Electronic Supplementary Information

Intramolecular oxidative cyclization of alkenes by rhodium/cobalt porphyrins in water

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EXPERIMENTAL

General

D_2O, CD_3OD, $CDCl_3$ were purchased from Cambridge Isotope Laboratory Inc.; tetra p-sulfonatophenyl porphyrin from Tokyo Chemical Industry (TCI); $(Rh(CO)_2Cl)_2$ from Stream Chemical Inc.; and all other chemicals were purchased from Aldrich or Alfa Aesar unless otherwise noted and used as received. Mass spectra were taken on a Bruker Apex IV FTMS. Room temperature ^1H NMR spectra were recorded on a Bruker AV-400 spectrometer. The chemical shifts were referenced to 3-trimethylsilyl-1-propanesulfonic acid sodium salt (DSS). GC-MS results were obtained by the Agilent 7980A/5975C GC/MSD system equipped with the DB-17MS (30 m, 0.25 mm, 0.25 μm) column. All reagents and solvents were of commercial quality and distilled or dried when necessary using standard procedures.

***Preparation of $Na_3[(TSPP)M^{III}(H_2O)_2]$ (M = Rh, and Co)*:** $Na_3[(TSPP)M^{III}(H_2O)_2]$ was synthesized by literature methods of Ashley[1]. The equilibrium distribution of $[(TSPP)Rh^{III}(D_2O)_2]^{-3}$, $[(TSPP)Rh^{III}(D_2O)(OD)]^{-4}$ and $[(TSPP)Rh^{III}(OD)_2]^{-5}$ were reported in the previously published paper.[2] $Na_3[(TSPP)Rh^{III}(H_2O)_2]$: ^{1}HNMR ($D_2O$, 400 MHz) δ (ppm): 9.15 (s, 8H, pyrrole), 8.44 (d, 8H, o-phenyl, J_{H-H} = 8 Hz), 8.25 (d, m-phenyl, J_{H-H} = 8 Hz). $Na_3[(TSPP)Co^{III}(H_2O)_2]$: ^{1}HNMR ($D_2O$, 400 MHz) δ (ppm): 9.37 (s, 8H, pyrrole), 8.41 (d, 8H, o-phenyl, J_{H-H} = 8 Hz), 8.22 (d, m-phenyl, J_{H-H} = 8 Hz).

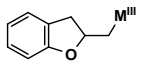
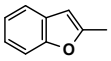
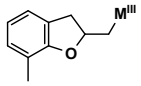
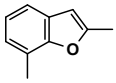
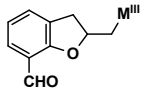
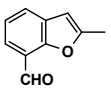
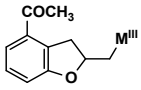
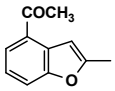
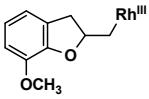
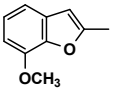
***Typical procedure for preparation of β-hetero-functionalized alkyl rhodium porphyrins*:** $Na_3[(TSPP)Rh^{III}(H_2O)_2]$ (1.1 mg, 0.001 mmol) and alkenes (10 equiv) were dissolved in 0.3 mL borate buffer D_2O solution (pH = 8.0) in vacuum adapted NMR tubes at room temperature, respectively. The progress of the reaction was monitored by ^1H NMR. After completion, the mixture was transformed to a 10 mL round-bottomed flask and the solvent was removed using the Schlenk line. The resulting solid was washed by ethyl ether and $CHCl_3$ to removed excess substrate.

***Typical procedure for preparation of β-hetero-functionalized alkyl cobalt porphyrins*:** $Na_3[(TSPP)Co^{III}(H_2O)_2]$ (1.1 mg, 0.001 mmol) and alkenes (10 equiv) were dissolved in 0.3 mL borate

buffer D_2O solution (pH = 9.0) in vacuum adapted NMR tubes at room temperature, respectively. The progress of the reaction was monitored by ^1H NMR. After completion, the mixture was transformed to a 10 mL round-bottomed flask wrapped with aluminum foil and the solvent was removed using the Schlenk line. The resulting solid was direct sent to ^1H NMR study.

***Typical procedure for production of 2-methylbenzofurans*:** purified β-phenoxyalkyl rhodium/cobalt porphyrin complexes were dissolved in 0.3 mL D_2O in vacuum adapted NMR tubes. After three freeze–thaw cycles, the solution was charged with N_2 in the glove box, heated at 333K. The elimination process was followed by ^1H NMR. After complete conversion of the rhodium alkyl complexes, 0.3 mL $CDCl_3$ was added to extract the formed product. GC-MS was also used to identify the 2-methylbenzofurans.

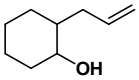
Table S1 Formation of heterocyclic unsaturated products[a]

Entry	Substrate	Product	Time(min)	Conv.(%)[b]
1			**1**: 30 **14**: <60	> 95
2			**1**: 45 **14**: <60	> 95
3			**1**: 20 **14**: <60	> 95
4			**1**: 15 **14**: <60	> 95
5			30	> 95

[a] 333K, D_2O (400 mL, pH 8.0 borate buffer), N_2 (1 atm) protection.

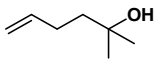
[b] Conversion of alkyl rhodium porphyrin intermediate was determined by 1H NMR. The conversion was almost quantitative. However, the yeild was not determined due to small amount of product.

Synthesis

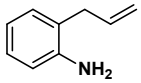


2-Allylcyclohexanol.[3] **A** 3-neck 100 mL round-bottom flask fitted with a mechanical stirrer, 25 mL addition funnel was charged with allyl magnesium bromide (1.0 M in Et_2O, 20 mL, 20 mmol, 3 equiv) and 16 mL Et_2O. Cyclohexene oxide (0.67 mL, 6.6 mmol, 1.0 equiv) was added dropwise. 30 min after addition, the mixture was refluxed for 3 hours which was then quenched by saturated NH_4Cl solution (30 mL) was carefully added. The solution was transferred to a separatory funnel and the organic layer was collected. The aqueous layer was extracted by Et_2O (30 mL × 3). The organic layers were combined, dried over Na_2SO_4, filtered and concentrated. The residue was purified by flash column chromatography to give a pale yellow oil (42% yeild). The spectral data match that of the literature compound.

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.85 (ddt, 1H), 5.08 (m, 1H), 5.03 (m, 1H), 3.26 (m, 1H), 2.45 (m, 1H), 2.01-1.94 (m, 2H), 1.79 (m, 2H), 1.63 (m, 2H), 1.38-1.18 (m, 4H), 0.95 (m, 1H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 137.60, 116.08, 74.71, 45.03, 35.70, 30.49, 29.80, 25.63, 25.02.

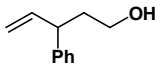


2-Methylhex-5-en-2-ol.[3] **A** 3-neck 50mL round-bottom flask fitted with a mechanical stirrer, 25 mL addition funnel was charged with methyl magnesium bromide (3.0 M in Et_2O, 7.0 mL, 21 mmol, 1.2 equiv) and 10 mL Et_2O. 5-hexen-2-one (2.0 mL, 17 mmol, 1.0 equiv) was added dropwise. One hour after addition was complete, saturated NH_4Cl solution (6 mL) was carefully added. The solution was transferred to a separatory funnel and the organic layer was collected. The aqueous layer was extracted by Et_2O (15 mL × 3). The organic layers were combined, dried over Na_2SO_4, filtered and concentrated to give a pale yellow oil as the pure product (56% yeild). The spectral data match that of the literature compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.75 (ddt, 1H), 4.94 (ddd, 1H), 4.85 (ddd, 1H), 2.05 (m, 2H), 1.48 (m, 1H), 1.13 (s, 6H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 139.98, 114.13, 70.68, 42.76, 29.06, 28.70.

