Supplementary Information

Microwave-assisted synthesis of tubulin assembly inhibitors as anticancer agents by aryl ring reversal and conjunctive approach

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Table S1. Docking score and interactions of compound **4**.

Table S2. ADME profile of compound **4**.

^{1}H and ^{13}C NMR spectra of compounds 3-30.

IR spectra of compounds 3-30.

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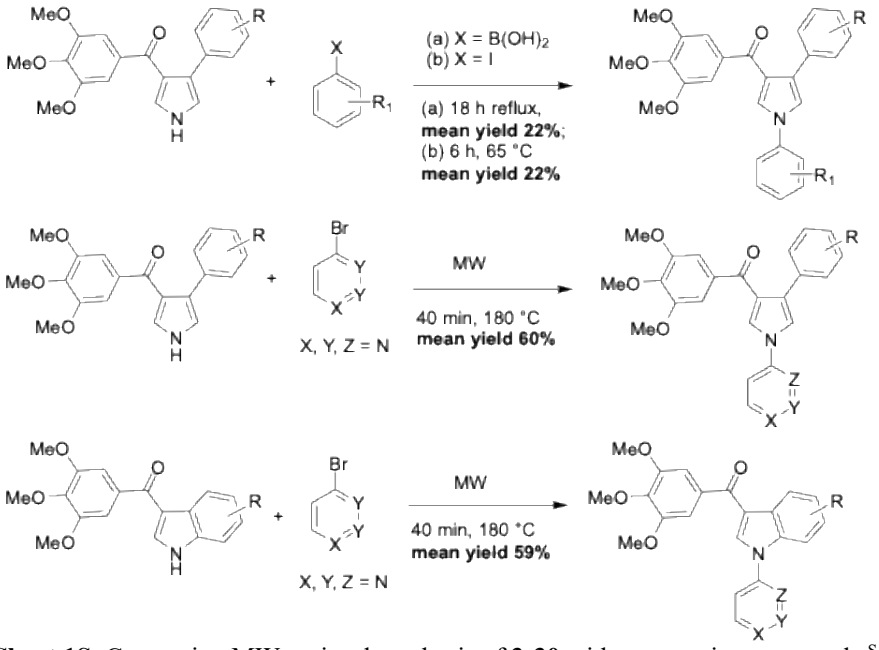


Chart 1S. Comparing MW-assisted synthesis of **3-30** with our previous protocols.[S1]

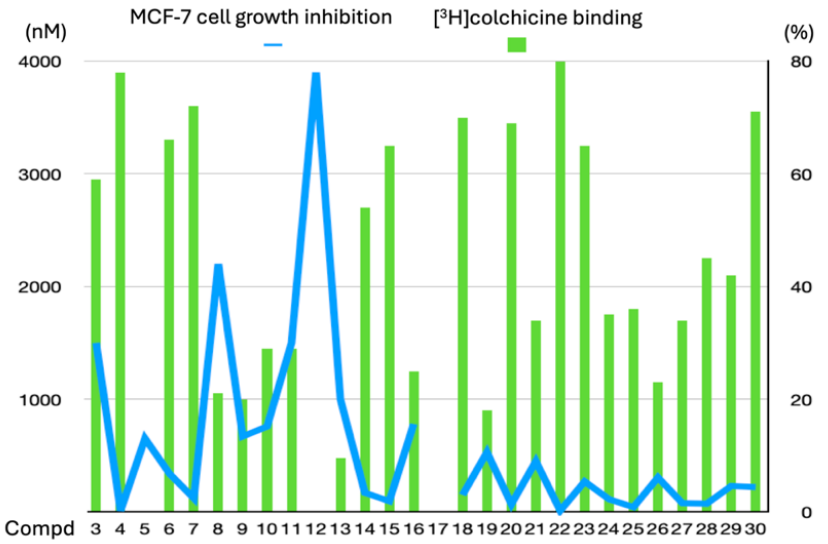


Figure S1. Correlation between the IC_{50} values of MCF-7 cancer cell growth inhibition and % values of [^{3}H]colchicine binding inhibition (Table 1 and Table 2).

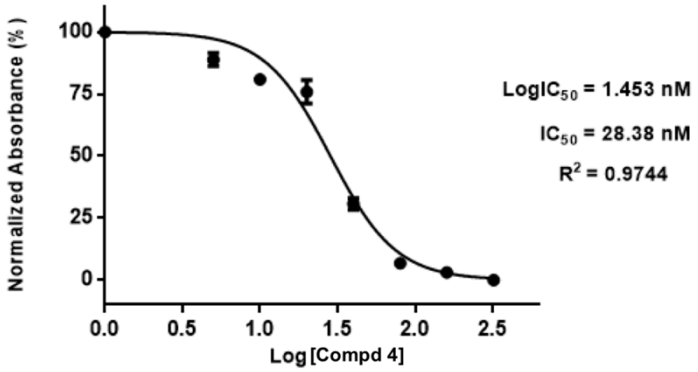


Figure S2. Inhibition of HCT116 cell growth by compound **4**.

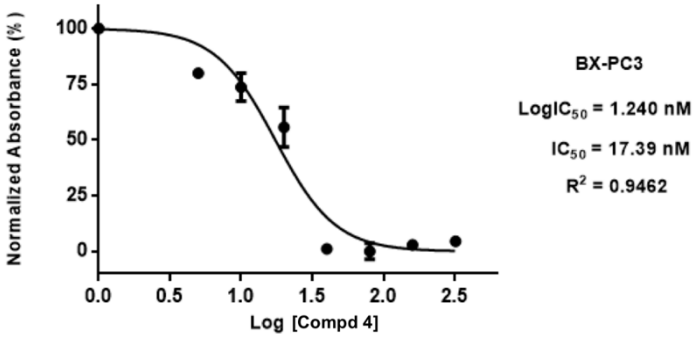


Figure S3. Inhibition of BX-PC3 cell growth by compound **4**.

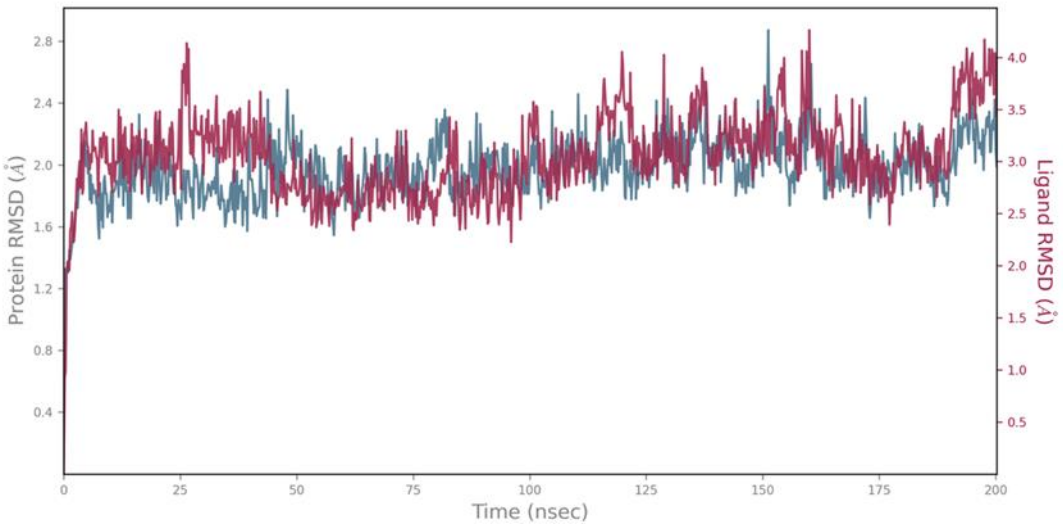


Figure S4. RMSD Plot.

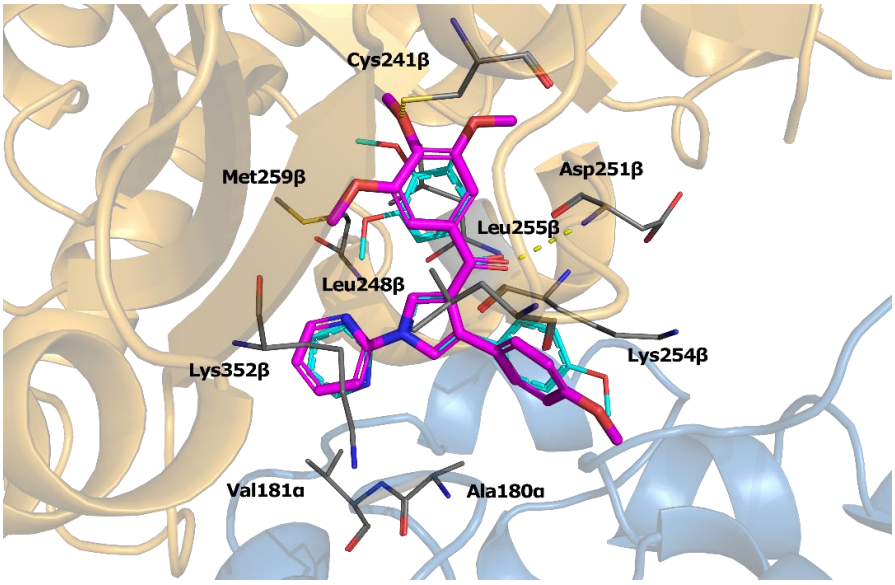
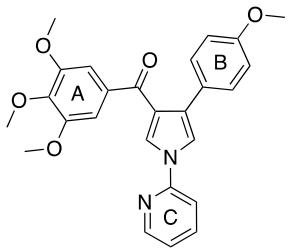


Figure S5. New hydrogen bond between the ketone group of compound **4** and Asp251β side chain, observed with 80% formation frequency during MD simulation.

Table S1. Docking score and interactions of compound **4**.



		Type of Interactions		
Cpd	Docking score[a]	H-bond	Hydrophobic[b]	Polar
4	-7.65	Ring A *p*OCH_3 Cys241β 3.1 Å	Ring A Leu254β 4.1 Å Ring B Leu248β 4.1 Å Ring B Lys252β 3.7 Å Ring C Met259β 3.8 Å Ring C Lys352β 3.7 Å Ring C Ala180α 4.4 Å Ring C Val181α 4.7 Å	Ring B OCH_3 Lys254β 4.2 Å

[a]Docking score is in Kcal/mol; [b] Distance are computed between the ring centroid and closest residue atom.

Table S2. ADME parameter for compound **4**.

Cpd	MW[a]	H don[b]	H Acc[c]	logP[d]	logS[e]	tPSA[f]	L r[g]	V r[h]
4	444.48	0	6	4.44	-5.38	71.81	0	0

Physicochemical properties predicted by QikProp:[S2,3] [a] Molecular Weight; [b] Number of H-bond acceptors; [c] Number of H-bond donors; [d] Octanol-water partition coefficient predictor by XLOGP3 method;[S4] [e] Logarithm of compounds water solubility by ESOL method;[S5] [f] Topological polar surface area; [g] L r: Lipinsky Rule deviation (log P <5, H-bond donors ≤5, H-bond acceptors ≤10, and a molecular weight <500);[S6] [h] V r: Veber rule deviation (rotable bonds ≤ 10, tPSA ≤ 140).[S7]

References of SI

(S1) G. La Regina, R. Bai, A. Coluccia, V. Famiglini, S. Passacantilli, V. Naccarato, G. Ortar, C. Mazzoccoli, V. Ruggieri, F. Agriesti, C. Piccoli, T Tataranni, M. Nalli, A. Brancale, S. Vultaggio, C. Mercurio, M. Varasi, C. Saponaro, S. Sergio, M. Maffia, A. M. L. Coluccia, E. Hamel, R. Silvestri. 3-Aroyl-1,4-diarylpyrroles inhibit chronic myeloid leukemia cell growth through an interaction with tubulin. *ACS Med. Chem. Lett*. 2017, **8**, 521-526. DOI: 10.1021/acsmedchemlett.7b00022.

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(S6) C. A. Lipinski, F. Lombardo, C. A. Dominy, P. J. Feeney. Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings. *Adv. Drug Delivery Rev*. 2001, **46**, 3-26. DOI: 10.1016/s0169-409x(00)00129-0.

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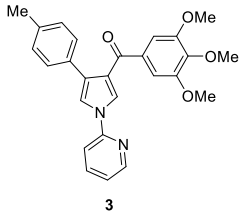
^{1}H and ^{13}C NMR Spectra of Pyrroles **3-24** and Indoles **25-30**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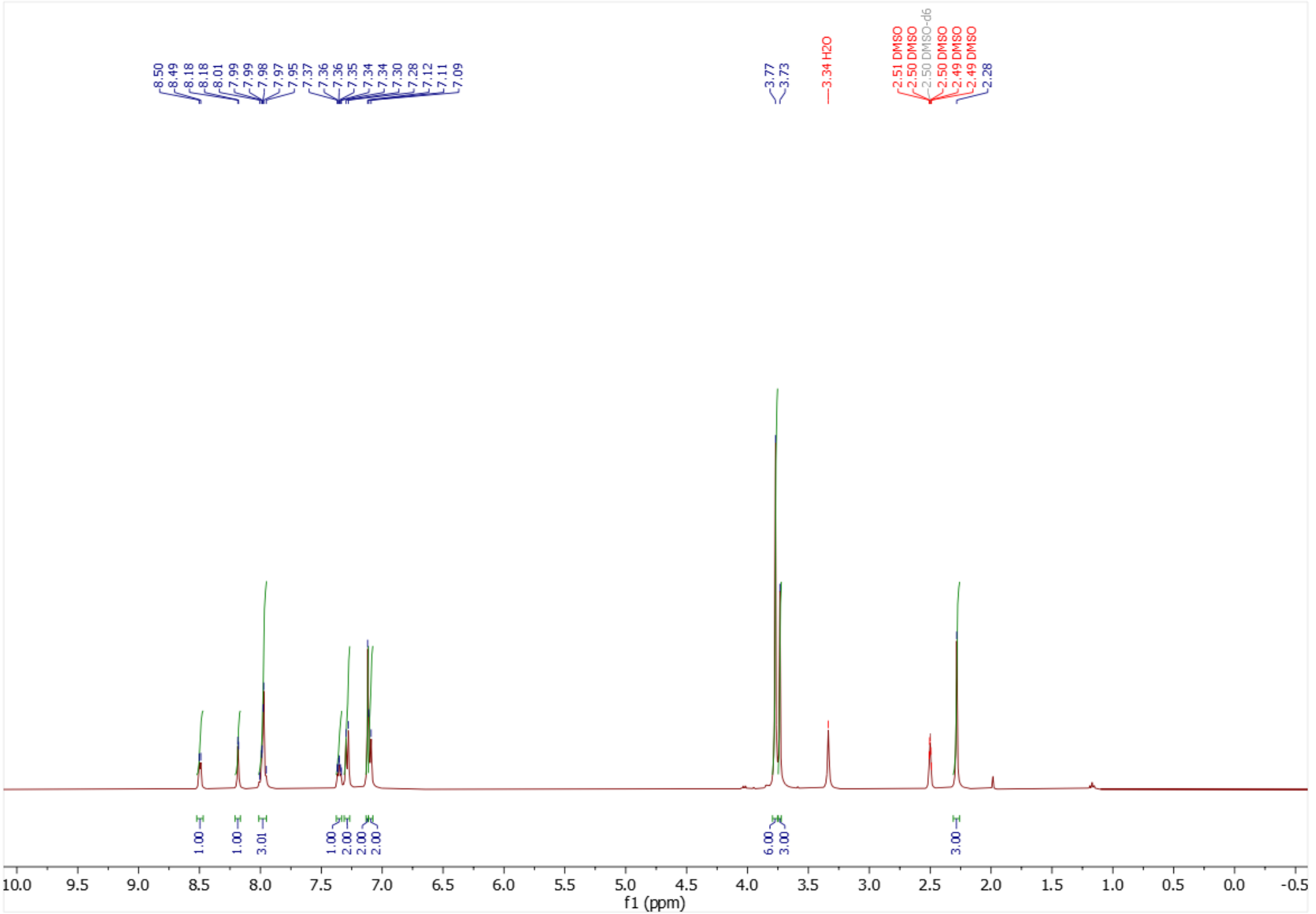
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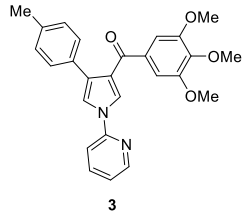
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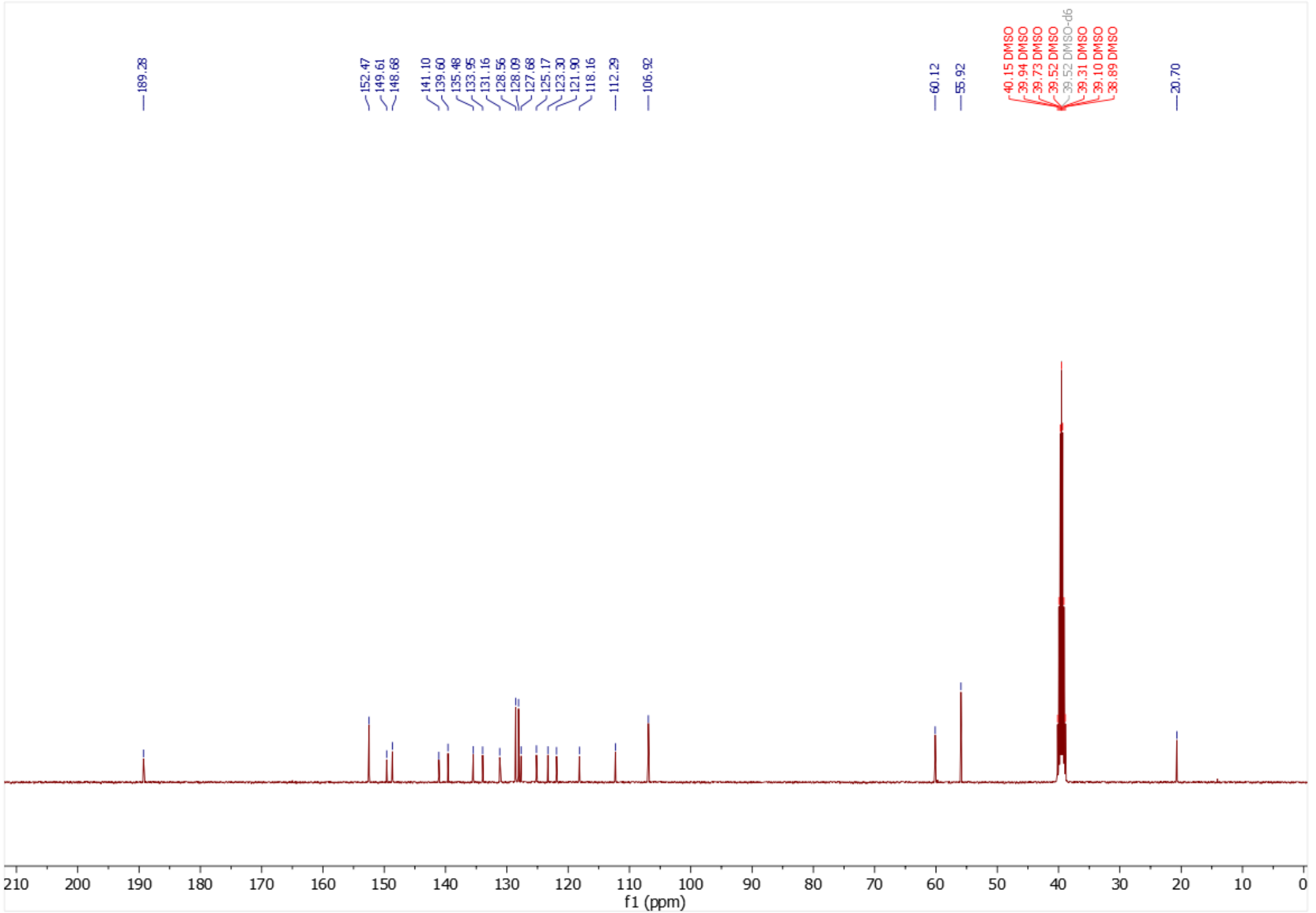
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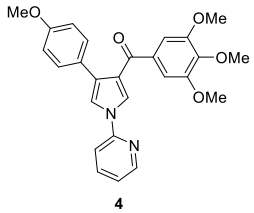
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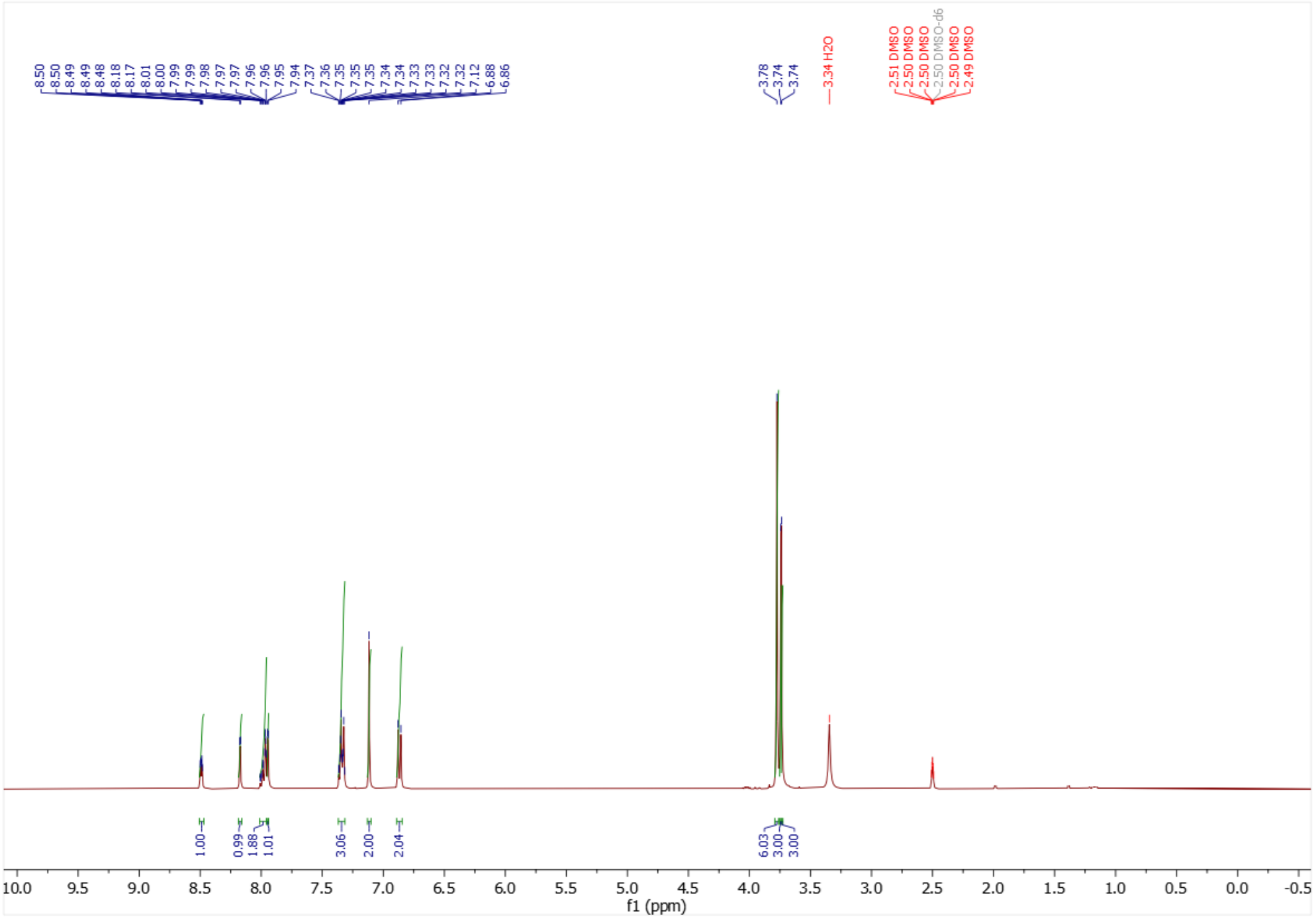
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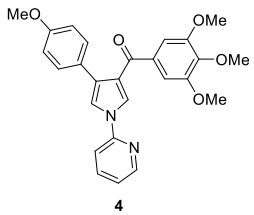
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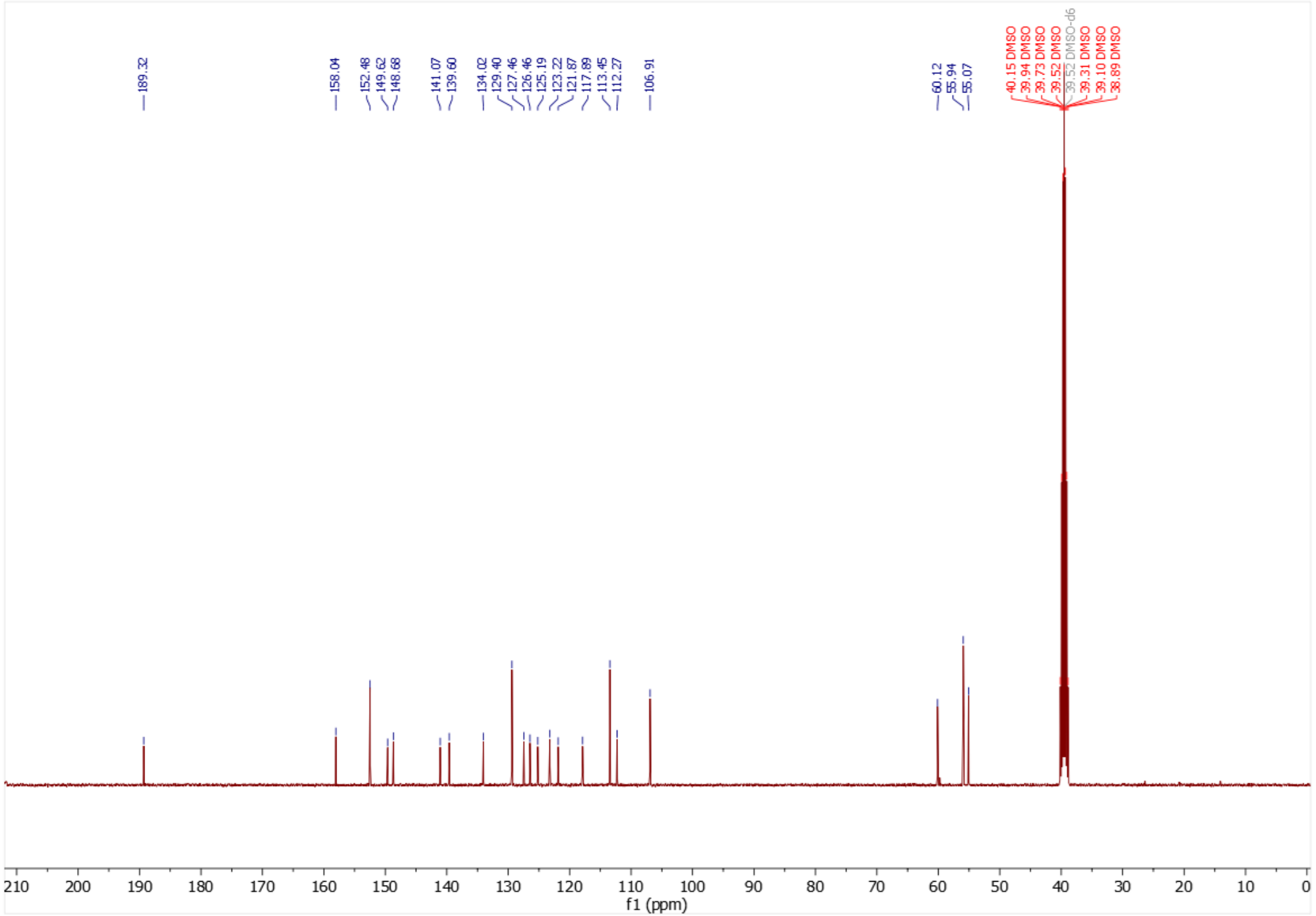
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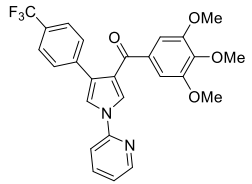
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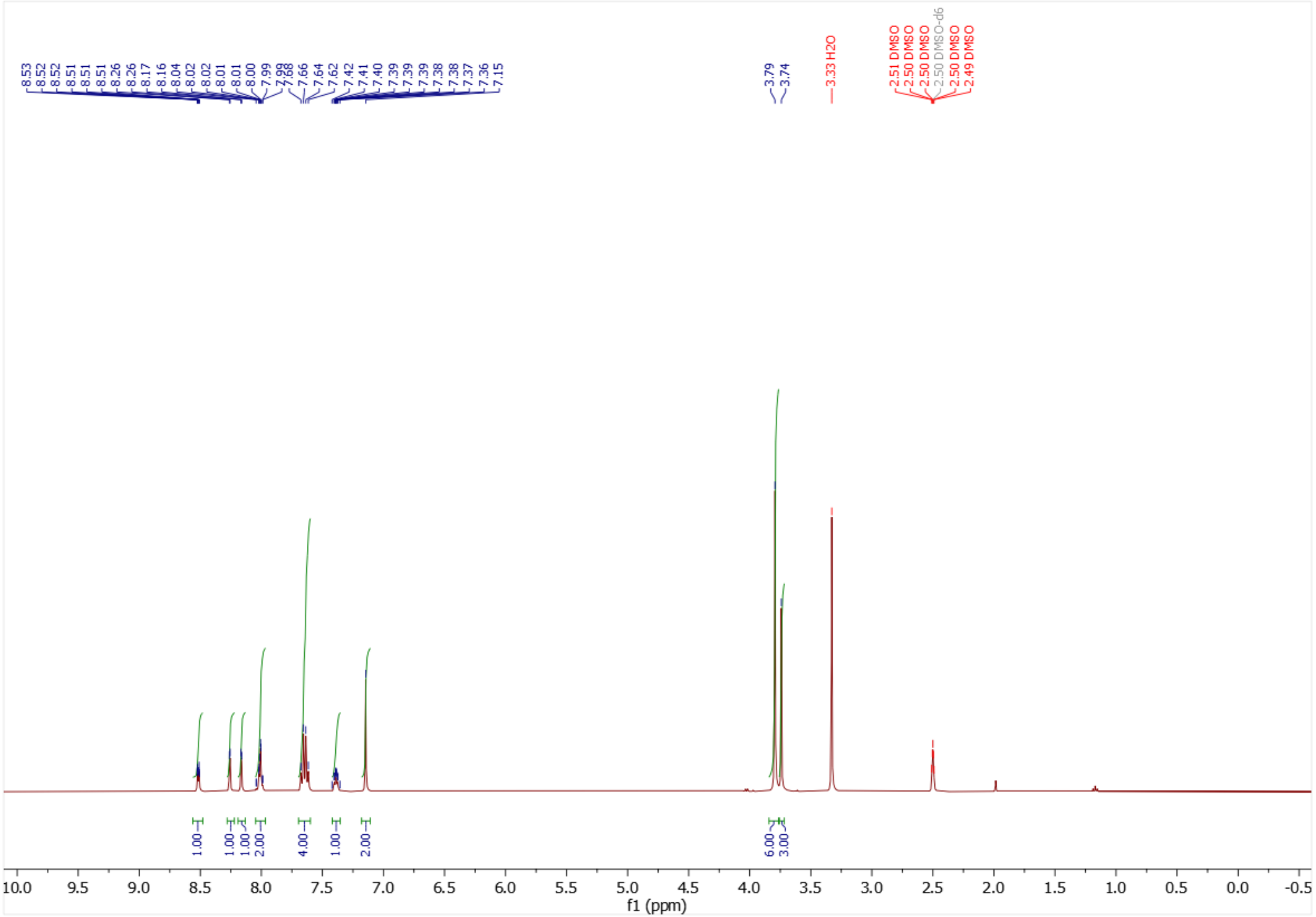
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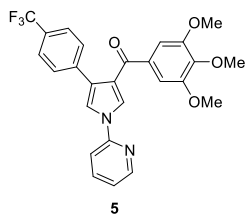
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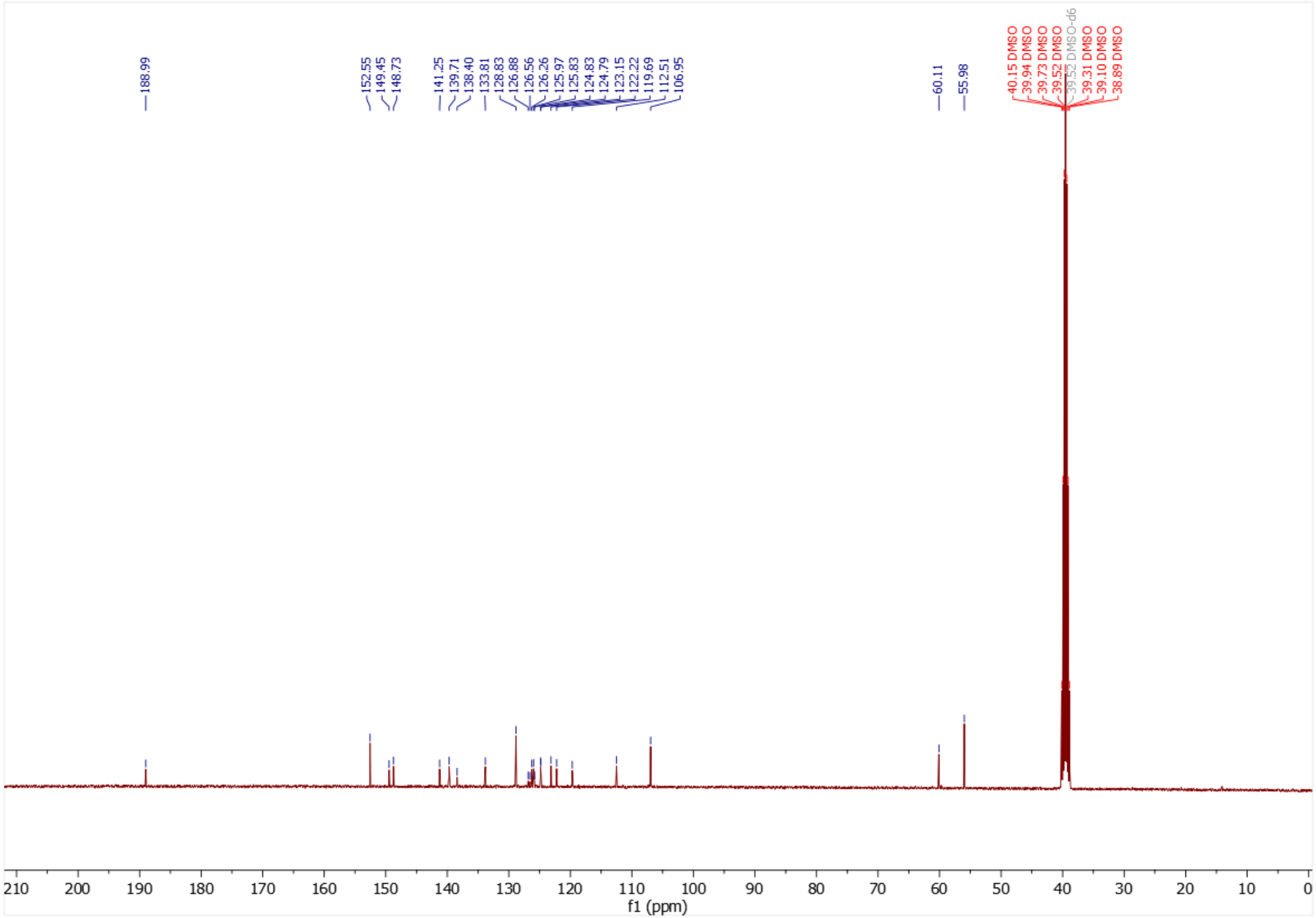
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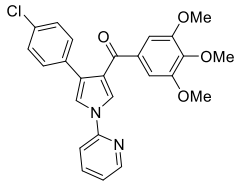
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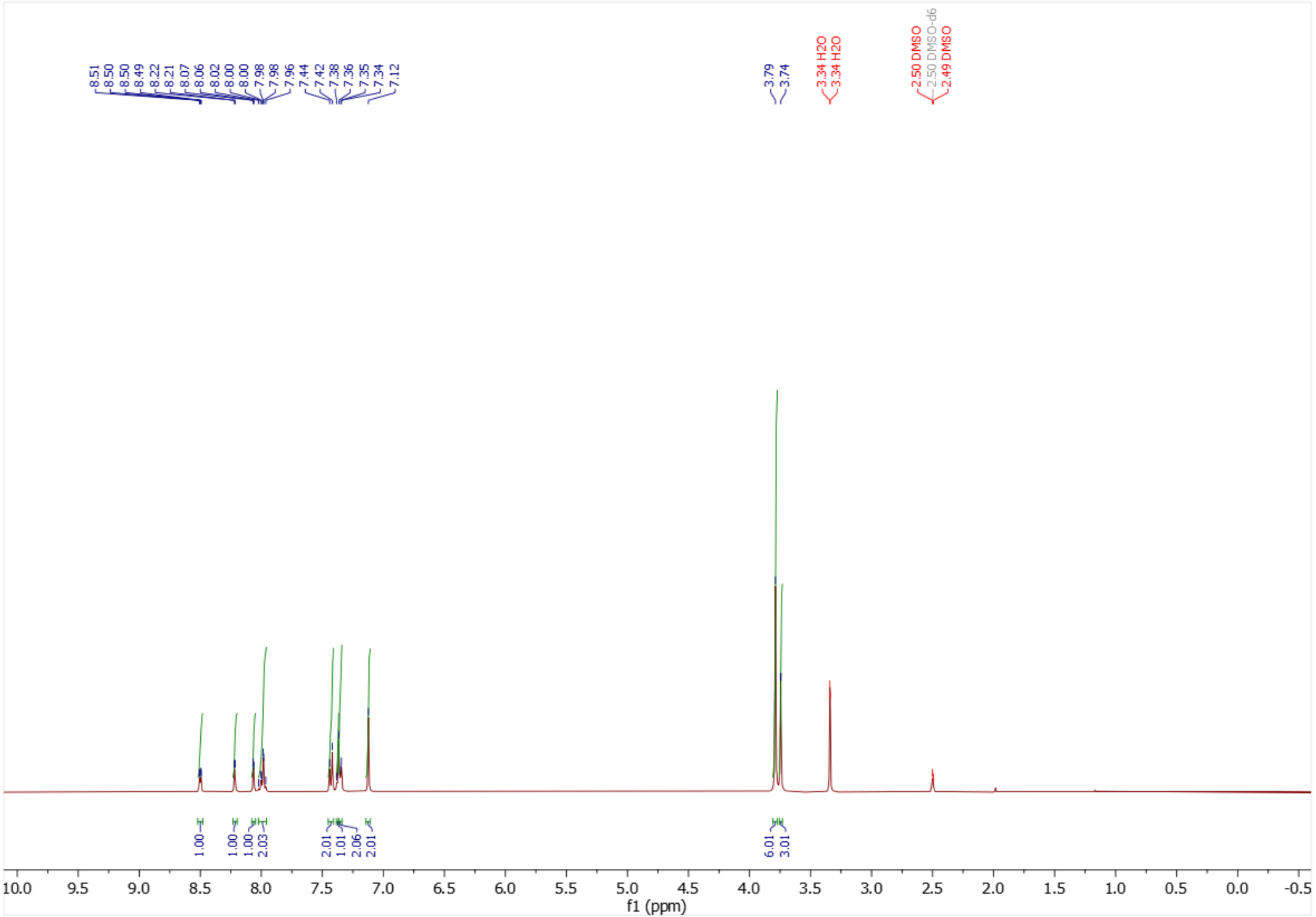
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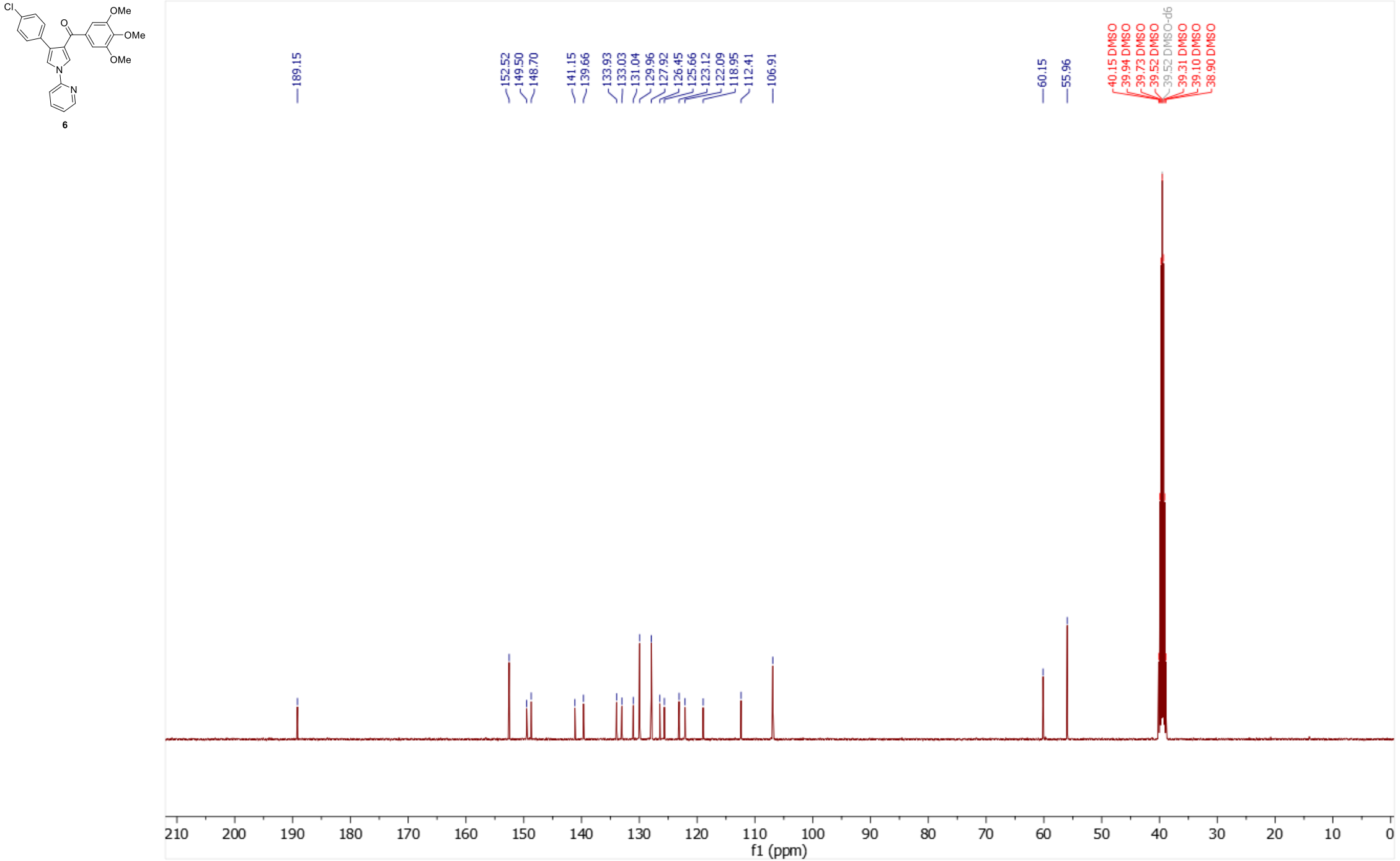
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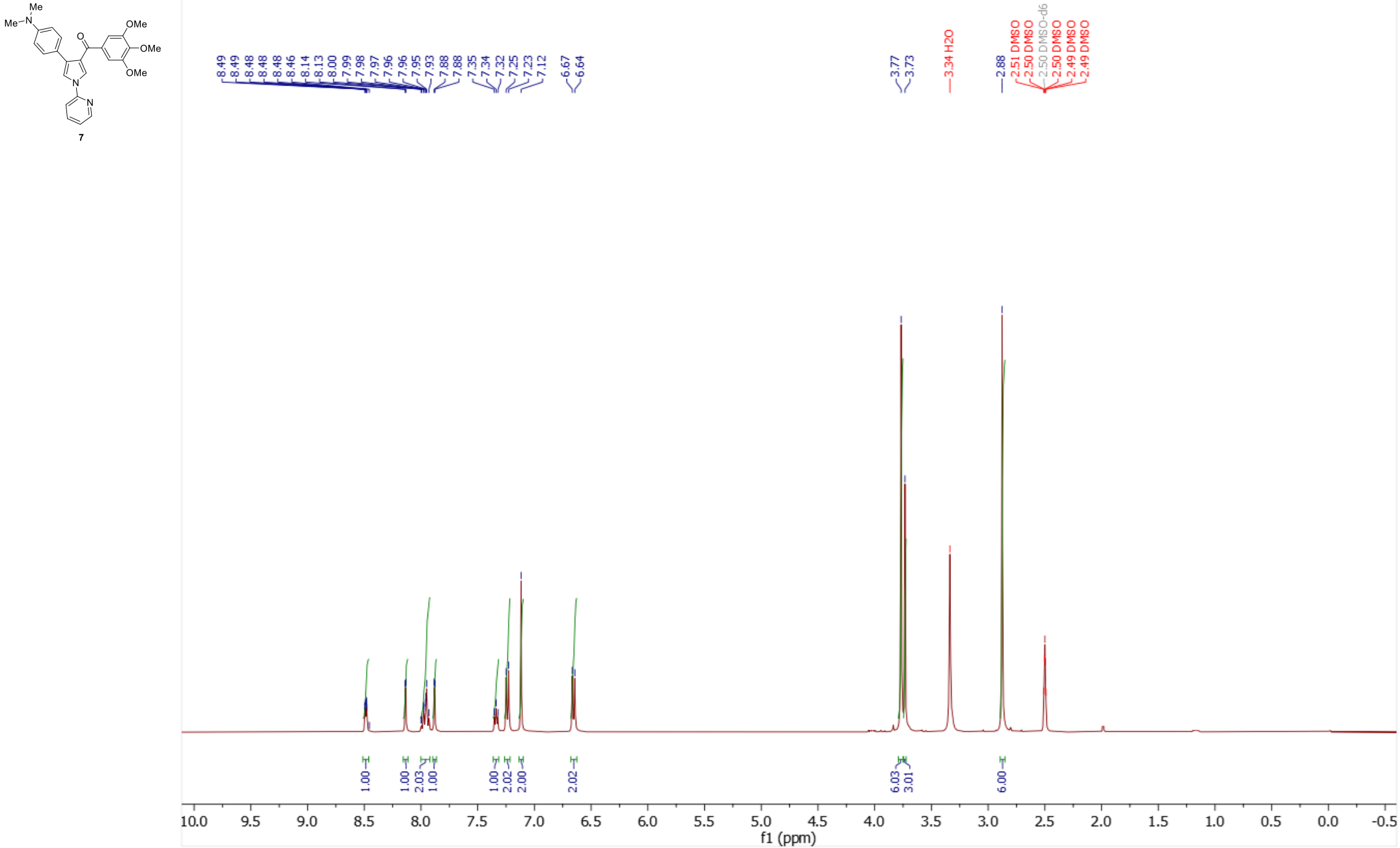
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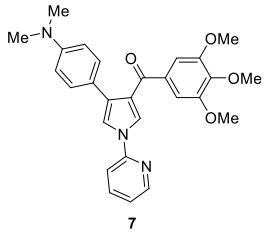
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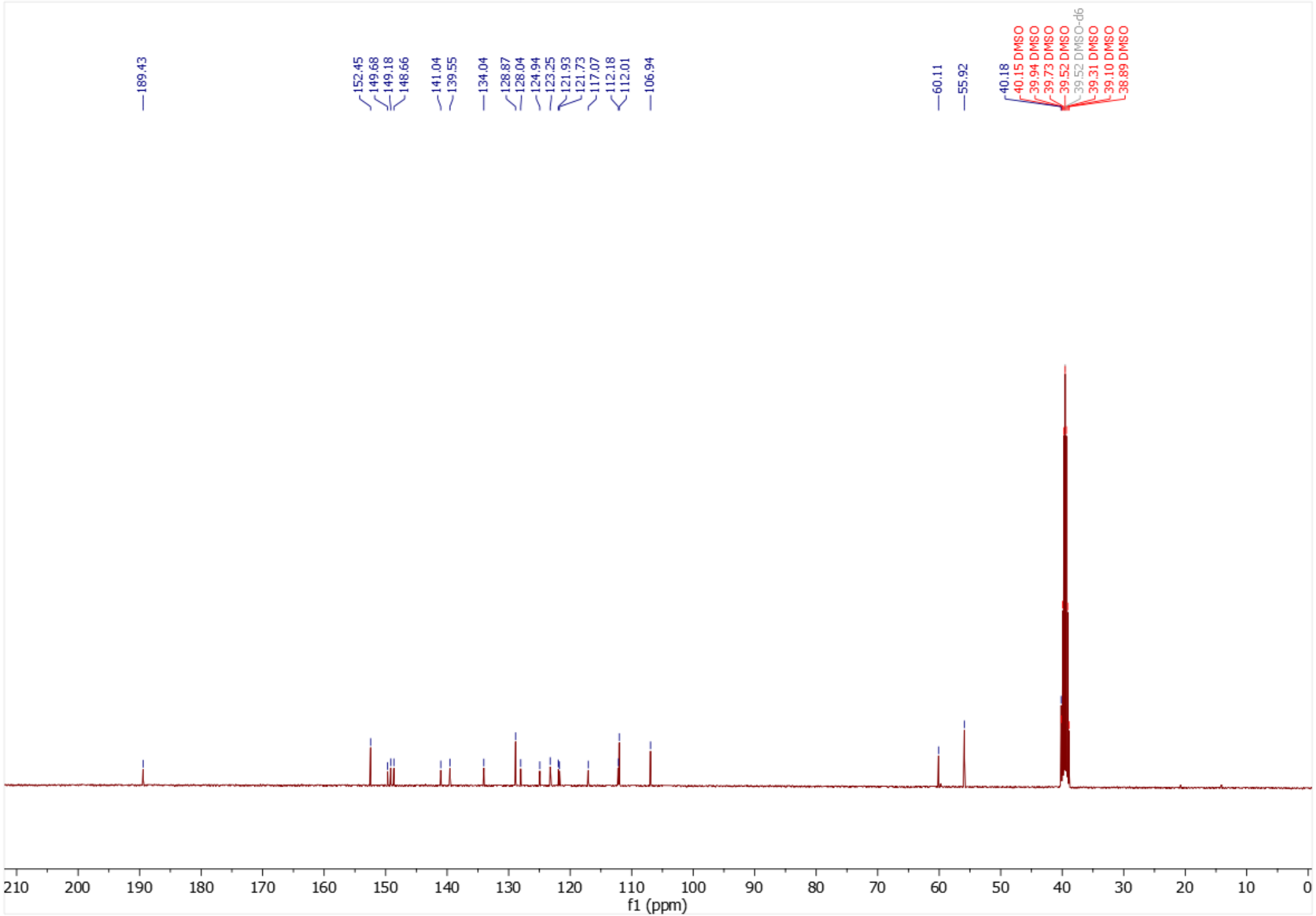
7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139.55
134.04
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128.04
124.94
123.25
121.93
121.73
117.07
112.18
112.01
106.94
60.11
55.92
40.18
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO
39.52 DMSO-d6
39.31 DMSO
39.10 DMSO
38.89 DMSO
210
200
190
180
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90
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70
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50
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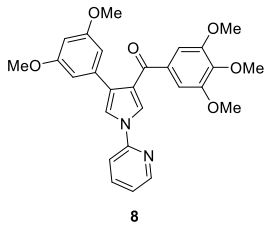
f1 (ppm)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MeO
OMe
OMe
O
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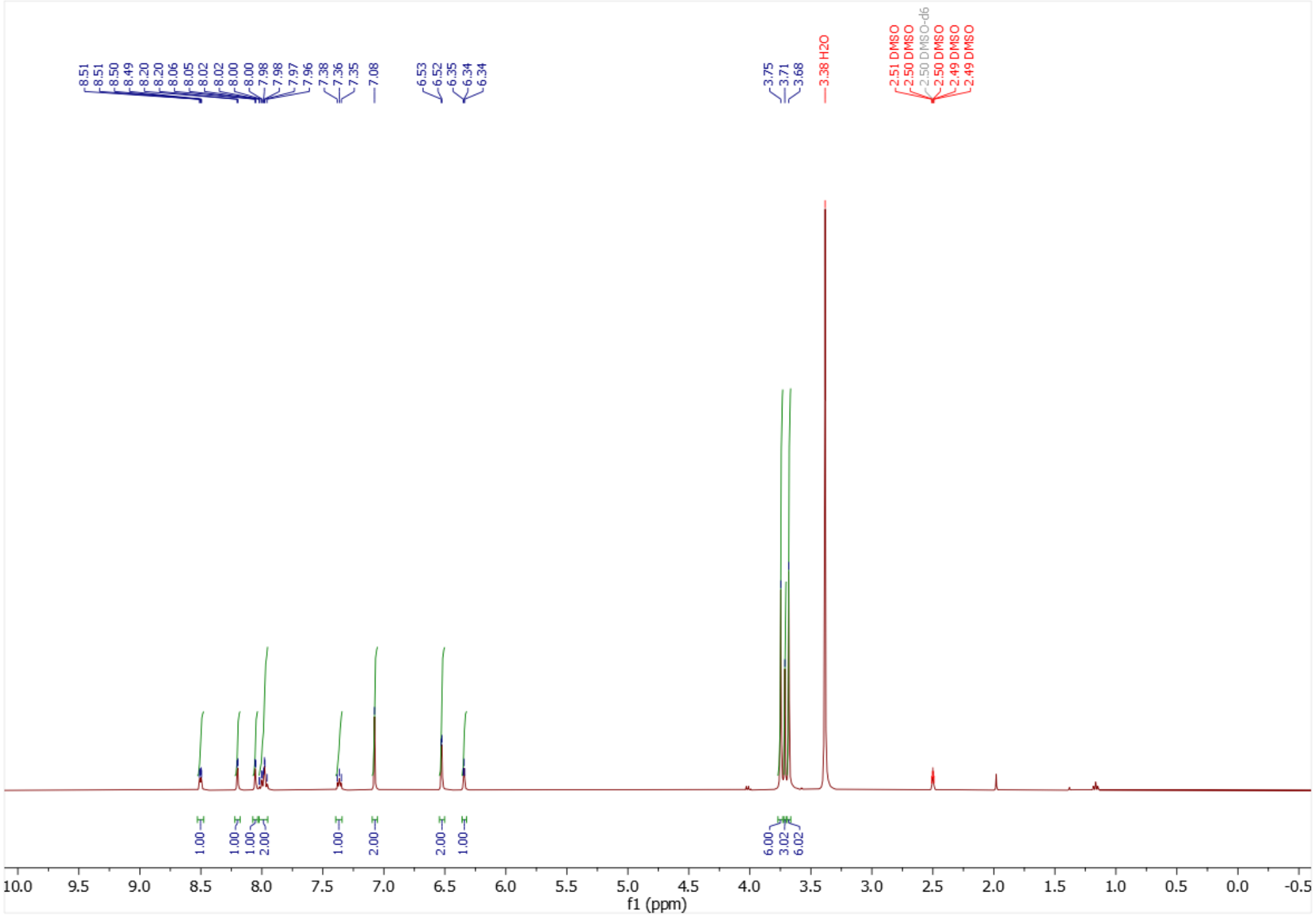
N

