Supporting Information

Catalyst-Free Direct Regiospecific Multicomponent Synthesis of C3-Functionalized Pyrroles

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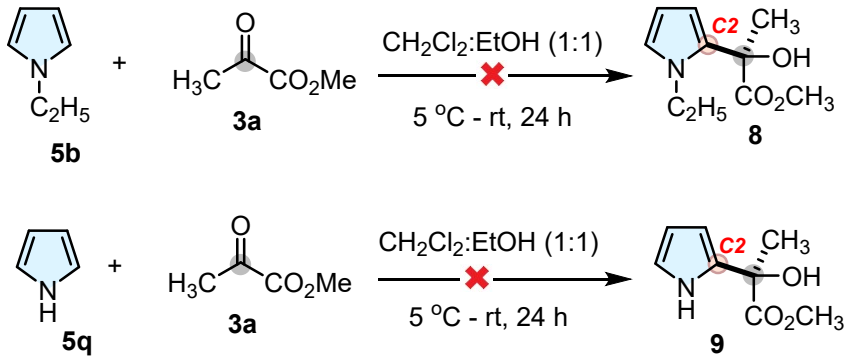
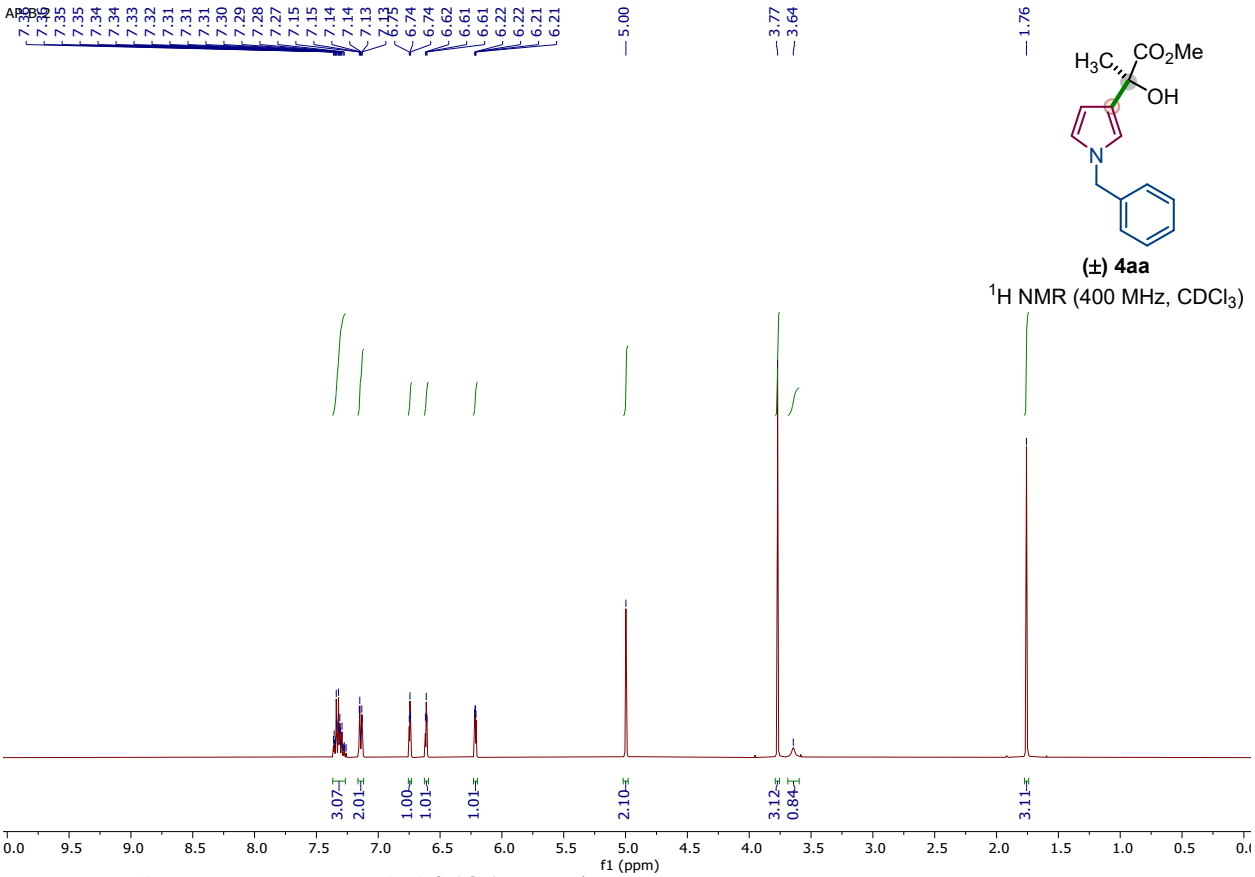
General procedure for the preparation of C3-substituted pyrrole (4/7): An over dried Schlenk tube (25 mL) was charged with succinaldehyde **1** (3.0 M sol, 0.6 mmol, 2.0 equiv.), amine **2** (0.3 mmol, 1.0 equiv.) and reactive carbonyls **3** (0.6 mmol, 2.0 equiv.) in CH_2Cl_2:EtOH (1:1) (3.0 mL) at 5 °C. The combined reaction mixture was stirred at the same temperature and monitored the reaction progress by TLC. Upon completion, solvents were removed under reduced pressure and the reaction was stirred between CH_2Cl_2 (5.0 mL) and water (5.0 mL) for five minutes. The organic layer was separated, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The product **4**/7 (up to 81% yield) was obtained by passing through the silica-gel column by eluting with petroleum ether/EtOAc.

pH-study during the progress of the reaction

(a) Standard buffer solution at 25 °C using digital pH-meter electrode (pH = 4.05)	(b) Succinaldehyde (3.0 M aqueous sol) at 25 °C using digital pH-meter electrode (pH = 2.41)
(c) Zero hour reaction in CH_2Cl_2:EtOH (1.:1) at 25 °C using digital pH-meter electrode (pH = 10.45)	(d) Reaction while completed CH_2Cl_2:EtOH (1.:1) at 25 °C using digital pH-meter electrode (pH = 7.88)

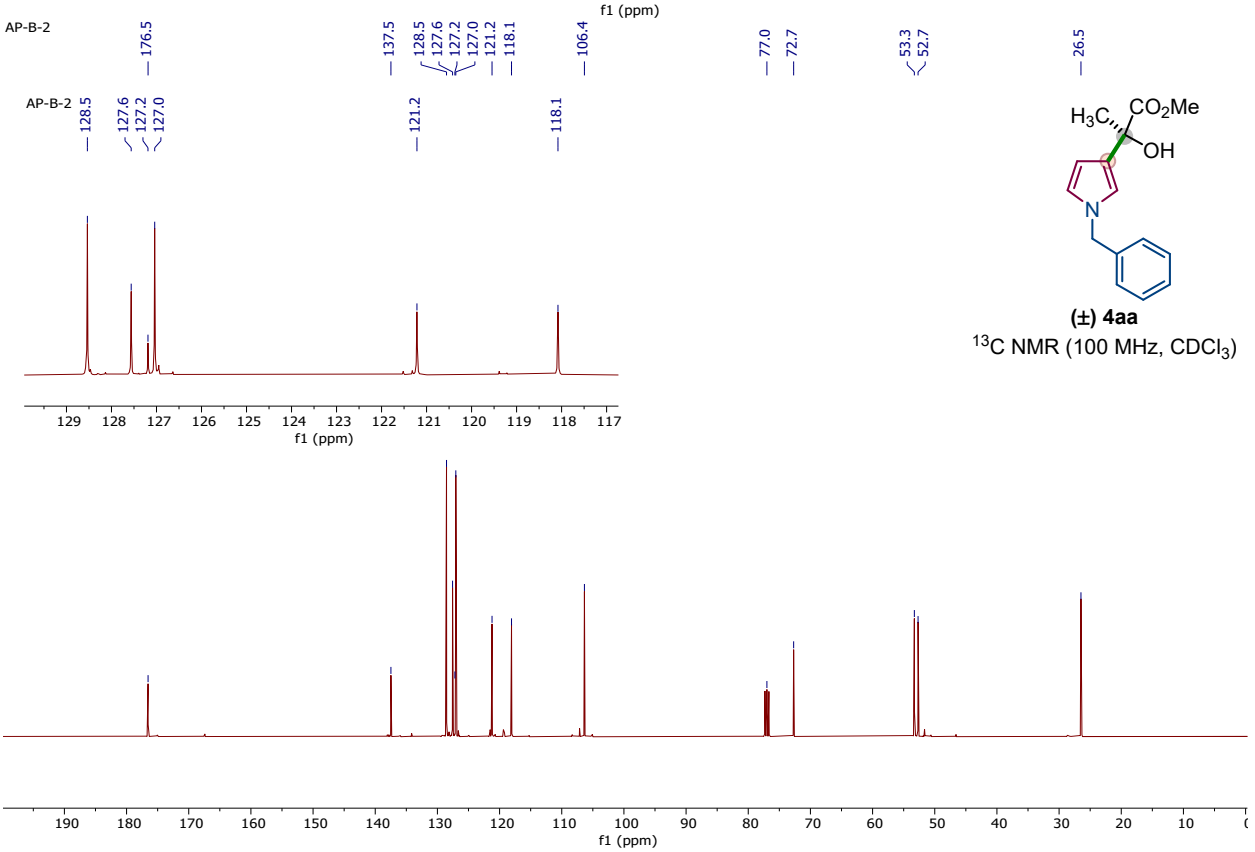
Controlled experiments: The model reaction between methyl pyruvate 3a and preformed N-ethyl pyrrole 5b/ pyrrole 5q: An over dried schlenk tube (25 mL) was charged with methyl pyruvate **3a** (0.3 mmol, 1.0 equiv.) and *N*-ethyl pyrrole **5b** (0.6 mmol, 2.0 equiv.)/pyrrole **5q** (0.6 mmol, 2.0 equiv.) in CH_2Cl_2:EtOH (1:1) (3.0 mL) and stirred initially at 5 °C and later at room temperature. However, no reactions were observed between them even after 24 h.





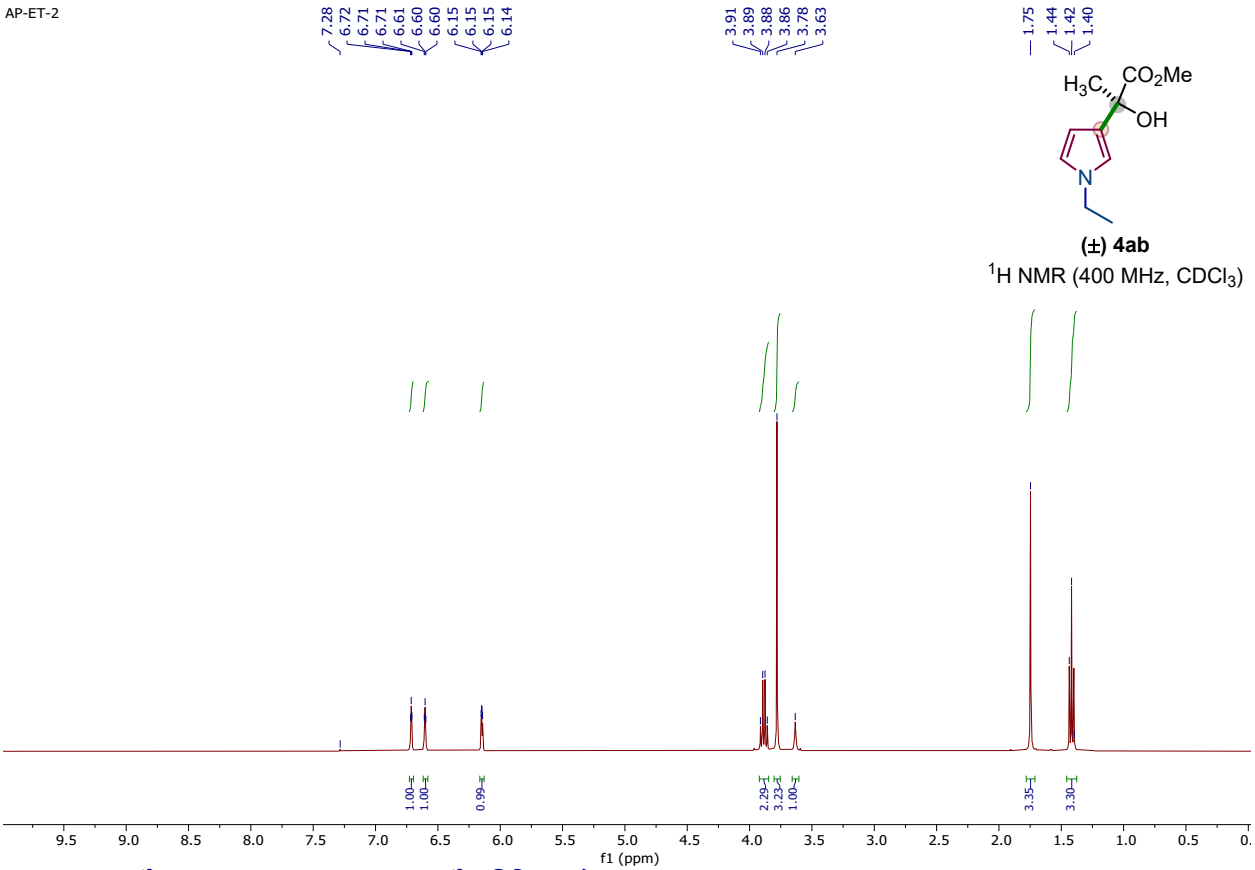
(±) 4aa

^{1}H NMR (400 MHz, $CDCl_3$)



(±) 4aa

^{13}C NMR (100 MHz, $CDCl_3$)



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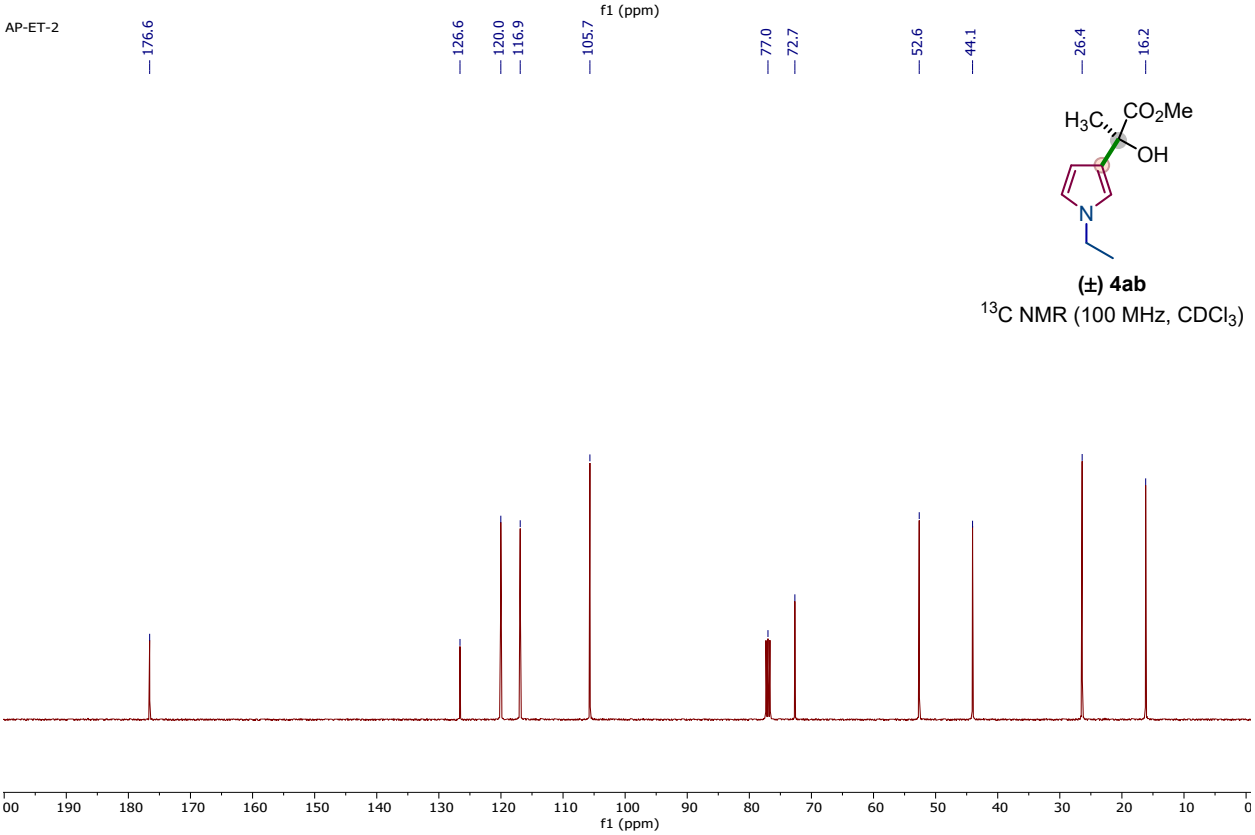

(±) 4ab

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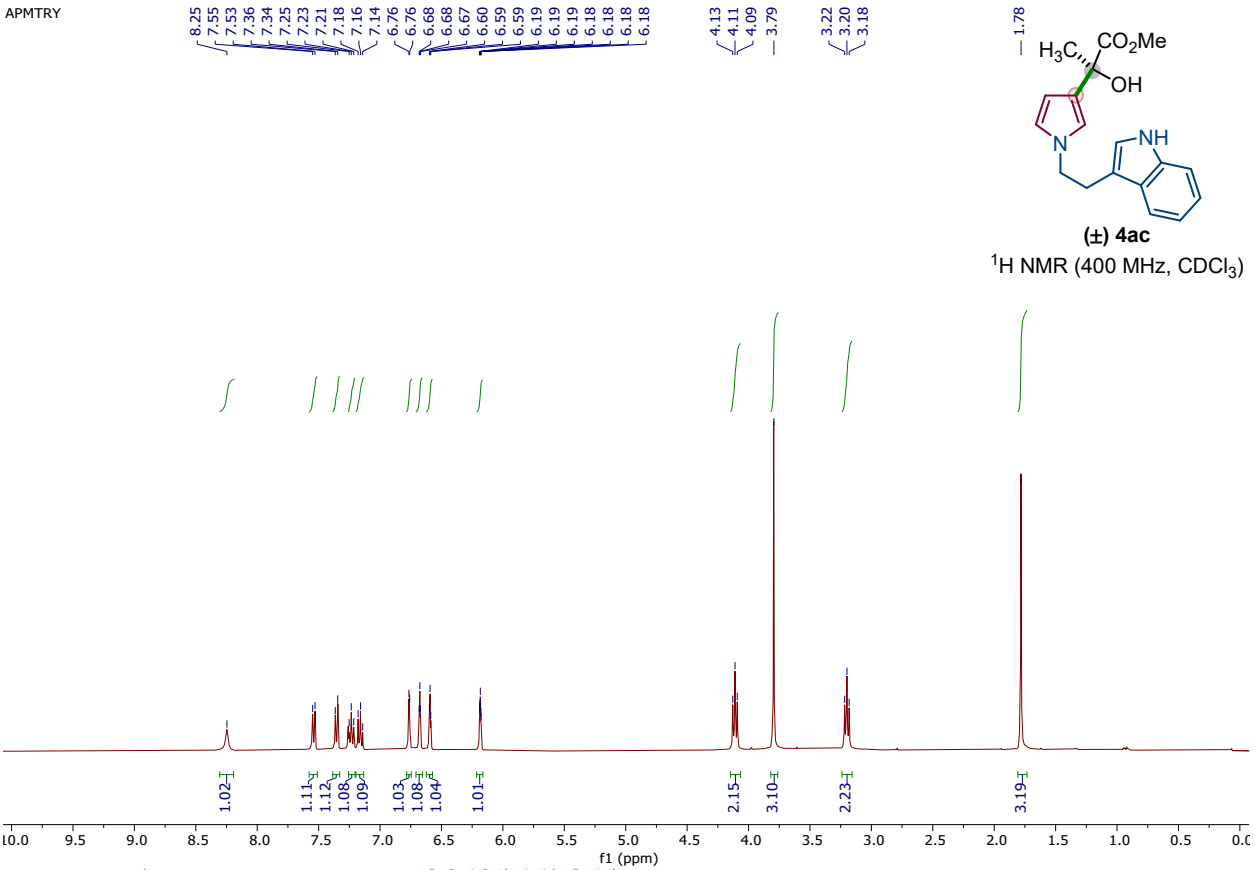

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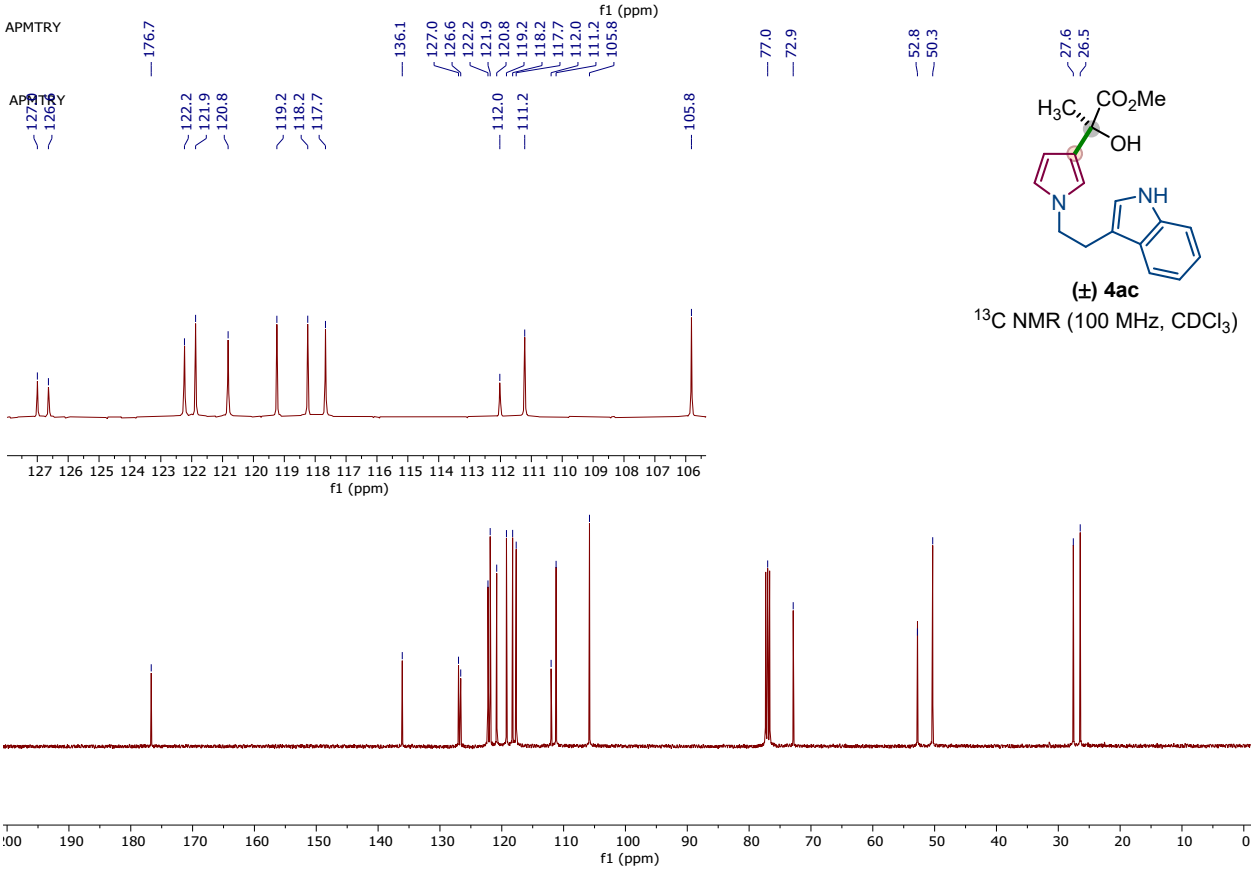

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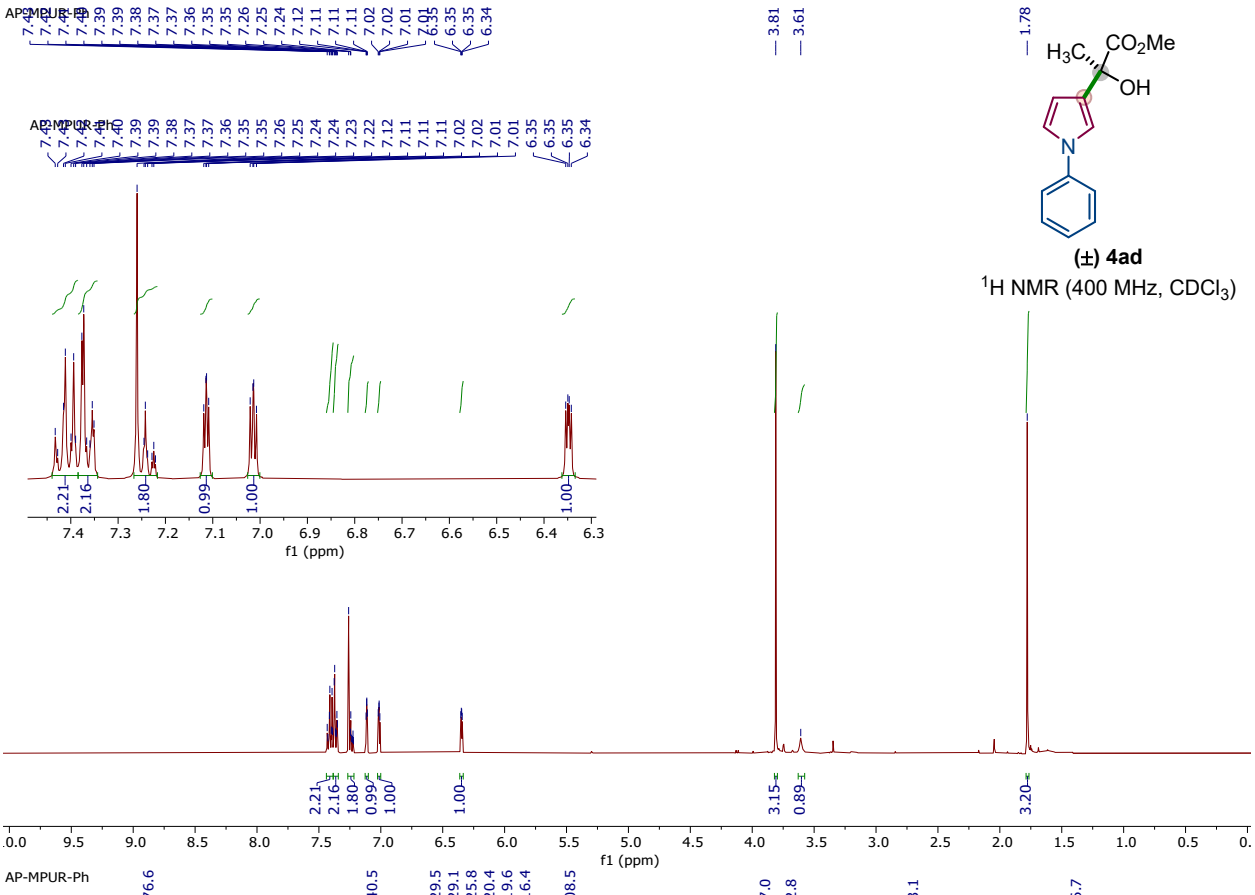
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1.78
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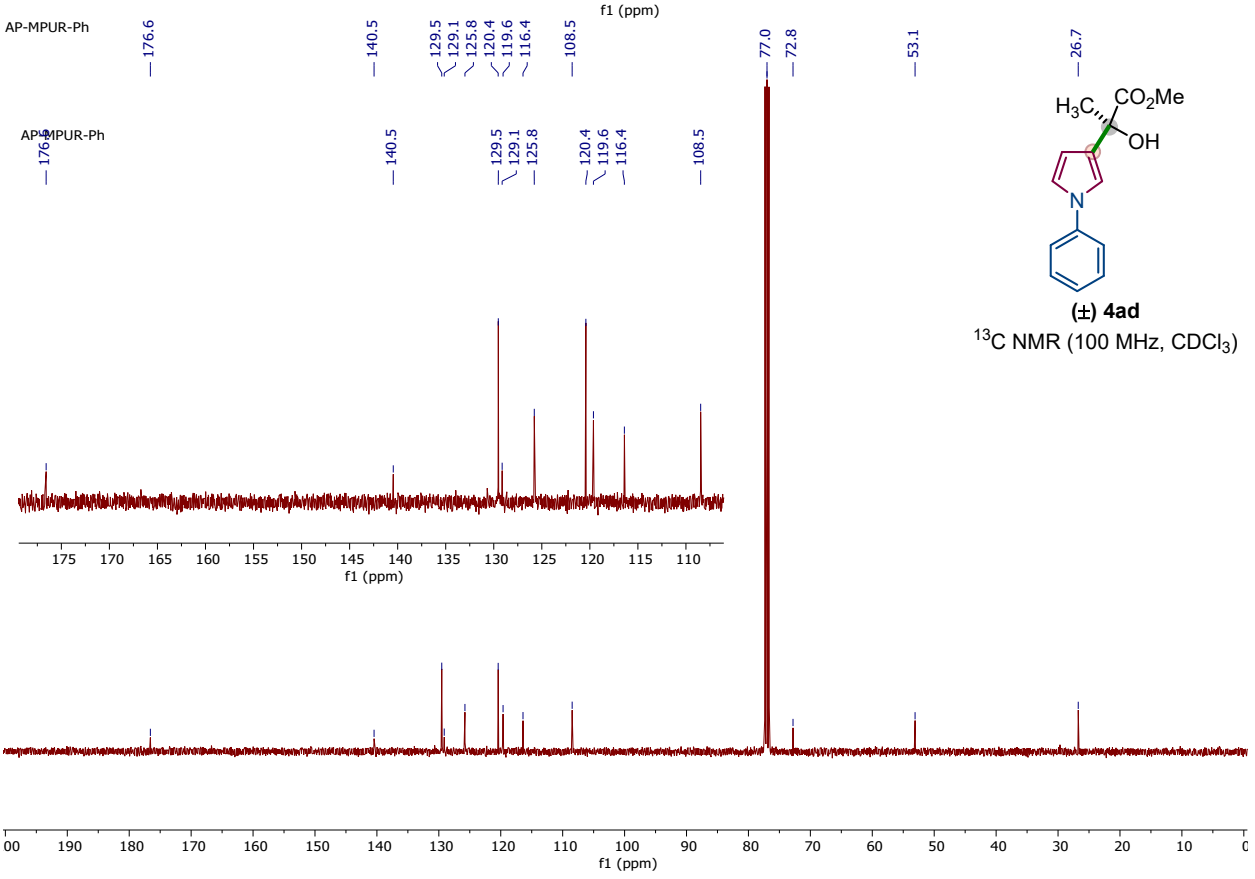
CO2Me
OH
N
(±) 4ad
1H NMR (400 MHz, CDCl3)
f1 (ppm)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140.5
129.5
129.1
125.8
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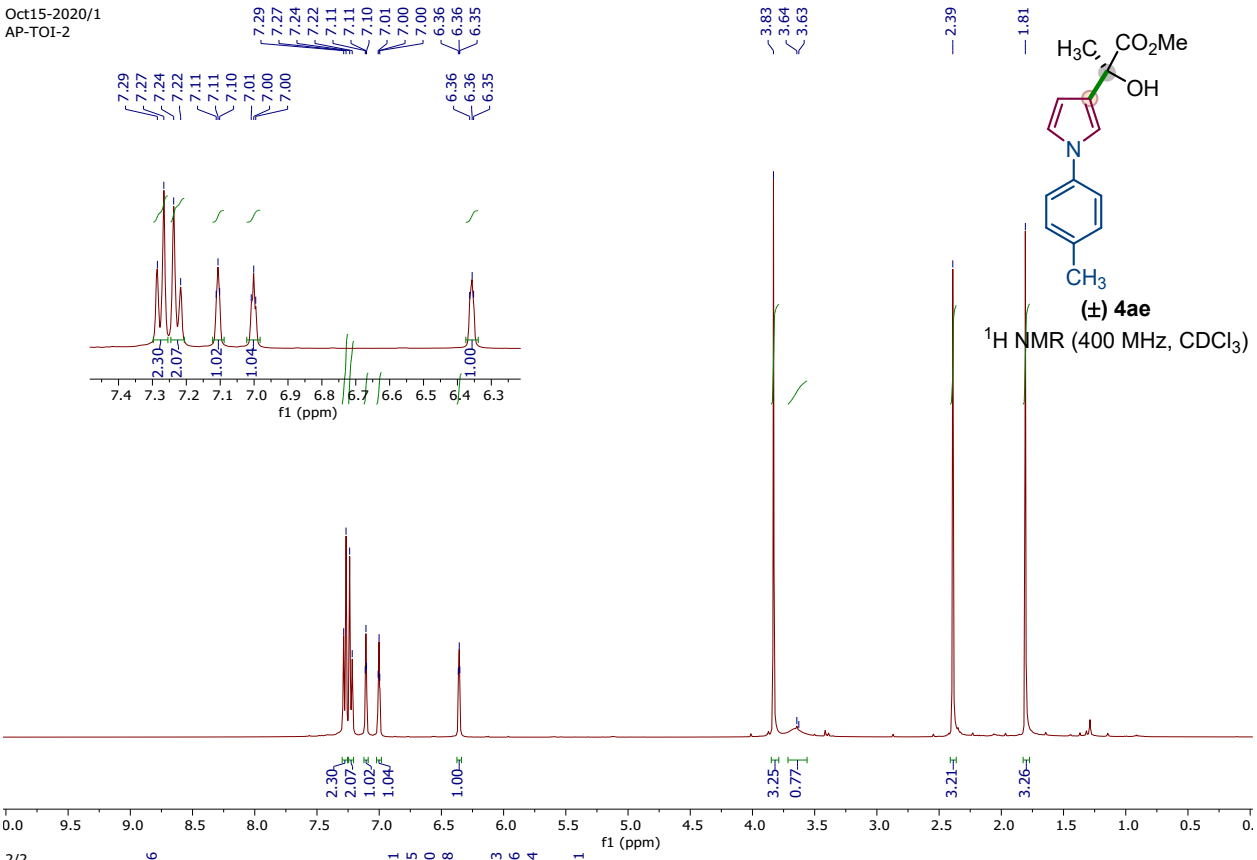
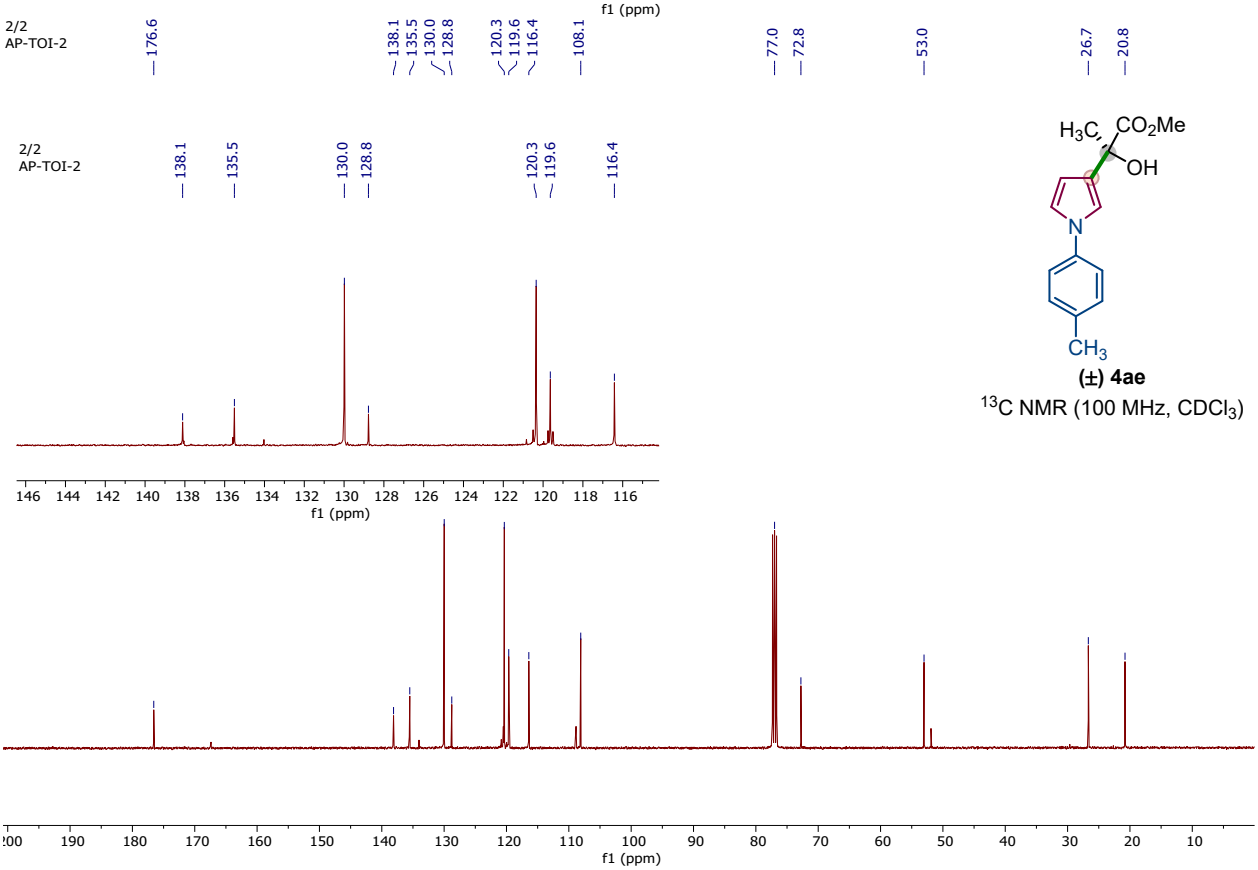
119.6
116.4
108.5
77.0
72.8
53.1
26.7
H3C
CO2Me
OH
N
(±) 4ad
13C NMR (100 MHz, CDCl3)
f1 (ppm)



(±) 4ae

^{1}H NMR (400 MHz, $CDCl_3$)



(±) 4ae

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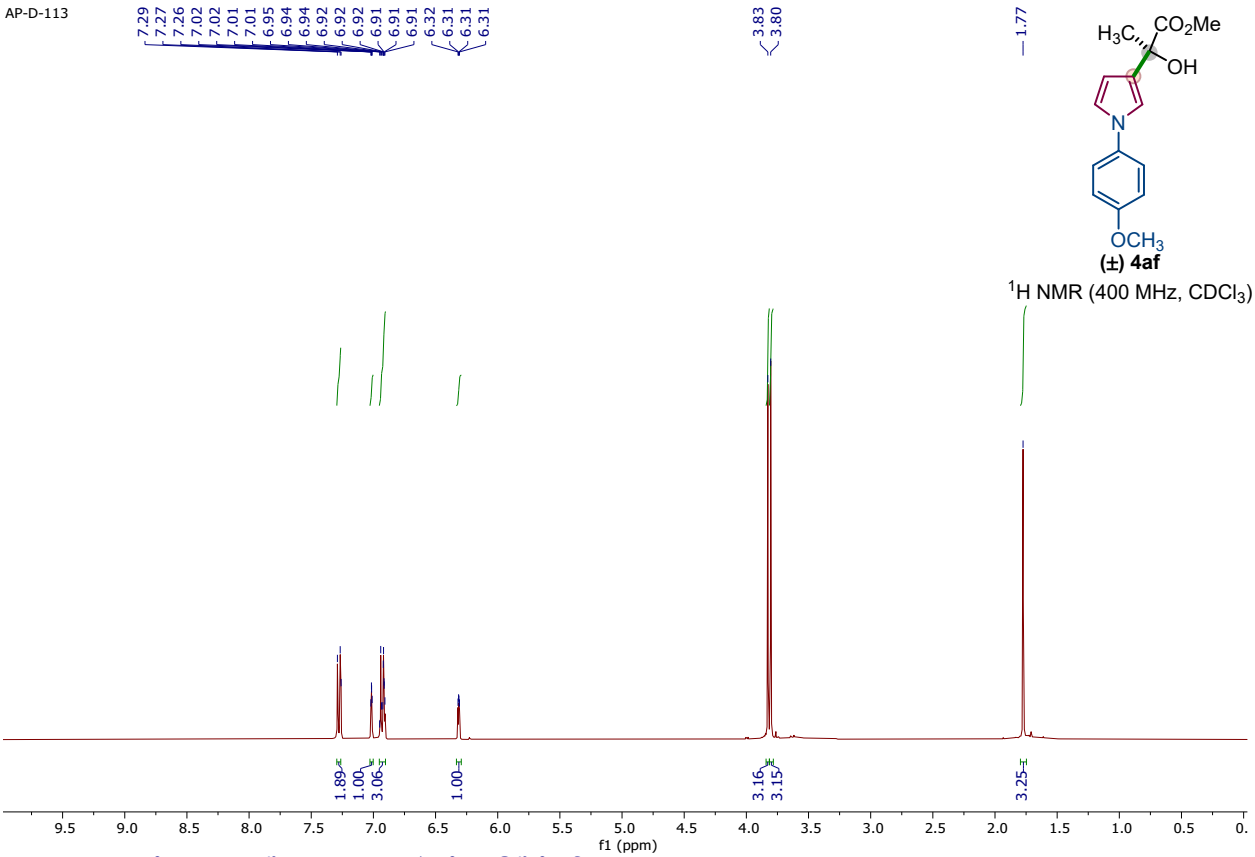

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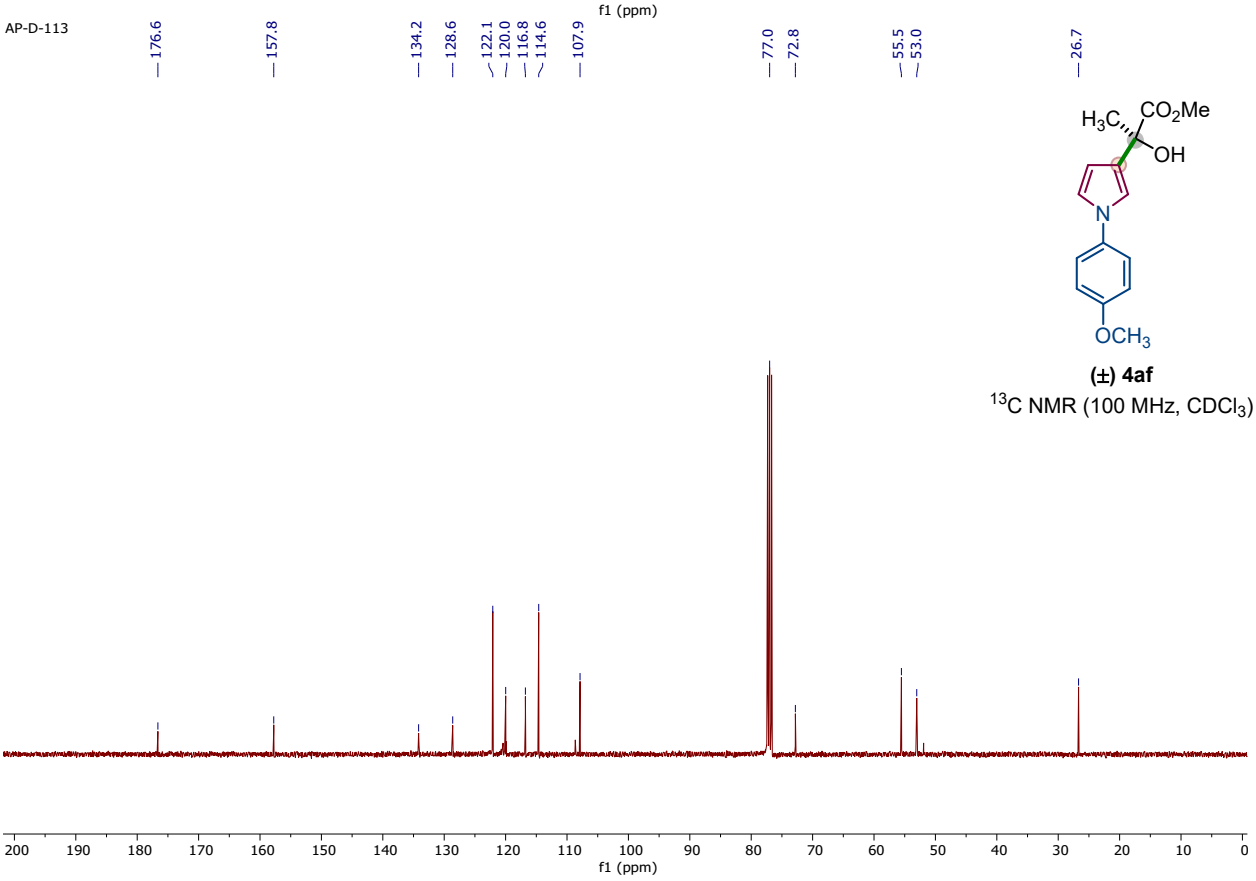