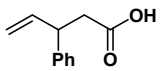


2-Allylaniline.[4] In a 100-mL seal-tube, a cold solution (at −78 °C) of N-allylaniline (1.33 g, 10.0 mmol) in m-xylene (20 mL) was added boron trifluoride etherate (1.5 mL, 12.0 mmol) under an argon atmosphere. After 5 min, the solution was warmed to room temperature and then heated to 180 °C. After 17 h, the reaction was cooled down to room temperature and quenched with 2 M NaOH solution (20 mL) at 0 °C. The organic layer was separated and the aqueous layer was extracted with diethyl ether (15 mL × 3). The combined organic layers were filtered and concentrated in vacuo. The residue was purified by flash column chromatography to give the product as a yellow oil (30% yeild).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.06-7.03 (m, 2H), 6.74 (t, 1H), 6.67 (d, 1H), 6.01-5.88 (m, 1H), 5.13-5.06 (m, 2H), 3.64 (bs, 2H), 3.30 (d, 2H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 144.92, 136.08, 130.29, 127.66, 124.15, 119.01, 116.21, 115.95, 36.60.

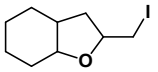


3-Phenylpent-4-en-1-ol.[5] A mixture of cynnamyl alcohol (18.7 mmol, 2.5 g), triethyl orthoacetate (107.4 mmol, 14 mL) and catalytic amount of propionic acid was heated at 150 °C overnight. The resulting mixture was concentrated and purified through silica gel column chromatography. The ester was then dissolved in THF (20 mL) and treated slowly with lithum aluminum hydride (12.5 mmol, 0.5 g) at 0 °C. The mixture was then warmed to room temperature and stired for 4 hours. The resulting mixture was poured into 1 M NaOH (aq, 50 mL) and ice with vigorous stirring to give white suspension. After filtration, the resulting solution was extracted with Et_2O (50 mL × 3). The combined organic layers were washed with 1 M HCl (aq, 30 mL× 2), brine (30 mL) and dried over Na_2SO_4. After filtration and concertation in vacuo, the residue was purified through silica gel column chromatography to give the final product (47% yeild). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.17 (m, 5H), 5.93 (m, 1H), 5.06 (m, 2H), 3.61 (m, 2H), 3.45 (q, 1H), 1.98 (m, 2H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 143.78, 141.89, 128.64, 127.66, 126.45, 114.45, 60.88, 46.30, 37.99, 36.60.



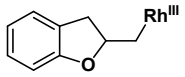
3-Phenyl-4-pentenoic acid.[5] The complex was prepared according to literature procedures [2]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.7 (br s, 1H), 7.29-7.11 (m, 5H), 5.85-6.02 (m, 1H), 5.02-4.98 (m, 2H),

4.95 (ddt, 1H), 4.03 (q, 1H), 2.68 (m, 2H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 178.06, 142.27, 140.08, 128.74, 127.62, 126.89, 115.11, 45.28, 40.05.

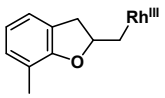


2-(iodomethyl)octahydrobenzofuran.[6] 2-allylphenol (1.0 mmol) and iodine (1.2 mmol) was added in ethanol/water (20 mL, 1/9). The mixture was stirred at 50 °C for 12 h. After completion, the reaction mixture was extracted with Et_2O and washed with water. The combined organic fraction was washed with aqueous sodium thiosulphate, dried over Na_2SO_4 and evaporated to generate the crude product, which was chromatographed to afford the product as yellow powder (81% yield).

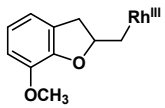
Formation of β-hetero-functionalized alkyl rhodium porphyrins



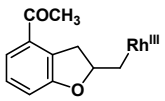
Reaction of (TSPP)Rh^{III} with 2-allylphenol. ^1H NMR (400 MHz, D_2O) δ 8.56 (8H, pyrrole), 8.20-7.97 (16H, phenyl), 6.16-5.87 (m, 3H), 5.24 (m, 1H), -0.65 (d, 2H), -1.75 (d, 1H), -2.40 (m, 1H), -5.67 (m, 1H), -5.81 (m, 1H). MS (ESI): *m*/*z*: 290.99903, *calcd.* 291.99900.



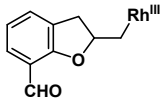
Reaction of (TSPP)Rh^{III} with 2-allyl-6-methylphenol. ^1H NMR (400 MHz, CD_3OD) δ 8.70 (8H, pyrrole), 8.12-8.01 (16H, phenyl), 6.17-6.03 (m, 3H), 5.24 (m, 1H), 1.09 (s, 3H), -0.52 (d, 2H), -1.49 (d, 1H), -2.51 (m, 1H), -5.57 (m, 1H), -5.74 (m, 1H). MS (ESI): *m*/*z*: 400.33510, *calcd.* 400.33399.



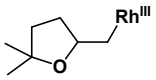
Reaction of (TSPP)Rh^{III} with 2-allyl-6-methoxyphenol. ^1H NMR (400 MHz, CD_3OD) δ 8.70 (8H, pyrrole), 8.12-8.01 (16H, phenyl), 8.68 (m, 2H), 5.85 (m, 1H), 3.03 (s, 3H), -0.49 (d, 2H), -1.50 (d, 1H), -2.51 (m, 1H), -5.63 (m, 1H), -5.76 (m, 1H). MS (ESI): *m*/*z*: 405.66726, *calcd.* 405.66563.



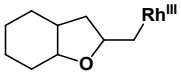
Reaction of (TSPP)Rh^{III} with 1-(2-allyl-3-hydroxyphenyl)ethanone. ^{1}H NMR (400 MHz, CD_3OD) δ 8.75 (8H, pyrrole), 8.26-8.24 (16H, phenyl), 7.15 (dd, 1H), 5.56 (d, 1H), 2.21 (s, 3H), -0.24 (q, 1H), -1.40 (m, 1H), -2.10 (dd, 1H), -5.52 (m, 1H), -5.71 (m, 1H). MS (ESI): *m*/*z*: 409.66760, *calcd.* 409.66563.



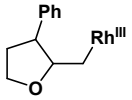
Reaction of (TSPP)Rh^{III} with 3-allyl-2-hydroxybenzaldehyde. ^{1}H NMR (400 MHz, CD_3OD) δ 8.68 (8H, pyrrole), 8.11-7.79 (16H, phenyl), 6.73 (d, 2H), 6.55 (d, 1H), 6.26 (t, 3H), 3.03 (s, 3H), -0.46 (dd, 2H), -1.31 (m, 1H), -2.51 (m, 1H), -5.55 (m, 1H), -5.77 (m, 1H). MS (ESI): *m*/*z*: 406.33963, *calcd.* 406.33751.



