Well-Defined Iron Catalysts for the Acceptorless Reversible Dehydrogenation-Hydrogenation of Alcohols and Ketones

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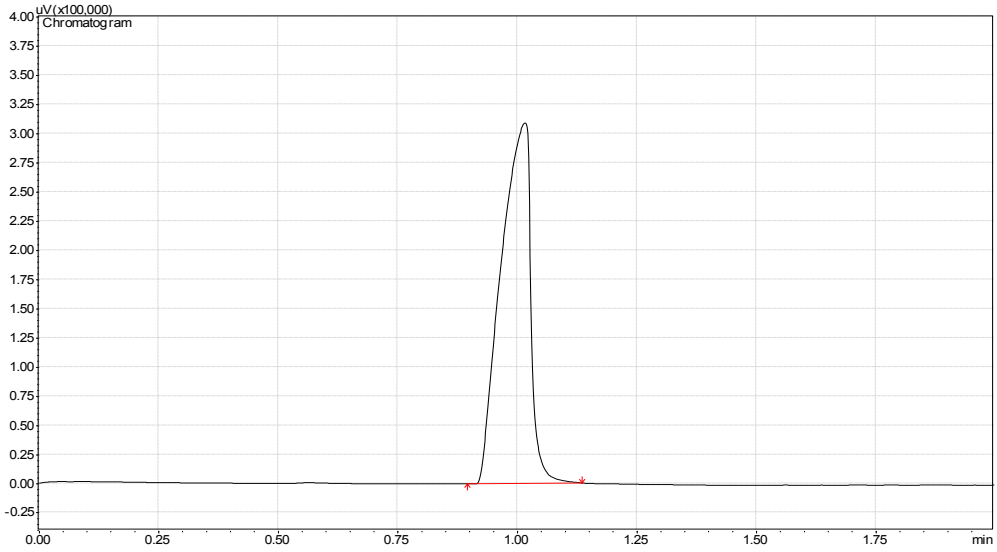
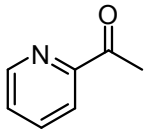
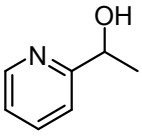
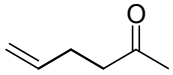
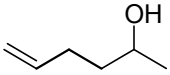
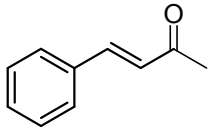
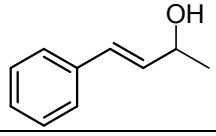
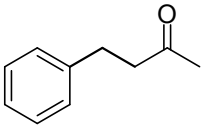
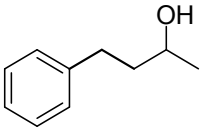
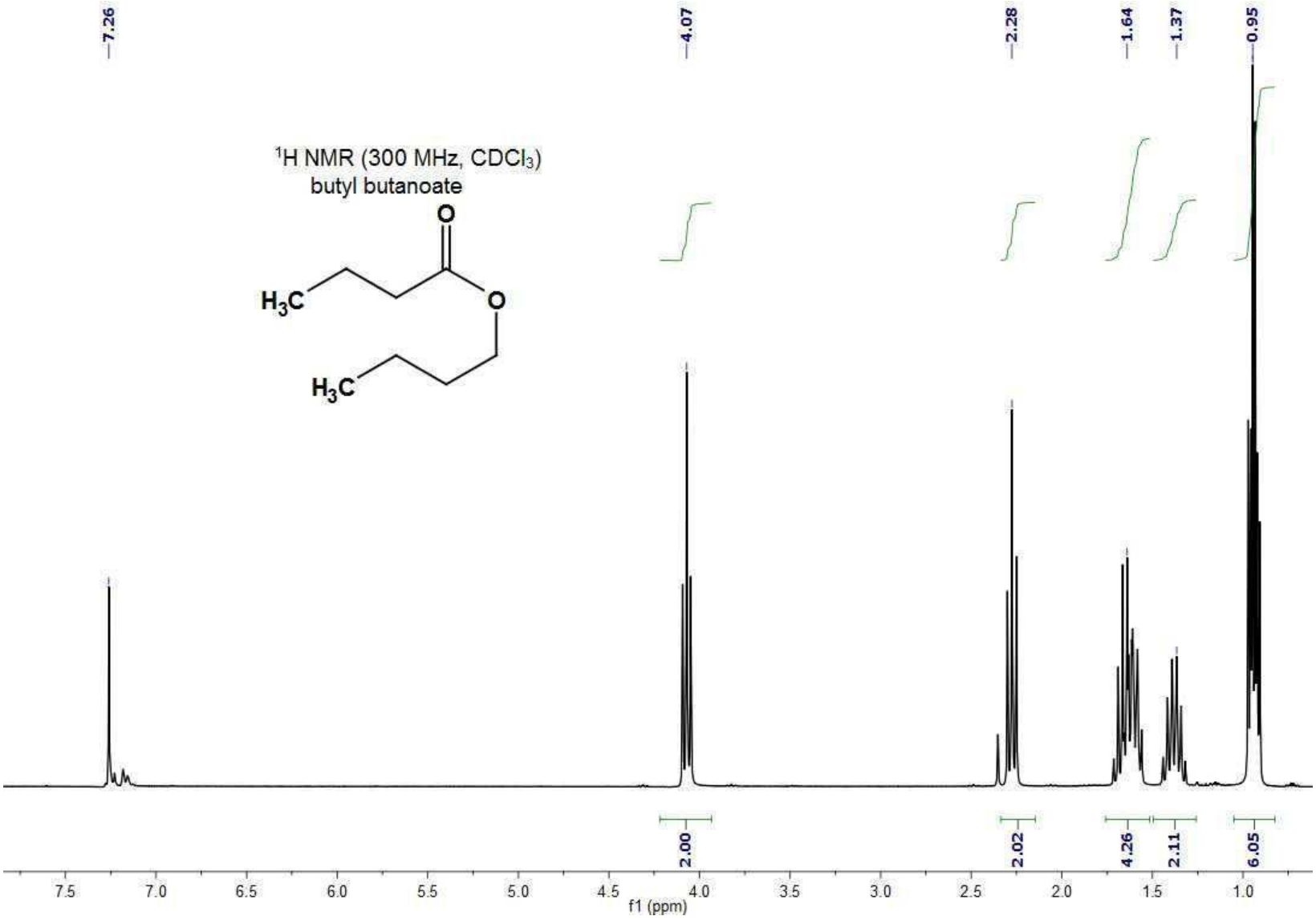


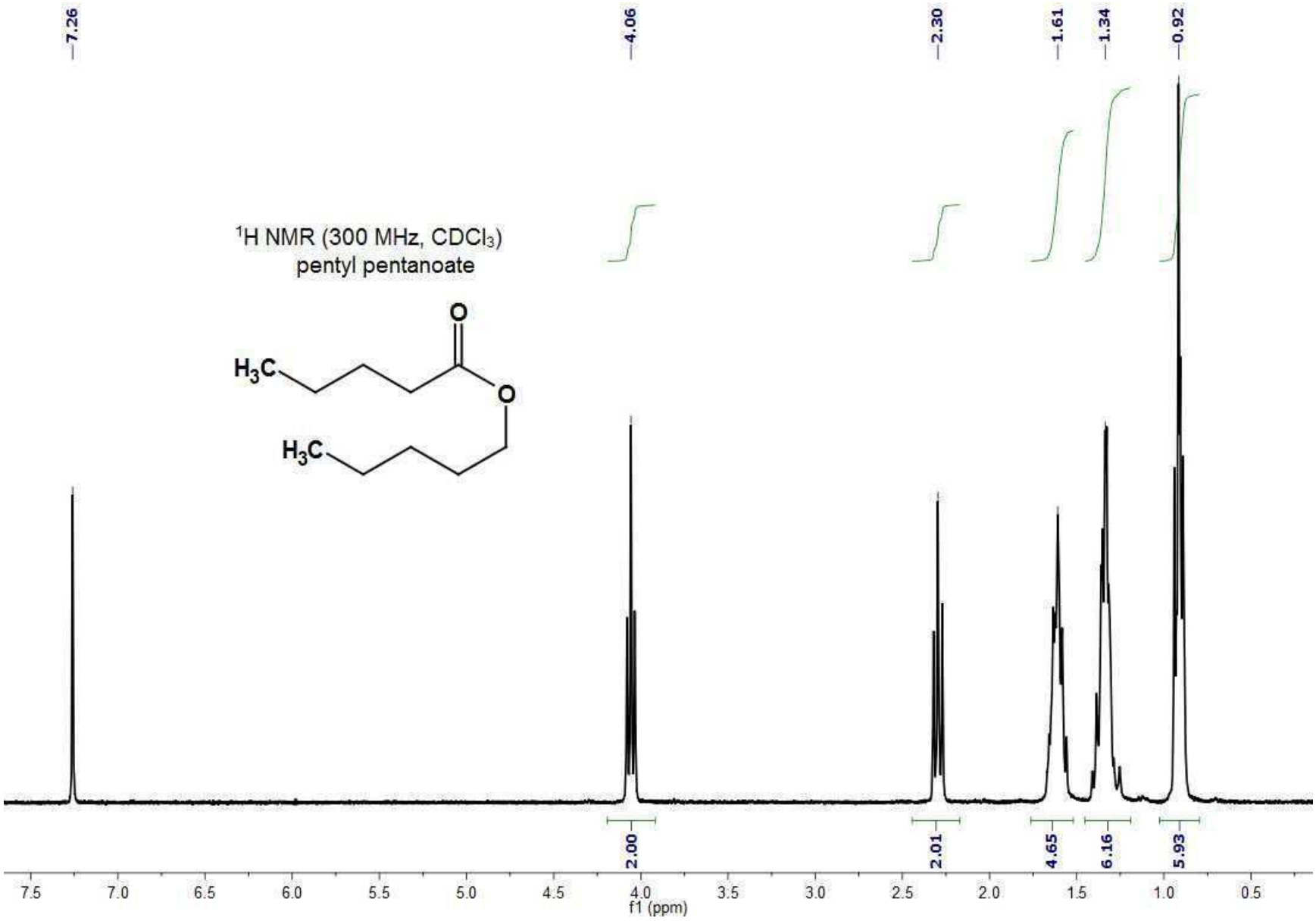
Figure S1. Detection of H_2 gas from the catalytic dehydrogenation of 1-phenylethanol (Richard Eisenberg Lab, helped by Amit Das) using a Shimadzu17A GC. GC parameters: injection temperature = 110 °C, column temperature = 28 °C, detector temperature = 140 °C. 5 Å molecular sieves column was used, and the carrier gas was N_2.

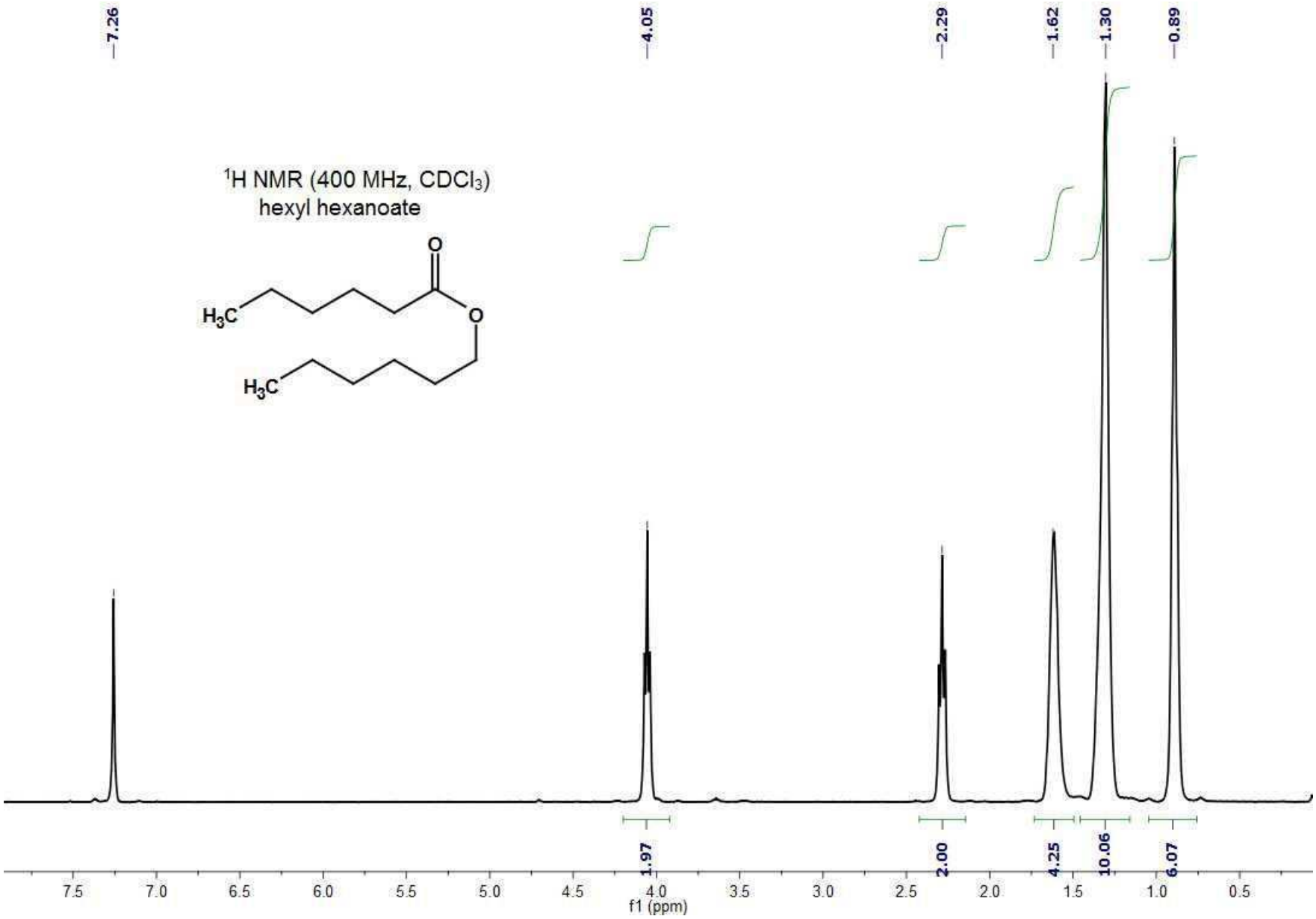
Table S1: Retention times (min) for all the substrates and products from hydrogenation studies reported from GC-FID analysis.

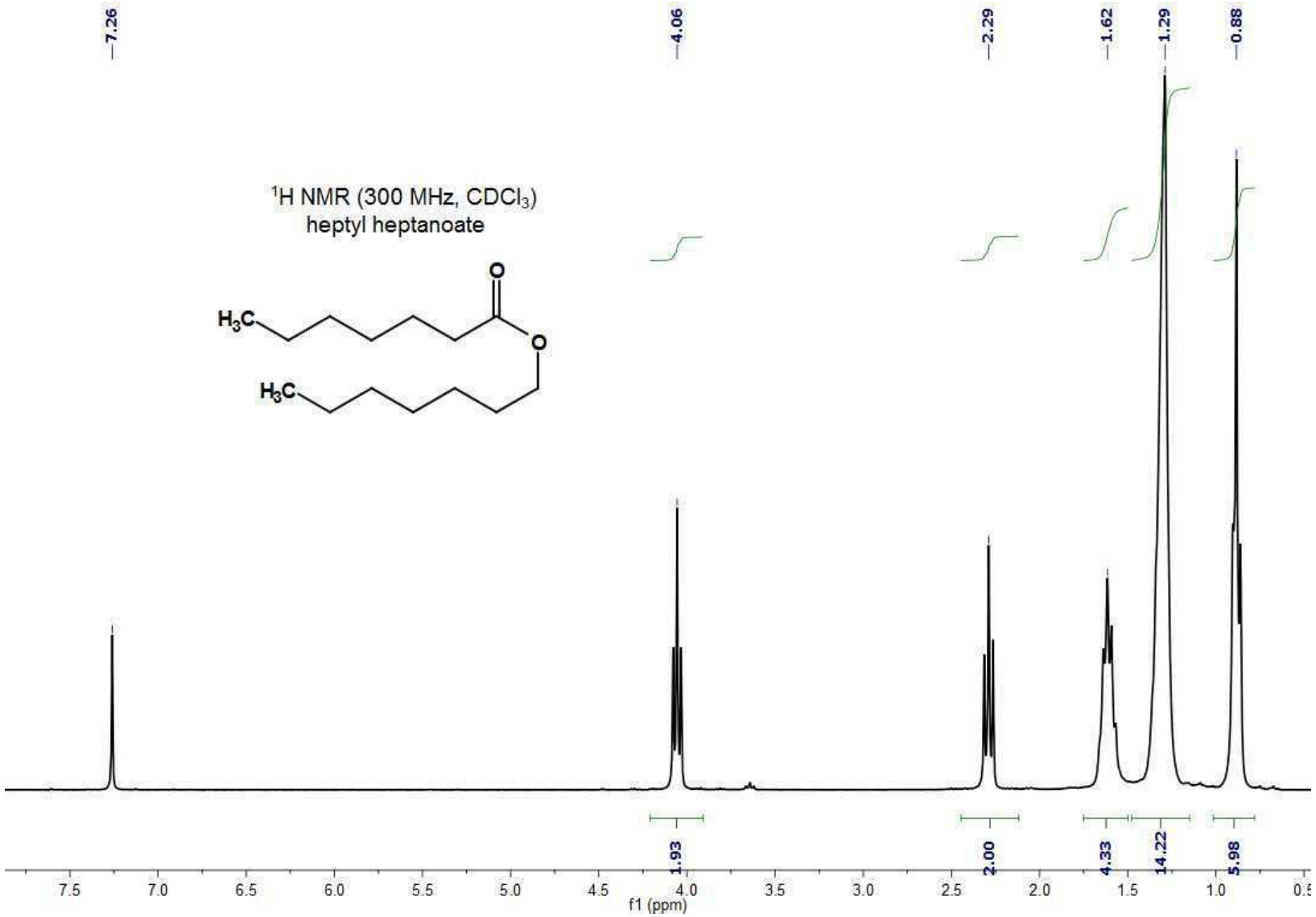
Substrate	t (min)	Product	t (min)
	6.91		7.30
	4.01		4.16
	10.08		9.78
			9.05
			9.18



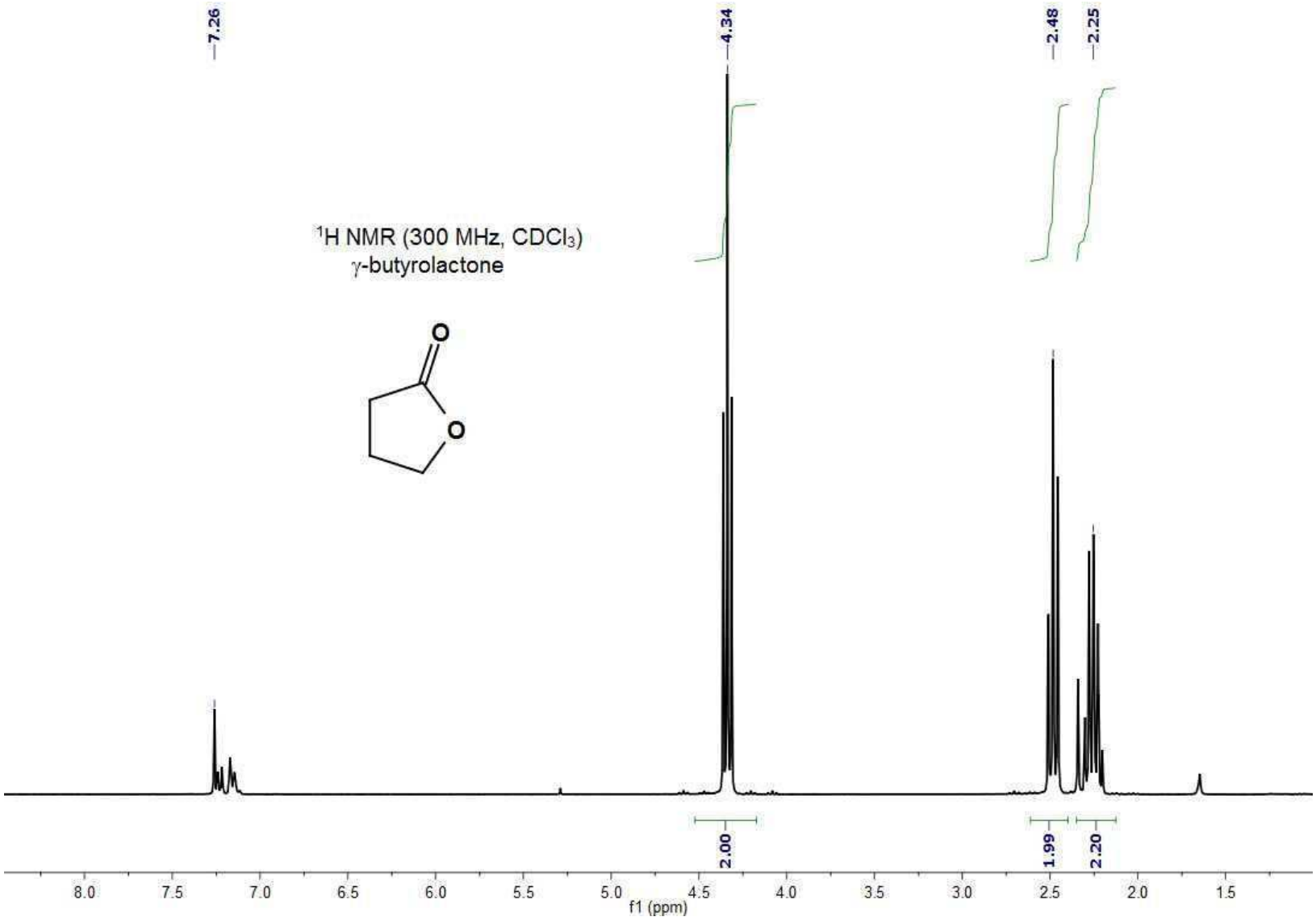
(with residual toluene solvent)


7.26
4.06
2.30
1.61
1.34
0.92
^{1}H NMR (300 MHz, $CDCl_3$)
pentyl pentanoate
O
H_3C
O
H_3C
2.00
2.01
4.65
6.16
5.93
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

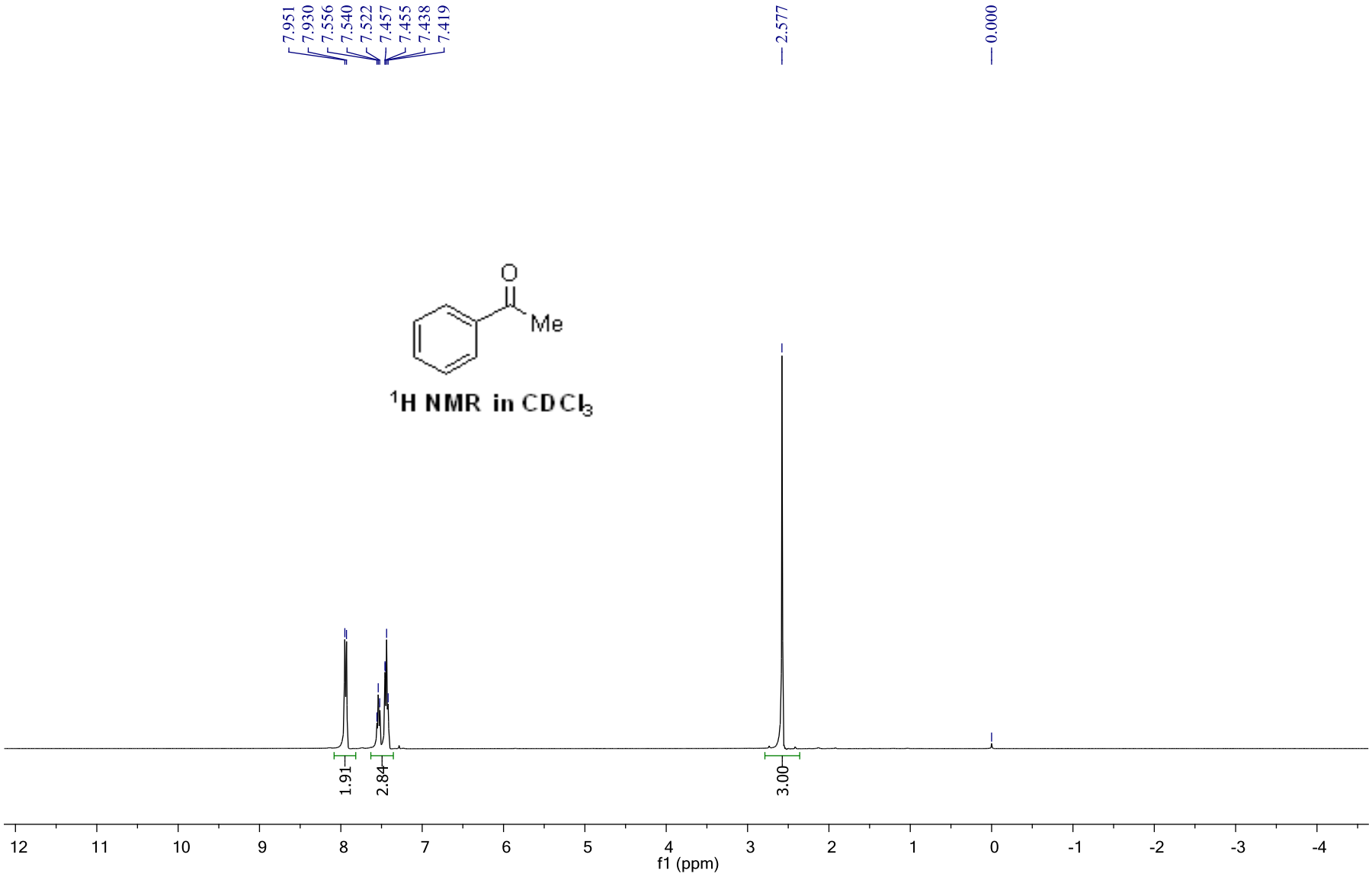

7.26
4.05
2.29
1.62
1.30
0.89
1H NMR (400 MHz, CDCl3)
hexyl hexanoate
O
H3C
O
H3C
1.97
2.00
4.25
10.06
6.07
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

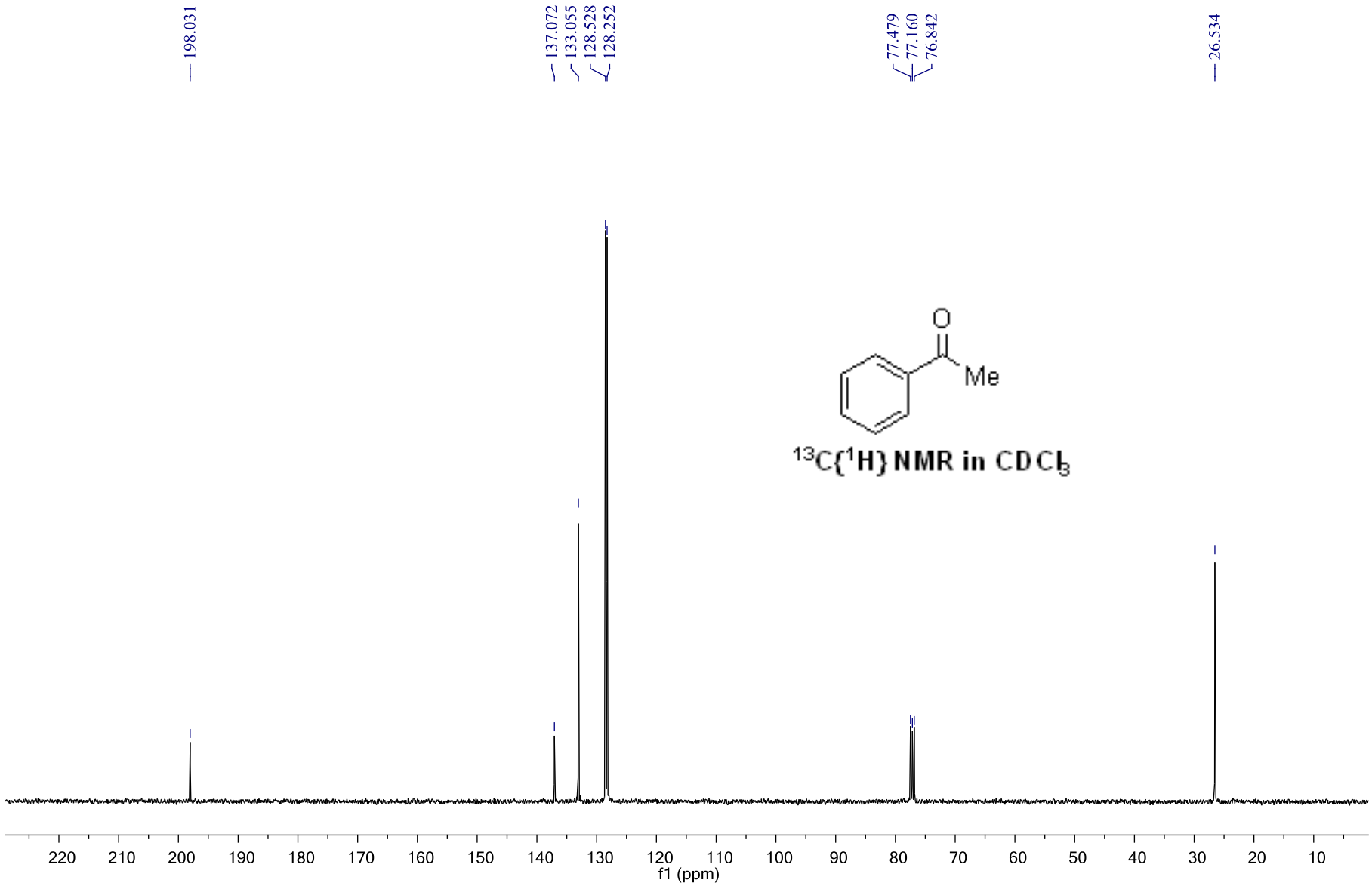


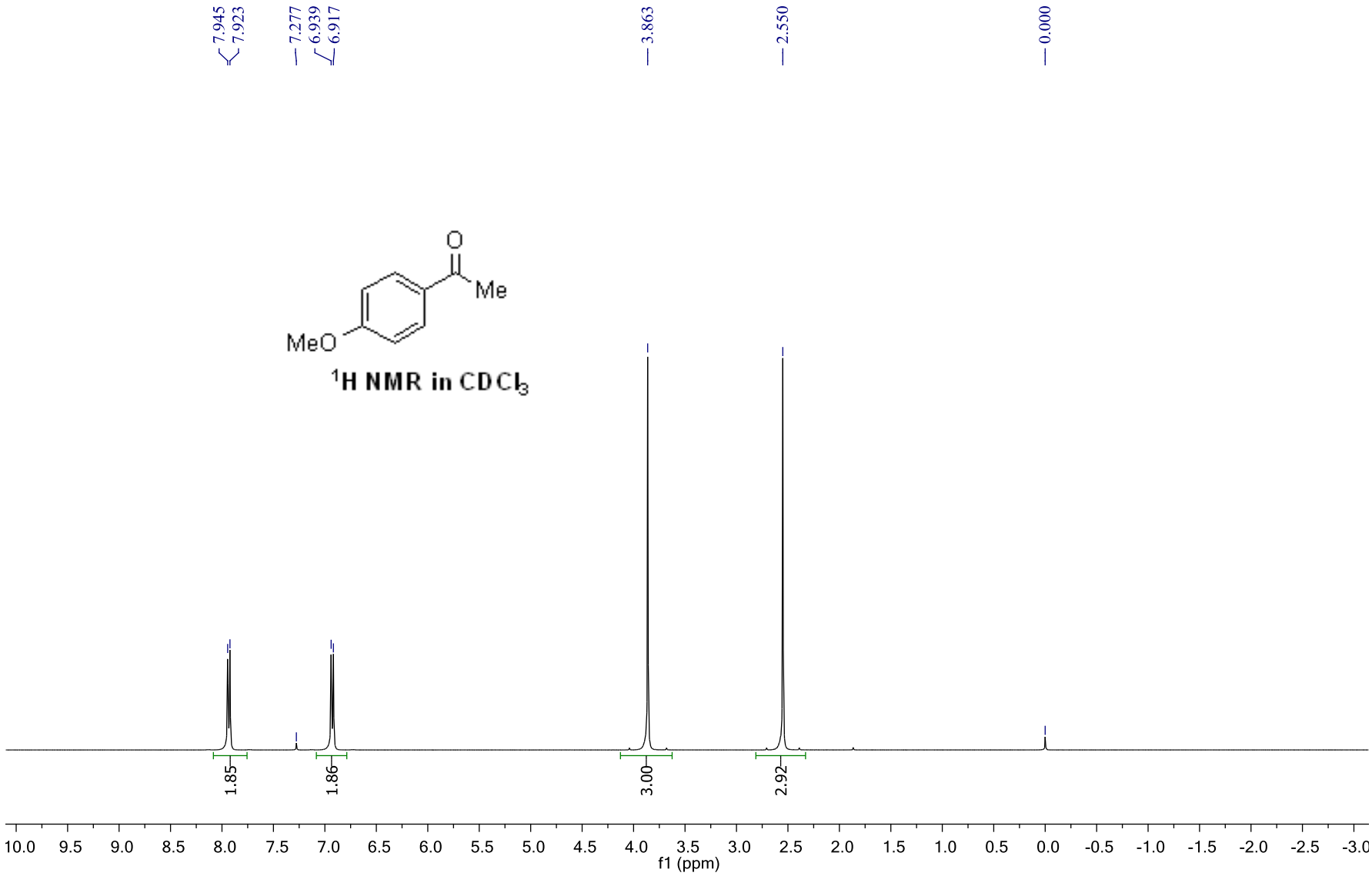
(with residual 1-heptanol)

