

## SUPPORTING INFORMATION

### A Green and Sustainable Procedure for the Functionalization of Morpholin-2-ones by Oxidative Imidation reactions

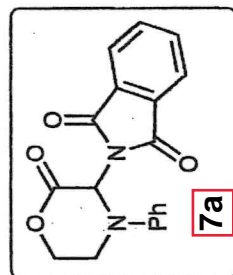
Ana Maria Faisca Phillips<sup>1\*</sup> and Armando J. L. Pombeiro<sup>1,2</sup>

<sup>1</sup>Coordination Chemistry and Catalysis Group, Centro de Química Estrutural, Institute of Molecular Sciences, Instituto Superior Técnico, Universidade de Lisboa,  
Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal

<sup>2</sup>Research Institute of Chemistry, Peoples' Friendship University of Russia (RUDN University),  
117198 Moscow, Russia

20211117-AMFP-21-2632set 1 1 D:\NMR-Files\IST-2021

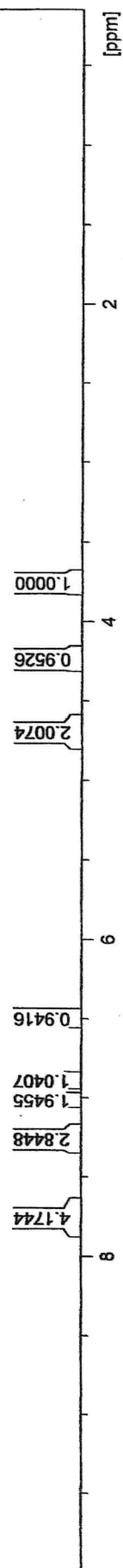
20211117-AMFP-21-2632set



7a

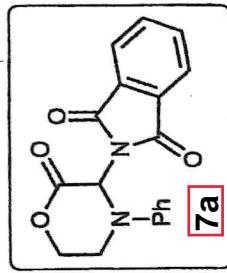
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

7.8459, 7.8383, 7.8322, 7.8246, 7.7395, 7.7319, 7.7259, 7.7182, 7.3001, 7.2856, 7.2818, 7.2785, 7.2600, 7.0310, 7.0097, 6.9298, 6.9115, 6.8933, 6.5155, 4.7731, 4.7654, 4.7594, 4.7460, 4.7381, 4.7322, 4.7090, 4.7013, 4.6820, 4.6742, 4.6548, 4.6470, 4.2831, 4.2750, 4.2561, 4.2491, 4.2418, 4.2228, 4.2146, 3.7774, 3.7714, 3.7505, 3.7442, 3.7379



20211117-AMFP-21-2632set 2 1 D:\NMR-Files\IST-2021

20211117-AMFP-21-2632set



$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

— 167.4293  
— 164.4076  
— 144.8259  
— 134.4214  
— 131.5255  
— 129.4108  
— 123.7844  
— 121.1281  
— 115.7801

— 69.3224  
— 61.7198

— 42.2703

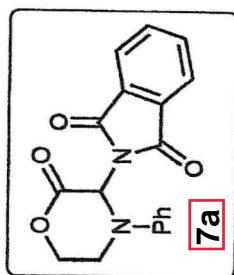
**7a**

[ppm]

50

100

150

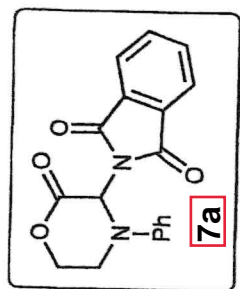


DEPT-135 NMR (100 MHz, CDCl<sub>3</sub>)

-134.4209  
 -129.4087  
 -123.7829  
 -121.1255  
 -115.7765  
 -69.3214  
 -61.7148  
 -42.2665

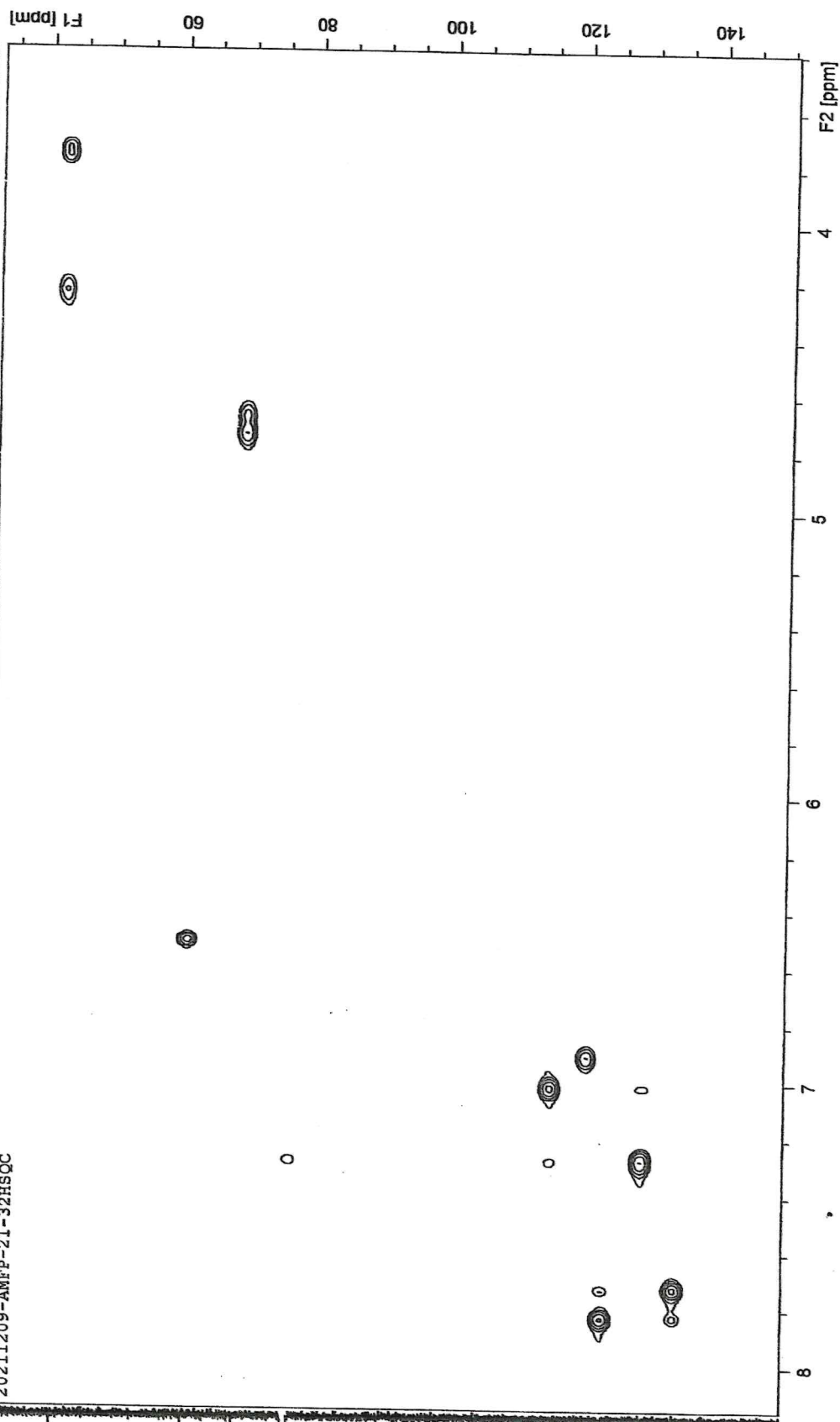
150 100 50 [ppm]

20211209-AMFP-21-32HSQC 1 1 D:\NMR-Files\IST-2021



HMQC (CDCl<sub>3</sub>)

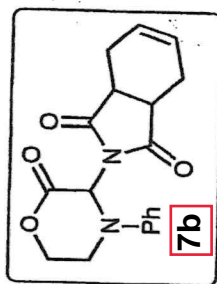
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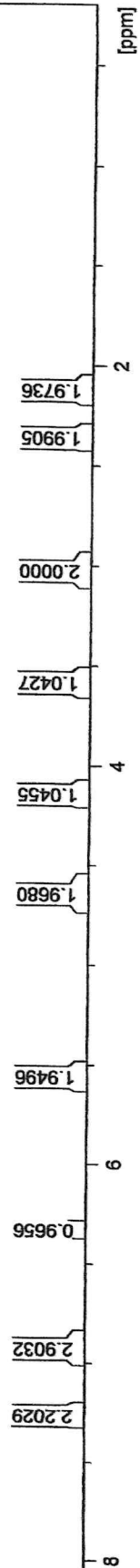
20220317-AMFP-21-87A 1 1 D:\NMR-Files\IST-2022

20220317-AMFP-21-87A

7.2763  
7.2579  
7.2392  
6.9518  
6.9342  
6.9168  
6.8898  
6.8703  
- 6.3267  
- 5.5365  
4.6715  
4.6441  
4.6048  
4.5695  
4.1680  
4.1362  
4.1091  
3.6001  
3.5676  
3.0769  
3.0567  
3.0374  
3.0041  
2.9848  
2.9642  
2.3799  
2.3452  
2.1559  
2.1395  
2.1185  
2.1020

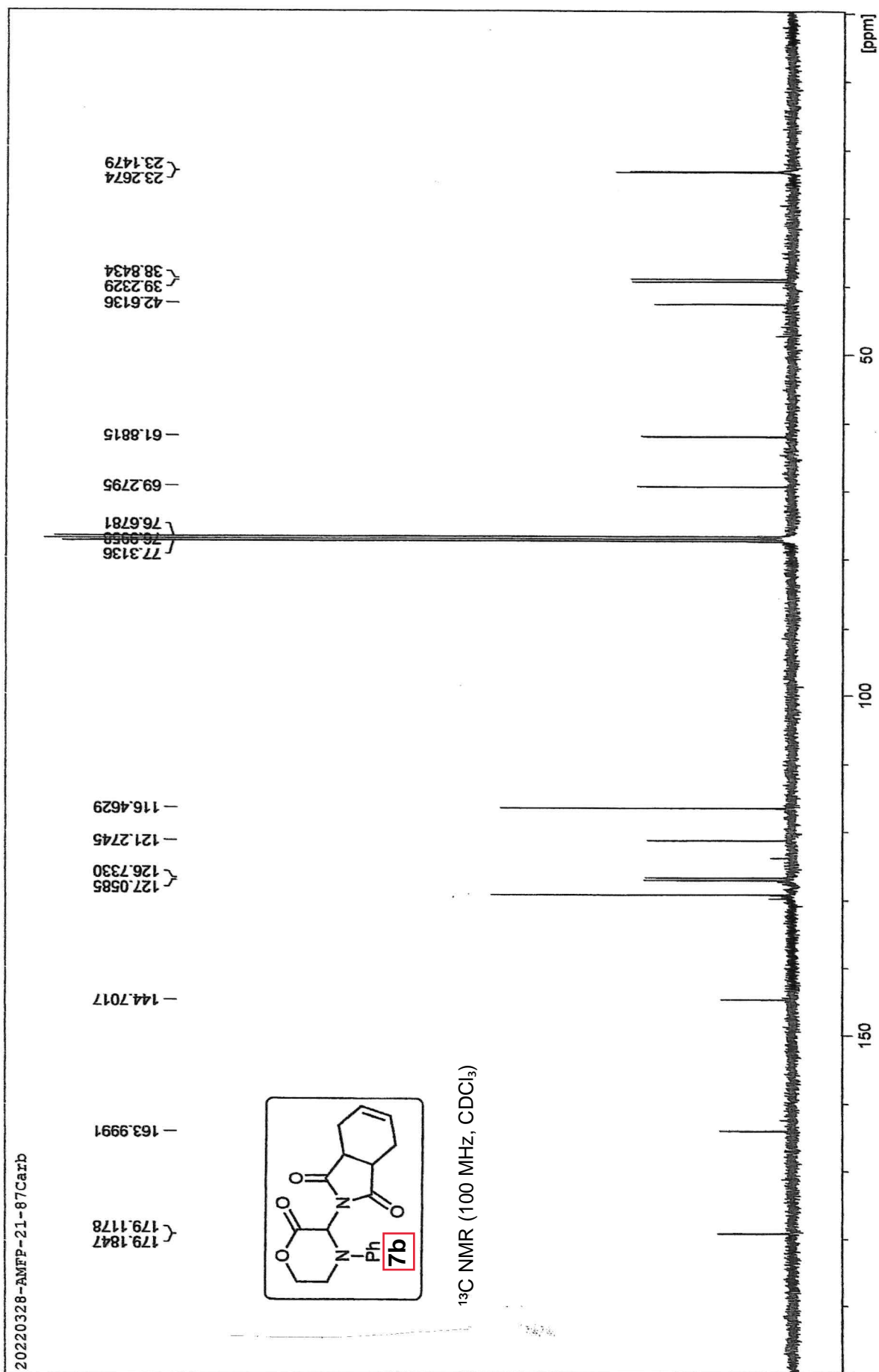


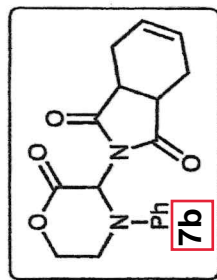
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



