

# **Supporting Information**

## **Ligand Controlled Product Selectivity in the Electrochemical Carbon Dioxide Reduction Using Manganese Bipyridine Catalysts**

Magnus H. Rønne,<sup>†</sup> Dasol Cho,<sup>§,||</sup> Monica R. Madsen,<sup>†,||</sup> Joakim B. Jakobsen,<sup>†,||</sup> Seunghwan Eom,<sup>§</sup> Émile Escoudé,<sup>†</sup> Hans Christian D. Hammershøj,<sup>†</sup> Dennis U. Nielsen,<sup>†</sup> Steen U. Pedersen,<sup>†</sup> Mu-Hyun Baik,<sup>\*,§</sup> Troels Skrydstrup,<sup>\*,†</sup> Kim Daasbjerg<sup>\*,†</sup>

<sup>†</sup>Carbon Dioxide Activation Center (CADIAC), Interdisciplinary Nanoscience Center, Department of Chemistry, Aarhus University, Gustav Wieds Vej 14, 8000 Aarhus C, Denmark

E-mail: [ts@chem.au.dk](mailto:ts@chem.au.dk), [kdaa@chem.au.dk](mailto:kdaa@chem.au.dk)

<sup>§</sup>Korean Institute for Advanced Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon, 3414, Republic of Korea

<sup>\*</sup>Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science (IBS), Daejeon 34141, Republic of Korea

E-mail: [mbaik2805@kaist.ac.kr](mailto:mbaik2805@kaist.ac.kr)

### **Table of Contents**

1. General Methods	S2
1.1 Cyclic Voltammetry	S2
1.2 Two-Electron Reduction of Mn Catalysts	S3
1.3 Infrared Spectroelectrochemistry	S3
1.4 Electrolysis under Catalytic Conditions	S3
1.5 Trapping Carbamate Intermediate	S4
1.6 Trapping of Mn–Hydride Intermediate	S4
1.7 Determination of the Kinetic Isotope Effect (KIE)	S4
1.8 Construction of Catalytic Tafel Plots	S4
2. X-Ray Crystallographic Data	S5
3. Figures Schemes, and Tables	S6
4. Computational Details	S28
4.1 Computational Methods	S28
4.2 Computational Details	S29
5. Synthesis of Starting Materials	S32
5.1 Synthesis of Manganese Complexes	S32
5.2 Synthesis of 2,9-Dichloro-1,10-phenanthroline	S37
5.3 Synthesis of <i>Fac</i> -Mn(CO) <sub>5</sub> OTf	S38
5.4 Synthesis of Ligands	S38
6. References	S46
7. NMR Spectra	S49
8. Computed Energy Components for DFT-Optimized Structures	S76

## 1. GENERAL METHODS

All analytical grade solvents and commercially available reagents were purchased from Sigma-Aldrich, TCI Chemicals, or Fluorochem and used without further purification, unless otherwise noted. Bu<sub>4</sub>NBF<sub>4</sub>, Bu<sub>4</sub>NOCHO, and [HDBU]<sup>+</sup>[CF<sub>3</sub>CH<sub>2</sub>OC(O)O]<sup>-</sup> were prepared according to literature.<sup>S1-S3</sup> Dry solvents were collected from a MBRAUN MB SP-800 purification system, and further dried over 3 Å molecular sieves. CO<sub>2</sub> was supplied by Air Liquide with a purity of 99.999%. Air-sensitive reactions were carried out either in an argon-filled glovebox or using standard Schlenk and vacuum techniques.

NMR spectra were recorded on a Bruker Ascend 400 spectrometer running at 400 MHz for <sup>1</sup>H, 367 MHz for <sup>19</sup>F, and 101 MHz for <sup>13</sup>C. Chemical shifts ( $\delta$ ) are reported in parts per million (ppm) relative to residual solvent signals (CDCl<sub>3</sub>, 7.26 ppm for <sup>1</sup>H NMR; CDCl<sub>3</sub>, 77.16 ppm for <sup>13</sup>C NMR; CD<sub>3</sub>CN, 1.94 ppm for <sup>1</sup>H NMR; CD<sub>3</sub>CN, 118.26 ppm for <sup>13</sup>C NMR; (CD<sub>3</sub>)<sub>2</sub>CO, 2.05 ppm for <sup>1</sup>H NMR; (CD<sub>3</sub>)<sub>2</sub>CO, 206.26 ppm for <sup>13</sup>C NMR; D<sub>2</sub>O, 4.79 ppm for <sup>1</sup>H NMR); (CD<sub>3</sub>)<sub>2</sub>SO, 2.50 ppm for <sup>1</sup>H NMR; (CD<sub>3</sub>)<sub>2</sub>SO, 39.52 ppm for <sup>13</sup>C NMR. The following abbreviations are used to indicate the multiplicity in NMR spectra: s, singlet; d, doublet; t, triplet; q, quartet; p, quintet; m, multiplet; bs, broad signal. <sup>13</sup>C NMR spectra were recorded in broad band decoupled mode.

Mass spectra were recorded on a Bruker Maxis Impact mass spectrometer using electrospray ionization (ESI<sup>+</sup>) (referenced to the mass of the charged species), and analyzed using Data Analysis (v4.1) by Bruker Daltonic GmbH to give the mSigma value as a measure for the isotope pattern. ATR FT-IR was recorded using a Perkin Elmer Spectrum Two instrument.

Cyclic voltammograms were recorded with a CH Instrument (601D) potentiostat. Electrolysis was performed with an Autolab PGSTAT302 potentiostat. A Nicolet 6700 (Thermo Fisher Scientific) instrument was used to record IR spectra in solution. A CH Instruments (601C) potentiostat was used to control and monitor electrochemical processes during infrared spectroelectrochemistry (IR-SEC) experiments.

Gaseous products produced in the electrolyses were quantified on an Agilent 7890B Gas Chromatograph equipped with TCD and FID detectors. Formate was quantified on a Dionex ICS-1100 Ion Chromatography System. Analytical thin layer chromatography (TLC) was performed using pre-coated aluminium-backed plates (Merck Kieselgel 60 F254) and visualized by UV radiation or KMnO<sub>4</sub> stain. For flash chromatography (FC) silica gel (Silica gel 60, 230-400 mesh, Sigma-Aldrich) was used.

Crystallographic single crystal X-ray data for **1a** was collected using an Oxford Diffraction Supernova instrument equipped with a Mo micro-focus X-ray source, an Atlas charge-coupled device detector, and a four-circle goniometer. The crystal was cooled to 100(1) K using an Oxford Cryosystems liquid nitrogen Cryostream device.

### 1.1 Cyclic Voltammetry

All cyclic voltammograms were recorded using a three-necked flask in a 5 mL 0.1 M Bu<sub>4</sub>NBF<sub>4</sub>/MeCN solution wrapped by an aluminium foil to shield the light-sensitive catalyst from light. The working electrode was a homemade glassy carbon disc electrode (Sigradur G, HTW, diameter = 1 mm) embedded in an epoxy resin (see Figure S23a). All voltammograms were recorded against either a non-aqueous Ag/AgI or a leak free aqueous saturated Ag/AgCl reference electrode. All potentials were referred to the ferrocenium/ferrocene (Fc<sup>+</sup>/Fc) redox couple, using Fc as internal standard. A Pt wire served as counter electrode. Unless otherwise noted, a sweep rate of 0.1 V s<sup>-1</sup> was employed.

## 1.2 Two-Electron Reduction of Mn Catalysts

Electrolyses were conducted in a two-chamber system with a glass frit separating the two compartments (see Figure S23b). Glassy carbon foam (Alfa Aesar, 500 pores per inch) was employed as working electrode using Teflon tape to demarcate the active electrode area ( $1.0\text{ cm} \times 1.0\text{ cm} \times 0.2\text{ cm}$ ). Teflon tape was used to attach the reference electrode (saturated Ag/AgCl) to the working electrode, while a Pt mesh served as the counter electrode. The two-chamber system was equipped with magnetic stir bars, and in each of the chambers  $\text{Bu}_4\text{NBF}_4$  (0.16 g, 0.1 M) was dissolved in MeCN (5 mL). In a glove box the desired catalyst (10 mM) was added to one of the chambers, which was sealed and equipped with the working and reference electrodes; the second chamber was equipped with the counter electrode and sealed. The electrochemical cell was wrapped with aluminum foil to shield the light-sensitive catalyst from light. The electrolysis was conducted at  $-2.07\text{ V}$  vs  $\text{Fc}^+/\text{Fc}$  until the current went below 2% of the initial current.

## 1.3 Infrared spectroelectrochemistry

An IR spectroelectrochemical cell with a design inspired by the one reported by Kubiak and coworkers<sup>S4</sup> was used for the IR-SEC experiments (see Figure S24). A 5 mm glassy carbon disk was used as working electrode surrounded by a Pt wire functioning as counter electrode. A Ag/AgCl reference electrode was positioned in-between the working and counter electrodes. The spectroelectrochemical experiments were conducted in 0.1 M  $\text{Bu}_4\text{NBF}_4$ /MeCN containing ~1 mM **1a** or **4**. Catalyst solutions were prepared under Ar in a glovebox and shielded from light until injection into the IR-SEC cell. Blank 0.1 M  $\text{Bu}_4\text{NBF}_4$ /MeCN solutions were used for background subtractions. Gas mixtures for experiments under  $\text{CO}_2$  were prepared by equal mixing of Ar and  $\text{CO}_2$  using two variable area flow meters (Key Instruments). In electrolysis experiments, a potential of  $-1.37\text{ V}$  vs  $\text{Fc}^+/\text{Fc}$  was applied for 5 s before stepping to  $-2.07\text{ V}$  vs  $\text{Fc}^+/\text{Fc}$  for 12 s. Multiple IR spectra were recorded during the experiment, making it possible to study the time-dependent appearance/disappearance of reactants, intermediates, and products.

## 1.4 Electrolysis under Catalytic Conditions

Electrolyses were conducted in a two-chamber system using a glass frit to separate the two compartments along with a bridge that allowed the equilibration of the gases above the two solutions (see Figure S23b). Carbon paper (Toray Paper 060 from FuelCellStore) was employed as working electrode using Teflon tape to demarcate the active electrode area ( $0.5\text{ cm} \times 0.27 \pm 0.02\text{ cm}$ ). Teflon tape was also used to attach the reference electrode (saturated Ag/AgCl) to the working electrode, while a Pt mesh served as the counter electrode (see Figure S23c).

The two-chamber system was equipped with magnetic stir bars, and in each of the chambers  $\text{Bu}_4\text{NBF}_4$  (0.33 g, 0.2 M) was dissolved in MeCN (3 mL). Either TFE (730  $\mu\text{L}$ , 2.0 M), phenol (470 mg, 1.0 M), or isopropanol (115  $\mu\text{L}$ , 0.3 M) was used as proton source, and MeCN was added to reach a total volume of 5 mL. In a glove box the given catalyst (1 mM) was added to one of the chambers, which was sealed and equipped with the working and reference electrodes; the second chamber was equipped with the counter electrode and sealed (see Figure S22d). The electrochemical cell was wrapped with aluminum foil to protect the light-sensitive catalyst from light. Prior to electrolysis, the two-chamber system was purged with  $\text{CO}_2$  for 10–15 min, after which the electrodes were connected to the potentiostat. The electrochemical cell was placed in a water bath at room temperature to avoid overheating of the membrane. Solutions were stirred during the 1 h electrolysis.

## 1.5 Trapping of Carbamates

In one chamber of a 20 mL COWARE reactor (SyTracks A/S), 0.015 mmol of either **1a** or **8** was dissolved in 1 mL  $(CD_3)_2SO$ . In the second chamber,  $Ba^{13}CO_3$  (198 mg, 1.0 mol) and camphor-10-sulfonic acid ( $\beta$ ) (464 mg, 2.0 mol) was added. It was covered with 0.7 mL 1,2-dichlorobenzene followed by slow addition of 0.6 mL  $H_2O$  before the reactor was closed. Both chambers were stirred for 4 h to let the catalyst have time to react with the liberated  $^{13}CO_2$  from the second chamber. The catalyst solution was analyzed by  $^{13}C$  NMR.

## 1.6 Trapping of Mn-Hydrides

After the electrochemical two-electron reduction of **1a** (see section 1.2), half of the solution from the working chamber was transferred to a vial and the solvent was removed. The dark blue residue was dissolved in 1.5 mL  $CD_3CN$  followed by adding 20  $\mu L$  TFE. The solution was stirred for 15 min before the sample was analyzed by  $^1H$  NMR. Another 80  $\mu L$  TFE was added and the solution was analyzed by  $^1H$  NMR once more.

## 1.7 Determination of the Kinetic Isotope Effect (KIE)

The KIE for **1a** was determined by cyclic voltammetry using TFE or  $CF_3CH_2OD$  as acids. The rate of the catalytic reactions was determined to be second order in the acid. Hence, plotting the observed rate vs  $[acid]^2$  allowed the determination of the average KIE effect according to eq S1.

$$KIE = \frac{k_H}{k_D} = \frac{TOF_{max,H}}{TOF_{max,D}} = \frac{\text{slope}_H}{\text{slope}_D} \quad (S1)$$

## 1.8 Construction of Catalytic Tafel Plots

A catalytic Tafel plot was constructed using eq S2.<sup>55</sup>

$$TOF = \frac{TOF_{max}}{1 + \exp\left[\frac{F}{RT}\left(E_{CO_2/HCOOH}^0 - E_{cat/2} - \eta\right)\right]} \quad (S2)$$

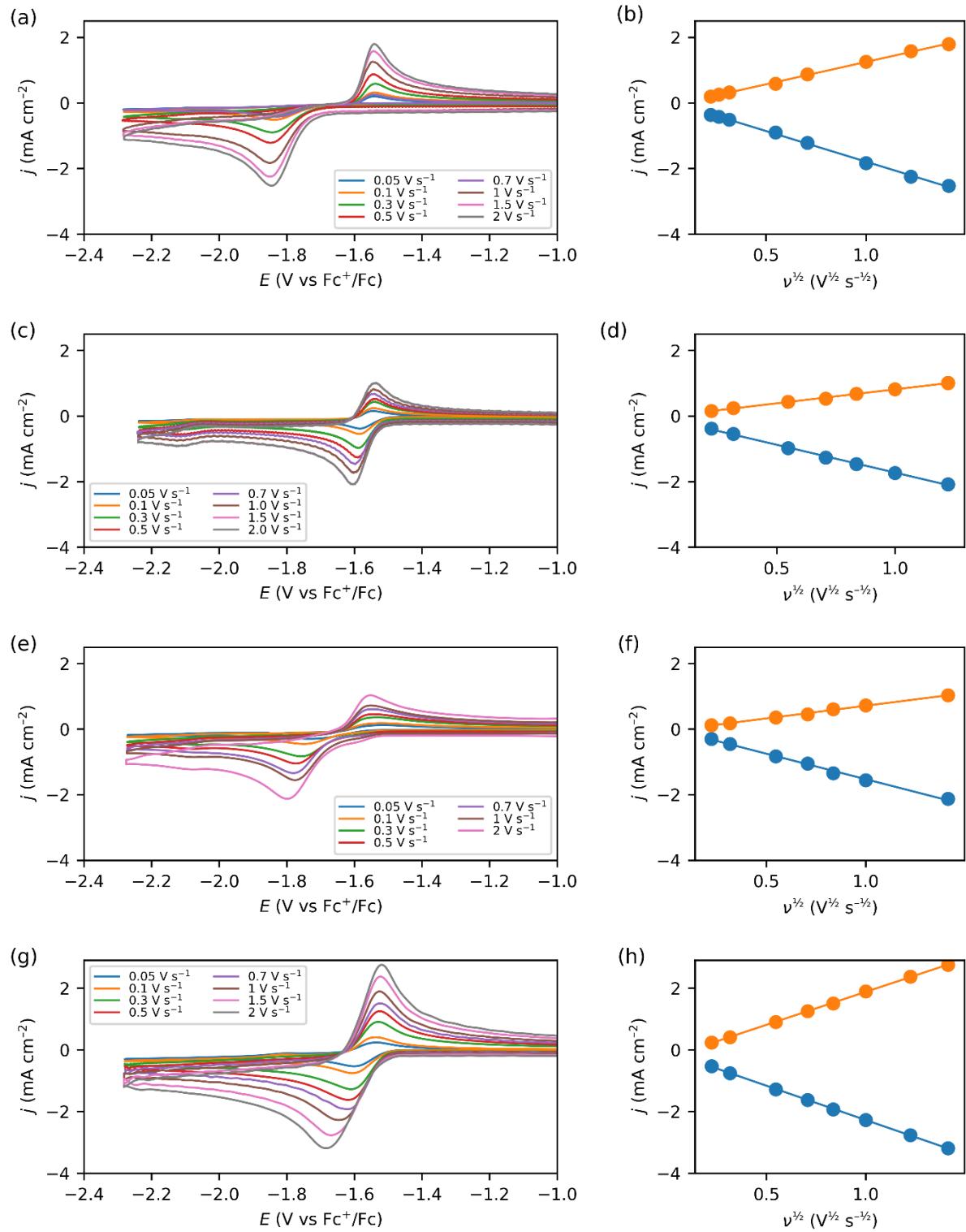
Here,  $F$  is the Faraday constant,  $R$  the gas constant,  $T$  the temperature, and  $E_{CO_2/HCOOH}^0$  the standard potential for the reduction of  $CO_2$  to  $HCOOH$  which has previously been determined to be  $-1.40$  and  $-1.45$  V vs  $Fc^+/Fc$  in MeCN and DMF, respectively.<sup>56</sup> The  $E_{cat/2}$  parameter is the standard potential of the catalytic cycle, determined as the potential, at which the catalyst reaches half of the maximum catalytic activity. The value of  $TOF_{max}$  is determined from the cyclic voltammograms using eq 1.

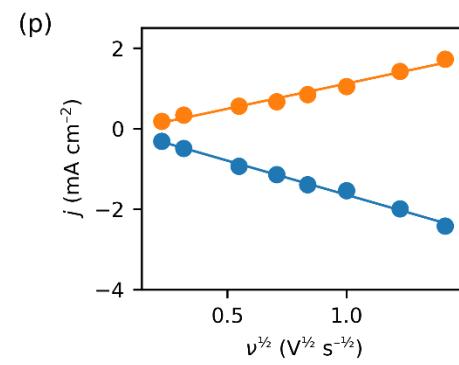
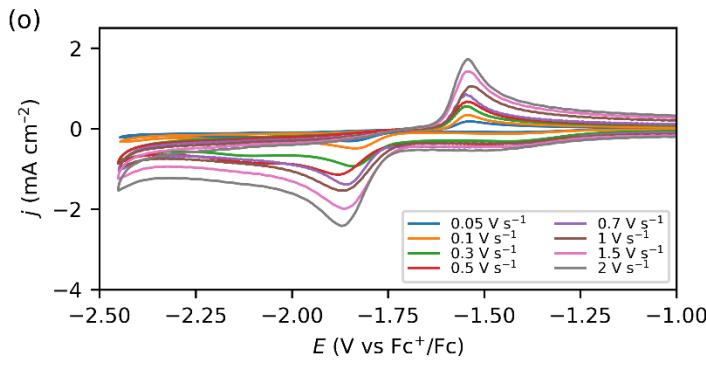
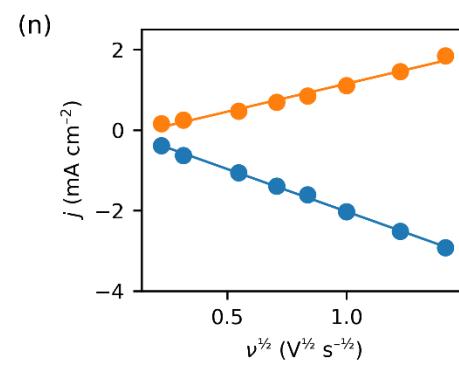
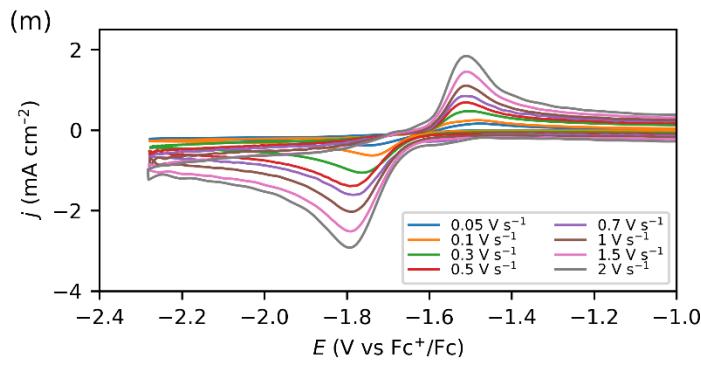
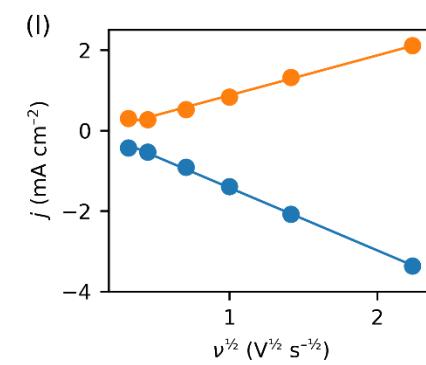
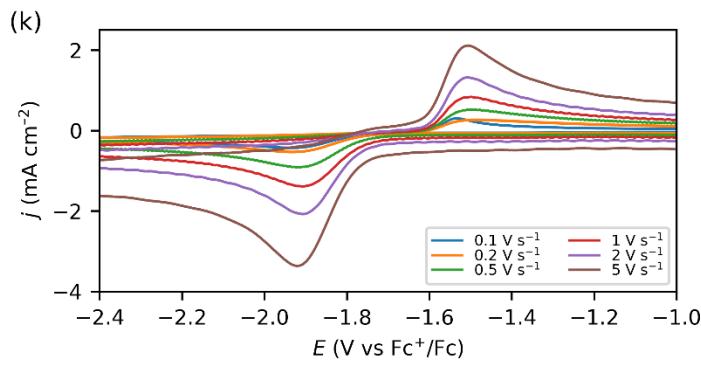
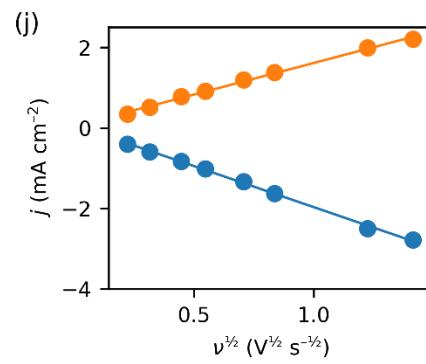
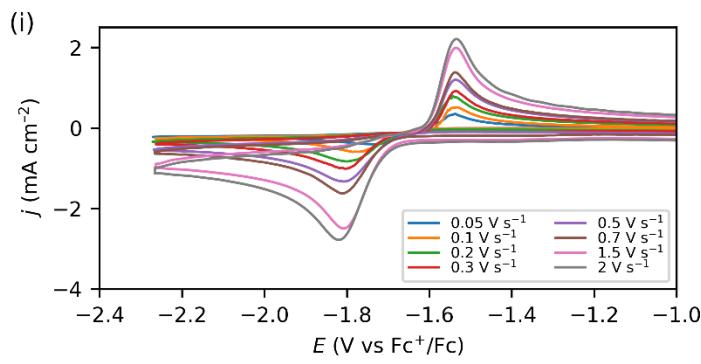
## 2. X-RAY CRYSTALLOGRAPHIC DATA

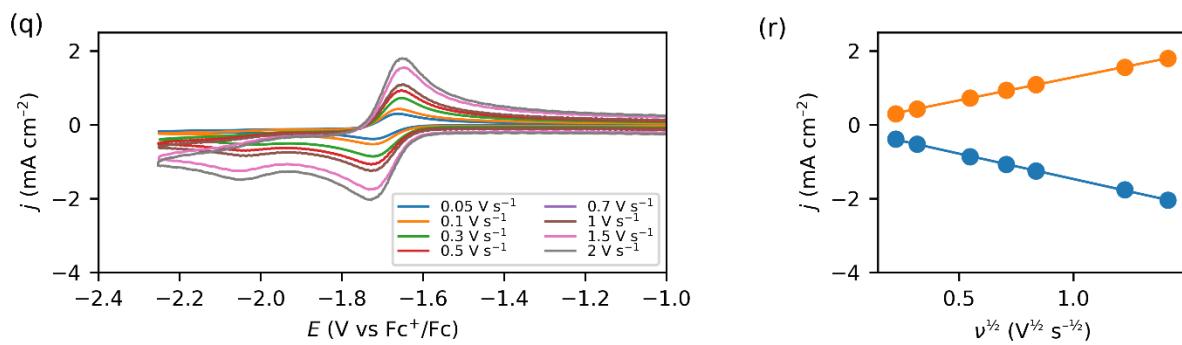
The intensities were empirically corrected for absorption using SCALE3 ABSPACK implemented in CrysAlisPRO.<sup>57</sup> The unit cell parameters were determined, and the Bragg intensities were integrated using CrysAlisPRO. The structure was solved and refined with SHELXS and SHELXL, respectively, in Olex2.<sup>58–510</sup> CCDC no. of **1a** is 1961900. The level B alert is originating from an uncertainty in the element type of one of the carbonyl carbons (C2). However, the identity of this atom is evidenced from both IR and HR-MS spectroscopy.

Item	Value
Molecular formula	C35 H38 Br Mn N4 O3
Formula weight	697.54
Crystal system	monoclinic
Space group	P 1 21/c 1
a (Å)	13.4608
b (Å)	29.8404
c (Å)	17.2593
α (°)	90
β (°)	103.92
γ (°)	90
Volume (Å <sup>3</sup> )	6729
Z	8
T (K)	100
ρ (g cm <sup>-1</sup> )	1.377
λ (Å)	0.71073
μ (mm <sup>-1</sup> )	1.619
# measured refl	84269
# unique refl	13754
R <sub>int</sub>	0.0432
# parameters	794
R(F <sup>2</sup> ), all refl	0.077
R <sub>w</sub> (F <sup>2</sup> ), all refl	0.1758
Goodness of fit	1.054

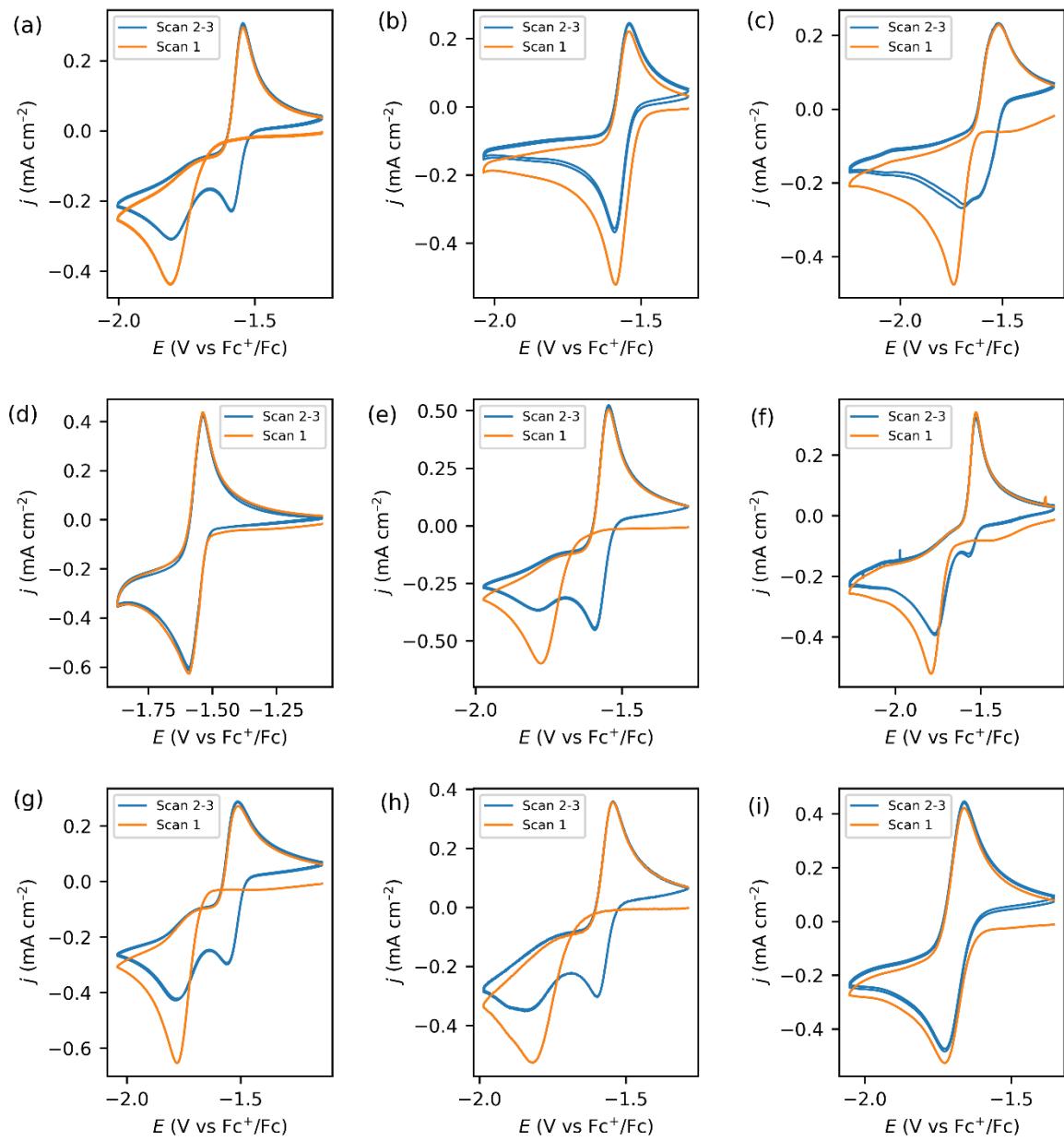
### 3. FIGURES, SCHEMES, AND TABLES



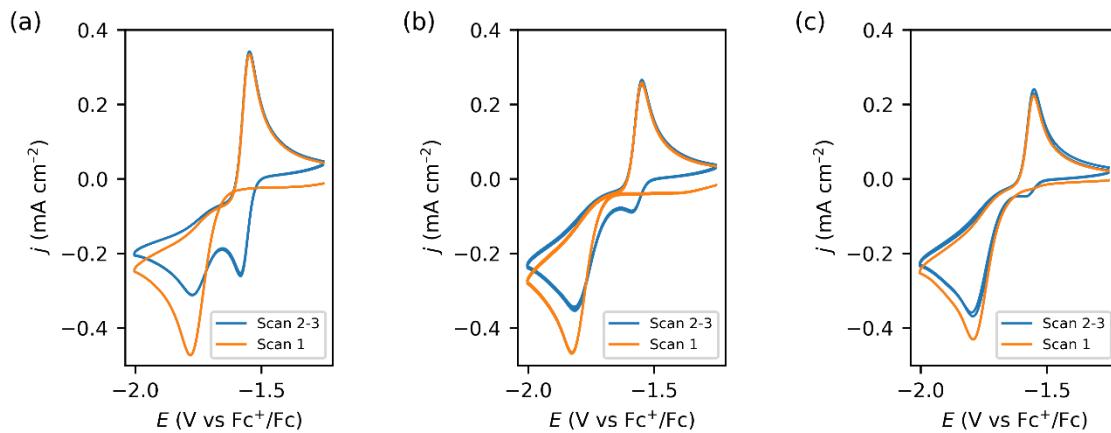




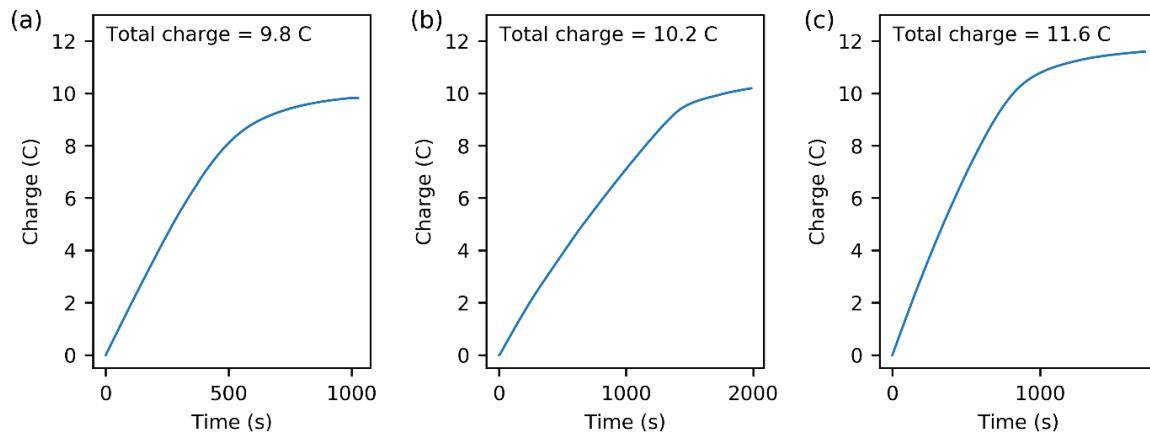
**Figure S1.** Cyclic voltammograms of 1 mM (a) **1a**, (c) **1b**, (e) **2**, (g) **3**, (i) **4**, (k) **5**, (m) **6**, (o) **7**, and (q) **8** recorded at a GC electrode (diameter = 1 mm) using various  $v$ 's in 0.1 M  $\text{Bu}_4\text{NBF}_4$ /MeCN under Ar. Plot of the peak currents [anodic (orange) and cathodic (blue)] vs  $v^{1/2}$  for (b) **1a**, (d) **1b**, (f) **2**, (h) **3**, (j) **4**, (l) **5**, (n) **6**, (p) **7**, and (r) **8** to show the linear dependency.



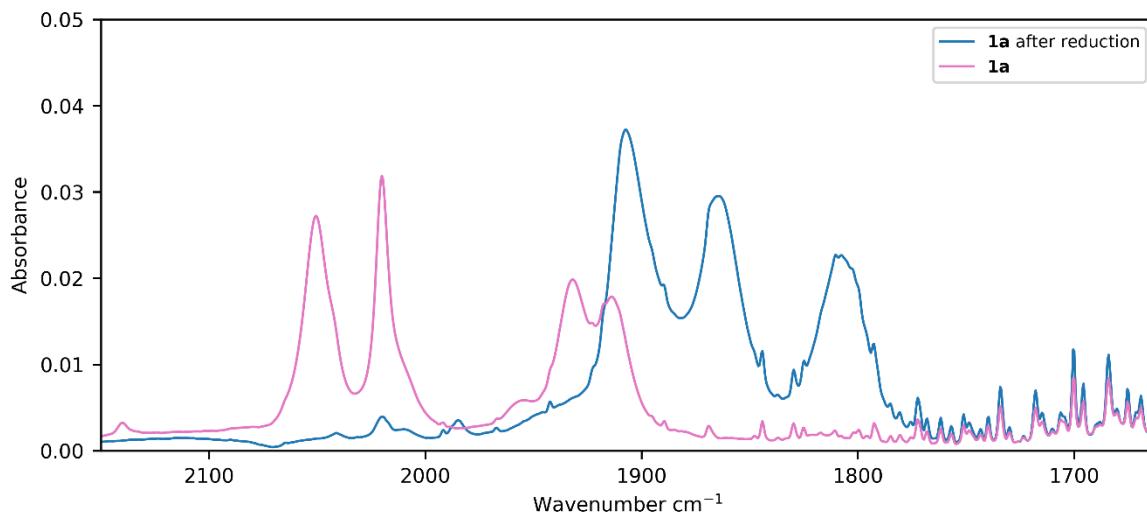
**Figure S2.** Three successive cyclic voltammograms of 1 mM (a) **1a**, (b) **1b**, (c) **2**, (d) **3**, (e) **4**, (f) **5**, (g) **6**, (h) **7**, and (i) **8** recorded at a GC electrode (diameter = 1 mm) using  $v = 0.1 \text{ V s}^{-1}$  in 0.1 M  $\text{Bu}_4\text{NBF}_4/\text{MeCN}$  under Ar.



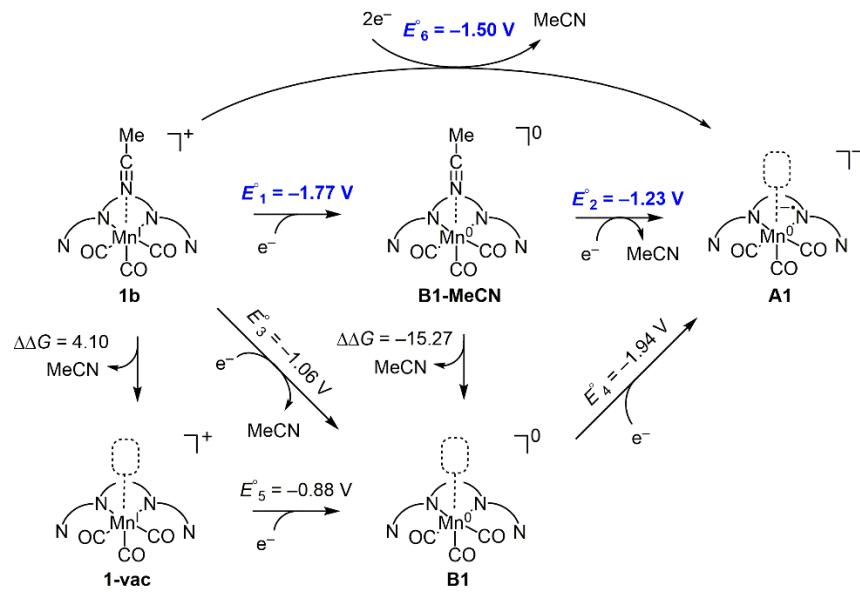
**Figure S3.** Three successive cyclic voltammograms recorded of 1 mM **1a** (using  $v = 0.1 \text{ V s}^{-1}$ ) containing (a) 0 equiv., (b) 2 equiv., and (c) 5 equiv.  $\text{Bu}_4\text{NBr}$  in 0.1 M  $\text{Bu}_4\text{NBF}_4$ /MeCN under Ar.



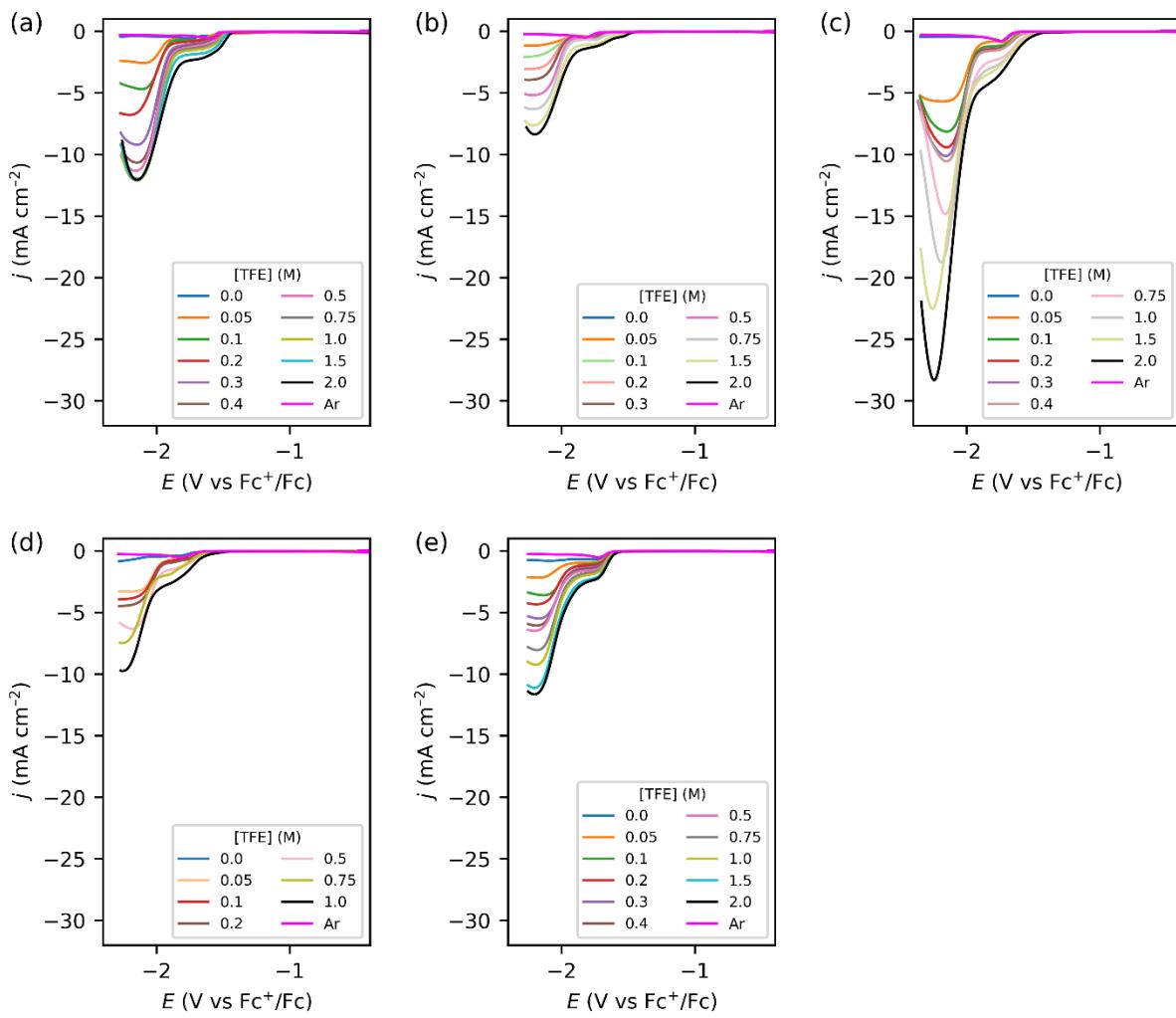
**Figure S4.** Electrolysis of 0.05 mmol (a) **1a** and (b) **2** at a GC foam working electrode ( $1 \text{ cm} \times 1 \text{ cm} \times 0.2 \text{ cm}$ ) applying a potential of  $-2.07 \text{ V vs Fc}^+/\text{Fc}$  in 5 mL 0.1 M  $\text{Bu}_4\text{NBF}_4/\text{CH}_3\text{CN}$  under Ar; the theoretically expected charge for a 2e reduction is 9.6 C. (c) Electrolysis of 0.06 mmol **4** under otherwise identical conditions as described for (a) and (b) with the theoretically expected charge being equal to 11.6 C for a 2e reduction.



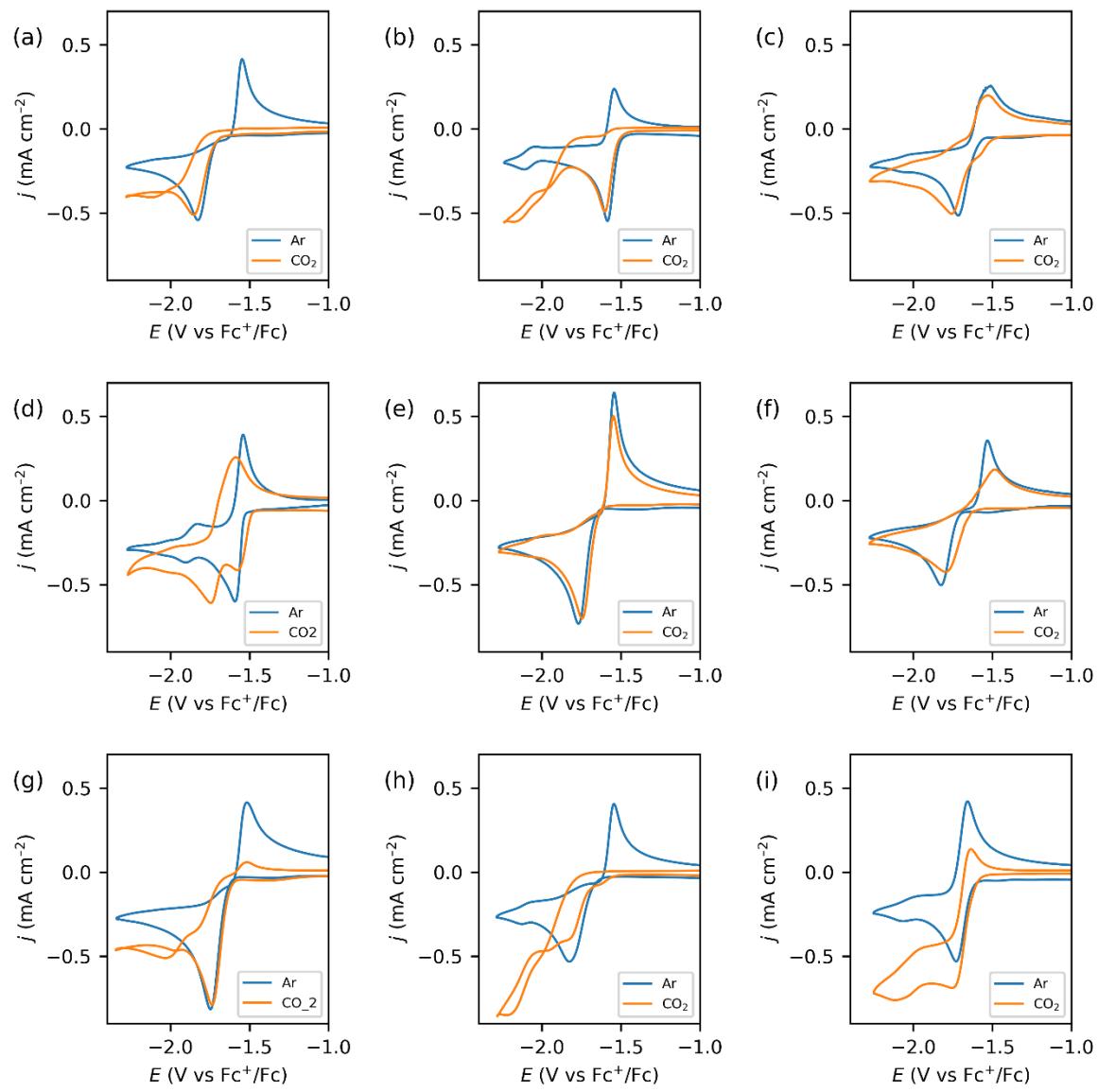
**Figure S5.** IR spectrum of **1a** before (purple) and after applying a potential of  $-2.07$  V vs  $\text{Fc}^+/\text{Fc}$  for  $12$  s (blue) in  $0.1$  M  $\text{Bu}_4\text{NBF}_4$ /MeCN under Ar.



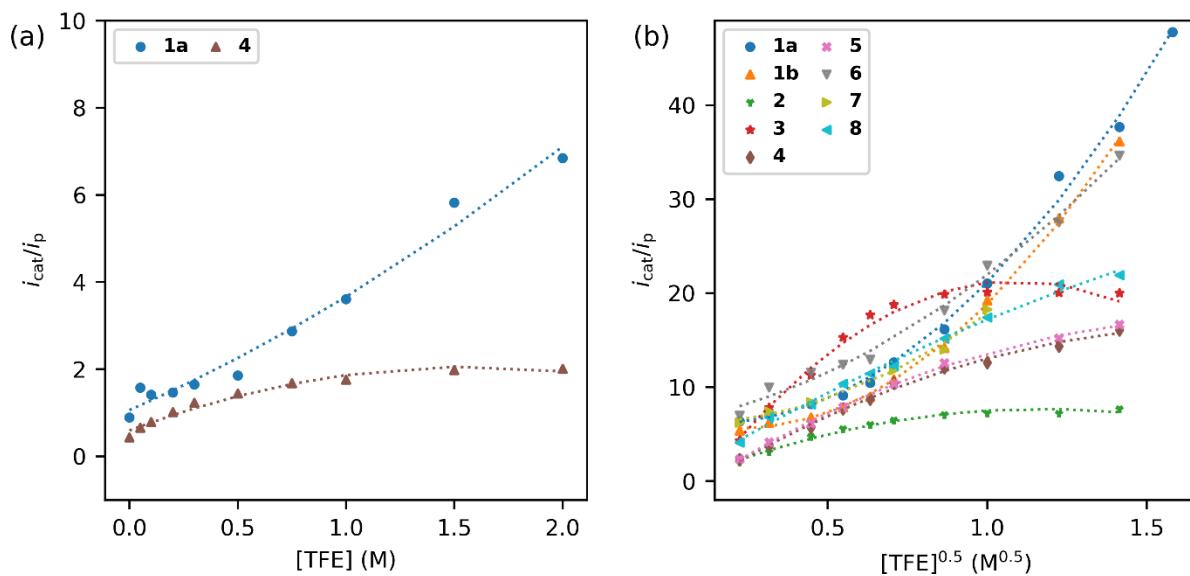
**Scheme S1.** Computational study on the reduction path of  $\text{Mn}(\text{bpy})^3(\text{CO})_3(\text{OTf})$  (**1b**); potential values are referenced vs  $\text{Fc}^+/\text{Fc}$  and energies are given in kcal/mol (see Section 4.2 for additional explanation).



**Figure S6.** Linear sweep voltammograms of 1 mM (a) **3**, (b) **5**, (c) **6**, (d) **7**, and (e) **8** under  $\text{CO}_2$  with increasing [TFE] recorded at a GC electrode (diameter = 1 mm) using  $v = 0.1 \text{ V s}^{-1}$  in 0.1 M  $\text{Bu}_4\text{NBF}_4$ /MeCN. A linear sweep voltammogram recorded under Ar without TFE (purple) is included.



**Figure S7.** Cyclic voltammograms of 1 mM (a) **1a**, (b) **1b**, (c) **2**, (d) **3**, (e) **4**, (f) **5**, (g) **6**, (h) **7**, and (i) **8** recorded under Ar (blue) and  $\text{CO}_2$  (yellow) at a GC electrode (diameter = 1 mm) using  $v = 0.1 \text{ V s}^{-1}$  in 0.1 M  $\text{Bu}_4\text{NBF}_4/\text{MeCN}$ .

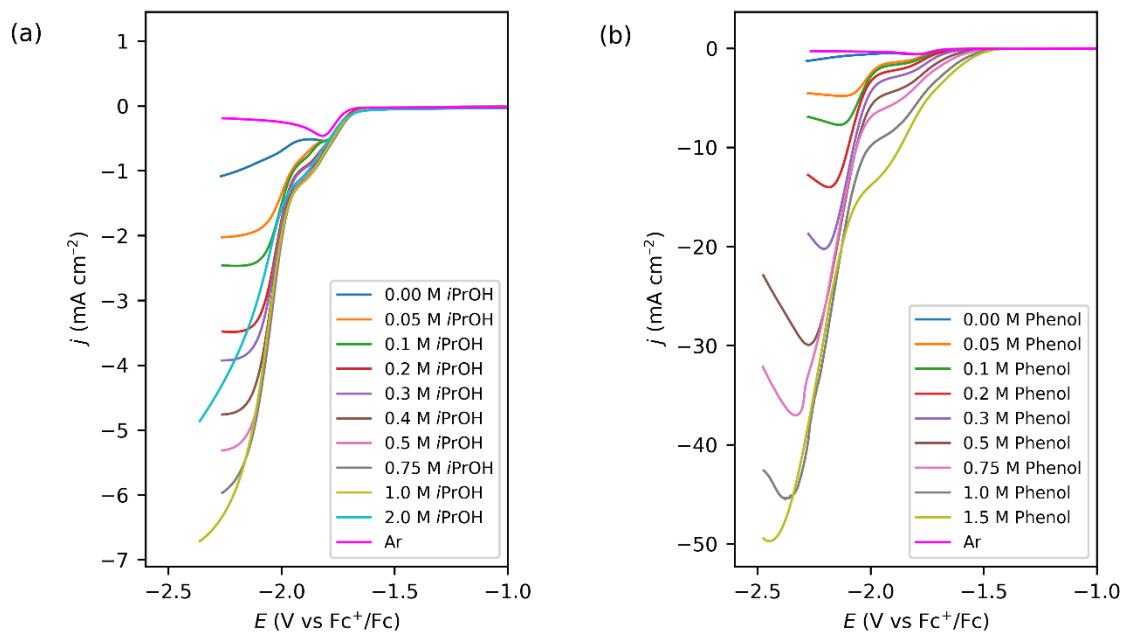


**Figure S8.** (a) Plot of the activity of **1a** and **4**,  $i_{\text{cat}}/i_p$ , vs [TFE] using  $v = 10 \text{ V s}^{-1}$ . (b) Plot of the activity of **1–8**,  $i_{\text{cat}}/i_p$ , vs  $[TFE]^{0.5}$  ( $M^{0.5}$ ) using  $v = 0.1 \text{ V s}^{-1}$ .

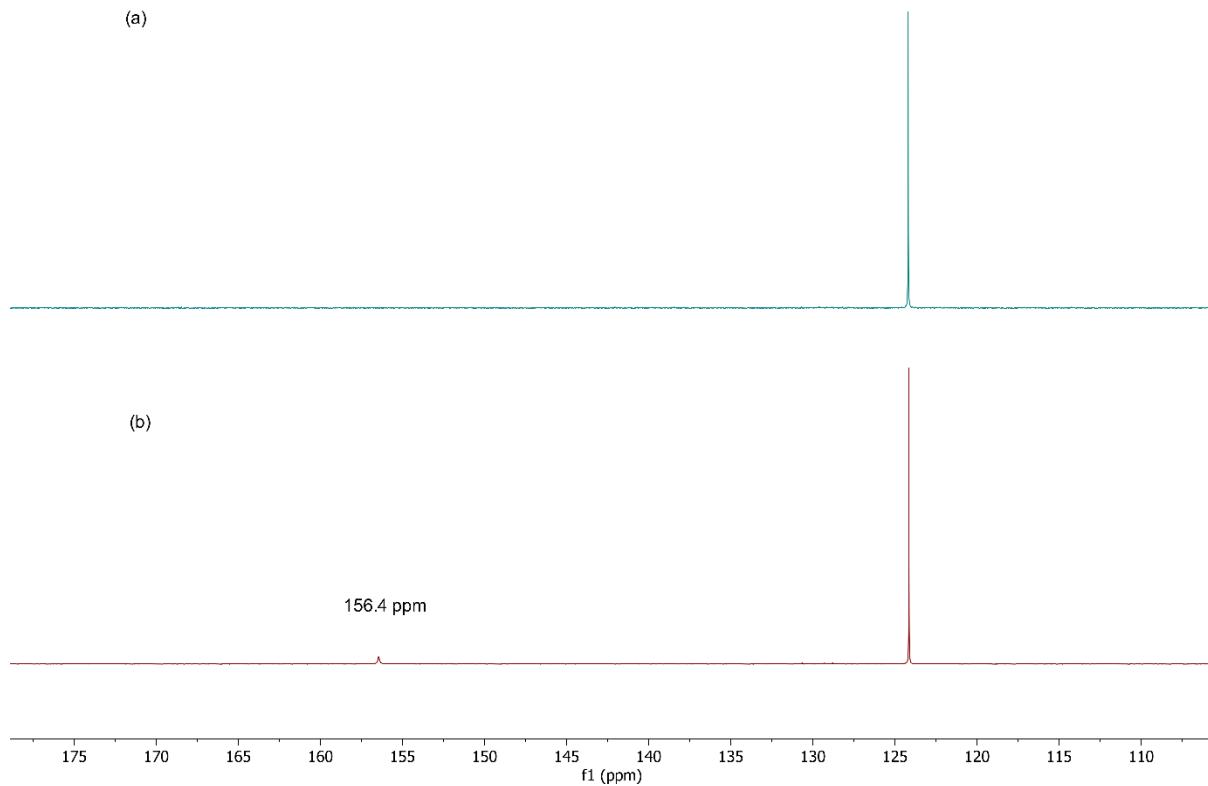
**Table S1. Electrolysis of 1–8 to Obtain the FE of the HCOOH, CO, and H<sub>2</sub> Production.<sup>a</sup>**

Catalyst <sup>b</sup>	E (V vs Fc <sup>+</sup> /Fc)	Acid	FE (%) <sup>c</sup>				Charge (C) <sup>d</sup>
			HCOOH	CO	H <sub>2</sub>	Total	
<b>1a</b>	-2.17	2.0 M TFE	71	4.8	6.4	82	40
<b>1b</b>	-2.17	2.0 M TFE	72	4.9	5.1	82	37
<b>2</b>	-2.17	2.0 M TFE	5.0	83	2.1	90	10
<b>3</b>	-2.17	2.0 M TFE	0.0	92	1.9	90	13
<b>4</b>	-2.17	2.0 M TFE	0.0	94	0.1	94	41
<b>5</b>	-2.17	2.0 M TFE	23	68	0.5	91	37
<b>6</b>	-2.17	2.0 M TFE	63	12.5	5.5	81	61
<b>7</b>	-2.17	2.0 M TFE	70	5.6	5.9	82	42
<b>8</b>	-2.17	2.0 M TFE	25	35	31	91	28
<b>1a</b>	-1.77	2.0 M TFE	90	6.9	7.3	104	11
<b>1a</b>	-2.17	0.3 M iPrOH	89	3.7	0.2	93	8
<b>1a</b>	-2.17	1.0 M Phenol	64	0	33	97	21
<b>4<sup>e</sup></b>	-2.17	2.0 M TFE	9.0	63	2	82	34
<b>4<sup>f</sup></b>	-2.17	2.0 M TFE	6.0	16	66	88	29
<b>1a<sup>g</sup></b>	-2.17	2.0 M TFE	0.0	0.0	94	94	40 <sup>h</sup>
<b>A7<sup>i</sup></b>	-2.17	2.0 M TFE	78	5.2	12	95	43

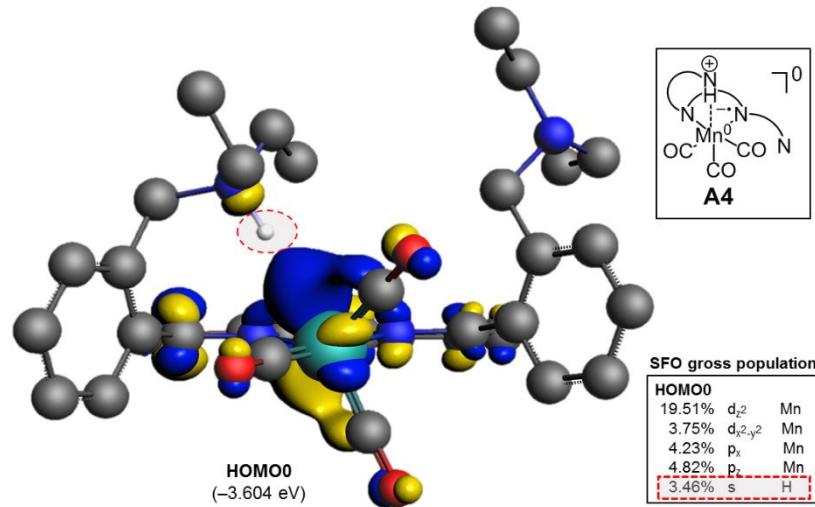
<sup>a</sup> Electrolysis was performed in CO<sub>2</sub> saturated 0.2 M Bu<sub>4</sub>NBF<sub>4</sub>/MeCN (5 ml); see electrochemical cell depicted in Figure S23d. <sup>b</sup> [Catalyst] = 1 mM. <sup>c</sup> The deviation of two measurements was in all cases <6 %. <sup>d</sup> The deviation of two measurements was <15%, the second last entry being an exception. <sup>e</sup> Addition of 0.1 M Et<sub>3</sub>N. <sup>f</sup> Addition of 0.1 M BnNH<sub>2</sub>. <sup>g</sup> Experiment carried out under Ar. <sup>h</sup> Uncertainty is 40 %. <sup>i</sup> A7 is the derivative of **1** with formate as displayed in Scheme 4.



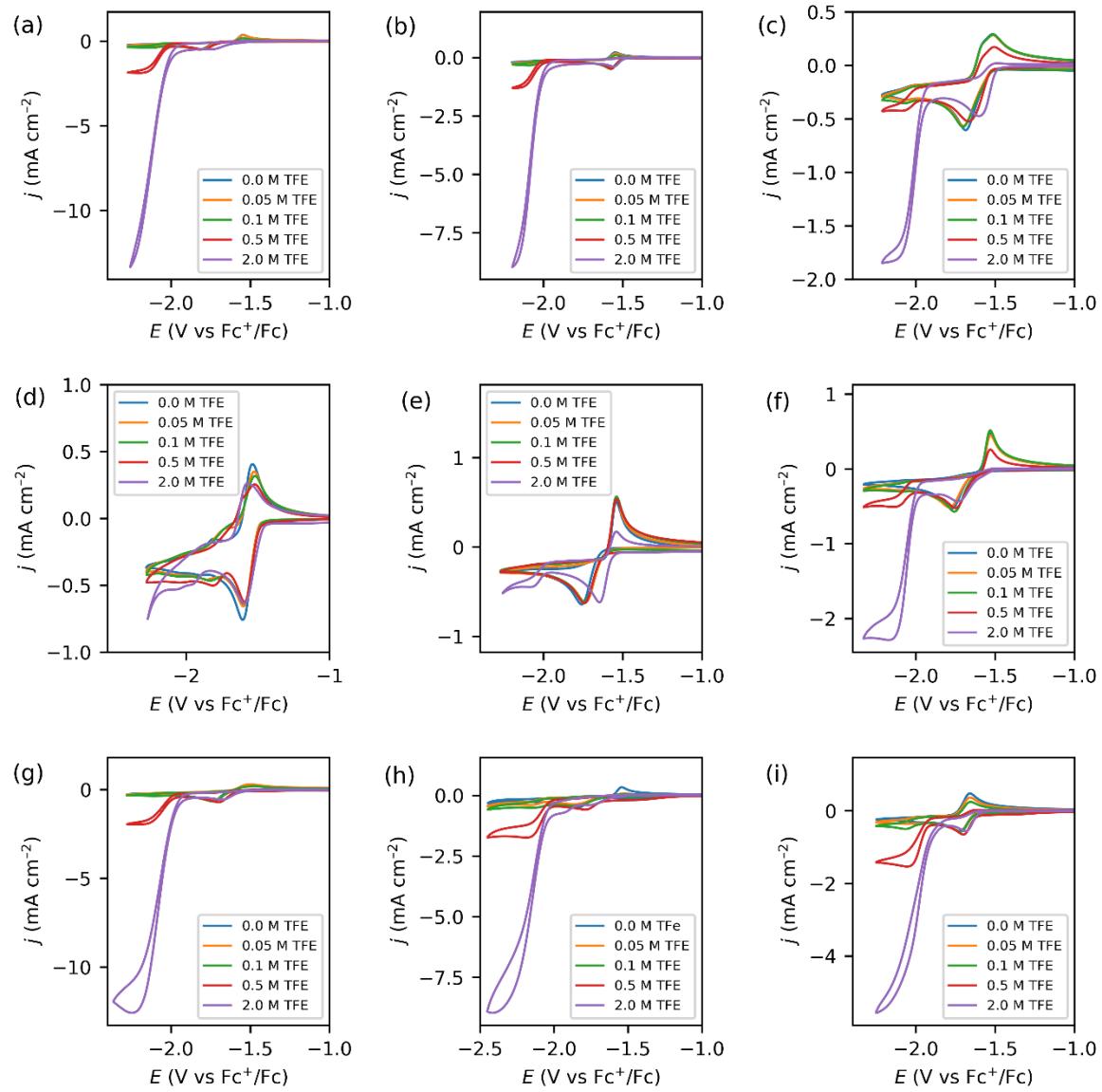
**Figure S9.** Linear sweep voltammograms of 1 mM **1a** recorded at a GC electrode (diameter = 1 mm) using  $\nu = 0.1 \text{ V s}^{-1}$  with increasing concentration of (a) 2-propanol and (b) phenol under  $\text{CO}_2$  in 0.1 M  $\text{Bu}_4\text{NBF}_4/\text{MeCN}$ . A linear sweep voltammogram recorded under Ar without acid (purple) is included.



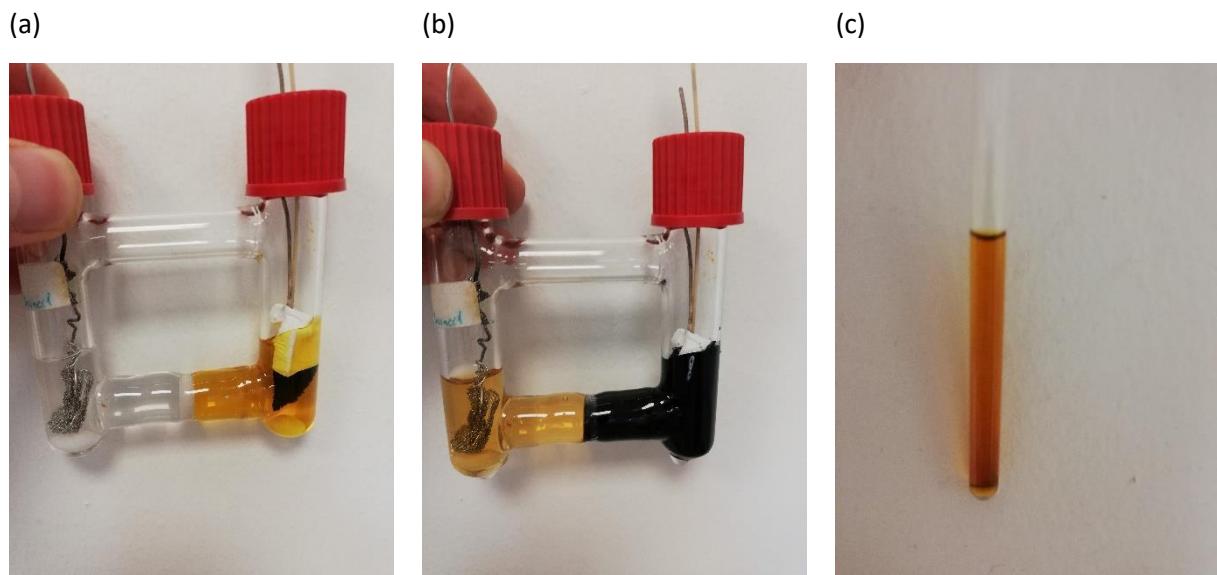
**Figure S10.** (a)  $^{13}\text{C}$  NMR spectra of 0.015 mmol **1a** in 1 mL  $(\text{CD}_3)_2\text{SO}$  after 4 h exposure to  $^{13}\text{CO}_2$ . (b)  $^{13}\text{C}$  NMR spectra of 0.015 mmol **8** in 1 mL  $(\text{CD}_3)_2\text{SO}$  after 4 h exposure to  $^{13}\text{CO}_2$ . The peak at 124 ppm is dissolved  $^{13}\text{CO}_2$ .



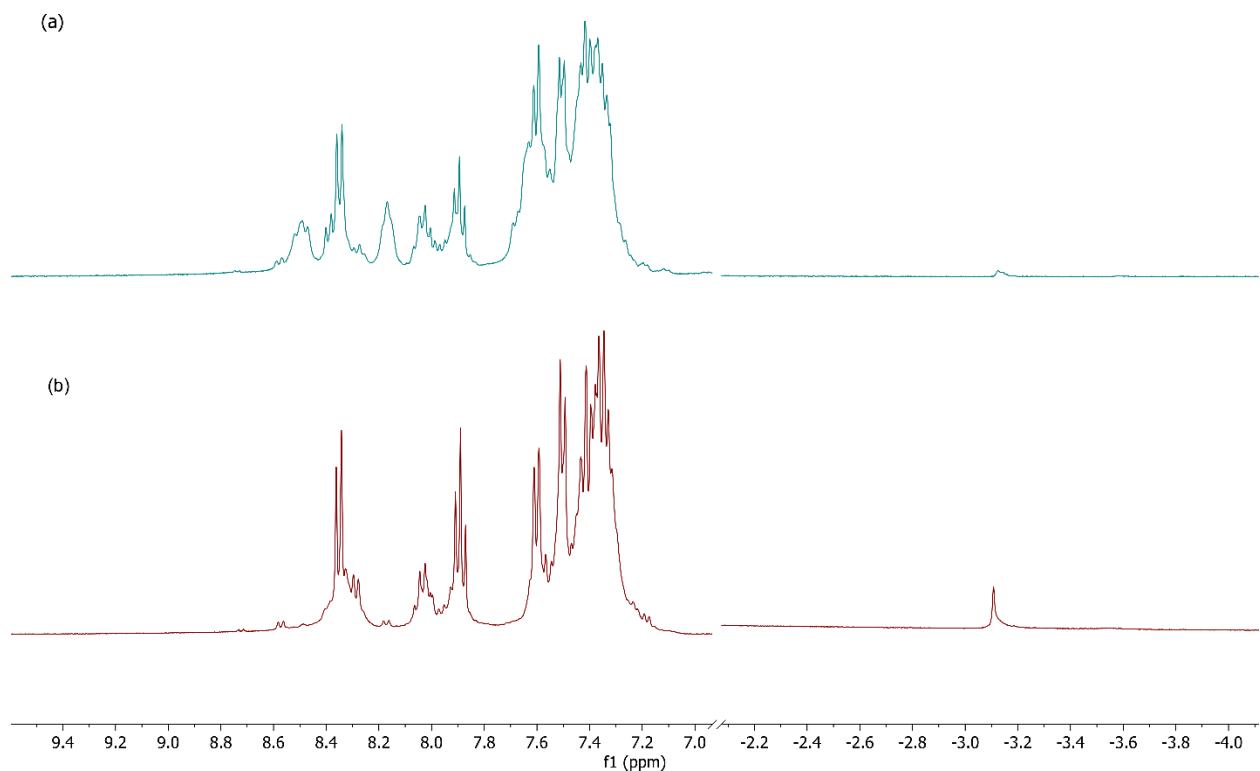
**Figure S11.** The orbital shape of HOMO0 and SFO gross analysis of this showing the origin of an interaction between tethered ammonium and manganese center (see Section 4.2 for additional explanation).



