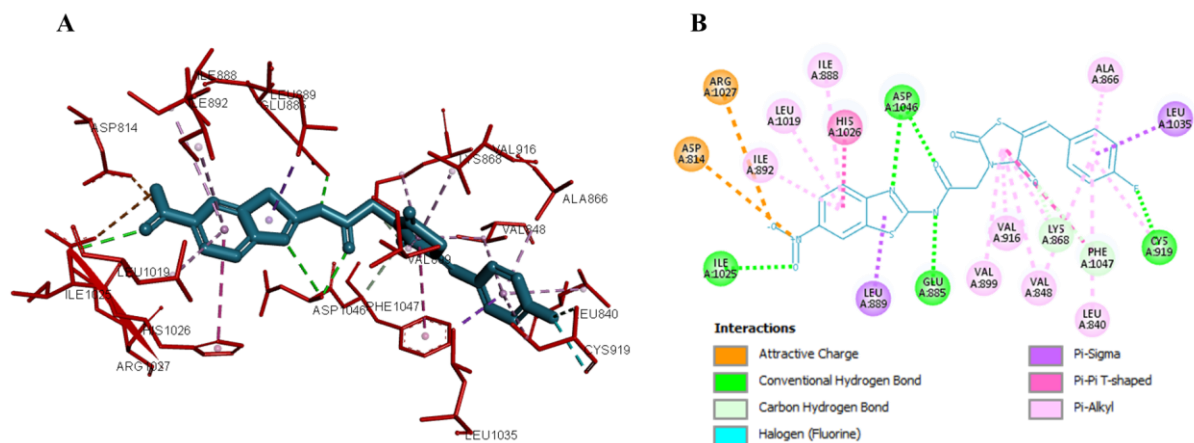


Supplementary file

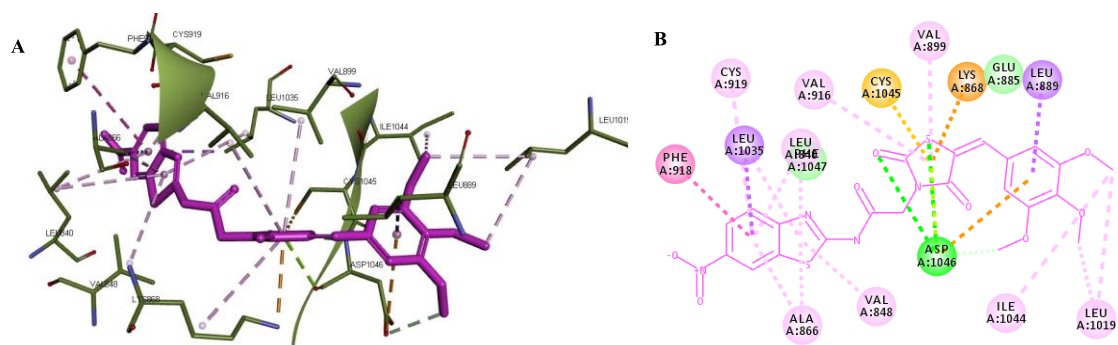
**New benzothiazole hybrids as Potential VEGFR-2 inhibitors: Design, Synthesis,  
Anticancer Evaluation and *In Silico* Study**

Mohammad M. Al-Sanea<sup>1,†,\*</sup>, Abdelrahman Hamdi<sup>2,†</sup>, Ahmed A. B. Mohamed<sup>3,†,\*</sup>, Hamed W. El-Shafey<sup>2</sup>, Mahmoud Moustafa<sup>4</sup>, Abdullah A. Elgazar<sup>5</sup>, Wagdy M. Eldehna<sup>6</sup>, Hidayat Ur Rahman<sup>7</sup>, Della G. T. Parambi<sup>1</sup>, Rehab M. Elbargisy<sup>8</sup>, Samy Selim<sup>9</sup>, Syed Nasir Abbas Bukhari<sup>1</sup>, Omnia Magdy Hendawy<sup>10</sup>, Samar S. Tawfik<sup>2</sup>

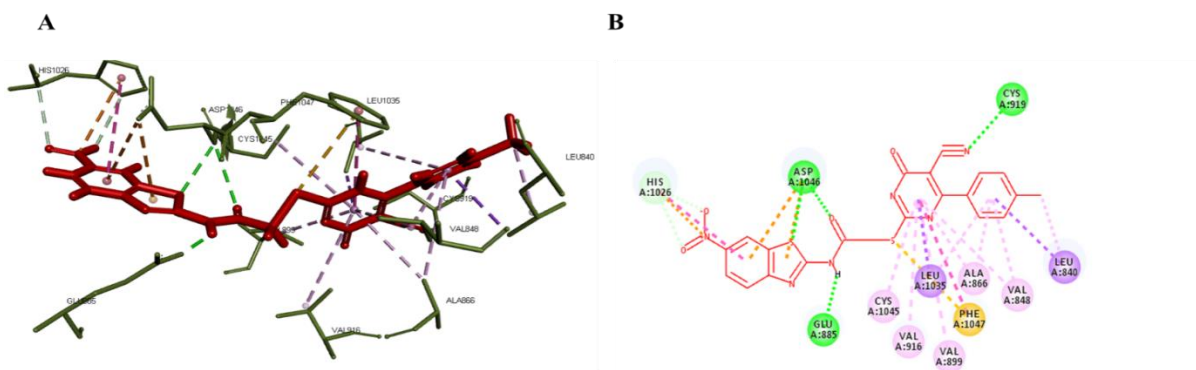
## Supplementary figures



**Fig. S1. A)** 3D interactions of **4a** (Turquoise) with the active site of VEGF2 **B)** 2D interactions of **4a** with amino acids in the active site of VEGFR-2.



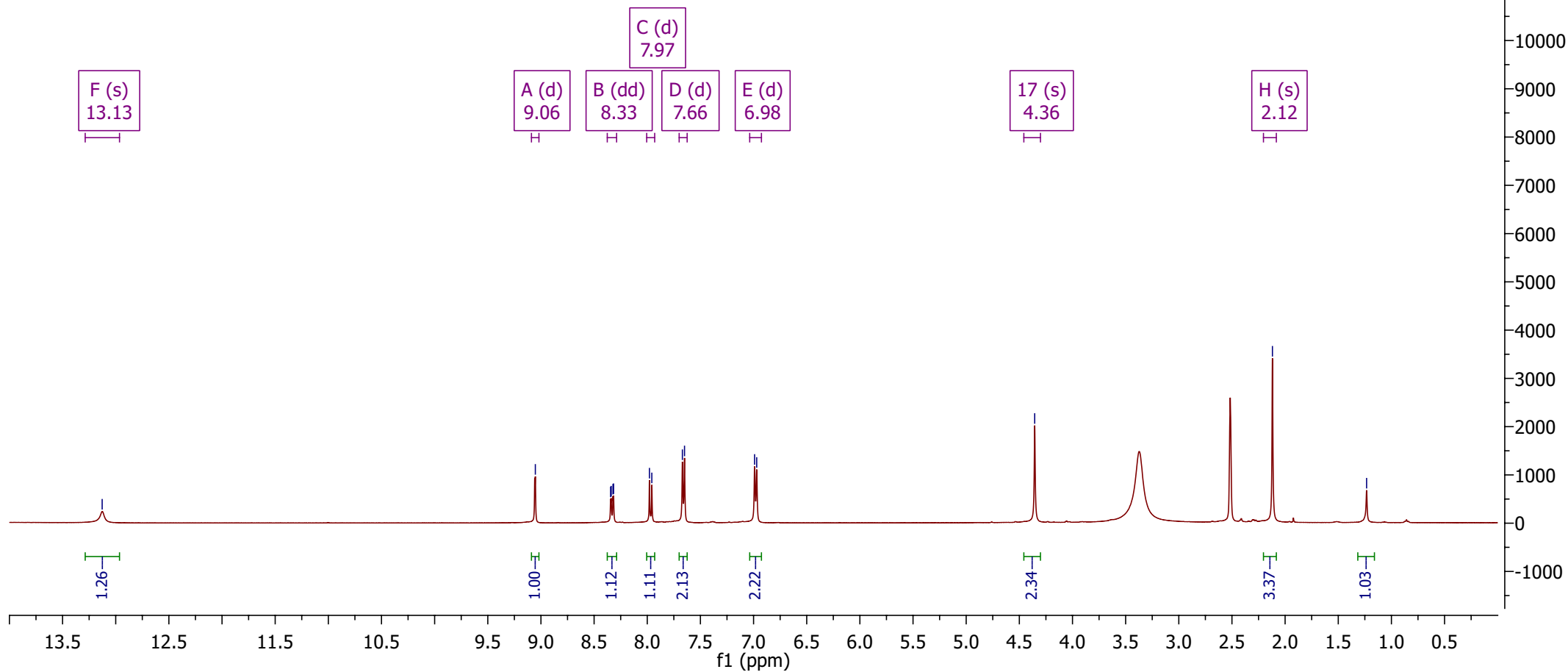
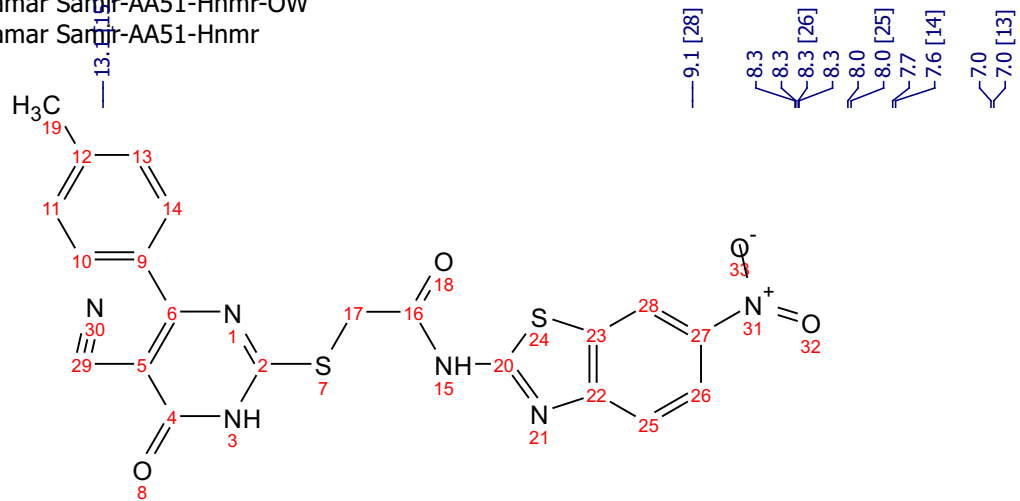
**Fig. S2.** A) 3D interactions of **4e** (magenta) with the active site of VEGFR-2. B) 2D interactions of **4e** with amino acids in the active site of VEGFR-2.



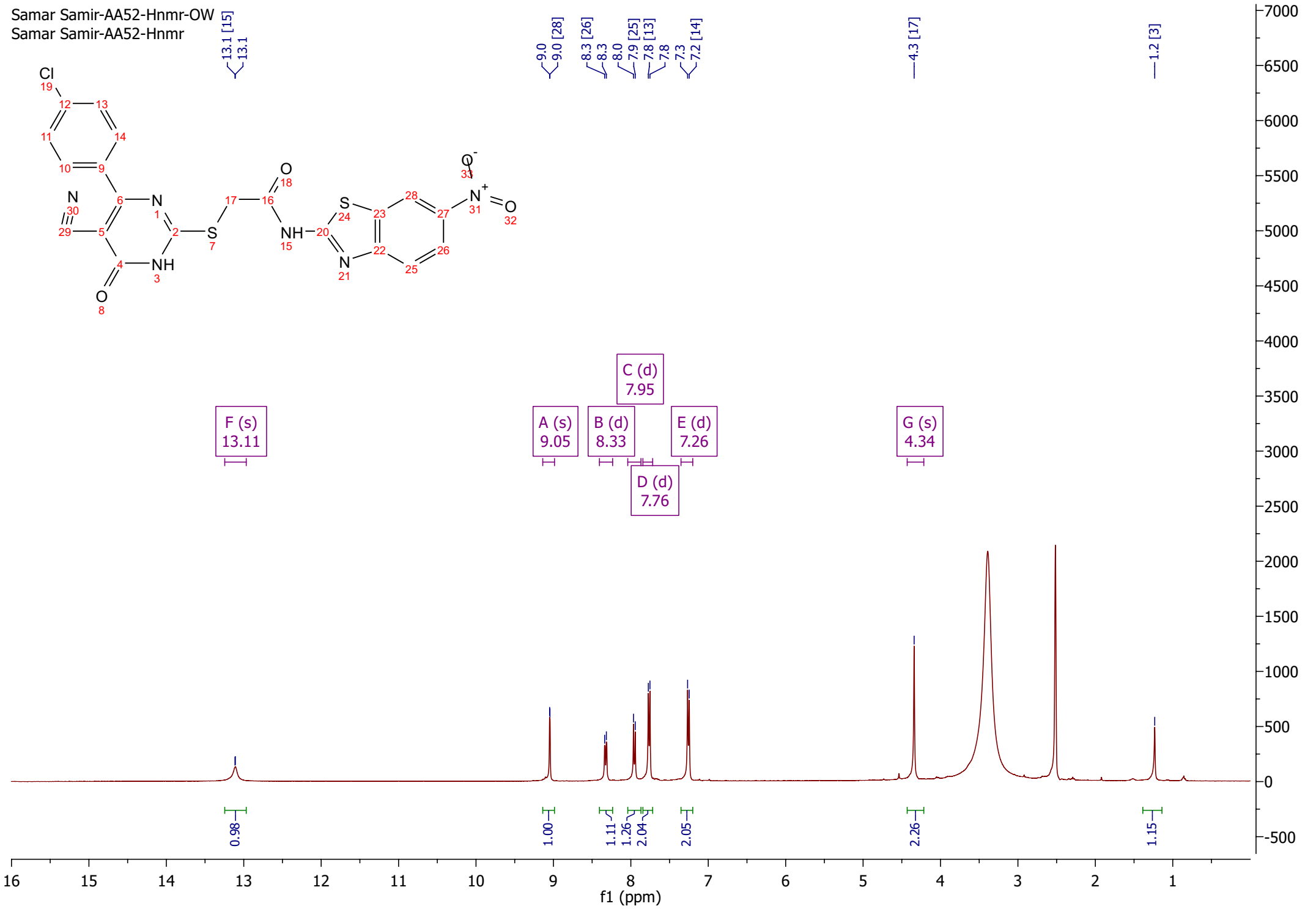
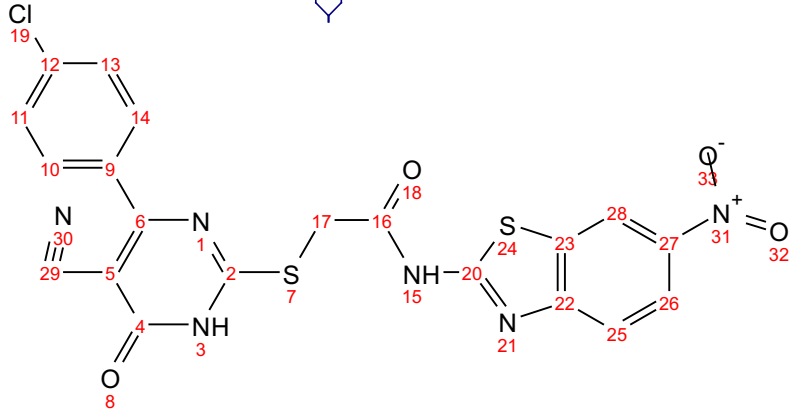
**Fig. S3.** A) 3D interactions of **8a** (Red) with the active site of VEGFR-2. B) 2D interactions of **8a** with amino acids in the active site of VEGFR-2.

