hz, 1H), (ddt, $^2J_{HH}$=15.35Hz, $^3J_{HH}$=7.69Hz, $^4J_{HH}$=1.31Hz, 1H). *^{13}C-NMR*: (*100MHz, $CDCl_3$, 25ºC)* δ (ppm): 25.1,



26.0, 33.5, 51.4, 69.3, 110.5, 111.3, 115.7, 117.3, 121.5, 133.7, 137.7, 145.7. _HRMS (ESI-TOF (m/z))_: calcd. for $C_{15}H_{22}NO$ 232.1696; found 232.1705 and calcd. for $C_{15}H_{21}NONa$ 254.1515; found 254.1514.

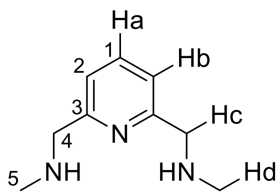
Synthesis of auxiliary ligands

L_3: *N,N'*-dimethyl-2,6-bis(aminomethyl)pyridine and hydrogen chloride salt (L_3.(HCl)$_2$). [1]

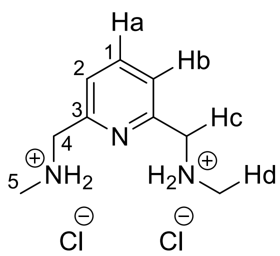


2,6-bis(chloromethyl)pyridine (1 g, 5.6 mmol) was added to aqueous methylamine (40%) (30 mL, 350 mmol) in a round-bottom flask and the mixture was stirred at room temperature for 2-3 days. The reaction was monitored by ^{1}H-NMR. Next, NaOH (0.470 g) was added and the mixture was concentrated under a reduced pressure. The crude was extracted with CH_2Cl_2 and the combined organic layers were dried with anhydrous $MgSO_4$. Finally, the solvent was evaporated under reduced pressure, obtaining **L_3** as a yellow oil (0.920 g, 90% yield).

Since the product is highly hygroscopic, the hydrochloric salt **L_3**.(HCl)$_2$ was prepared by dissolving the oil in $CHCl_3$ (1 mL) and hydrochloric acid 36.5% (0.85 mL). The aqueous phase was dried under vacuum to dryness and the crystallization was performed with a mixture of MeOH and Et_2O (0.660 g, 55% yield).

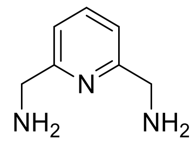


L_3 (oil): <u>^{1}H-NMR</u> (400 MHz, $CDCl_3$, 25 ºC) δ (ppm): 2.77 (s, 6 H, H^d), 3.84 (s, 4 H, H^c), 7.16 (d, 2 H, H^b), 7.60 (t, 1 H, H^a). <u>^{13}C-NMR</u> (100 MHz, $CDCl_3$, 25 ºC) δ (ppm): 36.15 (C_5), 57.17 (C_4), 120.39 (C_2), 136.72 (C_1), 159.17 (C_3).



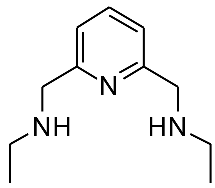
L_3.(HCl)$_2$ salt: <u>^{1}H-NMR</u> (400 MHz, D_2O, 25 ºC) δ (ppm): 2.83 (s, 6 H, H^d), 4.43 (s, 4 H, H^c), 7.46 (d, 2 H, H^b), 7.93 (t, 1 H, H^a). <u>EA:</u> calcd. for ($C_{19}H_{17}N_3Cl_2$•1.15 H_2O) C, 41.76; H, 7.51; N, 16.23; found C, 41.78; H, 7.37; N, 16.10. <u>HRMS (ESI-TOF (m/z))</u>: calcd. for $C_9H_{16}N_3$;166.1339; found 166.1345.

L_4: 2,6-pyridinediyldimethanamine

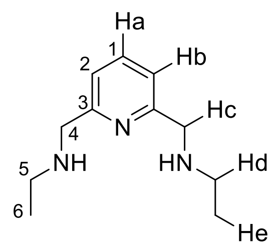


2,6-bis(chloromethyl)pyridine (0.5 g, 2.81 mmol) was dissolved in 30 mL of DMF. Sodium azide was then added (1.1 g, 16.95 mmol) and the mixture was stirred overnight at 80ºC. Next, the crude product was washed with AcOEt and H_2O, dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. Afterwards, the crude product was dissolved in THF (25 mL) and H_2O (5 mL). Then, triphenylphosphine (1.78 g, 6.75 mmols) was added and stirred overnight at room temperature. After completion of the reaction, the mixture was evaporated and extracted with CH_2Cl_2 and H_2O. The desired product remains in the aqueous phase which was dried under vaccum to dryness. The crystallization was performed with a mixture of MeOH and Et_2O (0.241 g, 62% yield). ^{1}H-NMR: (300 MHz, D_2O, 25 ºC) δ (ppm): 4.29 (s, 4 H, H^c), 7.35 (d, 2 H, *J*= 7.8Hz, H^b), 7.82 (t, 1 H, *J*= 7.8Hz, H^a). ^{13}C-NMR: (75 MHz, D_2O, 25 ºC) δ (ppm): 42.60 (C_4), 121.10 (C_2), 138.93 (C_1), 151.54 (C_3). HRMS (ESI-TOF (m/z)): calcd. for $C_7H_{12}N_3$ 138.1026; found 138.1035.

L_5: *N,N'*-diethyl-2,6-bis(aminomethylpyridine)

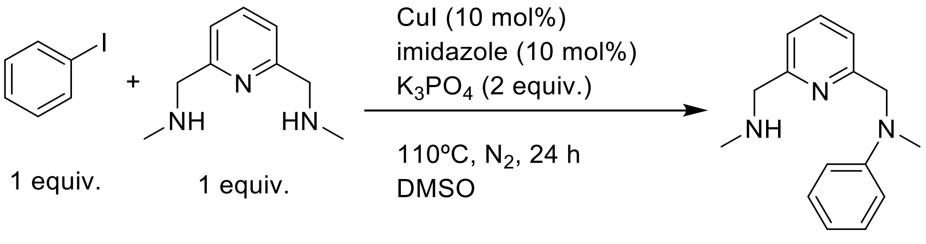


2,6-pyridinedicarboxyaldehyde (0.5 g, 3.53 mmol) was dissolved in dry MeOH (7 mL) under inert atmosphere. Next, ethylamine 2M in MeOH (3.75 mL, 7.5 mmol) was added dropwise. The reaction mixture was stirred at 40 ºC and monitored by ^{1}H-NMR. Afterwards, the reaction mixture was evaporated and the crude product was dissolved in 10 mL of TFE and 5 mL of CH_2Cl_2 and magnetically stirred at 40 ºC. After 5 min, $NaBH_4$ (168.92 mg, 4.23 mmol) was added and the progress of the reaction conversion was monitored by ^{1}H-NMR. After completion of the reaction, the mixture was filtered and solvent was evaporated. The crude was purified by silica gel column chromatography with CH_2Cl_2:MeOH:NH_3 (8:2:0.1) yielding *N,N'*-diethyl-2,6-bis(aminomethylpyridine) as a pale-yellow oil (0.188 g, 40% yield).



^{1}H-NMR: (300 MHz, $CDCl_3$, 25 ºC) δ (ppm): 1.10 (t, 6 H, *J*= 7.2 Hz, H^e), 1.79 (s, 2 H, NH), 2.66 (q, 4 H, *J*= 7.1 Hz, H^d), 3,84 (s, 4 H, H^c), 7.10 (d, 2 H, *J*= 7.8 Hz, H^b), 7.53 (t, 1 H, *J*= 7.7 Hz, H[a]). ^{13}C-NMR: (75 MHz, $CDCl_3$, 25 ºC) δ (ppm): 15.47 (C_6), 44.00 (C_5), 55.31 (C_4), 120.48 (C_2), 136.88 (C_1), 159.54 (C_3). HRMS (ESI-TOF (m/z)): calcd. for $C_{11}H_{20}N_3$ 194.1652; found 194.1661 and calcd. for $C_{11}H_{19}N_3Na$ 216.1471; found 216.1472.

L_3-C_6H_5: N-methyl-N-((6-((methylamino)methyl)pyridin-2-yl)methyl)benzenamine

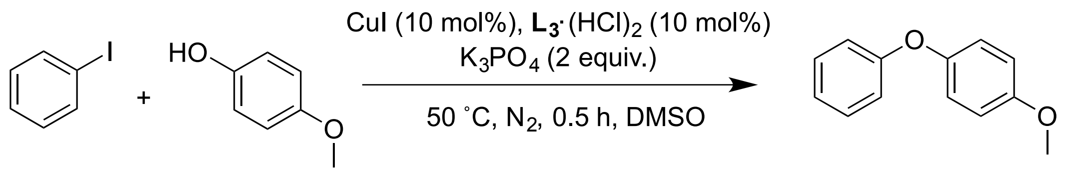


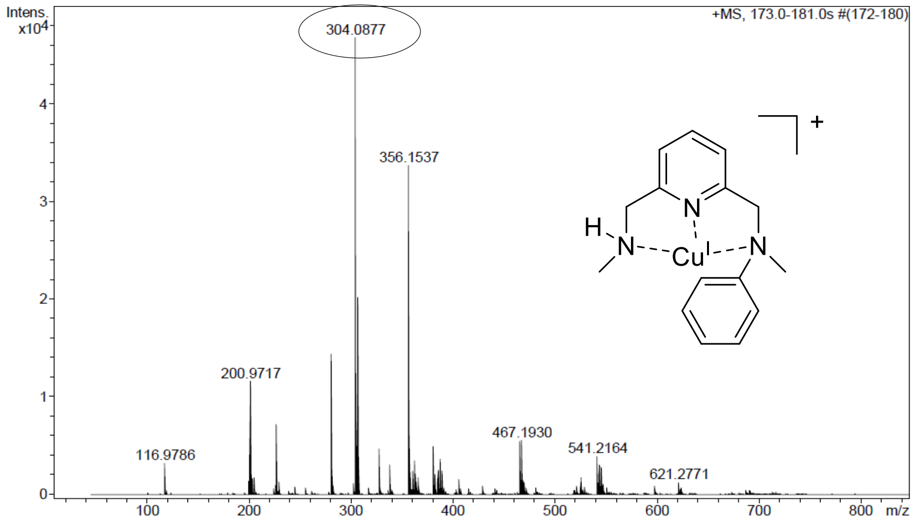
Following a modification of the general procedure for catalytic experiments, a vial was loaded with K_3PO_4 (1.8 mmol), the *N,N'*-dimethyl-2,6-bis(aminomethyl)pyridine (0.9 mmol) and imidazole ligand (10 mol%). Then, in an inert-atmosphere glovebox, copper(I) (10 mol-%) in DMSO and the aryl iodide (0.9 mmol) were added. The vial was sealed, and the reaction mixture was kept under an inert atmosphere and placed in a preheated oil bath under stirring for 24 h at 110ºC. After completion of the reaction, the mixture was quenched by the addition of CH_3CN (5 mL) and the crude product through silica gel using CH_3CN as eluent. Afterwards, the mixture was evaporated and extracted with CH_2Cl_2 and aqueous NH_3. The combined organic layers were dried with anhydrous $MgSO_4$ and the solvent was evaporated under reduced pressure, obtaining **L_3-C_6H_5** as a yellow oil (0.116 g, 90% yield). HRMS (ESI-TOF (m/z)): calcd. for $C_{15}H_{20}N_3$ 242.1652; found 242.1660, calcd. for $C_{15}H_{19}N_3Na$ 264.1471; found 264.1481, calcd. for $C_{15}H_{19}N_3K$ 280.1211; found 280.1229.

3. Supplementary Figures

3.1 Supplementary Figures - HRMS spectra

Figure S1. Determination of $[(\mathbf{L_3}\text{-}C_6H_5)\text{-}Cu^{I}]^{+}$ using the auxiliary ligand $\mathbf{L_3}$. HRMS spectrum (ESI-TOF) (*m/z*); Observed HRMS (top) with the theoretical isotope prediction (bottom).





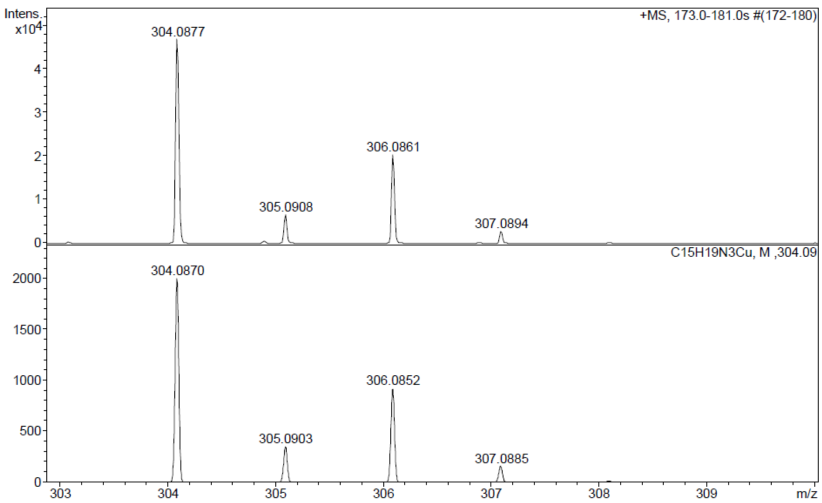
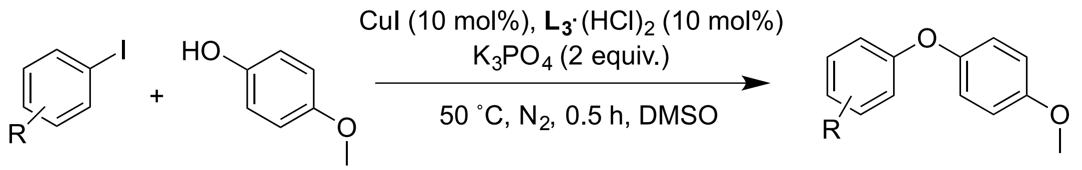


Figure S2. Determination of $[(\mathbf{L_3}\text{-}C_6H_5)\text{-}Cu^{I}]^{+}$ species using bromobenzene. HRMS spectrum (ESI-TOF) (*m/z*); Observed HRMS (top) with the theoretical isotope prediction (bottom).



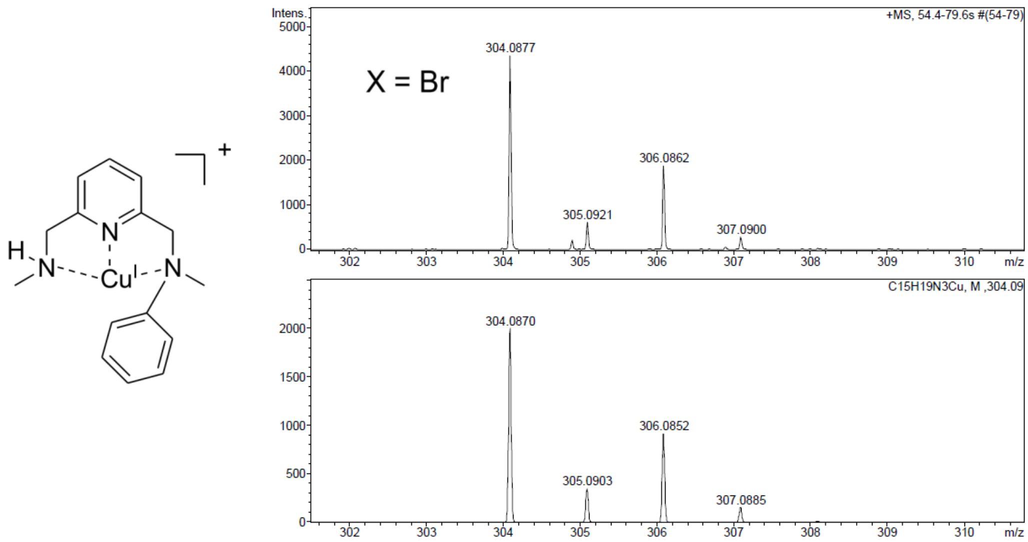


Figure S3. Determination of $[(\mathbf{L_3}\text{-}C_6H_4Me)\text{-}Cu^{I}]^{+}$ species using 1-iodo-4-methylbenzene. HRMS spectrum (ESI-TOF) (*m/z*); Observed HRMS (top) with the theoretical isotope prediction (bottom).

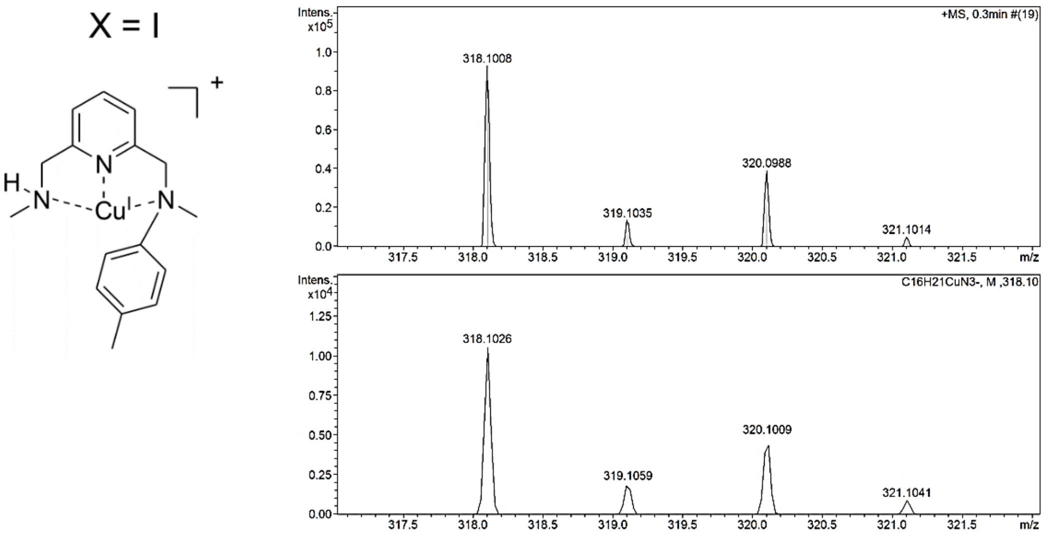


Figure S4. Determination of $[(\mathbf{L_3}\text{-}C_6H_3Me_2)\text{-}Cu^I]^+$ species using 1-iodo-3,5-dimethylbenzene. HRMS spectrum (ESI-TOF) (*m/z*); Observed HRMS (top) with the theoretical isotope prediction (bottom).