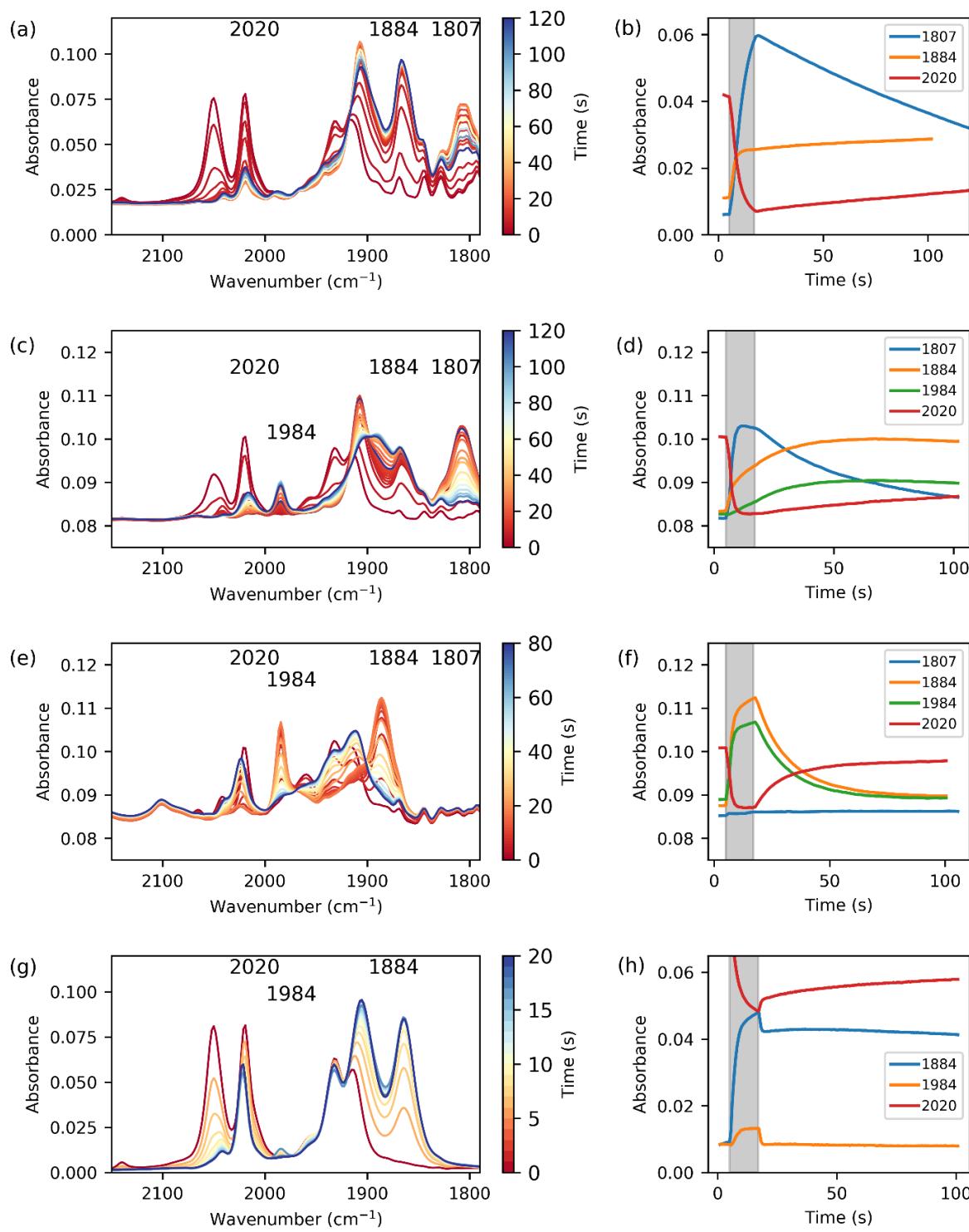
**Figure S12.** Cyclic voltammograms of 1 mM (a) **1a**, (b) **1b**, (c) **2**, (d) **3**, (e) **4**, (f) **5**, (g) **6**, (h) **7**, and (i) **8** with increasing [TFE] recorded at a GC electrode (diameter = 1 mm) using  $v = 0.1 \text{ V s}^{-1}$  in 0.1 M  $\text{Bu}_4\text{NBF}_4/\text{MeCN}$  under Ar.



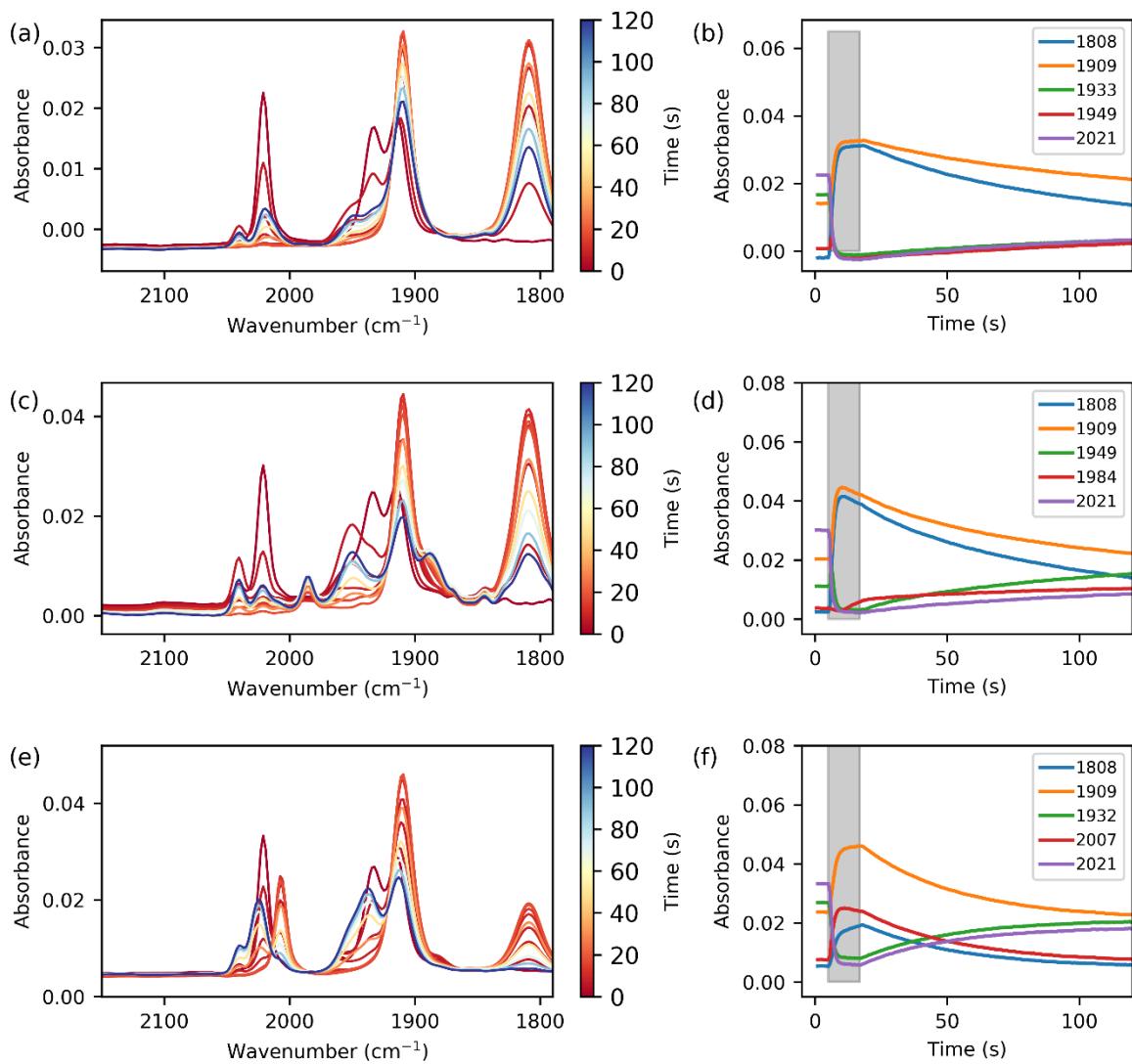
**Figure S13.** H-cell containing in the cathodic chamber (right-hand side) 10 mM **1a** (a) before and (b) after reduction at  $-2.07$  V vs  $\text{Fc}^+/\text{Fc}$  in 5 mL 0.1 M  $\text{Bu}_4\text{NBF}_4/\text{CH}_3\text{CN}$  under Ar with a GC foam working electrode (1 cm  $\times$  1 cm  $\times$  0.2 cm). During electrolysis some leakage of the complex to the counter chamber was observed due to the large concentration gradient across the membrane. (c) The electrochemically reduced solution after adding 10 equiv. TFE to form the **Mn–H** complex.



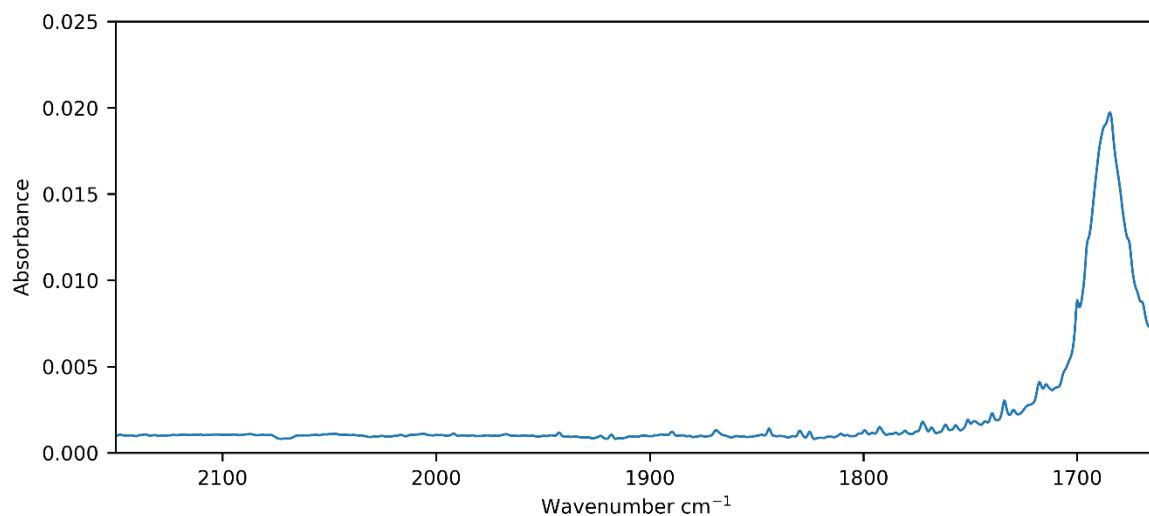
**Figure S14.**  ${}^1\text{H}$  NMR spectra of  $\sim 0.025$  mmol **1a** after electrochemical reduction and addition of (a) 50 equiv. and (b) 10 equiv. TFE.



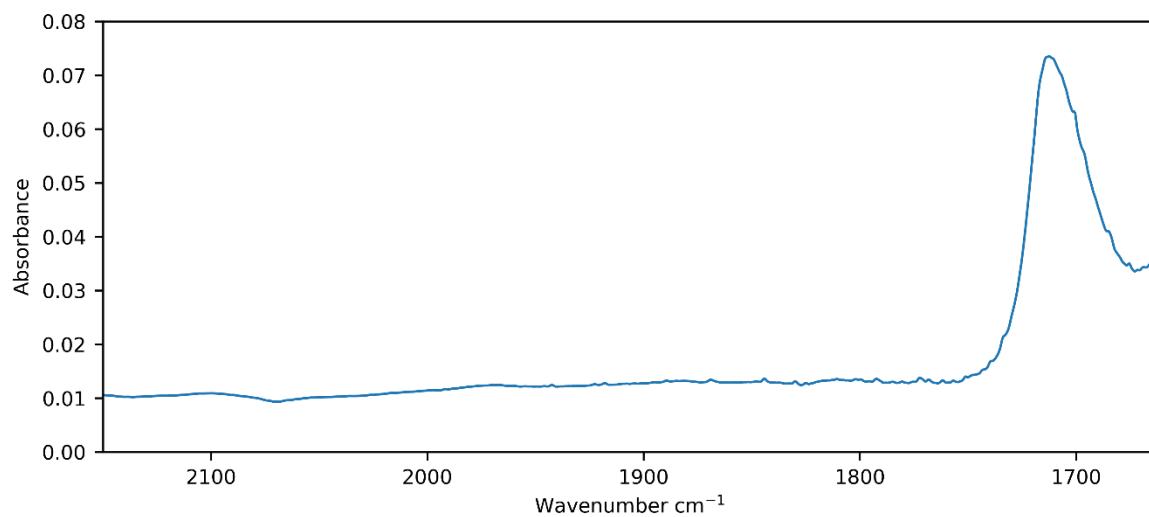
**Figure S15.** IR spectra of 1 mM **1a** recorded over 120 s with (a) 10 mM TFE (Ar), (c) 50 mM TFE (Ar), (e) 430 mM TFE (Ar), and (g) 10 mM TFE ( $\text{CO}_2$ ) in 0.1 M  $\text{Bu}_4\text{NBF}_4/\text{MeCN}$ . Initially, a pre-electrolysis potential of  $-1.37 \text{ V}$  vs  $\text{Fc}^+/\text{Fc}$  was applied for 5 s before the actual electrolysis was performed at  $-2.07 \text{ V}$  vs  $\text{Fc}^+/\text{Fc}$  for 12 s (grey region). From this point on the voltage was turned off and the kinetics were recorded, i.e. (b) 10 mM TFE (Ar), (d) 50 mM TFE (Ar), (f) 430 mM TFE (Ar), and (h) 10 mM TFE ( $\text{CO}_2$ ) in 0.1 M  $\text{Bu}_4\text{NBF}_4/\text{MeCN}$ .



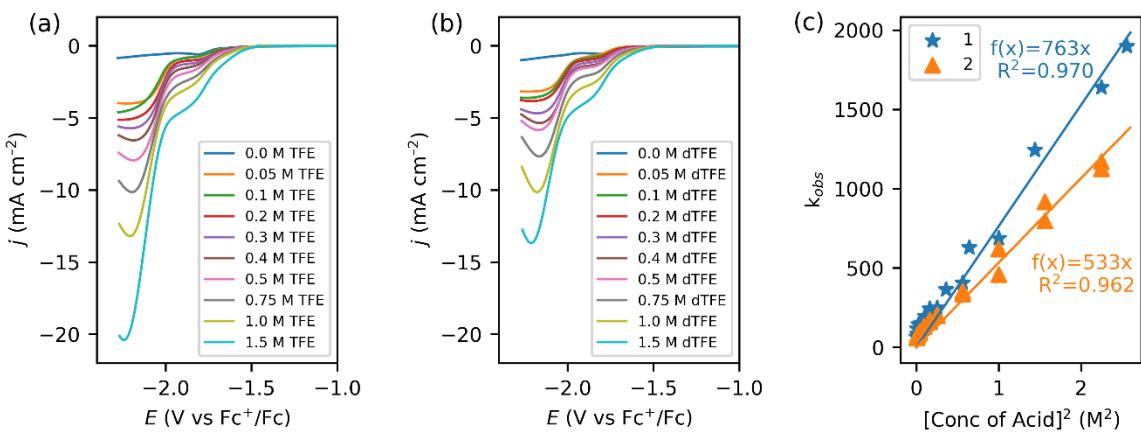
**Figure S16.** IR spectra of **4** recorded over 120 s with (a) 50 mM TFE (Ar), (c) 430 mM TFE (Ar), and (e) 50 mM TFE ( $\text{CO}_2$ ) in 0.1 M  $\text{Bu}_4\text{NBF}_4/\text{MeCN}$ . Initially a pre-electrolysis potential of  $-1.37 \text{ V}$  vs  $\text{Fc}^+/\text{Fc}$  was applied for 5 s before the actual electrolysis was performed at  $-2.07 \text{ V}$  vs  $\text{Fc}^+/\text{Fc}$  for 12 s (grey region). From this point on the voltage was turned off and the kinetics were recorded, i.e. (b) 50 mM TFE (Ar), (d) 430 mM TFE (Ar), and (f) 50 mM TFE ( $\text{CO}_2$ ).



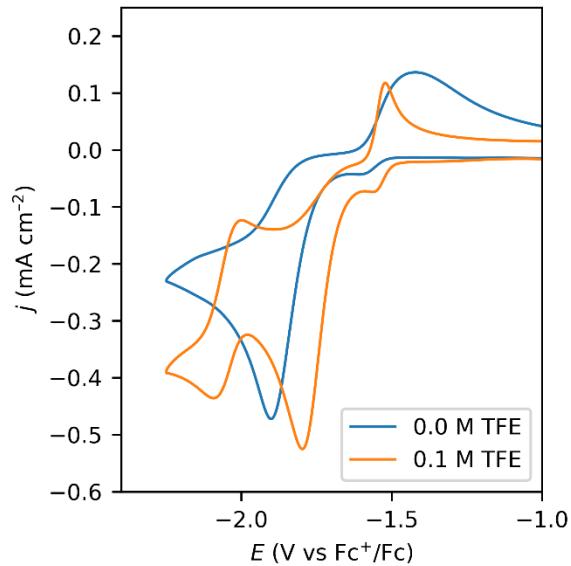
**Figure S17.** IR spectrum of  $[\text{Bu}_4\text{N}]^+[\text{HCOO}]^-$  in MeCN.



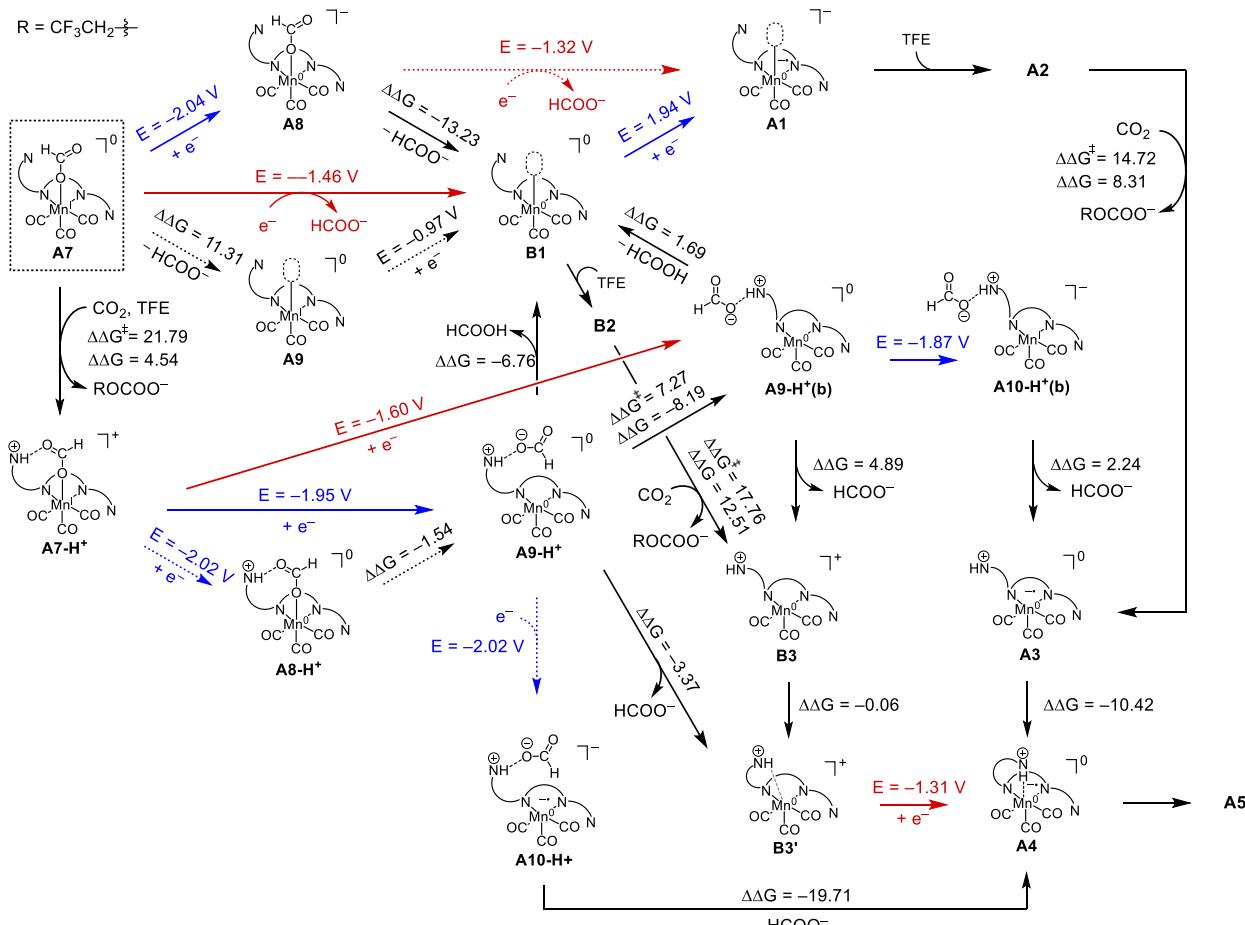
**Figure S18.** IR spectrum of  $[\text{HDBU}]^+[\text{CF}_3\text{CH}_2\text{OC(O)O}]^-$  in MeCN;  $[\text{HDBU}]^+$  refers to the protonated form of the base 1,8-diazabicyclo(5.4.0)undec-7-ene.



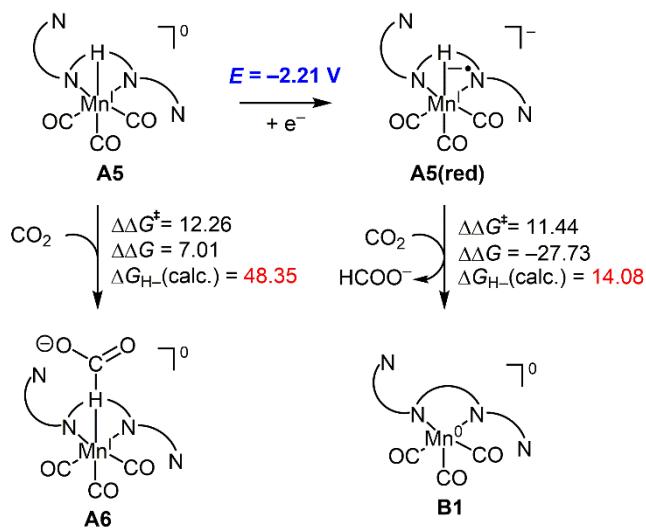
**Figure S19.** Linear sweep voltammograms of 1 mM **1a** recorded at a GC electrode (diameter = 1 mm) using  $v = 0.1 \text{ V s}^{-1}$  under  $\text{CO}_2$  with increasing concentration of (a) TFE or (b)  $\text{CF}_3\text{CH}_2\text{OD}$  (b) in 0.1 M  $\text{Bu}_4\text{NBF}_4/\text{MeCN}$ .



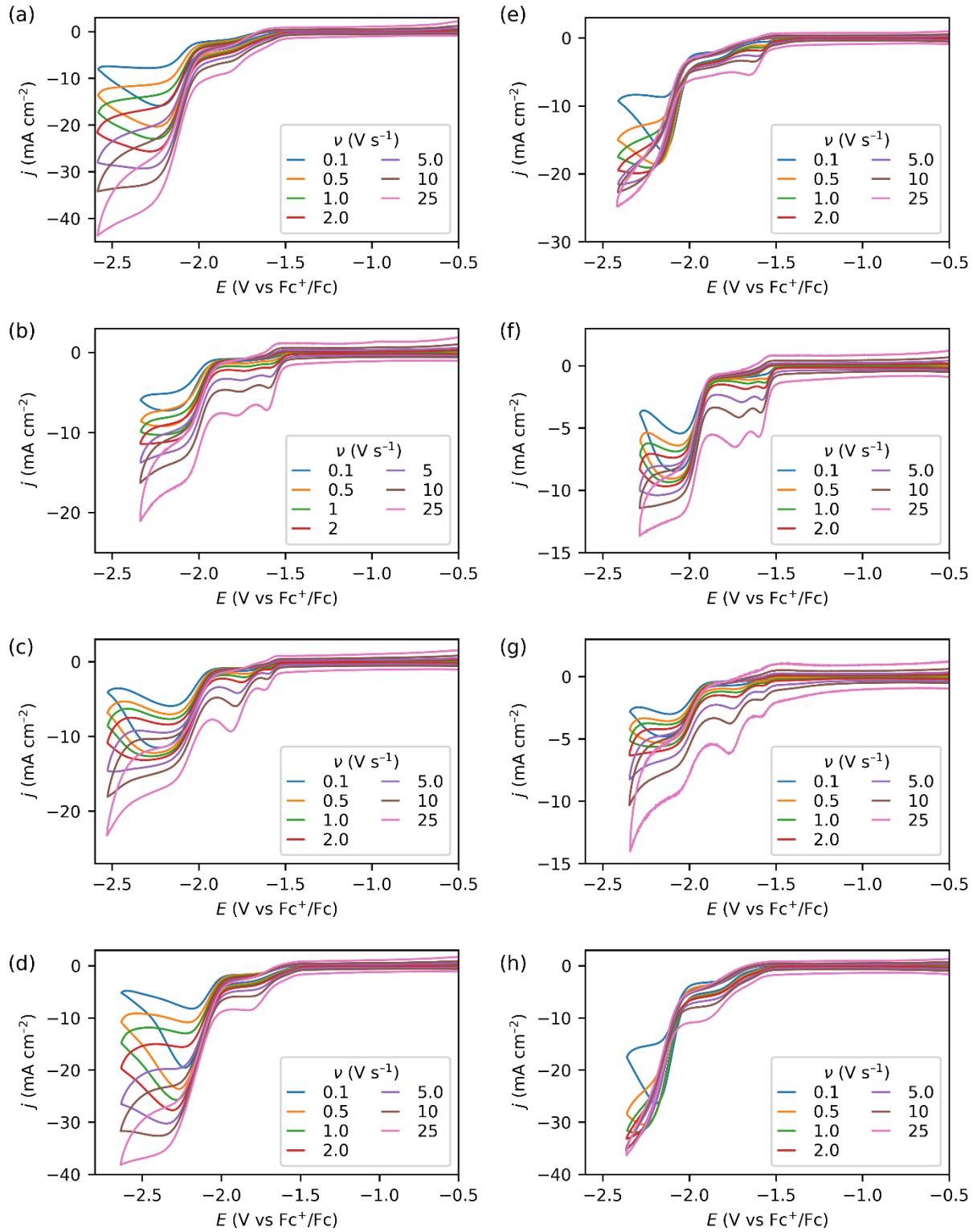
**Figure S20.** Cyclic voltammograms of 1 mM Mn(*N,N'*-((2,2'-bipyridine)-6,6'-diylbis(2,1-phenylene))bis(methylene))diethanamine)(CO)<sub>3</sub>O(CO)H (**A7**) recorded with no TFE (blue) and with 0.1 M TFE (yellow) at a GC electrode (diameter = 1 mm) using  $v = 0.1 \text{ V s}^{-1}$  in 0.1 M  $\text{Bu}_4\text{NBF}_4/\text{MeCN}$  under Ar.

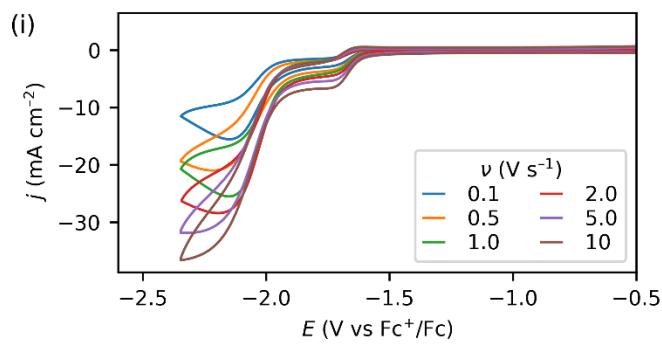


**Scheme S3.** Scheme showing computational results of the required potential for reduction of  $\text{Mn}^{\text{I}}-\text{H}$  and the reactivity of  $\text{Mn}^{\text{I}}-\text{H}$  and  $[\text{Mn}^{\text{I}}-\text{H}]^-$ , respectively; potential values are referenced vs  $\text{Fc}^+/\text{Fc}$  and energies are given in kcal/mol (see Section 4.2 for additional explanation).

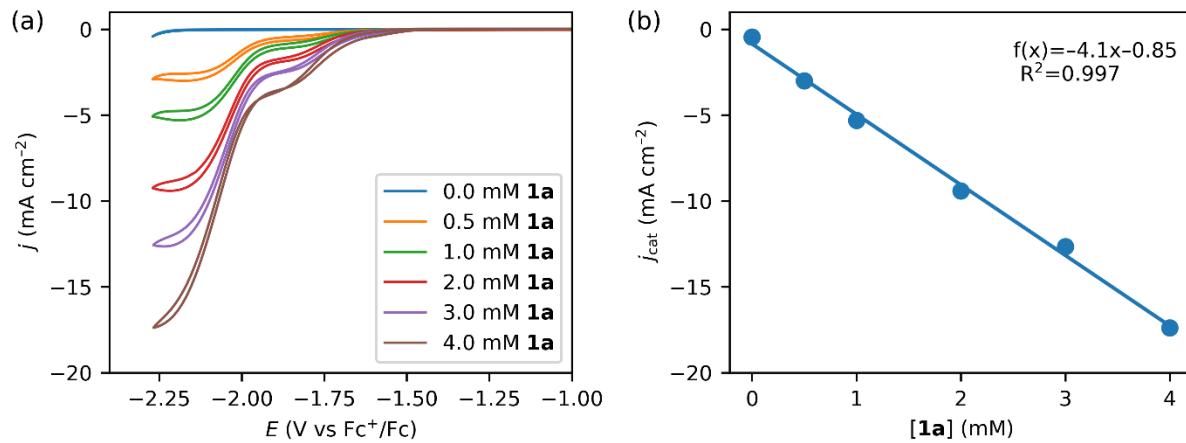


**Scheme S3.** Scheme showing computational results of the required potential for reduction of  $\text{Mn}^{\text{I}}-\text{H}$  and the reactivity of  $\text{Mn}^{\text{I}}-\text{H}$  and  $[\text{Mn}^{\text{I}}-\text{H}]^-$ , respectively; potential values are referenced vs  $\text{Fc}^+/\text{Fc}$  and energies are given in kcal/mol (see Section 4.2 for additional explanation).

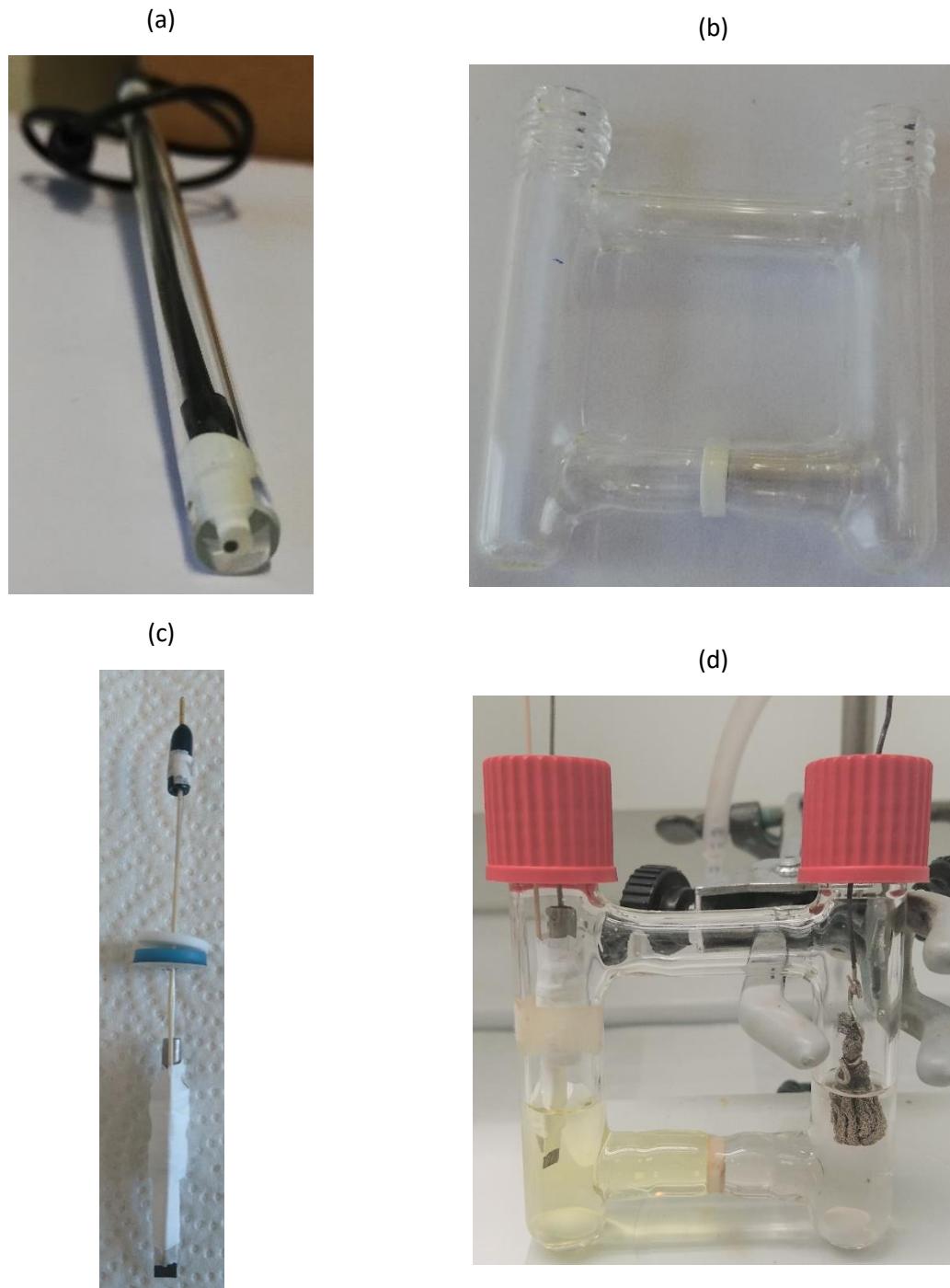




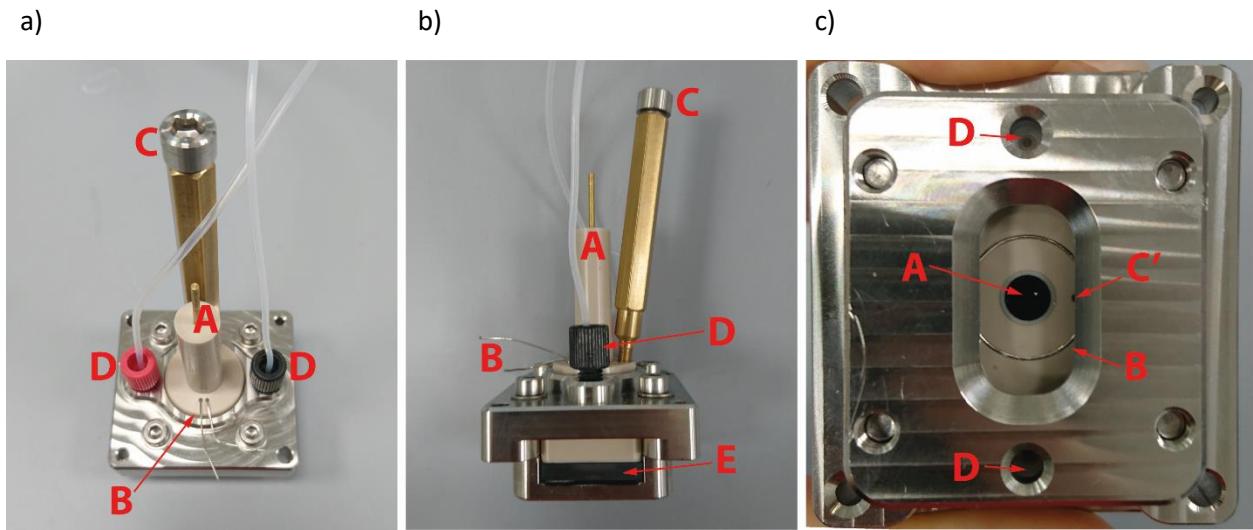
**Figure S21.** Cyclic voltammograms of 1 mM (a) **1a**, (b) **1b**, (e) **4**, (f) **5**, (g) **6**, (h) **7**, and (i) **8** recorded in a  $\text{CO}_2$  saturated solution containing 2.0 M TFE at a GC electrode (diameter = 1 mm) using various  $v$ 's in 0.1 M  $\text{Bu}_4\text{NBF}_4$ /MeCN. Cyclic voltammograms of 1 mM (c) **2** and (d) **3** in a  $\text{CO}_2$  saturated solution containing 1.0 M TFE at a GC electrode (diameter = 1 mm) using various  $v$ 's in 0.1 M  $\text{Bu}_4\text{NBF}_4$ /MeCN.



**Figure S22.** (a) Cyclic voltammograms of 0.5 M TFE recorded at a GC electrode (diameter = 1 mm) using  $v = 0.1 \text{ V s}^{-1}$  with **1a** in 0.1 M  $\text{Bu}_4\text{NBF}_4$ /MeCN under  $\text{CO}_2$ . (b) Plot of  $j_{\text{cat}}$  as function of **1a**.



**Figure S23.** Photos of (a) the homemade electrode used for the cyclic voltammetric studies, (b) the homemade cell used for the electrolysis experiments, (c) the working and reference electrodes, and (d) the electrolysis setup before wrapping it in aluminium foil.



**Figure S24.** Photos of the IR-SEC cell shown from (a) above, (b) the side, and (c) below where the dimension of the stainless steel platform is 5 × 4.5 cm. (A) GC working electrode, (B) Pt counter electrode, (C) holder for Ag/AgCl reference electrode, (C') tip of reference electrode, (D) inlet and outlet for the electrolyte solution, and (E) CaF<sub>2</sub> window.

## 4. COMPUTATIONAL METHODS AND DETAILS

### 4.1 Computational Methods

Density functional theory and Solvation

All calculations were implemented by the Jaguar 9.1 suite of programs<sup>S11</sup> and density functional theory (DFT).<sup>S12</sup> All geometries were optimized to the solvated structure in the solvent (acetonitrile) employed with solvation model called Poisson-Boltzmann Finite element (PBF) method ( $\epsilon = 37.5$ ,  $r = 2.18$ )<sup>S13, S14</sup> using the Becke's 3 parameter exchange functional<sup>S15, S16</sup> with Grimme's D3 dispersion correction (B3LYP-D3).<sup>S17</sup> The manganese was modelled with LACVP<sup>S18-S20</sup> basis set which includes the effective core potentials (not relativistic for first row transition metals) and the other atoms were modelled with the 6-31G\*\* basis set<sup>S21</sup>. Frequency calculations were carried out at the same level of theory as the geometry optimizations. Zero-point vibrational energies and entropy corrections were inferred from the vibrational frequencies calculations. The energies of the optimized structures were re-examined by single point calculations with cc-pVTZ(-f)<sup>S22</sup> basis set which contains Dunning's correlation-consistent triple- $\zeta$  quality and a double set of polarization functions. Solvation energies were calculated by the self-consistent reaction field (SCRF)<sup>S23-S25</sup> with the dielectric constants  $\epsilon = 37.5$  (acetonitrile) to get the solvation correction energy. Final Gibbs free energy of each optimized intermediates and transition state was computed as follows:

$$G(\text{Sol}) = G(\text{Gas}) + G(\text{Solv}) \quad (\text{S3})$$

$$G(\text{Gas}) = H(\text{Gas}) - TS(\text{Gas}) \quad (\text{S4})$$

$$H(\text{Gas}) = E(\text{SCF}) + \text{ZPE} \quad (\text{S5})$$

$$\Delta G(\text{Sol}) = \Sigma G(\text{Sol}) \text{ for products} - \Sigma G(\text{Sol}) \text{ for reactants} \quad (\text{S6})$$

$G(\text{Sol})$  is the solvation-corrected free energy;  $G(\text{Gas})$  is the free energy of the optimized structure using PBF method;  $G(\text{Solv})$  is the solvation free energy;  $H(\text{Gas})$  is the enthalpy in the optimized structure using PBF method;  $T$  is the temperature (298.15 K);  $S(\text{Gas})$  is the entropy in the optimized structure using PBF method;  $E(\text{SCF})$  is the electronic self-consistent field energy computed from the SCF convergence in the optimized structure using PBF method; and ZPE is the vibrational zero-point energy. Note that the entropy we report is specifically the vibrational, rotational, and translational entropies of the solute(s). The solvent entropies are implicitly included in the continuum model.

Computational reproduction of reduction potentials

Standard reduction potentials for various reduction processes were calculated as follows:

The general reduction process of A is expressed as,



where  $A^{n-}$  is the  $n^{\text{th}}$  reduced state of A, and  $n$  implies the number of electrons involved in the reaction.

The reduction potential relative to the ferrocenium/ferrocene couple was calculated as

$$E_{A/A^{n-}}^\circ (\text{vs } Fc^+/Fc) = E_{Fc^+/Fc}^\circ - \frac{\Delta G_{A/A^{n-}}^\circ}{nF} \quad (\text{S8})$$

where  $\Delta G_{A/A^{n-}}^\circ$  is the change of Gibbs free related with eq S7; and  $F$  is Faraday constant (23.0605 kcal/(mol V)). The absolute potential of saturated calomel electrode ( $E_{\text{SCE}}^\circ$ ) in acetonitrile is taken as –

4.422 V.<sup>S26</sup> The reference electrode potential  $E_{\text{Fc}^+/\text{Fc}}^0$  is taken as -4.804 V by considering the shift in acetonitrile, -0.382 V, from  $E_{\text{SCE}}^0$ .<sup>S27</sup>

## 4.2 Computational Details

### Details Regarding Scheme S1

To demonstrate a reduction path of the catalyst under conditions without CO<sub>2</sub> and TFE, computationally, we probed the reduction steps among the expected intermediate species. The calculated reduction potential ( $E_6 = -1.50$  V) involving a two-electron transfer traversing from **1b** ( $[\text{Mn}^{\text{I}}(\text{MeCN})]^+$ ) to **A1** ( $[\text{Mn}^0]$ ) could be assigned to the experimental standard potential of -1.55 V vs Fc<sup>+</sup>/Fc shown in the CV results in Figure S2a and S2b. The acetonitrile solvent is bound to  $[\text{Mn}^{\text{I}}]^+$  as a ligand stabilizing the cationic species thermodynamically with 4.10 kcal/mol. This effect of solvent environment which keeps acetonitrile bounded to Mn-center would be maintained in the reduction process. So we expected that a reduction path from **1b** to **B1-MeCN** ( $E_1 = -1.77$  V) would be the predominant reduction pathway due to this stabilization over the reduction to **1-vac** ( $E_3 = -1.06$  V). A strongly preserved MeCN-bound environment at the second reduction process was also examined. This makes the reduction of **B1-MeCN** to **A1** ( $E_2 = -1.23$  V) possible. Thus, once an acetonitrile is bound to  $[\text{Mn}^{\text{I}}]^+$ , most of the **1b** species are reduced to **A1** through **B1-MeCN**. This means that the two-electron reduction pathway through **1b**→**B1-MeCN**→**A1** is kinetically and electrochemically favoured.

### Details Regarding Figure S11

To investigate a characteristic of the interaction between ammonium and the two-electron-reduced active site, we employed a symmetry-adapted combination of fragment orbitals (SFO) gross population analysis. The SFO gross population analysis was performed by the Amsterdam Density Functional (ADF).<sup>S28</sup> The computation was carried out applying B3LYP-D3 density functional<sup>S17</sup> with a valence triple-ζ Slater-type basis set and polarization functions for all atoms (TZP) from the ADF library.<sup>S29</sup> Scalar relativity is considered with the zero-order regular approximation (ZORA) for relativistic effects.<sup>S30</sup> The Cartesian coordinate of **A4** (Figure S11) was utilized from the optimized geometry by Jaguar 9.1.

Determined by the SFO analysis, significant electron density of HOMO0 is located on the s orbital of the proton in ammonium. This density-occupation on antibonding orbital means that the d<sub>z<sup>2</sup></sub> orbital of the fully saturated Mn(0) center influenced by adjacent reduced bipyridine ligand (bpy<sup>-</sup>) donates electron density to ammonium. This delocalizes the electron density on LUMO-π\* of bpy to LUMO-σ\* of ammonium. The structural variation in bond length (R<sub>3</sub>NH<sup>+</sup>…Mn<sup>0</sup>) from 2.967 Å in **B3'** to 2.457 Å in **A4** supports this interpretation that the electron density on LUMO of bpy ligand makes an interaction by being dispersed to the LUMO of ammonium. This delocalization allows **B3** to be transformed to **A4** stabilizing the reduced active site with ~6 kcal/mol.

### Details Regarding Scheme S2

Calculation of the full set of catalytic paths from the **Mn<sup>I</sup>-HCOO<sup>-</sup>** complex (**A7**) to **Mn<sup>I</sup>-H** complex (**A5**) were fully covered in Scheme S2. Based on experimental results, the plain arrows are considered as expected reaction paths and the dashed arrows describe not preferred paths (Figure S20). The blue paths are associated with high overpotential, and the red paths with low overpotential. Note that the potential values of each steps were computationally reproduced within 150 mV error range showing similar tendency as the experimental results. Looking at the ΔΔG of 11.3 kcal/mol from **A7** to **A9**, it is evident that the liberation of formate from the manganese center needs a preceding reduction of **A7**. If not, the liberation requires a thermodynamic energy larger than 10 kcal/mol. This thermodynamic disadvantage,

however, would slow down the catalysis and the high performance of this system cannot be understood. The required reduction potential for going from **A7** to **A8** is around  $-2.04$  V, which is followed by liberation of formate along with a exergonic step with  $\sim 13$  kcal/mol to give **B1**. Contrarily **A7** could be reduced at the low overpotential of about  $-1.5$  V involving the simultaneous liberation of formate. But this event is slow due to the kinetic limitation of formate-liberation.

The protonation of the amine, coupled to the alkylcarbonate formation, from **B1** to **B3** is also possible with a barrier of  $17.8$  kcal/mol associated with **B2-TS**. This should be accessible at room temperature, even though it is  $\sim 3$  kcal/mol higher than the protonation from **A1** to **A3**. The **B3** intermediate would conduct an energetically favourable rearrangement to **B3'** of which the hydrogen of ammonium heads toward the manganese center. The **B3'** could easily undergo proton-coupled reduction at  $-1.31$  V offering an alternative path to **A4** and the Mn-hydride species **A5**. This alternative process explains one part of the experimentally observed early onset potential pathway in the cyclic voltammograms (Figure 3a) and is important for the catalytic low overpotential pathway.

A  $\text{CO}_2$ -involved protonation of **A7** is also possible. This will cause some changes to the electrochemical behaviour of  $[\text{Mn}^{\text{I}}-\text{HCOO}]^-$ . Our calculations show that the reduction of **A7-H<sup>+</sup>** requires  $100$  mV less negative potential than that of the non-protonated species ( $-1.95$  V,  $\text{A7-H}^+ \rightarrow \text{A9-H}^+$ ), which is in accordance with the positive shift in the cyclic voltammetry upon addition of TFE (Figure S20). This thermodynamic advantage by  $1.5$  kcal/mol originates from relieving the electrostatic repulsion between the formate and Mn-center by the structural rearrangement from **A8-H<sup>+</sup>** to **A9-H<sup>+</sup>**. This process is possible at the same time as the reduction, because the hydrogen bonding from the ammonium moiety assists the detachment of formate from the Mn center making the decoordination of formate kinetically achievable. **A9-H<sup>+</sup>** would be reduced at  $-2.02$  V to give **A10-H<sup>+</sup>**, or else, could fall into an intramolecular proton transfer pathway via the **B3'** intermediate. The protonated formate complex, **A7-H<sup>+</sup>**, is also reduced under low overpotential at  $-1.60$  V accompanying the intramolecular rearrangement of the ammonium-formate moiety to be **A9-H<sup>+(b)</sup>**. Interestingly, the rotational barrier is just  $\sim 7$  kcal/mol. Computationally, the possibility for obtaining formic acid as the product is predicted as well where the process is undertaken via proton transfer from ammonium to formate with liberation of formic acid (**A9-H<sup>+(b)</sup>**  $\rightarrow$  **B1**). The **A9-H<sup>+(b)</sup>** intermediate could be reduced when applying a potential over  $-1.87$  V (forming **A10-H<sup>+(b)</sup>**). The formate-liberation is also probable, but going through an endergonic path with  $\sim 5$  kcal/mol.

#### Details Regarding Scheme S3

As described in Scheme S3, the required potential to reduce  $\text{Mn}^{\text{I}}-\text{H}$  is not that high with  $-2.21$  V vs  $\text{Fc}^+/\text{Fc}$  (calc.). This amount of required overpotential originates from the non-innocent ligand feature of the bipyridine ligand. The additionally reduced  $[\text{Mn}^{\text{I}}-\text{H}]^-$  species makes a thermodynamic driving force for formate production. Comparing with the  $\text{CO}_2$  insertion at **A5** and **A5(red)**, the step barrier of this process is similar with  $12.3$  and  $11.4$  kcal/mol. However, with the simultaneous liberation of formate, **A5(red)** goes through exergonic formate formation with  $-27.8$  kcal/mol. On the contrary, the  $\text{CO}_2$  insertion to **A5** results in the endergonic reaction step with  $7.0$  kcal/mol without liberation. We estimated the increased reactivity by modelling the hydricity referring the parameterization (eq S9).<sup>S31</sup>

$$\Delta G^*_{\text{H}-} = 1.0752 \cdot \{G^*(\text{A}) - G^*(\text{AH}^-)\} - 443.7586 \text{ kcal/mol} \quad (\text{S9})$$

The asterisk symbol is denoted for the standard state of one mole per liter in solution distinguishing from one atmosphere of pressure in the gas phase. Calculations based on the least-squares linear fit (eq S9) approximated the hydricity of  $[\text{Mn}^{\text{I}}-\text{H}]^-$  species to be  $\sim 14.1$  kcal/mol which is enhanced by a factor of

three in comparison to the hydricity of the **Mn<sup>I</sup>-H** species (48.4 kcal/mol). This magnitude is comparable with the hypothetical hydride-accepted acetone species ( $\text{CH}_3\text{C}(\text{O})\text{HCH}_3^-$ ).<sup>531</sup> This result could give a plausible explanation for the enhanced TOF for the high overpotential pathway.

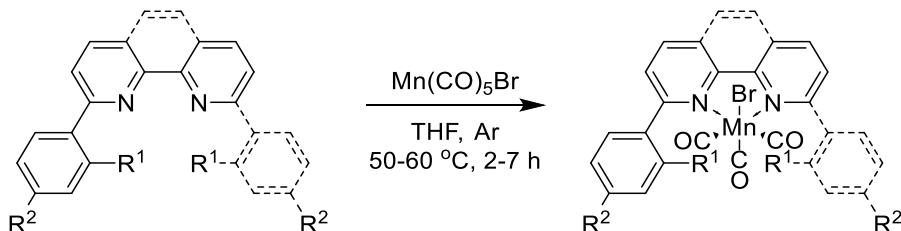
#### Calculated IR Stretches

Quantitatively matching vibrational frequencies using DFT calculations is challenging. The calculated CO stretching frequencies of the Mn-H species **A5** were calculated to be 1992, 1929, and 1928  $\text{cm}^{-1}$  that are notably red-shifted when compared to what is calculated for the Mn-Br complex (2024, 1971, and 1955  $\text{cm}^{-1}$ ). These values are in reasonable, but not perfect, agreement with the experimentally observed signals at 1984 and 1884  $\text{cm}^{-1}$ .

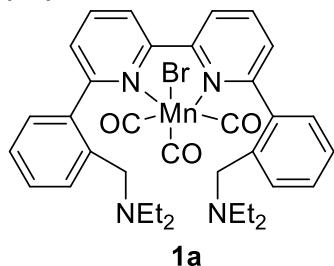
## 5. SYNTHESIS OF STARTING MATERIALS

### 5.1 Synthesis of Manganese Complexes

All the complexes were synthesized with a modified procedure adapted from Sampson and co-workers according to the general scheme below.<sup>532</sup> All complexes were shielded from light at all time and only handled in an argon filled glovebox or under inert atmosphere.



#### **Mn(*N,N'*-([2,2'-Bipyridine]-6,6'-diylbis(2,1-phenylene))bis(methylene))diethanamine)(CO)<sub>3</sub>Br (1a)**

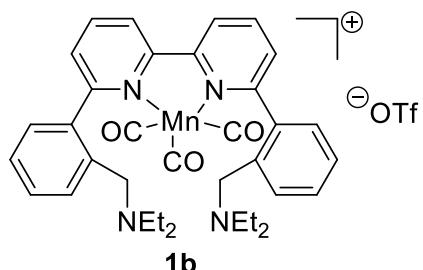


Compound **bpy**<sup>1</sup> (82 mg, 0.18 mmol, 1.0 equiv.) and Mn(CO)<sub>5</sub>Br (49 mg, 0.18 mmol, 1.0 equiv.) were dissolved in THF (1.0 mL) in a glovebox. The solution was heated to 55 °C and stirred for 2 h in an open 20 mL two-chamber system (COWARE) in amber glass. The solution was then concentrated to approximately 0.5 mL *in vacuo* and the complex was crystallized by vapor diffusion of pentane overnight. The product was collected by filtration and washed with pentane (3 x 5 mL), to give the title compound as a mixture of a yellow powder (105 mg, 85%).

**<sup>1</sup>H NMR** (400 MHz, CD<sub>3</sub>CN) ( $\delta$ ) ppm: 8.40 (d,  $J$  = 8.1 Hz, 2H)\*, 8.05 (t,  $J$  = 7.9 Hz, 2H)\*, 7.65 – 7.30 (m, 10H), 3.68 – 3.36 (m, 4H), 2.59 – 2.21 (m, 8H), 0.93 (t,  $J$  = 7.2 Hz 12H)\*. **<sup>13</sup>C NMR** (101 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  (ppm): 162.2 (2C), 157.1 (2C), 141.2 (2C), 138.5 (2C), 137.8 (2C), 129.6 (2C), 129.3 (2C), 129.1 (2C), 128.5 (2C), 125.6 (2C), 122.6 (2C), 55.2 (2C), 48.4 (4C), 12.9 (4C). **HRMS** (ESI<sup>+</sup>)  $m/z$  calcd. for C<sub>35</sub>H<sub>39</sub>BrMnN<sub>4</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 697.1581, found: 697.1590 (mSigma=11.5). **IR** (ATR, cm<sup>-1</sup>)  $\tilde{\nu}$  3058, 2968, 2793, 2011, 1920, 1901, 1606, 1567, 1447, 1385, 1225, 1203, 1167, 1059, 765, 625.

\*1–3 additional minor peaks with the exact same splitting was observed next to or underneath those peaks presumably due to rotamers.

#### **Mn(*N,N'*-([2,2'-Bipyridine]-6,6'-diylbis(2,1-phenylene))bis(methylene))diethanamine)(CO)<sub>3</sub>OTf (1b)**

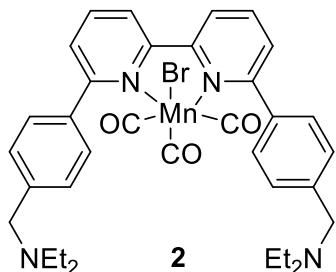


In an argon-filled glovebox, a 10 mL amber tube was charged with a magnetic stir bar, **12** (100 mg, 0.29 mmol, 1.0 equiv.), **bpy**<sup>1</sup> (139 mg, 0.29 mmol, 1.0 equiv.) and THF (1.5 mL) in a glovebox. The mixture was stirred at 55 °C for 3 h and was transferred to a 50 mL round bottom flask. The solvent was evaporated *in vacuo* to yield the product as a red oil. Et<sub>2</sub>O (2 mL) was added and was then evaporated, this was repeated three times to yield the product as a yellow solid (208 mg, 93%).

**<sup>1</sup>H NMR** (400 MHz, CD<sub>3</sub>CN) δ (ppm): 8.51 (d, *J* = 8.4 Hz, 2H)\*, 8.19 (t, *J* = 7.9 Hz, 2H)\*, 7.74 – 7.26 (m, 10H), 3.47 – 3.29 (m, 4H), 2.56 – 2.26 (m, 8H), 0.90 (t, *J* = 7.1 Hz, 12H)\*. **<sup>19</sup>F NMR** (376 MHz, CD<sub>3</sub>CN) δ (ppm): -78.9 (s, 3F). **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>35</sub>H<sub>39</sub>MnN<sub>4</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 617.2319, found: 617.2320. **IR** (ATR, cm<sup>-1</sup>)  $\tilde{\nu}$  2972, 2799, 2031, 1918, 1567, 1208, 1027, 762, 630.

\*1-3 additional minor peaks with the exact same splitting was observed next to or underneath those peaks presumably due to rotamers.

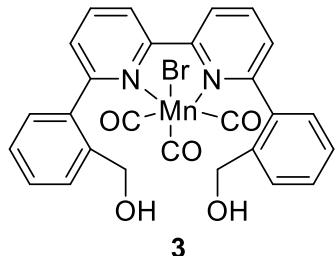
### Mn(*N,N'*-([2,2'-Bipyridine]-6,6'-diylbis(4,1-phenylene))bis(methylene))bis(*N*-ethylethanamine)(CO)<sub>3</sub>Br (2)



Compound **bpy**<sup>2</sup> (480 mg, 1.00 mmol, 1.0 equiv.) was added to a 8 mL vial followed by addition of THF (1 mL). A suspension of Mn(CO)<sub>5</sub>Br (275 mg, 1.00 mmol, 1.0 equiv.) in THF (2 mL) was added to the solution and an additional milliliter of THF was used to ensure complete transfer. The mixture was heated to 50 °C in an open vial in a glovebox and stirred in the dark. After 5 h the THF was removed by evaporation *in vacuo* and diethyl ether (4 mL) was added to the residue. The crude product was collected by filtration of the suspension and the solid was washed with diethyl ether to afford the pure product as a pale orange powder (260 mg, 37%).

**<sup>1</sup>H NMR** (400 MHz, CD<sub>3</sub>CN) δ (ppm): 8.41 (d, *J* = 7.9 Hz, 2H), 8.14 (t, *J* = 7.9 Hz, 2H), 7.63 – 7.49 (m, 10H), 3.66 (s, 4H), 2.53 (q, *J* = 6.0 Hz, 8H), 1.03 (t, *J* = 7.1 Hz, 12H). **<sup>13</sup>C NMR** (101 MHz, (CD<sub>3</sub>)<sub>2</sub>SO) δ (ppm): 164.4 (2C), 157.7 (2C), 141.5 (2C), 140.1 (2C), 139.1 (2C), 128.9 (8C), 127.1 (2C), 122.3 (2C), 62.4 (2C), 56.5 (4C), 11.6 (4C). **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>35</sub>H<sub>39</sub>BrMnN<sub>4</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 697.1581, found: 697.1488 (mSigma=34.4). **IR** (ATR, cm<sup>-1</sup>)  $\tilde{\nu}$  2967, 2871, 2014, 1928, 1902, 1563, 1455, 797, 627.

### Mn(*N,N'*-([2,2'-Bipyridine]-6,6'-diylbis(2,1-phenylene))dimethanol)(CO)<sub>3</sub>Br (3)

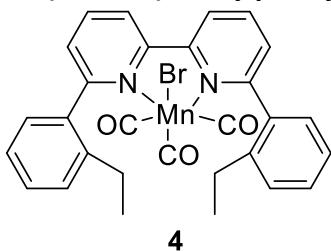


Compound **bpy**<sup>4</sup> (184 mg, 0.5 mmol, 1.0 equiv.) was suspended in THF (7 mL) in a 25 mL round bottomed flask in amber glass and heated to 55 °C. After solvation of the ligand, Mn(CO)<sub>5</sub>Br (137 mg, 0.5 mmol, 1.0 equiv.) dissolved in THF (3 mL) was added to the flask and the mixture was stirred for 3 h in an open flask in a glovebox at 55 °C. The solution was cooled to room temperature and filtered through a plug of celite aided by THF (1 mL). The complex was then crashed out by addition of pentane (10 mL) and cooling to -40 °C. The product was collected by suction filtration and washed with pentane (3 x 5 mL), to give the title compound as a yellow powder (228 mg, 77%).

**<sup>1</sup>H NMR** (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO) δ (ppm): 8.73 (d, *J* = 7.8 Hz, 2H)\*, 8.23 (t, *J* = 7.8 Hz, 2H)\*, 7.63 (t, *J* = 8.0 Hz, 4H)\*, 7.52 (t, *J* = 7.2 Hz, 2H)\*, 7.39 (t, *J* = 7.5 Hz, 2H)\*, 7.30 (d, *J* = 7.7 Hz, 2H)\*, 5.23 (t, *J* = 5.1 Hz, 2H)\*, 4.46 (d, *J* = 5.1 Hz, 4H)\*. **<sup>13</sup>C NMR** (101 MHz, (CD<sub>3</sub>)<sub>2</sub>SO) δ (ppm): 162.6 (2C)\*, 157.5 (2C)\*, 140.4 (2C)\*, 139.5 (2C)\*, 138.4 (2C)\*, 129.8 (2C)\*, 129.1 (2C)\*, 127.9 (2C)\*, 127.6 (2C)\*, 126.2 (2C)\*, 122.6 (2C)\*, 60.9 (2C)\*. **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>27</sub>H<sub>21</sub>MnN<sub>2</sub>O<sub>5</sub> [M+H]<sup>+</sup>: 507.0753; found: 507.0764. (Only the complex where bromide is already dissociated was observed in HRMS). **IR** (ATR, cm<sup>-1</sup>)  $\tilde{\nu}$  3468, 3077, 2930, 2873, 2022, 1916, 1567, 1450, 1224, 1015, 809, 764, 627.

\*1–3 additional minor peaks with the exact same splitting was observed next to or underneath those peaks presumably due to rotamers.

### Mn(6,6'-Bis(2-ethylphenyl)-2,2'-Bipyridine)(CO)<sub>3</sub>Br (4)



4

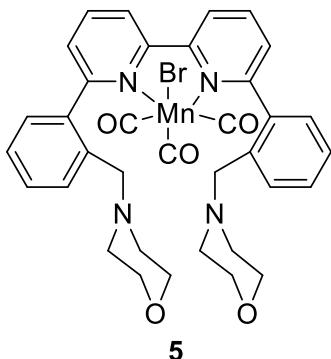
Compound **bpy**<sup>5</sup> (200 mg, 0.55 mmol, 1.0 equiv.) was added to an 8 mL vial followed by THF (2 mL). A suspension of Mn(CO)<sub>5</sub>Br (150 mg, 0.55 mmol, 1.0 equiv.) in THF (2 mL) was added to the solution and an additional milliliter of THF was used to achieve complete transfer. The mixture was heated to 50 °C in an open vial inside a glovebox and stirred in the dark. After 7 h the solution was allowed to cool and pentane (4 mL) was added.

The suspension was cooled to –30 °C for 12 h after which the crude product was collected by filtration and the solid was washed with diethyl ether to afford the pure product as a red crystalline powder (223 mg, 70%).

**<sup>1</sup>H NMR** (400 MHz, (CD<sub>3</sub>)<sub>2</sub>CO) δ (ppm): 8.64 (d, *J* = 8.1 Hz, 2H)\*, 8.21 (t, *J* = 7.9 Hz, 2H)\*, 7.61 – 7.27 (m, 10H), 2.80 – 2.40 (m, 4H), 1.26 (t, *J* = 7.6 Hz, 6H)\*. **<sup>13</sup>C NMR** (101 MHz, (CD<sub>3</sub>)<sub>2</sub>SO) δ (ppm): 163.5 (2C)\*, 157.7 (2C)\*, 141.7 (2C)\*, 140.9 (2C)\*, 138.4 (2C)\*, 129.9 (2C)\*, 129.4 (2C)\*, 128.5 (2C)\*, 127.7 (2C)\*, 125.3 (2C)\*, 122.1 (2C)\*, 25.7 (2C)\*, 14.1 (2C)\*. **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>29</sub>H<sub>25</sub>MnN<sub>2</sub>O<sub>3</sub>[M+H]<sup>+</sup>: 503.1162; found: 503.1171. (Only the debrominated complex could be observed in HRMS.) **IR** (ATR, cm<sup>–1</sup>)  $\tilde{\nu}$  3068, 2953, 2868, 2023, 1936, 1904, 1608, 1569, 1458, 1371, 1224, 802, 759, 622.

\*1–3 additional minor peaks with the exact same splitting was observed next to or underneath those peaks presumably due to rotamers.

### Mn(6,6'-Bis(2-(morpholinomethyl)phenyl)-2,2'-bipyridine)(CO)<sub>3</sub>Br (5)



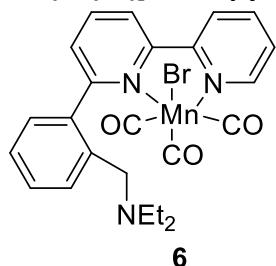
5

Compound **bpy**<sup>6</sup> (121 mg, 0.24 mmol, 1.0 equiv.) and Mn(CO)<sub>5</sub>Br (65 mg, 0.24 mmol, 1.0 equiv.) were dissolved in THF (4 mL) inside a glovebox. The solution was heated to 60 °C and stirred for 3 h in a closed 20 mL two-chamber system (COWare) in amber glass. After the reaction, impurities in the solution were crashed out by a slow vapor diffusion of pentane in at –30 °C overnight. The solution was collected and concentrated to approximately 0.5 mL and after vapor diffusion of pentane the product was collected by suction filtration and washed with pentane (3 x 5 mL), to give the title compound as a yellow powder (28 mg, 16%).

**<sup>1</sup>H NMR** (400 MHz, CD<sub>3</sub>CN) δ (ppm): 8.41 (d, *J* = 8.1 Hz, 2H)\*, 8.07 (t, *J* = 7.9 Hz, 2H)\*, 7.65 (d, *J* = 7.7 Hz, 2H)\*, 7.57 – 7.46 (m, 4H), 7.40 (d, *J* = 4.1 Hz, 4H)\*, 3.73 – 3.23 (m, 12H), 2.50 – 2.25 (m, 8H). **<sup>13</sup>C NMR** (101 MHz, (CD<sub>3</sub>)<sub>2</sub>SO) δ (ppm): 162.4 (2C)\*, 157.0 (2C)\*, 141.4 (2C)\*, 137.7 (2C)\*, 136.5 (2C)\*, 129.6 (2C)\*, 129.5 (2C)\*, 129.1 (2C)\*, 128.6 (2C)\*, 126.4 (2C)\*, 122.6 (2C)\*, 66.1 (4C)\*, 60.4 (2C)\*, 53.0 (4C)\*. **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>35</sub>H<sub>35</sub>BrMnN<sub>4</sub>O<sub>5</sub> [M+H]<sup>+</sup>: 725.1166; found: 725.1169 (*mSigma* = 13.5). **IR** (ATR, cm<sup>–1</sup>)  $\tilde{\nu}$  3066, 2965, 2810, 2017, 1935, 1902, 1565, 1429, 1112, 1006, 864, 812, 767, 632.

\*1–3 additional minor peaks with the exact same splitting was observed next to or underneath those peaks presumably due to rotamers.

**Mn(*N*-(2-([2,2'-Bipyridin]-6-yl)benzyl)-*N*-ethylethanamine)(CO)<sub>3</sub>Br (6)**



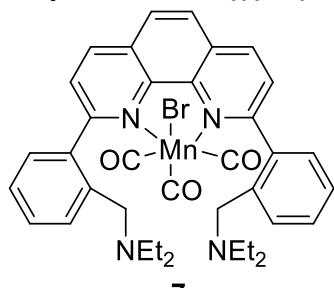
6

Compound **bpy**<sup>6</sup> (317 mg, 1.0 mmol, 1.0 equiv.) and Mn(CO)<sub>5</sub>Br (274 mg, 1.0 mmol, 1.0 equiv.) were dissolved in THF (3 mL). The solution was heated to 55 °C and stirred for 3 h in an open 20 mL two-chamber system (COWare) in amber glass inside a glovebox. The solution was concentrated to approximately 1.5 mL and the complex was crashed out by addition of pentane (5 mL). The product was collected by suction filtration and washed with pentane (3 x 5 mL), to give the title compound as a yellow powder (402 mg, 75%).

**<sup>1</sup>H NMR** (400 MHz, (CD<sub>3</sub>)<sub>2</sub>CO) δ (ppm): 9.29 (d, *J* = 5.4 Hz, 1H), 8.60 (dd, *J* = 8.4, 7.8 Hz, 2H), 8.25 – 8.15 (m, 2H)\*, 7.75 – 7.35 (m, 6H), 3.8 – 3.45 (m, 2H), 2.60 – 2.28 (m, 4H), 0.94 (t, *J* = 7.0 Hz 6H)\*. **<sup>13</sup>C NMR** (101 MHz, (CD<sub>3</sub>)<sub>2</sub>SO) δ (ppm): 162.9 (1C)\*, 156.6 (1C)\*, 155.5 (1C)\*, 153.0 (1C)\*, 141.6 (1C)\*, 139.2 (1C)\*, 138.4 (1C)\*, 137.9 (1C)\*, 129.7 (1C)\*, 129.3 (1C)\*, 129.2 (1C)\*, 128.8 (1C)\*, 126.3 (1C)\*, 126.2 (1C)\*, 123.7 (1C)\*, 122.2 (1C)\*, 55.3 (1C)\*, 46.4 (2C)\*, 11.8 (2C)\*. **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>24</sub>H<sub>24</sub>BrMnN<sub>3</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 536.0376; found: 536.0390 (mSigma=22.7). **IR** (ATR, cm<sup>-1</sup>) ̅ 3043, 2971, 2817, 2024, 1935, 1896, 1605, 1451, 1167, 779, 764, 624

\*1 additional set of minor peaks with the exact same splitting was observed next to this peak presumably due to rotamers.

**Mn(*N,N'*-((1,10-Phenanthroline-2,9-diyl)bis(2,1-phenylene))bis(methylene))bis(*N*-ethylethanamine)(CO)<sub>3</sub>Br (7)**



7

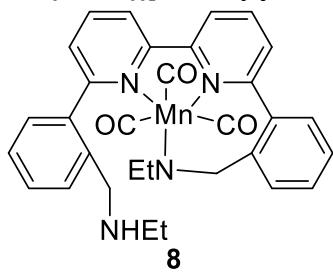
A solution of compound **bpy**<sup>7</sup> (306 mg, 0.61 mmol, 1.0 equiv.) in THF (2 mL) was added to an 8 mL vial. A suspension of Mn(CO)<sub>5</sub>Br (167 mg, 0.61 mmol, 1.0 equiv.) in THF (1 mL) was added to the solution and an additional milliliter of THF was used to achieve complete transfer. The mixture was heated to 50 °C in an open vial inside a glovebox and stirred in the dark. After 5 h the THF was removed by evaporation *in vacuo* and to the residue was added diethyl ether (4 mL) followed by pentane (3 mL). The clear solution was separated from the precipitated dark impurities and left to crystallize at –30 °C overnight. The liquid was then removed with a pipette and the remaining solid was washed with diethyl ether (2 mL) and dried *in vacuo* to yield the pure complex as a brown powder (146 mg, 33%).

**<sup>1</sup>H NMR** (400 MHz, (CD<sub>3</sub>)<sub>2</sub>CO) δ (ppm): 8.73 (d, *J* = 8.3 Hz, 2H)\*, 8.26 (s, 2H)\*, 8.01 (d, *J* = 8.4 Hz, 2H)\*, 7.72 (d, *J* = 7.9 Hz, 2H)\*, 7.58 – 7.36 (m, 6H), 3.84 – 3.43 (m, 4H), 2.61 – 2.23 (m, 8H), 0.92 (t, *J* = 7.1 Hz, 12H)\*.

**<sup>13</sup>C NMR** (101 MHz, (CD<sub>3</sub>)<sub>2</sub>CO) δ (ppm): 165.5 (2C)\*, 148.9 (2C)\*, 143.1 (2C)\*, 140.1 (2C)\*, 137.2 (2C)\*, 130.8 (2C)\*, 130.7 (2C)\*, 130.6 (2C)\*, 130.5 (2C)\*, 129.0 (2C)\*, 127.9 (2C)\*, 127.2 (2C)\*, 57.1 (2C)\*, 47.6 (4C)\*, 12.4 (4C)\*. **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>37</sub>H<sub>39</sub>BrMnN<sub>4</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 721.1581, found: 721.1606 (mSigma = 22.9). **IR** (ATR, cm<sup>-1</sup>) ̅ 2966, 2803, 2014, 1935, 1897, 1589, 1483, 1384, 1201, 1163, 861, 773, 627.

\*1–3 additional minor peaks with the exact same splitting was observed next to or underneath those peaks presumably due to rotamers

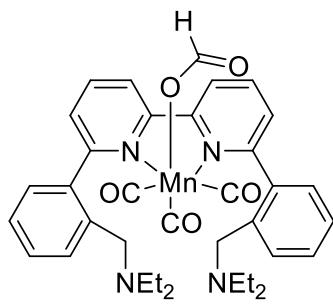
**Mn(*N,N'*-(([2,2'-Bipyridine]-6,6'-diyl)bis(2,1-phenylene))bis(methylene)diethanamine)(CO)<sub>3</sub> (8)**



which was evaporated *in vacuo* to give the title compound as a yellow powder (169 mg, 75%).

