Mechanistic Insights into the S$_N$2-type Reactivity of Aryl-Co(III) Masked-Carbenes for C-C Bond Forming Transformations

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1. General considerations

All reagents and solvents were purchased from Sigma Aldrich, Fisher Scientific or Fluorochem and used without further purification. Diazoacetates were synthesized using known procedures.[1,2] NMR data concerning product identity were collected with a Bruker 400 AVANCE (Serveis Tècnics, University of Girona) ($CDCl_3$, CD_3CN and DMSO-d_6) and calibrated relative the residual protons of the solvent. All NMR experiments (^1H, $^{13}C\{^1H\}$, COSY, HSQC, HMBC and NOESY) were recorded and processed using standard parameters and no more details are given. Quantification of reaction yields through integration of peaks was performed using an internal reference (1,3,5-trimethoxybenzene). Preparation and handling of air-sensitive materials were carried out in a N_2 drybox with O_2 and H_2O concentrations < 1 ppm. High resolution mass spectra (HRMS) were recorded on a Bruker MicrOTOF-Q IITM instrument using ESI or Cryospray ionization sources at Serveis Tècnics University of Girona.

XAS Data Acquisition and processing

Samples of **crude reaction mixture** (see Scheme were prepared as 15 mM solutions in trifluoroethanol and loaded into holders with Kapton windows. Data was collected at SOLEIL synchrotron, SAMBA beamline, under vacuum at 20 K using a liquid helium cryostat and Si(220) double crystal monochromator. Data was collected in fluorescence mode employing a 36-channel Ge fluorescence detector. Data calibration and normalization was carried out using the Athena software package.[3] The first inflection point of Co foil spectra taken as 7709.5 eV was used for energy calibration. A linear pre-edge function, followed by a quadratic polynomial for the post-edge, were used for background subtraction and normalization of the edge jump to unity. The AUTOBK algorithm with a spline between a k of 1.5 and 12.5 $Å^{-1}$ having a R_{bkg} value of 1.0 Å was used for EXAFS extraction. EXAFS analysis was carried out using the IFEFFIT engine and the FEFF6 code available in the Artemis software package.[3-5] The k^3-weighted data was fit in r-space over a r-range of 1 to 3 Å and a k-range of 2 to 12.5 $Å^{-1}$ using a Hannings window (dk=2). The S_0^2 value was set to 0.9, and a global ΔE_0 was employed with the initial E_0 value set to the inflection point of the rising edge. Scattering paths were fit in terms of a Δr_{eff} and σ^2 as previously described.[6,7] To assess the goodness of the fits both the R_{factor} (%R) and reduced χ^2 (χ^2_v) were minimized.

DFT Calculations

We used Gaussian 09 package[8] to perform all calculations. All geometry optimizations and frequency calculations were carry out with the BP86 functional[9,10] with the def2-TZVP basis set developed by Ahlrichs.[11,12] Empirical dispersion and solvation effects in 2,2,2-TriFluoroEthanol (TFE) were included using Grimme's DFT-D3 approach[13] and PCM-SMD method[14] respectively. All transition states were

connected to the corresponding reactants and products with IRC calculations. To refine the final free energy values we carried out Single Point Energy (SPE) calculations at the optimized geometries with the B3LYP[15-18] functional and def2-TZVP basis set including PCM-SMD and GD3-dispersion corrections (E_{B3LYP}). The free energy change associated to change from a standard-state gas concentration of 1 atm to a standard state gas phase concentration of 1 M for solutes ($\Delta G^{o/*}$) was also included in the final free energies values. In this case $\Delta G^{o/*}$ at 298.15 K is 1.89 kcal·mol^{-1} for 1 M standard state solutes. Entropic and Enthalpic correction were obtained from the frequency calculation at 298.15 K (G_{corr}). Then, the final total Gibbs free energy (G) was given by:

$$G = E_{B3LYP} + G_{corr.} + \Delta G^{o/*} \text{ (Equation 1)}$$

2. Protocol for the synthesis of Aryl-Co(III)-carboxylate complexes[19]
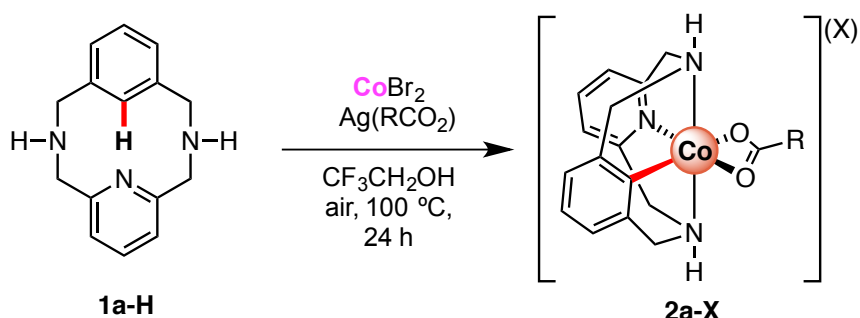
Scheme S1. Synthesis of aryl-Co(III) carboxylate complexes **2a-X**.

In a 10 mL vial, **1a-H** (50 mg, 0.21 mmol), Ag(RCOO$_2$) (0.63 mmol) and CoBr$_2$ (45.9 mg, 0.21 mmol) were mixed in CF$_3$CH$_2$OH (2.5 mL). The vial was then sealed with a septum and the mixture was warmed up to 100°C over 24h. Solvent was then removed, and the crude was dissolved in CHCl$_3$ and layered with pentane or diethyl ether. After 24 h at 4 °C, the resulting oil was dried under vacuum over 6h, obtaining a grey-red foam corresponding to the Co^{III} organometallic complex.

2.1 [**1a**-Co^{III}(OPiv)](OPiv) – (**2a-OPiv**)

Red foam (92% yield, 96 mg, 0.19 mmol). **^{1}H NMR** (400 MHz, CDCl$_3$, ppm) δ 7.47 (t, ^3J_H = 7.3 Hz, 1H), 7.04 (t, ^3J_H = 7.4 Hz, 1H), 6.95 (d, ^3J_H = 7.7 Hz, 2H), 6.89 (d, ^3J_H = 7.6 Hz, 2H), 4.85 (d, ^2J_H = 14.3 Hz, 2H), 4.74 (d, ^2J_H = 13.9 Hz, 2H), 3.76 (m, 4H), 1.24 (s, 9H, $^-$OPiv), 0.88 (s, 9H, OPiv). **^{13}C {^{1}H} NMR** (100 MHz, CDCl$_3$, ppm) 191.0, 180.8, 171.3,

161.6, 148.5, 138.8, 134.6, 124.2, 120.1, 118.2, 61.9, 61.4, 40.1, 29.7, 28.1. **HRMS** (ESI) calcd. for C$_{20}$H$_{25}$CoN$_3$O$_2^+$ [M-OPiv]$^+$: 398.1279; found: 398.1283.

2.2 [**1a**-Co^{III}(OBz)](OBz) – (**2a-OBz**)

Red foam (72% yield, 82 mg, 0.15 mmol). **^{1}H NMR** (400 MHz, CDCl$_3$, ppm) δ 8.10-7.80 (m, 5H), 7.66 (d, ^3J_H = 6.7 Hz, 2H) 7.46 (t, ^3J_H = 7.7 Hz, 1H), 7.22 (t, ^3J_H = 6.9 Hz, 1H), 7.14-7.10 (dd, 2H), 7.05 (t, ^3J_H = 7.3 Hz, 1H), 6.96 (d, ^3J_H = 7.7 Hz, 2H), 6.91 (d, ^3J_H = 7.3 Hz, 2H), 5.04 (d, ^2J_H = 13.9 Hz, 1H), 4.95 (d, ^2J_H = 14.5 Hz, 1H) 3.89 (m, 4H). **^{13}C {^{1}H} NMR** (100

MHz, CDCl$_3$, ppm) δ 170.0, 161.7, 148.6, 137.2, 130.1, 129.0, 127.3, 124.3, 120.5, 118.5, 62.4, 62.1. **HRMS** (ESI) calcd. for C$_{22}$H$_{21}$CoN$_3$O$_2^+$ [M-OBz]$^+$: 418.0966; found: 418.0952.

2.3 [**1a**-Co^{III}(OBz-NO$_2$)](OBz-NO$_2$) – (**2a-OBz-NO$_2$**)
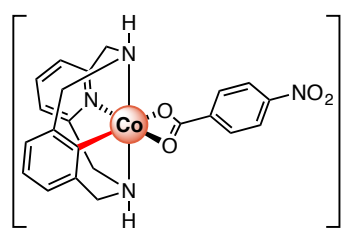
(OBz-NO$_2$) Orange-red foam (93% yield, 125 mg, 0.20 mmol). **^{1}H NMR** (400 MHz, CDCl$_3$, ppm) δ 8.28 (bs, 2H), 8.16 (bs, 2H), 7.99 (d, ^3J_H = 7.2 Hz, 2H), 7.78 (d, ^3J_H = 7.0 Hz, 2H), 7.57 (t, ^3J_H = 6.9 Hz, 1H), 7.10 (m, 1H), 7.01 (bs, 4H), 5.02 (dd, ^2J_H = 14.1 Hz, ^3J_H = 7.1 Hz, 2H), 4.93 (dd, ^2J_H = 14.0 Hz, ^3J_H = 6.9 Hz, 2H), 3.96 (m, 4H). **^{13}C {^{1}H} NMR** (100 MHz, CDCl$_3$, ppm) δ 191.4, 164.5, 156.8, 144.1, 143.6, 136.6, 133.0, 125.0, 120.0, 118.0, 116.1, 114.1, 57.7, 57.4. **HRMS** (ESI) calcd. for C$_{22}$H$_{20}$CoN$_4$O$_4$$^+$ [M-(OBz-NO$_2$)]$^+$: 463.0811; found: 463.0819.

2.4 [**1a**-Co^{III}(OBz-Acyl)](OBz-Acyl) – (**2a-OBz-COMe**)

(OBz-Acyl) Red foam (89% yield, 117 mg, 0.19 mmol). **^{1}H NMR** (400 MHz, CDCl$_3$, ppm) δ 7.71 (bs, 4H), 7.50 (t, ^3J_H = 6.8 Hz, 1H), 7.07 (t, ^3J_H = 7.2 Hz, 1H), 7.01 (bs, 4H), 6.99 (d, ^3J_H = 7.3 Hz, 2H), 6.94 (d, ^3J_H = 7.2 Hz, 1H), 5.01 (dd, ^2J_H = 14.2 Hz, ^3J_H = 7.4 Hz, 2H), 4.94 (dd, ^2J_H = 14.1 Hz, ^3J_H = 6.7 Hz, 2H), 3.85 (m, 4H), 2.49 (s, 3H). **^{13}C {^{1}H} NMR** (100 MHz, CDCl$_3$, ppm) δ 197.9, 161.7, 140.0, 138.1, 137.4, 129.0, 127.4, 124.5, 120.6, 118.5, 62.4, 62.1, 26.5. **HRMS** (ESI) calcd. for C$_{24}$H$_{23}$CoN$_3$O$_3$$^+$ [M-(OBz-Acyl)]$^+$: 460.1071; found: 460.1079.
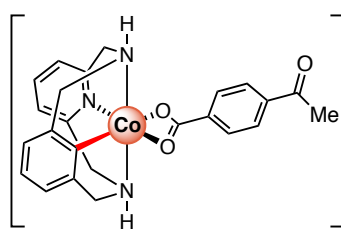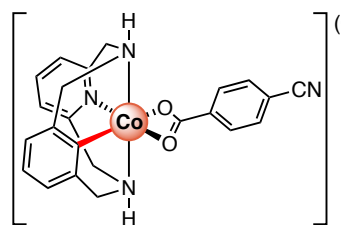
2.5 [**1a**-Co^{III}(OBz-CN)](OBz-CN) – (**2a-OBz-CN**)

(OBz-CN) Red foam (98% yield, 119 mg, 0.21 mmol). **^{1}H NMR** (400 MHz, CDCl$_3$, ppm) δ 8.23 (bs, 1H), 7.88 (bs, 2H), 7.72 (s, ^3J_H = 8.3 Hz, 2H), 7.60 (bs, 2H), 7.55 (t, ^3J_H = 7.9 Hz, 1H), 7.41 (d, ^3J_H = 8.1 Hz, 1H), 7.09 (m, 3H), 7.03 (m, 2H), 5.03 (dd, ^2J_H = 16.8 Hz, ^3J_H = 7.1 Hz, 2H), 4.93 (dd, ^2J_H = 16.3 Hz, ^3J_H = 6.8 Hz, 2H), 3.97 (d, ^2J_H = 17.6 Hz, 2H), 3.93 (d, ^2J_H = 16.8 Hz, 2H). **^{13}C {^{1}H} NMR** (100 MHz, CDCl$_3$, ppm) δ 178.1, 168.9, 161.5, 148.3, 139.5, 137.7, 131.4, 129.4, 124.8, 120.9, 118.8, 113.5, 62.5, 62.2. **HRMS** (ESI) calcd. for C$_{23}$H$_{20}$CoN$_4$O$_2$$^+$ [M-(OBz-CN)]$^+$: 443.0913; found: 443.0919.

2.6 [**1a**-Co^{III}(OBz-Me)](OBz-Me) – (**2a-OBz-Me**)
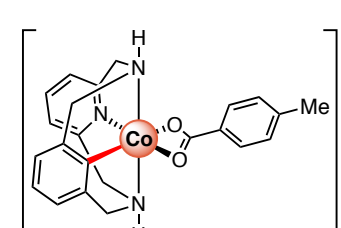
(OBz-Me) Red foam (95% yield, 118 mg, 0.20 mmol). **^{1}H NMR** (400 MHz, CDCl$_3$, ppm) δ 8.06 (bs, 1H), 7.58 (d, ^3J_H = 7.5 Hz, 2H), 7.43 (t, ^3J_H = 7.6 Hz, 2H), 7.33 (bs, 2H), 7.12 (bs, 2H), 7.03 (t, ^3J_H = 7.9 Hz, 2H), 6.97 (d, ^3J_H = 6.8 Hz, 2H), 6.95 (d, ^3J_H = 6.9 Hz, 2H), 6.88 (d, ^3J_H = 7.7 Hz, 2H), 4.99 (m, 2H), 4.91 (dd, ^2J_H = 15.2 Hz, ^3J_H = 6.1 Hz, 2H), 3.87 (d, ^2J_H = 13.8 Hz, 2H), 3.83 (d, ^2J_H = 13.9 Hz, 2H), 2.34 (bs, 3H),

2.25 (s, 3H). ^{13}C {^{1}H} NMR (100 MHz, CDCl$_3$, ppm) δ 170.7, 161.6, 148.5, 139.9, 137.1, 133.6, 129.6, 128.9, 128.0, 124.2, 120.4, 118.4, 62.2, 61.4, 21.3. **HRMS** (ESI) calcd. for C$_{23}$H$_{23}$CoN$_3$O$_2^+$ [M-(OBz-Me)]$^+$: 432.1117; found: 432.1120.

2.7 [**1a**-Co^{III}(TPA)](TPA) – (**2a-TPA**)
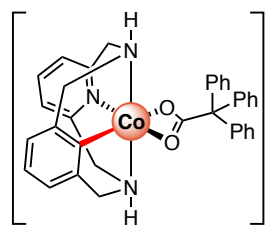
Red foam (92% yield, 166 mg, 0.19 mmol). ^{1}**H NMR** (400 MHz, CDCl$_3$, ppm) δ 7.56 (bs, 5H), 7.40 (t, ^3J_H = 7.4 Hz, 1H), 7.33 (bs, 2H), 7.23 (d, ^3J_H = 7.3 Hz, 4H), 7.05 (m, 10H), c6.97 (d, ^3J_H = 7.3 Hz, 2H), 6.95 (d, ^3J_H = 7.4 Hz, 2H), 6.88 (m, 6H), 6.69 (d, ^3J_H = 7.3 Hz, 2H), 6.61 (bs, 2H), 4.21 (dd, ^2J_H = 16.8 Hz, ^3J_H = 7.3 Hz, 2H), 4.10 (dd, ^2J_H = 14.2 Hz, ^3J_H = 6.1 Hz, 2H), 3.44 (d, ^2J_H = 16.6 Hz, 4H). ^{13}C {^{1}H} **NMR** (100 MHz, CDCl$_3$, ppm) 181.5, 170.8, 161.3, 148.6, 146.7, 145.9, 136.6, 130.7, 130.6, 128.3, 127.1, 126.9, 124.2, 120.3, 118.3, 70.6, 69.3, 61.9, 61.4. **HRMS** (ESI) calcd. for C$_{35}$H$_{31}$CoN$_3$O$_2^+$ [M-TPA]$^+$: 584.1748; found: 584.1754.

3. Evaluation of the scope of diazo acetate annulation

3.1 Aryl-Co(III) carboxylates
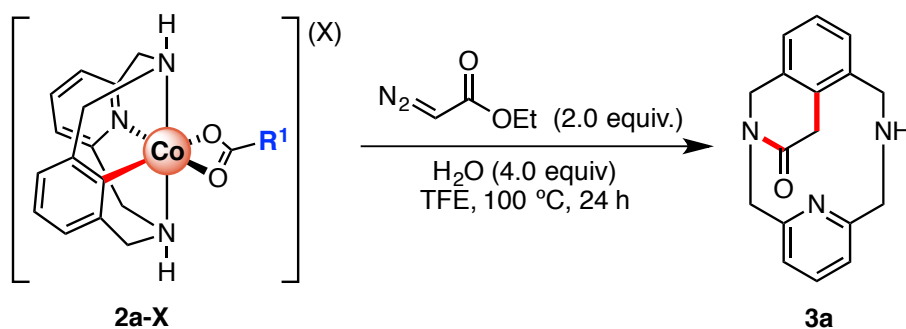
Scheme S2. Stoichiometric reaction of **2a-X** with EDA to furnish cyclic amide **3**.

In a 2 mL vial, **2a-X** (0.058 mmol), ethyl diazoacetate (14µl, 0.115 mmol) and H_2O (9 µl, 4.0 equiv.) were mixed in TFE (1.5 mL). The vial was then sealed with a septum and the mixture was stirred under air over 24h at 100ºC. Then, after removal of the solvent, NH_4OH (2 mL) was added and the solution was extracted using CH_2Cl_2 (2x5mL). Then, products were purified using silica gel chromatography (CH_2Cl_2, then CH_2Cl_2/MeOH 95:5) and characterized by NMR techniques.

Table S1. Reaction of **2a-OAc** with EDA (x equiv.) and water as additive (4.0 equiv.) to furnish cyclic amide **3**.

Entry	R^1 (R^1CO_2)	Yield of 3 (%)[a]
1	Me (OAc)	91%
2	Piv (OPiv)	23% (20%)[b]
3	CPh_3 (TPA)	traces
8	CF_3 (TFA)	75%
3	Ph (OBz)	78%
4	p-OMe-Ph (OBz-OMe)	71%
5	p-Me-Ph (OBz-Me)	72%
6	p-Cl-Ph (OBz-Cl)	81%
7	p-COMe-Ph (OBz-COMe)	85%
8	p-CN-Ph (OBz-CN)	80%
9	p-NO_2-Ph (OBz-NO_2)	81%

[a]Isolated yield after silica gel cromatography. [b]Reaction carried out in presence of 1.0 equiv. of LiOTf.

3.2 Alkyl diazoacetate substrate scope – α-substituted diazo acetates
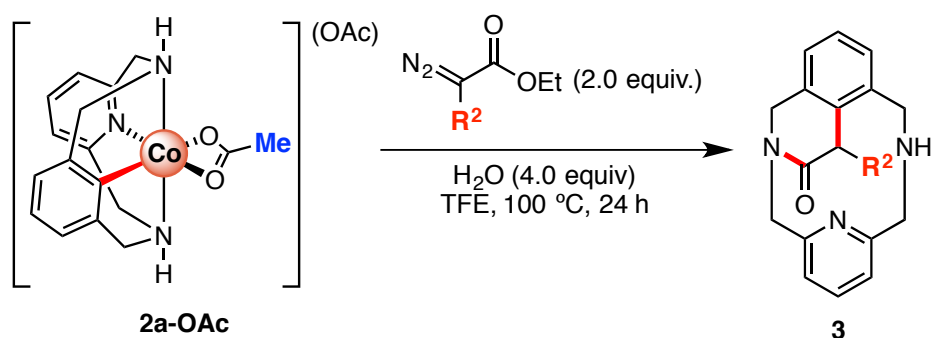
Scheme S3. Stoichiometric reaction of **2a-OAc** with alkyl to furnish cyclic amide **3**.

In a 2 mL vial, **2a-OAc** (30mg, 0.058 mmol), **α-substituted diazoacetate** (0.115 mmol) and H_2O (9 μl, 4.0 equiv.) were mixed in TFE (1.5 mL). The vial was then sealed with a septum and the mixture was stirred under air over 24h at 100ºC. Then, after removal of the solvent, NH_4OH (2 mL) was added and the solution was extracted using CH_2Cl_2 (2x5mL). Then, products were purified using silica gel chromatography (CH_2Cl_2, then CH_2Cl_2/MeOH 95:5) and characterized by NMR techniques.

Table S2. Reaction of **2a-OAc** with **α-substituted** diazoacetate (2.0 equiv.) and water as additive (4.0 equiv.) to furnish cyclic amide **3**.

Entry	R^2	Yield of 3x (%)[a]
1	H	91%
2	Me (**b**)	traces
3	Bn (**c**)	traces
4	EtOOC (**d**)	73% (**3a**)
5	CF_3 (**e**)	traces
6	NO_2 (**f**)	n.r
7	CN (**g**)	n.r
8	Ph (**h**)	traces[b]
9	p-OMe-Ph (**i**)	n.r.[b]
10	p-Br-Ph (**j**)	11% (65%)[b] (**3j**)
11	p-CF_3-Ph (**k**)	8% (74%)[b] (**3k**)
12	p-NO_2-Ph (**l**)	10% (73%)[b] (**3l**)
13[c]	p-NO_2-Ph (**l**)	traces

[a]Isolated yields. [b]Reaction carried out in presence of 4.0 equiv. of diazoester and 1.0 equiv. of LiOTf. [c]Reaction carried out in absence of additives.

3.3 Alkyl diazoacetate substrate scope – Influence of the ester substituent
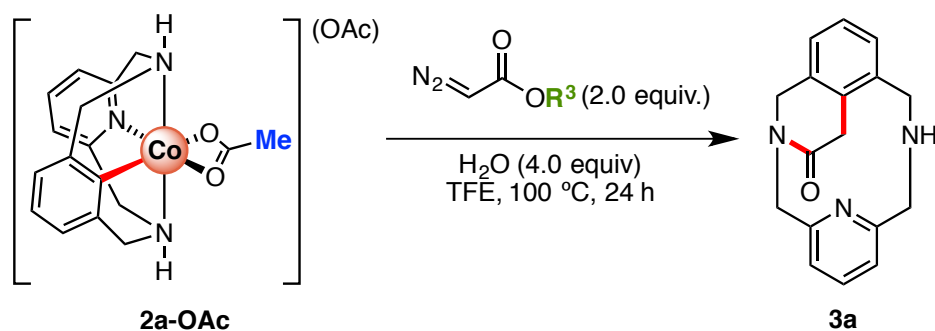
Scheme S4. Stoichometric reaction of **2a-OAc** with alkyl to furnish cyclic amide **3a**.

In a 2 mL vial, **2a-OAc** (30mg, 0.058 mmol), **alkyl diazoacetate** (0.115 mmol) and H_2O (9 μl, 4.0 equiv.) were mixed in TFE (1.5 mL). The vial was then sealed with a septum and the mixture was stirred under air over 24h at 100ºC. Then, after removal of the solvent, NH_4OH (2 mL) was added and the solution was extracted using CH_2Cl_2 (2x5mL). Then, products were purified using silica gel chromatography (CH_2Cl_2, then CH_2Cl_2/MeOH 95:5) and characterized by NMR techniques.

Table S3. Reaction of **2a-OAc** with alkyl diazoacetate (2.0 equiv.) and water as additive (4.0 equiv.) to furnish cyclic amide **3**.

Entry	R	Yield of 3 (%)[a]
1[b]	Et	10%[c]
2	Et	91%
3[b,d]	Et	31%
4[d]	Et	78%
5[b]	Me	18%[c]
6	Me	90%
7[b]	Bn	71%
8	Bn	89%
9[b]	tBu	87%
10	tBu	92%
11[b]	Ph	79%
12	Ph	78%

[a]Isolated yields. [b]No water was added. [c]Yield determined using 1,3,5-trimethoxybenzene as internal standard in a mixture of macrocyclic ligand and product. [d]HFIP as solvent.

4. Mechanistic insights

4.1 Competition experiments between electronically different α-substituted diazoacetates
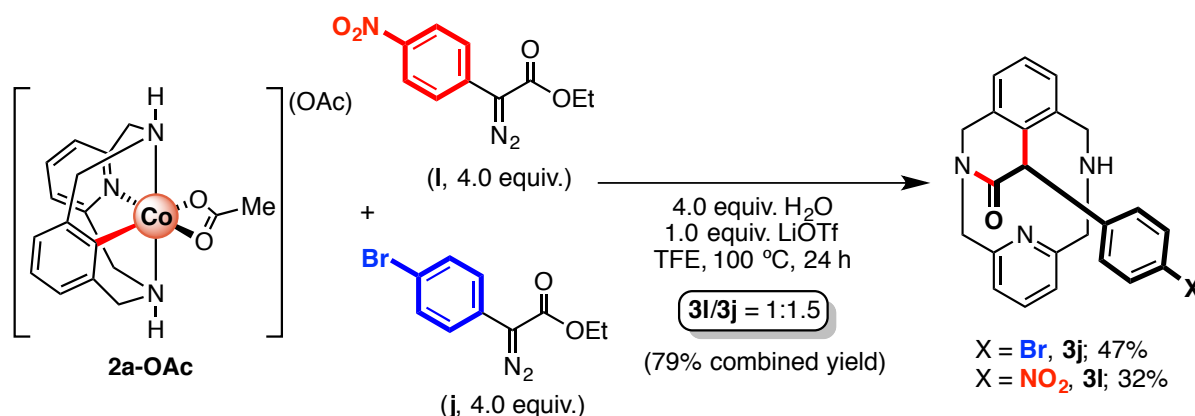
Scheme S5. Competition reaction of **2a-OAc** with electronically different diazo acetates.

In a 2 mL vial, **2a-OAc** (30 mg, 0.058 mmol) was mixed with **l** and **j** (0.232 mmol. 4.0 equiv. each), LiOTf (9 mg, 0.058 mmol, 1.0 equiv.) and H$_2$O (9 μl, 4.0 equiv.) were mixed in TFE (1.5 mL). The vial was then sealed with a septum and the mixture was stirred under air over 24h at 100ºC. Then, after removal of the solvent, NH$_4$OH (2 mL) was added and the solution was extracted using Et$_2$O (2x5mL). Then, reactions crudes were analyzed by NMR techniques using 1,3,5-trimethoxybenzene as internal standard.

4.2 Competition experiments between sterically different diazoacetates
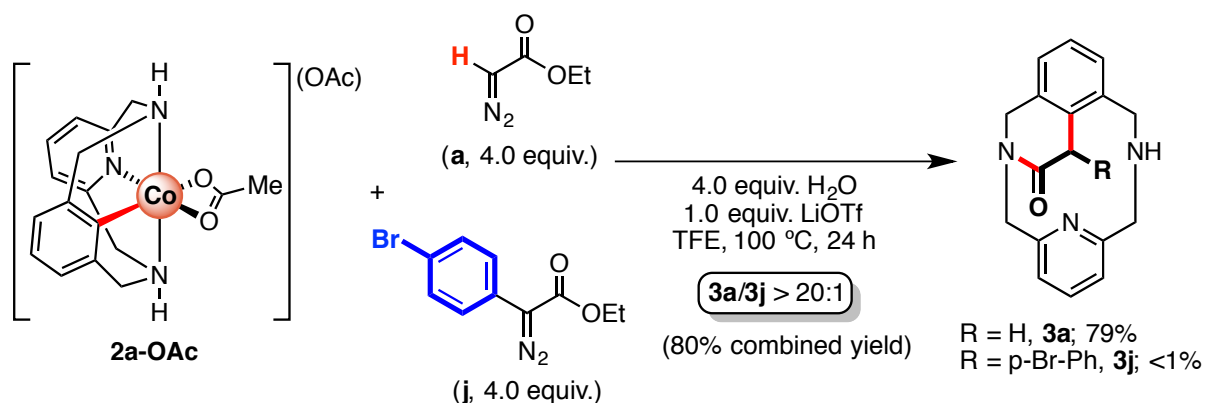
Scheme S6. Competition reaction of **2a-OAc** with sterically different diazo acetates.

In a 2 mL vial, **2a-OAc** (30 mg, 0.058 mmol) was mixed with **a** and **j** (0.232 mmol. 4.0 equiv. each), LiOTf (9 mg, 0.058 mmol, 1.0 equiv.) and H$_2$O (9 μl, 4.0 equiv.) were mixed in TFE (1.5 mL). The vial was then sealed with a septum and the mixture was stirred under air over 24h at 100ºC. Then, after removal of the solvent, NH$_4$OH (2 mL) was added and the solution was extracted using Et$_2$O (2x5mL). Then, reactions crudes were analyzed by NMR techniques using 1,3,5-trimethoxybenzene as internal standard.

4.3 Poisoning studies with electron-rich diazo acetates
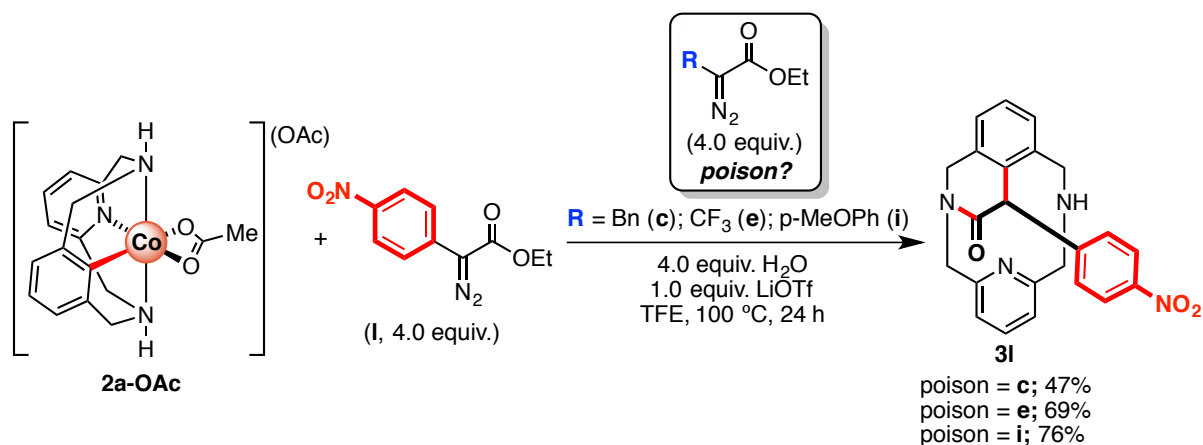
Scheme S7. Poisoning reactions of **2a-OAc** with non-reactive diazoesters **c**, **e** and **i**.

In a 2 mL vial, **2a-OAc** (30 mg, 0.058 mmol) was mixed with **l** and **poison** (0.232 mmol. 4.0 equiv. each), LiOTf (9 mg, 0.058 mmol, 1.0 equiv.) and H_2O (9 µl, 4.0 equiv.) were mixed in TFE (1.5 mL). The vial was then sealed with a septum and the mixture was stirred under air over 24h at 100ºC. Then, after removal of the solvent, NH_4OH (2 mL) was added and the solution was extracted using Et_2O (2x5mL). Then, reactions crudes were analyzed by NMR techniques using 1,3,5-trimethoxybenzene as internal standard.

4.4 Deuterium Incorporation experiments
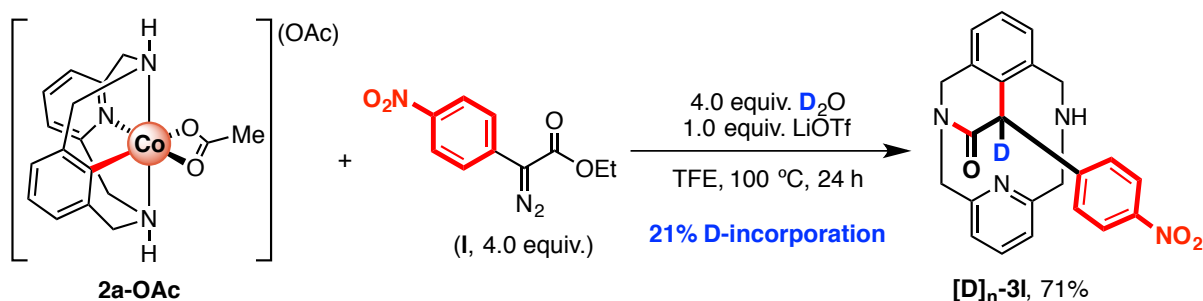
Scheme S8. Reaction of **2a-OAc** with EDA in presence of D_2O to furnish deuterated cyclic amide **D-3l**.

In a 2 mL vial, **2a-OAc** (0.058 mmol), ethyl diazoacetate (14 µl, 0.115 mmol) and D_2O (4.2 µl, 4.0 equiv.) and LiOTf (1.0 equiv) were mixed in TFE (0.5 mL). The vial was then sealed with a septum and the mixture was stirred under air over 24h at 100ºC. Then, after removal of the solvent, NH_4OH (2 mL) was added and the solution was extracted using CH_2Cl_2 (2x5mL). Then, products were purified using silica gel chromatography (CH_2Cl_2, then CH_2Cl_2/MeOH 90:10) and analyzed by NMR spectroscopy (Figure S1).
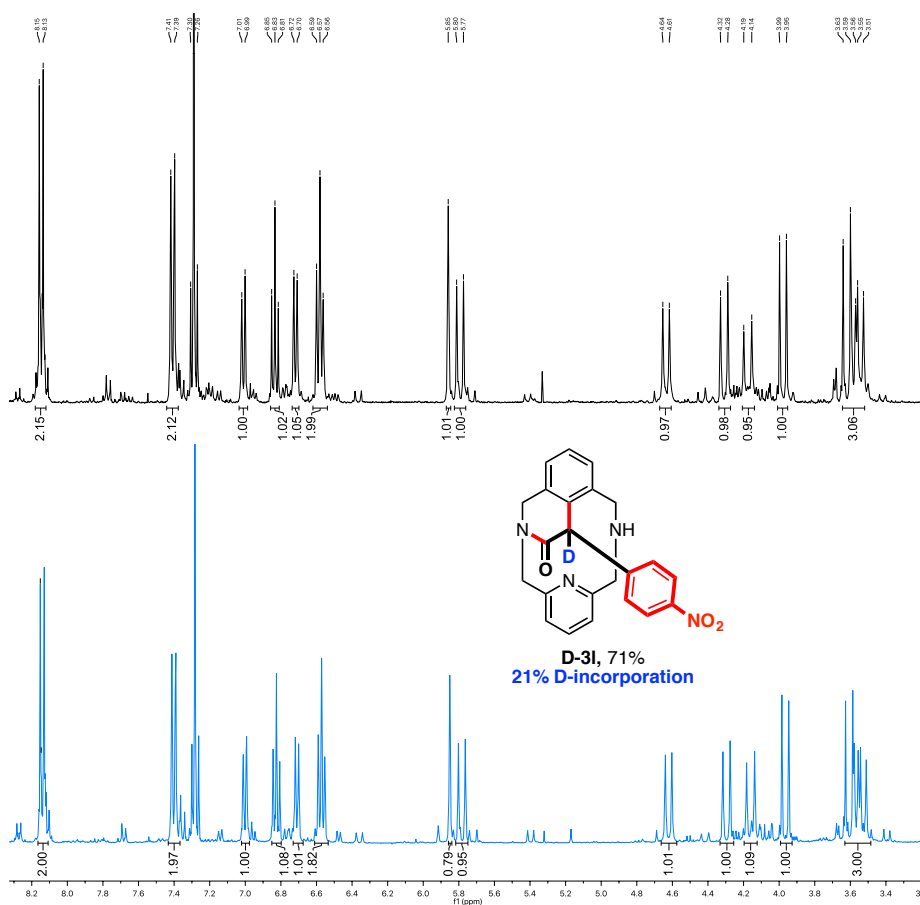
Figure S1. ^{1}H NMR spectrum of **3l** (up, black) and **D-3l** (down, blue) recorded at 298K using CDCl$_3$ as solvent. 21% of deuterium incorporation from D$_2$O (4.0 equiv.) using TFE as solvent.

5. Detection and isolation of reaction intermediates using EDA[19]
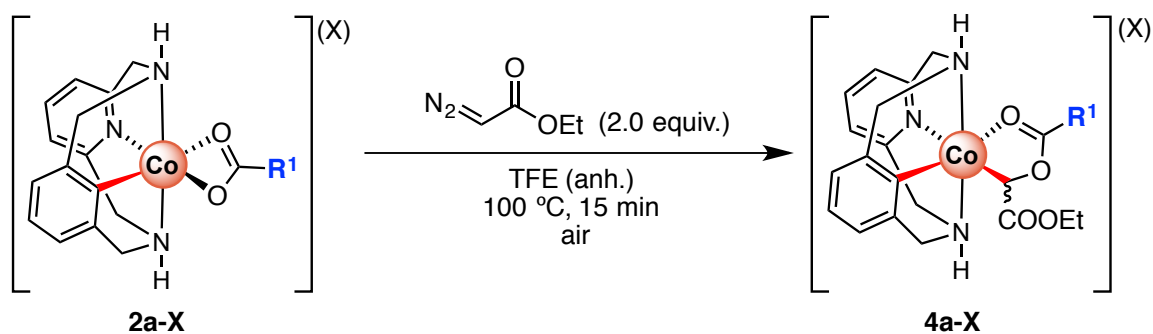
Scheme S9. Stoichometric reaction of **2a-X** with EDA to furnish intermediate species **5a-X**.

In a 2 mL vial, **2a-X** (0.06 mmol) and **ethyl diazoacetate** (2.0 equiv.) were mixed in TFE (1.5 mL). The vial was then sealed with a septum and the mixture was stirred under air over 15 min at 100ºC. After reaction completion, crude mixture was analyzed by HRMS and reaction intermediates were detected as major products. Then, recrystallization with $CHCl_3$ layered with pentane yielded the corresponding organometallic complex **4a-X**, which was characterized by NMR and X-Ray spectroscopy. When R = EWD, intermediate **4a-X** (X = OBz-NO_2, TFA) cannot be isolated.

5.1 [**1a**-Co^{III}(EDA-OPiv)](Br) – (**4a-OPiv**)
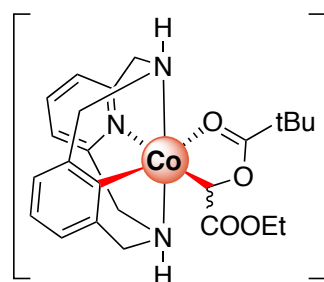
(Br) Orange crystaline solid (87% yield, 29 mg, 0.051 mmol). **¹H NMR (400 MHz, CDCl₃, ppm)** δ 7.90 (t, ^3J_H= 7.2 Hz, 1H), 7.43 (d, ^3J_H= 7.3 Hz, 1H), 7.34 (d, ^3J_H = 7.5 Hz, 1H), 6.83 (t, ^3J_H = 7.3 Hz, 1H), 6.78 (d, ^3J_H = 6.9 Hz, 1H), 6.65 (d, ^3J_H= 7.1 Hz, 1H), 5.77 (s, 1H), 5.40 (bt, ^3J_H= 6.4 Hz, 1H), 4.45 (bt, ^3J_H= 6.8 Hz, 1H), 4.15 (m, 1H), 4.14 (m, 3H), 4.02 (d, ^3J_H= 7.7 Hz, 1H), 3.92 (d, ^3J_H= 7.6 Hz, 1H),

3.80 (dq, ^2J_H= 10.9 Hz, ^3J_H= 7.3 Hz, 1H), 3.63 (d, ^3J_H= 7.3 Hz, 1H), 3.57 (d, ^3J_H= 7.4 Hz, 1H), 3.28 (dq, 1H), 1.37 (s, 9H), 0.78 (t, ^3J_H= 7.1 Hz, 3H). **¹³C {¹H} NMR** (100 MHz, CDCl₃, ppm) δ 193.0, 180.0, 150.4, 159.5, 146.4, 146.1, 139.0, 123.1, 120.4, 119.9, 119.5, 79.7, 64.7, 63.7, 62.7, 59.5, 38.8, 27.7, 14.0. **HRMS** (ESI) calcd. for C₂₄H₃₁CoN₃O₄$^+$ [M-OPiv]$^+$: 484.1641; found: 484.1654. **IR (ATR):** v̄ = 3020, 2864, 1686, 1617, 1358, 1035, 770, 598 cm^{-1}.
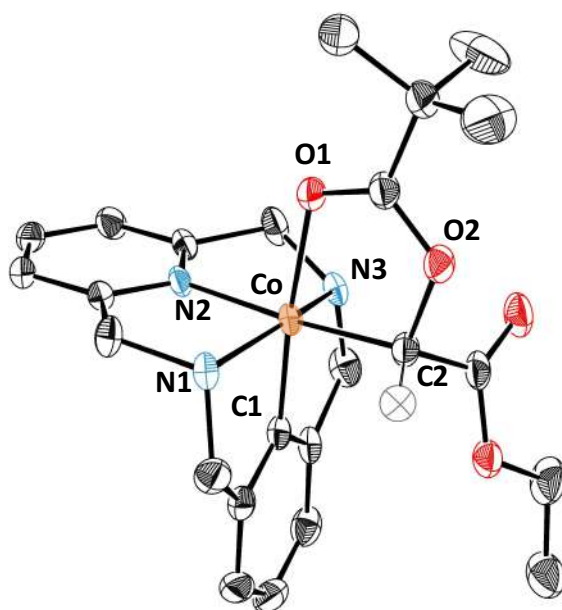
Figure S2. Solid state structures of aryl-Co(III)-EDA intermediate 4a-OPiv. Hydrogen atoms, anions and solvent molecules have been omitted for clarity; ellipsoids are set at 50% probability. Selected bond distances [Å] and angles [º]: Co-C(1) 1.840(6), Co-C(2) 1.962(4), Co-N(1) 2.002(4), Co-N(2) 1.892(3), Co-N(3) 1.994(4), Co-O(1) 2.023(4); C(1)-Co-C(2) 92.68(2), C(2)-Co-O(1) 82.12(2), C(1)-Co-N(2) 93.31(2), C(1)-Co-O(1) 174.79(2).

5.2 [**1a**-Co^{III}(EDA-OBz)](OBz) – (**4a-OBz**)
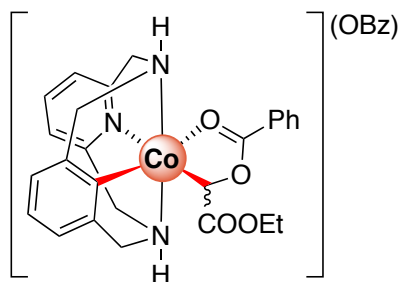
Orange crystaline solid (76% yield, 27.6 mg, 0.045 mmol). **^{1}H NMR** (400 MHz, CDCl$_3$, ppm) δ 8.19 (d, ^3J_H = 7.8 Hz, 1H), 7.93 (t, ^3J_H = 7.6 Hz, 1H), 7.80 (t, ^3J_H = 7.2 Hz, 1H), 7.62 (t, ^3J_H = 7.8 Hz, 2H), 7.45 (d, ^3J_H = 7.1 Hz, 1H), 7.38 (d, ^3J_H = 7.1 Hz, 1H), 6.85 (t, ^3J_H = 7.2 Hz, 1H), 6.81 (d, ^3J_H = 7.3 Hz, 1H), 6.68 (t, ^3J_H = 7.2 Hz, 1H), 6.06 (s, 1H), 5.61 (bt, ^3J_H = 6.7 Hz, 1H), 4.73 (bt, ^3J_H = 6.8 Hz, 1H), 4.53 5 (dd, ^2J_H = 16.1 Hz, ^3J_H = 7.7 Hz, 1H), 4.20 (m, 2H), 4.15 (dd, ^2J_H = 15.1 Hz, ^3J_H = 7.4 Hz, 1H), 4.04 (d, ^3J_H = 7.3 Hz, 1H), 3.95 (d, ^3J_H = 7.3 Hz, 1H), 3.82 (dq, ^2J_H = 10.9 Hz, ^3J_H = 7.3 Hz, 1H), 3.69 (d, ^3J_H = 7.3 Hz, 1H), 3.59 (d, ^3J_H = 7.3 Hz, 1H), 3.28 (dq, ^2J_H = 10.9 Hz, ^3J_H = 7.3 Hz, 1H), 0.78 (t, ^3J_H = 7.2 Hz, 3H) . **^{13}C {^{1}H} NMR** (100 MHz, CDCl$_3$, ppm) δ 180.2, 179.8, 160.6, 159.8, 146.6, 146.3, 139.0, 135.0, 130.8, 129.4, 128.0, 123.2, 120.5, 120.3, 119.8, 119.7, 77.2, 64.77, 63.8, 62.8, 62.5, 59.6, 14.0. **HRMS** (ESI) calcd. for C$_{26}$H$_{27}$CoN$_3$O$_4^+$ [M-OBn]$^+$: 504.1328; found: 504.1345. **IR (ATR):** ū (C=O) = 3227, 2927, 1683, 1629, 1598, 1553, 1379, 1040, 1023, 711, 657 cm^{-1}.
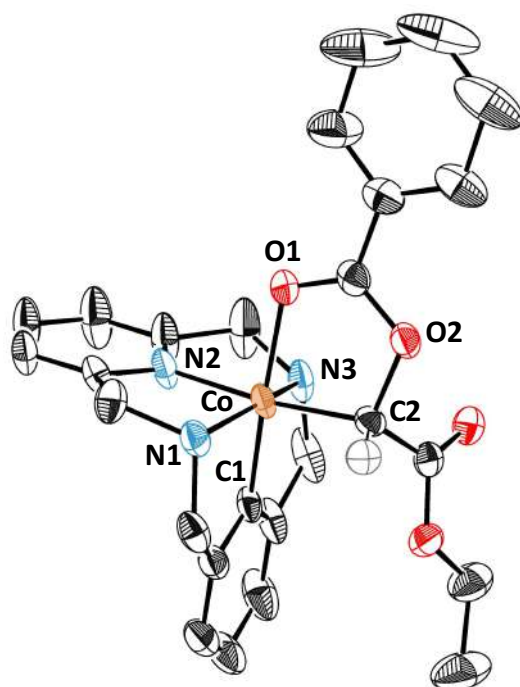
Figure S3. Solid state structures of aryl-Co(III)-EDA intermediate 4a-OBz. Hydrogen atoms, anions and solvent molecules have been omitted for clarity; ellipsoids are set at 50% probability. Selected bond distances [Å] and angles [º]: Co-C(1) 1.840(4), Co-C(2) 1.983(4), Co-N(1) 1.998(3), Co-N(2) 1.899(3), Co-N(3) 2.000(3), Co-O(1) 2.001(3); C(1)-Co-C(2) 95.60(2), C(2)-Co-O(1) 82.33 (2), C(1)-Co-N(2) 91.87(2), C(1)-Co-O(1) 177.49(2).

5.3 [**1a**-Co^{III}(EDA-OBz-NO$_2$)](OBz- NO$_2$) – (**4a-OBz-NO$_2$**)

Brown foam (21% yield, 8.7 mg, 0.012 mmol). **^{1}H NMR** (400 MHz, CDCl$_3$, ppm) δ 8.42 (m, 2H), 8.11 (d, ^3J_H = 7.4 Hz, 2H), 7.94 (t, ^3J_H = 6.9 Hz, 1H), 7.47 (d, ^3J_H = 7.1 Hz, 1H), 7.39 (d, ^3J_H = 7.2 Hz, 1H), 6.87 (d, ^3J_H = 6.6 Hz, 1H), 6.83 (d, ^3J_H = 7.4 Hz, 1H), 6.70 (d, ^3J_H = 7.3 Hz, 1H), 6.13 (s, 1H), 5.71 (t, ^3J_H = 7.2 Hz, 1H), 4.83 (d, ^3J_H = 7.2 Hz, 1H), 4.58 (dd, ^2J_H = 16.9 Hz, ^3J_H = 7.8 Hz, 1H), 4.29 (m, 2H), 4.18 (dd, ^2J_H = 15.7 Hz, ^3J_H = 7.2 Hz, 1H), 4.09 (d, ^2J_H = 18.4 Hz, 1H), 3.99 (d, ^2J_H = 18.1 Hz, 1H), 3.83 (dq, ^2J_H = 10.9 Hz, ^3J_H = 7.2 Hz, 1H), 3.73 (d, ^2J_H = 17.9 Hz, 1H), 3.64 (d, ^2J_H = 18.2 Hz, 1H), 3.30 (dq, ^2J_H = 10.8 Hz, ^3J_H = 7.3 Hz, 1H), 0.80 (t, ^3J_H = 7.0 Hz, 3H). **^{13}C {^{1}H} NMR** (100 MHz, CDCl$_3$, ppm) δ 179.9, 178.2, 169.6, 168.5, 151.2, 146.6, 146.3, 139.1, 133.3, 132.2, 131.1, 124.4, 123.8, 123.3, 120.5, 120.3, 119.9, 119.8, 78.3, 67.5, 64.8, 63.8, 62.6, 59.7, 14.0. **HRMS** (ESI) calcd. for C$_{26}$H$_{26}$CoN$_4$O$_6^+$ [M-(OBz-NO$_2$)]$^+$: 549.1179; found: 549.1167. **IR (ATR):** ῡ = 1620, 1578, 1517, 1338, 1275, 826, 723, 507 cm^{-1}.

Figure S4. Solid state structure of aryl-Co(III)-EDA intermediate 4a-OBz-NO$_2$. Hydrogen atoms, anions and solvent molecules have been omitted for clarity; ellipsoids are set at 50% probability. Selected bond distances [Å] and angles [º]: Co-C(1) 1.809(2), Co-C2 1.976(4), Co-N(1) 2.002(4), Co-N(2) 1.899(3), Co-N(3) 1.981(4), Co-O(1) 2.000(4), C(2)-O(2) 1.507(7); C(1)-Co-C(2) 94.1(1), C(1)-Co-O(1) 175.3(2).

5.4 [**1a**-Co^{III}(EDA-OBz-COMe)](OBz-COMe) – (**4a-OBz-COMe**)
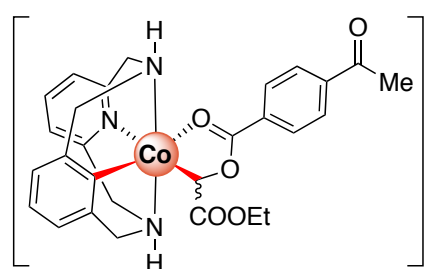
Orange crystalline solid (42% yield, 17.7 mg, 0.024 mmol). **^{1}H NMR** (400 MHz, CDCl$_3$, ppm) δ 8.29 (d, ^3J_H = 7.9 Hz, 2H), 8.12 (d, ^3J_H = 7.7 Hz, 2H), 7.92 (t, ^3J_H = 6.9 Hz, 1H), 7.45 (d, ^3J_H = 7.2 Hz, 1H), 7.38 (d, ^3J_H = 7.2 Hz, 1H), 6.86 (t, ^3J_H = 6.6 Hz, 1H), 6.81 (d, ^3J_H = 7.3 Hz, 1H), 6.68 (d, ^3J_H = 7.4 Hz, 1H), 6.11 (s, 1H), 5.81 (t, ^3J_H = 7.1 Hz, 1H), 4.79 (t, ^3J_H = 7.2 Hz, 1H), 4.56 (dd, ^2J_H = 17.1 Hz, ^3J_H = 7.8 Hz, 1H), 4.25 (m, 1H), 4.18 (dd, ^2J_H = 15.7 Hz, ^3J_H = 7.2 Hz, 1H), 4.06 (d, ^2J_H = 18.4 Hz, 1H), 3.96 (d, ^2J_H = 18.1 Hz, 1H), 3.83 (dq, ^2J_H = 10.9 Hz, ^3J_H = 7.2 Hz, 1H), 3.70 (d, ^2J_H = 17.9 Hz, 1H), 3.60 (d, ^2J_H = 18.2 Hz, 1H), 3.27 (dq, ^2J_H = 10.8 Hz, ^3J_H = 7.3 Hz, 1H), 2.67 (s, 3H), 0.78 (t, ^3J_H = 7.0 Hz, 3H). **^{13}C {^{1}H} NMR** (100 MHz, CDCl$_3$, ppm) δ 198.4, 198.1, 180.0, 179.0, 169.8, 166.3, 160.7, 159.9, 146.6, 146.4, 141.2, 139.0, 131.5, 131.1, 128.9, 123.1, 120.5, 120.3, 119.9, 119.7, 77.7, 64.8, 63.7, 62.7, 62.4, 59.9, 27.5, 14.0. **HRMS** (ESI) calcd. for C$_{28}$H$_{29}$CoN$_3$O$_5^+$ [M-(OBz-COMe)]$^+$: 546.1436; found: 546.1429. **IR (ATR):** ῡ = 1680, 1632, 1196, 752, 747, 695 cm^{-1}.
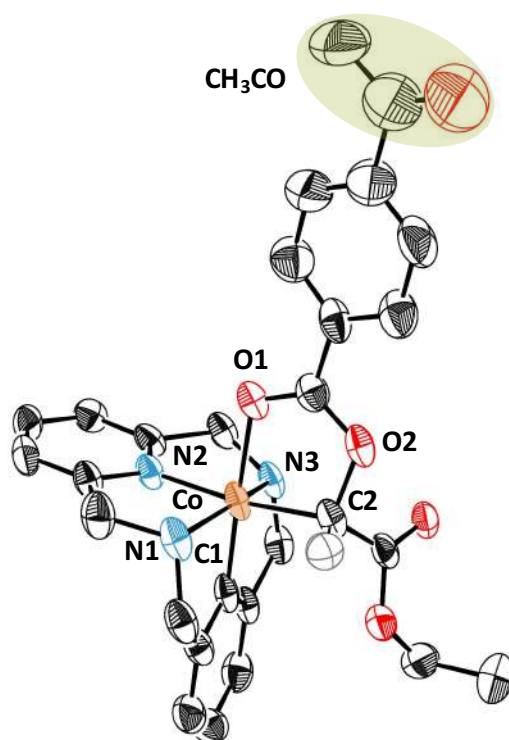
Figure S5. Solid state structure of aryl-Co(III)-EDA intermediate 4a-OBz-COMe. Hydrogen atoms, anions and solvent molecules have been omitted for clarity; ellipsoids are set at 50% probability. Selected bond distances [Å] and angles [°]: Co-C(1) 1.849(2), Co-C2 1.978(4), Co-N(1) 2.002(4), Co-N(2) 1.886(3), Co-N(3) 2.000(4), Co-O(1) 2.016(4), C(2)-O(2) 1.499 (7); C(1)-Co-C(2) 95.8(1), C(1)-Co-O(1) 177.9(2).

5.5 [1a-Co^{III}(EDA-OBz-Me)](OBz-Me) – (4a-OBz-Me)
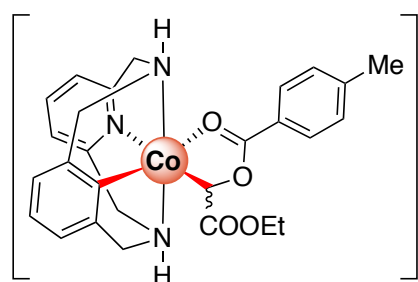
Orange crystalline solid (89% yield, 33.8 mg, 0.052 mmol). **¹H NMR** (400 MHz, CDCl₃, ppm) δ 8.03 (d, ^3J_H = 8.1 Hz, 2H), 7.88 (t, ^3J_H = 7.2 Hz, 1H), 7.80 (m, 2H), k7.41 (d, ^3J_H = 7.2 Hz, 1H), 7.38 (d, ^3J_H = 7.2 Hz, 2H), 7.34 (d, ^3J_H = 7.2 Hz, 2H), 7.24 (m, 2H), 6.82 (t, ^3J_H = 7.5 Hz, 1H), 6.78 (d, ^3J_H = 7.1 Hz, 1H), 6.64 (d, ^3J_H = 7.2 Hz, 1H), 6.05 (s, 1H), 5.92 (bt, 1H, NH), 5.92c (bt, 1H, NH), 4.68 (t, ^3J_H = 6.7 Hz, 1H, NH), 4.49 (dd, ^2J_H = 17.4 Hz, ^3J_H = 7.5 Hz, 1H), 4.20 (m, 2H), 4.13 (dd, ^2J_H = 16.7 Hz, ^3J_H = 7.4 Hz, 1H), 4.00 (d, ^2J_H = 18.1 Hz, 1H), 3.76 (dq, ^2J_H = 10.3 Hz, ^3J_H = 7.3 Hz, 1H), 3.63 (d, ^2J_H = 17.9 Hz, 1H), 3.55 (d, ^2J_H = 18.2 Hz, 1H), 3.23 (dq, ^2J_H = 10.3 Hz, ^3J_H = 7.3 Hz, 1H), 2.41 (s, 3H), 0.75 (t, ^3J_H = 7.1 Hz, 3H). **¹³C {¹H} NMR** (100 MHz, CDCl₃, ppm) δ180.3, 179.6, 170.1, 167.0, 160.8, 145.6, 138.9, 130.9, 129.9, 128.1, 125.3, 123.1, 120.4, 120.2, 119.8, 119.6, 76.9, 64.8, 63.8, 62.8, 62.5, 59.8, 21.8, 14.1. **HRMS** (ESI) calcd. for $C_{27}H_{29}CoN_3O_4^+$ [M-(OBz-Me)]⁺: 518.1485; found: 518.1478. **IR (ATR):** v̄ =1682, 1622, 1376, 1141, 1035, 750 cm⁻¹.
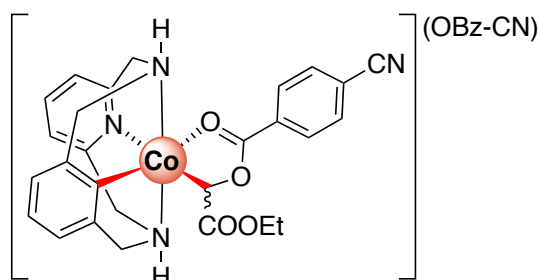
5.6 [1a-Co^{III}(EDA-OBz-CN)](OBz-CN) – (4a-OBz-CN)

Red foam (56% yield, 21.9 mg, 0.032 mmol). **¹H NMR** (400 MHz, CDCl₃, ppm) δ 8.30 (d, ^3J_H = 8.4 Hz, 2H), 8.05 (d, ^3J_H = 8.1 Hz, 1H), 7.92 (t, ^3J_H = 7.9 Hz, 1H), 7.71 (d, ^3J_H = 7.9 Hz, 1H), 7.44 (d, ^3J_H = 7.5 Hz, 1H), 7.37 (d, ^3J_H = 7.7 Hz, 1H), 6.85 (d, ^3J_H = 7.2 Hz, 1H), 6.68 (d, ^3J_H = 7.7 Hz, 1H), 6.12 (s, 1H), 5.82 (t, ^3J_H = 7.2 Hz, 1H), 4.78 (d, ^3J_H = 7.2 Hz, 1H), 4.56 (dd, ^2J_H = 17.5 Hz, ^3J_H = 7.8 Hz, 1H), 4.26 (dd, ^2J_H = 16.8 Hz, ^3J_H = 6.9 Hz, 1H), 4.08 (d, ^2J_H = 17.2 Hz, 1H), 3.96 (d, ^2J_H = 15.9 Hz, 1H), 3.85 (d, ^3J_H = 15.2 Hz, 1H), 3.76 (dq, ^2J_H = 10.8 Hz, ^3J_H = 7.3 Hz, 1H), 3.70 (d, ^2J_H = 15.9 Hz, 1H), 3.60 (d, ^2J_H = 15.9 Hz, 1H), 3.28 (dq, ^2J_H = 10.6 Hz, ^3J_H = 6.9 Hz, 1H), 0.78 (t, ^3J_H = 7.1 Hz, 3H). **¹³C {¹H} NMR** (100 MHz, CDCl₃, ppm) δ 179.9, 178.5, 160.7, 159.9, 146.6, 146.4, 139.1, 133.3, 131.3, 123.3, 120.5, 119.8, 118.4, 116.8, 78.2, 66.4, 64.8, 62.7, 62.4, 59.7, 14.0. **HRMS** (ESI) calcd. for $C_{27}H_{26}CoN_4O_4^+$ [M-(OBz-CN)]⁺: 529.1281; found: 529.1274. **IR (ATR):** v̄ = 2225, 1679, 1634, 1377, 1197, 753, 544 cm⁻¹.

6. Reactivity of C-metalated aryl-Co(III) enolate species

6.1 Evolution of organometallic **4a-X** species to cyclic amide **3a**
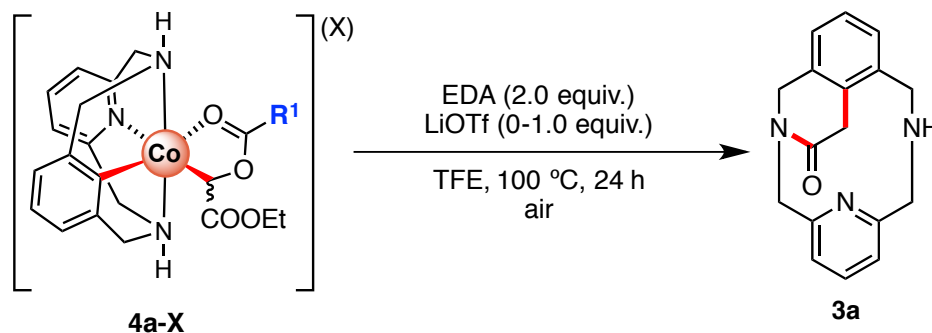
Scheme S10. Evolution of **4a-X** to **3** in presence/absence of LiOTf as additive.

In a 2 mL vial, **4a-OAc** (0.03 mmol) and LiOTf (0.0-1.0 equiv.) were mixed in freshly distilled TFE (0.5 mL). The vial was then sealed with a septum and the mixture was stirred under air over 24h at 100ºC. Then, after removal of the solvent, NH_4OH (2 mL) was added and the solution was extracted using Et_2O (2x5mL). Then, reactions crudes were analyzed by NMR techniques using 1,3,5-trimethoxybenzene as internal standard.

Table S4. Evolution of **4a-X** to **3** in presence/absence of LiOTf as additive.

entry	X	additive	yield of 3 (%)[a]
1	OAc	-	14%
2		-	52%[b]
3		Li(OTf)	89%
4	OPiv	-	traces
5		Li(OTf)	16%
6	OBz	-	67%
7		Li(OTf)	89%
8	OBz-NO2	-	76%
9		Li(OTf)	87%
10	OBz-CN	-	78%
11		Li(OTf)	88%
12	OBz-COMe	-	63%
13		Li(OTf)	79%
14	OBz-Cl	-	62%
15		Li(OTf)	85%
16	OBz-Me	-	28%
17		Li(OTf)	89%
18	OBz-OMe	-	24%
19		Li(OTf)	68%

[a]Yield determined using 1,3,5-trimethoxybenzene as internal standard.

6.2 Reaction yields of **4a-OBz-Y** (Y = OMe, Me, H, Cl, COMe, CN, NO$_2$) and correlation with Hammett parameters and leaving group pK$_a$ values
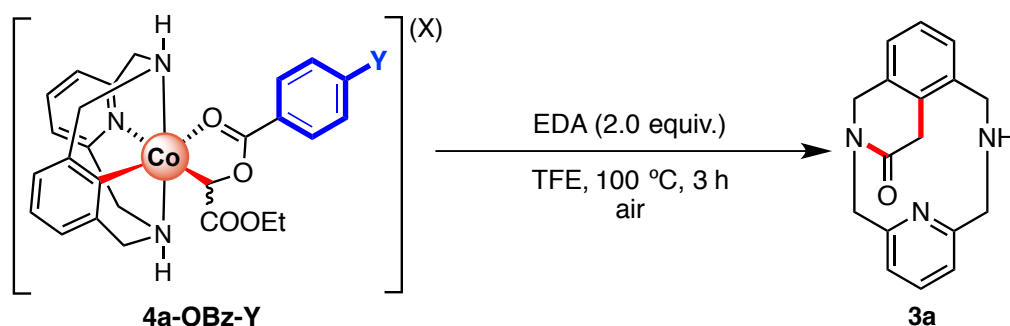
Scheme S11. Evolution of **4a-OBz-Y** to **3a** in absence of additives (3 h).

In a 2 mL vial, **4a-OBz-Y** (0.029 mmol) was mixed in freshly distilled TFE (0.5 mL). The vial was then sealed with a septum and the mixture was stirred under air over 3 h at 100 ºC. Then, after removal of the solvent, NH$_4$OH (2 mL) was added and the solution was extracted using Et$_2$O (2x5mL). Then, reactions crudes were analyzed by NMR techniques using 1,3,5-trimethoxybenzene as internal standard.

Table S5. Correlation of yield of **3a** from **4a-OBz-Y** with Hammett parameter and pK$_a$ of the corresponding leaving group.

Entry	Y	Yield 3a (%)[a]	R(%)/H(%)	Log(R/H)	σ_p	pK$_a$	$\Delta G^{\ddagger,b}$
1	OMe	11.3	0.518348624	-0.28537805	-0.268	4.47	29.96
2	Me	16.9	0.775229358	-0.11056978	-0.169	4.37	29.96
3	H	21.8	1	0	0	4.19	29.29
4	Cl	24.3	1.114678899	0.04714978	0.227	3.98	28.89
5	COMe	36.7	1.683486239	0.226209571	0.501	3.7	28.67
6	CN	46.8	2.146788991	0.331789359	0.658	3.55	27.92
7	NO$_2$	49.7	2.279816514	0.357899895	0.778	3.43	27.32

[a]Yield determined using 1,3,5-trimethoxybenzene as internal standard. [b]To avoid any error due to the harmonic approximation in the values of $\Delta G^{\ddagger}$, we obtained the corrected Gibbs free energies by applying the quasi-harmonic approximation to the vibrational entropy developed by Truhlar at 373 K and 1M concentration.[20a] This procedure was performed using the python program Goodvibes2.[20b] (See more information in the computational details section).

6.3 MS/MS experiments of **4a-OBz-Y** complexes (Y = OMe, Me, H, Cl, COMe, CN, NO$_2$)
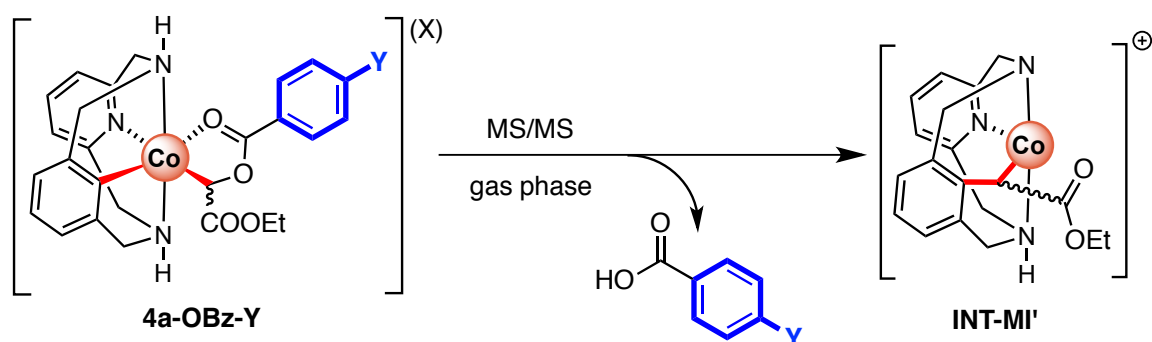
Scheme S12. Reactivity observed through MS/MS analysis of **4a-OBz-Y** intermediates.

4a-OBz-Y complexes were analyzed by high-resolution ESI-MS-QTOF analysis, isolating the peak corresponding to [(**4a-OBz-Y**)-(**OBz-Y**)] to subject it to tandem MS at different energies. As shown in Figures S6-13, one peak corresponding to [(**INT-MI**)-RCOOH)] (R = p-OMe-Ph, p-Me-Ph, p-H-Ph, p-Cl-Ph, p-COMe-Ph, p-CN-Ph and p-NO$_2$-Ph,) was observed (**INT-MI'**). As expected, the intensity of this peak increased with the energy applied. Significantly, when tandem MS experiments of **4a-OBz-Y** are compared when applying the same collision energy (15 eV), **4a-OBz-NO$_2$** generates relative higher amounts of **INT-MI'** than **4a-OBz-OMe**, which suggests p-NO$_2$-PhCOO$^-$ is a better leaving group.
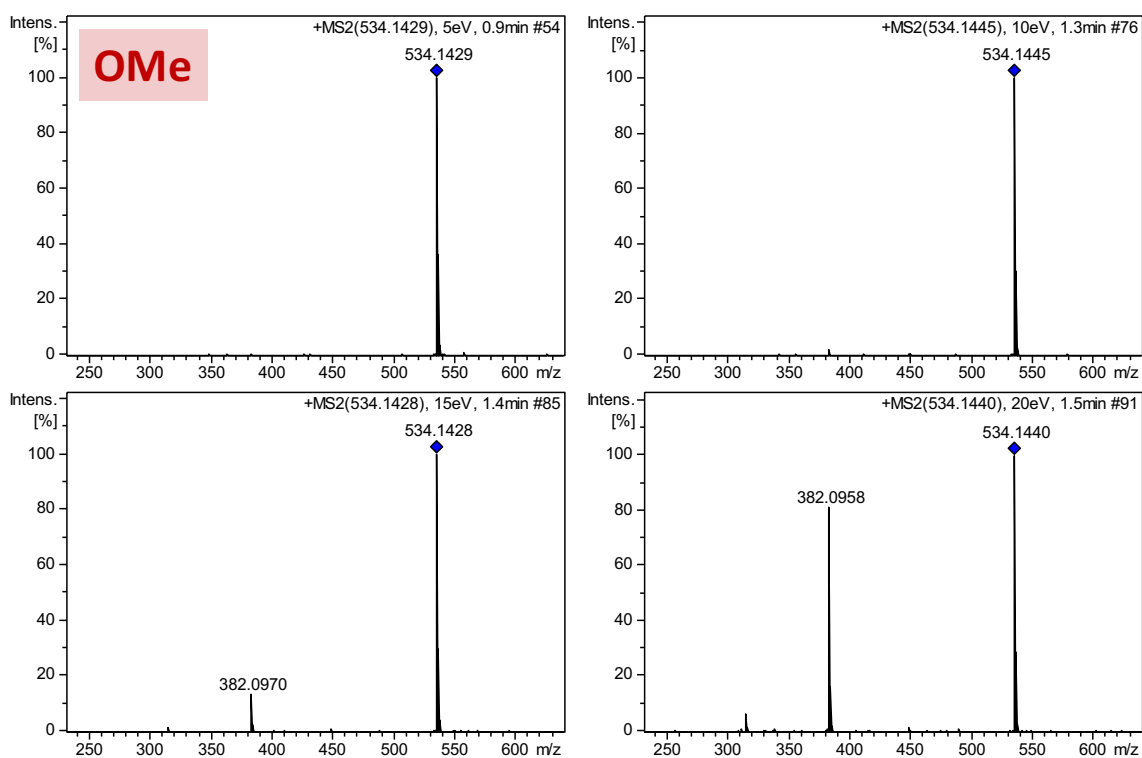
Figure S6. MS/MS spectrum of **4a-OBz-OMe** (m/z = 534.1440, 20 eV) showing a peak at m/z = 382.0958 (20 eV), which corresponds to **INT-MI'**.
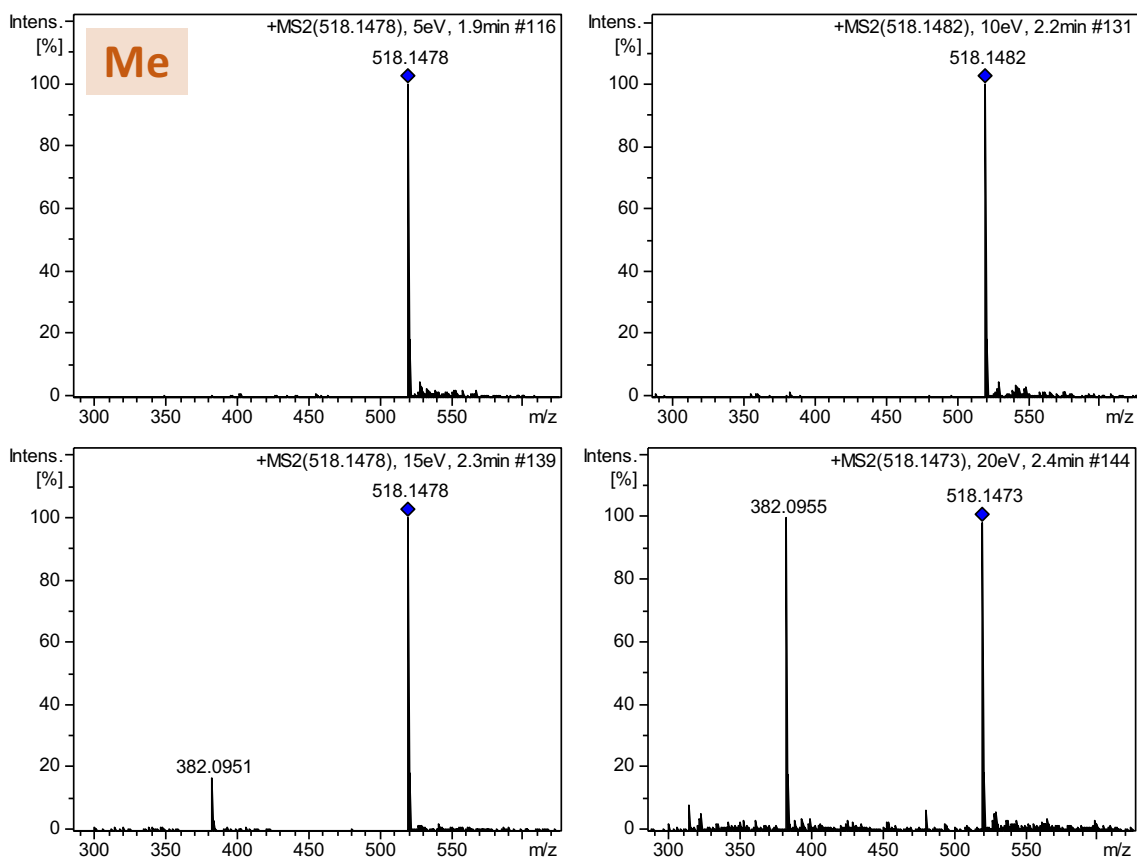
Figure S7. MS/MS spectrum of **4a-OBz-Me** (m/z = 5181473, 20 eV) showing a peak at m/z = 382.0955 (20 eV), which corresponds to **INT-MI'**.
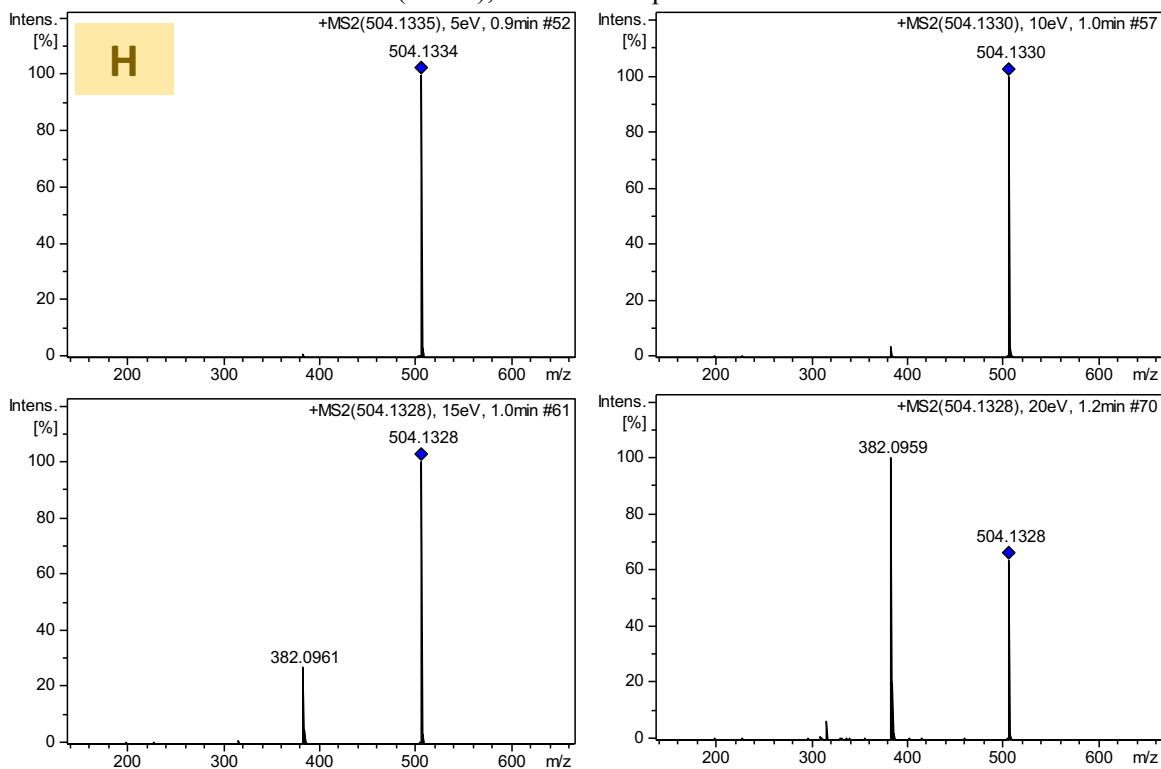
Figure S8. MS/MS spectrum of **4a-OBz-H** (m/z = 504.1328, 20 eV) showing a peak at m/z = 382.0959 (20 eV), which corresponds to **INT-MI'**.
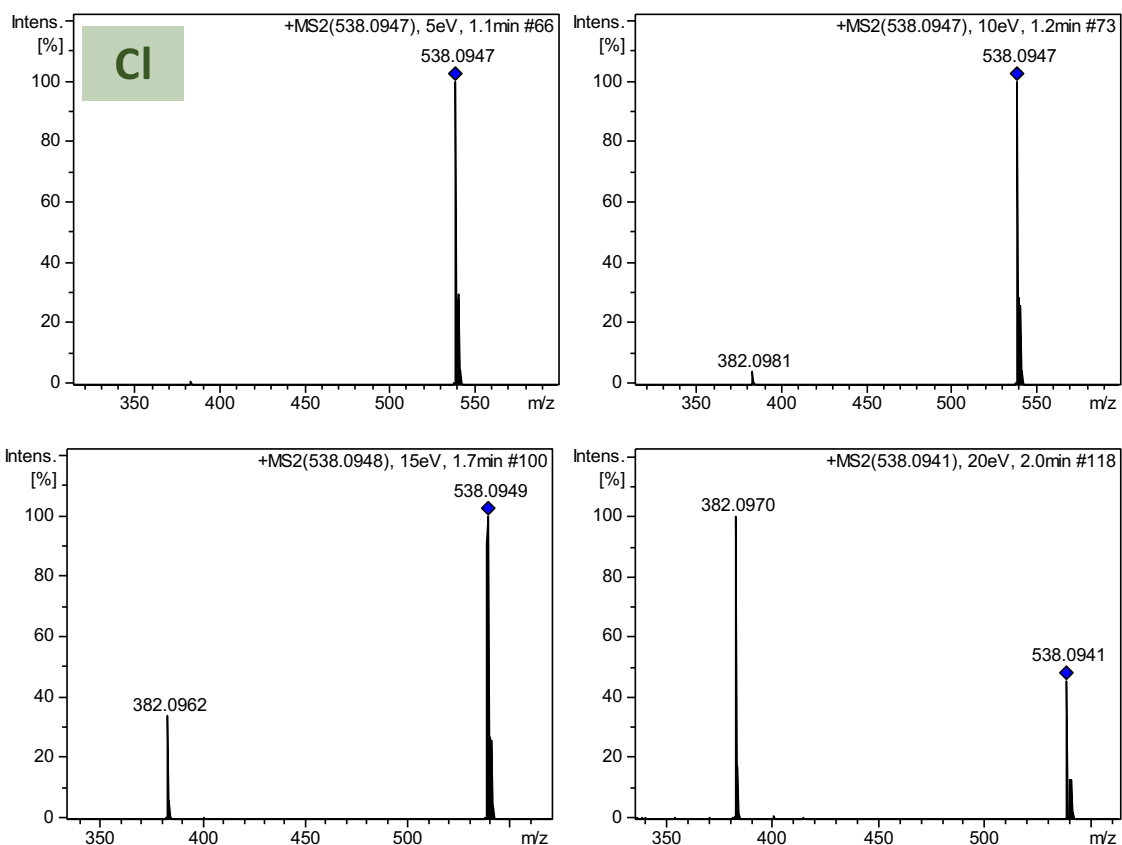
Figure S9. MS/MS spectrum of **4a-OBz-Cl** (m/z = 538.0941, 20 eV) showing a peak at m/z = 382.0970 (20 eV), which corresponds to **INT-MI'**.
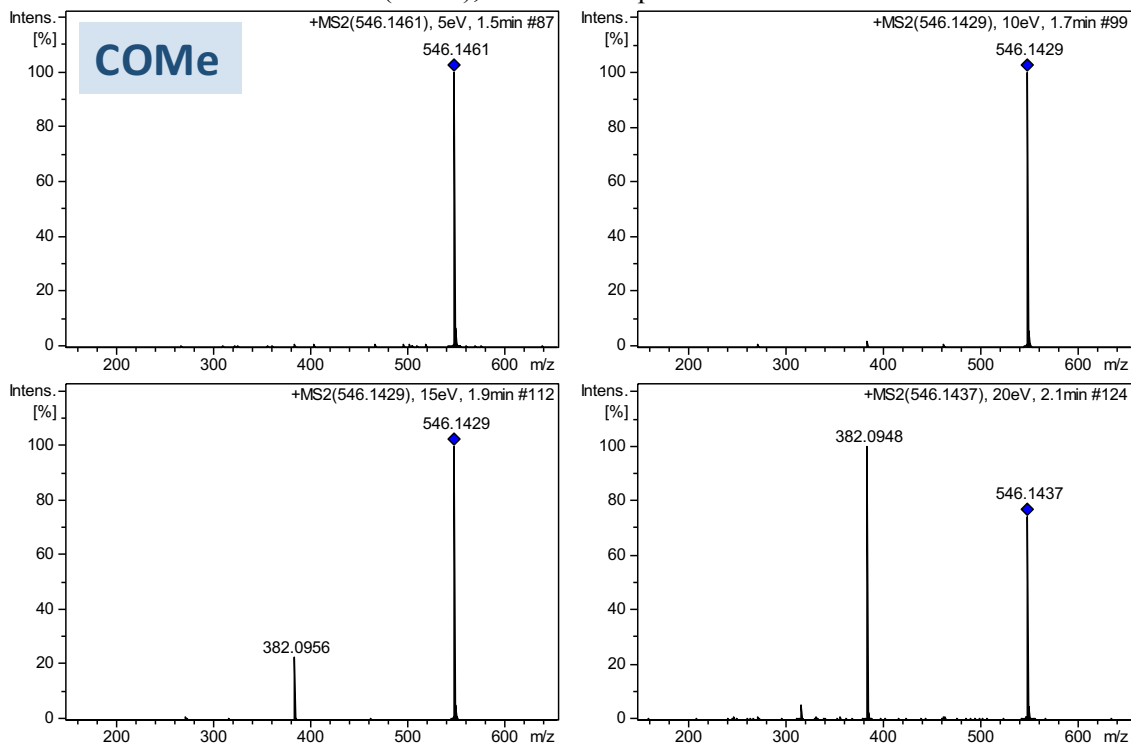
Figure S10. MS/MS spectrum of **4a-OBz-COMe** (m/z = 546.1437, 20 eV) showing a peak at m/z = 382.0948 (20 eV), which corresponds to **INT-MI'**.
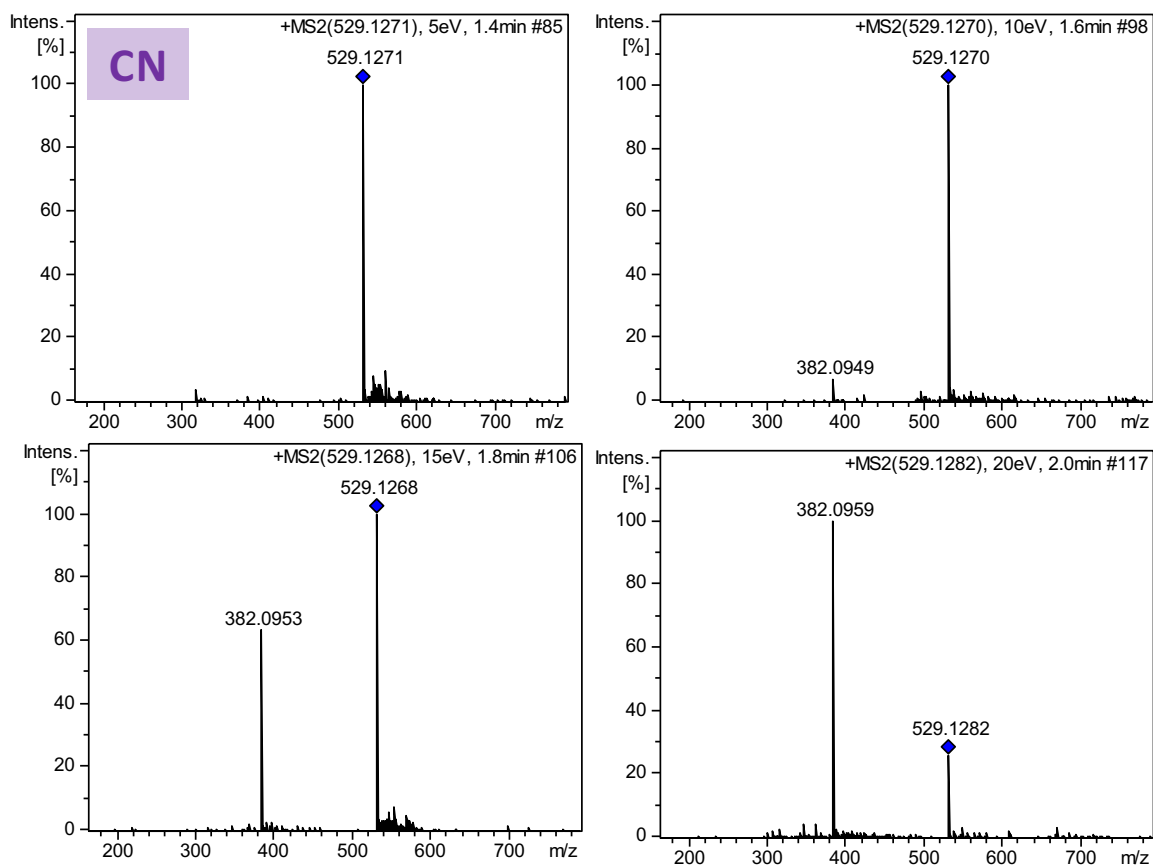
Figure S11. MS/MS spectrum of **4a-OBz-CN** (m/z = 529.1282, 20 eV) showing a peak at m/z = 382.0959 (20 eV), which corresponds to **INT-MI'**.
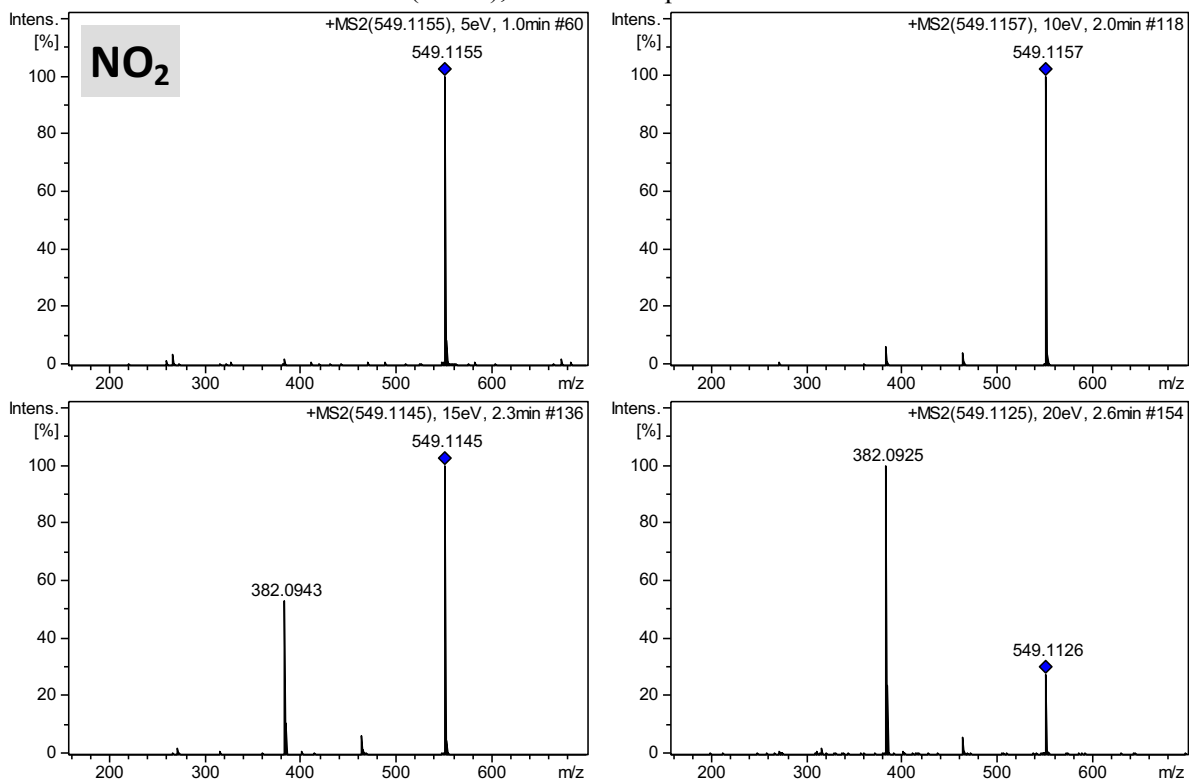
Figure S12. MS/MS spectrum of **4a-OBz-NO₂** (m/z = 549.1126, 20 eV) showing a peak at m/z = 382.0925 (20 eV), which corresponds to **INT-MI'**.
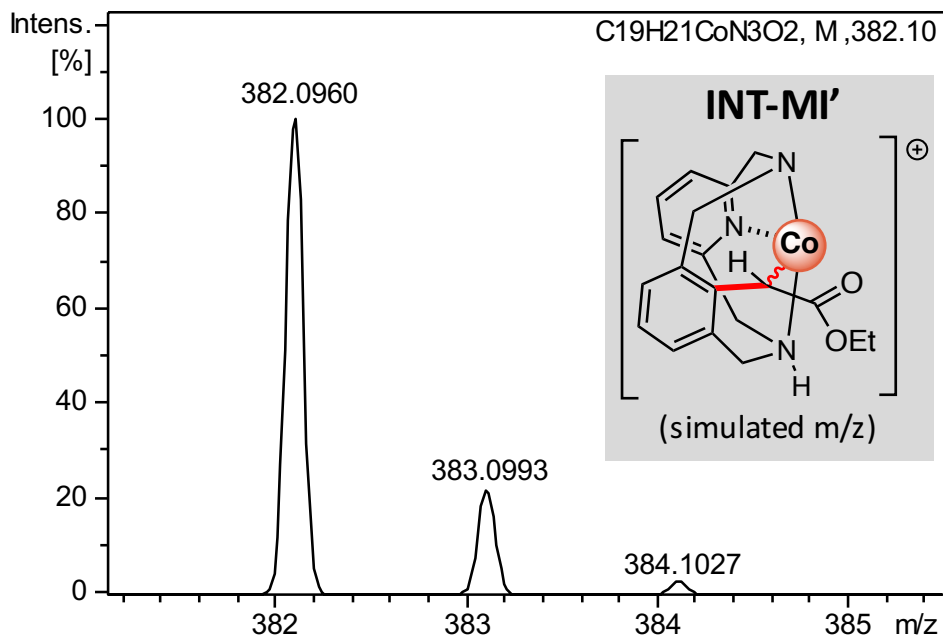
Figure S13. Simulated MS spectrum of **INT-MI'** showing a peak at m/z = 382.0960.

6.4 Detection of **4a-OAc-PhX** (X = OMe, NO$_2$) using HRMS and MS/MS studies
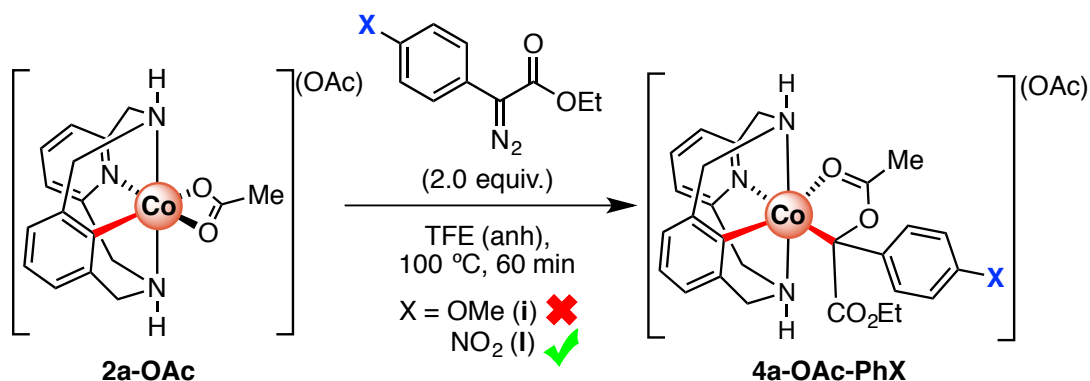
Scheme S13. Evolution of **4a-X** to **3** in presence of metal triflates as additives.

In a 2 mL vial, **2a-OAc** (0.029 mmol) and diazoacetate **i** and **l** (2.0 equiv.) were mixed in freshly distilled TFE (0.5 mL). The reactions crudes were analyzed by HRMS. When **i** was utilized as coupling partner, MS analysis only showed starting material (**2a-OAc**, m/z = 356.0815; Figure S14).
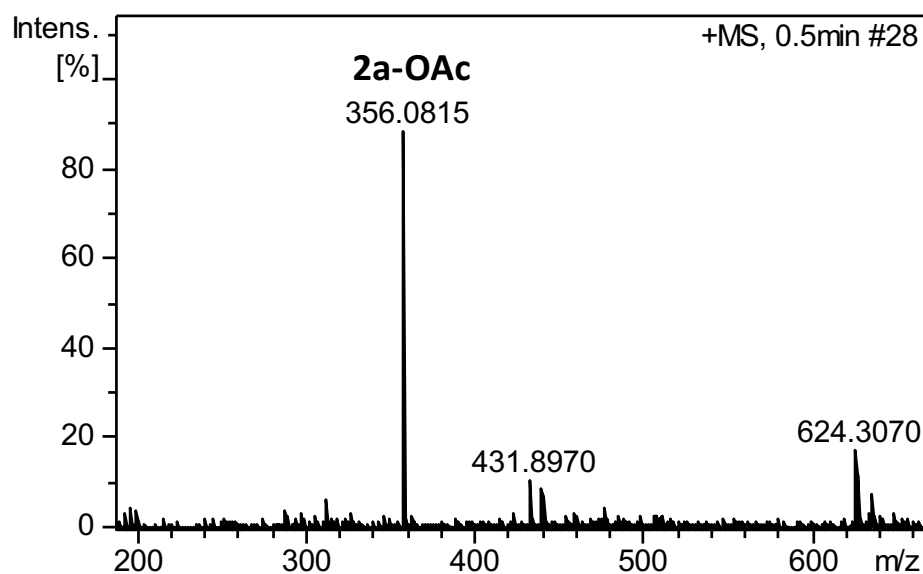
Figure S14. MS spectrum of crude reaction mixture after reaction of **2a-OAc** (m/z = 356.0815) with diazoacetate **i** (X = OMe).