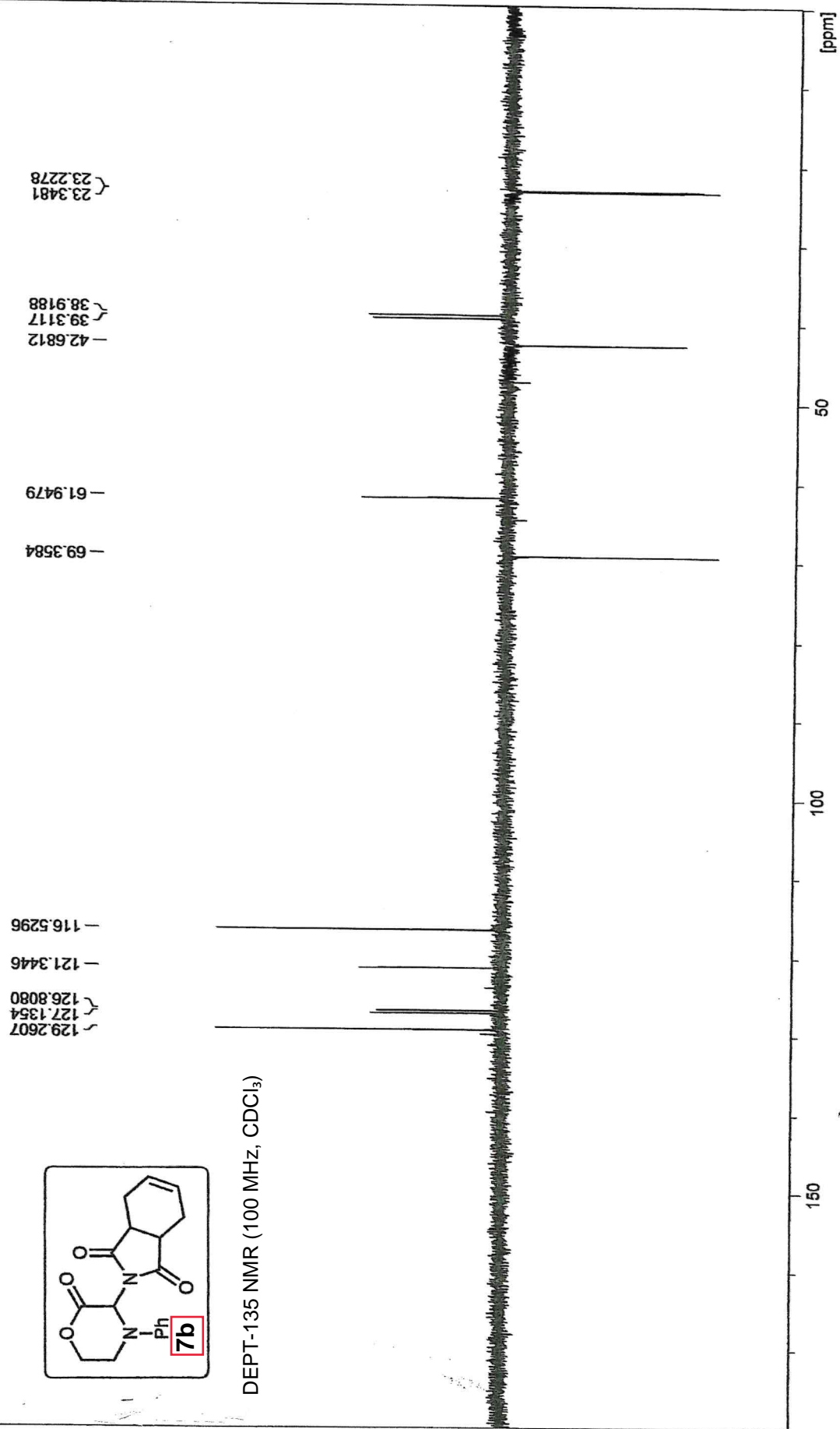
20220328-AMFP-21-87Carb 3 1 D:\NMR-Files\IST-2022

20220328-AMFP-21-87Carb





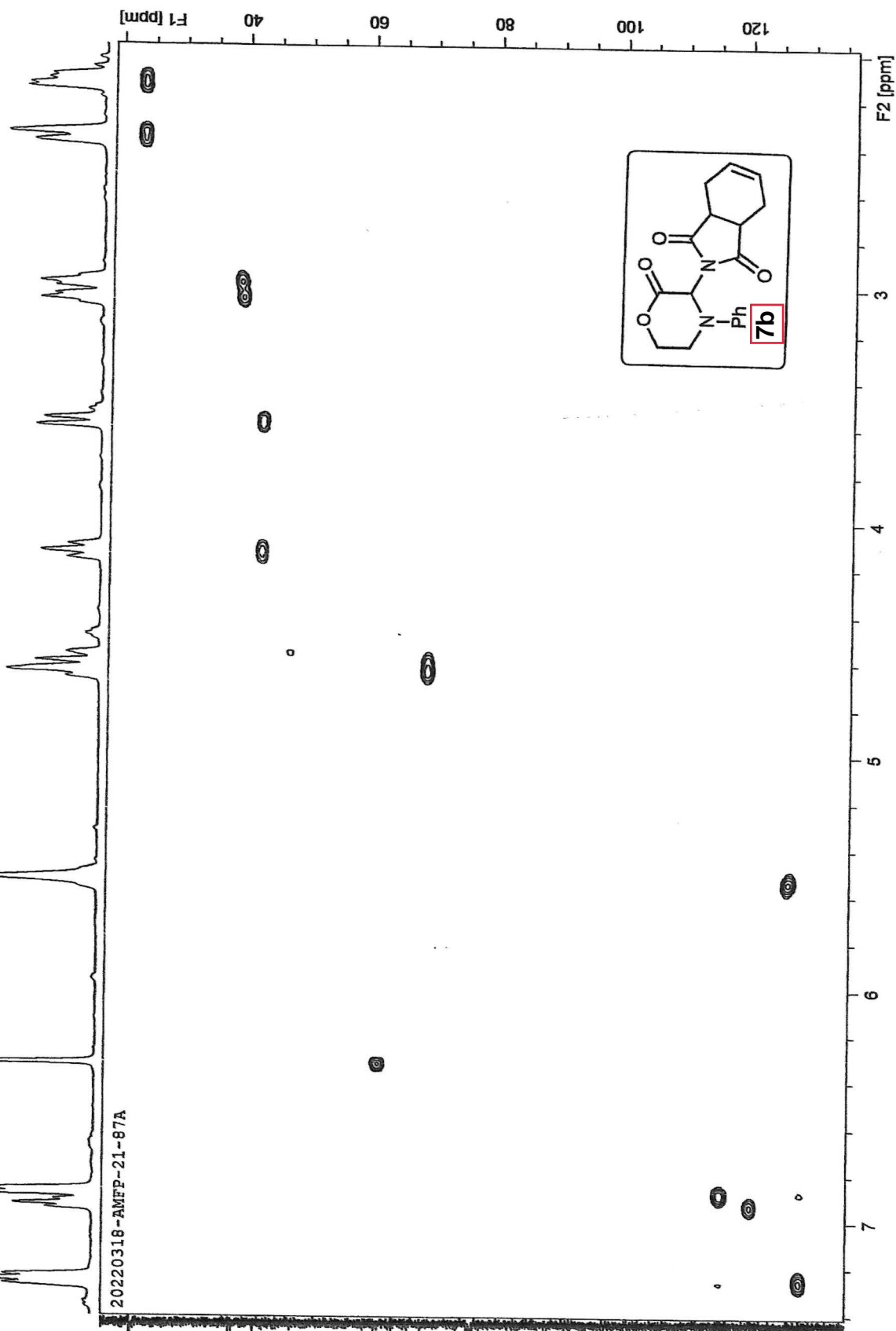
DEPT-135 NMR (100 MHz, CDCl<sub>3</sub>)

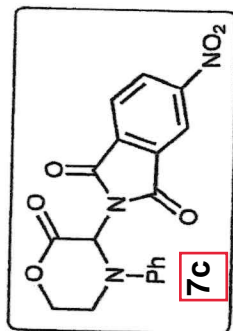




HMQC (CDCl<sub>3</sub>)

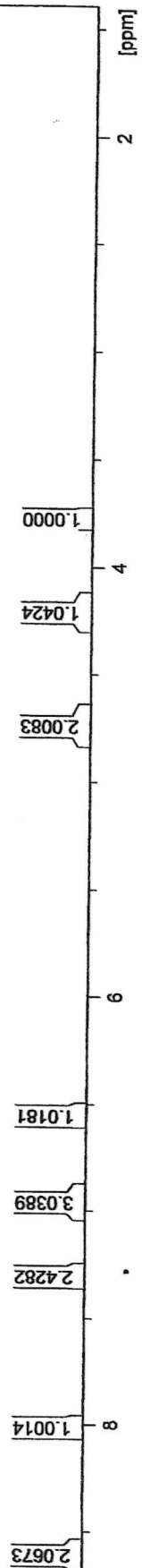
20220318-AMFP-21-87A 10 1 D:\NMR-Files\IST-2022





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

8.6349, 8.6066, 8.5864  
8.0380, 8.0179  
7.2944, 7.2784, 7.2589, 7.0039, 6.9844, 6.9413, 6.9233, 6.9058  
6.5490  
4.7708, 4.7456, 4.7187, 4.6916, 4.6647  
4.2427, 4.2125, 4.1837  
3.7845, 3.7511



20221109-AMFP-21-154set 3 1 D:\NMR-Files\IST-2022

20221109-AMFP-21-154set

165.3815  
165.0993  
163.9209

151.8900

144.5411

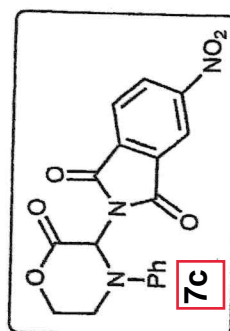
135.8443  
132.9228  
129.5841  
129.5395  
125.0609  
121.5807  
119.2010  
115.9269

77.3132  
76.5781

69.4438

62.2719

42.5504



$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

150 100 50 [ppm]

20221109-AMFP-21-154set 2 1 D:\NMR-Files\IST-2022

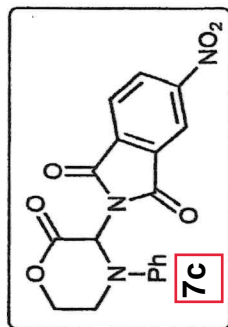
20221109-AMFP-21-154set

129.6273  
129.5819  
125.1055  
121.6207  
119.2443  
115.9640

69.4873

62.3089

42.5871



DEPT-135 NMR (100 MHz, CDCl<sub>3</sub>)

[ppm]

