

Development of new thiazolidine-2,4-dione hybrids as aldose reductase inhibitors endowed with antihyperglycemic activity: design, synthesis, biological investigations and in silico insights.

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Muhammad Yaseen (e-mail: muhammadyaseen.my907@gmail.com)

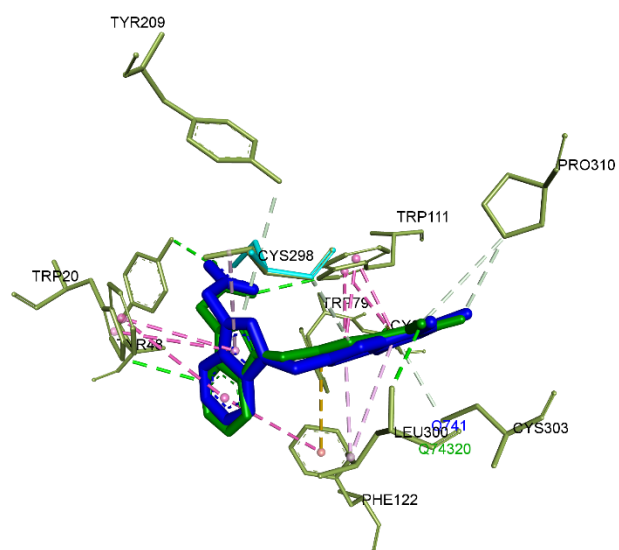
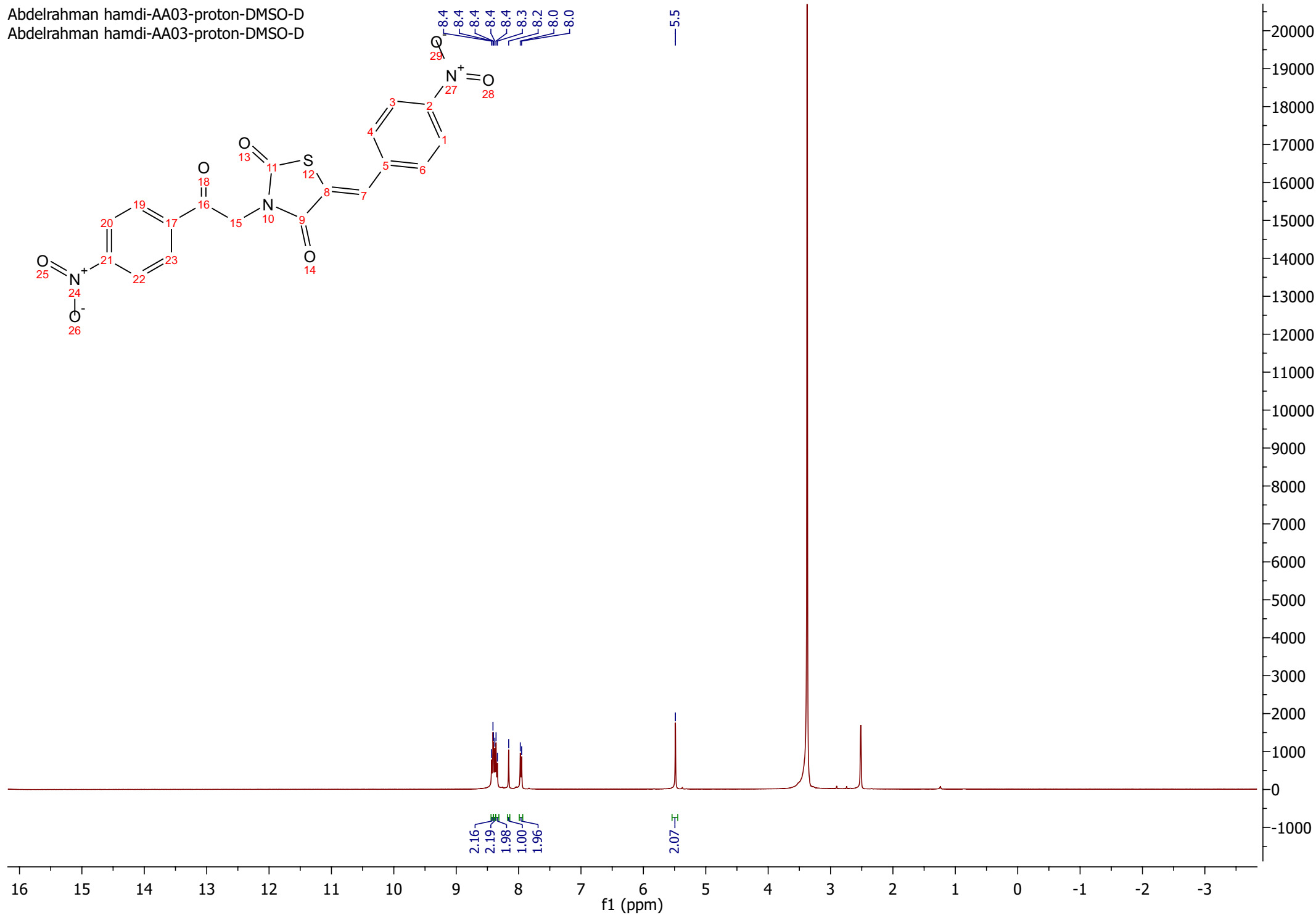
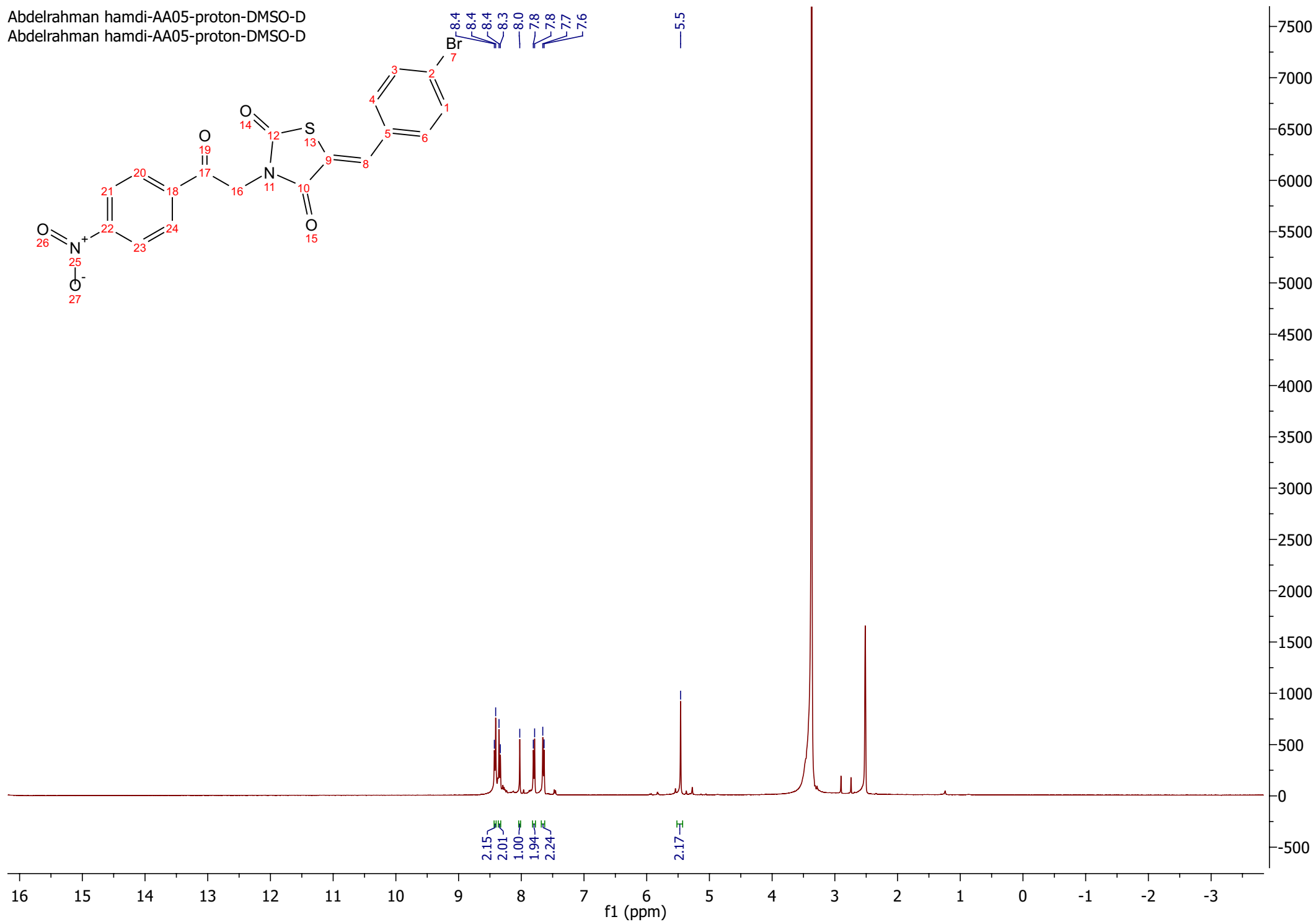


Fig.s1 Redocked co-crystallized ligand (blue) overlaid on the experimental pose (Green) showing RMSD=1.3 Å

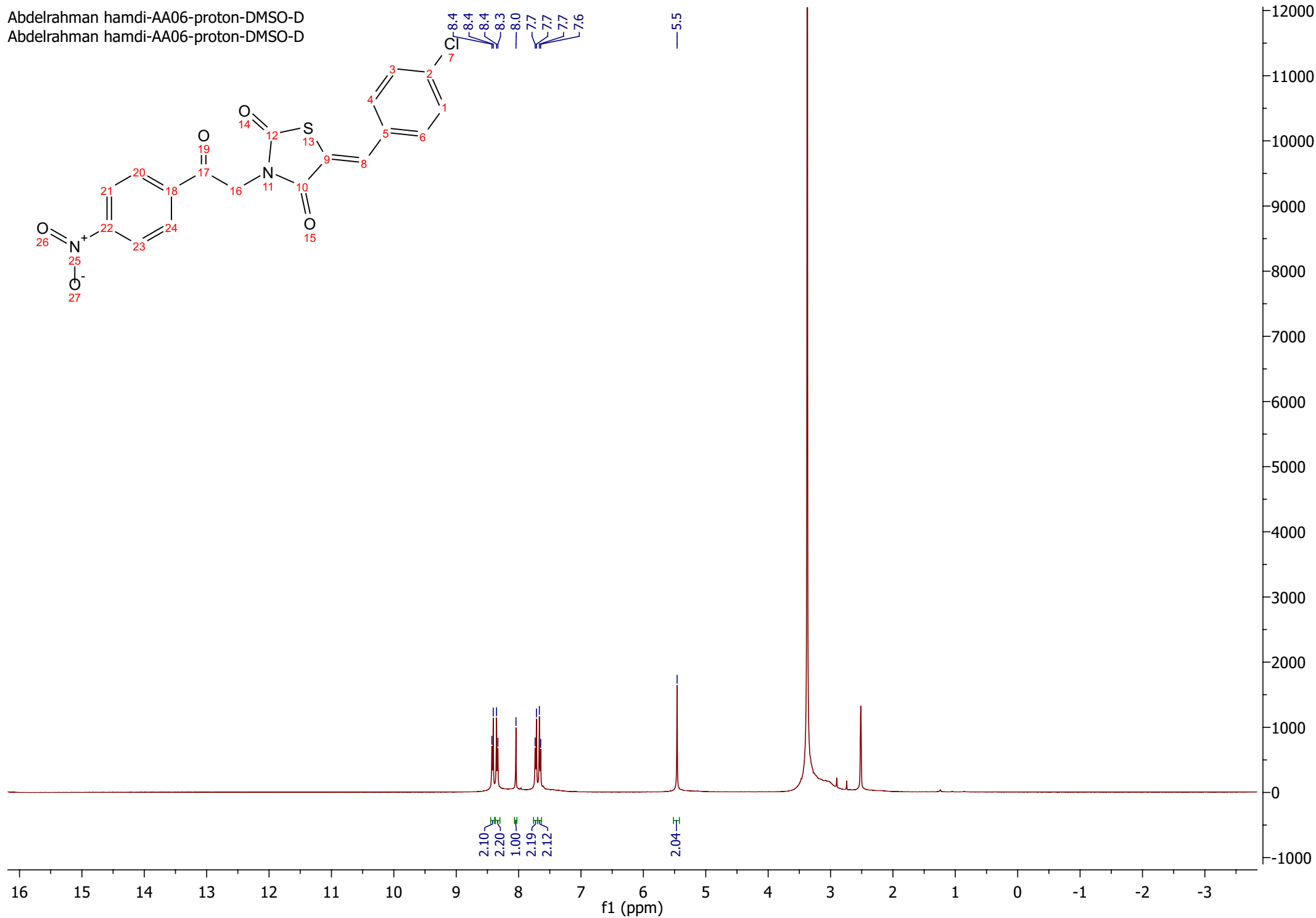
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Abdelrahman hamdi-AA03-proton-DMSO-D



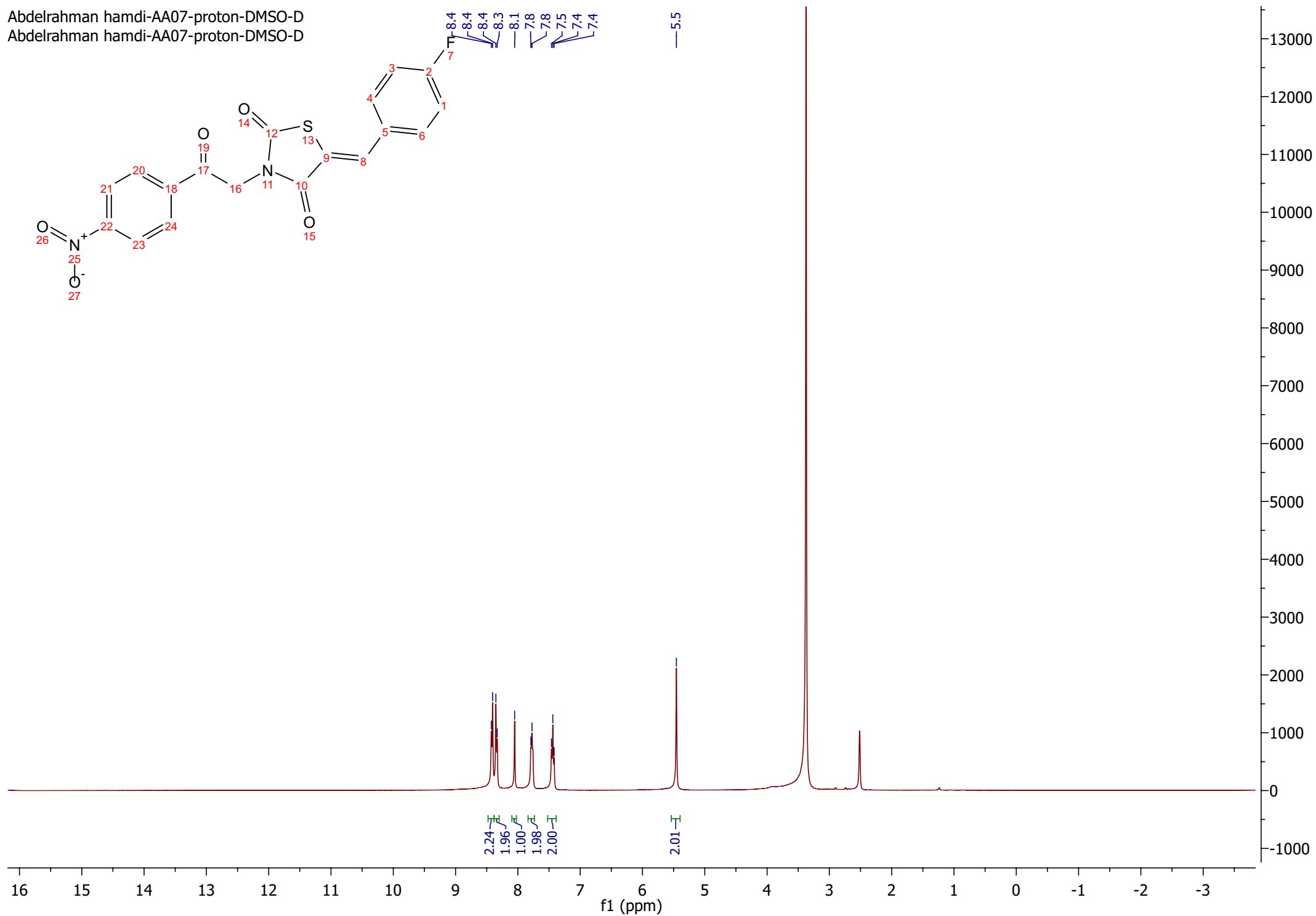
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Abdelrahman hamdi-AA05-proton-DMSO-D