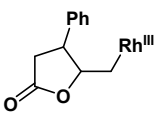
Reaction of (TSPP)Rh^{III} with 2-methylhex-5-en-2-ol. ^{1}H NMR (400 MHz, D_2O) δ 8.62 (8H, pyrrole), 8.39-8.12 (16H, phenyl), 0.15 (m, 1H), -0.03 (s, 3H), -0.13 (m, 1H), -0.18 (s, 3H), -1.91 (m, 1H), -2.62 (m, 1H), -3.23 (m, 1H), -5.82 (m, 1H), -5.91 (m, 1H). MS (ESI): *m*/*z*: 286.00632, *calcd.* 286.00682.



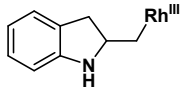
Reaction of (TSPP)Rh^{III} with 2-allylcyclohexanol. ^{1}H NMR (400 MHz, D_2O) δ 8.62 (8H, pyrrole), 8.39-8.12 (16H, phenyl), 0.39 (m, 1H), -0.09 (m, 1H), -1.03 (m, 1H), -1.96 (m, 1H), -2.35 (m, 1H), -3.65 (m, 1H), -5.68 (m, 1H), -5.83 (m, 1H).



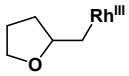
Reaction of (TSPP)Rh^{III} with 3-phenylpent-4-en-1-ol. ^{1}H NMR (400 MHz, D_2O) δ 8.36 (8H, pyrrole), 8.17-8.05 (16H, phenyl), 6.83 (m, 1H), 6.67 (m, 2H), 5.17 (m, 2H), -0.39 (m, 3H), -0.24 (m, 1H), -0.91 (m, 1H), -3.44 (m, 1H), -6.02 (m, 1H), -6.12 (m, 1H). MS (ESI): *m*/*z*: 298.00632, *calcd.* 298.00682.



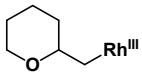
Reaction of (TSPP)Rh^{III} with 3-phenylpent-4-enoic acid. ^{1}H NMR (400 MHz, D_2O) δ 8.60 (8H, pyrrole), 8.31-8.00 (16H, phenyl), 6.86 (1H), 6.68 (2H), 5.05 (2H), 1.04 (1H), -0.58 (1H), -2.39 (1H), -5.82 (1H), -5.98 (1H). MS (ESI): *m*/*z*: 301.50235, *calcd.* 301.50164.



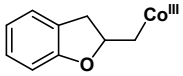
Reaction of (TSPP)Rh^{III} with 2-allylaniline. ^{1}H NMR (400 MHz, D_2O) δ 8.53 (8H, pyrrole), 8.17-8.04 (16H, phenyl), 6.74 (m, 1H), 6.63 (m, 2H), 5.45 (m, 2H), 0.07 (m, 1H), -1.36 (m, 1H), -2.64 (m, 1H), -5.87 (m, 1H), -5.89 (m, 1H).



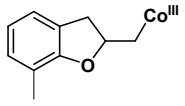
Reaction of (TSPP)Rh^{III} with pent-4-en-1-ol in methanol. ^{1}H NMR (400 MHz, CD_3OD) δ 8.78 (8H, pyrrole), 8.39-8.12 (16H, phenyl), 2.02 (m, 2H), 0.37 (m, 1H), 0.15 (m, 1H), -1.71 (m, 1H), -1.74 (m, 1H), -2.29 (m, 1H), -3.25 (dd, 1H), -5.58 (m, 1H), -5.81 (m, 1H).



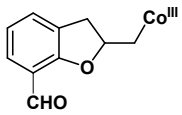
Reaction of (TSPP)Rh^{III} with hex-5-en-1-ol in methanol. ^{1}H NMR (400 MHz, CD_3OD) δ 8.67 (8H, pyrrole), 8.26-8.18 (16H, phenyl), 1.46 (m, 2H), 0.47 (m, 1H), 0.11 (m, 1H), -0.19 (m, 1H), -1.89 (m, 1H), -2.48 (m, 1H), -3.37 (m, 1H), -5.63 (m, 1H), -5.86 (m, 1H).



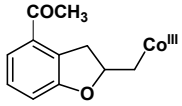
Reaction of (TSPP)Co^{III} with 2-allylphenol. ^{1}H NMR (400 MHz, CD_3OD) δ 8.23 (8H, pyrrole), 7.82-7.65 (16H, phenyl), 6.33-6.16 (m, 3H), 5.48 (m, 1H), -1.12 (m, 1H), -2.48 (m, 1H), -2.82 (m, 1H), -5.00 (m, 1H), -5.17 (m, 1H).



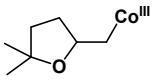
Reaction of (TSPP)Co^{III} with 2-allyl-6-methylphenol. ^{1}H NMR (400 MHz, D_2O) δ 8.83 (8H, pyrrole), 8.23-7.85 (16H, phenyl), 6.63 (br, 1H), 5.95 (br, 1H), 5.33(br, 1H), -0.42 (m, 1H), -1.42 (m, 1H), -2.19 (m, 1H), -4.01 (m, 1H), -4.46 (m, 1H).



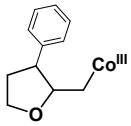
Reaction of (TSPP)Rh^{III} with 3-allyl-2-hydroxybenzaldehyde. ^{1}H NMR (400 MHz, D_2O) δ 8.84 (8H, pyrrole), 8.21-7.85 (16H, phenyl), 6.62 (br, 1H), 5.92 (br, 1H), 5.41(br, 1H), -0.34 (m, 1H), -1.23 (m, 1H), -2.16 (m, 1H), -4.03 (m, 1H), -4.53 (m, 1H).



Reaction of (TSPP)Rh^{III} with 1-(2-allyl-3-hydroxyphenyl)ethanone. ^{1}H NMR (400 MHz, D_2O) δ 8.83 (8H, pyrrole), 8.23-7.73 (16H, phenyl), 6.63 (br, 2H), 5.83 (br, 1H), -0.24 (m, 1H), 2.09 (s, 3H), -1.39 (m, 1H), -1.94 (m, 1H), -4.13 (m, 1H), -4.49 (m, 1H).



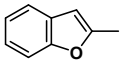
Reaction of (TSPP)Co^{III} with 2-methylhex-5-en-2-ol. ^{1}H NMR (400 MHz, D_2O) δ 8.62 (8H, pyrrole), 7.82-7.65 (16H, phenyl), 0.03 (m, 1H), -0.11 (s, 3H), -0.21 (m, 1H), -0.28 (s, 3H), -2.21 (m, 1H), -2.87 (m, 1H), -3.42 (m, 1H), -4.66 (m, 1H), -5.01 (m, 1H).



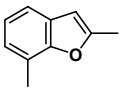
Reaction of (TSPP)Rh^{III} with 3-Phenyl-4-pentenoic acid. ^{1}H NMR (400 MHz, D_2O) δ 8.16 (b, 8H, pyrrole), 8.05 (b, 16H, phenyl), 6.73 (t,1H), 6.47 (t, 2H), 2.17 (1H), 0.86 (2H), 0.63 (1H), -0.64 (1H), -3.39 (1H), -4.87 (1H), -5.28 (1H).

β-H elimination product of Table 1

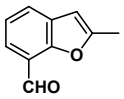
All BHE products of rhodium/cobalt alkyl complexes were carefully characterized by GC-MS.



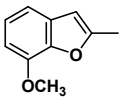
2-methylbenzofuran[7] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, 1H), 7.35 (d, 1H), 7.15 (m, 2H), 6.42 (1H), 2.42 (m, 3H).



