

Supplementary Data
for
Novel Thiazolactone Derivatives: Synthesis and Quantum Chemical Study

Behzad khalili^{1*}, Niloofar Bakhshi Boroon¹

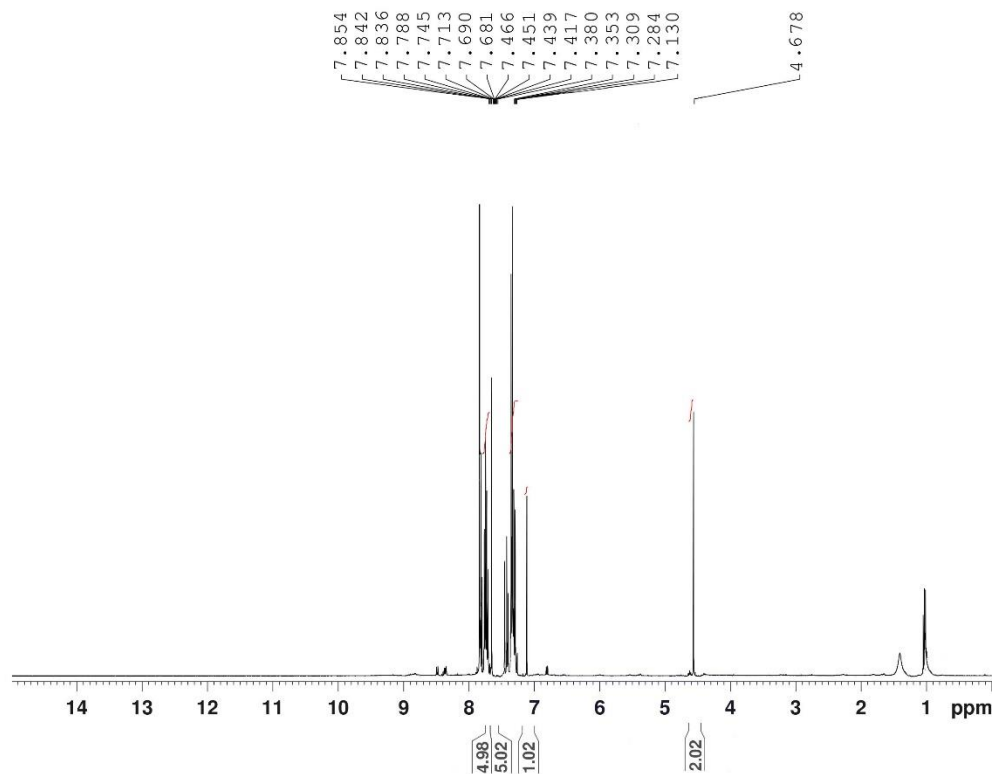
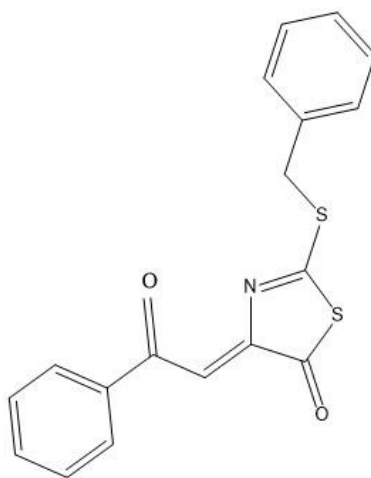
¹*Department of Chemistry, Faculty of Sciences, University of Guilan, P.O. Box 41335-1914,
Rasht, Iran. Tel.: +981333367262 and fax: +981333367262*

^{*} *Corresponding author's E-mail: b.khalili@guilan.ac.ir*

^1H NMR

for

(Z)-2-(benzylthio)-4-(2-oxo-2-phenylethylidene)thiazol-5(4H)-one(4H-Gly):



