CONCISE SYNTHESIS OF TPCA-1 AND RELATED THIOPHENE CARBOXAMIDES BY CROSS COUPLING

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Supporting Information

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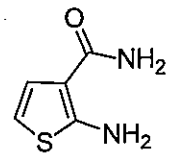
NH2
O
S

4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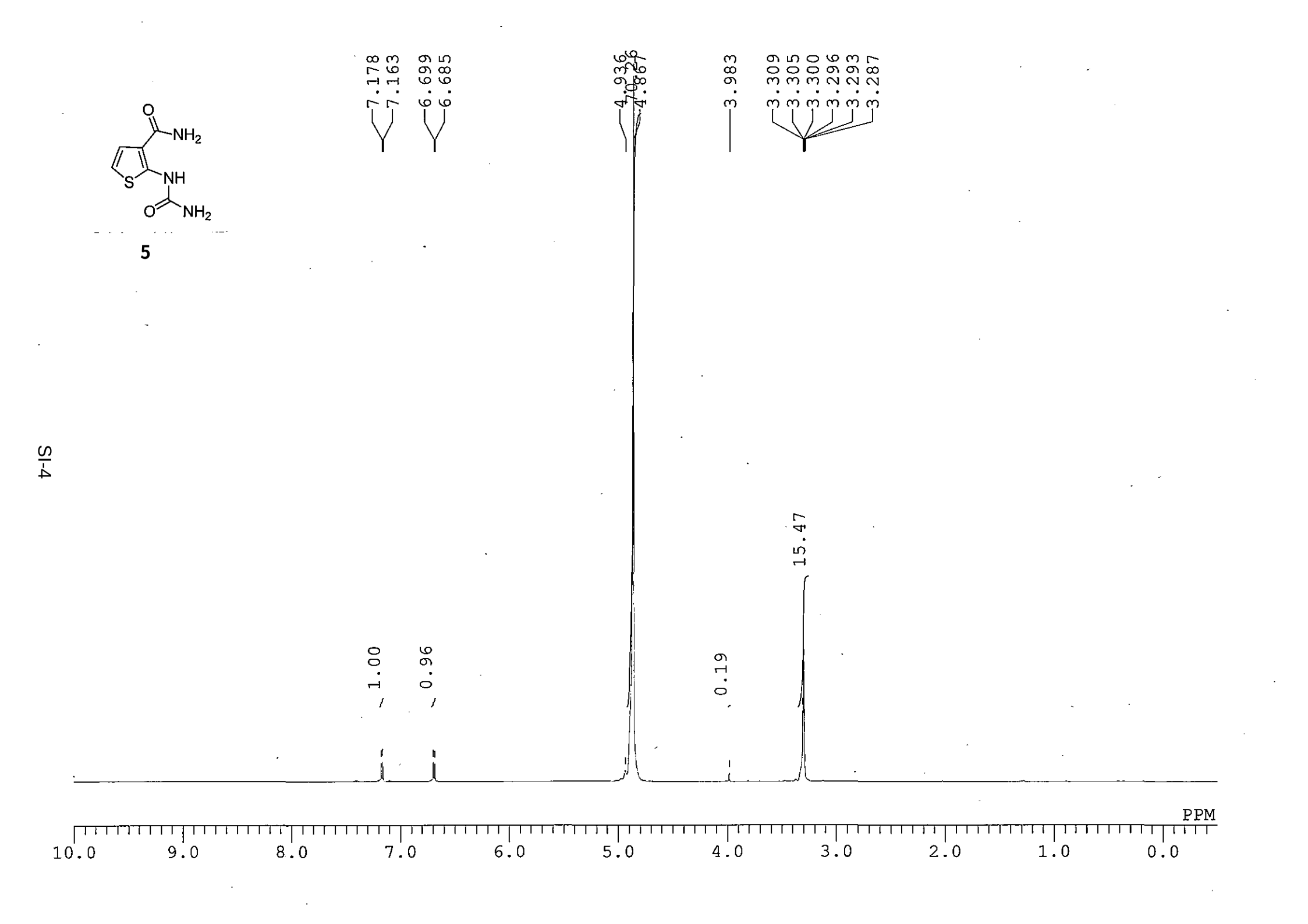
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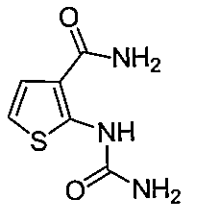

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49.000
48.786
48.572
48.358

SI-5

PPM

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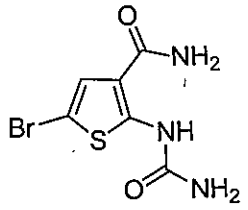