**<sup>1</sup>H NMR** (400 MHz, CD<sub>3</sub>CN) δ (ppm): 8.57–8.49 (m, 2H), 8.35 (t, *J* = 7.8 Hz, 1H), 8.22 (t, *J* = 7.7 Hz, 1H), 8.01–7.96 (m, 2H), 7.76 – 7.49 (m, 8H), 4.29 – 4.18 (m, 1H), 3.82 (d, *J* = 13.4 Hz, 1H), 3.70 – 3.60 (m, 2H), 3.18 – 2.90 (m, 3H), 2.52 – 2.46 (m, 2H), 1.49 (t, *J* = 6.9 Hz, 3H), 0.91 (t, *J* = 7.1 Hz, 3H). **<sup>13</sup>C NMR** (101 MHz, (CD<sub>3</sub>)<sub>2</sub>SO) δ (ppm): 164.7 (1C)\*, 162.6 (1C)\*, 156.4 (1C)\*, 155.8 (1C)\*, 141.5 (1C)\*, 141.3 (1C)\*, 141.2 (1C)\*, 139.8 (1C)\*, 139.8 (1C)\*, 136.3 (1C)\*, 133.1 (1C)\*, 131.4 (1C)\*, 130.8 (1C)\*, 130.1 (1C)\*, 129.9 (1C)\*, 129.8 (1C)\*, 129.7 (1C)\*, 129.1 (1C)\*, 128.8 (1C)\*, 126.8 (1C)\*, 123.3 (1C)\*, 121.8 (1C)\*, 51.0 (2C)\*, 48.5 (1C)\*, 47.6 (1C)\*, 43.8 (2C)\*, 15.2 (2C)\*, 14.0 (2C)\*. **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>31</sub>H<sub>30</sub>MnN<sub>4</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 561.1693, found: 561.1691. **IR** (ATR, cm<sup>-1</sup>)  $\tilde{\nu}$  3125, 3031, 2963, 2019, 1938, 1914, 1598, 1564, 1464, 1225, 1190, 1130, 1048, 816, 768.

**Mn(*N,N'*-(([2,2'-Bipyridine]-6,6'-diyl)bis(2,1-phenylene))bis(methylene)diethanamine)(CO)<sub>3</sub>O(CO)H (A7)**



**A7**

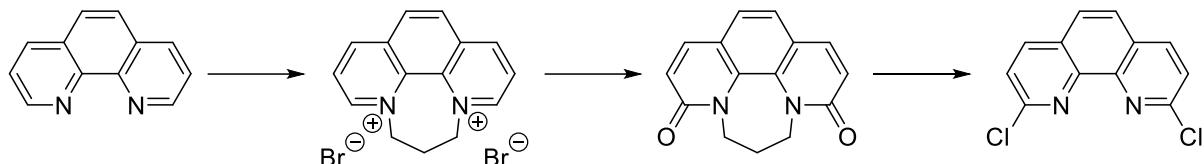
In an argon-filled glovebox, an amber 10 mL tube was charged with a magnetic stir bar, compound **1b** (80 mg, 0.10 mmol, 1.0 equiv.), and MeCN (2.5 mL). Tetrabutylammonium formate (30 mg, 0.10 mmol, 1.0 equiv.) was then added and the mixture was stirred at RT. After 72 hours the product had precipitated from the solution, and the reaction vessel was placed at –40 °C. After 24 hours, the product was collected by vacuum filtration and washed with pre-cooled pentane to yield the title compound as a yellow solid (26 mg, 38%).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 8.46 – 8.09 (m, 3H), 7.98 – 7.88 (m, 2H), 7.64 – 7.31 (m, 10H), 3.54 – 3.24 (m, 4H), 2.59 – 2.19 (m, 8H), 0.90 (t, *J* = 7.1 Hz, 12H)\*. **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm) 168.2\*, 164.4 (2C)\*, 157.5 (2C)\*, 141.2 (2C)\*, 138.8 (2C)\*, 136.6 (2C)\*, 130.7 (2C)\*, 129.9 (2C)\*, 129.9 (2C)\*, 128.6 (2C)\*, 126.6 (2C)\*, 121.3 (2C)\*, 55.7 (2C)\*, 46.7 (4C)\*, 11.9 (4C)\*. **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>36</sub>H<sub>40</sub>MnN<sub>4</sub>O<sub>5</sub> [M+H]<sup>+</sup>: 663.2374; found: 663.2379. **IR** (ATR, cm<sup>-1</sup>)  $\tilde{\nu}$  2958, 2809, 2016, 1934, 1898, 1610, 1567, 1470, 1307, 1222, 813, 769.

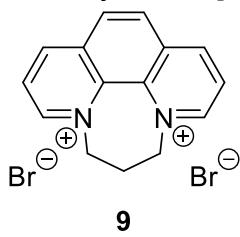
\*1–3 additional minor peaks with the exact same splitting was observed next to or underneath those peaks presumably due to rotamers.

## 5.2 Synthesis of 2,9-Dichloro-1,10-phenanthroline

2,9-Dichloro-1,10-phenanthroline was synthesized using a modified procedure of previously reported methods.<sup>S33, S34</sup> All spectroscopic data was in agreement with literature values.



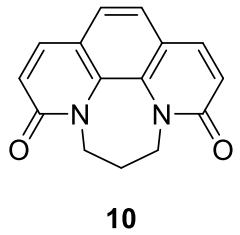
### 6,7-Dihydro-5*H*-[1,4]diazepino[1,2,3,4-*lmn*][1,10]phenanthroline-4,8-dium dibromide (9)



1,10-Phenanthroline (10 g, 55.5 mmol, 1.0 equiv.) was dissolved in chlorobenzene (80 mL) in a round-bottom flask equipped with a magnetic stir bar and the mixture was heated to 90°C. 1,3-Dibromopropane (11 mL, 107 mmol, 1.9 equiv.) was added to the clear solution dropwise over one hour, and the mixture was left to stir for 20 h. The crude product precipitated as a yellow solid which was collected by suction filtration, washed with CH<sub>2</sub>Cl<sub>2</sub> and dried *in vacuo* to yield the product as a yellow solid (19.7 g, 93%).

**<sup>1</sup>H NMR** (400 MHz, D<sub>2</sub>O) δ (ppm): 9.66 (d, *J* = 5.7 Hz, 2H), 9.45 (d, *J* = 8.4 Hz, 2H), 8.59 (d, *J* = 1.6 Hz, 2H), 8.54 (ddd, *J* = 7.8, 5.8, 1.6 Hz, 2H), 5.14 (t, *J* = 6.8 Hz, 4H), 3.42 (p, *J* = 6.6 Hz, 2H). **<sup>13</sup>C NMR** (101 MHz, D<sub>2</sub>O) δ (ppm): 153.5 (2C), 150.0 (2C), 136.7 (2C), 136.1 (2C), 132.9 (2C), 129.9 (2C), 63.0 (2C), 33.5. **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for [C<sub>15</sub>H<sub>14</sub>N<sub>2</sub>]<sup>2+</sup>: 222.1146, found: 222.1149.

### 6,7-Dihydro-5*H*-[1,4]diazepino[1,2,3,4-*lmn*][1,10]phenanthroline-3,9-dione (10)

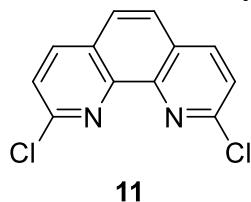


9 (18 g, 46 mmol, 1.0 equiv.) was suspended in *tert*-butanol (280 mL) in a round-bottom flask equipped with a magnetic stir bar and the mixture was heated to 40 °C. To this mixture was added potassium *tert*-butoxide (17.5 g, 156 mmol, 3.4 equiv.) and left to stir, open to air, at 40 °C overnight. Upon full conversion, the mixture was allowed to cool to room temperature and the solid was collected by suction filtration and washed with cold ethanol.\* The solid was taken up in chloroform, washed with water, and the chloroform layer was collected. The aqueous phase was extracted with chloroform and the combined organic layers were washed with brine, dried over magnesium sulfate, and concentrated *in vacuo* to give the product as a yellow solid (7.0 g, 59%).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 7.71 (d, *J* = 9.5 Hz, 2H), 7.36 (s, 2H), 6.80 (d, *J* = 9.5 Hz, 2H), 4.38 – 4.25 (m, 4H), 2.46 (p, *J* = 6.6 Hz, 2H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm): 162.8 (2C), 138.9 (2C), 132.3 (2C), 123.3 (2C), 123.0 (2C), 122.9 (2C), 45.9 (2C), 25.9. **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>15</sub>H<sub>13</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 253.0972, found: 253.0972.

\*The filtrate can be concentrated and taken up in water, then extracted with chloroform to give a less pure crop of product, which can be telescoped into the following chlorination (additionally 37%).

### 2,9-Dichloro-1,10-phenanthroline (11)

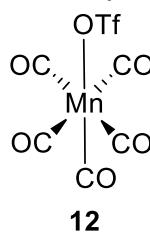


Compound **10** (6.50 g, 25.8 mmol, 1.0 equiv.) was mixed with phosphoryl chloride (78 mL, 834 mmol, 32.3 equiv.) in a round-bottom flask containing a magnetic stir bar. Phosphorus pentachloride (10.72 g, 51.5 mmol, 2.0 equiv.) was added, and the mixture was heated to reflux and left to stir overnight under an inert atmosphere. Upon full conversion, the phosphoryl chloride was distilled off and the residue was quenched with ice and basified to pH = 14 with 30% aqueous sodium hydroxide. The precipitate was filtered, washed copiously with water and then with diethyl ether (2 x 10 mL) to yield the chlorinated product as a yellow solid (5.1 g, 86%).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 8.20 (d, *J* = 8.4 Hz, 2H), 7.82 (s, 2H), 7.64 (d, *J* = 8.4 Hz, 2H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm): 152.2 (2C), 145.1 (2C), 138.9 (2C), 127.9 (2C), 126.4 (2C), 125.1 (2C). **HRMS (ESI<sup>+</sup>)** *m/z* calcd. for C<sub>12</sub>H<sub>7</sub>N<sub>2</sub>Cl<sub>2</sub> [M+H]<sup>+</sup>: 248.9981; found: 248.9987.

### 5.3 Synthesis of *Fac*-Mn(CO)<sub>5</sub>OTf

#### *Fac*-Mn(CO)<sub>5</sub>(OTf) (12)



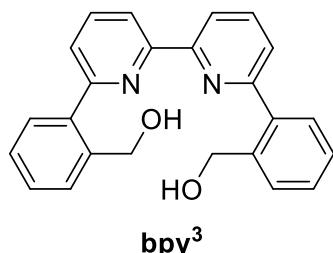
The title compound was synthesized according to a modified literature procedure. All spectroscopic data was in agreement with literature values.<sup>535</sup>

A 50 mL round bottom Schlenk flask equipped with a magnetic stir bar was charged with bromopentacarbonylmanganese(I) (400 mg, 1.46 mmol, 1.0 equiv.) and silver triflate (375 mg, 1.46 mmol, 1.0 equiv.) in an argon-filled glovebox. The flask was transferred out, attached to a Schlenk line and shielded from light. Hereafter, anhydrous dichloromethane (25 mL) was added via cannula and the reaction mixture was allowed to stir in the dark at room temperature. After 3 h, the reaction mixture was filtered through a cannula filter to remove the resulting AgBr precipitate. The filtrate was dried under vacuum, yielding the title compound as a yellow solid (335 mg, 89%).

**<sup>19</sup>F NMR** (376 MHz, CDCl<sub>3</sub>) δ (ppm): -76.3 (s, 3F). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm): 209.7, 202.4 (4C), 119.1 (q, *J* = 318.2 Hz). **IR (ATR, cm<sup>-1</sup>)**  $\tilde{\nu}$  2168, 2022, 1934, 1330, 1232, 1196, 1177, 1024.

### 5.4 Synthesis of Ligands

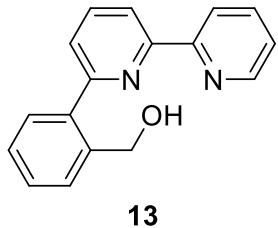
#### ([2,2'-Bipyridine]-6,6'-diylbis(2,1-phenylene))dimethanol (bpy<sup>3</sup>)



In an argon-filled glovebox, 6,6'-dibromo-2,2'-dipyridyl (1.6 g, 5.0 mmol, 1.0 equiv.), 2-(hydroxymethyl)phenylboronic acid (1.9 g, 12.5 mmol, 2.5 equiv.), Pd(PPh<sub>3</sub>)<sub>4</sub> (347 mg, 0.3 mmol, 6 mol%), and Na<sub>2</sub>CO<sub>3</sub> (2.7 g, 25 mmol, 5.0 equiv.) were added to a flame-dried flask followed by addition of a dioxane:H<sub>2</sub>O mixture (20:15 mL). The reaction mixture was sealed and removed from the glovebox and left to stir at 90 °C for 20 h under an atmosphere of argon. The reaction mixture was cooled and extracted with dichloromethane (3 x 50 mL). The combined organic layers were washed with brine (3 x 100 mL), dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated *in vacuo*. The light-green crude product was triturated in methanol to yield the title compound as a white solid (1.6 g, 85% yield).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 8.16 (dd, *J* = 7.9, 1.0 Hz, 2H), 7.99 (t, *J* = 7.9 Hz, 2H), 7.65 (dd, *J* = 7.8, 1.0 Hz, 2H), 7.60 – 7.52 (m, 4H), 7.50 – 7.42 (m, 4H), 5.85 (t, *J* = 6.9 Hz, 2H), 4.54 (d, *J* = 6.9 Hz, 4H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm): 159.7 (2C), 155.3 (2C), 140.3 (2C), 140.1 (2C), 139.0 (2C), 131.2 (2C), 130.5 (2C), 129.6 (2C), 128.4 (2C), 124.6 (2C), 120.7 (2C), 64.7 (2C). **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>24</sub>H<sub>21</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 369.1598; found: 369.1609.

### (2-([2,2'-Bipyridin]-6-yl)phenyl)methanol (13)

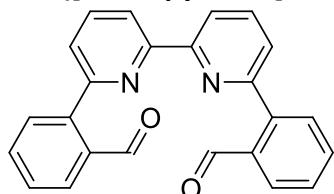


In an argon-filled glovebox, 6-bromo-2,2'-bipyridine (1.0 g, 4.3 mmol, 1.0 equiv.), 2-(hydroxymethyl)phenylboronic acid (807 mg, 5.3 mmol, 1.3 equiv.), Pd(PPh<sub>3</sub>)<sub>4</sub> (295 mg, 0.26 mmol, 6 mol%), and Na<sub>2</sub>CO<sub>3</sub> (1.1 g, 10.6 mmol, 2.5 equiv.) were added to a flame-dried flask followed by addition of a degassed dioxane:H<sub>2</sub>O mixture (17:14 mL). The reaction mixture was removed from the glovebox and left to stir at 90 °C for 20 h under an atmosphere of argon. The reaction mixture was cooled and extracted with dichloromethane (3 x 50 mL).

The combined organic layers were washed with brine (3 x 100 mL), dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated *in vacuo*. The deep-red crude product was purified by FC on silica gel eluting with 35% EtOAc in pentane to yield the title compound as a white solid (602 mg, 54% yield).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 8.73 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 8.33 (dd, *J* = 8.0, 1.0 Hz, 1H), 8.15 (dt, *J* = 8.3, 1.1 Hz, 1H), 7.99 (t, *J* = 7.9 Hz, 1H), 7.83 (td, *J* = 7.8, 1.8 Hz, 1H), 7.63 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.60 – 7.56 (m, 1H), 7.56 – 7.51 (m, 1H), 7.48 – 7.41 (m, 2H), 7.34 (ddd, *J* = 7.6, 4.8, 1.2 Hz, 1H), 6.02 (t, *J* = 7.0 Hz, 1H), 4.51 (d, *J* = 7.0 Hz, 2H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm): 159.3, 155.7, 155.6, 149.7, 140.4, 140.3, 138.5, 137.5, 131.1, 130.4, 129.4, 128.3, 124.2, 124.1, 121.3, 120.5, 64.8. **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>17</sub>H<sub>15</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 263.1179; found: 263.1188.

### **2,2'-(2,2'-Bipyridine]-6,6'-diyl)dibenzaldehyde (14a)**



**14a**

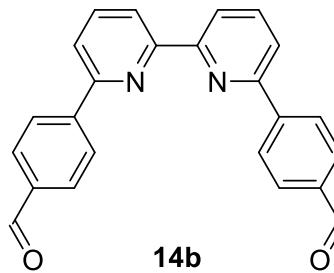
**Method 1:** **bpy**<sup>3</sup> (1.5 g, 4.0 mmol, 1.0 equiv.) was added to a flame-dried round bottom flask and dissolved in dry dichloromethane (50 mL). Dess-Martin periodinane (4.2 g, 10.0 mmol, 2.5 equiv.) was added and the mixture was stirred at RT. After 2 h, saturated aqueous NaHCO<sub>3</sub> solution (30 mL) was added and the reaction mixture was stirred for 15 min. The mixture was extracted with dichloromethane (3 x 30 mL) and the combined organic layers were washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated *in vacuo*. The crude-product was suspended in EtOAc and filtered to provide the pure product as a white solid (883 mg, 61% yield).

**Method 2:** 6,6'-Dibromo-2,2'-bipyridyl (1.0 g, 3.2 mmol, 1.0 equiv.) was added to a round bottom flask equipped with a magnetic stir bar and was dissolved in DME (104 mL). 2-Formylphenylboronic acid (1.2 g, 8.3 mmol, 2.6 equiv.), sodium carbonate (1.3 g, 12.0 mmol, 3.8 equiv.), and water (26 mL) was then added. The mixture was degassed by argon bubbling and tetrakis(triphenylphosphine)palladium(0) (184 mg, 0.16 mmol, 5 mol%) was added. The mixture was then heated to reflux over night under an argon atmosphere. The mixture was then cooled on an ice bath and the crude product was collected by suction filtration. The crude product was taken up in dichloromethane (1 L) and filtered over a celite pad to remove residue palladium. The filtrate was then evaporated to yield the pure product as a white crystalline solid (1.1 g, 96%).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 10.27 (s, 2H), 8.46 (dd, *J* = 7.9, 1.0 Hz, 2H), 8.03 (dd, *J* = 7.7, 1.4 Hz, 2H), 7.99 (t, *J* = 7.8 Hz, 2H), 7.77 (dd, *J* = 7.7, 1.1 Hz, 4H), 7.70 (td, *J* = 7.5, 1.4 Hz, 2H), 7.62 – 7.57 (m, 2H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm): 192.9 (2C), 155.5 (2C), 155.4 (2C), 142.9 (2C), 138.5 (2C), 136.0 (2C), 133.0 (2C), 129.7 (2C), 129.2 (2C), 128.4 (2C), 123.8 (2C), 120.2 (2C). **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>24</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 365.1285; found: 365.1289.

Additional note: The title compound seems to be very insoluble in most solvents, which complicates purification. If the Suzuki coupling is performed on a larger scale, soxhlet extraction with dichloromethane of the crude product is preferred.

### **4,4'-(2,2'-Bipyridine]-6,6'-diyl)dibenzaldehyde (14b)**



**14b**

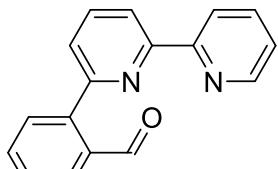
6,6'-Dibromo-2,2'-bipyridyl (1.00 g, 3.2 mmol, 1.0 equiv.) was added to a round bottom flask equipped with a magnetic stir bar and was dissolved in 1,2-dimethoxyethane (104 mL). 4-Formylphenylboronic acid (1.2 g, 8.3 mmol, 2.6 equiv.) was added followed by sodium carbonate (1.3 g, 12.0 mmol, 3.8 equiv) and water (26 mL). The mixture was degassed with argon and tetrakis(triphenylphosphine)palladium(0) (184 mg 0.16 mmol, 5 mol%) was added. The mixture was then stirred at reflux overnight under an atmosphere of argon. The mixture was then cooled on an ice bath and

the crude product was collected by filtration of the reaction mixture. The solid was washed with water and diethyl ether to yield the product as a white solid (1.1 g, 90%).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 10.12 (s, 2H), 8.68 (d, *J* = 7.8 Hz, 2H), 8.36 (d, *J* = 8.1 Hz, 4H), 8.05 (d, *J* = 8.2 Hz, 4H), 8.00 (t, *J* = 7.9 Hz, 2H), 7.90 (d, *J* = 7.8 Hz, 2H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm): 192.1 (2C), 156.1 (2C), 155.1 (2C), 145.0 (2C), 138.1 (2C), 136.7 (2C), 130.3 (4C), 127.7 (4C), 121.4 (2C), 120.8 (2C). **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>24</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 365.1285; found: 365.1290.

Additional note: The title compound seems to be very insoluble in most solvents, which complicates purification and characterization.

### 2-([2,2'-Bipyridin]-6-yl)benzaldehyde (14c)

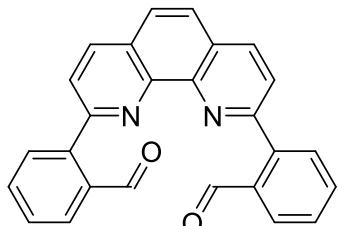


**14c**

**13** (475 mg, 1.81 mmol, 1.0 equiv.) was dissolved in dry dichloromethane (12 mL) in a flame dried round bottom flask. Dess-Martin periodinane (960 mg, 2.3 mmol, 1.2 equiv.) was added to this solution and the mixture was stirred at RT. After 3 h saturated aqueous NaHCO<sub>3</sub> solution (15 mL) was added and the reaction mixture was stirred for 15 min. The mixture was extracted with dichloromethane (3 x 15 mL), and the combined organic layers were washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated *in vacuo*. The crude product was purified by flash column chromatography on silica gel eluting with a gradient from 30% EtOAc in pentane to 40% EtOAc in pentane providing the product as a colorless solid (333 mg, 71% yield).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 10.25 (s, 1H), 8.69 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 8.50 (dd, *J* = 7.9, 1.0 Hz, 1H), 8.39 (dt, *J* = 8.0, 1.1 Hz, 1H), 8.02 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.98 (t, *J* = 7.8 Hz, 1H), 7.82 (td, *J* = 7.7, 1.8 Hz, 1H), 7.77 – 7.72 (m, 2H), 7.68 (td, *J* = 7.5, 1.4 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.32 (ddd, *J* = 7.5, 4.8, 1.2 Hz, 1H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm): 192.9, 156.0, 155.6, 155.5, 149.3, 143.0, 138.1, 137.3, 135.9, 133.0, 129.7, 129.1, 128.3, 124.2, 123.5, 121.5, 119.8. **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>17</sub>H<sub>13</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 261.1022; found: 261.1034.

### 2,2'-(1,10-Phenanthroline-2,9-diyl)dibenzaldehyde (14d)



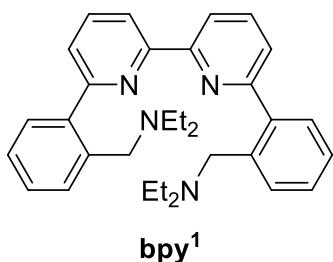
**14d**

**11** (930 mg, 3.7 mmol, 1.0 equiv.) was dissolved in DME (120 mL) in a round bottom flask equipped with a magnetic stir bar. 2-Formylphenylboronic acid (1.4 g, 9.6 mmol, 3.6 equiv.), sodium carbonate (1.5 g, 14.5 mmol, 3.9 equiv.), and water (30 mL) was added to the solution. The mixture was degassed with argon and tetrakis(triphenylphosphine)palladium(0) (224 mg, 0.2 mmol, 5 mol%) was added and the mixture was heated to reflux and stirred under an argon atmosphere. After 22 h, the mixture was cooled in an ice-bath and the precipitate was collected by suction filtration and

washed with diethyl ether to give the product as a white solid which was used directly in the following reaction. The spectral data was in accordance with the literature.<sup>536</sup>

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 10.43 (s, 2H), 8.41 (d, *J* = 8.3 Hz, 2H), 8.09 (d, *J* = 7.7 Hz, 2H), 7.98 (d, *J* = 8.3 Hz, 2H), 7.94 (d, *J* = 7.7 Hz, 2H), 7.93 (s, 2H), 7.74 (t, *J* = 7.5 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 2H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm): 192.6 (2C), 156.5 (2C), 146.1 (2C), 143.4 (2C), 136.8 (2C), 135.9 (2C), 133.3 (2C), 131.0 (2C), 129.3 (2C), 128.7 (2C), 127.9 (2C), 126.8 (2C), 124.0 (2C). **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>26</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 389.1285; found: 389.1295.

***N,N'-(*[(2,2'-Bipyridine]-6,6'-diyl*bis(2,1-phenylene))bis(methylene))bis(N-ethylethanamine)***  
**(bpy<sup>1</sup>)**



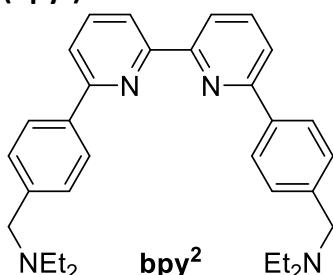
**Method 1:** To a solution of **14a** (600 mg, 1.7 mmol, 1.0 equiv.) in anhydrous 1,2-dichloroethane (6 mL), diethylamine (1.6 mL, 5.0 mmol, 3.0 equiv.), and acetic acid (236  $\mu$ L, 4.1 mmol, 2.8 equiv.) was added and mixed at RT for 15 min. The reaction mixture was then treated with sodium triacetoxyborohydride (1.1 g, 5.0 mmol, 3.0 equiv.) and the mixture was stirred at RT under an Ar atmosphere for 6 h. The reaction mixture was quenched by addition of cold aqueous saturated NaHCO<sub>3</sub>, and the product was extracted with EtOAc. The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>,

filtered, and concentrated *in vacuo*. The crude product was purified by FC on silica gel, eluting with a gradient from 5% EtOAc in pentane, containing 1% Et<sub>3</sub>N to 5% EtOAc in pentane, containing 10% Et<sub>3</sub>N to give the title compound as a colorless crystalline solid (459 mg, 58%).

**Method 2:** **14a** (1.1 g, 3.1 mmol, 1.0 equiv.) was suspended in 1,2-dichloroethane (15 mL) in a round bottom flask equipped with a magnetic stir bar. The mixture was degassed by bubbling argon through it and diethylamine (1.3 mL, 12.2 mmol, 4.0 equiv.) was added and the mixture was left to stir. After 5 min sodium triacetoxyborohydride (2.1 g, 9.8 mmol, 3.2 equiv.) was added and the mixture was left overnight at room temperature. Upon full conversion, determined from a homogeneous solution, water (10 mL) was added and the mixture was stirred for 1 h additionally. Then 30% sodium hydroxide solution (10 mL) was added and the mixture was diluted with water (20 mL) and extracted with dichloromethane (5 x 10 mL). The combined organic layers were then extracted with 4 M hydrochloric acid (4 x 10 mL) and the aqueous extracts were combined and basified with 30% sodium hydroxide to pH = 14. The amine was then extracted with dichloromethane (5 x 10 mL). The combined organic layers were dried over anhydrous sodium sulfate and concentrated *in vacuo* to afford the crude product which was recrystallized in ethanol to afford the pure product as a colorless solid (1.4 g, 93%).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 8.45 (dd, *J* = 7.9, 1.0 Hz, 2H), 7.84 (t, *J* = 7.8 Hz, 2H), 7.70 (dd, *J* = 7.5, 1.5 Hz, 2H), 7.49 (ddd, *J* = 6.8, 5.5, 1.4 Hz, 4H), 7.45 – 7.33 (m, 4H), 3.81 (s, 4H), 2.43 (q, *J* = 7.1 Hz, 8H), 0.89 (t, *J* = 7.1 Hz, 12H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 159.5 (2C), 155.5 (2C), 141.1 (2C), 138.8 (2C), 137.0 (2C), 130.1 (2C), 130.0 (2C), 128.2 (2C), 126.6 (2C), 124.3 (2C), 119.1 (2C), 55.2 (2C), 47.0 (4C), 12.0 (4C). **HRMS** (ESI<sup>+</sup>) *m/z* calcd. for C<sub>32</sub>H<sub>39</sub>N<sub>4</sub> [M+H]<sup>+</sup>: 479.3169; found: 479.3174.

***N,N'-(*[2,2'-Bipyridine]-6,6'-diyl*bis(4,1-phenylene))bis(methylene))bis(N-ethylethanamine)***  
**(bpy<sup>2</sup>)**



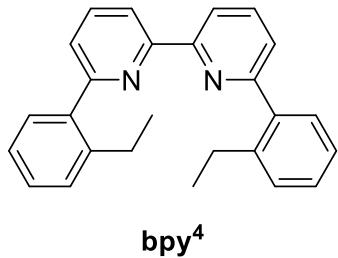
**14b** (1.0 g, 2.9 mmol, 1.0 equiv.) was suspended in 1,2-dichloroethane (15 mL) in a round bottom flask equipped with a magnetic stir bar. The suspension was degassed by bubbling argon through it for 5 min. Then diethylamine (1.2 mL, 11.6 mmol, 4.0 equiv.) was added and the mixture was left to stir for 5 min. Sodium triacetoxyborohydride (1.9 g, 9.2 mmol, 3.2 equiv.) was then added and the mixture was left to stir overnight at room temperature during which time the suspension became homogeneous. Then water (10 mL) was added and the mixture was left to stir for 10 min after which 30% sodium hydroxide in water (10 mL) was added and the mixture was diluted with water (20 mL) and extracted with dichloromethane (5 x 10 mL). The combined organic extracts were then extracted with 4 M hydrochloric acid (4 x 10 mL) after which the aqueous layers were combined and

filtered, and concentrated *in vacuo*. The crude product was purified by FC on silica gel, eluting with a gradient from 5% EtOAc in pentane, containing 1% Et<sub>3</sub>N to 5% EtOAc in pentane, containing 10% Et<sub>3</sub>N to give the title compound as a colorless crystalline solid (459 mg, 58%).

basified to pH = 14 with 30% sodium hydroxide. The combined aqueous mixture was then extracted with dichloromethane (5 x 10 mL). The combined organic layers were dried over anhydrous sodium sulfate and concentrated to give an oil which was added ethanol (10 mL) and the mixture was swirled in an ice bath for 10 min to crystallize the product. The crude product was collected by filtration, washed with cold ethanol and cold pentane to give the title compound as a colorless solid (967 mg, 71%).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 8.59 (d, J = 7.7 Hz, 2H), 8.12 (d, J = 8.2 Hz, 4H), 7.90 (t, J = 7.8 Hz, 2H), 7.78 (dd, J = 7.8, 1.0 Hz, 2H), 7.48 (d, J = 8.0 Hz, 4H), 3.65 (s, 4H), 2.57 (q, J = 7.1 Hz, 8H), 1.08 (t, J = 7.1 Hz, 12H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm): 156.5 (2C), 156.1 (2C), 141.2 (2C), 138.1 (2C), 137.7 (2C), 129.5 (4C), 126.9 (4C), 120.3 (2C), 119.5 (2C), 57.5 (2C), 47.0 (4C), 12.0 (4C). **HRMS** (ESI<sup>+</sup>) m/z calcd. for C<sub>32</sub>H<sub>39</sub>N<sub>4</sub> [M+H]<sup>+</sup>: 479.3169; found: 479.3185.

### 6,6'-Bis(2-ethylphenyl)-2,2'-bipyridine (**bpy**<sup>4</sup>)

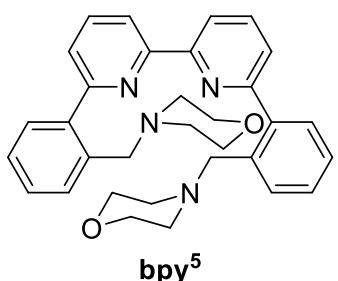


In an argon-filled glovebox to a flame-dried flask was added 6,6'-dibromo-2,2'-bipyridyl (628 mg, 2.0 mmol, 1.0 equiv.), (2-ethylphenyl)boronic acid (780 mg, 5.2 mmol, 2.6 equiv.), Pd(PPh<sub>3</sub>)<sub>4</sub> (139 mg, 0.12 mmol, 6 mol%), and Na<sub>2</sub>CO<sub>3</sub> (3.2 g, 30 mmol, 15.0 equiv.) followed by a toluene:ethanol:H<sub>2</sub>O mixture (14:3:14 mL). The reaction mixture was removed from the glovebox and left to stir at 85 °C for 17 h under an atmosphere of argon. The reaction mixture was allowed to cool to room temperature and NH<sub>4</sub>Cl (30 mL) was added and the mixture was extracted

with EtOAc (3 x 50 mL). The combined organic layers were washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated *in vacuo*. The light orange crude product was purified FC on silica gel, eluting with 2% EtOAc in pentane, containing 1 % Et<sub>3</sub>N to give the title compound as a colorless crystalline solid (658 mg, 90%).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 8.49 (dd, J = 7.9, 1.1 Hz, 2H), 7.86 (t, J = 7.8 Hz, 2H), 7.50 – 7.38 (m, 8H), 7.37 – 7.29 (m, 2H), 2.88 (q, J = 7.5 Hz, 4H), 1.22 (t, J = 7.5 Hz, 6H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm): 159.6 (2C), 155.7 (2C), 142.5 (2C), 140.4 (2C), 137.2 (2C), 130.1 (2C), 129.4 (2C), 128.6 (2C), 125.9 (2C), 124.2 (2C), 119.3 (2C), 26.4 (2C), 15.9 (2C). **HRMS** (ESI<sup>+</sup>) m/z calcd. for C<sub>26</sub>H<sub>25</sub>N<sub>2</sub> [M+H]<sup>+</sup>: 365.2012; found: 365.2036.

### 6,6'-Bis(2-(morpholinomethyl)phenyl)-2,2'-bipyridine (**bpy**<sup>5</sup>)

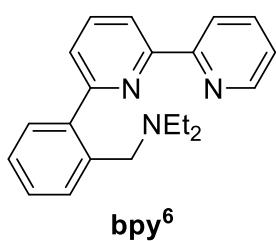


To a solution of **14a** (400 mg, 1.1 mmol, 1.0 equiv.) in anhydrous 1,2-dichloroethane (5.0 mL), morpholine (0.9 mL, 3.3 mmol, 3.0 equiv.) was added and mixed at RT for 15 min. The reaction mixture was then treated with sodium triacetoxyborohydride (653 mg, 3.1 mmol, 2.8 equiv.) and the mixture was stirred at RT under an Ar atmosphere for 3 h. The reaction mixture was quenched by addition of cold aqueous saturated NaHCO<sub>3</sub>, and the product was extracted with EtOAc (3 x 50 mL). The combined organic layers were dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated *in vacuo*. The

crude product was purified by FC eluting with EtOAc:Pentane (4:6), containing 1% Et<sub>3</sub>N. Following chromatography, the product was taken up in CHCl<sub>3</sub> and washed with 40% NaHSO<sub>3</sub>. The aqueous phase was extracted three times with CHCl<sub>3</sub> and the extracts were dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated *in vacuo* to give the title compound as an off-white solid (124 mg, 22% yield).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 8.46 (d, *J* = 7.8 Hz, 2H), 7.86 (t, *J* = 7.8 Hz, 2H), 7.60 – 7.51 (m, 6H), 7.44 – 7.38 (m, 4H), 3.76 (s, 4H), 3.55 (t, *J* = 4.6 Hz, 8H), 2.35 (t, *J* = 4.7 Hz, 8H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm): 159.4 (2C), 155.4 (2C), 141.3 (2C), 137.1 (2C), 136.2 (2C), 130.4 (2C), 130.2 (2C), 128.2 (2C), 127.3 (2C), 124.2 (2C), 119.0 (2C), 67.1 (4C), 60.6 (2C), 53.4 (4C). **HRMS (ESI<sup>+</sup>)** *m/z* calcd. for C<sub>32</sub>H<sub>35</sub>N<sub>4</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 507.2755; found: 507.2746.

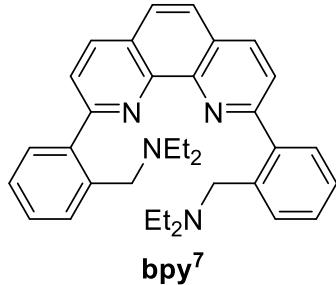
### ***N*-(2-([2,2'-Bipyridin]-6-yl)benzyl)-*N*-ethylethanamine (**bpy**<sup>6</sup>)**



To a solution of **14c** (350 mg, 1.3 mmol, 1.0 equiv.) in anhydrous 1,2-dichloroethane (7 mL), diethylamine (629 μL, 2.0 mmol, 1.5 equiv.) was added and mixed at RT for 15 min. The reaction mixture was then treated with sodium triacetoxyborohydride (426 mg, 2.0 mmol, 1.5 equiv.) and the mixture was stirred at RT under an Ar atmosphere for 4 h. The reaction mixture was quenched by addition of cold aqueous saturated NaHCO<sub>3</sub>, and the product was extracted with dichloromethane. The combined organic layers were dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated *in vacuo*. The crude product was purified by FC on silica gel, eluting with a gradient from 5% EtOAc in pentane, containing 1% Et<sub>3</sub>N to 10% EtOAc in pentane, containing 1% Et<sub>3</sub>N to give the title compound as a pale yellow solid (385 mg, 91%).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 8.69 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 8.48 (dt, *J* = 8.0, 1.1 Hz, 1H), 8.38 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.87 (t, *J* = 7.8 Hz, 1H), 7.79 (td, *J* = 7.8, 1.9 Hz, 1H), 7.67 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.51 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.46 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.40 (td, *J* = 7.5, 1.6 Hz, 1H), 7.34 (td, *J* = 7.6, 1.6 Hz, 1H), 7.30 (ddd, *J* = 7.5, 4.8, 1.2 Hz, 1H), 3.76 (s, 2H), 2.40 (q, *J* = 7.1 Hz, 4H), 0.86 (t, *J* = 7.1 Hz, 6H). **<sup>13</sup>C NMR** (101 MHz, CDCl<sub>3</sub>) δ (ppm): 159.6, 156.6, 155.2, 149.2, 141.0, 138.7, 137.1, 136.9, 130.1, 129.9, 128.3, 126.7, 124.5, 123.8, 121.4, 118.9, 55.2, 46.9 (2C), 12.0 (2C). **HRMS (ESI<sup>+</sup>)** *m/z* calcd. for C<sub>21</sub>H<sub>24</sub>N<sub>3</sub> [M+H]<sup>+</sup>: 318.1965; found: 318.1981.

### ***N,N'*-((1,10-Phenanthroline-2,9-diyl)bis(2,1-phenylene))bis(methylene))bis(*N*-ethylethanamine) (**bpy**<sup>7</sup>)**

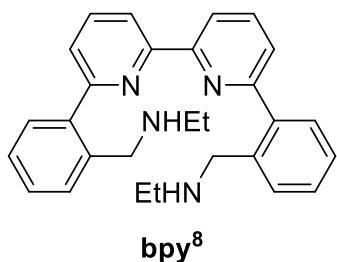


**14d** (1.75 g, 4.51 mmol, 1.0 equiv.) was added to a round bottom flask equipped with a magnetic stir bar followed by addition of 1,2-dichloroethane (20 mL). Argon was bubbled through the mixture for 5 min. Then diethylamine (2 mL, 19.3 mmol, 4.3 equiv.) was added and the mixture was stirred for 5 min, after which sodium triacetoxyborohydride (3.1 g, 14.4 mmol, 3.2 equiv.) was added slowly and the slurry was left to stir under an argon atmosphere. After 24 h, water (10 mL) was added and the mixture was left to stir for 10 min. Then 30% sodium hydroxide solution (10 mL) was added and the mixture was extracted with dichloromethane (5 x 10 mL). The combined organic layers were then extracted with 4 M HCl (3 x 20 mL) and the combined extracts were basified to pH = 14 by addition of 30% NaOH, and the mixture was extracted with dichloromethane (5 x 10 mL). The combined organic layers were dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated *in vacuo* to give the crude product as an oil which was added ethanol (10 mL) and the mixture was swirled. From this mixture the product slowly crystallized. After 10 min the mixture was cooled on ice and the crystals were collected by suction filtration, washed with cold ethanol followed by pentane to yield the title compound as a colorless solid (1.5 g, 66%).

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>) δ (ppm): 8.28 (d, *J* = 8.3 Hz, 2H), 7.89 (d, *J* = 8.2 Hz, 2H), 7.83 (s, 2H), 7.67 (d, *J* = 7.5 Hz, 2H), 7.59 (d, *J* = 7.3 Hz, 2H), 7.37 (t, *J* = 7.7 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 2H), 3.94 (s, 4H), 2.39 (q, *J* =

7.1 Hz, 8H), 0.80 (t,  $J$  = 7.1 Hz, 12H).  **$^{13}\text{C}$  NMR** (101 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 160.3 (2C), 145.9 (2C), 141.4 (2C), 139.4 (2C), 135.9 (2C), 130.7 (2C), 130.1 (2C), 128.2 (2C), 127.3 (2C), 126.5 (2C), 126.1 (2C), 124.3 (2C), 55.7 (2C), 46.9 (4C), 12.0 (4C). **HRMS (ESI $^+$ )**  $m/z$  calcd. for  $\text{C}_{34}\text{H}_{39}\text{N}_4$  [ $\text{M}+\text{H}]^+$ : 503.3169; found: 503.3190.

***N,N'*-((2,2'-Bipyridine)-6,6'-diylbis(2,1-phenylene))bis(methylene)diethanamine (bpy<sup>8</sup>)**



Compound **14a** (3.0 g, 8.2 mmol, 1.0 equiv.) was suspended in 1,2-dichloroethane (40 mL) in a round bottom flask equipped with a magnetic stir bar. The mixture was degassed by bubbling argon through it and ethylamine (2.0 M in THF, 13.2 mL, 26.4 mmol, 3.2 equiv.) was added followed by sodium triacetoxyborohydride (5.6 g, 26.3 mmol, 3.2 equiv.) and the mixture was degassed again by bubbling argon through it, where after the mixture was left to stir overnight at room temperature. Upon full conversion, determined by  $^1\text{H}$  NMR, water (10 mL) was added and the

mixture was stirred for 5 min additionally. Then 30% sodium hydroxide solution (20 mL) was added and the organic layer was collected. Then the aqueous phase was extracted with dichloromethane ( $5 \times 10$  mL). The combined organic layers were then extracted with 4 M hydrochloric acid ( $3 \times 20$  mL) and the aqueous extracts were combined and basified with 30% sodium hydroxide to pH = 14. Then the amine was extracted with dichloromethane ( $5 \times 20$  mL). The combined organic layers were dried over anhydrous sodium sulfate and concentrated *in vacuo* to afford the crude product as an oil. The crude product was dissolved in  $\text{Et}_2\text{O}$  to which pentane was added to precipitate a yellow sticky impurity. The clear solution was decanted into a round bottom flask and evaporated *in vacuo*. The resulting oil was crystallized by addition of  $\text{Et}_2\text{O}$  followed by pentane and the mixture was boiled, where after the mixture was cooled on ice. The resulting solid product was collected by vacuum filtration to afford the title compound as a colorless solid (2.4 g, 69%).

**$^1\text{H}$  NMR** (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 8.37 (dd,  $J$  = 7.9, 1.0 Hz, 2H), 7.89 (t,  $J$  = 7.8 Hz, 2H), 7.55 – 7.48 (m, 6H), 7.45 – 7.36 (m, 4H), 3.80 (s, 4H), 2.56 (q,  $J$  = 7.2 Hz, 4H), 2.04 (bs, 2H), 1.02 (t,  $J$  = 7.1 Hz, 6H).  **$^{13}\text{C}$  NMR** (101 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 159.5 (2C), 155.6 (2C), 140.8 (2C), 138.8 (2C), 137.6 (2C), 130.7 (2C), 130.1 (2C), 128.7 (2C), 127.2 (2C), 124.3 (2C), 119.6 (2C), 52.3 (2C), 43.7 (2C), 15.4 (2C). **HRMS (ESI $^+$ )**  $m/z$  calcd. for  $\text{C}_{28}\text{H}_{31}\text{N}_4$  [ $\text{M}+\text{H}]^+$ : 423.2543; found: 423.2560.

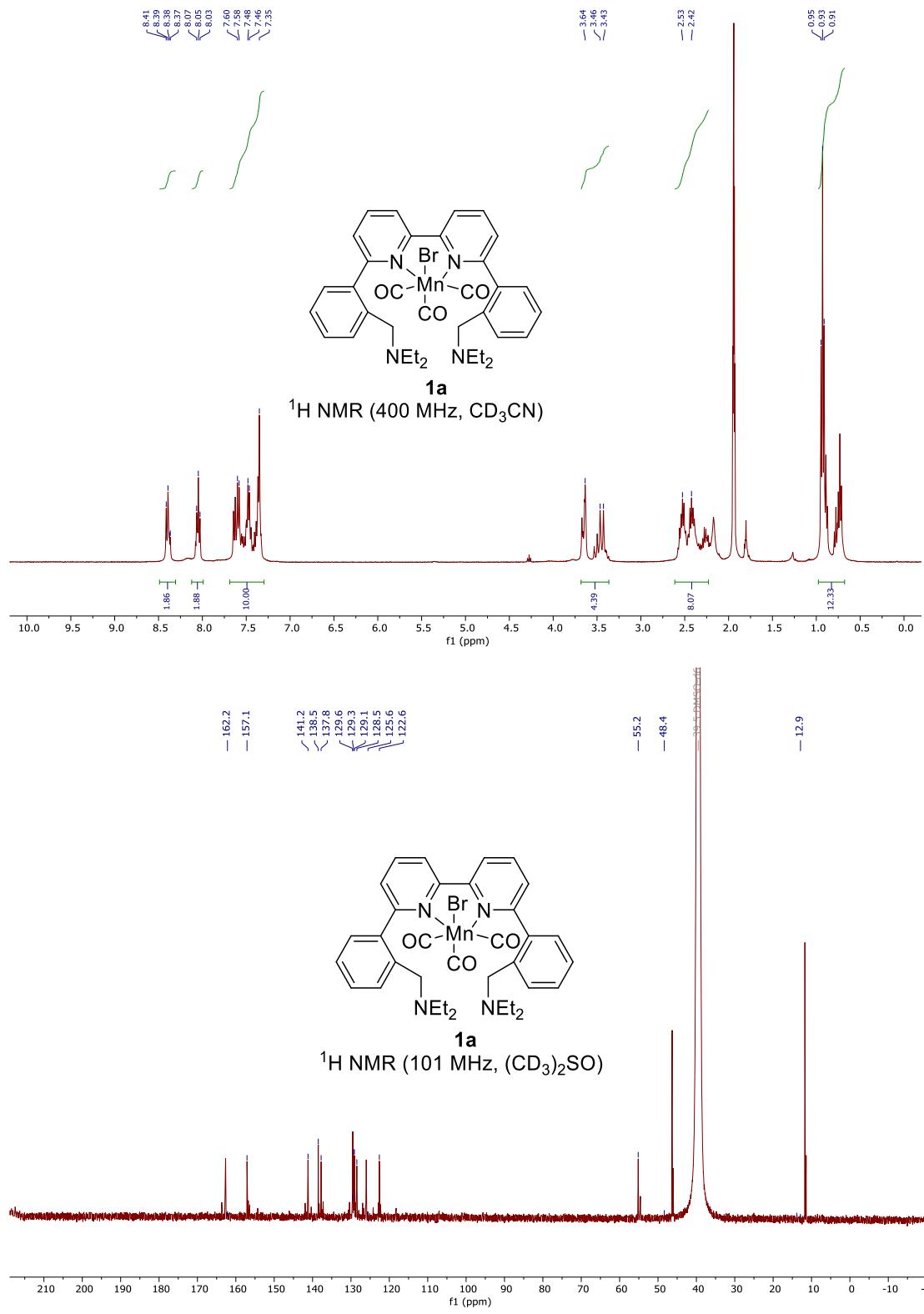
## 6. REFERENCES

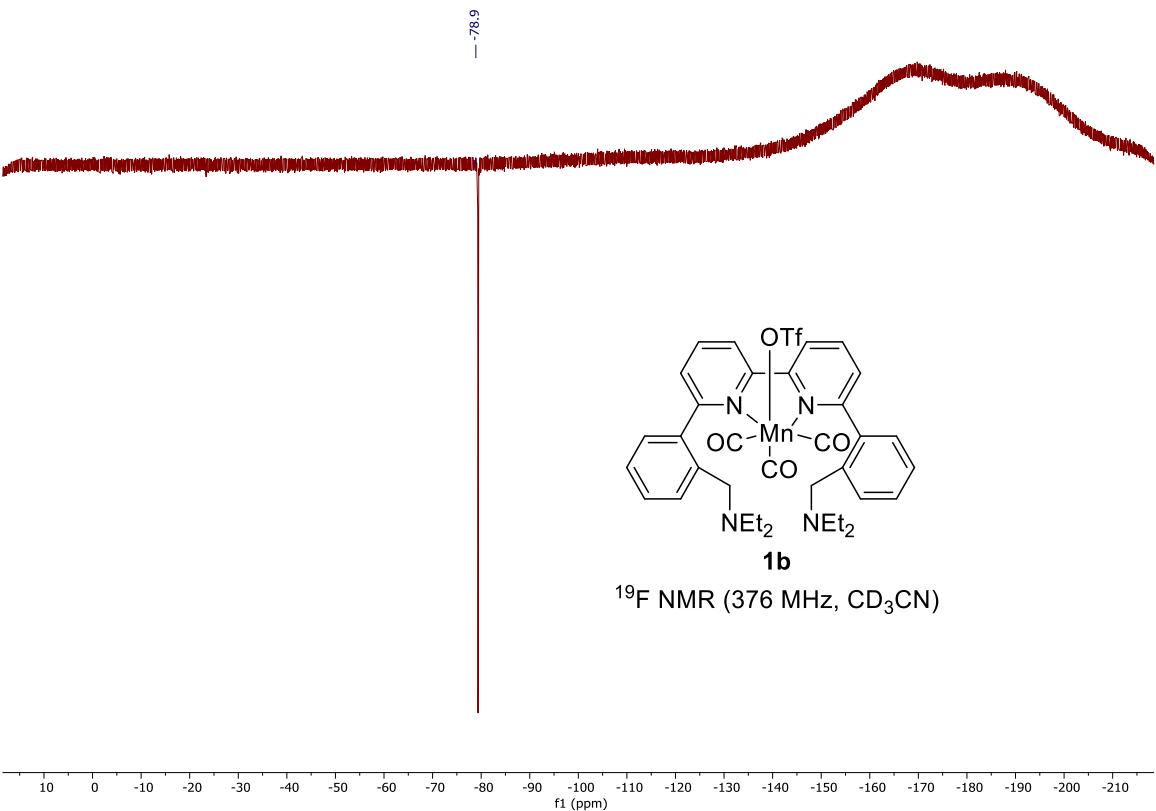
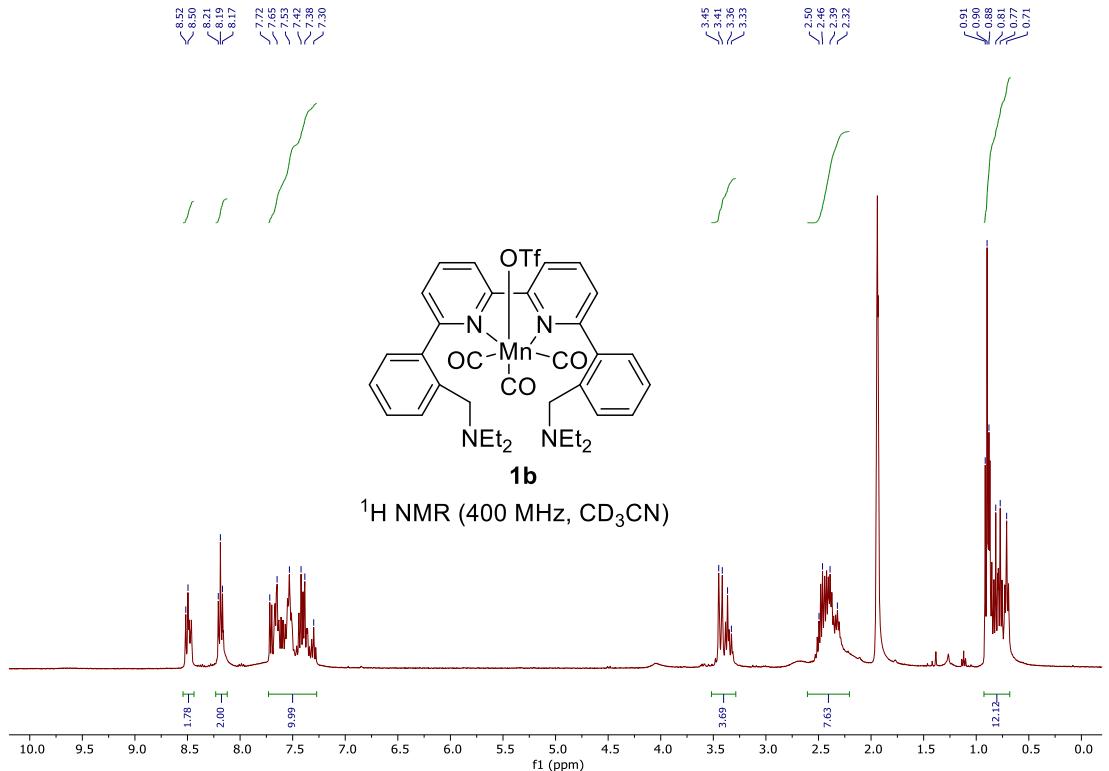
- (S1) Jensen, M. T.; Rønne, M. H.; Ravn, A. K.; Juhl, R. W.; Nielsen, D. U.; Hu, X. M.; Pedersen, S. U.; Daasbjerg, K.; Skrydstrup, T. Scalable carbon dioxide electroreduction coupled to carbonylation chemistry. *Nat. Commun.* **2017**, 8, 489.
- (S2) Grills, D. C.; Farrington, J. A.; Layne, B. H.; Lymar, S. V.; Mello, B. A.; Preses, J. M.; Wishart, J. F. Mechanism of the Formation of a Mn-Based CO<sub>2</sub> Reduction Catalyst Revealed by Pulse Radiolysis with Time-Resolved Infrared Detection. *J. Am. Chem. Soc.* **2014**, 136, 5563–5566.
- (S3) Zhao, Y.; Yu, B.; Yang, Z.; Zhang, H.; Hao, L.; Gao, X.; Liu, Z. A Protic Ionic Liquid Catalyzes CO<sub>2</sub> Conversion at Atmospheric Pressure and Room Temperature: Synthesis of Quinazoline-2,4(1H,3H)-diones. *Angew. Chem. Int. Ed.* **2014**, 53, 5922–5925.
- (S4) Machan, C. W.; Sampson, M. D.; Chabolla, S. A.; Dang, T.; Kubiak, C. P. Developing a Mechanistic Understanding of Molecular Electrocatalysts for CO<sub>2</sub> Reduction using Infrared Spectroelectrochemistry. *Organometallics* **2014**, 33, 4550–4559.
- (S5) Costentin, C.; Drouet, S.; Robert, M.; Savéant, J.-M. Turnover numbers, turnover frequencies, and overpotential in molecular catalysis of electrochemical reactions. Cyclic voltammetry and preparative-scale electrolysis. *J. Am. Chem. Soc.* **2012**, 134, 11235–11242.
- (S6) Roy, S.; Sharma, B.; Pecaut, J.; Simon, P.; Fontecave, M.; Tran, P. D.; Derat, E.; Artero, V. Molecular Cobalt Complexes with Pendant Amines for Selective Electrocatalytic Reduction of Carbon Dioxide to Formic Acid. *J. Am. Chem. Soc.* **2017**, 139, 3685–3696.
- (S7) CrysAlisPRO, Oxford Diffraction /Agilent Technologies UK Ltd, Yarnton, England.
- (S8) Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Cryst.* **2009**, 42, 339–341.
- (S9) Sheldrick, G.M. A short history of SHELX. *Acta Cryst.* **2008**, A64, 112–122.
- (S10) Sheldrick, G.M. Crystal structure refinement with SHELXL. *Acta Cryst.* **2015**, C71, 3–8.
- (S11) Bochevarov, A. D.; Harder, E.; Hughes, T. F.; Greenwood, J. R.; Braden, D. A.; Philipp, D. M.; Rinaldo, D.; Halls, M. D.; Zhang, J.; Friesner, R. A. Jaguar: A high-performance quantum chemistry software program with strengths in life and materials sciences. *Int. J. Quantum Chem.* **2013**, 113, 2110–2142.
- (S12) Parr, R. G.; Weitao, Y. *Density-Functional Theory of Atoms and Molecules*; Oxford University Press: Oxford, 1994.
- (S13) Tannor, D. J.; Marten, B.; Murphy, R.; Friesner, R. A.; Sitkoff, D.; Nicholls, A.; Ringnalda, M.; Goddard, W. A., III; Honig, B. Accurate First Principles Calculation of Molecular Charge Distributions and Solvation Energies from Ab Initio Quantum Mechanics and Continuum Dielectric Theory. *J. Am. Chem. Soc.* **1994**, 116, 11875–11882.
- (S14) Marten, B.; Kim, K.; Cortis, C.; Friesner, R. A.; Murphy, R. B.; Ringnalda, M. N.; Sitkoff, D.; Honig, B. New Model for Calculation of Solvation Free Energies: Correction of Self-Consistent Reaction Field Continuum Dielectric Theory for Short-Range Hydrogen-Bonding Effects. *J. Phys. Chem.* **1996**, 100, 11775–11788.
- (S15) Becke, A. D. A new mixing of Hartree–Fock and local density-functional theories. *J. Chem. Phys.* **1993**, 98, 1372.
- (S16) Becke, A. D. Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys. Rev. A* **1988**, 38, 3098.
- (S17) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010**, 132, 154104.
- (S18) Hay, P. J.; Wadt, W. R. Ab initio effective core potentials for molecular calculations. Potentials for K to Au including the outermost core orbitals. *J. Chem. Phys.* **1985**, 82, 299.

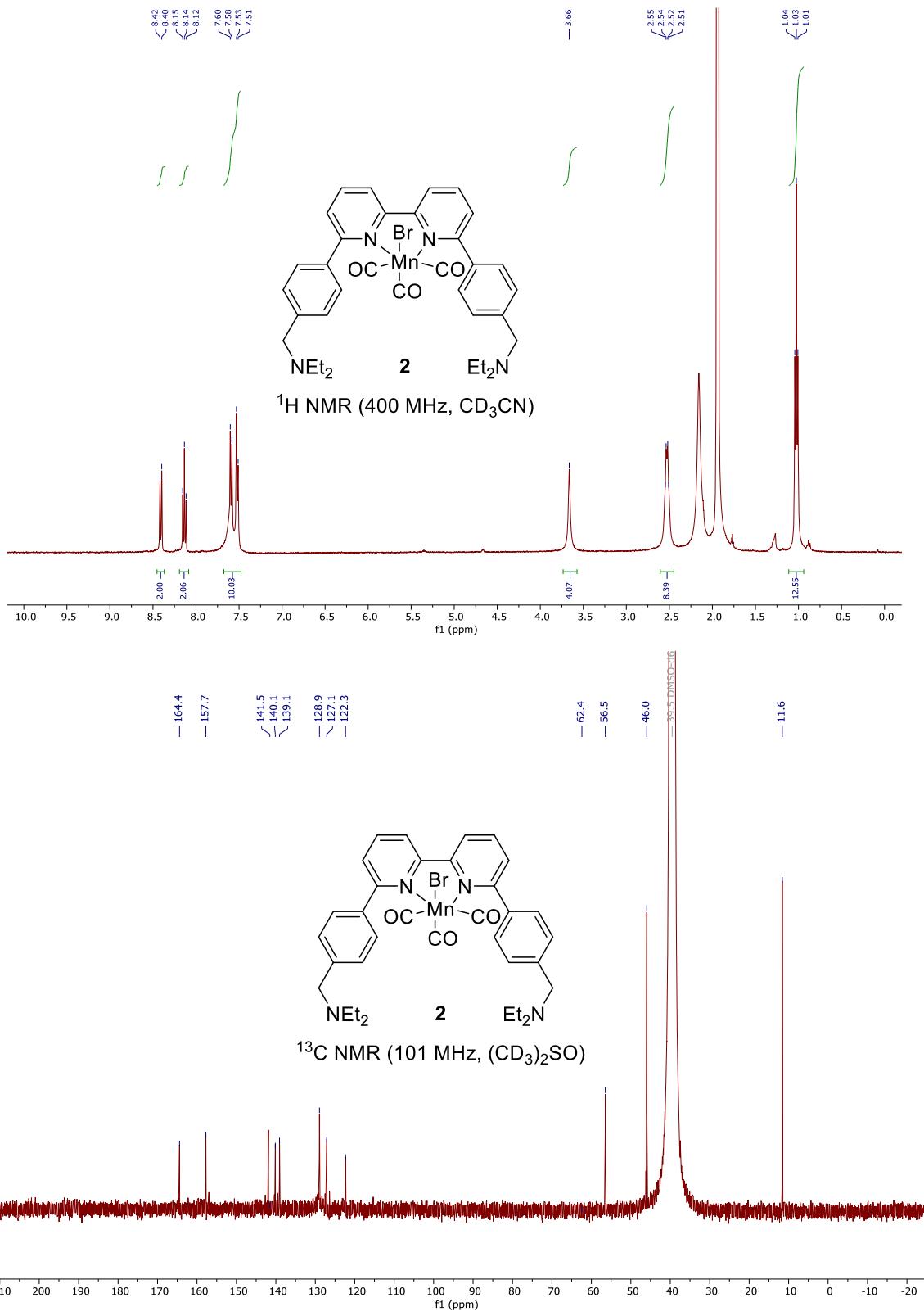
- (S19) Hay, P. J.; Wadt, W. R. Ab initio effective core potentials for molecular calculations. Potentials for the transition metal atoms Sc to Hg. *J. Chem. Phys.* **1985**, 82, 270.
- (S20) Wadt, W. R.; Hay, P. J. Ab initio effective core potentials for molecular calculations. Potentials for main group elements Na to Bi. *J. Chem. Phys.* **1985**, 82, 284.
- (S21) Ditchfield, R.; Hehre, W. J.; Pople, J. A. Self-Consistent Molecular-Orbital Methods. IX. An Extended Gaussian-Type Basis for Molecular-Orbital Studies of Organic Molecules. *J. Chem. Phys.* **1971**, 54, 724.
- (S22) Dunning, T. H. Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen. *J. Chem. Phys.* **1989**, 90, 1007.
- (S23) Marten, B.; Kim, K.; Cortis, C.; Friesner, R. A.; Murphy, R. B.; Ringnalda, M. N.; Sitkoff, D.; Honig, B. New Model for Calculation of Solvation Free Energies: Correction of Self-Consistent Reaction Field Continuum Dielectric Theory for Short-Range Hydrogen-Bonding Effects. *J. Phys. Chem.* **1996**, 100, 11775–11788.
- (S24) Edinger, S. R.; Cortis, C.; Shenkin, P. S.; Friesner, R. A. Solvation Free Energies of Peptides: Comparison of Approximate Continuum Solvation Models with Accurate Solution of the Poisson–Boltzmann Equation. *J. Phys. Chem. B* **1997**, 101, 1190–1197.
- (S25) Friedrichs, M.; Zhou, R.; Edinger, S. R.; Friesner, R. A. Poisson–Boltzmann Analytical Gradients for Molecular Modeling Calculations. *J. Phys. Chem. B* **1999**, 103, 3057–3061.
- (S26) Isse, A. A.; Gennaro, A. Absolute Potential of the Standard Hydrogen Electrode and the Problem of Interconversion of Potentials in Different Solvents. *J. Phys. Chem. B* **2010**, 114, 7894–7899.
- (S27) Aranzaes, J. R.; Daniel, M. -C.; Astruc, D. Metallocenes as references for the determination of redox potentials by cyclic voltammetry — Permethylated iron and cobalt sandwich complexes, inhibition by polyamine dendrimers, and the role of hydroxy-containing ferrocenes. *Can. J. Chem.* **2006**, 84, 288–299.
- (S28) te Velde, G.; Bickelhaupt, F. M; Baerends, E. J.; Fonseca G. C.; van Gisbergen, S. J.; Snijders, J. G.; Ziegler, T. Chemistry with ADF. *J. Comput. Chem.* **2001**, 22, 931–967.
- (S29) Lenthe, E. V.; Baerends, E.J. Optimized Slater-type basis sets for the elements 1–118. *J. Comput. Chem.* **2003**, 24, 1142–1156.
- (S30) Lenhe, E. V.; Snijders, J.G.; Baerends, E.J The zero-order regular approximation for relativistic effects: The effect of spin–orbit coupling in closed shell molecules. *J. Chem. Phys.* **1996**, 105, 6505.
- (S31) Muckerman, J. T.; Achord, P.; Creutz, C.; Polyansky, D. E.; Fujita, E. Calculation of thermodynamic hydricities and the design of hydride donors for CO<sub>2</sub> reduction. *PNAS* **2012**, 109, 15657–15662.
- (S32) Sampson, M. D.; Nguyen, A. D.; Grice, K. A.; Moore, C. E.; Rheingold, A. L.; Kubiak, C. P. Manganese Catalysts with Bulky Bipyridine Ligands for the Electrocatalytic Reduction of Carbon Dioxide: Eliminating Dimerization and Altering Catalysis. *J. Am. Chem. Soc.* **2014**, 136, 5460–5471.
- (S33) Borisova, N. E.; Kharcheva, A. V.; Patsaeva, S. V.; Korotkov, L. A.; Bakaev, S.; Reshetova, M. D.; Lyssenko, K. A.; Belova, E. V.; Myasoedov, B. F. Hard-and-soft phosphinoxide receptors for f-element binding: structure and photophysical properties of europium(III) complexes. *Dalton Trans.* **2017**, 46, 2238–2248.
- (S34) Huber, F. L.; Nauroozi, D.; Mengele, A. K.; Rau, S. Synthesis and Characterization of a Ruthenium(II) Complex for the Development of Supramolecular Photocatalysts Containing Multidentate Coordination Spheres. *Eur. J. Inorg. Chem.* **2017**, 34, 4020–4027.
- (S35) Nitschke, J.; Schmidt, S. P.; Troglar, W. C. Properties of (trifluoromethanesulfonato)pentacarbonylmanganese(I) and -rhenium(I). Reactions in superacid solvents. *Inorg. Chem.* **1985**, 24, 1972–1978.
- (S36) Gueddouda, N. M.; Hurtado, M. R.; Moreau, S.; Ronga, L.; Das, R. N.; Savrimoutou, S.; Rubio, S.; Marchand, A.; Mendoza, O.; Marchivie, M.; Elmi, L.; Chansavang, A.; Desplat, V.; Gabelica, V.; Bourdoncle, A.; Mergny, J.-L.; Guillou, J. Design, Synthesis, and Evaluation of 2,9-Bis((substituted-

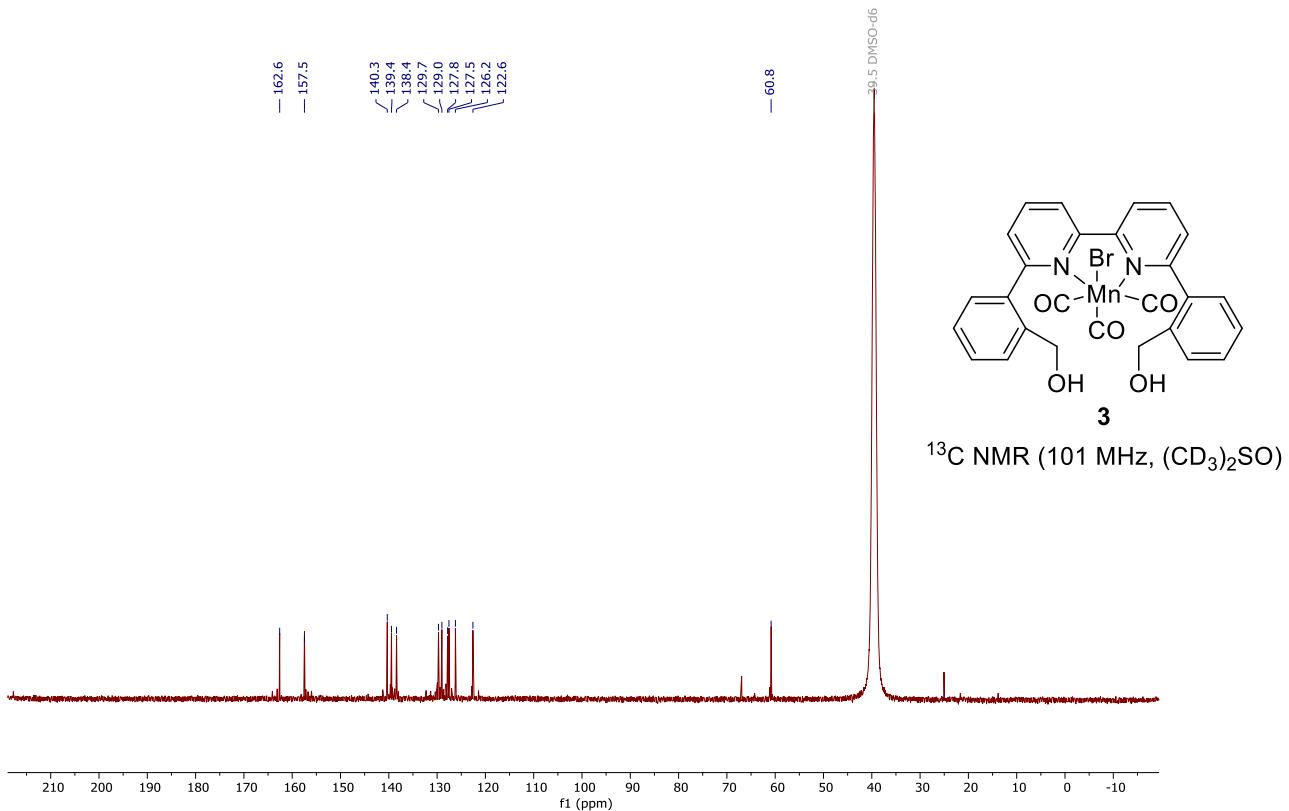
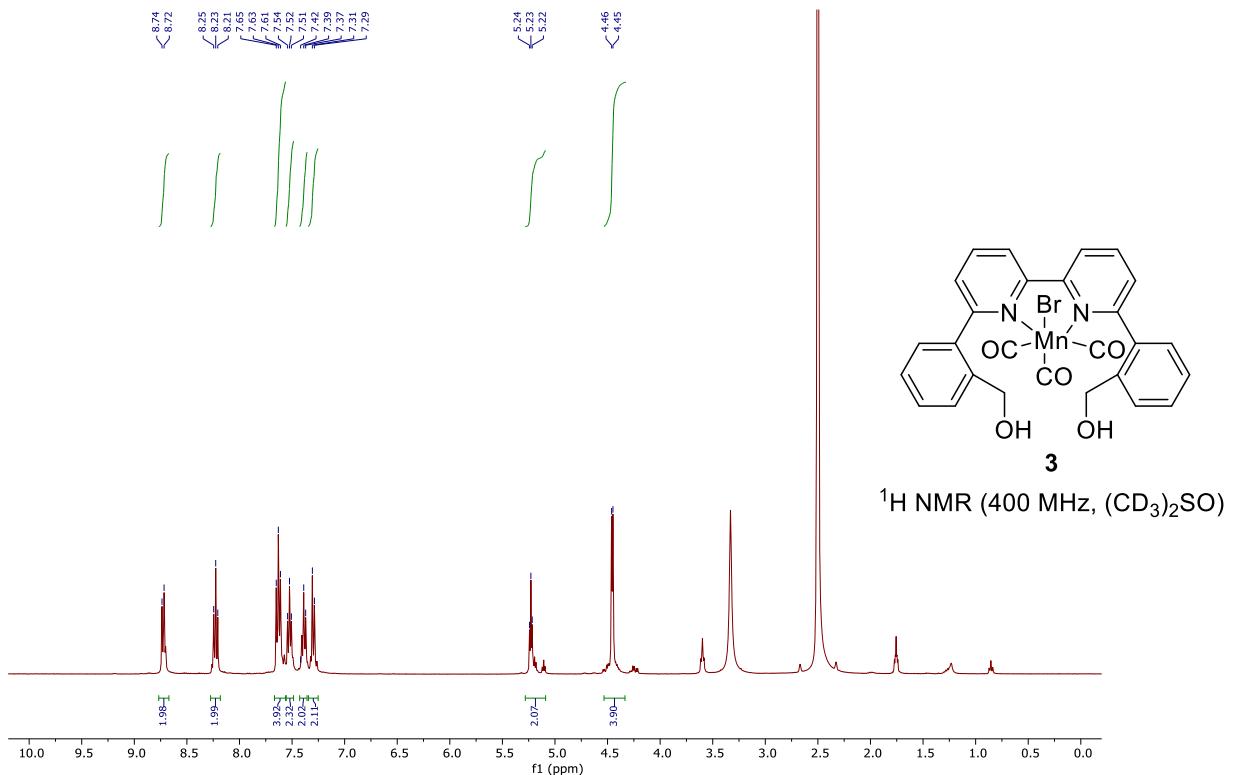
aminomethyl)phenyl))-1,10-phenanthroline Derivatives as G-Quadruplex Ligands. *ChemMedChem*. **2017**, 12, 146–160.

