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Supporting Information

Realization of an Asymmetric Non-Aqueous Redox Flow Battery through Molecular Design to Minimize Active Species Crossover and Decomposition

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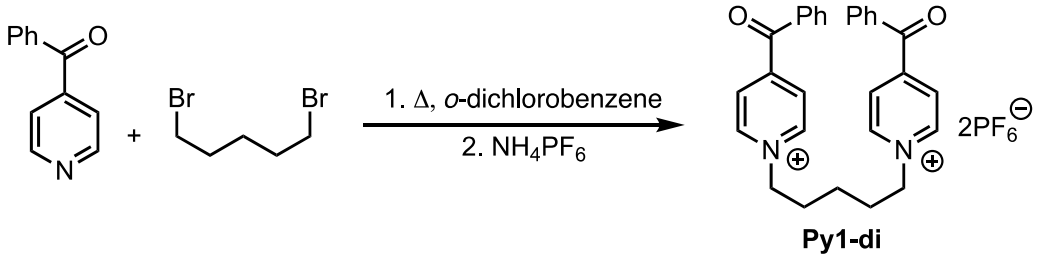
Contents

1. SYNTHESIS

Materials and Methods:

All commercial reagents and solvents were used as received, unless otherwise noted. Anhydrous CH_2Cl_2 was obtained from an SDS solvent system. All reactions were performed under nitrogen atmosphere unless otherwise noted. Biotage® SNAP Ultra column cartridges were used for flash column chromatography. NMR spectra were recorded on a Varian vnmrs 700 (700 MHz for ^1H; 176 MHz for ^{13}C) or a Varian vnmrs 500 (500 MHz for ^1H; 126 MHz for ^{13}C) spectrometer with the residual solvent peak (CD_3CN; δ = 1.94 ppm, ^{13}C: δ = 1.32 ppm or $CDCl_3$; ^1H: δ = 7.26 ppm, ^{13}C: δ = 77.16 ppm) as an internal reference, unless otherwise noted. Chemical shifts are reported in parts per million (ppm) relative to TMS. $CDCl_3$ and CD_3CN were purchased from Cambridge Isotope Laboratories, Inc. **Py1**,[1] **CP**,[2] and **CP-trimer**[Error! Bookmark not defined.] were synthesized using previously reported procedures.

Synthesis of Py1-di



Py1-di

4-Benzoyl pyridine (2.20 g, 12.4 mmol, 4.0 equiv) was dissolved in *o*-dichlorobenzene (3 mL) in a 20 mL vial. 1,5-Dibromopentane (0.420 mL, 3.10 mmol, 1.0 equiv) was added. The vial was sealed with a Teflon-lined cap, and the reaction was stirred at 90 ºC for 2 d, during which time a pale-yellow precipitate formed. The precipitate was dissolved in CH_3CN (10 mL), and then CH_2Cl_2 (~60 mL) was added until a solid formed. The solid was collected and then taken up in an aqueous solution of NH_4PF_6 (2.53 g, 15.5 mmol, 5.0 equiv in 75 mL of water). This solution was extracted with 10% CH_3CN in CH_2Cl_2 (4 x 100 mL). The organic extracts were dried over $MgSO_4$ and concentrated under vacuum. The product was purified via three recrystallizations from boiling CH_3OH to yield **Py1-di** as a white crystalline solid (788 mg, 35% yield).

^1H NMR (500 MHz, CD_3CN) δ 8.87 (d, *J* = 6.3 Hz, 4H), 8.25 (d, *J* = 6.1 Hz, 4H), 7.91-7.86 (m, 4H), 7.83 (t, *J* = 7.5 Hz, 2H), 7.66 (t, *J* = 7.7 Hz, 4H), 4.63 (t, *J* = 7.6 Hz, 4H), 2.11 (dd, *J* = 9.0, 6.7 Hz, 4H), 1.52 (p, *J* = 8.2 Hz, 2H).

^{13}C NMR (176 MHz, CD_3CN) δ 191.8, 152.6, 145.4, 135.0, 134.3, 130.3, 129.2, 127.6, 61.6, 30.1, 22.1.

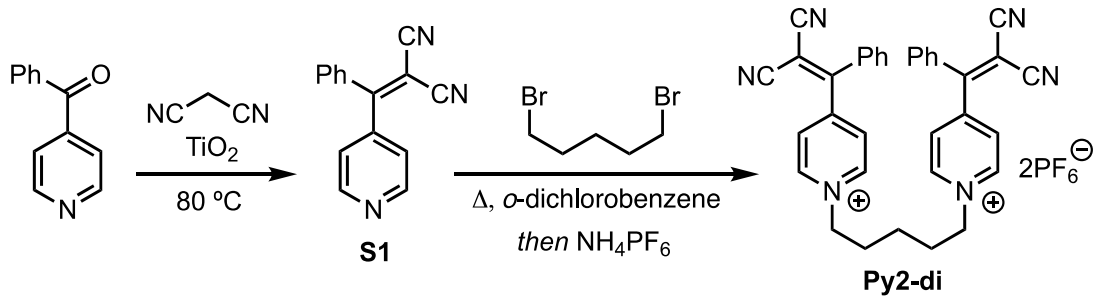
HRMS: $[M\text{-}PF_6]^+$ Calc. 581.1787, Measured: 581.1792

IR: 3131.89, 2954.84, 1664.16, 937.97 cm^{-1}

$E_{1/2}$: -1.01 V and -1.56 V vs Ag/Ag^+

SUPPORTING INFORMATION

Synthesis of Py2-di



4-Benzoyl pyridine (4.00 g, 21.8 mmol, 1.0 equiv), malononitrile (1.44 g, 21.8 mmol, 1.0 equiv), and titanium dioxide (1.74 g, 21.8 mmol, 1.0 equiv) were combined in a vial. The vial was sealed with a Teflon-lined cap, and the neat reaction mixture was heated to 80 °C overnight. The resulting gray paste was cooled, the organics were dissolved in ethyl acetate, and the TiO_2 was removed by filtration. The filtrate was concentrated under vacuum, and the resulting solids were purified via flash chromatography on silica gel, eluting with a gradient of 0-20% ethyl acetate in CH_2Cl_2. The fractions containing the product were collected and concentrated under vacuum. The product was further purified via recrystallization from CH_3OH to afford **S1** as a white powder (3.33 g, 66% yield).

^{1}H NMR (700 MHz, CD_3CN) δ 8.82-8.78 (m, 2H), 7.84 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.75-7.69 (m, 1H), 7.61-7.58 (m, 2H), 7.58-7.56 (m, 2H).

^{13}C NMR (176 MHz, CD_3CN) δ 171.8, 150.5, 143.7, 135.0, 132.9, 130.0, 129.0, 123.3, 113.4, 113.2, 84.9.

HRMS: Calc. 232.0869, Measured: 232.0870

IR: 3063.85, 2225.7, 1669.56, 820.74 cm^{-1}

Compound **S1** (800 mg, 3.46 mmol, 2.2 equiv) and dibromopentane (2.1 mL, 1.57 mmol, 1.0 equiv) were dissolved in *o*-dichlorobenzene (2 mL), and the reaction was heated at 90 °C for 3 d, during which time a pale yellow precipitate formed. The precipitate was dissolved in CH_3CN (10 mL), and then diethyl ether (150 mL) was added, resulting in the formation of a cream-colored precipitate. This precipitate was collected and then dissolved in an aqueous solution of NH_4PF_6 (1.28 g, 7.87 mmol, 5.0 equiv in 30 mL of water). The aqueous solution was extracted with 10% CH_3CN in CH_2Cl_2 (4 x 40 mL). The organic extracts were collected, dried over $MgSO_4$, and concentrated under vacuum. The product was purified via five recrystallizations from CH_3CN/diethyl ether to afford **Py2-di** as a white solid (258 mg, 20% yield).

^{1}H NMR (700 MHz, CD_3CN) δ 8.82 (d, *J* = 6.6 Hz, 4H), 8.10 (d, *J* = 6.4 Hz, 4H), 7.77-7.72 (m, 2H), 7.63 (dd, *J* = 8.7, 7.2 Hz, 4H), 7.57-7.53 (m, 4H), 4.58 (t, *J* = 7.7 Hz, 4H), 2.10-2.08 (m, 4H), 1.52 (p, *J* = 7.8 Hz, 2H).

^{13}C NMR (176 MHz, CD_3CN) δ 166.96, 152.05, 145.54, 133.79, 133.49, 130.19, 129.41, 128.84, 112.63, 112.26, 87.93, 61.75, 29.95, 22.24.

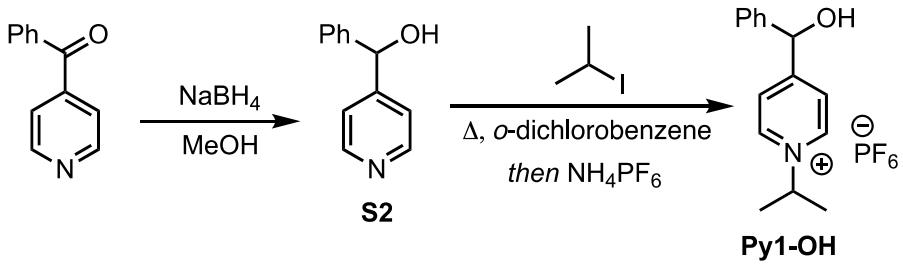
HRMS: $[M\text{-}PF_6]^+$ Calc.: 677.2012, Measured: 677.2013

IR: 3071.52, 2234.32, 1641.44, 1557.29, 828.55 cm^{-1}

$E_{1/2}$: -0.626 V and -0.976 V vs Ag/Ag^+

SUPPORTING INFORMATION

Synthesis of Py1-OH



4-Benzoyl pyridine (200 mg, 1.09 mmol, 1.0 equiv) was dissolved in CH_3OH (3 mL). The solution was cooled to 0 °C, and $NaBH_4$ (53.7 mg, 1.41 mmol, 1.3 equiv) was added. The reaction was allowed to warm to room temperature and stirred under nitrogen for 3 h. The reaction was quenched by the addition of water (2 mL), and the resulting mixture was extracted with ethyl acetate (3 x 20 mL). The organic extracts were collected, dried over $MgSO_4$, and concentrated under vacuum. The product was further purified by tituration with hexanes (2 x 15 mL) to afford **S2** as a white solid (190 mg, 95% yield).

^{1}H NMR (700 MHz, CD_3CN) δ 8.52-8.49 (m, 2H), 7.40 (d, *J* = 6.9 Hz, 2H), 7.38-7.34 (multiple peaks, 4H), 7.31-7.27 (m, 1H), 5.79 (d, *J* = 3.8 Hz, 1H), 4.04-4.02 (m, 1H).

^{13}C NMR (176 MHz, CD_3CN) δ 153.5, 149.7, 143.9, 128.5, 127.6, 126.5, 121.0, 73.9.

HRMS: Calc. 186.0913, Measured: 186.0916

IR: 3133.56, 2825.64, 2723.77, 1597.69, 1063.47 cm^{-1}

Compound **S2** (189 mg, 1.02 mmol, 1.0 equiv) was dissolved in *o*-dichlorobenzene (0.22 mL). *iso*-Propyl iodide (0.74 mL, 7.43 mmol, 7.3 equiv) was added, and the mixture was heated at 50 °C overnight. The reaction was cooled to room temperature, the resulting paste was transferred to an Erlenmeyer flask using CH_3CN (5 mL), and diethyl ether (50 mL) was added, resulting in the formation of a precipitate. The precipitate was collected via filtration and dissolved in CH_2Cl_2 to afford a bright red solution. The organic layer was washed with a solution of NH_4PF_6 (499 mg, 3.06 mmol, 3.0 equiv) in 1 : 1 H_2O : brine (3 x 50 mL) after which the organic layer turned light yellow. The organic extracts were collected, dried over $MgSO_4$, and concentrated under vacuum. The product was purified via flash chromatography (0-15% CH_3OH in CH_2Cl_2) followed by recrystallization from boiling CH_3OH (x 2). **Py1-OH** was obtained as a white solid (258 mg, 68% yield).