2,7-dimethylbenzofuran[8] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, 1H), 7.04 (t, 1H), 6.98 (d, 1H), 6.41 (s, 1H), 6.42 (1H), 2.42 (m, 6H).



2-methylbenzofuran-7-carbaldehyde ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, 1H), 7.24 (d, 1H), 7.16 (t, 1H), 6.46 (s, 1H), 2.46 (m, 3H).



7-methoxy-2-methylbenzofuran[8] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.10 (d, 1H), 7.02 (t, 1H), 6.69 (d, 1H), 6.19 (s, 1H), 3.71 (s, 3H), 2.29 (s, 3H).

Explanation of cobalt alkyl complexes

Elimination Charged with air or oxygen, (TSPP)Co^{III} mediated oxidative cyclization of 2-allylphenol derivatives gave cyclization product and mixture of (TSPP)Co^{II} and (TSPP)Co^{III} (Fig S1) :

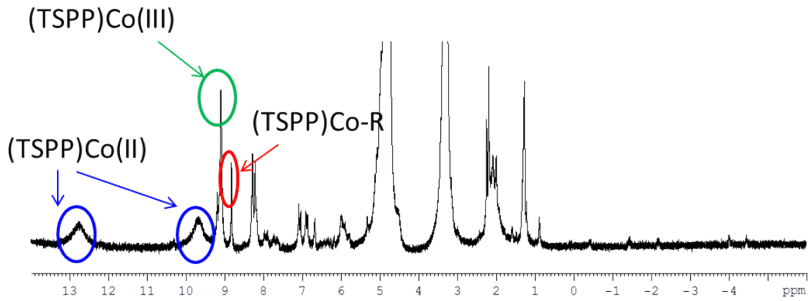


Figure S1 Elimination of Cobalt alkyls in air. Both (TSPP)Co(III) and (TSPP)Co(II) was observed.

ESI-MS results Due to weak Co-C bond, both ESI-MS and MALDI-TOF-MS failed to gave MS characterization of cobalt alkyl complexes. The spectra all showed *m/z* for (TSPP)Co shown in Fig. S2.

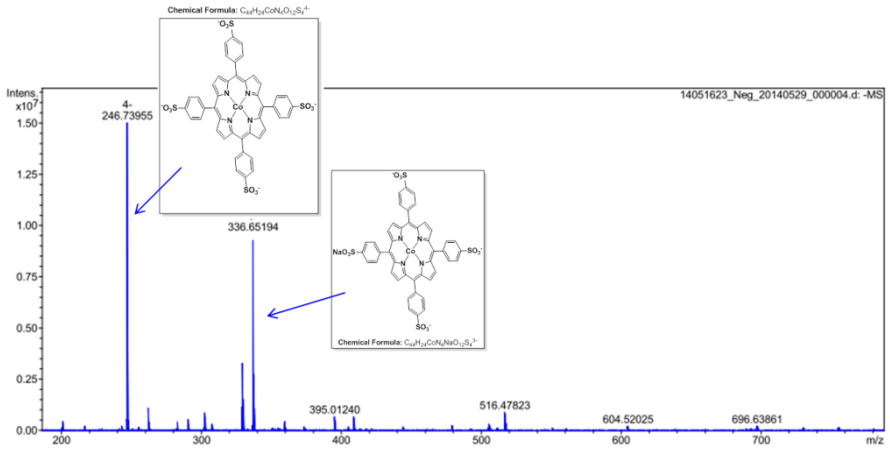


Figure S2 ESI-MS results for cobalt alkyl species. All reported cobalt alkyls in the manuscript gave almost the same spectra. The two highest m/z peaks correspond to (TSPP)Co with loss of 4 Na^+ and 3 Na^+.

Reference

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[3] N. Stefano, W. Jerome, *Org. Lett*. **2011**, *13*, 6324.

[4] H. Yamamoto, E. Ho, K. Namba, H. Imagawa, M. Nishizawa, *Chem. –Eur. J.* **2010**, *16*, 11271.