50

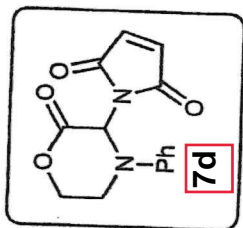
100

150

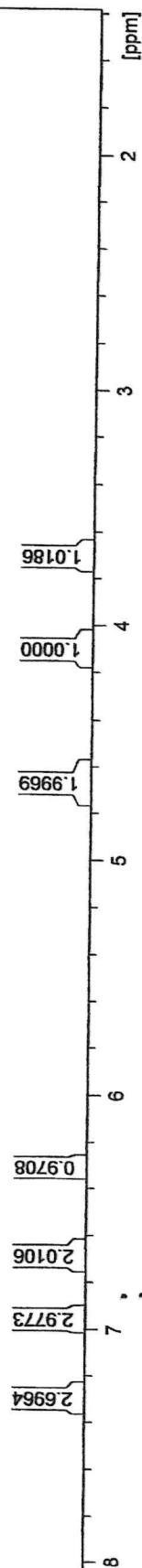
20220224-AMFP-21-75Ad 1 1 D:\NMR-Files\IST-2022

20220224-AMFP-21-75AD

7.3136  
7.2942  
7.2834  
7.2735  
6.9681  
6.9638  
6.9518  
6.9417  
6.6854  
6.2990  
4.7200  
4.7136  
4.7120  
4.7058  
4.6928  
4.6866  
4.6787  
4.6614  
4.6536  
4.6345  
4.6267  
4.6073  
4.5995  
4.1376  
4.1292  
4.1106  
4.1035  
4.0957  
4.0773  
4.0688  
3.7205  
3.7139  
3.7073  
3.6871  
3.6805  
3.6739

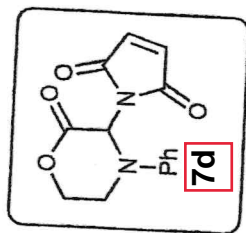


<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



20220224-AMFP-21-75Ad 1 1 D:\NMR-Files\IST-2022

20220224-AMFP-21-75AD

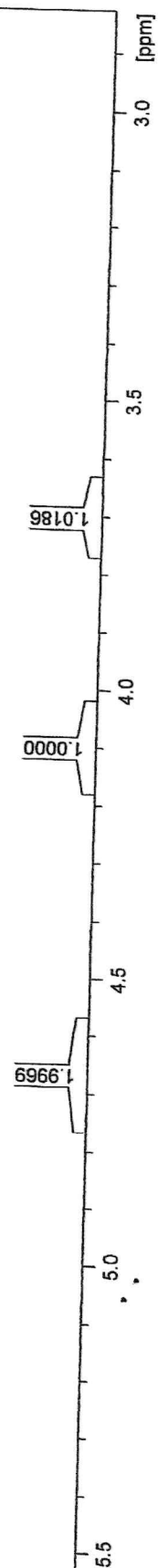


$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

3.7205  
3.7139  
3.7073  
3.6871  
3.6805  
3.6739

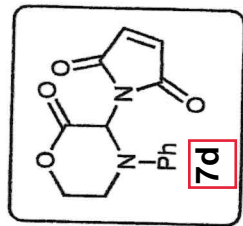
4.1376  
4.1292  
4.1106  
4.1035  
4.0957  
4.0773  
4.0688

4.7200  
4.7136  
4.7120  
4.7058  
4.6928  
4.6866  
4.6787  
4.6614  
4.6536  
4.6345  
4.6267  
4.6073  
4.5995



20220224-AMFP-21-75Ad 10 1 D:\NMR-Files\IST-2022

20220224-AMFP-21-75AD



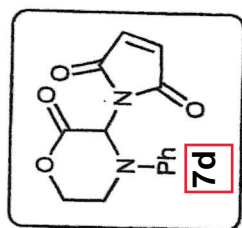
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

Chemical shift values (ppm):  
-169.7142  
-164.2222  
-144.7099  
-134.4123  
-129.4108  
-121.3470  
-115.9215  
77.3073  
76.9895  
76.6717  
-69.2724  
-61.6511  
-42.1587

[ppm]

20220224-AMFP-21-75Ad 2 1 D:\NMR-Files\IST-2022

20220224-AMFP-21-75AD



DEPT-135 NMR (100 MHz, CDCl<sub>3</sub>)

Chemical shift values (ppm):

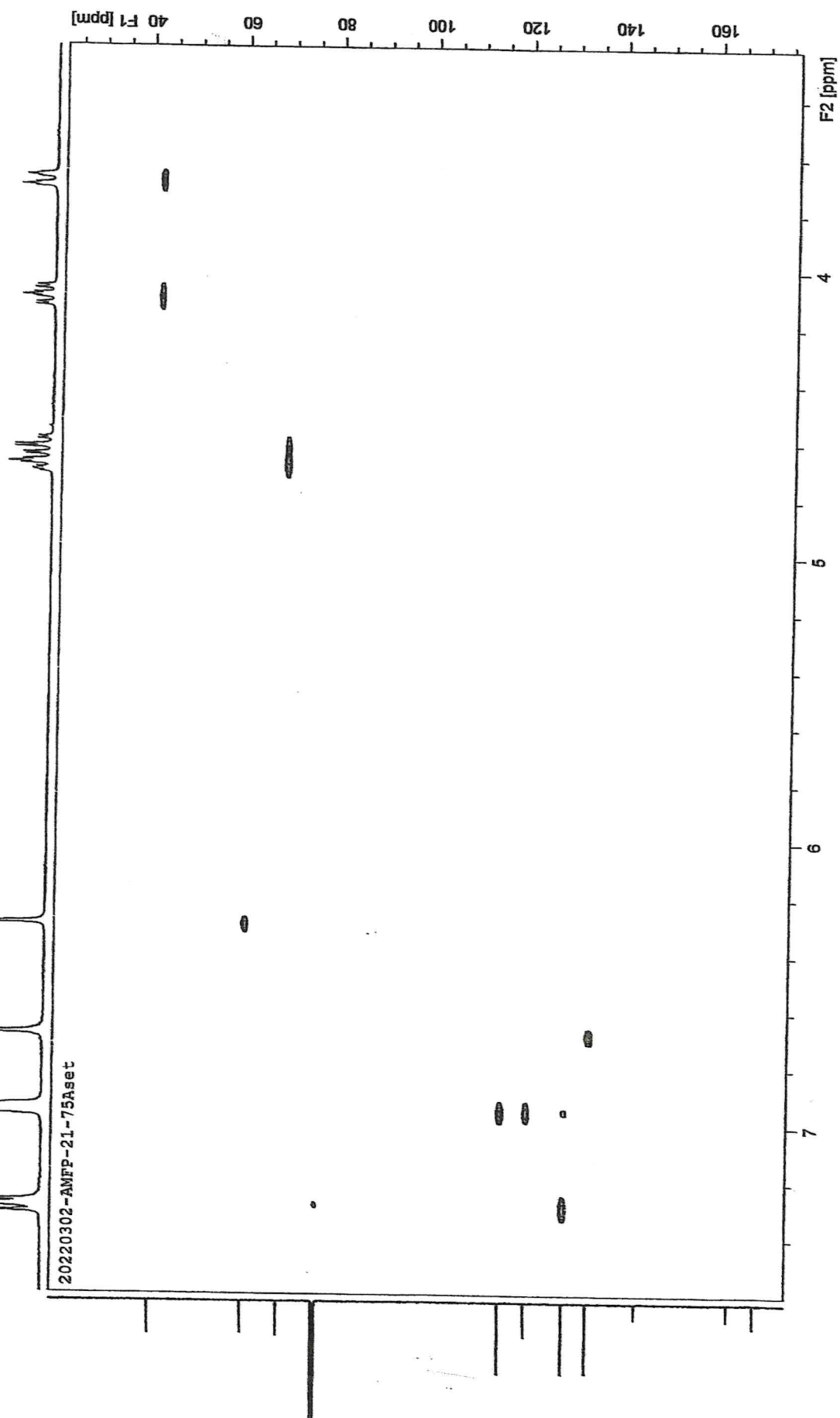
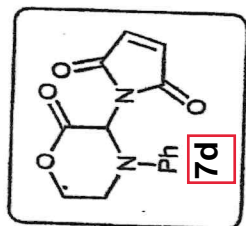
- 134.4854
- 129.4833
- 121.4169
- 115.9878
- 69.3476
- 61.7175
- 42.2247

[ppm]

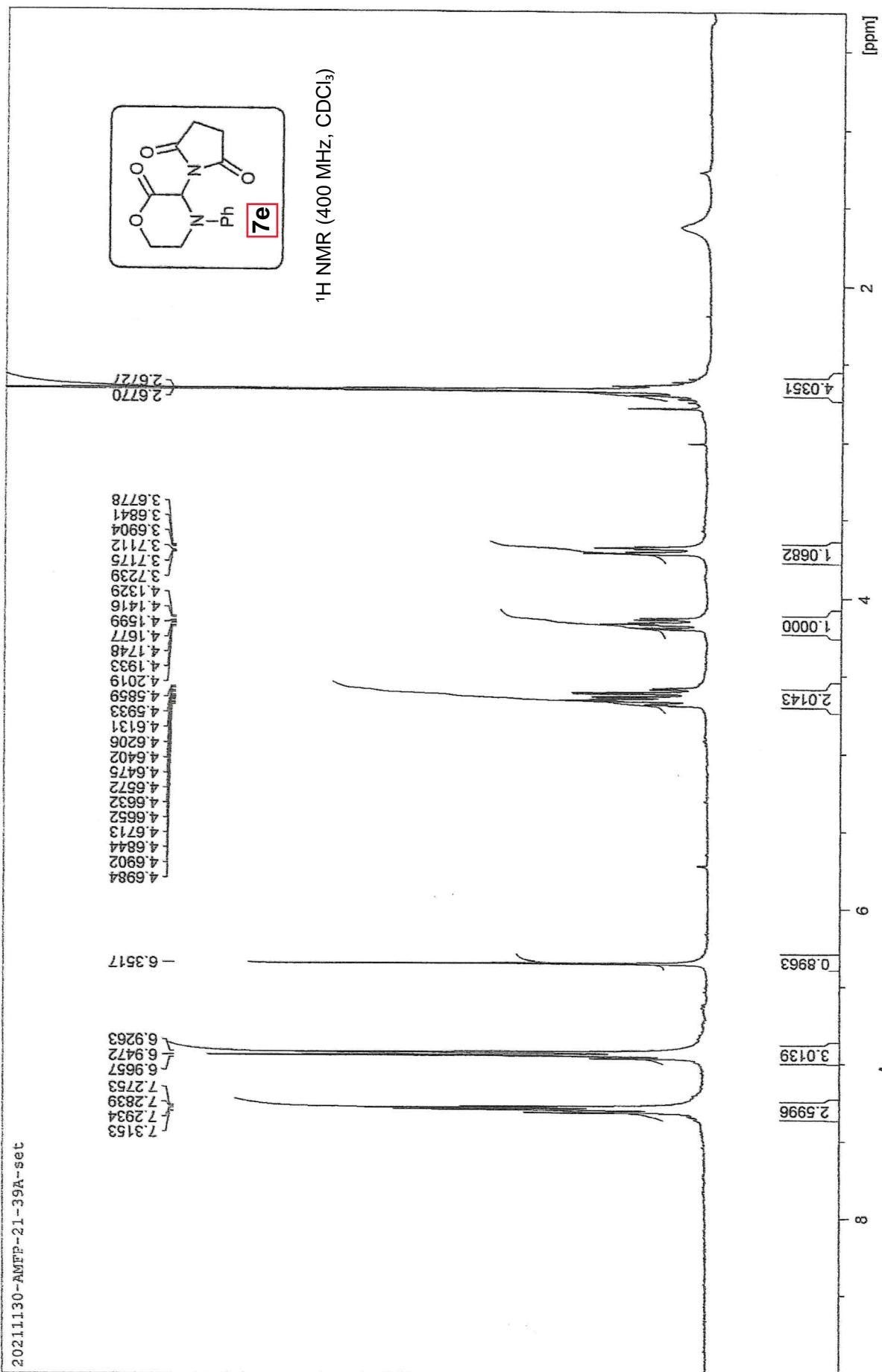


HMQC (CDCl<sub>3</sub>)

