Supporting Information

Stereospecific Copper(II)-Catalyzed Tandem Ring Opening/Oxidative Alkylation of Donor-Acceptor Cyclopropanes with Hydrazones: Synthesis of Tetrahydropyridazines

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Crystal Data and Structure Refinement

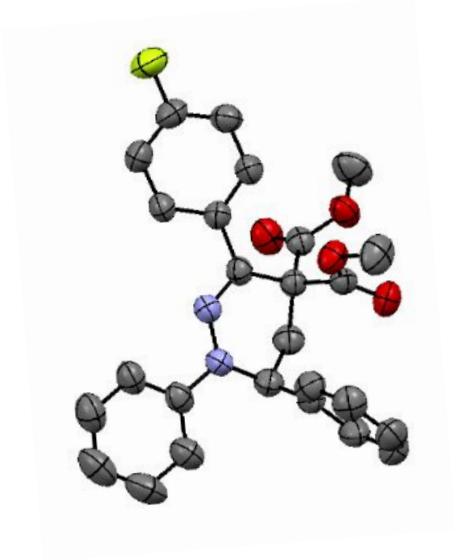


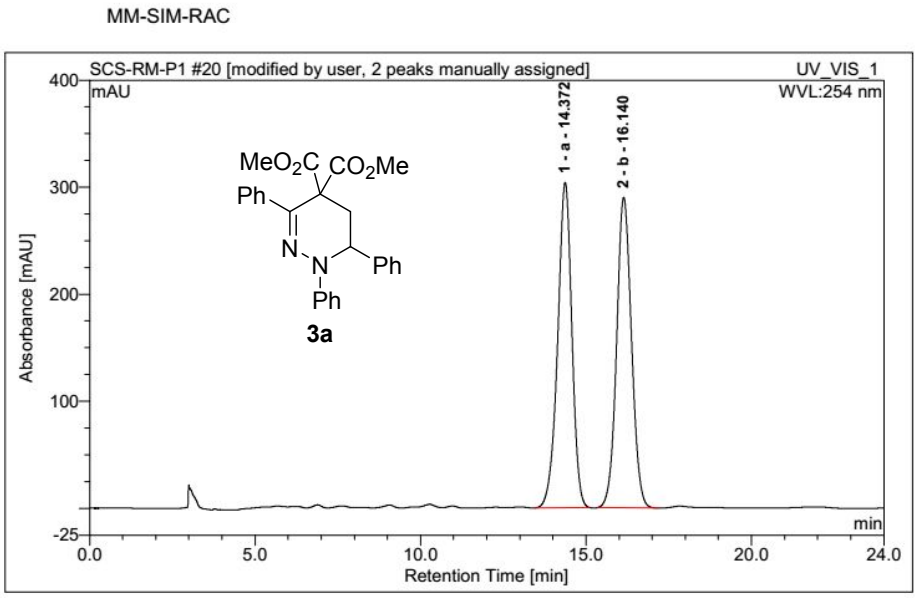
Figure S1. ORTEP diagram of dimethyl **3u′** with 50% ellipsoid. (CCDC 1895630). H-Atoms are omitted for clarity.

Solvent and Method for Crystal Growth. (*S*)-3-(4-Fluorophenyl)-1,6-diphenyl-5,6-dihydropyridazine-4,4(1H)-dicarboxylate **3u′** was dissolved in isopropanol and left at room temperature for slow evaporation. After 3 days, needle shaped colorless crystal growth was observed. Single crystal X-ray data were collected on a Bruker SMART APEX II equipped with a CCD area detector using Mo/Kα radiation and the structure was solved by direct method using SHELXL-16.

Identification code	**3u´**
CCDC Number	1895630
Empirical formula	$C_{26}H_{23}FN_2O_4$
Formula weight	446.46
Crystal habit, color	Needle / colorless
Crystal size, mm^3	0.29 x 0.24 x 0.18
Temperature, *T*/K	293 (2)
Wavelength, *λ*/Å	0.71073
Crystal system	orthorhombic
Space group	'P 21 21 21'
Unit cell dimensions	a = 10.2417(18)Å b = 10.911(2)Å c = 20.105(3)Å $\alpha = \beta = \gamma$ = 90.00°
Volume, V/$Å^3$	2246.7(7)

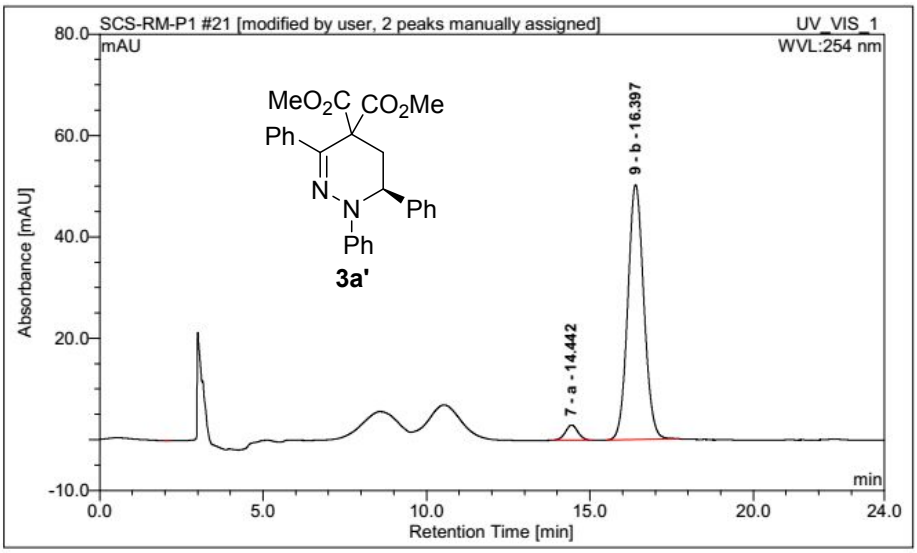
Z	4
Calculated density, Mg·m^{-3}	1.320
Absorption coefficient, μ/mm^{-1}	0.095
F(000)	936
θ range for data collection	2.03 to 25.991°
Limiting indices	$-12 \leq h \leq 12$, $-13 \leq k \leq 13$, $-24 \leq l \leq 24$
Reflection collected / unique	4435/2505 [R(int)= 0.1715]
Completeness to θ	100 % (θ= 25.991°)
Absorption correction	none
Max. and min. transmission	0.983/0.973
Refinement method	'SHELXL-2014/7 (Sheldrick, 2014)'
Data / restraints / parameters	4435/0/ 302
Goodness−of−fit on F^2	0.999
Final R indices [I>2sigma(I)]	$R1$ = 0.0608, $wR2$ = 0.1415
R indices (all data)	$R1$ = 0.1253, $wR2$ = 0.1802

HPLC Chromatograms



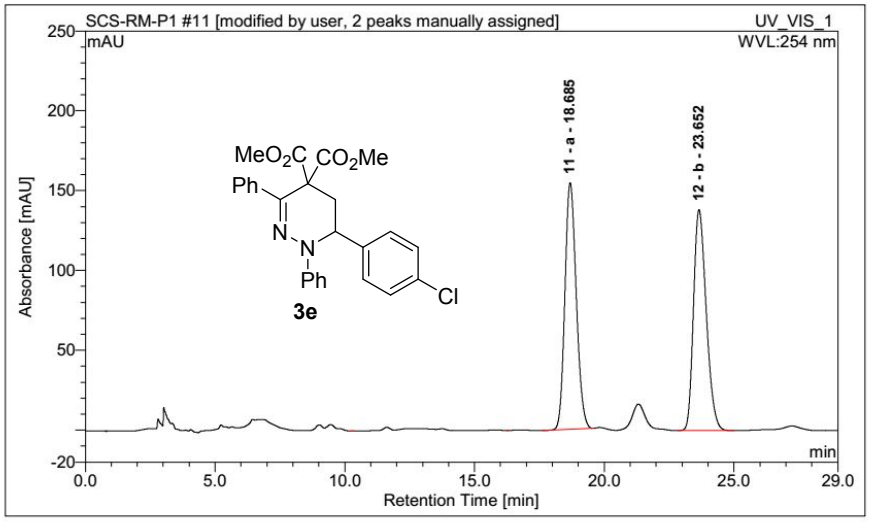
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	14.37	150.9201	49.98584341	303.9004	n.a.
2	b	16.14	151.006	50.01415659	290.215	n.a.

MM-SIM-CHI



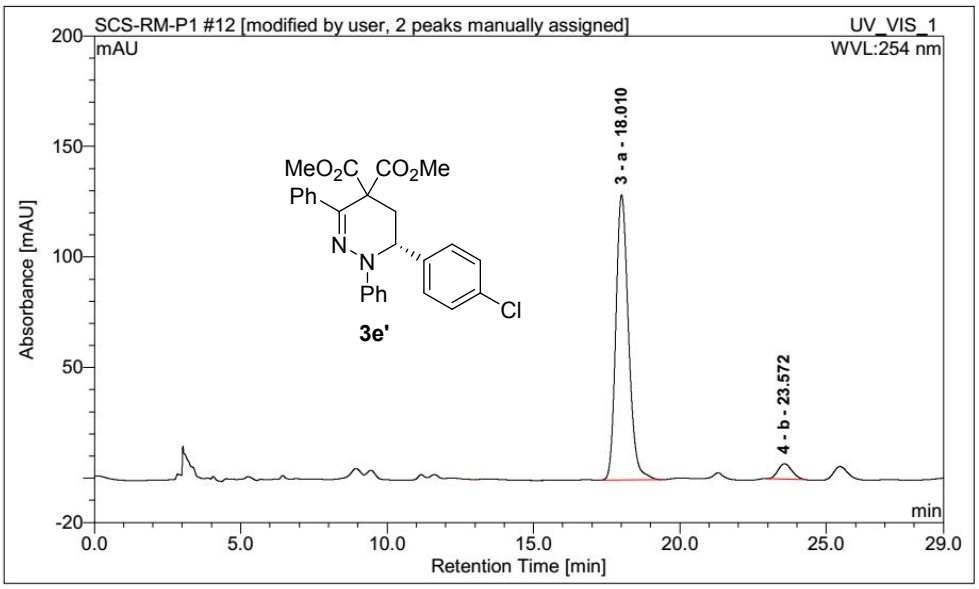
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
7	a	14.44	1.322518	4.408009872	2.99239	n.a.
9	b	16.40	28.680	95.59199013	50.352	n.a.

4Cl-CYP-RAC

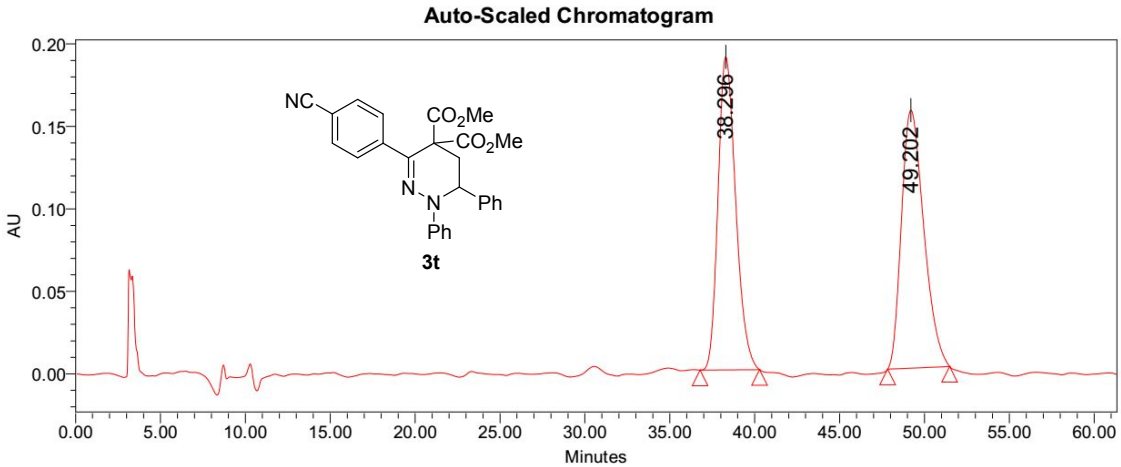


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
11	a	18.69	78.14179	49.85982381	154.5453	n.a.
12	b	23.65	78.581	50.14017619	138.316	n.a.

4Cl-CYP-CHI

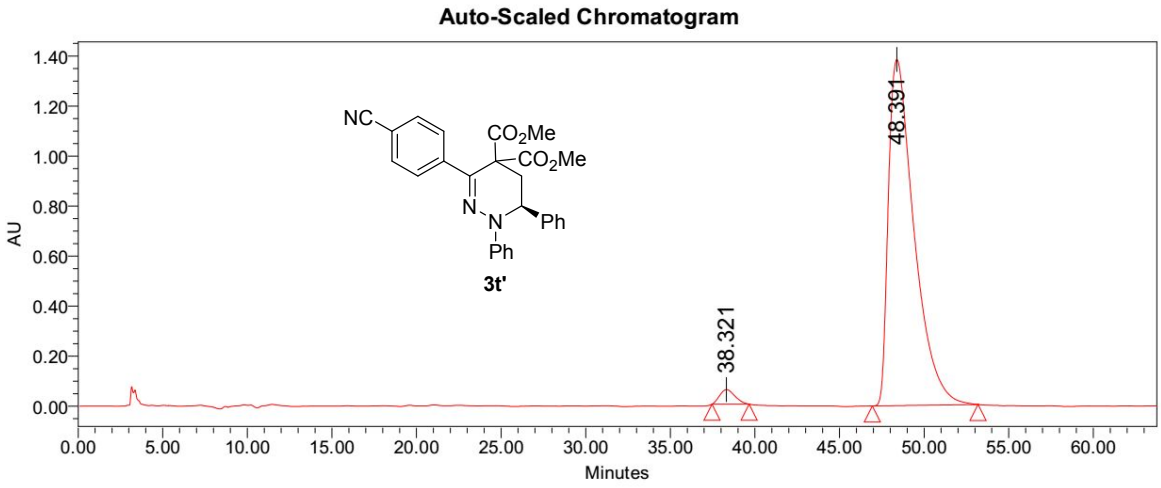


No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
3	a	18.01	64.47968	94.49482638	128.9899	n.a.
4	b	23.57	3.757	5.505173621	6.904	n.a.



Peak Results

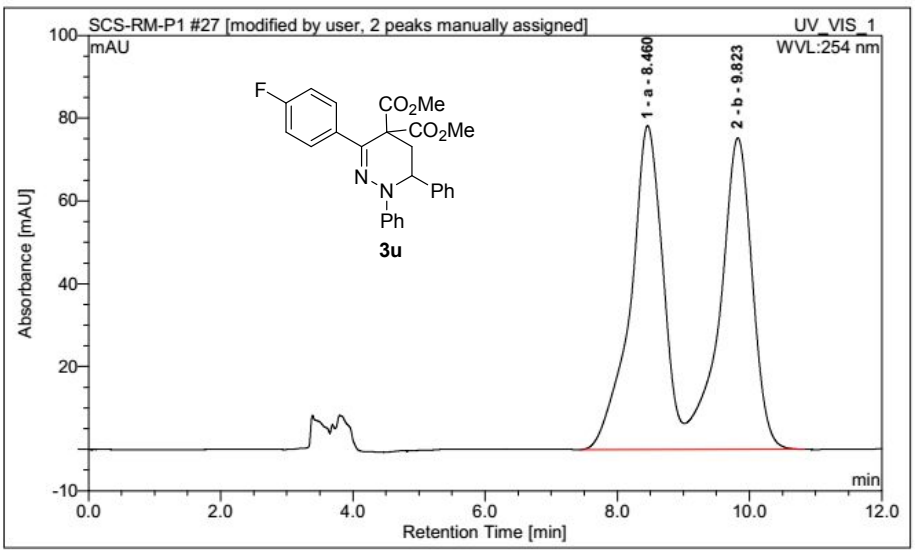
	RT	Height (µV)	% Area
1	38.296	189863	48.95
2	49.202	156465	51.05



Peak Results

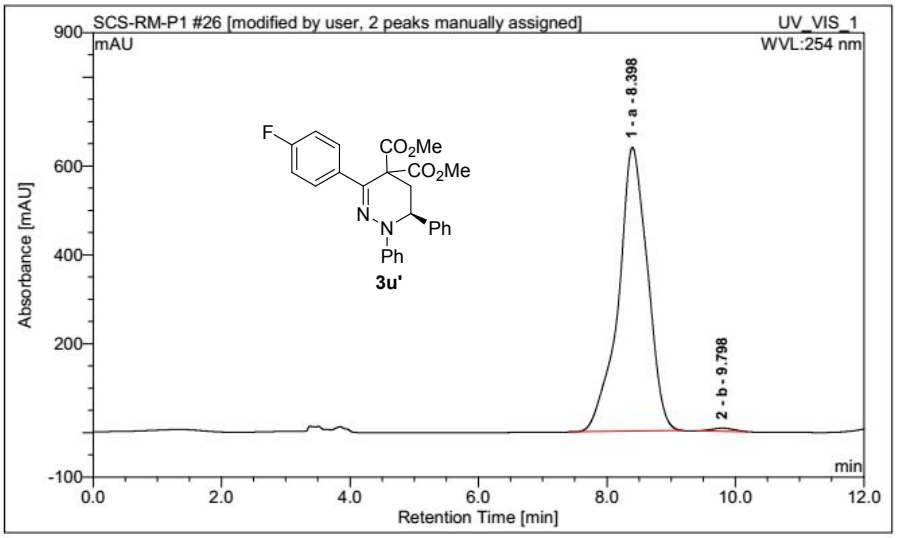
	RT	Height (μV)	% Area
1	38.321	58119	2.43
2	48.391	1384060	97.57

MM-4F-HYD-RAC



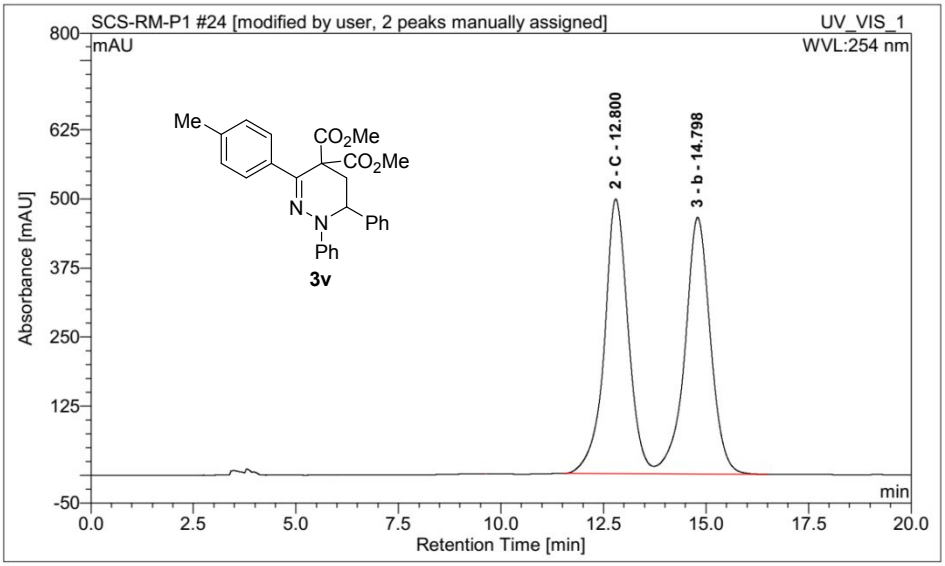
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	8.46	44.48181	50.93367303	78.23039	n.a.
2	b	9.82	42.851	49.06632697	75.281	n.a.

MM-4F-HYD-CHI



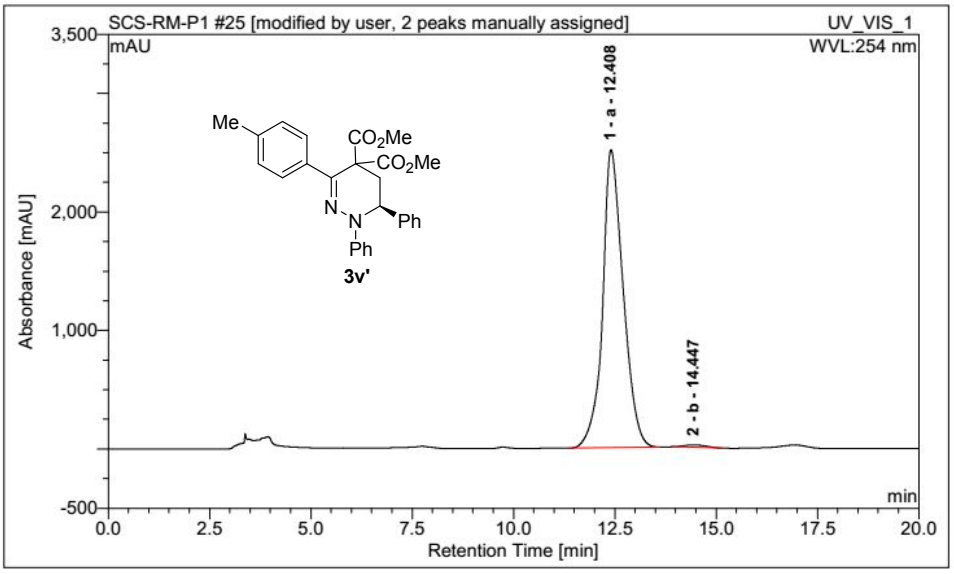
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	8.40	336.507	99.18884096	638.9039	n.a.
2	b	9.80	2.752	0.811159041	6.974	n.a.

MM-4Me-Rac



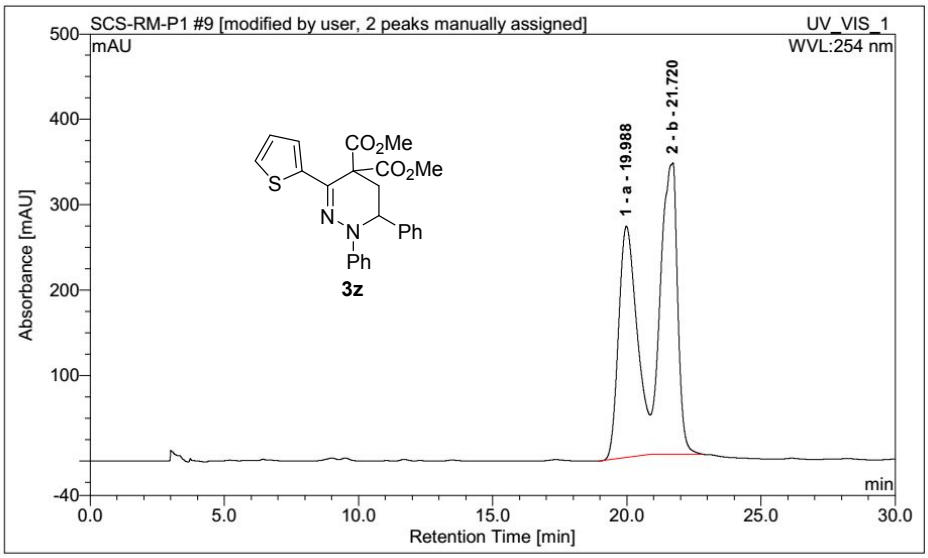
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
2	C	12.80	333.5791	49.84424434	497.2429	n.a.
3	b	14.80	335.664	50.15575566	464.511	n.a.

MM-4ME-HYD-CHI



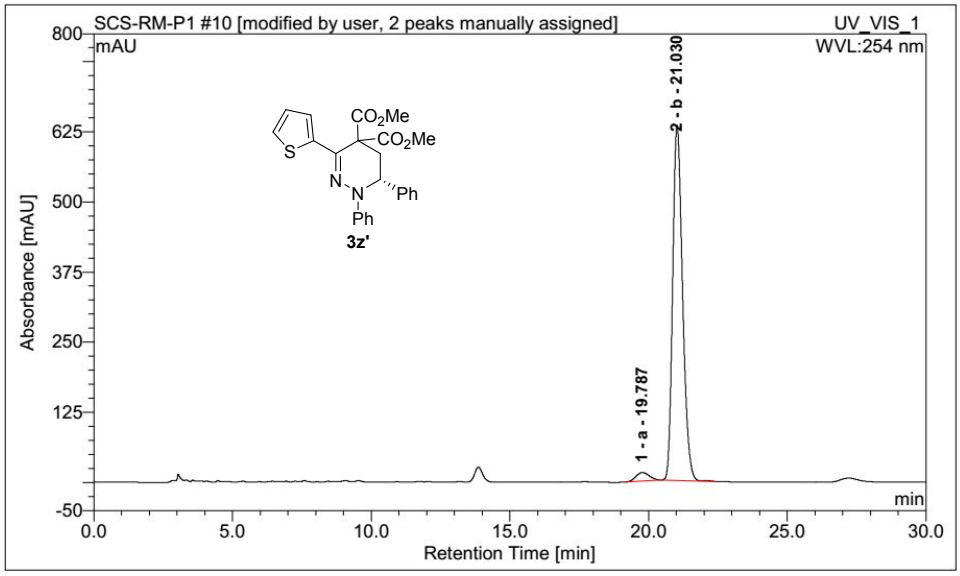
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	12.41	1483.083	99.15069274	2515.169	n.a.
2	b	14.45	12.704	0.8493072578	20.441	n.a.

THIO-HYD-RAC



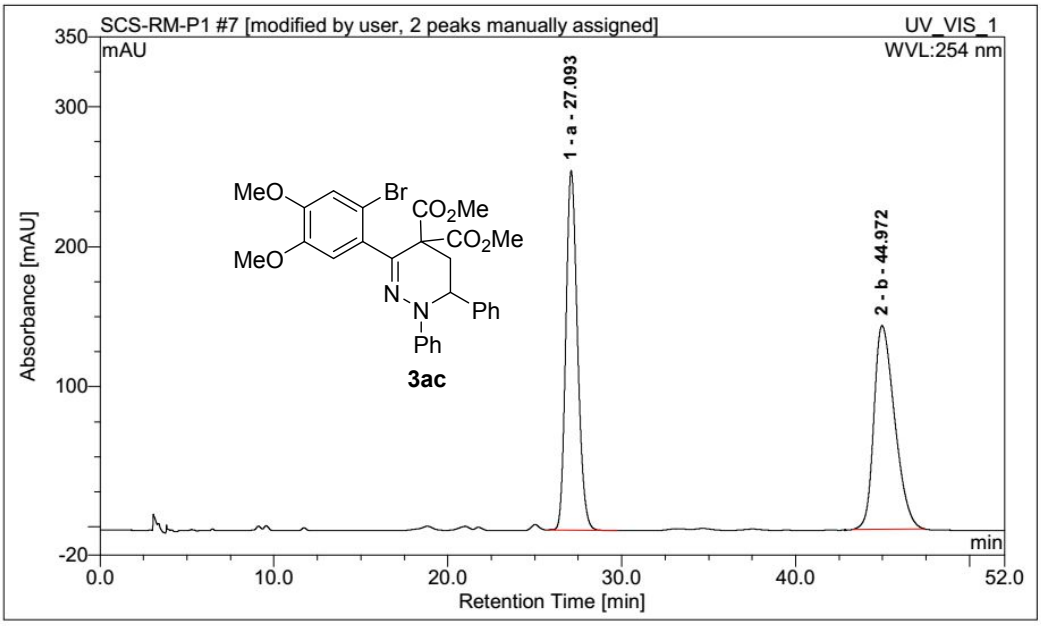
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	19.99	218.7637	46.80420822	270.7854	n.a.
2	b	21.72	248.638	53.19579178	340.856	n.a.

THIO-HYD-CHI



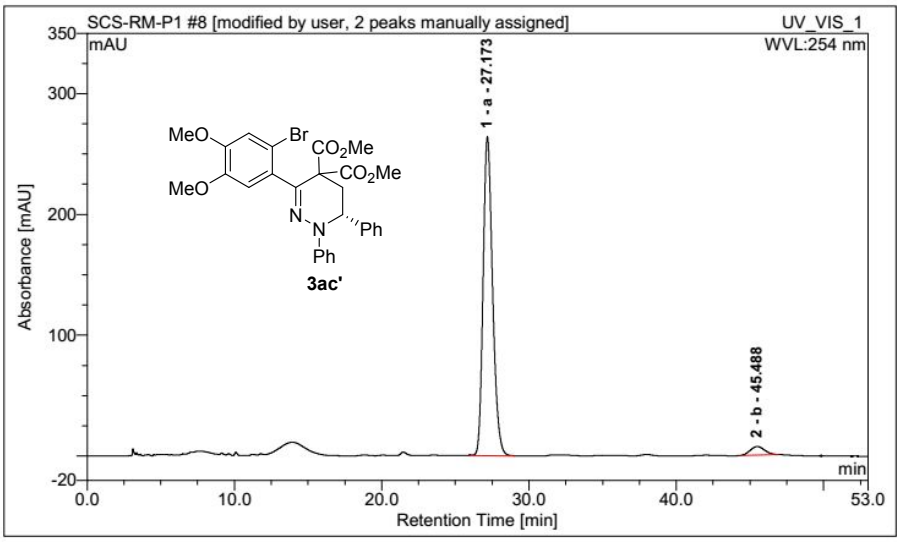
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	19.79	8.426532	3.123123564	15.22435	n.a.
2	b	21.03	261.385	96.87687644	633.353	n.a.

6-VERT-HYD-RAC

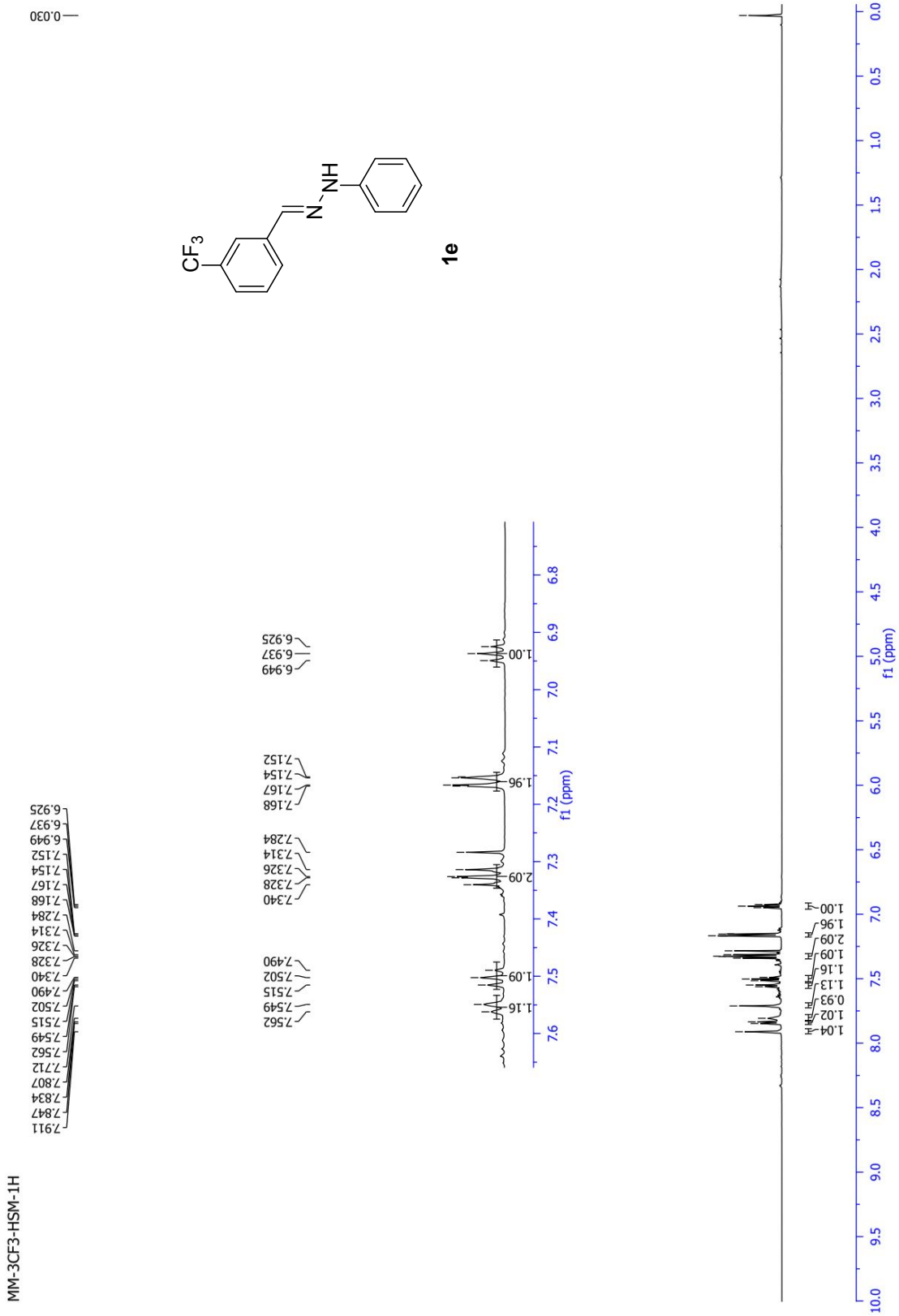


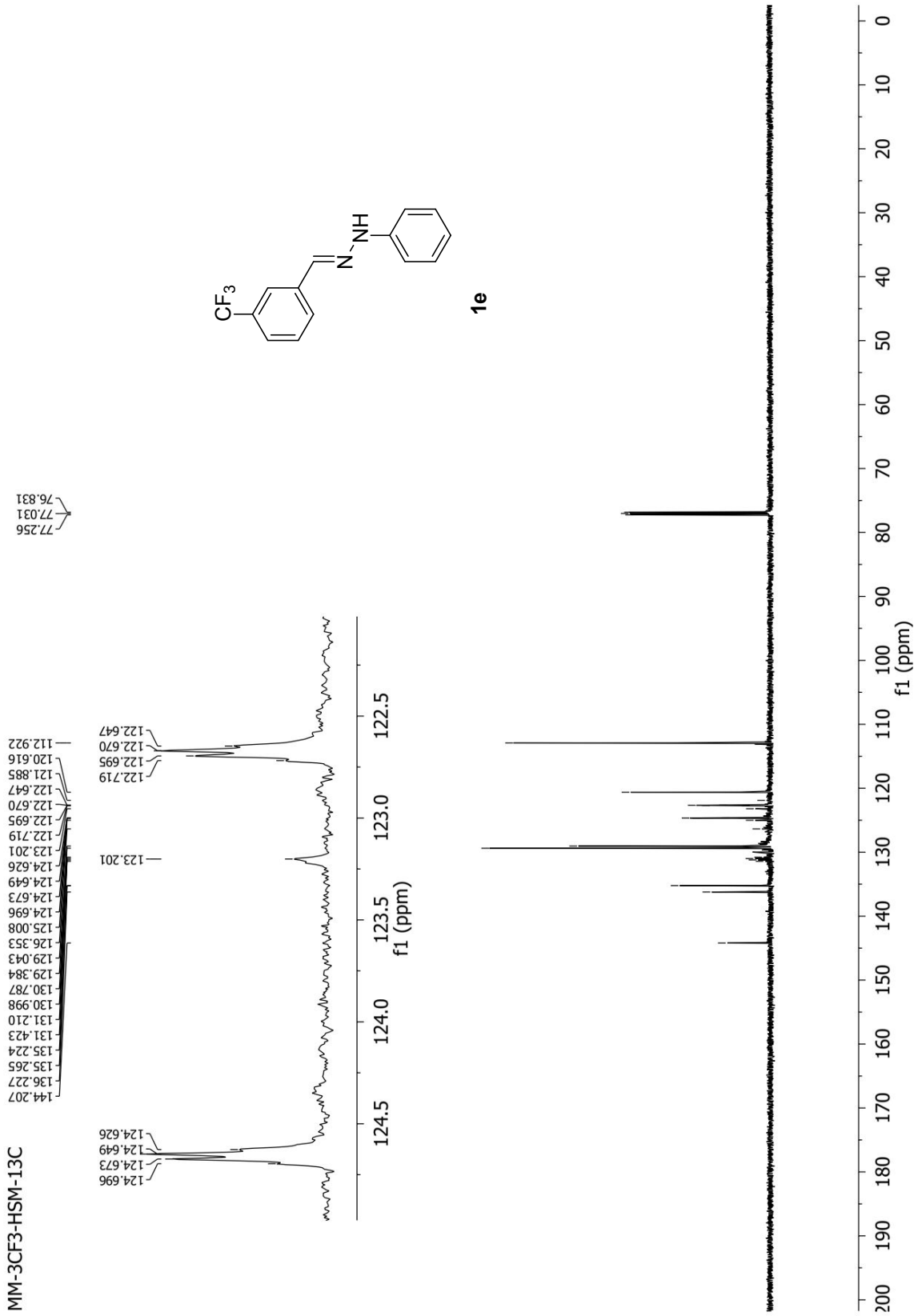
No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	27.09	198.7153	49.58249199	256.5834	n.a.
2	b	44.97	202.062	50.41750801	145.498	n.a.

6-VERT-HYD-CHI



No.	Peak Name	Ret.Time (detected) min	Area mAU*min	Rel.Area(ident.) %	Height mAU	Amount
1	a	27.17	195.826	96.10113654	263.6058	n.a.
2	b	45.49	7.945	3.898863462	6.976	n.a.


