Supplementary Material

Folic acid-sulfonamide conjugates as antibacterial agents: Design, synthesis and molecular docking studies

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, Muhammad Jadoon Khan [c], Asad Gulzar [d], Muhammad Muddassar [c*]

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1. Bacterial strains

The newly synthesized hybrids were investigated for antibacterial activities against gram negative bacteria *P. aeruginosa* (ATCC-27853), *E. coli* (ATCC-25922), and gram positive *S. aureus* (ATCC-25923) and *P. mirabilis* (ATCC 43071). The stock cultures were collected from the Institute of Biochemistry and Biotechnology, University of the Punjab, Lahore. Strains were recultured in the specific culture media i.e. tryptic soy broth. Inoculum was spread with the help of sterile L- shaped glass spreader and then placed in shaking incubator for 24 h at 37 °C. In the present work, $1\text{-}3\times10^8$ cfu/mL of gram positive (*S. aureus & P. mirabilis*) and gram negative (*E. coli & P. aeruginosa*) were obtained after setting with broth to an optical density at 0.3 to 0.4 and 0.2 to 0.3, respectively at 620 nm wavelength using spectrophotometer.

2. Antibacterial assay

2.1. Zone of Inhibition

A series of the 2 fold dilutions (0.5-0.00097 mg/mL) was prepared from stock solution of synthetic compounds as well as standard reference drug (ampicillin and trimethoprim) were used and concentrations were made in acetone which has no activity against the test microorganisms. Microfiltration of testing solutions was done with 0.2 μM pore size micro filter (Amicon, USA). 5 μL of each testing compounds' dilution was separately loaded on 6 mm sterilized disks of filter paper. Dimethylsulfoxide was used as a control. Sterilized forceps was used to place disk onto the medium. 100 μL microbial suspension of 0.5 McFarland nephelometry standard (10^8 cells/mL) was spread over the TSA media (20 mL in each petri plate) with the help of sterilized glass spreader to ensure the even growth of microorganism. The soaked discs were placed aseptically with the help of sterile forceps at equal distances over the inoculated plates. The plates were incubated at 37±1 °C for 24 h and distinct zone was visualized surrounding the discs. The zones of inhibition (mm) were measured using digital vernier caliper (Starrett 799A-6/150, USA), evaluated the antibacterial activities and all studies were performed in triplicates.

2.2. MIC Calculation

Biological activities of the synthesized compounds were also studied by measuring MIC values and comparison was made with standards. Minimum inhibitory concentration is the lowest concentration of compound that prevents visible growth. MIC quantifies the effectiveness of testing compound. Lower the minimum inhibitory concentration value, higher is the efficacy of a testing compound.

Minimum inhibitory concentration (MIC) value was calculated by using two fold serial dilution technique and concentration range 2000-1.95 μg/mL was used for MIC determination. 150 μL tryptic soy broth and 50 μL of bacterial suspension was added to each serially diluted concentration in 96-well plate then incubated at 37±1 °C. After 24 h of incubation the optical density of mixture in 96-well plate was recorded at 600 nm using a microplate reader (BioRad, USA). The lowest concentration of the derivative that prevented the development of visible growth (OD_{600} less than 0.05) is considered to be the MIC value

Table 1S. Antibacterial data as zone of inhibition at three gradient concentrations (n=3) for folic acid-sulfonamide hybrids for Gram (+) bacteria

	Gram (+) bacteria					
Compound	*S. aureus*			*P. mirabilis*		
	3 mg/mL	1.5 mg/mL	0.75 mg/mL	3 mg/mL	1.5 mg/mL	0.75 mg/mL
MS1	31.2,31.1,31.1	29.9,29.8,29.9	27.9,27.8,27.8	29.3, 29.4,29.3	27.9,27.8,27.9	22.0,21.8,22.1
MS2	29.9, 29.8,29.8	28.9,28.9,28.7	26.9,26.8,26.8	27.9,27.8,27.8	24.1,23.9,23.9	22.1,22.1,22.0
MS3	31.9,31.9,31.8	27.9,27.9,27.8	22.2,22.0,22.0	28.2,28.1,28.1	24.3,24.3,24.2	22.6,22.5,22.5
DS1	32.8,32.8,32.7	30.9,30.8,30.9	28.7,28.8,28.8	33.4,33.2,33.2	29.9,29.8,29.8	28.5,28.5,28.4
DS2	36.6,36.6,36.5	31.5,31.5,31.6	30.5,30.5,30.4	35.9,35.7,35.7	30.2,30.0,30.0	29.5,29.6,29.6
DS3	30.7,30.8,30.8	27.9,27.8,27.8	26.9,26.8,26.8	29.9,29.7,29.7	23.9,23.8,23.8	22.4,22.3,22.3
DS4	31.9,31.8,31.8	29.2,29.1,29.1	26.8,26.7,26.8	30.8,30.9,30.8	28.9,28.9,28.8	26.5,26.3,26.5
DS5	34.7,34.8,34.8	30.7,30.8,30.8	28.6,28.6,28.5	33.6,33.5,33.5	29.6,29.5,29.5	28.5,28.5,28.3
DS6	33.9,33.8,33.8	31.8,31.7,31.7	28.5,28.5,28.3	33.3,33.1,33.1	29.3,29.2,29.2	28.6,28.7,28.7
TS1	32.6,32.5,32.5	26.6,26.5,26.5	23.8,23.8,23.7	31.3,31.2,31.3	29.3,29.3,29.2	24.1,24.1,24.2
TS2	31.8,31.7,31.8	28.9,28.8,28.8	25.8,25.8,25.7	30.8,30.7,30.7	27.8,27.7,27.7	26.1,26.2,26.2
TS3	32.5,32.4,32.5	26.8,26.7,26.8	23.3,23.4,23.4	30.9,30.8,30.8	29.7,29.7,29.8	24.0,24.1,24.1
TS4	20.2,20.3,20.3	15.8,15.8,15.7	10.9,10.8,10.8	18.2,18.3,18.3	14.3,14.4,14.4	10.8,10.8,10.7
TS5	34.9,34.8,34.8	31.8,31.7,31.7	28.5,28.4,28.4	33.3,33.2,33.2	29.3,29.2,29.2	28.6,28.6,28.5
TS6	23.2,23.1,23.1	15.4,15.3,15.3	11.2,11.1,11.1	19.1,19.0,19.0	14.5,14.4,14.4	10.8,10.7,10.7
Folic acid	–	–	–	–	–	–
p-toluenesulfonyl chloride	–	–	–	–	–	–
benzenesulfonyl chloride	–	–	–	–	–	–
2,4-dibromo benzenesulfonyl chloride	–	–	–	–	–	–
[a] Ampicillin	29.8,29.8,29.7	28.0,28.1,28.1	26.7,26.7,26.8	30.5,30.6,30.5	29.5,29.5,29.4	28.2,28.2,28.1
[b] Trimethoprim	28.2,28.3,28.3	20.2,20.3,20.3	18.4,18.2,18.2	25.1,24.9,24.9	20.2,20.3,20.3	14.3,14.3,14.5

[a] Control drug, [b] Reference DHFR inhibitor, Zone of inhibition was measured in mm ±SD, Gradient concentration of 3 mg/mL, 1.5 mg/mL, and 0.75 mg/mL was used, *S. aureus* = *Staphylococcus aureus, E. coli* = *Escherichia coli*, *P. aerugenosa* = *Pseudomonas aerugenosa*, *P. mirabilis* = *Proteus mirabilis*

Table 2S. Antibacterial data as zone of inhibition at three gradient concentrations (n=3) for folic acid-sulfonamide hybrids for Gram (-) bacteria

Compound	Gram (-) bacteria					
	E. coli			*P. aeruginosa*		
	3 mg/mL	1.5 mg/mL	0.75 mg/mL	3 mg/mL	1.5 mg/mL	0.75 mg/mL
MS1	31.0,31.2,31.2	29.7,29.8,29.8	24.0,24.2,24.2	30.9,30.9,30.8	28.1,28.2,28.2	17.8,17.8,17.9
MS2	29.9,29.8,29.8	29.0,28.9,28.8	23.6,23.7,23.7	27.8,27.9,27.9	25.7,25.8,25.8	15.8,15.8,15.9
MS3	33.0,33.2,33.2	28.3,28.4,28.4	24.6,24.7,24.7	29.1,29.2,29.2	27.9,27.8,27.8	20.2,20.3,20.3
DS1	34.9,34.9,34.8	32.2,32.3,32.3	29.3,29.3,29.4	32.9,32.8,32.8	31.9,31.8,31.9	18.4,18.5,18.5
DS2	37.8,37.7,37.9	33.2,33.3,33.3	31.5,31.6,31.6	34.7,34.8,34.8	32.1,32.2,32.1	30.9,30.8,30.9
DS3	31.9,31.8,31.8	29.2,29.3,29.3	23.6,23.7,23.7	28.9,28.8,28.8	27.7,27.8,27.8	17.8,17.9,17.9
DS4	34.8,34.9,34.9	32.3,32.4,32.5	28.6,28.6,28.8	30.8,30.8,31.0	29.3,29.4,29.4	27.3,27.4,27.6
DS5	36.4,36.5,36.5	32.2,32.3,32.3	28.9,28.9,29.0	32.7,32.8,32.8	31.2,31.3,31.3	29.1,29.3,29.3
DS6	36.6,36.7,36.7	32.3,32.4,32.4	29.6,29.8,29.8	33.9,34.0,34.0	31.2,31.3,31.3	29.8,29.9,29.9
TS1	34.6,34.7,34.7	30.9,30.8,30.8	25.9,26.0,26.0	29.3,29.4,29.4	27.5,27.6,27.7	24.1,24.2,24.2
TS2	34.7,34.8,34.8	31.8,31.9,31.9	29.4,29.6,29.6	31.1,31.3,31.3	29.2,29.4,29.4	27.2,27.4,27.4
TS3	34.5,34.6,34.6	30.0,30.2,30.2	24.3,24.5,24.5	29.6,29.8,29.8	27.8,27.9,27.9	24.2,24.6,24.6
TS4	19.2,19.4,19.4	12.0,12.2,12.2	10.7,10.9,10.9	20.0,20.2,20.2	17.6,17.8,17.8	14.2,14.3,14.3
TS5	36.6,36.7,36.7	32.3,32.4,32.5	29.6,29.7,29.8	33.9,33.9,34.0	31.2,31.4,31.4	29.8,30.0,30.0
TS6	19.5,19.6,19.6	12.3,12.5,12.5	10.9,10.8,10.9	20.8,20.9,20.9	17.9,17.8,17.8	14.5,14.6,14.6
Folic acid	–, –, –	–, –, –	–	–	–	–
p-toluenesulfonyl chloride	–, –, –	–, –, –	–	–	–	–
benzenesulfonyl chloride	–, –, –	–, –, –	–	–	–	–
2,4-dibromo benzenesulfonyl chloride	–, –, –	–, –, –	–	–	–	–
[a] Ampicillin	33.5,33.8,33.6	30.0,30.2,30.1	29.0,29.2,29.1	29.1,29.3,29.2	27.2,27.3,27.3	26.2,26.1,26.3
[b] Trimethoprim	31.2,30.9,30.8	25.2,25.0,25.0	20.1,20.0,20.2	14.1,14.2,14.2	9.3,9.3,9.4	4.1,4.1,4.2

[a] Control drug, [b] Reference DHFR inhibitor, Zone of inhibition was measured in mm ±SD, Gradient concentration of 3 mg/mL, 1.5 mg/mL, and 0.75 mg/mL was used, *S. aureus = Staphylococcus aureus, E. coli = Escherichia coli*, *P. aerugenosa = Pseudomonas aerugenosa*, *P. mirabilis = Proteus mirabilis*

[1]HNMR and [13]CNMR

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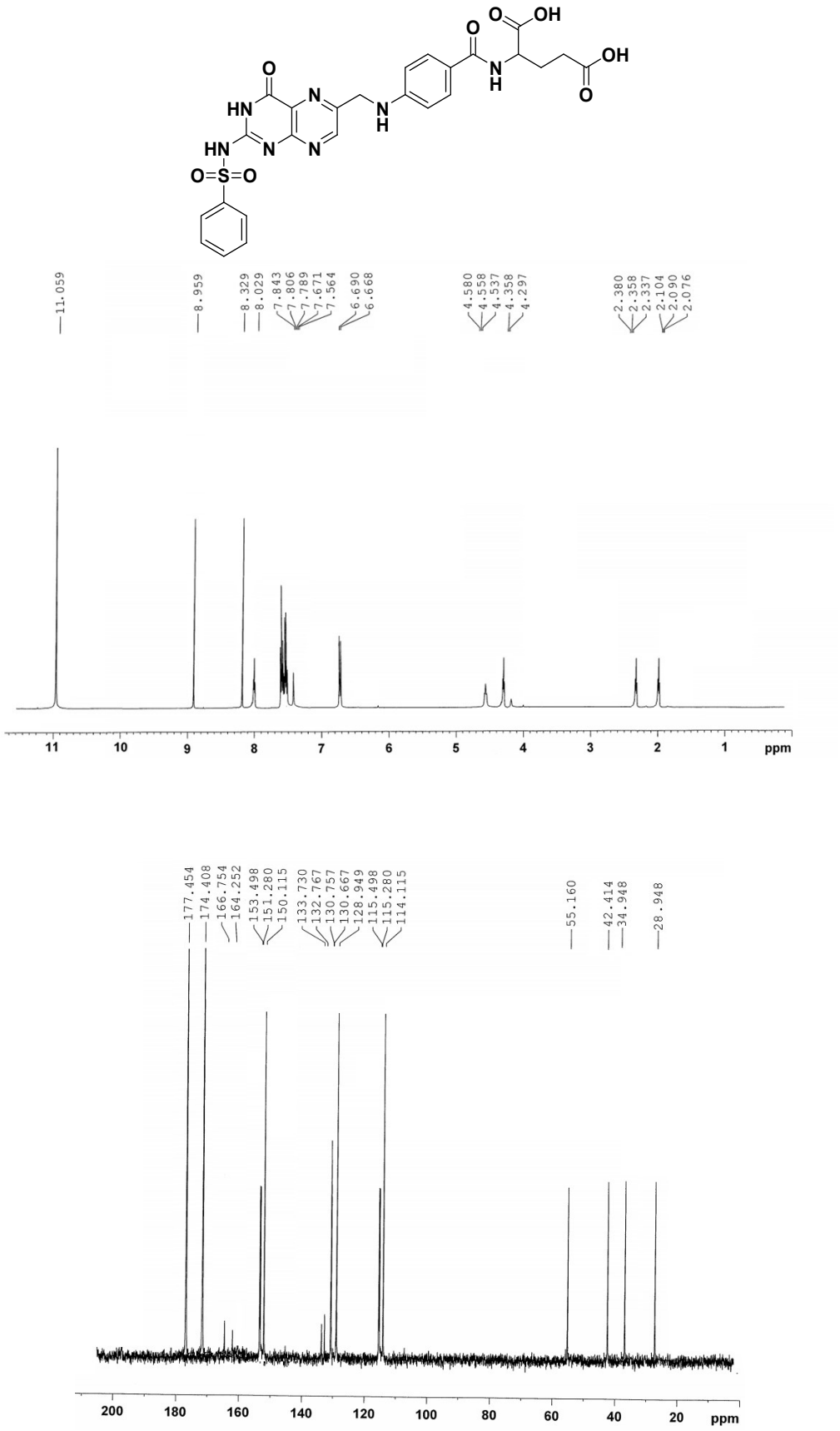