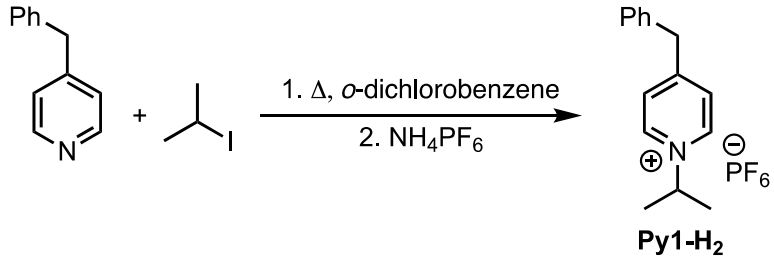
^{1}H NMR (700 MHz, CD_3CN) δ 8.65-8.62 (m, 2H), 8.02 (d, *J* = 6.2 Hz, 2H), 7.43-7.38 (multiple peaks, 4H), 7.35 (ddt, *J* = 9.7, 5.7, 1.8 Hz, 1H), 6.02 (d, *J* = 3.3 Hz, 1H), 4.85 (hept, *J* = 6.8 Hz, 1H), 4.52 (d, *J* = 3.8 Hz, 1H), 1.60 (dd, *J* = 6.6, 2.3 Hz, 6H).

^{13}C NMR (176 MHz, CD_3CN) δ 165.2, 143.3, 142.6, 130.0, 129.6, 128.0, 126.2, 74.3, 65.6, 22.9.

HRMS: Calc. 228.1383, Measured: 228.1384

IR: 3134.73, 1635.87, 878.06 cm^{-1}

Synthesis of Py1-H₂



Py1-H₂

4-Benzyl pyridine (1.18 mmol, 200 mg, 1.0 equiv) was dissolved in *o*-dichlorobenzene (0.25 mL). *iso*-Propyl iodide (0.86 mL, 8.6 mmol, 7.3 equiv) was added, and the mixture was heated at 50 °C overnight. The reaction was cooled to room temperature, the creamy paste was transferred to an Erlenmeyer flask using CH_3CN, and diethyl ether (50 mL) was added leading to the formation of a precipitate. The precipitate was collected via filtration and then dissolved in CH_2Cl_2, affording a bright red solution. The organic layer was washed with NH_4PF_6 (32.4 mmol, 3 equiv) in 1 : 1 H_2O : brine (50 mL x 3) after which the solution turned light yellow. The organic extracts were collected, dried over $MgSO_4$, and concentrated under vacuum. The product was purified via flash chromatography (0-15% CH_3OH in CH_2Cl_2) followed by recrystallization from boiling ethyl acetate. The product, **Py1-H₂**, was obtained as white solid (307 mg, 73% yield).

^{1}H NMR (700 MHz, CD_3CN) δ 8.60 (d, *J* = 6.5 Hz, 2H), 7.84 (d, *J* = 6.2 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.31 (d, *J* = 7.6 Hz, 2H), 4.84 (hept, *J* = 6.7 Hz, 1H), 4.28 (s, 2H), 1.61 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (176 MHz, CD_3CN) δ 163.1, 143.1, 138.1, 130.3, 130.1, 129.2, 128.4, 65.4, 41.7, 22.9.

HRMS: Calc. 212.1434, Measured: 212.1437

IR: 3570.84, 3071.27, 1672.30, 772.77 cm^{-1}

2. **ELECTROCHEMISTRY AND CYCLING STUDIES**

Materials:

Acetonitrile (99.8% anhydrous) was obtained from Sigma Aldrich and used as received. Potassium hexafluorophosphate (≥99%) was obtained from Sigma Aldrich and dried under high vacuum at 100 °C for 48 h before use. 0.5 M stock solutions of KPF_6 in MeCN were prepared in a nitrogen-filled glovebox and dried over activated 3Å molecular sieves for at least two days prior to use. The molecular sieves were activated by heating at 200 °C under vacuum. All organic electrolytes were dried at 80 °C under high vacuum for 19 h before use and were then stored in an inert-atmosphere drybox.

For the laboratory-scale flow battery, a peristaltic pump (Cole-Parmer) was used in combination with Solveflex and PFA tubing. The cycling was performed with a zero-gap flow cell comprised of graphite charge-collecting plates containing an interdigitated flow field. Two layers of non-woven carbon felt electrodes, Sicracet 29AA, were used in each half-cell. ePTFE gaskets were used to achieve ~20% compression of the carbon felt. The exposed area of the membrane in the gasket window was used as the active area (2.55 cm^2). Fumasep FAPQ-375PP was purchased from FuMa-Tech and was ion exchanged prior to use by soaking pre-cut membranes in a saturated aqueous solution of KPF_6 (3 x 8-16 h). After each soak, the membrane was rinsed

with deionized water. The membrane was stored outside the box, under ambient atmosphere. Prior to use, it was dried *in vacuo*, at 50 °C, along with the rest of the glassware for battery cycling. A sample of Celgard 2500 was generously provided by Celgard LLC, and used without any further treatment.

General Procedure for Cyclic Voltammetry

Cyclic voltammetry was performed in a nitrogen-filled drybox with a Biologic VSP multichannel potentiostat/galvanostat using a three-electrode setup. A glassy carbon electrode (0.07 cm^2, BASi) was used as the working electrode and a platinum wire was used as the counter electrode. An Ag/Ag^+ quasi-reference electrode (BASi) containing 0.01 M $AgBF_4$ (Sigma Aldrich) in 0.5 M KPF_6/MeCN was used. All potentials are referenced to Ag/Ag^+. The CVs were performed with a solution of 5 mM concentration of active species, a scan rate of 100 mV s^{-1}, using 0.5 M KPF_6 as supporting electrolyte in MeCN.

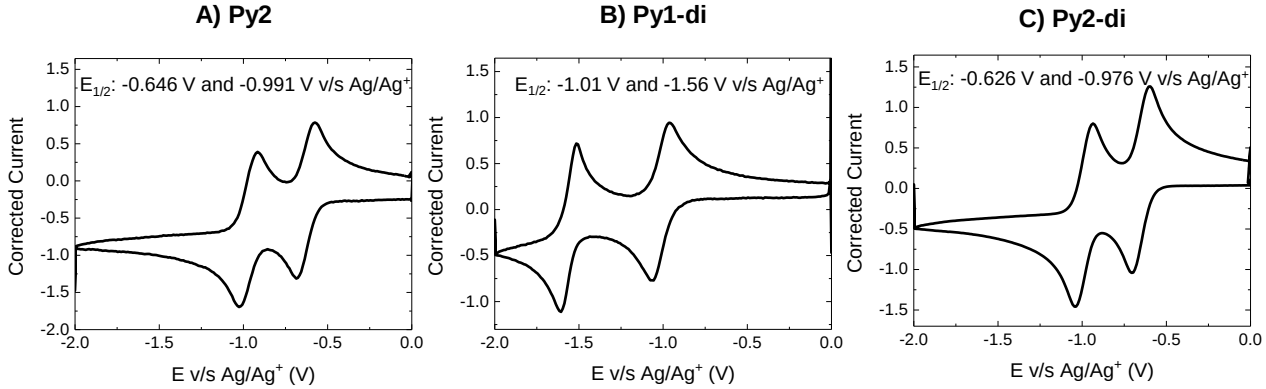


Figure S1. Representative cyclic voltammograms of **Py2**, **Py1-di** and **Py2-di** in MeCN with KPF_6 as the supporting electrolyte at 100 mVs^{-1}.

General Procedure for Flow Cell Cycling

All parts of the cell (including membrane, carbon felt electrodes, tubing) were dried in a vacuum oven at 50 °C overnight. The cell was assembled under ambient conditions and then brought into the glovebox. A 50 mM solution (per redox active unit) of the electrolyte was prepared in the glovebox using 0.5 M KPF_6 as the supporting electrolyte in MeCN (6 mL). To wet the membrane, the cell was pretreated by continuous flow of the electrolyte solution through the cell at 10 mL/min for 2 h. Electrochemical cycling was then performed under galvanostatic conditions using a BioLogic VSP galvanostat employing a charge/discharge current of 10 mA cm^{-2} (~4 C) using potential cutoffs of 1.7-2.2 V during charge and 1.0-0.5 V during discharge. Under these conditions, the battery typically reached ~80% state of charge. EIS was performed from 500 kHz to 1 Hz at OCV using a 10 mV sine perturbation. Aliquots of the solution were taken before and after the experiments to determine crossover (by CV) and decomposition (by ^1H NMR). Fade of capacity was calculated by subtracting the measured charge capacity at the end of cycling from the measured charge capacity at cycle 0 and dividing that by the theoretical capacity (8 mAh).

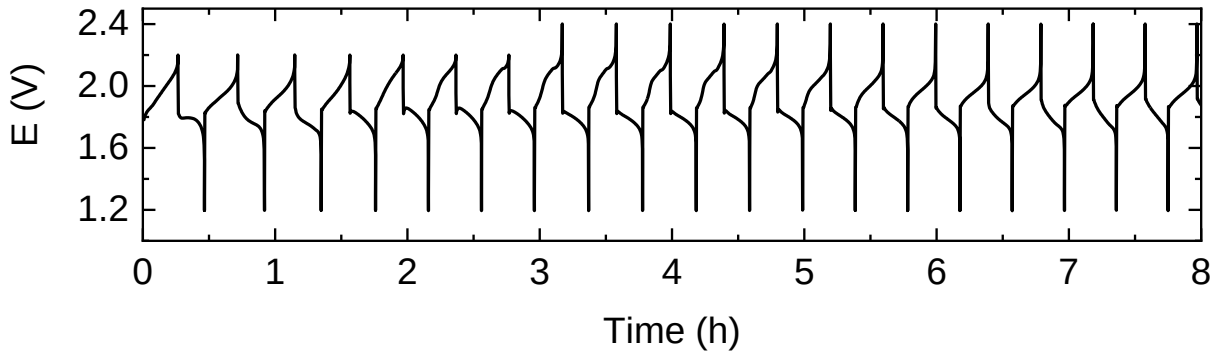


Figure S2. Flow cell cycling data showing the first few charge/discharge cycles of **Py1**/**CP** in a symmetric system (data in Figure 2b).