MM-3CF3-HSM-1H
CF3
N
NH
1e
f1 (ppm)


MM-3CF3-HSM-13C
CF3
N
NH
1e
f1 (ppm)
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124.649
124.626
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122.695
122.670
122.647
112.922
144.207
136.227
135.265
135.224
131.423
131.210
130.998
130.787
129.384
129.043
126.353
125.008
124.696
124.673
124.649
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122.719
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122.670
122.647
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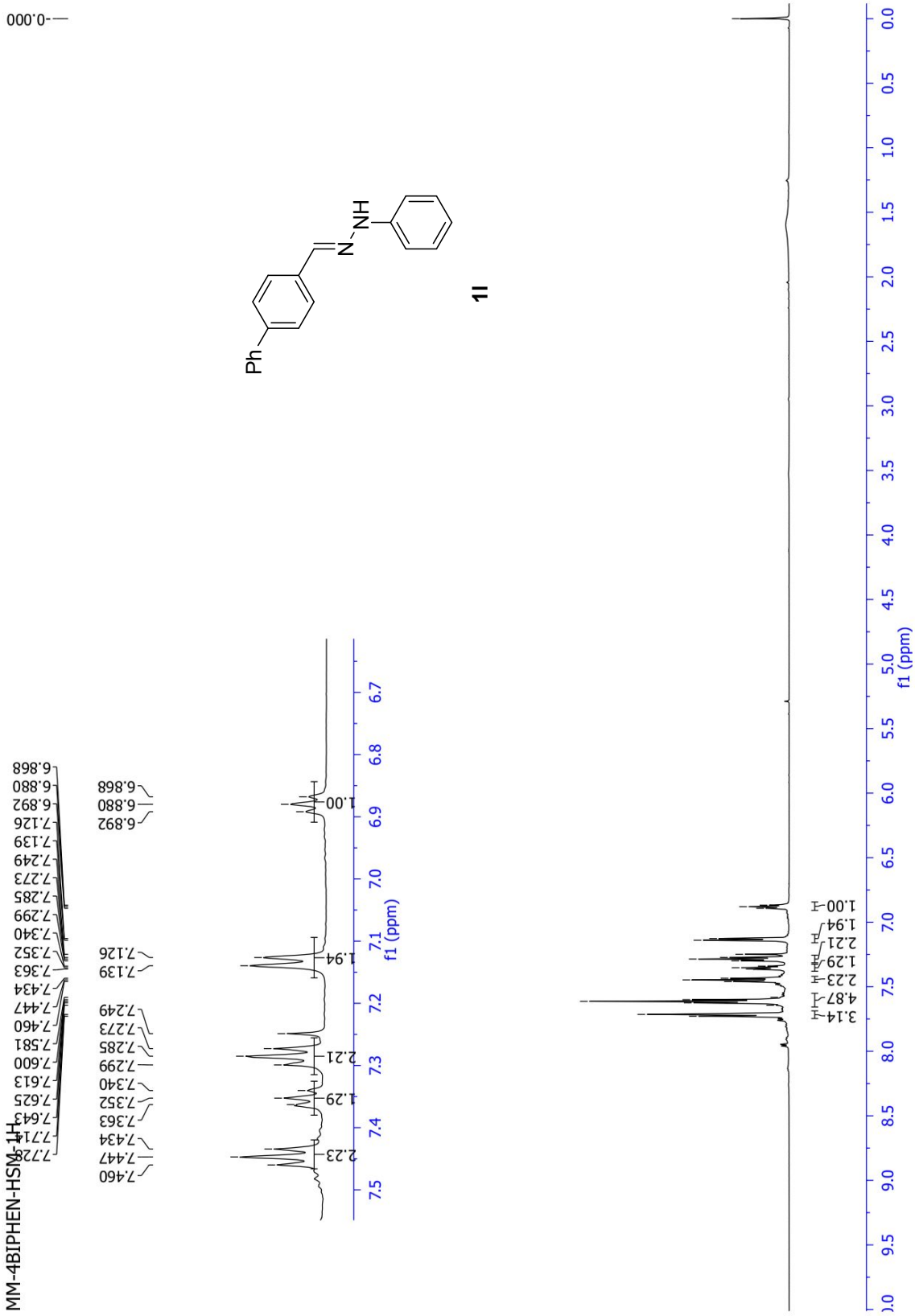
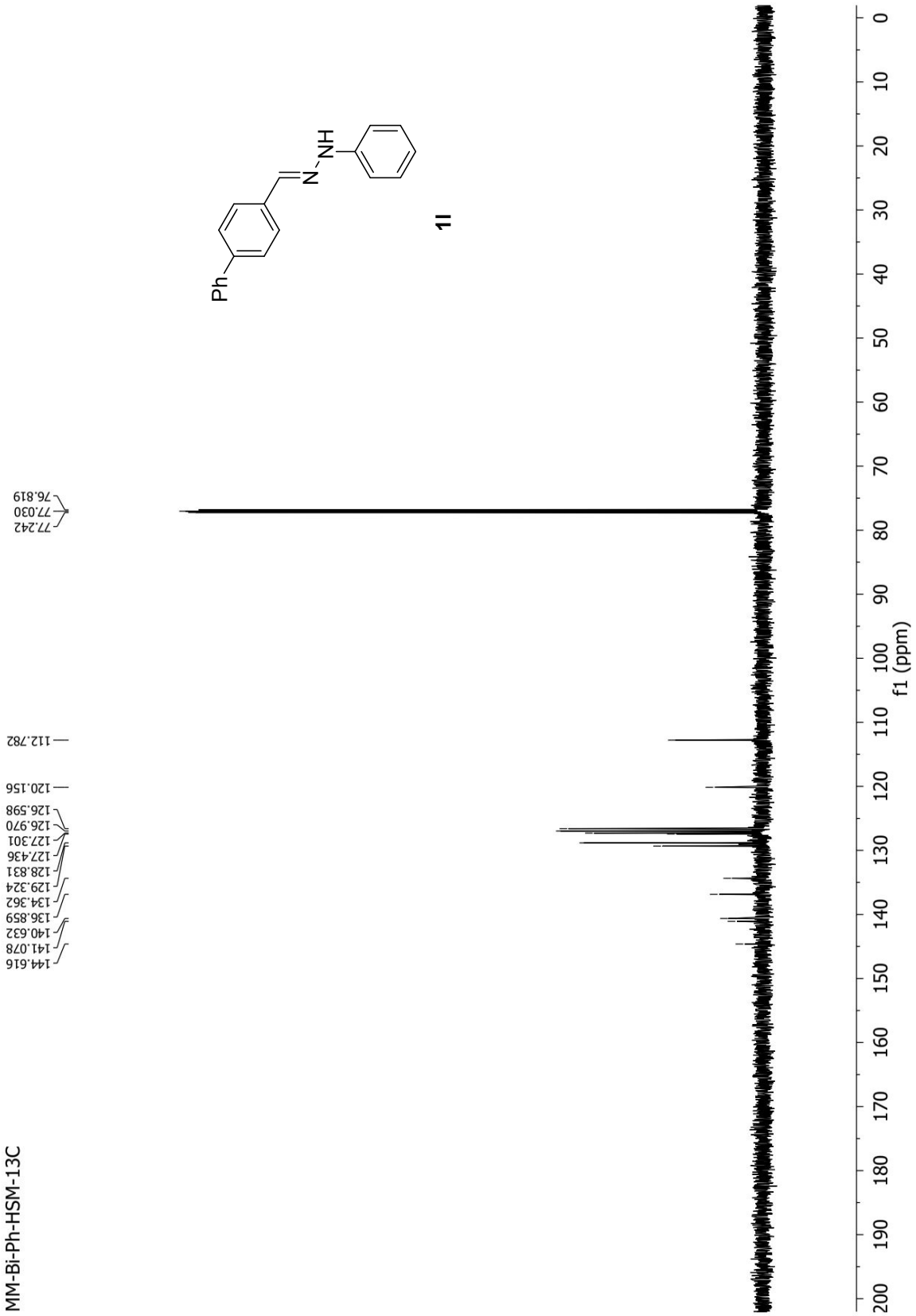
77.031
76.831


MM-4BIPHEN-HSM-1H
Ph
N
N
H
1l
f1 (ppm)
f1 (ppm)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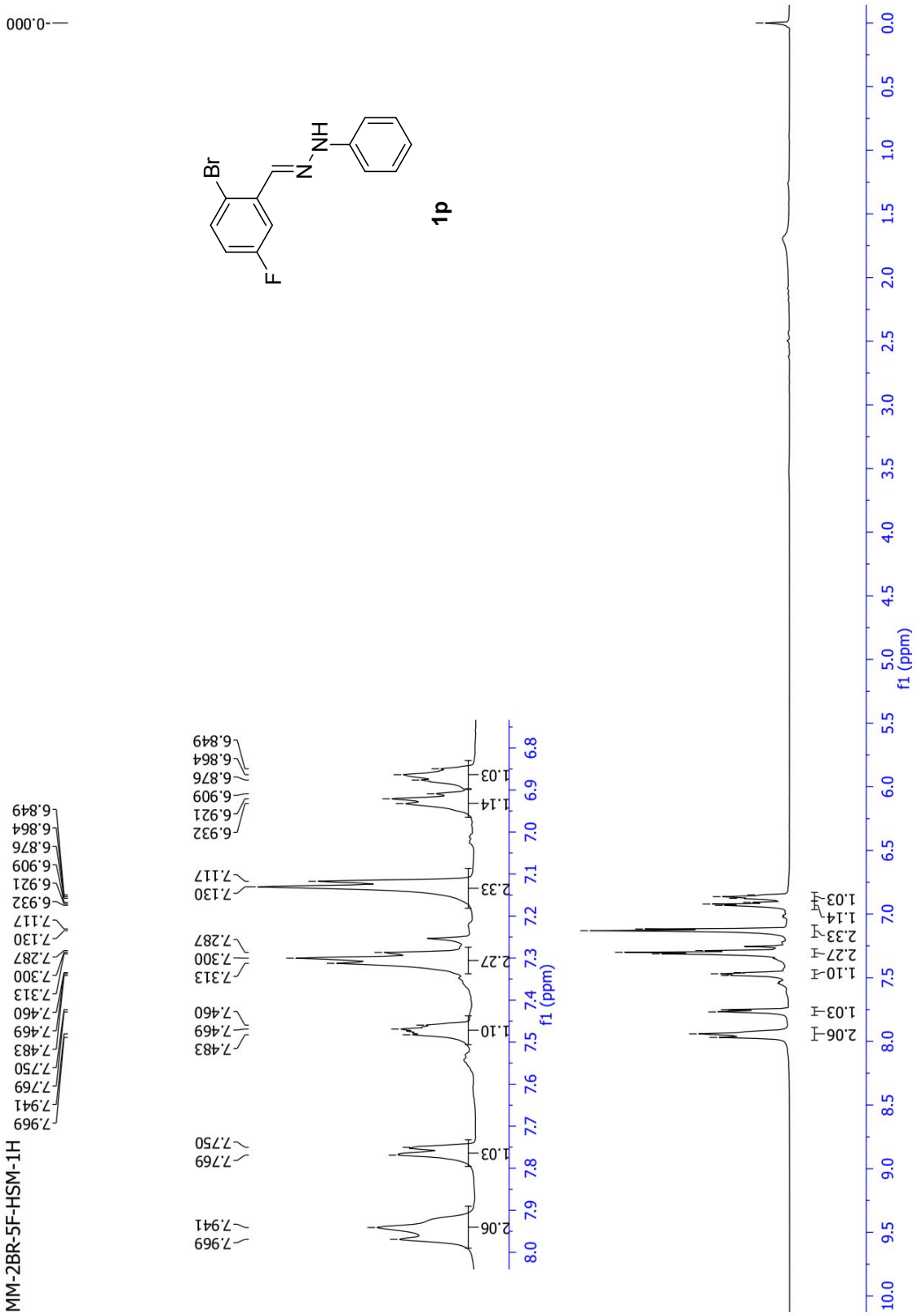
141.078
140.632
136.859
134.362
129.324
128.831
127.436
127.301
126.970
126.598
120.156
112.782
77.242
77.030
76.819
Ph
N
N
H
1l
f1 (ppm)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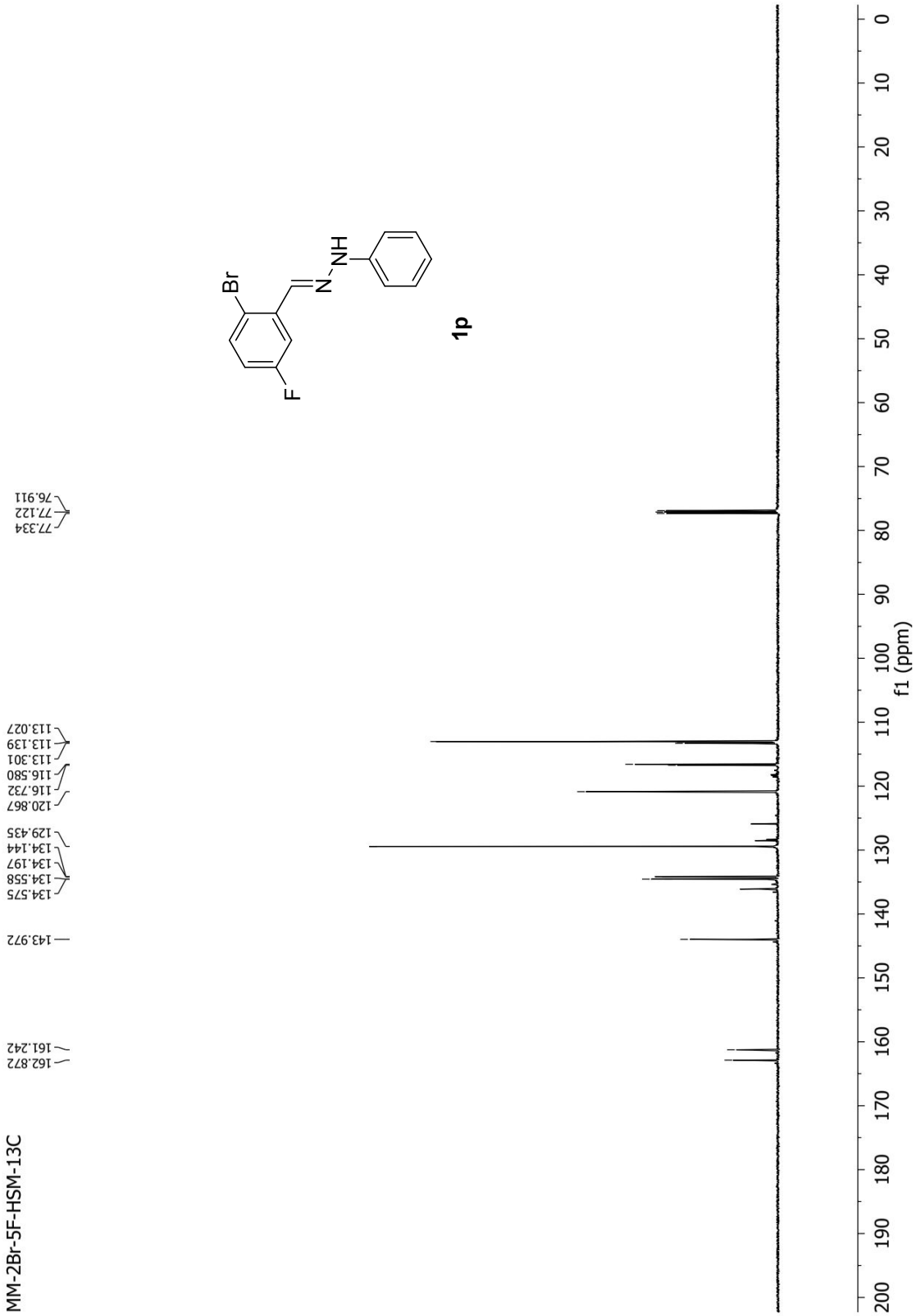
7.941
7.769
7.750
7.483
7.469
7.460
7.313
7.300
7.287
7.130
7.117
6.932
6.921
6.909
6.876
6.864
6.849
2.06
1.03
1.10
2.27
2.33
1.14
1.03
f1 (ppm)
Br
F
N
NH
1p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161.242
143.972
134.575
134.558
134.197
134.144
129.435
120.867
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116.580
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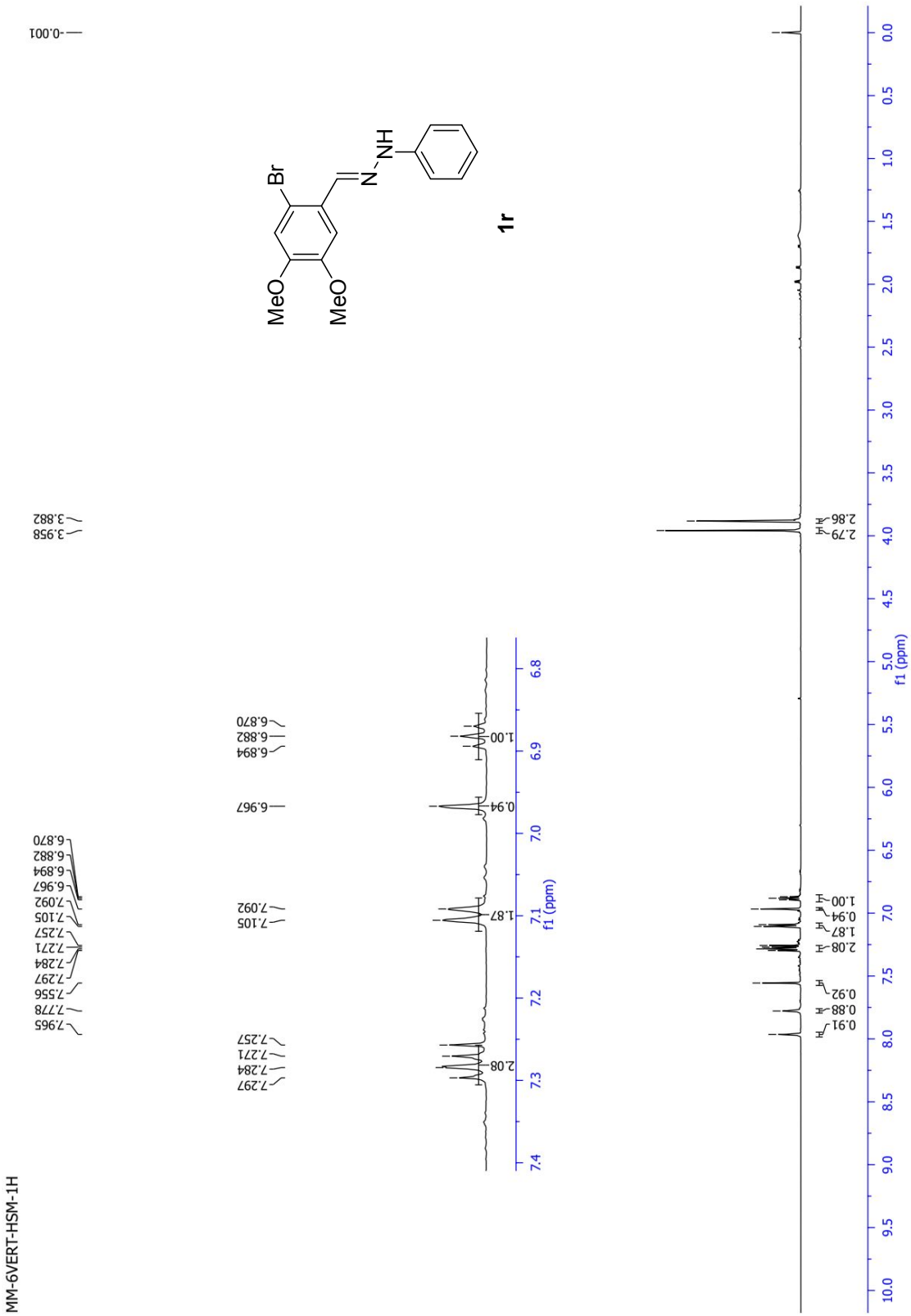
113.139
113.027
77.334
77.122
76.911
Br
F
N
NH
1p
f1 (ppm)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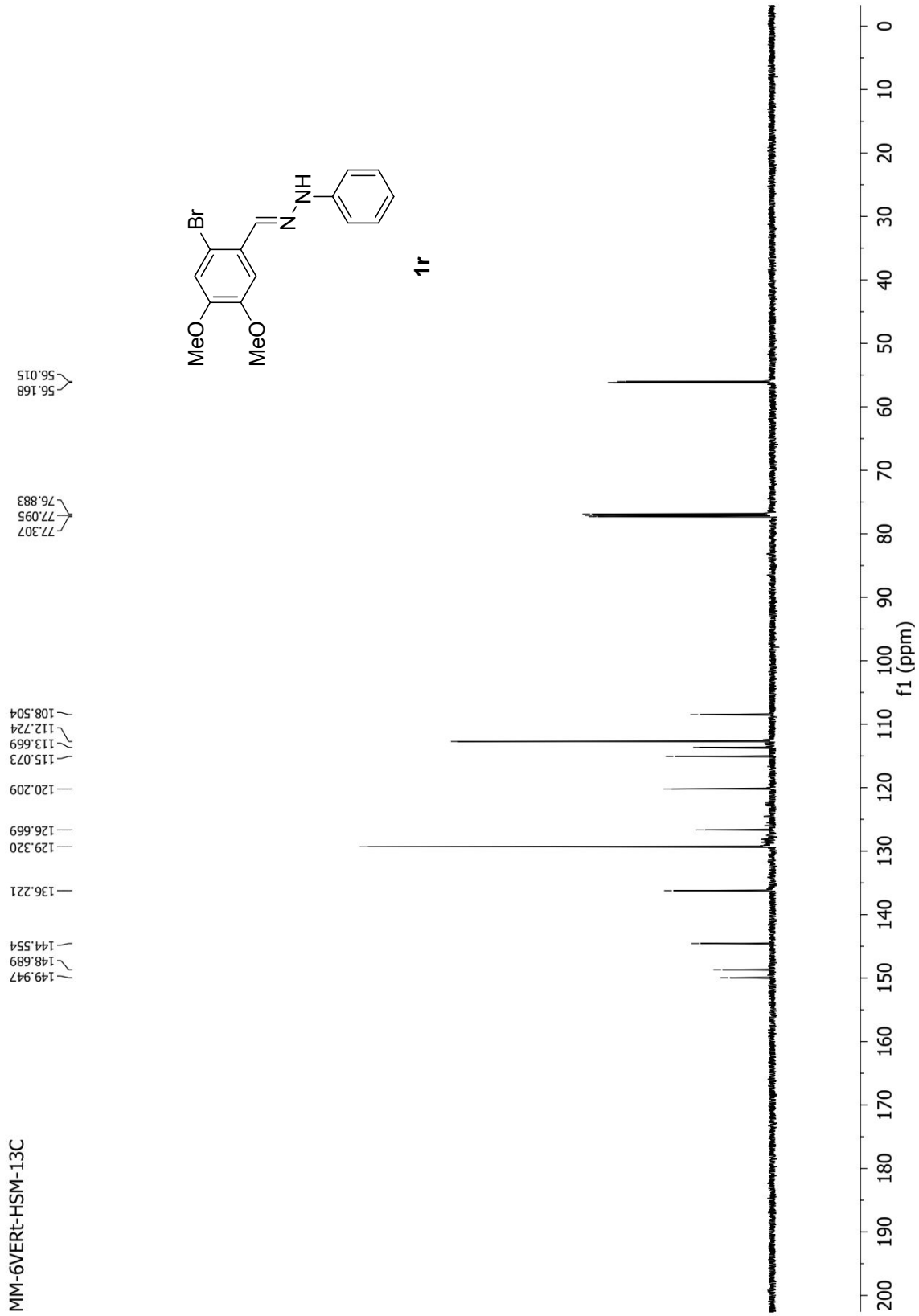
MeO
MeO
Br
N
NH
1r
f1 (ppm)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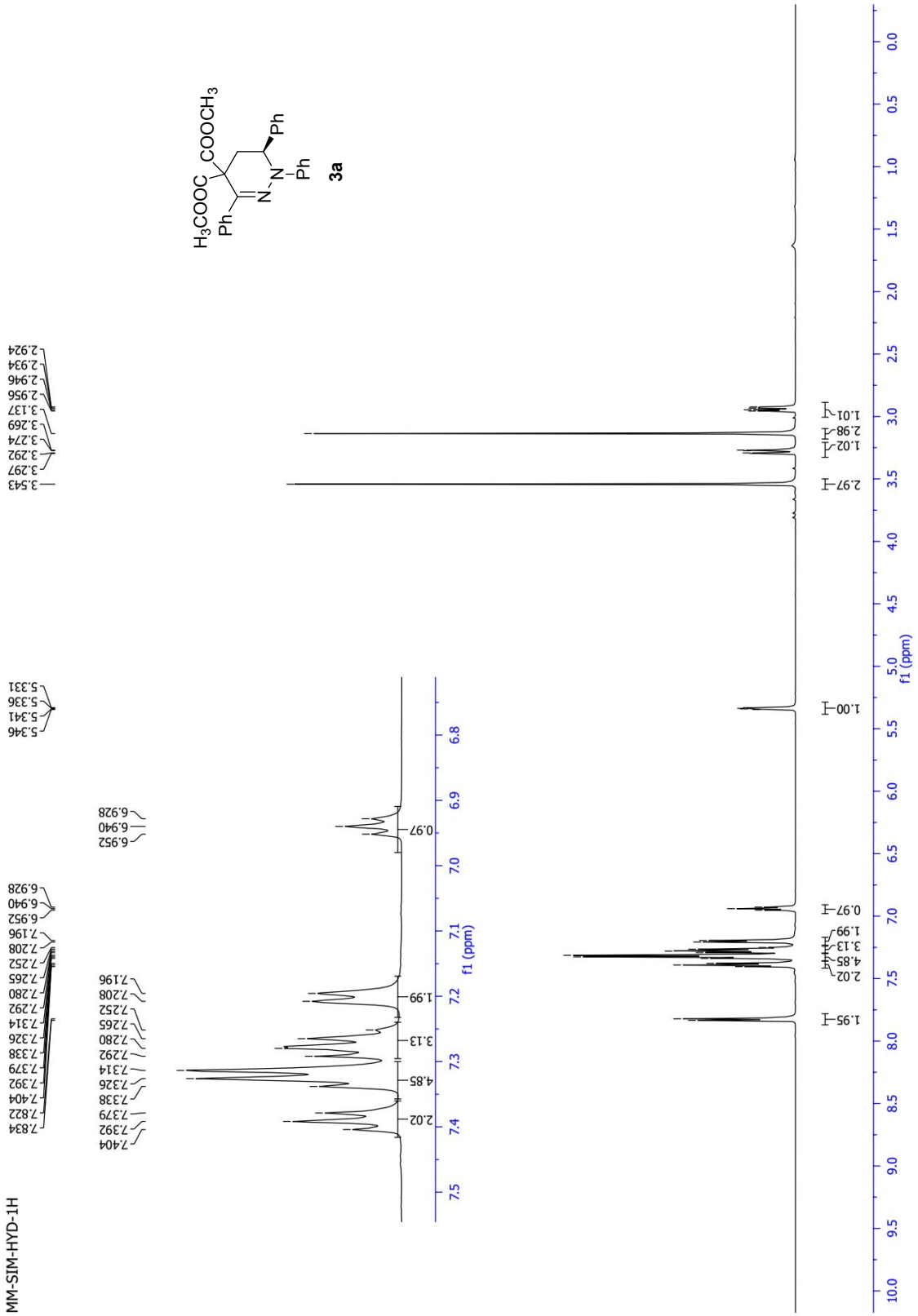
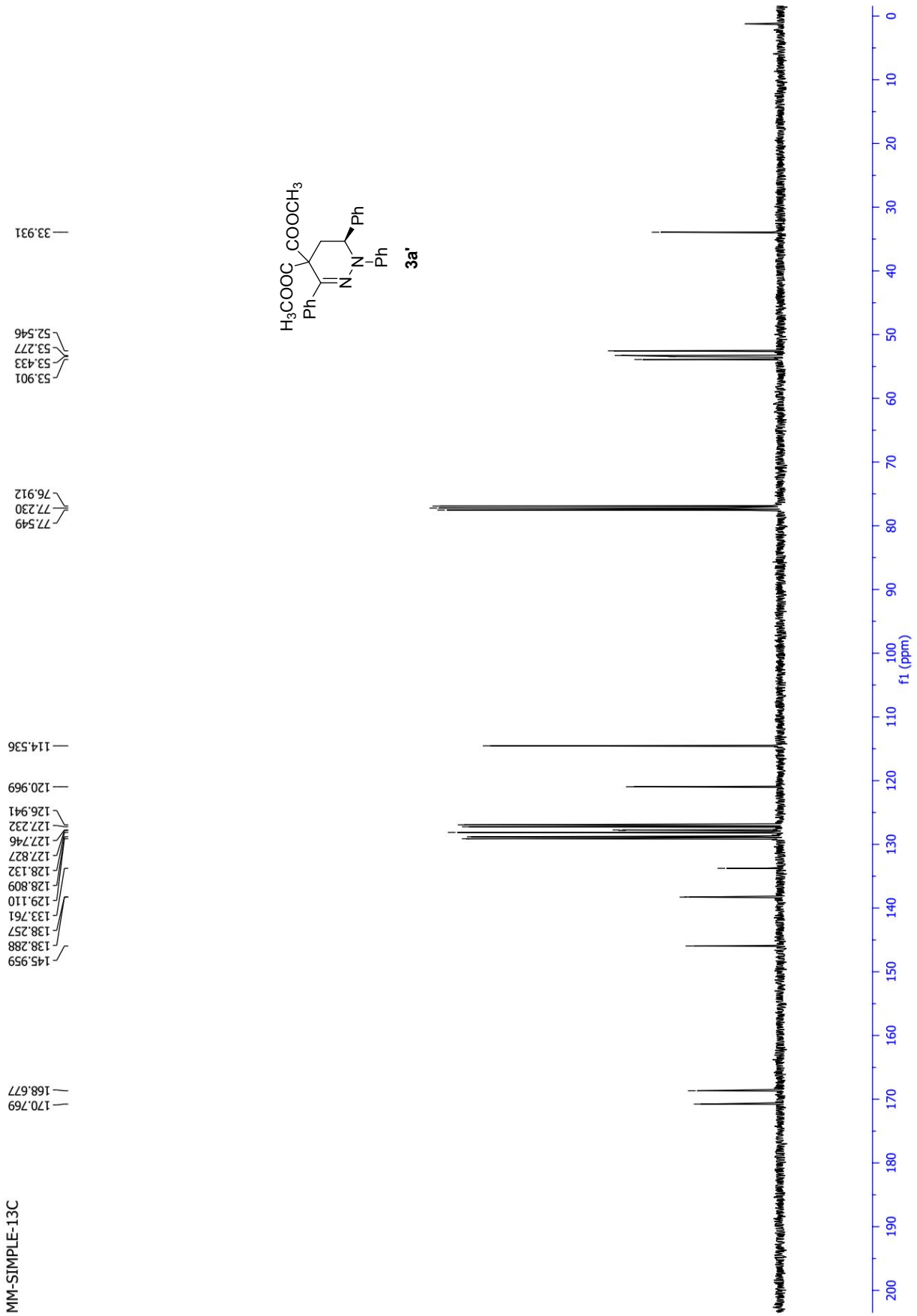
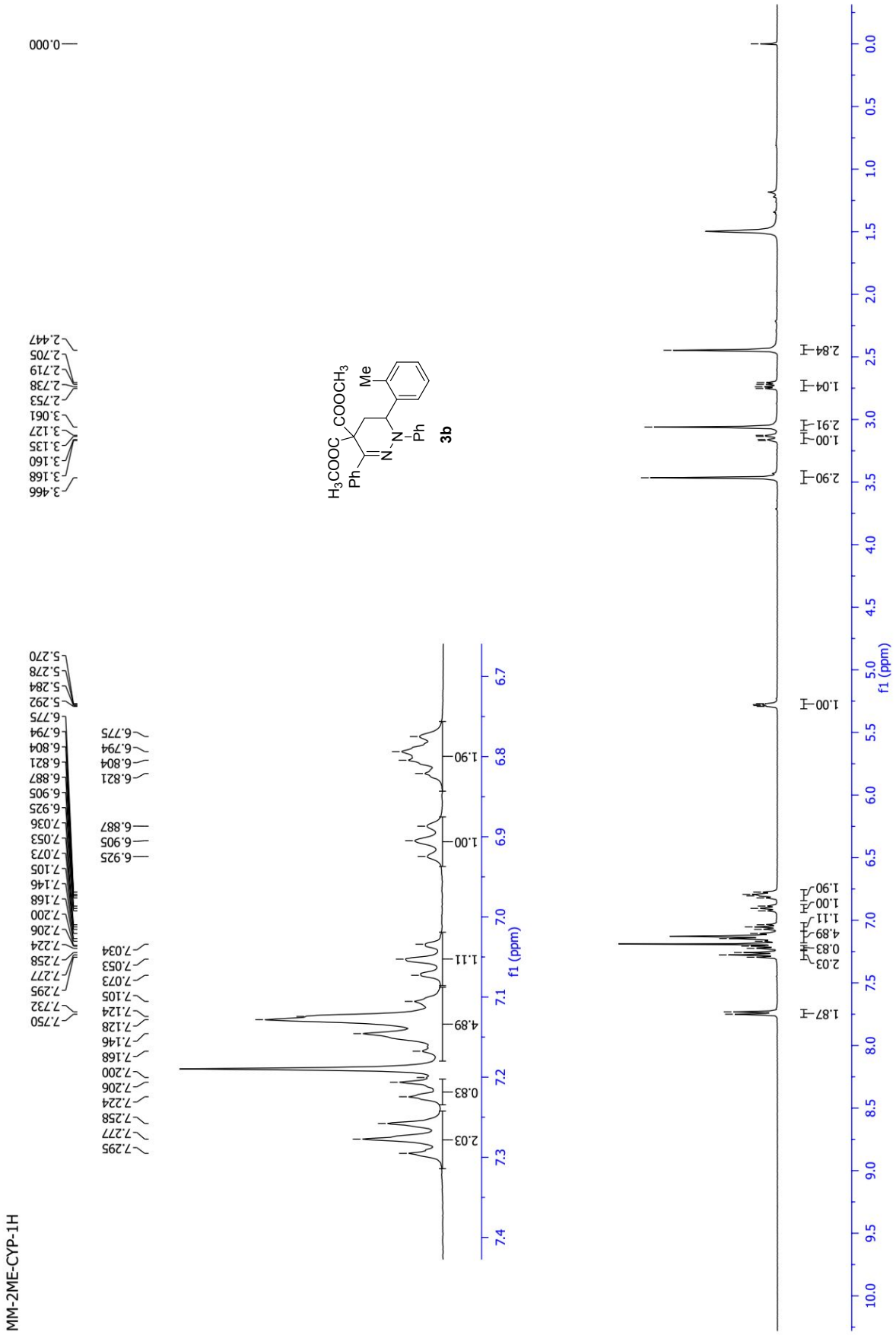
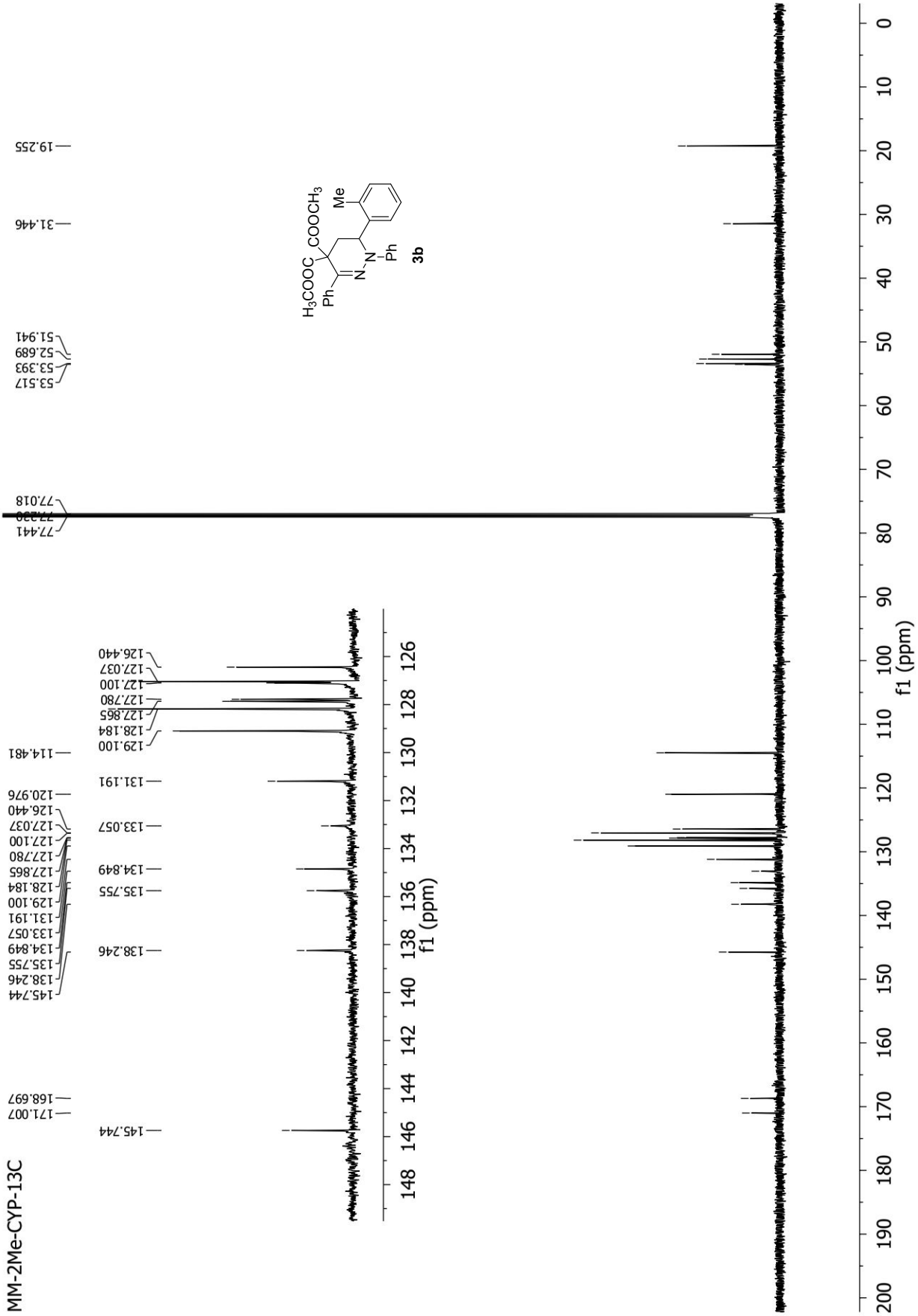
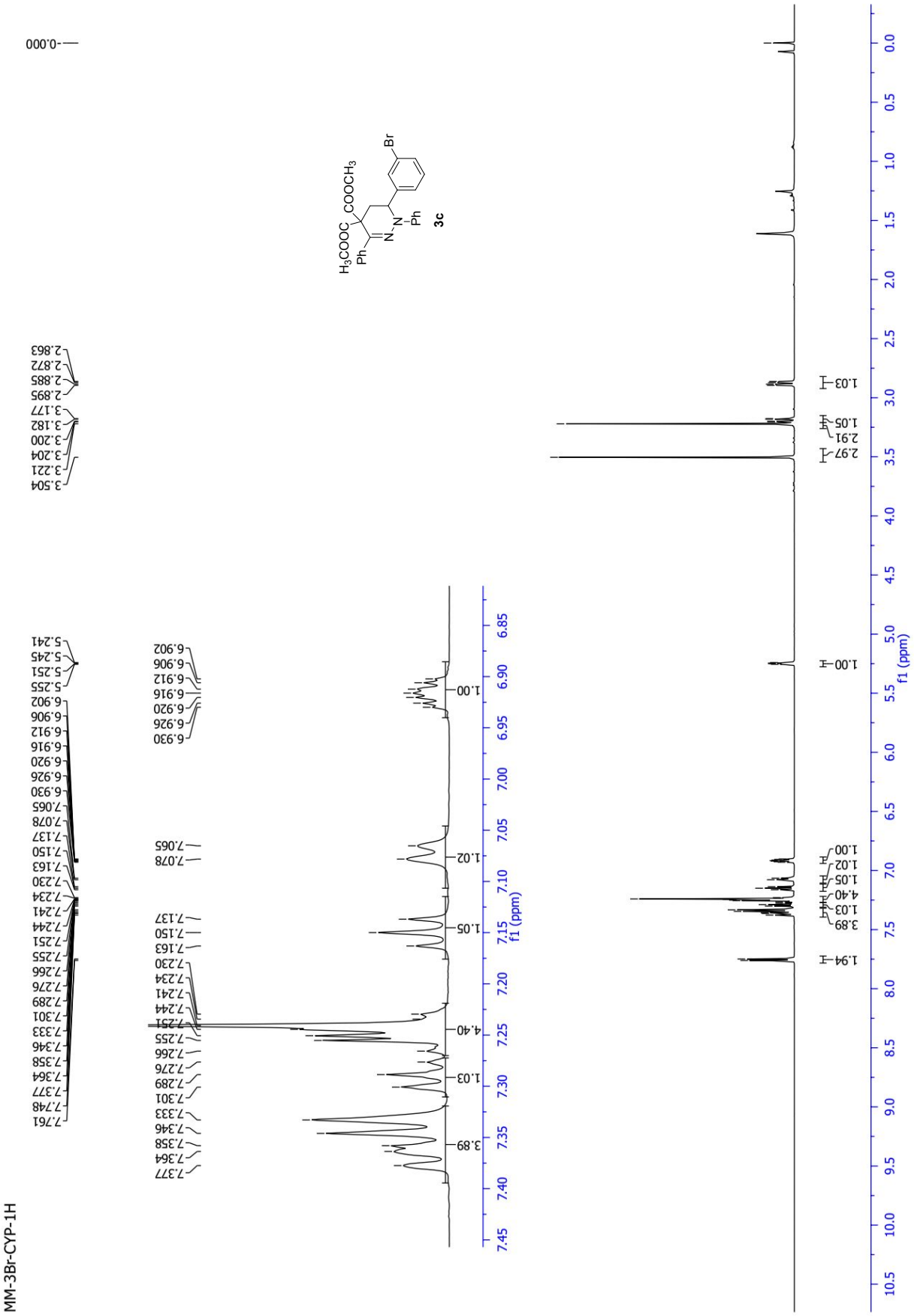
144.554
136.221
129.320
126.669
120.209
115.073
113.669
112.724
108.504
77.307
77.095
76.883
56.168
56.015
Br
MeO
MeO
N
NH
1r
f1 (ppm)