## **NMR Charts**

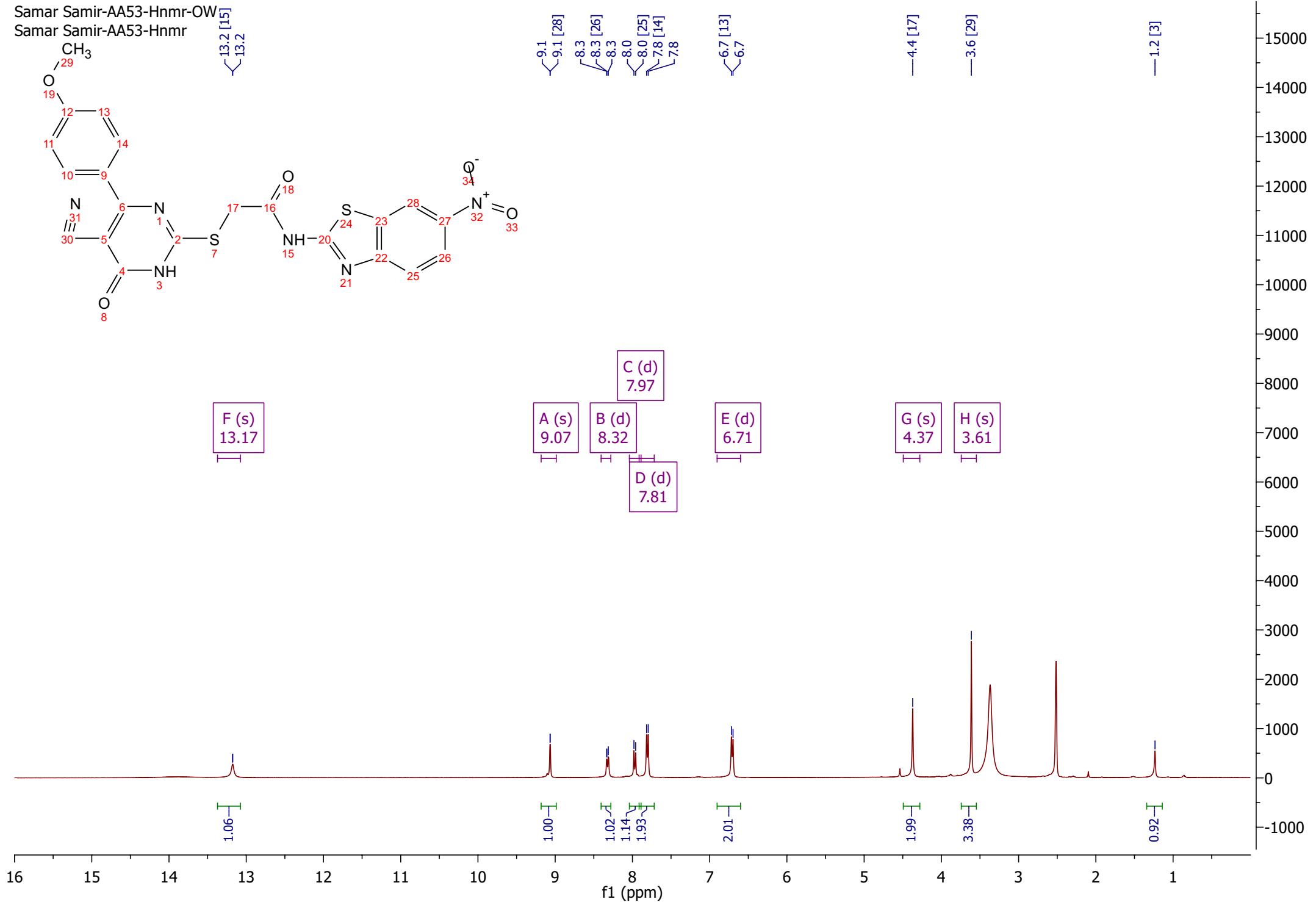
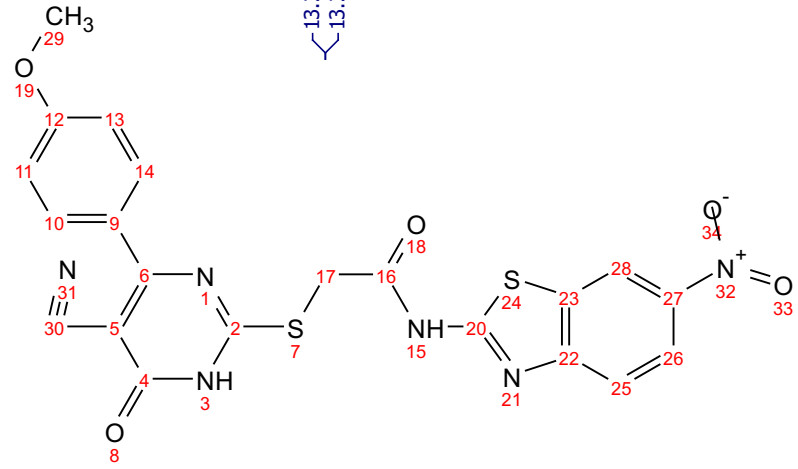
Samar Samir-AA51-Hnmr-OW  
 Samar Samir-AA51-Hnmr