(±) 4af

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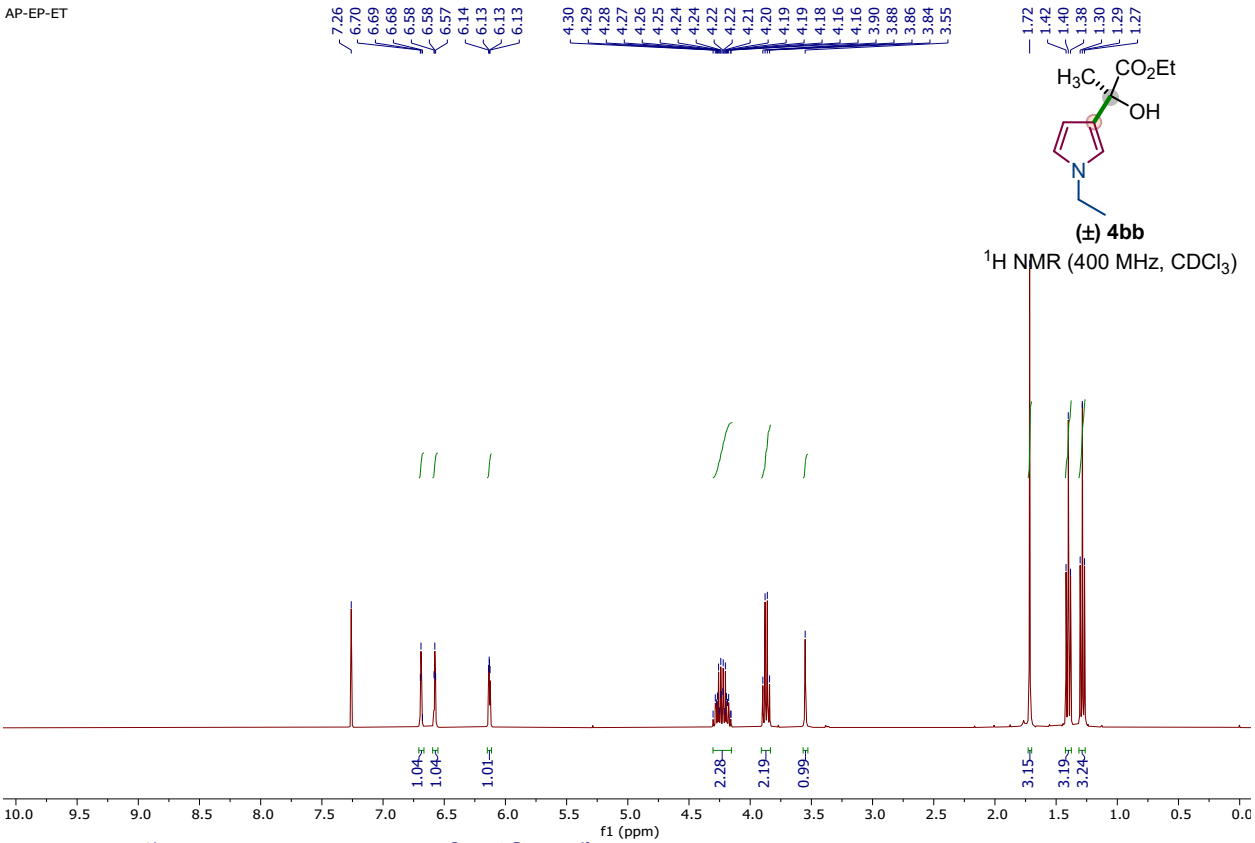

(±) 4bb

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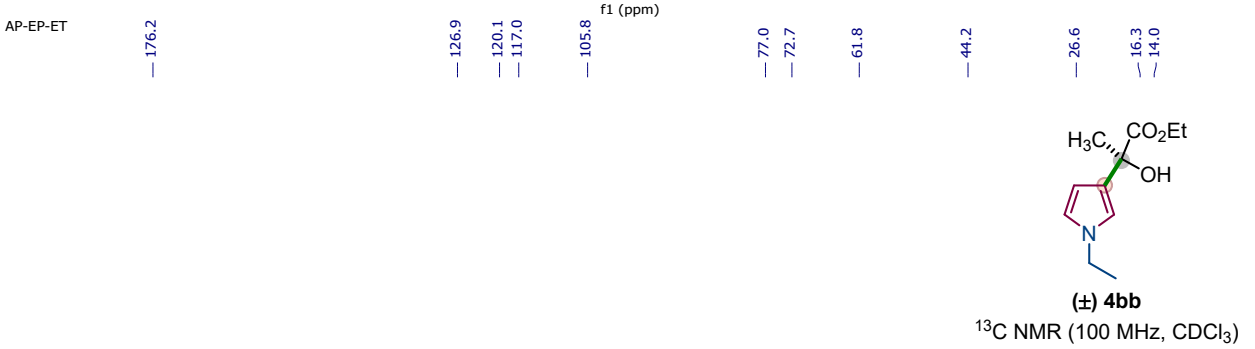
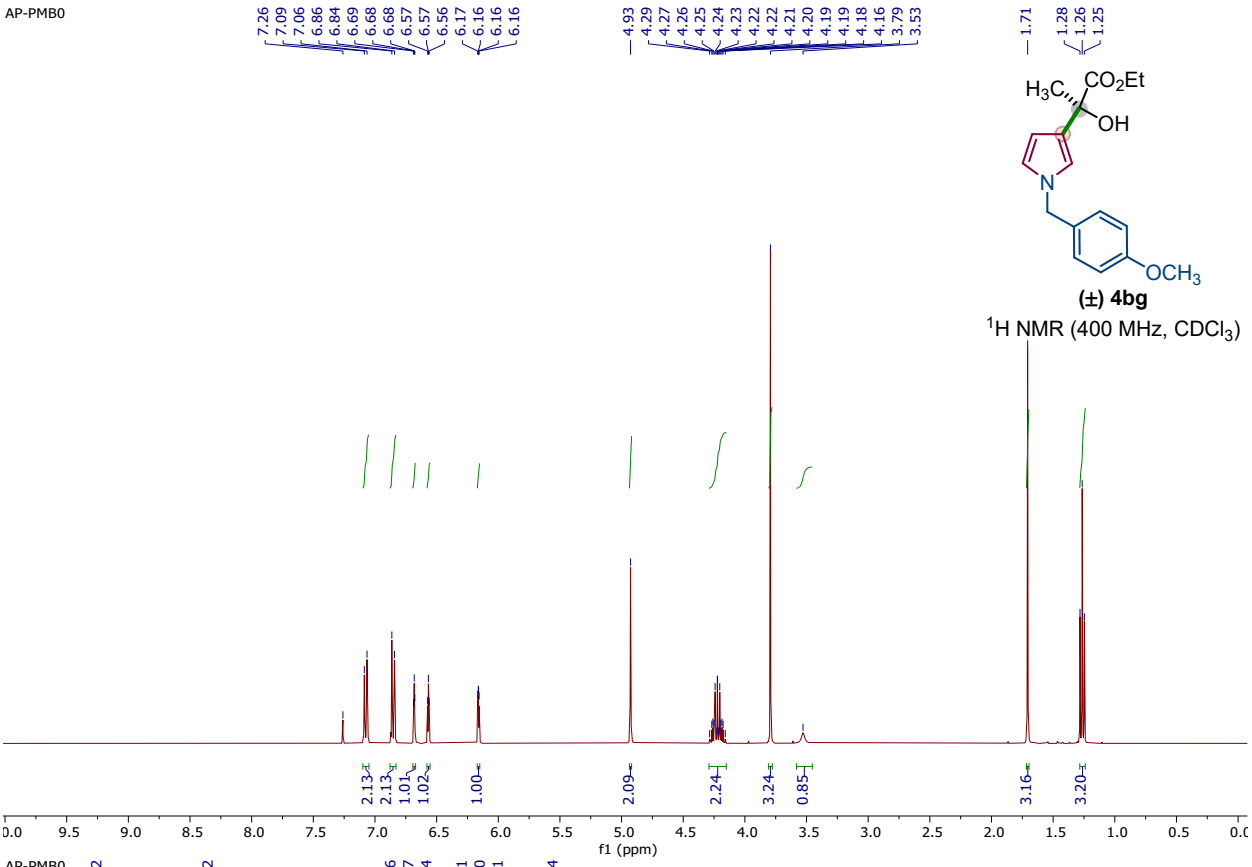


(±) 4bb

^{13}C NMR (100 MHz, $CDCl_3$)



(±) 4bg

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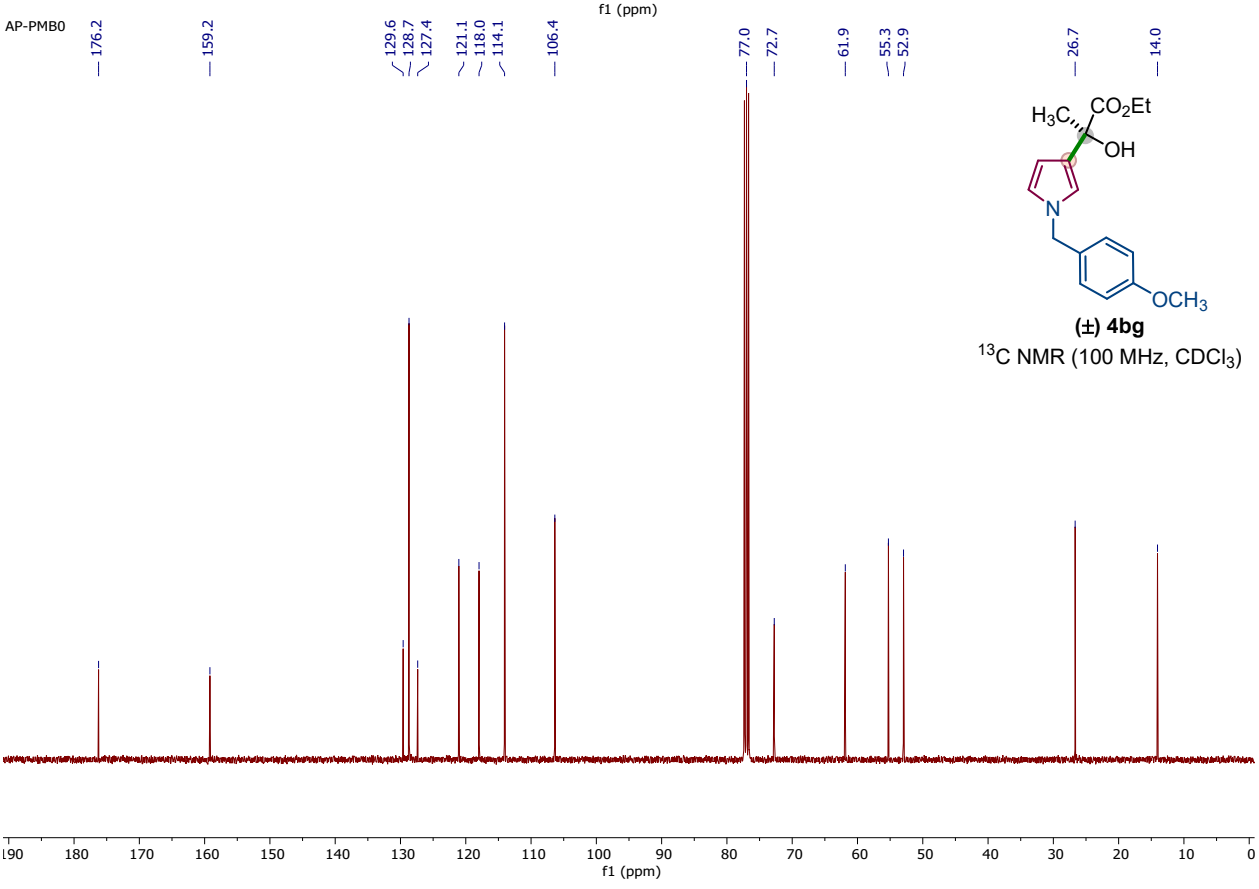

(±) 4bg

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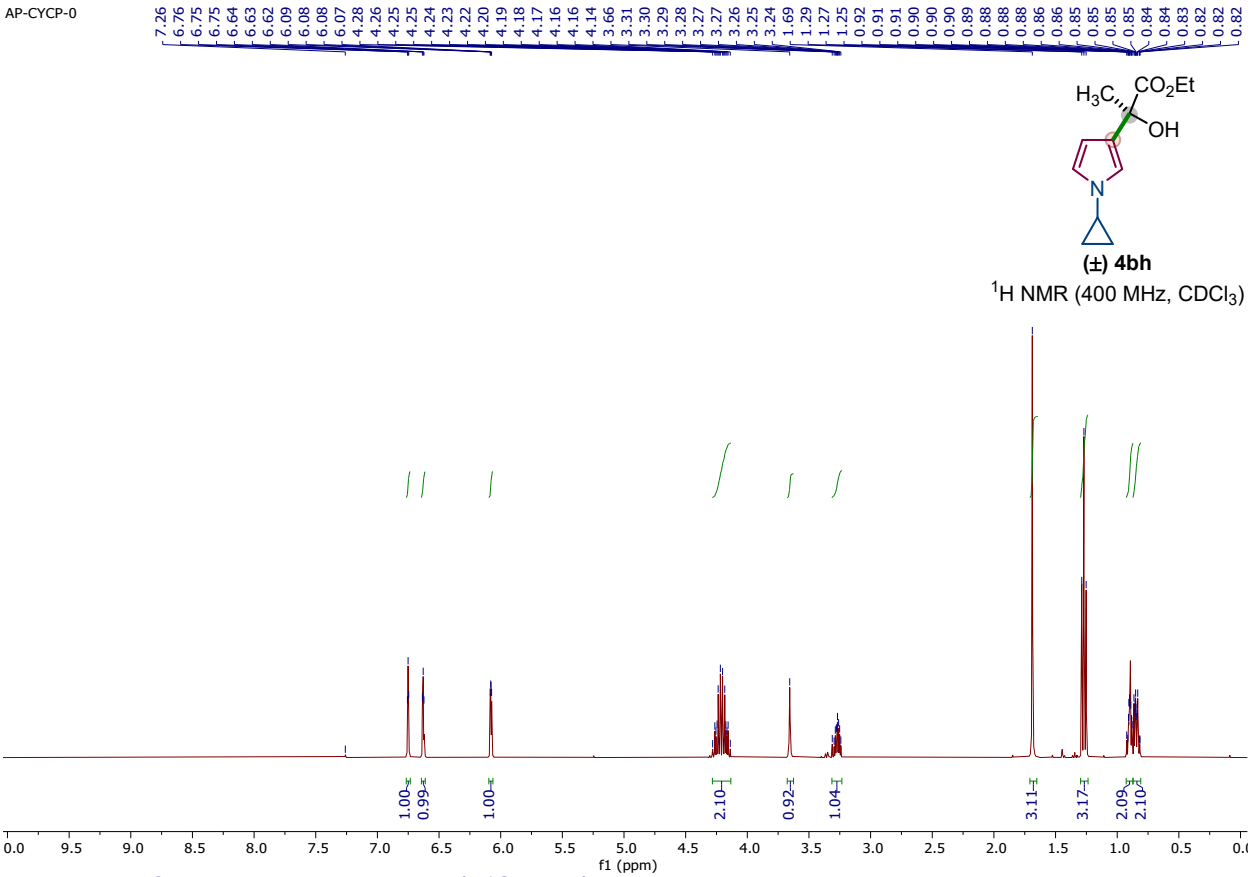
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H3C
CO2Et
OH
N
(±) 4bh
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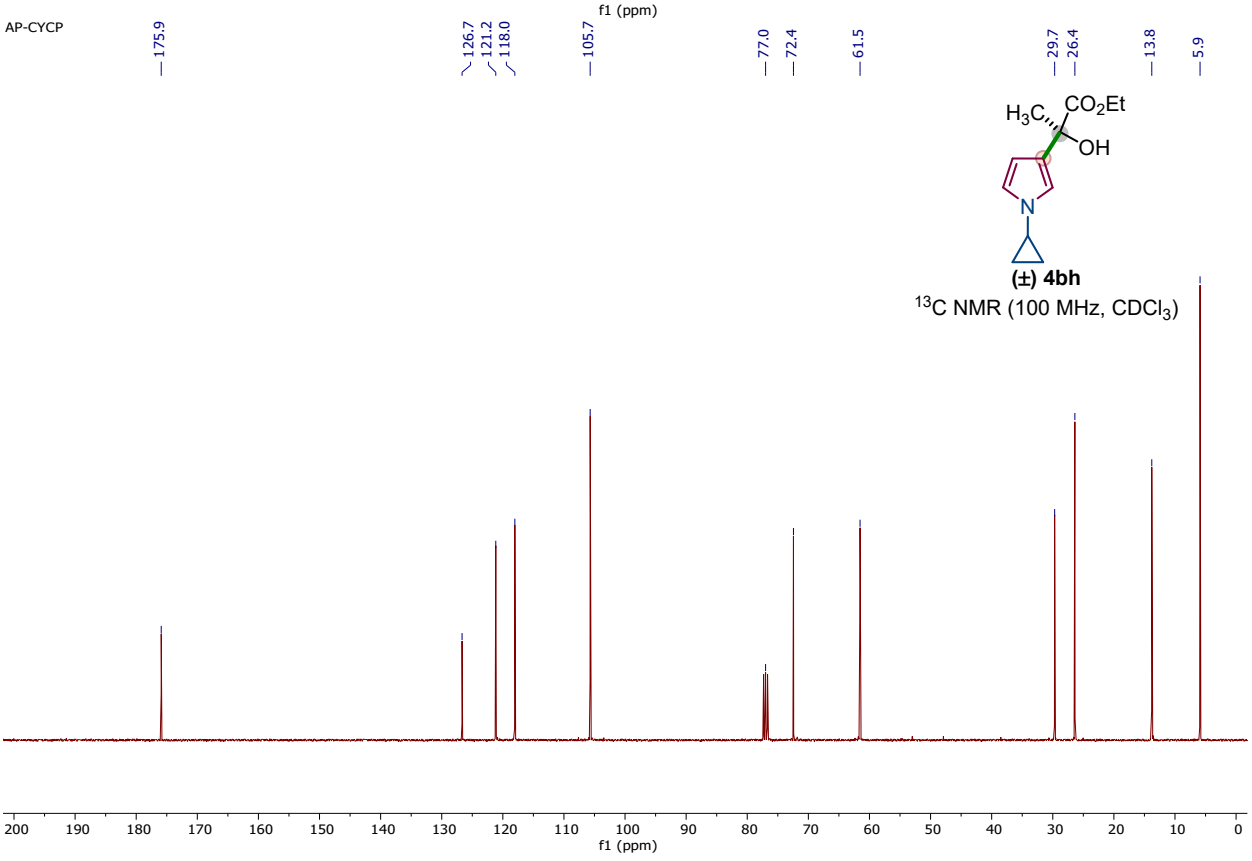
1.00 0.99 1.00 2.10 0.92 1.04 3.11 3.17 2.09 2.10
f1 (ppm)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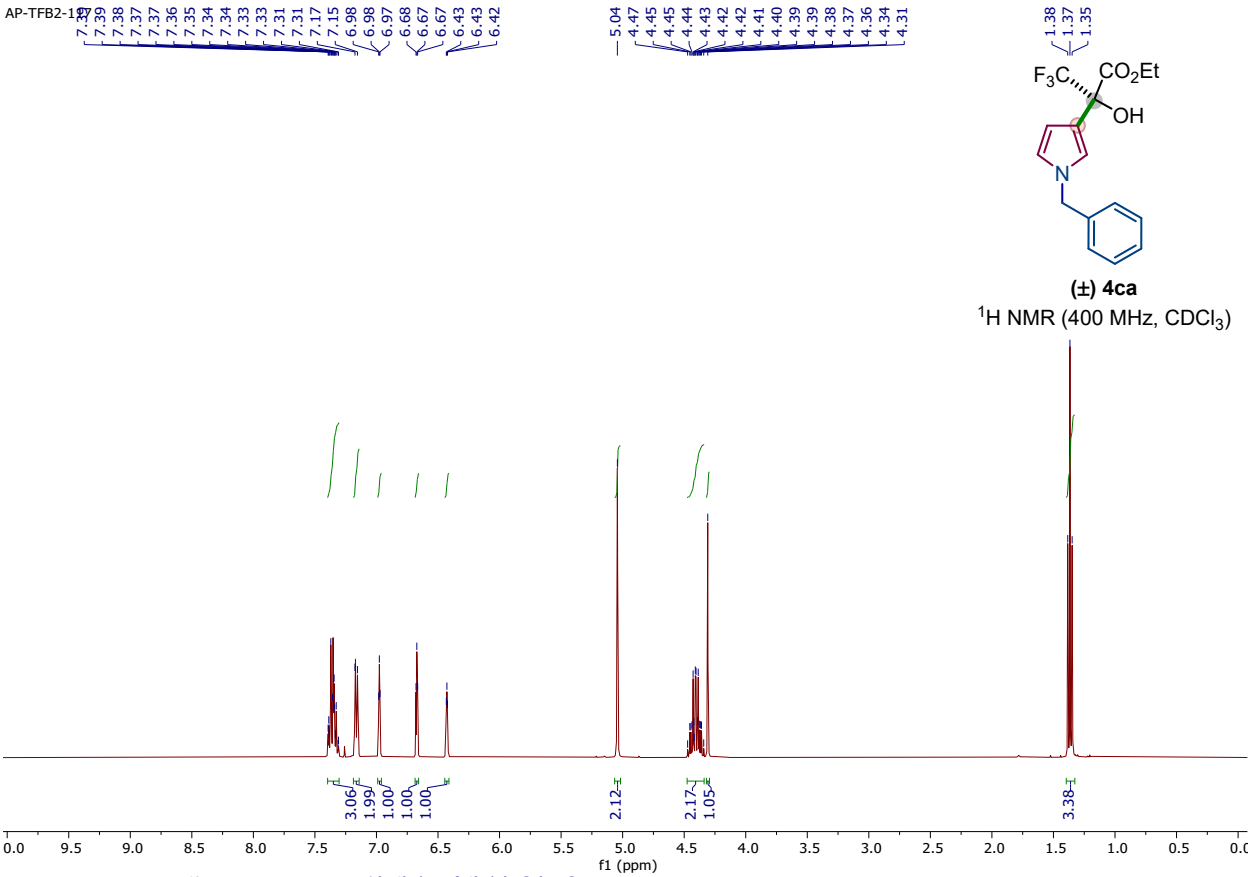
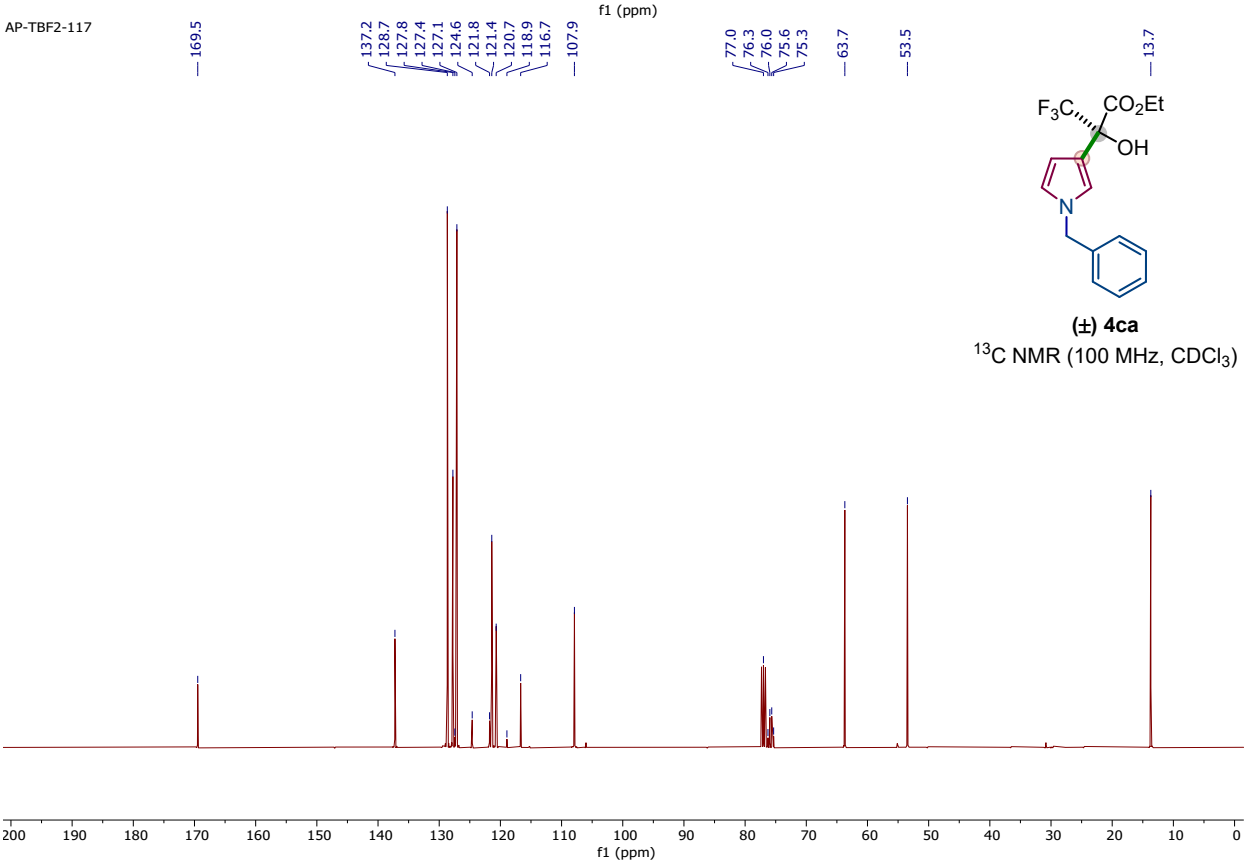
175.9 126.7 121.2 118.0 105.7 77.0 72.4 61.5 29.7 26.4 13.8 5.9
H3C
CO2Et
OH
N
(±) 4bh
13C NMR (100 MHz, CDCl3)
f1 (ppm)



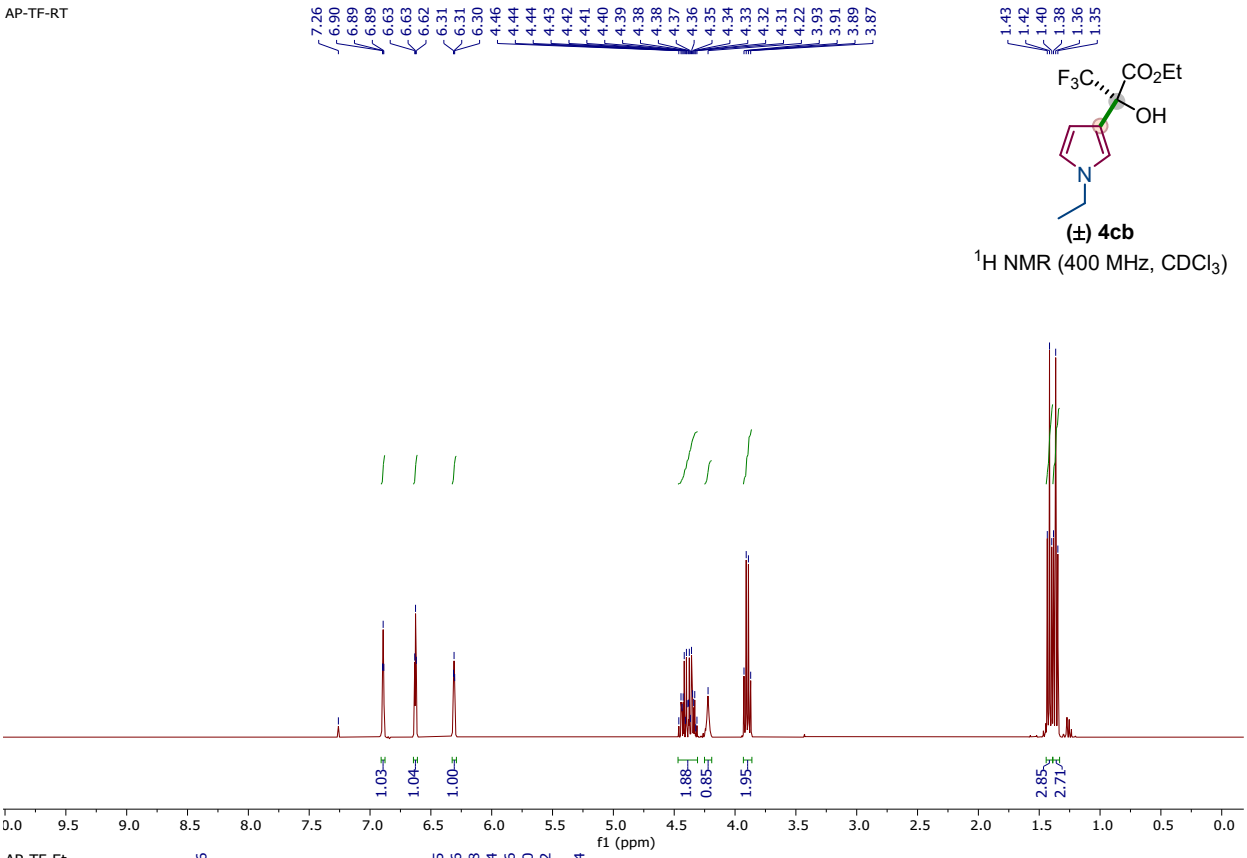
(±) 4ca

^{1}H NMR (400 MHz, $CDCl_3$)



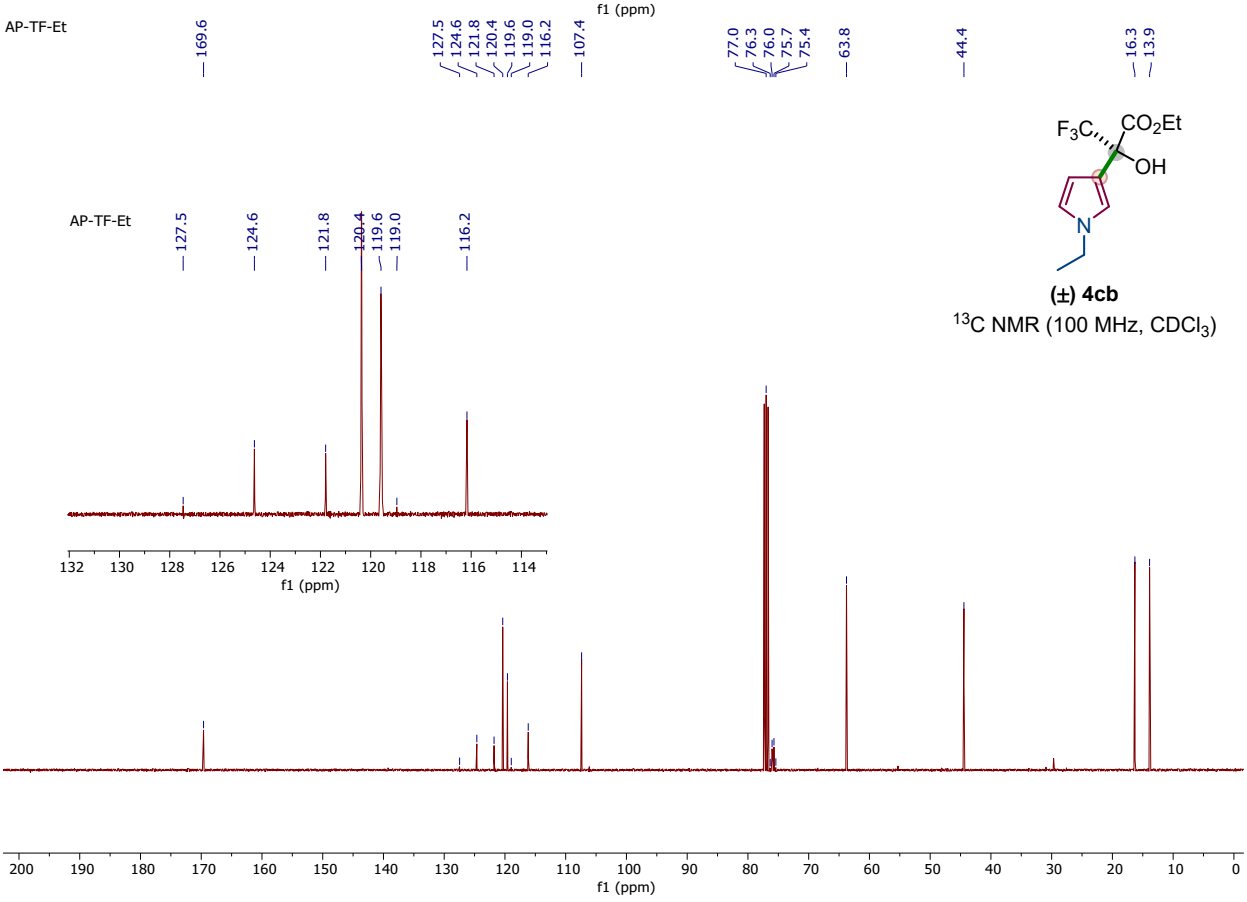
(±) 4ca

^{13}C NMR (100 MHz, $CDCl_3$)



(±) 4cb

^{1}H NMR (400 MHz, $CDCl_3$)



(±) 4cb

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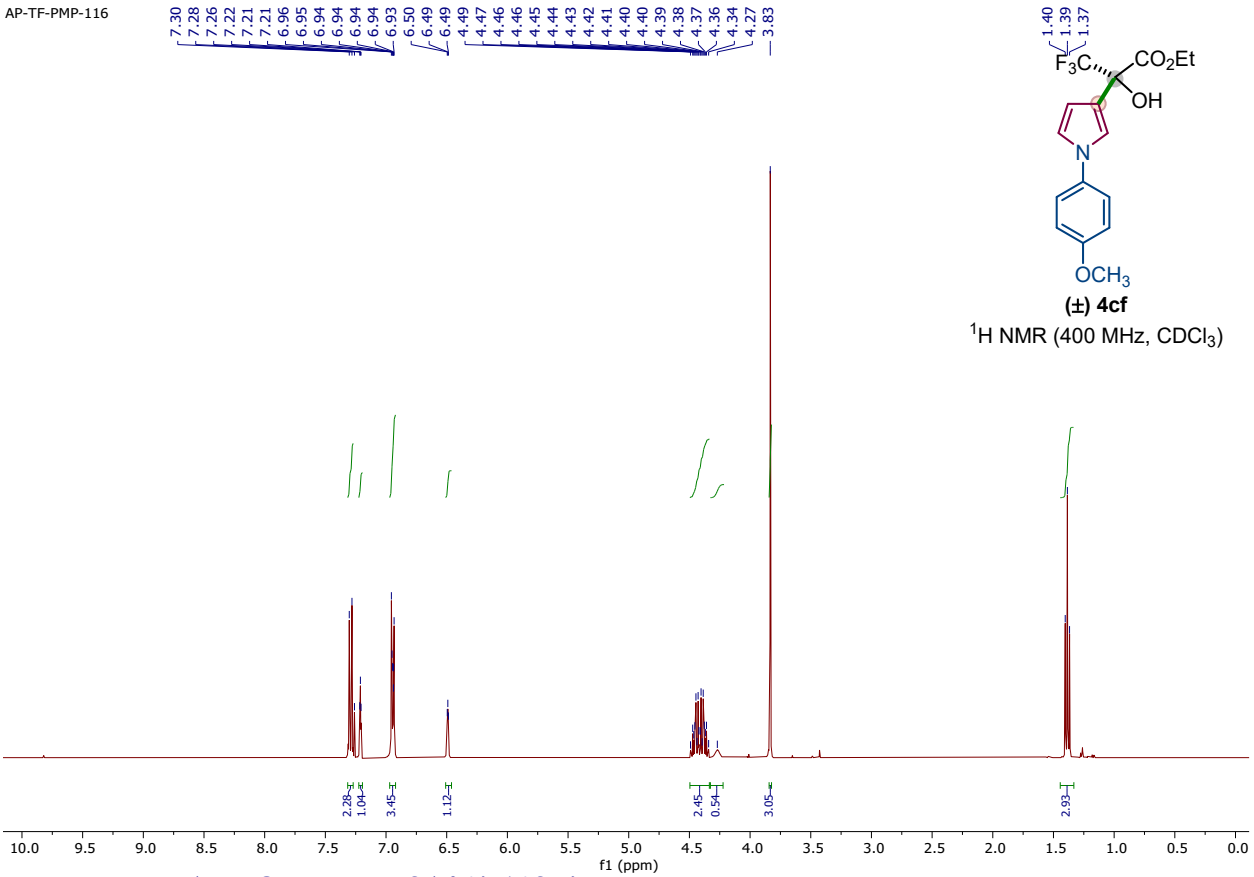

(±) 4cf

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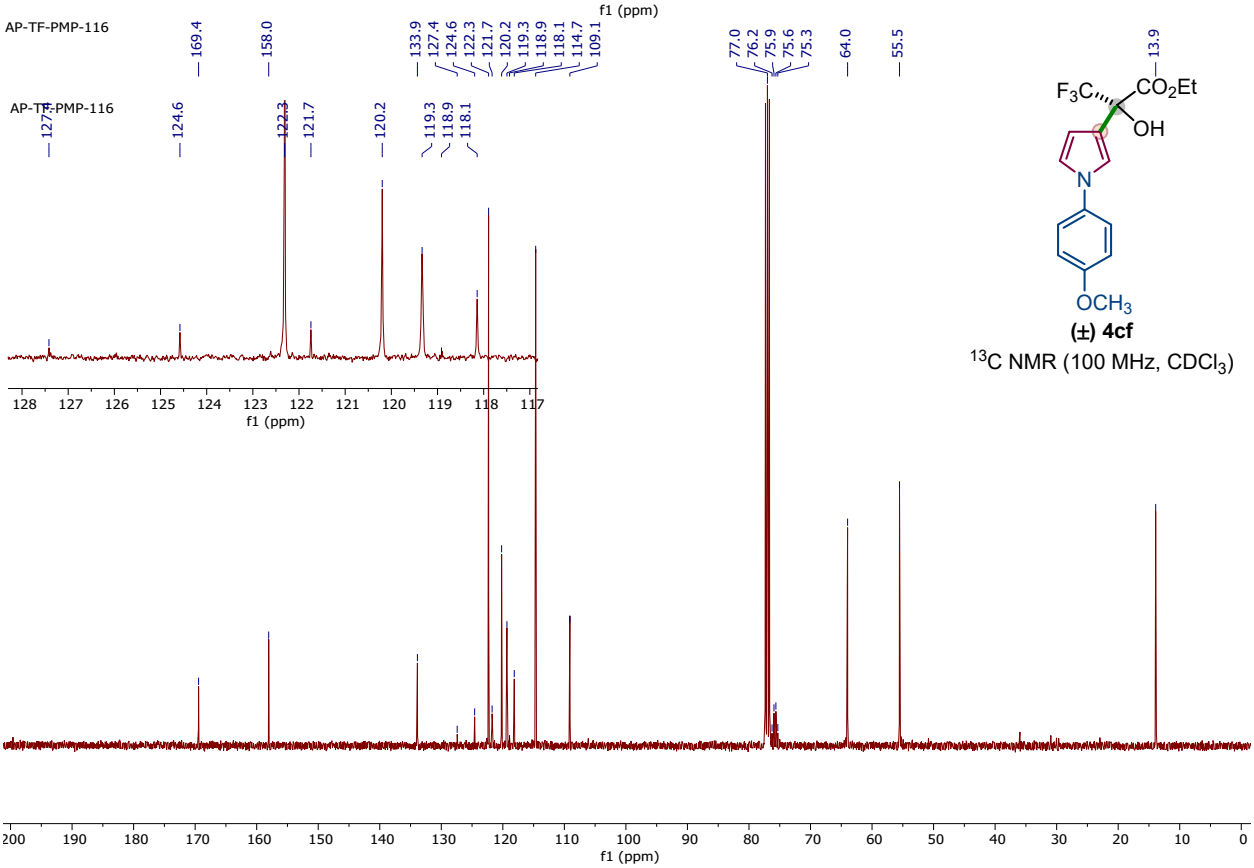

(±) 4cf

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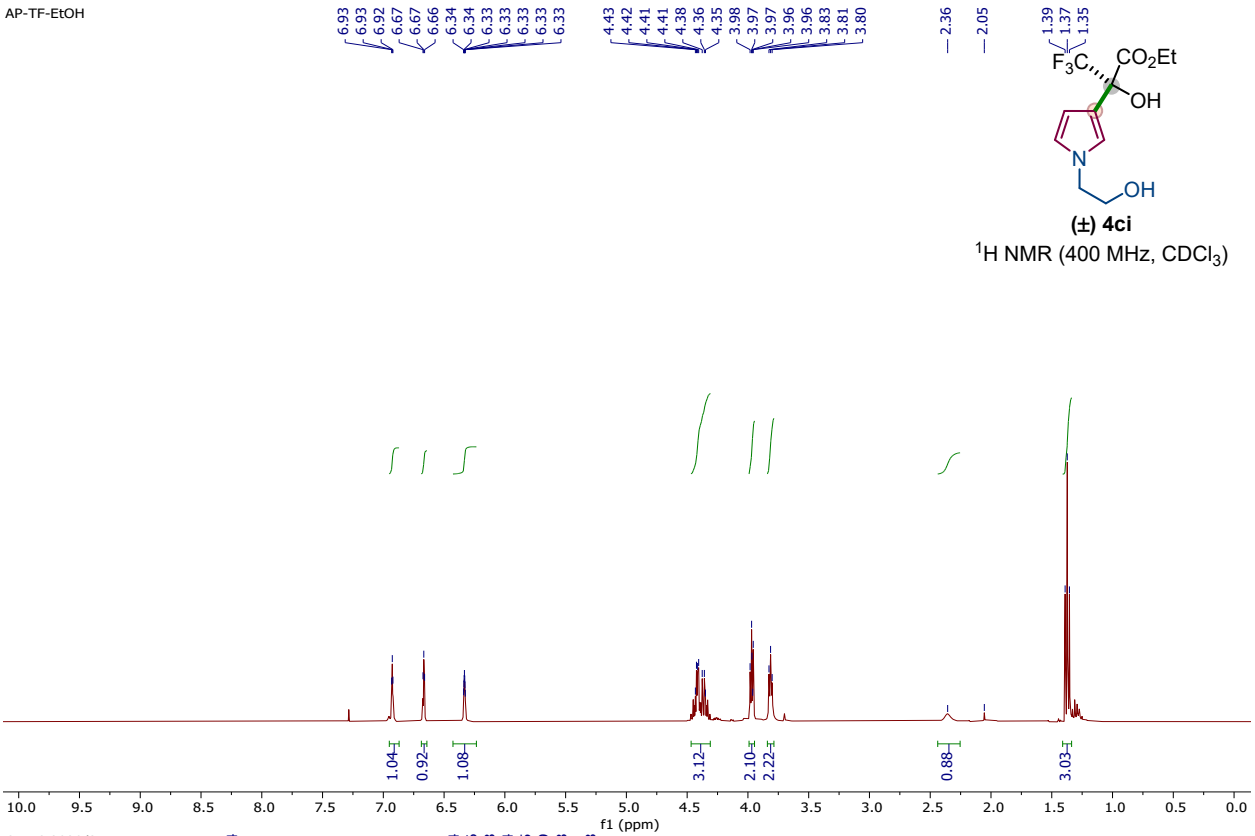

(±) 4ci

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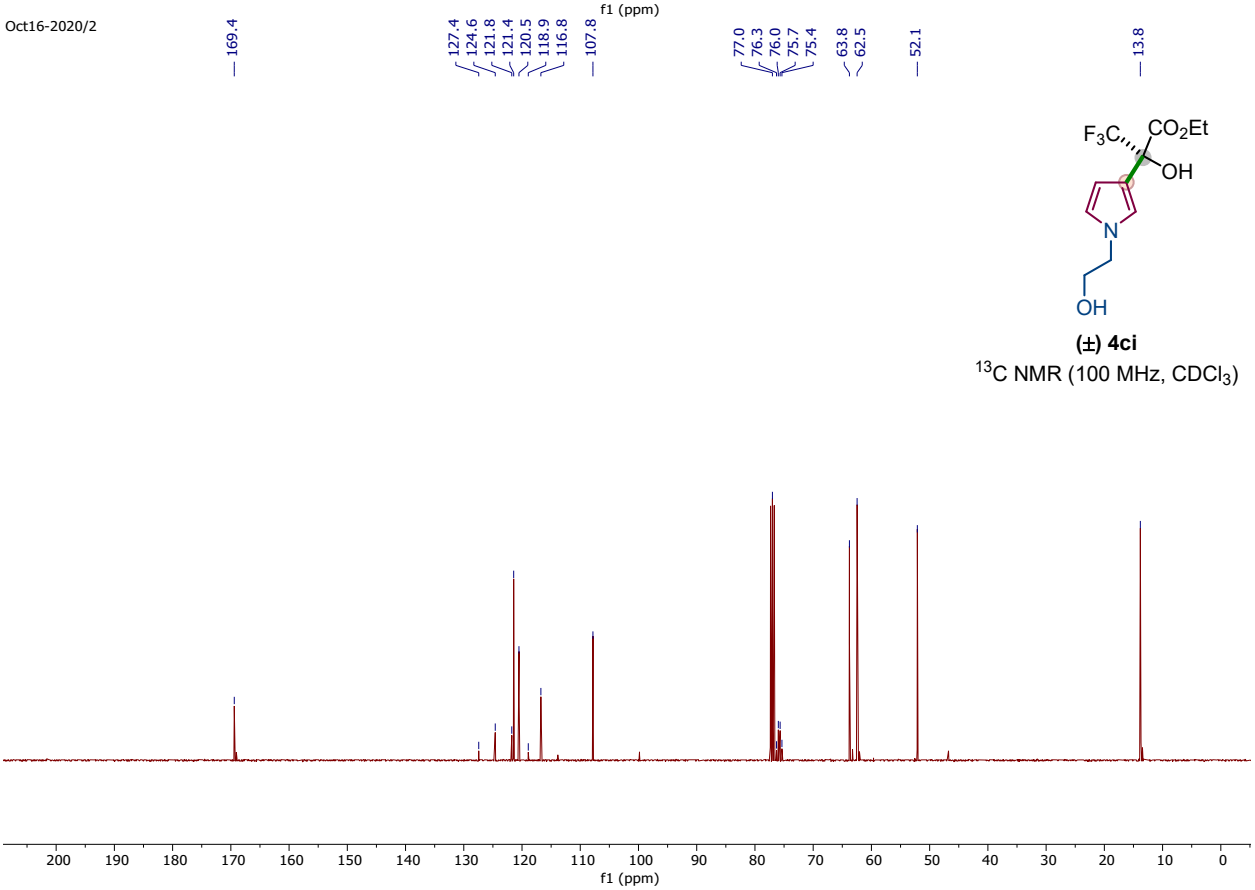