8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8.02
8.00
8.00
7.98
7.98
7.97
7.96
7.38
7.36
7.35
7.08
6.53
6.52
6.35
6.34
6.34
3.75
3.71
3.68
3.38 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.49 DMSO
2.49 DMSO
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1.00
1.00
2.00
1.00
2.00
2.00
1.00
6.00
3.02
6.02
10.0
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8.0
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6.5
6.0
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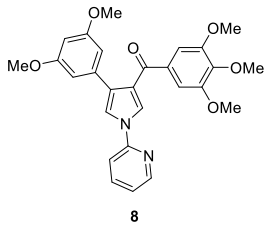
f1 (ppm)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OMe
OMe
O
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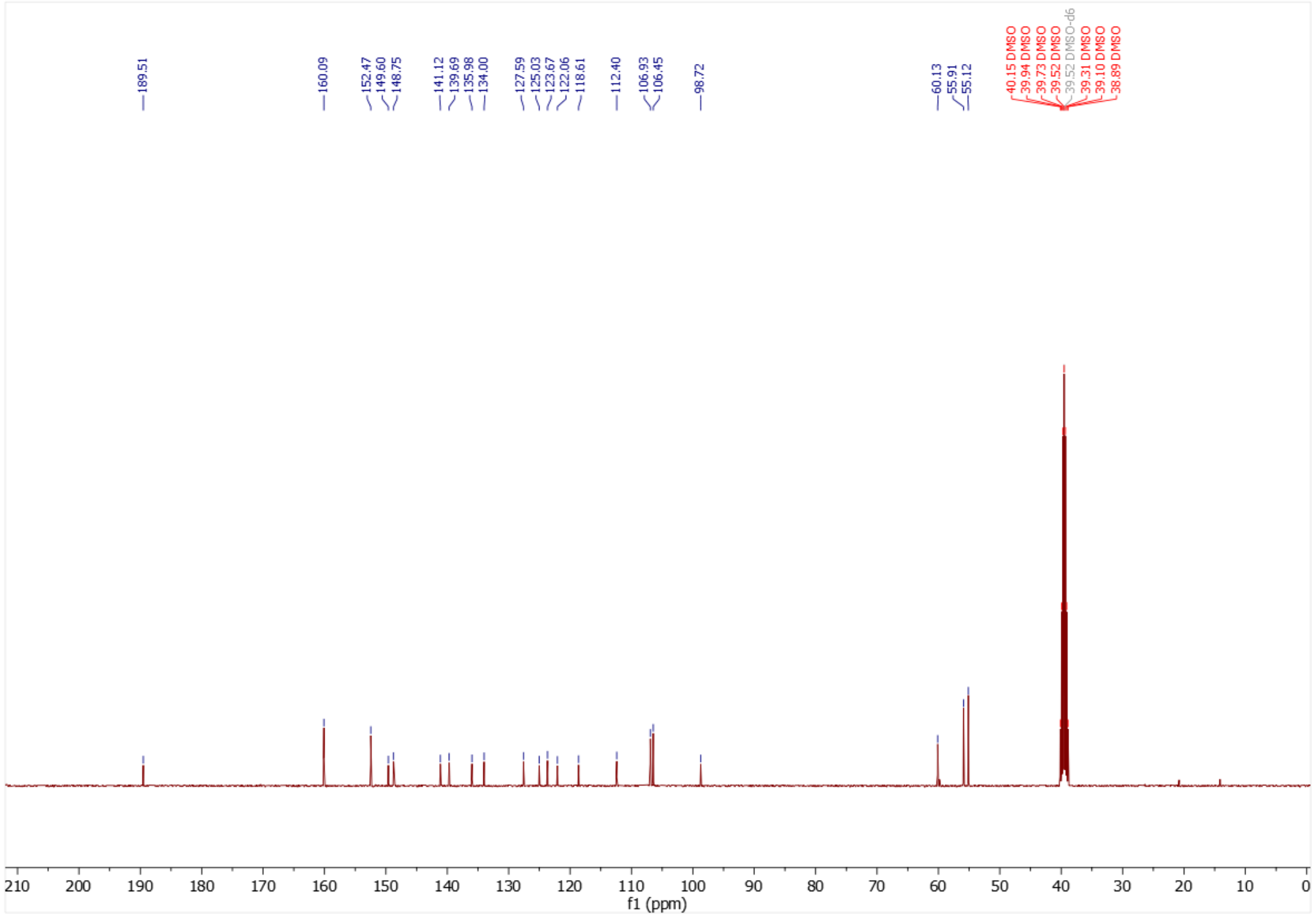
N

8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125.03
123.67
122.06
118.61
112.40
106.93
106.45
98.72
60.13
55.91
55.12
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO
39.52 DMSO-d6
39.31 DMSO
39.10 DMSO
38.89 DMSO
210
200
190
180
170
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50
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10
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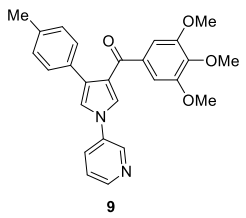
f1 (ppm)


Me
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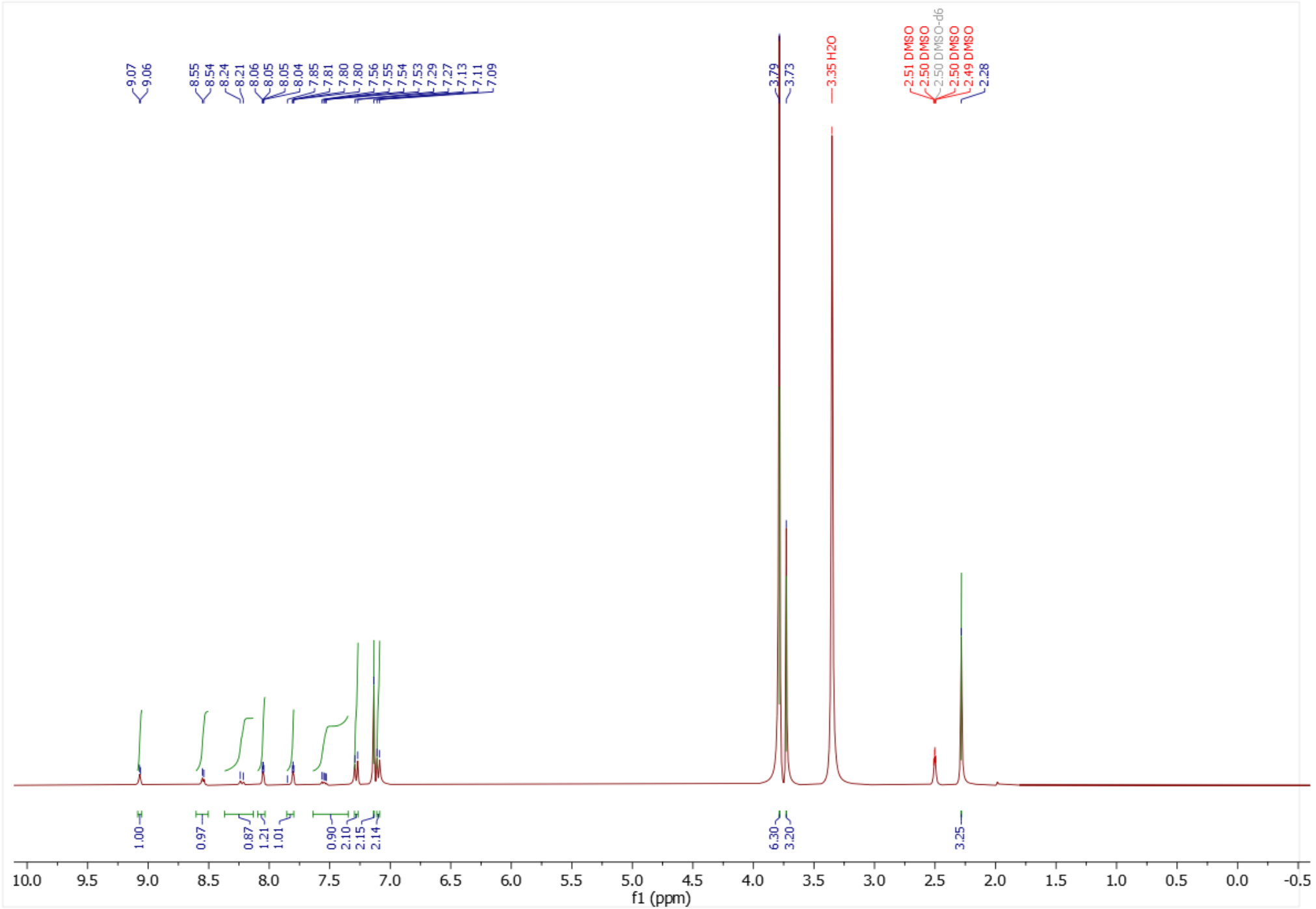
OMe
O
N
N

9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8.05
8.05
8.04
7.85
7.81
7.80
7.80
7.56
7.55
7.54
7.53
7.29
7.27
7.13
7.11
7.09
3.79
3.73
3.35 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.49 DMSO
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1.21
1.01
0.90
2.10
2.15
2.14
6.30
3.20
3.25
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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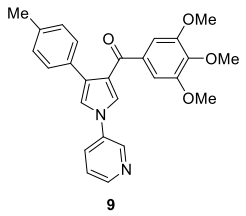
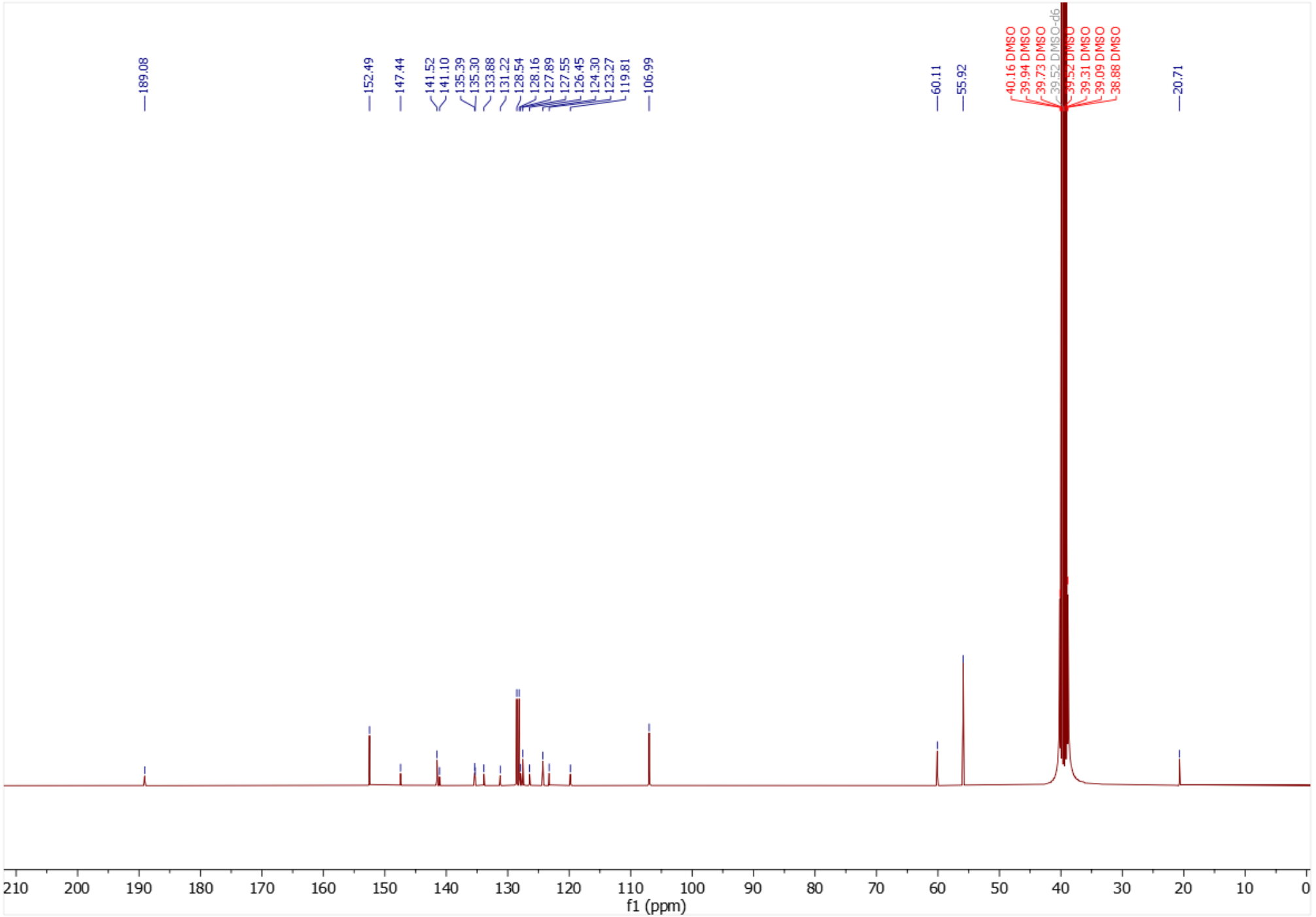
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Me
OMe
OMe
OMe
O
N
N

9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135.30
133.88
131.22
128.54
128.16
127.89
127.55
126.45
124.30
123.27
119.81
106.99
60.11
55.92
40.16 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO-d6
39.52 DMSO
39.31 DMSO
39.09 DMSO
38.88 DMSO
20.71
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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50
40
30
20
10
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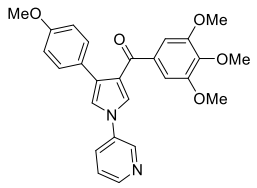
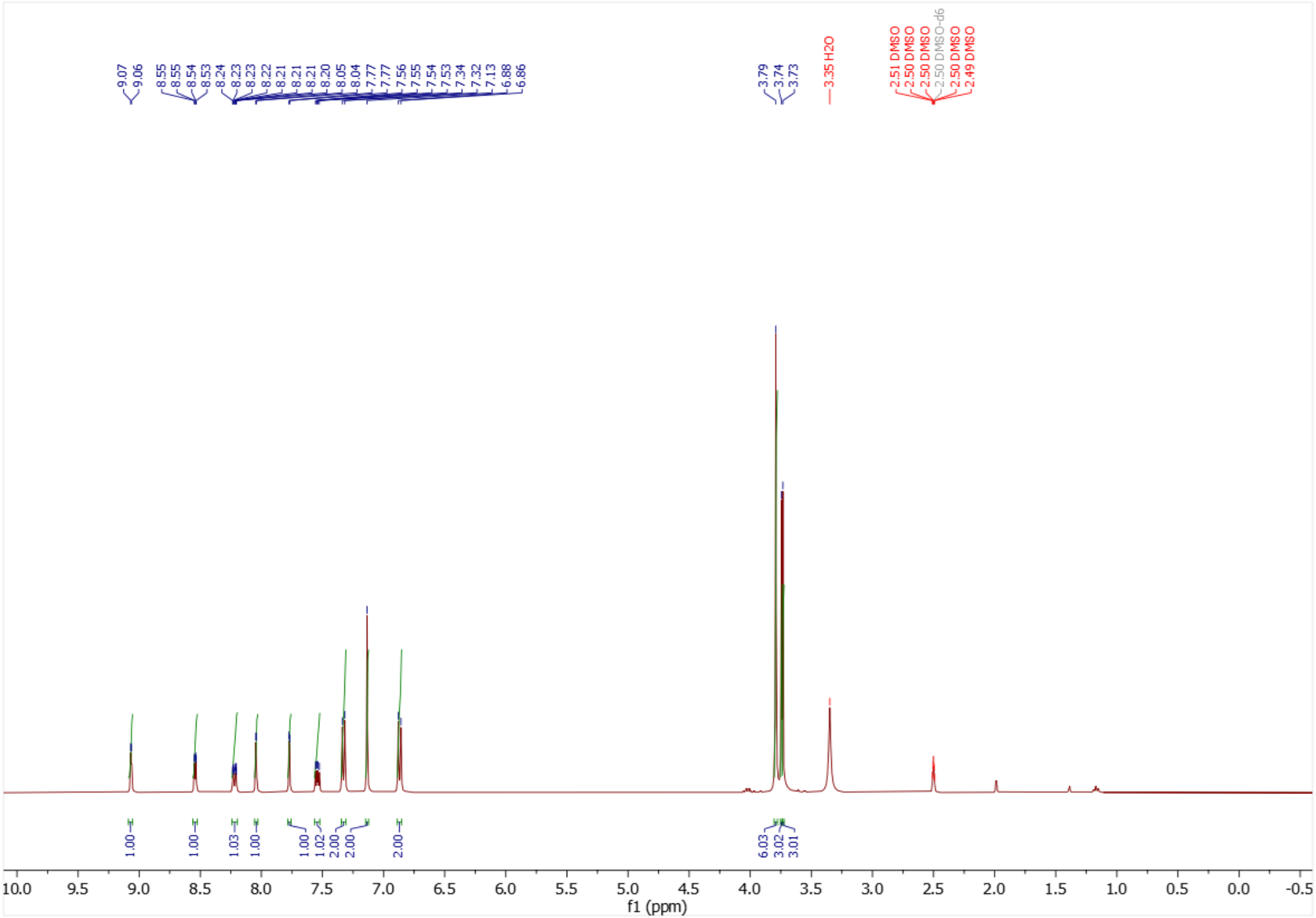
f1 (ppm)


MeO
OMe
OMe
OMe
O
N
N

10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9.06
8.55
8.55
8.54
8.53
8.24
8.23
8.23
8.22
8.21
8.21
8.21
8.20
8.05
8.04
7.77
7.77
7.56
7.55
7.54
7.53
7.34
7.32
7.13
6.88
6.86
3.79
3.74
3.73
3.35 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.49 DMSO
1.00
1.00
1.03
1.00
1.00
1.02
2.00
2.00
2.00
6.03
3.02
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
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2.0
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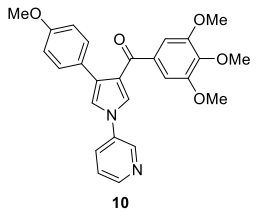
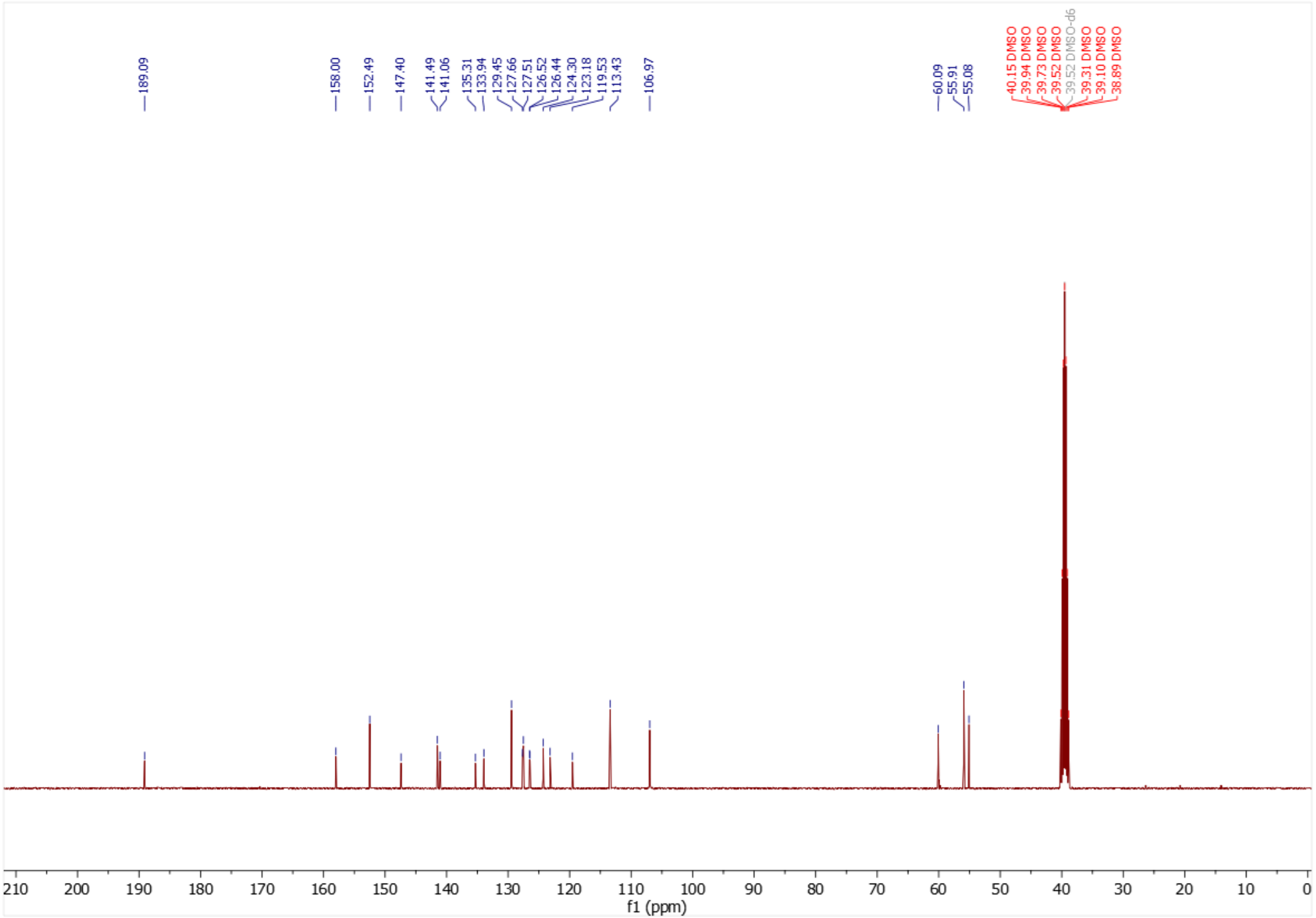
0.5
0.0
-0.5
f1 (ppm)


MeO
OMe
OMe
OMe
O
N
N

10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126.44
124.30
123.18
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113.43
106.97
60.09
55.91
55.08
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO
39.52 DMSO-d6
39.31 DMSO
39.10 DMSO
38.89 DMSO
210
200
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180
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150
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130
120
110
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90
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70
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50
40
30
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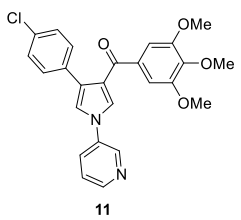
10
0
f1 (ppm)


Cl
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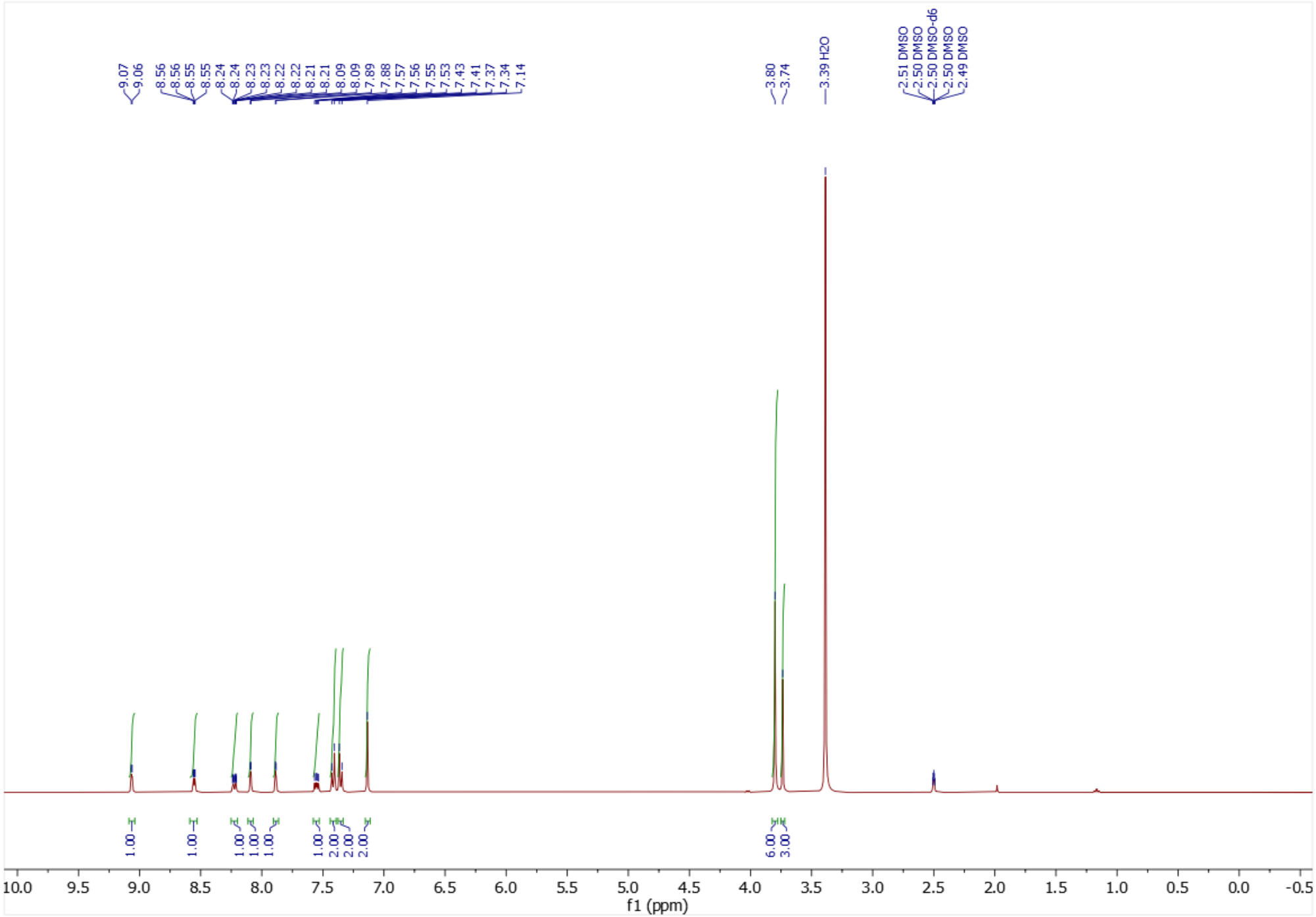
OMe
OMe
N
N

11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9.06
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8.24
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8.23
8.22
8.22
8.21
8.21
8.09
8.09
7.89
7.88
7.57
7.56
7.55
7.53
7.43
7.41
7.37
7.34
7.14
3.80
3.74
3.39 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.49 DMSO
1.00
1.00
1.00
1.00
1.00
1.00
2.00
2.00
2.00
6.00
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
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3.0
2.5
2.0
1.5
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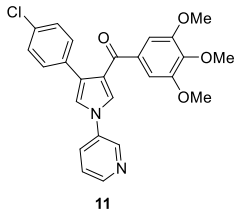
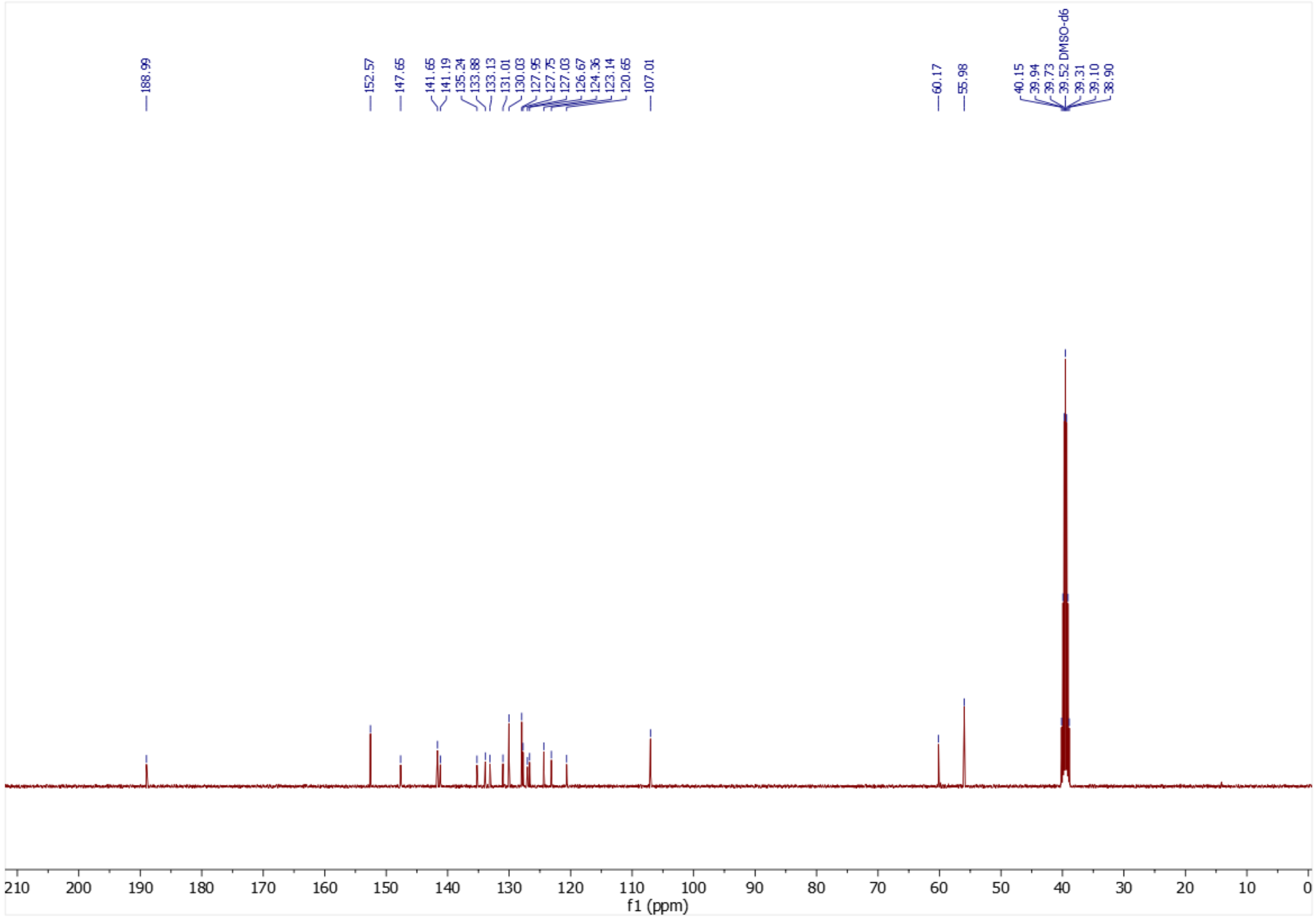
0.5
0.0
-0.5
f1 (ppm)


Cl
O
OMe
OMe
OMe
N
N

11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130.03
127.95
127.75
127.03
126.67
124.36
123.14
120.65
107.01
60.17
55.98
40.15
39.94
39.73
39.52 DMSO-d6
39.31
39.10
38.90
210
200
190
180
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130
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110
100
90
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50
40
30
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10
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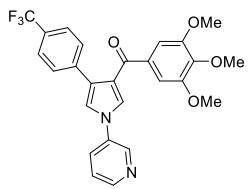
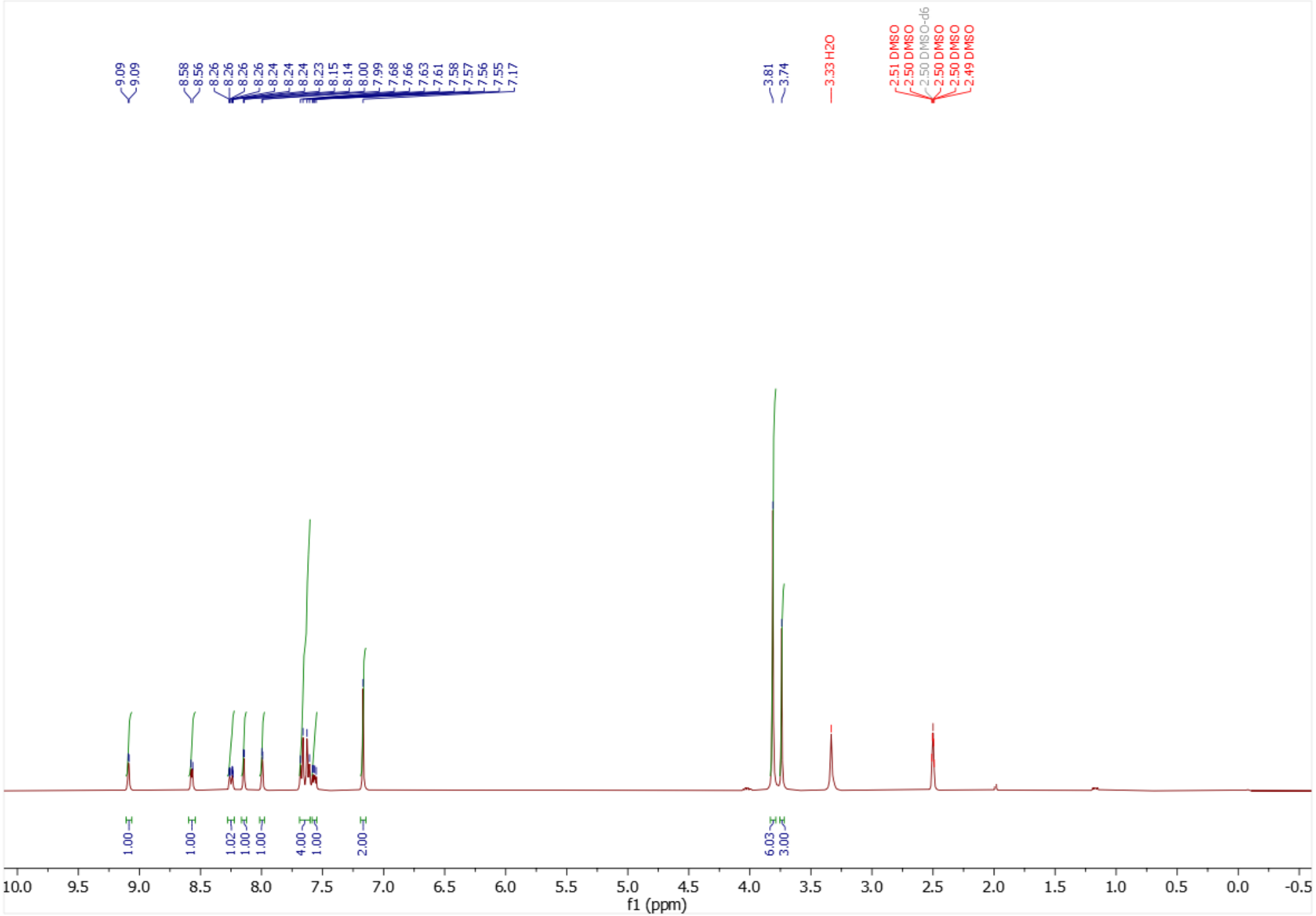
f1 (ppm)


F3C
OMe
OMe
OMe
O
N
N

12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8.14
8.00
7.99
7.68
7.66
7.63
7.61
7.58
7.57
7.56
7.55
7.17
3.81
3.74
3.33 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.50 DMSO
2.49 DMSO
1.00
1.00
1.02
1.00
1.00
4.00
1.00
2.00
6.03
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
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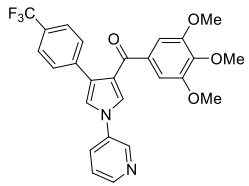
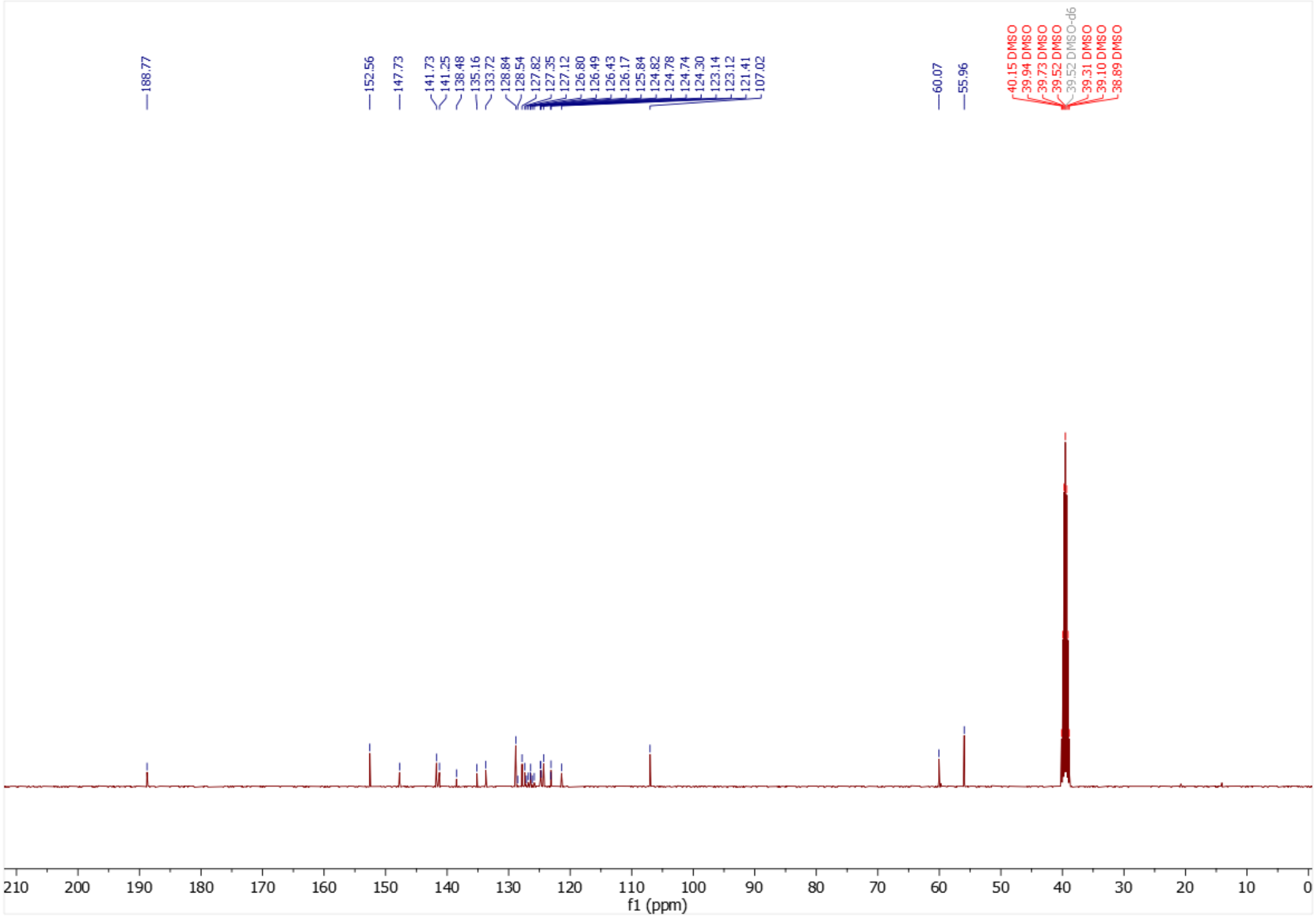
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


F3C
O
OMe
OMe
OMe
N
N

12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127.35
127.12
126.80
126.49
126.43
126.17
125.84
124.82
124.78
124.74
124.30
123.14
123.12
121.41
107.02
60.07
55.96
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO
39.52 DMSO-d6
39.31 DMSO
39.10 DMSO
38.89 DMSO
210
200
190
180
170
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150
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130
120
110
100
90
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70
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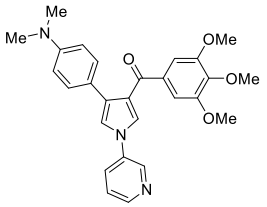
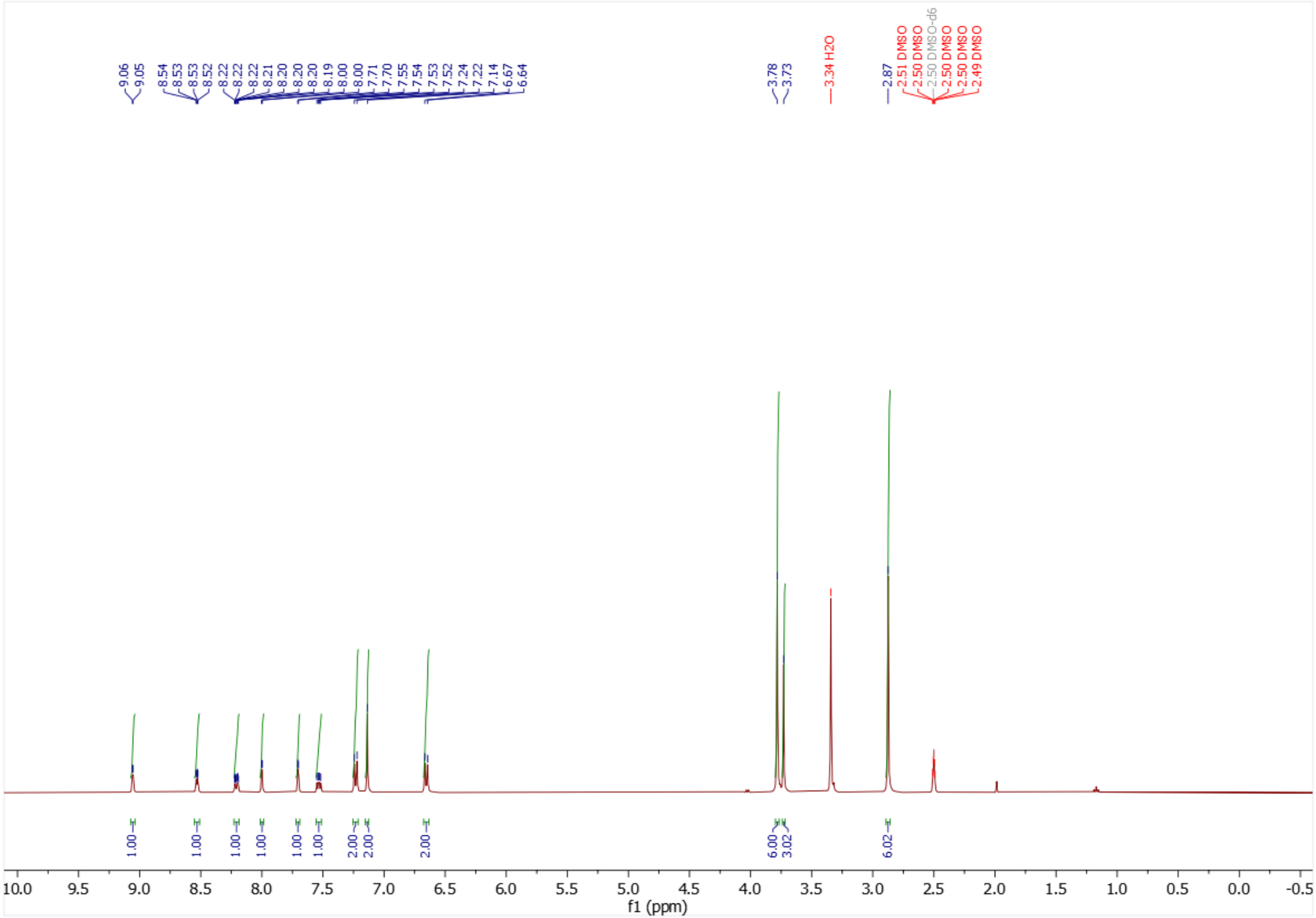
50
40
30
20
10
0
f1 (ppm)