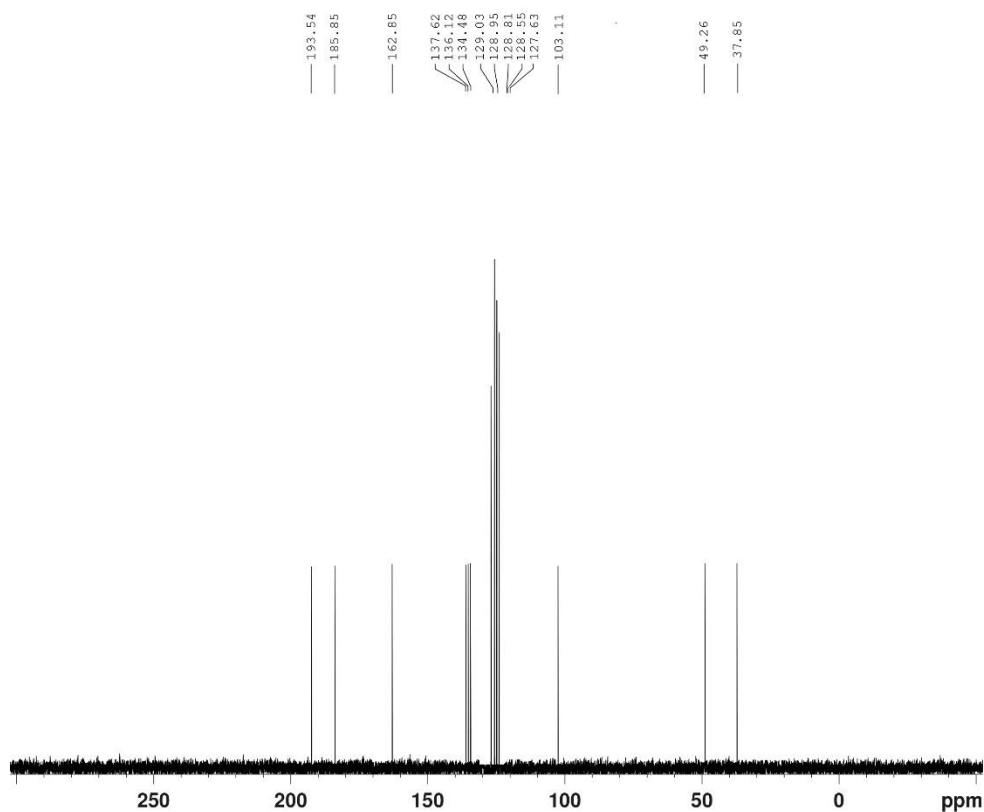
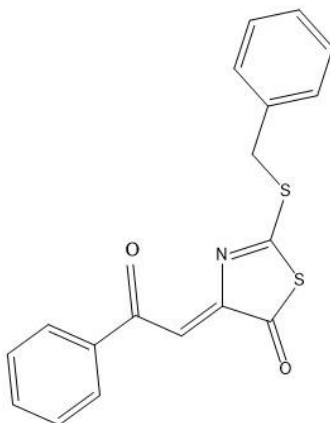
NAME Gilan UN
EXPNO 2128
PROCNO 1
Date_ 20170620
Time 13.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 20
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 181
DW 62.400 usec
DE 6.50 usec
TE 296.8 K
D1 4.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SF01 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR

for

(Z)-2-(benzylthio)-4-(2-oxo-2-phenylethylidene)thiazol-5(4H)-one(4H-Gly):



NAME Gilan UN
EXPNO 2340
PROCNO 1
Date_ 20170623
Time 19.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 731
DS 0
SWH 35714.285 Hz
FIDRES 0.544957 Hz
AQ 0.9175540 sec
RG 2050
DW 14.000 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