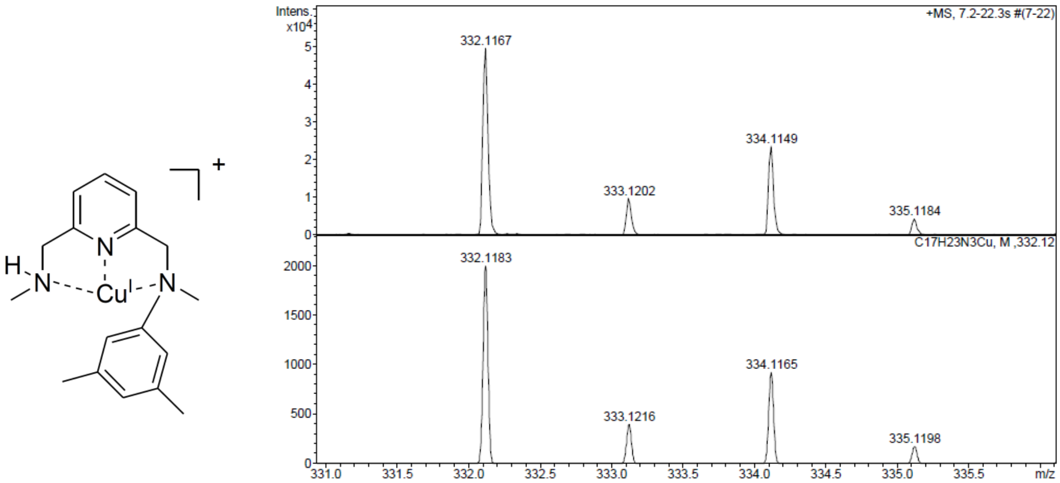
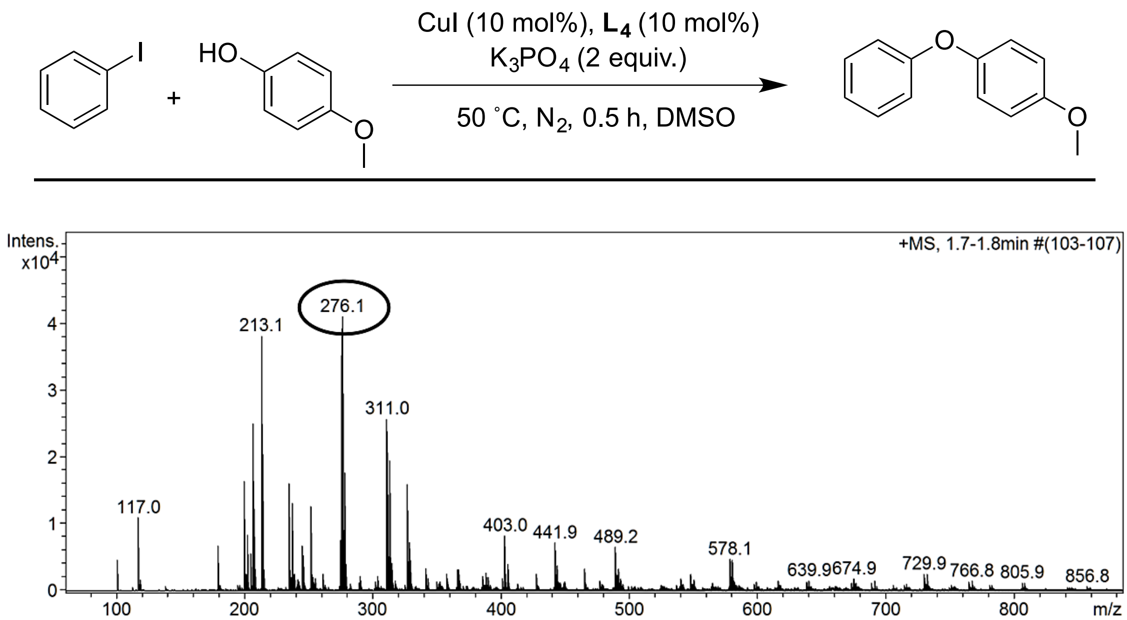


Figure S5. Determination of $[(\mathbf{L_4}\text{-}C_6H_5)\text{-}Cu^I]^+$ species using the auxiliary ligand $\mathbf{L_4}$. HRMS spectrum (ESI-TOF) (*m/z*); Observed HRMS (top) with the theoretical isotope prediction (bottom).



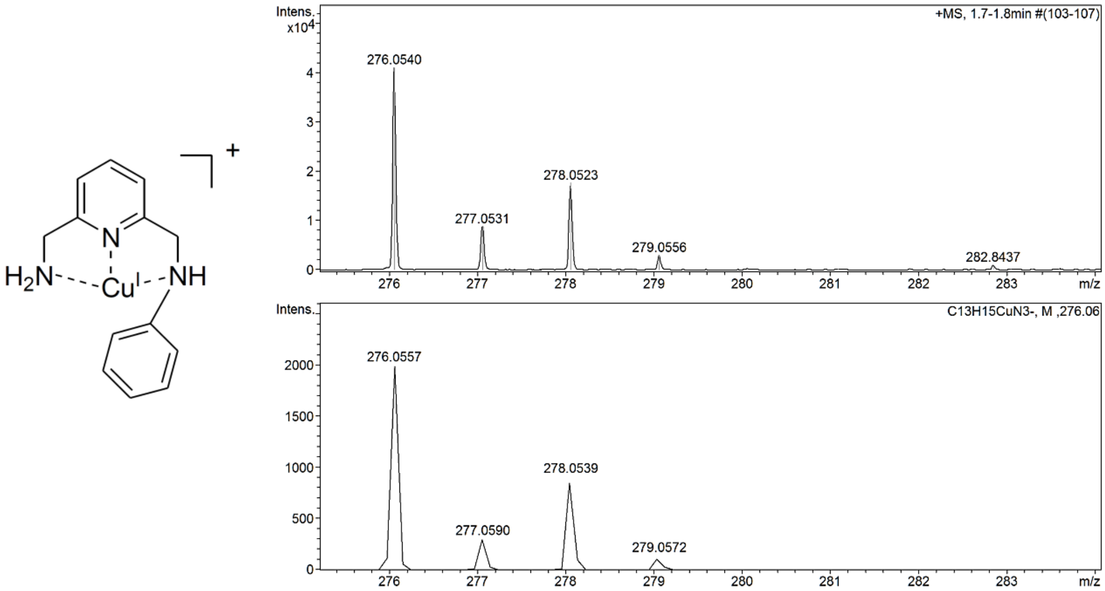
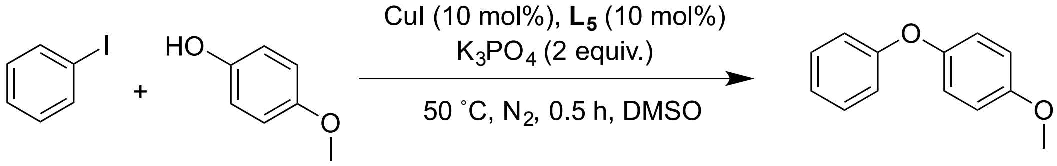
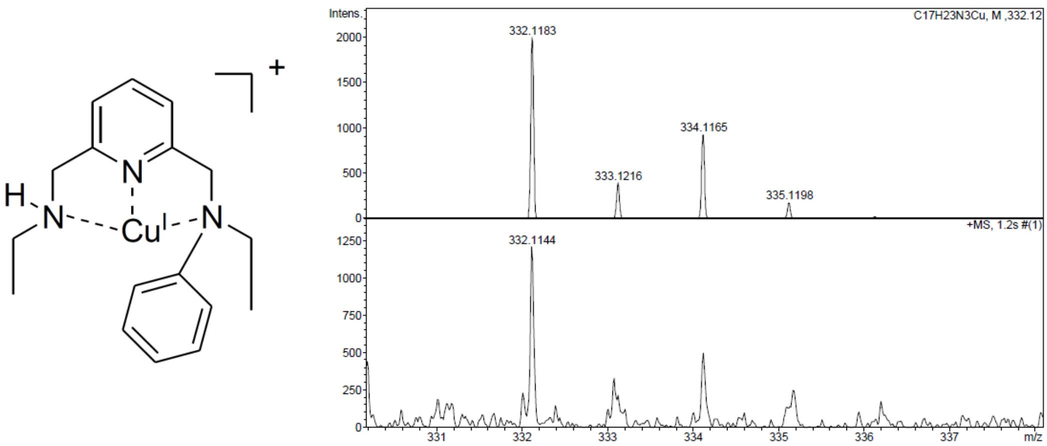


Figure S6. Determination of $[(\mathbf{L_5}\text{-}C_6H_5)\text{-}Cu^I]^+$ species using the auxiliary ligand $\mathbf{L_5}$. HRMS spectrum (ESI-TOF) (*m/z*); The theoretical isotope prediction (top) with the observed HRMS with (bottom).



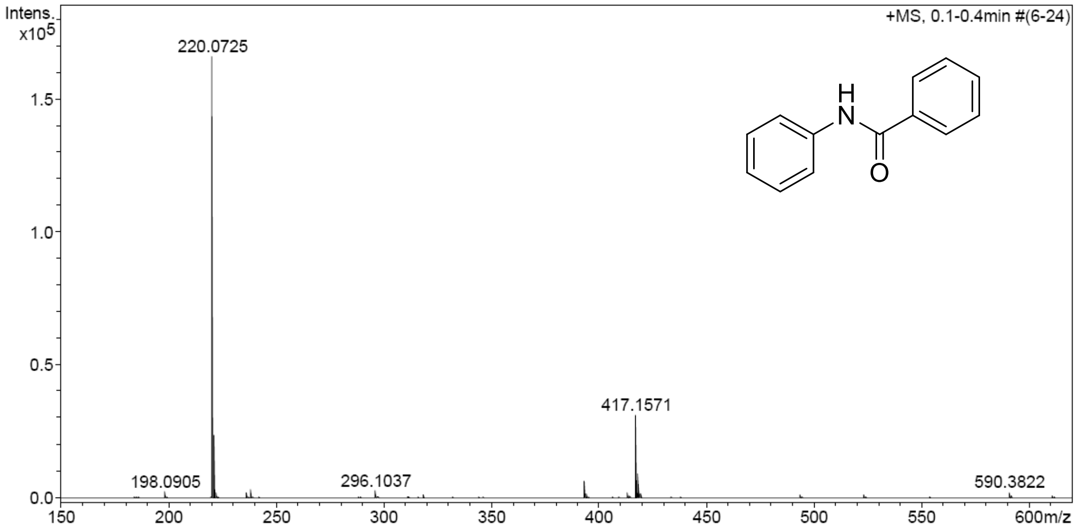


3.2 Supplementary Figures - ^{1}H NMR, ^{13}C NMR and ESI-TOF or GC-MS spectra

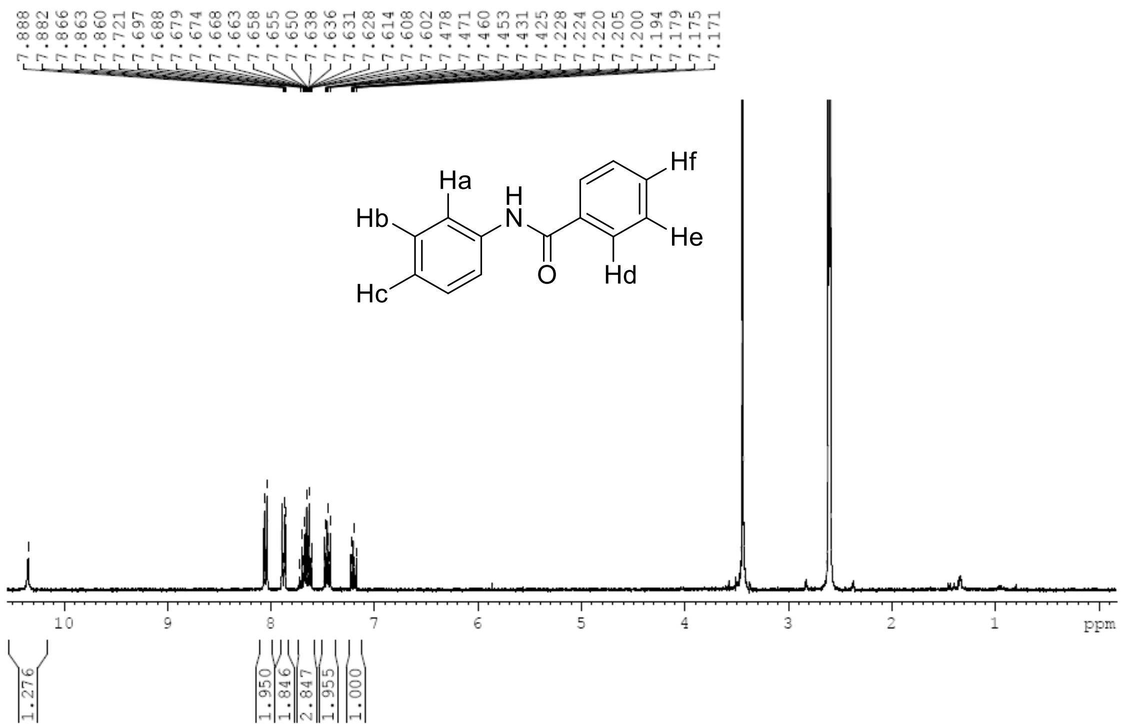
Amides

Figure S7. Benzanilide: a) HRMS (ESI-TOF) (*m/z*). b) ^{1}H-NMR spectrum (300 MHz, DMSO-d^{6}, 25 ºC). c) ^{13}C-NMR spectrum (75 MHz, DMSO-d^{6}, 25 ºC).

a)



b)



c)

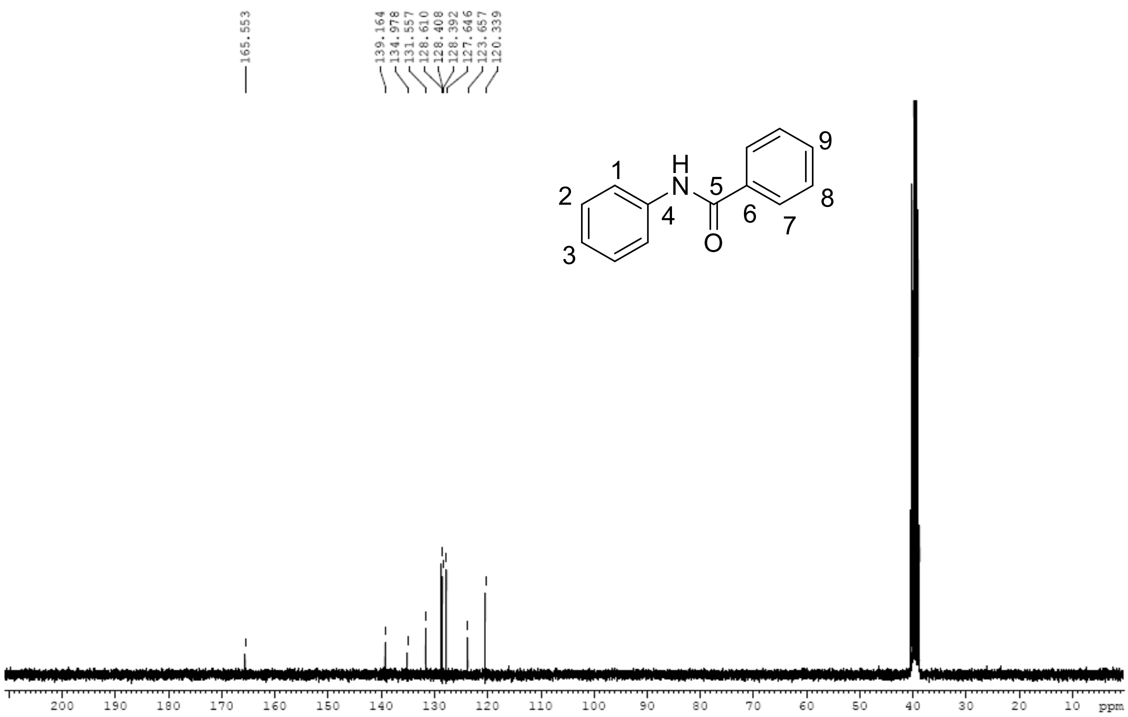
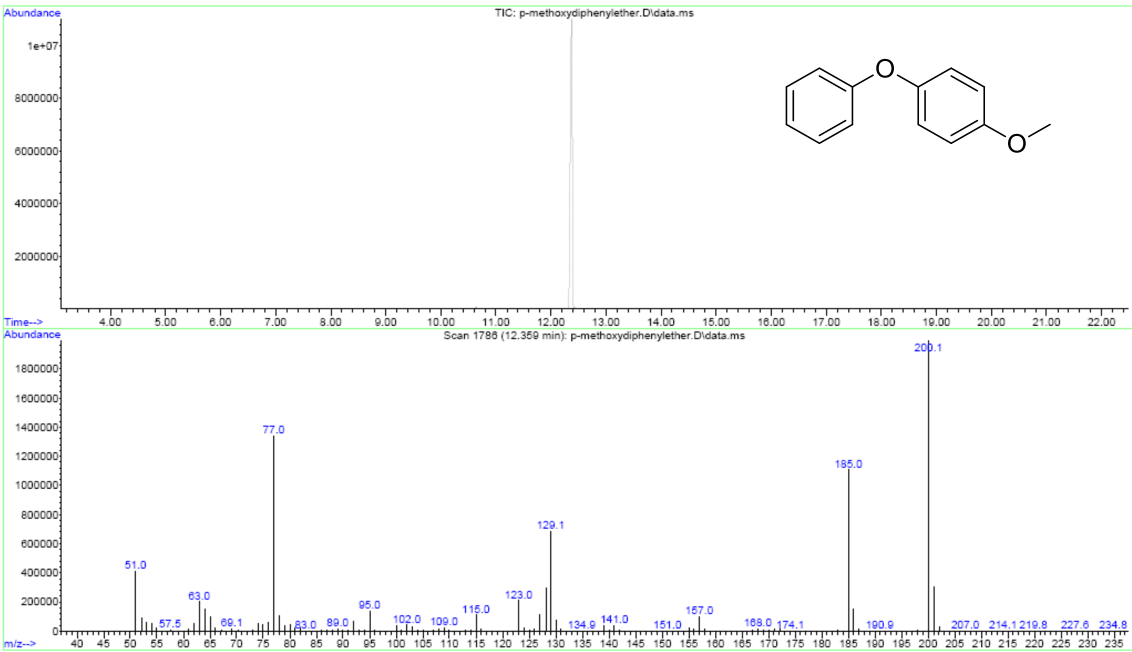
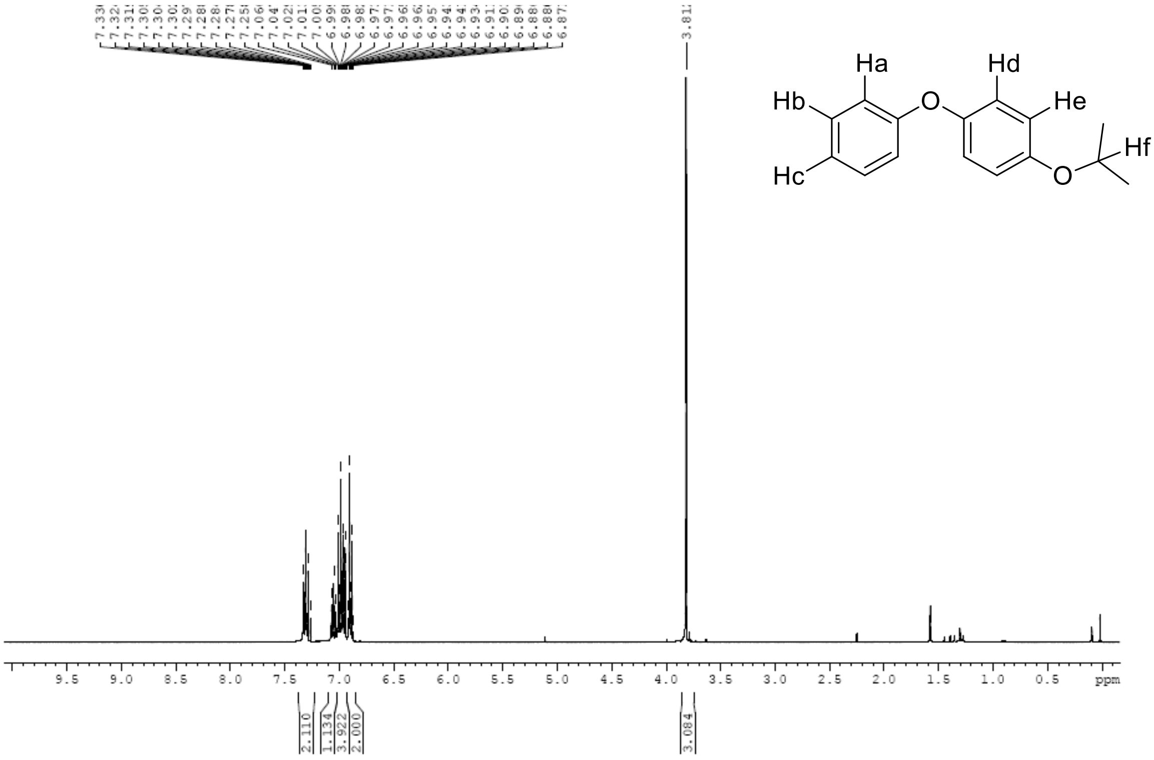