20220302-AMFP-21-75Aset 2 1 D:\NMR-Files\IST-2022



20211130-AMFP-21-39A-set 10 1 D:\NMR-Files\IST-2021  
20211130-AMFP-21-39A-set



20211130-AMFP-21-39A-set 4 1 D:\NMR-Files\IST-2021

20211130-AMFP-21-39A-set

176.1942

164.0337

144.6370

129.4274

121.1042

115.5848

77.3013

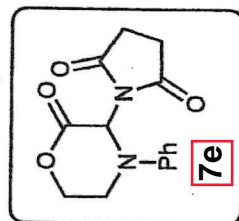
76.6659

69.3044

61.8730

42.5511

27.9831



$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

150

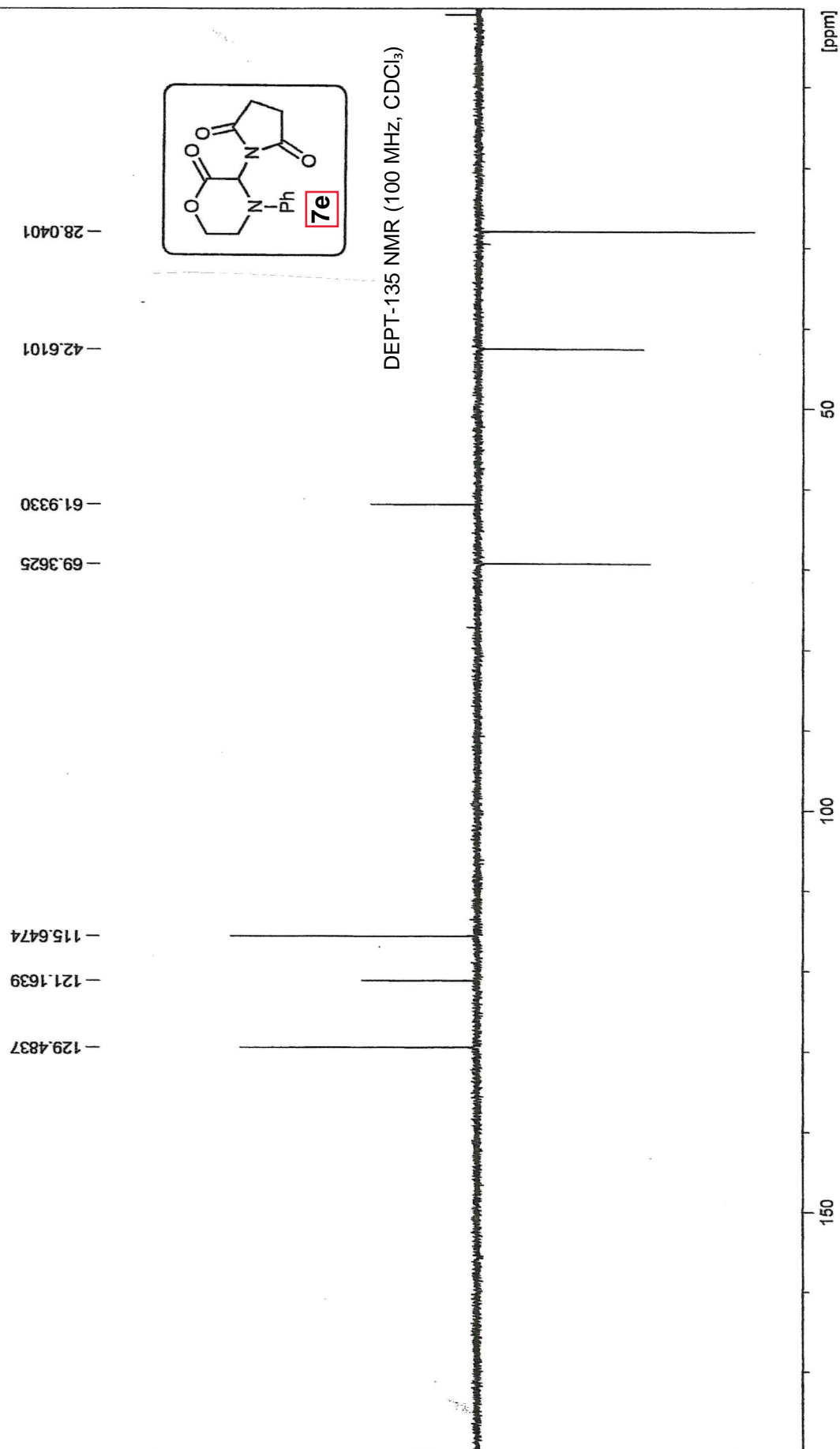
100

50

[ppm]

20211202-AMFP-21-39Aset2 3 1 D:\NMR-Files\IST-2021

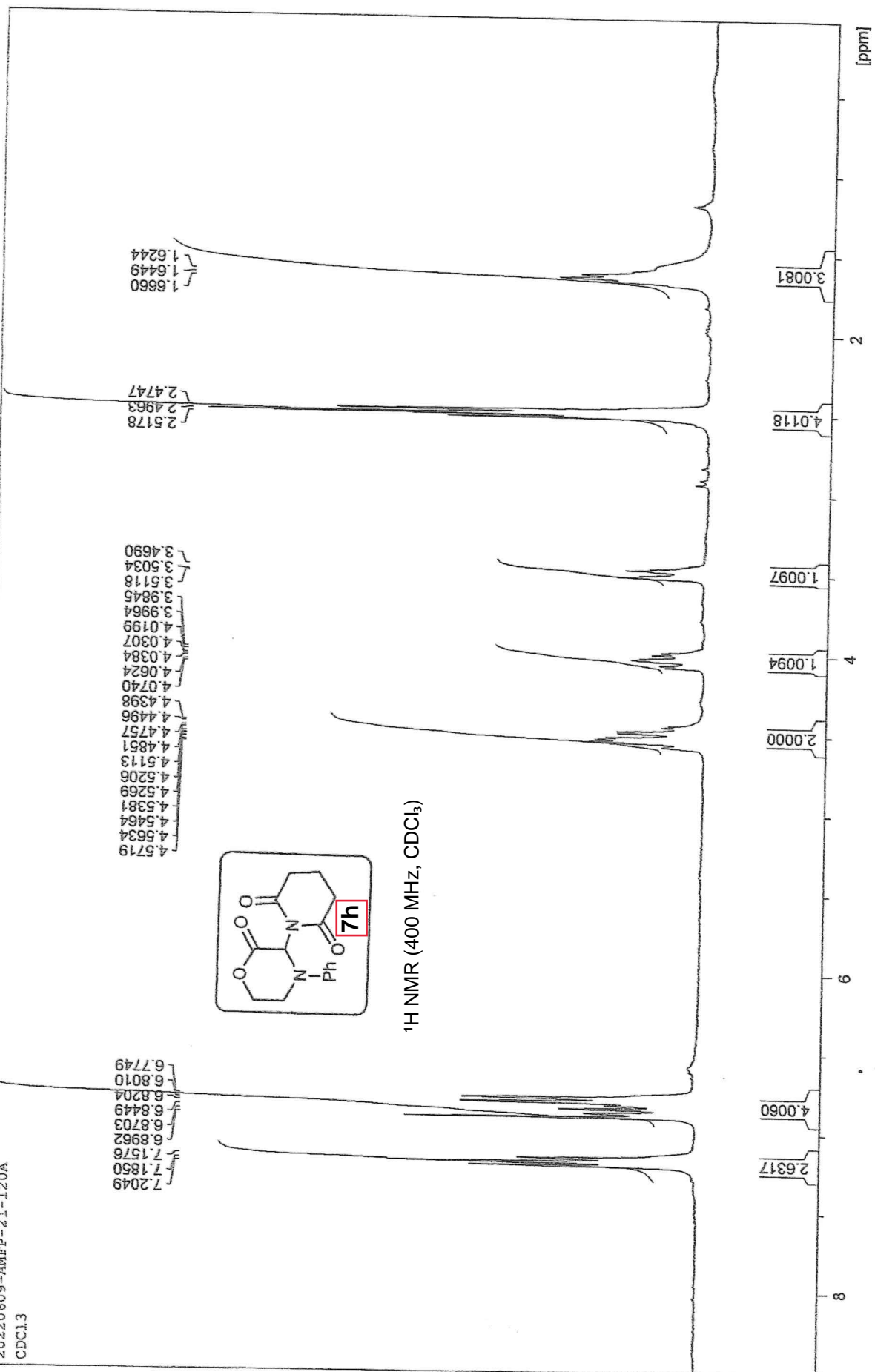
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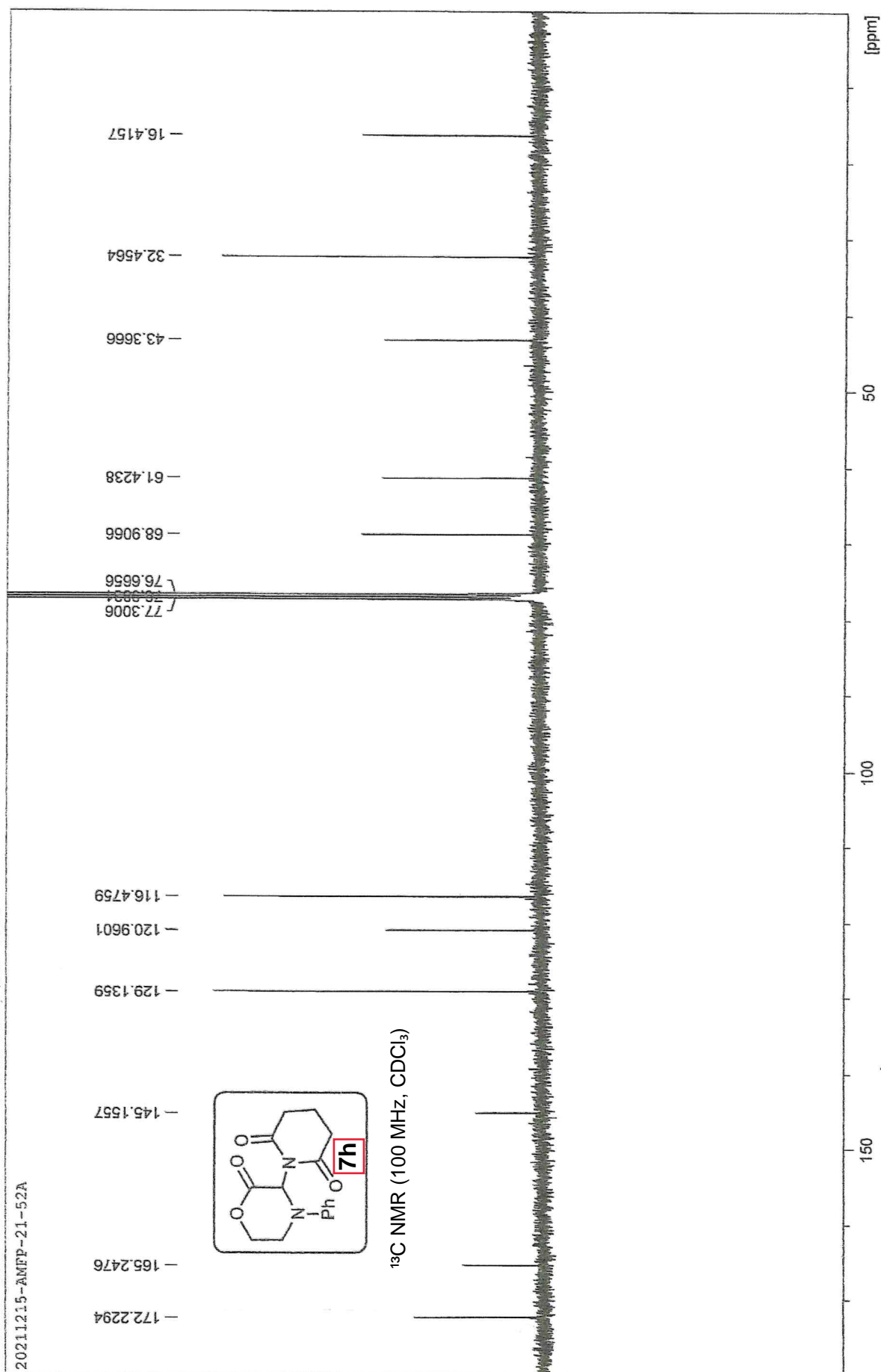
20220609-AMFP-21-120A