Samar Samir-AA52-Hnmr-OW  
Samar Samir-AA52-Hnmr

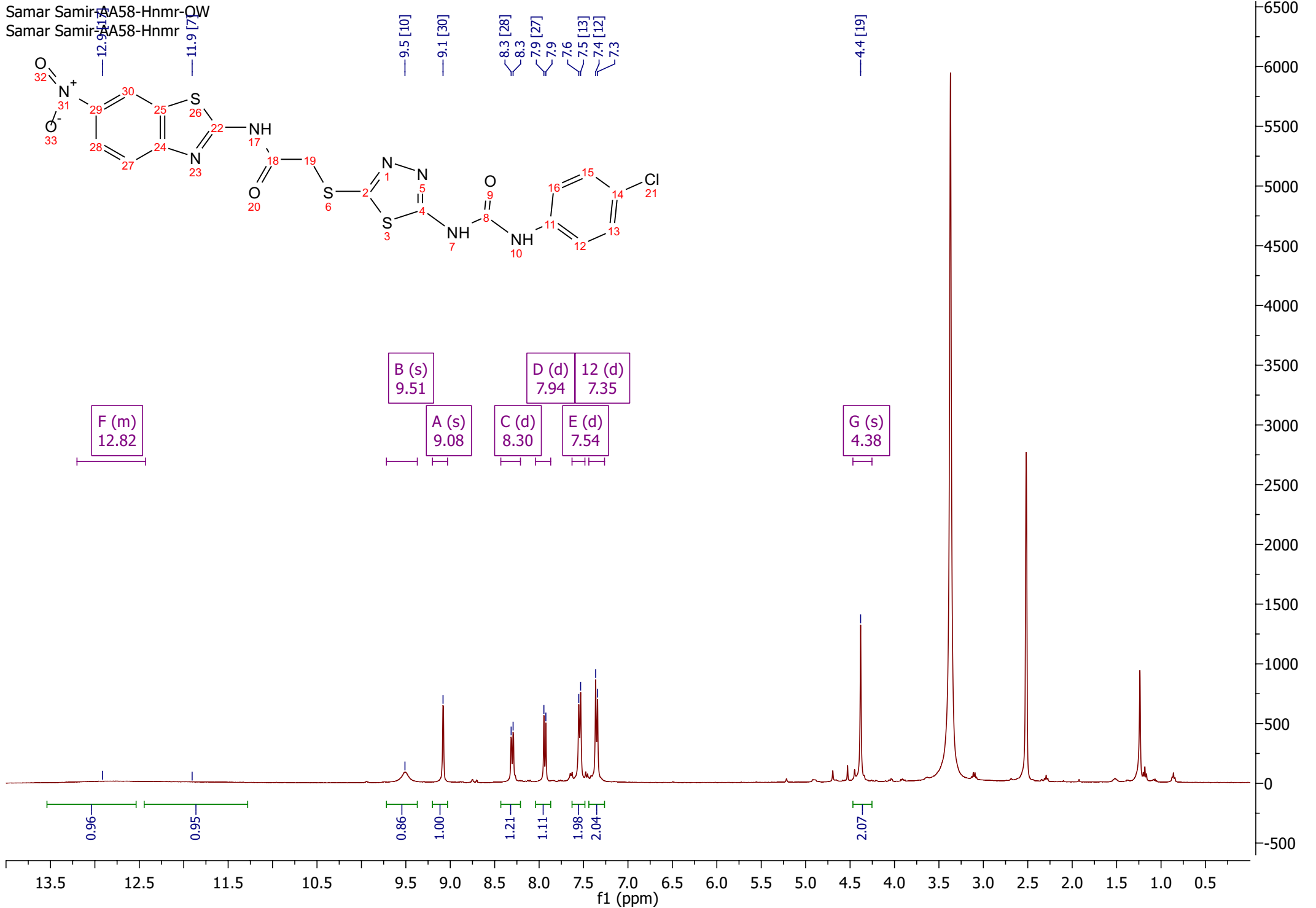


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Samar Samir-AA53-Hnmr

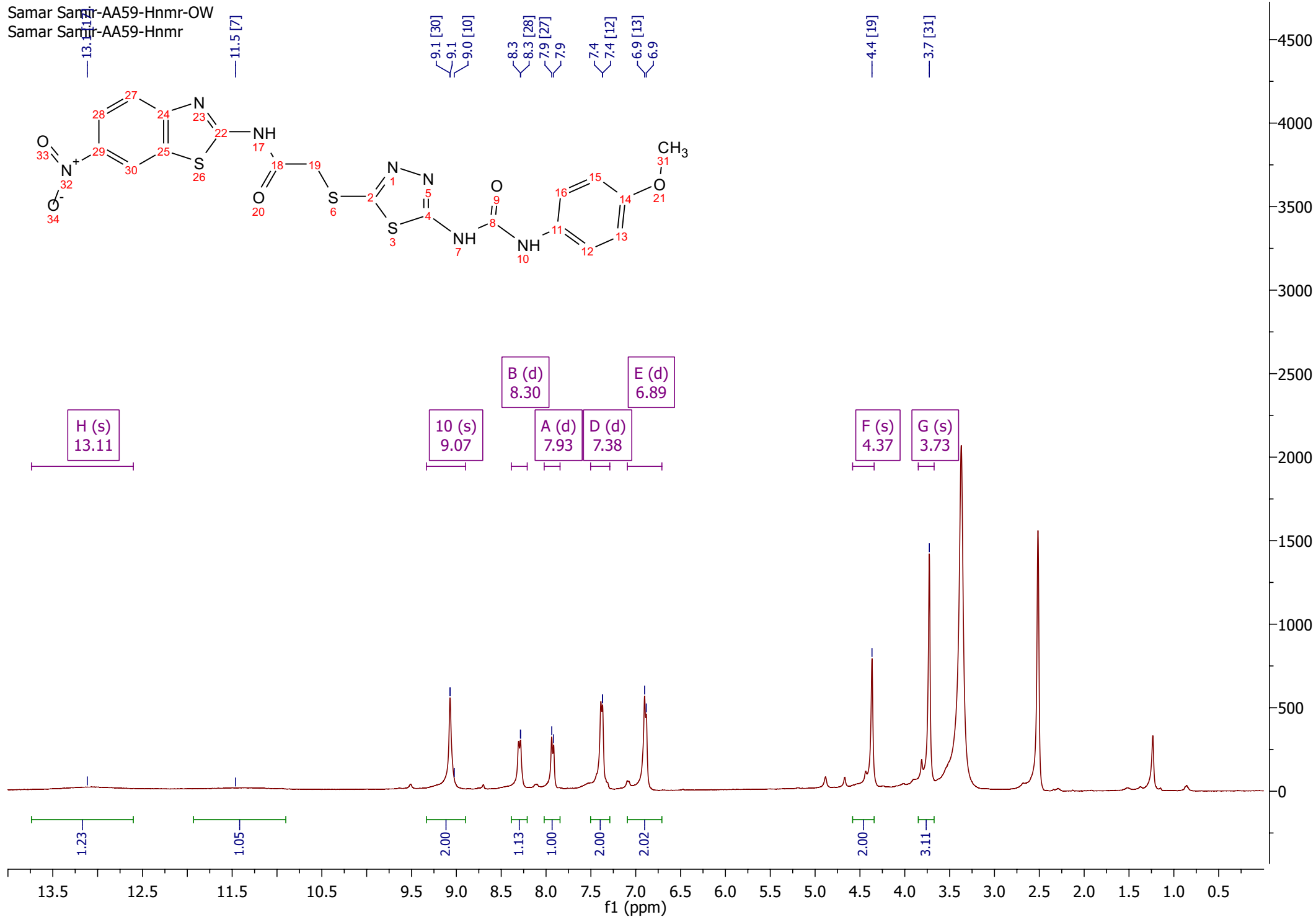




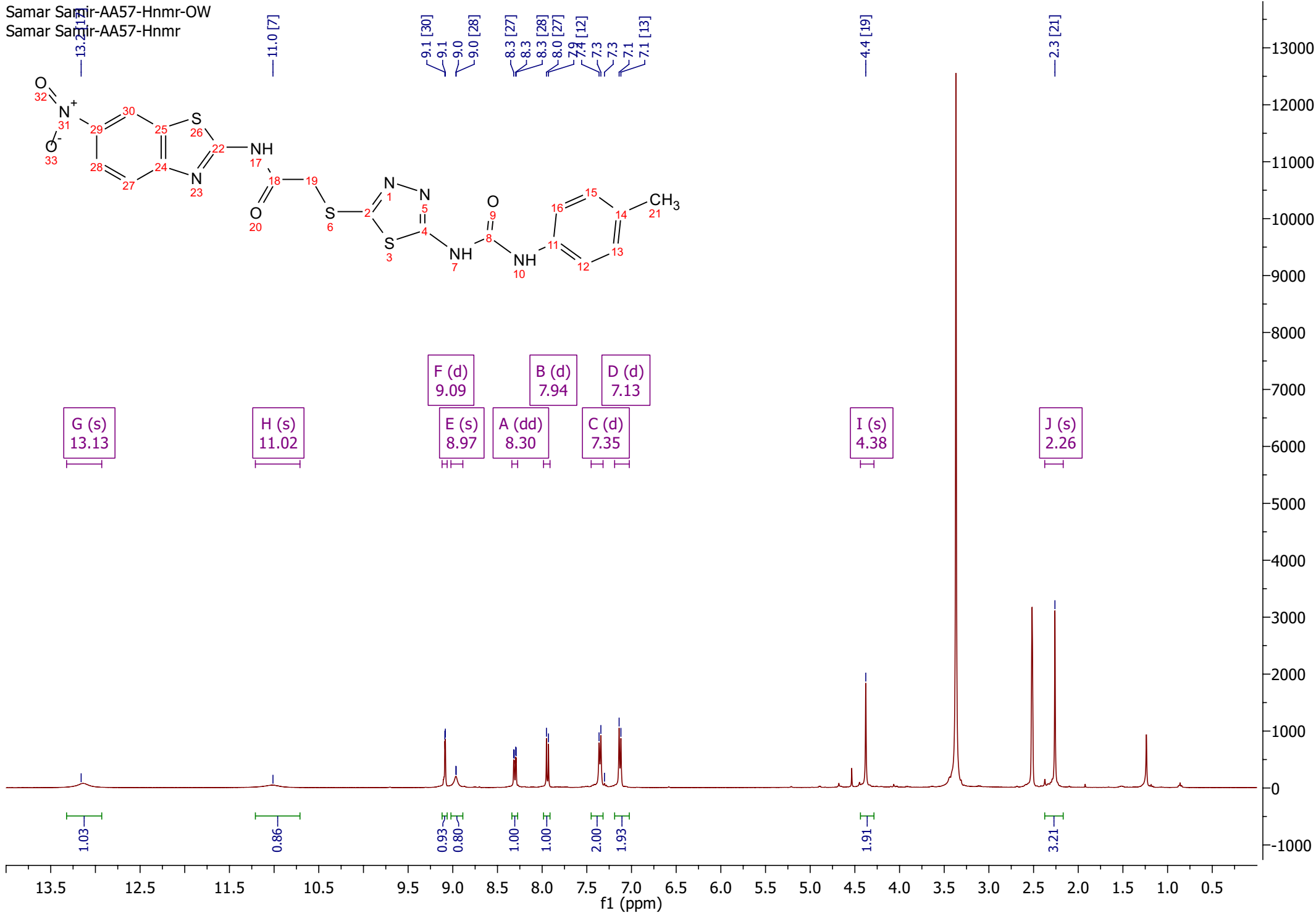
Samar Samir-AA58-Hnmr-QW  
Samar Samir-AA58-Hnmr



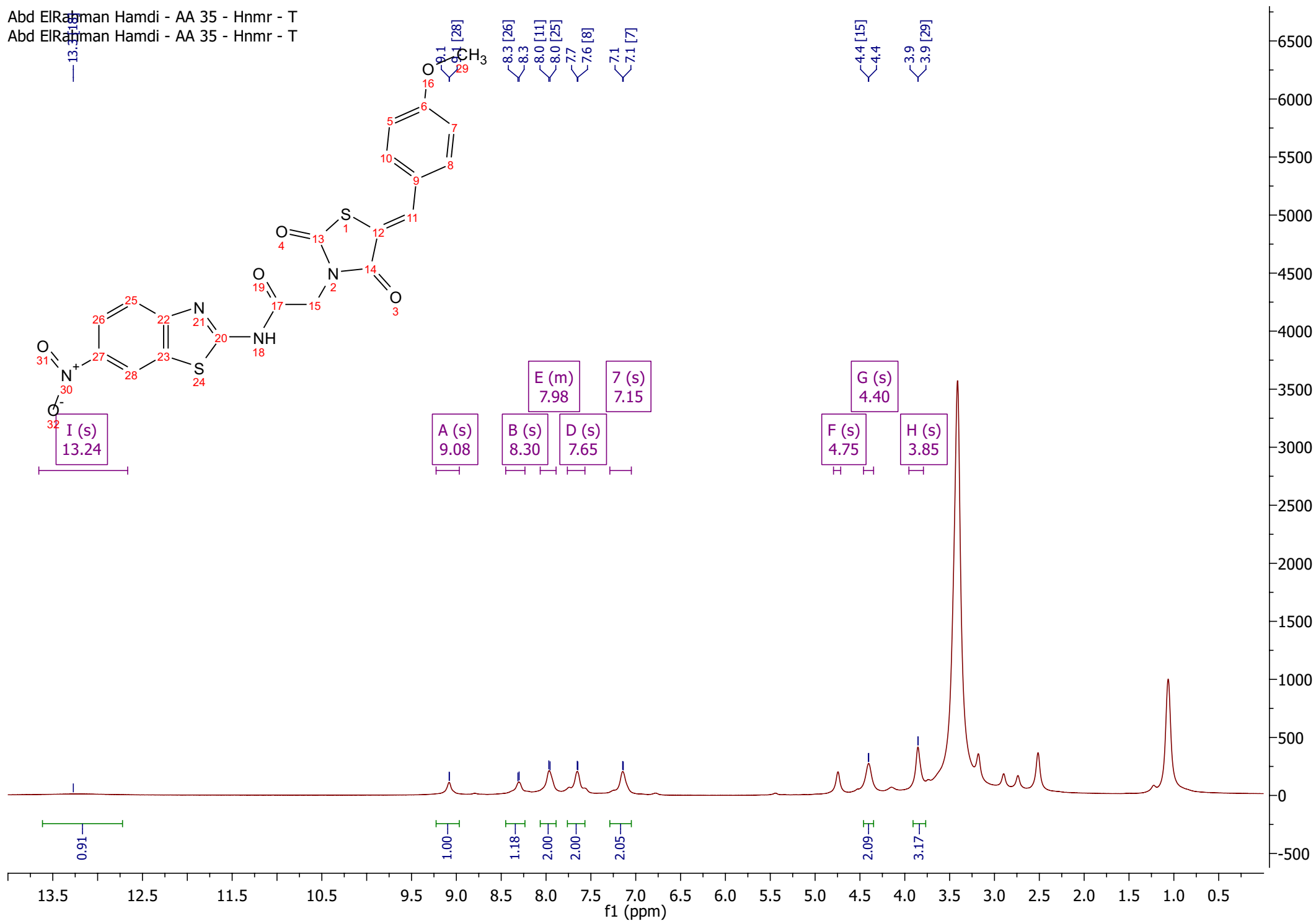
Samar Samir-AA59-Hnmr-OW  
Samar Samir-AA59-Hnmr



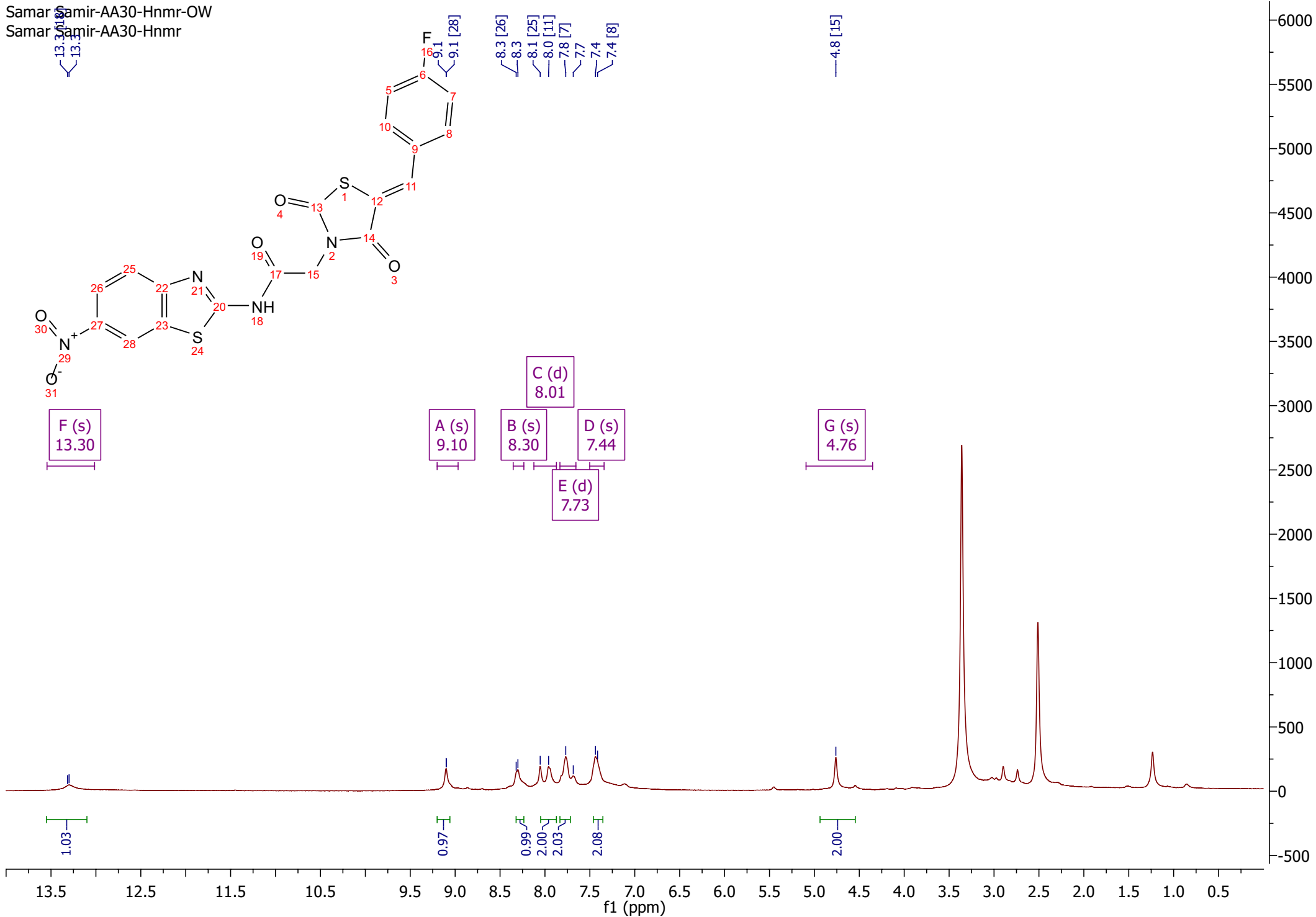
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 Samar Samir-AA57-Hnmr



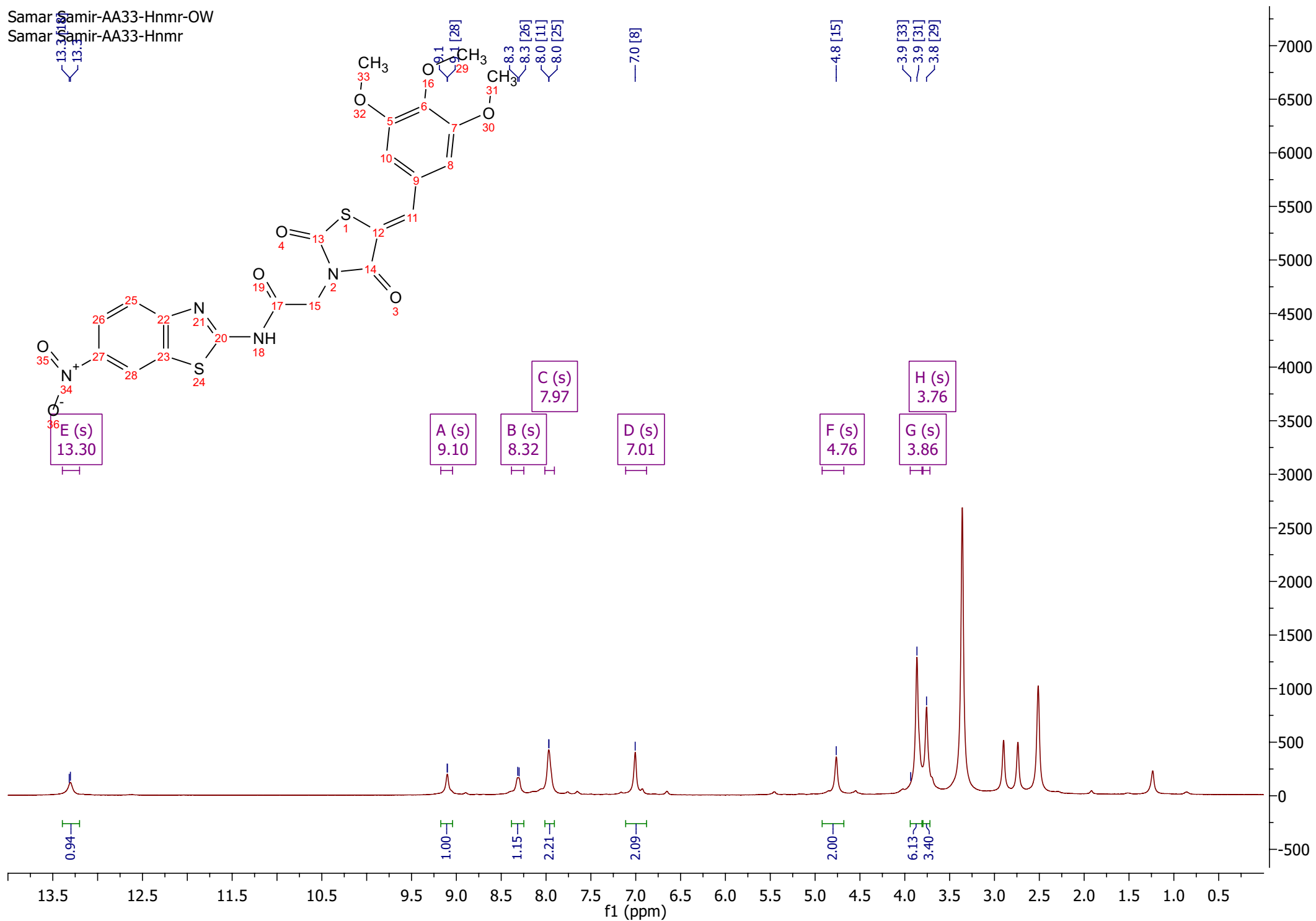
Abd ElRahman Hamdi - AA 35 - Hnmr - T  
Abd ElRahman Hamdi - AA 35 - Hnmr - T