However, when electron-poor diazoacetate l was utilized, a peak corresponding to **4a-OAc-PhNO$_2$** was detected (C$_{27}$H$_{28}$N$_4$O$_6$Co, experimental m/z = 563.1335; simulated m/z = 563.1335; Figure S15).
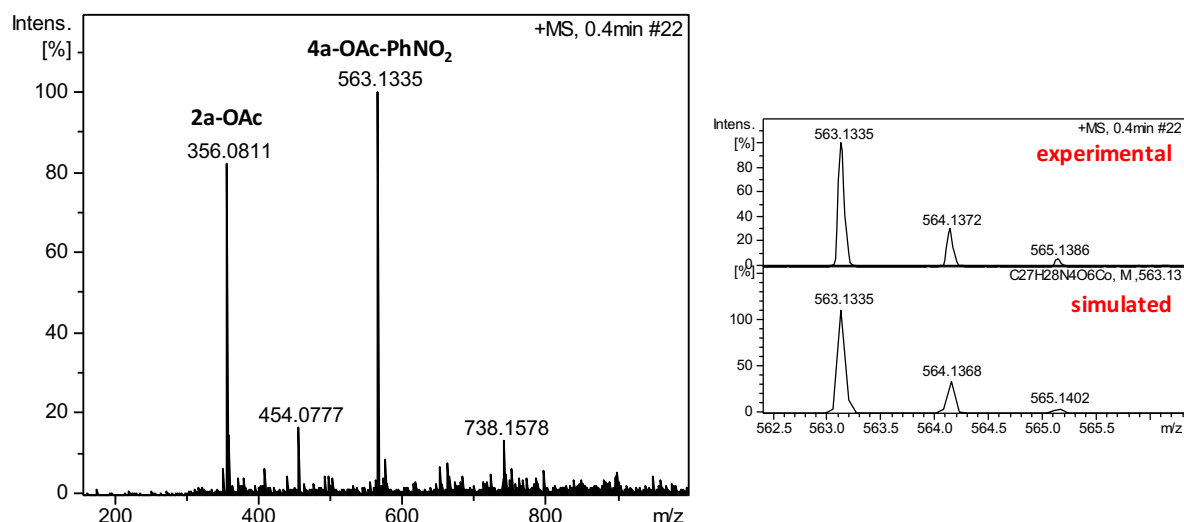
Figure S15. MS spectrum of **4a-OAc-PhNO₂** (m/z = 563.1335) after reaction of **2a-OAc** (m/z = 356.0811) with diazoacetate **l**.

Similarly to **4a-OBz-R** complexes, **4a-OAc-PhNO₂** was analyzed by high-resolution ESI-MS-QTOF analysis, isolating the peak corresponding to [(**4a-OAc-PhNO₂**)-(OAc)] to subject it to tandem MS at different energies. As shown in Figure S16, one peak corresponding to [(**INT-MI-PhNO₂**)-CH₃COOH)] was observed (**INT-MI-PhNO₂'**; $C_{25}H_{24}N_4O_4Co$, experimental m/z = 503.1128; simulated m/z = 503.1124) when MS/MS analysis was performed at a collision energy of 20 eV.
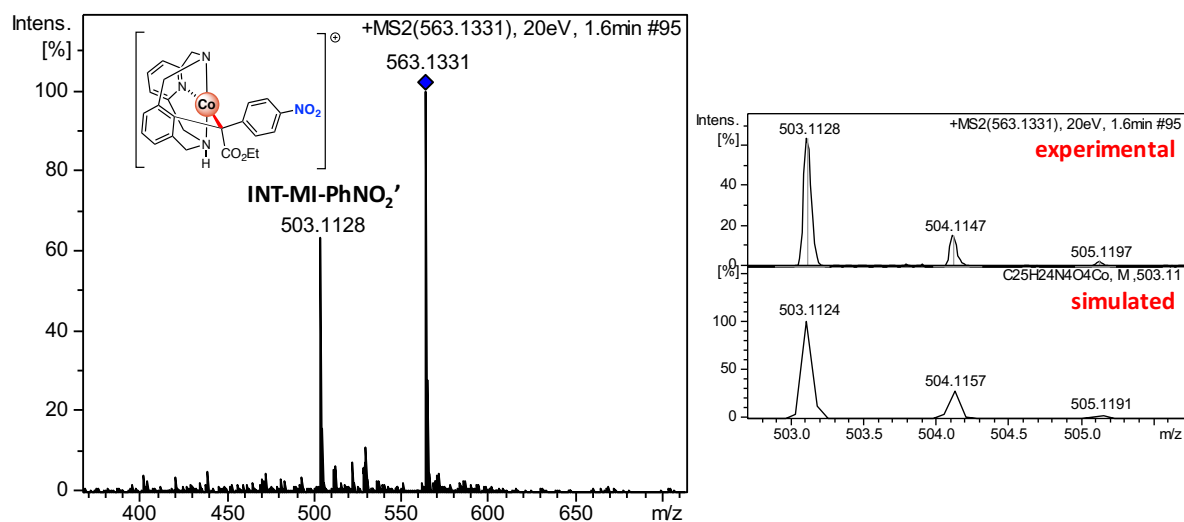
Figure S16. MS/MS spectrum of **4a-OAc-PhNO₂** (m/z = 563.1335, 20 eV) showing a peak at m/z = 503.1128 (20 eV), which corresponds to **INT-PhNO₂-MI'**.

6.5 Evaluation of several Lewis acids
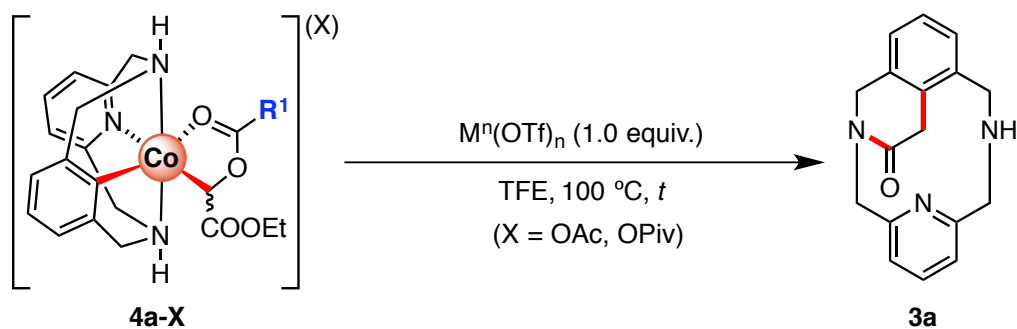
Scheme S14. Evolution of **4a-X** to **3a** in presence of metal triflates as additives.

In a 2 mL vial, **4a-X** (0.029 mmol, X = OAc and OPiv) and *Lewis acids* (1.0 equiv.) were mixed in freshly distilled TFE (0.5 mL). The vial was then sealed with a septum and the mixture was stirred under air at 100ºC. Then, after removal of the solvent, NH_4OH (2 mL) was added and the solution was extracted using Et_2O (2x5mL). Then, reactions crudes were analyzed by NMR techniques.

Table S6. Evolution of **4a-X** to **3a** in presence of several Lewis acids as additives.

Entry	4a-X	t	Lewis acid	Yield 3a (%)[a]
1	OAc	24h	HOTf	82%
2			LiOTf	89%
3			Mg(OTf)$_2$	67%
4			NaOTf	71%
5			KOTf	72%
6			Ba(OTf)$_2$	34%
7			B(C$_6$F$_5$)$_3$	26%
8	OAc	2h	HOTf	51%
9			LiOTf	61%
10			Mg(OTf)$_2$	24%
11			NaOTf	36%
12			KOTf	33%
13			Ba(OTf)$_2$	11%
14			B(C$_6$F$_5$)$_3$	7%
15	OPiv	24h	HOTf	14%
16			LiOTf	20%
17			Mg(OTf)$_2$	21%
18			NaOTf	8%
19			KOTf	traces
20			Ba(OTf)$_2$	8%
21			B(C$_6$F$_5$)$_3$	n.r.

[a]Yield determined by NMR using 1,3,5-trimethoxybenzene as internal standard.

7. XAS analysis of final reaction crude (RC)
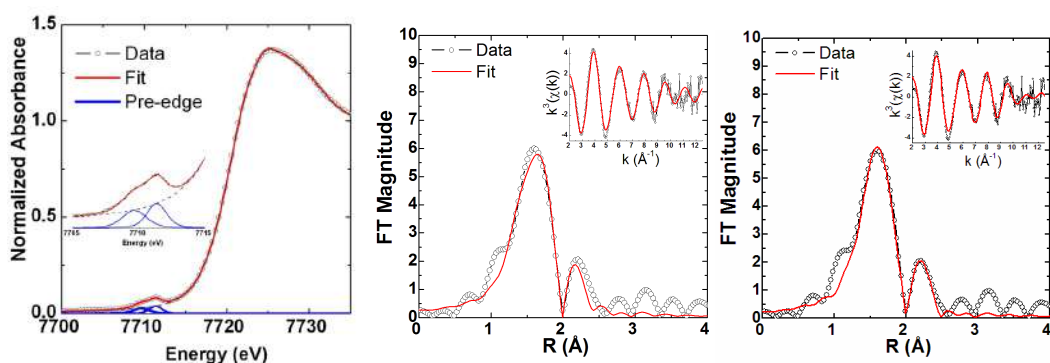
Figure S17. XAS of **RC**. *Left:* XANES region showing the rising edge of B1 at 7719.9 eV with a Lorentzian-Gaussian sum fitted pre-edge centered at 7710.6 eV having two features at 7709.66 eV and 7711.37 eV of 0.077 and 0.084 normalized intensity units respectively. *Right:* Fourier-transformed EXAFS spectra of **RC (model 9- center, model 10-right)**; Inset: k^3-weighted unfiltered EXAFS spectra.

Table S7. Selected EXAFS fits for **RC**. Fits carried out in r-space (Δk = 2-12.5 Å^{-1}; Δr = 1-3 Å) with a Hanning window (dk 2), a *k*-weight = 3 and S_0 = 0.9. Bond distances and disorder parameters (Δr_{eff} and σ^2) were allowed to float having initial values of 0.0 Å and 0.003 Å^2 respectively, with a universal E_0 and ΔE_0 = 0 eV. (Fits in bold are the best models; σ^2 reported as x10^3 Å^2)

FIT	Δk	Δr	Var.	%R	χ^2_v	ΔE_0	Co-O/N* N	r(Å)	σ^2	Co-O/N N	r(Å)	σ^2	Co-C N	r(Å)	σ^2	Co--C-O--Co N	r(Å)	σ^2
1	2-12.5	1-3	3	7.6	27.9	3.1				4	2.08(1)	8(1)						
2	2-12.5	1-3	3	5.1	18.7	2.6				5	2.08(1)	10(1)						
3	2-12.5	1-3	3	4.5	16.6	2.1				6	2.08(1)	12(1)						
4	2-12.5	1-3	3	7.0	25.6	3.3	2	2.01(1)	1(1)	2	2.15(1)	1(1)						
5	2-12.5	1-3	3	4.8	17.7	1.6	2	1.98(1)	4(1)	3	2.12(1)	4(1)						
6	2-12.5	1-3	3	4.7	17.1	0.8	2	1.97(1)	6(1)	4	2.11(1)	6(1)						
7	2-12.5	1-3	3	3.6	13.0	5.0	2	1.99(1)	6(1)	4	2.14(1)	6(1)	2	2.42(1)	6(1)			
8	2-12.5	1-3	3	3.8	15.6	4.7	-	-	-	6	2.09(1)	11(1)	2	2.37(1)	11(1)	4	2.66(14)	11(1)
9	**2-12.5**	**1-3**	**4**	**2.6**	**10.6**	**5.3**	**2**	**2.00(1)**	**5(1)**	**4**	**2.14(1)**	**5(1)**	**2**	**2.42(1)**	**5(1)**	**4**	**2.68(6)**	**5(1)**
10	**2-12.5**	**1-3**	**4**	**2.2**	**8.1**	**6.9**	**3**	**2.04(1)**	**5(1)**	**3**	**2.18(1)**	**5(1)**	**2**	**2.47(1)**	**5(1)**	**4**	**2.65(5)**	**5(1)**

*Chemical intuition was used to differentiate between N/C/O paths

8. Computational studies

8.1. Mechanistic insight in the formation of the aryl-Co(III) intermediates (4a-R complexes) bearing different carboxylate anions.

We computed the formation of the several aryl-Co(III) intermediates with different carboxylates without any additives based on the mechanism described in our previous report (Figure S18).[19] Therefore, the species **2a-X**, **2a-X-EDA**, **TS1**, **2a-carbene-X**, **TS1b**, **4a-X**, **TS2** and **INT-MI-Y** (X = TFA, OPiv, OBz-Y; Y =H, Me, OMe, Cl, COMe, CN, NO$_2$) were calculated and the values of the Gibbs Free Energy (ΔG) differences are collected in the table S8 along with the activation barrier (ΔG‡) for each derivative.

For X = TFA, B-pCl, B-pOMe and B-PNO$_2$ the optimized geometries of the species 2a-carbene-X were not found indicating that TS1 structures directly evolve to 4a-X intermediates. Due to the planarity and low value of TS1b-X barriers for X = OPiv, OBz (B), B-pCN, B-pMe and B-COMe our attempts to optimize TS1b-X geometries were all unsuccessful. Table S8 also shows that the ΔG of the equivalent species with different carboxylates are quite similar (excepting TFA).
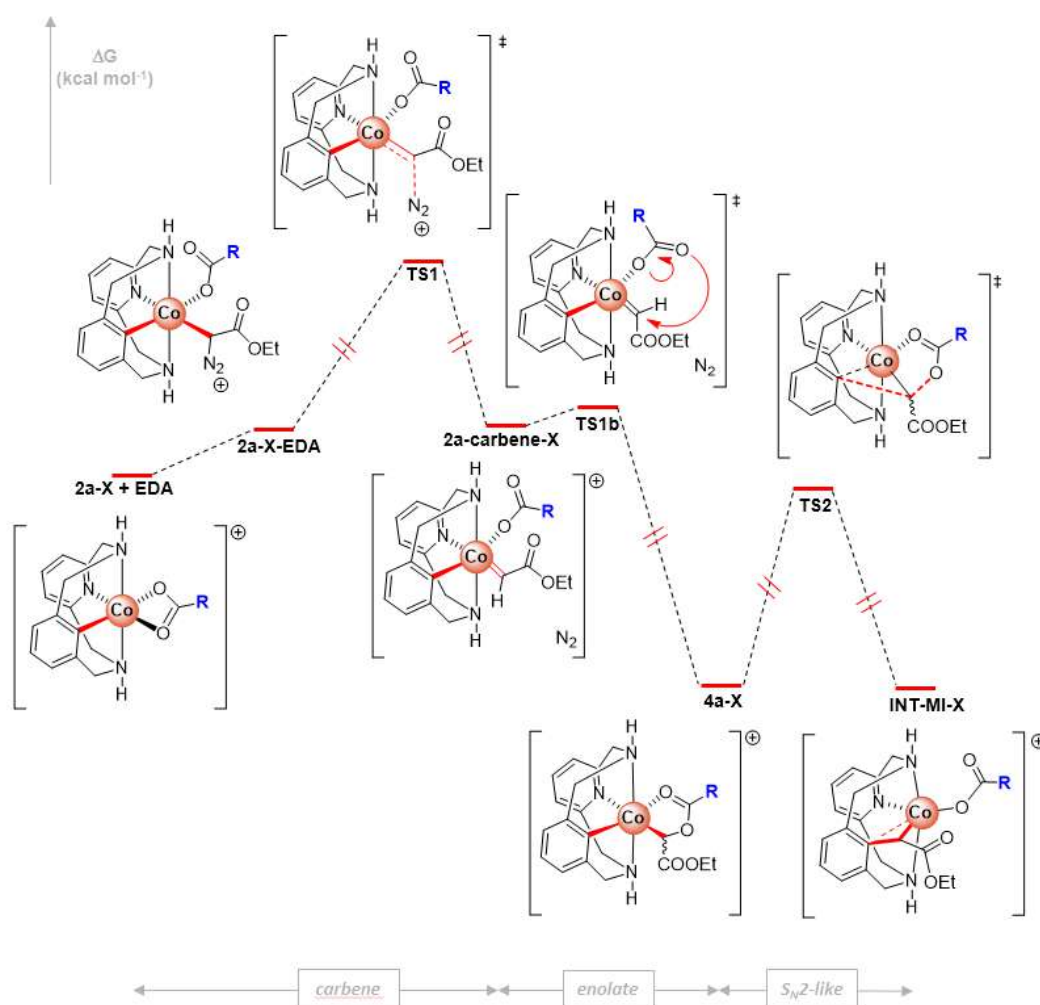
Figure S18. Energy profile sketch of the reaction for all the derivatives.

Table S8. Gibbs Energy (ΔG in kcal/mol) of the reaction of **2a-X** with EDA species. The symbol "--" represents that it was not possible to find the corresponding optimized species. The figures in blue correspond to the energies of the "masked-carbene" intermediates. The last row shows the values of the Activation barrier ($\Delta G^{\ddagger}$) of the intramolecular S_N2-type C-C bond forming event.

X=	Acetate[1]	TFA[1]	OPiv	OBz (B)	B-Cl	B-OMe	B-NO$_2$	B-CN	B-Me	B-COMe
2a-X + EDA	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	0.0	0.0
2a-X-EDA	8.9	1.8	7.3	8.3	8.2	9.5	6.5	7.4	8.3	7.9
TS1-X	23.1	13.7	21.3	21.6	20.8	22.5	19.9	20.6	21.6	21.7
2a-carbene-X	9.8	--	10.0	11.2	--	--	--	9.2	10.7	10.3
TS1b-X	10.6	--	--	--	--	--	--	--	--	--
4a-RX	-30.3	-25.3	-32.0	-29.8	-30.0	-30.2	-29.3	-29.9	-30.9	-31.0
TS2-X	-1.4	-5.6	-3.2	-1.4	-2.0	-1.1	-2.4	-2.0	-1.7	-1.44
INT-MI-X	-31.0	-35.2	-30.9	-31.0	-30.6	-29.2	-31.5	-31.2	-30.0	-29.93
$\Delta G^{\ddagger}$ (TS2)	**28.9**	**19.7**	**28.8**	**28.4**	**28.0**	**29.1**	**26.9**	**27.9**	**29.2**	**29.6**

[1]Data obtained from reference 19.

Table S9. Electronic Energy (ΔE in kcal/mol) of the reaction of **2a-X** with EDA species. The symbol "--" represents that it was not possible to find the corresponding optimized species. The figures in blue correspond to the energies of the "masked-carbene" intermediates. The last row shows the values of the Activation barrier ($\Delta E^{\ddagger}$) of the intramolecular S_N2-type C-C bond forming event. Electronic energies were used to construct the ΔE vs Hammett (σ_p) in Figure 2b (main text) in order to consider pure electronic effects only.

X=	Acetate[1]	TFA[1]	OPiv	OBz (B)	B-Cl	B-OMe	B-NO$_2$	B-CN	B-Me	B-COMe
2a-X + EDA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2a-X-EDA	**-5.3**	-12.4	-5.7	-6.0	-6.4	-5.5	-7.4	-7.1	-5.7	-6.8
TS1-X	9.9	2.7	9.5	9.2	8.6	9.6	7.6	7.9	9.3	8.3
2a-carbene-X	2.6	--	2.4	2.3	--	--	--	1.0	2.3	1.1
TS1b-X	2.3	--	--	--	--	--	--	--	--	--
4a-RX	-36.5	-31.8	-37.1	-36.1	-35.8	-36.4	-35.0	-35.2	-36.3	-35.5
TS2-X	-4.2	-8.4	-4.6	-4.2	-4.4	-3.8	-5.0	-4.8	-4.0	-4.7
INT-MI-X	-35.7	-41.2	-36.3	-34.1	-34.4	-33.7	-35.2	-35.0	-33.9	-34.7
$\Delta E^{\ddagger}$ (TS2)	**32.3**	**23.4**	**32.5**	**31.9**	**31.4**	**32.6**	**29.9**	**30.4**	**32.3**	**30.8**

[1]Data obtained from reference 19.
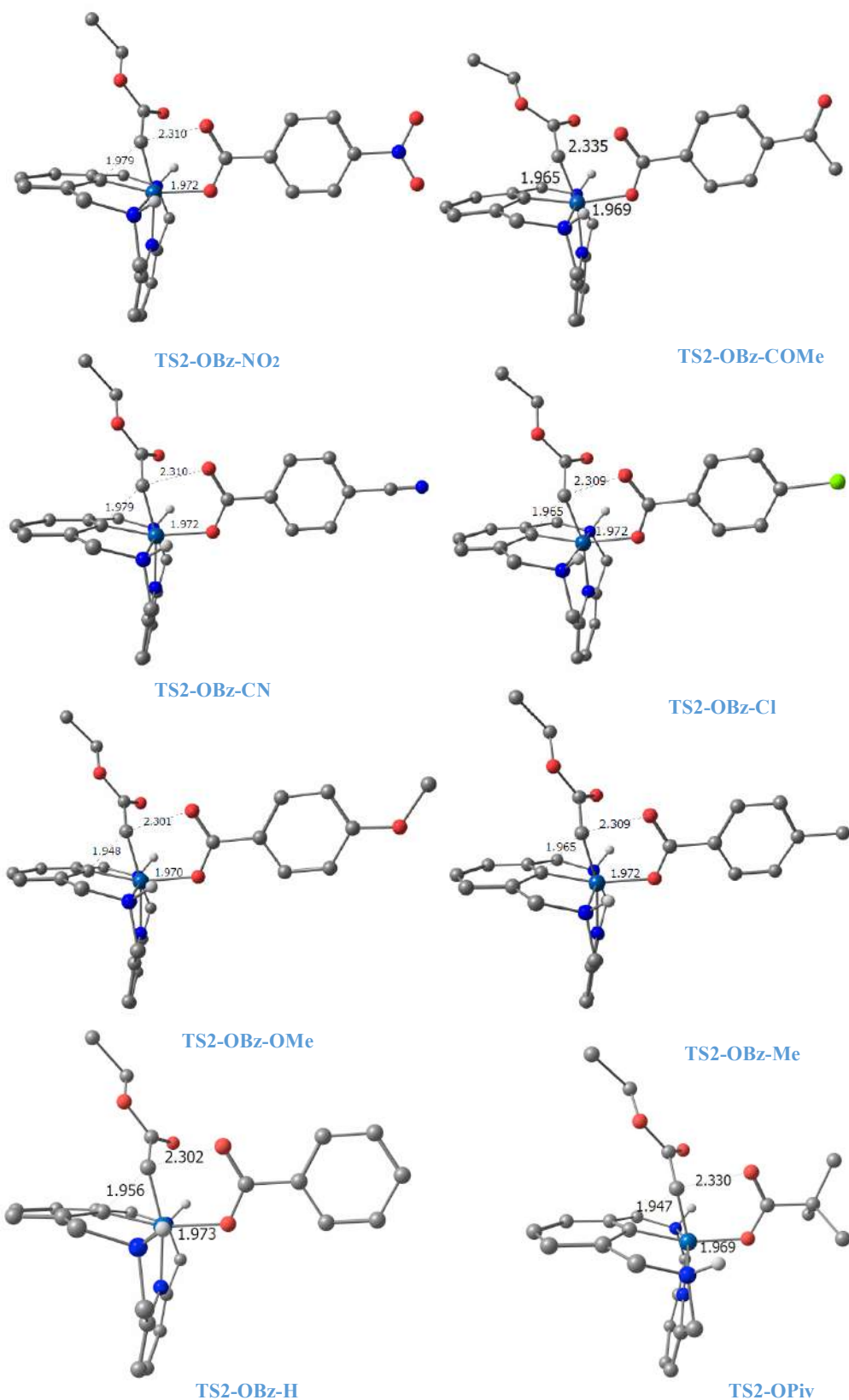
Figure S19. Structures of the optimized transition states TS2-X. The following color code illustrates the kind of atoms in the figure: Carbon, Nitrogen, Oxygen, Hydrogen, Cobalt. Most of hydrogens have been omitted for clarity.

8.2. Corrected values of the activation barrier by the quasi-harmonic approximation.

The correlation between electronic energy barriers of the S_N2-type transition states and Hammett parameters is excellent ($R^2 = 0.997$). On the contrary, if instead of electronic energies, the corresponding Gibbs energies given by gaussian09 code are used, the data show no correlation ($R^2 = 0.37$) (Figure S20a and S20b). Nevertheless, if the Gibbs energies are recomputed with the Goodvibes software[20b] using the quasi-harmonic approximation method developed by Truhlar[20a], the correlation is recovered ($R^2 = 0.949$, see Figure S20c)

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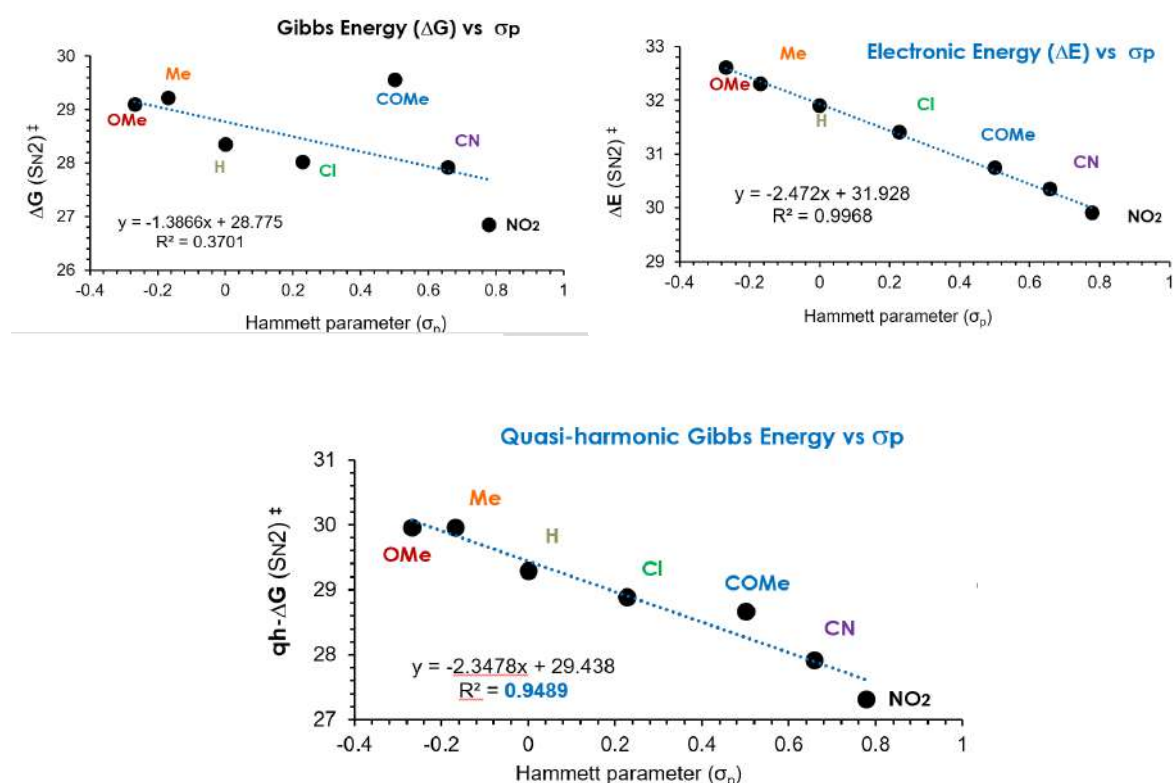
Figure S20. Hammett parameter plotted against **a)** Gibbs activation energy **b)** Electronic energy **c)** quasi-harmonic corrected Gibbs Energy values.

8.3. Computational studies on the effect in the mechanism of the Lewis acid as additive.

In our previous work, we calculated the LA-assisted S_N2-like pathway for the Lithium Triflate (LiOTf) with just adding explicitly a Lithium ion. Herein, we have evaluated the effect of others Lewis Acids and correlate the Gibbs energy barriers of the S_N2-type transition state with the Hammett parameters and experimental reaction rates. To achieve this goal, we simulated the LA-assisted S_N2-like pathway for the species Na(OTf), K(OTf) (see figure S21)
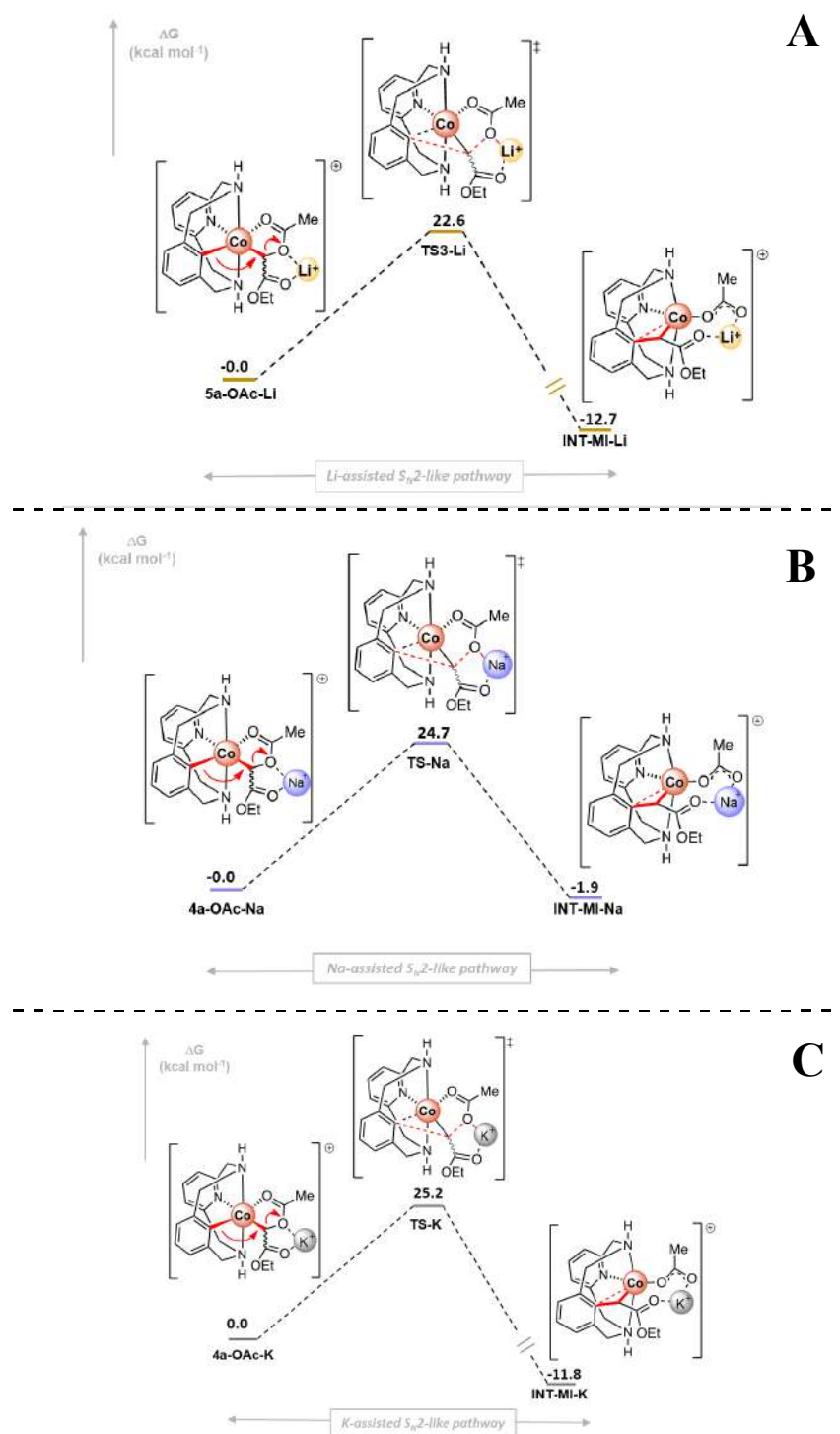
Figure S21. Gibbs energy profiles for the LA-assisted S$_N$2-like step starting from **4a-OAc** with different Lewis Acids. (A) Lithium, (B) Sodium, (C) Potassium.

In addition, to properly taking into account the effect of the solvent in the calculation of the alkali metal adduct formation, we computed the binding Gibbs energy considering the present of explicit molecules of solvent. Firstly, we explored the solvation of Lithium cation in different clusters of one, two and three molecules of TFE solvent (the most stable clusters from the those explored are shown in Figure

S22a). Afterwards, we calculated the Gibbs energy of the 4a-OAc-Li with one, two and three molecules of TFE coordinated to the alkali-metal (structures are shown in Figure S22b).

A

Li-TFE   Li-TFE$_2$ Li-TFE$_3$

B

4a-OAc-Li-TFE   4a-OAc-Li-TFE$_2$ 4a-OAc-Li-TFE$_3$
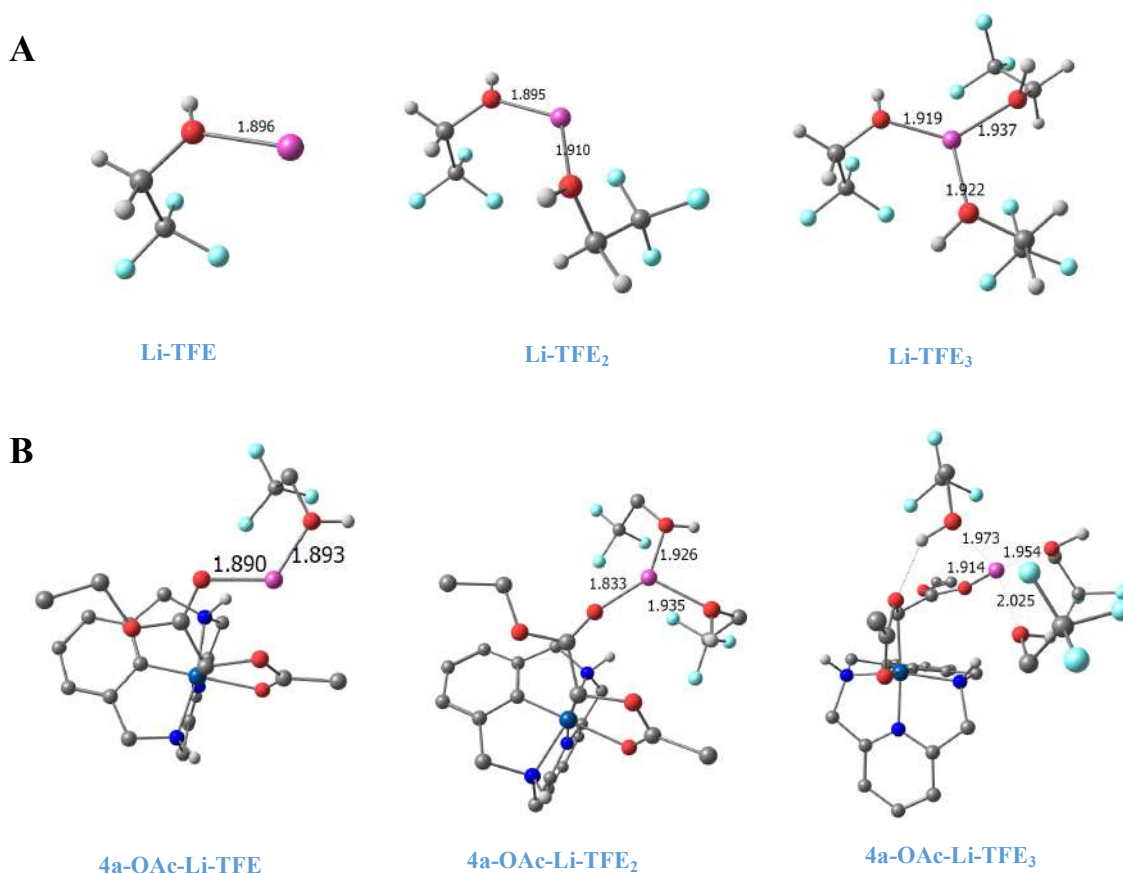
Figure S22. Structures of **A)** the most stable Lithium cation clusters with one, two and three molecules of solvent (TFE); **B)** Structures of the adducts formed when one two or three explicit molecules of solvent are coordinated to **4a-OAc-Li**.

The difference between the Gibbs energy of the adduct formation between **4a-OAc** and Li(TFE)$_n$ when 2 and 3 TFE molecules are included is only of 0.2 kcal/mol (-4.8 kcal/mol and -4.6 kcal/mol, respectively, Figure S23). Therefore, we concluded that including three TFE molecules is enough to properly consider the effect of the explicit solvent molecules in the adduct formation. Even though, the Gibbs energy value is not as exergonic as it was without explicit solvent molecules, the adduct formation still remains exergonic.
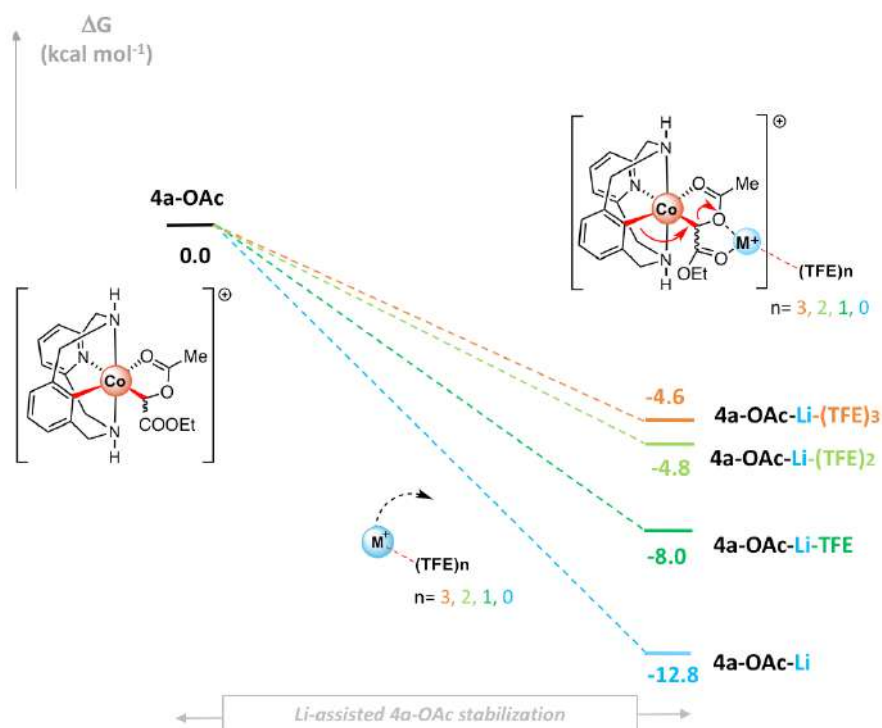
Figure S23. Gibbs energy of the TFE-solvated Lithium cation binding to **4a-OAc** when 0, 1, 2, 3 molecules of TFE are explicitly considered. Relative Gibbs energy values are given in kcal mol^{-1}; concentration of the solvated Li$^+$ = 0.039 mol l^{-1}.

With the previous information in hand, we calculated the most stable TFE-cluster-species (3 TFE molecules and **4a-OAc** coordinated to M$^+$) for the other 2 alkali-metals cation, Na$^+$ and K$^+$ (as shown in the Figure S24).
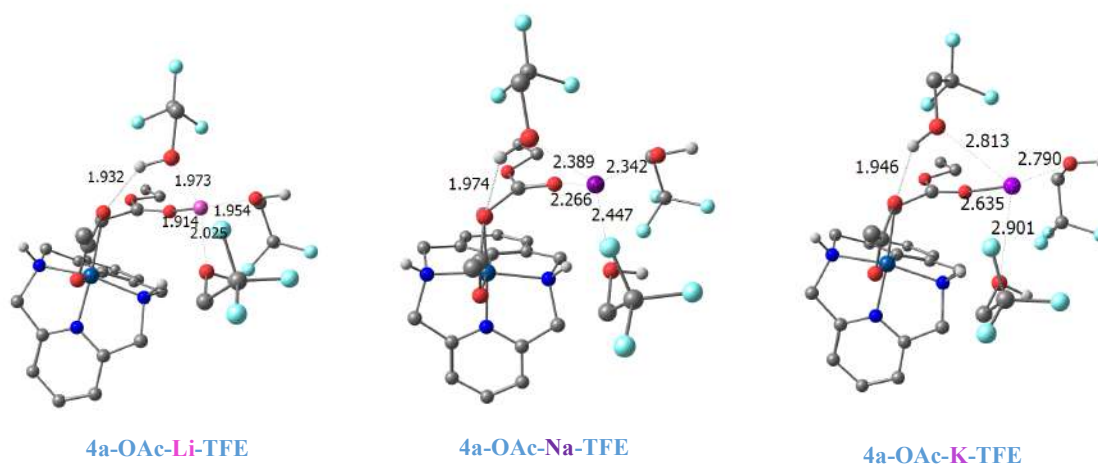
Figure S24. Structures of the **4a-OAc-M-TFE₃** intermediates, where M can be Lithium, Sodium or Potassium. The distance between the alkali cation and the carbonyl oxygen of the complex increases with the size of the metal.
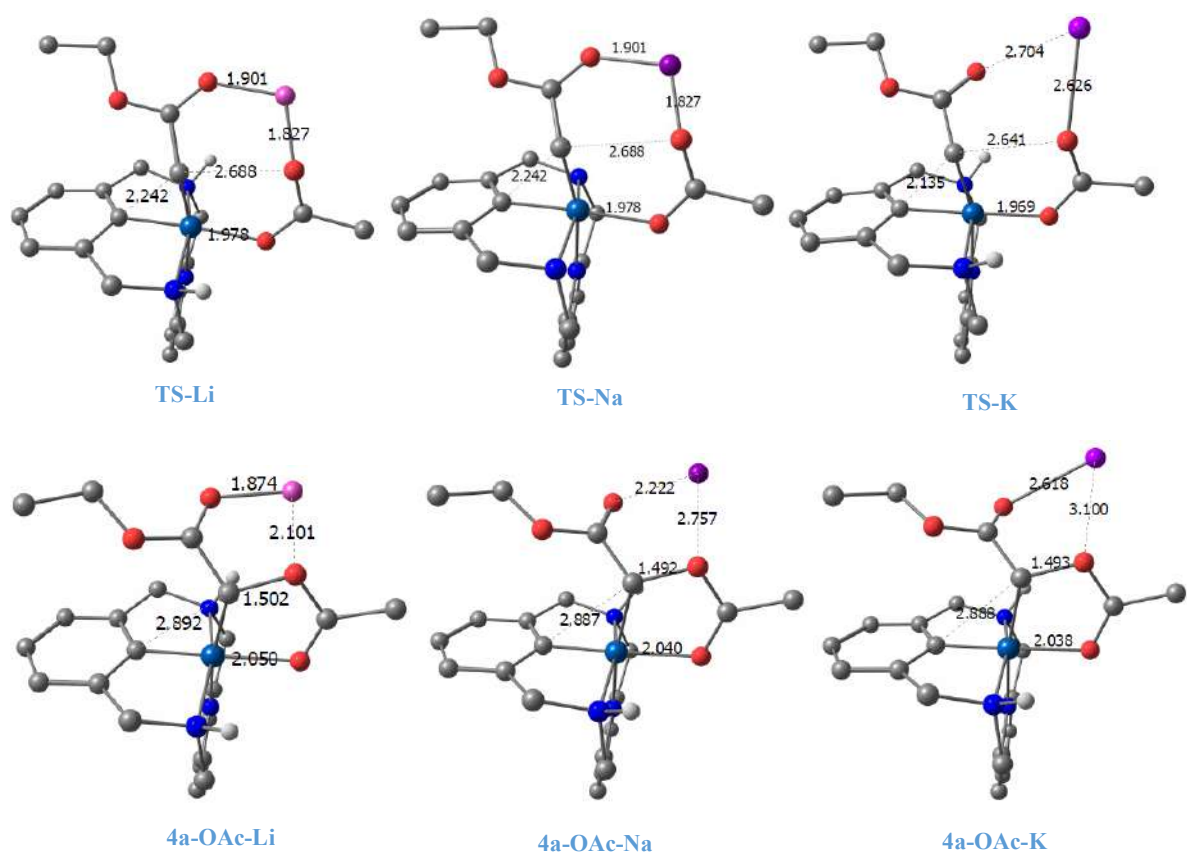
Figure S25. Transition state structures of the **TS-M** (M= Li, Na, K) and **4a-OAc-M** (M= Li, Na, K) structures. The size of the ion clearly affects the bond distance to the carbonyl groups. The following color code illustrates the kind of atoms in the figure: Carbon, Nitrogen, Oxygen, Hydrogen, Cobalt, Lithium, Sodium, Potassium. Most of hydrogens have been omitted for clarity.

8.4. Computational insight on the mechanism of the reaction with the electron poor α-p-NO₂-phenyl diazoacetate

As it is shown in the main text of the paper, we also studied the mechanism for the reaction of the α-p-NO2-phenyl diazoacetate (**l**). The Gibbs energy profile is already depicted in the main text (Figure 7). Here we present the optimized structures in detail (Figure S26). The figure shows that in the adduct the diazoacetate is quite far from the cobalt complex (3.2 Å). Another interesting feature is that the transition state **TS2** is strongly asynchronous, i.e., although it is a concerted transition state the C-O breaking takes place before reaching the TS2 geometry, which is determined by the C-C bon formation event. In this sense, **TS2** is very different from the other transition states like **TS2-M** and **TS2-X**, which are more reactive-like transition states instead of product-like.
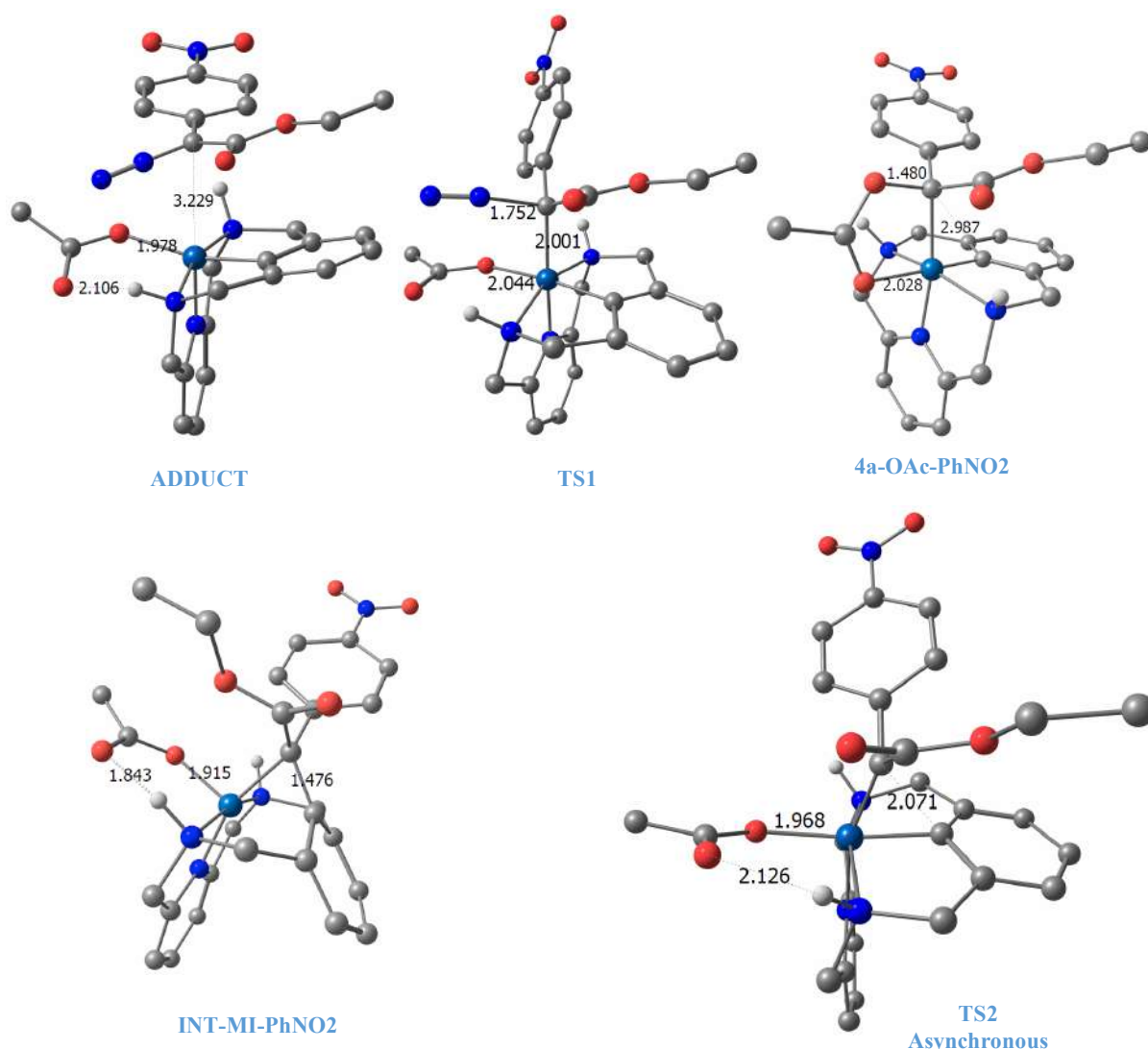
Figure S26. Optimized structures of the intermediates and Transition states generated in the reaction of **2a-OAc** and α-p-NO₂-phenyl diazoacetate. The following color code illustrates the kind of atoms in the figure: Carbon, Nitrogen, Oxygen, Hydrogen, Cobalt. Most of hydrogens have been omitted for clarity.

The IRC calculations presented in Figure S27 show that whereas **4a-OAc-PhNO$_2$** evolves to **INT-MI-PhNO$_2$** through a highly asynchronous late transition state, **4a-OAc** undergoes to corresponding product overcoming a synchronous transition state.
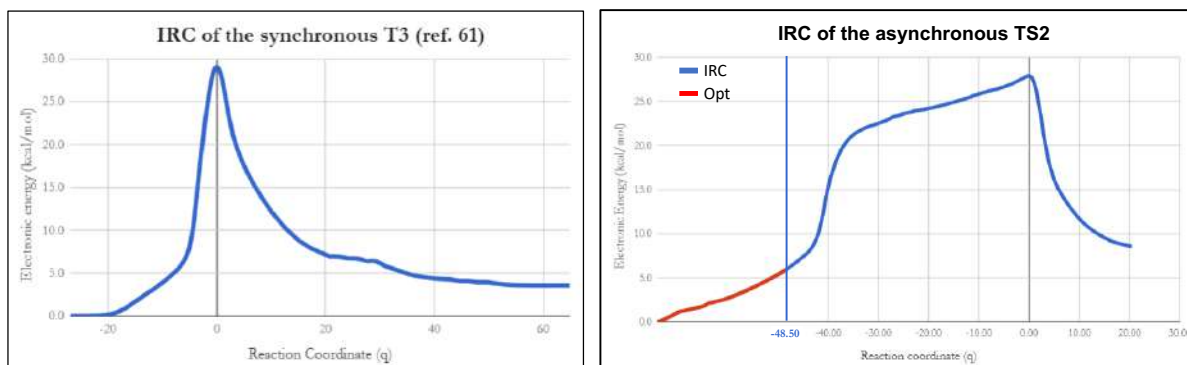
Figure S27. IRC profiles for the concerted S$_N$2-type C-C bond forming step with ethyl diazo acetate (left, synchronous) and diazo acetate **l** (right, highly asynchronous). In the latter, instead of the IRC algorithm, the last steps to achieve the equilibrium geometry of the **4a-OAc-PhNO$_2$** were obtained using the Gaussian09 optimization algorithm using a maximum step of only 0.02 Bohrs. We applied this approximation because due to the flatness of the PES in that region all our attempts to locate **4a-OAc-PhNO$_2$** minimum geometry using the IRC algorithm were unsuccessful. Nevertheless, the comparison of the very similar geometries of the last point of the rigorous IRC profile and the geometry of the **4a-OAc-PhNO$_2$** minimum, and the fact that both geometries are easily and quickly connected using optimization algorithm, shed no doubt that **TS2** and **4a-OAc-PhNO$_2$** are connected and there exist no intermediates between them.

The addition of the LA also changes the thermochemistry of the S$_N$2-like step, transforming an endergonic step (Figure 7, main text) to an exergonic step (Figure 9, main text). Figure S28 shows the structures of the species involved in Li-assisted S$_N$2-like event of 4a-OAc-PhNO$_2$-Li species.
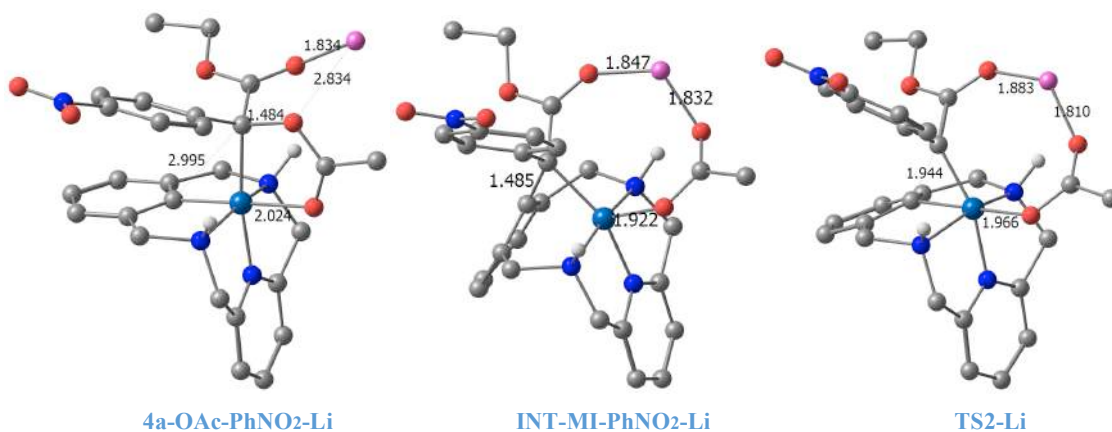
Figure S28. Optimized structures of the intermediates and transition state of the Lithium catalyzed S_N2-like reaction. The following color code illustrates the kind of atoms in the figure: Carbon, Nitrogen, Oxygen, Hydrogen, Cobalt, Lithium. Most of hydrogens have been omitted for clarity.
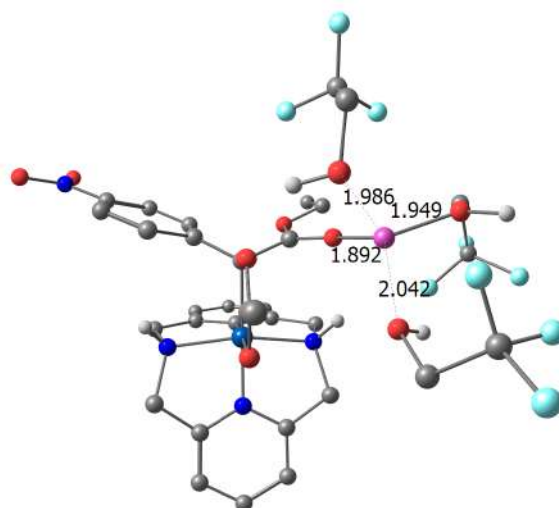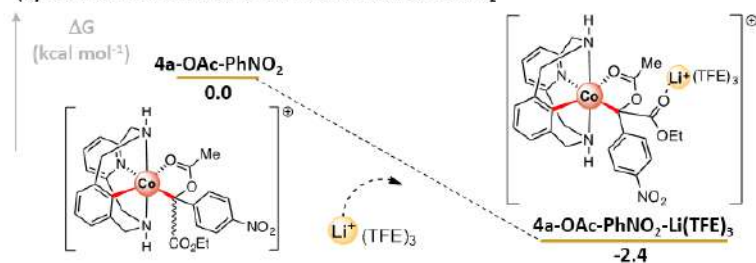
Figure S29. Structure of the complex (a) and Gibbs energy adduct formation (b) for **4a-OAc-PhNO₂-Li-TFE₃**. Relative Gibbs energy values are given in kcal mol^{-1}; concentration of the solvated Li$^+$ = 0.039 mol l^{-1}.

8.5. Computational study of the effect of the nucleophile strength on mechanism.

To study the electronic effect of para-substituted ligand scaffolds we considered the electron-donating –OMe and the electron-withdrawing -NO₂ groups, resulting in **4b** and **4c** (see Figure S30). As it is shown in the manuscript (figure 3, main text), the –OMe group induce a decrease of the barrier by 1.9 kcal mol^{-1}, whereas –NO₂ group causes an increase of the barrier by 5.8 kcal mol^{-1}.
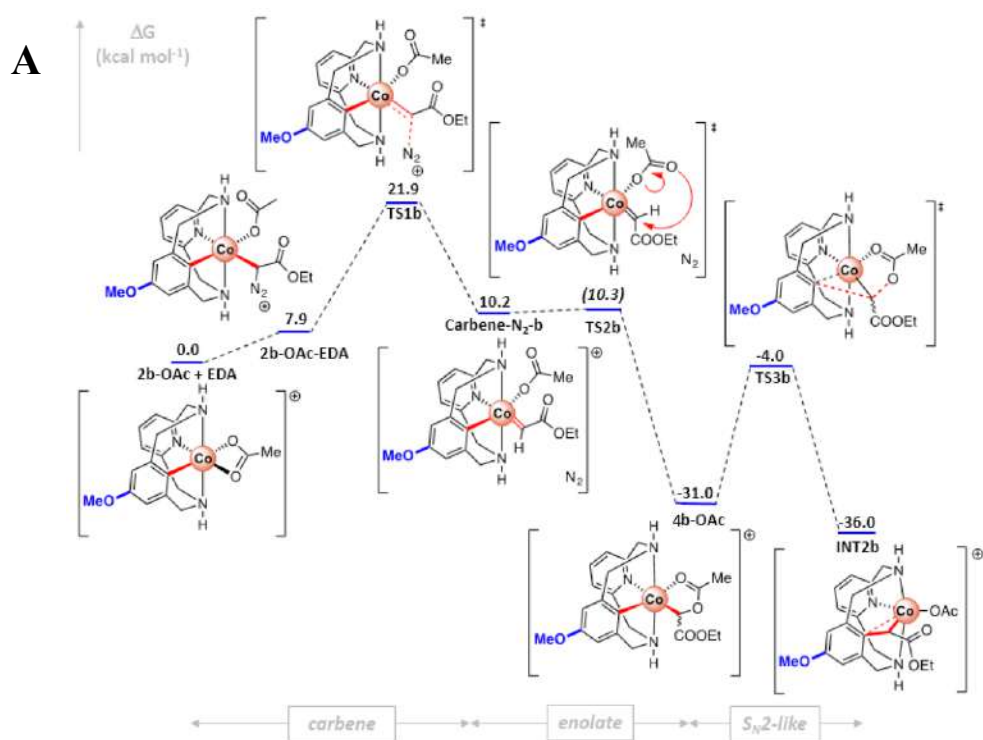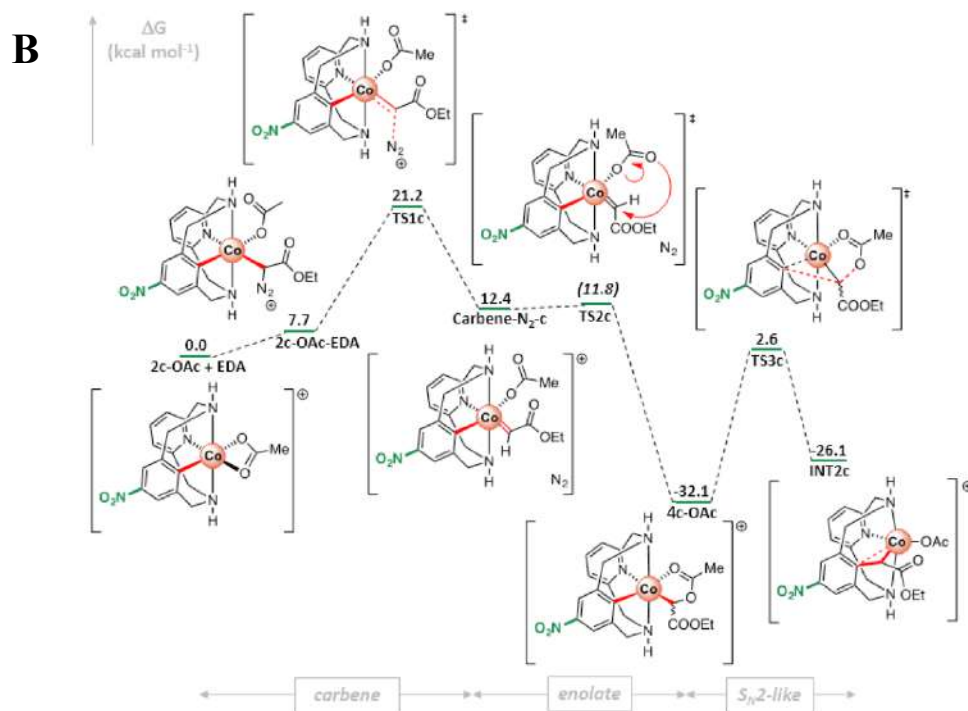
Figure S30. Gibbs energy profiles for: **A)** the reaction of the electron-rich *para*-OMe-substituted complex **2b-OAc** with EDA; **B)** the reaction of the electron-poor para-NO₂-substituted complex **2c-OAc** with EDA.

9. DFT XYZ coordinates of geometry optimized structures

Table S10. BP86/def2-TZVP structures

EDA

8	0.974401000	-0.435017000	-0.000058000
8	-0.376442000	1.414140000	-0.000021000
6	2.151200000	0.437016000	0.000089000
6	3.366415000	-0.462524000	-0.000040000
6	-0.229130000	0.191089000	-0.000048000
6	-1.294608000	-0.795135000	0.000016000
1	2.109956000	1.078630000	-0.893459000
1	2.109976000	1.078180000	0.893987000
1	4.275953000	0.157194000	-0.000614000
1	3.385637000	-1.101936000	0.895058000
1	3.384994000	-1.102584000	-0.894693000
1	-1.145636000	-1.873184000	0.000164000
7	-2.529782000	-0.363162000	0.000043000
7	-3.594191000	0.035740000	-0.000029000

2a-OAc

7	0.804859000	-1.216331000	-0.003207000
6	1.372680000	-1.543665000	-1.183408000
27	-0.732780000	-0.197878000	-0.012758000
7	-0.502635000	-0.146812000	1.977821000
6	2.587845000	-2.221563000	-1.204635000
1	3.049930000	-2.480940000	-2.157518000
7	-0.462905000	-0.118860000	-1.996362000
6	3.188573000	-2.559379000	0.013144000
1	4.147258000	-3.080228000	0.019842000
6	2.558272000	-2.244678000	1.222170000
1	2.996919000	-2.522407000	2.180906000
6	1.343810000	-1.566289000	1.184075000
6	0.449088000	-1.248548000	2.344402000
1	-0.156771000	-2.143365000	2.556761000
1	1.014309000	-1.001577000	3.254257000
1	-1.394149000	-0.343217000	2.445249000
6	-0.042294000	1.226310000	2.416942000
1	0.630919000	1.137758000	3.282797000
1	-0.941304000	1.768587000	2.746727000
6	0.572999000	1.928436000	1.239651000
6	0.249695000	1.363269000	0.007893000
6	0.590843000	1.948564000	-1.209644000
6	1.338995000	3.133984000	-1.194385000
1	1.624096000	3.623375000	-2.129767000
6	1.710376000	3.697245000	0.037422000
1	2.301476000	4.615692000	0.049293000
6	1.321107000	3.113935000	1.254259000
1	1.592602000	3.587848000	2.201584000
6	-0.008780000	1.264982000	-2.405803000
1	0.672001000	1.197823000	-3.267708000
1	-0.909361000	1.806855000	-2.731993000
1	-1.343604000	-0.317094000	-2.483335000
6	0.507002000	-1.205712000	-2.359888000
1	1.095014000	-0.935035000	-3.248301000
1	-0.085875000	-2.099938000	-2.608424000
8	-2.527979000	0.592518000	-0.033394000
8	-2.331219000	-1.592175000	-0.032388000
6	-3.094537000	-0.569241000	-0.031426000
6	-4.585392000	-0.680272000	0.004355000
1	-4.910108000	-0.681590000	1.057533000
1	-4.910222000	-1.620799000	-0.458800000
1	-5.051415000	0.177992000	-0.496896000

2a-OPiv

7	1.237345000	-1.300148000	0.005086000
6	1.782973000	-1.701369000	-1.162931000

27	-0.156681000	-0.095431000	-0.037253000
7	0.037699000	-0.065177000	1.958318000
6	2.909992000	-2.517535000	-1.159608000
1	3.354481000	-2.834823000	-2.103207000
7	0.160904000	-0.059563000	-2.014121000
6	3.446493000	-2.915459000	0.069991000
1	4.337810000	-3.544322000	0.096319000
6	2.837434000	-2.518728000	1.265717000
1	3.224692000	-2.837527000	2.233736000
6	1.712454000	-1.702112000	1.203152000
6	0.850457000	-1.265242000	2.349406000
1	0.144044000	-2.080496000	2.570726000
1	1.434793000	-1.070292000	3.259893000
1	-0.879702000	-0.153481000	2.408714000
6	0.645530000	1.248375000	2.400523000
1	1.266217000	1.093677000	3.296024000
1	-0.193218000	1.901075000	2.686662000
6	1.385215000	1.851171000	1.240227000
6	1.016529000	1.328550000	0.002561000
6	1.464123000	1.853168000	-1.208004000
6	2.369312000	2.922910000	-1.177790000
1	2.742404000	3.361635000	-2.107248000
6	2.787134000	3.435547000	0.061313000
1	3.501118000	4.261843000	0.084835000
6	2.290837000	2.920606000	1.270168000
1	2.603549000	3.357355000	2.222568000
6	0.801007000	1.252173000	-2.414794000
1	1.479980000	1.094882000	-3.266322000
1	-0.014544000	1.907351000	-2.756613000
1	-0.728093000	-0.142653000	-2.519051000
6	0.990783000	-1.262357000	-2.357720000
1	1.627105000	-1.070735000	-3.233246000
1	0.295060000	-2.075205000	-2.618099000
8	-1.835537000	0.916618000	-0.088743000
8	-1.913595000	-1.271390000	-0.095053000
6	-2.546104000	-0.162243000	-0.092840000
6	-4.063421000	-0.089190000	-0.022034000
6	-4.418331000	-0.149209000	1.484034000
1	-5.511304000	-0.098562000	1.605469000
1	-4.063327000	-1.087363000	1.936558000
1	-3.969400000	0.694789000	2.029480000
6	-4.676624000	-1.292241000	-0.756683000
1	-4.421692000	-1.275328000	-1.827547000
1	-4.323268000	-2.243243000	-0.333585000
1	-5.772872000	-1.260592000	-0.664112000
6	-4.563588000	1.230752000	-0.630669000
1	-4.269393000	1.316596000	-1.687748000
1	-5.662201000	1.267851000	-0.575882000
1	-4.163653000	2.101190000	-0.091224000

2a-OPiv-EDA

7	0.753291000	1.740971000	-0.075680000
6	0.899262000	2.320741000	-1.287308000
27	0.073388000	0.010810000	-0.005177000
7	0.266827000	0.219475000	1.988778000
6	1.360926000	3.628401000	-1.385516000
1	1.468775000	4.093506000	-2.365638000
7	-0.387593000	0.363469000	-1.943265000
6	1.680461000	4.315718000	-0.208798000
1	2.035829000	5.346133000	-0.258544000
6	1.553869000	3.681130000	1.028743000
1	1.817243000	4.188795000	1.957205000
6	1.083940000	2.368844000	1.067417000

6	0.975518000	1.512615000	2.288007000	6	0.918566000	1.535531000	2.270353000
1	1.992186000	1.262251000	2.625020000	1	1.978630000	1.319352000	2.471039000
1	0.472758000	2.046319000	3.106660000	1	0.484837000	1.977624000	3.177864000
1	0.885896000	-0.522338000	2.338654000	1	0.907150000	-0.499227000	2.287342000
6	-1.093576000	0.136159000	2.627250000	6	-1.094641000	0.067596000	2.599024000
1	-1.090165000	0.620779000	3.615526000	1	-1.112028000	0.570289000	3.577642000
1	-1.306370000	-0.934054000	2.773342000	1	-1.242481000	-1.010152000	2.765529000
6	-2.077834000	0.721545000	1.652672000	6	-2.118475000	0.579786000	1.626155000
6	-1.638051000	0.659860000	0.328800000	6	-1.689033000	0.530373000	0.300528000
6	-2.427626000	1.063877000	-0.745537000	6	-2.501500000	0.888672000	-0.771989000
6	-3.708641000	1.568958000	-0.483261000	6	-3.801899000	1.337212000	-0.503665000
1	-4.358093000	1.888619000	-1.302620000	1	-4.468417000	1.626692000	-1.320257000
6	-4.160700000	1.649018000	0.843722000	6	-4.249050000	1.401904000	0.825899000
1	-5.159050000	2.043347000	1.045657000	1	-5.263260000	1.750289000	1.032702000
6	-3.359276000	1.220982000	1.915241000	6	-3.420685000	1.020963000	1.893934000
1	-3.737594000	1.275754000	2.939591000	1	-3.791821000	1.068730000	2.921106000
6	-1.831602000	0.806972000	-2.100153000	6	-1.898846000	0.648183000	-2.126787000
1	-1.873714000	1.686067000	-2.760456000	1	-2.080204000	1.470503000	-2.834438000
1	-2.366941000	-0.010719000	-2.603927000	1	-2.318767000	-0.268801000	-2.565287000
1	-0.253168000	-0.472495000	-2.521176000	1	-0.143736000	-0.360181000	-2.593328000
6	0.599440000	1.382944000	-2.414394000	6	0.420581000	1.596495000	-2.405126000
1	0.245929000	1.903071000	-3.316181000	1	-0.024353000	2.103904000	-3.272743000
1	1.526208000	0.844455000	-2.666408000	1	1.406703000	1.207630000	-2.702068000
8	2.877555000	-0.833021000	1.489402000	8	2.928718000	-0.667401000	1.393164000
8	1.876183000	-0.736472000	-0.533843000	8	1.947257000	-0.498713000	-0.634027000
6	2.890676000	-0.949142000	0.240799000	6	2.952811000	-0.740075000	0.140170000
6	4.175922000	-1.387074000	-0.503973000	6	4.235829000	-1.228855000	-0.577150000
8	-2.778232000	-1.996423000	-0.903323000	8	-2.579939000	-2.224532000	-0.903334000
8	-2.459216000	-2.548597000	1.284532000	8	-2.098254000	-2.719508000	1.267220000
6	-4.236407000	-1.988468000	-0.689135000	6	-4.022881000	-2.359267000	-0.627677000
6	-4.878057000	-1.627447000	-2.006744000	6	-4.756178000	-1.978039000	-1.890875000
6	-2.037379000	-2.238569000	0.180842000	6	-1.768007000	-2.326967000	0.157754000
6	-0.584964000	-2.017913000	-0.149813000	6	-0.422863000	-1.787480000	-0.231112000
1	-4.531740000	-2.988256000	-0.338566000	1	-4.211284000	-3.400813000	-0.328908000
1	-4.452157000	-1.252187000	0.099211000	1	-4.263328000	-1.694231000	0.215453000
1	-5.971801000	-1.655676000	-1.890066000	1	-5.837489000	-2.096994000	-1.724837000
1	-4.594321000	-0.614092000	-2.324145000	1	-4.564028000	-0.929632000	-2.159061000
1	-4.596829000	-2.343049000	-2.793314000	1	-4.464198000	-2.625008000	-2.731123000
1	-0.283967000	-2.262030000	-1.176473000	1	-0.004027000	-2.272631000	-1.127780000
7	0.220712000	-2.697357000	0.718446000	7	0.610810000	-2.817201000	0.927251000
7	0.882777000	-3.182995000	1.478452000	7	1.389274000	-3.061615000	1.673947000
6	4.569975000	-0.263301000	-1.484025000	6	4.143325000	-2.771175000	-0.593827000
1	3.775749000	-0.082725000	-2.223399000	1	4.103704000	-3.177342000	0.428729000
1	4.759347000	0.681118000	-0.949266000	1	3.245345000	-3.107467000	-1.135950000
1	5.489177000	-0.537220000	-2.026193000	1	5.026101000	-3.196204000	-1.097603000
6	5.317587000	-1.640050000	0.487935000	6	4.313170000	-0.697139000	-2.017024000
1	6.225933000	-1.946817000	-0.054405000	1	3.464810000	-1.045285000	-2.622898000
1	5.554943000	-0.735286000	1.067392000	1	4.316059000	0.403871000	-2.034648000
1	5.059085000	-2.438556000	1.199272000	1	5.241128000	-1.047584000	-2.496373000
6	3.864797000	-2.681244000	-1.282715000	6	5.477908000	-0.786838000	0.212041000
1	3.529502000	-3.480544000	-0.602221000	1	6.389485000	-1.164223000	-0.277424000
1	3.076066000	-2.517090000	-2.031321000	1	5.545542000	0.311516000	0.259538000
1	4.767822000	-3.035109000	-1.805008000	1	5.456513000	-1.170576000	1.241872000

TS1-OPiv

7	0.586531000	1.858925000	-0.059211000
6	0.613595000	2.512353000	-1.236836000
27	0.076658000	0.014419000	-0.048035000
7	0.257088000	0.221990000	1.953254000
6	0.879638000	3.877035000	-1.277505000
1	0.891489000	4.403839000	-2.231762000
7	-0.406523000	0.421689000	-1.984662000
6	1.128933000	4.543330000	-0.071874000
1	1.329825000	5.615927000	-0.074416000
6	1.129863000	3.837418000	1.133719000
1	1.341414000	4.332473000	2.081881000
6	0.854575000	2.470505000	1.106684000

2a-carbene-OPiv

7	0.718938000	1.893743000	0.150796000
6	0.666768000	2.821737000	-0.819382000
27	0.049503000	0.105871000	-0.221323000
7	0.420182000	-0.159929000	1.727654000
6	1.048903000	4.134429000	-0.556384000
1	1.000505000	4.887975000	-1.342770000
7	-0.546233000	1.005201000	-1.944141000
6	1.494217000	4.450053000	0.732158000
1	1.786729000	5.474210000	0.969590000
6	1.576060000	3.457803000	1.714297000
1	1.942519000	3.678616000	2.717026000
6	1.180788000	2.163453000	1.382549000

6	1.306174000	0.939021000	2.234714000
1	2.343139000	0.575140000	2.155620000
1	1.100383000	1.140340000	3.294761000
1	0.990639000	-1.026259000	1.71897200
6	-0.869997000	-0.327094000	2.485423000
1	-0.742778000	0.015502000	3.522713000
1	-1.089586000	-1.404868000	2.506544000
6	-1.948423000	0.399119000	1.732967000
6	-1.646878000	0.607747000	0.388283000
6	-2.530591000	1.203865000	-0.506295000
6	-3.785981000	1.607926000	-0.032709000
1	-4.510312000	2.070915000	-0.707740000
6	-4.109054000	1.407482000	1.318954000
1	-5.087007000	1.725089000	1.687026000
6	-3.202185000	0.806740000	2.206574000
1	-3.475968000	0.656405000	3.254085000
6	-2.042462000	1.251488000	-1.923936000
1	-2.261829000	2.202501000	-2.430560000
1	-2.503680000	0.441658000	-2.507778000
1	-0.341672000	0.382621000	-2.731751000
6	0.275995000	2.243978000	-2.144297000
1	-0.255980000	2.962889000	-2.782783000
1	1.196164000	1.940163000	-2.666874000
8	2.446782000	-1.786506000	0.732159000
8	1.912627000	-0.325864000	-0.908000000
6	2.726773000	-1.122887000	-0.300803000
6	4.163162000	-1.173087000	-0.872830000
8	-2.742499000	-1.804714000	-1.345184000
8	-1.999414000	-2.764562000	0.590438000
6	-4.140117000	-2.183354000	-1.037899000
6	-5.006811000	-1.548301000	-2.098151000
6	-1.829188000	-2.102910000	-0.433940000
6	-0.490323000	-1.537996000	-0.643714000
1	-4.201245000	-3.280979000	-1.040336000
1	-4.369252000	-1.809556000	-0.029373000
1	-6.056307000	-1.822088000	-1.912727000
1	-4.927150000	-0.451900000	-2.066432000
1	-4.729086000	-1.901032000	-3.102092000
1	0.249544000	-2.252788000	-1.041427000
7	0.633828000	-4.185554000	1.456042000
7	0.519764000	-3.857933000	2.502218000
6	4.785793000	-2.556178000	-0.627395000
1	5.821397000	-2.572898000	-1.001503000
1	4.803116000	-2.804835000	0.443114000
1	4.220854000	-3.343786000	-1.150747000
6	4.949718000	-0.094918000	-0.092552000
1	5.992974000	-0.060959000	-0.444737000
1	4.504704000	0.901771000	-0.240207000
1	4.957917000	-0.315630000	0.986016000
6	4.185061000	-0.845813000	-2.373953000
1	3.574992000	-1.561011000	-2.947409000
1	3.802038000	0.164975000	-2.572922000
1	5.217921000	-0.900035000	-2.752964000

4a-OPiv

27	0.153521000	0.296573000	0.197217000
8	2.184079000	0.360934000	0.170463000
8	1.953641000	-1.846429000	0.500334000
8	0.206780000	-2.947821000	-1.329175000
8	-1.410510000	-2.887558000	0.276169000
7	0.060108000	2.143890000	-0.189044000
7	-0.017954000	0.107088000	-1.803333000
1	0.581721000	-0.650676000	-2.149250000
7	-0.117550000	0.886445000	2.106734000
1	0.603099000	0.485644000	2.715824000
6	-0.103033000	3.014466000	0.821073000
6	-0.264592000	4.373122000	0.549995000

1	-0.405165000	5.082313000	1.366365000
6	-0.234870000	4.795478000	-0.783253000
1	-0.371080000	5.851866000	-1.020747000
6	-0.017156000	3.872401000	-1.814318000
1	0.034057000	4.187366000	-2.856876000
6	0.135215000	2.530932000	-1.477731000
6	0.483303000	1.390507000	-2.392249000
1	0.109672000	1.537551000	-3.415935000
1	1.581563000	1.315849000	-2.436745000
6	-1.446597000	-0.213866000	-2.206592000
1	-1.734725000	0.416831000	-3.061159000
1	-1.461765000	-1.257303000	-2.553221000
6	-2.350678000	-0.033934000	-1.020418000
6	-3.750186000	-0.107296000	-1.021067000
1	-4.296762000	-0.267542000	-1.954683000
6	-4.450472000	0.020699000	0.189657000
1	-5.541329000	-0.033236000	0.186879000
6	-3.771056000	0.211627000	1.404272000
1	-4.332358000	0.302148000	2.338465000
6	-2.372063000	0.278568000	1.403484000
6	-1.688980000	0.154229000	0.192412000
6	-1.459238000	0.386578000	2.590836000
1	-1.840599000	1.033358000	3.395889000
1	-1.283869000	-0.611719000	3.022041000
6	0.022984000	2.384258000	2.179433000
1	1.033708000	2.602728000	2.557324000
1	-0.694159000	2.809446000	2.895928000
6	2.693450000	-0.771772000	0.287277000
6	0.499525000	-1.606704000	0.659481000
1	0.273134000	-1.812690000	1.715498000
6	-0.204370000	-2.554929000	-0.234505000
6	-2.325423000	-3.622269000	-0.596863000
1	-2.476496000	-3.033571000	-1.514486000
1	-1.857230000	-4.580754000	-0.868028000
6	-3.613250000	-3.809463000	0.172542000
1	-4.339577000	-4.347107000	-0.455444000
1	-3.445324000	-4.397924000	1.086795000
1	-4.047447000	-2.837037000	0.449126000
6	4.182249000	-1.041861000	0.166873000
6	4.392088000	-1.878808000	-1.117469000
1	5.466284000	-2.081489000	-1.242608000
1	3.859569000	-2.838676000	-1.057423000
1	4.036879000	-1.337379000	-2.007456000
6	4.651655000	-1.840367000	1.400558000
1	5.735425000	-2.014995000	1.326180000
1	4.455635000	-1.285105000	2.330422000
1	4.147951000	-2.814915000	1.463397000
6	4.940893000	0.287944000	0.069666000
1	6.019235000	0.084461000	-0.004294000
1	4.636667000	0.862051000	-0.817485000
1	4.767673000	0.910842000	0.959464000

TS2-OPiv

7	-1.050124000	2.004618000	-0.271568000
6	-1.352517000	2.814775000	0.758911000
27	-0.326624000	0.287780000	0.100475000
7	0.106072000	0.301585000	-1.871838000
6	-1.684262000	4.148441000	0.527563000
1	-1.921920000	4.808732000	1.362345000
7	-0.519223000	0.854217000	2.034519000
6	-1.704788000	4.610942000	-0.793812000
1	-1.951457000	5.653755000	-1.000208000
6	-1.411316000	3.741138000	-1.852860000
1	-1.431987000	4.082025000	-2.888408000
6	-1.086167000	2.421754000	-1.553014000
6	-0.812661000	1.297475000	-2.513663000
1	-1.762473000	0.774506000	-2.707891000
1	-0.415252000	1.648581000	-3.476784000

1	-0.095284000	-0.625248000	-2.263242000
6	1.576809000	0.591109000	-2.113274000
1	1.665819000	1.411170000	-2.840635000
1	2.031447000	-0.297536000	-2.574491000
6	2.253214000	0.958586000	-0.822602000
6	1.493035000	0.730964000	0.339879000
6	1.881225000	1.207957000	1.607293000
6	3.117019000	1.840097000	1.729197000
1	3.452148000	2.234497000	2.691299000
6	3.922799000	1.992658000	0.586129000
1	4.894634000	2.480862000	0.686052000
6	3.492813000	1.585508000	-0.688187000
1	4.112105000	1.790623000	-1.564729000
6	0.844027000	1.018011000	2.678391000
1	0.825231000	1.856757000	3.389518000
1	1.045592000	0.107819000	3.263670000
1	-1.020413000	0.125528000	2.553213000
6	-1.371045000	2.095926000	2.079631000
1	-1.069169000	2.747953000	2.911402000
1	-2.404852000	1.768980000	2.271946000
8	-0.998519000	-2.562946000	0.652956000
8	-2.042947000	-0.668922000	-0.031594000
6	-2.012984000	-1.921683000	0.271314000
6	-3.375884000	-2.652282000	0.151899000
8	2.711573000	-2.382853000	0.181954000
8	1.176146000	-2.366412000	-1.489806000
6	3.586873000	-3.237576000	-0.630732000
6	4.846158000	-3.473201000	0.170384000
6	1.549257000	-1.998243000	-0.380688000
6	0.789054000	-1.073639000	0.533049000
1	3.046051000	-4.171011000	-0.847874000
1	3.786376000	-2.717224000	-1.579989000
1	5.528861000	-4.112831000	-0.408944000
1	5.360560000	-2.524816000	0.384833000
1	4.622113000	-3.980059000	1.120592000
1	1.016219000	-1.318311000	1.579154000
6	-3.216246000	-4.155352000	0.412699000
1	-2.517151000	-4.612435000	-0.303351000
1	-2.839048000	-4.350377000	1.427287000
1	-4.191877000	-4.655302000	0.307637000
6	-3.926255000	-2.419420000	-1.268862000
1	-4.077363000	-1.348859000	-1.467684000
1	-3.238143000	-2.818737000	-2.030504000
1	-4.893749000	-2.933635000	-1.380671000
6	-4.324775000	-2.029648000	1.196677000
1	-3.930940000	-2.157612000	2.217279000
1	-4.466433000	-0.954666000	1.012832000
1	-5.308185000	-2.522838000	1.145720000

INT-MI-OPiv

7	1.747377000	1.281682000	-0.221890000
6	2.513277000	1.755996000	0.778263000
27	0.510198000	-0.065722000	0.154296000
7	0.314654000	-0.191703000	-1.796964000
6	3.410328000	2.792357000	0.525400000
1	4.027054000	3.193082000	1.330482000
7	1.108778000	0.152645000	2.062211000
6	3.508088000	3.285433000	-0.780691000
1	4.211451000	4.089358000	-1.003792000
6	2.715772000	2.752315000	-1.806263000
1	2.788561000	3.122029000	-2.829421000
6	1.815846000	1.740201000	-1.488432000
6	0.804001000	1.092194000	-2.394840000
1	-0.073912000	1.753626000	-2.466678000
1	1.191752000	0.935364000	-3.411825000
1	-0.700653000	-0.248765000	-1.982066000
6	1.039227000	-1.440133000	-2.204849000

1	1.839277000	-1.173722000	-2.908024000
1	0.339961000	-2.114832000	-2.710440000
6	1.671365000	-2.047867000	-0.967894000
6	0.993024000	-2.050129000	0.305544000
6	1.852393000	-2.024925000	1.480087000
6	3.176541000	-2.414654000	1.386950000
1	3.806436000	-2.395816000	2.279032000
6	3.735470000	-2.731762000	0.135039000
1	4.774582000	-3.058520000	0.067424000
6	3.014811000	-2.449722000	-1.021575000
1	3.511438000	-2.484884000	-1.994086000
6	1.344760000	-1.220362000	2.651859000
1	2.080048000	-1.173274000	3.466966000
1	0.397211000	-1.576355000	3.073142000
1	0.364528000	0.636498000	2.579798000
6	2.354990000	1.002459000	2.070508000
1	3.221075000	0.329544000	2.170369000
1	2.354083000	1.669679000	2.943582000
8	-2.274179000	0.651273000	-1.282654000
8	-0.945153000	1.126512000	0.494782000
6	-2.043129000	1.223806000	-0.198508000
6	-3.084464000	2.159328000	0.465521000
8	-2.721343000	-1.971987000	0.254905000
8	-1.469430000	-2.694939000	-1.498108000
6	-3.920108000	-2.221276000	-0.540409000
6	-5.116376000	-1.909070000	0.330173000
6	-1.533297000	-2.209514000	-0.368404000
6	-0.430256000	-1.807166000	0.514602000
1	-3.878551000	-1.577729000	-1.433386000
1	-3.914581000	-3.272211000	-0.868508000
1	-6.038083000	-2.088685000	-0.243710000
1	-5.136382000	-2.550444000	1.223991000
1	-5.111925000	-0.857217000	0.650398000
1	-0.763381000	-1.826445000	1.553473000
6	-4.371873000	2.188358000	-0.367598000
1	-5.108903000	2.848637000	0.115555000
1	-4.186093000	2.568156000	-1.382984000
1	-4.815723000	1.185790000	-0.455778000
6	-3.384947000	1.623244000	1.879329000
1	-2.486041000	1.636584000	2.512129000
1	-4.156423000	2.245687000	2.359296000
1	-3.758111000	0.588008000	1.835909000
6	-2.477949000	3.574460000	0.549043000
1	-2.233472000	3.959961000	-0.453401000
1	-3.201368000	4.264446000	1.011468000
1	-1.558989000	3.580267000	1.153066000

2a-OBz

7	-1.590890000	-1.299707000	-0.013871000
6	-2.099231000	-1.714633000	1.166156000
27	-0.194012000	-0.098091000	-0.003869000
7	-0.457531000	-0.041365000	-1.990266000
6	-3.226454000	-2.530162000	1.189072000
1	-3.640046000	-2.858786000	2.142750000
7	-0.447897000	-0.086452000	1.984759000
6	-3.803060000	-2.912747000	-0.027049000
1	-4.695602000	-3.540401000	-0.032105000
6	-3.232155000	-2.502505000	-1.236848000
1	-3.650457000	-2.809098000	-2.195821000
6	-2.104747000	-1.687766000	-1.200713000
6	-1.279825000	-1.238519000	-2.368871000
1	-0.578984000	-2.050231000	-2.618841000
1	-1.891884000	-1.035903000	-3.259173000
1	0.444969000	-0.121353000	-2.470980000
6	-1.082620000	1.276042000	-2.395712000
1	-1.738897000	1.128363000	-3.266505000
1	-0.256538000	1.931900000	-2.709840000

6	-1.776320000	1.867392000	-1.202018000
6	-1.364925000	1.329667000	0.015483000
6	-1.769887000	1.839530000	1.247100000
6	-2.673536000	2.910883000	1.261472000
1	-3.013659000	3.337508000	2.209026000
6	-3.132437000	3.440130000	0.044248000
1	-3.844901000	4.267983000	0.055566000
6	-2.679605000	2.939098000	-1.187130000
1	-3.024246000	3.387883000	-2.122721000
6	-1.070008000	1.221453000	2.423605000
1	-1.721685000	1.054588000	3.294472000
1	-0.241933000	1.869735000	2.748105000
1	0.456822000	-0.178493000	2.459078000
6	-1.269254000	-1.291358000	2.340240000
1	-1.877893000	-1.107878000	3.236927000
1	-0.568138000	-2.108685000	2.570607000
8	1.489161000	0.908571000	0.001249000
8	1.556179000	-1.285591000	-0.017724000
6	2.193656000	-0.177013000	-0.007381000
6	3.672373000	-0.111164000	-0.003948000
6	4.424702000	-1.297406000	0.043296000
6	4.326056000	1.132889000	-0.047589000
6	5.818827000	-1.238303000	0.046887000
6	5.720478000	1.185910000	-0.046336000
6	6.467767000	0.002088000	0.001172000
1	3.908977000	-2.258489000	0.080223000
1	3.735512000	2.050086000	-0.084665000
1	6.402147000	-2.160542000	0.085157000
1	6.228432000	2.151742000	-0.082841000
1	7.559069000	0.046316000	0.002663000

2a-OBz-EDA

7	-0.172356000	1.916490000	0.169302000
6	-0.305945000	2.398625000	1.424050000
27	0.195892000	0.103428000	-0.045965000
7	0.223969000	0.541503000	-2.017167000
6	-0.532564000	3.754370000	1.631412000
1	-0.631884000	4.138173000	2.646985000
7	0.534482000	0.172739000	1.949647000
6	-0.633468000	4.595192000	0.517107000
1	-0.804512000	5.663960000	0.655227000
6	-0.526534000	4.066023000	-0.770655000
1	-0.624629000	4.695816000	-1.655388000
6	-0.295288000	2.698933000	-0.918730000
6	-0.251972000	1.954700000	-2.214187000
1	-1.275687000	1.905573000	-2.613526000
1	0.374502000	2.473314000	-2.953586000
1	-0.455582000	-0.050306000	-2.509628000
6	1.609840000	0.310843000	-2.559200000
1	1.773172000	0.903651000	-3.471945000
1	1.669438000	-0.754053000	-2.832909000
6	2.578596000	0.605792000	-1.449070000
6	2.017492000	0.466819000	-0.178177000
6	2.763702000	0.602150000	0.990892000
6	4.127445000	0.909442000	0.884201000
1	4.743365000	1.018653000	1.780778000
6	4.702692000	1.067320000	-0.386585000
1	5.764436000	1.310714000	-0.466423000
6	3.941721000	0.908337000	-1.556383000
1	4.412360000	1.017337000	-2.537235000
6	2.015652000	0.292906000	2.255901000
1	2.168947000	1.044459000	3.044631000
1	2.339316000	-0.678837000	2.656300000
1	0.185442000	-0.667987000	2.420554000
6	-0.275562000	1.320976000	2.461819000
1	0.097107000	1.678165000	3.432474000
1	-1.304298000	0.954766000	2.601882000

8	-2.604068000	-0.073152000	-1.785639000
8	-1.750374000	-0.367644000	0.290155000
6	-2.720179000	-0.346579000	-0.565649000
8	2.575082000	-2.491623000	0.769665000
8	2.348314000	-2.703425000	-1.486802000
6	4.025917000	-2.717261000	0.643085000
6	4.616551000	-2.612971000	2.028095000
6	1.896994000	-2.455620000	-0.379187000
6	0.482377000	-2.008662000	-0.111550000
1	4.174646000	-3.711092000	0.196133000
1	4.422074000	-1.951823000	-0.040767000
1	5.696202000	-2.818071000	1.970485000
1	4.481786000	-1.604033000	2.442757000
1	4.162249000	-3.346752000	2.709973000
1	0.052245000	-2.324654000	0.847501000
7	-0.345739000	-2.420710000	-1.118337000
7	-0.999162000	-2.680406000	-1.988461000
6	-4.076096000	-0.711049000	-0.006290000
6	-4.221090000	-1.148075000	1.321397000
6	-5.213229000	-0.627126000	-0.826562000
6	-5.478863000	-1.500994000	1.816713000
6	-6.472073000	-0.972860000	-0.329313000
6	-6.607585000	-1.413284000	0.992853000
1	-3.339653000	-1.214475000	1.961273000
1	-5.100088000	-0.286984000	-1.857714000
1	-5.579823000	-1.845900000	2.848263000
1	-7.350332000	-0.901292000	-0.974779000
1	-7.591061000	-1.689131000	1.379895000

TS1-OBz

7	-0.236091000	1.872381000	0.038078000
6	-0.377349000	2.454753000	1.245066000
27	0.214953000	0.014136000	-0.032149000
7	0.228114000	0.329585000	-2.025587000
6	-0.638795000	3.817217000	1.340928000
1	-0.743518000	4.286391000	2.319387000
7	0.535936000	0.304100000	1.957096000
6	-0.764346000	4.555901000	0.158332000
1	-0.961956000	5.628099000	0.205372000
6	-0.645908000	3.923703000	-1.081331000
1	-0.758890000	4.475139000	-2.015107000
6	-0.378642000	2.554781000	-1.109539000
6	-0.309705000	1.701735000	-2.335265000
1	-1.332061000	1.573020000	-2.720091000
1	0.291207000	2.176735000	-3.123249000
1	-0.429616000	-0.329850000	-2.457557000
6	1.621970000	0.115932000	-2.551430000
1	1.756925000	0.639235000	-3.510036000
1	1.727883000	-0.964179000	-2.734840000
6	2.574165000	0.546890000	-1.472795000
6	2.022454000	0.470762000	-0.194141000
6	2.748102000	0.748339000	0.960916000
6	4.088012000	1.138484000	0.828442000
1	4.690154000	1.362006000	1.713002000
6	4.657645000	1.231505000	-0.451479000
1	5.701560000	1.536810000	-0.550668000
6	3.914059000	0.933327000	-1.604845000
1	4.378966000	1.000719000	-2.591902000
6	2.013235000	0.491260000	2.245205000
1	2.142510000	1.293320000	2.986709000
1	2.370844000	-0.443802000	2.700104000
1	0.209353000	-0.505878000	2.493563000
6	-0.308507000	1.468730000	2.369951000
1	0.061086000	1.915862000	3.303699000
1	-1.323751000	1.084256000	2.551245000
8	-2.539465000	-0.409480000	-1.762659000
8	-1.724965000	-0.441279000	0.349640000