CDCl<sub>3</sub>



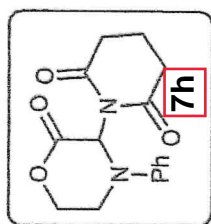
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20211215-ANFP-21-52A

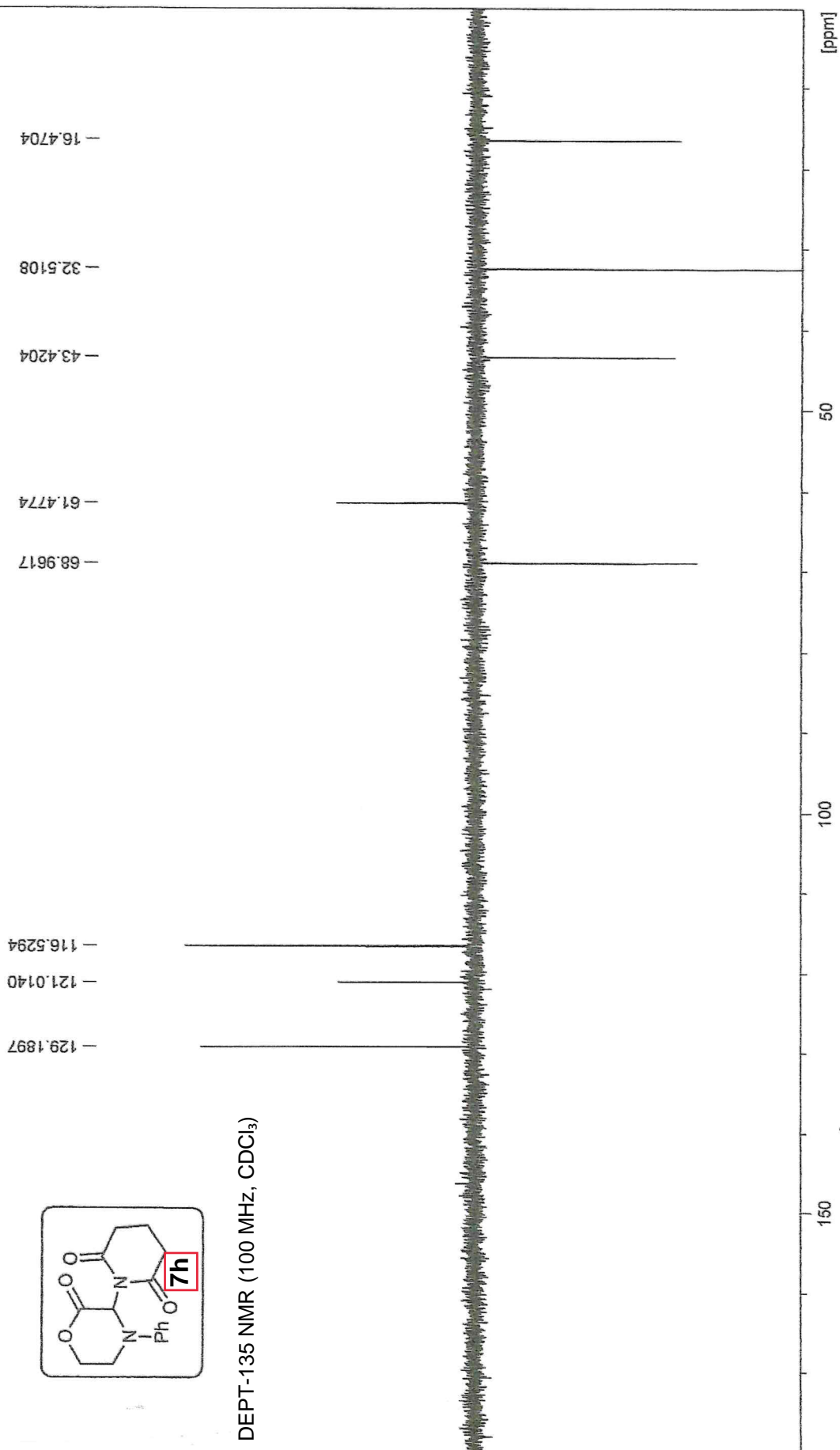


20211215-AMFP-21-52A 2 1 D:\NMR-Files\IST-2021

20211215-AMFP-21-52A

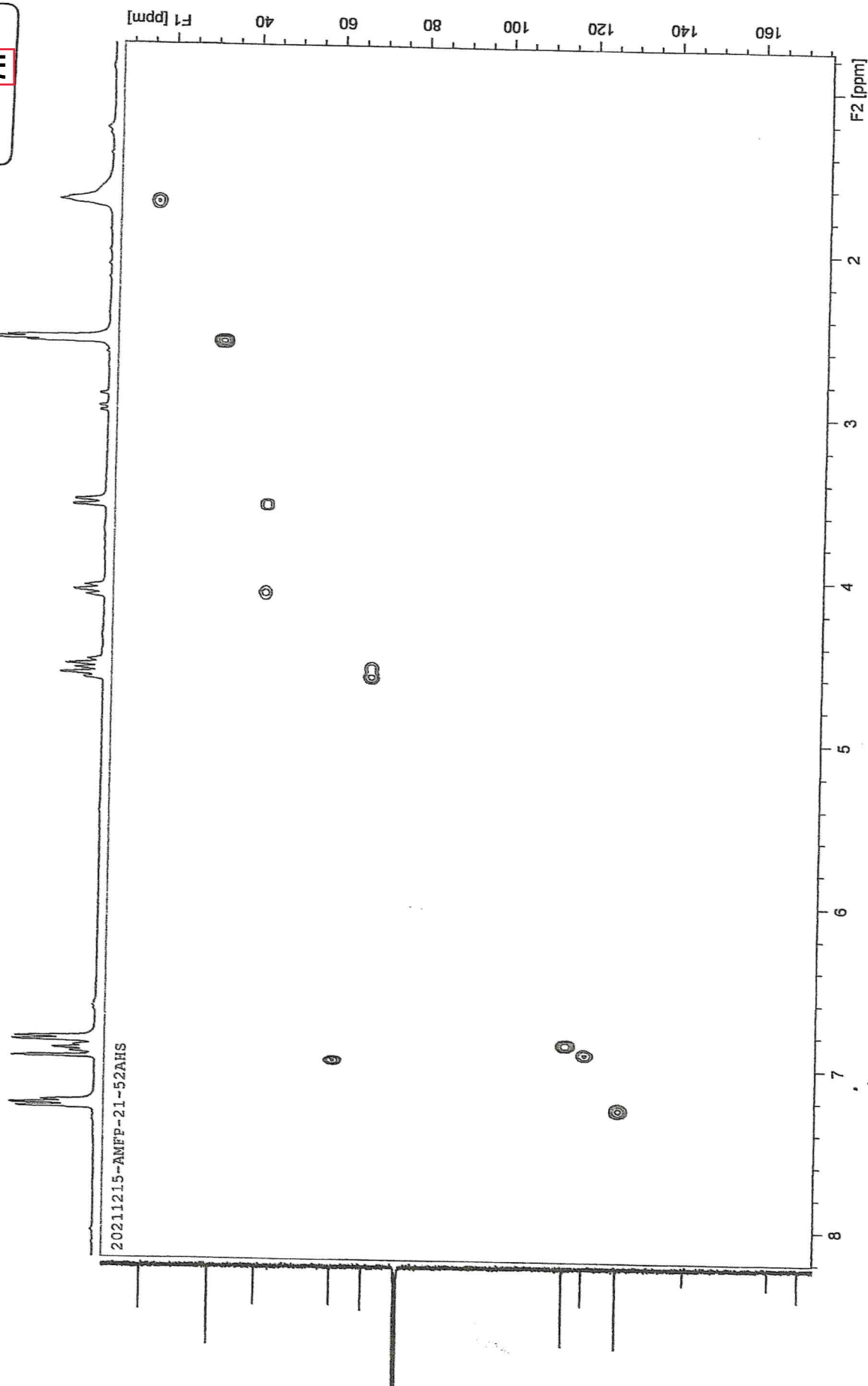
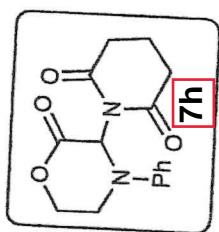


DEPT-135 NMR (100 MHz, CDCl<sub>3</sub>)

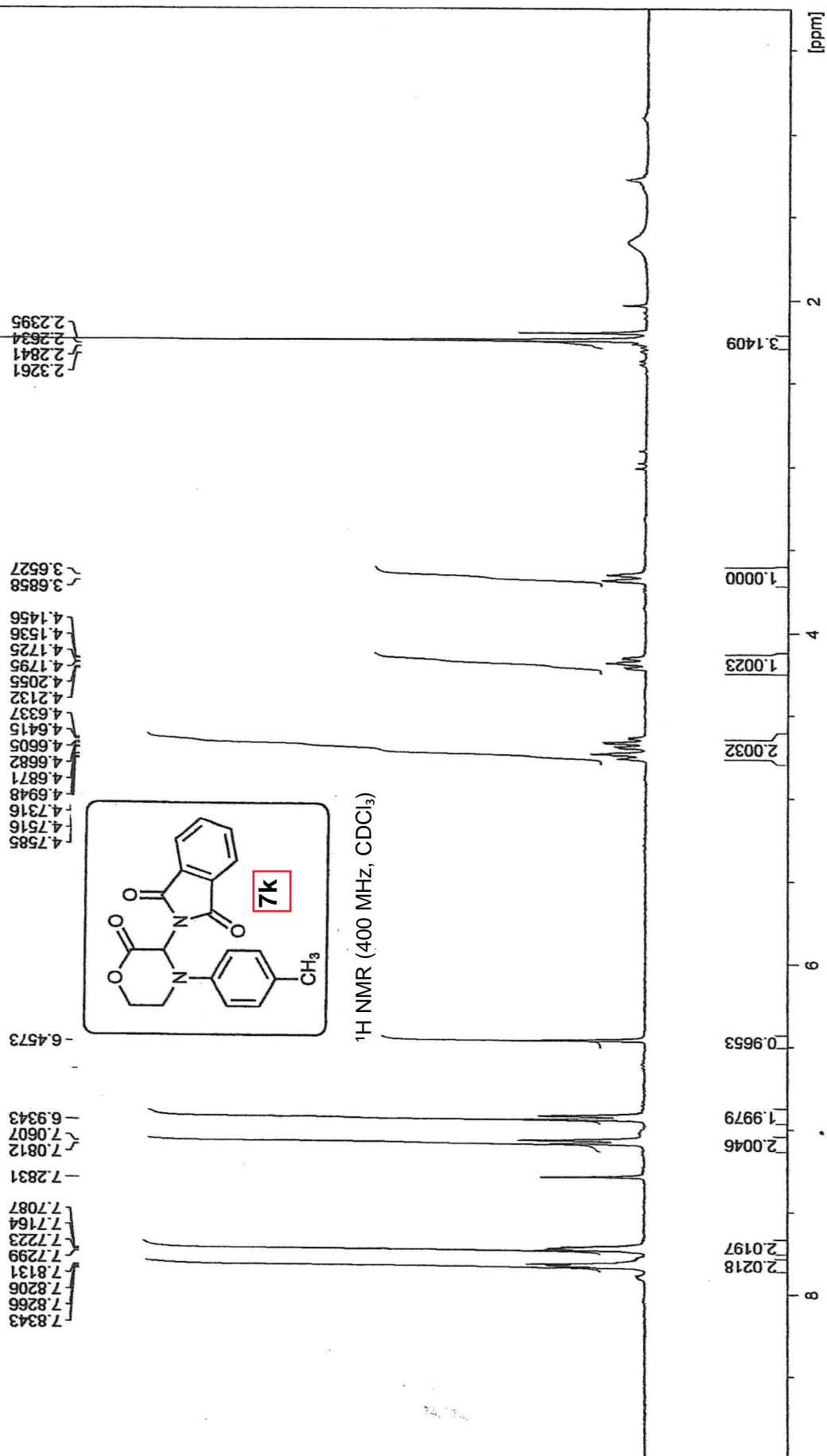


HMQC (CDCl<sub>3</sub>)