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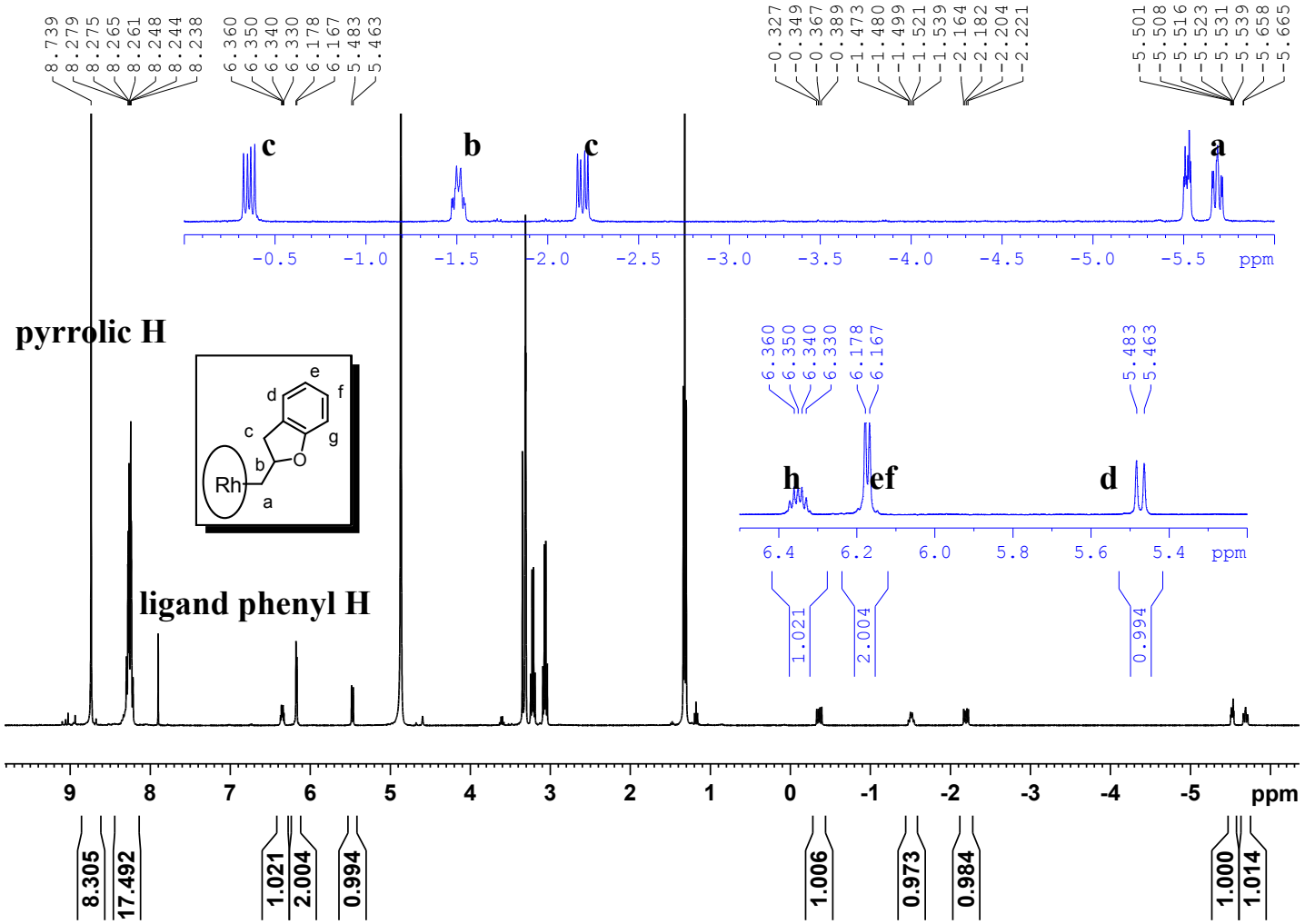
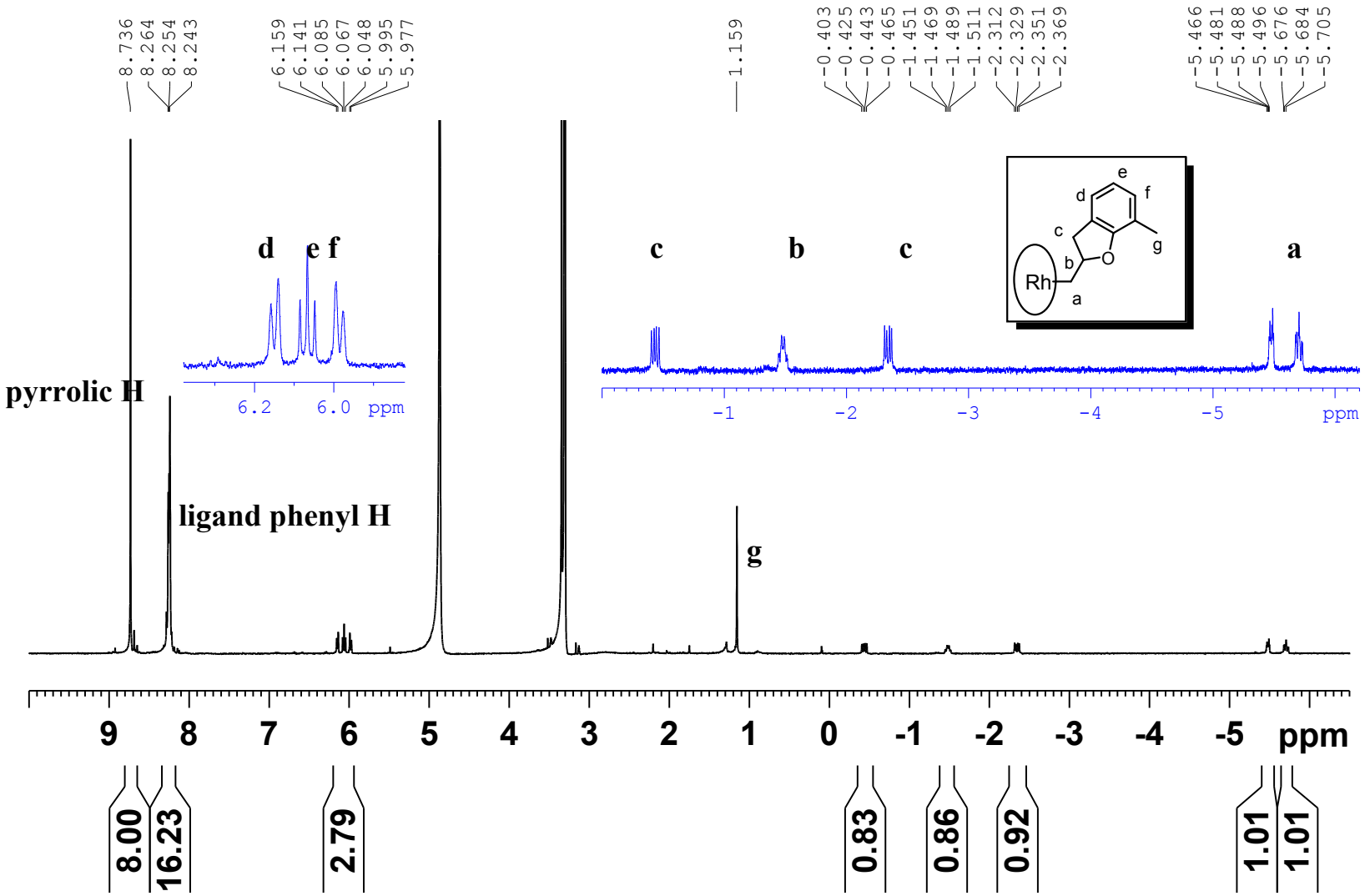
[8] A. Alemagna, C. Baldoli, P. Del Buttero, E. Licandro, S. Maiorana, *J. Chem. Soc., Chem. Commun*. **1985**, 417.

Representative ^{1}H NMR spctra :