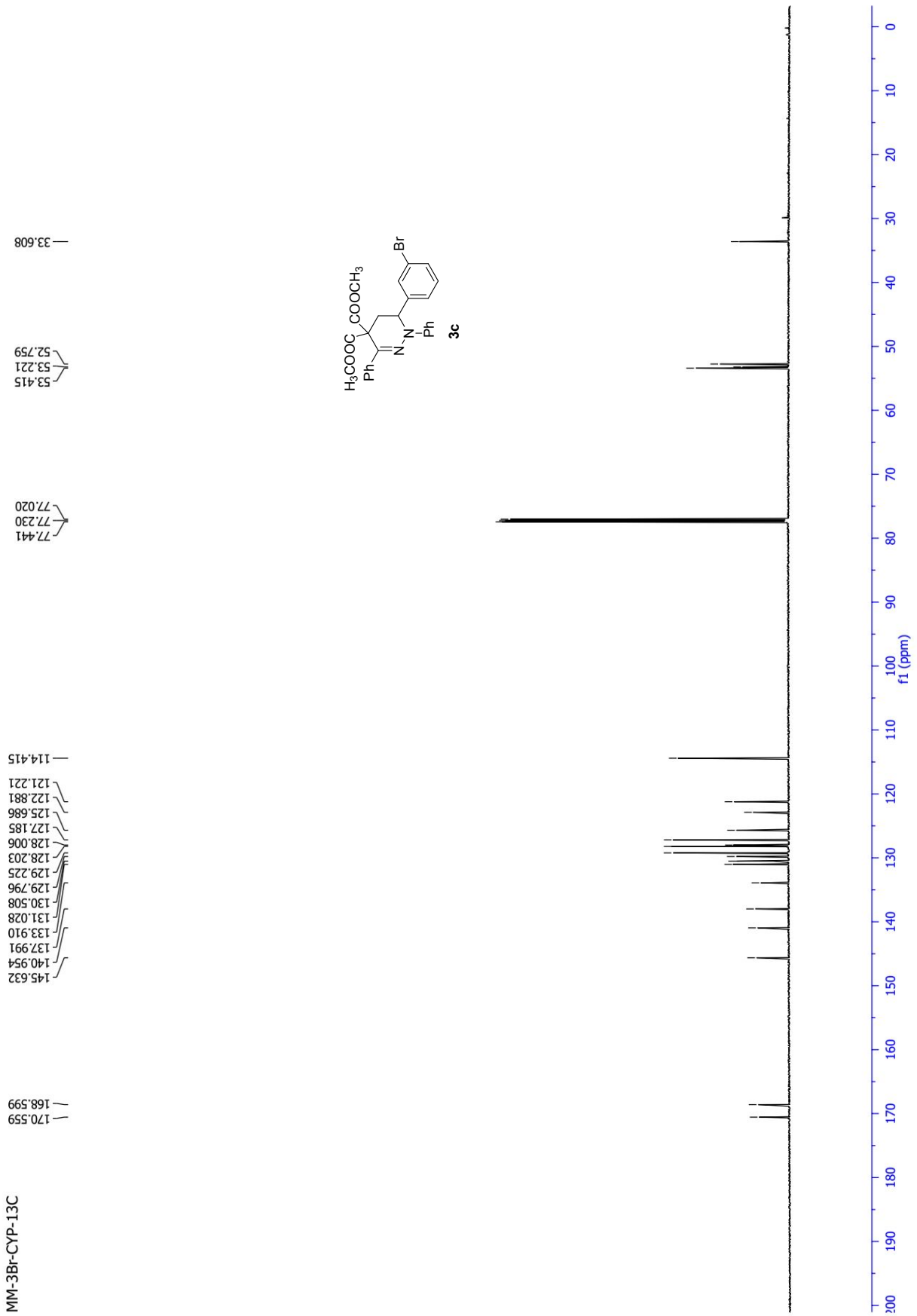

MM-SIM-HYD-1H
3a
f1 (ppm)


MM-SIMPLE-13C
170.769
168.677
145.959
138.288
138.257
133.761
129.110
128.809
128.132
127.827
127.746
127.232
126.941
120.969
114.536
77.549
77.230
76.912
53.901
53.433
53.277
52.546
33.931
H3COOC
COOCH3
Ph
N
N
Ph
Ph
3a'
f1 (ppm)


MM-2ME-CYP-1H
H3COOC
COOCH3
Ph
Ph
Me
3b
f1 (ppm)


MM-2Me-CYP-13C
145.744
171.007
168.697
145.744
138.246
135.755
134.849
133.057
131.191
129.100
128.184
127.865
127.780
127.100
127.037
126.440
120.976
114.481
77.441
77.230
77.018
53.517
53.393
52.689
51.941
31.446
19.255
f1 (ppm)
f1 (ppm)
H3COOC
COOCH3
Ph
Me
N
N
Ph
3b


MM-3Br-CYP-1H
3c
f1 (ppm)


MM-3Br-CYP-13C
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168.599
145.632
140.954
137.991
133.910
131.028
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128.006
127.185
125.686
122.881
121.221
114.415
77.441
77.230
77.020
53.415
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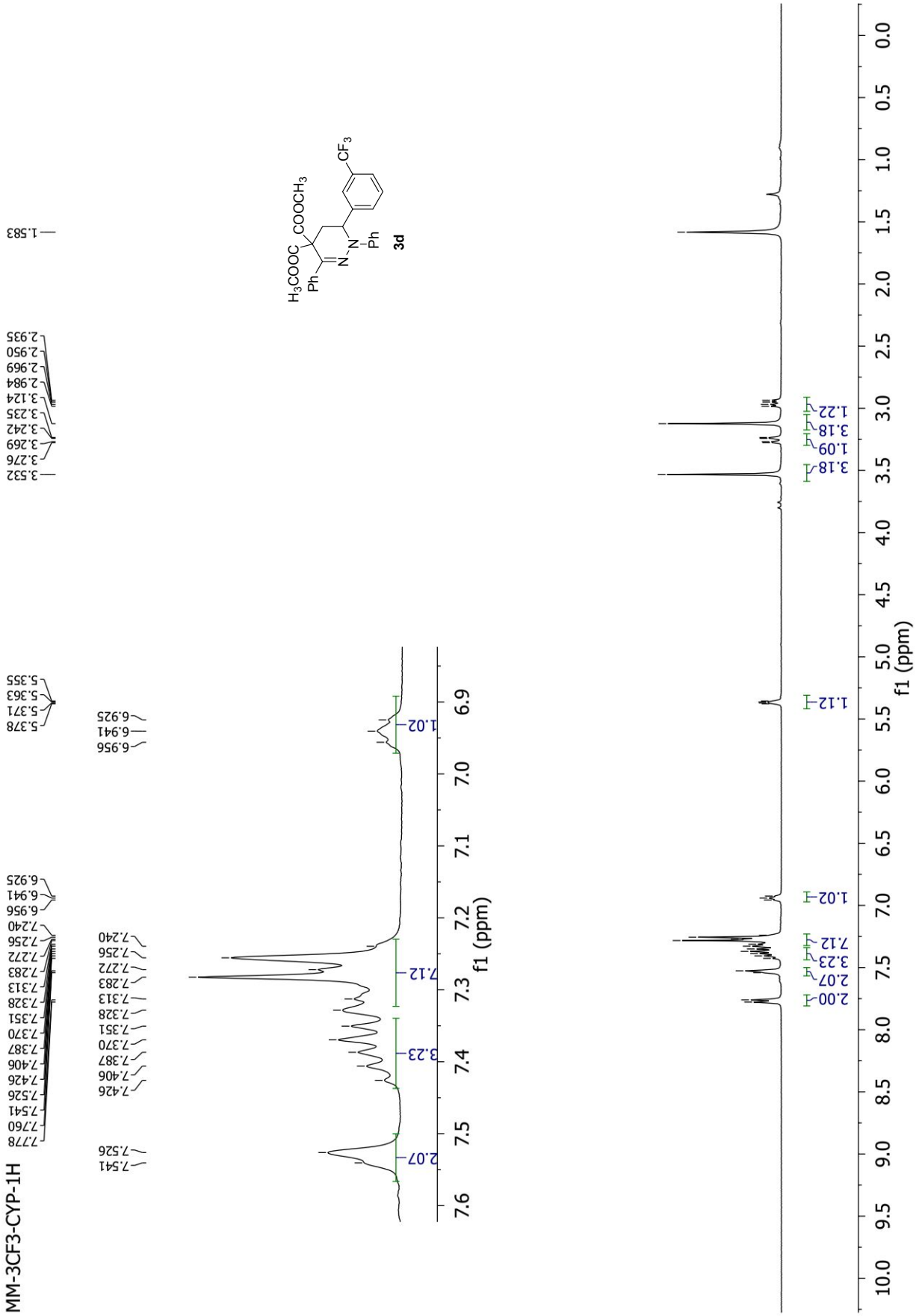
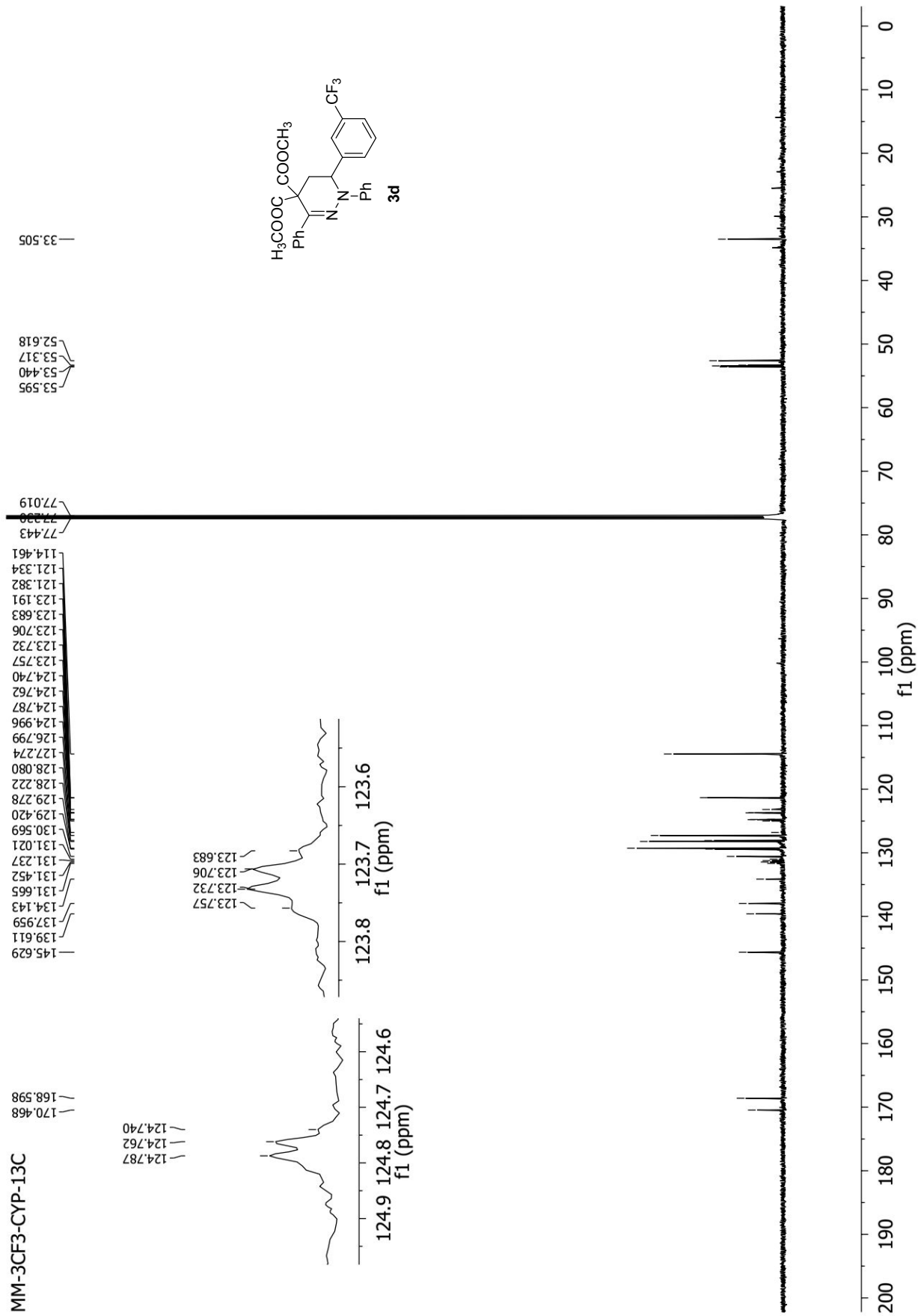
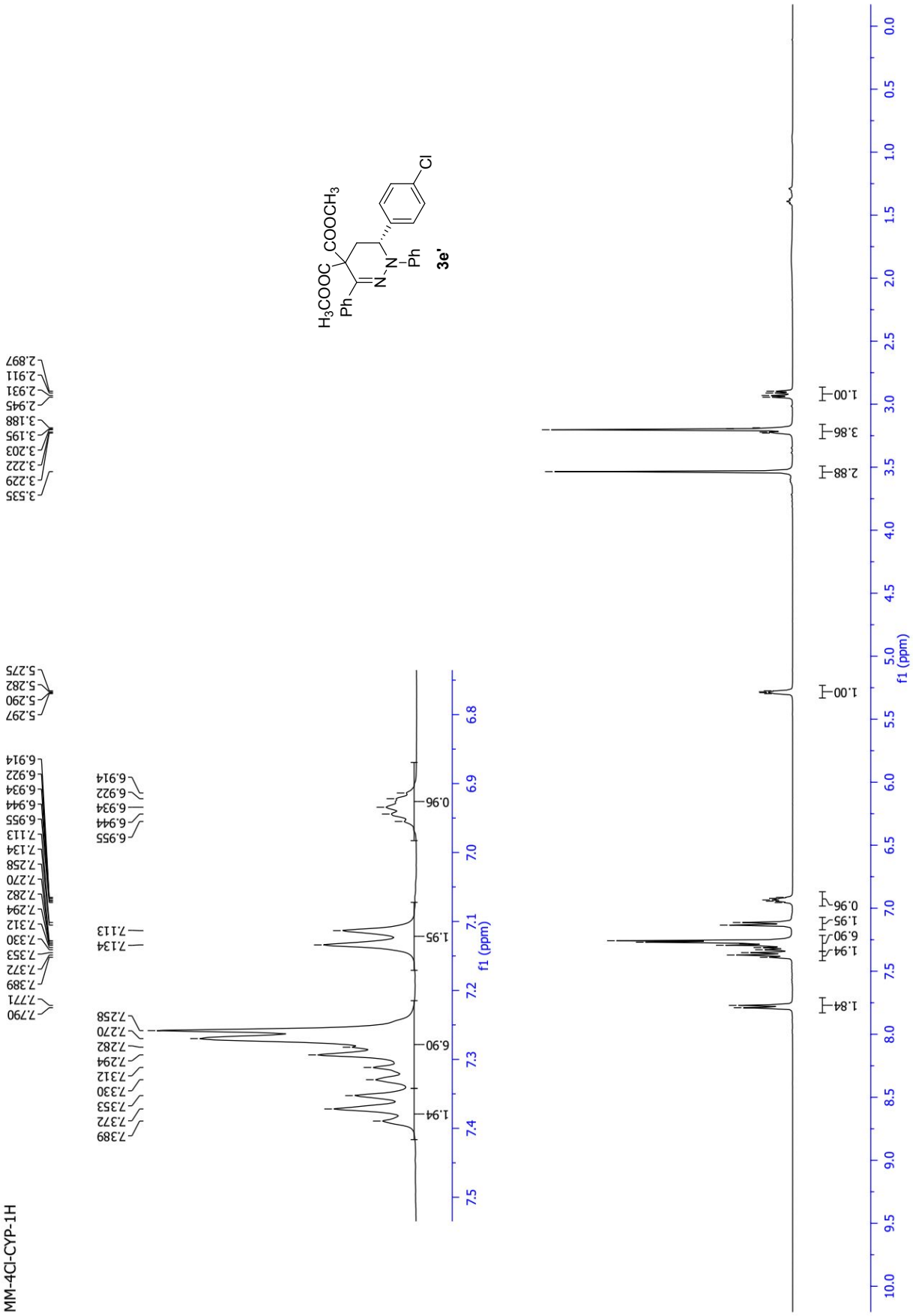
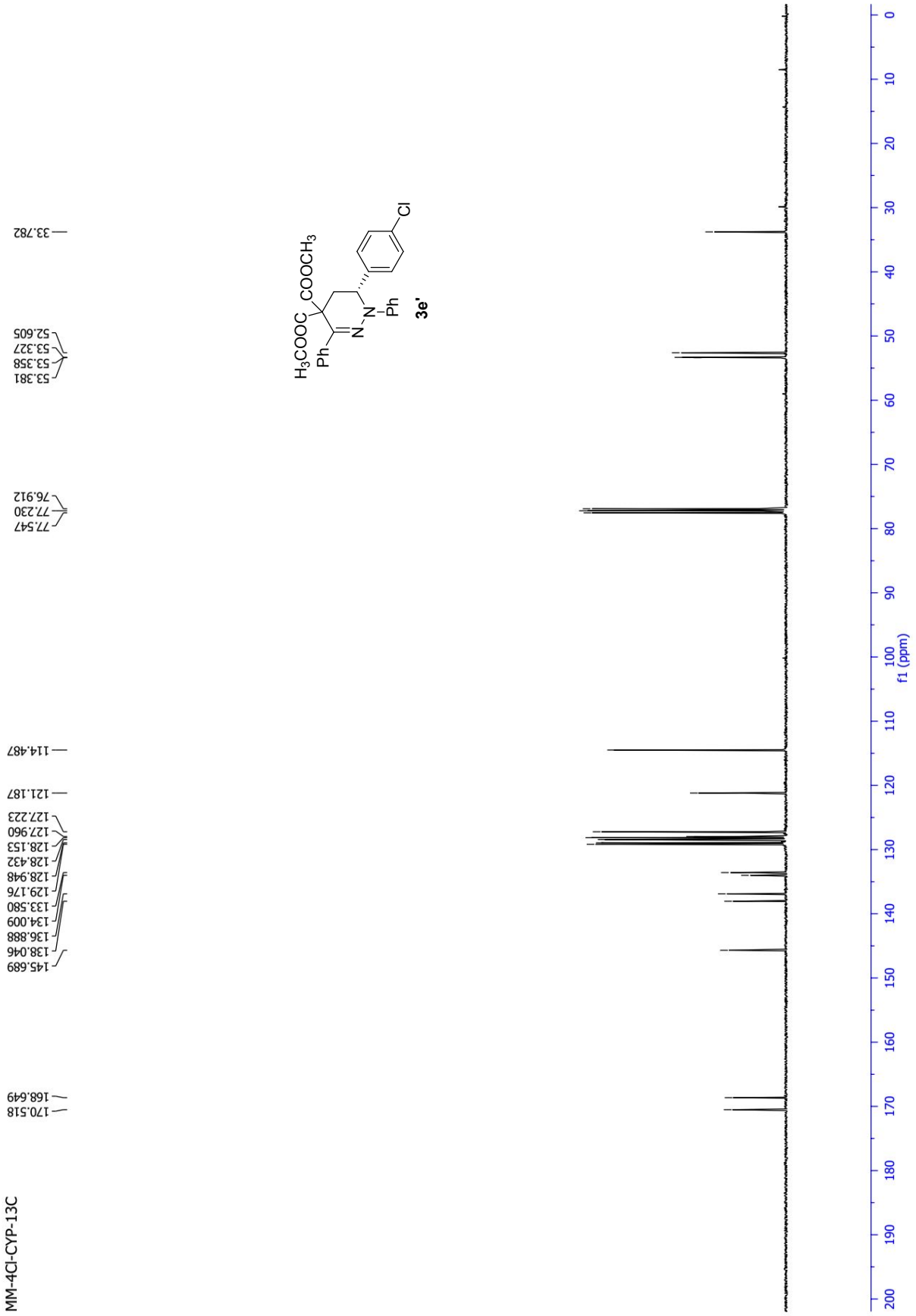
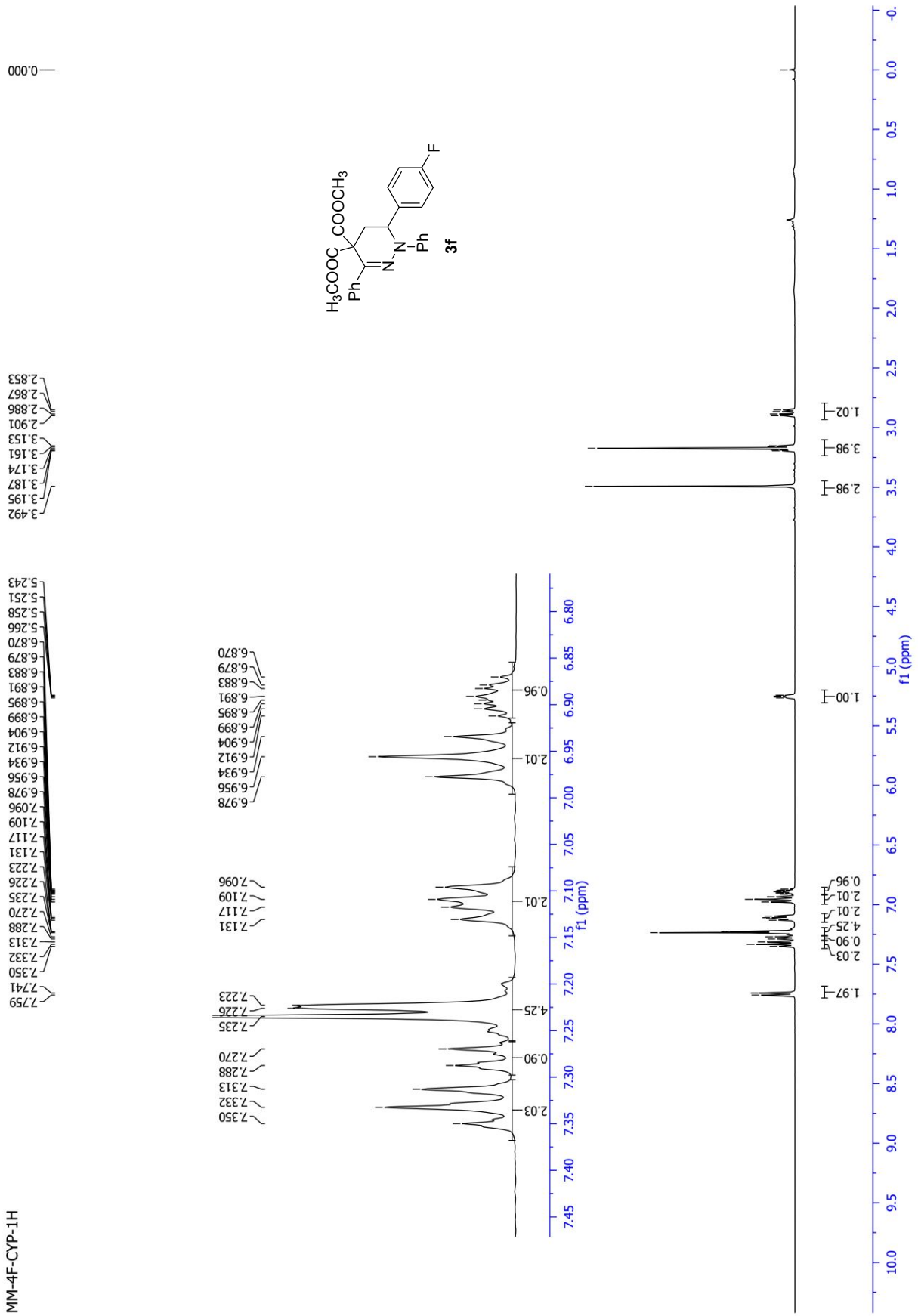
52.759
33.608
H3COOC
COOCH3
Ph
N
N
Ph
Br
3c
f1 (ppm)

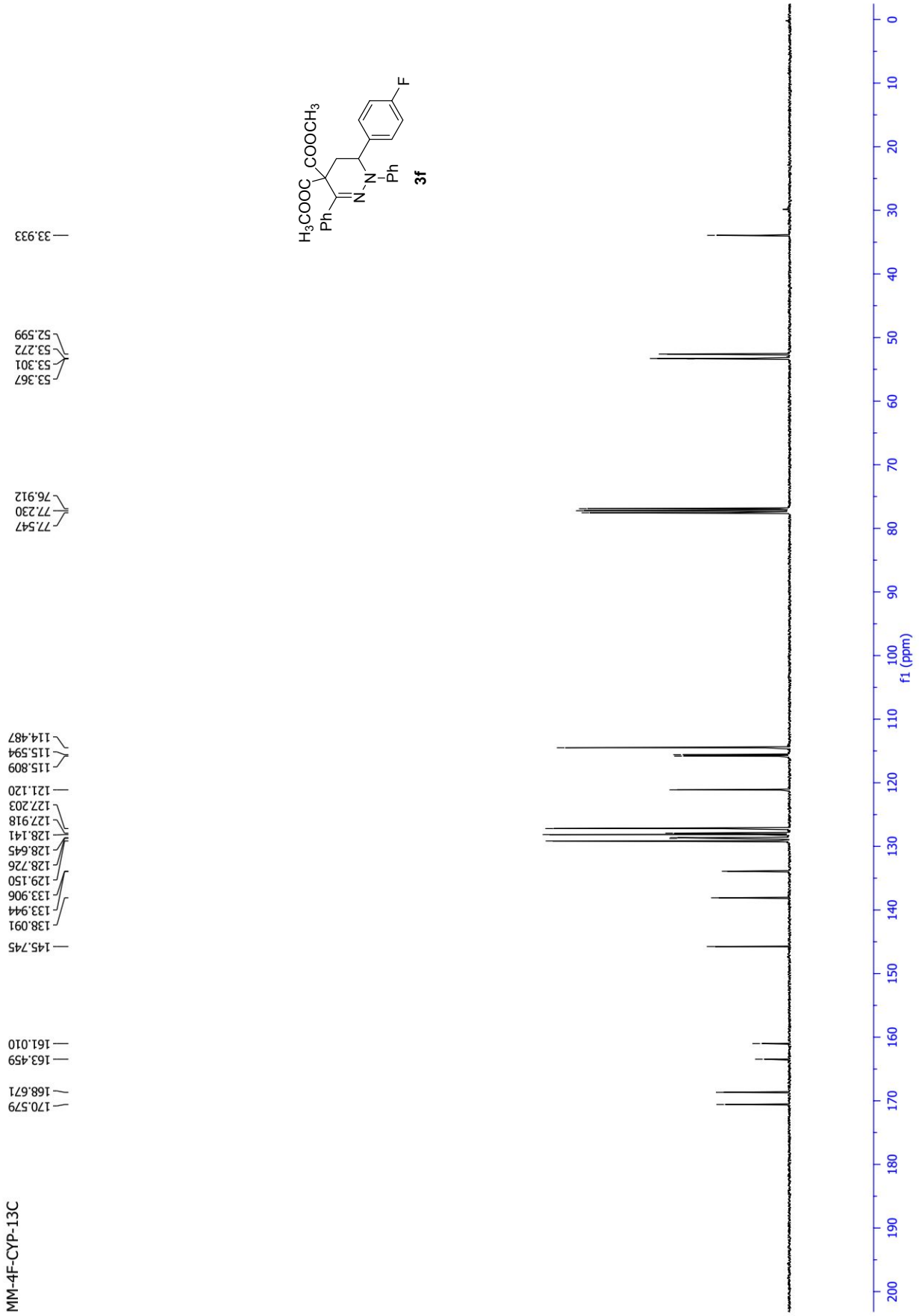

MM-3CF3-CYP-1H
H3COOC
COOCH3
Ph
N
N
Ph
CF3
3d
f1 (ppm)
f1 (ppm)

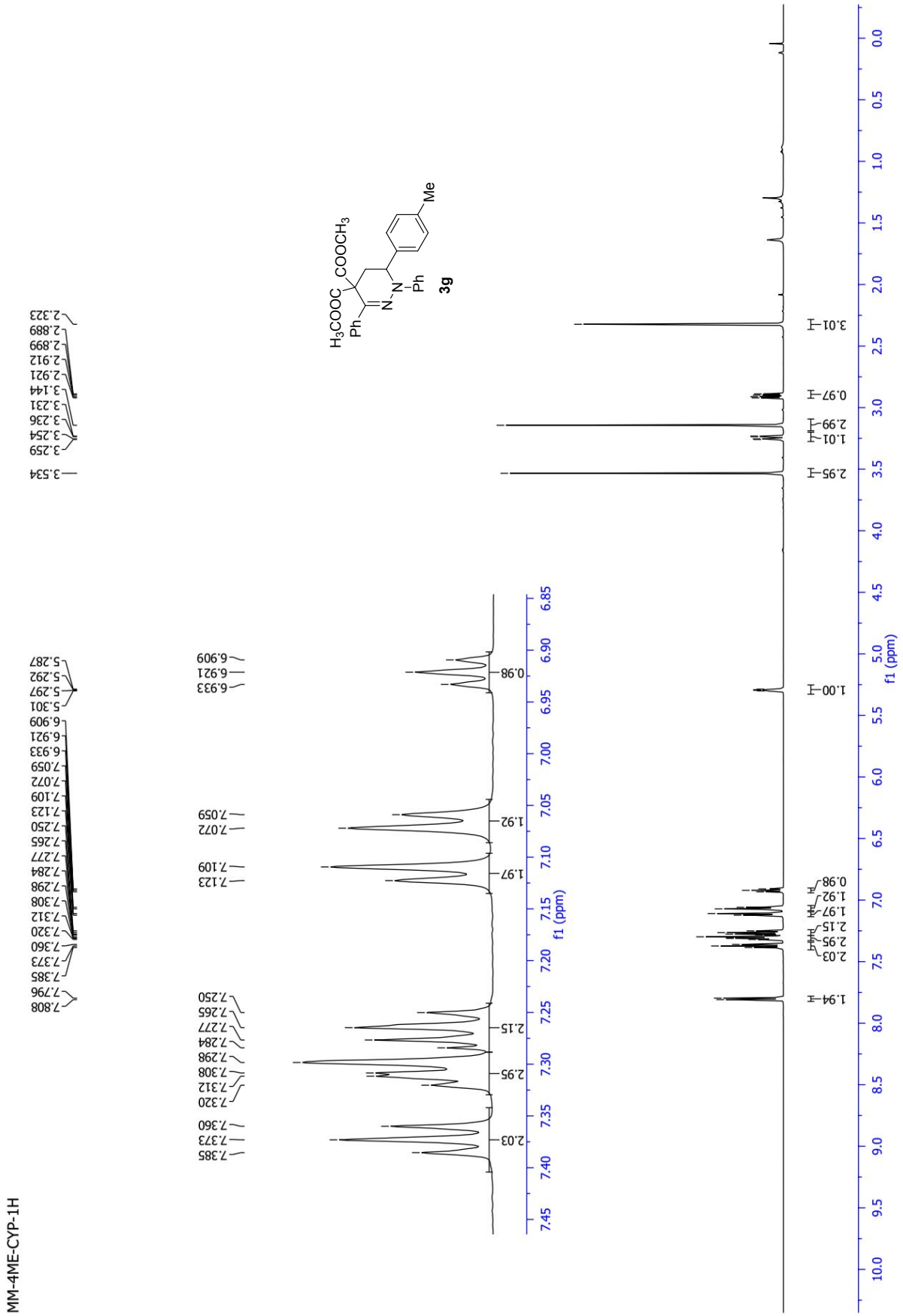

MM-3CF3-CYP-13C
170.468
168.598
124.787
124.762
124.740
145.629
139.611
137.959
134.143
131.665
131.452
131.237
131.021
130.569
129.420
129.278
128.222
128.080
127.274
126.799
124.996
124.787
124.762
124.740
123.757
123.732
123.706
123.683
123.191
121.382
121.334
114.461
77.443
77.230
77.019
53.595
53.440
53.317
52.618
33.505
124.9
124.8
124.7
124.6
f1 (ppm)
123.8
123.7
123.6
f1 (ppm)
f1 (ppm)
3d


MM-4Cl-CYP-1H
H3COOC
COOCH3
Ph
N
N
Ph
Cl
3e'
f1 (ppm)

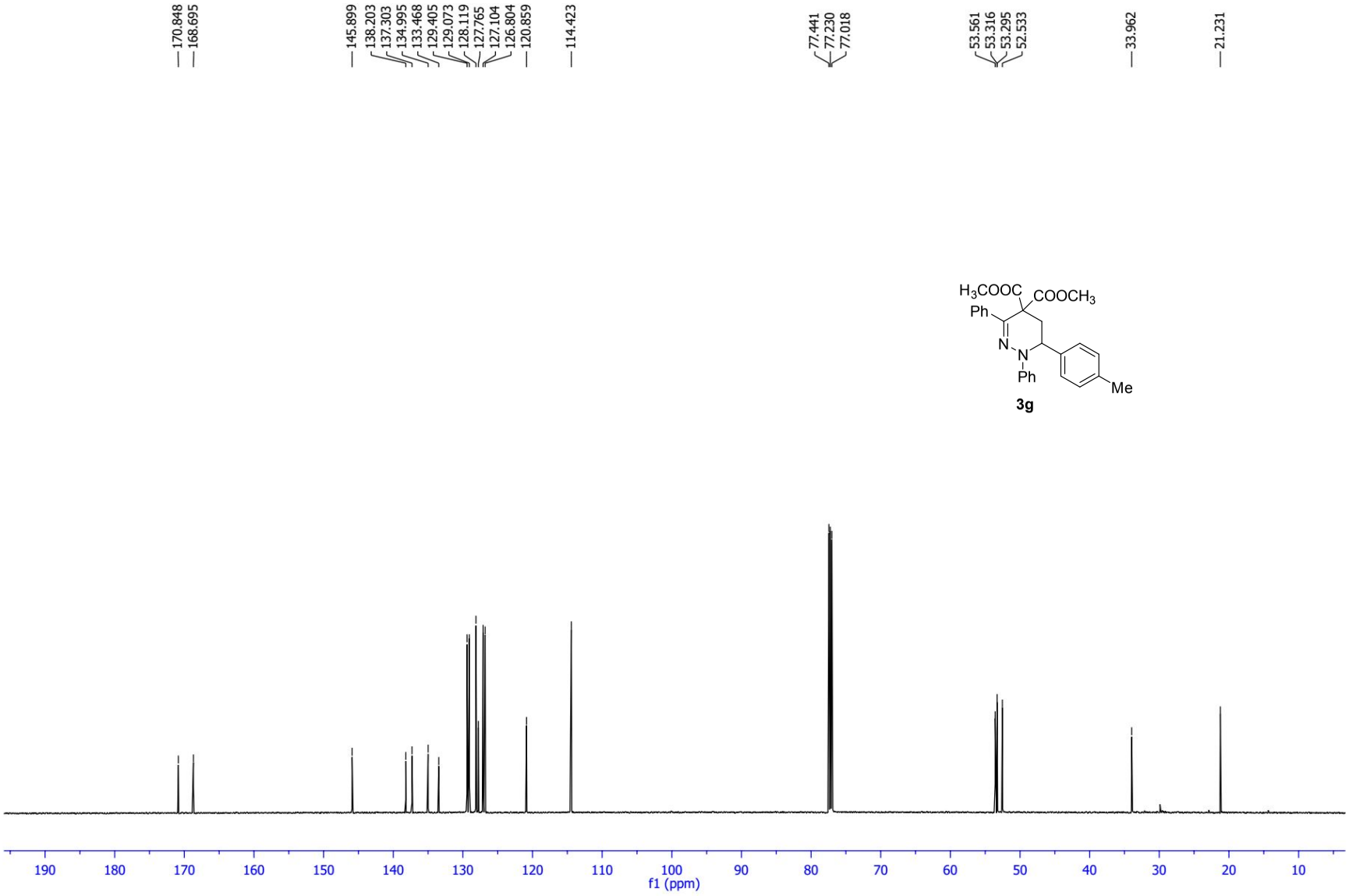

MM-4Cl-CYP-13C
170.518
168.649
145.689
138.046
136.888
134.009
133.580
129.176
128.948
128.432
128.153
127.960
127.223
121.187
114.487
77.547
77.230
76.912
53.381
53.358
53.327
52.605
33.782
H3COOC
COOCH3
Ph
N
N
Ph
Cl
3e'
f1 (ppm)

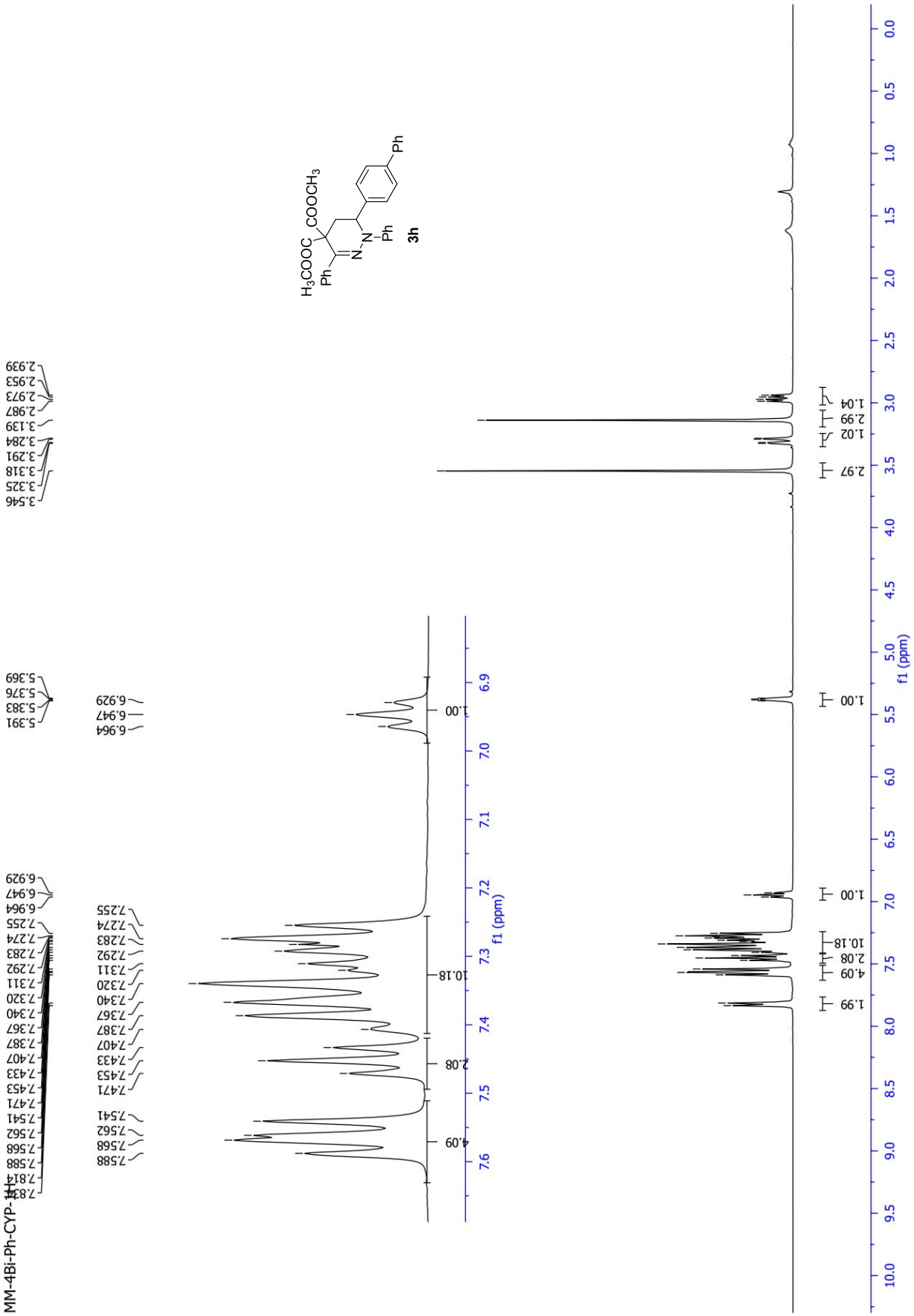

MM-4F-CYP-1H
3f
f1 (ppm)