Me
Me
N
O
OMe
OMe
OMe
N
N

13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8.22
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8.20
8.20
8.19
8.00
8.00
7.71
7.70
7.55
7.54
7.53
7.52
7.24
7.22
7.14
6.67
6.64
3.78
3.73
3.34 H2O
2.87
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.50 DMSO
2.49 DMSO
1.00
1.00
1.00
1.00
1.00
1.00
2.00
2.00
2.00
6.00
3.02
6.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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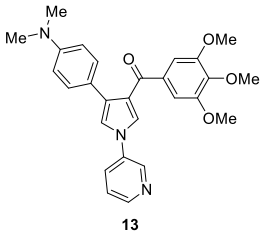
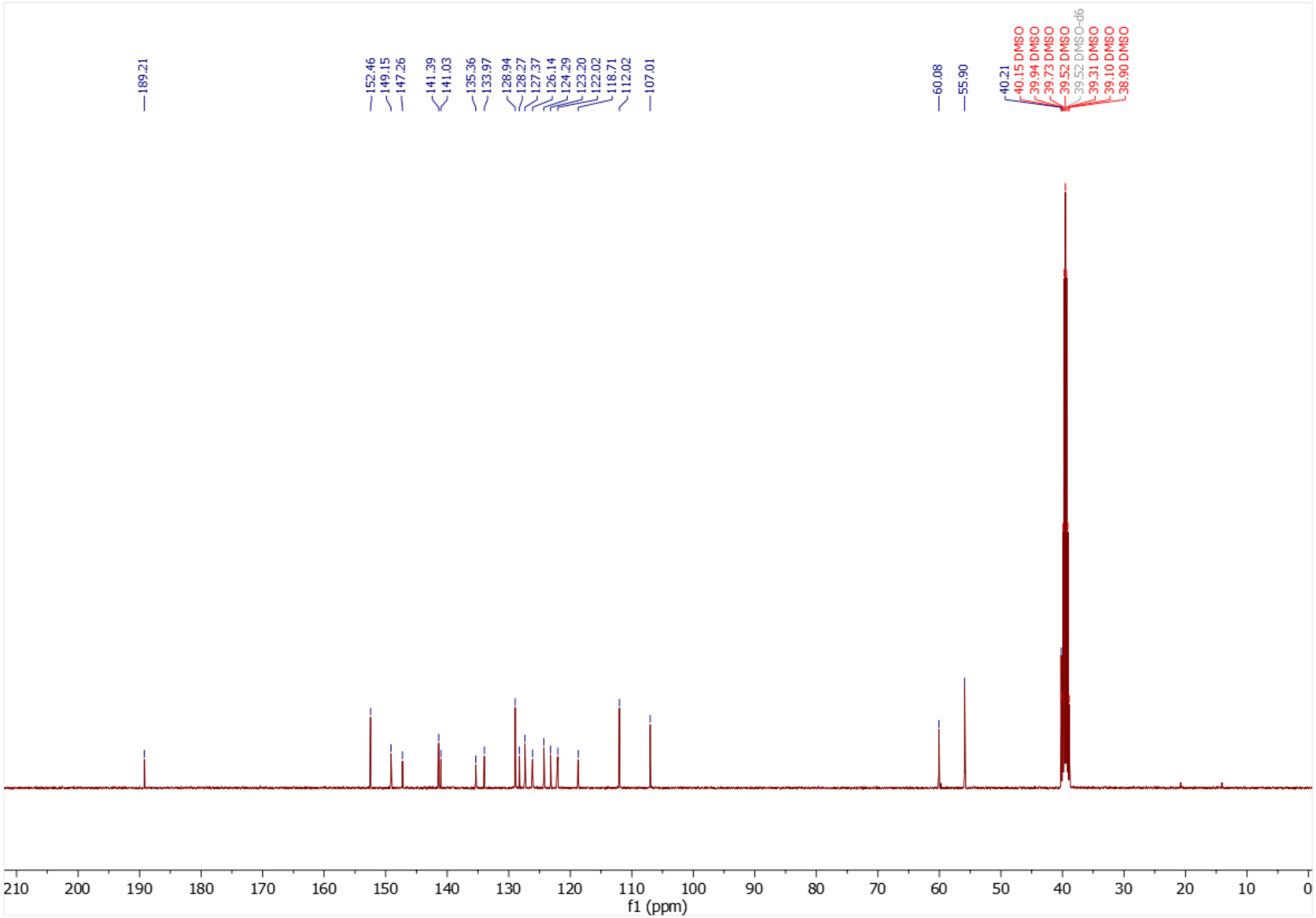
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Me
Me
N
O
OMe
OMe
OMe
N
13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149.15
147.26
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141.03
135.36
133.97
128.94
128.27
127.37
126.14
124.29
123.20
122.02
118.71
112.02
107.01
60.08
55.90
40.21
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO
39.52 DMSO-d6
39.31 DMSO
39.10 DMSO
38.90 DMSO
210
200
190
180
170
160
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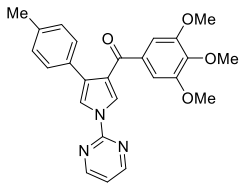
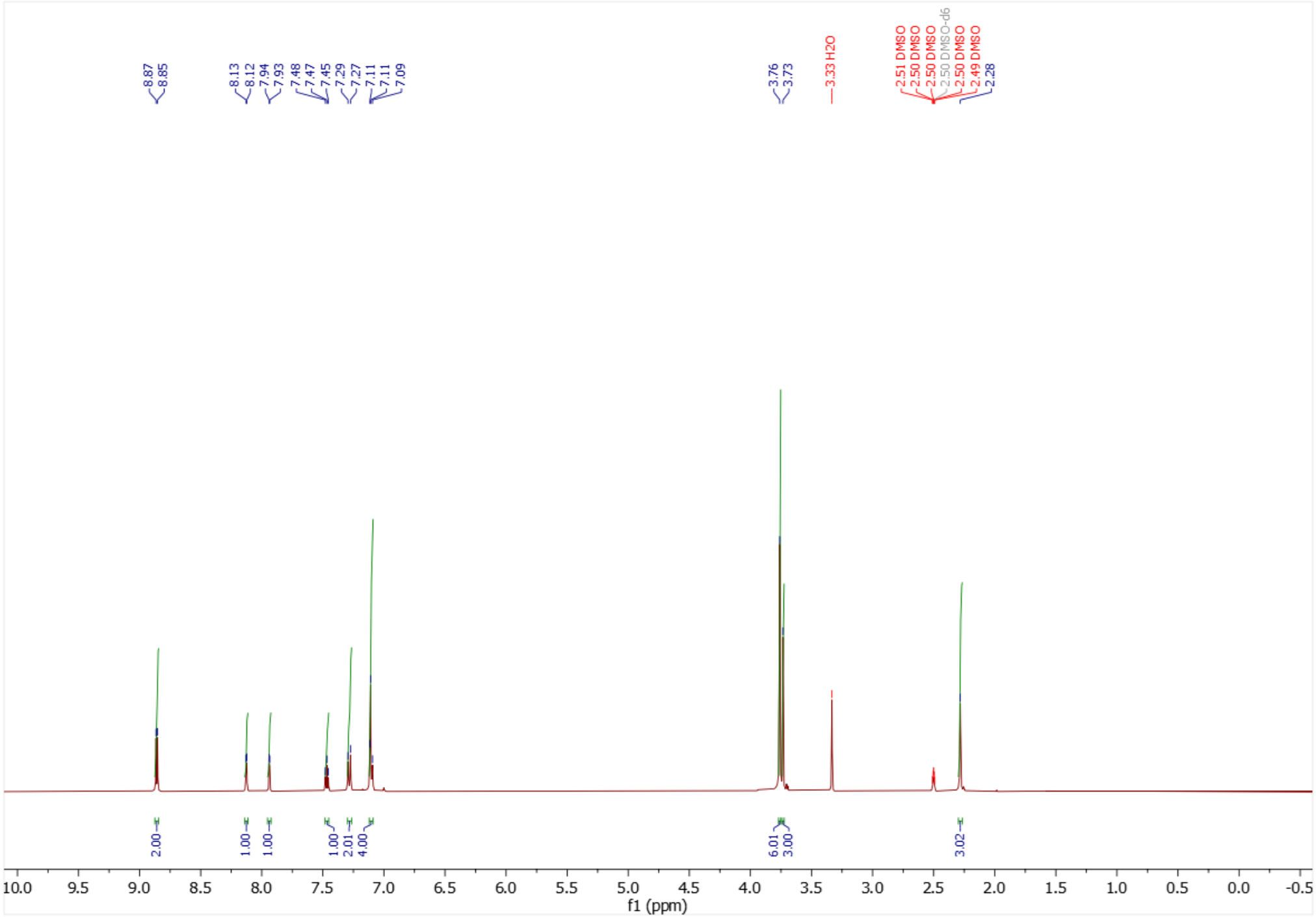
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Me
OMe
OMe
OMe
O
N
N
N

14


8.87
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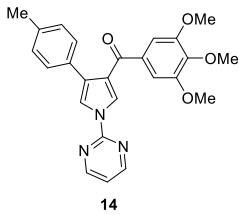
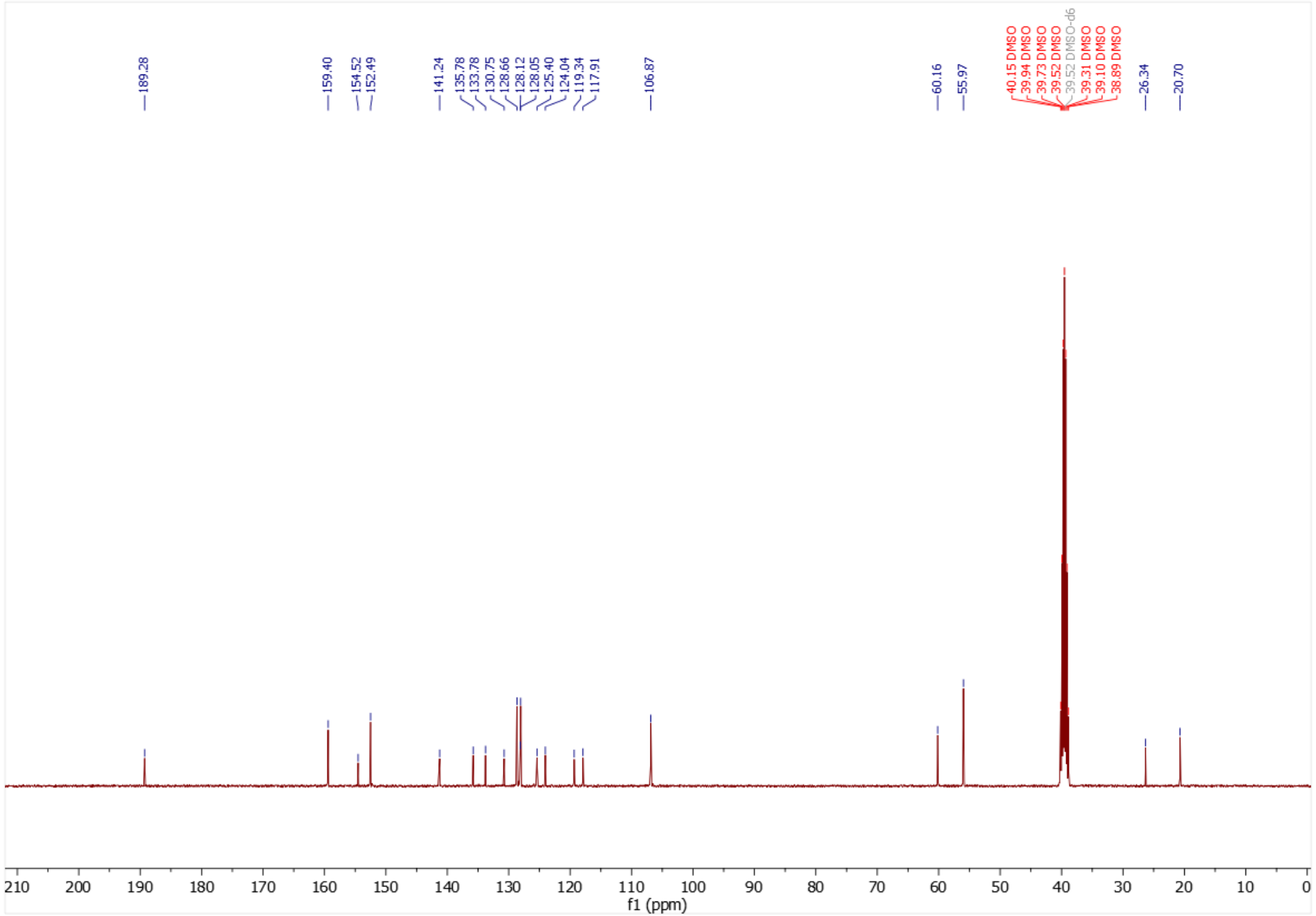
7.93
7.48
7.47
7.45
7.29
7.27
7.11
7.11
7.09
3.76
3.73
3.33 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.49 DMSO
2.28
2.00
1.00
1.00
1.00
2.01
4.00
6.01
3.00
3.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Me
OMe
OMe
OMe
O
N
N
N

14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152.49
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135.78
133.78
130.75
128.66
128.12
128.05
125.40
124.04
119.34
117.91
106.87
60.16
55.97
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO
39.52 DMSO-d6
39.31 DMSO
39.10 DMSO
38.89 DMSO
26.34
20.70
210
200
190
180
170
160
150
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130
120
110
100
90
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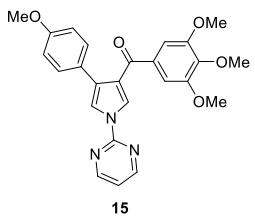
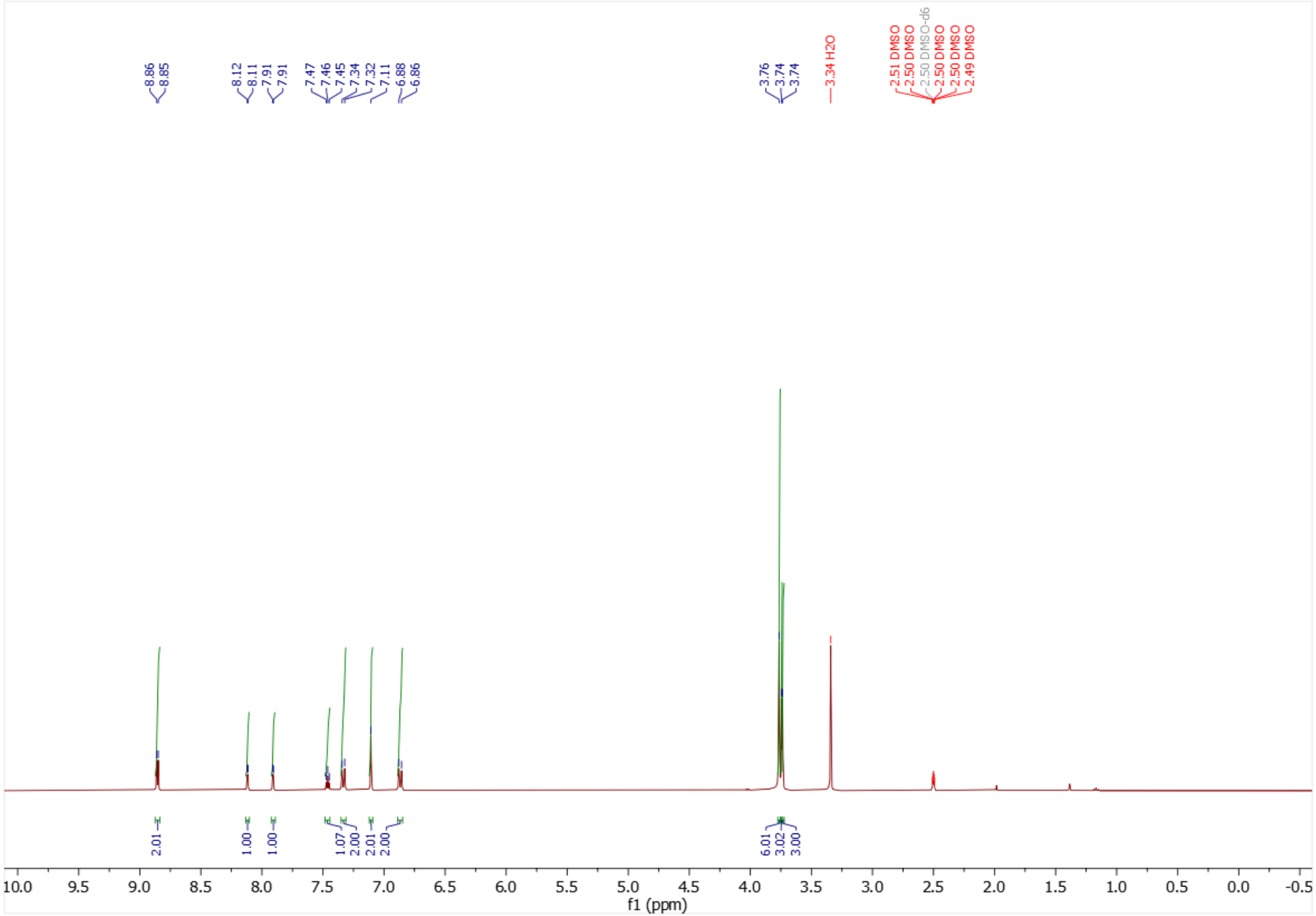
70
60
50
40
30
20
10
0
f1 (ppm)


MeO
OMe
OMe
OMe
O
N
N
N

15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8.85
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7.91
7.47
7.46
7.45
7.34
7.32
7.11
6.88
6.86
3.76
3.74
3.74
3.34 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.50 DMSO
2.49 DMSO
2.01
1.00
1.00
1.07
2.00
2.01
2.00
6.01
3.02
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
1.5
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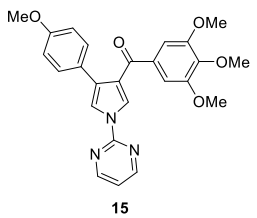
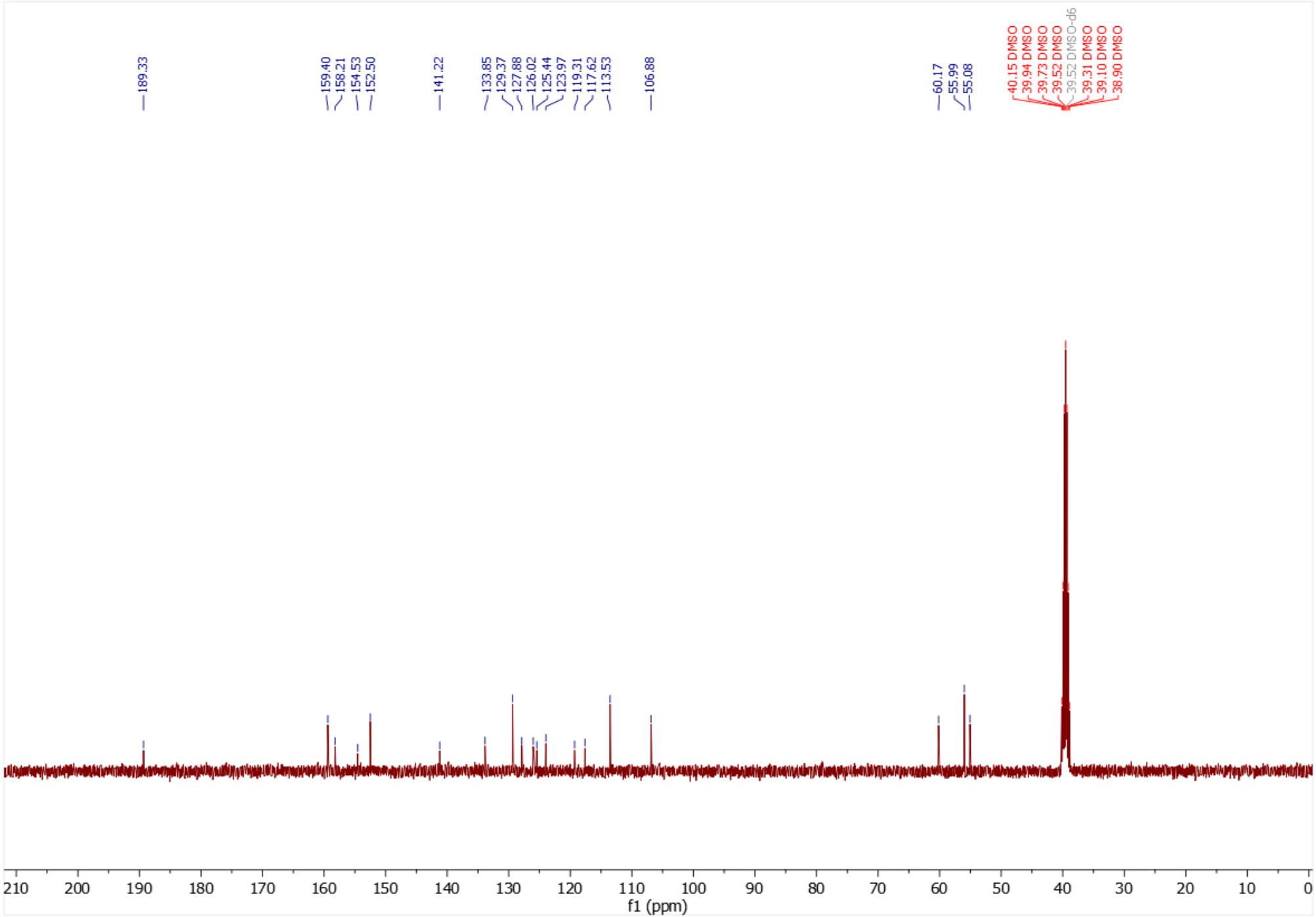
0.0
-0.5
f1 (ppm)


MeO
OMe
OMe
OMe
O
N
N
N

15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141.22
133.85
129.37
127.88
126.02
125.44
123.97
119.31
117.62
113.53
106.88
60.17
55.99
55.08
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO
39.52 DMSO-d6
39.31 DMSO
39.10 DMSO
38.90 DMSO
210
200
190
180
170
160
150
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130
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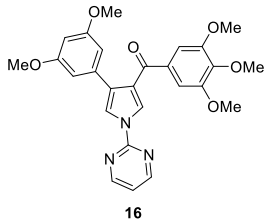
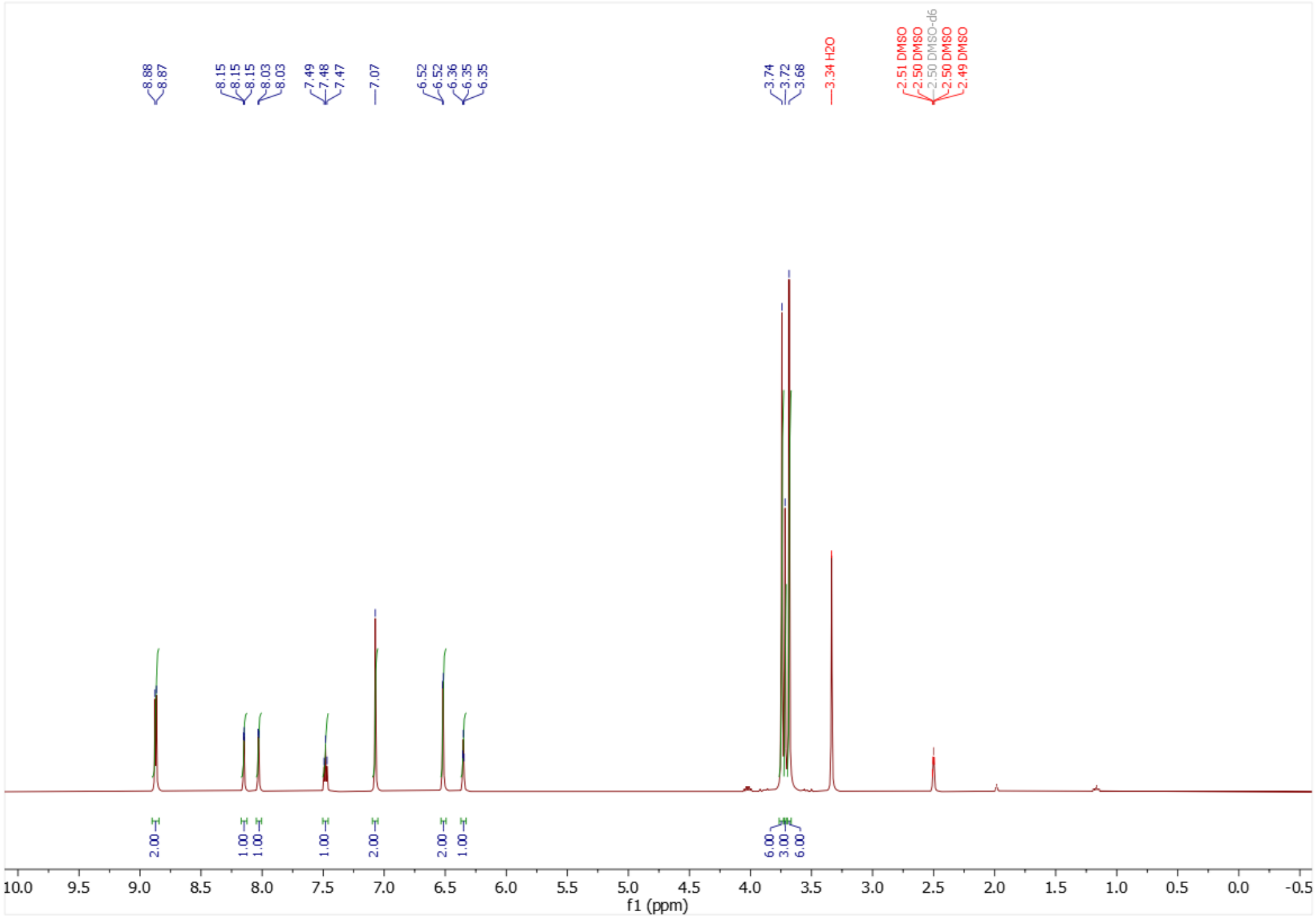
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OMe
MeO
OMe
OMe
OMe
O
N
N
N

16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8.87
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8.03
7.49
7.48
7.47
7.07
6.52
6.52
6.36
6.35
6.35
3.74
3.72
3.68
3.34 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.49 DMSO
2.00
1.00
1.00
1.00
2.00
2.00
1.00
6.00
3.00
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
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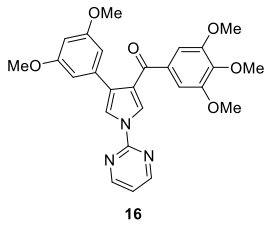
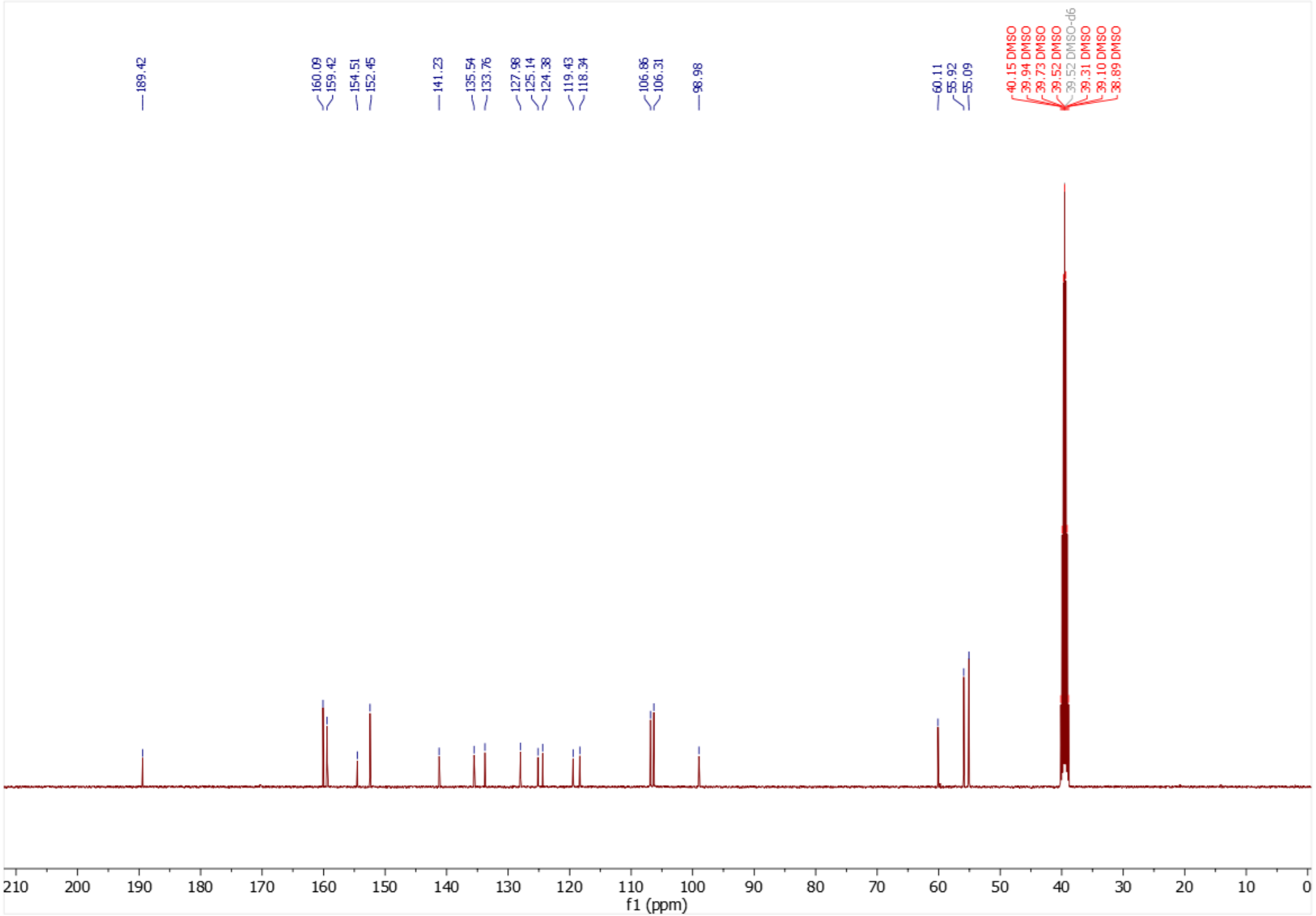
0.0
-0.5
f1 (ppm)


OMe
OMe
MeO
OMe
O
OMe
N
N
N

16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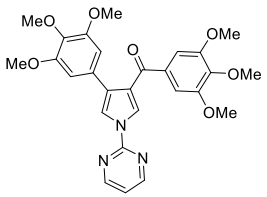
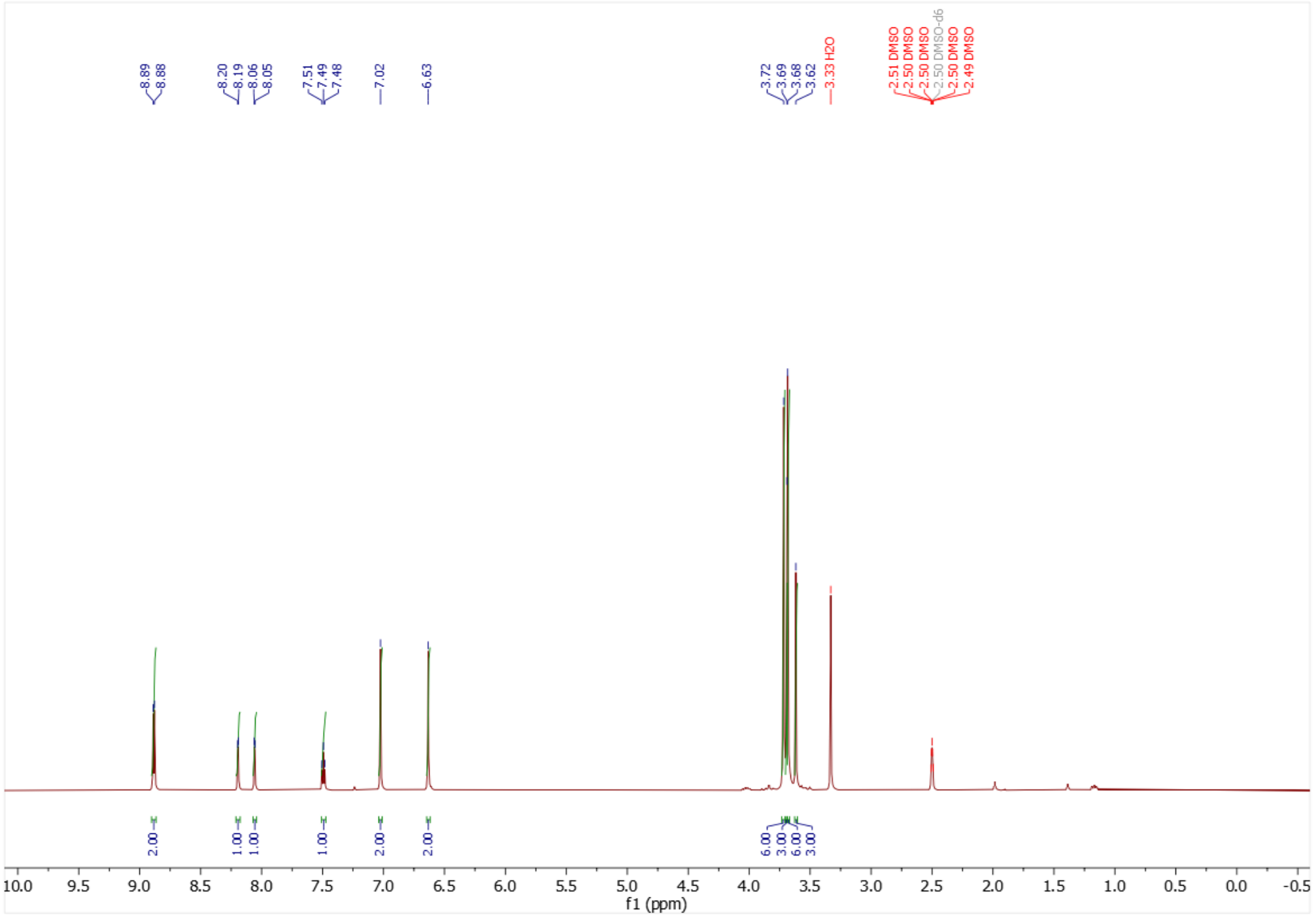
141.23
135.54
133.76
127.98
125.14
124.38
119.43
118.34
106.86
106.31
98.98
60.11
55.92
55.09
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO
39.52 DMSO-d6
39.31 DMSO
39.10 DMSO
38.89 DMSO
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


MeO
OMe
MeO
O
OMe
OMe
OMe
N
N
N

17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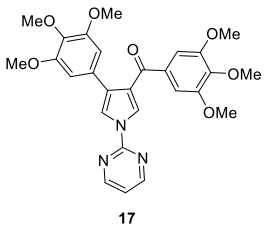
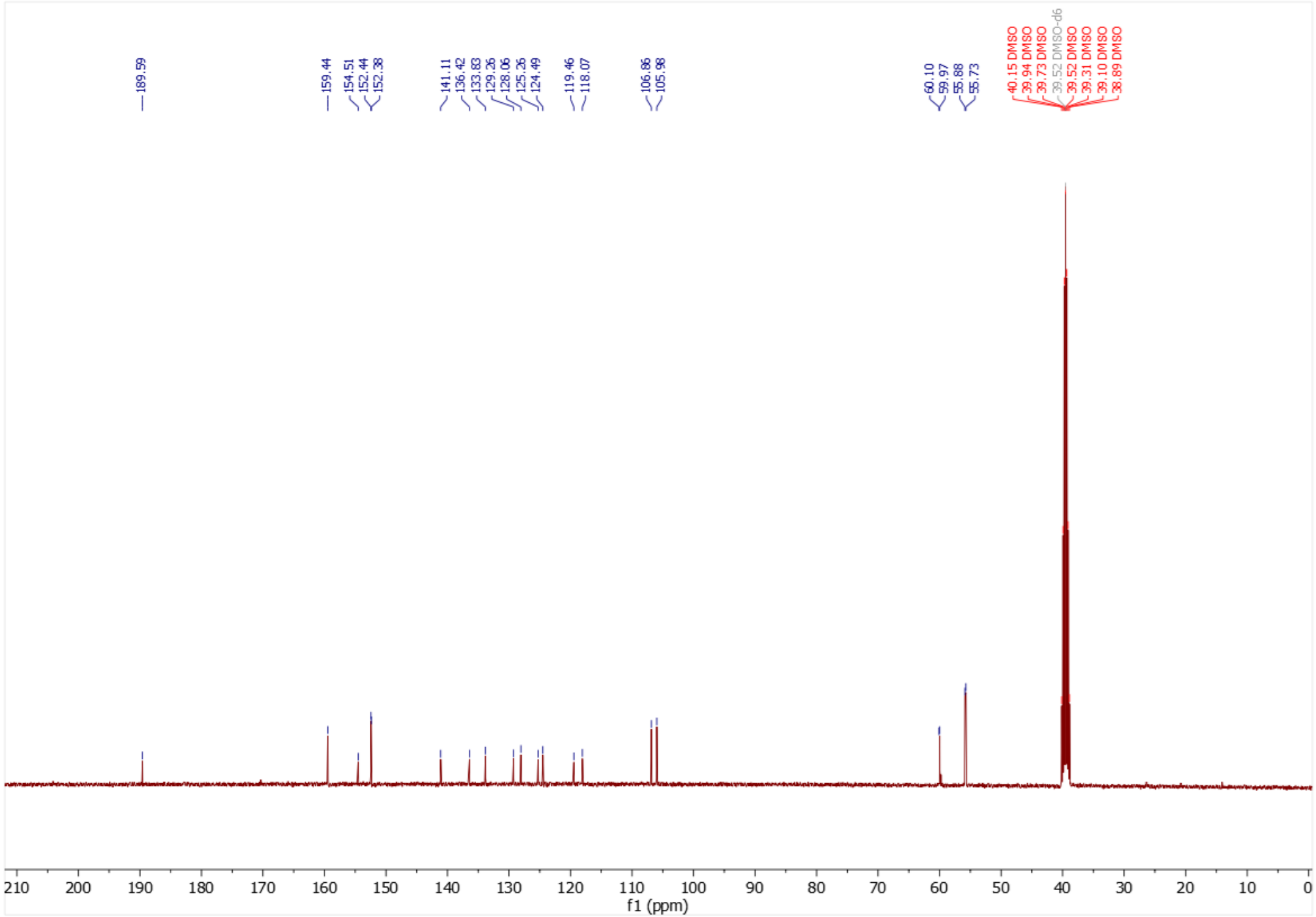
8.20
8.19
8.06
8.05
7.51
7.49
7.48
7.02
6.63
3.72
3.69
3.68
3.62
3.33 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.49 DMSO
2.00
1.00
1.00
1.00
2.00
2.00
6.00
3.00
6.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


MeO
OMe
MeO
O
OMe
OMe
OMe
N
N
N

17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152.38
141.11
136.42
133.83
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128.06
125.26
124.49
119.46
118.07
106.86
105.98
60.10
59.97
55.88
55.73
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO-d6
39.52 DMSO
39.31 DMSO
39.10 DMSO
38.89 DMSO
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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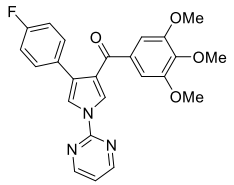
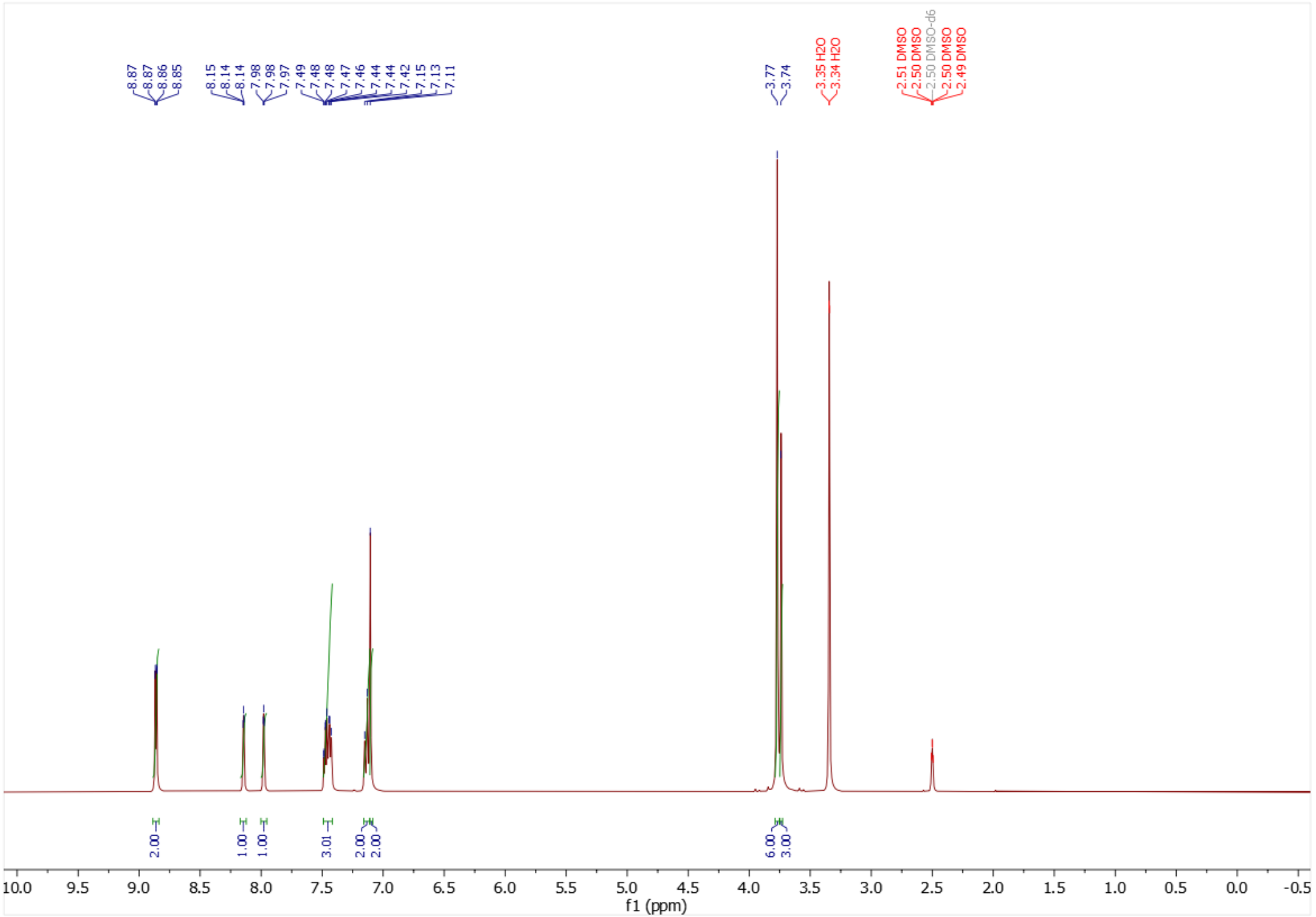
50
40
30
20
10
0
f1 (ppm)


F
O
OMe
OMe
OMe
N
N
N

18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7.98
7.97
7.49
7.48
7.48
7.47
7.46
7.44
7.44
7.42
7.15
7.13
7.11
3.77
3.74
3.35 H2O
3.34 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.49 DMSO
2.00
1.00
1.00
3.01
2.00
2.00
6.00
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
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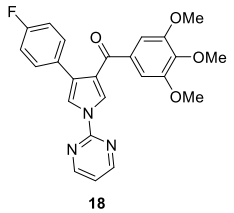
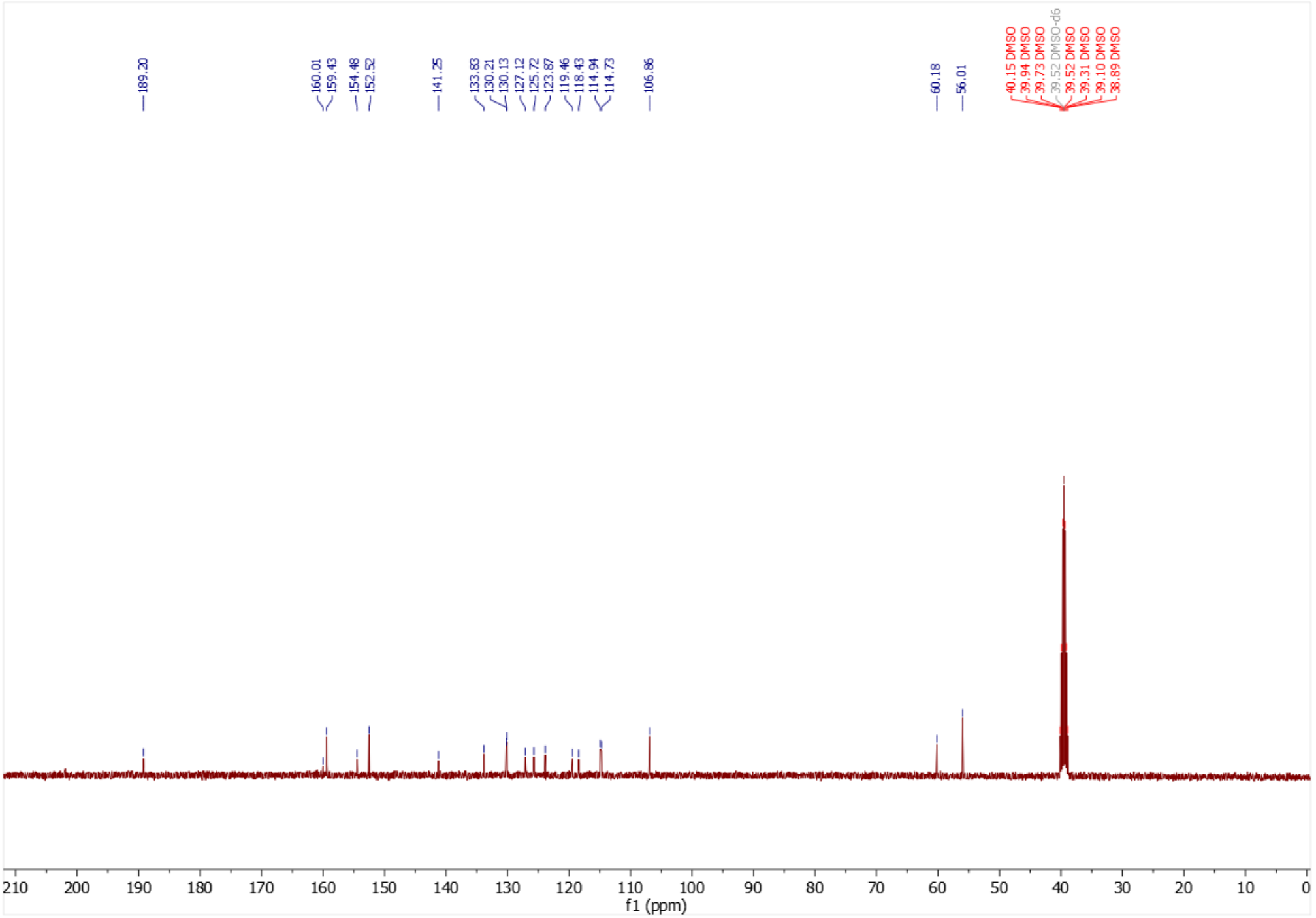
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