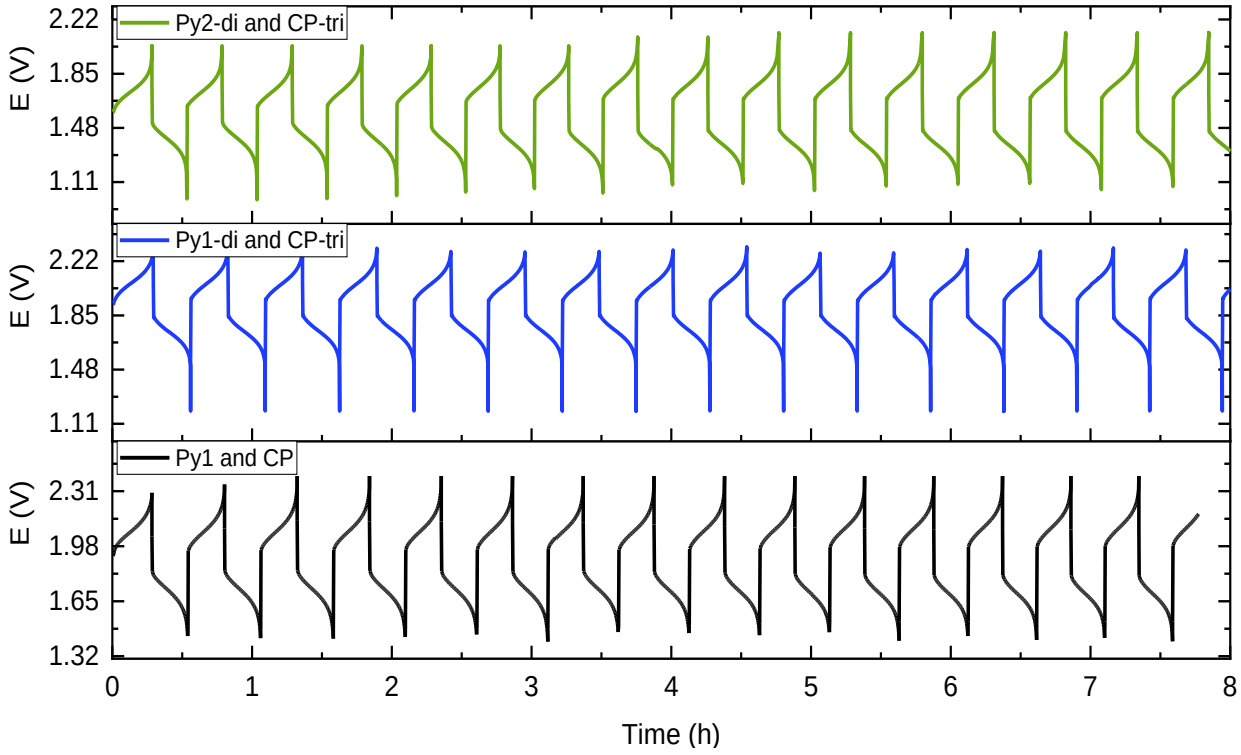


Figure S3. Flow cell cycling data showing the first few charge/discharge cycles for the asymmetric systems (data in Figure 3).

Deuterium Labeling Experiments

The deuterium labeling experiments conducted in custom glass H-cells equipped with stir bars and reticulated vitreous carbon (RVC) electrodes (100 ppi, ~70 cm^2 surface area, Duocell) in a nitrogen-filled glovebox with a BioLogic VSP galvanostat. A porous glass frit (P5, Adams and Chittenden) was used as a separator. H-cells, stir bars, and electrodes were dried in an oven at 150 °C for 30 min prior to use. A symmetrical configuration with 25 mM of each active species (5 mL in each chamber) was subjected on both halves of the cell. 0.5 M KPF_6 was used as a supporting electrolyte in CH_3CN or CD_3CN as solvent. Both chambers of the H-cell were stirred continously during the experiment. Electrochemical cycling was then performed under galvanostatic conditions employing a charge/discharge current of 1.2 mA cm^{-2} using potential cutoffs of 3.0 V during charge and 0.0 V during discharge.Three sets of experiments were run:

1) Using CD_3CN as a solvent and no added D_2O or H_2O
2) Using CH_3CN as the solvent and 10 equiv of D_2O added
3) Using CD_3CN as a solvent and 10 equiv of H_2O added

Integration of protons alpha to nitrogen was compared to that of H_a to track the amount of deuteration in the decomposition product.

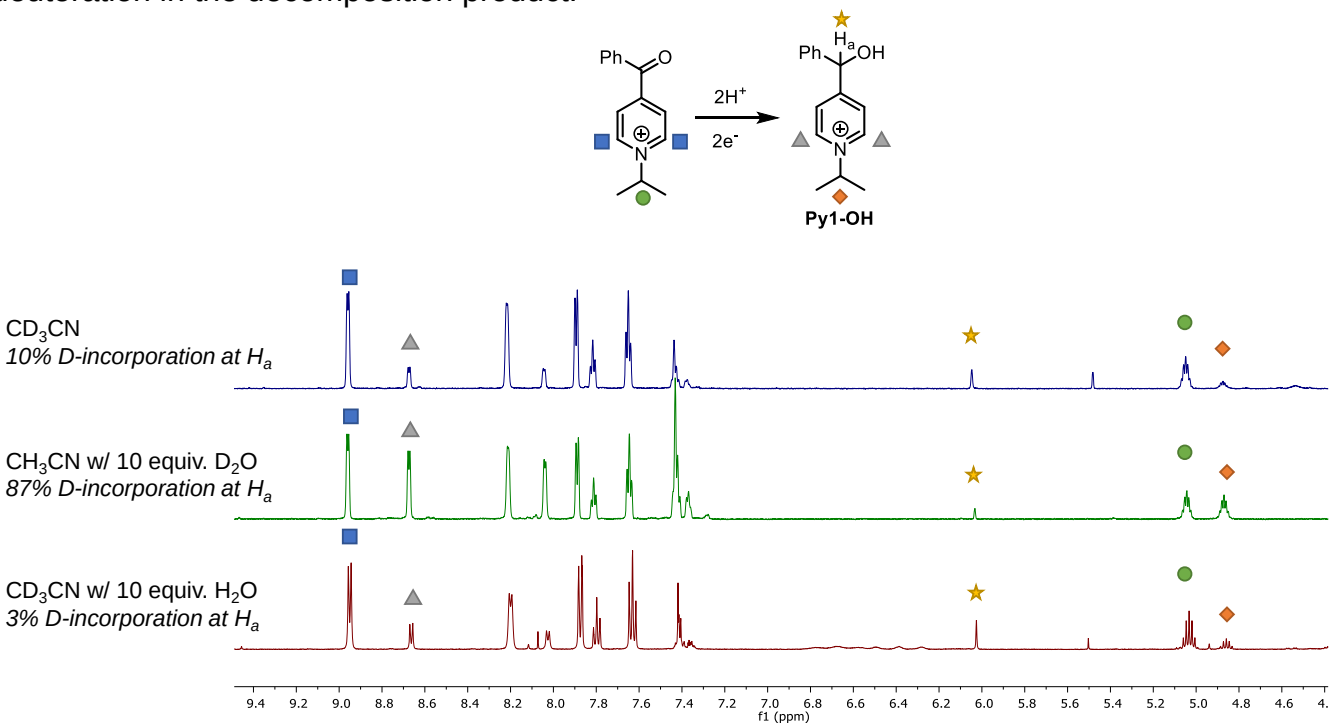


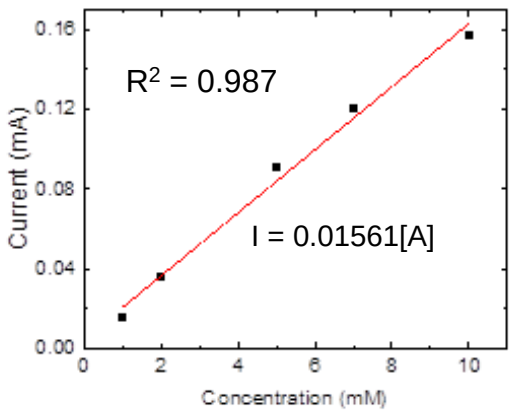
Figure S4. ^1H NMR of the deuterium labeling experiments.

General Procedure for Determining % Crossover

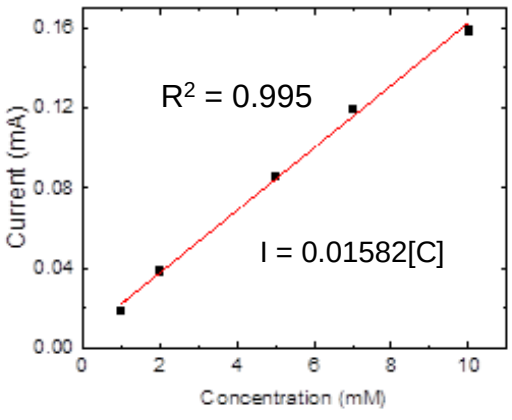
An aliquot of known amount was taken out for analysis before the start of the cycling experiment and at the end of the experiment. These aliquots were analyzed by cyclic voltammetry to determine % crossover. Volumes of solutions on both sides of the cell were measured (to account for any solvent lost to evaporation or transfer between half-cells).

Quantification of Crossover:

ANOLYTE:



CATHOLYTE



The aliquots collected at the beginning and end of the experiment were diluted with 0.5 M KPF_6 in MeCN solution (0.9 mL) and the cyclic voltammograms for each sample were measured. Calibration curves were used to calculate the concentration of this CV sample. This concentration was then normalized for the amount of aliquot taken out (by mass) and corrected for any volumetric change that occurred during the experiment (see calculation example below). Percent crossover was then calculated by dividing the concentration calculated for the blank side by the concentration of solution before the experiment.

To calculate crossover of CP monomer after 1 day of circulation:

-Mass of aliquot before experiment = 60 mg

-Mass of aliquot from crossover side after experiment = 61 mg

-Total volume of crossover side after the experiment = 5.67 mL

-Volumetric change = 5.67/6.0 = 0.945

*6.0 mL was the original volume of the solution

-CV peak height of sample before the experiment = 0.06659 mA. Concentration = 4.21 mM (by plugging peak height into the equation above)

-CV peak height of CV from the counter side sample after the experiment = 0.0175 mA. Concentration = 1.11 mM

-The peak heights were then normalized to their respective aliquot masses and the crossover calculated using the formula below.

$$\%crossover = \left(\frac{concentration(counter) * Volumetric\ change}{mass\ aliquot\ (counter)}\right) / \left(\frac{concentration(before)}{mass\ aliquote\ (before)}\right) * 100$$

For this example: Crossover = $\left(\frac{1.11*0.945}{61}\right) / \left(\frac{4.21}{60}\right) * 100$ = **24%**

- When plotting the CVs, *corrected/normalized current* was plotted. Current was normalized by dividing the voltammogram by the mass of the aliquot and multiplying for volumetric change

Author Contributions

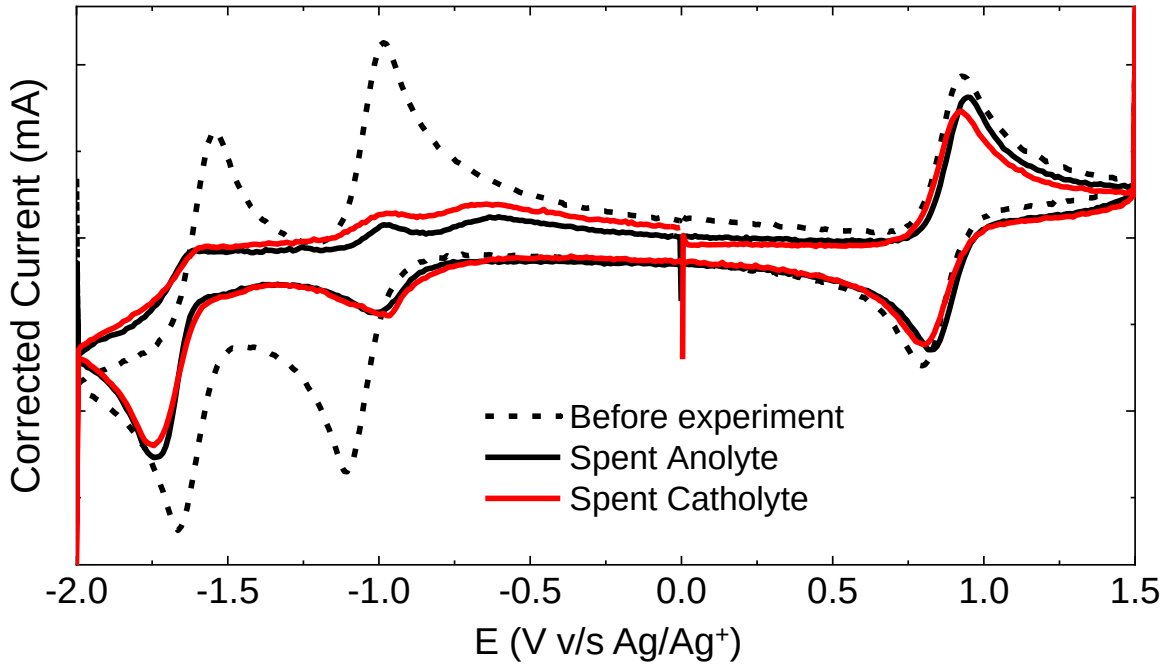
A. Shrestha: lead on electrochemical/flow cell cycling data collection and analysis, lead on synthesis and characterization of all new compounds, lead on writing drafts of manuscript and SI. **K. Hendriks**: lead on electrochemical/flow cell cycling data collection and analysis at initial stages of project, supporting in editing manuscript and SI. **S. Minteer, M. Sigman**: supporting on project administration, writing (equal contributions). **M. Sanford**: lead on funding acquisition, project administration, and writing/editing manuscript/SI.