(±) 4ci

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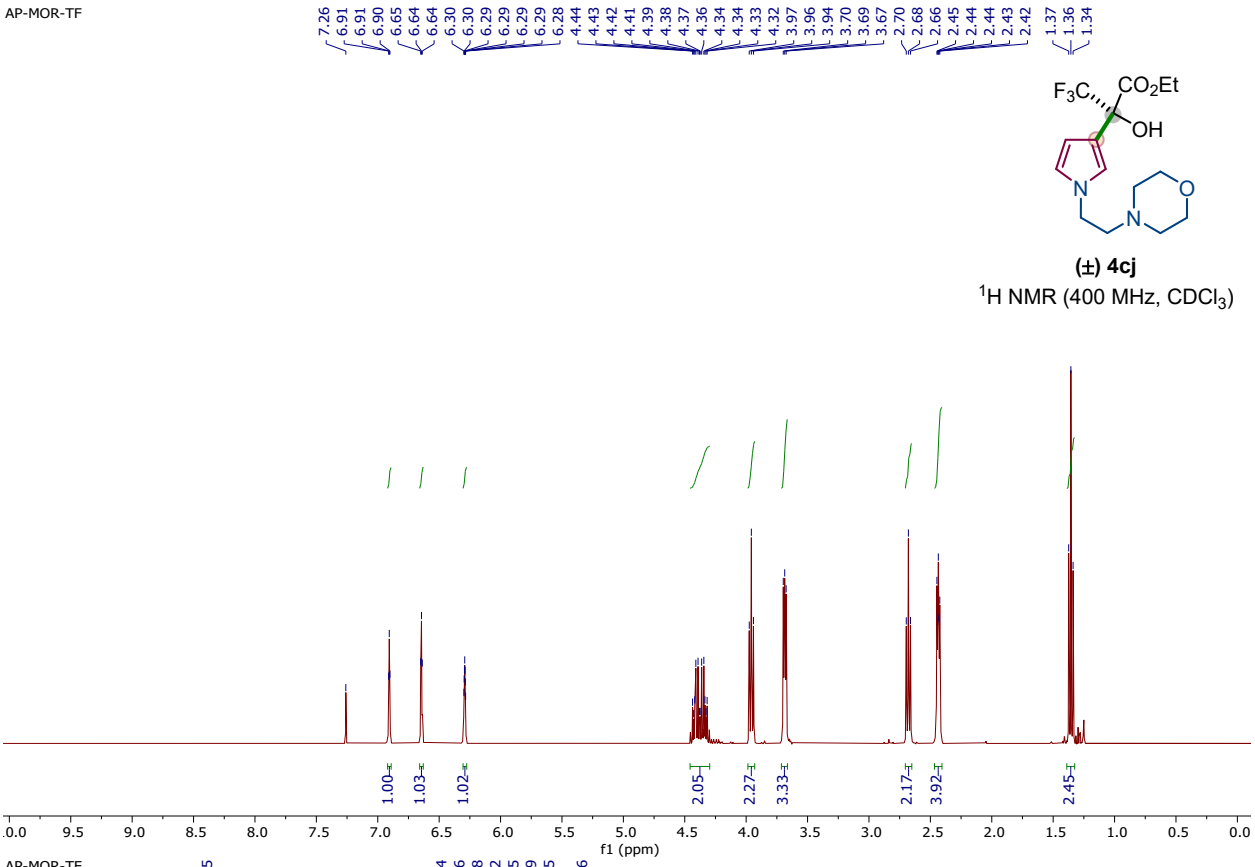
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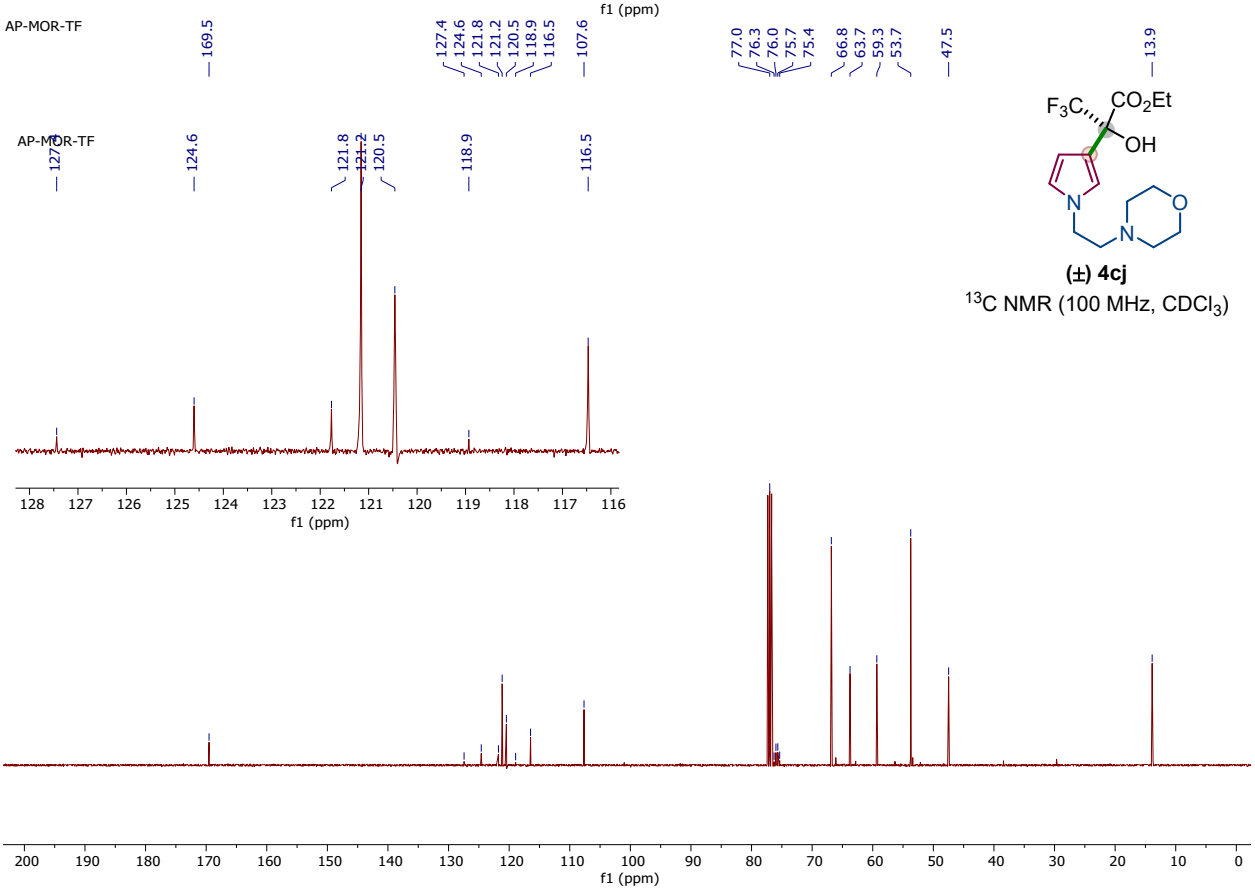
F3C CO2Et OH N O N
(±) 4cj
1H NMR (400 MHz, CDCl3)
1.00 1.03 1.02 2.05 2.27 3.33 2.17 3.92 2.45
f1 (ppm)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F3C CO2Et OH N O N
(±) 4cj
13C NMR (100 MHz, CDCl3)
AP-MOR-TF
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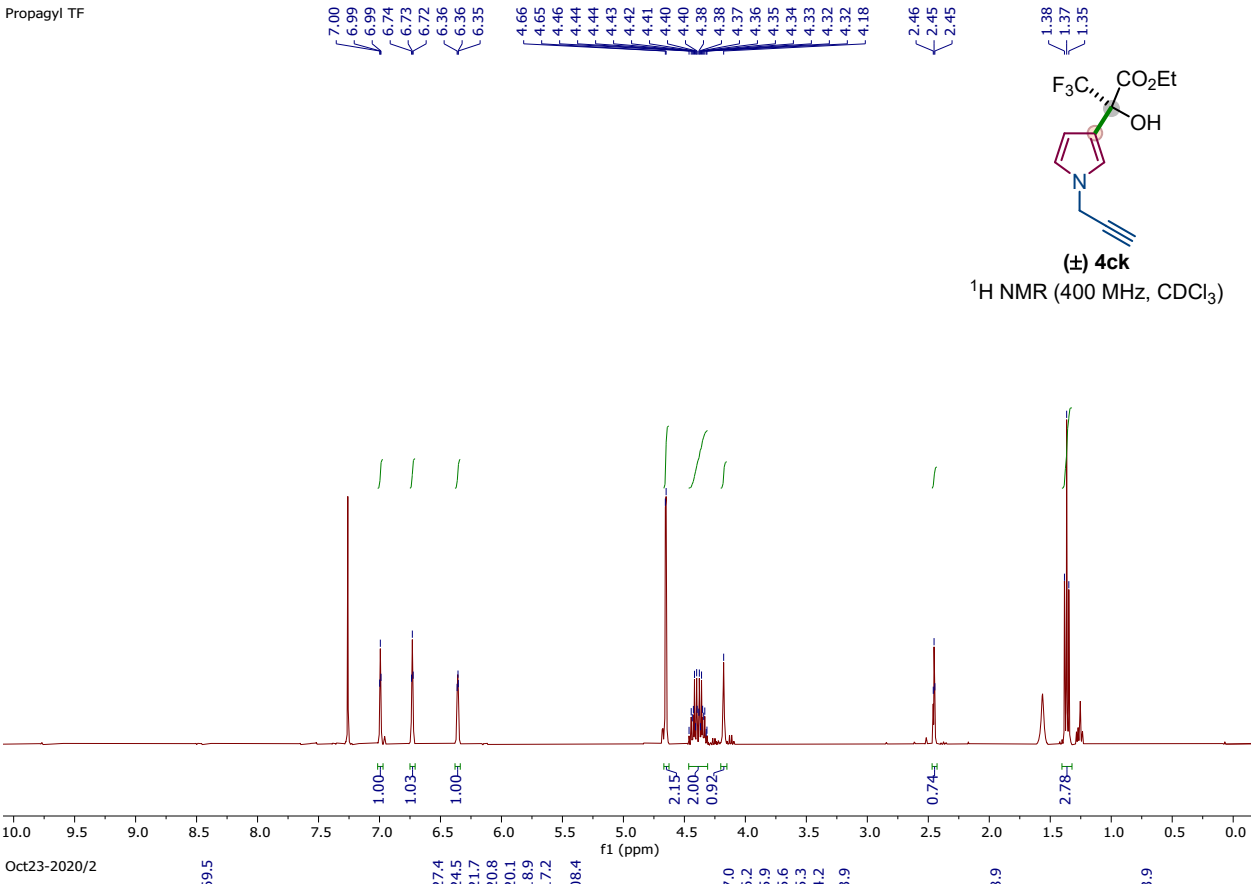
f1 (ppm)
f1 (ppm)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2.46 2.45 2.45
1.38 1.37 1.35
F3C CO2Et OH N
(±) 4ck
1H NMR (400 MHz, CDCl3)
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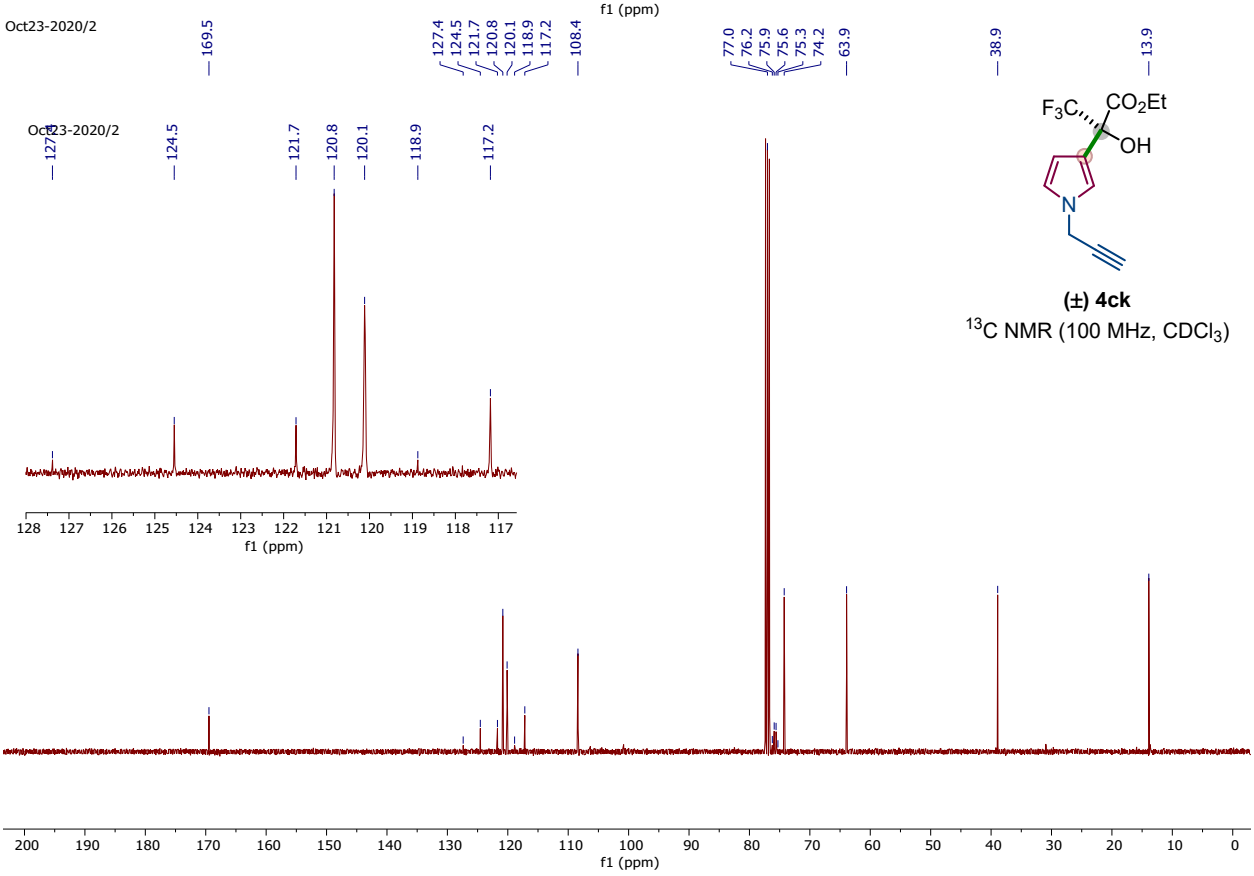
f1 (ppm)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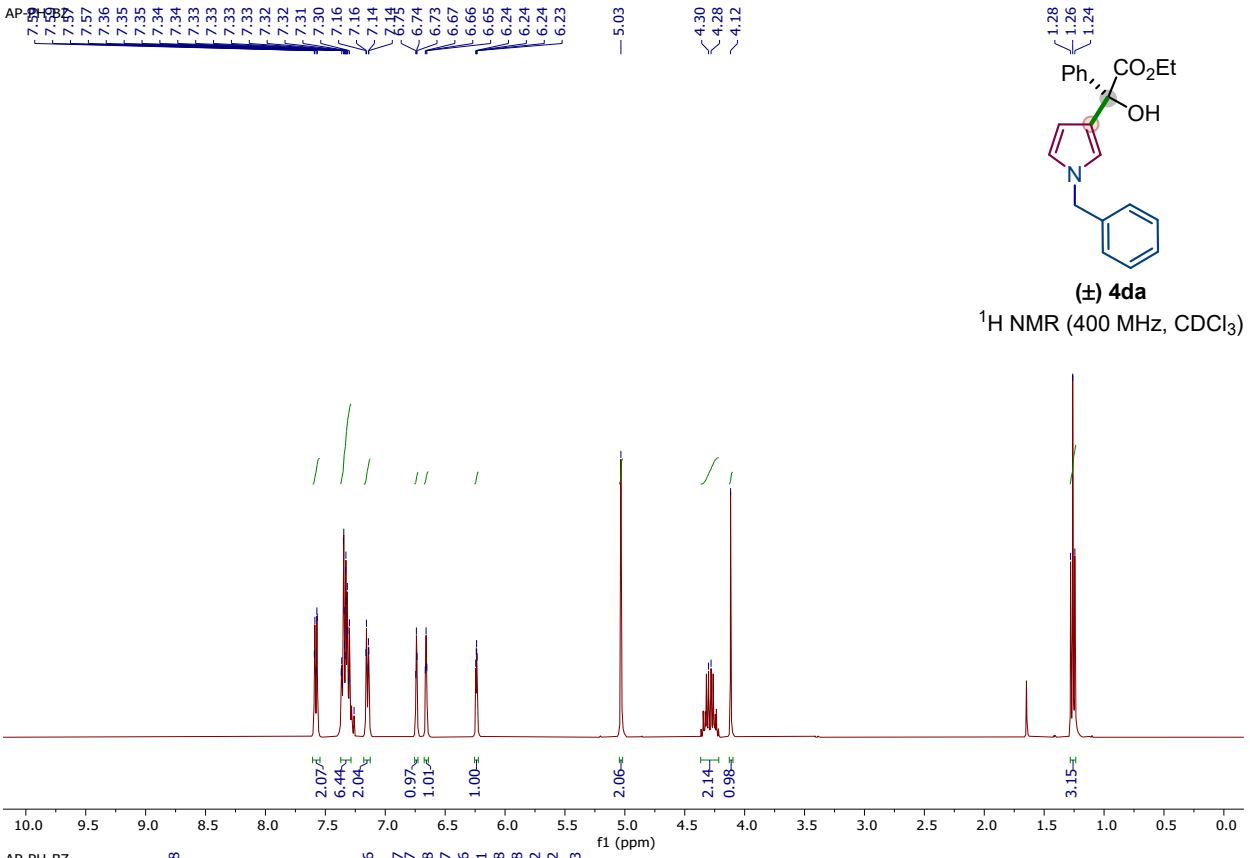
108.4
77.0 76.2 75.9 75.6 75.3 74.2
63.9
38.9
13.9
Oct23-2020/2
127.4 124.5 121.7 120.8 120.1 118.9 117.2
f1 (ppm)
F3C CO2Et OH N
(±) 4ck
13C NMR (100 MHz, CDCl3)
f1 (ppm)



(±) 4da

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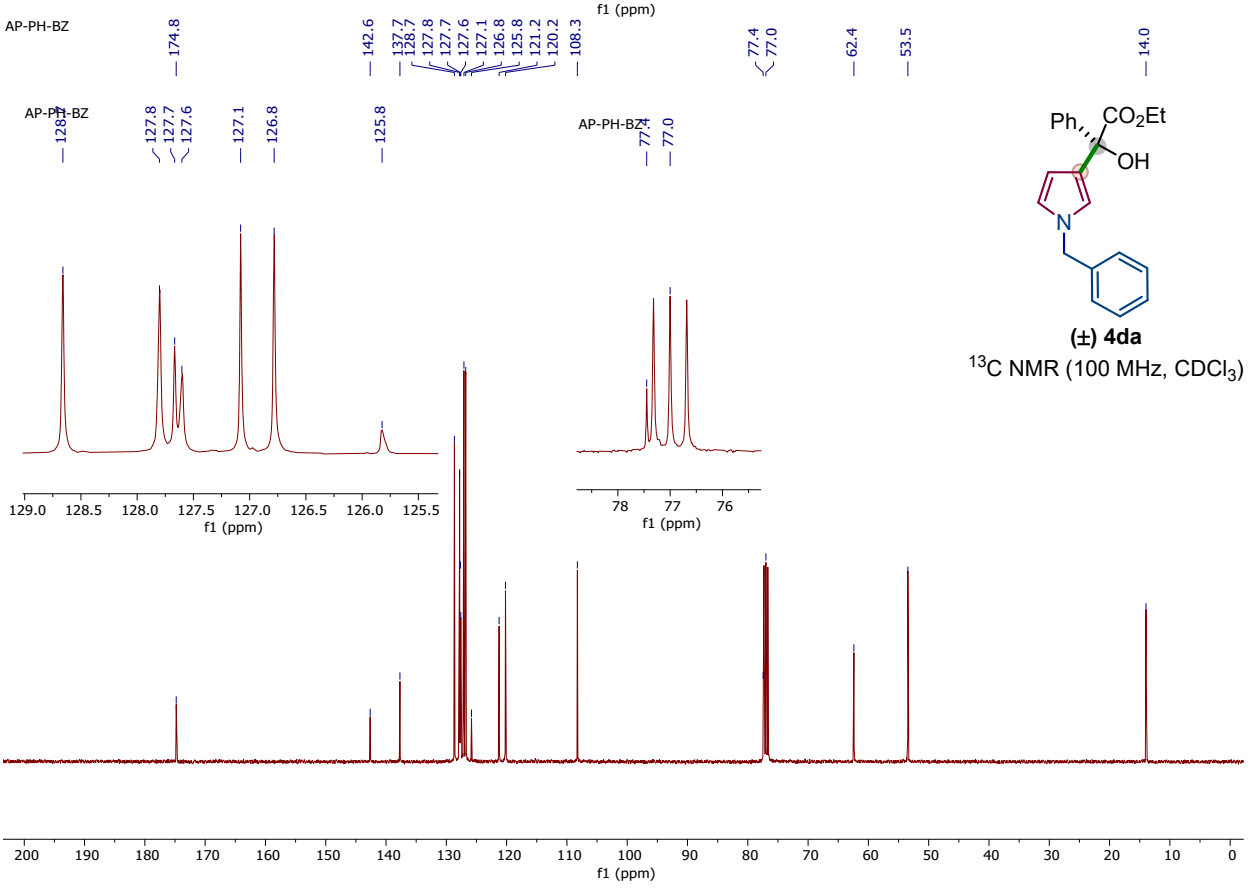

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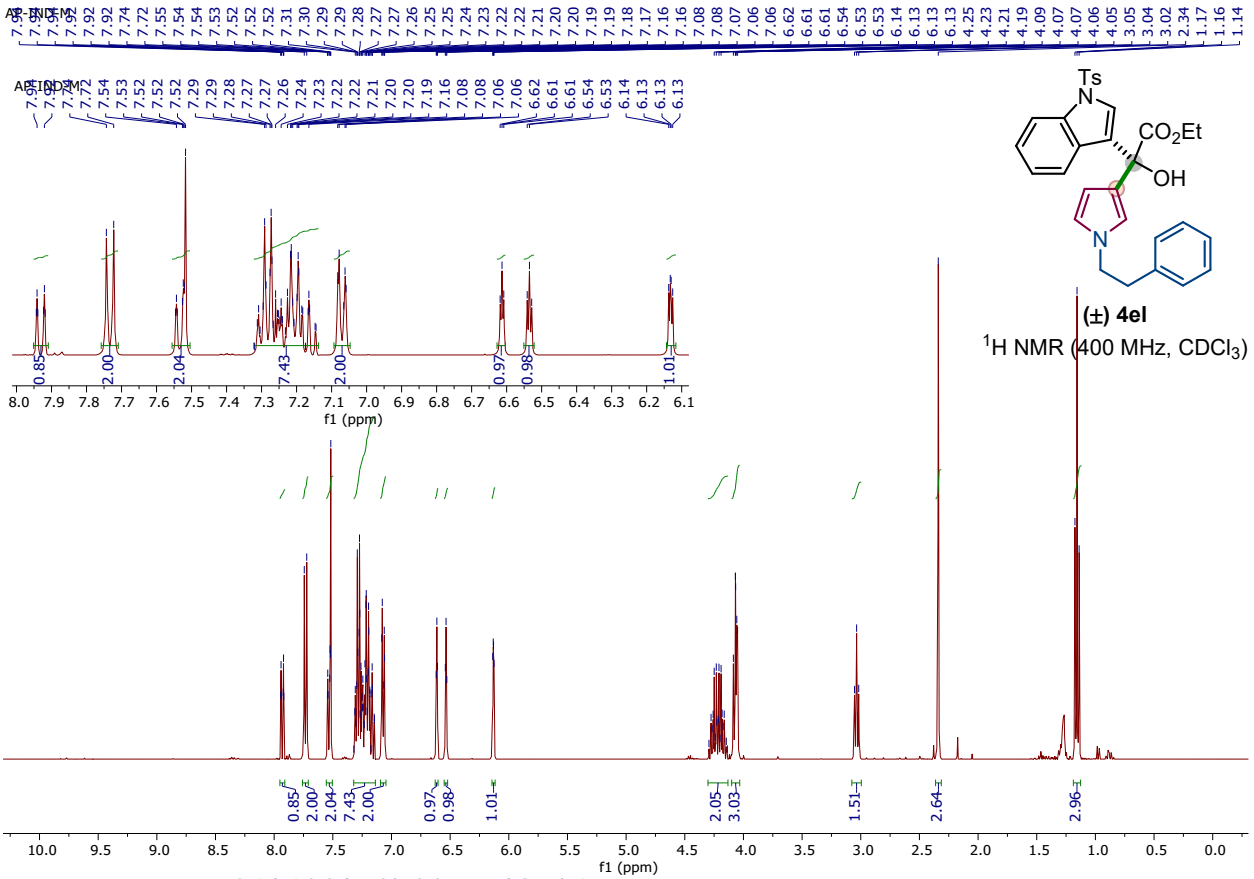
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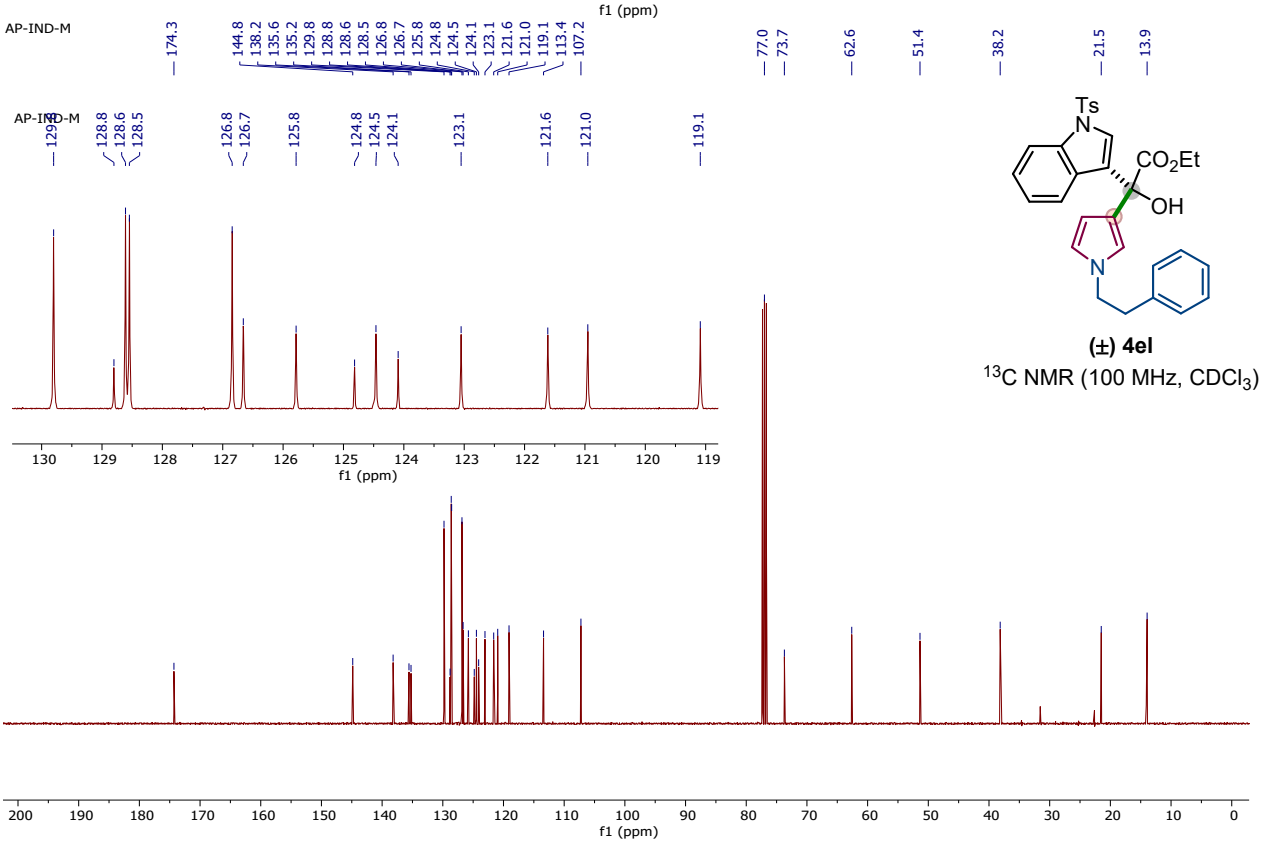
CO2Et
OH
N
(±) 4el
1H NMR (400 MHz, CDCl3)
f1 (ppm)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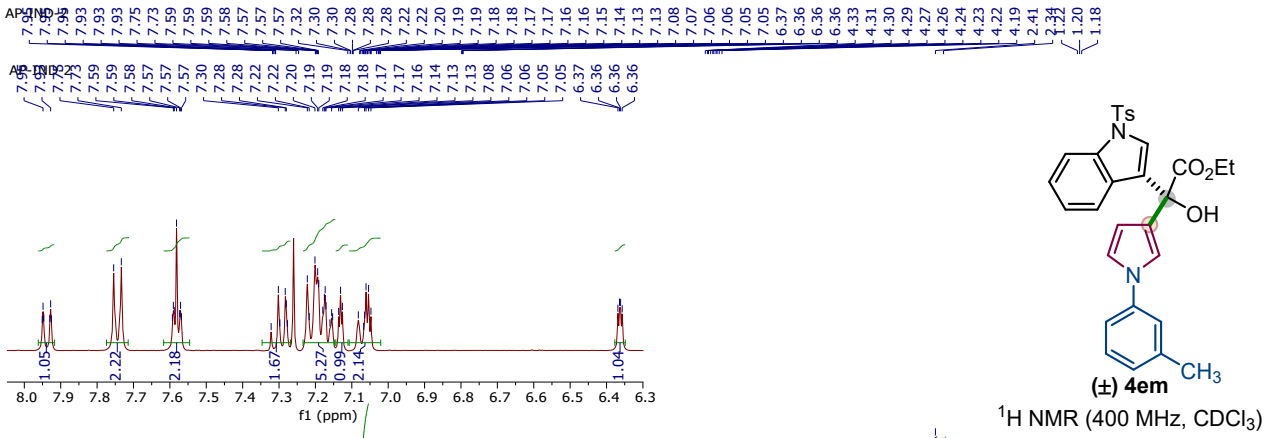
(±) 4el
13C NMR (100 MHz, CDCl3)
f1 (ppm)



(±) 4em

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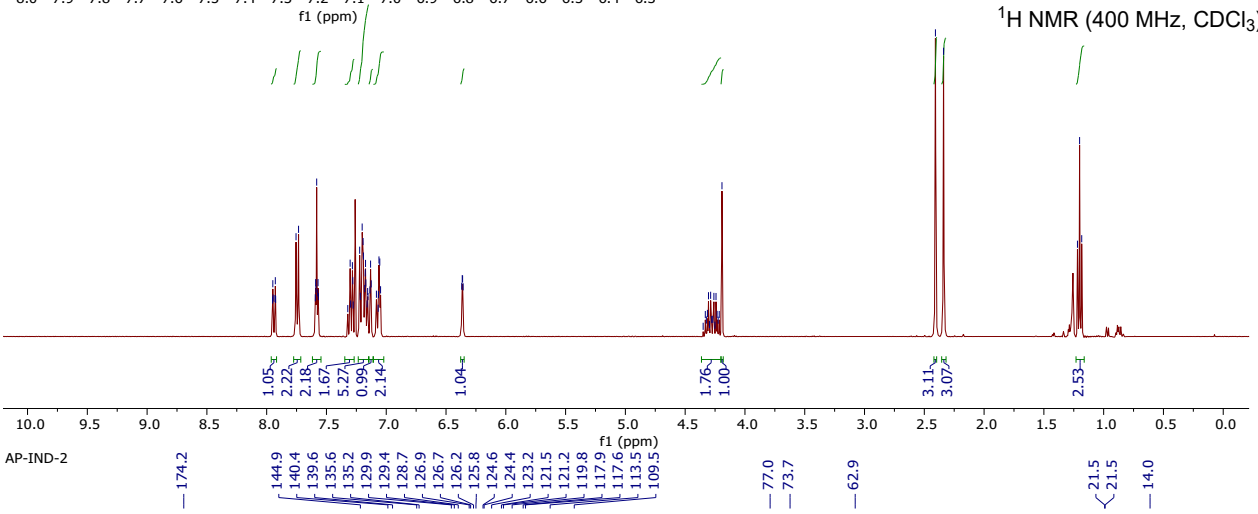

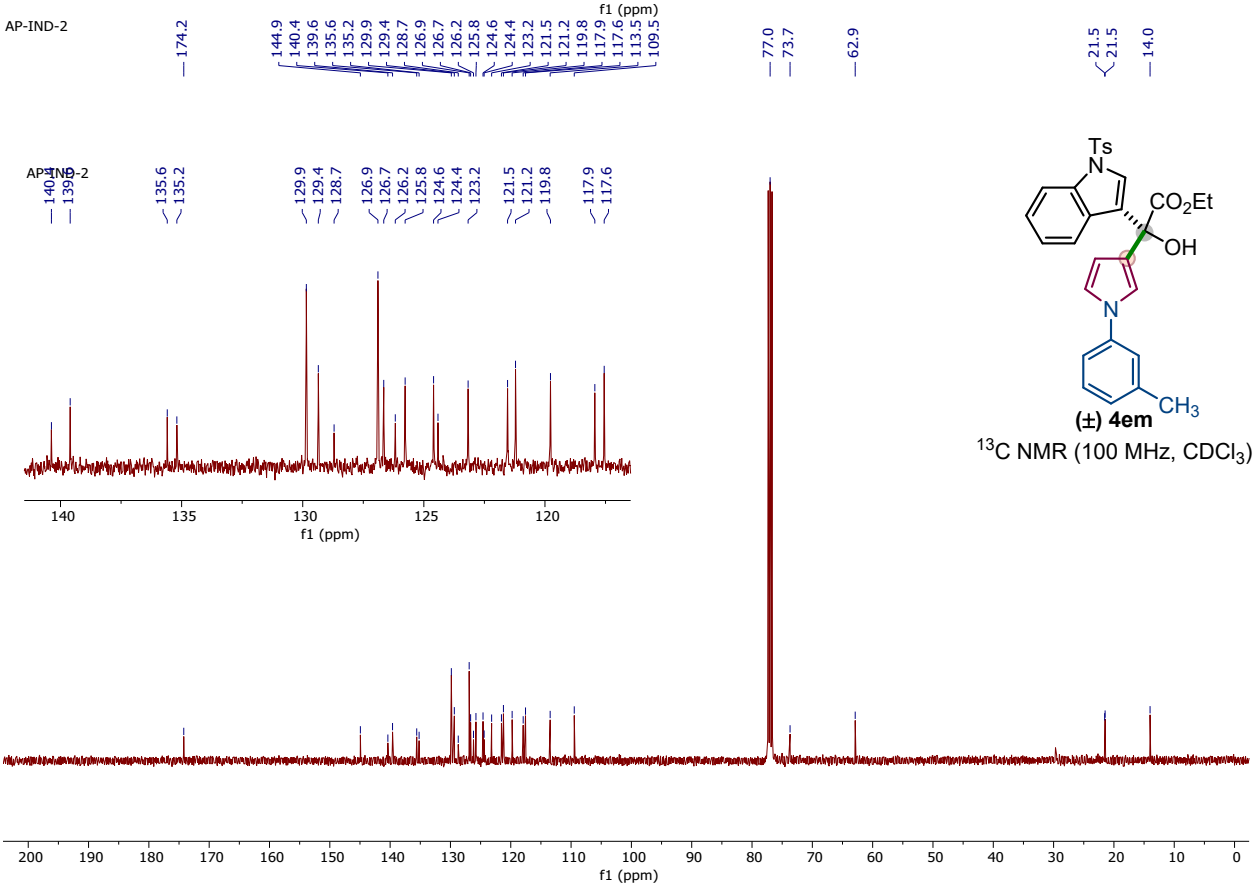

(±) 4em

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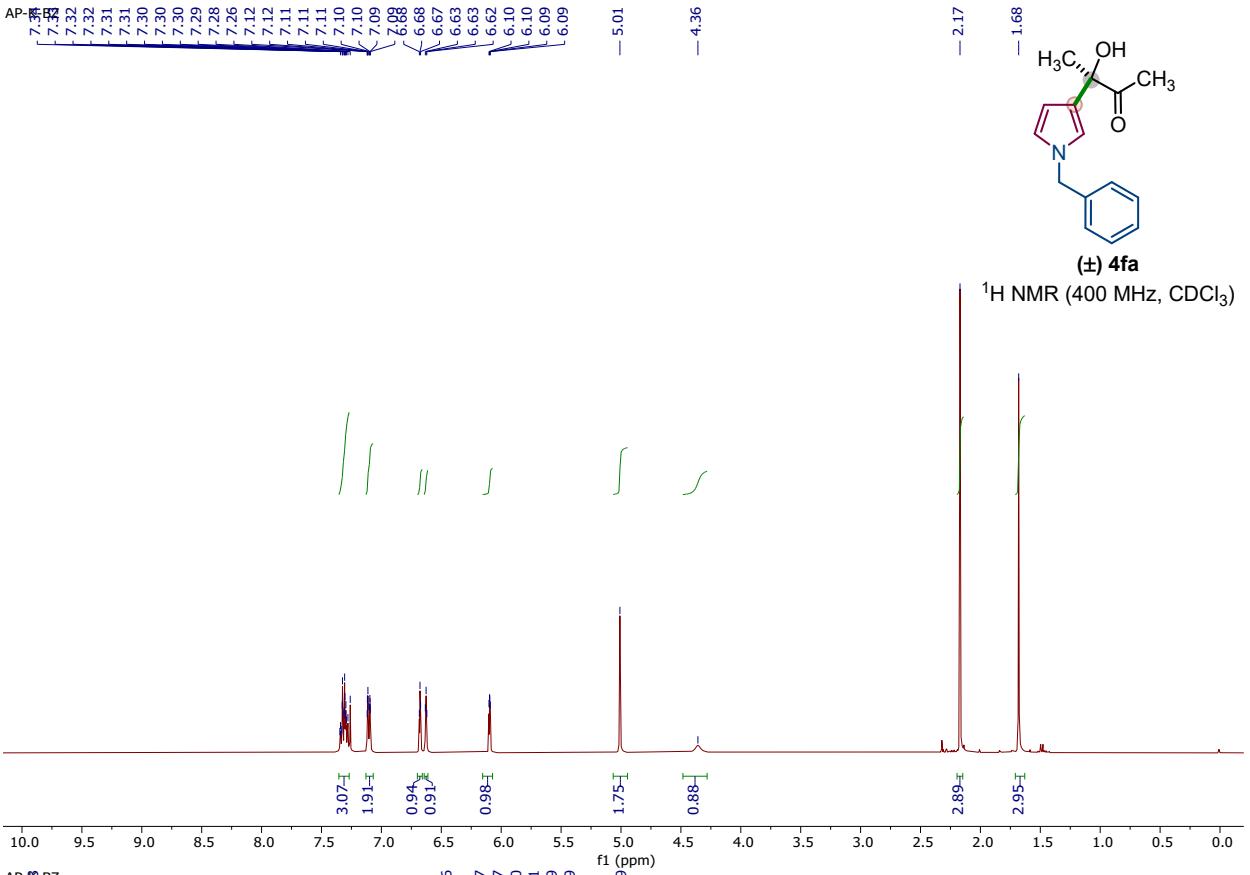
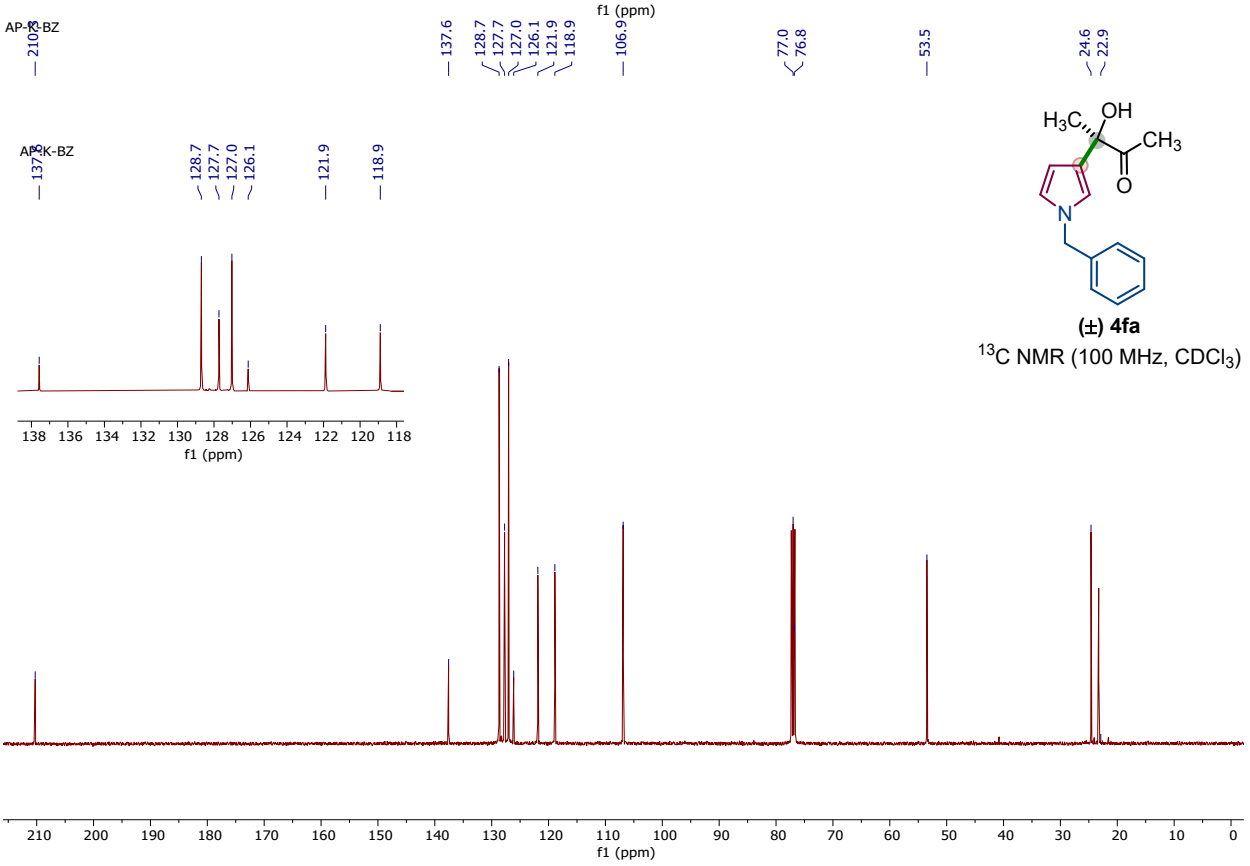


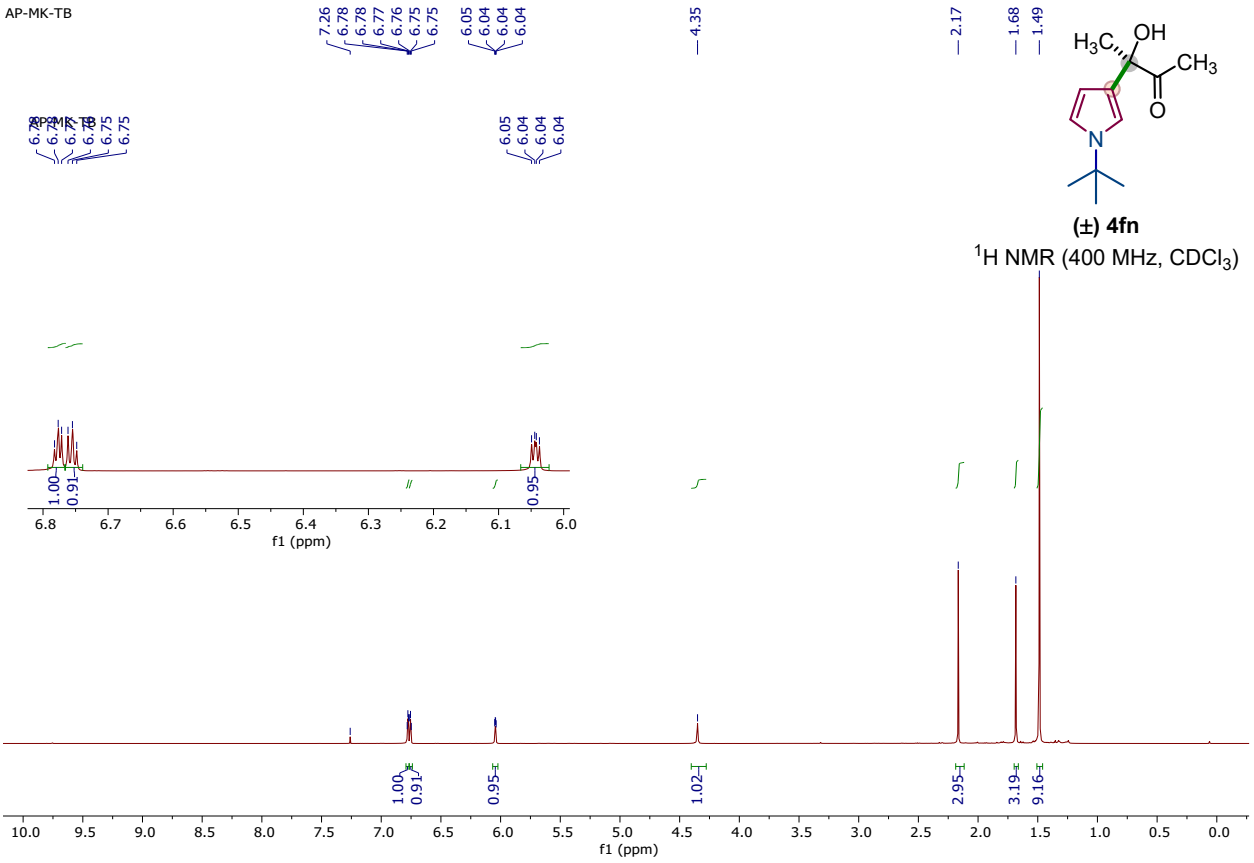
(±) 4fa

^{1}H NMR (400 MHz, $CDCl_3$)



(±) 4fa

^{13}C NMR (100 MHz, $CDCl_3$)