Figure S8. 1-methoxyl-4-phenoxybenzene: a) GC-MS (*m/z*). b) ^{1}H-NMR spectrum (400 MHz, $CDCl_3$, 25 ºC). c) ^{13}C-NMR spectrum (100 MHz, $CDCl_3$, 25 ºC).

a)



b)


3.812
Ha
Hb
Hc
Hd
He
Hf
O
O
2.110
1.134
3.922
2.000
3.084
ppm

c)

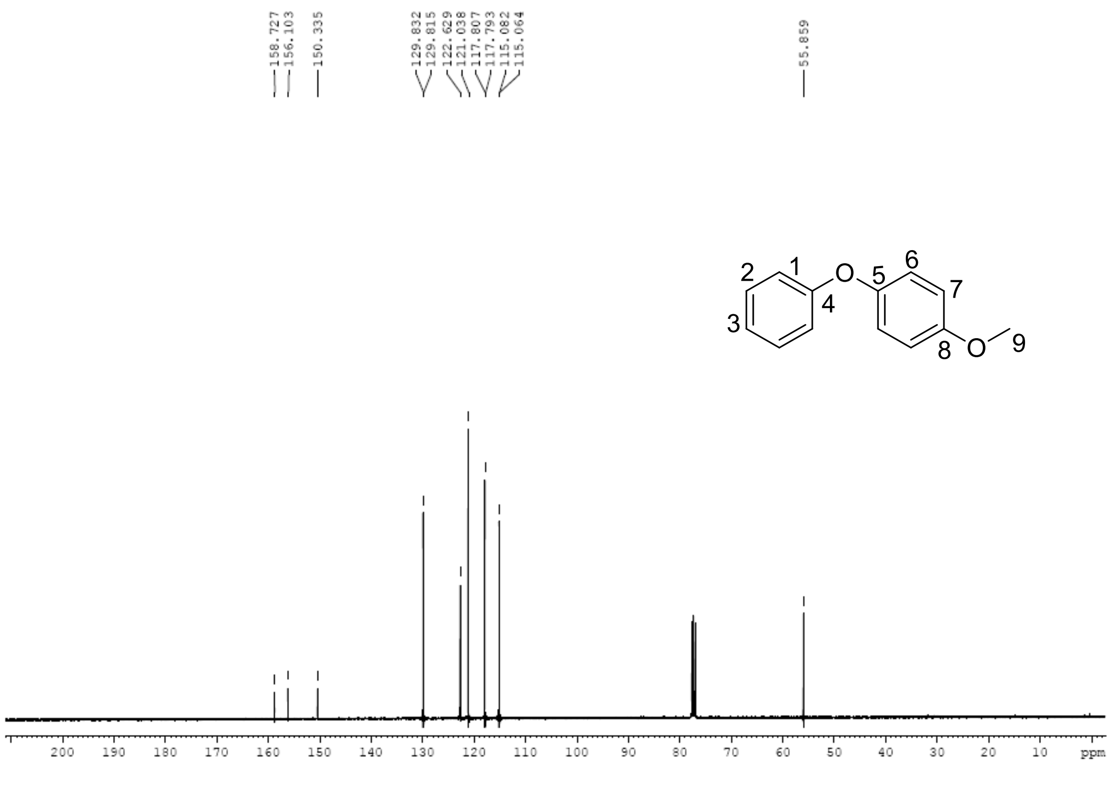
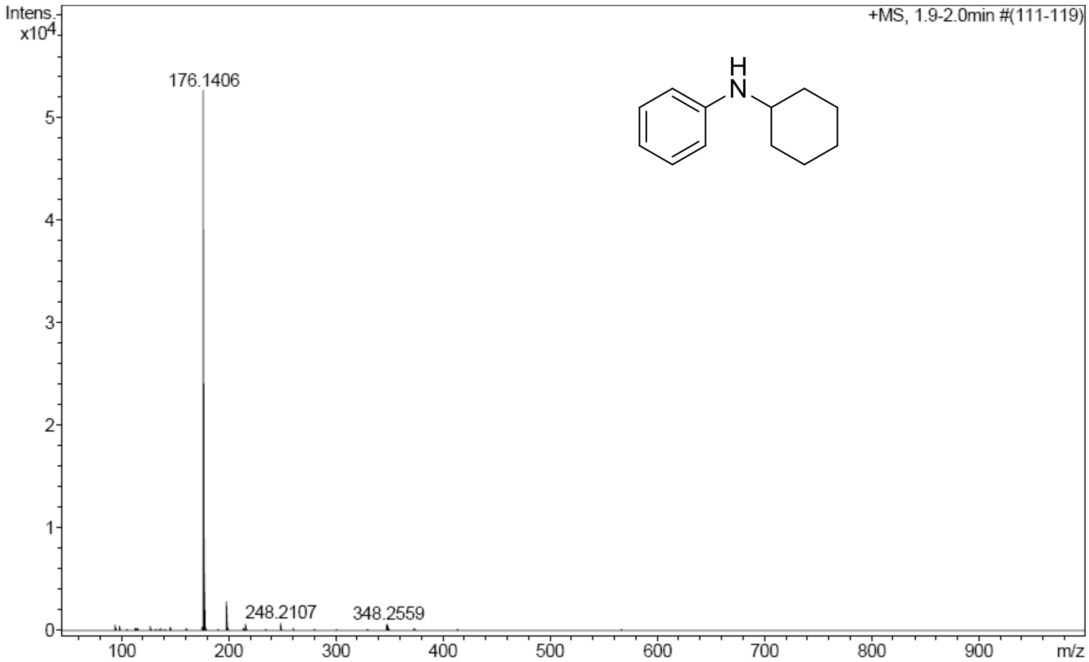
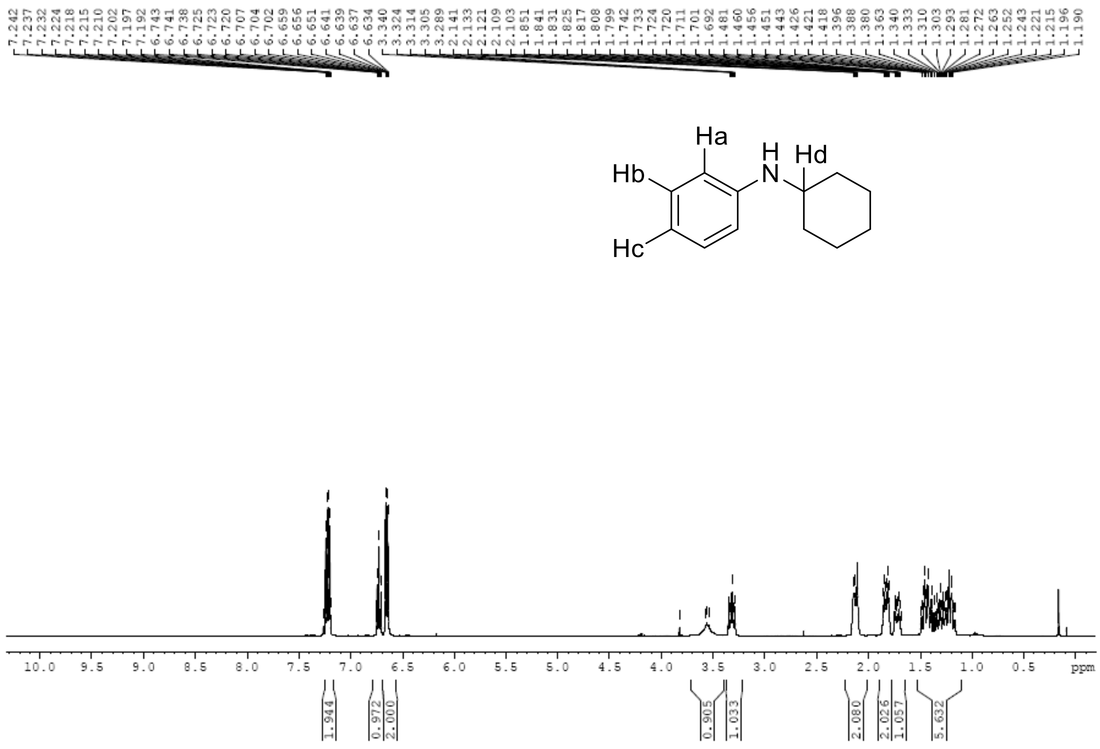

158.727
156.103
150.335
129.832
129.815
122.629
121.038
117.807
117.793
115.082
115.064
55.859
1
2
3
4
5
6
7
8
9
O
O
ppm

Figure S9. N-cyclohexylaniline: a) HRMS (ESI-TOF) (*m/z*). b) ^{1}H-NMR spectrum (400 MHz, $CDCl_3$, 25 ºC). c) ^{13}C-NMR spectrum (100 MHz, $CDCl_3$, 25 ºC).

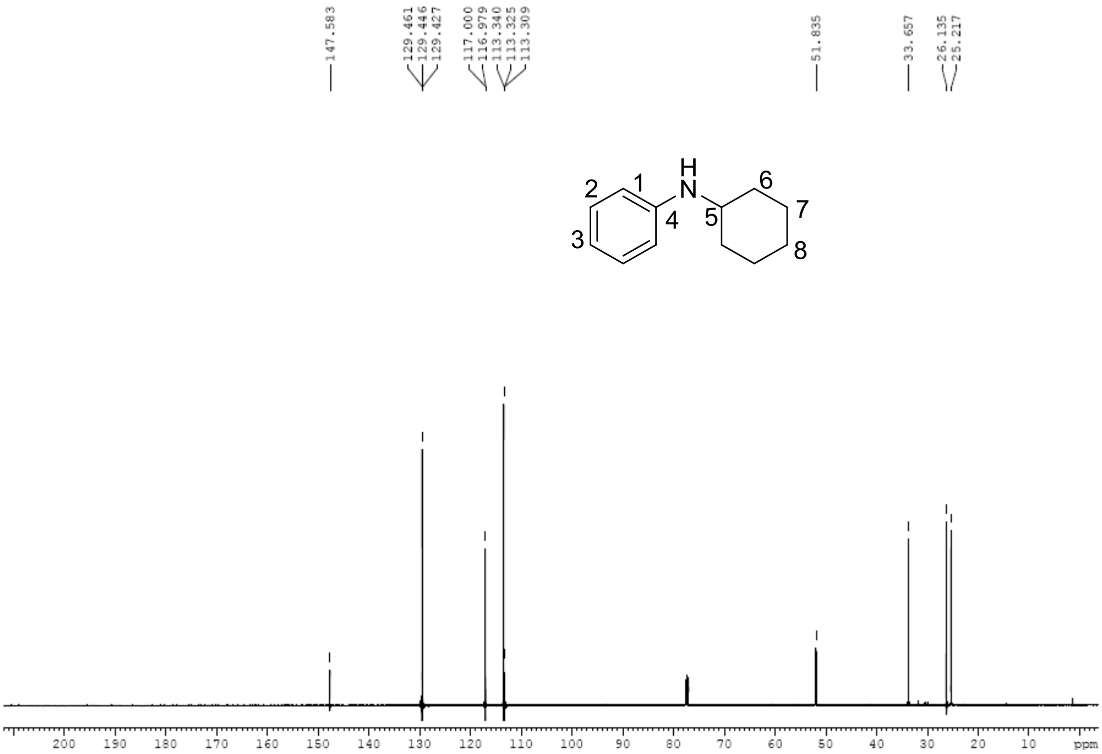
a)



b)



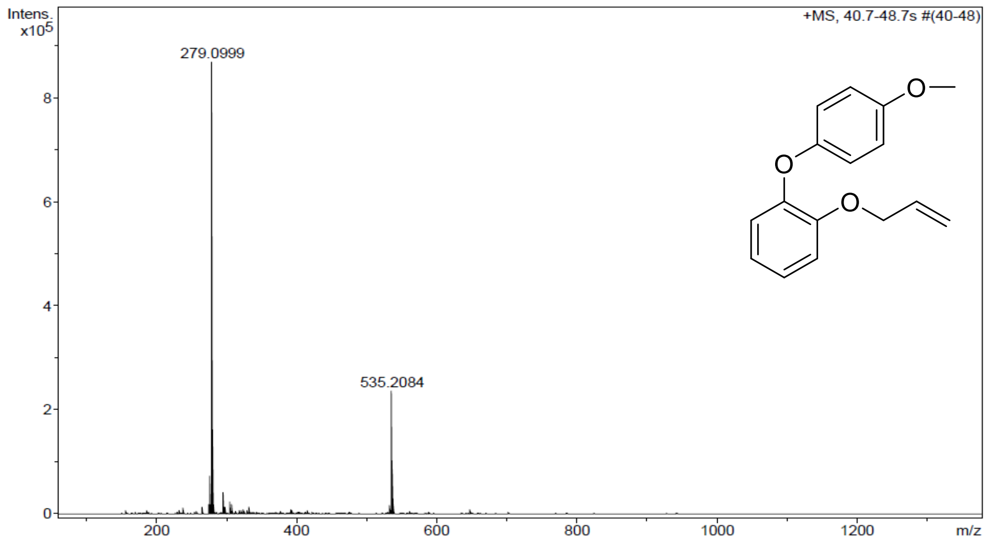
c)



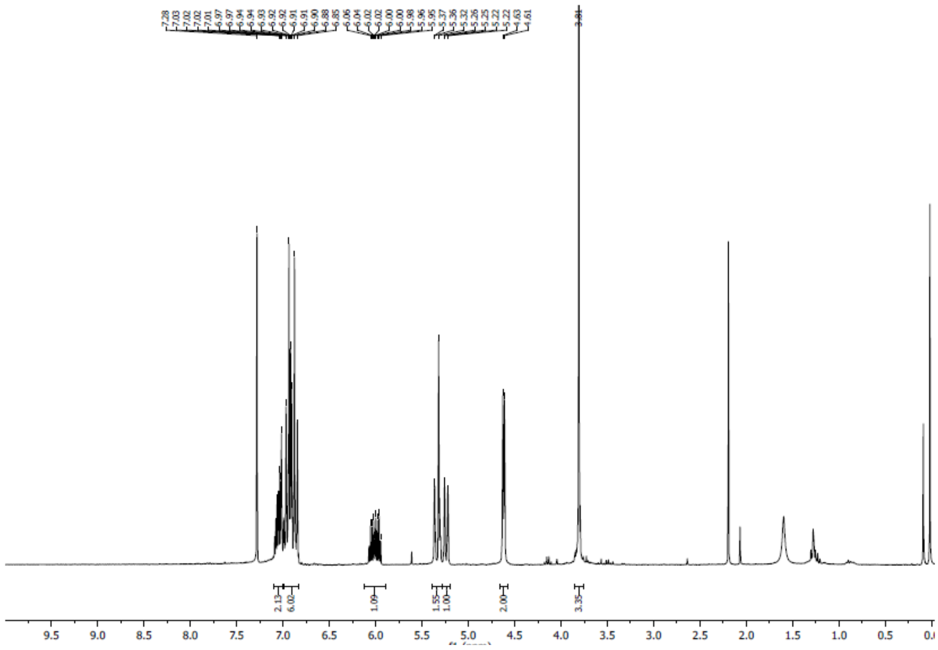
1-(allyloly)-2-iodobenzene (rc)

Figure S10. 1-(allyloxy)-2-(4-methoxyphenoxy)benzene (rc-2): a) HRMS (ESI-TOF) (*m/z*). b) ^{1}H-NMR spectrum (300 MHz, $CDCl_3$, 25 ºC). c) ^{13}C-NMR spectrum (75 MHz, $CDCl_3$, 25 ºC).

a)



b)



c)

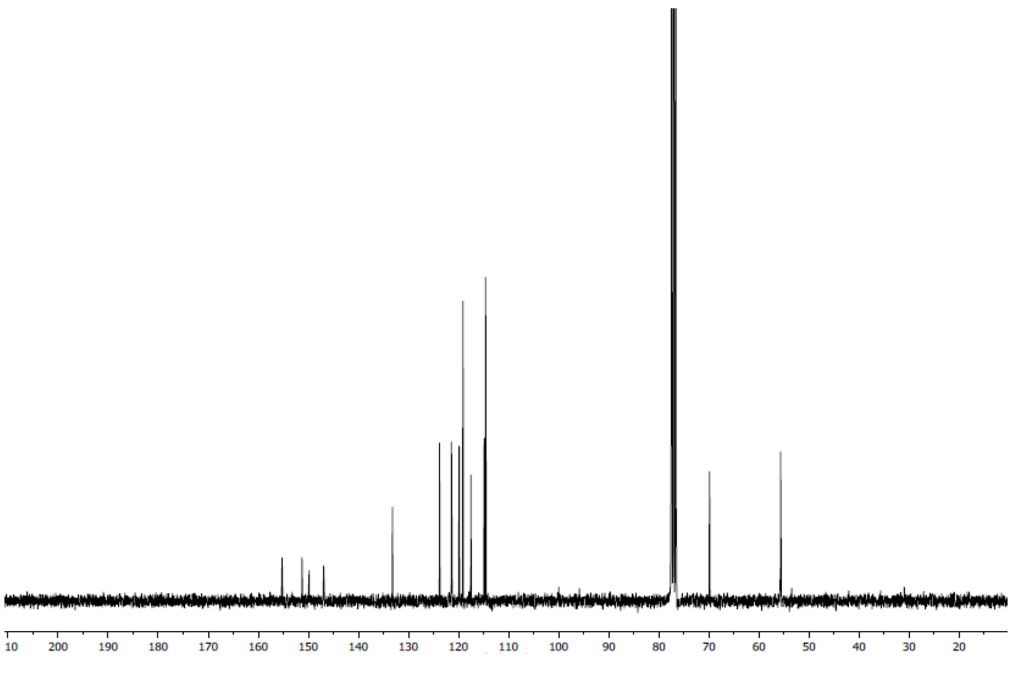
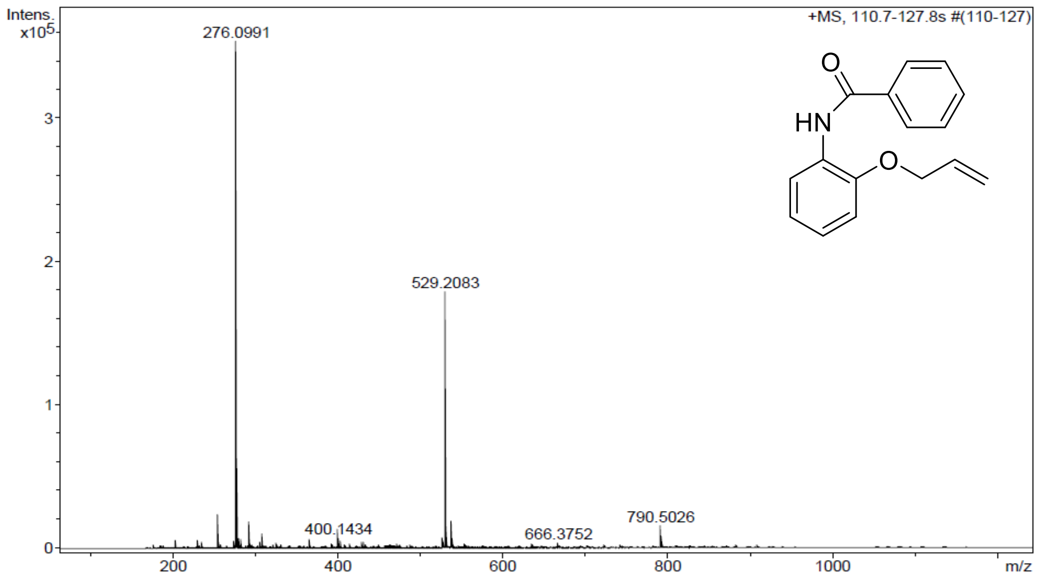
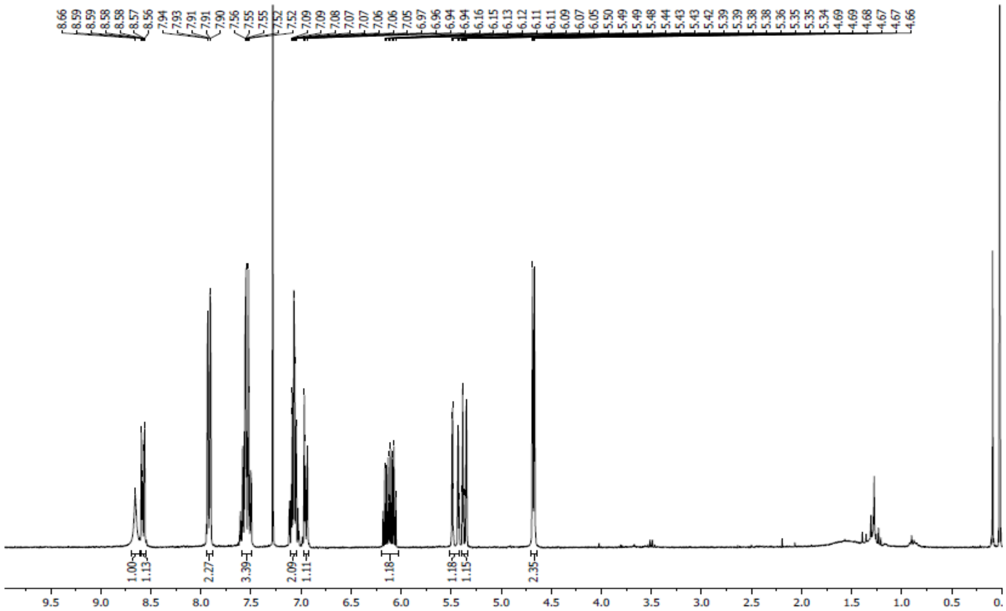