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-0.425
-0.443
-0.465
-1.451
-1.469
-1.489
-1.511
-2.312
-2.329
-2.351
-2.369
-5.466
-5.481
-5.488
-5.496
-5.676
-5.684
-5.705
d e f
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6.0
ppm
c b c
a
-1
-2
-3
-4
-5
ppm
e
d
f
c
g
b
O
Rh
a
pyrrolic H
ligand phenyl H
g
9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 ppm
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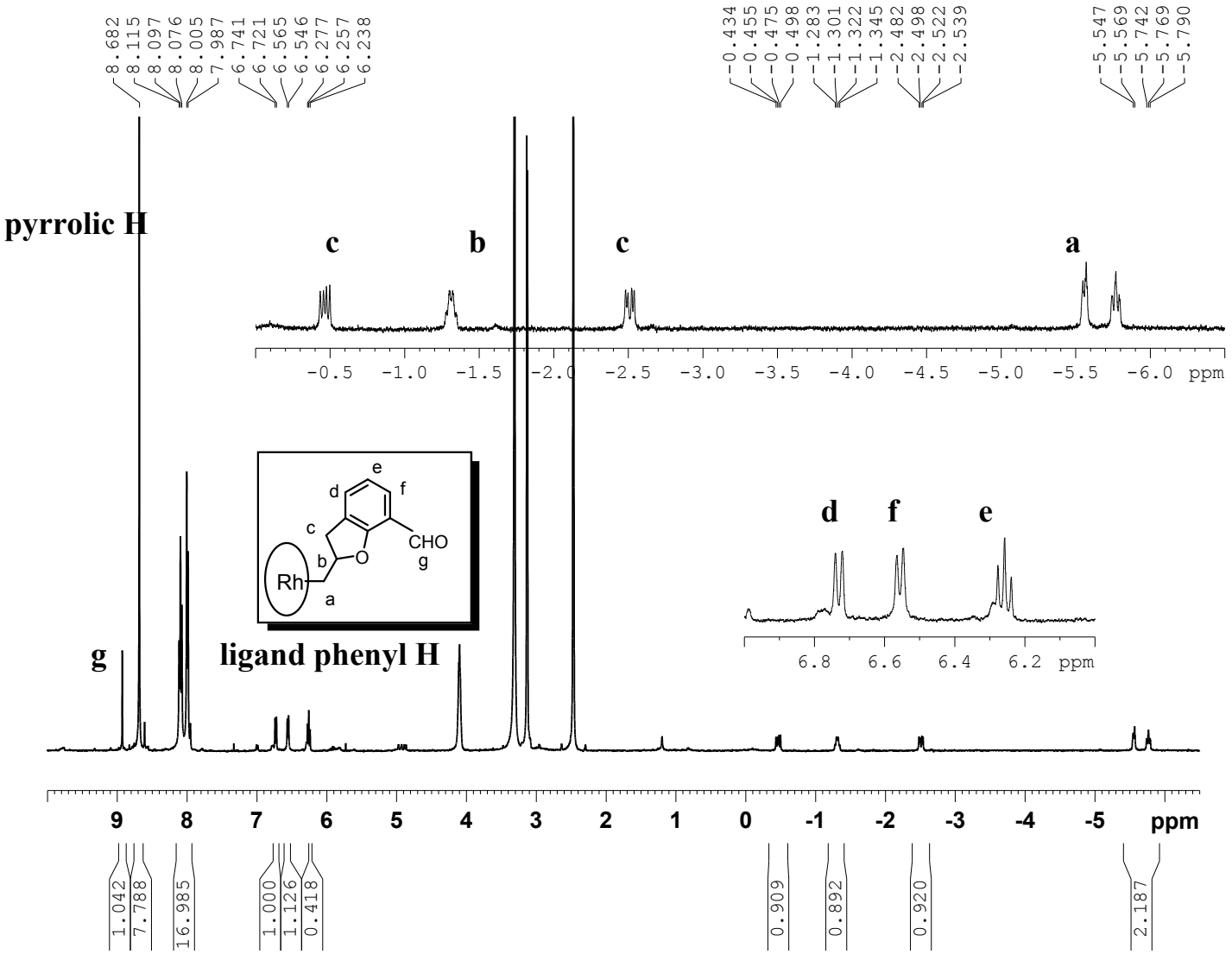
1.01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6.238
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-0.455
-0.475
-0.498
-1.283
-1.301
-1.322
-1.345
-2.482
-2.498
-2.522
-2.539
-5.547
-5.569
-5.742
-5.769
-5.790
pyrrolic H
c
b
c
a
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e
d
f
c
CHO
g
b
O
Rh
a
d
f
e
6.8 6.6 6.4 6.2 ppm
g
ligand phenyl H
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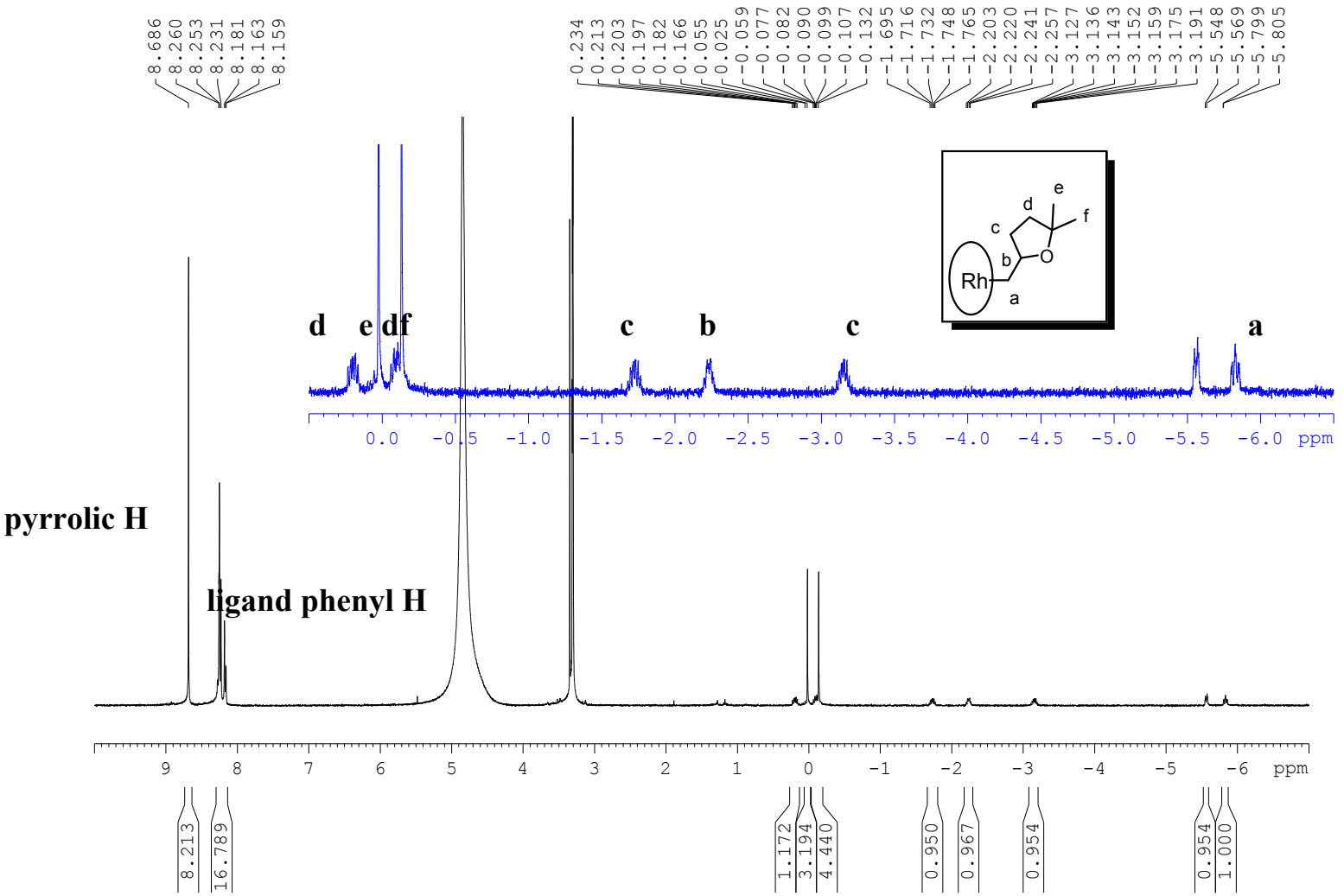