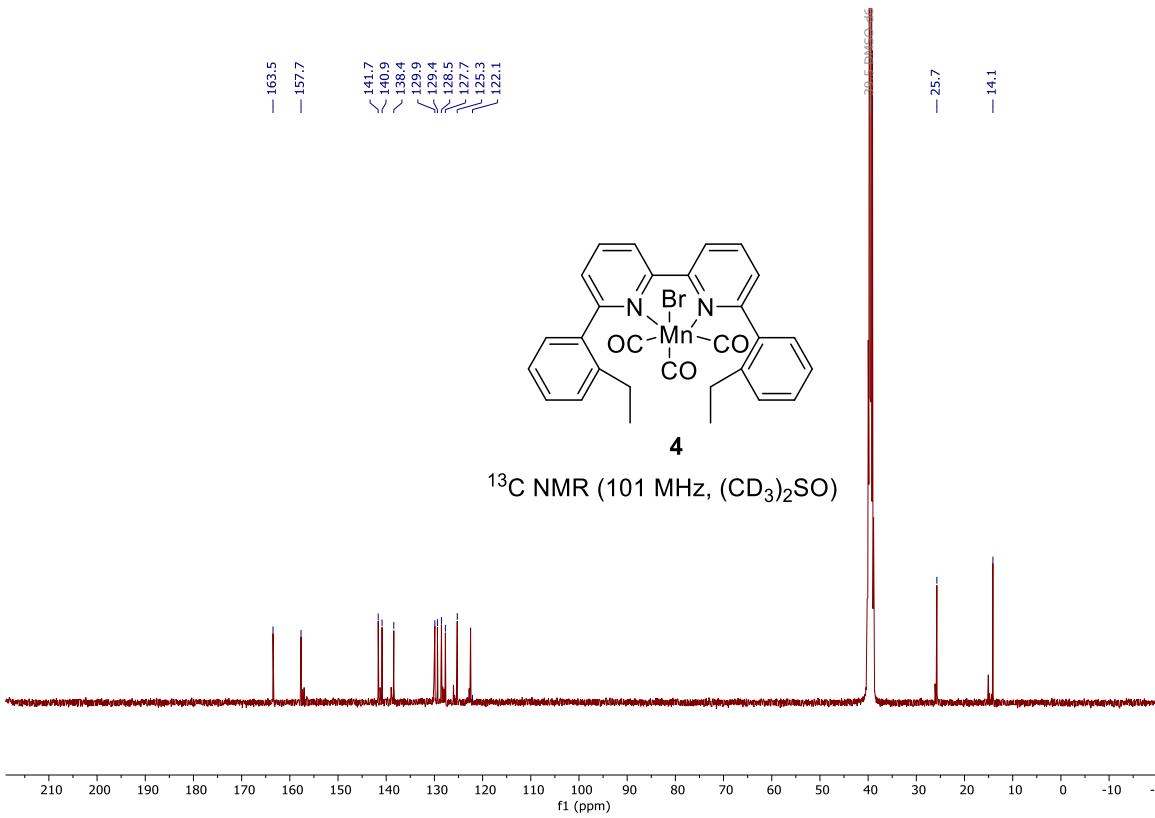
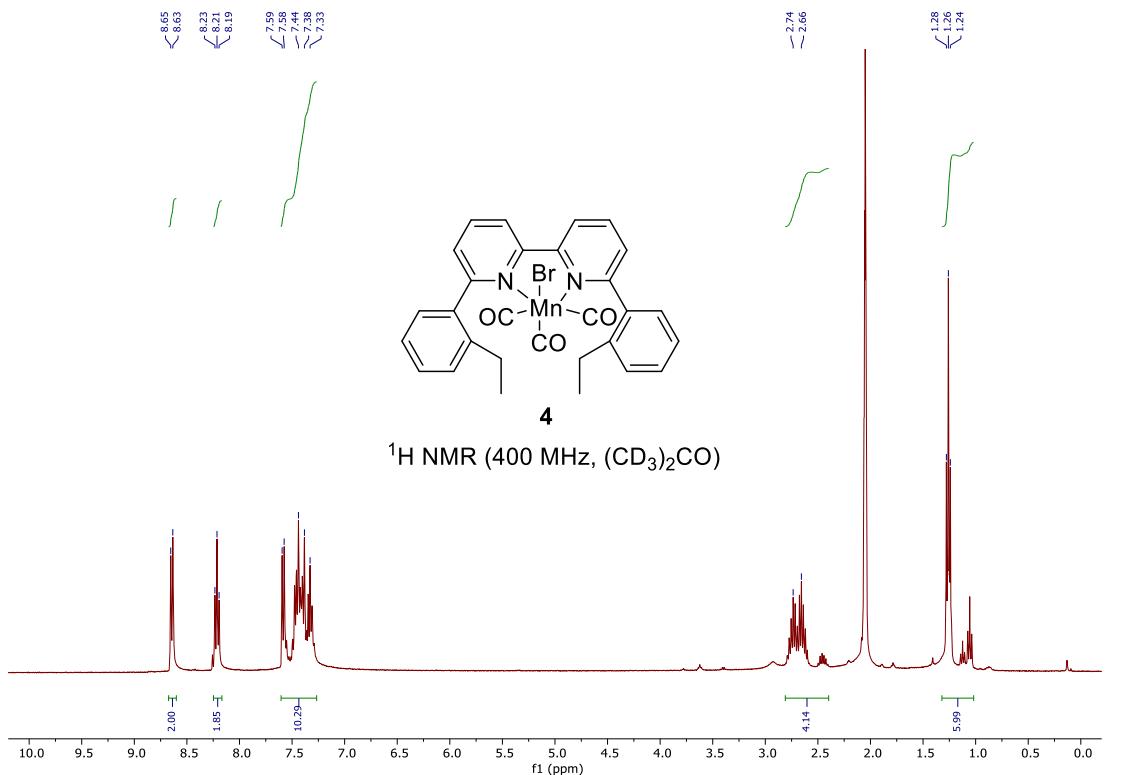
## 7. NMR SPECTRA

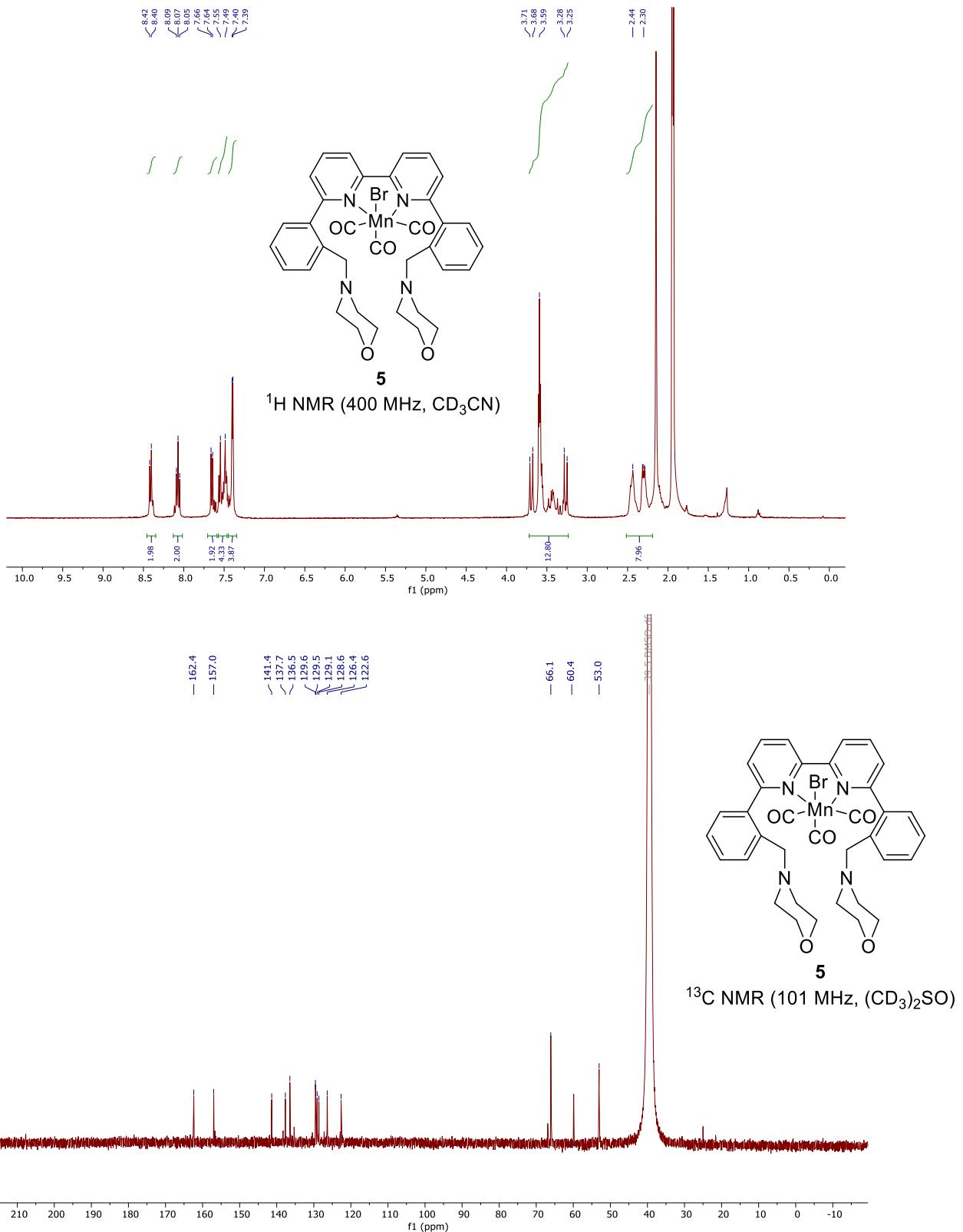


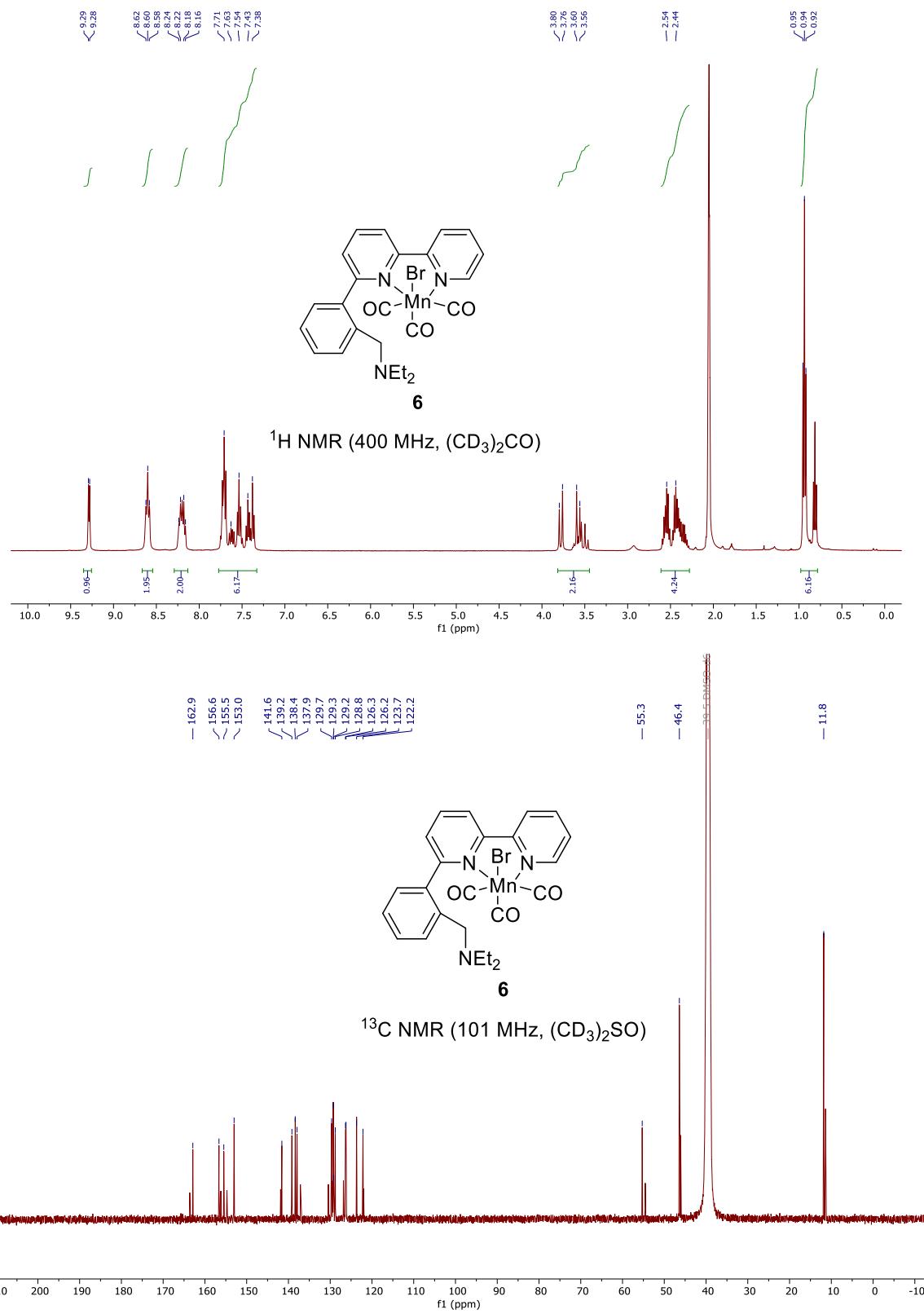


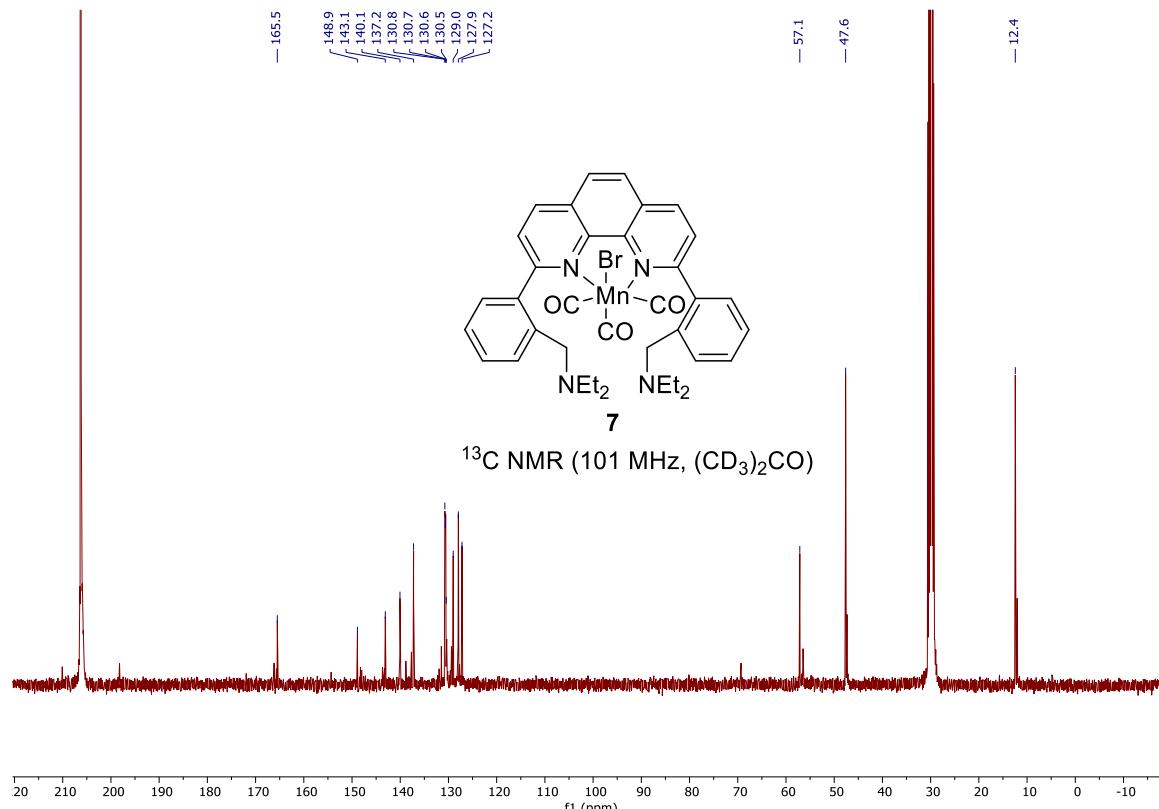
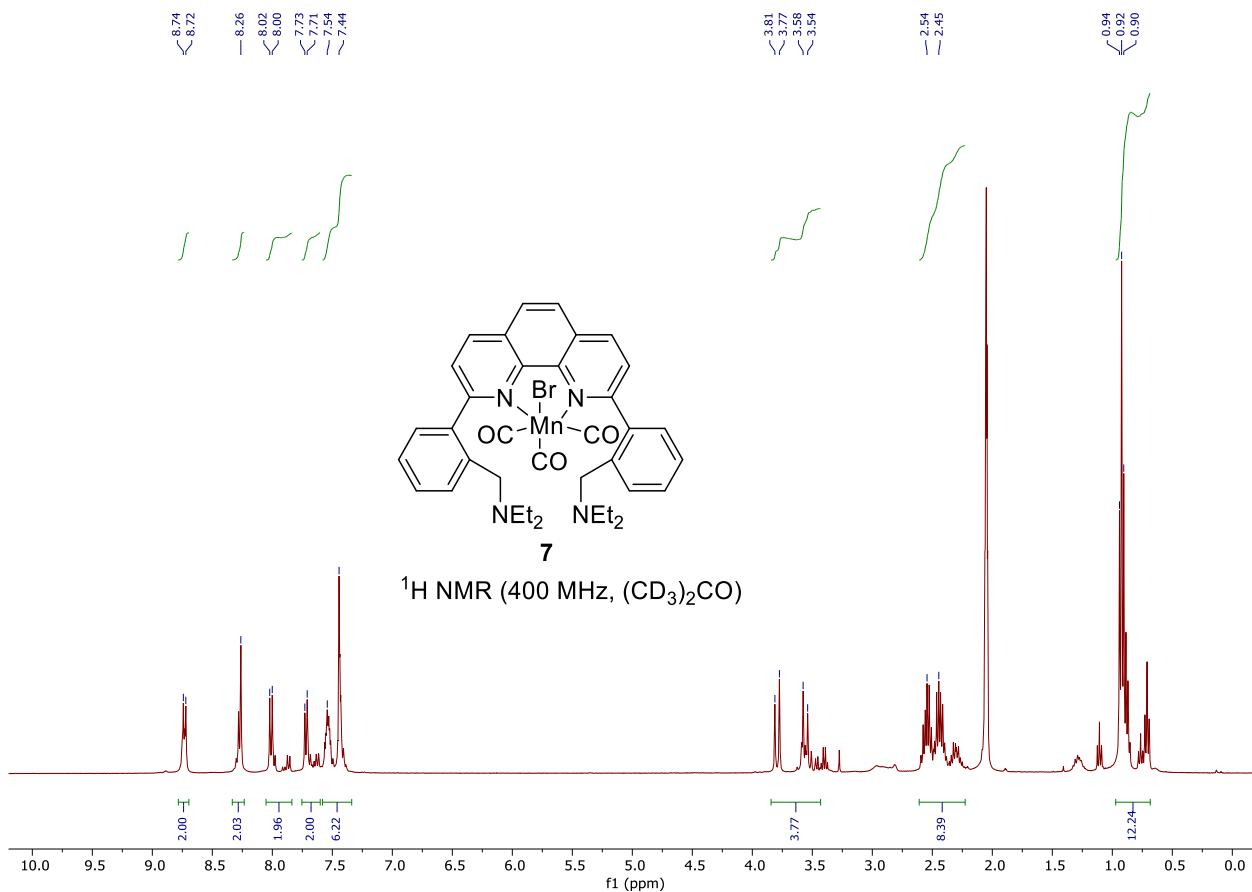


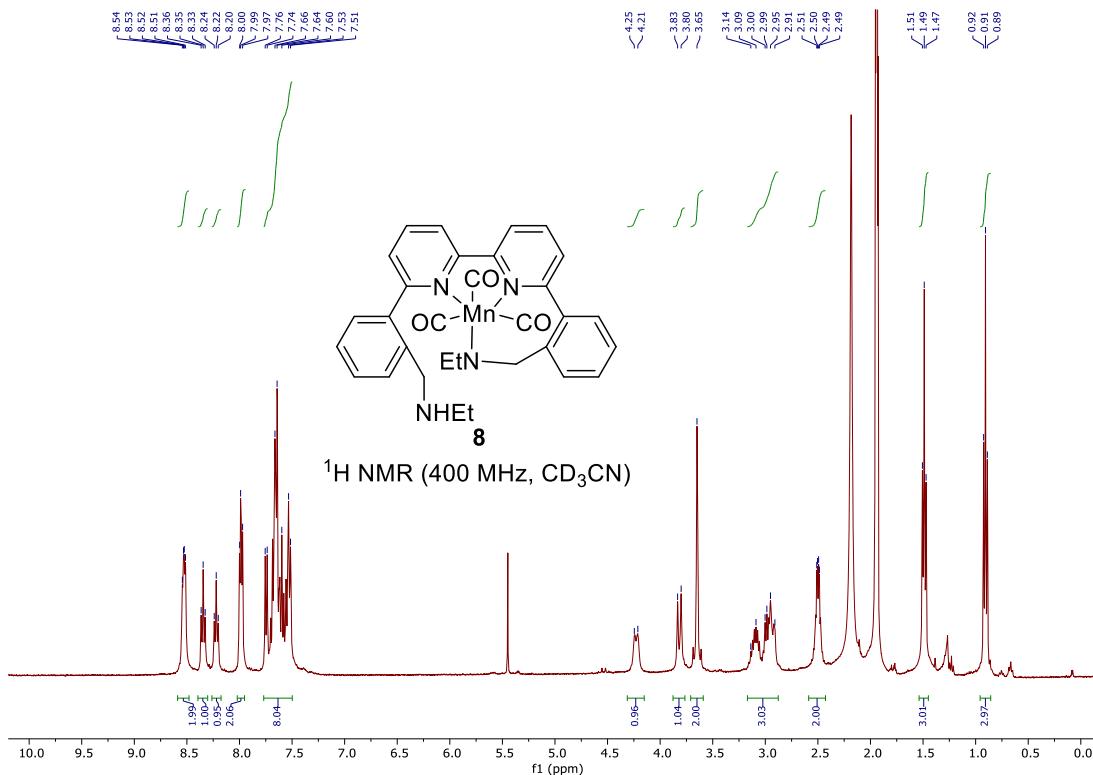




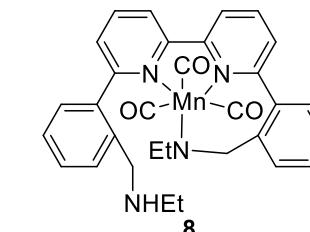




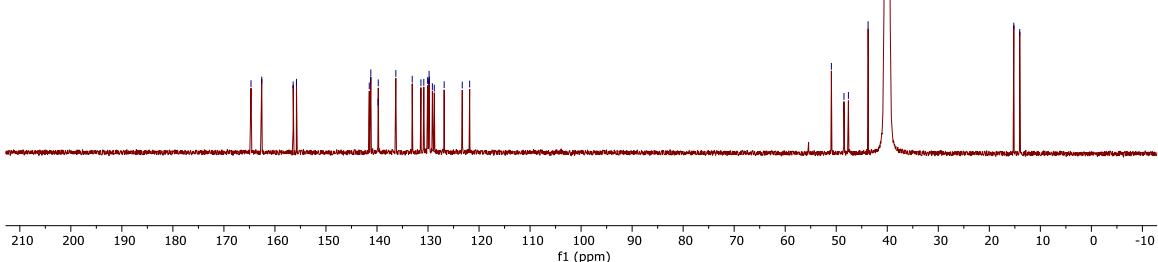


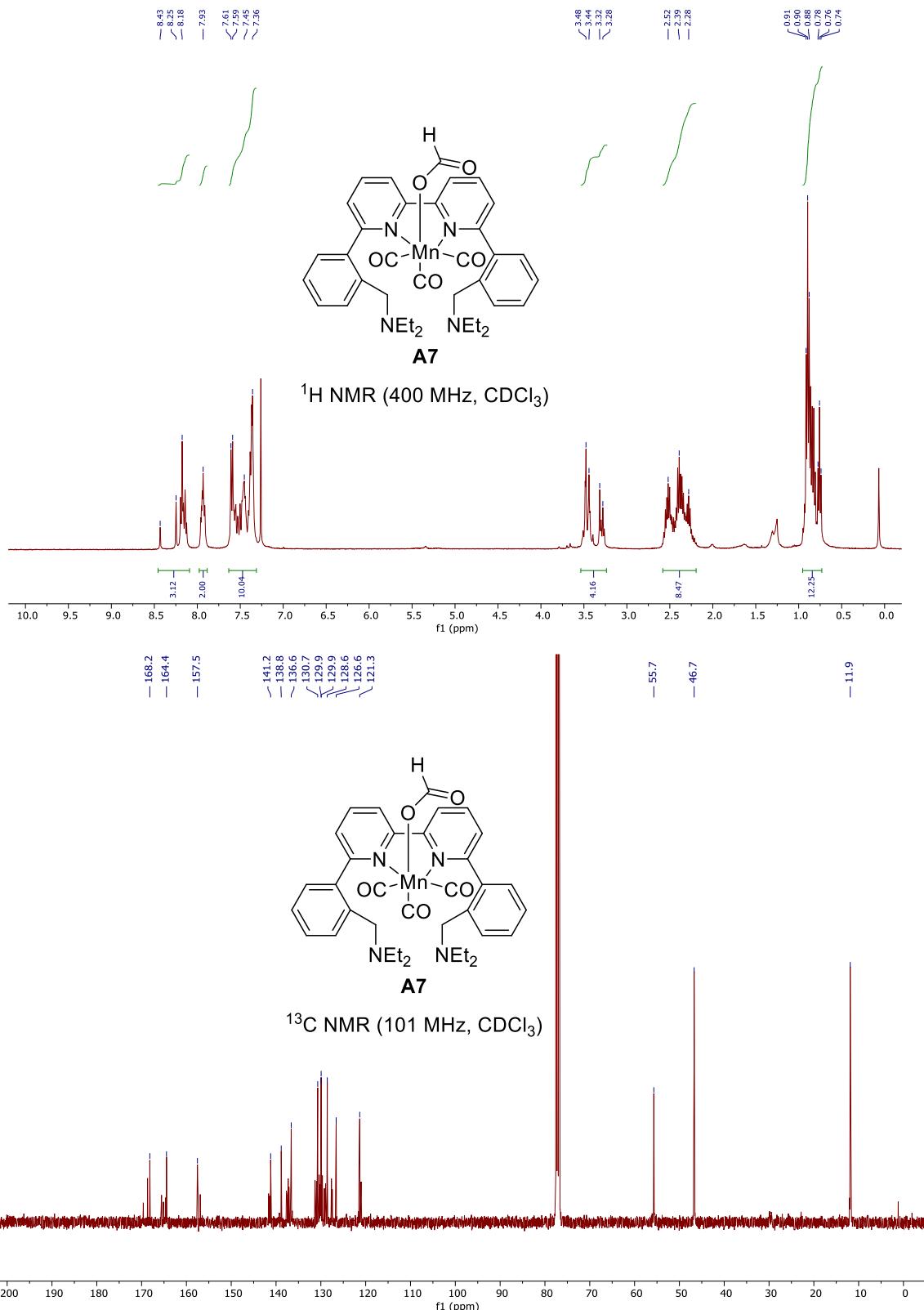


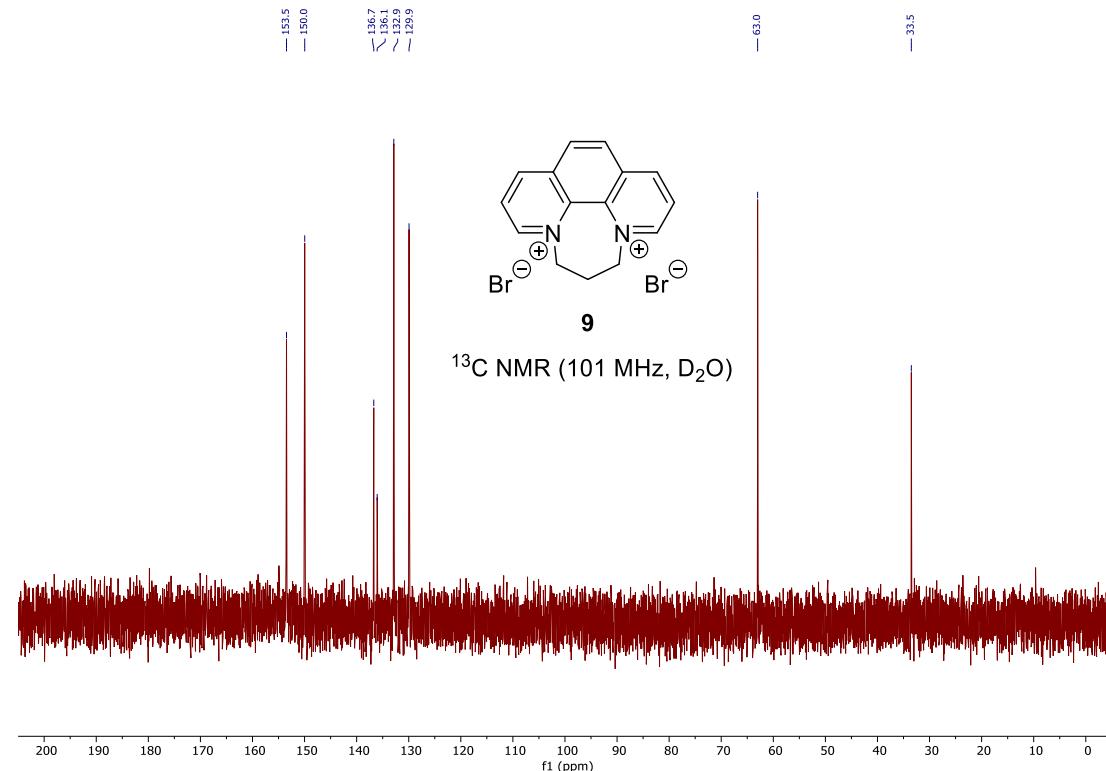
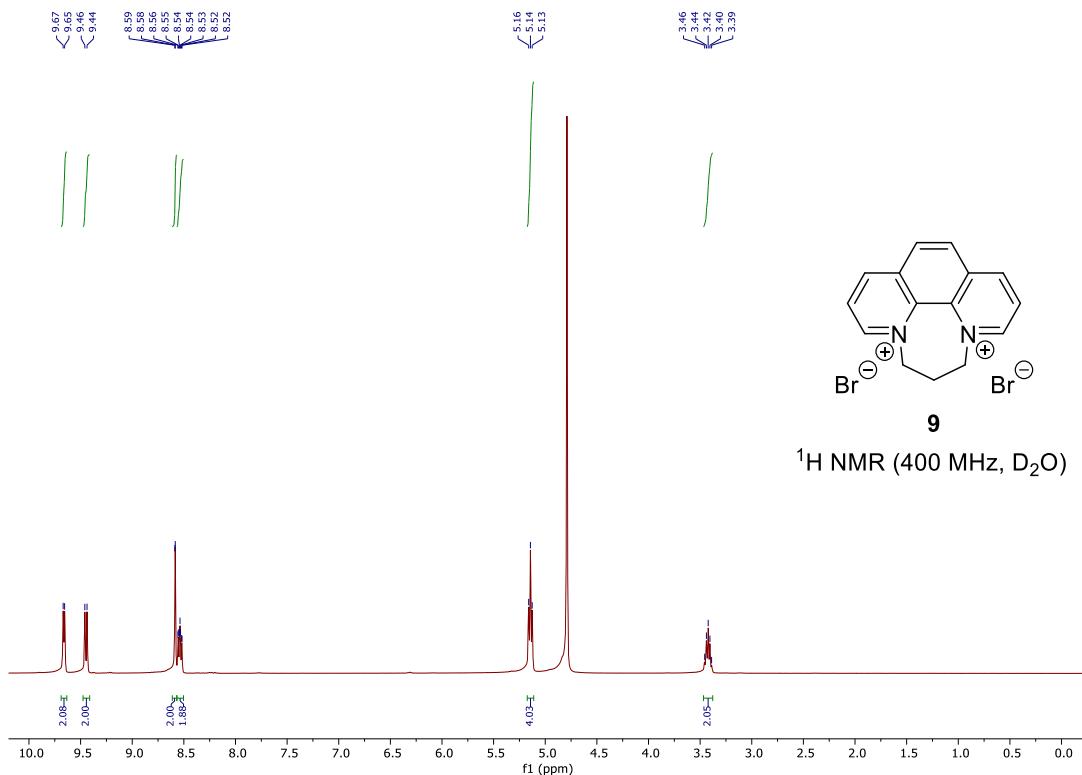
\*Extra peak from dichloromethane

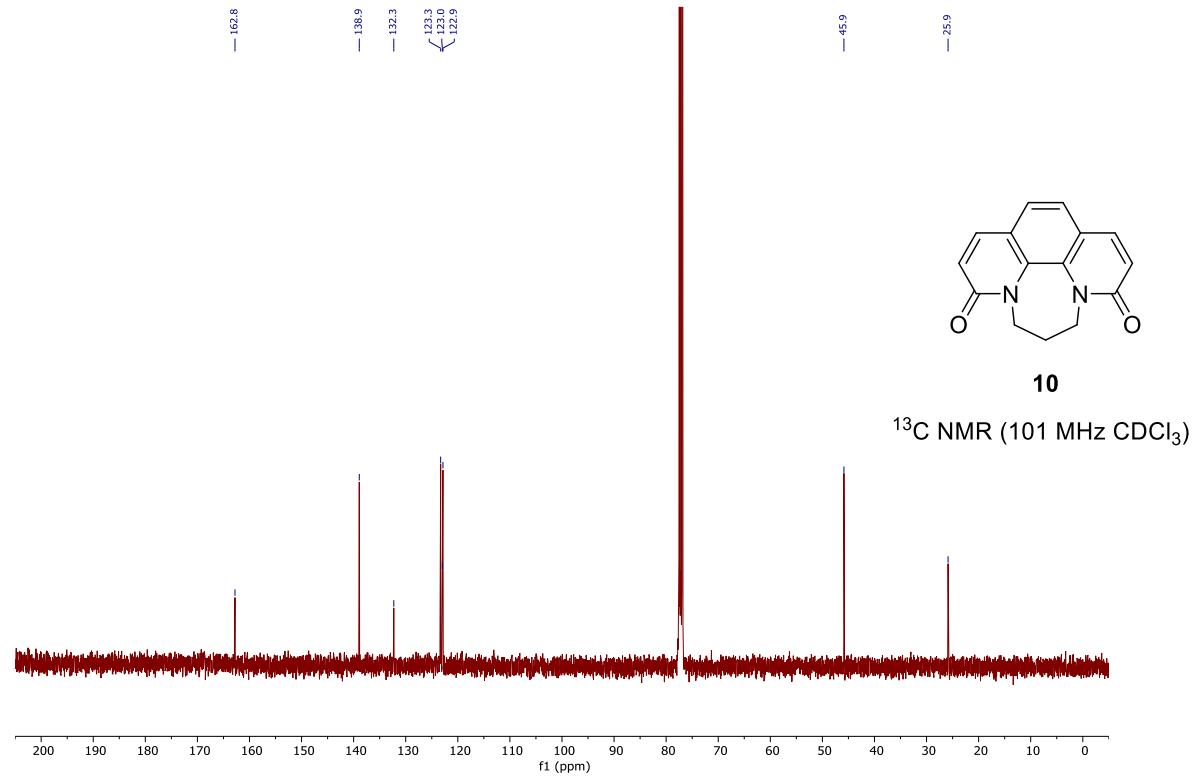
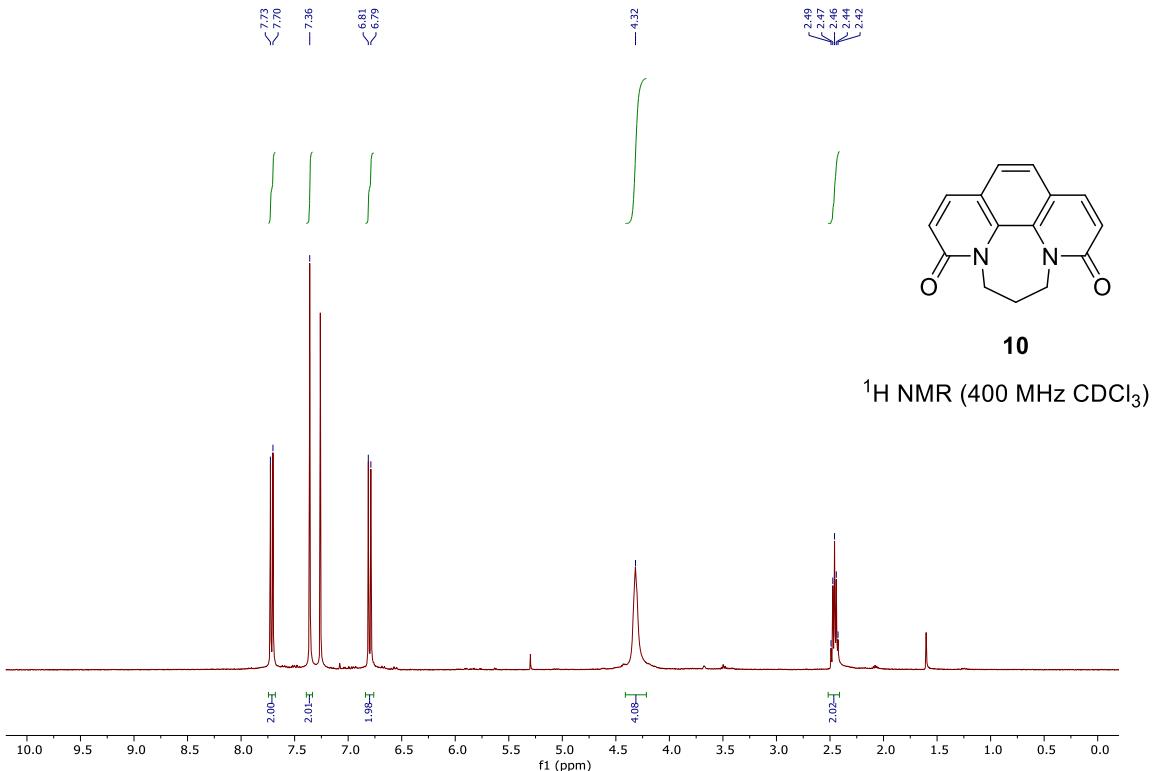


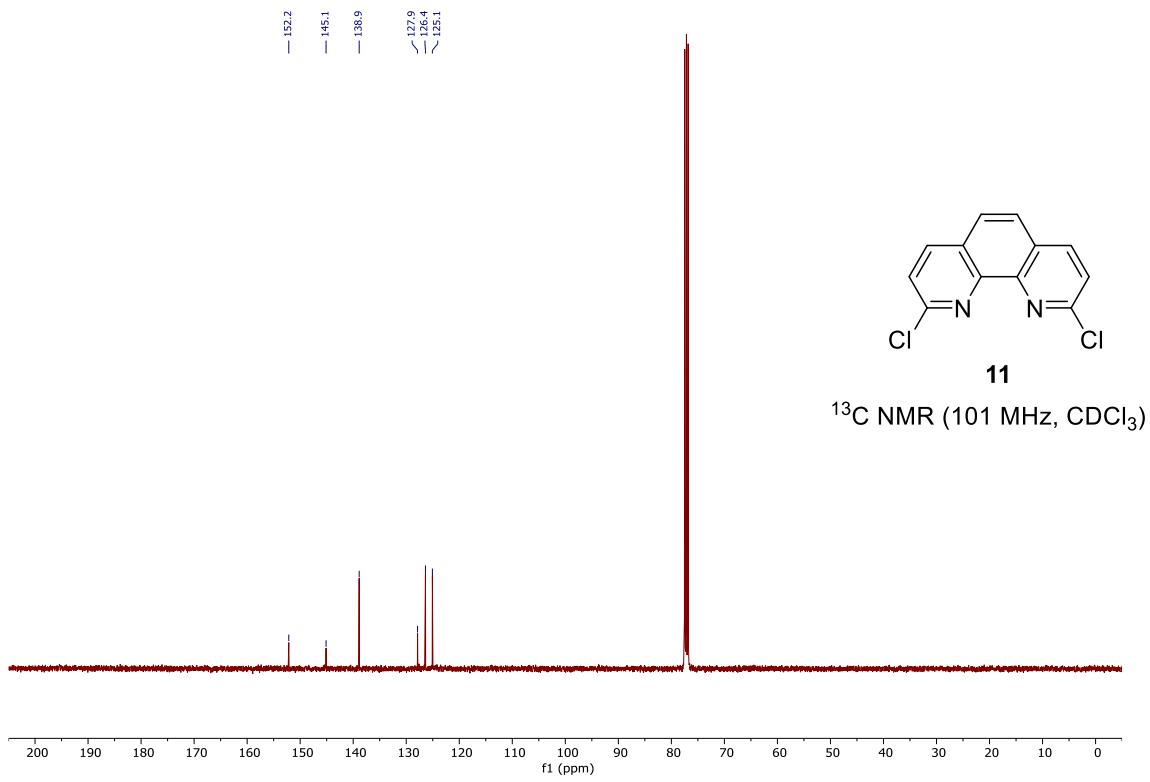
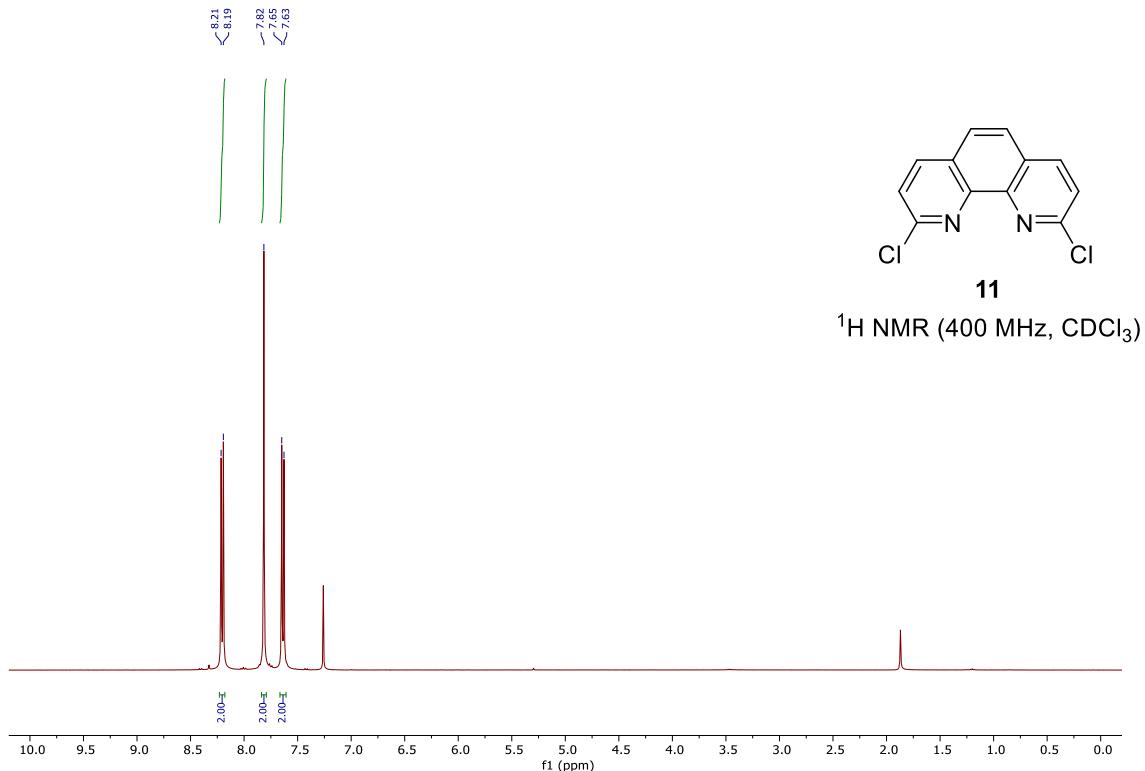
$^{13}\text{C}$  NMR (101 MHz,  $(\text{CD}_3)_2\text{SO}$ )

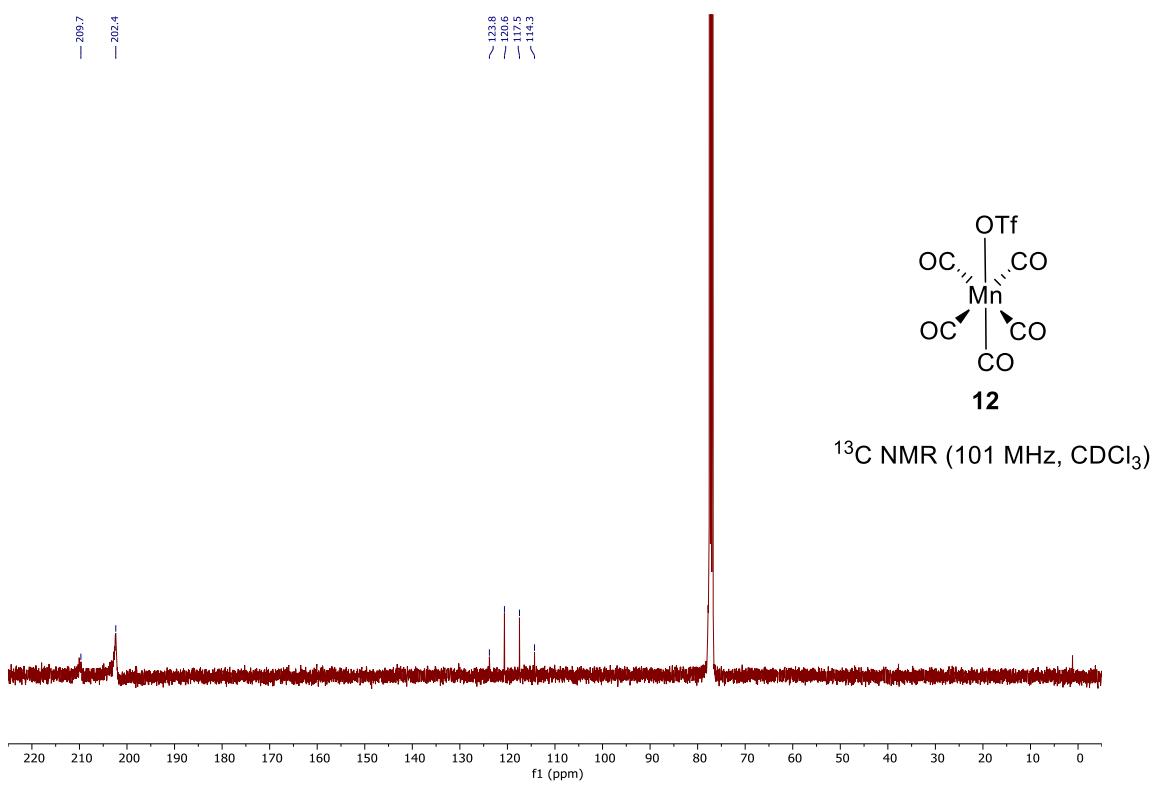
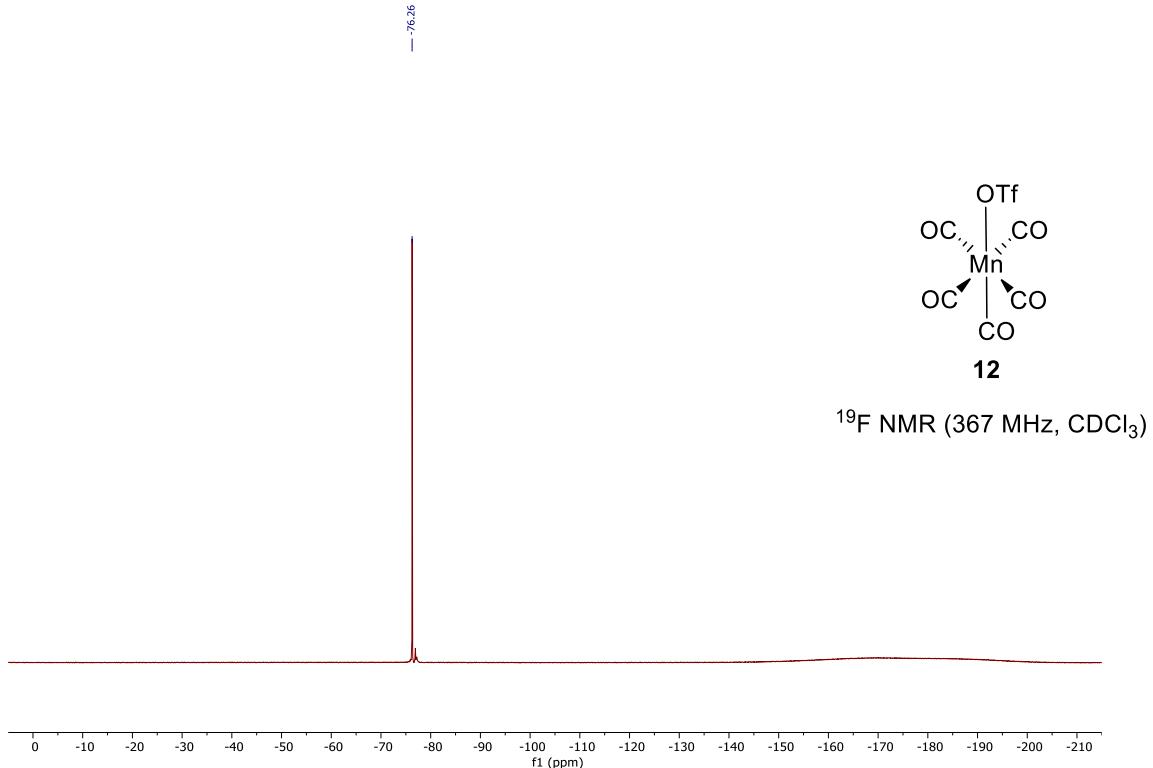


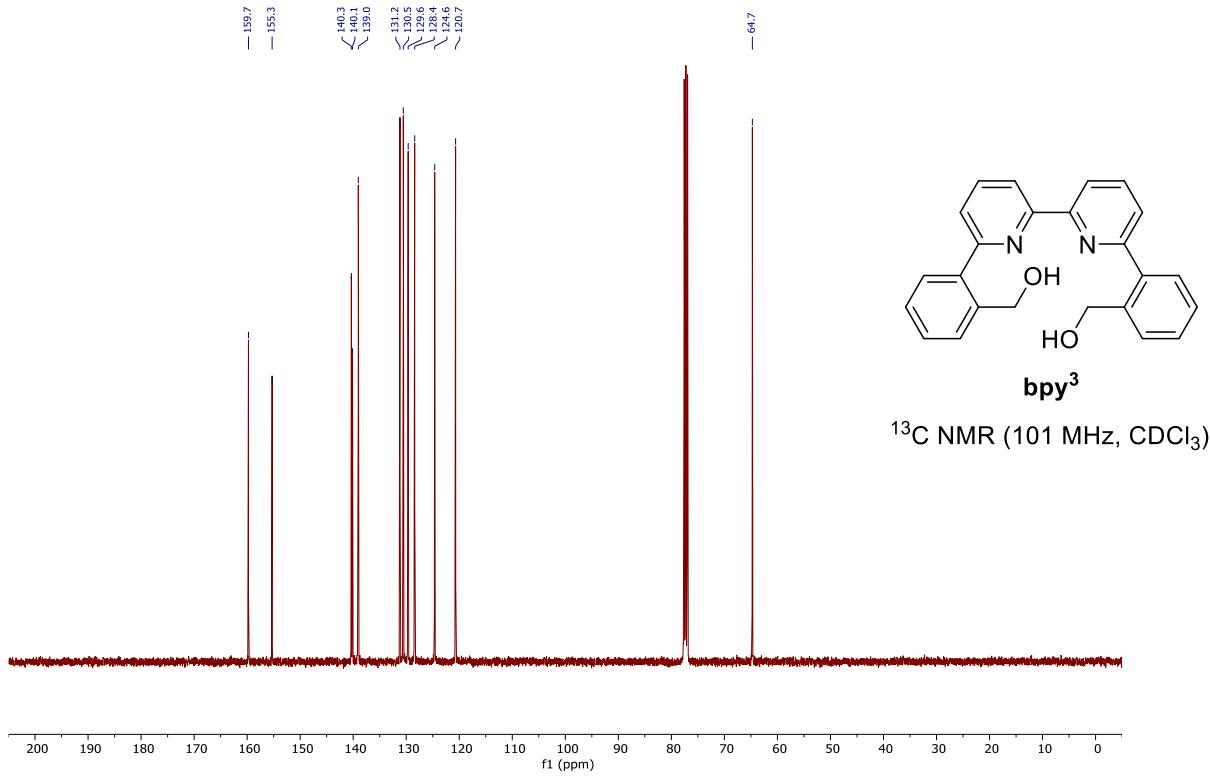
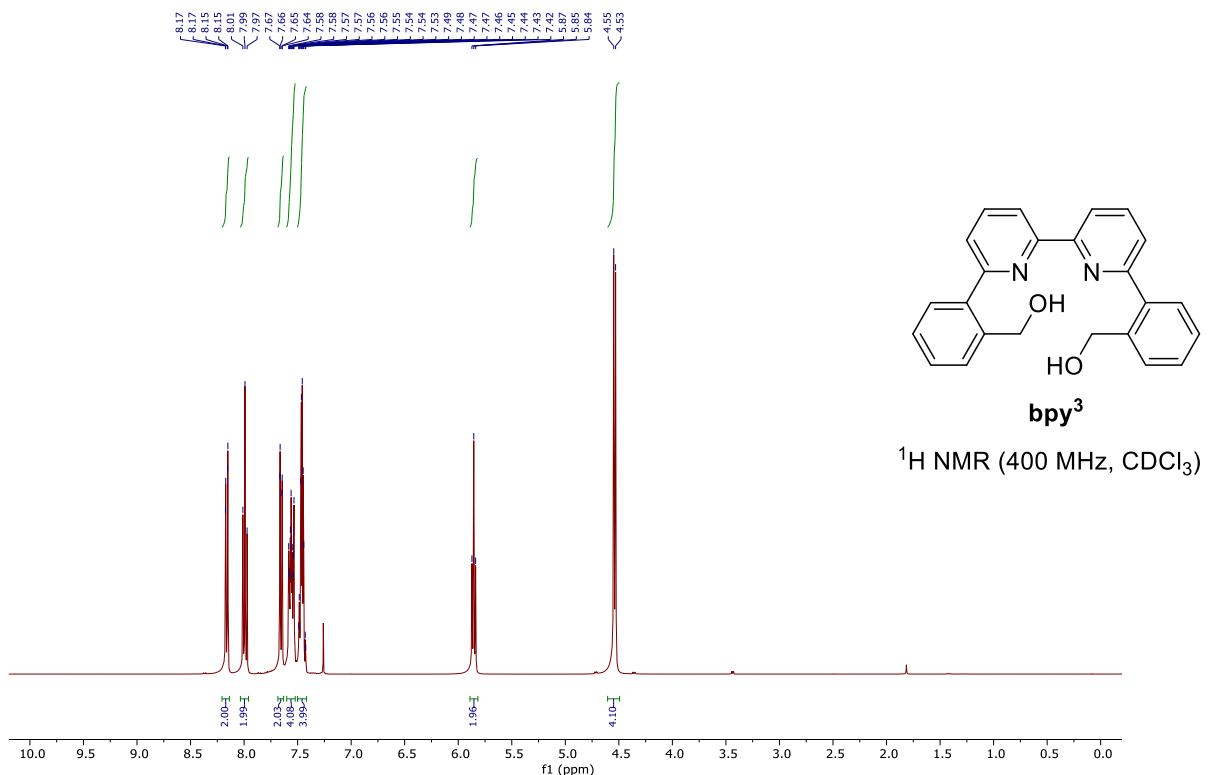


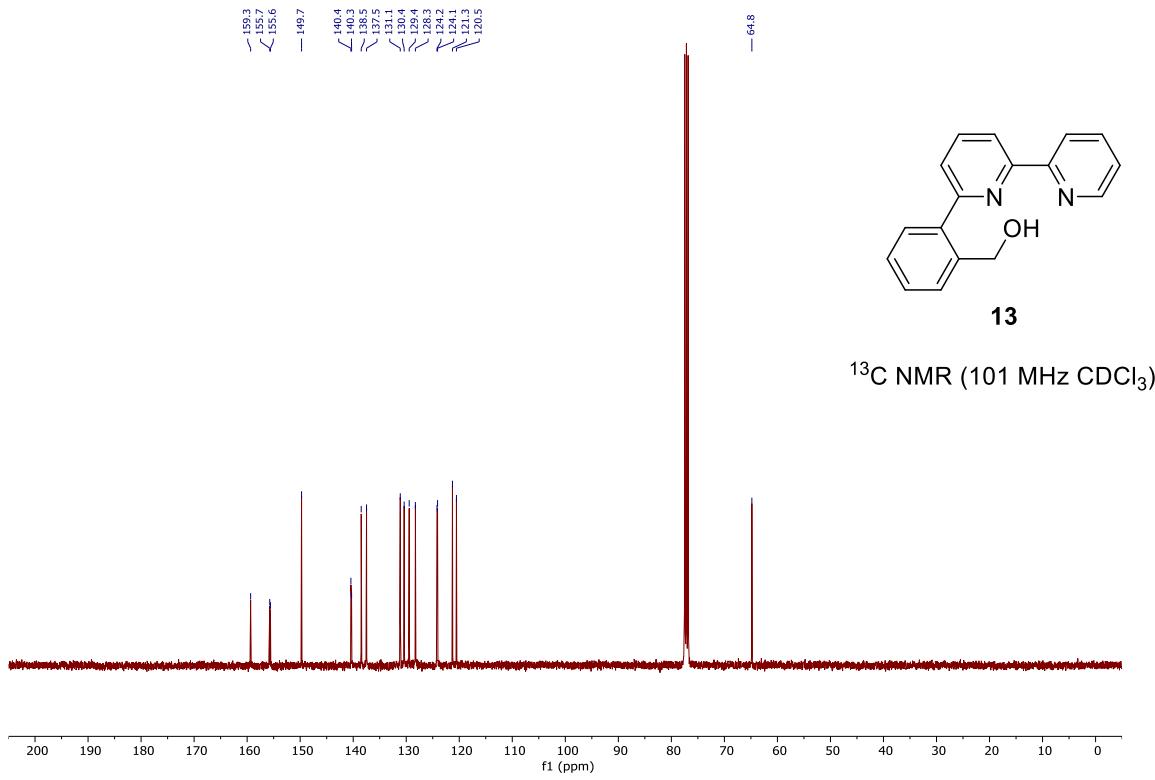
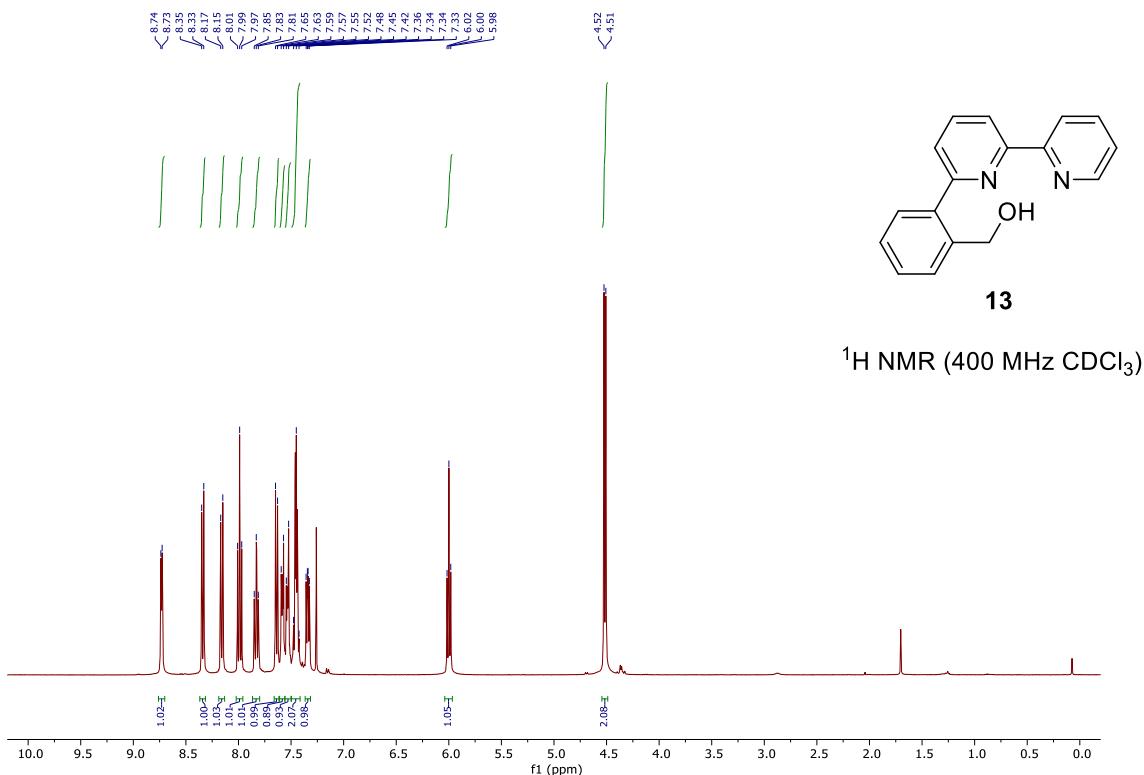


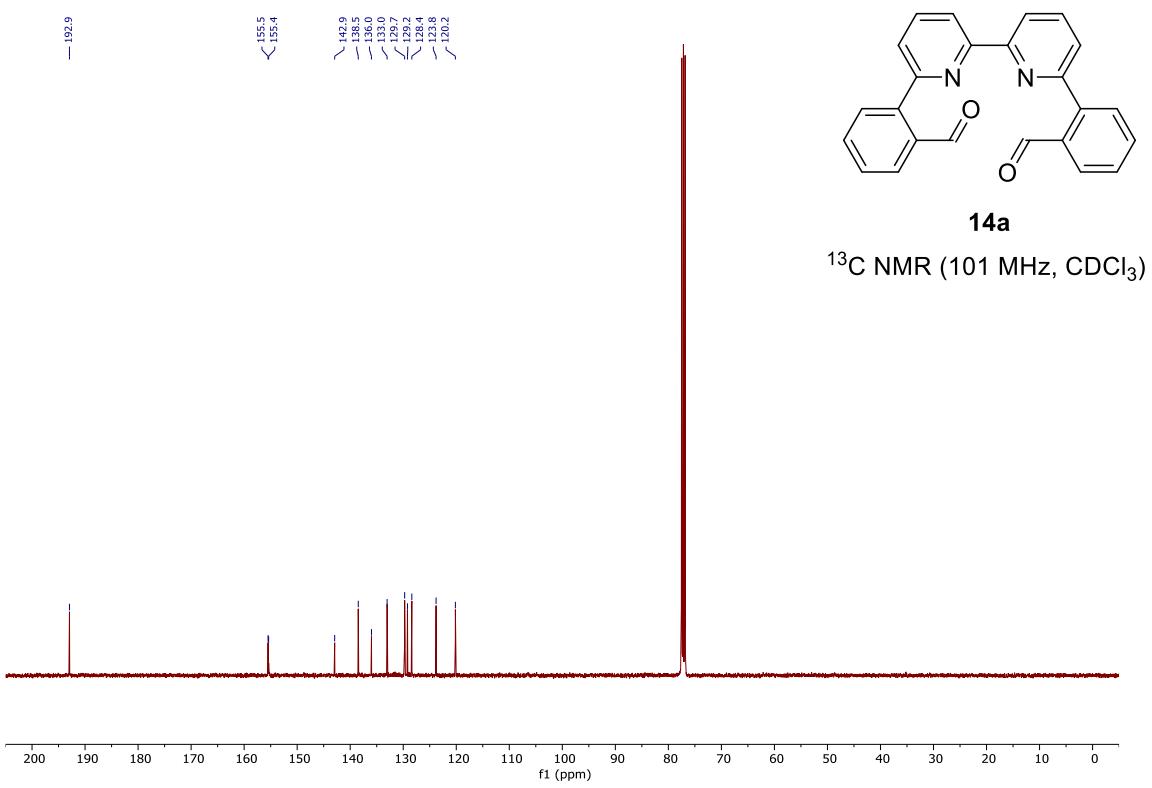
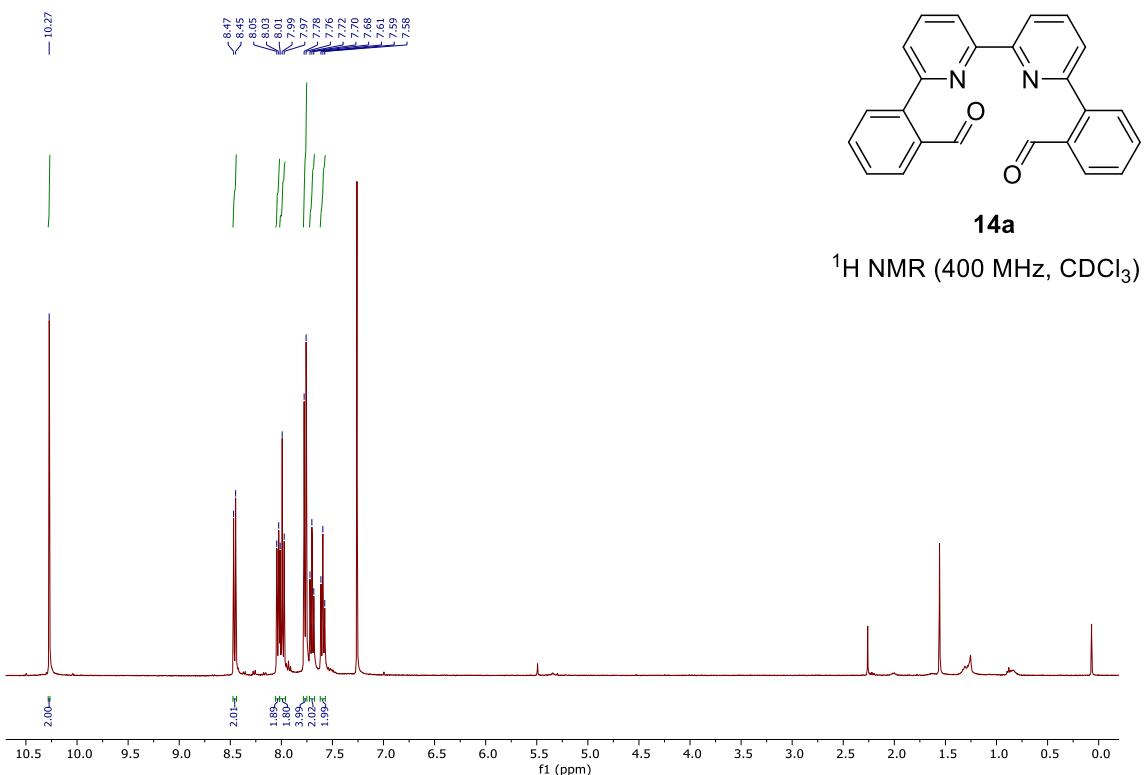