Figure S11. N-(2-(allyloxy)phenyl)benzamide (rc-3): a) HRMS (ESI-TOF) (*m/z*). b) ^{1}H-NMR spectrum (300 MHz, $CDCl_3$, 25 ºC). c) ^{13}C-NMR spectrum (75 MHz, $CDCl_3$, 25 ºC).

a)



b)



c)

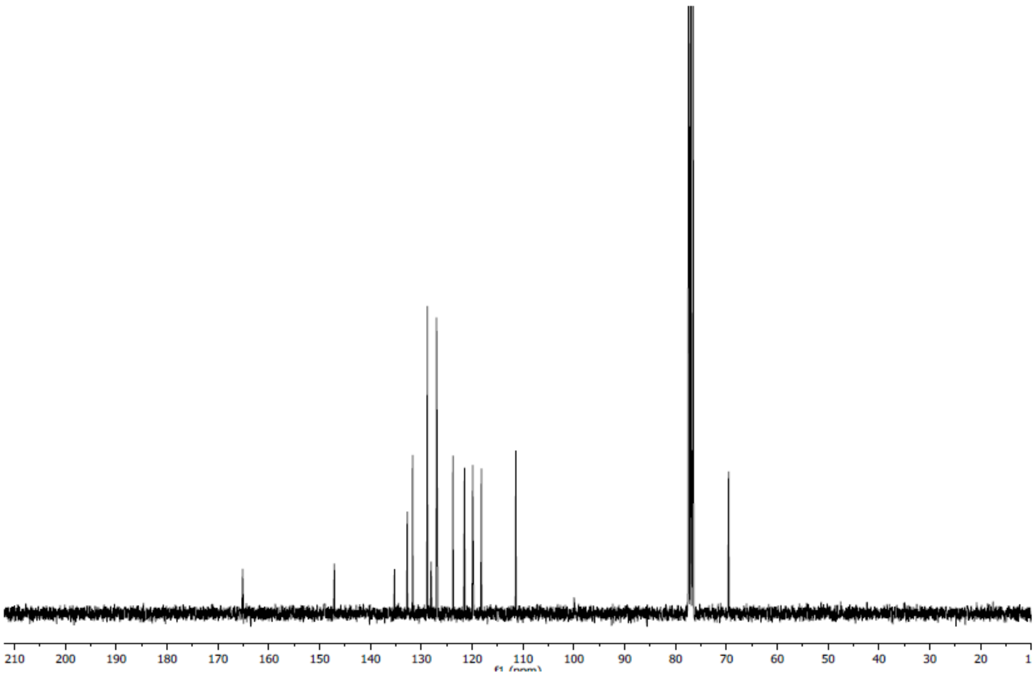
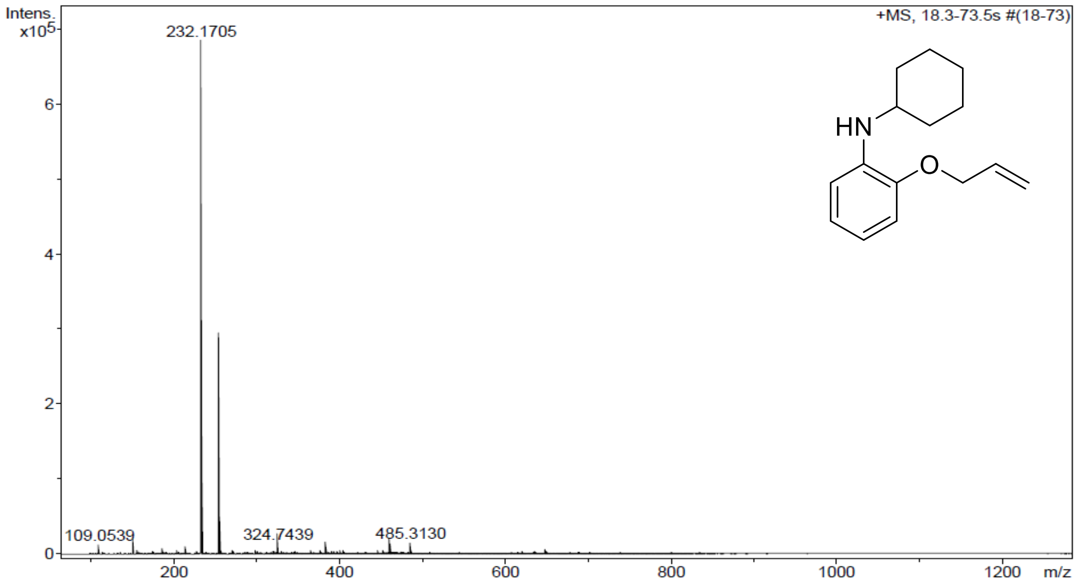
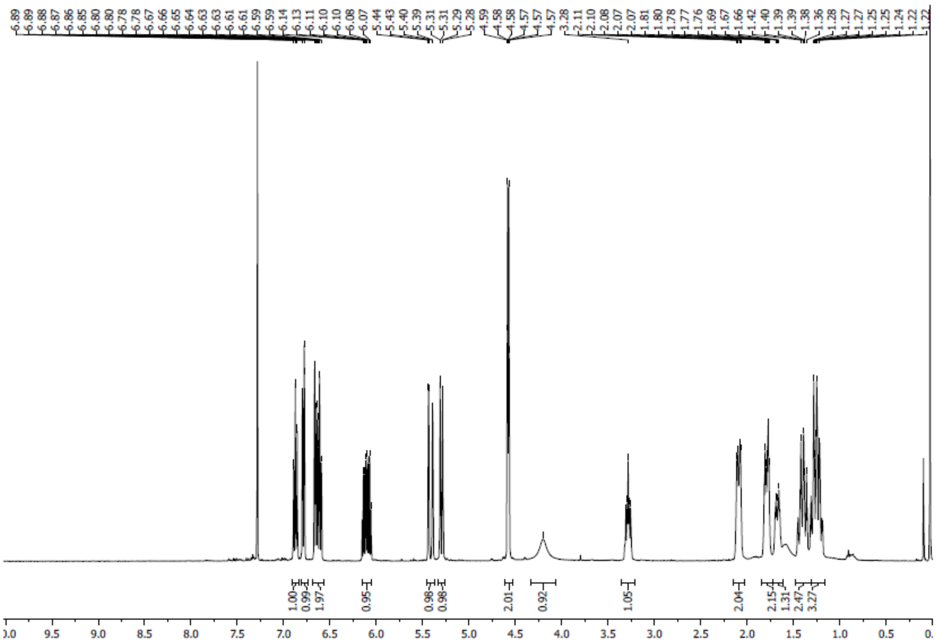


Figure S12. 2-(allyloxy)-N-cyclohexylaniline (rc-4): a) HRMS (ESI-TOF) (*m/z*). b) ^{1}H-NMR spectrum (400 MHz, $CDCl_3$, 25 ºC). c) ^{13}C-NMR spectrum (100 MHz, $CDCl_3$, 25 ºC).

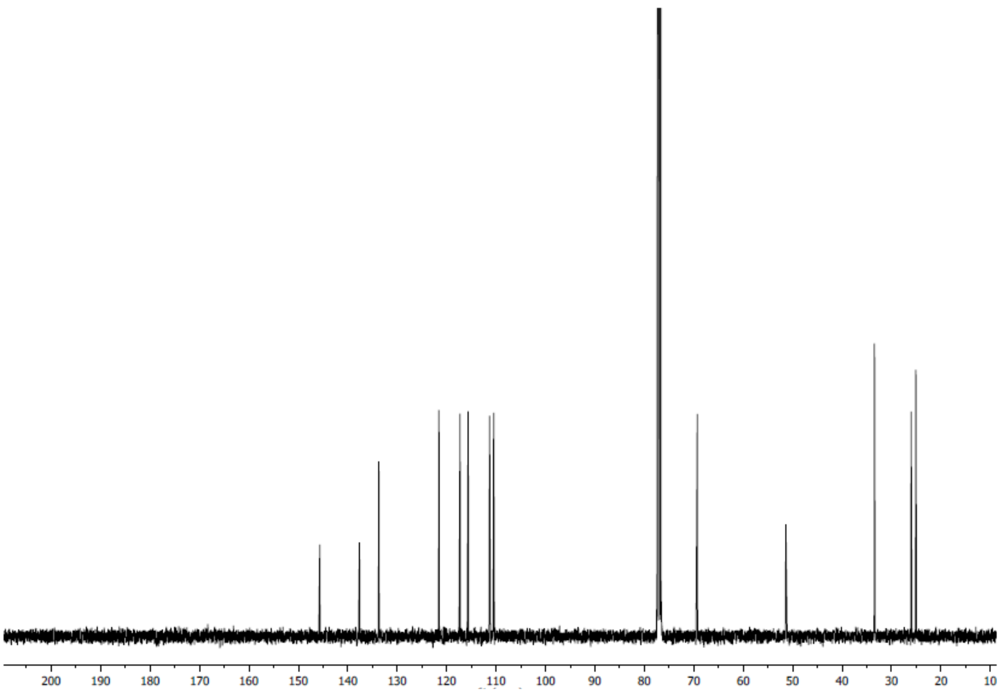
a)



b)



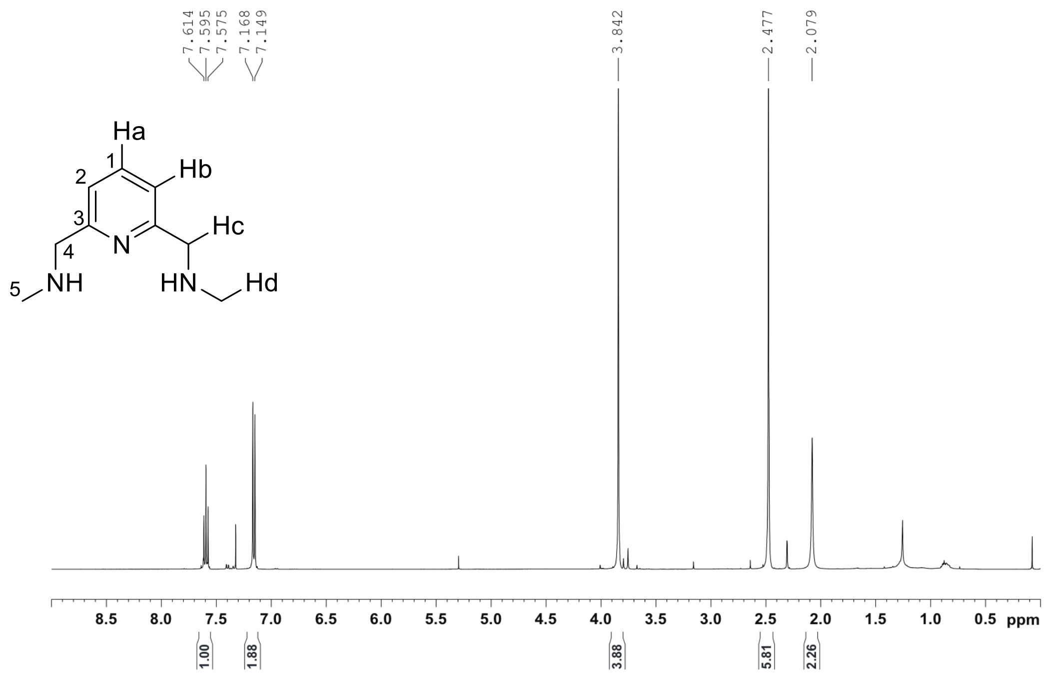
c)


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

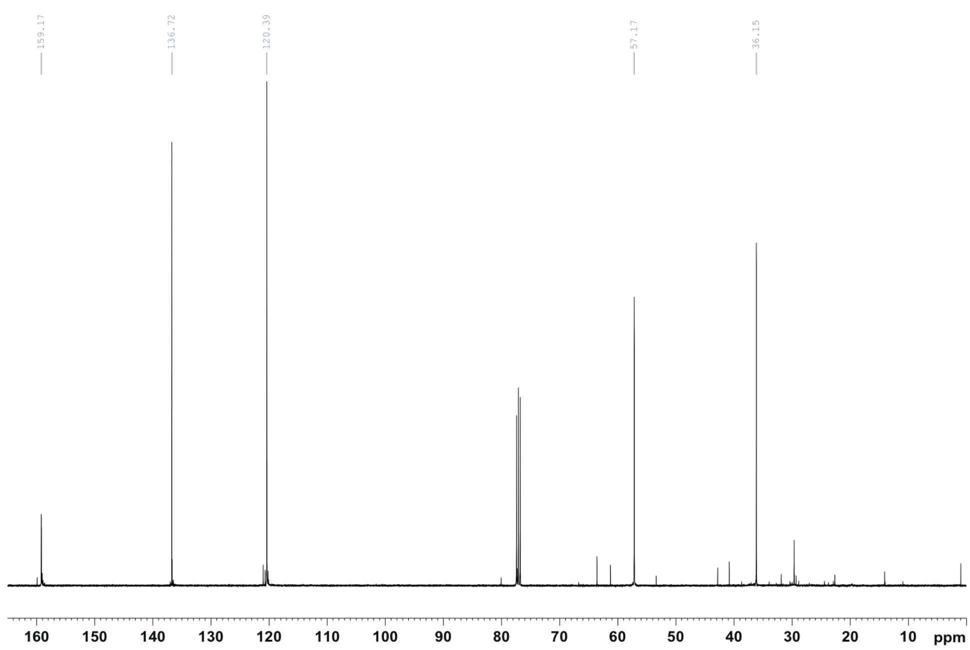
3.3. Supplementary Figures - Auxiliary ligands L_3, L_4, L_5 and L_3-C_6H_5

Figure S13. **L_3**: *N,N'*-dimethyl-2,6-bis(aminomethyl)pyridine; a) ^{1}H-NMR spectrum (400 MHz, $CDCl_3$, 25 ºC), b) ^{13}C-NMR spectrum (100 MHz, $CDCl_3$, 25 ºC), c) HRMS (ESI-TOF (*m/z*).