6	-2.681355000	-0.512543000	-0.517748000
8	2.699272000	-2.365738000	0.946680000
8	2.396507000	-2.774849000	-1.273969000
6	4.151613000	-2.576718000	0.804034000
6	4.772768000	-2.314874000	2.154710000
6	1.984969000	-2.397106000	-0.187016000
6	0.636443000	-1.808645000	0.103381000
1	4.309098000	-3.609256000	0.459552000
1	4.514031000	-1.880902000	0.032360000
1	5.857521000	-2.488293000	2.088746000
1	4.610895000	-1.274184000	2.469467000
1	4.361348000	-2.991061000	2.918372000
1	0.120779000	-2.311845000	0.937650000
7	-0.353982000	-2.759690000	-1.170312000
7	-1.138225000	-2.958556000	-1.924064000
6	-4.054128000	-0.745078000	0.060596000
6	-4.267470000	-0.787345000	1.447687000
6	-5.156110000	-0.917155000	-0.794582000
6	-5.549618000	-0.987428000	1.963794000
6	-6.433616000	-1.120209000	-0.274908000
6	-6.655865000	-1.154798000	1.114114000
1	-3.420311000	-0.662166000	2.124469000
1	-4.999595000	-0.891959000	-1.874907000
1	-5.697112000	-1.013170000	3.046852000
1	-7.278958000	-1.253696000	-0.955726000
1	-7.647283000	-1.305512000	1.515084000

2a-carbene-OBz

7	0.142604000	2.014367000	0.218864000
6	0.151800000	2.845716000	-0.839179000
27	-0.235127000	0.133845000	-0.083666000
7	-0.064671000	0.033920000	1.906280000
6	0.363108000	4.208495000	-0.657890000
1	0.361362000	4.883481000	-1.513922000
7	-0.754994000	0.846036000	-1.914736000
6	0.579386000	4.678149000	0.643525000
1	0.738313000	5.743833000	0.816564000
6	0.604105000	3.788519000	1.720710000
1	0.793645000	4.132478000	2.737838000
6	0.381310000	2.434610000	1.470117000
6	0.459185000	1.323618000	2.471681000
1	1.516996000	1.161174000	2.732008000
1	-0.077276000	1.572536000	3.397734000
1	0.686301000	-0.676824000	2.012594000
6	-1.374780000	-0.406237000	2.494756000
1	-1.440967000	-0.093638000	3.547067000
1	-1.385658000	-1.506316000	2.461897000
6	-2.464770000	0.144881000	1.620135000
6	-2.044010000	0.396675000	0.314630000
6	-2.892206000	0.865062000	-0.682380000
6	-4.238163000	1.086663000	-0.357310000
1	-4.937992000	1.448699000	-1.114971000
6	-4.682651000	0.837980000	0.950462000
1	-5.731093000	1.014468000	1.200110000
6	-3.808031000	0.370082000	1.944364000
1	-4.174566000	0.183535000	2.956951000
6	-2.261148000	1.015862000	-2.034055000
1	-2.472956000	1.992477000	-2.492777000
1	-2.622185000	0.237424000	-2.720929000
1	-0.456080000	0.179557000	-2.632958000
6	0.015571000	2.111619000	-2.138095000
1	-0.451328000	2.717037000	-2.927540000
1	1.022425000	1.821220000	-2.475275000
8	2.353019000	-1.174479000	1.322924000
8	1.742299000	-0.058948000	-0.551861000
6	2.606462000	-0.647045000	0.206610000
8	-2.518819000	-2.122376000	-1.559490000

8	-2.010813000	-2.994238000	0.490803000
6	-3.894311000	-2.665691000	-1.489056000
6	-4.653876000	-2.072991000	-2.651391000
6	-1.747925000	-2.312954000	-0.501320000
6	-0.474211000	-1.585991000	-0.471277000
1	-3.826563000	-3.761978000	-1.536629000
1	-4.316167000	-2.370047000	-0.517766000
1	-5.680680000	-2.468204000	-2.648858000
1	-4.706210000	-0.977648000	-2.565656000
1	-4.183994000	-2.337685000	-3.609707000
1	0.413474000	-2.215063000	-0.649115000
7	0.925622000	-3.917265000	1.682305000
7	0.555572000	-3.575576000	2.662593000
6	4.019475000	-0.684065000	-0.323558000
6	5.040713000	-1.254622000	0.454141000
6	4.334360000	-0.154466000	-1.586419000
6	6.353503000	-1.295058000	-0.021497000
6	5.646996000	-0.196681000	-2.062646000
6	6.659616000	-0.766353000	-1.281217000
1	4.795460000	-1.664502000	1.435580000
1	3.543938000	0.288628000	-2.194167000
1	7.140428000	-1.740112000	0.591448000
1	5.882367000	0.215611000	-3.046345000
1	7.686012000	-0.798352000	-1.653398000

4a-OBz

27	0.173457000	0.303245000	0.189271000
8	-1.826560000	0.597450000	0.154944000
8	-1.856904000	-1.636070000	0.422410000
8	-0.181687000	-2.865543000	-1.407838000
8	1.376346000	-3.036632000	0.247752000
7	0.462522000	2.136442000	-0.168119000
7	0.348568000	0.127340000	-1.813133000
1	-0.314393000	-0.568770000	-2.173532000
7	0.487038000	0.833842000	2.109058000
1	-0.284831000	0.511895000	2.702247000
6	0.705570000	2.971504000	0.855232000
6	0.998412000	4.312165000	0.605343000
1	1.204984000	4.991293000	1.433189000
6	1.014227000	4.755872000	-0.721008000
1	1.252785000	5.797659000	-0.941747000
6	0.712970000	3.873265000	-1.766775000
1	0.696172000	4.207122000	-2.804531000
6	0.429367000	2.548085000	-1.451202000
6	-0.026048000	1.460996000	-2.383774000
1	-1.126009000	1.493899000	-2.431223000
1	0.362721000	1.587626000	-3.404731000
6	1.746360000	-0.314415000	-2.209369000
1	2.103569000	0.312962000	-3.039565000
1	1.668967000	-1.343409000	-2.589260000
6	2.648046000	-0.253363000	-1.009135000
6	1.991942000	-0.030845000	0.201083000
6	2.669043000	0.000593000	1.421791000
6	4.055832000	-0.193939000	1.434892000
1	4.612136000	-0.176299000	2.376203000
6	4.729393000	-0.418507000	0.222767000
1	5.810473000	-0.573892000	0.229387000
6	4.035127000	-0.454210000	-0.997410000
1	4.576274000	-0.642369000	-1.928955000
6	1.754190000	0.174123000	2.600149000
1	2.188585000	0.752138000	3.430282000
1	1.461699000	-0.810268000	2.997639000
6	0.528649000	2.337052000	2.205941000
1	1.310800000	2.656815000	2.909103000
1	-0.436943000	2.671754000	2.614995000
6	-2.468096000	-0.473631000	0.248974000
6	-3.938601000	-0.529429000	0.177999000

6	-4.653275000	0.664372000	-0.031182000
1	-4.109978000	1.603996000	-0.142605000
6	-6.045549000	0.638229000	-0.093059000
1	-6.599273000	1.565204000	-0.253733000
6	-6.731247000	-0.574758000	0.051061000
6	-6.022047000	-1.764643000	0.256050000
1	-6.557969000	-2.709040000	0.368015000
6	-4.628826000	-1.747438000	0.320567000
1	-4.073262000	-2.671888000	0.482285000
6	-0.388774000	-1.558761000	0.613635000
1	-0.208960000	-1.804110000	1.669781000
6	0.232273000	-2.555669000	-0.288268000
6	2.246717000	-3.819314000	-0.629433000
1	2.429555000	-3.238814000	-1.546228000
1	1.725663000	-4.750080000	-0.901068000
6	3.523653000	-4.077171000	0.136543000
1	3.328948000	-4.661093000	1.048452000
1	4.004705000	-3.127975000	0.416183000
1	4.220144000	-4.647679000	-0.496259000
1	-7.822204000	-0.592265000	0.004127000

TS2-OBz

7	-0.669186000	-2.260323000	-0.236064000
6	-0.891102000	-3.074579000	0.811963000
27	-0.247764000	-0.438818000	0.098865000
7	-0.599397000	-0.238828000	-1.878535000
6	-1.390954000	-4.359312000	0.607623000
1	-1.578893000	-5.018257000	1.455965000
7	-0.433273000	-0.968971000	2.041616000
6	-1.640853000	-4.775799000	-0.705551000
1	-2.042143000	-5.773573000	-0.891029000
6	-1.375293000	-3.919735000	-1.782788000
1	-1.552019000	-4.232825000	-2.812318000
6	-0.877828000	-2.648926000	-1.509746000
6	-0.443194000	-1.597599000	-2.493294000
1	0.631943000	-1.737126000	-2.688192000
1	-0.973723000	-1.666950000	-3.453501000
1	0.113079000	0.386073000	-2.271597000
6	-1.954269000	0.395563000	-2.140328000
1	-2.515098000	-0.232211000	-2.848380000
1	-1.790270000	1.366456000	-2.629639000
6	-2.717180000	0.539730000	-0.855110000
6	-1.975831000	0.282608000	0.313874000
6	-2.578118000	0.157938000	1.582104000
6	-3.945196000	0.401425000	1.695520000
1	-4.453445000	0.304955000	2.657811000
6	-4.676746000	0.746283000	0.544240000
1	-5.746372000	0.946385000	0.637344000
6	-4.084264000	0.790152000	-0.728955000
1	-4.698630000	0.986843000	-1.610879000
6	-1.643800000	-0.300751000	2.666197000
1	-2.134576000	-0.995021000	3.363476000
1	-1.282026000	0.550172000	3.262960000
1	0.394298000	-0.651900000	2.557147000
6	-0.454043000	-2.472463000	2.118406000
1	-1.070136000	-2.813442000	2.962321000
1	0.580829000	-2.797524000	2.308223000
8	1.957033000	1.486356000	0.665934000
8	1.707840000	-0.667291000	-0.021190000
6	2.411812000	0.367723000	0.290056000
8	-0.885387000	3.591656000	0.153468000
8	0.113045000	2.513123000	-1.573970000
6	-0.944810000	4.813569000	-0.660157000
6	-1.635443000	5.871453000	0.168872000
6	-0.338799000	2.509208000	-0.433352000
6	-0.333328000	1.328107000	0.502801000
1	0.086118000	5.094004000	-0.924631000

1	-1.493099000	4.579928000	-1.585597000
1	-1.693140000	6.804677000	-0.411409000
1	-2.658978000	5.564977000	0.430368000
1	-1.077472000	6.075905000	1.094472000
1	-0.393497000	1.679403000	1.541135000
6	3.904530000	0.201899000	0.189990000
6	4.744032000	1.323500000	0.298206000
6	4.471467000	-1.068516000	-0.009207000
6	6.129595000	1.176725000	0.204816000
6	5.857922000	-1.213265000	-0.093978000
6	6.689509000	-0.091656000	0.011522000
1	4.302002000	2.309703000	0.449150000
1	3.819932000	-1.939658000	-0.091775000
1	6.775039000	2.054133000	0.283936000
1	6.292216000	-2.204236000	-0.243139000
1	7.773522000	-0.206405000	-0.056973000

INT-MI-OBz

7	0.910458000	-1.948790000	0.548714000
6	1.187601000	-2.949910000	-0.307645000
27	0.363816000	-0.294399000	-0.160648000
7	0.561091000	0.385476000	1.711340000
6	1.808000000	-4.106965000	0.159220000
1	2.040470000	-4.921612000	-0.527288000
7	0.446640000	-1.221121000	-1.934734000
6	2.125060000	-4.190210000	1.519933000
1	2.621544000	-5.081963000	1.906133000
6	1.815303000	-3.136654000	2.390326000
1	2.055250000	-3.190284000	3.452555000
6	1.192497000	-2.008335000	1.865738000
6	0.700331000	-0.803522000	2.623678000
1	-0.307355000	-1.030873000	3.004062000
1	1.337107000	-0.565331000	3.487082000
1	-0.287515000	0.894781000	1.981943000
6	1.731640000	1.334638000	1.710476000
1	2.343676000	1.180865000	2.608766000
1	1.347617000	2.360464000	1.743377000
6	2.531390000	1.027505000	0.465688000
6	1.853730000	0.983239000	-0.806499000
6	2.426590000	0.109502000	-1.801847000
6	3.728150000	-0.355600000	-1.666815000
1	4.143353000	-1.012483000	-2.433965000
6	4.469765000	-0.061001000	-0.514356000
1	5.495270000	-0.422007000	-0.417795000
6	3.839306000	0.551216000	0.571384000
1	4.345073000	0.603522000	1.537744000
6	1.465290000	-0.508117000	-2.783125000
1	1.968852000	-1.216897000	-3.453309000
1	0.940964000	0.229674000	-3.404593000
1	-0.503265000	-1.084249000	-2.324503000
6	0.713226000	-2.682965000	-1.712749000
1	1.428170000	-3.061898000	-2.456546000
1	-0.237094000	-3.217934000	-1.866693000
8	-2.213721000	-0.307235000	-2.021388000
8	-1.509322000	-0.474465000	0.130620000
6	-2.424912000	-0.378284000	-0.788214000
8	0.856762000	3.672844000	-0.136760000
8	-1.252115000	2.832919000	-0.054384000
6	0.383544000	4.905708000	0.501797000
6	1.584289000	5.811792000	0.652216000
6	-0.063570000	2.702161000	-0.339316000
6	0.493957000	1.493966000	-0.996803000
1	-0.396619000	5.346872000	-0.136815000
1	-0.066219000	4.643109000	1.471736000
1	1.272075000	6.756250000	1.122619000
1	2.353219000	5.347168000	1.287061000
1	2.027099000	6.044231000	-0.327675000

1	0.082610000	1.447455000	-2.010999000
6	-3.831366000	-0.371115000	-0.251420000
6	-4.089514000	-0.260058000	1.125913000
6	-4.907346000	-0.472142000	-1.148680000
6	-5.404591000	-0.249761000	1.595844000
6	-6.221445000	-0.465952000	-0.675992000
6	-6.473003000	-0.354819000	0.696795000
1	-3.255901000	-0.175493000	1.824512000
1	-4.703608000	-0.556562000	-2.217609000
1	-5.598106000	-0.158972000	2.666957000
1	-7.052318000	-0.547769000	-1.380142000
1	-7.501075000	-0.348640000	1.065670000

2a-OBz-Cl

7	2.162695000	-1.295341000	0.018670000
6	2.671751000	-1.713372000	-1.159989000
27	0.760213000	-0.100576000	0.004837000
7	1.024815000	-0.034392000	1.990667000
6	3.802689000	-2.523791000	-1.180263000
1	4.216764000	-2.855035000	-2.132814000
7	1.012398000	-0.096559000	-1.984068000
6	4.382203000	-2.898107000	0.037035000
1	5.277662000	-3.521557000	0.044090000
6	3.810472000	-2.485192000	1.245522000
1	4.231002000	-2.785636000	2.205469000
6	2.679262000	-1.675907000	1.206832000
6	1.852546000	-1.226349000	2.373546000
1	1.155239000	-2.040324000	2.626032000
1	2.463476000	-1.017925000	3.263273000
1	0.122997000	-0.116462000	2.472315000
6	1.644141000	1.287582000	2.390280000
1	2.303263000	1.146073000	3.259907000
1	0.815523000	1.940343000	2.704154000
6	2.332508000	1.878320000	1.193269000
6	1.923340000	1.333216000	-0.021631000
6	2.324776000	1.839557000	-1.255786000
6	3.222542000	2.915752000	-1.275397000
1	3.560027000	3.339687000	-2.225094000
6	3.679010000	3.453103000	-0.060860000
1	4.386902000	4.284792000	-0.076312000
6	3.229768000	2.954999000	1.172986000
1	3.572566000	3.409758000	2.106357000
6	1.629235000	1.211633000	-2.429596000
1	2.283342000	1.042551000	-3.298187000
1	0.798951000	1.854289000	-2.759559000
1	0.107706000	-0.194360000	-2.457264000
6	1.837968000	-1.299980000	-2.334824000
1	2.444012000	-1.118851000	-3.233719000
1	1.139707000	-2.121384000	-2.559396000
8	-0.928133000	0.898343000	-0.000800000
8	-0.987302000	-1.297212000	0.023299000
6	-1.626835000	-0.190424000	0.011315000
6	-3.104809000	-0.129929000	0.009088000
6	-3.854288000	-1.316346000	-0.053479000
6	-3.765181000	1.109032000	0.068217000
6	-5.246878000	-1.272359000	-0.059650000
6	-5.157376000	1.166923000	0.066572000
6	-5.882647000	-0.027676000	0.000853000
1	-3.340816000	-2.277779000	-0.101905000
1	-3.184208000	2.031272000	0.118665000
1	-5.833269000	-2.190341000	-0.110553000
1	-5.675266000	2.125330000	0.115634000
17	-7.632494000	0.035999000	-0.006635000

2a-OBz-Cl-EDA

7	0.385400000	1.950639000	0.146873000
6	0.209716000	2.426086000	1.398623000

27	0.661159000	0.120762000	-0.075434000
7	0.846625000	0.587257000	-2.032630000
6	0.067412000	3.792179000	1.614329000
1	-0.065420000	4.169895000	2.628327000
7	0.856127000	0.138334000	1.939543000
6	0.097625000	4.651984000	0.510656000
1	-0.000725000	5.728857000	0.656309000
6	0.243521000	4.131943000	-0.777137000
1	0.246697000	4.778431000	-1.655286000
6	0.382546000	2.753585000	-0.933635000
6	0.440969000	2.020175000	-2.234336000
1	-0.570729000	2.015211000	-2.667155000
1	1.112163000	2.516204000	-2.949403000
1	0.179206000	0.034217000	-2.583570000
6	2.257501000	0.307378000	-2.481420000
1	2.512693000	0.921196000	-3.358603000
1	2.286605000	-0.749597000	-2.788302000
6	3.159118000	0.515913000	-1.296735000
6	2.502259000	0.379526000	-0.072502000
6	3.169865000	0.435923000	1.149557000
6	4.553628000	0.658655000	1.147919000
1	5.109480000	0.703084000	2.088150000
6	5.226782000	0.813073000	-0.074475000
1	6.304539000	0.990200000	-0.073136000
6	4.542905000	0.733283000	-1.298677000
1	5.088141000	0.836773000	-2.240576000
6	2.316750000	0.134482000	2.347916000
1	2.470882000	0.839270000	3.178757000
1	2.538198000	-0.875420000	2.722919000
1	0.408973000	-0.679711000	2.365620000
6	0.102448000	1.337836000	2.419722000
1	0.441898000	1.656919000	3.415652000
1	-0.956532000	1.046295000	2.495379000
8	-1.985209000	0.049225000	-2.040394000
8	-1.329362000	-0.233906000	0.108666000
6	-2.221027000	-0.153353000	-0.824007000
8	2.857397000	-2.625346000	0.817214000
8	2.752738000	-2.754142000	-1.454457000
6	4.302540000	-2.915188000	0.765429000
6	4.810922000	-2.916625000	2.186297000
6	2.250392000	-2.518788000	-0.366066000
6	0.845153000	-2.007664000	-0.167062000
1	4.434269000	-3.888254000	0.270597000
1	4.774228000	-2.132687000	0.152851000
1	5.884384000	-3.158576000	2.178576000
1	4.686866000	-1.929826000	2.654691000
1	4.292381000	-3.672588000	2.794029000
1	0.348233000	-2.320654000	0.760322000
7	0.060729000	-2.367196000	-1.227616000
7	-0.546395000	-2.589967000	-2.140218000
6	-3.647301000	-0.345497000	-0.366670000
6	-3.957580000	-0.555499000	0.986646000
6	-4.689047000	-0.318116000	-1.307386000
6	-5.278274000	-0.737227000	1.398672000
6	-6.015438000	-0.498416000	-0.914870000
6	-6.294304000	-0.708118000	0.438815000
1	-3.156085000	-0.578721000	1.726210000
1	-4.453540000	-0.154122000	-2.360387000
1	-5.517279000	-0.901113000	2.450185000
1	-6.821951000	-0.478695000	-1.649100000
17	-7.957957000	-0.941321000	0.945655000

TS1-OBz-Cl

7	-0.332780000	1.916164000	-0.060820000
6	-0.143424000	2.454019000	-1.281799000
27	-0.676199000	0.037434000	0.066121000
7	-0.851561000	0.440429000	2.038546000

6	0.036505000	3.825567000	-1.424781000
1	0.180052000	4.257878000	-2.415225000
7	-0.866820000	0.218703000	-1.951109000
6	0.028633000	4.621772000	-0.273395000
1	0.158347000	5.701945000	-0.358565000
6	-0.136737000	4.037334000	0.984188000
1	-0.126913000	4.634979000	1.896076000
6	-0.316209000	2.656046000	1.059732000
6	-0.415189000	1.854069000	2.317255000
1	0.585898000	1.804336000	2.770561000
1	-1.092014000	2.324714000	3.043900000
1	-0.190963000	-0.159552000	2.546530000
6	-2.266332000	0.170496000	2.475867000
1	-2.498515000	0.730959000	3.394000000
1	-2.325672000	-0.903716000	2.708389000
6	-3.160054000	0.492721000	1.312254000
6	-2.513591000	0.389974000	0.080825000
6	-3.167393000	0.567980000	-1.135151000
6	-4.533186000	0.882516000	-1.117491000
1	-5.080823000	1.025673000	-2.052610000
6	-5.198921000	1.002517000	0.112954000
1	-6.262837000	1.248977000	0.123150000
6	-4.525831000	0.804020000	1.329340000
1	-5.064670000	0.890031000	2.276498000
6	-2.328156000	0.292626000	-2.349814000
1	-2.453936000	1.043566000	-3.143682000
1	-2.593031000	-0.687340000	-2.772977000
1	-0.449940000	-0.590347000	-2.422505000
6	-0.070780000	1.418308000	-2.360598000
1	-0.401646000	1.799515000	-3.337148000
1	0.976914000	1.094808000	-2.455399000
8	1.954292000	-0.151074000	2.012482000
8	1.313583000	-0.307260000	-0.154459000
6	2.197285000	-0.279629000	0.787127000
8	-2.951116000	-2.531855000	-0.951025000
8	-2.770305000	-2.817748000	1.301444000
6	-4.395630000	-2.822595000	-0.885336000
6	-4.942254000	-2.679407000	-2.284948000
6	-2.310930000	-2.467458000	0.224518000
6	-0.981825000	-1.813085000	-0.010288000
1	-4.515712000	-3.840920000	-0.487694000
1	-4.846140000	-2.105994000	-0.182073000
1	-6.016673000	-2.917264000	-2.274441000
1	-4.823444000	-1.650775000	-2.653905000
1	-4.442989000	-3.371578000	-2.978669000
1	-0.386857000	-2.320756000	-0.787115000
7	-0.025146000	-2.649038000	1.366277000
7	0.701570000	-2.775302000	2.189851000
6	3.628509000	-0.422489000	0.326497000
6	3.949193000	-0.535544000	-1.036005000
6	4.665392000	-0.431194000	1.272797000
6	5.276119000	-0.650125000	-1.451971000
6	5.997890000	-0.545684000	0.876332000
6	6.287684000	-0.652433000	-0.486980000
1	3.151240000	-0.533557000	-1.779830000
1	4.421721000	-0.344518000	2.333085000
1	5.523578000	-0.735320000	-2.510834000
1	6.801335000	-0.550919000	1.614181000
17	7.959881000	-0.792393000	-0.999557000

4a-OBz-Cl

27	-0.673665000	0.310270000	-0.193713000
17	7.985419000	-0.269086000	0.013664000
8	1.315159000	0.678617000	-0.167998000
8	1.426628000	-1.554920000	-0.420765000
8	-0.207975000	-2.845014000	1.401054000
8	-1.758779000	-3.064672000	-0.255337000

7	-1.024876000	2.133157000	0.160709000
7	-0.826363000	0.133337000	1.810628000
1	-0.135629000	-0.537047000	2.167470000
7	-1.020982000	0.824368000	-2.112347000
1	-0.242346000	0.529240000	-2.710649000
6	-1.302226000	2.957102000	-0.862844000
6	-1.632695000	4.289260000	-0.614524000
1	-1.865692000	4.959281000	-1.442765000
6	-1.651209000	4.736439000	0.710557000
1	-1.918451000	5.771485000	0.930131000
6	-1.315968000	3.866330000	1.756470000
1	-1.300911000	4.203620000	2.793135000
6	-0.994123000	2.549646000	1.442379000
6	-0.495320000	1.481493000	2.374559000
1	0.603056000	1.553300000	2.415369000
1	-0.881826000	1.598006000	3.397525000
6	-2.203971000	-0.357254000	2.219821000
1	-2.576000000	0.258871000	3.051763000
1	-2.086413000	-1.381912000	2.601106000
6	-3.117007000	-0.331150000	1.026913000
6	-2.478991000	-0.088724000	-0.189106000
6	-3.165914000	-0.085269000	-1.404452000
6	-4.545284000	-0.326558000	-1.406486000
1	-5.108849000	-0.330359000	-2.343587000
6	-5.200972000	-0.571371000	-0.188458000
1	-6.276154000	-0.763449000	-0.186056000
6	-4.496238000	-0.580801000	1.026156000
1	-5.023817000	-0.785196000	1.962038000
6	-2.265923000	0.114644000	-2.589872000
1	-2.728210000	0.669103000	-3.421012000
1	-1.939429000	-0.861111000	-2.982051000
6	-1.119856000	2.324564000	-2.213601000
1	-1.923122000	2.612638000	-2.906627000
1	-0.173535000	2.693821000	-2.637681000
6	1.993766000	-0.369669000	-0.255413000
6	3.463955000	-0.370319000	-0.183819000
6	4.133599000	0.847590000	0.030019000
1	3.559611000	1.767897000	0.146373000
6	5.523332000	0.885195000	0.092831000
1	6.047577000	1.826931000	0.257643000
6	6.238998000	-0.307975000	-0.059494000
6	5.593621000	-1.531221000	-0.269524000
1	6.171779000	-2.448263000	-0.384968000
6	4.202754000	-1.558003000	-0.331532000
1	3.689658000	-2.505396000	-0.498271000
6	-0.042845000	-1.529828000	-0.618273000
1	-0.208392000	-1.780898000	-1.675521000
6	-0.631128000	-2.547797000	0.281616000
6	-2.600593000	-3.878848000	0.621581000
1	-2.798072000	-3.308957000	1.542023000
1	-2.048640000	-4.793662000	0.886475000
6	-3.872592000	-4.174249000	-0.139103000
1	-3.664213000	-4.744648000	-1.056558000
1	-4.388290000	-3.240363000	-0.408286000
1	-4.544587000	-4.773258000	0.493975000

TS2-OBz-Cl

7	-1.100385000	-2.267814000	-0.212830000
6	-1.303370000	-3.076909000	0.842786000
27	-0.731271000	-0.431137000	0.104768000
7	-1.080536000	-0.263922000	-1.877078000
6	-1.760653000	-4.379142000	0.649738000
1	-1.933675000	-5.034132000	1.504300000
7	-0.911771000	-0.945253000	2.052641000
6	-1.986923000	-4.818298000	-0.660198000
1	-2.354191000	-5.830642000	-0.837005000
6	-1.741218000	-3.966354000	-1.745264000

1	-1.899849000	-4.296567000	-2.772378000
6	-1.287277000	-2.677029000	-1.483350000
6	-0.880330000	-1.623646000	-2.476115000
1	0.199383000	-1.732614000	-2.665369000
1	-1.404040000	-1.720099000	-3.437785000
1	-0.385129000	0.377746000	-2.273515000
6	-2.451842000	0.328846000	-2.150929000
1	-2.992182000	-0.322465000	-2.853649000
1	-2.312562000	1.298310000	-2.650773000
6	-3.223038000	0.467221000	-0.870071000
6	-2.480309000	0.241420000	0.304193000
6	-3.083489000	0.117589000	1.572046000
6	-4.456763000	0.327259000	1.677829000
1	-4.965859000	0.229623000	2.639545000
6	-5.192776000	0.639565000	0.520027000
1	-6.267493000	0.813313000	0.607069000
6	-4.596648000	0.684362000	-0.751409000
1	-5.212108000	0.856204000	-1.637730000
6	-2.140685000	-0.299971000	2.665120000
1	-2.614250000	-0.995568000	3.372961000
1	-1.802357000	0.569719000	3.248603000
1	-0.094183000	-0.602643000	2.567761000
6	-0.895500000	-2.448238000	2.145985000
1	-1.511901000	-2.795324000	2.987182000
1	0.145085000	-2.744711000	2.350944000
8	1.433640000	1.547991000	0.664858000
8	1.228852000	-0.616419000	-0.005554000
6	1.909831000	0.435101000	0.300157000
8	-1.423001000	3.593808000	0.118202000
8	-0.435273000	2.501155000	-1.606087000
6	-1.488714000	4.808486000	-0.705660000
6	-2.171950000	5.873659000	0.120023000
6	-0.878711000	2.506821000	-0.462214000
6	-0.859270000	1.336921000	0.487734000
1	-0.459943000	5.086013000	-0.981497000
1	-2.044856000	4.566840000	-1.624350000
1	-2.234823000	6.801799000	-0.467821000
1	-3.193095000	5.569404000	0.393230000
1	-1.605782000	6.086251000	1.038794000
1	-0.935853000	1.700434000	1.520939000
6	3.404603000	0.295440000	0.208789000
6	4.234500000	1.383041000	0.526070000
6	3.987371000	-0.918106000	-0.192072000
6	5.622137000	1.267699000	0.447123000
6	5.373094000	-1.049446000	-0.275791000
6	6.176388000	0.048607000	0.046255000
1	3.788553000	2.328335000	0.838667000
1	3.349331000	-1.766750000	-0.441405000
1	6.265934000	2.112860000	0.693416000
1	5.824682000	-1.991758000	-0.588059000
17	7.919990000	-0.107390000	-0.053889000

INT-MI-OBz-Cl

7	-1.368131000	-1.943006000	-0.565038000
6	-1.703439000	-2.942527000	0.272383000
27	-0.854479000	-0.293110000	0.179047000
7	-0.932920000	0.388005000	-1.703154000
6	-2.304077000	-4.094396000	-0.231509000
1	-2.582255000	-4.907998000	0.439033000
7	-1.050906000	-1.218542000	1.940849000
6	-2.541976000	-4.173824000	-1.608538000
1	-3.022039000	-5.061217000	-2.024358000
6	-2.173373000	-3.122185000	-2.457948000
1	-2.351505000	-3.172827000	-3.532440000
6	-1.572644000	-1.999727000	-1.896584000
6	-1.025233000	-0.799620000	-2.623041000
1	0.001559000	-1.034966000	-2.942624000

1	-1.606976000	-0.554589000	-3.522833000
1	-0.067323000	0.892313000	-1.924484000
6	-2.096082000	1.343144000	-1.774429000
1	-2.657057000	1.185896000	-2.704861000
1	-1.705747000	2.366491000	-1.789348000
6	-2.968693000	1.046809000	-0.577362000
6	-2.368053000	0.998130000	0.733046000
6	-3.009262000	0.131517000	1.694615000
6	-4.305268000	-0.319462000	1.483615000
1	-4.772886000	-0.970408000	2.225196000
6	-4.973622000	-0.018912000	0.288243000
1	-5.995426000	-0.368901000	0.130993000
6	-4.273061000	0.583733000	-0.758994000
1	-4.719088000	0.638225000	-1.754346000
6	-2.113052000	-0.499212000	2.729461000
1	-2.662134000	-1.205286000	3.366131000
1	-1.619486000	0.230775000	3.384215000
1	-0.125808000	-1.087904000	2.388516000
6	-1.310917000	-2.679245000	1.702614000
1	-2.068479000	-3.056763000	2.403606000
1	-0.372710000	-3.217498000	1.910366000
8	1.596933000	-0.314602000	2.204879000
8	1.035290000	-0.472240000	0.009608000
6	1.886579000	-0.371241000	0.987502000
8	-1.266938000	3.664261000	0.076345000
8	0.828660000	2.807859000	0.263383000
6	-0.705535000	4.881055000	-0.521397000
6	-1.861405000	5.819529000	-0.784655000
6	-0.387276000	2.690639000	0.404872000
6	-1.019964000	1.495914000	1.013211000
1	0.023515000	5.306763000	0.184347000
1	-0.174185000	4.600254000	-1.443887000
1	-1.479660000	6.750103000	-1.230871000
1	-2.584460000	5.373977000	-1.483781000
1	-2.383007000	6.074925000	0.149593000
1	-0.676638000	1.434789000	2.050842000
6	3.323273000	-0.338649000	0.544795000
6	3.670272000	-0.260329000	-0.814134000
6	4.340519000	-0.382612000	1.511162000
6	5.008219000	-0.226797000	-1.205889000
6	5.683379000	-0.351618000	1.136128000
6	6.001485000	-0.274037000	-0.222857000
1	2.887071000	-0.219911000	-1.571995000
1	4.074611000	-0.441806000	2.567769000
1	5.278444000	-0.162868000	-2.260561000
1	6.473044000	-0.386907000	1.887697000
17	7.686291000	-0.233798000	-0.707315000

2a-OBz-OMe

7	2.204406000	-1.259568000	0.011160000
6	2.718423000	-1.660796000	-1.171163000
27	0.767998000	-0.105642000	0.007843000
7	1.039158000	-0.040723000	1.992750000
6	3.868030000	-2.444344000	-1.199290000
1	4.285780000	-2.762475000	-2.154746000
7	1.012593000	-0.085910000	-1.982077000
6	4.460489000	-2.810677000	0.014278000
1	5.369910000	-3.413581000	0.015295000
6	3.883152000	-2.417462000	1.226743000
1	4.313218000	-2.713903000	2.183731000
6	2.733059000	-1.634794000	1.195619000
6	1.895468000	-1.215193000	2.365913000
1	1.217152000	-2.047771000	2.609786000
1	2.500091000	-1.000791000	3.258552000
1	0.141319000	-0.147265000	2.476841000
6	1.629221000	1.293110000	2.397435000
1	2.302558000	1.160760000	3.257646000

1	0.788499000	1.921924000	2.727564000
6	2.290139000	1.911589000	1.198578000
6	1.888861000	1.361291000	-0.016843000
6	2.272299000	1.883926000	-1.250199000
6	3.141233000	2.983564000	-1.268867000
1	3.464285000	3.420096000	-2.217938000
6	3.588488000	3.527754000	-0.053852000
1	4.274265000	4.377818000	-0.068490000
6	3.158776000	3.011588000	1.179584000
1	3.495157000	3.470158000	2.113501000
6	1.594330000	1.238939000	-2.425256000
1	2.254586000	1.088552000	-3.292685000
1	0.747723000	1.859359000	-2.756265000
1	0.108810000	-0.205558000	-2.451746000
6	1.866285000	-1.267211000	-2.339951000
1	2.460260000	-1.070947000	-3.243840000
1	1.186630000	-2.105680000	-2.558896000
8	-0.949581000	0.837868000	0.011059000
8	-0.926201000	-1.358250000	0.029137000
6	-1.614463000	-0.276276000	0.021693000
6	-3.085046000	-0.274330000	0.020279000
6	-3.801922000	0.933095000	0.065980000
6	-3.795532000	-1.491138000	-0.032010000
6	-5.195595000	0.941996000	0.057457000
6	-5.181803000	-1.496284000	-0.043662000
6	-5.892020000	-0.279239000	-0.001617000
1	-3.258872000	1.878795000	0.111802000
1	-3.246019000	-2.433411000	-0.069398000
1	-5.728599000	1.891239000	0.096296000
1	-5.743860000	-2.431160000	-0.087868000
8	-7.248879000	-0.391759000	-0.022905000
6	-8.038109000	0.815044000	-0.011462000
1	-7.866364000	1.392142000	0.911012000
1	-7.819248000	1.438856000	-0.892747000
1	-9.081619000	0.480798000	-0.046646000

2a-OBz-OMe-EDA

7	0.390953000	1.947115000	0.127746000
6	0.235461000	2.443797000	1.373968000
27	0.675644000	0.116362000	-0.067295000
7	0.812833000	0.544521000	-2.033602000
6	0.081892000	3.812084000	1.567045000
1	-0.034925000	4.207306000	2.576342000
7	0.919048000	0.174378000	1.942808000
6	0.079129000	4.651200000	0.447100000
1	-0.029569000	5.729378000	0.574687000
6	0.205197000	4.108890000	-0.833560000
1	0.182943000	4.738306000	-1.723758000
6	0.357487000	2.729476000	-0.967135000
6	0.401200000	1.972977000	-2.255211000
1	-0.615262000	1.959296000	-2.676458000
1	1.063434000	2.457609000	-2.986255000
1	0.130030000	-0.021212000	-2.552194000
6	2.211806000	0.254598000	-2.510860000
1	2.444466000	0.846617000	-3.409202000
1	2.234710000	-0.809801000	-2.792596000
6	3.141866000	0.494741000	-1.354350000
6	2.515128000	0.385463000	-0.111591000
6	3.211819000	0.474206000	1.092128000
6	4.594146000	0.703409000	1.051461000
1	5.172260000	0.773116000	1.976599000
6	5.236643000	0.831393000	-0.190395000
1	6.313207000	1.013483000	-0.219234000
6	4.523870000	0.718264000	-1.395464000
1	5.046176000	0.801454000	-2.352328000
6	2.388586000	0.197470000	2.317553000
1	2.553171000	0.927124000	3.124550000

1	2.630335000	-0.798564000	2.716447000
1	0.492838000	-0.641631000	2.393315000
6	0.161145000	1.373236000	2.416812000
1	0.516751000	1.714570000	3.399661000
1	-0.892599000	1.071175000	2.518990000
8	-2.012547000	-0.009094000	-1.969386000
8	-1.304156000	-0.250313000	0.167801000
6	-2.224824000	-0.188792000	-0.742318000
8	2.906929000	-2.597147000	0.837858000
8	2.754775000	-2.781981000	-1.426948000
6	4.351469000	-2.882259000	0.760130000
6	4.889818000	-2.855617000	2.169642000
6	2.273839000	-2.521846000	-0.334384000
6	0.871288000	-2.011677000	-0.118756000
1	4.476945000	-3.863779000	0.280523000
1	4.806274000	-2.109378000	0.122690000
1	5.963884000	-3.093698000	2.143999000
1	4.771102000	-1.861019000	2.622637000
1	4.386734000	-3.601974000	2.801735000
1	0.392669000	-2.307687000	0.823506000
7	0.068459000	-2.392821000	-1.157901000
7	-0.554273000	-2.630152000	-2.056282000
6	-3.631134000	-0.370398000	-0.245542000
6	-3.912320000	-0.552638000	1.123089000
6	-4.703338000	-0.363032000	-1.150318000
6	-5.217519000	-0.722337000	1.567560000
6	-6.021619000	-0.532256000	-0.722541000
6	-6.282268000	-0.715333000	0.646178000
1	-3.092225000	-0.561407000	1.842892000
1	-4.498647000	-0.221706000	-2.213446000
1	-5.440140000	-0.864039000	2.627352000
1	-6.829872000	-0.523295000	-1.453234000
8	-7.527170000	-0.895945000	1.180318000
6	-8.657958000	-0.881939000	0.287872000
1	-8.752396000	0.092410000	-0.218237000
1	-8.586231000	-1.687220000	-0.460915000
1	-9.535105000	-1.051114000	0.923689000

TS1-OBz-OMe

7	-0.353586000	1.916694000	-0.062219000
6	-0.184507000	2.461575000	-1.283053000
27	-0.691231000	0.036982000	0.059137000
7	-0.835278000	0.426954000	2.036569000
6	-0.006425000	3.833885000	-1.420769000
1	0.121265000	4.272046000	-2.410815000
7	-0.917024000	0.229340000	-1.953308000
6	0.005454000	4.623192000	-0.264622000
1	0.134701000	5.703752000	-0.345390000
6	-0.139559000	4.031287000	0.991993000
1	-0.114331000	4.623530000	1.907096000
6	-0.318440000	2.649587000	1.062402000
6	-0.397994000	1.840234000	2.316731000
1	0.609585000	1.790307000	2.755046000
1	-1.065900000	2.305643000	3.055021000
1	-0.166191000	-0.174821000	2.531063000
6	-2.242094000	0.150793000	2.495707000
1	-2.460872000	0.705262000	3.420825000
1	-2.294620000	-0.924972000	2.722729000
6	-3.155919000	0.477253000	1.349224000
6	-2.529544000	0.384891000	0.106597000
6	-3.204877000	0.568436000	-1.096882000
6	-4.571365000	0.877763000	-1.054079000
1	-5.135066000	1.025393000	-1.978916000
6	-5.216754000	0.986896000	0.188215000
1	-6.281285000	1.229151000	0.217923000
6	-4.522347000	0.783014000	1.391701000
1	-5.045357000	0.860459000	2.348476000

6	-2.385010000	0.303593000	-2.327237000
1	-2.525383000	1.059590000	-3.113901000
1	-2.655096000	-0.674152000	-2.752308000
1	-0.507257000	-0.576884000	-2.435949000
6	-0.128541000	1.431826000	-2.368686000
1	-0.474851000	1.818231000	-3.337850000
1	0.917798000	1.109473000	-2.481117000
8	1.986749000	-0.118467000	1.937815000
8	1.289458000	-0.307118000	-0.208237000
6	2.204403000	-0.263673000	0.707039000
8	-2.978264000	-2.531740000	-0.925096000
8	-2.746458000	-2.835386000	1.320841000
6	-4.419014000	-2.830519000	-0.831029000
6	-4.994598000	-2.687075000	-2.219138000
6	-2.312479000	-2.473955000	0.236915000
6	-0.992396000	-1.811839000	-0.022448000
1	-4.525798000	-3.850402000	-0.433466000
1	-4.859338000	-2.117968000	-0.117179000
1	-6.067679000	-2.929325000	-2.187525000
1	-4.887020000	-1.657138000	-2.588032000
1	-4.506326000	-3.375725000	-2.924140000
1	-0.410126000	-2.313619000	-0.812597000
7	0.001478000	-2.645780000	1.332142000
7	0.755501000	-2.753209000	2.133935000
6	3.614584000	-0.410033000	0.208944000
6	3.901515000	-0.554909000	-1.162985000
6	4.685429000	-0.395826000	1.115059000
6	5.211085000	-0.679199000	-1.609715000
6	6.008131000	-0.519627000	0.685165000
6	6.274789000	-0.662766000	-0.687206000
1	3.082178000	-0.569888000	-1.883572000
1	4.476763000	-0.283473000	2.180820000
1	5.438056000	-0.790435000	-2.672219000
1	6.815562000	-0.504974000	1.416663000
8	7.524686000	-0.793636000	-1.224063000
6	8.653689000	-0.775515000	-0.329573000
1	8.722245000	0.186208000	0.204410000
1	8.601257000	-1.602832000	0.396484000
1	9.536004000	-0.903889000	-0.967821000

4a-OBz-OMe

27	0.697555000	0.314917000	0.232846000
8	-1.273555000	0.770371000	0.300726000
8	-1.470664000	-1.464978000	0.481996000
8	0.106482000	-2.823527000	-1.331197000
8	1.657305000	-3.090733000	0.316417000
7	1.103402000	2.124250000	-0.133086000
7	0.723276000	0.144949000	-1.777539000
1	-0.013103000	-0.496255000	-2.094307000
7	1.182144000	0.799231000	2.128500000
1	0.427152000	0.543183000	2.773226000
6	1.478443000	2.928736000	0.874369000
6	1.839746000	4.250288000	0.612042000
1	2.150746000	4.905392000	1.426553000
6	1.788350000	4.706793000	-0.708874000
1	2.077719000	5.733472000	-0.939437000
6	1.355026000	3.857424000	-1.735566000
1	1.286285000	4.202798000	-2.767437000
6	1.005388000	2.551216000	-1.407982000
6	0.409662000	1.508905000	-2.312429000
1	-0.685601000	1.621975000	-2.284407000
1	0.737466000	1.618593000	-3.356289000
6	2.053231000	-0.396024000	-2.272911000
1	2.395437000	0.207969000	-3.126578000
1	1.874648000	-1.415676000	-2.644053000
6	3.037047000	-0.409587000	-1.137147000
6	2.482012000	-0.155757000	0.116581000

6	3.239512000	-0.193054000	1.289076000
6	4.606184000	-0.485641000	1.207388000
1	5.222862000	-0.523018000	2.109701000
6	5.178875000	-0.741164000	-0.049954000
1	6.243898000	-0.973633000	-0.117523000
6	4.403417000	-0.712136000	-1.220472000
1	4.866389000	-0.926952000	-2.187787000
6	2.412772000	0.018611000	2.524663000
1	2.943725000	0.525340000	3.345235000
1	2.057442000	-0.952180000	2.904760000
6	1.371177000	2.291171000	2.231038000
1	2.245221000	2.526791000	2.855004000
1	0.486890000	2.707811000	2.737030000
6	-1.999473000	-0.252564000	0.348960000
6	-3.457398000	-0.195390000	0.251026000
6	-4.086205000	1.058535000	0.089449000
1	-3.477983000	1.963376000	0.045009000
6	-5.463765000	1.144579000	-0.014889000
1	-5.961918000	2.107646000	-0.140850000
6	-6.250065000	-0.025724000	0.035164000
6	-5.635196000	-1.282258000	0.193492000
1	-6.225863000	-2.196495000	0.232511000
6	-4.249386000	-1.357056000	0.301397000
1	-3.776172000	-2.332050000	0.423550000
6	-0.005185000	-1.494102000	0.680120000
1	0.160542000	-1.735425000	1.740188000
6	0.544345000	-2.535517000	-0.214798000
6	2.469476000	-3.918682000	-0.575505000
1	2.672862000	-3.343710000	-1.491873000
1	1.891038000	-4.815964000	-0.844315000
6	3.740859000	-4.254057000	0.169803000
1	3.526991000	-4.826933000	1.084484000
1	4.282880000	-3.335909000	0.441296000
1	4.391513000	-4.864419000	-0.474633000
8	-7.590189000	0.163218000	-0.080708000
6	-8.449437000	-0.996313000	-0.067180000
1	-8.217140000	-1.667254000	-0.909090000
1	-8.364459000	-1.539483000	0.887001000
1	-9.466718000	-0.602959000	-0.177979000

TS2-OBz-OMe

7	-1.210693000	-2.249911000	-0.229091000
6	-1.442136000	-3.055149000	0.823758000
27	-0.746351000	-0.437680000	0.095628000
7	-1.108104000	-0.235334000	-1.879324000
6	-1.973218000	-4.328694000	0.628243000
1	-2.169070000	-4.980251000	1.480522000
7	-0.928183000	-0.955199000	2.041671000
6	-2.244820000	-4.743405000	-0.681266000
1	-2.671433000	-5.731931000	-0.859703000
6	-1.969121000	-3.897222000	-1.763899000
1	-2.162787000	-4.209505000	-2.790616000
6	-1.439371000	-2.637652000	-1.499683000
6	-0.988300000	-1.599641000	-2.490237000
1	0.081843000	-1.764322000	-2.692758000
1	-1.527920000	-1.659862000	-3.446032000
1	-0.384102000	0.371131000	-2.280150000
6	-2.449948000	0.429058000	-2.133287000
1	-3.029938000	-0.188067000	-2.835203000
1	-2.267684000	1.394396000	-2.627120000
6	-3.200034000	0.593797000	-0.842944000
6	-2.454829000	0.328402000	0.321812000
6	-3.051047000	0.217619000	1.594390000
6	-4.412639000	0.486121000	1.716318000
1	-4.916268000	0.400840000	2.682092000
6	-5.145630000	0.840987000	0.569016000
1	-6.210844000	1.060482000	0.668812000

6	-4.561442000	0.869321000	-0.708404000
1	-5.178600000	1.072939000	-1.586817000
6	-2.118677000	-0.258151000	2.673080000
1	-2.619401000	-0.938867000	3.376561000
1	-1.733675000	0.586648000	3.263933000
1	-0.089548000	-0.654179000	2.548839000
6	-0.980712000	-2.457748000	2.124226000
1	-1.596511000	-2.782370000	2.974739000
1	0.048569000	-2.804187000	2.306401000
8	1.500058000	1.440311000	0.641421000
8	1.200657000	-0.711972000	-0.032857000
6	1.933420000	0.308442000	0.272028000
8	-1.319907000	3.600533000	0.138499000
8	-0.335041000	2.506420000	-1.587047000
6	-1.368894000	4.820578000	-0.678284000
6	-2.053498000	5.885145000	0.147254000
6	-0.785027000	2.510621000	-0.445683000
6	-0.794045000	1.331878000	0.493222000
1	-0.335535000	5.093146000	-0.941496000
1	-1.917215000	4.588892000	-1.604205000
1	-2.103505000	6.817727000	-0.434761000
1	-3.079664000	5.586301000	0.407296000
1	-1.495995000	6.087283000	1.073655000
1	-0.836486000	1.686698000	1.530963000
6	3.413144000	0.106574000	0.175242000
6	4.290550000	1.187226000	0.355880000
6	3.956595000	-1.165356000	-0.095648000
6	5.673564000	1.021936000	0.269423000
6	5.330246000	-1.346873000	-0.180527000
6	6.199201000	-0.253414000	0.000422000
1	3.881675000	2.177844000	0.562204000
1	3.288918000	-2.016634000	-0.235178000
1	6.328277000	1.881328000	0.409339000
1	5.758298000	-2.330146000	-0.386676000
8	7.530791000	-0.535094000	-0.104842000
6	8.473173000	0.536163000	0.096738000
1	8.341322000	1.331051000	-0.654940000
1	8.382585000	0.958112000	1.110749000
1	9.463559000	0.081019000	-0.023711000

6	-4.310587000	0.500773000	-0.693294000
1	-4.782856000	0.539458000	-1.677187000
6	-2.040751000	-0.503353000	2.751842000
1	-2.556969000	-1.215616000	3.408663000
1	-1.553449000	0.248007000	3.387075000
1	-0.042569000	-1.034956000	2.363334000
6	-1.199568000	-2.673670000	1.737399000
1	-1.924274000	-3.064899000	2.465353000
1	-0.239479000	-3.180377000	1.923622000
8	1.646319000	-0.237880000	2.120117000
8	1.030548000	-0.450443000	-0.055929000
6	1.911983000	-0.315021000	0.895459000
8	-1.389822000	3.662358000	0.089296000
8	0.732910000	2.853885000	0.114792000
6	-0.903529000	4.904526000	-0.520479000
6	-2.103200000	5.808496000	-0.691371000
6	-0.466235000	2.706807000	0.342552000
6	-1.034529000	1.495950000	0.983609000
1	-0.143073000	5.340200000	0.145120000
1	-0.425630000	4.656410000	-1.480788000
1	-1.781546000	6.762279000	-1.135833000
1	-2.851691000	5.352422000	-1.356126000
1	-2.575099000	6.021971000	0.279280000
1	-0.656287000	1.457740000	2.010760000
6	3.327894000	-0.272654000	0.413952000
6	3.644188000	-0.224624000	-0.959026000
6	4.377845000	-0.280079000	1.344668000
6	4.965911000	-0.187932000	-1.382014000
6	5.711659000	-0.245579000	0.935917000
6	6.010084000	-0.200896000	-0.436865000
1	2.841079000	-0.210714000	-1.697226000
1	4.144580000	-0.314494000	2.410519000
1	5.217940000	-0.147889000	-2.443784000
1	6.504396000	-0.254123000	1.683175000
8	7.273501000	-0.166547000	-0.953337000
6	8.385129000	-0.180472000	-0.036384000
1	8.364690000	0.698883000	0.627440000
1	8.393584000	-1.105076000	0.563464000
1	9.283356000	-0.143930000	-0.664422000

INT-MI-OBz-OMe

7	-1.348060000	-1.970417000	-0.537048000
6	-1.627064000	-2.968289000	0.323034000
27	-0.854236000	-0.298912000	0.168318000
7	-1.000696000	0.355927000	-1.718052000
6	-2.208266000	-4.144054000	-0.146928000
1	-2.441682000	-4.956100000	0.542325000
7	-0.977960000	-1.203355000	1.948592000
6	-2.486378000	-4.249172000	-1.514833000
1	-2.952275000	-5.155911000	-1.904202000
6	-2.176753000	-3.198311000	-2.388246000
1	-2.387223000	-3.268433000	-3.455772000
6	-1.593035000	-2.050618000	-1.860264000
6	-1.110279000	-0.843830000	-2.621260000
1	-0.096041000	-1.058163000	-2.991432000
1	-1.742792000	-0.622747000	-3.492435000
1	-0.146316000	0.864890000	-1.970085000
6	-2.173202000	1.301127000	-1.763541000
1	-2.753598000	1.141309000	-2.681636000
1	-1.790572000	2.327689000	-1.787436000
6	-3.013885000	0.995455000	-0.545718000
6	-2.379759000	0.966704000	0.749565000
6	-2.975215000	0.091783000	1.730534000
6	-4.265331000	-0.391580000	1.553475000
1	-4.699259000	-1.047851000	2.310705000
6	-4.969896000	-0.114143000	0.374007000
1	-5.986575000	-0.489510000	0.244226000

2a-OBz-NO$_2$

7	2.374307000	-1.292222000	-0.030224000
6	2.886936000	-1.661725000	-1.223675000
27	0.964517000	-0.106131000	-0.001313000
7	1.226275000	-0.115369000	1.985835000
6	4.022028000	-2.464797000	-1.273419000
1	4.439306000	-2.756305000	-2.237518000
7	1.219729000	-0.024754000	-1.987681000
6	4.601724000	-2.883114000	-0.070684000
1	5.500428000	-3.501677000	-0.086548000
6	4.026141000	-2.520829000	1.152022000
1	4.446235000	-2.856971000	2.100173000
6	2.890953000	-1.716244000	1.143071000
6	2.060088000	-1.316727000	2.324506000
1	1.367518000	-2.143762000	2.546005000
1	2.668534000	-1.138469000	3.222249000
1	0.324058000	-0.222286000	2.461871000
6	1.836920000	1.193135000	2.438876000
1	2.499252000	1.020556000	3.300410000
1	1.004821000	1.826784000	2.781277000
6	2.519481000	1.836333000	1.266055000
6	2.117431000	1.336021000	0.029978000
6	2.515574000	1.892662000	-1.183056000
6	3.403023000	2.977391000	-1.158767000
1	3.737166000	3.441899000	-2.090427000
6	3.853330000	3.470634000	0.076497000
1	4.553721000	4.308555000	0.094724000

6	3.407684000	2.920354000	1.289105000
1	3.745888000	3.340023000	2.240386000
6	1.828608000	1.303836000	-2.381465000
1	2.487086000	1.171511000	-3.252917000
1	0.994773000	1.952388000	-2.690077000
1	0.315795000	-0.108803000	-2.465048000
6	2.051776000	-1.209524000	-2.383031000
1	2.656286000	-0.991621000	-3.274793000
1	1.357463000	-2.025658000	-2.636773000
8	-0.727746000	0.884664000	0.018403000
8	-0.787360000	-1.311596000	-0.021750000
6	-1.420531000	-0.204729000	-0.000039000
6	-2.904476000	-0.142153000	0.003650000
6	-3.650069000	-1.331758000	0.060077000
6	-3.556883000	1.101684000	-0.051483000
6	-5.040409000	-1.285727000	0.061774000
6	-4.946713000	1.161021000	-0.055556000
6	-5.665653000	-0.036730000	0.001547000
1	-3.133728000	-2.291070000	0.104900000
1	-2.970356000	2.019992000	-0.094230000
1	-5.634583000	-2.197478000	0.105324000
1	-5.470652000	2.114807000	-0.100983000
7	-7.138952000	0.020176000	-0.003977000
8	-7.682000000	1.129050000	-0.098798000
8	-7.768176000	-1.042839000	0.085131000

6	4.448409000	-2.939233000	0.776432000
6	4.918340000	-2.953282000	2.210630000
6	2.429716000	-2.513778000	-0.405162000
6	1.018718000	-2.007605000	-0.231937000
1	4.592891000	-3.907993000	0.276666000
1	4.937041000	-2.151775000	0.184182000
1	5.990931000	-3.198296000	2.229866000
1	4.785051000	-1.969618000	2.682904000
1	4.381725000	-3.712078000	2.798831000
1	0.500641000	-2.342325000	0.676076000
7	0.260240000	-2.350056000	-1.316920000
7	-0.329294000	-2.560684000	-2.243722000
6	-3.477144000	-0.294250000	-0.459036000
6	-3.794788000	-0.543440000	0.886836000
6	-4.508401000	-0.198589000	-1.408046000
6	-5.119338000	-0.698344000	1.285454000
6	-5.839186000	-0.346195000	-1.027555000
6	-6.123715000	-0.596515000	0.318185000
1	-2.995115000	-0.616306000	1.623930000
1	-4.257864000	-0.006363000	-2.451966000
1	-5.375627000	-0.891811000	2.326230000
1	-6.645420000	-0.274869000	-1.756725000
7	-7.527253000	-0.757476000	0.731760000
8	-7.763050000	-1.041073000	1.915114000
8	-8.413961000	-0.603081000	-0.119797000

2a-OBz-NO₂-EDA

7	0.553144000	1.941431000	0.168659000
6	0.353447000	2.387821000	1.427444000
27	0.830397000	0.115447000	-0.090577000
7	1.055547000	0.629063000	-2.032776000
6	0.213071000	3.749082000	1.672633000
1	0.060710000	4.103673000	2.692210000
7	0.982852000	0.086677000	1.928339000
6	0.270396000	4.634613000	0.590450000
1	0.174880000	5.708342000	0.759412000
6	0.439272000	4.144306000	-0.706221000
1	0.462702000	4.811589000	-1.568351000
6	0.574536000	2.769381000	-0.892563000
6	0.650086000	2.065361000	-2.208494000
1	-0.357143000	2.067295000	-2.651827000
1	1.327571000	2.577822000	-2.905770000
1	0.403420000	0.088701000	-2.613356000
6	2.476122000	0.361996000	-2.458845000
1	2.748782000	0.998522000	-3.314142000
1	2.511583000	-0.686377000	-2.793281000
6	3.352718000	0.539388000	-1.250792000
6	2.670972000	0.372971000	-0.044044000
6	3.312416000	0.401998000	1.192782000
6	4.695786000	0.624106000	1.225092000
1	5.232038000	0.647187000	2.177407000
6	5.394344000	0.805990000	0.020965000
1	6.471885000	0.982208000	0.048693000
6	4.736216000	0.756245000	-1.218678000
1	5.300514000	0.882432000	-2.146414000
6	2.434820000	0.077541000	2.366980000
1	2.570423000	0.768594000	3.212445000
1	2.650523000	-0.938039000	2.729316000
1	0.528767000	-0.740597000	2.329084000
6	0.218134000	1.275377000	2.418644000
1	0.532106000	1.568849000	3.430583000
1	-0.842925000	0.984342000	2.459428000
8	-1.788881000	0.088082000	-2.110940000
8	-1.164491000	-0.233467000	0.043578000
6	-2.036363000	-0.125567000	-0.901093000
8	3.002332000	-2.649417000	0.791829000
8	2.961930000	-2.722184000	-1.484485000

TS1-OBz-NO₂

7	0.518304000	1.915906000	0.025915000
6	0.319090000	2.471246000	1.237341000
27	0.845533000	0.032016000	-0.072327000
7	1.060972000	0.411562000	-2.048205000
6	0.154009000	3.846621000	1.360921000
1	0.002149000	4.293266000	2.343751000
7	0.999851000	0.232598000	1.945313000
6	0.188628000	4.628136000	0.200074000
1	0.072025000	5.710881000	0.270061000
6	0.364065000	4.025980000	-1.047879000
1	0.374799000	4.612581000	-1.966842000
6	0.526598000	2.641747000	-1.104028000
6	0.629403000	1.822039000	-2.349789000
1	-0.369945000	1.767935000	-2.806270000
1	1.310467000	2.279739000	-3.080757000
1	0.416083000	-0.195532000	-2.567540000
6	2.485117000	0.140440000	-2.455859000
1	2.734579000	0.699686000	-3.370079000
1	2.549561000	-0.934100000	-2.684675000
6	3.355920000	0.465622000	-1.276277000
6	2.685998000	0.371683000	-0.057047000
6	3.317167000	0.552929000	1.170406000
6	4.684051000	0.862462000	1.177433000
1	5.214255000	1.007540000	2.122210000
6	5.373553000	0.974287000	-0.040625000
1	6.438290000	1.217133000	-0.032013000
6	4.723096000	0.771765000	-1.268373000
1	5.279907000	0.850976000	-2.205631000
6	2.454778000	0.282085000	2.369478000
1	2.579199000	1.024166000	3.171774000
1	2.698087000	-0.705678000	2.787876000
1	0.558451000	-0.563868000	2.416205000
6	0.219401000	1.451335000	2.328687000
1	0.546167000	1.840772000	3.303261000
1	-0.834290000	1.146407000	2.418153000
8	-1.763400000	-0.145547000	-2.059436000
8	-1.153080000	-0.287830000	0.118474000
6	-2.018034000	-0.251614000	-0.836724000
8	3.093929000	-2.549806000	0.982715000
8	2.920668000	-2.842190000	-1.269725000

6   4.538268000   -2.843930000   0.925193000
6   5.076300000   -2.701533000   2.328146000
6   2.459686000   -2.485297000   -0.195795000
6   1.135089000   -1.819549000   0.031335000
1   4.658543000   -3.862487000   0.528252000
1   4.994279000   -2.128198000   0.224566000
1   6.151353000   -2.936608000   2.323789000
1   4.952466000   -1.673671000   2.697635000
1   4.574597000   -3.395851000   3.017927000
1   0.536015000   -2.315541000   0.812319000
7   0.172556000   -2.656821000   -1.341478000
7   -0.536274000   -2.771790000   -2.182068000
6   -3.464505000   -0.357763000   -0.393841000
6   -3.809858000   -0.343497000   0.968060000
6   -4.475511000   -0.460212000   -1.363729000
6   -5.142422000   -0.428219000   1.361656000
6   -5.812592000   -0.553020000   -0.989168000
6   -6.125389000   -0.535338000   0.373321000
1   -3.027413000   -0.262957000   1.722741000
1   -4.203849000   -0.465678000   -2.419869000
1   -5.420362000   -0.415895000   2.414717000
1   -6.602970000   -0.632933000   -1.734565000
7   -7.536105000   -0.636845000   0.780416000
8   -8.391030000   -0.811569000   -0.099383000
8   -7.809387000   -0.545461000   1.985991000

4a-OBz-NO₂

27   0.853929000   0.305432000   0.231373000
8   -1.130501000   0.682333000   0.283047000
8   -1.247382000   -1.555768000   0.476680000
8   0.367941000   -2.845995000   -1.354523000
8   1.939548000   -3.065670000   0.281994000
7   1.194915000   2.130558000   -0.123141000
7   0.900316000   0.147279000   -1.780337000
1   0.190312000   -0.519558000   -2.104835000
7   1.310203000   0.797479000   2.132331000
1   0.559941000   0.511529000   2.770074000
6   1.532044000   2.943388000   0.890928000
6   1.839034000   4.280514000   0.638276000
1   2.118637000   4.942422000   1.458610000
6   1.773783000   4.742863000   -0.679813000
1   2.021097000   5.782133000   -0.902744000
6   1.381178000   3.882569000   -1.713715000
1   1.302626000   4.231364000   -2.743706000
6   1.085083000   2.560785000   -1.395912000
6   0.538659000   1.501257000   -2.310831000
1   -0.560375000   1.571226000   -2.294186000
1   0.873031000   1.628754000   -3.350567000
6   2.252900000   -0.339052000   -2.269560000
1   2.576163000   0.281017000   -3.118947000
1   2.116579000   -1.363111000   -2.646571000
6   3.228836000   -0.319555000   -1.127892000
6   2.656862000   -0.099277000   0.124051000
6   3.406403000   -0.114174000   1.301712000
6   4.784719000   -0.348211000   1.226785000
1   5.396140000   -0.366371000   2.133154000
6   5.375708000   -0.567511000   -0.028685000
1   6.450207000   -0.752949000   -0.091094000
6   4.607661000   -0.561410000   -1.204146000
1   5.085832000   -0.746768000   -2.170053000
6   2.564590000   0.058028000   2.532748000
1   3.070688000   0.577945000   3.360586000
1   2.241759000   -0.927344000   2.903918000
6   1.447803000   2.294651000   2.243621000
1   2.314919000   2.555136000   2.867371000
1   0.551069000   2.678135000   2.753932000
6   -1.807084000   -0.366772000   0.342879000

6   -3.282608000   -0.358615000   0.254832000
6   -3.932872000   0.866370000   0.022980000
1   -3.346148000   1.778896000   -0.085053000
6   -5.318864000   0.912081000   -0.072474000
1   -5.840242000   1.850836000   -0.254152000
6   -6.035658000   -0.280226000   0.063419000
6   -5.413534000   -1.509369000   0.295141000
1   -6.006732000   -2.416628000   0.400369000
6   -4.025981000   -1.544588000   0.391999000
1   -3.518993000   -2.491505000   0.575597000
6   0.225857000   -1.534630000   0.666638000
1   0.396559000   -1.782070000   1.724003000
6   0.804190000   -2.551705000   -0.239736000
6   2.784908000   -3.851487000   -0.618122000
1   2.960707000   -3.260171000   -1.529550000
1   2.245690000   -4.770848000   -0.892896000
6   4.069878000   -4.137620000   0.123866000
1   3.880658000   -4.727806000   1.032886000
1   4.571598000   -3.199624000   0.404521000
1   4.745913000   -4.713286000   -0.526258000
7   -7.507191000   -0.237935000   -0.046451000
8   -8.128541000   -1.307452000   -0.006277000
8   -8.051363000   0.866361000   -0.174951000

TS2-OBz-NO₂

7   -1.264599000   -2.264605000   -0.230445000
6   -1.471253000   -3.084547000   0.815866000
27 -0.906991000   -0.428037000   0.107956000
7   -1.240217000   -0.244729000   -1.875822000
6   -1.917848000   -4.388003000   0.606750000
1   -2.093736000   -5.052040000   1.453654000
7   -1.103939000   -0.962173000   2.049053000
6   -2.129593000   -4.816213000   -0.709120000
1   -2.488145000   -5.829382000   -0.898601000
6   -1.880533000   -3.952655000   -1.784075000
1   -2.027983000   -4.274264000   -2.815551000
6   -1.438068000   -2.662726000   -1.506170000
6   -1.029940000   -1.598057000   -2.486021000
1   0.051372000   -1.700443000   -2.669701000
1   -1.547279000   -1.687707000   -3.451723000
1   -0.543354000   0.402774000   -2.260289000
6   -2.610734000   0.346781000   -2.156424000
1   -3.140542000   -0.295685000   -2.875068000
1   -2.469046000   1.324145000   -2.640059000
6   -3.395534000   0.464765000   -0.882052000
6   -2.663934000   0.225978000   0.296225000
6   -3.277267000   0.091028000   1.557600000
6   -4.651857000   0.297972000   1.653039000
1   -5.168977000   0.191984000   2.609547000
6   -5.378114000   0.619835000   0.491774000
1   -6.453800000   0.791280000   0.570817000
6   -4.770505000   0.679075000   -0.773545000
1   -5.377680000   0.860901000   -1.663563000
6   -2.342545000   -0.330220000   2.655707000
1   -2.817886000   -1.035037000   3.353121000
1   -2.015187000   0.536515000   3.249722000
1   -0.293428000   -0.619453000   2.575236000
6   -1.079576000   -2.465929000   2.128613000
1   -1.702168000   -2.824171000   2.960451000
1   -0.039370000   -2.758287000   2.341190000
8   1.252227000   1.545348000   0.720410000
8   1.054010000   -0.608274000   0.010649000
6   1.725905000   0.439960000   0.337180000
8   -1.608162000   3.591796000   0.141235000
8   -0.584719000   2.513572000   -1.571644000
6   -1.665726000   4.811128000   -0.677079000
6   -2.366031000   5.869371000   0.142969000

6	-1.048806000	2.511629000	-0.435893000
6	-1.038450000	1.335743000	0.507136000
1	-0.633556000	5.093435000	-0.934604000
1	-2.206146000	4.572064000	-1.605699000
1	-2.421459000	6.800494000	-0.440898000
1	-3.390864000	5.561006000	0.396933000
1	-1.816087000	6.078336000	1.072336000
1	-1.131001000	1.690123000	1.542342000
6	3.225687000	0.303979000	0.241676000
6	4.039838000	1.442899000	0.361035000
6	3.812981000	-0.955716000	0.033607000
6	5.423955000	1.333559000	0.267631000
6	5.195974000	-1.082534000	-0.053276000
6	5.981428000	0.068359000	0.062618000
1	3.580822000	2.418485000	0.522034000
1	3.179427000	-1.837789000	-0.058565000
1	6.064317000	2.210120000	0.355643000
1	5.662517000	-2.053518000	-0.214157000
7	7.444879000	-0.055818000	-0.039295000
8	8.126390000	0.978668000	-0.011559000
8	7.932552000	-1.189659000	-0.150146000

INT-MI-OBz-NO$_2$

7	-1.540164000	-1.937828000	-0.571783000
6	-1.903077000	-2.938357000	0.252186000
27	-1.034975000	-0.292677000	0.188631000
7	-1.070045000	0.393327000	-1.691536000
6	-2.475173000	-4.094759000	-0.275052000
1	-2.773464000	-4.910234000	0.384583000
7	-1.279073000	-1.221610000	1.944299000
6	-2.660817000	-4.175502000	-1.659523000
1	-3.118112000	-5.066400000	-2.093119000
6	-2.269683000	-3.120004000	-2.493949000
1	-2.408636000	-3.170195000	-3.574192000
6	-1.697023000	-1.994705000	-1.910218000
6	-1.134009000	-0.790950000	-2.617852000
1	-0.098607000	-1.020902000	-2.912519000
1	-1.693958000	-0.543741000	-3.530920000
1	-0.201964000	0.902569000	-1.891188000
6	-2.236350000	1.342923000	-1.784856000
1	-2.784921000	1.174614000	-2.720592000
1	-1.851096000	2.368116000	-1.803968000
6	-3.124425000	1.055040000	-0.597186000
6	-2.543124000	1.011759000	0.721808000
6	-3.208055000	0.161649000	1.683242000
6	-4.505234000	-0.276602000	1.458701000
1	-4.990243000	-0.916156000	2.199000000
6	-5.153127000	0.019747000	0.250188000
1	-6.176511000	-0.320240000	0.081790000
6	-4.431464000	0.603645000	-0.792684000
1	-4.863138000	0.654694000	-1.794483000
6	-2.328050000	-0.475928000	2.727417000
1	-2.890886000	-1.166230000	3.369306000
1	-1.821221000	0.249789000	3.376429000
1	-0.358582000	-1.124642000	2.408065000
6	-1.587087000	-2.673766000	1.700874000
1	-2.410435000	-3.002448000	2.350260000
1	-0.695341000	-3.255674000	1.981313000
8	1.393873000	-0.373356000	2.256564000
8	0.856851000	-0.478192000	0.051357000
6	1.690976000	-0.401711000	1.042250000
8	-1.405495000	3.663493000	0.062326000
8	0.677647000	2.786047000	0.287013000
6	-0.821441000	4.864492000	-0.546455000
6	-1.960013000	5.815717000	-0.837423000
6	-0.541387000	2.683711000	0.411672000
6	-1.195476000	1.499420000	1.018870000

1	-0.094219000	5.290729000	0.160733000
1	-0.284217000	4.561749000	-1.458518000
1	-1.558910000	6.731611000	-1.296866000
1	-2.683504000	5.369289000	-1.535521000
1	-2.486167000	6.096872000	0.086762000
1	-0.866973000	1.438938000	2.061159000
6	3.137982000	-0.354527000	0.614470000
6	3.492678000	-0.272597000	-0.743020000
6	4.140822000	-0.385789000	1.597499000
6	4.831465000	-0.227625000	-1.119444000
6	5.484330000	-0.335119000	1.238033000
6	5.808394000	-0.258608000	-0.119616000
1	2.714241000	-0.239174000	-1.505001000
1	3.859006000	-0.449821000	2.648938000
1	5.119338000	-0.160577000	-2.167735000
1	6.270594000	-0.360195000	1.991638000
7	7.226130000	-0.203917000	-0.510684000
8	7.505937000	-0.263621000	-1.716702000
8	8.079253000	-0.100522000	0.381936000

2a-OBz-CN

7	2.060899000	-1.290713000	-0.011840000
6	2.577734000	-1.674579000	-1.198891000
27	0.647297000	-0.109084000	-0.001740000
7	0.904848000	-0.090403000	1.986219000
6	3.716113000	-2.473786000	-1.235305000
1	4.136530000	-2.776956000	-2.194423000
7	0.906402000	-0.053885000	-1.988675000
6	4.294914000	-2.873252000	-0.025723000
1	5.196070000	-3.488421000	-0.031126000
6	3.715315000	-2.496230000	1.190650000
1	4.134900000	-2.817329000	2.144258000
6	2.576981000	-1.696392000	1.168215000
6	1.742155000	-1.284044000	2.342461000
1	1.051753000	-2.110418000	2.572943000
1	2.348001000	-1.092003000	3.239216000
1	0.002278000	-0.193758000	2.462295000
6	1.510221000	1.226286000	2.422273000
1	2.171035000	1.067804000	3.287687000
1	0.675299000	1.861946000	2.753946000
6	2.193406000	1.855484000	1.242162000
6	1.795765000	1.336521000	0.012259000
6	2.194586000	1.878164000	-1.207420000
6	3.078527000	2.965962000	-1.196277000
1	3.413329000	3.418456000	-2.133625000
6	3.524333000	3.477912000	0.033008000
1	4.221774000	4.318465000	0.041162000
6	3.077643000	2.942991000	1.252131000
1	3.411956000	3.377406000	2.198173000
6	1.512232000	1.270869000	-2.399392000
1	2.173500000	1.128550000	-3.267214000
1	0.677416000	1.912617000	-2.719398000
1	0.004089000	-0.147770000	-2.467205000
6	1.743527000	-1.241007000	-2.365986000
1	2.349517000	-1.033190000	-3.259175000
1	1.052736000	-2.062909000	-2.610677000
8	-1.046059000	0.879376000	0.004426000
8	-1.105386000	-1.317292000	-0.011131000
6	-1.739792000	-0.210274000	-0.002217000
6	-3.222686000	-0.146302000	0.000421000
6	-3.971652000	-1.334182000	0.037997000
6	-3.872797000	1.099066000	-0.035811000
6	-5.361539000	-1.284938000	0.038471000
6	-5.261907000	1.161792000	-0.037117000
6	-6.008159000	-0.033147000	-0.000215000
1	-3.456969000	-2.295251000	0.068723000
1	-3.283058000	2.016219000	-0.064657000

1   -5.951694000   -2.201529000   0.067796000
1   -5.776253000   2.122882000   -0.067248000
6   -7.434995000   0.026822000   -0.001898000
7   -8.600325000   0.075193000   -0.003362000

2a-OBz-CN-EDA

7   0.279038000   1.945832000   0.148503000
6   0.107875000   2.423573000   1.400044000
27   0.563150000   0.116712000   -0.070422000
7   0.734073000   0.578827000   -2.030550000
6   -0.041434000   3.789351000   1.612834000
1   -0.170612000   4.169021000   2.626570000
7   0.770809000   0.141226000   1.943275000
6   -0.023035000   4.646212000   0.506639000
1   -0.127182000   5.722851000   0.649945000
6   0.118432000   4.123602000   -0.780469000
1   0.112569000   4.767633000   -1.660521000
6   0.265085000   2.745709000   -0.934207000
6   0.321176000   2.009630000   -2.233556000
1   -0.691968000   2.000093000   -2.662908000
1   0.987711000   2.507029000   -2.952024000
1   0.067684000   0.020863000   -2.577526000
6   2.143575000   0.304136000   -2.486456000
1   2.390488000   0.915190000   -3.367909000
1   2.176316000   -0.754057000   -2.788689000
6   3.050916000   0.522491000   -1.308219000
6   2.402813000   0.386056000   -0.079431000
6   3.077534000   0.450559000   1.138236000
6   4.459852000   0.682078000   1.127010000
1   5.021139000   0.733034000   2.063630000
6   5.124194000   0.837164000   -0.100055000
1   6.200737000   1.021378000   -0.106030000
6   4.433168000   0.748854000   -1.319603000
1   4.971686000   0.852859000   -2.265292000
6   2.233805000   0.148000000   2.342811000
1   2.388449000   0.856699000   3.170178000
1   2.464169000   -0.859102000   2.719955000
1   0.331602000   -0.678430000   2.374493000
6   0.012917000   1.337567000   2.424758000
1   0.356624000   1.661272000   3.417711000
1   -1.043866000   1.040139000   2.507880000
8   -2.102099000   0.031189000   -2.016487000
8   -1.426751000   -0.246451000   0.128156000
6   -2.321590000   -0.173761000   -0.799120000
8   2.779453000   -2.613259000   0.818739000
8   2.663768000   -2.752876000   -1.451675000
6   4.225862000   -2.895936000   0.760252000
6   4.741304000   -2.891439000   2.178494000
6   2.165954000   -2.515428000   -0.361740000
6   0.758328000   -2.011692000   -0.158069000
1   4.359829000   -3.869536000   0.267075000
1   4.690207000   -2.112513000   0.143172000
1   5.815765000   -3.128768000   2.165965000
1   4.615329000   -1.904088000   2.645225000
1   4.229021000   -3.648177000   2.790536000
1   0.267284000   -2.325078000   0.772466000
7   -0.028304000   -2.380676000   -1.213775000
7   -0.639334000   -2.610730000   -2.121932000
6   -3.747379000   -0.381866000   -0.330842000
6   -4.042655000   -0.587854000   1.026899000
6   -4.789912000   -0.373295000   -1.271580000
6   -5.355723000   -0.785479000   1.444758000
6   -6.108339000   -0.570136000   -0.872676000
6   -6.393458000   -0.778373000   0.491348000
1   -3.233689000   -0.594570000   1.758064000
1   -4.555175000   -0.211998000   -2.324703000
1   -5.587828000   -0.946567000   2.498472000

1   -6.918634000   -0.566715000   -1.603076000
6   -7.742609000   -0.986480000   0.909556000
7   -8.844510000   -1.158474000   1.252175000

TS1-OBz-CN

7   -0.216743000   1.903554000   -0.032236000
6   -0.031042000   2.463470000   -1.243777000
27   -0.580543000   0.026489000   0.060888000
7   -0.738794000   0.392368000   2.042142000
6   0.165860000   3.835155000   -1.360727000
1   0.306768000   4.285709000   -2.343396000
7   -0.782834000   0.248816000   -1.951833000
6   0.179053000   4.607727000   -0.193391000
1   0.323269000   5.687509000   -0.257565000
6   0.016770000   4.000103000   1.053658000
1   0.042738000   4.579323000   1.976993000
6   -0.180624000   2.620050000   1.102977000
6   -0.278137000   1.793690000   2.344890000
1   0.726862000   1.719585000   2.785824000
1   -0.939803000   2.259044000   3.088721000
1   -0.087663000   -0.227911000   2.537513000
6   -2.155028000   0.136163000   2.483295000
1   -2.373886000   0.685411000   3.411310000
1   -2.228935000   -0.940539000   2.698977000
6   -3.050785000   0.489767000   1.331041000
6   -2.413995000   0.399608000   0.093748000
6   -3.073350000   0.608295000   -1.114309000
6   -4.434509000   0.941273000   -1.081465000
1   -4.986166000   1.109351000   -2.010073000
6   -5.090373000   1.048338000   0.155338000
1   -6.150606000   1.309431000   0.177138000
6   -4.411928000   0.819386000   1.363223000
1   -4.942757000   0.896369000   2.315658000
6   -2.246123000   0.342633000   -2.338854000
1   -2.370146000   1.105747000   -3.121226000
1   -2.523898000   -0.628627000   -2.773320000
1   -0.376587000   -0.554492000   -2.442098000
6   0.020161000   1.449603000   -2.344323000
1   -0.317590000   1.854341000   -3.308886000
1   1.063674000   1.118787000   -2.458061000
8   2.065475000   -0.235710000   1.985694000
8   1.406004000   -0.335340000   -0.179801000
6   2.292965000   -0.335529000   0.756368000
8   -2.889633000   -2.498855000   -0.989589000
8   -2.696115000   -2.825370000   1.256778000
6   -4.337752000   -2.769859000   -0.921200000
6   -4.890180000   -2.580874000   -2.313180000
6   -2.241198000   -2.461647000   0.182496000
6   -0.906894000   -1.817467000   -0.050896000
1   -4.470477000   -3.796422000   -0.549579000
1   -4.773172000   -2.065661000   -0.196292000
1   -5.968908000   -2.798344000   -2.302002000
1   -4.753187000   -1.545515000   -2.656113000
1   -4.408168000   -3.264410000   -3.027379000
1   -0.323449000   -2.316915000   -0.841607000
7   0.052736000   -2.689431000   1.302145000
7   0.789160000   -2.835921000   2.113656000
6   3.724816000   -0.476524000   0.281219000
6   4.041605000   -0.448815000   -1.087070000
6   4.753609000   -0.622146000   1.225914000
6   5.362868000   -0.556769000   -1.511275000
6   6.079751000   -0.736274000   0.820312000
6   6.386952000   -0.700686000   -0.554254000
1   3.243883000   -0.336250000   -1.821890000
1   4.504343000   -0.643099000   2.287723000
1   5.611396000   -0.529953000   -2.573097000
1   6.879914000   -0.849662000   1.553000000

6	7.745394000	-0.807262000	-0.979809000
7	8.855627000	-0.892853000	-1.327958000

2a-Carbene-OBz-CN

7	-0.299346000	2.047062000	0.282706000
6	-0.298702000	2.912112000	-0.745769000
27	-0.574116000	0.155040000	-0.083097000
7	-0.577252000	0.034246000	1.917826000
6	-0.214625000	4.281456000	-0.509762000
1	-0.222608000	4.983900000	-1.343422000
7	-0.937690000	0.869520000	-1.948131000
6	-0.118896000	4.721797000	0.815421000
1	-0.066502000	5.790539000	1.029698000
6	-0.080109000	3.799326000	1.865583000
1	0.018301000	4.121497000	2.902413000
6	-0.167668000	2.442868000	1.558806000
6	-0.022862000	1.296466000	2.509608000
1	1.053282000	1.124643000	2.672613000
1	-0.486155000	1.495433000	3.485545000
1	0.116995000	-0.709942000	2.104395000
6	-1.948846000	-0.336936000	2.415228000
1	-2.097358000	0.058838000	3.430375000
1	-1.978903000	-1.435403000	2.467921000
6	-2.952864000	0.160923000	1.415746000
6	-2.417813000	0.372852000	0.146447000
6	-3.180774000	0.777815000	-0.944155000
6	-4.555034000	0.977270000	-0.756484000
1	-5.188638000	1.289279000	-1.590604000
6	-5.114570000	0.768696000	0.514132000
1	-6.185318000	0.927108000	0.658932000
6	-4.326709000	0.361562000	1.602329000
1	-4.782538000	0.201435000	2.582807000
6	-2.426404000	0.865290000	-2.237202000
1	-2.685324000	1.752252000	-2.833311000
1	-2.626373000	-0.024560000	-2.851281000
1	-0.482890000	0.256108000	-2.631433000
6	-0.291965000	2.218062000	-2.073242000
1	-0.772725000	2.805879000	-2.867348000
1	0.756662000	2.047363000	-2.361921000
8	1.911618000	-1.168227000	1.471959000
8	1.435424000	0.028040000	-0.394678000
6	2.239360000	-0.575722000	0.412748000
8	-2.735010000	-2.249777000	-1.594459000
8	-2.249739000	-3.004111000	0.506330000
6	-4.079813000	-2.867374000	-1.549827000
6	-4.808092000	-2.402537000	-2.787859000
6	-1.989825000	-2.354178000	-0.506745000
6	-0.747352000	-1.571491000	-0.483823000
1	-3.948239000	-3.958303000	-1.516569000
1	-4.567671000	-2.531132000	-0.623543000
1	-5.812933000	-2.850496000	-2.803353000
1	-4.919453000	-1.308451000	-2.788418000
1	-4.277575000	-2.711832000	-3.700145000
1	0.164853000	-2.164534000	-0.665354000
7	0.470568000	-3.884607000	1.868903000
7	0.098193000	-3.557394000	2.853280000
6	3.698392000	-0.540771000	0.012236000
6	4.627848000	-1.330308000	0.707923000
6	4.136394000	0.281545000	-1.038832000
6	5.975873000	-1.307859000	0.363129000
6	5.482025000	0.323086000	-1.391660000
6	6.406184000	-0.475781000	-0.689395000
1	4.283299000	-1.966628000	1.524372000
1	3.414190000	0.897073000	-1.575964000
1	6.698576000	-1.924651000	0.898920000
1	5.826276000	0.965368000	-2.203423000
6	7.788302000	-0.439936000	-1.045766000

7	8.917361000	-0.410781000	-1.338068000

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27	-0.572052000	0.303992000	-0.218393000
8	1.418504000	0.664918000	-0.246163000
8	1.516857000	-1.573138000	-0.452265000
8	-0.121032000	-2.856006000	1.366143000
8	-1.682615000	-3.058210000	-0.282724000
7	-0.904271000	2.130319000	0.136332000
7	-0.651782000	0.139679000	1.791376000
1	0.047968000	-0.533149000	2.125571000
7	-0.991524000	0.806297000	-2.125394000
1	-0.233974000	0.513549000	-2.751318000
6	-1.218496000	2.949104000	-0.880445000
6	-1.523892000	4.286617000	-0.628028000
1	-1.785451000	4.953053000	-1.450634000
6	-1.480371000	4.743521000	0.692935000
1	-1.726927000	5.783021000	0.915634000
6	-1.110285000	3.877292000	1.730222000
1	-1.048217000	4.221700000	2.762808000
6	-0.815120000	2.555270000	1.412515000
6	-0.289520000	1.489329000	2.332210000
1	0.810140000	1.552150000	2.331736000
1	-0.637952000	1.615884000	3.367556000
6	-2.015991000	-0.338147000	2.256137000
1	-2.348597000	0.280711000	3.102689000
1	-1.893696000	-1.364731000	2.630963000
6	-2.973538000	-0.306169000	1.099071000
6	-2.379213000	-0.085405000	-0.142480000
6	-3.110010000	-0.088240000	-1.331943000
6	-4.491410000	-0.310450000	-1.280272000
1	-5.088498000	-0.318864000	-2.196307000
6	-5.104563000	-0.530346000	-0.035554000
1	-6.181524000	-0.706630000	0.008691000
6	-4.355472000	-0.536026000	1.152164000
1	-4.850915000	-0.721415000	2.109316000
6	-2.247684000	0.082965000	-2.549091000
1	-2.735751000	0.613813000	-3.380851000
1	-1.929972000	-0.903229000	-2.922343000
6	-1.109532000	2.305126000	-2.233656000
1	-1.957376000	2.578465000	-2.878017000
1	-0.195803000	2.680019000	-2.719682000
6	2.087375000	-0.389290000	-0.310589000
6	3.562066000	-0.396370000	-0.225521000
6	4.229047000	0.823026000	-0.013950000
1	3.653564000	1.744183000	0.083037000
6	5.615428000	0.853396000	0.072570000
1	6.141580000	1.794141000	0.237269000
6	6.342372000	-0.347398000	-0.053037000
6	5.679144000	-1.571955000	-0.264654000
1	6.253796000	-2.493520000	-0.360412000
6	4.291319000	-1.592272000	-0.349840000
1	3.771061000	-2.535764000	-0.514454000
6	0.045758000	-1.540010000	-0.650750000
1	-0.120056000	-1.785696000	-1.709321000
6	-0.546953000	-2.554473000	0.249136000
6	-2.539301000	-3.844149000	0.606166000
1	-2.719350000	-3.257814000	1.519963000
1	-2.007568000	-4.768254000	0.879618000
6	-3.819965000	-4.118794000	-0.147451000
1	-3.627163000	-4.705409000	-1.058039000
1	-4.313860000	-3.176372000	-0.427239000
1	-4.504530000	-4.693626000	0.494434000
6	7.767771000	-0.321557000	0.035512000
7	8.931434000	-0.299447000	0.107365000

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7	-0.980771000	-2.267586000	-0.236373000
6	-1.178738000	-3.090361000	0.809415000
27	-0.626463000	-0.431144000	0.102712000
7	-0.972825000	-0.244595000	-1.877824000
6	-1.622343000	-4.394830000	0.600102000
1	-1.791150000	-5.061293000	1.446556000
7	-0.808383000	-0.969349000	2.044489000
6	-1.840186000	-4.821108000	-0.715432000
1	-2.196524000	-5.835055000	-0.904952000
6	-1.599702000	-3.954654000	-1.790053000
1	-1.751767000	-4.274697000	-2.821357000
6	-1.159846000	-2.663887000	-1.511995000
6	-0.760370000	-1.595854000	-2.491870000
1	0.320430000	-1.693738000	-2.680934000
1	-1.282213000	-1.685589000	-3.455154000
1	-0.281779000	0.406937000	-2.265854000
6	-2.348198000	0.340296000	-2.148442000
1	-2.880702000	-0.305950000	-2.861703000
1	-2.215255000	1.317453000	-2.634913000
6	-3.123800000	0.456367000	-0.868155000
6	-2.382857000	0.219977000	0.304938000
6	-2.987160000	0.080933000	1.570301000
6	-4.361762000	0.282945000	1.675605000
1	-4.871893000	0.173701000	2.635514000
6	-5.097185000	0.603406000	0.519743000
1	-6.172905000	0.770875000	0.606502000
6	-4.498679000	0.665436000	-0.749861000
1	-5.112939000	0.845032000	-1.635470000
6	-2.043610000	-0.340469000	2.660996000
1	-2.512949000	-1.047174000	3.360591000
1	-1.713578000	0.525849000	3.254128000
1	0.005233000	-0.626241000	2.565560000
6	-0.781044000	-2.473186000	2.121178000
1	-1.398371000	-2.834101000	2.955814000
1	0.260775000	-2.764246000	2.327476000
8	1.531302000	1.554324000	0.682095000
8	1.335342000	-0.606429000	-0.005505000
6	2.007340000	0.445981000	0.309026000
8	-1.361366000	3.582381000	0.151784000
8	-0.342648000	2.521318000	-1.574588000
6	-1.446106000	4.801461000	-0.664281000
6	-2.138866000	5.853323000	0.170444000
6	-0.794812000	2.510323000	-0.434154000
6	-0.762860000	1.331593000	0.504580000
1	-0.422205000	5.093530000	-0.943002000
1	-2.003224000	4.557715000	-1.581833000
1	-2.216474000	6.783417000	-0.412487000
1	-3.154590000	5.534787000	0.447472000
1	-1.570570000	6.068656000	1.087252000
1	-0.842982000	1.682832000	1.541953000
6	3.506721000	0.311703000	0.214988000
6	4.318621000	1.454106000	0.308241000
6	4.097243000	-0.950672000	0.037361000
6	5.703080000	1.345042000	0.222500000
6	5.480632000	-1.076832000	-0.040535000
6	6.287133000	0.074863000	0.050808000
1	3.856453000	2.432405000	0.443717000
1	3.464803000	-1.835785000	-0.035212000
1	6.336348000	2.230693000	0.287585000
1	5.944204000	-2.055271000	-0.173055000
6	7.707108000	-0.046423000	-0.030533000
7	8.867516000	-0.146113000	-0.097036000

INT-MI-OBz-CN

7	1.218706000	-1.970819000	0.543342000
6	1.513628000	-2.969091000	-0.311093000
27	0.747776000	-0.295944000	-0.171447000

7	0.851083000	0.353764000	1.720414000
6	2.074063000	-4.149889000	0.171174000
1	2.319233000	-4.962163000	-0.513675000
7	0.915021000	-1.198395000	-1.950187000
6	2.316511000	-4.259579000	1.545405000
1	2.765555000	-5.170428000	1.944792000
6	1.992686000	-3.207896000	2.412408000
1	2.175878000	-3.280973000	3.484743000
6	1.430546000	-2.055218000	1.872119000
6	0.938859000	-0.847219000	2.624721000
1	-0.082406000	-1.056956000	2.977766000
1	1.557427000	-0.628281000	3.506440000
1	-0.007509000	0.863960000	1.955048000
6	2.023348000	1.297525000	1.795446000
1	2.580793000	1.136452000	2.727346000
1	1.642037000	2.324476000	1.809476000
6	2.892824000	0.991471000	0.599051000
6	2.290347000	0.964716000	-0.711419000
6	2.909981000	0.091565000	-1.679802000
6	4.194921000	-0.392406000	-1.471960000
1	4.647820000	-1.047231000	-2.219164000
6	4.869857000	-0.117291000	-0.274520000
1	5.882903000	-0.493178000	-0.120248000
6	4.184920000	0.495826000	0.777605000
1	4.632335000	0.532076000	1.773136000
6	2.000791000	-0.500782000	-2.725452000
1	2.532063000	-1.213862000	-3.369185000
1	1.532149000	0.252211000	-3.372555000
1	-0.003184000	-1.032494000	-2.398423000
6	1.126754000	-2.670499000	-1.735635000
1	1.870373000	-3.062567000	-2.443696000
1	0.170831000	-3.173740000	-1.950072000
8	-1.714136000	-0.216980000	-2.186345000
8	-1.145515000	-0.431153000	0.003103000
6	-1.994999000	-0.302370000	-0.970116000
8	1.277395000	3.660348000	-0.061218000
8	-0.843984000	2.856977000	-0.185024000
6	0.767379000	4.904418000	0.525802000
6	1.958409000	5.812377000	0.732162000
6	0.364067000	2.708982000	-0.359122000
6	0.954508000	1.499130000	-0.982090000
1	0.029509000	5.334715000	-0.168020000
1	0.256985000	4.659766000	1.470145000
1	1.619108000	6.769323000	1.156225000
1	2.683721000	5.364430000	1.427408000
1	2.464186000	6.018564000	-0.222860000
1	0.603759000	1.459249000	-2.018620000
6	-3.435132000	-0.274675000	-0.521528000
6	-3.773727000	-0.208021000	0.840485000
6	-4.450227000	-0.313783000	-1.491009000
6	-5.108088000	-0.182921000	1.234007000
6	-5.789161000	-0.292721000	-1.113663000
6	-6.119853000	-0.228400000	0.254212000
1	-2.985181000	-0.171554000	1.592426000
1	-4.179900000	-0.362443000	-2.546627000
1	-5.376680000	-0.129179000	2.289864000
1	-6.580907000	-0.325114000	-1.863340000
6	-7.490936000	-0.209139000	0.650855000
7	-8.611180000	-0.194946000	0.976198000

2a-OBz-Me

7	-1.888401000	-1.297043000	-0.007361000
6	-2.398773000	-1.703990000	1.174583000
27	-0.486275000	-0.101176000	-0.002880000
7	-0.750257000	-0.052305000	-1.989552000
6	-3.530104000	-2.513695000	1.201426000
1	-3.945324000	-2.835755000	2.156650000