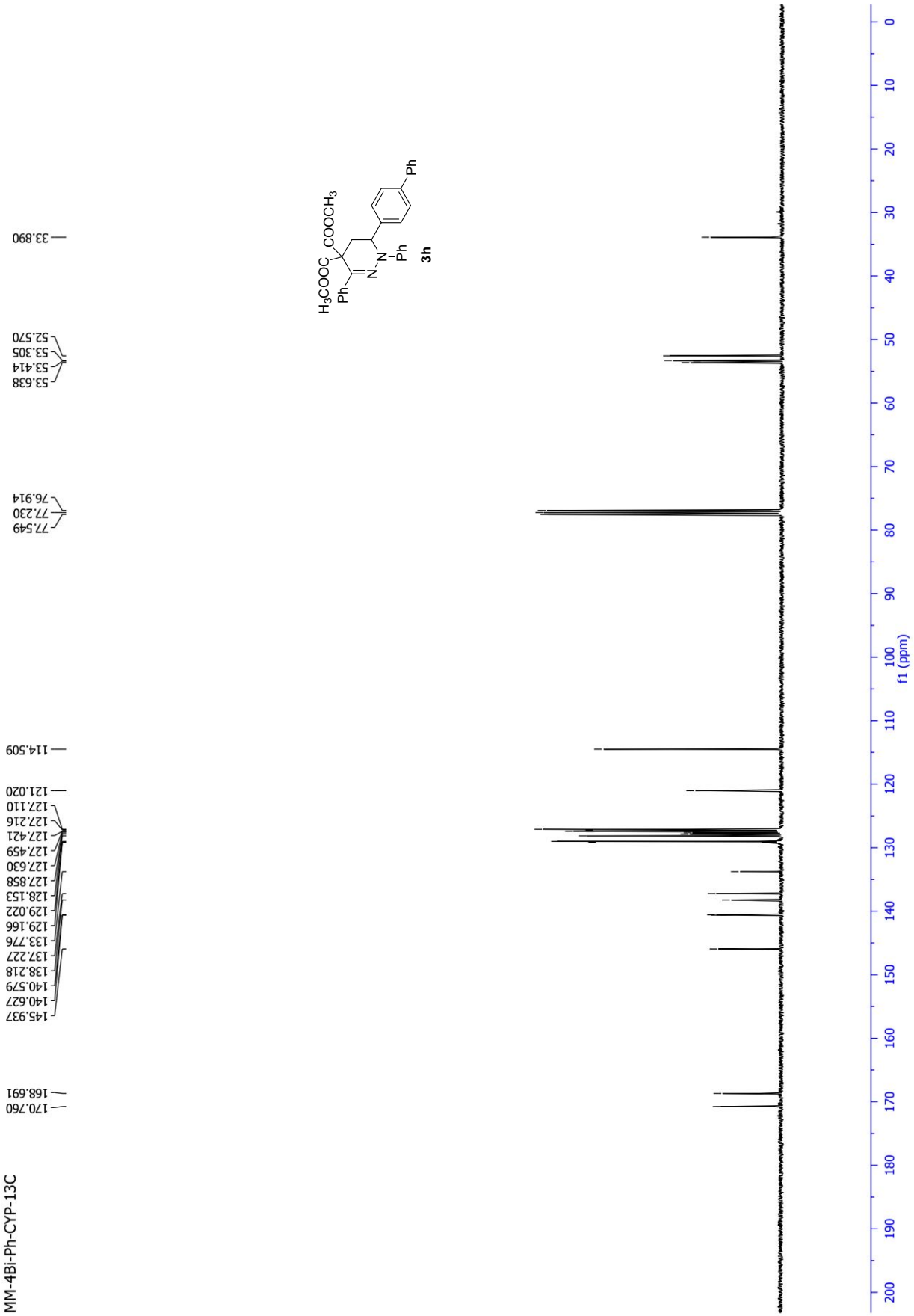

MM-4F-CYP-13C
170.579
168.671
163.459
161.010
145.745
138.091
133.944
133.906
129.150
128.726
128.645
128.141
127.918
127.203
121.120
115.809
115.594
114.487
77.547
77.230
76.912
53.367
53.301
53.272
52.599
33.933
H3COOC
COOCH3
Ph
N
N
Ph
F
3f
f1 (ppm)

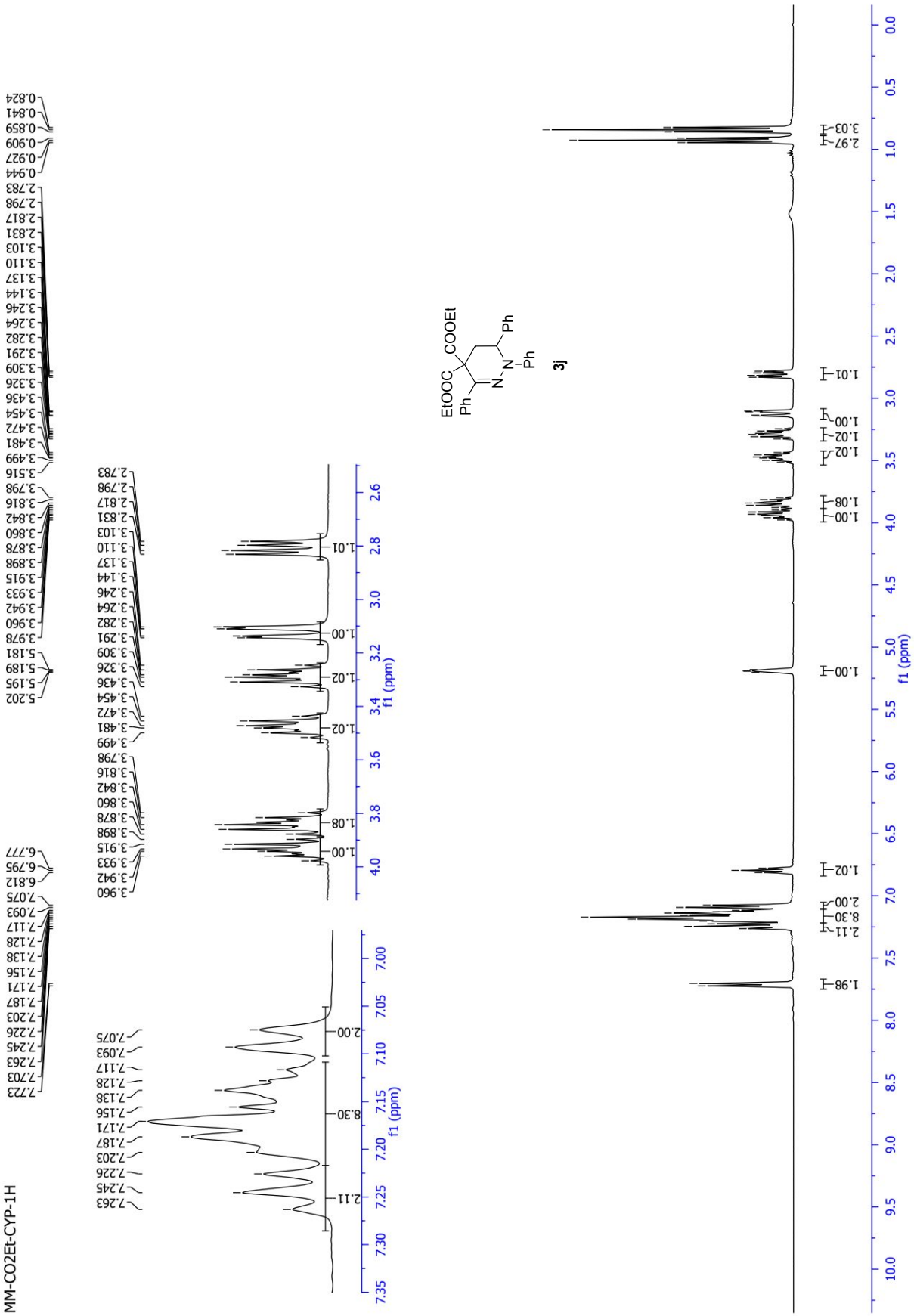

MM-4ME-CYP-1H
3g
f1 (ppm)

MM-4ME-CYP-13C

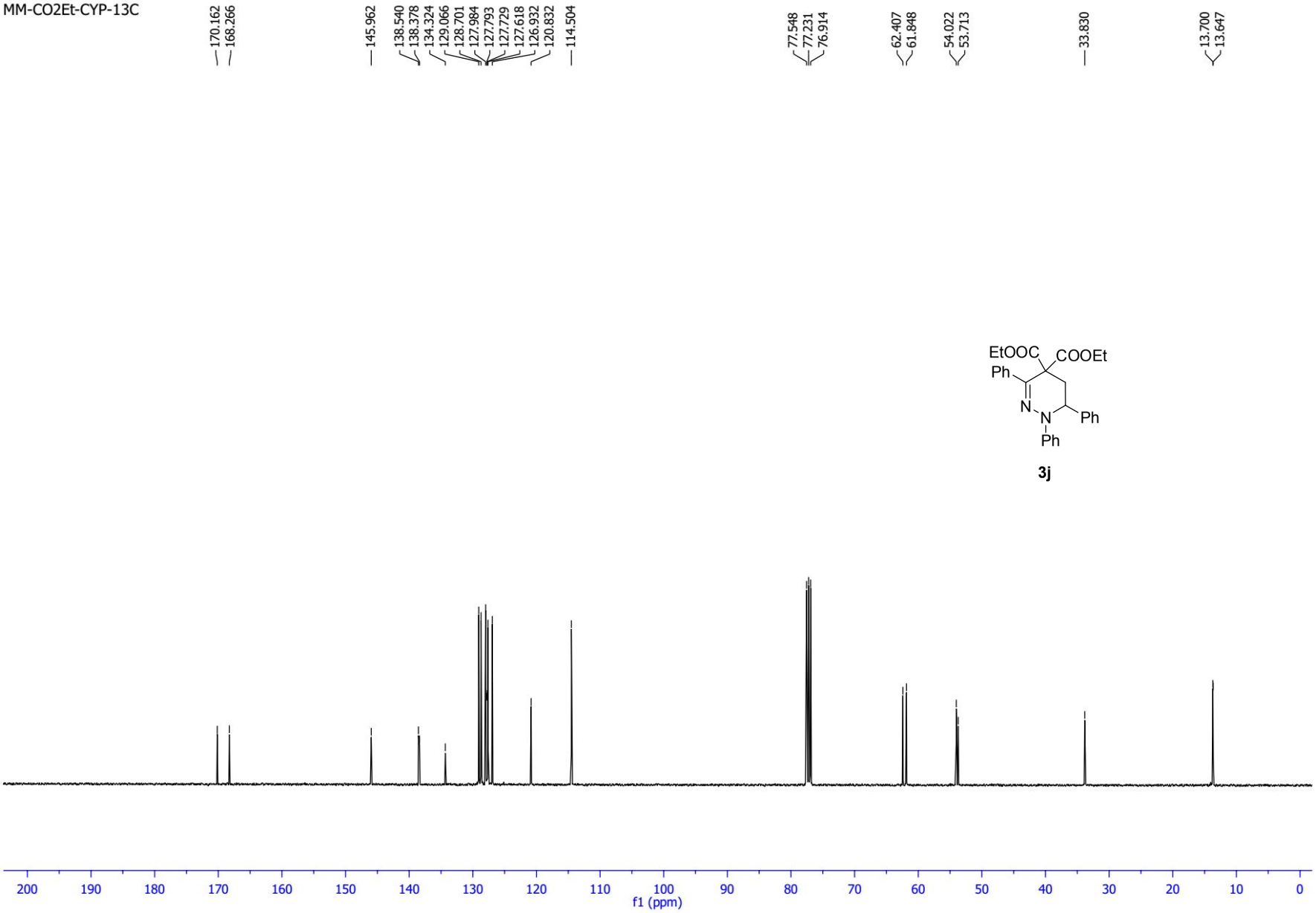



MM-4Bi-Ph-CYP-1H
3h
f1 (ppm)

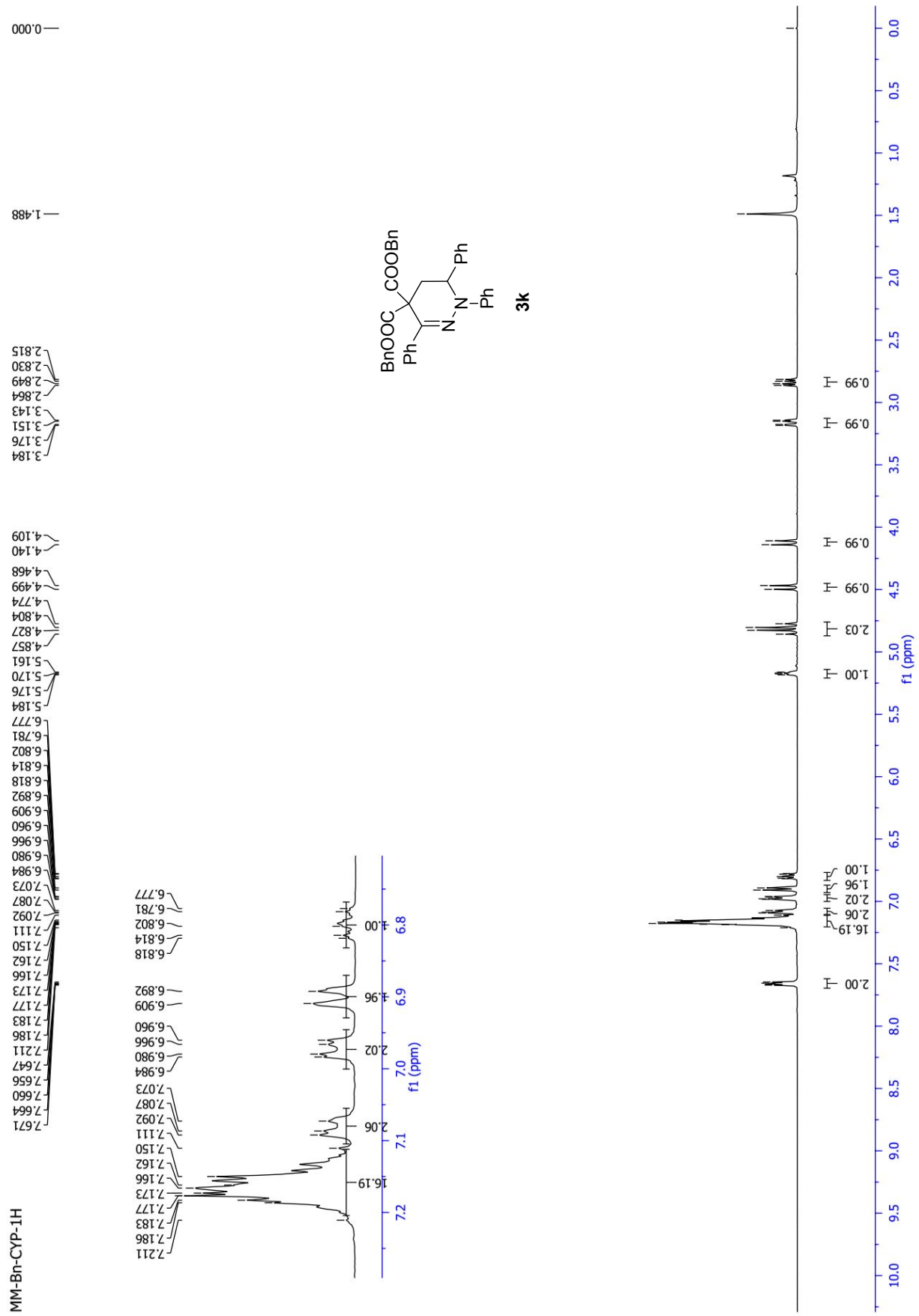

MM-4Bi-Ph-CYP-13C
170.760
168.691
145.937
140.627
140.579
138.218
137.227
133.776
129.166
129.022
128.153
127.858
127.630
127.459
127.421
127.216
127.110
121.020
114.509
77.549
77.230
76.914
53.638
53.414
53.305
52.570
33.890
H3COOC
COOCH3
Ph
N
N
Ph
Ph
3h
f1 (ppm)

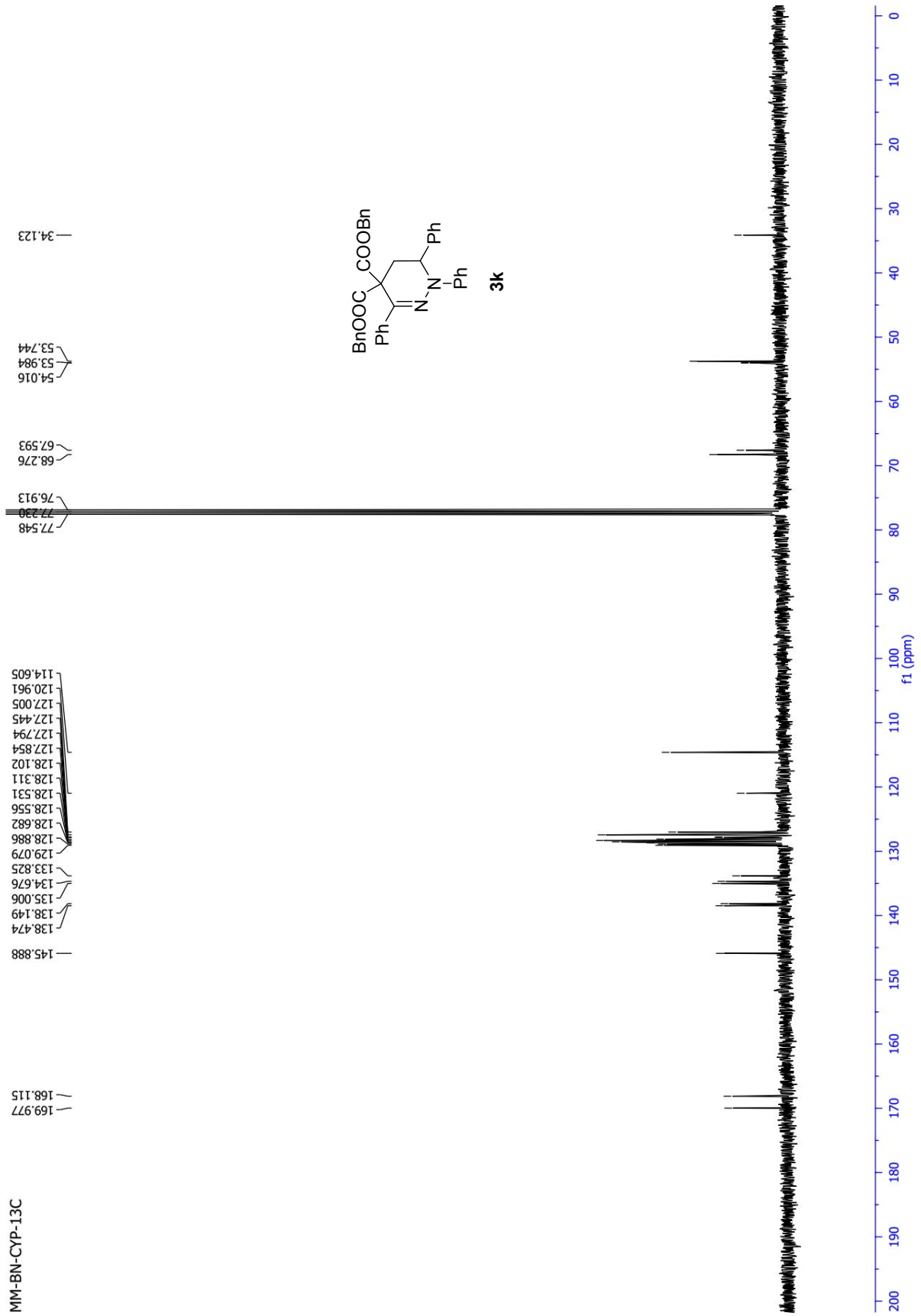

MM-CO2Et-CYP-1H
EtOOC
COOEt
Ph
Ph
Ph
Ph
3j
f1 (ppm)

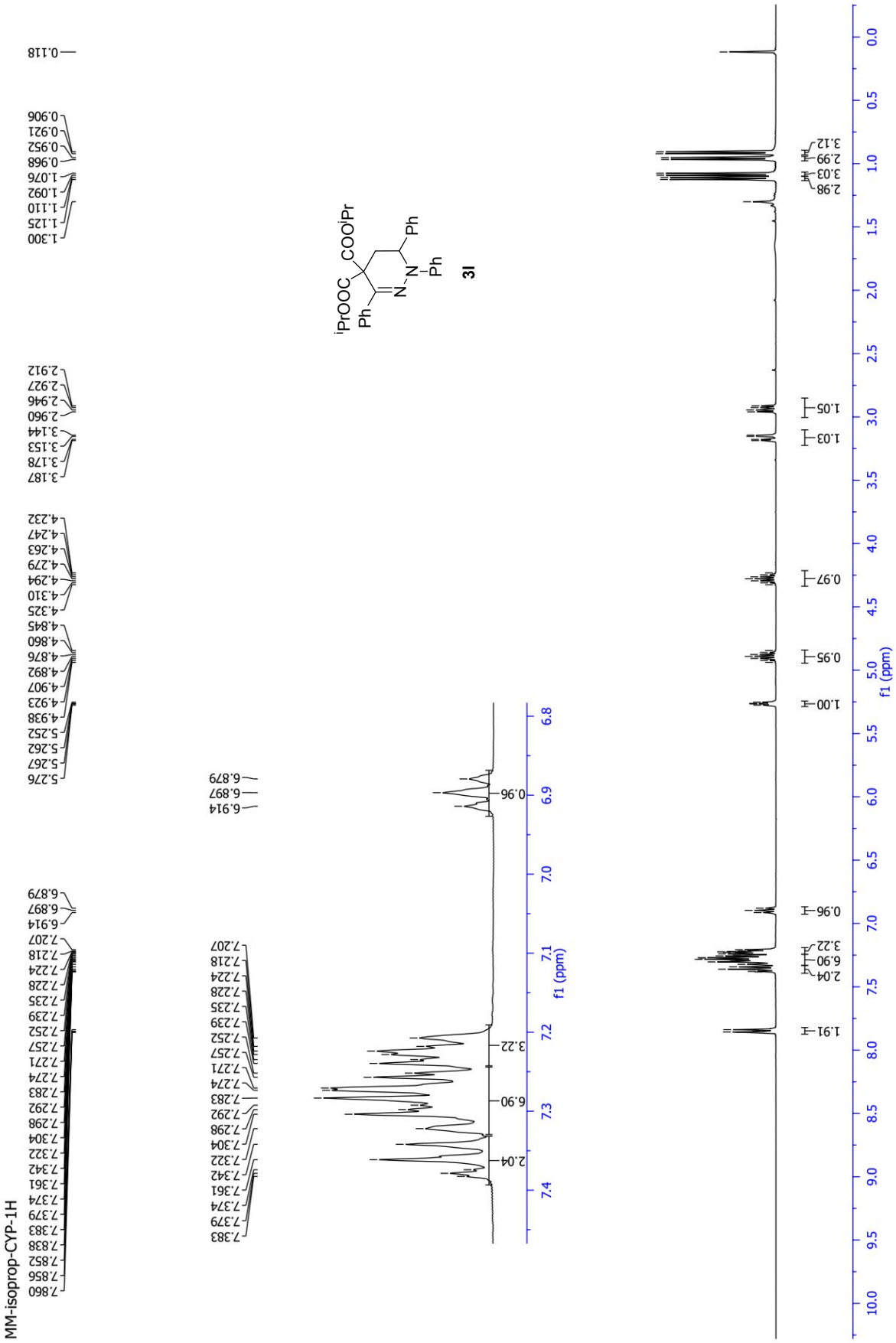
MM-CO2Et-CYP-13C



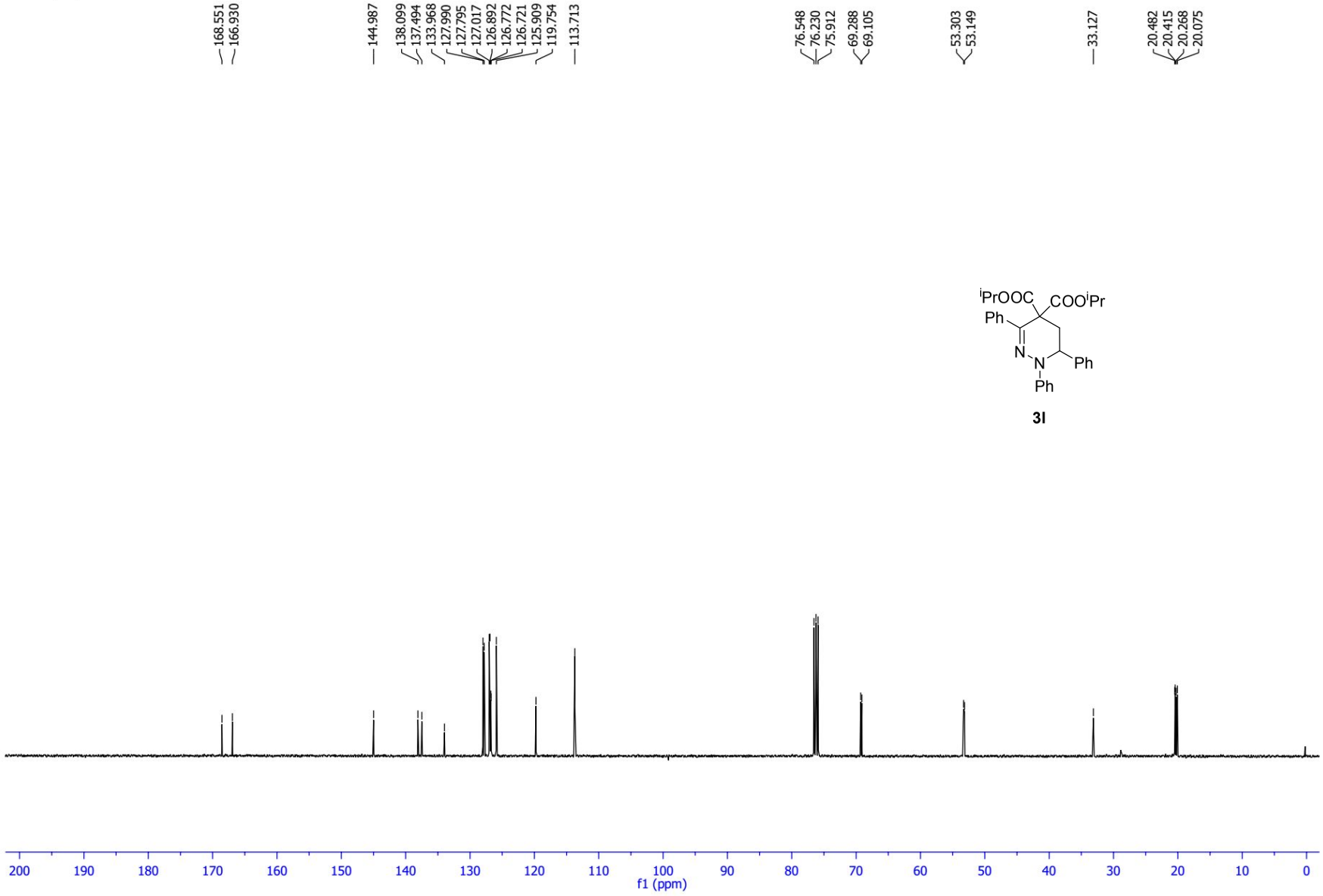
3j


MM-Bn-CYP-1H
BnOOC
COOBn
Ph
N
N
Ph
Ph
3k
f1 (ppm)

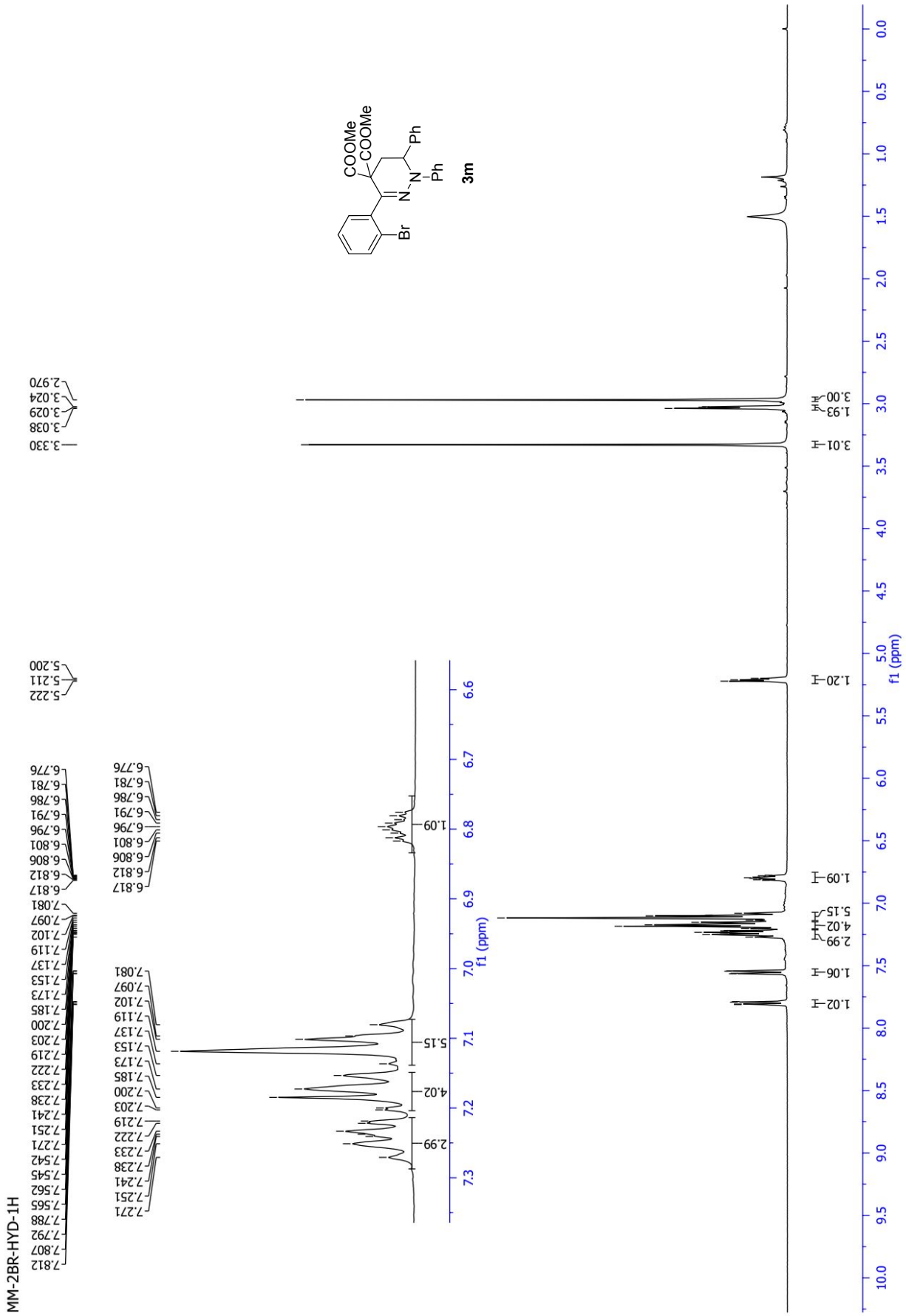

MM-BN-CYP-13C
169.977
168.115
145.888
138.474
138.149
135.006
134.676
133.825
129.079
128.886
128.682
128.556
128.531
128.311
128.102
127.854
127.794
127.445
127.005
120.961
114.605
77.548
77.230
76.913
68.276
67.593
54.016
53.984
53.744
34.123
BnOOC
COOBn
Ph
N
N
Ph
Ph
3k
f1 (ppm)

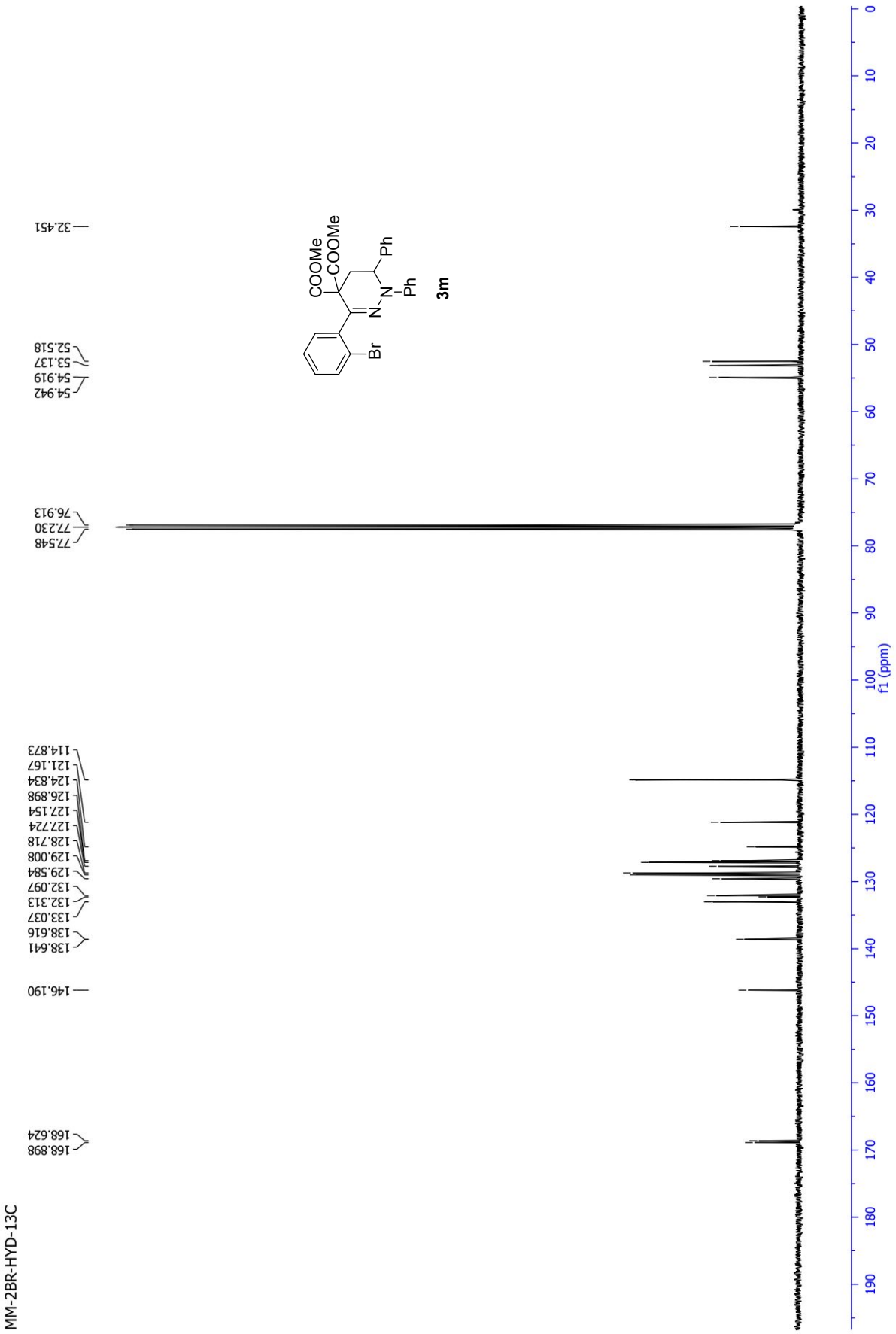

MM-isoprop-CYP-1H
7.860
7.856
7.852
7.838
7.383
7.379
7.374
7.361
7.342
7.322
7.304
7.298
7.292
7.283
7.274
7.271
7.257
7.252
7.239
7.235
7.228
7.224
7.218
7.207
6.914
6.897
6.879
5.276
5.267
5.262
5.252
4.938
4.923
4.907
4.892
4.876
4.860
4.845
4.325
4.310
4.294
4.279
4.263
4.247
4.232
3.187
3.178
3.153
3.144
2.960
2.946
2.927
2.912
1.300
1.125
1.110
1.092
1.076
0.968
0.952
0.921
0.906
0.118
iPrOOC
COOiPr
Ph
Ph
Ph
3l
f1 (ppm)
1.91
2.04
6.90
3.22
0.96
1.00
0.95
0.97
1.05
1.03
2.98
3.03
2.99
3.12