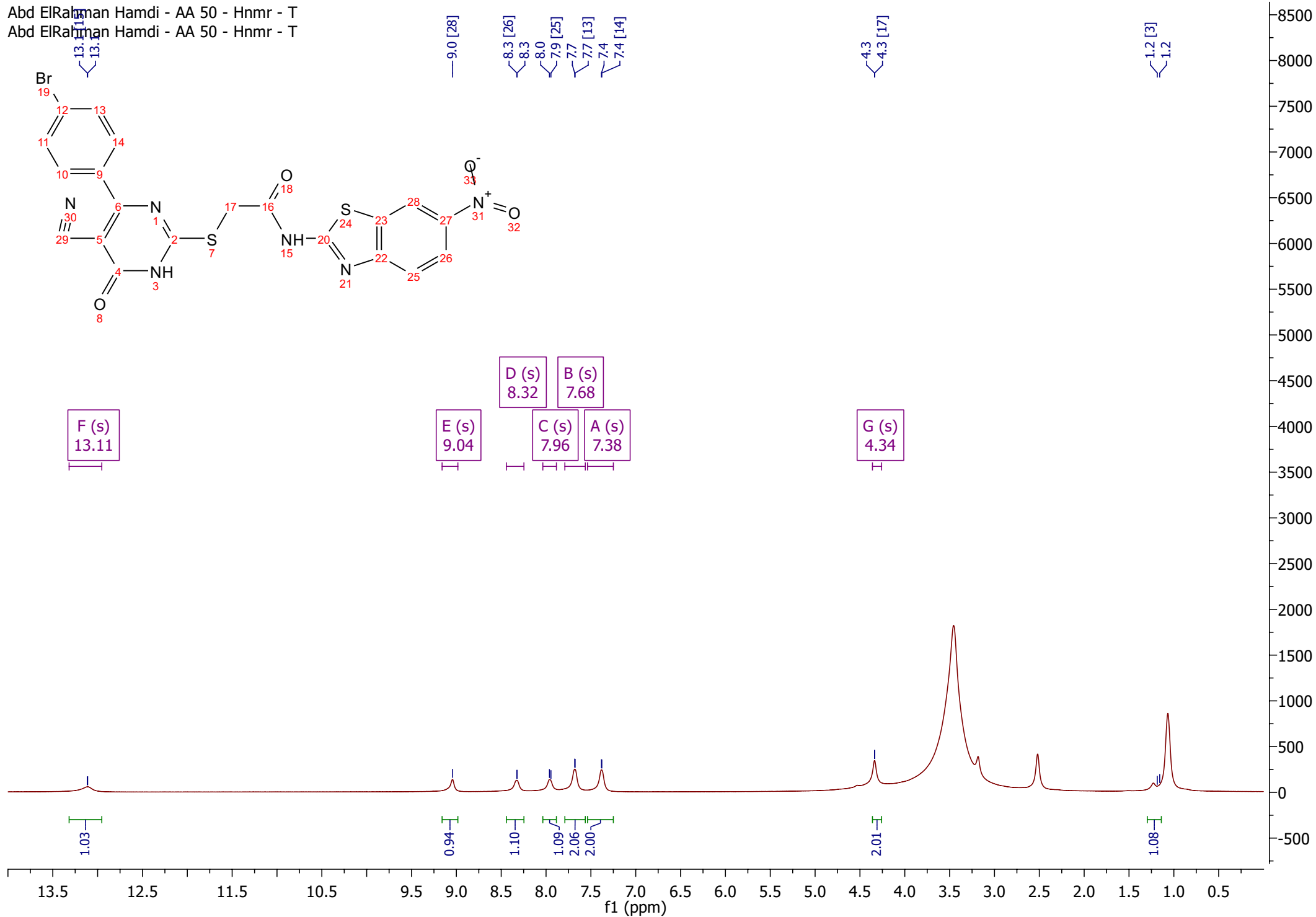
Samar Samir-AA30-Hnmr-OW  
Samar Samir-AA30-Hnmr



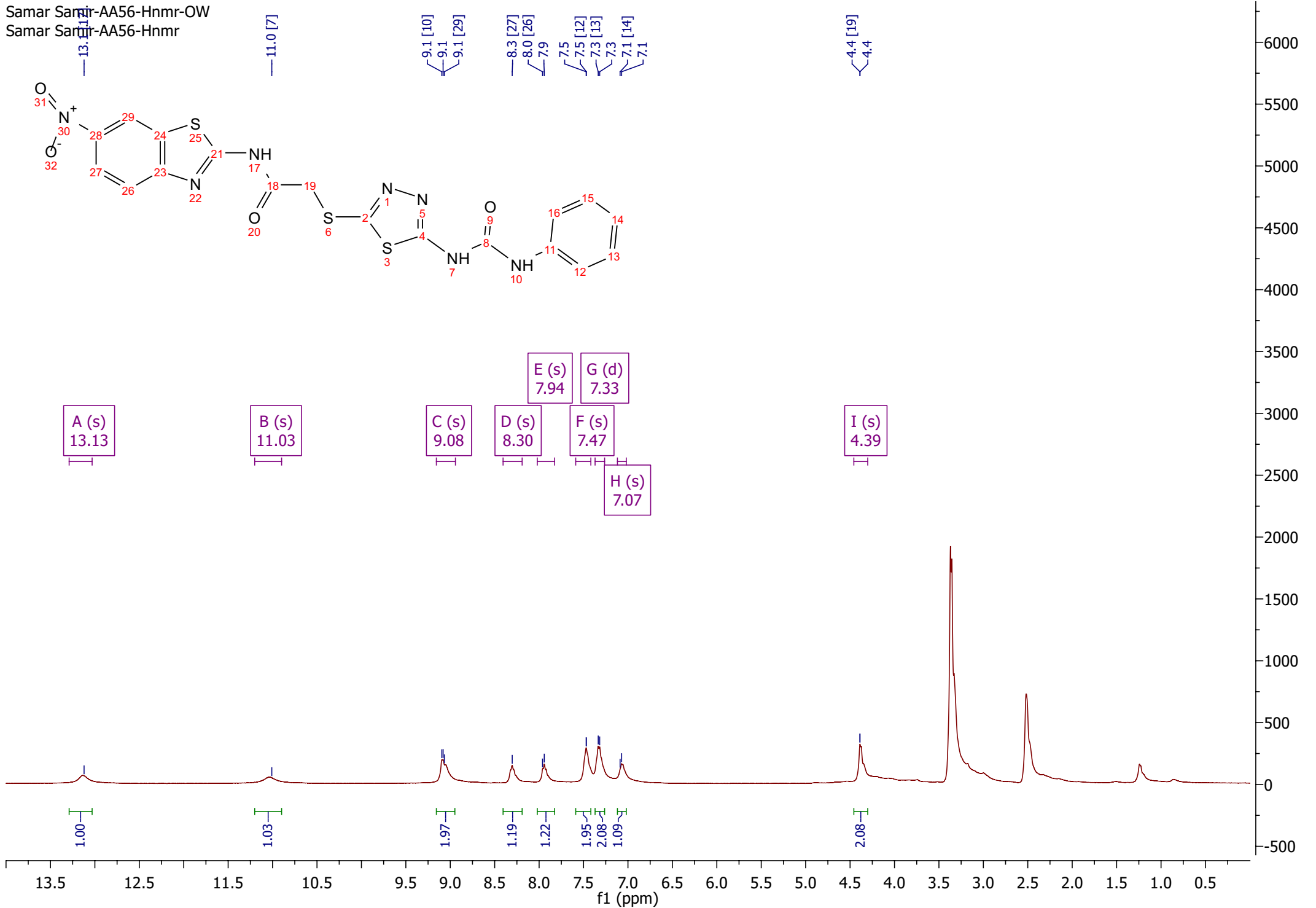
Samar Samir-AA33-Hnmr-OW  
Samar Samir-AA33-Hnmr



Abd ElRahman Hamdi - AA 50 - Hnmr - T  
Abd ElRahman Hamdi - AA 50 - Hnmr - T

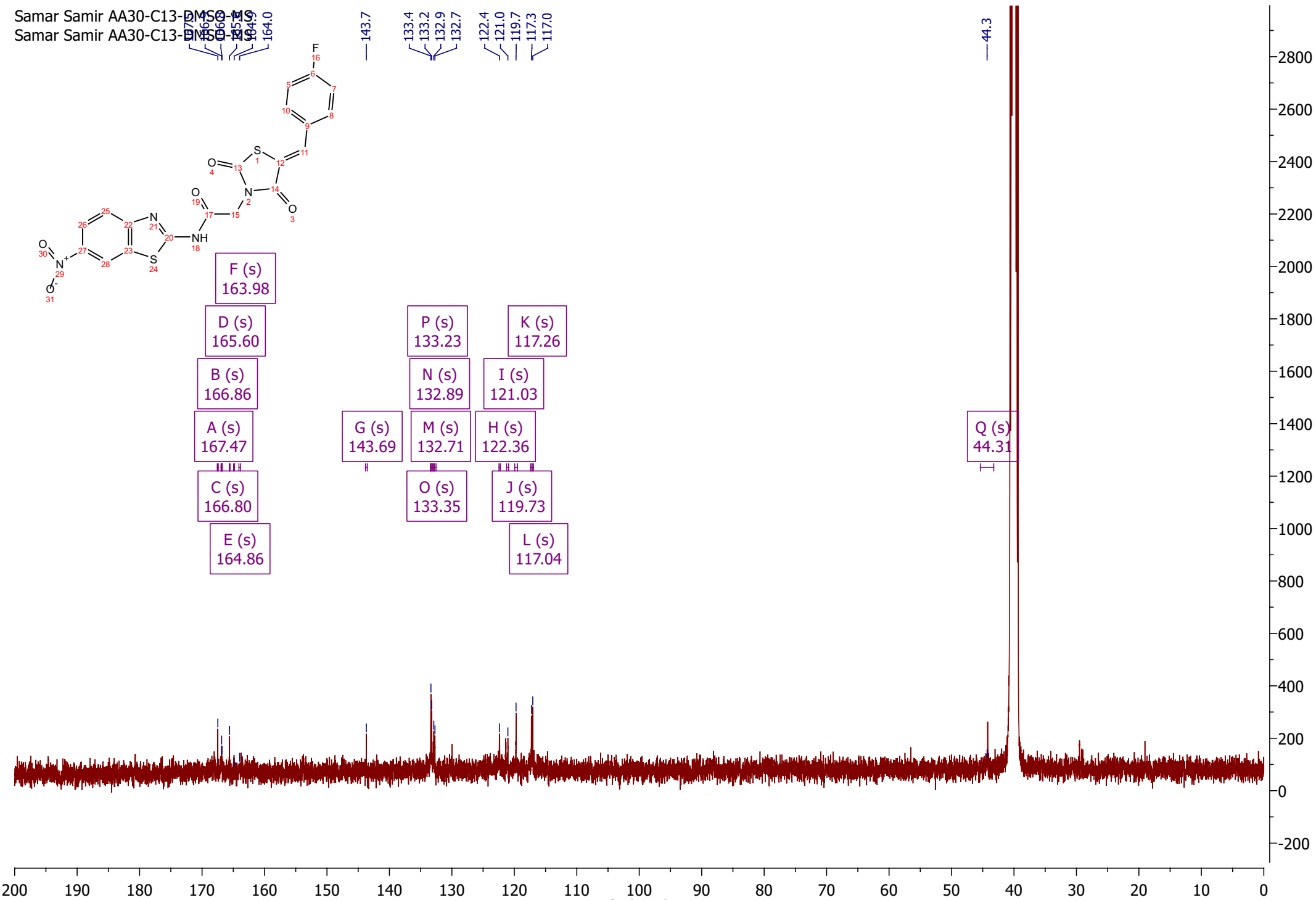
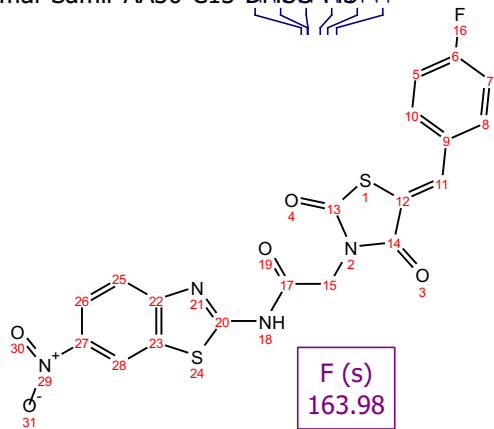