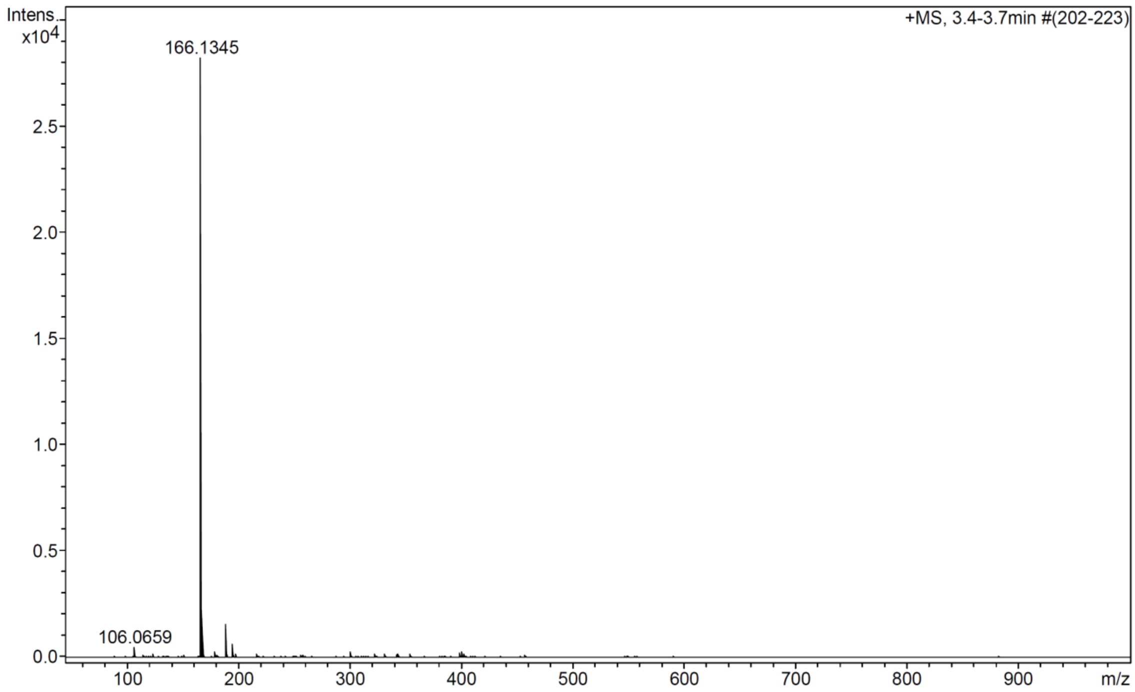
a)



b)



c)


Intens.
x10^4
+MS, 3.4-3.7min #(202-223)
166.1345
106.0659
2.5
2.0
1.5
1.0
0.5
0.0
100
200
300
400
500
600
700
800
900
m/z

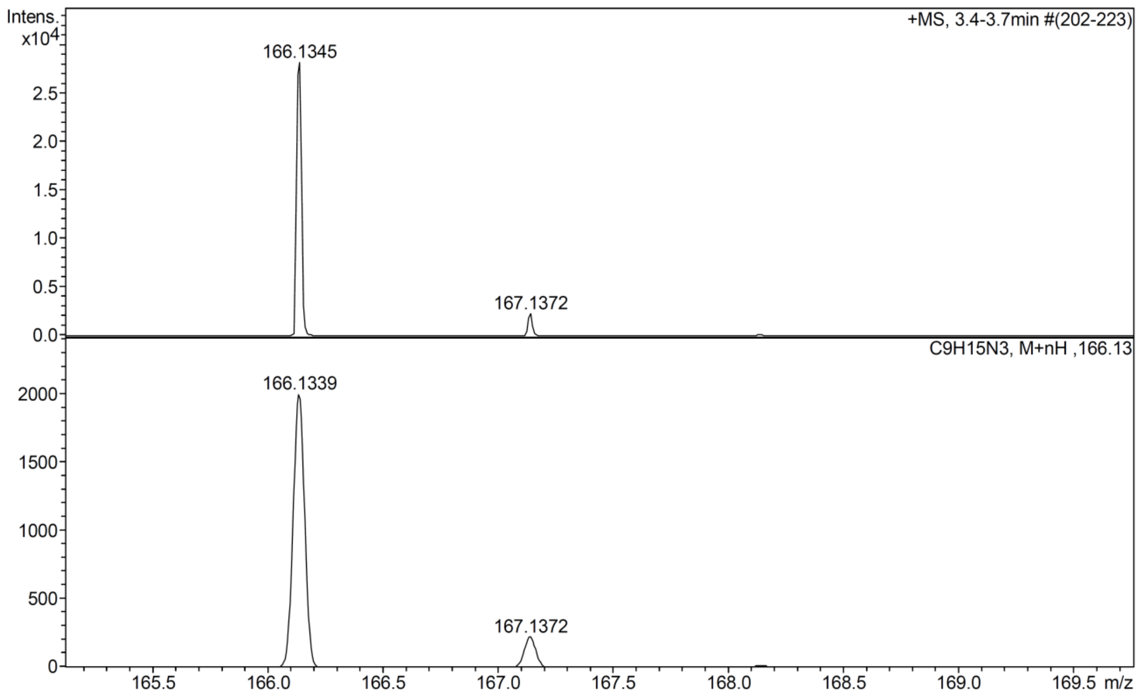
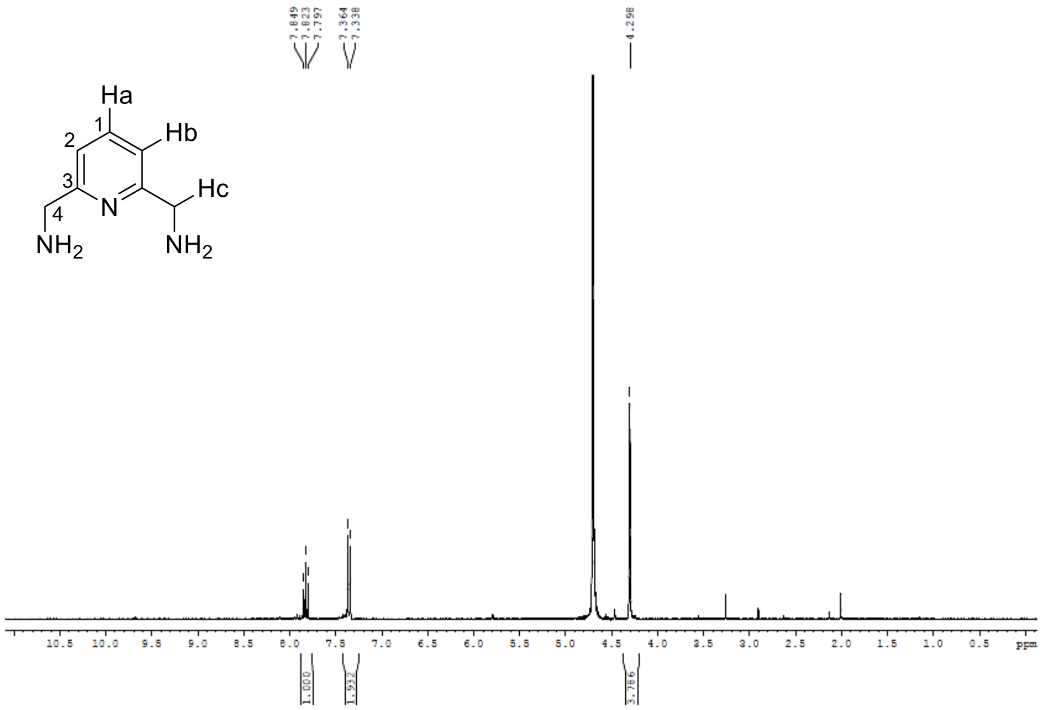
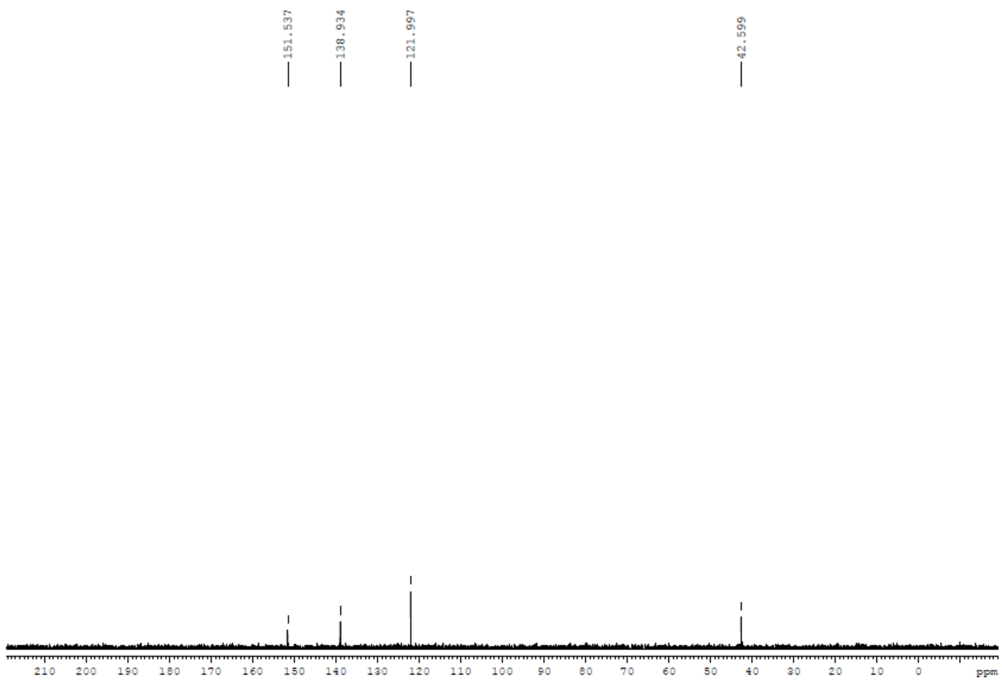

Intens.
x10^4
+MS, 3.4-3.7min #(202-223)
166.1345
167.1372
2.5
2.0
1.5
1.0
0.5
0.0
C9H15N3, M+nH ,166.13
166.1339
167.1372
2000
1500
1000
500
0
165.5
166.0
166.5
167.0
167.5
168.0
168.5
169.0
169.5
m/z

Figure S14. L$_4$: 2,6-pyridinediyldimethanamine; a) ^{1}H-NMR spectrum (300 MHz, D_2O, 25 ºC), b) ^{13}C-NMR spectrum (75 MHz, D_2O, 25 ºC), c) HRMS (ESI-TOF (*m/z*). Observed HRMS (top) with the theoretical isotope prediction (bottom).

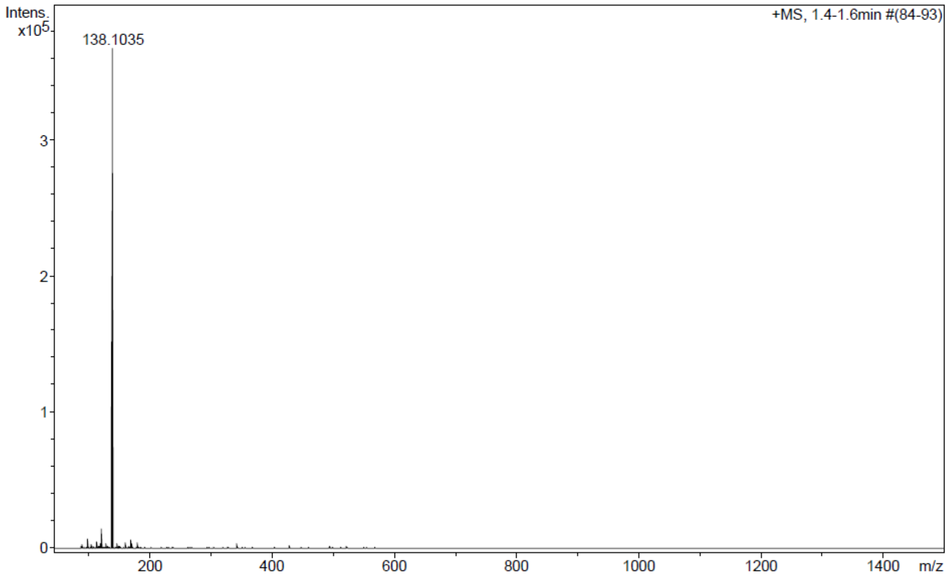
a)



b)



c)


Intens.
x10^5
+MS, 1.4-1.6min #(84-93)
138.1035
3
2
1
0
200
400
600
800
1000
1200
1400
m/z

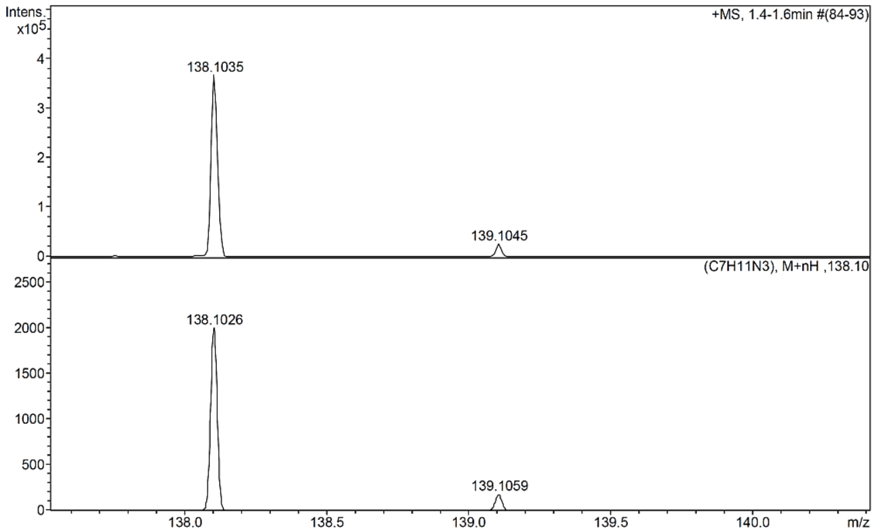
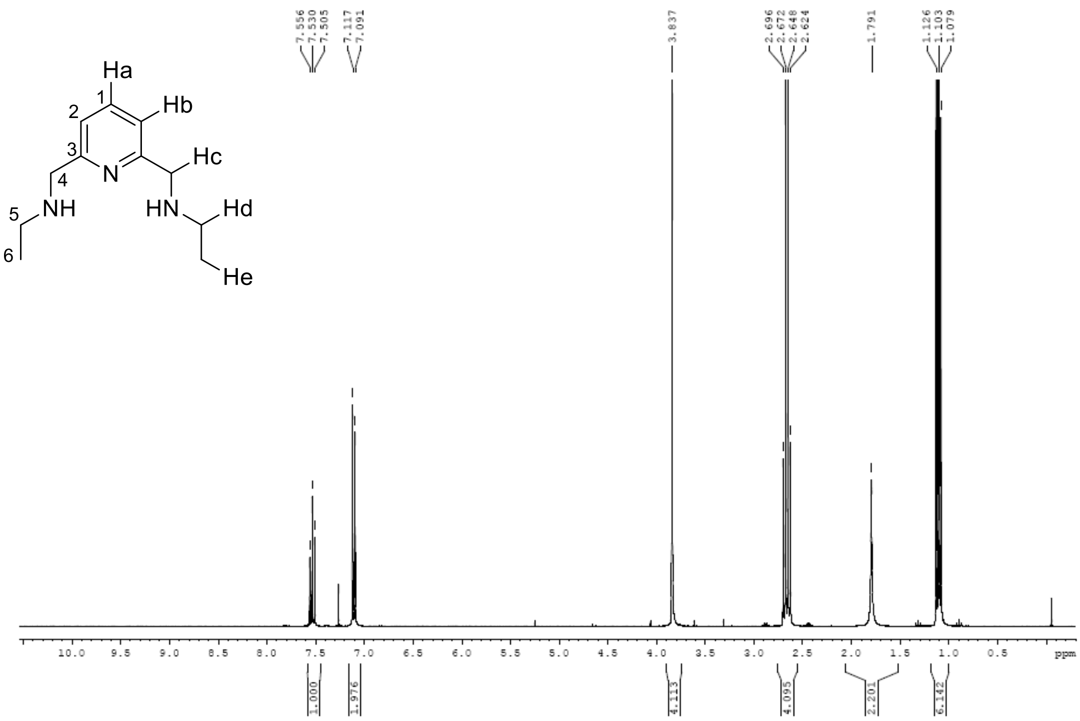
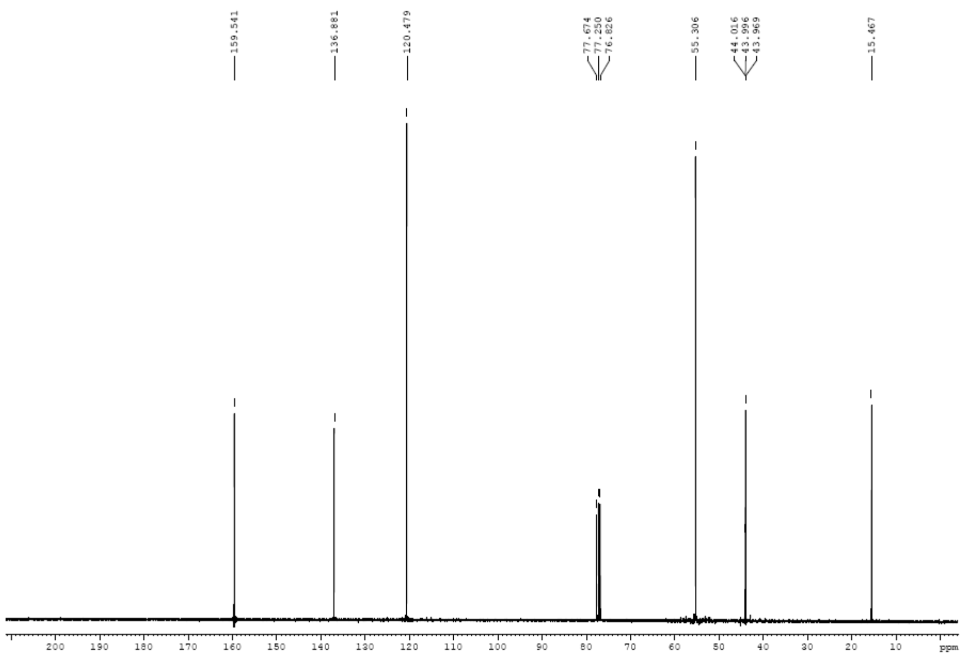

Intens.
x10^5
+MS, 1.4-1.6min #(84-93)
138.1035
139.1045
(C7H11N3), M+nH ,138.10
138.1026
139.1059
2500
2000
1500
1000
500
0
138.0
138.5
139.0
139.5
140.0
m/z

Figure S15. L$_5$: *N,N'*-diethyl-2,6-bis(aminomethylpyridine); a) ^{1}H-NMR spectrum (300 MHz, CDCl$_3$, 25 ºC), b) ^{13}C-NMR spectrum (75 MHz, CDCl$_3$, 25 ºC), c) HRMS (ESI-TOF) (*m/z*). Observed HRMS (top) with the theoretical isotope prediction (bottom).

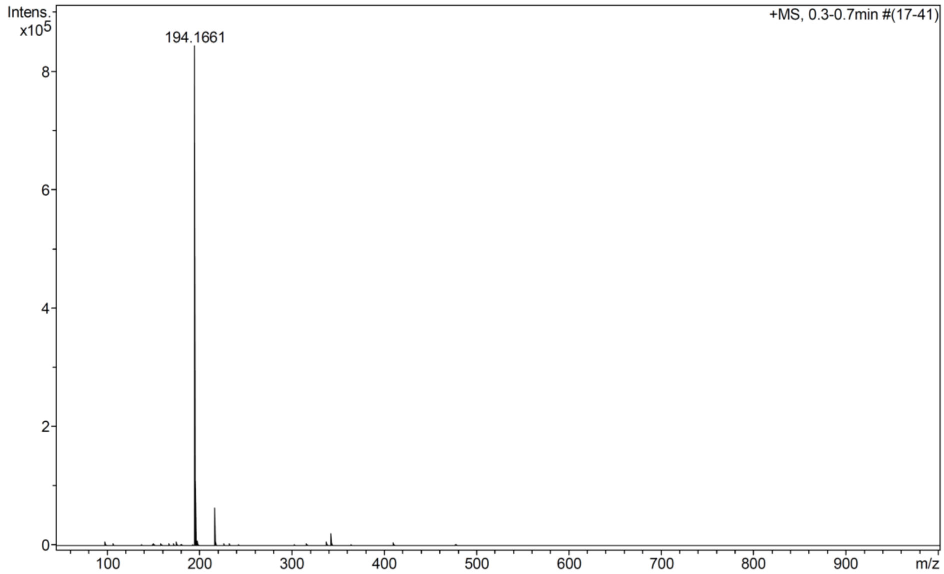
a)

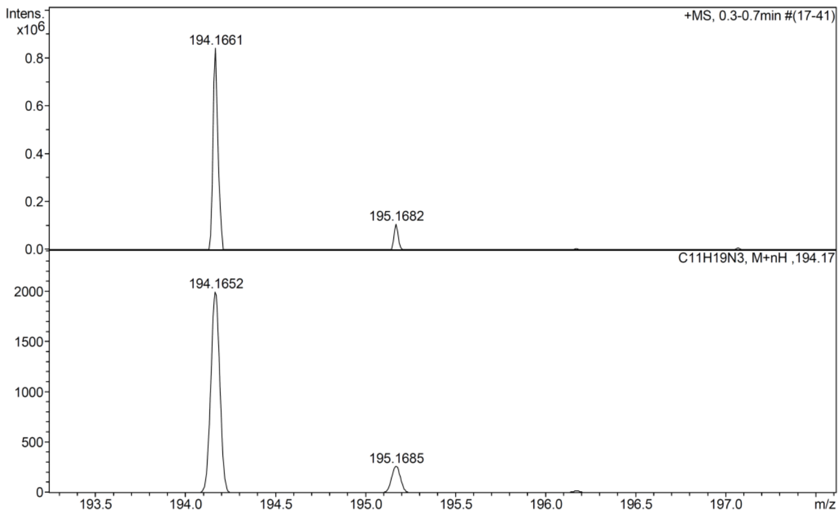


b)



c)