7	-0.740150000	-0.079485000	1.985747000
6	-4.108786000	-2.899037000	-0.012870000
1	-5.004481000	-3.522195000	-0.014936000
6	-3.535992000	-2.497188000	-1.224615000
1	-3.956005000	-2.806064000	-2.182110000
6	-2.404479000	-1.687964000	-1.192275000
6	-1.577340000	-1.247916000	-2.362388000
1	-0.879654000	-2.063683000	-2.608044000
1	-2.188230000	-1.047443000	-3.253980000
1	0.151835000	-0.138372000	-2.469921000
6	-1.370162000	1.265606000	-2.401119000
1	-2.028203000	1.116325000	-3.270347000
1	-0.541722000	1.916325000	-2.719727000
6	-2.060219000	1.865994000	-1.209710000
6	-1.650948000	1.331762000	0.010115000
6	-2.053492000	1.849293000	1.239379000
6	-2.952179000	2.924882000	1.249021000
1	-3.290220000	3.357493000	2.194620000
6	-3.408891000	3.450704000	0.029464000
1	-4.117508000	4.281905000	0.037091000
6	-2.958684000	2.941800000	-1.199661000
1	-3.301621000	3.387711000	-2.137274000
6	-1.356997000	1.232834000	2.418811000
1	-2.010163000	1.072218000	3.289749000
1	-0.526462000	1.878861000	2.741528000
1	0.164277000	-0.173046000	2.460255000
6	-1.566154000	-1.279588000	2.346487000
1	-2.173163000	-1.090409000	3.243142000
1	-0.867979000	-2.098817000	2.579033000
8	1.198277000	0.899771000	-0.001947000
8	1.257769000	-1.294815000	-0.013524000
6	1.901583000	-0.188267000	-0.008094000
6	3.376366000	-0.126228000	-0.007181000
6	4.133677000	-1.310276000	0.019830000
6	4.037918000	1.113847000	-0.036837000
6	5.525474000	-1.250571000	0.018339000
6	5.430505000	1.162898000	-0.039415000
6	6.198716000	-0.015180000	-0.009744000
1	3.622225000	-2.274354000	0.041199000
1	3.453314000	2.035478000	-0.062666000
1	6.106040000	-2.176448000	0.037863000
1	5.936486000	2.131140000	-0.067985000
6	7.701603000	0.042695000	0.022103000
1	8.064004000	0.015177000	1.063923000
1	8.149312000	-0.815909000	-0.499582000
1	8.080107000	0.969334000	-0.432701000

2a-OBz-Me-EDA

7	0.161415000	1.959166000	0.180030000
6	0.017043000	2.424990000	1.439481000
27	0.432561000	0.132255000	-0.061185000
7	0.558634000	0.608617000	-2.019745000
6	-0.123366000	3.788977000	1.668674000
1	-0.230975000	4.159093000	2.688453000
7	0.693488000	0.140066000	1.947014000
6	-0.124629000	4.656669000	0.570655000
1	-0.222513000	5.732164000	0.726474000
6	-0.010468000	4.146210000	-0.724198000
1	-0.031738000	4.799319000	-1.597180000
6	0.128520000	2.769364000	-0.894411000
6	0.157210000	2.045795000	-2.201868000
1	-0.862174000	2.050619000	-2.616121000
1	0.818192000	2.543895000	-2.924978000
1	-0.131491000	0.062567000	-2.549118000
6	1.951407000	0.318699000	-2.514148000
1	2.183214000	0.929603000	-3.399931000

1	1.963058000	-0.738736000	-2.820984000
6	2.892034000	0.523447000	-1.359650000
6	2.274174000	0.390199000	-0.114852000
6	2.980813000	0.449112000	1.084877000
6	4.364417000	0.669468000	1.038133000
1	4.949973000	0.715434000	1.960073000
6	4.998245000	0.819689000	-0.205553000
1	6.075816000	0.994886000	-0.238995000
6	4.275134000	0.738577000	-1.406986000
1	4.790192000	0.840061000	-2.366017000
6	2.166101000	0.155399000	2.311657000
1	2.337108000	0.874342000	3.126881000
1	2.409890000	-0.845914000	2.695513000
1	0.271024000	-0.686028000	2.382641000
6	-0.059615000	1.328345000	2.454627000
1	0.299558000	1.642350000	3.445254000
1	-1.114046000	1.026975000	2.551022000
8	-2.273509000	0.085829000	-1.936172000
8	-1.548934000	-0.231933000	0.184843000
6	-2.471893000	-0.164514000	-0.720639000
8	2.644567000	-2.612425000	0.773059000
8	2.486514000	-2.748055000	-1.495174000
6	4.087112000	-2.905549000	0.687535000
6	4.627455000	-2.907743000	2.096353000
6	2.009771000	-2.508950000	-0.396048000
6	0.610524000	-1.995805000	-0.166121000
1	4.205347000	-3.879027000	0.190085000
1	4.546297000	-2.124229000	0.063866000
1	5.700505000	-3.149631000	2.064770000
1	4.512739000	-1.921138000	2.567437000
1	4.122061000	-3.663729000	2.715027000
1	0.132174000	-2.308424000	0.771073000
7	-0.197214000	-2.350866000	-1.210349000
7	-0.825529000	-2.569918000	-2.109537000
6	-3.872583000	-0.437634000	-0.233868000
6	-4.125757000	-0.824632000	1.094188000
6	-4.957439000	-0.321085000	-1.116732000
6	-5.426651000	-1.087906000	1.521037000
6	-6.259142000	-0.581146000	-0.683657000
6	-6.518281000	-0.970102000	0.640915000
1	-3.291557000	-0.925087000	1.790754000
1	-4.772856000	-0.023770000	-2.151029000
1	-5.604638000	-1.392409000	2.556238000
1	-7.091224000	-0.484398000	-1.386175000
6	-7.920325000	-1.241438000	1.117659000
1	-8.635569000	-1.261307000	0.283281000
1	-7.981304000	-2.202929000	1.651180000
1	-8.249779000	-0.462857000	1.825809000

TS1-OBz-Me

7	0.080635000	1.908278000	0.055957000
6	-0.090648000	2.456560000	1.274965000
27	0.451249000	0.034531000	-0.058764000
7	0.571346000	0.414382000	-2.037341000
6	-0.295335000	3.825740000	1.406499000
1	-0.424549000	4.266831000	2.395041000
7	0.691762000	0.243856000	1.951843000
6	-0.332604000	4.607893000	0.245983000
1	-0.484241000	5.685934000	0.321508000
6	-0.184790000	4.011991000	-1.008417000
1	-0.229454000	4.598439000	-1.926495000
6	0.022264000	2.633872000	-1.072371000
6	0.110194000	1.819300000	-2.322805000
1	-0.897831000	1.750565000	-2.757581000
1	0.767740000	2.291736000	-3.065823000
1	-0.094253000	-0.199480000	-2.521297000
6	1.977296000	0.154103000	-2.506972000

1	2.179957000	0.701851000	-3.439648000
1	2.043430000	-0.923130000	-2.723055000
6	2.896430000	0.505028000	-1.372116000
6	2.282878000	0.412430000	-0.123070000
6	2.965543000	0.618152000	1.072513000
6	4.326217000	0.950261000	1.014279000
1	4.895833000	1.116597000	1.932350000
6	4.958465000	1.058940000	-0.234634000
1	6.018429000	1.318896000	-0.275942000
6	4.256903000	0.833422000	-1.430057000
1	4.769851000	0.911716000	-2.392199000
6	2.160895000	0.353151000	2.312607000
1	2.291063000	1.123596000	3.086759000
1	2.454911000	-0.611846000	2.750207000
1	0.304778000	-0.567400000	2.444412000
6	-0.118296000	1.431975000	2.366665000
1	0.226922000	1.830666000	3.331176000
1	-1.157002000	1.088958000	2.488470000
8	-2.235648000	-0.204566000	-1.925405000
8	-1.522712000	-0.343280000	0.219055000
6	-2.439858000	-0.341838000	-0.692517000
8	2.778780000	-2.488212000	0.947277000
8	2.561927000	-2.809729000	-1.297701000
6	4.225352000	-2.761112000	0.862948000
6	4.793922000	-2.572711000	2.248572000
6	2.117407000	-2.449345000	-0.217865000
6	0.784360000	-1.809210000	0.031844000
1	4.352577000	-3.787932000	0.490042000
1	4.653974000	-2.057757000	0.133180000
1	5.871769000	-2.793686000	2.225546000
1	4.664067000	-1.536573000	2.591888000
1	4.317648000	-3.253947000	2.968818000
1	0.208472000	-2.315252000	0.823930000
7	-0.186997000	-2.671216000	-1.317650000
7	-0.943334000	-2.808840000	-2.112471000
6	-3.847088000	-0.529729000	-0.185112000
6	-4.126521000	-0.607681000	1.188628000
6	-4.914583000	-0.622628000	-1.094579000
6	-5.438968000	-0.765304000	1.639116000
6	-6.222697000	-0.783548000	-0.640425000
6	-6.510766000	-0.853487000	0.735110000
1	-3.307093000	-0.543995000	1.906865000
1	-4.706918000	-0.569181000	-2.165211000
1	-5.637783000	-0.819801000	2.712864000
1	-7.040493000	-0.855479000	-1.362900000
6	-7.930769000	-0.998273000	1.214855000
1	-8.456757000	-1.799347000	0.672494000
1	-7.974317000	-1.221311000	2.290216000
1	-8.498328000	-0.068634000	1.040978000

2a-carbene-OBz-Me

7	-0.207890000	2.073733000	0.197678000
6	-0.214348000	2.876752000	-0.880893000
27	-0.455601000	0.161882000	-0.060873000
7	-0.417732000	0.144128000	1.940089000
6	-0.131038000	4.257251000	-0.728441000
1	-0.145053000	4.908385000	-1.602629000
7	-0.875409000	0.774600000	-1.950353000
6	-0.025662000	4.775933000	0.567681000
1	0.029295000	5.855379000	0.717768000
6	0.018467000	3.918215000	1.670305000
1	0.122384000	4.301426000	2.685673000
6	-0.072710000	2.544895000	1.446868000
6	0.055675000	1.464189000	2.474864000
1	1.122943000	1.348163000	2.722350000
1	-0.480059000	1.710204000	3.402080000
1	0.332438000	-0.546363000	2.132747000

6	-1.755817000	-0.290806000	2.468620000
1	-1.900244000	0.095050000	3.488243000
1	-1.734767000	-1.389930000	2.518314000
6	-2.800300000	0.156874000	1.486111000
6	-2.298491000	0.350108000	0.199854000
6	-3.094977000	0.704429000	-0.883753000
6	-4.470251000	0.871224000	-0.669556000
1	-5.130941000	1.142304000	-1.497011000
6	-4.995939000	0.683312000	0.618619000
1	-6.067275000	0.817004000	0.782882000
6	-4.173760000	0.327505000	1.699891000
1	-4.603272000	0.182560000	2.694453000
6	-2.373326000	0.785086000	-2.196114000
1	-2.636001000	1.680465000	-2.777887000
1	-2.601976000	-0.096458000	-2.811238000
1	-0.451462000	0.118786000	-2.613640000
6	-0.215136000	2.103705000	-2.163591000
1	-0.692221000	2.645571000	-2.991872000
1	0.831161000	1.903821000	-2.440987000
8	2.082822000	-0.986383000	1.527643000
8	1.547532000	0.051652000	-0.413396000
6	2.385865000	-0.488404000	0.409894000
8	-2.558832000	-2.295970000	-1.516857000
8	-2.093787000	-3.028531000	0.596321000
6	-3.884621000	-2.953585000	-1.493299000
6	-4.613112000	-2.505714000	-2.737637000
6	-1.827108000	-2.382892000	-0.418233000
6	-0.596427000	-1.583458000	-0.378957000
1	-3.717863000	-4.040006000	-1.464798000
1	-4.394969000	-2.639703000	-0.571224000
1	-5.594568000	-3.001727000	-2.775868000
1	-4.777001000	-1.418405000	-2.727586000
1	-4.053922000	-2.778503000	-3.644510000
1	0.327667000	-2.175054000	-0.489839000
7	0.762432000	-3.795961000	1.921165000
7	0.349950000	-3.426858000	2.874162000
6	3.822211000	-0.507914000	-0.042766000
6	4.820015000	-1.003858000	0.810301000
6	4.195939000	-0.040245000	-1.315129000
6	6.155020000	-1.033023000	0.401929000
6	5.529373000	-0.075614000	-1.719889000
6	6.534673000	-0.572728000	-0.869510000
1	4.541082000	-1.368089000	1.801036000
1	3.431067000	0.348387000	-1.989606000
1	6.918019000	-1.423205000	1.080782000
1	5.801373000	0.287063000	-2.715056000
6	7.971714000	-0.603533000	-1.318162000
1	8.618634000	-1.084698000	-0.571245000
1	8.077750000	-1.149617000	-2.269114000
1	8.352102000	0.416515000	-1.491577000

4a-OBz-Me

27	0.433492000	0.304929000	0.194613000
8	-1.557965000	0.648863000	0.172522000
8	-1.643336000	-1.585823000	0.423400000
8	0.005521000	-2.850817000	-1.405534000
8	1.560266000	-3.055048000	0.249278000
7	0.761168000	2.132331000	-0.158052000
7	0.587372000	0.132338000	-1.809660000
1	-0.093930000	-0.547693000	-2.166464000
7	0.775084000	0.821073000	2.113639000
1	0.000389000	0.515458000	2.711758000
6	1.028899000	2.958638000	0.866150000
6	1.342136000	4.295185000	0.618900000
1	1.567695000	4.967214000	1.447597000
6	1.352852000	4.744208000	-0.705682000
1	1.606534000	5.782847000	-0.924392000

6	1.026807000	3.871186000	-1.752093000
1	1.005448000	4.209668000	-2.788270000
6	0.722733000	2.549969000	-1.439089000
6	0.236498000	1.476166000	-2.371572000
1	-0.862866000	1.532715000	-2.409497000
1	0.619188000	1.599053000	-3.395310000
6	1.971806000	-0.337409000	-2.220300000
1	2.334670000	0.285805000	-3.051086000
1	1.869166000	-1.362887000	-2.603679000
6	2.885069000	-0.300573000	-1.027699000
6	2.243853000	-0.070240000	0.189054000
6	2.931662000	-0.058807000	1.404023000
6	4.314458000	-0.279785000	1.404833000
1	4.878713000	-0.277153000	2.341556000
6	4.973176000	-0.511931000	0.185898000
1	6.051119000	-0.687919000	0.182574000
6	4.267995000	-0.528965000	-1.028445000
1	4.798054000	-0.722997000	-1.965160000
6	2.029333000	0.127209000	2.590165000
1	2.484086000	0.686734000	3.422105000
1	1.715803000	-0.853340000	2.981013000
6	0.854878000	2.322302000	2.216368000
1	1.654452000	2.619792000	2.909713000
1	-0.096121000	2.679033000	2.640683000
6	-2.228325000	-0.406488000	0.260146000
6	-3.695457000	-0.424028000	0.189679000
6	-4.382726000	0.780676000	-0.051179000
1	-3.817725000	1.704530000	-0.186197000
6	-5.772149000	0.790277000	-0.113659000
1	-6.296884000	1.730662000	-0.299269000
6	-6.515813000	-0.392683000	0.060737000
6	-5.818172000	-1.589468000	0.302889000
1	-6.377968000	-2.516663000	0.446429000
6	-4.426820000	-1.612888000	0.365988000
1	-3.904132000	-2.550698000	0.558286000
6	-0.175565000	-1.543275000	0.617643000
1	-0.001963000	-1.793336000	1.673861000
6	0.425258000	-2.550765000	-0.285357000
6	2.413748000	-3.852764000	-0.630972000
1	2.602868000	-3.276074000	-1.548905000
1	1.875930000	-4.774721000	-0.900096000
6	3.689842000	-4.132658000	0.128758000
1	3.489533000	-4.710421000	1.043389000
1	4.191140000	-3.192364000	0.402737000
1	4.371193000	-4.718451000	-0.506660000
6	-8.015792000	-0.375582000	-0.037900000
1	-8.329322000	-0.403339000	-1.095471000
1	-8.465354000	-1.244048000	0.463790000
1	-8.436344000	0.542887000	0.397901000

TS2-OBz-Me

7	-0.887354000	-2.264821000	-0.231830000
6	-1.101566000	-3.080569000	0.816647000
27	-0.496803000	-0.436331000	0.101402000
7	-0.842255000	-0.246825000	-1.878573000
6	-1.576771000	-4.374604000	0.612196000
1	-1.758592000	-5.034755000	1.460944000
7	-0.683641000	-0.964726000	2.044450000
6	-1.809550000	-4.799032000	-0.701560000
1	-2.190860000	-5.804568000	-0.887246000
6	-1.552208000	-3.940840000	-1.779064000
1	-1.715785000	-4.259608000	-2.809039000
6	-1.080144000	-2.660417000	-1.505892000
6	-0.658974000	-1.603768000	-2.489438000
1	0.419428000	-1.724747000	-2.678702000
1	-1.183196000	-1.684942000	-3.452228000
1	-0.139048000	0.389802000	-2.269354000

6	-2.206426000	0.364123000	-2.147837000
1	-2.754813000	-0.276292000	-2.854356000
1	-2.056496000	1.335073000	-2.641536000
6	-2.976195000	0.502492000	-0.866010000
6	-2.235692000	0.262025000	0.307052000
6	-2.841964000	0.130264000	1.572831000
6	-4.213374000	0.351000000	1.679452000
1	-4.724450000	0.248034000	2.639571000
6	-4.945350000	0.680708000	0.523939000
1	-6.018588000	0.863170000	0.611573000
6	-4.347882000	0.730495000	-0.746679000
1	-4.961436000	0.913785000	-1.632046000
6	-1.905327000	-0.310767000	2.662148000
1	-2.388982000	-1.008513000	3.360973000
1	-1.557304000	0.547751000	3.256287000
1	0.137639000	-0.635501000	2.562366000
6	-0.684594000	-2.468341000	2.124991000
1	-1.303620000	-2.815574000	2.964225000
1	0.352842000	-2.778594000	2.325366000
8	1.677759000	1.522769000	0.672336000
8	1.461265000	-0.636845000	-0.008839000
6	2.151454000	0.409211000	0.301227000
8	-1.162066000	3.593668000	0.150880000
8	-0.175846000	2.512684000	-1.581611000
6	-1.219323000	4.816340000	-0.661473000
6	-1.904813000	5.875657000	0.170069000
6	-0.621202000	2.509336000	-0.438419000
6	-0.610861000	1.330220000	0.500049000
1	-0.188051000	5.093815000	-0.927818000
1	-1.770236000	4.585582000	-1.586089000
1	-1.961229000	6.809546000	-0.409268000
1	-2.928604000	5.571861000	0.433748000
1	-1.344091000	6.077702000	1.094536000
1	-0.681247000	1.684332000	1.536837000
6	3.642982000	0.263108000	0.206107000
6	4.474005000	1.388846000	0.318784000
6	4.232474000	-0.997572000	0.003217000
6	5.860755000	1.256708000	0.226628000
6	5.617656000	-1.122574000	-0.078991000
6	6.458367000	0.001170000	0.029405000
1	4.025829000	2.372288000	0.471069000
1	3.596346000	-1.879691000	-0.085198000
1	6.492360000	2.144979000	0.308897000
1	6.061526000	-2.110195000	-0.231307000
6	7.953470000	-0.152726000	-0.053336000
1	8.335248000	-0.729827000	0.805024000
1	8.246688000	-0.701854000	-0.962149000
1	8.462566000	0.821303000	-0.059639000

INT-MI-OBz-Me

7	1.086355000	-1.972393000	0.537833000
6	1.362277000	-2.972109000	-0.321185000
27	0.609935000	-0.296290000	-0.168836000
7	0.748313000	0.355050000	1.719474000
6	1.928089000	-4.154162000	0.151773000
1	2.158501000	-4.967740000	-0.536685000
7	0.739956000	-1.200077000	-1.949754000
6	2.195063000	-4.263530000	1.521543000
1	2.648753000	-5.175363000	1.913400000
6	1.889771000	-3.210366000	2.393621000
1	2.091859000	-3.283489000	3.462564000
6	1.321276000	-2.056418000	1.862667000
6	0.846119000	-0.845978000	2.622512000
1	-0.170349000	-1.052086000	2.991180000
1	1.479133000	-0.629917000	3.494617000
1	-0.104489000	0.868799000	1.967202000
6	1.925685000	1.293688000	1.772813000

1	2.498445000	1.131892000	2.695342000
1	1.548384000	2.322301000	1.792987000
6	2.773300000	0.981765000	0.561543000
6	2.148483000	0.957809000	-0.738373000
6	2.744728000	0.079401000	-1.715607000
6	4.029560000	-0.414267000	-1.528971000
1	4.464368000	-1.073325000	-2.283234000
6	4.727129000	-0.143095000	-0.343865000
1	5.739772000	-0.526618000	-0.206544000
6	4.064878000	0.476861000	0.718704000
1	4.529960000	0.511441000	1.706175000
6	1.813318000	-0.506922000	-2.744678000
1	2.328677000	-1.221637000	-3.399484000
1	1.336083000	0.249392000	-3.381638000
1	-0.190184000	-1.026000000	-2.372874000
6	0.949687000	-2.672314000	-1.738697000
1	1.678581000	-3.067413000	-2.460358000
1	-0.011914000	-3.172310000	-1.934903000
8	-1.881791000	-0.223274000	-2.136437000
8	-1.277844000	-0.433554000	0.042572000
6	-2.151506000	-0.304537000	-0.914275000
8	1.176563000	3.663188000	-0.090466000
8	-0.950806000	2.867068000	-0.113939000
6	0.696948000	4.909900000	0.515413000
6	1.901346000	5.807799000	0.684861000
6	0.247315000	2.712805000	-0.341721000
6	0.809123000	1.497793000	-0.981265000
1	-0.060689000	5.347635000	-0.152070000
1	0.216855000	4.667147000	1.475996000
1	1.584373000	6.764538000	1.126317000
1	2.646721000	5.349602000	1.351668000
1	2.375372000	6.015952000	-0.285907000
1	0.437208000	1.464229000	-2.010921000
6	-3.576078000	-0.275057000	-0.441579000
6	-3.899582000	-0.196985000	0.925266000
6	-4.616848000	-0.326017000	-1.381405000
6	-5.231347000	-0.171111000	1.333727000
6	-5.949104000	-0.304233000	-0.964731000
6	-6.281450000	-0.227251000	0.397753000
1	-3.099707000	-0.151051000	1.666011000
1	-4.374074000	-0.384898000	-2.444180000
1	-5.466760000	-0.106332000	2.399612000
1	-6.747529000	-0.347841000	-1.710072000
6	-7.715298000	-0.203945000	0.855597000
1	-8.412532000	-0.274426000	0.009068000
1	-7.923332000	-1.039511000	1.543378000
1	-7.938381000	0.724241000	1.406555000

2a-OBz-COMe

7	-2.378414000	-1.304491000	-0.012930000
6	-2.887607000	-1.718380000	1.167129000
27	-0.982285000	-0.101884000	-0.002894000
7	-1.244329000	-0.047321000	-1.989504000
6	-4.014489000	-2.534335000	1.189803000
1	-4.428778000	-2.862081000	2.143463000
7	-1.238025000	-0.088648000	1.985462000
6	-4.589918000	-2.918205000	-0.026416000
1	-5.482299000	-3.546073000	-0.031621000
6	-4.018253000	-2.508880000	-1.236116000
1	-4.435703000	-2.816354000	-2.195160000
6	-2.891249000	-1.693652000	-1.199896000
6	-2.066232000	-1.244829000	-2.367954000
1	-1.365292000	-2.056485000	-2.617767000
1	-2.678151000	-1.042308000	-3.258328000
1	-0.341341000	-0.127760000	-2.469277000
6	-1.868667000	1.269840000	-2.396792000
1	-2.524168000	1.121371000	-3.267978000

1	-1.042166000	1.925263000	-2.710653000
6	-2.563279000	1.862139000	-1.204322000
6	-2.153734000	1.325640000	0.014175000
6	-2.559102000	1.836527000	1.245044000
6	-3.462037000	2.908507000	1.257442000
1	-3.802450000	3.336260000	2.204346000
6	-3.919494000	3.436822000	0.039364000
1	-4.631372000	4.265173000	0.049267000
6	-3.465876000	2.934439000	-1.191084000
1	-3.809089000	3.382579000	-2.127475000
6	-1.860501000	1.219623000	2.422695000
1	-2.513138000	1.053216000	3.292861000
1	-1.032825000	1.868193000	2.747545000
1	-0.333598000	-0.179974000	2.460535000
6	-2.059409000	-1.293376000	2.341666000
1	-2.669311000	-1.108488000	3.237162000
1	-1.358480000	-2.110176000	2.574354000
8	0.698904000	0.907991000	0.002586000
8	0.777048000	-1.286867000	-0.015011000
6	1.404794000	-0.174788000	-0.005222000
6	2.885599000	-0.099976000	-0.002233000
6	3.644767000	-1.279941000	0.041519000
6	3.532420000	1.148428000	-0.044062000
6	5.036480000	-1.215223000	0.042202000
6	4.920886000	1.209157000	-0.043162000
6	5.690748000	0.030496000	-0.000091000
1	3.137222000	-2.244973000	0.077345000
1	2.938047000	2.062857000	-0.079286000
1	5.607698000	-2.143363000	0.078235000
1	5.429869000	2.173632000	-0.078754000
6	7.186525000	0.143251000	0.000397000
8	7.725031000	1.255755000	0.001644000
6	8.014887000	-1.113858000	-0.001338000
1	7.794185000	-1.722102000	0.890449000
1	7.776904000	-1.733375000	-0.880703000
1	9.079896000	-0.852544000	-0.011849000

2a-OBz-COMe-EDA

7	0.574554000	1.944775000	0.142451000
6	0.389365000	2.418313000	1.393492000
27	0.848558000	0.114218000	-0.081271000
7	1.055233000	0.585393000	-2.035606000
6	0.251369000	3.784642000	1.610727000
1	0.110906000	4.160952000	2.624207000
7	1.020984000	0.126582000	1.935855000
6	0.296082000	4.646522000	0.509179000
1	0.201914000	5.723575000	0.656220000
6	0.450865000	4.128455000	-0.778423000
1	0.464780000	4.776794000	-1.655086000
6	0.584538000	2.749805000	-0.936489000
6	0.647795000	2.017553000	-2.237613000
1	-0.363415000	2.010305000	-2.671774000
1	1.318954000	2.515033000	-2.951686000
1	0.395570000	0.032123000	-2.595688000
6	2.471705000	0.310557000	-2.469855000
1	2.735499000	0.930003000	-3.340435000
1	2.505785000	-0.744483000	-2.782647000
6	3.359804000	0.513488000	-1.274050000
6	2.689619000	0.371463000	-0.057712000
6	3.343559000	0.422406000	1.171919000
6	4.727196000	0.644887000	1.186656000
1	5.272682000	0.685135000	2.133132000
6	5.413849000	0.804621000	-0.027504000
1	6.491545000	0.981549000	-0.013566000
6	4.743602000	0.730700000	-1.259521000
1	5.299099000	0.838521000	-2.194886000
6	2.477208000	0.116080000	2.359405000

1   2.624817000   0.815314000   3.196090000
1   2.692066000   -0.896769000   2.730146000
1   0.565947000   -0.690248000   2.356005000
6   0.267342000   1.328265000   2.410949000
1   0.597807000   1.643671000   3.411035000
1   -0.793544000   1.040912000   2.475191000
8   -1.771696000   0.033221000   -2.085041000
8   -1.146148000   -0.230607000   0.075731000
6   -2.022751000   -0.149489000   -0.869337000
8   3.035554000   -2.637104000   0.824290000
8   2.953007000   -2.753723000   -1.448902000
6   4.481280000   -2.926423000   0.785807000
6   4.976086000   -2.930328000   2.211532000
6   2.440427000   -2.524020000   -0.364177000
6   1.033032000   -2.013723000   -0.175808000
1   4.617901000   -3.898511000   0.290354000
1   4.958678000   -2.142694000   0.179365000
1   6.049571000   -3.172221000   2.213561000
1   4.847778000   -1.944297000   2.680406000
1   4.451906000   -3.687301000   2.813131000
1   0.529318000   -2.329809000   0.746911000
7   0.257802000   -2.374336000   -1.242873000
7   -0.341129000   -2.598907000   -2.160350000
6   -3.460927000   -0.308916000   -0.425256000
6   -3.789557000   -0.485626000   0.930522000
6   -4.489512000   -0.275218000   -1.379396000
6   -5.118030000   -0.620202000   1.320389000
6   -5.821289000   -0.411326000   -0.991049000
6   -6.152814000   -0.583824000   0.365793000
1   -2.993149000   -0.515670000   1.675319000
1   -4.234656000   -0.139228000   -2.431715000
1   -5.373193000   -0.755082000   2.373218000
1   -6.601438000   -0.382290000   -1.752890000
6   -7.570618000   -0.729430000   0.823603000
8   -7.827038000   -0.883756000   2.023840000
6   -8.677535000   -0.684524000   -0.197232000
1   -8.552420000   -1.487118000   -0.941518000
1   -9.645538000   -0.798242000   0.305455000
1   -8.657921000   0.269143000   -0.748530000

TS1-OBz-COMe
7   0.523229000   1.911515000   0.029735000
6   0.314689000   2.463636000   1.241068000
27   0.859478000   0.029400000   -0.070514000
7   1.081604000   0.412699000   -2.043624000
6   0.141299000   3.837835000   1.366273000
1   -0.017907000   4.281830000   2.349145000
7   1.005254000   0.228221000   1.948484000
6   0.177138000   4.621628000   0.206981000
1   0.053675000   5.703535000   0.278222000
6   0.362332000   4.022647000   -1.041061000
1   0.374204000   4.610921000   -1.958947000
6   0.533221000   2.639430000   -1.098764000
6   0.648258000   1.822579000   -2.345324000
1   -0.346974000   1.766674000   -2.810559000
1   1.333962000   2.284074000   -3.069534000
1   0.435309000   -0.194976000   -2.561105000
6   2.507084000   0.144625000   -2.446813000
1   2.758324000   0.703683000   -3.360708000
1   2.575105000   -0.929908000   -2.674545000
6   3.372988000   0.473288000   -1.264235000
6   2.698500000   0.376891000   -0.047517000
6   3.324139000   0.561523000   1.182220000
6   4.689630000   0.877139000   1.194549000
1   5.215653000   1.025090000   2.141250000
6   5.383458000   0.991417000   -0.020871000
1   6.447070000   1.239016000   -0.008196000

6   4.738723000   0.785485000   -1.251153000
1   5.298931000   0.866943000   -2.186209000
6   2.458231000   0.287697000   2.378208000
1   2.574549000   1.032573000   3.179174000
1   2.706377000   -0.697331000   2.800179000
1   0.567704000   -0.571330000   2.417630000
6   0.215155000   1.441146000   2.330054000
1   0.534163000   1.830759000   3.307168000
1   -0.837082000   1.129340000   2.412793000
8   -1.717758000   -0.177726000   -2.082542000
8   -1.138383000   -0.298274000   0.104101000
6   -1.994021000   -0.272164000   -0.862104000
8   3.113944000   -2.542258000   0.995690000
8   2.953734000   -2.836169000   -1.257330000
6   4.559765000   -2.830000000   0.945550000
6   5.090491000   -2.680830000   2.350625000
6   2.485305000   -2.480683000   -0.186093000
6   1.156570000   -1.820618000   0.033948000
1   4.686605000   -3.849208000   0.552288000
1   5.015931000   -2.114415000   0.244858000
1   6.166728000   -2.910416000   2.352231000
1   4.959559000   -1.652526000   2.716402000
1   4.588963000   -3.375645000   3.040045000
1   0.556745000   -2.318382000   0.813197000
7   0.205147000   -2.667447000   -1.340981000
7   -0.494841000   -2.792853000   -2.187416000
6   -3.444820000   -0.373245000   -0.441305000
6   -3.817345000   -0.348057000   0.911866000
6   -4.444468000   -0.481601000   -1.423772000
6   -5.160829000   -0.427064000   1.277105000
6   -5.784628000   -0.561717000   -1.061594000
6   -6.162781000   -0.534873000   0.294538000
1   -3.048482000   -0.262091000   1.680742000
1   -4.155987000   -0.500701000   -2.475952000
1   -5.423513000   -0.401009000   2.335325000
1   -6.557065000   -0.647103000   -1.827970000
6   -7.615240000   -0.619055000   0.647528000
8   -8.473937000   -0.663720000   -0.241819000
6   -8.014551000   -0.647475000   2.100333000
1   -9.106399000   -0.712665000   2.179459000
1   -7.553753000   -1.507517000   2.611838000
1   -7.661617000   0.259704000   2.616036000

2a-Carbene-OBz-COMe
7   -0.645712000   2.069436000   0.329627000
6   -0.653766000   2.958283000   -0.677997000
27 -0.851763000   0.179248000   -0.084153000
7   -0.908157000   0.013978000   1.912682000
6   -0.619567000   4.323951000   -0.408973000
1   -0.632905000   5.044689000   -1.226826000
7   -1.183803000   0.920405000   -1.944789000
6   -0.566019000   4.735276000   0.927573000
1   -0.552602000   5.799780000   1.167353000
6   -0.519538000   3.789804000   1.956955000
1   -0.454547000   4.090564000   3.002784000
6   -0.554813000   2.438970000   1.617395000
6   -0.394582000   1.274385000   2.543529000
1   0.682662000   1.125278000   2.721156000
1   -0.877964000   1.440230000   3.516070000
1   -0.203619000   -0.720865000   2.099780000
6   -2.284911000   -0.392065000   2.367406000
1   -2.468092000   -0.012906000   3.383144000
1   -2.295710000   -1.491611000   2.405360000
6   -3.271540000   0.098588000   1.347080000
6   -2.706613000   0.342661000   0.096748000
6   -3.449456000   0.741453000   -1.010154000
6   -4.832537000   0.905083000   -0.859091000

1	-5.450252000	1.211479000	-1.707124000
6	-5.421746000	0.666518000	0.392799000
1	-6.499720000	0.796954000	0.509344000
6	-4.655027000	0.262801000	1.496997000
1	-5.134651000	0.077177000	2.461533000
6	-2.660354000	0.852668000	-2.280537000
1	-2.935776000	1.721702000	-2.895337000
1	-2.803977000	-0.052388000	-2.888907000
1	-0.679918000	0.343620000	-2.625727000
6	-0.597813000	2.299961000	-2.021845000
1	-1.093881000	2.888056000	-2.806519000
1	0.461338000	2.185405000	-2.299799000
8	1.603482000	-1.150537000	1.490981000
8	1.165027000	0.112095000	-0.339097000
6	1.956489000	-0.516278000	0.463654000
8	-2.941515000	-2.280362000	-1.623561000
8	-2.391500000	-3.054299000	0.454086000
6	-4.246343000	-2.977923000	-1.576797000
6	-5.007202000	-2.557131000	-2.810786000
6	-2.176023000	-2.372934000	-0.548938000
6	-0.966330000	-1.541599000	-0.528752000
1	-4.047172000	-4.058799000	-1.546484000
1	-4.750564000	-2.674781000	-0.647693000
1	-5.977158000	-3.076469000	-2.826574000
1	-5.195173000	-1.473606000	-2.806277000
1	-4.458051000	-2.825009000	-3.725222000
1	-0.036475000	-2.093523000	-0.748067000
7	0.206818000	-3.875259000	1.938571000
7	-0.175226000	-3.538306000	2.915990000
6	3.423751000	-0.455849000	0.100612000
6	4.373345000	-1.068284000	0.932656000
6	3.856639000	0.212890000	-1.058259000
6	5.730683000	-1.012292000	0.618946000
6	5.210060000	0.268912000	-1.373163000
6	6.166439000	-0.340127000	-0.538202000
1	4.038324000	-1.587927000	1.831642000
1	3.122123000	0.688663000	-1.709066000
1	6.448957000	-1.493825000	1.283586000
1	5.545668000	0.788632000	-2.272405000
6	7.614874000	-0.248352000	-0.906360000
8	7.962940000	0.359733000	-1.925613000
6	8.639548000	-0.904016000	-0.017713000
1	8.589211000	-0.490563000	1.002121000
1	8.444754000	-1.985234000	0.064340000
1	9.641968000	-0.741344000	-0.431705000

1	-0.950443000	1.622253000	3.362941000
6	-2.299508000	-0.356923000	2.259466000
1	-2.641172000	0.260570000	3.103417000
1	-2.157927000	-1.379125000	2.639410000
6	-3.260262000	-0.347717000	1.104475000
6	-2.673630000	-0.116762000	-0.138962000
6	-3.407468000	-0.136625000	-1.326475000
6	-4.783817000	-0.387255000	-1.270979000
1	-5.383012000	-0.409456000	-2.185416000
6	-5.388969000	-0.618608000	-0.024374000
1	-6.461833000	-0.817619000	0.022862000
6	-4.636803000	-0.607146000	1.161369000
1	-5.125793000	-0.801888000	2.119994000
6	-2.551550000	0.049081000	-2.546060000
1	-3.052315000	0.568478000	-3.377531000
1	-2.215807000	-0.931606000	-2.918052000
6	-1.455263000	2.293474000	-2.237630000
1	-2.311925000	2.549558000	-2.877392000
1	-0.551690000	2.684511000	-2.729822000
6	1.799202000	-0.335438000	-0.312862000
6	3.272161000	-0.311651000	-0.226169000
6	3.917981000	0.922869000	-0.027077000
1	3.323876000	1.833362000	0.062521000
6	5.303407000	0.973285000	0.054072000
1	5.811179000	1.926585000	0.208009000
6	6.070646000	-0.202253000	-0.056813000
6	5.418007000	-1.433335000	-0.249440000
1	5.989175000	-2.357743000	-0.337552000
6	4.028829000	-1.490569000	-0.336226000
1	3.529792000	-2.447376000	-0.490610000
6	-0.220272000	-1.525854000	-0.651777000
1	-0.381709000	-1.775196000	-1.710302000
6	-0.795409000	-2.548859000	0.249399000
6	-2.761793000	-3.875907000	0.608600000
1	-2.951111000	-3.290618000	1.521222000
1	-2.213643000	-4.789951000	0.883738000
6	-4.038669000	-4.174092000	-0.142583000
1	-3.837515000	-4.759269000	-1.052302000
1	-4.548865000	-3.240674000	-0.423375000
1	-4.712407000	-4.759189000	0.501517000
6	7.566232000	-0.101780000	0.030088000
8	8.106003000	1.003834000	0.138785000
6	8.386477000	-1.362229000	-0.020134000
1	8.086388000	-2.052656000	0.784035000
1	8.223027000	-1.889370000	-0.973933000
1	9.449519000	-1.113450000	0.083030000

4a-OBz-COMe

27	-0.874401000	0.305813000	-0.220970000
8	1.107465000	0.705002000	-0.253394000
8	1.249981000	-1.531015000	-0.451199000
8	-0.366799000	-2.838667000	1.368545000
8	-1.919692000	-3.077383000	-0.283011000
7	-1.237612000	2.126686000	0.131931000
7	-0.945081000	0.143450000	1.789181000
1	-0.232983000	-0.517066000	2.121797000
7	-1.308471000	0.797318000	-2.127103000
1	-0.547225000	0.518166000	-2.754731000
6	-1.568892000	2.938182000	-0.885166000
6	-1.895110000	4.271025000	-0.634203000
1	-2.170118000	4.931652000	-1.457125000
6	-1.854700000	4.730989000	0.685785000
1	-2.117310000	5.766782000	0.907406000
6	-1.466895000	3.872902000	1.723389000
1	-1.406847000	4.220199000	2.755121000
6	-1.150866000	2.555415000	1.407049000
6	-0.603829000	1.499968000	2.326520000
1	0.494561000	1.581697000	2.321719000

TS2-OBz-COMe

7	-1.118975000	-2.264268000	-0.268667000
6	-1.276173000	-3.121531000	0.756057000
27	-0.841722000	-0.423001000	0.116693000
7	-1.206170000	-0.195601000	-1.856336000
6	-1.674336000	-4.435060000	0.515048000
1	-1.809928000	-5.130065000	1.344333000
7	-0.986517000	-1.020972000	2.045443000
6	-1.890609000	-4.832947000	-0.809727000
1	-2.211785000	-5.853695000	-1.023911000
6	-1.693745000	-3.929421000	-1.862453000
1	-1.846027000	-4.226321000	-2.900610000
6	-1.298438000	-2.631399000	-1.552876000
6	-0.949039000	-1.522822000	-2.506766000
1	0.132947000	-1.573745000	-2.706973000
1	-1.476411000	-1.606566000	-3.467477000
1	-0.539677000	0.485947000	-2.236048000
6	-2.603907000	0.343397000	-2.103161000
1	-3.105194000	-0.281830000	-2.856331000
1	-2.512137000	1.351311000	-2.533848000

6	-3.386434000	0.357458000	-0.820535000		1	1.988816000	2.392601000	1.744450000
6	-2.629752000	0.133935000	0.345098000		6	3.185610000	1.011576000	0.536811000
6	-3.219643000	-0.076466000	1.606144000		6	2.591384000	0.960578000	-0.776701000
6	-4.603953000	0.037775000	1.719233000		6	3.223249000	0.071641000	-1.726207000
1	-5.103361000	-0.127257000	2.676831000		6	4.510854000	-0.394557000	-1.506904000
6	-5.360951000	0.340513000	0.573093000		1	4.970525000	-1.062943000	-2.237862000
1	-6.444972000	0.436030000	0.665085000		6	5.179956000	-0.089843000	-0.311455000
6	-4.770974000	0.473477000	-0.695559000		1	6.196834000	-0.450977000	-0.147542000
1	-5.398342000	0.637272000	-1.574922000		6	4.483909000	0.530578000	0.726698000
6	-2.246988000	-0.467214000	2.682292000		1	4.927750000	0.590285000	1.722758000
1	-2.673452000	-1.206975000	3.375136000		6	2.313050000	-0.570580000	-2.740403000
1	-1.956934000	0.406469000	3.285388000		1	2.849816000	-1.286510000	-3.376585000
1	-0.187666000	-0.654507000	2.573427000		1	1.808280000	0.149153000	-3.397240000
6	-0.889650000	-2.523840000	2.080310000		1	0.335220000	-1.177004000	-2.367463000
1	-1.478868000	-2.935728000	2.911653000		6	1.557839000	-2.722423000	-1.633737000
1	0.167086000	-2.771880000	2.265879000		1	2.395991000	-3.070608000	-2.253606000
8	1.230508000	1.626990000	0.747853000		1	0.671468000	-3.307852000	-1.923909000
8	1.120649000	-0.512803000	-0.016580000		8	-1.397652000	-0.487195000	-2.238082000
6	1.752486000	0.555510000	0.333712000		8	-0.843467000	-0.414297000	-0.036542000
8	-2.089023000	3.400501000	0.146445000		6	-1.688615000	-0.417804000	-1.021822000
8	-0.649807000	2.631256000	-1.432601000		8	1.530096000	3.637056000	-0.111842000
6	-2.415119000	4.551653000	-0.707826000		8	-0.579457000	2.870160000	-0.459872000
6	-3.511928000	5.324273000	-0.012870000		6	0.976873000	4.861476000	0.477983000
6	-1.226534000	2.499854000	-0.358489000		6	2.145335000	5.687134000	0.966289000
6	-1.076399000	1.317690000	0.562650000		6	0.638220000	2.702639000	-0.513169000
1	-1.499009000	5.146372000	-0.841636000		6	1.258001000	1.482830000	-1.079753000
1	-2.732145000	4.167141000	-1.689056000		1	0.391891000	5.380676000	-0.296145000
1	-3.788783000	6.193770000	-0.627781000		1	0.297716000	4.576367000	1.295544000
1	-4.406914000	4.699309000	0.123191000		1	1.768967000	6.621697000	1.408807000
1	-3.179244000	5.689431000	0.969879000		1	2.717402000	5.148209000	1.736020000
1	-1.154703000	1.643134000	1.609002000		1	2.821688000	5.945881000	0.138190000
6	3.254753000	0.482329000	0.230313000		1	0.915427000	1.389885000	-2.114653000
6	4.026822000	1.650267000	0.358990000		6	-3.130557000	-0.338190000	-0.588936000
6	3.896203000	-0.747420000	0.012932000		6	-3.481300000	-0.178800000	0.763772000
6	5.413167000	1.587172000	0.269574000		6	-4.142370000	-0.421417000	-1.557574000
6	5.286197000	-0.810748000	-0.068175000		6	-4.819132000	-0.106317000	1.135553000
6	6.062637000	0.356057000	0.058613000		6	-5.483383000	-0.348850000	-1.184390000
1	3.528099000	2.606150000	0.524854000		6	-5.838932000	-0.190711000	0.167891000
1	3.299662000	-1.655014000	-0.086491000		1	-2.697541000	-0.109004000	1.518742000
1	6.012309000	2.494591000	0.364660000		1	-3.869408000	-0.543110000	-2.606831000
1	5.762908000	-1.777917000	-0.230756000		1	-5.092579000	0.019268000	2.184744000
6	7.557878000	0.326615000	-0.021529000		1	-6.251338000	-0.415869000	-1.955809000
8	8.209850000	1.370639000	0.096560000		6	-7.267522000	-0.103804000	0.608562000
6	8.252884000	-0.991826000	-0.242485000		8	-7.543359000	0.037994000	1.805802000
1	8.014348000	-1.693428000	0.572781000		6	-8.359542000	-0.189211000	-0.425506000
1	7.911148000	-1.459329000	-1.179482000		1	-8.253216000	0.614675000	-1.171198000
1	9.337033000	-0.832080000	-0.283654000		1	-8.299938000	-1.143648000	-0.972556000
					1	-9.336681000	-0.107635000	0.065534000

INT-MI-OBz-COMe

7	1.507512000	-1.918379000	0.617128000		**4a-OAc-Na**			
6	1.839895000	-2.955812000	-0.173096000		7	-2.204015000	0.284227000	0.173545000
27	1.052688000	-0.283006000	-0.191178000		6	-3.097491000	-0.134837000	-0.738797000
7	1.113987000	0.457249000	1.665274000		27	-0.393783000	0.477299000	-0.335323000
6	2.358434000	-4.118654000	0.394529000		7	-0.094822000	0.686906000	1.653602000
1	2.630715000	-4.964217000	-0.237995000		6	-4.413462000	-0.394096000	-0.358017000
7	1.265665000	-1.275070000	-1.919459000		1	-5.137854000	-0.744097000	-1.094065000
6	2.524677000	-4.167126000	1.782675000		7	-1.042497000	-0.182260000	-2.126247000
1	2.940279000	-5.062956000	2.247007000		6	-4.773093000	-0.194584000	0.978591000
6	2.166433000	-3.073156000	2.581704000		1	-5.793908000	-0.403815000	1.302760000
1	2.290035000	-3.097525000	3.664707000		6	-3.832798000	0.280848000	1.901036000
6	1.646209000	-1.943551000	1.958761000		1	-4.099497000	0.462098000	2.942617000
6	1.122325000	-0.700208000	2.625541000		6	-2.535777000	0.520016000	1.458486000
1	0.075761000	-0.881925000	2.914637000		6	-1.405005000	1.124968000	2.238518000
1	1.682574000	-0.447645000	3.536956000		1	-1.460558000	2.218865000	2.121975000
1	0.271390000	1.012364000	1.851081000		1	-1.461119000	0.893745000	3.311843000
6	2.324573000	1.350714000	1.731867000		1	0.589003000	1.422480000	1.859639000
1	2.877327000	1.164279000	2.661807000		6	0.424288000	-0.602708000	2.263731000

1	-0.061430000	-0.771727000	3.236723000
1	1.498665000	-0.459733000	2.452968000
6	0.209892000	-1.727542000	1.292210000
6	-0.097378000	-1.318554000	-0.003833000
6	-0.242840000	-2.220175000	-1.058763000
6	-0.092582000	-3.588978000	-0.805726000
1	-0.198001000	-4.319196000	-1.612821000
6	0.208443000	-4.017577000	0.497798000
1	0.328111000	-5.084484000	0.698159000
6	0.370985000	-3.096908000	1.545334000
1	0.624431000	-3.448883000	2.549190000
6	-0.450552000	-1.547529000	-2.383713000
1	-1.081406000	-2.112562000	-3.086673000
1	0.523461000	-1.376808000	-2.869062000
1	-0.733332000	0.442090000	-2.878790000
6	-2.547645000	-0.179178000	-2.135284000
1	-2.934533000	-1.038990000	-2.700355000
1	-2.873674000	0.734044000	-2.656916000
8	1.591303000	2.407774000	-0.851357000
8	-0.648853000	2.471857000	-0.681421000
6	0.433794000	3.069537000	-0.807150000
6	0.552681000	4.552819000	-0.879361000
1	1.381947000	4.851162000	-1.532719000
1	0.753300000	4.935892000	0.135409000
1	-0.394762000	4.980748000	-1.226279000
8	2.813348000	-0.920850000	-0.586038000
8	3.059456000	0.832766000	0.827862000
6	3.693661000	-1.729308000	0.266882000
6	3.800329000	-3.090063000	-0.379390000
6	2.518253000	0.311993000	-0.163137000
6	1.443929000	0.927046000	-0.961604000
1	4.665937000	-1.219752000	0.339987000
1	3.241498000	-1.779839000	1.269063000
1	4.439923000	-3.735710000	0.240921000
1	2.809426000	-3.559838000	-0.463368000
1	4.248486000	-3.018527000	-1.381486000
1	1.548857000	0.686715000	-2.029953000
11	3.460971000	3.003039000	1.085401000

TS-Na

7	-2.145297000	-0.080749000	0.413953000
6	-3.101345000	-0.248239000	-0.513497000
27	-0.395271000	0.467435000	-0.152018000
7	0.083994000	0.055510000	1.778069000
6	-4.343295000	-0.764023000	-0.147490000
1	-5.121452000	-0.908914000	-0.897192000
7	-1.211438000	0.305608000	-2.010549000
6	-4.560685000	-1.078200000	1.198751000
1	-5.520136000	-1.495362000	1.509095000
6	-3.562828000	-0.846220000	2.153349000
1	-3.726857000	-1.057502000	3.210227000
6	-2.344902000	-0.329056000	1.719943000
6	-1.190467000	0.119281000	2.568398000
1	-1.355305000	1.176535000	2.828612000
1	-1.103765000	-0.452213000	3.503017000
1	0.711922000	0.773645000	2.155010000
6	0.780691000	-1.287820000	1.892533000
1	0.406441000	-1.818088000	2.780033000
1	1.850244000	-1.096322000	2.063471000
6	0.568961000	-2.074859000	0.631619000
6	0.151320000	-1.326482000	-0.472823000
6	-0.148490000	-1.888374000	-1.716702000
6	0.021511000	-3.267897000	-1.875364000
1	-0.208955000	-3.750740000	-2.828083000
6	0.475066000	-4.031568000	-0.788025000
1	0.608556000	-5.108076000	-0.913329000
6	0.733959000	-3.451831000	0.466520000

1	1.046016000	-4.078634000	1.305263000
6	-0.662034000	-0.908449000	-2.733236000
1	-1.439724000	-1.339040000	-3.380277000
1	0.150732000	-0.561811000	-3.388672000
1	-0.972999000	1.136616000	-2.562556000
6	-2.706635000	0.285883000	-1.860033000
1	-3.177208000	-0.265066000	-2.686065000
1	-3.048988000	1.330893000	-1.915217000
8	0.841165000	3.199493000	-0.828398000
8	-1.001689000	2.319228000	0.146876000
6	-0.273969000	3.305580000	-0.245746000
6	-0.817324000	4.686847000	0.060300000
1	-1.899448000	4.662777000	0.236088000
1	-0.573692000	5.378334000	-0.756746000
1	-0.323000000	5.053295000	0.974634000
8	3.129580000	-0.763880000	-0.140513000
8	3.138086000	1.434950000	0.394145000
6	4.412904000	-0.956414000	0.569020000
6	4.668590000	-2.444086000	0.601476000
6	2.597089000	0.449257000	-0.115538000
6	1.272871000	0.540813000	-0.795496000
1	5.183475000	-0.400298000	0.015857000
1	4.310773000	-0.523290000	1.574624000
1	5.617078000	-2.633313000	1.126121000
1	3.864639000	-2.969532000	1.137233000
1	4.746990000	-2.855804000	-0.415017000
1	1.428650000	0.635075000	-1.884569000
11	2.858585000	3.650938000	-0.011095000

INT-MI-Na

7	2.087973000	0.172297000	-0.565677000
6	3.042850000	0.561688000	0.299400000
27	0.287928000	0.358948000	-0.055993000
7	-0.112973000	-0.650186000	-1.737348000
6	4.375616000	0.246801000	0.045614000
1	5.154014000	0.551272000	0.745622000
7	1.036164000	1.162670000	1.630229000
6	4.681781000	-0.463658000	-1.120888000
1	5.717537000	-0.732720000	-1.334288000
6	3.670760000	-0.827123000	-2.019239000
1	3.896135000	-1.367151000	-2.939173000
6	2.357836000	-0.482914000	-1.711049000
6	1.139928000	-0.679051000	-2.571440000
1	1.081178000	0.169765000	-3.269824000
1	1.193071000	-1.600420000	-3.167615000
1	-0.835461000	-0.155582000	-2.271523000
6	-0.633876000	-2.007488000	-1.341694000
1	-0.215907000	-2.779490000	-2.000699000
1	-1.720156000	-2.005004000	-1.464948000
6	-0.191783000	-2.233100000	0.082778000
6	-0.446646000	-1.210155000	1.067072000
6	0.499083000	-1.119132000	2.154833000
6	1.366748000	-2.169476000	2.423862000
1	2.071889000	-2.084254000	3.253019000
6	1.394540000	-3.293245000	1.587926000
1	2.069466000	-4.121664000	1.810012000
6	0.681965000	-3.276749000	0.385552000
1	0.859995000	-4.051384000	-0.363230000
6	0.692756000	0.240835000	2.774939000
1	1.504651000	0.234039000	3.513787000
1	-0.206149000	0.625965000	3.273358000
1	0.575336000	2.071258000	1.770628000
6	2.510333000	1.391106000	1.436395000
1	3.059210000	1.206689000	2.370125000
1	2.642787000	2.452836000	1.176462000
8	-0.892335000	3.233931000	0.590786000
8	0.081154000	1.994379000	-1.031144000

6	-0.424426000	3.089909000	-0.569701000
6	-0.420325000	4.251544000	-1.538498000
1	-0.070256000	3.957030000	-2.534788000
1	0.236711000	5.037813000	-1.135798000
1	-1.435306000	4.670413000	-1.605942000
8	-3.205547000	-1.374567000	-0.043380000
8	-3.442611000	0.861761000	0.159817000
6	-4.532012000	-1.443981000	-0.674237000
6	-4.782664000	-2.895986000	-1.010102000
6	-2.751378000	-0.162266000	0.296744000
6	-1.413137000	-0.116298000	0.902722000
1	-5.269617000	-1.045480000	0.037959000
1	-4.520681000	-0.802460000	-1.567792000
1	-5.777641000	-2.994029000	-1.469559000
1	-4.036101000	-3.274442000	-1.723613000
1	-4.758539000	-3.520752000	-0.105230000
1	-1.484276000	0.555496000	1.761976000
11	-3.074279000	2.944143000	0.967991000

4a-OAc-K

7	2.123933000	-0.956127000	0.240925000
6	3.144017000	-0.908687000	-0.632097000
27	0.391216000	-0.490959000	-0.346214000
7	-0.045668000	-0.554437000	1.624861000
6	4.442839000	-1.176058000	-0.200795000
1	5.273735000	-1.132306000	-0.905703000
7	1.304120000	-0.125553000	-2.104290000
6	4.645234000	-1.503754000	1.143579000
1	5.654415000	-1.705189000	1.506694000
6	3.558436000	-1.587399000	2.023449000
1	3.694628000	-1.865268000	3.068923000
6	2.286889000	-1.310190000	1.531156000
6	0.977708000	-1.451032000	2.255033000
1	0.626568000	-2.486545000	2.121678000
1	1.069394000	-1.258426000	3.333729000
1	-0.967773000	-0.974574000	1.784712000
6	-0.063782000	0.837826000	2.230106000
1	0.448091000	0.819241000	3.203841000
1	-1.116133000	1.095720000	2.418649000
6	0.552134000	1.805087000	1.260406000
6	0.732723000	1.299353000	-0.025495000
6	1.220508000	2.080038000	-1.074512000
6	1.554442000	3.416910000	-0.826139000
1	1.937176000	4.053465000	-1.628663000
6	1.387328000	3.937930000	0.467780000
1	1.647418000	4.980163000	0.664796000
6	0.881229000	3.144474000	1.510020000
1	0.743157000	3.572574000	2.506761000
6	1.234788000	1.356366000	-2.389267000
1	2.050957000	1.655660000	-3.064472000
1	0.283191000	1.526517000	-2.917943000
1	0.827815000	-0.613928000	-2.869912000
6	2.712390000	-0.655593000	-2.048129000
1	3.404462000	0.020810000	-2.569651000
1	2.726296000	-1.617486000	-2.583507000
8	-2.094878000	-1.623720000	-1.056171000
8	-0.038517000	-2.453596000	-0.687700000
6	-1.244784000	-2.639674000	-0.928317000
6	-1.851418000	-3.995537000	-1.056218000
1	-2.741939000	-3.980473000	-1.696388000
1	-2.133645000	-4.351747000	-0.050875000
1	-1.103119000	-4.691554000	-1.454598000
8	-2.158157000	1.901386000	-0.613463000
8	-2.983649000	0.262707000	0.725391000
6	-2.732169000	2.919695000	0.273657000
6	-2.340980000	4.265409000	-0.290698000
6	-2.289046000	0.621283000	-0.238809000
6	-1.455484000	-0.274594000	-1.061730000

1	-3.822817000	2.777113000	0.302481000
1	-2.326364000	2.760192000	1.283924000
1	-2.737313000	5.059708000	0.359581000
1	-1.246566000	4.366804000	-0.333961000
1	-2.753818000	4.408446000	-1.300278000
1	-1.434916000	0.045612000	-2.113460000
19	-4.639938000	-1.765324000	0.708873000

TS-K

7	-2.213055000	0.688027000	0.391475000
6	-3.152219000	0.851690000	-0.554561000
27	-0.383803000	0.525643000	-0.146889000
7	-0.107365000	0.008922000	1.795024000
6	-4.501985000	0.819861000	-0.208788000
1	-5.269268000	0.943000000	-0.973173000
7	-1.168284000	0.638891000	-2.018458000
6	-4.837968000	0.631441000	1.136733000
1	-5.887869000	0.590361000	1.431594000
6	-3.837840000	0.505448000	2.108950000
1	-4.083386000	0.381523000	3.163922000
6	-2.508985000	0.544433000	1.695295000
6	-1.281916000	0.545389000	2.561327000
1	-1.047891000	1.591831000	2.812407000
1	-1.426580000	-0.005340000	3.501291000
1	0.734481000	0.461221000	2.168801000
6	0.065572000	-1.493116000	1.938186000
1	-0.483361000	-1.842887000	2.824496000
1	1.132032000	-1.689676000	2.129296000
6	-0.394218000	-2.178237000	0.682671000
6	-0.498854000	-1.347690000	-0.439506000
6	-0.965757000	-1.786807000	-1.683160000
6	-1.296339000	-3.137964000	-1.824248000
1	-1.671345000	-3.522985000	-2.775471000
6	-1.158501000	-3.994360000	-0.719871000
1	-1.414690000	-5.049997000	-0.831017000
6	-0.729809000	-3.524723000	0.534987000
1	-0.675212000	-4.209454000	1.384627000
6	-1.084419000	-0.703531000	-2.717609000
1	-1.959753000	-0.837597000	-3.368844000
1	-0.197033000	-0.683565000	-3.367563000
1	-0.631791000	1.317247000	-2.570074000
6	-2.570832000	1.167548000	-1.903533000
1	-3.197944000	0.797550000	-2.726670000
1	-2.509302000	2.263422000	-1.992921000
8	1.864278000	2.471022000	-0.856847000
8	-0.193218000	2.469872000	0.096197000
6	0.889340000	3.046571000	-0.302656000
6	0.966857000	4.537107000	-0.026947000
1	-0.034212000	4.975885000	0.067455000
1	1.535518000	5.045850000	-0.815832000
1	1.496027000	4.682803000	0.929184000
8	2.474624000	-1.970662000	-0.183626000
8	3.108527000	0.023863000	0.690066000
6	3.527726000	-2.669699000	0.579143000
6	3.282482000	-4.149119000	0.401880000
6	2.351583000	-0.658016000	-0.002376000
6	1.190684000	-0.080749000	-0.750713000
1	4.499554000	-2.347589000	0.177251000
1	3.453103000	-2.352175000	1.629848000
1	4.056712000	-4.709611000	0.947002000
1	2.299207000	-4.436073000	0.802150000
1	3.331474000	-4.434558000	-0.658959000
1	1.393002000	-0.108087000	-1.834997000
19	4.346381000	2.322634000	-0.013770000

INT-MI-K

7	2.207590000	0.461627000	-0.514588000

6	2.983265000	1.141330000	0.353733000
27	0.374174000	0.296689000	-0.127379000
7	0.316424000	-0.887911000	-1.749483000
6	4.367615000	1.112514000	0.215555000
1	5.001266000	1.652477000	0.919611000
7	0.813185000	1.356257000	1.519084000
6	4.916157000	0.377754000	-0.843240000
1	5.999341000	0.333054000	-0.967404000
6	4.085903000	-0.297078000	-1.744966000
1	4.497272000	-0.862509000	-2.581627000
6	2.707533000	-0.233073000	-1.552917000
6	1.649526000	-0.814233000	-2.449777000
1	1.528375000	-0.146526000	-3.316117000
1	1.937953000	-1.803473000	-2.831452000
1	-0.400974000	-0.542494000	-2.395638000
6	-0.062532000	-2.267754000	-1.282128000
1	0.454857000	-3.030010000	-1.879808000
1	-1.138656000	-2.391328000	-1.426759000
6	0.362661000	-2.331084000	0.163191000
6	-0.119446000	-1.313987000	1.066834000
6	0.757848000	-0.961921000	2.156536000
6	1.818012000	-1.791214000	2.507434000
1	2.466683000	-1.508691000	3.338913000
6	2.098838000	-2.934900000	1.752712000
1	2.926595000	-3.587342000	2.036264000
6	1.424434000	-3.147760000	0.545069000
1	1.778537000	-3.913236000	-0.148577000
6	0.646718000	0.438613000	2.704368000
1	1.425779000	0.635027000	3.451671000
1	-0.324193000	0.646522000	3.173377000
1	0.126749000	2.123338000	1.561694000
6	2.186008000	1.937226000	1.351045000
1	2.699514000	2.026492000	2.318514000
1	2.055303000	2.953871000	0.947569000
8	-1.311645000	2.960224000	0.311040000
8	-0.130334000	1.781097000	-1.221823000
6	-0.838376000	2.797388000	-0.841971000
6	-1.108221000	3.805188000	-1.940633000
1	-2.048939000	3.526902000	-2.443660000
1	-0.309314000	3.800636000	-2.693060000
1	-1.226633000	4.809177000	-1.513208000
8	-2.765617000	-2.086355000	-0.050385000
8	-3.392458000	0.086188000	-0.119701000
6	-4.032887000	-2.458642000	-0.693101000
6	-4.030906000	-3.963868000	-0.828732000
6	-2.545697000	-0.776875000	0.152547000
6	-1.262926000	-0.436577000	0.789993000
1	-4.856903000	-2.096513000	-0.060447000
1	-4.085719000	-1.948944000	-1.666992000
1	-4.971398000	-4.286293000	-1.300033000
1	-3.196169000	-4.304771000	-1.458699000
1	-3.953723000	-4.448909000	0.155588000
1	-1.495063000	0.271278000	1.589436000
19	-3.872335000	2.545071000	0.789613000

Ethyl 2-diazo-2-(4-nitrophenyl)acetate (l)

8	-3.458575000	-0.073922000	-0.039258000
8	-1.995327000	-1.803407000	0.200791000
6	-4.582881000	-1.009693000	0.084245000
6	-5.847479000	-0.185007000	0.010927000
6	-2.222451000	-0.608011000	0.052100000
6	-1.178225000	0.431416000	-0.035004000
1	-4.512246000	-1.742324000	-0.733678000
1	-4.484302000	-1.540522000	1.043026000
1	-6.718932000	-0.849491000	0.107986000
1	-5.883474000	0.552843000	0.825972000
1	-5.921138000	0.343126000	-0.951095000

7	-1.634241000	1.672981000	-0.114643000
7	-2.025214000	2.735344000	-0.187043000
6	0.270886000	0.241601000	-0.021406000
6	1.135147000	1.353534000	0.133616000
6	0.842239000	-1.043691000	-0.175667000
6	2.511094000	1.192525000	0.142631000
6	2.220386000	-1.209590000	-0.163697000
6	3.048599000	-0.092917000	-0.002204000
1	0.731131000	2.359500000	0.257237000
1	0.202064000	-1.911912000	-0.312186000
1	3.168293000	2.052229000	0.266730000
1	2.654451000	-2.201107000	-0.287338000
7	4.494065000	-0.268602000	0.014504000
8	4.956742000	-1.416523000	-0.111145000
8	5.214409000	0.736175000	0.154659000

Adduct (2a-OAc + l)

7	-2.585120000	-0.697499000	0.754206000
6	-2.491242000	-1.673363000	1.692121000
27	-1.066806000	-0.168436000	-0.079250000
7	-2.241248000	1.041586000	-1.160032000
6	-3.637658000	-2.122931000	2.333752000
1	-3.558216000	-2.900243000	3.094143000
7	-0.157109000	-1.112080000	1.441139000
6	-4.873589000	-1.570706000	1.976686000
1	-5.785405000	-1.910662000	2.469763000
6	-4.940954000	-0.593524000	0.982420000
1	-5.892537000	-0.162511000	0.669681000
6	-3.763510000	-0.164568000	0.372679000
6	-3.667216000	0.839912000	-0.730537000
1	-4.251827000	0.493034000	-1.594703000
1	-4.096717000	1.797845000	-0.404024000
1	-2.184569000	0.725330000	-2.137950000
6	-1.778793000	2.465877000	-1.014034000
1	-2.621238000	3.161285000	-1.149424000
1	-1.061859000	2.666140000	-1.823367000
6	-1.106378000	2.584993000	0.326383000
6	-0.777265000	1.358024000	0.911571000
6	-0.075419000	1.252167000	2.112338000
6	0.333405000	2.430080000	2.751698000
1	0.902770000	2.388828000	3.683902000
6	0.004167000	3.670258000	2.181921000
1	0.319361000	4.587504000	2.683405000
6	-0.706308000	3.759733000	0.973294000
1	-0.931199000	4.737624000	0.540003000
6	0.165422000	-0.156130000	2.575638000
1	-0.487998000	-0.399980000	3.426882000
1	1.202156000	-0.329738000	2.897469000
1	0.715658000	-1.547312000	1.124164000
6	-1.096708000	-2.199650000	1.843214000
1	-0.889399000	-2.566549000	2.858613000
1	-0.958573000	-3.033167000	1.137609000
8	-2.471088000	-1.244806000	-2.825394000
8	-0.892361000	-1.732362000	-1.277278000
6	-1.501271000	-1.921480000	-2.407971000
6	-0.928226000	-3.030787000	-3.270541000
1	-0.314506000	-3.728895000	-2.687472000
1	-0.293537000	-2.568338000	-4.044373000
1	-1.736149000	-3.569573000	-3.784546000
8	2.426923000	2.705491000	-0.375545000
8	1.192659000	3.253689000	-2.205164000
6	2.688203000	4.131153000	-0.128137000
6	3.481231000	4.214526000	1.154440000
6	1.682850000	2.417413000	-1.448090000
6	1.518134000	0.959466000	-1.652202000
1	3.240279000	4.528381000	-0.992919000
1	1.719969000	4.646392000	-0.056871000

1	3.700214000	5.270595000	1.372328000
1	2.911393000	3.799271000	1.998136000
1	4.435385000	3.674388000	1.067510000
7	0.783136000	0.700009000	-2.729426000
7	0.151144000	0.502405000	-3.648217000
6	2.127870000	-0.186419000	-0.973046000
6	2.716440000	-0.062384000	0.308191000
6	2.125274000	-1.459235000	-1.593899000
6	3.281612000	-1.164466000	0.937550000
6	2.680825000	-2.562793000	-0.967990000
6	3.259805000	-2.409264000	0.298372000
1	2.708694000	0.892781000	0.825028000
1	1.678788000	-1.595095000	-2.578566000
1	3.724801000	-1.063217000	1.927224000
1	2.670003000	-3.537327000	-1.453795000
7	3.834001000	-3.568434000	0.968548000
8	3.821396000	-4.662628000	0.378242000
8	4.312494000	-3.420177000	2.106818000

TS1

7	2.305468000	-1.179508000	-0.829669000
6	2.173541000	-1.381781000	-2.154829000
27	0.842818000	-0.416878000	0.133101000
7	2.170240000	-0.460668000	1.680493000
6	3.244510000	-1.858686000	-2.904313000
1	3.131788000	-2.013380000	-3.977569000
7	0.099298000	-0.153673000	-1.752816000
6	4.448938000	-2.134219000	-2.247859000
1	5.308432000	-2.495635000	-2.814808000
6	4.547545000	-1.961475000	-0.865117000
1	5.464976000	-2.197547000	-0.325322000
6	3.437064000	-1.483577000	-0.170680000
6	3.306272000	-1.369397000	1.311322000
1	3.053104000	-2.366429000	1.703078000
1	4.239919000	-1.041255000	1.788987000
1	1.725408000	-0.897734000	2.496988000
6	2.638836000	0.931258000	2.012960000
1	3.647159000	0.897404000	2.452120000
1	1.953463000	1.329151000	2.773742000
6	2.554916000	1.747415000	0.756714000
6	1.642441000	1.255560000	-0.176747000
6	1.387704000	1.901544000	-1.384513000
6	2.077769000	3.084195000	-1.676791000
1	1.896222000	3.614538000	-2.615380000
6	3.003216000	3.590152000	-0.749992000
1	3.543996000	4.510762000	-0.979751000
6	3.241971000	2.935013000	0.467235000
1	3.960196000	3.346513000	1.181437000
6	0.289780000	1.279337000	-2.194124000
1	0.462417000	1.316800000	-3.280025000
1	-0.657995000	1.797247000	-1.981667000
1	-0.905340000	-0.356179000	-1.803921000
6	0.778307000	-1.146807000	-2.640288000
1	0.742833000	-0.830741000	-3.692572000
1	0.224991000	-2.094774000	-2.547893000
8	0.902312000	-2.984134000	2.346119000
8	0.157680000	-2.334913000	0.305249000
6	0.270775000	-3.179265000	1.278114000
6	-0.487962000	-4.480070000	1.077446000
1	-0.015456000	-5.297342000	1.638125000
1	-0.566702000	-4.741765000	0.013928000
1	-1.508735000	-4.340673000	1.470314000
8	-0.884056000	2.623866000	0.434172000
8	-0.178656000	2.139601000	2.539703000
6	-0.532597000	4.040706000	0.617835000
6	-1.008530000	4.767796000	-0.616804000
6	-0.588579000	1.796547000	1.438994000

6	-0.790814000	0.362159000	0.986816000
1	-1.024152000	4.398143000	1.534261000
1	0.558575000	4.094439000	0.746654000
1	-0.774191000	5.838266000	-0.519123000
1	-0.505762000	4.386838000	-1.517135000
1	-2.096273000	4.662240000	-0.741473000
7	-0.883725000	-0.370630000	2.575163000
7	-0.957629000	-1.161638000	3.348196000
6	-2.181532000	0.060299000	0.488883000
6	-3.238841000	0.960695000	0.750802000
6	-2.457742000	-1.118920000	-0.230202000
6	-4.515309000	0.725858000	0.252758000
6	-3.729638000	-1.364492000	-0.738210000
6	-4.736076000	-0.428242000	-0.501352000
1	-3.074546000	1.856873000	1.349108000
1	-1.664539000	-1.854034000	-0.369295000
1	-5.328580000	1.423939000	0.446375000
1	-3.938268000	-2.269535000	-1.307213000
7	-6.082346000	-0.668713000	-1.061591000
8	-6.249903000	-1.673414000	-1.763493000
8	-6.975369000	0.148219000	-0.807061000

4a-OAc-Ph-NO$_2$

7	-2.637284000	-1.106065000	0.161771000
6	-2.565101000	-2.449261000	0.227426000
27	-1.108011000	-0.140405000	-0.389585000
7	-2.263409000	1.473578000	0.064837000
6	-3.646168000	-3.185654000	0.704760000
1	-3.581452000	-4.272269000	0.767000000
7	-0.218913000	-1.960630000	-0.292529000
6	-4.804674000	-2.499675000	1.086002000
1	-5.659645000	-3.052309000	1.478922000
6	-4.880444000	-1.110243000	0.938695000
1	-5.789254000	-0.560765000	1.185777000
6	-3.765838000	-0.431697000	0.451704000
6	-3.689193000	1.012001000	0.057166000
1	-4.048600000	1.089227000	-0.981236000
1	-4.322731000	1.657648000	0.681598000
1	-2.185371000	2.200431000	-0.656465000
6	-1.851376000	2.081895000	1.391133000
1	-2.752000000	2.311088000	1.980523000
1	-1.358043000	3.040006000	1.182171000
6	-0.935167000	1.133030000	2.105413000
6	-0.524592000	0.029089000	1.356947000
6	0.280315000	-0.973832000	1.901619000
6	0.743144000	-0.836050000	3.216443000
1	1.389711000	-1.599532000	3.657911000
6	0.377884000	0.295159000	3.961532000
1	0.744010000	0.407196000	4.984456000
6	-0.464875000	1.276977000	3.417444000
1	-0.756759000	2.143232000	4.017736000
6	0.614971000	-2.097236000	0.966323000
1	0.435161000	-3.085686000	1.414524000
1	1.673563000	-2.066286000	0.672659000
1	0.401255000	-2.111360000	-1.095656000
6	-1.304714000	-2.988719000	-0.378886000
1	-0.991372000	-3.941056000	0.072045000
1	-1.501919000	-3.166972000	-1.448008000
8	0.295683000	0.507290000	-2.778385000
8	-1.730765000	-0.342319000	-2.308711000
6	-0.872104000	0.001159000	-3.141827000
6	-1.051872000	-0.116125000	-4.614623000
1	-1.187926000	0.893915000	-5.032567000
1	-1.930701000	-0.729550000	-4.839732000
1	-0.149000000	-0.545022000	-5.071434000
8	0.839226000	2.872361000	-0.194572000
8	-0.507490000	2.897987000	-2.013756000

6	0.629946000	4.311721000	-0.013511000
6	1.261148000	4.675950000	1.310469000
6	0.233312000	2.290750000	-1.238837000
6	0.486413000	0.810867000	-1.342547000
1	1.098160000	4.831476000	-0.862986000
1	-0.450630000	4.520195000	-0.034853000
1	1.132838000	5.753588000	1.491049000
1	0.785729000	4.126438000	2.136580000
1	2.337657000	4.450209000	1.308466000
6	1.812555000	0.271314000	-0.934852000
6	2.411562000	0.604949000	0.304444000
6	2.476471000	-0.669694000	-1.759063000
6	3.607208000	0.026002000	0.702369000
6	3.674207000	-1.255541000	-1.369758000
6	4.232349000	-0.905468000	-0.135772000
1	1.919719000	1.300513000	0.977102000
1	2.044171000	-0.953312000	-2.717450000
1	4.048392000	0.280845000	1.665139000
1	4.171999000	-1.980283000	-2.012888000
7	5.478427000	-1.529872000	0.287946000
8	6.032272000	-2.336407000	-0.480378000
8	5.942999000	-1.236382000	1.403674000

TS2

7	2.602972000	-0.999368000	-0.552496000
6	2.578211000	-1.829919000	-1.608012000
27	0.950310000	-0.461731000	0.277088000
7	2.154623000	0.825067000	1.255395000
6	3.751840000	-2.122465000	-2.299984000
1	3.728260000	-2.789781000	-3.161974000
7	0.145994000	-1.571435000	-1.280168000
6	4.946916000	-1.547603000	-1.854064000
1	5.878208000	-1.749554000	-2.386055000
6	4.956583000	-0.728752000	-0.718828000
1	5.882006000	-0.296555000	-0.337629000
6	3.748013000	-0.477056000	-0.074799000
6	3.539630000	0.260311000	1.213890000
1	3.608052000	-0.465573000	2.039832000
1	4.291127000	1.043930000	1.385113000
1	1.847518000	0.804603000	2.238608000
6	2.072017000	2.222457000	0.679191000
1	3.086519000	2.634368000	0.578015000
1	1.550720000	2.866750000	1.402908000
6	1.371476000	2.181717000	-0.648683000
6	0.657957000	1.000284000	-0.914460000
6	0.081821000	0.724365000	-2.164579000
6	0.130901000	1.715029000	-3.147767000
1	-0.302264000	1.539121000	-4.135175000
6	0.770030000	2.933160000	-2.865313000
1	0.799384000	3.708258000	-3.634013000
6	1.416825000	3.162337000	-1.638111000
1	1.966028000	4.092214000	-1.473355000
6	-0.470499000	-0.662071000	-2.320306000
1	-0.282274000	-1.062498000	-3.327012000
1	-1.560742000	-0.675846000	-2.172092000
1	-0.590704000	-2.194899000	-0.934649000
6	1.230938000	-2.450974000	-1.825412000
1	1.046904000	-2.702797000	-2.879328000
1	1.203925000	-3.388293000	-1.247615000
8	1.428185000	-0.934292000	3.388170000
8	1.059022000	-2.042563000	1.443374000
6	1.208571000	-1.977575000	2.732502000
6	1.100440000	-3.309793000	3.454354000
1	0.291820000	-3.245790000	4.198164000
1	2.036536000	-3.497729000	4.001562000
1	0.902398000	-4.142423000	2.768397000
8	-1.024556000	2.793676000	0.933037000

8	-0.601147000	1.516136000	2.765098000
6	-1.223380000	3.982645000	1.781462000
6	-1.512019000	5.135010000	0.850001000
6	-0.714324000	1.655491000	1.552363000
6	-0.583079000	0.453974000	0.650491000
1	-2.055818000	3.770106000	2.468065000
1	-0.305520000	4.134452000	2.369351000
1	-1.660435000	6.049967000	1.442711000
1	-0.672052000	5.301944000	0.159586000
1	-2.424204000	4.949727000	0.264284000
6	-1.936483000	-0.043463000	0.300183000
6	-2.894780000	0.767261000	-0.346375000
6	-2.272668000	-1.363594000	0.665668000
6	-4.147001000	0.254736000	-0.662310000
6	-3.535817000	-1.874054000	0.383984000
6	-4.447434000	-1.059376000	-0.290958000
1	-2.636941000	1.786692000	-0.631938000
1	-1.528121000	-1.976784000	1.177165000
1	-4.885179000	0.861109000	-1.185700000
1	-3.807092000	-2.889706000	0.668993000
7	-5.774704000	-1.607321000	-0.629049000
8	-6.020325000	-2.779974000	-0.318091000
8	-6.580771000	-0.870404000	-1.211353000

INT-MI-PhNO$_2$

7	-2.622706000	-0.554314000	-0.956039000
6	-2.604212000	-1.615807000	-1.788875000
27	-0.981632000	0.045509000	-0.241029000
7	-2.109843000	1.350909000	0.777534000
6	-3.797476000	-2.208668000	-2.187226000
1	-3.787961000	-3.072623000	-2.852282000
7	-0.205283000	-1.518193000	-1.227480000
6	-4.999875000	-1.666854000	-1.712936000
1	-5.949468000	-2.118142000	-2.005337000
6	-4.991614000	-0.552522000	-0.868084000
1	-5.919315000	-0.114310000	-0.498716000
6	-3.762728000	-0.007314000	-0.498339000
6	-3.545097000	1.214529000	0.349113000
1	-3.794086000	2.104558000	-0.250706000
1	-4.205621000	1.213039000	1.226953000
1	-1.775112000	2.274738000	0.441664000
6	-1.881889000	1.150728000	2.246843000
1	-2.805072000	1.349338000	2.807737000
1	-1.139913000	1.878467000	2.591404000
6	-1.471740000	-0.295233000	2.388952000
6	-0.384734000	-0.769186000	1.557451000
6	-0.485997000	-2.136685000	1.108051000
6	-1.347709000	-3.020380000	1.762448000
1	-1.399393000	-4.056697000	1.422057000
6	-2.186152000	-2.578141000	2.784941000
1	-2.843040000	-3.282552000	3.298211000
6	-2.308109000	-1.201141000	3.024308000
1	-3.121216000	-0.826415000	3.649731000
6	0.153947000	-2.553809000	-0.196013000
1	-0.240930000	-3.530579000	-0.503761000
1	1.245479000	-2.640212000	-0.149104000
1	0.641729000	-1.236456000	-1.733950000
6	-1.214897000	-1.969605000	-2.243046000
1	-1.100039000	-3.040457000	-2.462263000
1	-1.005285000	-1.409498000	-3.167405000
8	-1.348613000	3.174880000	-1.109131000
8	-0.460904000	1.165233000	-1.704142000
6	-0.669775000	2.439658000	-1.861128000
6	0.032433000	3.025876000	-3.069063000
1	0.288729000	2.258010000	-3.809599000
1	0.963414000	3.500641000	-2.719356000
1	-0.595896000	3.803554000	-3.523872000

8	0.966987000	2.494689000	0.877637000
8	1.199841000	1.510125000	2.909993000
6	1.456970000	3.771881000	1.410978000
6	1.618729000	4.704513000	0.232094000
6	0.920073000	1.453246000	1.717075000
6	0.596611000	0.168457000	0.978751000
1	0.719304000	4.140767000	2.139588000
1	2.407291000	3.585374000	1.933333000
1	1.993008000	5.676416000	0.587490000
1	2.342561000	4.300035000	-0.490624000
1	0.658230000	4.868204000	-0.277451000
6	1.947224000	-0.293637000	0.500557000
6	2.491534000	0.239825000	-0.683191000
6	2.720889000	-1.181839000	1.274712000
6	3.757801000	-0.139660000	-1.115188000
6	3.989893000	-1.566453000	0.857821000
6	4.490347000	-1.045087000	-0.340507000
1	1.898899000	0.941995000	-1.270594000
1	2.314942000	-1.577260000	2.207029000
1	4.174788000	0.255278000	-2.040646000
1	4.588613000	-2.256983000	1.450381000
7	5.822248000	-1.455310000	-0.794856000
8	6.461365000	-2.263545000	-0.103102000
8	6.257805000	-0.978727000	-1.854909000

4a-OAc-PhNO₂-Li

7	2.575708000	-1.215933000	-0.185149000
6	2.438766000	-2.536631000	-0.409335000
27	1.066845000	-0.222573000	0.364084000
7	2.340032000	1.353729000	0.149062000
6	3.515776000	-3.279380000	-0.887065000
1	3.398523000	-4.345524000	-1.082877000
7	0.090830000	-1.968228000	0.023828000
6	4.737295000	-2.628936000	-1.091709000
1	5.591197000	-3.185518000	-1.481242000
6	4.876236000	-1.274398000	-0.768386000
1	5.831835000	-0.759903000	-0.871348000
6	3.762068000	-0.587115000	-0.295301000
6	3.726155000	0.800800000	0.270001000
1	3.954023000	0.725347000	1.345555000
1	4.466827000	1.471070000	-0.188378000
1	2.234354000	2.042854000	0.902059000
6	2.117783000	2.066550000	-1.174266000
1	3.087239000	2.189112000	-1.680144000
1	1.745422000	3.076732000	-0.960016000
6	1.156122000	1.276718000	-2.010140000
6	0.606157000	0.154813000	-1.390192000
6	-0.238201000	-0.726487000	-2.068974000
6	-0.608868000	-0.430664000	-3.387243000
1	-1.282795000	-1.095761000	-3.933994000
6	-0.105758000	0.725044000	-4.002984000
1	-0.397677000	0.958579000	-5.029172000
6	0.784845000	1.573874000	-3.328050000
1	1.191356000	2.455110000	-3.831634000
6	-0.684134000	-1.920301000	-1.279483000
1	-0.530276000	-2.861783000	-1.827823000
1	-1.753290000	-1.869201000	-1.032509000
1	-0.579386000	-2.168398000	0.775117000
6	1.113495000	-3.062835000	0.049917000
1	0.779305000	-3.938411000	-0.523355000
1	1.230738000	-3.373491000	1.100355000
8	-0.341214000	0.456666000	2.761866000
8	1.534954000	-0.686620000	2.277918000
6	0.715198000	-0.272142000	3.113085000
6	0.837618000	-0.522500000	4.575755000
1	-0.129324000	-0.421982000	5.081920000
1	1.538911000	0.217508000	4.995497000
1	1.264916000	-1.519795000	4.738592000

8	-0.665098000	2.793131000	0.085630000
8	0.287106000	2.897713000	2.115447000
6	-0.522077000	4.253563000	-0.050825000
6	-0.951895000	4.594045000	-1.457401000
6	-0.278129000	2.238075000	1.221581000
6	-0.512023000	0.765705000	1.320764000
1	-1.158112000	4.721535000	0.714480000
1	0.525447000	4.521647000	0.149272000
1	-0.849298000	5.678312000	-1.612473000
1	-0.324257000	4.075171000	-2.196170000
1	-2.002340000	4.318121000	-1.628039000
6	-1.837851000	0.235184000	0.884987000
6	-2.470297000	0.661710000	-0.306873000
6	-2.464459000	-0.783309000	1.641901000
6	-3.676269000	0.109822000	-0.715157000
6	-3.663897000	-1.353191000	1.233161000
6	-4.265001000	-0.898801000	0.055373000
1	-2.004448000	1.414124000	-0.934213000
1	-2.007732000	-1.138034000	2.565042000
1	-4.149658000	0.443465000	-1.637671000
1	-4.133447000	-2.139533000	1.822909000
7	-5.521041000	-1.497590000	-0.384213000
8	-5.991105000	-2.441524000	0.273666000
8	-6.072122000	-1.042561000	-1.400709000
3	0.195441000	2.974853000	3.945304000

TS2-Li

7	2.572538000	-1.025163000	-0.581242000
6	2.555078000	-1.764545000	-1.701620000
27	0.911636000	-0.486537000	0.236784000
7	2.138117000	0.665617000	1.352258000
6	3.743560000	-2.053339000	-2.370090000
1	3.727415000	-2.646156000	-3.284907000
7	0.121992000	-1.442123000	-1.426956000
6	4.942195000	-1.574140000	-1.832392000
1	5.884933000	-1.773735000	-2.344617000
6	4.940729000	-0.854933000	-0.631155000
1	5.867023000	-0.502113000	-0.177583000
6	3.718624000	-0.602579000	-0.015269000
6	3.489619000	0.020887000	1.327996000
1	3.474766000	-0.784093000	2.080502000
1	4.274109000	0.736920000	1.609481000
1	1.818539000	0.658250000	2.326837000
6	2.164854000	2.096475000	0.849157000
1	3.205085000	2.450065000	0.815630000
1	1.644857000	2.728700000	1.585059000
6	1.524149000	2.170364000	-0.506227000
6	0.744427000	1.059485000	-0.869846000
6	0.198791000	0.897803000	-2.152833000
6	0.353684000	1.937625000	-3.072548000
1	-0.053188000	1.849634000	-4.082477000
6	1.068158000	3.085659000	-2.696753000
1	1.185636000	3.897957000	-3.416794000
6	1.679849000	3.197155000	-1.435244000
1	2.289009000	4.072390000	-1.198124000
6	-0.437007000	-0.435360000	-2.406363000
1	-0.269077000	-0.782379000	-3.436058000
1	-1.526709000	-0.391484000	-2.260580000
1	-0.641733000	-2.069536000	-1.154341000
6	1.195520000	-2.307429000	-2.019688000
1	1.038227000	-2.447339000	-3.098027000
1	1.114363000	-3.294647000	-1.538658000
8	0.761975000	-1.335954000	3.320298000
8	1.016189000	-2.185589000	1.245324000
6	0.937141000	-2.299238000	2.520778000
6	1.088800000	-3.696312000	3.075014000
1	0.256583000	-3.909338000	3.761467000

1	2.019689000	-3.741070000	3.661636000
1	1.124203000	-4.448927000	2.278590000
8	-0.907335000	2.822221000	0.944239000
8	-0.737464000	1.480118000	2.749720000
6	-1.062040000	4.004896000	1.823260000
6	-1.058544000	5.211621000	0.918993000
6	-0.736616000	1.653076000	1.523593000
6	-0.607525000	0.463720000	0.611433000
1	-2.004449000	3.879379000	2.375429000
1	-0.222608000	4.001462000	2.533996000
1	-1.181118000	6.117332000	1.531423000
1	-0.107903000	5.288234000	0.371653000
1	-1.885380000	5.167371000	0.195587000
6	-1.961109000	0.002795000	0.225913000
6	-2.916198000	0.867185000	-0.353253000
6	-2.307687000	-1.337858000	0.500262000
6	-4.174730000	0.389452000	-0.697343000
6	-3.577807000	-1.814027000	0.192230000
6	-4.484464000	-0.944383000	-0.417272000
1	-2.651943000	1.902790000	-0.567292000
1	-1.569071000	-1.993981000	0.964376000
1	-4.910460000	1.038355000	-1.170377000
1	-3.858144000	-2.844218000	0.407562000
7	-5.822433000	-1.454604000	-0.784053000
8	-6.088524000	-2.634262000	-0.523608000
8	-6.610843000	-0.678063000	-1.336345000
3	-0.443012000	-0.073832000	3.791988000

INT-MI-PhNO$_2$-Li

7	2.733216000	-0.988373000	-0.194880000
6	2.816202000	-2.021203000	-1.054312000
27	1.016973000	-0.344730000	0.283675000
7	2.028321000	1.084803000	1.245398000
6	4.050313000	-2.384026000	-1.586647000
1	4.123399000	-3.213828000	-2.290052000
7	0.354258000	-1.796081000	-0.959701000
6	5.182462000	-1.660785000	-1.191290000
1	6.159589000	-1.917770000	-1.603528000
6	5.073245000	-0.617943000	-0.263506000
1	5.949441000	-0.062045000	0.071152000
6	3.810251000	-0.303512000	0.231621000
6	3.476332000	0.687881000	1.311275000
1	3.622693000	0.189238000	2.282770000
1	4.125811000	1.573656000	1.286529000
1	1.666887000	1.120800000	2.207610000
6	1.769831000	2.381097000	0.532724000
1	2.683039000	2.990345000	0.508839000
1	1.027954000	2.953554000	1.101525000
6	1.345291000	2.015871000	-0.870168000
6	0.288702000	1.045148000	-1.041713000
6	0.345596000	0.242344000	-2.238424000
6	1.141792000	0.643663000	-3.306275000
1	1.170159000	0.030110000	-4.208885000
6	1.967326000	1.767523000	-3.198684000
1	2.580995000	2.076226000	-4.046774000
6	2.130630000	2.387748000	-1.955370000
1	2.925415000	3.122051000	-1.810460000
6	-0.221124000	-1.151627000	-2.193683000
1	0.076978000	-1.717378000	-3.086177000
1	-1.313723000	-1.188213000	-2.128155000
1	-0.380666000	-2.340278000	-0.493193000
6	1.502125000	-2.727450000	-1.237175000
1	1.400695000	-3.185234000	-2.230486000
1	1.447623000	-3.531934000	-0.487553000
8	0.800932000	-0.261960000	3.525702000
8	0.846889000	-1.615352000	1.715939000
6	0.823384000	-1.405142000	2.982822000

6	0.811408000	-2.639578000	3.850456000
1	0.894583000	-3.558931000	3.259478000
1	-0.126764000	-2.653721000	4.426392000
1	1.640116000	-2.578278000	4.571232000
8	-1.304950000	3.008712000	0.288940000
8	-1.160874000	1.835814000	2.201522000
6	-1.774332000	4.177924000	1.057586000
6	-2.084061000	5.265433000	0.057991000
6	-1.019596000	1.905134000	0.977086000
6	-0.640225000	0.748914000	0.078742000
1	-2.659267000	3.867095000	1.631547000
1	-0.973709000	4.458863000	1.758265000
1	-2.443248000	6.154870000	0.596870000
1	-1.187795000	5.547046000	-0.513677000
1	-2.869502000	4.945275000	-0.642003000
6	-1.964065000	0.051213000	-0.138124000
6	-2.329831000	-1.028605000	0.682878000
6	-2.876315000	0.531513000	-1.098296000
6	-3.566140000	-1.649543000	0.528368000
6	-4.114261000	-0.078548000	-1.264882000
6	-4.440448000	-1.167008000	-0.448760000
1	-1.622740000	-1.395961000	1.427543000
1	-2.601383000	1.382225000	-1.723926000
1	-3.849441000	-2.496288000	1.152273000
1	-4.820782000	0.279667000	-2.012671000
7	-5.744909000	-1.821123000	-0.622252000
8	-6.533909000	-1.349070000	-1.453191000
8	-6.001489000	-2.817603000	0.069202000
3	-0.633520000	0.866337000	3.681993000

2c-OAc-EDA

7	-1.569695	1.527790	0.253542
6	-1.678439	2.096405	1.473115
27	-1.001960	-0.248808	0.154254
7	-1.154727	0.016452	-1.837602
6	-2.035977	3.435034	1.587922
1	-2.115034	3.892757	2.574130
7	-0.564253	0.026792	2.110643
6	-2.291616	4.162192	0.419821
1	-2.564203	5.216792	0.483433
6	-2.210947	3.538152	-0.826930
1	-2.430772	4.077618	-1.748686
6	-1.846646	2.193559	-0.882479
6	-1.814842	1.341384	-2.109896
1	-2.853207	1.131617	-2.407590
1	-1.321792	1.854810	-2.946692
1	-1.800016	-0.691556	-2.211572
6	0.207751	-0.107788	-2.463189
1	0.249303	0.431652	-3.420676
1	0.371176	-1.177007	-2.666761
6	1.209671	0.365187	-1.448216
6	0.740250	0.287401	-0.130199
6	1.542856	0.593439	0.973570
6	2.853761	1.009800	0.760161
1	3.518197	1.254259	1.588456
6	3.315950	1.095183	-0.565453
6	2.519369	0.772130	-1.679222
1	2.931665	0.838603	-2.685935
6	0.904426	0.342342	2.308903
1	1.009733	1.194859	2.995271
1	1.363652	-0.531496	2.790320
1	-0.785002	-0.809173	2.661937
6	-1.469577	1.119464	2.587150
1	-1.081697	1.593436	3.499739
1	-2.440106	0.657095	2.823487
8	-3.788452	-1.003954	-1.423226
8	-2.858316	-0.881185	0.637669

6	-3.849177	-1.089105	-0.173326
6	-5.143586	-1.494235	0.509793
1	-5.371009	-0.806922	1.337492
1	-5.022128	-2.500314	0.941484
1	-5.975541	-1.509310	-0.205138
8	1.687720	-2.466721	1.056215
8	1.416525	-2.890146	-1.166728
6	3.153290	-2.535311	0.893870
6	3.768929	-2.229898	2.237748
6	0.975731	-2.612016	-0.062708
6	-0.477017	-2.314522	0.225111
1	3.404385	-3.544355	0.536073
1	3.436183	-1.800879	0.125449
1	4.862774	-2.314101	2.153323
1	3.530518	-1.208154	2.564962
1	3.426142	-2.942575	3.002031
1	-0.837632	-2.595888	1.222747
7	-1.274742	-2.909651	-0.714218
7	-1.907512	-3.324143	-1.537242
7	4.690529	1.520972	-0.793506
8	5.109360	1.596366	-1.963539
8	5.403808	1.793864	0.190017