F
O
OMe
OMe
OMe
N
N
N

18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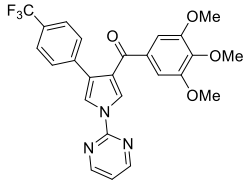
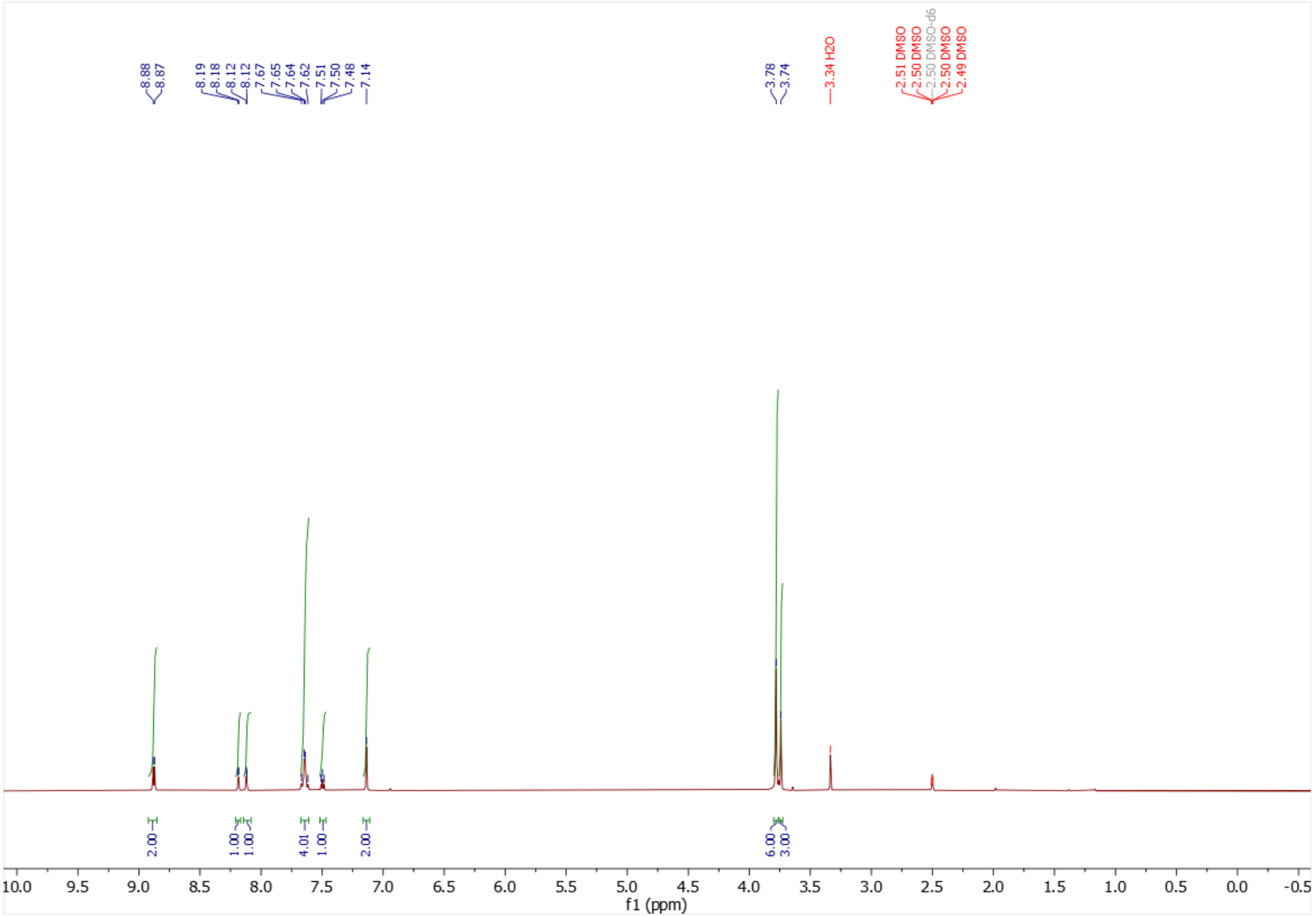
154.48
152.52
141.25
133.83
130.21
130.13
127.12
125.72
123.87
119.46
118.43
114.94
114.73
106.86
60.18
56.01
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO-d6
39.52 DMSO
39.31 DMSO
39.10 DMSO
38.89 DMSO
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


F3C
OMe
OMe
OMe
O
N
N
N

19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8.12
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7.64
7.62
7.51
7.50
7.48
7.14
3.78
3.74
3.34 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.49 DMSO
2.00
1.00
1.00
4.01
1.00
2.00
6.00
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
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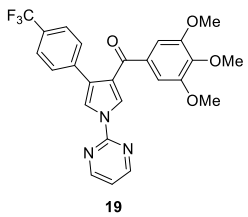
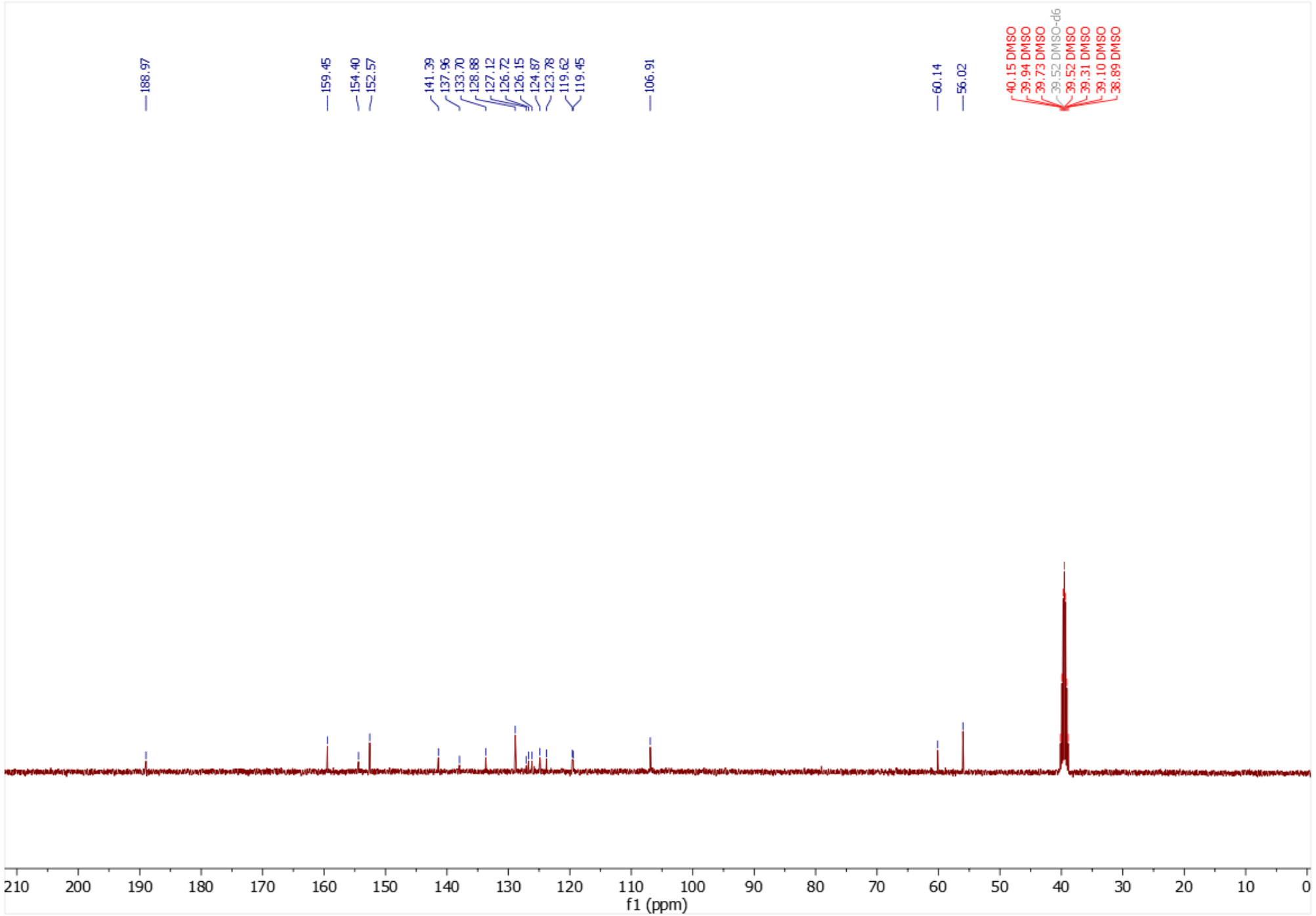
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


F3C
OMe
OMe
OMe
O
N
N
N

19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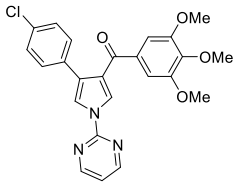
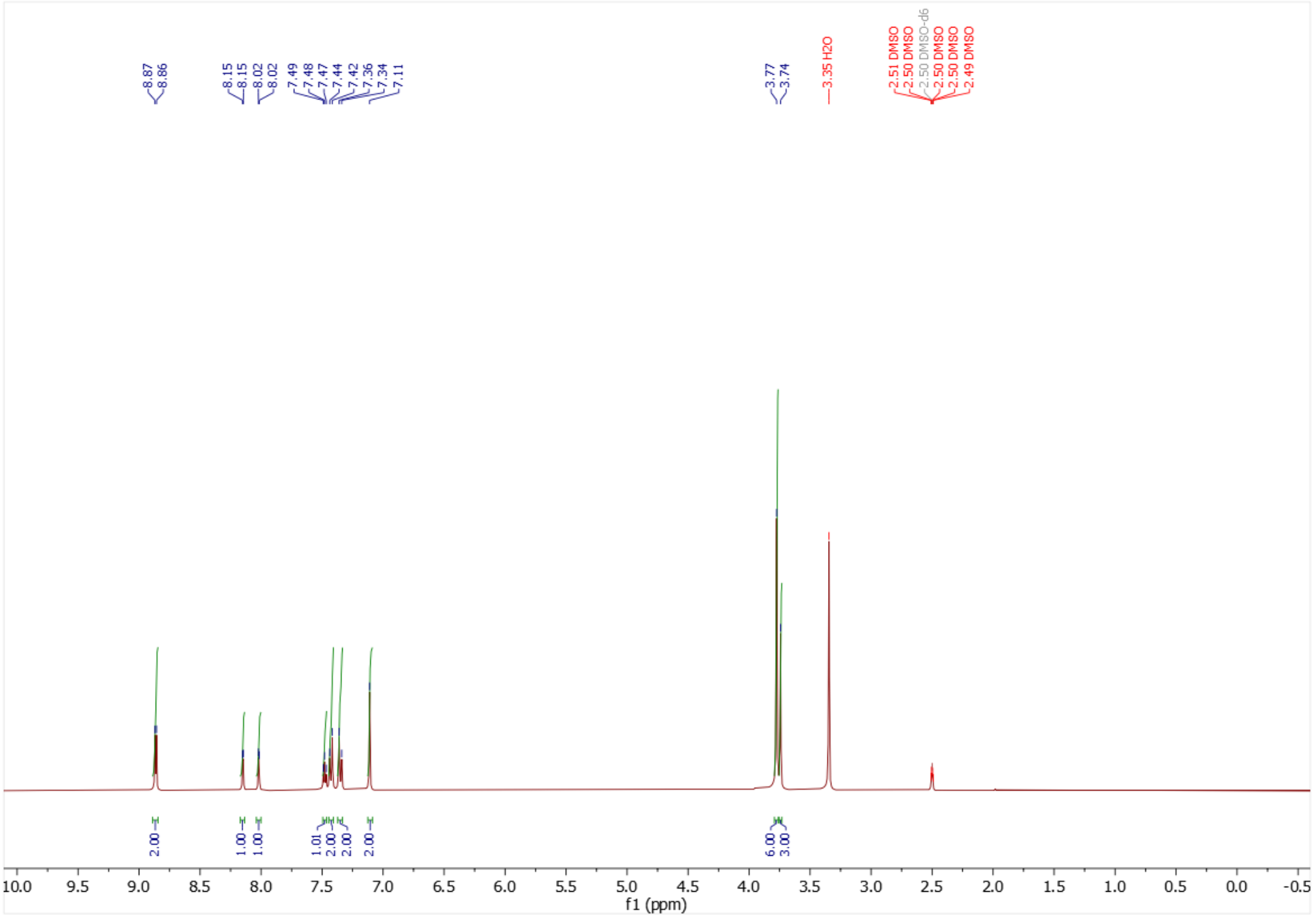
127.12
126.72
126.15
124.87
123.78
119.62
119.45
106.91
60.14
56.02
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO-d6
39.52 DMSO
39.31 DMSO
39.10 DMSO
38.89 DMSO
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Cl
O
OMe
OMe
OMe
N
N
N

20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8.02
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7.48
7.47
7.44
7.42
7.36
7.34
7.11
3.77
3.74
3.35 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.50 DMSO
2.49 DMSO
2.00
1.00
1.00
1.01
2.00
2.00
2.00
6.00
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
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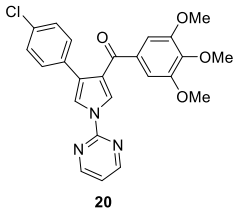
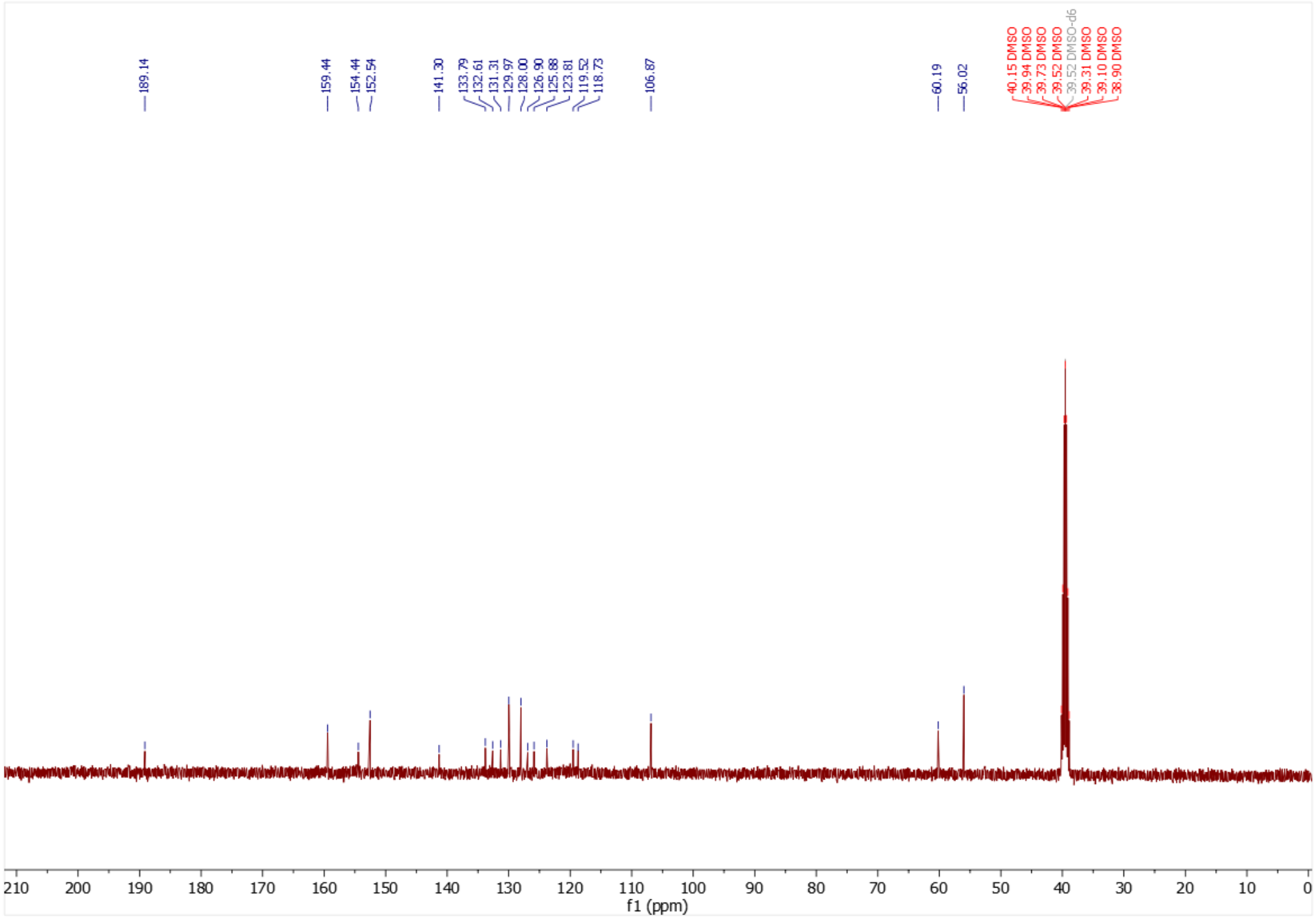
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Cl
O
OMe
OMe
OMe
N
N
N

20


189.14
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152.54
141.30
133.79
132.61
131.31
129.97
128.00
126.90
125.88
123.81
119.52
118.73
106.87
60.19
56.02
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO
39.52 DMSO-d6
39.31 DMSO
39.10 DMSO
38.90 DMSO
210
200
190
180
170
160
150
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130
120
110
100
90
80
70
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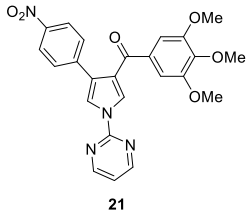
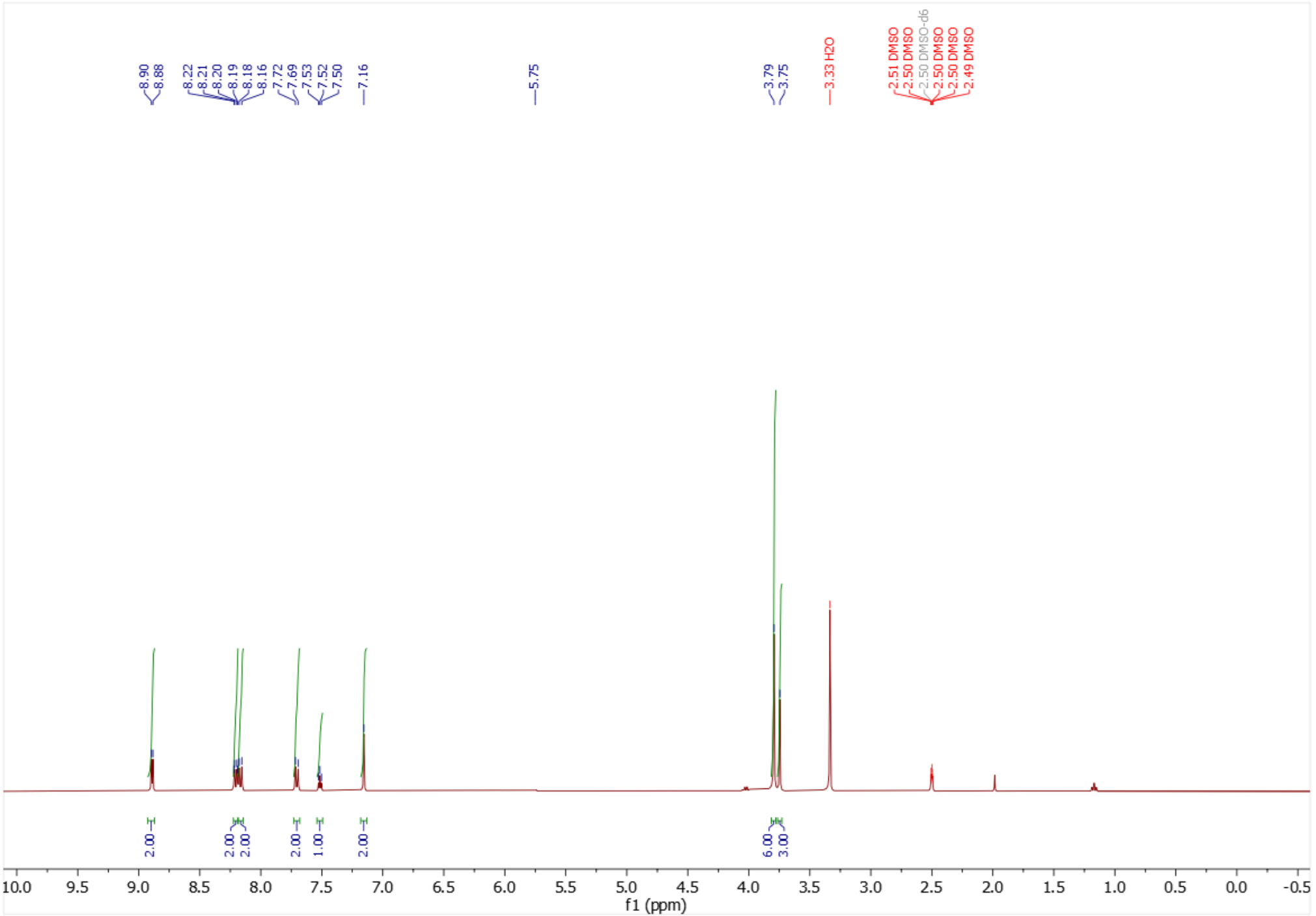
50
40
30
20
10
0
f1 (ppm)


O2N
OMe
OMe
OMe
O
N
N
N

21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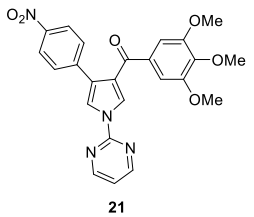
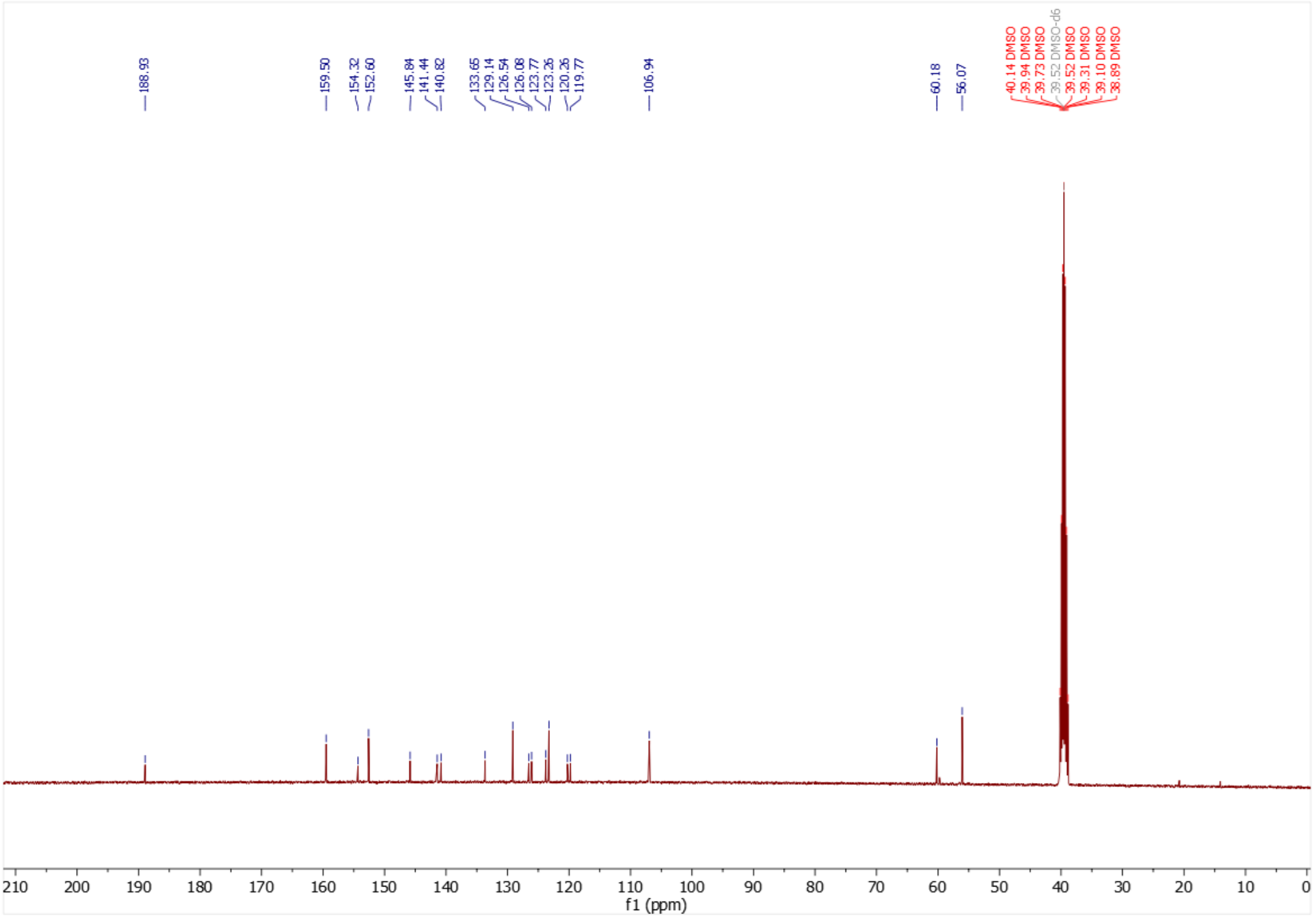
8.16
7.72
7.69
7.53
7.52
7.50
7.16
5.75
3.79
3.75
3.33 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.50 DMSO
2.49 DMSO
2.00
2.00
2.00
2.00
1.00
2.00
6.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


O2N
OMe
OMe
OMe
O
N
N
N

21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141.44
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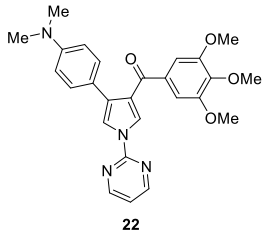
133.65
129.14
126.54
126.08
123.77
123.26
120.26
119.77
106.94
60.18
56.07
40.14 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO-d6
39.52 DMSO
39.31 DMSO
39.10 DMSO
38.89 DMSO
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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Me
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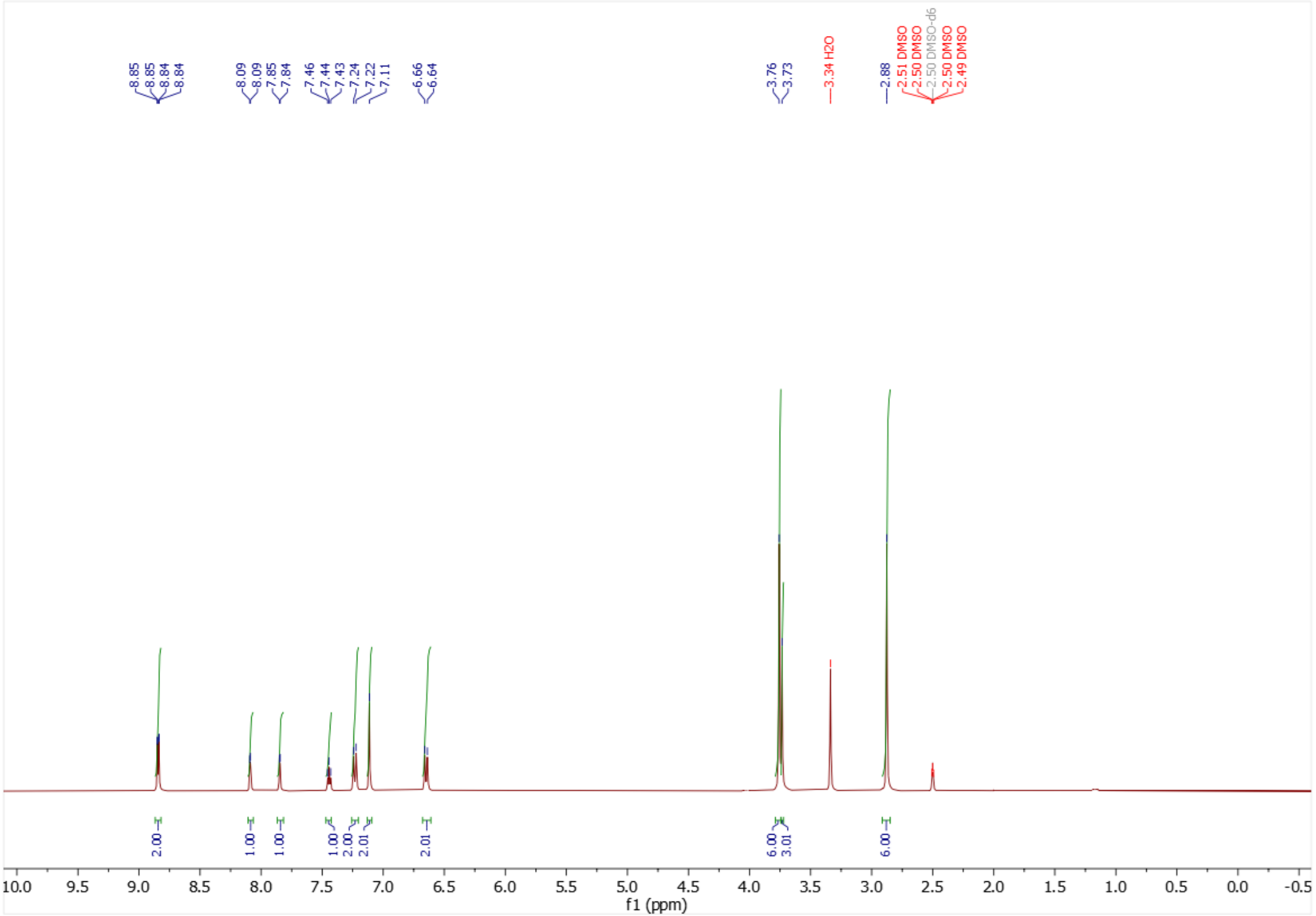
O
OMe
OMe
OMe
N
N
N

22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7.43
7.24
7.22
7.11
6.66
6.64
3.76
3.73
3.34 H2O
2.88
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.49 DMSO
2.00
1.00
1.00
1.00
2.00
2.01
2.01
6.00
3.01
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
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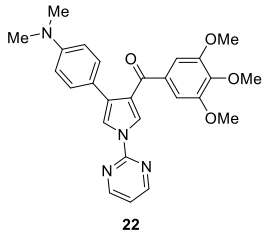
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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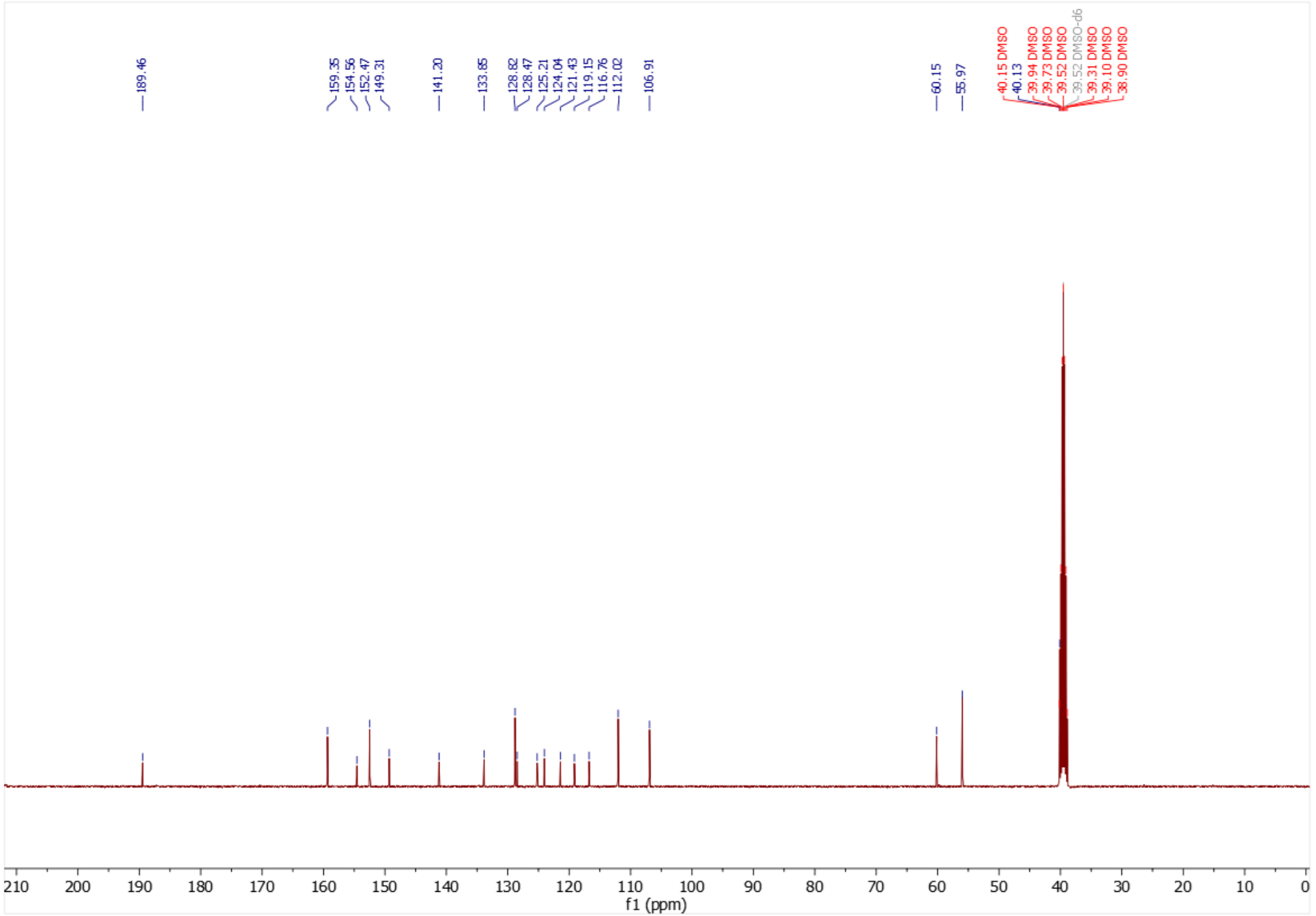
O
OMe
OMe
OMe
N
N
N

22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128.82
128.47
125.21
124.04
121.43
119.15
116.76
112.02
106.91
60.15
55.97
40.15 DMSO
40.13
39.94 DMSO
39.73 DMSO
39.52 DMSO
39.52 DMSO-d6
39.31 DMSO
39.10 DMSO
38.90 DMSO
210
200
190
180
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130
120
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90
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70
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50
40
30
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10
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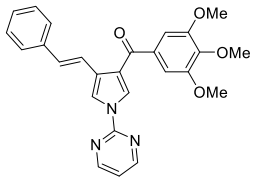
f1 (ppm)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O
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N
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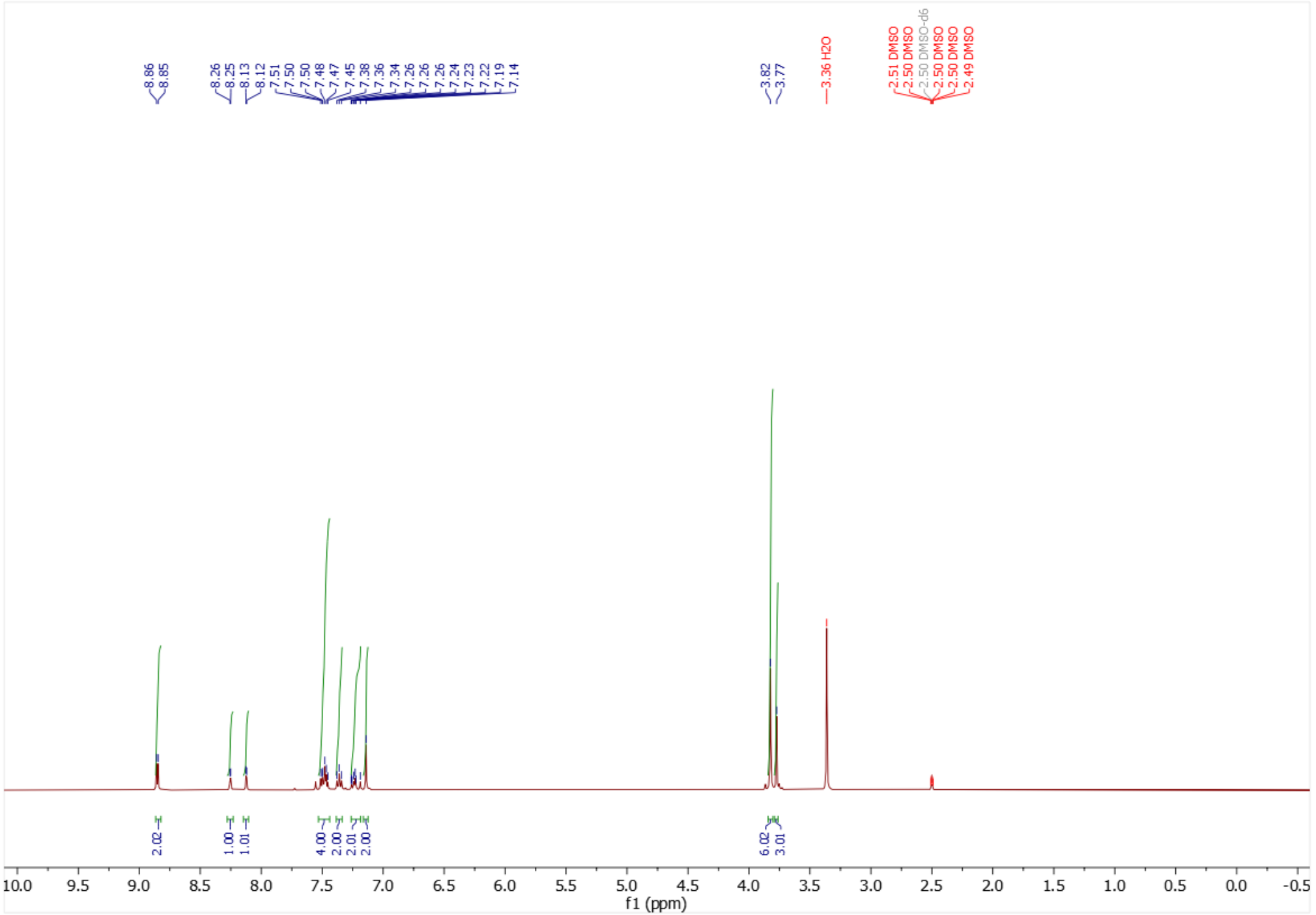
23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7.38
7.36
7.34
7.26
7.26
7.26
7.24
7.23
7.22
7.19
7.14
3.82
3.77
3.36 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.50 DMSO
2.49 DMSO
2.02
1.00
1.01
4.00
2.00
2.01
2.00
6.02
3.01
10.0
9.5
9.0
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.0
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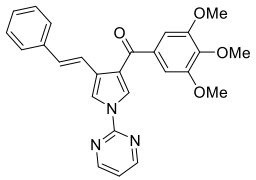
f1 (ppm)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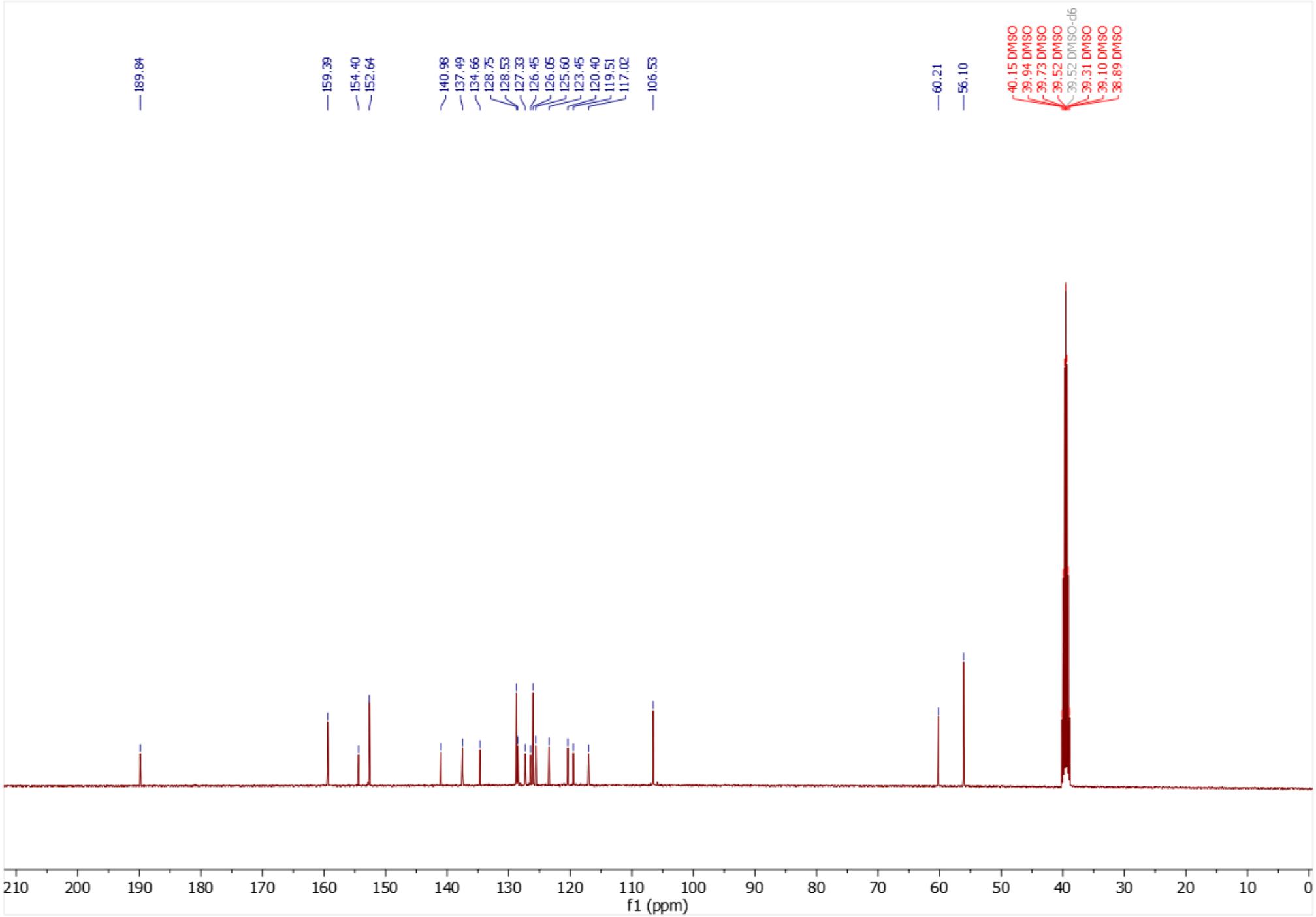
OMe
O
N
N
N

23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126.05
125.60
123.45
120.40
119.51
117.02
106.53
60.21
56.10
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO
39.52 DMSO-d6
39.31 DMSO
39.10 DMSO
38.89 DMSO
210
200
190
180
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160
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140
130
120
110
100
90
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50
40
30
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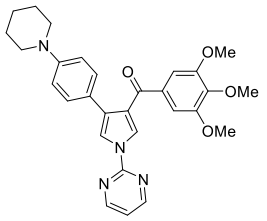
f1 (ppm)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OMe
OMe
O
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N
N
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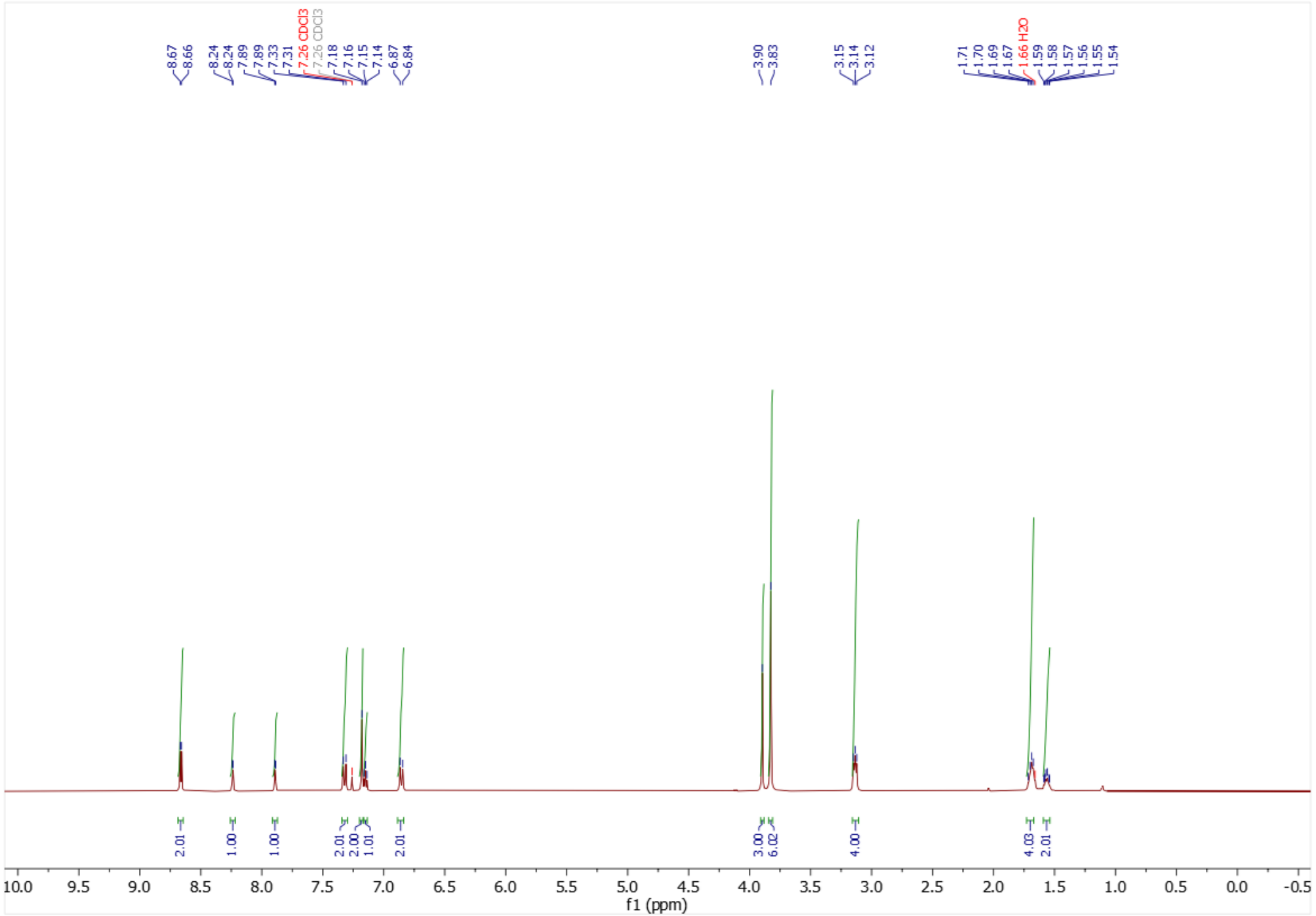
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7.89
7.33
7.31
7.26 CDCl3
7.26 CDCl3
7.18
7.16
7.15
7.14
6.87
6.84
3.90
3.83
3.15
3.14
3.12
1.71
1.70
1.69
1.67
1.66 H2O
1.59
1.58
1.57
1.56
1.55
1.54
2.01
1.00
1.00
2.01
2.00
1.01
2.01
3.00
6.02
4.00
4.03
2.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
1.5
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0.5
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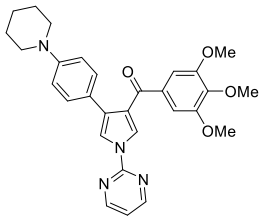
-0.5
f1 (ppm)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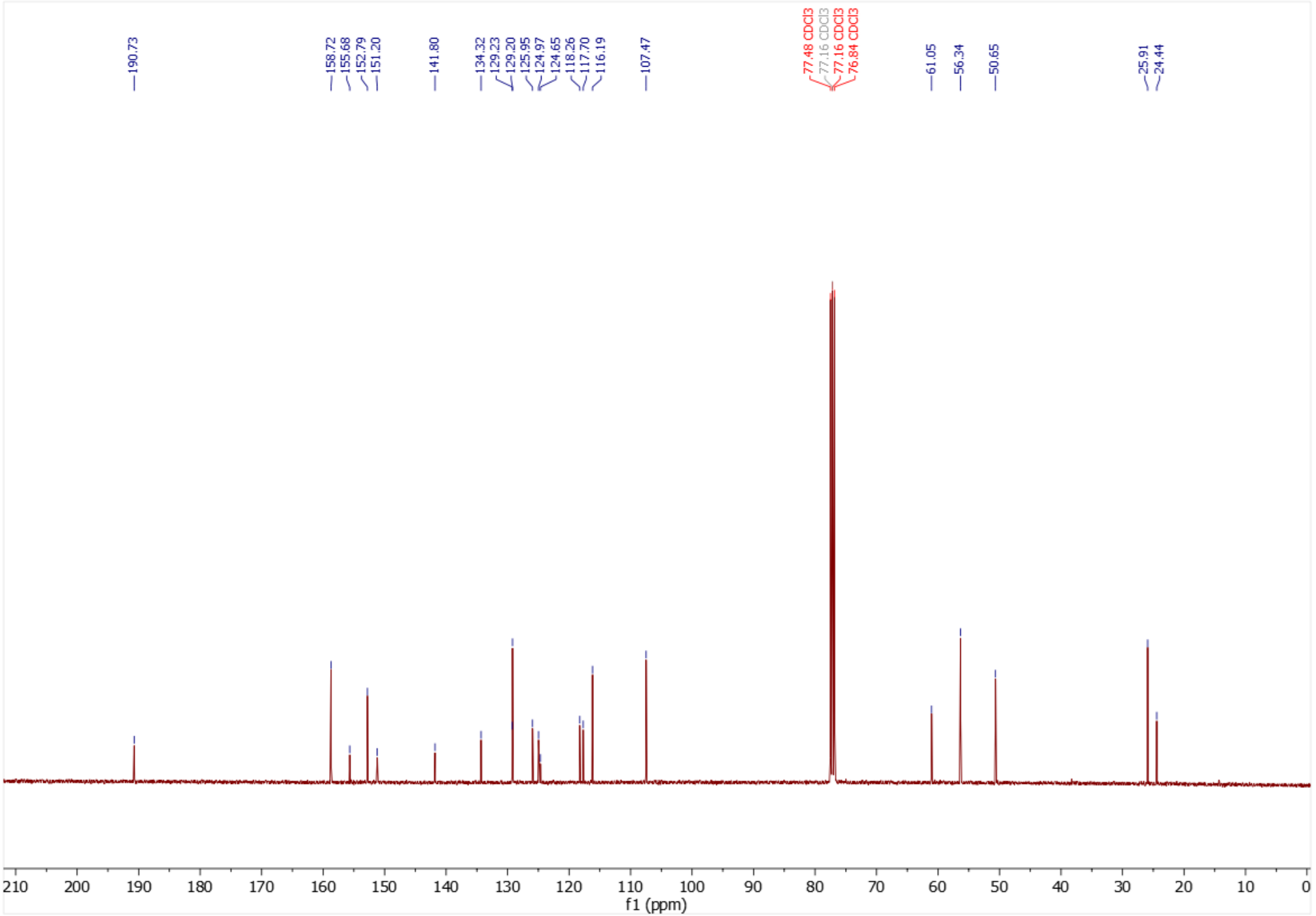
OMe
OMe
O
N
N
N