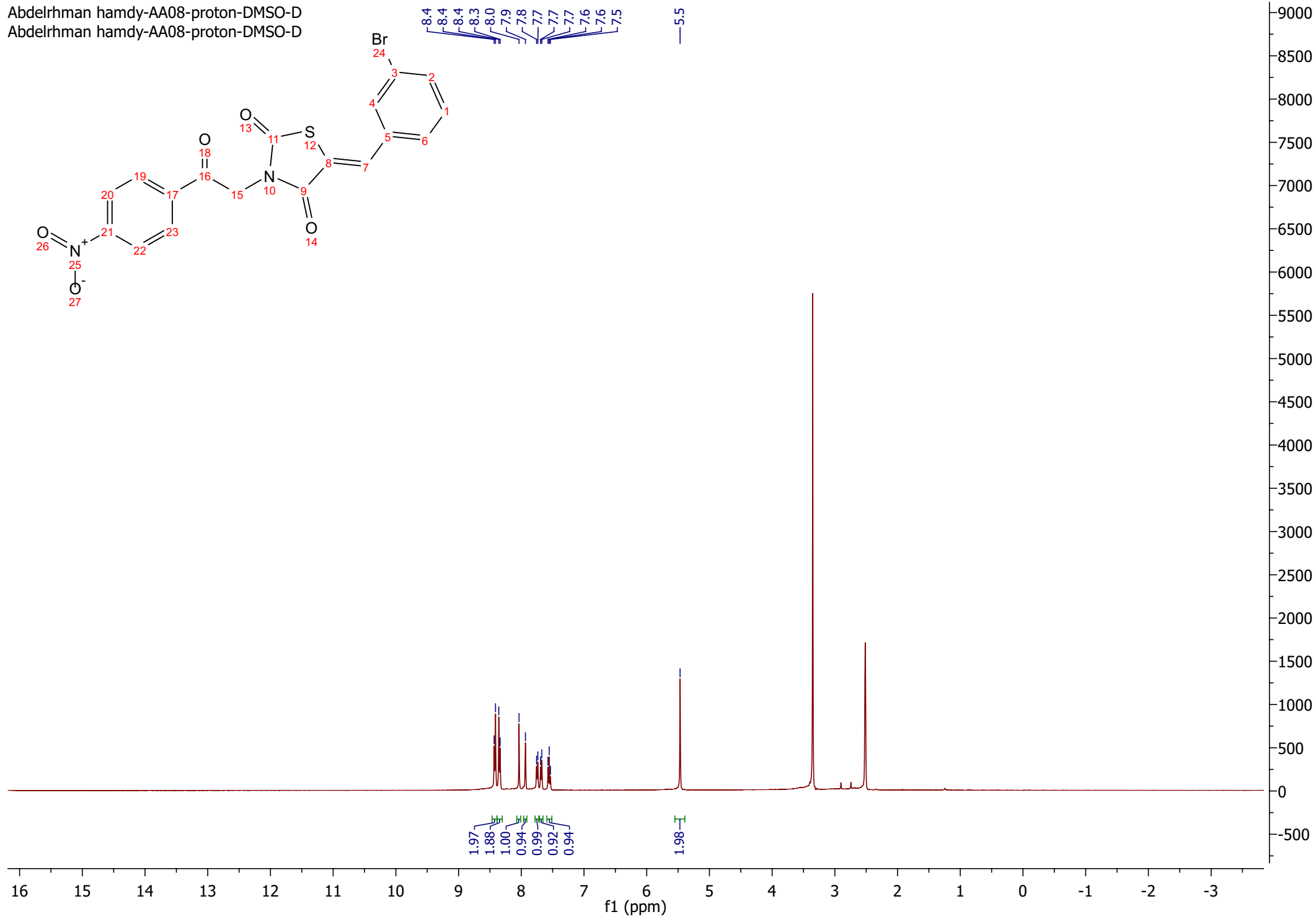
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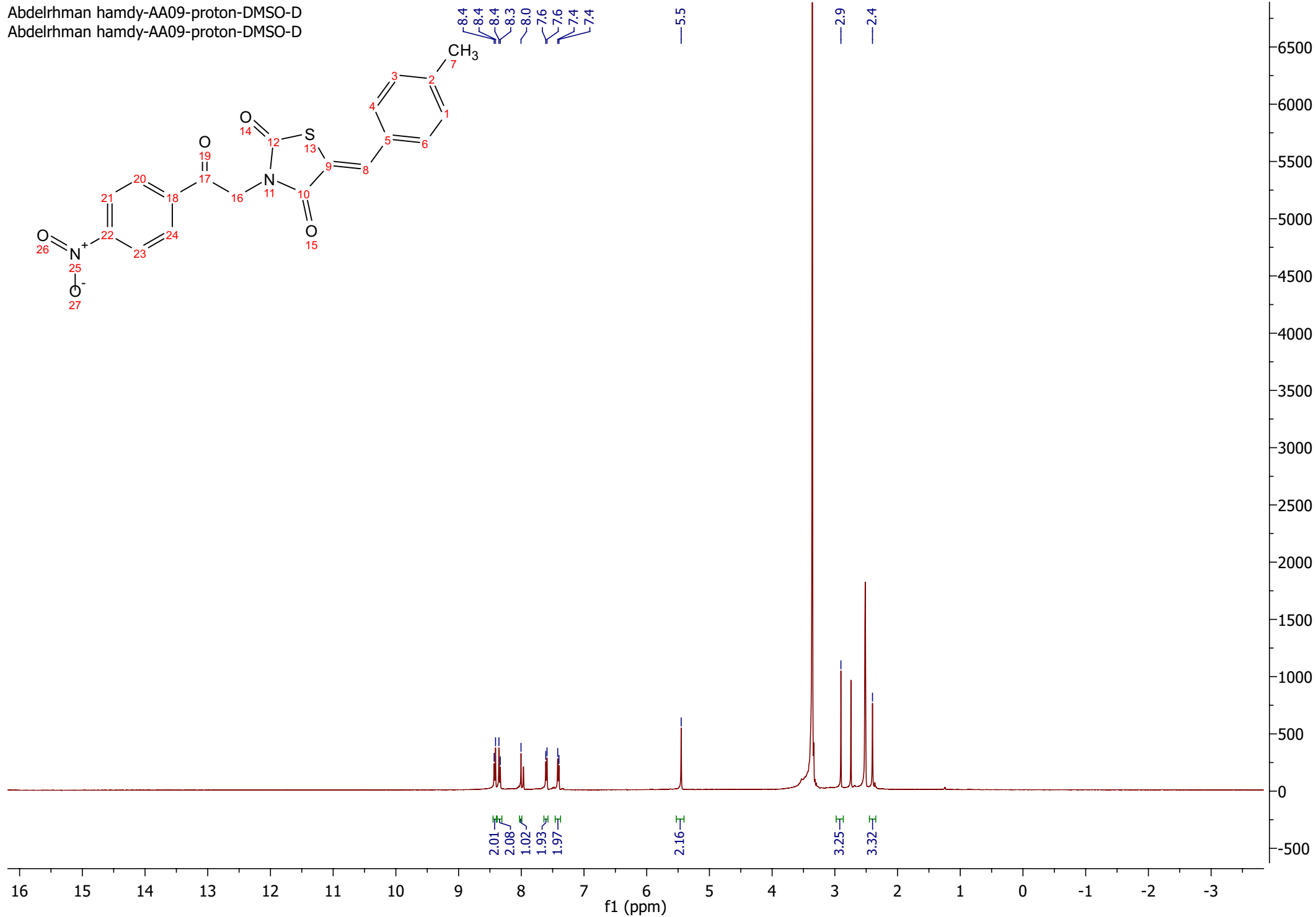
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Abdelrahman hamdi-AA07-proton-DMSO-D



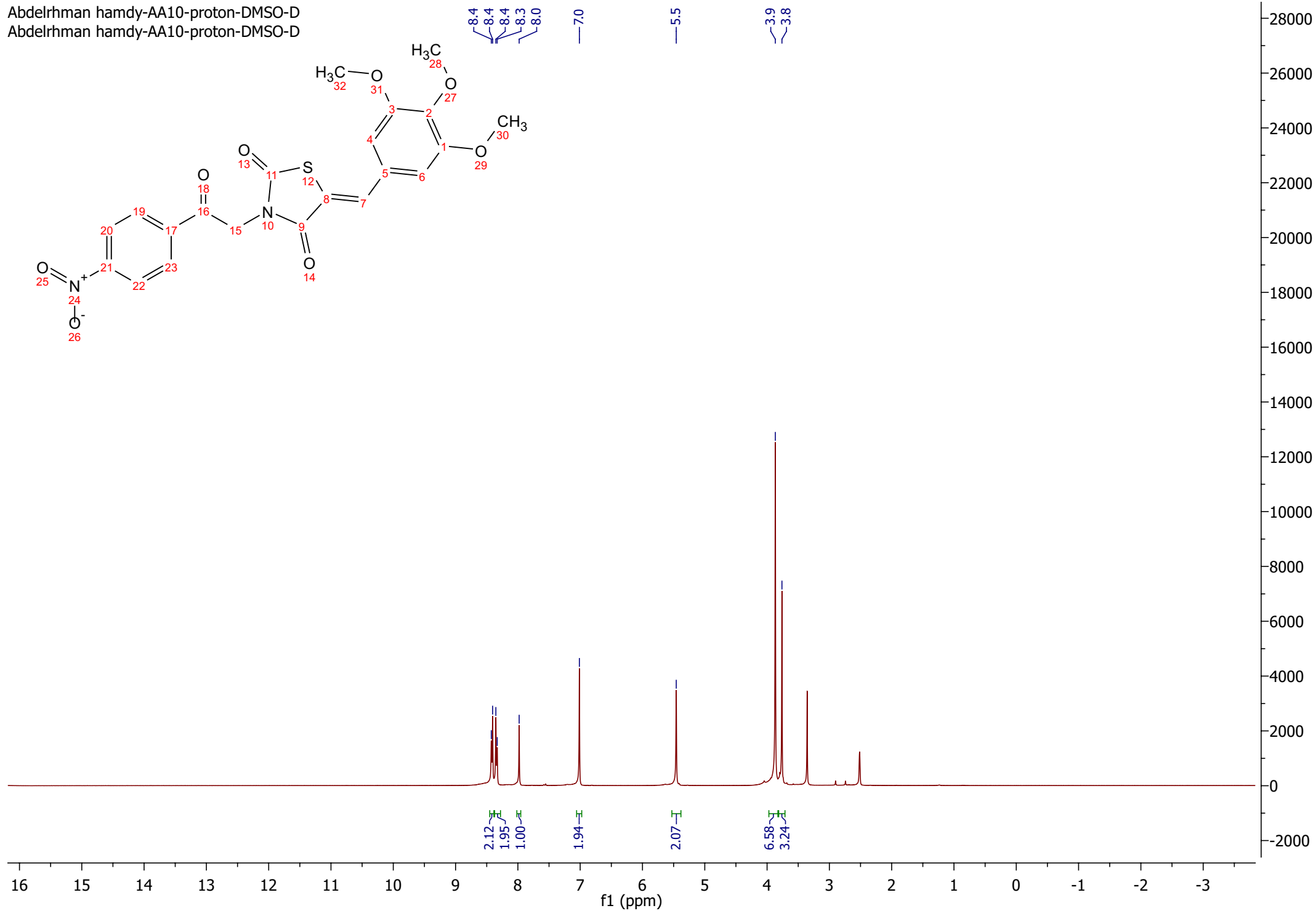
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Abdelrhman hamdy-AA08-proton-DMSO-D



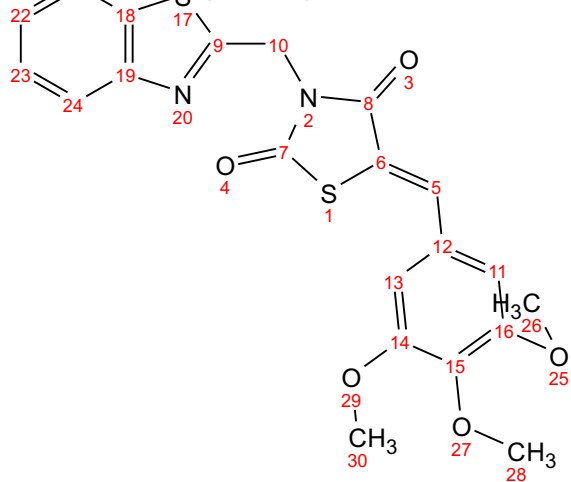
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Abdelrhman hamdy-AA09-proton-DMSO-D



Abdelrhman hamdy-AA10-proton-DMSO-D
Abdelrhman hamdy-AA10-proton-DMSO-D



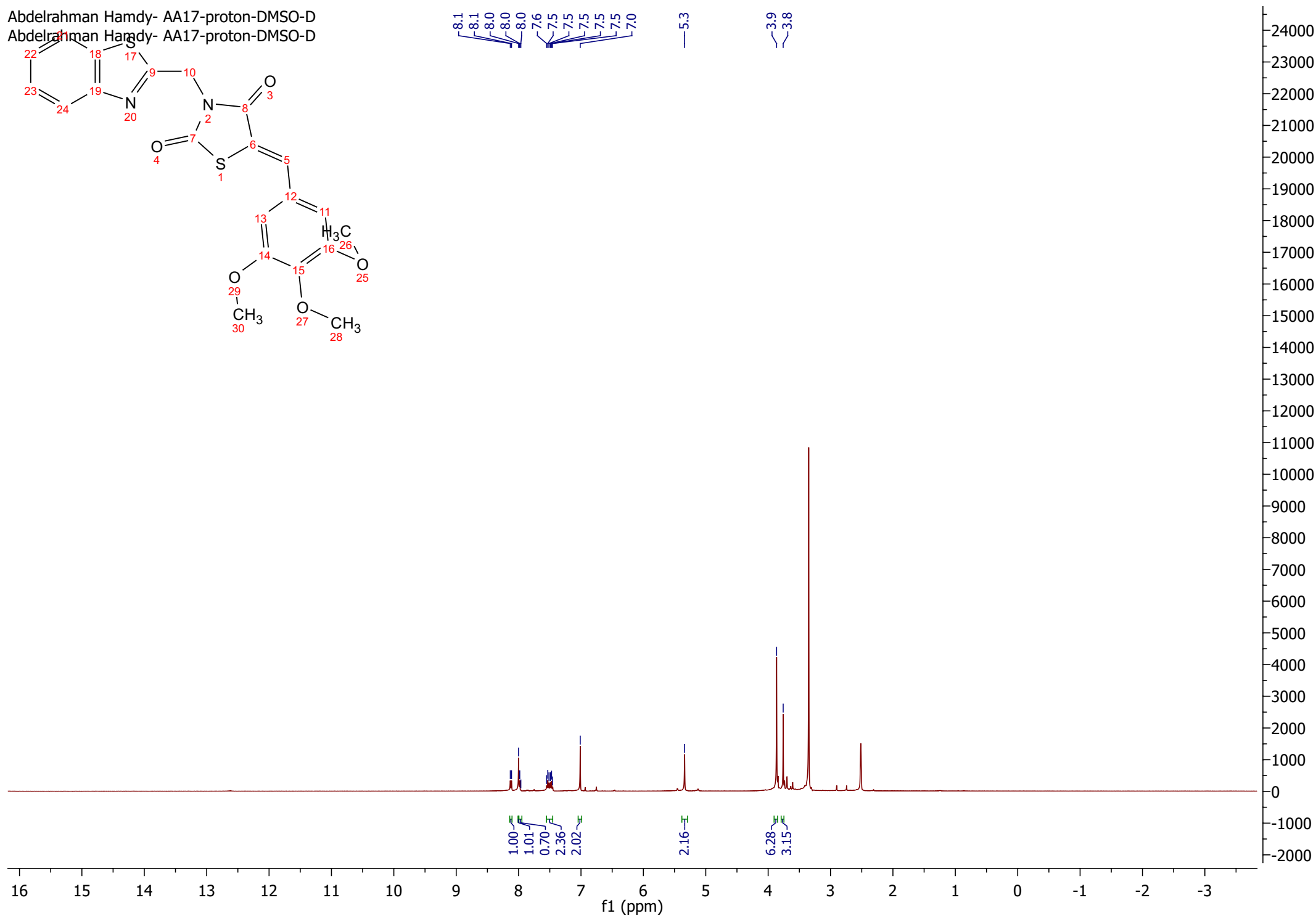
Abdelrahman Hamdy- AA17-proton-DMSO-D
Abdelrahman Hamdy- AA17-proton-DMSO-D