2c-OAc

7	-1.243584	1.341492	-0.001889
6	-1.262160	1.989568	1.181503
27	-1.158959	-0.504619	0.000782
7	-0.982604	-0.325515	-1.986996
6	-1.238267	3.380614	1.209322
1	-1.247020	3.905737	2.164620
7	-0.982937	-0.319929	1.987531
6	-1.209177	4.074974	-0.004873
1	-1.177761	5.165658	-0.006025
6	-1.235655	3.377897	-1.217533
1	-1.242309	3.900972	-2.173965
6	-1.259644	1.986840	-1.186687
6	-1.416125	1.064021	-2.357691
1	-2.487283	1.015262	-2.607976
1	-0.879121	1.421765	-3.246858
1	-1.614383	-0.981989	-2.458176
6	0.430791	-0.656126	-2.412514
1	0.718981	-0.049708	-3.283888
1	0.429698	-1.711568	-2.722896
6	1.337662	-0.483621	-1.228362
6	0.670465	-0.477559	0.000577
6	1.337648	-0.478419	1.229546
6	2.728246	-0.420505	1.238196
1	3.297428	-0.411796	2.167829
6	3.395809	-0.380312	0.000401
6	2.728265	-0.425534	-1.237266
1	3.297436	-0.420591	-2.166927
6	0.431133	-0.645551	2.414713
1	0.718386	-0.033274	3.282254
1	0.432016	-1.699040	2.731637
1	-1.613221	-0.977269	2.459637
6	-1.421015	1.069123	2.354035
1	-0.888407	1.429984	3.244592
1	-2.493088	1.018111	2.599972
8	-1.444918	-2.444460	0.008944
8	-3.168346	-1.093992	0.007031
6	-2.729015	-2.293328	0.009826
6	-3.640254	-3.476099	-0.003881
1	-4.051520	-3.593149	-1.019360
1	-4.481726	-3.304467	0.681726
1	-3.101422	-4.391080	0.271221
7	4.851073	-0.303018	0.000329
8	5.449688	-0.271472	-1.090714

8	5.449740	-0.270823	1.091336

4c-OAc

7	1.714429	1.572548	0.199001
6	1.836454	2.471627	-0.790928
27	1.138774	-0.183711	-0.221806
7	0.981750	-0.364469	1.779737
6	2.169401	3.792178	-0.491180
1	2.260988	4.529747	-1.289092
7	1.044477	0.517482	-2.109819
6	2.385486	4.137687	0.846787
1	2.636001	5.167602	1.106502
6	2.296634	3.168373	1.854135
1	2.486640	3.415236	2.898968
6	1.958222	1.868725	1.490388
6	1.909841	0.653938	2.373390
1	2.915268	0.204681	2.385869
1	1.632097	0.894022	3.409527
1	1.299297	-1.292728	2.082880
6	-0.455955	-0.199987	2.232979
1	-0.496856	0.479546	3.096532
1	-0.809660	-1.183034	2.574178
6	-1.283205	0.289907	1.079662
6	-0.621931	0.294811	-0.155930
6	-1.262213	0.669756	-1.346033
6	-2.597566	1.050912	-1.310150
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6	-3.258309	1.034768	-0.066441
6	-2.622565	0.657269	1.132021
1	-3.182131	0.652088	2.067545
6	-0.396173	0.512375	-2.561110
1	-0.562279	1.277879	-3.333288
1	-0.580920	-0.470311	-3.021339
1	1.570844	-0.092941	-2.743723
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6	3.147248	-2.052503	-0.450157
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1	4.565790	-3.298845	-1.425170
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8	-1.430543	-2.610867	-0.280141
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6	-0.169834	-2.743147	0.184786
6	0.792336	-2.078394	-0.728900
1	-2.388896	-4.097811	0.834667
1	-2.455377	-2.454631	1.537110
1	-4.663121	-3.062811	0.486067
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6	2.057239	3.694269	0.694180
1	2.640818	4.149755	1.494453

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6	1.982410	4.278444	-0.575670
1	2.513049	5.211765	-0.771446
6	1.246142	3.672851	-1.601975
1	1.197058	4.111249	-2.598959
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1	0.932445	-0.394621	-2.939589
1	-0.424895	-1.520496	-2.677333
6	1.012113	-1.356363	-1.032054
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6	2.385391	-1.561700	-1.189425
1	2.832954	-1.489670	-2.180862
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1	-0.049013	-1.254925	3.098216
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6	-3.052971	1.261622	0.126810
6	-4.180076	1.902146	0.912189
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6	-0.995307	-1.498465	0.571477
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1	-6.576782	-2.185606	-0.039843
1	-5.629411	-2.486814	1.440285
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7	-1.244755	-0.210193	-1.595491
6	-1.661490	3.984689	0.921261
1	-1.614488	4.680282	1.759299
7	-0.433708	0.653709	2.196575
6	-1.976884	4.417793	-0.371913
1	-2.165507	5.476326	-0.558310
6	-2.064698	3.500782	-1.423713
1	-2.336097	3.815265	-2.431635
6	-1.802012	2.158397	-1.156647
6	-1.961917	1.007541	-2.101162
1	-3.032087	0.749703	-2.148272
1	-1.629308	1.250990	-3.119445

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1	0.054188	-0.104893	-3.300826
1	0.176071	-1.585617	-2.318194
6	1.155172	0.090503	-1.417157
6	0.776395	0.277582	-0.083774
6	1.649031	0.753136	0.896501
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6	2.462506	0.387024	-1.792574
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1	-0.727594	-0.001046	2.928047
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6	-3.755834	-1.058456	0.228175
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6	3.772590	-2.188385	2.466162
6	0.659394	-2.472292	0.631850
6	-0.638009	-1.798696	0.754258
1	2.889361	-3.856374	1.364018
1	3.220618	-2.402657	0.367089
1	4.807446	-2.535947	2.328544
1	3.771559	-1.089074	2.437368
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6	-2.293594	3.166393	-1.857777
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1	-1.301536	-1.296475	-2.075734
6	0.454539	-0.205934	-2.230520
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1	0.806314	-1.189999	-2.570787
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6    2.623487    0.651010   -1.133831        8   -3.824781   -0.840998   -1.324560
1    3.181784    0.643478   -2.070100        8   -2.874533   -0.747477    0.728728
6    0.401218    0.516586    2.562202        6   -3.871795   -0.943055   -0.075092
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1    0.583831   -0.465554    3.024435        1   -6.029642   -1.046318    0.016463
1   -1.567519   -0.082516    2.747998        1   -5.227712   -1.002819    1.630201
6   -1.677951    1.889111    2.163280        1   -5.172692   -2.479092    0.634381
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8   -2.082978   -2.799617    0.658544        6    3.046029   -2.685975    0.857074
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6    0.160667   -2.745932   -0.176729        7   -2.353933   -3.301158   -1.609283
6   -0.795637   -2.075408    0.738912        7    4.736515    1.400978   -0.810930
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1    2.441239   -2.467407   -1.539596        8    5.457830    1.670420    0.166491
1    4.652103   -3.075661   -0.496486
1    3.909386   -1.699497    0.359336    TS2c
1    3.846415   -3.339900    1.073087        7   -1.481970   -1.803920    0.045354
1   -0.466744   -2.150828    1.784387        6   -1.390132   -2.786037   -0.865404
7    4.662500    1.398703    0.015193       27   -1.002901    0.006504   -0.467842
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1   -2.247960    5.349225    0.335870        1   -1.805735    1.203269    1.514615
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1   -2.207646    4.127151   -1.854764        1    0.075804    0.168125    3.193103
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6   -1.760101    1.342599   -2.117373        6    1.166366   -0.063197    1.314093
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6    0.773264    0.235447   -0.117444        6    1.009888   -0.914852   -2.340725
6    1.580532    0.545481    0.980360        1    1.335455   -1.785063   -2.927774
6    2.896751    0.939631    0.756166        1    1.271559   -0.003506   -2.899919
1    3.567622    1.187475    1.578242        1   -0.884093   -0.375791   -2.984643
6    3.354567    0.998549   -0.571923        6   -1.124342   -2.278129   -2.249244
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1    2.957918    0.725369   -2.687863        1   -2.092487   -2.169113   -2.761673
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8   5.099644   -0.885564   2.222170

TS36
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1   -0.972610   1.255685   2.223775
6   0.563555   -0.128394   2.269332
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6   2.279111   -1.675914   -1.388496
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6   0.921864   2.458516   0.436074
6   0.234381   1.484753   -0.486282
1   2.046385   4.800234   0.910542
1   3.107584   3.502069   1.530286
1   4.456681   5.246179   0.309321
1   4.539856   3.685287   -0.548564
1   3.479466   4.991759   -1.159586
1   0.568838   1.660382   -1.516204
7   4.163113   -2.682696   -0.153613
8   4.746973   -2.857670   0.925903
8   4.555219   -3.163815   -1.226986

2b-OAc
7   -1.587316   1.429789   0.284302
6   -1.768166   1.951676   1.517214
27   -0.877138   -0.282697   0.146300
7   -0.996426   0.032416   -1.843287
6   -2.231487   3.254273   1.664404
1   -2.366510   3.672424   2.662171
7   -0.488690   -0.028738   2.115896
6   -2.513588   3.998965   0.513384
1   -2.867865   5.027146   0.602233
6   -2.351234   3.424071   -0.749104
1   -2.585536   3.976742   -1.659522
6   -1.882840   2.113678   -0.836748
6   -1.745942   1.312201   -2.091587
1   -2.755312   1.039563   -2.435479
1   -1.264534   1.893923   -2.890366
1   -1.574515   -0.710725   -2.257317
6   0.389308   0.037698   -2.433131
1   0.405150   0.600661   -3.378815
1   0.643306   -1.009536   -2.659977
6   1.322799   0.568791   -1.380284
6   0.831364   0.415527   -0.087425
6   1.584336   0.757126   1.035438
6   2.867634   1.276914   0.858287
1   3.502055   1.546062   1.706388
6   3.371911   1.441375   -0.448128
6   2.612483   1.083830   -1.577975
1   3.012923   1.192831   -2.586212
6   0.944569   0.414605   2.350147
1   0.955380   1.252768   3.062710
1   1.468683   -0.427462   2.822953
1   -0.638473   -0.894828   2.643276
6   -1.497636   0.960350   2.605720
1   -1.176280   1.437276   3.542795
1   -2.427721   0.405541   2.802734
8   -3.544392   -1.227896   -1.536839
8   -2.692180   -1.106171   0.558408
6   -3.635681   -1.360481   -0.291479
6   -4.929635   -1.851521   0.335546
1   -5.395118   -1.024113   0.893993
1   -4.721678   -2.657349   1.054581
1   -5.630413   -2.206551   -0.430476
8   1.986445   -2.295767   1.069855
8   1.816624   -2.665662   -1.171337
6   3.455255   -2.258483   0.943292
6   4.020657   -1.964180   2.311426
6   1.318611   -2.457363   -0.075293
6   -0.160151   -2.303455   0.175450
1   3.782551   -3.234295   0.555433
1   3.705946   -1.477289   0.210767
1   5.119359   -1.980590   2.250977
1   3.713472   -0.969984   2.665608
1   3.704678   -2.721539   3.043697
1   -0.519784   -2.642334   1.154815
7   -0.873429   -2.935664   -0.802612

7	-1.445632	-3.373592	-1.659152
8	4.647432	1.960031	-0.513946
6	5.233117	2.144142	-1.812598
1	5.336461	1.184670	-2.346775
1	4.643212	2.846915	-2.424764
1	6.228213	2.568699	-1.630030

2b-OAc

7	-1.051960	1.365161	-0.062001
6	-1.098985	2.060205	1.094282
27	-1.040890	-0.473959	0.007351
7	-0.707608	-0.374321	-1.965524
6	-1.006981	3.448902	1.074354
1	-1.040041	4.008878	2.009274
7	-0.973349	-0.228385	1.997130
6	-0.876336	4.095576	-0.159415
1	-0.789936	5.182612	-0.196967
6	-0.867418	3.353839	-1.346058
1	-0.788887	3.839145	-2.319219
6	-0.963918	1.968131	-1.267426
6	-1.094138	1.005852	-2.409786
1	-2.155916	0.967900	-2.699813
1	-0.514724	1.318368	-3.290201
1	-1.311121	-1.038401	-2.462639
6	0.730762	-0.730984	-2.277815
1	1.086638	-0.140340	-3.135548
1	0.734422	-1.789960	-2.577457
6	1.552274	-0.551551	-1.032555
6	0.801272	-0.497278	0.133941
6	1.386851	-0.485509	1.399435
6	2.779083	-0.478029	1.499690
1	3.288437	-0.472012	2.466788
6	3.554003	-0.489601	0.320757
6	2.953830	-0.545645	-0.951174
1	3.555058	-0.592396	-1.859735
6	0.395591	-0.602997	2.522108
1	0.642013	0.007069	3.404269
1	0.329300	-1.651657	2.849466
1	-1.661947	-0.835435	2.454432
6	-1.358827	1.193384	2.290263
1	-0.848561	1.564922	3.190080
1	-2.441834	1.205546	2.488854
8	-1.373469	-2.413162	0.046989
8	-3.072787	-1.039707	-0.142969
6	-2.647420	-2.241968	-0.084514
6	-3.554756	-3.424765	-0.203583
1	-3.555903	-3.759172	-1.253738
1	-4.580244	-3.155226	0.078502
1	-3.188686	-4.254593	0.415557
8	4.917661	-0.455549	0.522519
6	5.765448	-0.460402	-0.636940
1	5.640075	-1.386887	-1.221912
1	5.571542	0.414731	-1.279546
1	6.791526	-0.408979	-0.251868

4b-OAc

7	-1.806229	1.397446	-0.172984
6	-2.079122	2.236823	0.839877
27	-1.025247	-0.279587	0.211494
7	-0.749350	-0.343932	-1.788508
6	-2.566037	3.516327	0.573946
1	-2.782518	4.201867	1.393906
7	-1.079290	0.357403	2.123247
6	-2.768712	3.888496	-0.759144
1	-3.135581	4.889269	-0.993363
6	-2.511956	2.980486	-1.795103
1	-2.684134	3.246407	-2.838495

6	-2.030883	1.717813	-1.462974
6	-1.790151	0.554331	-2.383822
1	-2.722771	-0.029082	-2.442638
1	-1.519932	0.868050	-3.402431
1	-0.909208	-1.292481	-2.147019
6	0.666684	0.053394	-2.169527
1	0.629614	0.782055	-2.993659
1	1.169155	-0.847125	-2.551430
6	1.375110	0.589053	-0.957950
6	0.670234	0.460290	0.232462
6	1.216913	0.852097	1.455851
6	2.510330	1.374188	1.493658
1	2.985298	1.673083	2.431622
6	3.238981	1.488347	0.292274
6	2.681584	1.103293	-0.939768
1	3.252559	1.180685	-1.865731
6	0.333860	0.539044	2.629371
1	0.358122	1.299778	3.424921
1	0.634909	-0.420196	3.078492
1	-1.536071	-0.336643	2.723925
6	-1.903542	1.615750	2.196395
1	-1.469394	2.324236	2.916254
1	-2.900265	1.336912	2.571765
8	-1.580093	-3.033625	0.479407
8	-2.835470	-1.198438	0.147595
6	-2.739678	-2.438355	0.253427
6	-3.899266	-3.364925	0.116589
1	-3.906618	-4.089881	0.942325
1	-3.789977	-3.930969	-0.821911
1	-4.833895	-2.794402	0.093383
8	1.875935	-2.343079	0.347365
8	0.522558	-3.089520	-1.327594
6	3.051853	-2.512690	-0.506216
6	4.255002	-2.126922	0.324290
6	0.669020	-2.594603	-0.207509
6	-0.424312	-2.120809	0.671566
1	3.094099	-3.559986	-0.841916
1	2.936140	-1.863550	-1.387614
1	5.167469	-2.229357	-0.281983
1	4.178812	-1.082397	0.661208
1	4.350027	-2.778975	1.205370
1	-0.149690	-2.203202	1.732654
8	4.523499	1.978175	0.432591
6	5.358212	1.990994	-0.735051
1	5.473558	0.977440	-1.155591
1	4.963861	2.671535	-1.508559
1	6.336016	2.356704	-0.396875

Carbene- N$_2$b

7	1.518585	-1.674827	0.081464
6	1.523725	-2.557089	1.094399
27	0.873032	0.132334	0.409060
7	1.084963	0.290618	-1.578338
6	1.865663	-3.887323	0.864517
1	1.861487	-4.605168	1.685075
7	0.407996	-0.676444	2.216547
6	2.211796	-4.267569	-0.437052
1	2.470918	-5.306433	-0.648069
6	2.236249	-3.321562	-1.467144
1	2.524714	-3.593788	-2.482615
6	1.883028	-2.007620	-1.167367
6	1.953214	-0.823627	-2.081009
1	2.988956	-0.447791	-2.069166
1	1.696483	-1.075178	-3.119040
1	1.635856	1.163605	-1.671114
6	-0.260275	0.389932	-2.248437
1	-0.203423	-0.028211	-3.264054

1	-0.494919	1.461547	-2.336098
6	-1.270202	-0.287139	-1.366279
6	-0.861281	-0.406324	-0.044140
6	-1.677994	-0.948016	0.945860
6	-2.958832	-1.378724	0.600439
1	-3.644163	-1.801018	1.339252
6	-3.389270	-1.260895	-0.738110
6	-2.554572	-0.717505	-1.732021
1	-2.889384	-0.623670	-2.765049
6	-1.086674	-0.908810	2.323755
1	-1.273203	-1.821709	2.907551
1	-1.499632	-0.056230	2.882307
1	0.677697	-0.015105	2.951434
6	1.234867	-1.912613	2.415343
1	0.746752	-2.594202	3.125591
1	2.192867	-1.592562	2.853403
8	3.187113	1.964606	-0.825531
8	2.776562	0.616991	0.949380
6	3.527446	1.404550	0.249616
6	4.932535	1.615280	0.784039
1	5.594124	0.869598	0.313575
1	4.978871	1.474939	1.871857
1	5.300110	2.613260	0.510619
8	-1.876140	2.092485	1.574917
8	-1.231776	2.944027	-0.443509
6	-3.287438	2.452464	1.310836
6	-4.106351	1.860006	2.432159
6	-1.008864	2.337355	0.604503
6	0.343115	1.790109	0.778096
1	-3.353964	3.549003	1.268184
1	-3.556102	2.033996	0.329862
1	-5.164875	2.116314	2.275354
1	-4.016711	0.764021	2.445733
1	-3.794609	2.259894	3.408030
1	1.095478	2.529761	1.100299
7	1.322141	4.354417	-1.510022
7	1.183099	3.916041	-2.511616
8	-4.667735	-1.713029	-0.973967
6	-5.179185	-1.620828	-2.313963
1	-5.206838	-0.575154	-2.663137
1	-4.582555	-2.230930	-3.012656
1	-6.201668	-2.015392	-2.266557

Carbene-b

7	-1.807327	1.396875	-0.173439
6	-2.080562	2.236111	0.839480
27	-1.025522	-0.279760	0.211075
7	-0.748988	-0.343720	-1.788884
6	-2.566994	3.515793	0.573593
1	-2.783653	4.201215	1.393604
7	-1.080437	0.357024	2.122946
6	-2.768933	3.888310	-0.759525
1	-3.135421	4.889230	-0.993710
6	-2.511865	2.980468	-1.795549
1	-2.683406	3.246661	-2.838977
6	-2.031176	1.717633	-1.463461
6	-1.789807	0.554393	-2.384436
1	-2.722235	-0.029284	-2.443716
1	-1.519264	0.868372	-3.402879
1	-0.908667	-1.292277	-2.147441
6	0.667043	0.053945	-2.169359
1	0.630144	0.782460	-2.993622
1	1.169946	-0.846502	-2.550850
6	1.374827	0.589917	-0.957519
6	0.669544	0.461056	0.232672
6	1.215794	0.852909	1.456231
6	2.509225	1.374939	1.494501

1	2.983856	1.673806	2.432650
6	3.238306	1.489084	0.293396
6	2.681284	1.104145	-0.938859
1	3.252593	1.181587	-1.864612
6	0.332386	0.539968	2.629528
1	0.355714	1.301341	3.424509
1	0.633896	-0.418655	3.079650
1	-1.536699	-0.337528	2.723429
6	-1.906041	1.614470	2.195865
1	-1.473691	2.322968	2.916792
1	-2.902987	1.334249	2.569636
8	-1.578231	-3.034119	0.481389
8	-2.834696	-1.200308	0.145977
6	-2.738103	-2.439983	0.253818
6	-3.897037	-3.367495	0.117882
1	-3.788439	-3.932666	-0.821242
1	-4.832150	-2.797694	0.096040
1	-3.902847	-4.093088	0.943038
8	1.877108	-2.341629	0.346325
8	0.523157	-3.089357	-1.327613
6	3.052807	-2.511867	-0.507451
6	4.256240	-2.126615	0.322867
6	0.670021	-2.593969	-0.207796
6	-0.423032	-2.120356	0.671805
1	3.094452	-3.559186	-0.843123
1	2.937293	-1.862684	-1.388847
1	5.168552	-2.229176	-0.283619
1	4.180367	-1.082134	0.660004
1	4.351319	-2.778840	1.203814
1	-0.147279	-2.201904	1.732648
8	4.522842	1.978729	0.434168
6	5.357875	1.991727	-0.733210
1	5.473454	0.978227	-1.153831
1	4.963711	2.672277	-1.506808
1	6.335549	2.357501	-0.394729

INT2b

7	0.917710	1.764980	-0.089890
6	1.661915	2.293687	0.898980
27	-0.244282	0.350335	0.297748
7	-0.433326	0.203981	-1.661478
6	2.524415	3.354336	0.624806
1	3.122533	3.794416	1.423482
7	0.373130	0.601086	2.201307
6	2.610577	3.823455	-0.690298
1	3.287518	4.645393	-0.928985
6	1.836042	3.242988	-1.703878
1	1.894046	3.595275	-2.734180
6	0.973610	2.205837	-1.365116
6	-0.015437	1.511334	-2.260529
1	-0.925895	2.129490	-2.318499
1	0.366038	1.378086	-3.283404
1	-1.445010	0.095614	-1.844064
6	0.358074	-0.995943	-2.094664
1	1.090366	-0.690627	-2.853358
1	-0.321231	-1.731043	-2.539843
6	1.091855	-1.536385	-0.886079
6	0.446610	-1.565694	0.402881
6	1.334909	-1.475938	1.553115
6	2.675444	-1.749911	1.431525
1	3.348578	-1.659183	2.286213
6	3.226088	-2.042842	0.157733
6	2.451835	-1.822161	-0.993218
1	2.919272	-1.787819	-1.977353
6	0.779195	-0.746520	2.751465
1	1.524321	-0.634529	3.550513
1	-0.110244	-1.220051	3.184167

1	-0.409394	0.976379	2.749830
6	1.508760	1.596935	2.223469
1	2.443317	1.056933	2.439248
1	1.355098	2.315277	3.041028
8	-3.064375	0.947897	-1.164888
8	-1.791368	1.464669	0.648207
6	-2.877473	1.520157	-0.067773
6	-3.959609	2.383414	0.555918
1	-3.580370	3.406348	0.700569
1	-4.225430	1.987843	1.547307
1	-4.849976	2.409444	-0.083717
8	-3.270017	-1.716930	0.410648
8	-2.007675	-2.495617	-1.311956
6	-4.475024	-1.999621	-0.361439
6	-5.630855	-1.362228	0.378014
6	-2.079073	-1.956486	-0.206725
6	-0.990304	-1.472365	0.650516
1	-4.353232	-1.577726	-1.370600
1	-4.586268	-3.091942	-0.449964
1	-6.567825	-1.558509	-0.164653
1	-5.728620	-1.771110	1.394718
1	-5.491400	-0.272875	0.444482
1	-1.293784	-1.537793	1.697248
8	4.532985	-2.368900	0.151678
6	5.186942	-2.600887	-1.117835
1	4.680630	-3.402358	-1.676590
1	5.215356	-1.675634	-1.713891
1	6.207249	-2.908578	-0.863184

TS1b

7	-1.492232	1.514127	0.259554
6	-1.612130	2.102767	1.465466
27	-0.869290	-0.293190	0.182833
7	-0.978032	0.000462	-1.814457
6	-1.963724	3.444933	1.561614
1	-2.050976	3.918475	2.539673
7	-0.477088	0.054910	2.152958
6	-2.198615	4.157460	0.379734
1	-2.465602	5.214572	0.425375
6	-2.097940	3.517631	-0.858049
1	-2.293662	4.049323	-1.789691
6	-1.739457	2.169925	-0.886402
6	-1.676577	1.302267	-2.102342
1	-2.706761	1.056032	-2.400554
1	-1.195452	1.818456	-2.944682
1	-1.585570	-0.731074	-2.203960
6	0.405542	-0.069609	-2.405205
1	0.440747	0.466908	-3.365365
1	0.612001	-1.132883	-2.600408
6	1.360102	0.455018	-1.369503
6	0.874198	0.339231	-0.072603
6	1.629232	0.699868	1.041586
6	2.916278	1.204137	0.848800
1	3.552762	1.492241	1.688982
6	3.419874	1.329956	-0.462473
6	2.653832	0.954867	-1.581948
1	3.050060	1.043144	-2.593799
6	0.987172	0.392082	2.364777
1	1.069510	1.217230	3.087306
1	1.458907	-0.493420	2.814277
1	-0.695751	-0.773376	2.716204
6	-1.407722	1.141380	2.594614
1	-1.040825	1.630541	3.508112
1	-2.374357	0.666010	2.821658
8	-3.614324	-1.063528	-1.444082
8	-2.737622	-0.945107	0.641497
6	-3.697388	-1.173468	-0.195655

6	-4.995273	-1.651863	0.433219
1	-5.853838	-1.351300	-0.182213
1	-5.111440	-1.276295	1.458507
1	-4.974455	-2.753459	0.471509
8	1.891729	-2.388944	1.081732
8	1.546965	-2.829402	-1.127079
6	3.352340	-2.436912	0.882793
6	3.991173	-2.103549	2.209136
6	1.140538	-2.497153	-0.023076
6	-0.254179	-2.060800	0.319671
1	3.610802	-3.446747	0.531853
1	3.605301	-1.707602	0.098687
1	5.085089	-2.158527	2.103858
1	3.728429	-1.085480	2.530230
1	3.682918	-2.817431	2.987054
1	-0.673936	-2.602457	1.182850
7	-1.173631	-3.124882	-0.905076
7	-1.912596	-3.384654	-1.686075
8	4.700065	1.833467	-0.543483
6	5.278910	1.993622	-1.848362
1	5.374075	1.025303	-2.367825
1	4.688988	2.690033	-2.467683
1	6.277302	2.415540	-1.678214

TS2b

7	-1.569943	-1.672611	0.050082
6	-1.575488	-2.677611	-0.839485
27	-0.889473	0.065824	-0.494196
7	-1.060451	0.450743	1.466339
6	-1.945759	-3.961128	-0.443389
1	-1.943173	-4.779756	-1.163419
7	-0.477467	-0.940755	-2.208991
6	-2.318565	-4.162977	0.889653
1	-2.601058	-5.161154	1.228391
6	-2.339715	-3.091056	1.788894
1	-2.646769	-3.223910	2.826466
6	-1.956968	-1.834358	1.326998
6	-2.006385	-0.537937	2.075977
1	-3.019977	-0.118657	1.969257
1	-1.802553	-0.658280	3.148822
1	-1.535194	1.369742	1.468596
6	0.290522	0.517652	2.134846
1	0.213617	0.133694	3.162362
1	0.570124	1.579460	2.192968
6	1.273928	-0.235633	1.285761
6	0.837537	-0.467822	-0.011079
6	1.633615	-1.091252	-0.970009
6	2.918604	-1.500667	-0.617367
1	3.587854	-1.981736	-1.334580
6	3.378787	-1.267314	0.696374
6	2.568134	-0.635302	1.656485
1	2.929084	-0.448788	2.667992
6	1.019952	-1.117419	-2.339256
1	1.239740	-2.028336	-2.915156
1	1.383050	-0.250614	-2.913249
1	-0.798592	-0.380780	-3.004960
6	-1.256290	-2.225265	-2.231945
1	-0.720268	-2.991259	-2.809484
1	-2.206290	-2.017247	-2.747913
8	-2.982103	2.239211	0.446325
8	-2.793442	0.539960	-1.039353
6	-3.439502	1.504687	-0.468783
6	-4.866924	1.705197	-0.944427
1	-5.525409	1.071094	-0.328391
1	-4.988662	1.403224	-1.992999
1	-5.175527	2.749965	-0.808244
8	1.962036	1.945642	-1.592495

8	1.072931	2.991437	0.232752
6	3.328118	2.356242	-1.198010
6	4.275784	1.727723	-2.190492
6	0.982142	2.270479	-0.761212
6	-0.326629	1.664407	-1.040302
1	3.370034	3.454701	-1.208168
1	3.492547	1.995840	-0.171652
1	5.306344	2.015798	-1.934074
1	4.206409	0.630732	-2.158319
1	4.064713	2.072487	-3.213240
1	-1.025178	2.316638	-1.590868
7	-1.220371	4.504820	1.648565
7	-1.111419	4.023670	2.634279
8	4.663126	-1.697572	0.940755
6	5.222016	-1.449306	2.241279
1	5.257106	-0.369419	2.462208
1	4.655598	-1.972775	3.029623
1	6.243879	-1.846454	2.202463

TS3b

7	-2.117248	1.047270	-0.318040
6	-2.627214	1.786397	0.684534
27	-1.014011	-0.435940	0.116202
7	-0.567989	-0.378273	-1.855854
6	-3.267638	2.993269	0.411296
1	-3.674332	3.596648	1.223659
7	-1.356444	0.133413	2.027073
6	-3.373949	3.404649	-0.922918
1	-3.862683	4.350701	-1.161965
6	-2.858201	2.606329	-1.952526
1	-2.941146	2.905755	-2.997807
6	-2.229421	1.412552	-1.611003
6	-1.676883	0.365861	-2.537615
1	-2.474338	-0.365957	-2.741517
1	-1.345756	0.782139	-3.499827
1	-0.550516	-1.336204	-2.222551
6	0.803169	0.228489	-2.097145
1	0.719286	1.014272	-2.862198
1	1.456275	-0.553717	-2.510765
6	1.350202	0.792535	-0.815548
6	0.634015	0.439135	0.339951
6	0.892289	1.043547	1.587939
6	1.946406	1.934769	1.698415
1	2.184875	2.442458	2.635914
6	2.731035	2.220013	0.553413
6	2.420517	1.678568	-0.713271
1	2.981851	1.970665	-1.600956
6	-0.085977	0.664031	2.665336
1	-0.323471	1.508730	3.328013
1	0.323556	-0.137379	3.298289
1	-1.660342	-0.678647	2.574195
6	-2.498027	1.114625	2.023010
1	-2.399313	1.838793	2.843862
1	-3.417941	0.535202	2.198935
8	-0.942590	-3.313306	0.837195
8	-2.443642	-1.807134	0.034094
6	-2.094679	-2.980859	0.429607
6	-3.164059	-4.055151	0.407291
1	-2.837493	-4.874492	-0.250094
1	-4.124392	-3.659580	0.056352
1	-3.281054	-4.470948	1.418907
8	2.584881	-2.207675	0.198372
8	1.039575	-2.772541	-1.366140
6	3.645833	-2.763026	-0.651647
6	4.965891	-2.358700	-0.037475
6	1.332263	-2.239457	-0.300136
6	0.368249	-1.521966	0.603898

1	3.512542	-3.855060	-0.687252
1	3.518549	-2.360789	-1.668044
1	5.788271	-2.764735	-0.645415
1	5.065025	-1.263460	-0.008849
1	5.066768	-2.751386	0.985065
1	0.664611	-1.649203	1.653536
8	3.762650	3.080468	0.773116
6	4.591965	3.463163	-0.342495
1	5.089306	2.585417	-0.784939
1	4.004700	3.991917	-1.109916
1	5.345512	4.141222	0.075103

K-TFE$_3$

6	3.002333	-2.219135	0.931040
6	3.357111	-1.493100	-0.359372
8	1.940323	-1.559197	1.613805
F	2.264144	-1.368093	-1.186170
1	3.915615	-2.294538	1.540700
1	2.665743	-3.229660	0.659862
1	2.320040	-0.831969	2.142820
F	3.816189	-0.231165	-0.139950
F	4.308606	-2.164678	-1.054706
6	-3.832477	0.131640	1.032197
6	-4.188473	-0.490339	-0.311497
8	-2.762829	-0.574969	1.655106
F	-3.098800	-0.532421	-1.152186
1	-4.742809	0.152998	1.650054
1	-3.503270	1.162883	0.841872
1	-3.135419	-1.333405	2.144016
F	-4.630452	-1.771141	-0.195180
F	-5.151692	0.224593	-0.944541
6	1.156925	2.065476	-1.237278
6	1.189841	2.581050	0.195401
8	0.010238	1.248689	-1.457899
F	0.135813	3.391822	0.485633
1	2.055312	1.451135	-1.387866
1	1.195074	2.933041	-1.913143
1	-0.740738	1.823392	-1.698737
F	1.144058	1.549414	1.103851
F	2.327296	3.279306	0.440679
K	-0.404181	-0.926439	0.200658

4a-OAc-K-TFE$_3$

7	-3.534524	1.109992	-0.013605
6	-4.680325	1.064590	-0.716899
27	-2.025876	0.169320	-0.667904
7	-1.243867	0.619479	1.146094
6	-5.843559	1.628223	-0.196908
1	-6.774229	1.584900	-0.763457
7	-3.287441	-0.409567	-2.132867
6	-5.782823	2.243803	1.058009
1	-6.683404	2.680798	1.492630
6	-4.570743	2.307662	1.755742
1	-4.499402	2.798675	2.726586
6	-3.444633	1.724230	1.181269
6	-2.037905	1.764885	1.700052
1	-1.573683	2.691585	1.331885
1	-1.995990	1.785407	2.798615
1	-0.271585	0.952241	1.078522
6	-1.265333	-0.595401	2.047954
1	-1.467119	-0.289596	3.085309
1	-0.254143	-1.023859	2.026434
6	-2.254816	-1.587615	1.508112
6	-2.610467	-1.370124	0.176932
6	-3.428559	-2.250136	-0.531266
6	-3.926183	-3.386192	0.120745
1	-4.566150	-4.096393	-0.410200

6	-3.589474	-3.609855	1.465699
1	-3.977654	-4.493552	1.976693
6	-2.750498	-2.723415	2.161215
1	-2.482451	-2.926886	3.201735
6	-3.586419	-1.884456	-1.978671
1	-4.576741	-2.118125	-2.398251
1	-2.836323	-2.419357	-2.582830
1	-2.864654	-0.274609	-3.057240
6	-4.512307	0.459917	-2.079919
1	-5.405537	-0.096542	-2.398084
1	-4.359980	1.282145	-2.796641
8	0.371458	0.408938	-2.134736
8	-1.295289	1.821753	-1.615531
6	-0.209462	1.603063	-2.184489
6	0.514271	2.622007	-2.994028
1	1.590668	2.418445	-3.031818
1	0.316091	3.624705	-2.599376
1	0.120388	2.568969	-4.022655
8	0.008195	-2.719485	-0.523696
8	1.332674	-0.972148	0.069812
6	0.618968	-3.554526	0.510563
6	-0.087545	-4.889883	0.465667
6	0.410186	-1.438997	-0.603272
6	-0.447974	-0.677631	-1.535801
1	1.694623	-3.640800	0.294999
1	0.491284	-3.052764	1.481731
1	0.334082	-5.553605	1.235328
1	-1.162880	-4.766092	0.663022
1	0.041839	-5.371846	-0.514979
1	-0.761118	-1.307829	-2.379854
6	3.402850	-1.660198	2.658247
6	2.511172	-0.822120	3.564147
8	4.334306	-0.848259	1.951486
F	3.203561	-0.222470	4.573729
1	2.751062	-2.150180	1.922456
1	3.891124	-2.425611	3.281327
1	5.079934	-0.635705	2.544063
F	1.882985	0.182677	2.878020
F	1.541418	-1.588484	4.132934
6	3.805714	-0.914460	-3.318934
6	3.711212	-2.175223	-2.467508
8	3.132436	0.180643	-2.716101
F	4.135581	-1.959480	-1.184072
1	3.413631	-1.157538	-4.319514
1	4.870733	-0.657058	-3.402695
1	2.161060	0.073059	-2.822607
F	2.436550	-2.653733	-2.380480
F	4.480949	-3.169526	-2.986608
6	0.855215	3.790416	0.635185
6	2.111684	4.465773	0.103598
8	1.169690	2.506991	1.173221
F	3.033170	4.689756	1.079499
1	0.159236	3.666195	-0.205076
1	0.402112	4.459486	1.381166
1	1.341149	2.612802	2.128299
F	2.739580	3.692446	-0.845273
F	1.821812	5.655198	-0.477857
K	3.243778	0.840876	0.016486

4a-OAc-Li-TFE₂

7	2.733779	-1.642857	-0.009495
6	3.921859	-1.936308	-0.567613
27	1.758283	-0.161220	-0.668900
7	0.605707	-0.496467	0.966522
6	4.717378	-2.944636	-0.026824
1	5.684555	-3.177601	-0.473311
7	3.353500	0.084534	-1.878306

6	4.244067	-3.642667	1.089381
1	4.855517	-4.426589	1.539247
6	2.984449	-3.347293	1.625137
1	2.587689	-3.894821	2.480409
6	2.238981	-2.328495	1.038867
6	0.834073	-1.922515	1.373007
1	0.150816	-2.542694	0.771141
1	0.586999	-2.080962	2.432151
1	-0.394451	-0.408357	0.763112
6	0.924079	0.492981	2.068799
1	0.916847	-0.021671	3.041249
1	0.103594	1.225287	2.085743
6	2.230561	1.164479	1.763584
6	2.683072	0.982834	0.456690
6	3.841680	1.595818	-0.021450
6	4.578037	2.420540	0.839175
1	5.488062	2.916243	0.490024
6	4.134992	2.609126	2.158084
1	4.708115	3.250939	2.830707
6	2.964565	1.989988	2.625068
1	2.628433	2.158022	3.651976
6	4.104978	1.334048	-1.475631
1	5.171585	1.230725	-1.725839
1	3.700775	2.155595	-2.087200
1	3.056086	0.201086	-2.852908
6	4.193361	-1.161548	-1.823528
1	5.259801	-0.922052	-1.941079
1	3.899239	-1.792184	-2.677114
8	-0.235730	0.622286	-2.522610
8	0.697958	-1.343984	-1.955132
6	-0.097953	-0.688996	-2.658675
6	-0.970659	-1.297403	-3.701023
1	-0.582242	-1.016874	-4.693038
1	-1.991769	-0.900931	-3.619308
1	-0.969498	-2.388067	-3.604633
8	0.634719	3.170809	-0.247784
8	-1.194363	1.838687	-0.224853
6	0.058110	4.008427	0.810593
6	1.115226	5.021800	1.183787
6	-0.057227	2.103846	-0.653468
6	0.716881	1.271427	-1.590482
1	-0.855490	4.475732	0.413481
1	-0.215983	3.364114	1.658445
1	0.734092	5.666756	1.989510
1	2.025530	4.517967	1.541594
1	1.374297	5.659016	0.325443
1	1.371059	1.893505	-2.215868
6	-3.394614	-2.274024	-0.312452
6	-3.336170	-2.835224	1.102014
8	-2.327348	-1.349643	-0.538991
F	-2.195850	-3.550333	1.323595
1	-4.345395	-1.736778	-0.426073
1	-3.363071	-3.114013	-1.021579
1	-1.507231	-1.847326	-0.722472
F	-3.373899	-1.855627	2.047216
F	-4.389398	-3.664692	1.327416
6	-5.144491	0.839542	1.025671
6	-5.826489	1.277035	-0.263122
8	-3.746184	1.119705	0.968843
F	-5.791050	2.626485	-0.439387
1	-5.274230	-0.245569	1.128129
1	-5.634281	1.346679	1.869059
1	-3.588347	2.045937	1.236030
F	-5.213859	0.726014	-1.359931
F	-7.126349	0.890439	-0.284654
Li	-2.558962	0.578403	-0.478459

4a-OAc-Li-TFE₃

7	-1.990216	-1.678786	-0.403851
6	-3.274089	-1.933082	-0.099159
27	-1.039282	-0.411915	0.620088
7	0.346226	-0.608301	-0.833398
6	-4.017474	-2.805622	-0.892977
1	-5.061425	-3.009836	-0.653215
7	-2.784101	-0.189199	1.599128
6	-3.391888	-3.407135	-1.989718
1	-3.957008	-4.083979	-2.632703
6	-2.041041	-3.154827	-2.261322
1	-1.530786	-3.632647	-3.097989
6	-1.353220	-2.275491	-1.431032
6	0.113212	-1.950012	-1.462911
1	0.637797	-2.692986	-0.841445
1	0.534856	-1.995706	-2.477017
1	1.295202	-0.614189	-0.445863
6	0.267070	0.538870	-1.823453
1	0.401251	0.155208	-2.845812
1	1.115828	1.205510	-1.610329
6	-1.030407	1.268075	-1.626810
6	-1.690880	0.957827	-0.440248
6	-2.857363	1.609518	-0.038329
6	-3.400062	2.597502	-0.869170
1	-4.312433	3.126840	-0.581305
6	-2.753531	2.911035	-2.076471
1	-3.175547	3.680243	-2.726787
6	-1.567729	2.262059	-2.455934
1	-1.067663	2.535629	-3.389123
6	-3.316511	1.198247	1.329712
1	-4.407165	1.228133	1.474610
1	-2.859398	1.856437	2.086173
1	-2.646990	-0.281703	2.611160
6	-3.728192	-1.283848	1.177216
1	-4.756304	-0.903522	1.097032
1	-3.720712	-2.050080	1.967887
8	1.008953	-0.213868	2.537970
8	-0.291546	-1.897857	1.813075
6	0.645246	-1.508120	2.525168
6	1.443715	-2.391114	3.417522
1	1.226861	-2.128221	4.464706
1	2.519578	-2.230702	3.253327
1	1.184715	-3.438820	3.233788
8	0.098133	2.865667	0.990707
6	0.721145	3.897015	0.146509
6	-0.283734	5.014289	0.002138
6	0.807079	1.765101	1.225339
6	0.023134	0.704776	1.879139
1	1.648872	4.226588	0.636474
1	0.971571	3.432788	-0.819179
1	0.147296	5.804305	-0.631023
1	-1.206465	4.653182	-0.475384
1	-0.532093	5.451862	0.980263
1	-0.617780	1.099841	2.680211
8	1.997331	1.633474	0.873165
6	5.284102	0.194101	-0.021675
6	4.812113	-0.592470	-1.237807
8	4.646310	-0.270518	1.169200
F	5.106516	-1.918790	-1.147072
1	5.006886	1.245761	-0.173103
1	6.378022	0.107981	0.043375
1	5.110633	-1.058529	1.510029
F	3.459142	-0.503766	-1.409845
F	5.397221	-0.116597	-2.367667
Li	2.975374	0.327772	1.826553

4a-OAc-PhNO₂-Li-TFE₃

7	1.467484	-3.261456	-0.490475
6	2.510118	-3.732350	-1.201410
27	1.265302	-1.394050	-0.295678
7	-0.269203	-1.930898	0.916468
6	2.720125	-5.104844	-1.308682
1	3.573533	-5.483691	-1.871598
7	3.080546	-1.347436	-1.197305
6	1.808845	-5.969862	-0.693076
1	1.961069	-7.048930	-0.748750
6	0.687566	-5.456502	-0.031809
1	-0.061601	-6.113208	0.411177
6	0.534103	-4.074595	0.041122
6	-0.663708	-3.322935	0.536900
1	-1.371243	-3.237130	-0.303729
1	-1.178515	-3.832918	1.363156
1	-1.088976	-1.338138	0.748518
6	0.112250	-1.803658	2.378617
1	-0.203386	-2.712005	2.912861
1	-0.466181	-0.973523	2.805268
6	1.590898	-1.573292	2.484834
6	2.250692	-1.381746	1.270376
6	3.636135	-1.223930	1.193509
6	4.378616	-1.184669	2.381088
1	5.462746	-1.045573	2.350793
6	3.720391	-1.325380	3.612134
1	4.298356	-1.290091	4.538216
6	2.333145	-1.530697	3.672108
1	1.838821	-1.662961	4.638321
6	4.188588	-1.086105	-0.195066
1	5.016221	-1.786434	-0.382173
1	4.577154	-0.075459	-0.381579
1	3.119623	-0.604840	-1.904441
6	3.249970	-2.646864	-1.922329
1	4.311554	-2.883544	-2.078578
1	2.780098	-2.529477	-2.911916
8	0.104158	0.821923	-1.669130
8	0.230574	-1.391600	-2.035843
6	-0.137003	-0.264715	-2.400957
6	-0.873071	-0.000174	-3.667024
1	-0.401863	0.832032	-4.208428
1	-1.903710	0.305150	-3.427646
1	-0.887097	-0.904428	-4.283978
8	0.446435	1.384889	1.829501
8	-1.332636	0.910397	0.548397
6	-0.455810	1.757135	2.929453
6	0.408619	1.948065	4.153109
6	-0.106753	1.012167	0.679576
6	0.868403	0.661946	-0.404140
1	-0.980638	2.675460	2.628225
1	-1.197950	0.956863	3.062926
1	-0.230630	2.216922	5.007292
1	0.946937	1.021405	4.400944
1	1.140355	2.754757	4.002130
6	2.125515	1.458339	-0.518634
6	2.913639	1.798078	0.608061
6	2.610904	1.825396	-1.796698
6	4.116948	2.473755	0.466927
6	3.822561	2.487629	-1.949506
6	4.570066	2.809781	-0.813057
1	2.600066	1.505006	1.603775
1	2.036455	1.586941	-2.690721
1	4.715521	2.717186	1.343819
1	4.184090	2.759309	-2.940605
7	5.849870	3.492261	-0.966989
8	6.250043	3.753533	-2.114612
8	6.493310	3.784658	0.055043
6	-4.337333	1.266405	1.937693

6	-4.377707	-0.102041	2.604934
8	-4.374121	1.151513	0.519394
F	-5.510781	-0.793181	2.300587
1	-3.390837	1.745639	2.218299
1	-5.178522	1.858750	2.327221
1	-5.288080	0.984831	0.222247
F	-3.326731	-0.895860	2.228586
F	-4.319524	0.022189	3.956575
6	-2.636731	3.741508	-1.703783
6	-2.164238	4.327753	-0.378712
8	-2.318495	2.357318	-1.804782
F	-2.797244	3.776248	0.693576
1	-2.172921	4.325745	-2.513408
1	-3.727735	3.848467	-1.753997
1	-1.344539	2.260895	-1.882205
F	-0.825988	4.130575	-0.188330
F	-2.391100	5.668483	-0.339134
6	-3.540691	-1.848475	-1.950055
6	-4.846634	-1.155191	-2.312043
8	-2.915957	-1.180227	-0.854294
F	-5.763871	-1.225978	-1.305625
1	-2.871946	-1.791424	-2.817467
1	-3.758368	-2.902323	-1.724874
1	-3.311439	-1.510599	-0.023393
F	-4.651217	0.176803	-2.565425
F	-5.405161	-1.705143	-3.418696
Li	-2.820975	0.845779	-0.617817

4a-OAc-Li-TFE

7	-3.460893	1.329463	0.045987
6	-4.678009	1.270045	-0.521013
27	-2.070980	0.254552	-0.650170
7	-1.098483	0.827955	1.021158
6	-5.742637	1.974847	0.039141
1	-6.733511	1.921105	-0.412802
7	-3.493228	-0.395739	-1.926849
6	-5.504995	2.746291	1.181485
1	-6.325648	3.296338	1.644999
6	-4.217323	2.824979	1.727310
1	-4.007978	3.438666	2.603901
6	-3.197909	2.095913	1.122603
6	-1.735740	2.109992	1.462799
1	-1.264476	2.919159	0.882912
1	-1.550886	2.305874	2.528824
1	-0.107156	1.043618	0.837987
6	-1.147926	-0.253468	2.080822
1	-1.331621	0.200750	3.066060
1	-0.151648	-0.715959	2.115821
6	-2.180912	-1.273763	1.698187
6	-2.630918	-1.174430	0.382696
6	-3.526525	-2.088779	-0.172787
6	-3.998738	-3.141782	0.620507
1	-4.698046	-3.876293	0.211500
6	-3.557469	-3.252545	1.949472
1	-3.923469	-4.073601	2.569733
6	-2.646833	-2.331196	2.491288
1	-2.302549	-2.443039	3.523246
6	-3.787037	-1.848334	-1.631294
1	-4.804736	-2.108122	-1.960446
1	-3.080402	-2.439560	-2.234745
1	-3.168965	-0.333707	-2.897706
6	-4.702653	0.491389	-1.804552
1	-5.628226	-0.091926	-1.911531
1	-4.670028	1.212123	-2.636327
8	0.241862	0.327275	-2.258178
8	-1.363432	1.813781	-1.752009
6	-0.290083	1.546032	-2.320157

6	0.498048	2.524224	-3.117852
1	1.538273	2.545791	-2.760900
1	0.048337	3.519355	-3.041695
1	0.516918	2.199528	-4.169468
8	-0.184688	-2.718704	-0.506378
8	1.218635	-1.011369	-0.021783
6	0.405021	-3.511295	0.578298
6	-0.323097	-4.835194	0.595112
6	0.256982	-1.464546	-0.658782
6	-0.593572	-0.702133	-1.589333
1	1.480324	-3.624967	0.376181
1	0.271941	-2.956056	1.518992
1	0.082827	-5.463412	1.402030
1	-1.397448	-4.685191	0.778491
1	-0.193044	-5.368943	-0.358070
1	-0.984144	-1.342978	-2.391726
6	3.653825	-1.218056	2.060472
6	3.154315	-0.623387	3.369736
8	3.883537	-0.200988	1.090616
F	4.054122	0.236627	3.923141
1	2.872179	-1.884855	1.674071
1	4.562930	-1.799846	2.274969
1	4.722244	0.259249	1.281796
F	1.991918	0.084313	3.207451
F	2.903306	-1.601538	4.277937
6	3.907476	-0.729209	-2.796258
6	3.593857	-2.173715	-2.422030
8	3.030525	0.186497	-2.149479
F	3.761538	-2.415795	-1.092591
1	3.848544	-0.645038	-3.892090
1	4.933316	-0.513474	-2.469441
1	2.139886	0.134314	-2.564286
F	2.305655	-2.512799	-2.724370
F	4.409459	-3.028436	-3.097826
6	1.636627	3.272162	0.459617
6	2.989594	3.790618	-0.006497
8	1.711637	1.878471	0.764208
F	3.941198	3.692270	0.964336
1	0.918369	3.410770	-0.357592
1	1.318681	3.863843	1.329490
1	2.034834	1.771140	1.680895
F	3.454615	3.089420	-1.082447
F	2.904772	5.095904	-0.371224
Li	2.558332	0.337775	-0.240039

Na-TFE$_3$

6	3.000613	-1.710995	0.893601
6	3.130979	-0.841454	-0.350043
8	1.626405	-1.980113	1.174694
F	2.670876	-1.459595	-1.470205
1	3.423712	-1.150877	1.738810
1	3.583050	-2.630355	0.735836
1	1.344556	-2.754626	0.650613
F	2.403692	0.319885	-0.221760
F	4.420472	-0.486579	-0.571281
6	-3.010913	-0.570850	0.127873
6	-2.498932	-1.892136	-0.427657
8	-2.273112	-0.203196	1.293801
F	-1.147624	-1.832845	-0.680322
1	-4.087367	-0.671219	0.328225
1	-2.853212	0.198257	-0.640333
1	-2.704170	-0.600605	2.074131
F	-2.682123	-2.927373	0.435755
F	-3.112882	-2.209928	-1.593329
6	-0.839956	2.886505	1.038297
6	-0.533926	2.813684	-0.451661
8	0.071469	2.082622	1.786455

F	0.676335	3.348145	-0.766160
1	-1.851584	2.484620	1.188940
1	-0.815436	3.943126	1.343304
1	0.900158	2.581492	1.919317
F	-0.509811	1.512711	-0.895768
F	-1.476605	3.468142	-1.175482
Na	0.090368	-0.208718	1.280550

4a-OAc-Na-TFE₃

7	-3.423054	1.270492	-0.000671
6	-4.580035	1.297811	-0.685206
27	-1.988373	0.234370	-0.671676
7	-1.158992	0.631323	1.131043
6	-5.690008	1.953284	-0.154716
1	-6.630867	1.970214	-0.705628
7	-3.300205	-0.261902	-2.121917
6	-5.562469	2.582356	1.088209
1	-6.421094	3.090780	1.530012
6	-4.336440	2.569838	1.764476
1	-4.211904	3.071980	2.724333
6	-3.266297	1.897997	1.180995
6	-1.848366	1.849260	1.668879
1	-1.323306	2.725419	1.258616
1	-1.777417	1.899802	2.764855
1	-0.162806	0.878260	1.048461
6	-1.277024	-0.565628	2.050858
1	-1.492610	-0.229874	3.076178
1	-0.291239	-1.050751	2.072433
6	-2.308682	-1.508908	1.503073
6	-2.655461	-1.270599	0.173585
6	-3.524382	-2.102380	-0.532723
6	-4.079667	-3.211874	0.118465
1	-4.761415	-3.883736	-0.410376
6	-3.747478	-3.458517	1.460475
1	-4.179873	-4.321748	1.971036
6	-2.860527	-2.619397	2.154900
1	-2.600710	-2.838731	3.194321
6	-3.675273	-1.720161	-1.976519
1	-4.681199	-1.895864	-2.387059
1	-2.962127	-2.290855	-2.592337
1	-2.882381	-0.139030	-3.050205
6	-4.481507	0.665745	-2.043165
1	-5.408253	0.143943	-2.321593
1	-4.319646	1.469164	-2.778642
8	0.394141	0.343910	-2.178333
8	-1.182994	1.843819	-1.622604
6	-0.120318	1.570285	-2.209327
6	0.662198	2.551565	-3.009898
1	1.738507	2.422342	-2.839848
1	0.348015	3.572269	-2.768045
1	0.467038	2.355336	-4.076878
8	-0.082330	-2.739677	-0.509620
8	1.305252	-1.035241	0.046033
6	0.509465	-3.572371	0.540073
6	-0.229347	-4.890567	0.515418
6	0.361529	-1.478673	-0.618301
6	-0.466514	-0.697417	-1.558235
1	1.582609	-3.686930	0.326097
1	0.393885	-3.051691	1.502291
1	0.177510	-5.552778	1.294253
1	-1.301187	-4.738306	0.712545
1	-0.112413	-5.389188	-0.458391
1	-0.822525	-1.323042	-2.388052
6	3.415438	-1.320589	2.545347
6	2.577049	-0.662866	3.632892
8	4.018265	-0.347359	1.697531
F	3.327772	0.075809	4.497896

1	2.740237	-1.935158	1.935004
1	4.158805	-1.967143	3.035650
1	4.823501	-0.000949	2.125853
F	1.635508	0.184670	3.116622
F	1.915759	-1.601524	4.362704
6	3.976548	-0.896619	-3.050674
6	3.754500	-2.228042	-2.344030
8	3.193029	0.138734	-2.469936
F	4.009206	-2.143946	-1.004416
1	3.755225	-1.040218	-4.119715
1	5.035893	-0.631656	-2.932074
1	2.257690	0.041273	-2.755191
F	2.470435	-2.673925	-2.470397
F	4.570759	-3.188348	-2.854588
6	1.283915	3.523262	0.518115
6	2.593509	4.088476	-0.012506
8	1.479008	2.199081	1.015893
F	3.512725	4.278799	0.971716
1	0.570371	3.482618	-0.314739
1	0.901985	4.209054	1.287877
1	1.740627	2.254927	1.955475
F	3.174811	3.237424	-0.922803
F	2.399760	5.275717	-0.636245
Na	2.892834	0.570274	-0.139938

TFE₂

6	1.394519	-0.463350	0.878193
6	2.505970	-0.196809	-0.129622
8	0.891672	0.737697	1.431687
F	2.073402	0.532948	-1.202047
1	1.831197	-1.074749	1.682103
1	0.622415	-1.057836	0.361433
1	0.217202	1.098458	0.797914
F	3.548168	0.494823	0.413476
F	3.009729	-1.367371	-0.620061
6	-2.287347	1.202909	-0.379726
6	-2.478929	-0.266545	-0.024300
8	-0.912029	1.554380	-0.488403
F	-1.911389	-1.098729	-0.945718
1	-2.725867	1.798913	0.431875
1	-2.838334	1.396686	-1.313133
1	-0.563169	1.221648	-1.337656
F	-1.934541	-0.588370	1.182203
F	-3.806021	-0.570742	0.034804

TFE

6	-0.910521	0.766692	-0.098947
6	0.413671	0.017854	-0.001712
8	-2.017367	-0.094959	0.117335
F	0.581964	-0.583705	1.209521
1	-0.938020	1.268493	-1.080328
1	-0.912451	1.528661	0.693632
1	-2.162093	-0.623403	-0.690169
F	0.523069	-0.964380	-0.944905
F	1.465256	0.867934	-0.182156

TFE₃

6	-1.976622	-0.891946	0.643073
6	-3.310993	-0.894932	-0.087663
8	-0.946059	-1.451581	-0.171897
F	-3.272662	-0.138185	-1.223248
1	-2.077895	-1.524540	1.534482
1	-1.753997	0.141504	0.952074
1	-0.709270	-0.801379	-0.862671
F	-3.696545	-2.146029	-0.463332
F	-4.293121	-0.385645	0.706927
6	0.927926	2.332669	1.089817

6	0.177011	2.353309	-0.236056
8	0.469978	1.306361	1.946312
F	0.380737	1.214887	-0.969883
1	0.742289	3.304686	1.572070
1	2.002081	2.257276	0.852886
1	0.887943	0.438394	1.690291
F	-1.171778	2.470657	-0.073285
F	0.583745	3.399852	-1.009441
6	2.442870	-1.824788	0.966615

6	2.961100	-1.167184	-0.305273
8	1.230744	-1.245432	1.417361
F	2.089788	-1.303218	-1.347339
1	3.205933	-1.684723	1.745004
1	2.336779	-2.902128	0.756715
1	0.484644	-1.472174	0.791639
F	3.185038	0.168018	-0.151285
F	4.141068	-1.733057	-0.690200

10. Crystallographic data information

10.1 X-Ray structure of **4a-OPiv** (CCDC-1825084)

Orange crystals of **(C$_{24}$H$_{31}$CoN$_3$O$_4$)Br**, were grown from slow diffusion of pentane in a CHCl$_3$ solution of the compound, and used for low temperature (100(2) K) X-ray structure determination. The measurement was carried out on a *BRUKER SMART APEX CCD* diffractometer using graphite-monochromated Mo *K*α radiation ($\lambda = 0.71073$ Å) from an x-Ray Tube. The measurements were made in the range 1.8 to 27.500° for θ. Hemi-sphere data collection was carried out with ω and φ scans. A total of 11797 reflections were collected of which 5423 [R(int) = 0.031] were unique. Programs used: data collection, Smart[21]; data reduction, Saint+[22]; absorption correction, SADABS[23]. Structure solution and refinement was done using SHELXTL[24]. The structure was solved by direct methods and refined by full-matrix least-squares methods on F^2. The non-hydrogen atoms were refined anisotropically. The H-atoms were placed in geometrically optimized positions and forced to ride on the atom to which they are attached.

Table S11. Crystallographic parameters for **4a-OPiv**.

Chemical formula	C$_{24}$H$_{31}$CoN$_3$O$_4$Br
fw (g mol^{-1})	564.36
T (K)	100 (2)
Space group	Triclinic, P-1
a (Å)	10.302(4)
b (Å)	10.479(4)
c (Å)	12.612(4)
α (deg.)	72.875(6)
β (deg.)	70.700(6)
γ (deg.)	76.245(6)
V (Å^3)	1213.1(8)
ρ$_{calcd.}$ (g cm^{-3})	1.545
λ (Å)	0.71073
R$_1$ [I>2sigma(I)]	0.0663
*w*R$_2$ [I>2sigma(I)]	0.1820

10.2 X-Ray structure of **4a-OBz** (CCDC-1825085)

Orange crystals of $(C_{33}H_{30}CoN_3O_6)(C_7O_2H_5)$, were grown from slow diffusion of pentane in a $CHCl_3$ solution of the compound, and used for low temperature (100(2) K) X-ray structure determination. The measurement was carried out on a *BRUKER SMART APEX CCD* diffractometer using graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0.71073$ Å) from an x-Ray Tube. The measurements were made in the range 1.576 to 28.274° for θ. Full-sphere data collection was carried out with ω and φ scans. A total of 13012 reflections were collected of which 8251 [R(int) = 0.0378] were unique. Programs used: data collection, Smart[21]; data reduction, Saint+[22]; absorption correction, SADABS[23]. Structure solution and refinement was done using SHELXTL[24]. The structure was solved by dual-space algorithm and refined by full-matrix least-squares methods on F^2. The non-hydrogen atoms were refined anisotropically. The H-atoms were placed in geometrically optimized positions and forced to ride on the atom to which they are attached. A considerable amount of electron density attributable to a heavylly disordered Benzoate counterion molecule per asymmetric unit was removed with the SQUEEZE option of PLATON.[25] Those Benzoate molecules are, however, included in the reported chemical formula and derived values (e.g. formula weight, F(000), etc.).

Table S12. Crystallographic parameters for **4a-OBz**.

Chemical formula	$C_{33}H_{30}CoN_3O_6$
fw (g mol^{-1})	623.53
T (K)	100 (2)
Space group	Triclinic, P-1
a (Å)	11.416(3)
b (Å)	13.616(4)
c (Å)	13.991(3)
α (deg.)	73.027(5)
β (deg.)	70.324(4)
γ (deg.)	69.364(5)
V (Å^3)	1879.0(8)
$\rho_{calcd.}$ (g cm^{-3})	1.102
λ (Å)	0.71073
R_1 [I>2sigma(I)]	0.0695
wR_2 [I>2sigma(I)]	0.2061

10.3 X-Ray structure of **4a-OBz-NO₂** (CCDC-1825086)

Orange crystals of $(C_{26}H_{26}CoN_4O_6)_2(C_7H_4O_2)$ + [solvent], were grown from slow diffusion of pentane in a CHCl₃ solution of the compound, and used for low temperature (100(2) K) X-ray structure determination. The measurement was carried out on a *BRUKER SMART APEX CCD* diffractometer using graphite-monochromated Mo *K*α radiation (λ = 0.71073 Å) from an x-Ray Tube. The measurements were made in the range 1.396 to 24.500° for θ. Hemi-sphere data collection was carried out with ω and φ scans. A total of 13983 reflections were collected of which 7327 [R(int) = 0.1749] were unique. Programs used: data collection, Smart[21]; data reduction, Saint+[22]; absorption correction, SADABS[23]. Structure solution and refinement was done using SHELXTL[24]. The structure was solved by direct methods and refined by full-matrix least-squares methods on F^2. The non-hydrogen atoms were refined anisotropically. The H-atoms were placed in geometrically optimized positions and forced to ride on the atom to which they are attached. A considerable amount of electron density attributable to a disordered solvent molecules, which cannot be identified, was removed with the SQUEEZE option of PLATON.[25]

Table S13. Crystallographic parameters for **4a-OBz-NO₂**.

Chemical formula	$C_{40}H_{34}CoN_6O_{14}$
fw (g mol⁻¹)	881.66
T (K)	100 (2)
Space group	Triclinic, P-1
a (Å)	11.724(2)
b (Å)	14.00(2)
c (Å)	15.95(3)
α (deg.)	66.86(5)
β (deg.)	76.56(3)
γ (deg.)	68.44(3)
V (Å³)	2228(6)
ρ_calcd. (g cm⁻³)	1.314
λ (Å)	0.71073
R₁ [I>2sigma(I)]	0.1186
*w*R₂ [I>2sigma(I)]	0.2708

10.4 X-Ray structure of **4a-COMe** (CCDC-1825087)

Orange crystals of $(C_{28}H_{29}CoN_3O_5)(C_9H_8O_3)(C_9H_7O_3)$, were grown from slow diffusion of pentane in a CHCl$_3$ solution of the compound, and used for low temperature (100(2) K) X-ray structure determination. The measurement was carried out on a *BRUKER SMART APEX CCD* diffractometer using graphite-monochromated Mo *K*α radiation (λ = 0.71073 Å) from an x-Ray Tube. The measurements were made in the range 2.196to 26.900° for θ. Full-sphere data collection was carried out with ω and φ scans. A total of 36681 reflections were collected of which 11005 [R(int) = 0.1300] were unique. Programs used: data collection, Smart[21]; data reduction, Saint+;[22] absorption correction, SADABS.[23] Structure solution and refinement was done using SHELXTL.[24] The structure was solved by direct methods and refined by full-matrix least-squares methods on F^2. The non-hydrogen atoms were refined anisotropically. The H-atoms were placed in geometrically optimized positions and forced to ride on the atom to which they are attached. Spurious electron density peaks non attribuitable to any solvent molecule were removed using the SQUEEZE option in PLATON.[25]

Table S14. Crystallographic parameters for **4a-OBz-COMe**.

Chemical formula	$C_{46}H_{44}CoN_3O_{11}$
fw (g mol^{-1})	873.77
T (K)	100 (2)
Space group	Triclinic, P-1
a (Å)	11.930(9)
b (Å)	14.213(11)
c (Å)	17.277(13)
α (deg.)	98.862(12)
β (deg.)	101.804(13)
γ (deg.)	112.978(12)
V (Å^3)	2550(3)
$\rho_{calcd.}$ (g cm^{-3})	1.138
λ (Å)	0.71073
R$_1$ [I>2sigma(I)]	0.1128
*w*R$_2$ [I>2sigma(I)]	0.3113

11. Description of organic products
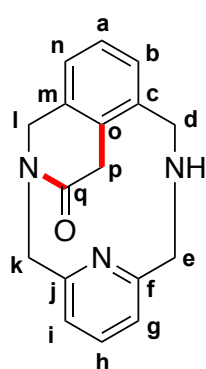
3a, ^{1}H NMR (400 MHz, CDCl$_3$, ppm) δ 7.23 (t, ^3J_H = 6.0 Hz, 1H, **Hh**), 6.85 (d, ^3J_H = 7.2 Hz, 1H, **Hb**), 6.69 (t, ^3J_H = 7.5 Hz, 1H, **Ha**), 6.66 (t, ^3J_H = 7.6 Hz 1H, **Hi**), 6.53-6.52 (m, 2H, **Hn**, **Hg**), 5.67 (d, ^2J_H = 15.8 Hz, 1H, **Hk**), 4.75 (d, ^2J_H = 15.4 Hz, 1H, **Hl**), 4.61 (d, ^2J_H = 14.3 Hz, 1H, **Hd**), 4.19 (d, ^2J_H = 15.8 Hz, 1H, **Hp**), 4.10 (d, ^2J_H = 15.9 Hz, 1H, **He**), 3.92 (d, ^2J_H = 15.9 Hz, 1H, **Hk'**), 3.82 (d, ^2J_H = 15.5 Hz, 1H, **Hl'**), 3.53 (d, ^2J_H = 16.1Hz, 1H, **Hp'**), 3.48 (d, ^2J_H = 14.8 Hz, 1H, **He'**), 3.44 (d, ^2J_H = 15.1Hz, 1H, **Hd'**).

^{13}C {^{1}H} NMR (100 MHz, CDCl$_3$, ppm) δ 180.5 (**Cq**), 158.2 (**Cj**), 152.6 (**Cf**), 137.7 (**Cm**), 137.4 (**Co**), 136.3 (**Ch**), 135.2 (**Cc**), 128.5 (**Cb**), 124.5 (**Ca**), 123.8 (**Cn**), 119.0 (**Cg**), 118.6 (**Ci**), 58.8 (**Ck**), 54.3 (**Cl**), 52.9 (**Cd**), 51.3 (**Ce**), 39.5 (**Cp**).

HRMS (ESI-QTOF) calcd. for C$_{17}$H$_{18}$N$_3$O$^+$ [M+H]$^+$: 280.1445; found: 280.1439.

IR (ATR): ῡ (C=O) = 1670 cm^{-1}.

3l, ^{1}H NMR (400 MHz, CDCl$_3$, ppm) δ 8.16 (d, ^3J_H = 7.1 Hz, 1H, **Hu**), 7.41 (d, ^3J_H = 7.2 Hz, 1H, **Hs**), 7.28 (t, **Hh**), 7.00 (d, ^3J_H = 6.6 Hz, 1H, **Hn**), 6.83 (t, ^3J_H = 7.9 Hz, 1H, **Ha**), 6.71 (d, ^3J_H = 7.4 Hz, 1H, **Hg**), 6.58 (d, ^3J_H = 7.2 Hz 1H, **Hi**), 6.56 (d, ^3J_H = 7.7 Hz, 1H, **Hb**), 5.85 (s, **Hp**), 5.78 (d, ^2J_H = 16.3 Hz, 1H, **Hk**), 4.62 (d, ^2J_H = 15.2 Hz, 1H, **Hl**), 4.30 (d, ^2J_H = 14.7 Hz, 1H, **Hd**), 4.16 (d, ^2J_H = 15.6 Hz, 1H, **He**), 3.99 (d, ^2J_H = 15.2 Hz, 1H, **Hk'**), 3.61 (d, ^2J_H = 15.6 Hz, 1H, **Hl'**), 3.57 (d, ^2J_H = 15.2 Hz, 1H, **Hd'**), 3.53 (d, ^2J_H = 15.7Hz, 1H, **He'**).

^{13}C {^{1}H} NMR (100 MHz, CDCl$_3$, ppm) δ 178.9 (**Cq**), 158.7 (**Cj**), 152.1 (**Cf**), 147.1 (**Cu**), 143.9 (**Cr**), 138.6 (**Cm**), 137.7 (**Co**), 136.2 (**Ch**), 130.5 (**Cc**), 129.0 (**Cn**), 128.2 (**Cs**), 125.8 (**Ca**), 124.6 (**Cb**), 123.8 (**Ct**), 119.3 (**Ci**), 118.6 (**Cg**), 59.1 (**Ck**), 54.0 (**Cp**), 52.8 (**Cl**), 52.7 (**Cd**), 51.3 (**Ce**).

HRMS (ESI-QTOF) calcd. for C$_{23}$H$_{20}$N$_4$O$_3$$^+$ [M+H]$^+$: 401.1608; found: 401.1609.

IR (ATR): ῡ = 1668 (C=O), 1516 (NO$_2$), 1343 (NO$_2$) cm^{-1}

3j, ^{1}H NMR (400 MHz, CDCl$_3$, ppm) δ 8.16 (d, ^3J_H= 7.1 Hz, 1H, **Hu**), 7.41 (d, ^3J_H= 7.2 Hz, 1H, **Hs**), 7.28 (t, **Hh**), 7.00 (d, ^3J_H= 6.6 Hz, 1H, **Hn**), 6.83 (t, ^3J_H= 7.9 Hz, 1H, **Ha**), 6.71 (d, ^3J_H= 7.4 Hz, 1H, **Hg**), 6.58 (d, ^3J_H= 7.2 Hz 1H, **Hi**), 6.56 (d, ^3J_H= 7.7 Hz, 1H, **Hb**), 5.85 (s, **Hp**), 5.78 (d, ^2J_H= 16.3 Hz, 1H, **Hk**), 4.62 (d, ^2J_H= 15.2 Hz, 1H, **Hl**), 4.30 (d, ^2J_H= 14.7 Hz, 1H, **Hd**), 4.16 (d, ^2J_H= 15.6 Hz, 1H, **He**), 3.99 (d, ^2J_H= 15.2 Hz, 1H, **Hk'**), 3.61 (d, ^2J_H= 15.6 Hz, 1H, **Hl'**), 3.57 (d, ^2J_H= 15.2 Hz, 1H, **Hd'**), 3.53 (d, ^2J_H= 15.7Hz, 1H, **He'**).

^{13}C {^{1}H} NMR (100 MHz, CDCl$_3$, ppm) δ 178.9 (**Cq**), 158.7 (**Cj**), 152.1 (**Cf**), 147.1 (**Cu**), 143.9 (**Cr**), 138.6 (**Cm**), 137.7 (**Co**), 136.2 (**Ch**), 130.5 (**Cc**), 129.0 (**Cn**), 128.2 (**Cs**), 125.8 (**Ca**), 124.6 (**Cb**), 123.8 (**Ct**), 119.3 (**Ci**), 118.6 (**Cg**), 59.1 (**Ck**), 54.0 (**Cp**), 52.8 (**Cl**), 52.7 (**Cd**), 51.3 (**Ce**).

HRMS (ESI-QTOF) calcd. for C$_{23}$H$_{20}$N$_4$O$_3^+$ [M+H]$^+$: 401.1608; found: 401.1609.

IR (ATR): ῡ = 1671 (C=O) cm^{-1}.

3k, ^{1}H NMR (400 MHz, CDCl$_3$, ppm) δ 8.16 (d, ^3J_H= 7.1 Hz, 1H, **Hu**), 7.41 (d, ^3J_H= 7.2 Hz, 1H, **Hs**), 7.28 (t, **Hh**), 7.00 (d, ^3J_H= 6.6 Hz, 1H, **Hn**), 6.83 (t, ^3J_H= 7.9 Hz, 1H, **Ha**), 6.71 (d, ^3J_H= 7.4 Hz, 1H, **Hg**), 6.58 (d, ^3J_H= 7.2 Hz 1H, **Hi**), 6.56 (d, ^3J_H= 7.7 Hz, 1H, **Hb**), 5.85 (s, **Hp**), 5.78 (d, ^2J_H= 16.3 Hz, 1H, **Hk**), 4.62 (d, ^2J_H= 15.2 Hz, 1H, **Hl**), 4.30 (d, ^2J_H= 14.7 Hz, 1H, **Hd**), 4.16 (d, ^2J_H= 15.6 Hz, 1H, **He**), 3.99 (d, ^2J_H= 15.2 Hz, 1H, **Hk'**), 3.61 (d, ^2J_H= 15.6 Hz, 1H, **Hl'**), 3.57 (d, ^2J_H= 15.2 Hz, 1H, **Hd'**), 3.53 (d, ^2J_H= 15.7Hz, 1H, **He'**).

^{13}C {^{1}H} NMR (100 MHz, CDCl$_3$, ppm) δ 178.9 (**Cq**), 158.7 (**Cj**), 152.1 (**Cf**), 147.1 (**Cu**), 143.9 (**Cr**), 138.6 (**Cm**), 137.7 (**Co**), 136.2 (**Ch**), 130.5 (**Cc**), 129.0 (**Cn**), 128.2 (**Cs**), 125.8 (**Ca**), 124.6 (**Cb**), 123.8 (**Ct**), 119.3 (**Ci**), 118.6 (**Cg**), 59.1 (**Ck**), 54.0 (**Cp**), 52.8 (**Cl**), 52.7 (**Cd**), 51.3 (**Ce**).

HRMS (ESI-QTOF) calcd. for C$_{23}$H$_{20}$N$_4$O$_3^+$ [M+H]$^+$: 401.1608; found: 401.1609.

IR (ATR): ῡ = 1671 (C=O) cm^{-1}.