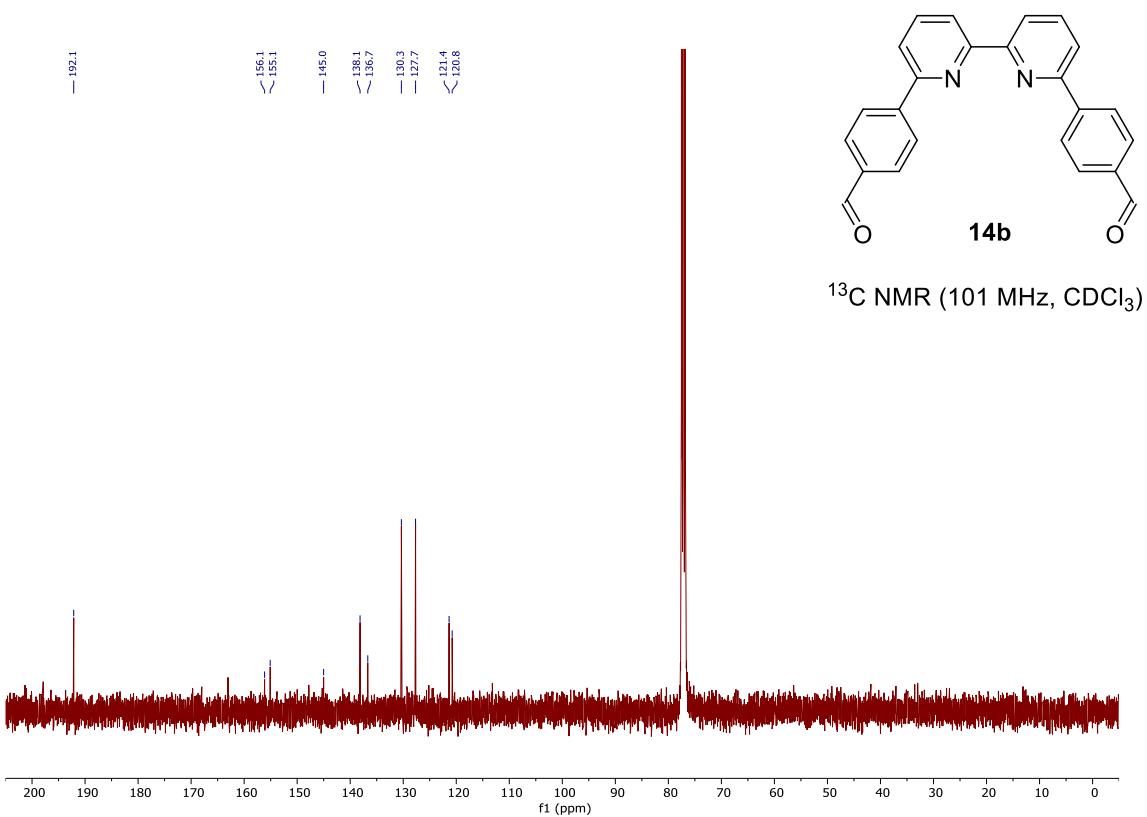
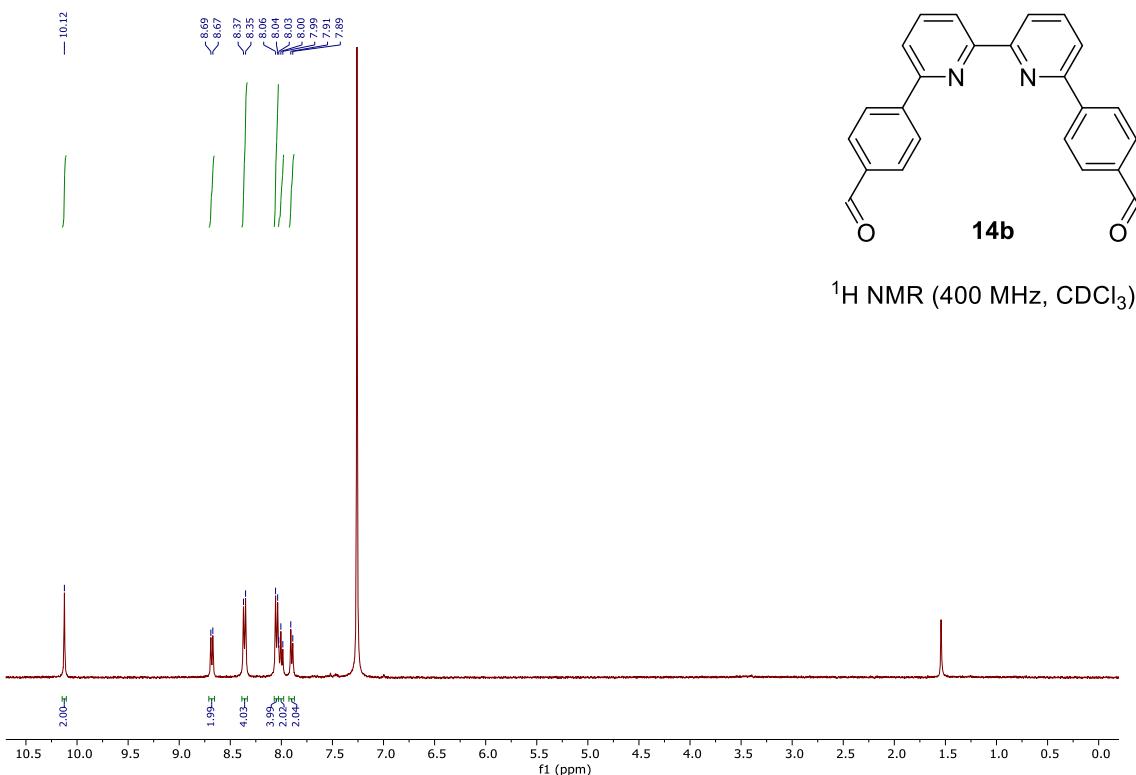




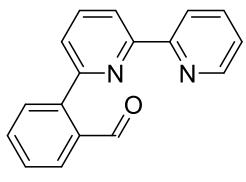
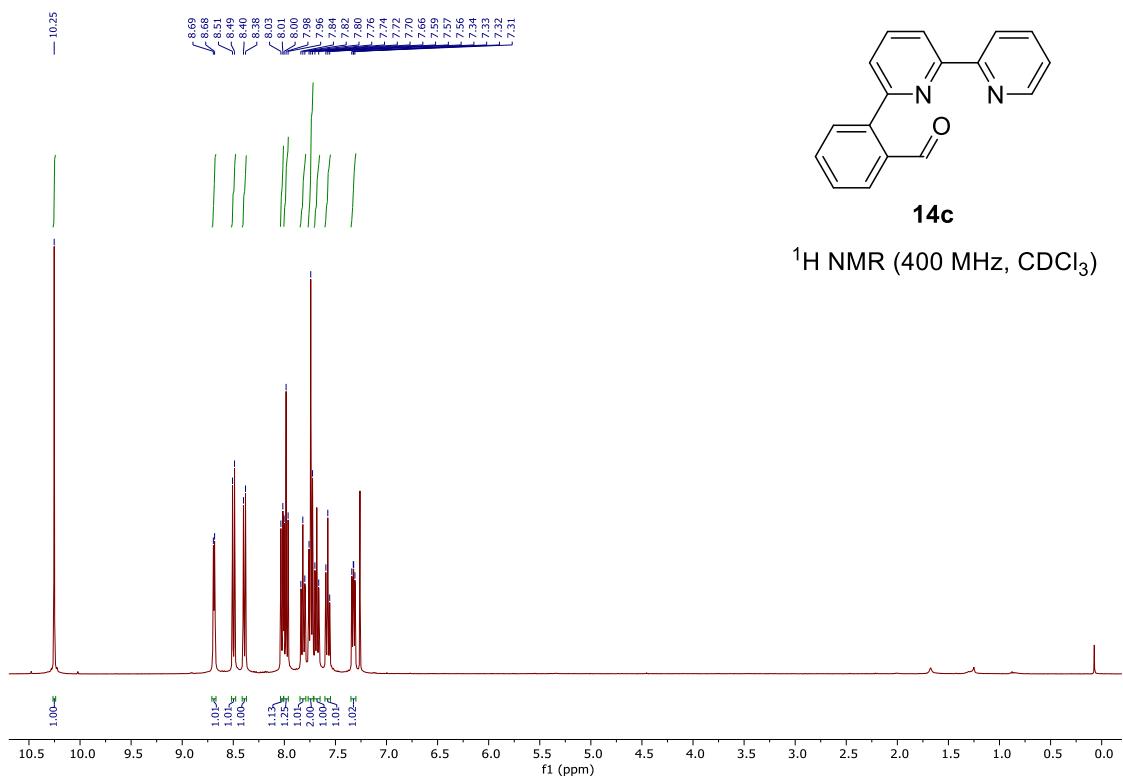




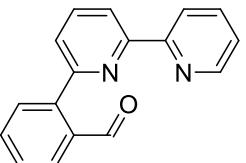
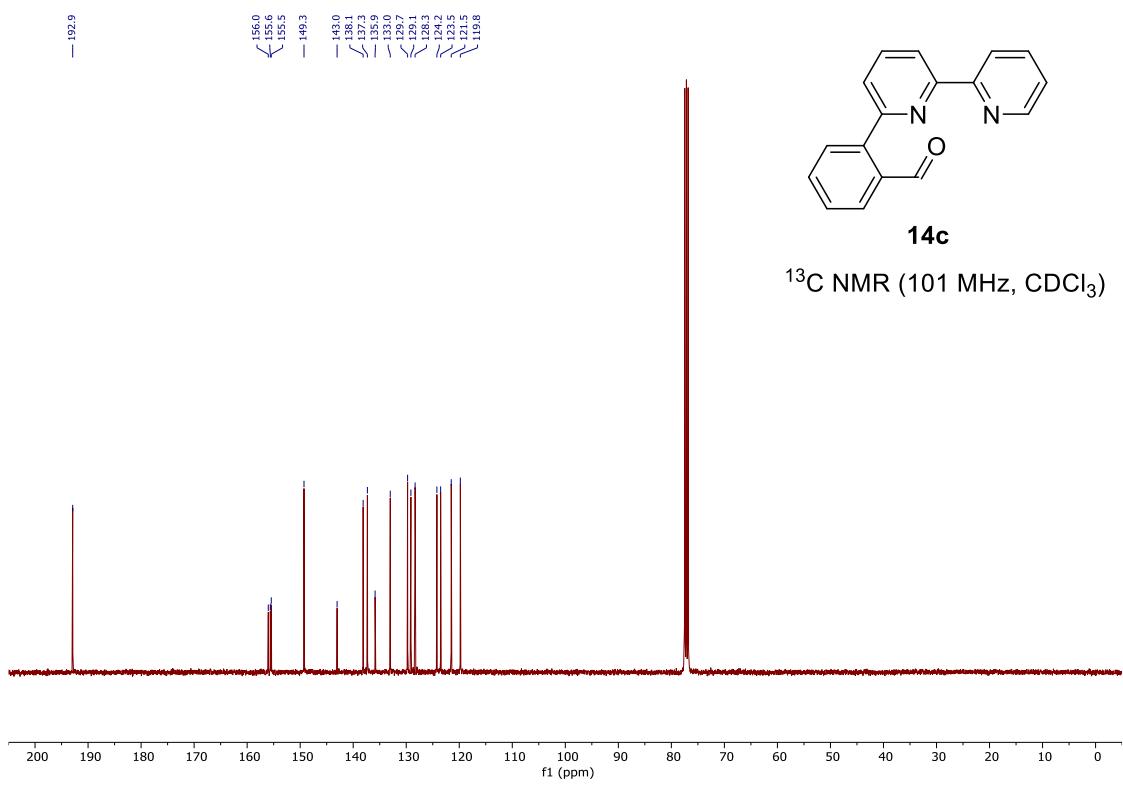




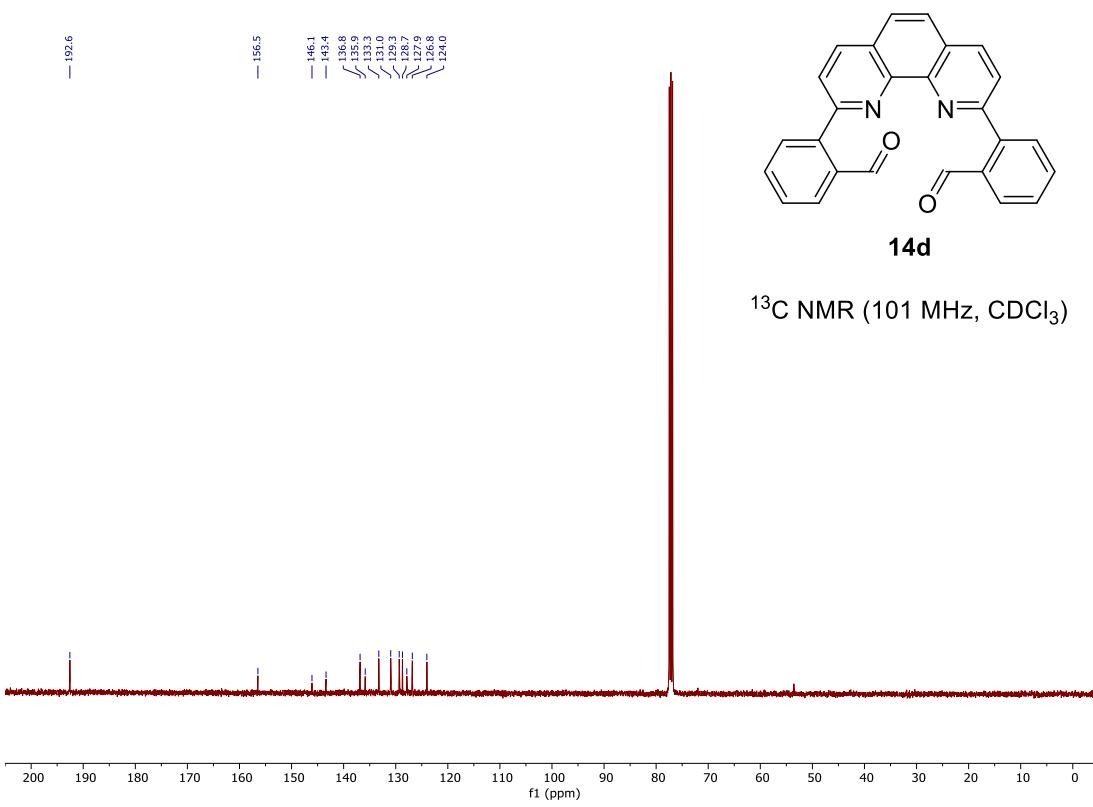
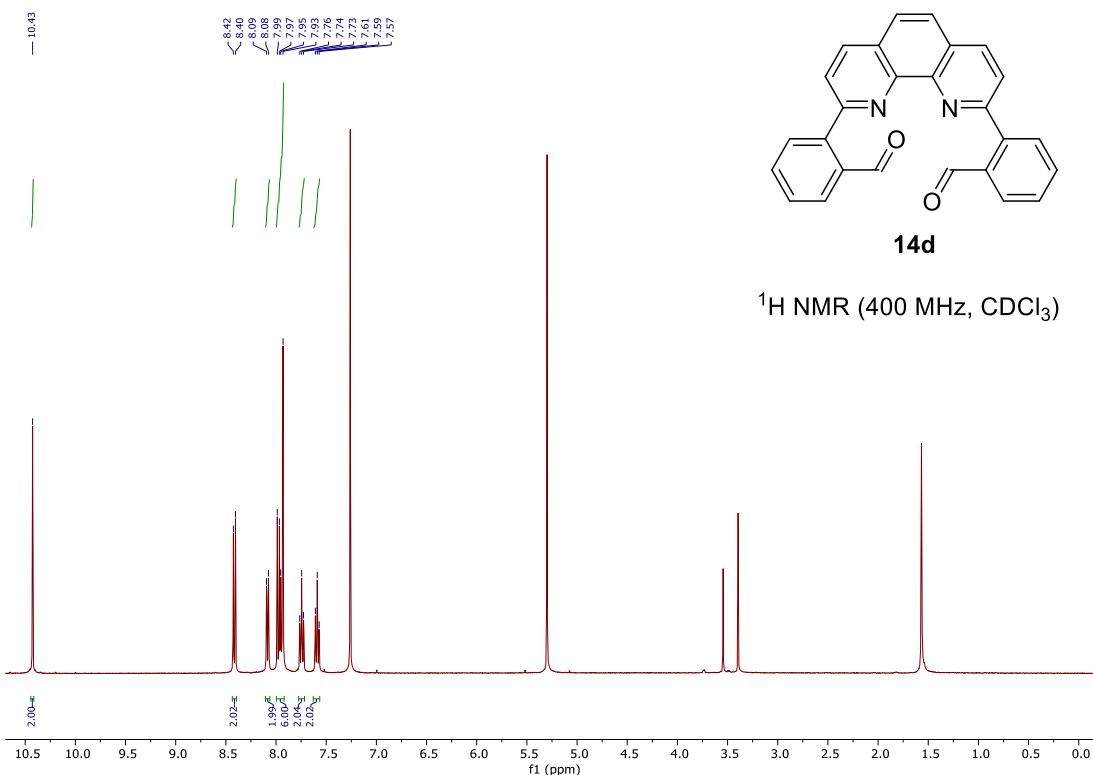
\* Due to very low solubility of the aldehyde, only a <sup>13</sup>C-NMR of low intensity was obtainable.  
 Peaks assigned based on two overlapped spectra.



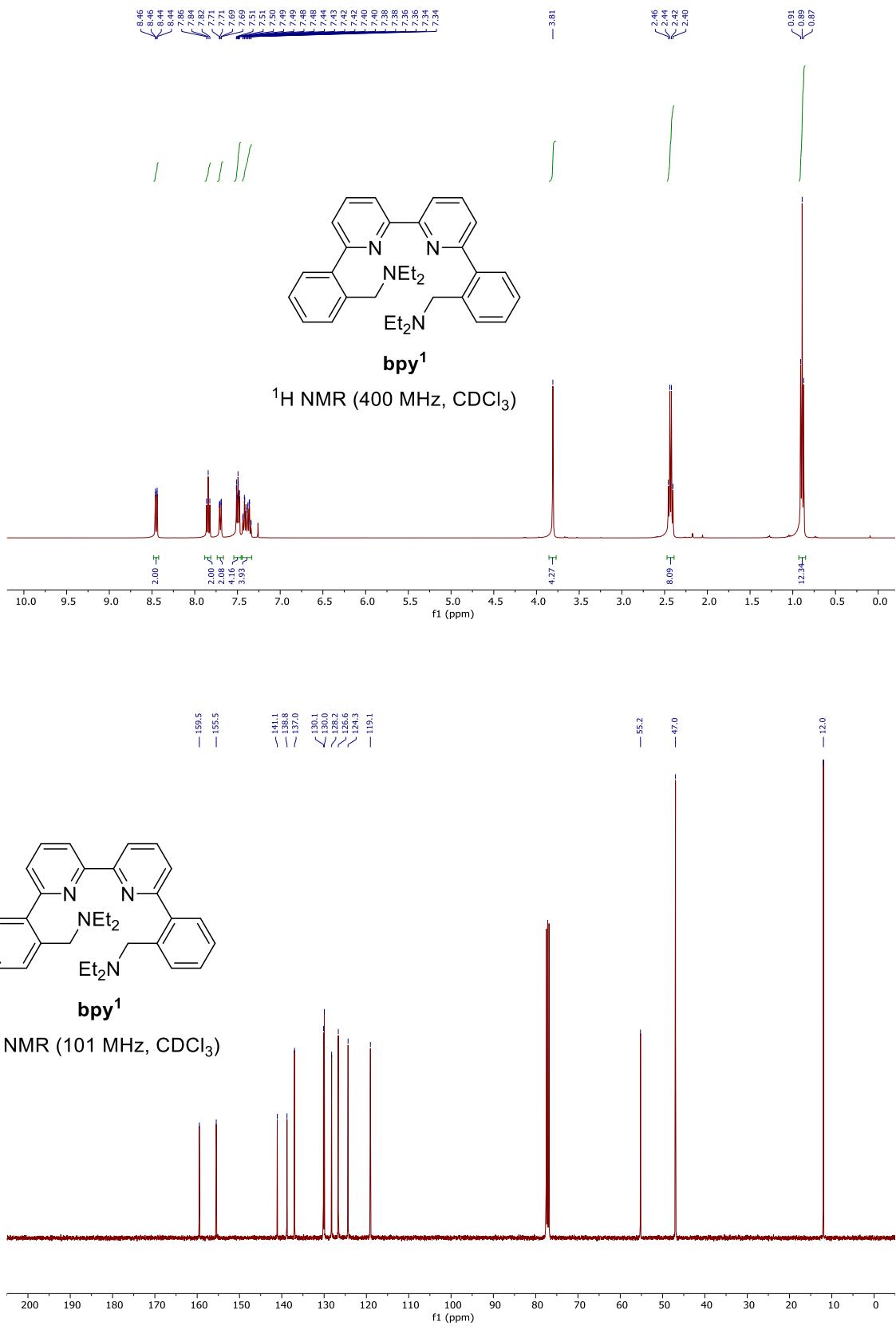
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

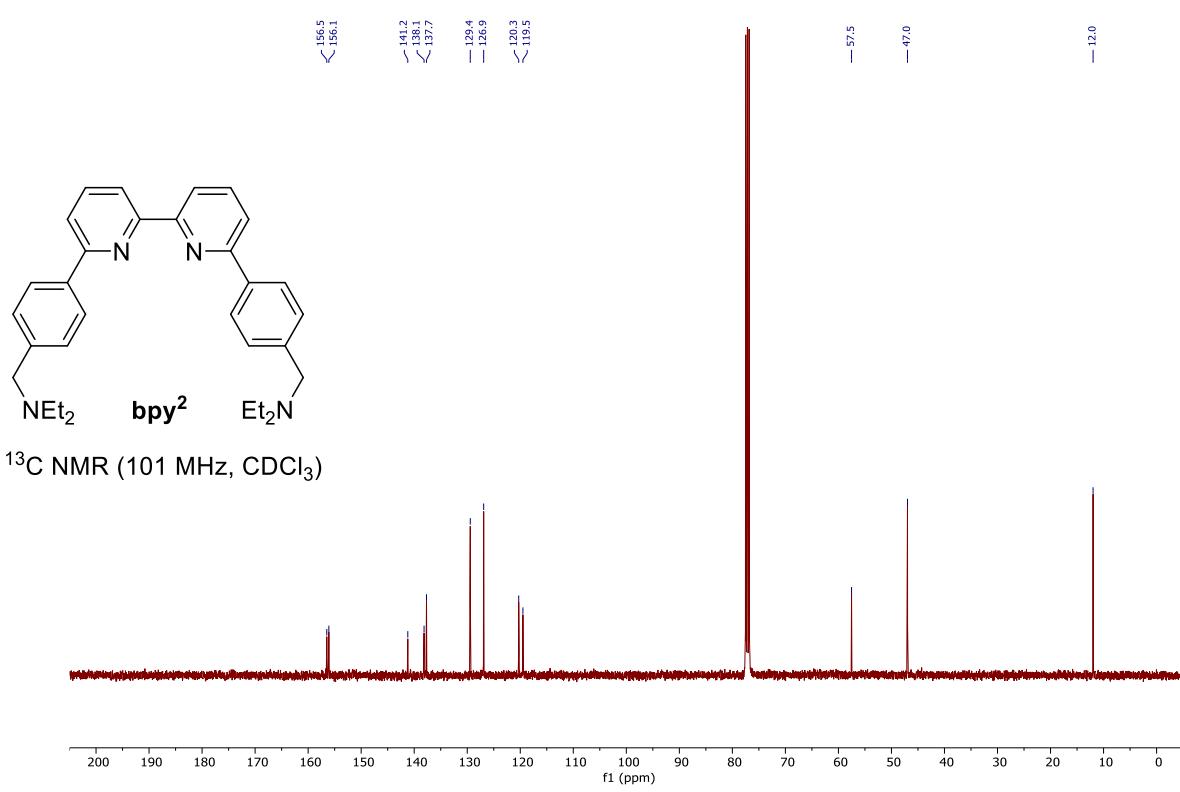
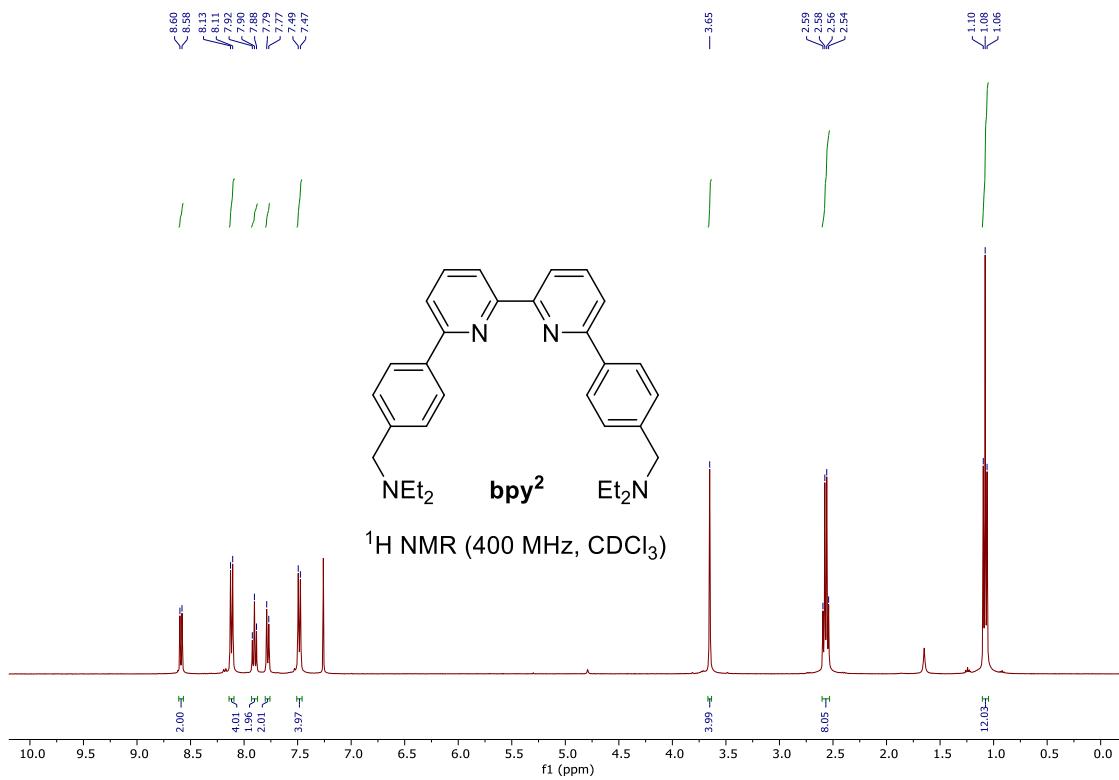


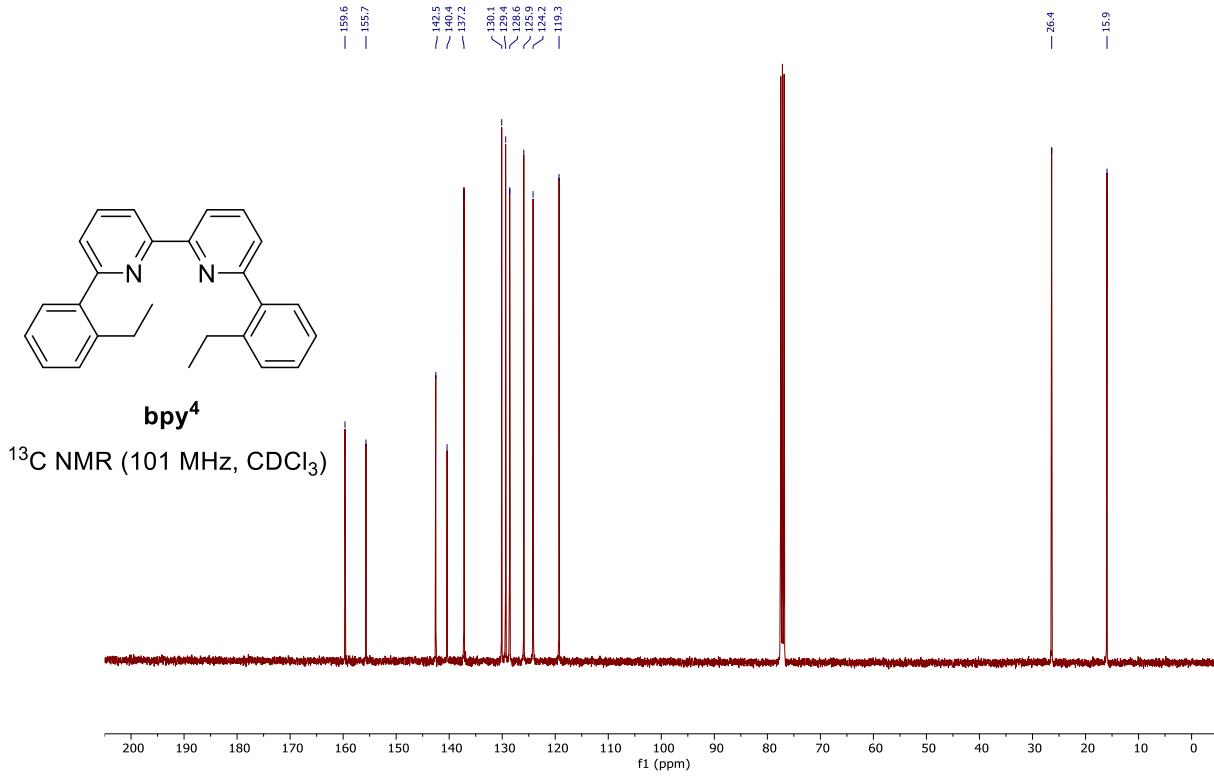
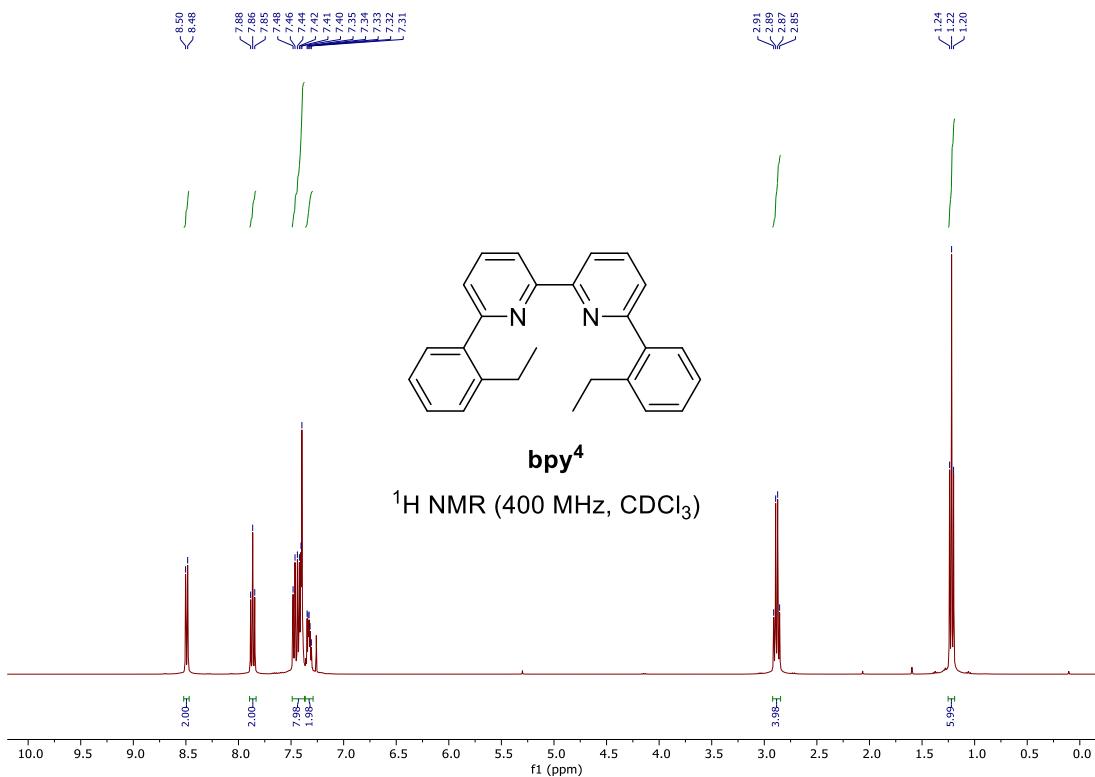
<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)

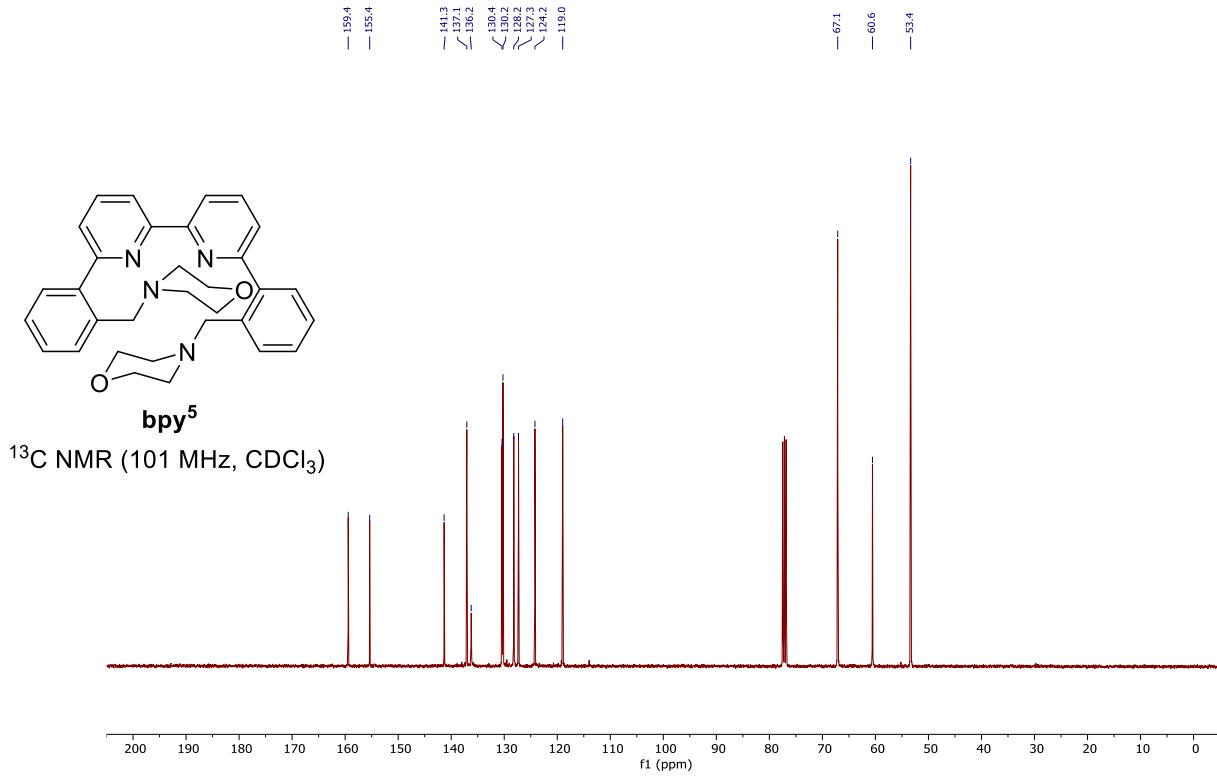
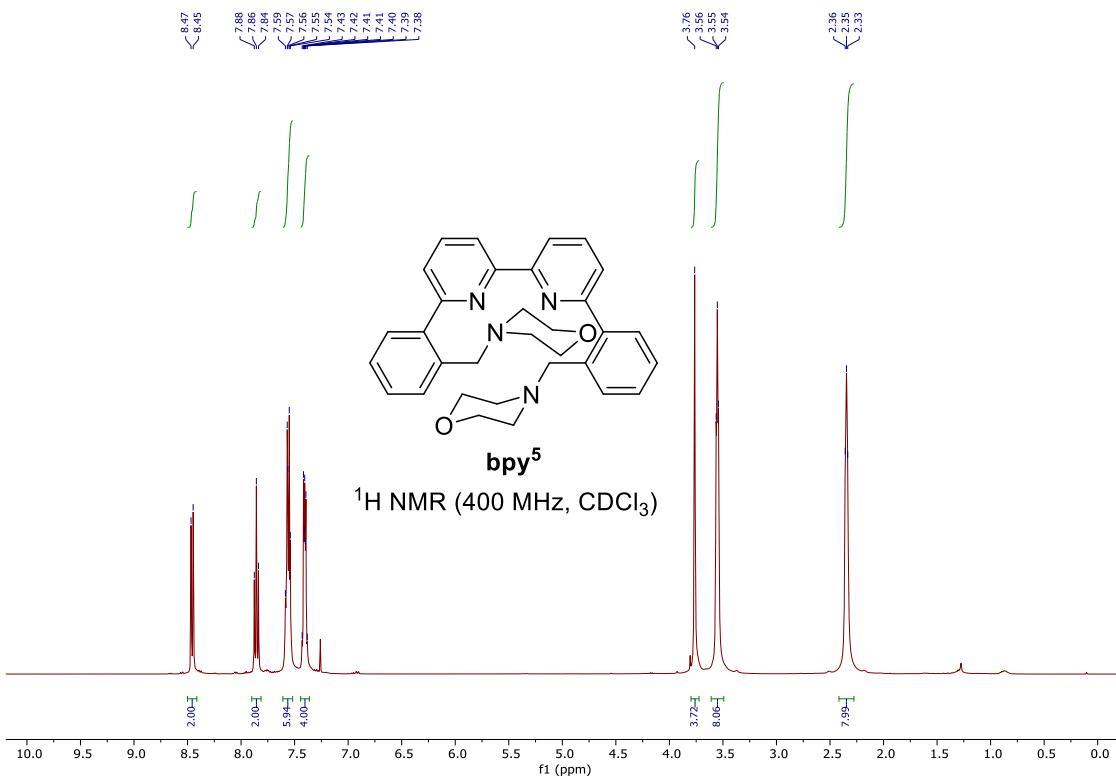


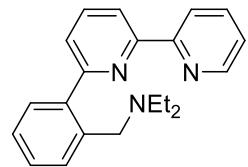
\*Extra peaks originates from dimethoxyethane, dichloromethane, and water.





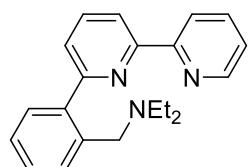
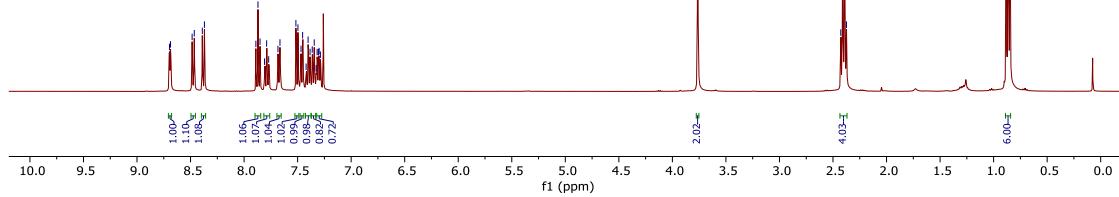






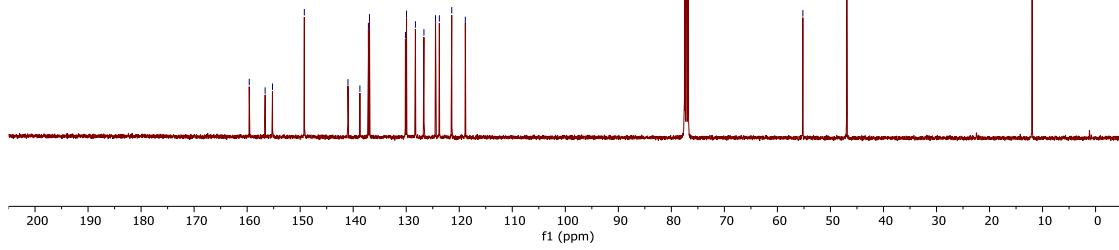
bpy<sup>6</sup>

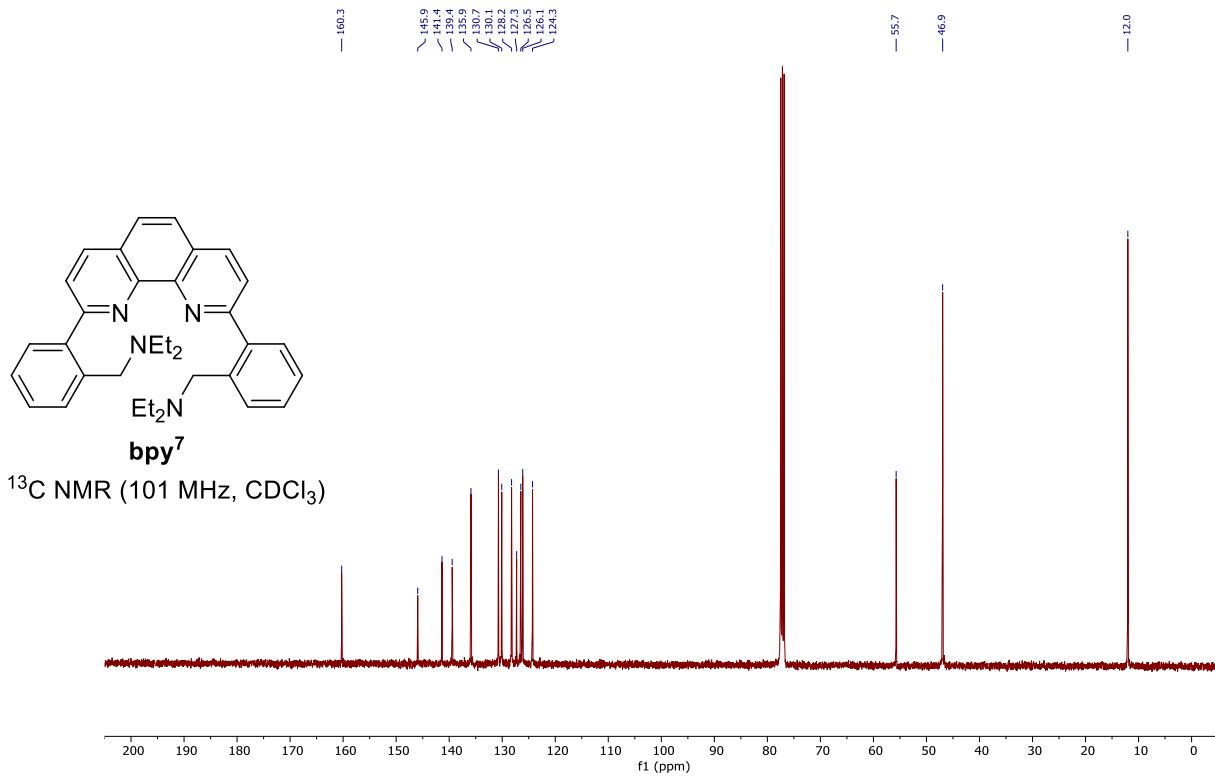
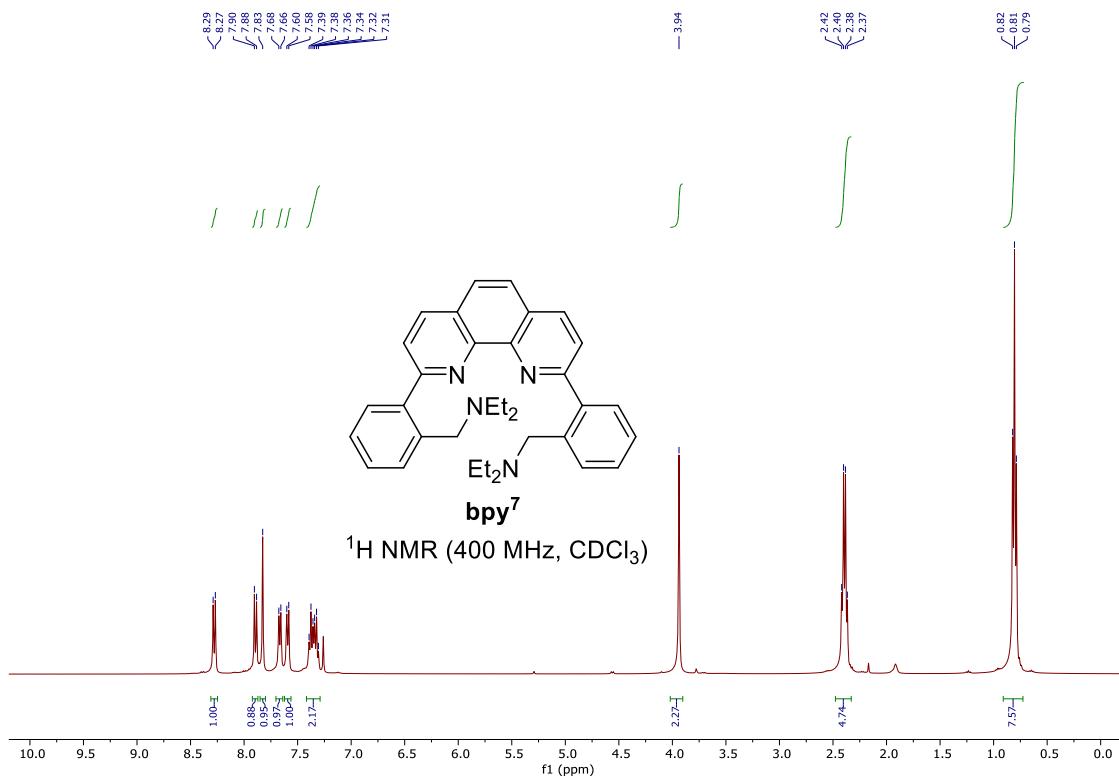
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

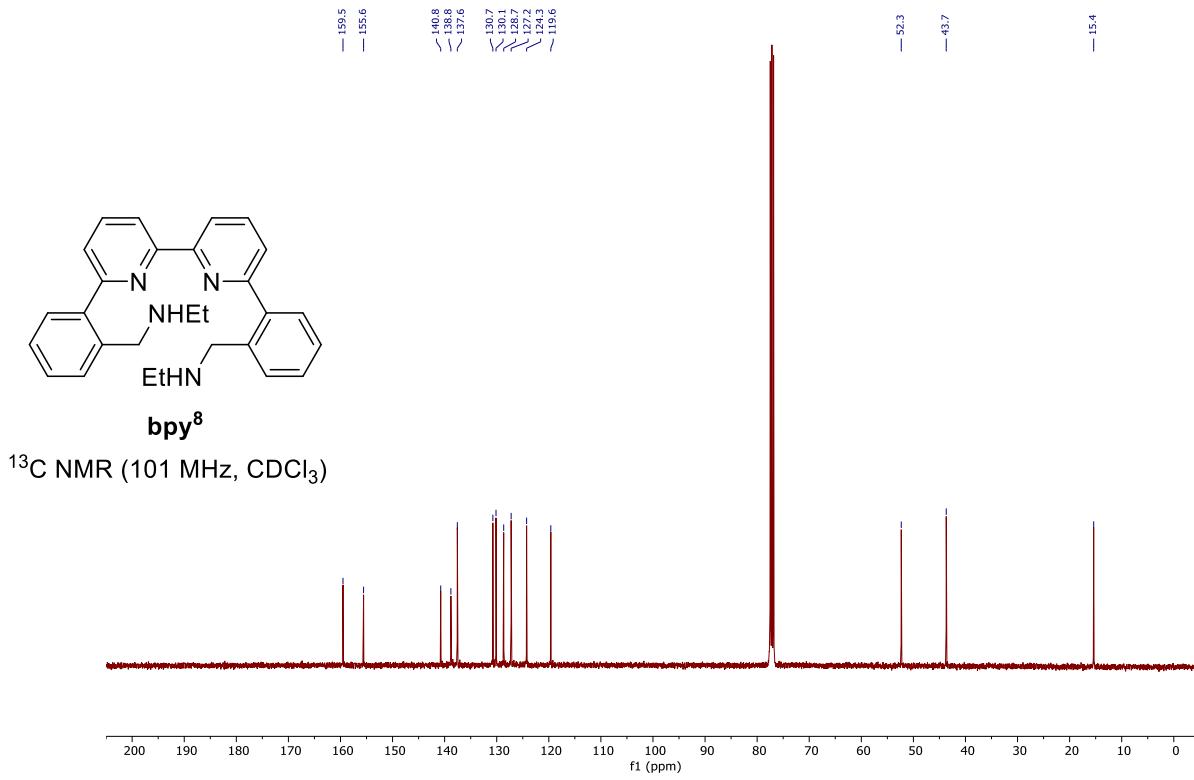
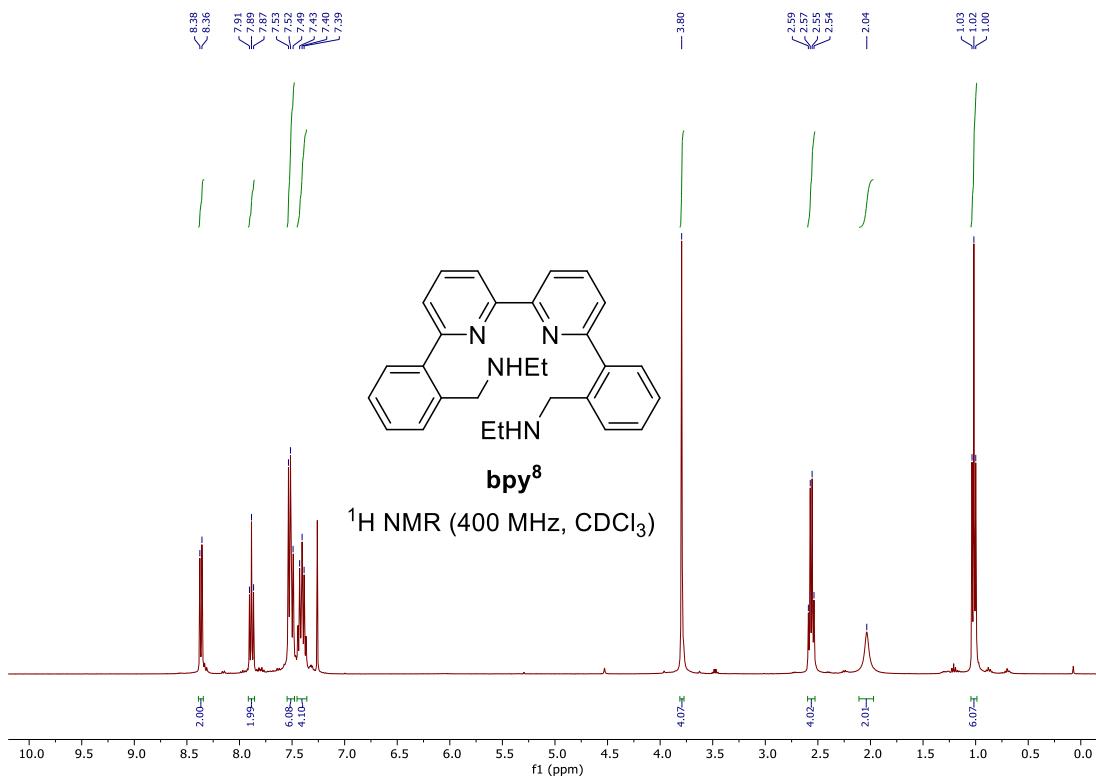


bpy<sup>6</sup>

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)







## 8. COMPUTED ENERGY COMPONENTS FOR DFT-OPTIMIZED STRUCTURES

**Table S2.** Computed energy components for DFT-optimized structures.

	E(SCF)/(eV)	ZPE/(kcal/mol)	S(gas)/(cal/mol·K)	G(solv)/(kcal/mol)
	cc-pVTZ(-f)/LACV3P**	6-31G**/LACVP**	6-31G**/LACVP**	6-31G**/LACVP**
<b>CO<sub>2</sub></b>	-5133.566	7.29	52.54	-2.57
<b>MeCN</b>	-3613.76	28.45	57.86	-17.25
<b>TFE</b>	-12325.194	36.02	76.52	-7.91
<b>FC<sub>3</sub>CH<sub>2</sub>O<sup>-</sup></b>	-12308.994	26.67	75.34	-69.49
<b>HCOO<sup>-</sup></b>	-5150.204	12.77	58.38	-76.18
<b>HCOOH</b>	-5165.695	21.21	59.26	-9.23
<b>CF<sub>3</sub>CH<sub>2</sub>OCOO<sup>-</sup></b>	-17443.859	37.24	92.93	-67.40
<b>1a</b>	-52224.156	418.51	261.08	-19.07
<b>1b</b>	-55473.543	448.01	267.50	-43.79
<b>1-vac</b>	-51858.668	418.25	244.63	-45.43
<b>A1</b>	-51865.199	415.85	243.05	-49.36
<b>A2</b>	-64191.285	453.78	277.12	-49.92
<b>A2-TS</b>	-69324.820	460.31	292.89	-50.04
<b>A2-TS''</b>	-64189.742	450.24	276.87	-56.67
<b>A3(A3')</b>	-51878.023	425.04	249.75	-43.93
<b>A4</b>	-51879.469	425.88	240.08	-24.37
<b>A4-TS</b>	-51879.211	421.31	238.87	-18.92
<b>A5</b>	-51879.758	421.76	249.46	-18.84
<b>A5-TS</b>	-57013.555	430.18	262.22	-16.82
<b>A5(red)</b>	-51881.113	419.98	245.17	-45.64
<b>A5(red)-TS</b>	-57014.836	429.53	269.03	-43.96
<b>A6</b>	-57013.641	433.15	257.56	-24.44
<b>A7</b>	-57014.539	433.92	259.92	-20.03
<b>A8</b>	-57015.859	431.08	266.64	-48.58
<b>A9</b>	-51858.883	418.69	242.81	-43.50
<b>A7-TS</b>	-74473.594	478.73	304.56	-28.59
<b>A7-H<sup>+</sup></b>	-57026.242	443.82	257.51	-47.64
<b>A8-H<sup>+</sup></b>	-57030.176	441.89	258.87	-18.84

<b>A9-H<sup>+</sup></b>	-57029.539	440.13	268.00	-30.59
<b>A9-H<sup>+</sup>-TS</b>	-57029.039	439.72	264.16	-35.58
<b>A9-H<sup>+</sup>(b)</b>	-57030.023	440.56	264.09	-29.21
<b>A10-H<sup>+</sup></b>	-57031.219	439.67	260.32	-57.97
<b>A10-H<sup>+</sup>(b)</b>	-57031.793	439.57	261.26	-55.86
<b>B1-MeCN</b>	-55477.676	446.20	270.70	-15.70
<b>B1</b>	-51863.711	416.85	249.35	-16.75
<b>B2</b>	-64189.762	455.31	278.24	-20.27
<b>B2-TS</b>	-69323.094	461.50	288.57	-23.23
<b>B3</b>	-51874.430	426.42	249.36	-58.03
<b>B3'</b>	-51874.965	427.34	244.72	-48.06

---

**Table S3.** Cartesian coordinates of the optimized geometries.

<b>CO<sub>2</sub></b>	H 0.104010656 0.225272417 -0.654933035
	O -1.384815574 -1.043683290 -1.466361642
	F -0.108311899 -0.091480784 -3.917389631
	F 1.311007261 -1.083662868 -2.601850748
	F 1.260613561 1.095320106 -2.699011326
<b>MeCN</b>	
	<b>HCOO<sup>-</sup></b>
C -1.251215100 2.816294432 -2.586167812	C -0.691797853 -0.347317129 -2.689039230
N -1.251084924 2.816349268 -3.747890234	O -0.686929405 -0.439962626 -3.946885824
C -1.251357079 2.816273928 -1.126851678	O -0.104967989 0.494798481 -1.957220912
H -0.219961464 2.816500664 -0.757072687	H -1.303341389 -1.126842618 -2.144594193
H -1.766994596 1.923071146 -0.756710529	
H -1.766755104 3.709515333 -0.756654322	
<b>TFE</b>	<b>HCOOH</b>
	C -0.966720521 -0.013352667 0.360521942
C 0.465664893 -0.015315662 -2.689784527	O -1.583956242 0.026635595 -0.826538324
C -0.497938007 0.100095846 -1.523824930	O -1.527693868 -0.009070893 1.437698603
H -1.076425076 1.021819115 -1.682487011	H 0.126898050 -0.051930286 0.225676805
H 0.113398209 0.226717472 -0.619768679	H -2.556084394 0.061309054 -0.694943428
O -1.301231861 -1.063988447 -1.495285034	
H -1.845063925 -1.035507321 -0.690665185	
F -0.174083069 -0.128454715 -3.874742746	<b>CF<sub>3</sub>CH<sub>2</sub>OCOO<sup>-</sup></b>
F 1.285091758 -1.082128167 -2.576359749	C -2.127453804 -1.202791691 -1.481776595
F 1.242744327 1.091308355 -2.750893831	C -2.410697460 -2.346045732 -1.889745951
<b>CF<sub>3</sub>CH<sub>2</sub>O<sup>-</sup></b>	O -2.009429455 -3.472097397 -1.530089855
	C -5.268181324 -3.742760897 -2.880410671
C 0.466216624 -0.022721818 -2.685961962	C -3.885252953 -3.511925220 -3.461391449
C -0.567409098 0.017843857 -1.543267488	H -3.991169930 -3.461877584 -4.551158428
H -1.040906787 1.031888604 -1.718762279	H -3.259426117 -4.365709782 -3.189683676
	O -3.354443550 -2.292230844 -2.984540462

F	-6.140557289	-2.768109560	-3.229139805
F	-5.252087116	-3.792335033	-1.530387640
F	-5.781383038	-4.916139126	-3.326528549

---

**1a**

---



---

Br	-0.706541419	12.747546196	5.802068710
Mn	-0.048095442	14.937510490	4.397644043
O	0.546206832	17.366558075	2.849995852
O	2.556396246	13.644273758	3.824009895
O	-0.614067793	13.304308891	1.994174004
N	-5.034264565	12.019864082	3.211404562
N	-1.948389769	15.692969322	4.906384945
N	0.370149195	15.809917450	6.287236691
N	4.461111546	12.547880173	7.397015095
C	0.329126656	16.404132843	3.457746506
C	1.585214972	14.195224762	4.118086338
C	-0.492725521	13.983008385	2.920435190
C	-7.359641552	11.869465828	2.275529146
H	-7.658302307	10.952566147	2.794190407
H	-6.948359013	11.590360641	1.299243689
H	-8.267063141	12.461444855	2.111151457
C	-6.338581562	12.688970566	3.067536354
H	-6.164531708	13.629247665	2.534449339
H	-6.754120827	12.964045525	4.056821823
C	-5.094521999	10.898303032	4.161509991
H	-5.977260113	10.300591469	3.916536570
H	-5.244284153	11.262070656	5.197607517
C	-3.867180109	9.984683037	4.102150917
H	-4.036527157	9.094181061	4.717405796
H	-2.960226059	10.473484039	4.472203732
H	-3.685521364	9.660343170	3.071587801
C	-4.005658150	12.991490364	3.593766212
H	-3.094492912	12.459106445	3.885446072
H	-4.308173180	13.561067581	4.490816116
C	-3.619374275	13.943547249	2.472723961

C	-3.677590847	13.522501945	1.138927460
H	-4.084037781	12.537239075	0.931133986
C	-3.225014448	14.338392258	0.101911418
H	-3.283994436	13.987197876	-0.926212966
C	-2.694306612	15.600637436	0.383433968
H	-2.341393709	16.243059158	-0.419749916
C	-2.628396749	16.036830902	1.706230164
H	-2.228358984	17.020929337	1.937773347
C	-3.079142332	15.215397835	2.751067638
C	-3.068720818	15.744004250	4.147572041
C	-4.263497829	16.295778275	4.629530430
H	-5.128878593	16.320680618	3.974482536
C	-4.321413994	16.801597595	5.921528339
H	-5.234839916	17.245000839	6.309750080
C	-3.176703691	16.733415604	6.707852840
H	-3.190539837	17.137380600	7.713416576
C	-2.010443449	16.170137405	6.179012775
C	-0.766114712	16.099020004	6.974071980
C	-0.765456736	16.331905365	8.354081154
H	-1.691344500	16.506116867	8.889764786
C	0.442867428	16.323150635	9.043358803
H	0.469387114	16.501007080	10.115448952
C	1.614166975	16.114427567	8.325572014
H	2.583347797	16.164714813	8.811171532
C	1.553833485	15.861154556	6.947229385
C	2.837672234	15.761136055	6.194972038
C	3.100277185	16.744979858	5.227292538
H	2.345463037	17.499586105	5.026089191
C	4.309596539	16.766422272	4.534852028
H	4.492457390	17.527574539	3.780015945
C	5.282463551	15.809803009	4.832489014
H	6.235760212	15.816204071	4.308045864
C	5.034789085	14.842991829	5.808286190
H	5.785403252	14.095064163	6.044039249
C	3.816201925	14.788774490	6.494913101

C	3.559166908	13.693765640	7.525293827	N	-0.518762469	1.896169066	-0.753912449
H	3.711647034	14.115880013	8.526651382	H	2.851483822	2.098796368	-1.080981255
H	2.493424892	13.407320976	7.487874508	H	2.396250725	0.448645949	-2.877156973
C	5.614215374	10.688866615	8.612087250	H	0.042330060	-0.363534898	-3.190096855
H	5.319176197	9.859419823	7.961116791	C	-2.128531694	0.371071309	-1.849912286
H	5.766514301	10.280285835	9.616815567	C	-2.933732510	0.574479163	-2.987325430
H	6.571554661	11.081995964	8.251565933	C	-2.559995174	-0.500064254	-0.833831429
C	4.561149120	11.797768593	8.656623840	C	-4.174962521	-0.074937232	-3.048922777
H	3.590162992	11.368046761	8.966080666	C	-3.795792818	-1.137176991	-0.912217021
H	4.836703777	12.516018867	9.439218521	C	-4.609601498	-0.917986333	-2.027562380
C	4.176716805	11.713090897	6.212888718	H	-1.907811046	-0.685870051	0.014989185
H	4.133697987	12.379820824	5.347836971	H	-4.792230129	0.090902172	-3.926789284
H	5.039268017	11.058581352	6.047027588	H	-4.114531517	-1.805300117	-0.115661301
C	2.892965555	10.868344307	6.251521111	H	-5.578278065	-1.407730222	-2.103695631
H	2.907381535	10.136658669	7.067102432	C	-2.558286190	1.542452574	-4.099092960
H	2.796255589	10.312390327	5.311662197	H	-1.483076096	1.784030676	-4.053008556
H	1.995211482	11.485673904	6.355895519	H	-3.079395294	2.484417915	-3.896459818

---

### 1b

---

C	0.276493549	0.413762093	-2.470065594	N	-2.978432894	1.070122004	-5.420274734
Mn	-1.879661083	3.108592987	0.298248380	C	-2.220948458	-0.101171233	-5.889071941
C	0.984793484	3.152443886	0.658653319	H	-2.279633760	-0.865795255	-5.105583668
C	2.252019405	3.619956017	1.018128157	H	-2.752410412	-0.510008693	-6.757962704
C	2.407179117	4.312952042	2.216212988	C	-0.749321282	0.137458742	-6.267152309
C	1.297083020	4.489058971	3.033359528	H	-0.659787655	0.852113068	-7.091969013
C	0.040060308	4.037639141	2.609081268	H	-0.165351331	0.523334622	-5.425410748
N	-0.116789483	3.416822672	1.414348602	H	-0.286898315	-0.802953303	-6.586821079
H	3.114627600	3.437234402	0.387999207	C	-3.068365335	2.148406506	-6.414929867
H	3.386348248	4.673381329	2.521453619	H	-2.175648928	2.800035954	-6.404196262
H	1.385974407	4.945596218	4.013529778	H	-3.091727734	1.681308389	-7.406635284
C	0.768499315	2.272527933	-0.515058637	C	-4.332607746	2.995589018	-6.242464066
C	1.833277583	1.783265591	-1.277715206	H	-4.358233929	3.511093378	-5.275838375
C	1.581619382	0.850914180	-2.280303478	H	-4.387009144	3.761704922	-7.024096489
C	-0.760420144	0.952594995	-1.696925521	H	-5.225337029	2.364690065	-6.310399532
				C	-1.110030293	4.114661694	3.559335947
				C	-1.565430641	2.890697956	4.083536625
				C	-1.680817842	5.323002815	4.006413460

C	-2.599075079	2.847084522	5.015015602	H	-1.269809127	7.282392502	-2.664964914
C	-2.723633051	5.258635044	4.941944599	H	0.100235291	6.311952591	-3.284943342
C	-3.184775591	4.042316914	5.442195892	=====	=====	=====	=====
H	-1.086319923	1.970092654	3.762241364	<b>1-vac</b>	=====	=====	=====
H	-2.937329769	1.891361833	5.408246517	C	0.346536577	1.191607952	-2.648625374
H	-3.162215948	6.193556786	5.277207851	Mn	-1.362348676	1.812646985	1.303443432
H	-3.995552063	4.026450634	6.167540073	C	0.982674599	3.245068073	0.977964759
C	-1.290769935	6.683176994	3.445257187	C	2.177484035	3.815325260	1.419804573
H	-0.316139787	6.625077724	2.933716059	C	2.146528482	4.660197258	2.528944969
H	-2.015560627	6.930959702	2.662109613	C	0.922393262	4.959043503	3.123580694
N	-1.338622808	7.738925934	4.459126472	C	-0.246346503	4.350974083	2.650642872
C	-1.468384147	9.087239265	3.889924288	N	-0.192809209	3.447693110	1.639582038
H	-0.748060048	9.265371323	3.070738077	H	3.114172459	3.614612341	0.910995543
H	-1.213887572	9.803574562	4.680158615	H	3.063796043	5.111769676	2.898443699
C	-2.890718222	9.379736900	3.402859926	H	0.854369462	5.667927265	3.943189383
H	-3.195889711	8.712132454	2.589302778	C	0.857157052	2.448965549	-0.266146600
H	-3.606289387	9.259474754	4.223324776	C	1.899884105	2.294449568	-1.181796312
H	-2.960378647	10.406967163	3.027633190	C	1.639557004	1.639151931	-2.384517193
C	-0.277309239	7.623725891	5.470880508	C	-0.661030293	1.360056400	-1.691074610
H	-0.541228235	8.287487984	6.304291248	N	-0.388981819	1.944386601	-0.497095942
H	-0.312700123	6.602329254	5.868098736	H	2.888664722	2.690024614	-0.974987805
C	1.153216124	7.946956635	5.007182121	H	2.430159807	1.504765630	-3.118608475
H	1.857991457	7.800262451	5.833095074	H	0.100520782	0.715687990	-3.592795134
H	1.473680615	7.304353237	4.180570602	C	-2.038654327	0.863258243	-1.979330897
H	1.239053488	8.986586571	4.674460888	C	-3.125034809	1.724629283	-2.231513500
C	-3.287803411	2.938619137	-0.836894333	C	-2.219189882	-0.529634118	-2.056910992
O	-4.219047070	2.939321518	-1.516536117	C	-4.381721973	1.155753493	-2.488777161
C	-2.465767384	1.753704190	1.338743210	C	-3.474411726	-1.074895263	-2.313547611
O	-2.848187685	0.893558681	2.002980471	C	-4.566248417	-0.224707708	-2.517355680
C	-2.915731192	4.315454006	1.179690123	H	-1.366272688	-1.182523608	-1.888822317
O	-3.634242058	5.090277672	1.639960885	H	-5.214047909	1.822348952	-2.699869156
C	-0.821586967	5.562846661	-1.557016373	H	-3.600495577	-2.154104471	-2.353125095
N	-1.160331607	4.672893524	-0.898970962	H	-5.552779198	-0.637610614	-2.716302872
C	-0.394813955	6.685899734	-2.381143570	C	-3.008068323	3.236418962	-2.332953215
H	0.304407597	7.313004971	-1.815500855				

H	-1.990450144	3.571679354	-2.070573092	H	-4.708364964	6.911022186	-0.429929465
H	-3.675183296	3.683025837	-1.590546012	H	-4.535938740	8.556124687	0.202939078
N	-3.440749884	3.705825567	-3.655385971	H	-4.410442352	8.246626854	-1.544351339
C	-2.538655996	3.304038048	-4.745110512	C	-0.942376256	7.611781120	1.351105571
H	-2.436701775	2.212815285	-4.706341267	H	-0.963764250	8.707466125	1.406236529
H	-3.046351910	3.532423496	-5.690769196	H	-0.786562383	7.257654190	2.376678705
C	-1.142994523	3.948504925	-4.750442982	C	0.241892025	7.175163746	0.471036702
H	-1.208163261	5.039624214	-4.818497181	H	1.181250572	7.551376820	0.890166998
H	-0.573700249	3.698129416	-3.849410295	H	0.328156143	6.085880280	0.405139714
H	-0.567660630	3.591617584	-5.611804008	H	0.146104500	7.565915108	-0.547449470
C	-3.785023451	5.135621071	-3.666001320	C	-2.985578537	2.440121889	0.947787702
H	-3.044729948	5.744107246	-3.115502596	O	-4.037446022	2.863939047	0.735948205
H	-3.749018431	5.481615543	-4.705492020	C	-1.904762387	0.082521126	1.067089200
C	-5.189179420	5.392991543	-3.112402916	O	-2.211158037	-1.023719668	1.012543440
H	-5.288460732	5.072114468	-2.069524050	C	-1.809167385	1.593784571	3.062470675
H	-5.425157070	6.461925507	-3.149873734	O	-2.092434645	1.374984980	4.154736996
H	-5.934507370	4.849346638	-3.702951670	=====			
C	-1.563529968	4.699672222	3.249084234	<b>A1</b>			
C	-1.736411214	4.482813358	4.628152370	=====			
C	-2.601014614	5.293230057	2.494986296	C	-0.680835903	1.861526132	-5.569907665
C	-2.940378189	4.792639732	5.254493237	Mn	-3.500311136	1.206906915	-2.295587301
C	-3.800071239	5.608701706	3.150223732	C	-0.866968393	2.091146946	-1.409151077
C	-3.982513189	5.351590157	4.507438183	C	0.154428229	2.602607965	-0.575135410
H	-0.923451781	4.041445732	5.199647427	C	0.001478462	2.598497868	0.792806804
H	-3.066526651	4.597265244	6.316668987	C	-1.167019725	2.015251637	1.322222114
H	-4.597864628	6.076626301	2.577229738	C	-2.129890680	1.491966724	0.475113809
H	-4.929055214	5.596070290	4.984263897	N	-2.041775703	1.580040216	-0.893436491
C	-2.470684528	5.712250233	1.038858891	H	1.062930584	2.999268770	-1.014760971
H	-1.687164426	5.136257172	0.523990333	H	0.775617063	2.994947672	1.445110083
H	-3.407723427	5.458947659	0.535690844	H	-1.306803346	1.921135068	2.394668102
N	-2.276403666	7.166030407	0.920470178	C	-0.780916572	2.069777012	-2.839374781
C	-2.652442932	7.671620369	-0.409778208	C	0.325979710	2.592742682	-3.542046070
H	-2.272874594	7.022279739	-1.219590545	C	0.371106178	2.532060862	-4.917646885
H	-2.165728807	8.644008636	-0.548434496	C	-1.736320615	1.330071092	-4.846976280
C	-4.165061951	7.854049206	-0.551362455	N	-1.886725783	1.521852612	-3.481775522

H	1.145077229	3.048051357	-2.995060921	C	-0.490415096	-1.490694404	2.492184401
H	1.209663749	2.941788435	-5.474739552	H	0.398095489	-1.065012932	1.985924721
H	-0.650619447	1.697096944	-6.642364025	C	-0.414263487	-3.272134542	0.842737973
C	-2.713526011	0.510214627	-5.612987995	H	0.275681525	-3.719608068	1.564349413
C	-2.884909630	-0.878048003	-5.399838924	C	-4.711929798	1.195251346	-3.600746393
C	-3.388955832	1.127639294	-6.677285671	O	-5.607029915	1.232897758	-4.361674786
C	-3.771472454	-1.574496627	-6.230242729	C	-4.552118778	2.339214325	-1.461252451
C	-4.261505127	0.417349100	-7.499935150	O	-5.274765491	3.069885254	-0.874727488
C	-4.462328434	-0.944064438	-7.268326759	C	-4.116805077	-0.344833195	-1.739413619
H	-3.232517719	2.191236973	-6.843191624	O	-4.656826019	-1.356652379	-1.453285456
H	-3.904604197	-2.643463373	-6.070405960	H	-1.112681270	-0.637293696	2.777914286
H	-4.777949810	0.924400985	-8.312134743	H	0.216616601	-2.745263577	0.100232378
H	-5.138826370	-1.516913772	-7.898882866	H	1.127114177	-2.069442987	-4.674198151
C	-2.185520172	-1.631902933	-4.283812046	H	-0.518708408	-2.422165871	-2.272603273
H	-2.381458044	-2.713938713	-4.408670425	C	-0.071405314	-2.232911348	3.762105227
H	-2.674600363	-1.325824738	-3.354642153	H	-0.953090847	-2.623287916	4.281843662
N	-0.753117621	-1.368567109	-4.122049809	H	0.600377798	-3.073487043	3.557977915
C	-0.382040203	-1.408162236	-2.702819109	H	0.455211997	-1.550915718	4.439336300
H	-1.084697247	-0.748688817	-2.185960293	C	-1.189531088	-4.400442123	0.159054339
C	0.084182031	-2.216401815	-4.968811989	H	-0.491783291	-5.125338554	-0.274879903
H	-0.136493295	-3.292368889	-4.802343845	H	-1.823208094	-4.922437668	0.884266198
C	-3.237027168	0.723532498	1.119891405	H	-1.828363895	-4.036673546	-0.652109861
C	-4.293935776	1.404092431	1.740008712	C	1.039556980	-0.922834635	-2.412807226
C	-3.129524946	-0.674439907	1.259761930	H	1.154228568	-0.748712480	-1.337041736
C	-5.256546021	0.711530983	2.474525690	H	1.809313536	-1.642387986	-2.712284803
C	-4.097464561	-1.356243253	2.007740259	H	1.223540187	0.022448733	-2.932007551
C	-5.157995701	-0.677611947	2.609968185	C	-0.033834420	-1.893297672	-6.460723877
H	-4.354867935	2.483711243	1.638688207	H	0.689158618	-2.486690998	-7.032291889
H	-6.070669651	1.255332112	2.948807240	H	-1.031940937	-2.105716228	-6.852125168
H	-3.995100975	-2.432067871	2.126455545	H	0.170695707	-0.831294239	-6.628294945
H	-5.897481441	-1.225468397	3.189848661	=====			
C	-2.005805492	-1.461578369	0.612689435	<b>A2</b>			
H	-2.451064825	-2.092420578	-0.160608426	=====			
H	-1.313617229	-0.781257689	0.093342744	C	-1.648405075	1.748772502	-4.199356556
N	-1.277813315	-2.321625233	1.564357758	Mn	-3.354001045	1.798325896	-0.206273481