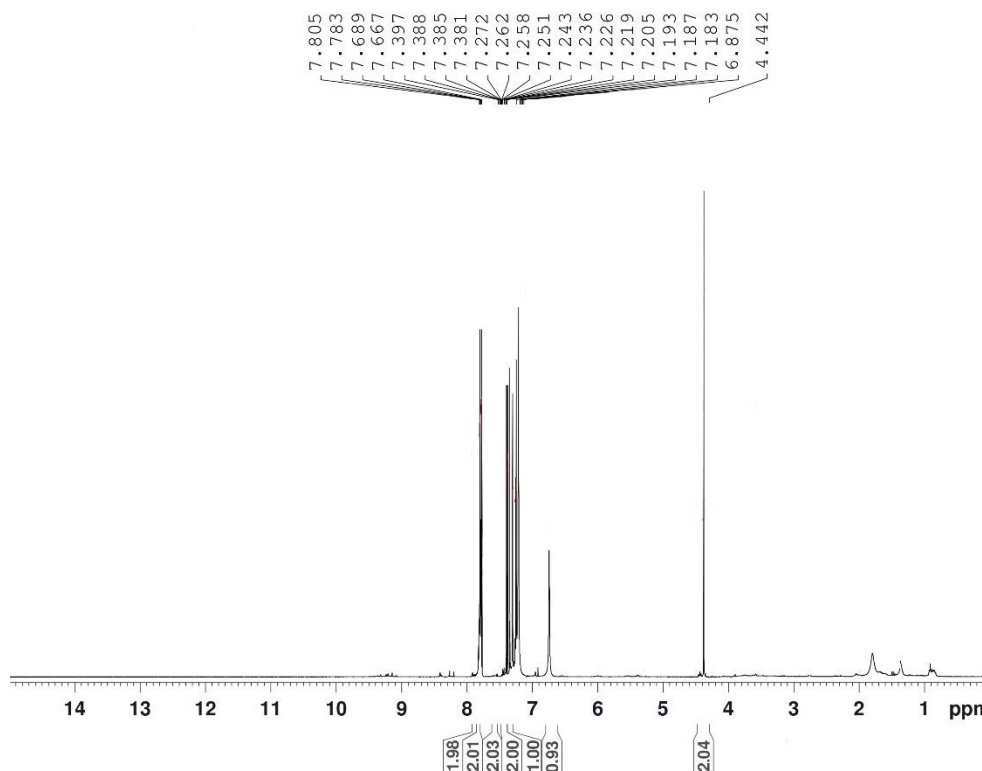
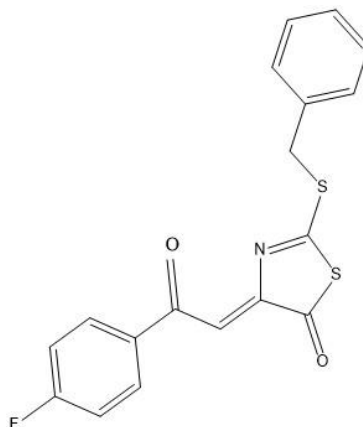
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR

For

(Z)-2-(benzylthio)-4-(2-(4-fluorophenyl)-2-oxoethylidene)thiazol-5(4H)-one(4F-Gly):

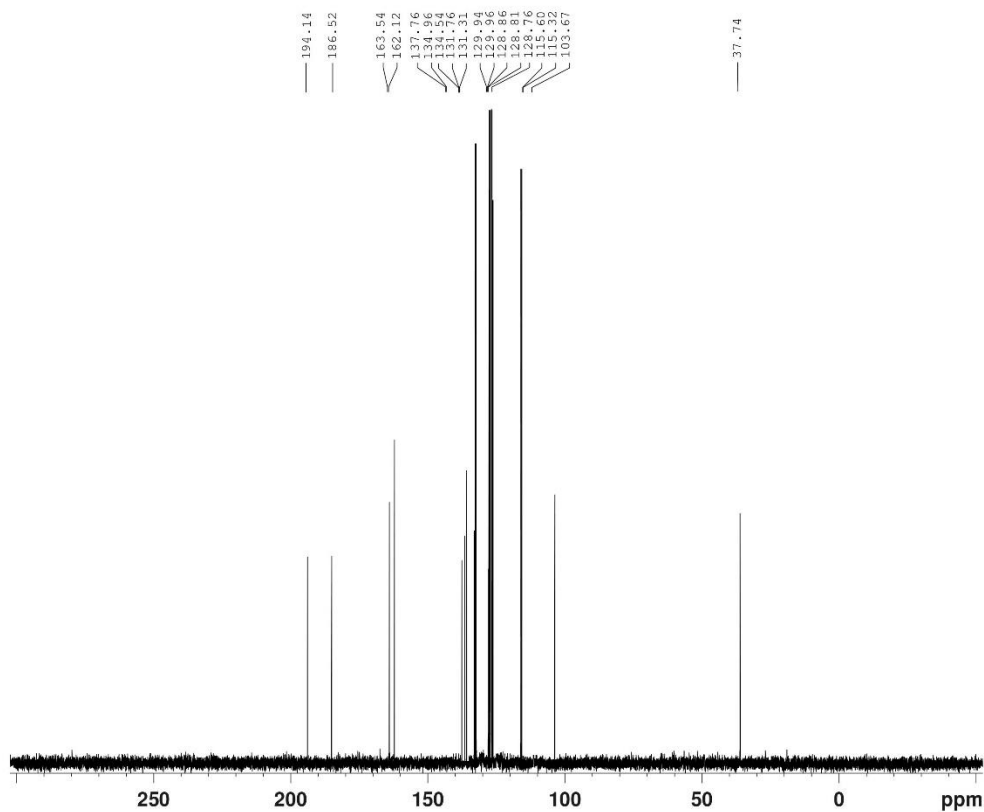
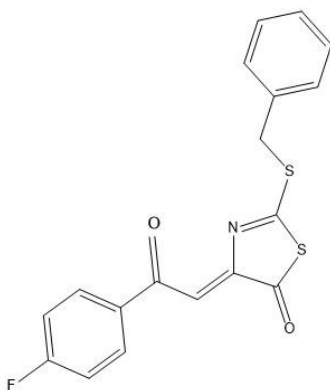