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13. Original NMR and FT-IR spectra
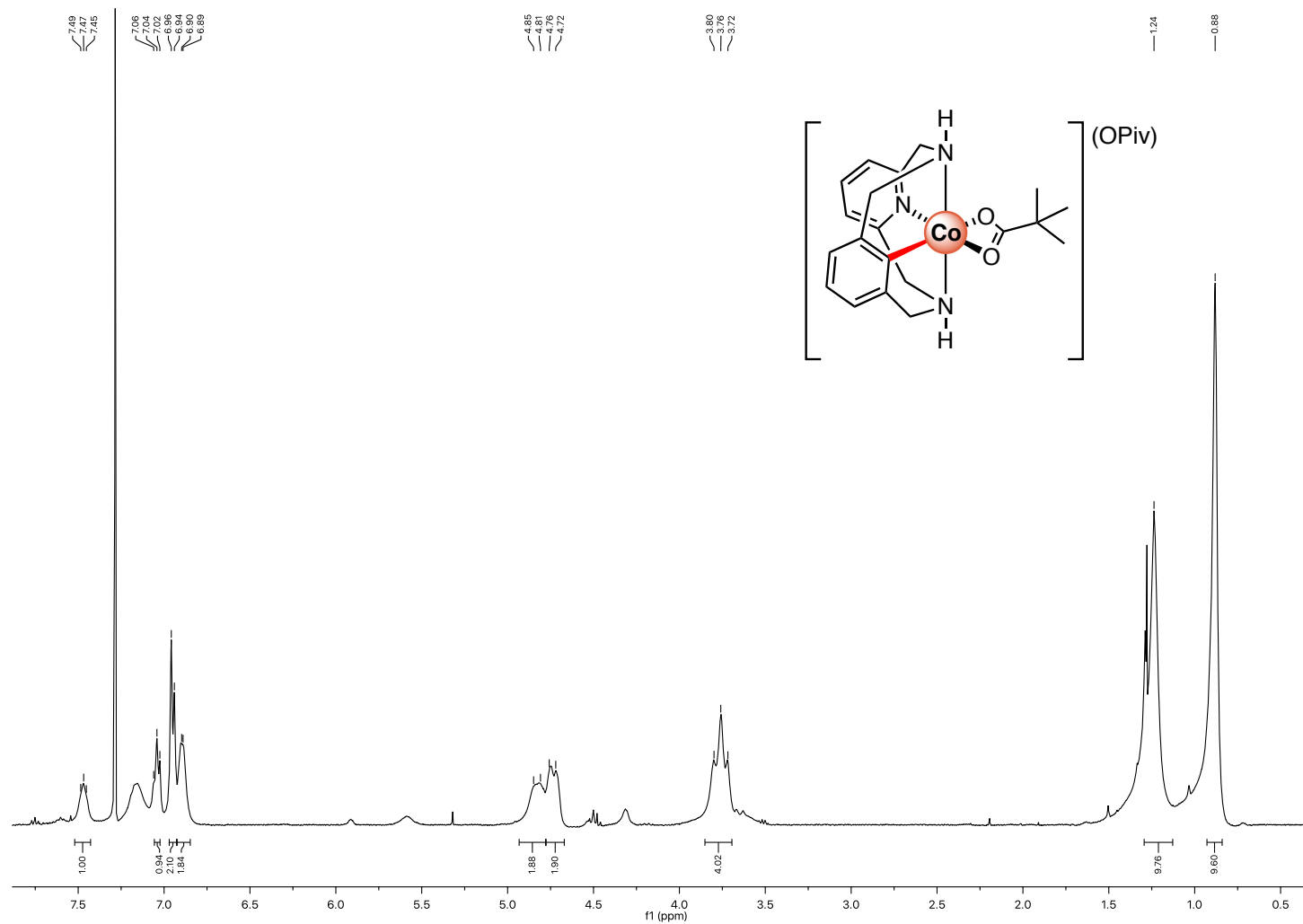
Figure S31. 400 MHz ^{1}H NMR spectrum of **2a-OPiv** in CDCl$_3$, 298 K.
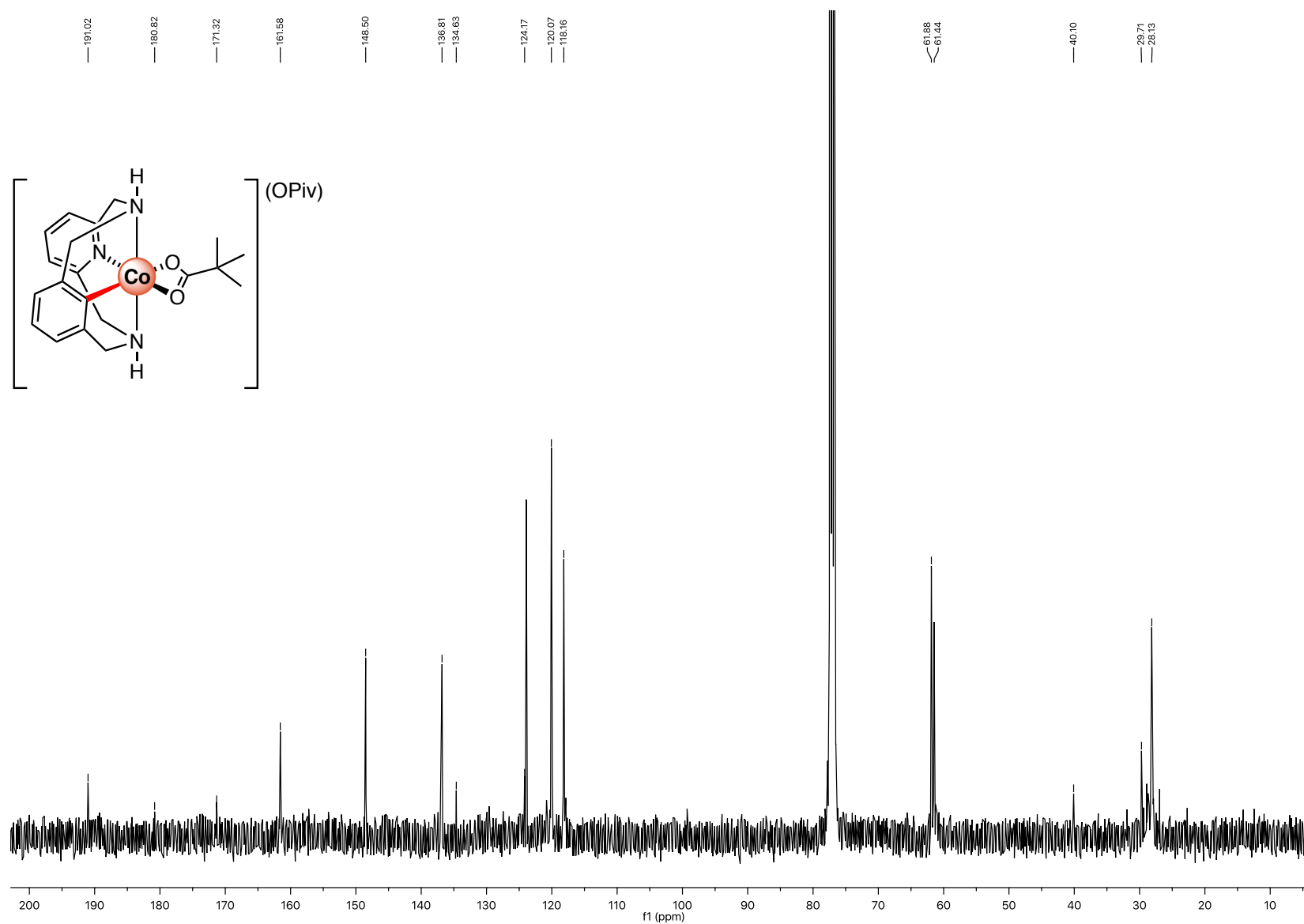
Figure S32. 100 MHz ^{13}C {^{1}H} NMR spectrum of **2a-OPiv** in CDCl$_3$, 298 K.
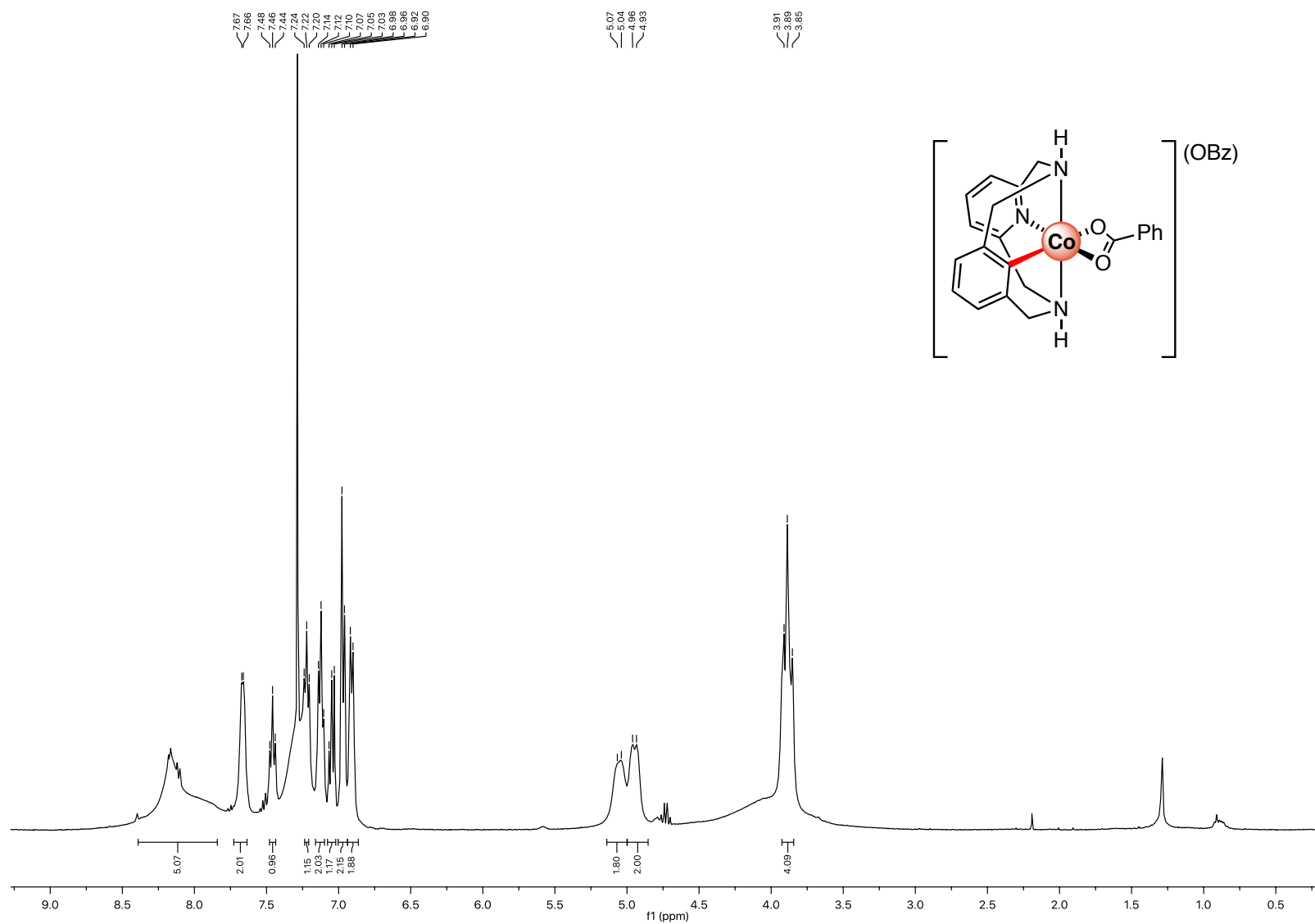
Figure S33. 400 MHz ^{1}H NMR spectrum of **2a-OBz** in CDCl$_3$, 298 K.
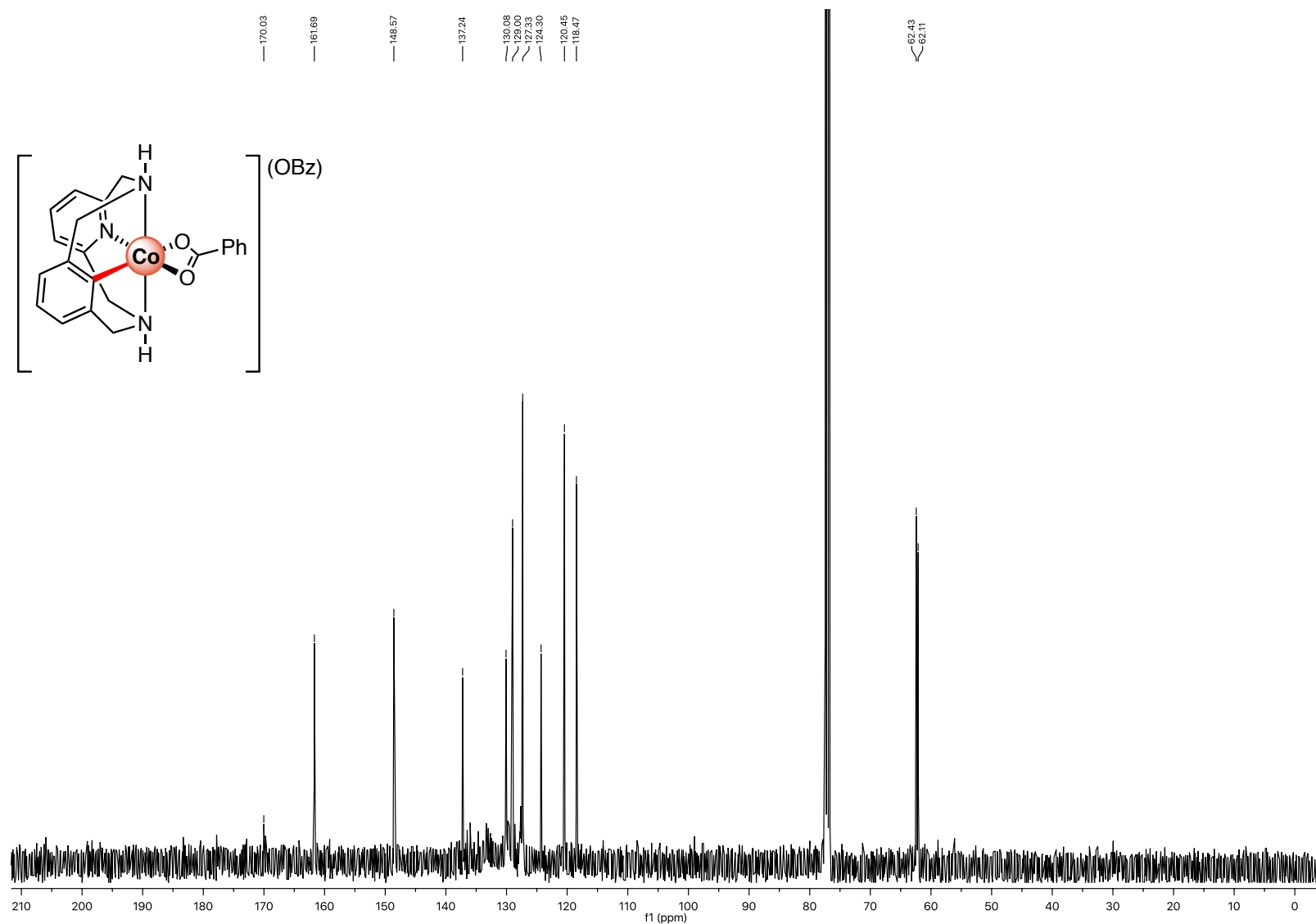
Figure S34. 100 MHz ^{13}C {H} NMR spectrum of **2a-OBz** in CDCl$_3$, 298 K.
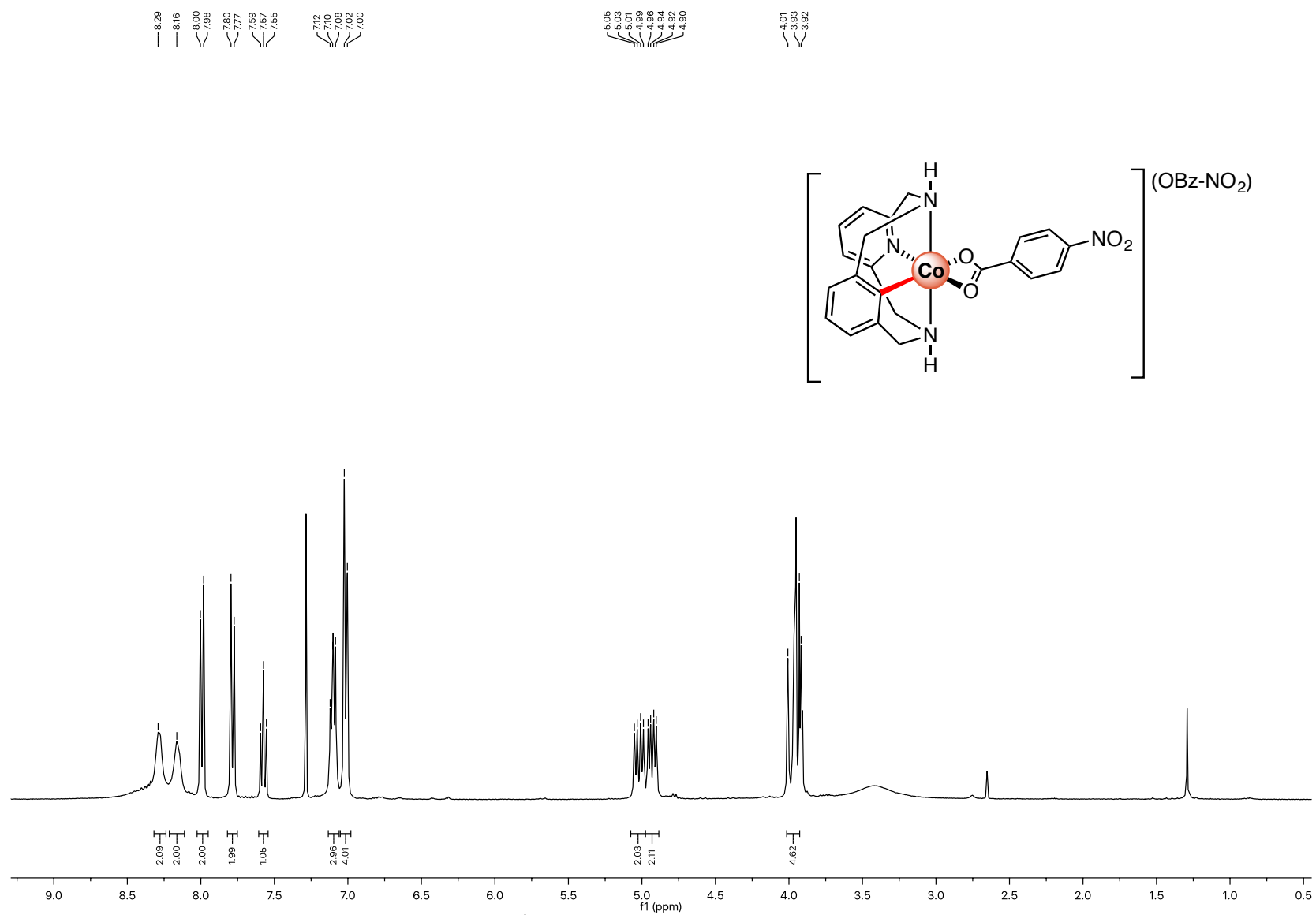
Figure S35. 400 MHz ^{1}H NMR spectrum of **2a-OBz-NO$_2$** in CDCl$_3$, 298 K.
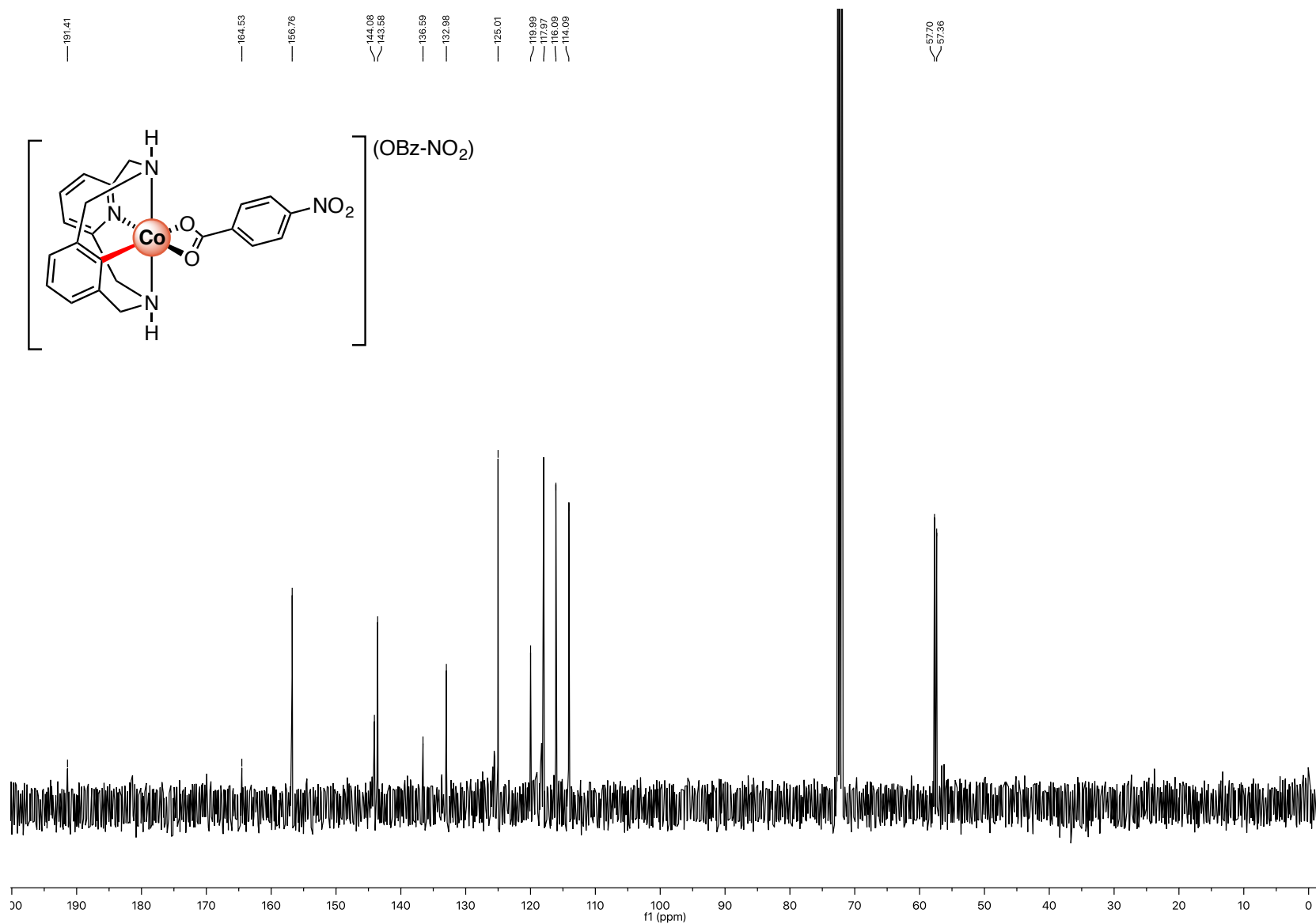
Figure S36. 100 MHz ^{13}C {H} NMR spectrum of **2a-OBz-NO$_2$** in CDCl$_3$, 298 K.
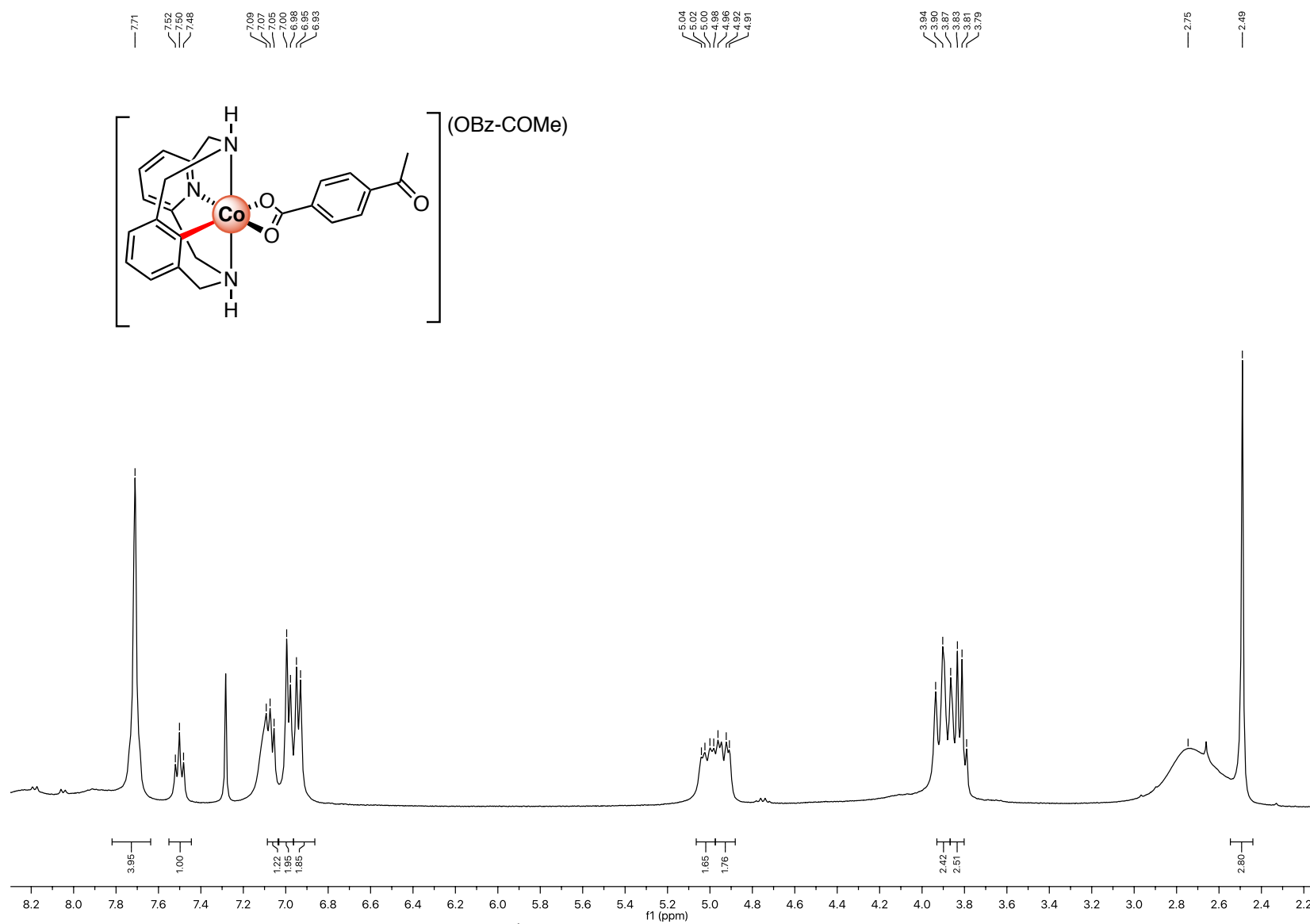
Figure S37. 400 MHz ^{1}H NMR spectrum of **2a-OBz-COMe** in CDCl$_3$, 298 K.
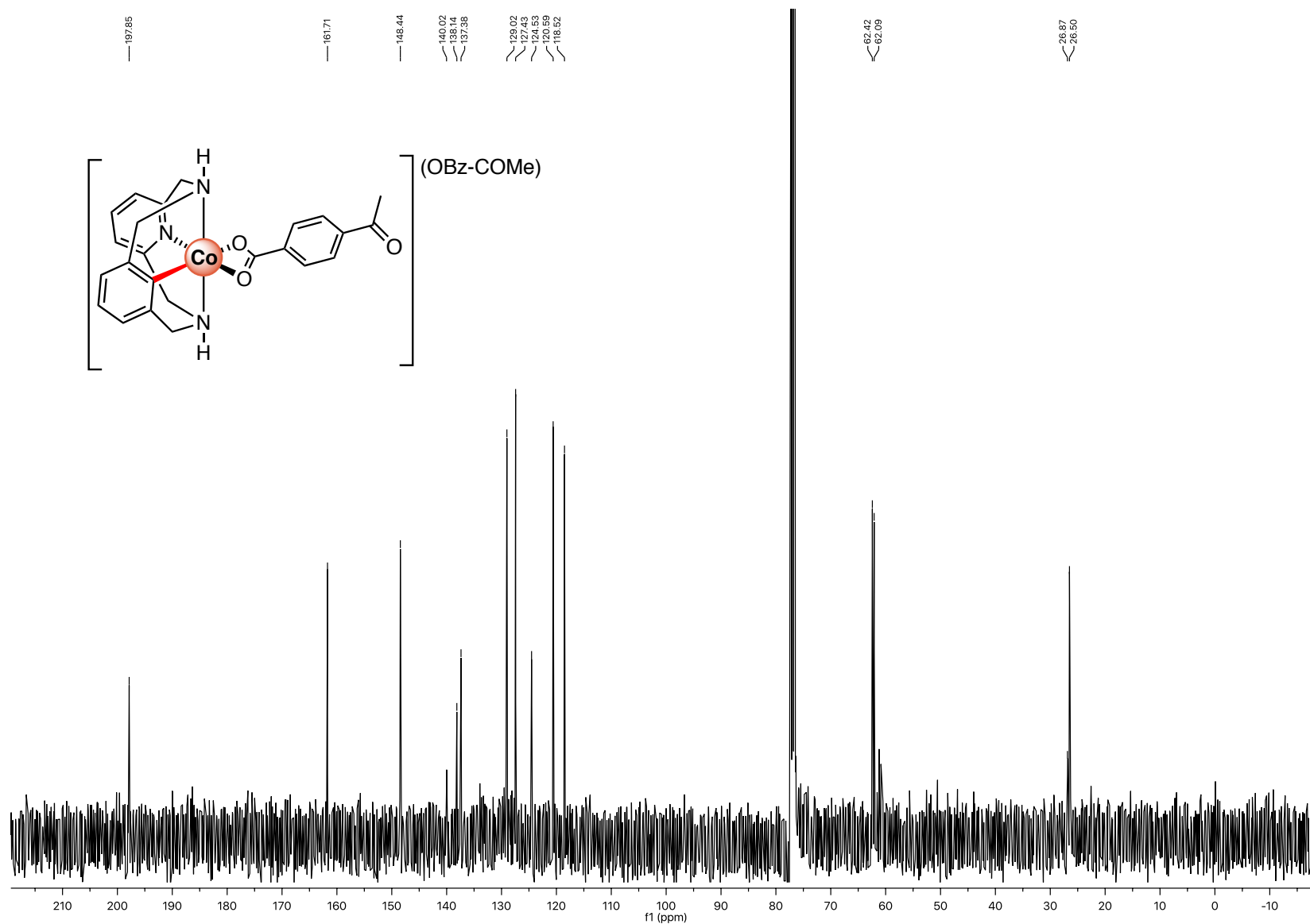
Figure S38. 100 MHz ^{13}C {H} NMR spectrum of **2a-OBz-COMe** in CDCl$_3$, 298 K.
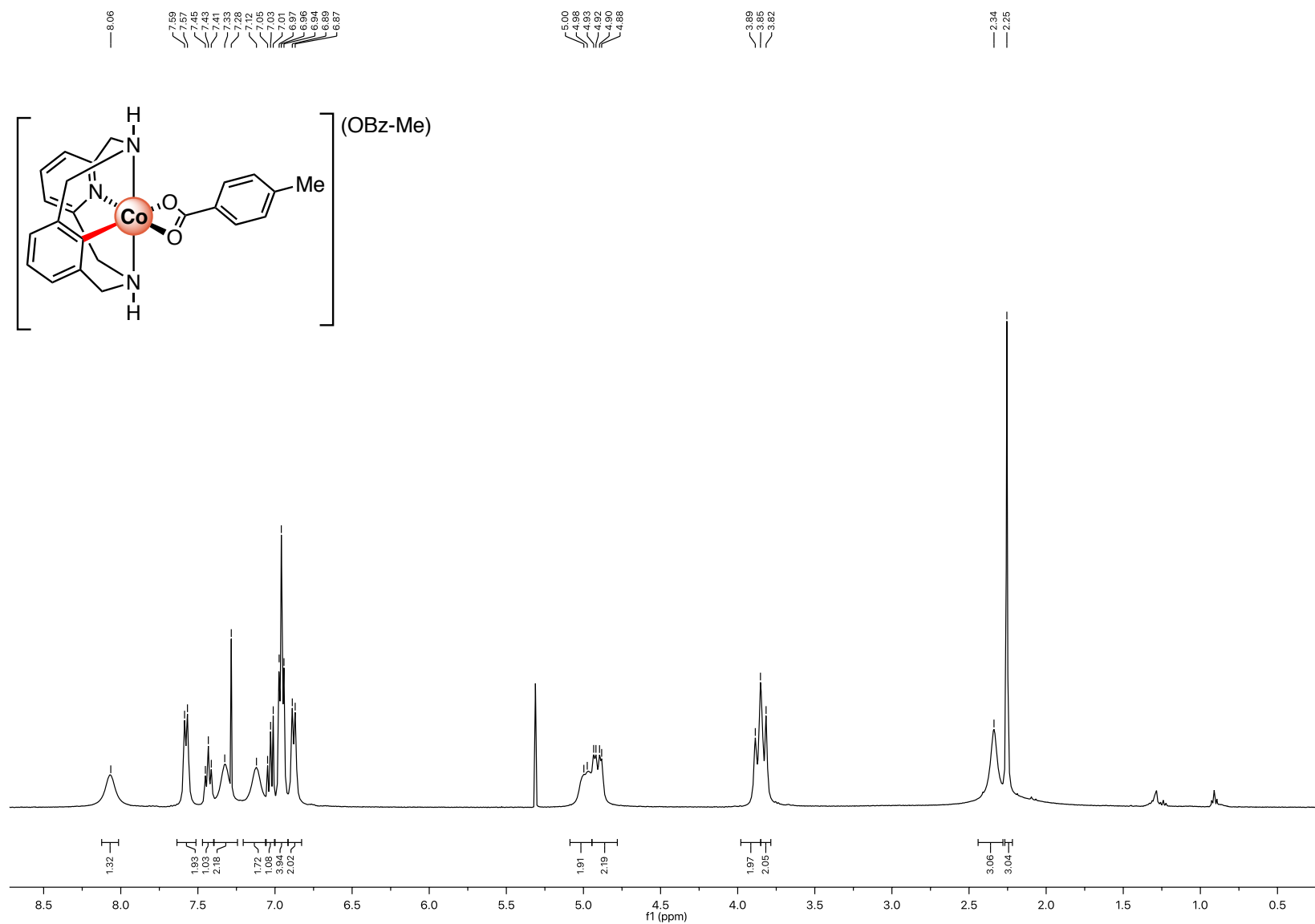
Figure S39. 400 MHz ^{1}H NMR spectrum of **2a-OBz-Me** in CDCl$_3$, 298 K.
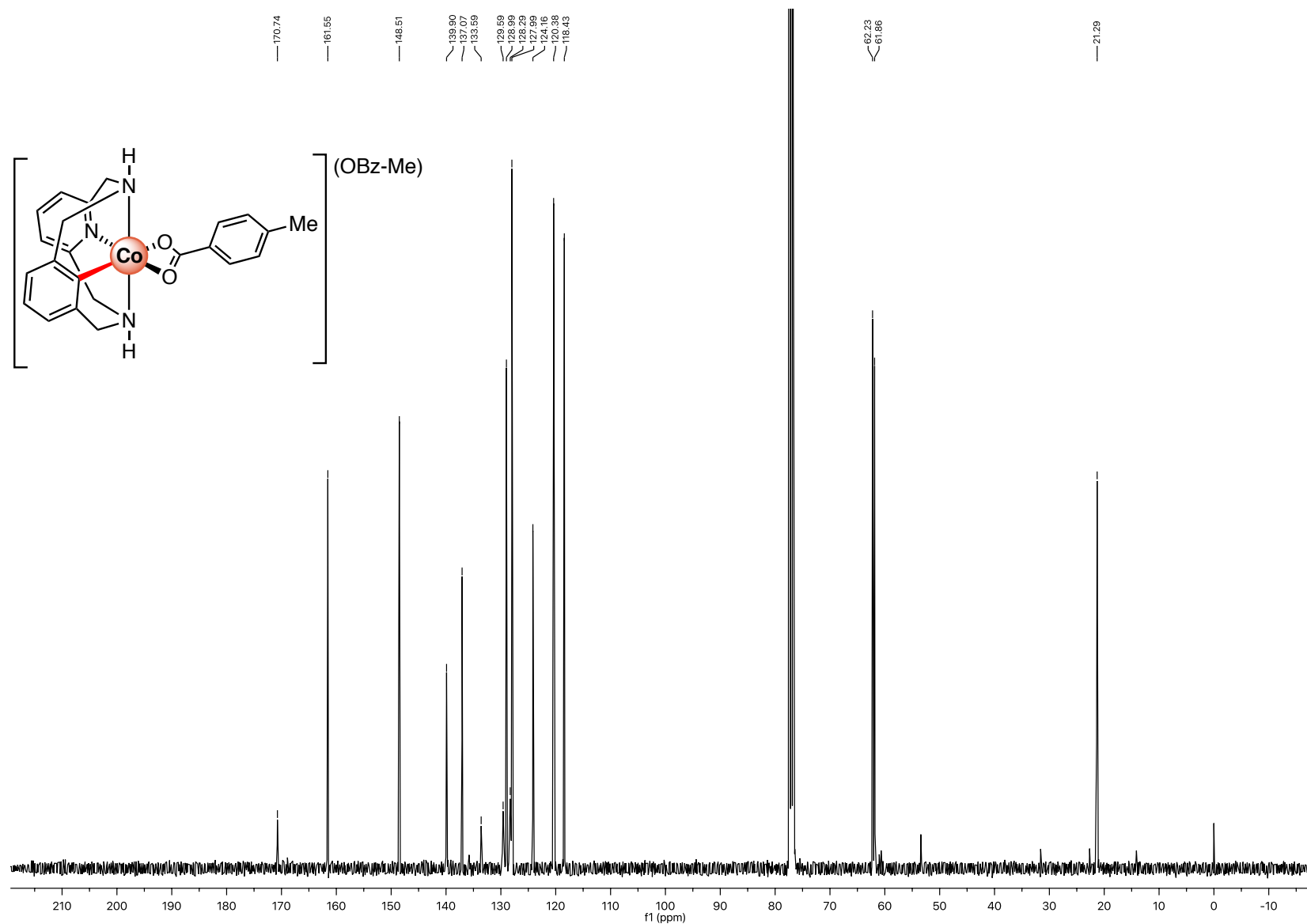
Figure S40. 100 MHz ^{13}C {H} NMR spectrum of **2a-OBz-Me** in CDCl$_3$, 298 K.
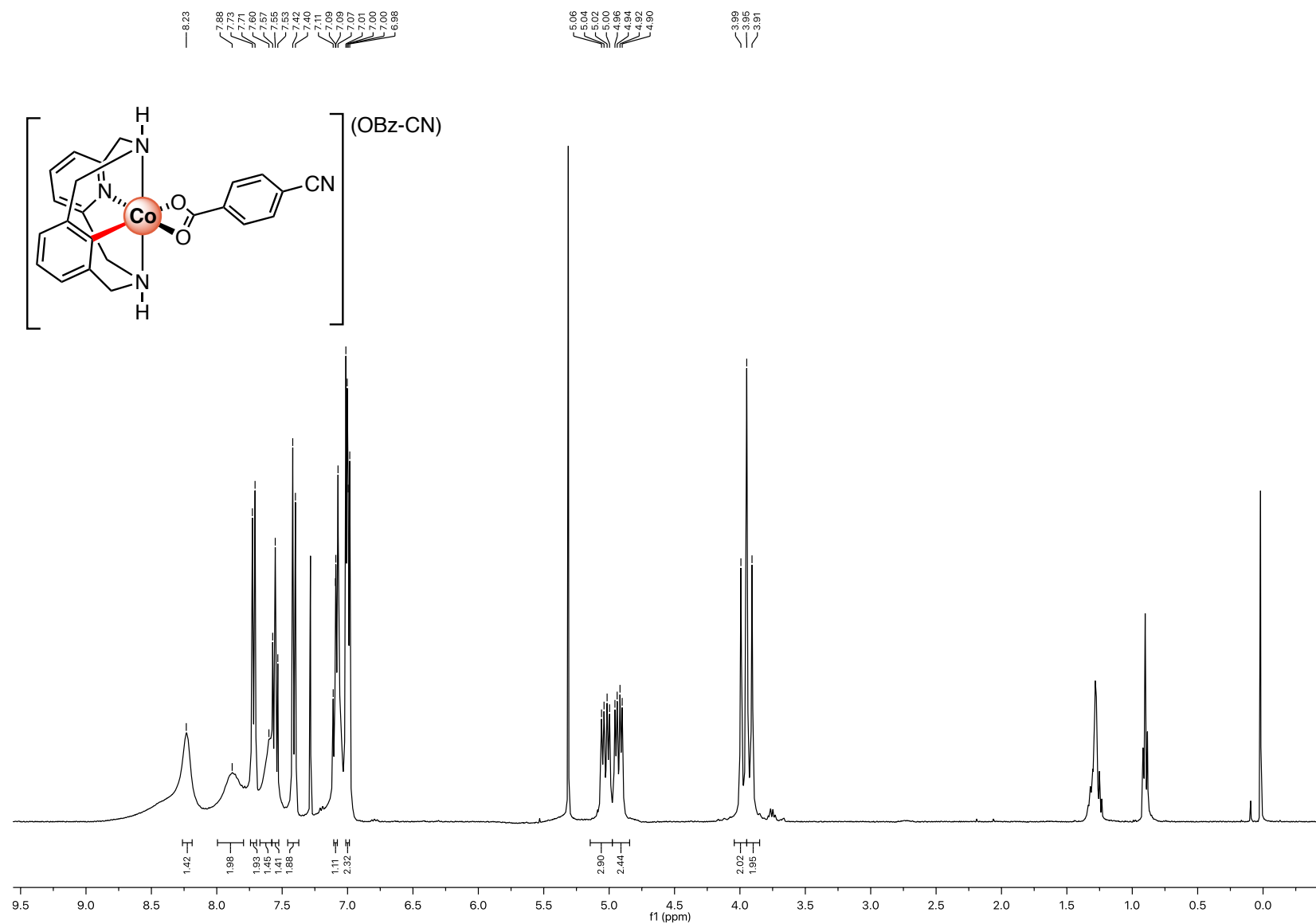
Figure S41. 400 MHz ^{1}H NMR spectrum of **2a-OBz-CN** in CDCl$_3$, 298 K.
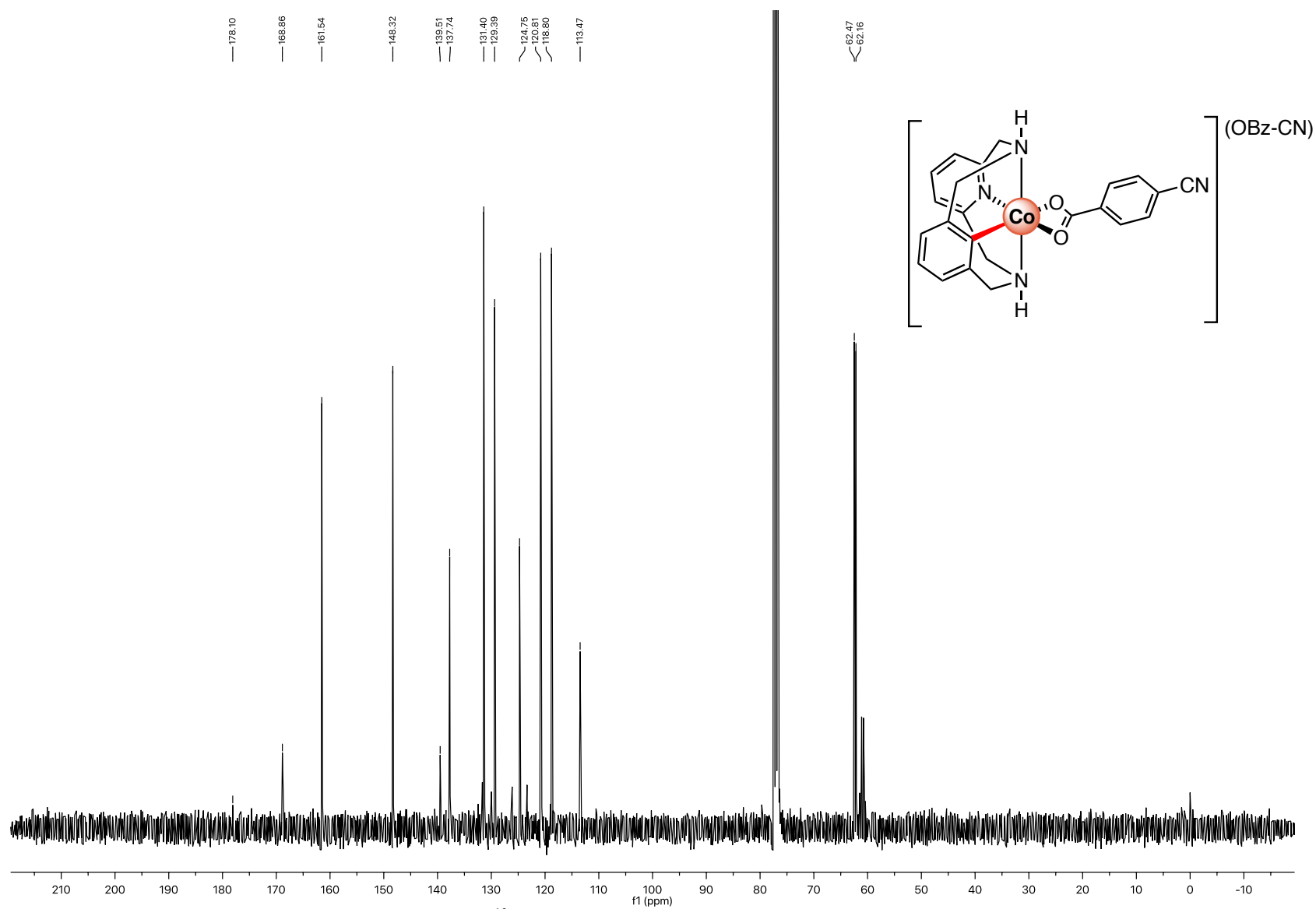
Figure S42. 100 MHz ^{13}C {H} NMR spectrum of **2a-OBz-CN** in CDCl$_3$, 298 K.
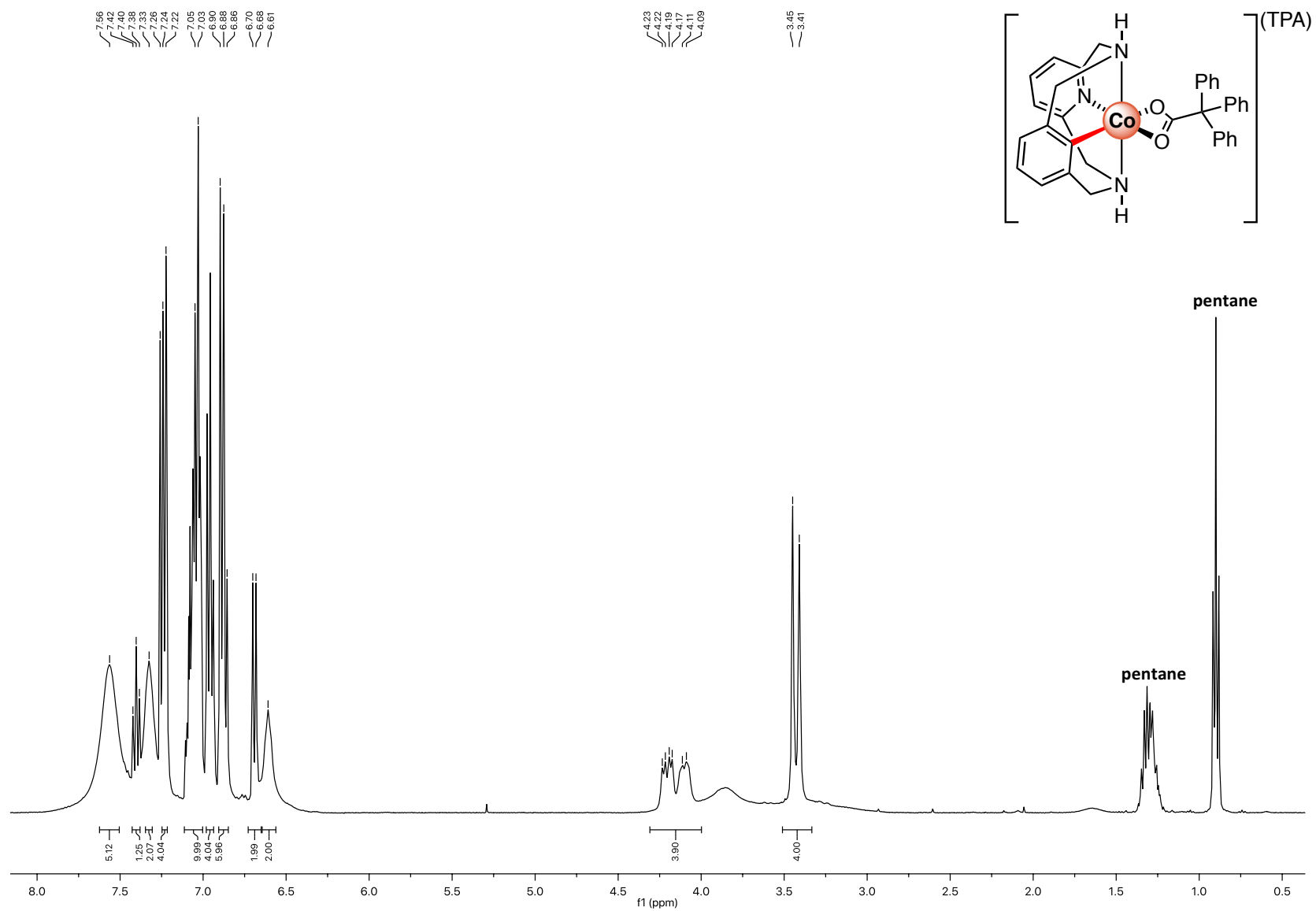
Figure S43. 400 MHz ^{1}H NMR spectrum of **2a-TPA** in CDCl$_3$, 298 K.
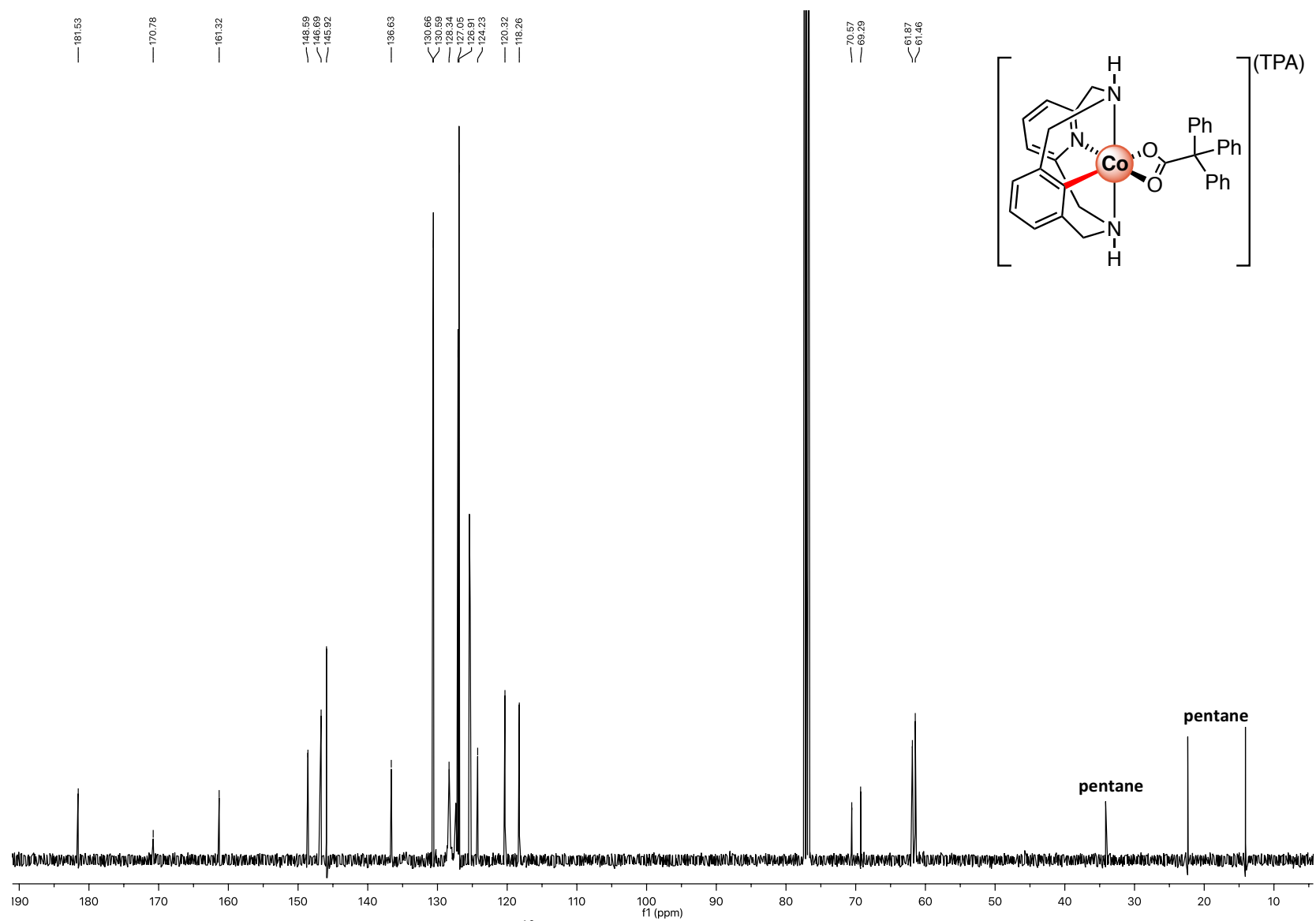
Figure S44. 100 MHz ^{13}C {H} NMR spectrum of **2a-TPA** in CDCl$_3$, 298 K.
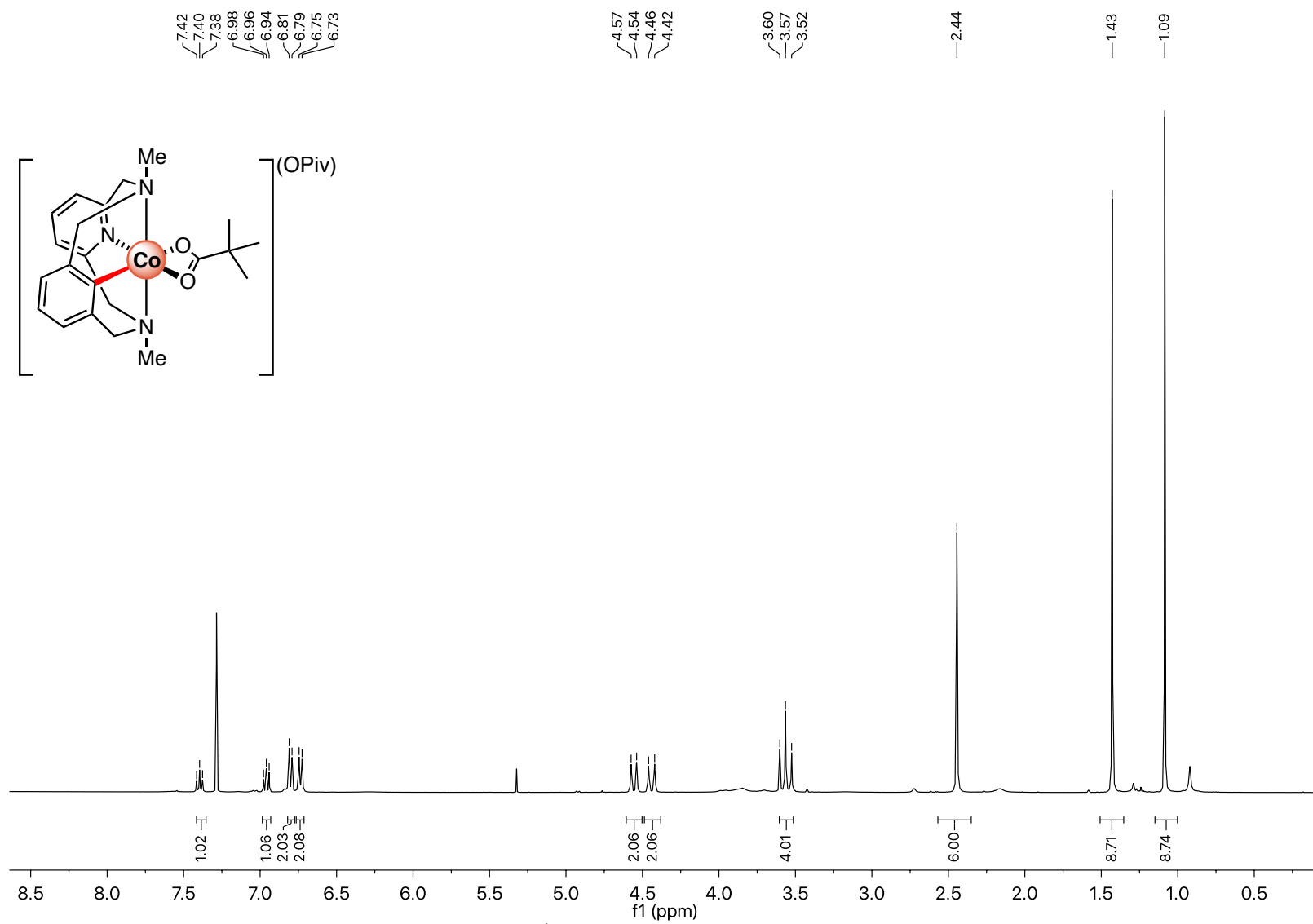
Figure S45. 400 MHz ^{1}H NMR spectrum of **2b-OPiv** in CDCl$_3$, 298 K.
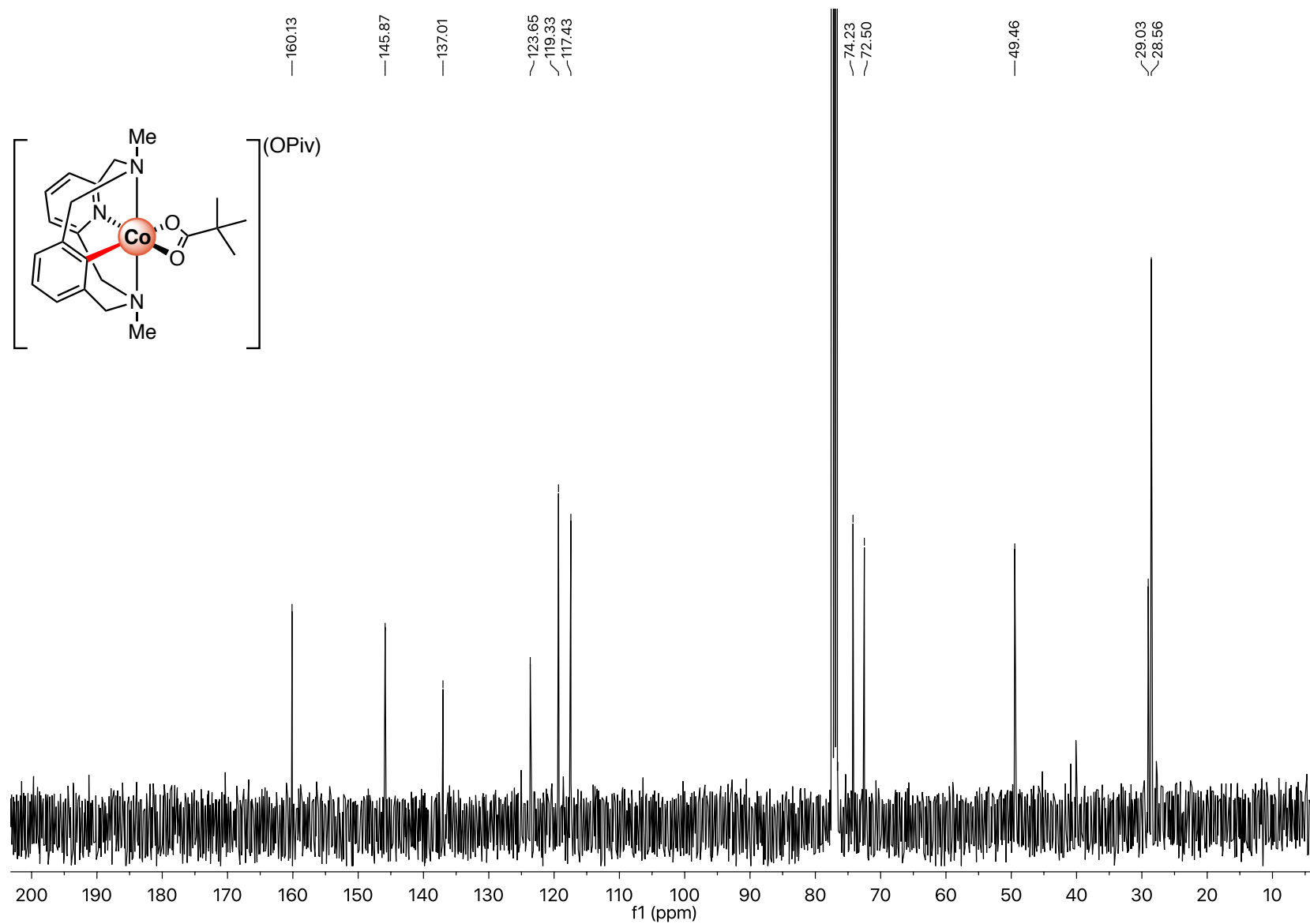
Figure S46. 100 MHz ^{13}C {^{1}H} NMR spectrum of **2b-OPiv** in CDCl$_3$, 298 K.

Peak labels: 160.13, 145.87, 137.01, 123.65, 119.33, 117.43, 74.23, 72.50, 49.46, 29.03, 28.56
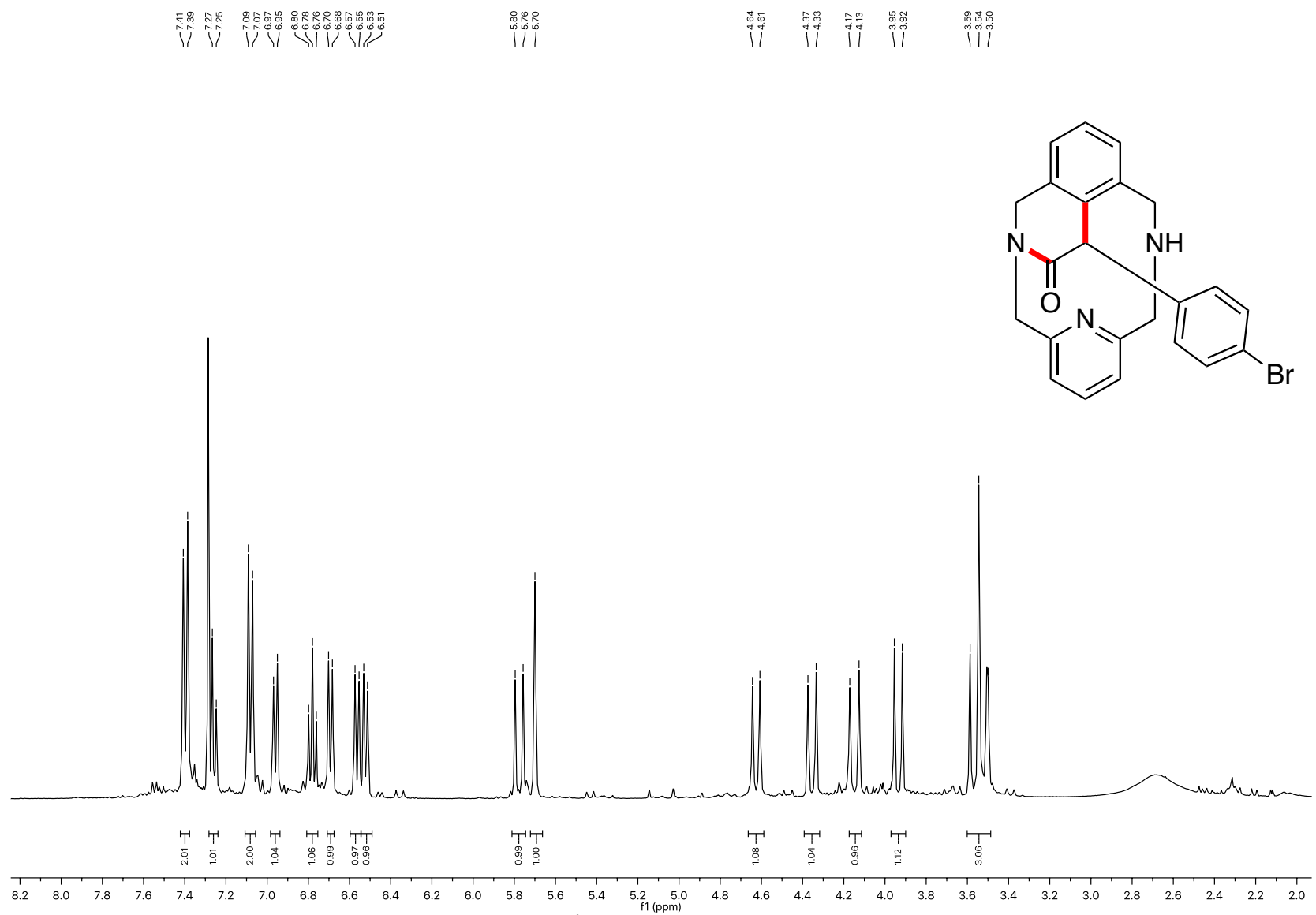
Figure S47. 400 MHz ^{1}H NMR spectrum of **3j** in CDCl$_3$, 298 K.
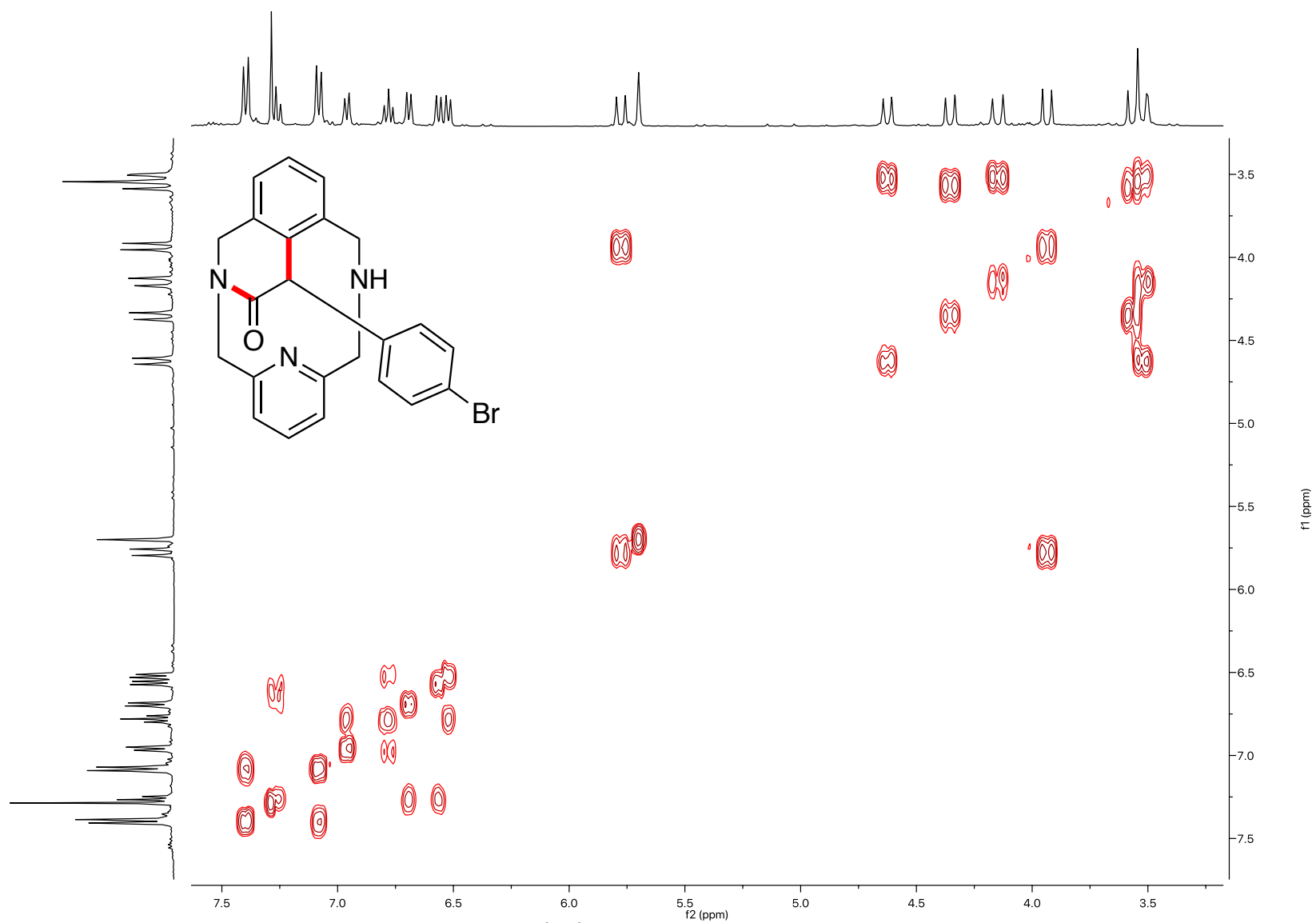
Figure S48. 400 MHz ^{1}H-^{1}H COSY spectrum of **3j** in CDCl$_3$, 298 K.
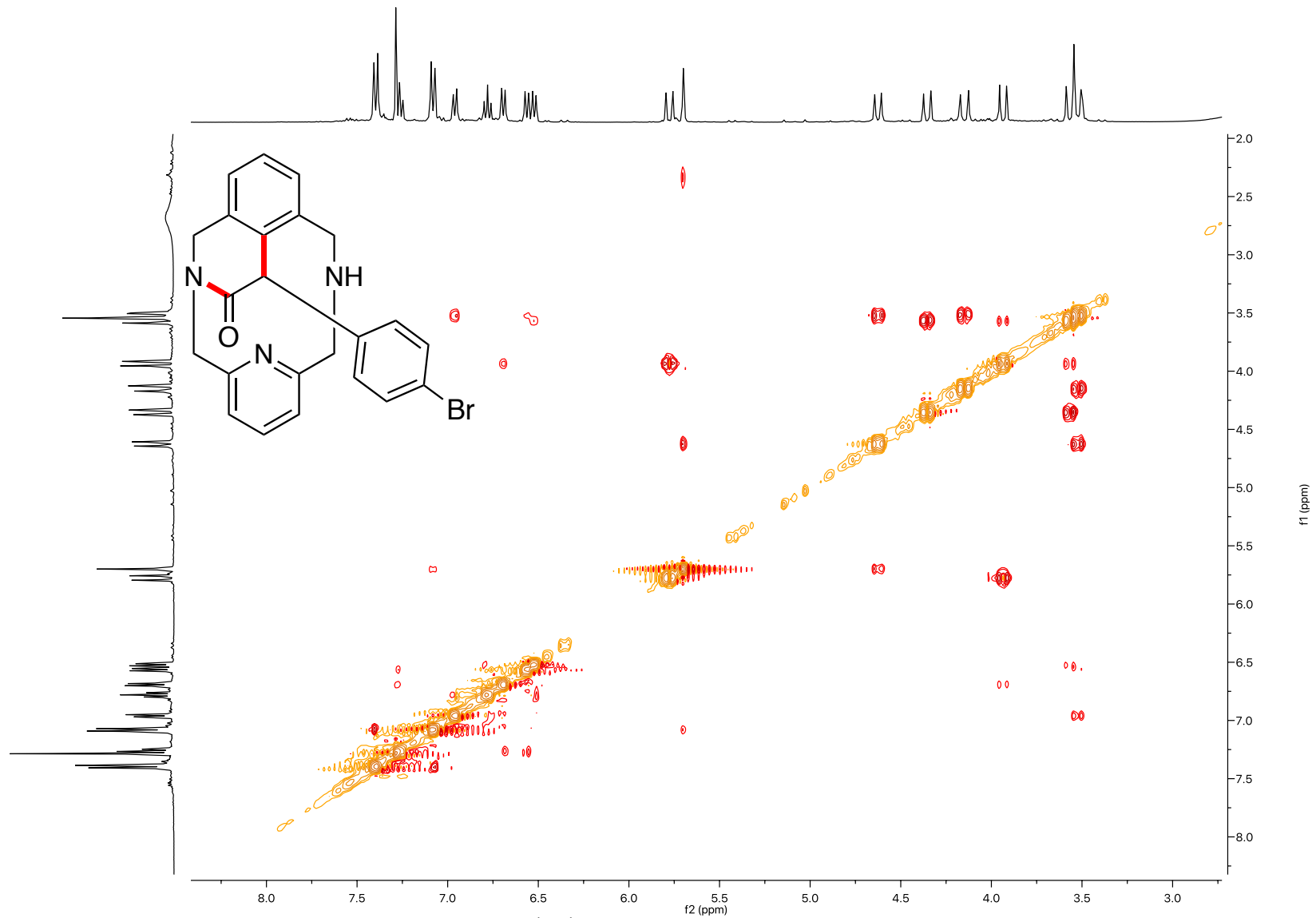
Figure S49. 400 MHz ^{1}H-^{1}H NOESY spectrum of **3j** in CDCl$_3$, 298 K.
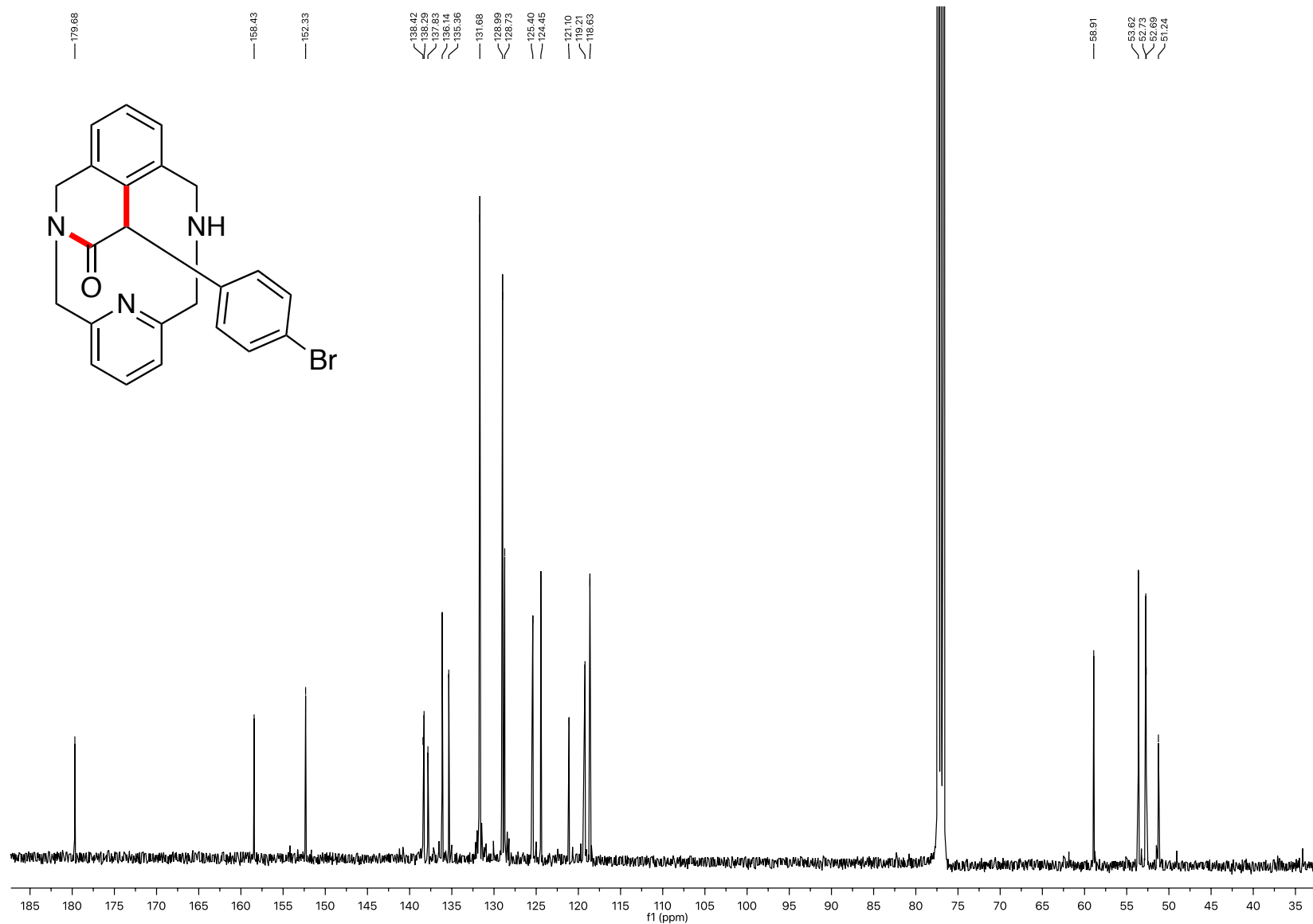
Figure S50. 100 MHz ^{13}C-{H} NMR spectrum of **3j** in CDCl$_3$, 298 K.
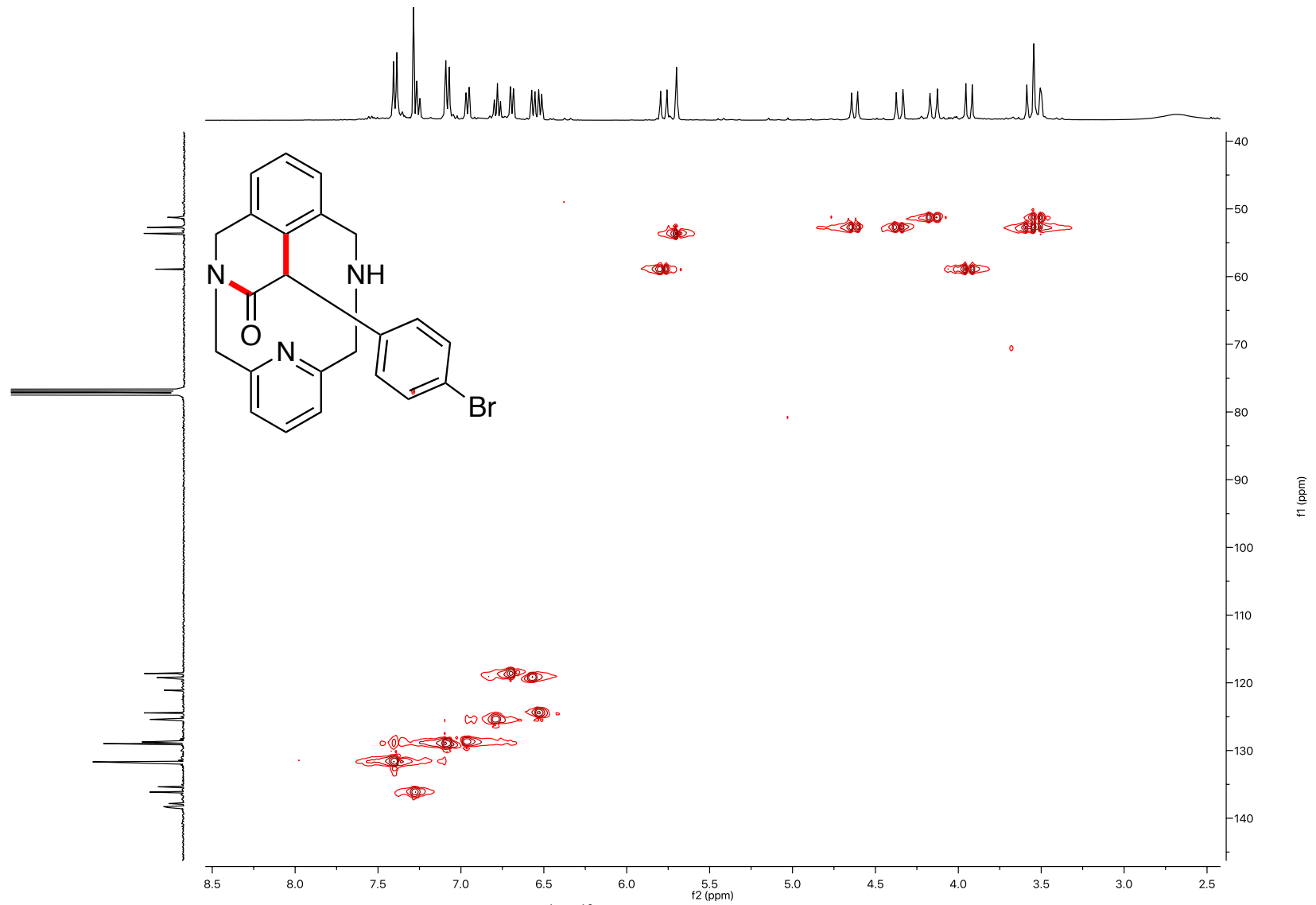
Figure S51. 400 MHz ^{1}H-^{13}C HSQC spectrum of **3j** in CDCl$_3$, 298 K.
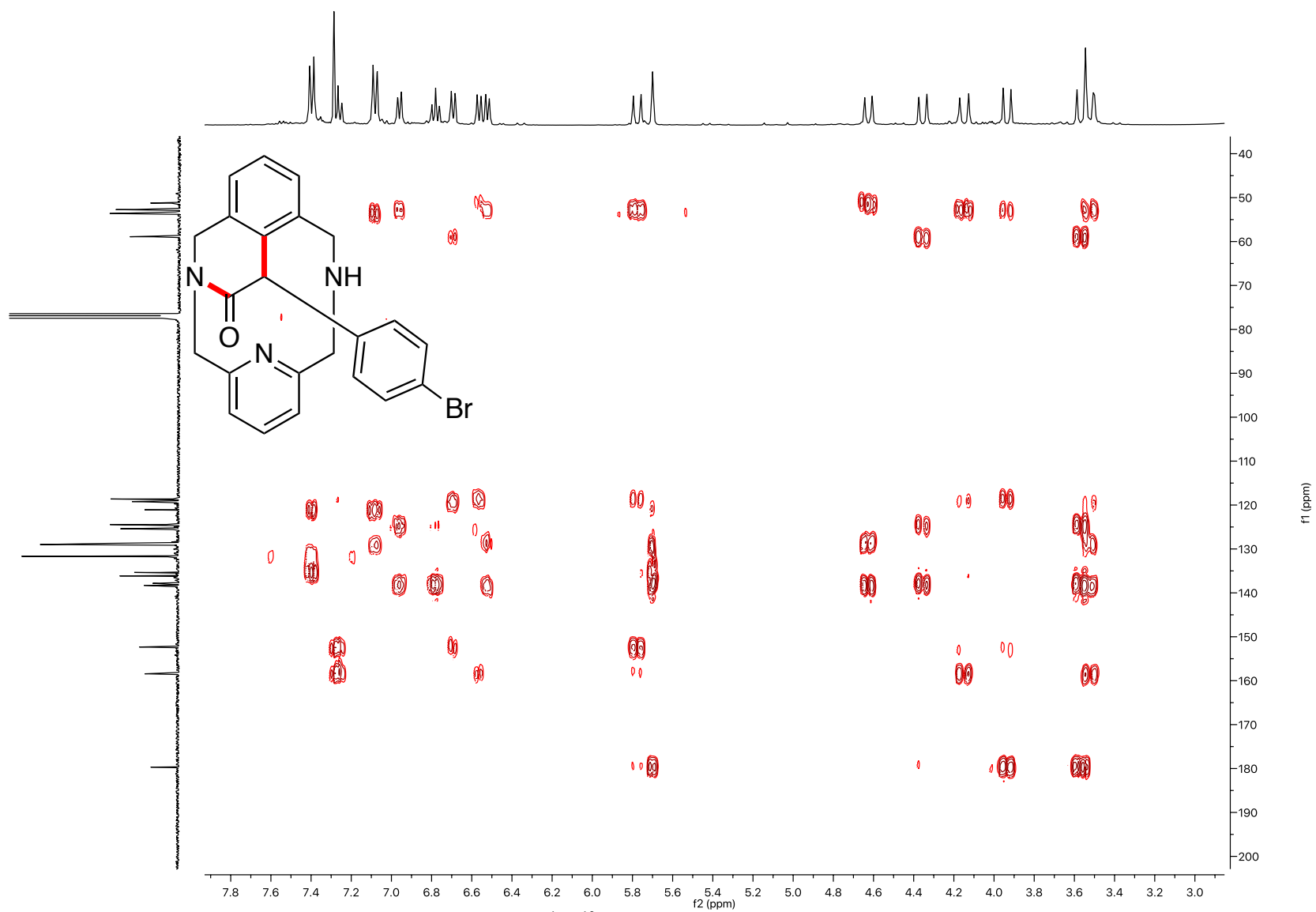
Figure S52. 400 MHz ^1H-^{13}C HSQC spectrum of **3j** in CDCl$_3$, 298 K.
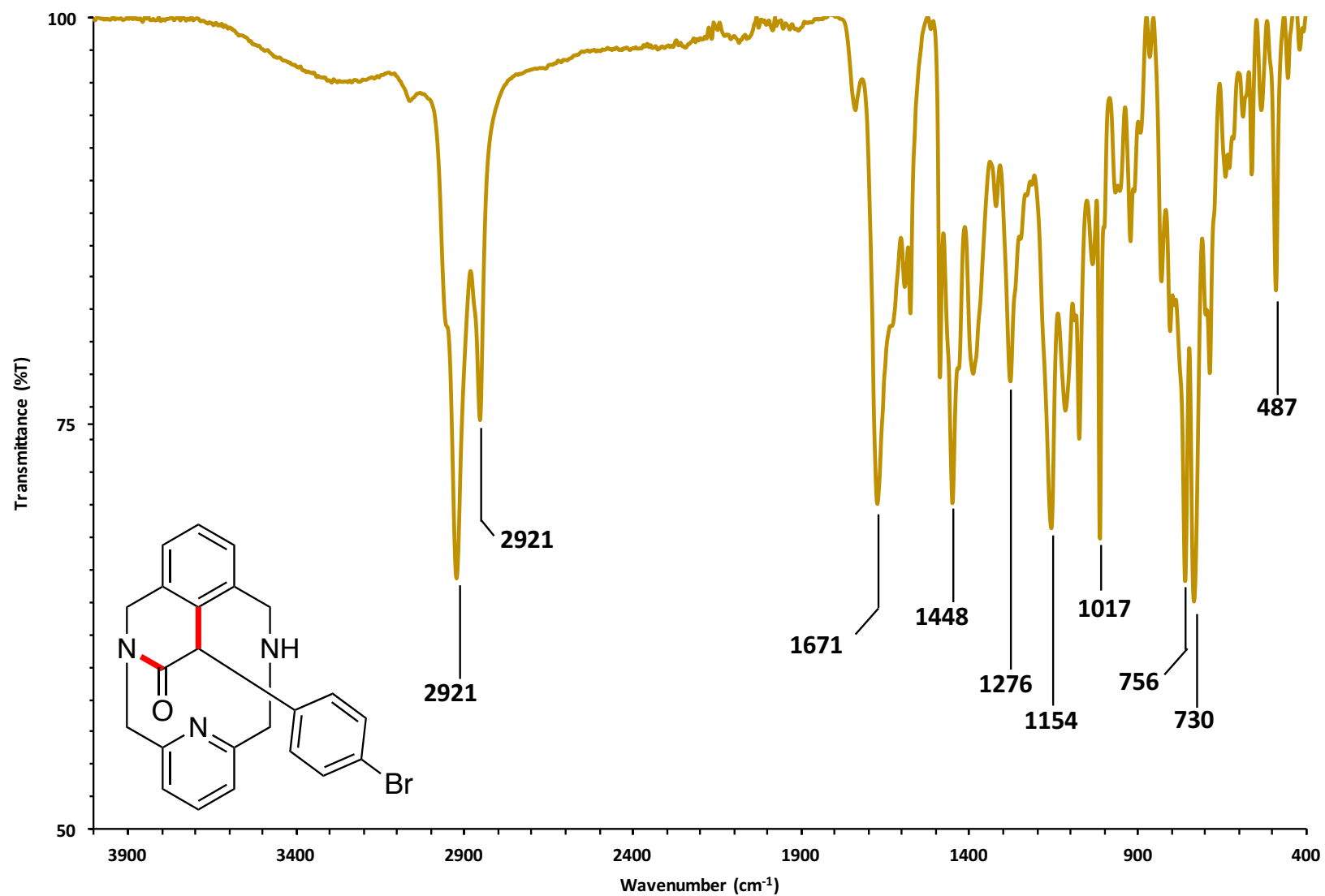
Figure S53. FT-IR spectrum of **3j** in solid state, 298 K.
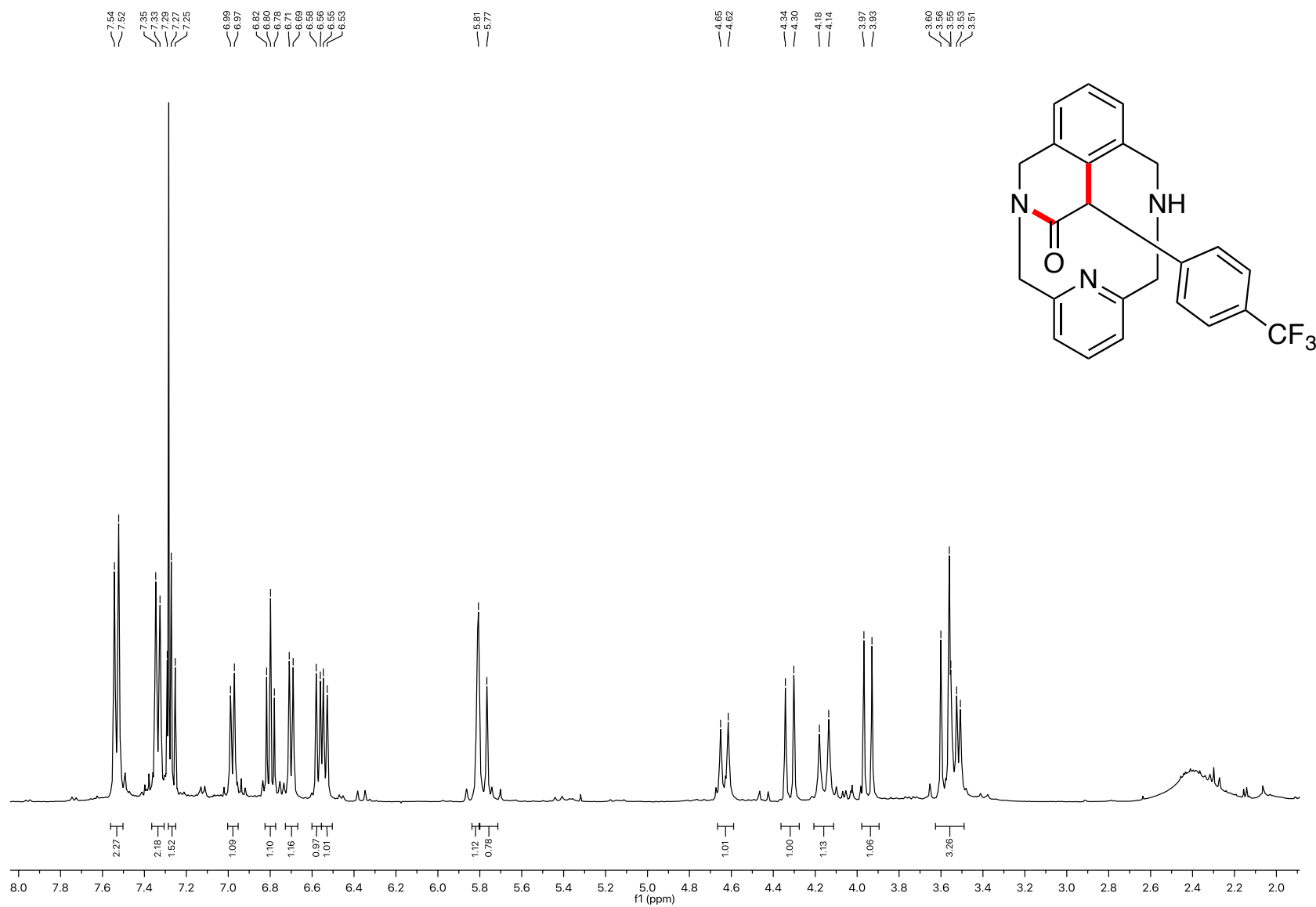
Figure S54. 400 MHz ^{1}H NMR spectrum of **3k** in CDCl$_3$, 298 K.
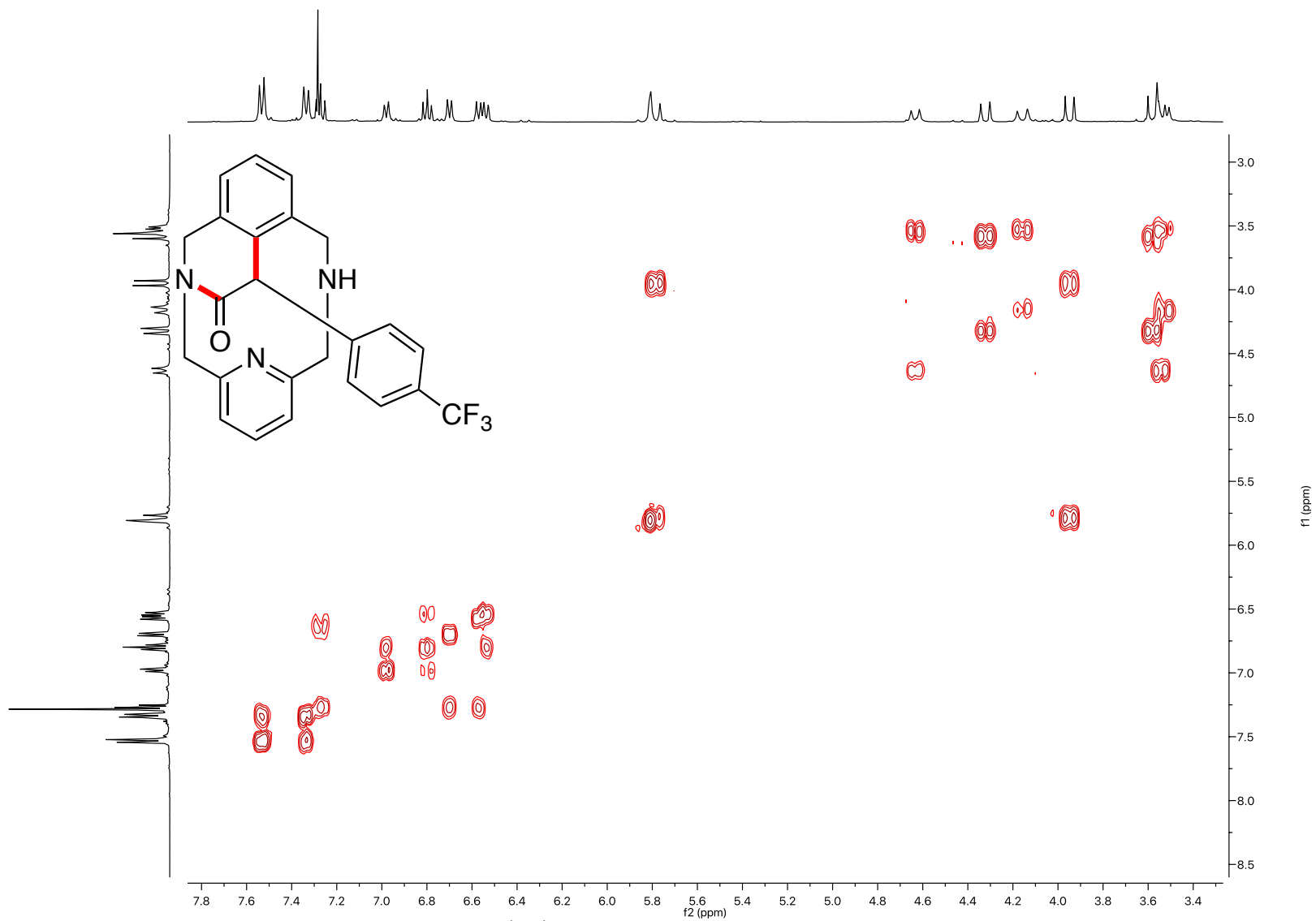
Figure S55. 400 MHz ^{1}H-^{1}H COSY NMR spectrum of **3k** in CDCl$_3$, 298 K.
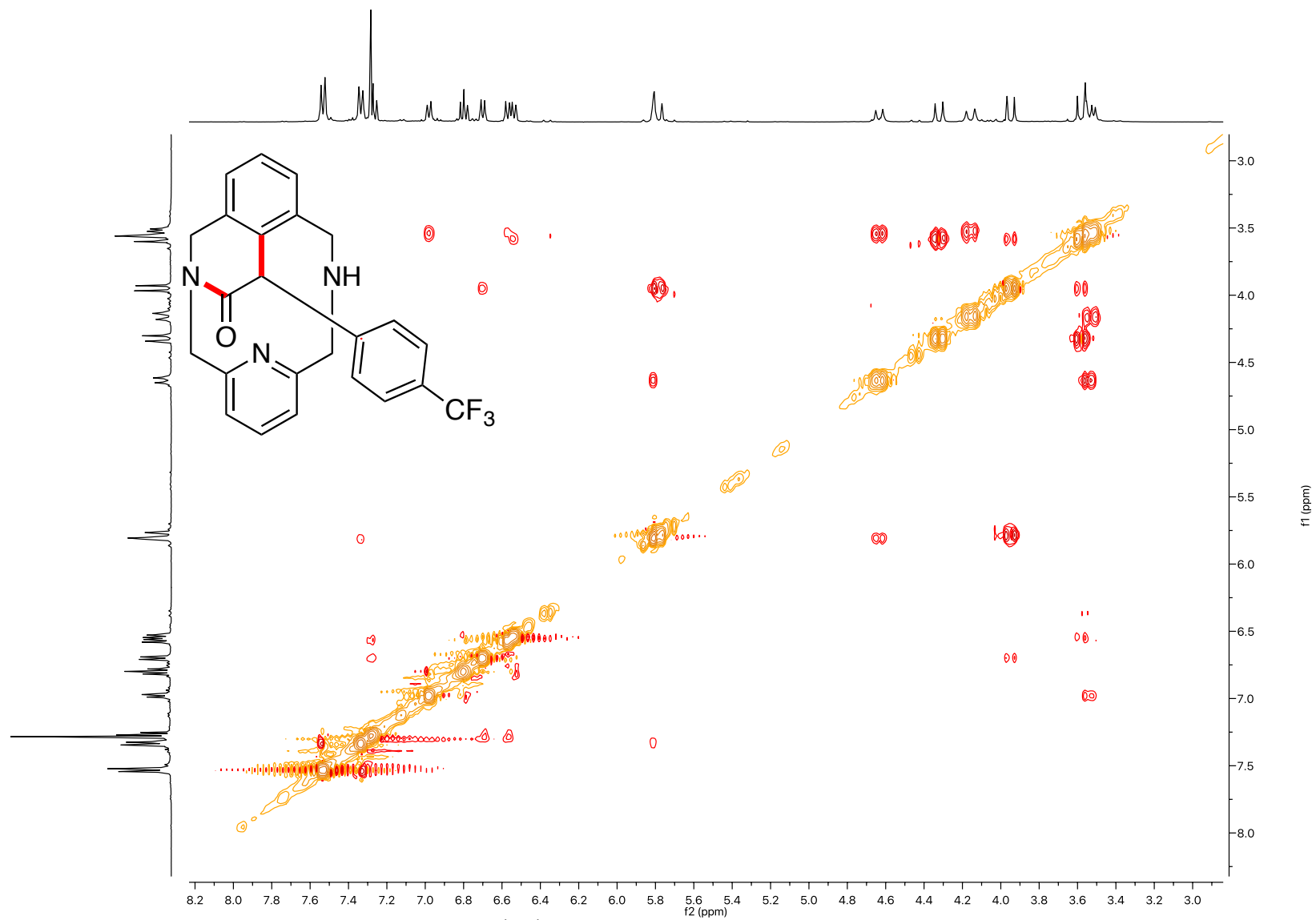
Figure S56. 400 MHz ^{1}H-^{1}H NOESY NMR spectrum of **3k** in CDCl$_3$, 298 K.
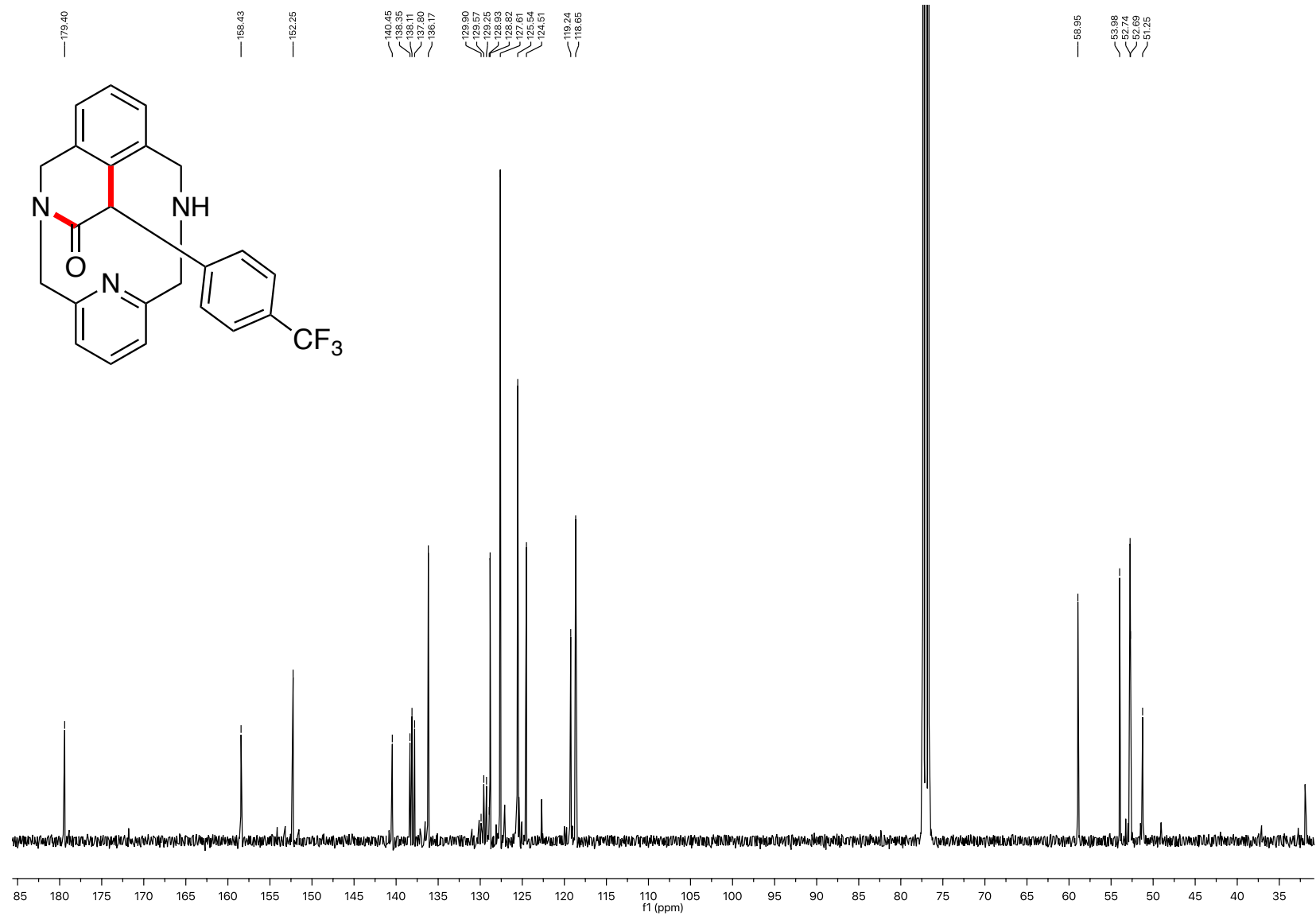
Figure S57. 100 MHz ^{13}C-{H} NMR spectrum of **3k** in CDCl$_3$, 298 K.
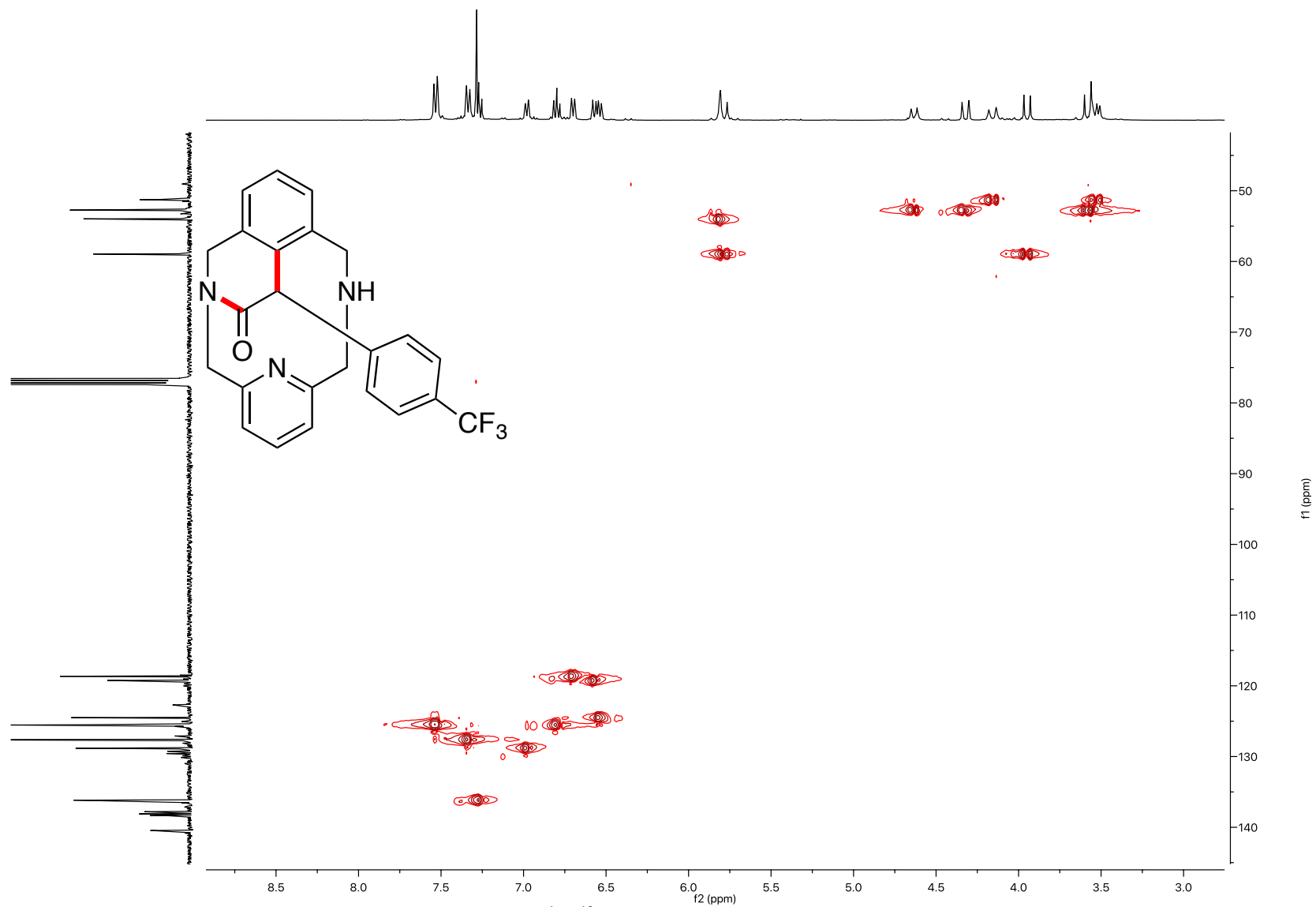
Figure S58. 400 MHz ^{1}H-^{13}C HSQC spectrum of **3k** in CDCl$_3$, 298 K.
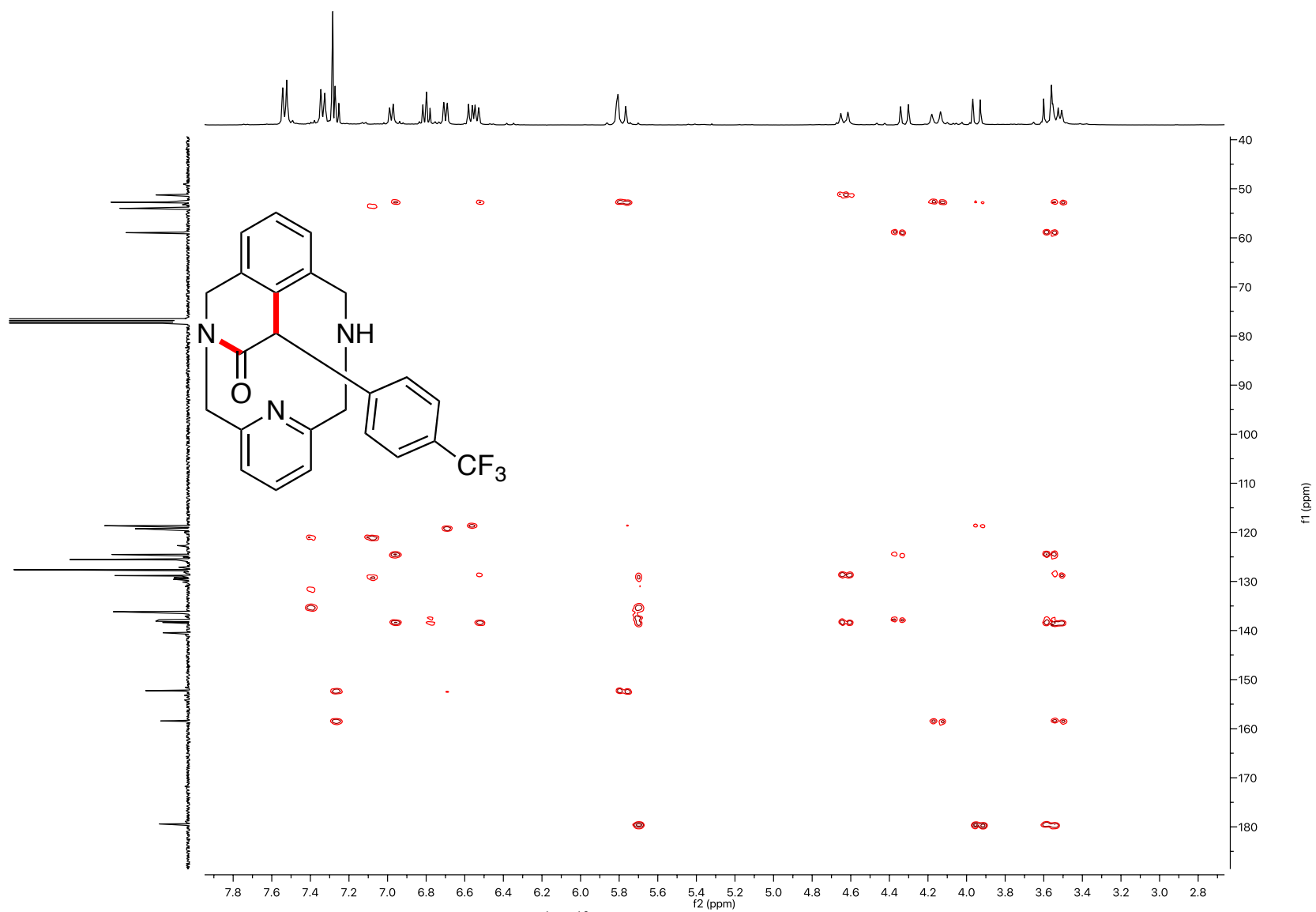
Figure S59. 400 MHz ^{1}H-^{13}C HMBC spectrum of **3k** in CDCl$_3$, 298 K.
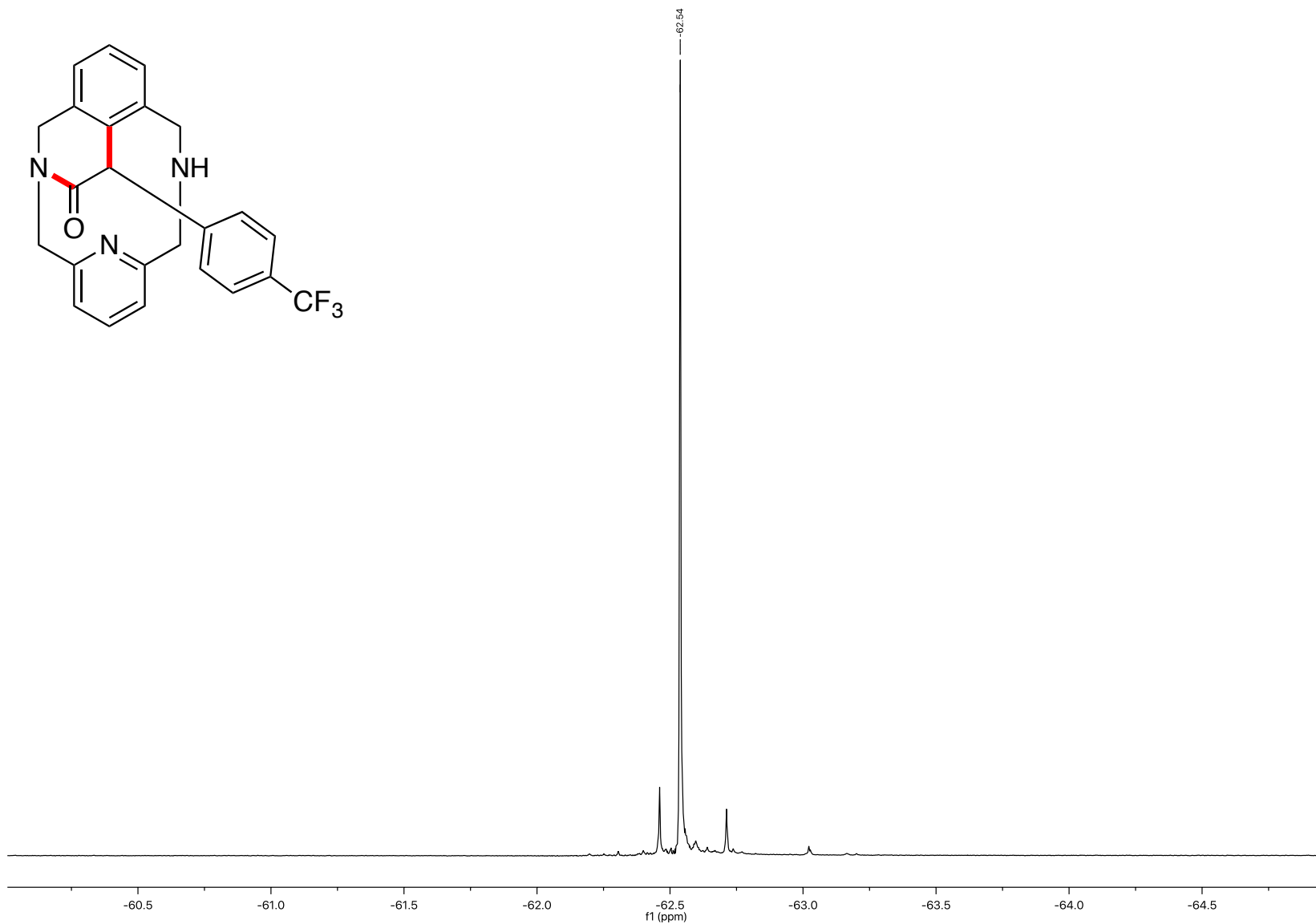
Figure S60. 100 MHz ^{19}F-{H} NMR spectrum of **3k** in CDCl$_3$, 298 K.
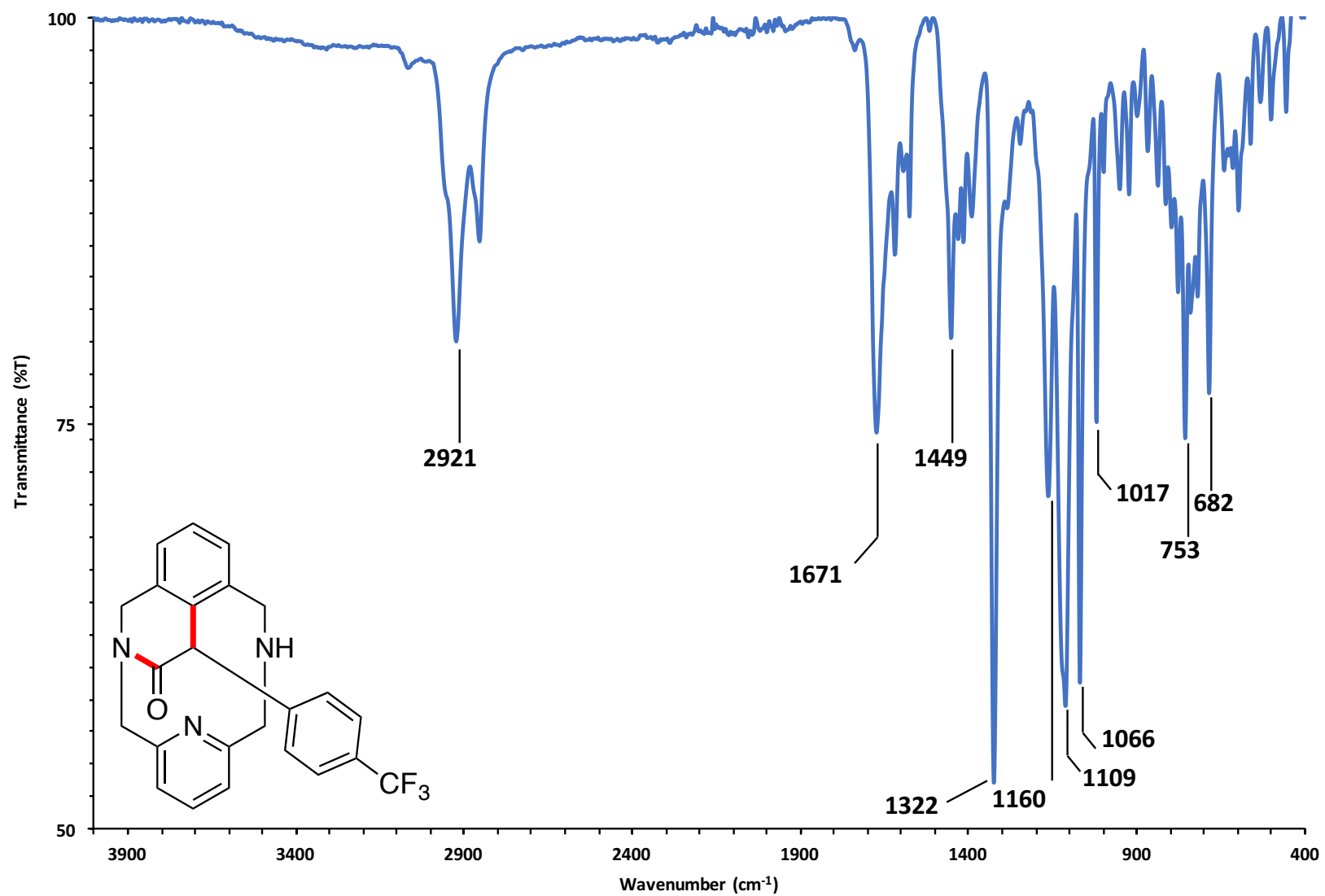
Figure S61. FT-IR spectrum of **3k** in solid state, 298 K.
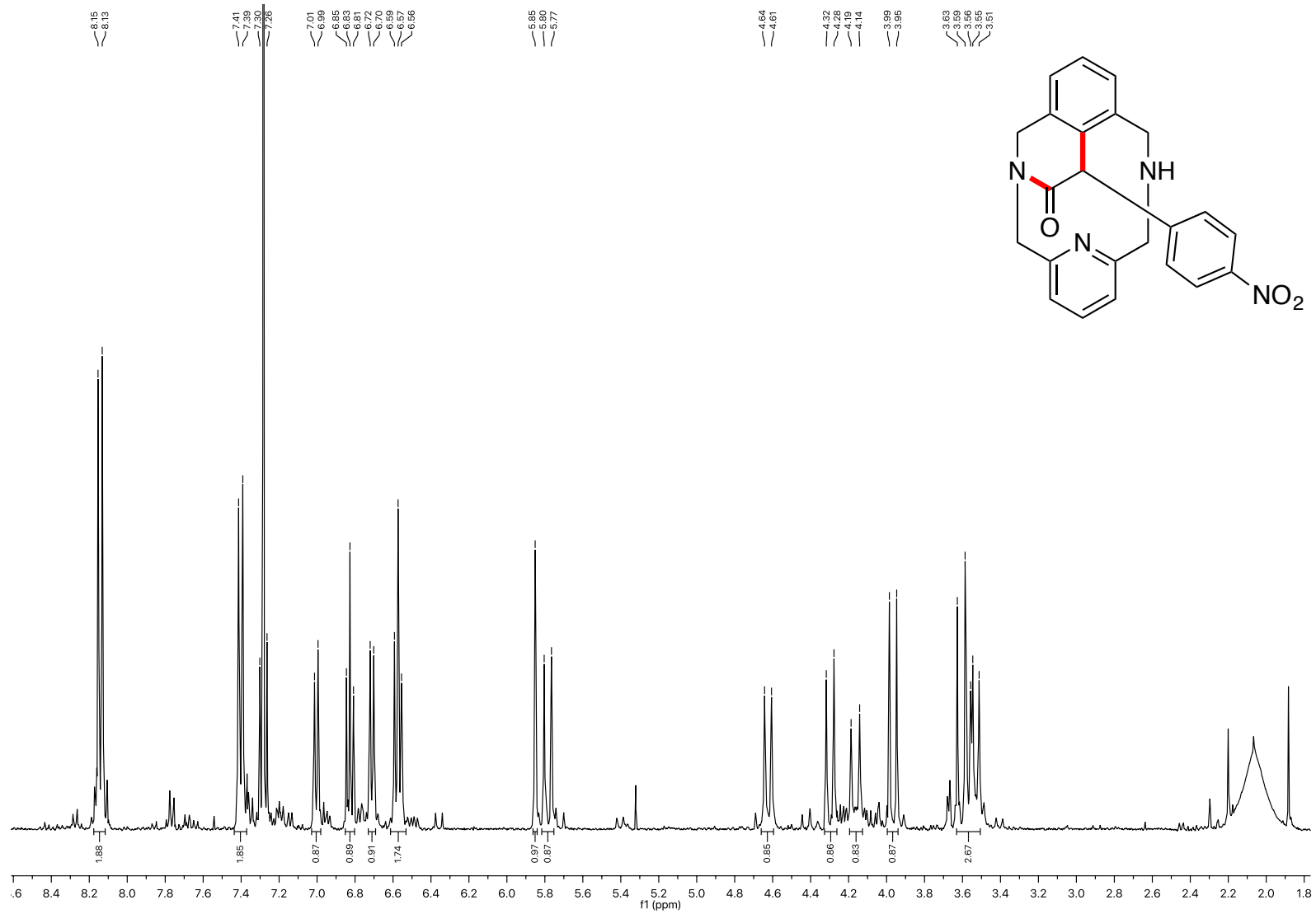
Figure S62. 400 MHz ^{1}H NMR spectrum of **3l** in CDCl$_3$, 298 K.
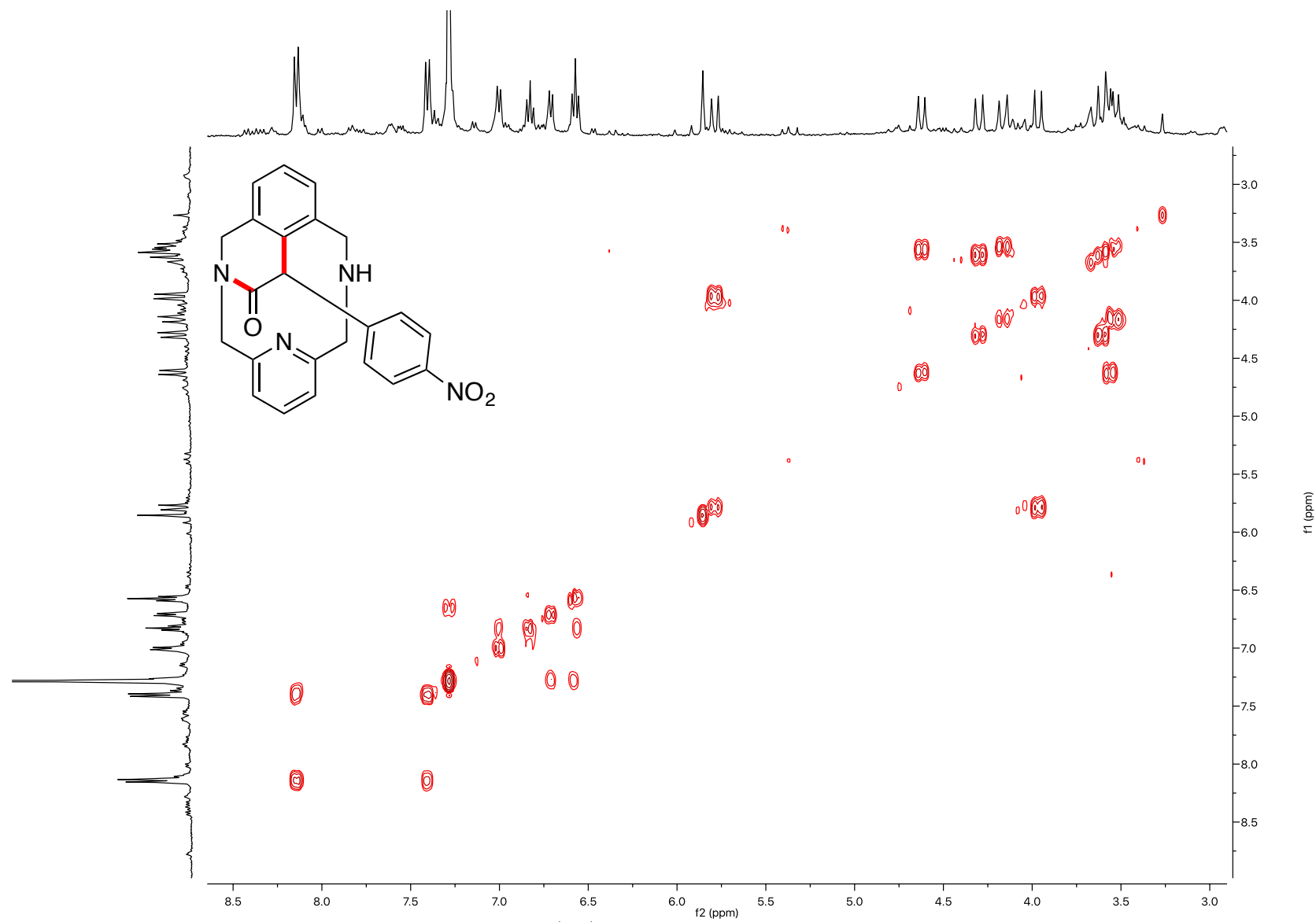
Figure S63. 400 MHz ^1H-^1H COSY spectrum of **3l** in CDCl$_3$, 298 K.
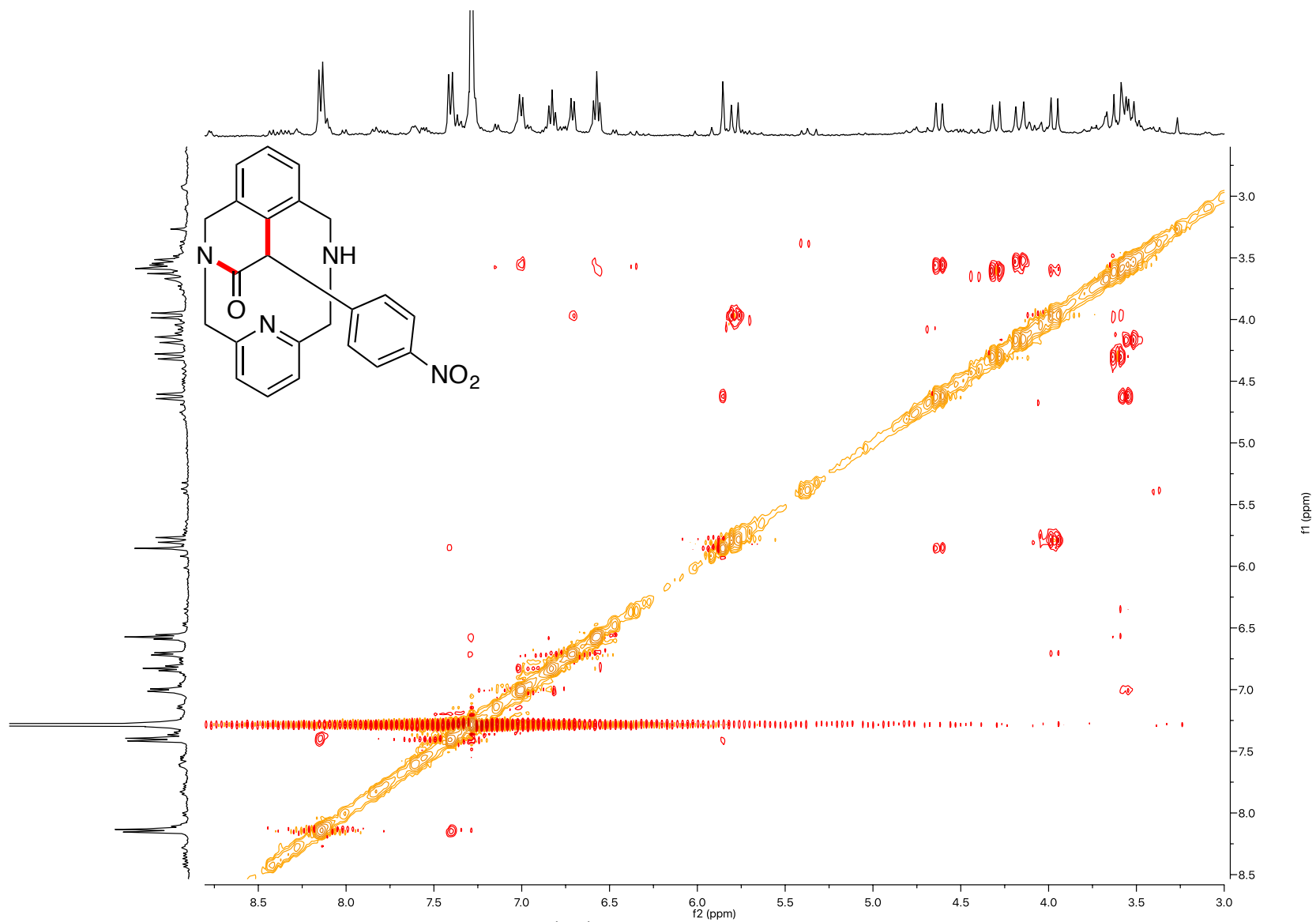
Figure S64. 400 MHz ^{1}H-^{1}H COSY spectrum of **3l** in CDCl$_3$, 298 K.
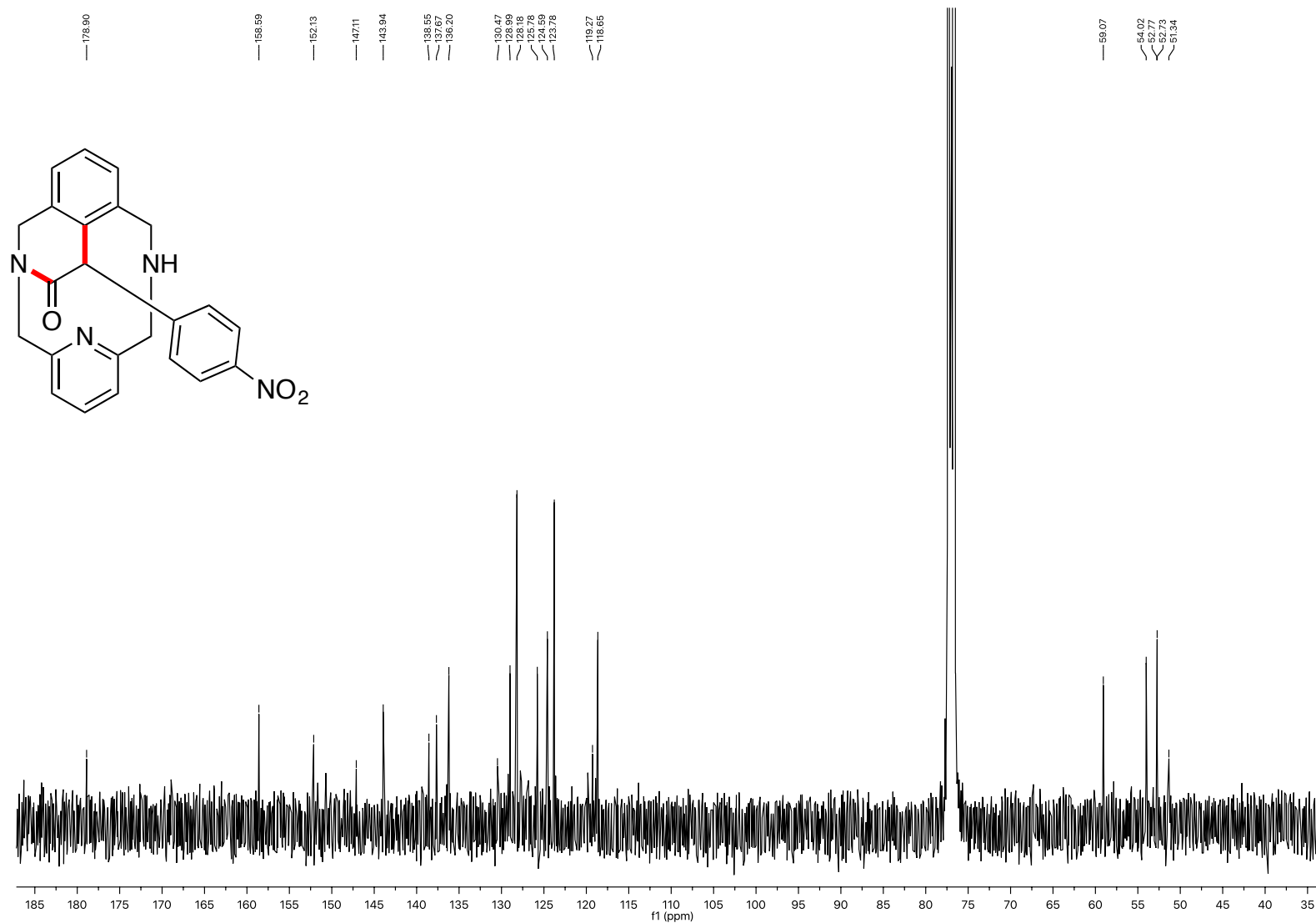
Figure S65. 100 MHz ^{13}C-{H} NMR spectrum of **3l** in CDCl$_3$, 298 K.
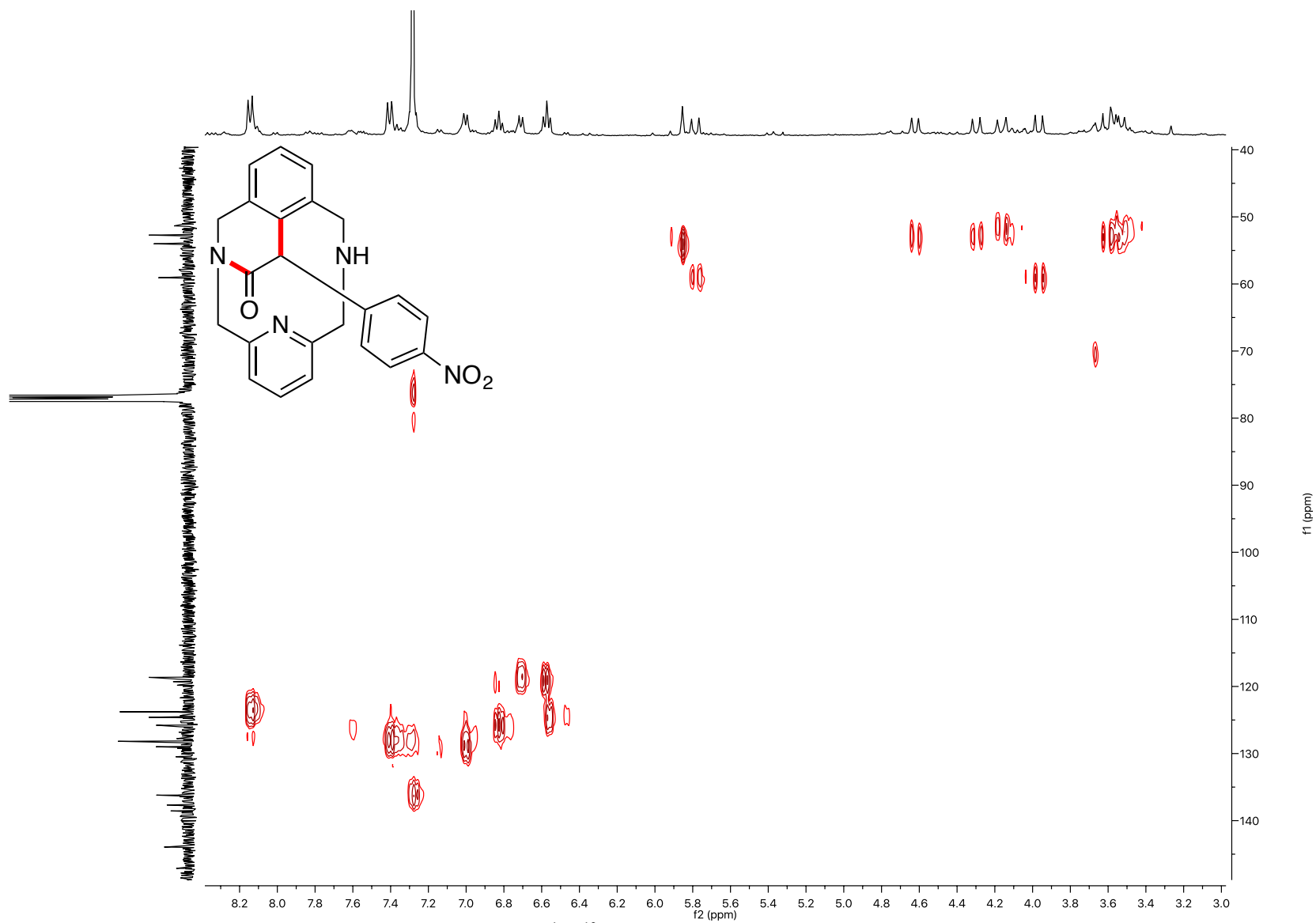
Figure S66. 400 MHz ^{1}H-^{13}C HSQC spectrum of **3l** in CDCl$_3$, 298 K.