C	-0.661093593	2.914717436	-0.314069659	H	1.035672784	-1.495698094	-0.917173684
C	0.534807205	3.557585239	0.058138352	C	-2.131874084	2.126419544	3.023716927
C	0.821990430	3.783947706	1.386956573	C	-2.670926332	3.043549538	3.940347195
C	-0.103475839	3.304298639	2.335497618	C	-2.334818125	0.744149566	3.226746321
C	-1.267949462	2.668241739	1.937992573	C	-3.422082901	2.620390892	5.034893036
N	-1.627986073	2.514788389	0.607998610	C	-3.111562252	0.334884405	4.318835258
H	1.244330049	3.850055456	-0.708630741	C	-3.650504589	1.256063104	5.219013691
H	1.746531725	4.264990807	1.694470048	H	-2.497497559	4.104524612	3.776692152
H	0.105198659	3.383723259	3.398012638	H	-3.828644276	3.350120783	5.731773376
C	-0.975525260	2.600239277	-1.676125884	H	-3.275461674	-0.726206660	4.476416588
C	-0.243633226	3.069409370	-2.789373636	H	-4.241678238	0.906217277	6.062560081
C	-0.615108848	2.695453882	-4.064542770	C	-1.730193973	-0.304622561	2.313391447
C	-2.303871632	1.281136751	-3.072220087	H	-2.547224998	-0.865250349	1.859370112
N	-2.090864897	1.812767029	-1.824936032	H	-1.194282413	0.172889471	1.485745907
H	0.595394373	3.741045713	-2.641332150	N	-0.866162181	-1.288676500	3.017705679
H	-0.082063958	3.071254730	-4.934607506	C	0.255900502	-0.653279364	3.755003214
H	-1.888725400	1.315232515	-5.165518284	H	0.697740912	-1.429595351	4.387405872
C	-3.176594019	0.085588120	-3.215408325	C	-0.367446065	-2.317255974	2.071014881
C	-2.758853912	-1.157879949	-2.681560993	H	0.366927087	-2.918544054	2.617293835
C	-4.334805489	0.153340712	-3.998209000	C	-4.406033516	2.244376183	1.156792879
C	-3.538485765	-2.288446903	-2.943104744	O	-5.188244343	2.536296606	1.984169602
C	-5.106342316	-0.985212386	-4.240475178	C	-3.878494024	0.133412272	-0.043477248
C	-4.706456661	-2.212311745	-3.708959103	O	-4.364934921	-0.932576120	0.118833236
H	-4.632593632	1.115080953	-4.407632351	C	-4.597217083	2.391977072	-1.299633503
H	-3.220459461	-3.249372959	-2.542105675	O	-5.429938316	2.720767260	-2.072645426
H	-6.007344723	-0.912547588	-4.845856667	H	-0.181794167	0.093053877	4.424709797
H	-5.292046070	-3.109585762	-3.897516012	H	0.160698131	-1.844999433	1.228845716
C	-1.521384835	-1.288171530	-1.809752226	H	0.279021055	0.059206583	-0.553521335
H	-1.389122128	-2.353897095	-1.543768883	C	-0.729751587	-3.945297480	5.973575115
H	-1.717172265	-0.753990829	-0.873467028	C	-1.839710951	-2.907933950	5.939634323
N	-0.313066572	-0.695580721	-2.379557133	H	-1.404871464	-1.953873634	6.270105839
C	0.113755055	-1.285374165	-3.647315502	H	-2.589875460	-3.211610556	6.679339409
H	-0.751505971	-1.259917617	-4.319491863	O	-2.424047947	-2.841172218	4.664098740
H	0.859091222	-0.621490061	-4.098773003	H	-1.838530183	-2.257859707	4.082764149
C	0.725557327	-0.529006243	-1.364805222	F	0.263165295	-3.652763367	5.092293739

F	-1.175756335	-5.179773331	5.660216331	C	-2.209687710	1.426039815	-3.133179426
F	-0.165108874	-4.013445854	7.202007294	N	-2.042348862	1.789794207	-1.819046140
C	-1.459614635	-3.240551233	1.526684999	H	0.859824598	3.531799316	-2.238183260
H	-0.998201013	-4.009017467	0.896599352	H	0.322206199	3.148506880	-4.629270554
H	-1.989804149	-3.737936974	2.344096422	H	-1.627364159	1.634722352	-5.174132824
H	-2.189923286	-2.708607197	0.909812450	C	-3.191142321	0.364019662	-3.488193750
C	1.352440119	0.002672410	2.901205540	C	-2.955798388	-0.977384567	-3.101489544
H	2.077518702	0.496739864	3.558271646	C	-4.265719891	0.663907588	-4.334181786
H	1.897878051	-0.732500792	2.300629854	C	-3.833114624	-1.965466976	-3.556734800
H	0.946990788	0.764716446	2.229842901	C	-5.136211872	-0.335332304	-4.777289867
C	1.969279170	0.206234053	-1.866409302	C	-4.921004295	-1.656268954	-4.380977154
H	2.620020866	0.447114825	-1.018638849	H	-4.418885231	1.696134567	-4.637048721
H	2.553717136	-0.395416945	-2.571385384	H	-3.654484510	-2.999570847	-3.266669989
H	1.683034182	1.139433861	-2.360754728	H	-5.969310760	-0.081541285	-5.428750992
C	0.672521532	-2.717476845	-3.583734751	H	-5.585471153	-2.447210789	-4.722052097
H	-0.067372836	-3.420410633	-3.185887337	C	-1.793580294	-1.353035331	-2.198923349
H	0.955163121	-3.060956001	-4.585489273	H	-1.825918674	-2.441163301	-2.004421711
H	1.563515544	-2.772601128	-2.948158026	H	-1.947823524	-0.861881673	-1.234031677

---

## A2-TS

---

C	-1.424404740	1.938952327	-4.152032375	N	-0.495662391	-0.890889168	-2.691309690
Mn	-3.408558846	1.667961836	-0.283961594	C	-0.068283327	-1.523863196	-3.941588163
C	-0.665555656	2.656072855	-0.107263006	H	-0.883761883	-1.372602820	-4.658447742
C	0.503593564	3.245303392	0.415340781	H	0.781658471	-0.961125553	-4.341554165
C	0.674592495	3.377849102	1.776452422	C	0.499654979	-0.899458230	-1.618702531
C	-0.327506214	2.837712049	2.608914614	H	0.677131116	-1.918329835	-1.216675639
C	-1.454754591	2.246715546	2.066693783	C	-2.404695511	1.597802639	3.009616375
N	-1.715828300	2.221949816	0.702438176	C	-3.017493010	2.392075062	3.989884138
H	1.282368898	3.579671144	-0.262298733	C	-2.652363777	0.208066151	2.993343115
H	1.571843266	3.826308489	2.194035769	C	-3.890208960	1.839409590	4.926365852
H	-0.205991030	2.832871675	3.688317299	C	-3.560844660	-0.326693535	3.913969755
C	-0.883628726	2.467481852	-1.511115193	C	-4.173432827	0.473745525	4.880600929
C	-0.022138719	2.964299917	-2.514711142	H	-2.814806700	3.460209370	3.996567965
C	-0.317334265	2.751394987	-3.844674587	H	-4.355359077	2.475336313	5.676455021
				H	-3.767584801	-1.390938997	3.886430740
				H	-4.865063667	0.030280586	5.592904091
				C	-1.945608258	-0.732870221	2.039280415

H	-2.666909695	-1.454291463	1.650769711	H	0.634075046	0.468368471	1.287361383
H	-1.532039881	-0.203521609	1.182065964	C	1.842245817	-0.282930970	-2.013391972
N	-0.864943147	-1.541010618	2.707423925	H	2.479330301	-0.194168121	-1.126027226
C	0.331045210	-0.724029541	3.100432158	H	2.384461403	-0.894910336	-2.742774248
H	0.932396352	-1.347314715	3.763051748	H	1.690634012	0.714118242	-2.438741207
C	-0.537653029	-2.733846188	1.856917024	C	0.287519991	-3.022670269	-3.872631550
H	-1.471102953	-3.294975042	1.762047648	H	-0.405723244	-3.574488878	-3.229537725
C	-4.527801514	2.087836742	1.029801965	H	0.272599757	-3.476094246	-4.869207382
O	-5.351065636	2.375338316	1.817350388	H	1.289373279	-3.171795130	-3.452477217
C	-3.972027063	0.009470358	-0.252031446	=====			
O	-4.483009338	-1.053913951	-0.182834104	<b>A2-TS”</b>			
C	-4.601685047	2.349609375	-1.386815071	=====			
O	-5.405174732	2.768934727	-2.143637180	C	1.071349740	-0.114796840	-1.441923261
H	-0.048694480	0.111851744	3.694061518	Mn	-1.758655906	2.539523840	0.689327300
H	-0.243931562	-2.393056870	0.858403265	C	0.959285498	3.676450253	0.337255925
H	0.078694887	-0.306205302	-0.799715757	C	2.060665846	4.548950195	0.329559535
C	-0.234321579	-2.590697050	6.648834229	C	2.048625231	5.680477619	1.124969125
C	-1.475292444	-2.015590191	5.991900921	C	0.929531038	5.890340328	1.928427100
H	-1.331499457	-0.928656101	5.894006729	C	-0.167341515	5.030975819	1.851395726
H	-2.308391571	-2.177059889	6.690967083	N	-0.189419881	3.940308332	1.030801535
O	-1.705977917	-2.639013052	4.772916794	H	2.926048994	4.337585926	-0.286943048
H	-1.295117259	-2.030388355	3.734225273	H	2.895154238	6.361802101	1.144992828
F	0.872600377	-2.447724104	5.873226643	H	0.892897904	6.714338779	2.632131815
F	-0.362168193	-3.912289143	6.900163174	C	1.007274628	2.384669542	-0.341079742
F	0.028069891	-1.976205111	7.829170704	C	2.209312201	1.892537594	-0.878744185
O	-3.119508028	-4.266483307	3.514192104	C	2.254901648	0.622301519	-1.425515294
O	-3.569129229	-4.047727108	5.781188011	C	-0.102615066	0.433296829	-0.923216820
C	-3.147439003	-3.974311113	4.669764519	N	-0.151866853	1.660774231	-0.336913496
C	0.529503942	-3.632209301	2.475413322	H	3.111846924	2.490945339	-0.844291151
H	0.237299591	-3.923376799	3.488216877	H	3.179343700	0.218616813	-1.830601096
H	0.619942129	-4.538723946	1.867975950	H	1.034589648	-1.110485435	-1.873000622
H	1.514451027	-3.157660007	2.511962414	C	-1.337393999	-0.375832736	-1.118487954
C	1.185469508	-0.204738855	1.945528388	C	-2.057353020	-0.223451495	-2.319973707
H	2.027075052	0.359931022	2.359228849	C	-1.668986678	-1.388381124	-0.212093383
H	1.601224542	-1.020418644	1.345765710	C	-3.115106821	-1.101502657	-2.576984406

C	-2.729906559	-2.253430843	-0.481154114	H	-1.168693781	7.174547672	0.876992106
C	-3.449387312	-2.110734701	-1.671723366	H	-2.913843155	7.220242977	0.937371731
H	-1.082937360	-1.500067830	0.697495997	N	-2.036675215	8.837243080	1.926663399
H	-3.672268391	-0.978214860	-3.501334667	C	-2.446577787	9.724710464	0.829396844
H	-2.981296301	-3.042117834	0.224620432	H	-1.889397264	9.515447617	-0.102117233
H	-4.269886971	-2.789252758	-1.895788908	H	-2.182316303	10.749435425	1.117973924
C	-1.764401197	0.951754332	-3.234664440	C	-3.951222181	9.664676666	0.556200624
H	-0.727852046	1.286985040	-3.093058825	H	-4.271019459	8.674327850	0.214995936
H	-2.374867916	1.795653105	-2.894474745	H	-4.513072014	9.905734062	1.464916587
N	-2.049975634	0.684148192	-4.651244640	H	-4.223286629	10.384546280	-0.223630965
C	-1.124707341	-0.312535048	-5.222341537	C	-0.789830208	9.272838593	2.577409506
H	-1.208163619	-1.221038580	-4.615167618	H	-0.992973506	10.224894524	3.085646152
H	-1.491142154	-0.571092784	-6.224429131	H	-0.565470815	8.545584679	3.366435766
C	0.361860454	0.082018413	-5.320344925	C	0.440553427	9.450709343	1.669368029
H	0.508515358	0.954813242	-5.965042591	H	1.320419192	9.696978569	2.274747849
H	0.791427135	0.308691770	-4.339221954	H	0.670232952	8.543293953	1.103256702
H	0.937879026	-0.747094870	-5.747530460	H	0.293238491	10.264294624	0.951772273
C	-2.086084604	1.927676201	-5.439536572	C	-3.100306749	1.633165836	-0.021943873
H	-1.190207243	2.549434662	-5.269492626	O	-4.084431171	1.164037347	-0.453594923
H	-2.072297335	1.640231133	-6.498898983	C	-1.622823596	1.586305380	2.183517218
C	-3.331509113	2.771930933	-5.157457829	O	-1.716535568	0.925897360	3.153281689
H	-3.320729733	3.201239109	-4.149952412	C	-3.040443420	3.683395147	1.124593019
H	-3.377172709	3.606630087	-5.866489887	O	-3.943137169	4.407920837	1.308472753
H	-4.235527039	2.164004564	-5.279745579	H	-2.433380604	3.301144600	-0.767357349
C	-1.283886313	5.309072971	2.801551580	H	-1.707689047	5.374331474	-0.945755959
C	-1.434863925	4.440123558	3.894863605	C	-2.170693159	5.175354958	-1.939629078
C	-2.063357830	6.477759361	2.725124359	H	-2.563001156	6.157655239	-2.286051035
C	-2.353568077	4.709871769	4.904294014	C	-0.972471893	4.917847633	-2.851944447
C	-2.986303806	6.735810280	3.749385357	O	-3.088560343	4.164251328	-1.927648425
C	-3.134597301	5.868717670	4.829792023	F	-0.032963708	5.902400494	-2.726548433
H	-0.815460682	3.549974680	3.944507360	F	-1.307183027	4.883301258	-4.172499180
H	-2.451289654	4.029562473	5.747319698	F	-0.340105385	3.748797655	-2.591612101
H	-3.581001282	7.642915726	3.685277939	=====			
H	-3.853798389	6.094851494	5.614210129	<b>A3(A3')</b>			
C	-2.017400980	7.420997620	1.533391953	=====			

C	-1.574466705	1.827570677	-4.898163795	C	-0.741599619	-1.802740455	-5.468175411
Mn	-3.756384850	1.139851689	-1.192540288	H	0.133385584	-1.368962884	-4.946490765
C	-1.157486916	2.414155960	-0.788548827	C	-3.358830929	1.835626841	2.179942608
C	-0.021426108	2.996461391	-0.174550265	C	-4.412977695	2.760344028	2.237572432
C	0.020315660	3.174102545	1.187172771	C	-3.396188498	0.709112227	3.025614977
C	-1.102265000	2.765623569	1.937828302	C	-5.498760223	2.568186998	3.087460518
C	-2.184482098	2.172518015	1.310753822	C	-4.507068634	0.509957969	3.861622810
N	-2.239820004	1.965734720	-0.050191026	C	-5.551229000	1.431147814	3.900713682
H	0.823478043	3.299512148	-0.782494724	H	-4.369626522	3.640768051	1.604581594
H	0.883542955	3.623805046	1.670434356	H	-6.300434589	3.302509546	3.116442919
H	-1.142273068	2.938512087	3.007585049	H	-4.559572697	-0.381819874	4.486082554
C	-1.271910071	2.237737179	-2.203979969	H	-6.399497986	1.265774846	4.560703754
C	-0.323111713	2.768779039	-3.109066010	C	-2.295299530	-0.324860692	3.036355019
C	-0.470418721	2.592580318	-4.464003563	H	-2.701111317	-1.300197363	2.765172958
C	-2.480679989	1.312677741	-3.991945267	H	-1.483269930	-0.078896202	2.348333836
N	-2.408092022	1.543951392	-2.623829126	N	-1.647314906	-0.489900440	4.417334080
H	0.520062149	3.336732626	-2.730677128	C	-1.110565901	0.830552280	4.951841354
H	0.243499607	3.005126715	-5.171570301	H	-0.246476725	1.082644820	4.330281734
H	-1.713740230	1.606620669	-5.952159882	C	-0.565729558	-1.560992479	4.396225929
C	-3.545616150	0.441897124	-4.563762665	H	-0.118278414	-1.564659834	5.390972137
C	-3.463867903	-0.961776674	-4.484187603	C	-5.016753674	0.329180211	-2.162579298
C	-4.562255383	1.035672426	-5.327738762	O	-5.955250263	-0.211210102	-2.616884708
C	-4.411637783	-1.732924700	-5.167738914	C	-4.943421841	2.375730991	-0.821681976
C	-5.505546570	0.256415486	-5.995125771	O	-5.785735130	3.172057867	-0.593940914
C	-5.427885056	-1.137135625	-5.915172577	C	-4.050296783	-0.164440468	-0.035333667
H	-4.600797176	2.120407820	-5.394679070	O	-4.306398392	-1.067686319	0.682489872
H	-4.326950073	-2.816404819	-5.123540401	H	-1.896119833	1.567323446	4.778167248
H	-6.288239002	0.732203960	-6.581853867	H	0.188196093	-1.220058203	3.679608583
H	-6.152011395	-1.756384015	-6.440410614	H	-1.333104730	-0.952557445	-5.819466114
C	-2.379714489	-1.667021155	-3.693018198	H	-0.228432342	-2.936927080	-2.928613424
H	-2.866135359	-2.254824638	-2.908518076	H	-2.374315023	-0.812177122	5.075175762
H	-1.742412806	-0.933978796	-3.173290968	C	-1.103828073	-2.945029974	4.059442997
N	-1.582492113	-2.575872660	-4.538236141	H	-0.300381958	-3.669021845	4.227950573
C	-0.779311061	-3.491051197	-3.714242935	H	-1.940951109	-3.214396715	4.713935375
H	-0.016907560	-3.944646358	-4.354814529	H	-1.420300603	-3.037193060	3.017072916

C	-0.762423635	0.780719638	6.433669567	C	-3.025215149	2.749933481	0.742329121
H	-1.617120743	0.440588802	7.030072212	C	-1.767984748	2.283770561	2.770823240
H	0.100193337	0.144675881	6.650256634	C	-4.208695412	2.559622765	1.466808438
H	-0.513782382	1.798026800	6.754101753	C	-2.953271389	2.086411238	3.477673054
C	-1.608847260	-4.611895084	-3.084475279	C	-4.180535316	2.232818127	2.821800709
H	-2.137738466	-5.174076080	-3.861665964	H	-0.809524357	2.190782070	3.273734808
H	-0.956639946	-5.303168774	-2.539445639	H	-5.155417442	2.686861753	0.948799551
H	-2.352703333	-4.233353615	-2.375376463	H	-2.919906855	1.838211536	4.536375046
C	-0.289966673	-2.615248919	-6.682377338	H	-5.111455917	2.096183062	3.368259907
H	0.340894550	-3.467455864	-6.406961918	C	-3.099557877	3.023986578	-0.748889625
H	-1.161175966	-2.999693394	-7.223832130	H	-2.099995375	3.274898052	-1.138510823
H	0.290232778	-1.984057546	-7.365042686	H	-3.378239155	2.079320908	-1.227085829

---

#### A4

---

C	-0.141873255	4.313150406	0.825130105	C	-3.762162209	5.383059025	-0.632336259
Mn	0.009512896	-0.002708871	0.009315610	H	-3.572041273	5.310330391	0.444627434
C	1.995175362	1.542649627	-1.463369608	H	-4.655741692	6.010241985	-0.749184847
C	3.103046179	1.876372457	-2.272726536	C	-2.570299149	6.077353954	-1.315246105
C	3.764759779	0.904191256	-2.989115953	H	-2.747319221	6.217818737	-2.387049913
C	3.274028778	-0.412285328	-2.893260956	H	-1.642866373	5.510233879	-1.192797303
C	2.178156137	-0.701670289	-2.099870205	H	-2.411654711	7.067306042	-0.871909797
N	1.512538075	0.243343368	-1.337965846	C	-4.434243202	3.996598005	-2.540544510
H	3.436317205	2.906273127	-2.333590031	H	-3.526862860	3.976167440	-3.173131704
H	4.620909214	1.143177152	-3.613771439	H	-4.954885960	4.930103302	-2.786289215
H	3.735186815	-1.220013499	-3.454420805	C	-5.341476917	2.818551302	-2.906425714
C	1.291388154	2.532335281	-0.692186177	H	-4.860637665	1.851380229	-2.721843481
C	1.695363045	3.886375904	-0.630746365	H	-5.604547977	2.857509375	-3.969426632
C	0.993503034	4.783137798	0.142938897	H	-6.263992310	2.849462509	-2.317009211
C	-0.519635916	2.982485056	0.720273077	C	1.714696050	-2.118866205	-2.126289368
N	0.202013269	2.061412573	0.004404584	C	2.403865814	-3.069643497	-1.364758849
H	2.568035364	4.220375061	-1.180260181	C	0.702798426	-2.540706158	-3.016741753
H	1.299144745	5.823928356	0.212455004	C	2.081987143	-4.424987316	-1.452022433
H	-0.752120852	4.983488083	1.422431231	C	0.396817178	-3.904639244	-3.104252577
C	-1.792895675	2.609411955	1.407332182	H	1.074128866	-4.843607903	-2.322574615

H	-0.366435945	-4.239442825	-3.803853750	C	-0.945309162	-5.484096527	-2.738368511
H	0.824419796	-5.898721695	-2.405250072	C	0.224368930	-4.789819717	-2.441653490
C	-0.019848742	-1.544607043	-3.892586946	N	0.310851842	-3.879624367	-1.423369527
H	-0.429177403	-2.014168739	-4.789981842	H	-2.858140707	-4.301295757	-0.234297261
H	0.650703251	-0.744287252	-4.209252834	H	-3.008942366	-5.843843460	-2.169223547
N	-1.180165648	-0.869716525	-3.172514915	H	-0.938282967	-6.184609890	-3.567895174
C	-1.675812483	0.352086365	-3.917865038	C	-0.672260344	-2.822338581	0.487503529
H	-1.769260287	0.082020156	-4.973466396	C	-1.752824306	-2.513081551	1.333182812
H	-2.676548719	0.564517915	-3.532723665	C	-1.574673295	-1.628714442	2.381407022
C	-0.760820925	1.554995894	-3.704894781	C	0.738566339	-1.420507193	1.702632070
H	0.240811735	1.397521973	-4.115200996	N	0.570500314	-2.278476715	0.656150877
H	-0.666926324	1.784080148	-2.639159203	H	-2.729250908	-2.951158762	1.161990762
H	-1.196561337	2.421153784	-4.213246822	H	-2.398581982	-1.371293664	3.042024851
C	-2.296131849	-1.827906728	-2.798554420	H	-0.106084943	-0.380050123	3.370424986
H	-2.973056078	-1.255594730	-2.162156105	C	2.056199074	-0.772837698	1.976910591
H	-1.838299274	-2.600054026	-2.177174807	C	2.981755018	-1.346442342	2.864418268
C	-3.031710625	-2.425066233	-3.989495277	C	2.290964127	0.505472600	1.447598577
H	-3.823494196	-3.075381517	-3.603802919	C	4.126308441	-0.615021467	3.208535671
H	-2.383664131	-3.036942720	-4.623935223	C	3.440176964	1.216058850	1.787172794
H	-3.501843452	-1.656103611	-4.609671593	C	4.358170986	0.653837919	2.681151867
C	-1.754585028	-0.052672826	0.028643427	H	1.561014414	0.938043177	0.768495262
O	-2.923023224	-0.231195837	0.058092590	H	4.830132008	-1.059456229	3.906938791
C	0.432859033	-0.056937870	1.715281010	H	3.610373020	2.206349373	1.370649695
O	0.632435977	-0.120042920	2.876003504	H	5.251991749	1.205594540	2.964510679
C	-0.154427841	-1.775922894	-0.001635589	C	2.817473650	-2.760123014	3.387320757
O	-0.410920590	-2.917619705	0.113038853	H	1.820409894	-3.149347067	3.125217676
H	-0.807938695	-0.527501047	-2.247701883	H	3.533204556	-3.381943464	2.839078665

---

#### A4-TS

---

C	-0.304258674	-1.077282071	2.562253475	N	3.106148958	-2.884014130	4.821219444
Mn	1.889663458	-2.643117428	-0.940989137	C	2.129819632	-2.173778057	5.665217400
C	-0.804460645	-3.741780758	-0.636660457	H	2.100833893	-1.132784724	5.323262215
C	-2.001235247	-4.437238693	-0.883928955	H	2.530512810	-2.154335499	6.687007427
C	-2.089702606	-5.304271221	-1.956900716	C	0.699483931	-2.740051985	5.697131157
				H	0.681825876	-3.763894320	6.085362434
				H	0.239319667	-2.744559288	4.704425335
				H	0.069063969	-2.124604225	6.349096298

C	3.306413651	-4.283110142	5.225344181	C	3.404984713	-2.440568924	-0.065281592
H	2.513056040	-4.945164680	4.830839157	O	4.482168198	-2.359594584	0.405614704
H	3.225346327	-4.328728199	6.318040848	C	1.539633870	-1.005322099	-1.540133238
C	4.679246426	-4.820540428	4.811859131	O	1.446476460	0.102187261	-1.923256040
H	4.808992863	-4.834155560	3.724016666	C	2.955000401	-2.911912203	-2.340170145
H	4.808910847	-5.847726345	5.170413971	O	3.755607367	-2.965694427	-3.193331480
H	5.475821972	-4.199380398	5.235144615	H	2.548177004	-4.301557541	-0.457048893
C	1.414305568	-5.131330490	-3.269120455	=====			
C	1.447628498	-4.707932949	-4.603459358	<b>A5</b>			
C	2.416340828	-5.996460438	-2.777600765	=====			
C	2.485205173	-5.097608089	-5.450702667	C	0.727216899	0.226923123	-2.101773262
C	3.438714027	-6.393951416	-3.647879124	Mn	-2.089140415	2.716166019	0.277865767
C	3.486127138	-5.942789078	-4.969146252	C	0.632133186	3.796417475	0.128459170
H	0.653712690	-4.061803818	-4.971187592	C	1.697429061	4.704812050	0.162613302
H	2.503099680	-4.753638744	-6.482385635	C	1.680210471	5.742716789	1.087959290
H	4.202310562	-7.082642078	-3.293246269	C	0.603324592	5.826214314	1.961390257
H	4.292188168	-6.266813755	-5.623404980	C	-0.465543032	4.926812172	1.844335198
C	2.362270594	-6.549052238	-1.365665078	N	-0.469748169	3.942496538	0.912823021
H	2.808272123	-7.552673817	-1.346427798	H	2.537523985	4.604598522	-0.514880359
H	1.322316051	-6.659954548	-1.055872321	H	2.503471136	6.450438023	1.143697619
N	3.035012245	-5.692627430	-0.345743328	H	0.575796008	6.568429947	2.752126455
C	2.726544857	-6.124989986	1.040782809	C	0.669804394	2.587314367	-0.720431030
H	2.940443516	-7.196599960	1.159471631	C	1.839637995	2.210383892	-1.392946005
H	3.418516397	-5.584196568	1.694395185	C	1.871530175	1.013754010	-2.096993208
C	1.292175293	-5.807868958	1.465029359	C	-0.427189678	0.661900997	-1.436133623
H	0.550112009	-6.374657154	0.894672275	N	-0.462798595	1.832764030	-0.752954245
H	1.088265300	-4.743651867	1.335290313	H	2.729944706	2.825642109	-1.346349359
H	1.163371921	-6.064418316	2.521948099	H	2.775102854	0.694998920	-2.610342741
C	4.494514942	-5.524571419	-0.578837812	H	0.709327221	-0.734940469	-2.603369236
H	4.834136009	-4.771004677	0.135060117	C	-1.598971009	-0.265681893	-1.456544638
H	4.609211445	-5.084084034	-1.572668910	C	-2.385150433	-0.434617579	-2.611232758
C	5.345865726	-6.788210869	-0.444354683	C	-1.826732993	-1.071177840	-0.327740073
H	6.392479420	-6.532815456	-0.641706109	C	-3.392177343	-1.410184979	-2.596071720
H	5.057666779	-7.568824768	-1.154980302	C	-2.838486195	-2.028768539	-0.325209975
H	5.287940502	-7.208983421	0.564407527	C	-3.622406244	-2.200431347	-1.471052289

H	-1.194660902	-0.946829915	0.546575308	N	-2.639524221	8.563652992	2.577299356
H	-3.993184090	-1.539752126	-3.491913557	C	-3.178617477	9.570423126	1.652943969
H	-3.003751278	-2.644224644	0.555869043	H	-2.635799170	9.585295677	0.690296829
H	-4.411574364	-2.949230909	-1.486261368	H	-3.016777992	10.554918289	2.108392000
C	-2.255293369	0.464878172	-3.830781937	C	-4.677747250	9.389185905	1.399641633
H	-1.364667654	1.108643532	-3.742959261	H	-4.902880192	8.435551643	0.909829974
H	-3.111966133	1.147826314	-3.816362858	H	-5.230214119	9.421587944	2.344892740
N	-2.288277626	-0.284265339	-5.092771053	H	-5.051865578	10.188323021	0.749934971
C	-1.085188389	-1.106111407	-5.301564217	C	-1.449361563	9.022523880	3.310083866
H	-0.942600131	-1.710047960	-4.397598267	H	-1.754737973	9.858408928	3.953312635
H	-1.301733971	-1.812982559	-6.113322735	H	-1.148294926	8.211353302	3.983390331
C	0.215463847	-0.352145702	-5.630449772	C	-0.244283974	9.460616112	2.459465265
H	0.138011739	0.180597886	-6.583705425	H	0.596209347	9.729151726	3.108972549
H	0.474031955	0.378561169	-4.858022213	H	0.095739409	8.666196823	1.787535071
H	1.049113154	-1.059218287	-5.709202766	H	-0.485189617	10.334733963	1.846035480
C	-2.613592386	0.561862290	-6.250909805	C	-3.408531904	1.875398397	-0.583195388
H	-2.005437136	1.484464169	-6.275174618	O	-4.340158939	1.450652003	-1.132826686
H	-2.347795248	-0.000847510	-7.154018879	C	-1.983164549	1.553995728	1.661481619
C	-4.100257397	0.921429753	-6.318603992	O	-1.937093019	0.797868013	2.542562485
H	-4.421111107	1.523426533	-5.461561680	C	-3.395213842	3.721454382	0.969832003
H	-4.307161808	1.503700018	-7.223620415	O	-4.314121246	4.345561504	1.311687946
H	-4.712281704	0.013349435	-6.341996670	H	-2.143611908	3.733258486	-0.962084353
C	-1.554417014	5.010759830	2.861558676	=====			
C	-1.637843013	3.962592840	3.794555426	<b>A5-TS</b>			
C	-2.409205914	6.123714924	2.981805801	=====			
C	-2.562575579	3.997058392	4.834192753	C	0.876392305	-0.071455188	-1.469022155
C	-3.332048893	6.143932343	4.037694931	Mn	-2.031378984	2.527003288	0.640455782
C	-3.415184259	5.099042416	4.956050873	C	0.765423238	3.316828012	1.034142375
H	-0.955665588	3.122356653	3.703371048	C	1.927687168	4.002238274	1.413275719
H	-2.609346151	3.177861214	5.547962189	C	1.844886303	5.041585445	2.329675674
H	-3.985927105	7.006911755	4.125088692	C	0.592890859	5.372992992	2.827811718
H	-4.141398907	5.143345356	5.765103817	C	-0.544092298	4.677864552	2.392899513
C	-2.459693909	7.246838570	1.956739306	N	-0.465777189	3.653437376	1.507533193
H	-1.585175395	7.206282616	1.287875891	H	2.894472361	3.726467848	1.010239244
H	-3.325697184	7.050538540	1.314520597	H	2.736843348	5.574140072	2.649885654

H	0.473524690	6.160988331	3.564972162	H	-2.820279598	3.221010923	-6.807314396
C	0.828437626	2.160438299	0.116271295	H	-3.800591707	1.913950443	-6.107741833
C	2.053350925	1.683535457	-0.370464593	C	-1.833790541	5.061073303	3.036425829
C	2.082647800	0.549448311	-1.170601368	C	-2.376689434	4.195915222	3.996310949
C	-0.324013650	0.467250139	-0.989584267	C	-2.429966927	6.320310593	2.799483776
N	-0.355462372	1.569953322	-0.200866580	C	-3.532212019	4.542266369	4.697596073
H	2.983593225	2.176741600	-0.116633281	C	-3.588959932	6.647754192	3.511953831
H	3.025318861	0.155662253	-1.542303681	C	-4.144090176	5.771475792	4.448913574
H	0.840079963	-0.974640965	-2.069738865	H	-1.887180328	3.244707584	4.188872814
C	-1.572823405	-0.263584197	-1.359365225	H	-3.947171688	3.857701778	5.433788776
C	-2.157877922	-0.132019579	-2.632882357	H	-4.067924023	7.607101440	3.324483156
C	-2.097366333	-1.181301951	-0.434443712	H	-5.048219681	6.052323341	4.984630108
C	-3.270675421	-0.926203251	-2.940278292	C	-1.875363946	7.295121670	1.770962834
C	-3.204108477	-1.963079572	-0.756816983	H	-2.348904848	8.280943871	1.928595185
C	-3.791017294	-1.833994508	-2.019712925	H	-0.808831096	7.449842453	1.951519489
H	-1.625710011	-1.277443409	0.540548205	N	-2.035547495	6.800936699	0.399890959
H	-3.721816063	-0.816217184	-3.922315598	C	-1.116276622	7.412631989	-0.565880716
H	-3.601048946	-2.670494556	-0.032397419	H	-1.138862729	8.518134117	-0.524371624
H	-4.654851437	-2.439574480	-2.285498857	H	-1.477109075	7.142336845	-1.566079736
C	-1.707529068	0.927083075	-3.625085831	C	0.324925840	6.920248985	-0.419691116
H	-0.713553071	1.315009594	-3.346628904	H	0.766432285	7.204802513	0.539942026
H	-2.397644758	1.769440174	-3.515147686	H	0.361082286	5.831066608	-0.499730259
N	-1.766487598	0.481685132	-5.022020340	H	0.950860798	7.350891590	-1.210137606
C	-0.828950047	-0.613105893	-5.325232506	C	-3.430948734	6.804340839	-0.060877591
H	-1.045176506	-1.432366490	-4.630442142	H	-3.479438543	6.174902916	-0.957174361
H	-1.076396227	-0.986632884	-6.327320576	H	-4.031926632	6.300297737	0.698950648
C	0.671421289	-0.277301192	-5.271451473	C	-4.049080372	8.181127548	-0.362720907
H	0.941981137	0.480945289	-6.013495445	H	-5.093989372	8.060744286	-0.670802355
H	0.973299265	0.093918607	-4.287433624	H	-4.038165569	8.835989952	0.515888751
H	1.262453675	-1.175846219	-5.481015682	H	-3.519352674	8.696024895	-1.171375751
C	-1.654721975	1.601891875	-5.968465805	C	-3.300723791	1.798948765	-0.388457119
H	-0.752749145	2.213779211	-5.780967236	O	-4.222137928	1.486223340	-1.023250103
H	-1.526090384	1.168207169	-6.967905045	C	-2.148632765	1.332822204	1.990180969
C	-2.889606714	2.508562326	-5.977624416	O	-2.234441757	0.563525200	2.857527971
H	-2.989054441	3.092015266	-5.056567669	C	-3.405450106	3.525654554	1.206356287

O	-4.398048401	4.071335316	1.461545467	H	-4.594886780	0.598123610	-8.110601425
H	-1.850425601	3.606871605	-0.537993431	H	-4.781661510	-1.852711320	-7.678803921
C	-1.585769176	4.123569012	-2.246430397	C	-1.661062360	-1.694298267	-4.175125122
O	-0.402706236	4.117740631	-2.276764154	H	-1.992056370	-2.734631300	-4.003137589
O	-2.705775023	4.264133453	-2.608549118	H	-1.784986854	-1.165243149	-3.228176117
<hr/>				N	-0.253767371	-1.599537134	-4.579296589
<b>A5(red)</b>				C	0.667622387	-1.492093444	-3.449360609
<hr/>				H	0.280649215	-0.696298957	-2.805703640
C	-0.505023956	1.795757651	-5.268551350	C	0.124530926	-2.548606873	-5.627149582
Mn	-3.613687992	1.180844307	-2.165163994	H	-0.642511070	-2.491611481	-6.407906055
C	-0.970689714	1.881846189	-1.100700617	C	-3.422777414	0.379527599	1.280566692
C	0.028573820	2.345612764	-0.194467679	C	-4.321009159	1.043029308	2.123209000
C	-0.149634540	2.224737406	1.161649466	C	-3.569512129	-1.008604407	1.059750795
C	-1.321307540	1.595896840	1.638226390	C	-5.389084816	0.363154501	2.714863062
C	-2.261495113	1.131384730	0.719991267	C	-4.646237850	-1.674283147	1.650636554
N	-2.147890091	1.310194731	-0.616837204	C	-5.559561729	-0.999056876	2.468626738
H	0.945565820	2.779987574	-0.578803599	H	-4.184017658	2.107302904	2.302844763
H	0.613901019	2.575390816	1.853289604	H	-6.081933498	0.897225618	3.361698627
H	-1.475165248	1.405136943	2.694334507	H	-4.760375023	-2.744035006	1.481154680
C	-0.813502491	1.943104982	-2.513163090	H	-6.386929512	-1.540168285	2.922790289
C	0.304234236	2.564544439	-3.145463228	C	-2.528554916	-1.764987707	0.258557290
C	0.448836237	2.514827013	-4.509729385	H	-2.913955688	-2.772072792	0.013848120
C	-1.584092736	1.208954811	-4.613929272	H	-2.386110067	-1.244660378	-0.691815674
N	-1.805846572	1.336890340	-3.283959866	N	-1.243719816	-1.799893737	0.961713314
H	1.040935636	3.088869333	-2.545563459	C	-0.101115122	-1.847613454	0.052375194
H	1.297859430	2.993017912	-4.994051456	H	-0.051437169	-2.791878939	-0.525362909
H	-0.380577862	1.636423349	-6.333788395	C	-1.209965467	-2.732431412	2.088190556
C	-2.491295099	0.353113949	-5.430928230	H	-0.364459097	-2.470564842	2.735340834
C	-2.558833122	-1.041545033	-5.209898472	H	-2.111796141	-2.551745653	2.684451103
C	-3.210578918	0.920695961	-6.487485409	C	-4.721756458	0.897075355	-3.525244951
C	-3.396107674	-1.810919762	-6.021610737	O	-5.540988445	0.669874489	-4.324872971
C	-4.036015034	0.137628928	-7.298694611	C	-3.780615807	2.981697559	-2.193085194
C	-4.140593052	-1.232015967	-7.056418419	O	-3.967741728	4.133379936	-2.230149269
H	-3.132750273	1.992115974	-6.659334660	C	-5.043765545	0.920934796	-1.139137268
H	-3.449099779	-2.885663509	-5.853534698	O	-6.052651882	0.721205413	-0.587089717

H	-0.252057999	-1.045991182	-0.676524639	C	-0.275443763	2.009248257	-3.121520519
H	1.054361463	-2.203736067	-6.094711304	C	-0.236239433	1.958573818	-4.495438099
H	0.698570609	-2.410588264	-2.831389427	C	-2.210709810	0.569331110	-4.445179939
H	-3.465138435	-0.401746899	-2.157789707	N	-2.347934723	0.726938605	-3.106151342
C	1.238775134	-1.612642884	0.751118779	H	0.485328913	2.563561916	-2.580075979
H	1.513861895	-2.433866501	1.422809482	H	0.552455604	2.470705748	-5.042668819
H	2.032705784	-1.521799207	0.001053854	H	-1.142588258	1.010679007	-6.250808239
H	1.202071786	-0.684115827	1.330811501	C	-3.109504700	-0.399566084	-5.135633945
C	-1.127206564	-4.228044033	1.732661724	C	-3.089289427	-1.764403224	-4.760391712
H	-0.200239033	-4.462272644	1.197905421	C	-3.915432930	0.011651343	-6.201294422
H	-1.149339199	-4.836887360	2.643679380	C	-3.932974815	-2.656792164	-5.425661087
H	-1.966082931	-4.542449474	1.101991057	C	-4.745440483	-0.895347476	-6.866935730
C	2.090997458	-1.116863489	-3.865922689	C	-4.766947746	-2.231357336	-6.466626167
H	2.693989992	-0.912009597	-2.973787308	H	-3.905977011	1.059506178	-6.493475914
H	2.591770172	-1.916241765	-4.423995018	H	-3.922664642	-3.705981016	-5.135673523
H	2.074724197	-0.214701176	-4.486547470	H	-5.375359535	-0.555753589	-7.686282635
C	0.297998995	-4.015112877	-5.189846516	H	-5.414562225	-2.945694447	-6.970965862
H	-0.613527834	-4.412321568	-4.729794979	C	-2.106525660	-2.255847931	-3.715739965
H	0.535411000	-4.644224167	-6.055522442	H	-2.326531172	-3.302492142	-3.455631018
H	1.113184452	-4.124335289	-4.465948582	H	-2.254041433	-1.672744751	-2.804333448

---

### A5(red)-TS

---

C	-1.207428932	1.188020110	-5.182510376	N	-0.721059084	-2.052106619	-4.167057037
Mn	-4.142754555	0.661034763	-1.906318188	C	0.199465036	-2.057442665	-3.029842138
C	-1.382766485	1.280709267	-0.982689559	H	-0.124460630	-1.250821352	-2.362855196
C	-0.337234318	1.742935538	-0.132372409	C	-0.352705479	-2.918307543	-5.290592194
C	-0.437311143	1.607669711	1.231777549	H	-1.063132405	-2.722826242	-6.101232529
C	-1.581460953	0.978372574	1.774674296	C	-3.744398117	-0.181862682	1.511013985
C	-2.578165293	0.532143712	0.911142170	C	-4.609369755	0.515935481	2.361295462
N	-2.528328896	0.704318523	-0.430303037	C	-3.943443060	-1.563284755	1.294820189
H	0.553128302	2.186780930	-0.566931248	C	-5.700448990	-0.122374758	2.956881523
H	0.363750815	1.955442309	1.880839705	C	-5.047367096	-2.185524225	1.883891940
H	-1.678035498	0.790900648	2.838475466	C	-5.930949211	-1.474583507	2.703244448
C	-1.319913864	1.354851604	-2.406132221	H	-4.430640697	1.574125290	2.540102720
				H	-6.369626999	0.437541991	3.606778145
				H	-5.207204342	-3.248416662	1.710704446
				H	-6.781723022	-1.981243134	3.153892279

C	-2.918947220	-2.362976074	0.520264089	H	-1.514307141	-5.333047867	1.560191154
H	-3.348685741	-3.326597452	0.208247691	H	-2.232811689	-5.394702911	3.179618359
H	-2.679698706	-1.825658917	-0.399669021	H	-3.218386650	-4.931708813	1.787777781
N	-1.674591899	-2.515873909	1.299106121	=====			
C	-0.579614043	-2.894893885	0.400528640	<b>A6</b>			
H	-0.776818812	-3.854232073	-0.117754951	=====			
C	-1.837076783	-3.366914988	2.485003471	C	0.923558414	-0.062949136	-1.691560507
H	-0.900033653	-3.354165554	3.049710751	Mn	-1.952957034	2.589970827	0.359200984
H	-2.601254940	-2.906898975	3.120383501	C	0.827901840	3.369759321	0.756165028
C	-5.311869144	0.586745620	-3.248225212	C	1.984466076	4.057693958	1.141252637
O	-6.140463352	0.539280832	-4.064425945	C	1.891041279	5.094192505	2.062037468
C	-4.178699017	2.459876776	-1.841859579	C	0.637850344	5.418565273	2.563683748
O	-4.281323910	3.621172905	-1.801450491	C	-0.494285315	4.719527245	2.125813007
C	-5.537830353	0.449658066	-0.812273920	N	-0.404036731	3.703745127	1.230733156
O	-6.514092445	0.281023711	-0.201695591	H	2.953828096	3.787652731	0.739906251
H	-0.522687614	-2.121558189	-0.368559480	H	2.780169487	5.628534794	2.387243986
H	0.631140590	-2.609265566	-5.656140327	H	0.514531851	6.202243328	3.304901123
H	0.162219599	-3.003516436	-2.456377506	C	0.890651822	2.204560518	-0.152714550
H	-4.216364384	-1.022341609	-1.953471065	C	2.111529827	1.709694862	-0.624675393
C	-5.304619789	-2.574259758	-2.195007563	C	2.131739378	0.557462275	-1.401459455
O	-4.457680225	-3.389272928	-2.064779758	C	-0.274205685	0.492141813	-1.225162148
O	-6.378783226	-2.105067015	-2.354742527	N	-0.294209391	1.609747648	-0.458141595
C	1.655671954	-1.778102875	-3.413707495	H	3.044843674	2.200626373	-0.377398700
H	2.271344662	-1.717865705	-2.508967161	H	3.072523355	0.148801729	-1.762059808
H	2.083093882	-2.571827173	-4.036053181	H	0.883264005	-0.977656782	-2.274388075
H	1.732704163	-0.831106067	-3.958976984	C	-1.534239769	-0.220798641	-1.586588025
C	-0.325974494	-4.437769413	-5.010267258	C	-2.126499653	-0.054065160	-2.853557348
H	-1.335879087	-4.853609085	-4.931535244	C	-2.065887451	-1.143074155	-0.670281231
H	0.182152003	-4.967500687	-5.824354172	C	-3.258935213	-0.819200516	-3.162200451
H	0.206961751	-4.668174744	-4.081363678	C	-3.193571091	-1.894063950	-0.995045841
C	0.790506244	-2.989550352	1.080728412	C	-3.789167404	-1.731029868	-2.250063181
H	0.806249440	-3.715746403	1.899923086	H	-1.584744096	-1.267489314	0.297199100
H	1.551585317	-3.283039331	0.349583864	H	-3.718004704	-0.683456421	-4.137403965
H	1.074173689	-2.018507481	1.504675031	H	-3.600298405	-2.604424238	-0.279008597
C	-2.223289490	-4.840229034	2.234627485	H	-4.669373989	-2.312504768	-2.516155481

C	-1.641718864	1.006722689	-3.826327324	C	0.306759953	6.880754471	-0.707425952
H	-0.622000456	1.332225680	-3.563370466	H	0.730342150	7.192507744	0.251977354
H	-2.270479918	1.888803363	-3.670769453	H	0.372577697	5.793676376	-0.782658041
N	-1.761469722	0.611757338	-5.234594822	H	0.927462995	7.319262028	-1.497364283
C	-0.925098121	-0.547965705	-5.589343548	C	-3.455630541	6.729411602	-0.368257374
H	-1.195757985	-1.368472934	-4.915852547	H	-3.500450134	6.064122677	-1.237683058
H	-1.219138861	-0.866641879	-6.597916126	H	-4.065632343	6.267662048	0.411279917
C	0.599119246	-0.343573540	-5.551376343	C	-4.060883045	8.097059250	-0.727963686
H	0.924558282	0.409902334	-6.275706768	H	-5.105314255	7.969710350	-1.034408569
H	0.943683743	-0.027965087	-4.561725616	H	-4.048591614	8.788357735	0.122144349
H	1.107150793	-1.283381701	-5.795094013	H	-3.525840998	8.572974205	-1.556223392
C	-1.553971648	1.751826763	-6.141396046	C	-3.270307541	1.778956175	-0.595079005
H	-0.590798318	2.259766817	-5.949409485	O	-4.225918770	1.412290812	-1.127847552
H	-1.491003156	1.346995234	-7.159273148	C	-2.060553074	1.431834936	1.722164750
C	-2.684105873	2.784223318	-6.080084801	O	-2.092904568	0.683468223	2.602747679
H	-2.691010237	3.337639093	-5.135255337	C	-3.357272148	3.563697100	0.971829712
H	-2.561735392	3.514506102	-6.887922764	O	-4.364607334	4.042455673	1.268934131
H	-3.656689644	2.294431925	-6.203531742	H	-1.754176974	3.794527054	-1.001416683
C	-1.791336536	5.076353550	2.769794464	C	-1.575169683	4.073801517	-2.159131289
C	-2.301199198	4.209467888	3.747402906	O	-0.379301399	4.107269287	-2.463819981
C	-2.431063414	6.309804440	2.510615349	O	-2.640695572	4.281449318	-2.761064529
C	-3.465306997	4.530109406	4.447201729	=====			
C	-3.595624447	6.612368584	3.224273920	<b>A7</b>			
C	-4.116671085	5.735229015	4.180681705	=====			
H	-1.777560711	3.280357122	3.958769560	C	-1.004152298	1.877667665	-5.739841461
H	-3.854679823	3.845417738	5.197002411	Mn	-3.371494293	0.527604342	-2.151265383
H	-4.106789589	7.552038670	3.022849798	C	-0.795296252	1.895725489	-1.535832524
H	-5.026392937	5.996446133	4.716871738	C	0.384538800	2.264899254	-0.878527105
C	-1.911616087	7.273958206	1.456425667	C	0.426434547	2.227607489	0.511329651
H	-2.416134596	8.247698784	1.584445953	C	-0.719426572	1.839711070	1.195136070
H	-0.849829257	7.465951443	1.631570697	C	-1.865116954	1.461693645	0.481147259
N	-2.059832096	6.731562614	0.100435436	N	-1.896371603	1.463980675	-0.869880378
C	-1.143601656	7.333662987	-0.878014565	H	1.263287902	2.554501295	-1.443960667
H	-1.192935109	8.438287735	-0.865087807	H	1.331187367	2.503789186	1.047345161
H	-1.489936233	7.021651745	-1.870093346	H	-0.748787105	1.823505878	2.280004978

C	-0.877117515	1.940086842	-3.011760235	H	-6.174769402	0.558083951	3.558782816
C	-0.034947351	2.777034283	-3.751748323	C	-2.332933187	-1.278393984	1.647379160
C	-0.116980672	2.761664391	-5.141597271	H	-2.878803492	-1.958072066	0.988589823
C	-1.827739239	1.068206310	-4.943513870	H	-1.441883206	-0.955038428	1.081161022
N	-1.804689765	1.137140393	-3.593690157	N	-1.979022980	-2.008618355	2.866267920
H	0.651565671	3.451780558	-3.253125191	C	-1.097945809	-1.205961227	3.727011919
H	0.511490941	3.415772200	-5.741017342	H	-1.451291680	-0.170481399	3.681659222
H	-1.073324800	1.794240117	-6.819908619	H	-0.059775099	-1.197290778	3.341757536
C	-2.744512796	0.121868022	-5.639523983	C	-1.404124260	-3.322266579	2.545863390
C	-2.526638031	-1.272909880	-5.603999138	H	-0.588107467	-3.226133347	1.801973104
C	-3.785372019	0.649863899	-6.415353775	H	-0.942574084	-3.720785141	3.453923225
C	-3.386850595	-2.098123789	-6.335855484	C	-4.453696728	-0.382367253	-3.285650253
C	-4.640515327	-0.191057637	-7.130167484	O	-5.236889362	-0.964118302	-3.903277636
C	-4.440997601	-1.571677208	-7.087299347	C	-4.179553032	2.094292164	-2.499341249
H	-3.931345701	1.727720618	-6.445650578	O	-4.682536125	3.114459753	-2.722676277
H	-3.221242428	-3.173692226	-6.318206787	C	-4.639063835	0.090079531	-0.932625532
H	-5.452564716	0.231027260	-7.717777252	O	-5.546281815	-0.211947262	-0.284928858
H	-5.095786095	-2.237869978	-7.644814491	O	-2.205729961	-1.103790522	-1.746297240
C	-1.391167641	-1.874002695	-4.801898956	C	-2.601832628	-2.301367044	-1.505787134
H	-1.493655682	-2.977173090	-4.808685303	O	-3.765059710	-2.726204395	-1.407912374
H	-1.497842789	-1.552862287	-3.765738010	H	0.550860524	-3.002665281	-6.599751949
N	-0.065952145	-1.449425936	-5.268393040	H	1.942317605	-1.784982800	-4.807003498
C	0.973726988	-1.823711872	-4.298724174	H	-1.755037665	-3.009341240	-1.370648503
H	0.843381107	-2.874965906	-3.973112583	C	-2.447025061	-4.329325676	2.052679300
C	0.233715966	-1.941936970	-6.618856430	H	-1.981233597	-5.310692787	1.908898830
H	-0.693093061	-1.911613345	-7.199812412	H	-3.250383615	-4.431663513	2.789864302
C	-3.089101553	1.135194778	1.271117210	H	-2.896065235	-4.035931587	1.097841382
C	-4.035348892	2.157812357	1.455430746	C	-1.123206139	-1.654594302	5.189030647
C	-3.257441521	-0.106121883	1.908516884	H	-2.147686958	-1.617231488	5.574162960
C	-5.147881508	1.954866529	2.268531561	H	-0.749294460	-2.675342560	5.321073532
C	-4.375817299	-0.289917171	2.733179331	H	-0.497098953	-0.993076503	5.798476696
C	-5.312794685	0.725315988	2.916211367	C	1.024657488	-0.901543081	-3.077873230
H	-3.885472059	3.114808798	0.960142732	H	0.087023444	-0.903418362	-2.514395475
H	-5.876480579	2.751044512	2.403250456	H	1.827264309	-1.218904138	-2.401730299
H	-4.494169712	-1.248881459	3.230409145	H	1.227547050	0.126383454	-3.393624544

C 1.281128049 -1.084257841 -7.332294941  
 H 2.245755672 -1.089203835 -6.812957287  
 H 1.451434612 -1.453834295 -8.349995613  
 H 0.936153412 -0.046578154 -7.388854980

---

### A8

---

C -0.647239804 1.612269044 -5.582138538  
 Mn -3.568783760 0.852616966 -2.253907919  
 C -0.956249177 1.994786382 -1.415506482  
 C 0.072443351 2.583185196 -0.621117055  
 C -0.054036524 2.667594910 0.741242349  
 C -1.215656281 2.127786398 1.342646837  
 C -2.174711943 1.518075943 0.540324390  
 N -2.097565889 1.463871002 -0.811827242  
 H 0.975336730 2.950168610 -1.096326947  
 H 0.730706573 3.116174698 1.346494675  
 H -1.354557276 2.139294624 2.417478085  
 C -0.851487219 1.908949494 -2.832908630  
 C 0.188627094 2.566559315 -3.554100275  
 C 0.287672669 2.433274984 -4.916286469  
 C -1.652707100 0.993957162 -4.844709396  
 N -1.812488079 1.159447193 -3.508661270  
 H 0.891753376 3.202608585 -3.028034210  
 H 1.073497295 2.944918394 -5.468008518  
 H -0.576996803 1.418701887 -6.646623135  
 C -2.573580980 0.107488573 -5.614449978  
 C -2.530762672 -1.300441861 -5.501365662  
 C -3.415876865 0.701877058 -6.563322544  
 C -3.377693892 -2.059259892 -6.317438602  
 C -4.253771782 -0.070053577 -7.369454384  
 C -4.240870476 -1.459048748 -7.238771915  
 H -3.417409897 1.785952330 -6.655127525  
 H -3.345728874 -3.144626379 -6.238267422  
 H -4.908069611 0.410876304 -8.093457222

H -4.885088921 -2.075898409 -7.861767292  
 C -1.590797305 -1.996928453 -4.537969112  
 H -1.822755337 -3.082293272 -4.536764145  
 H -1.804635167 -1.626147866 -3.537393808  
 N -0.170012549 -1.756830812 -4.810342312  
 C 0.656922102 -2.205506563 -3.684107304  
 H 0.375839561 -3.233619213 -3.374099255  
 C 0.265873939 -2.319056511 -6.090161800  
 H -0.547181606 -2.175791740 -6.808726311  
 C -3.316012859 0.885485530 1.266926527  
 C -4.333150387 1.712252140 1.766584873  
 C -3.305849075 -0.486257017 1.587261319  
 C -5.360330105 1.187814116 2.548569202  
 C -4.346296310 -0.999190867 2.373588085  
 C -5.368607521 -0.177939937 2.849176407  
 H -4.310480118 2.773638964 1.528944731  
 H -6.146572113 1.838938475 2.924299955  
 H -4.328862667 -2.056325912 2.630443811  
 H -6.164190292 -0.598669946 3.460360289  
 C -2.188722610 -1.418796897 1.158904791  
 H -2.644495010 -2.248266220 0.617432356  
 H -1.519822478 -0.915864110 0.443904579  
 N -1.444028020 -1.988983989 2.303893566  
 C -0.748815477 -0.923409641 3.045180082  
 H -1.491100907 -0.151638418 3.267593145  
 H 0.021163937 -0.435383588 2.416438580  
 C -0.499043494 -3.013295412 1.828386545  
 H 0.167694628 -2.604789019 1.041637182  
 C -4.693062305 0.258650571 -3.541044235  
 O -5.509200096 -0.101812802 -4.279647350  
 C -3.971072197 2.561106205 -2.560861111  
 O -4.208549023 3.683073282 -2.755628347  
 C -4.989804268 0.638879716 -1.155259371  
 O -5.986083031 0.517437220 -0.576717138  
 O -2.917728662 -1.101667523 -1.854601026

C	-3.651674986	-2.143312216	-1.751058459	H	-0.957982063	1.634616733	2.398839951
O	-4.890218258	-2.247465611	-1.814133644	C	-0.791051388	1.985215783	-2.883270025
H	0.148923963	-3.290988207	2.664400816	C	0.226145267	2.506693602	-3.682744026
H	0.427923381	-3.414191484	-6.022858143	C	0.204964712	2.234246016	-5.053163052
H	1.694839597	-2.269533157	-4.027273178	C	-1.751448512	0.868048012	-4.708738327
H	-3.050959349	-3.069077730	-1.583612800	N	-1.820414186	1.270578384	-3.416910887
C	0.597293735	-1.264050126	-2.477516174	H	1.020904303	3.109246016	-3.255828857
H	-0.415986925	-1.158356905	-2.080044985	H	0.973675489	2.645750523	-5.702887535
H	1.240885735	-1.644011140	-1.674582124	H	-0.756309628	1.069344401	-6.603913307
H	0.943022549	-0.265912354	-2.760488987	C	-2.726674318	-0.150032178	-5.179074287
C	1.519088626	-1.629367352	-6.636112213	C	-2.760347843	-1.427996397	-4.570067883
H	2.390549421	-1.775560856	-5.988331318	C	-3.564044952	0.130684555	-6.266414642
H	1.775583267	-2.023799896	-7.626328468	C	-3.672086000	-2.371989965	-5.049859524
H	1.338749051	-0.552854180	-6.719089031	C	-4.475557327	-0.823102176	-6.725688457
C	-0.128010064	-1.386029601	4.365630150	C	-4.535139561	-2.074357986	-6.109480381
H	-0.860261023	-1.944691777	4.959795952	H	-3.513959408	1.108533502	-6.739644527
H	0.752069712	-2.022054911	4.224679947	H	-3.697548866	-3.360450745	-4.594446182
H	0.191499248	-0.513913393	4.947071552	H	-5.130959034	-0.588908076	-7.561143875
C	-1.177714825	-4.286943913	1.316618443	H	-5.237375736	-2.825993538	-6.463470459
H	-1.741112471	-4.127157688	0.391947776	C	-1.808790684	-1.793526649	-3.444533110
H	-0.419188231	-5.049339771	1.106901169	H	-1.945425749	-2.859360695	-3.189754486
H	-1.866026282	-4.684716702	2.070605516	H	-2.086448669	-1.232270837	-2.548595667
<hr/>							
<b>A9</b>				N	-0.420802176	-1.440117121	-3.740807295
<hr/>							
C	-0.767009199	1.378460526	-5.563046455	C	0.408010155	-1.457132459	-2.531629086
Mn	-3.430365324	1.584691167	-2.220499992	H	-0.111300215	-0.840031564	-1.787928462
C	-0.811072826	2.054630280	-1.402526021	H	0.485312521	-2.467766762	-2.088589430
C	0.265581697	2.516669035	-0.644662440	C	0.144399703	-2.135543823	-4.904838562
C	0.210210517	2.390925884	0.742560267	H	-0.543363869	-1.976462841	-5.742767811
C	-0.901731670	1.786648512	1.325346947	H	1.074475169	-1.627796292	-5.180987358
C	-1.964822650	1.355011940	0.521739662	C	-3.153012276	0.721794546	1.165905714
N	-1.928272605	1.526234508	-0.823051691	C	-3.934767008	1.534352183	2.007640839
H	1.141438484	2.943058252	-1.122874618	C	-3.462302923	-0.647620559	1.029170513
H	1.038014770	2.734589577	1.358203173	C	-5.044884205	1.018578529	2.671921730
				C	-4.577999592	-1.151084542	1.714851141
				C	-5.370474339	-0.333978593	2.518540859

H	-3.670879841	2.582910538	2.122169971	H	-0.302379817	-4.920578957	1.545364380
H	-5.648133278	1.663954020	3.305495501				
H	-4.802260399	-2.211426735	1.623339176				
H	-6.232359409	-0.752008200	3.034101963				
C	-2.630867004	-1.630149007	0.223405764				
H	-3.279530764	-2.091709614	-0.527479231				
H	-1.844199061	-1.098708510	-0.333196938				
N	-2.102000237	-2.720525026	1.051664352				
C	-1.085892558	-2.261943340	2.015963078				
H	-1.533036113	-1.442651749	2.590437651				
C	-1.682396054	-3.854871035	0.212069735				
H	-0.874551177	-3.577771664	-0.490009129				
C	-4.303359032	0.045663998	-2.073114157				
O	-4.883428097	-0.949566782	-2.008188486				
C	-4.493466854	2.043259382	-3.629632950				
O	-5.159929276	2.369881630	-4.507284164				
C	-4.614377975	2.406550884	-1.100341320				
O	-5.358985424	2.978296518	-0.437219769				
H	-2.544271946	-4.127084732	-0.410419881				
H	-0.909355164	-3.069839001	2.734115839				
C	1.810195804	-0.885474682	-2.742038488				
H	2.308129787	-0.769095361	-1.773271680				
H	2.438521385	-1.535355091	-3.360093594				
H	1.753085494	0.097052433	-3.222358465				
C	0.406033456	-3.640884399	-4.737978458				
H	-0.513612509	-4.187255383	-4.501530170				
H	0.809754074	-4.056396008	-5.668041229				
H	1.130514383	-3.839800596	-3.940856695				
C	0.261093020	-1.798954844	1.433052659				
H	0.924448788	-1.475985289	2.242892742				
H	0.767523170	-2.601739168	0.886936903				
H	0.142707527	-0.951012909	0.750665307				
C	-1.249807119	-5.079884052	1.019522667				
H	-2.012888432	-5.344391823	1.760476470				
H	-1.112843990	-5.933858871	0.347301155				

---

				A7-TS			
C	-1.238653898	1.698845029	-5.819327354				
Mn	-3.428773403	0.520821869	-2.070410728				
C	-0.784800529	1.815306187	-1.633939028				
C	0.444981158	2.130266190	-1.041816235				
C	0.540215731	2.161023140	0.345025420				
C	-0.605470061	1.907337904	1.092328072				
C	-1.804332018	1.588233113	0.441072822				
N	-1.886522651	1.508230448	-0.905200541				
H	1.317832470	2.327382565	-1.654350519				
H	1.484198213	2.393915415	0.831830740				
H	-0.591357172	1.970494986	2.175989628				
C	-0.933629632	1.800767779	-3.105309010				
C	-0.087390207	2.563595295	-3.916518211				
C	-0.267866403	2.540461302	-5.297613144				
C	-2.034282923	0.932278275	-4.952173233				
N	-1.945502043	1.050659776	-3.607161045				
H	0.676655352	3.194949865	-3.477051497				
H	0.354403496	3.150986671	-5.947486401				
H	-1.382593393	1.598454475	-6.890371323				
C	-2.987195253	-0.030324748	-5.575276375				
C	-2.735678911	-1.421038866	-5.532790184				
C	-4.058258057	0.463587701	-6.331295013				
C	-3.586905241	-2.274505377	-6.242321491				
C	-4.912387848	-0.406249106	-7.012041569				
C	-4.673150063	-1.781480432	-6.971016884				
H	-4.229019642	1.537505746	-6.372185230				
H	-3.395465136	-3.345971107	-6.217507839				
H	-5.750205517	-0.009296385	-7.580607891				
H	-5.321549416	-2.467884302	-7.510847569				
C	-1.632043362	-1.997868180	-4.666799545				
H	-1.575936675	-3.088982582	-4.835732460				

H	-1.935498118	-1.859593630	-3.628730536	H	-2.447218895	-3.582523108	2.187621832
N	-0.346113741	-1.321749568	-4.811223507	H	-0.449784279	-1.746119618	4.420288563
C	0.505999267	-1.525260329	-3.635210276	H	-1.852057219	-2.987957239	-1.072885036
H	-0.096150063	-1.244300246	-2.763906002	H	-2.905340195	-1.941105843	3.701567888
H	0.776536584	-2.590361357	-3.497368574	O	-4.016543388	-2.516164303	4.311081409
C	0.293024004	-1.512056470	-6.113983154	C	-4.202340603	-2.417552471	5.674127579
H	-0.465946585	-1.300338268	-6.875898838	H	-4.057514191	-1.399967670	6.083190918
H	1.061552048	-0.739935458	-6.234337807	H	-5.209319592	-2.747880220	5.977383614
C	-3.031890154	1.432634830	1.276623011	C	-3.207002878	-3.303765297	6.404006958
C	-3.890719652	2.541721344	1.355771303	F	-3.341733217	-3.218989372	7.750301838
C	-3.291692972	0.283269972	2.045796394	F	-1.922033191	-2.943717957	6.113524437
C	-5.003796101	2.519980431	2.192191601	F	-3.325474977	-4.605772018	6.066717148
C	-4.413866520	0.278787315	2.886761904	C	-5.615487099	-3.154110670	3.126582384
C	-5.256011963	1.385542750	2.969084263	O	-5.057369232	-3.252373934	2.085517168
H	-3.670912981	3.424324751	0.759310484	O	-6.505777359	-3.186316967	3.908624172
H	-5.663930416	3.382817984	2.242850304	C	-0.335972130	-3.216625214	1.796713471
H	-4.621773243	-0.607582271	3.477714062	H	-0.148049712	-4.271851540	1.573341012
H	-6.119182587	1.356887341	3.630427599	H	-0.452571779	-2.694357157	0.842480302
C	-2.500572205	-0.988080978	1.807067275	H	0.549280703	-2.819770098	2.302226782
H	-3.160230160	-1.688697934	1.286708117	C	-1.425756812	0.154929414	4.656564236
H	-1.651245713	-0.795084238	1.150075555	H	-1.840149045	0.977020323	4.071574688
N	-2.008923054	-1.712704897	3.027608395	H	-2.190433979	-0.186077431	5.360674858
C	-0.926027060	-0.994383216	3.786293030	H	-0.581049621	0.540001810	5.237503529
H	-0.175125629	-0.648920953	3.067943096	C	1.784050703	-0.685242355	-3.654858828
C	-1.582327485	-3.120621681	2.669945478	H	2.289600134	-0.759510219	-2.685628414
H	-1.433001876	-3.629122496	3.625748396	H	2.492461443	-1.015284896	-4.422372341
C	-4.539444447	-0.465464830	-3.112098694	H	1.547264934	0.367053181	-3.839443922
O	-5.328801632	-1.089261413	-3.677751541	C	0.910597980	-2.895554066	-6.375800610
C	-4.248215675	2.066861868	-2.478229284	H	1.337133050	-2.933890343	-7.384333611
O	-4.753602505	3.078253031	-2.731539726	H	1.714999199	-3.115910530	-5.665473461
C	-4.656255245	0.165648654	-0.786818147	H	0.164371878	-3.693612814	-6.296814442
O	-5.539245605	-0.086593144	-0.086452350	=====			
O	-2.248784542	-1.091304421	-1.554517627	<b>A7-H<sup>+</sup></b>			
C	-2.678000927	-2.276121378	-1.292798877	=====			
O	-3.847475529	-2.685176849	-1.266237617	C	-0.304580063	0.109377831	1.979143977

Mn	1.798819661	-2.756873369	-0.718867481	C	0.925278127	-0.946739078	6.229206562
C	-1.132615447	-3.023094893	-0.735251009	H	0.450542092	-1.841356158	6.645782948
C	-2.384850502	-3.645417213	-0.810282648	H	0.325316101	-0.610022426	5.377041817
C	-2.622158289	-4.574895859	-1.816782117	H	0.884069443	-0.160241425	6.990861416
C	-1.612964630	-4.831910133	-2.739428282	C	2.231369972	-3.613531113	5.347277164
C	-0.362278283	-4.217442513	-2.589951515	H	1.144482017	-3.785901308	5.240918159
N	-0.114809982	-3.356017590	-1.568713784	H	2.440819263	-3.642422676	6.423170567
H	-3.164952755	-3.411861658	-0.094769344	C	3.000632048	-4.747748852	4.664342403
H	-3.590377808	-5.061927319	-1.902230740	H	2.800483942	-4.793200493	3.588451147
H	-1.796172500	-5.472745895	-3.596781731	H	2.710870504	-5.713428974	5.093748093
C	-0.867659688	-1.935212255	0.239730194	H	4.079056740	-4.615253925	4.801455021
C	-1.919981003	-1.249864697	0.857516348	C	0.658335388	-4.375061512	-3.669999123
C	-1.635571957	-0.205501214	1.732791781	C	1.073636532	-3.185279608	-4.294095039
C	0.710090101	-0.612780273	1.336405396	C	1.136926770	-5.613403320	-4.164265156
N	0.431869835	-1.603582144	0.458410740	C	1.973131657	-3.194099665	-5.357058525
H	-2.951010466	-1.502671123	0.637690842	C	2.023550987	-5.601796150	-5.252551079
H	-2.438961744	0.349715382	2.210702896	C	2.454410553	-4.412038803	-5.839291573
H	-0.029436020	0.906562328	2.663702488	H	0.666058779	-2.243466616	-3.940640926
C	2.126458168	-0.275403470	1.671397686	H	2.281022310	-2.256848812	-5.814628601
C	2.756612301	-0.889245689	2.774196386	H	2.382000923	-6.547006607	-5.653180599
C	2.800142765	0.698593438	0.921311021	H	3.148159981	-4.440102100	-6.676165581
C	4.071148396	-0.519496202	3.077728987	C	0.748918951	-6.959169865	-3.586986303
C	4.108561516	1.060561061	1.244565964	H	0.771025538	-7.730503082	-4.361314774
C	4.742898941	0.447221816	2.327812910	H	-0.255694896	-6.948613167	-3.172661543
H	2.293529749	1.169815063	0.082476057	N	1.656379342	-7.439188957	-2.462660074
H	4.566655159	-1.015850544	3.906445980	C	1.107133508	-8.695113182	-1.807156324
H	4.625432491	1.815918088	0.657331824	H	0.951776683	-9.436083794	-2.595998526
H	5.764354229	0.717412353	2.587620020	H	1.898241520	-9.053465843	-1.142708063
C	2.056794643	-2.004874706	3.533875704	C	-0.172197714	-8.437605858	-1.017943740
H	0.974674702	-1.795057178	3.586760283	H	-1.023460746	-8.184906960	-1.656861901
H	2.131054640	-2.908210278	2.917360783	H	-0.024931105	-7.639322758	-0.285247445
N	2.627424002	-2.285687208	4.852354050	H	-0.430855632	-9.352681160	-0.475842625
C	2.387856722	-1.213131666	5.835152626	C	3.116059780	-7.608839512	-2.850519180
H	2.824975967	-0.290782243	5.437294960	H	3.648534060	-7.737011909	-1.903810740
H	2.964546442	-1.463895202	6.734307289	H	3.433302641	-6.659321785	-3.279728413