Intens.
x10^5
+MS, 0.3-0.7min #(17-41)
194.1661
m/z


Intens.
x10^6
+MS, 0.3-0.7min #(17-41)
194.1661
195.1682
C11H19N3, M+nH ,194.17
194.1652
195.1685
m/z

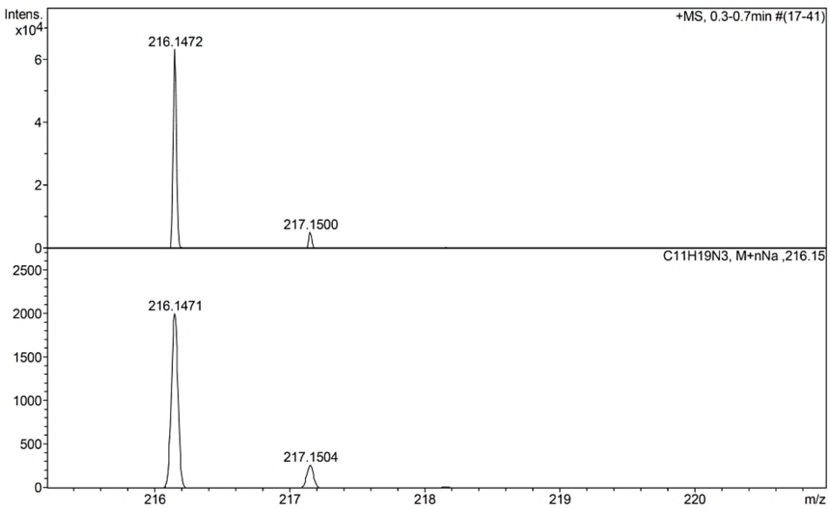
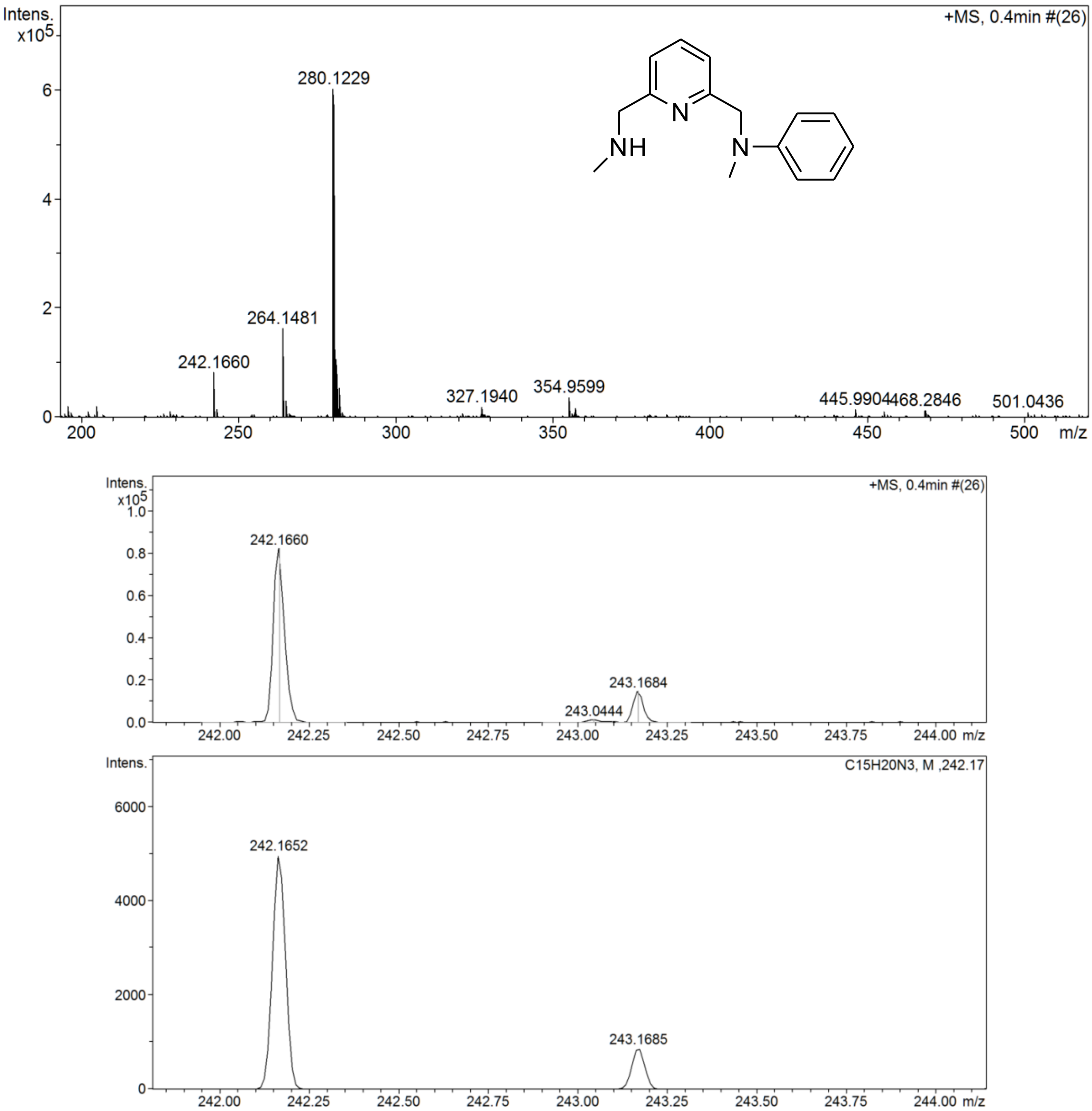
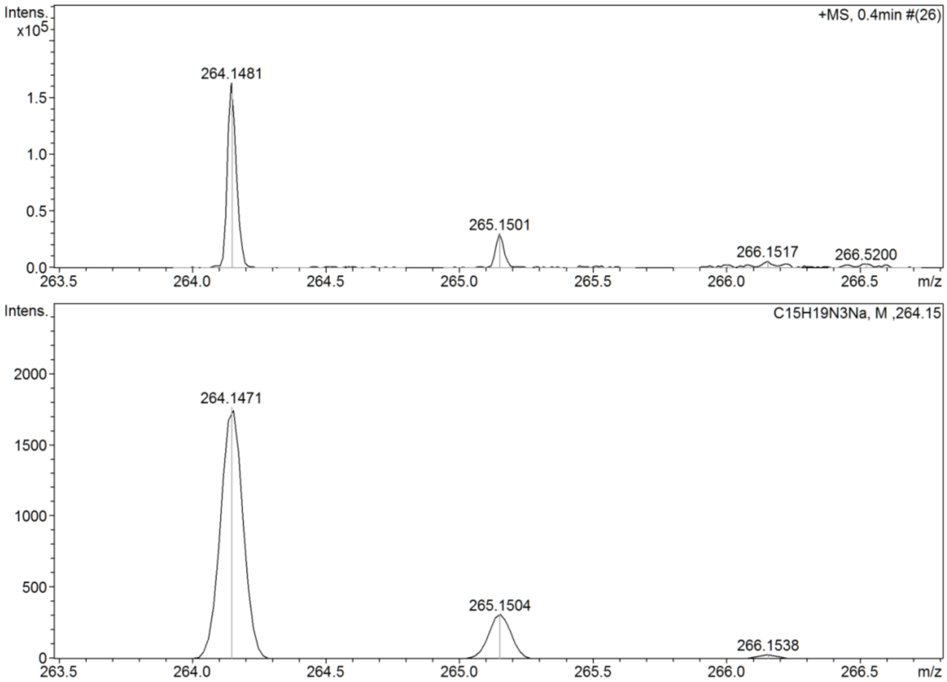
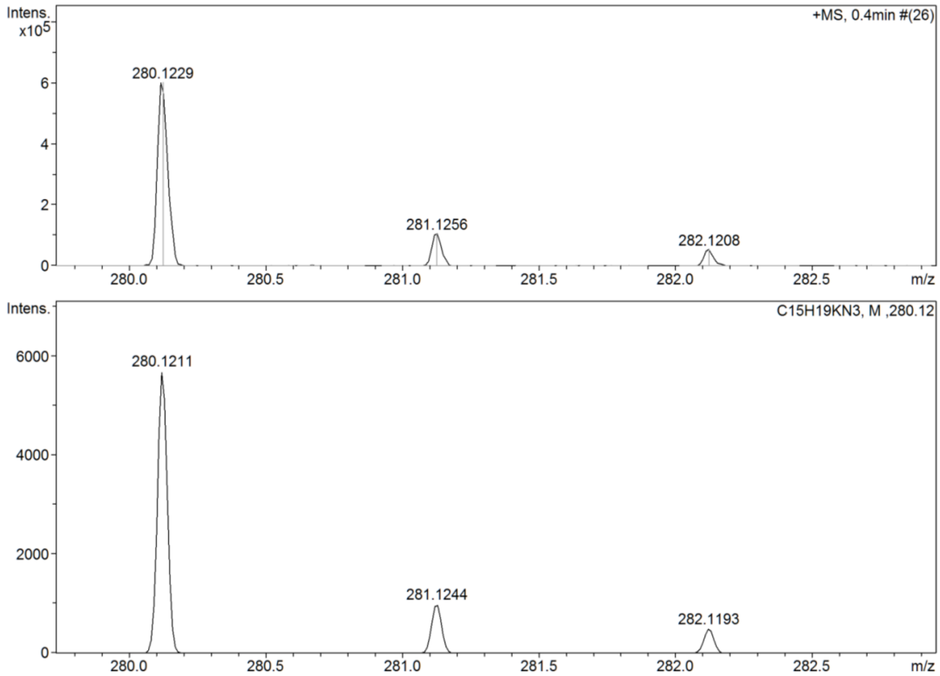

Intens.
x10^4
+MS, 0.3-0.7min #(17-41)
216.1472
217.1500
C11H19N3, M+nNa ,216.15
216.1471
217.1504
m/z

Figure S16. L_3-C_6H_5: *N*-methyl-*N*-((6-((methylamino)methyl)pyridin-2-yl)methyl)benzenamine: a) HRMS (ESI-TOF) (*m/z*). Observed HRMS (top) with the theoretical isotope prediction (bottom).

a)




Intens.
x10^5
+MS, 0.4min #(26)
264.1481
265.1501
266.1517
266.5200
m/z
C15H19N3Na, M ,264.15
264.1471
265.1504
266.1538


Intens.
x10^5
+MS, 0.4min #(26)
280.1229
281.1256
282.1208
m/z
C15H19KN3, M ,280.12
280.1211
281.1244
282.1193

3.4. Supplementary Figures - Crystal structures of L_3-containing compounds

Figure S17. Crystal structure of $\mathbf{L_3}$·2HCl (ellipsoid representation is at 50% probability). Crystal data: $P2_12_12_1$; a 9.439(5) b 10.181(5) c 13.024(7), α 90.00 β 90.00 γ 90.00, R-Factor (%) = 3.81; CCDC code:1054559.

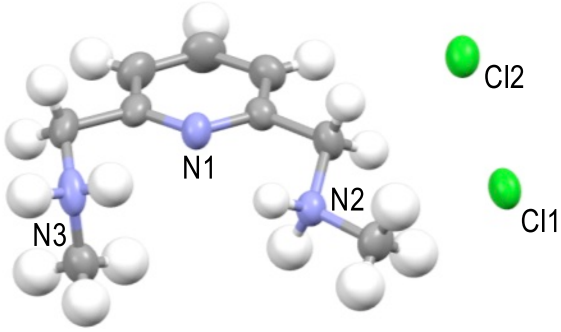


Figure S18. Crystal structure of $\mathbf{[(L_3)Cu^{I}(Br)]_n}$ (ellipsoid representation is at 50% probability). Crystal data: $P2_1/c$; a 9.533(12) b 15.50(2) c 8.885(11), α 90.00 β 113.710(19) γ 90.00, R-Factor (%) = 4.26; CCDC code: 1054555.

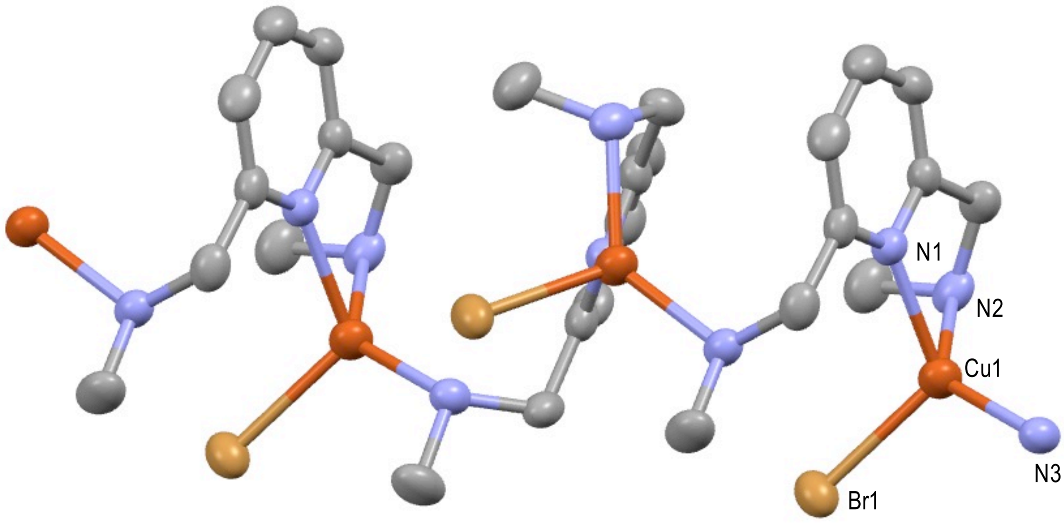
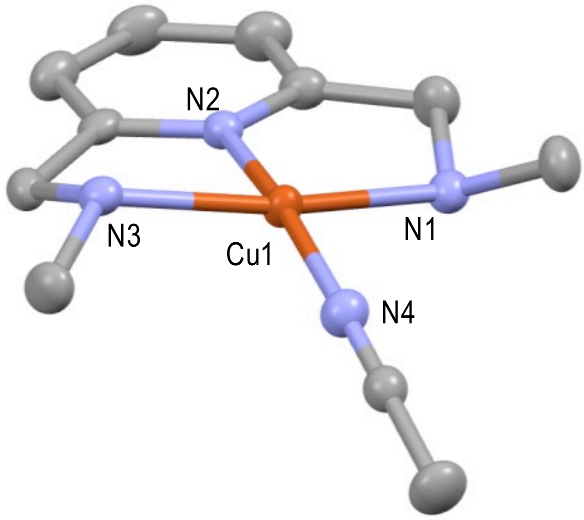
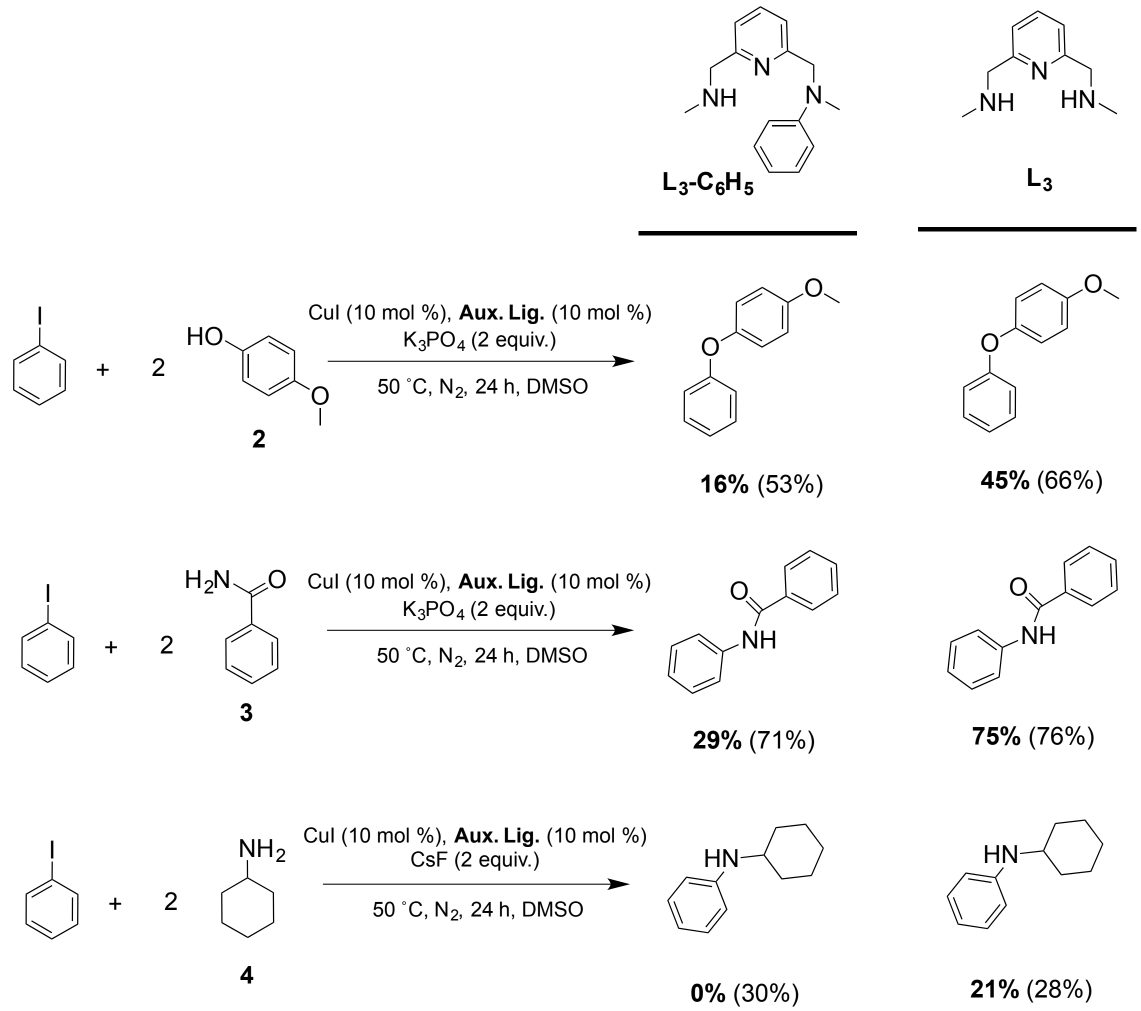


Figure S19. Crystal structure of **[L_3-Cu^{II}($OTf)_2$]** (ellipsoid representation is at 50% probability, H atoms and OTf anions have been omitted for clarity). Crystal data: P-1; a 8.1838(11) b 9.3740(14) c 14.364(2), α 98.975(2) β 94.759(2) γ 93.248(2), R-Factor (%) = 3.89; CCDC code: 1054556.



3.5. Coupling catalysis using $[(L_3\text{-}C_6H_5)\text{-}Cu^I]^+$ as catalyst

Figure S20. Cross coupling catalysis using independently synthesized **L_3-C_6H_5** auxiliary ligand and p-MeO-phenol, benzamide and cyclohexylamine, in comparison to the same reactions using **L_3**.



4. Supplementary Tables

Table S1. Optimized xyz cartesian coordinates of all the DFT optimized intermediates and transition states. The absolute free energy values (G) are in atomic units (hartrees). The imaginary frequencies (cm^{-1}) associated to the transition states are also tabulated.