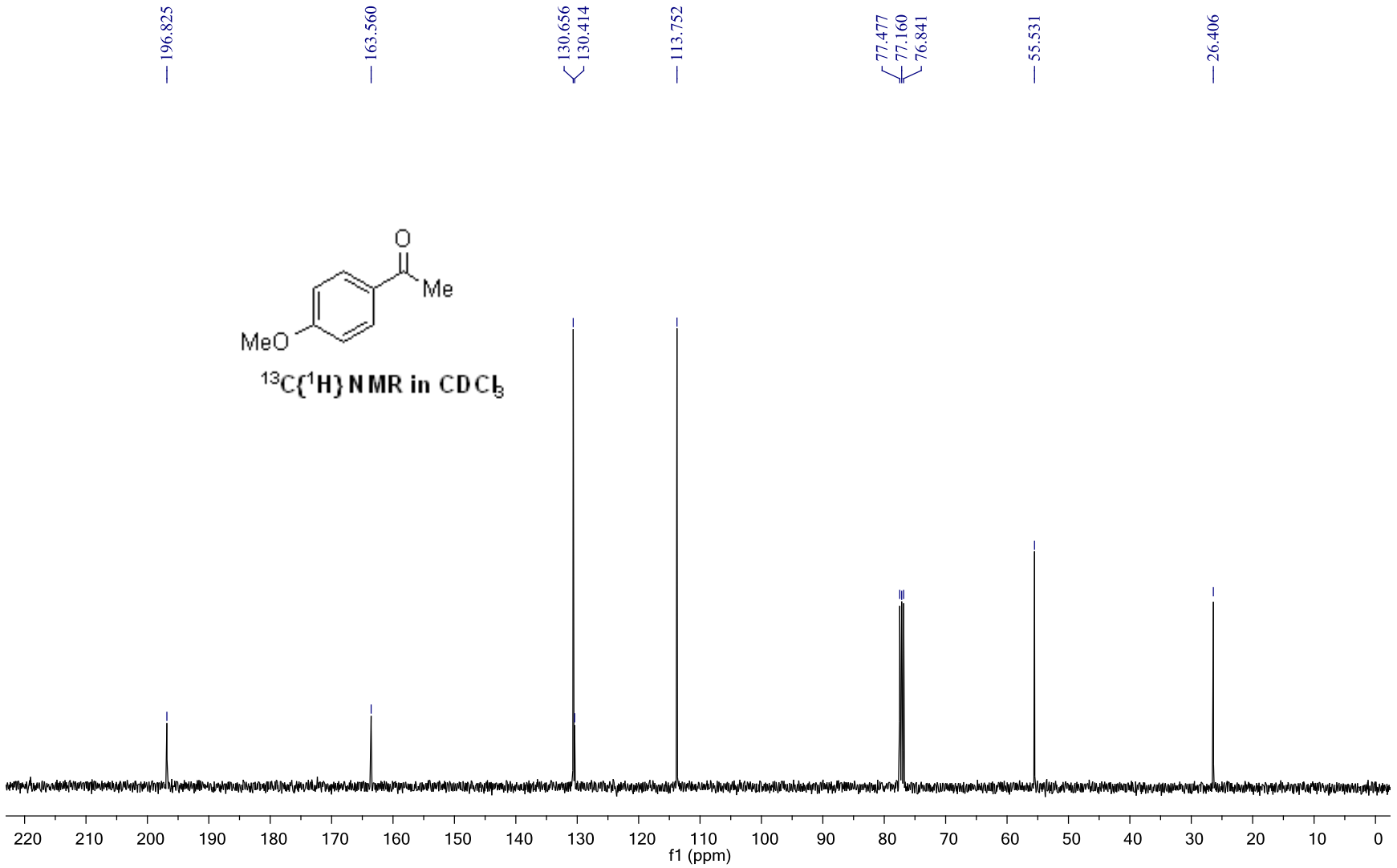


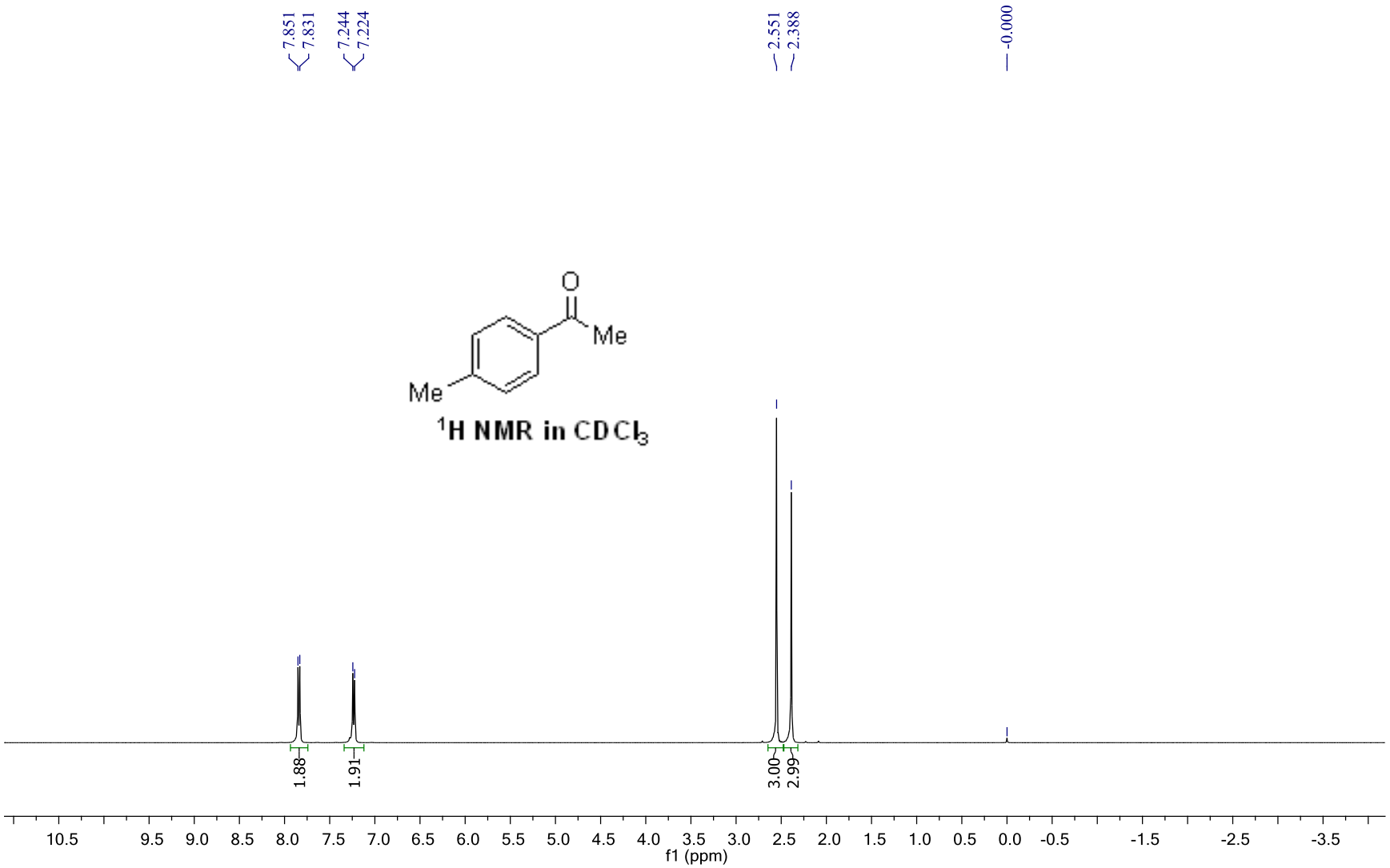
(with residual toluene solvent)

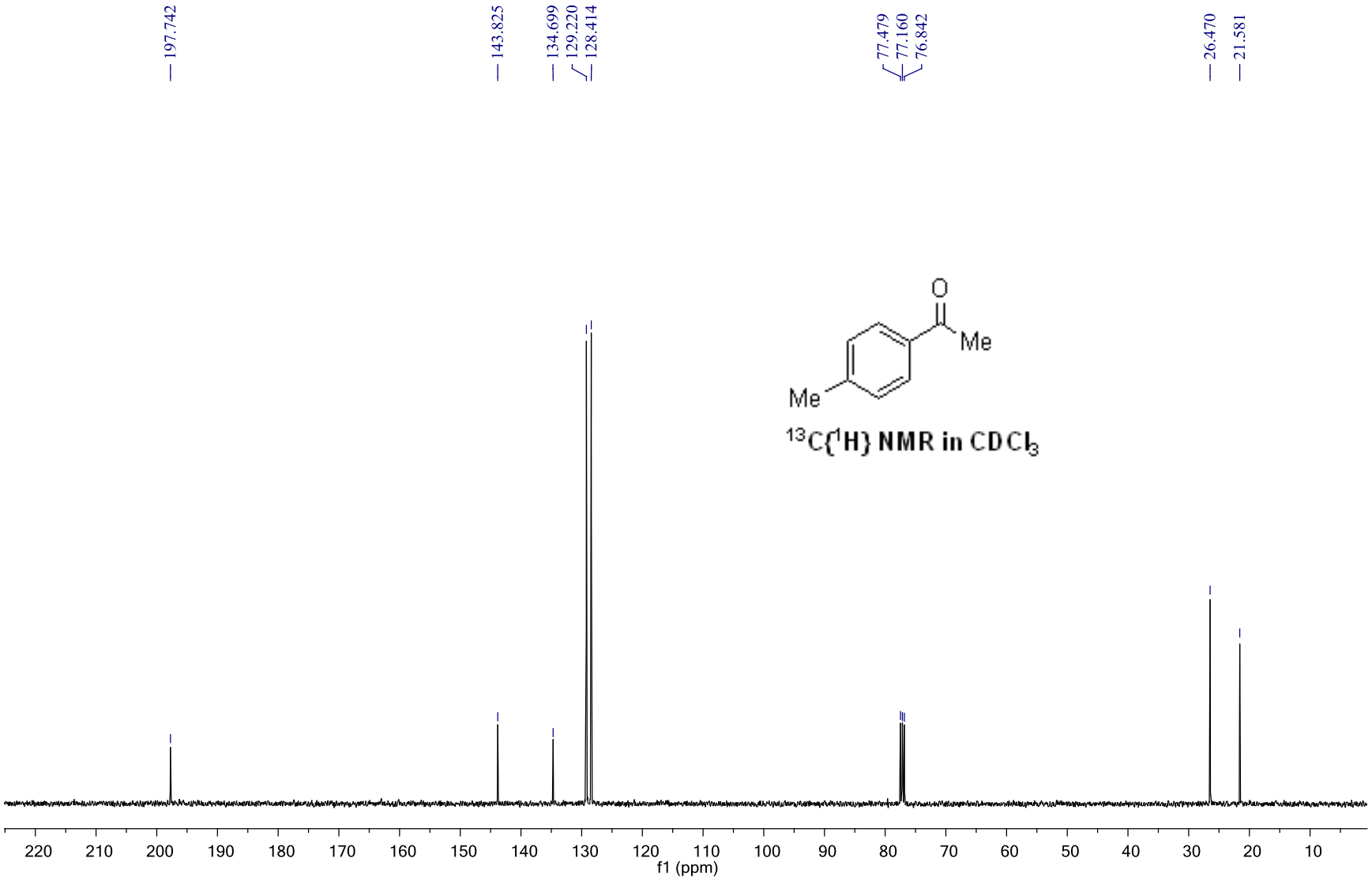

7.951
7.930
7.556
7.540
7.522
7.457
7.455
7.438
7.419
2.577
0.000
O
Me
1H NMR in CDCl3
1.91
2.84
3.00
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

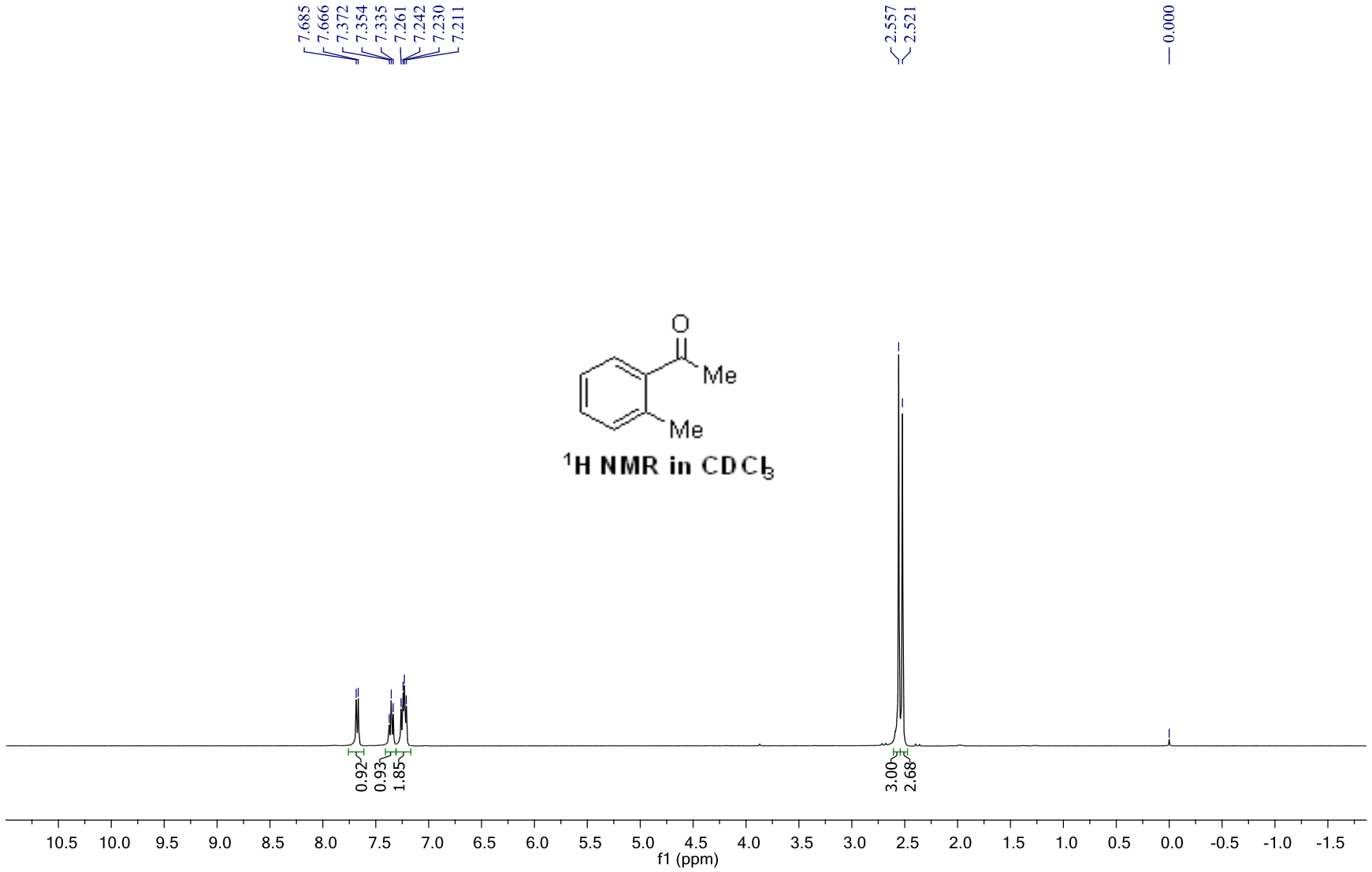

198.031
137.072
133.055
128.528
128.252
77.479
77.160
76.842
26.534
O
Me
13C{1H} NMR in CDCl3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

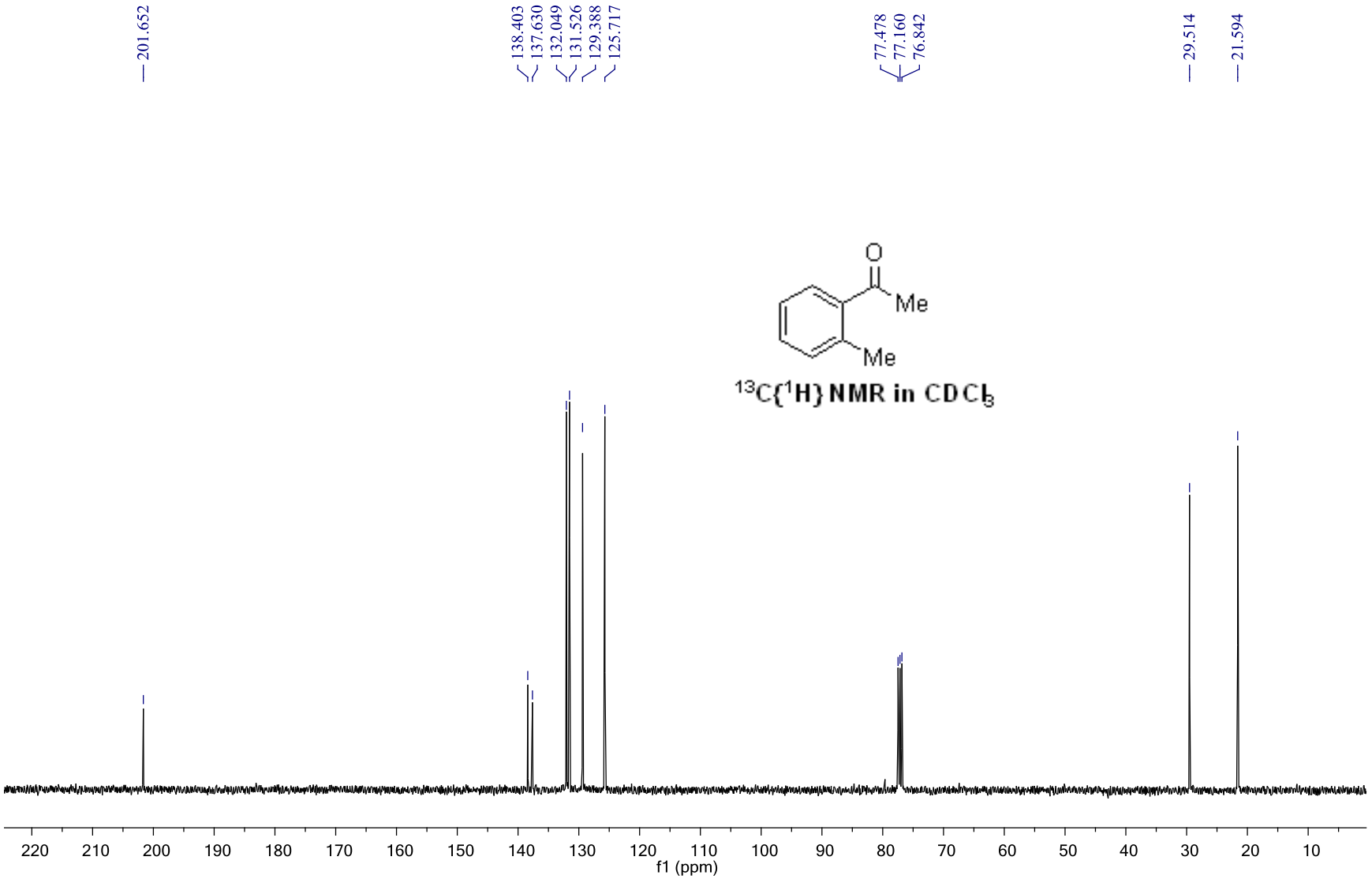

7.945
7.923
7.277
6.939
6.917
3.863
2.550
0.000
O
Me
MeO
^{1}H NMR in CDCl$_3$
1.85
1.86
3.00
2.92
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5 -3.0
f1 (ppm)


196.825
163.560
130.656
130.414
113.752
77.477
77.160
76.841
55.531
26.406
O
Me
MeO
$^{13}C\{^{1}H\}$ NMR in $CDCl_3$
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.851
7.831
7.244
7.224
2.551
2.388
-0.000
O
Me
Me
1H NMR in CDCl3
1.88
1.91
3.00
2.99
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.5
-2.5
-3.5
f1 (ppm)


197.742
143.825
134.699
129.220
128.414
77.479
77.160
76.842
26.470
21.581
O
Me
Me
13C{1H} NMR in CDCl3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.685
7.666
7.372
7.354
7.335
7.261
7.242
7.230
7.211
2.557
2.521
0.000
O
Me
Me
¹H NMR in CDCl₃
0.92
0.93
1.85
3.00
2.68
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)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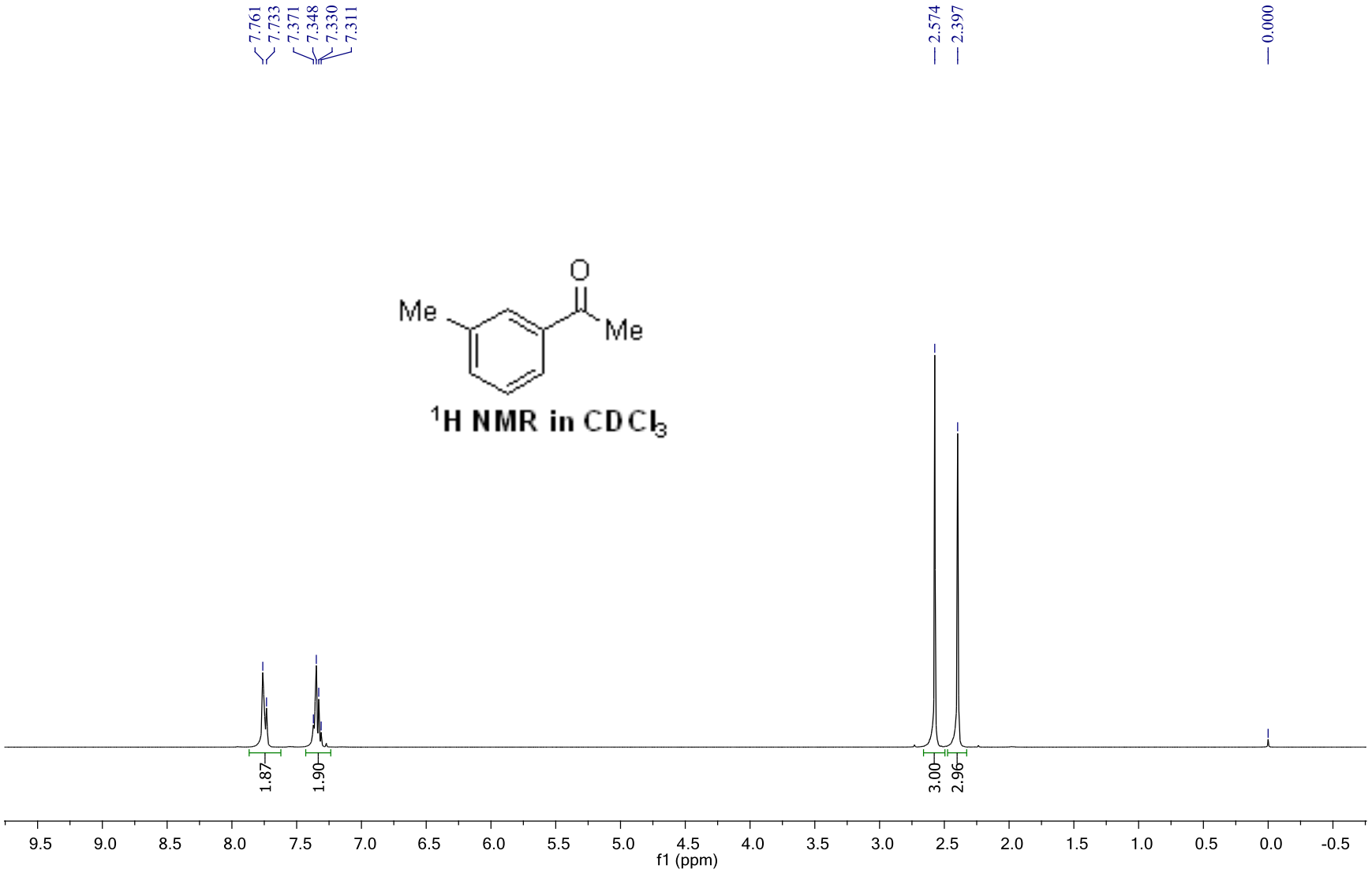
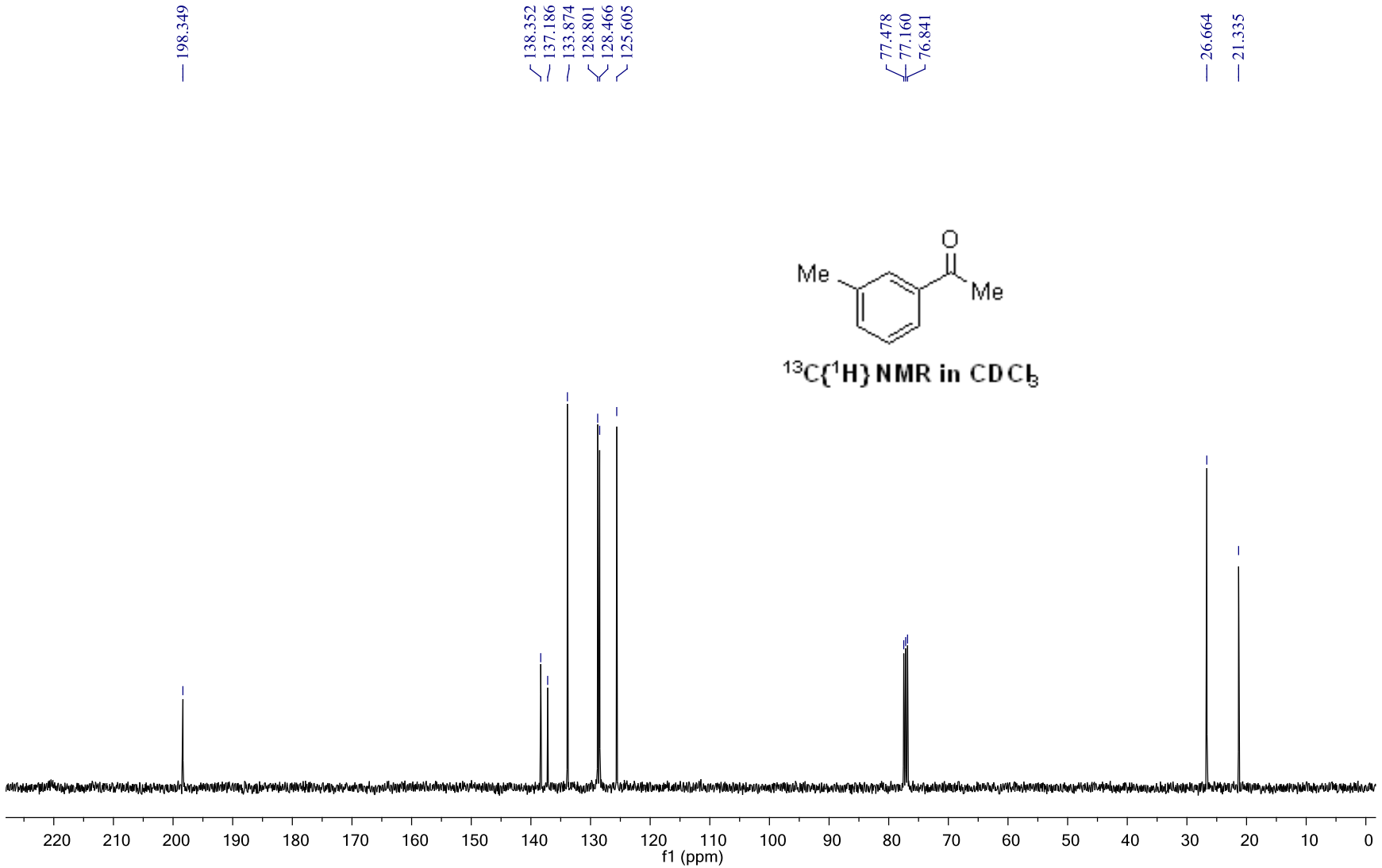
138.403
137.630
132.049
131.526
129.388
125.717
77.478
77.160
76.842
29.514
21.594
O
Me
Me
13C{1H} NMR in CDCl3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.761
7.733
7.371
7.348
7.330
7.311
2.574
2.397
0.000
O
Me
Me
1H NMR in CDCl3
1.87
1.90
3.00
2.96
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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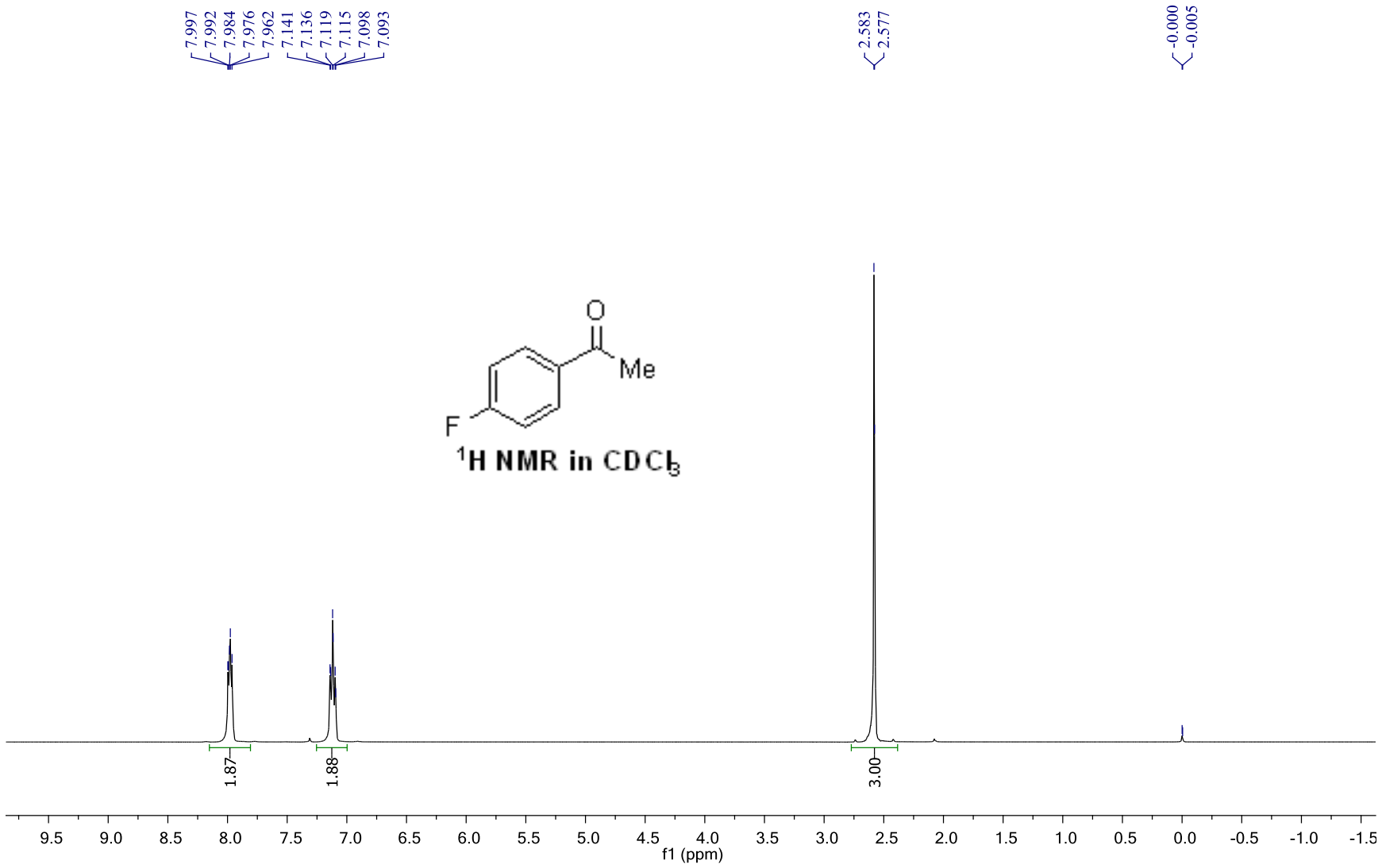
138.352
137.186
133.874
128.801
128.466
125.605
77.478
77.160
76.841
26.664
21.335
O
Me
Me
13C{1H} NMR in CDCl3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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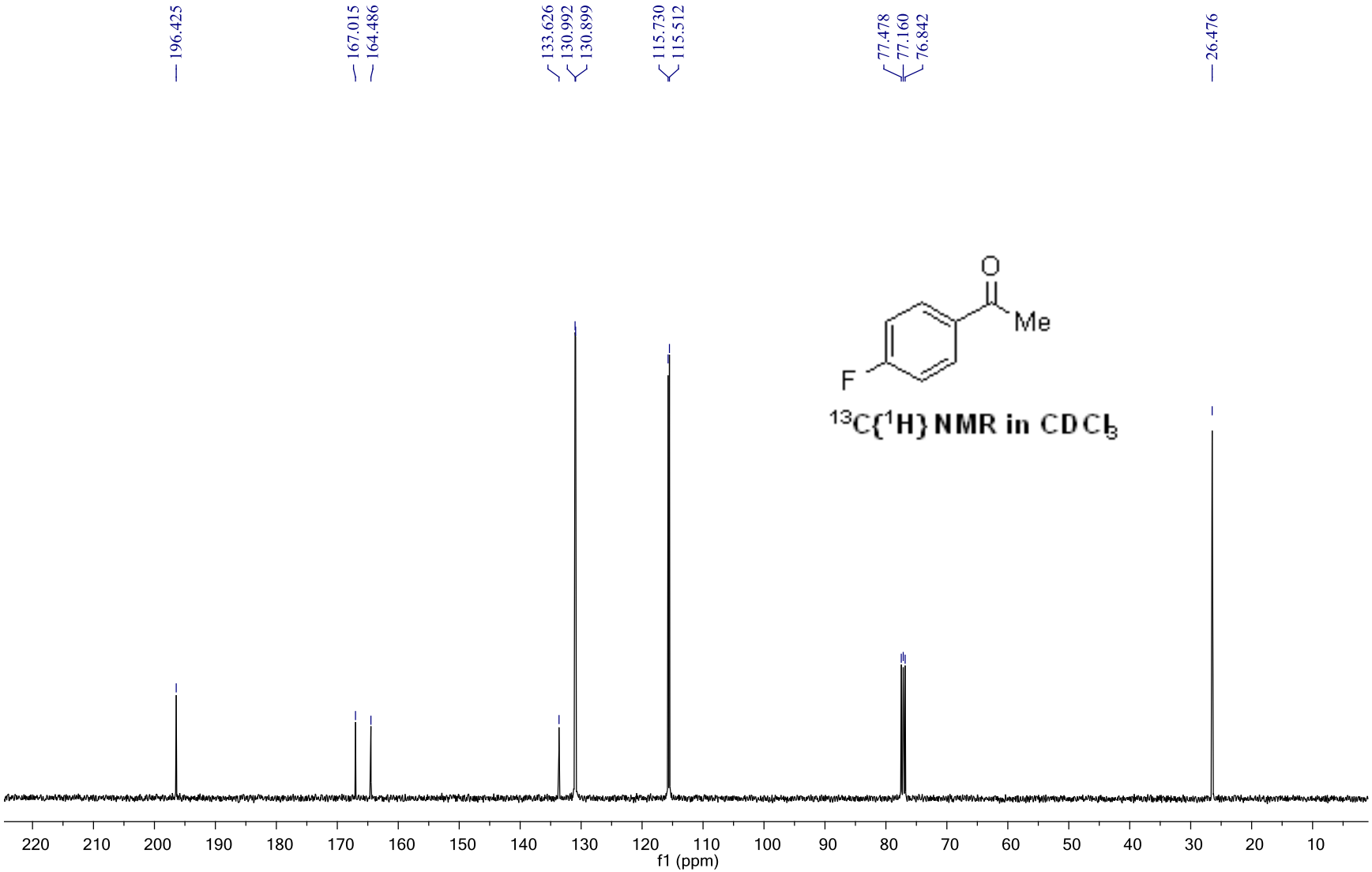
7.992
7.984
7.976
7.962
7.141
7.136
7.119
7.115
7.098
7.093
2.583
2.577
-0.000
-0.005
O
Me
F
1H NMR in CDCl3
1.87
1.88
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)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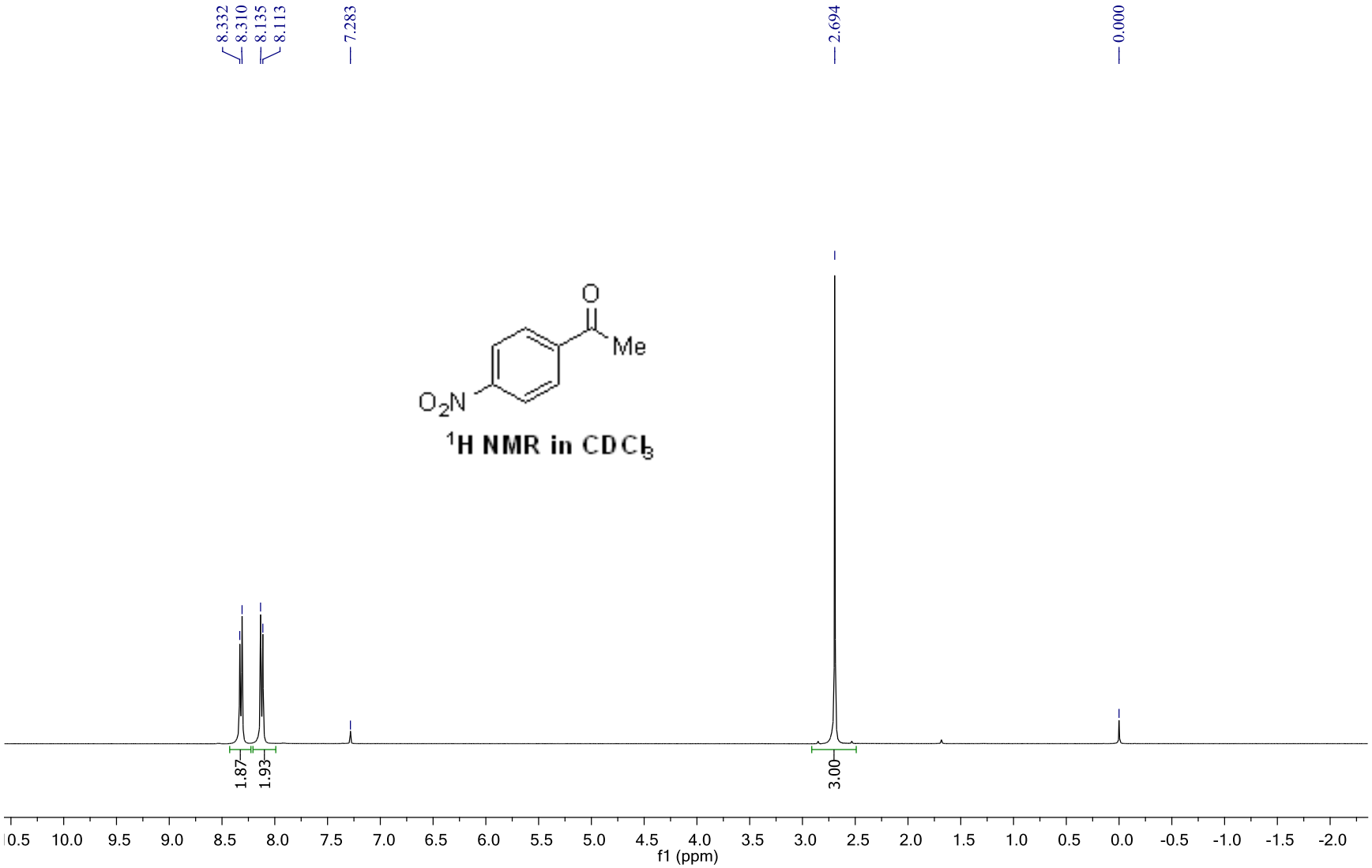
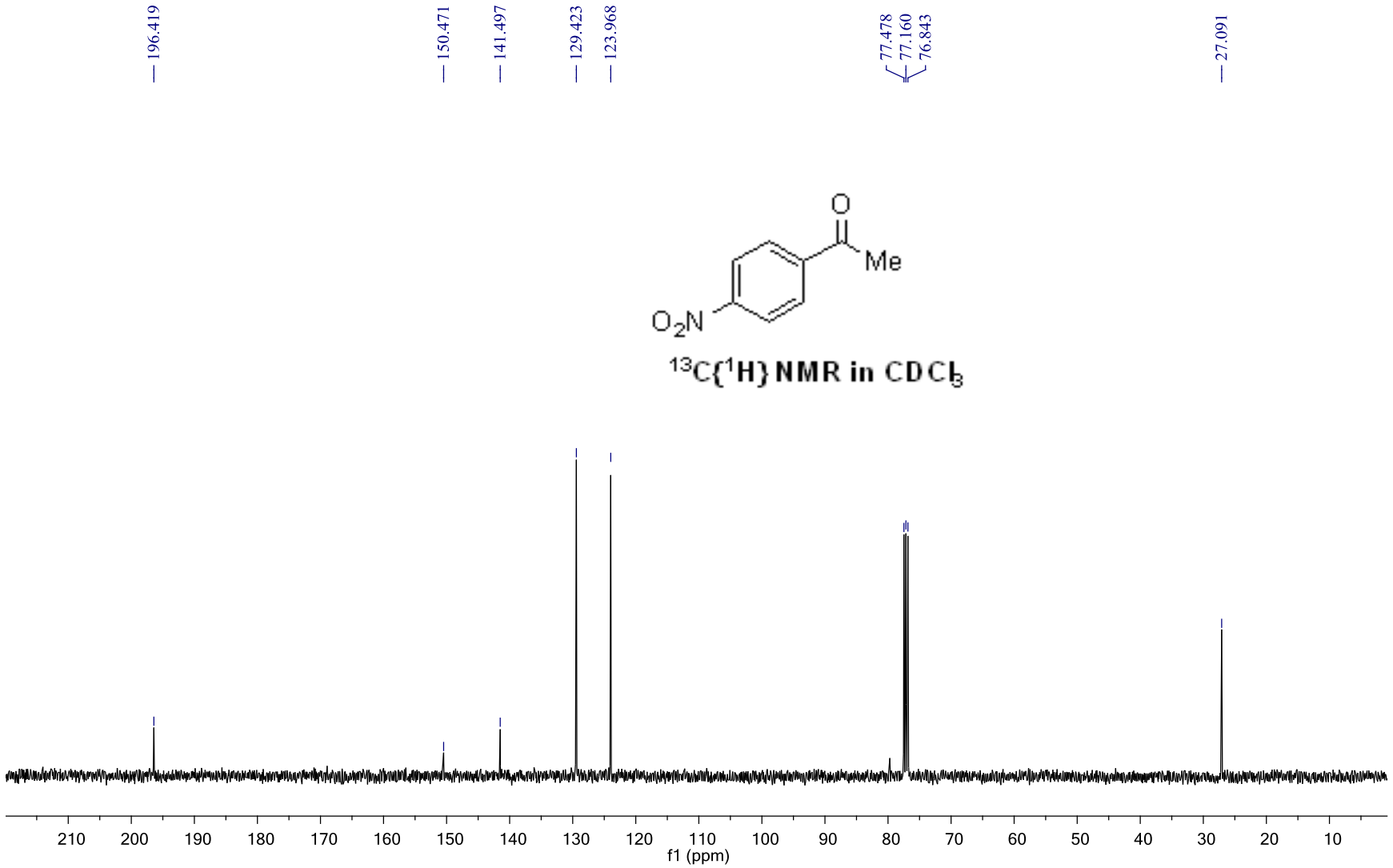
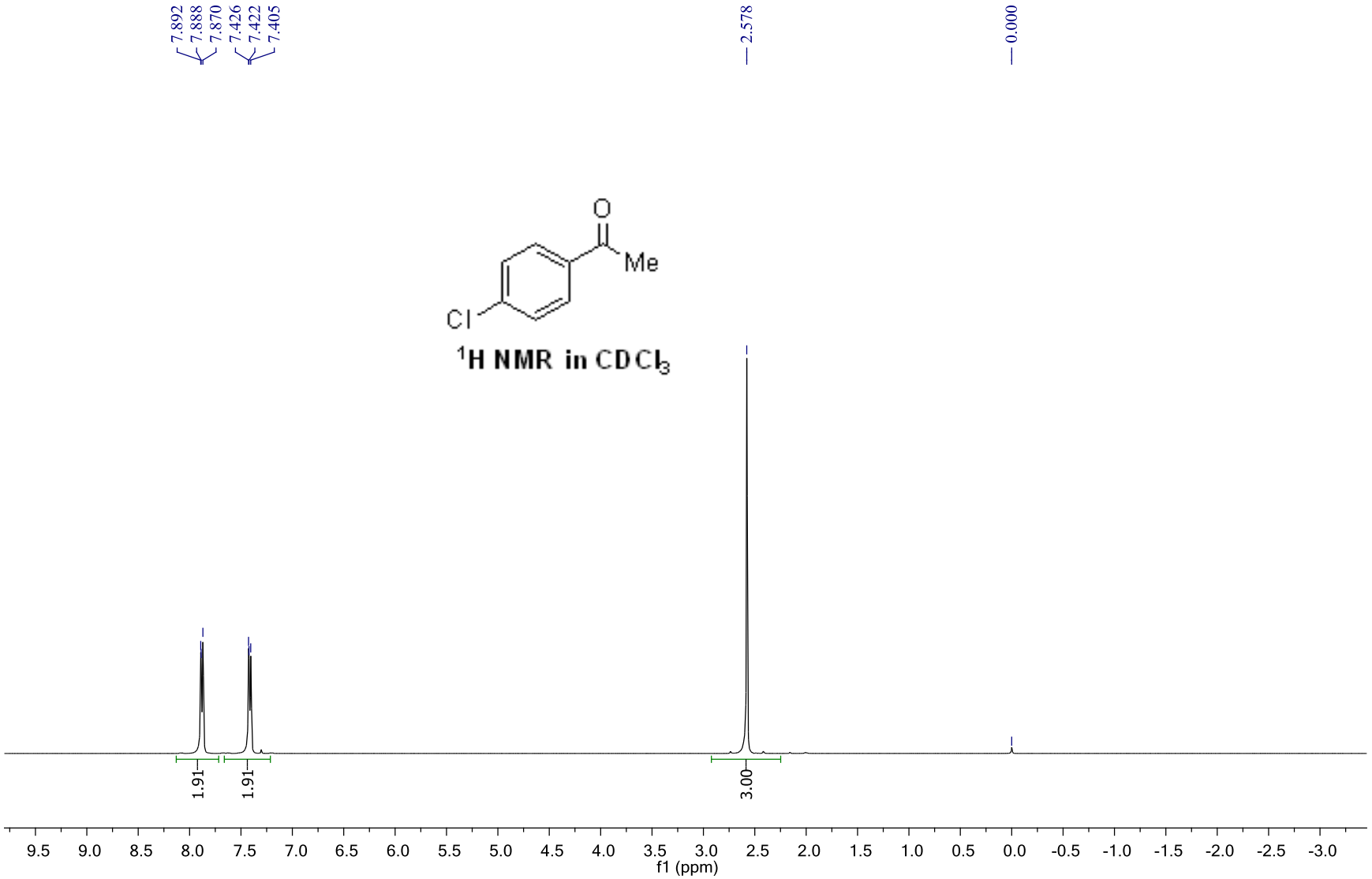
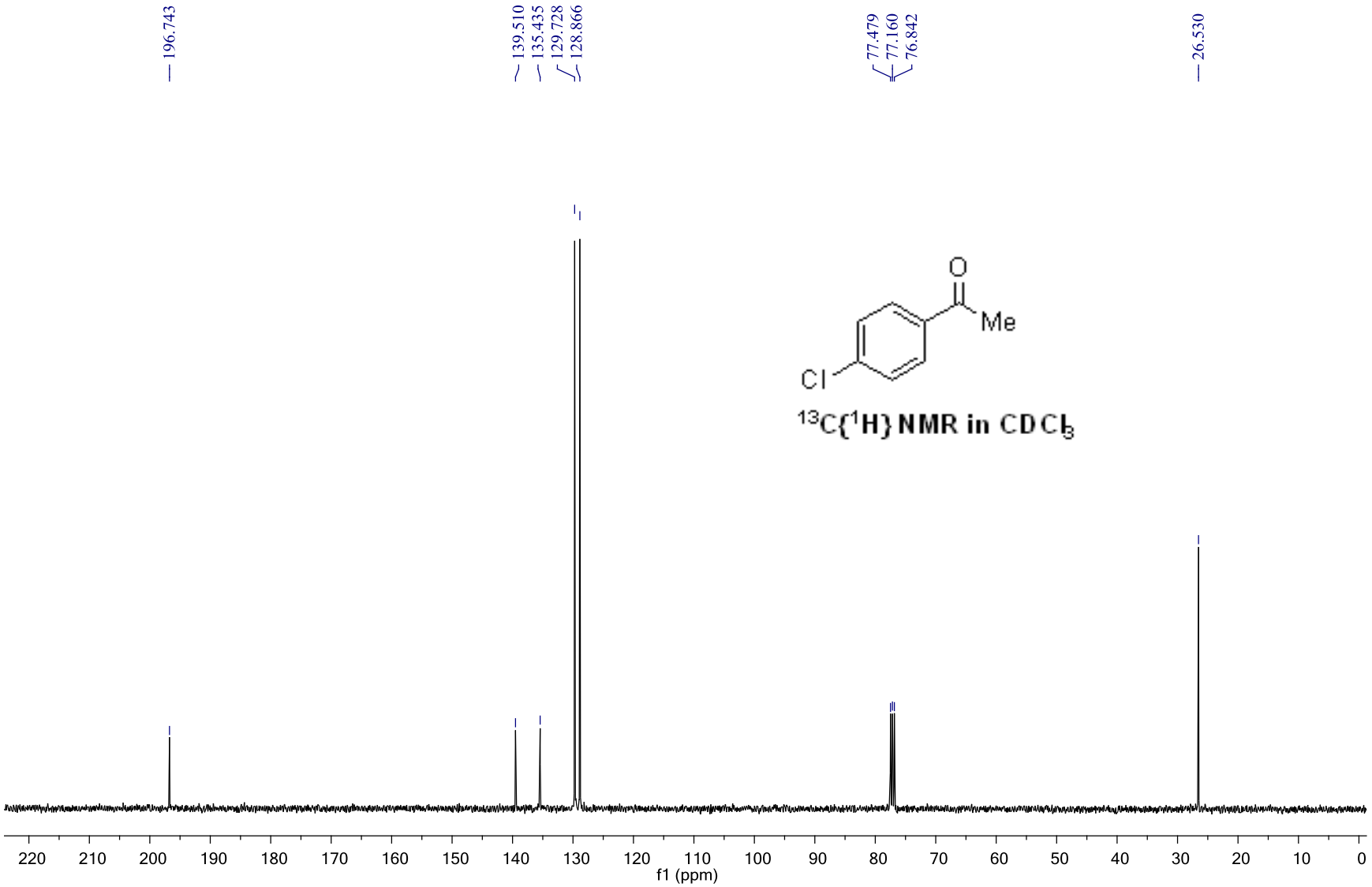
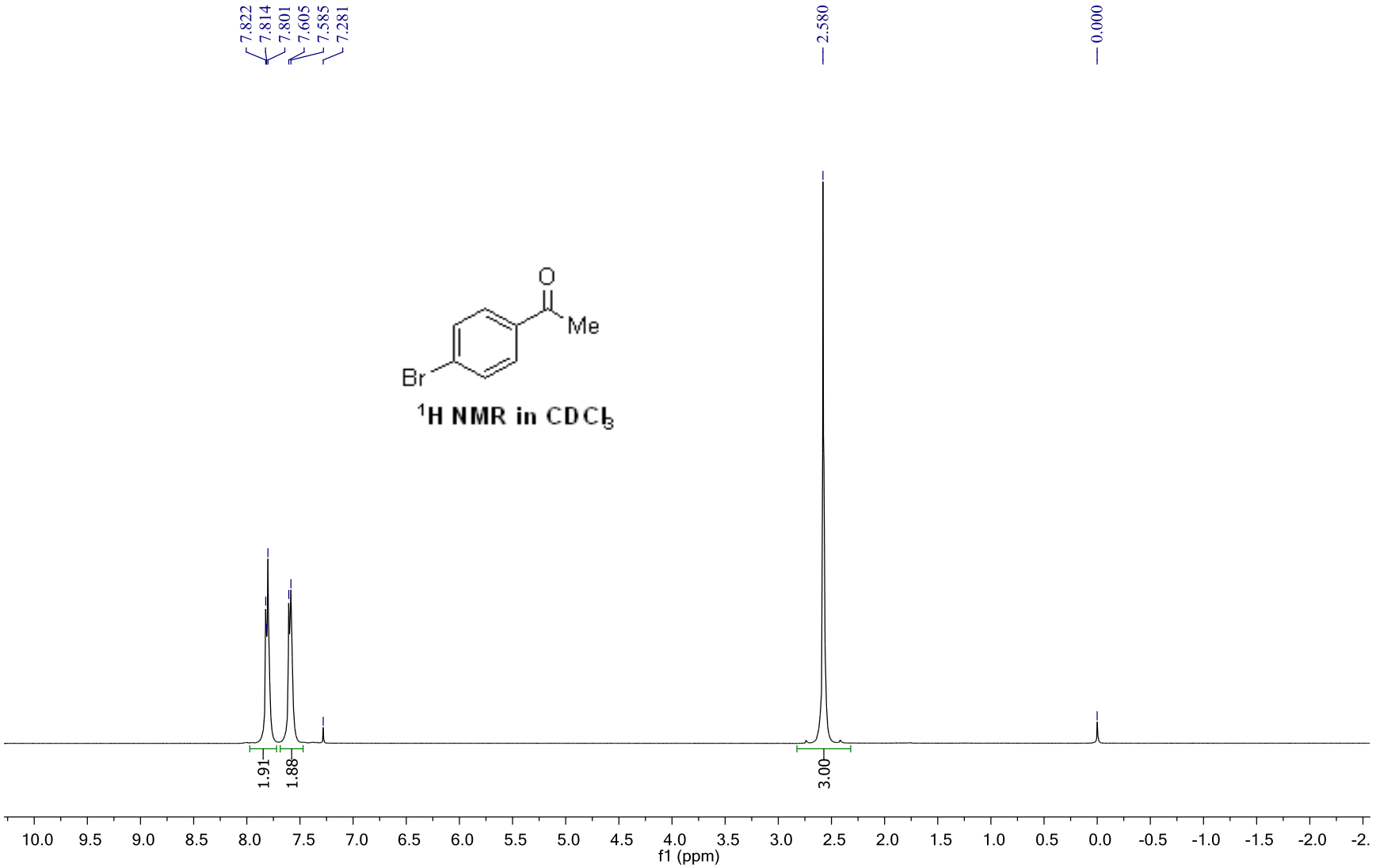
167.015
164.486
133.626
130.992
130.899
115.730
115.512
77.478
77.160
76.842
26.476
O
Me
F
13C{1H} NMR in CDCl3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