References

[1] Sevov, C. S.; Hickey, D. P.; Cook, M. E.; Robinson, S. G.; Barnett, S.; Minteer, S. D.; Sigman, M. S.; Sanford, M. S. Physical Organic Approach to Persistent, Cyclable, Low-Potential Electrolytes for Flow Battery Applications. *J. Am. Chem. Soc.* **2017**, *139*, 2934-2927.

[2] Sevov, C. S.; Samaroo, S. K.; Sanford, M. S. Cyclopropenium Salts as Cyclable, High-Potential, Catholytes in Nonaqueous Media. *Adv. Energy Mater.* **2017**, *7*, 1602027.

Figure S5. CVs before and after the cycling experiments in symmetric system (Figure 1b)



CVs of the spent solutions indicate complete anolyte decomposition.

Figure S6. ^{1}H NMR spectra obtained after the symmetrical cycling experiment in Figure 1b along with independent spectra of **Py1**, **Py1-OH** and **Py1-H$_2$**

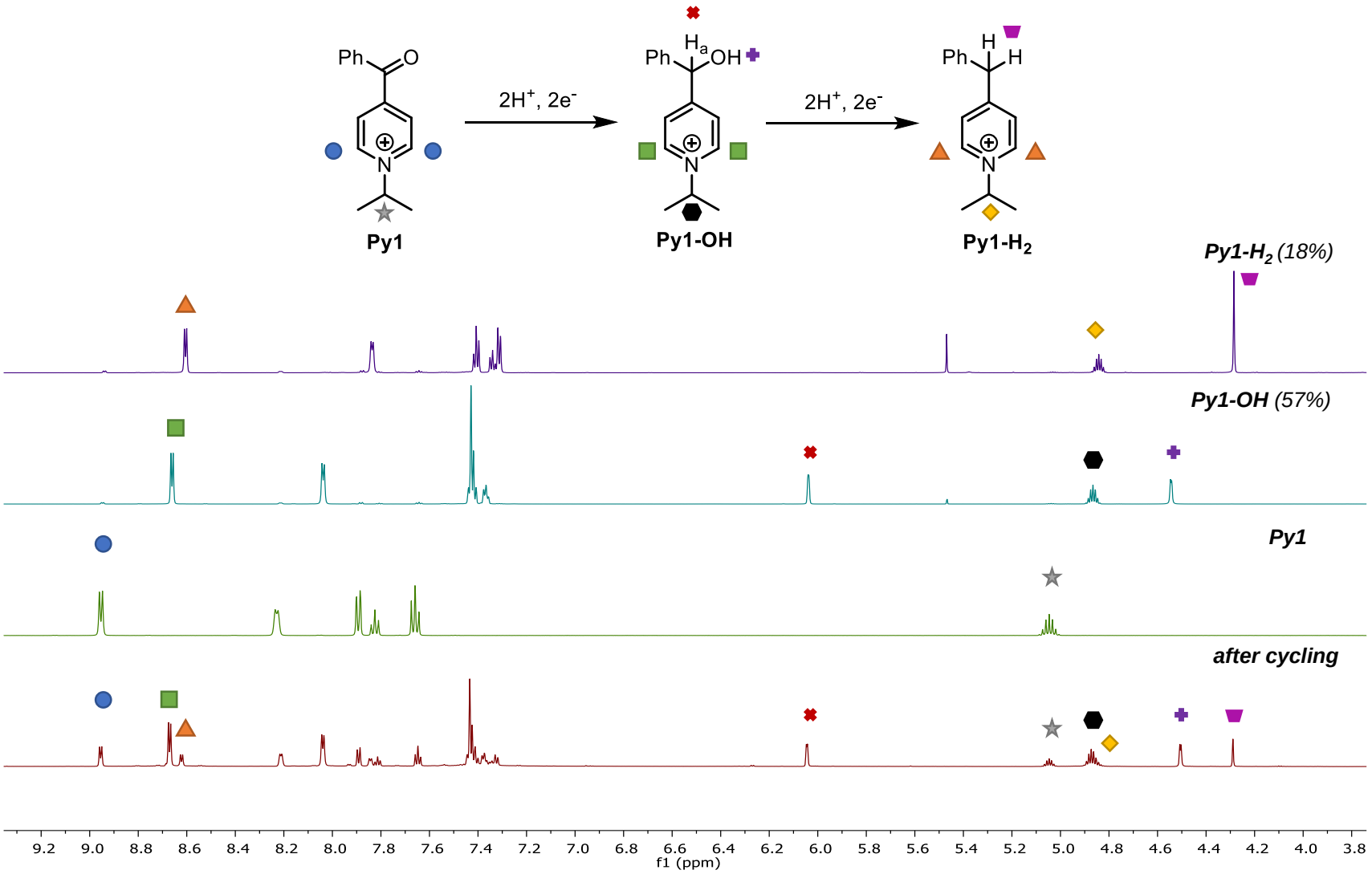
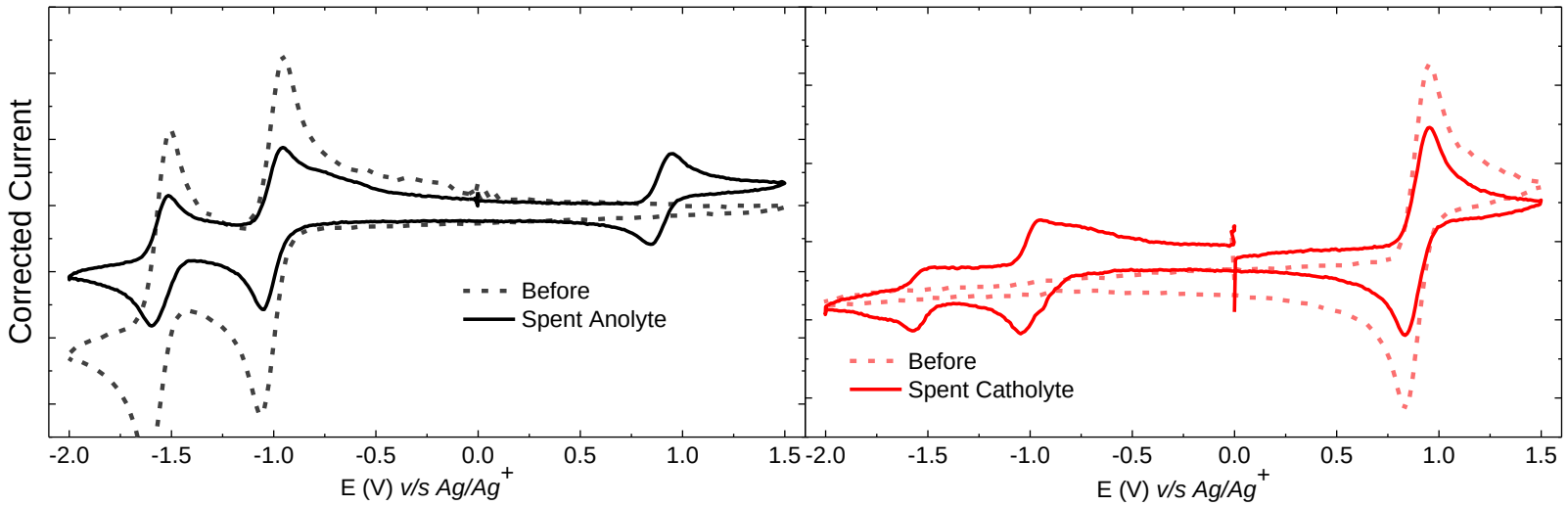


Figure S7. CVs after the cycling experiments in asymmetric system

A) Py1 and CP (Figure 3c, black)



B) Py1-di and CP-tri (Figure 3c, blue)

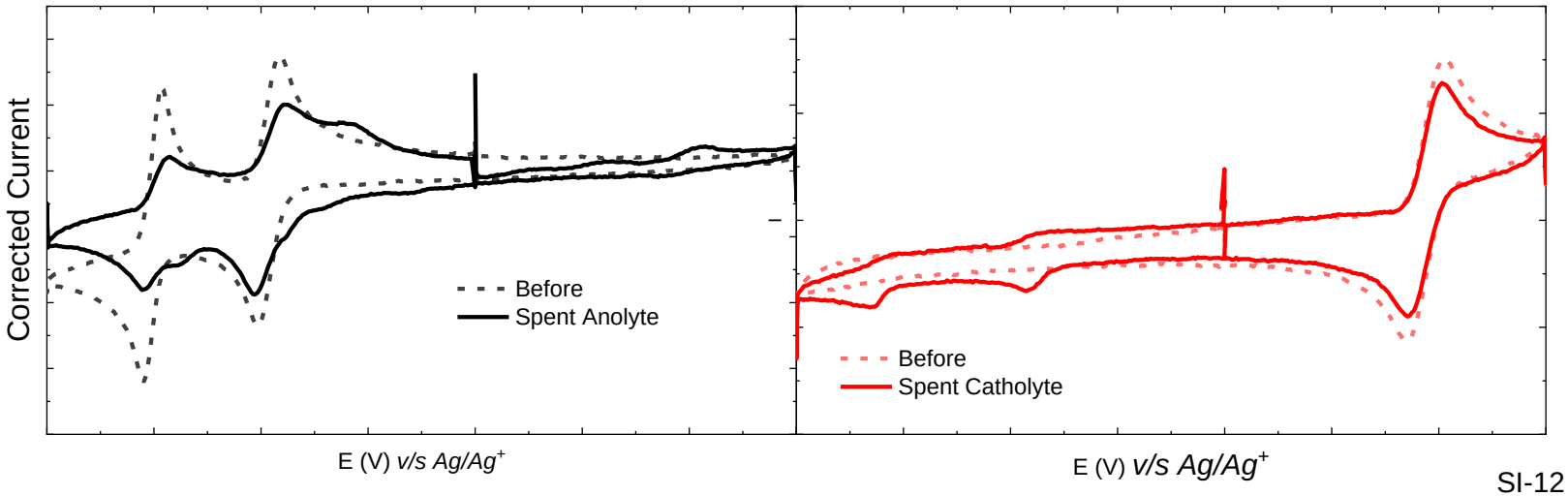


Figure S8. ^{1}H NMR spectrum of the anolyte solution after the electrochemical cycling of **Py1**/**CP** in asymmetric system (Figure 3c, black)