A (G = -2721.725926)

29	5.042113000	-1.030337000	2.720792000
7	6.456836000	-2.065551000	3.851375000
6	7.108718000	-3.273750000	3.329027000
1	7.786266000	-3.736423000	4.061298000
1	7.680190000	-3.009019000	2.435682000
1	6.344659000	-4.005069000	3.050181000
7	4.383756000	-0.521689000	4.473744000
6	5.749563000	-2.335934000	5.134012000
1	6.438781000	-2.664537000	5.921273000
1	5.039142000	-3.150551000	4.943445000
7	4.462639000	0.935820000	2.238804000
6	5.021182000	-1.077724000	5.526061000
6	5.071819000	-0.448530000	6.763260000
1	5.593511000	-0.917448000	7.591386000
6	4.465881000	0.804138000	6.905554000
1	4.493002000	1.321344000	7.859500000
6	3.886506000	1.413614000	5.787206000
1	3.470873000	2.414753000	5.845988000
6	3.870955000	0.722257000	4.582661000
6	3.417176000	1.258956000	3.248158000
1	2.498517000	0.751890000	2.931342000
1	3.213046000	2.335657000	3.300058000
6	5.589388000	1.882005000	2.294503000
1	5.267003000	2.926826000	2.174086000
1	6.300885000	1.631358000	1.503482000
1	6.097071000	1.779742000	3.257677000
8	4.681887000	-2.095902000	1.048759000
16	3.384006000	-2.950254000	0.932537000
6	3.282204000	-3.880084000	2.483998000
1	4.073760000	-4.632672000	2.478582000
1	3.431063000	-3.170231000	3.304073000
1	2.303979000	-4.364597000	2.553188000
6	2.013664000	-1.810349000	1.264276000
1	2.004046000	-1.062807000	0.467333000
1	1.075257000	-2.372553000	1.261529000
1	2.182949000	-1.335781000	2.235285000
1	4.033070000	1.010236000	1.317346000
1	7.192261000	-1.385295000	4.067775000
53	8.742091000	0.708669000	5.113018000

B (G = -2411.563674)

29	5.938385000	-0.519404000	2.816712000
7	6.200795000	-2.369961000	3.935595000
6	4.965030000	-3.140085000	4.142246000
1	5.117312000	-4.008821000	4.798683000
1	4.598797000	-3.483286000	3.170891000
1	4.201310000	-2.494889000	4.584358000
7	5.601796000	0.035738000	4.801207000
6	6.826131000	-1.947313000	5.210667000
1	7.847714000	-1.622709000	4.983803000
1	6.880367000	-2.767508000	5.937334000
7	4.102885000	0.587805000	2.729236000
6	6.021365000	-0.792696000	5.762807000
6	5.627862000	-0.616993000	7.085560000
1	5.968901000	-1.297838000	7.858589000
6	4.752700000	0.433750000	7.377726000
1	4.421485000	0.595424000	8.399133000
6	4.248416000	1.228158000	6.346397000
1	3.504723000	1.994513000	6.537901000
6	4.693565000	0.982638000	5.048610000
6	4.154818000	1.621542000	3.793275000
1	3.166241000	2.059182000	3.978722000
1	4.818725000	2.420273000	3.446432000
6	3.621107000	1.154765000	1.463011000
1	2.631655000	1.620257000	1.572992000
1	3.558663000	0.360538000	0.715649000
1	4.327120000	1.911644000	1.112731000
1	3.404143000	-0.096179000	3.037321000
6	7.018627000	0.311220000	1.354507000
6	7.758067000	-0.770406000	1.918737000
6	6.443321000	0.176623000	0.060951000
6	7.873772000	-1.973804000	1.170571000
1	8.450333000	-0.594390000	2.735967000
6	6.524313000	-1.031227000	-0.603559000
1	5.936943000	1.019819000	-0.393656000
6	7.245729000	-2.114149000	-0.050020000
1	8.479589000	-2.780545000	1.574441000
1	6.055584000	-1.134654000	-1.578093000
1	7.337664000	-3.041222000	-0.608025000
53	1.171289000	-1.049146000	4.488731000
53	7.519967000	2.325956000	1.990155000
1	6.866916000	-2.959324000	3.440207000

C (G = -2411.561193) (93.72i cm^{-1})

29	5.896325000	-0.237538000	2.990580000
7	6.335194000	-2.160586000	3.899580000
6	5.170965000	-3.057033000	3.859687000
1	5.335998000	-3.983652000	4.428311000
1	4.957297000	-3.307486000	2.817124000
1	4.298788000	-2.542280000	4.271989000
7	5.453475000	0.110651000	4.926125000
6	6.763629000	-1.841838000	5.278471000
1	7.785917000	-1.449768000	5.221457000
1	6.775442000	-2.726600000	5.927602000
7	4.070753000	0.909479000	2.822842000
6	5.848866000	-0.777875000	5.844642000
6	5.391718000	-0.699974000	7.156245000
1	5.712968000	-1.425832000	7.895891000
6	4.492284000	0.319038000	7.482376000
1	4.114512000	0.404046000	8.496796000
6	4.038757000	1.195405000	6.494312000
1	3.295885000	1.955129000	6.712760000
6	4.540408000	1.048250000	5.203816000
6	4.097330000	1.825006000	3.988650000
1	3.117828000	2.286887000	4.163949000
1	4.812441000	2.625843000	3.766112000
6	3.623021000	1.600454000	1.607418000
1	2.681764000	2.145447000	1.767130000
1	3.468072000	0.862992000	0.816586000
1	4.389489000	2.309898000	1.284806000
1	3.365930000	0.197203000	3.040590000
6	7.032288000	-0.108926000	1.384567000
6	8.093152000	-0.997253000	1.670268000
6	6.239029000	-0.316521000	0.235651000
6	8.220802000	-2.174086000	0.933559000
1	8.773667000	-0.784019000	2.487075000
6	6.378490000	-1.499581000	-0.484573000
1	5.499229000	0.417690000	-0.057141000
6	7.360693000	-2.435763000	-0.136502000
1	9.009723000	-2.876757000	1.187531000
1	5.727925000	-1.682875000	-1.335288000
1	7.474217000	-3.346520000	-0.716633000
53	1.278687000	-1.150921000	4.309478000
53	7.490095000	2.057907000	1.945472000
1	7.111350000	-2.614902000	3.422979000

D (G = -2411.580401)

29	0.692510000	-0.381369000	0.032186000
7	1.397517000	-1.967282000	0.912042000
6	0.476781000	-3.112594000	0.699604000
1	0.839093000	-3.979235000	1.260280000
1	0.439833000	-3.346682000	-0.363366000
1	-0.520932000	-2.836161000	1.044196000
7	0.097391000	0.094234000	1.755715000
6	1.562898000	-1.642695000	2.370370000
1	2.534668000	-1.152263000	2.485336000
1	1.560706000	-2.561157000	2.961941000
7	-0.574163000	0.964305000	-0.585614000
6	0.485283000	-0.677961000	2.779844000
6	-0.061366000	-0.469105000	4.038116000
1	0.235878000	-1.084205000	4.879599000
6	-1.005565000	0.554332000	4.181594000
1	-1.455266000	0.733361000	5.153004000
6	-1.380804000	1.347407000	3.093878000
1	-2.110271000	2.142169000	3.199608000
6	-0.796509000	1.083051000	1.860591000
6	-0.970181000	1.833780000	0.572754000
1	-1.992541000	2.191340000	0.426245000
1	-0.296922000	2.697031000	0.578257000
6	-0.274388000	1.784158000	-1.779813000
1	-1.087800000	2.497358000	-1.947958000
1	-0.176114000	1.132242000	-2.646186000
1	0.660863000	2.321972000	-1.614479000
1	-1.383175000	0.360236000	-0.790953000
6	1.140652000	-1.004805000	-1.686615000
6	2.433908000	-0.836015000	-2.167246000
6	0.152874000	-1.638535000	-2.435321000
6	2.742728000	-1.312723000	-3.447992000
1	3.194317000	-0.343991000	-1.569197000
6	0.474386000	-2.110799000	-3.713153000
1	-0.852897000	-1.763794000	-2.043345000
6	1.766291000	-1.946848000	-4.217849000
1	3.750283000	-1.186770000	-3.835393000
1	-0.288916000	-2.604649000	-4.308483000
1	2.012042000	-2.314855000	-5.209944000
53	-3.329540000	-1.348497000	0.083543000
53	3.147871000	1.831175000	0.763323000
1	2.315224000	-2.206344000	0.532693000

E (G = -2399.483362)

29	0.538622000	-0.471750000	0.013699000
7	1.219633000	-2.103940000	0.898453000
6	0.226287000	-3.180158000	0.677299000
1	0.540474000	-4.099138000	1.182306000
1	0.133341000	-3.361434000	-0.394218000
1	-0.740374000	-2.860097000	1.073004000
7	0.090909000	0.033604000	1.770591000
6	1.432124000	-1.819470000	2.353489000
1	2.452778000	-1.439844000	2.466482000
1	1.336343000	-2.733917000	2.945464000
7	-0.648757000	0.864697000	-0.525822000
6	0.472983000	-0.744568000	2.791256000
6	0.039565000	-0.444705000	4.075488000
1	0.332717000	-1.061222000	4.917769000
6	-0.781438000	0.676962000	4.246474000
1	-1.138551000	0.929460000	5.240063000
6	-1.145259000	1.477760000	3.160238000
1	-1.772018000	2.352634000	3.291453000
6	-0.679437000	1.119788000	1.898682000
6	-0.825869000	1.823257000	0.583477000
1	-1.803259000	2.316204000	0.484808000
1	-0.068705000	2.629269000	0.566141000
6	-0.486496000	1.611287000	-1.765169000
1	-1.340055000	2.297240000	-1.881931000
1	-0.476116000	0.936260000	-2.621830000
1	0.429035000	2.226636000	-1.795268000
6	1.104104000	-0.957252000	-1.712772000
6	2.427760000	-0.737091000	-2.097728000
6	0.230142000	-1.625124000	-2.573045000
6	2.874543000	-1.181191000	-3.348576000
1	3.115849000	-0.220909000	-1.433284000
6	0.678468000	-2.071380000	-3.820748000
1	-0.806071000	-1.789494000	-2.285748000
6	2.001770000	-1.848351000	-4.210099000
1	3.905925000	-1.005313000	-3.644666000
-1	-0.006821000	-2.589168000	-4.487308000
1	2.349909000	-2.192338000	-5.180343000
53	3.400505000	1.699456000	1.154423000
1	2.110153000	-2.395547000	0.495269000

F (G = -2399.466612) (239.14i cm^{-1})

29	1.771821000	-0.053295000	0.389237000
7	2.019045000	-1.882649000	1.377633000
6	1.393731000	-3.014224000	0.668494000
1	1.508512000	-3.951717000	1.226675000
1	1.855518000	-3.117780000	-0.315976000
1	0.328941000	-2.811021000	0.532061000
7	0.349886000	0.129758000	1.833561000
6	1.471961000	-1.721081000	2.760727000
1	2.236327000	-1.205431000	3.351557000
1	1.276674000	-2.694144000	3.224002000
7	0.990100000	1.517036000	-0.266951000
6	0.218597000	-0.870634000	2.707137000
6	-0.984688000	-1.066678000	3.373250000
1	-1.108124000	-1.877798000	4.083259000
6	-2.044888000	-0.200137000	3.069831000
1	-2.999925000	-0.325407000	3.571316000
6	-1.904692000	0.781983000	2.087159000
1	-2.742759000	1.407733000	1.797122000
6	-0.663453000	0.907017000	1.458713000
6	-0.355536000	1.770950000	0.247928000
1	-1.139442000	1.599900000	-0.509396000
1	-0.409414000	2.837707000	0.508542000
6	1.352700000	2.421525000	-1.341424000
1	0.686725000	2.362378000	-2.217118000
1	2.376759000	2.226677000	-1.663427000
1	1.315042000	3.448831000	-0.952301000
6	0.944609000	-0.271711000	-1.314003000
6	1.830463000	-0.369972000	-2.392954000
6	-0.327139000	-0.844796000	-1.397617000
6	1.463621000	-1.097715000	-3.527165000
1	2.806979000	0.101861000	-2.347560000
6	-0.690227000	-1.564041000	-2.540170000
1	-1.033222000	-0.761763000	-0.577812000
6	0.202246000	-1.695087000	-3.605900000
1	2.166918000	-1.192782000	-4.350316000
1	-1.675807000	-2.019170000	-2.591729000
1	-0.084538000	-2.250699000	-4.494059000
53	4.799007000	0.717881000	0.729445000
1	3.017154000	-2.071501000	1.463675000

G (G = -2399.532354)

29	1.640688000	-0.663334000	-0.000938000
7	1.936303000	-2.358851000	1.098677000
6	1.097753000	-3.425210000	0.519444000
1	1.142468000	-4.348583000	1.112171000
1	1.434156000	-3.628288000	-0.499884000
1	0.061077000	-3.081141000	0.479385000
7	0.356206000	-0.164623000	1.419254000
6	1.534777000	-2.002892000	2.474403000
1	2.402703000	-1.536646000	2.954115000
1	1.261701000	-2.887478000	3.062536000
7	0.505008000	1.616046000	-0.787720000
6	0.397715000	-1.001834000	2.477348000
6	-0.513287000	-0.901287000	3.519629000
1	-0.467981000	-1.595064000	4.352513000
6	-1.476366000	0.108684000	3.466908000
1	-2.200911000	0.216067000	4.268400000
6	-1.500433000	0.974626000	2.379261000
1	-2.236071000	1.769960000	2.312159000
6	-0.561026000	0.810288000	1.357247000
6	-0.596852000	1.743777000	0.160785000
1	-1.584571000	1.638948000	-0.322443000
1	-0.569021000	2.769562000	0.544251000

6	0.456932000	2.689774000	-1.784783000
1	-0.463821000	2.657097000	-2.392580000
1	1.316433000	2.602070000	-2.453255000
1	0.505826000	3.658808000	-1.278400000
6	0.652547000	0.320143000	-1.400912000
6	1.933283000	-0.050272000	-1.926426000
6	-0.478262000	-0.457190000	-1.802618000
6	2.039154000	-1.139422000	-2.826711000
1	2.758902000	0.650683000	-1.839561000
6	-0.330855000	-1.549785000	-2.636549000
1	-1.464792000	-0.192969000	-1.436718000
6	0.931536000	-1.897117000	-3.163354000
1	3.012377000	-1.371663000	-3.250869000
1	-1.206505000	-2.133617000	-2.908147000
1	1.026323000	-2.742699000	-3.837875000
53	4.424302000	0.639879000	1.285124000
1	2.902175000	-2.679943000	1.125680000

DMSO (G = -553.273805)

16	0.249917000	1.197848000	-0.026023000
8	1.757492000	1.148847000	0.192050000
6	-0.263042000	2.947926000	0.032775000
1	-1.328568000	3.019485000	-0.206047000
1	-0.090701000	3.307156000	1.050913000
1	0.332194000	3.532629000	-0.675476000
6	-0.058673000	0.963695000	-1.808878000
1	0.228986000	-0.060385000	-2.062473000
1	-1.123997000	1.108209000	-2.013578000
1	0.544606000	1.674030000	-2.382717000

PhI (G = -243.118314)

6	-2.434710000	-0.213805000	0.000077000
6	-1.038727000	-0.216237000	0.000535000
6	-0.342712000	0.993856000	-0.000035000
6	-1.033558000	2.208738000	-0.001050000
6	-2.428313000	2.190685000	-0.001499000
6	-3.141356000	0.991836000	-0.000947000
1	-2.984225000	-1.150993000	0.000508000
1	-0.495784000	-1.156738000	0.001308000
1	0.743735000	1.000861000	0.000309000
1	-0.490737000	3.147664000	-0.001492000
1	-4.225952000	0.991042000	-0.001308000
53	-3.495981000	4.040052000	-0.003184000

K_3PO_4 (G = -2442.607734)

15	0.186240000	0.654919000	0.103346000
8	-1.062405000	-0.242437000	0.125146000
8	0.397984000	1.366553000	-1.309870000
8	0.111738000	1.820275000	1.191048000
8	1.524572000	-0.161021000	0.404648000
19	2.602149000	0.257729000	-1.836299000
19	2.089792000	1.042727000	2.547519000
19	0.114848000	3.726270000	-0.460641000

K_2HPO_4 (G = -1843.207589)

15	0.453297000	0.245282000	-0.422746000
8	-0.981445000	-0.142792000	-0.895537000
8	1.124697000	1.236449000	-1.390033000
8	0.154282000	1.084025000	1.008378000
8	1.285081000	-0.995967000	-0.054537000
1	1.013537000	1.391198000	1.342960000
19	-0.575686000	-2.672527000	-0.603827000
19	-0.860413000	1.325656000	-3.010021000

KI (G = -611.503901)

19	-0.008069000	1.075085000	0.000000000
53	-3.368996000	1.075085000	0.000000000

H (G = -2821.569347)

29	0.463872000	-0.088820000	-0.415295000
7	1.191938000	-1.736241000	0.370584000
6	0.202623000	-2.834397000	0.405280000
1	0.633208000	-3.716772000	0.890376000
1	-0.078959000	-3.076589000	-0.621039000
1	-0.685129000	-2.512230000	0.952096000
7	-0.101937000	0.190105000	1.463318000
6	1.690023000	-1.332902000	1.720223000
1	2.611283000	-0.761493000	1.568195000
1	1.922253000	-2.216183000	2.322841000
7	-1.964490000	0.376405000	-0.418478000
6	0.637637000	-0.471508000	2.366112000
6	0.373897000	-0.359291000	3.724907000
1	0.971443000	-0.901147000	4.449566000
6	-0.696808000	0.447796000	4.118386000
1	-0.932332000	0.557368000	5.172414000
6	-1.500505000	1.063180000	3.158285000
1	-2.377840000	1.634022000	3.442058000
6	-1.183523000	0.897963000	1.812053000
6	-2.009907000	1.386525000	0.650931000
1	-3.031300000	1.611042000	0.988720000
1	-1.574645000	2.308029000	0.251472000
6	-2.574570000	0.857929000	-1.657098000
1	-3.599951000	1.236119000	-1.516899000
1	-2.604734000	0.040240000	-2.382696000
1	-1.957075000	1.662267000	-2.066705000
1	-2.481036000	-0.441196000	-0.088532000
6	1.111218000	-0.598458000	-2.103459000
6	2.440097000	-0.401024000	-2.460400000
6	0.219112000	-1.245389000	-2.954020000
6	2.885563000	-0.853290000	-3.708034000
1	3.129245000	0.104085000	-1.789052000
6	0.670999000	-1.688256000	-4.203842000
1	-0.815031000	-1.407921000	-2.664415000
6	2.001028000	-1.491783000	-4.580244000
1	3.923972000	-0.704387000	-3.992617000
1	-0.021941000	-2.184973000	-4.878016000
1	2.348526000	-1.838055000	-5.549640000
53	-3.799280000	-2.148763000	1.847585000
1	1.993056000	-2.039269000	-0.183252000
6	1.669673000	2.277715000	-1.045469000
6	2.590284000	2.217610000	0.026924000
6	2.042665000	3.011636000	-2.185058000
6	3.819367000	2.858067000	-0.047774000
1	2.327980000	1.650339000	0.916066000
6	3.268416000	3.675174000	-2.258695000
1	1.350481000	3.058157000	-3.020932000
6	4.170343000	3.596983000	-1.189330000
1	4.525299000	2.802828000	0.775969000
1	3.512862000	4.235825000	-3.153662000
8	0.467831000	1.694550000	-0.982876000
8	5.399196000	4.191547000	-1.163110000
6	5.781908000	4.964301000	-2.296214000
1	5.091951000	5.800782000	-2.464661000
1	6.775472000	5.356981000	-2.071187000
1	5.833862000	4.350601000	-3.204428000

I (G = -2821.555570)