8.1
8.1
8.0
8.0
8.0
7.6
7.5
7.5
7.5
7.5
7.0

5.3

3.9
3.8



1.00
1.01
0.70
2.36
2.02

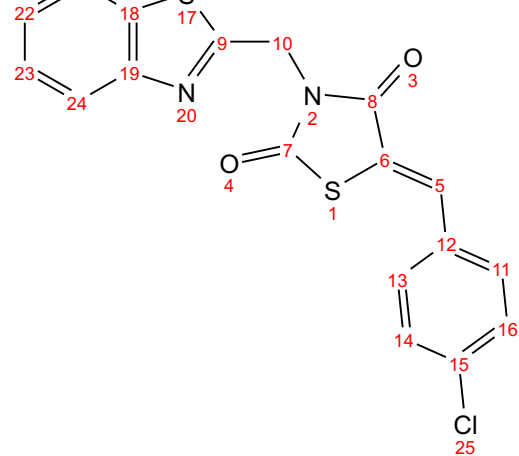
2.16

6.28
3.15

16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3

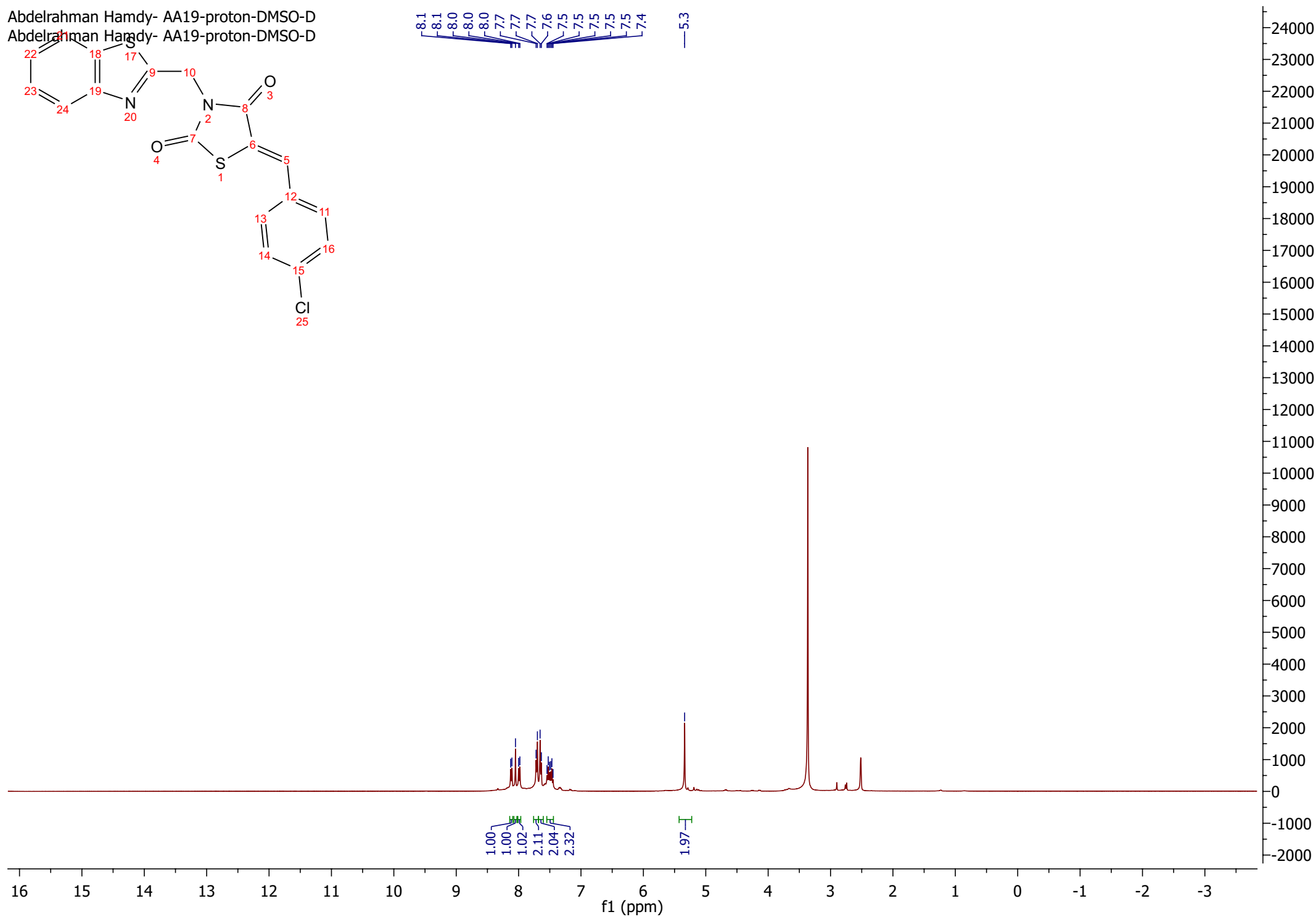
f1 (ppm)

Abdelrahman Hamdy- AA19-proton-DMSO-D
Abdelrahman Hamdy- AA19-proton-DMSO-D

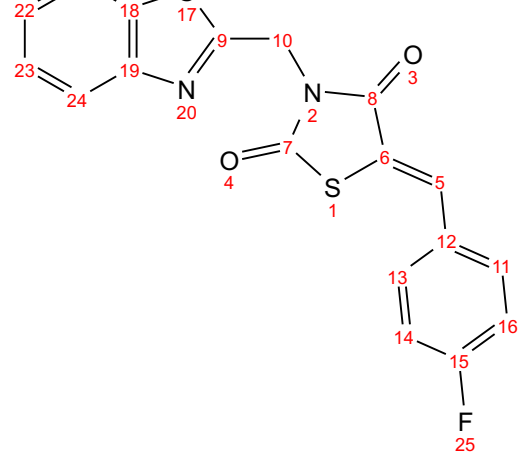


8.1
8.1
8.0
8.0
7.7
7.7
7.7
7.6
7.5
7.5
7.5
7.5
7.4

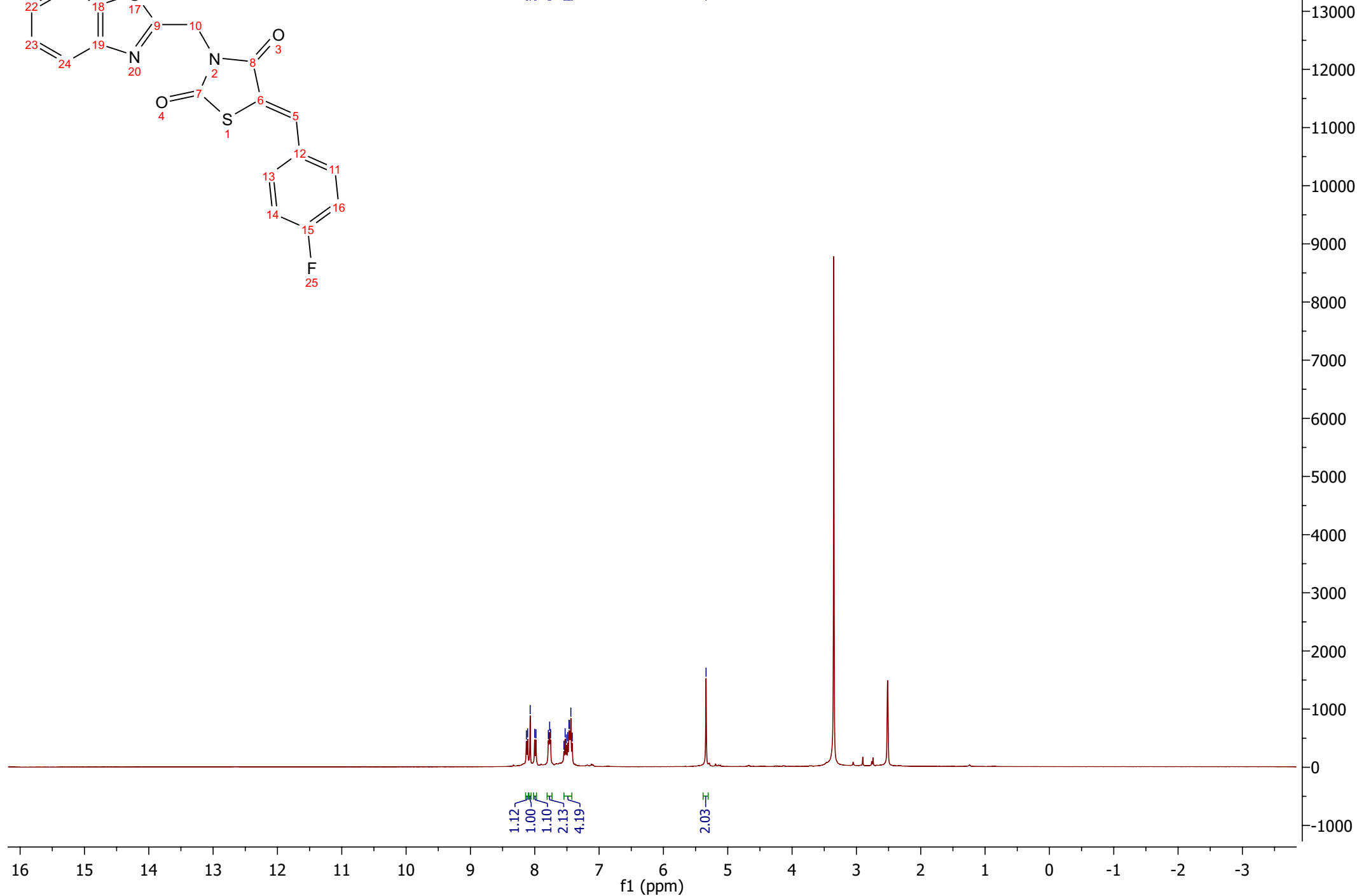
5.3



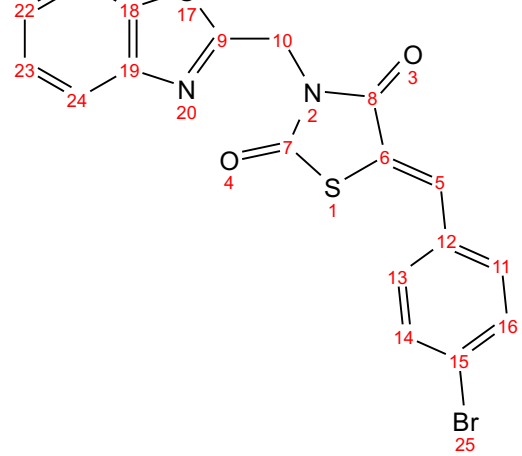
Abdelrahman Hamdy- AA20-proton-DMSO-D
Abdelrahman Hamdy- AA20-proton-DMSO-D



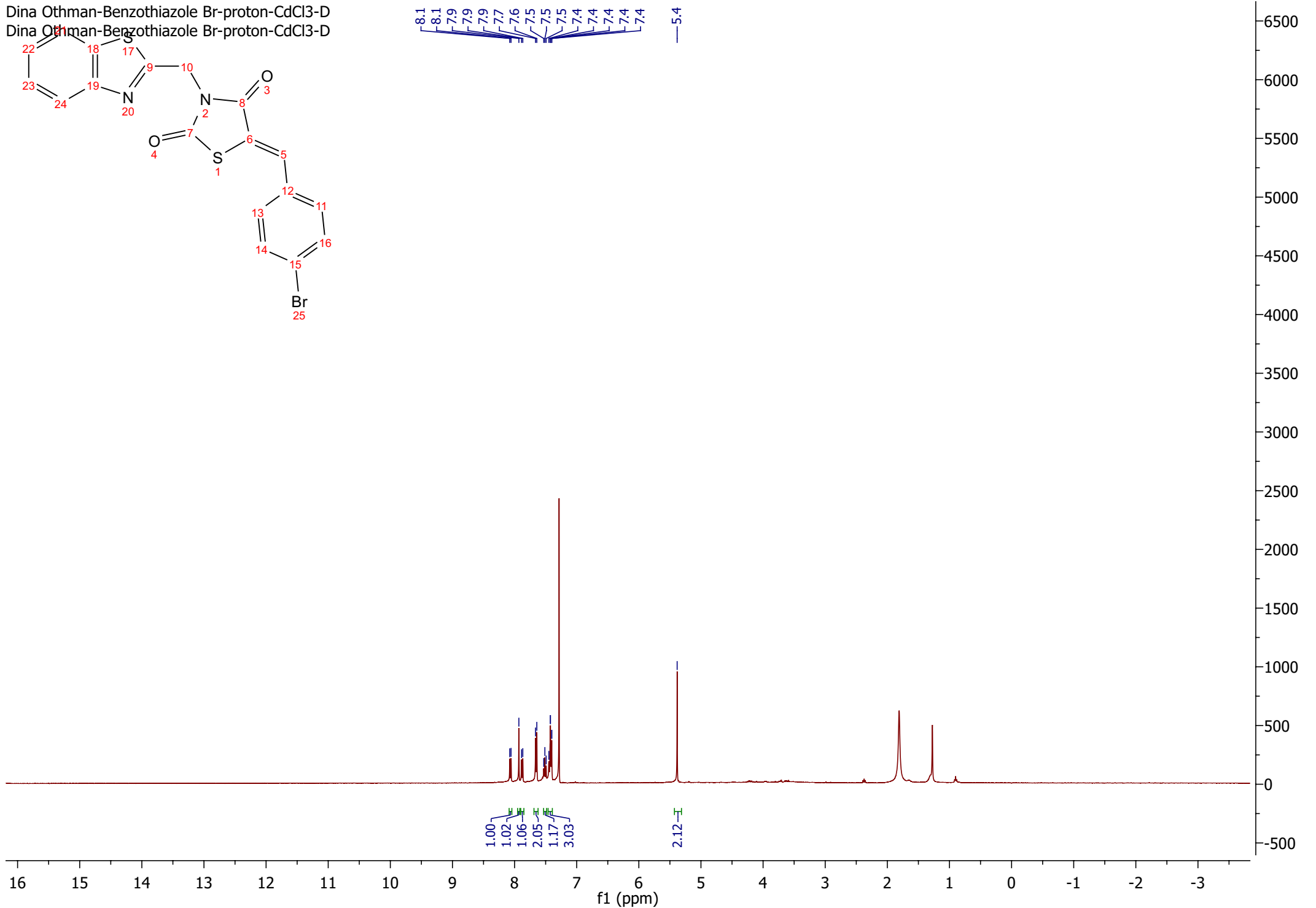
8.1
8.1
8.1
8.0
8.0
7.8
7.8
7.8
7.5
7.5
7.5
7.5
7.5
7.4
7.4
5.3