(±) 4fn

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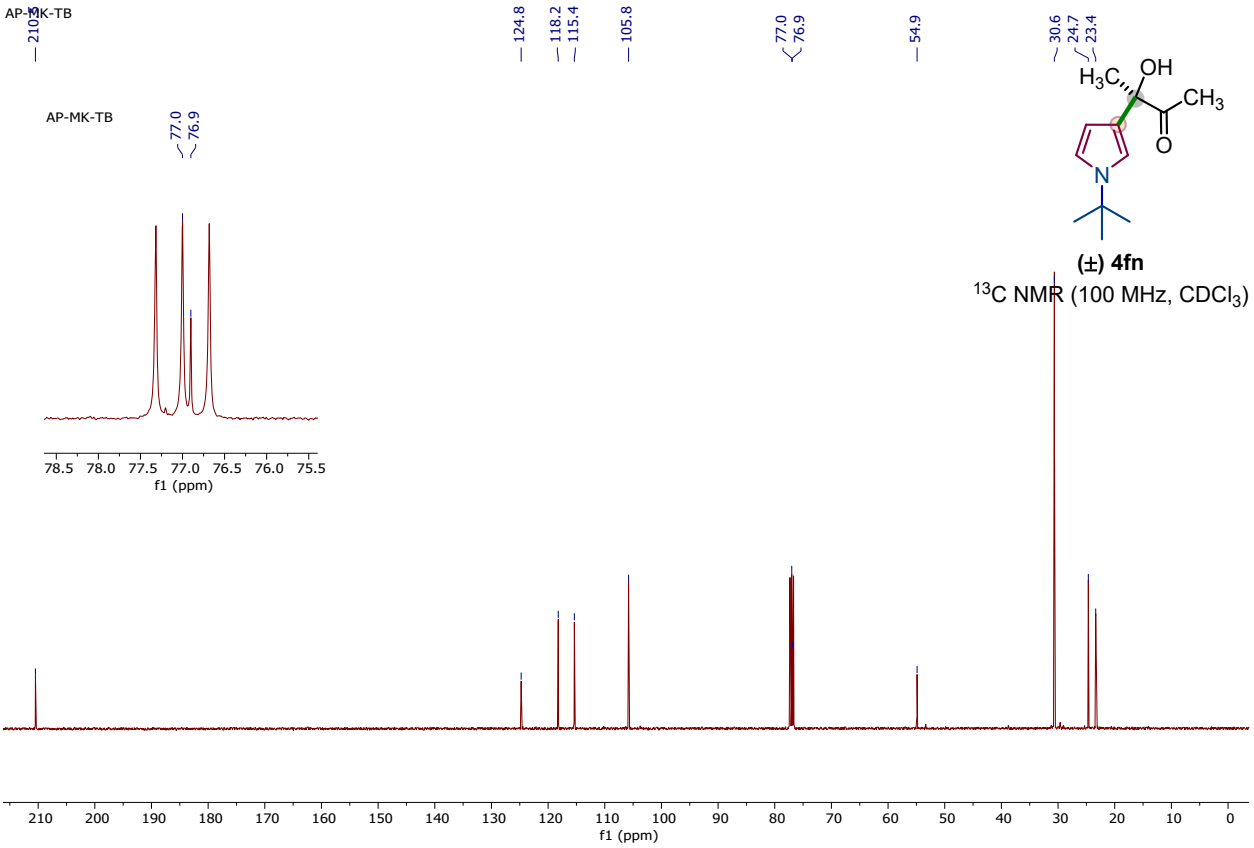
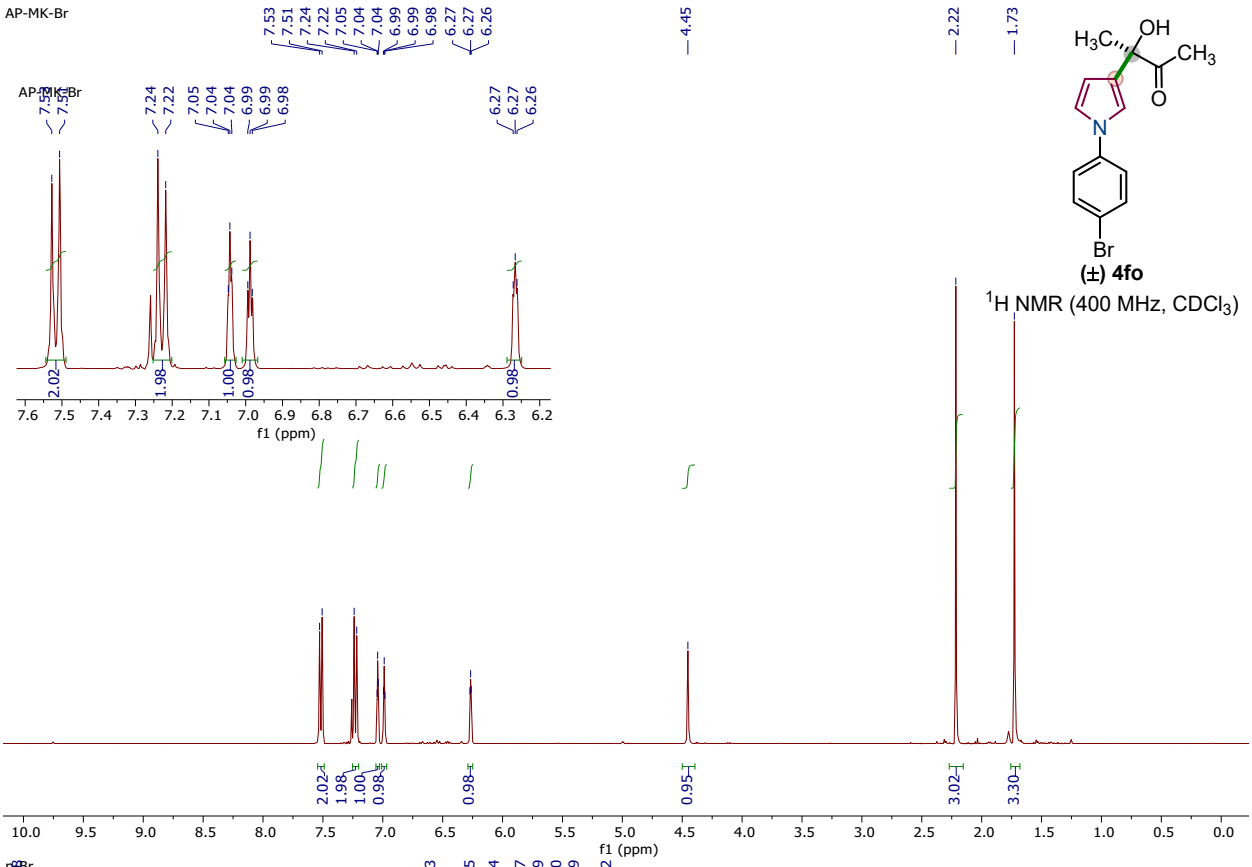


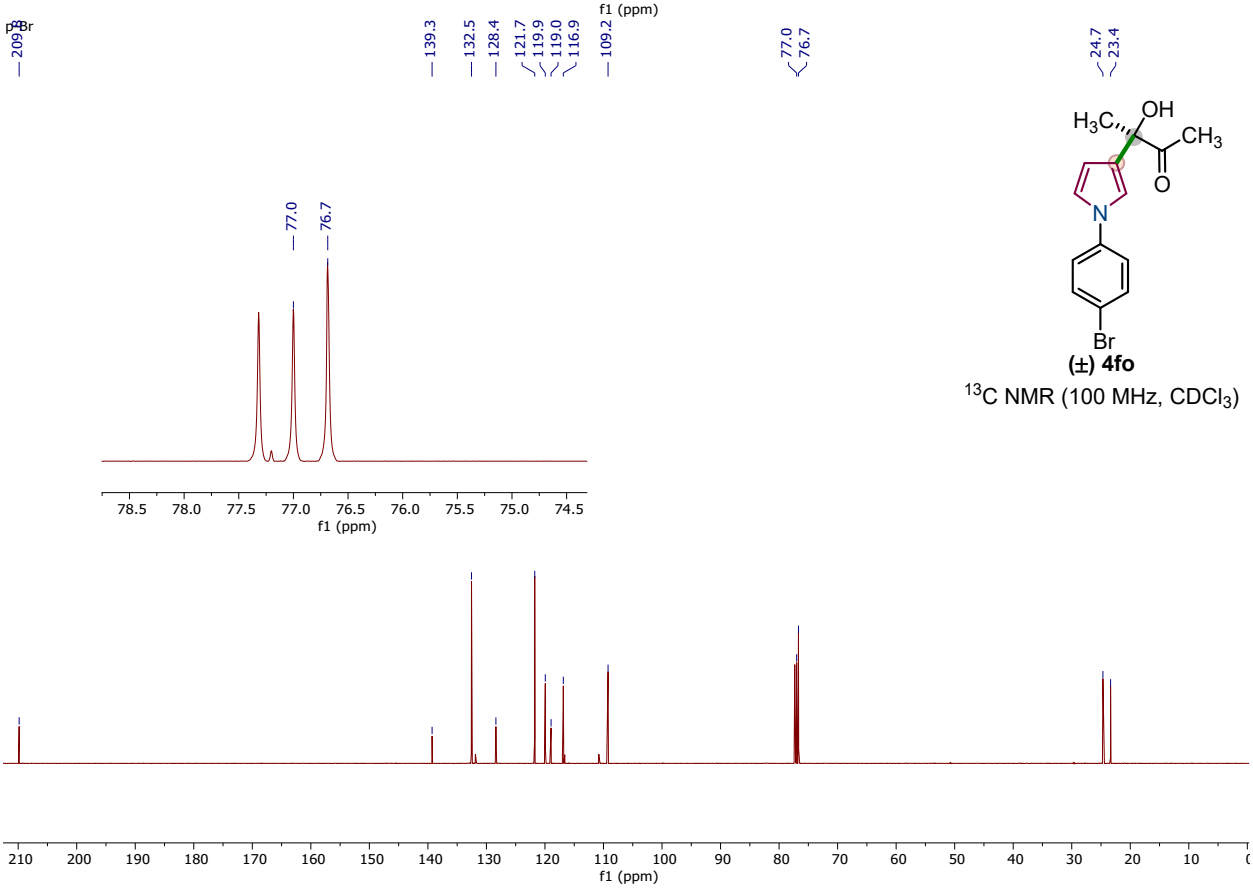
(±) 4fn

^{13}C NMR (100 MHz, $CDCl_3$)



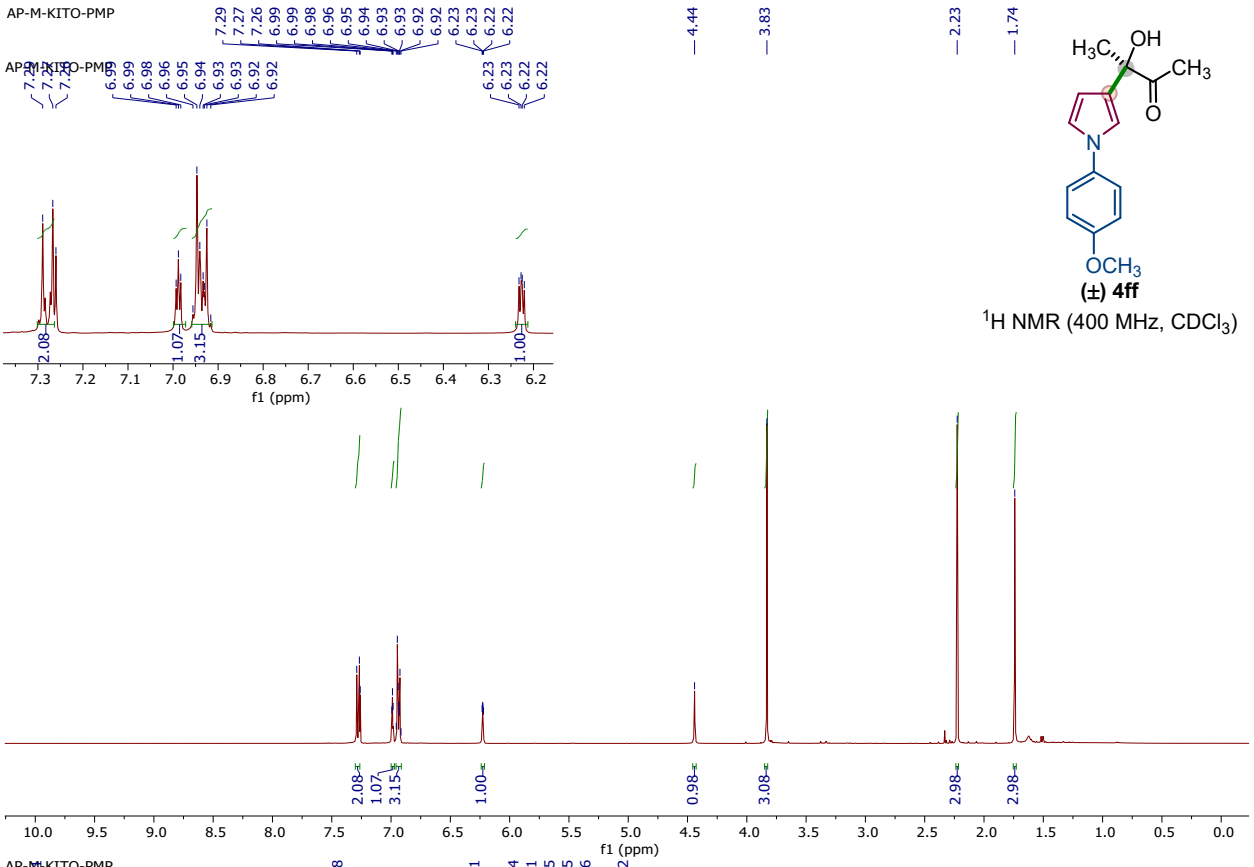
(±) 4fo

^{1}H NMR (400 MHz, $CDCl_3$)



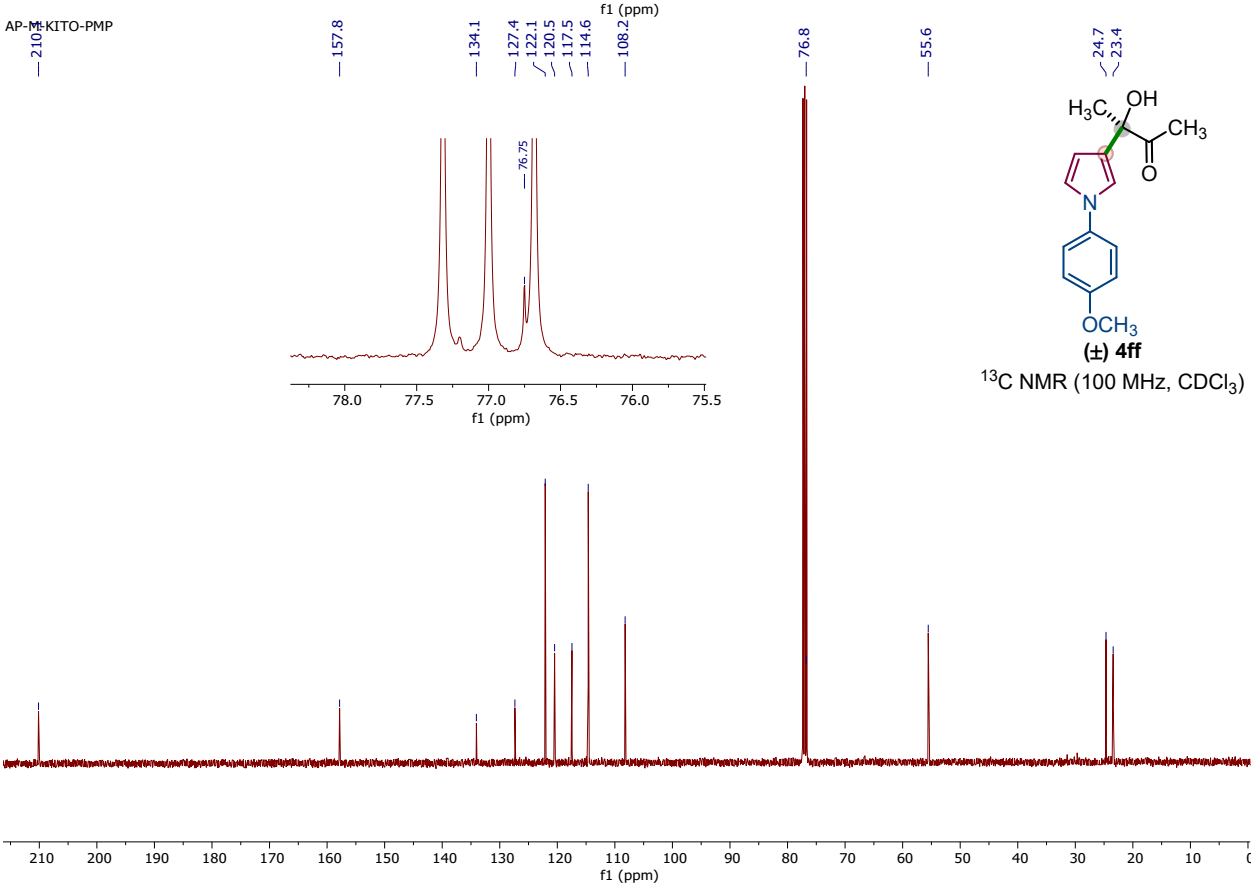
(±) 4fo

^{13}C NMR (100 MHz, $CDCl_3$)



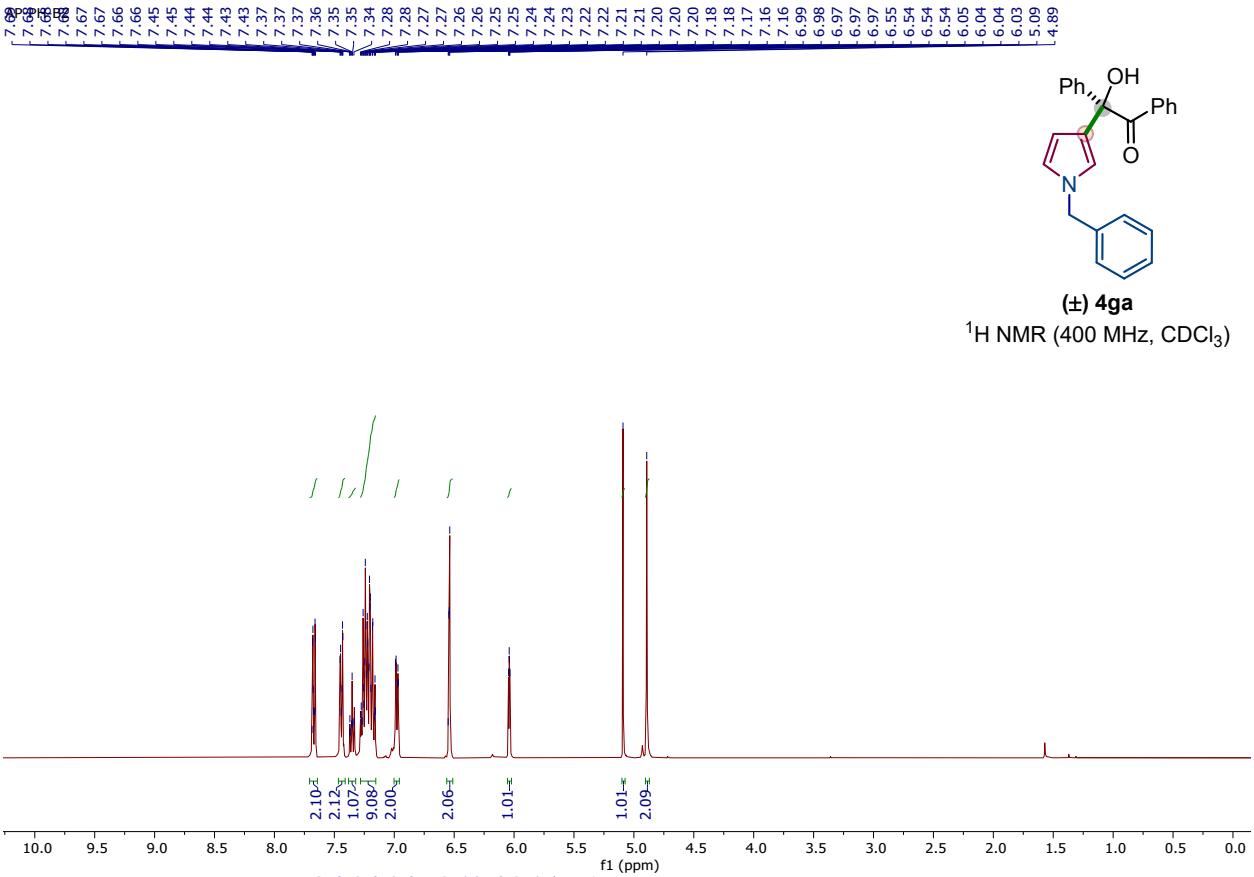
(±) 4ff

^{1}H NMR (400 MHz, $CDCl_3$)



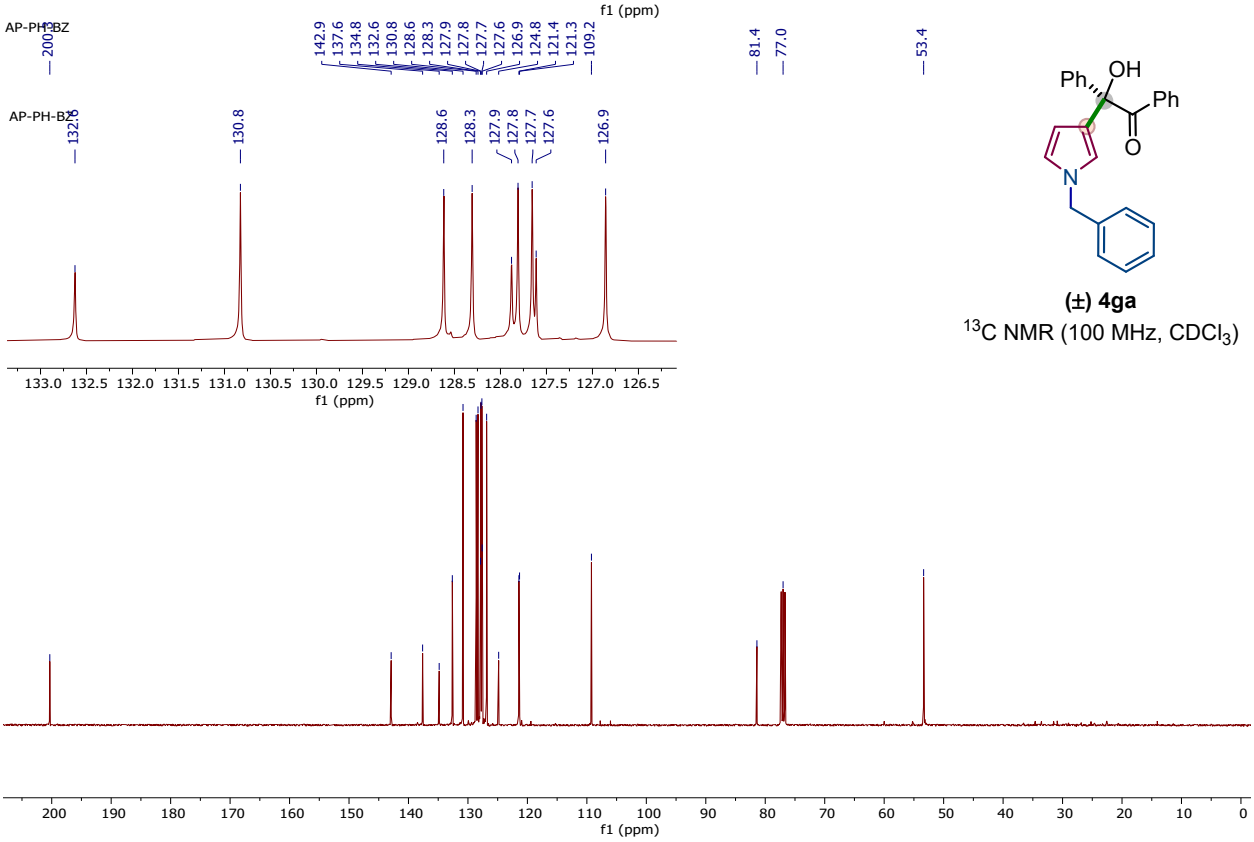
(±) 4ff

^{13}C NMR (100 MHz, $CDCl_3$)



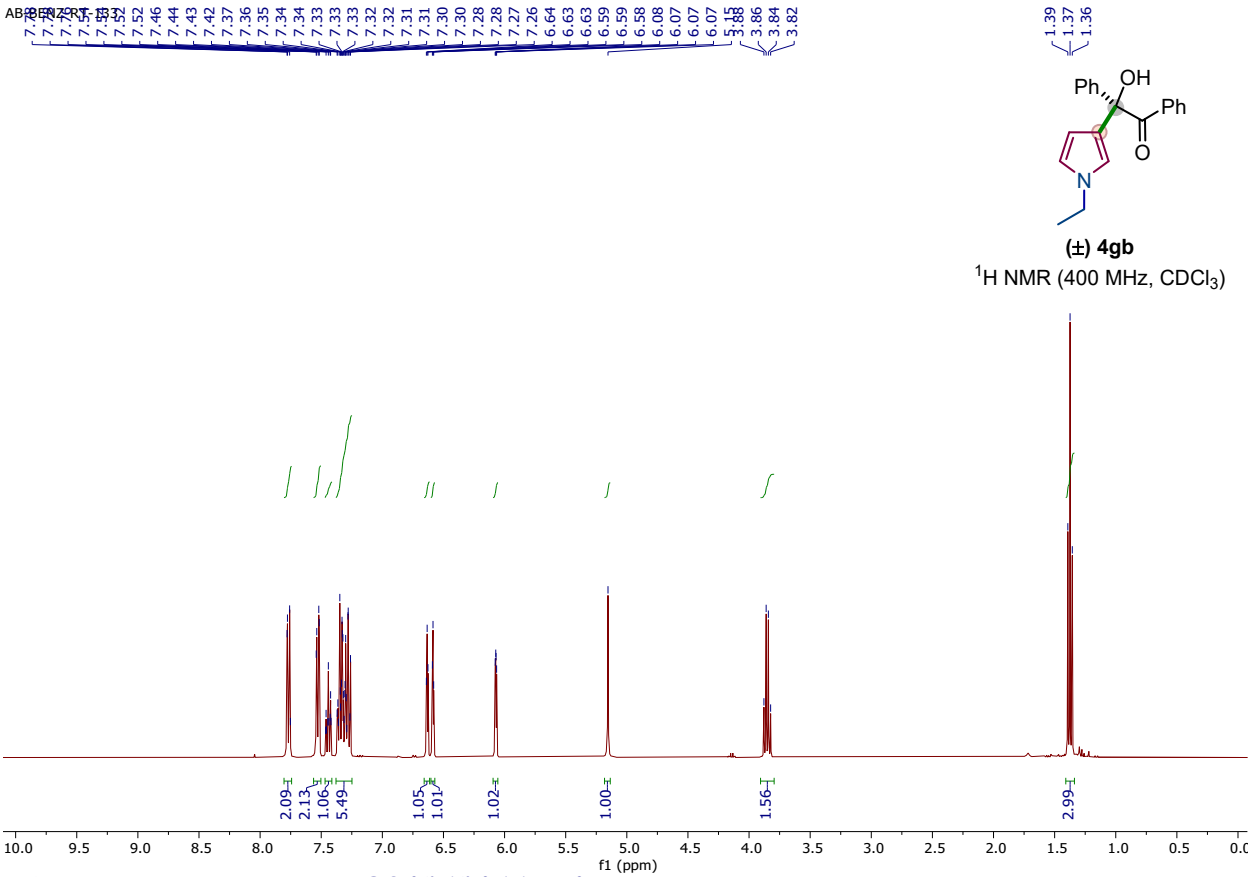
(±) 4ga

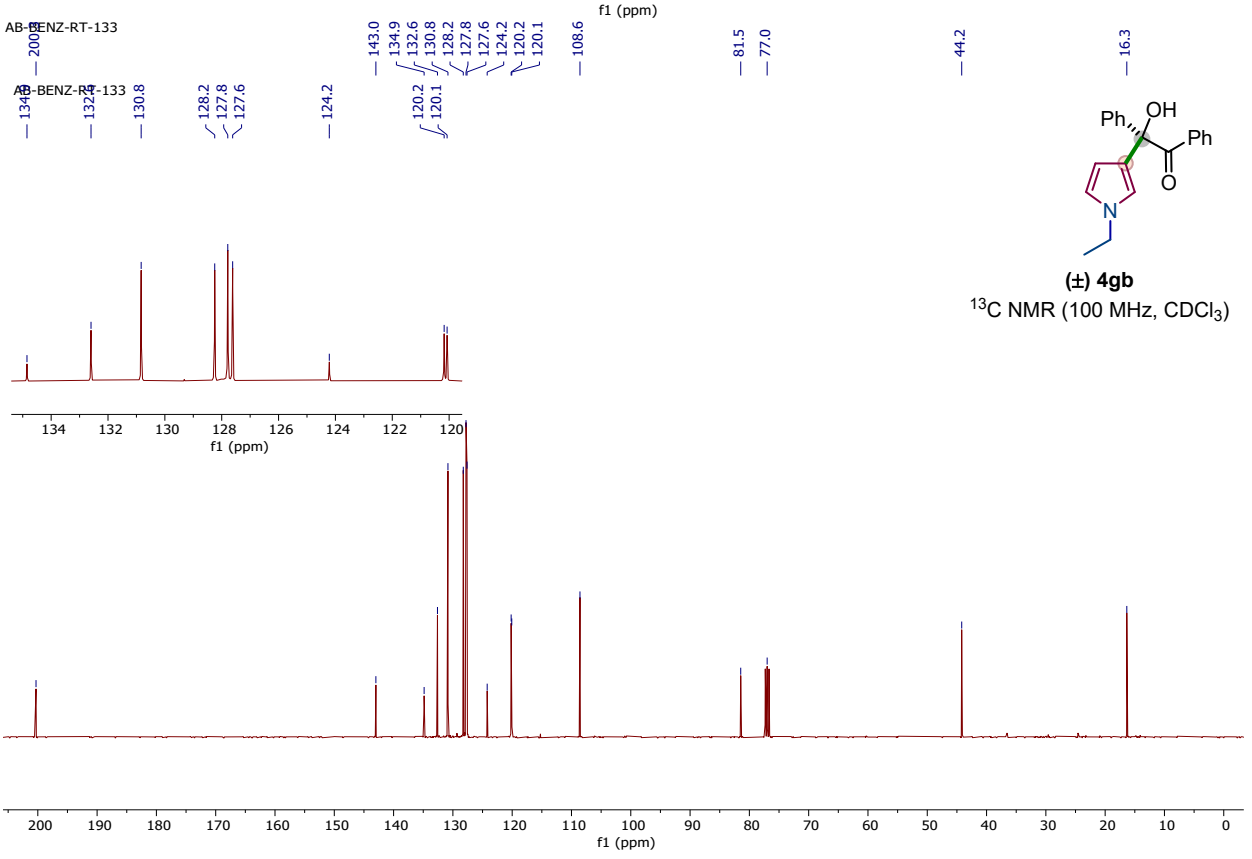
^{1}H NMR (400 MHz, $CDCl_3$)

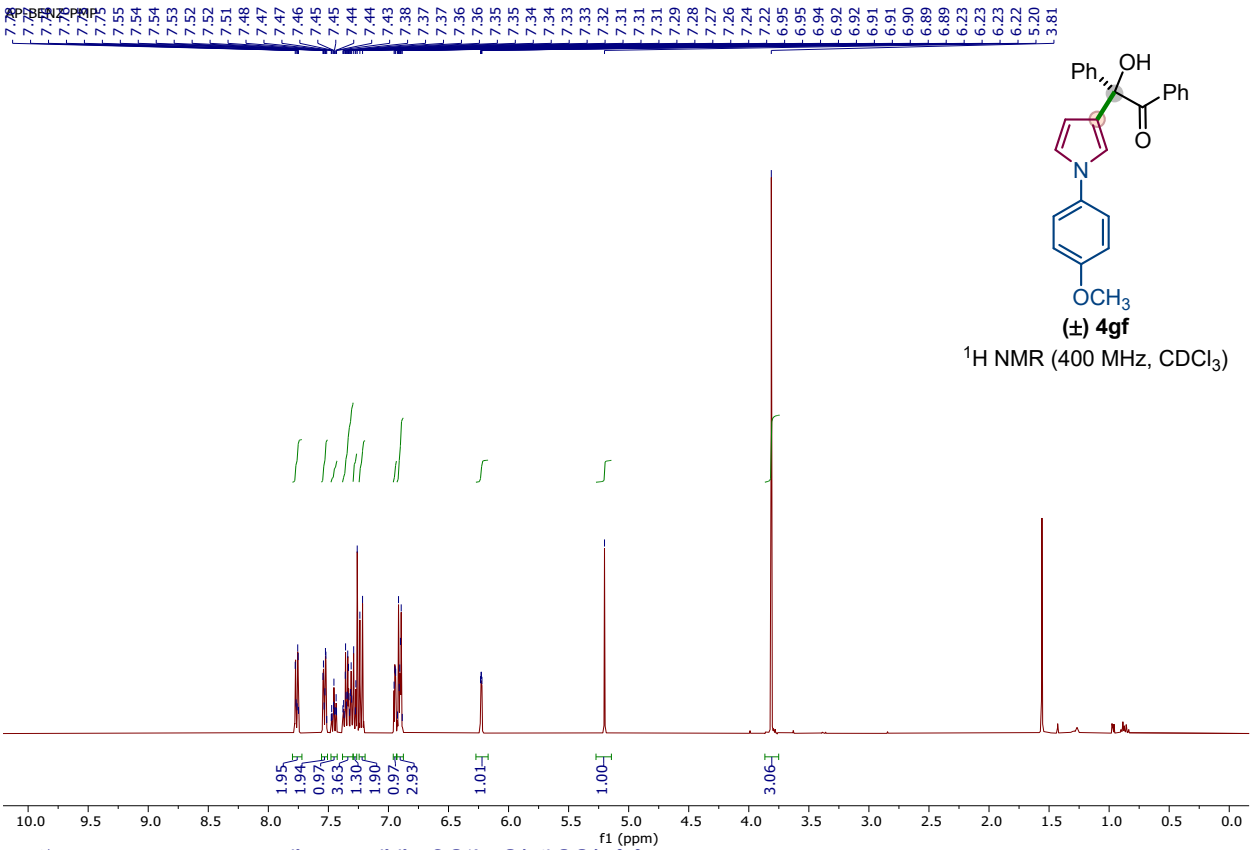


(±) 4ga

^{13}C NMR (100 MHz, $CDCl_3$)

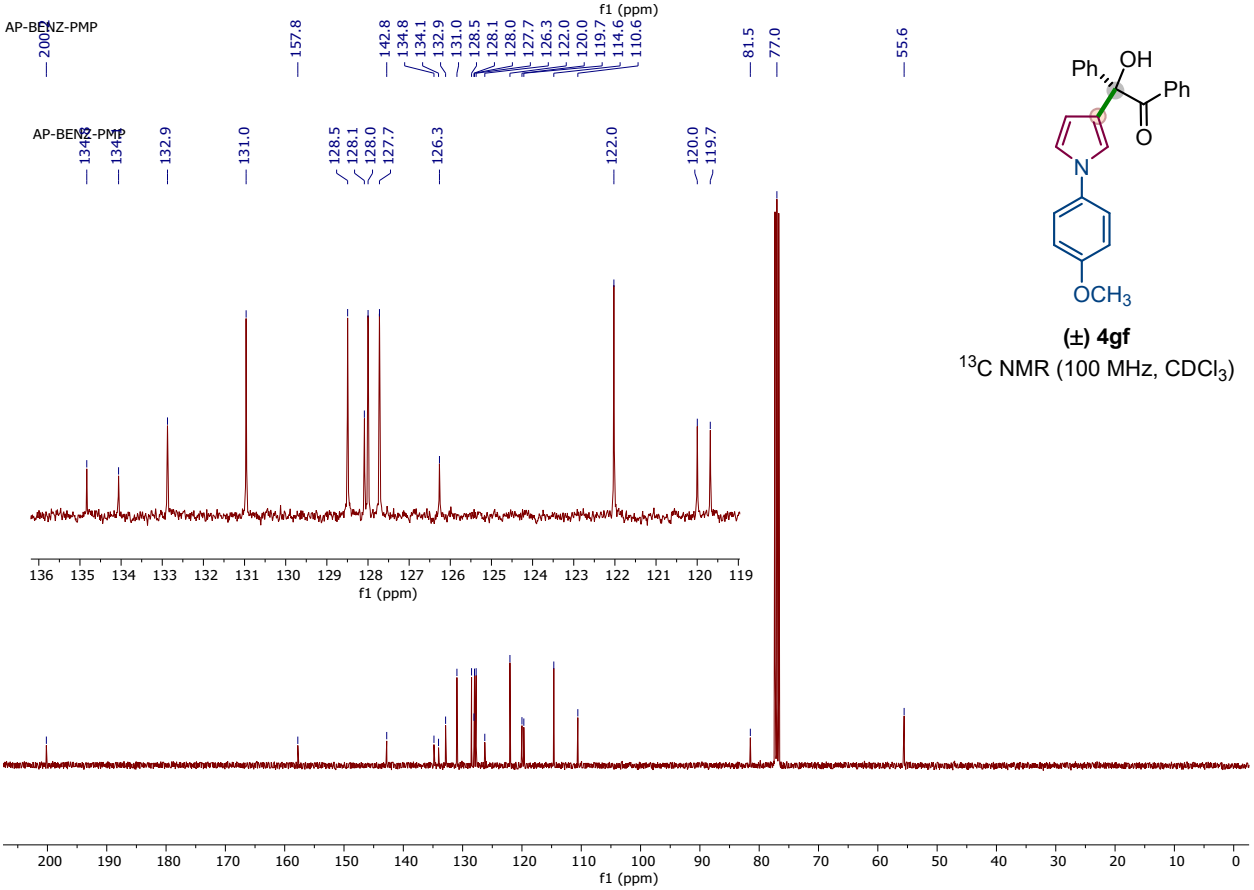

AB-BENZ-RT-133
Ph
OH
Ph
O
N
(±) 4gb
^{1}H NMR (400 MHz, $CDCl_3$)
f1 (ppm)


AB-BENZ-RT-133
Ph
OH
Ph
O
N
(±) 4gb
^{13}C NMR (100 MHz, $CDCl_3$)
f1 (ppm)



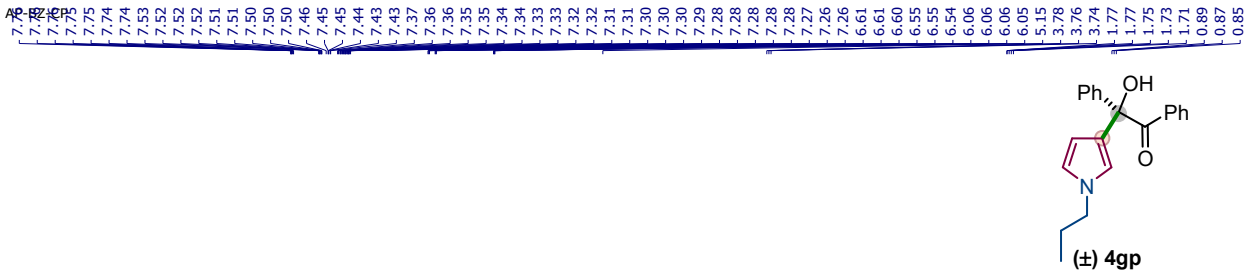
(±) 4gf

^{1}H NMR (400 MHz, $CDCl_3$)



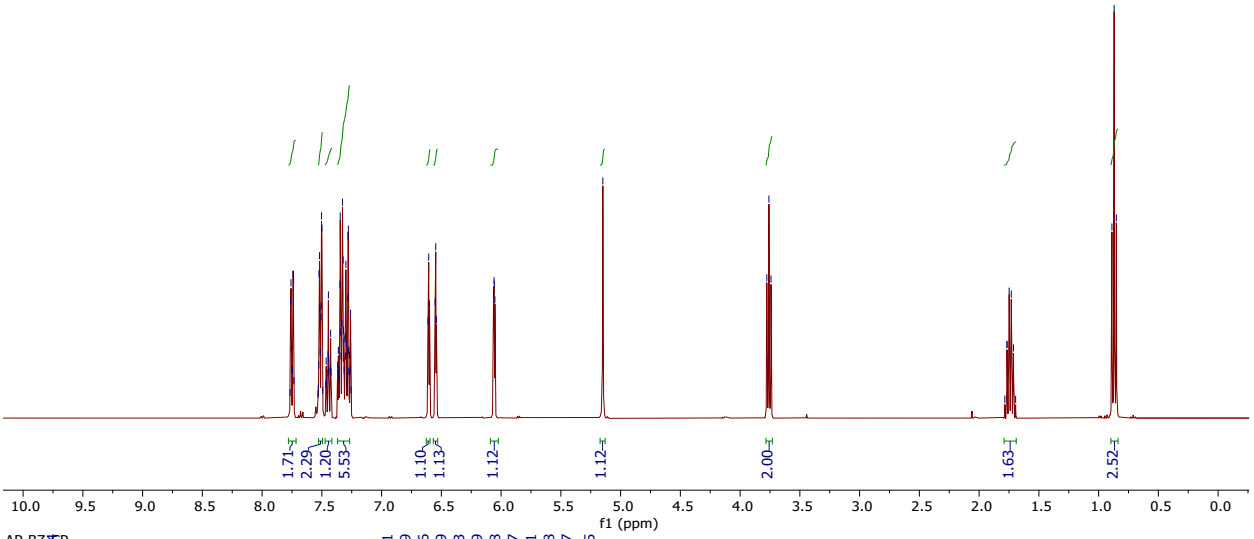
(±) 4gf

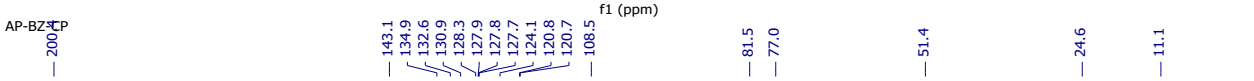
^{13}C NMR (100 MHz, $CDCl_3$)

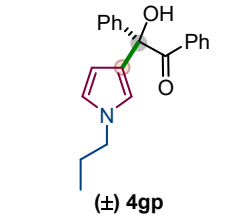


(±) 4gp

^{1}H NMR (400 MHz, $CDCl_3$)