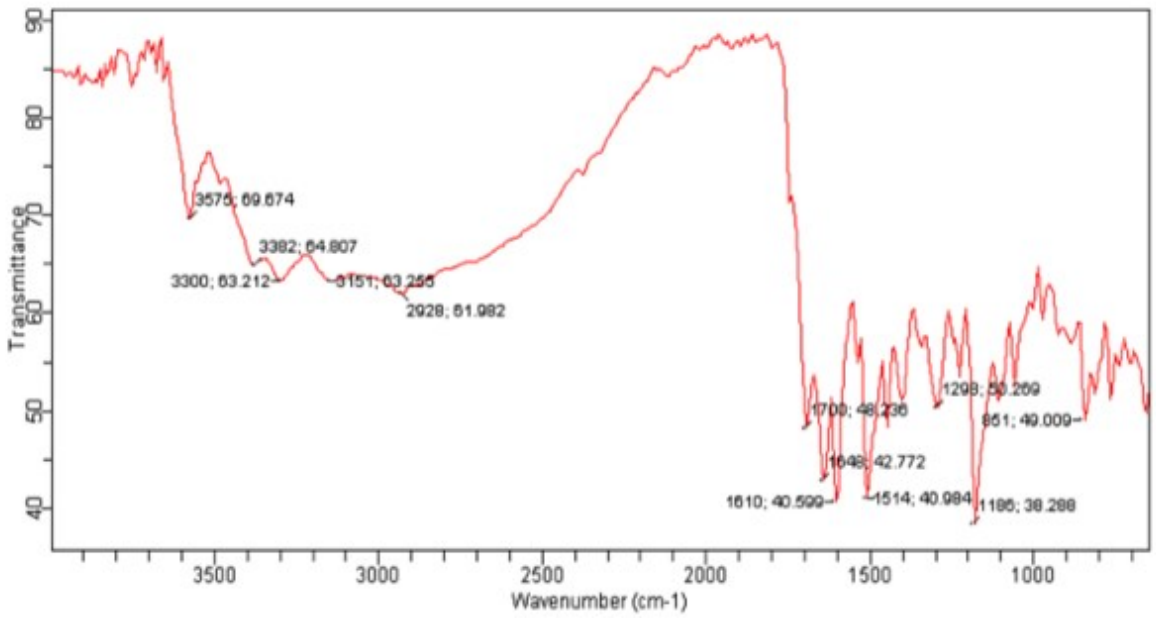
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Wavenumber (cm-1)
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3382; 64.807
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3151; 63.255
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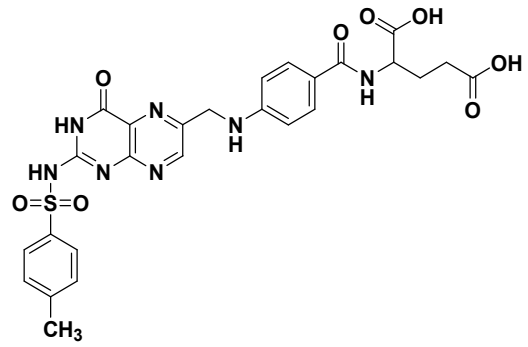
1610; 40.599
1514; 40.984
1298; 50.269
1186; 38.288
1151; 49.009

MS2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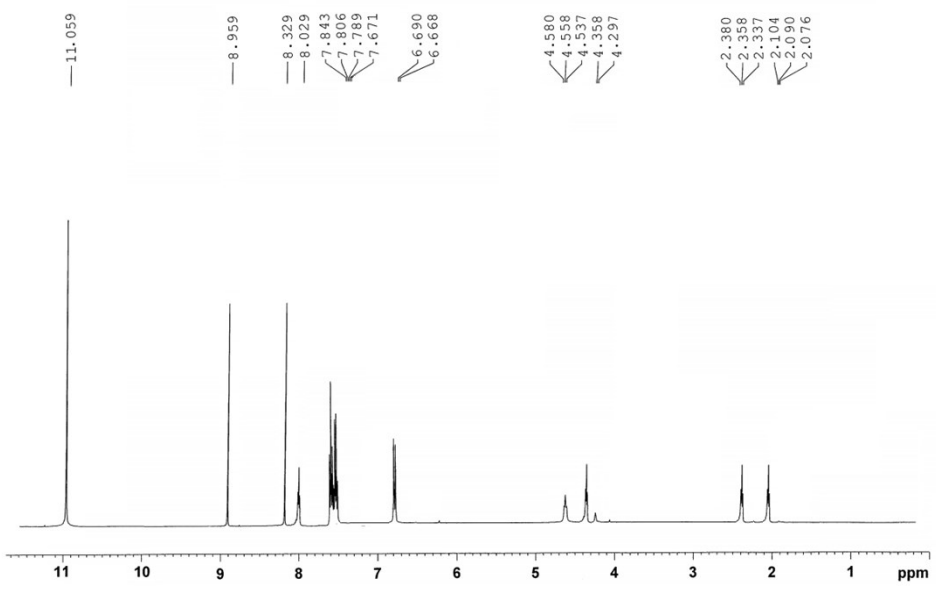
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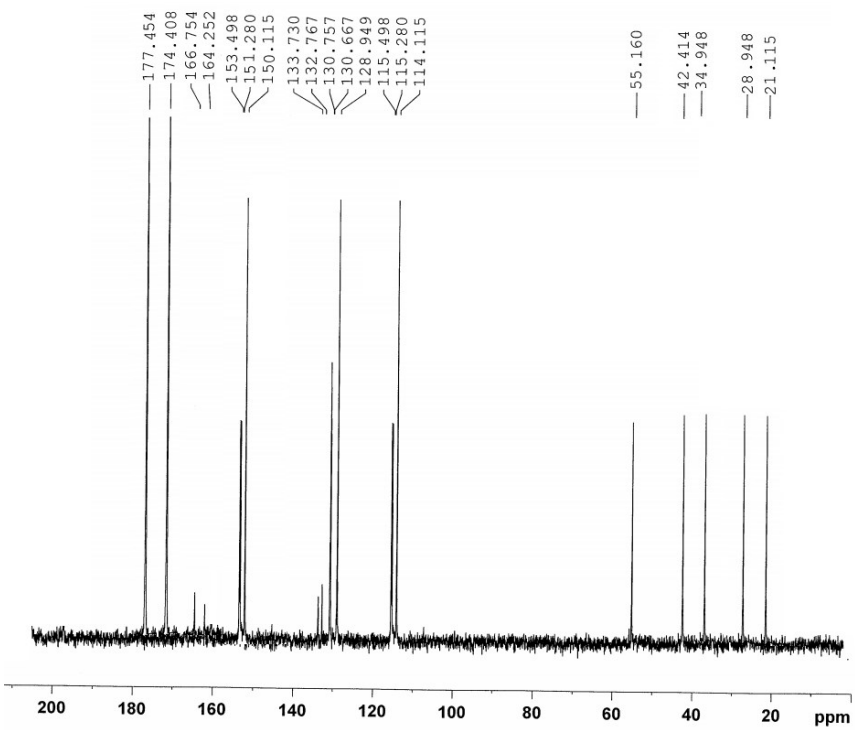
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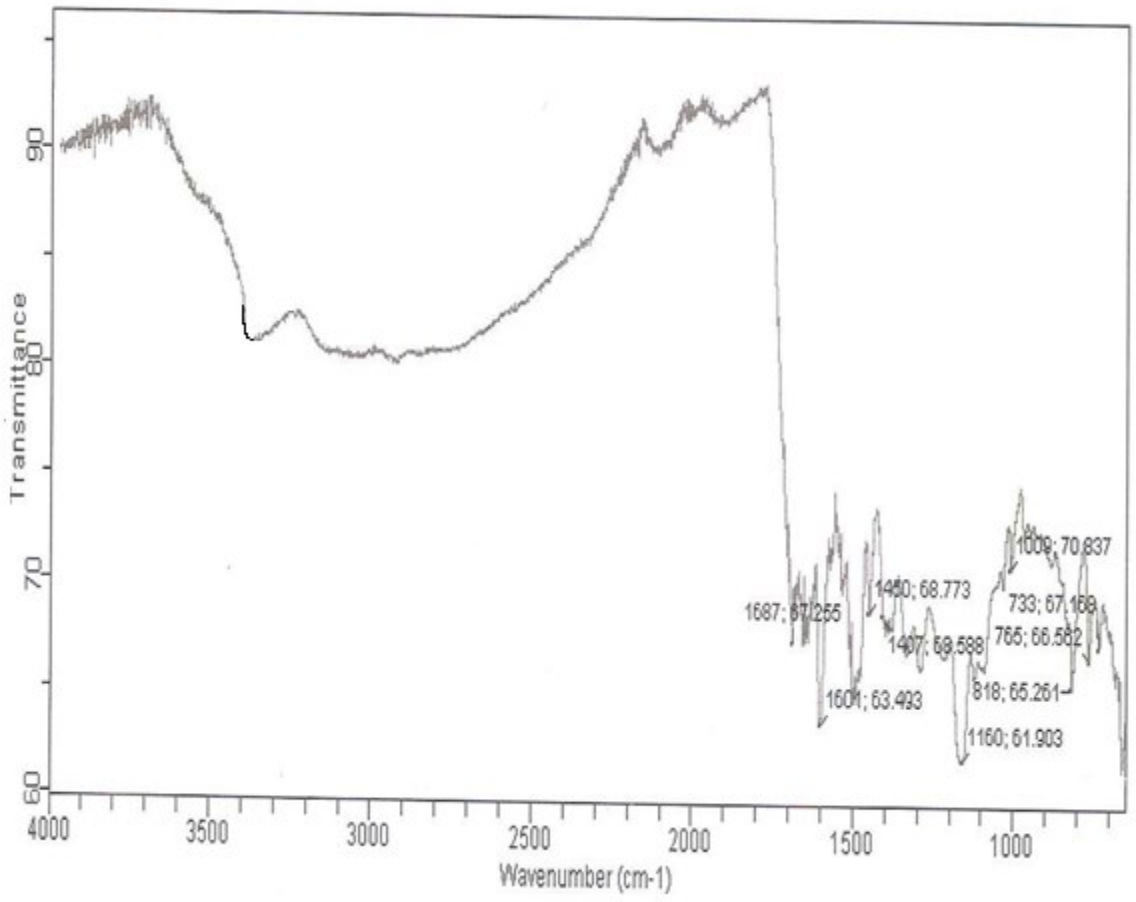
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1160; 61.903
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Wavenumber (cm-1)