NAME Gilan UN
EXPNO 2488
PROCNO 1
Date_ 20170911
Time 10.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 20
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 181
DW 62.400 usec
DE 6.50 usec
TE 296.8 K
D1 4.00000000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR

For

(Z)-2-(benzylthio)-4-(2-(4-fluorophenyl)-2-oxoethylidene)thiazol-5(4H)-one(4F-Gly):



NAME Gilan UN
EXPNO 2361
PROCNO 1
Date_ 20170920
Time 19.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 0
SWH 35714.285 Hz
FIDRES 0.544957 Hz
AQ 0.9175540 sec
RG 2050
DW 14.000 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

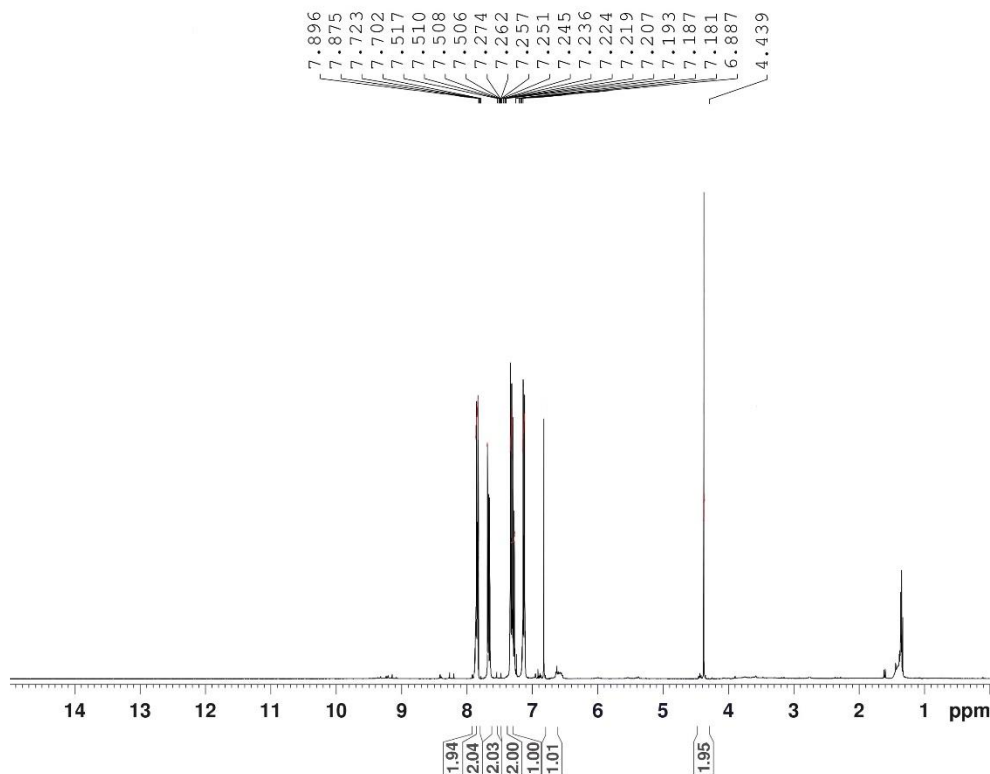
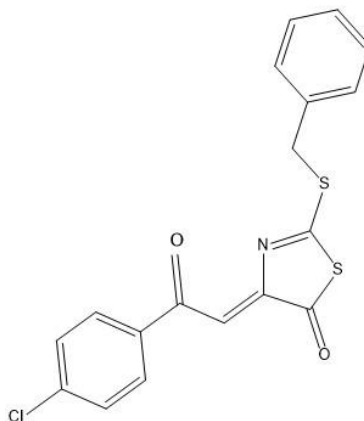
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^1H NMR