C	3.385549307	-8.768606186	-3.799718857	H	0.286639154	3.522012711	-5.582249641
H	4.447728157	-8.745830536	-4.063402176	H	-1.459209085	2.065109015	-6.700576782
H	2.814257145	-8.694205284	-4.730264187	C	-3.050927401	0.315553397	-5.595771790
H	3.175376654	-9.737677574	-3.339438438	C	-2.760151386	-1.040310860	-5.862997532
C	3.349195719	-2.469064236	0.177744508	C	-4.207025051	0.897981167	-6.134057045
O	4.398249626	-2.429631472	0.655449390	C	-3.658347368	-1.768833041	-6.651537895
C	2.055493355	-1.344869494	-1.798653841	C	-5.096994400	0.154378623	-6.913453102
O	2.200349331	-0.411388874	-2.466619253	C	-4.816479206	-1.188148022	-7.174917698
C	2.839939117	-3.816198111	-1.755354285	H	-4.404995918	1.949018478	-5.934750080
O	3.614760876	-4.394103050	-2.389530182	H	-3.440479517	-2.814888000	-6.861677647
C	1.545627475	-5.427174568	0.736410499	H	-5.991042614	0.622227371	-7.319400787
O	2.116298676	-6.085195065	-0.164950758	H	-5.491065025	-1.781558037	-7.788763523
O	1.278366089	-4.184978008	0.748605490	C	-1.563421726	-1.743050218	-5.239502430
H	1.227732301	-5.966977596	1.651919484	H	-1.610880494	-2.815523863	-5.510913372
H	1.686209083	-6.720927715	-1.702540874	H	-1.690368414	-1.685265541	-4.155045033

---

#### A8-H<sup>+</sup>

---

C	-1.316272378	2.048801899	-5.625560760	C	0.682352483	-1.302235007	-4.423682690
Mn	-3.281881332	0.221220002	-2.046438217	H	0.121671066	-1.060725808	-3.517557383
C	-0.845879197	1.726645947	-1.469125032	H	1.043261886	-2.346048117	-4.312496662
C	0.346354008	2.082701683	-0.782862008	C	0.312434494	-1.676824212	-6.810107231
C	0.381956130	2.096603632	0.589607358	H	1.368404508	-1.394190907	-6.847692966
C	-0.811730742	1.801086068	1.297874928	C	-3.232923031	1.309670687	1.347814322
C	-1.944873929	1.410701275	0.594197214	C	-4.263749123	2.171961546	0.934205353
N	-1.969390750	1.292987227	-0.765771329	C	-3.436421394	0.514166653	2.500199556
H	1.237929463	2.320081949	-1.355175972	C	-5.474169254	2.248433828	1.617624164
H	1.293244123	2.356383324	1.122320414	C	-4.651012897	0.626003921	3.196673632
H	-0.870034754	1.943571448	2.371722460	C	-5.669818878	1.472774148	2.762746334
C	-0.960157275	1.821801186	-2.890692472	H	-4.092708588	2.798887253	0.065537348
C	-0.129812226	2.693053246	-3.647392273	H	-6.250739574	2.926055908	1.269798636
C	-0.319949359	2.829303265	-5.002963543	H	-4.798081398	0.031780422	4.096065998
C	-2.088092327	1.186769843	-4.854598522	H	-6.601668358	1.534150362	3.319679022
N	-1.973774910	1.098781466	-3.504334211	C	-2.401597738	-0.460242987	3.019643307
H	0.614776790	3.296650887	-3.138501883	H	-1.398882866	-0.125791207	2.775747061
				H	-2.474722385	-0.571281493	4.106451035
				N	-2.523443937	-1.865445256	2.444119453

C -3.860160351 -2.499562979 2.772225857  
 H -4.617600918 -1.797053099 2.428448200  
 H -3.916305065 -2.570501566 3.863791704  
 C -1.364977837 -2.738853216 2.889522314  
 H -1.461657166 -2.871249437 3.972264290  
 H -1.514715791 -3.703034639 2.404188395  
 C -4.224703789 -0.878041089 -3.127000809  
 O -4.890865803 -1.652174711 -3.674685001  
 C -4.402033806 1.578635335 -2.312791586  
 O -5.088222980 2.491010189 -2.527679205  
 C -4.259875298 -0.521022081 -0.725686193  
 O -4.972503662 -1.031672239 0.034686238  
 O -1.700374365 -1.224232554 -1.989074469  
 C -1.456822753 -2.158352852 -1.174388766  
 O -2.095754623 -2.488838673 -0.144305572  
 H 0.292730182 -2.786666155 -6.834692955  
 H -0.558479726 -2.759837151 -1.433433294  
 H -2.448579311 -1.829247355 1.397454381  
 C -0.367598623 -1.123476386 -8.065509796  
 H 0.172872096 -1.451002836 -8.961345673  
 H -1.403986454 -1.456744313 -8.155261993  
 H -0.369549751 -0.028961934 -8.039016724  
 C 1.878466845 -0.350364894 -4.511353970  
 H 2.467125654 -0.410933763 -3.588406563  
 H 2.553182364 -0.582207799 -5.343083858  
 H 1.524548292 0.677568913 -4.629052162  
 C -4.077433109 -3.848819017 2.094485760  
 H -3.452957630 -4.642036915 2.514338493  
 H -5.123548985 -4.135902882 2.241752148  
 H -3.887110949 -3.776541710 1.020710826  
 C -0.000778350 -2.181667089 2.492011070  
 H 0.298056036 -1.311405063 3.082651854  
 H 0.748969376 -2.963224411 2.652756691  
 H 0.010924683 -1.915650129 1.430929184

**A9-H<sup>+</sup>**

C 0.006716091 -0.082154959 2.205251455  
 Mn 1.969834685 -2.735443354 -0.721356273  
 C -0.908008277 -3.119078159 -0.561725259  
 C -2.163106680 -3.737620592 -0.641972184  
 C -2.453230381 -4.536205292 -1.738657355  
 C -1.486415744 -4.674627304 -2.731467485  
 C -0.220407486 -4.106104851 -2.564649820  
 N 0.086613499 -3.360841036 -1.461938858  
 H -2.904076099 -3.589356184 0.135409102  
 H -3.425445080 -5.010856628 -1.839190483  
 H -1.723101139 -5.191995621 -3.654772997  
 C -0.611331165 -2.109216928 0.472344369  
 C -1.633955717 -1.507090807 1.217961788  
 C -1.324789882 -0.474780470 2.094358444  
 C 0.994832158 -0.734510839 1.462381244  
 N 0.693504632 -1.733634710 0.588706970  
 H -2.666103840 -1.810406923 1.084244847  
 H -2.104854107 0.023804296 2.663866997  
 H 0.299281150 0.734945714 2.857109785  
 C 2.403147221 -0.257736593 1.627319932  
 C 3.202934504 -0.666125655 2.710934401  
 C 2.884481430 0.705635786 0.726720512  
 C 4.492164135 -0.126738325 2.831137419  
 C 4.165008068 1.236179709 0.863302827  
 C 4.975862026 0.810642302 1.920767188  
 H 2.243633032 1.036540866 -0.085365914  
 H 5.102694035 -0.445124716 3.671477556  
 H 4.524489403 1.980026603 0.156122267  
 H 5.978672028 1.216077209 2.039752960  
 C 2.740859747 -1.699857116 3.723655462  
 H 1.656395197 -1.875991225 3.624600649  
 H 3.218795538 -2.648981094 3.461593628  
 N 3.133470297 -1.357947230 5.097160816

C	2.491849184	-0.133411884	5.602533340	C	2.675500631	-7.502755165	-2.796861172
H	2.699885368	0.667580485	4.884324074	H	2.914435148	-7.853326321	-1.788223863
H	3.004755020	0.145855725	6.532277107	H	3.003729105	-6.467645645	-2.871593714
C	0.978008509	-0.203090414	5.865660667	C	3.352820873	-8.368281364	-3.853236437
H	0.738537192	-0.938876152	6.640264511	H	4.435762882	-8.239388466	-3.754250765
H	0.419026971	-0.471223503	4.963968754	H	3.079699993	-8.076214790	-4.871387959
H	0.611283600	0.772139668	6.205207825	H	3.131074667	-9.431141853	-3.725915194
C	3.000456333	-2.497437239	6.016130924	C	3.284621477	-2.978277922	0.467415661
H	2.016847849	-2.993189335	5.921214581	O	4.191175461	-3.211926222	1.170000315
H	3.044723511	-2.103519678	7.038825035	C	2.601846218	-1.315681696	-1.619893789
C	4.116628170	-3.530807018	5.839329720	O	3.064228058	-0.453159183	-2.260200024
H	4.093519688	-4.001721859	4.850728512	C	2.976916075	-3.810891867	-1.725820541
H	4.014903069	-4.327919483	6.584248543	O	3.761527061	-4.431267262	-2.332323313
H	5.097160339	-3.059428453	5.966171265	C	-0.183062449	-6.399415970	0.313399136
C	0.770314932	-4.178533077	-3.680091381	O	0.826912522	-6.470139503	-0.462561727
C	1.276313066	-2.946237803	-4.130835533	O	-1.243938446	-7.057026386	0.282535702
C	1.162615538	-5.364574432	-4.349813461	H	-0.073961630	-5.637355804	1.124291658
C	2.183094740	-2.861630917	-5.182991982	H	0.891543090	-6.962951183	-1.943899393
C	2.078953981	-5.256531239	-5.409624100	=====	=====	=====	=====
C	2.598212004	-4.029877663	-5.822471142	<b>A9-H<sup>+</sup>-TS</b>	=====	=====	=====
H	0.944769144	-2.042399406	-3.631847620	=====	=====	=====	=====
H	2.554660082	-1.890765786	-5.502461910	C	-0.747750759	-0.185555801	2.296776056
H	2.379376650	-6.157060146	-5.940164566	Mn	1.556001902	-2.938506603	-0.261277318
H	3.304475784	-3.989009142	-6.648711681	C	-1.248494864	-2.868874788	-0.904178441
C	0.613104761	-6.754738808	-4.073725700	C	-2.488727808	-3.286753893	-1.402338028
H	0.806522429	-7.396961212	-4.937776566	C	-2.542626143	-3.964939117	-2.613577366
H	-0.464868814	-6.731639385	-3.938307047	C	-1.354765296	-4.177654743	-3.310953379
N	1.164761901	-7.470146179	-2.860187054	C	-0.136056796	-3.776286125	-2.754656553
C	0.574822307	-8.857842445	-2.732293606	N	-0.078200415	-3.166289568	-1.537870169
H	0.846081972	-9.418978691	-3.630878448	H	-3.404084206	-3.075035810	-0.861852229
H	1.081683755	-9.312691689	-1.875931025	H	-3.495237589	-4.289674282	-3.024041891
C	-0.934675634	-8.853288651	-2.515141964	H	-1.364282489	-4.636510372	-4.295085430
H	-1.482770681	-8.528001785	-3.404983759	C	-1.120804310	-2.019535303	0.297280073
H	-1.203367114	-8.223734856	-1.660932779	C	-2.233113050	-1.528304696	0.990181804
H	-1.247850060	-9.880393028	-2.299505949	C	-2.043510675	-0.608574450	2.016266108

C	0.335313916	-0.734207988	1.602368116	C	1.573323250	-5.115589142	-4.133789539
N	0.155400038	-1.673874974	0.635679245	C	2.844370127	-2.666465044	-4.763753414
H	-3.237636566	-1.836654663	0.722534776	C	2.659066200	-5.063691616	-5.020639896
H	-2.893049479	-0.201108664	2.558077574	C	3.298204184	-3.860294819	-5.324775219
H	-0.558480978	0.593337119	3.027114153	H	1.362969160	-1.768753409	-3.486208439
C	1.696688533	-0.170036986	1.835786939	H	3.327887535	-1.721918464	-5.000348568
C	2.356733799	-0.202495664	3.080657005	H	3.022500515	-5.962739468	-5.501647949
C	2.274836302	0.524362326	0.758083880	H	4.141150951	-3.861232996	-6.011805534
C	3.591886044	0.454227567	3.194890261	C	0.840601623	-6.405337334	-3.804291010
C	3.497493982	1.173581123	0.891399026	H	0.147862688	-6.678607941	-4.607128620
C	4.161735535	1.135327935	2.121656895	H	0.234882563	-6.241127491	-2.917979717
H	1.742198110	0.555136621	-0.188147962	N	1.645333648	-7.654803276	-3.505636692
H	4.091834545	0.430493951	4.158757210	C	0.758402050	-8.657793045	-2.774935961
H	3.924938202	1.708608031	0.046867847	H	-0.151718870	-8.788173676	-3.367411375
H	5.118306637	1.639032841	2.244249344	H	1.329324961	-9.586396217	-2.763626575
C	1.849631429	-0.982064545	4.287261963	C	0.462655574	-8.230261803	-1.340121388
H	0.808744550	-1.307723999	4.132841587	H	-0.181860298	-7.348598480	-1.271128535
H	2.437408209	-1.904205561	4.341148853	H	1.393388033	-8.025510788	-0.803946435
N	2.036861420	-0.244000375	5.541675091	H	-0.052636746	-9.054140091	-0.836142004
C	1.119880676	0.894900262	5.689464092	C	2.327064514	-8.318945885	-4.697759628
H	1.176012278	1.481087446	4.764406681	H	2.665252924	-9.284078598	-4.318310738
H	1.512891293	1.540886521	6.485795975	H	3.226195335	-7.738102913	-4.905855179
C	-0.348663747	0.559169471	6.002570152	C	1.447161913	-8.464009285	-5.930271626
H	-0.443535775	0.054387286	6.969403267	H	1.997197866	-9.051534653	-6.672800064
H	-0.794281363	-0.091357097	5.243308544	H	1.202949643	-7.500455856	-6.389774799
H	-0.944007874	1.478039622	6.044985771	H	0.514957964	-8.994064331	-5.710086823
C	2.092986822	-1.107891798	6.728216648	C	2.498812437	-3.112857103	1.247179627
H	1.271815300	-1.847237229	6.746562004	O	3.128417492	-3.254543543	2.222091436
H	1.946023464	-0.469383150	7.607711792	C	2.787787437	-1.930196285	-1.096930861
C	3.439830303	-1.823116302	6.864136219	O	3.639596224	-1.321982145	-1.613954425
H	3.636732101	-2.496681452	6.022935867	C	2.214006662	-4.514774799	-0.780665040
H	3.460898161	-2.424753666	7.779849529	O	2.624635935	-5.551269531	-1.130917311
H	4.254968643	-1.092820406	6.908608437	C	4.145139694	-9.378890991	-1.911652684
C	1.108620405	-3.896960497	-3.576196194	O	3.902655125	-8.135529518	-1.978751302
C	1.746531487	-2.692556858	-3.908425331	O	3.506023407	-10.341814041	-2.407967806

H	5.061294079	-9.644662857	-1.324552059	H	-2.377349138	-2.979959726	-2.290816545
H	2.445133686	-7.489840031	-2.841678381	H	-2.428546906	-1.259473443	-1.915760398
<hr/>				N	-0.665924788	-1.792666554	-2.848919153
<b>A9-H<sup>+</sup>(b)</b>				C	0.027540166	-1.579618096	-1.579493761
<hr/>				H	-0.518993914	-0.781739593	-1.059856772
C	-0.562551558	0.769598186	-5.097618103	H	-0.009010555	-2.467322350	-0.920199037
Mn	-3.616355658	1.441961050	-2.038416624	C	-0.044558316	-2.755462170	-3.763978243
C	-0.991730154	2.301797867	-1.200332522	H	-0.628618717	-2.741233349	-4.691117764
C	0.014067817	2.973303318	-0.495475411	H	0.949085295	-2.379847765	-4.030744076
C	-0.188463986	3.288035393	0.843228221	C	-3.583233833	1.745363355	1.403808832
C	-1.375328183	2.882632017	1.452350974	C	-4.496671200	2.720600367	1.829523921
C	-2.341119051	2.199359417	0.707225800	C	-3.818064451	0.391659886	1.723350883
N	-2.173577070	1.951756477	-0.617425084	C	-5.649887085	2.365077019	2.529096842
H	0.945540071	3.242923737	-0.981090307	C	-4.977867126	0.047654361	2.431556702
H	0.574007988	3.819146633	1.407608867	C	-5.893604755	1.022431612	2.830768824
H	-1.560054183	3.076636553	2.504504919	H	-4.304719925	3.763051271	1.589908481
C	-0.827678144	1.868632436	-2.602113008	H	-6.353376389	3.135529518	2.836067200
C	0.300237805	2.182882309	-3.367635965	H	-5.150841236	-0.995206773	2.684754372
C	0.413574100	1.654150248	-4.651788712	H	-6.789629936	0.735677302	3.375784636
C	-1.657840729	0.473350435	-4.277941227	C	-2.864086151	-0.711905360	1.323073626
N	-1.837505341	1.093520641	-3.084234953	H	-3.438496590	-1.536448359	0.901008487
H	1.076568127	2.832593918	-2.978052855	H	-2.149024963	-0.375578672	0.570073664
H	1.270575523	1.898007035	-5.274928570	N	-2.071802855	-1.279574871	2.480966330
H	-0.474235147	0.273386478	-6.058887482	C	-1.364944577	-0.192348421	3.250938892
C	-2.641118526	-0.550611615	-4.721753120	H	-2.146472692	0.486142993	3.599025011
C	-2.874629259	-1.715780377	-3.954588890	H	-0.733696818	0.349591583	2.538376331
C	-3.283102989	-0.389857322	-5.955964565	C	-1.122583985	-2.365373135	2.031282187
C	-3.793439865	-2.655720711	-4.429114342	H	-0.313016504	-1.886511803	1.470012069
C	-4.197653294	-1.339252591	-6.416045666	H	-0.722041965	-2.799462080	2.947275162
C	-4.463909626	-2.469950199	-5.642915249	C	-4.640584946	1.424902081	-3.503602266
H	-3.082110882	0.501377821	-6.546171188	O	-5.359651566	1.459136963	-4.422565460
H	-3.970906734	-3.558535337	-3.847445488	C	-4.714303493	2.724605083	-1.450360298
H	-4.697328091	-1.193231225	-7.370956898	O	-5.442195415	3.570684195	-1.099647999
H	-5.173223972	-3.217651844	-5.990979195	C	-4.469997406	0.012695920	-1.366173029
C	-2.105512619	-1.979531765	-2.672705173	O	-5.094832897	-0.905407190	-0.997525454

H	-2.771547318	-1.786015749	3.148856401	C	-0.501893461	-1.850162864	0.468173236
O	-3.776254654	-2.652579069	3.958879948	C	-1.436175823	-1.260554552	1.354450941
C	-3.220774889	-3.513953686	4.723799706	C	-1.024103761	-0.334337562	2.282768011
O	-2.000833035	-3.726219893	4.886284828	C	1.239050746	-0.633028030	1.465347528
H	-3.940451860	-4.138079166	5.306436062	N	0.839947701	-1.517465115	0.490001887
C	-0.550484478	-0.703946888	4.434705257	H	-2.485972881	-1.523108006	1.284710526
H	-1.133946896	-1.397725821	5.045120239	H	-1.732042193	0.137995675	2.958749056
H	0.364916593	-1.211823225	4.118461132	H	0.736339033	0.673266590	3.072452545
H	-0.263540268	0.156404540	5.048289776	C	2.680696011	-0.283055663	1.663097620
C	-1.810011625	-3.463296652	1.225065112	C	3.449770927	-0.937491596	2.644676208
H	-1.114235878	-4.301681519	1.120817184	C	3.214873314	0.825597346	0.989824831
H	-2.702207804	-3.821763039	1.747203350	C	4.743009567	-0.468003541	2.914054632
H	-2.095193624	-3.142803669	0.219831720	C	4.503996849	1.278346539	1.263223886
C	1.482723475	-1.138954759	-1.745931983	C	5.272109509	0.627590895	2.234868526
H	1.888763309	-0.831554651	-0.775639296	H	2.605674505	1.334166884	0.249254361
H	2.119105816	-1.943818808	-2.128855944	H	5.320692539	-0.970359981	3.685453415
H	1.545468211	-0.289902270	-2.434353590	H	4.900479317	2.143049955	0.735647738
C	0.069162942	-4.201230526	-3.253225803	H	6.275703430	0.979250133	2.465917826
H	-0.912896514	-4.622891903	-3.012933493	C	2.952171087	-2.167979240	3.383834600
H	0.525758803	-4.837208271	-4.019780636	H	1.892729998	-2.353429794	3.146375656
H	0.690749526	-4.262877464	-2.353280067	H	3.502128601	-3.024906874	2.982554197
<hr/>				N	3.202039719	-2.098137617	4.831970692
<b>A10-H<sup>+</sup></b>				C	2.376955986	-1.085984707	5.510815620
<hr/>				H	2.510765553	-0.142231852	4.969652176
				H	2.798889160	-0.932307720	6.513179302
				C	0.874272943	-1.390900493	5.642851353
				H	0.699573576	-2.294693947	6.236154079
				H	0.397974342	-1.524361253	4.667366982
				H	0.366707146	-0.559792817	6.145944118
				C	3.140104294	-3.415662289	5.480193138
				H	2.239506721	-3.984218359	5.183304787
				H	3.051153898	-3.250203848	6.560998917
				C	4.390754223	-4.258379459	5.216006279
				H	4.516137123	-4.489920616	4.152936459
				H	4.327502251	-5.210499763	5.754781246

H	5.287135124	-3.726809740	5.553185940	C	-2.448886156	-7.668935776	-1.623627543
C	0.676631808	-4.344485283	-3.542951107	O	-1.554339170	-7.402587414	-0.757720470
C	0.950895488	-3.257970810	-4.392508984	O	-2.328621626	-7.784728050	-2.865856886
C	1.204780817	-5.616766930	-3.853994131	H	-3.471583366	-7.818494320	-1.198642850
C	1.743308425	-3.393886328	-5.526404858	H	-0.061918985	-7.159064293	-1.330711365
C	2.038604736	-5.724162102	-4.984500408	=====			
C	2.306654453	-4.638581276	-5.815396309	<b>A10-H<sup>+</sup>(b)</b>			
H	0.538734078	-2.289057255	-4.125628948	=====			
H	1.929280758	-2.535696030	-6.168676853	C	-0.672293901	0.849794269	-5.156658649
H	2.469920397	-6.693058491	-5.228711605	Mn	-3.647380829	1.347044230	-2.035623550
H	2.946382523	-4.767173290	-6.685769081	C	-0.974322915	2.188325405	-1.220337868
C	0.829077244	-6.948668957	-3.217004538	C	0.065684371	2.784191370	-0.474098086
H	1.450839639	-7.710212231	-3.691407442	C	-0.134633943	3.129771709	0.843773961
H	-0.215375170	-7.194796562	-3.437135935	C	-1.383624792	2.821907520	1.421192050
N	0.945669115	-7.189943314	-1.711507082	C	-2.370709896	2.209503651	0.666392982
C	1.412744045	-8.607998848	-1.449313045	N	-2.221776962	1.935474157	-0.672990799
H	2.390670538	-8.720044136	-1.925457358	H	1.028504610	2.962813377	-0.941361606
H	1.548872232	-8.688049316	-0.366227180	H	0.654949129	3.591954708	1.430533409
C	0.441874713	-9.676955223	-1.939246774	H	-1.576306105	3.022781849	2.470547676
H	0.245179400	-9.604029655	-3.012393236	C	-0.838971853	1.803643823	-2.592436075
H	-0.507581949	-9.611097336	-1.406636238	C	0.311410278	2.074652195	-3.364339113
H	0.888890862	-10.657289505	-1.744182706	C	0.380824476	1.653210521	-4.675106049
C	1.767314196	-6.213123798	-0.907424390	C	-1.761915922	0.567017138	-4.352754116
H	1.553864479	-6.449586391	0.140122309	N	-1.952408433	1.169905424	-3.119718313
H	1.383209229	-5.214005470	-1.093779325	H	1.137491822	2.625945568	-2.926623821
C	3.263393641	-6.260614872	-1.189587951	H	1.248681664	1.871762395	-5.292041779
H	3.738359690	-5.464556217	-0.610706747	H	-0.602951765	0.371139735	-6.128701687
H	3.473251820	-6.065469742	-2.244058371	C	-2.697261333	-0.492584914	-4.815880299
H	3.717781067	-7.211188316	-0.898633838	C	-2.838617086	-1.710670471	-4.103957176
C	3.343536854	-2.722137928	-0.050589088	C	-3.338701487	-0.343183994	-6.053390026
O	4.333728790	-3.045274258	0.505315781	C	-3.662108660	-2.705838680	-4.639214039
C	2.362207413	-0.751121283	-1.736861706	C	-4.152070522	-1.349380016	-6.575845718
O	2.707768202	0.274027795	-2.213998795	C	-4.325674534	-2.533921719	-5.859031677
C	2.940777779	-3.117836475	-2.293488264	H	-3.207150936	0.587883770	-6.599924564
O	3.763281822	-3.554448128	-3.011988163	H	-3.767686605	-3.644889116	-4.098149300

H	-4.645885468	-1.205607891	-7.534558296	O	-5.368977547	3.569031239	-1.165918112
H	-4.955739498	-3.328438044	-6.252985954	C	-4.450335979	-0.016392957	-1.277903914
C	-2.108899355	-1.964249015	-2.798732281	O	-5.105201721	-0.911502421	-0.867811561
H	-2.317723274	-2.999227047	-2.467072248	H	-2.774374247	-1.714011312	3.213675261
H	-2.534154177	-1.295376062	-2.043496132	O	-3.757310629	-2.596269131	4.089688301
N	-0.679890275	-1.664943457	-2.866756439	C	-3.161087513	-3.440519094	4.840667725
C	-0.099018313	-1.475214958	-1.540668845	O	-1.935065627	-3.665629387	4.929091454
H	-0.700053930	-0.699985385	-1.049641490	H	-3.845827579	-4.038833618	5.490355015
H	-0.174262241	-2.385079622	-0.912438631	C	-1.888444304	-3.398877859	1.265457630
C	0.072940834	-2.520573378	-3.782916069	H	-1.205451488	-4.244938850	1.139167547
H	-0.441111594	-2.487201929	-4.750322342	H	-2.769897938	-3.750808001	1.810359120
H	1.054108858	-2.063290596	-3.951036453	H	-2.195596457	-3.068643808	0.269814163
C	-3.616071939	1.810814142	1.388499618	C	-0.552722096	-0.656653881	4.471847534
C	-4.507615566	2.811617851	1.797322989	H	-1.157509565	-1.310608268	5.104912281
C	-3.838143349	0.479491472	1.799264073	H	0.337610155	-1.210170865	4.160631180
C	-5.618646622	2.505536079	2.583148956	H	-0.222478896	0.204109758	5.062820911
C	-4.956876278	0.181425542	2.587316513	C	1.357750297	-1.010419726	-1.564589500
C	-5.844036579	1.185384274	2.980553389	H	1.666830420	-0.714953899	-0.555454910
H	-4.322836876	3.836006165	1.486518502	H	2.040817976	-1.797904134	-1.901395559
H	-6.301091671	3.296339512	2.886705875	H	1.467302442	-0.146365270	-2.227024078
H	-5.118484020	-0.843508601	2.911937952	C	0.256498426	-3.985366106	-3.349353552
H	-6.705760956	0.937975705	3.596118450	H	-0.706622183	-4.491658211	-3.223571539
C	-2.908756971	-0.641541243	1.390829086	H	0.828107178	-4.538322926	-4.103311539
H	-3.503599167	-1.460546136	0.988350749	H	0.798142672	-4.056154251	-2.399504423
H	-2.211641073	-0.318130642	0.616826653	=====			
N	-2.094912052	-1.216123819	2.531802177	<b>B1-MeCN</b>			
C	-1.355541110	-0.138212726	3.282996416	=====			
H	-2.117023945	0.567185760	3.621603251	C	0.213193908	0.471237421	-2.458992004
H	-0.715872824	0.378519714	2.560547829	Mn	-1.947193384	3.127788782	0.335131109
C	-1.168629766	-2.311220407	2.057754517	C	0.912303507	3.205862522	0.635426104
H	-0.370266080	-1.839297771	1.475590467	C	2.188043833	3.717549801	1.009499907
H	-0.749967396	-2.752722979	2.962015152	C	2.346174002	4.373896599	2.205026627
C	-4.708151817	1.231474638	-3.455415487	C	1.227753162	4.509320736	3.063101530
O	-5.470902920	1.226087213	-4.349661350	C	-0.016718971	4.062838554	2.635941029
C	-4.673575878	2.680872679	-1.516913772	N	-0.207575858	3.475084305	1.424388289

H	3.040998697	3.574407339	0.355300248	C	-4.326192379	2.682639837	-6.433878899
H	3.319768190	4.755768299	2.502968073	H	-4.490742207	3.233299494	-5.501304150
H	1.324700713	4.931928635	4.056206226	H	-4.403133392	3.401305914	-7.257407665
C	0.705988884	2.371063232	-0.499916911	H	-5.131520748	1.947428703	-6.537181854
C	1.766973019	1.914782166	-1.333767891	C	-1.146739721	4.127195358	3.616108418
C	1.525910378	0.979434192	-2.309590101	C	-1.575537086	2.906304121	4.167320251
C	-0.811492145	0.986355782	-1.673979282	C	-1.710810184	5.330248833	4.083099842
N	-0.603727698	1.951602817	-0.739484727	C	-2.565686703	2.859208584	5.144909859
H	2.774973154	2.281405687	-1.175029874	C	-2.705975056	5.267155170	5.070437908
H	2.334787607	0.610844970	-2.935866594	C	-3.137679815	4.052420139	5.598502159
H	-0.009178409	-0.321797997	-3.163300037	H	-1.108163834	1.987338662	3.825939894
C	-2.166195154	0.368952394	-1.828872681	H	-2.880073071	1.902678728	5.556313038
C	-2.963937283	0.547567487	-2.975303650	H	-3.130085468	6.202094078	5.426179409
C	-2.591264963	-0.515020847	-0.821952879	H	-3.911184788	4.034309387	6.363633156
C	-4.176702976	-0.152150497	-3.067041159	C	-1.356449962	6.694578648	3.511340618
C	-3.799520254	-1.199618816	-0.924518704	H	-0.474190533	6.618928432	2.857883930
C	-4.598822594	-1.014860749	-2.057745695	H	-2.184923172	6.999127388	2.863030672
H	-1.951591134	-0.671619713	0.041760549	N	-1.205363512	7.713800907	4.558447838
H	-4.780601501	-0.012657309	-3.959565163	C	-1.363274455	9.084441185	4.056060314
H	-4.108386517	-1.880538464	-0.134545341	H	-0.766411960	9.265995979	3.143497944
H	-5.543286324	-1.546387076	-2.154757261	H	-0.964930415	9.764020920	4.819270134
C	-2.611482859	1.527823210	-4.082359314	C	-2.828750372	9.445138931	3.796799421
H	-1.587465763	1.907730222	-3.945234776	H	-3.277505875	8.819518089	3.017517090
H	-3.270689249	2.395266533	-3.969810486	H	-3.419253349	9.318842888	4.710630417
N	-2.833699942	0.960995257	-5.419290543	H	-2.911794901	10.487726212	3.469928026
C	-1.872493148	-0.099170007	-5.761025429	C	0.004318755	7.527606487	5.373696327
H	-1.868758917	-0.814356625	-4.929854870	H	-0.101968654	8.146125793	6.274899960
H	-2.268656731	-0.639351130	-6.631199360	H	0.008848109	6.485595226	5.714277744
C	-0.431027442	0.347095400	-6.062444687	C	1.347225547	7.854246616	4.697772980
H	-0.388871431	0.989328384	-6.948287964	H	2.175185919	7.631609440	5.380626202
H	0.009565216	0.895450056	-5.224414825	H	1.500037551	7.265579700	3.788004637
H	0.200223118	-0.528199971	-6.254443645	H	1.411350250	8.913972855	4.429909706
C	-2.962540627	1.986637235	-6.462853909	C	-3.344937325	2.928507566	-0.797646821
H	-2.156917334	2.741588116	-6.407120228	O	-4.276177883	2.904716253	-1.483887434
H	-2.844401121	1.488001466	-7.432552338	C	-2.486877680	1.776080728	1.373102546

O	-2.830427170	0.899250805	2.044292688	C	-4.341362476	-0.320322931	-6.988192081
C	-2.969469070	4.328302860	1.221704483	C	-4.447892189	-1.606630921	-6.458170891
O	-3.683037043	5.103785038	1.699565411	H	-3.357870102	1.591441870	-6.821052551
C	-0.848415375	5.585344791	-1.573033452	H	-3.673652887	-3.010132313	-5.017458916
N	-1.229094386	4.718543053	-0.908402979	H	-4.968334675	-0.012684212	-7.821712017
C	-0.359975904	6.674230576	-2.411665916	H	-5.159543037	-2.315229416	-6.876206398
H	-1.168501973	7.028553009	-3.061272383	C	-1.772589684	-1.586094022	-3.724675417
H	0.471530765	6.317389011	-3.030511379	H	-1.963041544	-2.659193754	-3.539412498
H	-0.012497593	7.499809742	-1.780202746	H	-2.059736729	-1.057010651	-2.813516378
<hr/>				N	-0.346350878	-1.320054412	-3.957212687
<b>B1</b>				C	0.374763519	-1.093520522	-2.696776867
<hr/>				H	-0.262495607	-0.461575955	-2.071587324
C	-0.717880607	1.820664525	-5.560715199	C	0.301871628	-2.347054005	-4.784494400
Mn	-3.532698631	1.470179796	-2.240529299	H	0.091301128	-3.359329224	-4.385390282
C	-0.913965046	2.290124655	-1.381993532	C	-3.164367437	0.704853594	1.107061028
C	0.115501463	2.809900284	-0.590902627	C	-4.116310596	1.394134641	1.875261068
C	0.042250883	2.669892788	0.791643202	C	-3.237812042	-0.696941555	0.994859457
C	-1.039284825	1.981672406	1.338912606	C	-5.163808823	0.713245988	2.492562056
C	-2.041043758	1.480115771	0.501528382	C	-4.292067051	-1.367362380	1.630468369
N	-2.000917196	1.670830727	-0.841293752	C	-5.255945206	-0.676942647	2.363956690
H	0.970219791	3.299151897	-1.045769691	H	-4.036820889	2.473896027	1.970151782
H	0.829653144	3.065760374	1.428294420	H	-5.900542736	1.263681293	3.072925329
H	-1.113510251	1.811486244	2.408766747	H	-4.330778599	-2.450867891	1.555780411
C	-0.858842432	2.275950670	-2.858502150	H	-6.067386150	-1.219621778	2.843788862
C	0.132938370	2.920059204	-3.603145599	C	-2.218365192	-1.522097349	0.230786905
C	0.177412078	2.716381788	-4.982563972	H	-2.728282452	-1.978883743	-0.619913220
C	-1.694749594	1.210991383	-4.763541698	H	-1.433305979	-0.873819411	-0.189920753
N	-1.819572330	1.513946772	-3.448901653	N	-1.644454479	-2.593193054	1.058746934
H	0.859830976	3.566609144	-3.122673512	C	-0.748375356	-2.028427839	2.081373930
H	0.930080354	3.217015028	-5.586753845	H	0.225296021	-1.740265608	1.639169812
H	-0.664798856	1.573018193	-6.616381645	C	-0.963368952	-3.606781960	0.238212883
C	-2.625790358	0.208385810	-5.346270561	H	-0.391150087	-4.253374100	0.910311401
C	-2.688861370	-1.111159801	-4.841741085	C	-4.634882450	1.854378939	-3.593224049
C	-3.428634405	0.578233600	-6.432457447	O	-5.395678997	2.134673119	-4.435008526
C	-3.617877245	-1.993065596	-5.401080132	C	-4.671849728	2.389882803	-1.218186617

O	-5.433907986	3.003898621	-0.576217651	H	1.867174387	4.326004505	1.489201307
C	-4.264120102	-0.157218620	-2.002442122	H	0.297153503	3.265151739	3.131963491
O	-4.833837032	-1.173099041	-1.899192095	C	-0.814924717	2.822209597	-2.023267984
H	-1.203710914	-1.101754785	2.446174622	C	-0.097320646	3.391361237	-3.080284834
H	-0.223717198	-3.137478828	-0.438228577	C	-0.415672272	3.022181749	-4.385841846
H	1.383761764	-2.208955526	-4.704514980	C	-2.034273148	1.478670597	-3.484740734
H	0.527949870	-2.036342144	-2.136994600	N	-1.837988853	1.954211473	-2.232757092
C	-0.537550628	-2.962641001	3.273707867	H	0.685376465	4.118822575	-2.894614935
H	-1.499696970	-3.199852467	3.739916563	H	0.106478252	3.471307278	-5.227177143
H	-0.057761613	-3.904694319	2.987853527	H	-1.589528799	1.650286198	-5.579418182
H	0.101683281	-2.482130289	4.022879601	C	-2.956965208	0.327384621	-3.682878971
C	-1.922749281	-4.483829975	-0.569369555	C	-2.645803452	-0.936843634	-3.130141973
H	-1.363370776	-5.270177841	-1.088585138	C	-4.089360237	0.477983534	-4.492833614
H	-2.655584335	-4.958739281	0.091927782	C	-3.504940271	-2.007532597	-3.393928289
H	-2.469715357	-3.917755127	-1.330795646	C	-4.945236206	-0.599730253	-4.733839035
C	1.716960669	-0.380433202	-2.877618790	C	-4.650897503	-1.846859097	-4.179265022
H	2.129152536	-0.116858236	-1.896723628	H	-4.307585716	1.453588486	-4.919708729
H	2.461528063	-0.998747289	-3.389733076	H	-3.270174503	-2.985336542	-2.976935863
H	1.579656601	0.539024472	-3.453612328	H	-5.828084469	-0.465018094	-5.354207516
C	-0.072299458	-2.285738230	-6.267397881	H	-5.303213120	-2.697258949	-4.365312099
H	0.545873880	-2.989734173	-6.835962296	C	-1.428077579	-1.140505910	-2.244461298
H	-1.120087266	-2.538566828	-6.442413807	H	-1.350571036	-2.210692167	-1.980155468
H	0.099256814	-1.277671695	-6.658957005	H	-1.602455497	-0.606827497	-1.304749131

---

## B2

---

C	-1.370803595	2.030234814	-4.586301804	N	-0.197505072	-0.596849084	-2.816825151
Mn	-3.198594332	2.012389660	-0.647745728	C	0.246263757	-1.269065619	-4.041179657
C	-0.494526207	3.061203718	-0.602459490	H	-0.618661880	-1.315575600	-4.712084770
C	0.674865842	3.717433214	-0.203375310	H	0.977249086	-0.622216582	-4.538841248
C	0.963227093	3.823871374	1.153108358	C	0.831458092	-0.384166986	-1.799239755
C	0.087867923	3.242896080	2.067004681	H	1.160085678	-1.328843355	-1.323763847
C	-1.069180608	2.595606565	1.615310788	C	-1.980785847	1.994935155	2.630015373
N	-1.379502892	2.534230947	0.292972624	C	-2.496168137	2.864085197	3.607991457
H	1.360681415	4.124038696	-0.938756645	C	-2.297514200	0.620626152	2.681855440
				C	-3.348278046	2.403022051	4.608709812
				C	-3.173258781	0.177465245	3.683596611
				C	-3.697025537	1.049972057	4.637912273

H	-2.235913277	3.918832541	3.560760736	H	0.083010092	-3.865930557	3.060934305
H	-3.742396832	3.093917131	5.350102425	H	0.562728703	-4.361745834	1.423942089
H	-3.428642750	-0.877521932	3.721351624	H	1.496455789	-3.131621599	2.282682419
H	-4.370904446	0.672275841	5.403646946	C	2.059351921	0.367823422	-2.314111471
C	-1.704009056	-0.411820352	1.742483497	H	2.702185631	0.641470432	-1.470268130
H	-2.514529228	-1.031853318	1.350057602	H	2.658963203	-0.234998256	-3.004495621
H	-1.239376307	0.074619293	0.877686977	H	1.755998850	1.284339905	-2.829985142
N	-0.757329464	-1.337380409	2.415392399	C	0.838654935	-2.677971363	-3.869292736
C	0.436248690	-0.643893480	2.958520651	H	0.123245135	-3.362933159	-3.401319027
H	0.948309362	-1.342053533	3.622839451	H	1.110939860	-3.094865084	-4.845522881
C	-0.433311701	-2.453657627	1.492612720	H	1.742347479	-2.661763668	-3.250107050
H	-1.388385057	-2.920715094	1.223087311	=====			
C	-4.247982979	2.580687284	0.682355523	<b>B2-TS</b>			
O	-4.987807274	2.953954697	1.505051136	=====			
C	-3.846180916	0.344857246	-0.493097425	C	-1.416115761	1.943109155	-4.170056343
O	-4.373973370	-0.692713261	-0.375940919	Mn	-3.389516830	1.696019173	-0.300949246
C	-4.449422359	2.598899364	-1.777722001	C	-0.651946485	2.679072857	-0.093396366
O	-5.269457817	2.957087755	-2.532872200	C	0.499072552	3.303270817	0.403983504
H	0.066964693	0.166374490	3.594868898	C	0.678133368	3.410953999	1.778171062
H	0.003711048	-2.075659037	0.555209756	C	-0.267803490	2.827850103	2.619263411
H	0.365237832	0.211539790	-1.005514383	C	-1.386019468	2.191538572	2.072219372
C	-0.665396690	-3.172504425	6.100591660	N	-1.621468663	2.183760405	0.730145872
C	-1.919512272	-2.500262499	5.566702366	H	1.247767329	3.703260660	-0.270404577
H	-1.796004891	-1.417638540	5.711087227	H	1.555587053	3.907277107	2.185520649
H	-2.753345490	-2.832063913	6.197291374	H	-0.133688360	2.827420712	3.696824074
O	-2.162917376	-2.858415604	4.229537010	C	-0.885688543	2.484028101	-1.536007524
H	-1.616650462	-2.259226561	3.633454323	C	-0.043494686	3.008294821	-2.523871899
F	0.446419656	-2.793568373	5.418100357	C	-0.347156972	2.780056477	-3.863234043
F	-0.731811941	-4.518376827	6.012936115	C	-2.179362774	1.390726328	-3.137119532
F	-0.462633491	-2.854929686	7.400361061	N	-1.990663409	1.755239367	-1.844732285
C	1.429821014	-0.082509346	1.931141376	H	0.826233387	3.599288940	-2.258115530
H	2.240865946	0.434961498	2.454952955	H	0.270651847	3.207669020	-4.649242401
H	1.878736854	-0.872349560	1.320767522	H	-1.634081006	1.659921288	-5.195405960
H	0.964407861	0.641820848	1.257871270	C	-3.167119503	0.324161530	-3.462296963
C	0.484154552	-3.510071278	2.108011246	C	-2.918114662	-1.008579373	-3.059327841

C	-4.263258934	0.612832069	-4.282801628	C	-4.510935783	2.117988825	1.028506637
C	-3.805010080	-2.007338285	-3.470638275	O	-5.317098141	2.387984276	1.827293754
C	-5.144505024	-0.396783382	-4.676803589	C	-4.012388706	0.016294898	-0.270781636
C	-4.914555073	-1.711592674	-4.268837452	O	-4.510200500	-1.040501475	-0.203966558
H	-4.432694435	1.638735414	-4.599443436	C	-4.623233795	2.367174864	-1.406451344
H	-3.621476889	-3.034541845	-3.160398483	O	-5.435224056	2.794763088	-2.131403923
H	-5.999857903	-0.155641958	-5.303844929	H	-0.037616882	0.002145886	3.690463543
H	-5.589397907	-2.507595778	-4.576127052	H	-0.237961650	-2.513226748	0.854104042
C	-1.741855741	-1.355552197	-2.165618896	H	0.156310812	-0.327735126	-0.799355924
H	-1.751523495	-2.440942764	-1.958268642	C	-0.283125639	-2.476283312	6.679025650
H	-1.893734574	-0.863261402	-1.199787140	C	-1.530256867	-1.968927264	5.979133606
N	-0.463030934	-0.870804369	-2.684338093	H	-1.419138551	-0.884275258	5.834534645
C	-0.077073313	-1.464972496	-3.969165802	H	-2.368921757	-2.129050732	6.670785427
H	-0.890641570	-1.260226011	-4.674519539	O	-1.726591945	-2.654988527	4.784016609
H	0.789208055	-0.912641644	-4.347638130	H	-1.331978202	-2.102007151	3.761241674
C	0.563042939	-0.899381280	-1.641072392	F	0.829970598	-2.335810184	5.911988735
H	0.748879313	-1.922651649	-1.257664919	F	-0.375589401	-3.786671400	6.991436005
C	-2.346800089	1.525711536	2.993889570	F	-0.059587359	-1.796875000	7.830266953
C	-2.954848528	2.316487789	3.981970549	O	-3.201993465	-4.204577446	3.511774302
C	-2.636164665	0.145471334	2.931148291	O	-3.557424545	-4.080119133	5.803391933
C	-3.867767096	1.767397881	4.879848003	C	-3.184297085	-3.967934608	4.679133415
C	-3.587128878	-0.381806046	3.815584898	C	0.488503993	-3.739775896	2.503647804
C	-4.193549156	0.412247390	4.788666725	H	0.222899213	-3.936805964	3.546574116
H	-2.725456476	3.378772974	4.021176338	H	0.517388940	-4.692334175	1.964915395
H	-4.331961155	2.396733999	5.635663033	H	1.494605184	-3.309585571	2.474612236
H	-3.834995985	-1.436004519	3.747288227	C	1.174558520	-0.285450548	1.921754837
H	-4.919952393	-0.026032286	5.469088554	H	1.966092348	0.348582774	2.333044529
C	-1.933204055	-0.811985314	1.991130948	H	1.643422008	-1.086456776	1.342539430
H	-2.661840200	-1.526542544	1.603100777	H	0.596462905	0.341251105	1.239382386
H	-1.499565005	-0.299888790	1.132246137	C	1.890766025	-0.267689228	-2.057334900
N	-0.878251910	-1.625424027	2.684681654	H	2.540129423	-0.167435229	-1.180516362
C	0.328514338	-0.823925257	3.074221611	H	2.427490473	-0.871803582	-2.796513319
H	0.935176253	-1.457559943	3.721127033	H	1.721142054	0.728122413	-2.480106592
C	-0.554579377	-2.833536148	1.853643537	C	0.231586441	-2.970489502	-3.964837790
H	-1.495586753	-3.380819559	1.749276876	H	-0.648761630	-3.565051079	-3.698166847

H	0.553108335	-3.288439035	-4.963023186	H	-1.951097131	-2.982258797	-3.904457808
H	1.034264088	-3.216194153	-3.261013746	H	-2.218030930	-1.516284108	-2.959426403
<hr/>				N	-0.456774622	-1.444931865	-4.054591179
<b>B3</b>				C	0.269642949	-1.435625196	-2.783590078
<hr/>				H	-0.309130698	-0.809515238	-2.093283892
C	-0.872952938	1.704402089	-5.515076637	C	0.226324096	-2.082630396	-5.182620525
Mn	-3.479038239	0.928598762	-2.061833382	H	-0.456599921	-2.025315046	-6.037827492
C	-0.878702402	2.049104929	-1.324548602	C	-3.354884386	1.393673182	1.364887714
C	0.253195643	2.465157270	-0.609455168	C	-4.321345329	2.411714315	1.370037556
C	0.207459375	2.499560595	0.776303053	C	-3.618245840	0.198159605	2.065459728
C	-0.977380693	2.123475790	1.408729434	C	-5.549984455	2.238657475	2.001904488
C	-2.068476677	1.690907121	0.651867986	C	-4.872606754	0.023294616	2.671508789
N	-2.020192862	1.635402918	-0.709627986	C	-5.835359573	1.029818177	2.642395496
H	1.162388444	2.741872311	-1.131855130	H	-4.101935863	3.344491482	0.858397067
H	1.070254326	2.821635008	1.353557229	H	-6.285046101	3.039412260	1.983100176
H	-1.071258903	2.186258554	2.487574816	H	-5.105945587	-0.919290423	3.166525841
C	-0.877410531	1.994356275	-2.797971487	H	-6.799966812	0.873348951	3.119021177
C	0.069944903	2.691610575	-3.554100752	C	-2.612392902	-0.923669875	2.185047865
C	0.049744908	2.570431232	-4.940560341	H	-3.021902561	-1.839759350	1.757072210
C	-1.788210392	1.016259909	-4.706821918	H	-1.662195921	-0.696994185	1.694719911
N	-1.851874471	1.227995515	-3.364353418	N	-2.268198252	-1.234334350	3.644775391
H	0.794251263	3.341001034	-3.074900627	C	-1.631878376	-0.036814708	4.336679935
H	0.757839680	3.120202065	-5.555827141	H	-2.184982061	0.840532780	3.997522831
H	-0.879418075	1.527476311	-6.585937023	H	-0.604828238	0.021876782	3.963294268
C	-2.700958967	0.046135187	-5.372421265	C	-1.395578384	-2.478199959	3.753504515
C	-2.724741697	-1.325856447	-5.026833534	H	-0.544776320	-2.313585281	3.085089684
C	-3.489156008	0.504471064	-6.438334465	H	-1.022621036	-2.508864164	4.778086662
C	-3.563604593	-2.182097435	-5.745940685	C	-4.679961681	0.376634479	-3.273279905
C	-4.327325344	-0.363226444	-7.139348984	O	-5.571609974	0.037070565	-3.944046736
C	-4.368914127	-1.712819457	-6.787349224	C	-4.761434555	2.092274666	-1.598929048
H	-3.457237720	1.558420181	-6.705807209	O	-5.645788193	2.829372168	-1.388575792
H	-3.571910143	-3.241463423	-5.494833946	C	-3.864782810	-0.534254134	-1.095767856
H	-4.937842369	0.013478241	-7.956923485	O	-4.140508175	-1.513552547	-0.514536440
H	-5.009765625	-2.402920723	-7.331992626	H	0.404349476	-3.160968304	-5.008114815
C	-1.844889760	-1.882113576	-3.922062874	H	1.223229051	-0.918900430	-2.935338736

H	-3.146181345	-1.440134048	4.146793842	N	-2.307622433	0.640917659	-3.074030876
C	-2.159664154	-3.757487774	3.434410572	H	1.012714863	0.384069264	-2.409996033
H	-1.500362873	-4.607841015	3.635478735	H	1.051396966	-0.273654997	-4.813930035
H	-3.043061495	-3.860453367	4.075587749	H	-1.106904626	-0.186071247	-6.111943722
H	-2.472535849	-3.821624279	2.388449907	C	-3.494142056	0.625584006	-5.237302780
C	-1.700404167	-0.132846847	5.855375290	C	-4.041210651	-0.326612443	-6.128562450
H	-2.737016678	-0.243787691	6.194952488	C	-4.076055050	1.901399612	-5.149612904
H	-1.103502393	-0.954636812	6.260363102	C	-5.197539806	0.022763191	-6.842263699
H	-1.309445977	0.801109433	6.272203445	C	-5.205053329	2.238770485	-5.893506050
C	0.525613248	-2.807210445	-2.135924816	C	-5.781149387	1.286705017	-6.737156391
H	-0.413735569	-3.336214542	-1.938513160	H	-3.624142647	2.637315035	-4.491473675
H	1.144847751	-3.446780682	-2.774774313	H	-5.648378372	-0.719613135	-7.497651577
H	1.049108386	-2.683571815	-1.181107521	H	-5.630981445	3.235687494	-5.810248852
C	1.539141536	-1.392051578	-5.557949543	H	-6.670341969	1.525949597	-7.315968037
H	2.314039230	-1.526746988	-4.795821667	C	-3.460307598	-1.715425134	-6.325731277
H	1.926249743	-1.805158257	-6.496108532	H	-4.277494431	-2.402646780	-6.614725590
H	1.373958707	-0.317766607	-5.691573620	H	-3.073563576	-2.079894543	-5.369799137
<hr/>				N	-2.355103254	-1.775219321	-7.308924198
<b>B3'</b>				C	-2.788144588	-1.442305207	-8.676625252
<hr/>				H	-3.479759455	-0.599002957	-8.619144440
C	-1.070145130	0.059672717	-5.055785179	C	-1.701834917	-3.096339226	-7.254184246
Mn	-3.953599215	0.510414243	-1.732514143	H	-2.457127333	-3.903971195	-7.214775562
C	-1.215320468	1.205470681	-1.016604185	H	-1.152961373	-3.244729519	-8.187923431
C	-0.098119594	1.738147378	-0.361786544	C	-3.901178837	1.624791622	1.510122180
C	-0.239284530	2.266183138	0.915543139	C	-4.850414276	2.628508329	1.288986206
C	-1.500711679	2.233989477	1.507920504	C	-4.168309689	0.596458137	2.442025423
C	-2.580906630	1.684227824	0.814359426	C	-6.068629742	2.610157967	1.970799923
N	-2.456013918	1.182857037	-0.446296513	C	-5.390407085	0.594617903	3.123728275
H	0.865103722	1.770610809	-0.858699322	C	-6.337930202	1.594343543	2.890498400
H	0.611515760	2.699898958	1.434340715	H	-4.632354259	3.419497252	0.576336801
H	-1.664654493	2.630010843	2.505908728	H	-6.802504063	3.390866756	1.785090446
C	-1.127038360	0.710807920	-2.401858568	H	-5.602241993	-0.198142737	3.838177919
C	0.097273335	0.375484079	-2.992034912	H	-7.284848213	1.577587485	3.424590349
C	0.118684456	0.010505807	-4.332839966	C	-3.177058458	-0.524523735	2.651865482
C	-2.267757893	0.395483196	-4.415659904	H	-2.152472496	-0.155640095	2.737231255

H -3.404455423 -1.108960867 3.546562195  
 N -3.198599339 -1.492697597 1.460309744  
 C -4.317088127 -2.513543367 1.613799810  
 H -4.102716446 -3.091805696 2.515492678  
 C -1.830399990 -2.079226732 1.152998805  
 H -1.915183306 -2.581593752 0.186095387  
 H -1.165022016 -1.220773697 1.024002075  
 C -4.804812431 -0.640322864 -2.820401192  
 O -5.380529404 -1.417512059 -3.471481323  
 C -4.839591503 2.035979509 -2.104001045  
 O -5.430848598 3.016244888 -2.316172361  
 C -5.211165428 0.015880002 -0.568708599  
 O -6.132273674 -0.326729119 0.069110006  
 H -5.220741272 -1.927175999 1.789251447  
 H -3.352643728 -2.278455973 -9.132012367  
 H -3.440977812 -0.933056295 0.625699461  
 C -4.477121353 -3.395695210 0.382213295  
 H -3.650495052 -4.101844311 0.261567533  
 H -5.399938107 -3.973844290 0.491702676  
 H -4.564699173 -2.796394587 -0.530110896  
 C -1.317592263 -3.019035339 2.233220100  
 H -1.927681684 -3.923298597 2.315883636  
 H -0.302026778 -3.324486494 1.962940454  
 H -1.272444844 -2.530113220 3.211389065  
 C -0.714954197 -3.239016294 -6.093585968  
 H -1.191871047 -3.092883825 -5.119144917  
 H -0.270862043 -4.240666389 -6.099527836  
 H 0.091100827 -2.504402876 -6.184364319  
 C -1.623026371 -1.030764103 -9.581282616  
 H -0.891422629 -1.833358884 -9.723223686  
 H -1.998491526 -0.750445604 -10.572309494  
 H -1.099009633 -0.168660030 -9.154260635

**Table S4.** Vibrational frequencies (in cm<sup>-1</sup>) of the optimized structures.

	1a						
<b>CO<sub>2</sub></b>							
	15.35	22.71	27.49	32.41	38.30	40.13	
641.88	641.88	1372.90	2440.51				
	48.26	51.89	57.23	59.71	66.00	69.56	
	75.07	79.59	80.16	85.49	93.34	96.08	
<b>MeCN</b>							
	104.12	104.87	107.80	115.29	129.86	136.63	
395.78	395.93	936.04	1069.30	1069.54	1419.38		
1483.69	1483.73	2368.06	3040.03	3120.65	3121.05		
	144.28	148.29	158.87	166.22	177.30	182.41	
	189.10	210.45	214.96	228.86	232.57	242.74	
	249.36	255.03	261.45	269.30	273.43	289.39	
	298.96	310.31	318.52	328.55	344.00	349.43	
<b>TFE</b>							
	362.81	384.86	392.53	404.88	413.05	445.09	
121.21	232.80	329.05	354.13	414.51	525.82		
543.20	645.42	826.34	982.46	1104.44	1176.50		
1193.90	1275.27	1310.42	1320.00	1498.56	1518.10		
3014.00	3059.20	3748.33					
	451.36	460.60	467.96	470.58	475.39	480.23	
	488.20	492.13	494.70	503.96	522.45	535.53	
	538.80	542.00	572.17	585.61	612.37	618.95	
	624.10	641.66	642.88	644.93	647.85	655.55	
	690.84	705.76	708.95	742.50	743.58	762.54	
	770.61	779.01	786.27	788.45	792.24	793.58	
<b>CF<sub>3</sub>CH<sub>2</sub>O<sup>-</sup></b>							
	804.97	814.85	821.84	823.61	833.14	838.92	
136.74	228.95	315.65	402.54	506.09	520.63		
655.48	788.25	975.59	1127.17	1170.39	1179.55		
1257.26	1273.13	1417.35	1478.82	2572.27	2648.11		
	842.67	846.78	877.65	900.70	907.44	924.11	
	926.99	928.69	931.97	966.78	974.52	992.22	
	1003.10	1007.79	1010.50	1011.65	1013.91	1016.61	
	1018.86	1019.69	1025.23	1044.95	1064.32	1070.21	
	1075.65	1080.76	1084.91	1092.09	1095.30	1105.56	
	1113.38	1128.94	1137.32	1137.99	1151.24	1153.07	
	1157.67	1162.02	1197.82	1198.03	1201.17	1202.83	
<b>HCOO<sup>-</sup></b>							
	1213.06	1217.49	1221.76	1225.34	1236.80	1237.41	
	1276.21	1278.64	1286.53	1291.24	1303.62	1305.78	
	1315.94	1321.45	1329.40	1330.80	1332.75	1343.49	
	1347.04	1363.47	1375.92	1391.31	1405.00	1408.46	
	1409.78	1418.19	1422.42	1428.26	1434.19	1438.24	
	1439.98	1443.55	1451.68	1482.54	1483.46	1491.77	
	1493.35	1496.55	1503.28	1505.88	1507.27	1508.04	
<b>HCOOH</b>							
	1510.11	1514.25	1514.89	1518.11	1519.27	1523.81	
	1527.16	1528.88	1529.03	1534.36	1539.98	1610.37	
	1617.63	1620.75	1621.71	1640.31	1644.97	1653.21	
	1655.47	2034.29	2050.75	2105.60	2918.36	2925.78	
	2942.40	2953.39	2965.52	3037.16	3038.80	3040.30	
<b>CF<sub>3</sub>CH<sub>2</sub>OCOO<sup>-</sup></b>							
	1807.46	3043.64	3117.68				

3088.78	3100.23	3110.70	3113.25	3113.47	3116.53	1512.60	1512.78	1517.66	1518.29	1520.73	1521.39
3118.07	3118.87	3123.44	3130.79	3168.16	3168.69	1525.96	1527.98	1528.92	1531.24	1605.15	1612.19
3179.29	3184.34	3187.14	3188.14	3193.88	3200.10	1620.32	1621.44	1638.77	1643.94	1650.35	1651.29
3205.39	3207.81	3209.56	3212.87	3217.45	3230.53	2064.20	2069.01	2125.40	2384.92	2945.01	2945.47
<hr/>											
<b>1b</b>						2968.36	2975.46	3036.74	3038.28	3038.77	3039.19
<hr/>											
19.99	28.31	30.32	32.58	34.05	34.78	3039.28	3044.30	3045.06	3065.07	3065.82	3071.82
43.35	48.29	55.67	61.24	62.62	65.88	3072.54	3076.87	3078.47	3108.51	3108.98	3113.68
79.37	81.68	87.46	92.43	100.88	109.02	3114.73	3120.24	3120.35	3120.53	3121.47	3122.30
110.90	115.89	127.12	132.83	136.90	142.87	3123.79	3174.54	3175.52	3186.20	3187.28	3193.08
144.17	151.61	151.94	166.63	172.44	177.90	3194.21	3199.19	3199.88	3208.68	3210.14	3216.53
179.07	188.65	205.29	208.25	218.62	225.05	3220.82	3222.09	3232.49			
<hr/>											
<b>1-vac</b>											
<hr/>											
21.18	27.52	28.96	35.19	40.19	51.37						
55.21	60.67	65.54	69.99	72.69	80.15						
84.03	100.64	102.47	107.39	111.71	116.37						
124.17	129.10	133.31	140.66	142.95	150.90						
160.37	174.94	185.67	188.99	195.13	218.57						
225.40	233.53	237.30	246.65	258.11	261.68						
266.83	282.05	295.89	308.17	313.47	326.10						
340.68	343.69	349.87	390.79	391.03	401.66						
406.45	417.89	430.27	436.55	440.61	446.57						
447.52	453.12	469.31	482.01	484.81	509.89						
515.81	524.03	528.79	537.07	538.41	563.19						
584.20	615.48	617.60	619.19	623.57	630.93						
642.88	648.29	651.52	688.66	701.63	704.28						
740.68	749.14	762.13	765.74	775.16	786.40						
786.98	796.01	799.51	813.83	815.50	816.08						
819.09	825.57	834.14	839.09	848.81	866.61						
899.24	899.91	917.83	919.87	934.95	942.79						
970.95	971.73	976.74	981.15	996.00	999.16						
1008.17	1013.45	1013.62	1024.99	1025.90	1030.45						
1040.58	1056.68	1061.66	1068.09	1080.82	1084.90						
1085.81	1091.71	1111.38	1115.18	1116.00	1118.94						
1123.52	1136.13	1138.55	1152.10	1168.19	1197.23						
1202.80	1206.14	1208.07	1216.67	1219.94	1224.01						
1225.53	1232.11	1234.77	1274.04	1274.87	1286.78						
1292.93	1307.55	1314.49	1315.53	1319.27	1324.88						

1325.23	1351.70	1354.92	1359.98	1374.69	1377.05		1133.08	1141.32	1150.99	1161.49	1163.96	1189.19	
1386.65	1390.21	1401.81	1404.33	1409.39	1414.57		1192.02	1194.27	1197.68	1200.14	1203.18	1221.03	
1419.41	1423.23	1424.61	1433.48	1437.29	1443.66		1224.25	1230.30	1239.08	1277.32	1279.32	1296.28	
1481.29	1485.37	1492.50	1496.36	1497.27	1499.79		1310.64	1312.28	1315.58	1323.30	1328.46	1329.10	
1502.70	1503.29	1504.30	1507.63	1509.46	1515.01		1330.87	1335.59	1340.04	1351.72	1370.91	1378.81	
1515.47	1519.50	1522.78	1525.73	1528.33	1529.63		1394.00	1395.20	1401.02	1404.85	1406.39	1408.72	
1532.49	1533.72	1597.60	1604.87	1617.52	1619.76		1418.64	1422.24	1434.73	1438.26	1439.18	1447.28	
1637.54	1642.24	<b>1649.76</b>	1650.85	2064.86	2090.47		1460.22	1478.71	1481.06	1484.82	1487.63	1501.62	
2139.53	2945.18	2953.73	2969.50	3001.77	3038.14		1502.42	1503.18	1503.78	1506.80	1507.04	1508.20	
3039.56	3042.37	3043.67	3043.76	3046.92	3067.78		1512.67	1517.57	1521.16	1523.74	1526.19	1528.19	
3068.67	3076.86	3081.12	3098.98	3099.95	3110.38		1531.30	1534.03	1555.89	1580.67	1613.34	1616.71	
3113.37	3115.92	3116.23	3119.86	3120.83	3122.83		1622.61	1626.61	1649.53	1654.41	1875.09	1898.76	
3123.04	3172.97	3174.39	3178.04	3181.94	3188.78		1958.41	2879.20	2895.43	2923.44	2924.80	2932.62	
3194.17	3194.20	3195.28	3200.83	3201.78	3212.28		3007.04	3037.73	3037.93	3040.42	3043.06	3079.41	
3215.51	3218.17	3225.35					3079.57	3085.65	3087.48	3093.38	3106.27	3108.36	
<hr/>													
<b>A1</b>							3109.52	3110.31	3115.22	3116.97	3123.37	3130.89	
<hr/>													
25.88	34.65	38.19	42.46	43.20	50.40		3140.61	3148.05	3158.38	3160.19	3167.49	3169.64	
55.67	58.19	62.74	72.13	75.31	85.37		3173.08	3174.35	3186.59	3188.06	3190.58	3195.57	
85.59	91.62	96.61	105.07	107.00	109.23		3199.87	3200.56	3211.91				
118.53	123.25	128.92	134.63	147.03	157.73		<hr/>						
172.08	175.69	183.12	191.70	208.78	216.04	<b>A2</b>							
221.18	233.18	236.31	243.01	252.25	265.44		16.02	25.43	29.40	35.48	37.65	44.15	
269.70	285.18	296.63	303.60	312.23	323.98		44.51	52.22	54.54	56.26	62.35	66.20	
329.89	343.88	346.80	385.22	389.33	407.81		73.91	79.56	83.51	88.98	95.02	97.86	
410.35	417.03	420.22	431.12	451.71	461.17		103.05	109.43	112.67	114.89	117.32	127.34	
471.21	478.66	486.15	491.97	506.74	515.77		131.15	134.23	139.55	143.89	158.75	160.69	
525.75	539.24	548.51	550.35	573.57	574.58		165.72	170.28	183.19	195.28	211.72	216.31	
583.30	597.36	614.82	623.51	626.58	640.44		225.21	236.60	241.76	244.49	248.26	249.51	
643.75	651.78	670.53	678.60	701.50	703.55		261.86	273.99	277.19	286.99	299.02	304.29	
727.94	737.68	744.64	747.06	759.42	766.21		319.39	323.10	332.13	344.84	350.64	354.16	
775.83	778.46	793.77	794.54	804.47	817.76		369.61	402.37	406.50	410.97	417.83	420.58	
823.89	827.81	833.72	842.95	847.32	866.91		429.51	445.42	448.09	469.63	482.02	486.89	
872.06	873.48	879.71	888.60	911.31	926.04		493.38	504.40	508.87	519.84	522.68	537.48	
927.61	935.26	941.33	942.39	970.59	972.67		538.41	545.07	551.86	564.39	572.12	578.49	
980.37	994.60	1002.47	1004.97	1012.14	1019.79		584.50	594.42	611.85	614.69	622.38	635.51	
1040.95	1061.86	1069.16	1077.49	1081.12	1086.42		640.85	645.35	657.66	668.76	673.82	692.39	
1088.90	1094.52	1106.21	1109.32	1125.98	1131.06		703.38	724.55	736.11	739.79	744.18	756.38	
							759.68	770.20	782.94	788.67	791.35	797.28	

798.12	816.52	818.16	826.06	834.32	842.62	332.60	342.48	348.62	354.04	374.88	375.84
847.12	861.34	866.87	880.66	882.26	897.11	380.95	408.97	414.91	422.70	428.51	436.71
913.83	922.64	922.99	932.40	937.76	959.19	447.26	466.91	468.35	476.30	483.93	494.69
966.60	971.80	974.11	978.54	987.50	990.75	503.80	507.90	518.98	519.87	542.15	545.81
992.54	999.08	1013.06	1027.59	1033.15	1055.52	548.67	549.47	557.31	573.38	581.53	587.28
1065.27	1069.77	1075.82	1083.62	1087.84	1088.69	593.21	611.71	616.73	624.82	640.62	645.57
1102.75	1109.04	1110.36	1118.75	1123.78	1134.68	647.35	648.81	659.62	667.93	674.35	689.95
1141.67	1148.69	1159.83	1164.21	1180.16	1184.26	702.36	703.08	725.48	726.69	740.66	744.11
1193.09	1194.75	1196.51	1197.19	1200.45	1210.98	755.37	758.77	767.60	772.56	784.69	790.97
1220.52	1224.21	1232.88	1241.36	1274.01	1278.05	792.77	798.66	803.03	814.25	827.51	830.91
1290.74	1295.38	1305.75	1311.98	1313.71	1322.38	843.54	846.31	863.09	864.45	873.62	882.70
1325.97	1328.48	1332.61	1335.92	1349.65	1354.99	884.97	894.54	914.53	922.56	923.22	934.91
1367.82	1372.88	1375.17	1384.86	1389.73	1394.84	939.06	954.26	972.73	973.43	977.39	978.83
1401.58	1408.38	1411.57	1415.93	1418.07	1422.32	983.28	985.01	999.76	1005.53	1012.17	1037.85
1426.72	1432.33	1445.67	1449.58	1452.92	1481.53	1039.91	1061.35	1064.48	1068.82	1077.72	1082.79
1484.92	1486.45	1491.37	1493.12	1496.12	1503.12	1084.92	1104.21	1107.52	1110.25	1126.50	1132.54
1508.60	1511.02	1513.42	1514.99	1516.33	1517.89	1140.76	1147.71	1160.14	1165.13	1174.70	1183.66
1520.52	1521.40	1523.88	1526.22	1533.55	1534.81	1184.00	1186.41	1193.84	1197.57	1198.49	1199.90
1537.12	1550.79	1577.05	1595.77	1612.67	1616.66	1208.01	1218.36	1221.37	1224.91	1235.50	1274.19
1621.51	1629.59	1651.31	1652.73	1873.48	1897.84	1276.95	1292.96	1296.94	1306.98	1313.32	1315.58
1957.74	2891.32	2927.83	2941.50	3012.51	3029.47	1320.50	1326.20	1328.67	1330.65	1332.46	1348.00
3035.68	3038.91	3044.34	3047.73	3051.42	3054.61	1348.37	1357.50	1366.44	1371.27	1377.85	1384.09
3064.91	3068.00	3071.73	3081.74	3082.13	3084.87	1389.15	1393.72	1400.95	1404.69	1409.66	1415.90
3103.26	3103.65	3105.10	3113.83	3115.26	3116.56	1422.12	1427.65	1439.05	1442.46	1444.72	1454.46
3129.62	3138.24	3141.46	3150.22	3152.10	3157.58	1462.42	1484.07	1486.34	1488.09	1490.57	1491.00
3164.49	3166.18	3171.63	3172.65	3179.95	3186.25	1497.35	1498.71	1505.30	1506.98	1512.33	1514.66
3189.74	3193.05	3193.95	3199.47	3208.13	3209.32	1518.78	1520.08	1521.40	1524.46	1526.81	1531.39
<hr/>											
<b>A2-TS</b>											
<hr/>											
-515.55	15.48	24.92	27.74	28.49	34.80	1614.93	1617.93	1624.53	1631.37	1650.40	1652.37
37.19	38.81	42.87	47.96	50.36	58.24	1738.45	1884.27	1906.65	1962.55	2214.54	2891.52
62.86	65.25	70.81	73.08	76.57	85.32	2935.30	3003.19	3037.04	3037.39	3051.05	3052.07
88.65	91.50	95.32	104.65	107.56	110.85	3052.22	3057.70	3071.01	3074.20	3080.94	3086.68
113.77	120.08	125.50	127.89	132.86	142.36	3096.08	3101.96	3106.15	3108.59	3115.65	3119.60
144.89	148.06	159.18	168.30	171.31	182.84	3121.00	3127.41	3128.11	3145.45	3151.39	3153.39
186.62	192.51	205.00	213.74	219.08	234.45	3164.01	3166.55	3167.03	3168.11	3171.42	3173.42
240.07	248.86	251.09	261.45	265.26	274.14	3180.38	3181.74	3187.68	3191.81	3195.26	3196.37
278.50	285.27	302.35	313.09	314.55	327.51	3200.27	3211.58	3220.78			
<hr/>											
<b>A2-TS''</b>											