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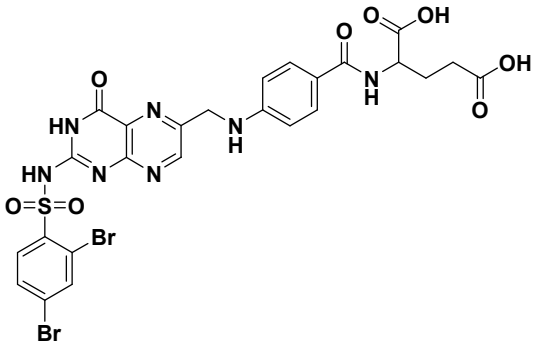
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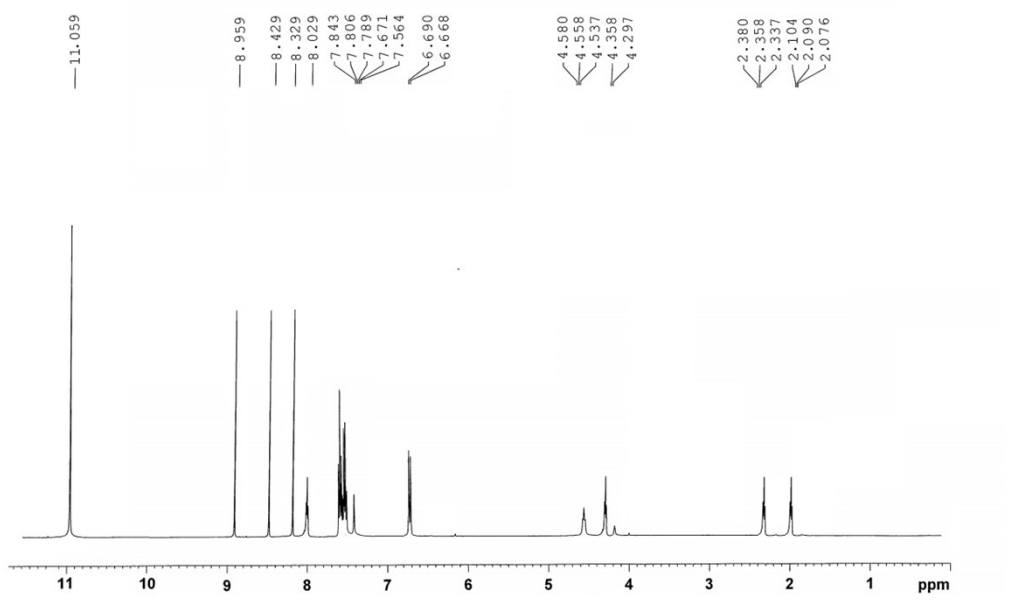
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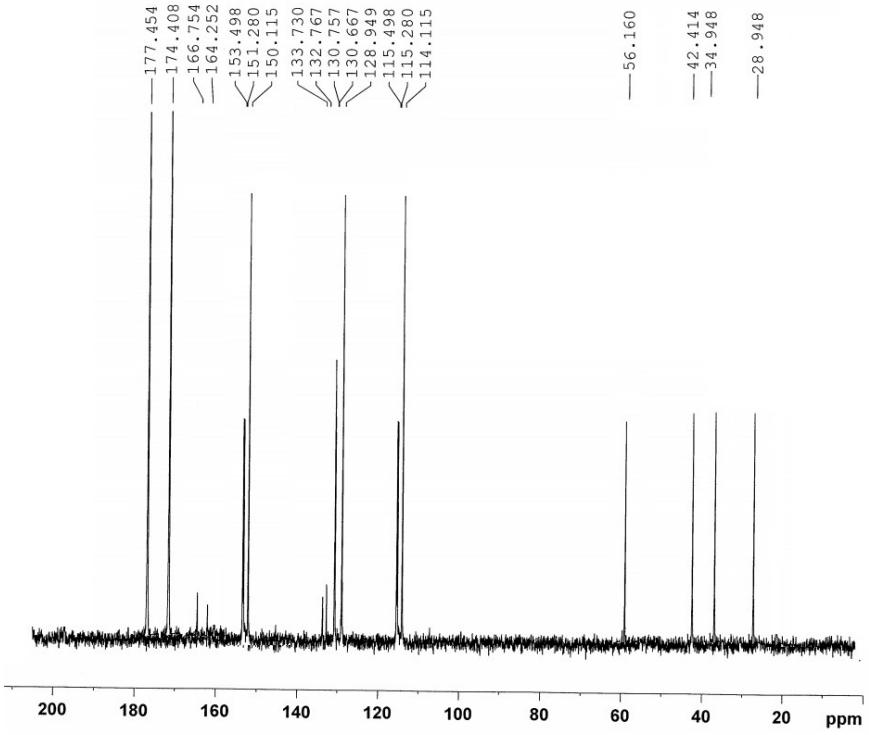
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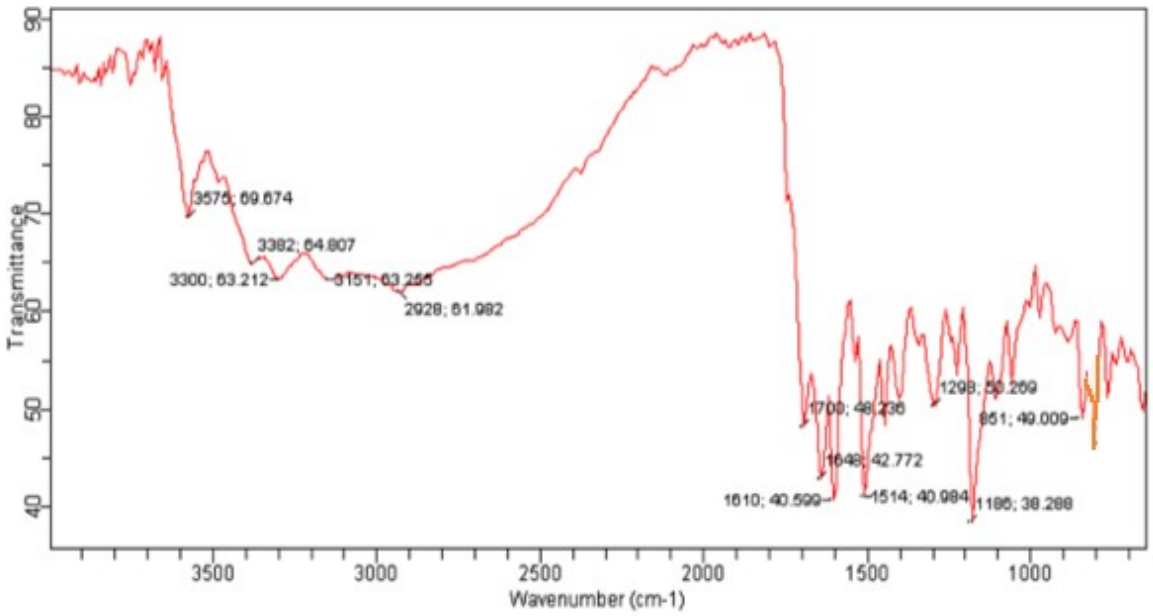
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Wavenumber (cm-1)
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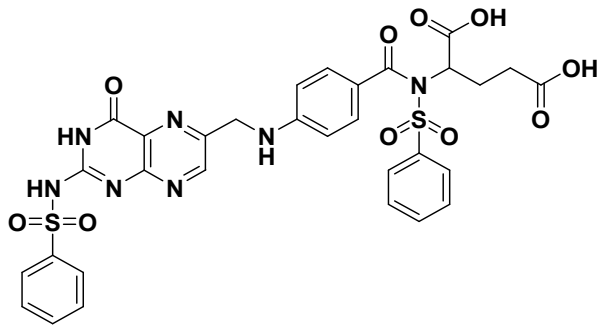
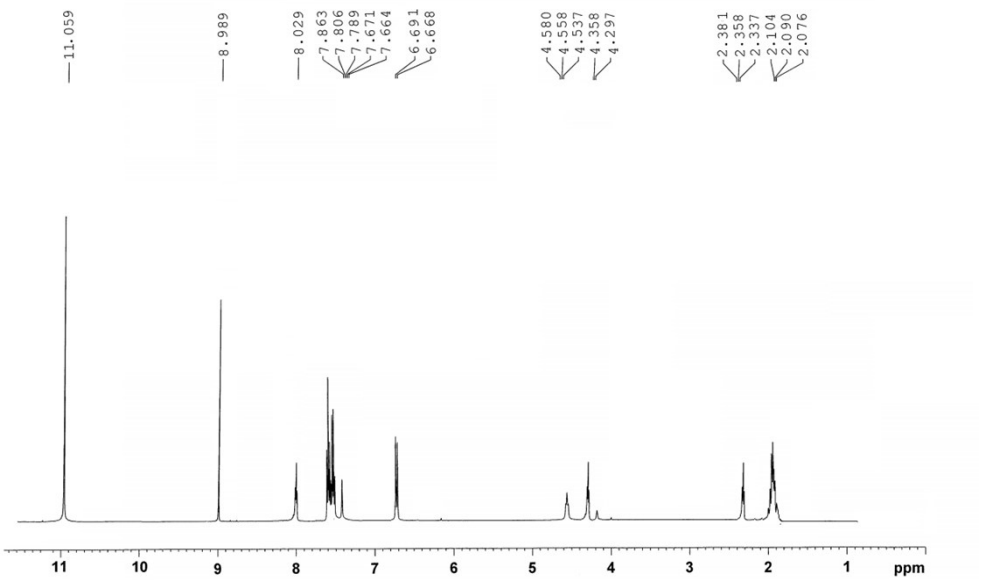
1186; 38.288

DS1

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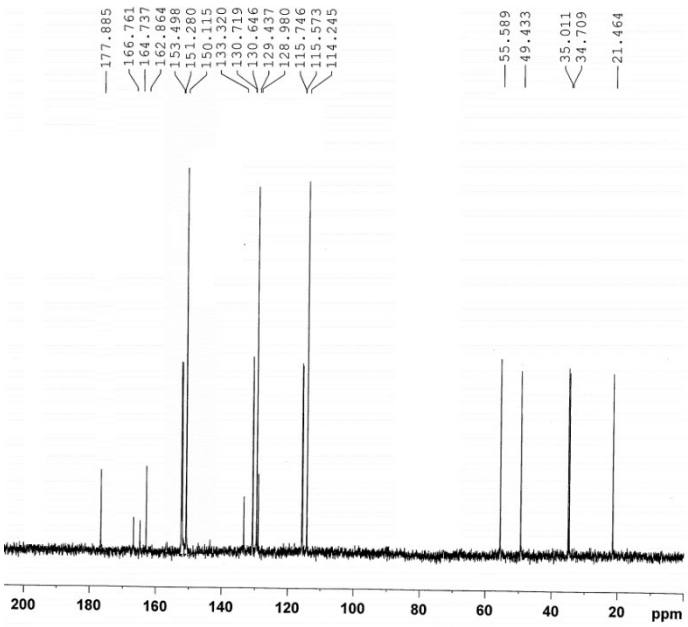
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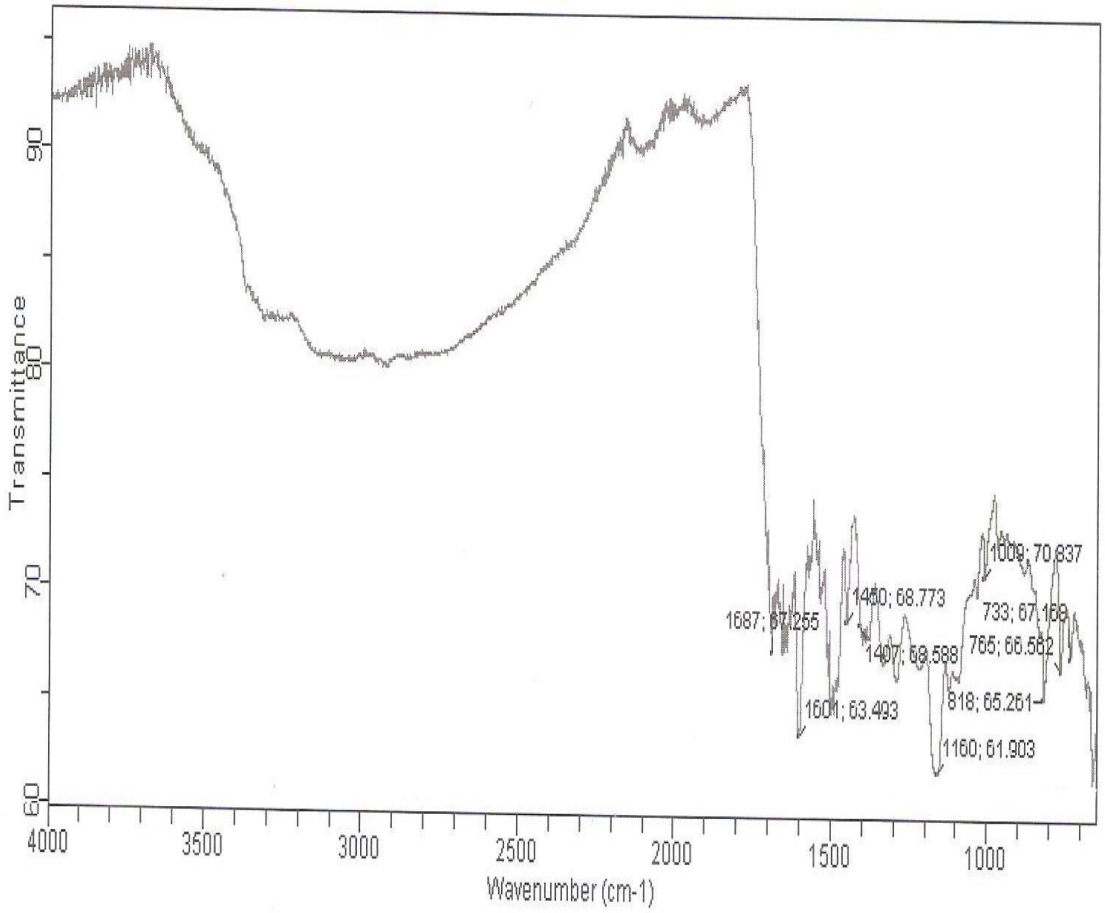
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Wavenumber (cm-1)
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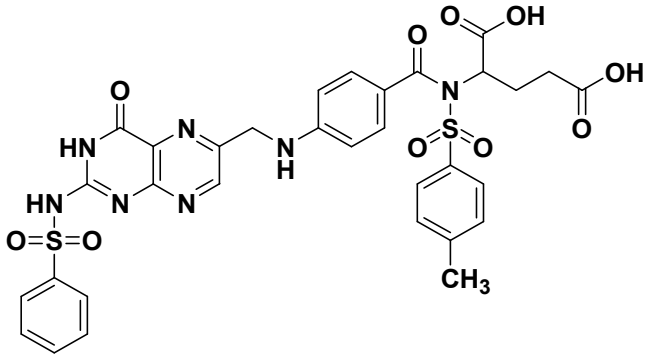
733; 67.169