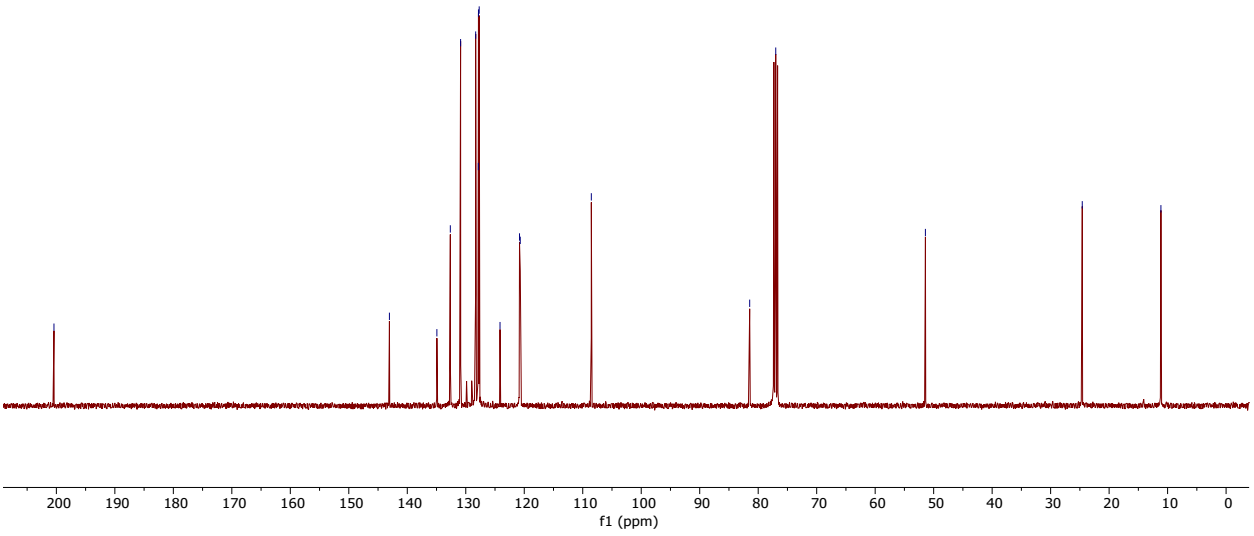


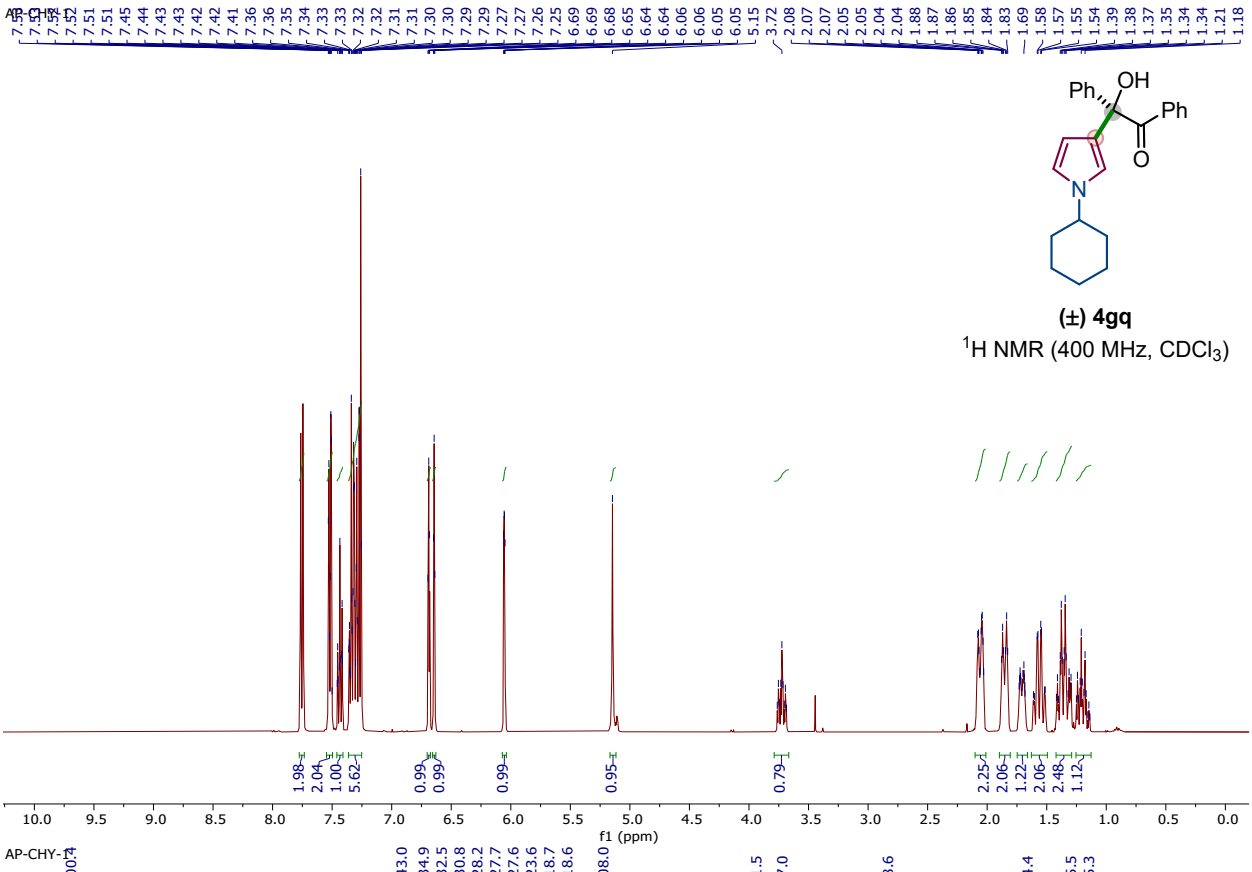




(±) 4gp

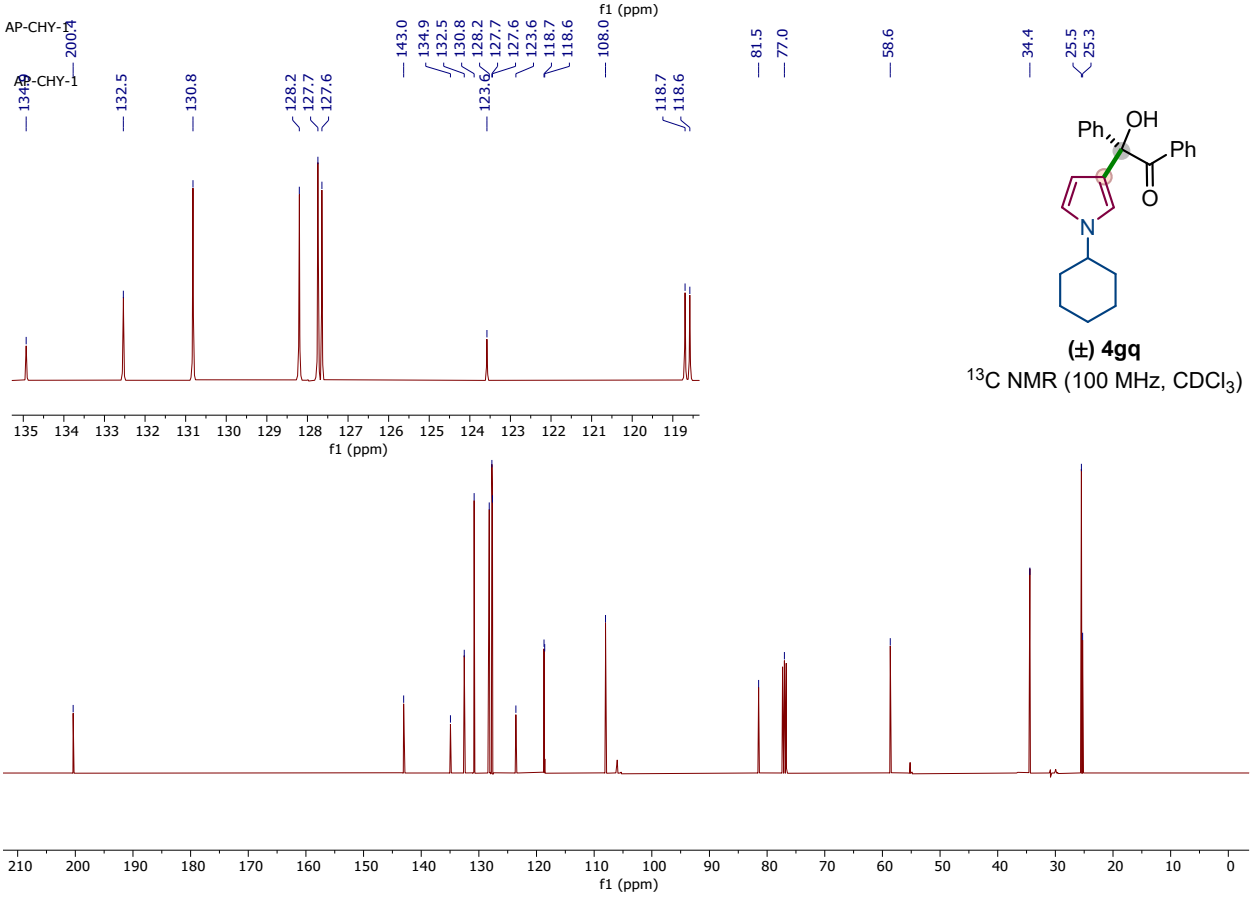
^{13}C NMR (100 MHz, $CDCl_3$)





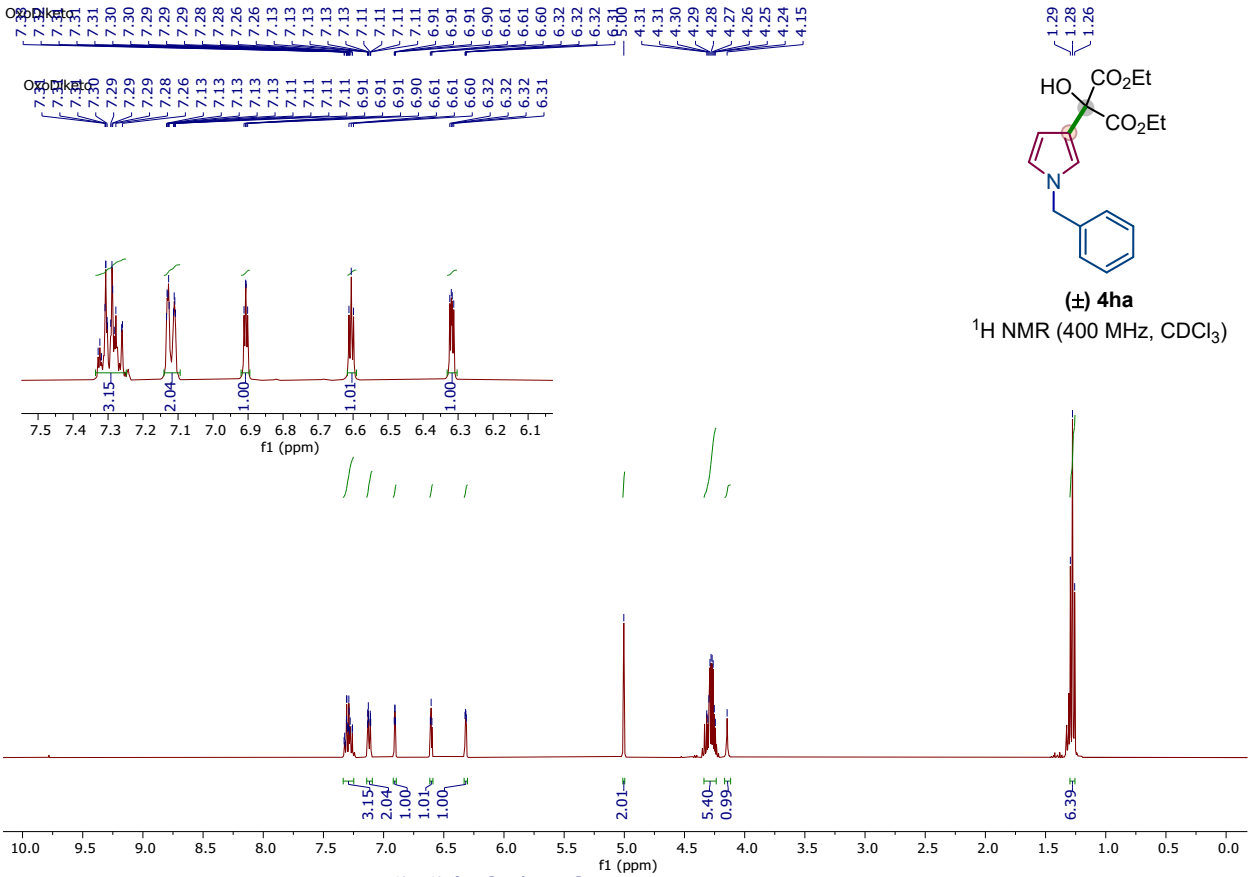
(±) 4gq

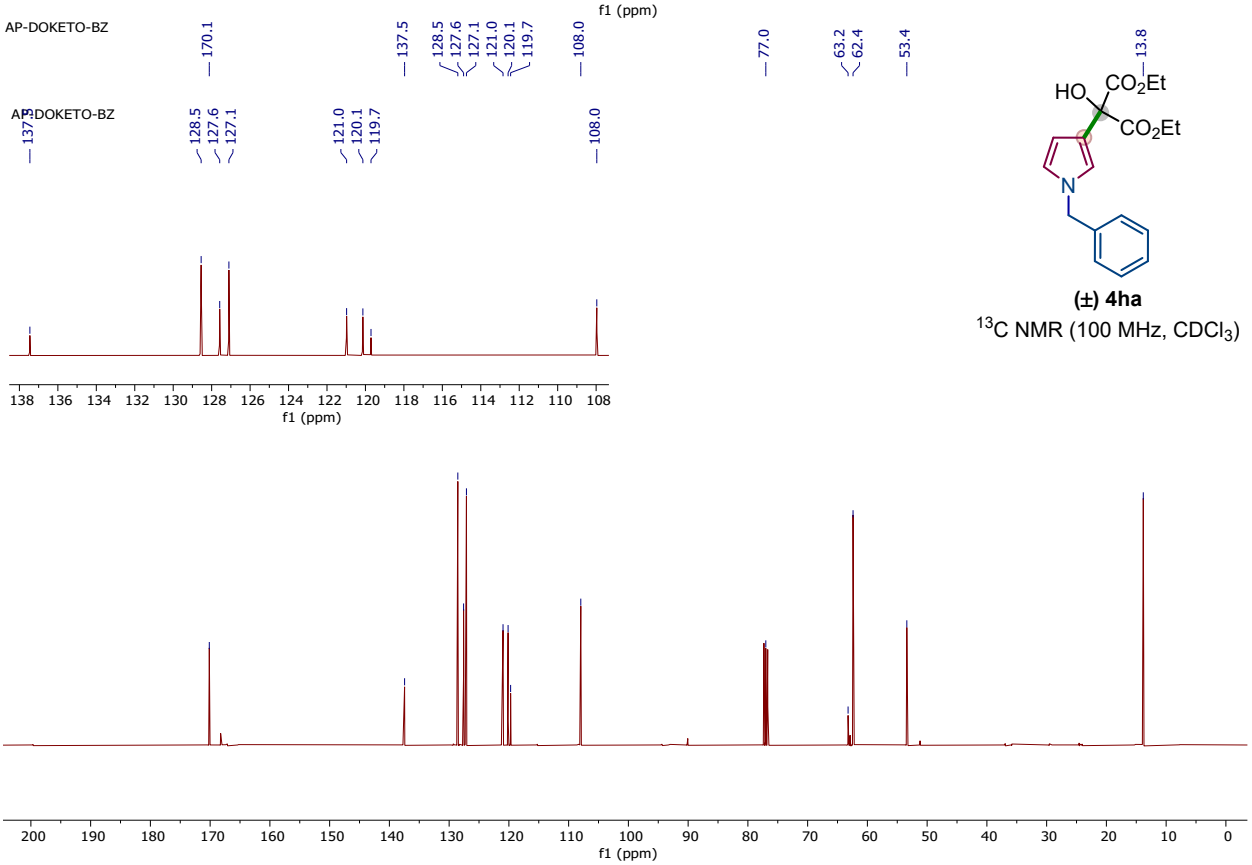
^{1}H NMR (400 MHz, $CDCl_3$)

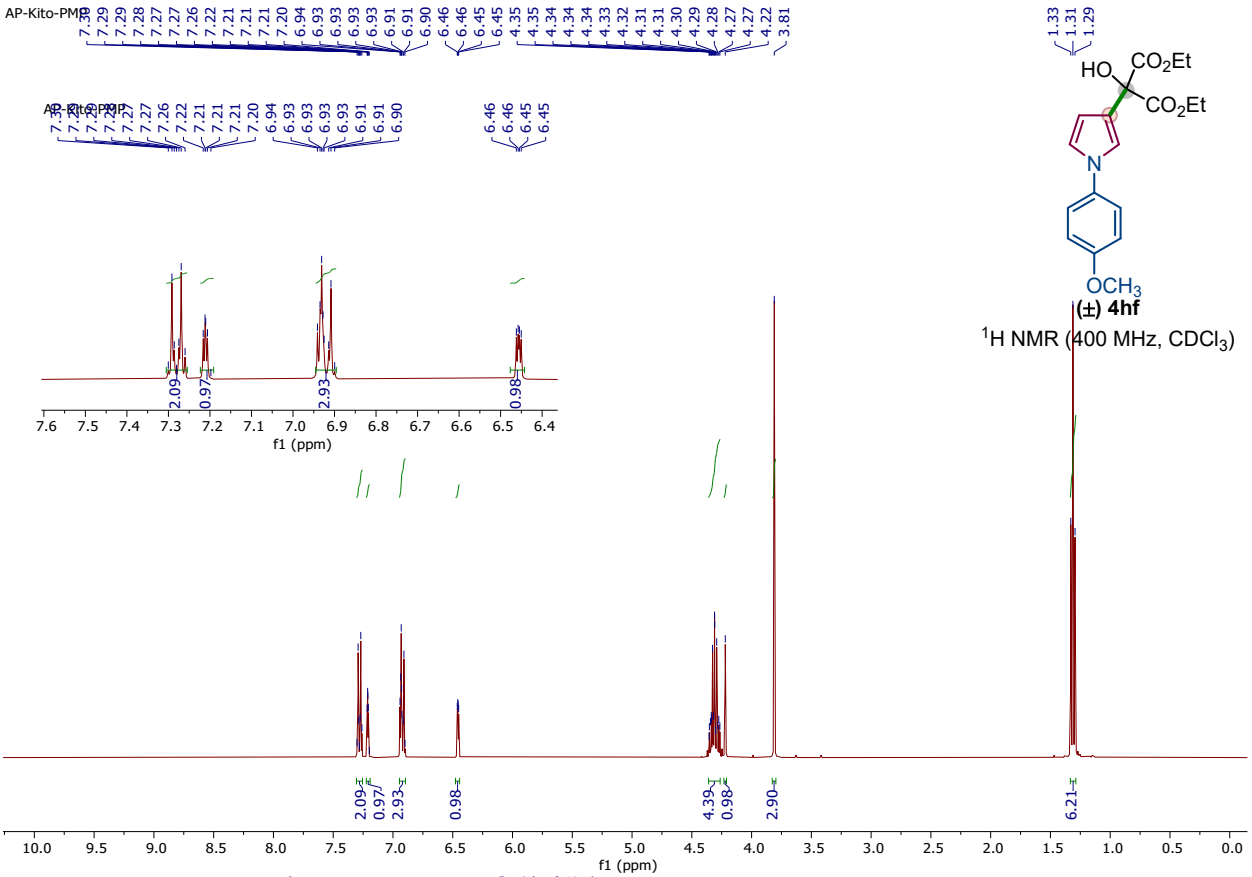


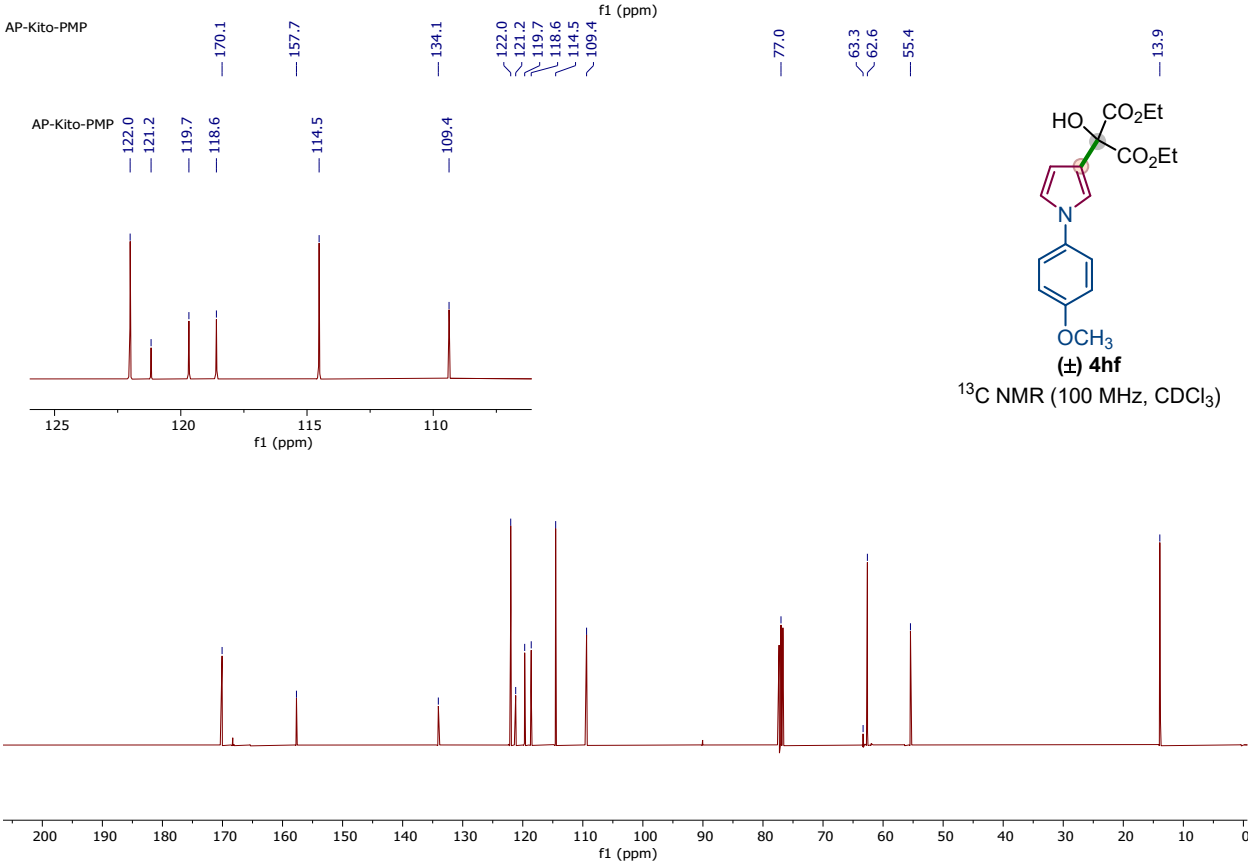
(±) 4gq

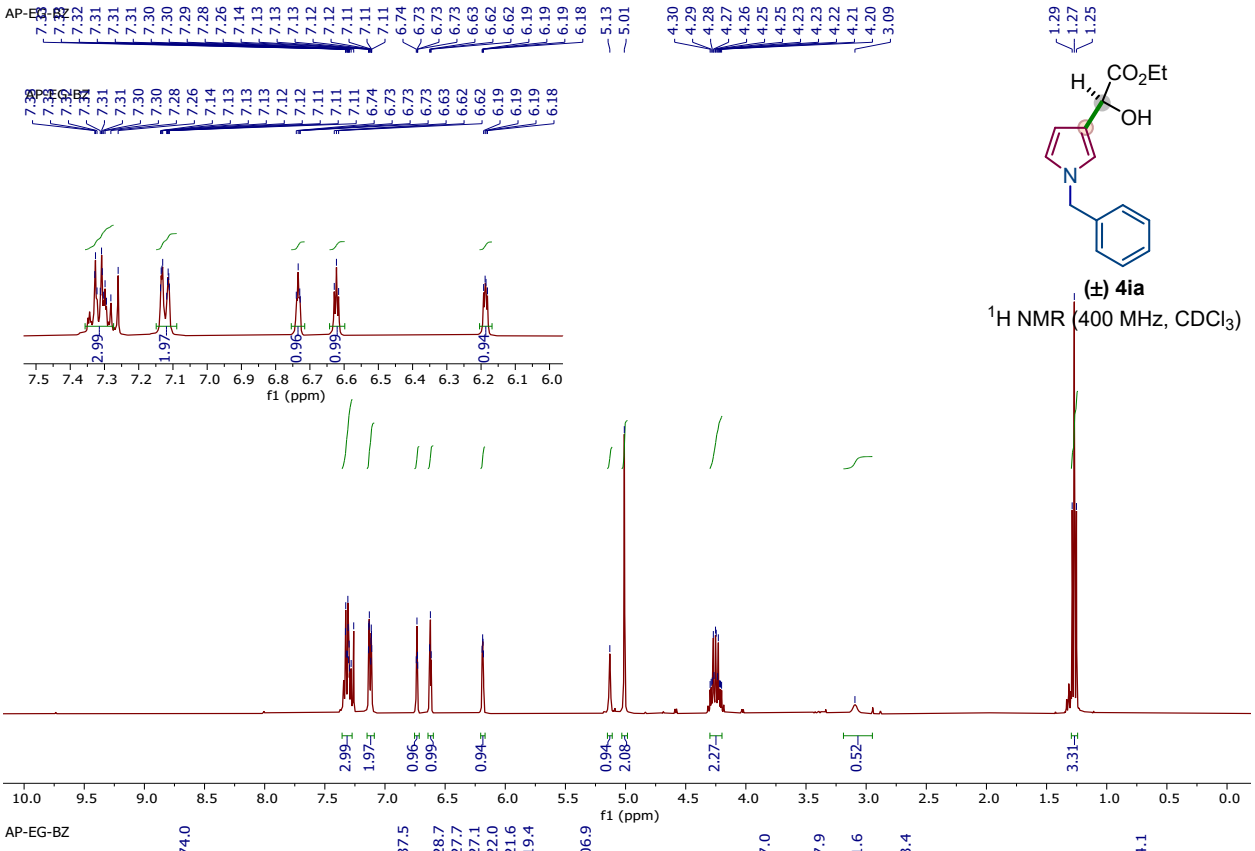
^{13}C NMR (100 MHz, $CDCl_3$)

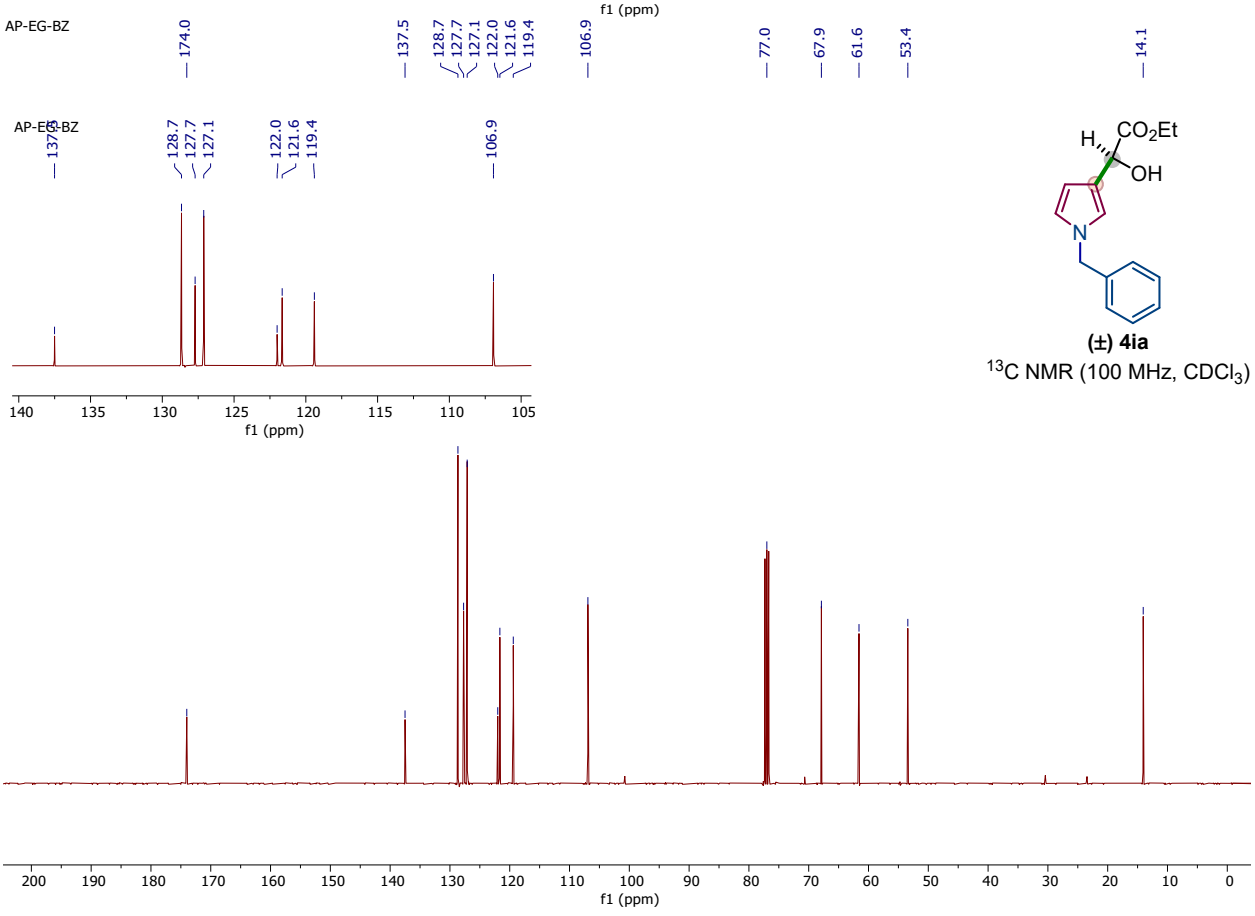

OzpDiketo
OzpDiketo
HO
CO2Et
CO2Et
N
(±) 4ha
1H NMR (400 MHz, CDCl3)
f1 (ppm)

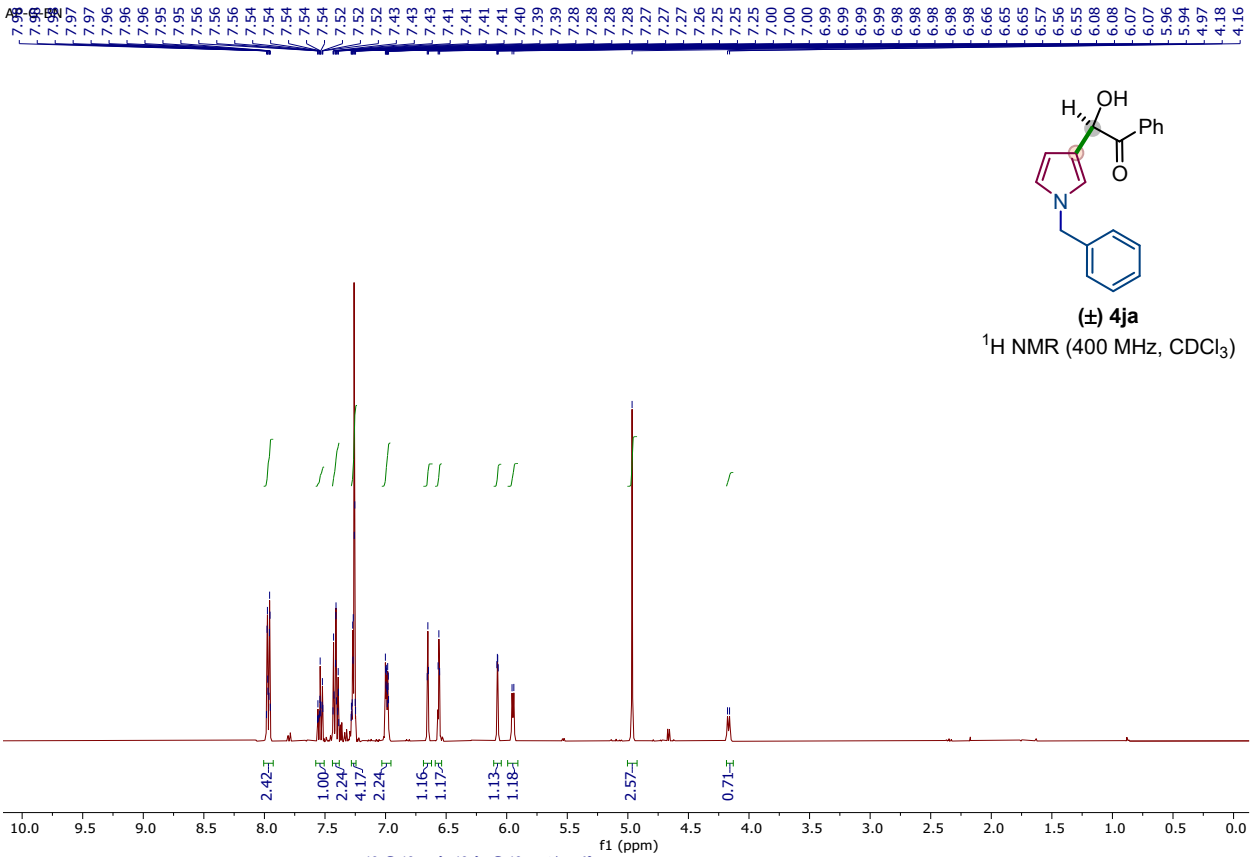

AP-DOKETO-BZ
AP-DOKETO-BZ
HO
CO2Et
CO2Et
N
(±) 4ha
13C NMR (100 MHz, CDCl3)
f1 (ppm)


AP-Kito-PMP
HO
CO2Et
CO2Et
N
OCH3
(±) 4hf
1H NMR (400 MHz, CDCl3)
f1 (ppm)


AP-Kito-PMP
HO
CO2Et
CO2Et
N
OCH3
(±) 4hf
13C NMR (100 MHz, CDCl3)
f1 (ppm)

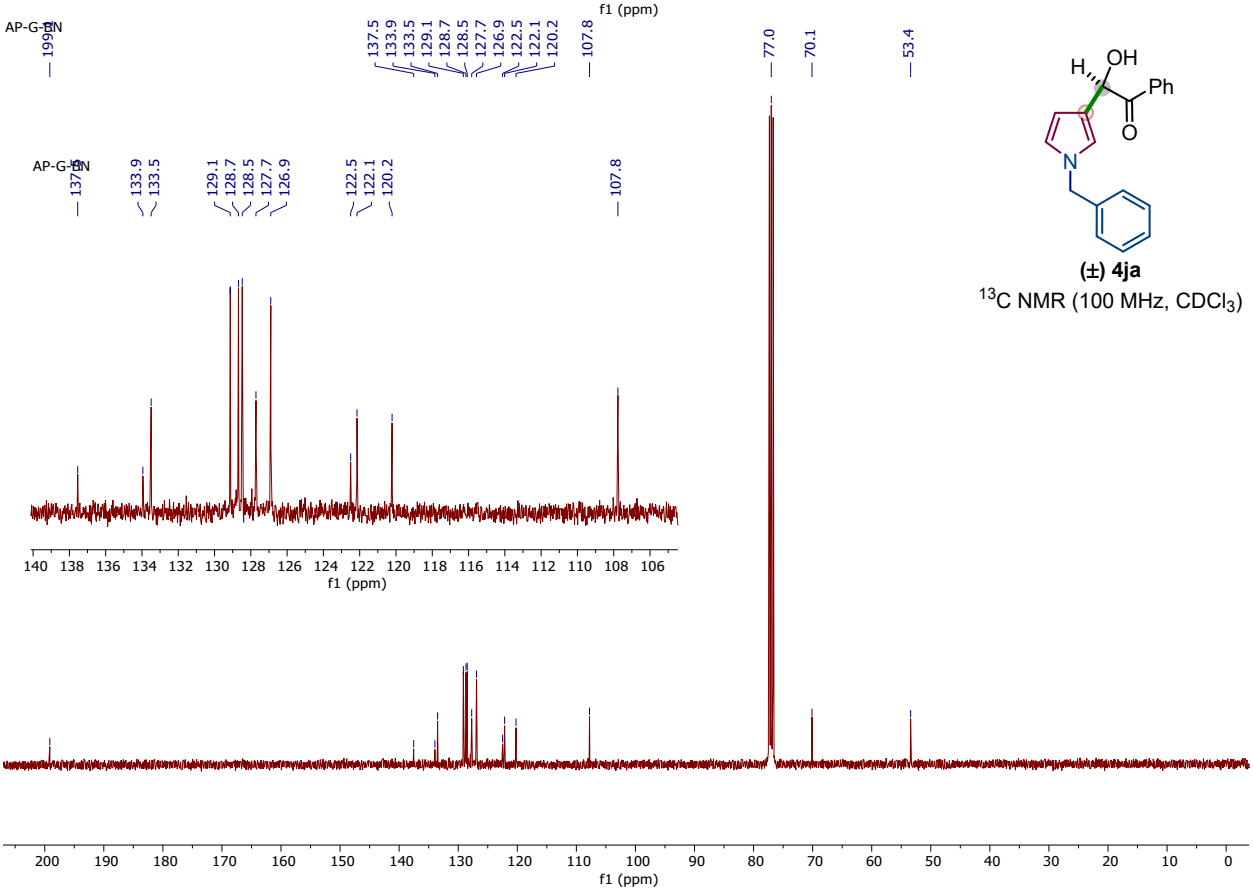

AP-EG-BZ
H
CO2Et
OH
N
(±) 4ia
1H NMR (400 MHz, CDCl3)
f1 (ppm)


AP-EG-BZ
H
CO2Et
OH
N
(±) 4ia
13C NMR (100 MHz, CDCl3)
f1 (ppm)



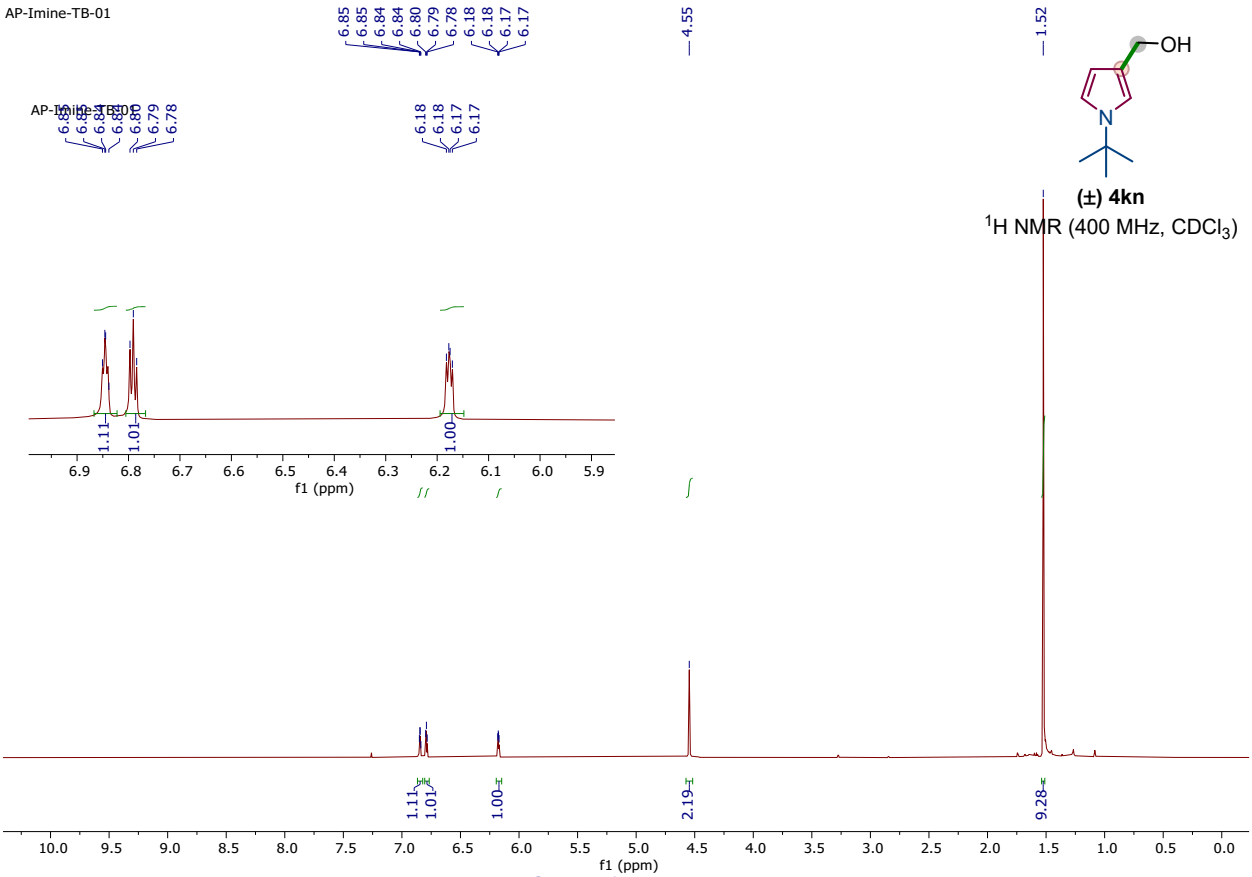
(±) 4ja

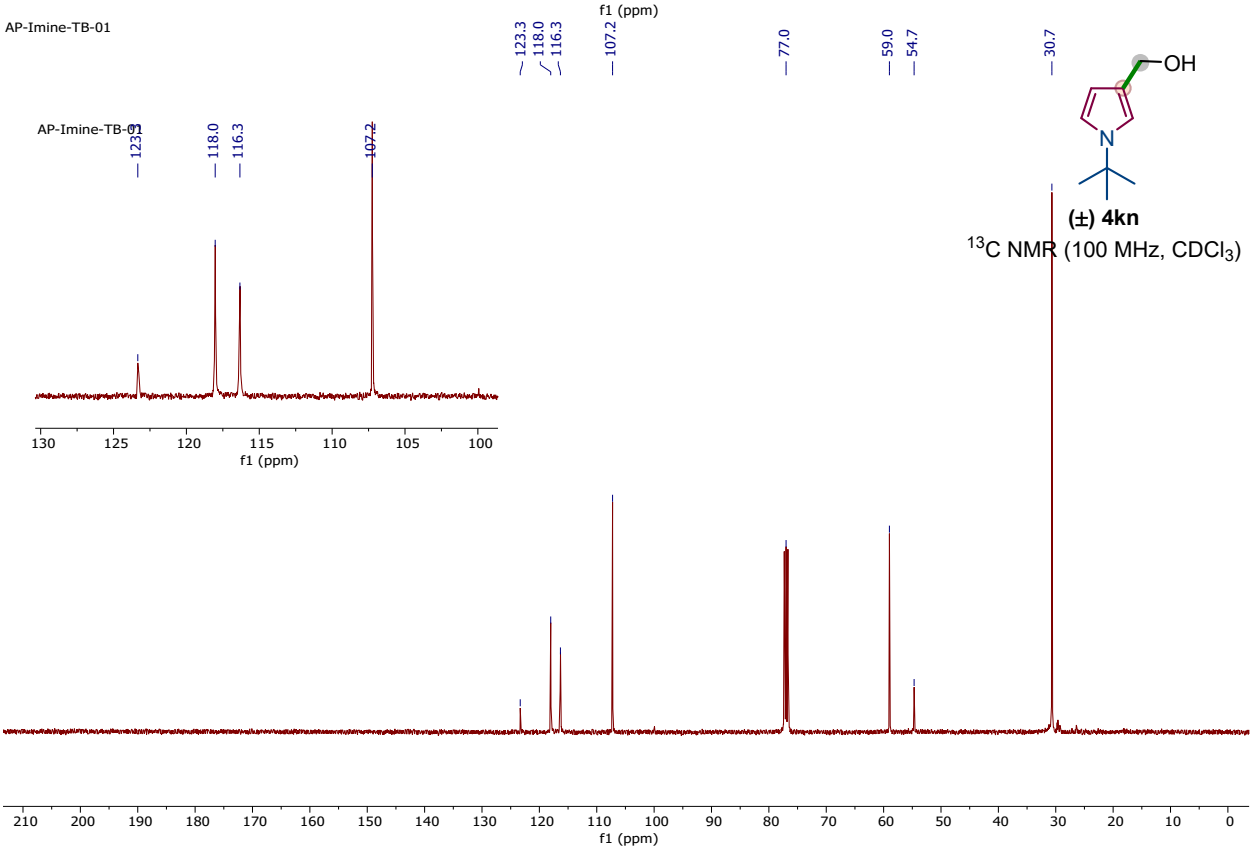
^{1}H NMR (400 MHz, $CDCl_3$)

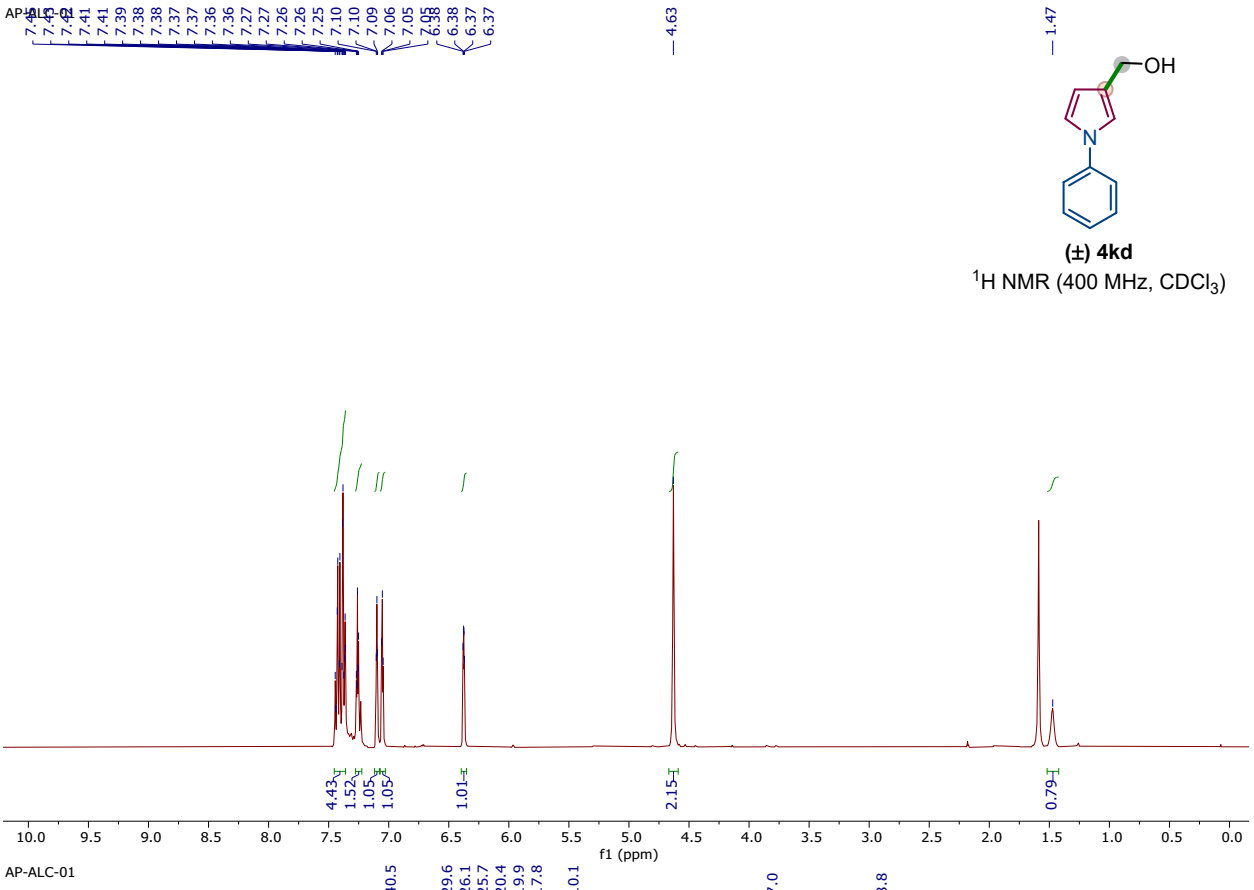


(±) 4ja

^{13}C NMR (100 MHz, $CDCl_3$)

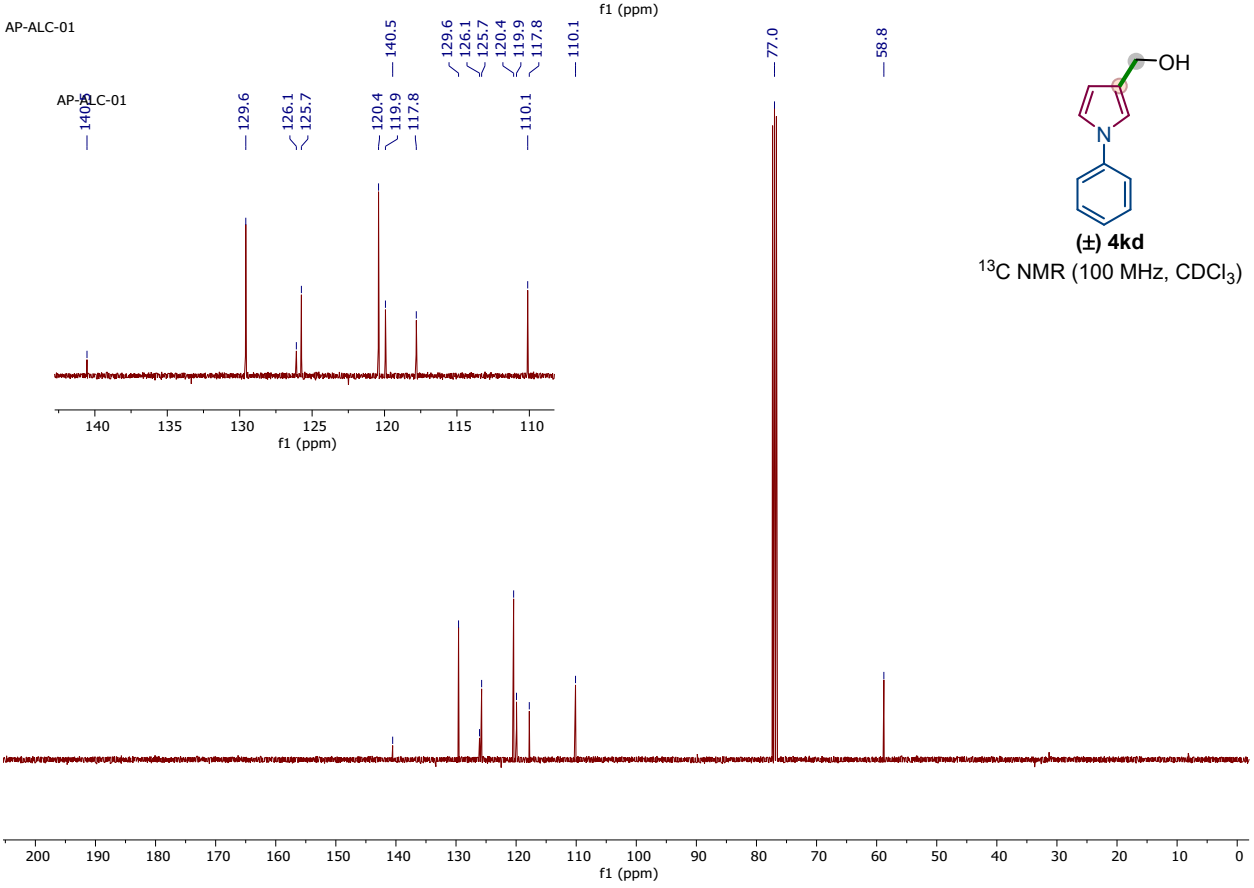

AP-Imine-TB-01
6.85
6.85
6.84
6.84
6.80
6.79
6.78
6.18
6.18
6.17
6.17
4.55
1.52
OH
N
(±) 4kn
^{1}H NMR (400 MHz, CDCl$_3$)
1.11
1.01
1.00
2.19
9.28
f1 (ppm)