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NH
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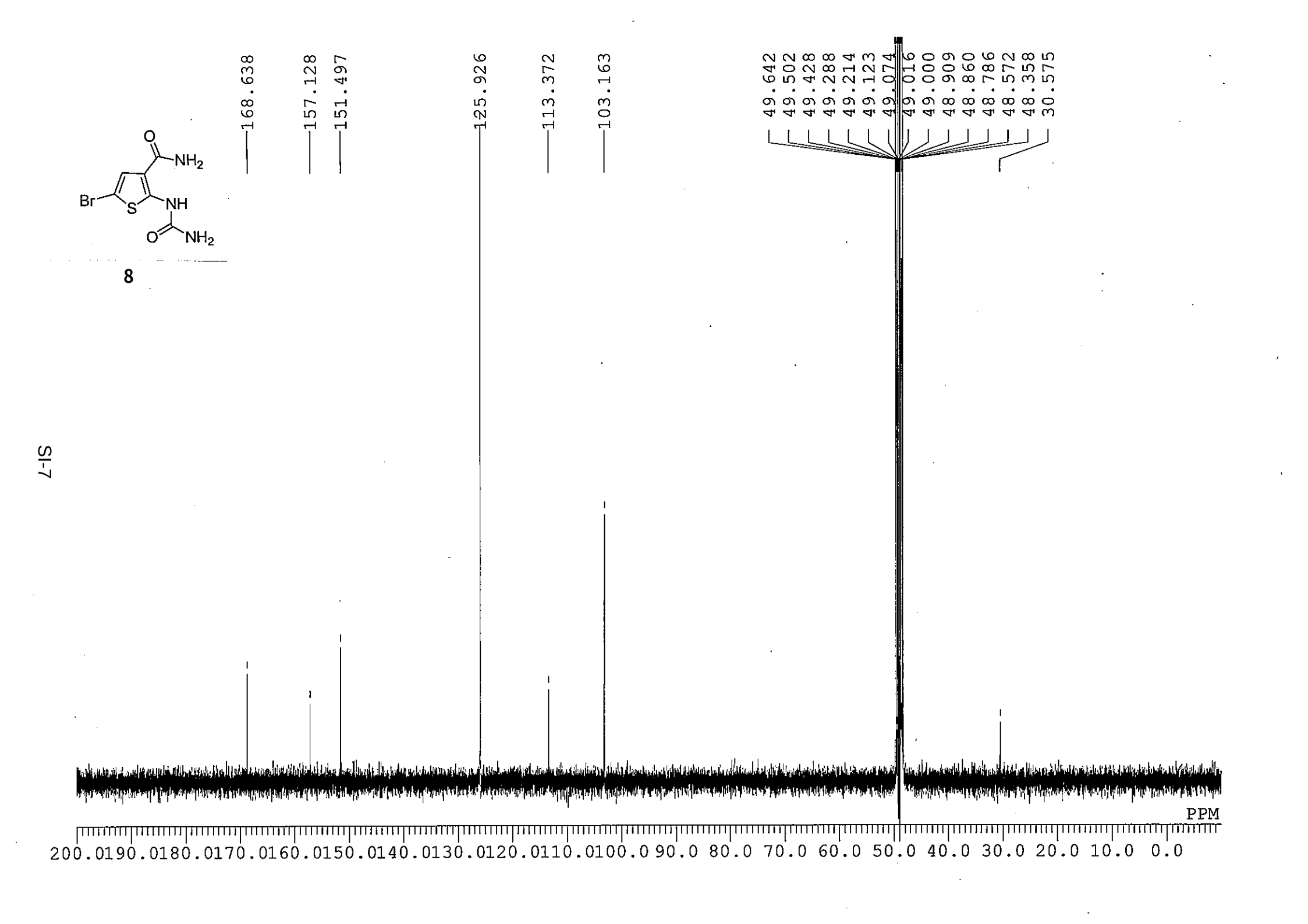
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49.016
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48.909
48.860
48.786
48.572
48.358
30.575
O
NH2
Br
S
NH
O
NH2
8
PPM
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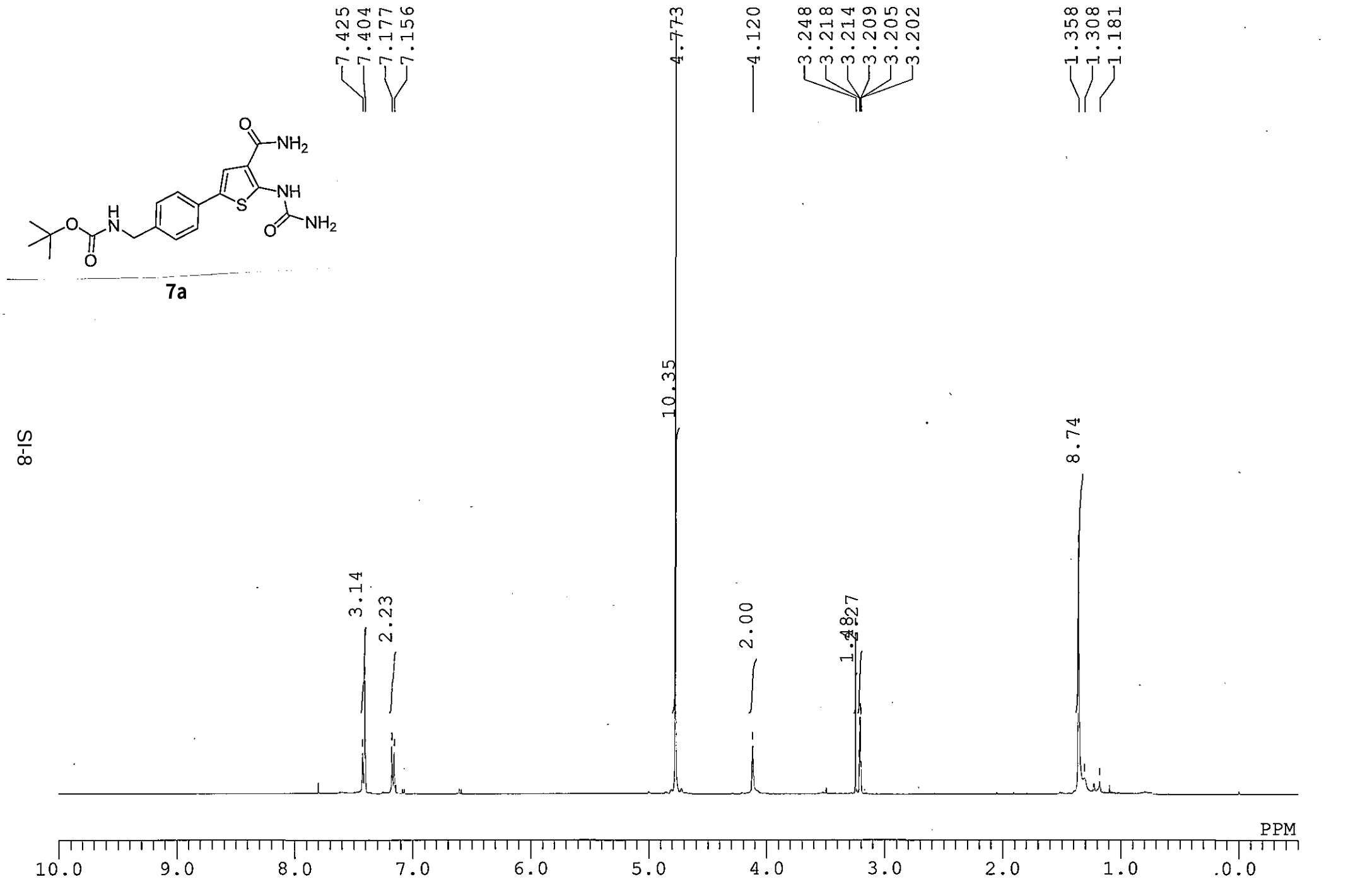
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1.181
10.35
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3.14
2.23
2.00
1.48
1.27
8-IS