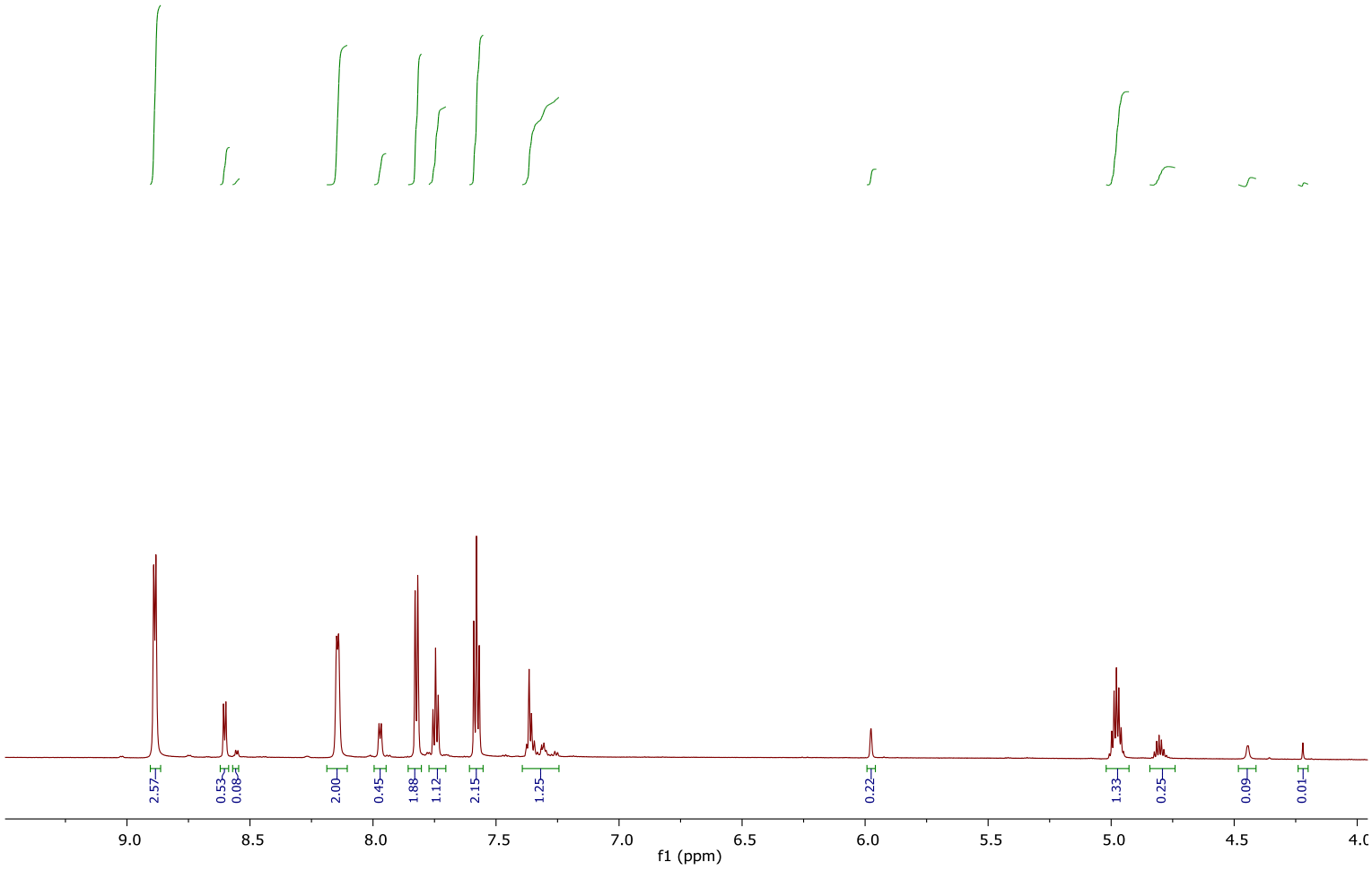


Figure S9. ^{1}H NMR spectrum of the anolyte solution after the electrochemical cycling of **Py1-di**/**CP-tri** in asymmetric system (Figure 3c, blue)

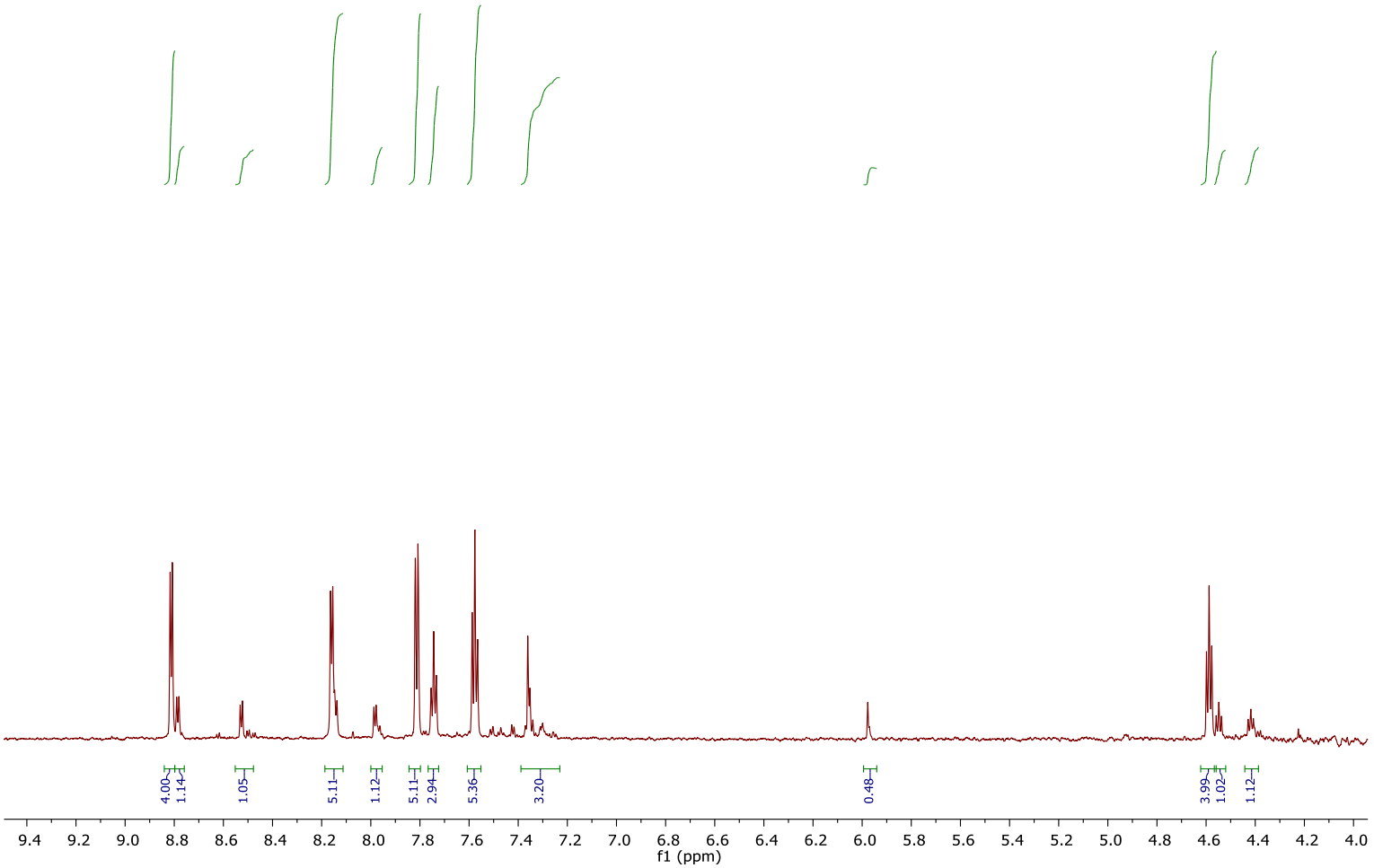


Figure S10. EIS spectrum at 0% SOC of flow battery with Fumasep FAPQ-375-PP with **Py2-di/CP-tri**

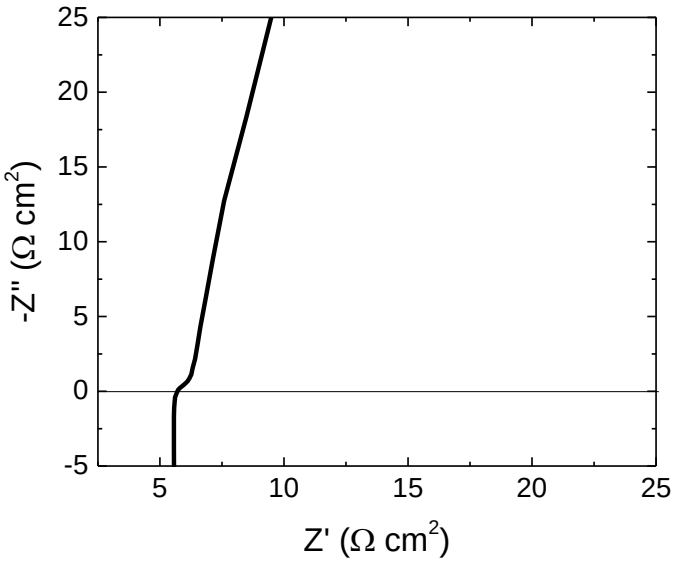


Figure S11. Discharge capacity, coulombic efficiency and energy efficiency of RFB with **Py2-di/CP-tri**

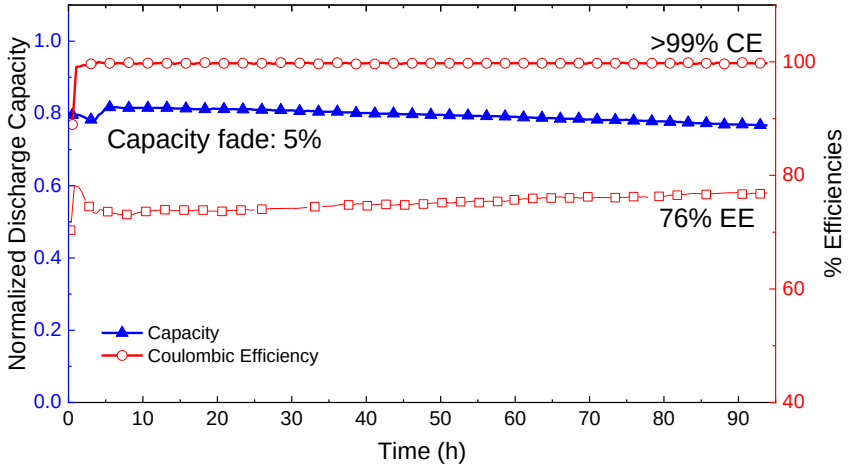


Figure S12. CVs after the cycling experiment with **Py2-di/CP-tri** (Figure 3c, green)