For

(Z)-2-(benzylthio)-4-(2-(4-chlorophenyl)-2-oxoethylidene)thiazol-5(4H)-one(4Cl-Gly):



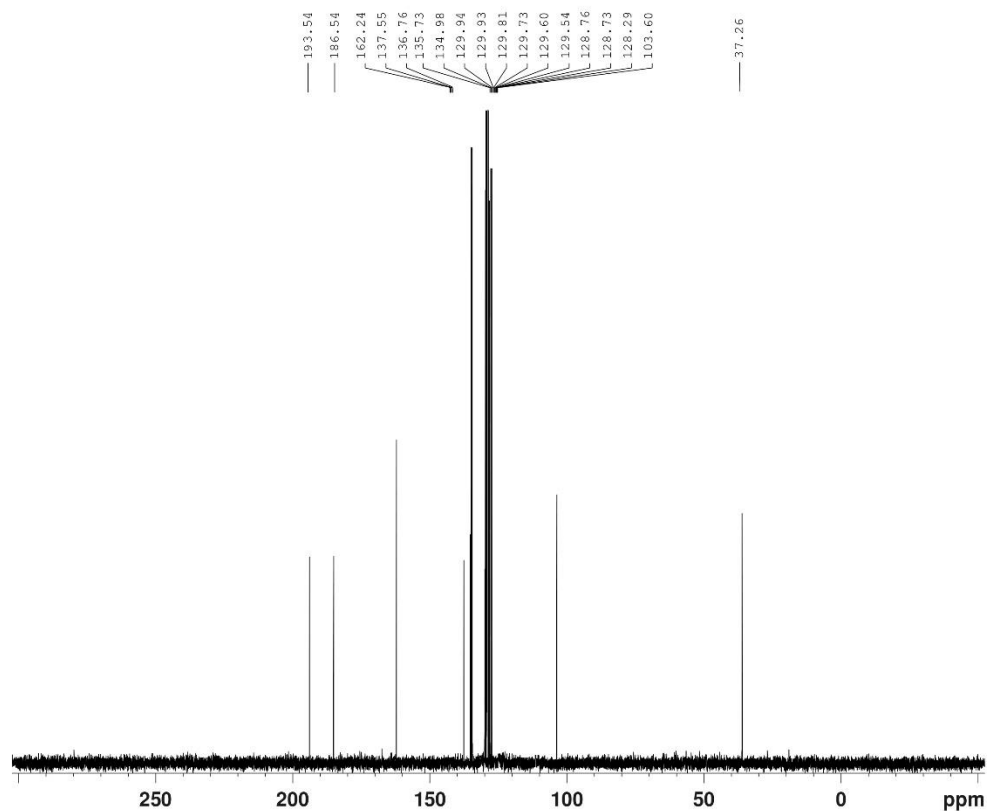
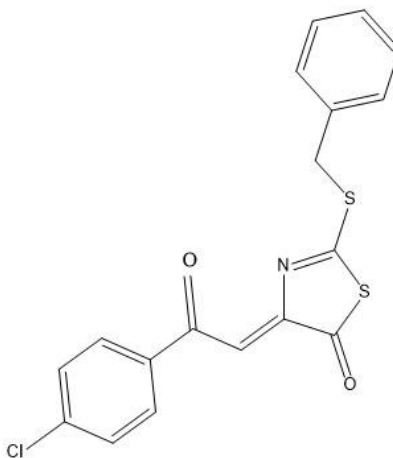
```
NAME      Gilan UN
EXPNO     2266
PROCNO    1
Date_     20171002
Time      13.36
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS         20
DS         0
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894966 sec
RG         181