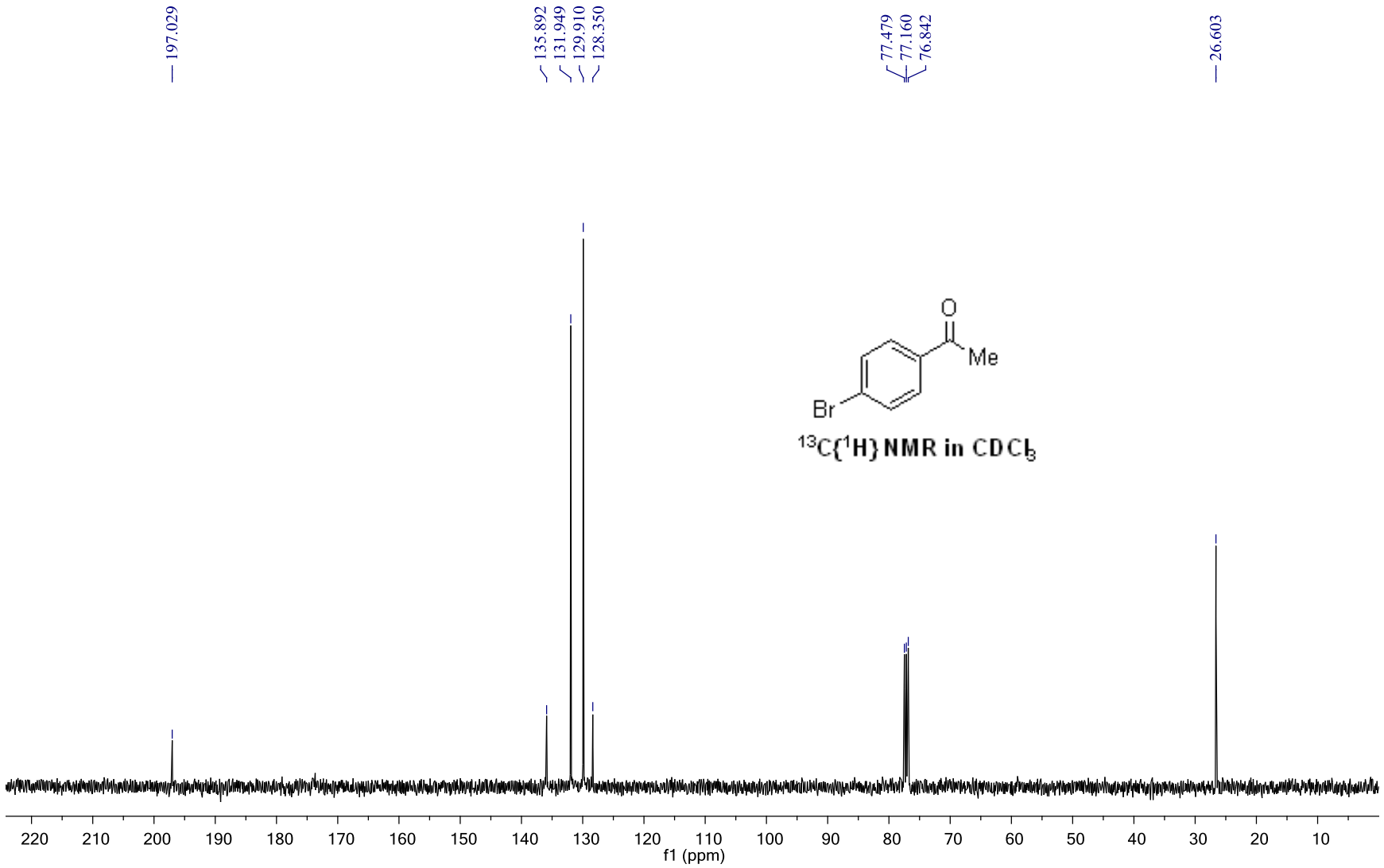

8.332
8.310
8.135
8.113
7.283
2.694
0.000
O
Me
O2N
1H NMR in CDCl3
1.87
1.93
3.00
f1 (ppm)

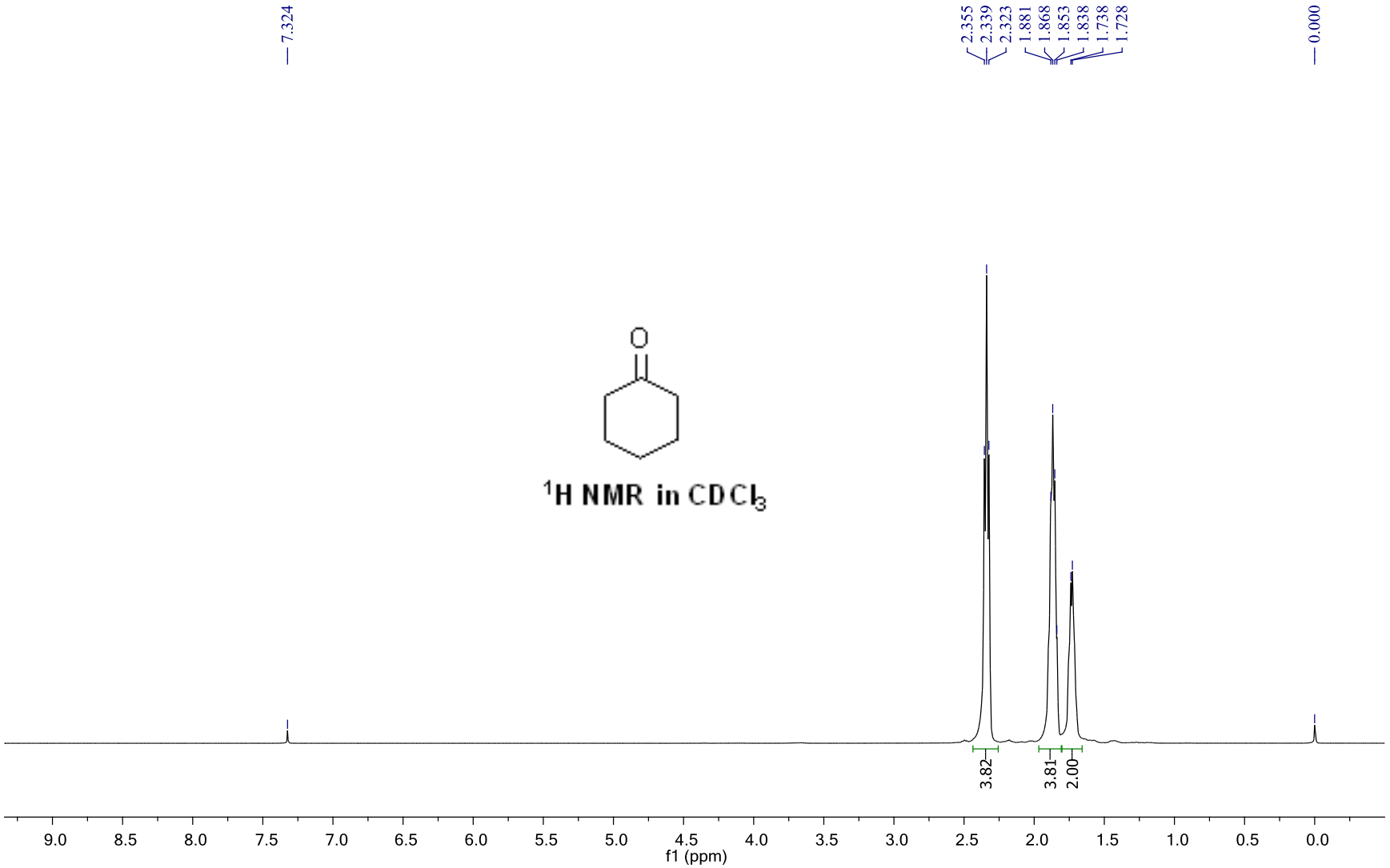

196.419
150.471
141.497
129.423
123.968
77.478
77.160
76.843
27.091
O
Me
O2N
13C{1H} NMR in CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.892
7.888
7.870
7.426
7.422
7.405
2.578
0.000
O
Me
Cl
1H NMR in CDCl3
1.91
1.91
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5 -3.0
f1 (ppm)


196.743
139.510
135.435
129.728
128.866
77.479
77.160
76.842
26.530
O
Me
Cl
13C{1H} NMR in CDCl3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.822
7.814
7.801
7.605
7.585
7.281
2.580
0.000
O
Me
Br
^{1}H NMR in CDCl$_3$
1.91
1.88
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.
f1 (ppm)


197.029
135.892
131.949
129.910
128.350
77.479
77.160
76.842
26.603
O
Me
Br
13C{1H} NMR in CDCl3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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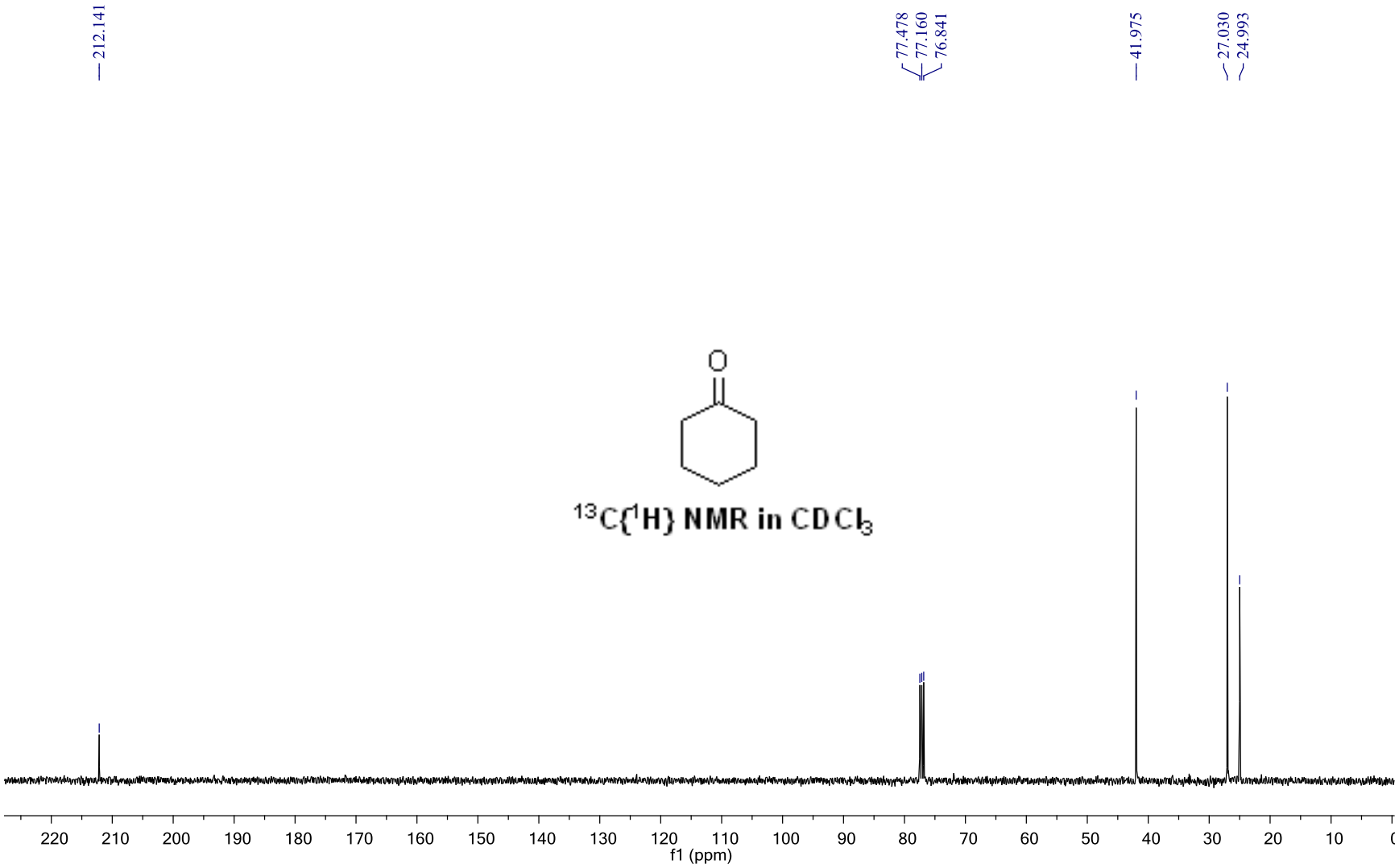
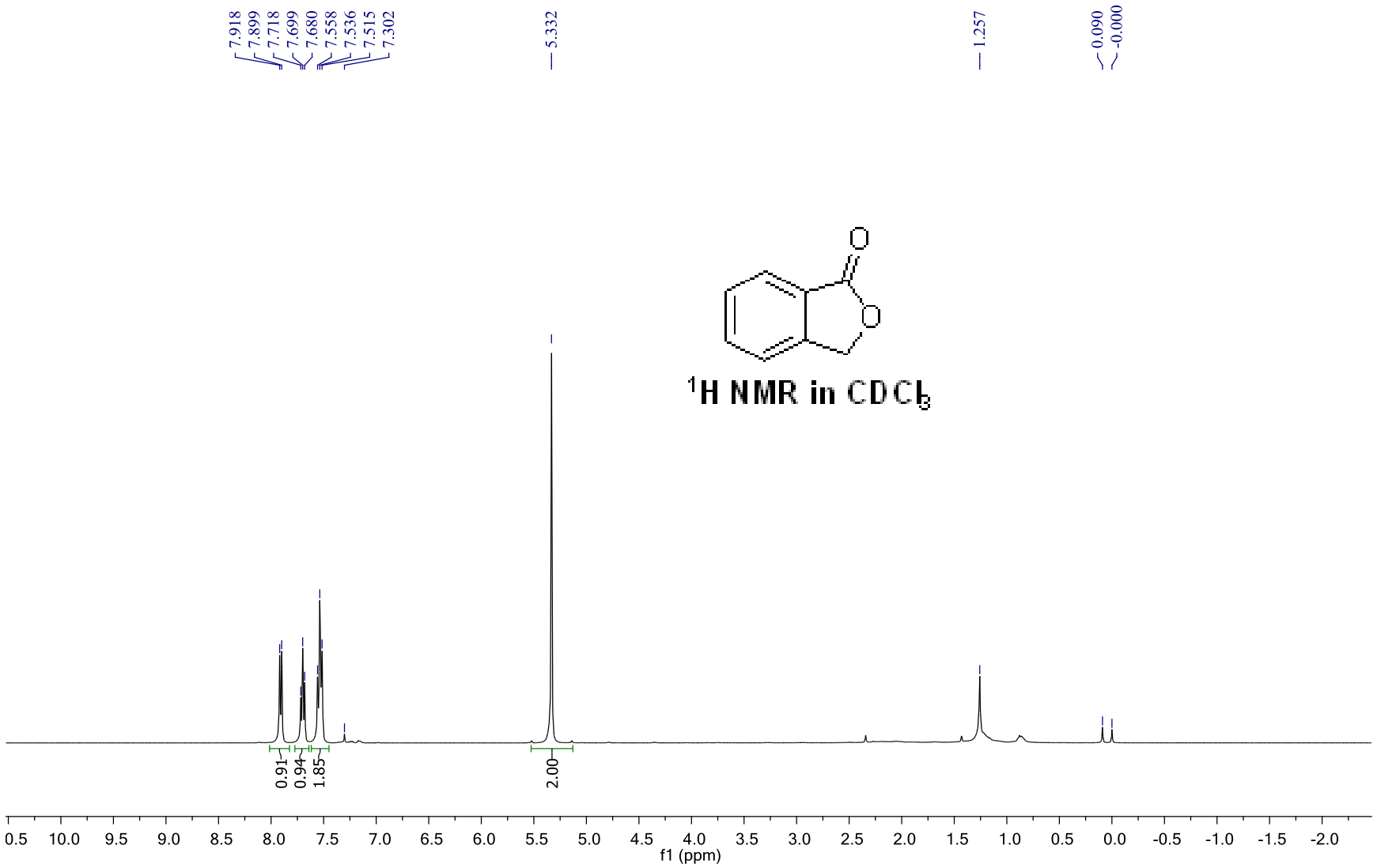
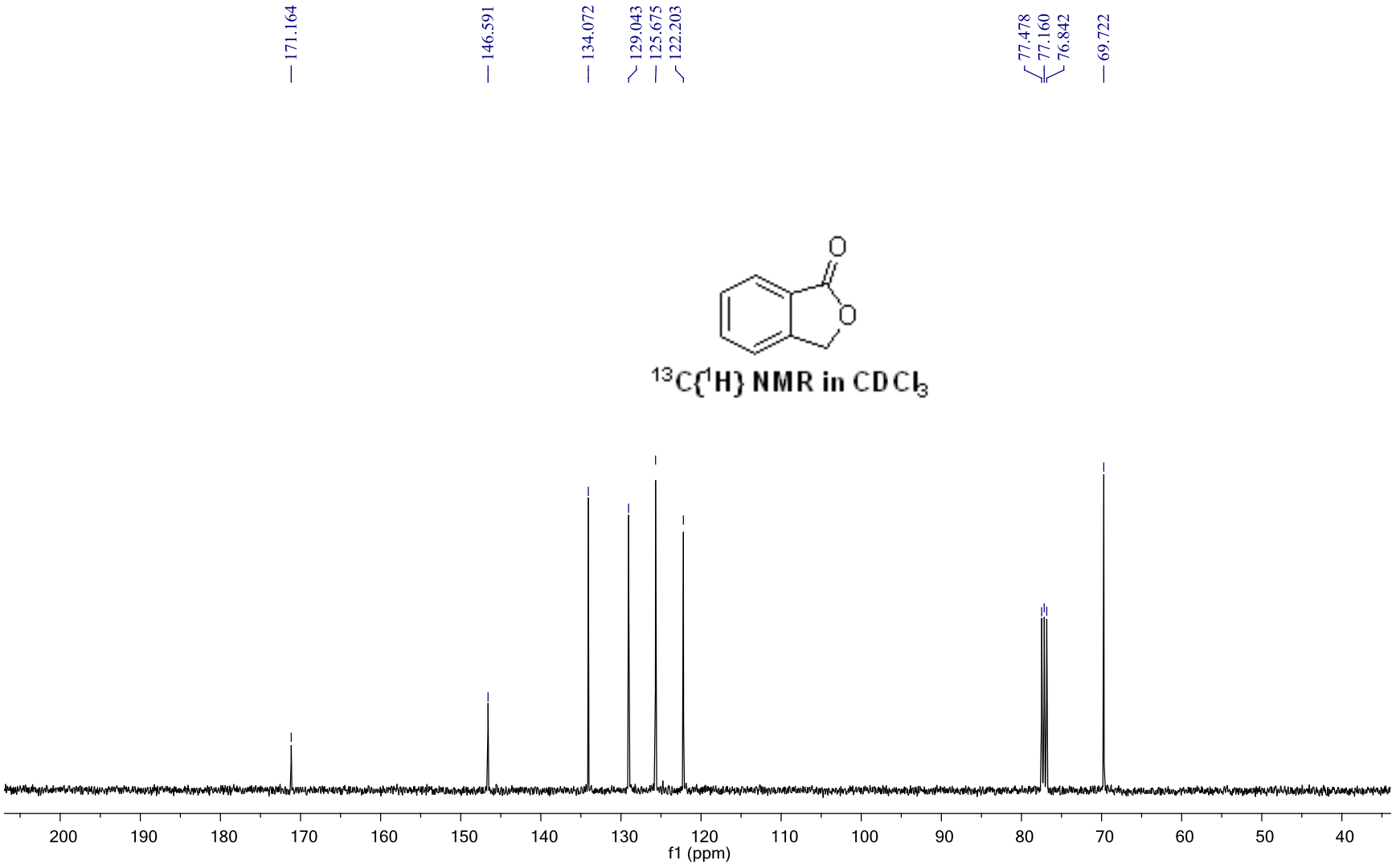
2.355
2.339
2.323
1.881
1.868
1.853
1.838
1.738
1.728
0.000
O
^{1}H NMR in $CDCl_3$
3.82
3.81
2.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


212.141
77.478
77.160
76.841
41.975
27.030
24.993
O
$^{13}C\{^{1}H\}$ NMR in $CDCl_3$
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