20211215-AMFP-21-52AHS 1 1 D:\NMR-Files\IST-2021

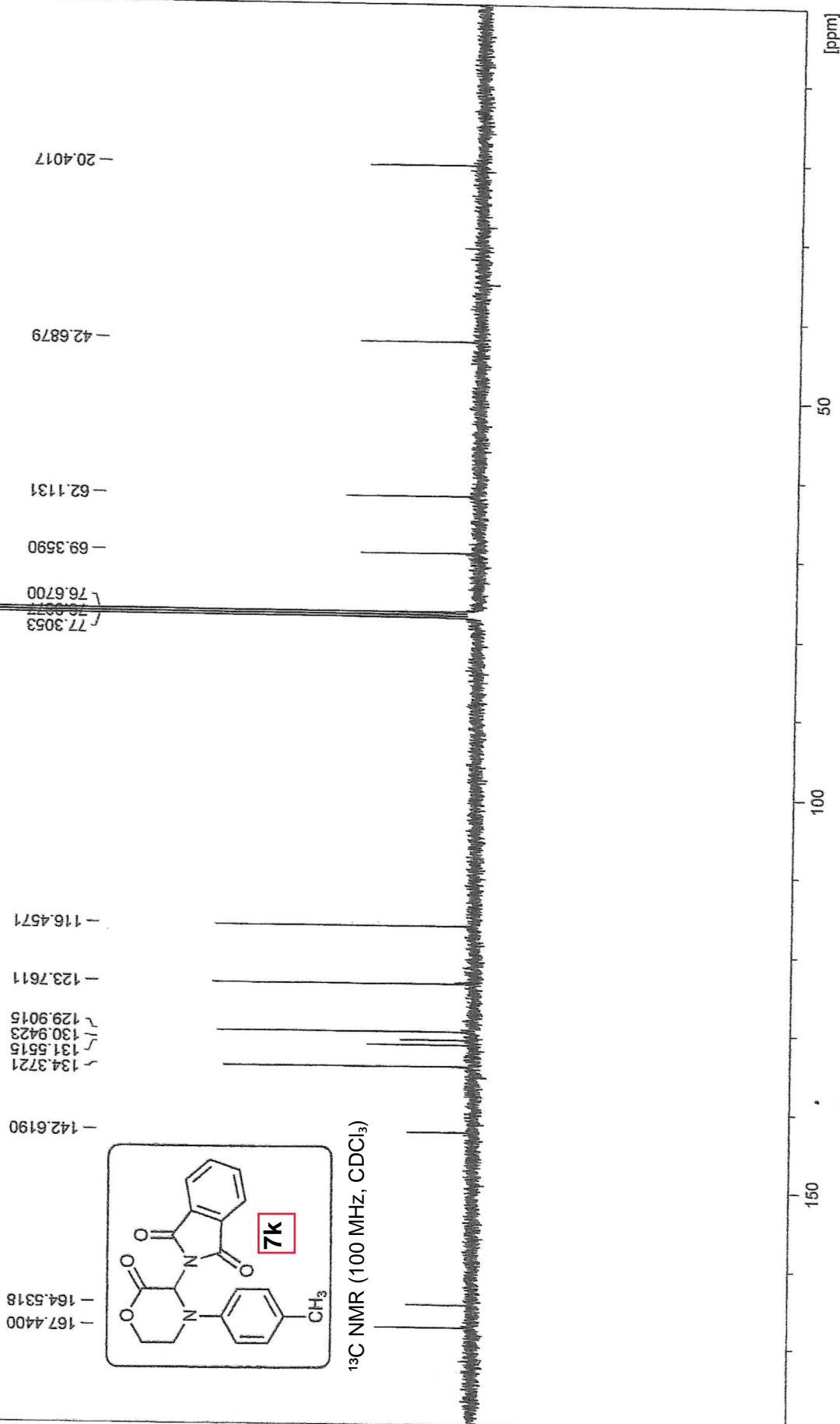






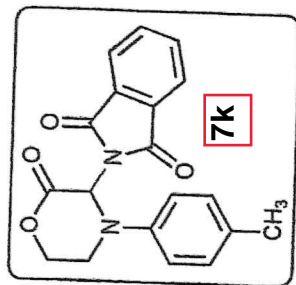
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20220427-ANFP-21-103ccB-carb

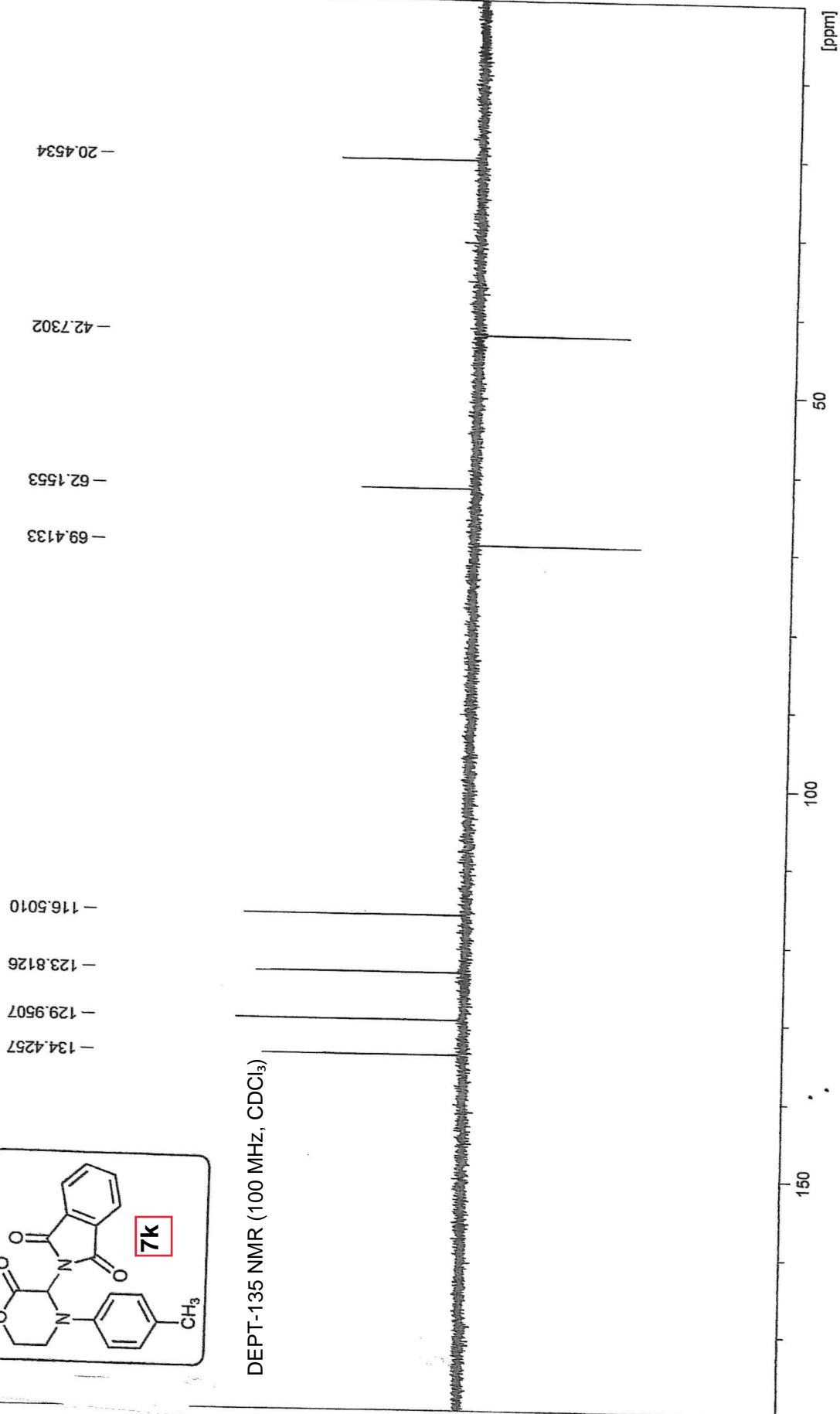


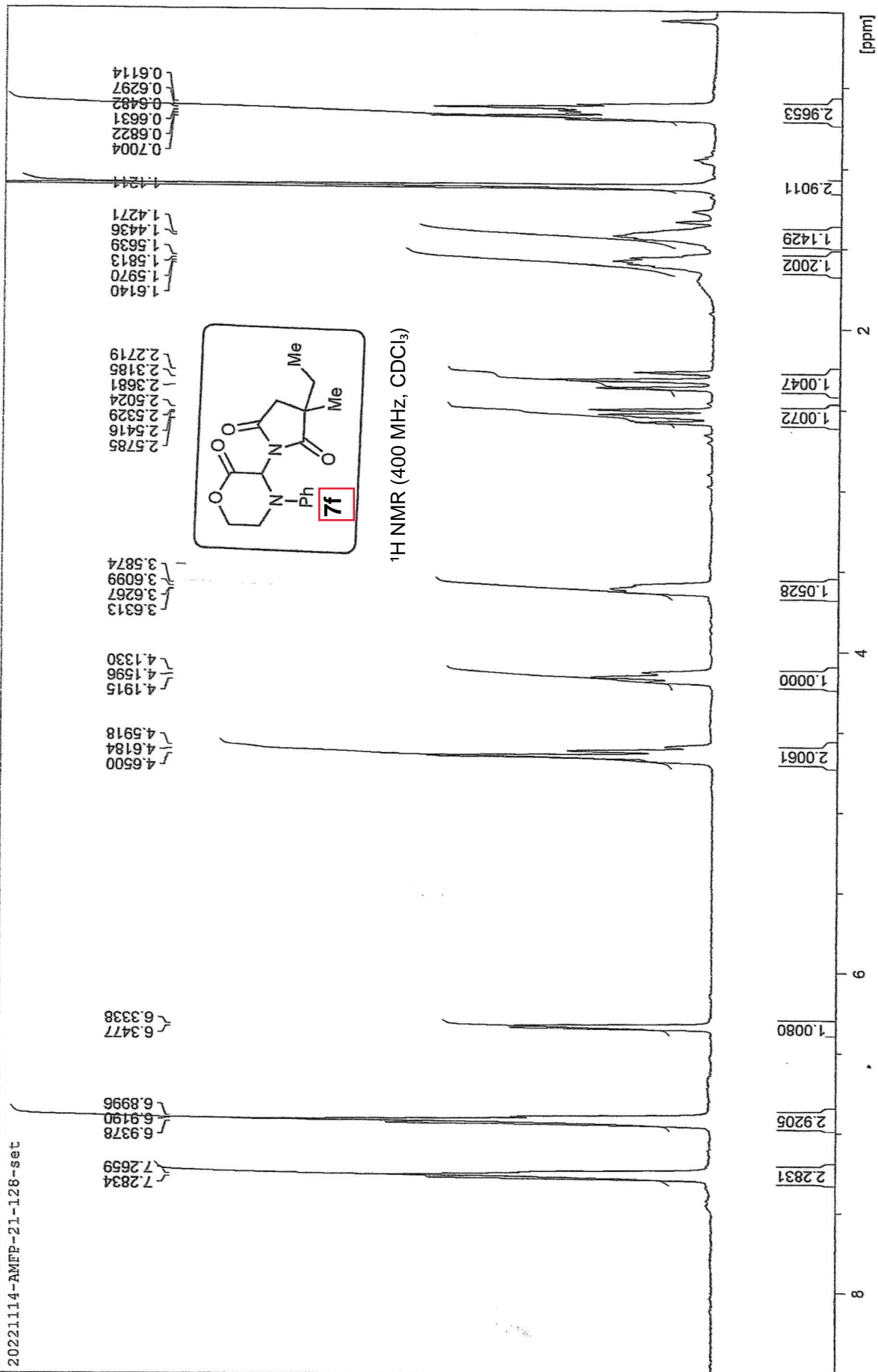
20220412-AMFP-21-103ccb 4 1 D:\NMR-Files\IST-2022