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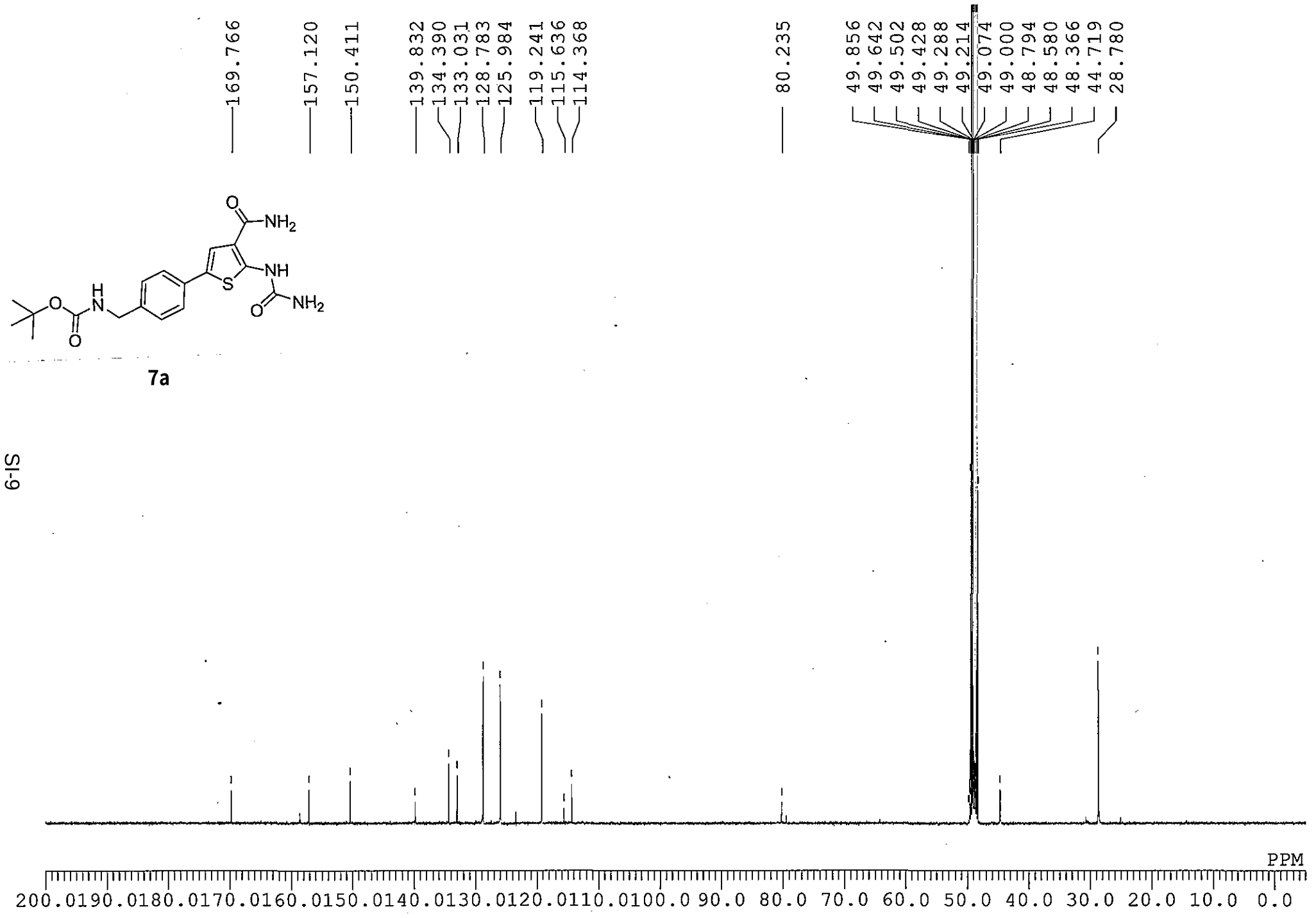
7a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49.214
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28.780
O
NH2
NH
S
O
NH2
H
N
O
O
7a
6-IS
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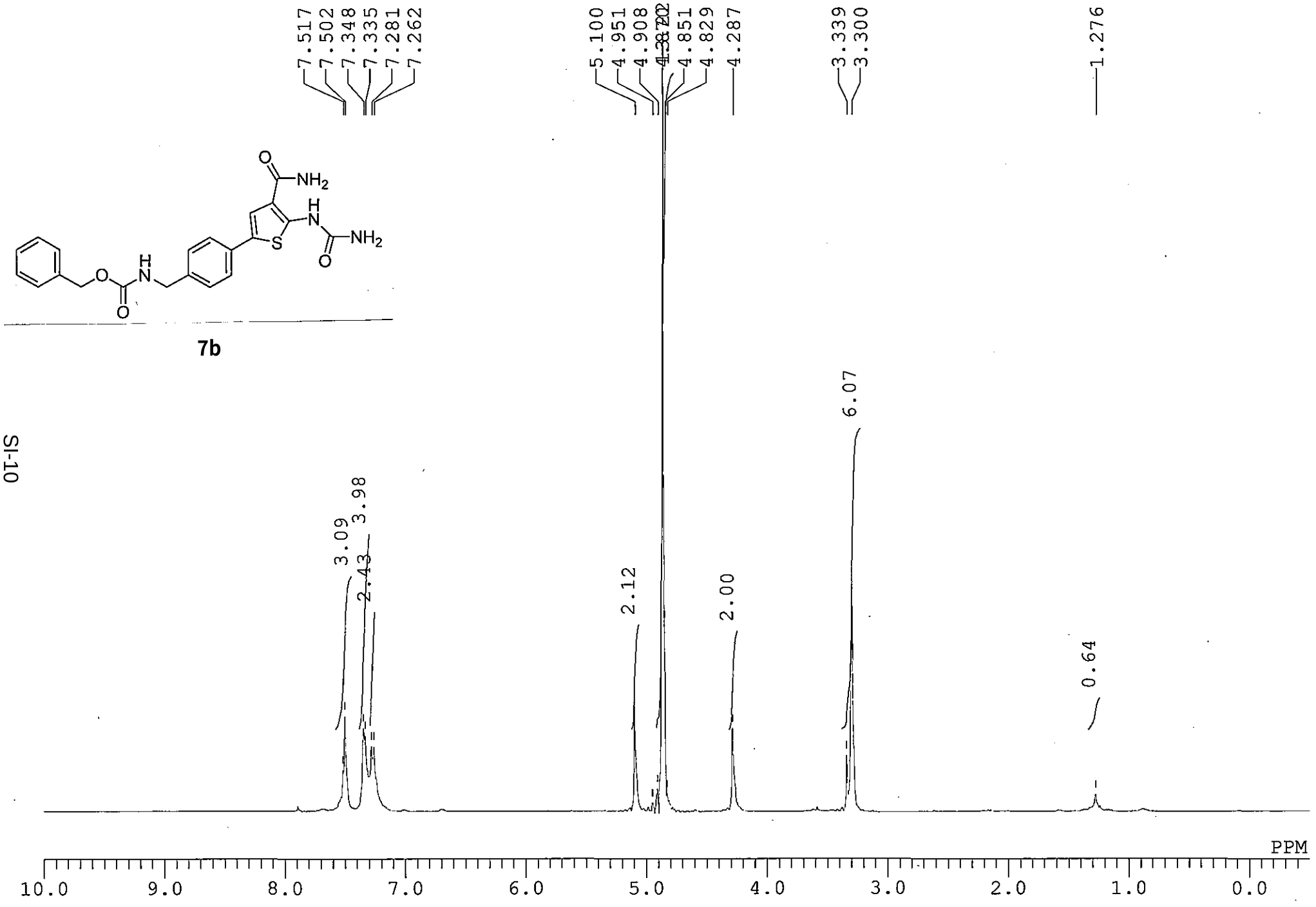
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3.300
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NH2
O
S
7b
SI-10
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2.00
6.07
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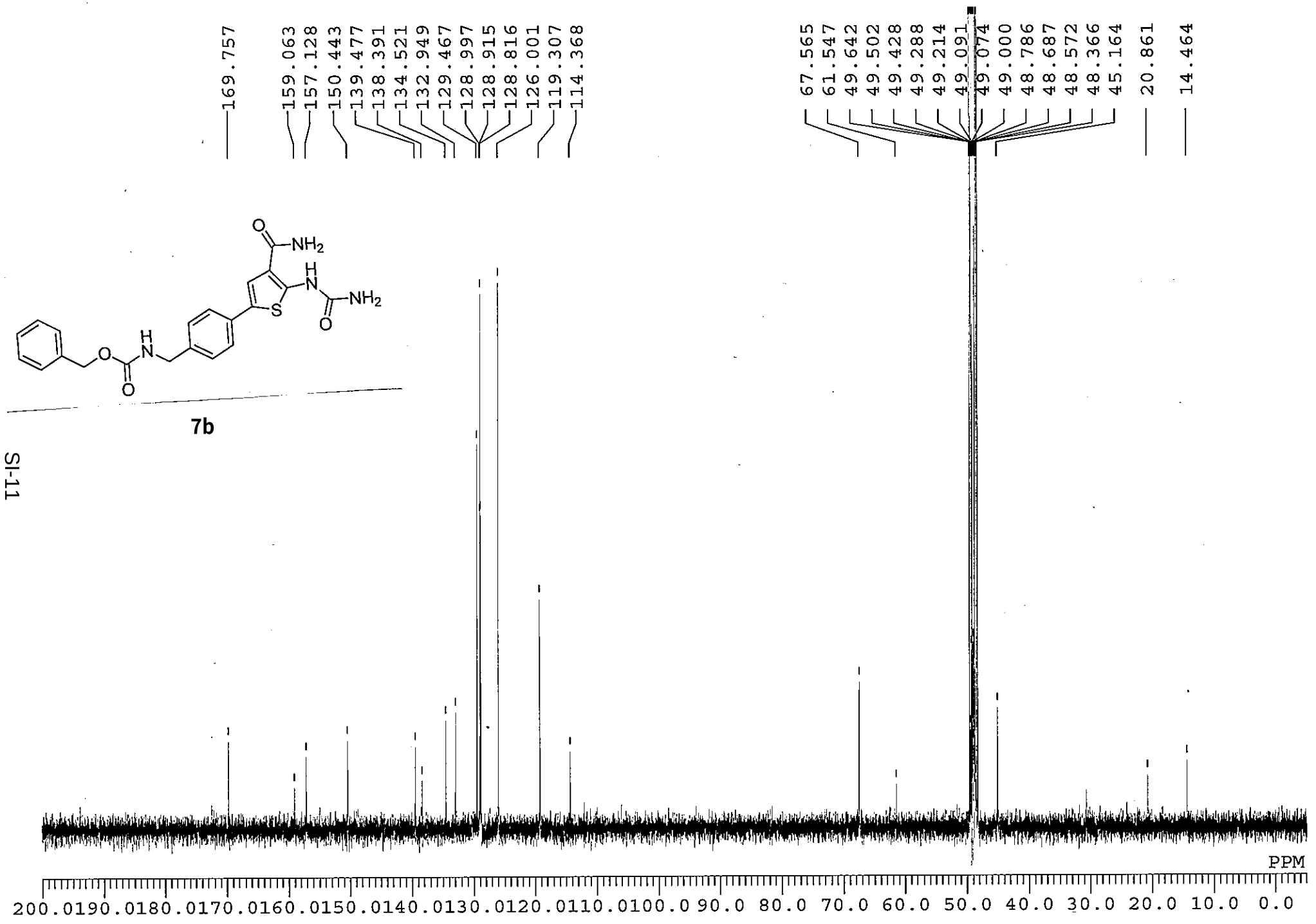