Samar Samir-AA56-Hnmr-OW  
Samar Samir-AA56-Hnmr

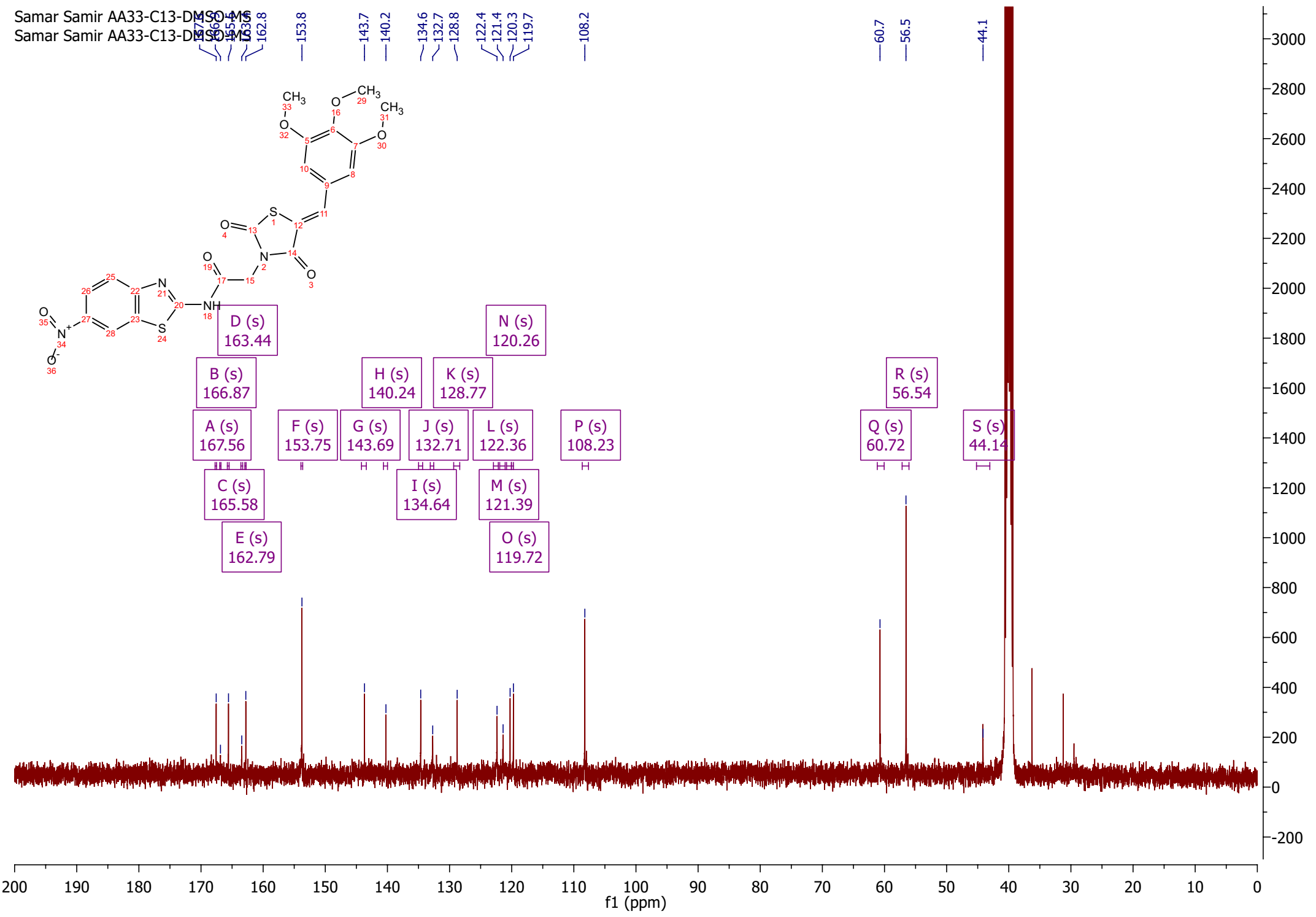




Samar Samir AA30-C13-DMSO-MG  
Samar Samir AA30-C13-DMSO-MG



Samar Samir AA33-C13-DMSO-d6  
Samar Samir AA33-C13-DMSO-d6



samarsamir-AA35-13C-DMSO-d6  
samarsamir-AA35-13C-DMSO-d6

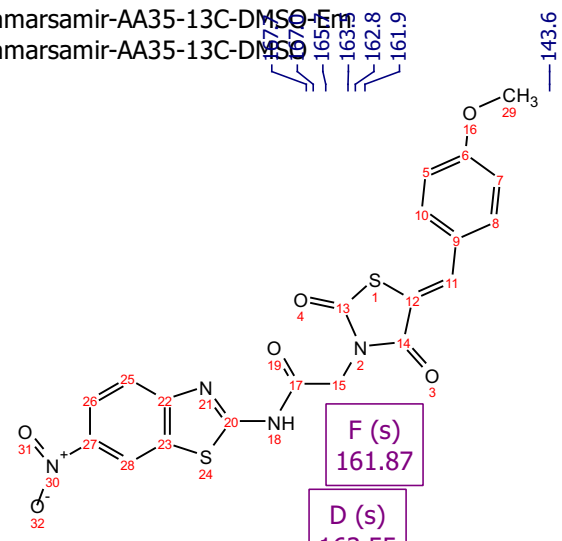
167.74  
165.74  
163.55  
162.82  
162.8  
161.9

143.6

134.4  
132.9  
132.7  
132.5  
125.7  
122.3  
121.3  
119.7  
117.9  
115.5

56.0

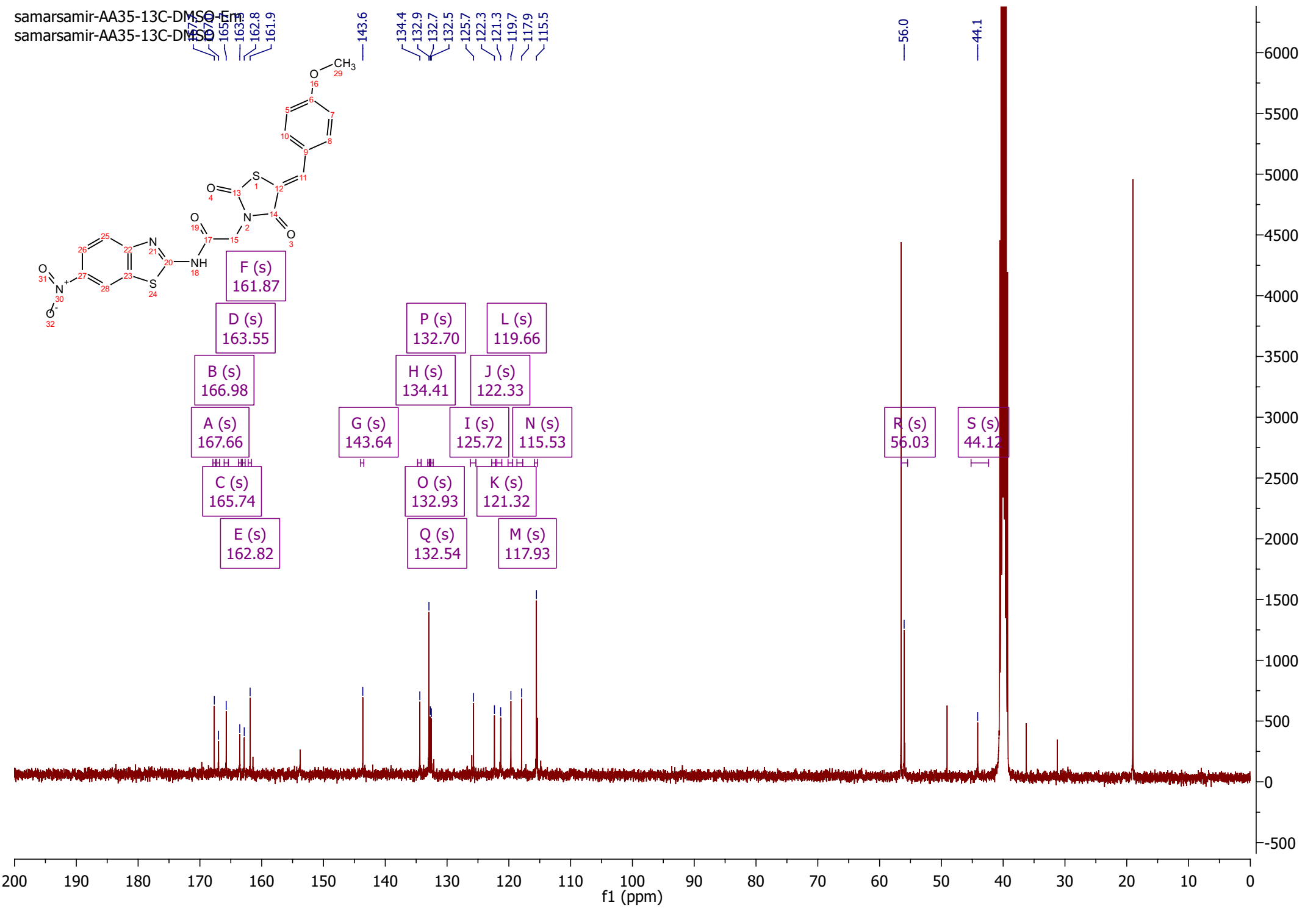
44.1



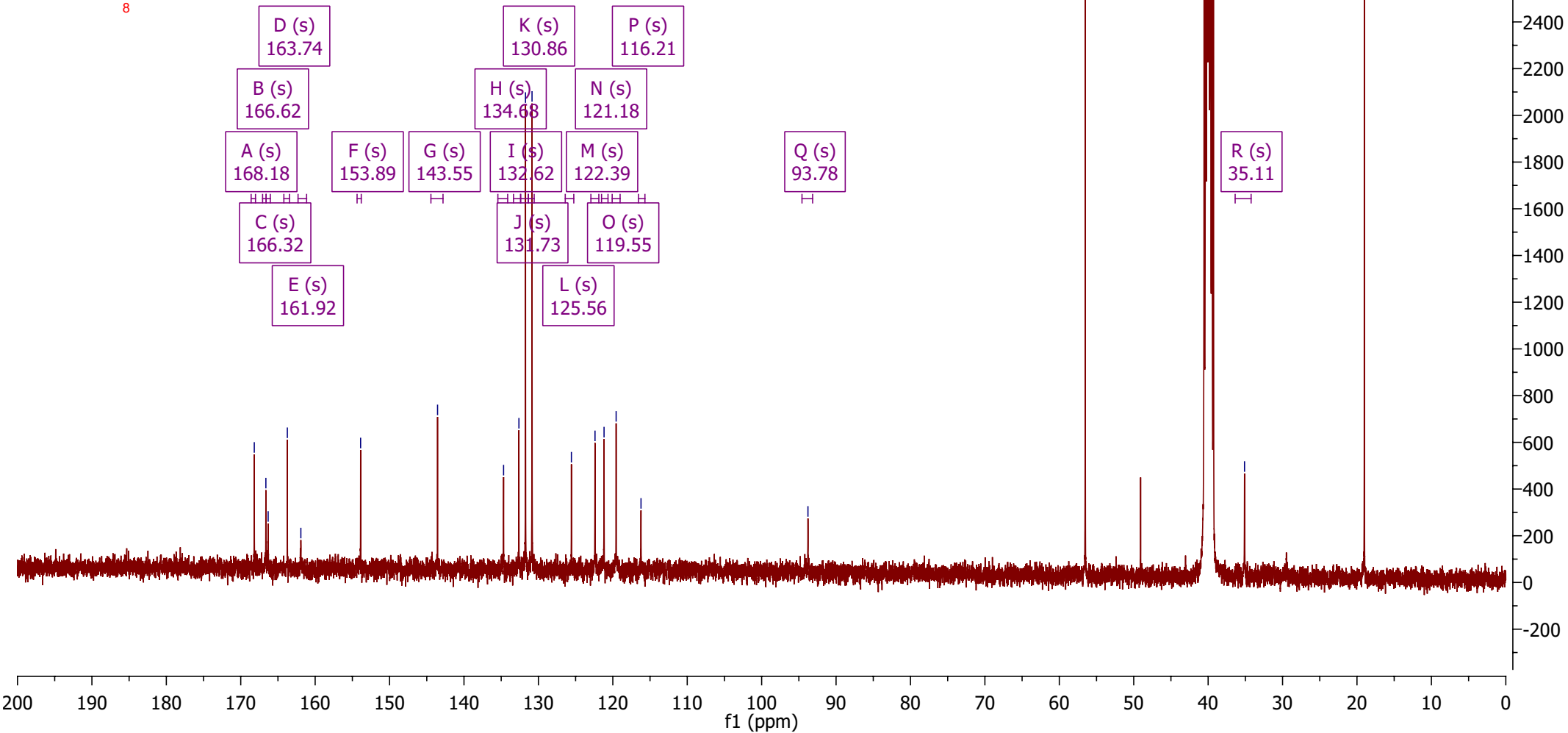
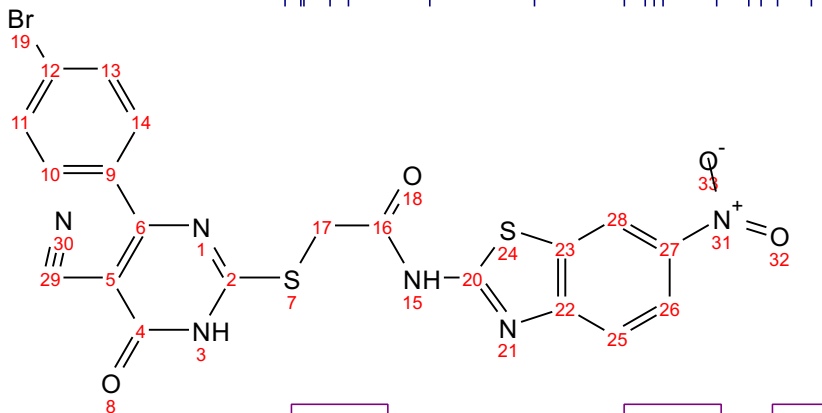
F (s)  
161.87  
D (s)  
163.55  
B (s)  
166.98  
A (s)  
167.66  
C (s)  
165.74  
E (s)  
162.82

P (s)  
132.70  
L (s)  
119.66  
H (s)  
134.41  
J (s)  
122.33  
G (s)  
143.64  
I (s)  
125.72  
N (s)  
115.53  
O (s)  
132.93  
K (s)  
121.32  
Q (s)  
132.54  
M (s)  
117.93

R (s)  
56.03  
S (s)  
44.12

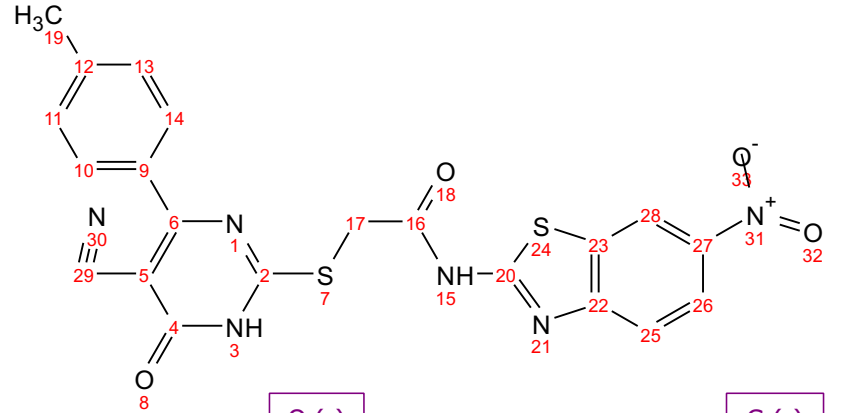


samarsamir-AA50-13C-DMSO-d6  
samarsamir-AA50-13C-DMSO-d6



Samar Samir AA51-C13-DMSO-M8  
Samar Samir AA51-C13-DMSO-M8

167.58 165.67 161.86 153.97 143.52 142.1 132.7 129.27 129.0 122.33 121.12 119.59 116.44 93.13 35.09 21.28



O (s) 167.58  
L (s) 161.86  
M (s) 163.82  
N (s) 165.67  
P (s) 168.11  
K (s) 153.97  
J (s) 143.52  
I (s) 142.13  
H (d) 132.69  
Q (s) 129.27  
R (s) 128.96  
G (s) 122.33  
F (s) 121.12  
E (s) 119.59  
D (s) 116.44