24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134.32
129.23
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125.95
124.97
124.65
118.26
117.70
116.19
107.47
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
61.05
56.34
50.65
25.91
24.44
210
200
190
180
170
160
150
140
130
120
110
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90
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50
40
30
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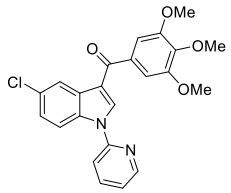
f1 (ppm)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OMe
OMe
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Cl
N
N

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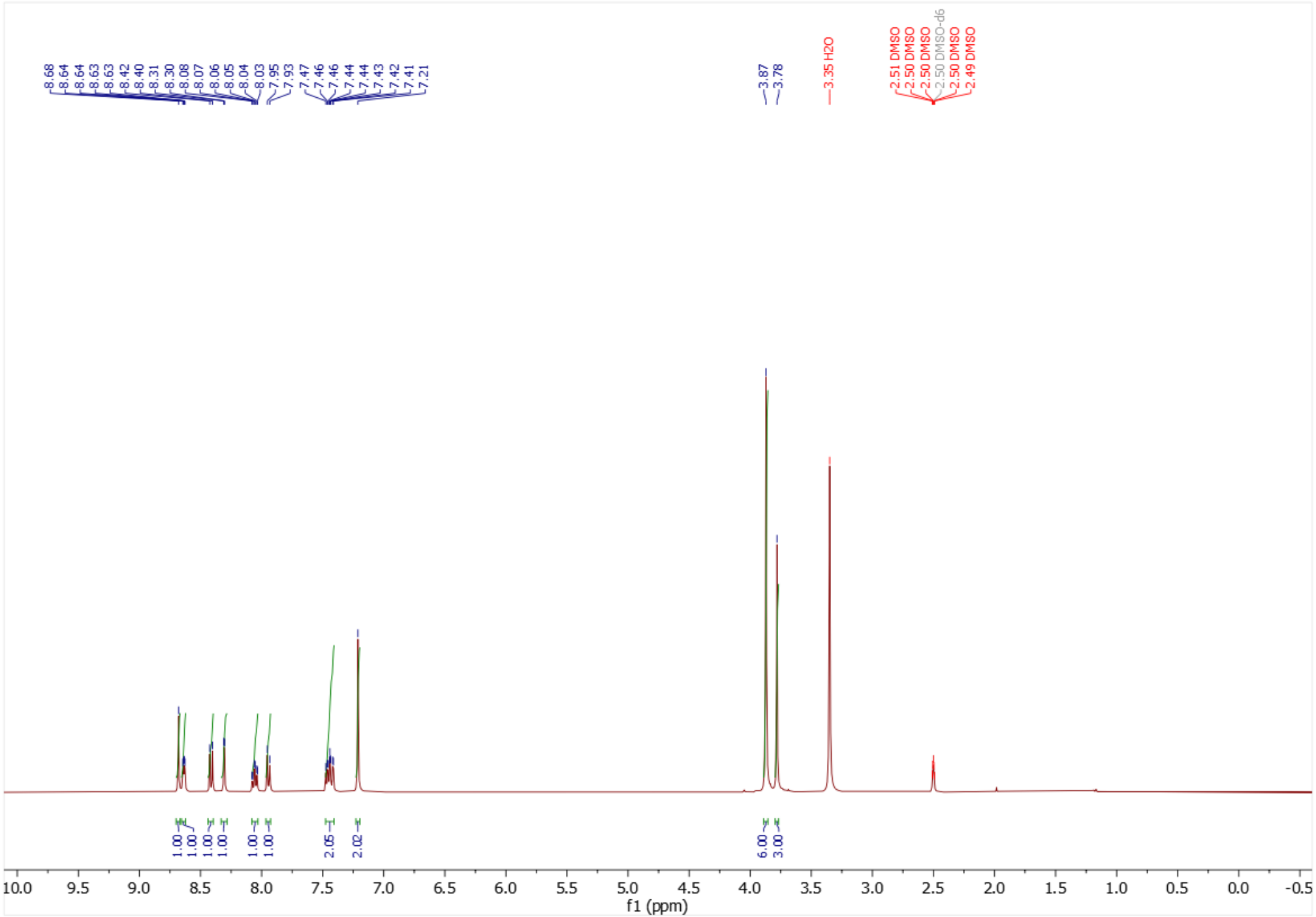
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8.08
8.07
8.06
8.05
8.04
8.03
7.95
7.93
7.47
7.46
7.46
7.44
7.44
7.43
7.42
7.41
7.21
3.87
3.78
3.35 H2O
2.51 DMSO
2.50 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
2.49 DMSO
1.00
1.00
1.00
1.00
1.00
1.00
2.05
2.02
6.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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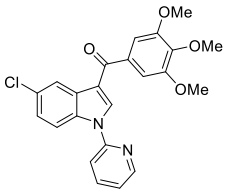
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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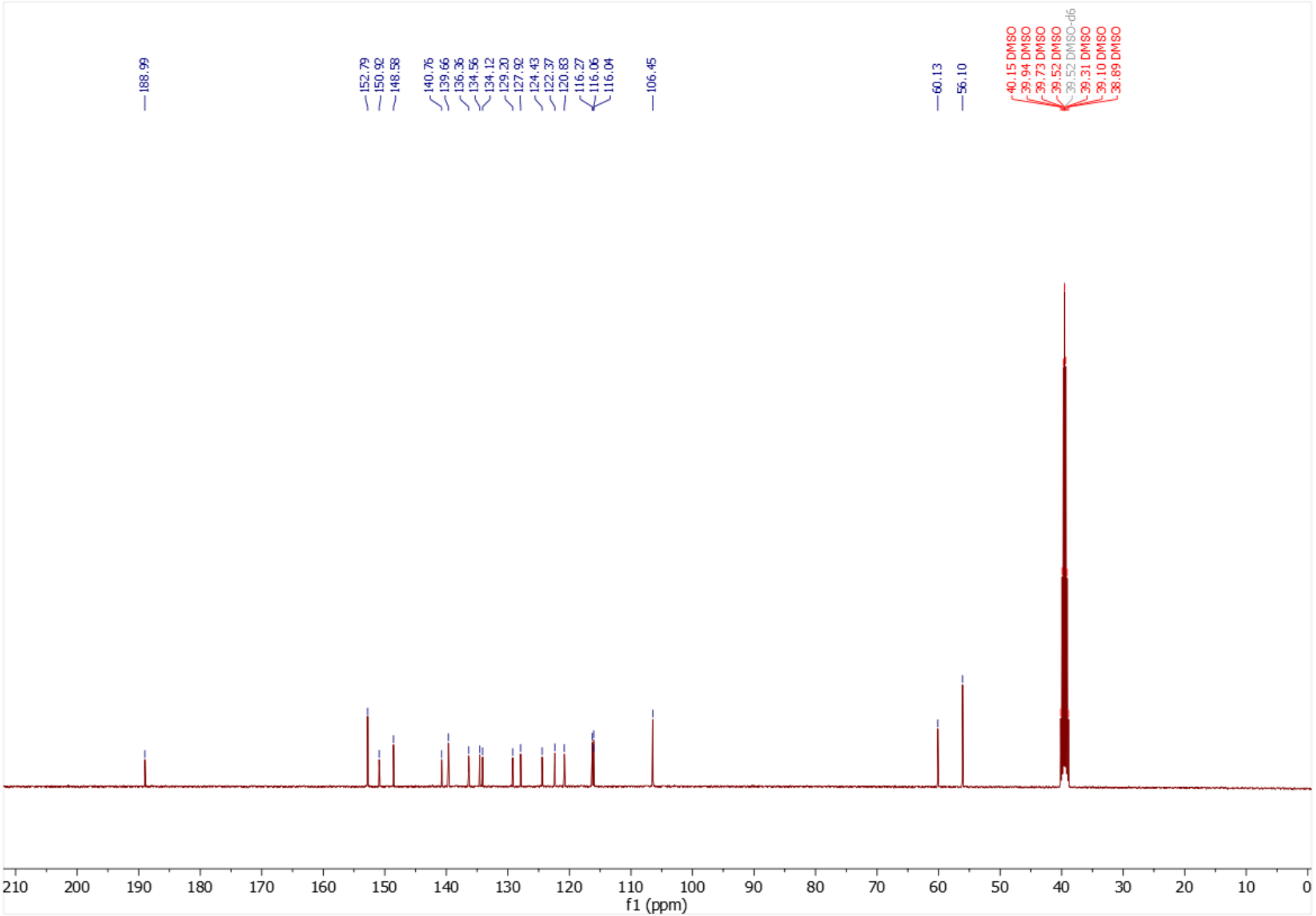
OMe
OMe
O
Cl
N
N

25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134.56
134.12
129.20
127.92
124.43
122.37
120.83
116.27
116.06
116.04
106.45
60.13
56.10
40.15 DMSO
39.94 DMSO
39.73 DMSO
39.52 DMSO
39.52 DMSO-d6
39.31 DMSO
39.10 DMSO
38.89 DMSO
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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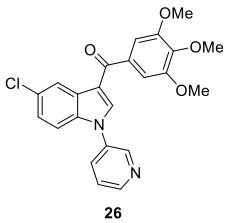
50
40
30
20
10
0
f1 (ppm)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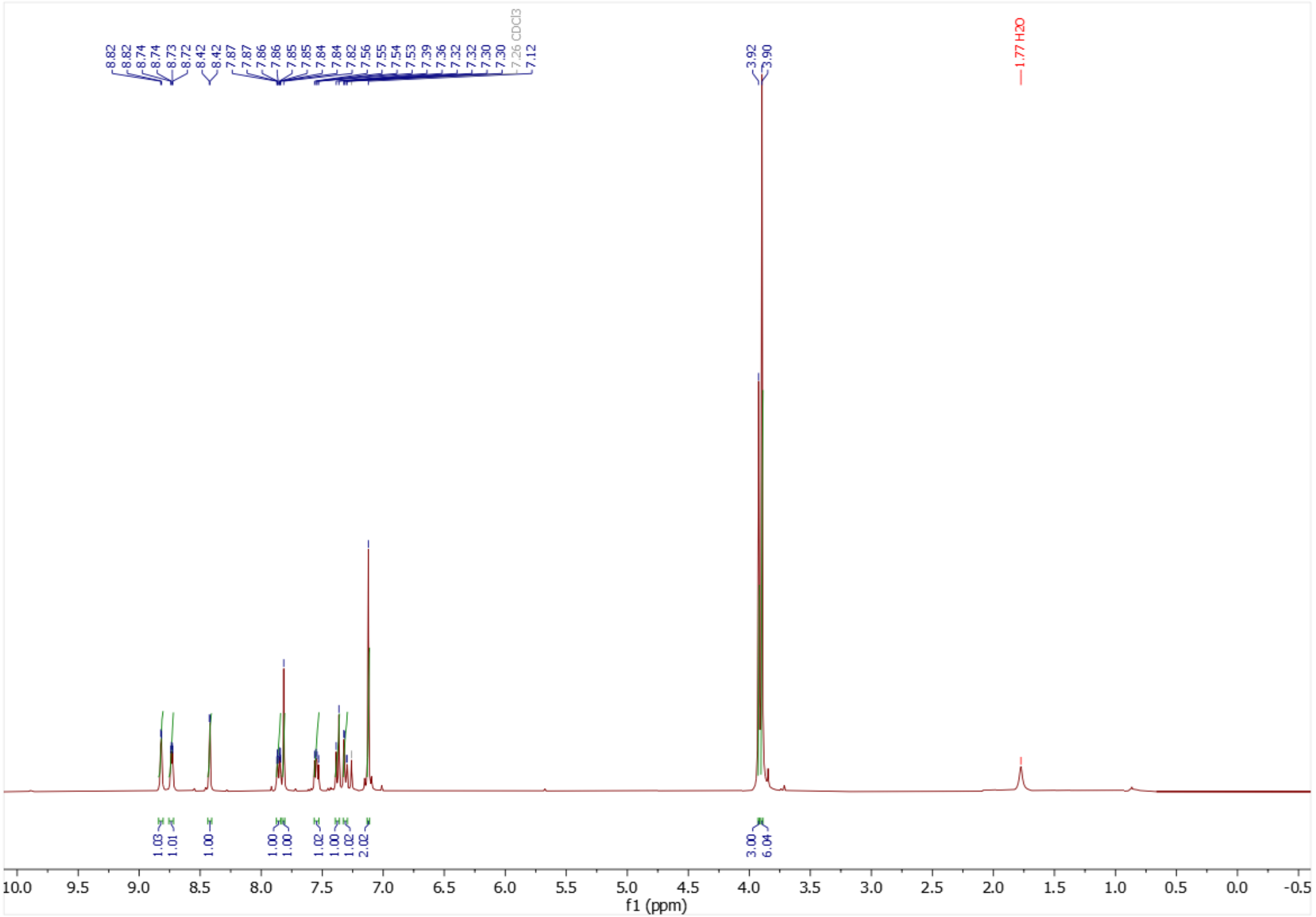
OMe
OMe
O
Cl
N
N

26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8.42
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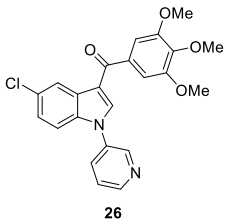
7.87
7.86
7.86
7.85
7.85
7.84
7.84
7.82
7.56
7.55
7.54
7.53
7.39
7.36
7.32
7.30
7.30
7.26 CDCl3
7.12
3.92
3.90
1.77 H2O
1.03
1.01
1.00
1.00
1.00
1.02
1.00
1.02
2.02
3.00
6.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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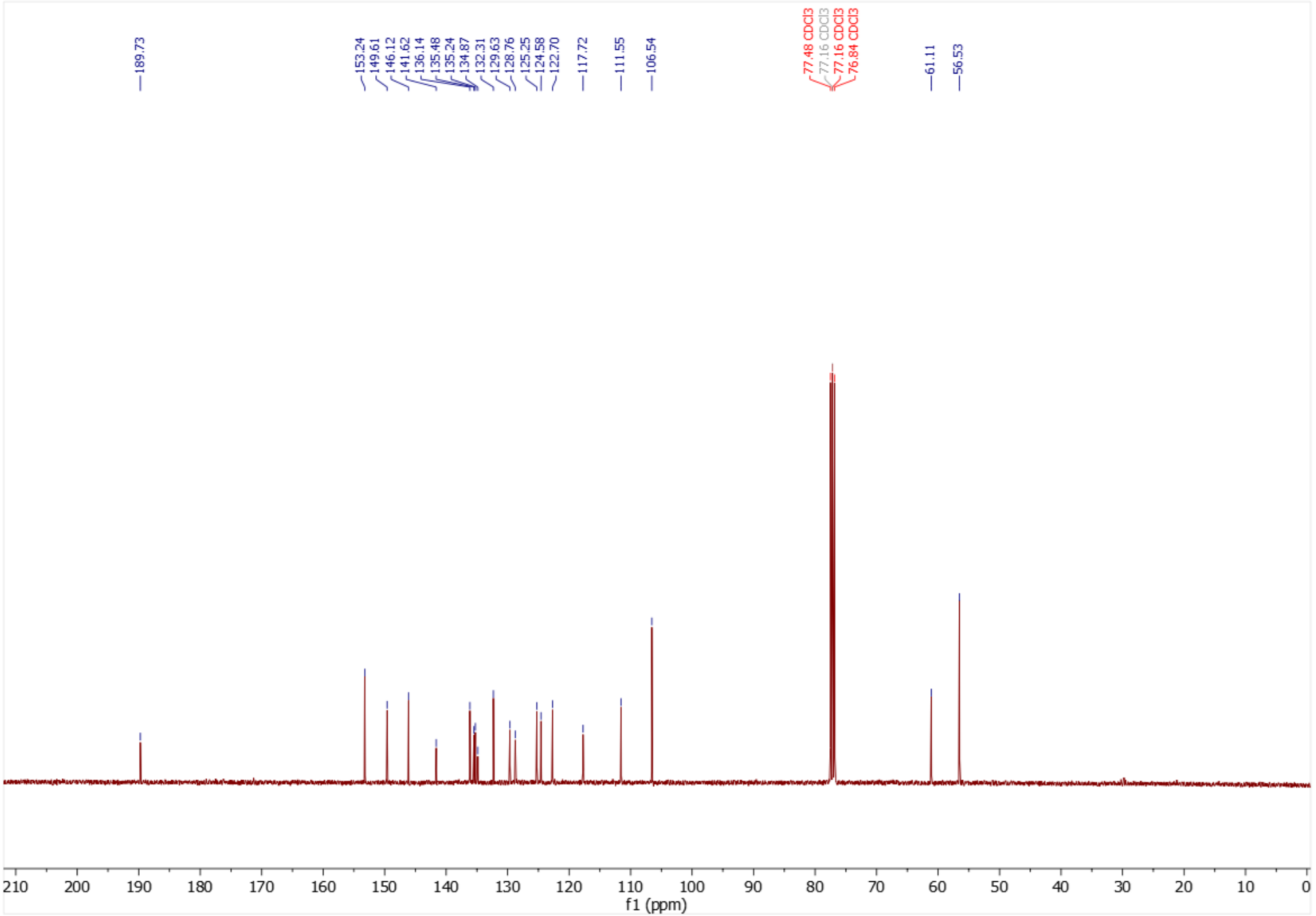
OMe
OMe
O
Cl
N
N

26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136.14
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135.24
134.87
132.31
129.63
128.76
125.25
124.58
122.70
117.72
111.55
106.54
77.48 CDCl3
77.16 CDCl3
77.16 CDCl3
76.84 CDCl3
61.11
56.53
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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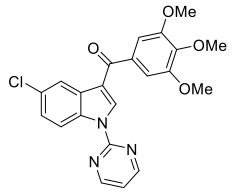
50
40
30
20
10
0
f1 (ppm)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OMe
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Cl
N
N
N

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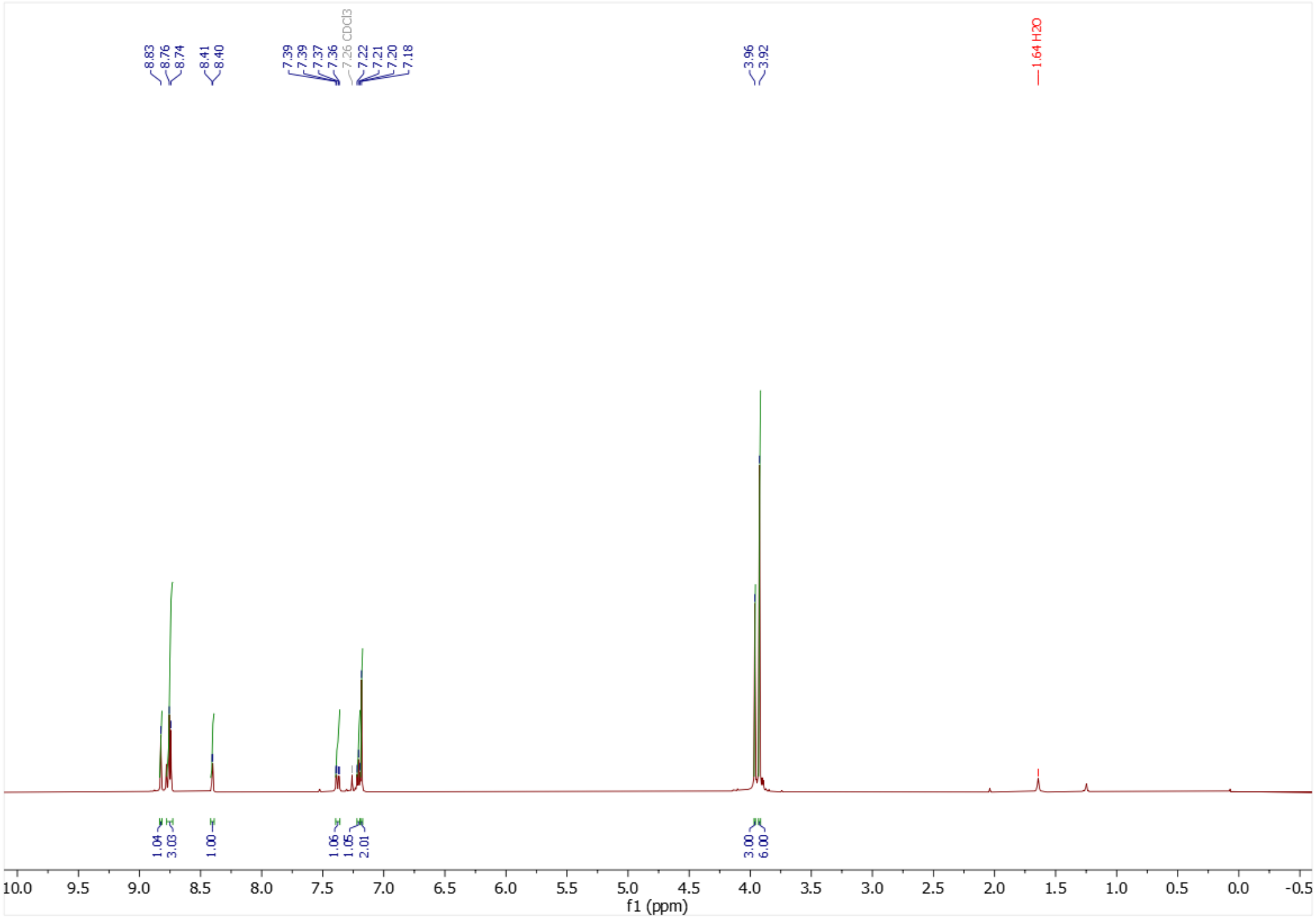
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7.39
7.37
7.36
7.26 CDCl3
7.22
7.21
7.20
7.18
3.96
3.92
1.64 H2O
1.04
3.03
1.00
1.06
1.05
2.01
3.00
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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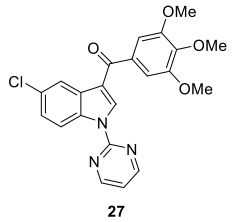
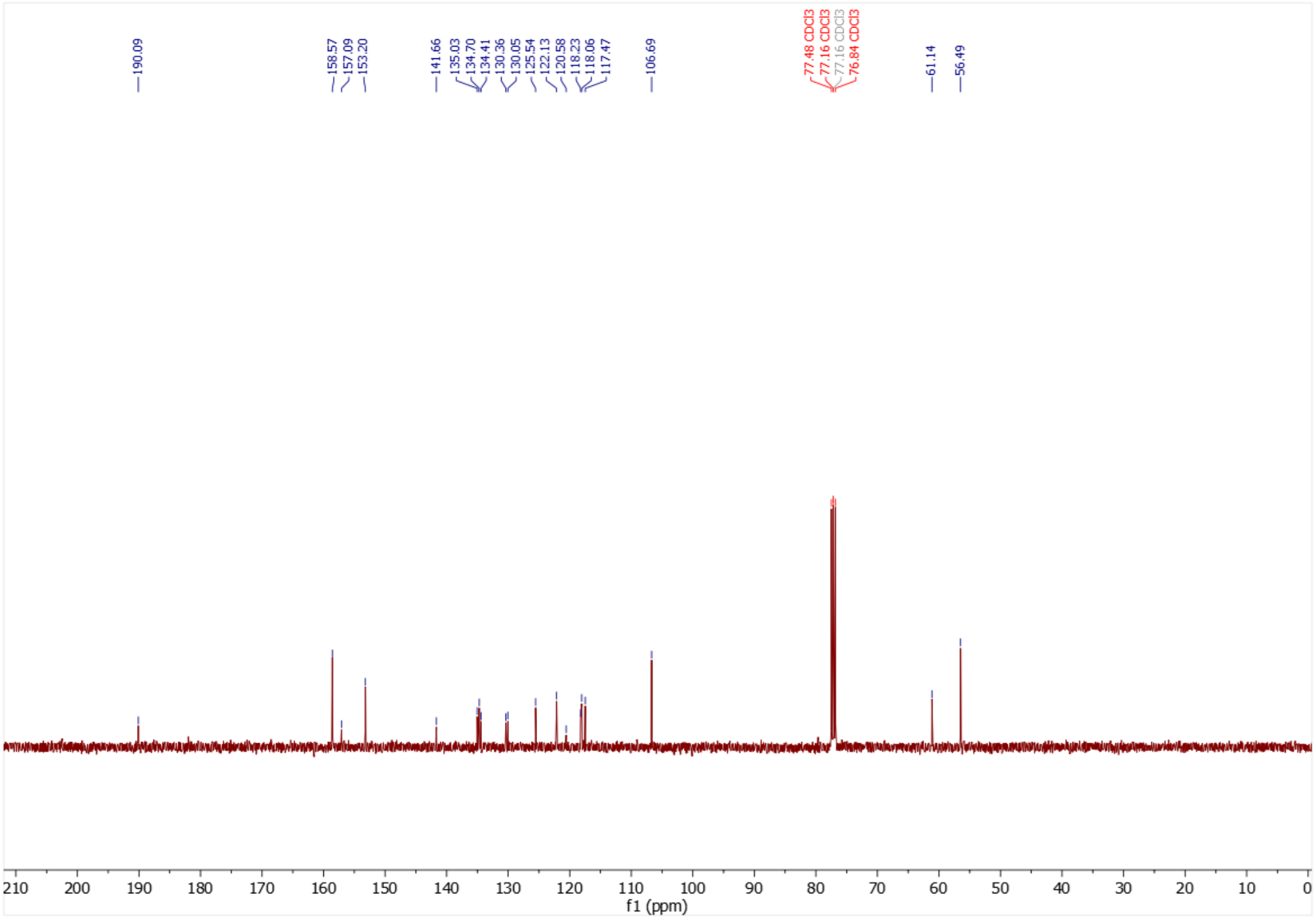
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


OMe
OMe
OMe
O
Cl
N
N
N

27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134.41
130.36
130.05
125.54
122.13
120.58
118.23
118.06
117.47
106.69
77.48 CDCl3
77.16 CDCl3
77.16 CDCl3
76.84 CDCl3
61.14
56.49
210
200
190
180
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140
130
120
110
100
90
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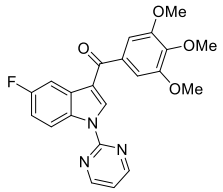
70
60
50
40
30
20
10
0
f1 (ppm)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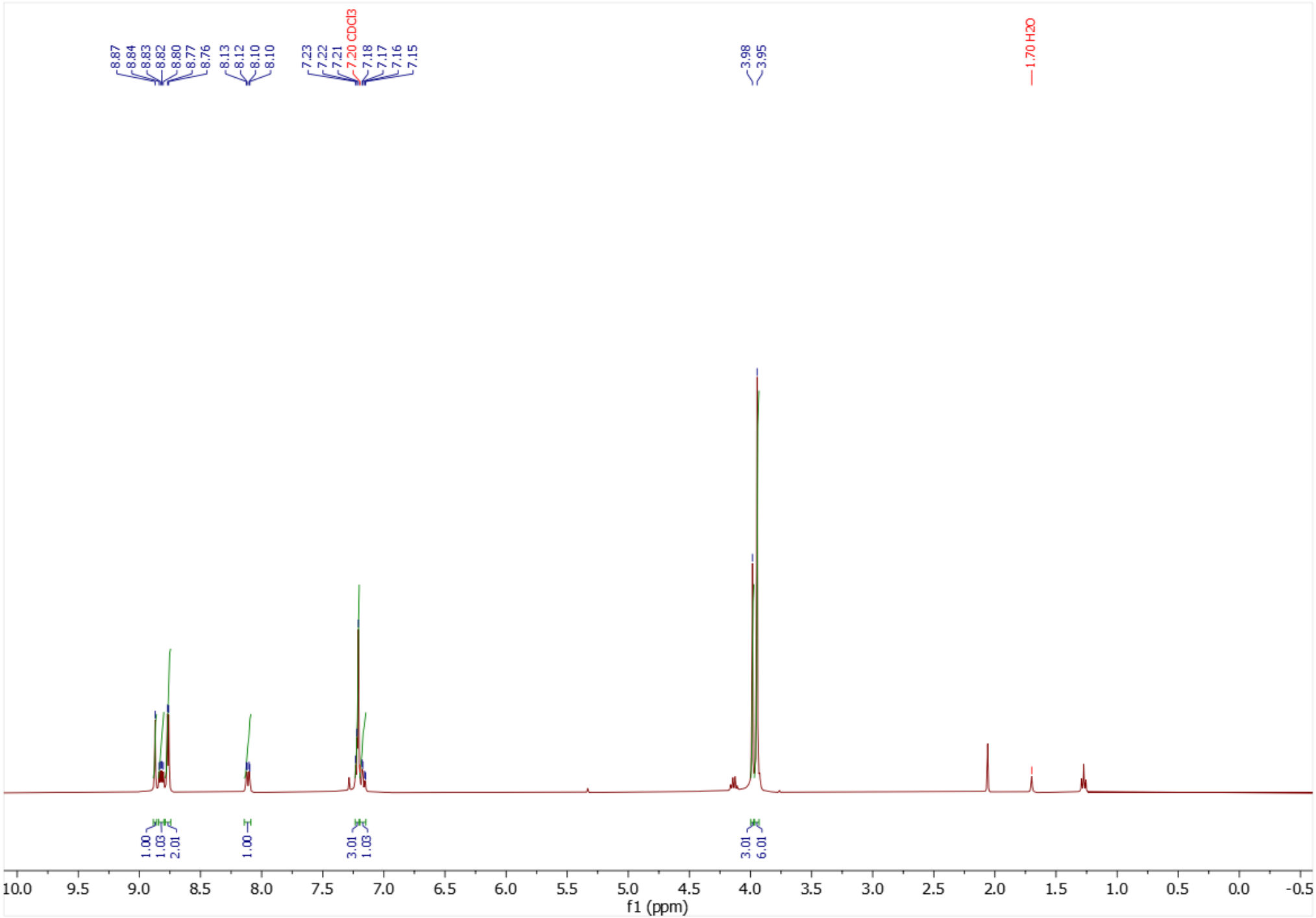
OMe
OMe
O
F
N
N
N

28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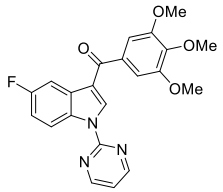
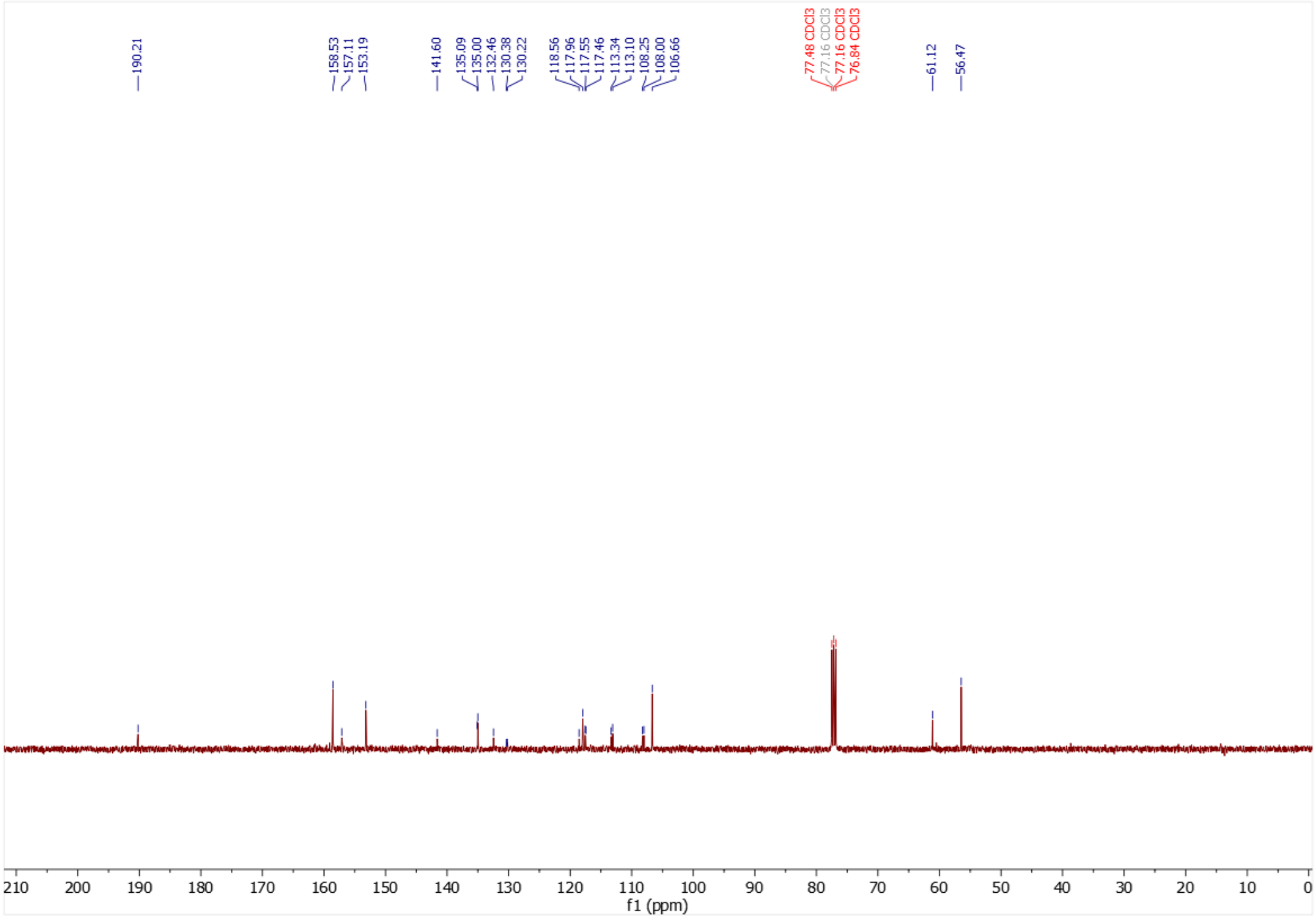
8.10
8.10
7.23
7.22
7.21
7.20 CDCl3
7.18
7.17
7.16
7.15
3.98
3.95
1.70 H2O
1.00
1.03
2.01
1.00
3.01
1.03
3.01
6.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


OMe
OMe
OMe
O
F
N
N
N

28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118.56
117.96
117.55
117.46
113.34
113.10
108.25
108.00
106.66
77.48 CDCl3
77.16 CDCl3
77.16 CDCl3
76.84 CDCl3
61.12
56.47
210
200
190
180
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130
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110
100
90
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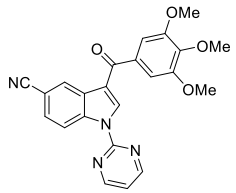
50
40
30
20
10
0
f1 (ppm)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OMe
OMe
O
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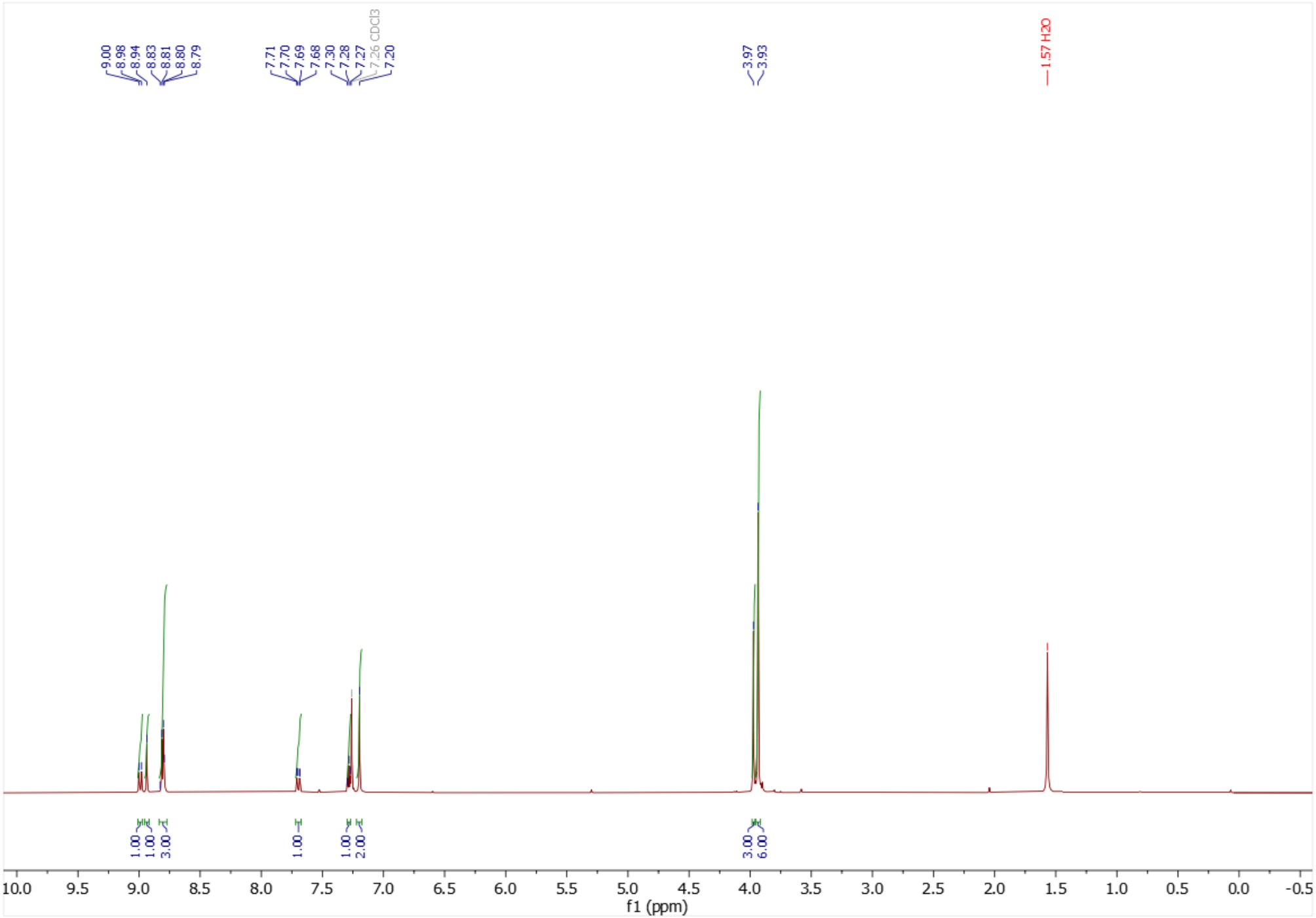
N
N
N

29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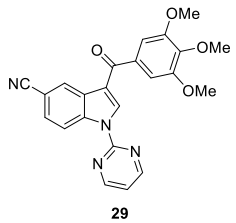
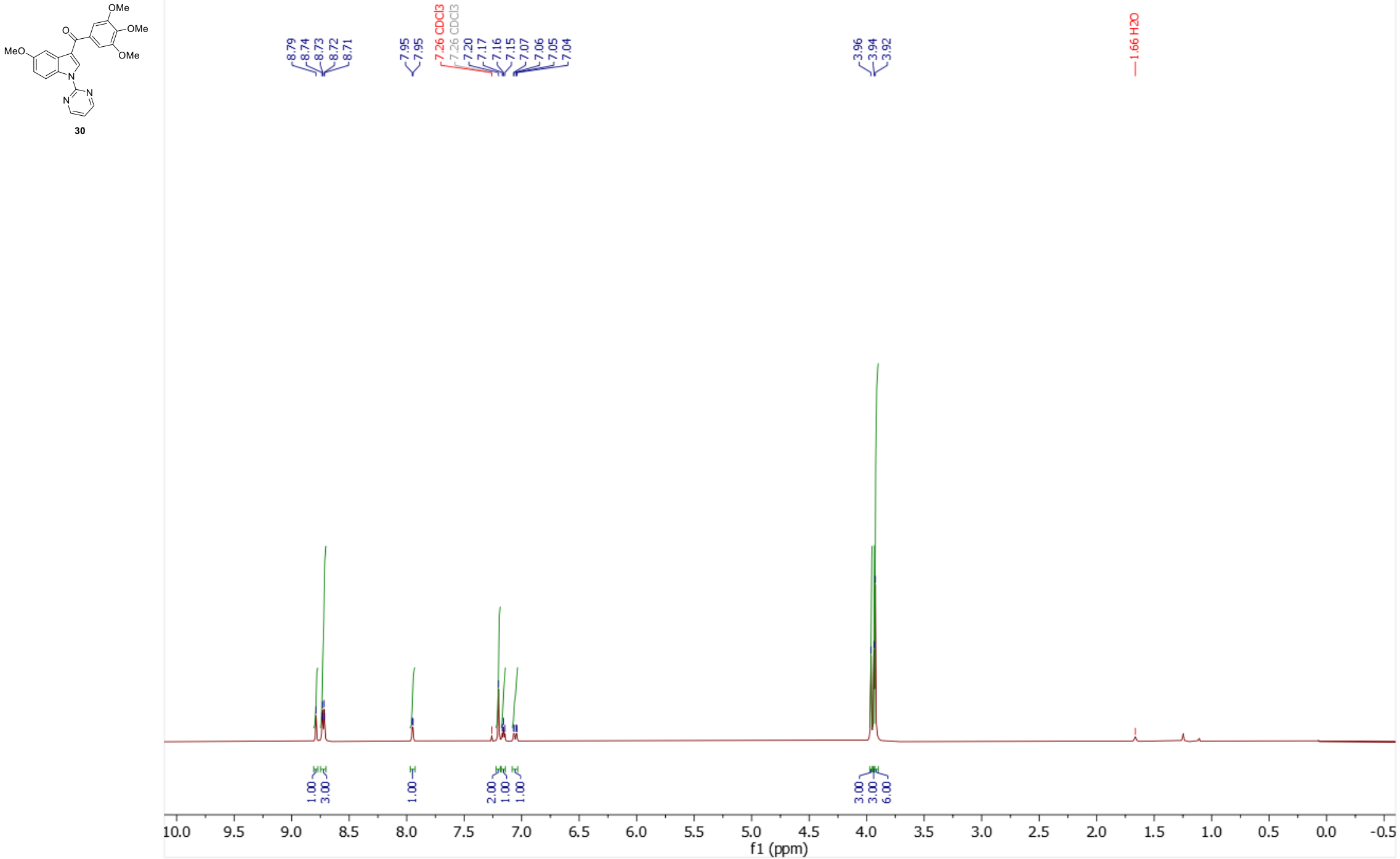
7.69
7.68
7.30
7.28
7.27
7.26 CDCl3
7.20
3.97
3.93
1.57 H2O
1.00
1.00
3.00
1.00
1.00
2.00
3.00
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

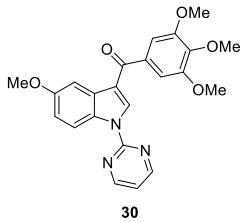


29

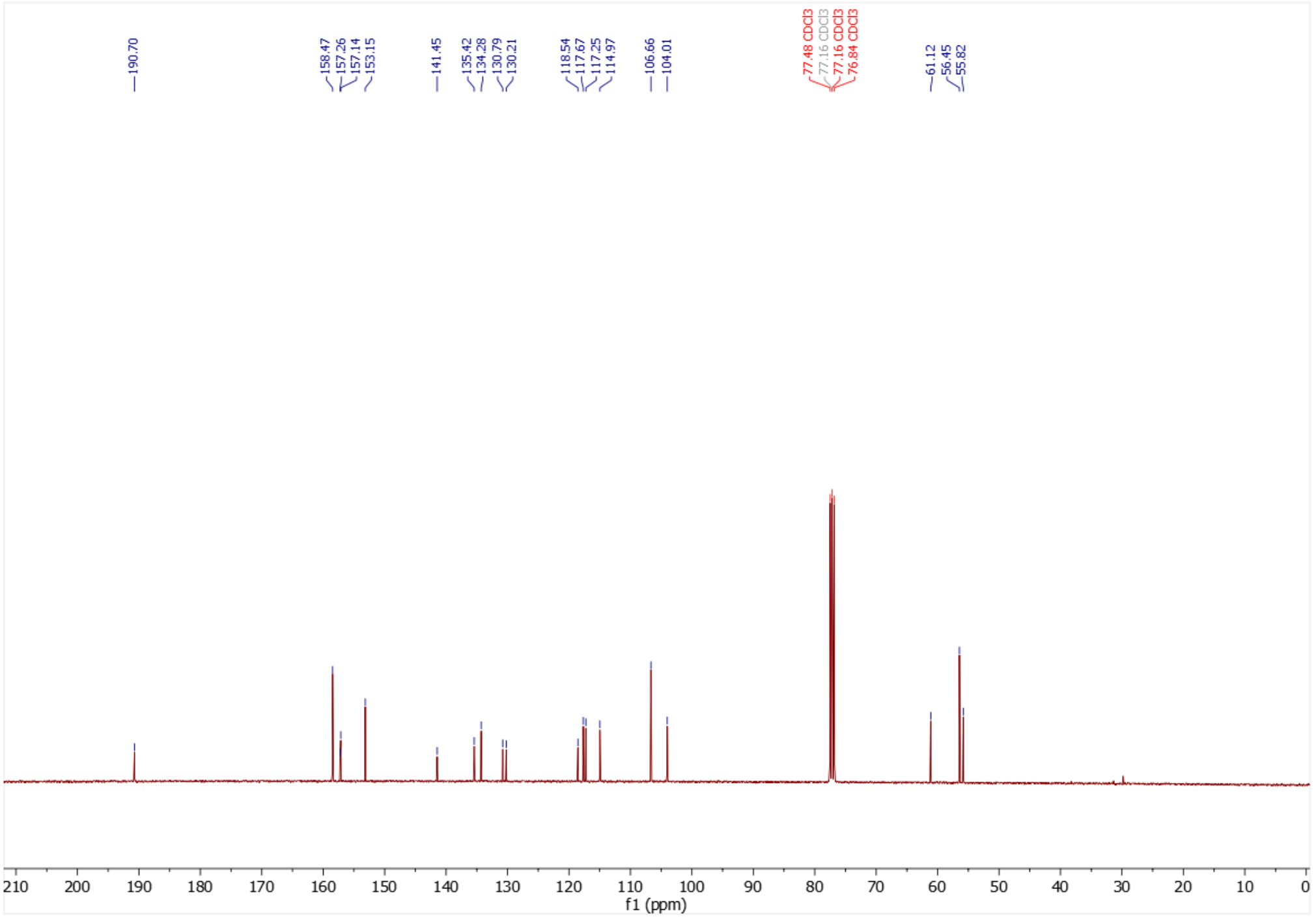
189.76
158.75
156.89
153.28
141.95
137.68
135.26
134.59
129.26
128.32
127.60
119.84
118.64
118.50
117.38
107.54
106.72
77.48 CDCl3
77.16 CDCl3
77.16 CDCl3
76.84 CDCl3
61.15
56.51

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

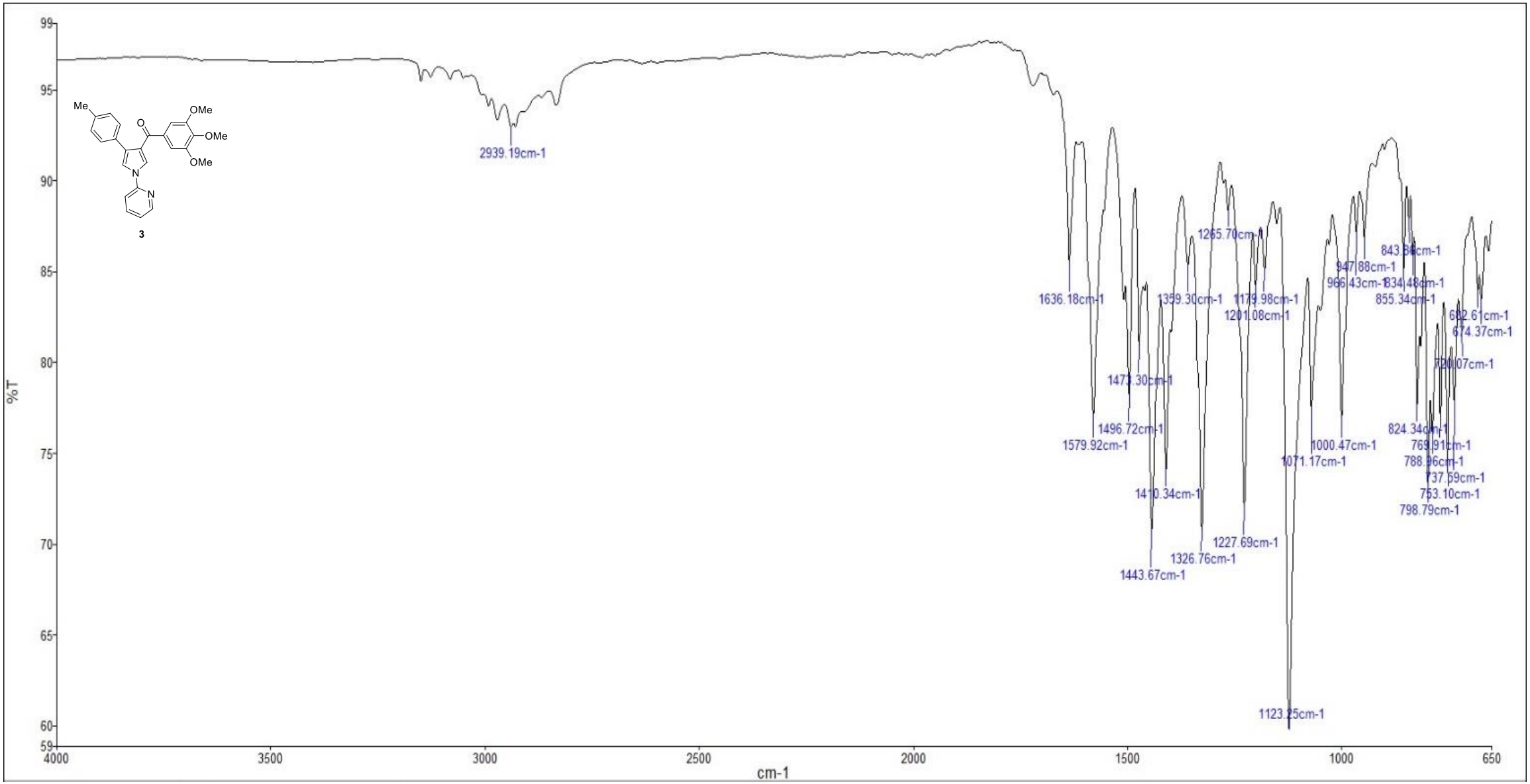

OMe
OMe
OMe
MeO
O
N
N
N
30
8.79
8.74
8.73
8.72
8.71
7.95
7.95
7.26 CDCl3
7.26 CDCl3
7.20
7.17
7.16
7.15
7.07
7.06
7.05
7.04
3.96
3.94
3.92
1.66 H2O
1.00
3.00
1.00
2.00
1.00
1.00
3.00
3.00
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