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49.428
49.288
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49.074
49.000
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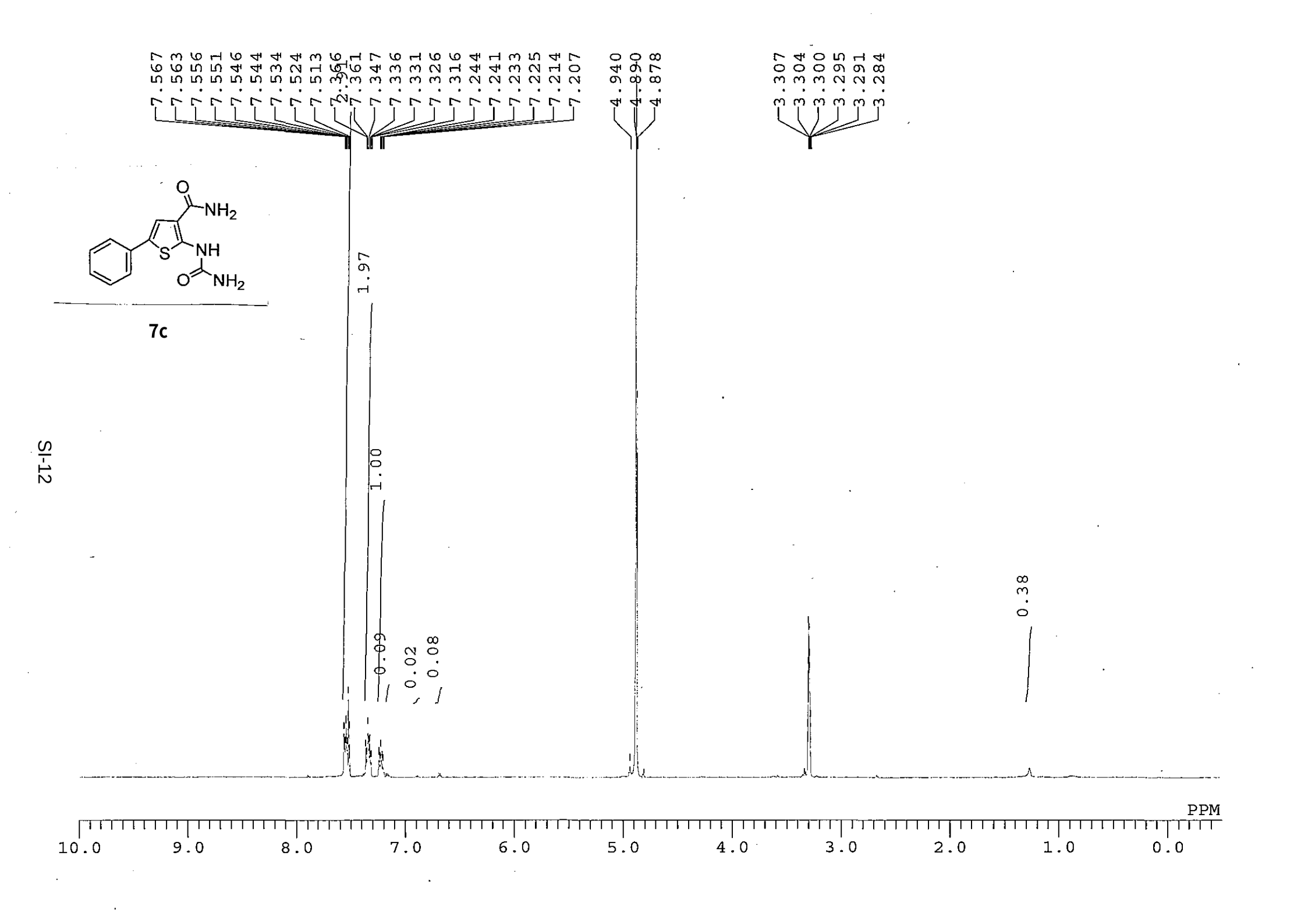
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7.241
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7.225
7.214
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3.295
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3.284
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0.02
0.08
0.38
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NH
NH2
O
O
S