C (s) 93.13

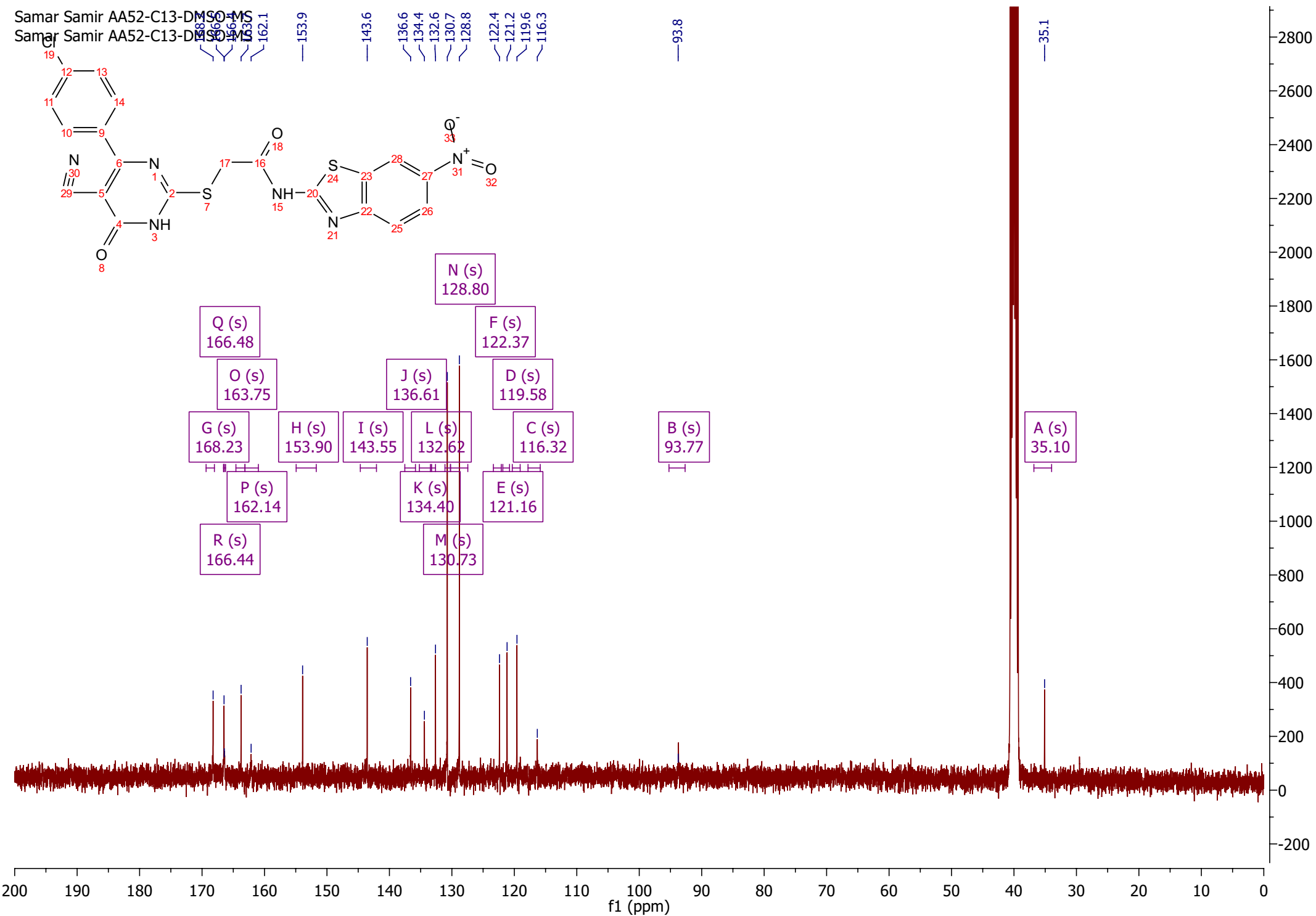
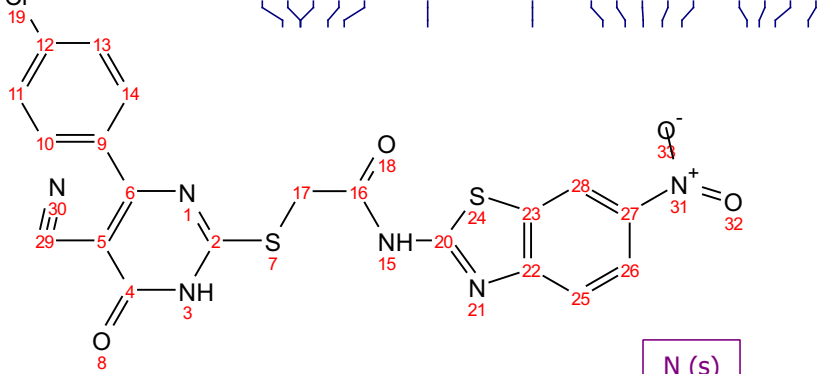
A (s) 35.09

B (s) 21.28

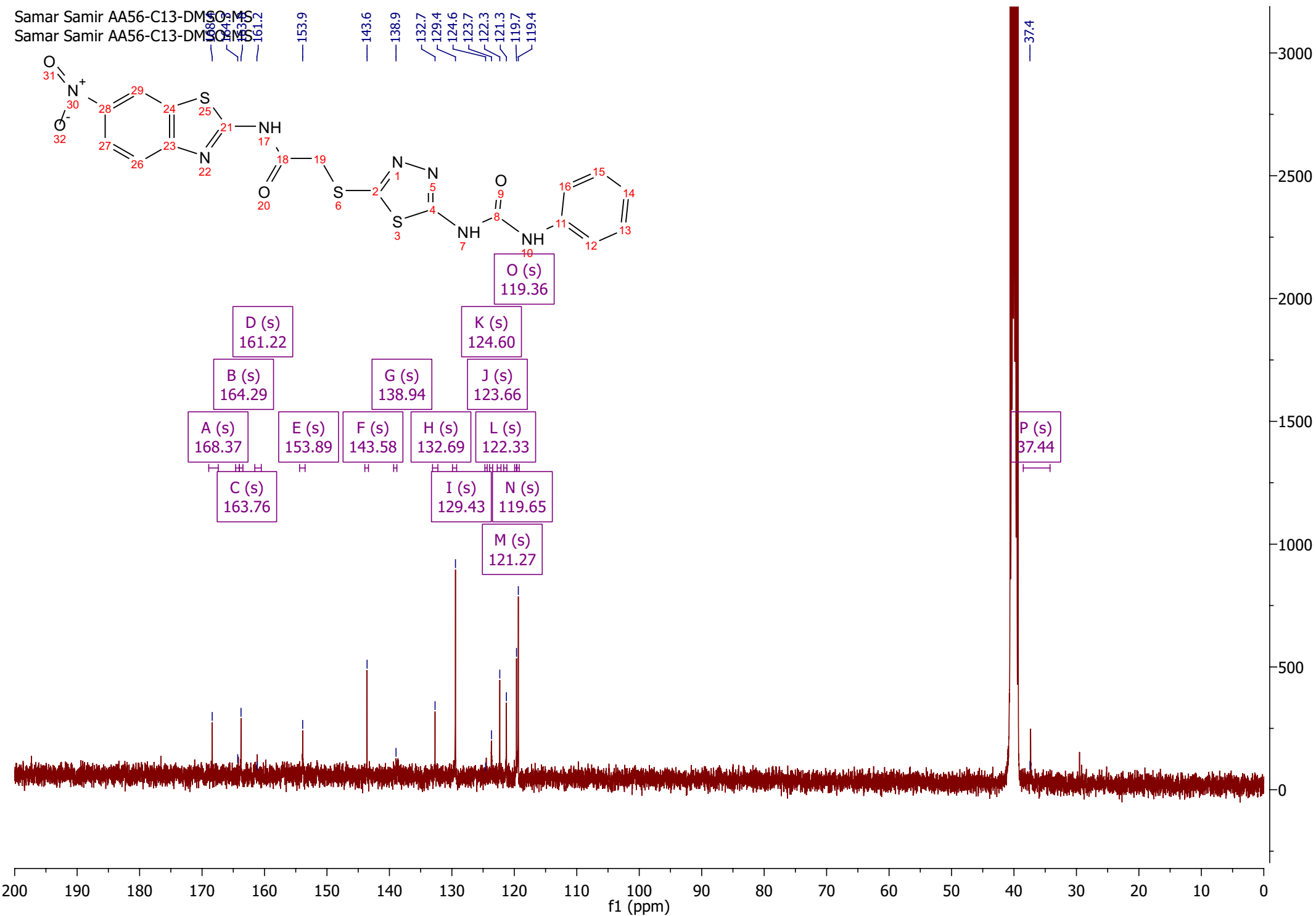
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0  
f1 (ppm)

4500  
4000  
3500  
3000  
2500  
2000  
1500  
1000  
500  
0

Samar Samir AA52-C13-DMSO-M5  
Samar Samir AA52-C13-DMSO-M5

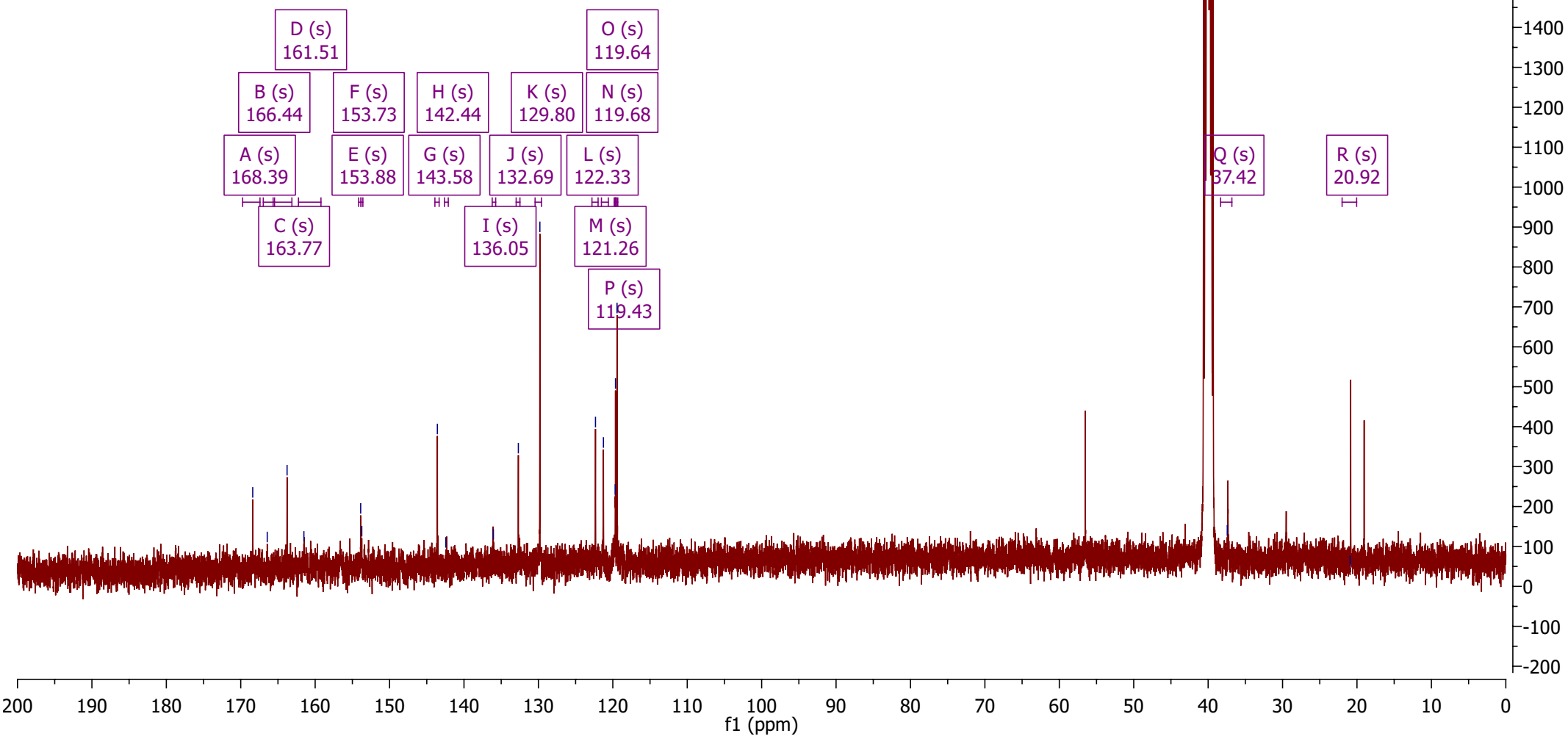
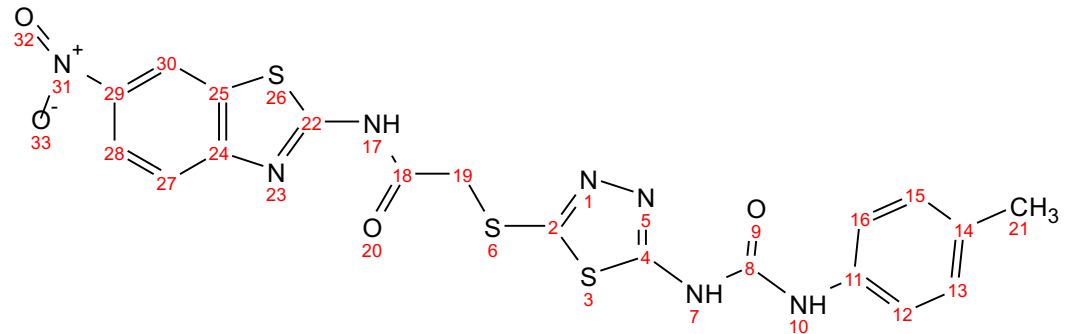


Samar Samir AA56-C13-DMSO-d6 MS  
Samar Samir AA56-C13-DMSO-d6 MS



Samar Samir AA57-C13-DMFMS  
Samar Samir AA57-C13-DMFMS

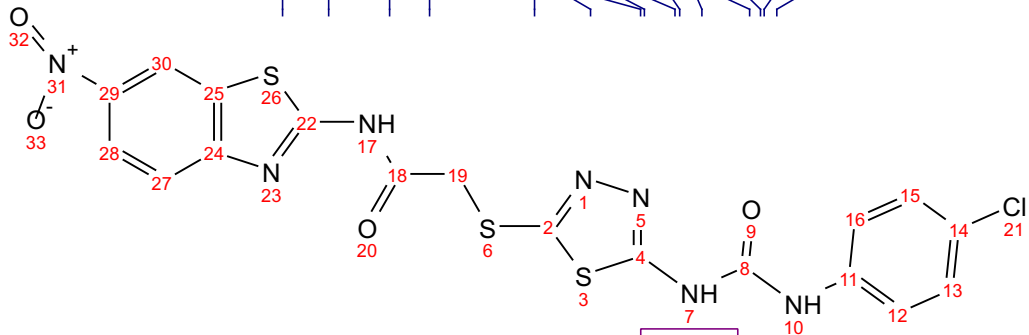
188.6  
186.6  
183.3  
181.2  
153.9  
153.7  
143.6  
142.4  
136.1  
132.7  
129.8  
122.3  
121.3  
119.7  
119.6  
119.4