Figure S66. 400 MHz ^{1}H-^{13}C HMBC spectrum of **3l** in CDCl$_3$, 298 K.
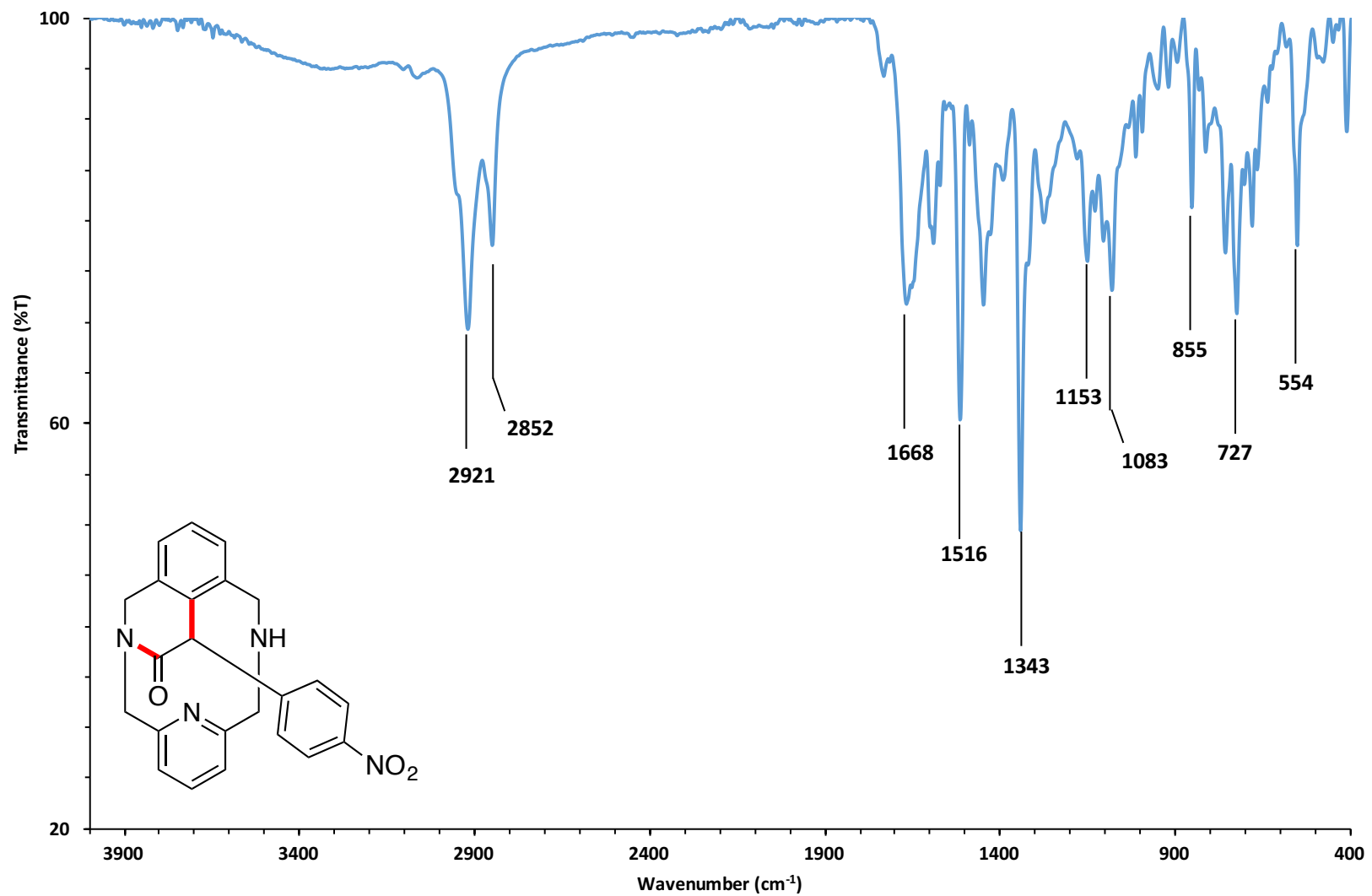
Figure S67. FT-IR spectrum of **3l** in solid state, 298 K.
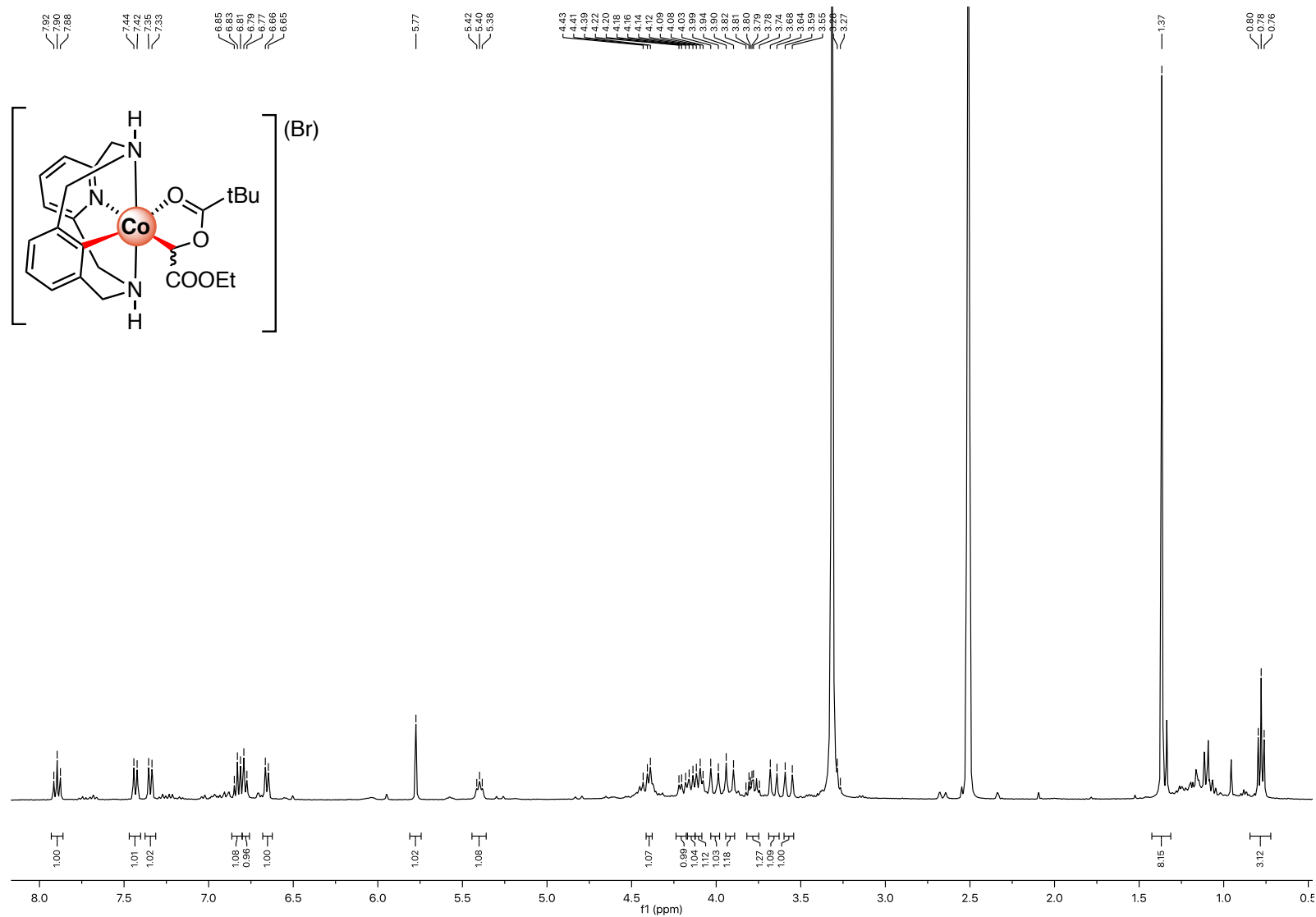
Figure S68. 400 MHz ^{1}H NMR spectrum of **4a-OPiv** in DMSO-d$_6$, 298 K.
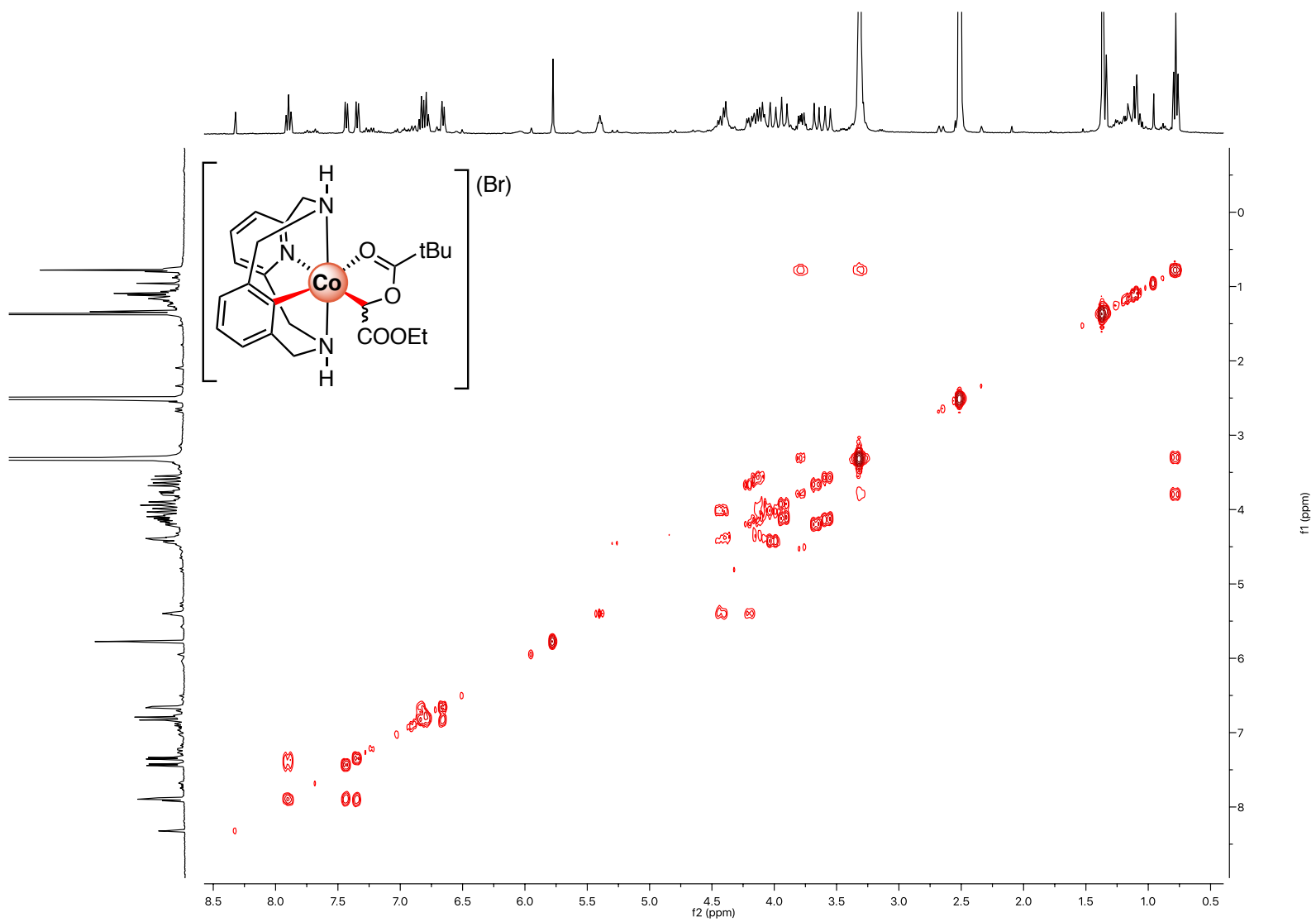
Figure S69. 400 MHz ^{1}H-^{1}H COSY spectrum of **4a-OPiv** in DMSO-d$_6$, 298 K.
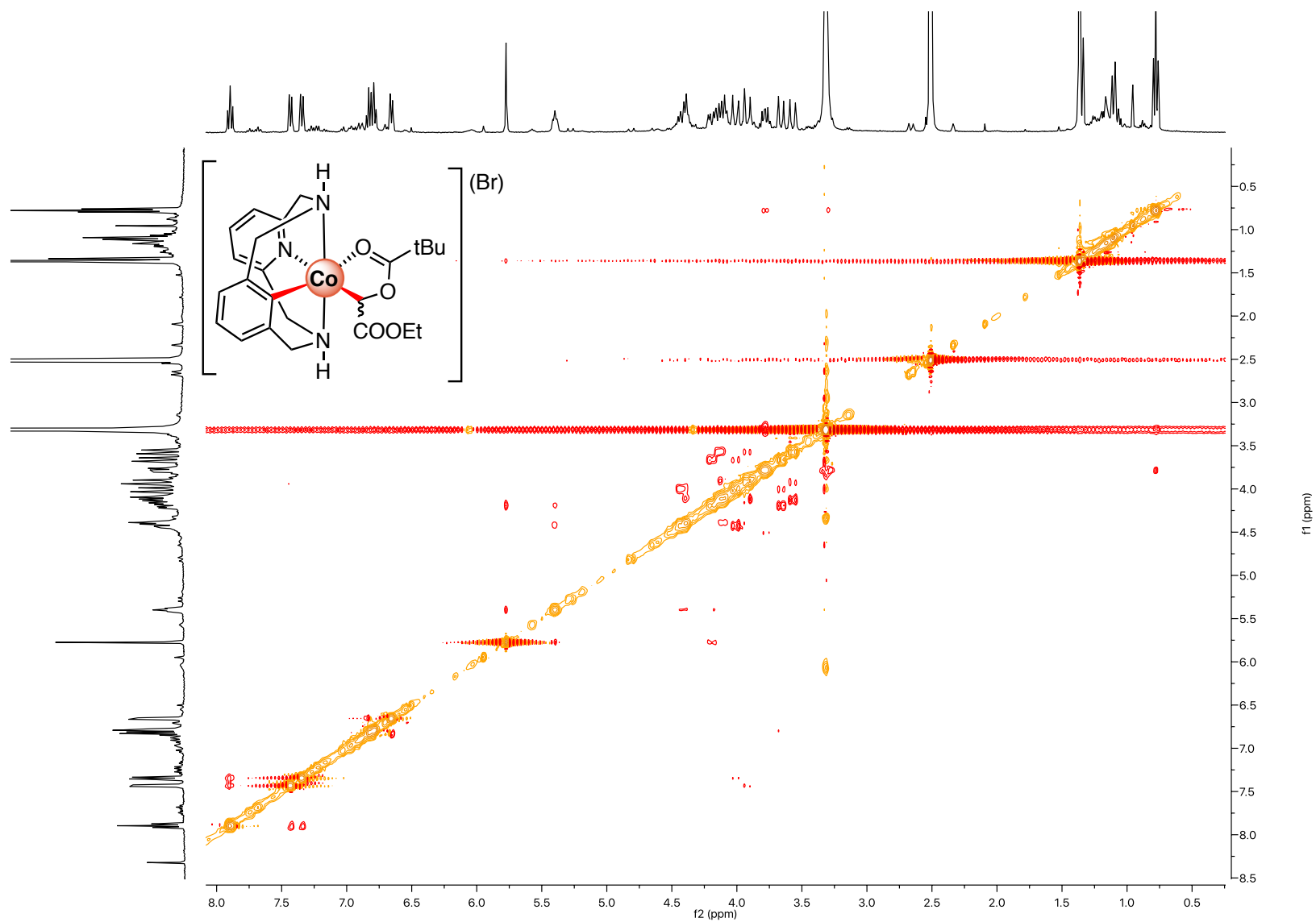
Figure S70. 400 MHz ^{1}H-^{1}H NOESY spectrum of **4a-OPiv** in DMSO-d$_6$, 298 K.
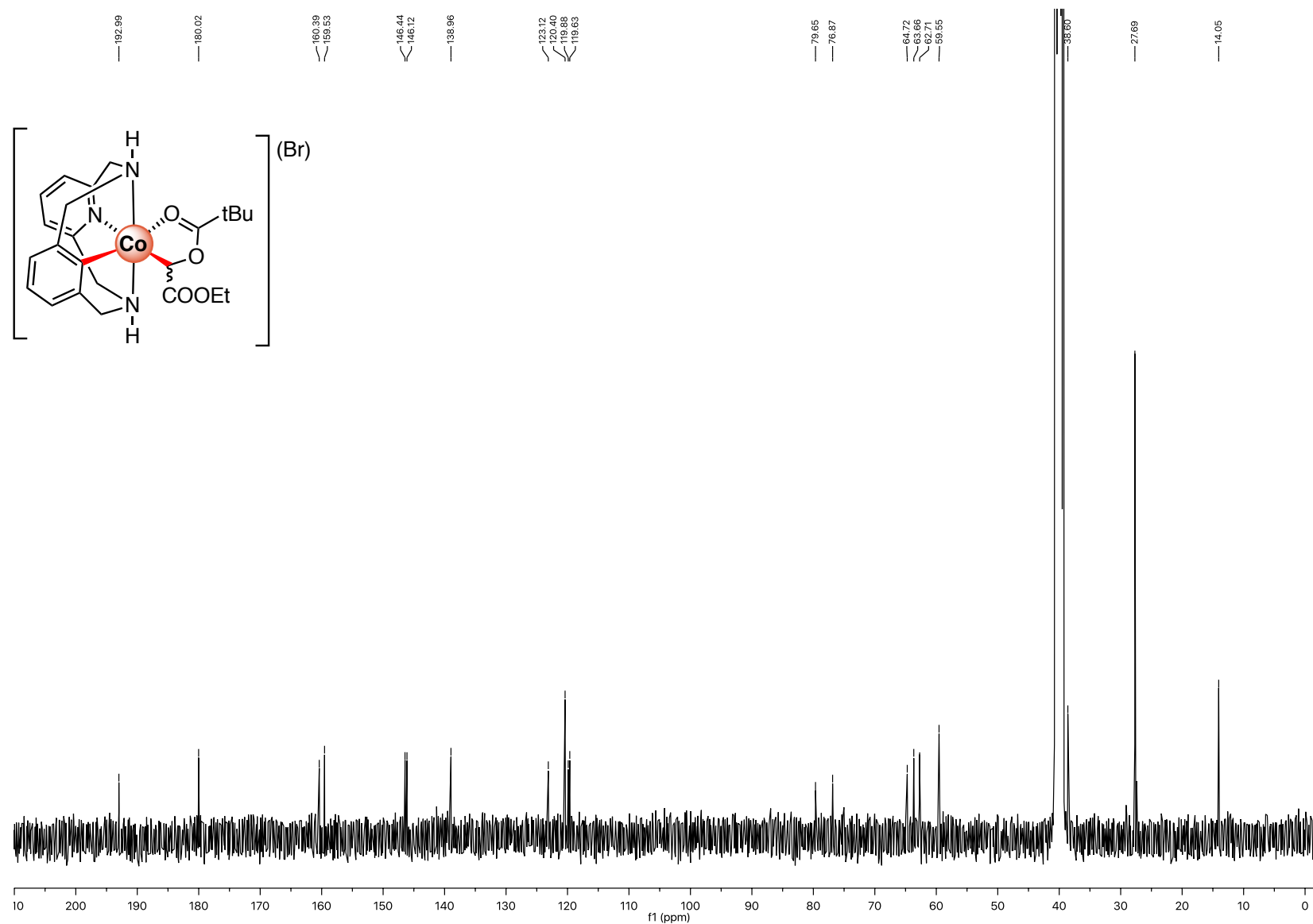
Figure S71. 100 MHz ^{13}C {1H} NMR spectrum of **4a-OPiv** in DMSO-d$_6$, 298 K.

Figure S72. 400 MHz ^{1}H-^{13}C HSQC spectrum of **4a-OPiv** in DMSO-d$_6$, 298 K.
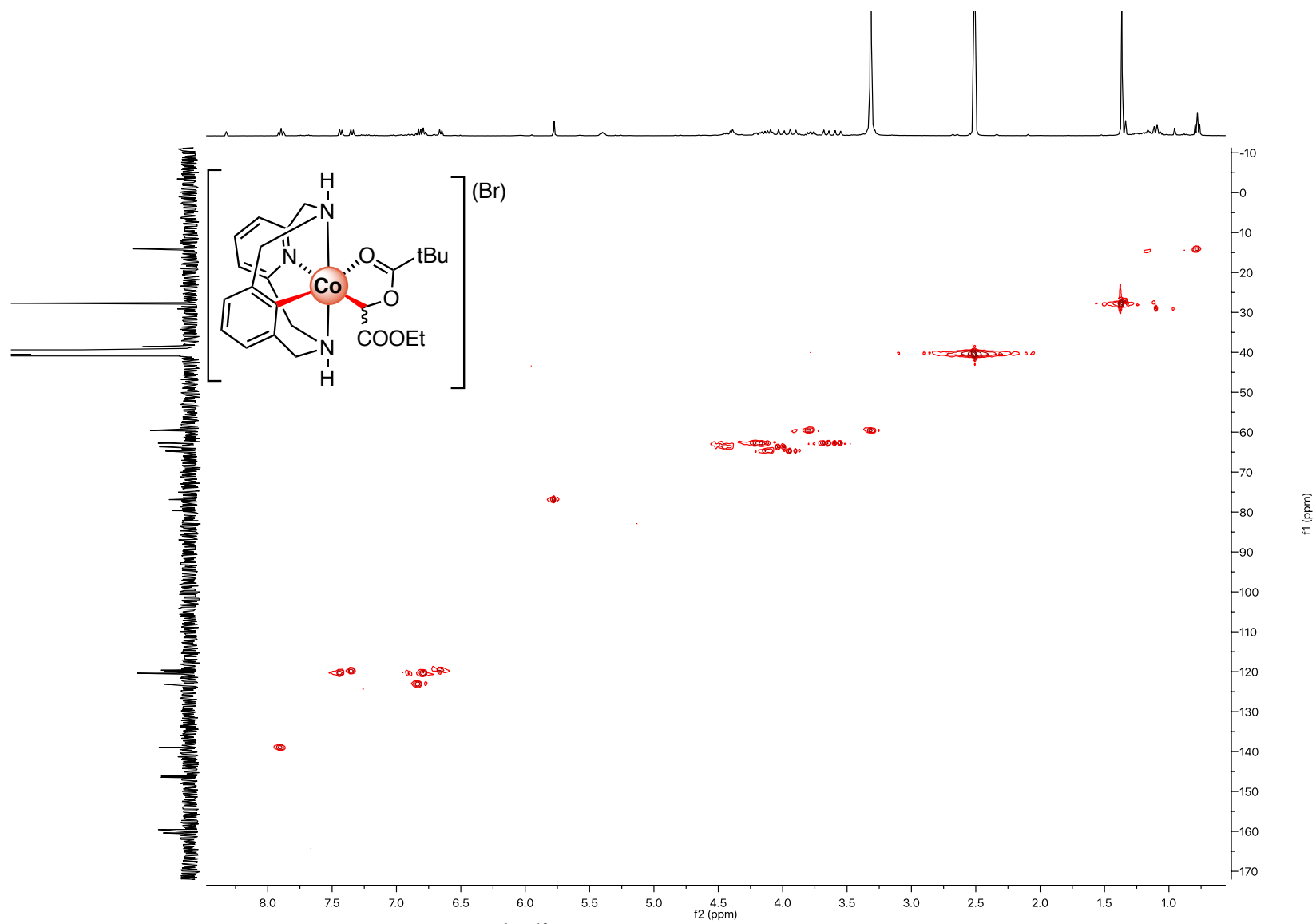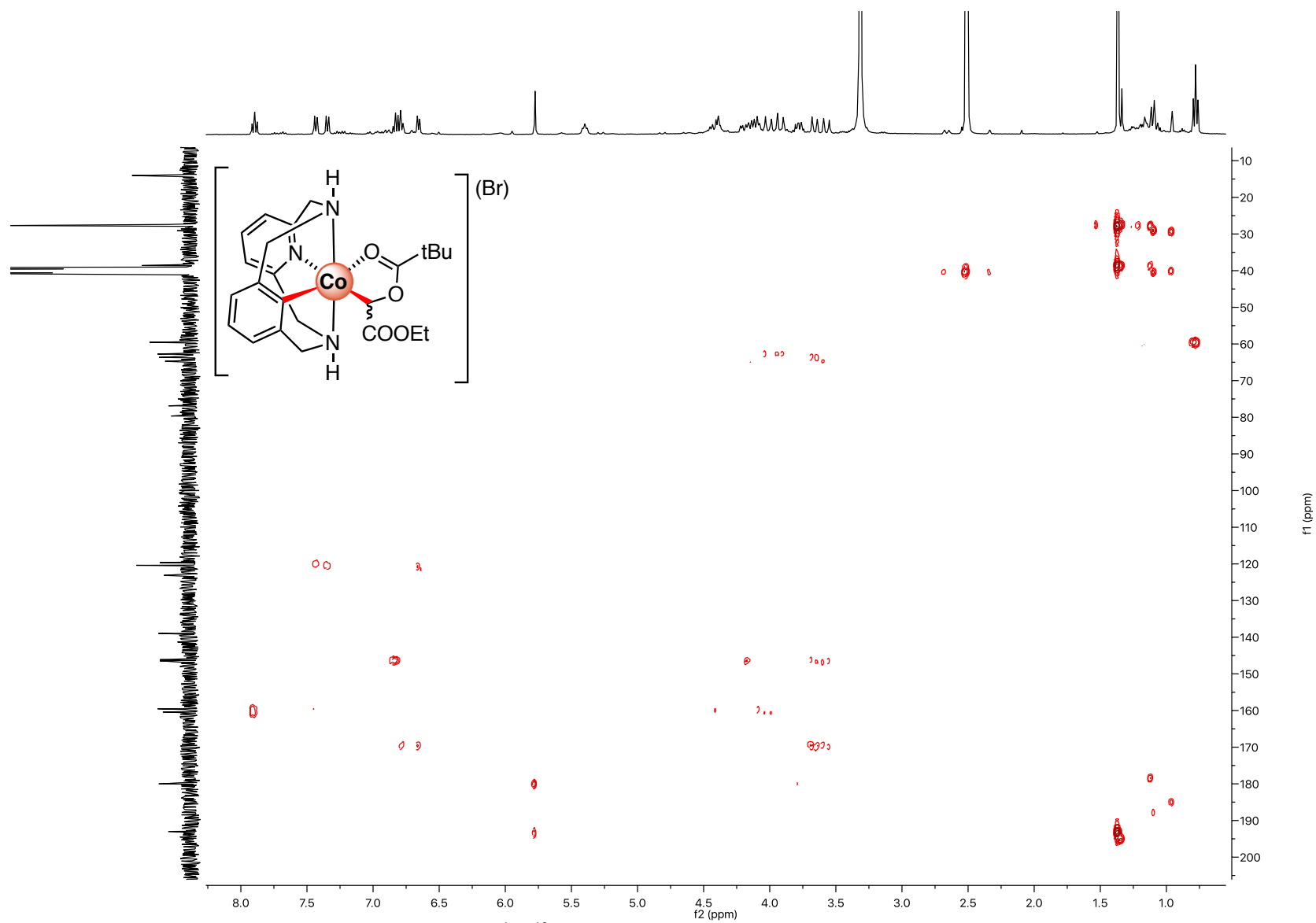
Figure S73. 400 MHz ^{1}H-^{13}C HMBC spectrum of **4a-OPiv** in DMSO-d$_6$, 298 K.
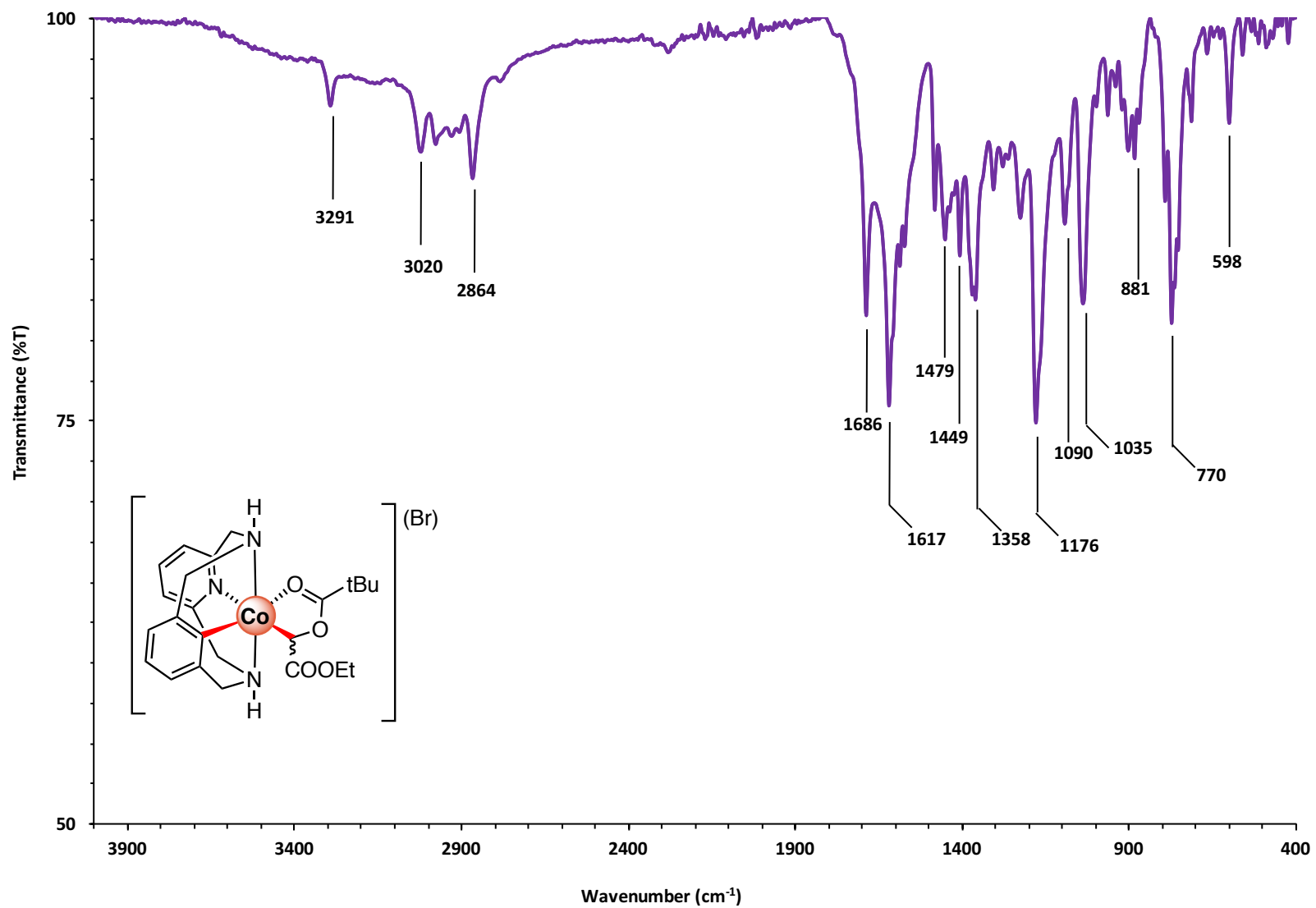
Figure S74. FT-IR spectrum of **4a-OPiv** in solid state, 298 K.
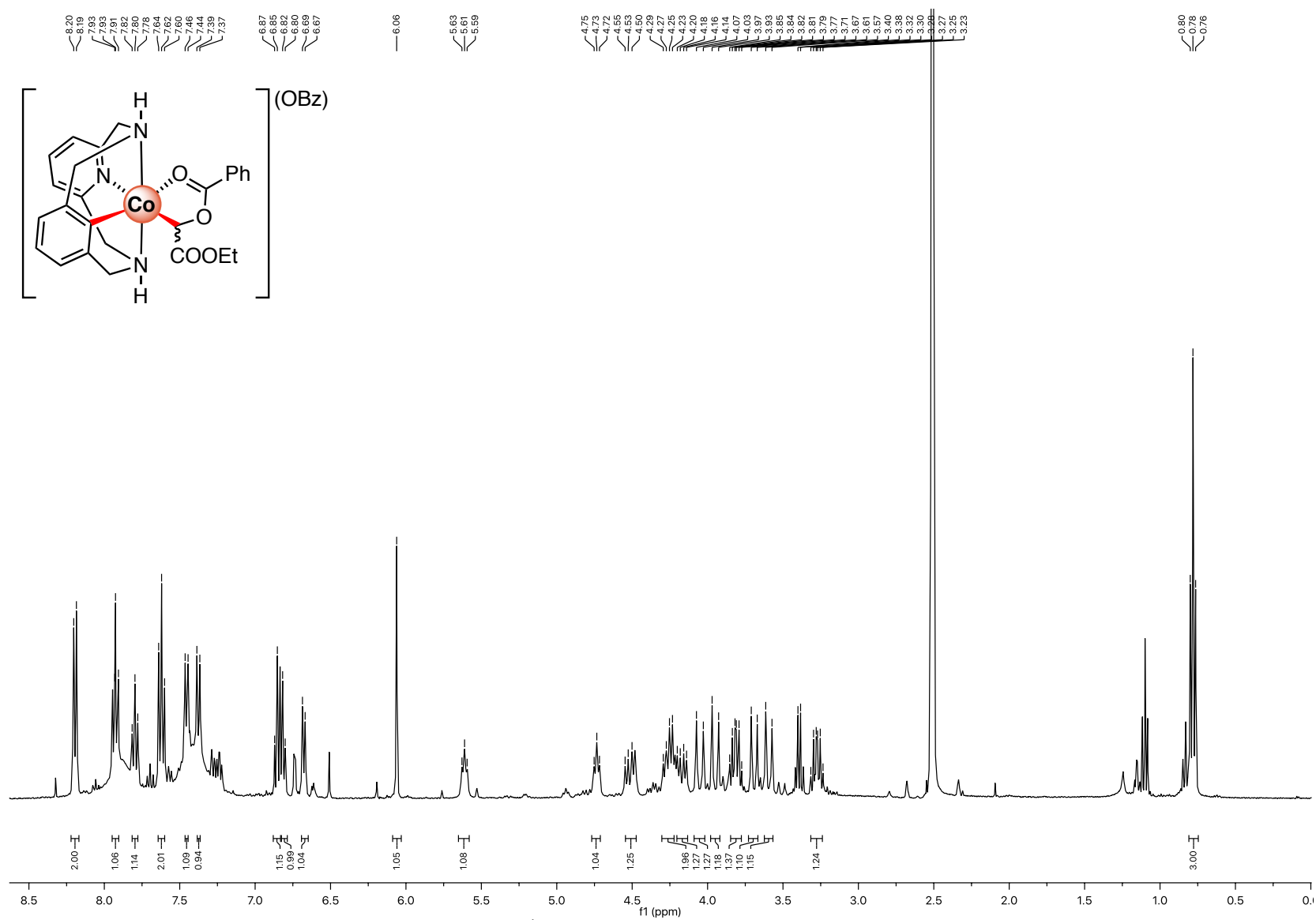
Figure S75. 400 MHz ^{1}H NMR spectrum of **4a-OBz** in DMSO-d$_6$, 298 K.
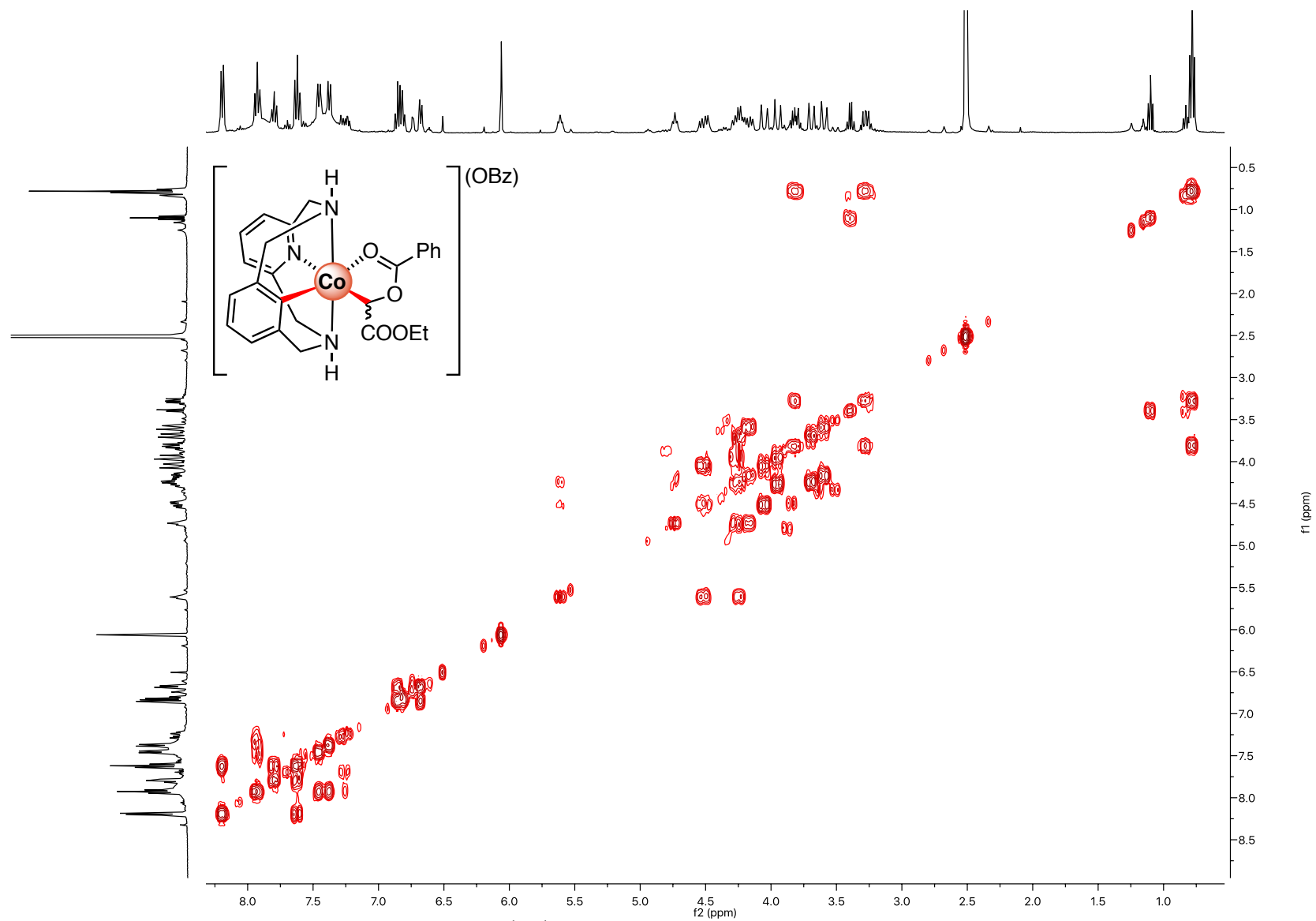
Figure S76. 400 MHz ^{1}H-^{1}H COSY spectrum of **4a-OBz** in DMSO-d$_6$, 298 K.

Figure S77. 400 MHz ^{1}H-^{1}H NOESY spectrum of **4a-OBz** in DMSO-d$_6$, 298 K.
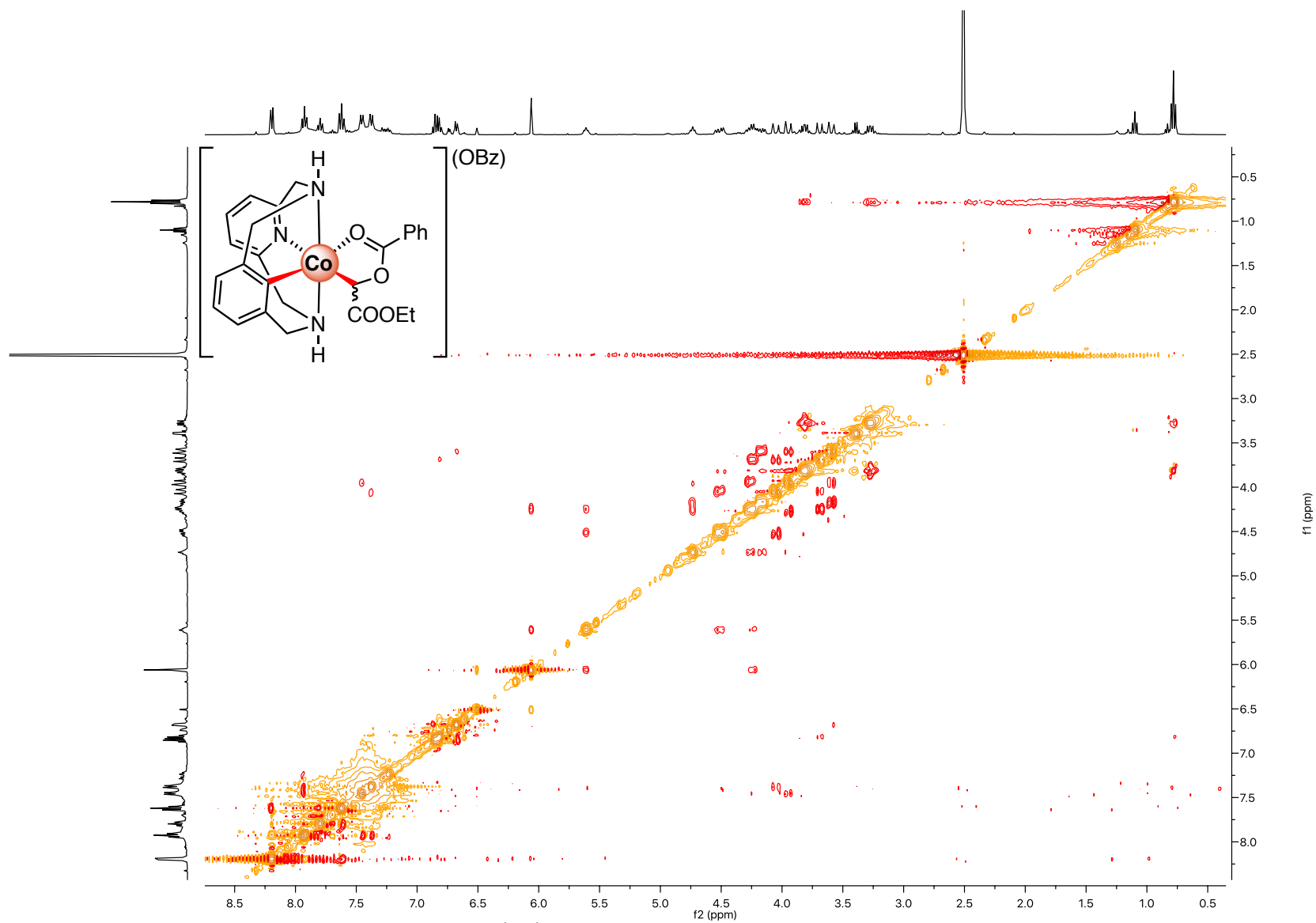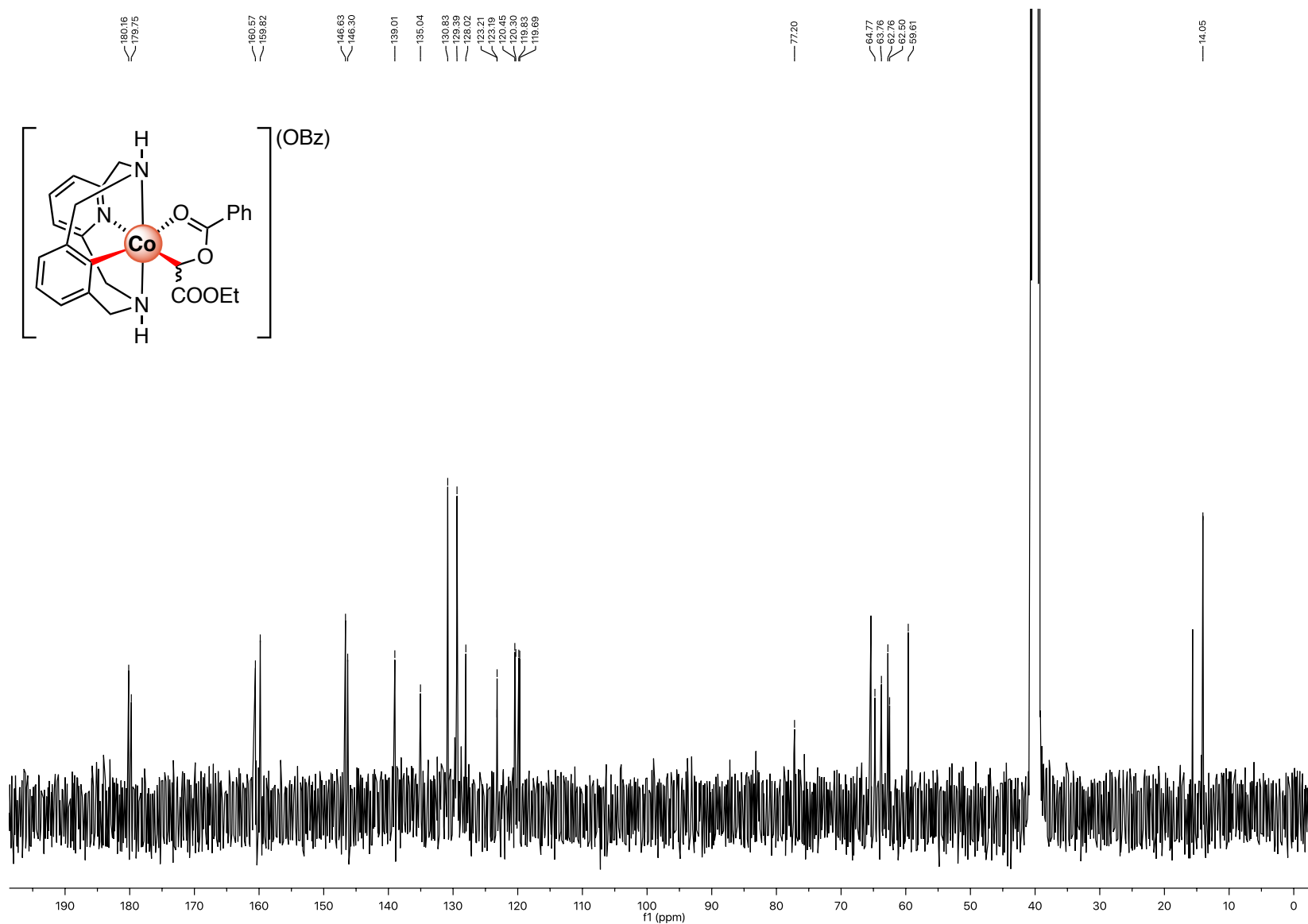
Figure S78. 100 MHz ^{13}C {1H} NMR spectrum of **4a-OBz** in DMSO-d$_6$, 298 K.
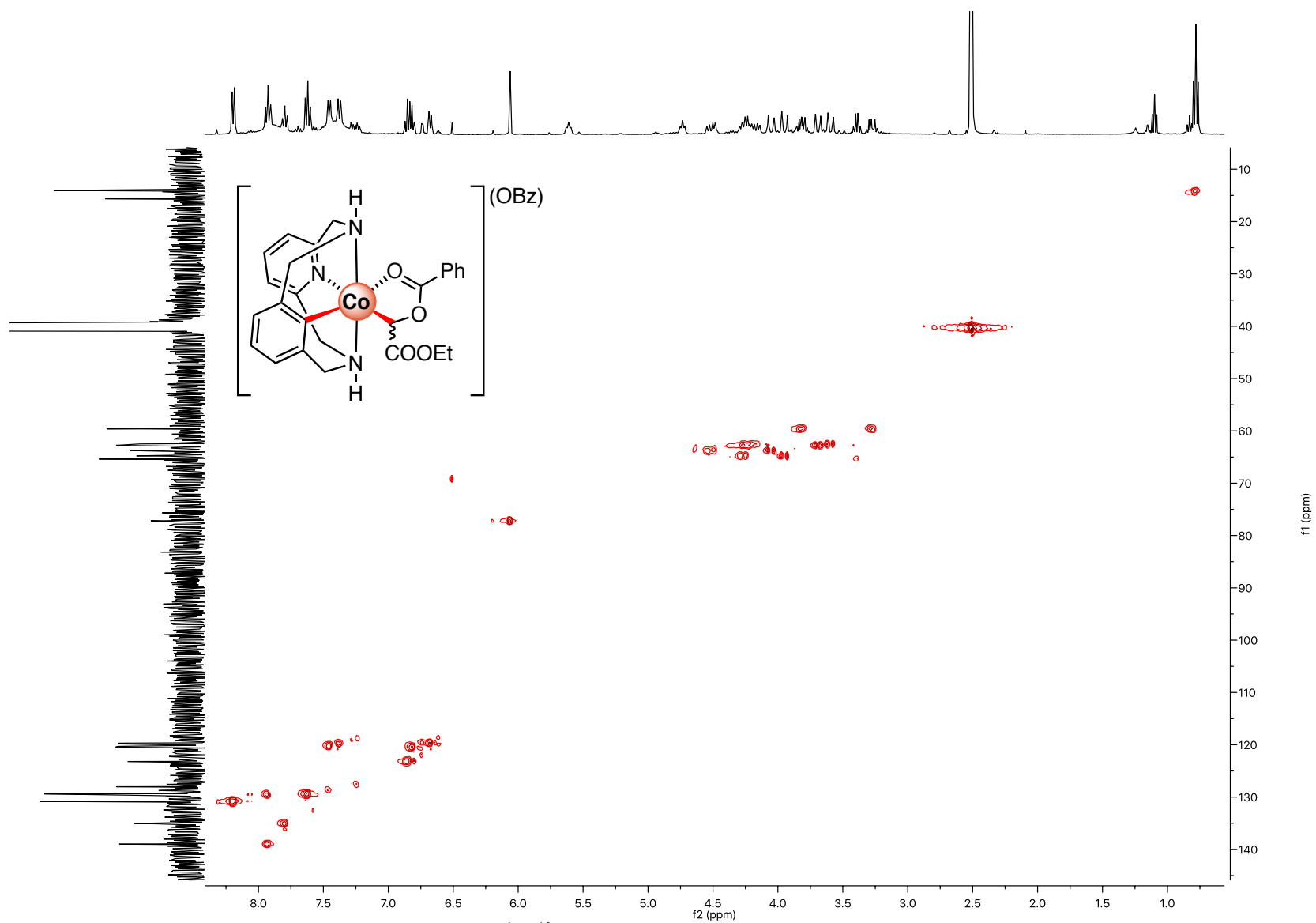
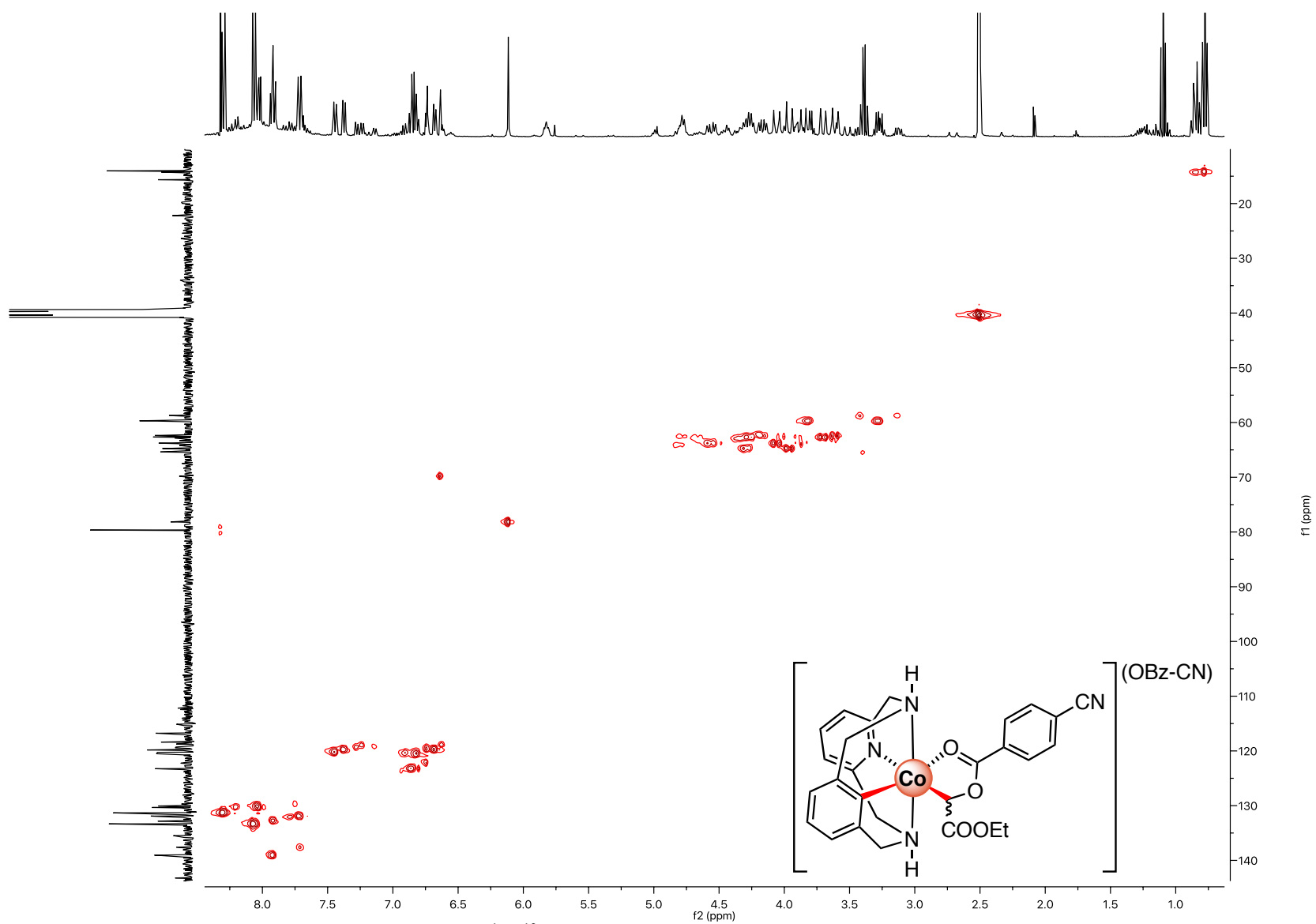**Figure S79.** 400 MHz ^{1}H-^{13}C HSQC spectrum of **4a-OBz** in DMSO-d$_6$, 298 K.
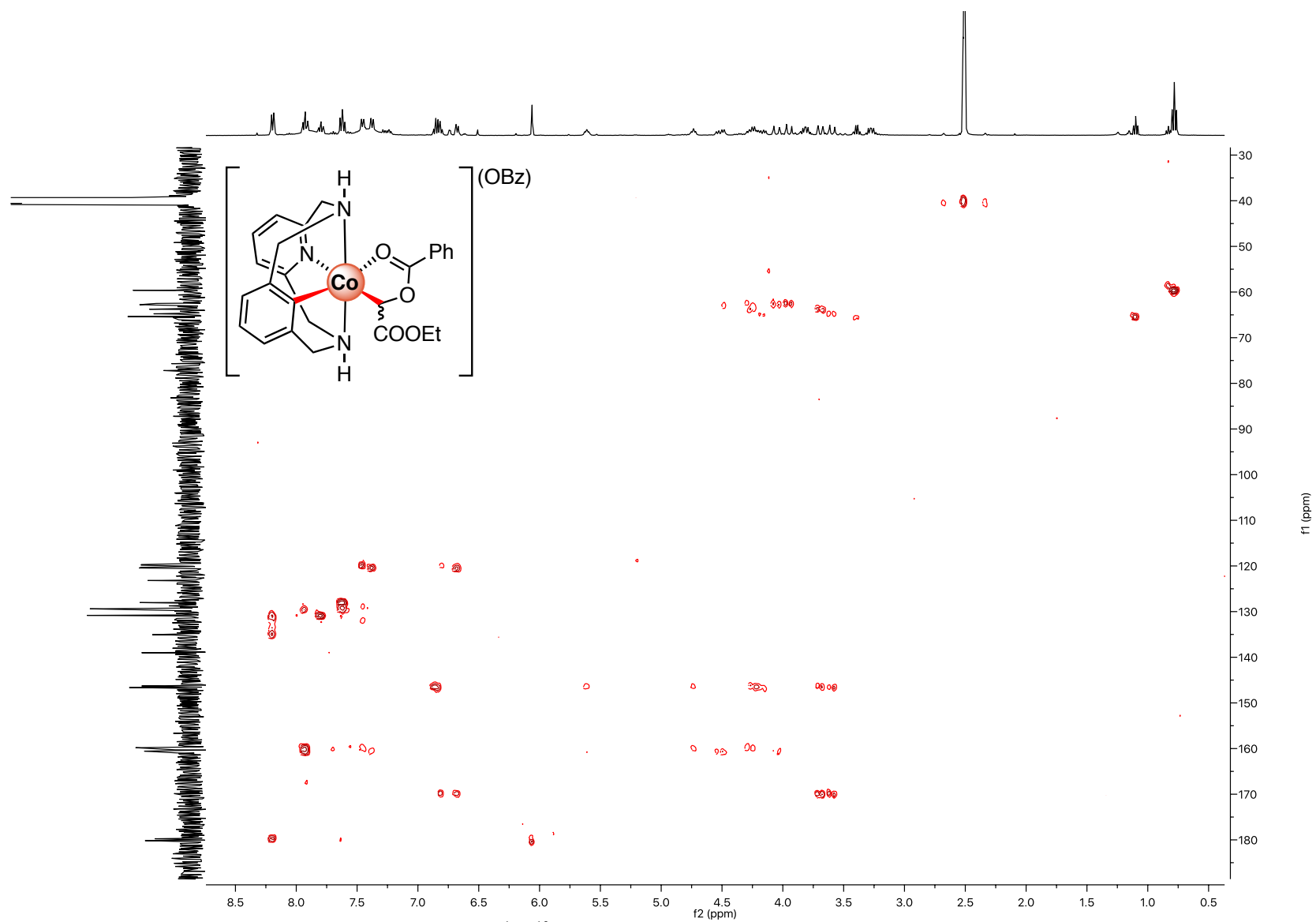
Figure S80. 400 MHz ^{1}H-^{13}C HMBC spectrum of **4a-OBz** in DMSO-d$_6$, 298 K.
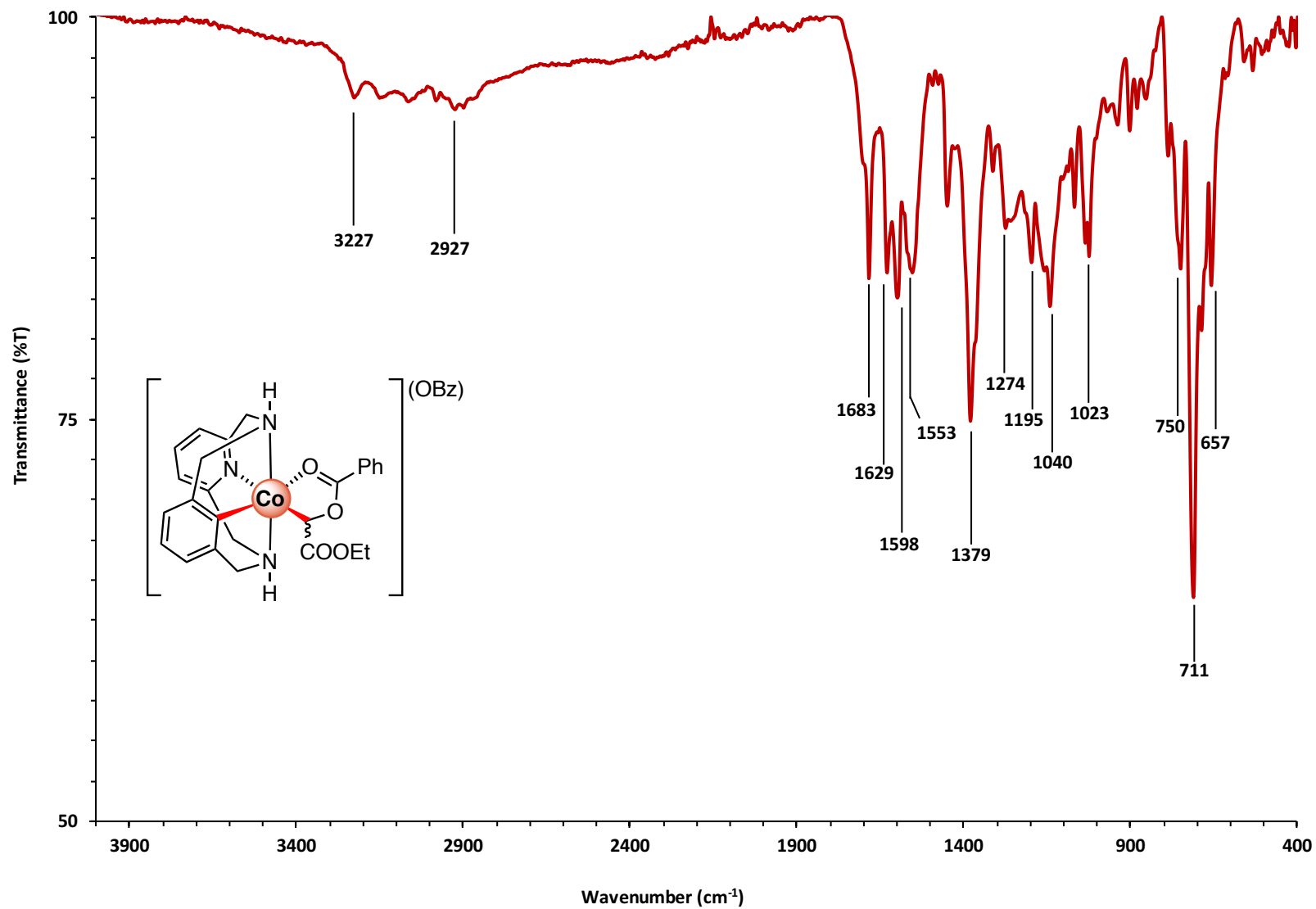
Figure S81. FT-IR spectrum of **4a-OBz** in solid state, 298 K.
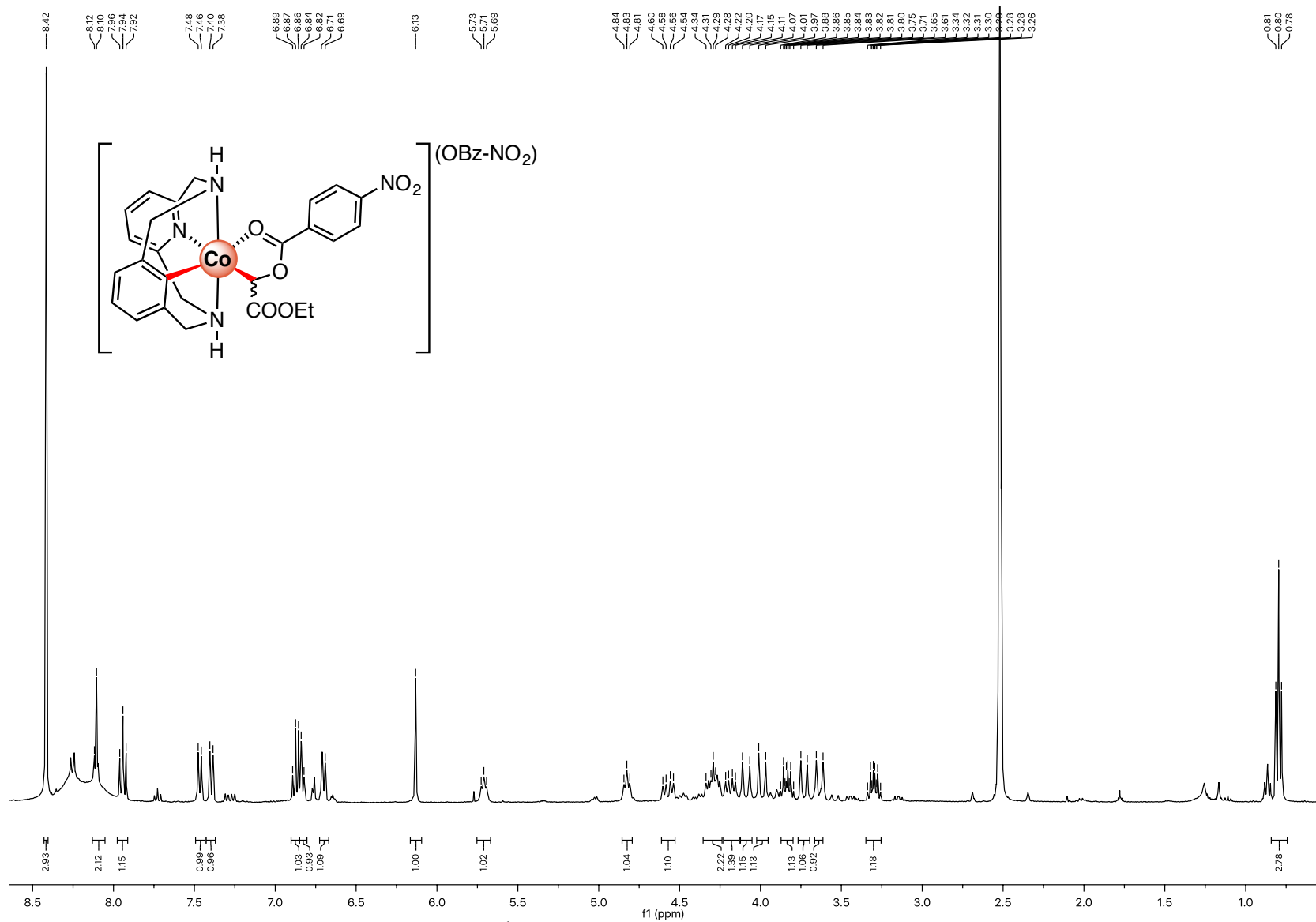
Figure S82. 400 MHz ^{1}H NMR spectrum of **4a-OBz-NO$_2$** in DMSO-d$_6$, 298 K.
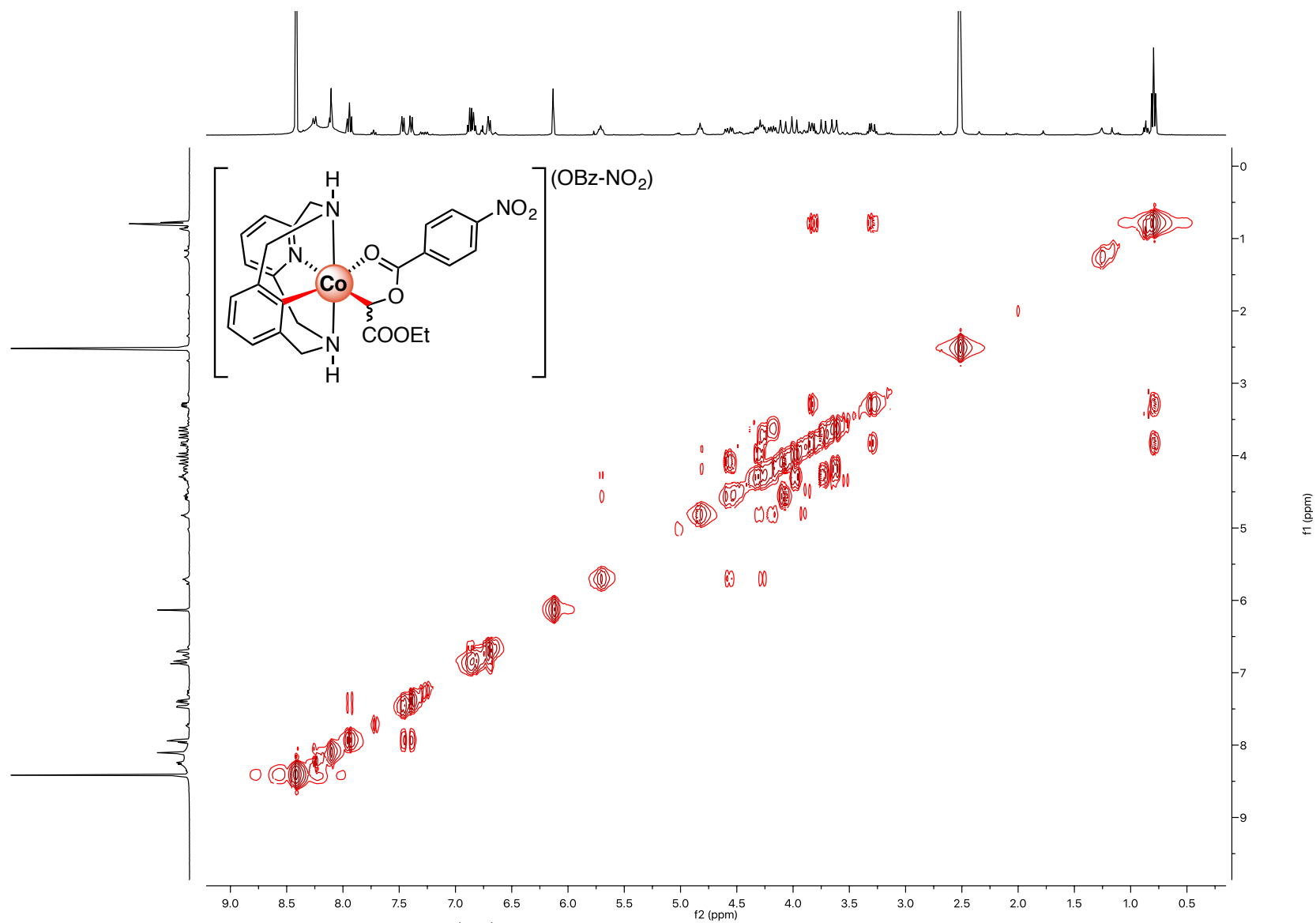
Figure S83. 400 MHz ^{1}H-^{1}H COSY NMR spectrum of **4a-OBz-NO$_2$** in DMSO-d$_6$, 298 K.
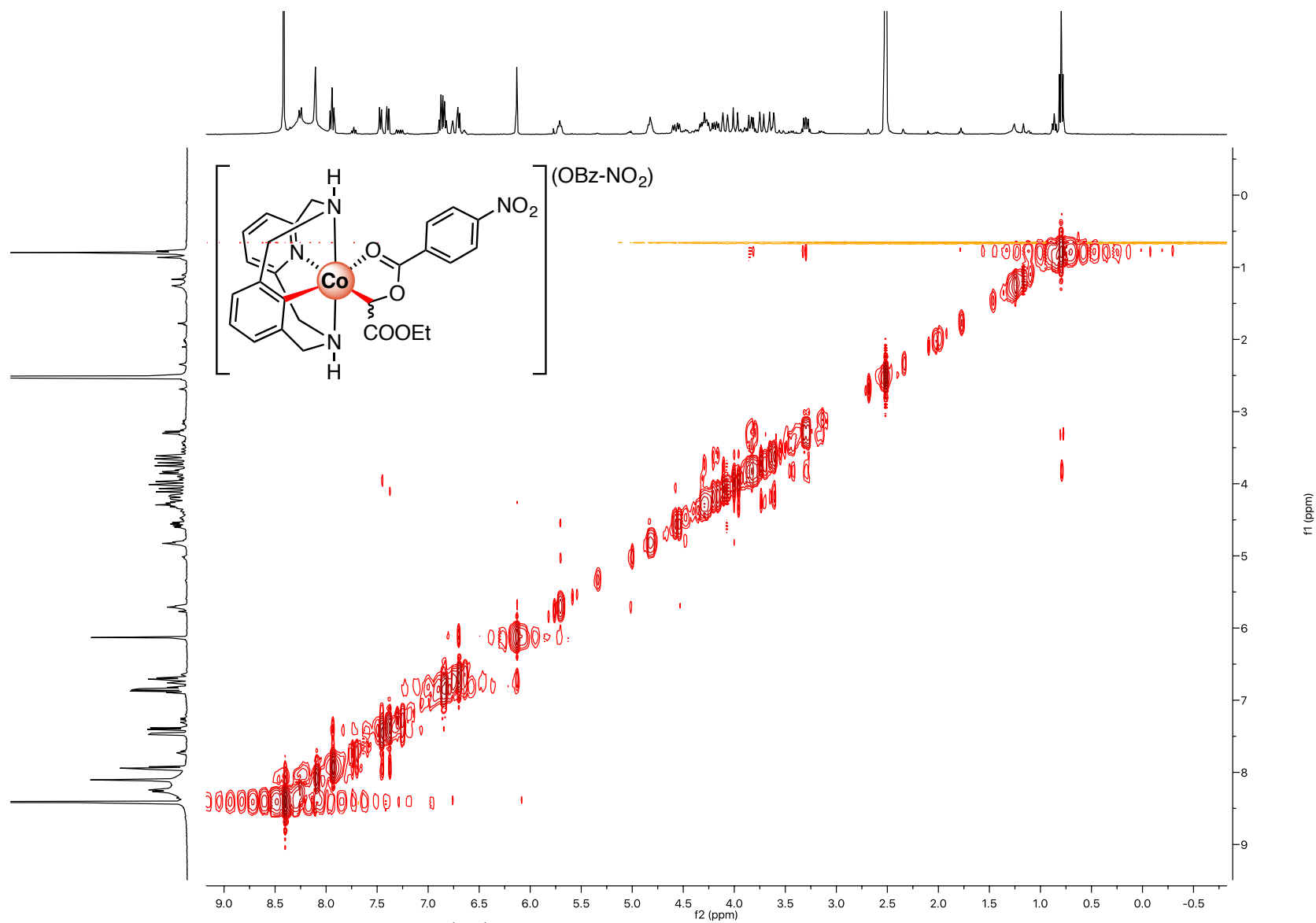
Figure S84. 400 MHz ^{1}H-^{1}H NOESY NMR spectrum of **4a-OBz-NO$_2$** in DMSO-d$_6$, 298 K.
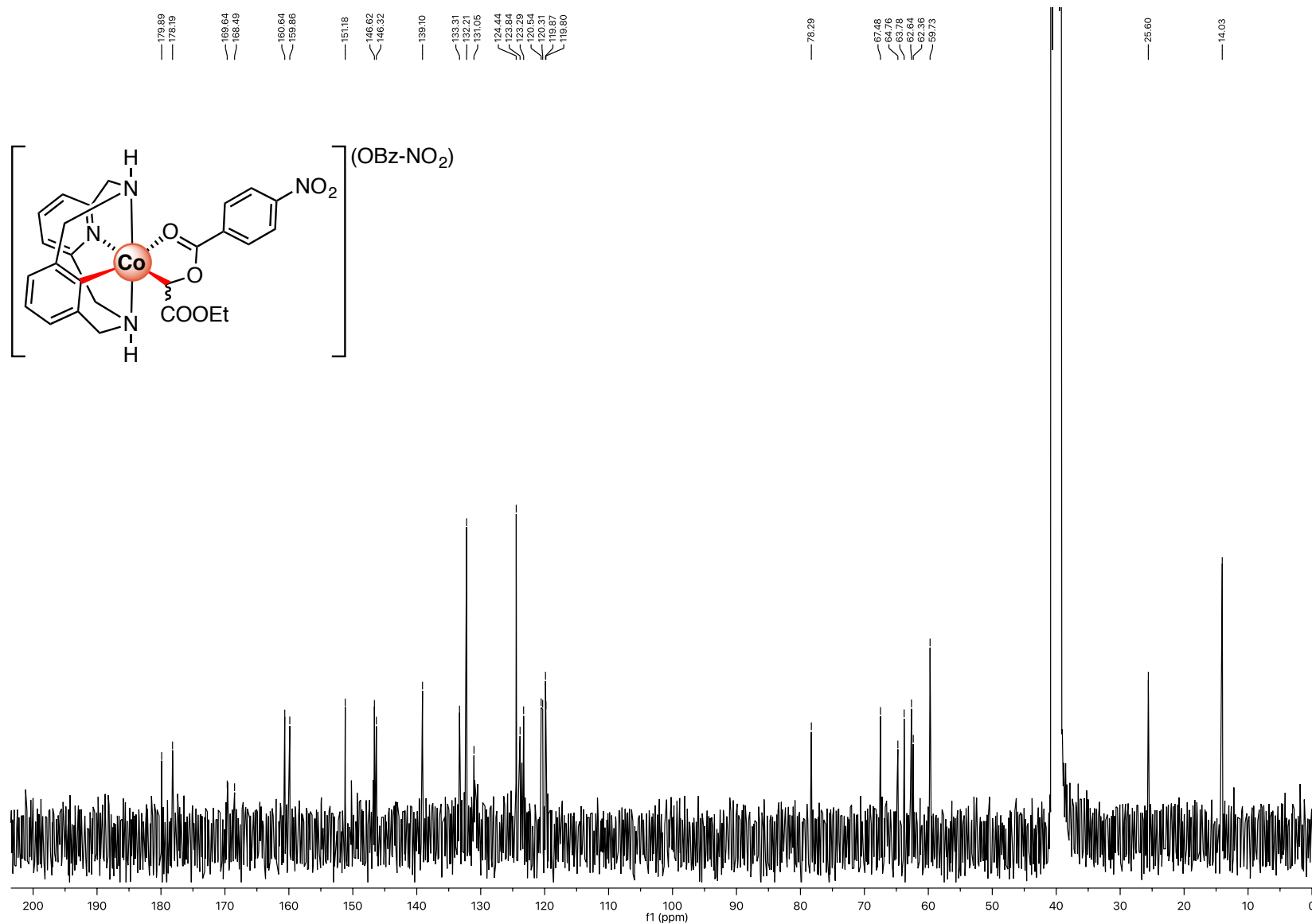
Figure S85. 100 MHz ^{13}C {^{1}H} NMR spectrum of **4a-OBz-NO$_2$** in DMSO-d$_6$, 298 K.
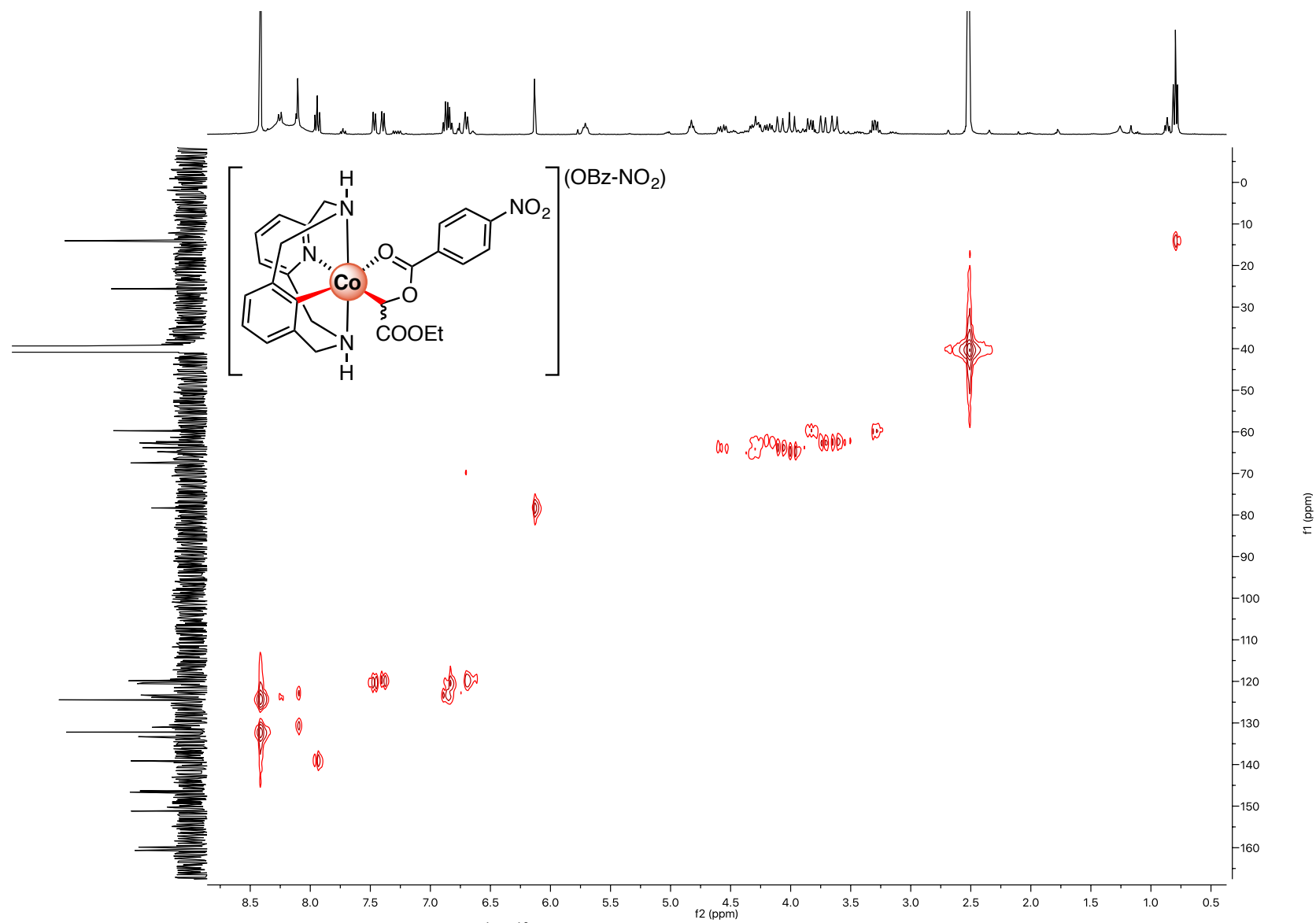
Figure S86. 400 MHz ^{1}H-^{13}C HSQC spectrum of **4a-OBz-NO$_2$** in DMSO-d$_6$, 298 K.
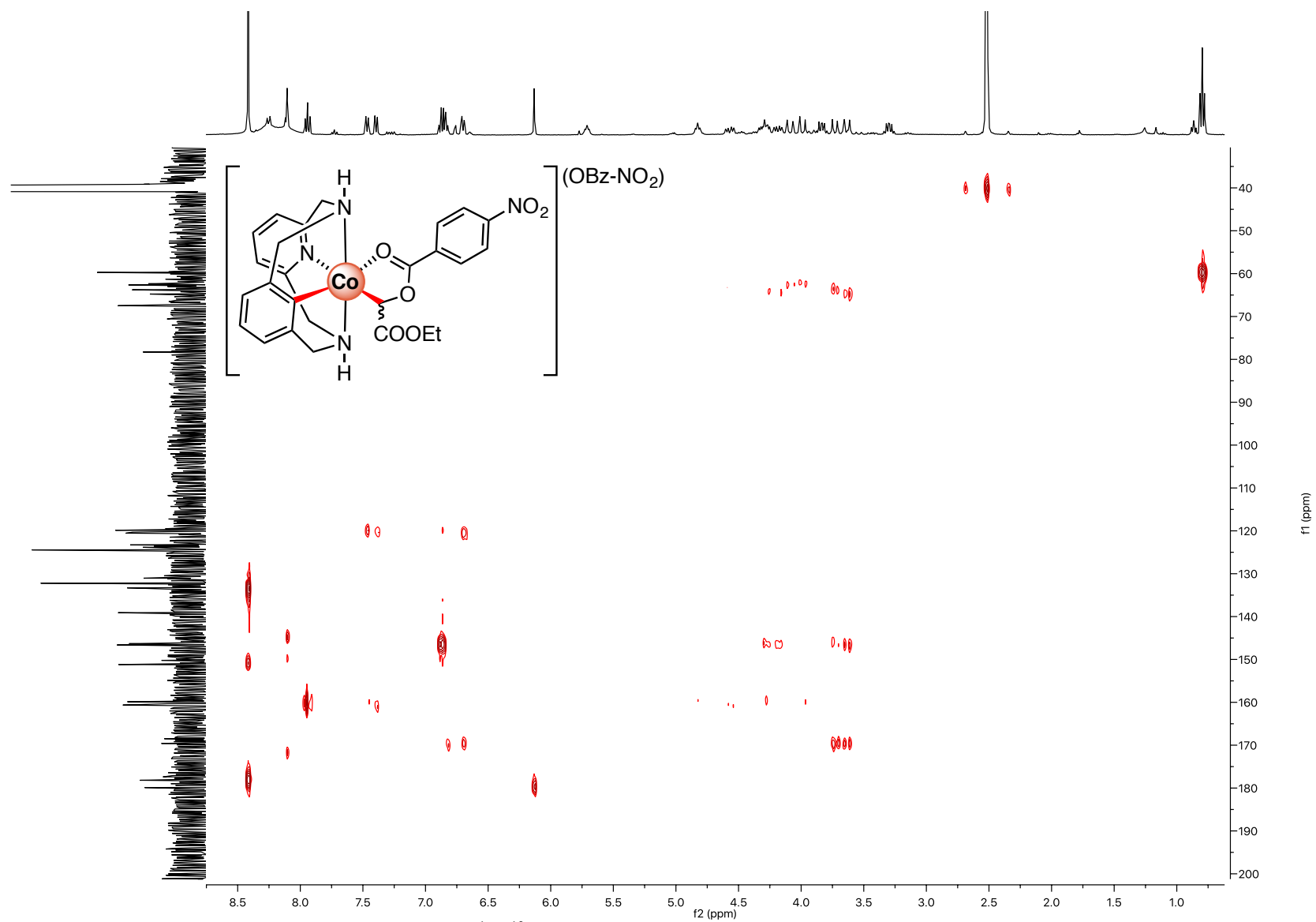
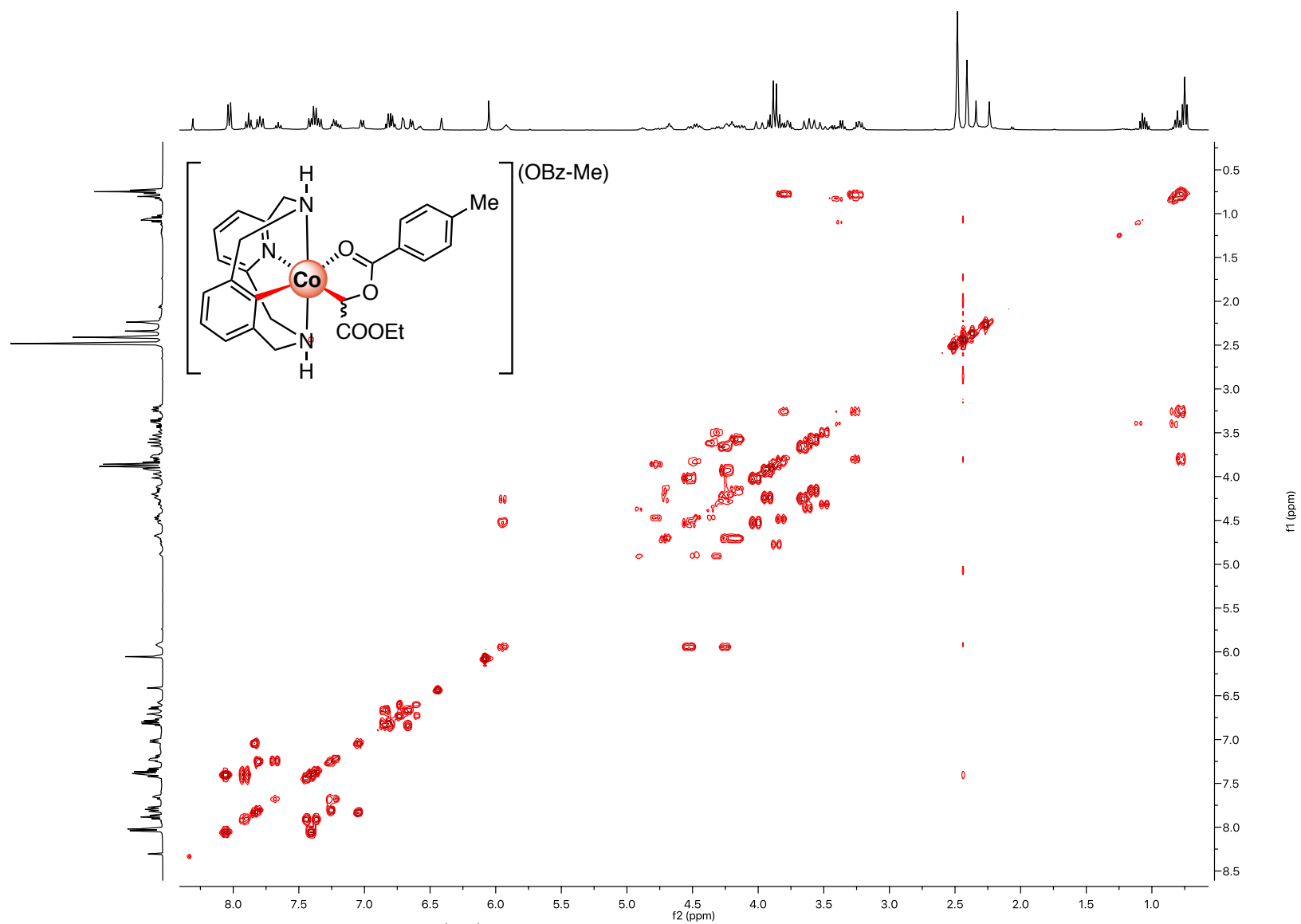**Figure S87.** 400 MHz ^1H-^{13}C HMBC spectrum of **4a-OBz-NO$_2$** in DMSO-d$_6$, 298 K.
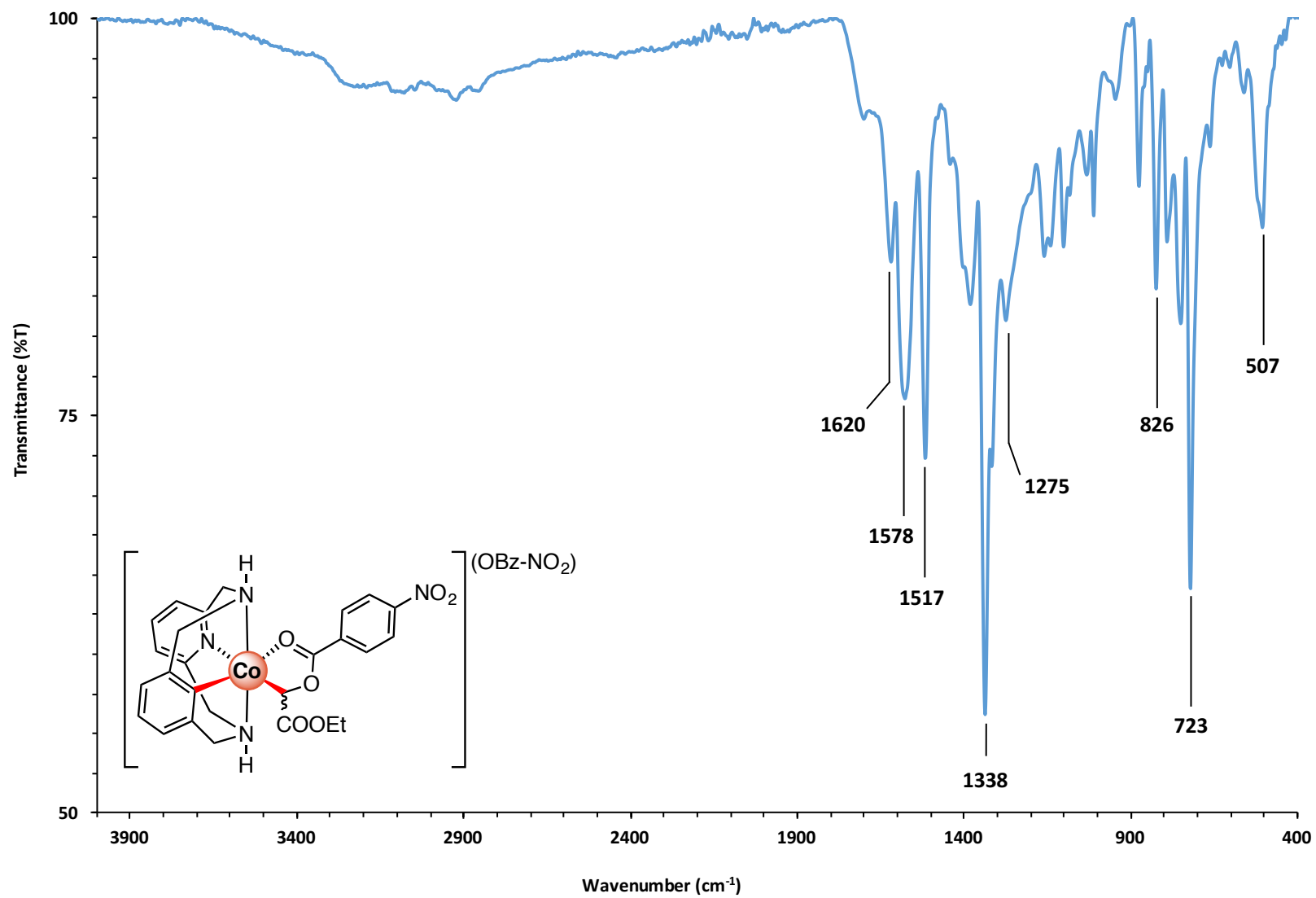
Figure S88. FT-IR spectrum of **4a-OBz-NO₂** in solid state, 298 K.
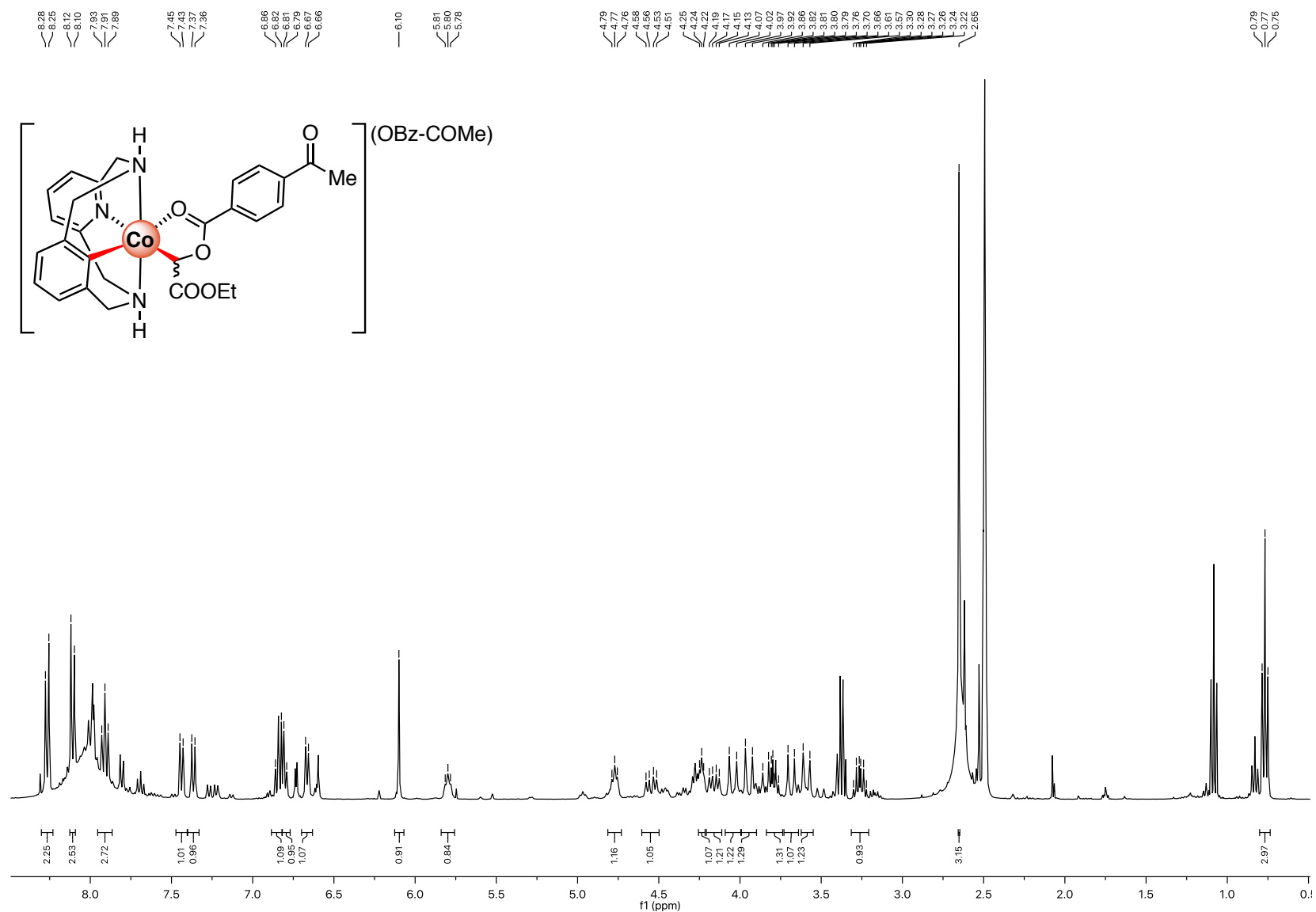
Figure S89. 400 MHz ^{1}H NMR spectrum of **4a-OBz-COMe** in DMSO-d$_6$, 298 K. (Residual ether peaks at 1.1(t) and 3.4(q) ppm)