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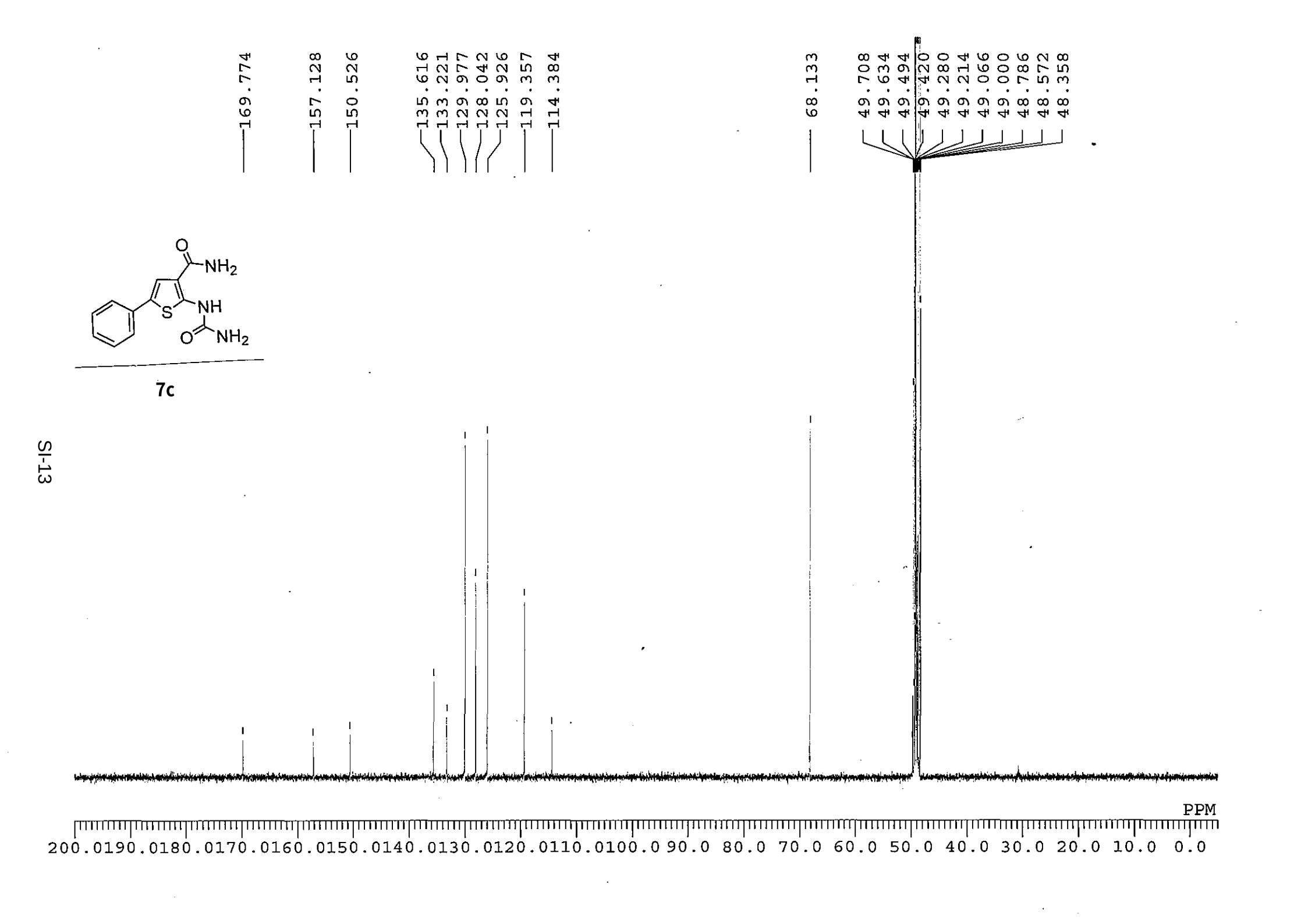
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49.420
49.280
49.214
49.066
49.000
48.786
48.572
48.358
O
NH2
NH
S
O
NH2
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0

7c

PPM
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4.784
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O
S
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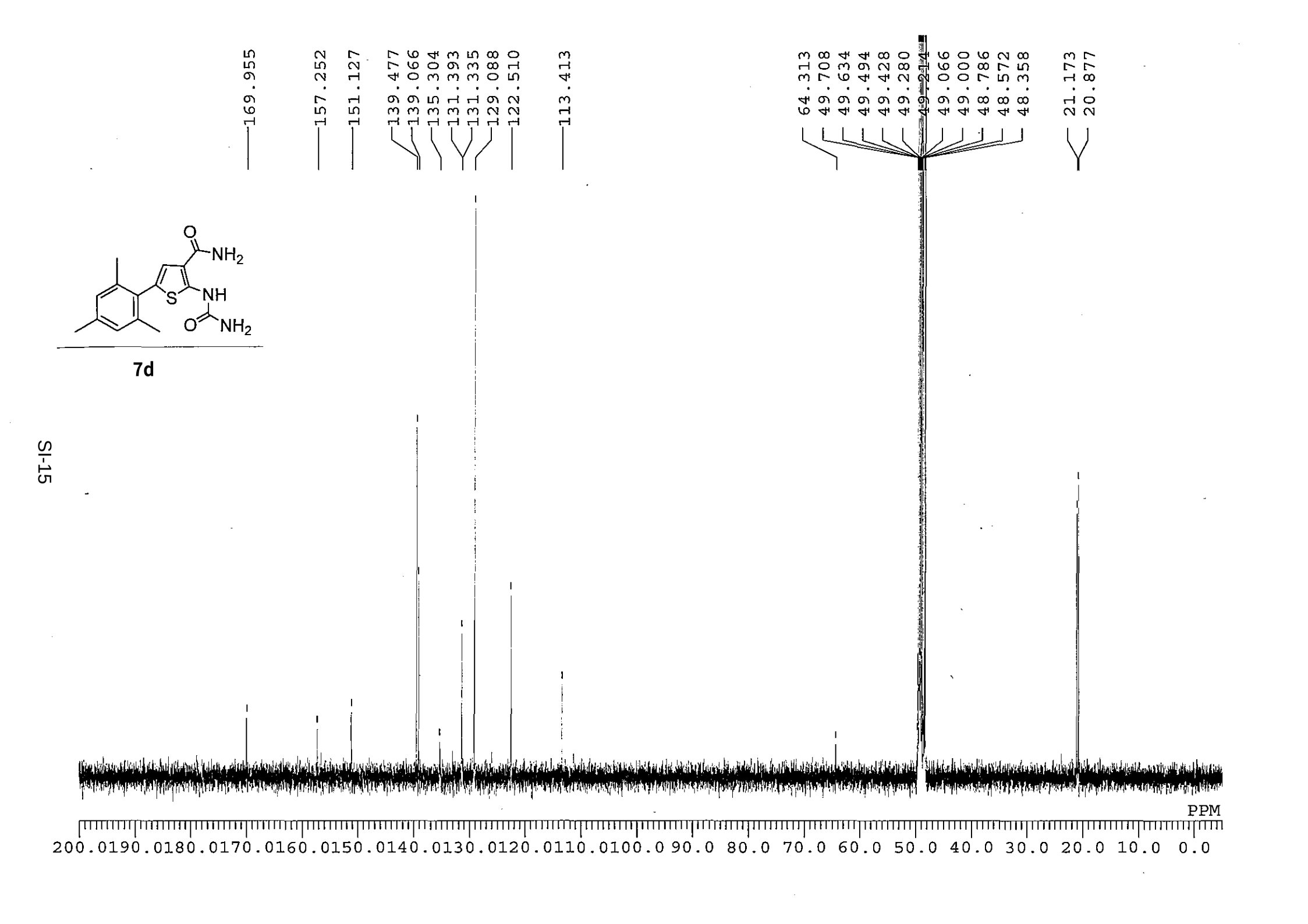
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49.428
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49.066
49.000
48.786
48.572
48.358