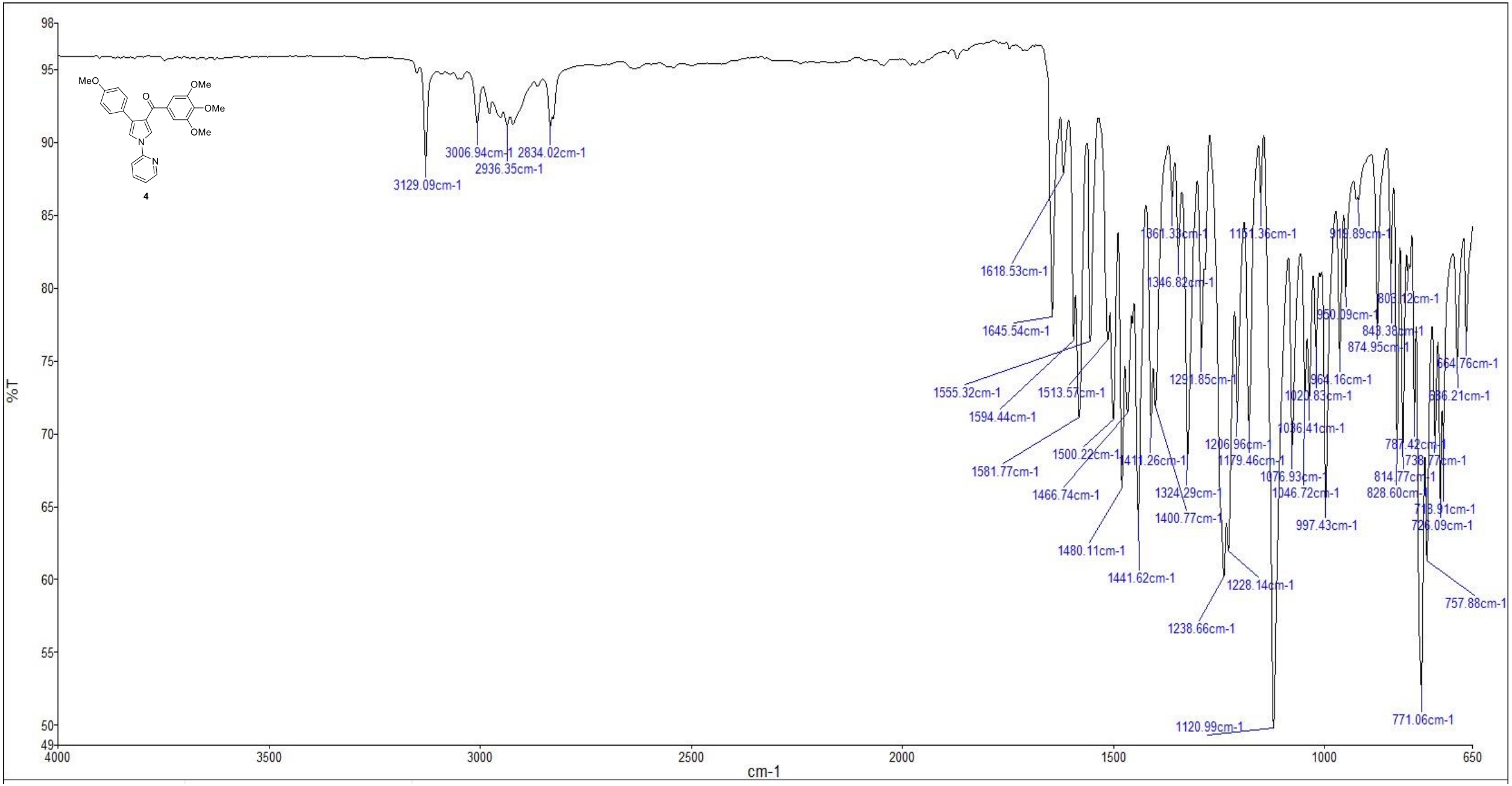

OMe
OMe
OMe
MeO
O
N
N
N

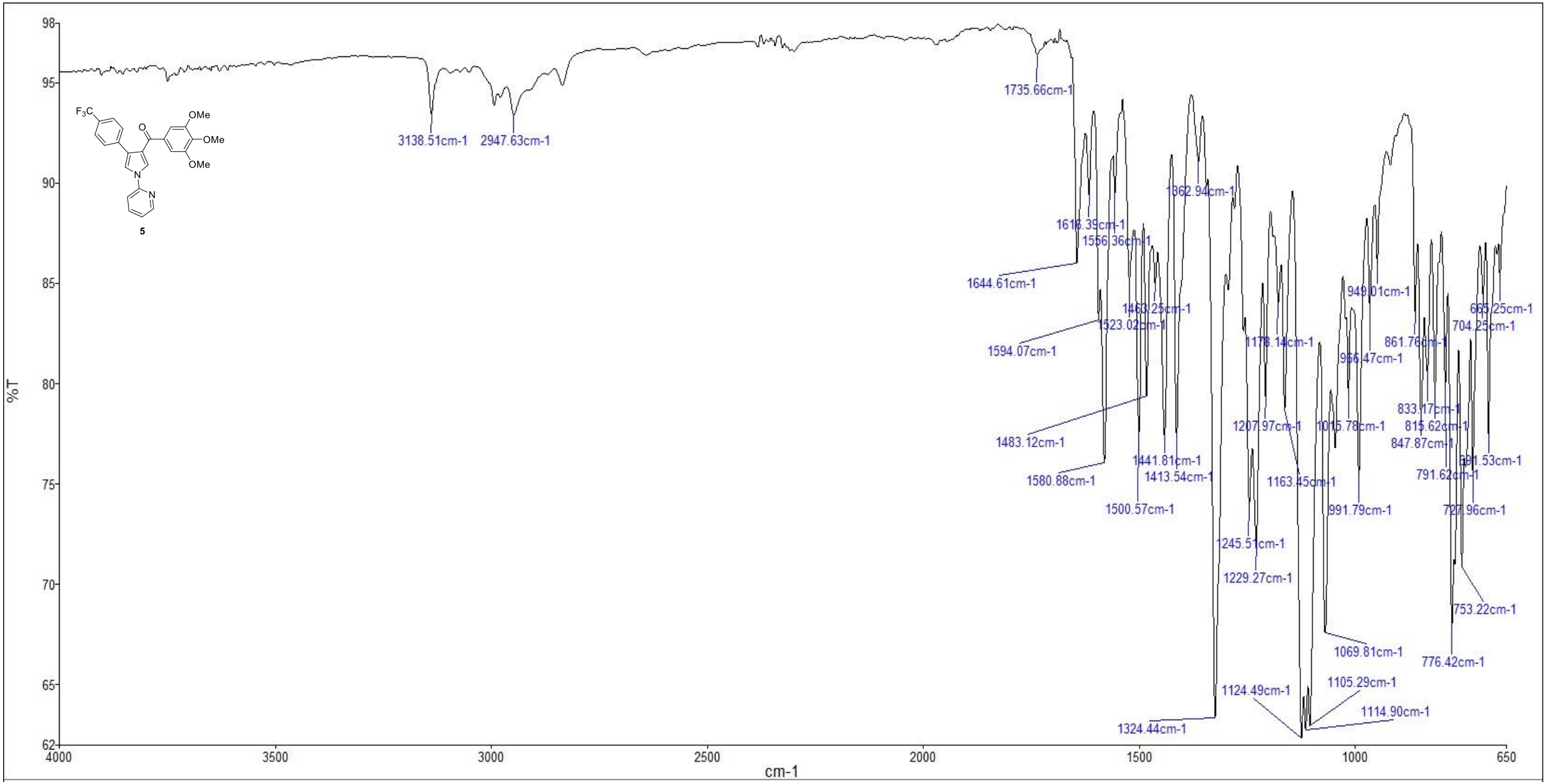
30

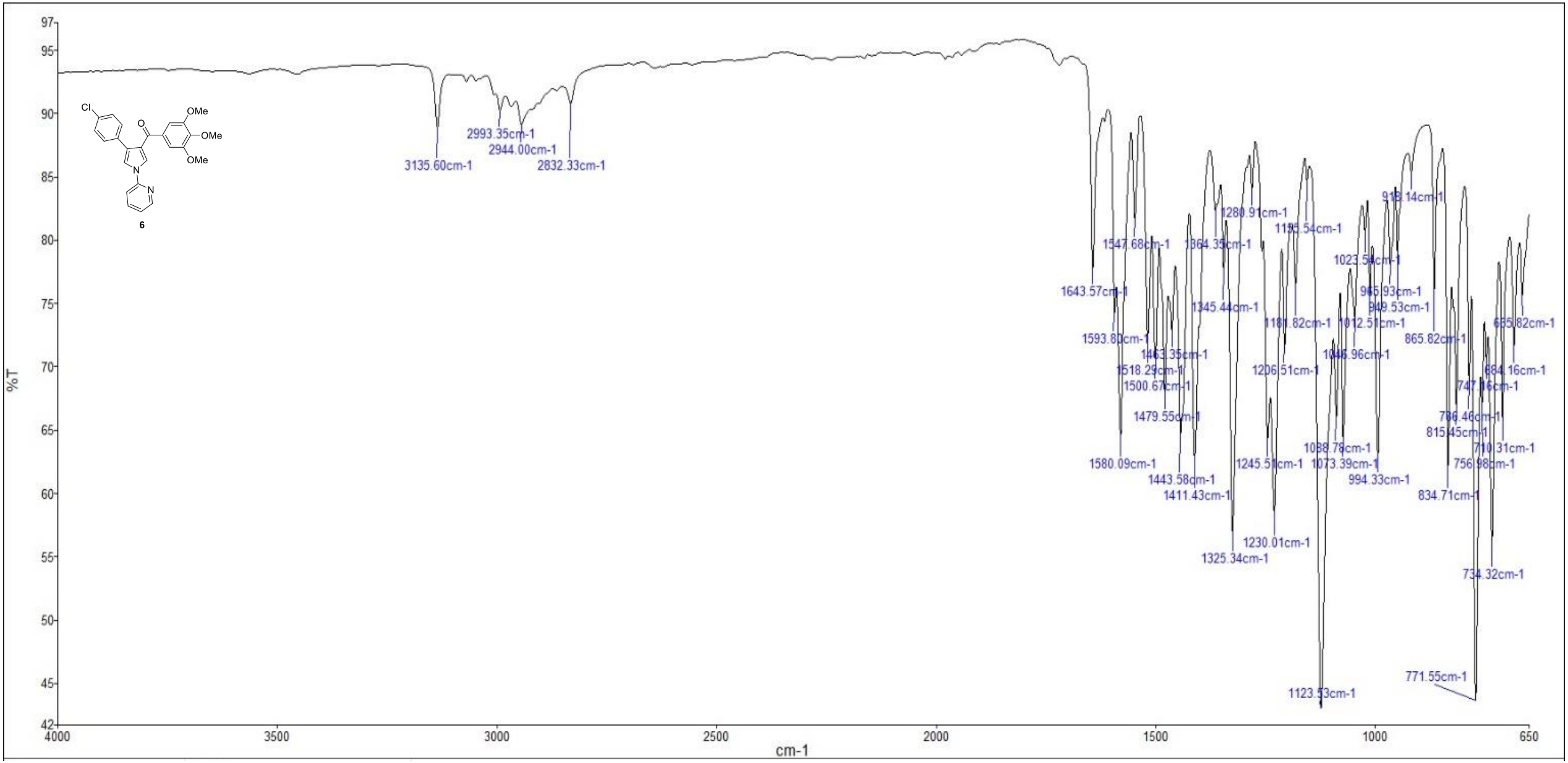

190.70
158.47
157.26
157.14
153.15
141.45
135.42
134.28
130.79
130.21
118.54
117.67
117.25
114.97
106.66
104.01
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
61.12
56.45
55.82
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

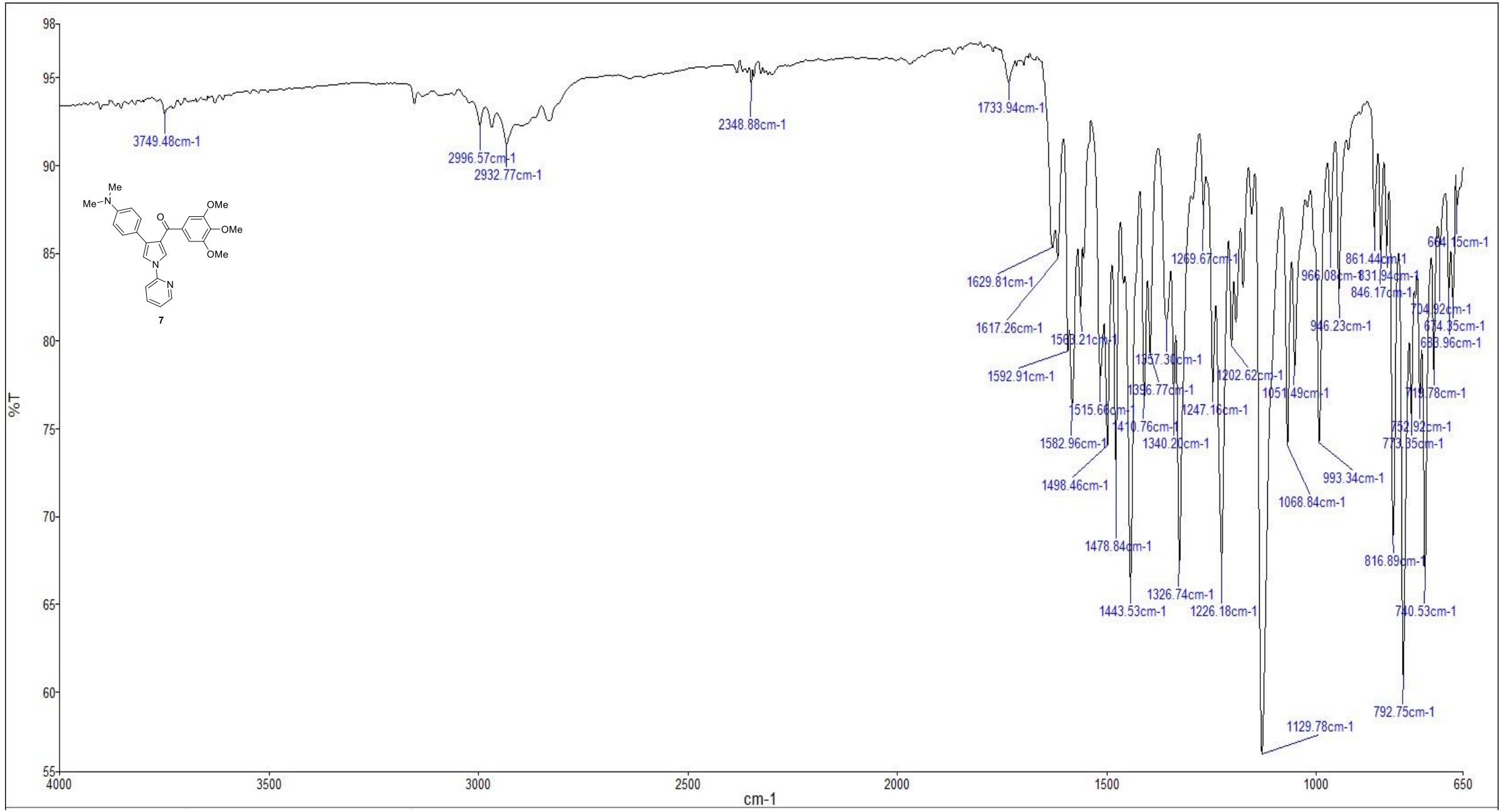
IR Spectra of Pyrroles **3-24** and Indoles **25-30**


Me
OMe
OMe
OMe
O
N
N
3
%T
cm-1
2939.19cm-1
1636.18cm-1
1579.92cm-1
1496.72cm-1
1473.30cm-1
1443.67cm-1
1410.34cm-1
1359.30cm-1
1326.76cm-1
1265.70cm-1
1227.69cm-1
1201.08cm-1
1179.98cm-1
1123.25cm-1
1071.17cm-1
1000.47cm-1
966.43cm-1
947.88cm-1
855.34cm-1
843.84cm-1
834.48cm-1
824.34cm-1
798.79cm-1
788.96cm-1
769.91cm-1
753.10cm-1
737.59cm-1
720.07cm-1
682.61cm-1
674.37cm-1
99
95
90
85
80
75
70
65
60
59
4000
3500
3000
2500
2000
1500
1000
650


MeO
OMe
OMe
OMe
O
N
N
4
%T
cm-1
3129.09cm-1
3006.94cm-1
2936.35cm-1
2834.02cm-1
1618.53cm-1
1645.54cm-1
1555.32cm-1
1594.44cm-1
1581.77cm-1
1513.57cm-1
1500.22cm-1
1466.74cm-1
1480.11cm-1
1441.62cm-1
1411.26cm-1
1361.33cm-1
1346.82cm-1
1324.29cm-1
1400.77cm-1
1291.85cm-1
1238.66cm-1
1228.14cm-1
1206.96cm-1
1179.46cm-1
1151.36cm-1
1120.99cm-1
1076.93cm-1
1046.72cm-1
1036.41cm-1
1020.83cm-1
997.43cm-1
964.16cm-1
950.09cm-1
919.89cm-1
874.95cm-1
843.38cm-1
808.12cm-1
787.42cm-1
771.06cm-1
757.88cm-1
738.77cm-1
726.09cm-1
718.91cm-1
814.77cm-1
828.60cm-1
836.21cm-1
664.76cm-1
4000
3500
3000
2500
2000
1500
1000
650
98
95
90
85
80
75
70
65
60
55
50
49


98
95
90
85
80
75
70
65
62
%T
4000
3500
3000
2500
2000
1500
1000
650
cm-1
F3C
O
OMe
OMe
OMe
N
N
5
3138.51cm-1
2947.63cm-1
1735.66cm-1
1644.61cm-1
1616.39cm-1
1556.36cm-1
1362.94cm-1
1594.07cm-1
1523.02cm-1
1463.25cm-1
1483.12cm-1
1580.88cm-1
1500.57cm-1
1441.81cm-1
1413.54cm-1
1245.51cm-1
1229.27cm-1
1178.14cm-1
1207.97cm-1
1163.45cm-1
1124.49cm-1
1324.44cm-1
1105.29cm-1
1114.90cm-1
1069.81cm-1
991.79cm-1
956.47cm-1
949.01cm-1
1015.78cm-1
861.76cm-1
833.17cm-1
815.62cm-1
847.87cm-1
791.62cm-1
704.25cm-1
665.25cm-1
691.53cm-1
727.96cm-1
753.22cm-1
776.42cm-1


Cl
O
OMe
OMe
OMe
N
N
6
3135.60cm-1
2993.35cm-1
2944.00cm-1
2832.33cm-1
1643.57cm-1
1593.80cm-1
1580.09cm-1
1547.68cm-1
1518.29cm-1
1500.67cm-1
1479.55cm-1
1463.35cm-1
1443.58cm-1
1411.43cm-1
1364.35cm-1
1345.44cm-1
1325.34cm-1
1280.91cm-1
1245.51cm-1
1230.01cm-1
1206.51cm-1
1185.54cm-1
1181.82cm-1
1123.53cm-1
1073.39cm-1
1046.96cm-1
1023.54cm-1
1012.51cm-1
994.33cm-1
965.93cm-1
949.53cm-1
918.14cm-1
865.82cm-1
834.71cm-1
815.45cm-1
786.46cm-1
771.55cm-1
756.98cm-1
747.96cm-1
734.32cm-1
710.31cm-1
684.16cm-1
655.82cm-1
%T
cm-1
97
95
90
85
80
75
70
65
60
55
50
45
42
4000
3500
3000
2500
2000
1500
1000
650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2932.77cm-1
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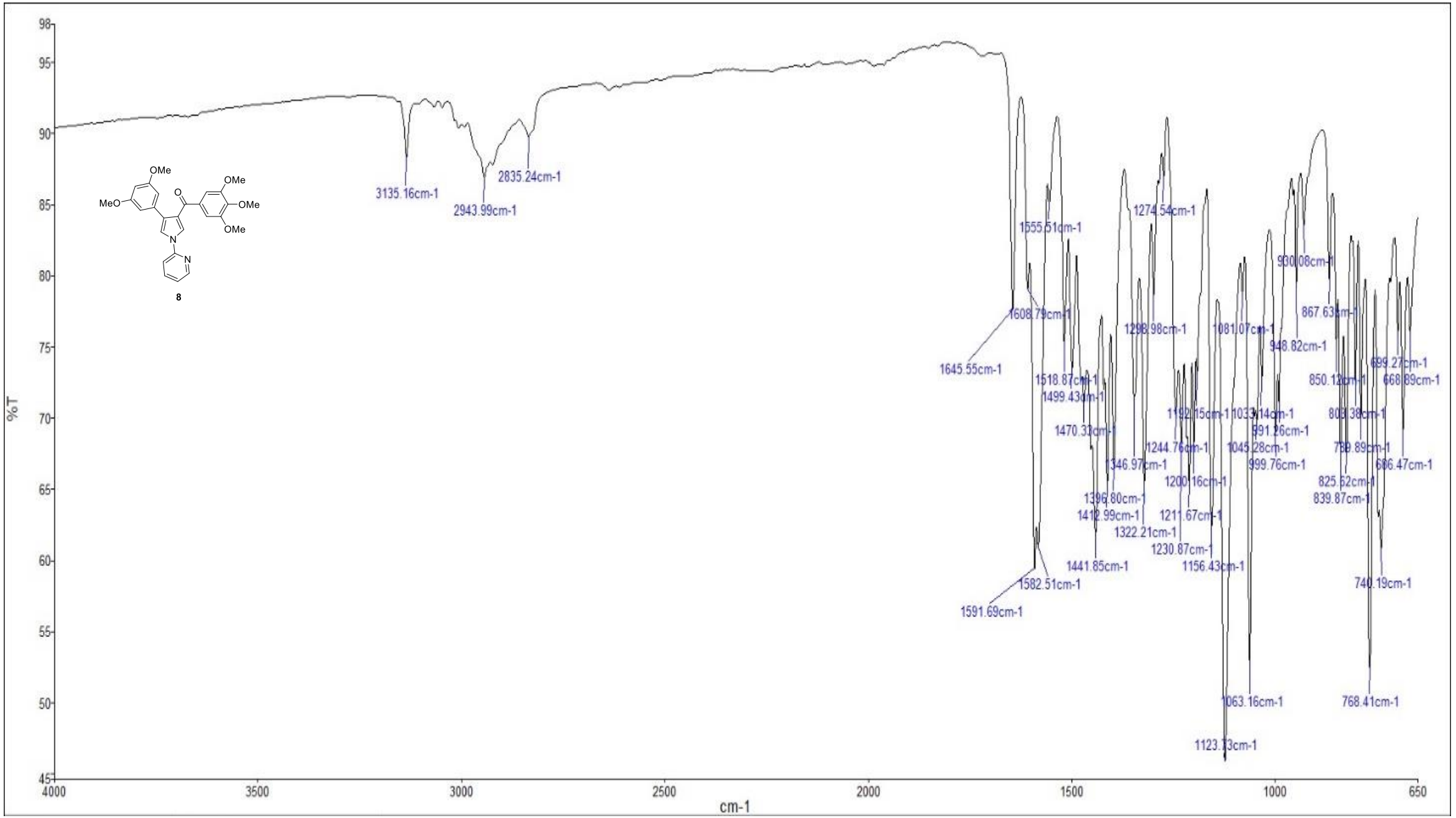
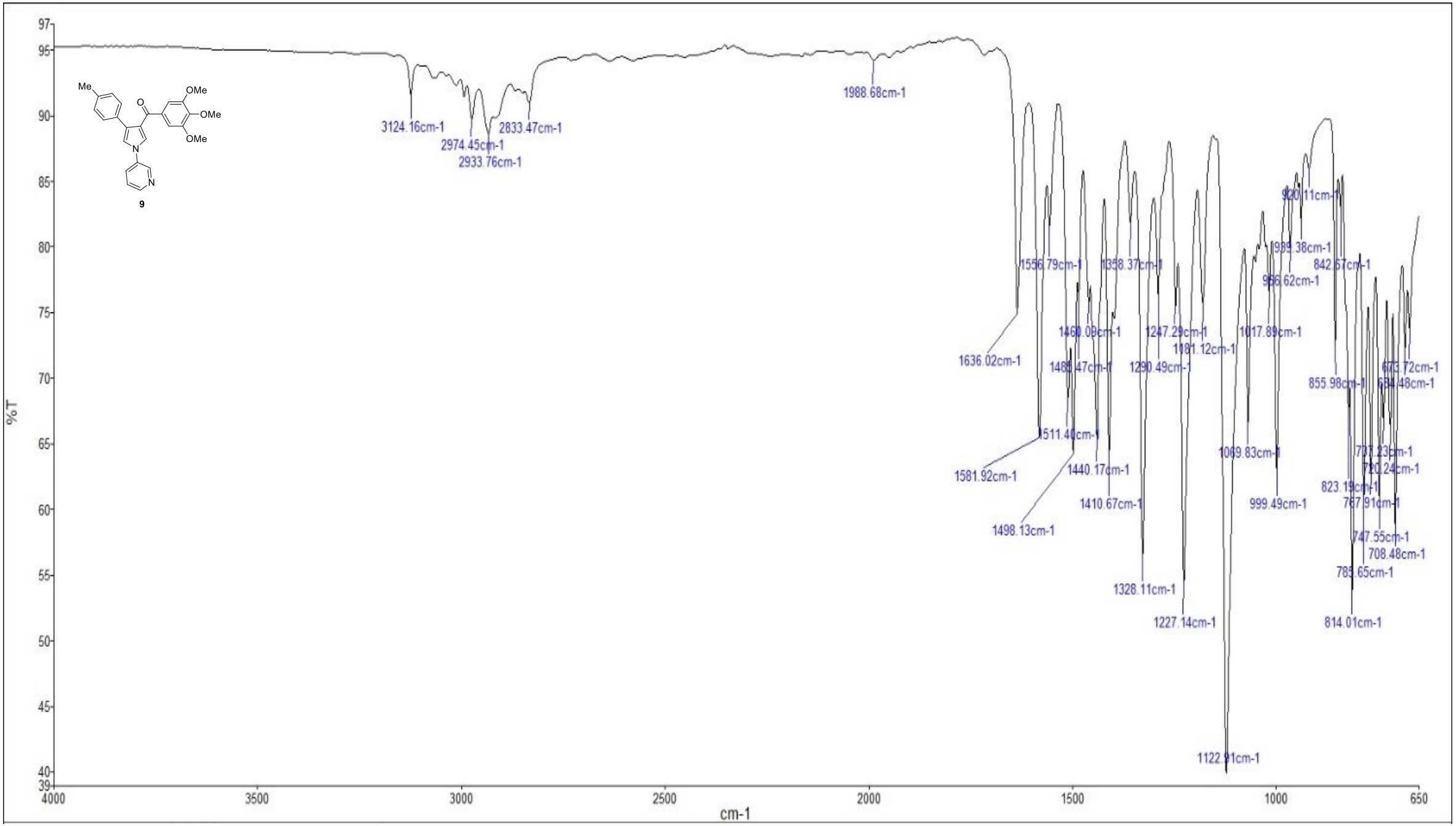
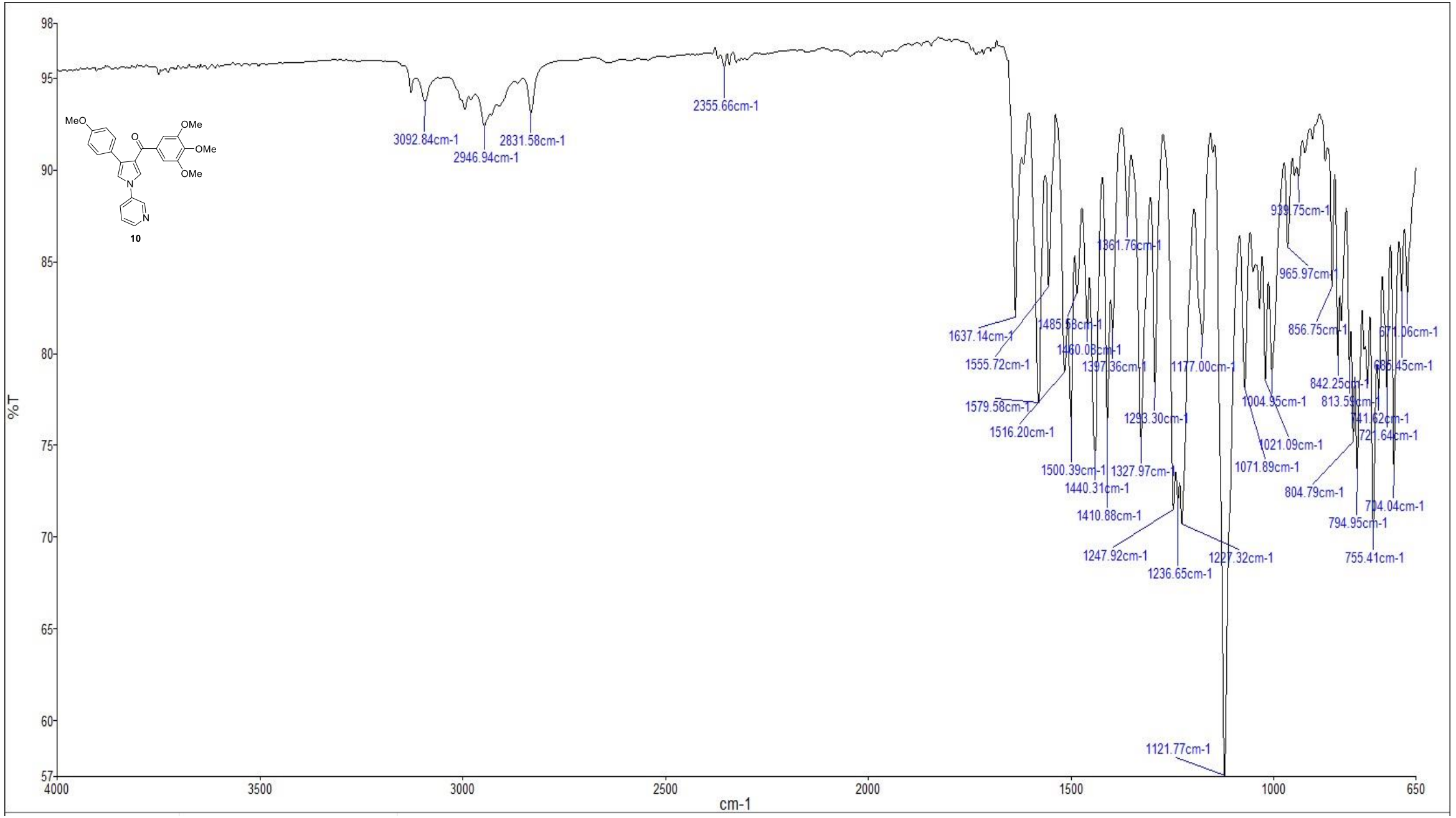
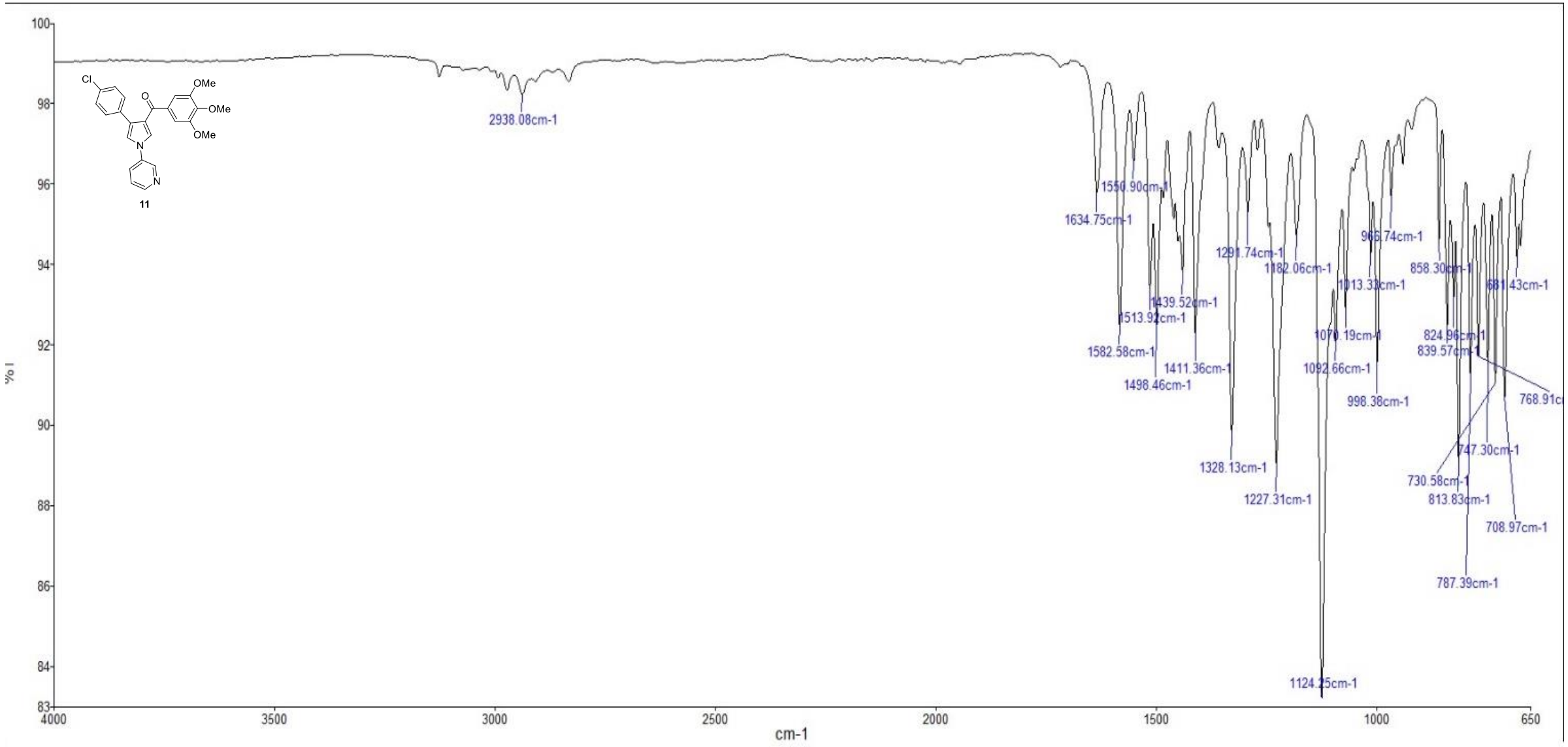
1733.94cm-1
1629.81cm-1
1617.26cm-1
1592.91cm-1
1582.96cm-1
1498.46cm-1
1478.84cm-1
1443.53cm-1
1515.66cm-1
1410.76cm-1
1340.20cm-1
1326.74cm-1
1226.18cm-1
1396.77cm-1
1357.30cm-1
1269.67cm-1
1247.16cm-1
1202.62cm-1
1129.78cm-1
1068.84cm-1
1051.49cm-1
993.34cm-1
966.08cm-1
946.23cm-1
861.44cm-1
846.17cm-1
831.94cm-1
816.89cm-1
792.75cm-1
752.92cm-1
740.53cm-1
719.78cm-1
704.92cm-1
674.35cm-1
664.15cm-1
633.96cm-1
773.35cm-1
Me
Me
N
OMe
OMe
OMe
O
N
7
%T
cm-1
98
95
90
85
80
75
70
65
60
55
4000
3500
3000
2500
2000
1500
1000
650


OMe
MeO
OMe
OMe
OMe
O
N
N
8
3135.16cm-1
2943.99cm-1
2835.24cm-1
1645.55cm-1
1608.79cm-1
1591.69cm-1
1582.51cm-1
1555.51cm-1
1518.87cm-1
1499.43cm-1
1470.33cm-1
1441.85cm-1
1412.99cm-1
1396.80cm-1
1346.97cm-1
1322.21cm-1
1274.54cm-1
1244.76cm-1
1230.87cm-1
1211.67cm-1
1200.16cm-1
1192.15cm-1
1156.43cm-1
1123.33cm-1
1081.07cm-1
1063.16cm-1
1045.28cm-1
1033.14cm-1
999.76cm-1
991.26cm-1
948.82cm-1
930.08cm-1
867.63cm-1
850.12cm-1
839.87cm-1
825.52cm-1
803.38cm-1
768.41cm-1
759.89cm-1
740.19cm-1
699.27cm-1
686.47cm-1
668.89cm-1
%T
cm-1
98
95
90
85
80
75
70
65
60
55
50
45
4000
3500
3000
2500
2000
1500
1000
650


Me
OMe
OMe
OMe
O
N
N
9
3124.16cm-1
2974.45cm-1
2933.76cm-1
2833.47cm-1
1988.68cm-1
1636.02cm-1
1581.92cm-1
1556.79cm-1
1511.46cm-1
1498.13cm-1
1488.47cm-1
1468.09cm-1
1440.17cm-1
1410.67cm-1
1358.37cm-1
1328.11cm-1
1290.49cm-1
1247.29cm-1
1227.14cm-1
1181.12cm-1
1122.91cm-1
1069.83cm-1
1017.89cm-1
999.49cm-1
956.62cm-1
939.38cm-1
920.11cm-1
855.98cm-1
842.67cm-1
823.19cm-1
814.01cm-1
783.65cm-1
767.91cm-1
747.55cm-1
737.23cm-1
720.24cm-1
708.48cm-1
673.72cm-1
634.48cm-1
%T
cm-1
97
95
90
85
80
75
70
65
60
55
50
45
40
39
4000
3500
3000
2500
2000
1500
1000
650


MeO
OMe
OMe
OMe
O
N
N
10
%T
cm-1
3092.84cm-1
2946.94cm-1
2831.58cm-1
2355.66cm-1
1637.14cm-1
1555.72cm-1
1579.58cm-1
1516.20cm-1
1500.39cm-1
1485.68cm-1
1460.08cm-1
1440.31cm-1
1410.88cm-1
1397.36cm-1
1361.76cm-1
1327.97cm-1
1293.30cm-1
1247.92cm-1
1236.65cm-1
1227.32cm-1
1177.00cm-1
1121.77cm-1
1071.89cm-1
1021.09cm-1
1004.95cm-1
965.97cm-1
939.75cm-1
856.75cm-1
842.25cm-1
813.59cm-1
804.79cm-1
794.95cm-1
755.41cm-1
741.62cm-1
721.64cm-1
704.04cm-1
685.45cm-1
671.06cm-1


Cl
OMe
OMe
OMe
O
N
N
11
2938.08cm-1
1634.75cm-1
1550.90cm-1
1513.92cm-1
1582.58cm-1
1439.52cm-1
1411.36cm-1
1498.46cm-1
1328.13cm-1
1291.74cm-1
1227.31cm-1
1182.06cm-1
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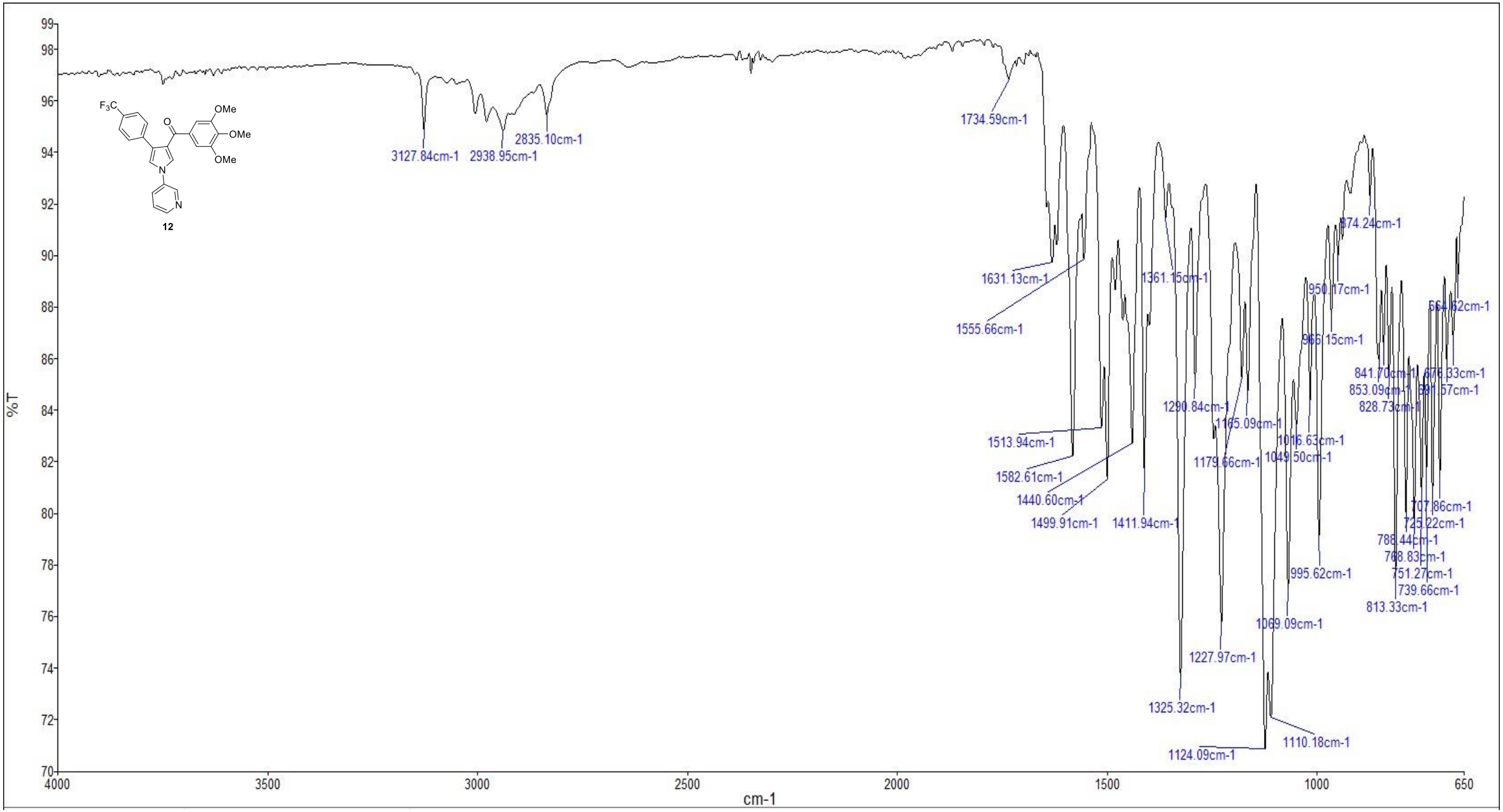
1092.66cm-1
1070.19cm-1
1013.32cm-1
998.38cm-1
965.74cm-1
858.30cm-1
824.96cm-1
839.57cm-1
768.91cm-1
747.30cm-1
730.58cm-1
813.83cm-1
787.39cm-1
708.97cm-1
681.43cm-1
%T
100
98
96
94
92
90
88
86
84
83
4000
3500
3000
2500
2000
1500
1000
650
cm-1


12
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2938.95cm-1
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1631.13cm-1
1555.66cm-1
1513.94cm-1
1582.61cm-1
1440.60cm-1
1499.91cm-1
1411.94cm-1
1361.15cm-1
1325.32cm-1
1290.84cm-1
1227.97cm-1
1179.66cm-1
1165.09cm-1
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1049.50cm-1
1016.63cm-1
995.62cm-1
950.17cm-1
874.24cm-1
841.70cm-1
828.73cm-1
813.33cm-1
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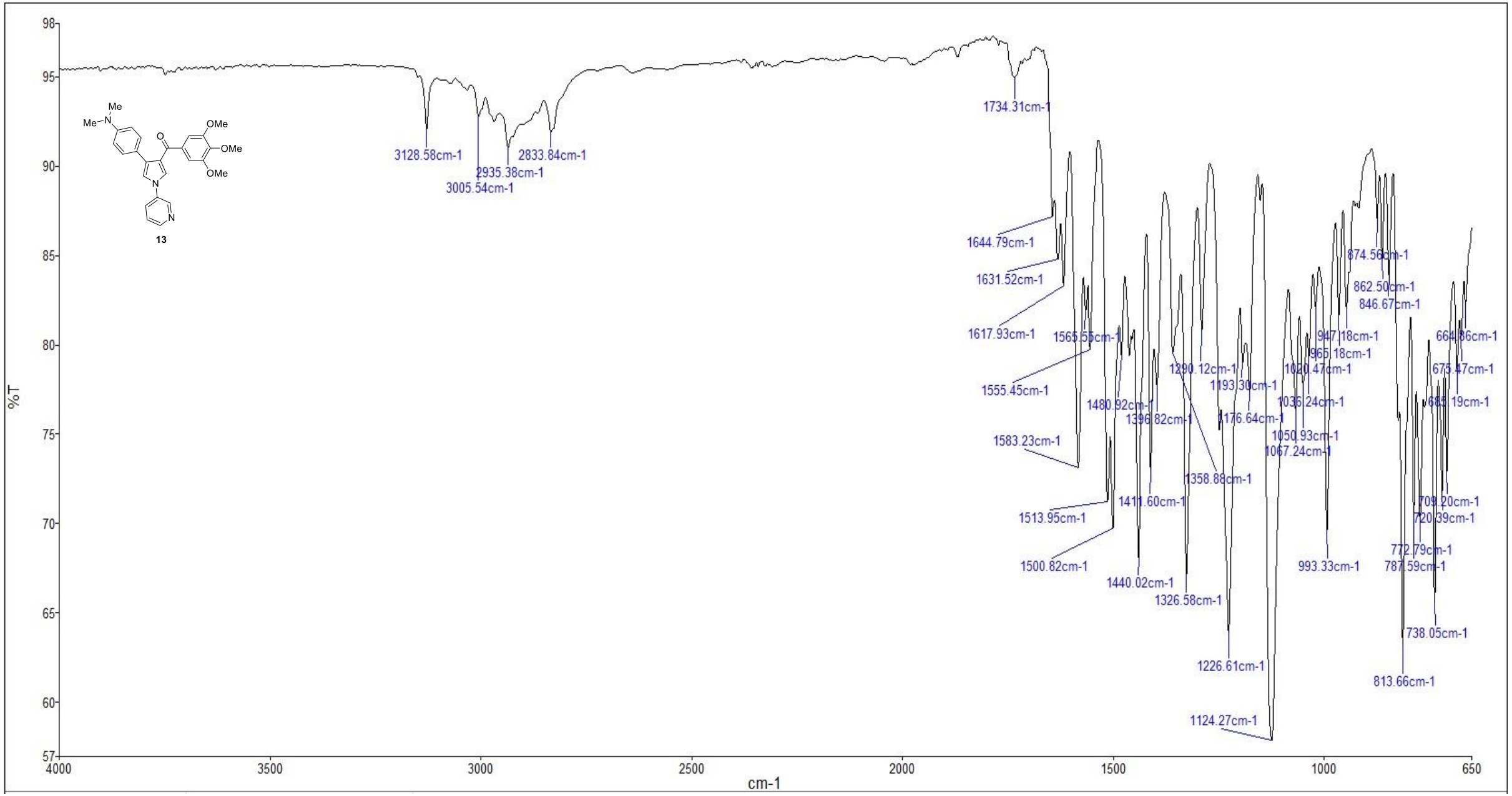
768.83cm-1
751.27cm-1
739.66cm-1
725.22cm-1
707.86cm-1
%T
cm-1