DS2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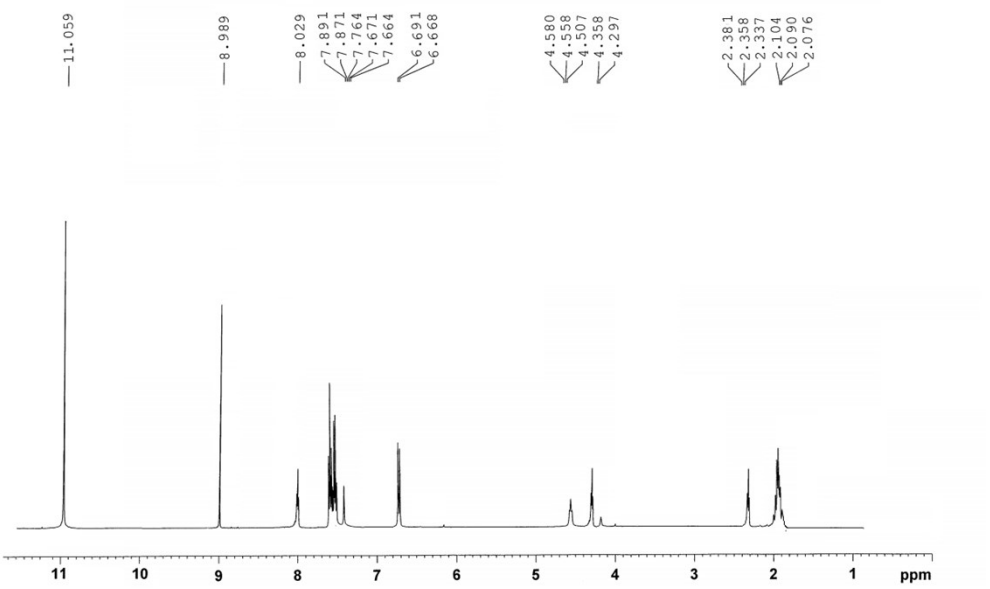
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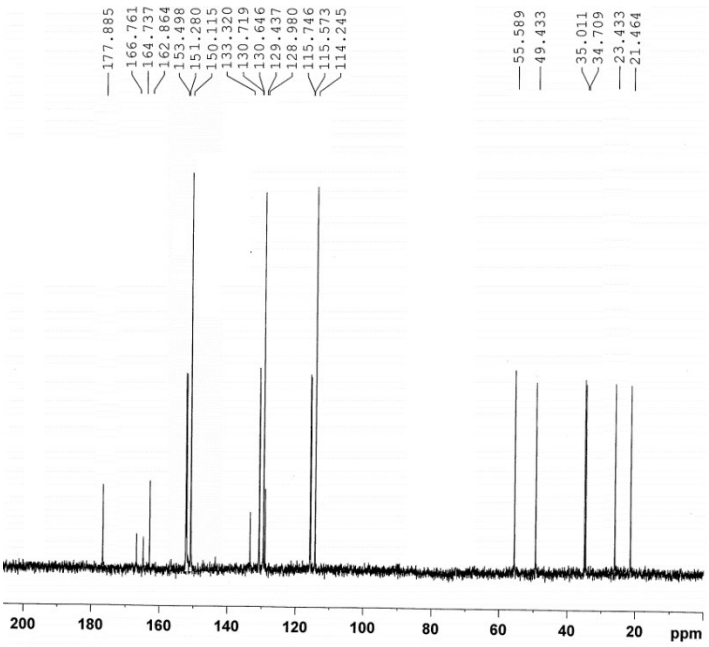
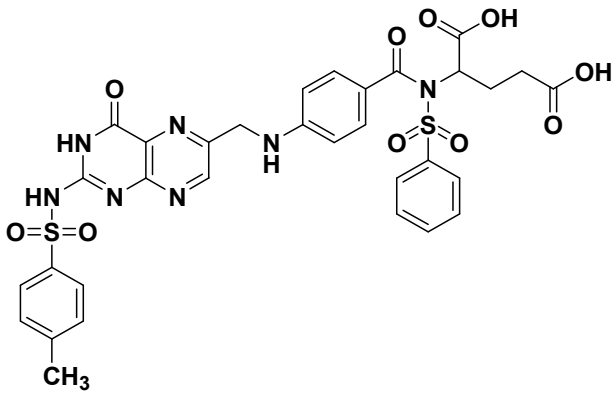
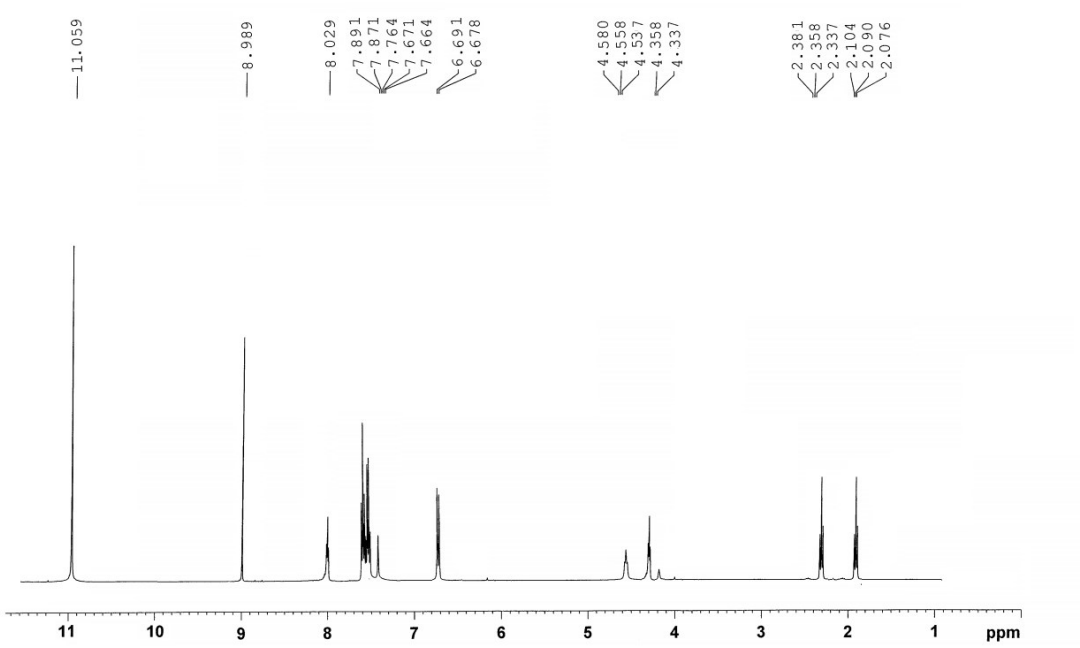
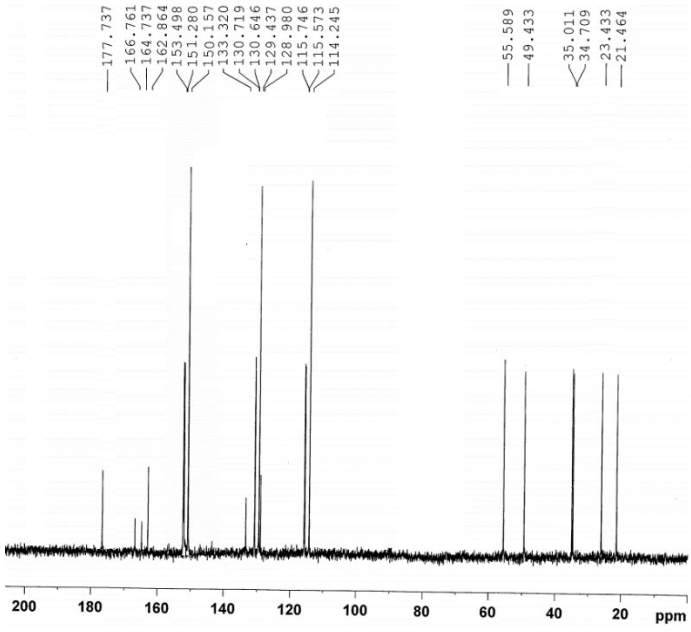
ppm

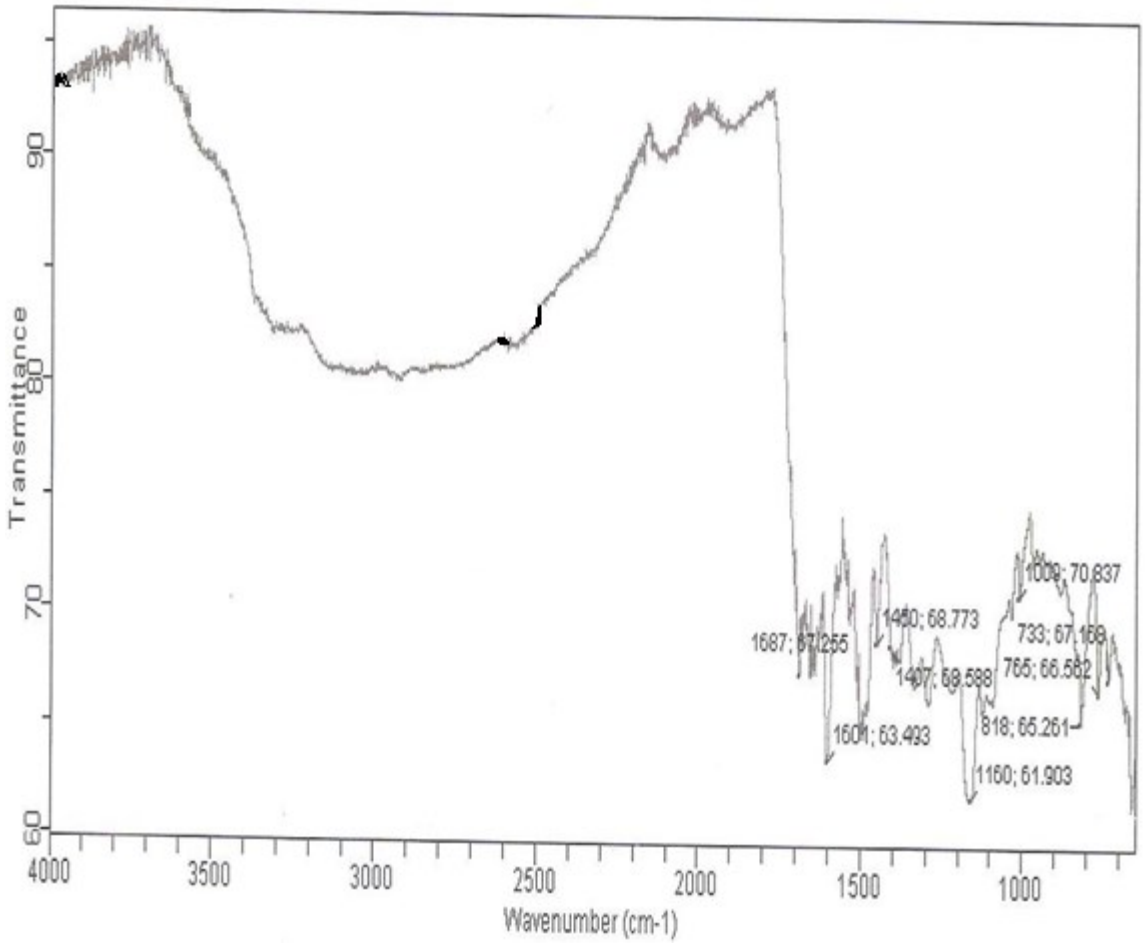

177.885
166.761
164.737
162.864
153.498
151.280
150.115
133.320
130.719
130.646
129.437
128.980
115.746
115.573
114.245
55.589
49.433
35.011
34.709
23.433
21.464
200
180
160
140
120
100
80
60
40
20
ppm

DS3

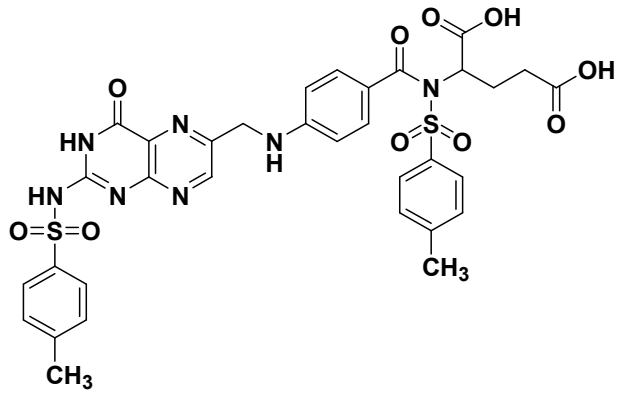


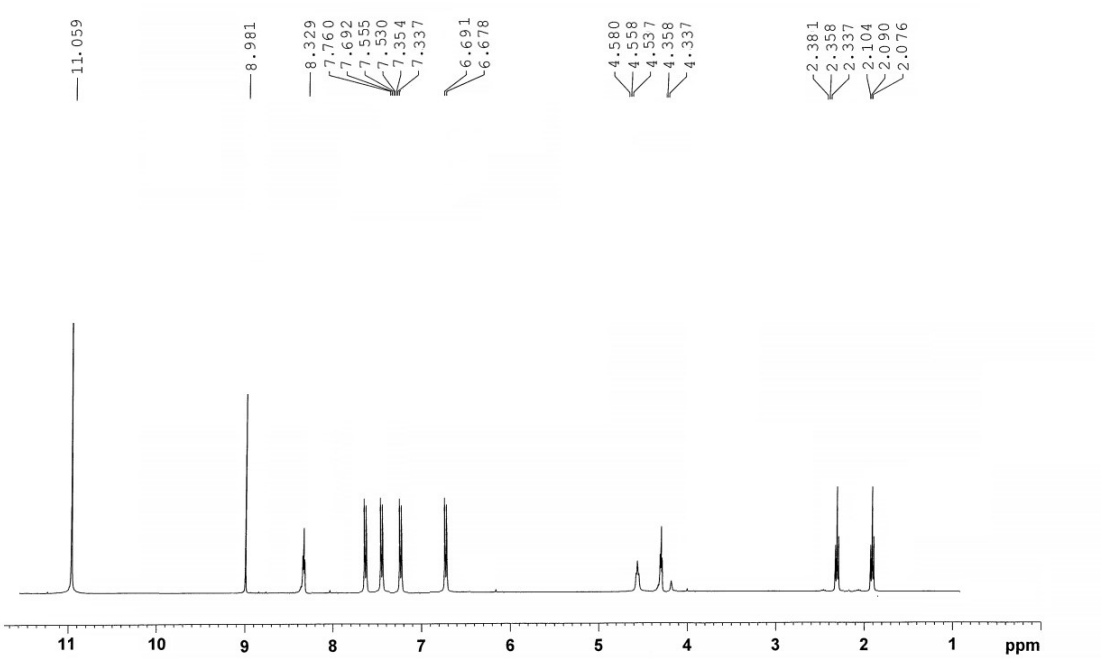

11.059
8.989
8.029
7.891
7.871
7.764
7.671
7.664
6.691
6.678
4.580
4.558
4.537
4.358
4.337
2.381
2.358
2.337
2.104
2.090
2.076
11
10
9
8
7
6
5
4
3
2
1
ppm

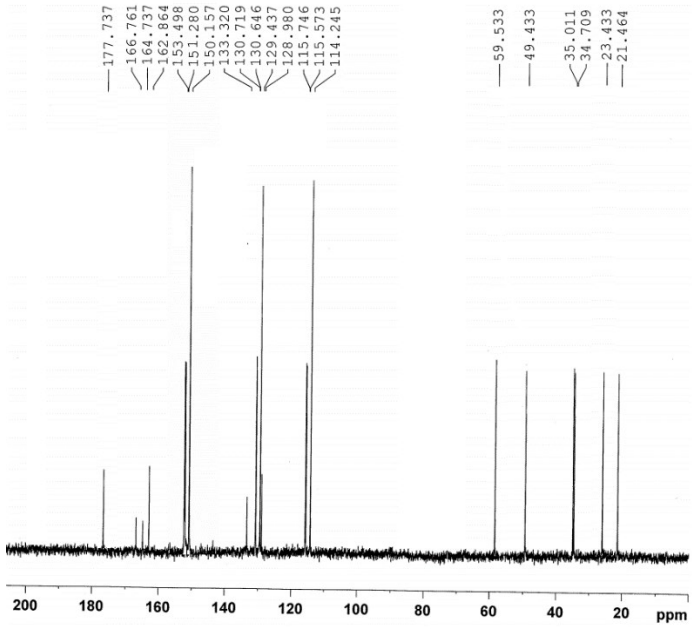

177.737
166.761
164.737
162.864
153.498
151.280
150.157
133.320
130.719
130.646
129.437
128.980
115.746
115.573
114.245
55.589
49.433
35.011
34.709
23.433
21.464
200
180
160
140
120
100
80
60
40
20
ppm


Transmittance
90
80
70
60
4000
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)
1687; 67.255
1601; 63.493
1480; 68.773
1407; 68.588
1160; 61.903
1009; 70.837
818; 65.261
765; 66.582
733; 67.168