7.918
7.899
7.718
7.699
7.680
7.558
7.536
7.515
7.302
5.332
1.257
0.090
-0.000
O
O
^{1}H NMR in CDCl$_3$
0.91
0.94
1.85
2.00
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)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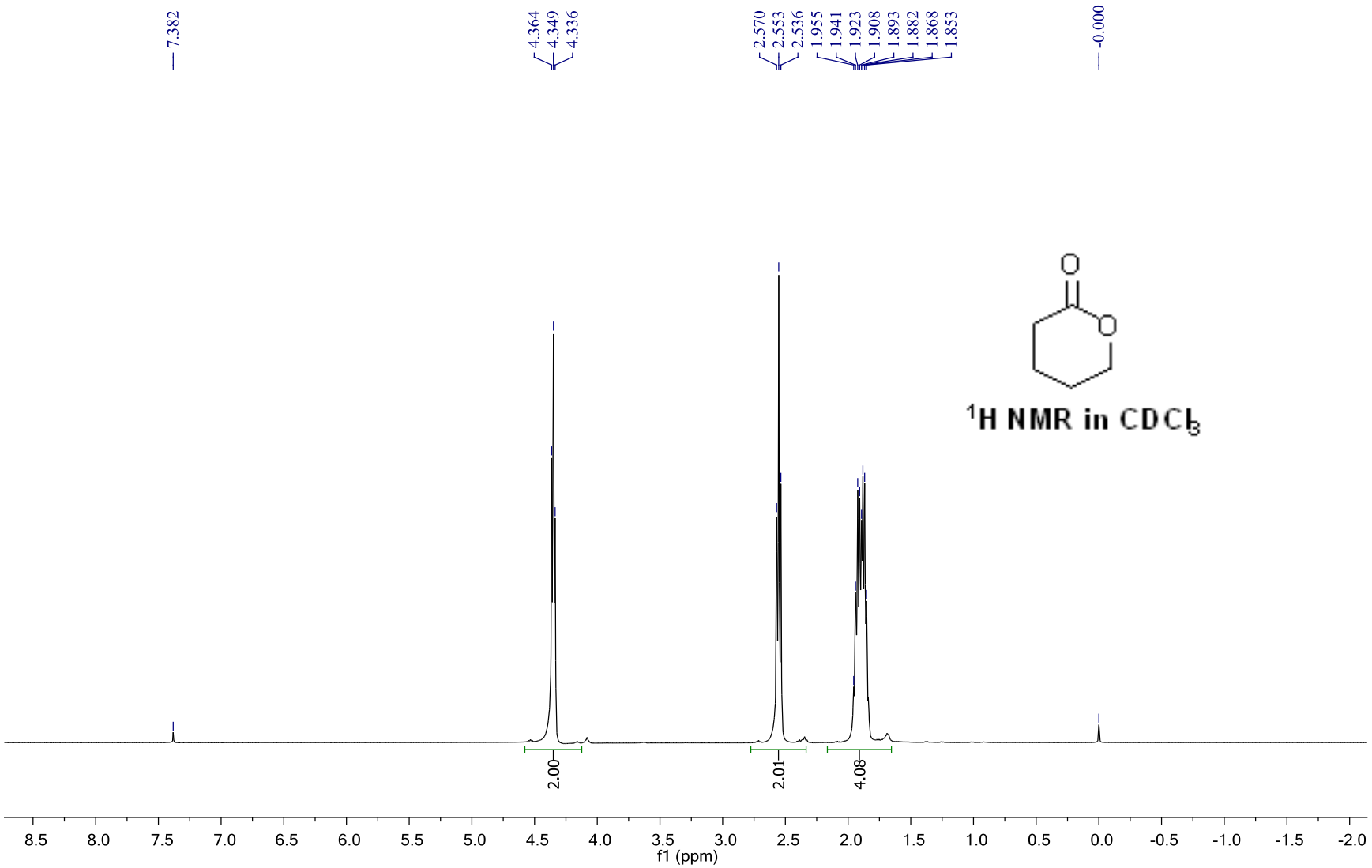
146.591
134.072
129.043
125.675
122.203
77.478
77.160
76.842
69.722
O
O
$^{13}C\{^{1}H\}$ NMR in $CDCl_3$
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
f1 (ppm)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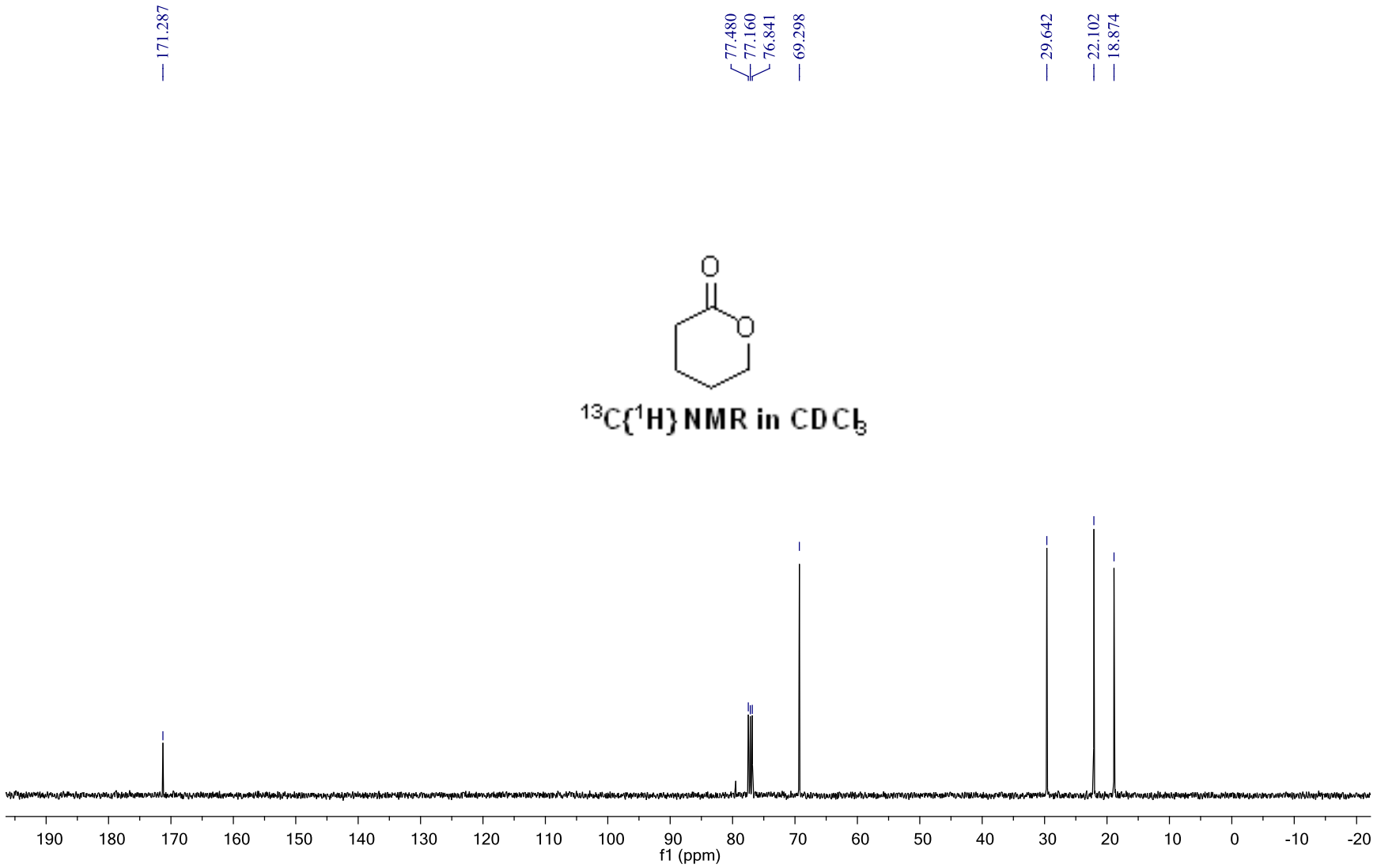
4.364
4.349
4.336
2.570
2.553
2.536
1.955
1.941
1.923
1.908
1.893
1.882
1.868
1.853
-0.000
^{1}H NMR in CDCl$_3$
2.00
2.01
4.08
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)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76.841
69.298
29.642
22.102
18.874
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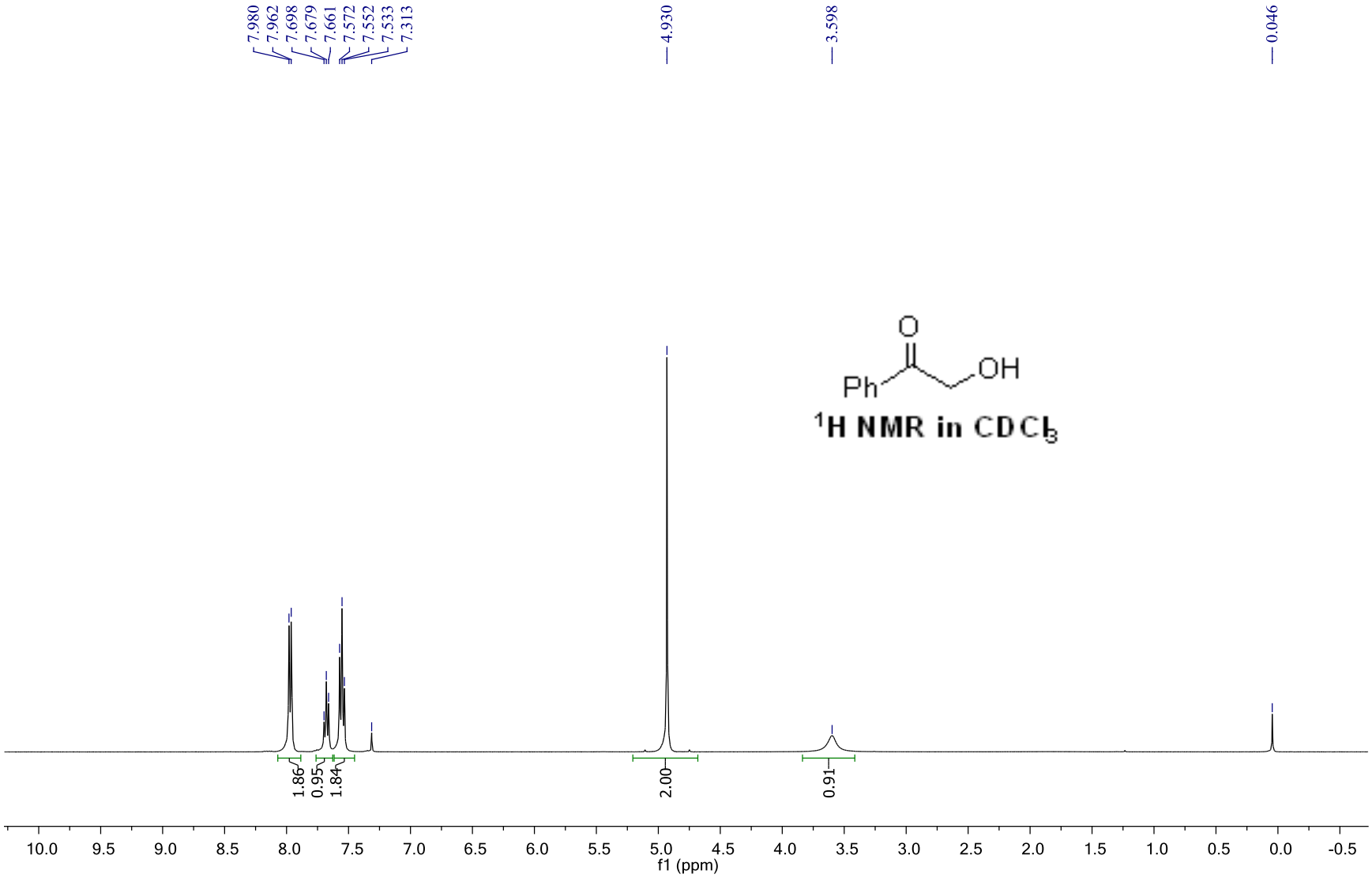
O
13C{1H} NMR in CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)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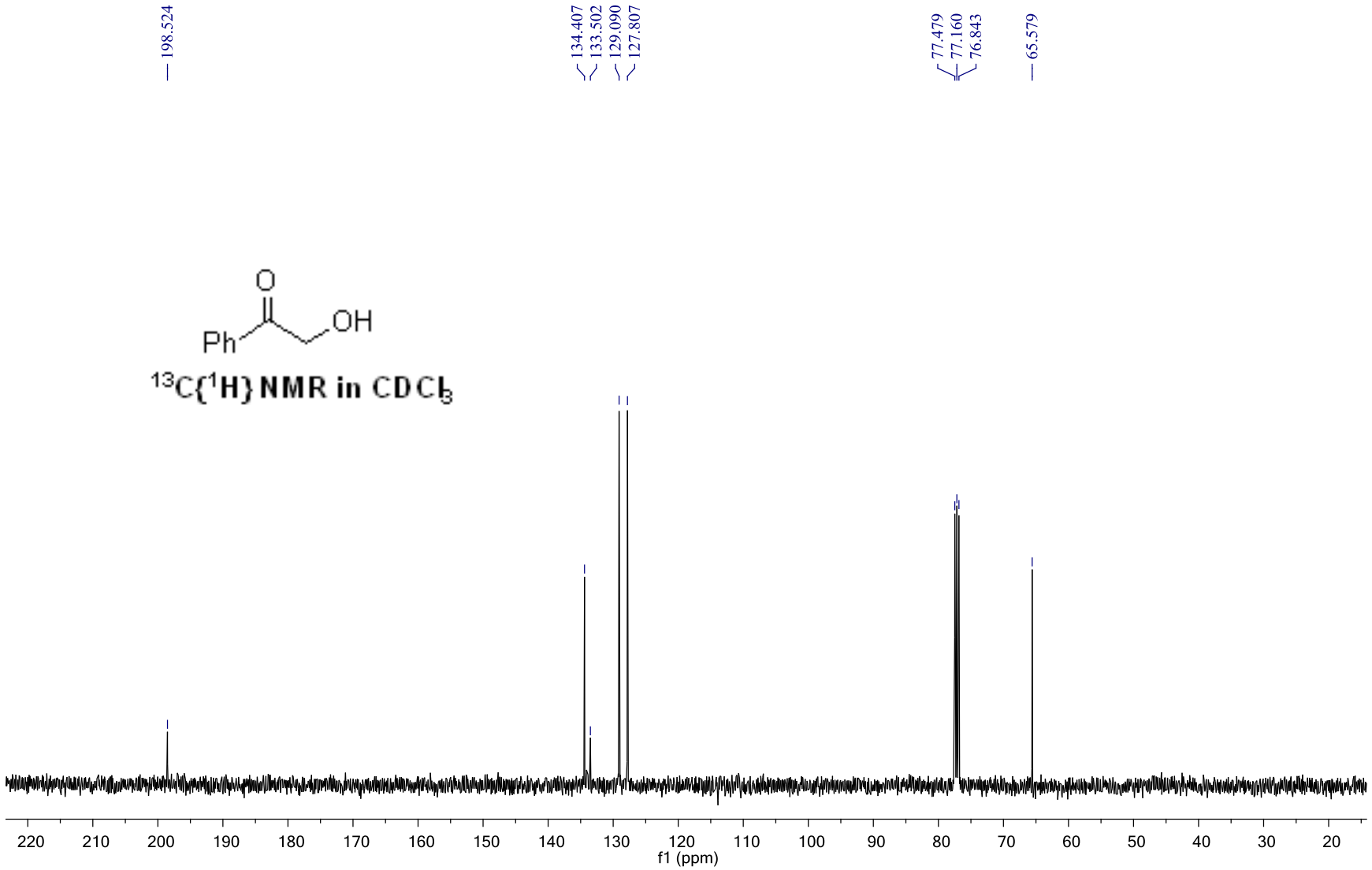
7.698
7.679
7.661
7.572
7.552
7.533
7.313
4.930
3.598
0.046
O
Ph
OH
1H NMR in CDCl3
1.86
0.95
1.84
2.00
0.91
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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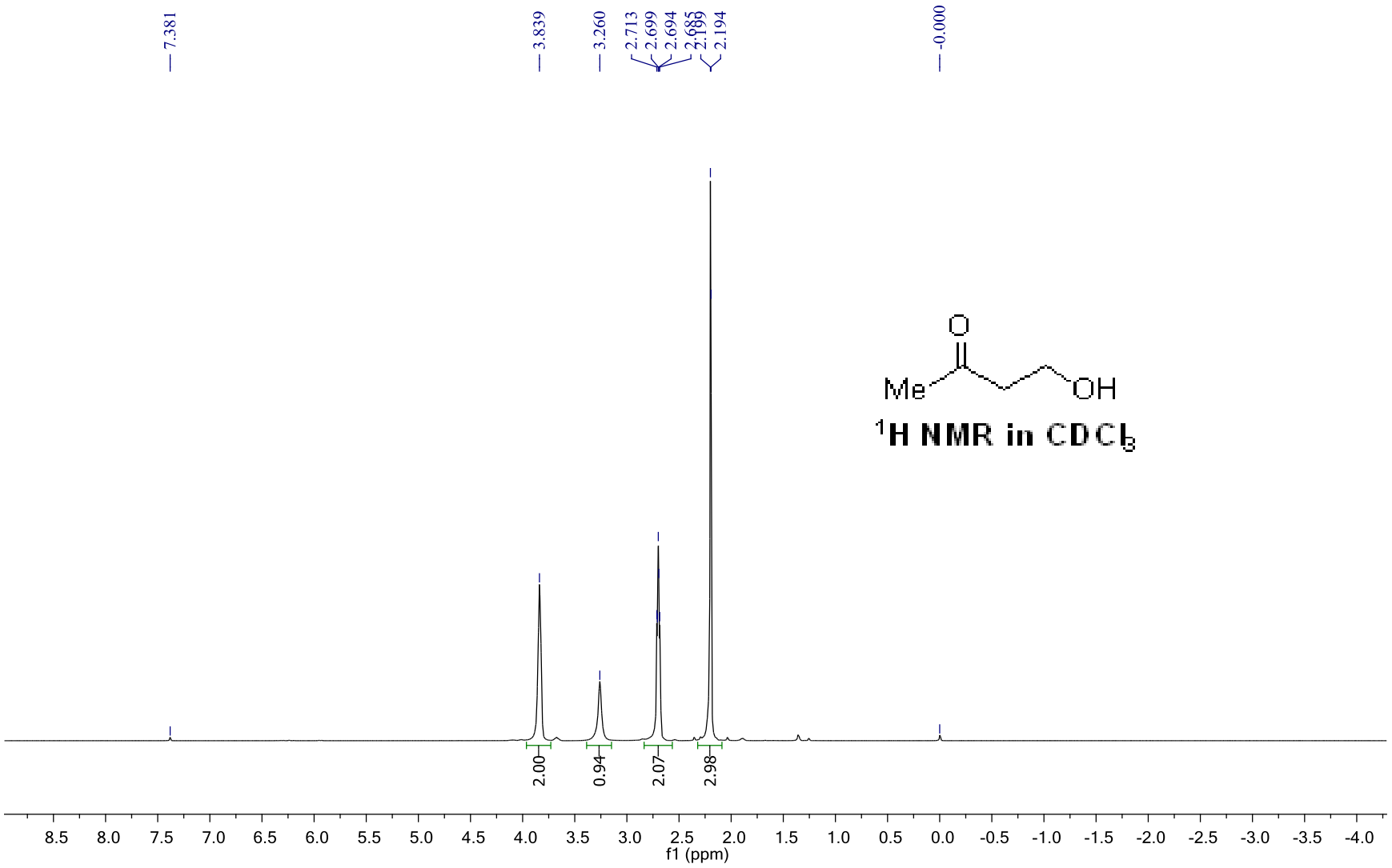
134.407
133.502
129.090
127.807
77.479
77.160
76.843
65.579
O
Ph
OH
13C{1H} NMR in CDCl3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)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3.839
3.260
2.713
2.699
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2.194
-0.000
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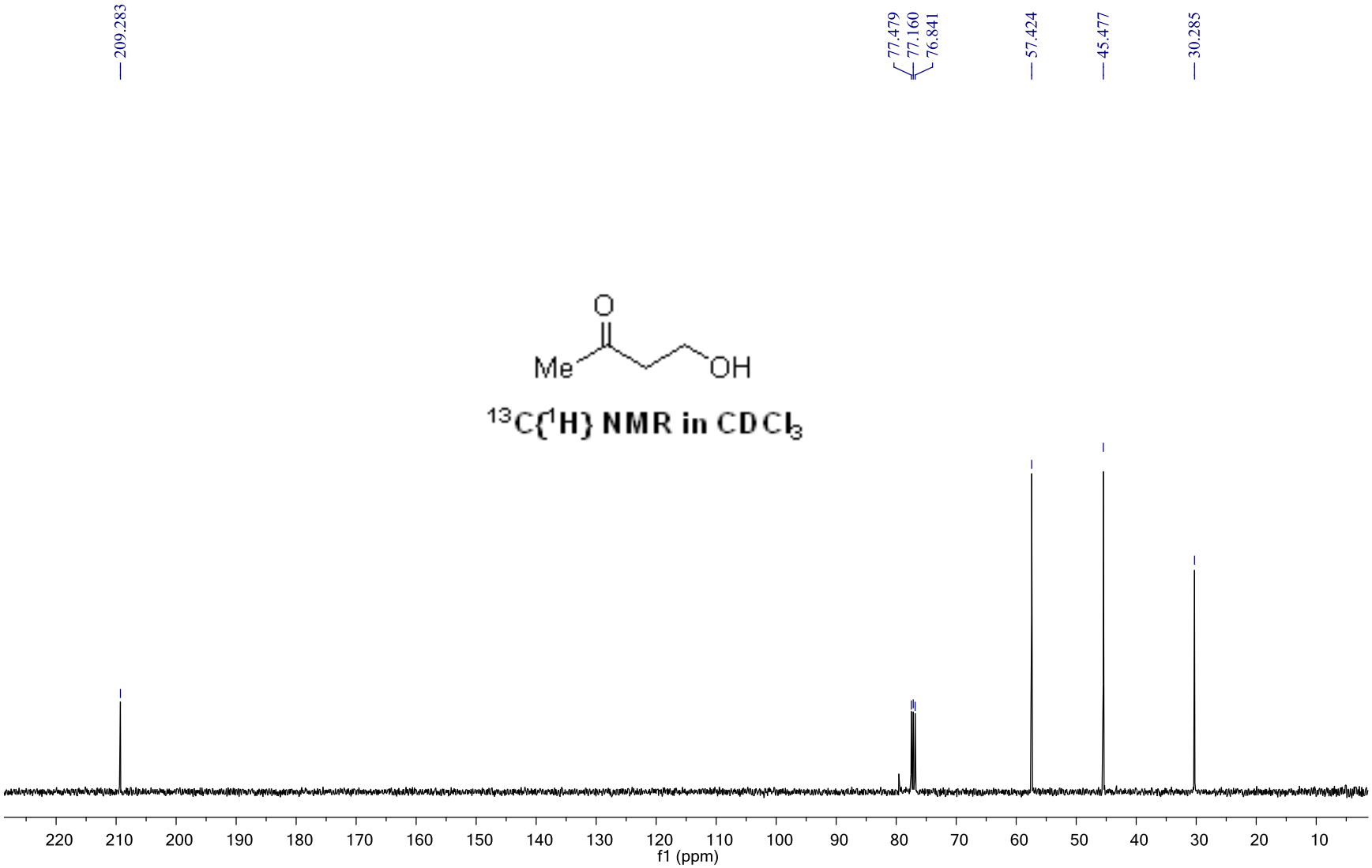
Me
OH
^{1}H NMR in CDCl$_3$
2.00
0.94
2.07
2.98
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5 -3.0 -3.5 -4.0
f1 (ppm)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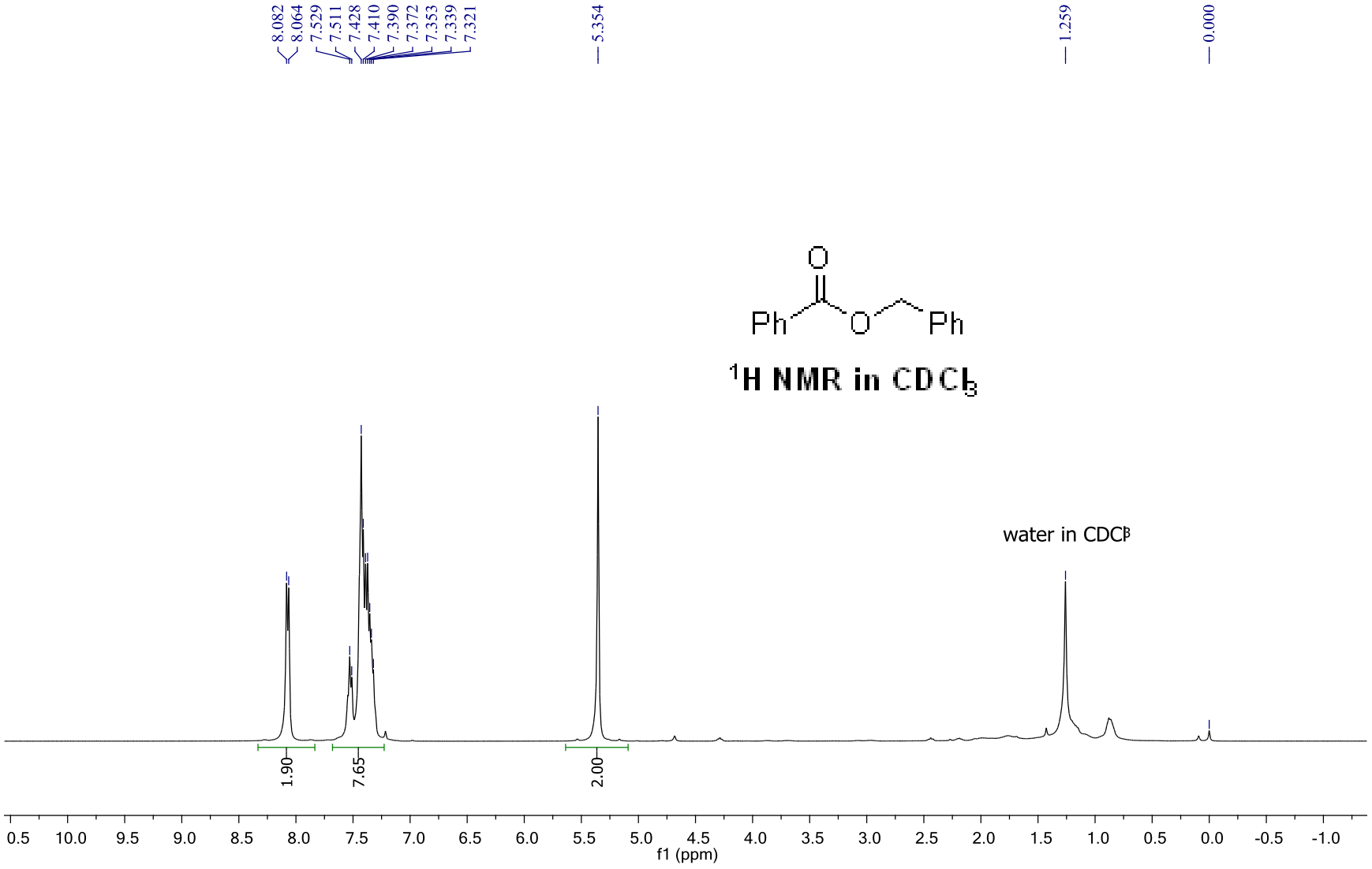
76.841
57.424
45.477
30.285
O
Me
OH
13C{1H} NMR in CDCl3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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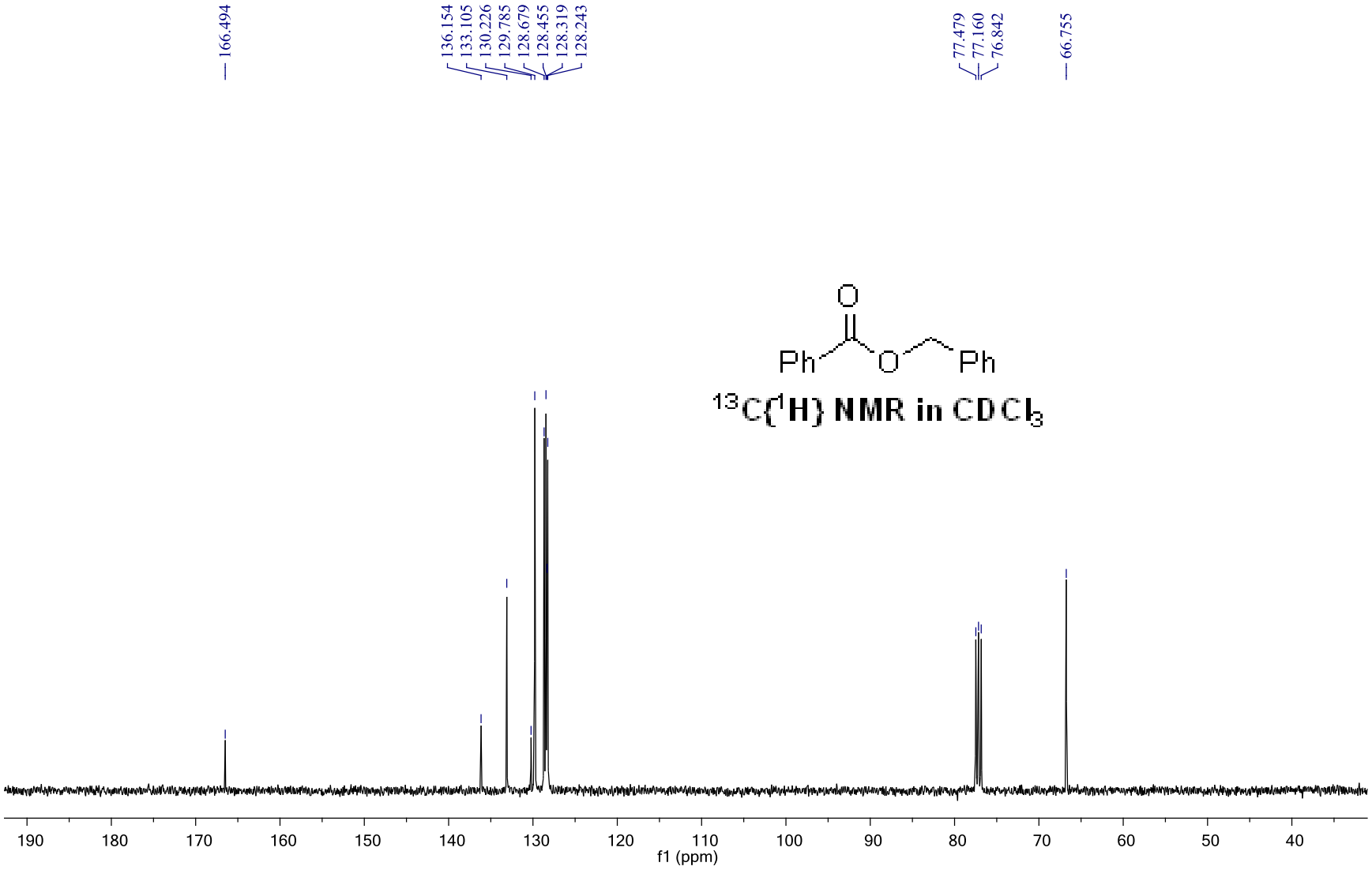
8.064
7.529
7.511
7.428
7.410
7.390
7.372
7.353
7.339
7.321
5.354
1.259
0.000
O
Ph
O
Ph
¹H NMR in CDCl₃
water in CDCl₃
1.90
7.65
2.00
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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136.154
133.105
130.226
129.785
128.679
128.455
128.319
128.243
77.479
77.160
76.842
66.755
O
Ph
O
Ph
13C{1H} NMR in CDCl3
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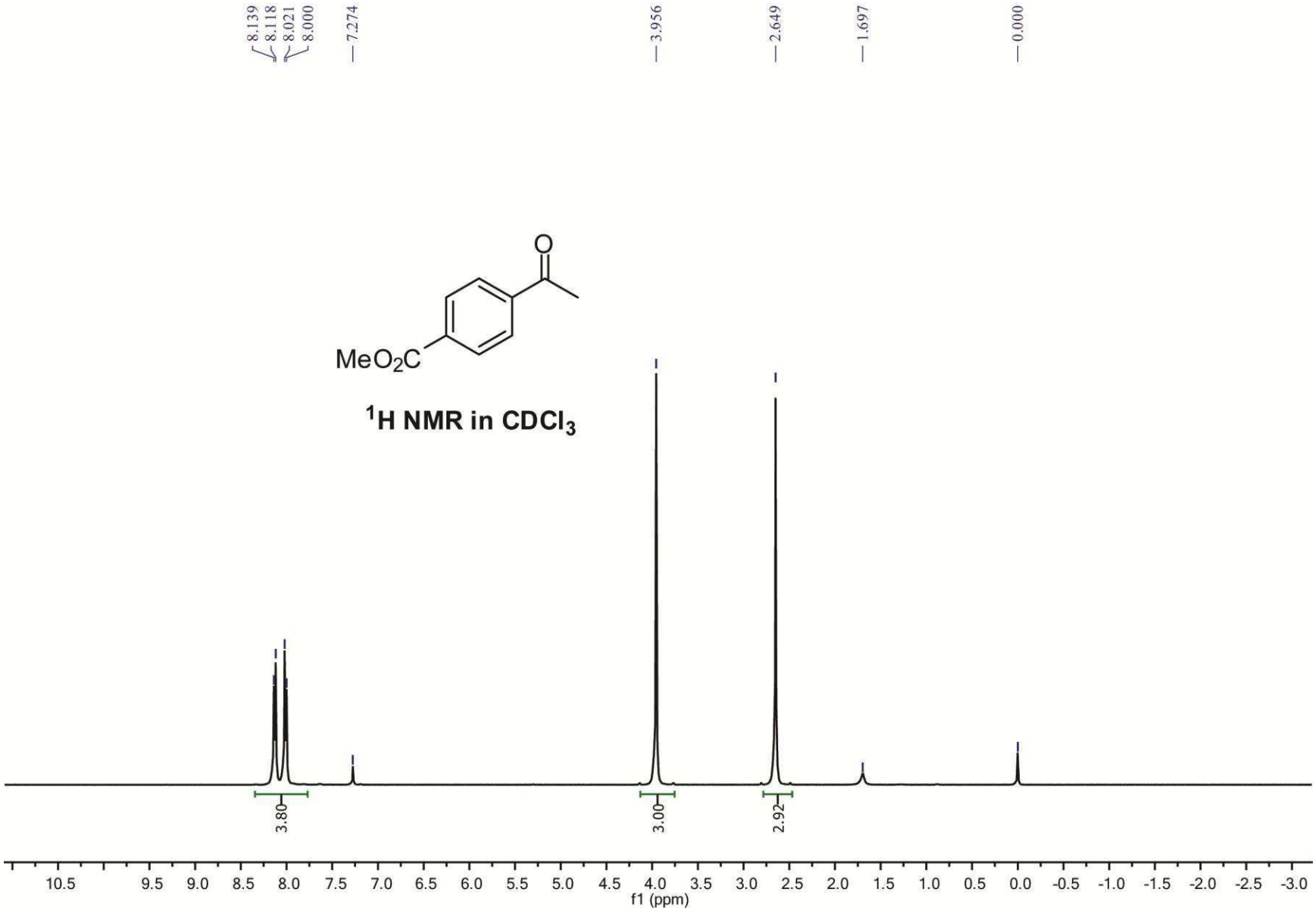
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
f1 (ppm)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8.000
7.274
3.956
2.649
1.697
0.000
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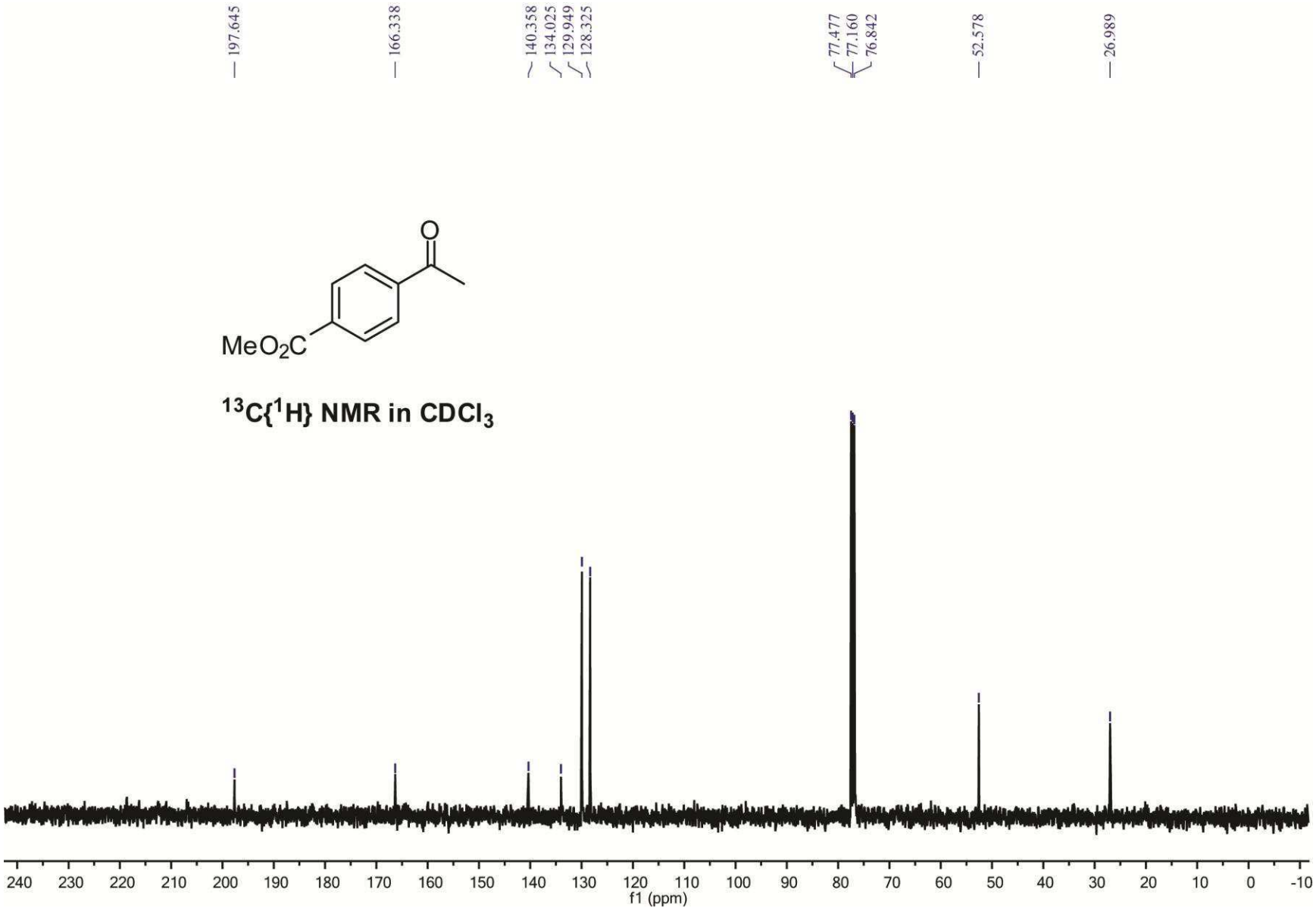
MeO2C
1H NMR in CDCl3
3.80
3.00
2.92
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5 -3.0
f1 (ppm)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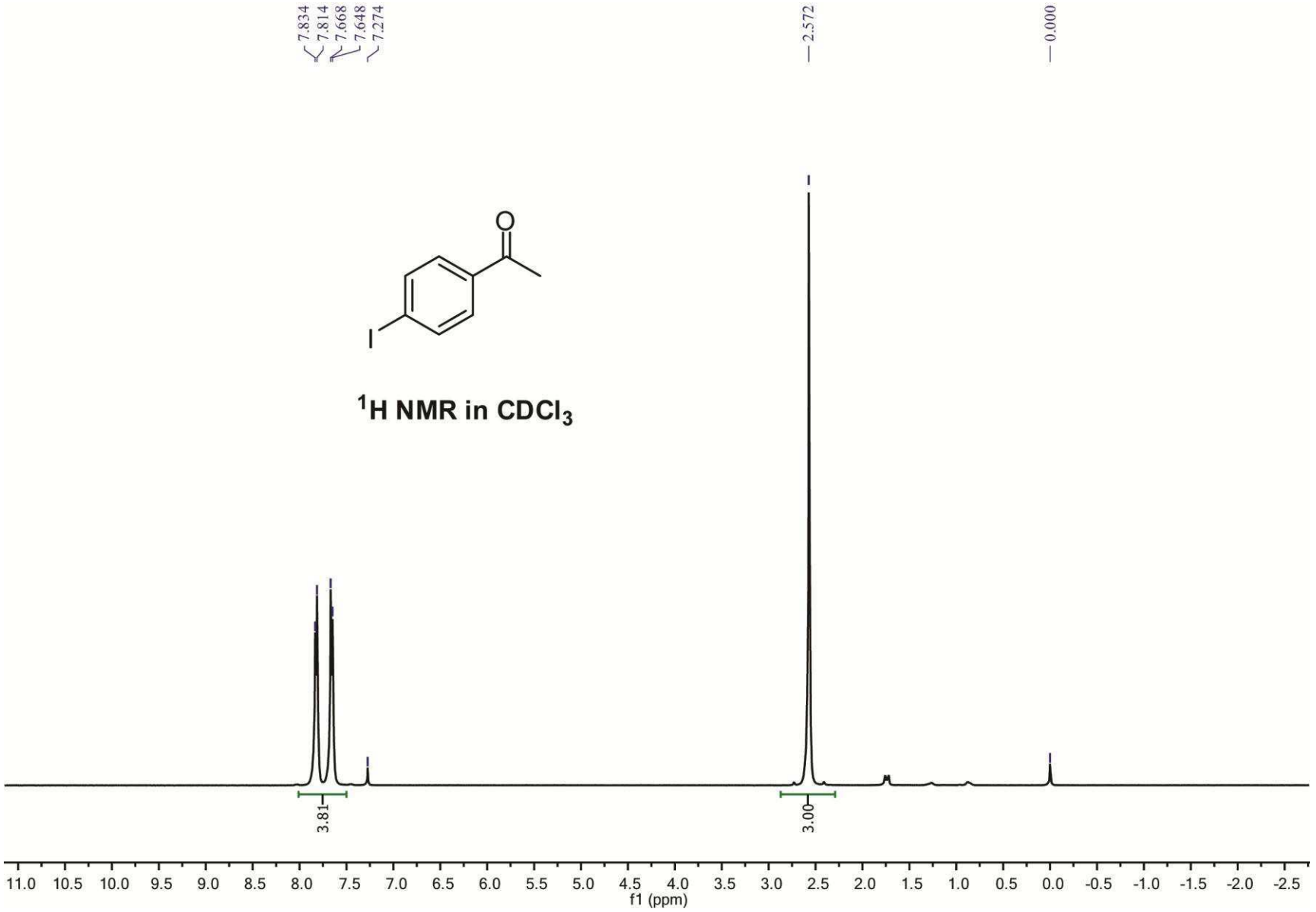
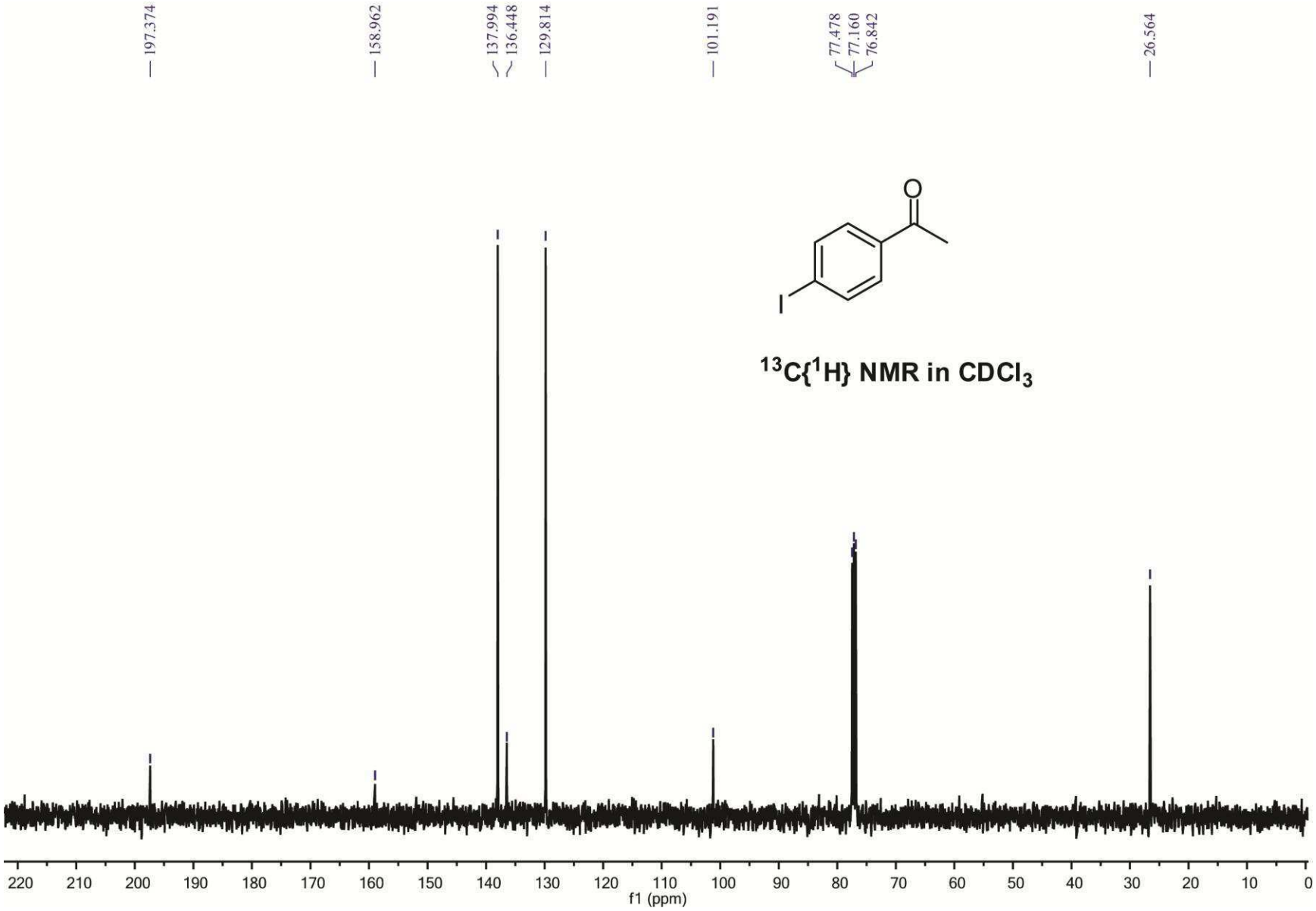
134.025
129.949
128.325
77.477
77.160
76.842
52.578
26.989
O
MeO2C
13C{1H} NMR in CDCl3
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.834
7.814
7.668
7.648
7.274
2.572
0.000
O
I
^{1}H NMR in CDCl$_3$
3.81
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5
f1 (ppm)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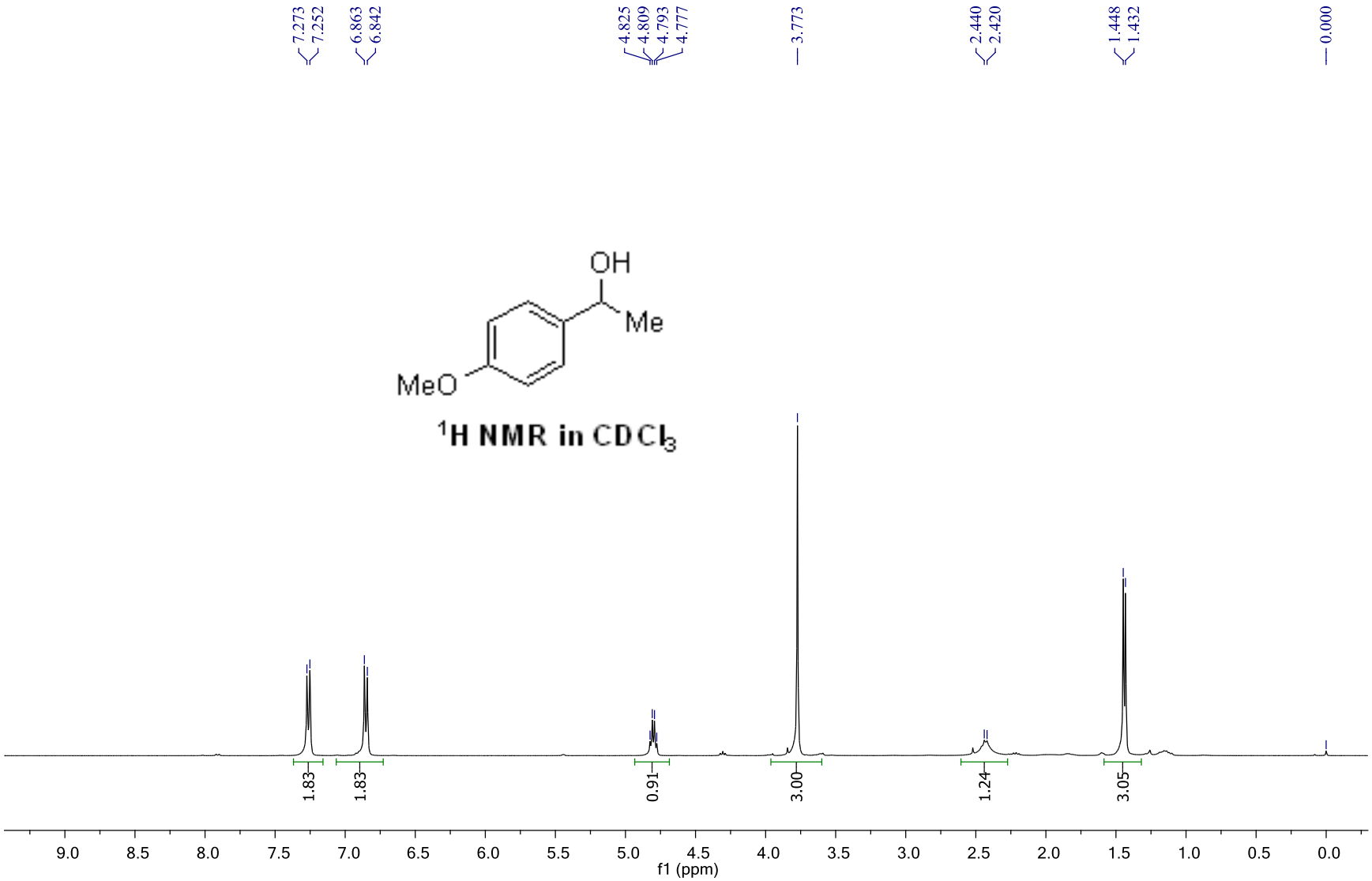
137.994
136.448
129.814
101.191
77.478
77.160
76.842
26.564
O
I
$^{13}C\{^{1}H\}$ NMR in $CDCl_3$
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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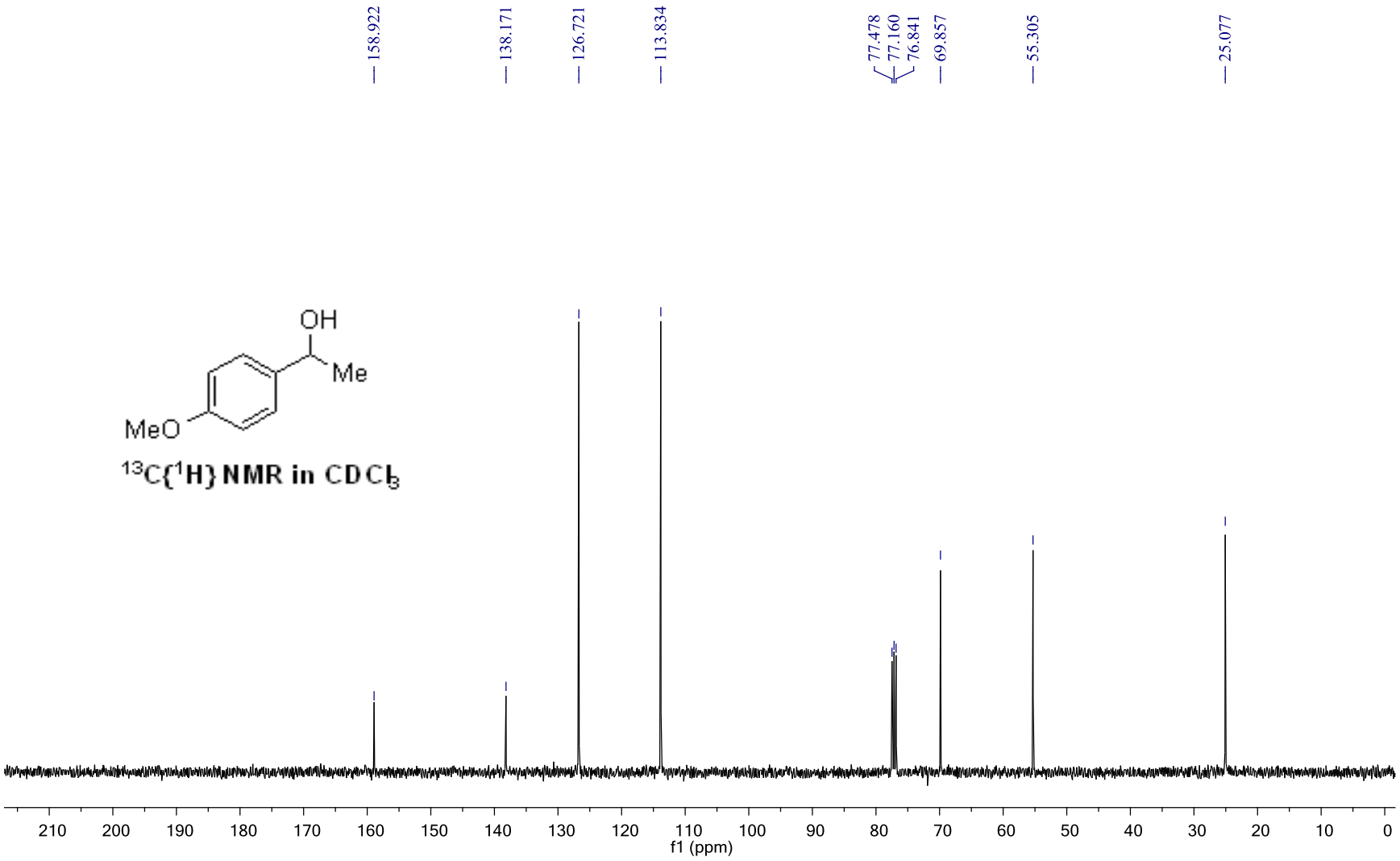
6.842
4.825
4.809
4.793
4.777
3.773
2.440
2.420
1.448
1.432
0.000
OH
Me
MeO
1H NMR in CDCl3
1.83
1.83
0.91
3.00
1.24
3.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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138.171
126.721
113.834
77.478
77.160
76.841
69.857
55.305
25.077
OH
Me
MeO
13C{1H} NMR in CDCl3
210
200
190
180
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160
150
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120
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90
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50
40
30
20
10
0
f1 (ppm)