20220412-AMFP-21-103ccb



DEPT-135 NMR (100 MHz, CDCl<sub>3</sub>)





20221114-AMFP-21-128-set 2 1 D:\NMR-Files\IST-2022

20221114-AMFP-21-128-set

175.2197  
175.1164

164.0637

144.7861  
144.7156

129.2314

121.4472  
121.2628  
116.5368  
116.1079

77.3134  
76.9933  
76.6782

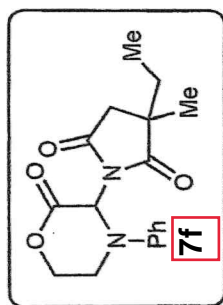
69.2934  
69.2340  
61.9393  
61.7621

44.3362  
44.1661  
42.7133  
42.6717  
40.0649  
39.9848

30.7202  
30.4831

23.8440  
23.6375

8.2442  
8.1418



$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

[ppm]

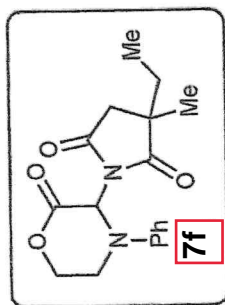
50

100

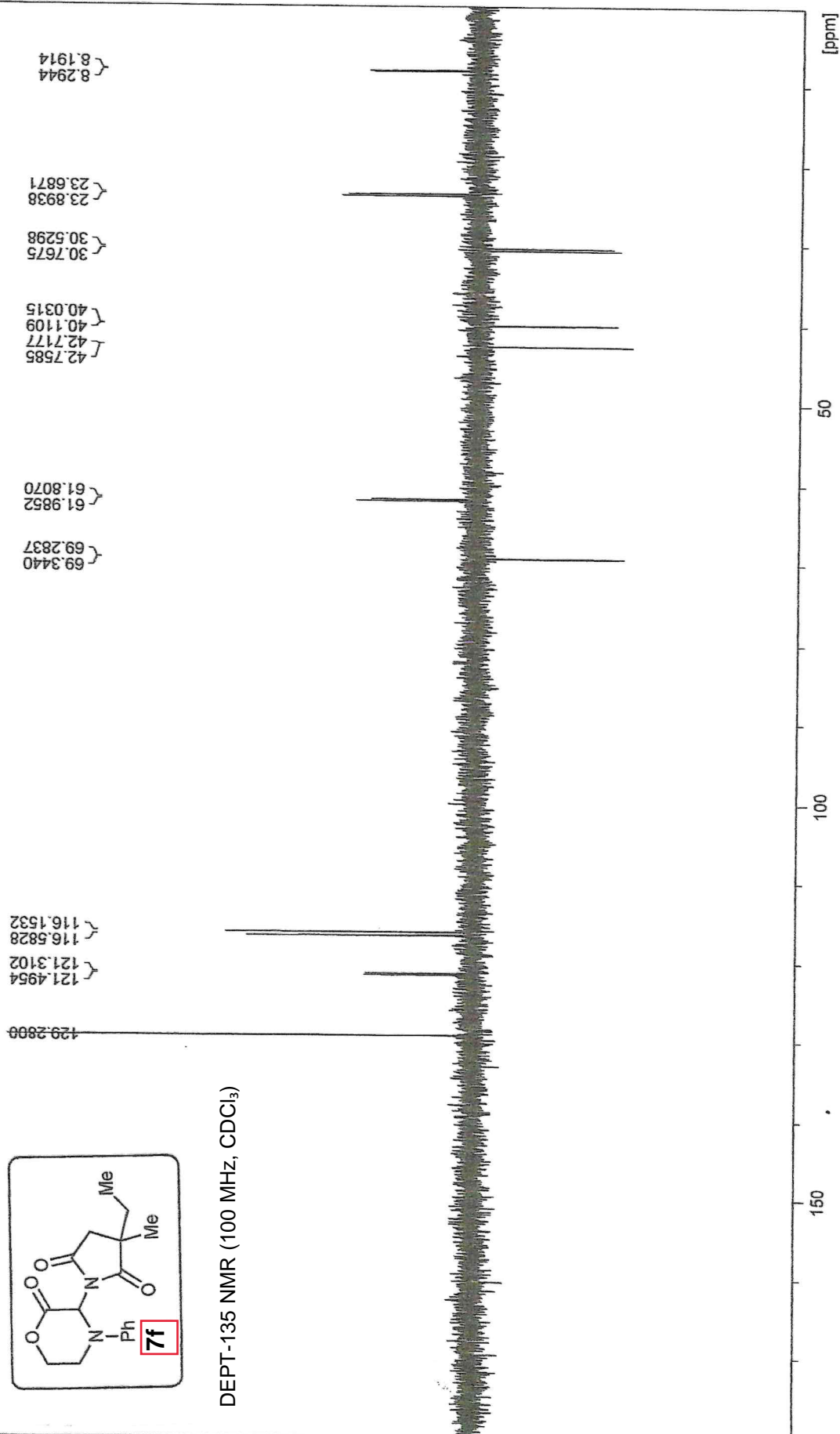
150

20221114-AMFP-21-128-set 5 1 D:\NMR-Files\IST-2022

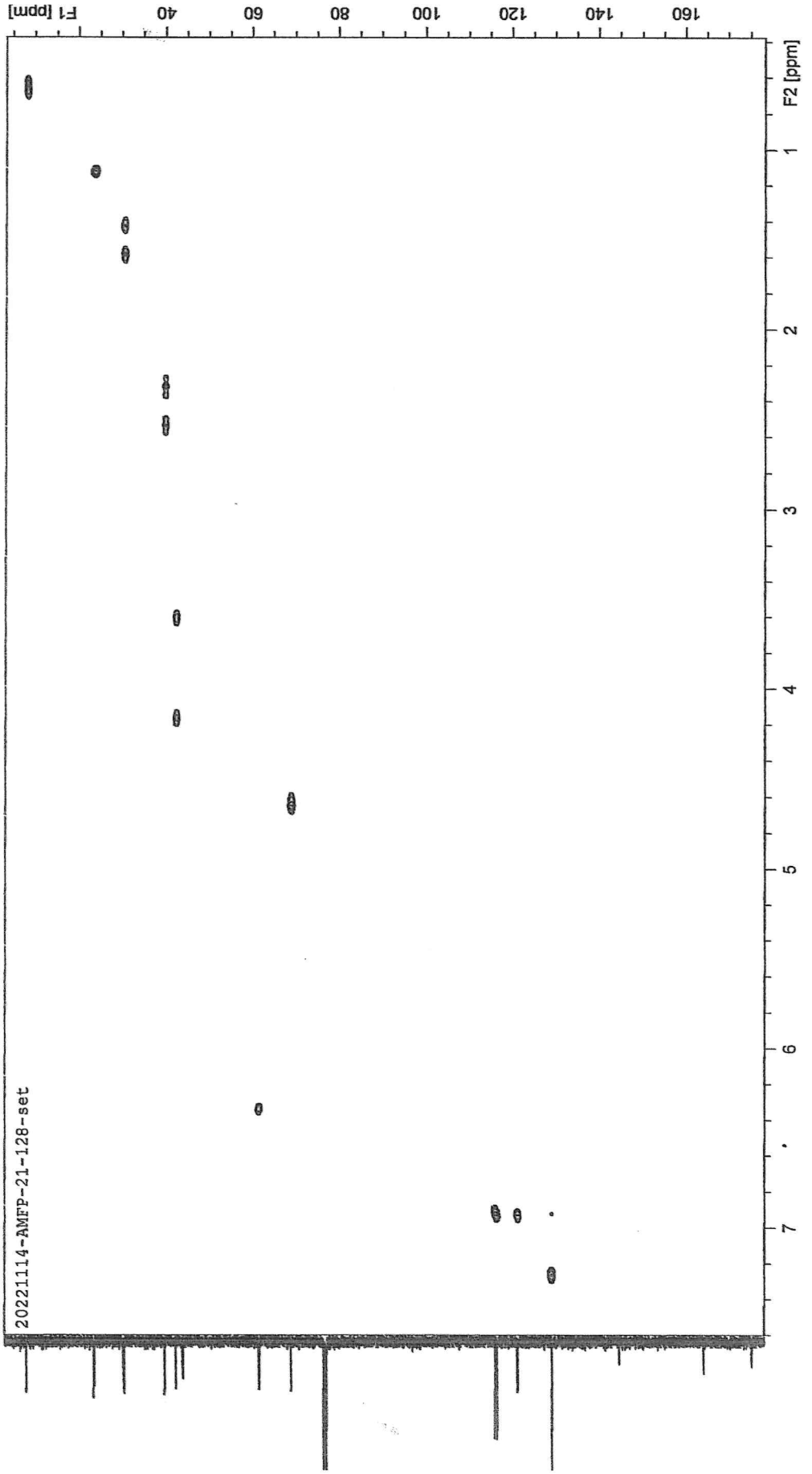
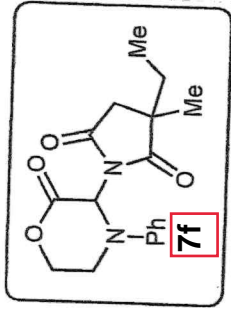
20221114-AMFP-21-128-set



DEPT-135 NMR (100 MHz, CDCl<sub>3</sub>)



20221114-AMFP-21-128-set 1 1 D:\NMR-Files\IST-2022







20211019-AMFP-21-24A 21 1 D:\NMR-Files\IST-2021

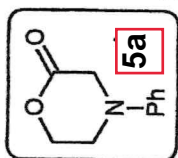
20211019-AMFP-21-24a

7.3661  
7.3611  
7.3476  
7.3445  
7.3259  
7.2848  
6.9592  
6.9409  
6.9225  
6.8403  
6.8203

4.6027  
4.5902  
4.5775

4.1505

3.5435  
3.5308  
3.5183



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

1.9463

0.9516  
2.0072

1.9651

2.0000

2.0048

[ppm]