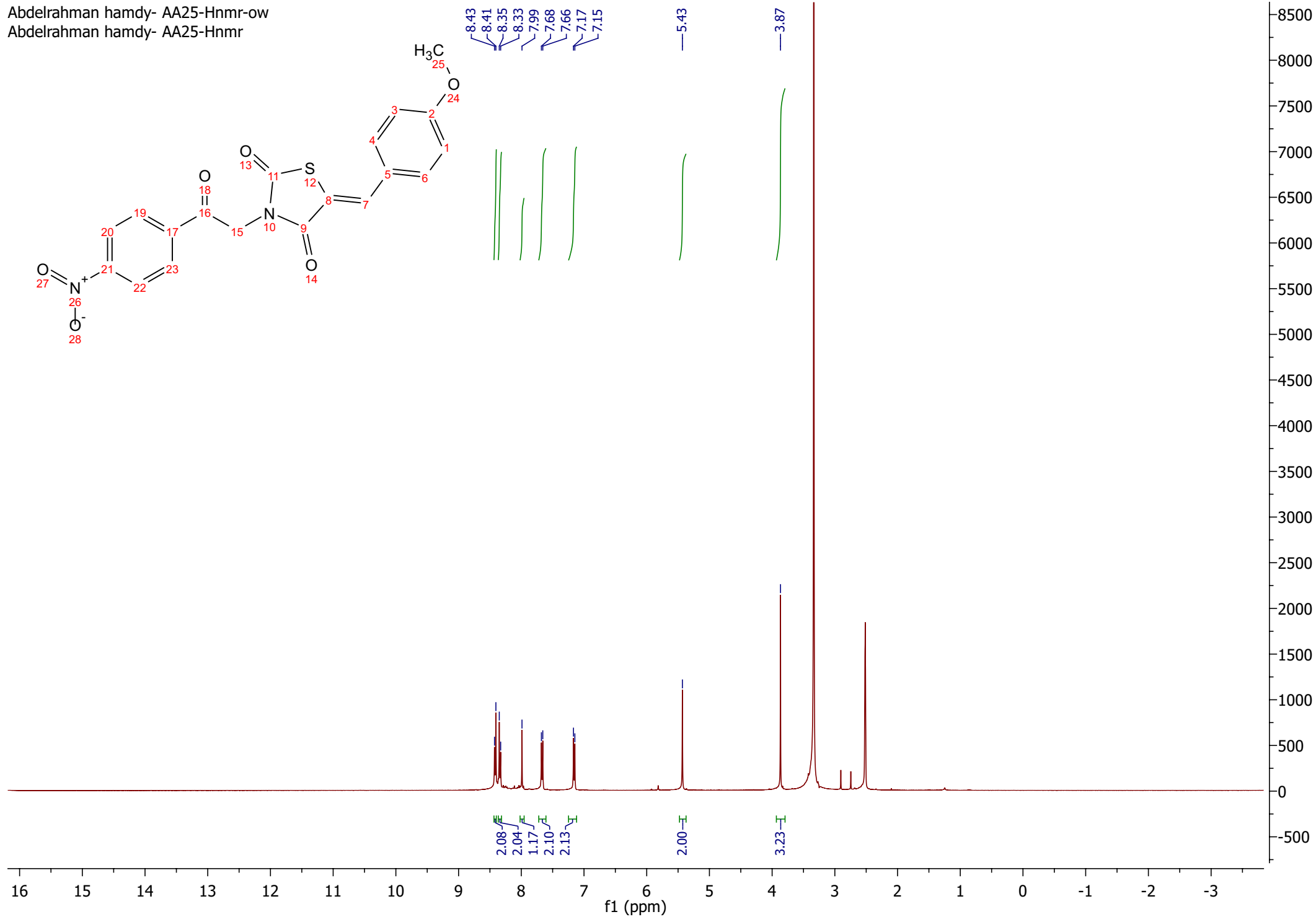
Dina Othman-Benzothiazole Br-proton-CdCl3-D
Dina Othman-Benzothiazole Br-proton-CdCl3-D



8.1
8.1
7.9
7.9
7.9
7.7
7.6
7.5
7.5
7.5
7.4
7.4
7.4
7.4
5.4



Abdelrahman hamdy- AA25-Hnmr-ow
Abdelrahman hamdy- AA25-Hnmr



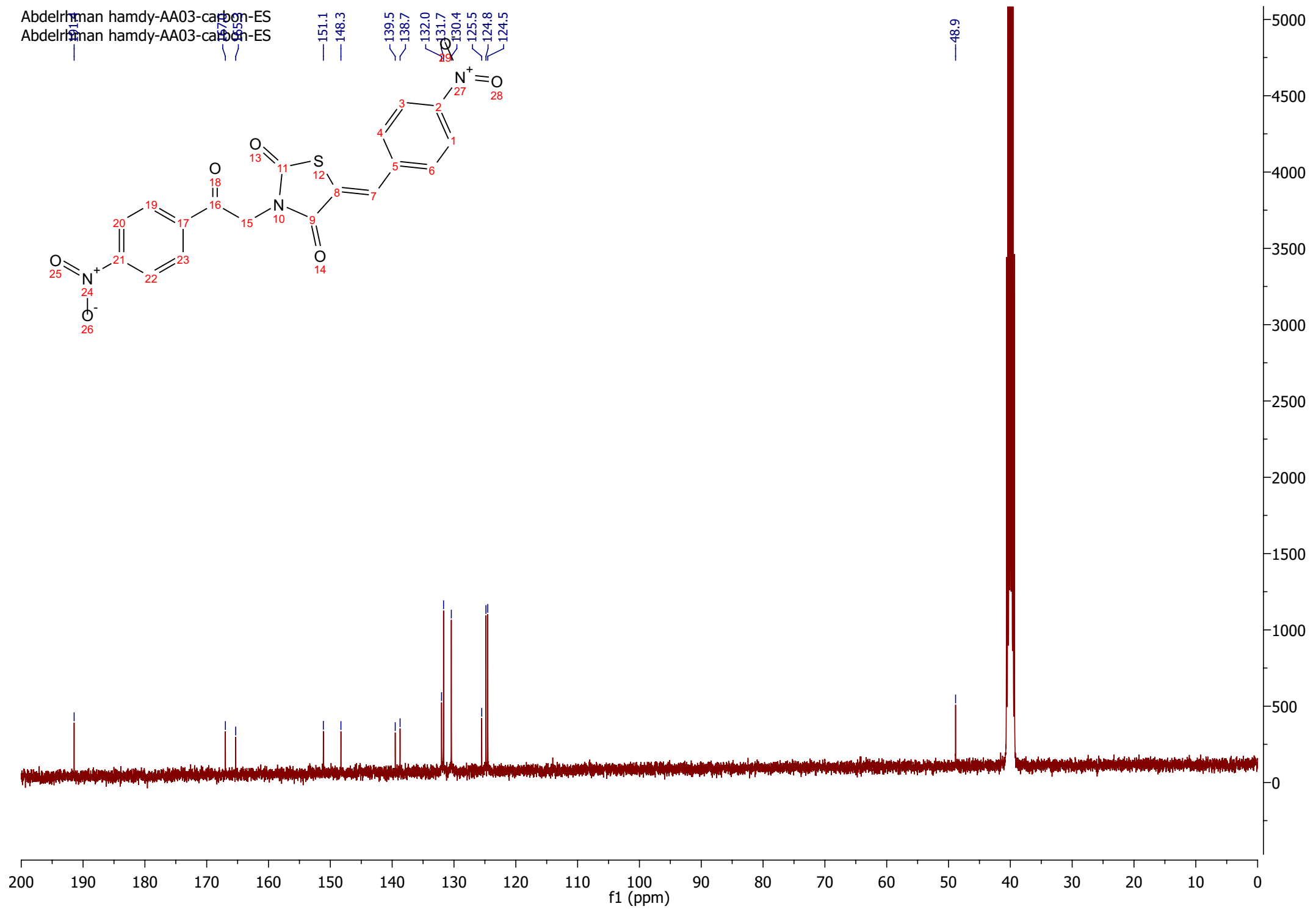
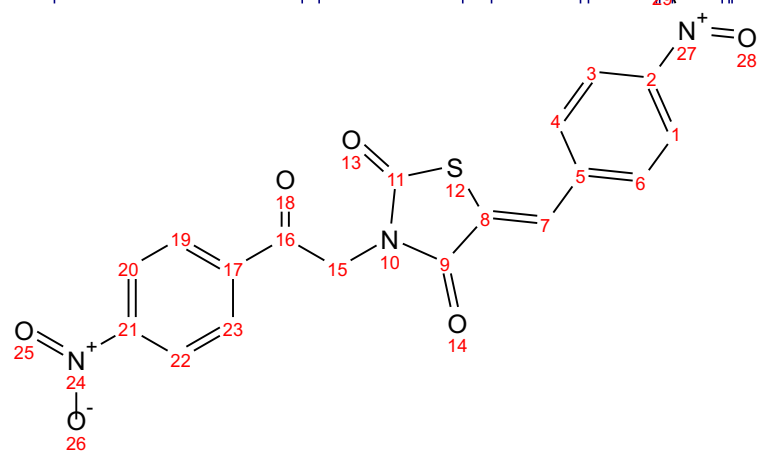
Abdelrhman hamdy-AA03-carbon-ES
Abdelrhman hamdy-AA03-carbon-ES

151.1
148.3

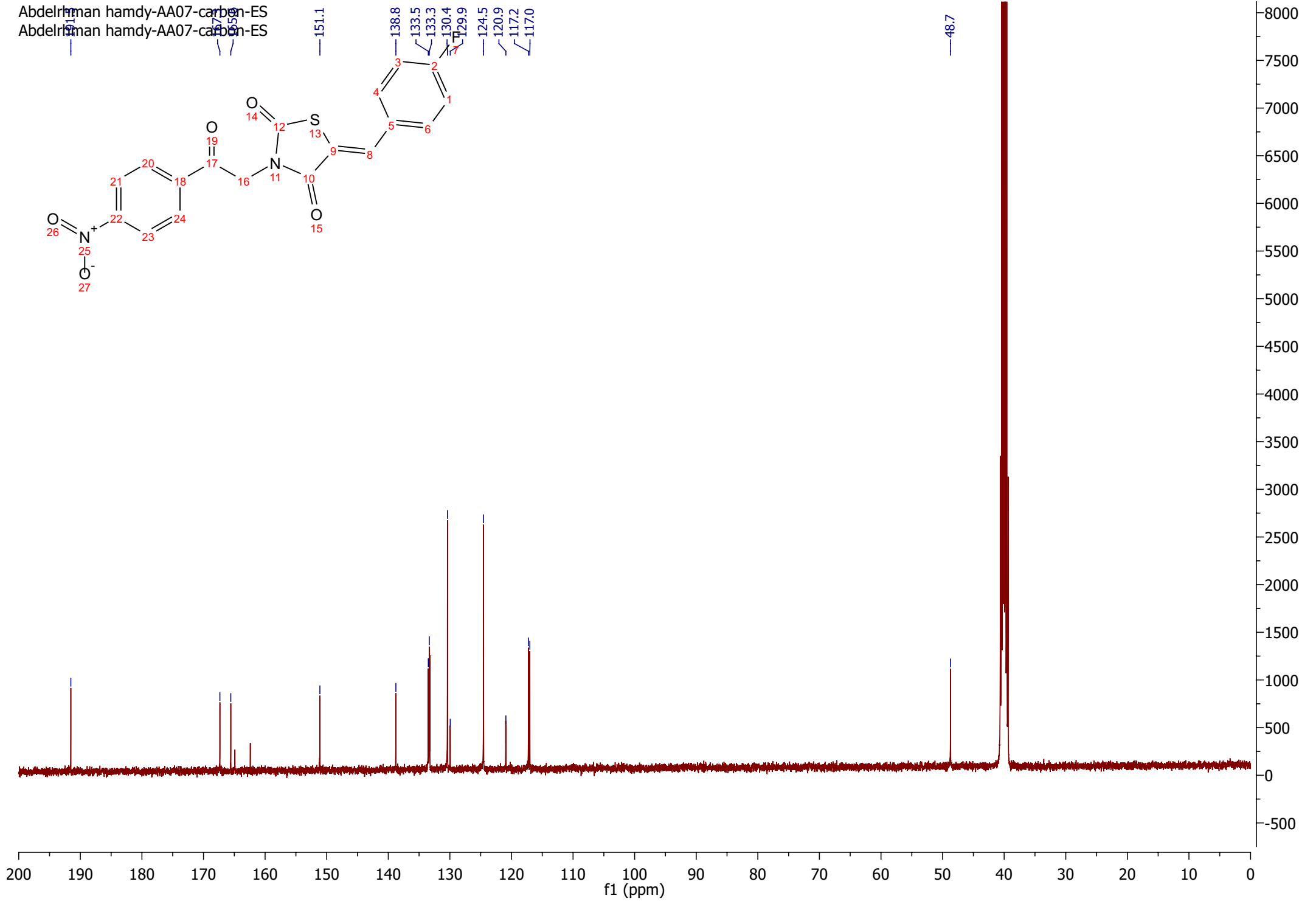
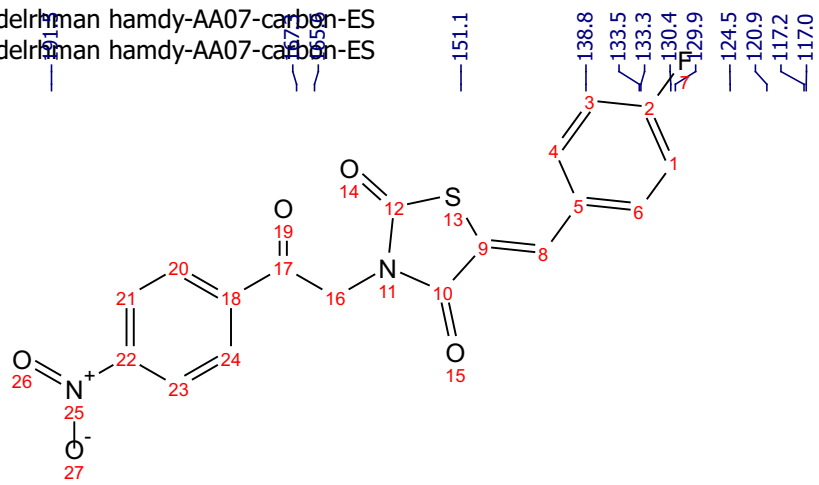
139.5
138.7
132.0
131.7
130.4