13
3128.58cm-1
3005.54cm-1
2935.38cm-1
2833.84cm-1
1734.31cm-1
1644.79cm-1
1631.52cm-1
1617.93cm-1
1565.55cm-1
1555.45cm-1
1583.23cm-1
1513.95cm-1
1500.82cm-1
1480.92cm-1
1440.02cm-1
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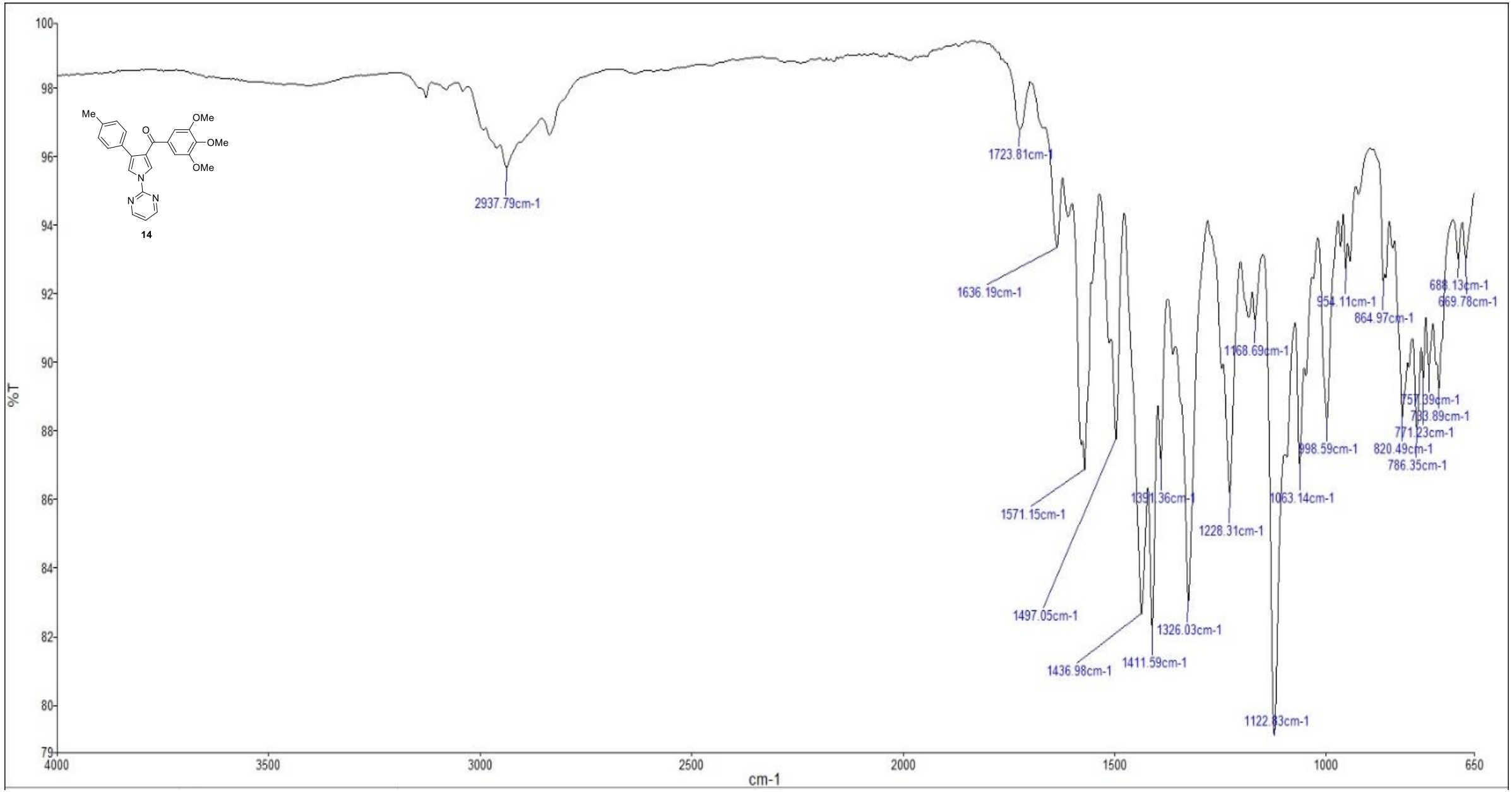
1396.82cm-1
1358.88cm-1
1326.58cm-1
1290.12cm-1
1226.61cm-1
1193.30cm-1
1176.64cm-1
1124.27cm-1
1067.24cm-1
1050.93cm-1
1036.24cm-1
1020.47cm-1
993.33cm-1
965.18cm-1
947.18cm-1
874.56cm-1
862.50cm-1
846.67cm-1
813.66cm-1
787.59cm-1
772.79cm-1
738.05cm-1
720.39cm-1
709.20cm-1
685.19cm-1
675.47cm-1
664.86cm-1
%T
cm-1


Me
OMe
OMe
OMe
O
N
N
N
14
%T
100
98
96
94
92
90
88
86
84
82
80
79
4000
3500
3000
2500
2000
1500
1000
650
cm-1
2937.79cm-1
1723.81cm-1
1636.19cm-1
1571.15cm-1
1497.05cm-1
1436.98cm-1
1411.59cm-1
1391.36cm-1
1326.03cm-1
1228.31cm-1
1168.69cm-1
1122.83cm-1
1063.14cm-1
998.59cm-1
954.11cm-1
864.97cm-1
820.49cm-1
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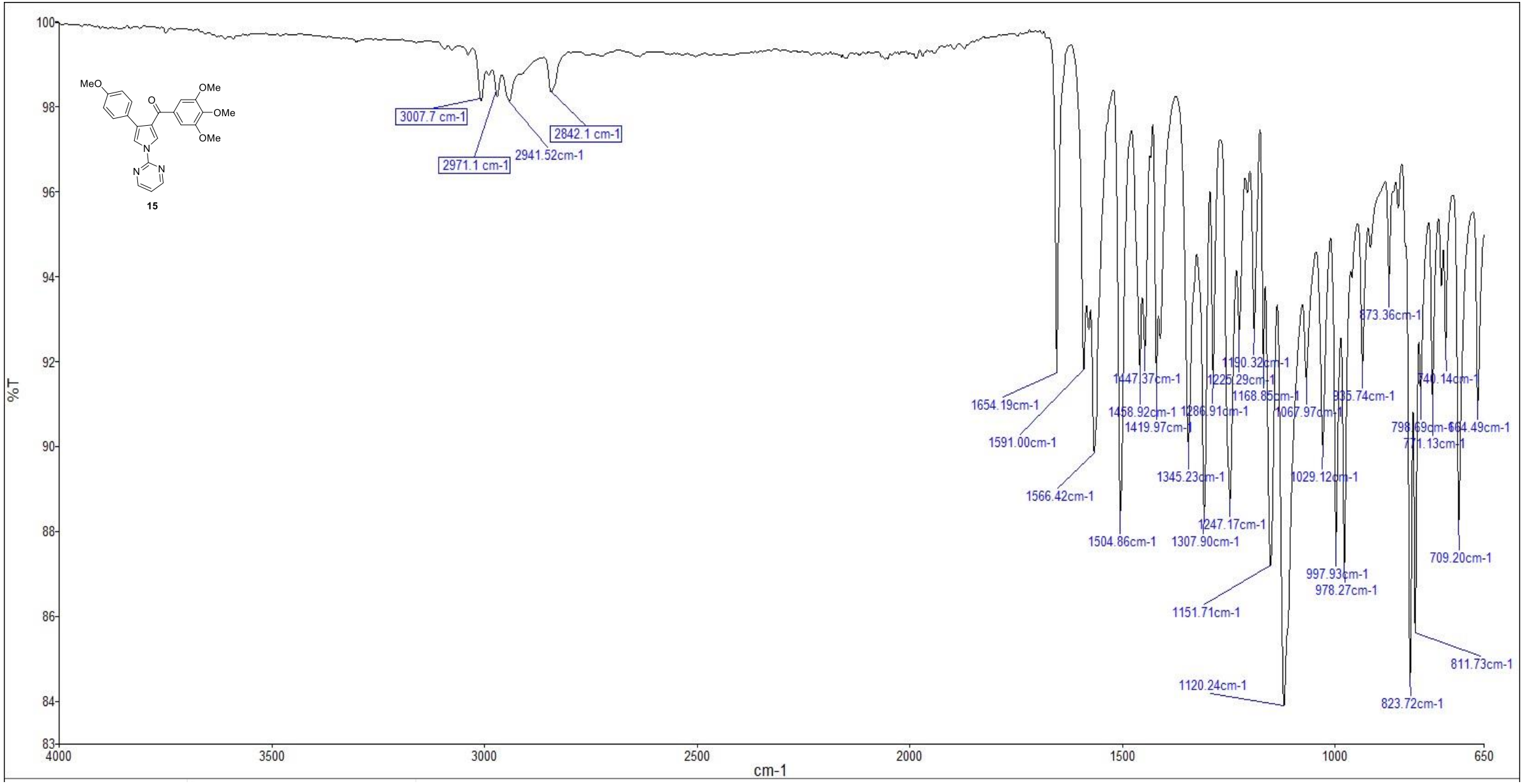
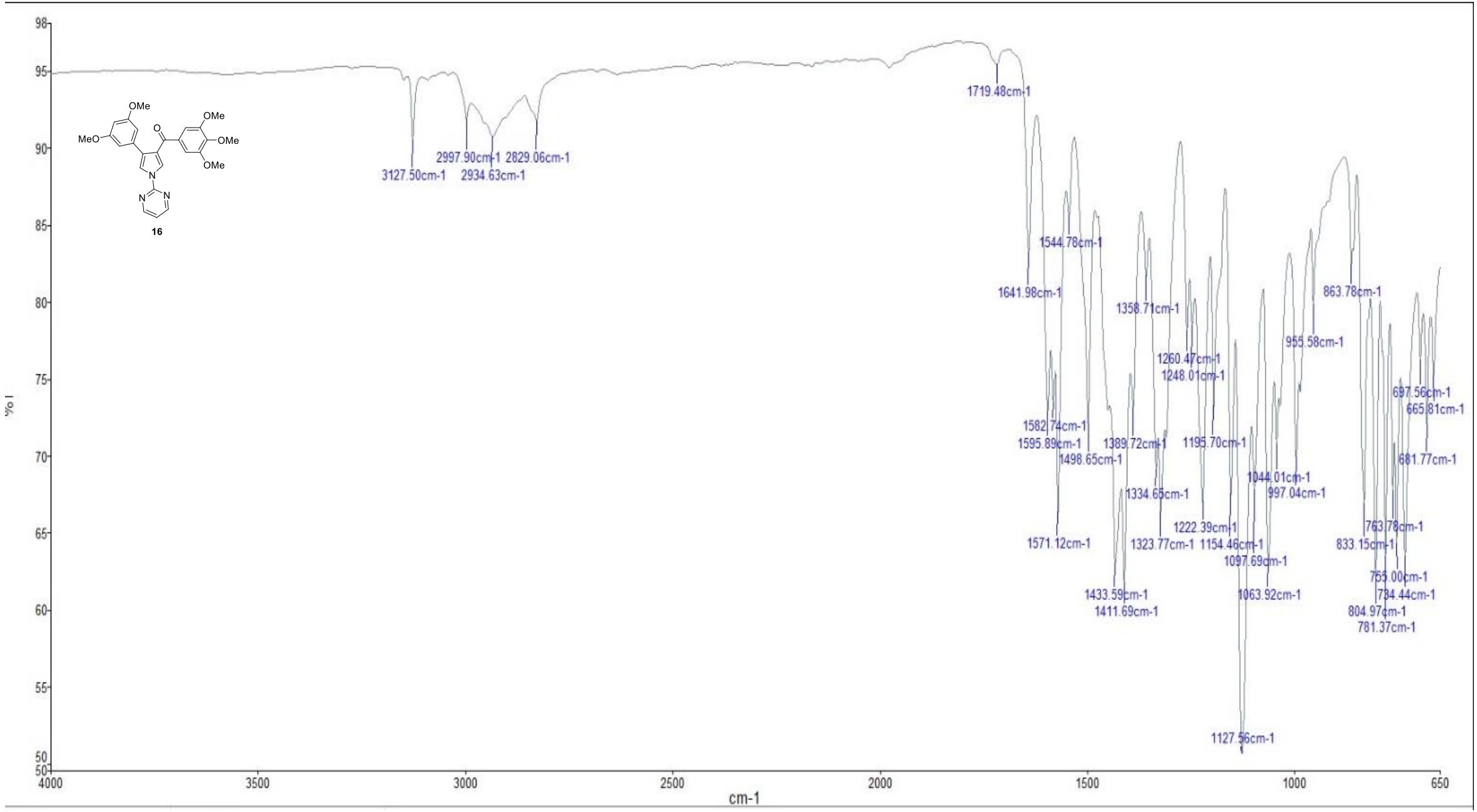
771.23cm-1
757.39cm-1
733.89cm-1
688.13cm-1
669.78cm-1


MeO
OMe
OMe
OMe
O
N
N
N
15
3007.7 cm-1
2971.1 cm-1
2941.52cm-1
2842.1 cm-1
1654.19cm-1
1591.00cm-1
1566.42cm-1
1504.86cm-1
1458.92cm-1
1447.37cm-1
1419.97cm-1
1345.23cm-1
1307.90cm-1
1286.91cm-1
1247.17cm-1
1225.29cm-1
1190.32cm-1
1168.85cm-1
1151.71cm-1
1120.24cm-1
1067.97cm-1
1029.12cm-1
997.93cm-1
978.27cm-1
935.74cm-1
873.36cm-1
823.72cm-1
811.73cm-1
798.69cm-1
771.13cm-1
740.14cm-1
709.20cm-1
664.49cm-1
%T
100
98
96
94
92
90
88
86
84
83
4000
3500
3000
2500
2000
1500
1000
650
cm-1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1582.74cm-1
1595.89cm-1
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1411.69cm-1
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1358.71cm-1
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1222.39cm-1
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997.04cm-1
955.58cm-1
863.78cm-1
833.15cm-1
804.97cm-1
781.37cm-1
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755.00cm-1
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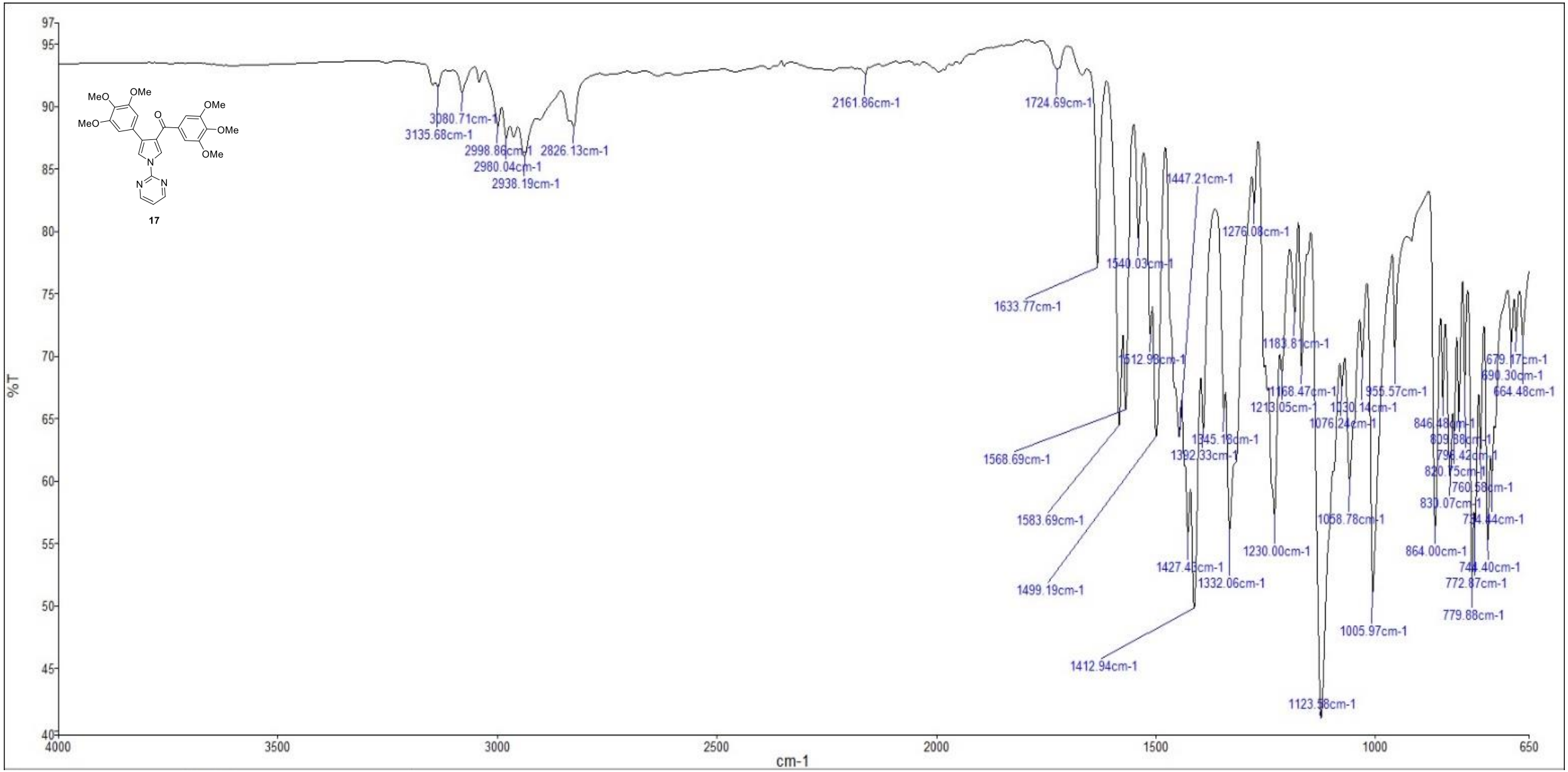
%T
cm-1
4000
3500
3000
2500
2000
1500
1000
650


17
%T
cm-1
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3500
3000
2500
2000
1500
1000
650
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2938.19cm-1
2826.13cm-1
2161.86cm-1
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1540.03cm-1
1512.98cm-1
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1427.46cm-1
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1412.94cm-1
1276.08cm-1
1213.05cm-1
1230.00cm-1
1183.81cm-1
1168.47cm-1
1130.14cm-1
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1058.78cm-1
1123.58cm-1
1005.97cm-1
955.57cm-1
846.48cm-1
809.68cm-1
796.42cm-1
820.75cm-1
760.58cm-1
830.07cm-1
754.44cm-1
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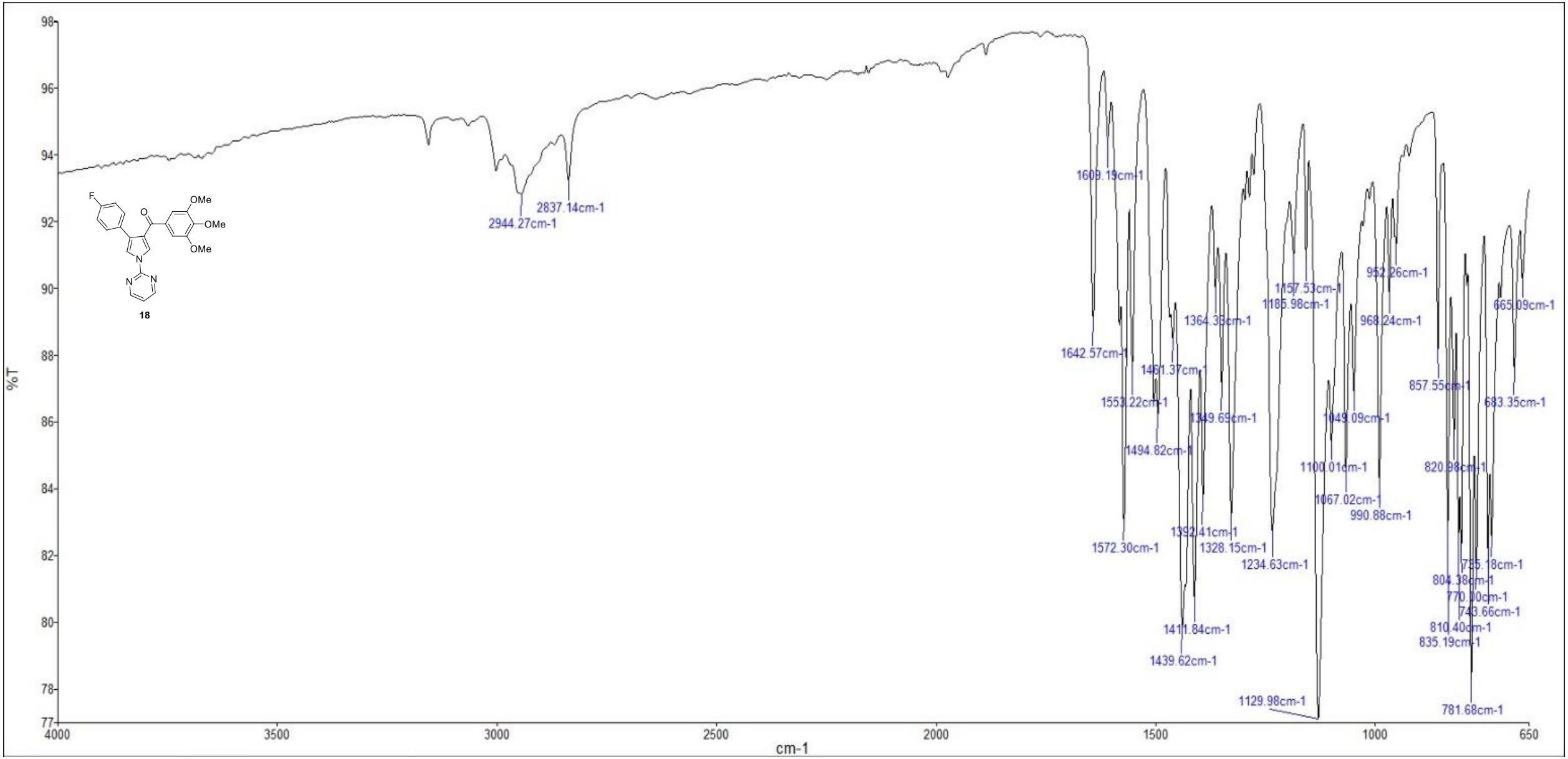
664.48cm-1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1461.37cm-1
1439.62cm-1
1411.84cm-1
1392.41cm-1
1364.33cm-1
1349.69cm-1
1328.15cm-1
1234.63cm-1
1185.98cm-1
1157.53cm-1
1129.98cm-1
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1067.02cm-1
1049.09cm-1
990.88cm-1
968.24cm-1
952.26cm-1
857.55cm-1
835.19cm-1
820.98cm-1
810.40cm-1
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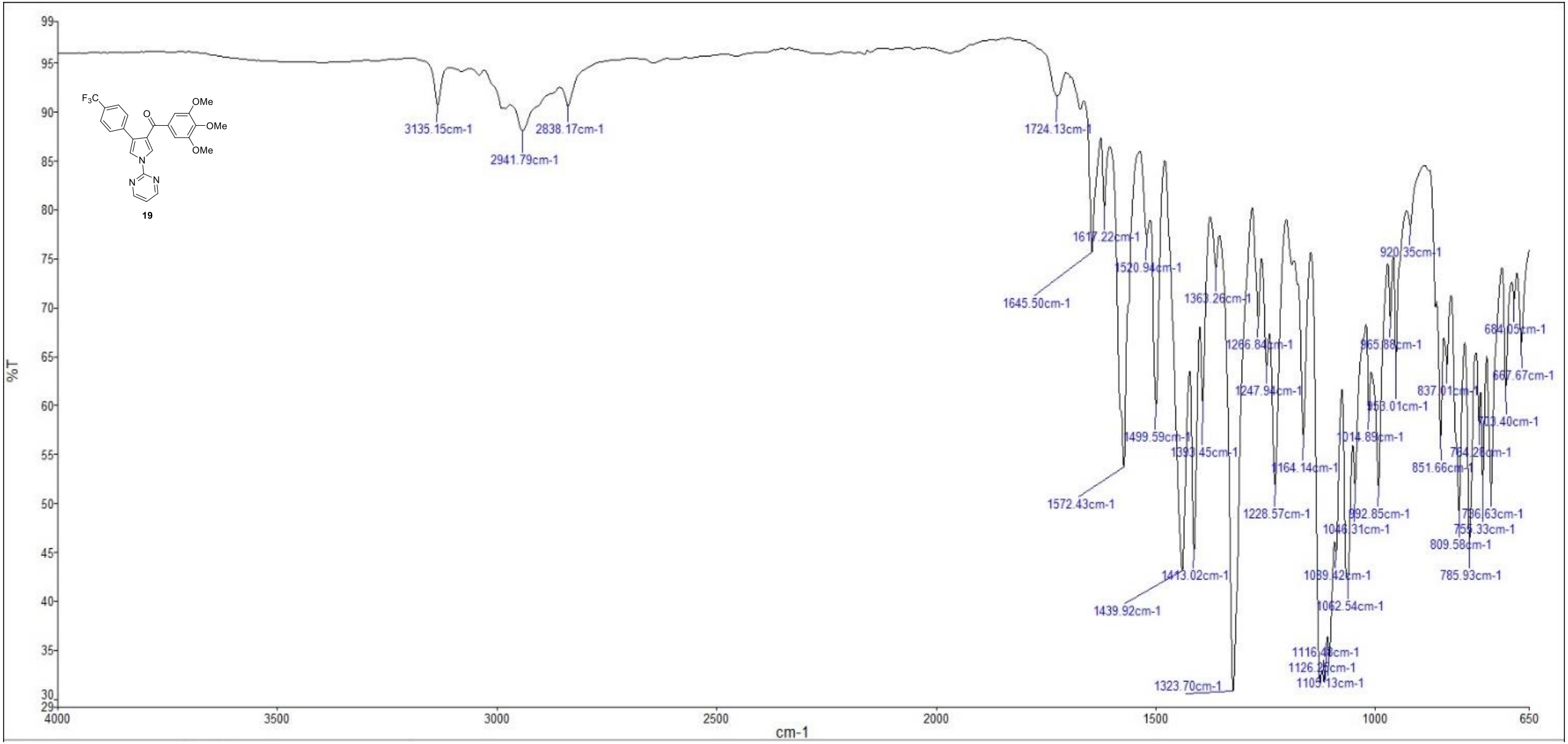
F3C
OMe
OMe
OMe
O
N
N
N
19
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1413.02cm-1
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1363.26cm-1
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1228.57cm-1
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851.66cm-1
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755.33cm-1
736.63cm-1
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667.67cm-1
%T
cm-1
4000
3500
3000
2500
2000
1500
1000
650
99
95
90
85
80
75
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65
60
55
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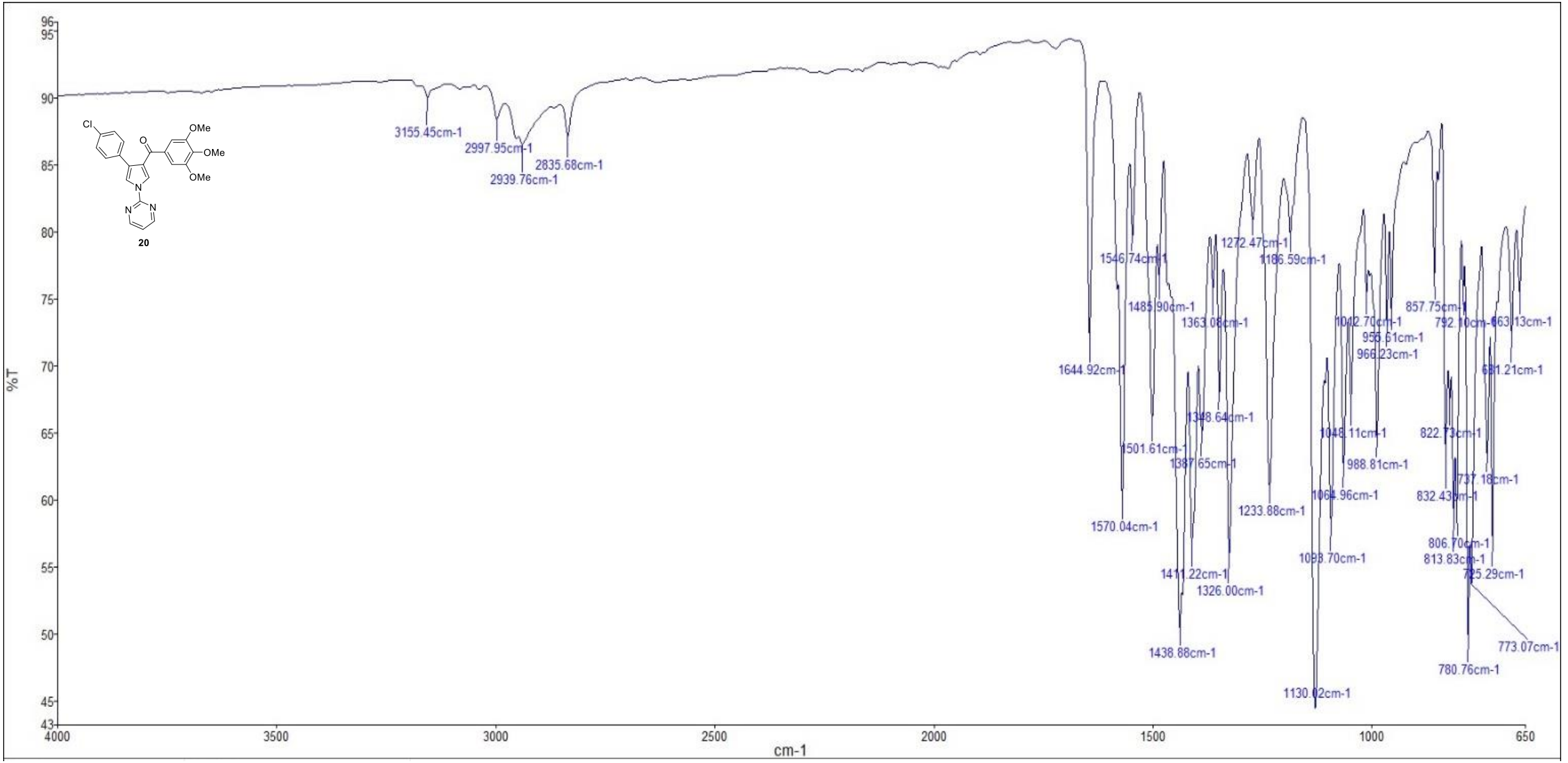
35
30
29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1501.61cm-1
1485.90cm-1
1438.88cm-1
1411.22cm-1
1387.65cm-1
1363.08cm-1
1348.64cm-1
1326.00cm-1
1272.47cm-1
1233.88cm-1
1186.59cm-1
1130.62cm-1
1093.70cm-1
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1048.11cm-1
1002.70cm-1
988.81cm-1
966.23cm-1
956.61cm-1
857.75cm-1
832.43cm-1
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806.70cm-1
792.10cm-1
780.76cm-1
773.07cm-1
737.18cm-1
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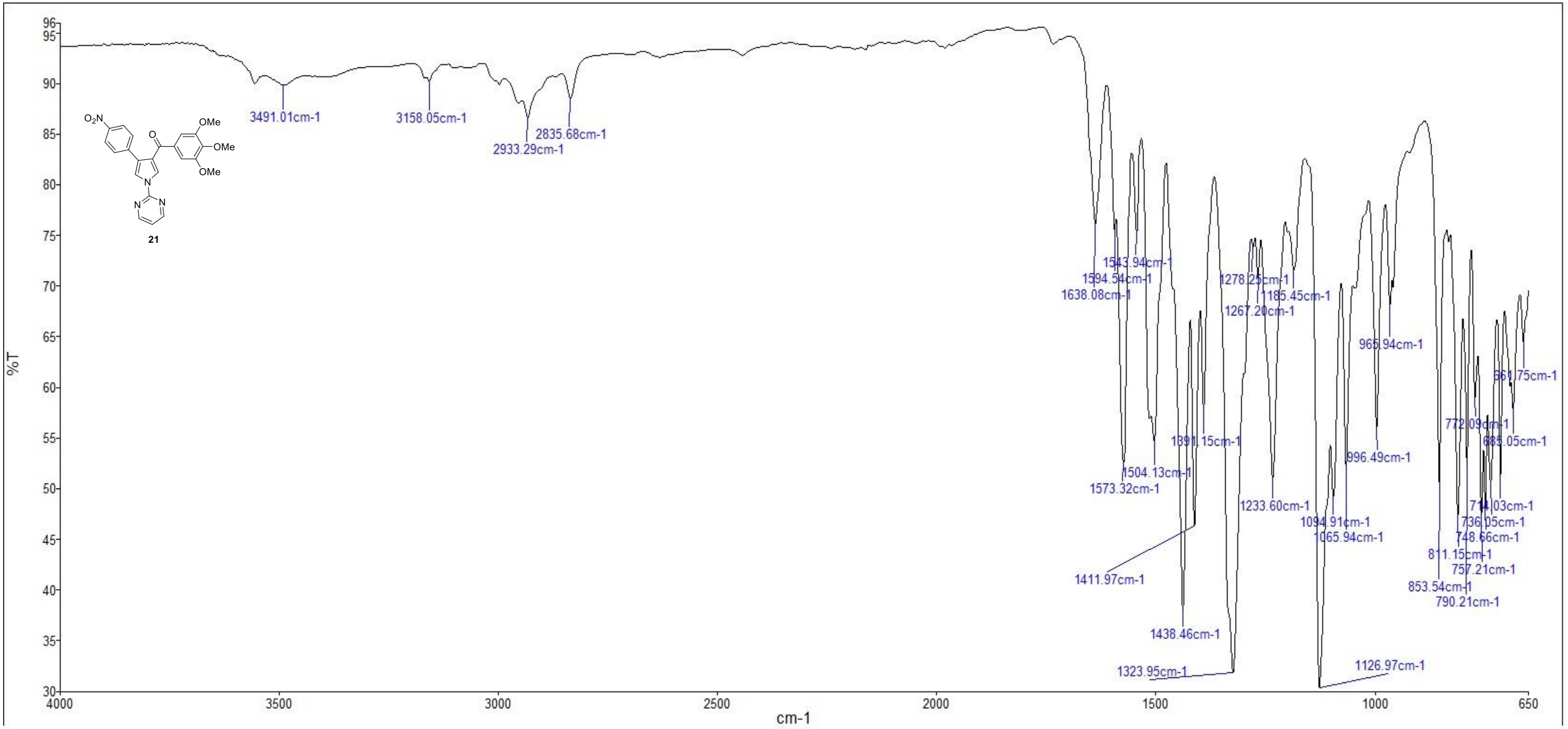
%T
cm-1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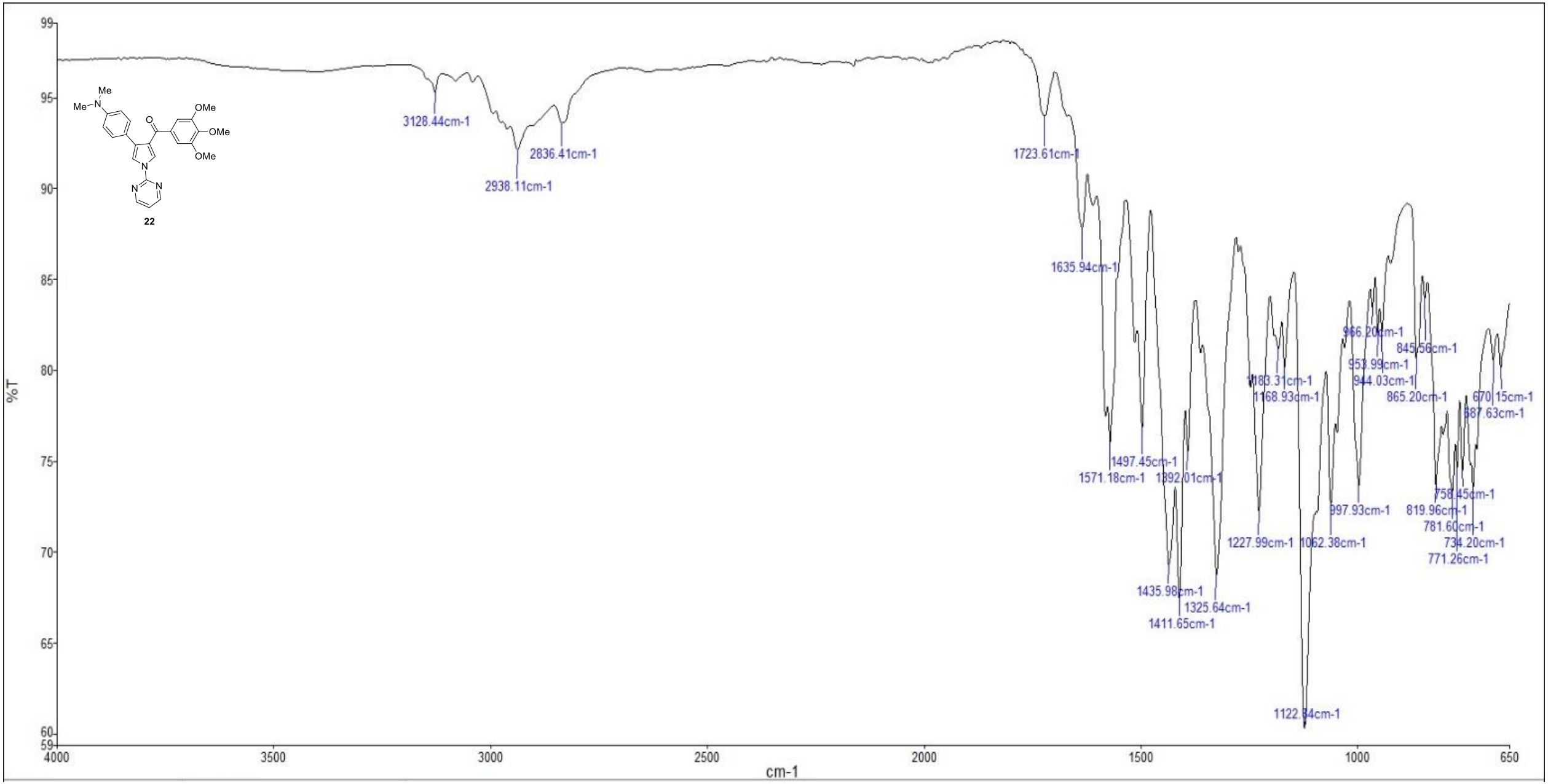
1438.46cm-1
1391.15cm-1
1323.95cm-1
1278.25cm-1
1267.20cm-1
1185.45cm-1
1233.60cm-1
1126.97cm-1
1094.91cm-1
1065.94cm-1
996.49cm-1
965.94cm-1
853.54cm-1
811.15cm-1
790.21cm-1
772.09cm-1
757.21cm-1
748.66cm-1
736.05cm-1
714.03cm-1
685.05cm-1
661.75cm-1
%T
cm-1
4000
3500
3000
2500
2000
1500
1000
650
96
95
90
85
80
75
70
65
60
55
50
45
40
35
30


22
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1571.18cm-1
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1435.98cm-1
1411.65cm-1
1392.01cm-1
1325.64cm-1
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1168.93cm-1
1122.84cm-1
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997.93cm-1
966.20cm-1
953.99cm-1
944.03cm-1
865.20cm-1
758.45cm-1
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670.15cm-1
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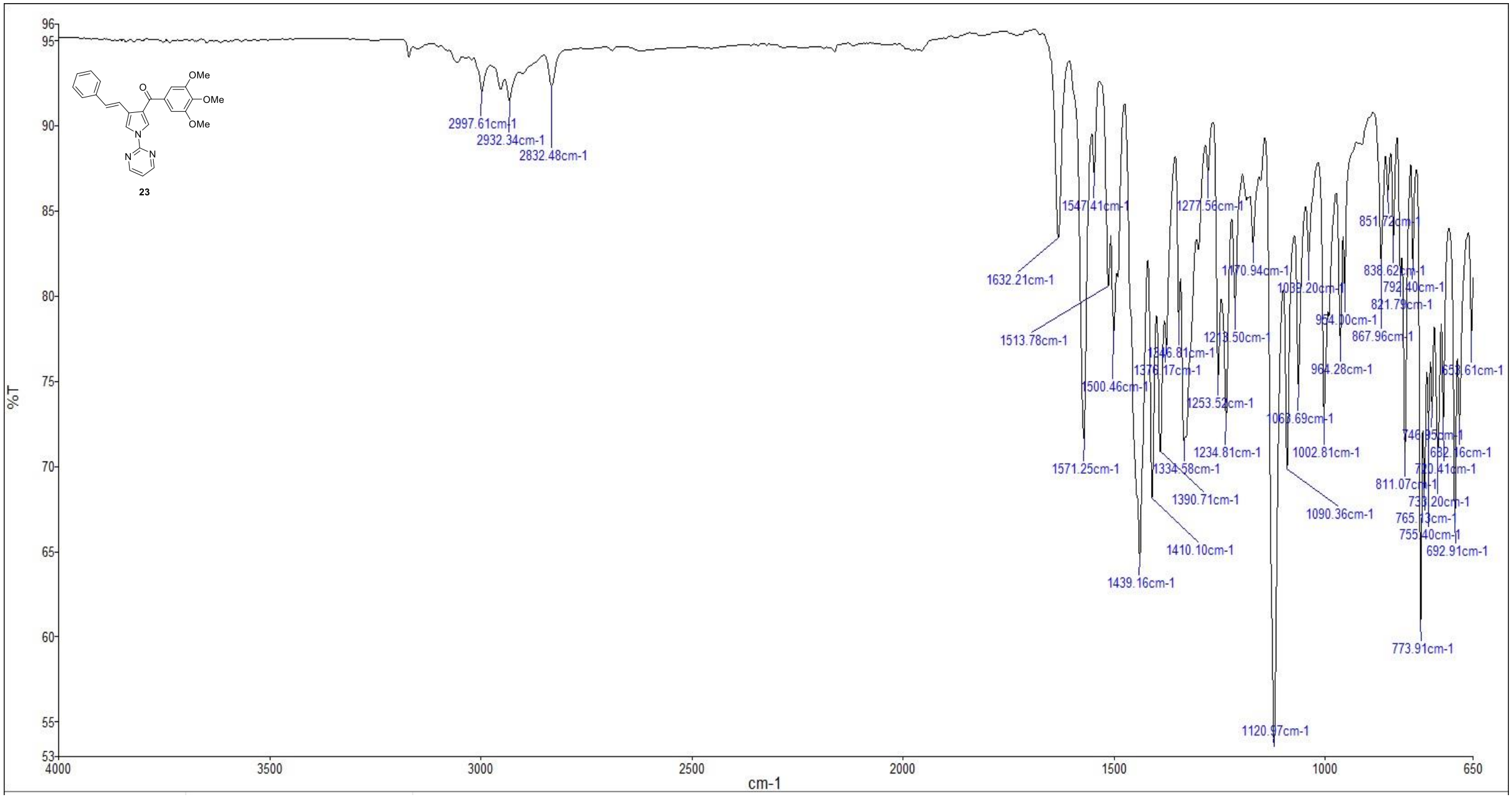
%T
cm-1


23
%T
cm-1
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1632.21cm-1
1547.41cm-1
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1571.25cm-1
1500.46cm-1
1439.16cm-1
1410.10cm-1
1390.71cm-1
1376.17cm-1
1346.81cm-1
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1234.81cm-1
1213.50cm-1
1170.94cm-1
1120.97cm-1
1090.36cm-1
1063.69cm-1
1033.20cm-1
1002.81cm-1
964.28cm-1
954.00cm-1
867.96cm-1
851.72cm-1
838.62cm-1
821.79cm-1
792.40cm-1
773.91cm-1
755.40cm-1
746.85cm-1
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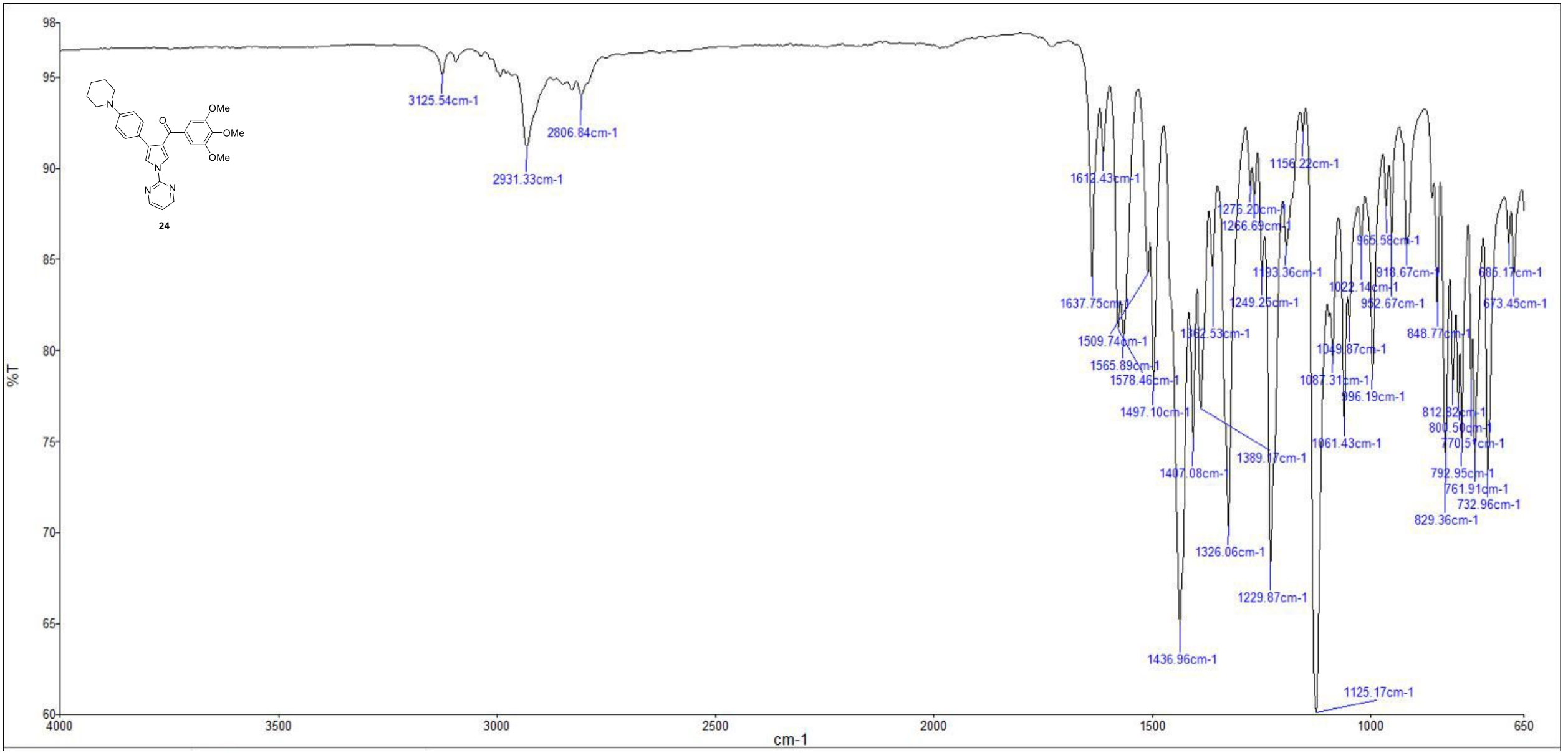
765.13cm-1