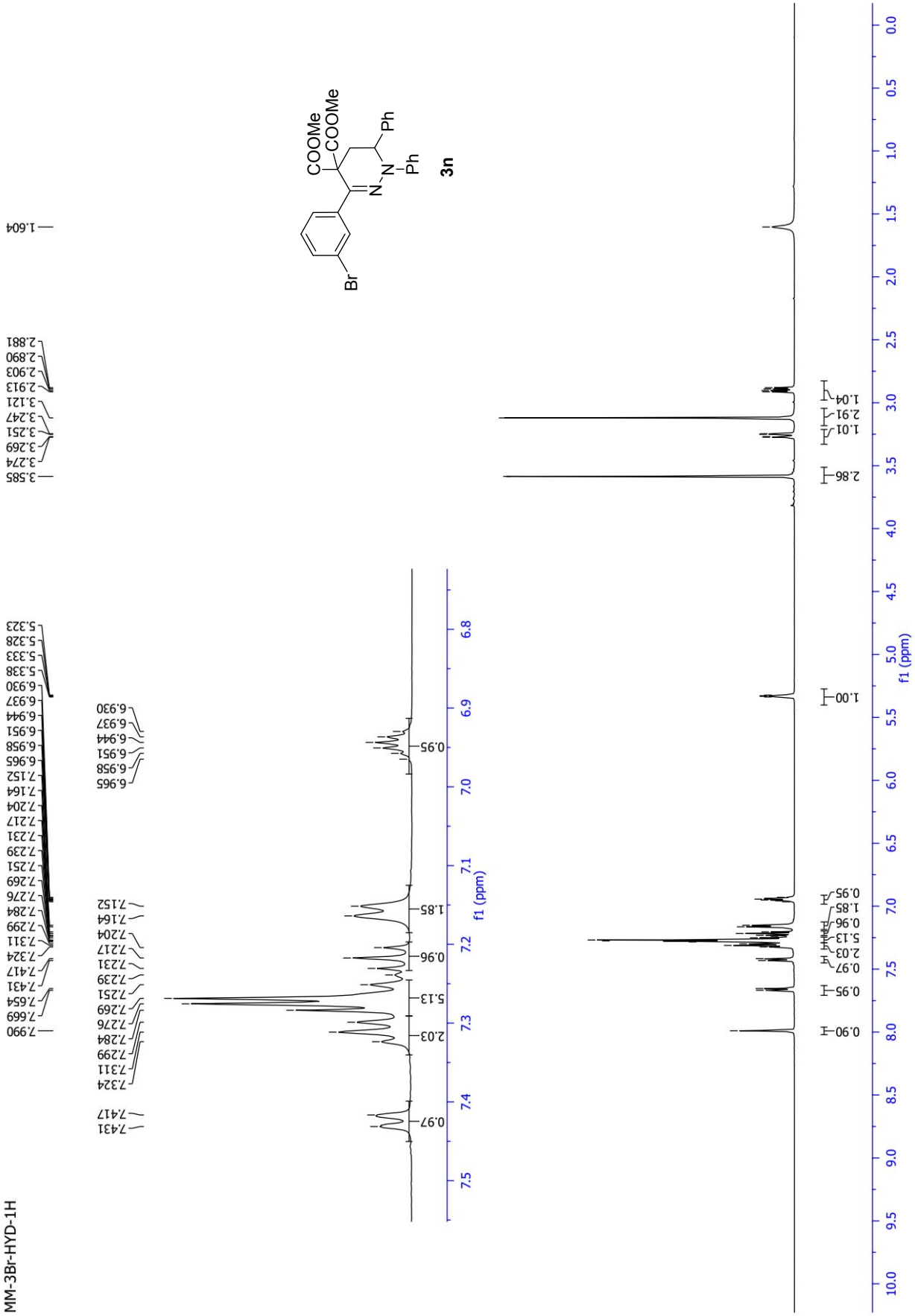
MM-isoprop-CYP-13C

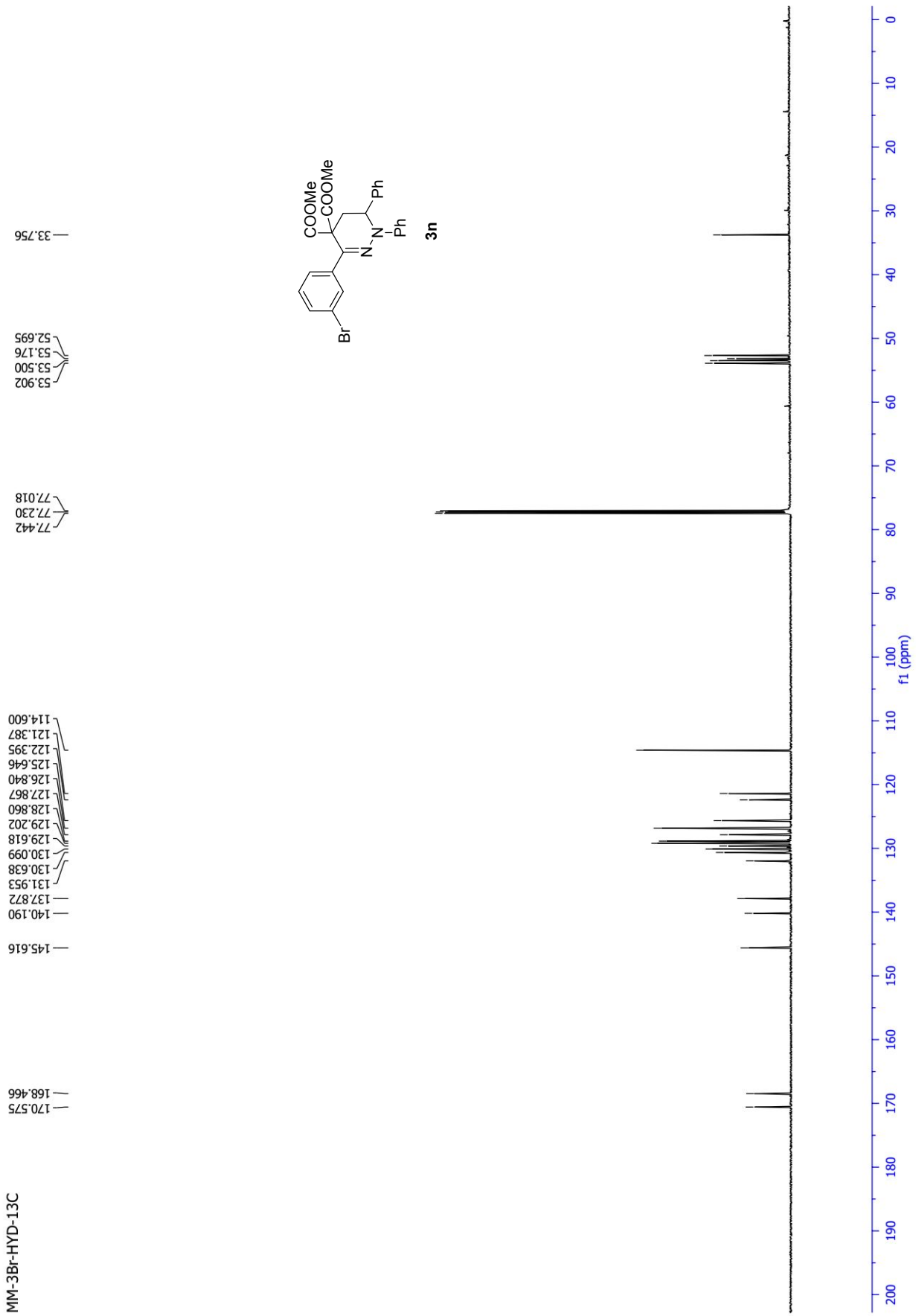


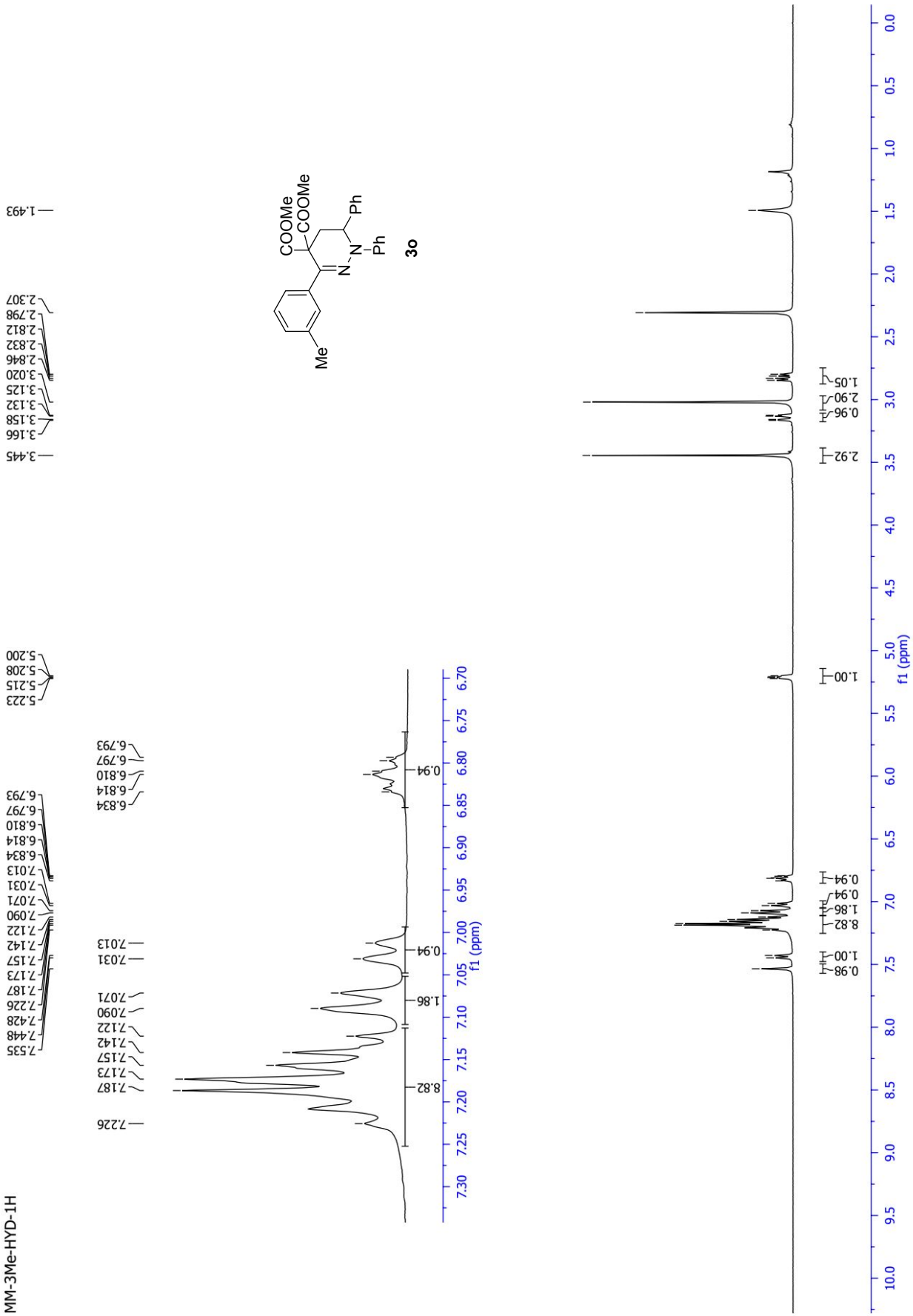
3l

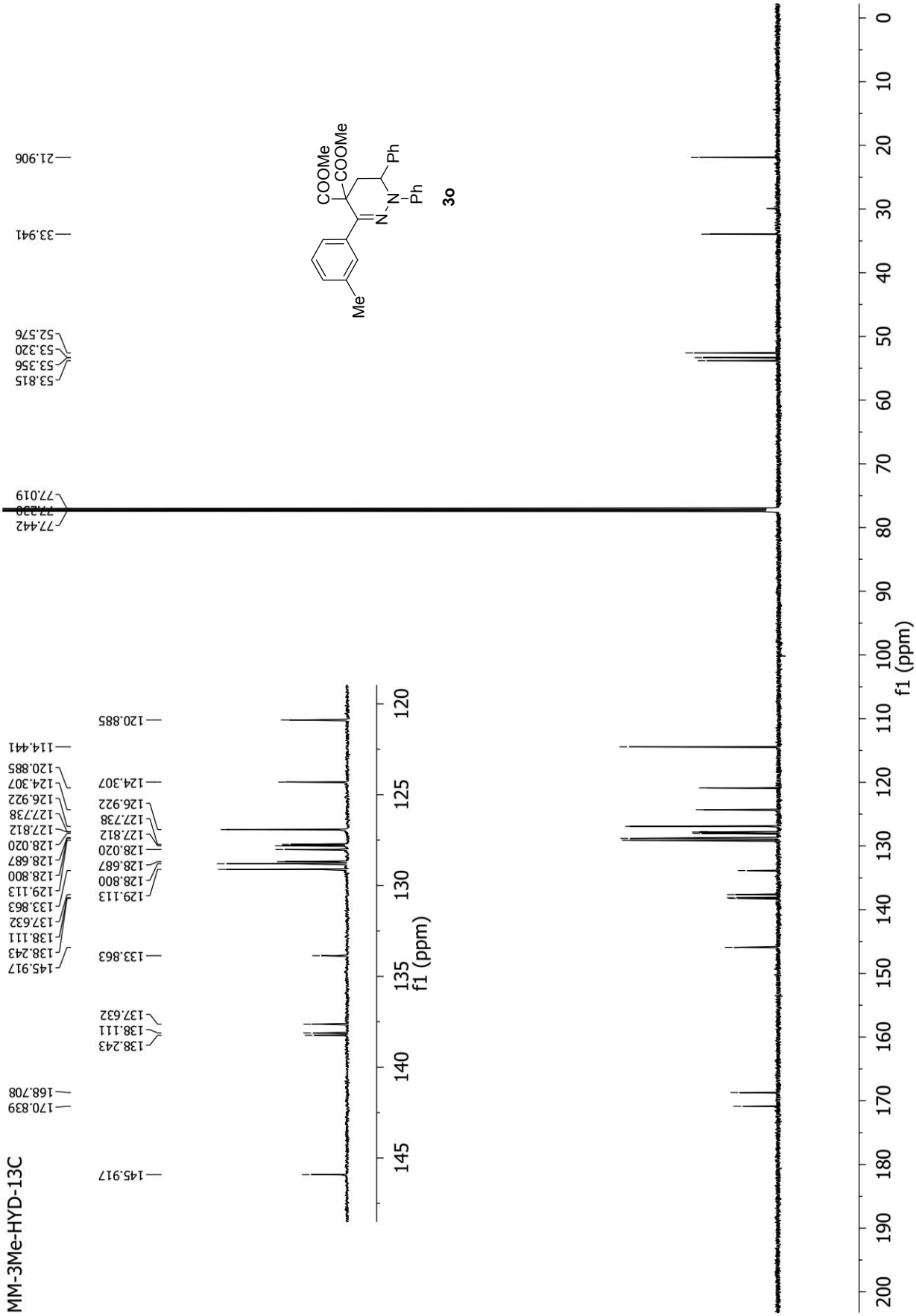

MM-2BR-HYD-1H
COOMe
COOMe
Ph
Ph
Br
3m
f1 (ppm)


MM-2BR-HYD-13C
168.898
168.624
146.190
138.641
138.616
133.037
132.313
132.097
129.584
129.008
128.718
127.724
127.154
126.898
124.834
121.167
114.873
77.548
77.230
76.913
54.942
54.919
53.137
52.518
32.451
COOMe
COOMe
Ph
Ph
N
N
Br
3m
f1 (ppm)

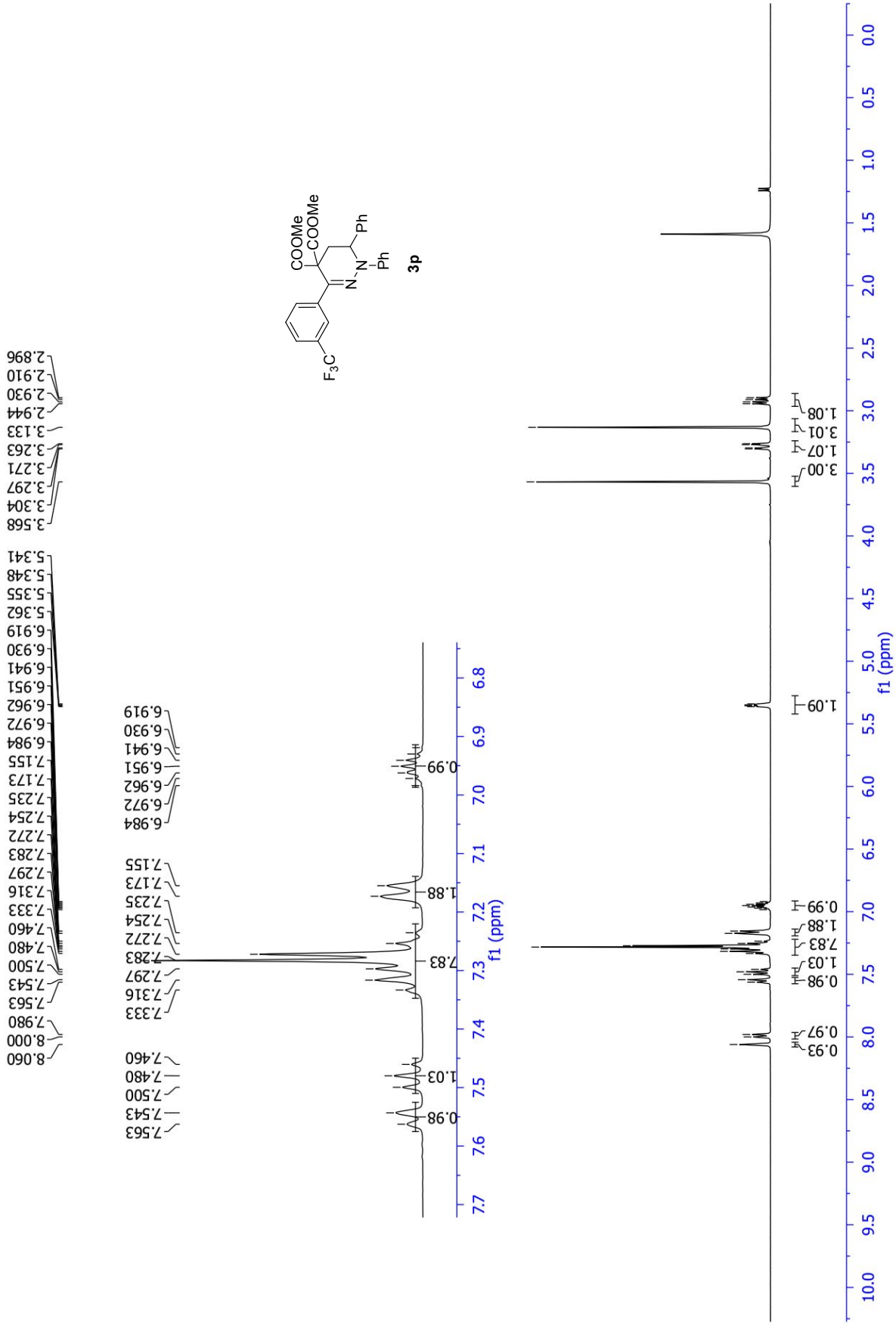

MM-3Br-HYD-1H
COOMe
COOMe
Ph
Ph
Br
3n
f1 (ppm)

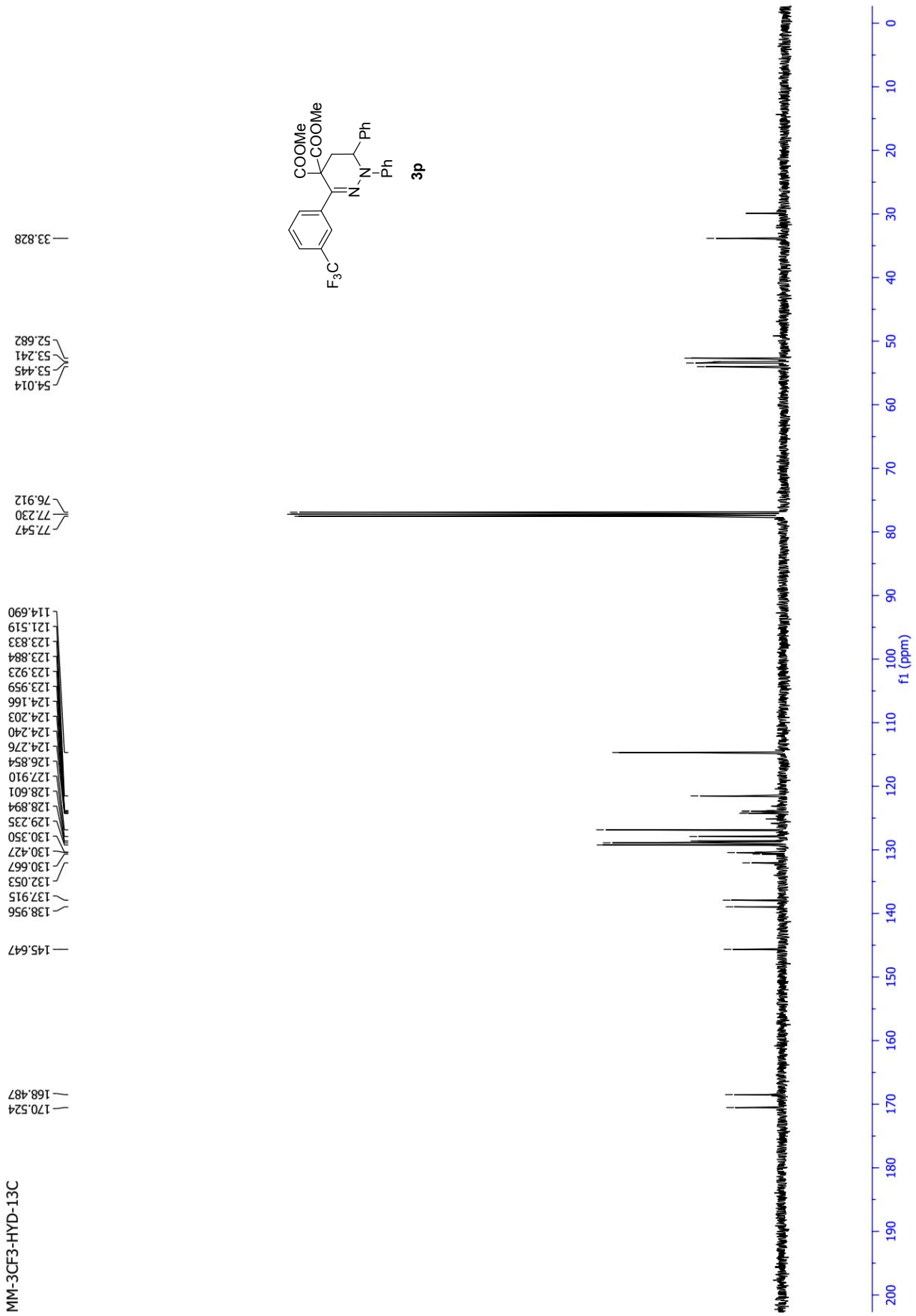

MM-3Br-HYD-13C
170.575
168.466
145.616
140.190
137.872
131.953
130.638
130.099
129.618
129.202
128.860
127.867
126.840
125.646
122.395
121.387
114.600
77.442
77.230
77.018
53.902
53.500
53.176
52.695
33.756
COOMe
COOMe
Ph
Ph
N
N
Br
3n
f1 (ppm)

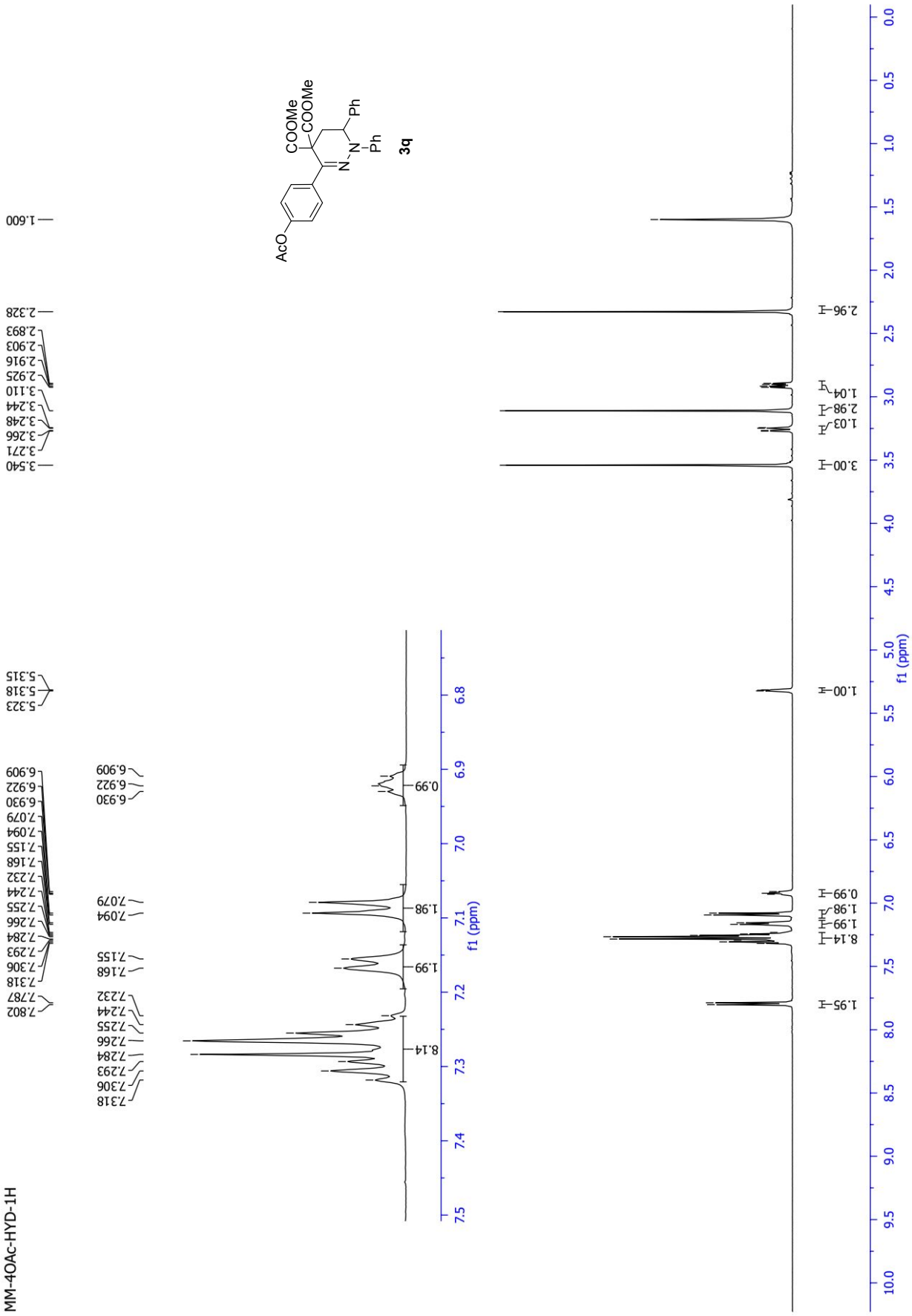

MM-3Me-HYD-1H
COOMe
COOMe
Ph
N
N
Ph
Me
3o
f1 (ppm)

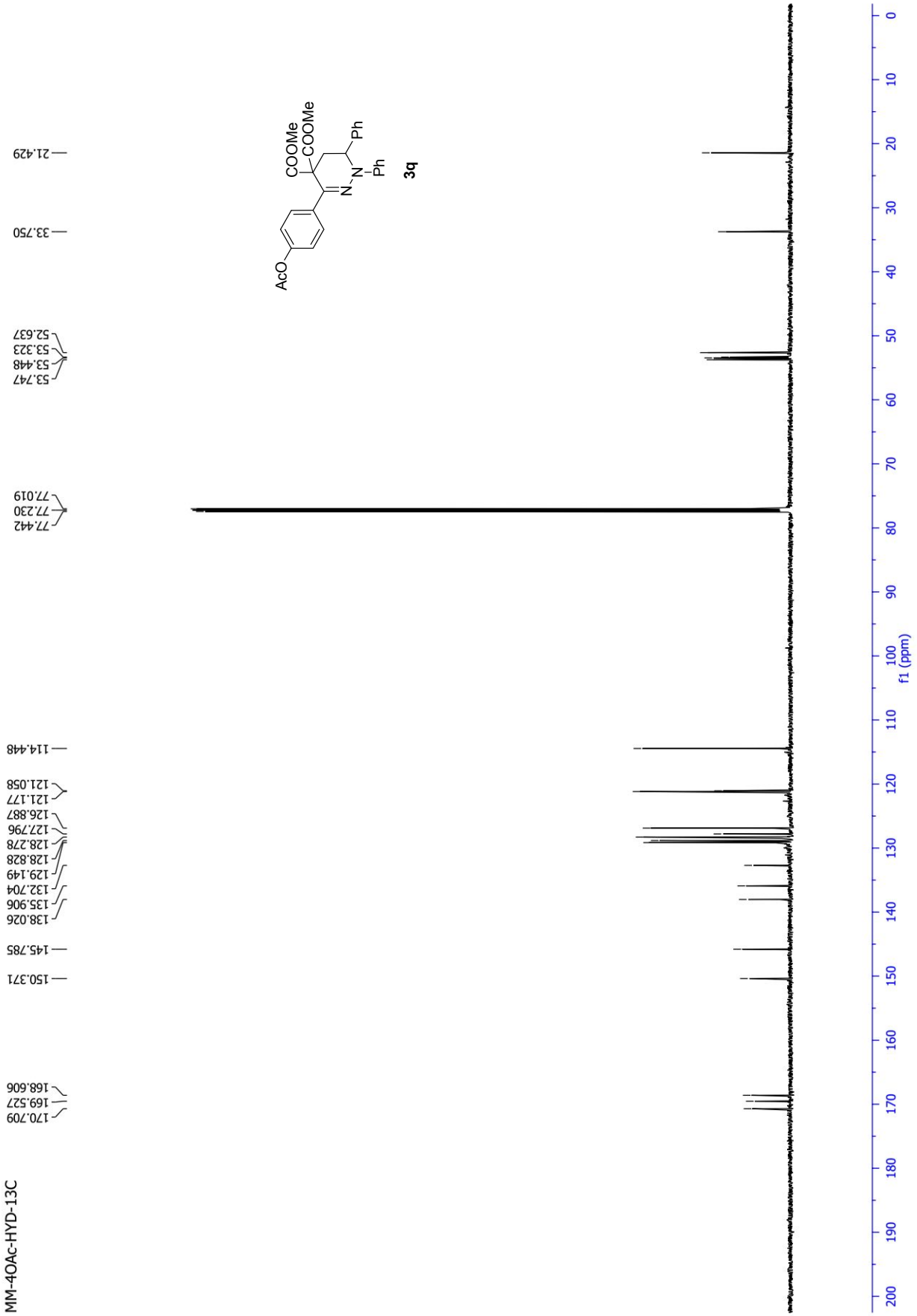

MM-3Me-HYD-13C
145.917
170.839
168.708
138.243
138.111
137.632
133.863
129.113
128.800
128.687
128.020
127.812
127.738
126.922
124.307
120.885
114.441
120.885
124.307
126.922
127.738
127.812
128.020
128.687
128.800
129.113
133.863
137.632
138.111
138.243
145.917
77.442
77.230
77.019
53.815
53.356
53.320
52.576
33.941
21.906
COOMe
COOMe
Ph
Ph
N
N
Me
3o
f1 (ppm)
f1 (ppm)

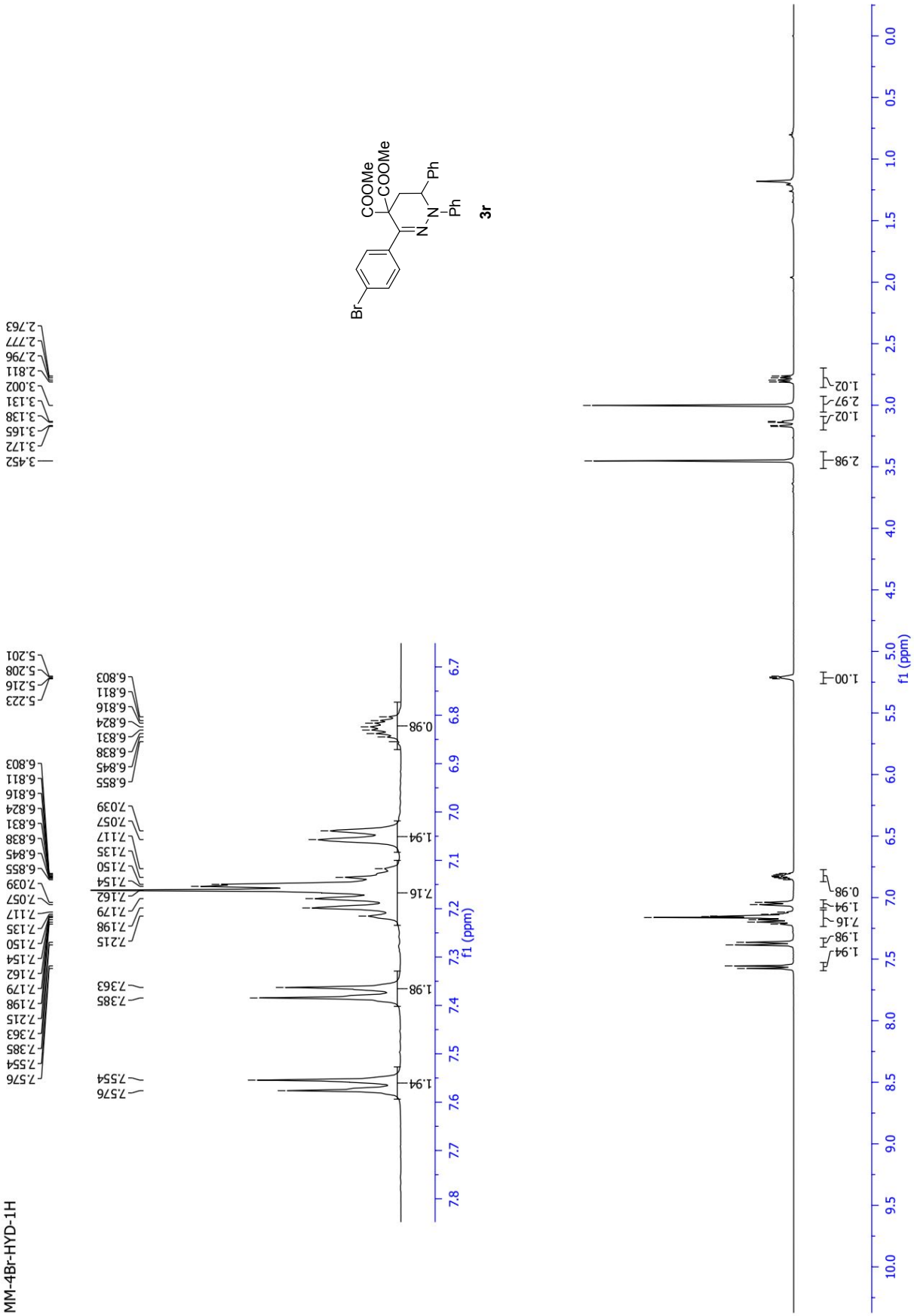
MM-3CF3-HYD-1H

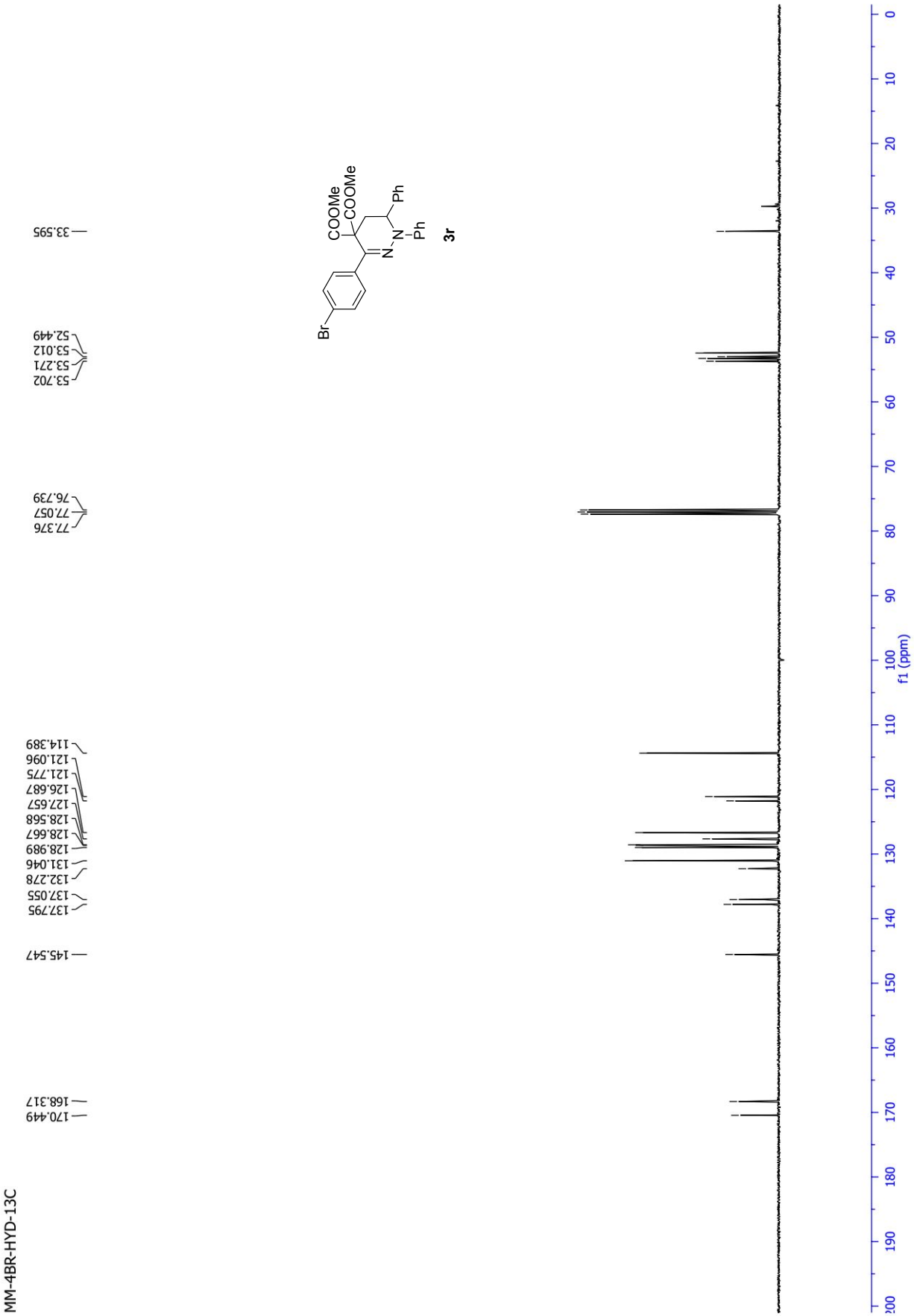


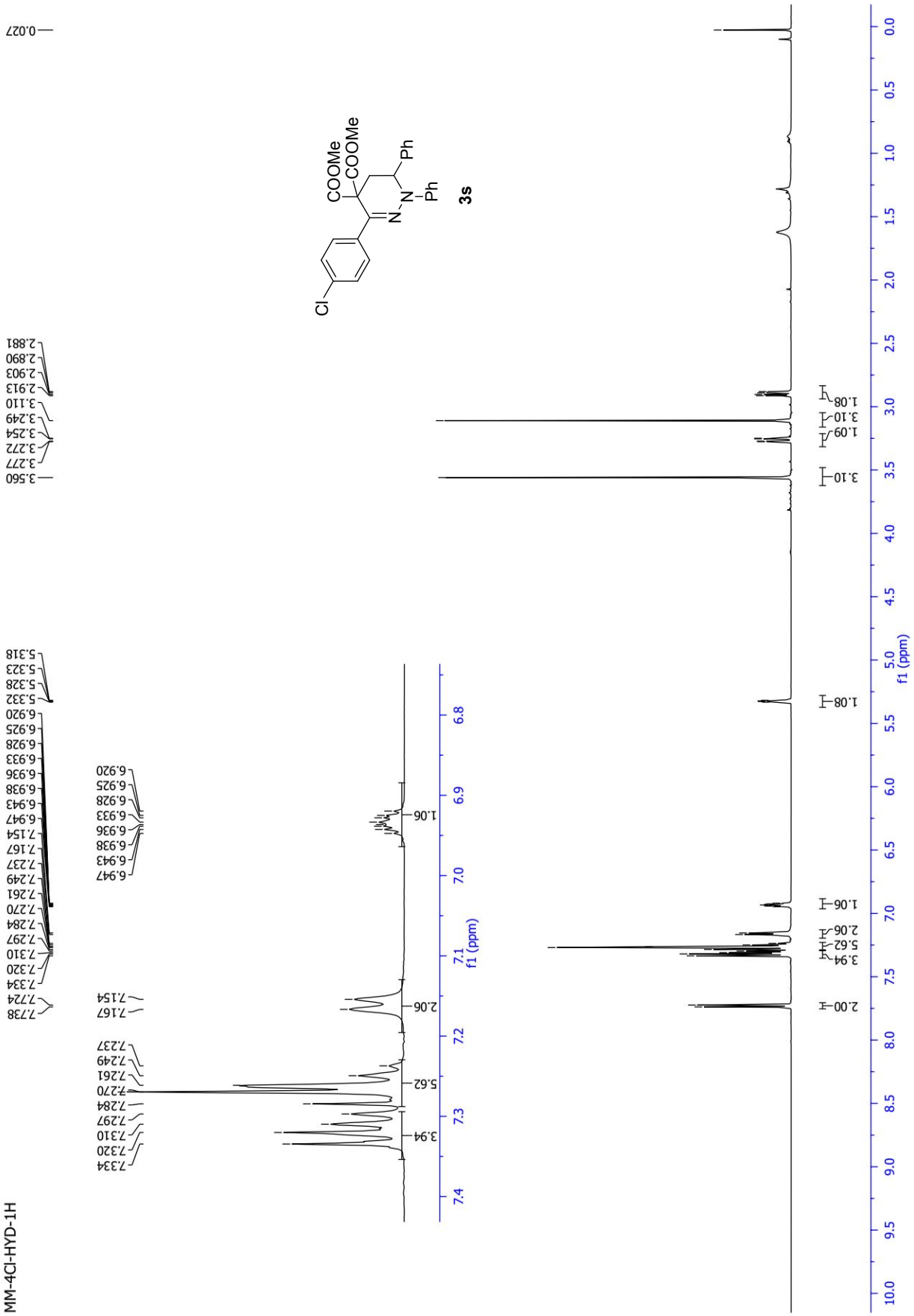

MM-3CF3-HYD-13C
170.524
168.487
145.647
138.956
137.915
132.053
130.667
130.427
130.350
129.235
128.894
128.601
127.910
126.854
124.276
124.240
124.203
124.166
123.959
123.923
123.884
123.833
121.519
114.690
77.547
77.230
76.912
54.014
53.445
53.241
52.682
33.828
COOMe
COOMe
Ph
Ph
N
N
F3C
3p
f1 (ppm)

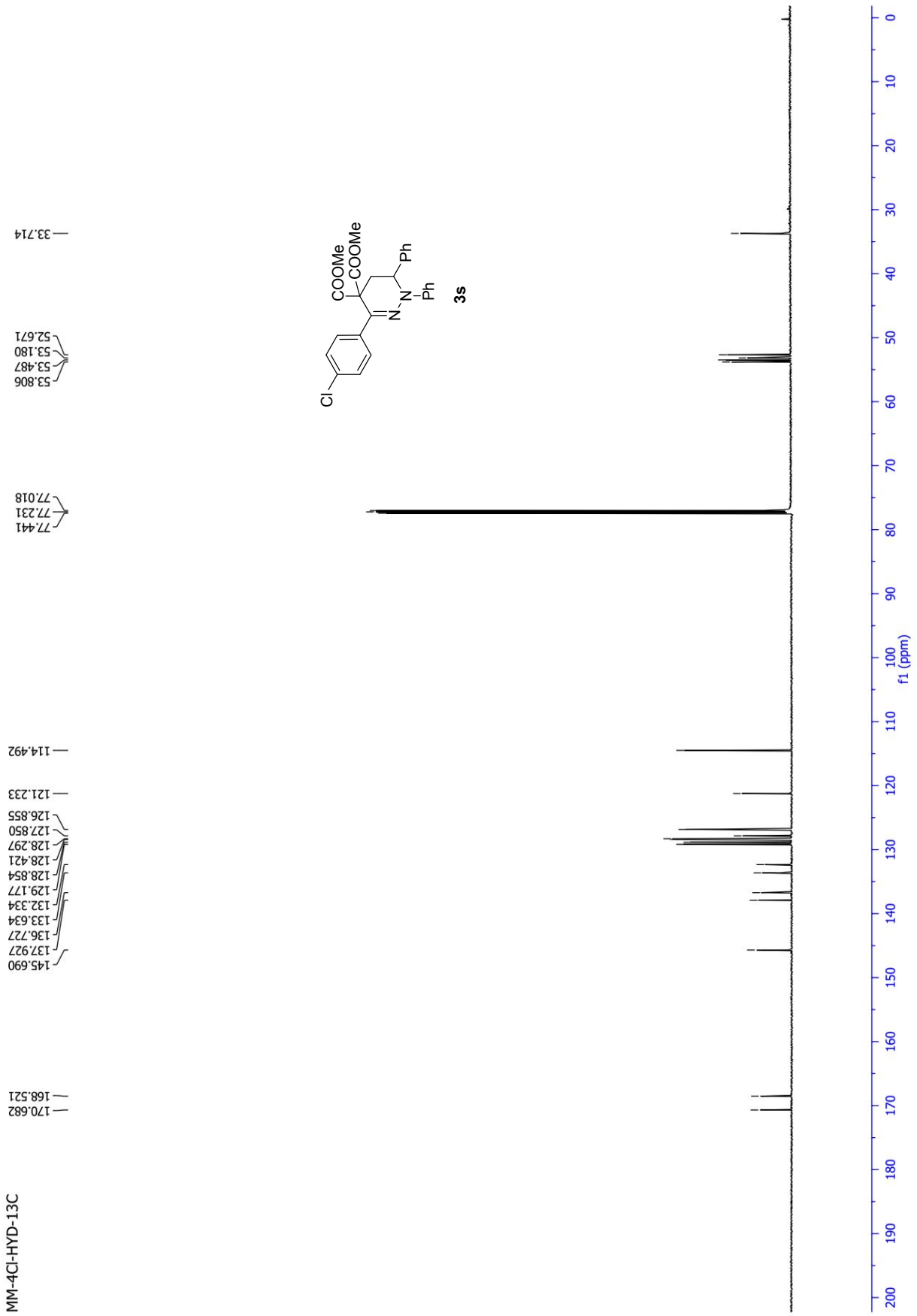

MM-4OAc-HYD-1H
AcO
COOMe
COOMe
Ph
Ph
3q
f1 (ppm)