1508.49	1512.15	1514.00	1514.20	1521.24	1522.67		1390.07	1390.69	1397.06	1400.31	1401.22	1409.38										
1527.52	1527.71	1530.89	1532.04	1556.64	1581.80		1415.52	1417.22	1424.56	1432.88	1433.46	1442.41										
1610.85	1615.60	1621.33	1633.93	1650.48	1654.70		1456.92	1474.47	1480.18	1482.59	1489.36	1490.86										
1878.53	1904.82	1962.81	2916.66	2930.93	2997.92		1495.73	1497.14	1500.79	1504.99	1508.90	1510.99										
3037.39	3040.11	3044.77	3048.54	3080.67	3085.73		1512.87	1514.26	1516.26	1519.12	1522.19	1524.03										
3087.33	3092.37	3093.11	3105.23	3110.00	3111.05		1528.61	1530.48	1533.45	1533.97	1559.66	1592.01										
3117.87	3119.55	3120.10	3123.14	3129.65	3135.59		1618.28	1622.61	1628.75	1632.14	1653.59	1657.24										
3137.30	3158.27	3160.12	3163.85	3167.82	3171.46		1879.79	1907.47	1960.55	2825.12	2929.80	2988.92										
3175.42	3177.54	3178.28	3181.55	3190.99	3193.66		3031.23	3037.61	3042.35	3053.43	3054.01	3058.85										
3194.31	3203.08	3206.80	3217.07	3219.18	3360.26		3076.47	3078.29	3080.07	3097.50	3105.15	3107.98										
<hr/>																						
<b>A4</b>							3110.96	3119.00	3122.41	3127.35	3129.54	3130.65										
<hr/>																						
25.54	28.17	35.69	37.67	47.10	60.26		3131.07	3147.37	3152.63	3164.06	3164.08	3168.74										
60.87	63.61	72.89	78.82	85.22	86.02		3174.75	3179.73	3179.93	3181.14	3187.20	3194.36										
93.70	101.88	109.34	112.60	117.55	120.68		3195.53	3197.83	3200.34	3202.62	3209.00	3223.52										
123.18	131.06	135.82	140.58	153.09	162.92		<hr/>															
166.38	175.38	184.36	193.32	201.19	213.95		<b>A4-TS</b>															
225.92	232.49	238.44	249.18	250.74	257.44		-1028.54	25.86	29.75	34.46	37.58	48.83										
274.05	295.94	303.82	310.82	315.39	333.24		61.39	63.64	68.18	73.11	81.76	88.25										
341.64	352.28	355.55	388.82	397.05	401.80		92.54	98.37	102.53	110.74	117.19	117.47										
408.53	418.08	431.43	435.82	451.17	460.08		123.02	127.06	132.57	141.59	147.67	152.83										
481.54	484.77	496.15	499.78	509.94	513.69		162.38	166.51	177.62	184.75	194.07	203.04										
538.92	539.96	550.94	565.74	574.78	578.49		217.15	225.61	231.86	235.86	246.08	250.58										
586.31	602.22	613.25	622.36	624.72	642.51		260.10	274.87	286.94	294.80	302.17	308.41										
647.01	651.29	671.24	688.36	699.99	706.40		326.34	343.53	347.40	355.73	383.96	399.73										
739.21	742.65	745.84	757.47	767.12	778.00		404.69	415.24	422.42	439.01	452.55	457.39										
784.39	786.14	794.00	796.89	810.83	814.67		471.61	477.88	487.85	497.03	501.02	506.68										
815.96	818.53	824.79	835.74	845.84	873.62		515.56	540.26	542.50	549.07	561.26	573.46										
890.95	892.66	894.80	903.66	912.88	918.46		577.58	584.02	607.88	619.11	625.06	627.67										
936.81	941.34	958.12	961.02	967.52	979.17		636.55	642.93	646.81	675.89	696.06	696.52										
980.42	982.02	993.22	998.35	1000.90	1004.63		702.98	737.73	744.02	749.66	761.74	768.59										
1026.65	1042.22	1057.66	1060.61	1065.10	1076.36		782.39	785.98	793.17	798.82	806.05	814.33										
1081.23	1083.49	1092.67	1111.37	1116.27	1119.31		815.83	818.99	824.26	829.33	835.58	847.91										
1124.85	1134.22	1140.13	1151.16	1163.96	1178.67		867.77	894.54	896.66	909.04	919.28	920.10										
1195.52	1196.90	1197.30	1201.48	1203.02	1214.44		921.41	951.03	963.05	964.74	971.65	981.22										
1223.12	1225.04	1238.07	1259.30	1278.10	1295.46		985.05	987.58	988.09	995.91	996.17	998.60										
1306.50	1308.91	1312.89	1315.04	1317.36	1320.48		1005.63	1030.53	1036.87	1047.59	1061.28	1064.44										
1324.85	1346.57	1350.62	1362.58	1368.64	1374.09		1066.17	1077.12	1085.16	1090.05	1092.36	1115.48										
							1119.52	1121.35	1124.22	1135.39	1140.92	1147.39										

1150.93	1160.44	1192.61	1197.04	1198.34	1202.66	998.18	1000.50	1001.06	1002.81	1003.88	1006.26						
1206.27	1219.72	1224.73	1225.18	1227.65	1237.91	1008.28	1015.26	1025.62	1053.05	1060.66	1062.26						
1273.34	1276.21	1290.81	1302.22	1306.76	1311.11	1072.69	1082.82	1090.57	1092.63	1115.01	1115.75						
1315.18	1320.50	1323.77	1325.97	1347.86	1354.20	1119.30	1119.64	1128.18	1132.72	1136.37	1150.79						
1371.90	1373.83	1386.01	1388.25	1390.70	1401.36	1153.09	1197.43	1198.06	1198.67	1198.74	1210.40						
1402.04	1405.81	1417.44	1424.32	1425.04	1432.26	1216.84	1218.66	1222.52	1237.74	1239.02	1269.56						
1434.21	1435.24	1440.98	1478.75	1484.73	1491.78	1272.63	1280.20	1285.17	1296.98	1305.28	1308.04						
1494.23	1496.42	1498.04	1501.71	1505.08	1506.90	1315.51	1321.35	1324.39	1345.26	1347.91	1353.69						
1509.58	1512.45	1514.09	1518.50	1519.37	1523.12	1373.63	1374.78	1388.91	1389.89	1402.55	1402.82						
1525.75	1529.71	1532.33	1534.34	1536.57	1579.37	1405.76	1416.34	1417.27	1423.82	1424.44	1436.56						
1608.75	1621.19	1624.59	1629.61	1636.73	1655.08	1436.73	1445.11	1476.93	1478.83	1488.01	1497.06						
1656.70	1909.94	1932.38	1991.74	2935.48	2987.02	1497.44	1500.84	1502.27	1502.56	1505.97	1506.12						
3014.02	3024.11	3033.97	3039.43	3043.34	3049.36	1514.14	1514.54	1519.94	1520.02	1522.68	1523.50						
3055.03	3059.75	3075.13	3078.90	3089.90	3096.39	1527.45	1528.14	1530.84	1532.00	1606.47	1615.67						
3108.69	3109.95	3117.52	3118.06	3119.21	3121.12	1621.46	1622.21	1632.63	1637.54	1639.18	1653.50						
3127.82	3133.74	3149.58	3165.92	3166.36	3166.78	1654.22	2005.58	2006.80	2072.88	2947.26	2947.55						
3174.26	3180.73	3183.32	3184.49	3184.78	3194.28	2981.44	2988.42	3030.41	3030.69	3039.91	3040.02						
3195.80	3199.27	3203.15	3206.28	3212.47	3227.98	3044.47	3044.92	3057.51	3057.91	3073.02	3073.59						
<hr/>																	
<b>A5</b>																	
<hr/>																	
19.12	25.02	25.74	32.22	35.27	38.54	3118.36	3118.46	3123.33	3127.07	3168.51	3169.23						
47.97	53.24	58.57	66.88	74.85	79.34	3184.06	3185.02	3186.29	3187.65	3198.33	3199.81						
84.82	88.58	99.53	102.63	108.32	112.57	3203.45	3203.85	3213.56	3216.48	3218.81	3232.60						
123.72	126.46	127.84	140.51	151.65	155.80	<hr/>											
163.83	166.65	179.42	182.85	194.21	209.84	<b>A5-TS</b>											
214.39	222.16	230.41	243.63	247.55	261.51	-172.43	13.74	25.18	30.95	33.52	34.36						
270.97	273.40	278.62	293.07	299.80	322.72	43.50	47.95	59.00	60.04	66.41	71.45						
330.80	343.02	356.80	375.44	389.69	395.38	74.50	81.61	82.19	86.39	86.74	93.24						
400.25	412.81	438.04	443.10	448.97	456.59	104.94	111.70	115.20	123.93	125.63	134.26						
468.80	481.47	485.88	488.73	492.64	503.43	139.29	150.99	154.29	155.56	163.43	171.38						
504.35	534.22	535.87	540.80	544.16	569.00	179.76	189.28	193.13	205.79	216.22	224.03						
582.02	606.61	612.76	614.56	616.00	631.17	230.21	240.95	245.33	250.92	257.02	269.67						
640.43	648.23	656.51	684.36	692.42	702.05	286.02	291.36	299.14	302.18	306.33	324.81						
727.93	746.96	751.61	759.34	774.99	781.34	346.91	348.48	362.03	377.66	397.99	403.88						
785.42	786.66	792.00	796.13	801.77	812.52	407.56	431.13	439.25	450.09	455.52	464.43						
812.77	817.74	818.68	825.20	830.18	831.17	467.49	478.38	486.68	489.60	497.49	509.36						
844.38	859.23	900.25	903.91	916.44	917.92	511.19	536.68	538.35	548.50	556.41	573.94						
921.93	932.59	968.55	972.54	978.54	980.62	586.65	608.24	610.05	624.46	627.19	637.03						
						646.04	648.98	660.73	661.47	694.43	700.92						

703.39	739.92	747.18	750.76	762.18	775.48	404.99	427.39	432.46	455.29	462.85	465.49
779.59	785.22	788.24	791.94	801.94	811.31	473.55	478.01	489.44	489.94	493.30	502.96
815.70	818.04	824.40	826.43	835.28	843.20	511.28	543.81	546.85	548.19	552.39	570.25
848.68	870.53	899.56	899.88	907.36	917.23	585.87	591.86	614.38	618.65	625.50	625.78
919.32	921.09	933.39	961.94	967.23	980.03	642.03	648.81	661.49	664.56	688.40	701.88
984.13	996.50	999.17	1003.10	1003.85	1004.73	717.65	726.66	745.14	746.25	750.64	758.91
1008.96	1011.29	1012.50	1039.06	1063.96	1064.53	763.12	779.76	781.83	794.58	795.56	797.70
1065.37	1077.88	1088.69	1094.77	1097.23	1116.25	800.81	802.14	810.27	816.97	824.23	825.97
1118.96	1121.86	1126.08	1134.01	1136.16	1146.61	834.51	843.25	847.17	867.94	888.46	890.72
1156.82	1158.28	1195.74	1199.00	1201.07	1201.90	914.38	917.08	926.47	941.17	941.25	941.54
1212.32	1220.73	1223.73	1230.17	1237.42	1238.51	971.45	971.84	977.78	980.31	981.11	1007.69
1272.68	1273.41	1277.17	1279.53	1285.43	1301.62	1011.16	1015.63	1039.05	1059.98	1062.36	1065.55
1309.44	1312.82	1320.37	1325.68	1326.60	1346.67	1073.92	1077.29	1081.00	1084.50	1091.65	1104.50
1350.58	1360.66	1375.27	1385.32	1393.86	1402.17	1106.43	1121.54	1129.69	1140.81	1153.87	1164.89
1405.35	1405.92	1414.00	1420.90	1422.77	1426.36	1165.72	1190.49	1192.45	1192.56	1197.66	1204.87
1428.26	1438.56	1438.79	1447.70	1481.82	1484.97	1215.65	1220.86	1222.81	1235.62	1239.39	1273.39
1493.72	1499.23	1501.28	1504.88	1506.16	1506.64	1278.58	1284.25	1301.24	1304.40	1304.58	1306.91
1507.97	1510.17	1515.24	1516.47	1518.65	1521.93	1313.58	1332.87	1335.03	1343.44	1348.98	1351.61
1524.13	1525.07	1531.40	1531.60	1533.93	1537.38	1368.33	1369.39	1384.10	1385.34	1395.22	1398.99
1612.11	1618.77	1622.11	1623.10	1640.70	1641.98	1404.03	1410.38	1411.66	1417.22	1417.42	1418.56
1655.13	1655.70	1684.08	2005.06	2006.38	2072.48	1441.91	1446.94	1465.16	1486.44	1486.92	1493.51
2265.19	2932.87	2941.23	2950.65	2979.02	3035.24	1497.64	1498.78	1501.34	1511.95	1513.08	1513.68
3037.60	3040.89	3046.15	3047.59	3053.86	3057.51	1514.66	1517.67	1518.14	1519.83	1520.07	1521.60
3064.90	3079.77	3090.03	3099.21	3104.73	3107.66	1525.82	1530.49	1531.60	1540.78	1550.88	1567.84
3111.51	3112.87	3113.24	3122.98	3128.41	3140.18	1609.14	1614.02	1622.53	1623.23	1653.96	1654.43
3149.75	3162.29	3167.68	3173.76	3179.36	3185.30	1686.48	1973.69	1974.69	2049.64	2905.82	2921.27
3185.67	3186.74	3192.69	3196.90	3202.59	3207.03	2937.92	2945.00	3032.37	3032.61	3035.07	3036.27
3212.19	3219.48	3237.82				3042.51	3042.79	3076.00	3076.60	3081.85	3088.01

#### A5(red)

9.83	19.25	27.08	36.23	38.40	41.78
44.71	52.73	57.99	67.96	72.59	78.59
78.89	82.76	87.22	90.82	92.84	107.01
109.49	110.66	137.02	139.94	144.21	145.99
155.62	173.74	176.16	186.01	193.61	213.37
218.80	235.37	241.19	243.91	252.20	254.88
260.17	283.51	300.61	304.24	307.25	317.32
326.89	350.67	351.14	379.15	382.11	397.81

404.99	427.39	432.46	455.29	462.85	465.49
473.55	478.01	489.44	489.94	493.30	502.96
511.28	543.81	546.85	548.19	552.39	570.25
585.87	591.86	614.38	618.65	625.50	625.78
642.03	648.81	661.49	664.56	688.40	701.88
717.65	726.66	745.14	746.25	750.64	758.91
763.12	779.76	781.83	794.58	795.56	797.70
800.81	802.14	810.27	816.97	824.23	825.97
834.51	843.25	847.17	867.94	888.46	890.72
914.38	917.08	926.47	941.17	941.25	941.54
971.45	971.84	977.78	980.31	981.11	1007.69
1011.16	1015.63	1039.05	1059.98	1062.36	1065.55
1073.92	1077.29	1081.00	1084.50	1091.65	1104.50
1106.43	1121.54	1129.69	1140.81	1153.87	1164.89
1165.72	1190.49	1192.45	1192.56	1197.66	1204.87
1215.65	1220.86	1222.81	1235.62	1239.39	1273.39
1278.58	1284.25	1301.24	1304.40	1304.58	1306.91
1313.58	1332.87	1335.03	1343.44	1348.98	1351.61
1368.33	1369.39	1384.10	1385.34	1395.22	1398.99
1404.03	1410.38	1411.66	1417.22	1417.42	1418.56
1441.91	1446.94	1465.16	1486.44	1486.92	1493.51
1497.64	1498.78	1501.34	1511.95	1513.08	1513.68
1514.66	1517.67	1518.14	1519.83	1520.07	1521.60
1525.82	1530.49	1531.60	1540.78	1550.88	1567.84
1609.14	1614.02	1622.53	1623.23	1653.96	1654.43
1686.48	1973.69	1974.69	2049.64	2905.82	2921.27
2937.92	2945.00	3032.37	3032.61	3035.07	3036.27
3042.51	3042.79	3076.00	3076.60	3081.85	3088.01
3098.17	3101.54	3102.61	3103.34	3107.18	3112.97
3113.57	3116.70	3118.22	3119.49	3148.30	3148.51
3156.37	3158.33	3159.65	3159.90	3172.55	3172.88
3185.51	3185.77	3189.29	3204.57	3208.51	3209.59

#### A5(red)-TS

-164.24	16.51	19.34	28.33	31.05	33.29
38.41	43.93	48.13	54.89	61.73	63.60
65.52	75.83	77.55	80.20	82.66	87.59
93.21	95.28	101.71	107.42	110.99	117.24

134.38	136.40	144.09	149.21	158.87	160.67
164.04	187.35	190.87	209.54	218.51	221.98
229.92	231.35	234.60	243.19	247.39	253.02
282.62	292.25	305.44	313.87	320.78	334.70
356.24	357.03	381.00	387.21	396.16	411.50
427.01	433.29	441.89	449.73	462.96	470.45
477.88	485.66	487.85	493.47	508.99	511.45
521.40	533.34	543.74	547.77	551.09	572.12
586.11	595.34	605.88	616.78	620.32	621.28
641.94	653.36	655.70	663.47	665.59	697.95
718.37	720.85	729.61	746.14	747.15	752.37
754.59	760.35	765.80	780.58	783.16	791.02
793.22	798.23	804.26	811.08	817.40	827.98
834.23	845.76	849.07	867.09	870.59	887.91
890.31	914.82	917.12	929.05	942.09	943.27
944.20	971.96	973.16	973.31	975.40	977.96
1011.15	1013.16	1017.19	1038.42	1054.77	1059.70
1061.25	1071.40	1073.93	1076.84	1078.08	1088.13
1103.13	1104.63	1114.23	1129.96	1140.93	1158.71
1164.14	1167.19	1190.00	1193.32	1193.98	1201.33
1206.49	1211.77	1221.29	1225.85	1226.05	1229.05
1270.87	1273.60	1282.01	1300.65	1301.49	1305.08
1308.42	1312.63	1319.37	1332.31	1334.42	1347.05
1347.29	1351.91	1367.52	1368.90	1381.34	1382.09
1394.16	1396.01	1403.06	1410.49	1411.25	1412.86
1416.39	1417.19	1441.38	1446.35	1466.64	1487.81
1488.26	1492.83	1493.85	1496.88	1499.42	1510.28
1511.23	1512.29	1515.35	1518.36	1519.02	1520.07
1522.82	1524.60	1527.39	1530.38	1531.58	1538.86
1551.12	1570.19	1592.24	1610.41	1621.26	1623.72
1654.78	1655.27	1979.35	1992.05	2057.42	2286.95
2910.58	2922.78	2984.23	3001.01	3008.35	3035.18
3035.56	3038.03	3040.54	3055.78	3057.53	3069.67
3090.21	3093.13	3100.53	3101.67	3103.83	3107.40
3109.16	3115.71	3117.21	3119.64	3120.34	3122.95
3127.59	3152.17	3152.98	3157.45	3159.84	3161.80
3163.79	3173.73	3174.19	3184.72	3186.58	3187.57
3198.18	3202.73	3206.77			

#### A6

25.38	30.49	38.03	40.91	46.24	48.64
58.61	61.52	62.89	69.43	76.29	81.46
83.36	87.15	92.74	97.50	105.61	110.04
114.69	118.72	127.02	131.33	133.42	137.05
147.73	159.00	162.93	170.24	172.80	177.79
184.04	194.89	197.26	207.14	217.91	226.90
232.18	241.92	247.30	256.58	267.19	275.64
288.81	295.20	305.77	309.49	321.56	343.42
348.86	357.77	377.36	399.95	401.92	410.52
430.46	438.81	441.61	446.72	453.40	459.38
473.33	478.73	483.38	487.29	495.17	510.90
536.19	538.36	540.81	541.56	570.08	583.38
587.41	608.09	623.95	626.24	638.47	640.49
644.72	651.01	652.84	692.60	703.52	713.95
740.77	748.04	756.30	761.02	763.32	780.56
786.22	788.81	792.74	804.25	811.66	816.89
824.41	826.41	832.15	839.81	844.48	849.80
870.90	900.25	901.72	918.53	920.95	922.31
934.18	963.77	965.82	981.12	985.22	999.47
1000.30	1001.16	1003.03	1007.79	1009.24	1013.40
1014.50	1039.76	1064.15	1064.86	1065.96	1073.40
1077.03	1089.14	1094.55	1096.13	1118.37	1120.74
1123.45	1128.89	1133.45	1136.55	1147.74	1156.12
1159.44	1190.51	1195.55	1198.52	1201.77	1204.68
1213.56	1220.90	1223.88	1229.50	1237.03	1237.91
1273.59	1277.41	1281.15	1287.72	1292.64	1301.32
1312.42	1313.11	1322.01	1326.60	1330.89	1348.10
1350.24	1361.44	1376.58	1393.53	1395.51	1400.14
1407.58	1409.01	1418.83	1421.89	1422.72	1433.13
1436.71	1441.91	1442.60	1449.45	1482.30	1484.86
1495.24	1499.08	1501.72	1502.37	1508.65	1508.85
1510.58	1513.04	1516.39	1517.71	1518.95	1520.59
1523.54	1524.51	1530.92	1532.98	1535.38	1539.97
1612.47	1617.50	1620.12	1620.99	1641.94	1644.84
1653.77	1654.91	1808.42	2048.05	2053.64	2110.33
2602.34	2939.62	2946.45	2960.05	2986.81	3034.13
3036.68	3038.99	3045.75	3049.02	3050.13	3070.85

3074.61	3080.16	3093.37	3096.01	3104.56	3108.24	1508.76	1511.69	1513.70	1518.40	1518.80	1523.26						
3110.98	3111.35	3112.47	3122.86	3127.61	3137.65	1524.99	1530.52	1532.49	1535.44	1537.65	1543.40						
3160.86	3163.95	3166.66	3173.82	3176.97	3184.29	1614.54	1618.44	1623.22	1624.28	1639.30	1644.84						
3186.65	3187.55	3191.44	3196.28	3202.99	3207.83	1653.93	1654.57	1679.37	2032.61	2050.53	2108.01						
3213.10	3220.11	3237.09				2902.96	2916.50	2918.48	2921.99	2927.97	2933.44						
<hr/>																	
<b>A7</b>						2966.22	3038.38	3040.06	3040.49	3040.84	3072.53						
<hr/>																	
22.69	27.77	30.13	37.76	45.06	48.44	3079.89	3084.93	3086.27	3109.18	3110.37	3111.11						
52.37	55.79	65.95	66.99	74.67	77.28	3111.21	3114.12	3118.25	3120.74	3124.13	3131.36						
80.78	88.99	93.23	95.20	99.74	105.71	3140.42	3163.01	3164.64	3168.60	3174.10	3180.23						
110.74	113.40	119.03	124.85	130.53	135.11	3184.73	3185.69	3189.00	3194.57	3200.27	3209.26						
142.47	154.99	158.92	163.29	168.74	171.83	3211.23	3215.10	3224.12									
183.37	191.73	203.71	216.71	224.86	230.31	<hr/>											
236.59	242.86	257.00	258.69	266.78	272.03	<b>A8</b>											
280.56	299.66	310.68	318.98	327.11	339.91	14.31	22.50	31.01	34.59	38.14	46.64						
345.01	352.79	370.78	386.60	395.42	413.84	50.71	53.16	63.40	67.58	72.53	76.15						
422.69	441.26	444.44	448.69	457.10	463.53	78.07	81.02	83.86	87.88	95.03	98.04						
470.52	471.47	473.65	482.73	485.63	491.10	99.99	103.18	116.17	120.58	123.67	127.15						
520.41	527.13	533.21	538.27	555.96	577.75	143.70	149.25	153.26	158.26	164.99	173.53						
591.17	624.34	627.74	632.14	638.77	643.48	185.98	188.14	197.91	213.26	216.44	221.15						
649.01	655.34	666.34	700.24	709.22	742.79	230.59	236.89	246.03	256.76	260.27	262.83						
752.78	767.61	771.76	773.47	775.83	784.28	285.06	292.37	296.02	309.53	319.58	331.72						
786.43	796.64	797.42	818.17	822.98	828.22	345.77	347.97	372.80	384.57	392.52	406.88						
832.66	833.07	838.06	846.40	852.53	858.29	417.21	421.13	449.19	451.74	454.35	458.94						
880.48	896.67	899.83	927.13	930.48	932.26	471.74	475.32	477.76	480.97	490.77	494.34						
937.06	959.48	965.03	997.38	1003.23	1007.60	526.26	529.08	536.62	542.78	557.06	583.52						
1008.07	1008.56	1011.34	1016.17	1019.79	1021.63	591.86	601.17	622.17	626.11	629.99	642.58						
1046.38	1048.55	1066.21	1074.38	1078.00	1086.05	646.50	657.70	663.36	668.99	700.81	724.09						
1092.22	1093.63	1095.12	1112.83	1115.60	1130.98	734.28	741.99	750.59	755.18	768.44	769.84						
1132.14	1135.13	1138.99	1150.90	1155.65	1165.78	771.99	778.97	784.54	796.65	799.13	815.48						
1198.81	1201.90	1205.58	1207.28	1209.33	1215.24	818.44	819.49	822.65	830.37	831.24	834.27						
1216.68	1225.78	1231.36	1241.35	1241.68	1276.56	848.38	852.66	870.74	885.10	891.29	933.96						
1278.83	1282.65	1297.48	1303.99	1312.94	1319.08	934.40	934.91	946.31	946.62	947.24	975.88						
1325.08	1330.09	1332.80	1333.69	1337.23	1353.75	976.12	976.44	996.28	1004.99	1014.19	1016.38						
1357.40	1360.20	1374.79	1400.87	1403.17	1405.83	1039.67	1042.66	1057.65	1066.85	1073.15	1077.88						
1408.75	1412.74	1426.58	1433.32	1436.65	1438.32	1087.17	1087.86	1094.16	1094.74	1107.08	1114.86						
1440.32	1442.65	1451.51	1452.90	1481.85	1487.65	1115.73	1127.88	1133.70	1152.39	1156.16	1165.08						
1496.76	1500.46	1502.41	1504.79	1505.54	1508.37	1167.64	1191.96	1193.89	1195.27	1197.72	1209.47						
						1221.29	1222.46	1225.63	1228.29	1241.61	1268.11						

1274.47	1284.77	1300.33	1306.90	1311.55	1314.76		1044.04	1064.85	1068.54	1073.55	1074.57	1079.05	
1317.77	1328.12	1329.06	1331.34	1337.63	1341.33		1085.47	1089.17	1103.67	1107.07	1124.09	1135.65	
1354.42	1359.37	1384.26	1400.37	1402.50	1405.47		1138.47	1148.27	1157.29	1160.12	1172.10	1202.68	
1408.21	1409.10	1411.71	1420.80	1423.58	1432.63		1205.79	1206.53	1208.99	1215.83	1219.88	1225.50	
1434.80	1438.92	1439.74	1444.93	1465.91	1485.10		1227.81	1229.37	1237.74	1272.75	1274.76	1289.04	
1485.65	1498.81	1501.39	1505.28	1506.07	1506.94		1294.39	1310.37	1314.44	1316.22	1320.15	1328.54	
1508.25	1509.22	1510.19	1514.62	1522.04	1523.41		1331.21	1350.52	1352.64	1361.63	1366.97	1367.83	
1524.72	1525.16	1526.52	1530.52	1531.93	1536.74		1387.50	1390.13	1396.25	1402.82	1413.77	1419.65	
1555.64	1572.65	1610.06	1617.19	1621.70	1622.55		1421.22	1423.40	1429.45	1443.60	1446.70	1447.15	
1653.62	1654.95	1689.42	2006.11	2024.51	2087.40		1482.09	1488.41	1495.11	1499.19	1499.59	1499.74	
2842.79	2889.98	2893.53	2908.02	2909.32	2932.23		1500.21	1502.58	1511.03	1513.19	1514.18	1514.45	
3016.38	3035.55	3036.29	3037.28	3039.95	3070.54		1519.30	1524.21	1524.61	1529.60	1531.76	1532.54	
3079.99	3083.13	3090.49	3103.94	3106.86	3107.66		1535.49	1538.33	1595.49	1605.14	1618.20	1620.40	
3113.75	3114.72	3120.80	3122.38	3137.72	3139.09		1638.76	1644.45	1649.67	1652.01	2065.80	2091.17	
3150.35	3153.04	3156.63	3161.36	3162.62	3163.73		2139.62	2941.18	2949.43	2964.00	2998.18	3041.13	
3167.46	3174.39	3178.07	3187.78	3188.75	3196.22		3041.97	3043.32	3044.34	3045.45	3049.51	3054.94	
3207.21	3211.44	3216.03					3057.26	3088.43	3088.74	3089.58	3098.16	3113.49	
<hr/>													
<b>A9</b>							3114.78	3115.22	3116.39	3117.17	3118.81	3121.60	
<hr/>													
29.13	33.51	37.93	43.01	46.56	52.78		3122.85	3167.83	3174.08	3177.04	3180.21	3186.79	
56.02	60.22	61.96	67.98	70.92	77.36		3191.12	3191.14	3192.63	3200.54	3201.69	3209.80	
81.47	91.59	95.38	99.10	107.70	112.61		3213.22	3215.83	3221.85				
115.27	120.50	127.11	135.13	141.98	157.77		<hr/>						
159.48	166.92	178.03	203.71	210.69	228.25	<b>A7-TS</b>							
232.69	241.63	248.86	255.34	262.78	266.32		-110.51	7.21	18.93	20.13	26.11	31.08	
273.70	284.58	301.13	308.99	317.90	324.31		34.05	38.01	46.03	48.37	49.55	54.52	
327.44	347.71	355.38	376.34	379.74	399.61		61.75	62.97	67.50	70.73	72.77	74.54	
409.99	417.11	420.33	436.83	450.83	451.23		78.11	83.56	90.02	90.62	93.50	99.82	
467.28	474.42	479.24	484.78	488.06	498.18		100.94	106.12	113.39	118.74	123.62	125.48	
500.44	525.41	530.60	544.33	546.67	565.75		126.99	133.88	142.65	152.79	158.26	159.70	
583.78	610.23	618.45	625.33	628.21	632.50		164.02	165.97	171.09	174.27	189.01	192.62	
644.22	651.93	656.26	691.39	693.49	709.82		212.17	219.67	226.21	233.59	241.42	245.54	
744.66	747.23	758.84	762.85	772.99	787.07		249.13	252.24	259.21	268.62	270.62	272.71	
787.18	792.35	794.84	799.93	801.61	822.56		282.02	294.44	300.60	309.77	325.15	343.90	
832.49	838.96	840.13	843.20	848.07	877.22		348.37	350.41	358.28	367.63	379.88	387.28	
900.20	904.25	922.05	926.04	928.35	939.17		396.48	403.12	413.98	431.18	441.43	445.38	
970.36	972.59	986.46	993.01	1011.12	1013.82		449.22	462.49	467.77	470.81	482.68	486.30	
1014.87	1016.07	1018.36	1022.27	1026.19	1032.00		488.87	497.78	504.75	519.89	525.40	533.53	

610.46	619.12	623.89	629.26	637.74	642.43		146.55	148.86	154.06	169.35	172.74	178.50
648.77	655.08	660.28	665.01	678.85	699.95		191.04	193.47	202.29	215.74	229.93	233.86
704.72	742.04	749.93	764.78	768.32	773.02		237.18	244.96	255.80	263.16	271.69	274.24
776.81	784.05	792.29	796.18	801.20	811.14		282.60	298.40	304.45	308.41	322.05	343.83
812.08	820.31	823.46	826.86	837.88	842.50		346.81	351.13	370.41	393.52	400.49	410.71
845.27	846.79	857.01	878.70	896.96	907.17		415.68	430.72	442.02	447.22	458.76	461.33
913.53	920.92	922.04	929.69	957.57	972.96		471.30	479.82	480.91	484.04	494.90	508.52
978.82	987.38	991.93	995.11	998.09	1005.93		531.49	535.62	540.80	555.04	561.16	578.26
1010.84	1016.31	1019.81	1040.56	1044.12	1046.85		592.67	615.71	618.94	622.38	637.06	643.72
1048.85	1064.25	1069.07	1071.88	1078.70	1079.47		647.49	654.90	662.88	697.23	708.66	735.86
1088.29	1091.95	1107.84	1123.83	1129.29	1134.07		745.35	754.03	764.07	772.52	782.42	788.34
1138.76	1144.05	1148.44	1162.20	1167.86	1170.77		790.32	793.76	799.49	810.80	814.39	817.73
1179.61	1194.70	1197.30	1201.56	1206.28	1213.03		823.75	826.16	829.83	837.09	851.77	871.26
1215.06	1216.04	1217.47	1226.07	1227.51	1242.17		892.24	903.13	905.29	912.44	922.66	938.41
1259.95	1278.55	1282.48	1289.77	1295.99	1302.16		940.17	945.88	969.92	975.55	984.65	988.15
1306.49	1312.35	1315.21	1322.43	1329.24	1332.45		1007.16	1010.26	1019.95	1020.70	1022.58	1023.54
1334.97	1345.34	1354.14	1354.78	1362.67	1369.98		1031.84	1035.25	1052.62	1060.00	1063.25	1066.57
1373.88	1388.86	1394.53	1398.31	1409.89	1412.42		1079.29	1083.91	1089.41	1095.56	1115.39	1122.80
1414.93	1419.44	1425.02	1436.20	1440.50	1446.00		1123.67	1133.67	1137.95	1139.55	1154.66	1162.71
1447.11	1453.96	1460.24	1477.65	1484.13	1487.94		1174.30	1200.61	1200.65	1203.41	1211.06	1215.51
1494.89	1497.88	1499.42	1500.71	1503.36	1505.71		1219.72	1223.72	1226.28	1234.90	1239.25	1269.19
1509.18	1512.43	1514.28	1515.60	1518.07	1518.67		1280.60	1286.67	1296.15	1308.70	1312.53	1316.32
1519.37	1524.32	1528.51	1532.83	1536.97	1540.47		1320.21	1321.31	1322.24	1343.77	1346.67	1356.10
1545.07	1613.21	1618.45	1621.42	1625.80	1638.71		1367.83	1380.80	1396.79	1401.62	1403.17	1404.33
1643.78	1650.38	1654.25	1659.46	1688.13	1813.29		1408.07	1412.09	1417.16	1425.59	1427.60	1436.11
2035.16	2052.33	2108.82	2271.26	2900.54	2923.63		1440.01	1447.47	1451.79	1475.13	1481.17	1483.33
2935.97	2946.33	3013.50	3040.13	3041.18	3046.63		1487.18	1491.70	1495.38	1499.47	1500.14	1505.99
3053.77	3059.58	3066.54	3075.06	3077.68	3085.39		1507.37	1508.71	1512.65	1512.77	1514.57	1516.78
3093.96	3109.55	3110.66	3116.80	3121.64	3125.07		1517.35	1518.00	1524.55	1526.31	1529.10	1531.31
3125.67	3127.92	3129.41	3140.56	3145.04	3151.81		1534.58	1538.24	1611.48	1615.82	1619.82	1620.93
3162.20	3162.87	3167.49	3168.96	3179.47	3180.62		1636.76	1642.59	1650.78	1654.57	1666.51	2037.07
3184.54	3185.42	3191.81	3195.41	3198.01	3209.77		2052.17	2111.31	2943.53	2946.20	2962.94	3037.97
=====												
<b>A7-H<sup>+</sup></b>												
=====												
22.85	26.04	34.55	40.35	44.56	48.56		3040.94	3042.33	3042.63	3057.15	3059.56	3064.88
54.51	62.14	68.76	69.07	75.76	80.89		3068.63	3083.69	3084.59	3101.60	3105.81	3110.57
88.11	96.82	103.50	107.94	110.40	111.06		3111.79	3120.11	3121.33	3126.09	3130.77	3135.79
115.13	121.71	124.99	127.77	132.98	134.80		3138.82	3154.12	3171.14	3177.07	3180.32	3180.83
=====												

**A8-H<sup>+</sup>**

29.38	32.02	38.24	42.82	51.05	51.81	3075.74	3084.28	3086.42	3095.19	3099.30	3112.93
56.79	57.87	63.85	70.63	78.03	84.88	3120.68	3125.04	3126.12	3139.14	3143.97	3144.75
85.46	94.00	95.69	101.85	105.26	107.81	3153.47	3154.20	3164.04	3166.24	3166.96	3170.02
109.63	115.78	121.19	129.03	130.98	142.07	3173.32	3176.07	3177.51	3178.65	3190.88	3193.38
145.32	149.05	151.20	158.21	169.50	179.75	3194.63	3200.27	3205.11	3206.65	3212.10	3220.03
184.03	193.36	210.07	217.38	223.61	227.32	<hr/>					
231.75	244.39	254.47	256.78	261.92	279.86	<b>A9-H<sup>+</sup></b>					
287.61	290.30	298.70	303.95	306.88	337.51	18.14	22.83	28.09	34.49	36.28	39.50
345.09	349.29	366.55	381.41	408.44	413.13	45.18	49.26	55.58	62.35	72.32	74.77
422.99	424.33	436.15	450.85	457.50	465.03	81.17	84.99	90.33	94.63	99.80	104.60
473.18	474.25	479.73	486.72	491.82	495.89	108.33	109.59	121.17	124.97	129.57	132.43
528.50	537.70	541.57	544.63	560.18	573.46	136.32	140.96	151.80	155.02	164.09	176.10
603.62	607.11	620.78	623.56	626.62	644.98	184.21	187.72	192.13	199.50	210.30	213.62
650.49	654.85	662.37	675.05	699.66	727.40	222.04	229.76	238.51	245.43	260.85	274.20
741.50	745.26	751.87	760.65	762.20	764.58	277.07	294.23	296.38	301.90	322.83	327.32
779.89	786.57	794.46	797.28	802.80	812.15	336.75	347.29	356.85	382.79	397.76	404.67
817.37	827.79	831.54	840.22	847.76	850.19	406.72	418.53	421.35	428.21	438.77	452.15
862.72	873.04	895.58	902.72	905.68	917.51	461.10	473.10	476.62	482.80	494.36	502.00
929.29	953.51	953.75	958.72	965.92	974.68	510.71	535.39	537.13	538.36	552.75	566.10
980.23	982.10	987.96	1000.15	1008.81	1015.67	576.54	601.32	612.41	622.77	627.94	632.72
1037.09	1039.09	1050.80	1058.33	1062.14	1076.59	638.94	648.02	651.57	681.56	699.59	702.87
1083.32	1085.55	1094.21	1095.35	1095.82	1111.98	735.79	744.52	752.76	756.74	763.64	771.04
1122.67	1125.45	1139.88	1150.35	1154.38	1164.26	781.39	786.27	792.67	795.34	809.10	812.57
1170.66	1192.63	1197.05	1199.66	1201.78	1202.96	813.20	819.66	828.31	835.24	838.38	844.05
1203.89	1222.56	1224.39	1240.36	1242.50	1262.68	876.38	895.96	901.31	920.06	921.29	923.33
1277.37	1282.77	1299.90	1307.96	1308.88	1313.32	929.68	958.42	967.66	970.00	981.49	982.27
1315.80	1318.86	1334.12	1339.25	1340.92	1347.74	988.14	995.42	999.22	1000.74	1003.94	1006.55
1373.58	1385.20	1397.27	1398.70	1402.56	1405.58	1009.66	1038.06	1042.64	1062.48	1063.22	1064.19
1409.14	1411.08	1415.05	1415.95	1423.20	1439.54	1067.13	1080.68	1089.78	1094.60	1096.57	1116.44
1444.83	1450.44	1463.09	1466.76	1472.10	1483.71	1122.35	1126.70	1132.78	1139.60	1145.59	1153.85
1485.87	1496.87	1497.15	1500.86	1505.10	1505.92	1160.58	1176.61	1198.34	1201.97	1202.50	1206.29
1507.34	1509.13	1512.36	1512.67	1514.62	1518.04	1211.54	1215.39	1223.21	1224.20	1238.07	1269.53
1519.69	1526.04	1526.59	1528.03	1528.30	1537.27	1275.14	1288.47	1288.93	1299.18	1309.49	1314.32
1545.50	1548.18	1555.56	1563.65	1581.59	1613.68	1319.21	1320.99	1322.79	1342.08	1346.40	1355.86
1615.89	1620.38	1651.01	1652.45	1693.50	2006.38	1360.26	1371.48	1374.89	1385.56	1393.73	1402.91
2016.18	2080.17	2888.43	2897.17	2911.50	2922.57	1404.46	1408.66	1408.96	1417.27	1421.54	1424.46
2984.64	3038.57	3044.02	3057.37	3058.73	3071.69	1436.41	1440.64	1442.24	1459.99	1477.97	1479.69
						1487.01	1491.94	1493.75	1498.35	1503.40	1506.09

1507.89	1510.15	1514.18	1515.17	1519.58	1520.71		1279.01	1287.85	1297.08	1298.29	1307.39	1308.36									
1523.14	1525.15	1527.45	1529.89	1533.32	1534.18		1316.81	1317.71	1324.48	1334.12	1339.15	1350.52									
1539.74	1580.28	1597.48	1606.01	1617.38	1622.37		1351.18	1358.28	1374.40	1376.51	1380.52	1389.56									
1628.96	1632.15	1652.08	1655.16	1690.83	1943.08		1402.88	1406.05	1408.82	1415.68	1423.79	1426.28									
1948.16	2011.66	2430.01	2834.49	2944.39	2973.62		1434.00	1436.86	1442.79	1446.08	1458.12	1474.93									
3032.82	3032.89	3040.68	3045.01	3056.71	3056.97		1477.93	1486.67	1488.47	1492.68	1497.49	1502.58									
3072.40	3080.01	3088.75	3088.85	3096.68	3110.40		1504.03	1506.04	1507.09	1512.94	1514.09	1515.99									
3111.60	3112.39	3118.99	3119.27	3127.20	3127.61		1520.15	1523.74	1524.18	1526.02	1527.72	1531.52									
3133.43	3136.66	3166.62	3168.61	3181.33	3182.52		1550.57	1555.22	1571.07	1599.36	1618.33	1620.29									
3183.82	3186.23	3188.29	3191.80	3194.38	3197.27		1621.96	1630.09	1653.19	1653.43	1689.54	1955.99									
3201.57	3209.14	3212.10	3216.31	3219.99	3227.25		1957.02	2013.57	2821.89	2948.77	2957.28	2989.79									
<hr/>																					
<b>A9-H<sup>+</sup>-TS</b>																					
<hr/>																					
-20.52	27.45	31.75	32.20	37.36	39.42		3112.75	3116.14	3117.81	3117.84	3122.50	3124.35									
41.19	51.96	53.91	59.81	67.28	69.25		3143.58	3155.95	3162.82	3169.81	3178.30	3183.76									
76.09	79.47	81.86	85.07	89.55	100.12		3184.47	3185.46	3188.08	3192.56	3197.35	3203.63									
103.98	111.17	111.81	123.06	125.64	133.38		3203.73	3206.04	3212.03	3223.12	3227.00	3242.36									
134.46	143.26	146.34	154.35	160.14	160.26		<hr/>														
175.97	176.98	185.58	192.07	196.21	215.54		<b>A9-H<sup>+(b)</sup></b>														
226.40	240.72	245.86	254.93	258.76	267.42		29.13	32.08	36.45	41.97	45.18	45.91									
271.90	278.21	285.38	293.00	295.57	324.81		52.91	58.84	59.76	67.49	70.29	73.89									
333.92	340.13	356.41	377.61	390.01	395.90		81.41	83.82	84.62	90.56	95.80	102.65									
405.94	410.72	418.06	431.86	444.16	449.94		106.79	109.15	114.59	122.68	125.19	128.87									
462.99	470.43	481.89	484.66	490.52	498.62		130.38	141.09	147.45	158.77	160.14	169.81									
505.49	516.79	535.16	540.59	555.48	565.04		175.19	188.13	200.96	208.84	213.85	224.71									
577.79	601.60	607.03	613.16	614.32	623.46		230.06	241.71	248.62	252.35	260.64	263.05									
637.59	640.30	643.79	690.31	691.75	694.25		278.97	291.68	300.09	301.54	309.89	318.50									
727.72	743.30	751.04	759.13	762.00	767.49		333.59	347.97	350.53	381.01	396.98	401.75									
780.17	782.26	784.65	793.82	800.65	810.76		410.87	414.69	419.63	431.74	444.82	460.38									
814.16	816.79	824.52	831.13	831.83	834.01		467.83	479.95	482.27	484.03	490.57	496.07									
859.67	885.11	894.48	900.06	916.43	918.60		500.63	526.15	533.95	538.07	548.48	568.06									
929.93	953.00	967.15	968.10	980.02	983.36		579.12	601.71	606.43	624.15	624.38	638.29									
987.07	988.87	993.49	996.68	1001.79	1002.87		641.08	648.26	651.53	681.74	696.81	703.38									
1005.22	1023.09	1027.26	1052.12	1061.50	1063.14		745.65	749.49	751.37	762.50	765.46	767.57									
1070.07	1076.46	1083.40	1086.19	1092.64	1116.04		782.39	787.92	791.78	796.85	800.92	811.78									
1119.10	1119.81	1122.85	1134.04	1138.49	1148.93		822.57	831.77	836.53	844.75	850.53	855.76									
1154.34	1161.94	1197.24	1199.80	1200.47	1207.51		878.62	897.00	902.98	911.14	924.76	925.56									
1209.78	1211.18	1218.88	1221.52	1239.44	1270.45		932.72	959.73	973.94	986.58	990.03	990.48									

996.07	998.41	998.74	1008.33	1011.78	1012.76		646.29	648.48	667.99	679.22	695.43	704.72								
1018.52	1045.17	1046.32	1067.94	1068.94	1070.48		723.44	734.40	742.28	748.91	764.44	764.87								
1072.58	1081.09	1087.81	1090.58	1107.58	1108.63		768.62	776.21	779.67	781.31	794.58	801.97								
1125.29	1130.06	1142.46	1144.99	1156.76	1164.21		810.68	813.33	819.51	828.71	835.77	843.31								
1168.98	1183.58	1202.06	1202.13	1206.77	1210.44		872.07	873.49	874.73	886.88	916.91	917.61								
1212.69	1214.16	1224.64	1230.81	1239.78	1273.99		919.41	938.26	944.03	950.70	952.21	953.14								
1275.48	1291.07	1298.51	1307.55	1312.60	1322.85		971.67	977.90	978.74	979.21	983.89	997.95								
1326.84	1328.28	1330.45	1344.79	1349.83	1355.62		1002.21	1036.36	1046.65	1058.55	1059.42	1061.60								
1357.33	1365.94	1367.63	1385.44	1388.21	1399.96		1064.18	1077.50	1084.22	1092.17	1092.64	1107.76								
1402.04	1407.16	1409.14	1417.03	1420.06	1425.59		1116.24	1118.55	1129.36	1134.89	1137.70	1146.26								
1442.16	1444.08	1447.26	1459.37	1482.51	1484.59		1160.23	1182.50	1190.28	1193.85	1198.52	1198.82								
1489.25	1493.03	1495.44	1497.93	1499.04	1505.90		1204.85	1207.65	1217.04	1222.68	1238.51	1273.41								
1508.28	1511.90	1511.99	1514.92	1518.88	1521.43		1277.53	1298.05	1305.62	1307.09	1315.38	1320.80								
1524.43	1525.70	1529.23	1532.78	1537.10	1542.57		1322.14	1323.69	1335.43	1337.72	1347.84	1362.81								
1583.29	1583.93	1604.65	1621.63	1622.08	1624.95		1370.19	1372.52	1374.51	1388.20	1396.89	1398.96								
1632.28	1634.79	1653.25	1654.06	1684.48	1944.06		1401.01	1401.53	1403.49	1407.93	1417.91	1424.27								
1962.44	2016.78	2283.05	2865.38	2938.11	2952.71		1434.03	1438.13	1444.79	1454.67	1468.68	1475.22								
3040.43	3040.66	3041.47	3053.76	3054.50	3057.87		1485.05	1489.03	1495.20	1498.38	1501.96	1505.44								
3064.57	3068.63	3085.55	3089.58	3107.72	3110.12		1507.17	1511.97	1513.88	1516.61	1520.67	1521.17								
3111.31	3117.62	3119.53	3124.63	3129.24	3136.77		1522.59	1526.55	1528.28	1528.58	1532.98	1538.39								
3140.47	3154.88	3163.22	3163.95	3169.88	3171.81		1556.30	1559.23	1585.19	1612.77	1616.91	1619.00								
3174.48	3182.17	3182.71	3185.02	3186.65	3194.76		1622.94	1638.83	1652.84	1656.72	1678.47	1880.99								
3196.07	3202.05	3205.19	3208.27	3211.42	3221.55		1899.20	1958.70	2496.33	2841.37	2942.61	2998.63								
<hr/>																				
<b>A10-H<sup>+</sup></b>																				
<hr/>																				
23.71	28.27	36.30	36.73	41.79	51.11		3023.04	3038.75	3042.08	3046.31	3051.97	3058.81								
57.01	59.58	68.50	72.25	77.36	80.03		3061.93	3070.00	3076.54	3080.12	3088.92	3106.38								
86.45	88.03	90.98	101.39	103.35	109.53		3108.60	3113.64	3118.58	3120.24	3129.76	3134.41								
114.70	119.95	125.68	127.98	135.25	137.80		3138.06	3153.88	3154.19	3157.30	3167.62	3172.41								
142.41	150.94	160.42	169.12	172.64	176.02		3174.52	3176.53	3184.62	3185.54	3191.55	3196.92								
183.41	189.84	194.21	205.19	216.18	222.82		3198.69	3200.22	3203.09	3208.01	3215.73	3223.45								
226.36	232.17	237.53	244.53	254.51	267.66		<hr/>													
272.56	292.71	301.07	306.26	325.86	329.57		<b>A10-H<sup>(b)</sup></b>													
333.79	355.24	358.86	378.34	392.14	404.71		<hr/>													
413.36	416.19	417.87	447.48	450.74	453.55		26.58	30.00	36.28	43.54	43.57	46.37								
478.22	485.96	493.26	500.21	501.36	508.56		52.34	59.07	63.80	69.10	72.41	74.84								
528.19	539.30	555.34	570.65	574.02	579.07		81.98	82.94	89.71	95.11	98.49	103.27								
582.58	598.89	610.48	622.51	637.93	640.97		105.68	113.65	121.07	122.43	126.96	132.56								
							136.99	145.15	155.81	163.45	169.44	175.84								
							180.83	188.67	197.58	210.08	217.14	224.96								
							231.54	240.93	249.39	253.62	256.71	262.87								

283.30	290.80	303.43	304.99	311.13	328.76		39.93	41.16	53.47	59.50	63.81	66.07	
330.86	351.15	352.64	381.09	406.76	411.05		79.48	81.74	85.77	92.20	99.02	106.80	
413.53	418.94	422.10	445.04	448.11	472.70		110.08	116.88	124.52	131.58	132.30	139.35	
481.78	487.03	490.26	493.18	505.70	518.23		146.74	155.66	156.07	157.58	167.53	173.38	
536.03	539.32	549.86	552.96	572.77	577.24		173.58	185.49	187.37	204.08	219.57	221.78	
585.75	597.48	616.63	624.36	624.59	640.82		226.43	231.53	234.10	242.92	249.76	265.34	
643.72	651.39	667.61	676.13	702.33	703.32		276.50	277.85	292.67	299.58	308.07	324.24	
728.09	741.79	743.57	749.70	760.23	763.41		334.36	349.80	356.94	380.45	389.84	396.03	
765.49	775.93	783.52	791.00	792.97	796.02		401.41	404.00	416.84	418.68	437.16	448.73	
798.91	822.50	833.36	844.65	848.09	855.14		450.41	456.55	474.69	481.15	484.08	487.64	
869.60	872.16	875.39	888.27	893.18	914.94		491.40	498.26	505.26	537.28	538.01	545.16	
921.52	930.65	935.62	940.90	959.91	973.55		547.67	570.02	587.23	596.38	615.82	619.10	
980.70	982.87	986.96	991.79	999.09	1000.83		629.10	638.41	645.04	648.30	655.10	666.59	
1014.98	1040.33	1045.96	1062.97	1063.45	1069.29		693.36	710.21	728.09	738.47	741.80	752.43	
1070.35	1078.88	1084.04	1089.06	1104.17	1107.71		762.89	769.67	780.22	788.35	789.51	795.35	
1109.74	1124.37	1129.12	1140.51	1154.27	1163.14		798.26	807.03	815.10	815.78	819.69	824.27	
1166.97	1185.09	1190.45	1194.46	1194.98	1200.57		836.29	843.36	851.63	861.71	904.17	904.61	
1202.91	1214.84	1221.15	1228.11	1239.75	1275.47		918.03	918.79	938.88	949.42	962.26	971.74	
1278.24	1296.46	1305.32	1313.33	1322.63	1326.13		973.81	977.09	980.74	981.57	999.92	1001.14	
1327.86	1330.26	1332.61	1348.59	1350.66	1357.52		1003.80	1003.97	1012.92	1029.41	1054.77	1061.28	
1367.29	1368.28	1373.27	1384.54	1394.59	1400.74		1061.51	1064.01	1065.74	1074.13	1082.22	1090.99	
1401.08	1406.40	1409.14	1411.70	1415.84	1418.74		1092.62	1092.97	1113.91	1115.95	1118.33	1119.06	
1420.29	1444.38	1447.64	1456.25	1458.54	1483.21		1119.88	1132.04	1141.20	1163.13	1192.67	1197.76	
1486.40	1488.57	1489.44	1493.41	1496.45	1504.56		1197.89	1198.32	1199.10	1216.59	1218.03	1221.49	
1505.20	1510.44	1510.48	1513.57	1515.78	1519.03		1238.79	1239.14	1264.60	1272.46	1286.57	1301.39	
1521.80	1522.83	1525.54	1528.94	1536.50	1538.61		1302.52	1304.24	1308.33	1310.11	1321.31	1322.81	
1553.36	1576.36	1587.29	1613.08	1615.55	1616.99		1347.51	1348.38	1351.74	1374.29	1374.78	1390.54	
1624.50	1628.08	1649.80	1655.00	1688.08	1879.47		1390.90	1401.51	1401.82	1407.04	1409.75	1414.09	
1903.75	1959.93	2416.27	2846.58	2910.16	2924.16		1415.54	1417.00	1424.62	1424.86	1435.02	1435.19	
3036.82	3037.73	3051.34	3053.19	3054.66	3057.99		1465.19	1477.64	1479.09	1480.52	1483.56	1497.05	
3068.34	3071.84	3077.21	3082.42	3103.01	3104.97		1497.14	1502.47	1502.62	1506.85	1506.98	1513.67	
3115.53	3116.93	3118.17	3126.38	3129.27	3137.90		1513.70	1520.68	1521.07	1521.96	1522.86	1523.77	
3138.83	3151.79	3156.26	3162.90	3163.43	3164.63		1526.46	1527.10	1529.72	1530.42	1553.31	1571.70	
3168.29	3171.84	3176.78	3178.64	3180.77	3188.78		1600.08	1613.47	1620.53	1621.45	1653.77	1654.06	
3189.53	3193.28	3194.78	3198.93	3199.39	3208.53		2033.08	2038.96	2100.10	2390.83	2941.76	2942.26	
<hr/>													
<b>B1-MeCN</b>							2998.21	3001.13	3028.63	3028.80	3038.74	3039.38	
<hr/>													
19.71	26.04	29.68	32.29	35.28	36.68		3039.50	3042.56	3042.88	3057.61	3058.09	3073.33	
<hr/>													
3074.16	3075.22	3075.93	3109.29	3109.47	3109.91		3110.04	3117.93	3118.02	3120.29	3122.14	3125.20	

3127.74	3165.82	3165.90	3174.25	3176.10	3181.72		2015.02	2916.91	2924.36	2927.62	2940.83	2946.95								
3182.05	3196.00	3197.02	3201.54	3202.32	3202.73		2992.01	3040.84	3040.95	3043.98	3047.05	3075.65								
3216.78	3221.97	3222.36					3083.77	3088.64	3092.19	3107.11	3109.45	3111.99								
<hr/>																				
<b>B1</b>							3113.51	3114.55	3117.26	3120.82	3124.33	3136.88								
<hr/>																				
23.70	25.86	33.38	34.82	40.38	41.55		3147.88	3162.45	3169.05	3172.73	3180.88	3181.74								
52.77	55.66	58.31	64.87	71.84	76.49		3182.41	3183.68	3192.16	3196.46	3198.81	3203.40								
80.55	86.47	90.89	98.51	100.86	112.14		3207.00	3209.98	3217.61											
113.58	122.26	123.85	127.14	135.40	144.16		<hr/>													
156.41	165.61	174.69	189.20	205.68	213.22		19.70	25.97	31.92	34.80	38.48	39.70								
222.03	228.27	237.42	241.77	253.97	258.10		44.80	53.22	55.48	62.13	65.79	68.54								
265.33	277.41	299.97	308.45	312.90	313.19		76.31	80.81	84.04	88.74	94.01	95.80								
324.77	337.69	340.57	381.45	389.34	398.26		98.70	108.54	110.36	114.78	117.64	120.59								
401.85	414.19	426.91	429.11	439.87	456.57		124.77	131.26	135.55	144.79	153.00	164.18								
458.17	469.15	474.14	481.81	484.03	489.49		166.51	169.30	176.05	197.38	212.43	218.53								
499.80	525.33	525.89	532.50	544.62	567.77		228.37	238.27	244.12	244.81	253.26	257.33								
578.30	599.96	609.40	621.13	623.85	638.60		262.94	269.73	273.39	286.63	295.37	308.45								
641.76	648.38	651.82	681.93	698.36	703.95		310.91	324.68	332.02	342.26	352.41	353.50								
743.85	749.14	752.59	764.07	769.76	780.14		372.03	376.61	396.64	402.15	412.24	417.35								
782.16	794.80	801.32	811.39	816.43	816.59		429.84	433.84	460.04	467.21	477.72	480.43								
830.25	832.29	835.68	839.97	848.04	877.34		490.15	492.31	494.66	502.33	521.14	521.24								
889.61	894.56	912.61	922.56	928.60	931.09		533.14	535.55	541.25	542.15	548.91	568.77								
956.45	958.05	989.93	994.74	994.95	995.12		582.02	594.54	611.36	616.64	617.94	632.08								
1002.61	1006.07	1010.15	1012.71	1015.13	1015.48		640.71	643.81	647.05	658.94	681.95	692.92								
1045.12	1067.85	1072.87	1078.49	1083.84	1088.57		695.28	742.42	746.29	752.00	755.63	764.12								
1092.27	1093.11	1109.87	1118.72	1121.99	1130.94		779.34	790.15	791.69	793.57	800.49	804.07								
1136.21	1144.70	1151.52	1154.78	1166.50	1197.05		811.53	826.26	829.26	831.65	843.45	844.78								
1199.14	1200.16	1201.49	1208.97	1211.47	1223.57		846.21	872.71	891.71	909.13	911.39	922.88								
1226.10	1234.49	1237.57	1276.96	1278.59	1293.96		925.22	928.43	955.93	967.51	977.62	979.79								
1296.71	1305.57	1314.94	1316.81	1322.08	1327.93		988.77	990.51	995.64	997.01	1001.21	1001.92								
1330.44	1333.86	1336.95	1352.13	1356.54	1375.10		1004.57	1007.97	1016.05	1029.58	1036.03	1056.11								
1384.42	1386.92	1403.55	1403.69	1407.24	1420.20		1065.31	1071.37	1072.60	1078.71	1087.77	1089.17								
1420.92	1436.76	1438.03	1438.26	1442.23	1445.13		1107.96	1108.57	1114.73	1123.98	1135.67	1141.45								
1481.53	1484.48	1490.74	1493.71	1496.07	1502.20		1149.21	1161.56	1165.21	1170.85	1181.53	1195.37								
1503.57	1504.18	1504.89	1505.89	1510.10	1511.74		1198.23	1200.57	1206.41	1207.68	1211.82	1214.01								
1512.14	1518.64	1521.44	1523.54	1528.80	1532.78		1219.16	1224.90	1228.56	1239.93	1272.78	1275.84								
1533.21	1534.73	1584.29	1603.27	1621.34	1621.83		1289.34	1294.35	1298.35	1306.79	1311.24	1318.92								
1633.00	1634.43	1653.73	1654.04	1946.21	1957.37		1319.40	1327.09	1329.02	1334.18	1348.76	1354.50								

1356.17	1367.80	1369.46	1384.92	1387.79	1394.06	974.78	983.22	987.91	991.65	993.41	997.77									
1396.34	1402.85	1417.37	1424.76	1426.55	1428.73	1001.25	1005.81	1008.56	1013.70	1018.07	1039.39									
1433.79	1441.69	1445.34	1452.09	1480.33	1482.54	1045.43	1065.75	1071.18	1073.88	1081.16	1087.21									
1491.29	1493.05	1495.29	1497.10	1498.96	1500.91	1090.13	1107.79	1108.81	1125.69	1136.51	1143.01									
1505.18	1512.08	1513.97	1514.85	1517.32	1519.77	1143.52	1148.62	1162.44	1168.00	1175.27	1180.85									
1524.00	1526.76	1530.83	1532.84	1534.91	1538.22	1187.29	1199.97	1202.15	1206.88	1211.53	1213.17									
1541.07	1576.49	1583.91	1604.07	1619.57	1620.24	1214.31	1216.92	1226.48	1229.98	1237.43	1274.60									
1630.77	1635.19	1652.27	1654.04	1942.77	1960.31	1275.03	1290.93	1295.65	1301.16	1309.64	1314.23									
2015.35	2921.37	2949.99	2997.61	3012.67	3039.58	1324.08	1324.77	1325.56	1329.87	1331.52	1347.19									
3042.44	3050.24	3050.70	3051.02	3052.28	3059.65	1350.03	1356.94	1358.67	1368.13	1375.92	1384.93									
3062.92	3068.69	3078.86	3083.41	3084.04	3087.87	1389.06	1390.93	1401.96	1404.43	1417.43	1425.54									
3109.94	3111.63	3113.58	3116.11	3117.30	3117.69	1430.78	1437.91	1442.79	1444.59	1446.91	1460.10									
3125.99	3130.22	3142.84	3149.92	3161.58	3170.23	1482.31	1484.76	1491.14	1491.79	1495.62	1497.40									
3174.80	3179.39	3182.29	3183.61	3184.88	3194.53	1498.10	1499.12	1503.20	1511.68	1512.89	1515.32									
3197.56	3203.52	3205.26	3207.95	3211.02	3220.52	1519.02	1522.15	1522.84	1526.65	1532.16	1533.21									
<hr/>																				
<b>B2-TS</b>																				
<hr/>																				
-671.28	3.97	19.51	24.63	29.27	35.35	2951.69	3011.01	3040.58	3041.08	3050.21	3054.90									
37.06	39.03	43.85	47.04	50.92	58.75	3056.10	3060.80	3062.42	3066.44	3079.55	3087.00									
61.36	65.16	69.68	70.64	75.36	81.28	3091.77	3105.23	3110.14	3111.38	3111.47	3118.92									
85.15	90.27	92.46	98.57	103.05	107.74	3123.20	3127.01	3128.95	3140.33	3143.25	3159.35									
112.32	117.99	124.24	125.84	134.36	142.09	3162.66	3168.10	3171.59	3174.36	3182.14	3182.97									
143.12	149.38	158.34	166.16	171.93	179.24	3183.58	3186.08	3196.23	3197.79	3204.26	3206.64									
187.45	204.07	208.46	215.38	231.47	238.33	3212.00	3216.99	3224.30	<hr/>											
247.02	248.59	257.11	261.86	267.21	273.27	<hr/>														
277.80	288.18	302.27	305.18	315.02	320.47	<b>B3</b>														
331.74	339.49	351.37	352.10	367.24	377.75	<hr/>														
378.92	399.46	410.02	412.53	422.63	435.50	19.71	28.55	31.09	37.90	40.71	43.99									
438.91	464.47	468.65	469.88	479.21	479.95	49.88	52.38	62.33	66.75	70.53	72.55									
487.93	496.35	500.09	504.06	520.06	525.67	83.18	85.94	89.44	95.34	103.79	107.71									
537.03	546.94	549.37	550.93	570.35	583.06	114.10	124.46	127.79	136.74	140.97	148.85									
595.76	610.92	613.68	627.38	634.21	640.43	157.68	162.07	180.78	191.93	205.26	212.60									
643.99	647.92	650.07	666.10	681.66	682.86	224.90	238.37	243.83	247.62	256.60	260.79									
691.48	697.35	702.27	745.93	750.46	758.47	270.44	279.03	296.10	309.15	310.49	312.98									
764.05	769.07	781.55	788.18	791.39	799.27	327.70	343.60	347.95	380.28	387.81	391.05									
800.48	811.59	813.51	829.87	830.20	834.43	403.68	407.89	416.96	434.68	454.64	458.39									
841.92	849.31	864.08	878.56	893.70	902.37	464.79	466.43	469.25	476.92	486.86	492.04									
909.70	923.20	926.09	926.58	957.58	970.67	503.45	526.67	533.10	536.44	540.20	565.71									

572.57	598.76	609.47	621.11	631.52	636.94		335.72	344.05	349.72	367.07	387.75	402.37	
641.07	646.68	650.18	672.66	698.08	701.15		409.53	424.58	434.31	438.73	448.55	451.88	
742.17	749.60	756.16	762.33	769.59	780.09		463.04	466.53	471.04	476.00	487.55	497.28	
785.06	792.57	793.49	801.51	812.77	814.94		517.79	527.55	538.20	541.46	547.49	564.47	
830.39	834.01	837.32	842.40	848.62	878.55		577.95	594.14	613.26	618.92	632.31	633.39	
890.39	901.58	902.97	919.77	921.43	927.36		645.91	648.50	653.41	682.08	702.43	704.28	
930.14	966.05	973.04	986.62	988.92	995.36		743.35	747.38	759.37	767.37	772.74	783.48	
999.68	1004.94	1008.08	1011.32	1014.67	1016.82		788.03	793.60	801.46	811.39	812.91	822.21	
1027.16	1035.48	1044.21	1066.05	1070.58	1079.34		831.42	835.72	844.21	849.87	856.33	876.96	
1081.41	1086.87	1092.92	1107.91	1115.57	1131.06		896.83	900.41	912.53	925.80	934.18	939.18	
1141.48	1147.07	1153.49	1158.18	1167.56	1173.37		949.06	975.77	979.57	984.49	996.39	1002.90	
1198.49	1204.27	1205.77	1209.94	1215.04	1217.83		1006.99	1007.56	1008.85	1015.25	1018.27	1021.16	
1225.85	1227.51	1240.71	1263.51	1280.28	1287.24		1025.36	1044.43	1049.20	1064.07	1067.99	1080.91	
1293.51	1299.52	1299.68	1312.18	1316.76	1319.84		1088.00	1088.54	1094.15	1109.68	1121.53	1127.34	
1327.96	1338.77	1344.53	1347.06	1361.08	1378.87		1132.72	1149.45	1153.86	1161.82	1165.01	1168.71	
1387.75	1387.91	1392.07	1396.04	1407.99	1419.57		1194.74	1204.73	1207.02	1208.97	1216.15	1223.21	
1419.90	1422.99	1432.52	1441.03	1442.32	1443.64		1225.55	1229.27	1232.68	1261.07	1274.86	1290.25	
1448.10	1451.10	1480.23	1484.69	1491.88	1492.80		1294.31	1303.37	1312.54	1315.74	1320.27	1325.34	
1494.09	1498.21	1503.29	1506.08	1507.77	1508.01		1332.97	1336.56	1338.38	1355.64	1357.06	1364.42	
1510.07	1513.24	1515.99	1516.33	1519.49	1523.88		1377.11	1396.20	1399.28	1405.23	1407.65	1416.12	
1525.93	1532.88	1536.82	1537.67	1585.13	1606.56		1421.51	1436.33	1439.40	1439.66	1443.87	1447.69	
1621.34	1621.57	1631.34	1634.78	1652.62	1652.97		1455.24	1477.79	1483.48	1485.59	1494.94	1500.61	
1934.13	1961.84	2017.81	2936.80	2944.32	3035.75		1501.45	1503.80	1505.10	1506.26	1507.90	1511.62	
3038.71	3043.18	3046.77	3048.35	3067.82	3071.97		1513.01	1514.91	1517.08	1517.75	1523.19	1528.00	
3081.22	3085.70	3090.77	3099.89	3105.26	3112.75		1528.13	1532.41	1533.36	1536.88	1588.02	1606.09	
3116.39	3120.88	3121.77	3123.84	3133.81	3136.33		1618.70	1620.15	1631.35	1640.75	1650.79	1654.09	
3143.16	3157.47	3160.83	3161.84	3166.52	3170.40		1949.05	1976.31	2033.42	2936.63	2940.83	2948.27	
3181.54	3186.69	3186.89	3189.35	3195.70	3198.13		3039.39	3044.41	3053.50	3056.51	3085.66	3090.83	
3208.25	3209.84	3213.27	3215.60	3224.67	3360.09		3092.43	3096.28	3100.63	3103.41	3113.26	3116.87	
<hr/>													
<b>B3*</b>							3123.39	3125.94	3126.00	3129.13	3134.41	3135.90	
<hr/>													
23.72	27.68	31.55	39.57	44.10	47.00		3144.82	3147.45	3163.01	3169.43	3171.91	3181.46	
55.29	57.71	70.54	76.46	83.09	86.30		3184.54	3188.14	3192.16	3193.87	3196.21	3203.34	
90.05	96.98	98.16	102.16	105.33	112.84		3204.92	3205.04	3206.34	3211.54	3224.96	3238.42	
116.97	123.05	134.28	143.39	148.08	157.56								
170.55	173.11	178.06	188.52	208.07	222.39								
226.66	231.89	237.83	249.10	259.95	274.45								
278.87	293.47	302.40	313.47	326.69	330.74								