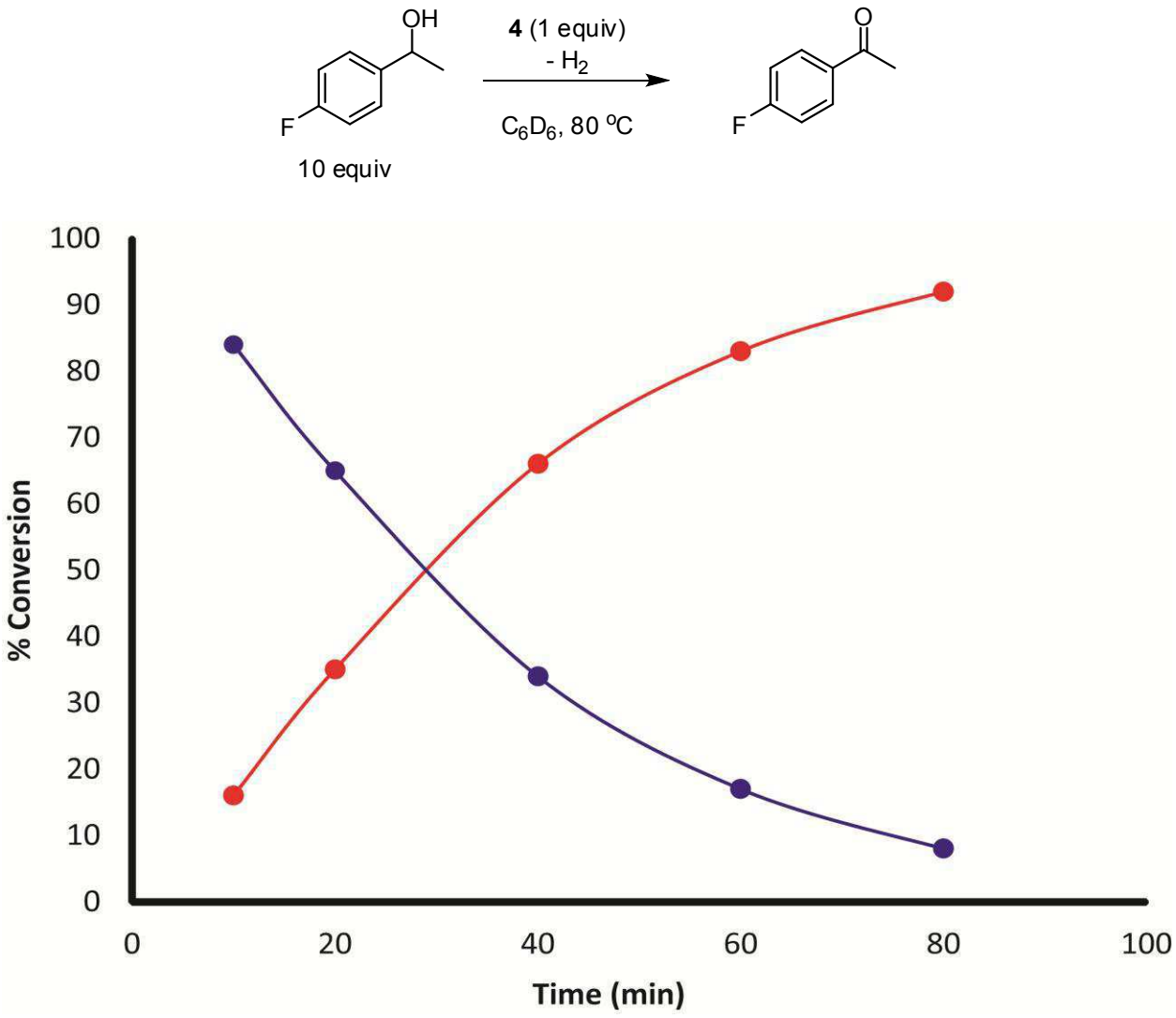

Figure S2: Reaction profile of the dehydrogenation of **F** by catalyst **4** via ^{19}F NMR analysis in C_6D_6 at 80 ^{o}C (red: formation of p-fluoroacetophenone; blue: consumption of **F**).

2 Computational Details

DFT calculations were performed to explore reaction pathways for the methanol and hemiacetal dehydrogenation by an Fe–PNP complex employing a truncated ligand model system, where the P*i*Pr$_2$-groups are replaced by PMe$_2$. Geometry optimizations, analytic harmonic frequency analyses and intrinsic reaction coordinate (IRC) following calculations were conducted using the B3LYP[1–3] hybrid functional in combination with the def2-SVP[4] basis set using the Gaussian09[5] program package. Unscaled zero-point vibrational energies as well as thermal and entropic corrections were obtained from computed Hessians using the standard procedures implemented in Gaussian09 and were used to obtain Gibbs free energies at 393.15 K (1 bar atmospheric pressure).

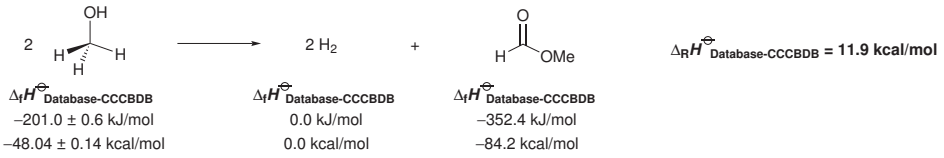

Figure S3: Experimental reaction enthalpy of the overall AAD cycle at standard conditions (HOF of substrate and products as tabulated in the CCCBDB database).

In order to assess the performance of the B3LYP/def2-SVP level of theory, we benchmarked the calculated reaction enthalpy against tabulated experimental data as listed in the CCCBDB database[6] (figure S3). The experimental reaction enthalpy is calculated to be $\Delta_\mathrm{R}H^\ominus_\mathrm{database} = 11.9$ kcal mol^{-1} (with $\Delta_\mathrm{f}H^\ominus_{\mathrm{CH_3OH}} = -201.0 \pm 0.6$ kJ mol^{-1} [7] and $\Delta_\mathrm{f}H^\ominus_{\mathrm{HCO(OCH_3)}} = -352.4$ kJ mol^{-1} [8]). As listed in table S2, the B3LYP/def2-SVP values show a large deviation of 7.9 kcal mol^{-1} to the experimental reaction enthalpy. The deviation to the experiment can be reduced to 3.2 kcal mol^{-1} by using a quadruple zeta basis set and adding a dispersion correction. The best results are obtained by RI-B3PW91-D3BJ/def2-QZVPP singlepoint calculations with an excellent agreement to the experimental value. Therefore, all the reported free energies correspond to the sum of electronic energies calculated at the RI-B3PW91-D3BJ/def2-QZVPP level of theory and enthalpy/free energy corrections calculated at the B3LYP/def2-SVP level of theory. The single point energy calculations on the optimized structures were performed with the B3PW91 hybrid functional[2,3,9–13] in conjunction with the empirical dispersion correction D3BJ[14] (atom-pairwise dispersion correction with Becke-Johnson damping)[15] and the def2-QZVPP basis set[4] as implemented in the ORCA[16] program package. The RIJCOSX approximation was used in these calculations with the def2-QZVPP/J auxiliary basis set.[17] The enthalpies and free energies shown were computed as the sum of electronic energies calculated at the RI-B2GP-PLYP-D3BJ/def2-QZVPP level of theory and enthalpy/free energy corrections calculated at the B3LYP/def2-SVP level of theory.

Table S2: Benchmarking the calculated reaction enthalpy against tabulated experimental values at standard conditions (see figure S3). The geometry optimizations were performed at the B3LYP/def2-SVP level of theory.

Method	$\Delta_\mathrm{R}H_{calculated}$	$\Delta\Delta_\mathrm{R}H_{database}$
B3LYP/def2-SVP	4.0	7.9
RI-B3LYP-D3BJ/def2-QZVPP // B3LYP/def2-SVP	8.7	3.2
RI-B3PW91-D3BJ/def2-QZVPP // B3LYP/def2-SVP	10.9	1.0

Table S3: Overall reaction free energy and enthalpy at catalytic conditions (T = 120 °C) calculated at the RI-B3PW91-D3BJ/def2-QZVPP//B3LYP/def2-SVP level of theory.

Method	$\Delta_\mathrm{R}H_{393.15\ K}$	$\Delta_\mathrm{R}G_{393.15\ K}$
RI-B3PW91-D3BJ/def2-QZVPP // B3LYP/def2-SVP	11.6	4.0

2.1 Proton Shuffling Mechanism vs. Direct H_2 Transfer

We investigated the influence of a methanol-assisted proton shuffling mechanism on the barrier height in comparison to a direct H_2 elimination from the trans dihydride complex **4** (figure S4). The proton shuffling mechanism via **TS_5** is associated with a lowering of the activation barrier of 3.0 kcal mol^{-1} at the RI-B3PW91-D3BJ/def2-QZVPP level of theory.

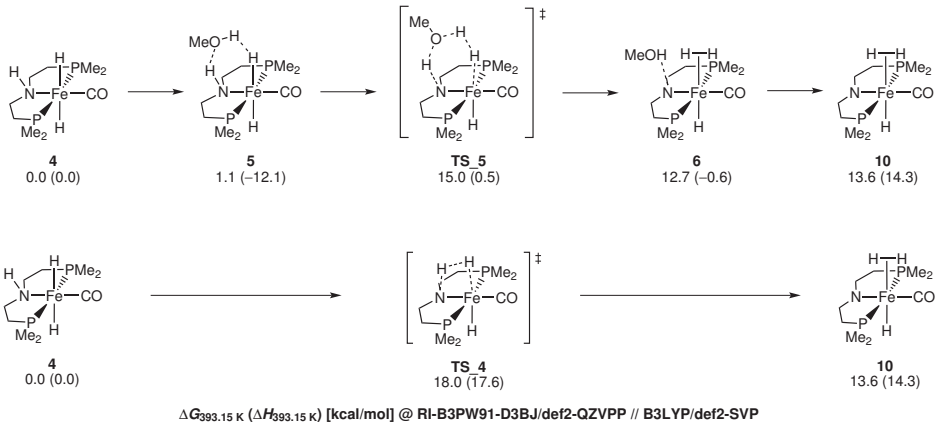

Figure S4: Comparison between the barrier heights for the H_2 heterolysis with (**TS_5**) and without methanol assisted proton shuffling (**TS_4)**

2.2 Influence of Ligand System Truncation

We used a truncated PMe_2 model system for the theoretical investigations to reduce the computational costs and to avoid conformational problems by rotation of the iPr$_2$-groups. However, in order to assess the influence of ligand truncation on the studied systems, we compared the reaction cascade for the H_2 elimination from complex **4** and ***i*Pr-4** (figure S5). In general, the relative free energies do not change significantly when substituting the PiPr$_2$ ligand by a truncated PMe_2 model system. The calculated barriers for the H_2 splitting and H_2 release are in excellent agreement. The largest deviation of 5.4 kcal mol^{-1} is observed for the relative stability of the five-coordinate complex **1** and ***i*Pr-1**. The increased relative stability of complex ***i*Pr-1** in comparison to **1** indicates the stronger donor capability of the iPr$_2$-group when compared to the iPr$_2$ system. Thus, the subvalent five-coordinate Fe complex can be better stabilized by the iPr$_2$-groups. In summary, the results in figure S5 indicate, that it is sufficient to investigate the underlying reaction mechanism using a truncated PMe_2 model system.

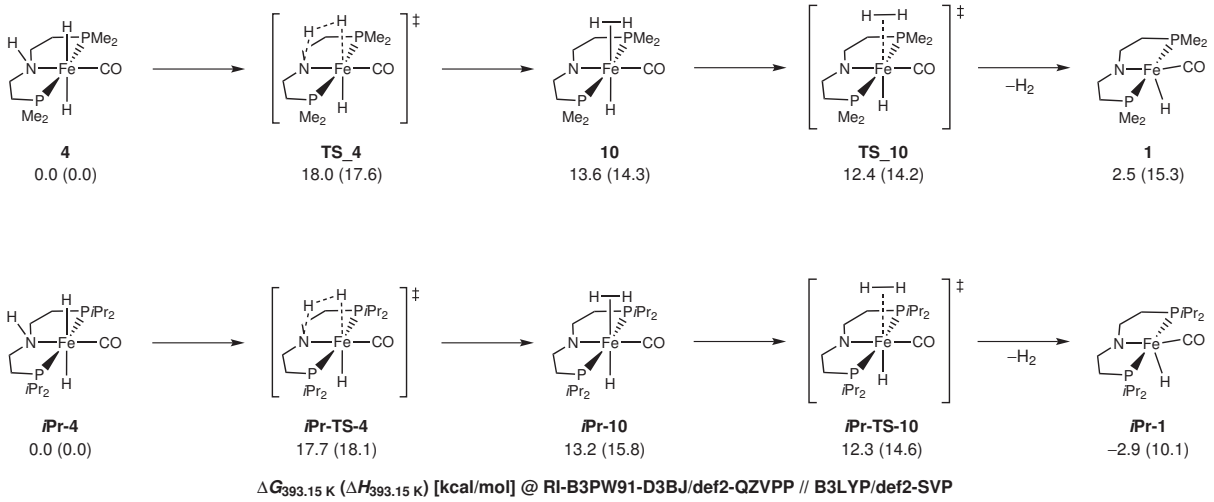

Figure S5: Comparison of PMe_2 and PiPr$_2$ ligand systems: relative energies for H_2 release from complexes **4** and ***i*Pr-4**.

2.3 Relative Isomer Stability of Dihydride Complex 4

We further investigated the relative free energies of three isomers of the dihydride comples **4** with employing the PMe_2 and the $PiPr_2$ ligand system. The results given in figure S6 show, that the *trans* isomer **4** is slightly more stable than the corresponding *cis* isomers **4a** and **4b**. Qualitatively, the same applies for the computations on the full molecular model. These findings are in alignment with previously reported results by Schneider and Hazari[18] and emphasize the role of the *trans* dihydride complex **4** as an active species in the catalytic cylce (see main text for further discussion).

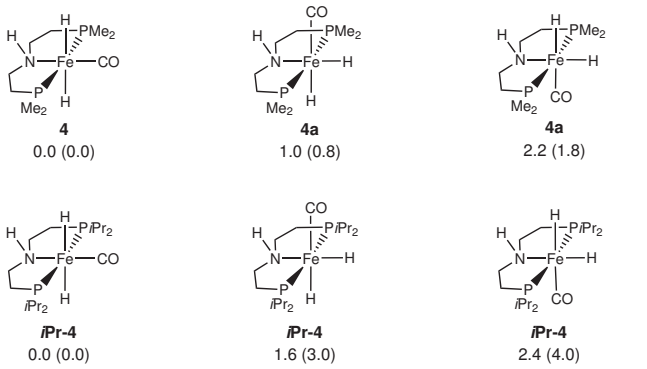

Figure S6: Calculated relative enthalpies and Gibbs free energies for three possible isomers of dihydrido complexes ***i*4** and ***i*Pr-4**.

2.4 Hemi-Acetal Formation

We investigated the hemi-acetal formation from methanol and formaldehyde via non-catalyzed and iron catalyzed reaction pathways by complex **A1** (figure S7). Both pathways (a) and (b) exhibit large barriers of 41.6 and 30.6 kcal mol^{-1} and are not feasible at the reaction conditions ($T = 120$ °C). The iron catalyzed reaction sequence shown in (c) exhibits a low effective barrier of 8.9 kcal mol^{-1}. Note that both the addition of methanol along the Fe–N bond via **TS_A10** and the proton shift to form the hemi-acetal via **TS_A13** are barrierless at the ΔG surface. The results shown in figure S7 clearly emphasize the formation of the hemi-acetal in via the iron-catalyzed pathway (c).

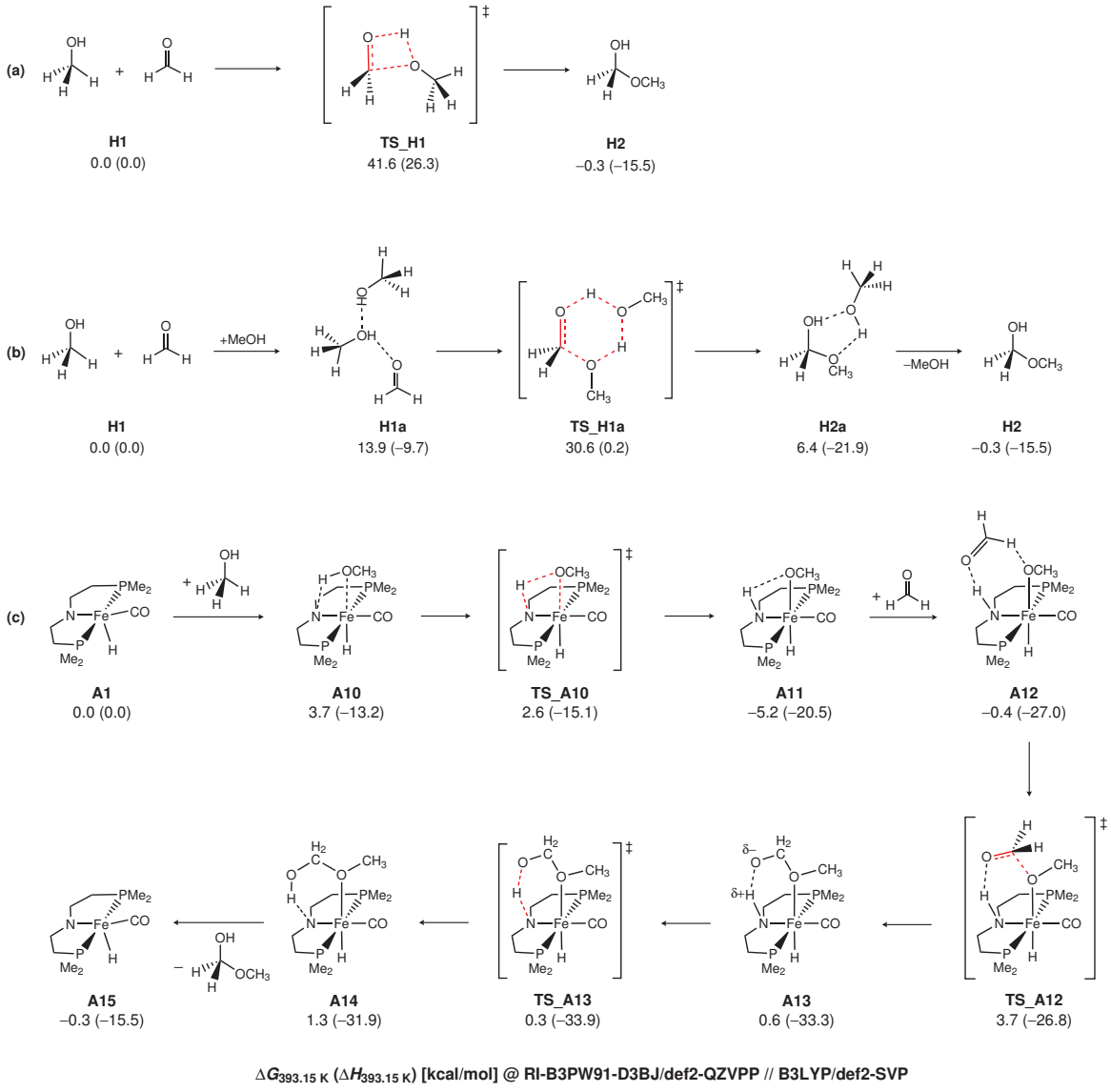

Figure S7: Computed reaction pathways for hemi-acetal formation: (a) direct formation from methanol and formaldehyde; (b) methanol-assisted proton shuffling; (c) iron-catalyzed reaction sequence.