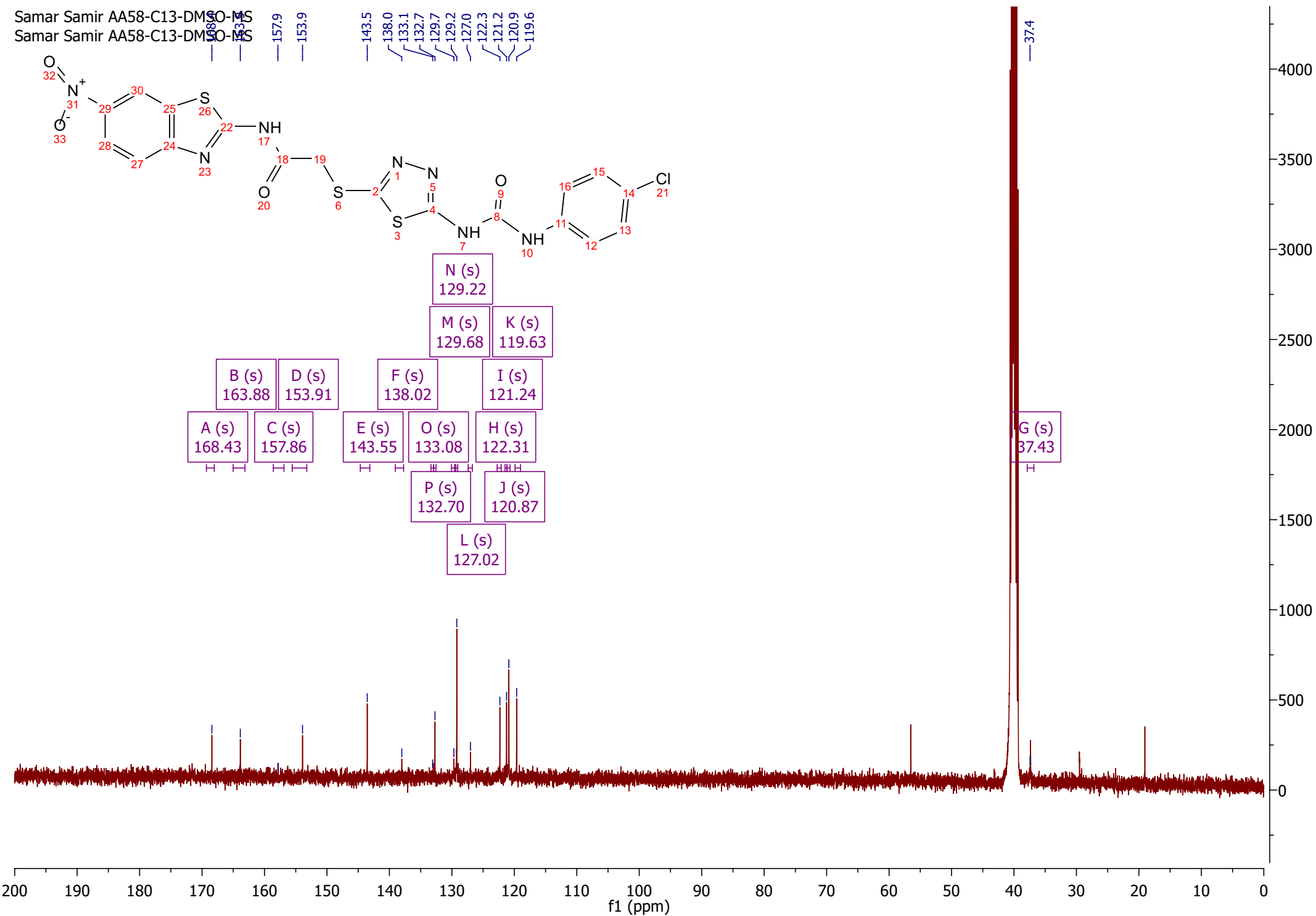


Samar Samir AA58-C13-DMSO-MS  
Samar Samir AA58-C13-DMSO-MS

157.9  
153.9  
143.5  
138.0  
133.1  
132.7  
129.7  
129.2  
127.0  
122.3  
121.2  
120.9  
119.6



N (s) 129.22	
M (s) 129.68	K (s) 119.63
B (s) 163.88	D (s) 153.91
A (s) 168.43	C (s) 157.86
E (s) 143.55	
F (s) 138.02	I (s) 121.24
O (s) 133.08	H (s) 122.31
P (s) 132.70	J (s) 120.87
L (s) 127.02	



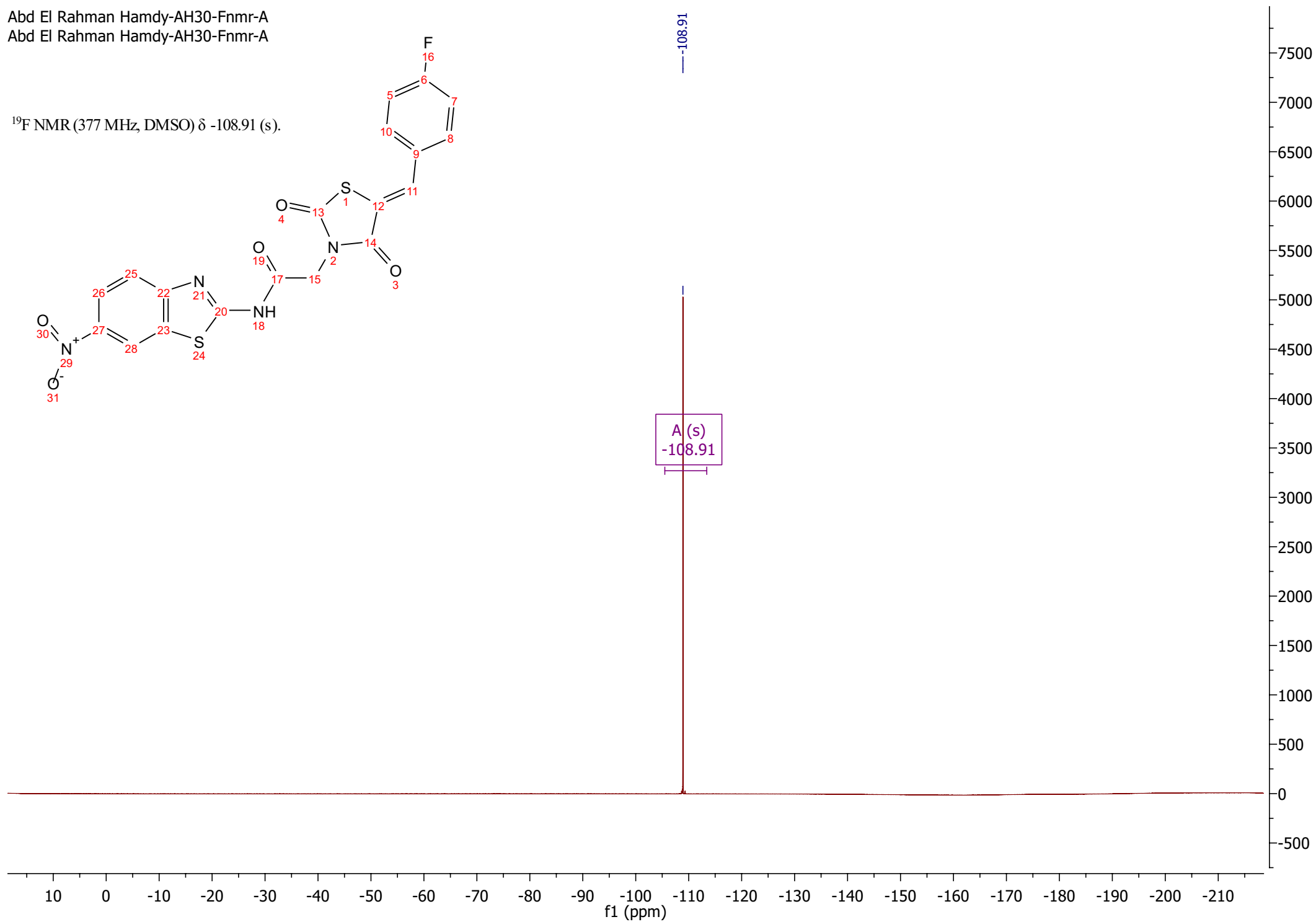
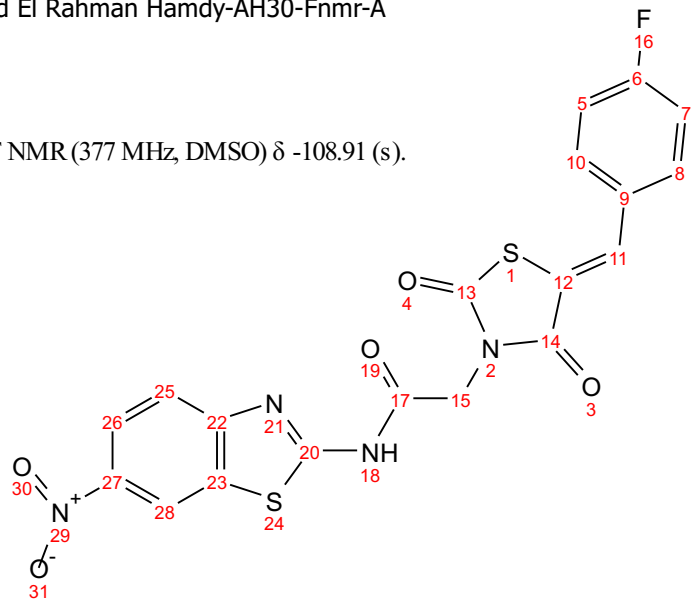
37.4

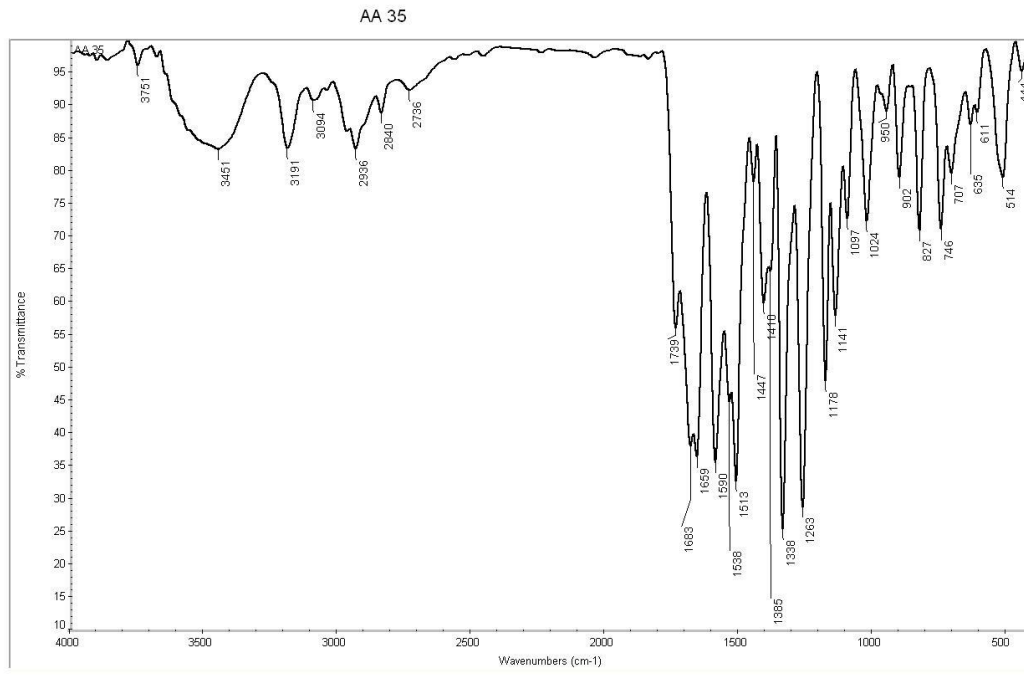
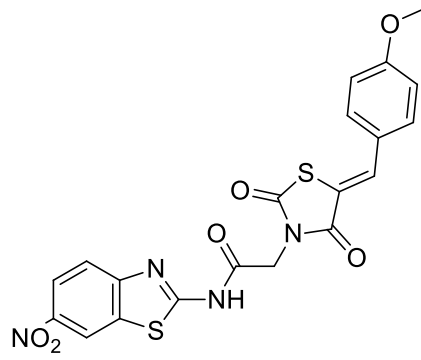
G (s)  
37.43

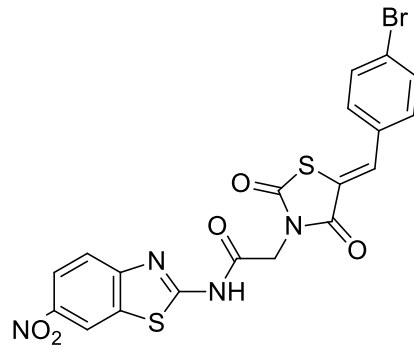
f1 (ppm)

Abd El Rahman Hamdy-AH30-Fnmr-A  
Abd El Rahman Hamdy-AH30-Fnmr-A

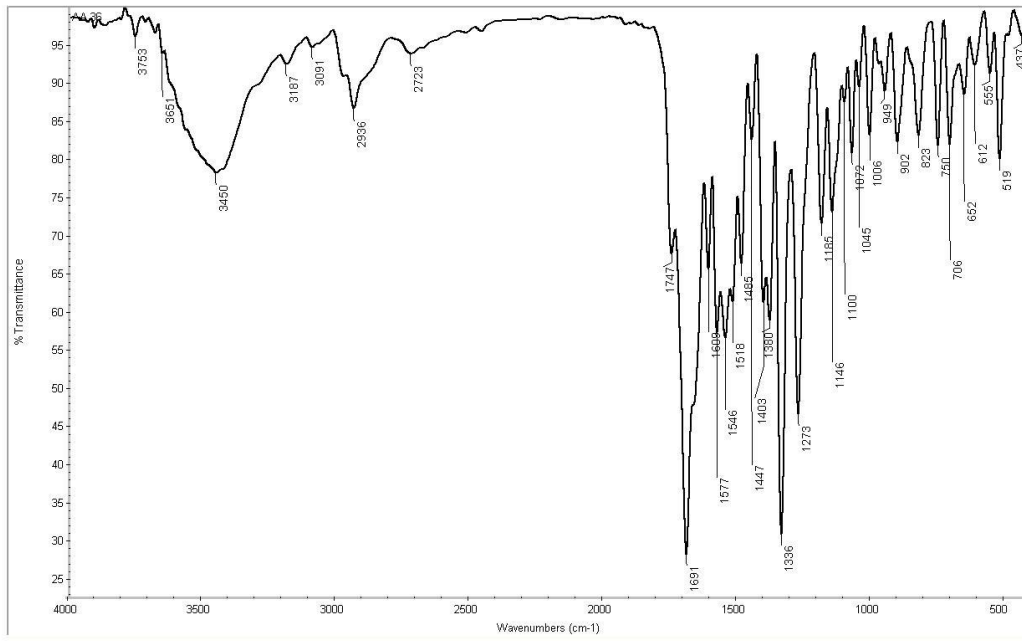
$^{19}\text{F}$  NMR (377 MHz, DMSO)  $\delta$  -108.91 (s).