125.5
124.8
124.5

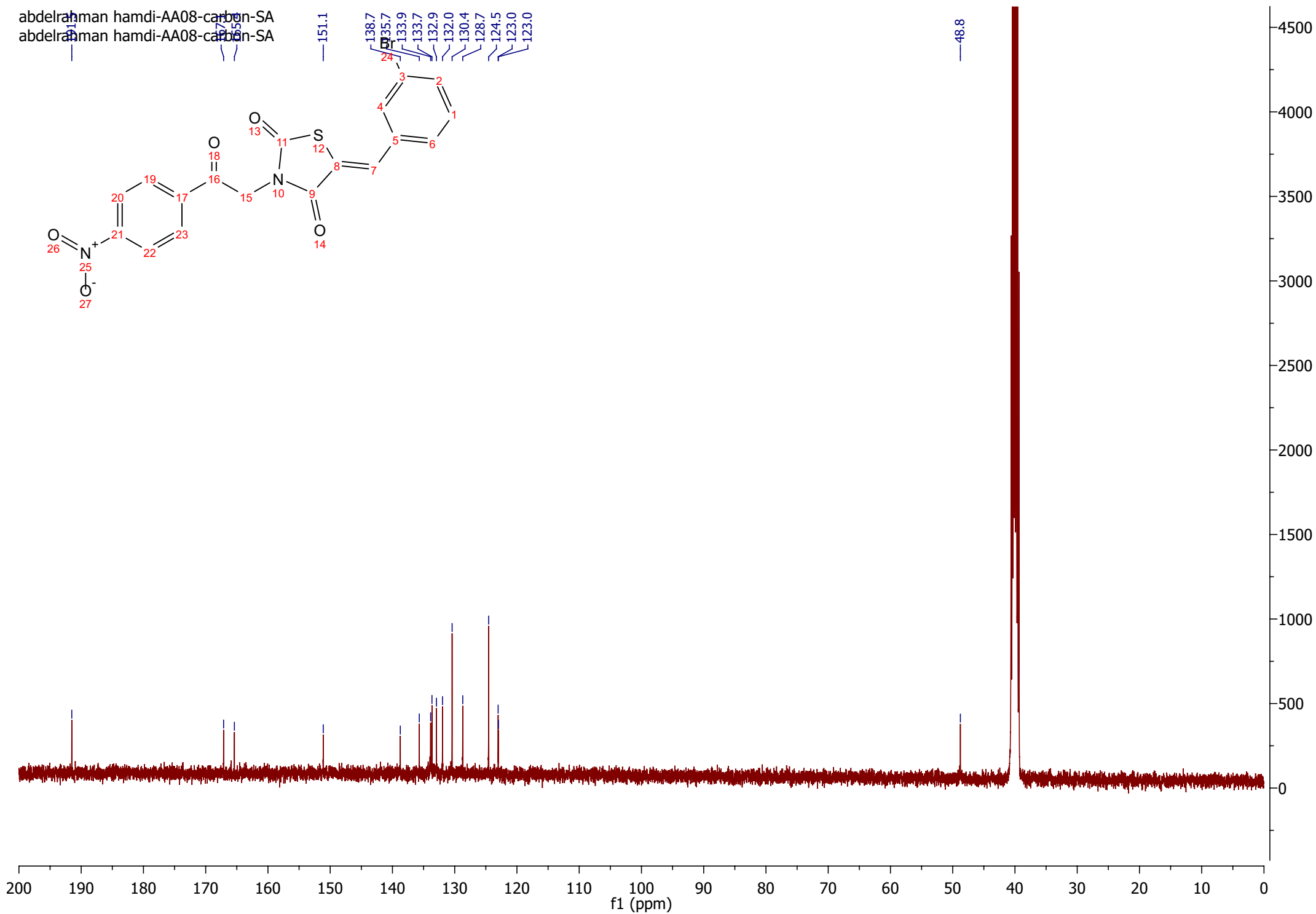
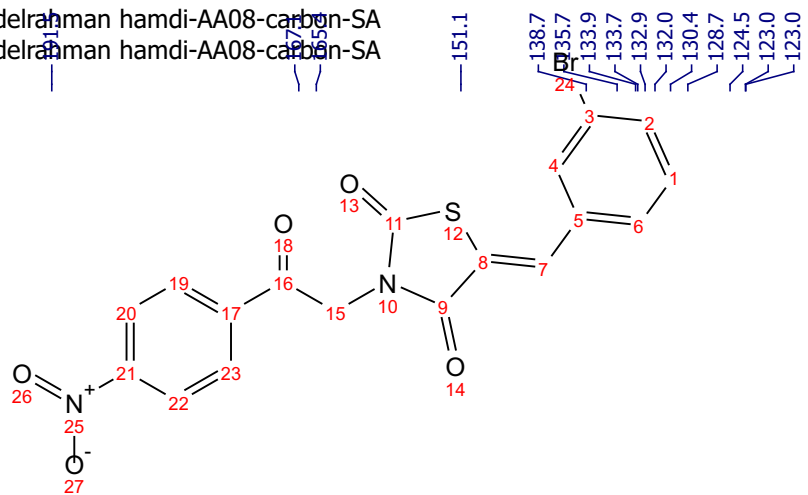
48.9



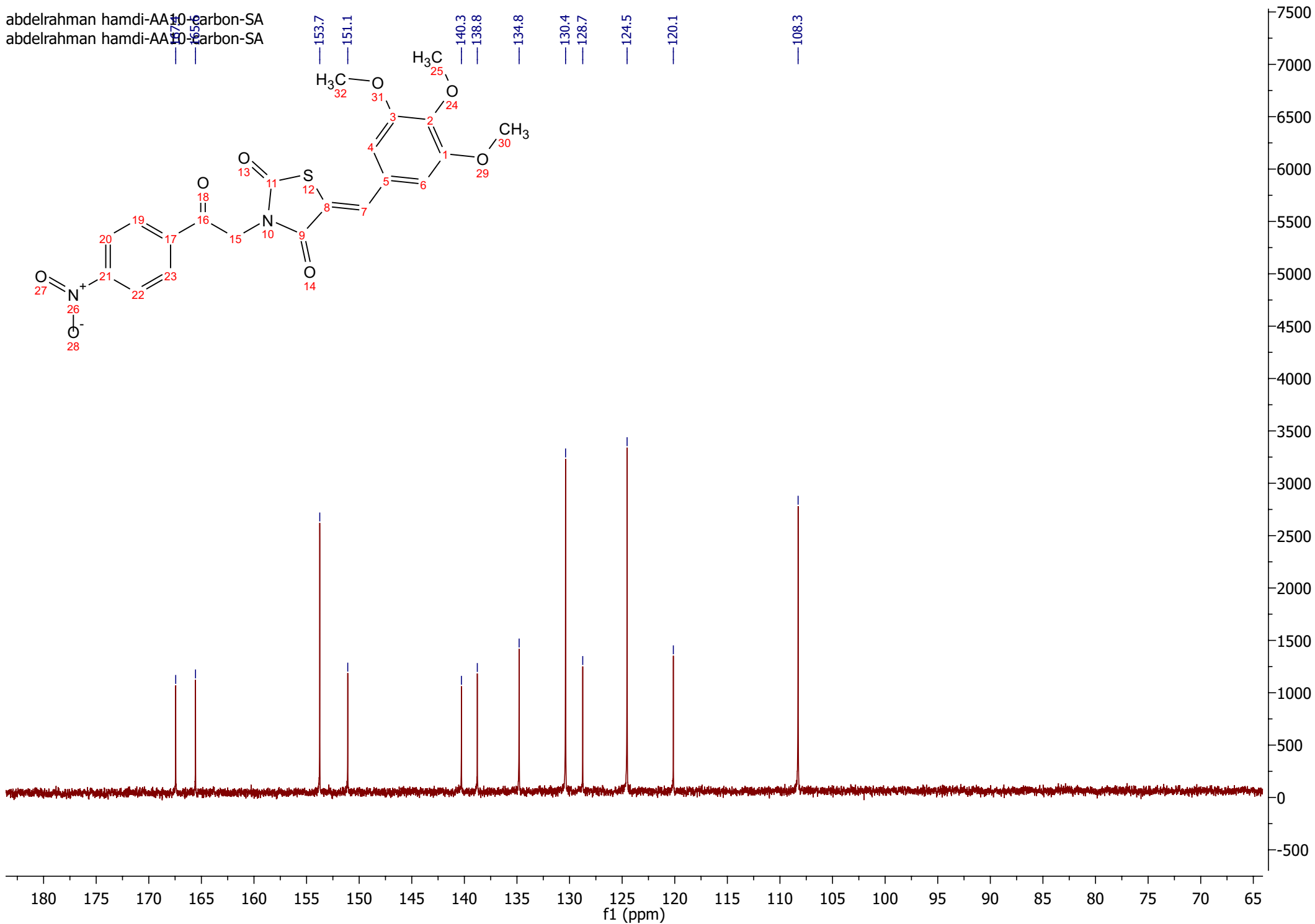
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Abdelrhman hamdy-AA07-carbon-ES



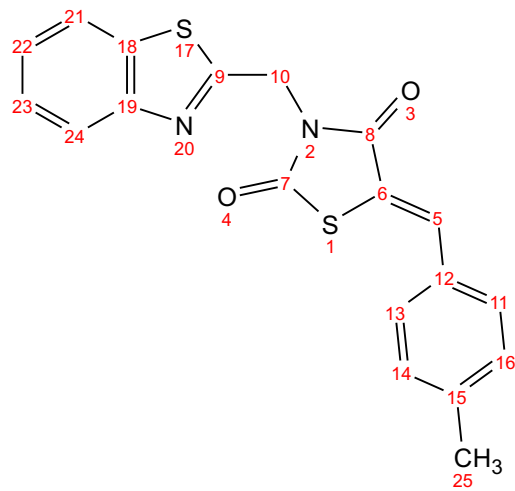
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abdelrahman hamdi-AA08-carbon-SA



abdelrahman hamdi-AA-10-carbon-SA
abdelrahman hamdi-AA-10-carbon-SA

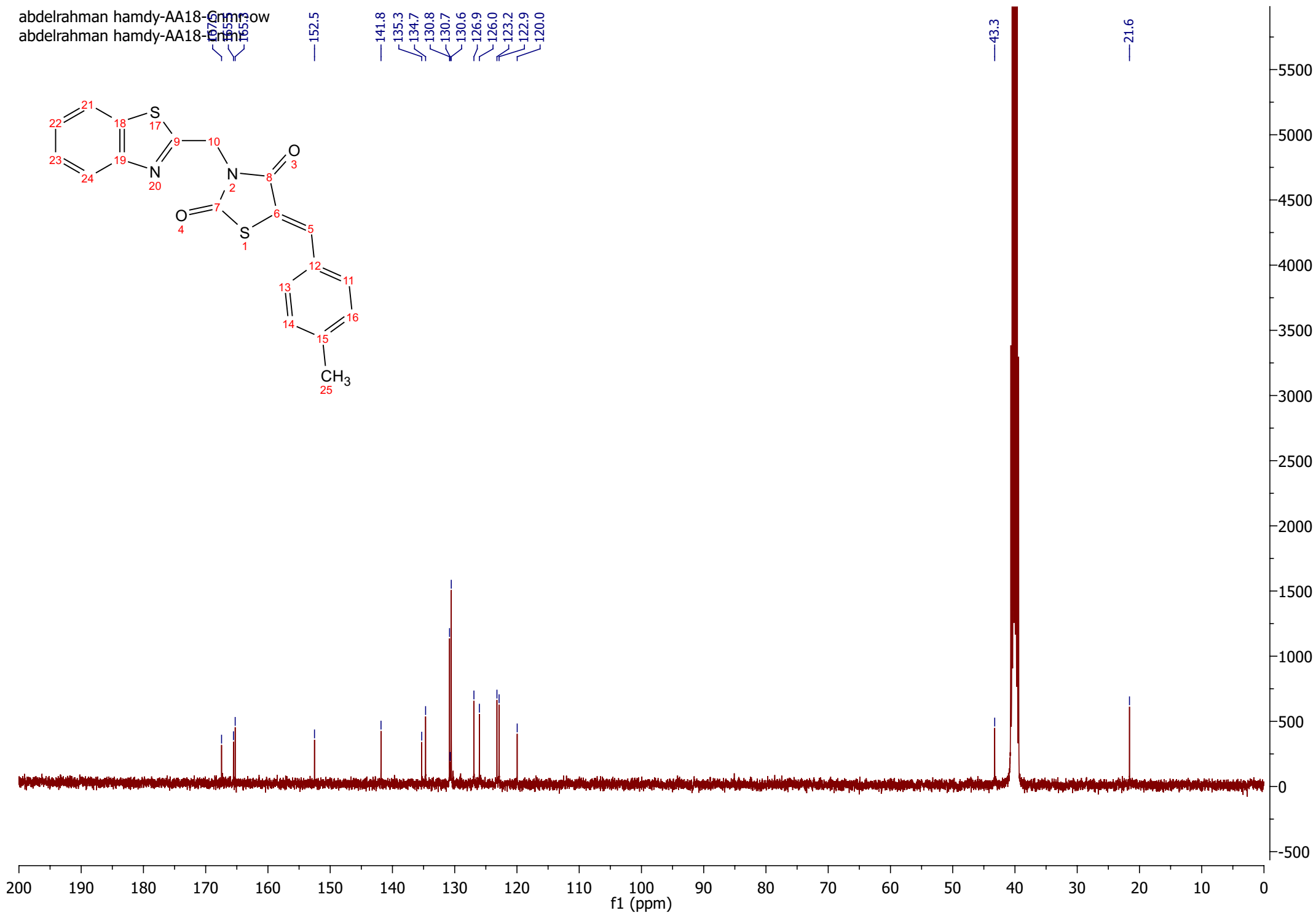


abdelrahman hamdy-AA18-Orinow
abdelrahman hamdy-AA18-Orinow

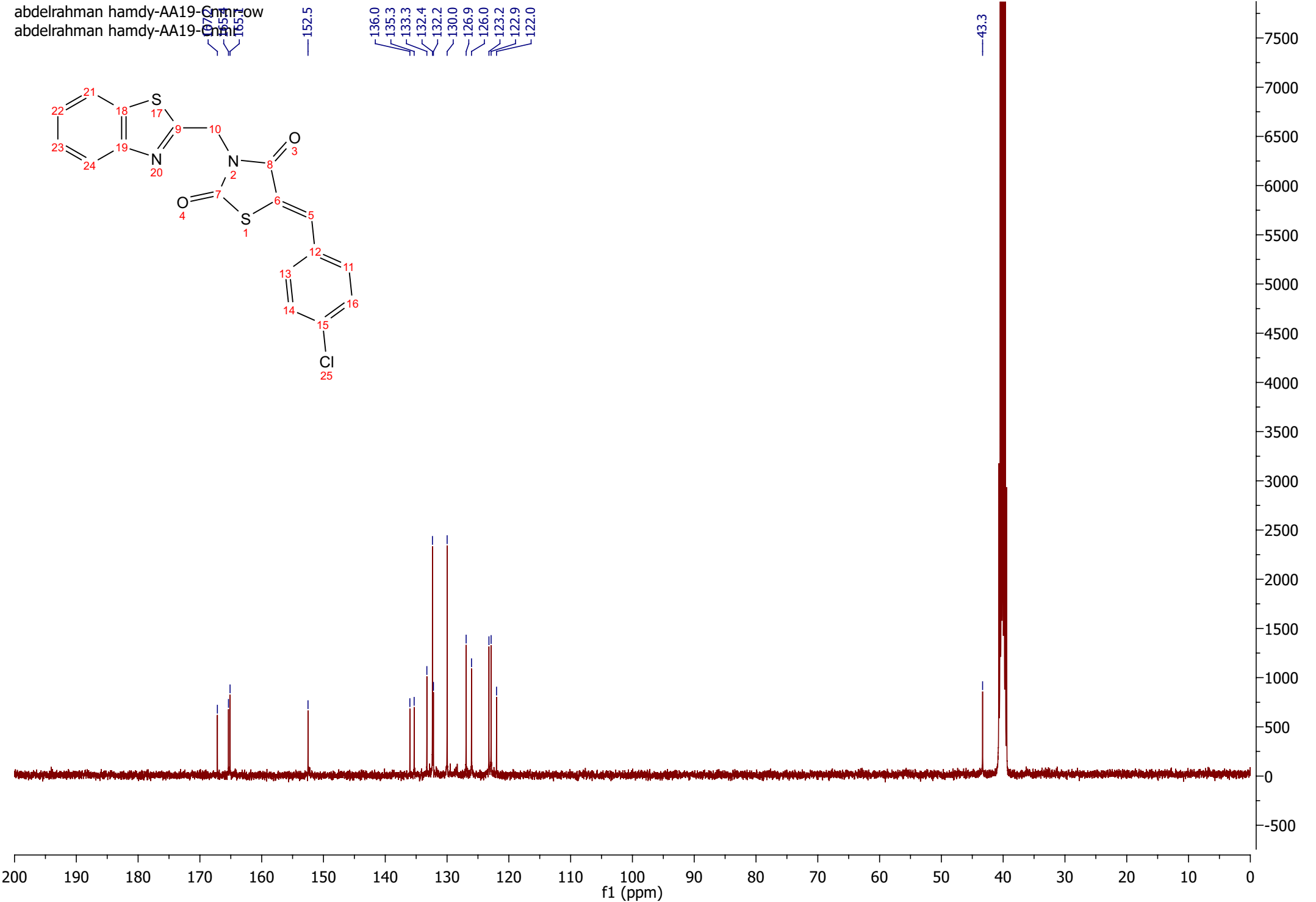
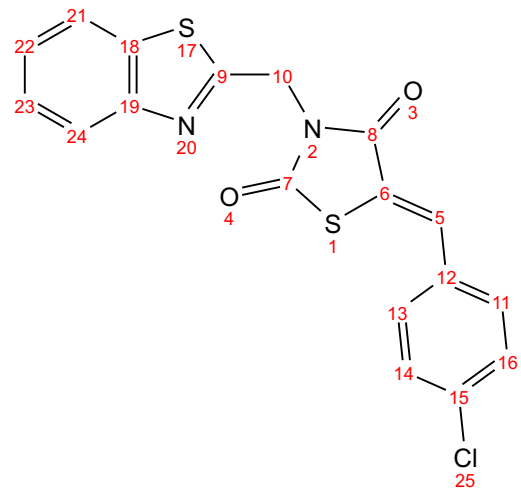