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0.166
0.055
0.025
-0.059
-0.077
-0.082
-0.090
-0.099
-0.107
-0.132
-1.695
-1.716
-1.732
-1.748
-1.765
-2.203
-2.220
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-5.799
-5.805
d e d f
c
b
c
a
Rh
O
a
b
c
d
e
f
0.0 -0.5 -1.0 -1.5 -2.0 -2.5 -3.0 -3.5 -4.0 -4.5 -5.0 -5.5 -6.0 ppm
pyrrolic H
ligand phenyl H
9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 ppm
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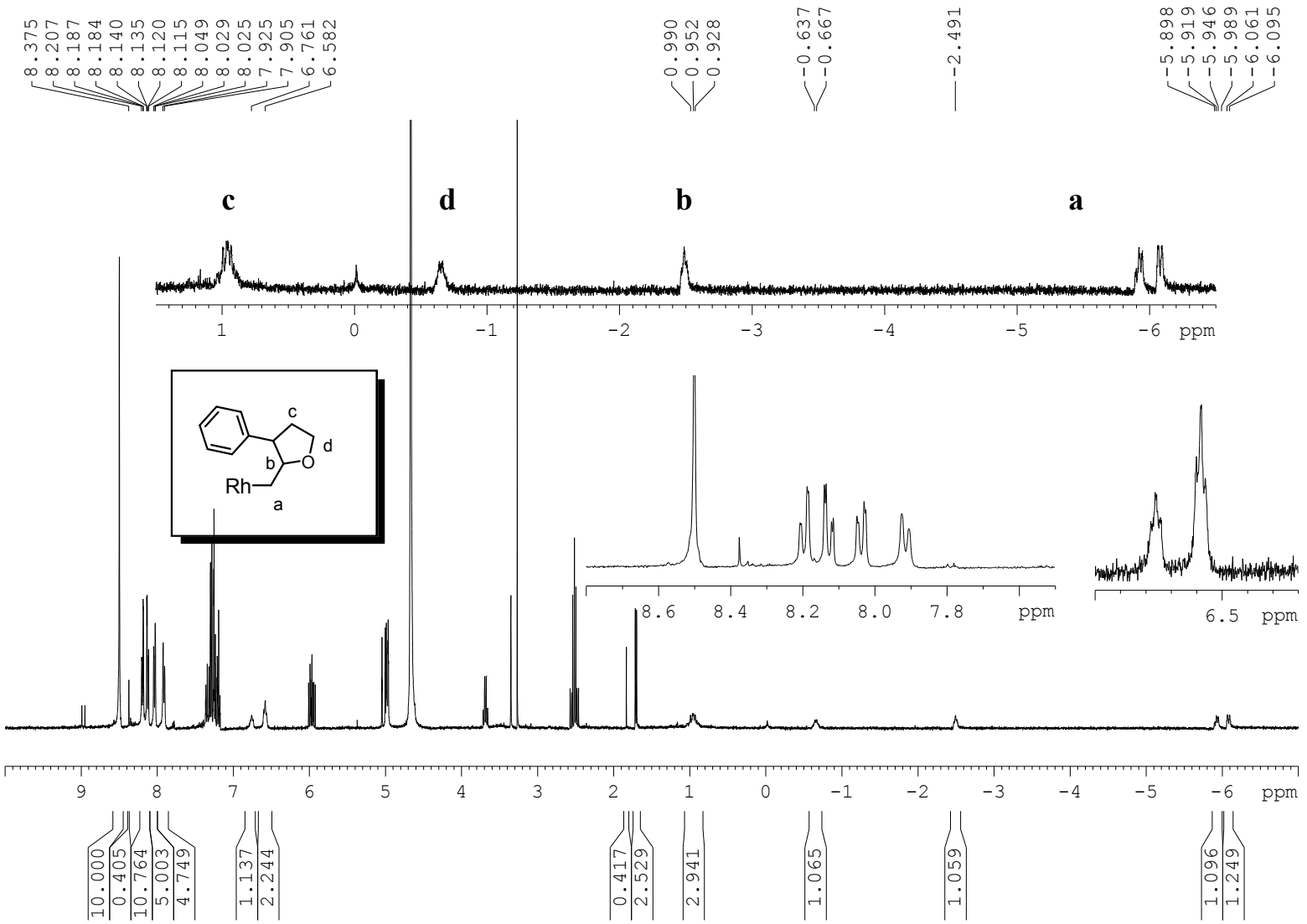
1.000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6.761
6.582
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0.952
0.928
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d
b
a
ppm
c
d
b
O
Rh
a
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8.2
8.0
7.8
ppm
6.5
ppm
9
8
7
6
5
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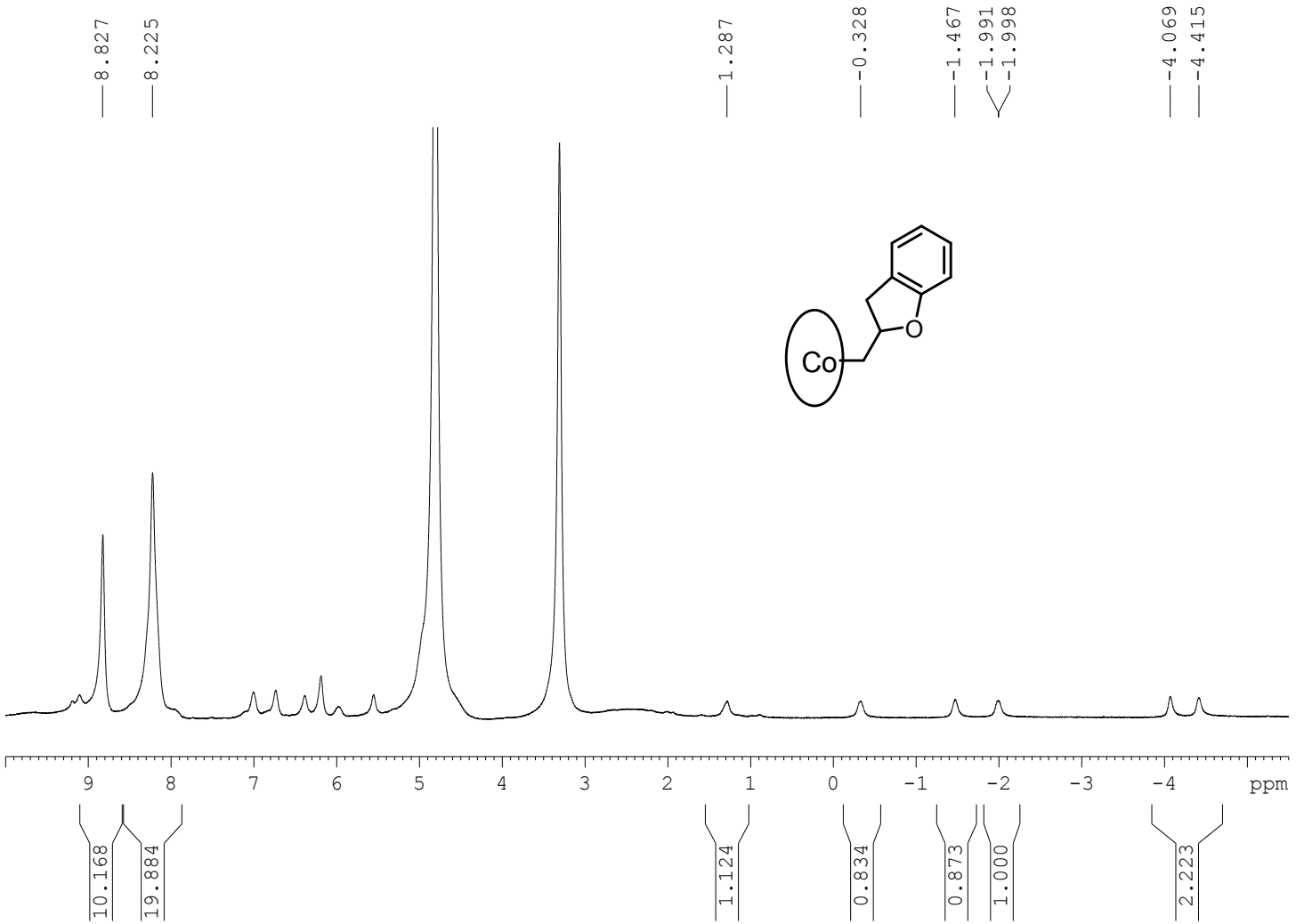
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Co
O