1

2

3

4

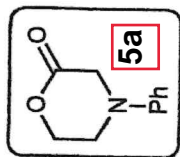
5

6

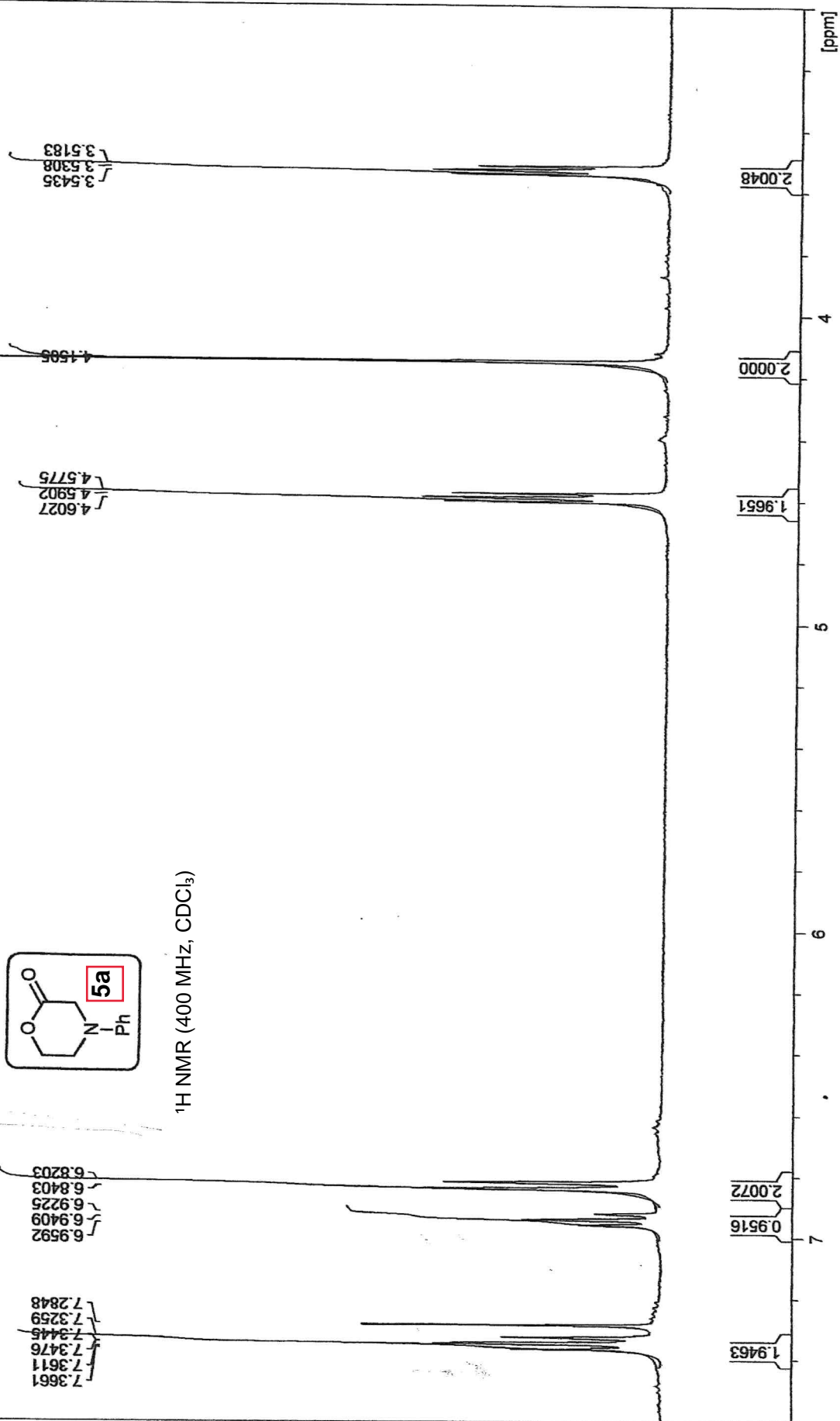
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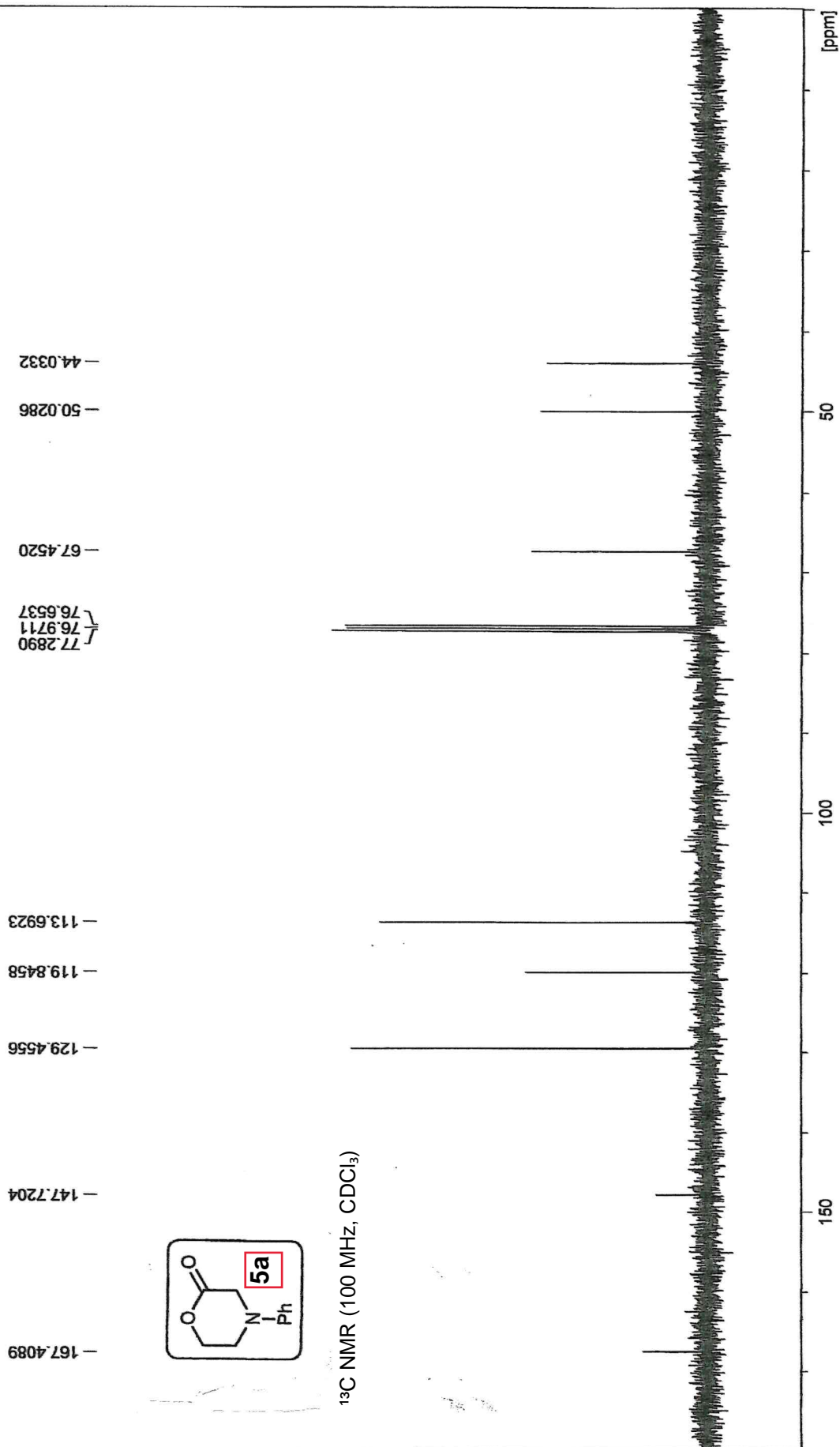
20211019-AMFP-21-24A 21 1 D:\NMR-Files\IST-2021

20211019-AMFP-21-24a



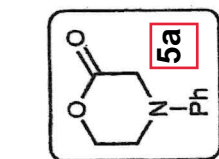
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )





2021-09-28-AMFP-21-16B 1 1 D:\NMR-Files\IST-2021

2021-09-28-AMFP-21-16B



DEPT-135 NMR (100 MHz, CDCl<sub>3</sub>)

129.5794  
119.9922  
113.8242  
67.5719  
50.1704  
44.1720

[ppm]

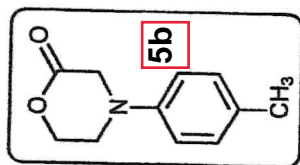
50

100

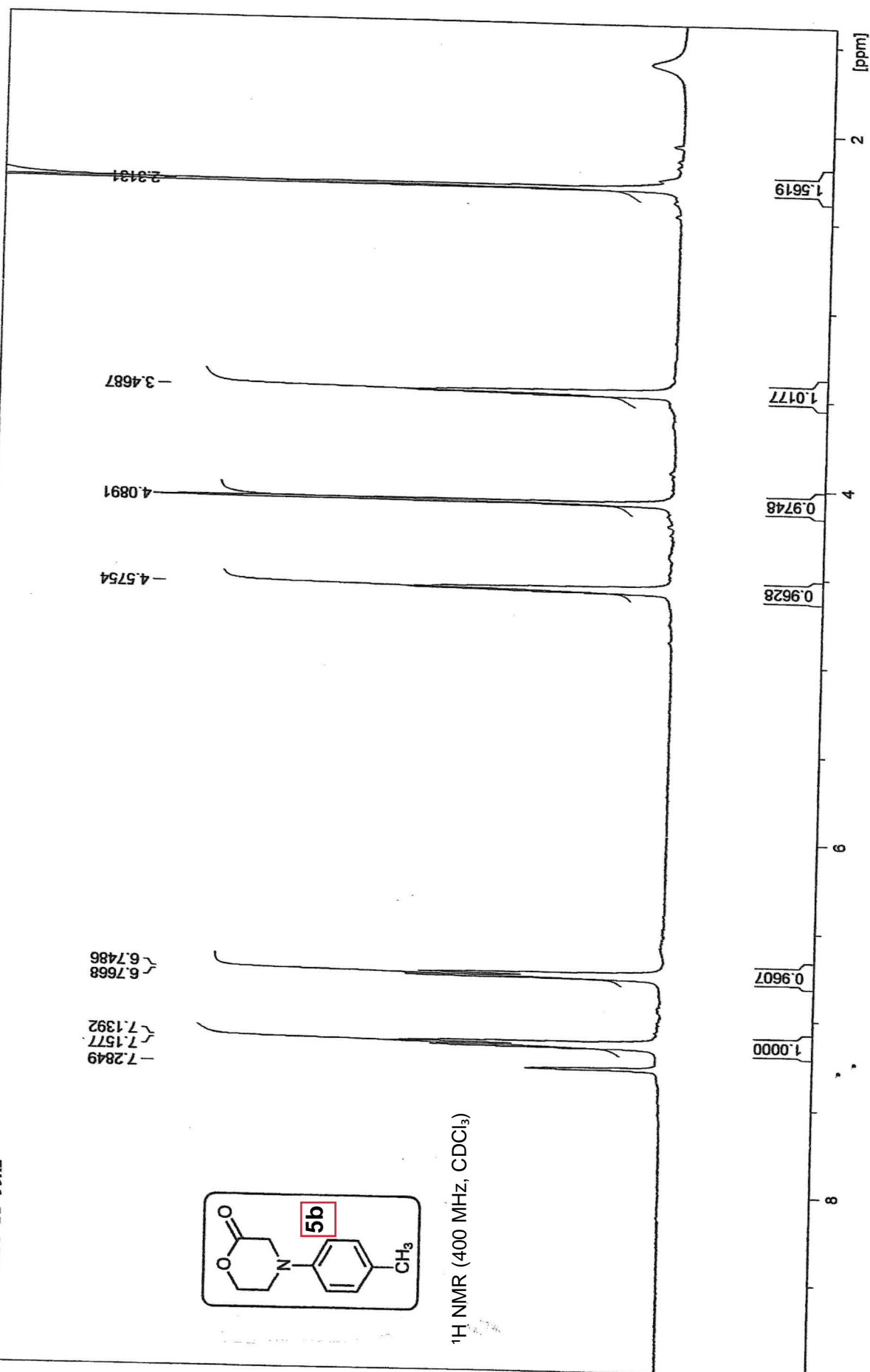
150

20220406-AMFP-21-99AL 3 1 D:\NMR-Files\IST-2022

20220406-AMFP-21-99AL

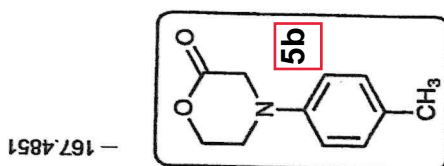


<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



20220406-AMFP-21-99AL-13C 1 1 D:\NMR-Files\IST-2022

20220406-AMFP-21-99AL-13C



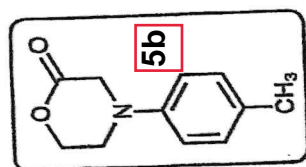
<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)



[ppm]

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DEPT-135 NMR (100 MHz, CDCl<sub>3</sub>)