2.5 Cartesian Coordinates of Optimized Geometries

The cartesian coordinates are given in Å, together with the point groups, the electronic state and electronic energies (at the B3LYP/def2-SVP and the RI-B3PW91-D3BJ/def2-QZVPP//B3LYP/def2-SVP level of theory) in Hartree and the thermal corrections at the B3LYP/def2-SVP level of theory. The imaginary frequencies in cm^{-1} are added for transition state structures. Figure S8 shows the relation between the nomenclature of the optimized structures and the intermediates in the main text.

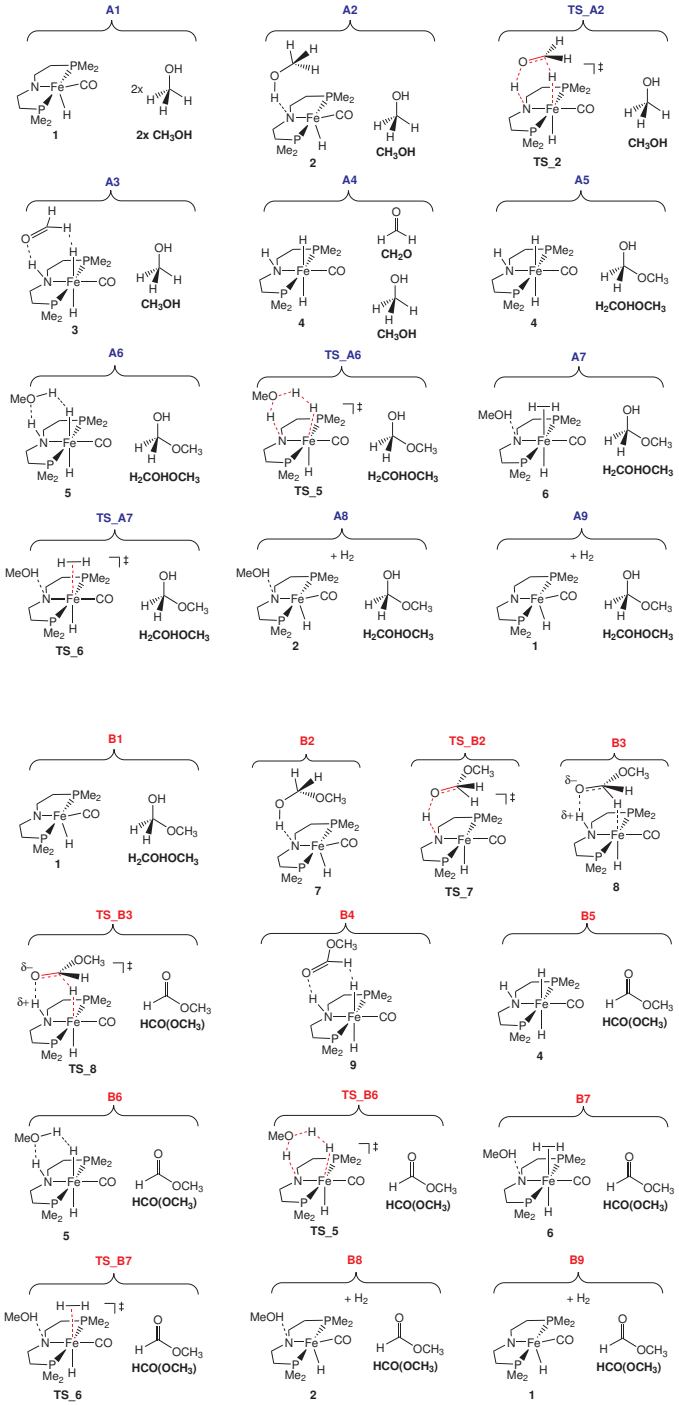

Figure S8: Relation between nomenclature of intermediates in the main text and molecular structures.

H_2 $^1\Sigma_g^+$ $D_{\infty h}$ ZPVE = 0.009962
E(B3LYP) = -1.17379008386 E(B3PW91) = -1.179577123977
thermal correction (393.15 K): H = 0.014319 G = -0.00645

H	0.000000000000	0.000000000000	0.380319749312
H	0.000000000000	0.000000000000	-0.380319749312

CH_3OH $^1A'$ C_S ZPVE = 0.051031
E(RB3LYP) = -115.631895804 E(B3PW91) = -115.742858439179
thermal correction (393.15 K): H = 0.057049 G = 0.019451

C	-0.046580541070	0.653154457590	0.000000000000
H	-1.095946502369	0.986180582575	0.000000000000
H	0.439108217090	1.090471360949	0.895818939899
H	0.439108217090	1.090471360949	-0.895818939899
O	-0.046580541070	-0.753781138039	0.000000000000
H	0.869857643170	-1.055800945707	0.000000000000

CH_2O $^1A_1$ C_{2v} ZPVE = 0.026537
E(B3LYP) = -114.415498156 E(B3PW91) = -114.514289760472
thermal correction (393.15 K): H = 0.03168 G = -0.002573

O	0.000000000000	0.000000000000	0.675299875000
C	0.000000000000	0.000000000000	-0.524383125000
H	0.000000000000	0.944691000000	-1.128050125000
H	0.000000000000	-0.944691000000	-1.128050125000

$HCOHOCH_3$ ^1A C_1 ZPVE = 0.085212
E(B3LYP) = -230.077543296 E(B3PW91) = -230.28744778044
thermal correction (393.15 K): H = 0.094274 G = 0.046763

C	0.672461328732	0.548921428549	0.246851638359
H	0.565535691923	0.598165146876	1.347927453061
H	1.188491713988	1.459672815815	-0.108798614184
O	1.415679057753	-0.609376838417	-0.004719812420
H	1.596089638013	-0.642461579154	-0.954822528879
O	-0.573529287921	0.564307961518	-0.381936424080
C	-1.483594663651	-0.398488544373	0.105389720097
H	-1.090963689743	-1.424584642474	-0.000651808152
H	-1.719472331407	-0.227812062624	1.174664243920
H	-2.410079171917	-0.305025968302	-0.478517004509

$HCO(OCH_3)$ $^1A'$ C_S ZPVE = 0.061892
E(B3LYP) = -228.893205470 E(B3PW91) = -229.092588938055
thermal correction (393.15 K): H = 0.069987 G = 0.024293

O	0.000000000000	0.863811812224	0.000000000000
O	-0.720424167142	-1.277149978725	0.000000000000
C	-0.932251576291	-0.095423263358	0.000000000000
C	1.361265745798	0.423185414709	0.000000000000
H	1.976961520611	1.330720865045	0.000000000000
H	1.575236041612	-0.183417543615	0.893075000000
H	1.575236041612	-0.183417543615	-0.893075000000
H	-1.938125283742	0.376246646094	0.000000000000

1 ^{1}A′ C_S ZPVE = 0.287454

E(B3LYP) = -2431.38285736 E(B3PW91) = -2432.19772795281

thermal correction (393.15 K): H = 0.320102 G = 0.218134

N	-1.475943360305	-0.439786843714	0.000000000000
P	0.133922688870	0.160545208372	2.186665869347
P	0.133922688870	0.160545208372	-2.186665869347
C	-1.477878106043	-0.710915193640	-2.449721611277
H	-1.239106942405	-1.785365050638	-2.516779569682
H	-1.993274875972	-0.414781852711	-3.378563311767
C	-2.313884438732	-0.441754932752	-1.196222755570
H	-3.112717404953	-1.208494610905	-1.112606874367
H	-2.855105224169	0.525601141370	-1.311973316567
C	-2.313884438732	-0.441754932752	1.196222755570
H	-3.112717404953	-1.208494610905	1.112606874367
H	-2.855105224169	0.525601141370	1.311973316567
C	-1.477878106043	-0.710915193640	2.449721611277
H	-1.239106942405	-1.785365050638	2.516779569682
H	-1.993274875972	-0.414781852711	3.378563311767
C	1.288541056423	-0.578250117824	-3.420545466259
C	-0.133476432495	1.855984664586	-2.863607245031
C	1.288541056423	-0.578250117824	3.420545466259
C	-0.133476432495	1.855984664586	2.863607245031
H	-0.915968634454	2.353847697051	2.272390092993
H	0.793651038733	2.437167277402	2.748080775428
H	-0.426582084513	1.837472997366	3.925627238482
H	0.904479691160	-0.488686448162	4.449380215834
H	2.263360819037	-0.070917084065	3.355442539498
H	1.443965716578	-1.641017281043	3.181898279711
H	-0.915968634454	2.353847697051	-2.272390092993
H	-0.426582084513	1.837472997366	-3.925627238482
H	0.793651038733	2.437167277402	-2.748080775428
H	0.904479691160	-0.488686448162	-4.449380215834
H	2.263360819037	-0.070917084065	-3.355442539498
H	1.443965716578	-1.641017281043	-3.181898279711
Fe	0.363507791176	-0.000587865540	0.000000000000
C	2.063303216829	-0.400087033333	0.000000000000
H	0.844429551882	1.420414652069	0.000000000000
O	3.194180285583	-0.666610363623	0.000000000000

2 ^{1}A′ C_S ZPVE = 0.340385

E(B3LYP) = -2547.03068141 E(B3PW91) = -2547.96613512878

thermal correction (393.15 K): H = 0.38002 G = 0.258589

N	0.977313963683	-1.038931916936	0.000000000000
P	-0.539920010139	-0.229267278092	2.197992448892
P	-0.539920010139	-0.229267278092	-2.197992448892
C	1.188749664627	-0.841830320346	-2.444787058765
H	1.835078206821	0.051150968945	-2.471674005642
H	1.329903525180	-1.402004963487	-3.383695945752
C	1.535034935460	-1.666065746739	-1.203292253193
H	2.636278618338	-1.756377338790	-1.117398836857
H	1.156945316074	-2.705383744630	-1.318020533034
C	1.535034935460	-1.666065746739	1.203292253193
H	2.636278618338	-1.756377338790	1.117398836857
H	1.156945316074	-2.705383744630	1.318020533034
C	1.188749664627	-0.841830320346	2.444787058765
H	1.835078206821	0.051150968945	2.471674005642
H	1.329903525180	-1.402004963487	3.383695945752
C	-0.738277857928	1.154662974129	-3.398766443253
C	-1.619836262207	-1.539536247212	-2.918544108851
C	-0.738277857928	1.154662974129	3.398766443253
C	-1.619836262207	-1.539536247212	2.918544108851
H	-1.477467636006	-2.474521125578	2.357149728861
H	-2.672042590310	-1.237885106783	2.806497501056
H	-1.398845789917	-1.712930123173	3.983915963518
H	-0.526325513630	0.835605720098	4.431639774526
H	-1.767724553841	1.540826773190	3.344896968948
H	-0.054729763294	1.971681069232	3.123971855854
H	-1.477467636006	-2.474521125578	-2.357149728861
H	-1.398845789917	-1.712930123173	-3.983915963518
H	-2.672042590310	-1.237885106783	-2.806497501056
H	-0.526325513630	0.835605720098	-4.431639774526
H	-1.767724553841	1.540826773190	-3.344896968948
H	-0.054729763294	1.971681069232	-3.123971855854
Fe	-0.600304847049	0.026598851176	0.000000000000
C	-1.437184863270	1.557267636070	0.000000000000
H	-1.989010767374	-0.535433490632	0.000000000000
O	-1.992412511705	2.576851406432	0.000000000000
C	2.603038259559	2.448201403520	0.000000000000
H	2.014570919676	2.749852369872	-0.891873732045
H	2.014570919676	2.749852369872	0.891873732045
H	3.525935332124	3.051431288860	0.000000000000
O	2.960838566452	1.093017106948	0.000000000000
H	2.145547963604	0.544414572153	0.000000000000

3 ^{1}A′ C_S ZPVE = 0.336465

E(RB3LYP) = -2547.00635972 E(B3PW91) = -2547.93599618938

thermal correction (393.15 K): H = 0.376123 G = 0.256891

H	-0.000130042553	-1.290903992496	1.340820367653
H	-0.000012993842	0.215635131238	-1.422740741428
N	0.000030713587	1.262278552630	0.991229372239
H	0.000048427758	1.958463642270	0.236911292746
P	-2.177845637122	-0.468934354584	0.072960175987
P	2.177730754937	-0.469206111155	0.073043249613
C	2.454531651793	1.168934639276	0.927113520484
H	2.555274170852	1.939764637078	0.144353124451
H	3.379032460309	1.187328577739	1.527169995112
C	1.225669905617	1.455702275832	1.786550749638
H	1.268871825481	2.480743538751	2.204878241227
H	1.182682542419	0.753598348677	2.634713825905
C	-1.225603376105	1.455807974109	1.786536939483
H	-1.268699532353	2.480836927028	2.204905650464
H	-1.182724206522	0.753660179248	2.634669438053
C	-2.454465419003	1.169229193591	0.927038842458
H	-2.555050012770	1.940089015513	0.144285146550
H	-3.378995408037	1.187747270721	1.527046086982
C	3.272780788323	-0.361674569865	-1.412047882222
C	3.115051346518	-1.671325643948	1.119402093400
C	-3.272810427067	-0.361248592114	-1.412179666143
C	-3.115358778823	-1.670948177496	1.119268494464
H	-2.664642409023	-1.693358690408	2.121694493354
H	-3.007384304234	-2.677388489250	0.685867226232
H	-4.186450370093	-1.421492301735	1.193277183234
H	-4.315832192914	-0.118553346723	-1.151623305966
H	-3.251657866999	-1.327979829792	-1.938930335256
H	-2.871362414891	0.401148182756	-2.095112829700
H	2.664304884426	-1.693652185068	2.121816482567
H	4.186175694823	-1.422016782346	1.193435349053
H	3.006948473668	-2.677760225833	0.686020179692
H	4.315811925392	-0.119071386530	-1.151442051761
H	3.251564250481	-1.328421422672	-1.938766878674
H	2.871444904121	0.400737436261	-2.095030010623
Fe	-0.000062514583	-0.608319653707	-0.073608526065
C	-0.000140842375	-2.113064581057	-0.928567424129
O	-0.000192537607	-3.121448397854	-1.506654819432
O	0.000457204677	3.455994460562	-1.203146450525
C	0.000480252609	3.050119266219	-2.341590873387
H	0.000348421485	1.957483948034	-2.567164994319
H	0.000639444364	3.760270722645	-3.206626852169

4 ^{1}A′ C_S ZPVE = 0.308252

E(B3LYP) = -2432.57887838 E(B2PW91) = -2433.40894698382

thermal correction (393.15 K): H = 0.341603 G = 0.239317

H	0.115698530859	1.509018903774	0.000000000000
H	0.433629902294	-1.620585096749	0.000000000000
N	-1.771674740875	-0.260973476777	0.000000000000
H	-1.851231878816	-1.279499045515	0.000000000000
P	0.174320982017	-0.040167371114	2.176747490944
P	0.174320982017	-0.040167371114	-2.176747490944
C	-1.659934380478	-0.287607437605	-2.453036470212
H	-1.838516040938	-1.372606115603	-2.549588967665
H	-2.020371001321	0.185672001023	-3.380835429692
C	-2.392911159009	0.259880889337	-1.230983589248
H	-3.472167795952	0.011128933048	-1.269458553659
H	-2.307328003528	1.357414429413	-1.195561356070
C	-2.392911159009	0.259880889337	1.230983589248
H	-3.472167795952	0.011128933048	1.269458553659
H	-2.307328003528	1.357414429413	1.195561356070
C	-1.659934380478	-0.287607437605	2.453036470212
H	-1.838516040938	-1.372606115603	2.549588967665
H	-2.020371001321	0.185672001023	3.380835429692
C	0.936485181403	-1.344833193589	-3.238803913569
C	0.556039013648	1.487099741990	-3.146389804576
C	0.936485181403	-1.344833193589	3.238803913569
C	0.556039013648	1.487099741990	3.146389804576
H	-0.000882561051	2.330172409359	2.713074437995
H	1.628857415874	1.711065013706	3.040378877811
H	0.311384779339	1.382818406884	4.216115950930
H	0.592618787777	-1.293813386740	4.284607728210
H	2.030767452059	-1.224713451454	3.216051880743
H	0.698952950270	-2.329517607346	2.811306306443
H	-0.000882561051	2.330172409359	-2.713074437995
H	0.311384779339	1.382818406884	-4.216115950930
H	1.628857415874	1.711065013706	-3.040378877811
H	0.592618787777	-1.293813386740	-4.284607728210
H	2.030767452059	-1.224713451454	-3.216051880743
H	0.698952950270	-2.329517607346	-2.811306306443
Fe	0.364696238249	-0.044480474985	0.000000000000
C	2.087167734121	0.125027392541	0.000000000000
O	3.243264092532	0.242438429694	0.000000000000

4a ^{1}A′ C_S ZPVE = 0.30833

E(B3LYP) = -2432.57770474 E(B3PW91) = -2433.4078234157

thermal correction (393.15 K): H = 0.341755 G = 0.239732

Fe	-0.405586137528	0.234739270071	0.000000000000
N	1.352819011069	-1.012808753266	0.000000000000
C	2.151836725459	-0.823051014263	1.230372823810
H	2.938813507317	-1.598220141046	1.318889748443
C	1.256957464079	-0.806198229635	2.469337502378
P	-0.155601386463	0.387093653352	2.150170739708
C	2.151836725459	-0.823051014263	-1.230372823810
C	1.256957464079	-0.806198229635	-2.469337502378
H	1.841960875640	-0.563368574934	-3.372438965752
P	-0.155601386463	0.387093653352	-2.150170739708
H	2.662206290994	0.147356727575	-1.128931230150
H	0.810411976207	-1.802792302956	-2.631817976367
H	2.938813507317	-1.598220141046	-1.318889748443
H	0.981774594979	-1.964357473529	0.000000000000
H	2.662206290994	0.147356727575	1.128931230150
H	1.841960875640	-0.563368574934	3.372438965752
H	0.810411976207	-1.802792302956	2.631817976367
H	-1.455536009623	1.329940747492	0.000000000000
H	0.586215409553	1.447759369162	0.000000000000
C	-1.748671915090	-0.889700704441	0.000000000000
O	-2.702005467653	-1.559213688438	0.000000000000
C	-1.437107302603	-0.171836247678	3.360803333607
H	-1.054115234258	-0.212933379836	4.393348282386
H	-2.285503889706	0.528864727134	3.322665658238
H	-1.810731471762	-1.163526516235	3.065506109693
C	0.401926977111	1.961846854305	2.935584768368
H	1.320627174871	2.305079477706	2.439309475801
H	-0.370949246913	2.726370956139	2.763225821774
H	0.575181497829	1.854701720816	4.018649905161
C	0.401926977111	1.961846854305	-2.935584768368
H	1.320627174871	2.305079477706	-2.439309475801
H	0.575181497829	1.854701720816	-4.018649905161
H	-0.370949246913	2.726370956139	-2.763225821774
C	-1.437107302603	-0.171836247678	-3.360803333607
H	-2.285503889706	0.528864727134	-3.322665658238
H	-1.054115234258	-0.212933379836	-4.393348282386
H	-1.810731471762	-1.163526516235	-3.065506109693

4b ^{1}A′ C_S ZPVE = 0.308391

E(B3LYP) = -2432.57634208 E(B3PW91) = -2433.40615811464

thermal correction (393.15 K): H = 0.341718 G = 0.240086

Fe	0.429261327945	0.263364420911	0.000000000000
N	-1.605281817743	-0.357617212866	0.000000000000
C	-1.965273422588	-1.047156190053	1.249502687635
H	-3.049578387439	-1.276179408267	1.288939527433
C	-1.551435869753	-0.178533659137	2.442518120953
P	0.215408079402	0.415244979541	2.161897883845
C	-1.965273422588	-1.047156190053	-1.249502687635
C	-1.551435869753	-0.178533659137	-2.442518120953
H	-1.673080102960	-0.724031494105	-3.392094242597
P	0.215408079402	0.415244979541	-2.161897883845
H	-1.427119981251	-2.008867033986	-1.264773535333
H	-2.200265710516	0.713199264876	-2.498004071720
H	-3.049578387439	-1.276179408267	-1.288939527433
H	-2.055889054629	0.558995379273	0.000000000000
H	-1.427119981251	-2.008867033986	1.264773535333
H	-1.673080102960	-0.724031494105	3.392094242597
H	-2.200265710516	0.713199264876	2.498004071720
H	1.759817955861	0.991750213150	0.000000000000
H	-0.120797565059	1.735840800587	0.000000000000
C	1.372365828706	-1.212657557277	0.000000000000
O	2.095890304512	-2.125511010418	0.000000000000
C	0.269375399508	2.028973018478	3.053704838397
H	-0.017478683646	1.937277945778	4.113846383057
H	1.294326069012	2.425299873371	2.990464936864
H	-0.394938678837	2.740322764430	2.542803854077
C	1.201200784339	-0.651567913753	3.309809161450
H	1.130339285707	-1.701219782357	2.988193080728
H	2.259827323734	-0.356492058281	3.241898690990
H	0.869511052636	-0.563630007611	4.357016522049
C	1.201200784339	-0.651567913753	-3.309809161450
H	1.130339285707	-1.701219782357	-2.988193080728
H	0.869511052636	-0.563630007611	-4.357016522049
H	2.259827323734	-0.356492058281	-3.241898690990
C	0.269375399508	2.028973018478	-3.053704838397
H	1.294326069012	2.425299873371	-2.990464936864
H	-0.017478683646	1.937277945778	-4.113846383057
H	-0.394938678837	2.740322764430	-2.542803854077

5 ^{1}A C_1 ZPVE = 0.361695

E(RB3LYP) = -2548.23556482 E(B3PW91) = -2548.54884543111

thermal correction (393.15 K): H = 0.401492 G = 0.282663

P	-2.078928256908	-0.669397766969	-0.114109617187
P	2.272244651959	-0.246405827645	0.021039656695
N	-0.023015395681	1.098300969703	-1.225488092509
C	-2.451465886236	0.738661238404	-1.280340485534
C	-1.199654584465	1.005525088635	-2.112142748168
C	1.227794310171	1.327881602188	-1.970460626741
C	2.418829245932	1.299308760488	-1.016185595834
C	-3.238170355972	-0.357683712955	1.288843271163
C	-2.836889478300	-2.149222765285	-0.917604078932
C	3.364783618392	-1.459309367945	-0.844699551598
C	3.277653300040	0.147307216391	1.519163671475
H	-3.328019504853	0.544312359296	-1.919166471271
H	-2.669373099412	1.617271793195	-0.652164449537
H	-1.017924670015	0.179931583228	-2.818545949223
H	-1.316964984580	1.932655866116	-2.707178197911
H	1.321633339899	0.523850659941	-2.718171457043
H	3.374682094840	1.359216477833	-1.562030435263
H	-3.129054440105	-1.159120003092	2.035539593990
H	-2.331127665388	-2.331156918372	-1.876561487105
H	3.344298367622	-2.411554982102	-0.292297625927
H	2.770644548958	0.940717949324	2.086846054497
H	0.211285722916	-1.457066827323	-1.160846791146
H	1.188574553852	2.286492817489	-2.524520843128
H	2.376745759471	2.162688776133	-0.330320987266
H	0.045991716413	0.383863935324	1.399425774500
H	-0.179916177871	1.891454843581	-0.589977055621
H	2.959908090936	-1.651268409071	-1.848611804569
H	4.406399257641	-1.107389462658	-0.920673340736
H	3.326051257627	-0.746193627835	2.160826946403
H	4.303433992688	0.462296525873	1.267993889759
H	-2.951801386499	0.594651946416	1.757522691384
H	-4.289532485341	-0.309930836774	0.962011695447
H	-2.663793846886	-3.028865714094	-0.278208331193
H	-3.920016216302	-2.028235191922	-1.080640721861
H	-0.635519906331	1.690981446336	1.306842885622
O	-1.019614059794	2.589621882158	1.094111238058
C	0.206837922147	-1.997612841751	1.117310030748
O	0.273539556916	-2.964689500788	1.755777188440
C	-0.631294759597	3.513356413558	2.079865005433
H	0.469100421937	3.604340878437	2.178234209824
H	-1.022900563508	4.505995836768	1.803640881123
H	-1.035863615637	3.262144522914	3.079672903067
Fe	0.107402973550	-0.579687229039	0.124393219772

6 ^{1}A C_1 ZPVE = 0.358297

E(RB3LYP) = -2548.21325647 E(B3PW91) = -2549.1524535417

thermal correction (393.15 K): H = 0.398305 G = 0.279704

P	-2.049109568398	-0.743481692379	-0.166480000982
P	2.311709729490	-0.170278444460	-0.008189766025
N	-0.071170904562	1.206724968427	-0.877145584731
C	-2.437016547896	0.681146654674	-1.284721440325
C	-1.114252296195	1.146682090678	-1.893157710048
C	1.135151415162	1.744653848413	-1.488295742217
C	2.339087444805	1.592789367620	-0.560914856562
C	-3.254026186176	-0.562992789609	1.217612701204
C	-2.637854689564	-2.254296684252	-1.040129278887
C	3.229475363051	-1.096209846726	-1.309297861425
C	3.482392890786	-0.246840531976	1.417398511018
H	-3.184694704483	0.412840983656	-2.048040975992
H	-2.852933548434	1.476646692955	-0.648047996730
H	-0.830046660639	0.468237614798	-2.731752127320
H	-1.267020709024	2.144607731064	-2.358686702640
H	1.371114881423	1.229924734275	-2.451268709204
H	3.289004642844	1.879427625029	-1.041923476166
H	-3.108693266607	-1.367308016736	1.955064066486
H	-2.083187916837	-2.360754462318	-1.983361956161
H	3.231491334390	-2.167419789396	-1.056696239528
H	3.098044915946	0.372495153958	2.241901366739
H	0.244895366399	-1.293977353626	-1.099748833162
H	1.006617853625	2.815010820456	-1.760763549745
H	2.211143301228	2.214614612839	0.341527955893
H	0.377771847286	0.252809279618	1.667440983611
H	-0.831558989107	2.124180190280	0.362312930408
H	2.707689394186	-0.977308711662	-2.269178852915
H	4.268282763828	-0.742078555562	-1.405333274978
H	3.558635105544	-1.284878291663	1.776349996961
H	4.486924335470	0.109489829755	1.138359489602
H	-3.057250547017	0.408057531100	1.697027988029
H	-4.294786979020	-0.589111209021	0.856615129903
H	-2.431702084202	-3.141347800640	-0.421536114022
H	-3.717868338777	-2.202591859181	-1.249961593659
H	-0.409104386675	0.415931960410	1.484230140519
O	-1.436476474405	2.481570095251	1.094757744099
C	0.287099975400	-2.145120954166	0.948636174552
O	0.389791722398	-3.231433076454	1.335277221744
C	-0.794035936056	3.508755460082	1.787999128718
H	0.132774881929	3.177197971168	2.307681142944
H	-0.511478717022	4.365532555577	1.140057150843
H	-1.471163361513	3.902693805212	2.565739787913
Fe	0.137832419884	-0.561388138752	0.213115399527

7 ^{1}A C_1 ZPVE = 0.374428

E(RB3LYP) = -2661.47896433 E(B3PW91) = -2662.514307302

hermal correction (393.15 K): H = 0.417232 G = 0.286431

N	0.287561325933	-0.583851076176	-1.468787901812
P	2.424617737719	-0.079325964282	0.282219078565
P	-1.796284490308	-1.360088162844	0.251654111900
C	-2.126543654281	-1.086121165966	-1.551105390856
H	-2.524321475758	-0.061050803625	-1.629751578163
H	-2.880569486575	-1.775148545420	-1.965747719839
C	-0.780219917984	-1.188213001859	-2.269012617695
H	-0.849868406589	-0.698963351309	-3.263258447489
H	-0.552327931363	-2.255378121848	-2.486444096618
C	1.529470346379	-0.545834449788	-2.248149781239
H	1.346247990958	-0.110995314729	-3.252590955342
H	1.904197650279	-1.575924470177	-2.437207054056
C	2.600657582093	0.276278024458	-1.527877064089
H	2.388375943627	1.350209059696	-1.653884831361
H	3.615054419108	0.077945567963	-1.910715906281
C	-3.239182396347	-0.589987482308	1.096516641576
C	-2.057502349052	-3.165452923584	0.522745745253
C	3.154020406666	1.397243837425	1.109862882834
C	3.656262583996	-1.403756274824	0.641187274990
H	3.399230269642	-2.301923543579	0.060932084536
H	3.601792558849	-1.666088964126	1.708437984681
H	4.681549255834	-1.085670823714	0.393537798535
H	4.195899448642	1.572599068010	0.797718183626
H	3.119998488746	1.263920831778	2.201989335762
H	2.542335061425	2.273881310065	0.849107274498
H	-1.328146161152	-3.730256995580	-0.076249473378
H	-3.078735416141	-3.476344068745	0.250437509936
H	-1.873783111433	-3.398380195269	1.582373872783
H	-4.192037395917	-1.042304213861	0.778403547369
H	-3.132808645042	-0.698124683435	2.186764600439
H	-3.236605944194	0.481220036183	0.844809929143
Fe	0.271848706473	-0.584913414676	0.452972862495
C	0.071421408996	0.052241130720	2.064061050945
H	0.644519181743	-1.846663370020	1.156485619178
O	-0.061237365189	0.478463302238	3.136360698664
C	-1.296386534267	2.807900089035	-1.361668569769
H	-1.208232767555	3.899412188397	-1.533821999103
H	-1.856763739348	2.357224213034	-2.202747457356
O	-0.007887341530	2.309265543026	-1.257717786372
H	-0.030732499740	1.318909414920	-1.294622278914
O	-2.103703289109	2.568642526809	-0.230753376351
C	-1.687395744194	3.254380494134	0.931632277699
H	-0.669249862904	2.963628982828	1.239617221411
H	-1.710236315894	4.352168081455	0.780186658461
H	-2.385761895660	2.994976291575	1.740092222960

8 ^{1}A C_1 ZPVE = 0.373846

E(RB3LYP) = -2661.47868613 E(B3PW91) = -2662.51134715774

thermal correction (393.15 K): H = 0.415172 G = 0.294643

H	-0.679155768590	-1.887510933396	0.482919416724
H	0.271501609384	0.891922341695	-1.001579092648
N	-0.111965040286	0.386046037008	1.579930638951
H	0.015684332854	1.384206502447	1.172520563880
P	-2.398468992148	-0.011227845382	-0.139948034642
P	1.862036762902	-1.208121968189	0.144088511599
C	2.302801509399	-0.105744032645	1.568521321569
H	2.571381844278	0.862739614127	1.116351200290
H	3.160513423608	-0.475031065921	2.154037832378
C	1.049600863103	0.051437667362	2.426581667351
H	1.203327630648	0.833880986781	3.194526633928
H	0.833084266370	-0.886378845632	2.968133680693
C	-1.363368789464	0.420329348985	2.362135166761
H	-1.253286541633	1.091532936628	3.235882089052
H	-1.567906633247	-0.590586833378	2.754218644225
C	-2.505692296129	0.906131339046	1.472293607978
H	-2.342201252739	1.966515675031	1.225492374471
H	-3.487123207435	0.799055648915	1.960930638680
C	3.175655861943	-0.914778659218	-1.107570312691
C	2.212007868187	-2.919092807626	0.733525089030
C	-3.125200063251	1.168460234849	-1.355202609357
C	-3.672507215056	-1.337717460765	-0.038134083349
H	-3.662616933115	-1.921801845073	-0.971261458273
H	-4.680964872400	-0.923488596511	0.119231415907
H	-3.418597971652	-2.018152234995	0.787165360858
H	-2.495056597908	2.069816926021	-1.377182448007
H	-4.154175663443	1.451148673937	-1.081115590367
H	-3.130996681373	0.714522988712	-2.357875267952
H	1.573600890107	-3.146538820240	1.599200055681
H	3.271015454907	-3.043654898200	1.010660976403
H	1.960857332407	-3.633793669518	-0.065033421235
H	4.182363276972	-1.072035046015	-0.688234629553
H	3.028383968988	-1.599917504612	-1.956691069690
H	3.066794254326	0.122694658748	-1.457066863466
Fe	-0.256385373147	-0.630372385705	-0.230120691982
C	-0.415946575910	-1.540263347375	-1.710920218339
O	-0.547065977297	-2.209666414274	-2.646857031860
O	-0.024660337555	2.598473086013	0.214441522124
C	0.445972201084	2.077525203891	-0.864874812927
O	1.891933001046	2.099733115804	-1.008699549148
C	2.398659752881	3.413574576466	-1.052233155004
H	2.040375593924	3.960768797306	-1.949016014701
H	2.102182651884	3.990870170080	-0.159462685757
H	3.496818816283	3.352399219520	-1.101142428216
H	0.016903008825	2.456931448223	-1.829903043846

9 ^{1}A C_1 ZPVE = 0.3716

E(RB3LYP) = -2661.48482999 E(B3PW91) = -2662.51560161956

thermal correction (393.15 K): H = 0.414562 G = 0.285645

H	-2.234601495444	0.000331371761	0.766934202391
H	0.271988736118	-0.000129384237	-1.140286699219
N	0.241320788351	-0.000104712589	1.506053664884
H	1.190302579309	-0.000195163789	1.112866953316
P	-0.951275854234	2.176811911332	-0.047442392985
P	-0.951971154877	-2.176577857865	-0.047518202785
C	0.192383786639	-2.451365035690	1.402120770937
H	1.217602868141	-2.536394122513	1.003903514516
H	-0.027658478864	-3.381140892365	1.951913603051
C	0.090553033153	-1.226587486963	2.308651456969
H	0.851041223844	-1.269618883498	3.113371328839
H	-0.899720131517	-1.189392036380	2.790555040605
C	0.090817470073	1.226347330271	2.308756887362
H	0.851282362560	1.269112628662	3.113513838378
H	-0.899485823184	1.189362530379	2.790613075889
C	0.193026122514	2.451171392337	1.402332316228
H	1.218299660648	2.535936013041	1.004198789554
H	-0.026808043609	3.380968108645	1.952170155973
C	-0.240556733868	-3.265778355709	-1.360448974067
C	-2.473187851646	-3.122360222124	0.411608390375
C	-0.239336636651	3.265840837464	-1.360236226077
C	-2.472246074355	3.123060355569	0.411505218559
H	-2.907066763982	2.676604938671	1.317112421780
H	-3.212382922700	3.017882363649	-0.396955225988
H	-2.268860502512	4.193323488134	0.578904067300
H	-0.125898713839	4.310412796118	-1.027502257063
H	-0.901745812237	3.240364609218	-2.239467181975
H	0.736988721347	2.862617541569	-1.665174057153
H	-2.907702646705	-2.675848301357	1.317335933618
H	-2.270137373525	-4.192708796907	0.578876661271
H	-3.213441858400	-3.016873995393	-0.396705188632
H	-0.127397549395	-4.310398867639	-1.027774764159
H	-0.903079206226	-3.240060117756	-2.239587699180
H	0.735850884008	-2.862838103949	-1.665497449554
Fe	-1.026523500876	0.000132386321	-0.236487978224
C	-2.056084102045	0.000314414743	-1.627277185338
O	-2.746973653987	0.000432935396	-2.561990079791
O	4.387419410273	-0.000422442939	-1.371934342821
O	3.116785001354	-0.000445246499	0.483571830318
C	3.227186710853	-0.000366088534	-0.723057680979
C	5.576333601988	-0.000597045673	-0.573369997053
H	6.416779447786	-0.000608458881	-1.277488949873
H	5.614137511419	0.892844172794	0.067828210982
H	5.613979945974	-0.894158223878	0.067669910404
H	2.365622000913	-0.000217614127	-1.421296642036