21.173
20.877
O
NH2
S
NH
O
NH2
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0

7d

PPM
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2.21
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1.565
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3.200
3.205
3.209
3.213
3.218
3.248
3.381
3.495
3.542
4.008
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4.898
6.980
6.988
6.993
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7.010
7.027
7.032
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NH
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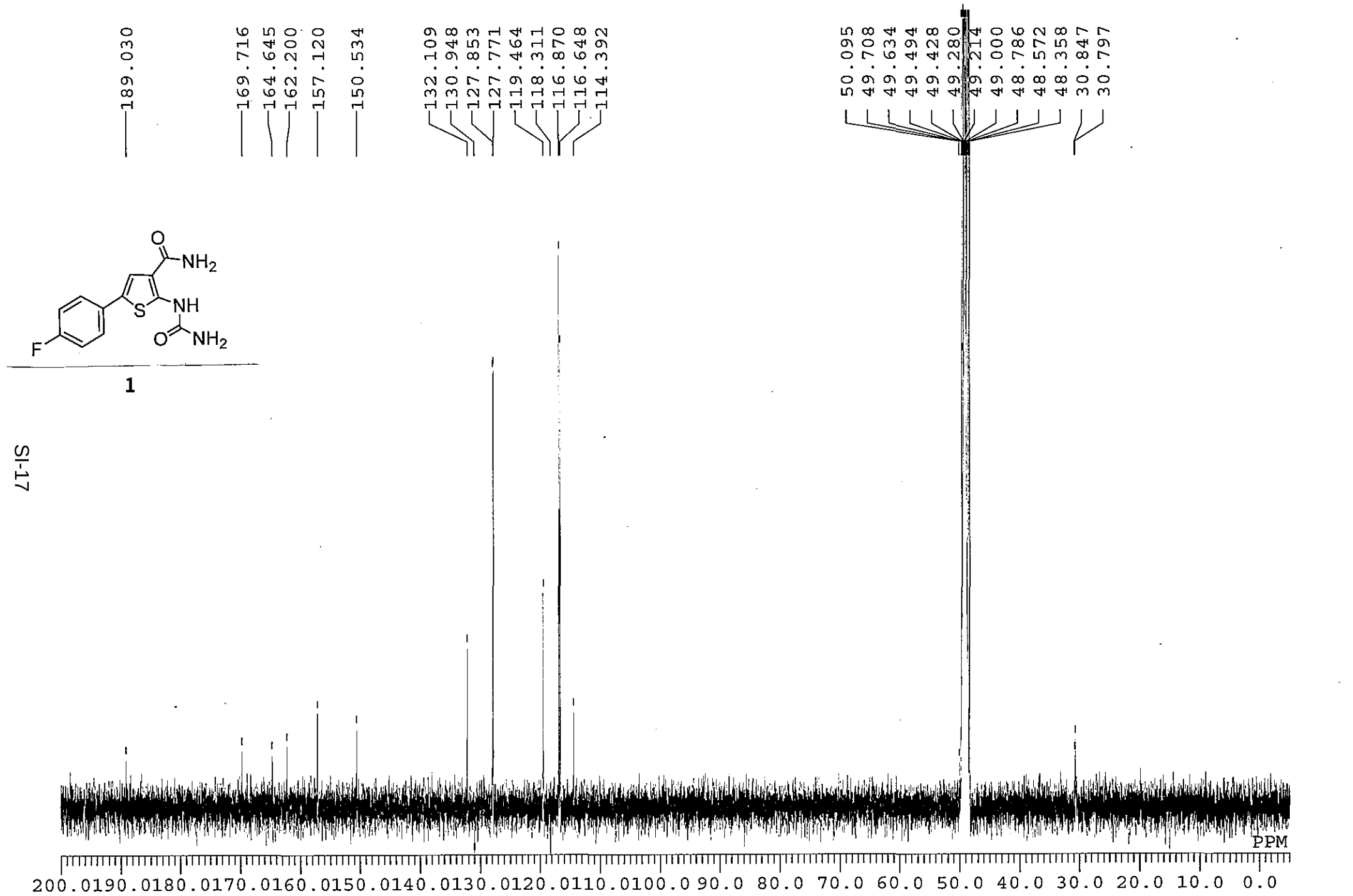