AP-Imine-TB-01
123.3
118.0
116.3
107.2
77.0
59.0
54.7
30.7
OH
N
(±) 4kn
^{13}C NMR (100 MHz, CDCl$_3$)
f1 (ppm)



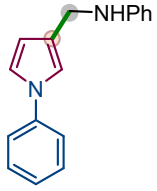
(±) 4kd

^{1}H NMR (400 MHz, $CDCl_3$)



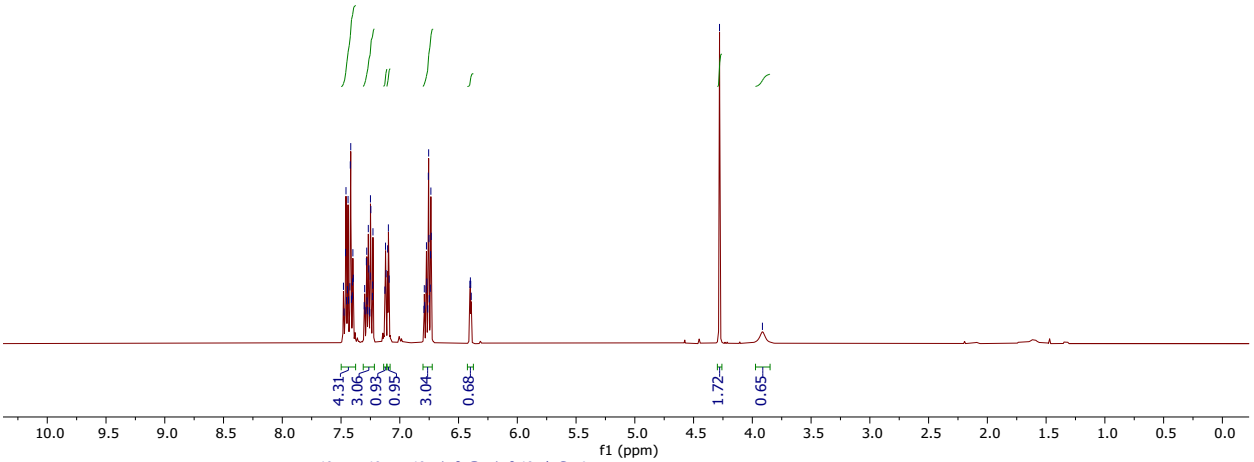
(±) 4kd

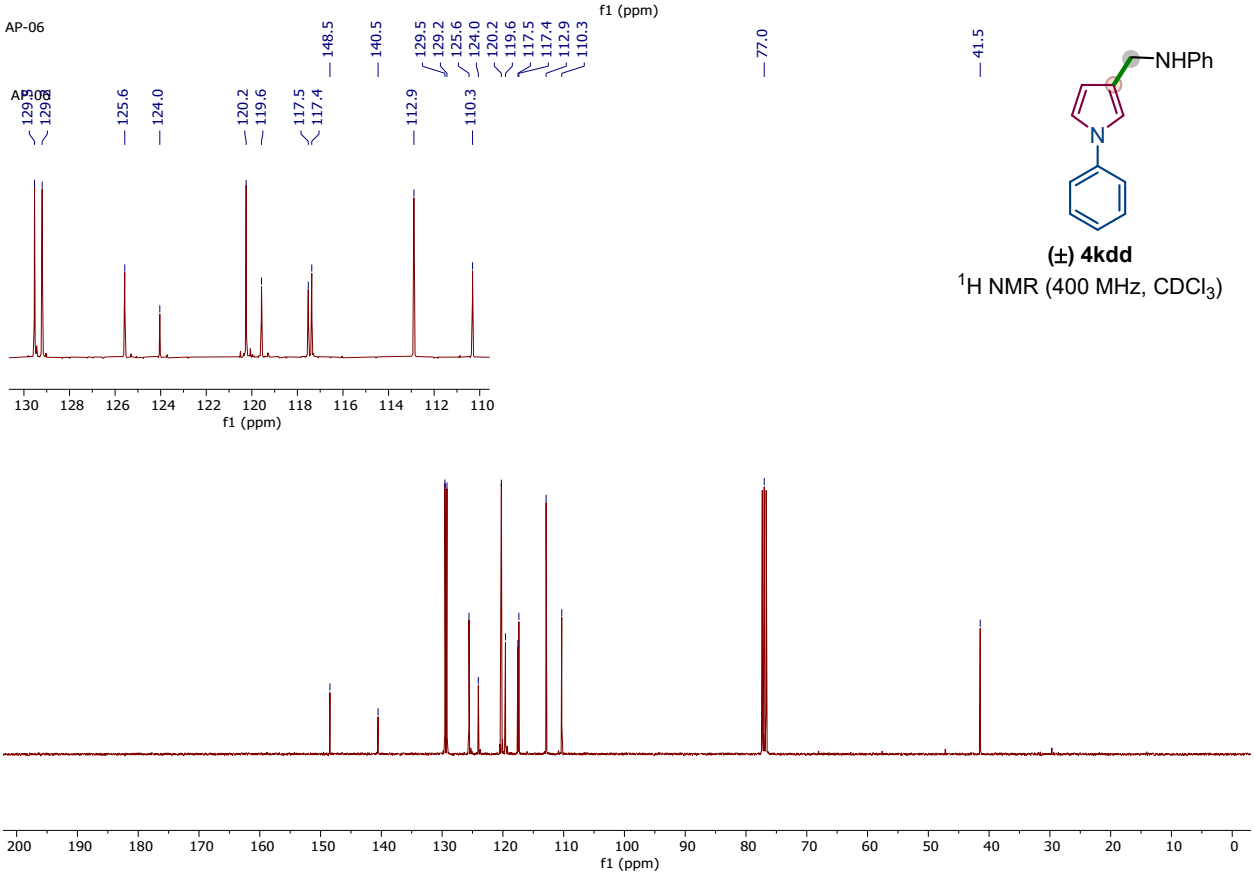
^{13}C NMR (100 MHz, $CDCl_3$)



(±) 4kdd

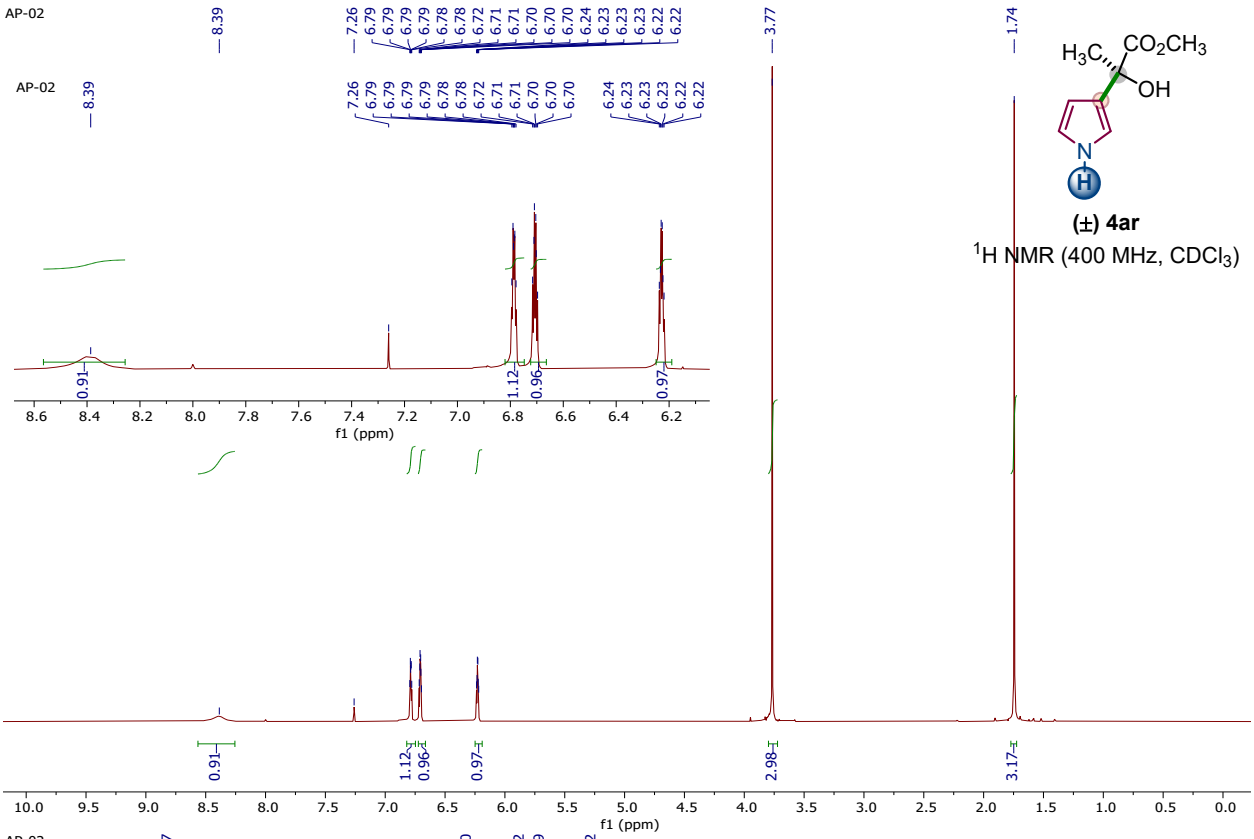
^{13}C NMR (100 MHz, $CDCl_3$)





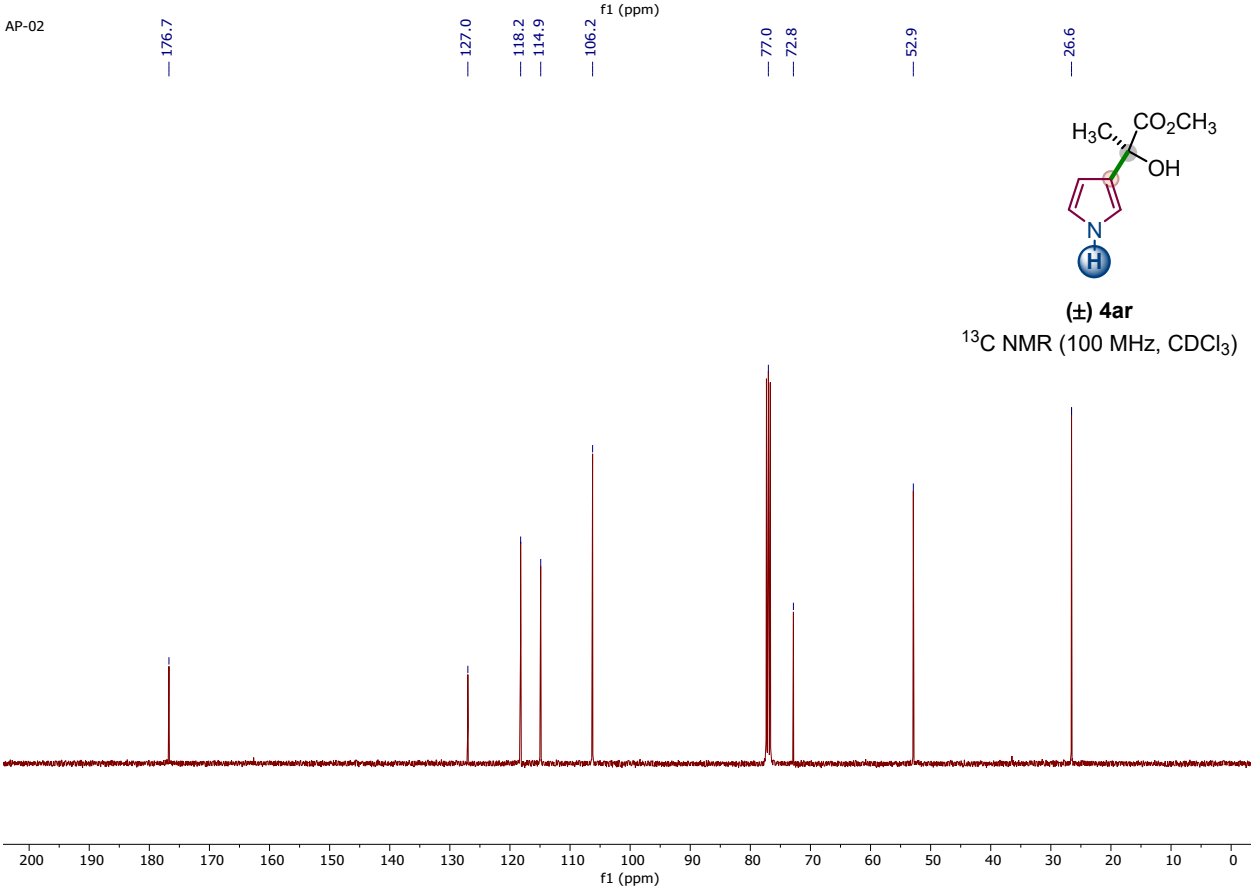
(±) 4kdd

^{1}H NMR (400 MHz, $CDCl_3$)



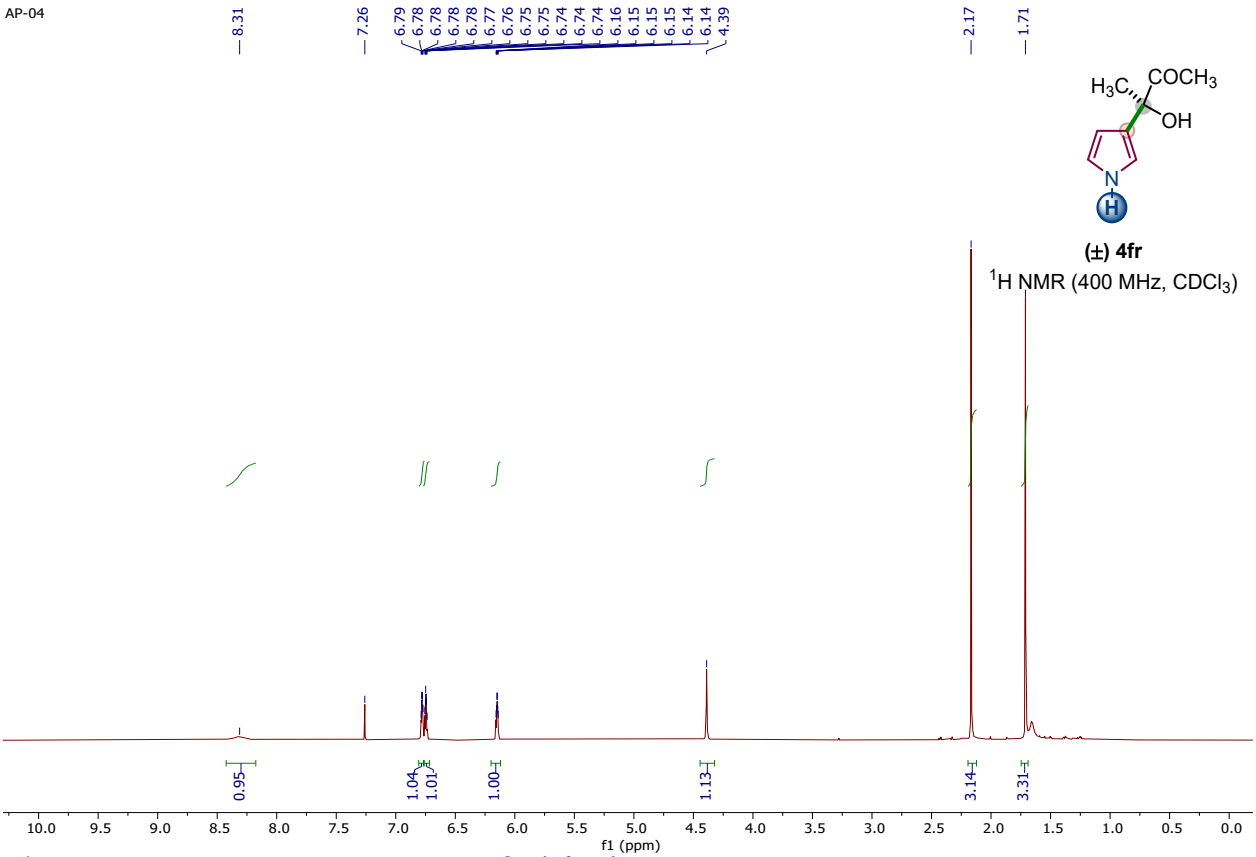
(±) 4ar

^{1}H NMR (400 MHz, $CDCl_3$)



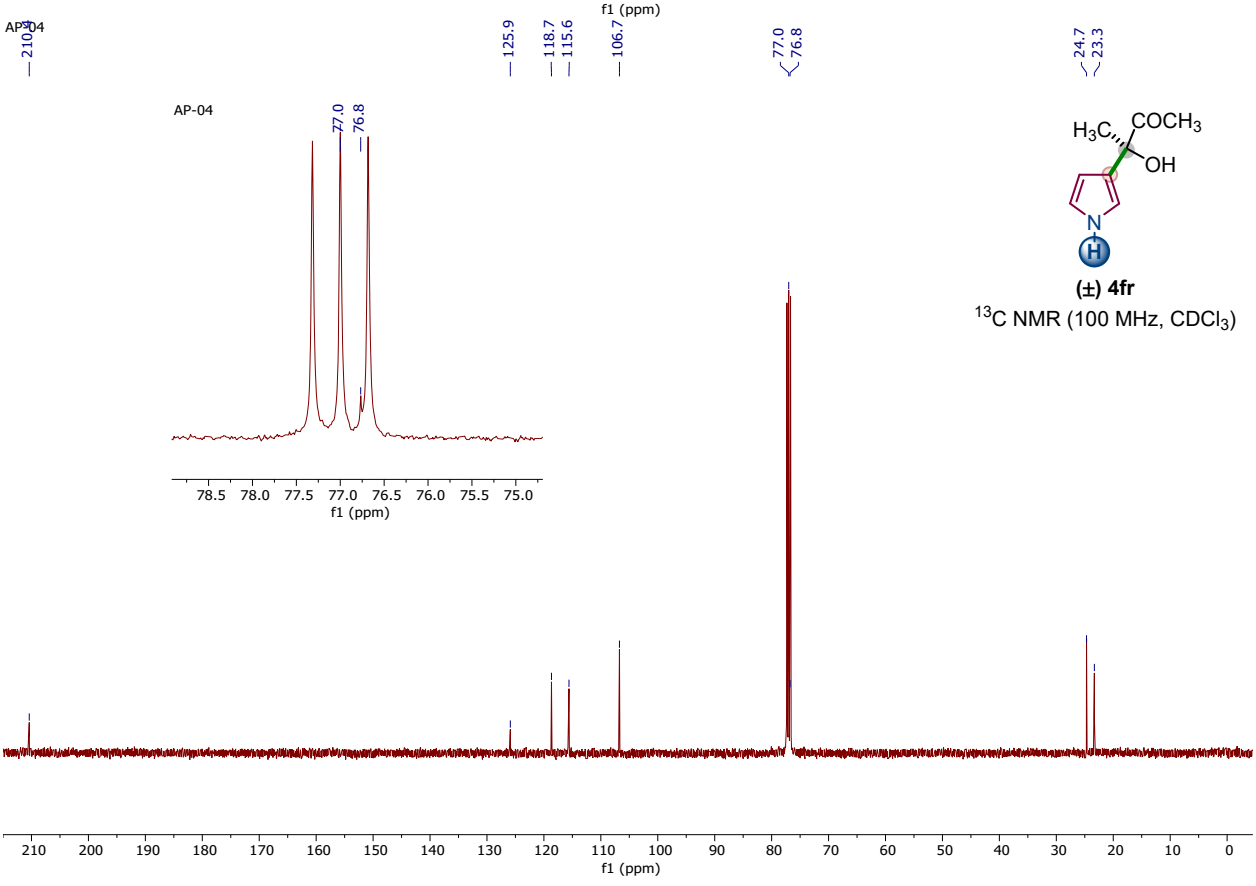
(±) 4ar

^{13}C NMR (100 MHz, $CDCl_3$)



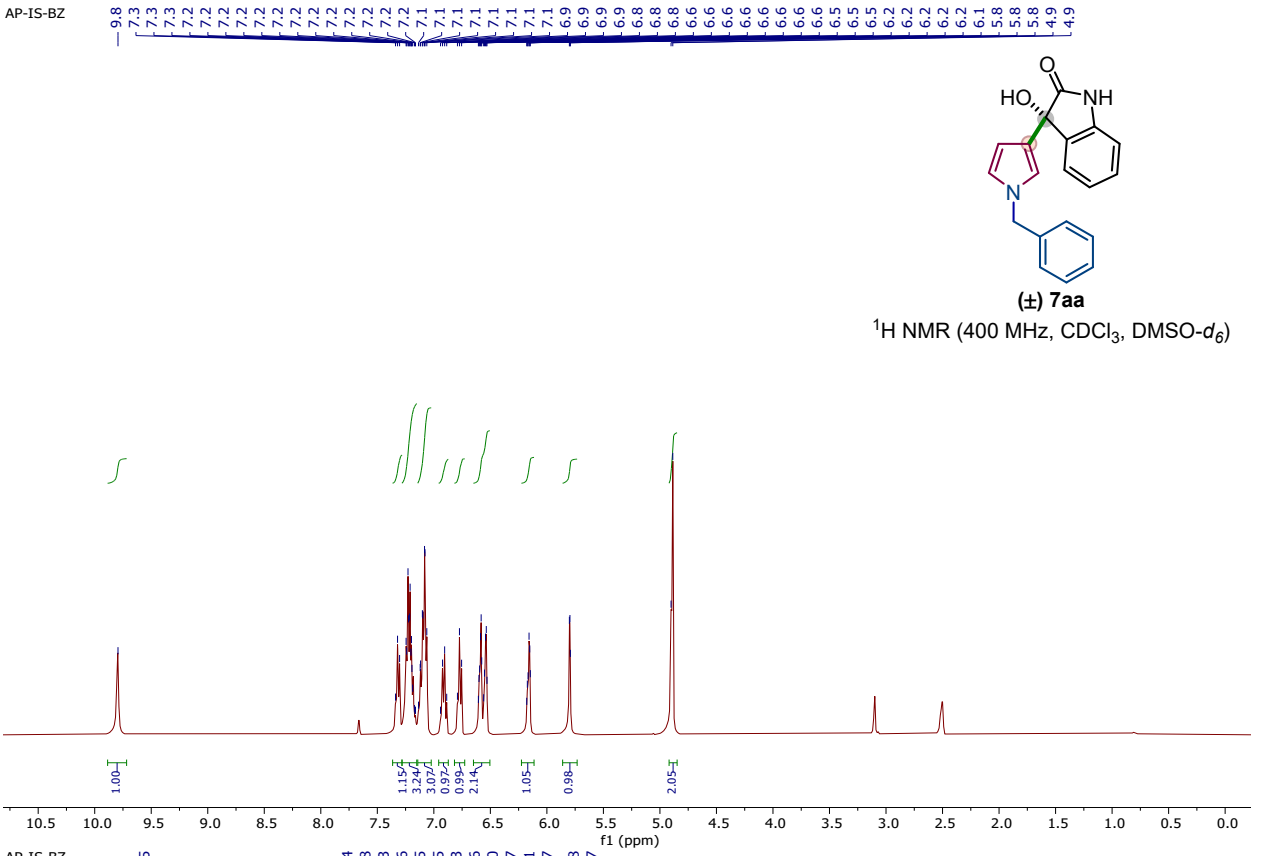
(±) 4fr

^{1}H NMR (400 MHz, $CDCl_3$)



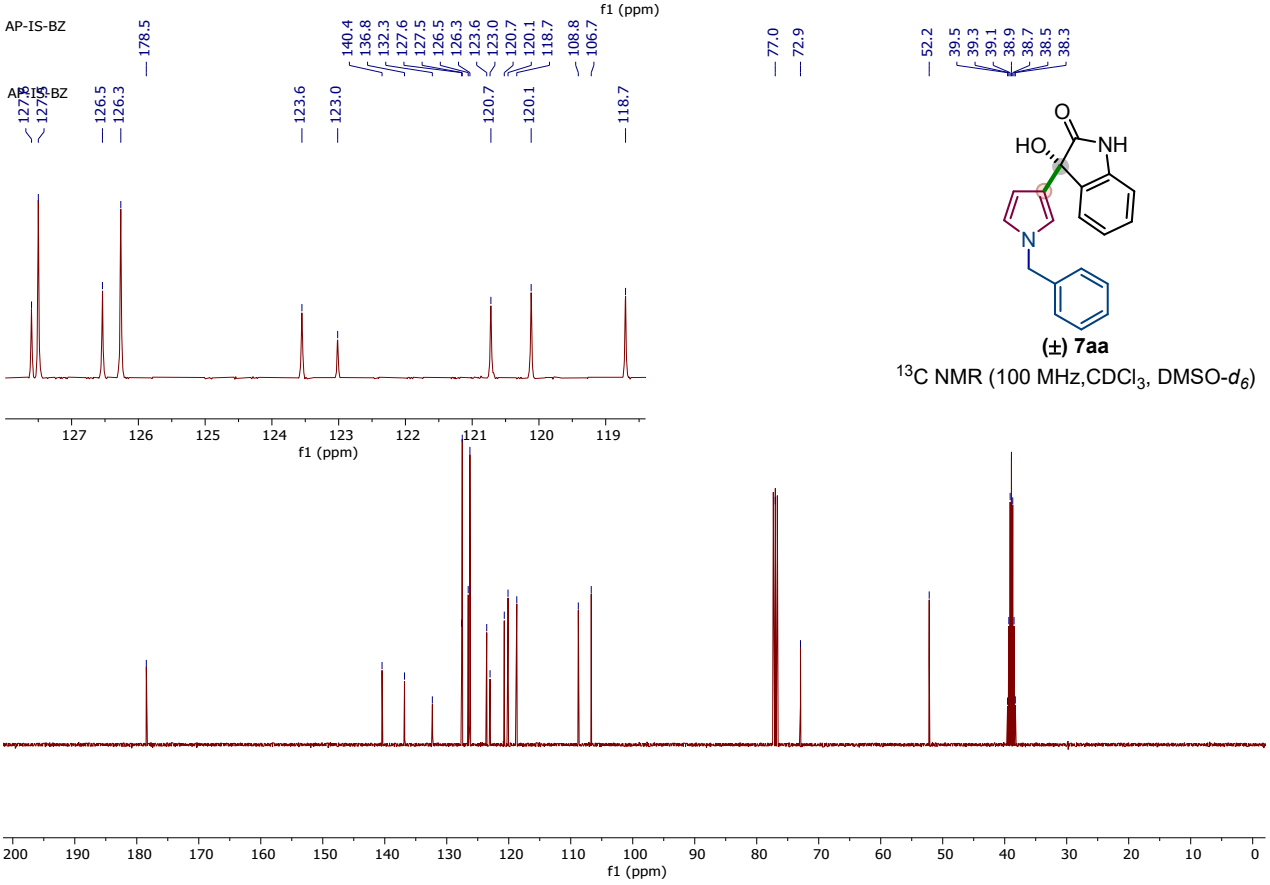
(±) 4fr

^{13}C NMR (100 MHz, $CDCl_3$)



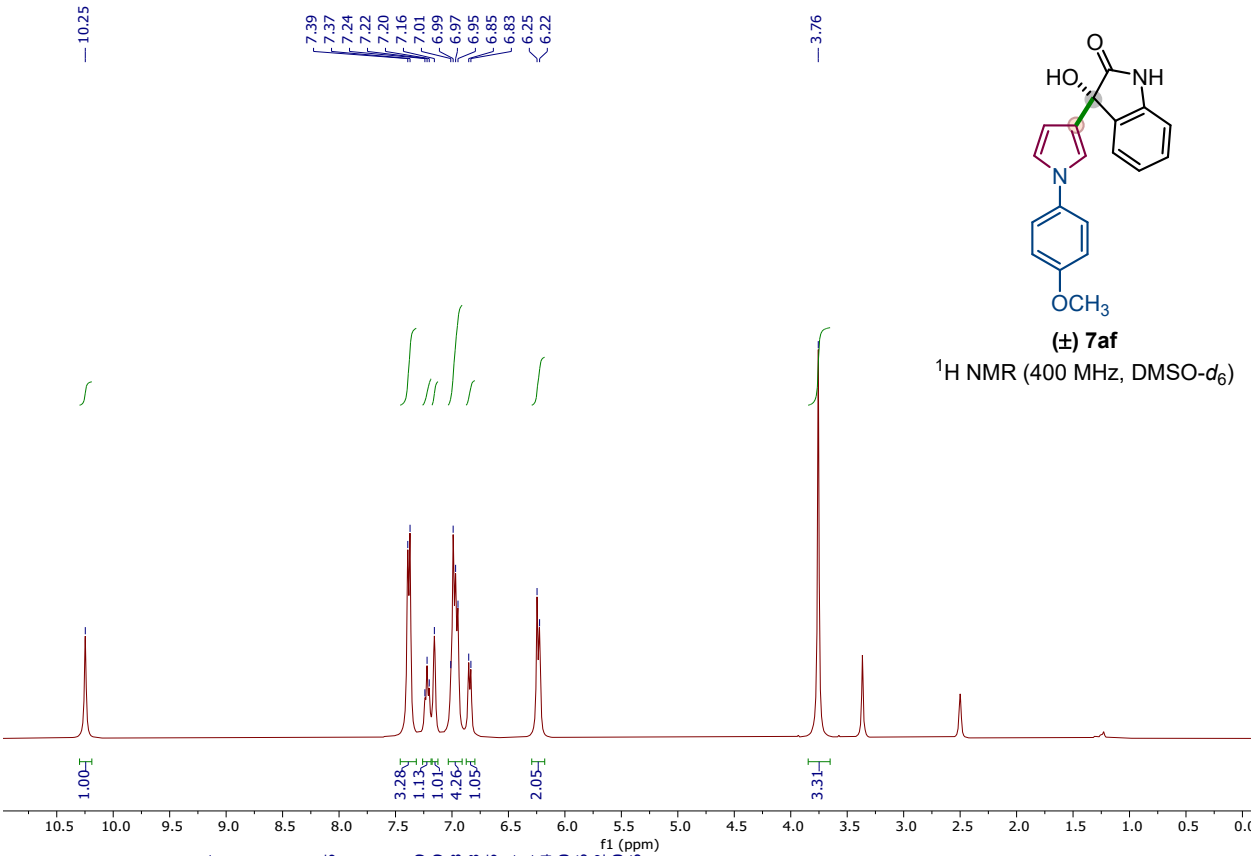
(±) 7aa

^{1}H NMR (400 MHz, $CDCl_3$, DMSO-d_6)



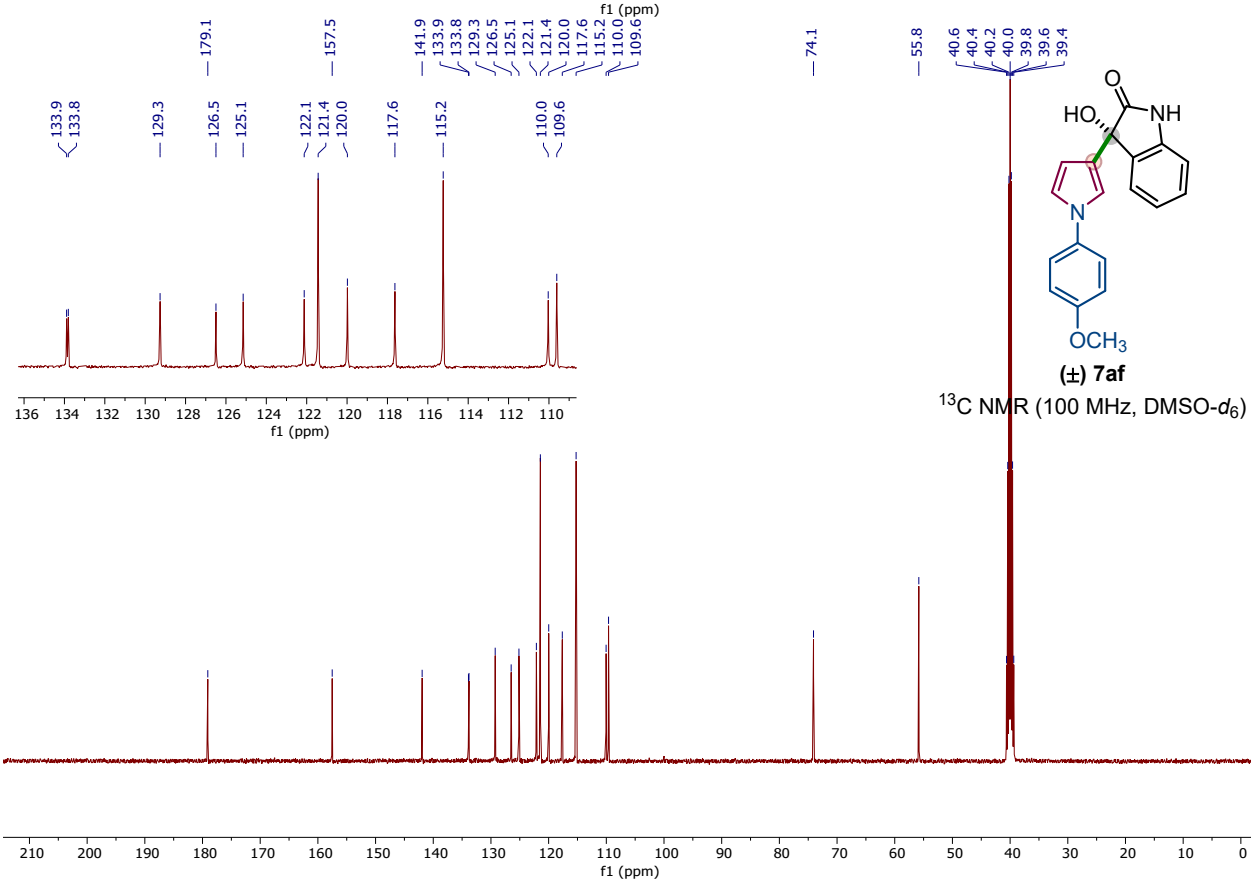
(±) 7aa

^{13}C NMR (100 MHz,$CDCl_3$, DMSO-d_6)



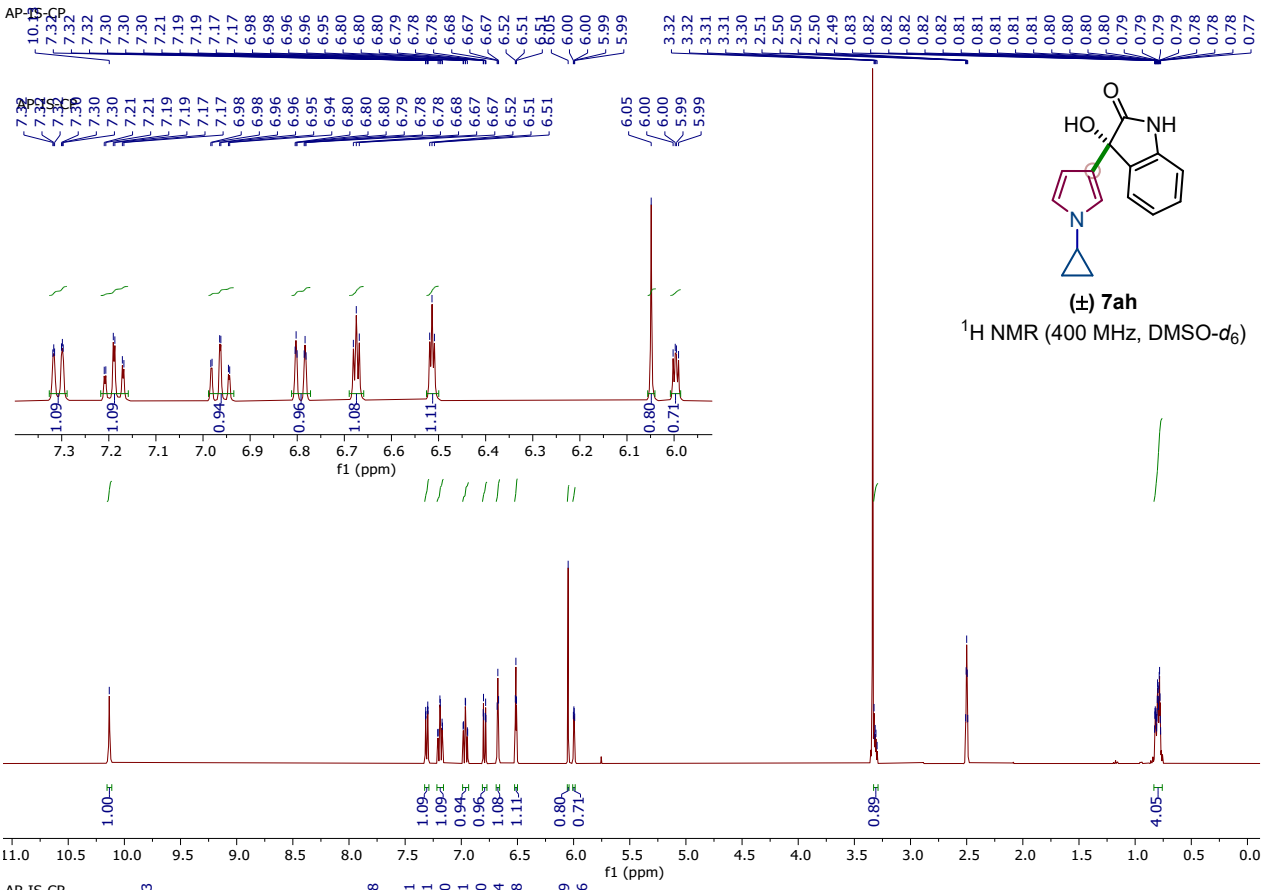
(±) 7af

^{1}H NMR (400 MHz, DMSO-d_6)



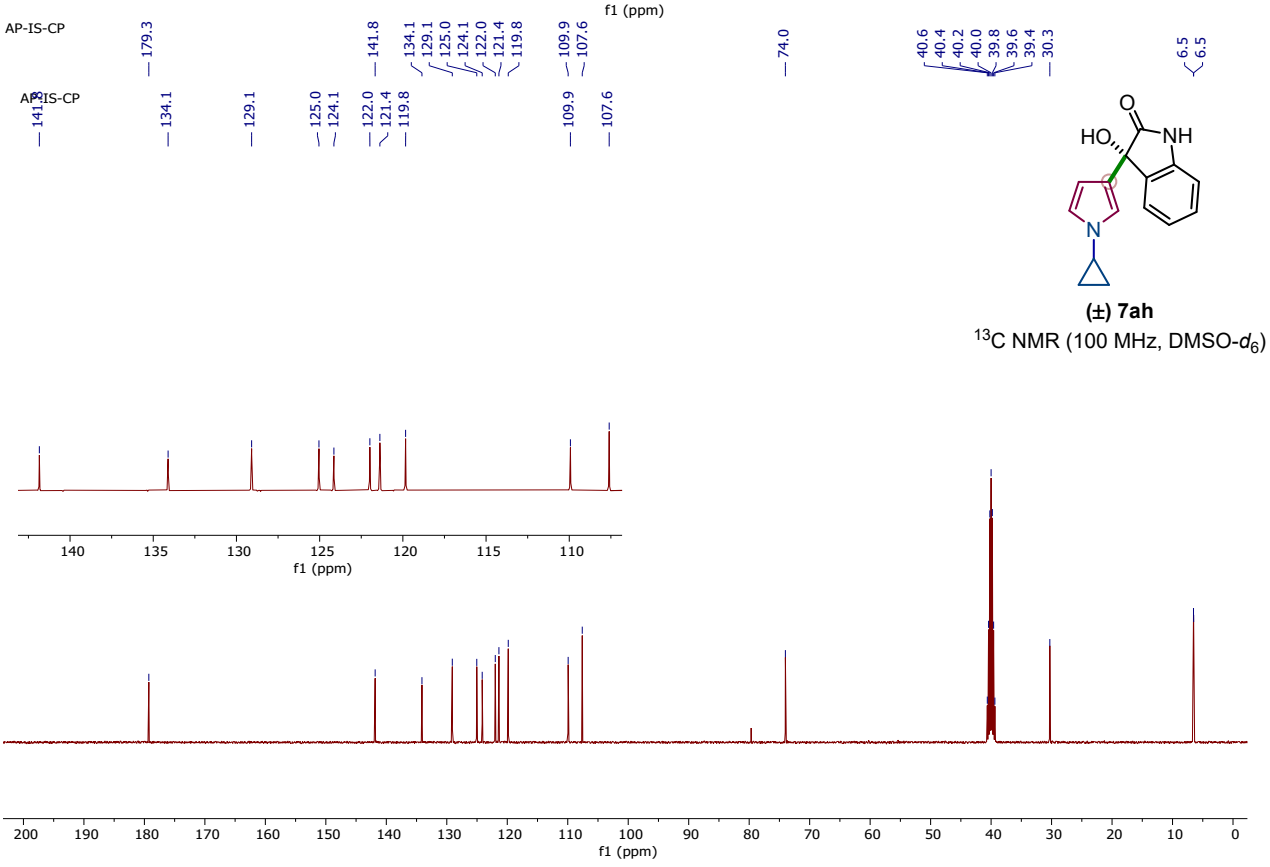
(±) 7af

^{13}C NMR (100 MHz, DMSO-d_6)



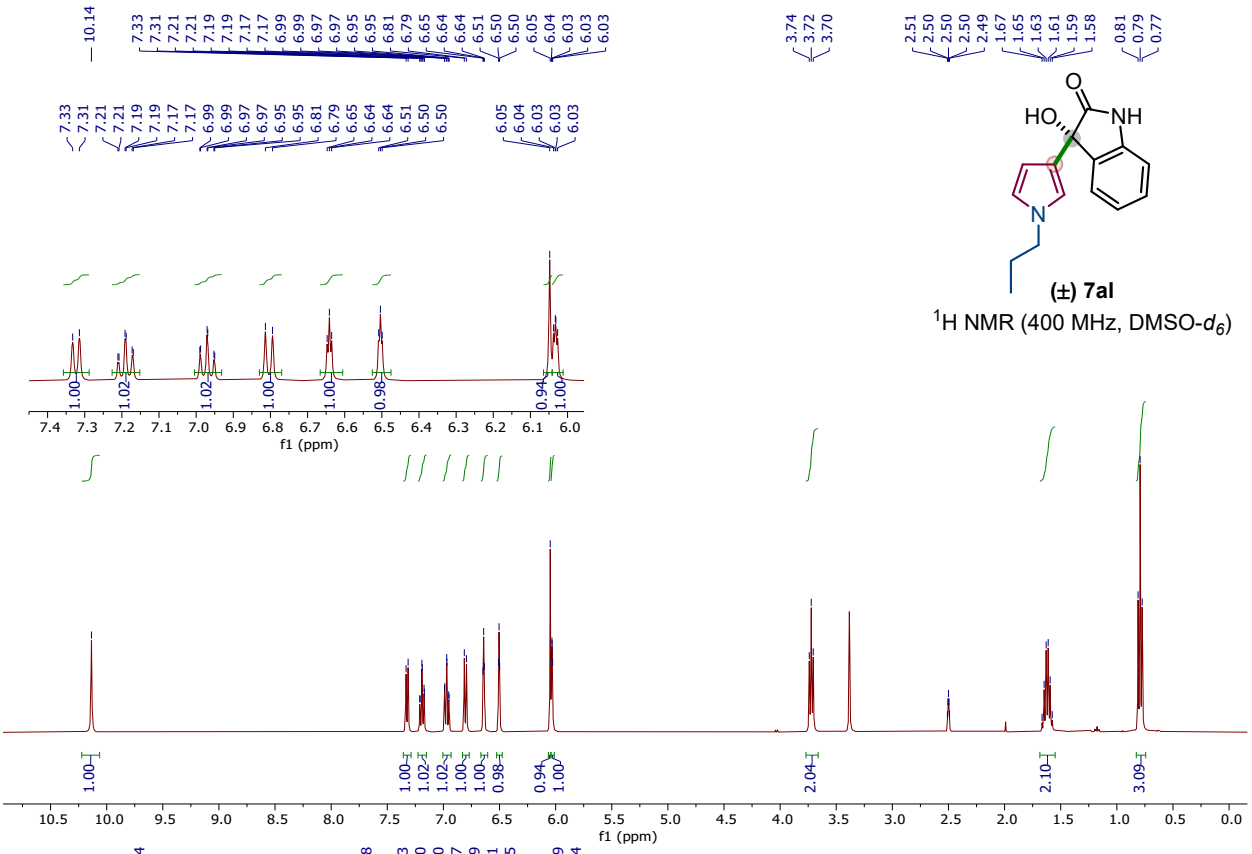
(±) 7ah

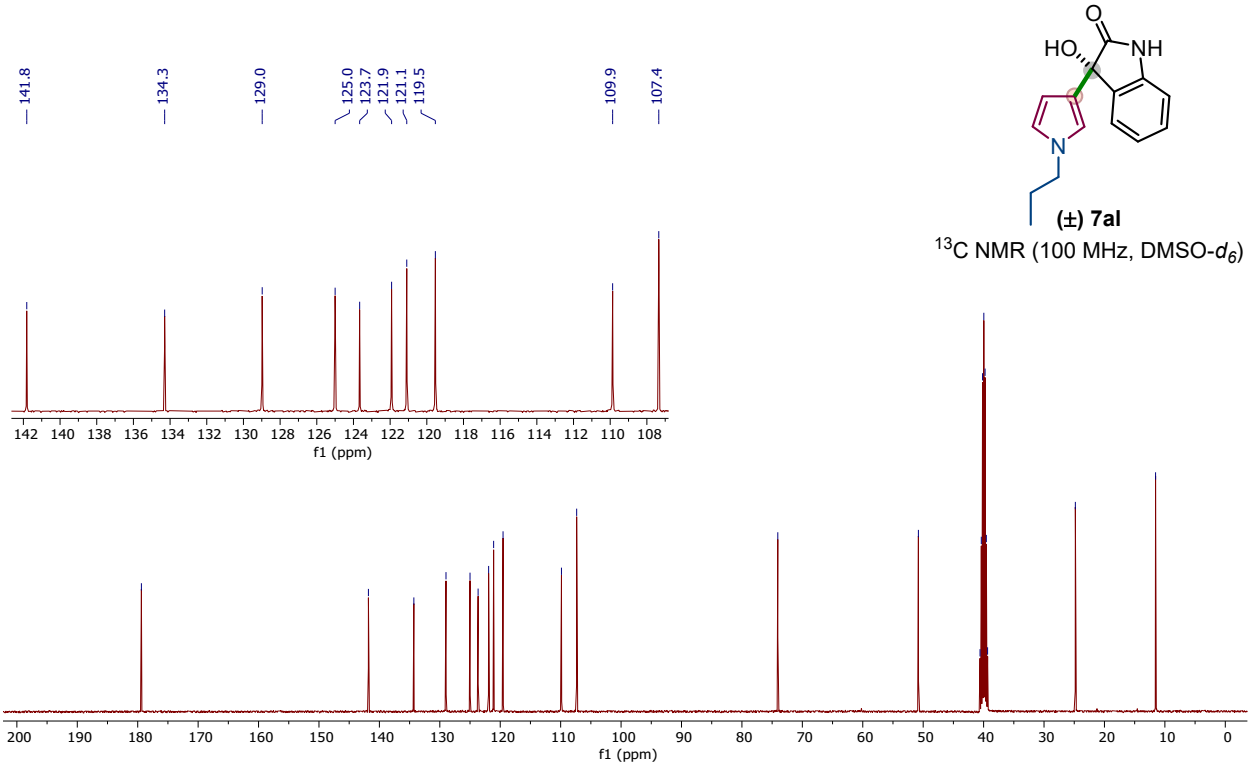
^{1}H NMR (400 MHz, DMSO-d_6)