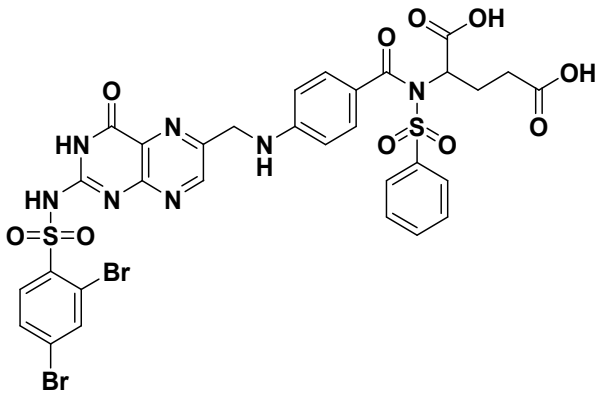
DS4

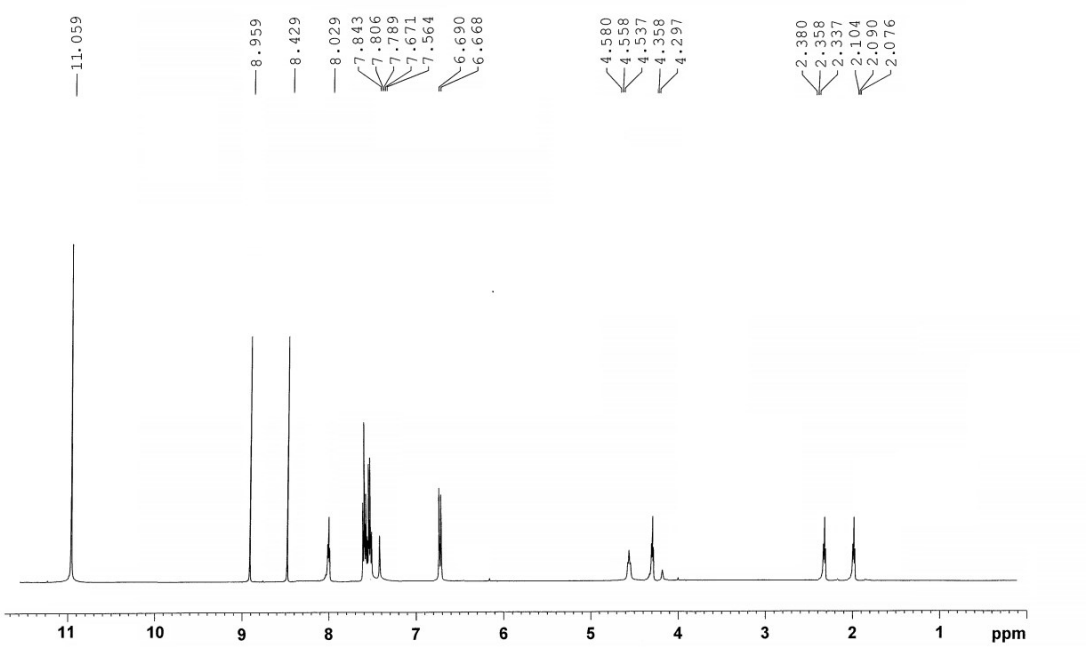

O
OH
O
N
OH
O
S
O
O
HN
N
N
N
H
HN
O=S=O
CH3
CH3

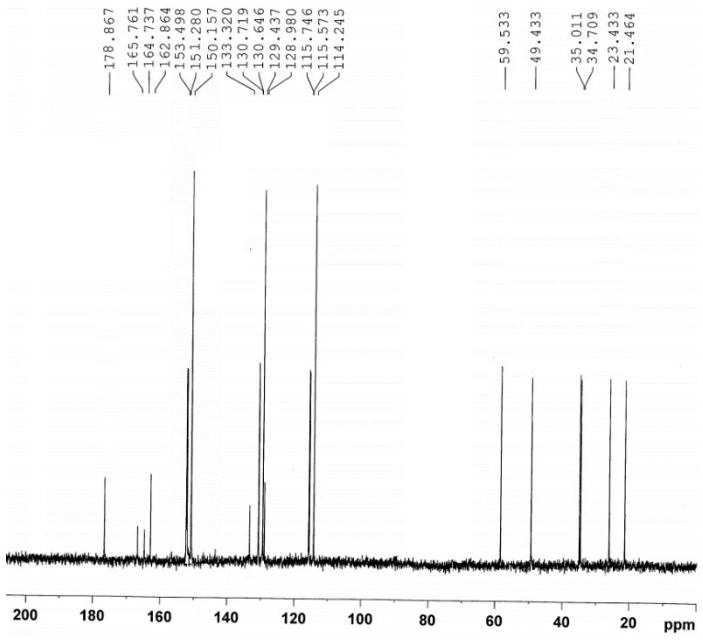

11.059
8.981
8.329
7.760
7.692
7.555
7.530
7.354
7.337
6.691
6.678
4.580
4.558
4.537
4.358
4.337
2.381
2.358
2.337
2.104
2.090
2.076
11
10
9
8
7
6
5
4
3
2
1
ppm

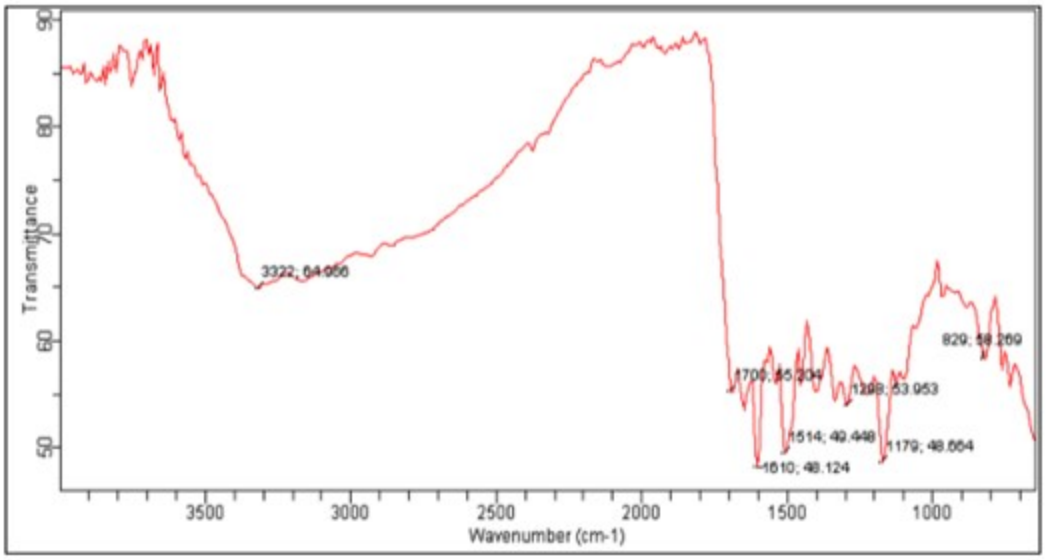

177.737
166.761
164.737
162.864
153.498
151.280
150.157
133.320
130.719
130.646
129.437
128.980
115.746
115.573
114.245
59.533
49.433
35.011
34.709
23.433
21.464
200
180
160
140
120
100
80
60
40
20
ppm

DS5

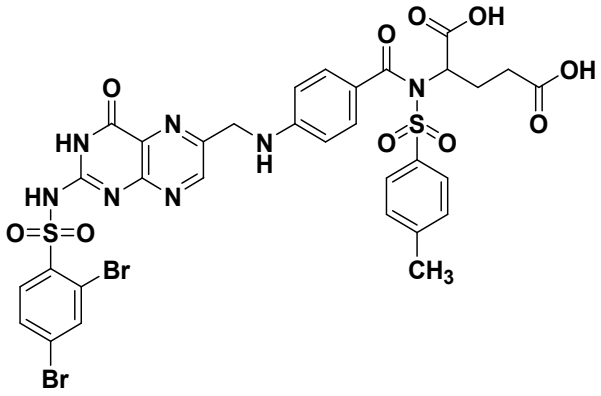


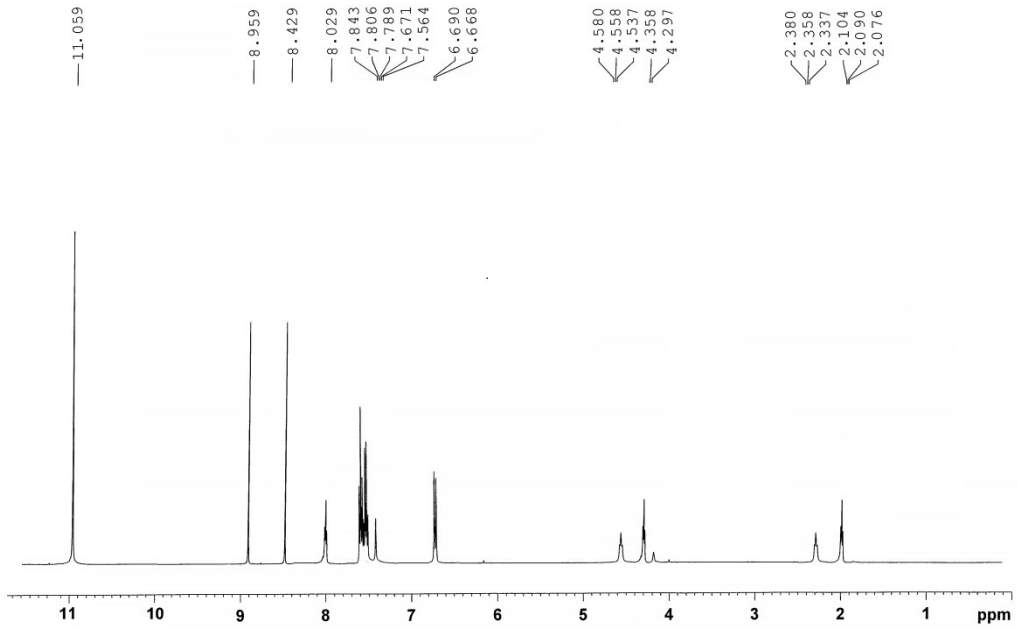

11.059
8.959
8.429
8.029
7.843
7.806
7.789
7.671
7.564
6.690
6.668
4.580
4.558
4.537
4.358
4.297
2.380
2.358
2.337
2.104
2.090
2.076
11
10
9
8
7
6
5
4
3
2
1
ppm

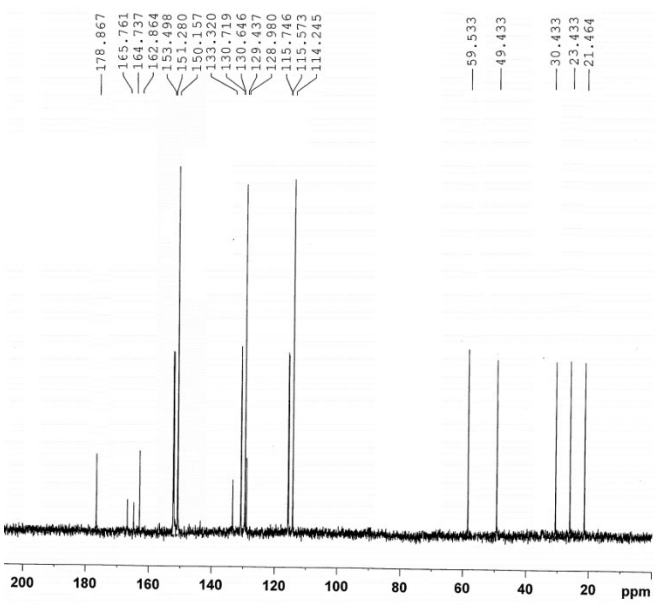

178.867
165.761
164.737
162.864
153.498
151.280
150.157
133.320
130.719
130.646
129.437
128.980
115.746
115.573
114.245
59.533
49.433
35.011
34.709
23.433
21.464
200
180
160
140
120
100
80
60
40
20
ppm


Transmittance
Wavenumber (cm-1)
3322; 64.966
1610; 48.124
1514; 49.448
1179; 48.664