29	5.798362000	0.254574000	2.859951000
7	6.801962000	-1.319440000	3.650970000
6	5.955184000	-2.526066000	3.710425000
1	6.488120000	-3.368220000	4.168860000
1	5.657740000	-2.792030000	2.692975000
1	5.055000000	-2.310626000	4.291229000
7	5.464732000	0.606181000	4.811889000
6	7.301257000	-0.890905000	4.982981000
1	8.181832000	-0.261668000	4.813314000
1	7.605476000	-1.747343000	5.594681000
7	3.587205000	0.870110000	2.965890000
6	6.226538000	-0.082282000	5.671030000
6	5.981234000	-0.030378000	7.038870000
1	6.596089000	-0.594775000	7.731823000

6	4.909665000	0.747554000	7.485759000
1	4.690011000	0.805941000	8.547429000
6	4.091145000	1.409586000	6.568271000
1	3.222430000	1.972618000	6.891928000
6	4.396496000	1.301853000	5.214380000
6	3.587445000	1.855479000	4.069317000
1	2.572243000	2.107920000	4.402170000
1	4.051763000	2.776175000	3.694363000
6	2.850368000	1.378881000	1.804565000
1	1.863751000	1.782322000	2.077726000
1	2.699659000	0.564592000	1.091496000
1	3.433287000	2.167933000	1.322232000
1	3.097701000	0.042517000	3.316066000
6	6.484277000	0.110444000	1.071353000
6	7.849165000	-0.163387000	0.914659000
6	5.552476000	-0.337537000	0.128176000
6	8.259810000	-0.992670000	-0.129879000
1	8.575903000	0.244311000	1.610550000
6	5.981912000	-1.166105000	-0.909902000
1	4.510688000	-0.051951000	0.205380000
6	7.332441000	-1.502007000	-1.044319000
1	9.315163000	-1.233382000	-0.228438000
1	5.251973000	-1.536019000	-1.625355000
1	7.660847000	-2.136889000	-1.861633000
53	1.880413000	-1.820685000	5.081475000
1	7.606952000	-1.521763000	3.058437000
6	7.238300000	2.539377000	1.854132000
6	7.816379000	2.678758000	3.126441000
6	7.830487000	3.188495000	0.766175000
6	8.946879000	3.466415000	3.302395000
1	7.373497000	2.166688000	3.975010000
6	8.964989000	3.984220000	0.935894000
1	7.392175000	3.069491000	-0.220122000
6	9.531616000	4.125935000	2.209854000
1	9.395685000	3.580713000	4.284536000
1	9.397609000	4.479019000	0.074423000
8	6.105308000	1.807227000	1.655311000
8	10.639614000	4.870100000	2.486266000
6	11.280259000	5.533879000	1.399959000
1	10.611561000	6.260244000	0.922087000
1	12.133787000	6.060373000	1.831442000
1	11.638408000	4.820111000	0.647733000

J (G = -2821.607023)

29	5.856004000	0.104617000	2.040478000
7	6.564285000	-1.529328000	3.477544000
6	5.469899000	-2.100370000	4.267300000
1	5.822627000	-2.769150000	5.067883000
1	4.808947000	-2.662361000	3.601170000
1	4.886118000	-1.294058000	4.721990000
7	6.262690000	1.075517000	3.748132000
6	7.569027000	-0.837335000	4.301593000
1	8.473592000	-0.724965000	3.694132000
1	7.839264000	-1.402100000	5.204924000
7	4.114334000	1.282067000	2.263341000
6	7.048392000	0.531460000	4.682256000
6	7.287324000	1.190635000	5.884303000
1	7.932901000	0.747586000	6.635752000
6	6.654705000	2.417009000	6.104338000
1	6.822110000	2.956174000	7.031799000
6	5.758889000	2.918276000	5.158269000
1	5.198289000	3.829059000	5.339744000
6	5.577378000	2.200048000	3.979124000
6	4.592525000	2.538218000	2.887036000
1	3.764389000	3.134808000	3.289309000
1	5.083983000	3.128913000	2.106992000
6	3.226321000	1.546084000	1.125392000
1	2.363781000	2.166068000	1.407203000
1	2.863535000	0.594518000	0.728282000
1	3.783210000	2.064164000	0.338990000
1	3.563745000	0.797318000	2.979192000
6	7.216258000	-0.287315000	0.399068000
6	7.957397000	-1.483496000	0.538535000
6	5.823680000	-0.335971000	0.100684000
6	7.314954000	-2.707999000	0.483361000
1	9.031176000	-1.421364000	0.682775000
6	5.207008000	-1.615660000	-0.009192000
1	5.352428000	0.529099000	-0.356651000
6	5.929074000	-2.773605000	0.214907000
1	7.885631000	-3.623289000	0.610765000
1	4.158366000	-1.667644000	-0.287919000
1	5.440699000	-3.740753000	0.139987000
53	2.196684000	0.559138000	5.454586000
1	7.029449000	-2.272971000	2.962740000
6	8.220021000	1.745857000	1.129113000
6	9.174157000	1.403868000	2.091388000
6	7.593167000	2.985232000	1.178779000
6	9.439494000	2.275257000	3.139862000
1	9.689062000	0.451271000	2.029841000
6	7.865164000	3.872635000	2.223541000
1	6.874914000	3.249699000	0.409227000
6	8.770453000	3.506342000	3.226601000
1	10.155876000	2.012487000	3.911671000
1	7.350182000	4.824924000	2.255423000
8	7.915792000	0.884969000	0.081064000
8	9.069900000	4.271595000	4.312657000
6	8.356031000	5.494672000	4.474254000
1	7.274279000	5.323652000	4.515469000
1	8.692133000	5.915279000	5.423811000
1	8.582975000	6.200323000	3.665416000

K (G = -2809.460652)

29	0.634821000	-0.464290000	-0.499790000
7	1.876367000	-1.967399000	0.064771000
6	1.195945000	-3.274470000	-0.048602000
1	1.848344000	-4.082456000	0.301003000
1	0.926023000	-3.450215000	-1.089381000
1	0.287389000	-3.258138000	0.558654000
7	0.752464000	-0.013617000	1.334470000
6	2.392201000	-1.733364000	1.453717000
1	3.431580000	-1.402246000	1.386893000
1	2.379456000	-2.669581000	2.020165000
7	-0.966678000	0.544430000	-0.462828000
6	1.579320000	-0.675848000	2.147136000
6	1.653158000	-0.317013000	3.490765000
1	2.319943000	-0.843189000	4.165077000
6	0.853668000	0.737046000	3.936777000
1	0.891976000	1.034430000	4.980270000
6	0.003414000	1.414956000	3.055451000
1	-0.617066000	2.237427000	3.393839000
6	-0.024765000	1.003556000	1.728393000
6	-0.771357000	1.584745000	0.564154000
1	-1.746458000	1.994043000	0.865806000
1	-0.176944000	2.438177000	0.189052000
6	-1.513552000	1.175767000	-1.653494000
1	-2.436248000	1.713923000	-1.381864000
1	-1.769245000	0.427070000	-2.404681000
1	-0.838845000	1.916205000	-2.119267000
6	0.405570000	-1.012994000	-2.287527000
6	1.250720000	-0.527479000	-3.286062000
6	-0.575697000	-1.955527000	-2.605912000
6	1.123482000	-0.996761000	-4.599394000
1	1.994481000	0.217980000	-3.021499000
6	-0.701977000	-2.424680000	-3.917980000
1	-1.252105000	-2.326997000	-1.838935000
6	0.149646000	-1.945822000	-4.917430000
1	1.786405000	-0.617046000	-5.373817000
1	-1.467183000	-3.159105000	-4.158075000
1	0.051056000	-2.307945000	-5.937488000
1	2.682320000	-1.960079000	-0.561489000
8	2.253930000	1.096990000	-0.916343000
6	3.375095000	0.815681000	-0.317589000
6	4.325024000	-0.098136000	-0.859862000
6	3.729263000	1.377181000	0.948132000
6	5.493435000	-0.464954000	-0.182761000
1	4.114227000	-0.536682000	-1.833464000
6	4.890503000	1.016555000	1.621344000
1	3.041465000	2.087658000	1.401506000
6	5.782357000	0.082721000	1.072819000
1	6.167869000	-1.179708000	-0.643823000
1	5.122766000	1.446094000	2.593437000
8	6.899449000	-0.213150000	1.825997000
6	7.780951000	-1.194495000	1.306716000

1	8.580100000	-1.311454000	2.042781000
1	7.277560000	-2.161480000	1.167407000
1	8.220883000	-0.883285000	0.349154000

L (G = -2809.450865)

29	-0.573953000	0.327227000	-0.566906000
7	0.178778000	-1.117597000	0.759657000
6	0.046580000	-2.530191000	0.361328000
1	0.463308000	-3.192767000	1.129966000
1	0.574555000	-2.686822000	-0.580311000
1	-1.008462000	-2.772542000	0.217101000
7	-2.086618000	0.190635000	0.804519000
6	-0.441722000	-0.865099000	2.098298000
1	0.088391000	-0.017338000	2.544755000
1	-0.309896000	-1.731518000	2.754677000
7	-1.797052000	1.507134000	-1.376831000
6	-1.902339000	-0.509228000	1.920627000
6	-2.991605000	-0.831891000	2.722799000
1	-2.870748000	-1.407005000	3.634904000
6	-4.257439000	-0.400369000	2.299066000
1	-5.129746000	-0.632805000	2.902919000
6	-4.419102000	0.294009000	1.096392000
1	-5.403658000	0.592486000	0.750846000
6	-3.274271000	0.566759000	0.344184000
6	-3.179626000	1.146487000	-1.052075000
1	-3.605645000	0.403676000	-1.752555000
1	-3.805551000	2.045598000	-1.156699000
6	-1.701068000	1.942792000	-2.757285000
1	-2.109667000	1.229141000	-3.492000000
1	-0.656976000	2.142993000	-3.013529000
1	-2.260832000	2.885416000	-2.870236000
6	-0.756118000	-0.766894000	-2.094091000
6	0.271566000	-0.751382000	-3.040847000
6	-1.804832000	-1.676685000	-2.230073000
6	0.262082000	-1.662292000	-4.104030000
1	1.082937000	-0.031286000	-2.963126000
6	-1.818681000	-2.583457000	-3.295178000
1	-2.613960000	-1.700138000	-1.503956000
6	-0.783288000	-2.579462000	-4.232873000
1	1.070591000	-1.649746000	-4.831149000
1	-2.637918000	-3.292372000	-3.388750000
1	-0.793206000	-3.283691000	-5.060483000
1	1.175553000	-0.908896000	0.845079000
8	0.715242000	1.708159000	0.202750000
6	1.885080000	1.369585000	0.692385000
6	2.315223000	1.802872000	1.972789000
6	2.802006000	0.538106000	-0.016667000
6	3.557959000	1.450081000	2.507088000
1	1.645051000	2.436488000	2.549551000
6	4.037734000	0.181021000	0.514808000
1	2.515928000	0.178789000	-1.003434000
6	4.432227000	0.632512000	1.781087000
1	3.829753000	1.814550000	3.492408000
1	4.717962000	-0.454262000	-0.047355000
8	5.673530000	0.225533000	2.214227000
6	6.072224000	0.637913000	3.512258000
1	7.066523000	0.215364000	3.675456000
1	6.131069000	1.731766000	3.593188000
1	5.390552000	0.259467000	4.286149000

M (G = -2809.449926)

29	-0.457373000	0.377671000	-0.598863000
7	0.273341000	-1.097351000	0.735355000
6	0.237747000	-2.502461000	0.293268000
1	0.681824000	-3.162175000	1.049031000
1	0.791736000	-2.596422000	-0.642451000
1	-0.795934000	-2.806422000	0.118720000
7	-2.028947000	0.194607000	0.759174000
6	-0.416338000	-0.916803000	2.051085000
1	0.073578000	-0.079010000	2.558694000
1	-0.295113000	-1.808471000	2.674994000
7	-1.692303000	1.574570000	-1.392694000
6	-1.876780000	-0.580028000	1.828878000
6	-2.989578000	-0.987417000	2.557089000
1	-2.893146000	-1.625569000	3.429474000
6	-4.247517000	-0.556154000	2.109337000
1	-5.138633000	-0.851982000	2.655327000
6	-4.374794000	0.216845000	0.951798000
1	-5.351338000	0.513721000	0.582282000
6	-3.205045000	0.568885000	0.272362000
6	-3.083696000	1.239543000	-1.082476000
1	-3.542827000	0.566450000	-1.830590000
1	-3.675812000	2.167428000	-1.115904000
6	-1.577800000	2.027367000	-2.765211000
1	-1.994487000	1.331462000	-3.513099000
1	-0.527935000	2.210454000	-3.012130000
1	-2.117659000	2.982449000	-2.873579000
6	-0.866539000	-0.769131000	-2.038197000
6	0.086068000	-0.819776000	-3.060383000
6	-1.941655000	-1.657032000	-2.056302000
6	-0.021794000	-1.773118000	-4.079209000
1	0.914644000	-0.115271000	-3.075364000
6	-2.055372000	-2.605369000	-3.078939000
1	-2.694471000	-1.634953000	-1.272687000
6	-1.093837000	-2.668126000	-4.090011000
1	0.730330000	-1.809978000	-4.863711000
1	-2.894721000	-3.296709000	-3.080628000
1	-1.181956000	-3.405234000	-4.883616000
1	1.253430000	-0.845040000	0.873696000
8	0.765716000	1.751069000	0.174974000
6	1.927758000	1.411615000	0.692826000
6	2.312134000	1.820943000	1.993194000
6	2.872692000	0.610192000	-0.010264000
6	3.543241000	1.470533000	2.555496000
1	1.617173000	2.432144000	2.564383000
6	4.095855000	0.253224000	0.548754000
1	2.617727000	0.270659000	-1.012637000
6	4.447307000	0.679717000	1.836605000
1	3.781919000	1.815047000	3.556241000
1	4.799368000	-0.361216000	-0.007505000
8	5.678627000	0.276062000	2.296454000
6	6.041300000	0.671546000	3.610849000
1	7.035514000	0.256046000	3.790955000
1	6.086401000	1.764392000	3.710234000
1	5.344893000	0.273595000	4.361346000

N (G = -2809.452089)

29	1.508130000	0.583804000	0.362335000
7	2.122839000	-0.973446000	1.734077000
6	2.032200000	-2.352513000	1.234716000
1	2.384018000	-3.079079000	1.979434000
1	2.634377000	-2.444026000	0.327380000
1	0.994339000	-2.581362000	0.982888000
7	-0.185123000	0.342480000	1.590842000
6	1.348854000	-0.781158000	2.989605000
1	1.799235000	0.064162000	3.521110000
1	1.414121000	-1.662525000	3.638310000
7	0.210190000	1.566281000	-0.674041000
6	-0.093393000	-0.454008000	2.654852000
6	-1.241471000	-0.926772000	3.280836000
1	-1.181874000	-1.584920000	4.141768000
6	-2.479512000	-0.542759000	2.745787000
1	-3.396806000	-0.892657000	3.210269000
6	-2.544071000	0.244573000	1.594749000
1	-3.497602000	0.499363000	1.142592000
6	-1.340126000	0.665224000	1.021743000
6	-1.189072000	1.366530000	-0.316320000
1	-1.746741000	0.782432000	-1.072136000
1	-1.672046000	2.355269000	-0.283464000
6	0.349577000	2.218939000	-1.958830000
1	-0.115314000	1.669232000	-2.795888000
1	1.406230000	2.371084000	-2.190314000
1	-0.124916000	3.210579000	-1.905960000
6	0.892607000	-0.363633000	-1.152736000
6	1.879903000	-0.389108000	-2.150822000
6	-0.093068000	-1.357664000	-1.144084000
6	1.921126000	-1.433577000	-3.077956000
1	2.621187000	0.403295000	-2.205123000
6	-0.057264000	-2.390008000	-2.084811000
1	-0.875606000	-1.361989000	-0.393748000

6	0.951079000	-2.438518000	-3.050597000
1	2.708414000	-1.451724000	-3.827477000
1	-0.821576000	-3.162687000	-2.054267000
1	0.973723000	-3.243053000	-3.780185000
1	3.101743000	-0.773114000	1.939477000
8	2.728405000	1.930367000	1.161541000
6	3.906664000	1.573350000	1.625913000
6	4.408153000	2.077496000	2.850701000
6	4.759308000	0.664236000	0.935737000
6	5.660092000	1.712730000	3.355699000
1	3.787939000	2.774511000	3.409891000
6	6.003200000	0.294386000	1.437759000
1	4.416811000	0.252821000	-0.012198000
6	6.470185000	0.813674000	2.652521000
1	5.988402000	2.132772000	4.300802000
1	6.633962000	-0.402959000	0.891763000
8	7.713010000	0.385504000	3.061589000
6	8.198820000	0.897216000	4.292399000
1	9.184931000	0.450862000	4.441685000
1	8.301535000	1.990753000	4.268007000
1	7.549459000	0.620125000	5.134076000

O (G = -2809.519101)

29	1.521239000	0.477063000	0.229765000
7	2.050151000	-1.203491000	1.566315000
6	1.640014000	-2.557366000	1.184233000
1	1.794606000	-3.290257000	1.991174000
1	2.210336000	-2.868060000	0.305394000
1	0.579276000	-2.554926000	0.916505000
7	-0.190376000	0.319425000	1.327100000
6	1.406605000	-0.737315000	2.801247000
1	1.984021000	0.119954000	3.165943000
1	1.404892000	-1.500726000	3.592097000
7	-0.424031000	1.564477000	-1.187851000
6	-0.013439000	-0.303359000	2.512859000
6	-1.068282000	-0.538003000	3.383975000
1	-0.892098000	-1.052473000	4.322938000
6	-2.346956000	-0.111467000	3.017939000
1	-3.192667000	-0.277582000	3.678381000
6	-2.525980000	0.506222000	1.786644000
1	-3.509040000	0.828331000	1.457350000
6	-1.418374000	0.704459000	0.955404000
6	-1.630743000	1.329756000	-0.408545000
1	-2.368995000	0.710507000	-0.949800000
1	-2.115858000	2.301764000	-0.263956000
6	-0.731240000	2.320251000	-2.405606000
1	-1.402383000	1.765241000	-3.083876000
1	0.193926000	2.543526000	-2.941501000
1	-1.213771000	3.264938000	-2.135595000
6	0.386926000	0.402832000	-1.459231000
6	1.760791000	0.624596000	-1.791362000
6	-0.178591000	-0.878485000	-1.717297000
6	2.511098000	-0.433776000	-2.362141000
1	2.124650000	1.642832000	-1.892425000
6	0.599256000	-1.905917000	-2.219106000
1	-1.225656000	-1.055553000	-1.494261000
6	1.955394000	-1.688475000	-2.543829000
1	3.541180000	-0.245503000	-2.652836000
1	0.155620000	-2.885056000	-2.379063000
1	2.550677000	-2.496773000	-2.958901000
1	3.058872000	-1.183758000	1.705653000
8	2.796281000	1.746116000	1.002577000
6	3.959554000	1.347401000	1.465372000
6	4.505617000	1.884699000	2.657333000
6	4.756489000	0.363772000	0.810341000
6	5.742763000	1.477897000	3.167785000
1	3.930666000	2.640654000	3.187923000
6	5.985670000	-0.045478000	1.317639000
1	4.381760000	-0.075404000	-0.110707000
6	6.494605000	0.503375000	2.502328000
1	6.104915000	1.926042000	4.087409000
1	6.572181000	-0.800873000	0.799776000
8	7.717186000	0.025590000	2.921531000
6	8.226135000	0.541731000	4.140435000
1	9.180576000	0.038061000	4.311982000
1	8.399701000	1.625335000	4.085608000
1	7.553340000	0.333251000	4.983677000

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