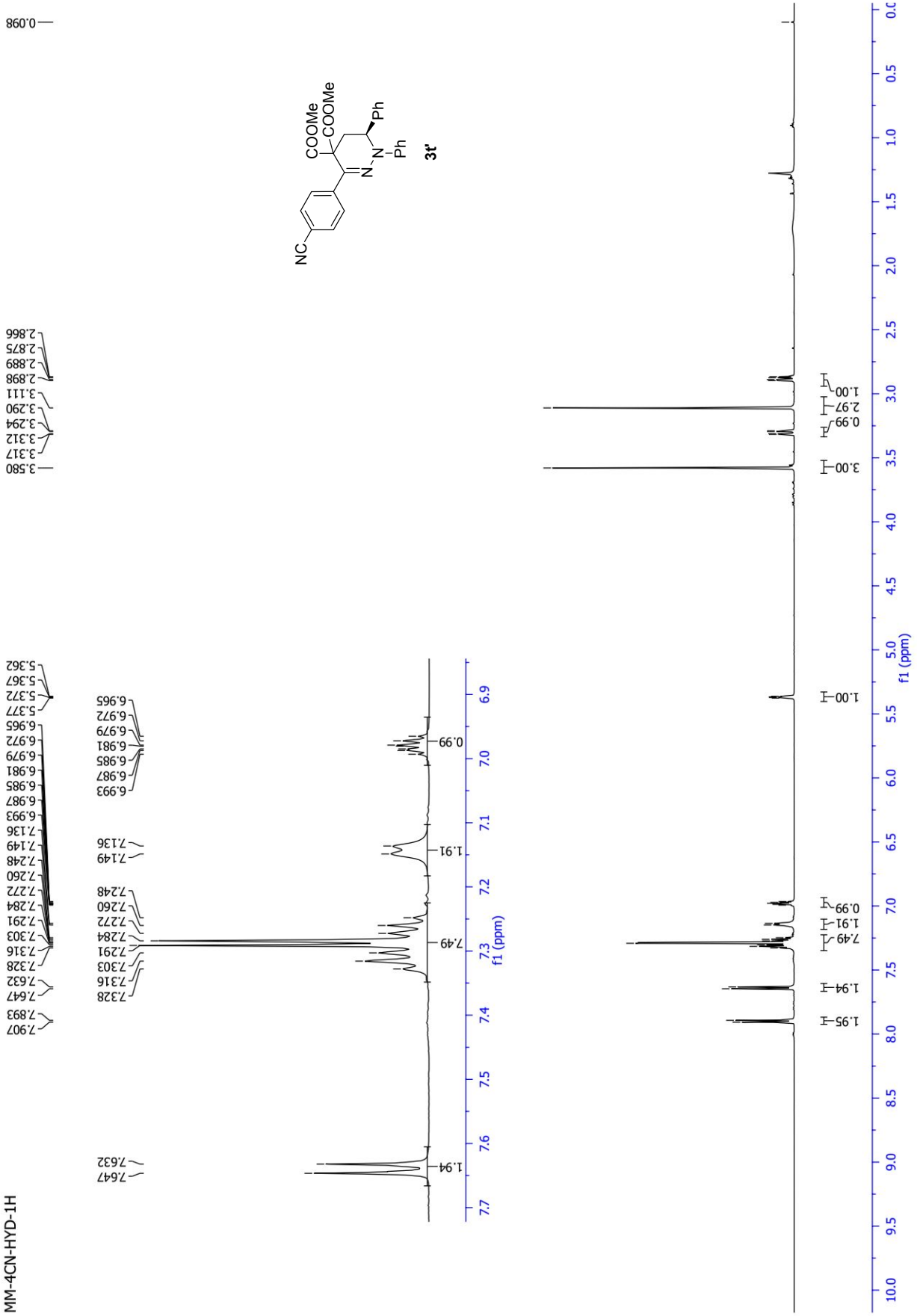

MM-4OAc-HYD-13C
170.709
169.527
168.606
150.371
145.785
138.026
135.906
132.704
129.149
128.828
128.278
127.796
126.887
121.177
121.058
114.448
77.442
77.230
77.019
53.747
53.448
53.323
52.637
33.750
21.429
AcO
COOMe
COOMe
Ph
N
N
Ph
3q
f1 (ppm)


MM-4Br-HYD-1H
COOMe
COOMe
Ph
Ph
N
N
Br
3r
f1 (ppm)
f1 (ppm)

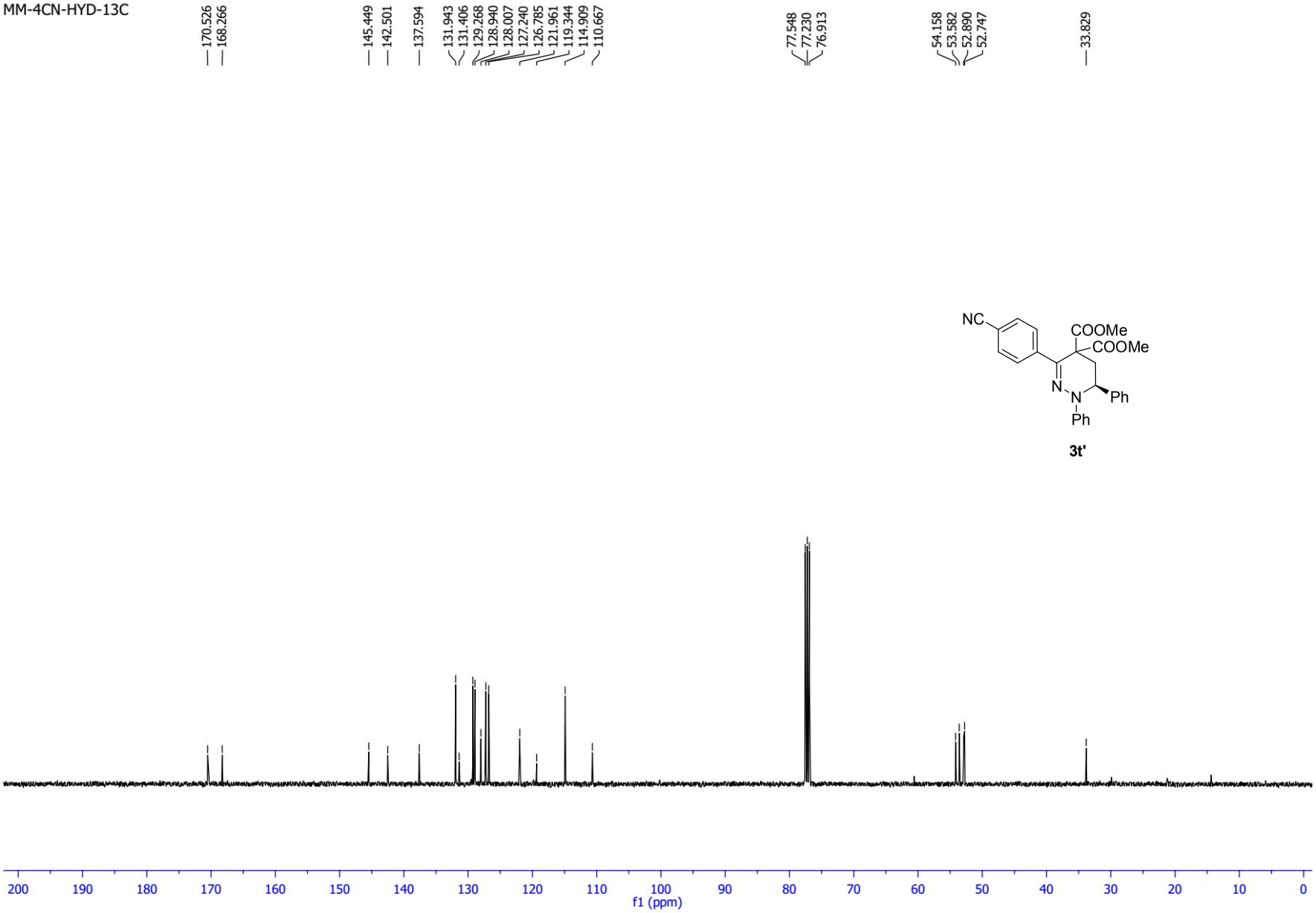

MM-4BR-HYD-13C
170.449
168.317
145.547
137.795
137.055
132.278
131.046
128.989
128.667
128.568
127.657
126.687
121.775
121.096
114.389
77.376
77.057
76.739
53.702
53.271
53.012
52.449
33.595
COOMe
COOMe
Ph
Ph
N
N
Br
3r
f1 (ppm)


MM-4Cl-HYD-1H
COOMe
COOMe
Ph
N
N
Ph
Cl
3s
f1 (ppm)


MM-4Cl-HYD-13C
170.682
168.521
145.690
137.927
136.727
133.634
132.334
129.177
128.854
128.421
128.297
127.850
126.855
121.233
114.492
77.441
77.231
77.018
53.806
53.487
53.180
52.671
33.714
COOMe
COOMe
Ph
N
N
Ph
Cl
3s
f1 (ppm)

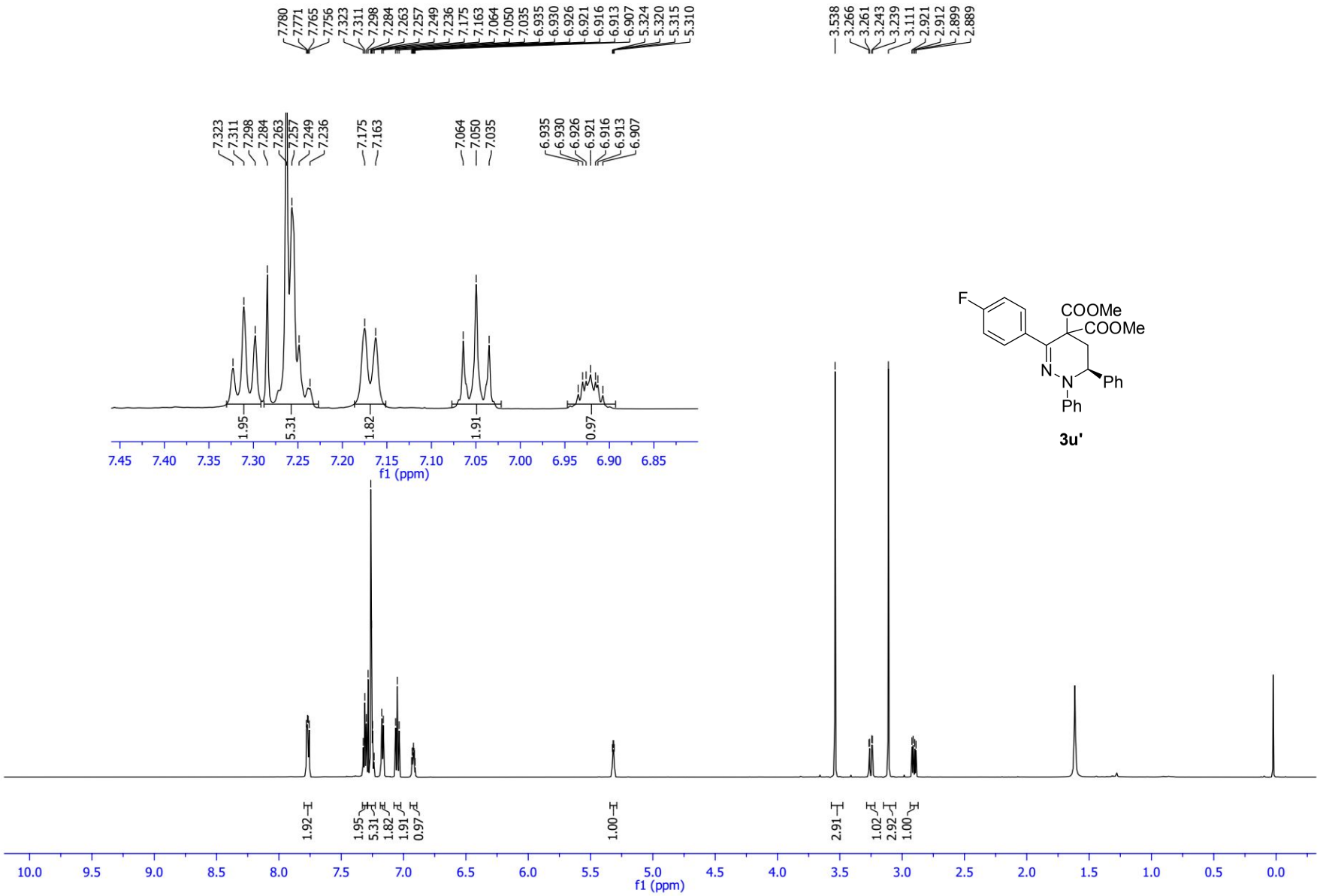

MM-4CN-HYD-1H
NC
COOMe
COOMe
Ph
N
N
Ph
3t'
f1 (ppm)

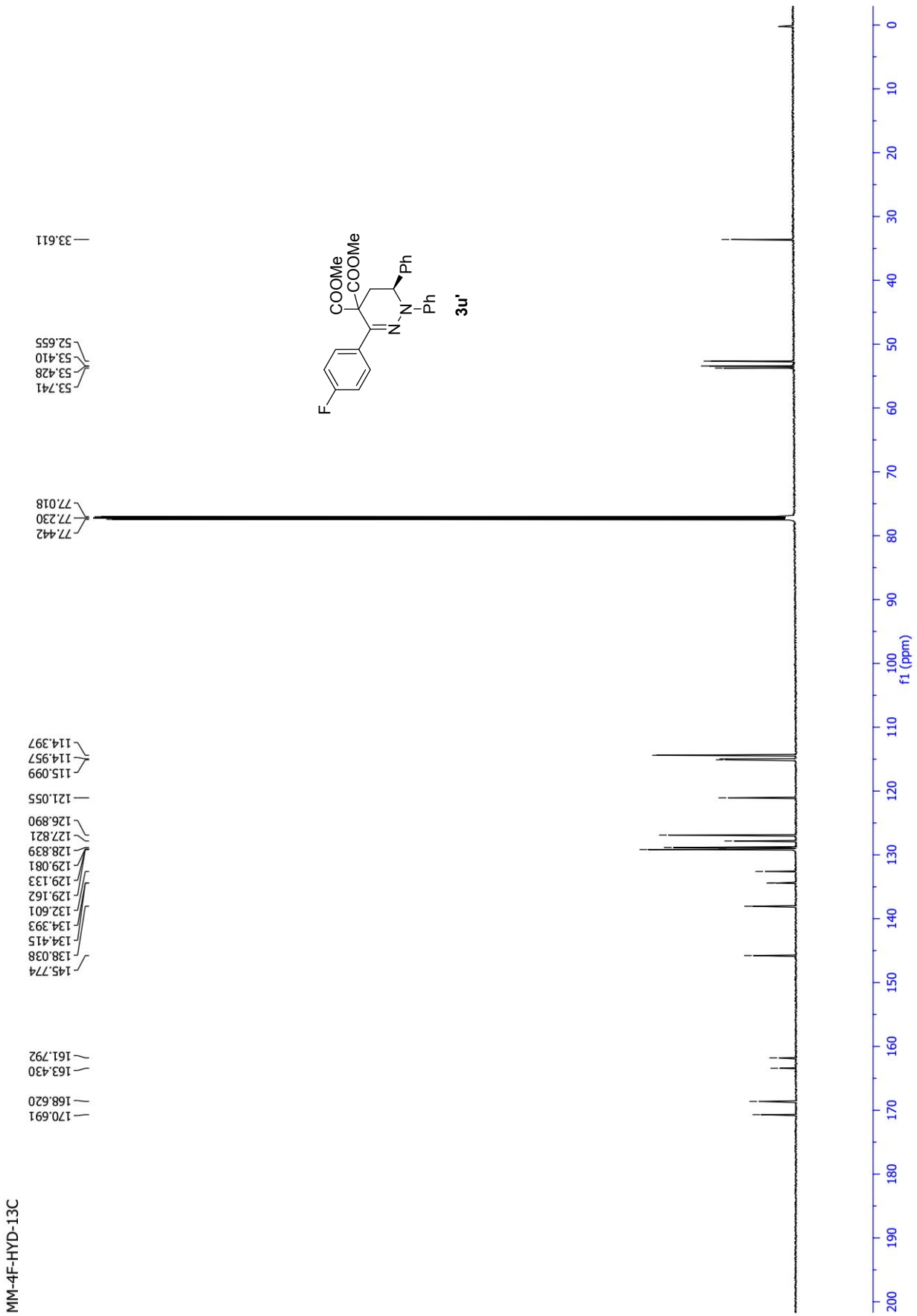
MM-4CN-HYD-13C

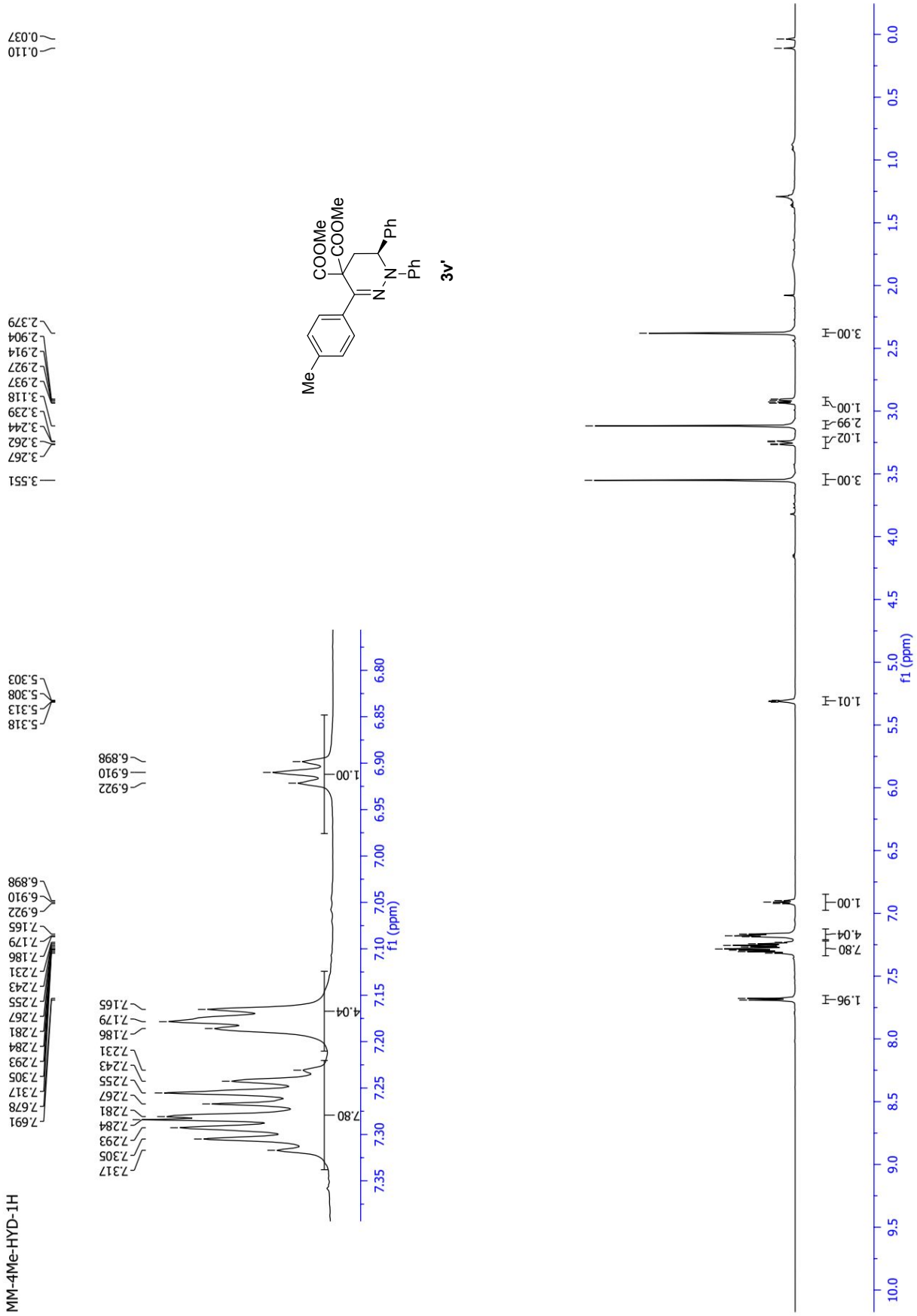


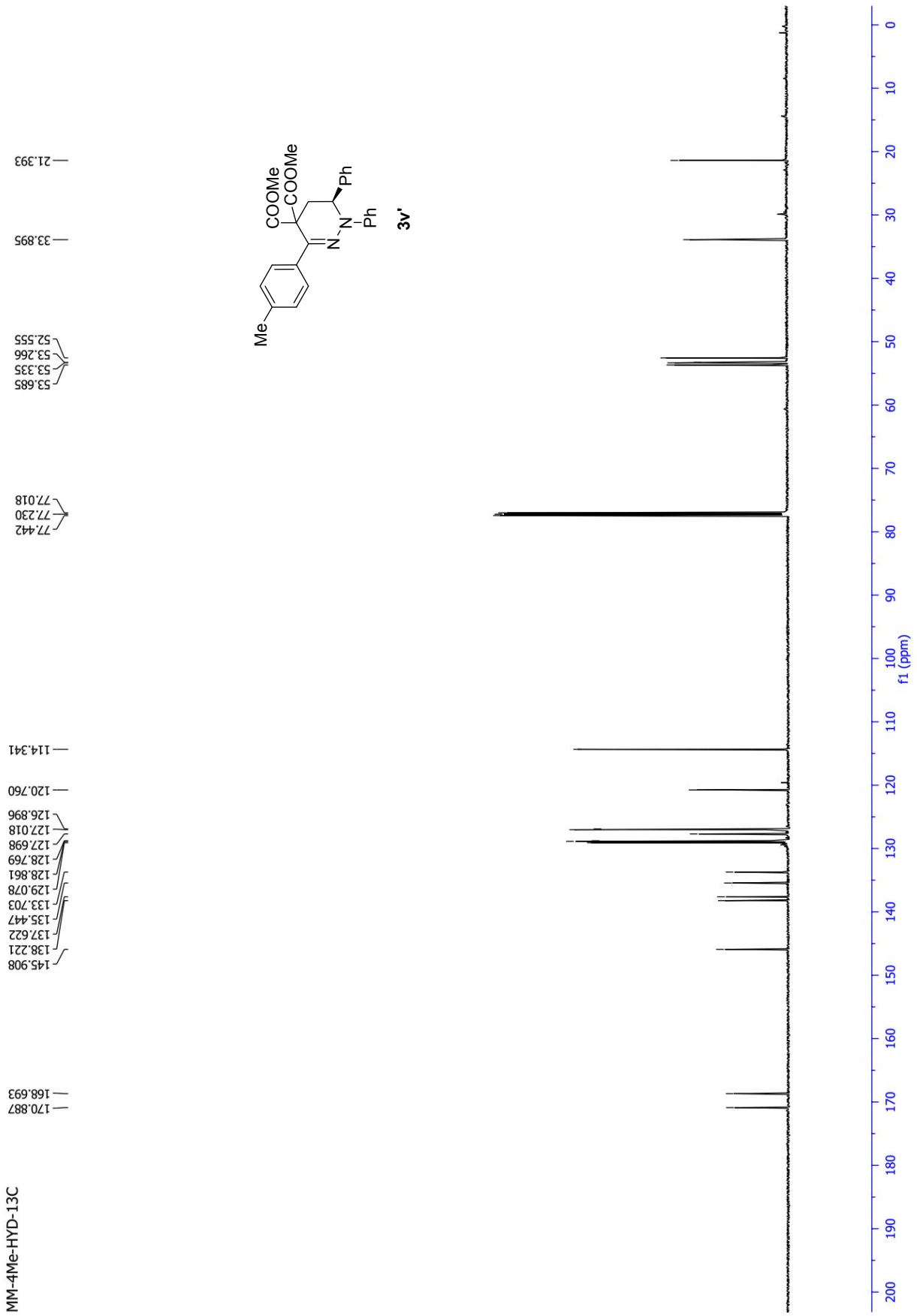
3t'

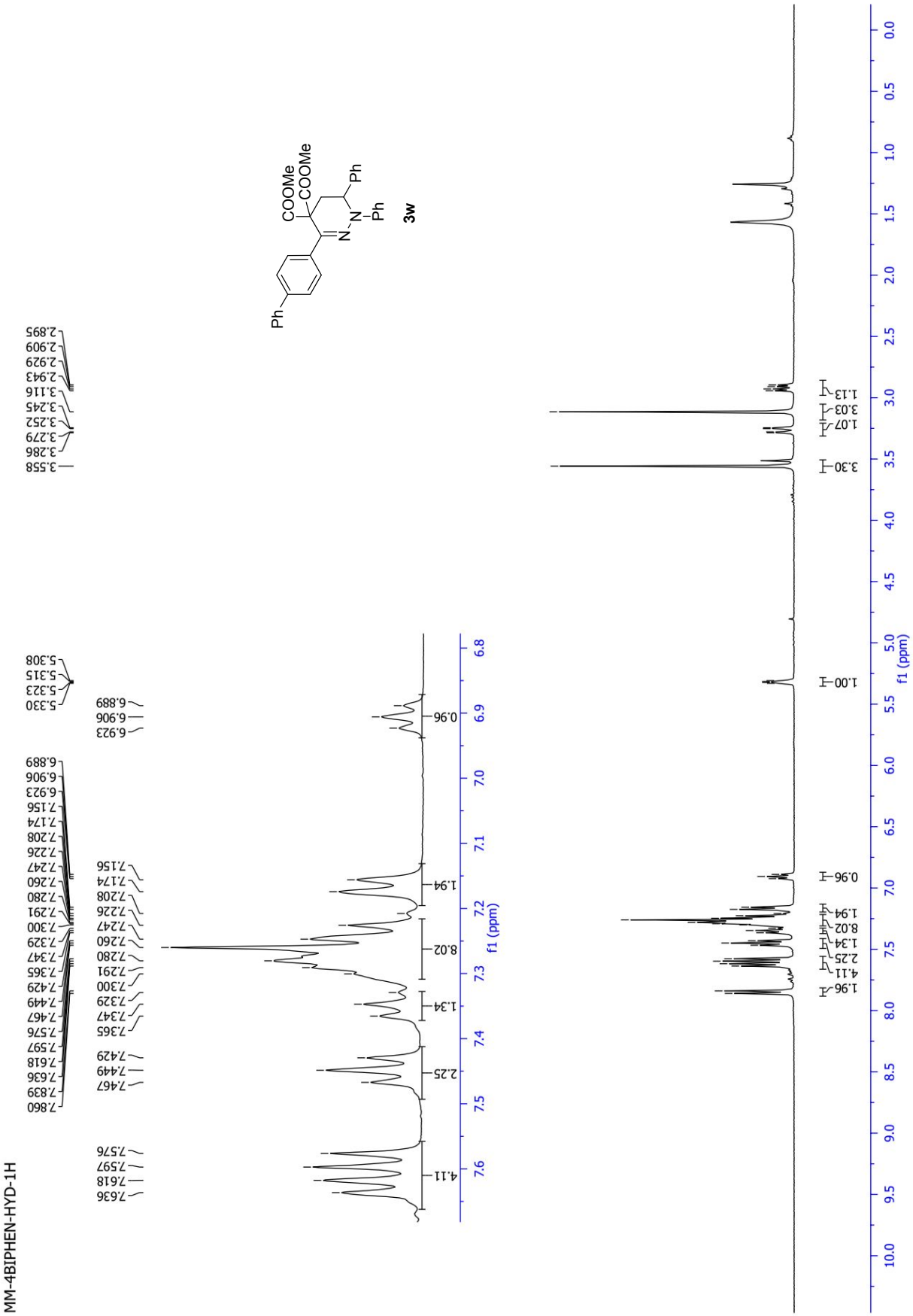
MM-4F-HYD-1H

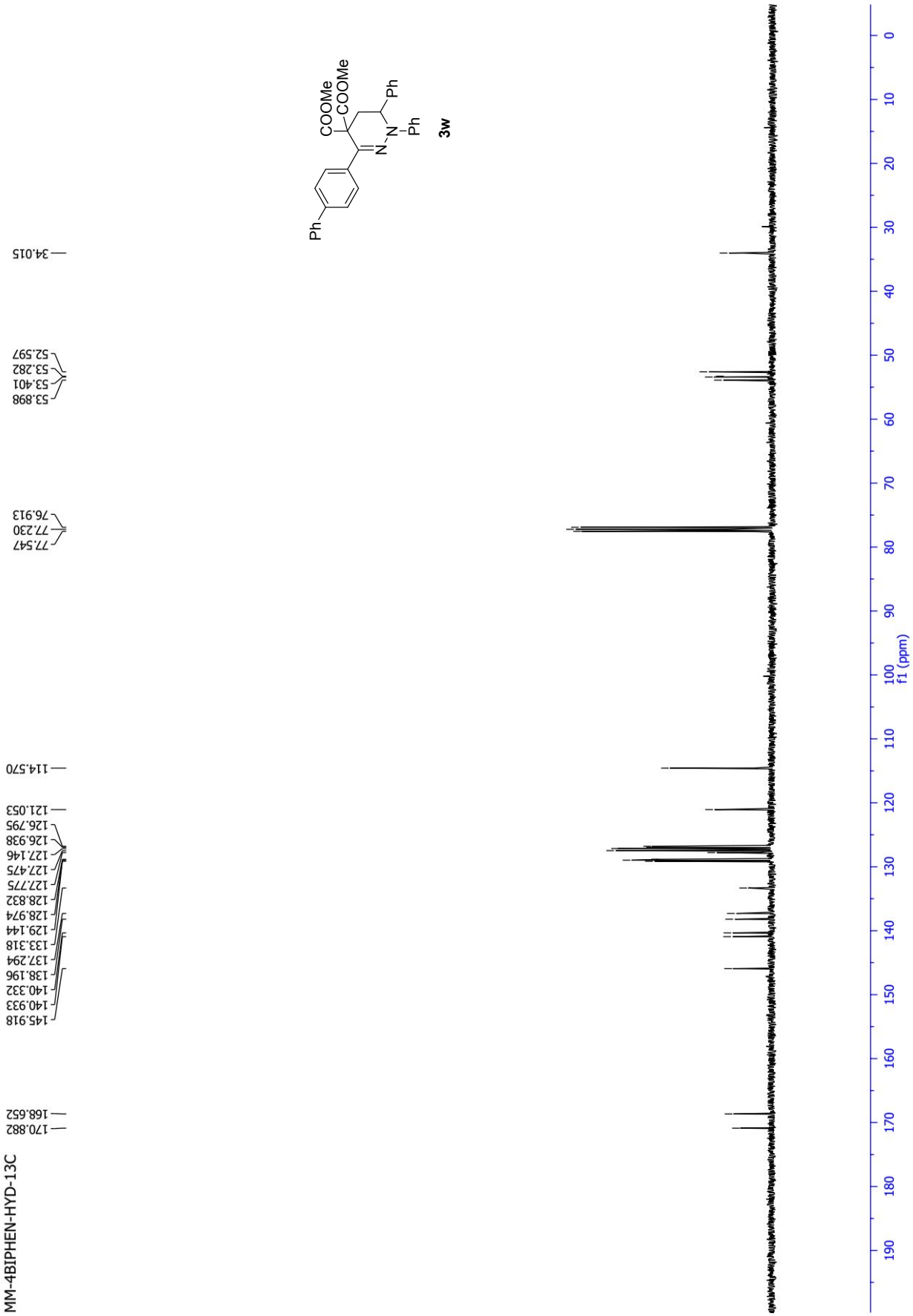

7.780
7.771
7.765
7.756
7.323
7.311
7.298
7.284
7.263
7.257
7.249
7.236
7.175
7.163
7.064
7.050
7.035
6.935
6.930
6.926
6.921
6.916
6.913
6.907
5.324
5.320
5.315
5.310
3.538
3.266
3.261
3.243
3.239
3.111
2.921
2.912
2.899
2.889
1.95
5.31
1.82
1.91
0.97
7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85
f1 (ppm)
1.92
1.95
5.31
1.82
1.91
0.97
1.00
2.91
1.02
2.92
1.00
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
f1 (ppm)
F
COOMe
COOMe
N
N
Ph
Ph
3u'

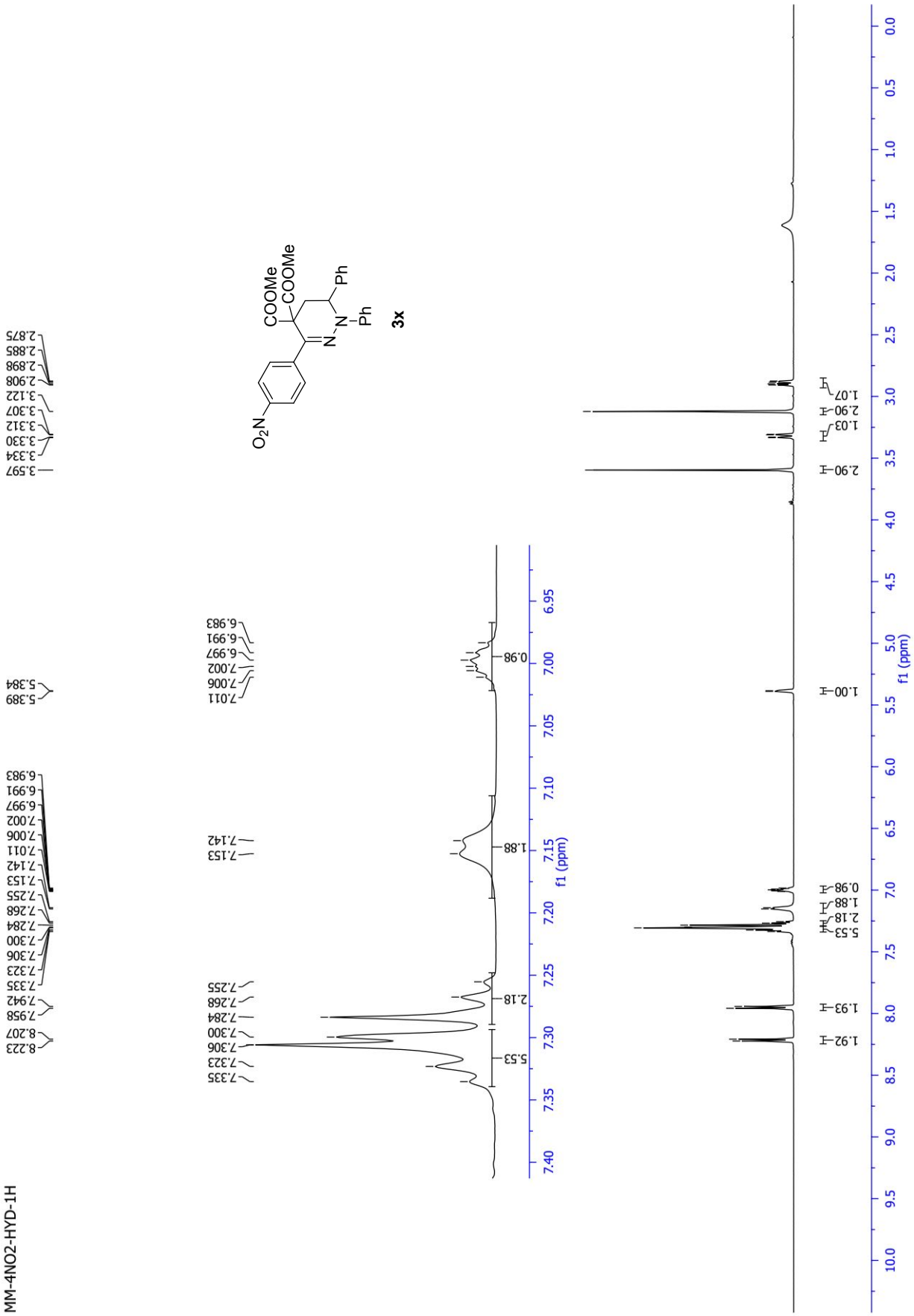

MM-4F-HYD-13C
170.691
168.620
163.430
161.792
145.774
138.038
134.415
134.393
132.601
129.162
129.133
129.081
128.839
127.821
126.890
121.055
115.099
114.957
114.397
77.442
77.230
77.018
53.741
53.428
53.410
52.655
33.611
COOMe
COOMe
Ph
Ph
N
N
F
3u'
f1 (ppm)

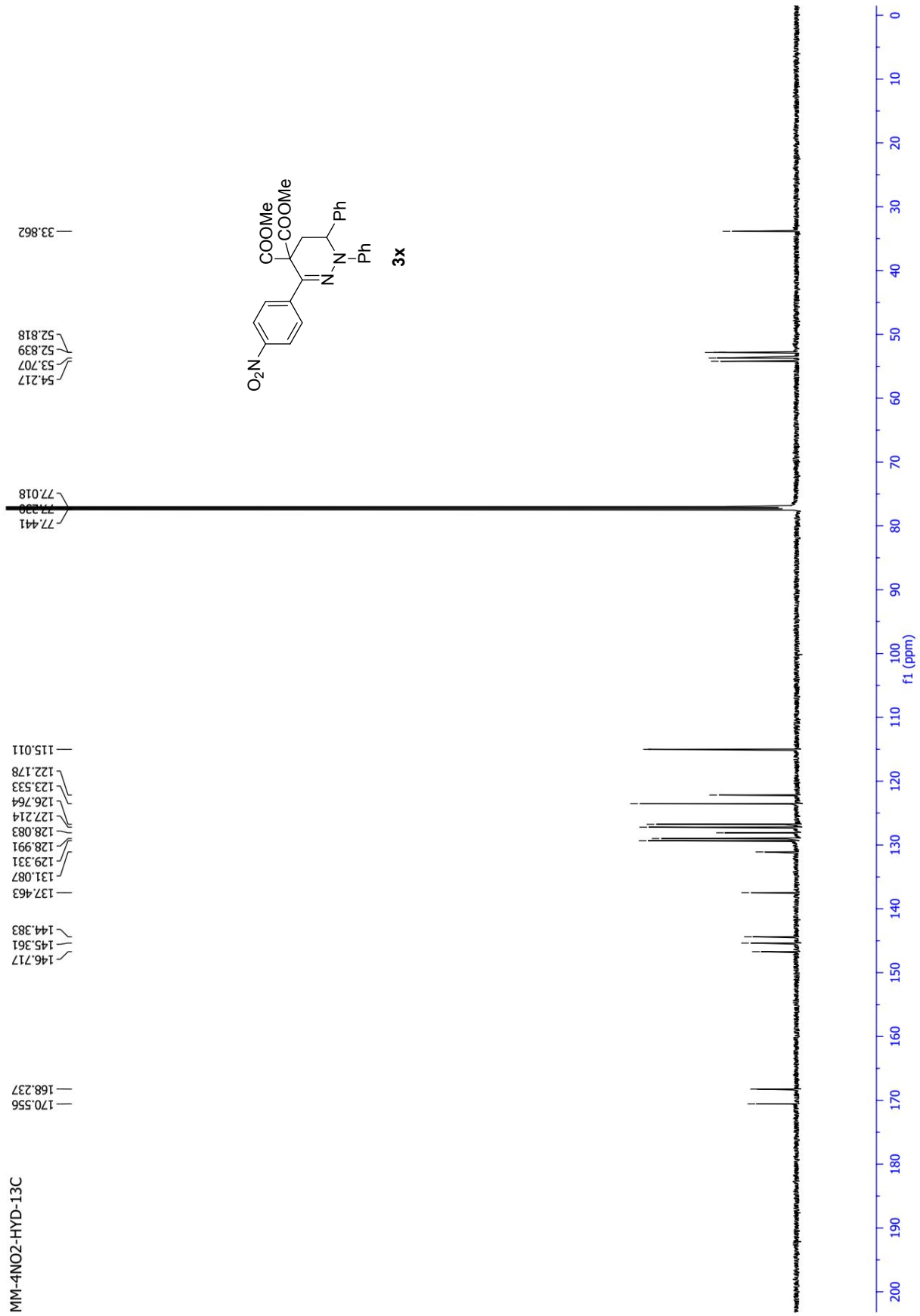

MM-4Me-HYD-1H
COOMe
COOMe
Ph
Ph
Me
3v'
f1 (ppm)