24
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1578.46cm-1
1497.10cm-1
1436.96cm-1
1407.08cm-1
1362.53cm-1
1326.06cm-1
1276.20cm-1
1266.69cm-1
1249.25cm-1
1229.87cm-1
1389.17cm-1
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1193.36cm-1
1125.17cm-1
1061.43cm-1
1087.31cm-1
1049.87cm-1
1022.14cm-1
996.19cm-1
965.58cm-1
952.67cm-1
918.67cm-1
848.77cm-1
829.36cm-1
812.32cm-1
800.50cm-1
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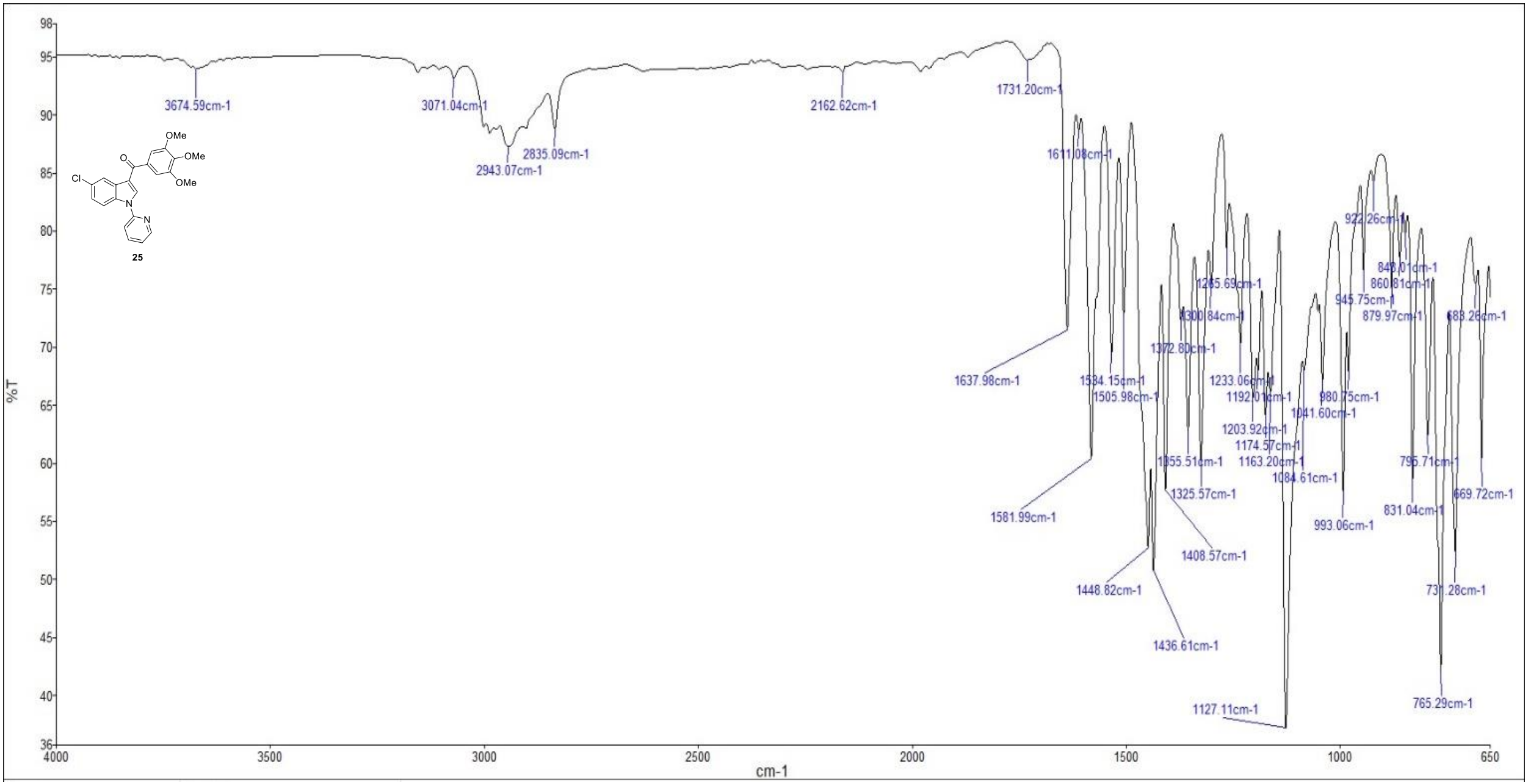
761.91cm-1
732.96cm-1
685.17cm-1
673.45cm-1
%T
cm-1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1448.82cm-1
1436.61cm-1
1408.57cm-1
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1355.51cm-1
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1300.84cm-1
1265.69cm-1
1233.06cm-1
1203.92cm-1
1192.01cm-1
1174.57cm-1
1163.20cm-1
1127.11cm-1
1084.61cm-1
1041.60cm-1
993.06cm-1
980.75cm-1
945.75cm-1
922.26cm-1
879.97cm-1
860.81cm-1
848.01cm-1
831.04cm-1
796.71cm-1
765.29cm-1
731.28cm-1
683.26cm-1
669.72cm-1
OMe
OMe
OMe
Cl
O
N
N
25
%T
cm-1
98
95
90
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70
65
60
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50
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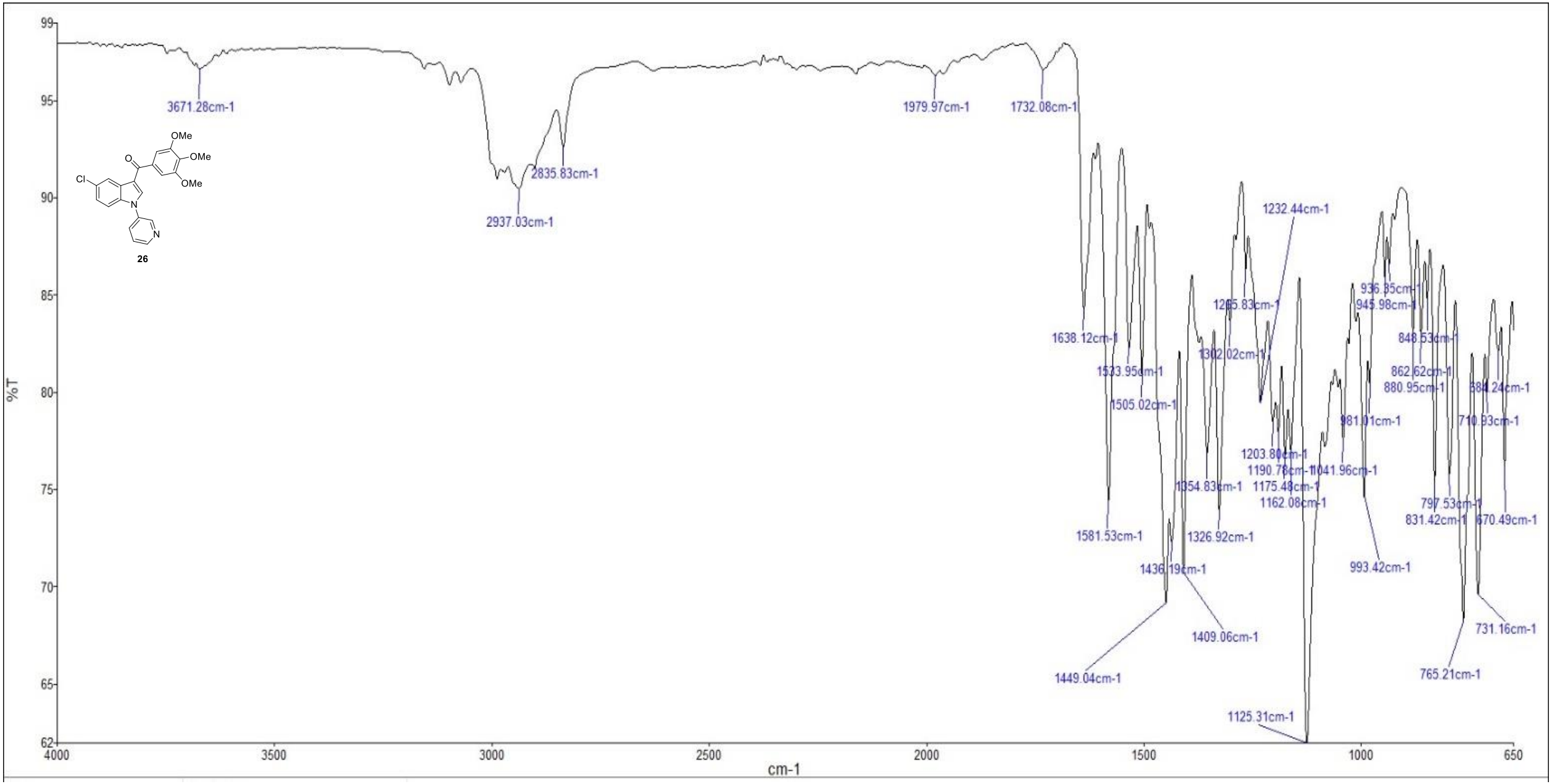
40
36
4000
3500
3000
2500
2000
1500
1000
650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1533.95cm-1
1505.02cm-1
1449.04cm-1
1436.19cm-1
1409.06cm-1
1354.83cm-1
1326.92cm-1
1302.02cm-1
1285.83cm-1
1232.44cm-1
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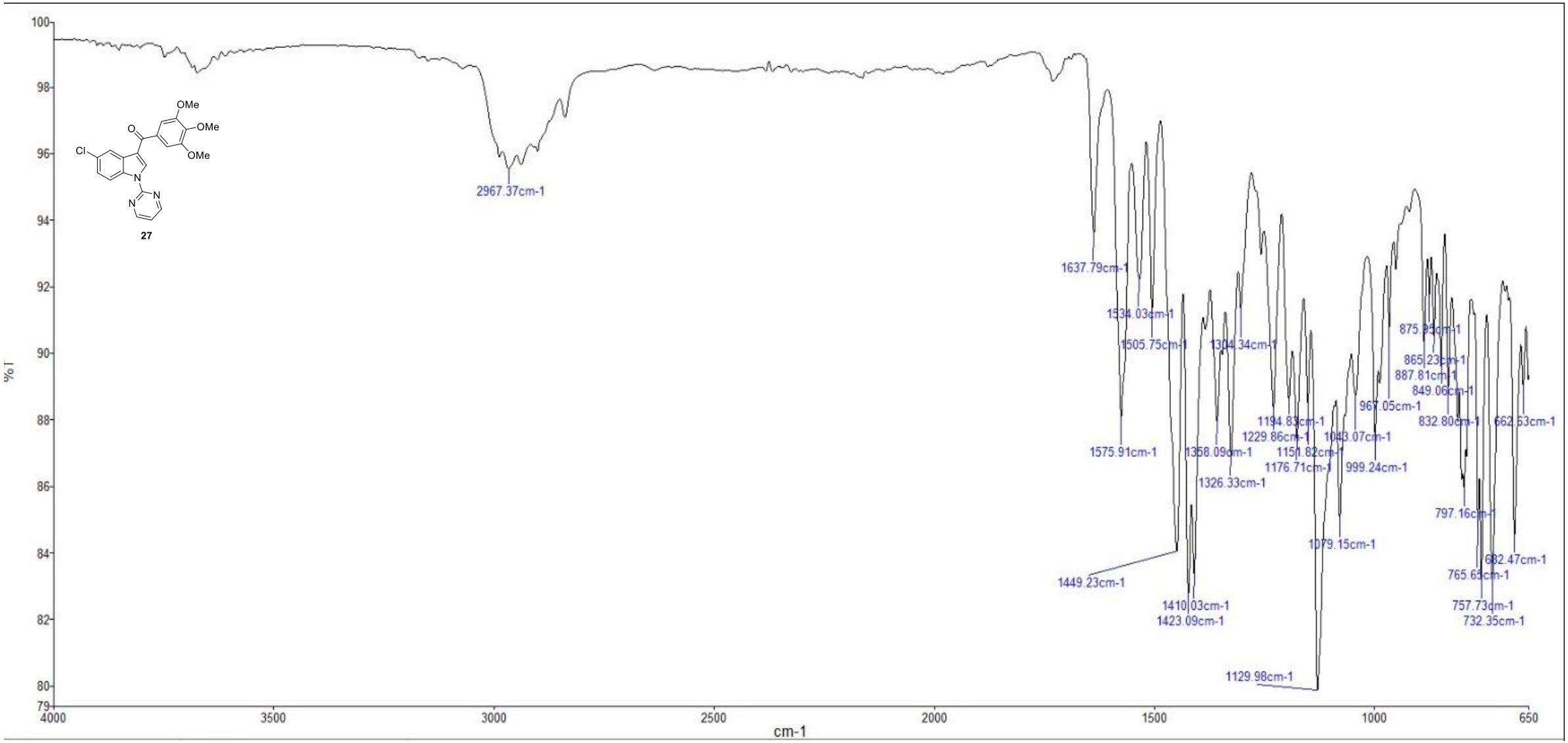
797.53cm-1
765.21cm-1
731.16cm-1
710.93cm-1
670.49cm-1
%T
cm-1
99
95
90
85
80
75
70
65
62
4000
3500
3000
2500
2000
1500
1000
650
OMe
OMe
OMe
O
Cl
N
N
26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OMe
OMe
O
Cl
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N
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999.24cm-1
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682.47cm-1
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765.65cm-1
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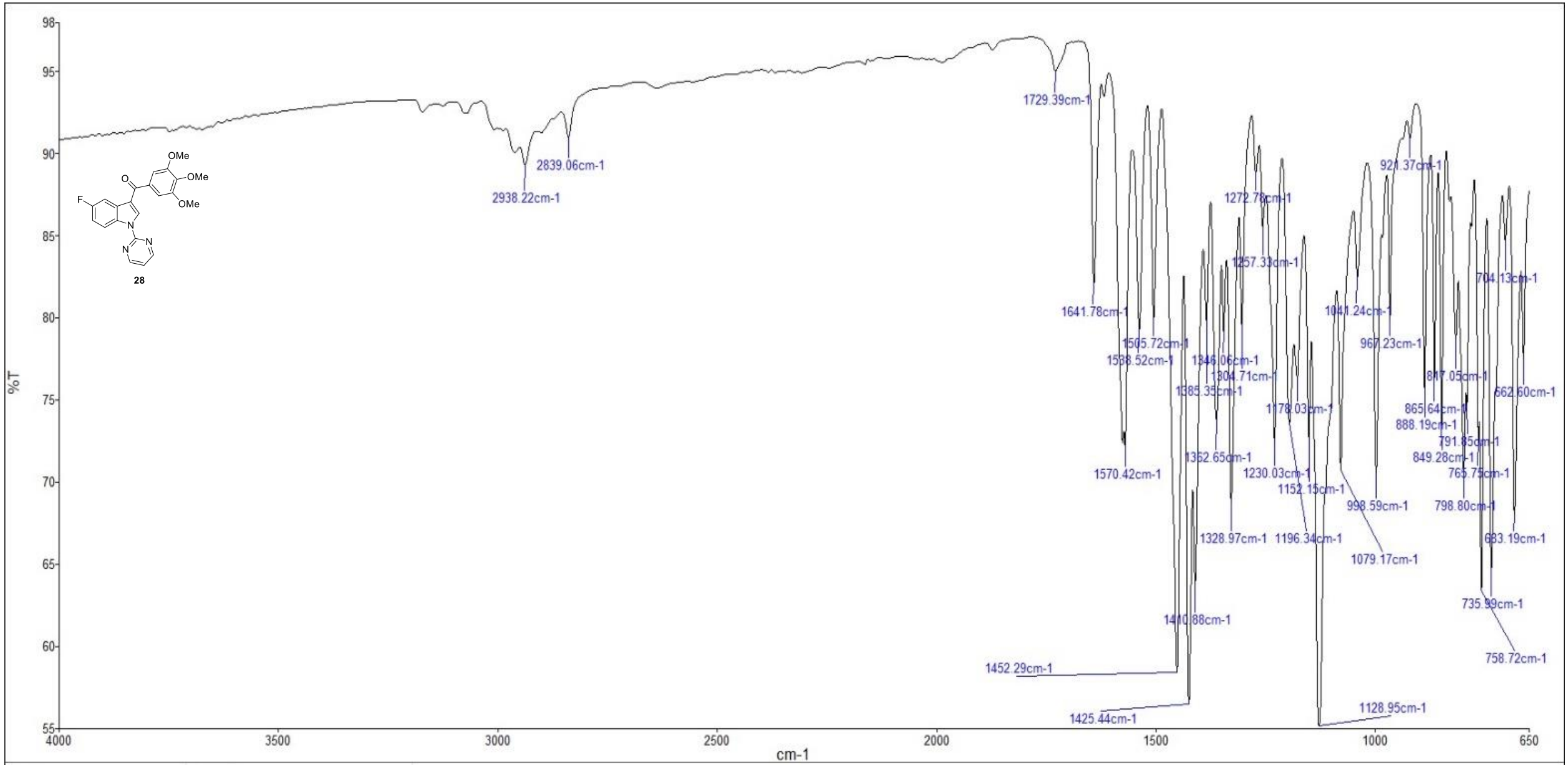
757.73cm-1
1423.09cm-1
732.35cm-1
1129.98cm-1
100
98
96
94
92
90
88
86
84
82
80
79
%T
4000
3500
3000
2500
2000
1500
1000
650
cm-1


28
%T
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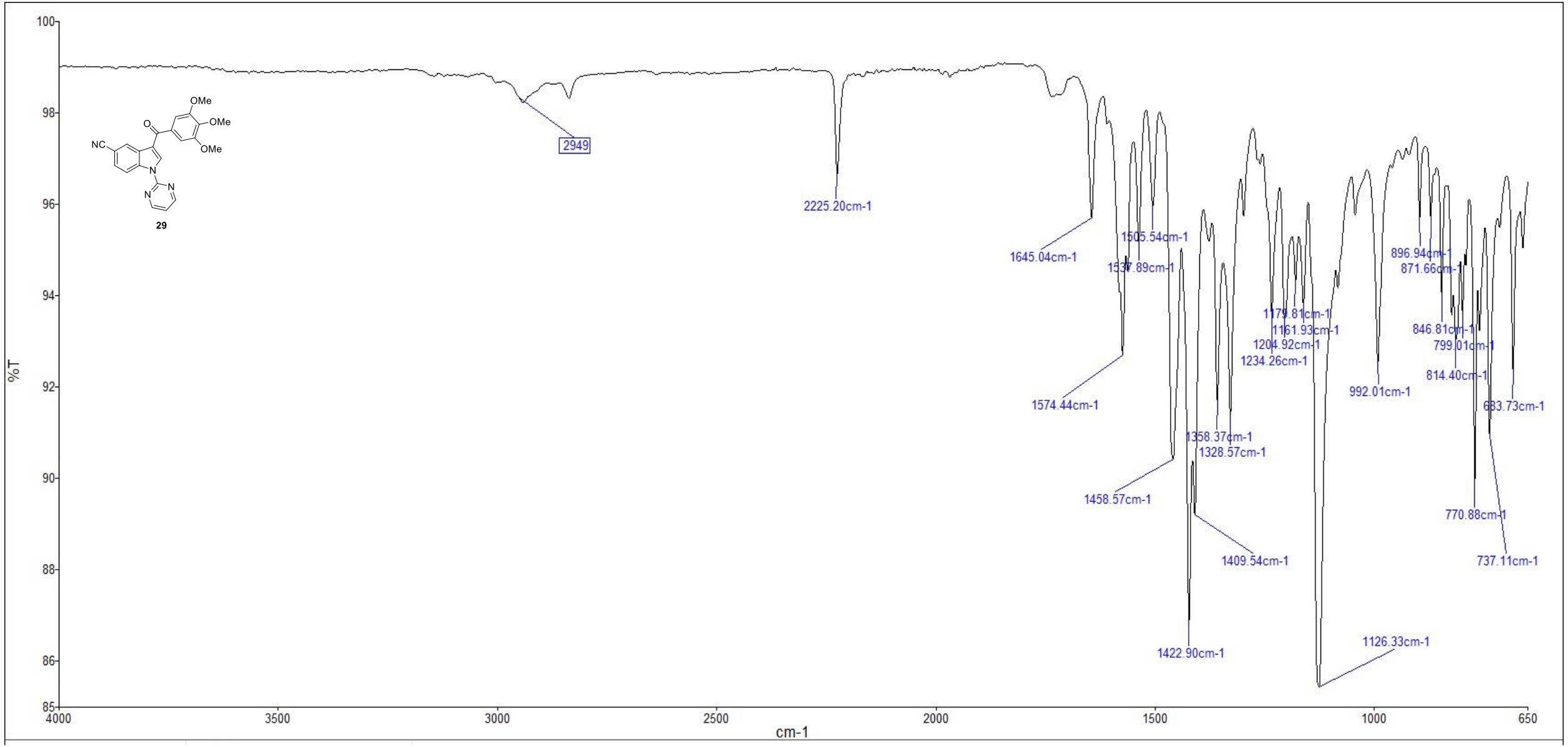
29
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1234.26cm-1
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683.73cm-1
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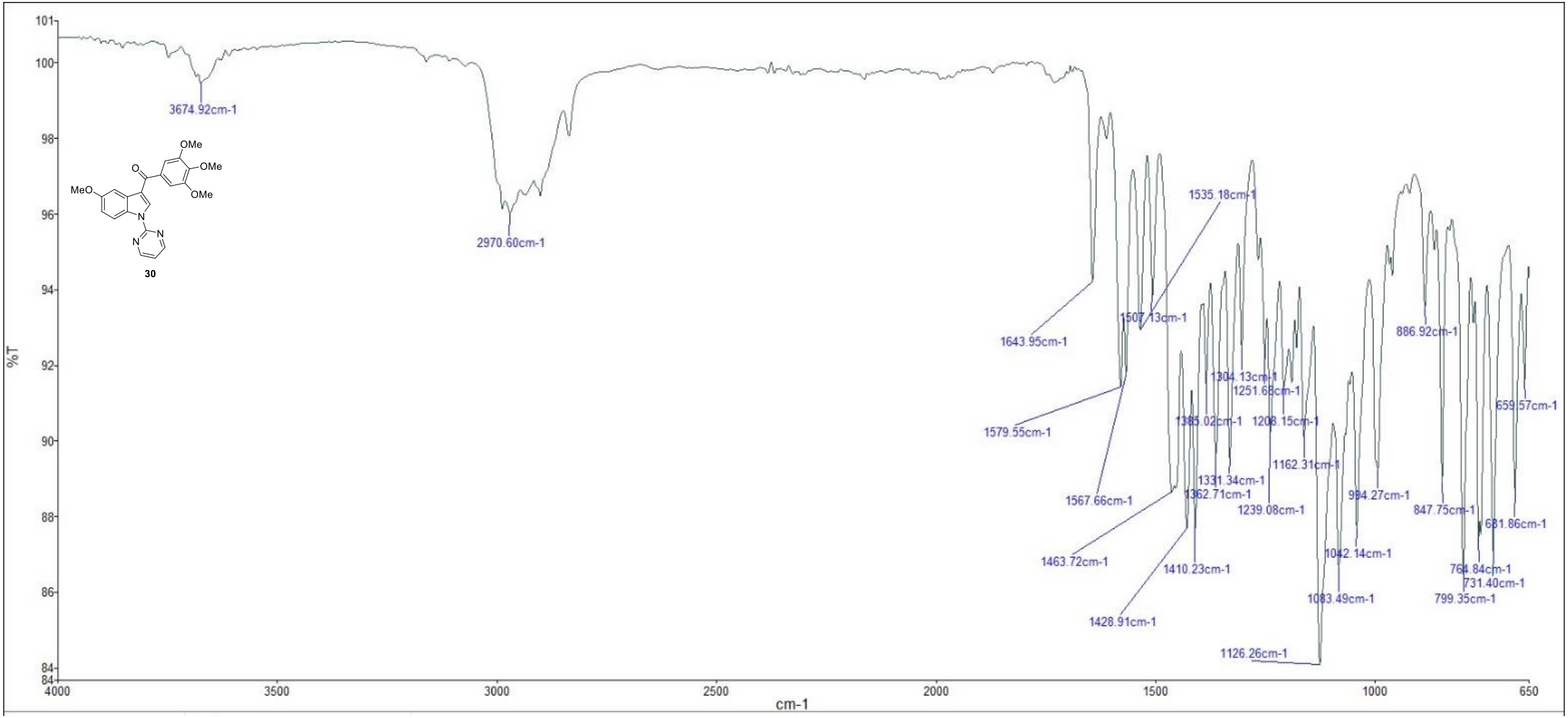
cm-1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1304.13cm-1
1251.68cm-1
1239.08cm-1
1208.15cm-1
1162.31cm-1
1126.26cm-1
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886.92cm-1
847.75cm-1
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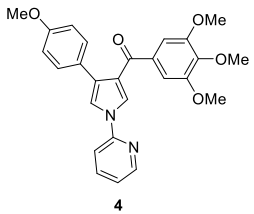
731.40cm-1
681.86cm-1
659.57cm-1
%T
cm-1
4000
3500
3000
2500
2000
1500
1000
650
101
100
98
96
94
92
90
88
86
84
OMe
OMe
OMe
MeO
O
N
N
N
30

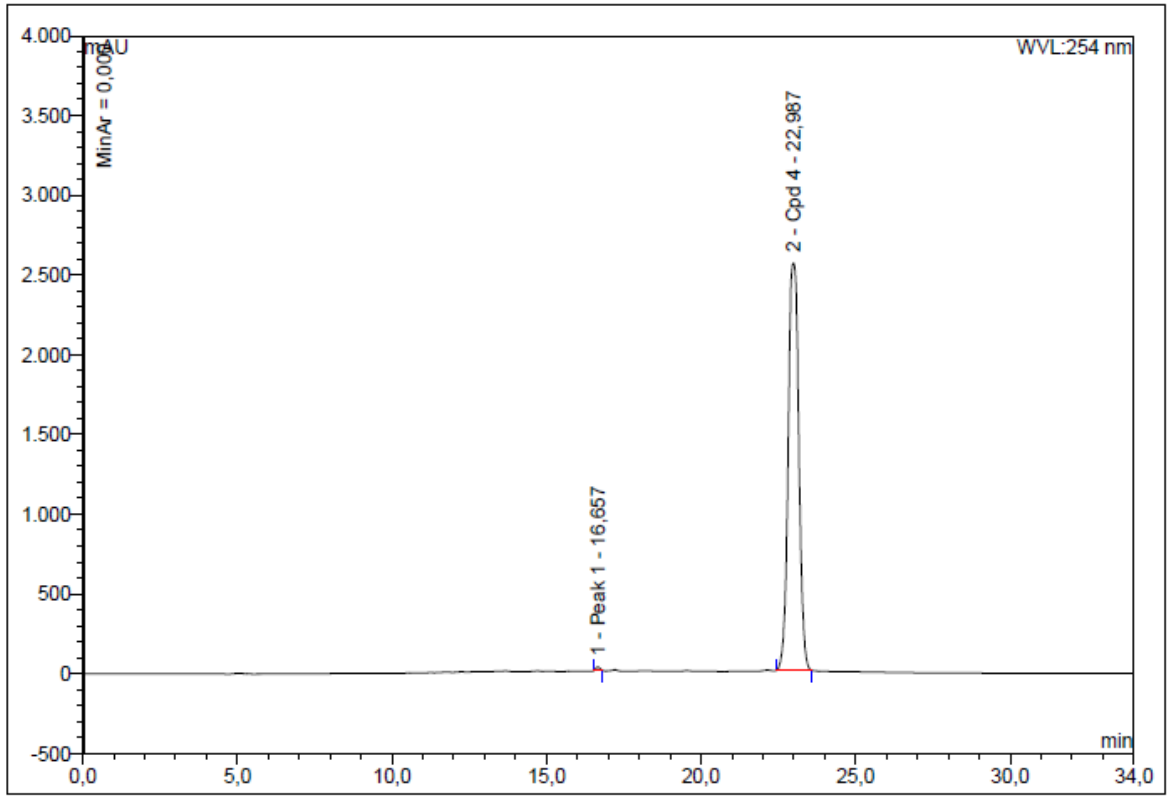
HPLC Chromatograms of Compounds **4**, **14**, **15**, **18**, **20**, **22** and **24**



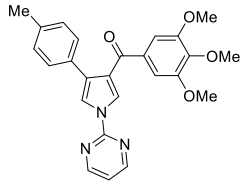
4

Cpd 4

Sample Name:	**Cpd 4**	*Injection Volume:*	**20,0**
Vial Number:	**22**	*Channel:*	**UV_VIS_3**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:		*Bandwidth:*	**4**
Quantif. Method:	**default_0_05**	*Dilution Factor:*	**1,0000**
Run Time (min):	**34,00**	*Sample Weight:*	**1,0000**
		Sample Amount:	**1,0000**



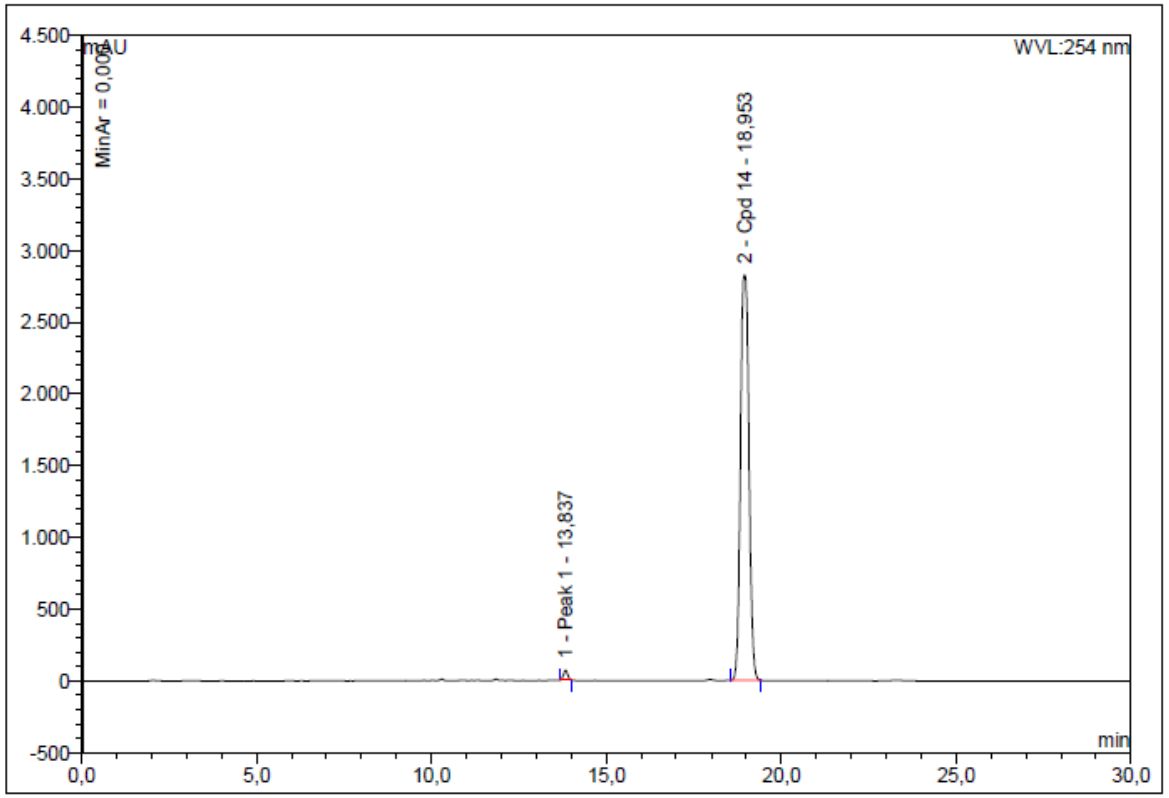
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16,66	Peak 1	24,048	3,637	0,36	n.a.	BM *^
2	22,99	Cpd 4	2554,339	1018,404	99,64	n.a.	BMB*
Total:			2578,388	1022,040	100,00	0,000	



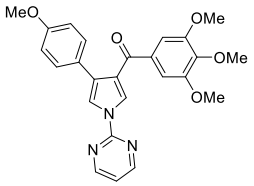
14

Cpd 14

Sample Name:	**Cpd 14**	*Injection Volume:*	**20,0**
Vial Number:	**53**	*Channel:*	**UV_VIS_3**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:		*Bandwidth:*	**4**
Quantif. Method:	**default_0_05**	*Dilution Factor:*	**1,0000**
Run Time (min):	**34,00**	*Sample Weight:*	**1,0000**
		Sample Amount:	**1,0000**



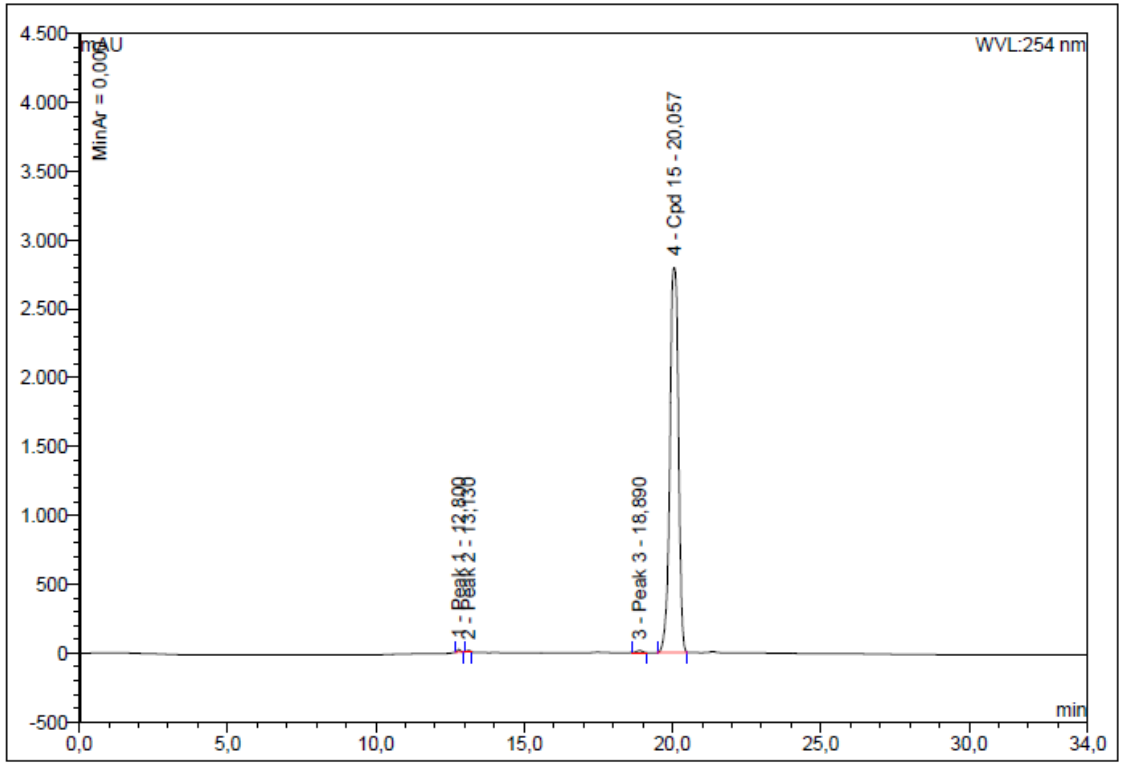
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13,84	Peak 1	66,801	9,145	1,14	n.a.	BMB*^
2	18,95	Cpd 14	2827,333	793,189	98,86	n.a.	BMB*^
Total:			2894,135	802,334	100,00	0,000	



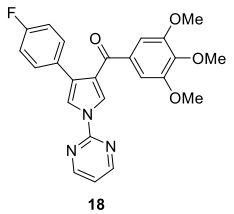
15

Cpd 15

Sample Name:	**Cpd 15**	*Injection Volume:*	**20,0**
Vial Number:	**29**	*Channel:*	**UV_VIS_3**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:		*Bandwidth:*	**4**
Quantif. Method:	**default_0_05**	*Dilution Factor:*	**1,0000**
Run Time (min):	**34,00**	*Sample Weight:*	**1,0000**
		Sample Amount:	**1,0000**



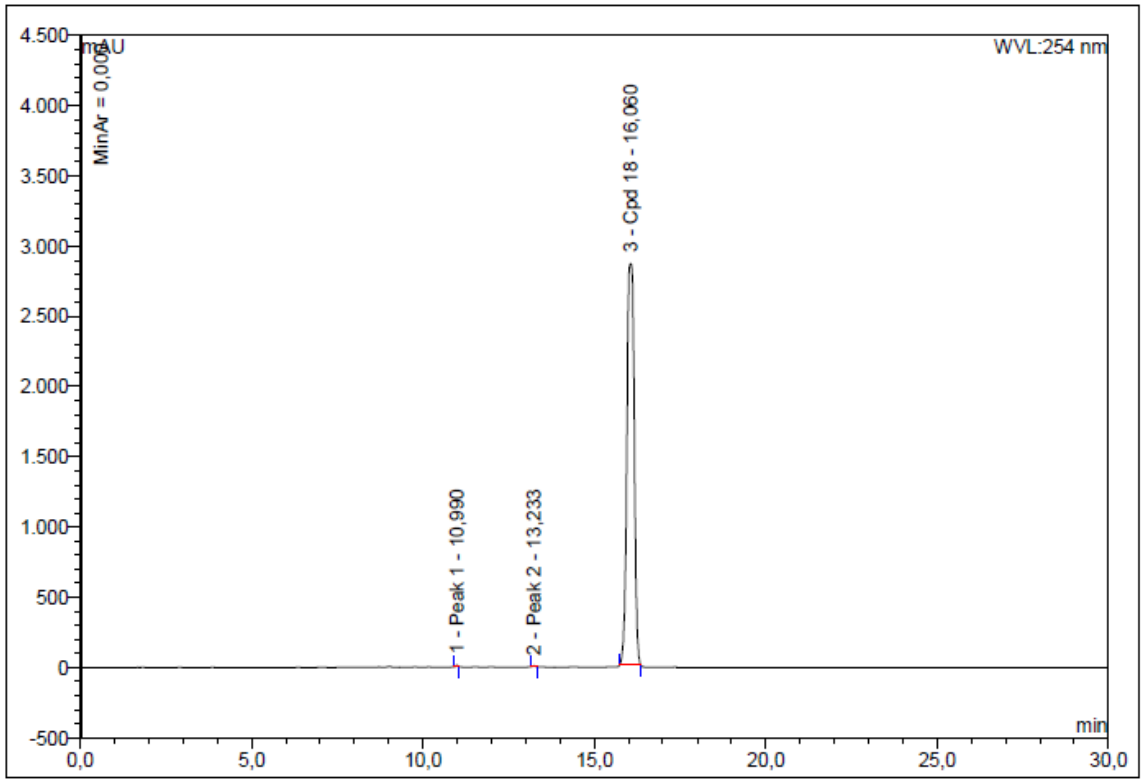
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12,80	Peak 1	19,435	2,288	0,24	n.a.	BMB*^
2	13,13	Peak 2	11,621	1,247	0,13	n.a.	BMB*^
3	18,89	Peak 3	15,285	3,348	0,35	n.a.	BMB*^
4	20,06	Cpd 15	2797,019	938,075	99,27	n.a.	BMB*
Total:			2843,361	944,958	100,00	0,000	



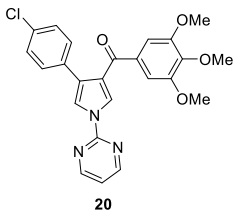
18

Cpd 18

Sample Name:	**Cpd 18**	*Injection Volume:*	**20,0**
Vial Number:	**53**	*Channel:*	**UV_VIS_3**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:		*Bandwidth:*	**4**
Quantif. Method:	**default_0_05**	*Dilution Factor:*	**1,0000**
Run Time (min):	**30,00**	*Sample Weight:*	**1,0000**
		Sample Amount:	**1,0000**



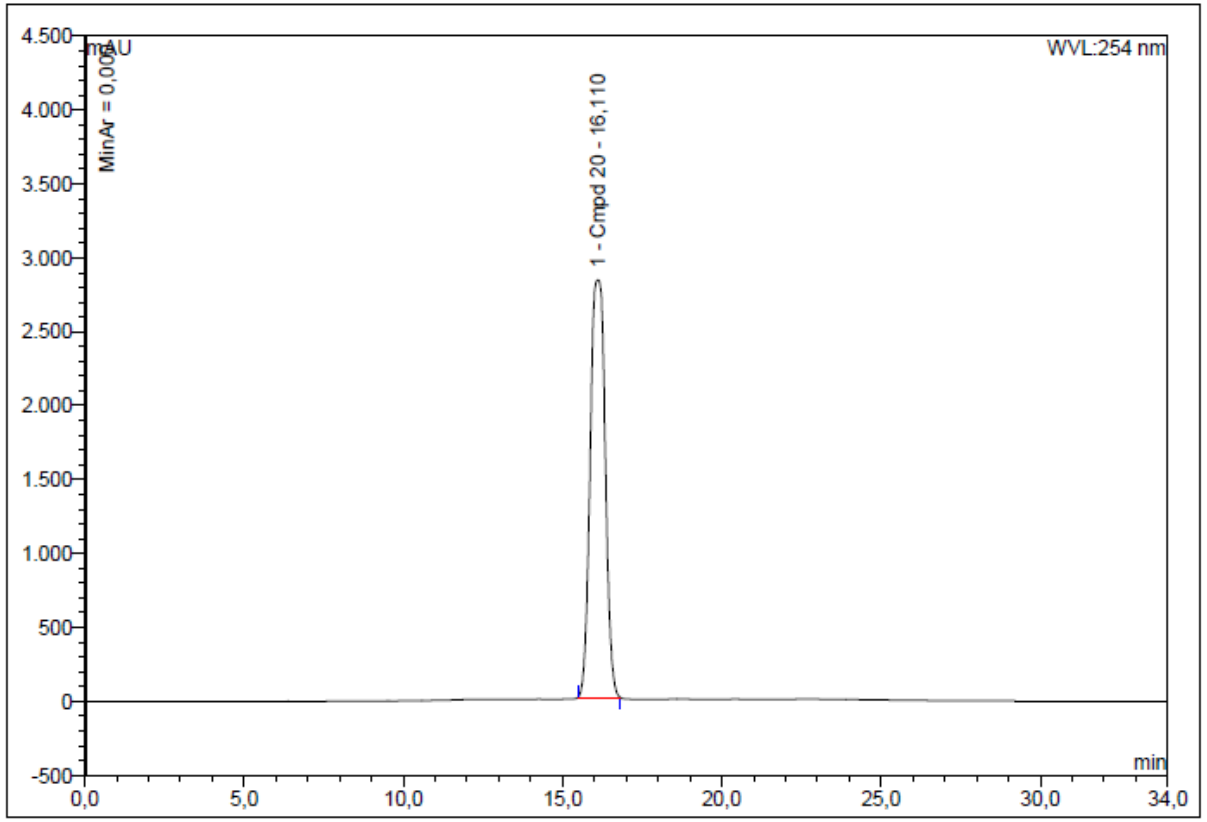
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10,99	Peak 1	10,376	0,773	0,11	n.a.	BMB*^
2	13,23	Peak 2	4,346	0,388	0,05	n.a.	BMB*^
3	16,06	Cpd 18	2857,142	708,472	99,84	n.a.	BMB*^
Total:			2871,864	709,633	100,00	0,000	



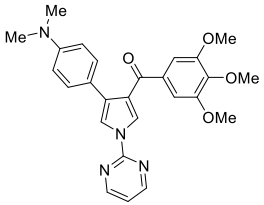
20

Cpd 20

Sample Name:	**Cpd 20**	*Injection Volume:*	**20,0**
Vial Number:	**41**	*Channel:*	**UV_VIS_3**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:		*Bandwidth:*	**4**
Quantif. Method:	**default_0_05**	*Dilution Factor:*	**1,0000**
Run Time (min):	**34,00**	*Sample Weight:*	**1,0000**
		Sample Amount:	**1,0000**



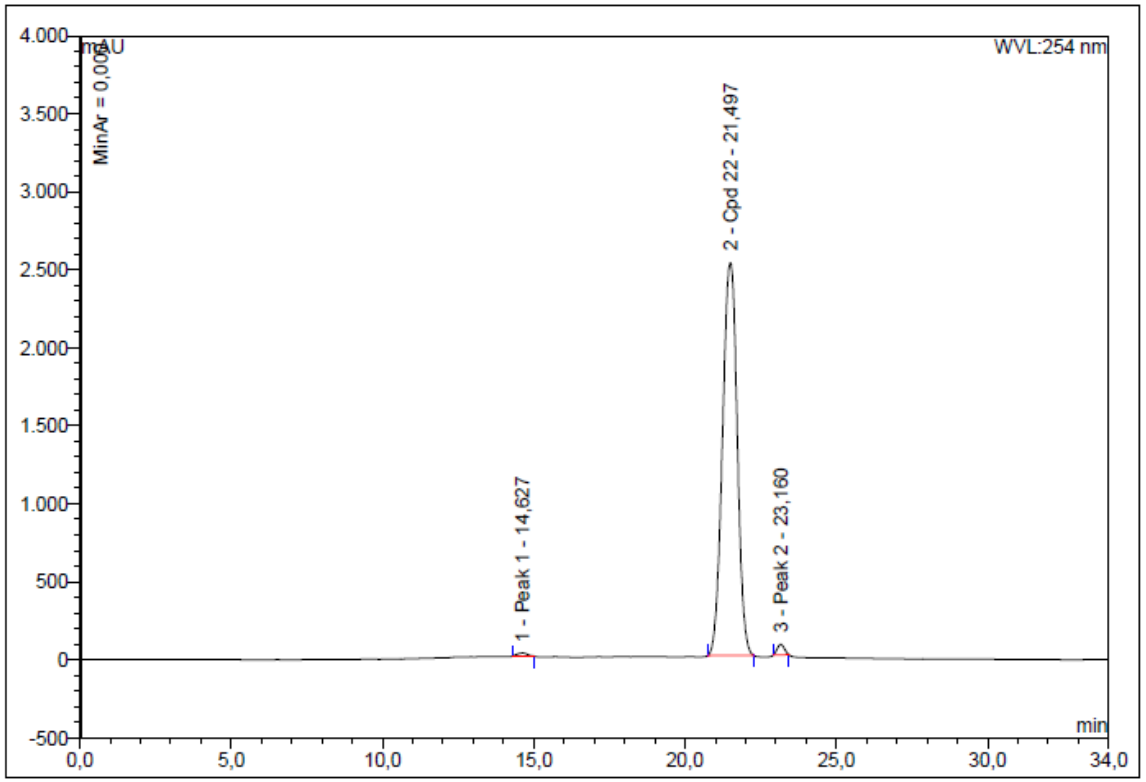
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16,11	Cmpd 20	2822,964	1543,254	100,00	n.a.	BMB*
Total:			2822,964	1543,254	100,00	0,000	



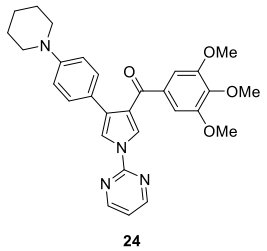
22

Cpd 22

Sample Name:	**Cpd 22**	*Injection Volume:*	**20,0**
Vial Number:	**25**	*Channel:*	**UV_VIS_3**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:		*Bandwidth:*	**4**
Quantif. Method:	**default_0_05**	*Dilution Factor:*	**1,0000**
Run Time (min):	**34,00**	*Sample Weight:*	**1,0000**
		Sample Amount:	**1,0000**



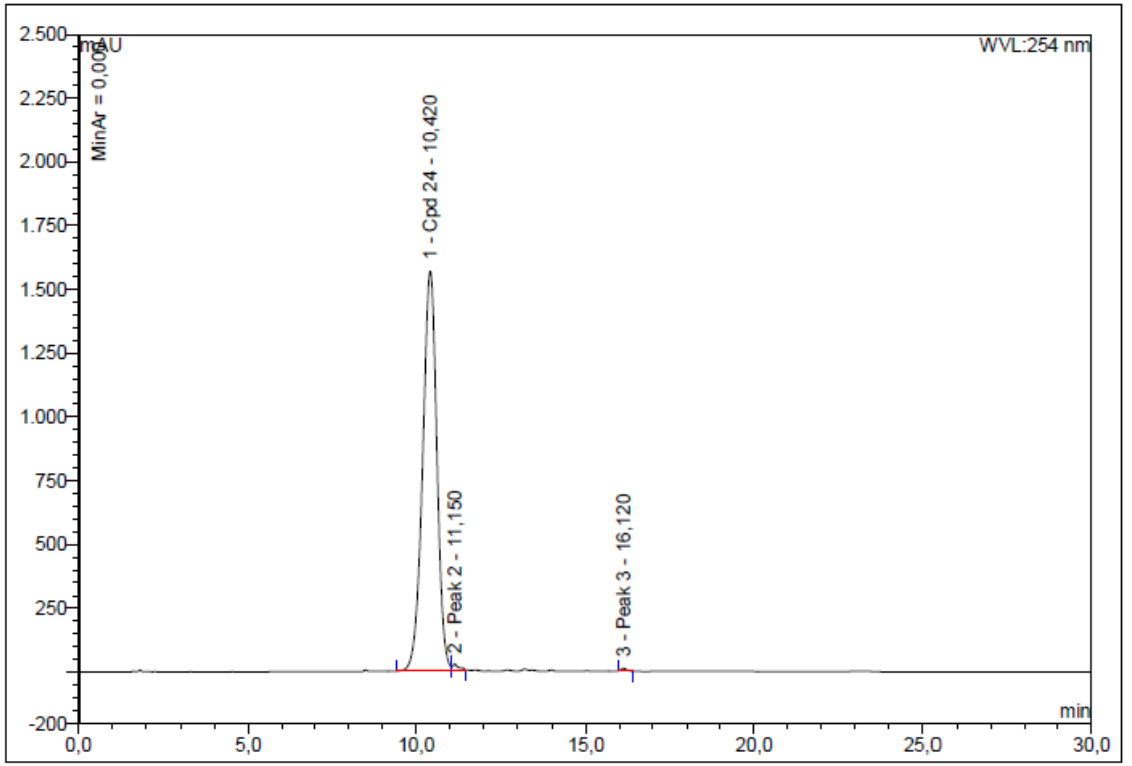
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	14,63	Peak 1	21,719	8,777	0,61	n.a.	BMB*^
2	21,50	Cpd 22	2516,590	1417,760	98,13	n.a.	BMB*^
3	23,16	Peak 2	66,965	18,311	1,27	n.a.	BMB*^
Total:			2605,274	1444,848	100,00	0,000	



24

Cpd 24

Sample Name:	**Cpd 24**	*Injection Volume:*	**20,0**
Vial Number:	**55**	*Channel:*	**UV_VIS_3**
Sample Type:	**unknown**	*Wavelength:*	**254.0**
Control Program:		*Bandwidth:*	**4**
Quantif. Method:	**default_0_05**	*Dilution Factor:*	**1,0000**
Run Time (min):	**30,00**	*Sample Weight:*	**1,0000**
		Sample Amount:	**1,0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10,42	Cpd 24	1567,201	769,437	98,09	n.a.	BM *
2	11,15	Peak 2	27,614	6,519	0,83	n.a.	M *^
3	16,12	Peak 3	10,508	2,019	0,26	n.a.	BMB*^
Total:			1605,323	777,975	100,00	0,000	