10 ^{1}A′ C_S ZPVE = 0.304165

E(RB3LYP) = -2432.55438085 E(B3PW91) = -2433.38289719542

thermal correction (393.15 K): H = 0.338278 G = 0.234917

P	0.124531026209	-0.046409075969	2.202653000000
P	0.124531026209	-0.046409075969	-2.202653000000
N	-1.699218976713	-0.238739046755	0.000000000000
C	-1.694047477212	-0.271492046786	-2.443798500000
H	-2.062497969933	0.203601459052	-3.367916500000
H	-1.878298995164	-1.356668544052	-2.515182000000
C	-2.347466468369	0.284296963869	-1.178224000000
H	-2.321792950701	1.405720463356	-1.228196500000
H	-3.430527972812	0.026161980515	-1.186306500000
C	-1.694047477212	-0.271492046786	2.443798500000
H	-1.878298995164	-1.356668544052	2.515182000000
H	-2.062497969933	0.203601459052	3.367916500000
C	-2.347466468369	0.284296963869	1.178224000000
H	-3.430527972812	0.026161980515	1.186306500000
H	-2.321792950701	1.405720463356	1.228196500000
H	-0.116060002425	-1.836385072448	0.000000000000
H	0.689043996733	-1.905490085360	0.000000000000
Fe	0.367086023773	-0.187533080471	0.000000000000
C	2.101257028309	0.088955891184	0.000000000000
H	0.275228047932	1.311543920527	0.000000000000
O	3.218419033718	0.397217873679	0.000000000000
C	0.521684552456	1.563548416727	-3.003889500000
H	-0.047462435564	2.358035425722	-2.500865500000
H	1.593222055763	1.780922399269	-2.876554000000
H	0.275423051756	1.555408420770	-4.077579500000
C	0.910206507044	-1.259425588778	-3.353549500000
H	2.003712008551	-1.132045606988	-3.335512500000
H	0.679102990752	-2.281533585182	-3.017219000000
H	0.552487009228	-1.132089582985	-4.387970000000
C	0.910206507044	-1.259425588778	3.353549500000
H	0.552487009228	-1.132089582985	4.387970000000
H	0.679102990752	-2.281533585182	3.017219000000
H	2.003712008551	-1.132045606988	3.335512500000
C	0.521684552456	1.563548416727	3.003889500000
H	-0.047462435564	2.358035425722	2.500865500000
H	0.275423051756	1.555408420770	4.077579500000
H	1.593222055763	1.780922399269	2.876554000000

TS_2 ^{1}A C_1 i = 145 ZPVE = 0.336355

E(B3LYP) = -2547.00522963 E(B3PW91) = -2547.93559541059

thermal correction (393.15 K): H = 0.375033 G = 0.258266

H	0.142721883334	-1.233093752393	-1.371424372245
H	-0.022003122874	0.183271186899	1.435873287406
N	-0.036813530207	1.300755262317	-0.957959282387
H	-0.114434384748	1.978163746896	-0.190800016664
P	2.234534329698	-0.303523227592	-0.039370769966
P	-2.111750137428	-0.592642044279	-0.130220187273
C	-2.477971007081	1.041191847029	-0.957802455391
H	-2.639944335343	1.788778998419	-0.163298772334
H	-3.389250304062	1.011377398348	-1.577237732731
C	-1.252652725275	1.425477369767	-1.783423854409
H	-1.354980798210	2.453689043457	-2.182909250833
H	-1.139246281844	0.744865785340	-2.642259223347
C	1.191743105665	1.605769759684	-1.712693447540
H	1.171195547349	2.643080353257	-2.101543245821
H	1.222820576858	0.928336347360	-2.581065160842
C	2.413960090671	1.381399927583	-0.826234152909
H	2.433293987192	2.128263828277	-0.013955557266
H	3.351509394708	1.491651780151	-1.395298650969
C	-3.239569110010	-0.586627760603	1.333886039534
C	-2.948299918678	-1.832715670588	-1.216651107456
C	3.300737917458	-0.184505704821	1.466240113128
C	3.265489682086	-1.398725552329	-1.115156450594
H	2.832780629156	-1.411363024782	-2.125638565251
H	3.216436960024	-2.426230570547	-0.722433891136
H	4.319039533779	-1.077868010304	-1.160042330337
H	4.330707388951	0.129831894800	1.231594042250
H	3.330834790793	-1.169884174444	1.956770316197
H	2.845852461516	0.525836512584	2.171636162150
H	-2.480062118993	-1.805769940870	-2.210853188227
H	-4.031912667590	-1.651758019097	-1.305838849296
H	-2.782357963555	-2.838298956064	-0.799923227032
H	-4.290604975778	-0.407214471394	1.054914468007
H	-3.165702287684	-1.559792871208	1.843727521837
H	-2.903162293155	0.187766778976	2.037835613317
Fe	0.068999216604	-0.591701082033	0.059159668297
C	0.153953183817	-2.116614439124	0.873264010135
O	0.211257615366	-3.138806408833	1.423425795243
O	-0.666490435261	3.252477524585	1.304867914308
C	-0.411765391742	2.825937479489	2.405826430588
H	0.461000350170	2.166092241895	2.605382895436
H	-1.054472176588	3.068795806610	3.288335260381

TS_4 ^{1}A C_1 i = 964 ZPVE = 0.302525

E(B3LYP) = -2432.54653024 E(B3PW91) = -2433.3747930623

thermal correction (393.15 K): H = 0.33548 G = 0.233891

P	-2.196090090938	-0.146375243750	0.024561490993
P	2.196090301865	-0.146375320999	0.024561378106
N	-0.000000103391	1.716761767870	-0.324122604445
C	2.450525482414	1.650560556826	-0.368898366487
H	3.373741667891	2.056190405638	0.075973711806
H	2.543703275690	1.725993526289	-1.465483944794
C	1.201487116331	2.396786992906	0.104093264212
H	1.235820337438	2.488845008028	1.216702761174
H	1.231318431456	3.440107067991	-0.280074189294
C	-2.450525497646	1.650560179479	-0.368899160066
H	-2.543702346230	1.725992776412	-1.465484810407
H	-3.373742009223	2.056190271435	0.075971959383
C	-1.201487482123	2.396786821066	0.104093026852
H	-1.231318708988	3.440106941102	-0.280074265550
H	-1.235820999462	2.488844588715	1.216702530237
H	-0.000000694081	0.722976963814	-1.397626106291
H	-0.000000329967	-0.164578784862	-1.786752041604
Fe	0.000000145535	-0.376141479984	-0.111932491776
C	-0.000000347116	-2.122311380808	-0.045638223257
H	0.000000697370	-0.358324150316	1.412935294556
O	-0.000000851243	-3.276882372969	0.053652014767
C	3.014503239493	-0.397190059511	1.656045962735
H	2.513441944505	0.231745828118	2.405333976234
H	2.891507747169	-1.446962806533	1.963112851050
H	4.087573109151	-0.149696000915	1.618750174537
C	3.341736648915	-1.024944499378	-1.125374097400
H	3.316252369929	-2.104434666776	-0.910305649533
H	2.996002425765	-0.876789521070	-2.159184275062
H	4.378863201472	-0.665048710193	-1.030865571068
C	-3.341736133984	-1.024945025816	-1.125373793938
H	-4.378862625226	-0.665048881766	-1.030865977849
H	-2.996001469012	-0.876790720372	-2.159183902879
H	-3.316252260465	-2.104435075255	-0.910304723998
C	-3.014503132613	-0.397188904205	1.656046128029
H	-2.513442825177	0.231748634252	2.405333414683
H	-4.087573274763	-0.149696134143	1.618749788449
H	-2.891506441386	-1.446961083457	1.963114414808

TS_5 ^{1}A C_1 i = 824 ZPVE = 0.353766

E(B3LYP) = -2548.20652990 E(B3PW91) = -2549.14544243469

thermal correction (393.15 K): H = 0.393165 G = 0.276267

P	-2.153070716217	-0.524674699422	-0.102763793715
P	2.268368020791	-0.322775732638	-0.023939355788
N	-0.020522024883	1.238883623833	-0.908069993646
C	-2.446027097642	0.977220243039	-1.151498727057
C	-1.133617372592	1.306539628015	-1.862075348073
C	1.224260518937	1.675913492570	-1.542679994333
C	2.416612593661	1.425935224481	-0.621306035304
C	-3.220116666982	-0.242942726033	1.369401679046
C	-2.970194656797	-1.918457572060	-0.986446391600
C	3.186653345093	-1.326519226021	-1.266363909139
C	3.379490503938	-0.403040841086	1.446161782998
H	-3.282082204438	0.839799649663	-1.855152302992
H	-2.687002379216	1.793094104828	-0.453353469079
H	-0.958204963538	0.605033787235	-2.700960585709
H	-1.201181967019	2.320615529344	-2.306397859654
H	1.375978246555	1.127299995716	-2.494579504153
H	3.379484684153	1.628476883139	-1.118790842259
H	-3.134999823213	-1.089427640767	2.067781786422
H	-2.483989374958	-2.056907420379	-1.963067249769
H	3.131273088362	-2.389158577181	-0.984625696534
H	2.977078142257	0.243365044880	2.240253650482
H	0.111867476356	-1.277418360913	-1.200911498179
H	1.173014885772	2.749891145860	-1.814257297554
H	2.353352426578	2.075279118090	0.268012098877
H	0.193765265986	0.027120579897	1.726551733740
H	-0.355509814747	1.919460722231	0.065804501496
H	2.703581309824	-1.214618741976	-2.247390977120
H	4.243473036036	-1.023538519539	-1.336516541668
H	3.408624878827	-1.435540486717	1.827128455124
H	4.404667786215	-0.082318771312	1.201435115326
H	-2.844372791131	0.671001294103	1.854843295737
H	-4.277208975831	-0.109261265147	1.089153055903
H	-2.841289786525	-2.846486003490	-0.408405339307
H	-4.045472888191	-1.729927931684	-1.132914469760
H	-0.257465475302	0.659150959005	1.427515382988
O	-0.909050735998	2.324249368568	1.144831078815
C	0.097311947879	-2.211278263793	0.780985611319
O	0.110259481223	-3.323042822722	1.101843028831
C	-0.210005125497	3.243318850417	1.901409009576
H	0.612124905593	2.789634627511	2.514551429273
H	0.278262708330	4.044300042817	1.295406418711
H	-0.863744869241	3.771506164919	2.629010565425
Fe	0.067088199087	-0.582332309231	0.141845939097

TS_6 ^{1}A C_1 i = 188 ZPVE = 0.354392

E(RB3LYP) = -2548.20264720 E(B3PW91) = -2549.14260077106

thermal correction (393.15 K): H = 0.395759 G = 0.27321

P	2.133511335105	-0.700364822046	0.150541164966
P	-2.276947763810	-0.363338968453	0.079540245254
N	0.044758384649	1.112660745271	0.793788350030
C	2.497096090954	0.965190614465	0.865801184191
C	1.230055460772	1.406580389200	1.600316770769
C	-1.134919627677	1.669996207101	1.449445695654
C	-2.389249429009	1.403737449056	0.617478343216
C	3.271905810053	-0.845311079233	-1.293431775684
C	2.831514645089	-1.916416836680	1.346318463218
C	-3.154755146927	-1.316036301123	1.390966199161
C	-3.437594014936	-0.495289170413	-1.349266627460
H	3.390904659718	0.970236046186	1.510340429911
H	2.669809621349	1.640912783221	0.013029256913
H	1.176212484212	0.910119324688	2.595902069962
H	1.297081524728	2.493782318635	1.818727240490
H	-1.275274478749	1.241502985946	2.468997112371
H	-3.320360831599	1.633011031783	1.161361134916
H	3.169411734687	-1.843064997044	-1.747346710665
H	2.326237999437	-1.795297732028	2.315239721379
H	-3.112729205549	-2.388800129843	1.149275978321
H	-3.059974618912	0.116974864819	-2.181791167007
H	-0.156698259515	-1.497590463685	1.125479147263
H	-1.021402840583	2.763671574413	1.610305205818
H	-2.370723343451	2.014907789037	-0.300710791515
H	-0.127480245879	0.127791665388	-2.518703156119
H	0.461375210222	2.169666995503	-0.617069391357
H	-2.637832763072	-1.166298556700	2.349590667077
H	-4.206842075771	-1.003356187062	1.485434424723
H	-3.483714612399	-1.541662782356	-1.688473443291
H	-4.452457175632	-0.158334011238	-1.083742155573
H	2.987484915217	-0.092585817135	-2.043774611282
H	4.322784785454	-0.687657885503	-1.002253440934
H	2.633366454096	-2.937373555444	0.986224107222
H	3.916774005329	-1.779451401051	1.476659348412
H	0.102924651398	0.851390378792	-2.418240489093
O	0.849704115519	2.701726679610	-1.368333057807
C	-0.173153957769	-2.171410192502	-0.970487216045
O	-0.240605738866	-3.217394234280	-1.468856221159
C	0.332126302872	4.002484715088	-1.361215158985
H	-0.773438428687	4.037799362881	-1.462447288449
H	0.595311155475	4.571820325586	-0.445278796730
H	0.750932298124	4.556610942148	-2.218333649522
Fe	-0.079784180591	-0.659138752375	-0.093237745893

TS_7 ^{1}A C_1 i = 824 ZPVE = 0.370705

E(RB3LYP) = -2661.47682340 E(B3PW91) = -2662.51009391765

thermal correction (393.15 K): H = 0.411641 G = 0.291831

H	-0.788445014574	-1.859429924906	0.385283403945
H	0.304591503469	1.016081774704	-1.035490078491
N	-0.130665237391	0.391067989823	1.533465591332
H	0.151033779976	1.534673980698	1.044749237602
P	-2.426667045406	0.075287978100	-0.159202526269
P	1.765677791791	-1.310535747062	0.179850167403
C	2.239741957595	-0.259341626704	1.628087722847
H	2.602156669001	0.689347928894	1.200804216703
H	3.042214414771	-0.700414177308	2.241557428082
C	0.963132594688	-0.010738411223	2.429650334667
H	1.144159711485	0.772839966993	3.192938594749
H	0.680521408616	-0.925057956021	2.988803808351
C	-1.371498594659	0.595404568915	2.295799931662
H	-1.204754148510	1.316159528103	3.121543420363
H	-1.691171389460	-0.352805909097	2.771214739281
C	-2.464896217207	1.124079312077	1.367427146707
H	-2.200989685691	2.144404146633	1.047206947694
H	-3.455319191073	1.147137380944	1.849559324268
C	3.138832566452	-1.119188927522	-1.028535124315
C	1.956980072982	-3.049356561146	0.760513982095
C	-3.194880680066	1.130183949666	-1.463088685401
C	-3.708991705721	-1.221109399459	0.107668544899
H	-3.725199446241	-1.900510713996	-0.758179722627
H	-4.709769743574	-0.781235020763	0.244113090084
H	-3.442063715701	-1.813095209733	0.994765229076
H	-2.546805287325	1.998296251082	-1.654868650105
H	-4.194111419148	1.484954751928	-1.163917746587
H	-3.283591359425	0.552912799455	-2.396257327882
H	1.284945226698	-3.226739178560	1.612304927288
H	2.995755862585	-3.263764113942	1.058499352105
H	1.663266836577	-3.735350796418	-0.048493089864
H	4.115454714711	-1.354337086124	-0.575890806685
H	2.967837501351	-1.790172749519	-1.884538084537
H	3.125793643330	-0.077620320764	-1.381541269170
Fe	-0.304209754744	-0.595480785251	-0.241762946068
C	-0.450087107753	-1.427362782022	-1.773108122899
O	-0.573133043063	-2.048595141825	-2.743512542868
O	0.323036685163	2.546282686520	0.390531443563
C	0.645979952106	2.104671500193	-0.813781878121
O	2.053459451341	2.011307617335	-1.072851728368
C	2.690991190966	3.268541752045	-1.067856624209
H	2.320182493241	3.916010291105	-1.888993406706
H	2.531819402354	3.799639515307	-0.113513910294
H	3.768205553413	3.101061170111	-1.217443762284
H	0.184501844613	2.694093148220	-1.642353769122

TS_8 ^{1}A C_1 i = 351 ZPVE = 0.371146

E(RB3LYP) = -2661.47115324 E(B3PW91) = -2662.50794897091

thermal correction (393.15 K): H = 0.412291 G = 0.291567

H	-0.625950004908	-1.920870128469	0.520110005576
H	0.273710414994	0.786799015588	-0.899343109046
N	-0.080195065668	0.349271526381	1.629927633846
H	0.104793310150	1.322162261551	1.306831837817
P	-2.370925957186	-0.089299901606	-0.116101325138
P	1.870558617880	-1.197519391076	0.094759444630
C	2.311808075507	-0.255331819370	1.641318203804
H	2.668565679614	0.738499639847	1.326778453589
H	3.121377653755	-0.730783209965	2.218733936522
C	1.039304431498	-0.113130966361	2.472852781744
H	1.202285127033	0.578632292180	3.321972513433
H	0.755918916211	-1.088494409945	2.901664263891
C	-1.351297475359	0.387766199375	2.382598077261
H	-1.258477369062	1.045770555897	3.268467730883
H	-1.559069814862	-0.630213284534	2.750786022449
C	-2.473976734482	0.875534781324	1.471614492637
H	-2.291901181879	1.929217858918	1.206693742432
H	-3.459159632257	0.798876247408	1.959338071245
C	3.186450115892	-0.738841081389	-1.112403957577
C	2.305832143817	-2.945381714843	0.496660967726
C	-3.224323917400	1.007517848299	-1.333050149631
C	-3.603087450813	-1.449167373834	0.079532796208
H	-3.300608233389	-2.087353586900	0.921849669259
H	-3.596858633208	-2.071536800904	-0.828657013615
H	-4.621485142890	-1.063356315335	0.247285134312
H	-4.252505439765	1.244929978701	-1.016214373295
H	-3.258729778039	0.507926027194	-2.313393159399
H	-2.659221073904	1.944551483345	-1.441357283435
H	1.699716967475	-3.279540966719	1.350924693428
H	3.376483606364	-3.065798019440	0.728040206403
H	2.047172590850	-3.582212668836	-0.363207248081
H	4.199666640227	-0.852354051709	-0.694693041622
H	3.091690160622	-1.384979663121	-1.999085738424
H	3.021268658494	0.298940149408	-1.435185628633
Fe	-0.228728518351	-0.636348259774	-0.235098963501
C	-0.375516567264	-1.460774352008	-1.757681191471
O	-0.487815907569	-2.038334221380	-2.757567616066
O	1.497178800426	2.611439973436	-1.476885897908
O	0.003400121571	2.753727848780	0.252411471451
C	0.268547002942	2.352609553750	-0.896377993666
C	2.486855292445	3.176521162076	-0.638536638415
H	3.270491078868	3.570763686619	-1.300902000140
H	2.072611451848	3.983817602399	-0.015487717460
H	2.942711628428	2.425880663973	0.032482984679
H	-0.476354170499	2.344566873738	-1.714053122564

*i*Pr-1 ^{1}A′ C_S ZPVE = 0.515851

E(B3LYP) = -2745.64362772 E(B3PW91) = -2746.77447008458

thermal correction (393.15 K): H = 0.565781 G = 0.42791

N	-1.153653614870	-1.523590111821	0.000000000000
P	-0.101138786093	-0.153885618221	2.218079845660
P	-0.101138786093	-0.153885618221	-2.218079845660
C	-1.063423943869	-1.725663776566	-2.466363780562
H	-0.316442686433	-2.519158567928	-2.620313326547
H	-1.701381309575	-1.700695243444	-3.364659456757
C	-1.855494720248	-2.004337205667	-1.188435443511
H	-2.044522661623	-3.095908703645	-1.108523954743
H	-2.865261621959	-1.543870451214	-1.261664097251
C	-1.855494720248	-2.004337205667	1.188435443511
H	-2.044522661623	-3.095908703645	1.108523954743
H	-2.865261621959	-1.543870451214	1.261664097251
C	-1.063423943869	-1.725663776566	2.466363780562
H	-0.316442686433	-2.519158567928	2.620313326547
H	-1.701381309575	-1.700695243444	3.364659456757
C	1.361714274939	-0.433958048260	-3.382486613194
C	-1.115781588655	1.194576268537	-3.062688661682
C	1.361714274939	-0.433958048260	3.382486613194
C	-1.115781588655	1.194576268537	3.062688661682
H	-0.990042828883	1.035026194856	4.149821636229
H	0.910020816899	-0.852248582871	4.301531192736
H	-0.990042828883	1.035026194856	-4.149821636229
H	0.910020816899	-0.852248582871	-4.301531192736
Fe	0.095745526445	-0.109447399526	0.000000000000
C	1.668771428113	0.635041736298	0.000000000000
H	-0.422429823176	1.287735515352	0.000000000000
O	2.721386383918	1.135673980546	0.000000000000
C	2.325431566551	-1.475408956950	-2.792177914944
H	1.822514758456	-2.406489218925	-2.490432960549
H	3.092363292190	-1.740865690518	-3.539063702380
H	2.843232739469	-1.073841748846	-1.908038861106
C	2.132066690643	0.838066311953	-3.761732493015
H	2.517779925453	1.358093624350	-2.870624590727
H	3.000968305357	0.570467982315	-4.386377867010
H	1.523384158353	1.545398569058	-4.342830373133
C	2.325431566551	-1.475408956950	2.792177914944
H	2.843232739469	-1.073841748846	1.908038861106
H	3.092363292190	-1.740865690518	3.539063702380
H	1.822514758456	-2.406489218925	2.490432960549
C	2.132066690643	0.838066311953	3.761732493015
H	1.523384158353	1.545398569058	4.342830373133
H	3.000968305357	0.570467982315	4.386377867010
H	2.517779925453	1.358093624350	2.870624590727
C	-0.622356298578	2.602537944835	2.695137803175
H	-1.206943423669	3.359660851539	3.244554875427
H	0.437750175353	2.765635851938	2.929529752565
H	-0.750948363931	2.781620457950	1.617158994258
C	-2.606323508206	1.063414557371	2.714742196145
H	-2.756291063622	1.105569882094	1.624074619982
H	-3.051415558812	0.129658970648	3.087606332902
H	-3.170226797245	1.898560220895	3.162840312038
C	-2.606323508206	1.063414557371	-2.714742196145
H	-3.170226797245	1.898560220895	-3.162840312038
H	-3.051415558812	0.129658970648	-3.087606332902
H	-2.756291063622	1.105569882094	-1.624074619982
C	-0.622356298578	2.602537944835	-2.695137803175
H	-0.750948363931	2.781620457950	-1.617158994258

H	0.437750175353	2.765635851938	-2.929529752565
H	-1.206943423669	3.359660851539	-3.244554875427

*i*Pr-4 ^{1}A′ C_S ZPVE = 0.536928

E(B3LYP) = -2746.83876136 E(B3PW91) = -2747.97742322603

thermal correction (393.15 K): H = 0.587437 G = 0.449524

N	-1.380357207632	-1.636807268359	0.000000000000
P	-0.078332553340	-0.162562846700	2.198192342418
P	-0.078332553340	-0.162562846700	-2.198192342418
C	-1.314487144416	-1.548989299112	-2.459247538059
H	-0.736920800471	-2.478823148948	-2.583100266680
H	-1.916020960699	-1.425512212758	-3.372978143637
C	-2.201500444680	-1.651811474714	-1.224092179868
H	-2.832613198199	-2.562035045666	-1.265526068895
H	-2.878026901978	-0.786482295280	-1.166949576340
C	-2.201500444680	-1.651811474714	1.224092179868
H	-2.832613198199	-2.562035045666	1.265526068895
H	-2.878026901978	-0.786482295280	1.166949576340
C	-1.314487144416	-1.548989299112	2.459247538059
H	-0.736920800471	-2.478823148948	2.583100266680
H	-1.916020960699	-1.425512212758	3.372978143637
C	1.312701366408	-0.706911613327	-3.363572950708
C	-0.810932777082	1.314680331031	-3.134505506873
C	1.312701366408	-0.706911613327	3.363572950708
C	-0.810932777082	1.314680331031	3.134505506873
H	-0.558347406517	1.153614861449	4.198660328816
H	0.810286675290	-0.937895029153	4.322115071718
H	-0.558347406517	1.153614861449	-4.198660328816
H	0.810286675290	-0.937895029153	-4.322115071718
Fe	0.119010331197	-0.089711356311	0.000000000000
C	1.432876477623	1.030417552039	0.000000000000
H	-1.076227135005	0.938662112060	0.000000000000
O	2.353203596351	1.744101116914	0.000000000000
C	2.015273393624	-1.972495424045	-2.856927544975
H	1.328905396006	-2.824824492353	-2.735358999050
H	2.794260034810	-2.281065376904	-3.574378160693
H	2.487085940932	-1.790774842025	-1.880127785464
C	2.345067881253	0.402853175343	-3.614624996956
H	2.801875626735	0.748323990614	-2.673607558580
H	3.156371585208	0.019095948257	-4.255710316784
H	1.913617557206	1.275486175959	-4.125676440475
C	2.015273393624	-1.972495424045	2.856927544975
H	2.487085940932	-1.790774842025	1.880127785464
H	2.794260034810	-2.281065376904	3.574378160693
H	1.328905396006	-2.824824492353	2.735358999050
C	2.345067881253	0.402853175343	3.614624996956
H	1.913617557206	1.275486175959	4.125676440475
H	3.156371585208	0.019095948257	4.255710316784
H	2.801875626735	0.748323990614	2.673607558580
C	-0.176680689339	2.628380290299	2.652093644821
H	-0.545593221820	3.472043450103	3.259883696669
H	0.920315145807	2.627268857806	2.709454140972
H	-0.449531868165	2.810919771139	1.601876007334
C	-2.337290606688	1.411936241274	3.007745238745
H	-2.633583896407	1.504446781275	1.950616900490
H	-2.864068198755	0.551523849252	3.447463577234
H	-2.696546544844	2.313099054917	3.532448708150
C	-2.337290606688	1.411936241274	-3.007745238745
H	-2.696546544844	2.313099054917	-3.532448708150
H	-2.864068198755	0.551523849252	-3.447463577234
H	-2.633583896407	1.504446781275	-1.950616900490
C	-0.176680689339	2.628380290299	-2.652093644821
H	-0.449531868165	2.810919771139	-1.601876007334

H	0.920315145807	2.627268857806	-2.709454140972
H	-0.545593221820	3.472043450103	-3.259883696669
H	-0.774747679705	-2.458950979400	0.000000000000
H	1.157553943431	-1.256521152960	0.000000000000

*i*Pr-4a ^{1}A′ C_S ZPVE = 0.536818

E(B3LYP) = -2746.83499675 E(B3PW91) = -2747.97299753569

thermal correction (393.15 K): H = 0.587732 G = 0.447683

N	0.407744584481	2.033114224451	0.000000000000
P	0.108045575602	-0.000557032888	2.170605501886
P	0.108045575602	-0.000557032888	-2.170605501886
C	0.471282299889	1.820213069911	-2.472257895278
H	-0.492947546572	2.325454505453	-2.632879796630
H	1.083985609244	2.005810700439	-3.370375896128
C	1.145783726372	2.397497955640	-1.227490066544
H	1.250003114400	3.497507798122	-1.315885501843
H	2.158742821854	1.985296045709	-1.120760548419
C	1.145783726372	2.397497955640	1.227490066544
H	1.250003114400	3.497507798122	1.315885501843
H	2.158742821854	1.985296045709	1.120760548419
C	0.471282299889	1.820213069911	2.472257895278
H	-0.492947546572	2.325454505453	2.632879796630
H	1.083985609244	2.005810700439	3.370375896128
C	-1.264925507883	-0.424275591511	-3.415807914233
C	1.582751967537	-0.875266756696	-2.976961622726
C	-1.264925507883	-0.424275591511	3.415807914233
C	1.582751967537	-0.875266756696	2.976961622726
H	1.467010686883	-0.697852382097	4.061851618000
H	-0.751421574842	-0.620893596400	4.374056801896
H	1.467010686883	-0.697852382097	-4.061851618000
H	-0.751421574842	-0.620893596400	-4.374056801896
Fe	-0.204368029881	-0.029391179146	0.000000000000
C	-1.941257627646	0.123252123353	0.000000000000
H	1.306886762691	-0.430856567580	0.000000000000
O	-3.109977184573	0.145963119289	0.000000000000
C	-2.271210510630	0.713615824401	-3.640936343357
H	-1.824077484084	1.589514674967	-4.134647605850
H	-3.088912009073	0.359136560201	-4.290664526986
H	-2.731692793207	1.040092420593	-2.694692058608
C	-2.013375687114	-1.699835072814	-2.991497060806
H	-2.600887118119	-1.524659679837	-2.079211308192
H	-2.709412223976	-2.005466412429	-3.791167189554
H	-1.341968783148	-2.545373770214	-2.789728185364
C	-2.271210510630	0.713615824401	3.640936343357
H	-2.731692793207	1.040092420593	2.694692058608
H	-3.088912009073	0.359136560201	4.290664526986
H	-1.824077484084	1.589514674967	4.134647605850
C	-2.013375687114	-1.699835072814	2.991497060806
H	-1.341968783148	-2.545373770214	2.789728185364
H	-2.709412223976	-2.005466412429	3.791167189554
H	-2.600887118119	-1.524659679837	2.079211308192
C	1.538830912182	-2.386466276475	2.710336247976
H	2.434005846515	-2.873019775618	3.133187181006
H	0.660548237850	-2.869239067458	3.161885025550
H	1.514496545875	-2.583342202404	1.627313253774
C	2.937212457801	-0.302662451879	2.543494054504
H	3.062238037942	-0.377645000090	1.452081215602
H	3.070025739870	0.749288216930	2.839948044555
H	3.751491002127	-0.875824388466	3.017817454824
C	2.937212457801	-0.302662451879	-2.543494054504
H	3.751491002127	-0.875824388466	-3.017817454824
H	3.070025739870	0.749288216930	-2.839948044555
H	3.062238037942	-0.377645000090	-1.452081215602
C	1.538830912182	-2.386466276475	-2.710336247976
H	1.514496545875	-2.583342202404	-1.627313253774

H	0.660548237850	-2.869239067458	-3.161885025550
H	2.434005846515	-2.873019775618	-3.133187181006
H	-0.483584848657	2.530669179547	0.000000000000
H	-0.416601371058	-1.529365934861	0.000000000000

*i*Pr-4b ^{1}A′ C_S ZPVE = 0.536481

E(B3LYP) = -2746.83384078 E(B3PW91) = -2747.9710715277

thermal correction (393.15 K): H = 0.587529 G = 0.446945

N	0.043909935195	2.016029643009	0.000000000000
P	-0.202885588481	0.057622654420	2.182138729766
P	-0.202885588481	0.057622654420	-2.182138729766
C	-0.089248085194	1.924887335525	-2.446069521399
H	-1.116006268823	2.318349431717	-2.508166133025
H	0.407815757003	2.198415739976	-3.388370225682
C	0.621368334299	2.552101406829	-1.244435428882
H	0.545885547957	3.658006459632	-1.279575135483
H	1.692076272501	2.295589243959	-1.248447425439
C	0.621368334299	2.552101406829	1.244435428882
H	0.545885547957	3.658006459632	1.279575135483
H	1.692076272501	2.295589243959	1.248447425439
C	-0.089248085194	1.924887335525	2.446069521399
H	-1.116006268823	2.318349431717	2.508166133025
H	0.407815757003	2.198415739976	3.388370225682
C	-1.829480769490	-0.345002644616	-3.067277272796
C	1.065727018527	-0.654871132482	-3.403590276218
C	-1.829480769490	-0.345002644616	3.067277272796
C	1.065727018527	-0.654871132482	3.403590276218
H	0.578011703059	-0.621831554494	4.395521711984
H	-1.698069700766	0.037378817133	4.096937178001
H	0.578011703059	-0.621831554494	-4.395521711984
H	-1.698069700766	0.037378817133	-4.096937178001
Fe	0.049223352032	-0.112601832956	0.000000000000
C	1.744210236366	-0.525156710991	0.000000000000
H	-1.505396157148	-0.104228847366	0.000000000000
O	2.845621077421	-0.918259878330	0.000000000000
C	-3.040622703926	0.355873368314	-2.439427899248
H	-2.951203523141	1.453264853414	-2.431389758022
H	-3.949521543921	0.111669094550	-3.014503563842
H	-3.186507126822	0.023014984959	-1.400967222755
C	-2.085880753918	-1.857921047201	-3.131833432712
H	-2.064315931188	-2.300187376656	-2.122852441864
H	-3.080739427783	-2.052487402113	-3.566469504310
H	-1.351344385562	-2.386184644888	-3.755425036559
C	-3.040622703926	0.355873368314	2.439427899248
H	-3.186507126822	0.023014984959	1.400967222755
H	-3.949521543921	0.111669094550	3.014503563842
H	-2.951203523141	1.453264853414	2.431389758022
C	-2.085880753918	-1.857921047201	3.131833432712
H	-1.351344385562	-2.386184644888	3.755425036559
H	-3.080739427783	-2.052487402113	3.566469504310
H	-2.064315931188	-2.300187376656	2.122852441864
C	1.410708791357	-2.115463204807	3.065115297830
H	2.039916742402	-2.543193286709	3.864295323112
H	0.525837178423	-2.755933927374	2.956811119951
H	1.975119037837	-2.175012853202	2.124125935267
C	2.360183505320	0.169168016133	3.476905248150
H	2.857829721463	0.222174696400	2.496530316369
H	2.201166661202	1.193706047328	3.844573243001
H	3.067079680522	-0.315481169409	4.171224799459
C	2.360183505320	0.169168016133	-3.476905248150
H	3.067079680522	-0.315481169409	-4.171224799459
H	2.201166661202	1.193706047328	-3.844573243001
H	2.857829721463	0.222174696400	-2.496530316369
C	1.410708791357	-2.115463204807	-3.065115297830
H	1.975119037837	-2.175012853202	-2.124125935267

H	0.525837178423	-2.755933927374	-2.956811119951
H	2.039916742402	-2.543193286709	-3.864295323112
H	-0.956188382133	2.224508438614	0.000000000000
H	-0.208379375477	-1.604279256288	0.000000000000

*i*Pr-10 ^{1}A′ C_S ZPVE = 0.531354

E(B3LYP) = -2746.80993594 E(B3PW91) = -2747.94806916874

thermal correction (393.15 K): H = 0.583315 G = 0.441259

P	-0.090177737134	-0.204659245733	2.218514982194
P	-0.090177737134	-0.204659245733	-2.218514982194
N	-1.241653014761	-1.661132767214	0.000000000000
C	-1.248818365606	-1.636022210678	-2.452956991070
H	-1.867746255630	-1.539682421117	-3.359288958310
H	-0.617291374681	-2.529706891316	-2.576857695344
C	-2.074736765532	-1.766189633405	-1.174303135370
H	-2.889533820076	-0.999611647007	-1.190561052680
H	-2.609691941100	-2.743554074118	-1.195365268359
C	-1.248818365606	-1.636022210678	2.452956991070
H	-0.617291374681	-2.529706891316	2.576857695344
H	-1.867746255630	-1.539682421117	3.359288958310
C	-2.074736765532	-1.766189633405	1.174303135370
H	-2.609691941100	-2.743554074118	1.195365268359
H	-2.889533820076	-0.999611647007	1.190561052680
H	0.892569128584	-1.755067749305	0.000000000000
H	1.560182797670	-1.303399726216	0.000000000000
Fe	0.208631155246	-0.187127316245	0.000000000000
C	1.402416912528	1.099371627061	0.000000000000
H	-0.870394425588	0.859432601605	0.000000000000
O	2.144102936151	1.991892268294	0.000000000000
C	-0.918926798016	1.282514265726	-3.041539957250
H	-0.712751914967	1.160667664220	-4.120851264362
C	1.296091131318	-0.620460934091	-3.437647871947
H	0.766920742962	-0.919576658046	-4.361782598393
C	1.296091131318	-0.620460934091	3.437647871947
H	0.766920742962	-0.919576658046	4.361782598393
C	-0.918926798016	1.282514265726	3.041539957250
H	-0.712751914967	1.160667664220	4.120851264362
C	2.131119619835	-1.813451811513	-2.951697482886
H	1.518900534453	-2.686157903209	-2.678602827407
H	2.826780762351	-2.133786265366	-3.745004777690
H	2.735253457959	-1.539477075047	-2.072678118883
C	2.215997710071	0.562975470673	-3.768456178682
H	2.697316267346	0.966592760164	-2.862862265972
H	3.018985575425	0.232121500866	-4.448385897726
H	1.686296981908	1.385899292811	-4.268849415989
C	-0.313709102812	2.611569152183	-2.564252370377
H	-0.573365618030	2.792175825890	-1.510572271906
H	0.781004721642	2.647242502874	-2.642743845520
H	-0.721271517423	3.444127970289	-3.162206189671
C	-2.441001410848	1.312448035859	-2.847268083249
H	-2.946993565253	0.437483189036	-3.279461967458
H	-2.702116884162	1.366269483425	-1.779138209752
H	-2.855386905242	2.209020702168	-3.338387325623
C	-0.313709102812	2.611569152183	2.564252370377
H	-0.721271517423	3.444127970289	3.162206189671
H	0.781004721642	2.647242502874	2.642743845520
H	-0.573365618030	2.792175825890	1.510572271906
C	-2.441001410848	1.312448035859	2.847268083249
H	-2.702116884162	1.366269483425	1.779138209752
H	-2.946993565253	0.437483189036	3.279461967458
H	-2.855386905242	2.209020702168	3.338387325623
C	2.131119619835	-1.813451811513	2.951697482886
H	2.735253457959	-1.539477075047	2.072678118883
H	2.826780762351	-2.133786265366	3.745004777690
H	1.518900534453	-2.686157903209	2.678602827407