152.5
141.8
135.3
134.7
130.8
130.7
130.6
126.9
126.0
123.2
122.9
120.0

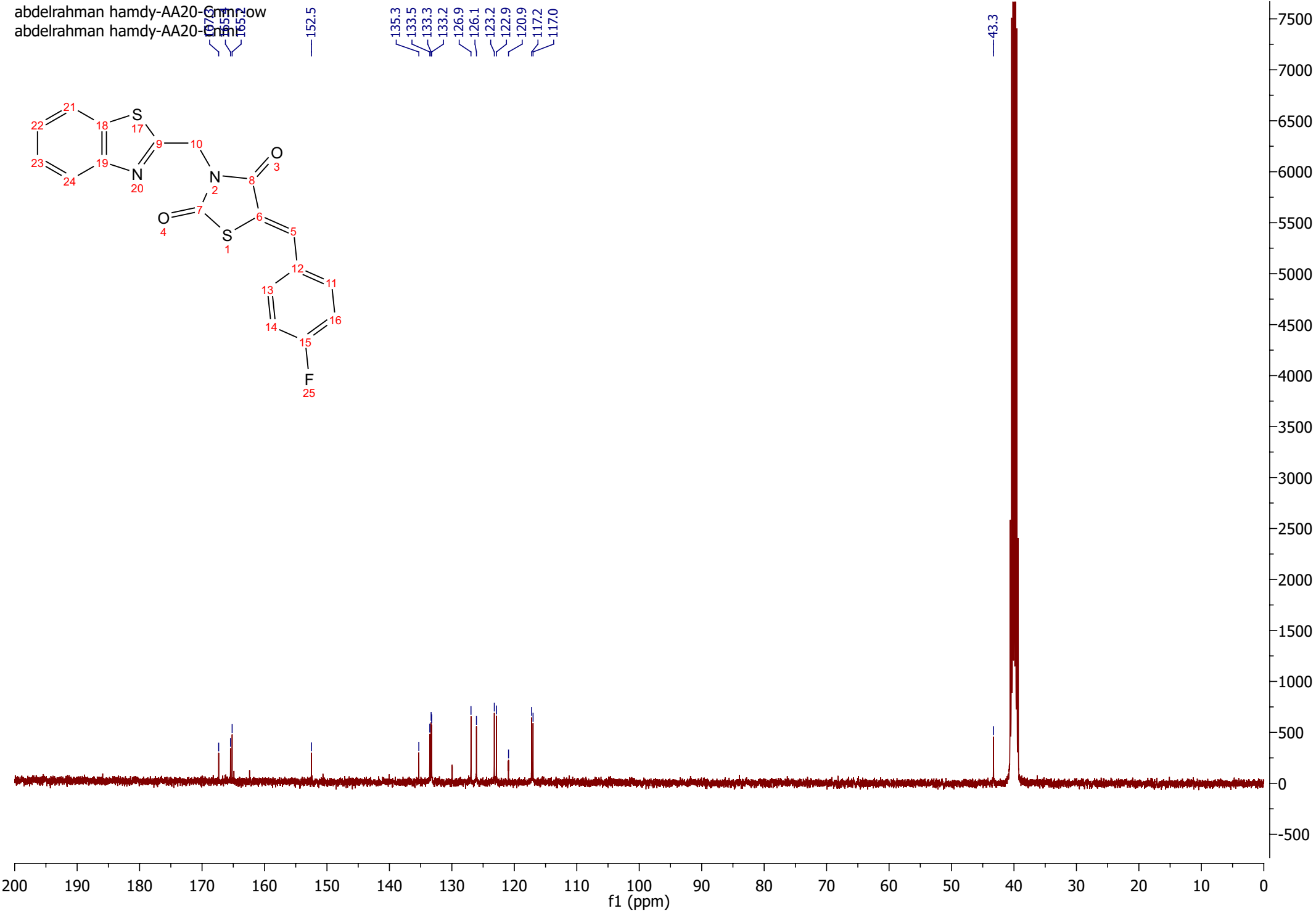
43.3
21.6



abdelrahman hamdy-AA19-Ornlow
abdelrahman hamdy-AA19-Ornlow



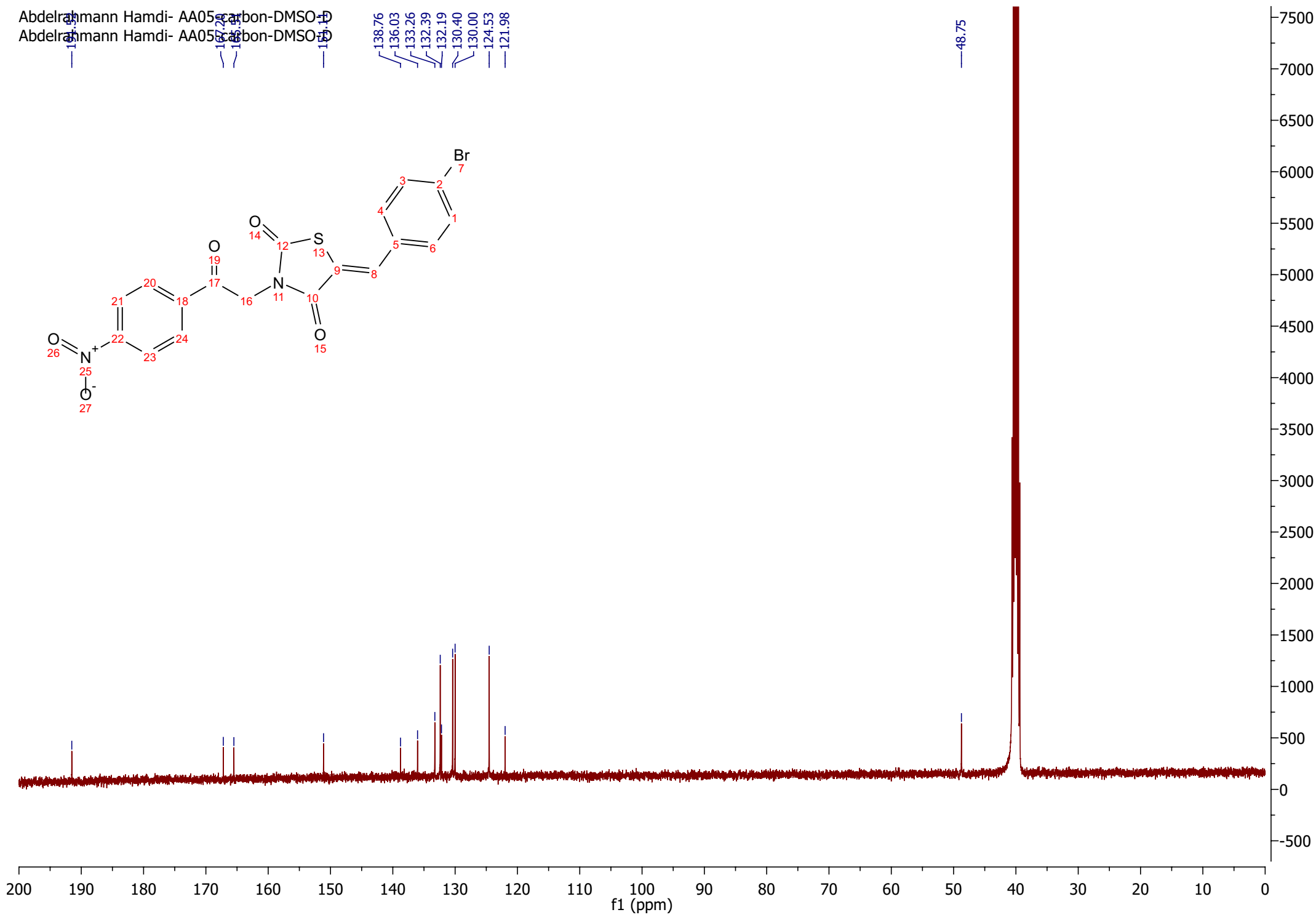
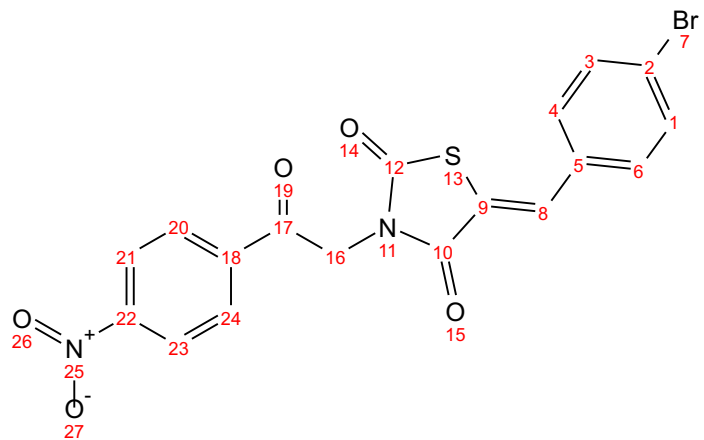
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abdelrahman hamdy-AA20-Orinlow



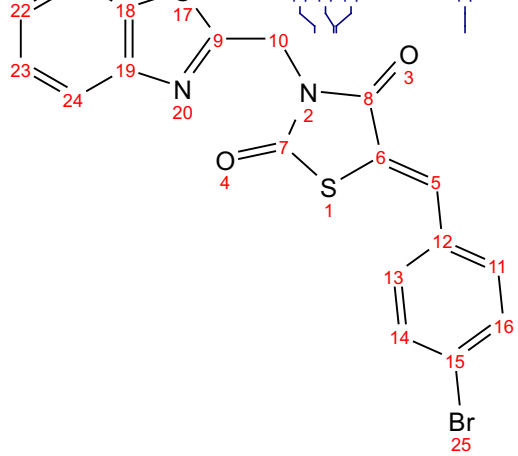
Abdelrahman Hamdi- AA05 carbon-DMSO-D
Abdelrahman Hamdi- AA05 carbon-DMSO-D