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8
7
6
5
4
3
2
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-1
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-3
-4
ppm
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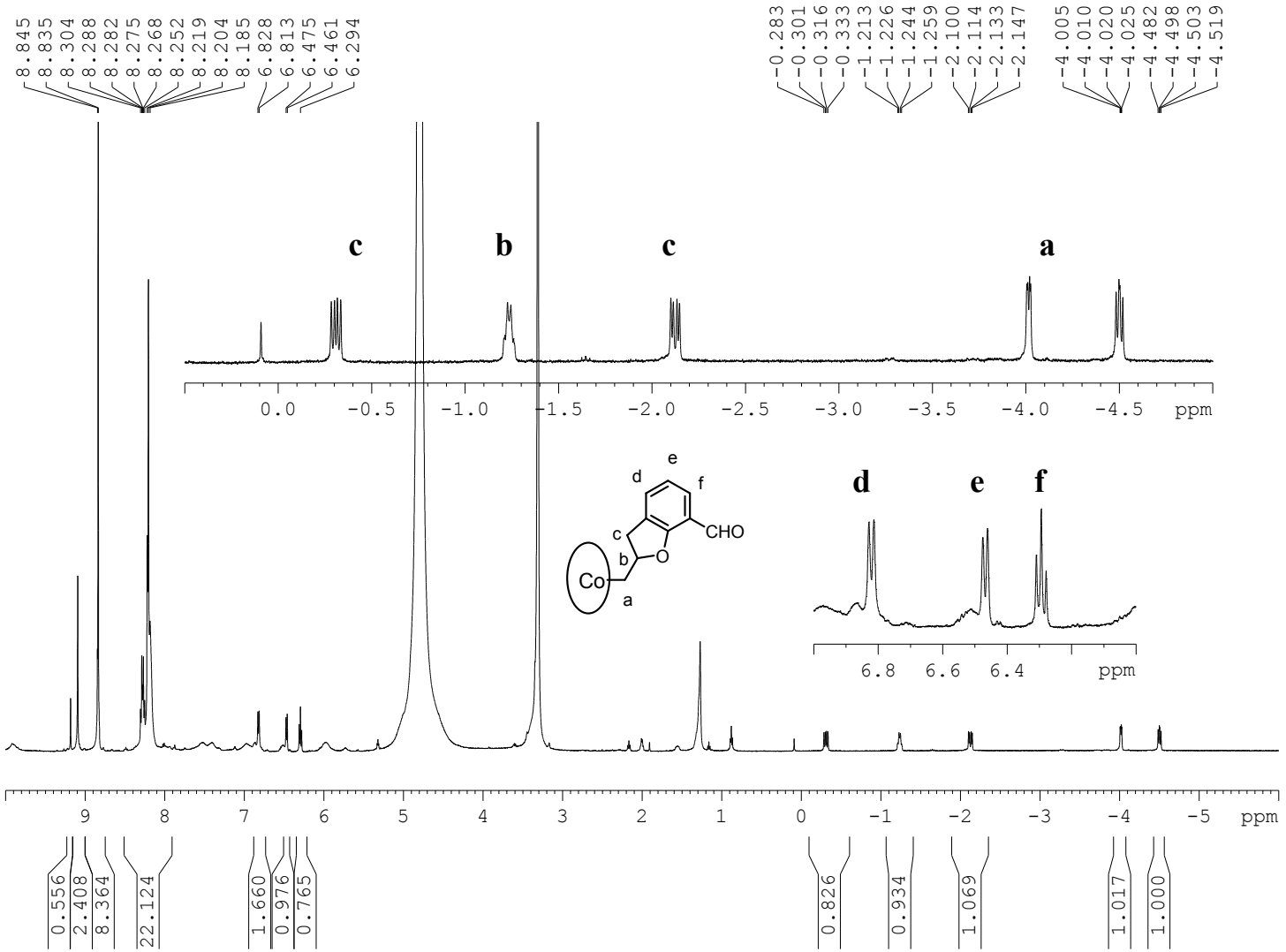
2.223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8.204
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6.813
6.475
6.461
6.294
-0.283
-0.301
-0.316
-0.333
-1.213
-1.226
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-2.100
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c
b
c
a
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-4.5
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e
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CHO
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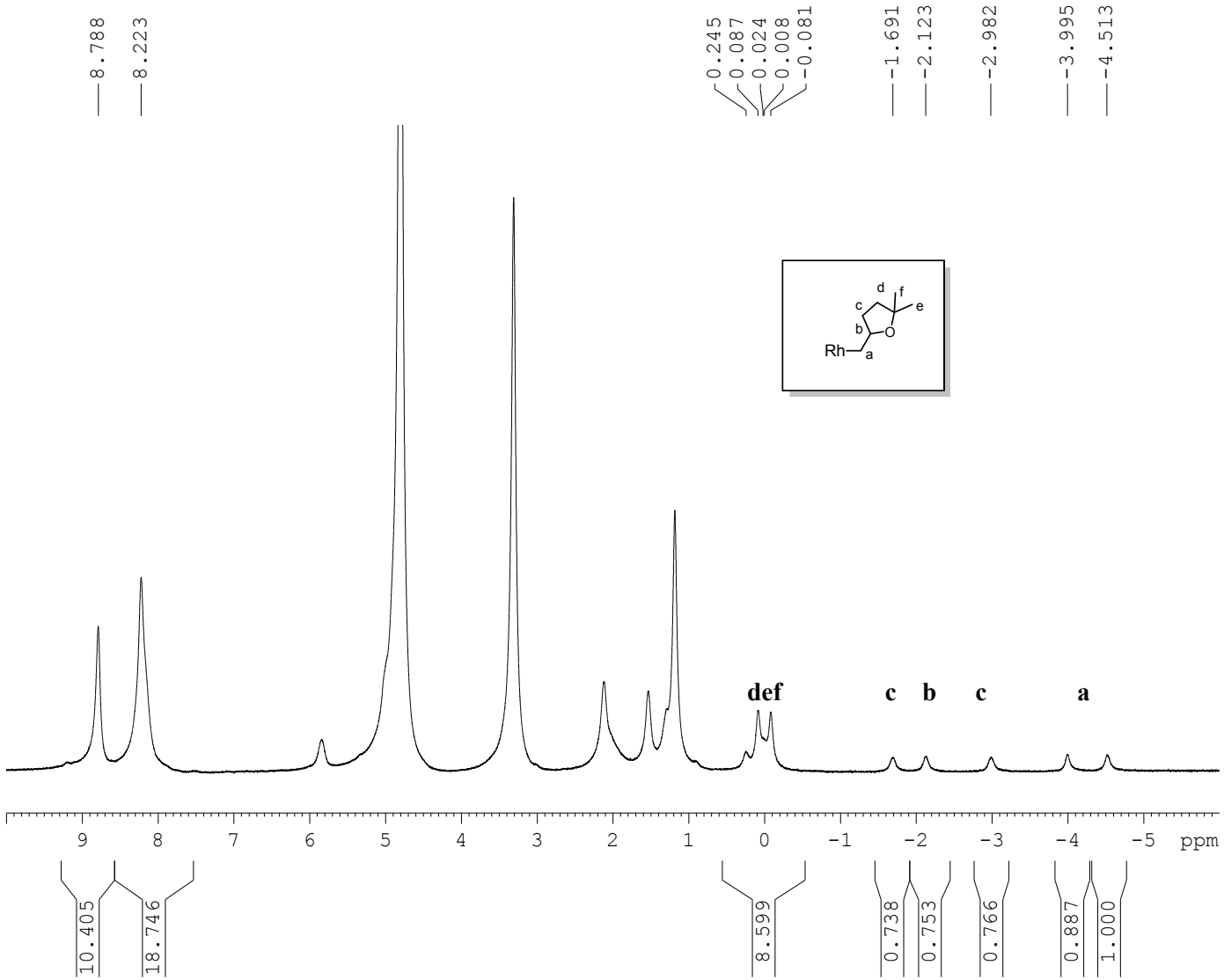
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c
e
b
O
Rh
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