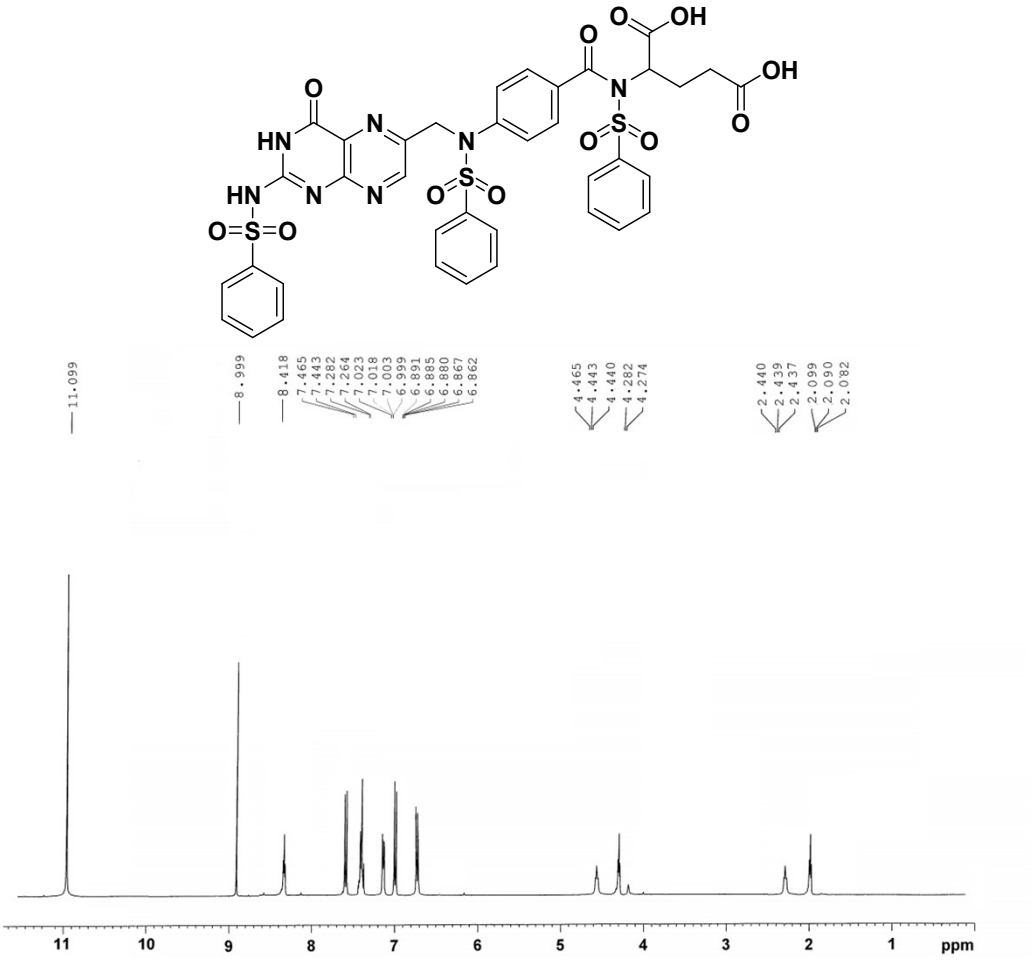
DS6

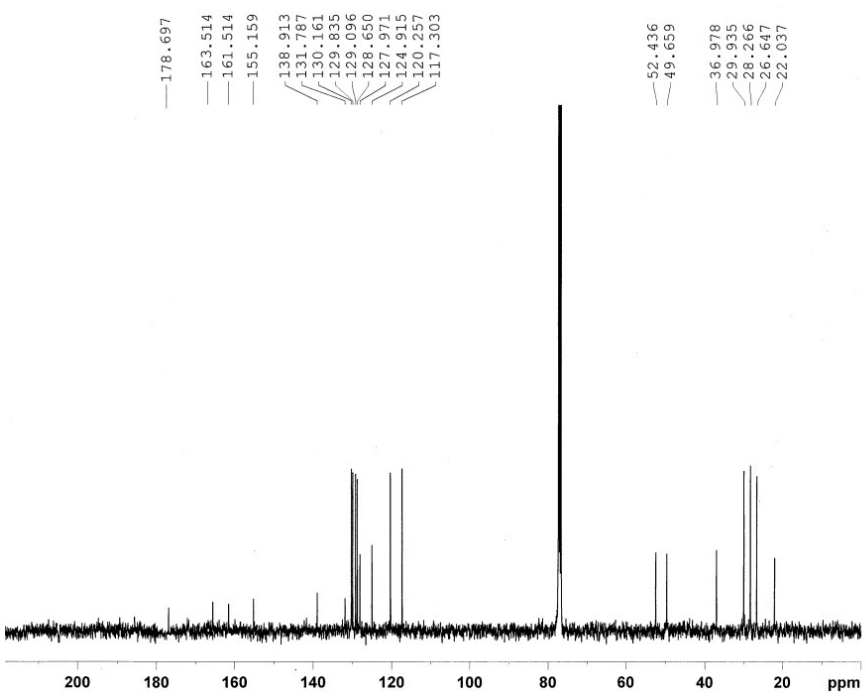

O
OH
OH
O
N
S
O
O
HN
N
N
HN
N
N
O=S=O
Br
Br
CH3

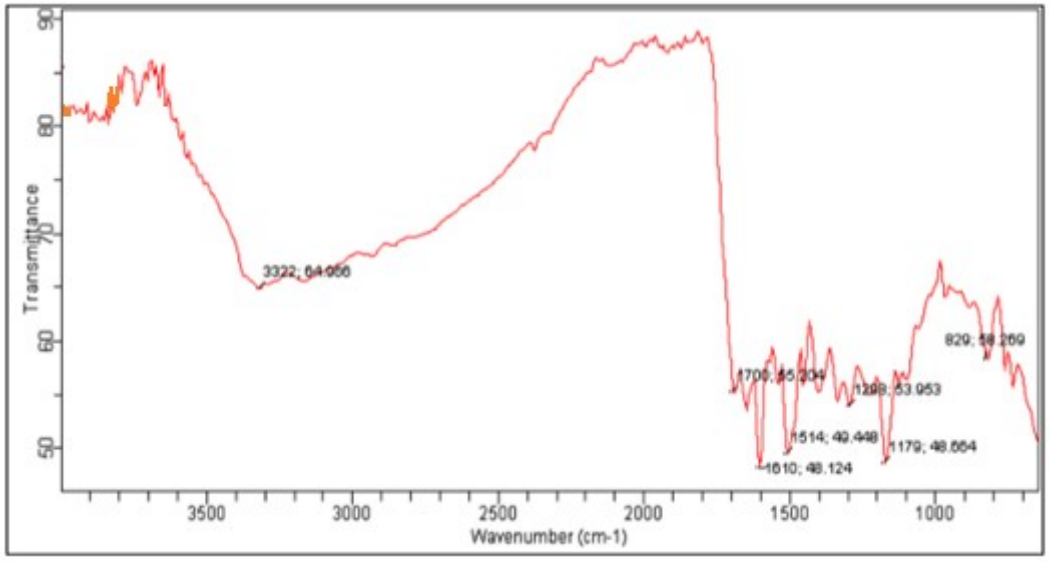

11.059
8.959
8.429
8.029
7.843
7.806
7.789
7.671
7.564
6.690
6.668
4.580
4.558
4.537
4.358
4.297
2.380
2.358
2.337
2.104
2.090
2.076
ppm


178.867
165.761
164.737
162.864
153.498
151.280
150.157
133.320
130.719
130.646
129.437
128.980
115.746
115.573
114.245
59.533
49.433
30.433
23.433
21.464
200
180
160
140
120
100
80
60
40
20
ppm

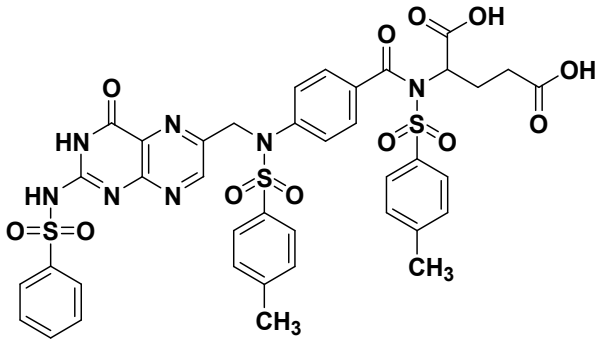
TS1

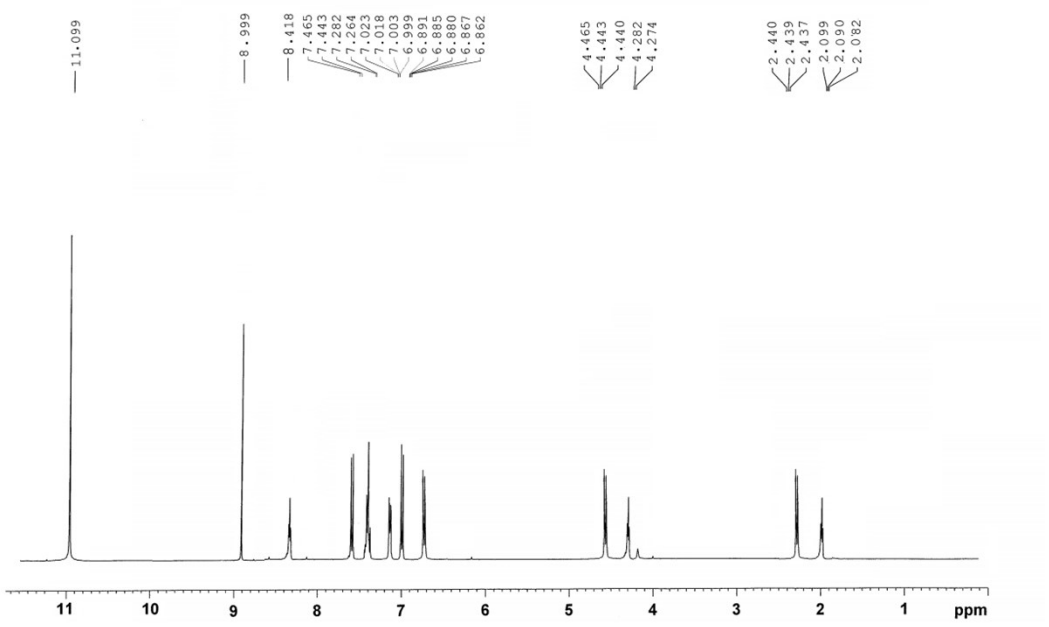

11.099
8.999
8.418
7.465
7.443
7.282
7.264
7.023
7.018
7.003
6.999
6.891
6.885
6.880
6.867
6.862
4.465
4.443
4.440
4.282
4.274
2.440
2.439
2.437
2.099
2.090
2.082
11
10
9
8
7
6
5
4
3
2
1
ppm

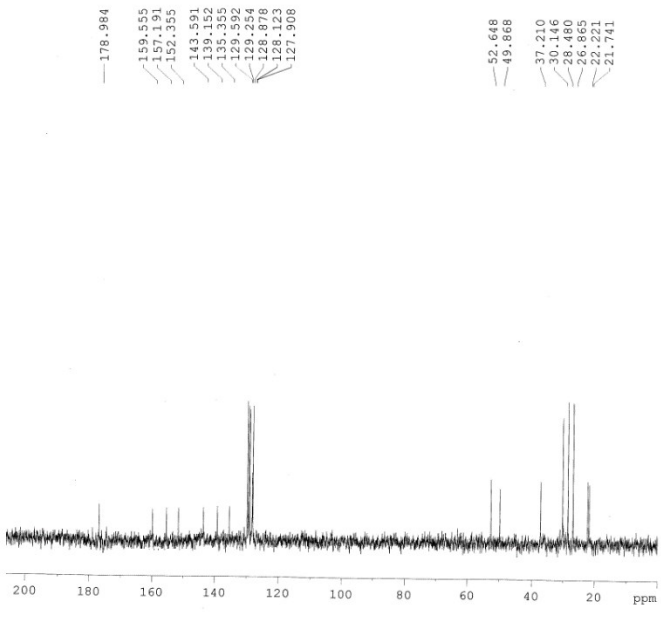

178.697
163.514
161.514
155.159
138.913
131.787
130.161
129.835
129.096
128.650
127.971
124.915
120.257
117.303
52.436
49.659
36.978
29.935
28.266
26.647
22.037
200
180
160
140
120
100
80
60
40
20
ppm

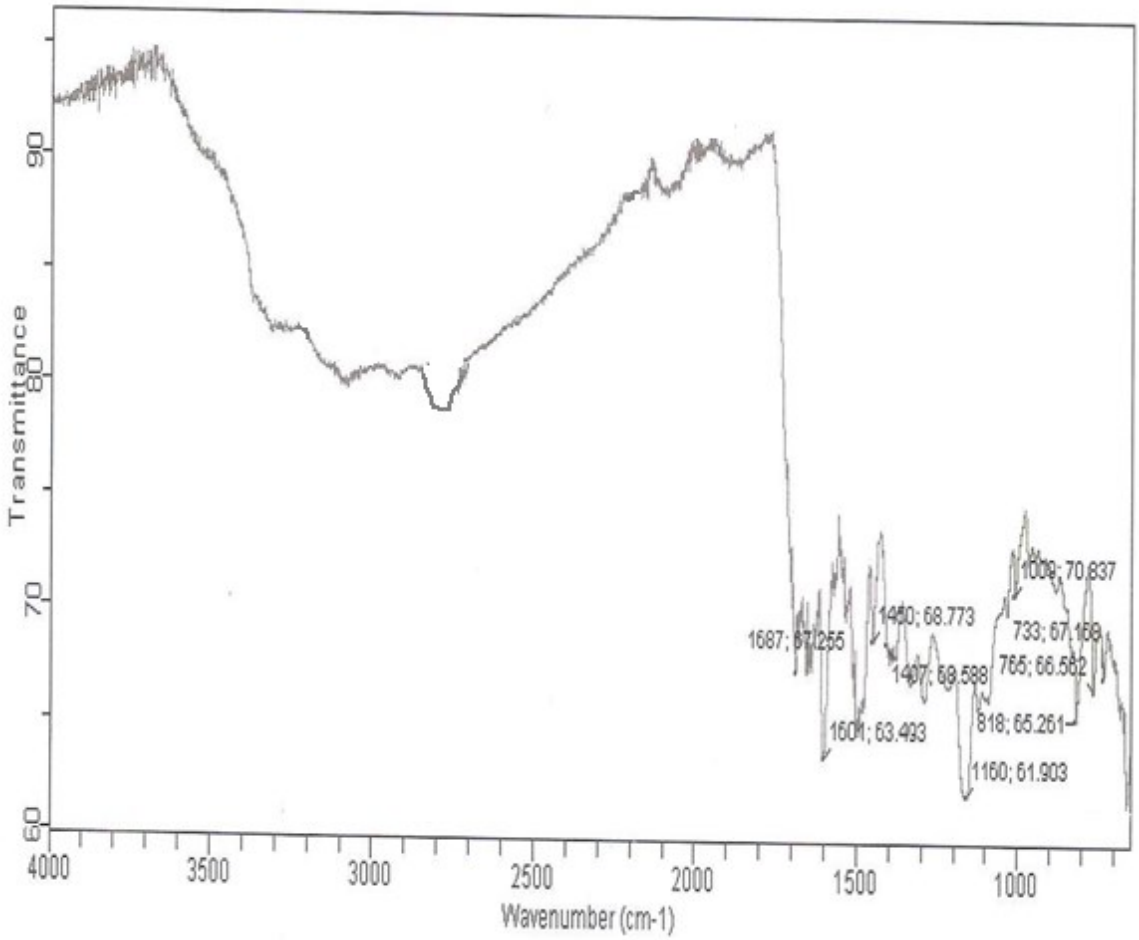

Transmittance
Wavenumber (cm-1)
3500
3000
2500
2000
1500
1000
3322; 64.956
1700; 55.204
1610; 48.124
1514; 49.448
1298; 53.953
1179; 48.664
829; 58.269

TS2

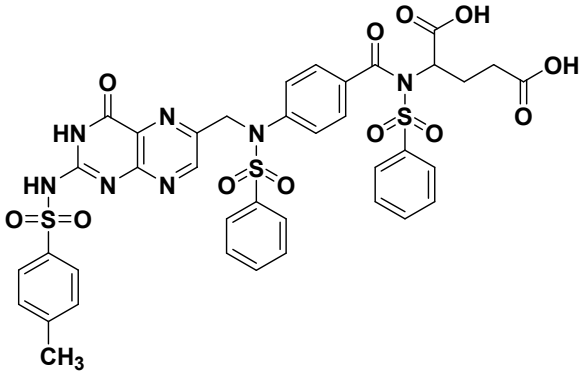

O
OH
O
OH
O
HN
N
N
HN
N
N
O=S=O
N
S
O
O
O
N
S
O
O
CH3
CH3

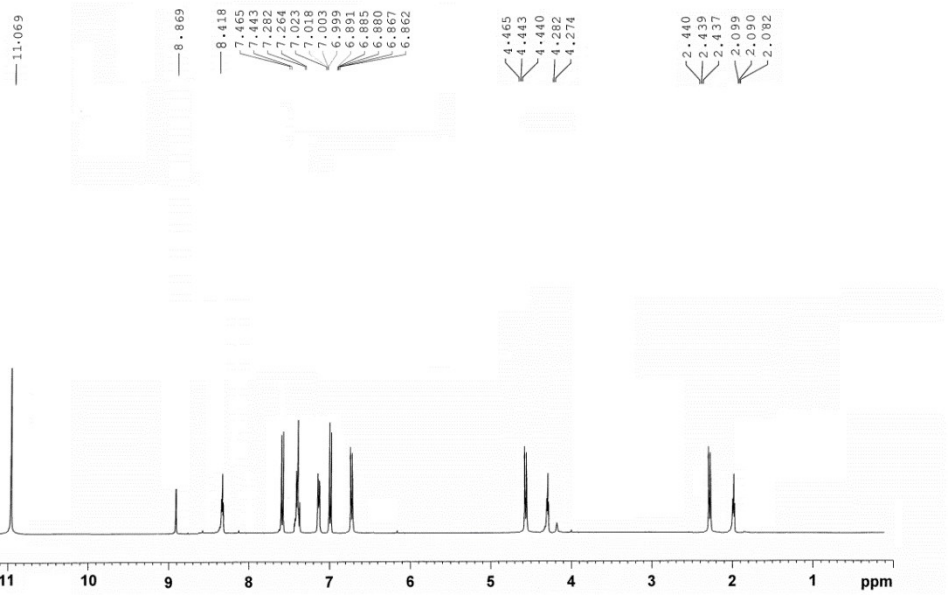

11.099
8.999
8.418
7.465
7.443
7.282
7.264
7.023
7.018
7.003
6.999
6.891
6.885
6.880
6.867
6.862
4.465
4.443
4.440
4.282
4.274
2.440
2.439
2.437
2.099
2.090
2.082
11
10
9
8
7
6
5
4
3
2
1
ppm