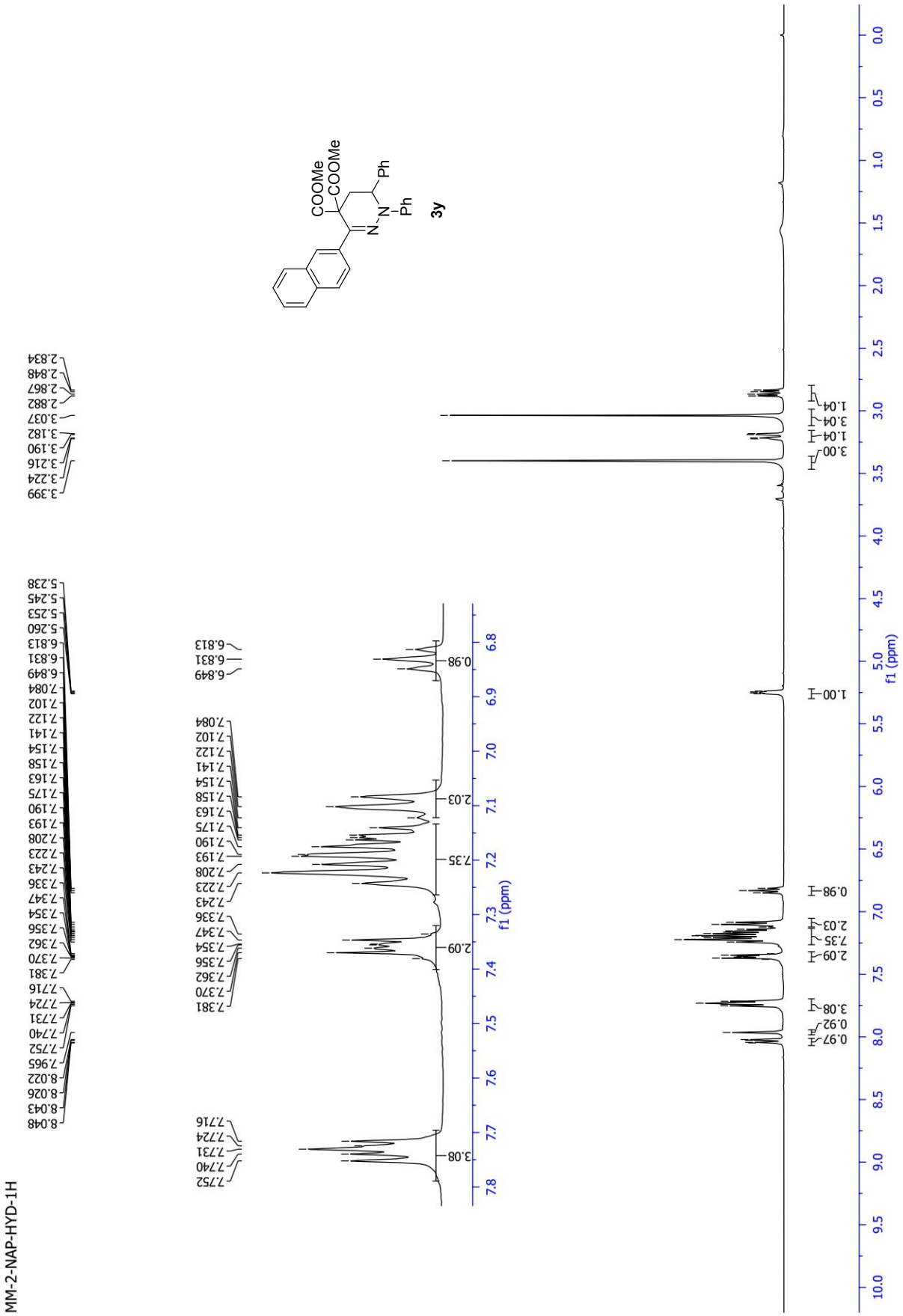

MM-4Me-HYD-13C
170.887
168.693
145.908
138.221
137.622
135.447
133.703
129.078
128.861
128.769
127.698
127.018
126.896
120.760
114.341
77.442
77.230
77.018
53.685
53.335
53.266
52.555
33.895
21.393
COOMe
COOMe
Ph
Ph
N
N
Me
3v'
f1 (ppm)

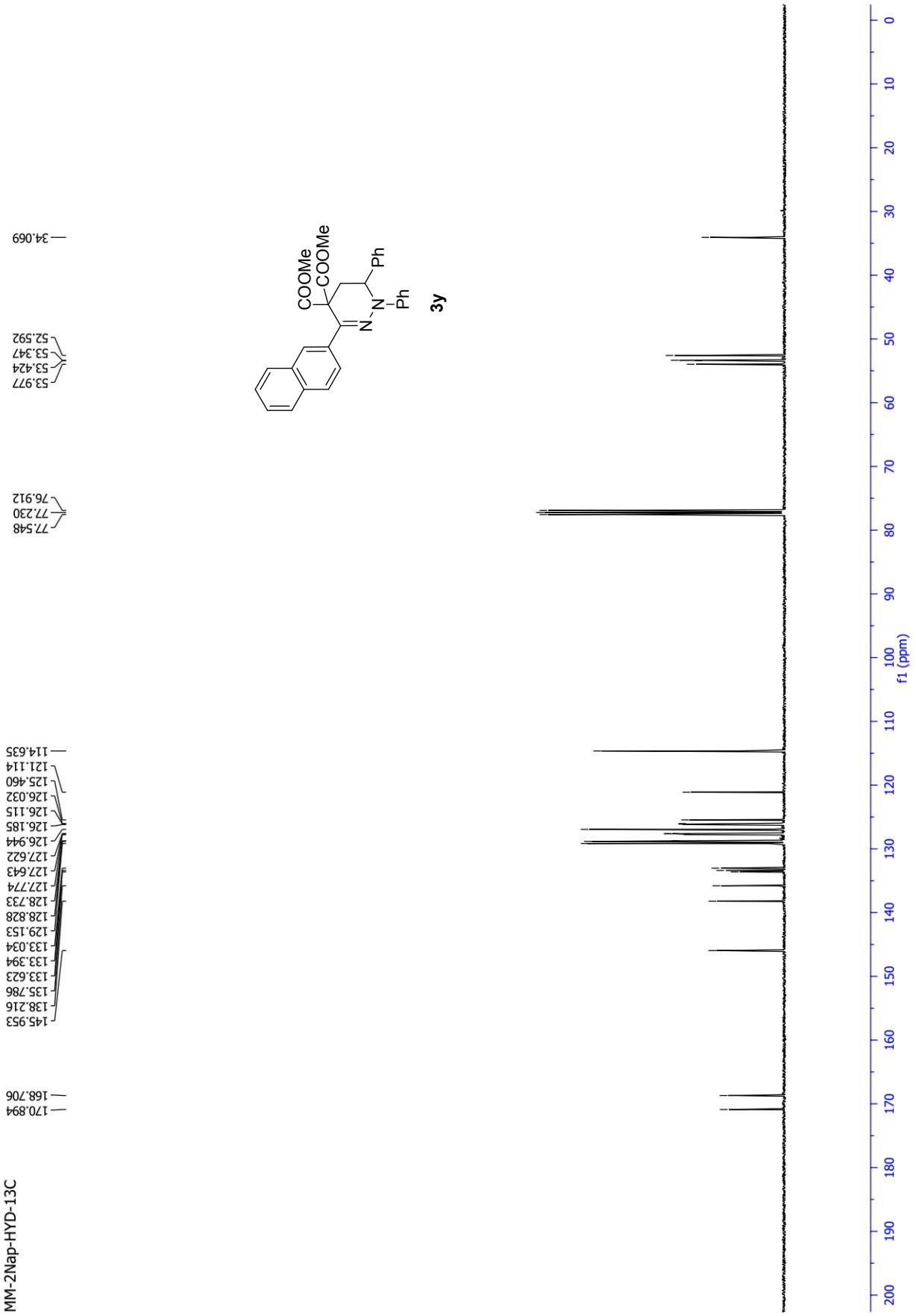

MM-4BIPHEN-HYD-1H
COOMe
COOMe
Ph
Ph
Ph
N
N
3w
f1 (ppm)
f1 (ppm)

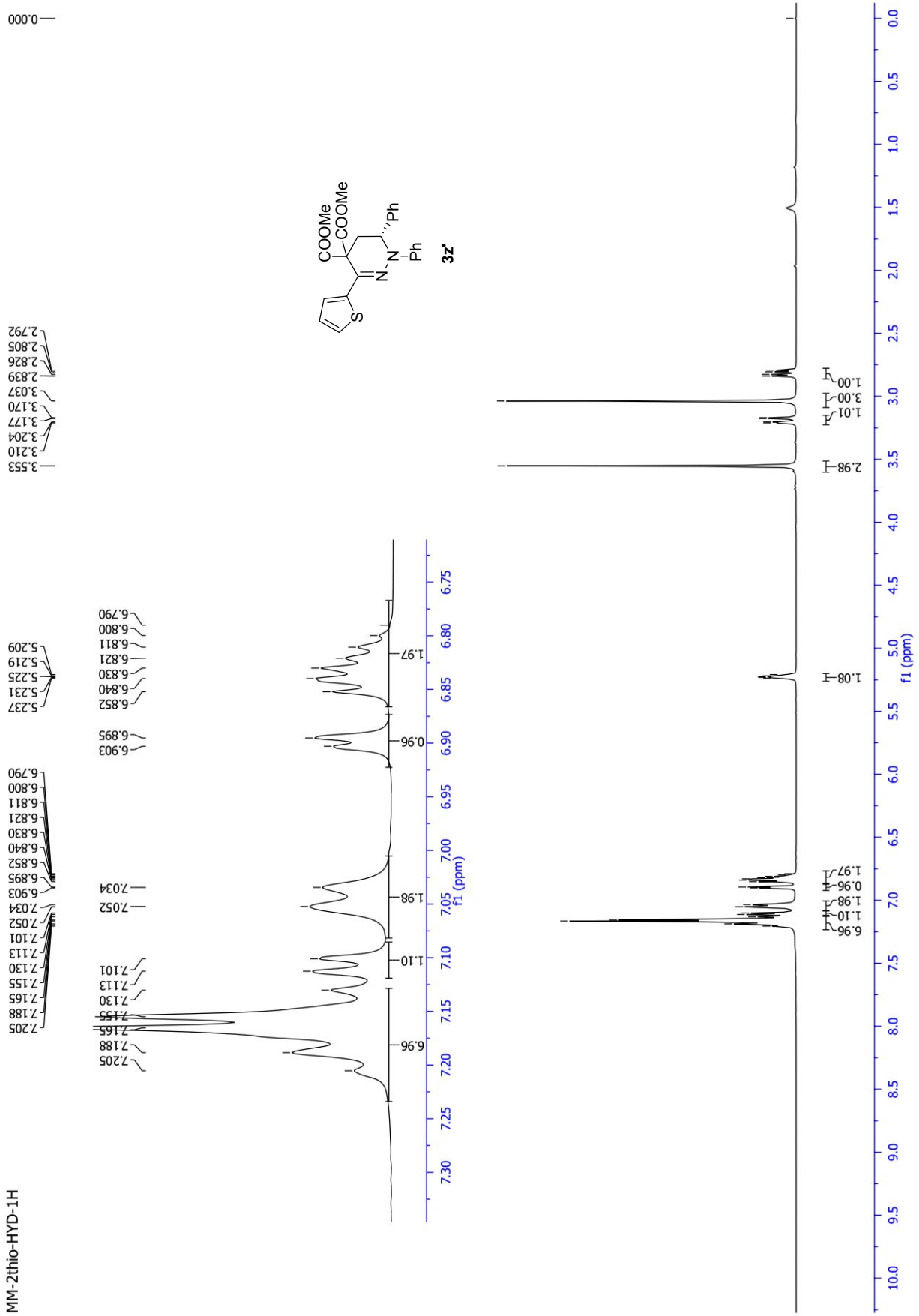

MM-4BIPHEN-HYD-13C
170.882
168.652
145.918
140.933
140.332
138.196
137.294
133.318
129.144
128.974
128.832
127.775
127.475
127.146
126.938
126.795
121.053
114.570
77.547
77.230
76.913
53.898
53.401
53.282
52.597
34.015
COOMe
COOMe
Ph
Ph
Ph
N
N
3w
f1 (ppm)

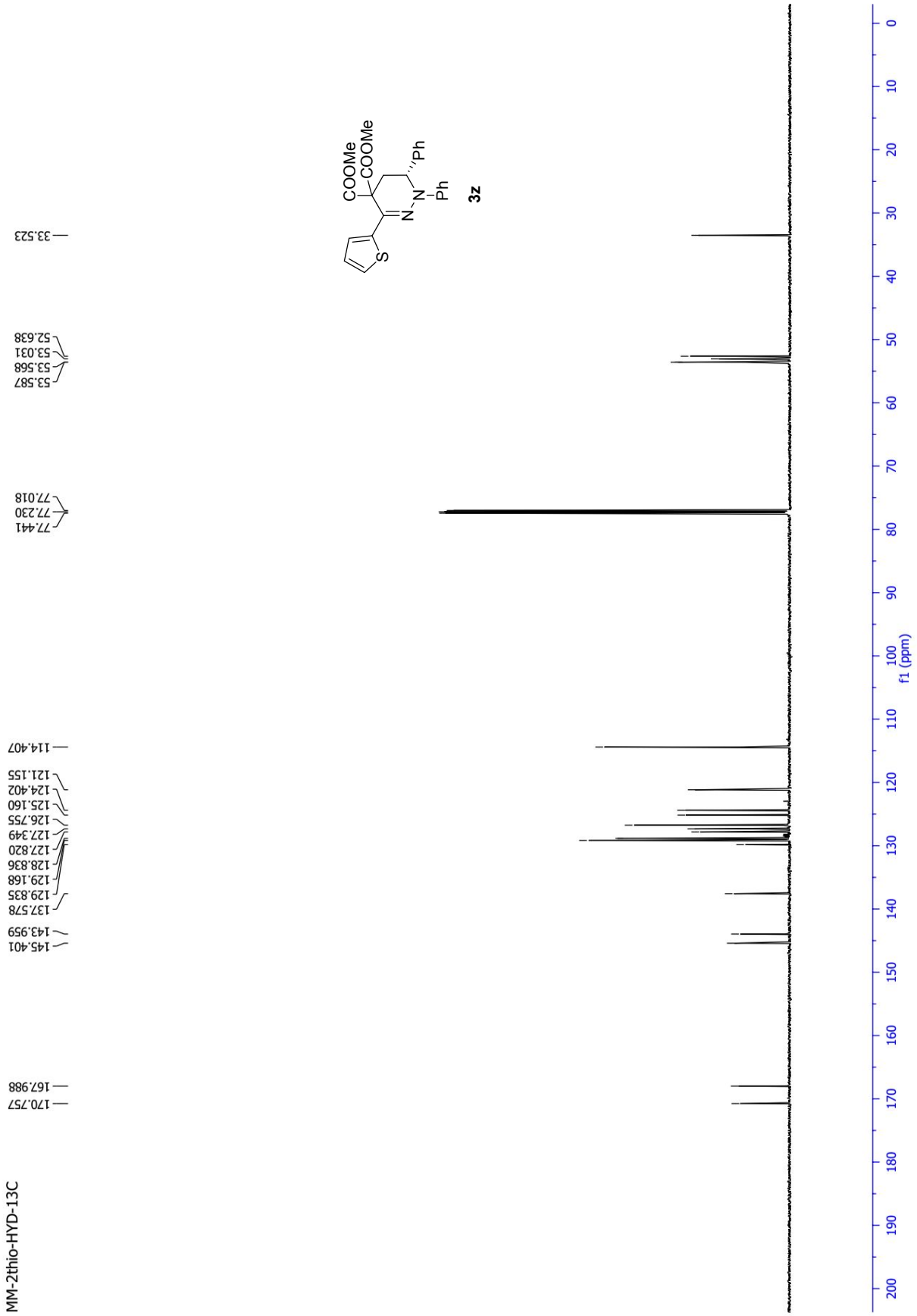

MM-4NO2-HYD-1H
3x
COOMe
COOMe
Ph
Ph
N
N
O2N
8.223
8.207
7.958
7.942
7.335
7.323
7.306
7.300
7.284
7.268
7.255
7.153
7.142
7.011
7.006
7.002
6.997
6.991
6.983
5.389
3.597
3.334
3.330
3.312
3.307
3.122
2.908
2.898
2.885
2.875
7.335
7.323
7.306
7.300
7.284
7.268
7.255
7.153
7.142
7.011
7.006
7.002
6.997
6.991
6.983
5.53
2.18
1.88
0.98
f1 (ppm)
1.92
1.93
5.53
2.18
1.88
0.98
1.00
2.90
1.03
2.90
1.07
f1 (ppm)

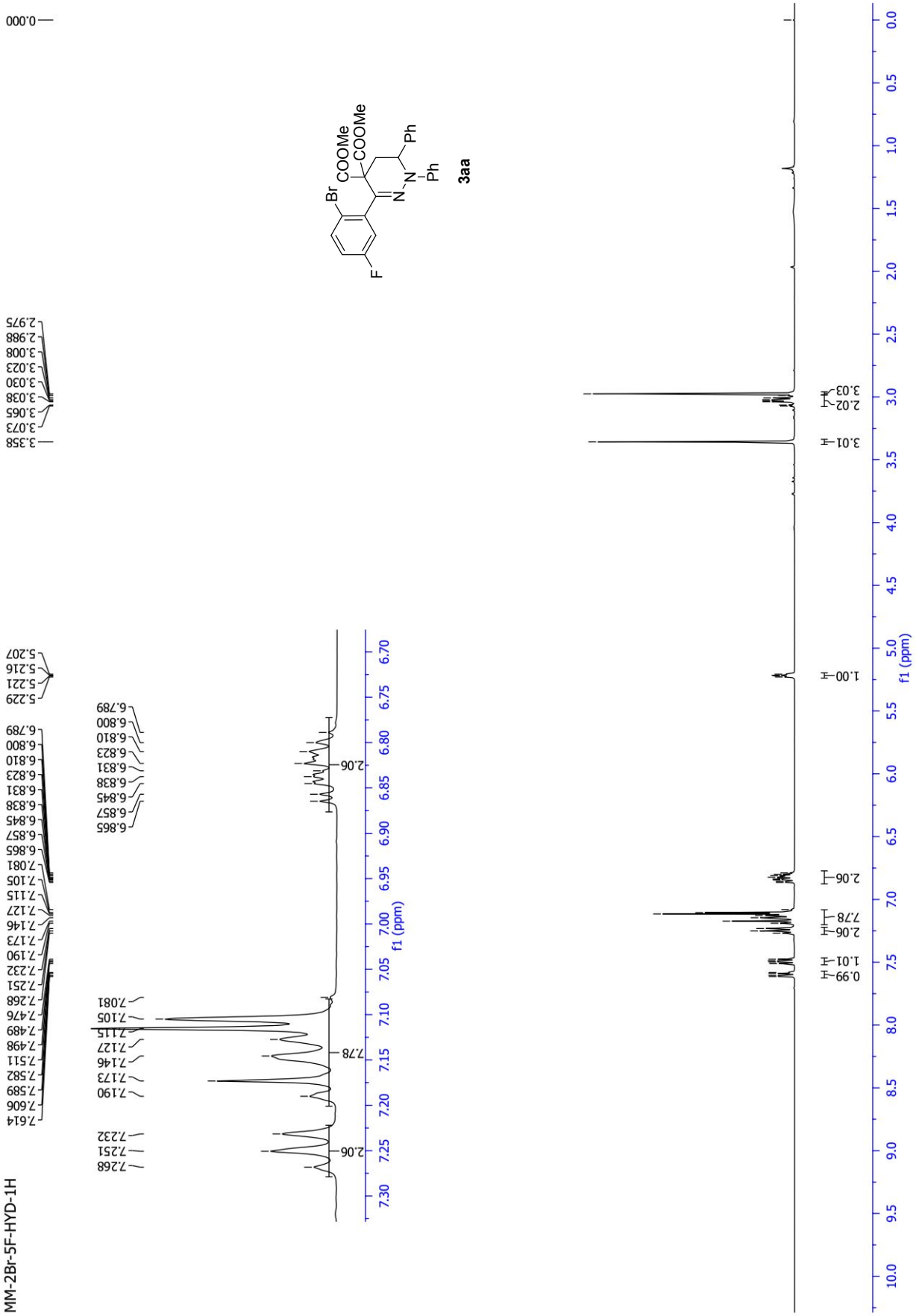

MM-4NO2-HYD-13C
170.556
168.237
146.717
145.361
144.383
137.463
131.087
129.331
128.991
128.083
127.214
126.764
123.533
122.178
115.011
77.441
77.338
77.018
54.217
53.707
52.839
52.818
33.862
COOMe
COOMe
Ph
Ph
N
N
O_2N
3x
f1 (ppm)

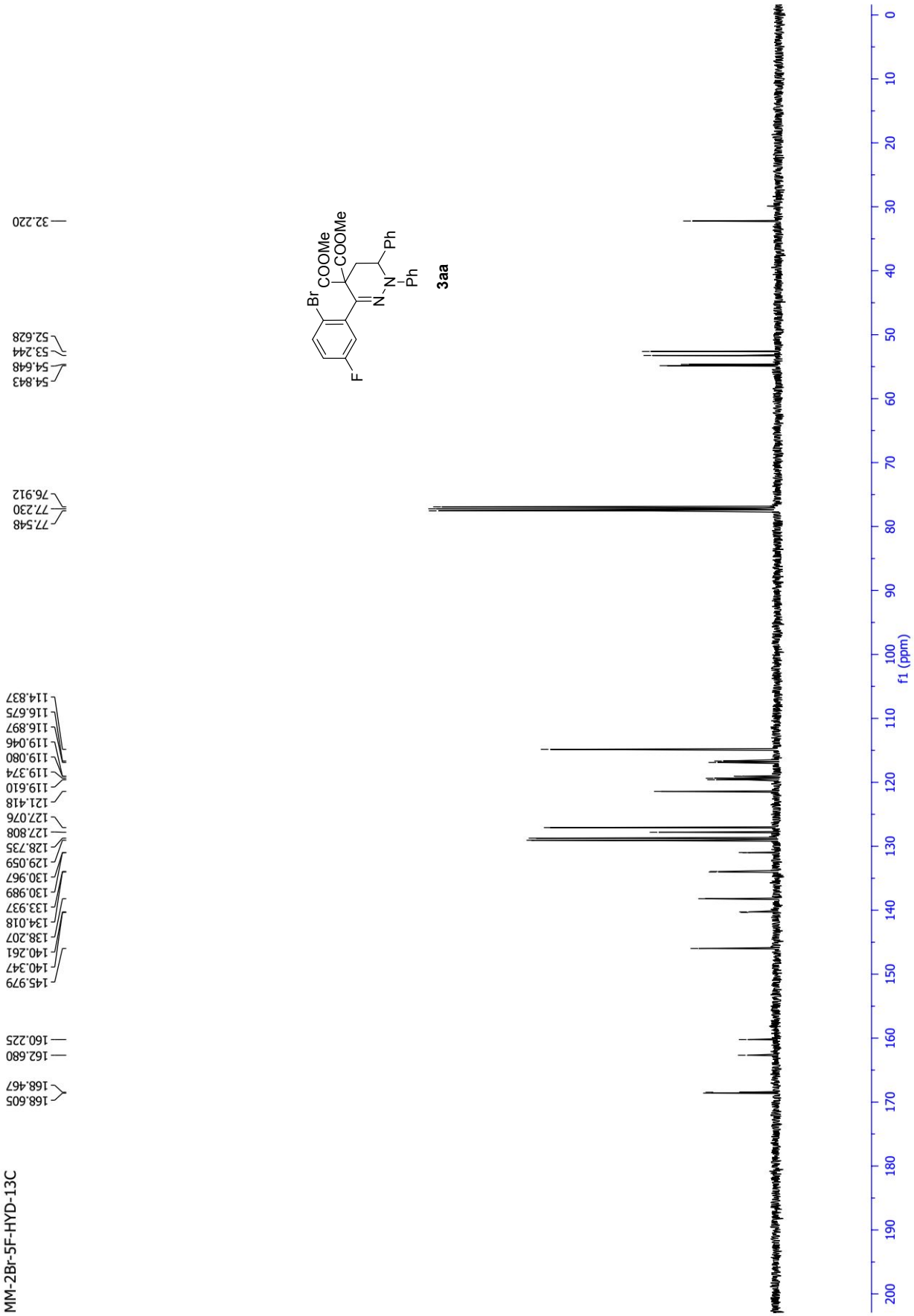

MM-2-NAP-HYD-1H
COOMe
COOMe
Ph
Ph
N
N
3y
f1 (ppm)

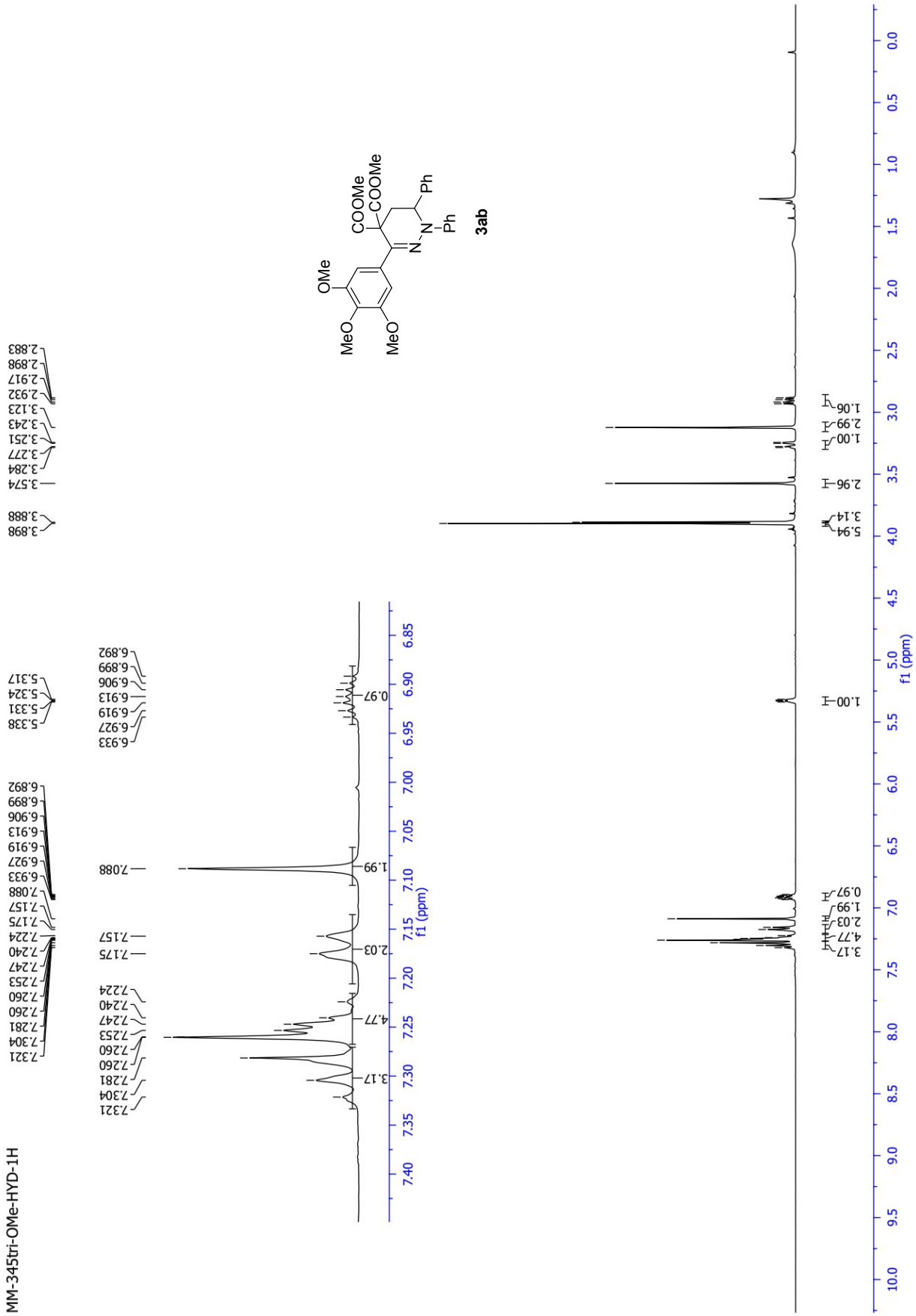

MM-2Nap-HYD-13C
170.894
168.706
145.953
138.216
135.786
133.623
133.394
133.034
129.153
128.828
128.733
127.774
127.643
127.622
126.944
126.185
126.115
126.032
125.460
121.114
114.635
77.548
77.230
76.912
53.977
53.424
53.347
52.592
34.069
COOMe
COOMe
Ph
N
N
Ph
3y
f1 (ppm)

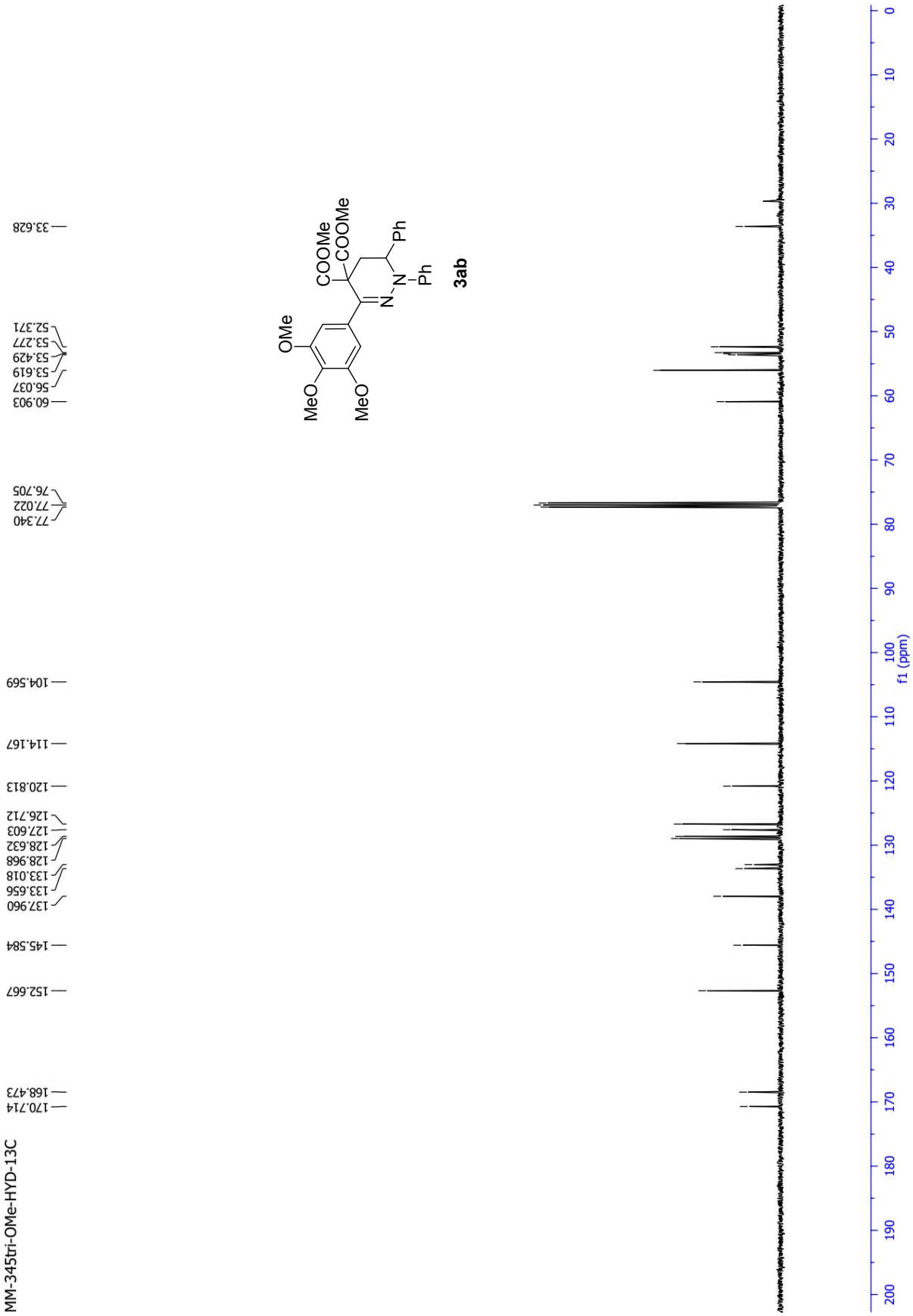

MM-2thio-HYD-1H
COOMe
COOMe
Ph
N
N
Ph
S
3z'
f1 (ppm)

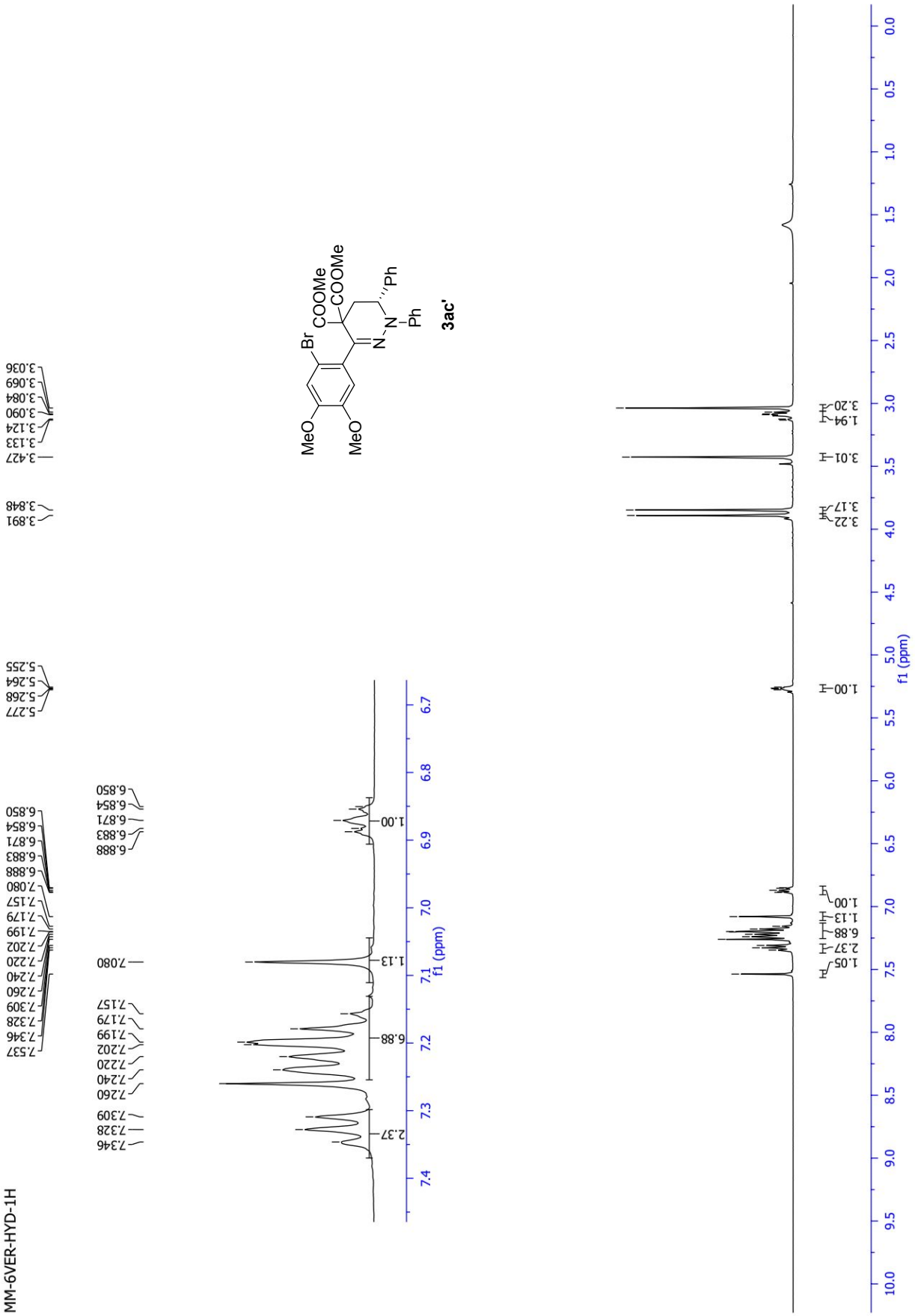

MM-2thio-HYD-13C
170.757
167.988
145.401
143.959
137.578
129.835
129.168
128.836
127.820
127.349
126.755
125.160
124.402
121.155
114.407
77.441
77.230
77.018
53.587
53.568
53.031
52.638
33.523
COOMe
COOMe
Ph
Ph
3z
f1 (ppm)

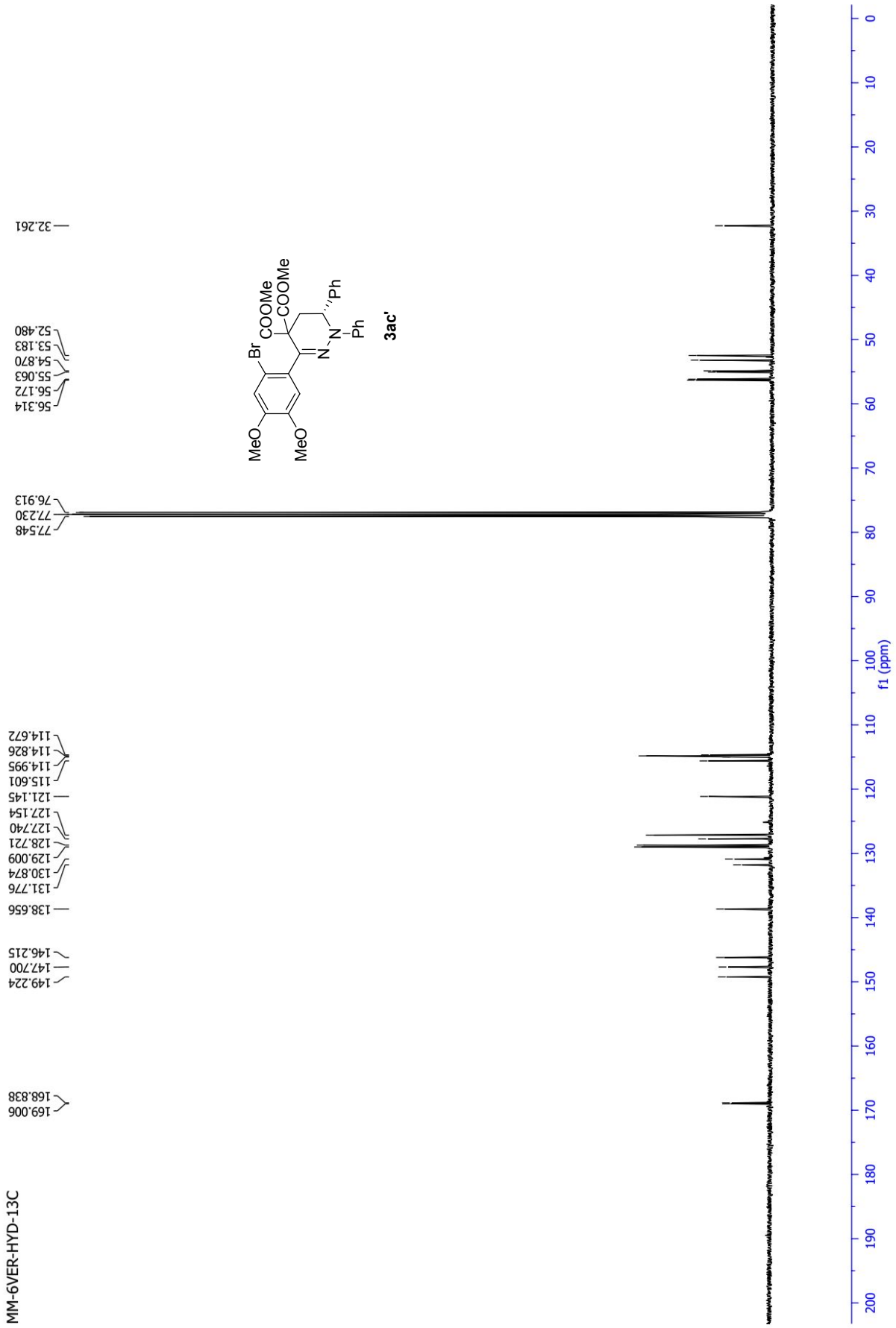

MM-2Br-5F-HYD-1H
3aa
f1 (ppm)