Figure S90. 400 MHz ^{1}H-^{1}H COSY NMR spectrum of **4a-OBz-COMe** in DMSO-d$_6$, 298 K.
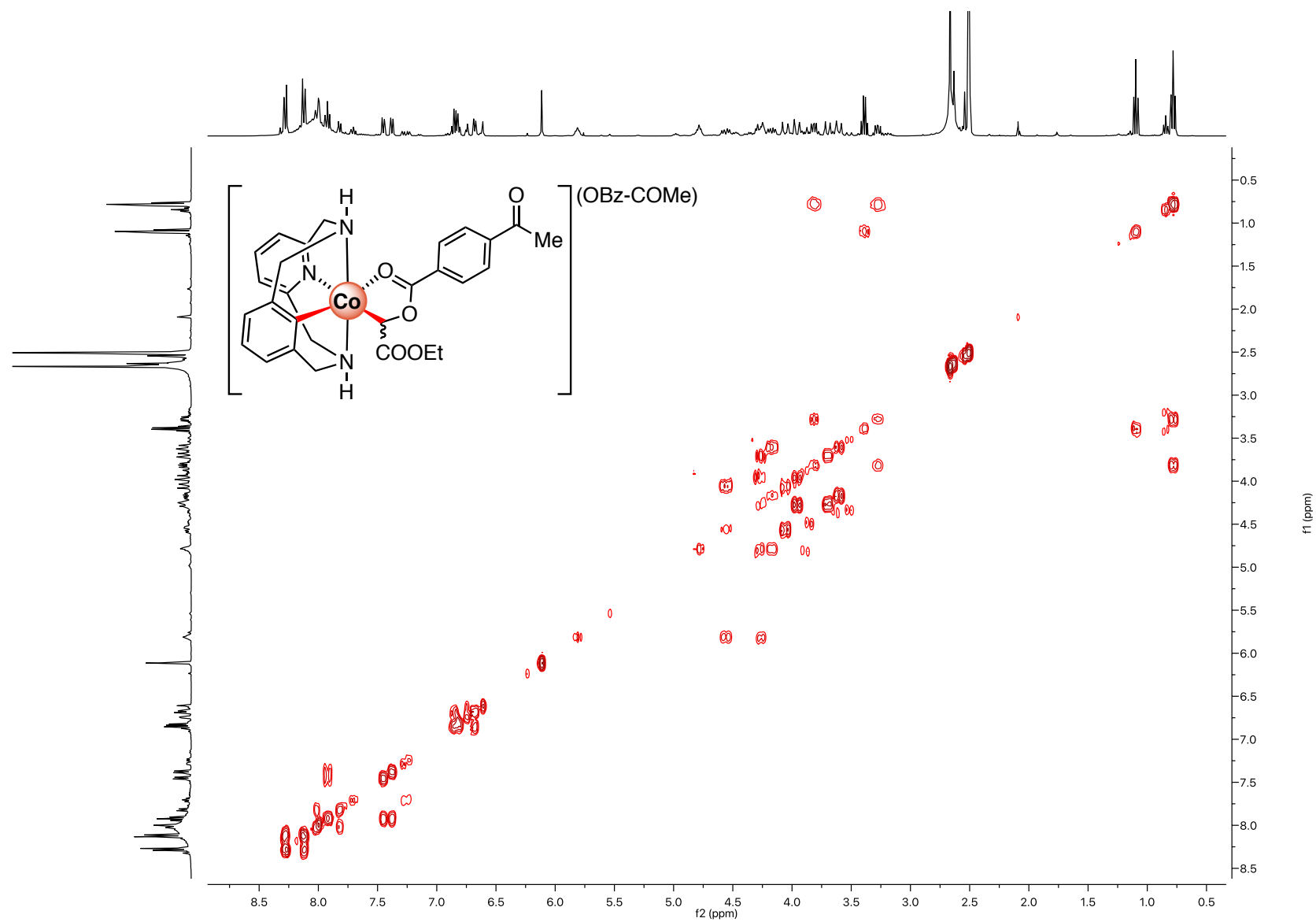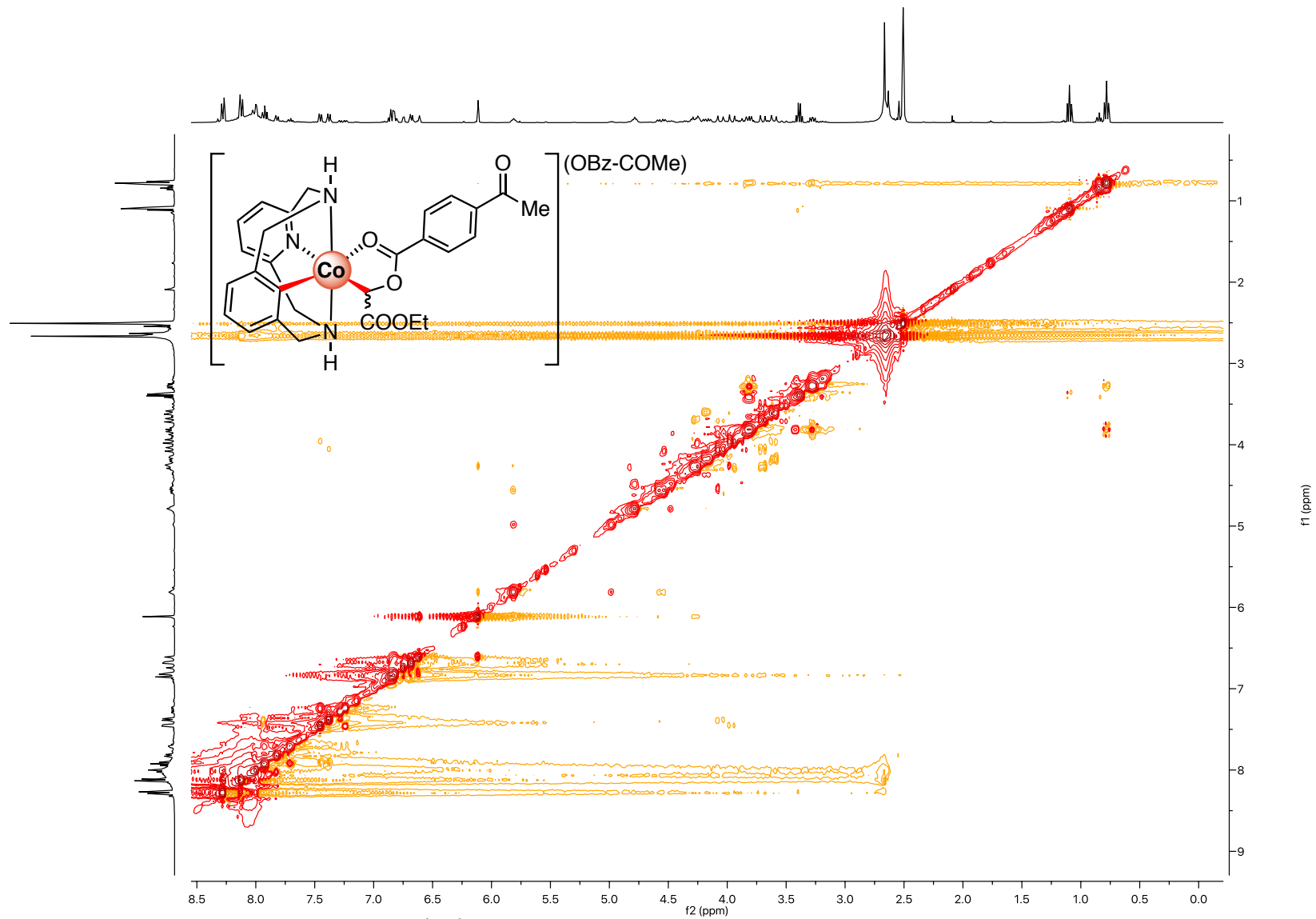
Figure S91. 400 MHz ^{1}H-^{1}H NOESY NMR spectrum of **4a-OBz-COMe** in DMSO-d$_6$, 298 K.
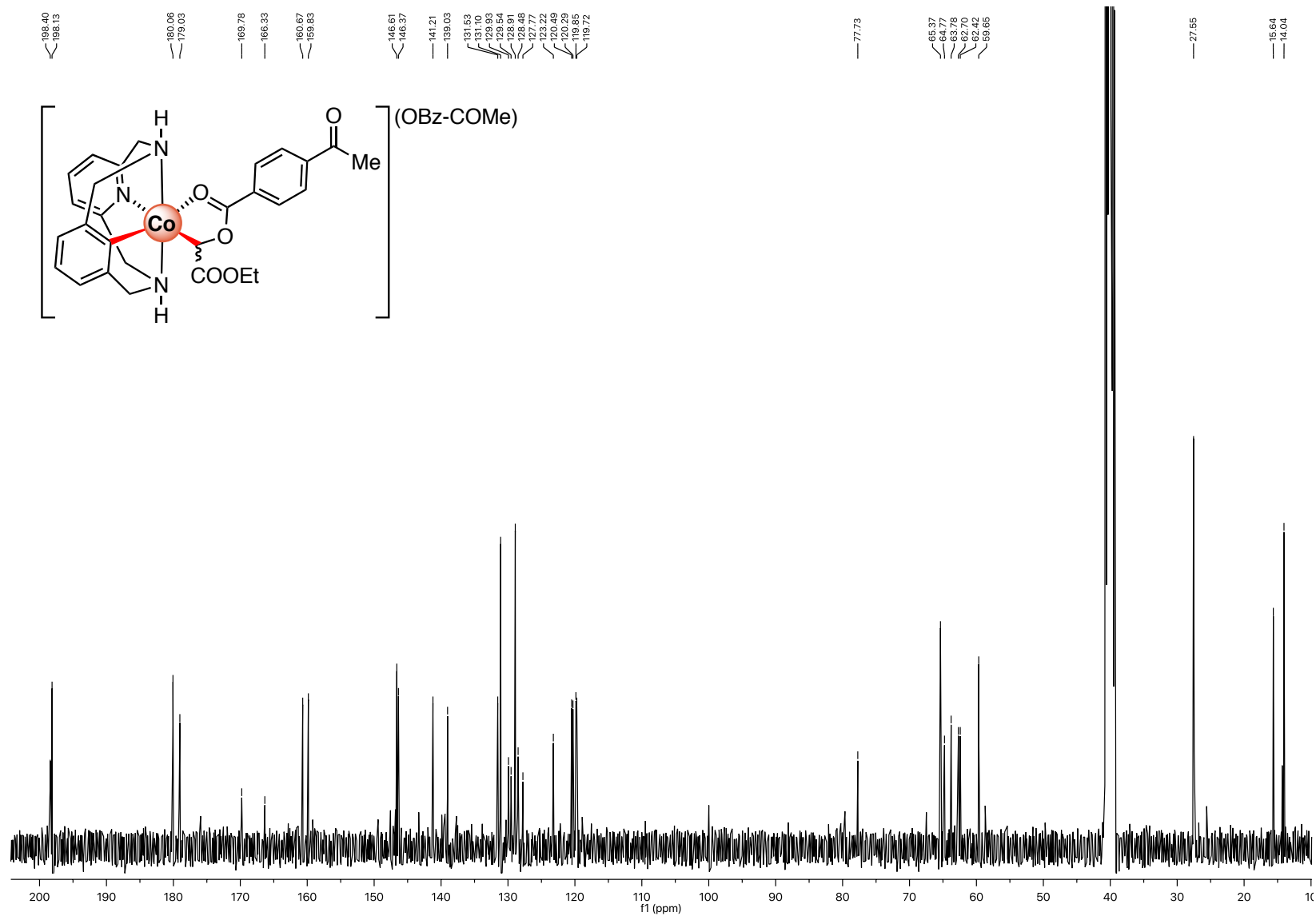
Figure S92. 100 MHz ^{13}C {^1H} NMR spectrum of **4a-OBz-COMe** in DMSO-d$_6$, 298 K.

Figure S93. 400 MHz ^{1}H-^{13}C HSQC spectrum of **4a-OBz-COMe** in DMSO-d$_6$, 298 K.
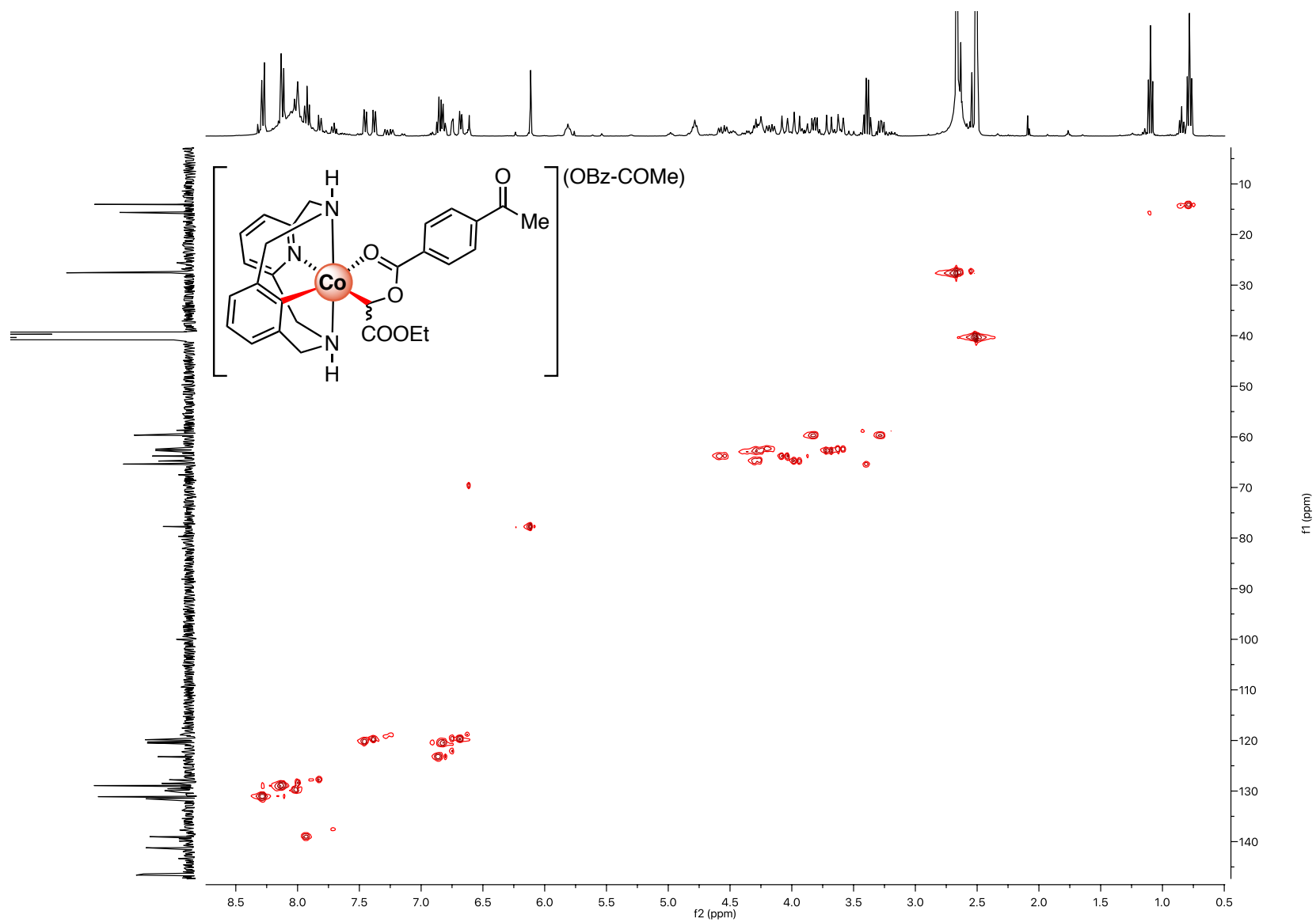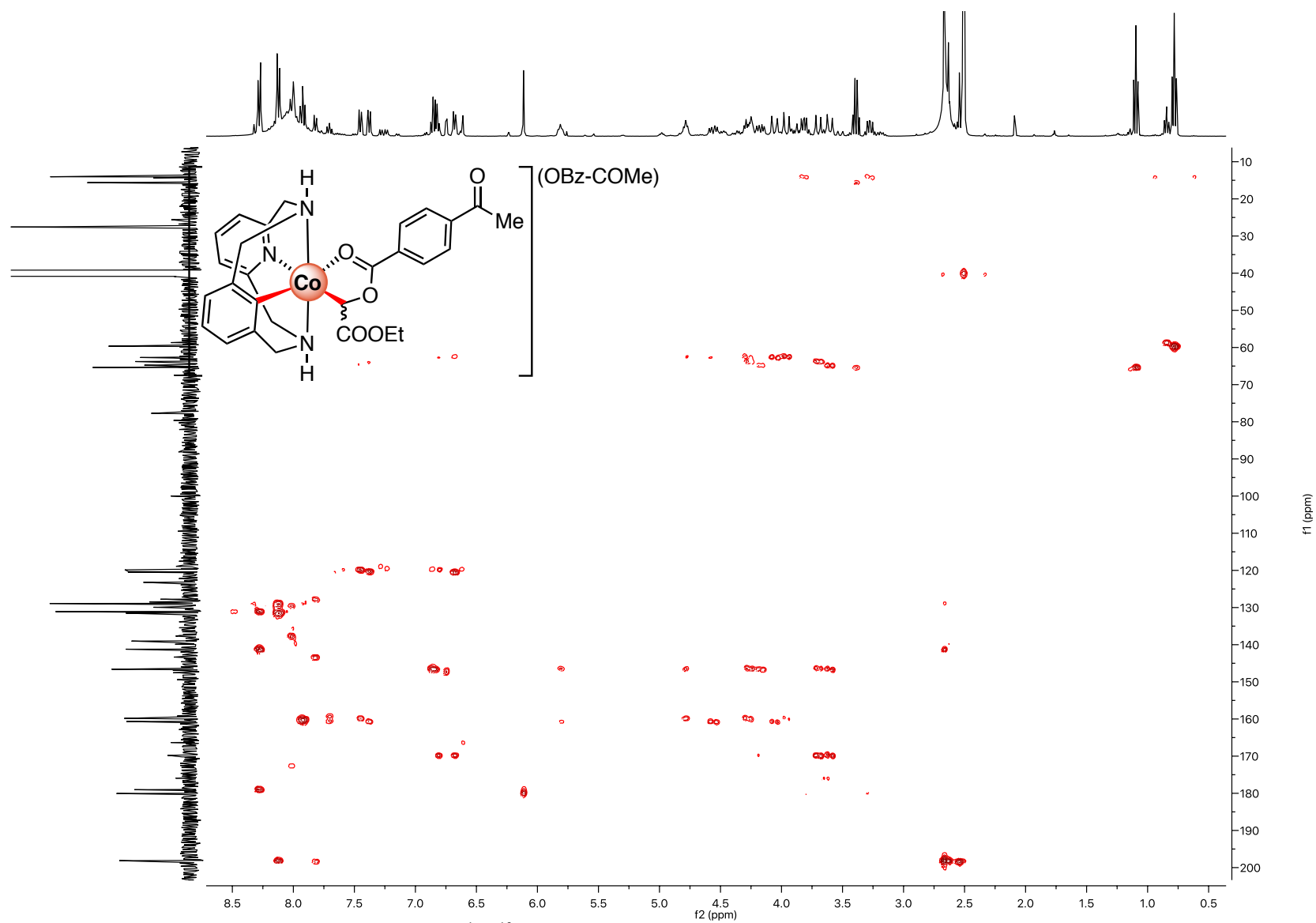
Figure S94. 400 MHz ^{1}H-^{13}C HMBC spectrum of **4a-OBz-COMe** in DMSO-d$_6$, 298 K.
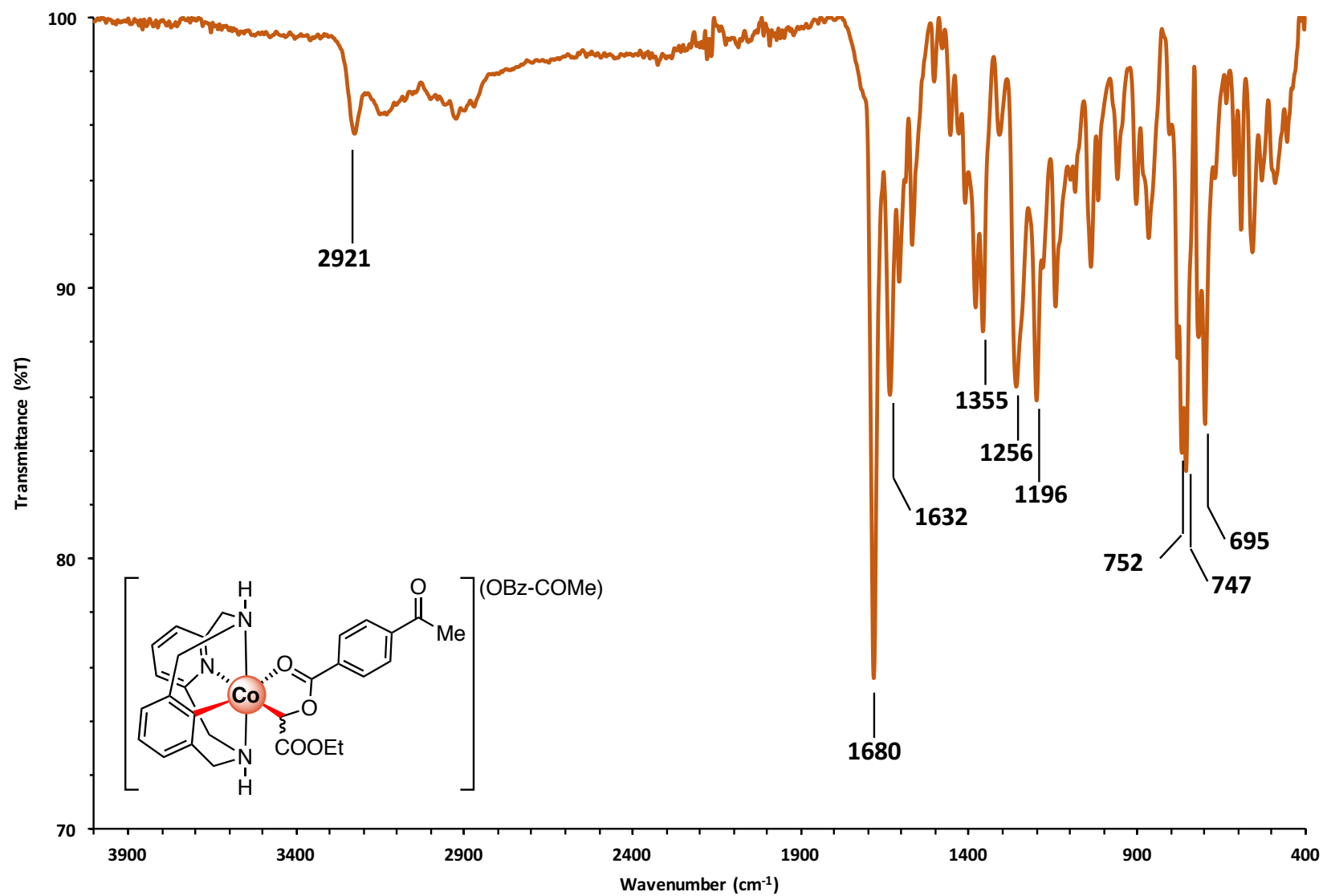
Figure S95. FT-IR spectrum of **4a-OBz-COMe** in solid state, 298 K.
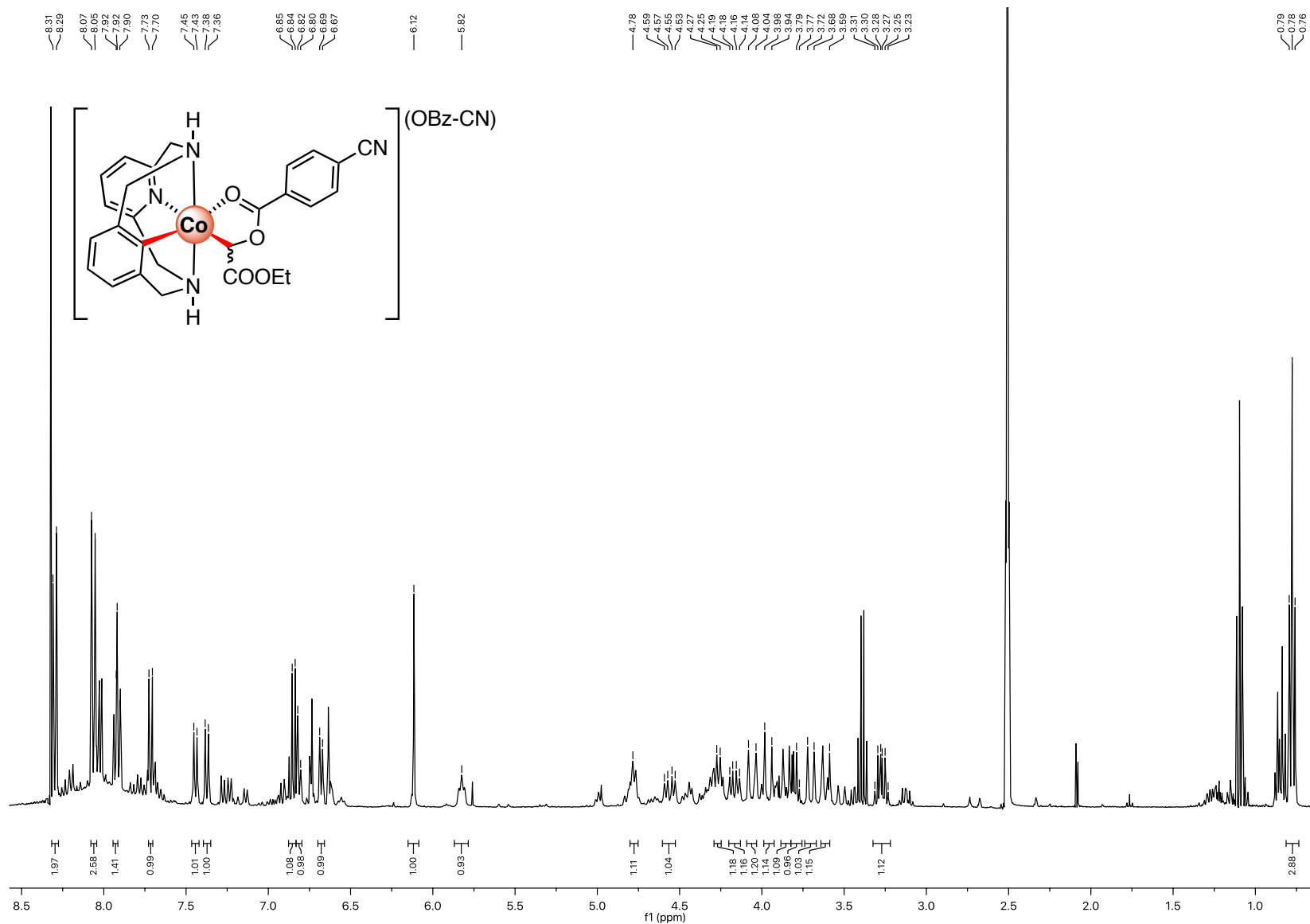
Figure S96. 400 MHz ^{1}H NMR spectrum of **4a-OBz-CN** in DMSO-d$_6$, 298 K. (Residual ether peaks at 1.1(t) and 3.4(q) ppm)
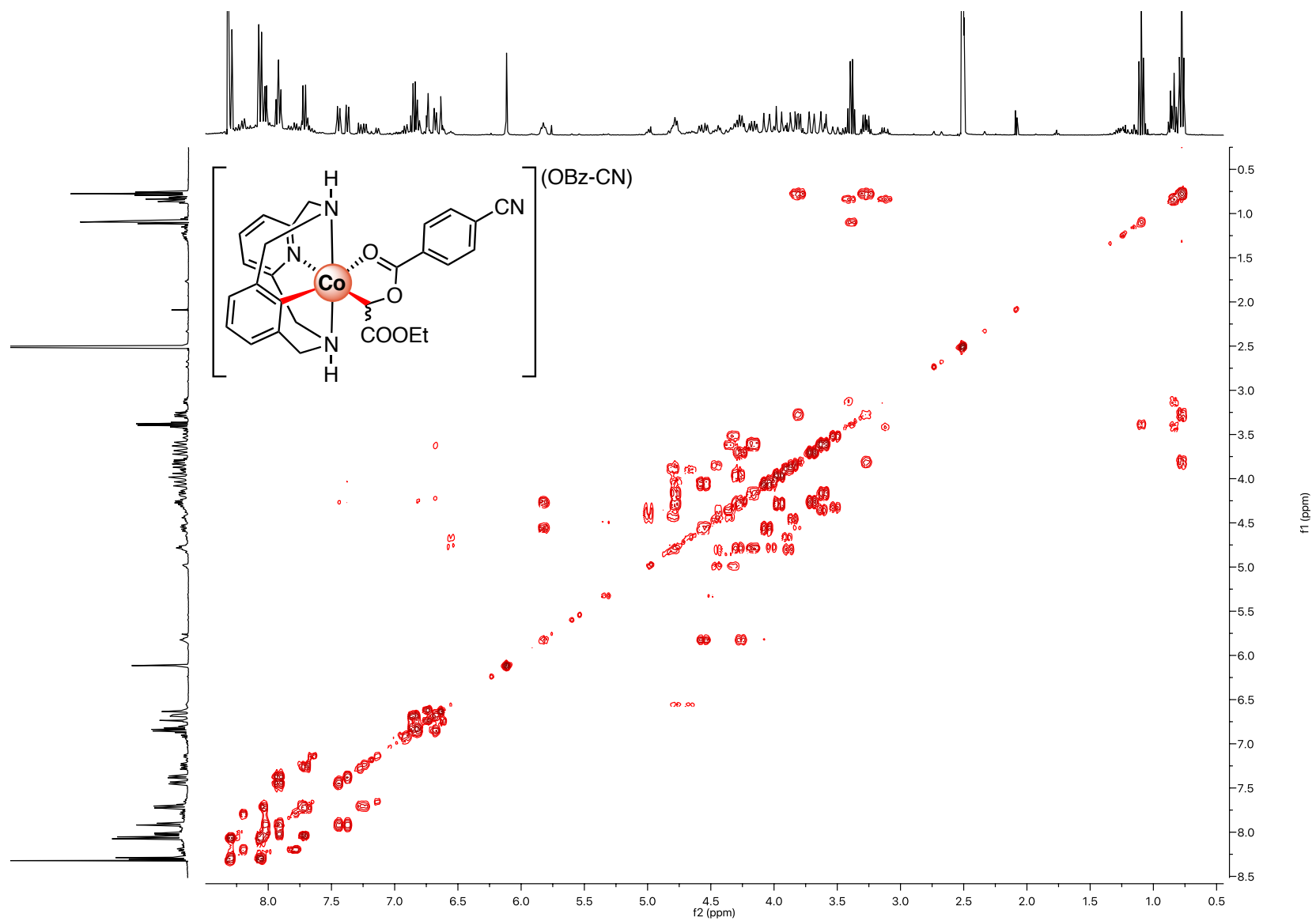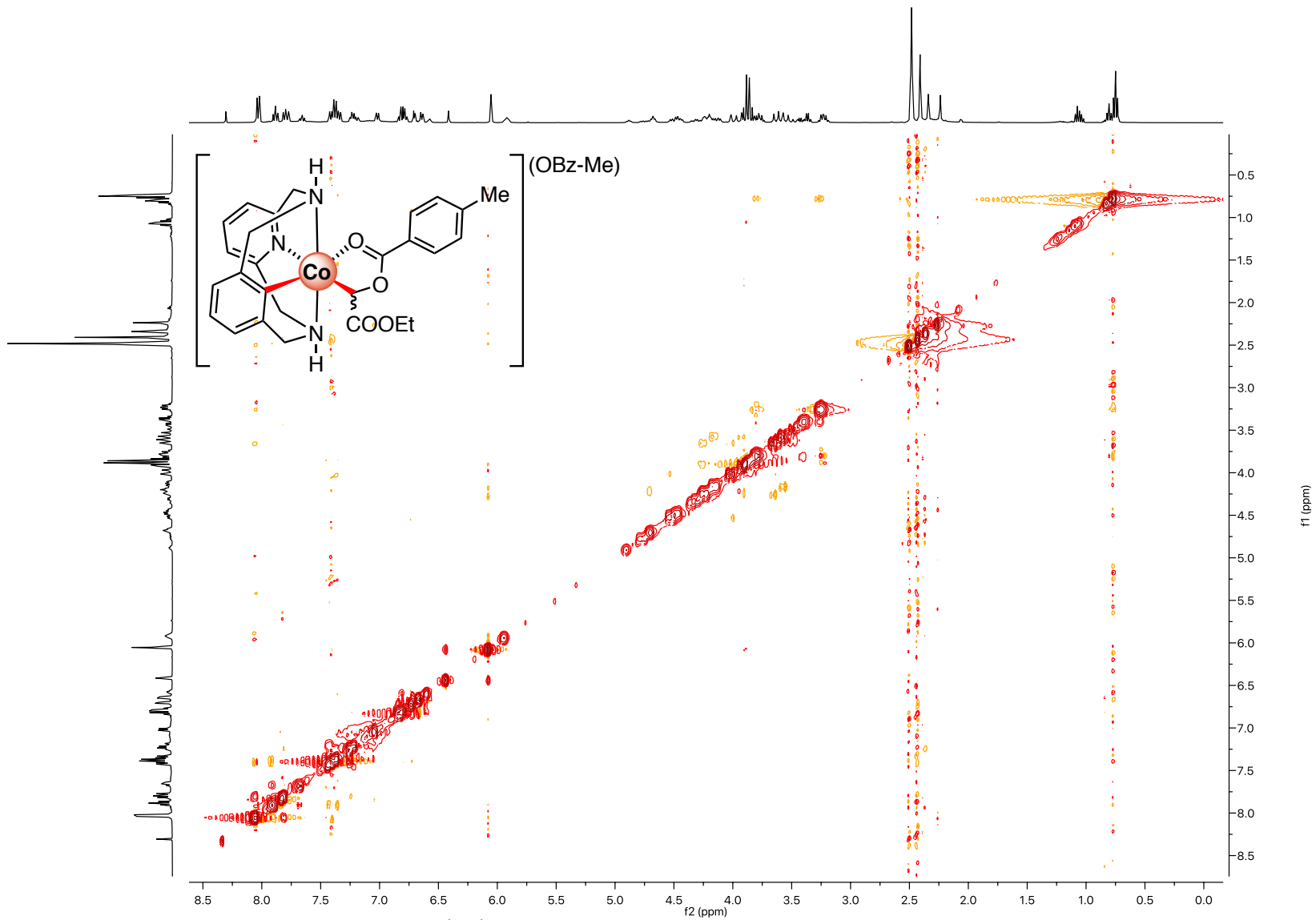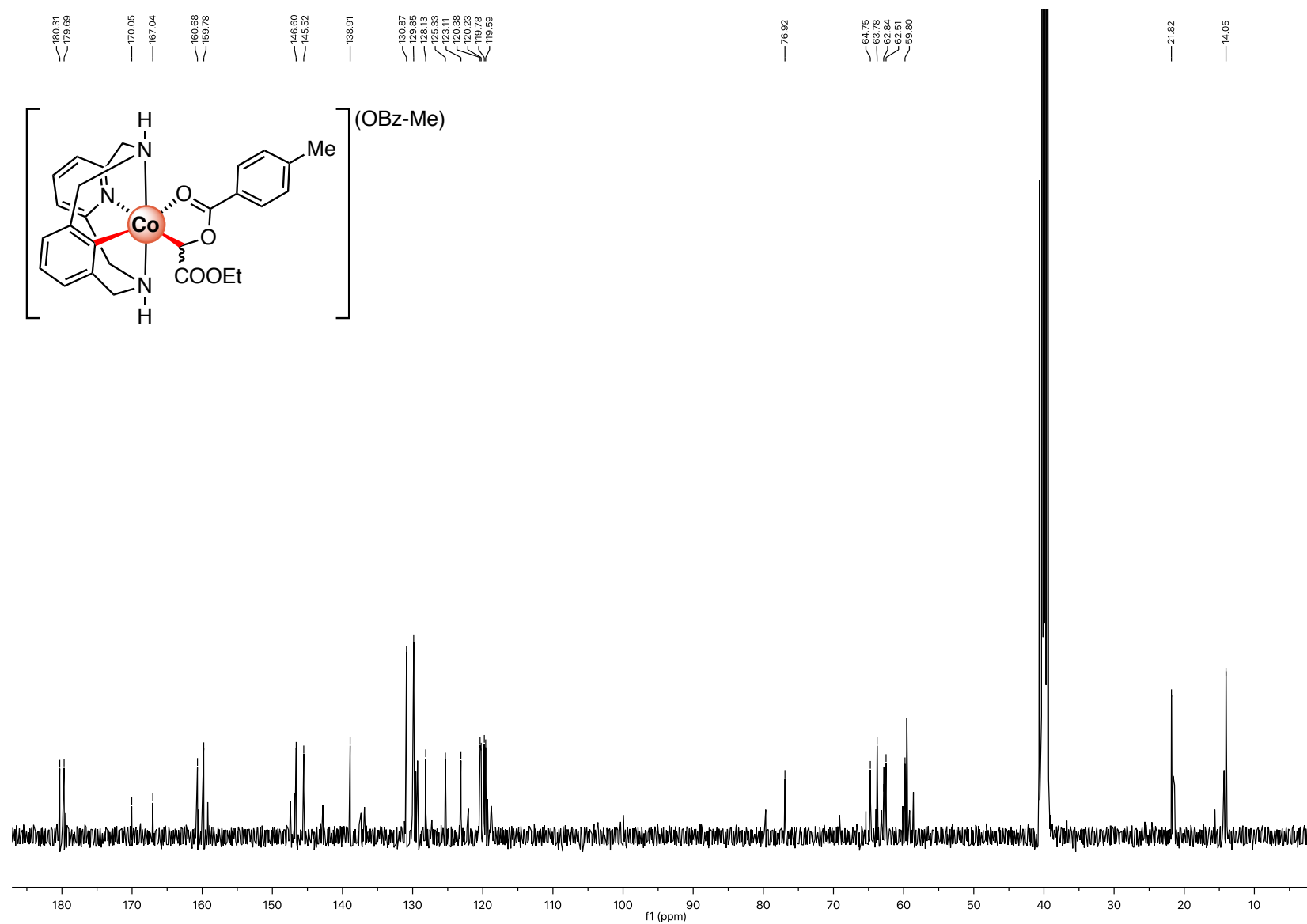
Figure S97. 400 MHz ^{1}H-^{1}H COSY NMR spectrum of **4a-OBz-CN** in DMSO-d$_6$, 298 K.

Figure S98. 400 MHz ^{1}H-^{1}H NOESY NMR spectrum of **4a-OBz-CN** in DMSO-d$_6$, 298 K.
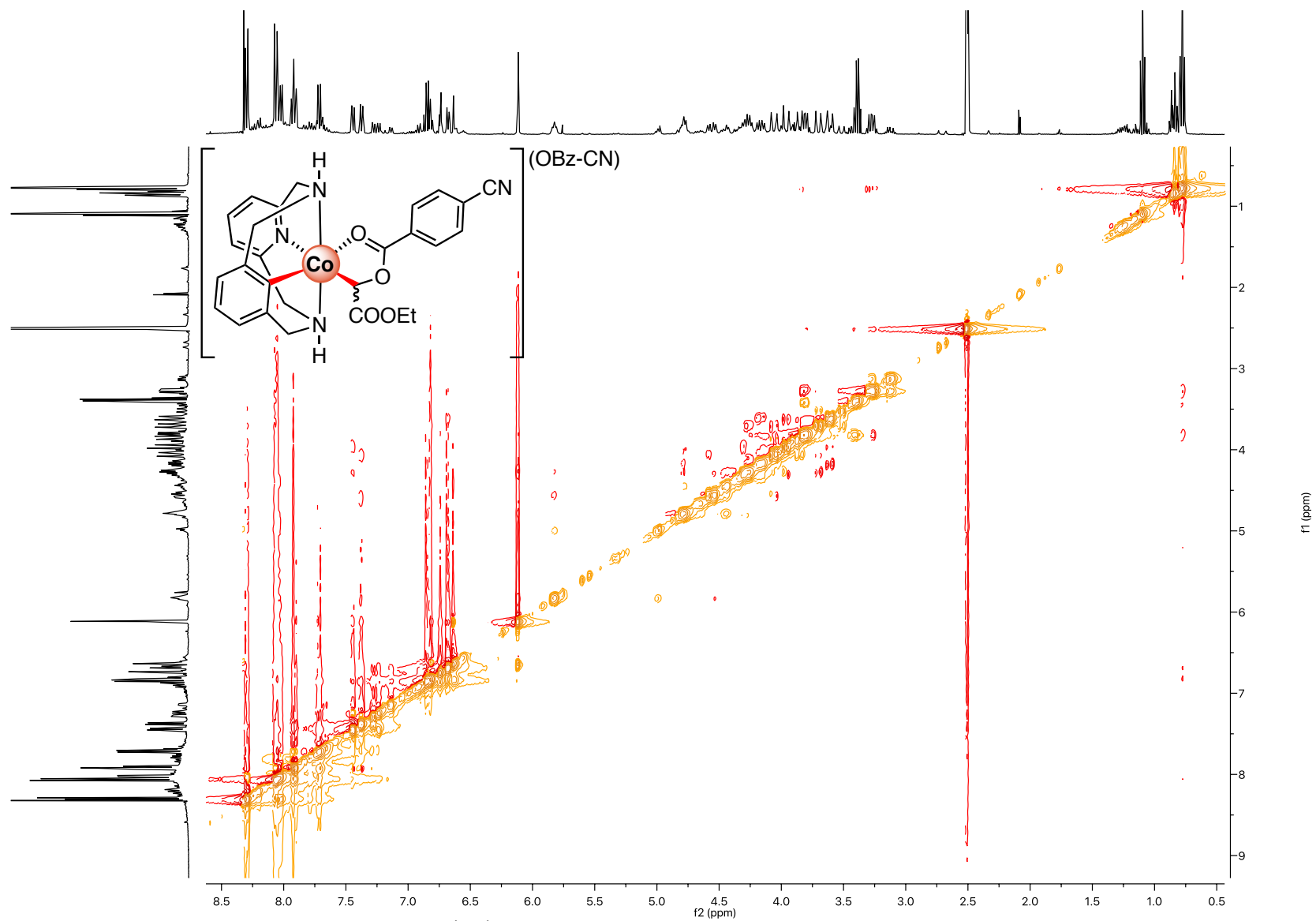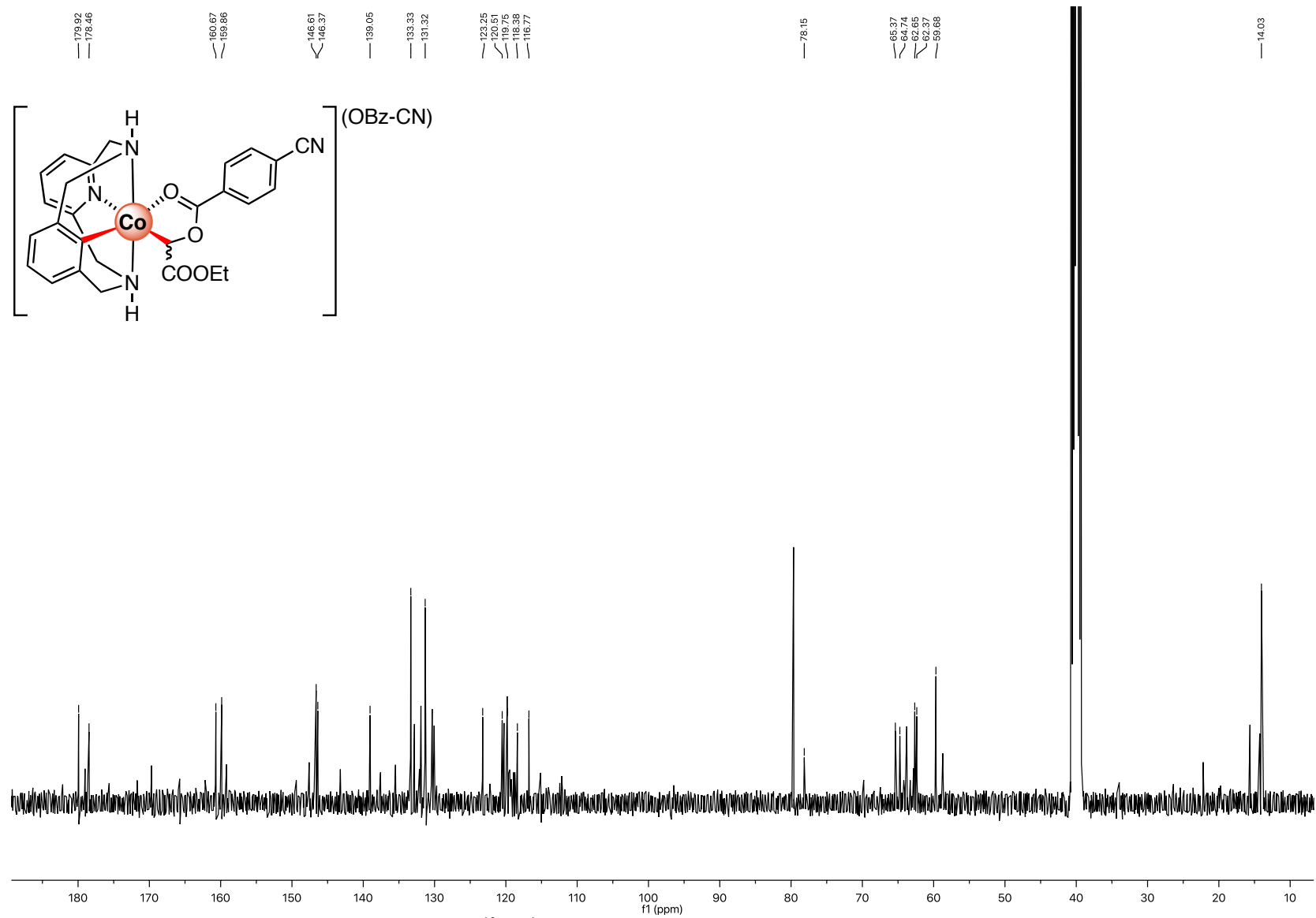
Figure S99. 100 MHz ^{13}C {^1H} NMR spectrum of **4a-OBz-CN** in DMSO-d_6, 298 K.

Figure S100. 400 MHz ^{1}H-^{13}C HSQC spectrum of **4a-OBz-CN** in DMSO-d$_6$, 298 K.
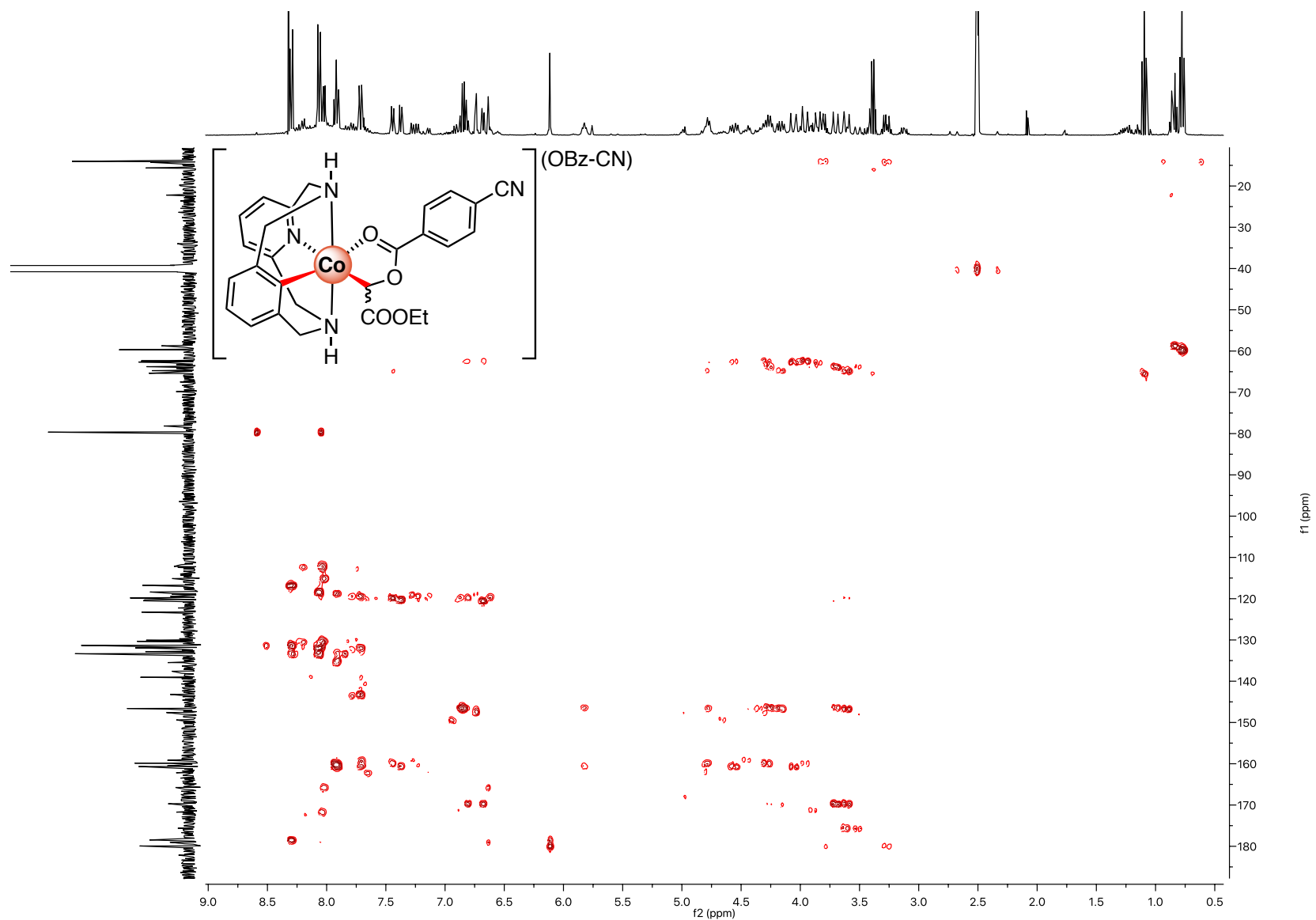
Figure S101. 400 MHz ^{1}H-^{13}C HMBC spectrum of **4a-OBz-CN** in DMSO-d$_6$, 298 K.
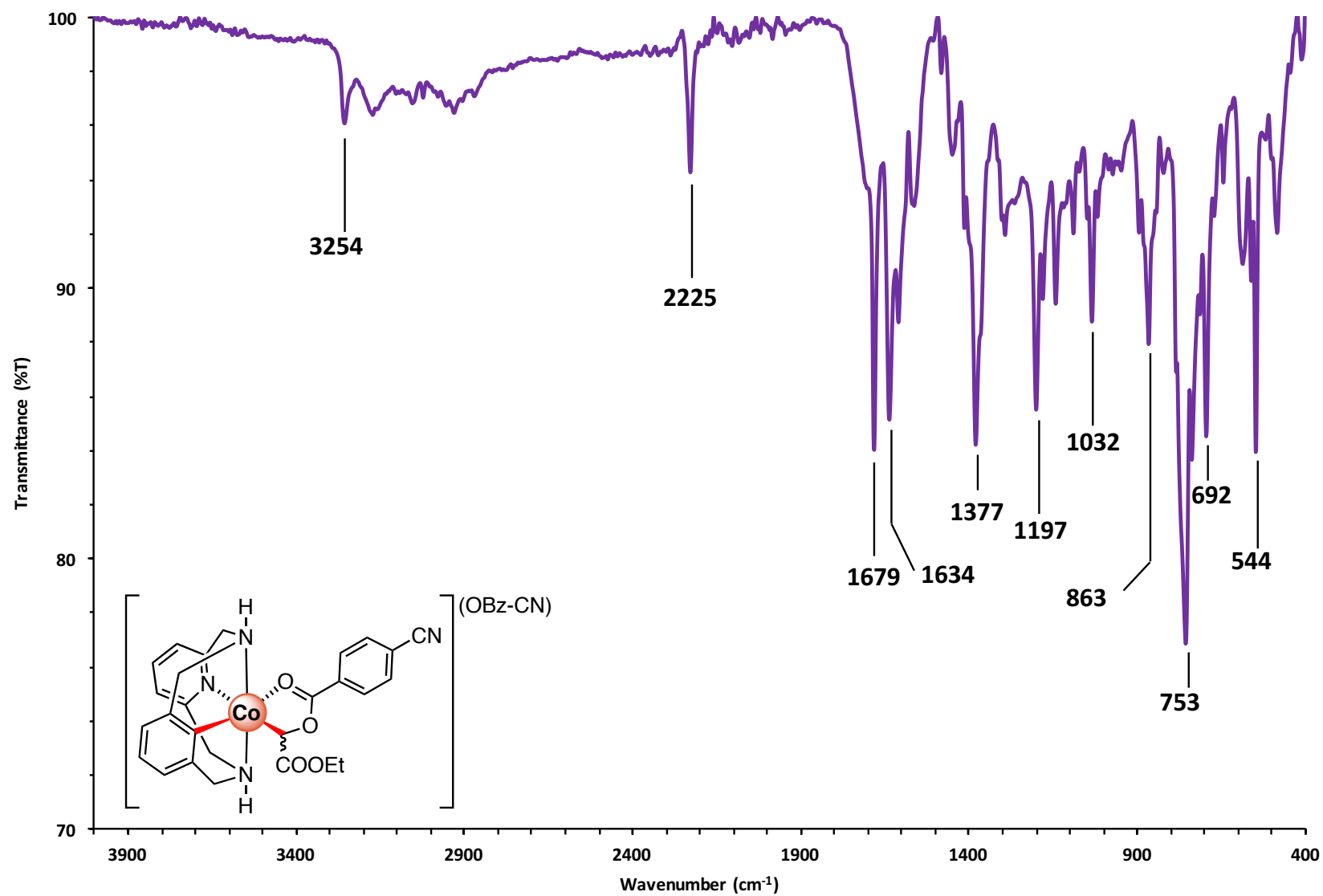
Figure S102. FT-IR spectrum of **4a-OBz-CN** in solid state, 298 K.
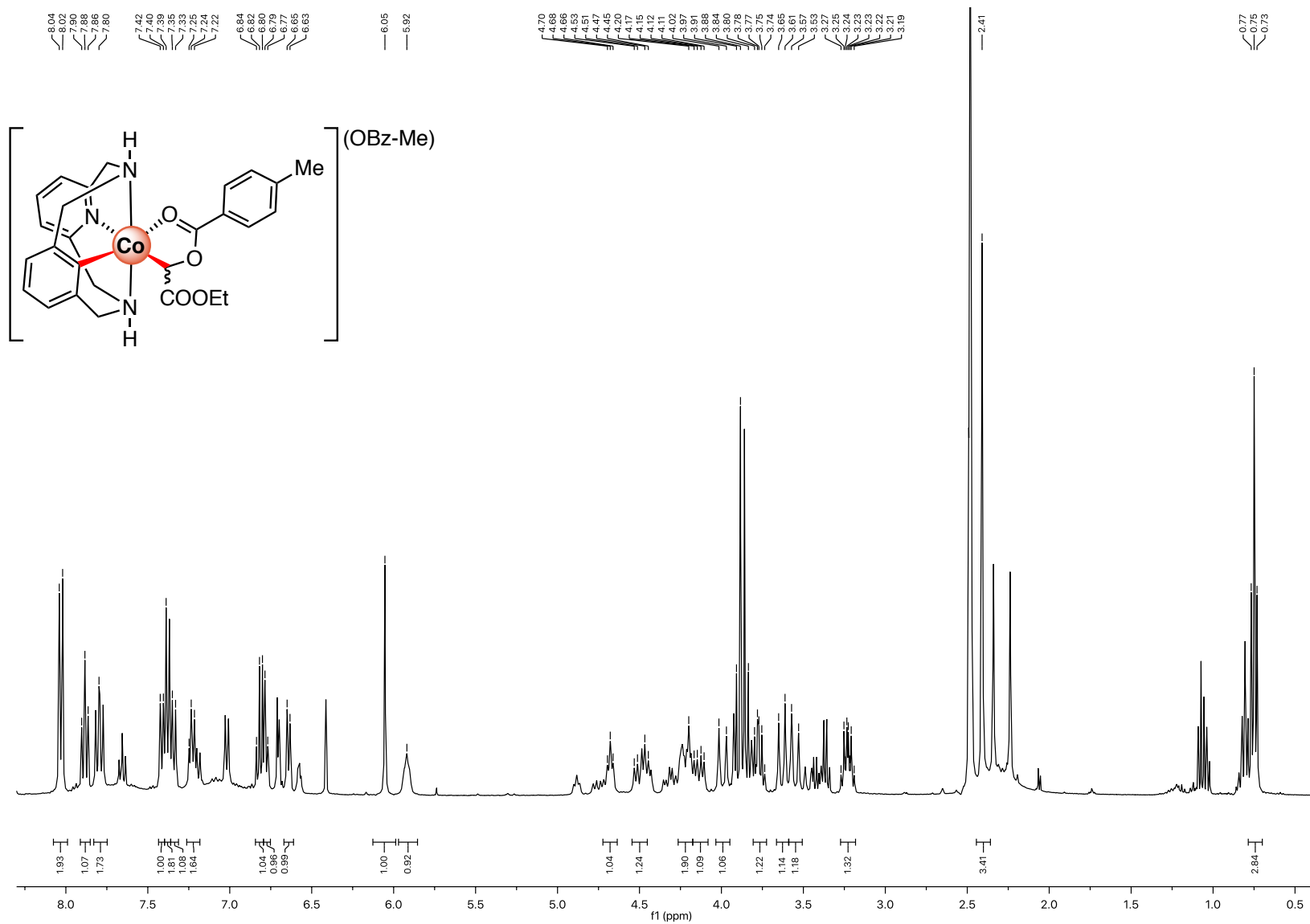
Figure S103. 400 MHz ^{1}H NMR spectrum of **4a-OBz-Me** in DMSO-d$_6$, 298 K. (Residual ether peaks at 1.1(t) and 3.4(q) ppm)

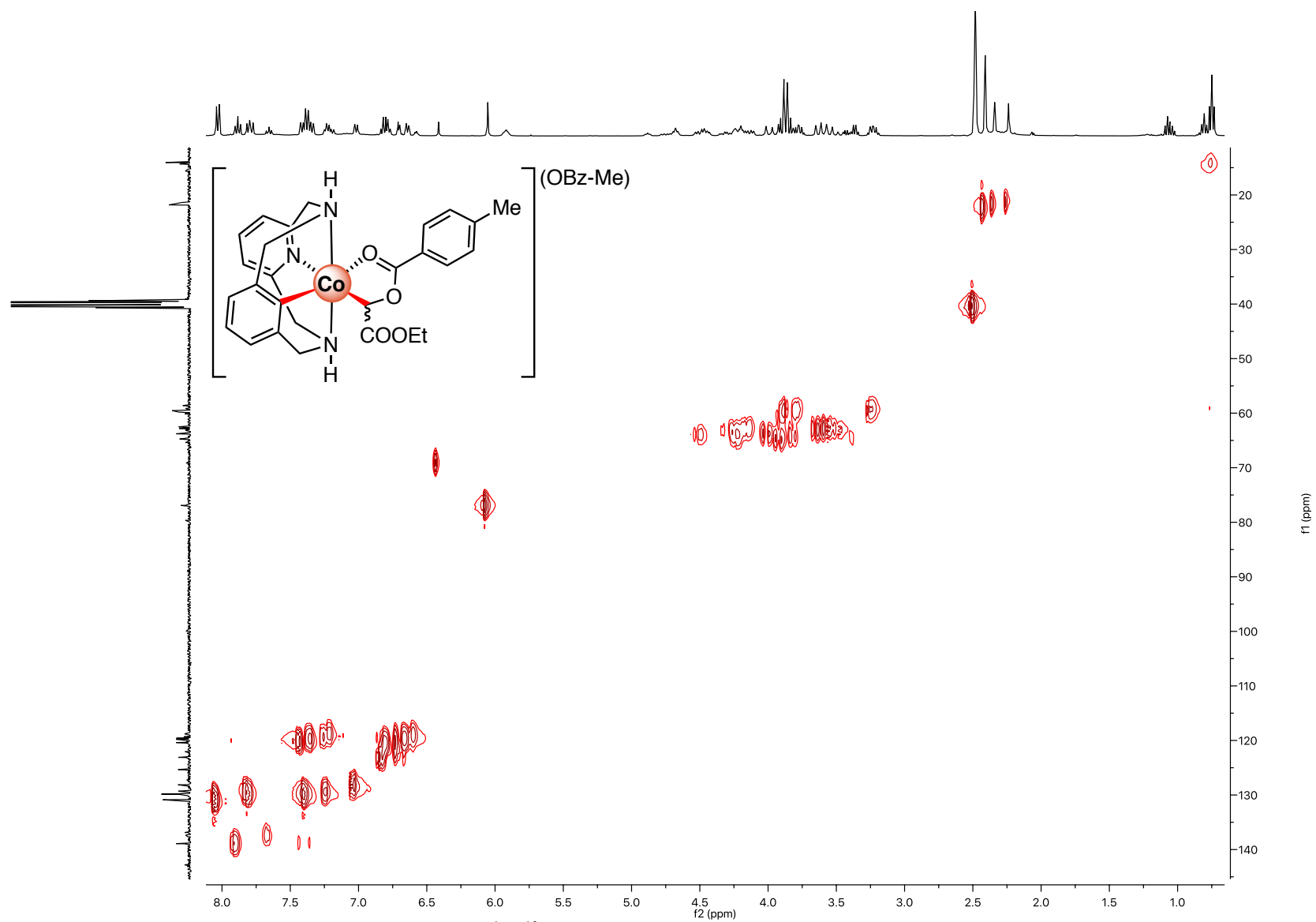**Figure S104.** 400 MHz ^{1}H-^{1}H COSY NMR spectrum of **4a-OBz-Me** in DMSO-d$_6$, 298 K.

Figure S105. 400 MHz ^1H-^1H NOESY NMR spectrum of **4a-OBz-Me** in DMSO-d$_6$, 298 K.

Figure S106. 100 MHz $^{13}C\ \{^1H\}$ NMR spectrum of **4a-OBz-Me** in DMSO-d$_6$, 298 K.

Figure S107. 400 MHz ^{1}H-^{13}C HSQC spectrum of **5a-OBz-Me** in DMSO-d$_6$, 298 K.

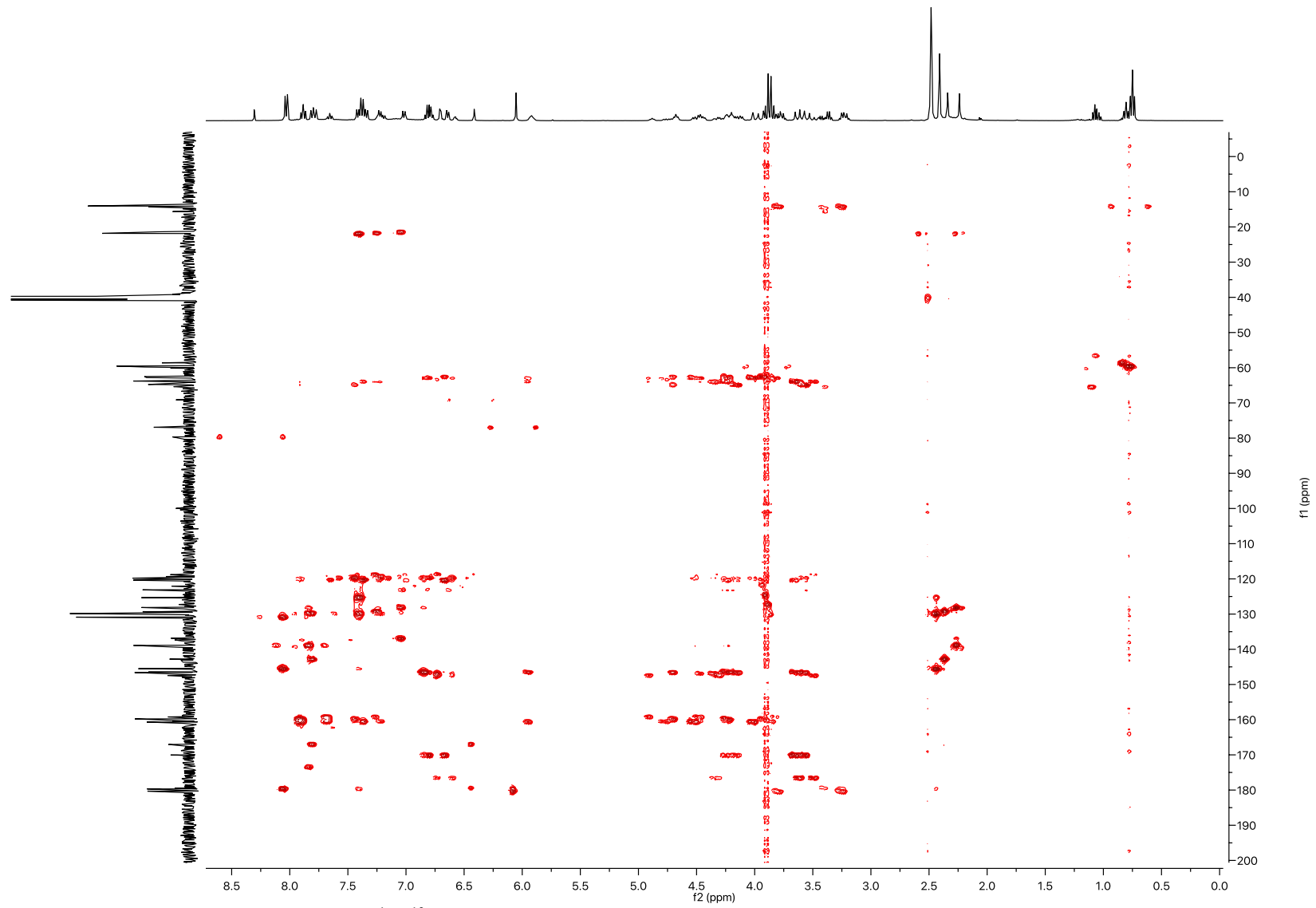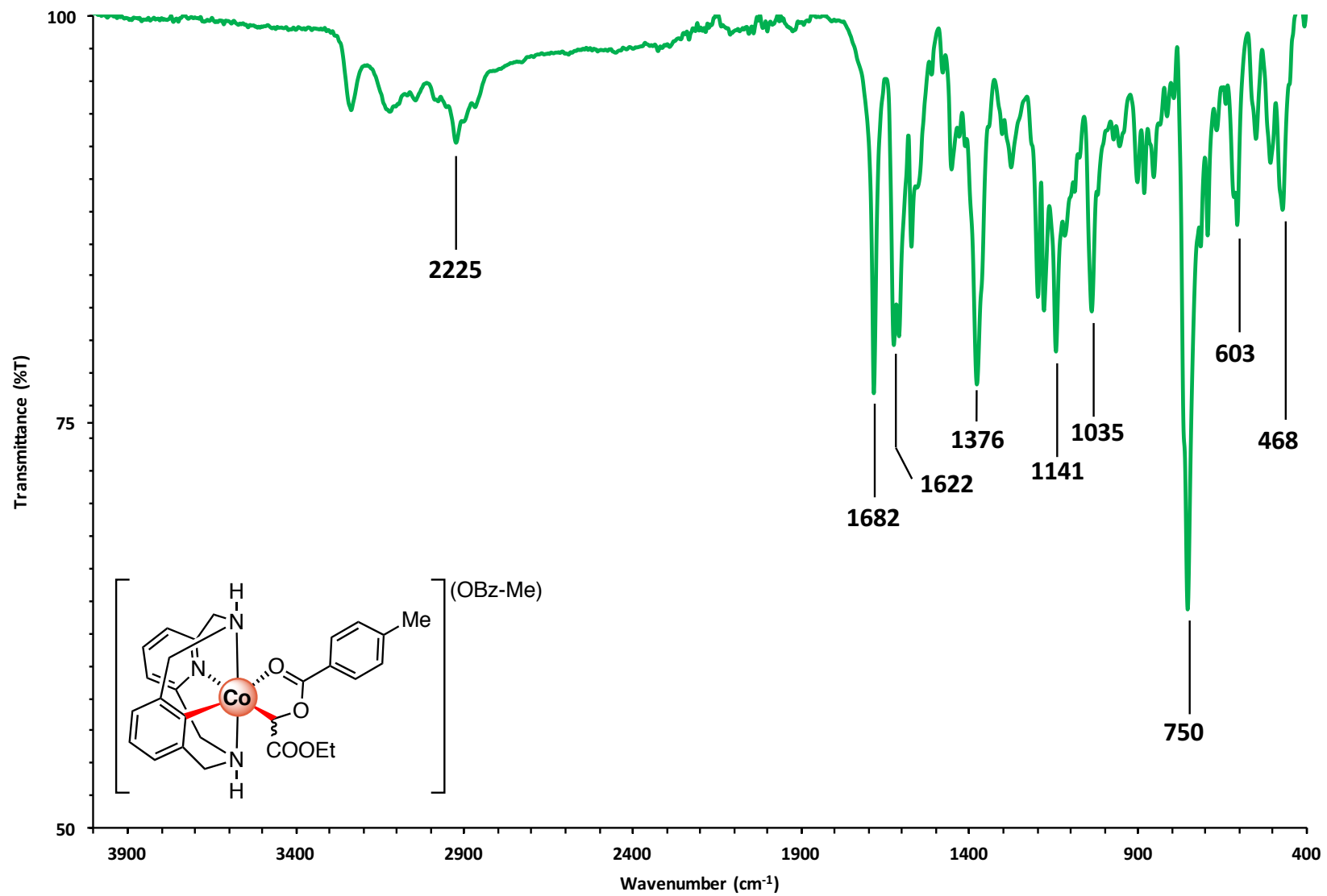**Figure S108.** 400 MHz ^{1}H-^{13}C HMBC spectrum of **4a-OBz-Me** in DMSO-d$_6$, 298 K. insertar ChemDraw?

Figure S109. FT-IR spectrum of **4a-OBz-Me** in solid state, 298 K.