138.76
136.03
133.26
132.39
132.19
130.40
130.00
124.53
121.98

48.75

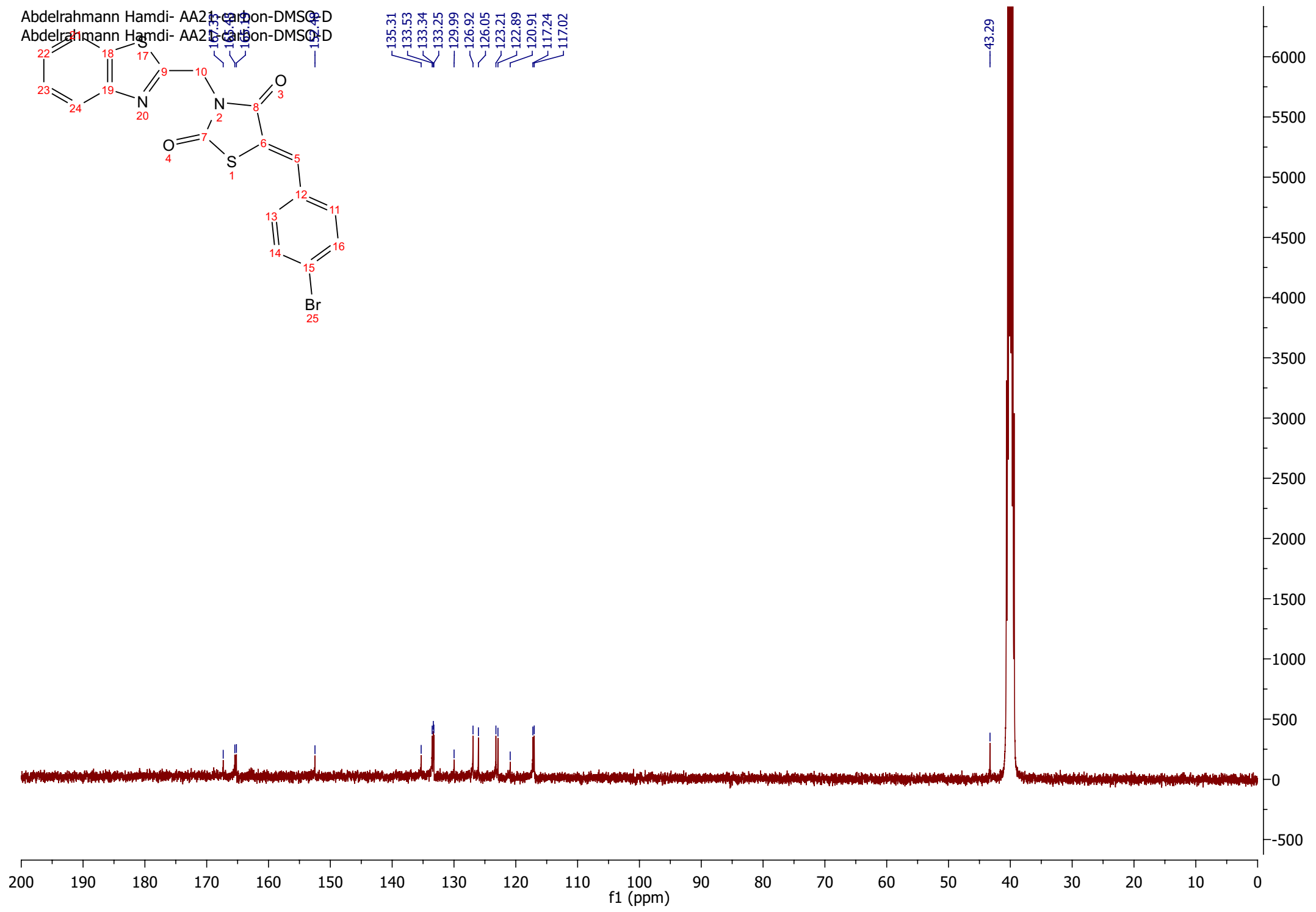


Abdelrahmann Hamdi- AA21 Carbon-DMSO-D
Abdelrahmann Hamdi- AA21 Carbon-DMSO-D



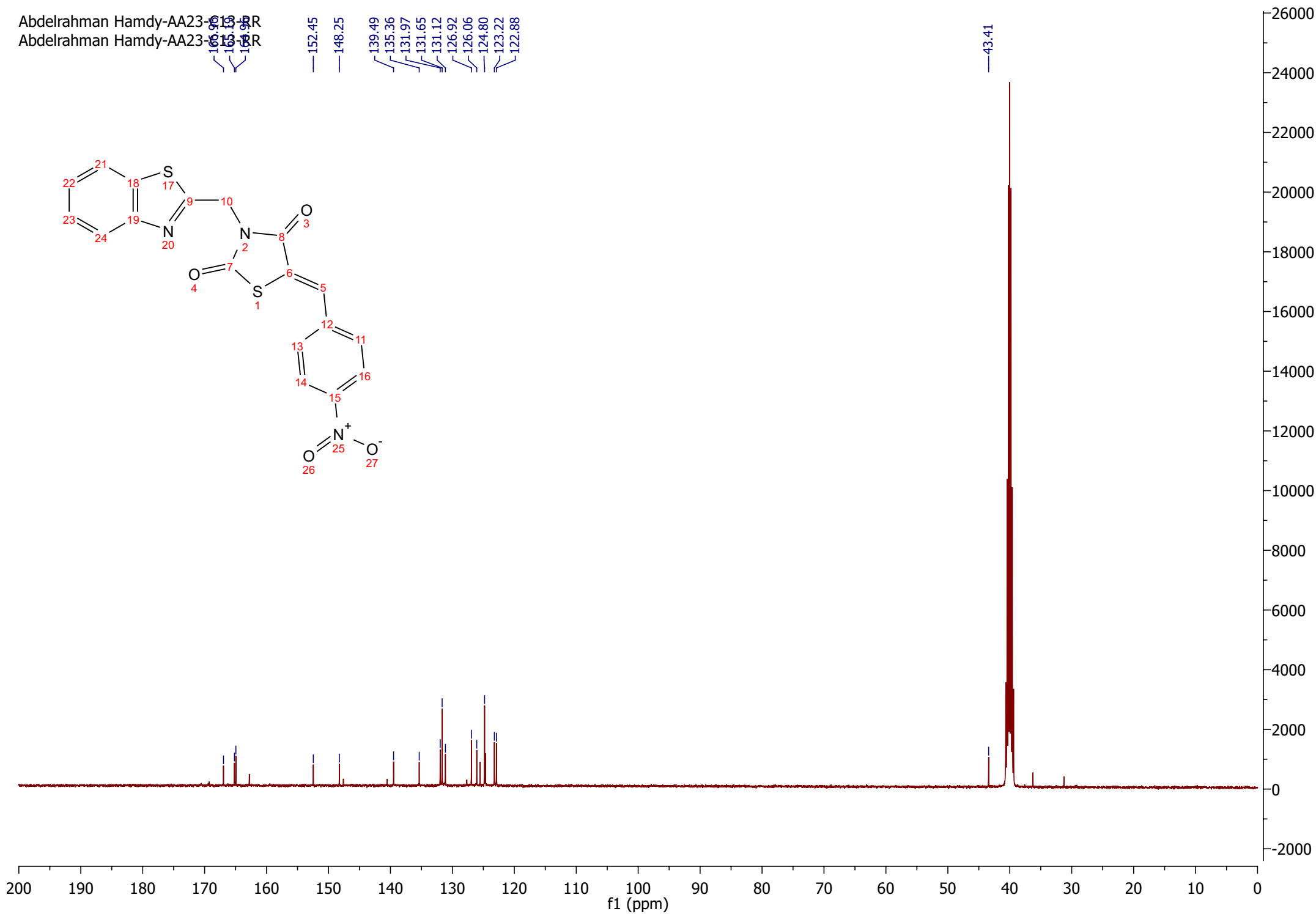
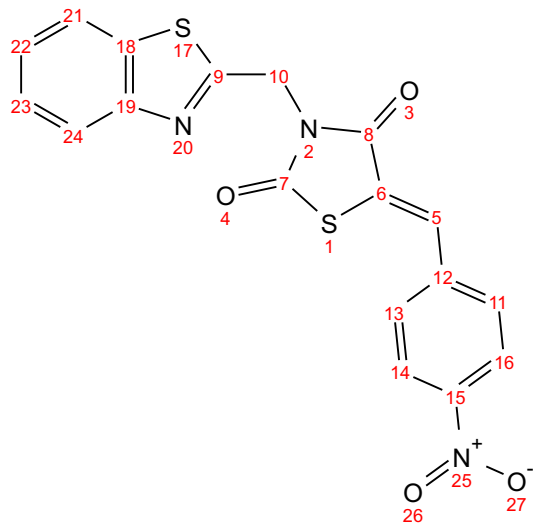
135.31
133.53
133.34
133.25
129.99
126.92
126.05
123.21
122.89
120.91
117.24
117.02

43.29



Abdelrahman Hamdy-AA23-013-9R
Abdelrahman Hamdy-AA23-013-9R

152.45
148.25
139.49
135.36
131.97
131.65
131.12
126.92
126.06
124.80
123.22
122.88
43.41

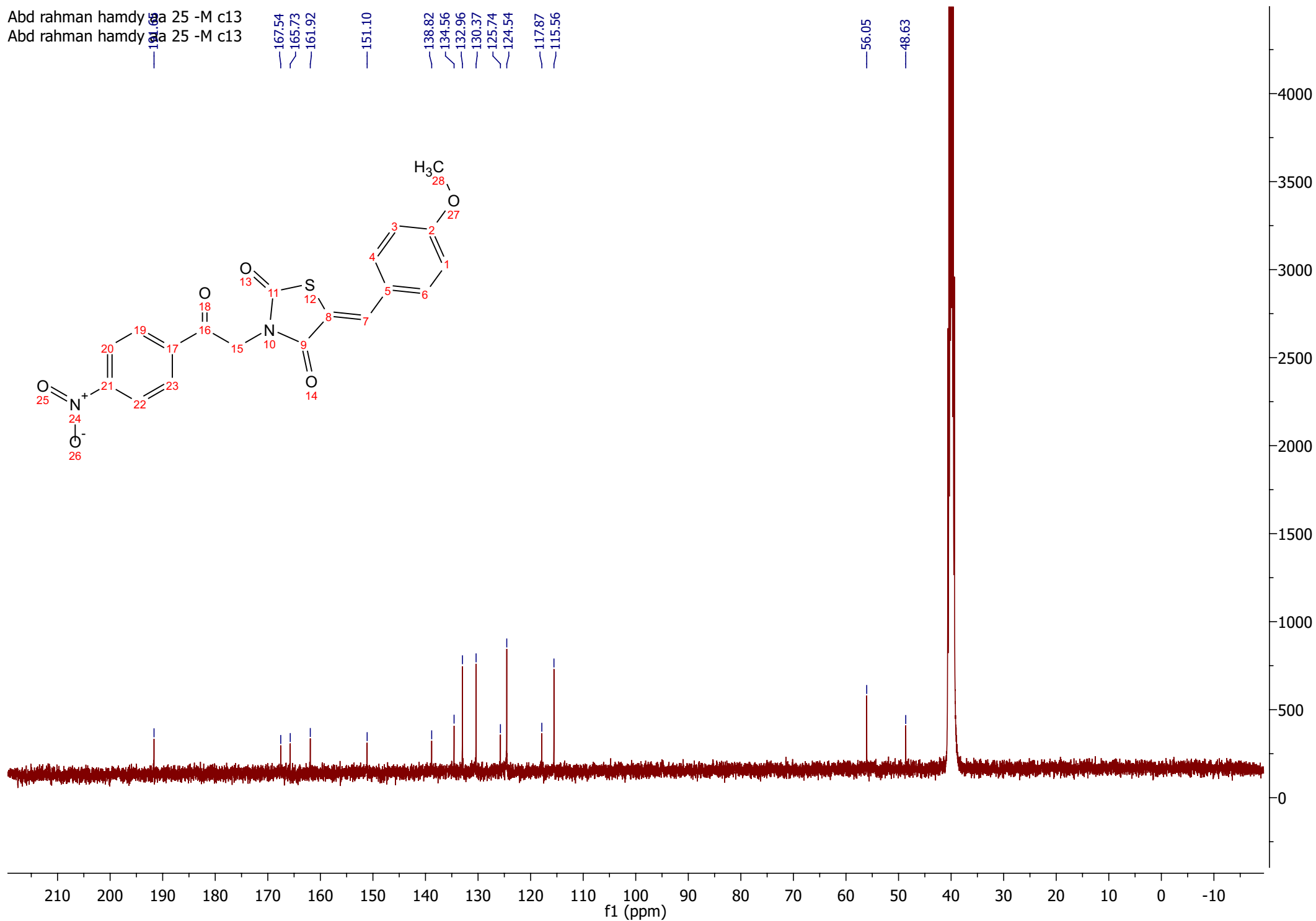
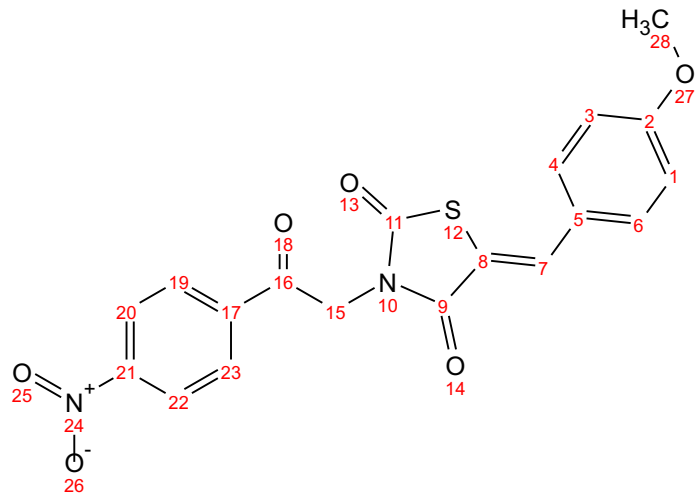


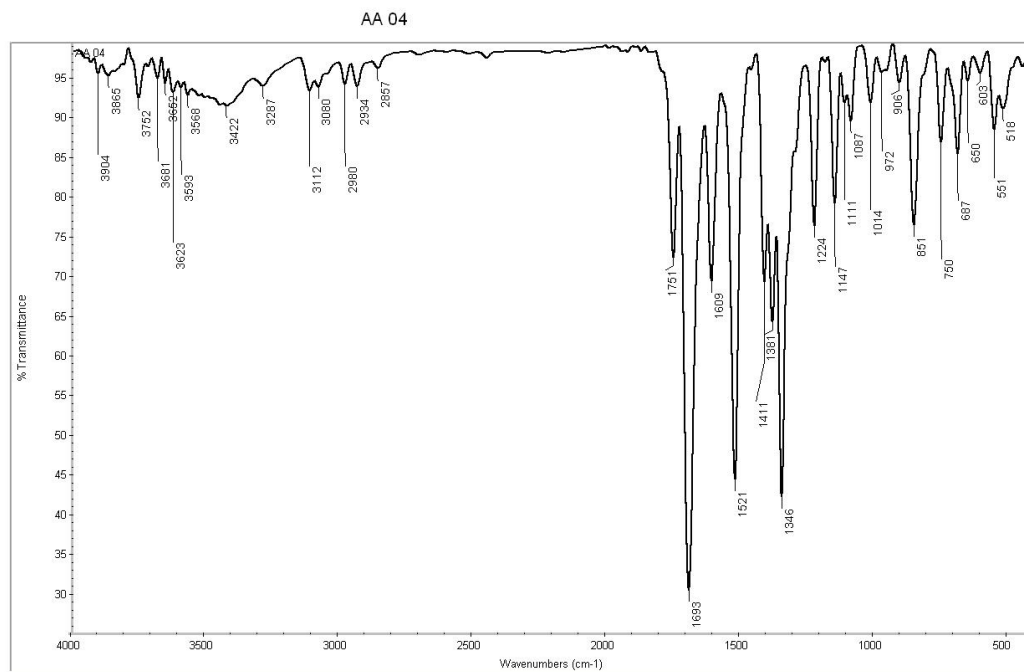
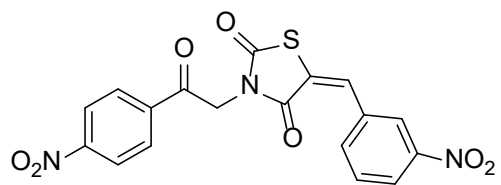
Abd rahman hamdy
Abd rahman hamdy

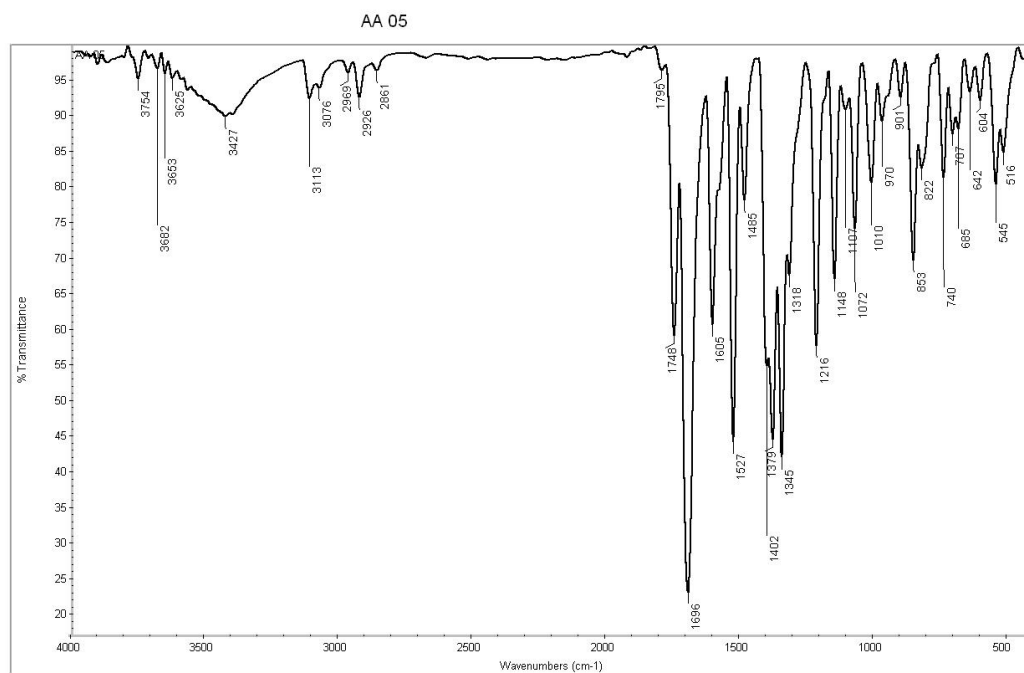
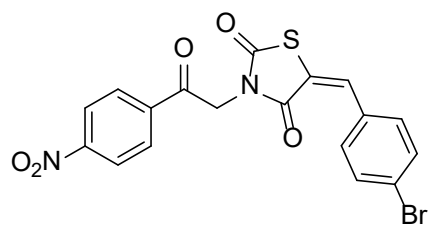
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25 -M c13