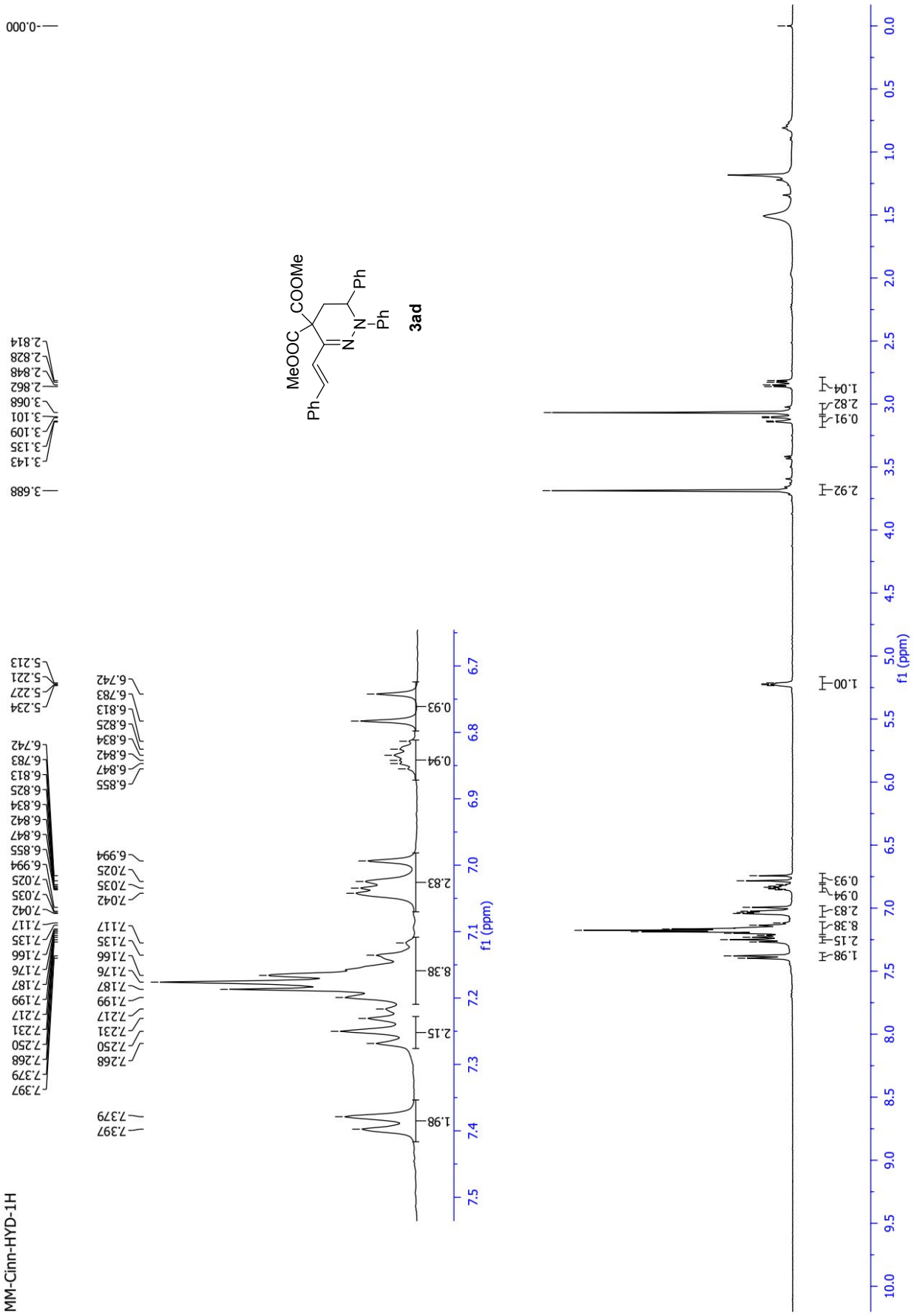

MM-2Br-5F-HYD-13C
168.605
168.467
162.680
160.225
145.979
140.347
140.261
138.207
134.018
133.937
130.989
130.967
129.059
128.735
127.808
127.076
121.418
119.610
119.374
119.080
119.046
116.897
116.675
114.837
77.548
77.230
76.912
54.843
54.648
53.244
52.628
32.220
Br
COOMe
COOMe
N
N
Ph
Ph
F
3aa
f1 (ppm)

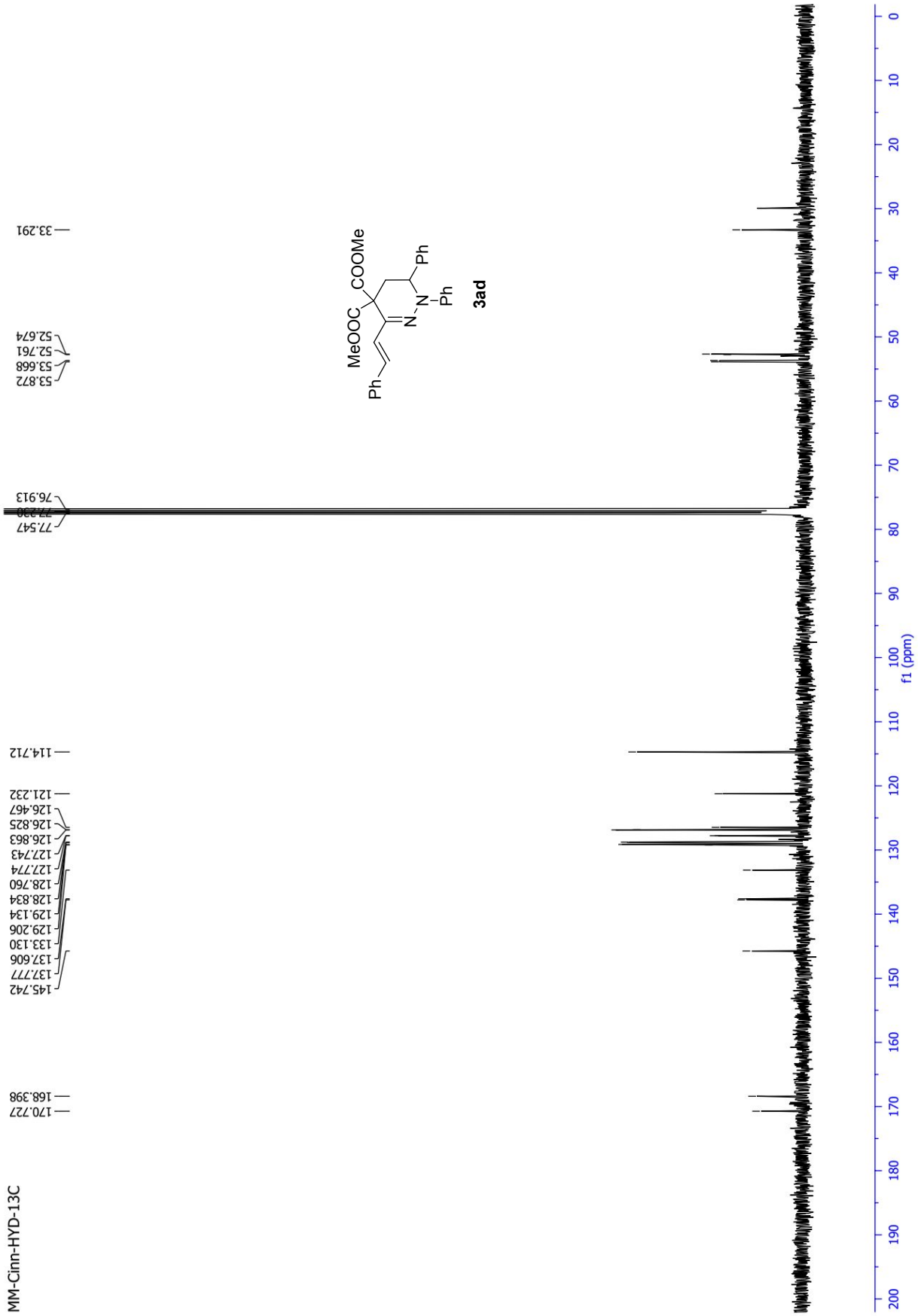

MM-345tri-OMe-HYD-1H
3ab
f1 (ppm)

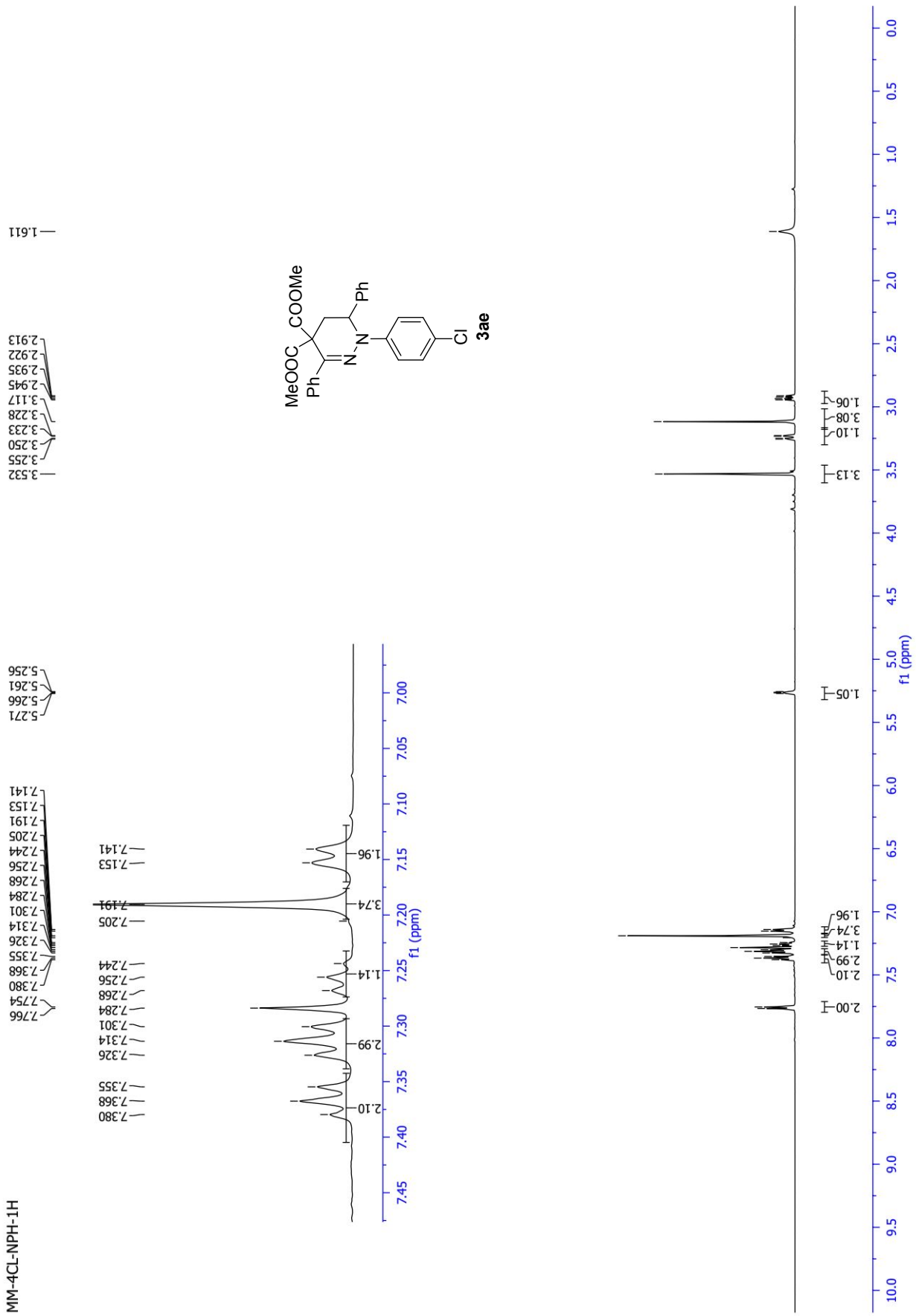

MM-345tri-OMe-HYD-13C
170.714
168.473
152.667
145.584
137.960
133.656
133.018
128.968
128.632
127.603
126.712
120.813
114.167
104.569
77.340
77.022
76.705
60.903
56.037
53.619
53.429
53.277
52.371
33.628
MeO
MeO
OMe
COOMe
COOMe
N
N
Ph
Ph
3ab
f1 (ppm)

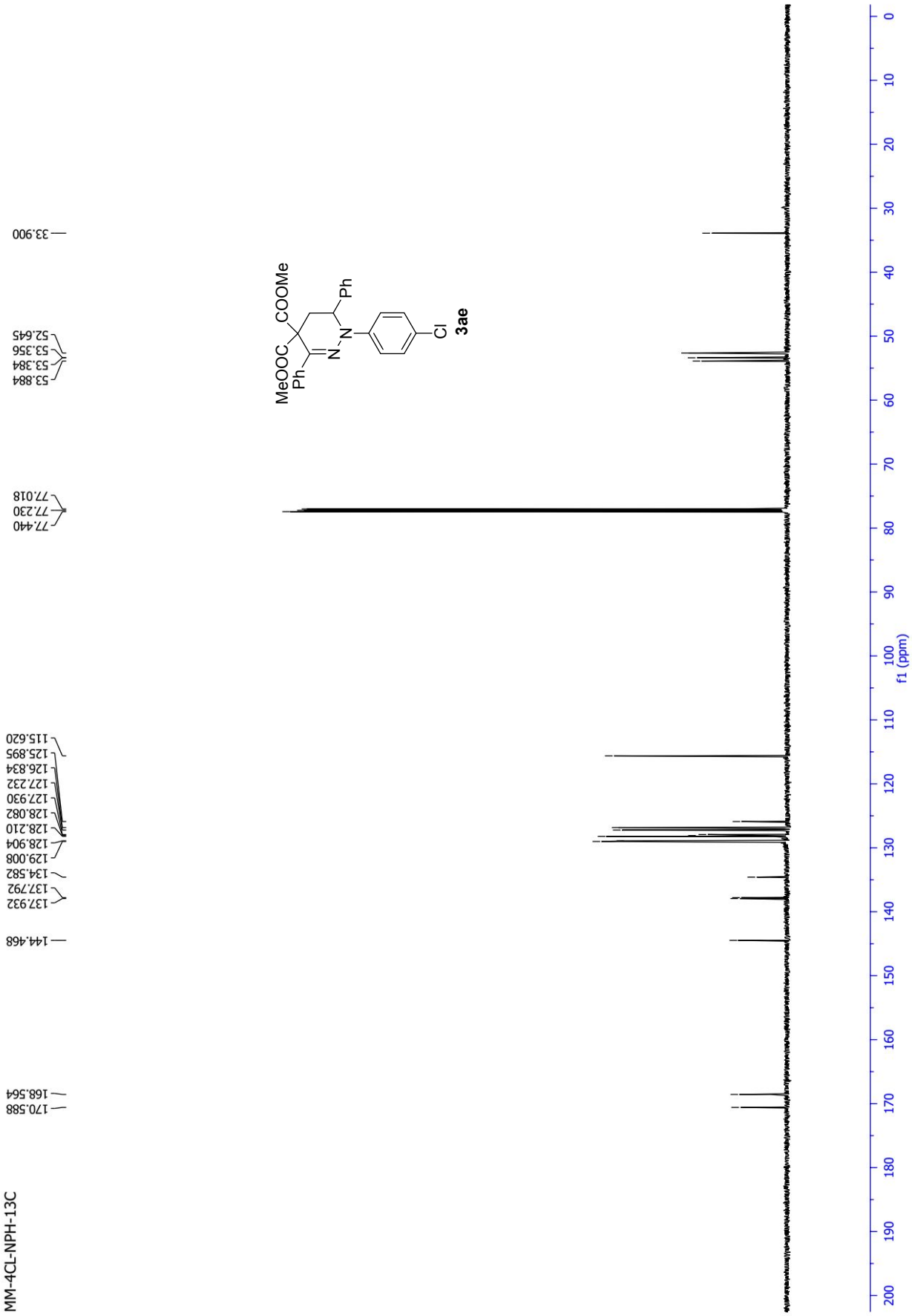

MM-6VER-HYD-1H
3ac'
f1 (ppm)

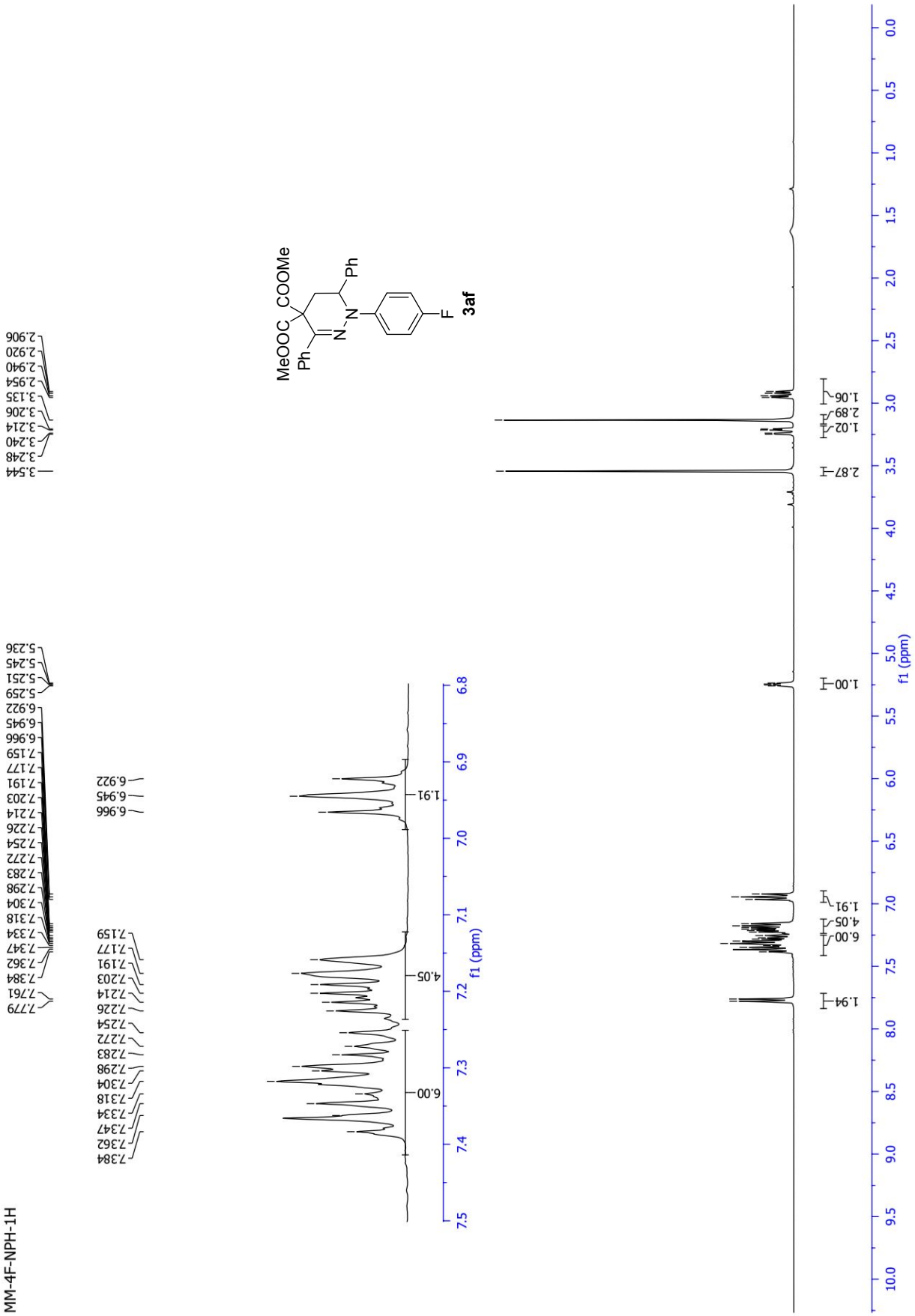

MM-6VER-HYD-13C
169.006
168.838
149.224
147.700
146.215
138.656
131.776
130.874
129.009
128.721
127.740
127.154
121.145
115.601
114.995
114.826
114.672
77.548
77.230
76.913
56.314
56.172
55.063
54.870
53.183
52.480
32.261
MeO
MeO
Br
COOMe
COOMe
N
N
Ph
Ph
3ac'
f1 (ppm)

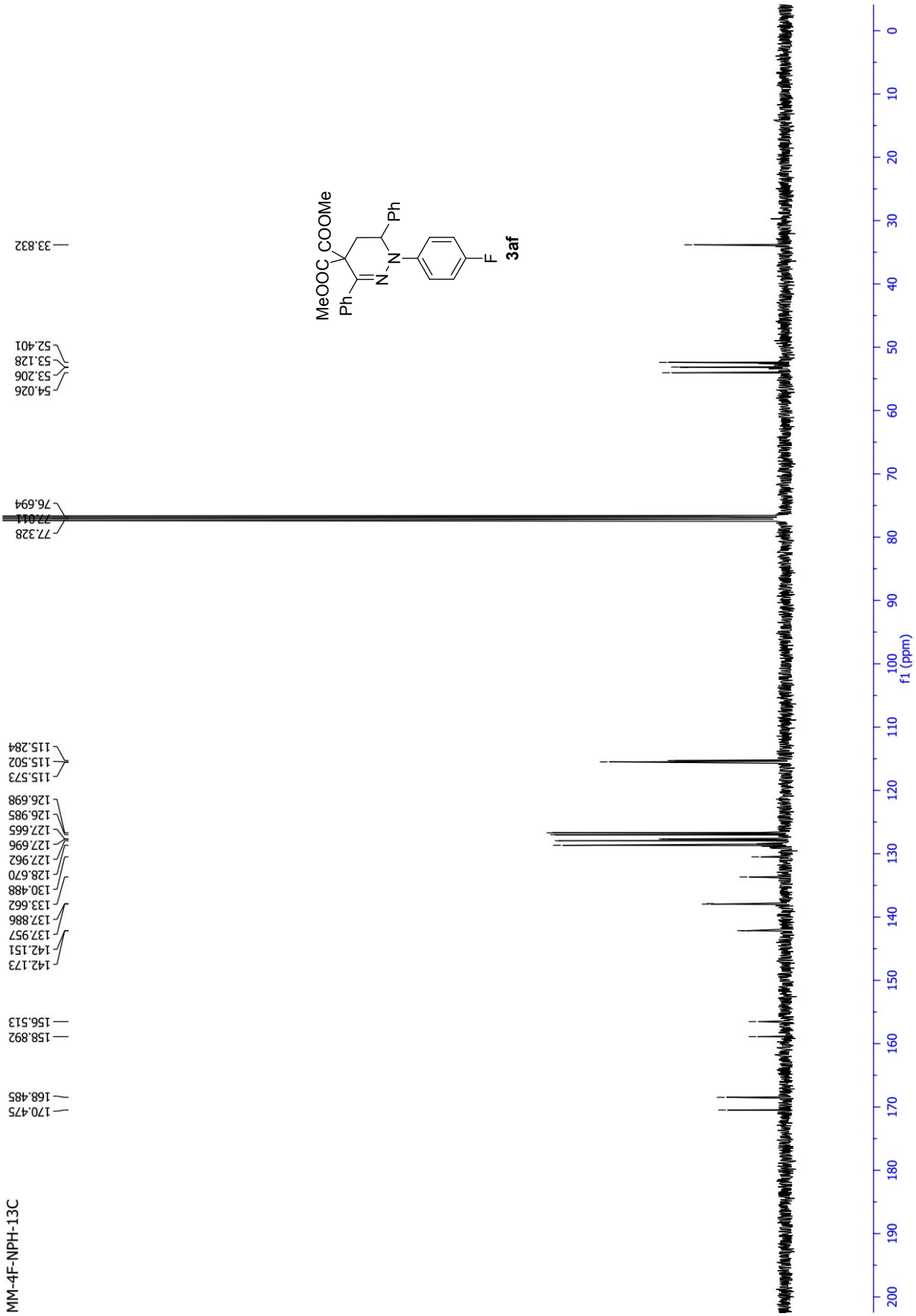

MM-Cinn-HYD-1H
MeOOC
COOMe
Ph
Ph
Ph
Ph
3ad
f1 (ppm)

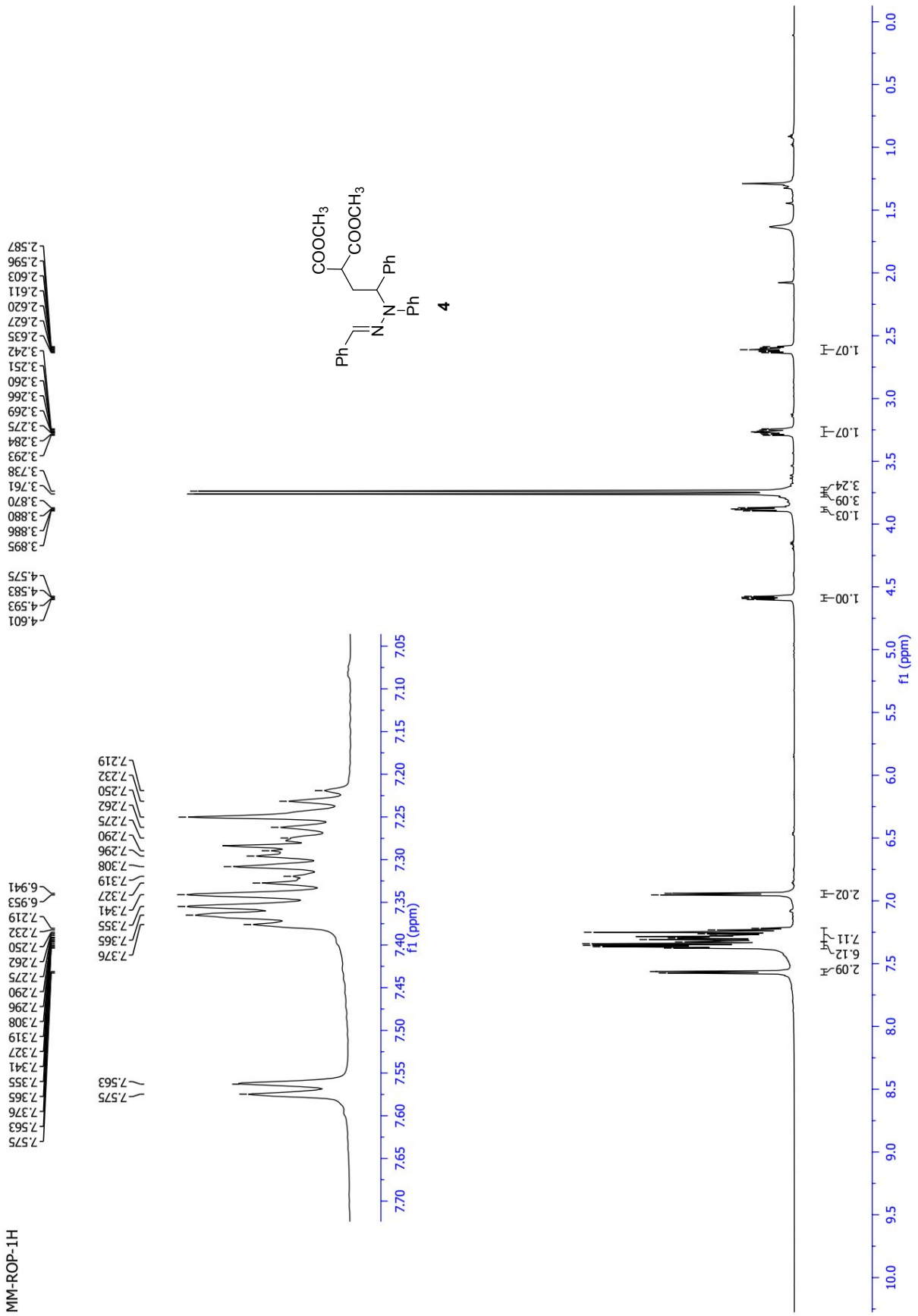

MM-Cinn-HYD-13C
170.727
168.398
145.742
137.777
137.606
133.130
129.206
129.134
128.834
128.760
127.774
127.743
126.863
126.825
126.467
121.232
114.712
77.547
76.913
53.872
53.668
52.761
52.674
33.291
MeOOC
COOMe
Ph
N
N
Ph
Ph
3ad
f1 (ppm)

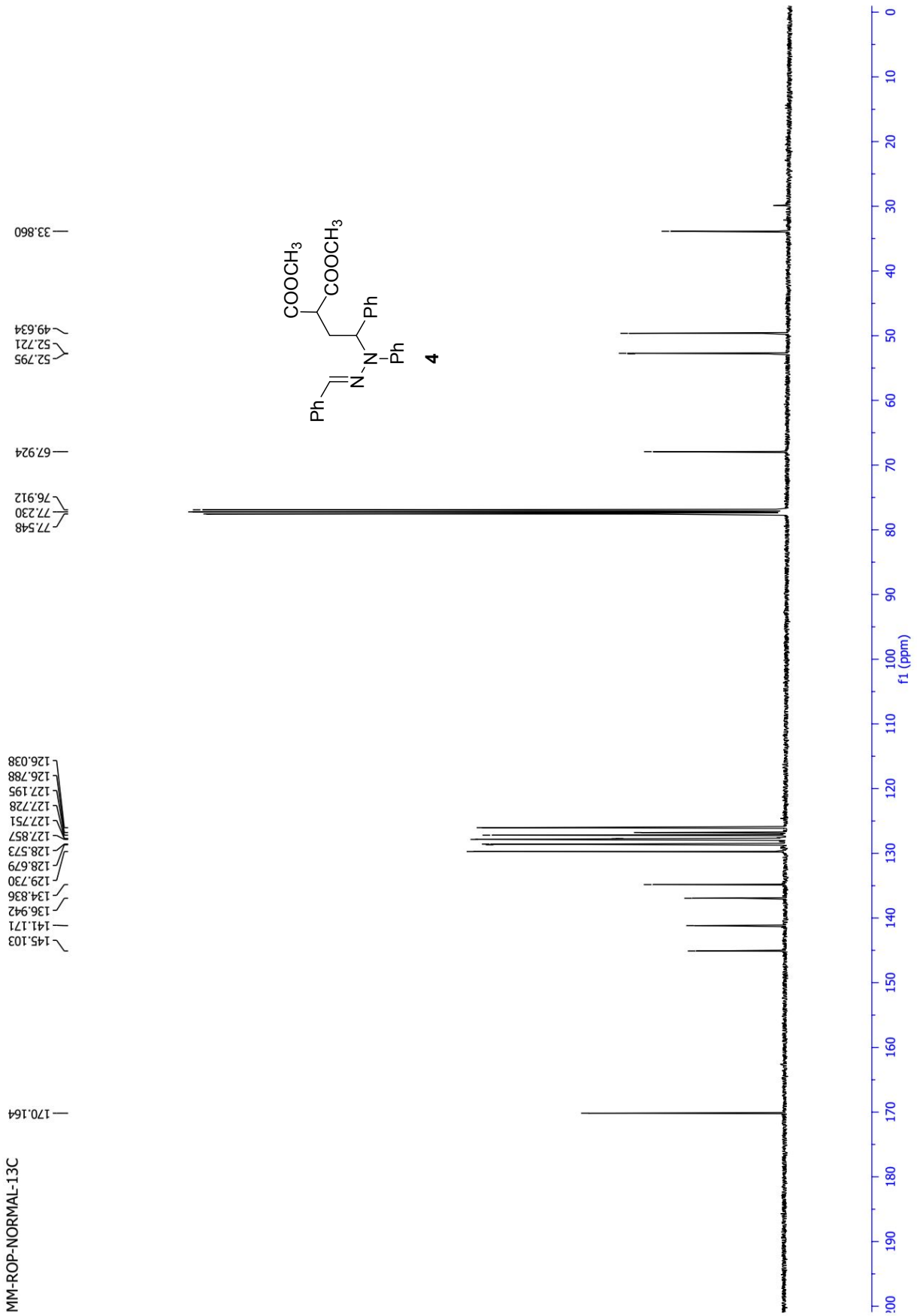

MM-4Cl-NPH-1H
MeOOC
COOMe
Ph
Ph
N
N
Cl
3ae
f1 (ppm)

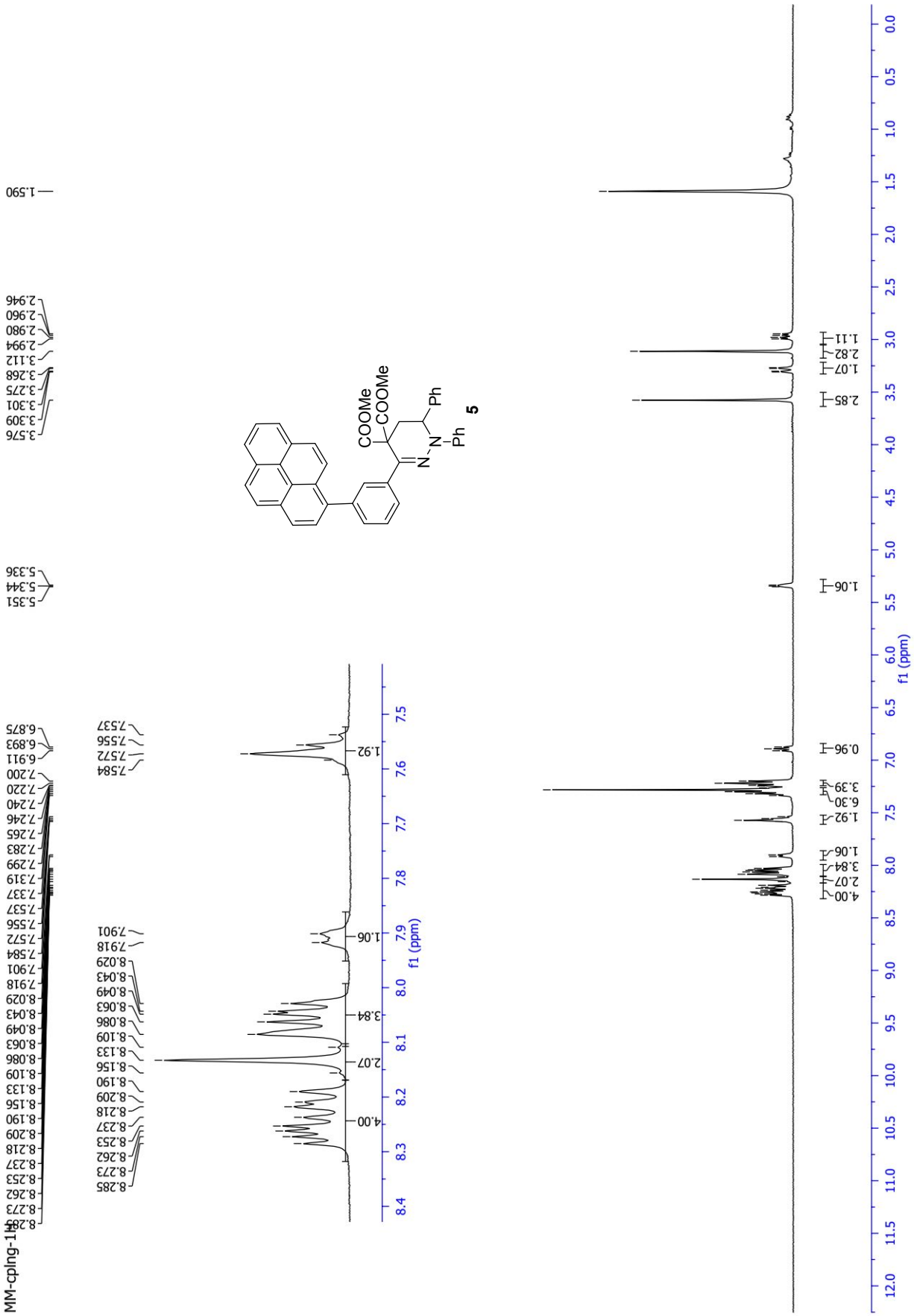

MM-4CL-NPH-13C
170.588
168.564
144.468
137.932
137.792
134.582
129.008
128.904
128.210
128.082
127.930
127.232
126.834
125.895
115.620
77.440
77.230
77.018
53.884
53.384
53.356
52.645
33.900
MeOOC
COOMe
Ph
Ph
N
N
Cl
3ae
f1 (ppm)

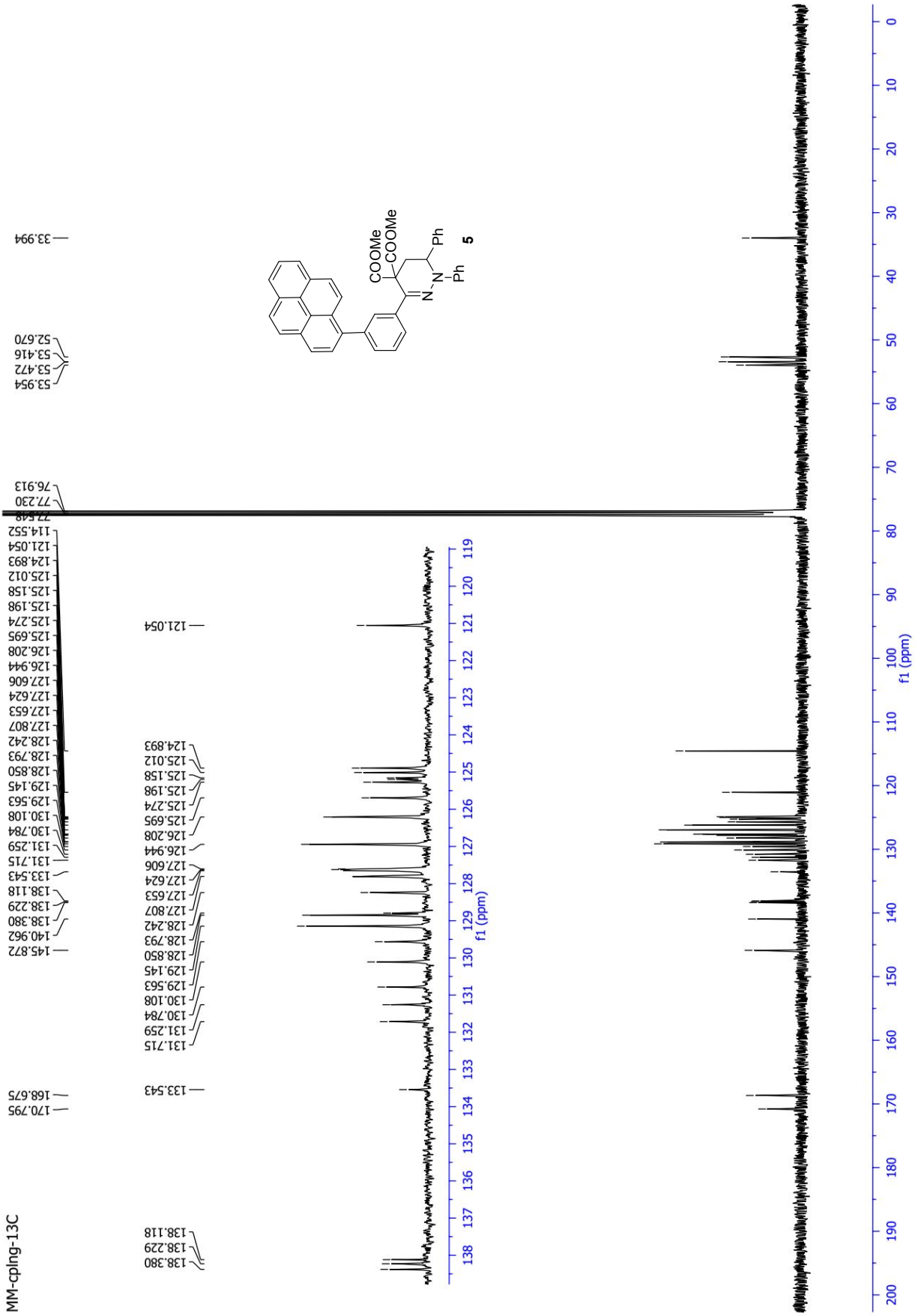

MM-4F-NPH-1H
MeOOC
COOMe
Ph
Ph
N
N
F
3af
f1 (ppm)


MM-4F-NPH-13C
170.475
168.485
158.892
156.513
142.173
142.151
137.957
137.886
133.662
130.488
128.670
127.962
127.696
127.665
126.985
126.698
115.573
115.502
115.284
77.328
77.011
76.694
54.026
53.206
53.128
52.401
33.832
MeOOC
COOMe
Ph
Ph
N
N
F
3af
f1 (ppm)


MM-ROP-1H
COOCH3
COOCH3
Ph
Ph
N
N
Ph
Ph
4
f1 (ppm)
f1 (ppm)


MM-ROP-NORMAL-13C
170.164
145.103
141.171
136.942
134.836
129.730
128.679
128.573
127.857
127.751
127.728
127.195
126.788
126.038
77.548
77.230
76.912
67.924
52.795
52.721
49.634
33.860
COOCH3
COOCH3
Ph
Ph
N
N
Ph
Ph
4
f1 (ppm)


MM-cplng-1H
COOMe
COOMe
Ph
Ph
5


MM-cpIng-13C
COOMe
COOMe
Ph
Ph
5
f1 (ppm)