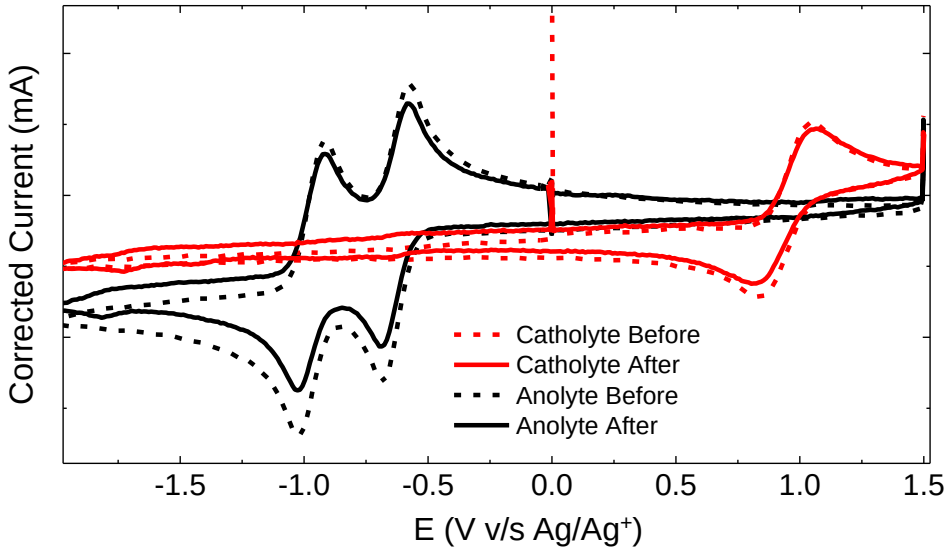


Figure S13. ^{1}H NMR spectra after the cycling experiments comparing **Py1/CP** to **Py2-di/CP-tri**

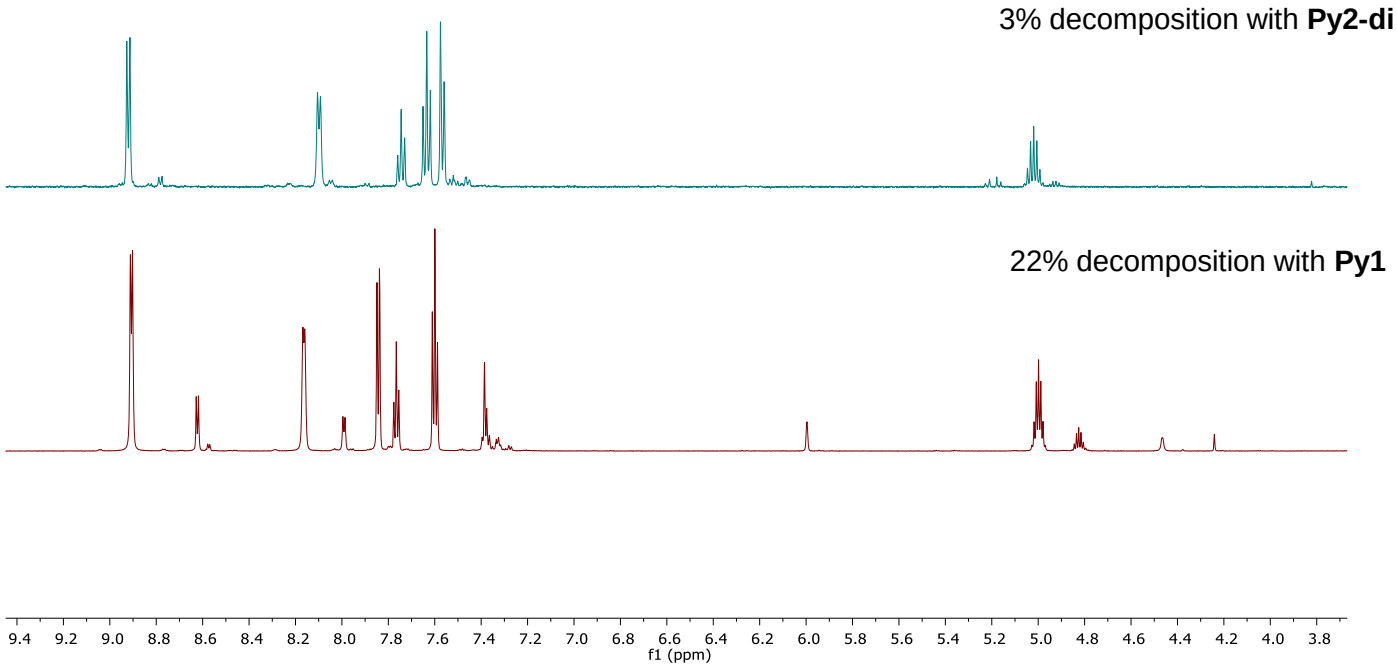
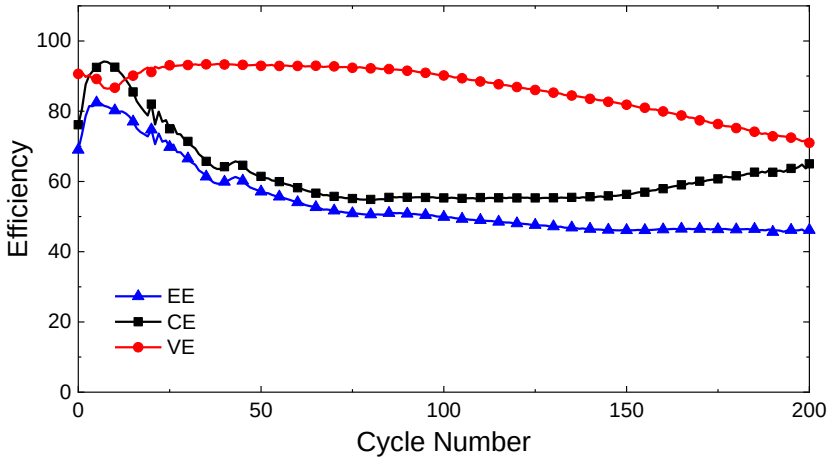
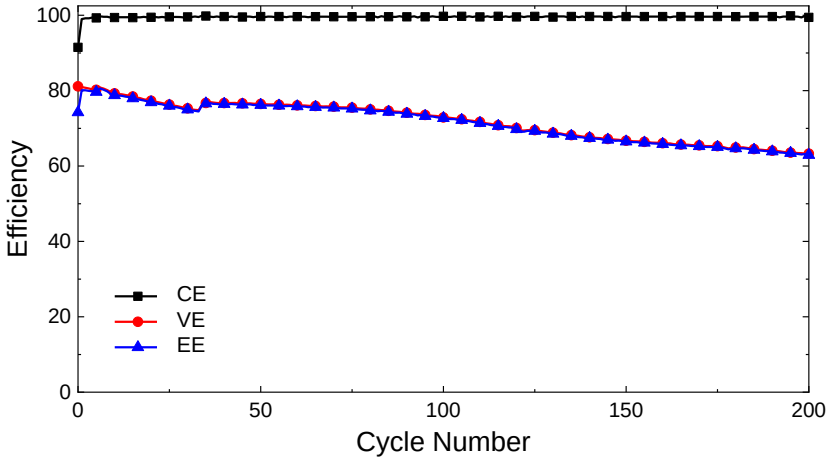


Figure S14. Coulombic, voltaic and energy efficiencies

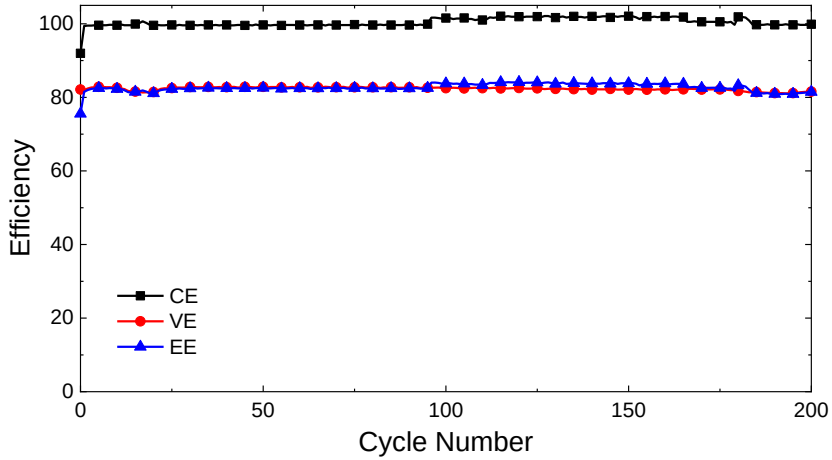
A) Py1/CP in symmetric battery (Figure 1b)



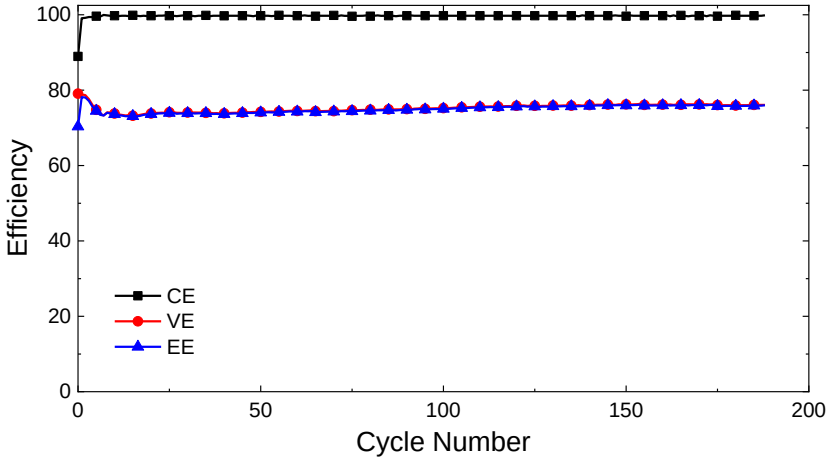
B) Py1/CP in asymmetric battery (Figure 3c, black)



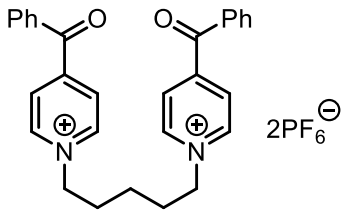
C) Py1-di/CP-tri in asymmetric battery (Figure 3c, blue)



D) Py2-di/CP-tri in asymmetric battery (Figure 3c, green)