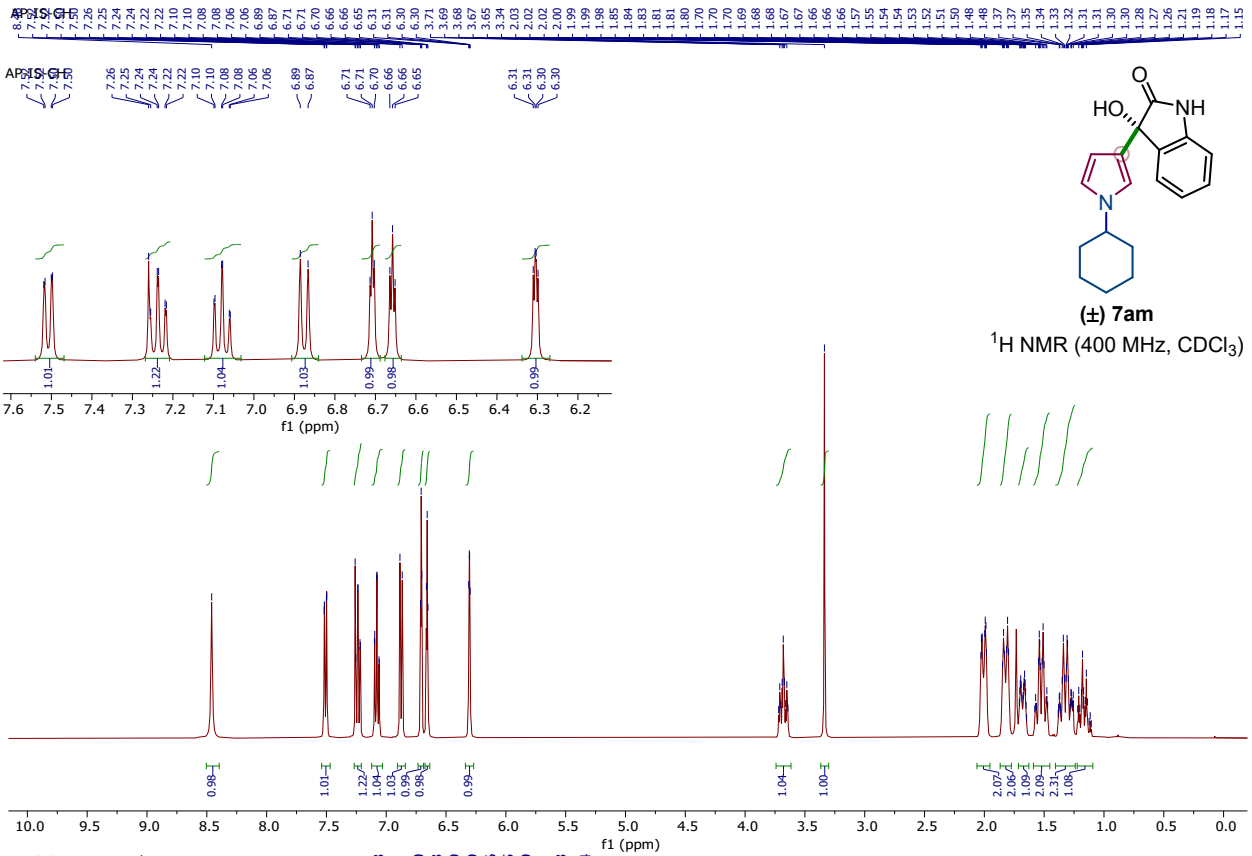


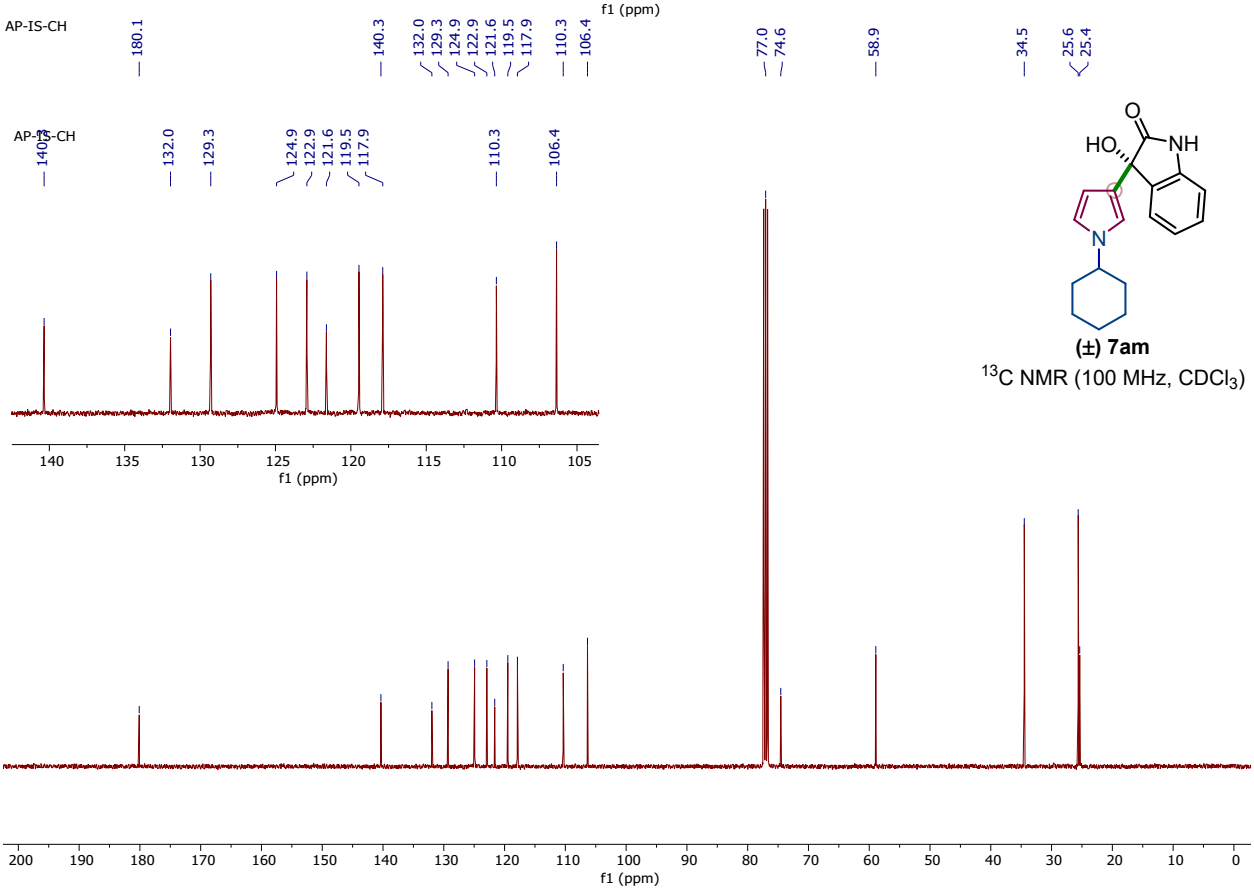
(±) 7ah

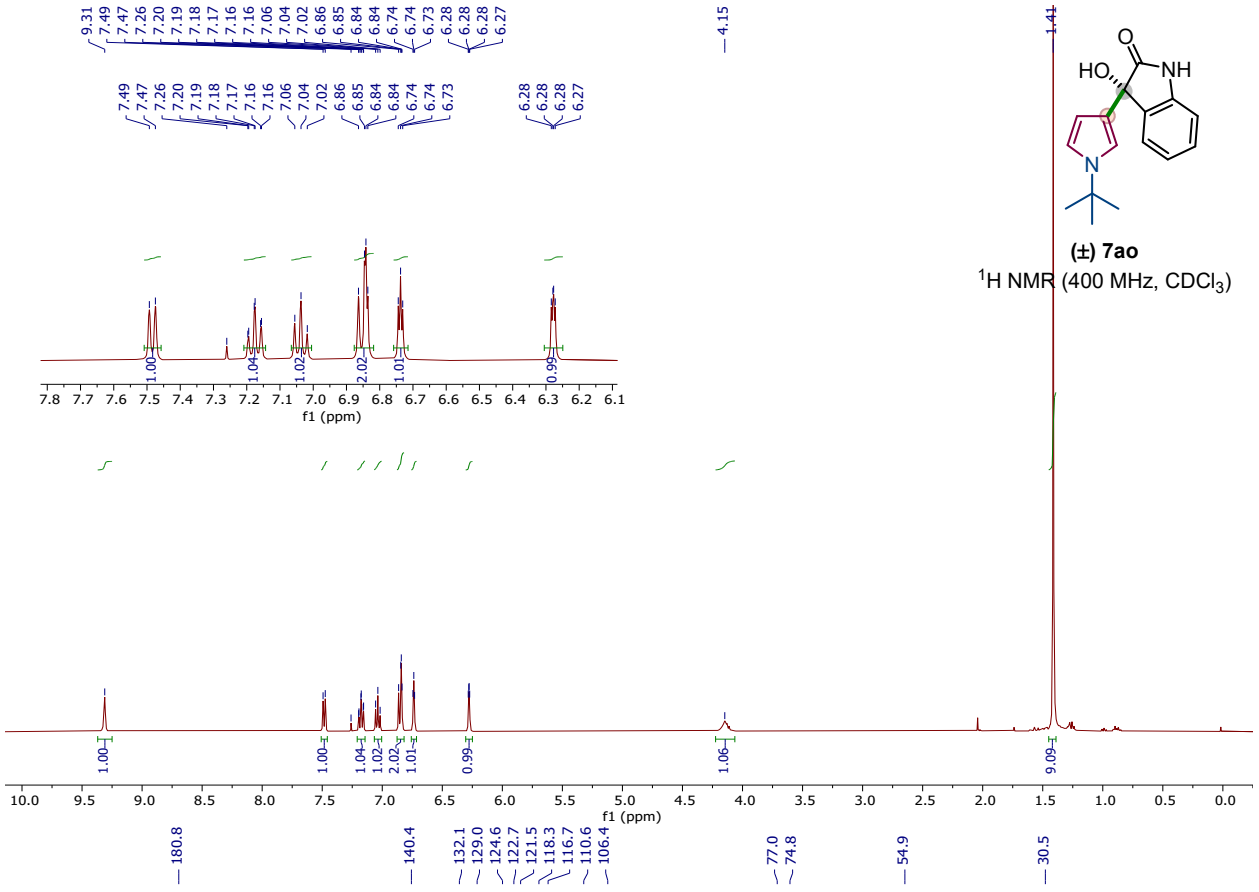
^{13}C NMR (100 MHz, DMSO-d_6)

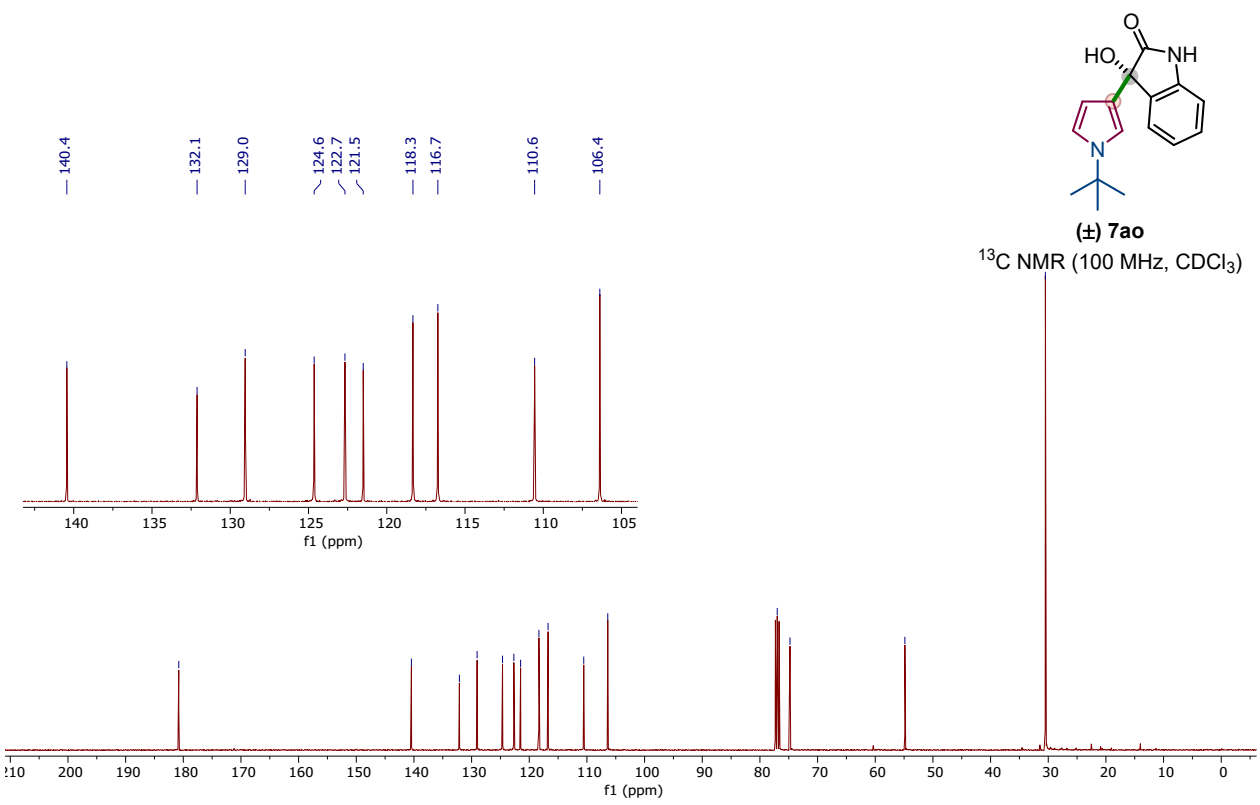

HO
O
NH
N
(±) 7al
^{1}H NMR (400 MHz, DMSO-d_6)
f1 (ppm)

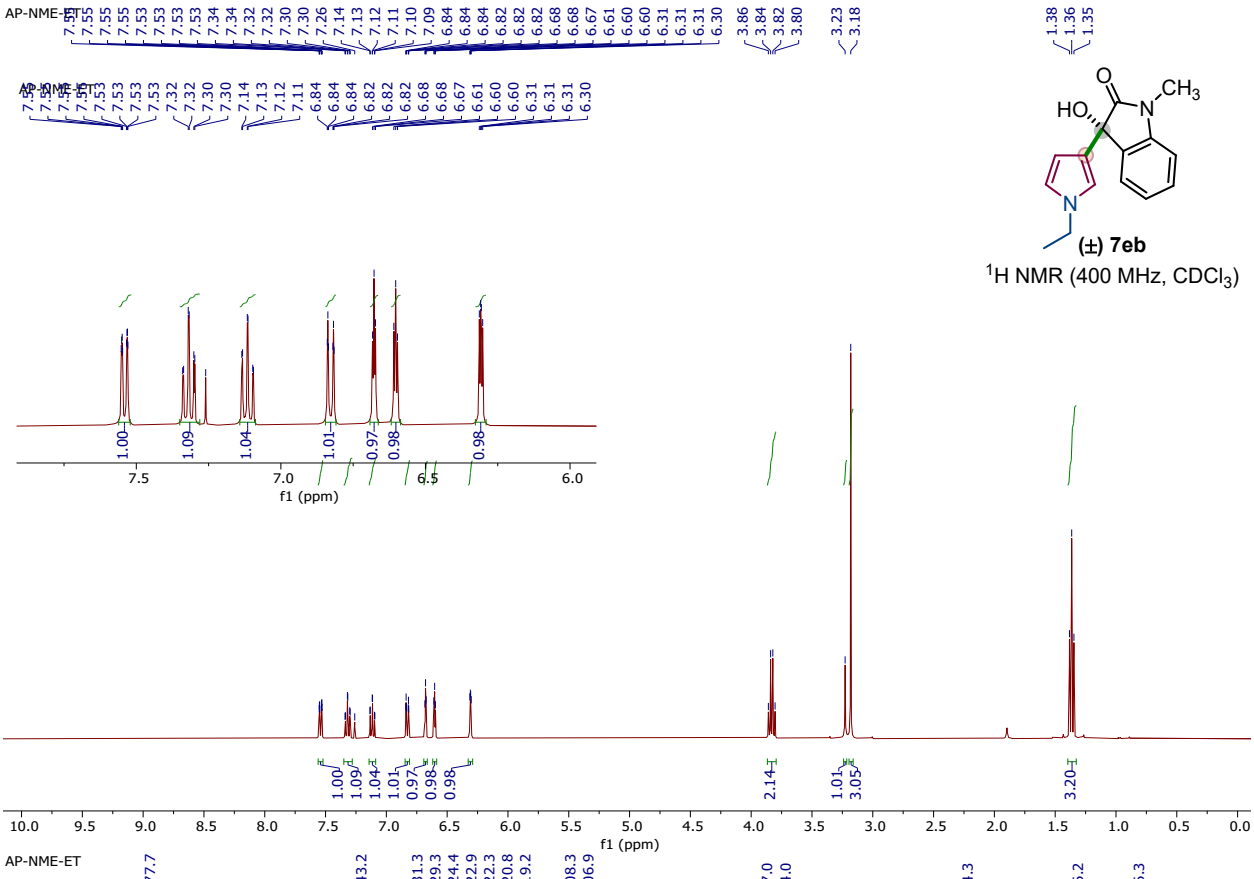

HO
O
NH
N
(±) 7al
^{13}C NMR (100 MHz, DMSO-d_6)
f1 (ppm)


AP-IS-CH
HO
NH
O
N
(±) 7am
^{1}H NMR (400 MHz, CDCl$_3$)
f1 (ppm)


AP-IS-CH
HO
NH
O
N
(±) 7am
^{13}C NMR (100 MHz, CDCl$_3$)
f1 (ppm)

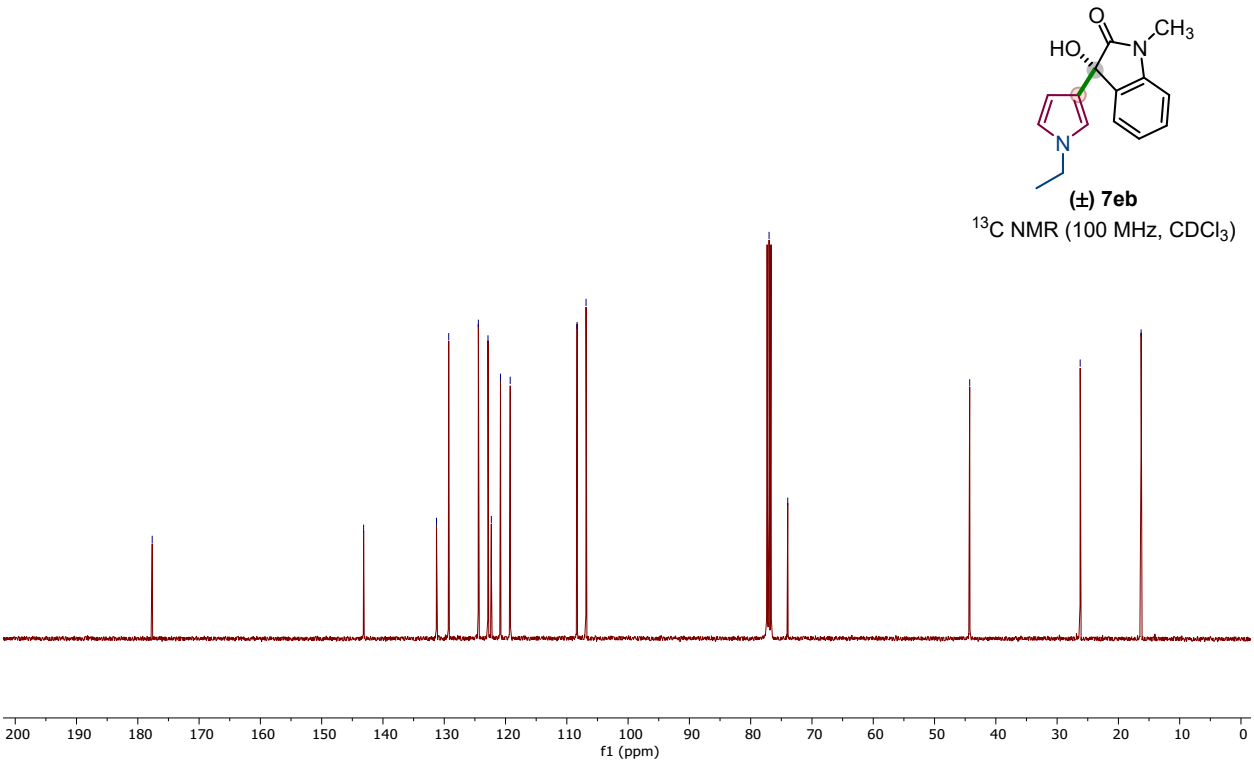

HO
O
NH
N
(±) 7ao
^{1}H NMR (400 MHz, CDCl$_3$)
f1 (ppm)


HO
O
NH
N
(±) 7ao
^{13}C NMR (100 MHz, CDCl$_3$)
f1 (ppm)



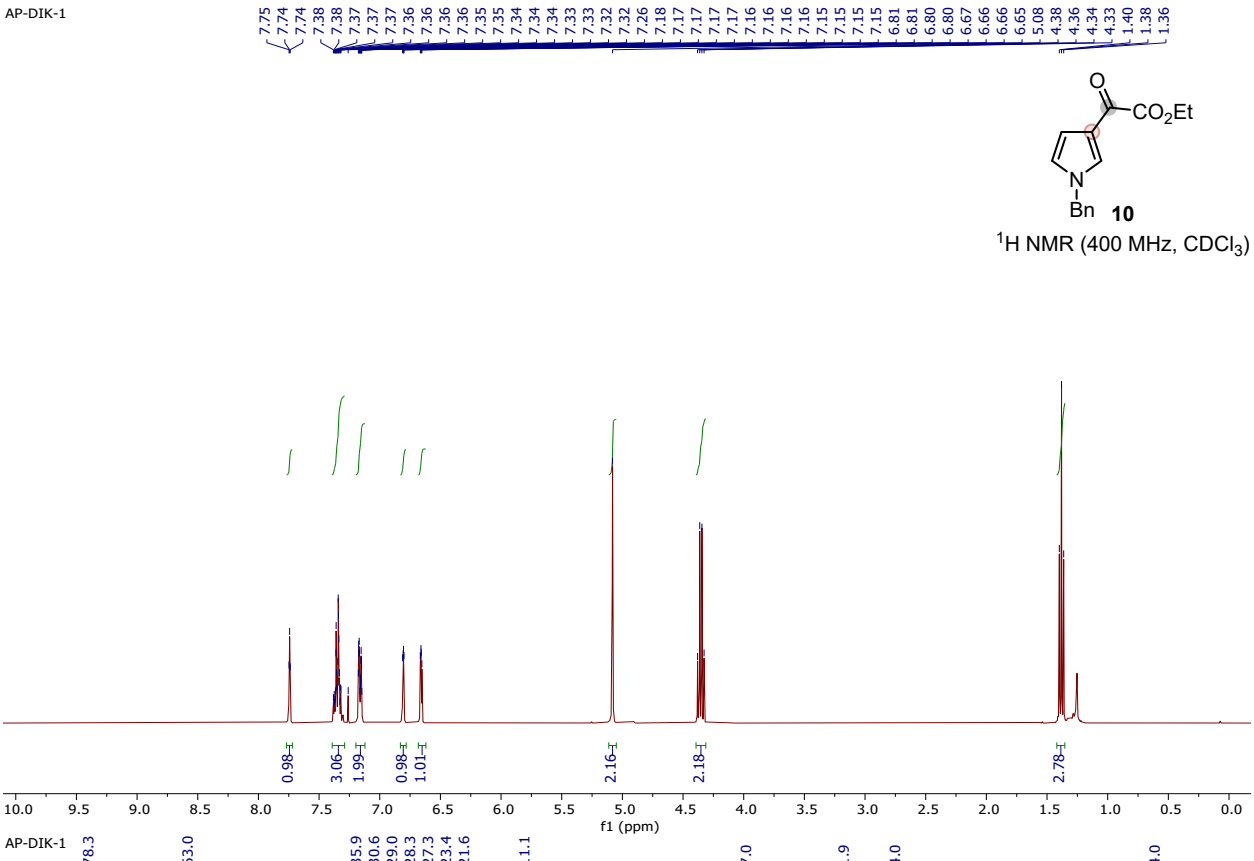
(±) **7eb**

^{1}H NMR (400 MHz, $CDCl_3$)

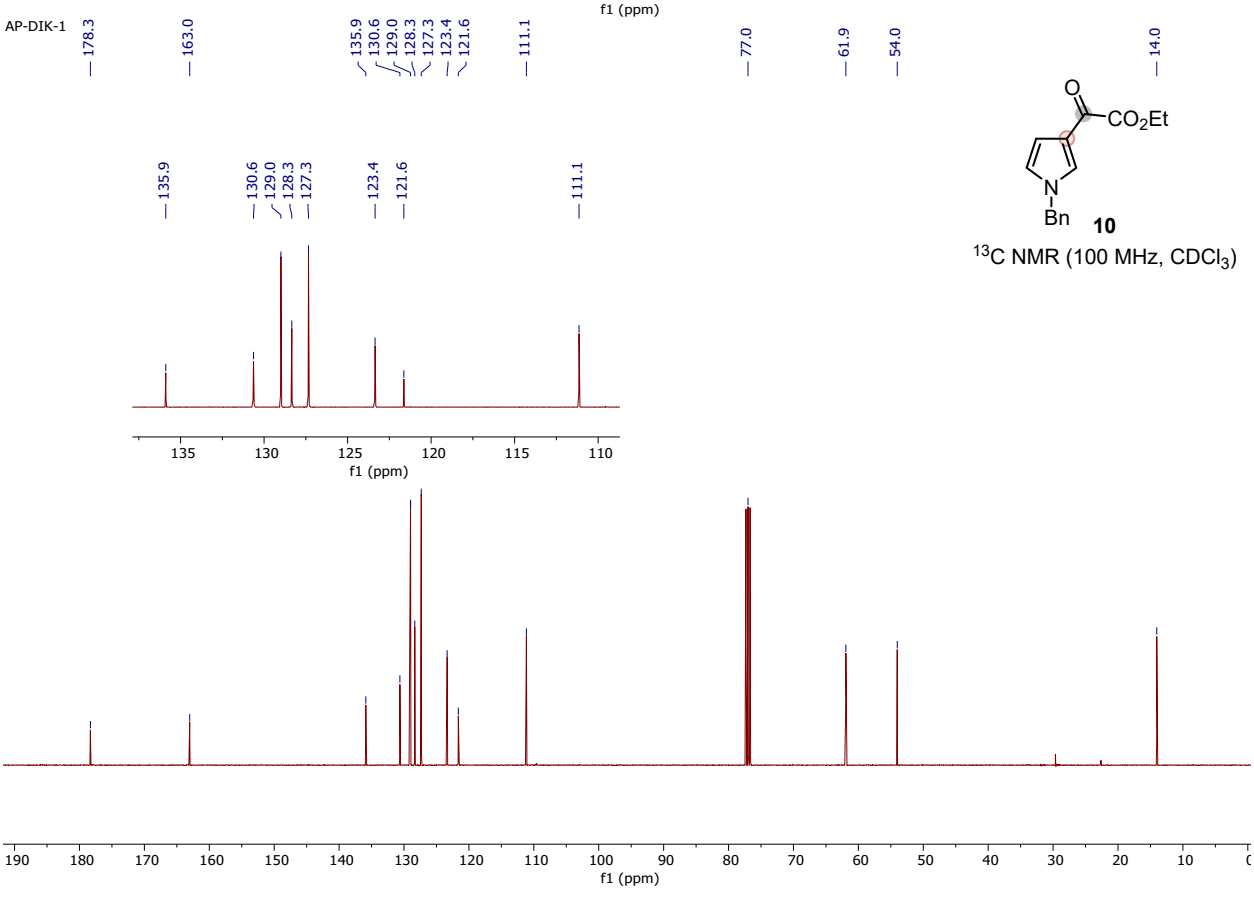


(±) **7eb**

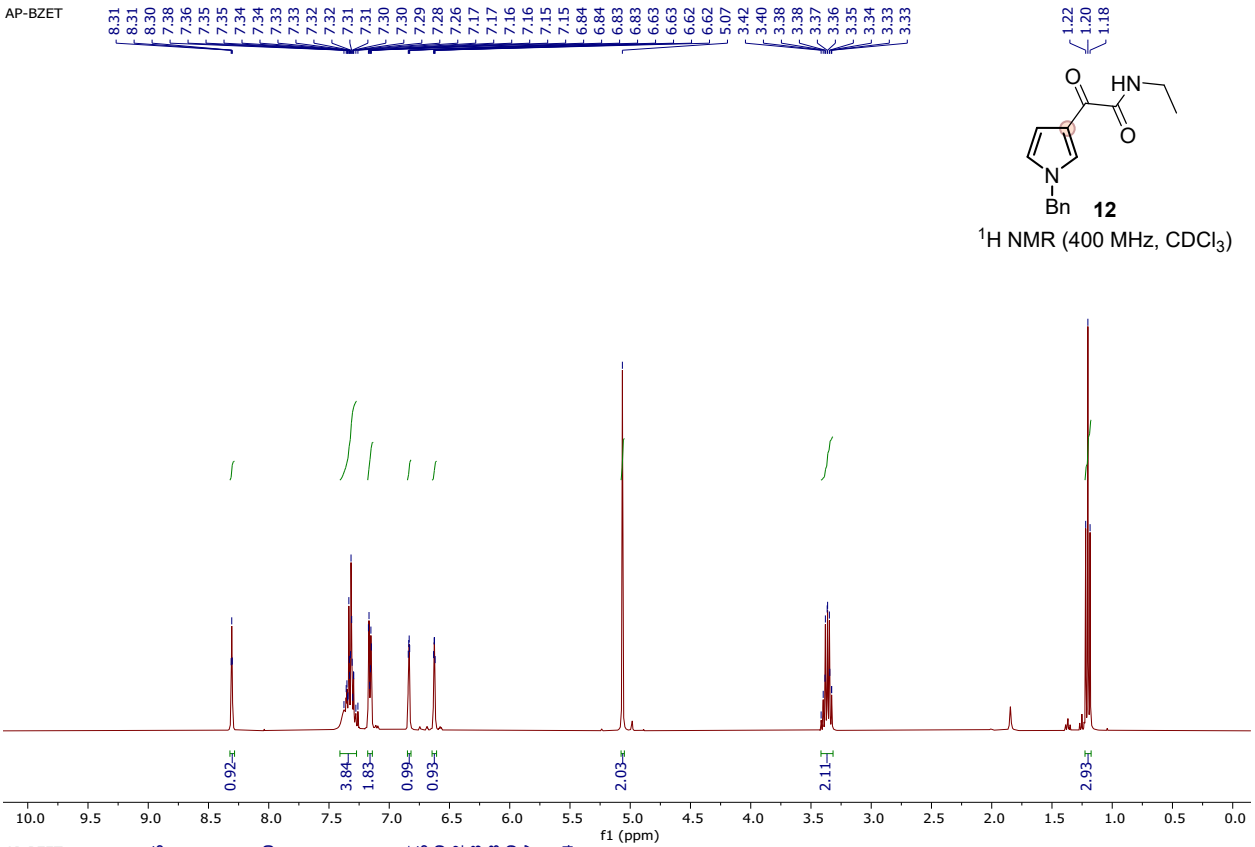
^{13}C NMR (100 MHz, $CDCl_3$)



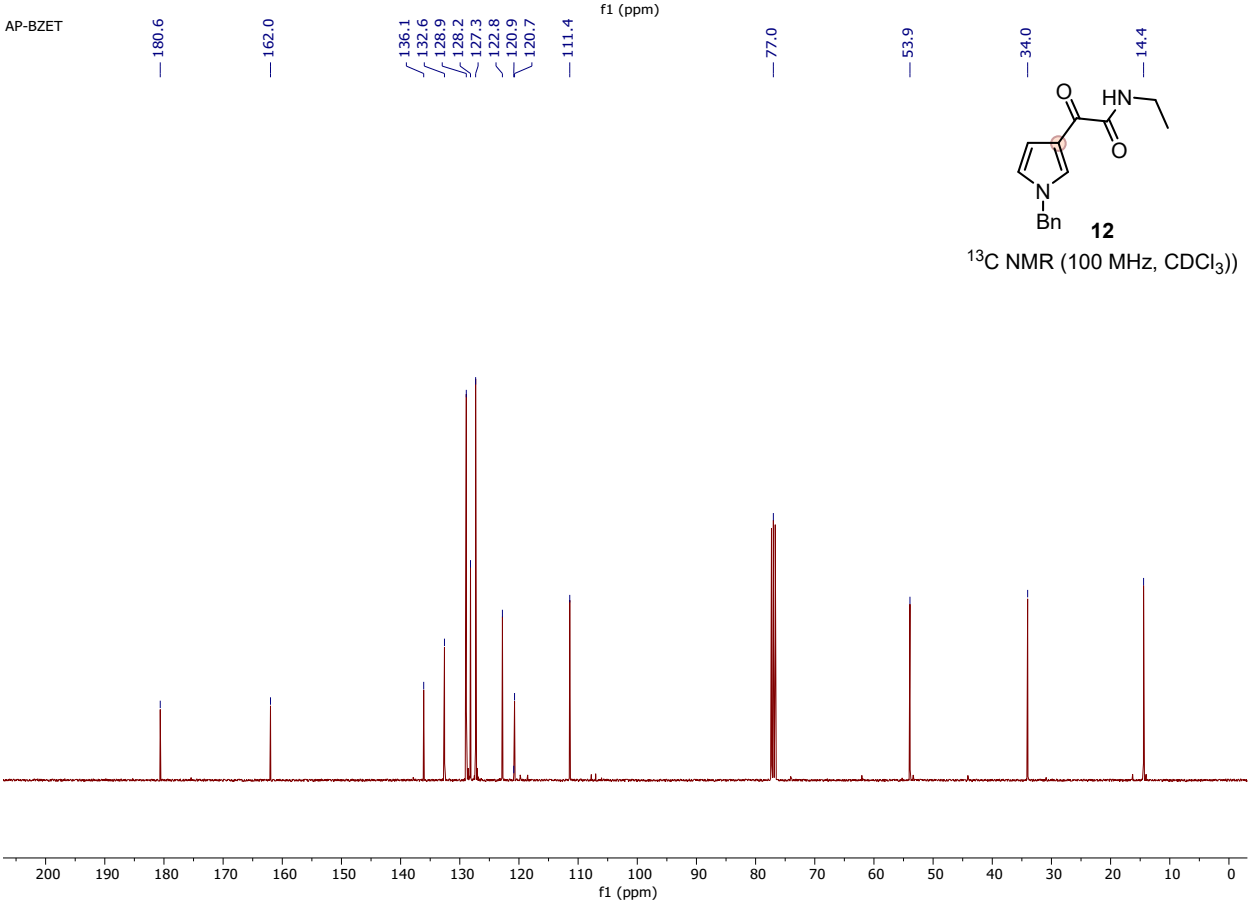
^{1}H NMR (400 MHz, $CDCl_3$)



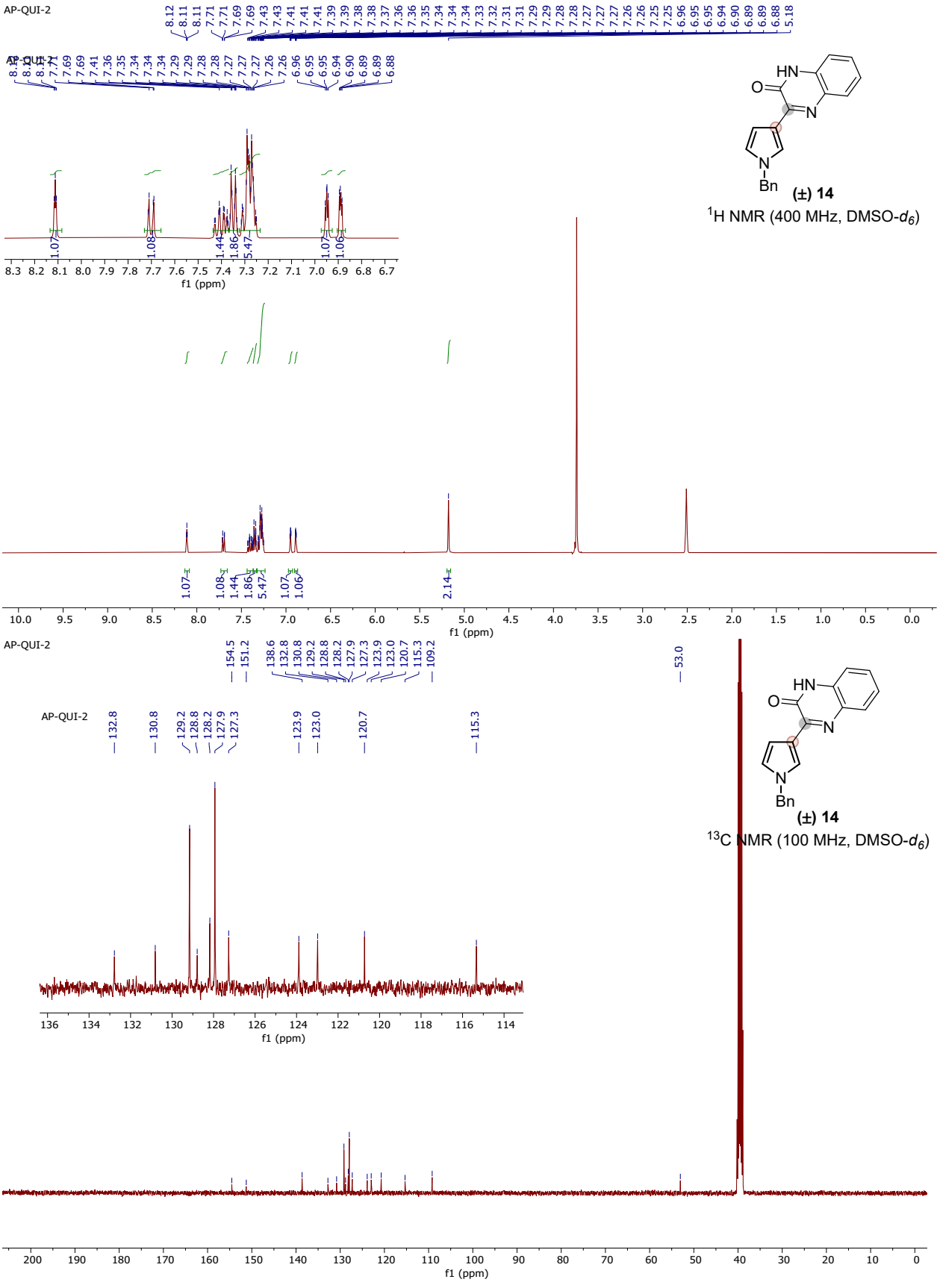
^{13}C NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$))


AP-QUI-2
HN
O
N
N
Bn
(±) 14
1H NMR (400 MHz, DMSO-d6)
f1 (ppm)
AP-QUI-2
13C NMR (100 MHz, DMSO-d6)
f1 (ppm)

Single crystal X-ray Diffraction Experiment and Analysis

Single Crystal XRD Experiments for 7ah: The single crystal XRD data collection and data reduction were performed using CrysAlis PRO on a single crystal Rigaku Oxford XtaLab Pro Kappa dual home/near diffractometer. The crystals were kept at 93(2) K during data collection using CuKα (λ = 1.54184 Å) radiation. Using Olex2[1], the structure was solved with the ShelXT[2] structure solution program using Intrinsic Phasing and refined with the ShelXL[3] refinement package using Least Squares minimisation.

Single Crystal structure, Cell parameters and structure data of compound (7ah):

The single crystal of compound (**7ah**) $C_{15}H_{14}N_2O_2$ **[exp_968_IK-APIS-CP]** was crystalize as colorless block through the slow evaporation of (ethyl acetate + hexane + acetone) solvent mixture solution at room temperature. The compound **[exp_968_IK-APIS-CP]** crystallized in monoclinic crystal system with $P2_1/c$ space group. One molecule appeared in structure solution in an asymmetric unit (Z'=1) with following crystal unit cell data.

Crystal Data for $C_{15}H_{14}N_2O_2$ (M =254.28 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 11.1124(2) Å, b = 11.30100(10) Å, c = 10.6161(2) Å, β = 109.698(2)°, V = 1255.17(4) Å^3, Z = 4, T = 93(2) K, μ(Cu Kα) = 0.737 mm^{-1}, $Dcalc$ = 1.346 g/cm^3, 13555 reflections measured (8.452° ≤ 2Θ ≤ 159.236°), 2695 unique (R_{int} = 0.0296, R_{sigma} = 0.0230) which were used in all calculations. The final R_1 was 0.0386 (I > 2σ(I)) and wR_2 was 0.0980 (all data). The crystallographic details of the compound **7ah** are deposited to the Cambridge Crystallographic (CCDC 2166129). The ORTEP diagram as crystal structure of **7ah [exp_968_IK-APIS-CP]** is illustrated in Figure S1. The molecule has one chiral center (C7–*R*).

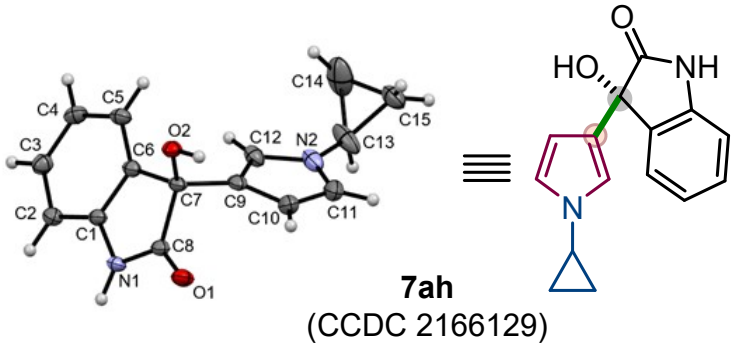


Figure S1: The ORTEP diagram of compound **7ah** (CCDC 2166129) **[exp_968_IK-APIS-CP]**. (The thermal ellipsoid is drawn at the 50 % probability level.)

The compound crystallized as colorless block in a monoclinic, $P2_1/c$ space group (CCDC 2166129). One neutral molecule $C_{15}H_{14}N_2O_2$ found in an asymmetric unit and four molecules are found in a unit cell. The compound has two hydrogen bond donors, N1-H and O2-H, and two hydrogen bond acceptors, O1 and O2. The 3D supramolecular structure is stabilized by hydrogen bond and non-covalent bond interactions.

Table S1: Crystal data and structure refinement for (7ah) exp_968_IK_APIS-CP_autored.