C	2.215997710071	0.562975470673	3.768456178682
H	1.686296981908	1.385899292811	4.268849415989
H	3.018985575425	0.232121500866	4.448385897726
H	2.697316267346	0.966592760164	2.862862265972

*i*Pr-TS-4 ^{1}A′ i = 897 C_S ZPVE = 0.530768

E(B3LYP) = -2746.80474528 E(B3PW91) = -2747.94227860082

thermal correction (393.15 K): H = 0.581179 G = 0.442558

P	-0.100389701859	-0.173023178011	2.215847945664
P	-0.100389701859	-0.173023178011	-2.215847945664
N	-1.321479508211	-1.637537293578	0.000000000000
C	-1.274084199065	-1.600340609134	-2.457479553990
H	-1.886916778225	-1.497861797086	-3.366801725613
H	-0.647490778985	-2.496747046225	-2.587290341523
C	-2.126119246003	-1.745040938810	-1.196068866566
H	-2.927587351357	-0.970596311706	-1.207453721940
H	-2.659595130397	-2.721179114543	-1.232180269924
C	-1.274084199065	-1.600340609134	2.457479553990
H	-0.647490778985	-2.496747046225	2.587290341523
H	-1.886916778225	-1.497861797086	3.366801725613
C	-2.126119246003	-1.745040938810	1.196068866566
H	-2.659595130397	-2.721179114543	1.232180269924
H	-2.927587351357	-0.970596311706	1.207453721940
H	0.150654180532	-1.832846146913	0.000000000000
H	1.062971262598	-1.571445275882	0.000000000000
Fe	0.168728514426	-0.149978222868	0.000000000000
C	1.529017033966	0.943333548051	0.000000000000
H	-0.804016714448	1.025150125410	0.000000000000
O	2.418963538705	1.688616811583	0.000000000000
C	-0.900330274476	1.310334125727	-3.070485318307
H	-0.688014837715	1.173663240575	-4.146789920380
C	1.297671332758	-0.634803979993	-3.403885705696
H	0.782636060012	-0.941922396541	-4.333546606523
C	1.297671332758	-0.634803979993	3.403885705696
H	0.782636060012	-0.941922396541	4.333546606523
C	-0.900330274476	1.310334125727	3.070485318307
H	-0.688014837715	1.173663240575	4.146789920380
C	2.106275724345	-1.828193373297	-2.876805988238
H	1.478913388342	-2.696884566102	-2.626789772609
H	2.832524286958	-2.154524942803	-3.639949626520
H	2.667073418860	-1.554149667302	-1.970391149985
C	2.239198987775	0.531453891148	-3.737112136459
H	2.713523555944	0.939681545465	-2.830303785063
H	3.046386596741	0.178569884727	-4.400692688208
H	1.728246692095	1.354306502111	-4.257051122220
C	-0.276403107907	2.631695252801	-2.596411092893
H	-0.517698159851	2.803528507920	-1.536905127891
H	0.817676633815	2.653930350916	-2.691847563683
H	-0.682960579396	3.471824643317	-3.184347420543
C	-2.422539616686	1.361888124171	-2.882802844676
H	-2.824757846943	2.259373501261	-3.382030511989
H	-2.938398117467	0.490336269003	-3.311283170122
H	-2.685735158857	1.428244294505	-1.815675231211
C	-0.276403107907	2.631695252801	2.596411092893
H	-0.682960579396	3.471824643317	3.184347420543
H	0.817676633815	2.653930350916	2.691847563683
H	-0.517698159851	2.803528507920	1.536905127891
C	-2.422539616686	1.361888124171	2.882802844676
H	-2.685735158857	1.428244294505	1.815675231211
H	-2.938398117467	0.490336269003	3.311283170122
H	-2.824757846943	2.259373501261	3.382030511989
C	2.239198987775	0.531453891148	3.737112136459
H	1.728246692095	1.354306502111	4.257051122220
H	3.046386596741	0.178569884727	4.400692688208
H	2.713523555944	0.939681545465	2.830303785063

C	2.106275724345	-1.828193373297	2.876805988238
H	1.478913388342	-2.696884566102	2.626789772609
H	2.667073418860	-1.554149667302	1.970391149986
H	2.832524286958	-2.154524942803	3.639949626520

*i*Pr-TS-10 $^1A'$ C_S ZPVE = 0.529225

E(B3LYP) = -2746.80594389 E(B3PW91) = -2747.9480391919

thermal correction (393.15 K): H = 0.581291 G = 0.439751

P	-0.095712704558	-0.186227447836	2.215886797251
P	-0.095712704558	-0.186227447836	-2.215886797251
N	-1.218917460039	-1.586255289460	0.000000000000
C	-1.212573611004	-1.648990379138	-2.464142795079
H	-1.848291184378	-1.555720173758	-3.359454013505
H	-0.549090706649	-2.513266600759	-2.624031028325
C	-2.020514332567	-1.847130829148	-1.180008106250
H	-2.934104085729	-1.205992586181	-1.216388769754
H	-2.414883039957	-2.888526531683	-1.165044312294
C	-1.212573611004	-1.648990379138	2.464142795079
H	-0.549090706649	-2.513266600759	2.624031028325
H	-1.848291184378	-1.555720173758	3.359454013505
C	-2.020514332567	-1.847130829148	1.180008106250
H	-2.414883039957	-2.888526531683	1.165044312294
H	-2.934104085729	-1.205992586181	1.216388769754
H	1.024346323605	-2.137520940989	0.000000000000
H	1.763942672556	-1.925900736222	0.000000000000
Fe	0.202337434200	-0.203422630062	0.000000000000
C	1.565203520360	0.893661841408	0.000000000000
H	-0.698934906513	0.968141061716	0.000000000000
O	2.426935108026	1.675618848530	0.000000000000
C	-0.996202900317	1.293326768665	-2.970858709893
H	-0.846547371821	1.197972216365	-4.062133415222
C	1.269054528056	-0.524399655295	-3.482976800383
H	0.726548207684	-0.827079350527	-4.398270252754
C	1.269054528056	-0.524399655295	3.482976800383
H	0.726548207684	-0.827079350527	4.398270252754
C	-0.996202900317	1.293326768665	2.970858709893
H	-0.846547371821	1.197972216365	4.062133415222
C	2.162973214805	-1.691322051465	-3.040222262631
H	1.595203578800	-2.596864129983	-2.778802445091
H	2.857767374702	-1.961050001423	-3.853024933933
H	2.768558204541	-1.411583708626	-2.164152197633
C	2.135947444316	0.697549379595	-3.816891354631
H	2.624607032936	1.104953291398	-2.917289961854
H	2.933510063396	0.404665773512	-4.520287967282
H	1.565830675202	1.506594014123	-4.294843231500
C	-0.398888822440	2.627979760464	-2.497646924210
H	-0.610148317790	2.781966773136	-1.429091973650
H	0.690000735228	2.689058600176	-2.626465800341
H	-0.852215301549	3.461778241114	-3.059931714490
C	-2.505447698194	1.276313259668	-2.690395394947
H	-3.011625093277	0.399667570468	-3.119246244565
H	-2.705445592830	1.293532891063	-1.607615773152
H	-2.972275118552	2.173915002372	-3.129899758140
C	2.162973214805	-1.691322051465	3.040222262631
H	2.768558204541	-1.411583708626	2.164152197633
H	2.857767374702	-1.961050001423	3.853024933933
H	1.595203578800	-2.596864129983	2.778802445091
C	2.135947444316	0.697549379595	3.816891354631
H	2.933510063396	0.404665773512	4.520287967282
H	2.624607032936	1.104953291398	2.917289961854
H	1.565830675202	1.506594014123	4.294843231500
C	-0.398888822440	2.627979760464	2.497646924210
H	-0.852215301549	3.461778241114	3.059931714490
H	0.690000735228	2.689058600176	2.626465800341
H	-0.610148317790	2.781966773136	1.429091973650

C	-2.505447698194	1.276313259668	2.690395394947
H	-2.705445592830	1.293532891063	1.607615773152
H	-3.011625093277	0.399667570468	3.119246244565
H	-2.972275118552	2.173915002372	3.129899758140

H1a ^{1}A C_1 ZPVE = 0.134708

E(B3LYP) = -345.710204665 E(B3PW91) = -346.021934211198

thermal correction (393.15 K): H = 0.152246 G = 0.080392

C	0.738750196814	1.733626770458	0.448152719733
C	2.008959856506	-1.292778596597	-0.373933374042
O	1.213938002799	-0.786458708722	0.673078660804
O	0.143005056503	1.787367224403	-0.604518698586
H	0.249286408489	1.448277864817	1.405374629810
H	1.805322049890	-2.361353025101	-0.580026904410
H	3.067130584098	-1.206714752804	-0.079096189617
H	0.274080843685	-0.884889206340	0.408947543147
O	-1.328214079284	-0.533222775391	-0.365805693763
H	-1.092004473306	0.378092801306	-0.630600449472
H	1.811089475120	2.025917458281	0.532722866751
H	1.873311234304	-0.734018193711	-1.321279282859
C	-2.623845033299	-0.552750807328	0.191748158970
H	-3.396701085985	-0.258891577464	-0.543080559788
H	-2.841853974909	-1.582672887679	0.513017936755
H	-2.722683021660	0.106181397172	1.076181234078

H2a ^{1}A C_1 ZPVE = 0.139541

E(B3LYP) = -345.729588741 E(B3PW91) = -346.043832504855

thermal correction (393.15 K): H = 0.154685 G = 0.090353

C	0.974686449008	0.835532128839	0.629847717606
C	1.972016587868	-1.103625341713	-0.324534801677
O	0.963348782349	-0.583505899238	0.525027515251
O	0.624307557386	1.469040813687	-0.546330135462
H	0.280437419317	1.050623201277	1.464031122551
H	1.828436923370	-2.191669306566	-0.384458306571
H	2.978378284243	-0.900060726534	0.088248283666
H	-0.845052645491	-0.706038519247	-0.130805876051
O	-1.576903262792	-0.213873174099	-0.551157050331
H	-0.292056395795	1.187879513364	-0.747386017151
H	1.989076839172	1.180437913501	0.903312476417
H	1.911722256876	-0.668143095784	-1.335977797696
C	-2.733996023584	-0.297344032923	0.250821615470
H	-3.523304960143	0.303727480069	-0.226059327355
H	-3.109534928066	-1.334658071519	0.337628160023
H	-2.580369488779	0.097231163416	1.274337458102

TS_H1 ^{1}A C_1 i = 1655 ZPVE = 0.078369

E(B3LYP) = -230.003412947 E(B3PW91) = -230.213853044576

thermal correction (393.15 K): H = 0.087308 G = 0.039804

O	1.509506795456	-0.537911988950	0.181191261840
C	0.930553169554	0.613790274527	0.064246664284
H	1.226590232491	1.313143317515	-0.748191380507
H	0.572418400999	1.159564121670	0.969960889777
O	-0.488364704057	-0.063588744121	-0.565642837040
H	0.330285724557	-0.870419874333	-0.309919243570
C	-1.658945611741	-0.052664548575	0.241275675571
H	-2.356609635329	-0.812724665527	-0.142557691872
H	-1.425785659259	-0.276578550842	1.298482184029
H	-2.145681141523	0.932267160379	0.174703804605

TS_H1a ^{1}A C_1 i = 1266 ZPVE = 0.13206

E(B3LYP) = -345.686168029 E(B3PW91) = -346.000066512298

thermal correction (393.15 K): H = 0.146094 G = 0.08515

C	0.829827489034	1.154699263192	0.486648055172
C	1.853194610701	-1.096564734360	-0.300335041032
O	0.910593037244	-0.536710716362	0.609575053040
O	0.233666731102	1.457982435998	-0.610315724530
H	0.300526547564	1.290796103484	1.455771180535
H	1.643132189276	-2.170519575768	-0.419057866172
H	2.870116284740	-0.976540659714	0.105575488585
H	-0.171308977794	-0.698387439079	0.188239056951
O	-1.218857444617	-0.425356876734	-0.460733120556
H	-0.738820254934	0.588986077888	-0.663842556129
H	1.903905540546	1.416692283151	0.574680433790
H	1.787885740569	-0.601905103975	-1.284344026325
C	-2.450406700998	-0.355527733135	0.229408983820
H	-3.228968083936	0.071292502309	-0.425105055570
H	-2.772142929006	-1.368655958733	0.521405646305
H	-2.393237039280	0.265282253040	1.144136046638

A10 ^{1}A C_1 ZPVE = 0.340659

E(B3LYP) = -2547.03720185 E(B3PW91) = -2547.96309665519

thermal correction (393.15 K): H = 0.378689 G = 0.266018

H	0.037183660353	-0.330843802839	-1.632041007433
N	0.013904295728	1.679877090142	0.096146480931
P	2.232564052186	-0.136213661062	-0.271215232118
P	-2.168019756168	-0.135918901956	-0.375820556513
C	-2.444835798092	1.640941299332	0.082316754955
H	-2.573781194236	1.674565057844	1.177627800209
H	-3.355001508489	2.063735652324	-0.374484677989
C	-1.179042446533	2.397424702903	-0.325066118400
H	-1.206748492021	3.422160442081	0.105877241390
H	-1.190725663682	2.547330337832	-1.429767928714
C	1.204766929025	2.394677411386	-0.341859953523
H	1.218858462868	3.432381469427	0.057502419549
H	1.221475478195	2.508348065359	-1.450627165825
C	2.472779819407	1.665347705313	0.107652725918
H	2.585224296977	1.742495507370	1.201602121372
H	3.383776315124	2.078448240595	-0.355524031151
C	-3.460176408467	-1.065968489306	0.566893741196
C	-2.818684967624	-0.268154890978	-2.096562836548
C	3.345867638340	-1.003286564453	0.914827923762
C	3.065277932960	-0.401148630249	-1.892266775403
H	2.571264828410	0.217995639419	-2.654726071137
H	2.951637829532	-1.454994323675	-2.188939886818
H	4.136703785728	-0.148127925006	-1.848141901232
H	4.376557035656	-0.615002108947	0.884578785100
H	3.359060169720	-2.079684379589	0.683899519208
H	2.926784276710	-0.871826022361	1.922973648802
H	-2.246109823130	0.406593164329	-2.748271216768
H	-3.889916456981	-0.015315652698	-2.147470881117
H	-2.666411302341	-1.295234792329	-2.461288890224
H	-4.471621641254	-0.674884360619	0.371097534532
H	-3.425272616816	-2.126680154951	0.273221397900
H	-3.253101742655	-1.006740849367	1.645189176000
Fe	0.027334244673	-0.379350628054	-0.129096189957
C	0.034266212434	-2.122447998443	-0.249674796162
O	0.035654963469	-3.272440571920	-0.405238147859
C	-0.589102249005	-0.207632082086	3.072456980701
H	-0.605482310596	-1.295280937380	3.249468564978
H	-0.228873265602	0.279563671933	3.998552780657
H	-1.633142935670	0.122656210196	2.906646154915
O	0.253854435641	0.075133053052	1.985096031786
H	0.098702774799	1.004252365160	1.530889965251

A11 ^{1}A C_1 ZPVE = 0.342065

E(B3LYP) = -2547.05056580 E(B3PW91) = -2547.97663649646

thermal correction (393.15 K): H = 0.380471 G = 0.265338

H	0.000085739443	0.097601197911	-1.730217459289
N	0.000004869670	1.764913887523	0.307988474306
H	0.000028623357	1.465297677833	1.300048943421
P	2.211457789066	-0.063453798059	-0.250428024362
P	-2.211452211582	-0.063466661906	-0.250483715464
C	-2.444532542842	1.669173598037	0.396674145300
H	-2.483662399110	1.581856827864	1.494980748782
H	-3.386690024063	2.130374114232	0.059382929053
C	-1.230504526438	2.502704857880	-0.006774705274
H	-1.247644093864	3.485570344262	0.504989452228
H	-1.239702896460	2.704989346036	-1.091017883948
C	1.230471819700	2.502734343480	-0.006861332999
H	1.247608583950	3.485618088783	0.504868255973
H	1.239607527456	2.704980520636	-1.091111144528
C	2.444550320136	1.669259252479	0.396550107487
H	2.483799437308	1.582055386868	1.494863062453
H	3.386668903873	2.130451378651	0.059138614980
C	-3.295109700340	-1.064934243646	0.853265600117
C	-3.136680693680	-0.082061830852	-1.846243750116
C	3.295261803067	-1.064747436265	0.853354925805
C	3.136605199629	-0.082220226691	-1.846233220647
H	2.672760076202	0.633933901276	-2.539845281475
H	3.050631781237	-1.083211912158	-2.296601825437
H	4.202370970160	0.164036608740	-1.713325265712
H	4.325827958872	-0.676185243678	0.885805905371
H	3.314806513884	-2.106199661330	0.497811462349
H	2.859615654633	-1.054428155980	1.862354198670
H	-2.672860704584	0.634154190316	-2.539810543999
H	-4.202432011471	0.164215075259	-1.713253757181
H	-3.050767227323	-1.083010416571	-2.296719412300
H	-4.325682491369	-0.676407008035	0.885902922314
H	-3.314660598221	-2.106337120775	0.497577552680
H	-2.859310045907	-1.054724410400	1.862199117939
Fe	0.000008230909	-0.290314053002	-0.239994778600
C	0.000034183460	-1.946809318676	-0.765339725601
O	0.000066694122	-3.026504810611	-1.189859213818
O	-0.000267101557	-0.304453317756	1.778892544148
C	0.000006425180	-1.435754959286	2.560038848940
H	-0.885703865391	-2.100573396130	2.405458717136
H	0.886029004984	-2.100158528932	2.405466768579
H	-0.000066638952	-1.182722931633	3.645822942084

A12 ^{1}A C_1 ZPVE = 0.37078

E(B3LYP) = -2661.47783003 E(B3PW91) = -2662.50422610971

thermal correction (393.15 K): H = 0.415152 G = 0.28371

H	0.004622115538	-1.376174177647	-1.447815183147
N	-0.004261913956	1.159292808085	-1.140283720596
H	-0.011516730670	1.838034690404	-0.367489802998
P	2.217387172286	-0.518083831861	-0.223229565706
P	-2.211613850390	-0.534783653808	-0.222907571459
C	-2.457031036206	1.103594288640	-1.077060299327
H	-2.537583853111	1.868481376047	-0.287041324280
H	-3.384303401312	1.140461863154	-1.671463268286
C	-1.226368947827	1.381673131830	-1.934797283519
H	-1.252822512949	2.415190632195	-2.329928297492
H	-1.194515423721	0.697811546339	-2.798509715299
C	1.219825425724	1.398100120701	-1.926894989177
H	1.237383319125	2.433486593216	-2.317608866660
H	1.200081360683	0.717838547784	-2.793888816984
C	2.448737132686	1.129042695683	-1.063827788808
H	2.514964202068	1.888619774793	-0.267397117927
H	3.379024133901	1.181744642689	-1.652298010865
C	-3.270442064292	-0.380259820111	1.276710092679
C	-3.148397197706	-1.736537655669	-1.261731515813
C	3.273037687904	-0.368220728941	1.278755324438
C	3.163932004413	-1.703471567982	-1.272074981310
H	2.715068127493	-1.733351228746	-2.275444989380
H	3.076479154200	-2.711802163272	-0.838436905840
H	4.229557085710	-1.434002971004	-1.348837844131
H	4.296631082023	-0.040436941367	1.036710730816
H	3.317909712519	-1.338912145073	1.794995987727
H	2.791393917217	0.357226259916	1.949134554793
H	-2.698172530193	-1.772104642261	-2.264282824101
H	-4.215800313365	-1.475255500308	-1.341913740975
H	-3.054248753979	-2.740247816959	-0.818867200794
H	-4.296599455098	-0.064009544504	1.030147937503
H	-3.307381053431	-1.346305301658	1.802168977049
H	-2.797026356058	0.355916699485	1.941249521350
Fe	0.003638451399	-0.681156053145	-0.070465371360
C	0.009752700573	-2.292102685446	0.584119633345
O	0.013775218020	-3.400893688903	0.925259126070
O	0.005215323911	0.539116093492	1.547395383307
C	0.000562819430	-0.012633981969	2.810212450612
H	-0.887498641036	-0.654419924893	3.027718474963
H	0.885185972101	-0.657539507460	3.032781309158
H	-0.000310815951	0.776929627759	3.601618922832
O	-0.034146477142	3.809783586029	0.452009559346
C	-0.017197034726	3.572698500346	1.640861118016
H	-0.022703054489	4.409467866657	2.386440321492
H	0.003595087500	2.516030047492	2.001456811879

A13 ^{1}A C_1 ZPVE = 0.375422

E(B3LYP) = -2661.48461298 E(B3PW91) = -2662.51609453913

thermal correction (393.15 K): H = 0.417003 G = 0.29723

H	-0.092265946513	-0.096039343320	-1.838548571564
N	0.050846350126	1.761772273688	-0.135156051791
H	0.352120195994	1.772818176064	0.883209601040
P	2.150635107989	-0.198530842258	-0.544051913234
P	-2.288441462745	0.003354207200	-0.348191859326
C	-2.380917255262	1.754475775117	0.260246851022
H	-2.282796042284	1.707628829689	1.357548334898
H	-3.341761196023	2.241389094302	0.025239449704
C	-1.197863859968	2.510473714474	-0.337850582745
H	-1.124124819470	3.525233054804	0.098979812509
H	-1.351383222957	2.645884052664	-1.423351062634
C	1.160622305954	2.343030836427	-0.912712480978
H	1.256268084741	3.425911400795	-0.699631808452
H	0.922907859903	2.242115255810	-1.985397872306
C	2.470890675558	1.632963268846	-0.578755650448
H	2.783962950835	1.900462555248	0.440228503308
H	3.268969207902	1.902904093795	-1.288473721167
C	-3.479657066536	-0.884406731967	0.746045186917
C	-3.185035252089	0.024381905612	-1.959459926036
C	3.326816788398	-0.814185651132	0.732971465324
C	2.880426167883	-0.840952406680	-2.112380480957
H	2.354288710061	-0.389939334089	-2.965943404490
H	2.732395635680	-1.930814945558	-2.163923544993
H	3.957246860007	-0.619884250754	-2.183207025629
H	4.369146899612	-0.581545907300	0.461670275698
H	3.222251603450	-1.903270212833	0.851988559321
H	3.068580486086	-0.310853723059	1.675060758253
H	-2.648864963625	0.674468555160	-2.665441743869
H	-4.223868125346	0.374192244496	-1.848628902623
H	-3.188913585399	-0.992256636588	-2.381852870108
H	-4.479446963546	-0.423070708360	0.710301193611
H	-3.562176931706	-1.935847219756	0.431056436783
H	-3.105154281797	-0.857805767210	1.778816229730
Fe	-0.075271260143	-0.357530054247	-0.346233026666
C	-0.144671832400	-2.024877730069	-0.844441073988
O	-0.189711167447	-3.091138237787	-1.297284709868
O	-0.179910226388	-0.593507436103	1.770043307502
C	-0.397019449134	-1.866351399107	2.318921722528
H	-1.160183578085	-2.405786951475	1.738220463086
H	0.523128783200	-2.485281268176	2.328235242823
H	-0.760095305132	-1.788386129096	3.363446387072
O	1.211362767379	1.313155263835	2.179088710601
C	0.657547450099	0.337853465794	2.793461117311
H	-0.163418549823	0.563613879393	3.527763292973
H	1.340646845030	-0.427320777621	3.253388277715

A14 ^{1}A C_1 ZPVE = 0.373681

E(B3LYP) = -2661.48048656 E(B3PW91) = -2662.51209025714

thermal correction (393.15 K): H = 0.415245 G = 0.29436

H	-0.034688297273	-0.395248104887	-1.788592240706
N	0.020023431071	1.681439500488	-0.388160134013
H	0.206273186681	1.928556066168	1.079457724313
P	2.206315150295	-0.210028917539	-0.465236326303
P	-2.219752444259	-0.139725458850	-0.453678984541
C	-2.437019266309	1.698670893991	-0.377743474258
H	-2.530533334496	1.971813475984	0.686820145011
H	-3.348324387707	2.042043360705	-0.894579537652
C	-1.163398877099	2.306760007762	-0.963257682200
H	-1.162150779086	3.403450040251	-0.783600137285
H	-1.182273062954	2.189146972244	-2.070974162625
C	1.212857464179	2.250752441105	-1.010730046704
H	1.249427048800	3.351245341787	-0.860898541726
H	1.201658846635	2.100280339441	-2.114214816404
C	2.473894831412	1.618992262163	-0.420534942265
H	2.561765728880	1.896132787225	0.641742286949
H	3.392160507011	1.928810060492	-0.945589535085
C	-3.463731068362	-0.788009677960	0.753991765165
C	-2.980603971934	-0.632991521508	-2.059350494343
C	3.322567849430	-0.882247291252	0.838846304389
C	3.006033464893	-0.779713022196	-2.024337764557
H	2.518169319747	-0.286817799427	-2.877537917704
H	2.860234250794	-1.865467087202	-2.133681314478
H	4.084303869398	-0.554405099692	-2.036843679556
H	4.355310924232	-0.516275939652	0.724975073106
H	3.325208874077	-1.982398151601	0.792463948694
H	2.926930111234	-0.575050463224	1.817375482889
H	-2.440451514524	-0.136014790789	-2.877402559741
H	-4.048439268245	-0.365964697656	-2.104079891678
H	-2.870795646899	-1.719907597349	-2.195262436658
H	-4.480200817816	-0.436059316220	0.514703343111
H	-3.455380314366	-1.888836427903	0.738737015998
H	-3.203434520137	-0.455138690365	1.769570143229
Fe	-0.008483232178	-0.403416390075	-0.290893667364
C	-0.022612607756	-2.135758751757	-0.489366070877
O	-0.026910270466	-3.265463021856	-0.760897945142
O	0.171971969110	-0.367219063965	1.955666042724
C	-0.186158043780	-1.528768350132	2.675547390434
H	0.194889133300	-2.404808955371	2.136432317003
H	0.257397204770	-1.508442648584	3.688273527524
H	-1.282965595584	-1.632644054564	2.779374013586
O	0.462473051237	1.912705341453	2.120449489313
C	-0.177232059317	0.868813594394	2.662250651876
H	-1.293673758710	0.932007848997	2.619783370172
H	0.113677429631	0.725869262844	3.723999816804

TS_A10 ^{1}A C_1 i = 629 ZPVE = 0.337735

E(B3LYP) = -2547.03679422 E(B3PW91) = -2547.96276706383

thermal correction (393.15 K): H = 0.375227 G = 0.263889

H	0.033527251036	-0.385291096492	-1.638636228039
N	0.013809563881	1.685795781305	0.059726643635
P	2.234588622782	-0.151023088122	-0.268205185138
P	-2.170269682160	-0.153697674759	-0.367673886674
C	-2.446288914904	1.632975041935	0.060666458903
H	-2.575046717909	1.683836320965	1.155036563759
H	-3.358215221788	2.046205323040	-0.401044726778
C	-1.187584629374	2.394487412227	-0.359977025769
H	-1.217300661427	3.421959831344	0.062285125326
H	-1.196380319854	2.528729030501	-1.463991306761
C	1.212889205640	2.391809842257	-0.377402463471
H	1.228902102979	3.432269390039	0.012603022516
H	1.227567883181	2.489191057122	-1.485151335685
C	2.472690700475	1.657409407250	0.087177537384
H	2.578033934351	1.745830455868	1.180555403771
H	3.387051799100	2.063419894697	-0.375252372643
C	-3.450757760760	-1.063727053018	0.608251597869
C	-2.839493454511	-0.317779273475	-2.078600385444
C	3.333044707909	-0.994759633862	0.946226302119
C	3.083365058806	-0.439235756048	-1.876984764461
H	2.592423711060	0.163121911355	-2.654858292639
H	2.977568768572	-1.498711976658	-2.156086750333
H	4.153209199776	-0.180239467032	-1.828922997169
H	4.363535778004	-0.605594907912	0.923885726759
H	3.350319748617	-2.075105288124	0.735115186765
H	2.896382262766	-0.843604190142	1.944036855900
H	-2.272818036058	0.342398789676	-2.750181443304
H	-3.911018673627	-0.064805346791	-2.123353029239
H	-2.692444549336	-1.352109396200	-2.424498070255
H	-4.464374763615	-0.675156050940	0.419083496640
H	-3.420288365025	-2.129427007049	0.332823099050
H	-3.227214468466	-0.984980699670	1.681789341738
Fe	0.027673589840	-0.389963170421	-0.129404425234
C	0.034016539095	-2.134234945149	-0.192017608020
O	0.034884493553	-3.289173817216	-0.301258232351
C	-0.576359735701	-0.098745501027	3.016083450095
H	-0.611614113830	-1.184292661153	3.217701802248
H	-0.207167754594	0.395889391829	3.936604849672
H	-1.622458424491	0.240984376298	2.864055193597
O	0.254166380872	0.169344461801	1.924383671338
H	0.081317942790	1.124203317228	1.335473405802

TS_A12 ^{1}A C_1 i = 171 ZPVE = 0.371389

E(B3LYP) = -2661.47670485 E(B3PW91) = -2662.50307330779

thermal correction (393.15 K): H = 0.414394 G = 0.289054

H	-0.326816114254	-1.360817401342	-1.416739007093
N	0.121098033564	1.152431391303	-1.182363574058
H	0.320543977322	1.813458715709	-0.420060214756
P	2.025014232173	-0.880105599630	-0.291644879807
P	-2.331868606701	-0.108485955048	-0.168899106860
C	-2.291580137919	1.570246905349	-0.975944921301
H	-2.175626113017	2.307463354520	-0.164293093515
H	-3.223049254528	1.808898115729	-1.514699456338
C	-1.078160348669	1.621881409078	-1.899308871662
H	-0.926166461851	2.646604051719	-2.290481803953
H	-1.229025652762	0.961899643757	-2.769118379789
C	1.309132664778	1.111065091526	-2.055854157328
H	1.504637255236	2.106599380153	-2.498173519782
H	1.091746275336	0.415867758556	-2.882667961296
C	2.519703117657	0.637003197023	-1.257735682269
H	2.802923461630	1.413986347951	-0.529714866844
H	3.388983103494	0.456264581944	-1.910447811184
C	-3.327747747281	0.189123683205	1.352162511442
C	-3.485251017211	-1.090148831752	-1.221383302417
C	3.155854958036	-0.831383287407	1.162863305096
C	2.692506691709	-2.290344886778	-1.274140626798
H	2.203189662376	-2.305274467498	-2.258634450585
H	2.441381511942	-3.232590407326	-0.762748578674
H	3.785097253265	-2.227868476267	-1.401885189422
H	4.209225286801	-0.705039610318	0.865615877775
H	3.053120156079	-1.762659347390	1.739965493994
H	2.842283097785	0.005631487781	1.802176665980
H	-3.060068655050	-1.185785409845	-2.230832653328
H	-4.486314243264	-0.633529663589	-1.280516740671
H	-3.574600499453	-2.104073822509	-0.801453581011
H	-4.289129229559	0.679535434797	1.130195576405
H	-3.522184843844	-0.768192383467	1.858833277798
H	-2.729214479426	0.820308167377	2.023484642083
Fe	-0.175689549990	-0.640065240742	-0.061562308855
C	-0.427028596916	-2.204708540009	0.653412262786
O	-0.600423293149	-3.283784680602	1.042390248701
O	0.037913347511	0.613731327071	1.508735214340
C	0.015882250001	0.114118047777	2.791517333858
H	-0.932917478435	-0.409478374014	3.064799616227
H	0.826128325454	-0.623294926684	3.011883488130
H	0.135313334239	0.925499779742	3.551673921208
O	1.426696604964	3.368712890967	0.521661672573
C	1.130179388443	3.242515819560	1.687675949449
H	0.155379118442	2.820908663698	2.007156482160
H	1.843778278386	3.533740702236	2.500127225080

TS_A13 ^{1}A C_1 i = 509 ZPVE = 0.371165

E(B3LYP) = -2661.48032950 E(B3PW91) = -2662.5121658981

thermal correction (393.15 K): H = 0.412168 G = 0.292757

H	-0.035615248386	-0.457961379767	-1.774090683477
N	0.014335180704	1.671159967538	-0.448552261710
H	0.141813100348	1.949785200981	0.870313513997
P	2.210573617142	-0.223351449420	-0.446409921899
P	-2.220466359072	-0.170059583864	-0.436543707278
C	-2.441909817228	1.670379597941	-0.437238467241
H	-2.531149812551	1.985795220480	0.615649957120
H	-3.356546545248	1.989893621398	-0.963246435954
C	-1.175114172896	2.264455809024	-1.050872887300
H	-1.179976520275	3.366633146011	-0.915828764543
H	-1.184675921566	2.095293848949	-2.149529600367
C	1.213684585183	2.217568095795	-1.084654037524
H	1.246616552978	3.322144084899	-0.976676480340
H	1.204526900261	2.018528960668	-2.178080230238
C	2.465721026896	1.608240372706	-0.454417841796
H	2.525085884083	1.917138476593	0.601143233008
H	3.392132677898	1.909502812265	-0.969869968816
C	-3.450751499442	-0.766485068369	0.809595267425
C	-2.992130342567	-0.736008347066	-2.012674082177
C	3.320463853365	-0.844466717680	0.887071897580
C	3.025770100669	-0.836899820712	-1.980570731118
H	2.537600854691	-0.380798776994	-2.853789924437
H	2.893392323920	-1.927556351068	-2.052323639348
H	4.101531462695	-0.599933688958	-1.994967349473
H	4.352102549803	-0.477553496081	0.766739175645
H	3.328573904999	-1.945484623627	0.879196317098
H	2.916498413129	-0.504735185946	1.851244365815
H	-2.458805588848	-0.277706143254	-2.857324200969
H	-4.060662704458	-0.472545244843	-2.061513132113
H	-2.882273555723	-1.828037159407	-2.098836945426
H	-4.469873987777	-0.424751250132	0.566812288549
H	-3.441768505888	-1.866922205890	0.840273115510
H	-3.177094800976	-0.391219376126	1.806557649028
Fe	-0.006598247537	-0.419459846146	-0.273270745701
C	-0.018222708456	-2.155970911788	-0.424474270362
O	-0.022219982920	-3.292604357023	-0.662342366428
O	0.183398032500	-0.286328981865	1.935658610161
C	-0.137011912565	-1.420934387264	2.711126214271
H	0.260816344049	-2.312587310838	2.209914503250
H	0.316091372108	-1.343016256979	3.716979425335
H	-1.229677347760	-1.549377098439	2.835050116071
O	0.393301265840	2.016170969375	1.994024056218
C	-0.186071501695	0.990267246227	2.601330759434
H	-1.308386796399	0.994650736134	2.590329997218
H	0.136924103925	0.881044909486	3.661030028936

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