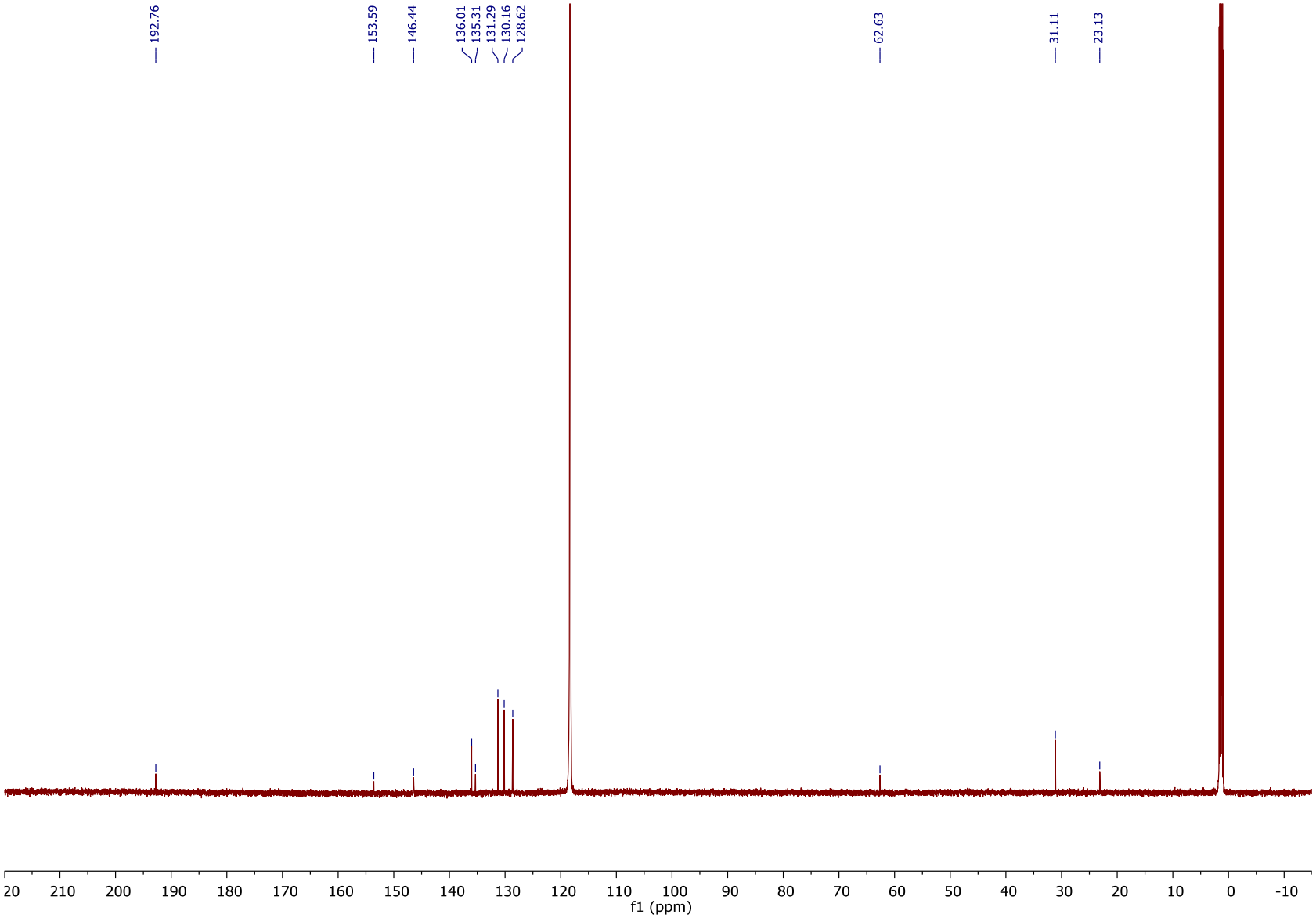


^{1}H NMR

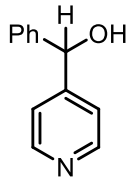


$2PF_6^{\ominus}$

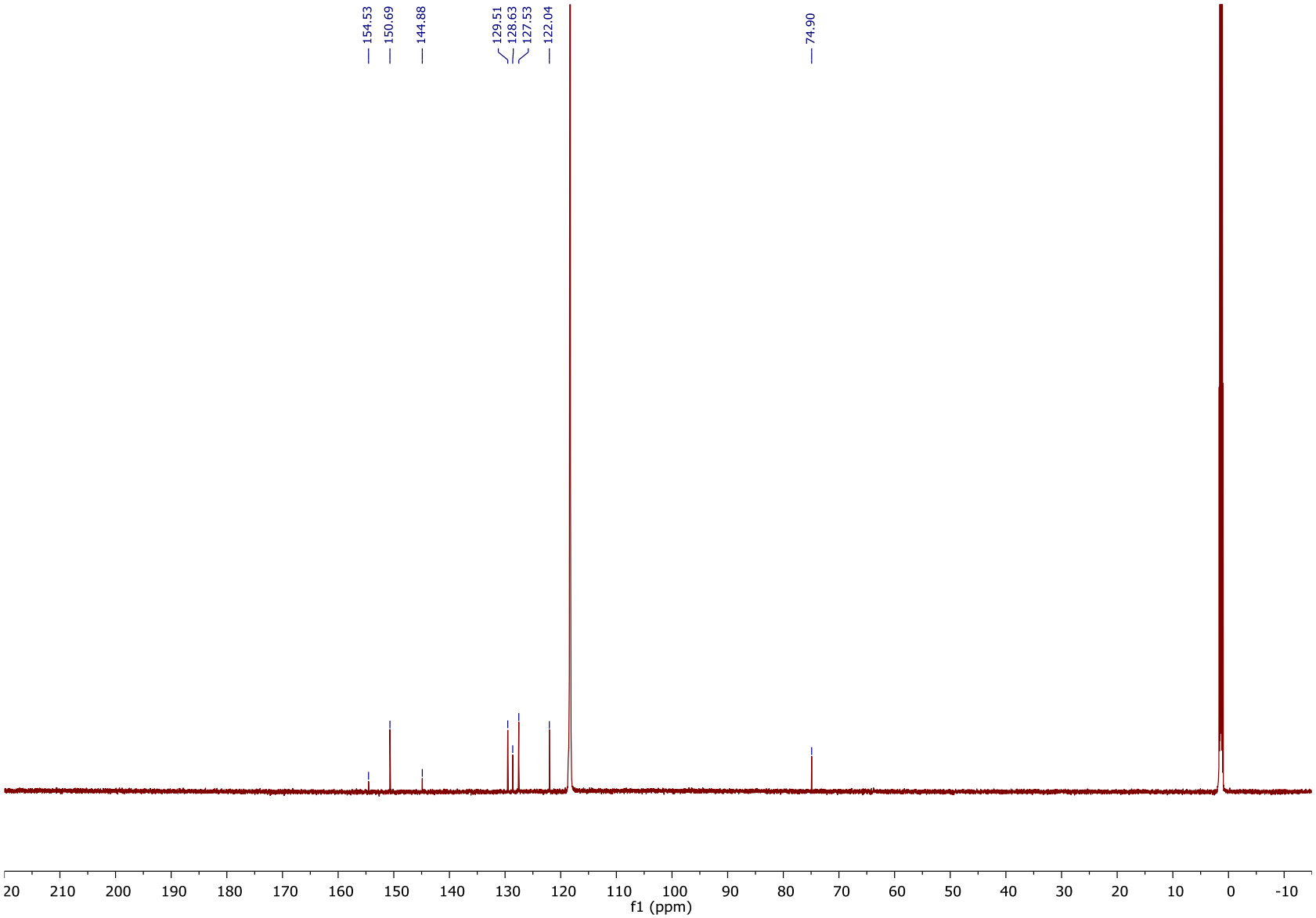
^{13}C NMR


192.76
153.59
146.44
136.01
135.31
131.29
130.16
128.62
62.63
31.11
23.13
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

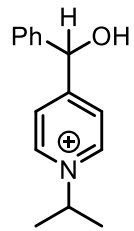
^{1}H NMR



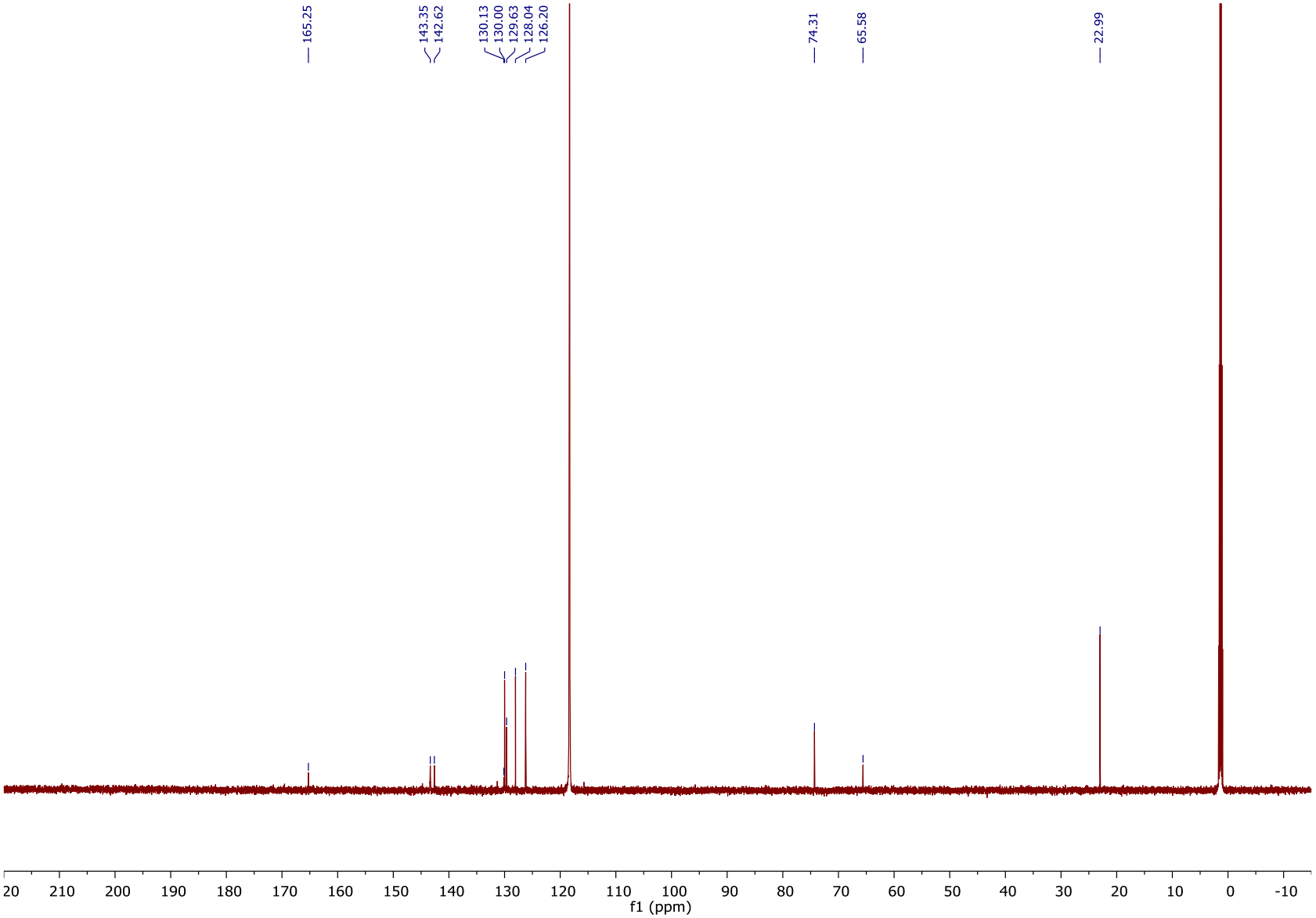
^{13}C NMR


154.53
150.69
144.88
129.51
128.63
127.53
122.04
74.90
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