NH2
O
F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30.797
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O
NH2
F
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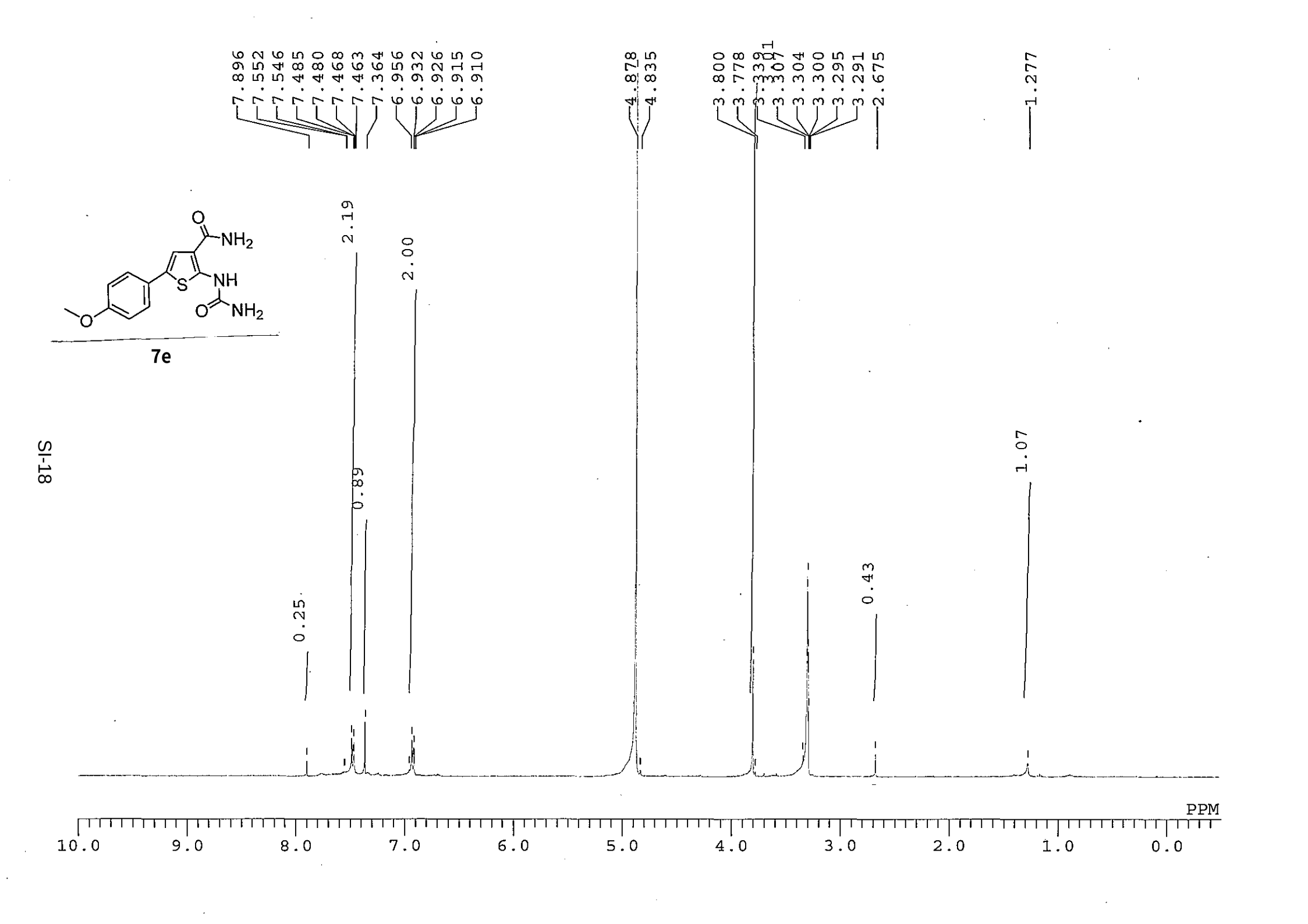
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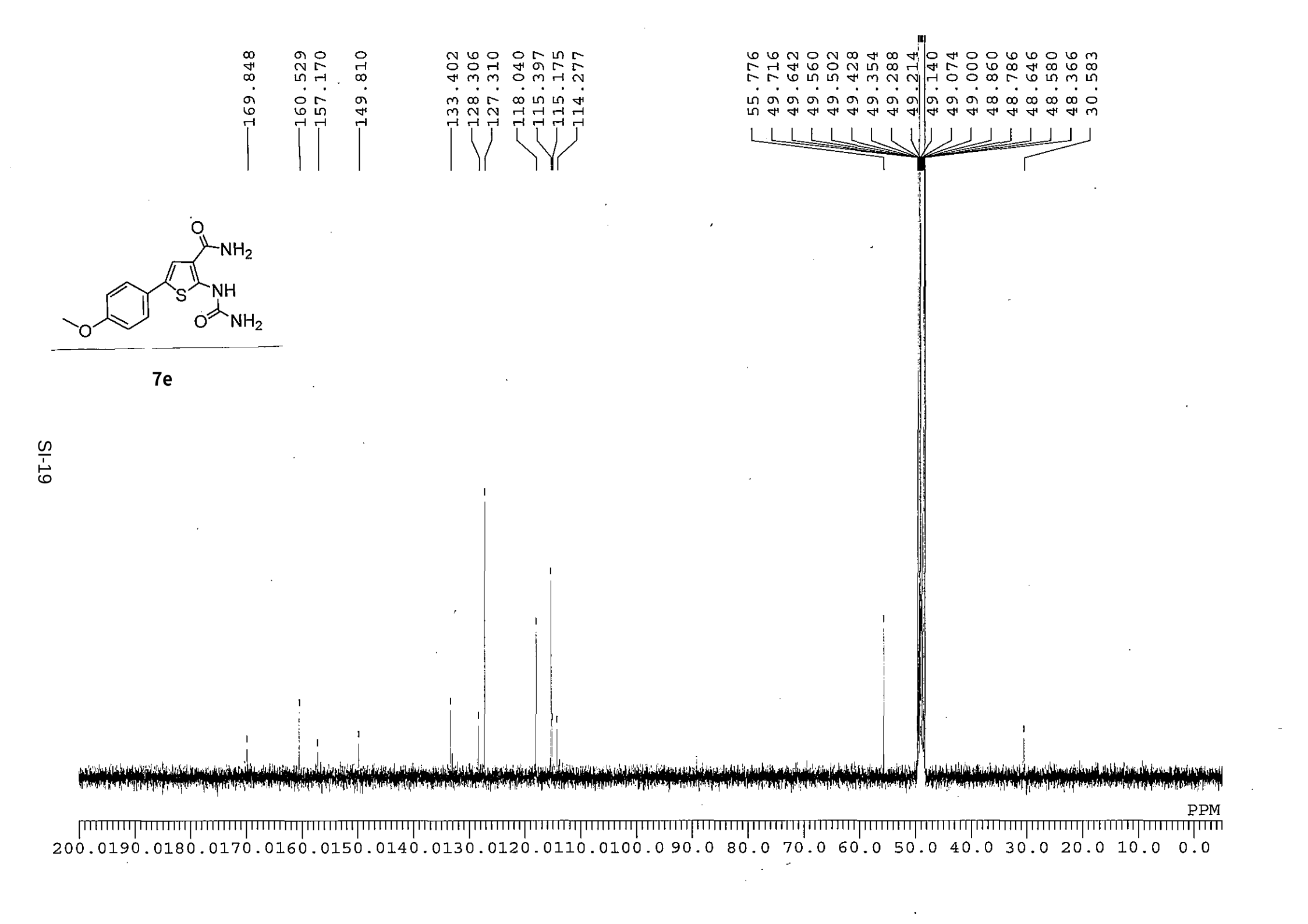
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7e
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PPM
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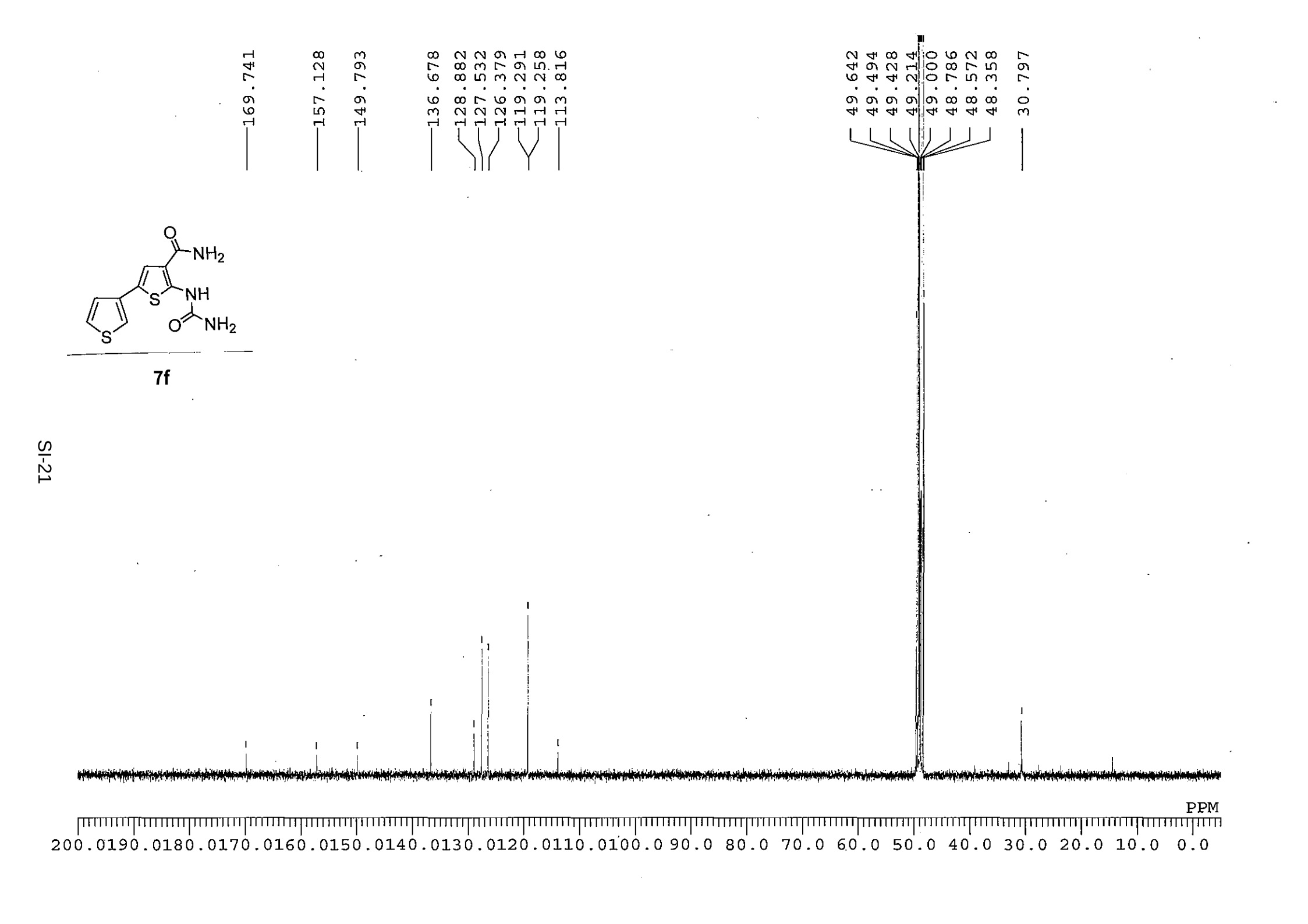
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48.572
48.358
30.797
NH2
NH
NH2
S
S
O
O
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7f

Summary of DFT calculation

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Freq RB3LYP 6-31+G
Number of atoms 19
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6 18 -502
Charge 0
Multiplicity 1
Number of electrons 96
Number of alpha electrons 48
Number of beta electrons 48
Number of basis functions 174
Number of independent functions 174
Number of point charges in /Mol/ 0
Number of translation vectors 0
Atomic numbers N= 19
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8 7 1 1 1 1
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