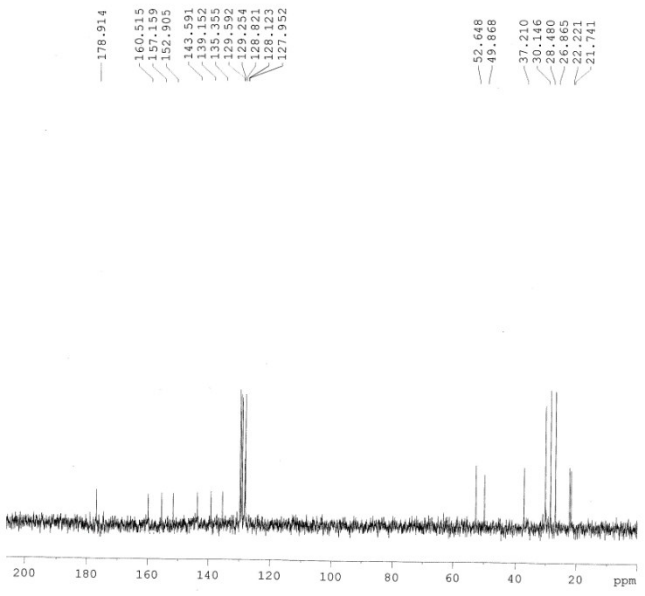

178.984
159.555
157.191
152.355
143.591
139.152
135.355
129.592
129.254
128.878
128.123
127.908
52.648
49.868
37.210
30.146
28.480
26.865
22.221
21.741
200
180
160
140
120
100
80
60
40
20
ppm

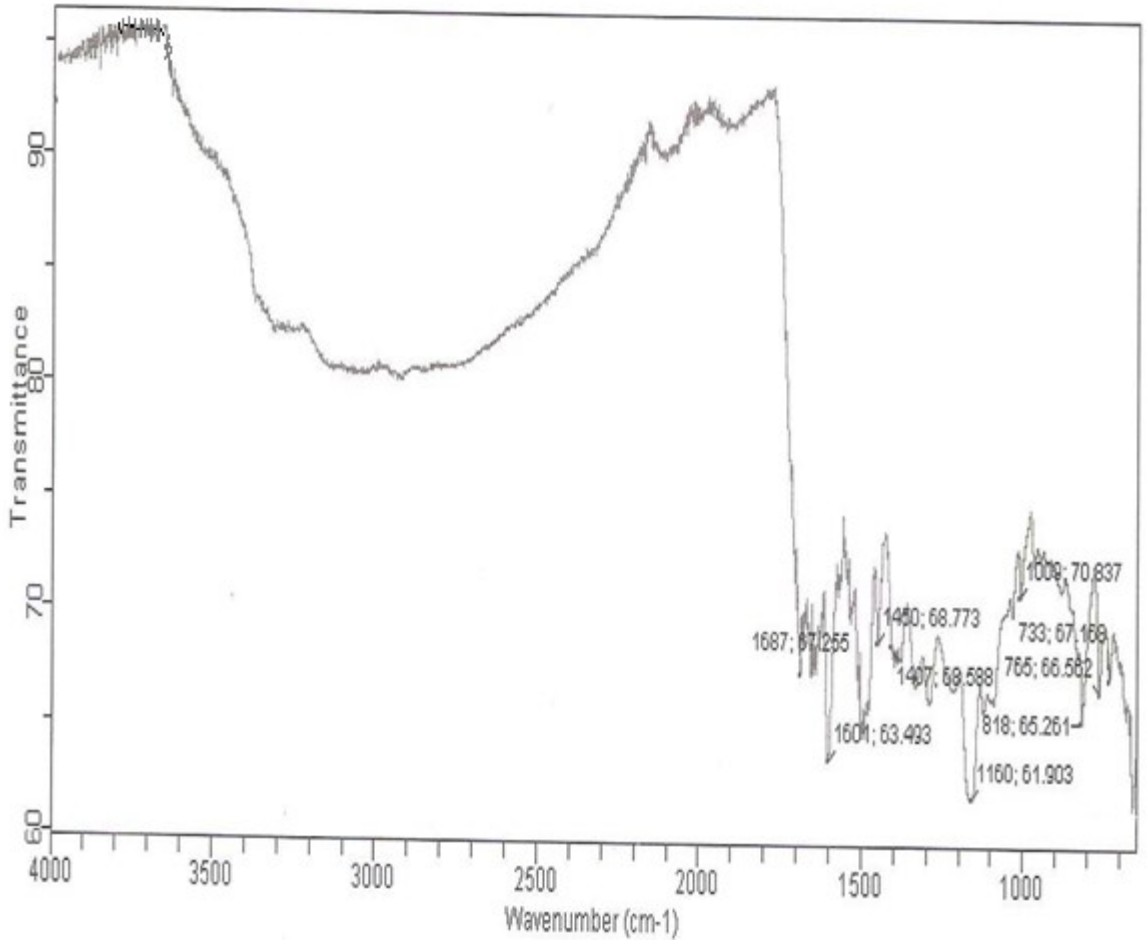

Transmittance
90
80
70
60
4000
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)
1687; 67.255
1601; 63.493
1450; 68.773
1407; 68.588
1160; 61.903
1009; 70.837
818; 65.261
765; 66.562
733; 67.168

TS3

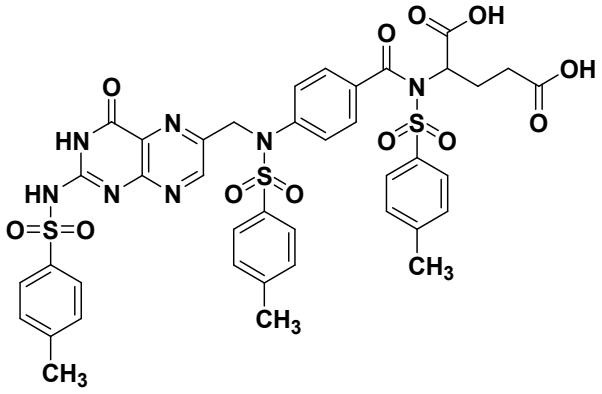


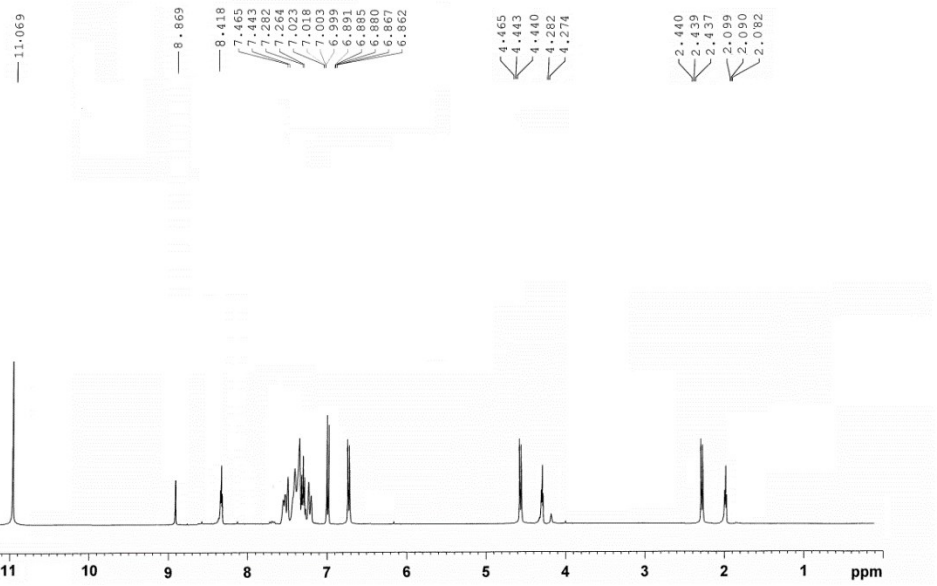

11.069
8.869
8.418
7.465
7.443
7.282
7.264
7.023
7.018
7.003
6.999
6.891
6.885
6.880
6.867
6.862
4.465
4.443
4.440
4.282
4.274
2.440
2.439
2.437
2.099
2.090
2.082
11
10
9
8
7
6
5
4
3
2
1
ppm

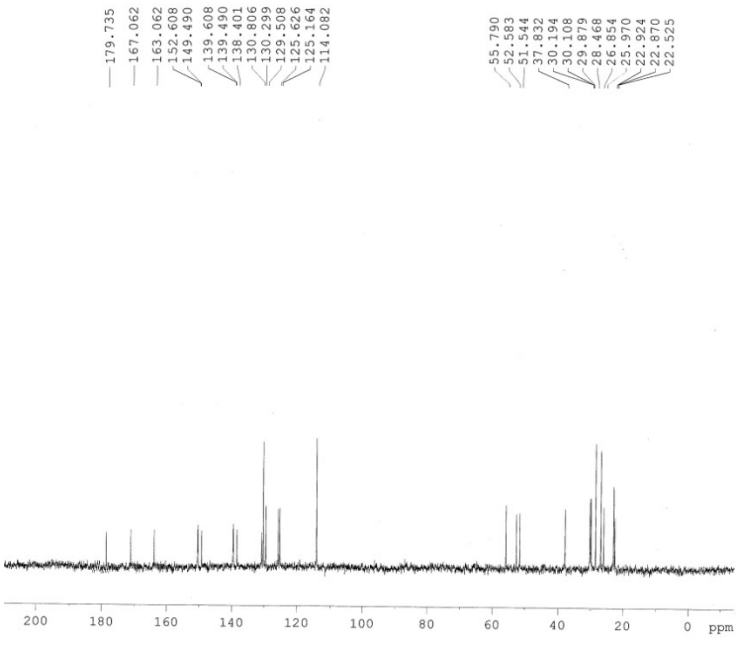

178.914
160.515
157.159
152.905
143.591
139.152
135.355
129.392
129.264
128.821
128.123
127.952
52.648
49.868
37.210
30.446
28.480
26.865
22.221
21.741
200
180
160
140
120
100
80
60
40
20
ppm

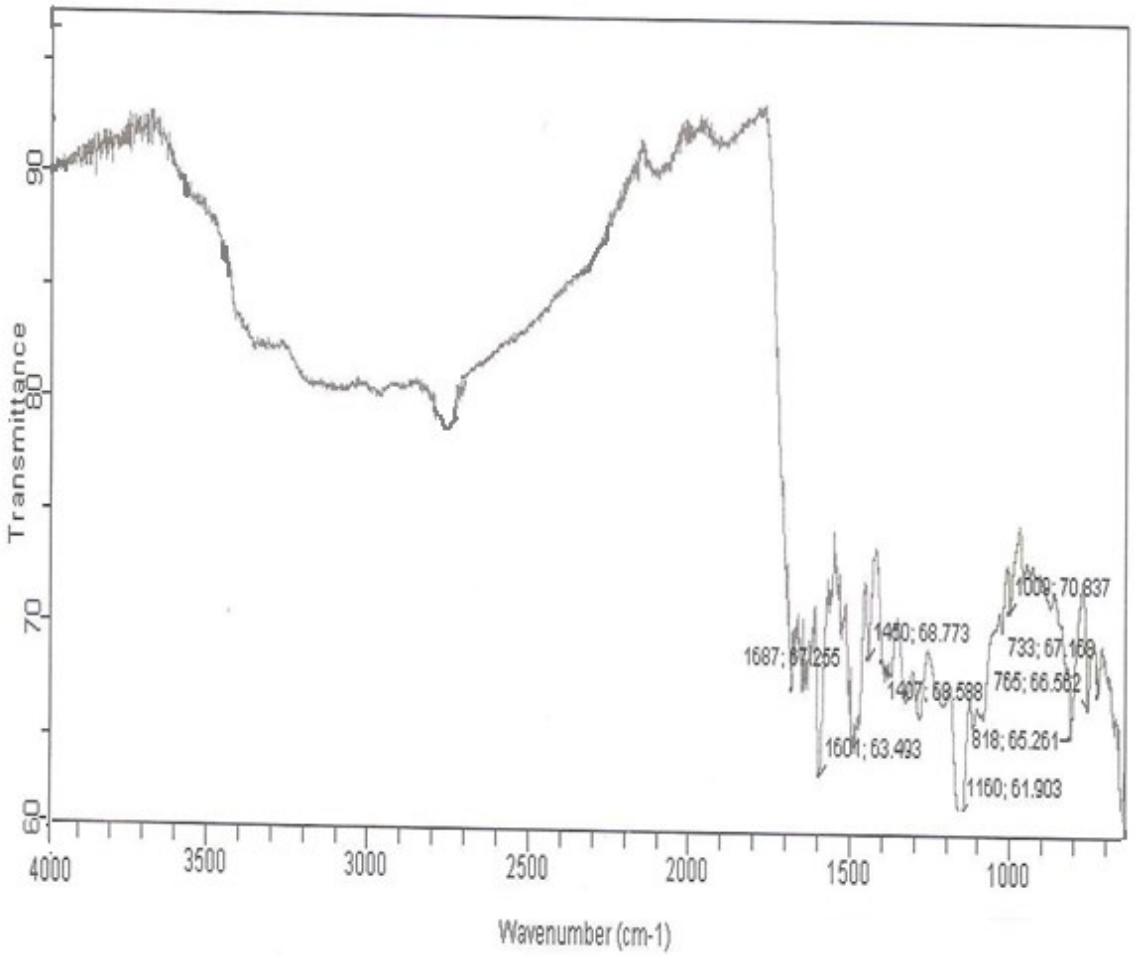

Transmittance
90
80
70
60
4000
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)
1687; 67.255
1601; 63.493
1460; 68.773
1407; 68.588
1160; 61.903
1009; 70.837
733; 67.169
765; 66.582
818; 65.261