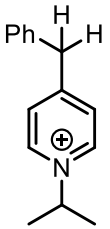
^{1}H NMR



^{13}C NMR

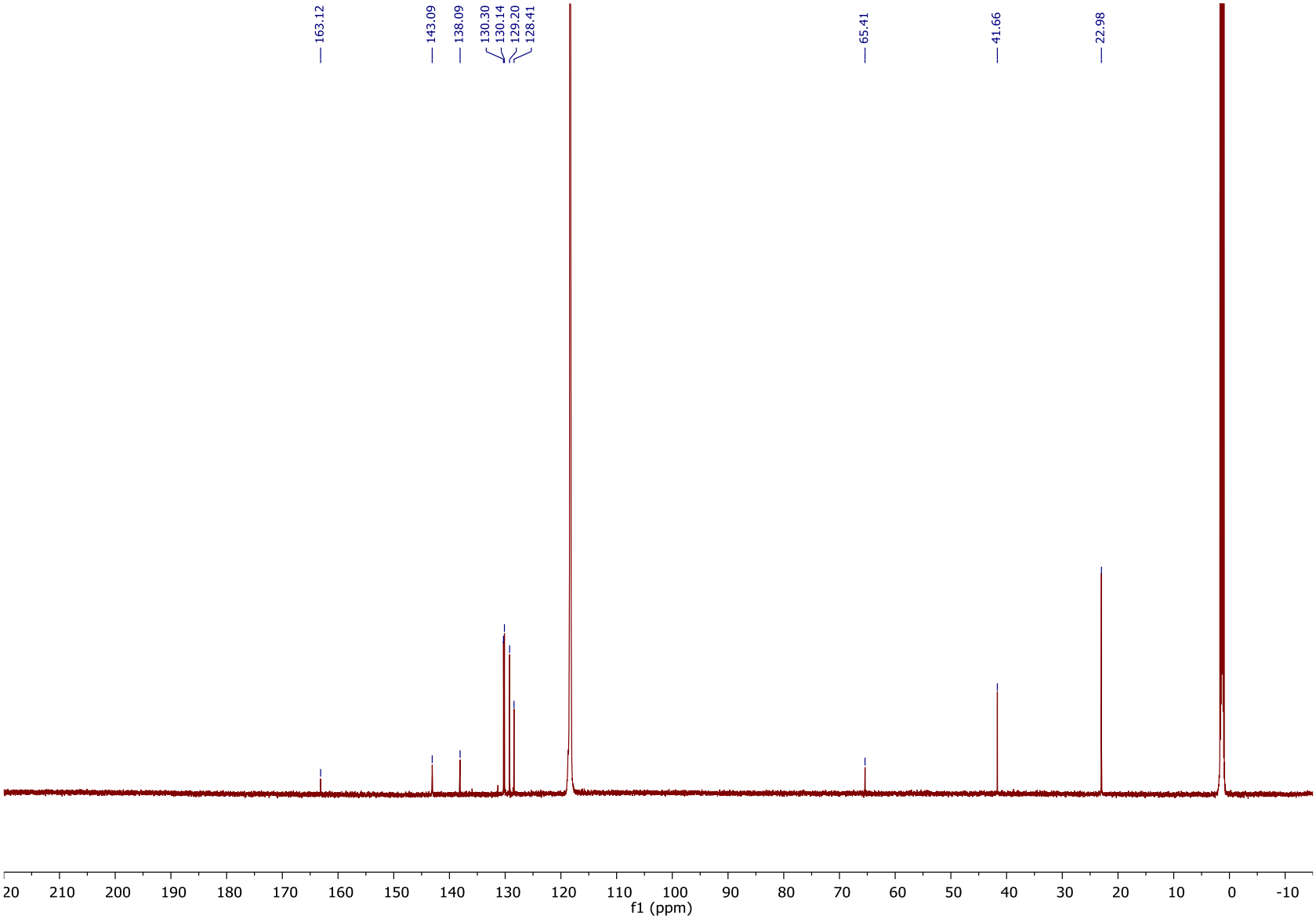

165.25
143.35
142.62
130.13
130.00
129.63
128.04
126.20
74.31
65.58
22.99
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

^{1}H NMR

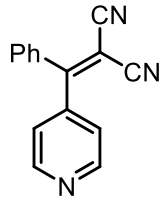

H
Ph
H
N

8.61
8.60
7.84
7.83
7.42
7.41
7.40
7.35
7.34
7.33
7.32
7.31
4.88
4.87
4.87
4.86
4.85
4.84
4.83
4.82
4.81
4.28
1.62
1.61
2.00
1.99
1.88
1.05
1.90
1.07
2.02
5.84
f1 (ppm)

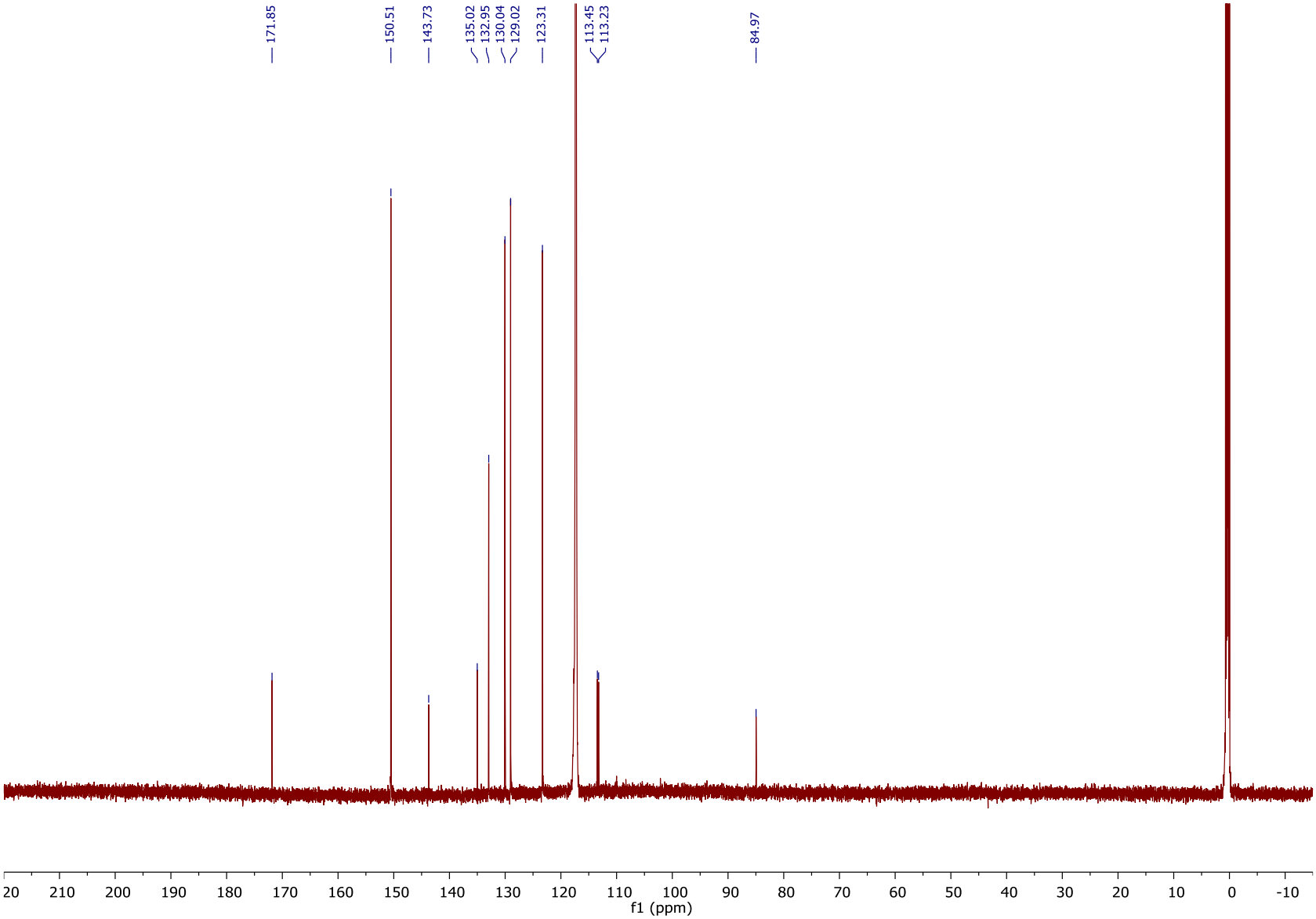
^{13}C NMR


163.12
143.09
138.09
130.30
130.14
129.20
128.41
65.41
41.66
22.98
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

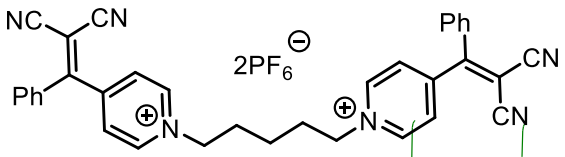
^{1}H NMR



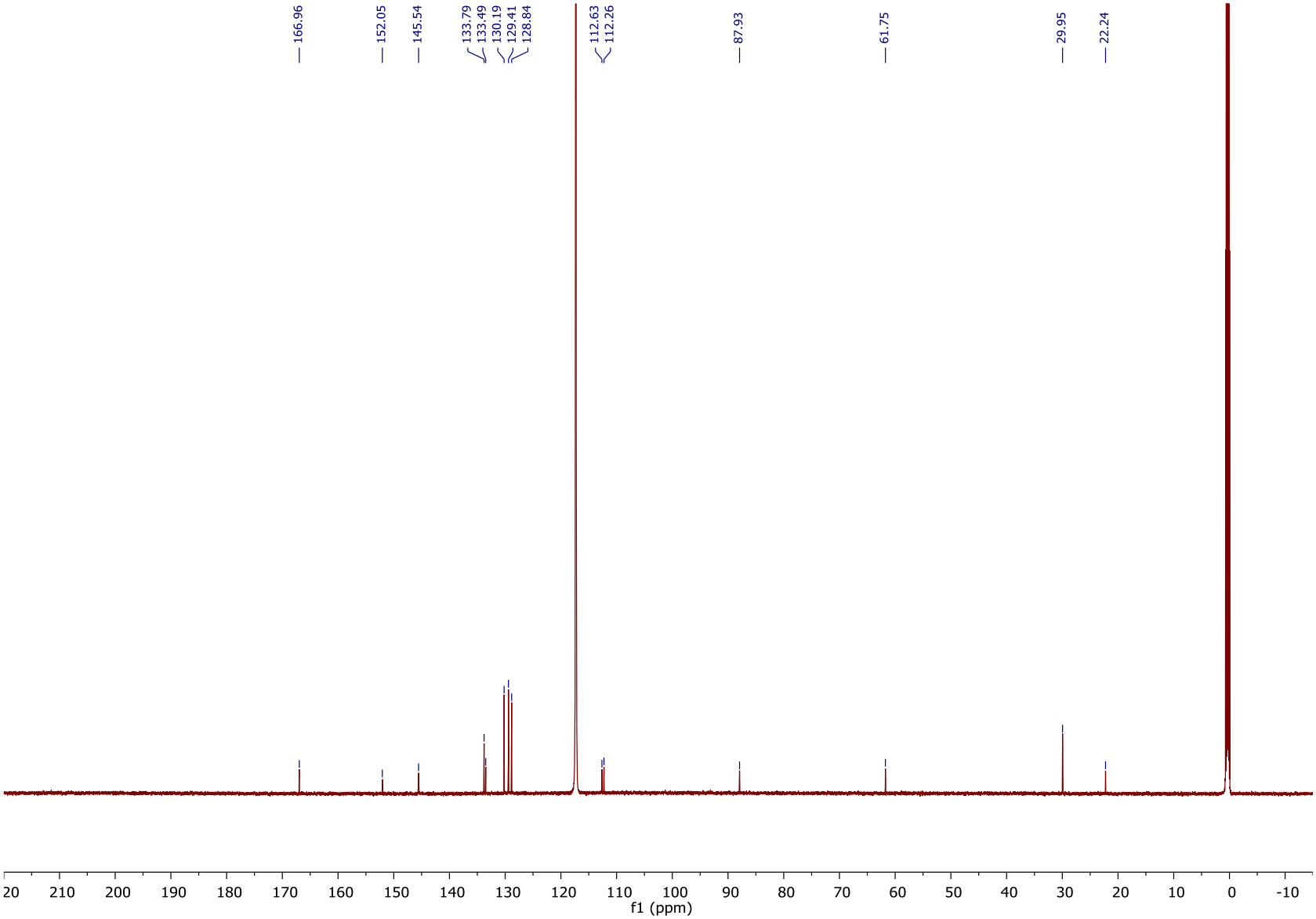
^{13}C NMR


171.85
150.51
143.73
135.02
132.95
130.04
129.02
123.31
113.45
113.23
84.97
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

^{1}H NMR



^{13}C NMR


166.96
152.05
145.54
133.79
133.49
130.19
129.41
128.84
112.63
112.26
87.93
61.75
29.95
22.24
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)