DW         62.400 usec
DE         6.50 usec
TE         296.8 K
D1         4.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.00 usec
PL1        -2.00 dB
PL1W       11.86359406 W
SF01       400.2236020 MHz
SI         32768
SF         400.2200000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

¹³C NMR

For

(Z)-2-(benzylthio)-4-(2-(4-chlorophenyl)-2-oxoethylidene)thiazol-5(4H)-one(4Cl-Gly):



NAME Gilan UN
EXPNO 1921
PROCNO 1
Date_ 20170920
Time 10.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 0
SWH 35714.285 Hz
FIDRES 0.544957 Hz
AQ 0.9175540 sec
RG 2050
DW 14.000 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

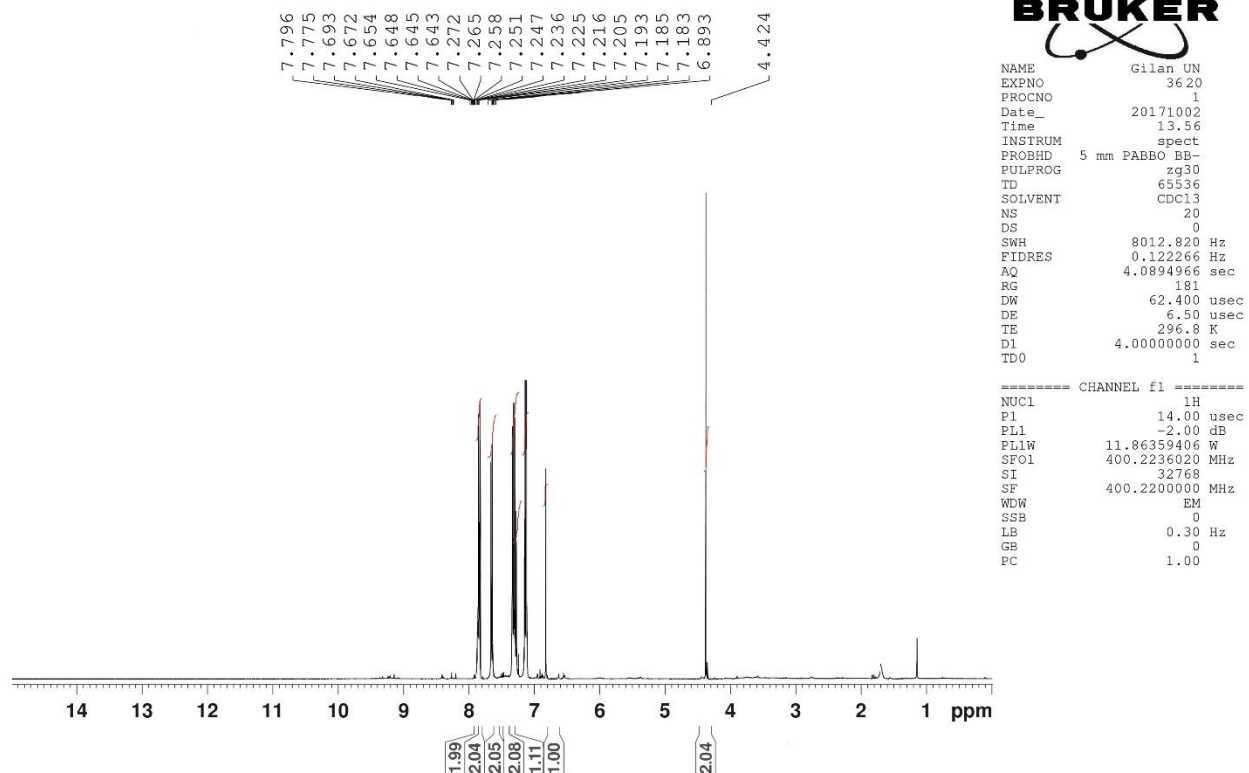
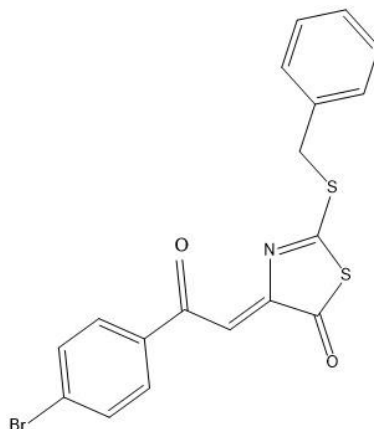
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^1H NMR

For

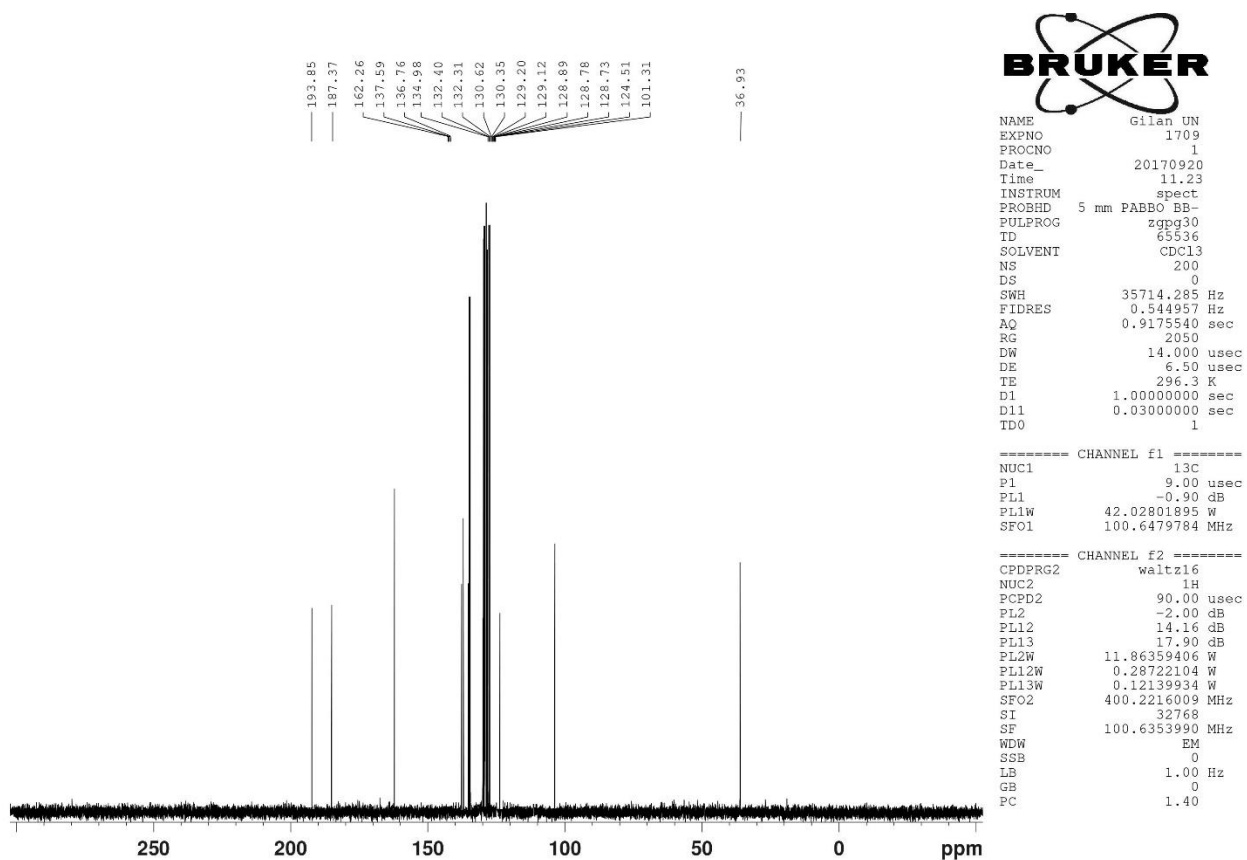