TS4

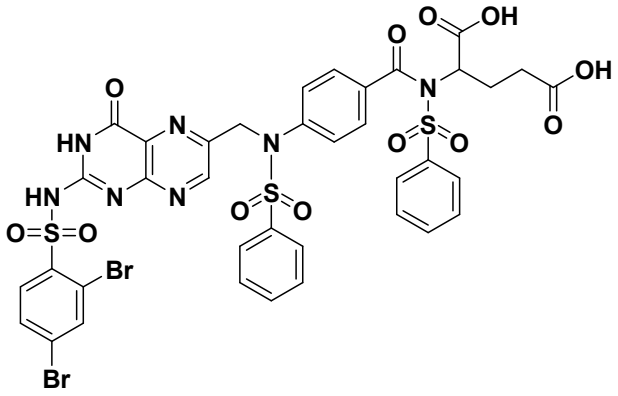

O
OH
O
OH
O
N
HN
N
N
S
O
O
HN
N
N
O=S=O
CH3
CH3
CH3

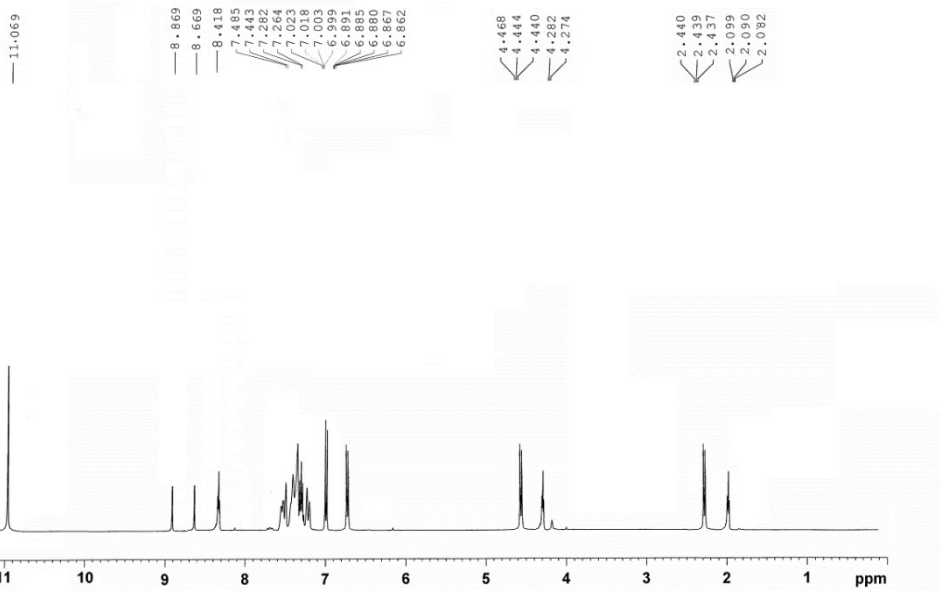

11.069
8.869
8.418
7.465
7.443
7.282
7.264
7.023
7.018
7.003
6.999
6.891
6.885
6.880
6.867
6.862
4.465
4.443
4.440
4.282
4.274
2.440
2.439
2.437
2.099
2.090
2.082
11
10
9
8
7
6
5
4
3
2
1
ppm

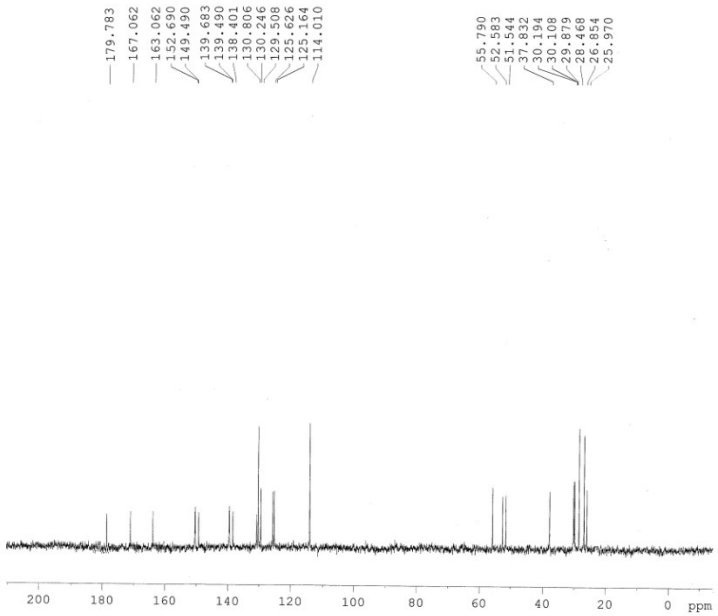

179.735
167.062
163.062
152.608
149.490
139.608
139.490
138.401
130.806
130.299
129.508
125.626
125.164
114.082
55.790
52.583
51.544
37.832
30.194
30.108
29.879
28.468
26.854
25.970
22.924
22.870
22.525
200
180
160
140
120
100
80
60
40
20
0
ppm

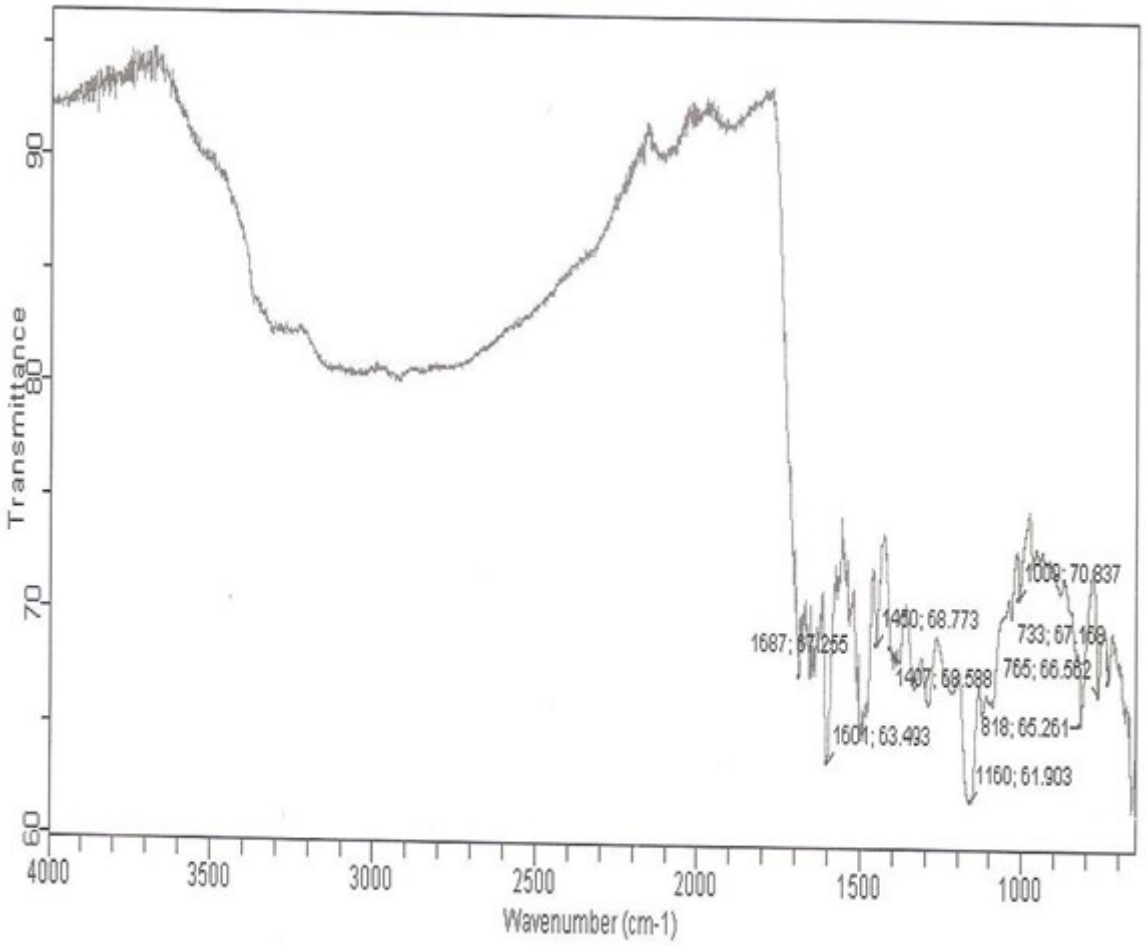

Transmittance
90
80
70
60
4000
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)
1687; 67.255
1601; 63.493
1460; 68.773
1407; 69.588
1160; 61.903
818; 65.261
765; 66.582
733; 67.169
1009; 70.837

TS5

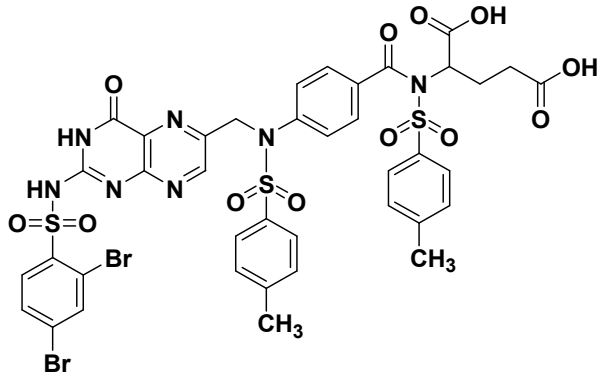

O
OH
O
OH
N
O
HN
N
N
S
O
O
HN
N
N
N
S
O
O
O=S=O
Br
Br

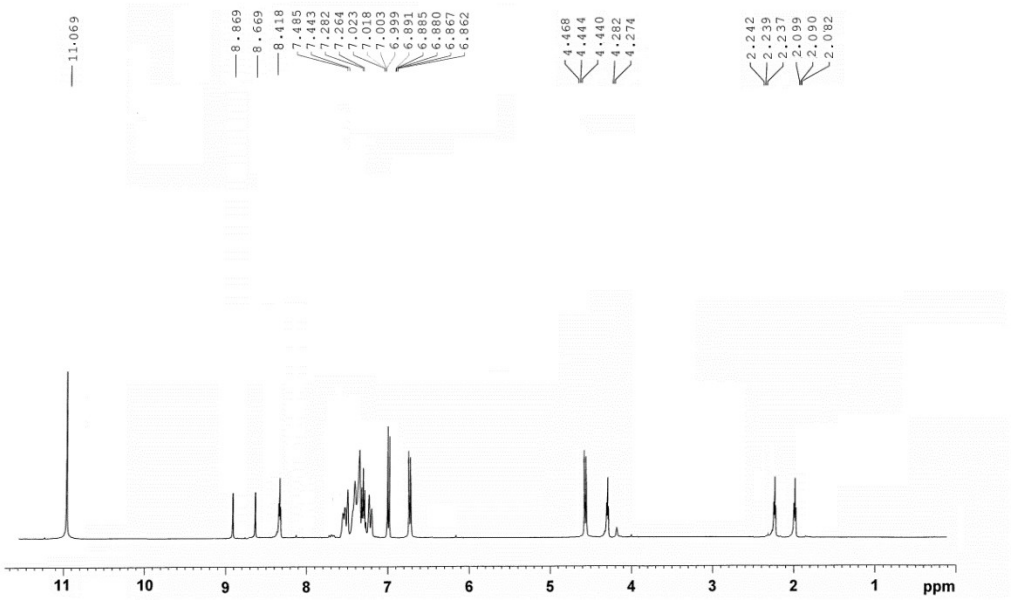

11.069
8.869
8.669
8.418
7.485
7.443
7.282
7.264
7.023
7.018
7.003
6.999
6.891
6.885
6.880
6.867
6.862
4.468
4.444
4.440
4.282
4.274
2.440
2.439
2.437
2.099
2.090
2.082
11
10
9
8
7
6
5
4
3
2
1
ppm

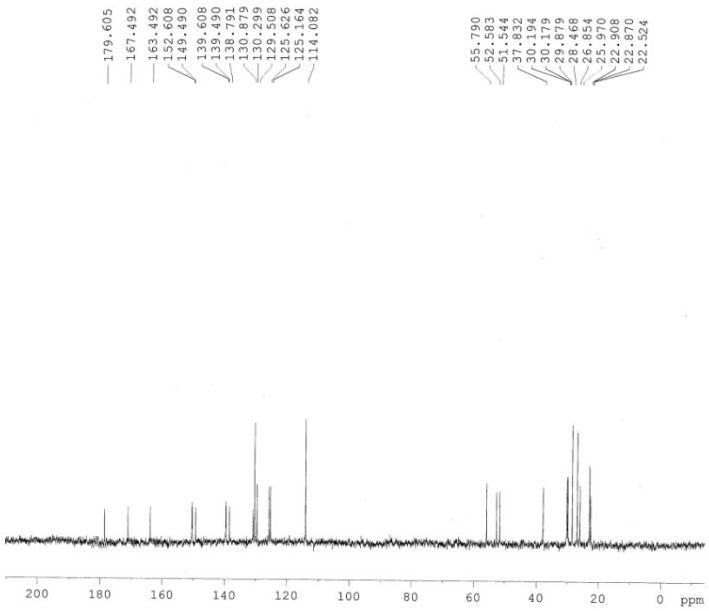

179.783
167.062
163.062
152.690
149.490
139.683
139.490
138.401
130.801
130.246
129.508
125.626
125.164
114.010
55.790
52.583
51.544
37.832
30.194
30.108
29.879
28.468
26.854
25.970
200
180
160
140
120
100
80
60
40
20
0
ppm


Transmittance
90
80
70
60
4000
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)
1687; 67.255
1601; 63.493
1460; 68.773
1407; 68.588
1160; 61.903
1009; 70.837
818; 65.261
765; 66.582
733; 67.168

TS6


O
OH
O
OH
N
O
HN
N
N
N
HN
N
N
S
O
O
O
S
O
O
O=S=O
Br
Br
CH3
CH3


11.069
8.869
8.669
8.418
7.485
7.443
7.282
7.264
7.023
7.018
7.003
6.999
6.891
6.885
6.880
6.867
6.862
4.468
4.444
4.440
4.282
4.274
2.242
2.239
2.237
2.099
2.090
2.082
11
10
9
8
7
6
5
4
3
2
1
ppm


179.605
167.492
163.492
152.608
149.490
139.608
139.490
138.791
130.879
130.299
129.508
125.626
125.164
114.082
55.790
52.583
51.544
37.832
30.194
30.179
29.879
28.468
26.854
25.970
22.908
22.870
22.524
200
180
160
140
120
100
80
60
40
20
0
ppm