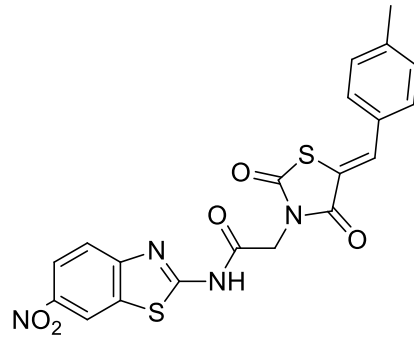




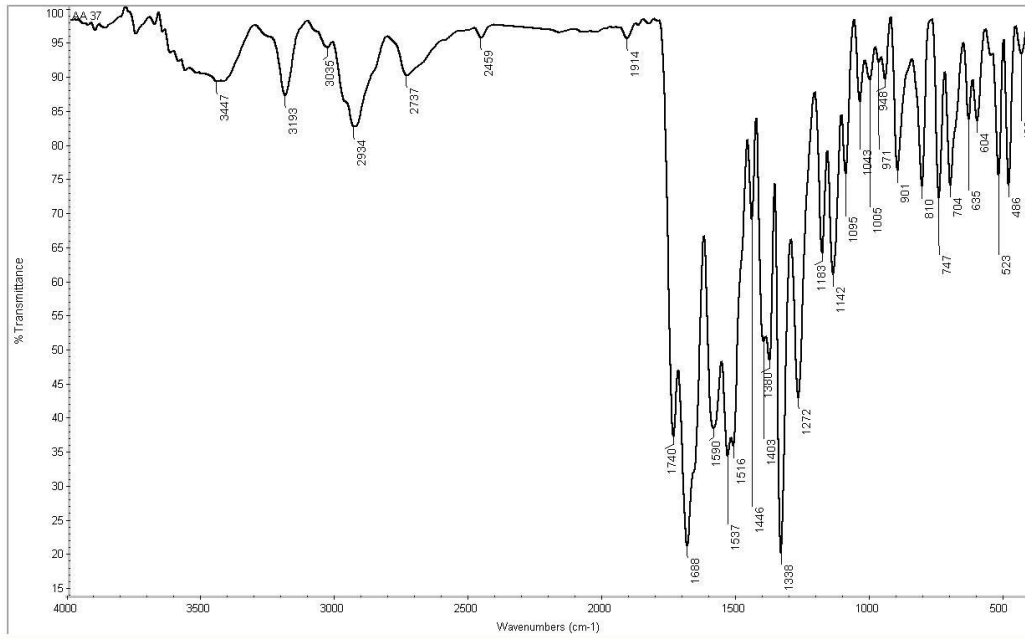


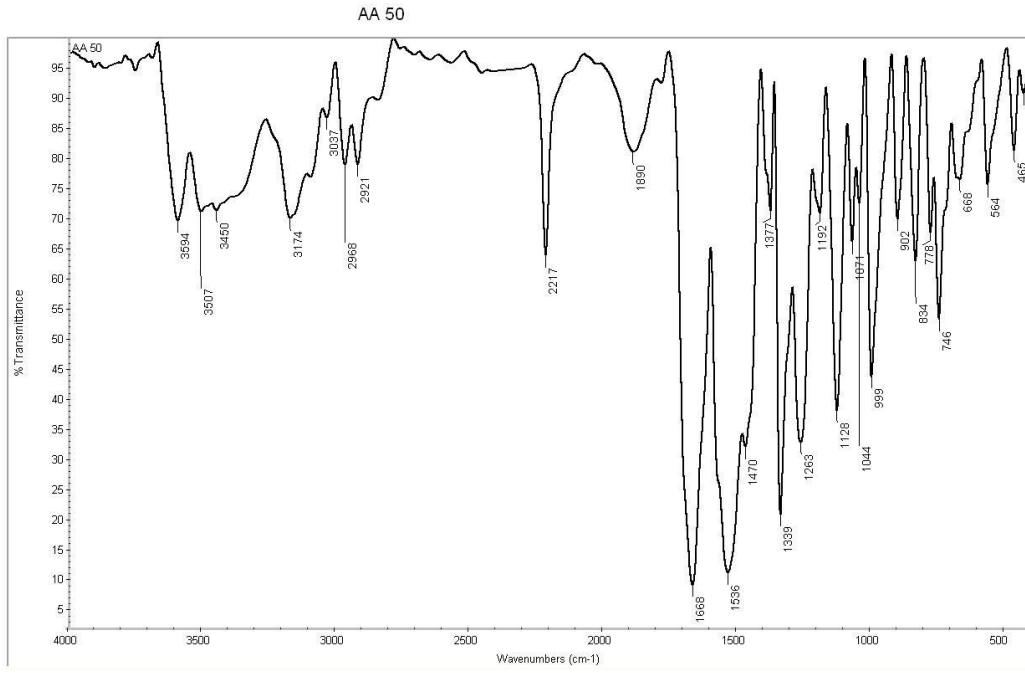
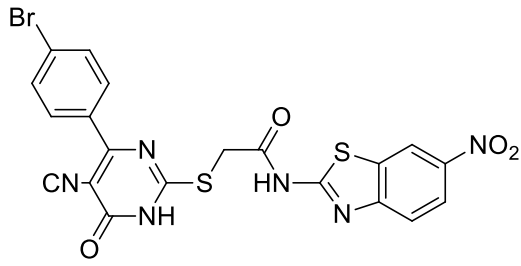
AA 36

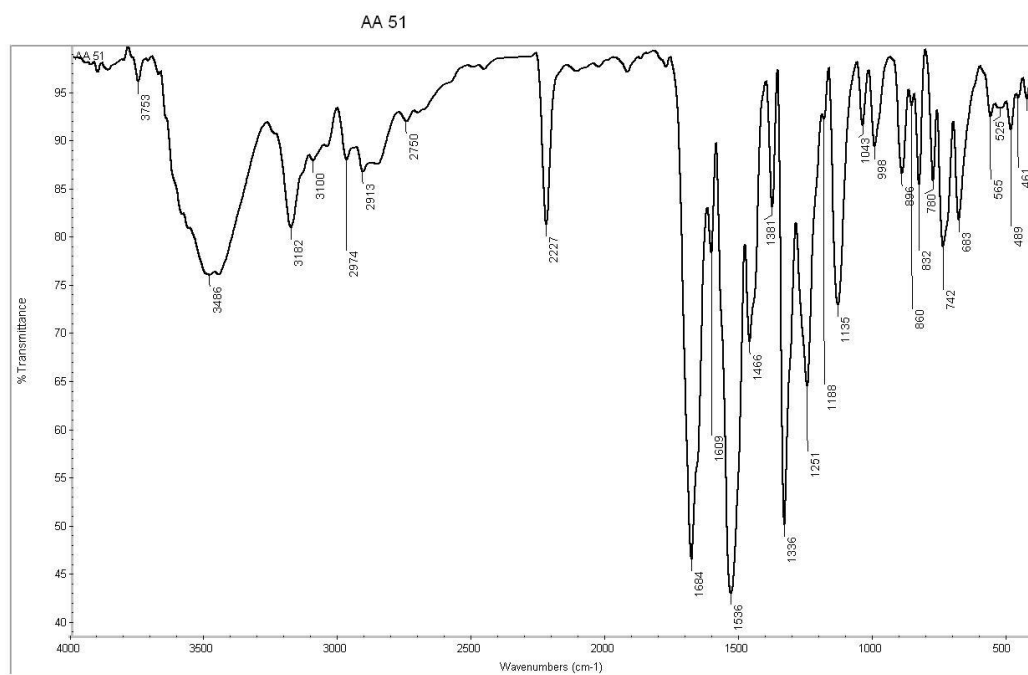
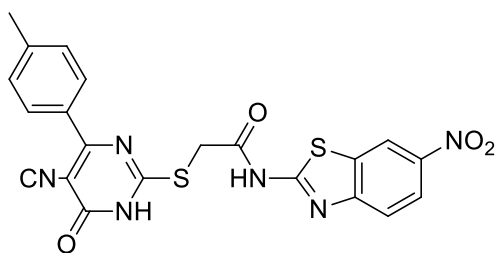


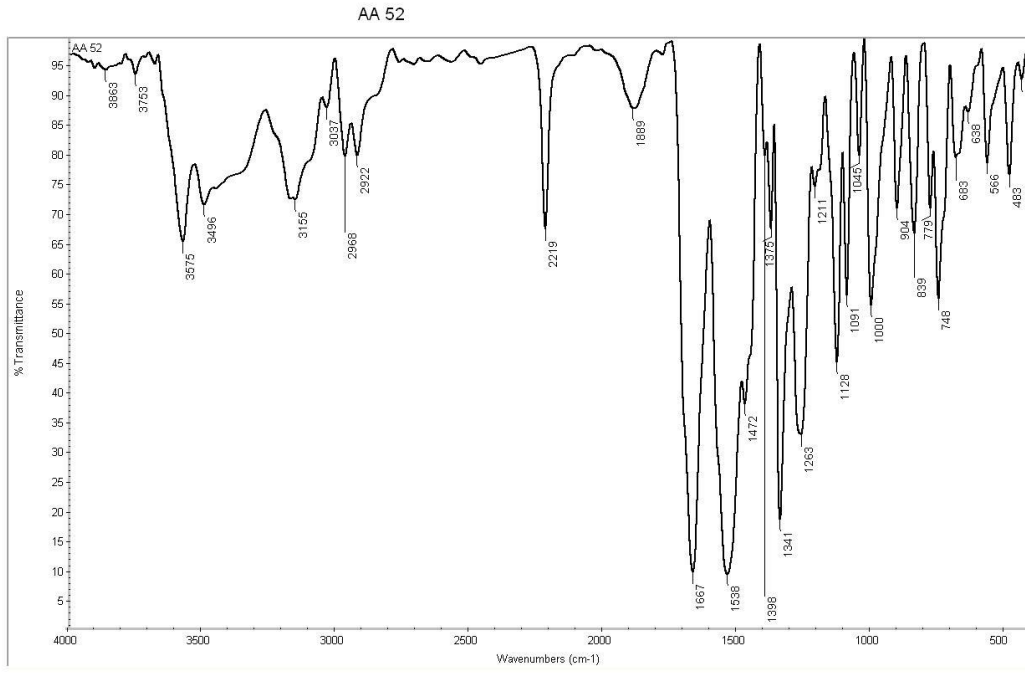
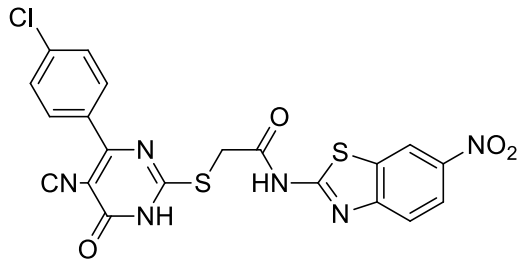


AA 37

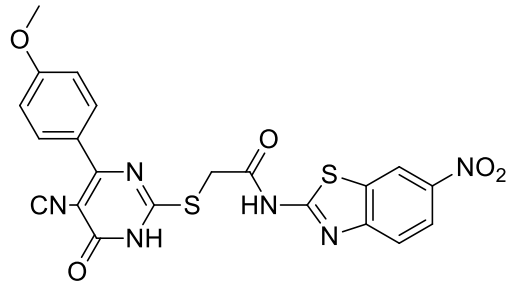




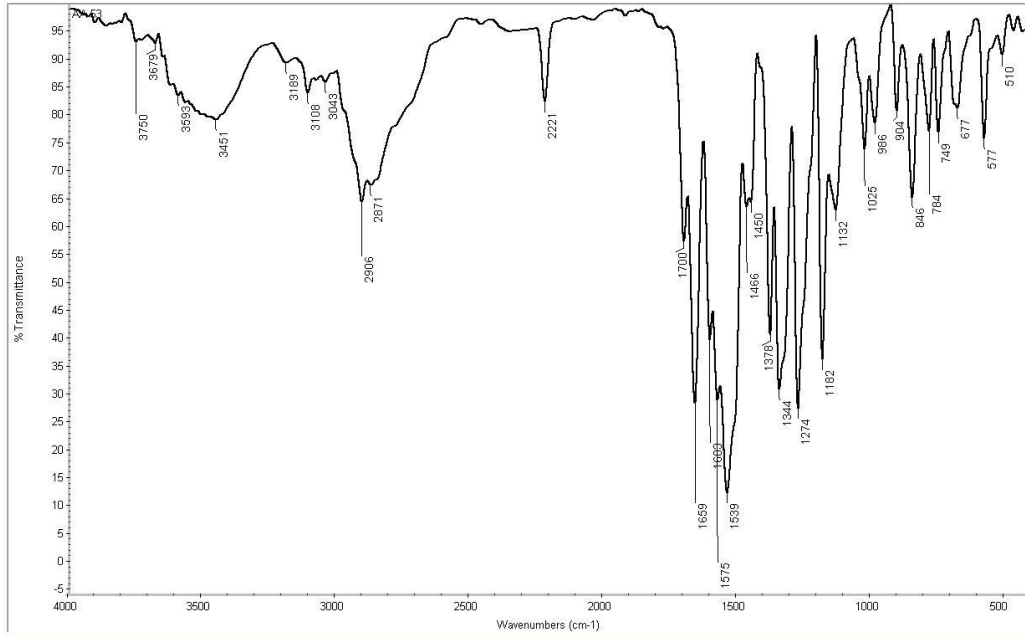


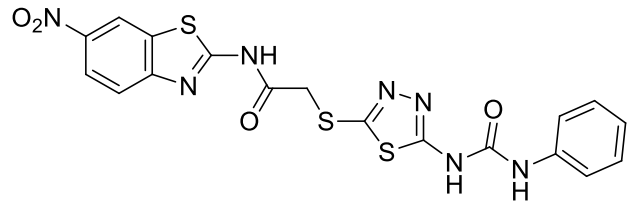






AA 53





AA 56