Identification code	exp_968_IK_APIS-CP_autored
Empirical formula	$C_{15}H_{14}N_2O_2$
Formula weight	254.28
Temperature/K	93(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.1124(2)
b/Å	11.30100(10)
c/Å	10.6161(2)
α/°	90
β/°	109.698(2)
γ/°	90
Volume/Å^3	1255.17(4)
Z	4
ρ_{calc}g/cm^3	1.346
μ/mm^{-1}	0.737
F(000)	536.0
Crystal size/mm^3	0.2 × 0.15 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.452 to 159.236
Index ranges	$-14 \le h \le 13$, $-13 \le k \le 14$, $-12 \le l \le 13$
Reflections collected	13555
Independent reflections	2695 [R_{int} = 0.0296, R_{sigma} = 0.0230]
Data/restraints/parameters	2695/0/173
Goodness-of-fit on F^2	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0386, wR_2 = 0.0964
Final R indexes [all data]	R_1 = 0.0411, wR_2 = 0.0980
Largest diff. peak/hole / e Å^{-3}	0.27/-0.34
CCDC	2166129

Crystal structure determination of 7ah [exp_968_IK_APIS-CP_autored]

Crystal Data for compound **7ah** $C_{15}H_{14}N_2O_2$ (*M* =254.28 g/mol): monoclinic, space group $P2_1/c$ (no. 14), *a* = 11.1124(2) Å, *b* = 11.30100(10) Å, *c* = 10.6161(2) Å, *β* = 109.698(2)°, *V* =

1255.17(4) Å^3, Z = 4, T = 93(2) K, μ(Cu Kα) = 0.737 mm^{-1}, *Dcalc* = 1.346 g/cm^3, 13555 reflections measured (8.452° ≤ 2Θ ≤ 159.236°), 2695 unique (R_{int} = 0.0296, R_{sigma} = 0.0230) which were used in all calculations. The final R_1 was 0.0386 (I > 2σ(I)) and wR_2 was 0.0980 (all data).

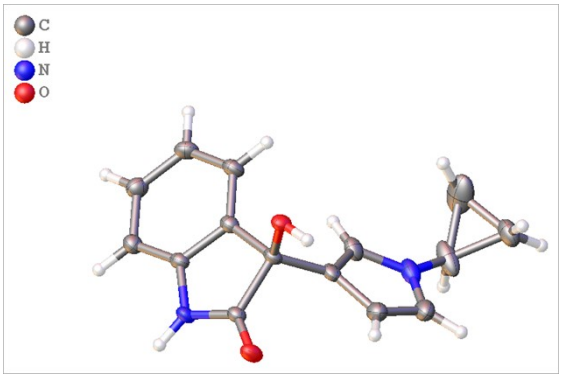
Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups, All N(H) groups
 At 1.5 times of:
  All O(H) groups
2.a Ternary CH refined with riding coordinates:
 C13(H13)
2.b Secondary CH2 refined with riding coordinates:
 C14(H14A,H14B), C15(H15A,H15B)
2.c Aromatic/amide H refined with riding coordinates:
 N1(H1), C2(H2A), C3(H3), C4(H4), C5(H5), C10(H10), C11(H11), C12(H12)
2.d Idealised tetrahedral OH refined as rotating group:
 O2(H2)
```

This report has been created with Olex2, compiled on 2020.11.12 svn.r5f609507 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.



References:

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (**2009**), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (**2015**). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (**2015**). Acta Cryst. C71, 3-8.

Supporting information for the Theoretical Calculation at the DFT-Level

All the calculations were performed using B3LYP functional[1] with def2-TZVP basis set[2] with RIJCOSX approximation. A correction for dispersion interaction is added using Grimme D3 with Becke-Johnson damping.[3] All the calculations, including geometry optimization and frequencies, were performed using ORCA 4.2 program in the gas phase, with RIJCOSX approximation for Coulomb and exchange integrals.[4]

From the transition states, the paths to the reactants and products were traced back using intrinsic reaction coordinates (IRC) calculations.

References:

[1] K. Kim, K. D. Jordan, *J. Phys. Chem.* **1994**, *98*, 10089–10094.

[2] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297–3305.

[3] B. R. Brooks, C. L. Brooks III,; A. D. Mackerell Jr, L. Nilsson, R. J. Petrella, B. Roux, Y. Won, G. Archontis, C. Bartels, S. Boresch, A. Caflisch, L. Caves, Q. Cui, A. R. Dinner, M. Feig, S. Fischer, J. Gao, M. Hodoscek, W. Im, K. Kuczera, T. Lazaridis, J. Ma, V. Ovchinnikov, E. Paci, R. W. Pastor, C. B. Post, J. Z. Pu, M. Schaefer, B. Tidor, R. M. Venable, H. L. Woodcock, X. Wu, W. Yang, D. M. York, M. Karplus, B. *J. Comput. Chem.* **2009**, *30*, 1545–1614.

[4] a) F. Neese, *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, *2*, 73–78; b) F. Neese, *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2018**, *8*, 1–6.

Table S5: The optimized structures of the molecules.

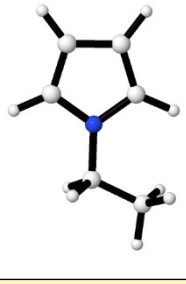
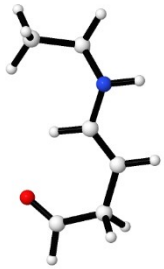
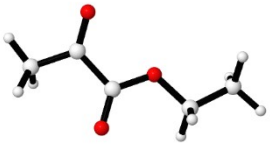
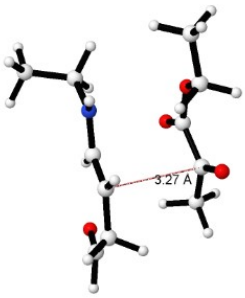
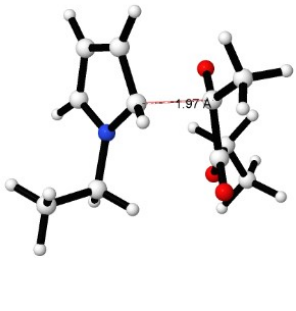
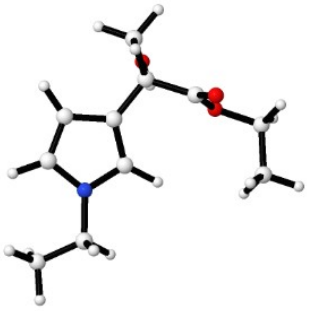
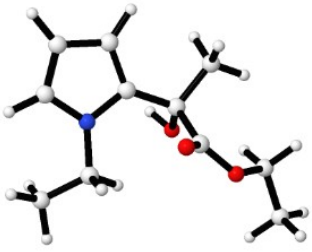
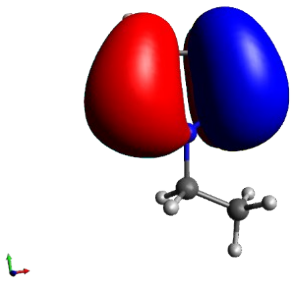
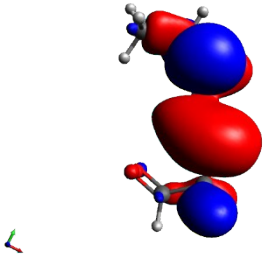
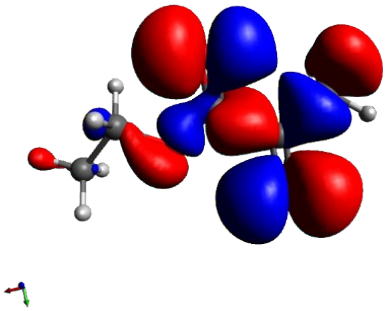
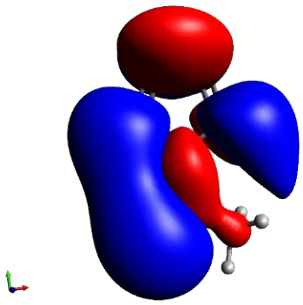
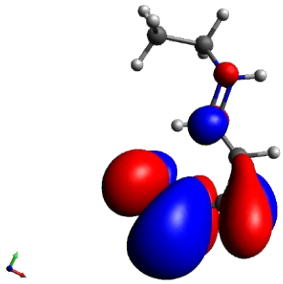
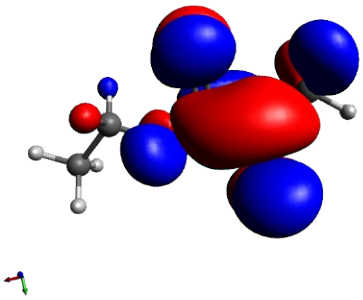
Pyrrole **5b**	Enamine **A**
	
Carbonyl **3b**	
	
TS-1 C-3 substituted pyrrole	**TS-2** C-2 substituted pyrrole
	
Compound **4bb** C-3 substituted Pyrrole	Compound **8** C-2 substituted Pyrrole
	

Figure S6: The pictures of the frontier orbitals are given below

		
a) OMO of preformed Pyrrole **5b** (–5.6 eV)	b) OMO of in situ enamine-**A** (–5.37 eV)	c) HOMO of carbonyl **3b** (–7.1 eV)
		
e) LUMO of preformed pyrrole **5b** (–0.73 eV)	f) LUMO of in situ enamine-**A** (–0.68eV)	g) LUMO Isatin **3b** (–2.04 eV)

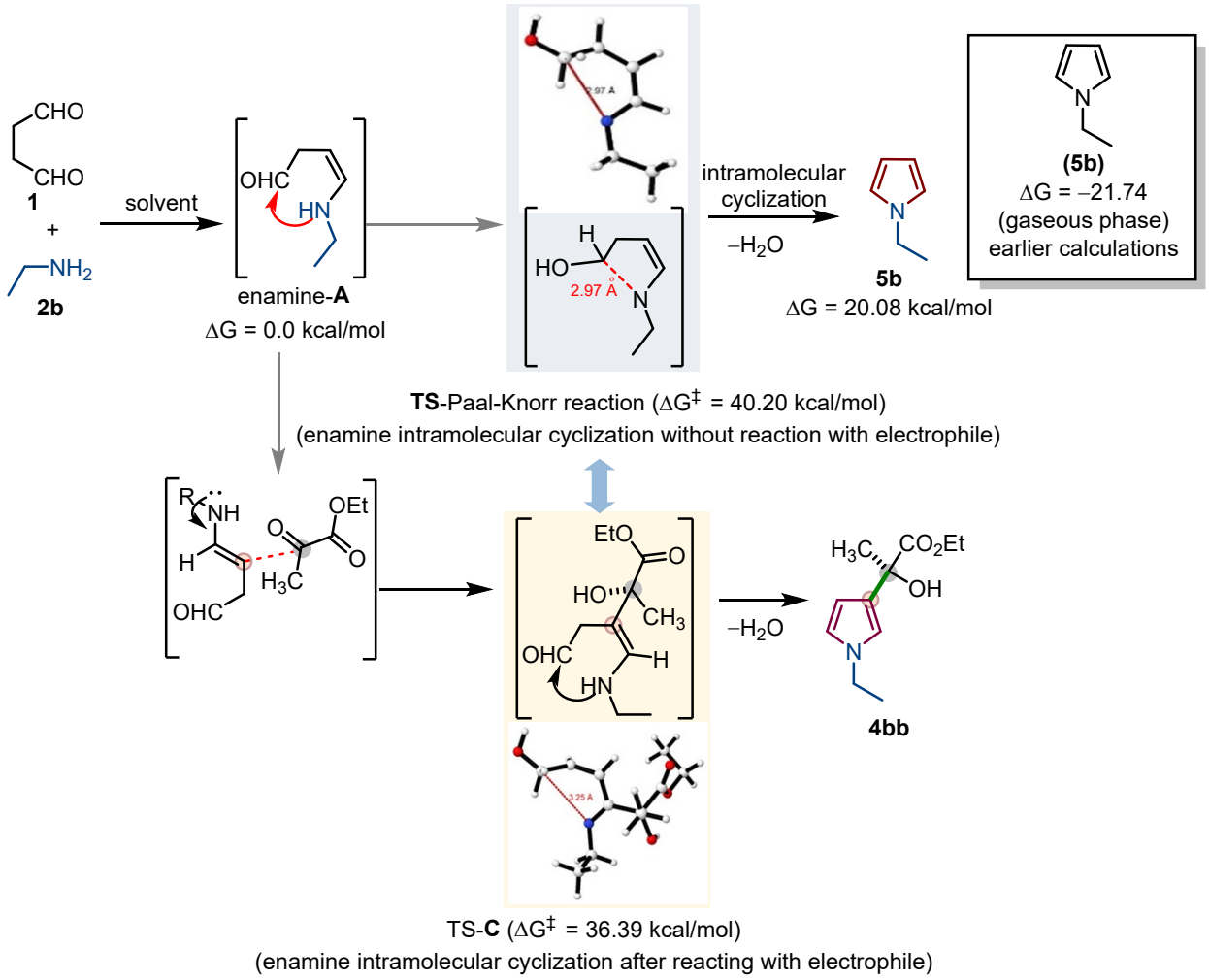
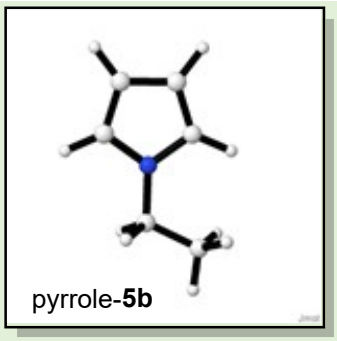


Figure S7: Separate DFT-Calculations were performed for the comparison between the TS-Paal-Knorr reaction (cyclization without reaction with reactive carbonyls) and TS-**C** (cyclization after reaction with reactive carbonyls) in EtOH as suggested to show the comparison between cyclization steps.

XYZ coordinates, energies, and frequencies

Note: All thermochemistry calculations are done at 298.15K and 1.00 atm

Pyrrole 5b



GIBBS FREE ENERGY

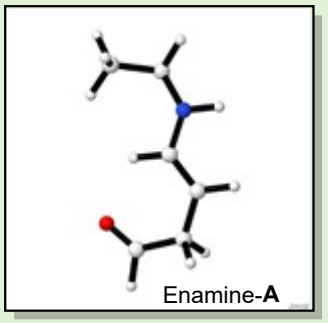
The Gibbs free energy is G = H - T*S

Total enthalpy ... -288.59189803 Eh
Total entropy correction ... -0.03630735 Eh -22.78 kcal/mol

Final Gibbs free energy ... -288.62820538 Eh

C	-6.44938131080991	2.08976375490413	-0.01401379259410
C	-5.03658755337243	1.96247900504482	-0.00380859766865
C	-6.97114542771052	0.81788632815014	-0.00771567667738
C	-4.74710255785369	0.61710952257081	0.00853714105486
N	-5.93124096553293	-0.07871852436392	0.00518789622844
C	-6.11327785552268	-1.52654186552911	0.03871334324288
C	-4.81387030159236	-2.31225011171962	-0.00960083767943
H	-7.01738226019185	3.00505330178139	-0.02645574955572
H	-4.31291392676473	2.76043881406363	-0.00738647226326
H	-7.99228655986177	0.47406684115632	-0.01086517734016
H	-3.79881939663624	0.11199208339819	0.01716208424690
H	-6.74347630116981	-1.81041649391319	-0.80811026605862
H	-6.66283452699028	-1.78535292487801	0.94798407469695
H	-4.25510665815108	-2.10822510027289	-0.92358984536166
H	-5.04524225683625	-3.37807597501285	0.01574230353045
H	-4.17527214100341	-2.08805865537984	0.84517957219850

Enamine A



GIBBS FREE ENERGY

The Gibbs free energy is G = H - T*S
Total enthalpy ... -364.97203725 Eh
Total entropy correction ... -0.04526842 Eh -28.41 kcal/mol

Final Gibbs free energy ... -365.01730566 Eh

C	-7.68869262374191	3.39050976181050	0.27470219910227
C	-6.32321000444829	3.86274477398972	-0.21124366643282
N	-5.20682821832376	3.14462970455977	0.40177328696638

C	-5.01408547205674	1.80220312260684	0.13531192468407
H	-5.91978851475246	1.22944146845852	-0.00008779985664
C	-3.82072909589716	1.19641051979073	0.08605972054396
C	-3.55593525667982	-0.26980941542049	-0.04241438338372
C	-4.66617924681410	-1.22971897539466	-0.36211280686736
O	-5.82003333970990	-0.96580511946825	-0.58565926221135
H	-4.32446077698447	-2.28891298821473	-0.38265872512038
H	-8.47364204713658	3.96972009080371	-0.21491719527599
H	-7.78388998913074	3.52574749829683	1.35389912266869
H	-7.86309574233248	2.33974528835842	0.03729082897747
H	-6.20019412248842	4.91346576365122	0.05864422639940
H	-6.28168665696585	3.80192514454775	-1.30821834411296
H	-4.35131441150701	3.68073393061466	0.41650885970703
H	-2.92724046920435	1.80447020744928	0.21074655560858
H	-3.08868455647035	-0.67354538085738	0.87126831657672
H	-2.79195945535545	-0.46348539558252	-0.81146285797338

Carbonyl 3b

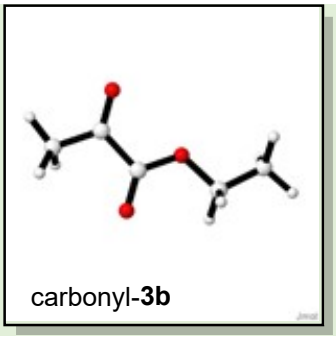
GIBBS FREE ENERGY

The Gibbs free energy is G = H - T*S

Total enthalpy ... -420.85187437 Eh

Total entropy correction ... -0.04463288 Eh -28.01 kcal/mol

Final Gibbs free energy ... -420.89650725 Eh



C	-8.32240629167295	2.66786043948642	-0.25712174566105
C	-7.03592832017822	3.43847867702001	-0.18447028853187
C	-5.81292225439737	2.61691927915379	0.28825919121762
O	-5.93285970738520	1.59325438501548	0.91628604576484
O	-4.66299349467938	3.18077374488621	-0.06215591645271
C	-3.46042109355526	2.50958734230496	0.39092595374772
C	-2.26944881705589	3.19028200878813	-0.23786447022732
O	-6.92915266034633	4.61012445170145	-0.43539150595262
H	-8.23109356157753	1.87192152638982	-1.00092907392663
H	-9.13299373315147	3.34061776036995	-0.52569496238843
H	-8.51988030549289	2.17282169301353	0.69509467101600
H	-3.52677693034968	1.45820282350464	0.10805413954693
H	-3.43552111357089	2.57044527164312	1.48044415351876
H	-2.29791643815795	3.10564493100973	-1.32503279240618
H	-1.35420334564422	2.71374822507872	0.11895172803509
H	-2.23424193278467	4.24618744063401	0.03419487269986

Compound 4bb

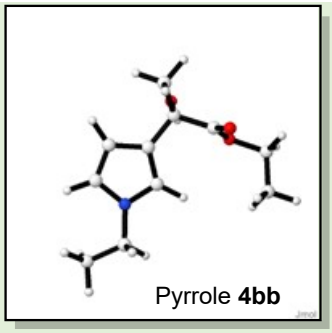
GIBBS FREE ENERGY

The Gibbs free energy is G = H - T*S

Total enthalpy ... -709.45985728 Eh

Total entropy correction ... -0.05587660 Eh -35.06 kcal/mol

Final Gibbs free energy ... -709.51573388 Eh



C	-5.11568043446146	1.92168647445038	-0.13120799394969
C	-3.81898204775734	1.33681275282077	-0.05196959423962
C	-6.03192278867211	0.89986591207020	-0.10390444899715
C	-4.00537326099624	-0.02749389769475	0.00594469128230
N	-5.35066300376423	-0.29136504077146	-0.02584163781691
C	-5.91631566993722	-1.61884943700305	0.18647557280803
C	-7.36679070411274	-1.73402214966304	-0.25107474129669
C	-2.51058611695563	2.08973505196779	-0.05441815227467
C	-2.55766122685516	3.29202556296156	0.88303332157728
O	-2.22119240871215	2.62122224427501	-1.34934435662375
C	-1.38476752866017	1.14264470160543	0.40571731130998
O	-1.07126219642694	0.95447036443186	1.55267400491546
O	-0.80084226446174	0.52395394788091	-0.64012329872922
C	0.26671530488554	-0.40125961447288	-0.33640240946824
C	-0.27107487802917	-1.78618917157468	-0.03522664131450
H	-5.34940057786922	2.96913526230777	-0.21981623981882
H	-7.10526874003048	0.93465952860547	-0.14971240221009
H	-5.82756474842560	-1.88178104379320	1.24540658478315
H	-5.30177123369848	-2.32705082179919	-0.37293386276181
H	-8.01398542066188	-1.07487118428488	0.32742641432565
H	-7.71044643706775	-2.75587745208218	-0.08520698946906
H	-7.48674393123044	-1.49177403511622	-1.30835534955918
H	-3.33131887156918	3.97750265922429	0.54204611708747
H	-1.60058072896731	3.81318232789975	0.86862573783789
H	-2.77852692004687	2.96981496625229	1.89784593476094
H	-2.17109638243723	1.88313318596179	-1.96753991456097
H	0.83854482531419	-0.00879137069359	0.50300659369879
H	0.88908575902393	-0.39874247108156	-1.22983703682720
H	-0.89914421112053	-1.77178278330894	0.85539737542013
H	0.55987379933013	-2.47076224447193	0.14709710728499
H	-0.85147817381481	-2.16794311483327	-0.87664353572864
H	-3.29133878181142	-0.82949911007048	0.08865183855408

Compound 8

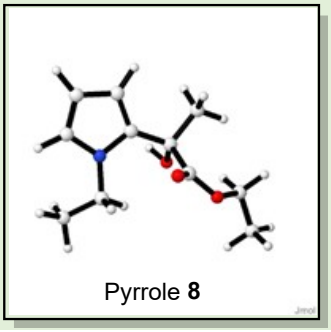
GIBBS FREE ENERGY

The Gibbs free energy is G = H - T*S

Total enthalpy ... -709.46325075 Eh

Total entropy correction ... -0.05877106 Eh -36.88 kcal/mol

Final Gibbs free energy ... -709.52202181 Eh



C	-6.28737338405470	2.60749527605171	0.18209572904559
C	-4.88265327539720	2.77226939515001	0.18020559412357
C	-6.53278737991120	1.25819449294884	0.09860260108777
C	-4.30838768833968	1.51851574484477	0.09394091401276
N	-5.33575847500712	0.59369730148341	0.03458649540568
C	-5.18488943009238	-0.86167302737860	0.05780049143947
C	-6.35601385982159	-1.59811478326670	-0.57508516704725
C	-2.85409845836065	1.15793520825115	-0.00335540317371
C	-1.98126478652600	2.41114034083559	0.14752789153226
O	-2.59433519897681	0.52432680686381	-1.28103654535435
C	-2.44093775132415	0.16304676704212	1.11775858117921
O	-3.09833108966049	0.06018640833439	2.11868180946133
O	-1.33507821964298	-0.59126786544846	0.99978175100919
C	-0.22152845008354	-0.39138293128732	0.09989481605219
C	0.40573870793913	-1.74593429761455	-0.14941873689803
H	-7.03232133593001	3.38374960981574	0.23430689303618
H	-4.35325806288103	3.70700989783878	0.24275421061835
H	-7.46599719493411	0.72616326277419	0.06914790750224
H	-5.04634943874633	-1.18335401921404	1.09133806202623
H	-4.27112147074308	-1.10113984714769	-0.48385704641801
H	-7.27755079061788	-1.46740850146891	-0.00799084444839
H	-6.13209521705826	-2.66582603216770	-0.58866723144868
H	-6.53117191857112	-1.26809755384596	-1.60070647525059
H	-2.28461105121461	3.16109405458372	-0.58181250408799
H	-0.93749374547717	2.16597934033755	-0.03316825811822
H	-2.08357970934558	2.83347491486760	1.14704333565517
H	-3.09813255555656	1.02455868269947	-1.93448483170758
H	0.47985910062481	0.27437006078857	0.61021631829178
H	-0.55404662837190	0.06482215255993	-0.82646152830427
H	0.68648006563487	-2.22322094129469	0.78985575702825
H	1.30307099943272	-1.63169917109220	-0.76076350375373
H	-0.28933230698521	-2.39765074684457	-0.67977108249641

TS-1

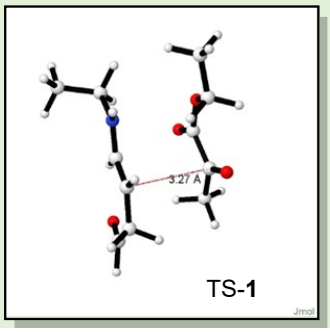
GIBBS FREE ENERGY

The Gibbs free energy is G = H - T*S

Total enthalpy ... -785.82742070 Eh

Total entropy correction ... -0.06329099 Eh -39.72 kcal/mol

Final Gibbs free energy ... -785.89071169 Eh



C	-5.29133752571890	5.04178394837014	-0.71835832780240
C	-3.80426535349049	4.67945940948909	-0.75116685228423
N	-3.38365651310053	3.78681919061243	0.31097722264852
C	-3.45538686414169	2.42141774131178	0.22063657730331
H	-3.80754089054184	2.04731431346972	-0.74304309439051
C	-3.09563683944884	1.55100379909344	1.19286913884512
C	-3.20774096126491	0.05558283843794	1.16458500840468
C	-3.78252954712974	-0.65024845626035	-0.03532213261965
O	-4.00870084914298	-0.17651054637403	-1.12371970825549
H	-3.98407222140329	-1.73981392118007	0.15347315814429
H	-5.54325876354297	5.75393947349902	-1.52088628976095
H	-5.56631696979766	5.50764600222223	0.24315074991692
H	-5.91686045397941	4.14415736850711	-0.85022105683365
H	-3.18938410308886	5.59328011309438	-0.69348840872703
H	-3.53790138317894	4.20531966102906	-1.70871071697005
H	-3.23310740697015	4.19128559613507	1.22800944704228
H	-2.70868129639419	1.95556658604785	2.13685966684515
H	-3.78843057504510	-0.31779744410460	2.03321275032246
H	-2.21425805682510	-0.42515896218809	1.31561315788976
C	-0.25486752583522	1.55731333573309	-0.42573494136081
C	-0.57120726975885	0.31051588831647	-1.20364509984048
O	0.35692612631444	1.56203377413314	0.61820363470221
C	-0.71009870415444	2.86492298929053	-1.12426532977047
O	-1.26895693601182	2.80344127568055	-2.19204076964937
O	-0.43383113081460	4.04757431477340	-0.57463209432933
C	0.00592945480154	4.27256068880128	0.77844403982302
C	-0.07448505218950	5.76507335227649	1.01389816216329
H	-1.62474944631433	0.29567260353015	-1.51310526866667
H	-0.31307456415987	-0.56717985784850	-0.59702143254310
H	0.02249118863109	0.30857704006591	-2.13279331680601
H	1.02926108629356	3.89335115497950	0.90827265236158
H	-0.63898071743318	3.71214847204225	1.47007735093977
H	0.56247453793667	6.30746145195129	0.29927509250991
H	0.26607471078318	6.00634130255869	2.03331819928958
H	-1.10755918388007	6.12541550250004	0.88907883145829

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.000000000 (already applied!)

0:	0.00 cm**-1	36:	704.54 cm**-1	73:	1468.09 cm**-1
1:	0.00 cm**-1	37:	707.62 cm**-1	74:	1481.28 cm**-1
2:	0.00 cm**-1	38:	724.29 cm**-1	75:	1490.89 cm**-1
3:	0.00 cm**-1	39:	788.19 cm**-1	76:	1495.53 cm**-1
4:	0.00 cm**-1	40:	826.34 cm**-1	77:	1498.01 cm**-1
5:	0.00 cm**-1	41:	835.64 cm**-1	78:	1504.63 cm**-1
6:	-58.75 cm**-1	42:	851.91 cm**-1	79:	1516.06 cm**-1
imaginary mode		43:	860.66 cm**-1	80:	1521.41 cm**-1
7:	46.32 cm**-1	44:	917.88 cm**-1	81:	1525.95 cm**-1
8:	56.63 cm**-1	45:	947.36 cm**-1	82:	1688.86 cm**-1
9:	68.89 cm**-1	46:	992.26 cm**-1	83:	1759.94 cm**-1
10:	78.74 cm**-1	47:	1038.60 cm**-1	84:	1765.88 cm**-1
11:	86.02 cm**-1	48:	1044.78 cm**-1	85:	1778.53 cm**-1
12:	99.53 cm**-1	49:	1049.80 cm**-1	86:	2754.64 cm**-1
13:	115.21 cm**-1	50:	1054.89 cm**-1	87:	2851.82 cm**-1
14:	127.22 cm**-1	51:	1058.79 cm**-1	88:	2892.23 cm**-1
15:	146.68 cm**-1	52:	1068.45 cm**-1	89:	2938.94 cm**-1
16:	170.80 cm**-1	53:	1116.49 cm**-1	90:	2949.84 cm**-1
17:	174.07 cm**-1	54:	1139.89 cm**-1	91:	2955.37 cm**-1
18:	190.73 cm**-1	55:	1170.78 cm**-1	92:	2963.76 cm**-1
19:	209.23 cm**-1	56:	1180.25 cm**-1	93:	2976.91 cm**-1
20:	231.41 cm**-1	57:	1188.87 cm**-1	94:	2981.39 cm**-1
21:	269.39 cm**-1	58:	1246.92 cm**-1	95:	3001.64 cm**-1
22:	280.45 cm**-1	59:	1271.00 cm**-1	96:	3002.57 cm**-1
23:	297.99 cm**-1	60:	1299.67 cm**-1	97:	3008.30 cm**-1
24:	337.75 cm**-1	61:	1307.68 cm**-1	98:	3018.50 cm**-1
25:	355.23 cm**-1	62:	1320.19 cm**-1	99:	3022.44 cm**-1
26:	359.20 cm**-1	63:	1347.65 cm**-1	100:	3024.99 cm**-1
27:	368.71 cm**-1	64:	1366.66 cm**-1	101:	3030.48 cm**-1
28:	386.72 cm**-1	65:	1395.34 cm**-1	102:	3068.10 cm**-1
29:	410.00 cm**-1	66:	1410.61 cm**-1	103:	3109.70 cm**-1
30:	424.31 cm**-1	67:	1414.23 cm**-1	104:	3521.12 cm**-1
31:	439.20 cm**-1	68:	1416.63 cm**-1		
32:	482.74 cm**-1	69:	1429.08 cm**-1		
33:	518.86 cm**-1	70:	1433.33 cm**-1		
34:	561.97 cm**-1	71:	1439.80 cm**-1		
35:	620.93 cm**-1	72:	1450.50 cm**-1		

TS-2

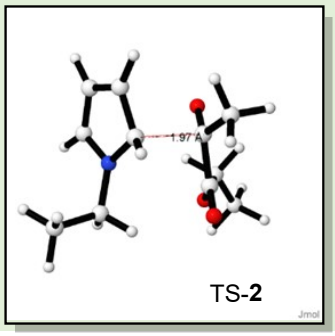
GIBBS FREE ENERGY

The Gibbs free energy is G = H - T*S

Total enthalpy ... -709.43509124 Eh

Total entropy correction ... -0.05773824 Eh -36.23 kcal/mol

Final Gibbs free energy ... -709.49282948 Eh



C	-5.20139091652128	1.90154914003427	-1.80204903854822
C	-4.59119508431160	2.53478647917973	-0.71604133090565
C	-5.38688541382182	0.56670572994587	-1.46555490098565
C	-4.33025328847540	1.50758000551729	0.31777668551074
N	-4.90520260860648	0.34075529057403	-0.17465415503159
C	-5.25858099721471	-0.82621034522594	0.62487134222106
C	-6.66561063652616	-0.71857326038373	1.21368819454015
C	-2.36571957752660	1.45809389070201	0.32749816253754
C	-1.97686117493546	2.62536855900009	1.21928879706243
O	-2.18625219891002	1.58301019917433	-0.95966635328915
C	-2.21688904120407	0.10090519697078	0.97716077932218
O	-2.42217213156625	-0.05292979218749	2.16411611821118
O	-2.02785255701637	-0.98230143815383	0.20084129814318
C	-1.30520271582218	-0.98585871717390	-1.04173749017907
C	-0.52061330638494	-2.28445916894071	-1.09527660209496
H	-5.46114562592078	2.35683314522615	-2.75593917906816
H	-4.29379147743965	3.57629218974996	-0.62508032499492
H	-5.82205279305907	-0.24990803021717	-2.03869047609438
H	-4.51118258192352	-0.93779193428093	1.42134897710417
H	-5.16462174068060	-1.71426601254667	-0.02028817848911
H	-6.74217771148363	0.14825337415014	1.88922431697048
H	-6.91440032868560	-1.62177096803169	1.79292816172104
H	-7.42096968105206	-0.59588546560680	0.42093351550804
H	-2.42150939460031	3.55404185218630	0.82965996367945
H	-0.88174853709233	2.75585698517291	1.20180875814703
H	-2.28943552667477	2.46484433712124	2.26003646209917
H	-0.63945871407253	-0.11259866186153	-1.10089068819710
H	-2.02397365180595	-0.89768963012225	-1.87038911898956
H	0.20236990870624	-2.33685719626919	-0.26607237007673
H	0.03379931493725	-2.36074106932066	-2.04457924276468
H	-1.19613127769447	-3.14989395292323	-1.01043593034000
H	-4.43420853261122	1.69140926854038	1.39626384727113

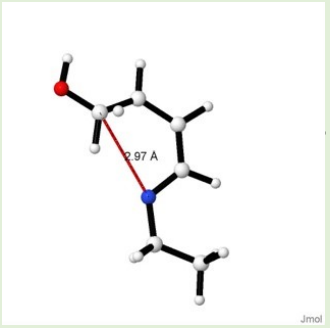
VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.000000000 (already applied!)

0:	0.00 cm**-1	43:	975.62 cm**-1	87:	3001.48 cm**-1
1:	0.00 cm**-1	44:	985.67 cm**-1	88:	3011.80 cm**-1
2:	0.00 cm**-1	45:	1022.49 cm**-1	89:	3012.65 cm**-1
3:	0.00 cm**-1	46:	1050.87 cm**-1	90:	3023.00 cm**-1
4:	0.00 cm**-1	47:	1074.33 cm**-1	91:	3037.44 cm**-1
5:	0.00 cm**-1	48:	1090.53 cm**-1	92:	3040.89 cm**-1
6:	-345.76 cm**-1	49:	1106.26 cm**-1	93:	3137.39 cm**-1
imaginary mode		50:	1111.05 cm**-1	94:	3151.41 cm**-1
7:	49.35 cm**-1	51:	1124.02 cm**-1	95:	3164.73 cm**-
8:	62.88 cm**-1	52:	1130.52 cm**-1		
9:	106.22 cm**-1	53:	1143.42 cm**-1		
10:	116.98 cm**-1	54:	1189.38 cm**-1		
11:	132.34 cm**-1	55:	1199.07 cm**-1		
12:	142.78 cm**-1	56:	1248.68 cm**-1		
13:	150.52 cm**-1	57:	1260.46 cm**-1		
14:	175.11 cm**-1	58:	1289.56 cm**-1		
15:	208.73 cm**-1	59:	1316.12 cm**-1		
16:	217.90 cm**-1	60:	1323.74 cm**-1		
17:	257.59 cm**-1	61:	1368.12 cm**-1		
18:	297.00 cm**-1	62:	1384.26 cm**-1		
19:	302.97 cm**-1	63:	1410.51 cm**-1		
20:	323.76 cm**-1	64:	1411.92 cm**-1		
21:	339.95 cm**-1	65:	1416.02 cm**-1		
22:	360.32 cm**-1	66:	1430.36 cm**-1		
23:	375.82 cm**-1	67:	1434.98 cm**-1		
24:	399.08 cm**-1	68:	1444.37 cm**-1		
25:	416.92 cm**-1	69:	1486.69 cm**-1		
26:	432.12 cm**-1	70:	1491.71 cm**-1		
27:	556.54 cm**-1	71:	1493.76 cm**-1		
28:	569.97 cm**-1	72:	1500.32 cm**-1		
29:	587.21 cm**-1	73:	1501.44 cm**-1		
30:	597.89 cm**-1	74:	1502.14 cm**-1		
31:	640.49 cm**-1	75:	1508.06 cm**-1		
32:	703.88 cm**-1	76:	1524.80 cm**-1		
33:	717.81 cm**-1	77:	1527.03 cm**-1		
34:	742.24 cm**-1	78:	1706.11 cm**-1		
35:	759.68 cm**-1	79:	2948.08 cm**-1		
36:	833.41 cm**-1	80:	2948.84 cm**-1		
37:	846.46 cm**-1	81:	2951.00 cm**-1		
38:	854.39 cm**-1	82:	2967.37 cm**-1		
39:	902.75 cm**-1	83:	2968.67 cm**-1		
40:	927.40 cm**-1	84:	2993.61 cm**-1		
41:	937.15 cm**-1	85:	2994.73 cm**-1		
42:	963.99 cm**-1	86:	2998.72 cm**-1		

TS-Paal-Knorr cyclization

GIBBS FREE ENERGY



The Gibbs free energy is G = H - T*S

Total enthalpy **:** -364.9206796 **Eh**

Total entropy correction : -0.04267934 Eh -26.78 kcal/mol

Final Gibbs free energy : -364.96335891 Eh

Xyz coordinates

C	-1.97270210333040	-0.57580951822897	0.09097337490660
C	-1.79594873403213	0.78286392844580	-0.05908304134773
C	-0.51578444265479	1.44961720308210	0.12206103412973
C	0.76518728436389	0.87091205708422	0.04881537287464
N	0.96893566327021	-0.39374181809837	-0.24863189881249
C	2.29982631786412	-0.95109266561643	-0.25160509029623
C	3.49603996884709	-0.05522212785513	0.07293898806133
O	-3.14898745864219	-1.20984556443372	-0.08839004080138
H	-1.10113406279017	-1.23828002758972	0.04507412503515
H	-2.68394455981246	1.42067693310508	-0.14926205061769
H	-3.85997512139717	-0.55706164353667	-0.17423493506045
H	-0.55130117056799	2.52555859428717	0.31654967311088
H	1.60440301010674	1.55624498445625	0.25607070073712
H	-1.71476073998640	-0.63928465011339	1.78653653829565
H	2.28554486532063	-1.81045885042418	0.44888027670966
H	2.44900151709002	-1.42105760668798	-1.24397512892297
H	3.59177999185555	0.78024748890605	-0.63967345844625
H	3.42973154184863	0.37024439103889	1.08742386592078
H	4.42448823264680	-0.64521110782100	0.01923169452366

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.000000000 (already applied!)

0:	0.00 cm**-1	8:	120.52 cm**-1	17:	536.63 cm**-1
1:	0.00 cm**-1	9:	173.79 cm**-1	18:	575.95 cm**-1
2:	0.00 cm**-1	10:	223.02 cm**-1	19:	739.88 cm**-1
3:	0.00 cm**-1	11:	235.32 cm**-1	20:	755.21 cm**-1
4:	0.00 cm**-1	12:	275.06 cm**-1	21:	807.76 cm**-1
5:	0.00 cm**-1	13:	325.67 cm**-1	22:	836.98 cm**-1
6:	-1039.38 cm**-1	14:	389.12 cm**-1	23:	910.79 cm**-1
imaginary mode		15:	436.16 cm**-1	24:	956.04 cm**-1
7:	108.92 cm**-1	16:	451.66 cm**-1	25:	984.01 cm**-1

26: 1012.43 cm**-1
27: 1027.68 cm**-1
28: 1057.75 cm**-1
29: 1096.46 cm**-1
30: 1145.32 cm**-1
31: 1147.40 cm**-1
32: 1182.02 cm**-1
33: 1216.60 cm**-1
34: 1295.04 cm**-1
35: 1317.20 cm**-1
36: 1321.36 cm**-1
37: 1348.07 cm**-1
38: 1400.24 cm**-1
39: 1415.91 cm**-1
40: 1419.29 cm**-1
41: 1463.87 cm**-1
42: 1477.41 cm**-1
43: 1486.34 cm**-1
44: 1496.34 cm**-1
45: 1552.77 cm**-1
46: 1618.06 cm**-1
47: 2893.97 cm**-1
48: 2899.71 cm**-1
49: 2944.36 cm**-1
50: 2969.72 cm**-1
51: 2997.41 cm**-1
52: 3004.80 cm**-1
53: 3049.03 cm**-1
54: 3073.25 cm**-1
55: 3083.08 cm**-1
56: 3732.52 cm**-1

TS-C

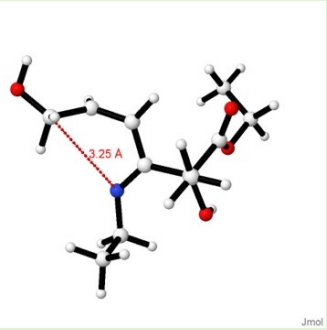
GIBBS FREE ENERGY

The Gibbs free energy is G = H - T*S

Total enthalpy **:** -785.72930296 **Eh**

Total entropy correction : -0.06109137 Eh -38.34 kcal/mol

Final Gibbs free energy : -785.79039432 Eh



C	-1.45968968598785	-0.42333009324673	1.44763998300493
C	-1.83378813078774	0.27994234593954	0.18079929090182
C	-1.02013087787744	1.35722925348894	-0.37865816911443
C	0.24199782203921	1.11865347507376	-0.99558904749358
N	0.65745068872653	-0.12380580189241	-1.00392849476568
C	1.93840436316877	-0.61814755454417	-1.45568240458805
C	2.95558957674632	-0.60911359480517	-0.30691818187236
O	-2.54942593203810	-1.06956010004245	2.07200126318452
H	-0.72065053611211	-1.21226941757496	1.20530304855177
H	-2.55831172264173	-0.23902882596172	-0.46246457137672
H	-3.23383661111239	-0.40299042705632	2.22016073340955
H	-1.37669854190591	2.39121228283144	-0.29443587532884
H	-0.93849852160214	0.28224217841265	2.13036942991680
H	1.78097301052280	-1.66554887860434	-1.76720886405643
H	2.36317404798669	-0.06486019828948	-2.30344511199335
H	3.21846362698857	0.42237234781069	-0.02635989567362
H	2.54714646883923	-1.11646770963493	0.58126935120622
H	3.87944668976228	-1.12587610765550	-0.61149268365668
H	1.58008688058682	1.84687025075873	-3.28717595467942
C	0.99787975919528	2.38340841663111	-1.52451097017635
C	1.64349498305372	3.13296129942430	-0.36127319223844
C	-0.04400750408912	3.28138066009583	-2.22007751904134
O	2.01783357353940	2.08699086085342	-2.45713313410666
O	-0.26909107631237	2.83262728088658	-3.47000835958500
O	-0.60463041267810	4.22902466485177	-1.73040635729688
H	2.36801428514308	2.47598918769567	0.13907483623982
H	2.16973881508199	4.02044579354637	-0.74155467951968
H	0.88550091924115	3.45223918816468	0.36476303214100
C	-1.29127571291777	3.49212429157253	-4.24582921122097
C	-2.66133418584883	2.91718875723629	-3.93656025040433
H	-1.00409949436542	3.31935379445130	-5.29264159554573
H	-1.25213170277273	4.57012917665320	-4.03227669201895
H	-2.67838656255031	1.82969594169768	-4.10734200802937
H	-3.41898002986208	3.38321671580241	-4.58659630157354
H	-2.93912826915971	3.11510054542920	-2.89061144319994

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.000000000 (already applied!)

0:	0.00 cm**-1	32:	501.78 cm**-1	65:	1341.83 cm**-1
1:	0.00 cm**-1	33:	530.88 cm**-1	66:	1365.63 cm**-1
2:	0.00 cm**-1	34:	574.93 cm**-1	67:	1381.05 cm**-1
3:	0.00 cm**-1	35:	603.54 cm**-1	68:	1382.77 cm**-1
4:	0.00 cm**-1	36:	626.96 cm**-1	69:	1400.20 cm**-1
5:	0.00 cm**-1	37:	689.96 cm**-1	70:	1406.32 cm**-1
6:	-201.39 cm**-1	38:	739.89 cm**-1	71:	1415.93 cm**-1
imaginary mode		39:	750.52 cm**-1	72:	1417.16 cm**-1
7:	12.24 cm**-1	40:	801.76 cm**-1	73:	1423.34 cm**-1
8:	20.92 cm**-1	41:	835.88 cm**-1	74:	1430.03 cm**-1
9:	43.75 cm**-1	42:	852.38 cm**-1	75:	1473.52 cm**-1
10:	62.26 cm**-1	43:	863.90 cm**-1	76:	1477.44 cm**-1
11:	92.98 cm**-1	44:	879.61 cm**-1	77:	1480.25 cm**-1
12:	99.14 cm**-1	45:	909.04 cm**-1	78:	1483.38 cm**-1
13:	108.15 cm**-1	46:	931.27 cm**-1	79:	1486.04 cm**-1
14:	126.84 cm**-1	47:	968.11 cm**-1	80:	1486.80 cm**-1
15:	170.44 cm**-1	48:	1019.38 cm**-1	81:	1489.76 cm**-1
16:	172.62 cm**-1	49:	1023.47 cm**-1	82:	1502.39 cm**-1
17:	211.32 cm**-1	50:	1037.40 cm**-1	83:	1507.64 cm**-1
18:	247.17 cm**-1	51:	1070.70 cm**-1	84:	1515.87 cm**-1
19:	290.82 cm**-1	52:	1085.67 cm**-1	85:	1764.97 cm**-1
20:	298.62 cm**-1	53:	1094.48 cm**-1	86:	2871.66 cm**-1
21:	302.70 cm**-1	54:	1115.32 cm**-1	87:	2899.38 cm**-1
22:	307.79 cm**-1	55:	1121.87 cm**-1	88:	2922.24 cm**-1
23:	337.15 cm**-1	56:	1149.83 cm**-1	89:	2945.85 cm**-1
24:	353.17 cm**-1	57:	1165.31 cm**-1	90:	2955.75 cm**-1
25:	355.96 cm**-1	58:	1177.64 cm**-1	91:	2975.32 cm**-1
26:	365.57 cm**-1	59:	1180.62 cm**-1	92:	2983.43 cm**-1
27:	376.30 cm**-1	60:	1205.07 cm**-1	93:	2998.20 cm**-1
28:	403.84 cm**-1	61:	1209.66 cm**-1	94:	3008.34 cm**-1
29:	409.92 cm**-1	62:	1246.83 cm**-1	95:	3012.28 cm**-1
30:	421.96 cm**-1	63:	1291.19 cm**-1	96:	3017.17 cm**-1
31:	456.98 cm**-1	64:	1317.18 cm**-1		