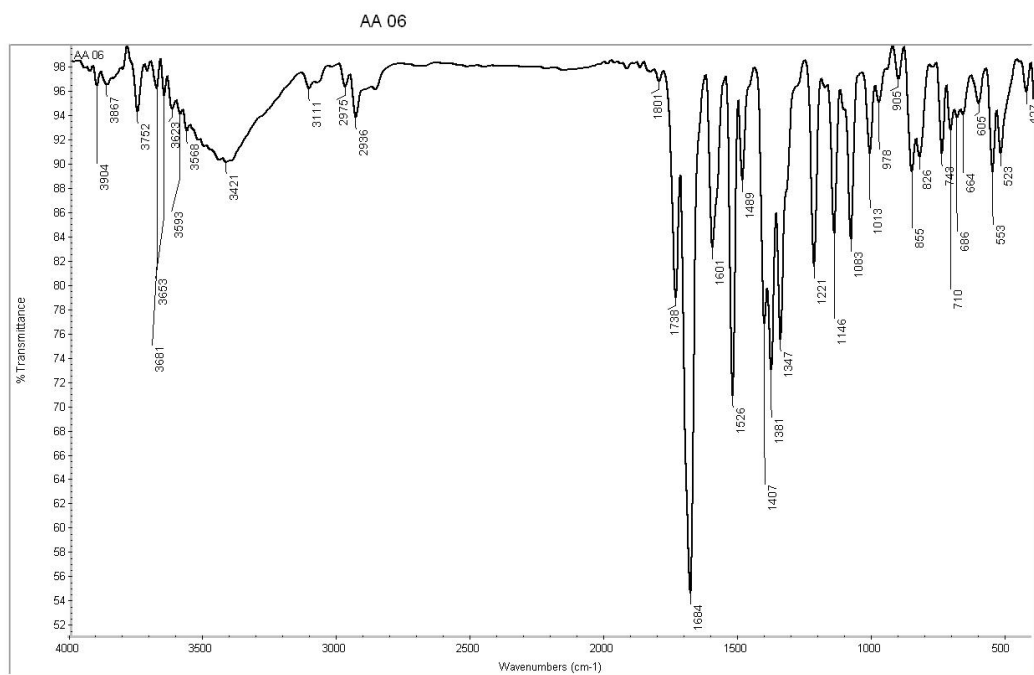
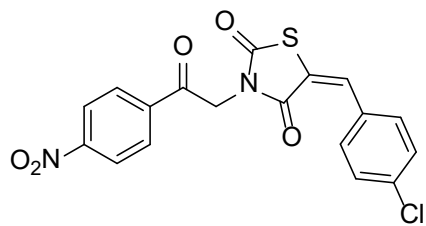
167.54
165.73
161.92
151.10
138.82
134.56
132.96
130.37
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124.54
117.87
115.56

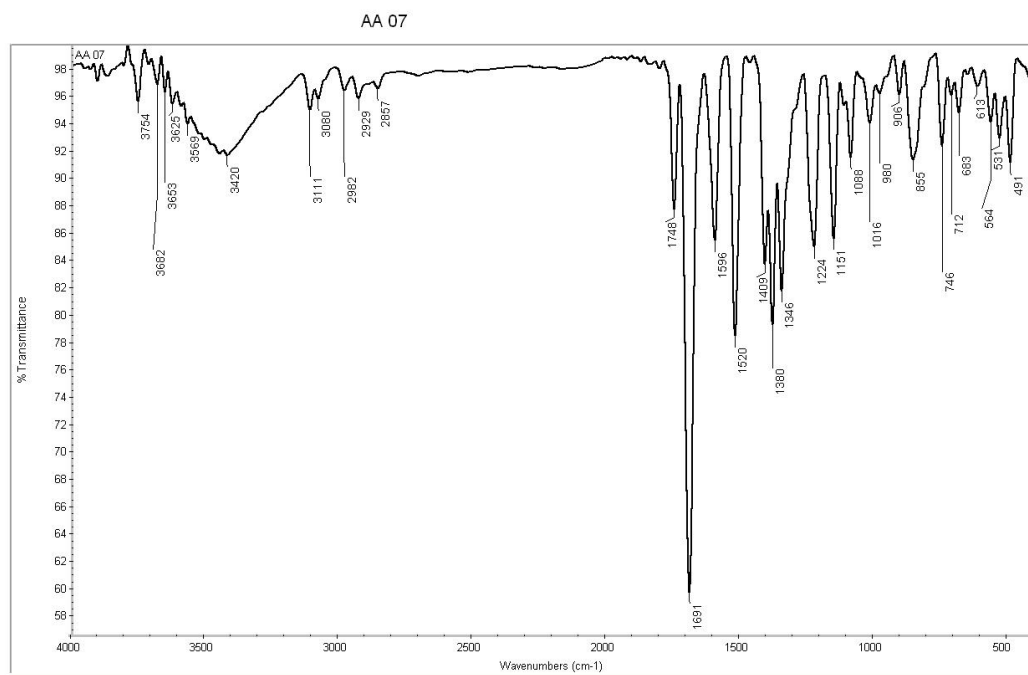
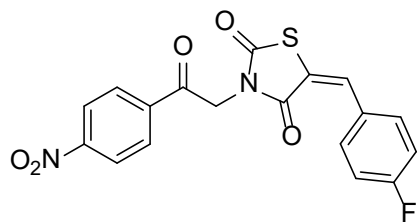
56.05
48.63

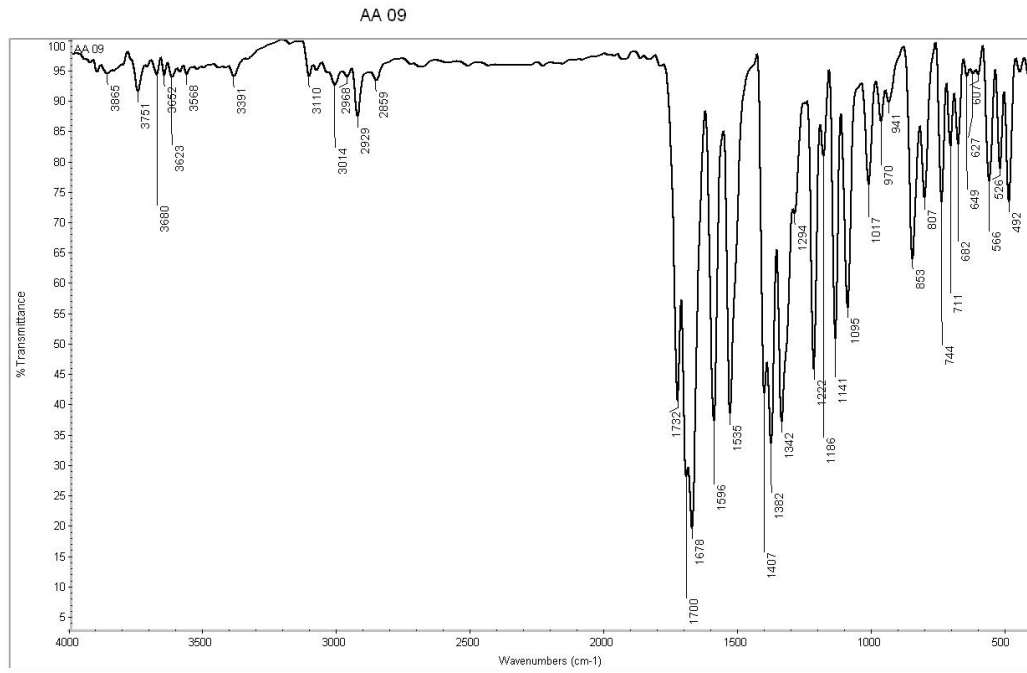
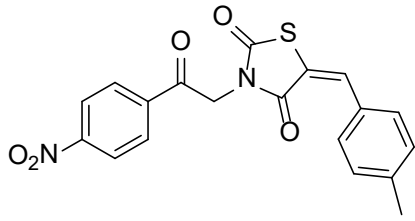


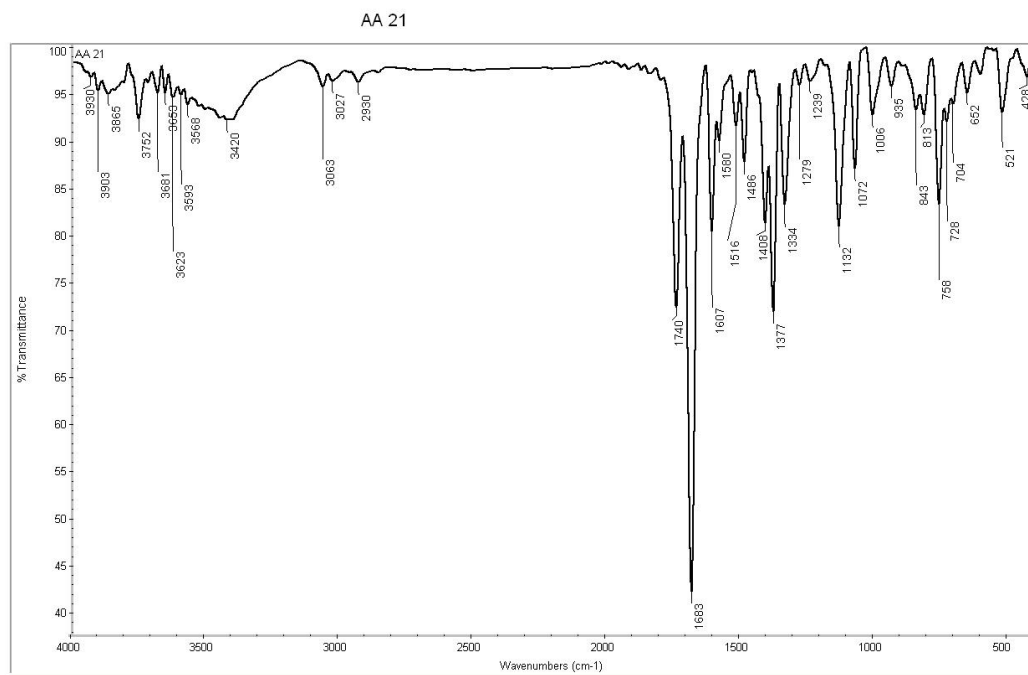
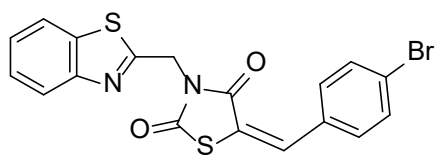






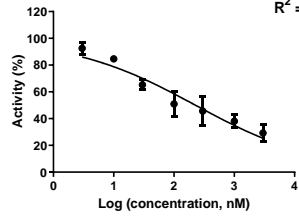






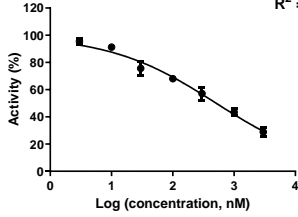
Best-fit values	
LogIC50	2.357
HillSlope	-0.4199
IC50	227.4

AA03 $IC_{50} = 227.4$
 $R^2 = 0.8926$



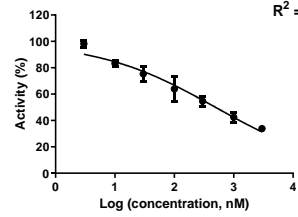
Best-fit values	
LogIC50	2.709
HillSlope	-0.4960
IC50	511.7

AA04 $IC_{50} = 511.7$
 $R^2 = 0.9715$



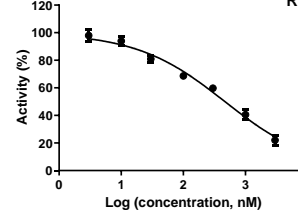
Best-fit values	
LogIC50	2.693
HillSlope	-0.4353
IC50	493.7

AA05 $IC_{50} = 493.7$
 $R^2 = 0.9403$



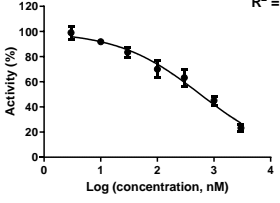
Best-fit values	
LogIC50	2.670
HillSlope	-0.6081
IC50	468.0

AA06 $IC_{50} = 468.0$
 $R^2 = 0.9794$



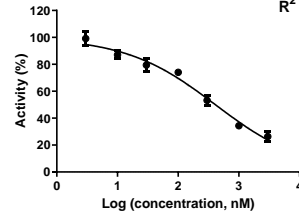
Best-fit values	
LogIC50	2.760
HillSlope	-0.5977
IC50	575.1

AA07 $IC_{50} = 575.1$
 $R^2 = 0.9605$



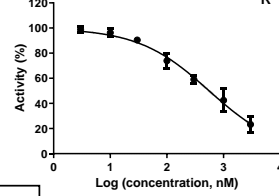
Best-fit values	
LogIC50	2.613
HillSlope	-0.5861
IC50	410.2

AA08 $IC_{50} = 410.2$
 $R^2 = 0.9710$



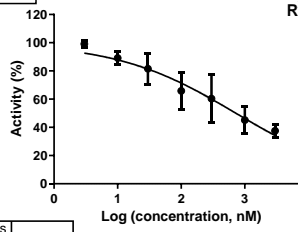
Best-fit values	
LogIC50	2.747
HillSlope	-0.6936
IC50	558.0

AA09 $IC_{50} = 558.0$
 $R^2 = 0.9713$



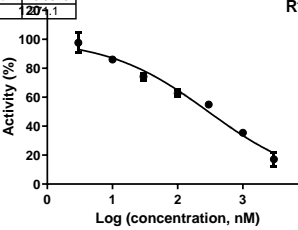
Best-fit values	
LogIC50	2.861
HillSlope	-0.4612
IC50	726.7

AA10 $IC_{50} = 726.7$
 $R^2 = 0.8431$



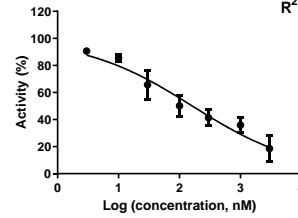
Best-fit values	
LogIC50	2.472
HillSlope	-0.5624
IC50	296.4

AA18 $IC_{50} = 296.4$
 $R^2 = 0.9677$



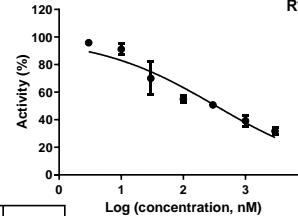
Best-fit values	
LogIC50	2.212
HillSlope	-0.4885
IC50	163.0

AA19 $IC_{50} = 163.0$
 $R^2 = 0.9170$



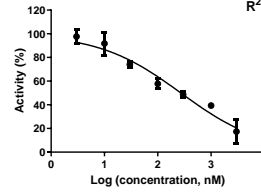
Best-fit values	
LogIC50	2.525
HillSlope	-0.4516
IC50	335.1

AA20 $IC_{50} = 335.1$
 $R^2 = 0.9057$



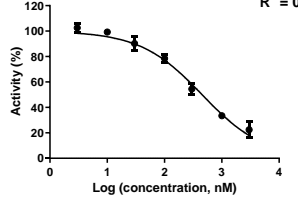
Best-fit values	
LogIC50	2.433
HillSlope	-0.5646
IC50	271.1

AA17 $IC_{50} = 271.1$
 $R^2 = 0.9343$



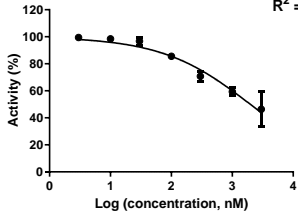
Best-fit values	
LogIC50	2.656
HillSlope	-0.8046
IC50	452.6

AA22 $IC_{50} = 452.6$
 $R^2 = 0.9762$



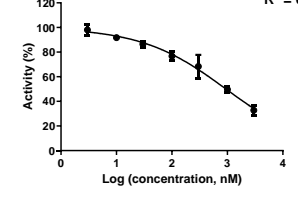
Best-fit values	
LogIC50	3.297
HillSlope	-0.5953
IC50	1980

AA23 $IC_{50} = 1980$
 $R^2 = 0.9297$



Best-fit values	
LogIC50	2.975
HillSlope	-0.5687
IC50	944.9

AA24 $IC_{50} = 944.9$
 $R^2 = 0.9656$



Best-fit values	
LogIC50	2.334
HillSlope	-0.4244
IC50	215.6

AA21 $IC_{50} = 215.6$
 $R^2 = 0.9490$