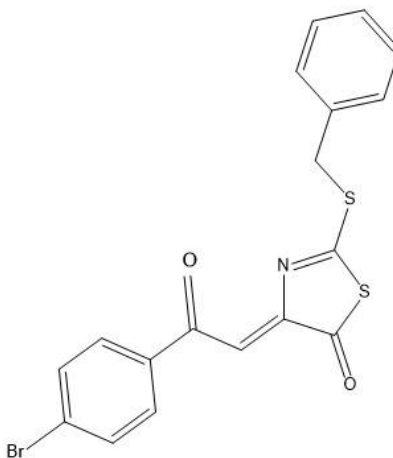
(Z)-2-(benzylthio)-4-(2-(4-bromophenyl)-2-oxoethylidene)thiazol-5(4H)-one(4Br-Gly):



¹³C NMR

For

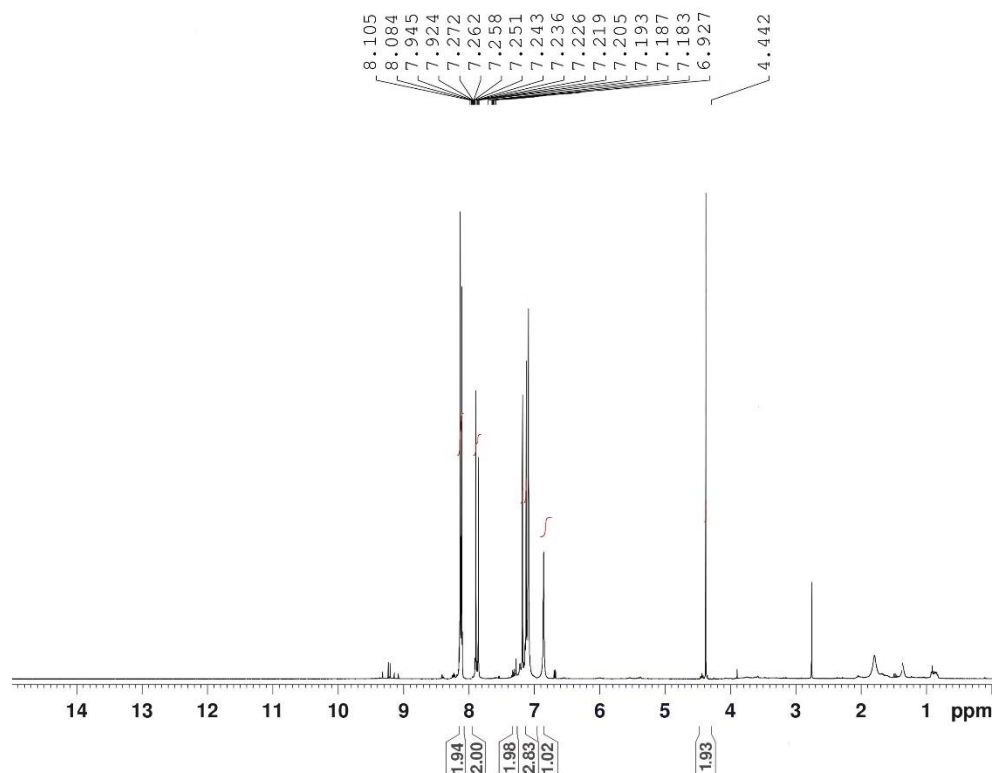
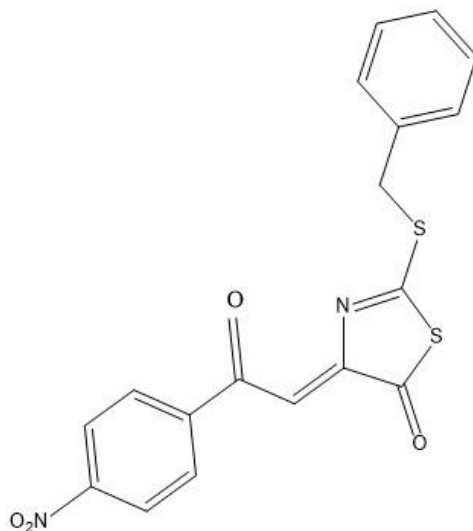
(Z)-2-(benzylthio)-4-(2-(4-bromophenyl)-2-oxoethylidene)thiazol-5(4H)-one(4Br-Gly):



^1H NMR

For

(Z)-2-(benzylthio)-4-(2-(4-nitrophenyl)-2-oxoethylidene)thiazol-5(4H)-one(4NO₂-Gly):



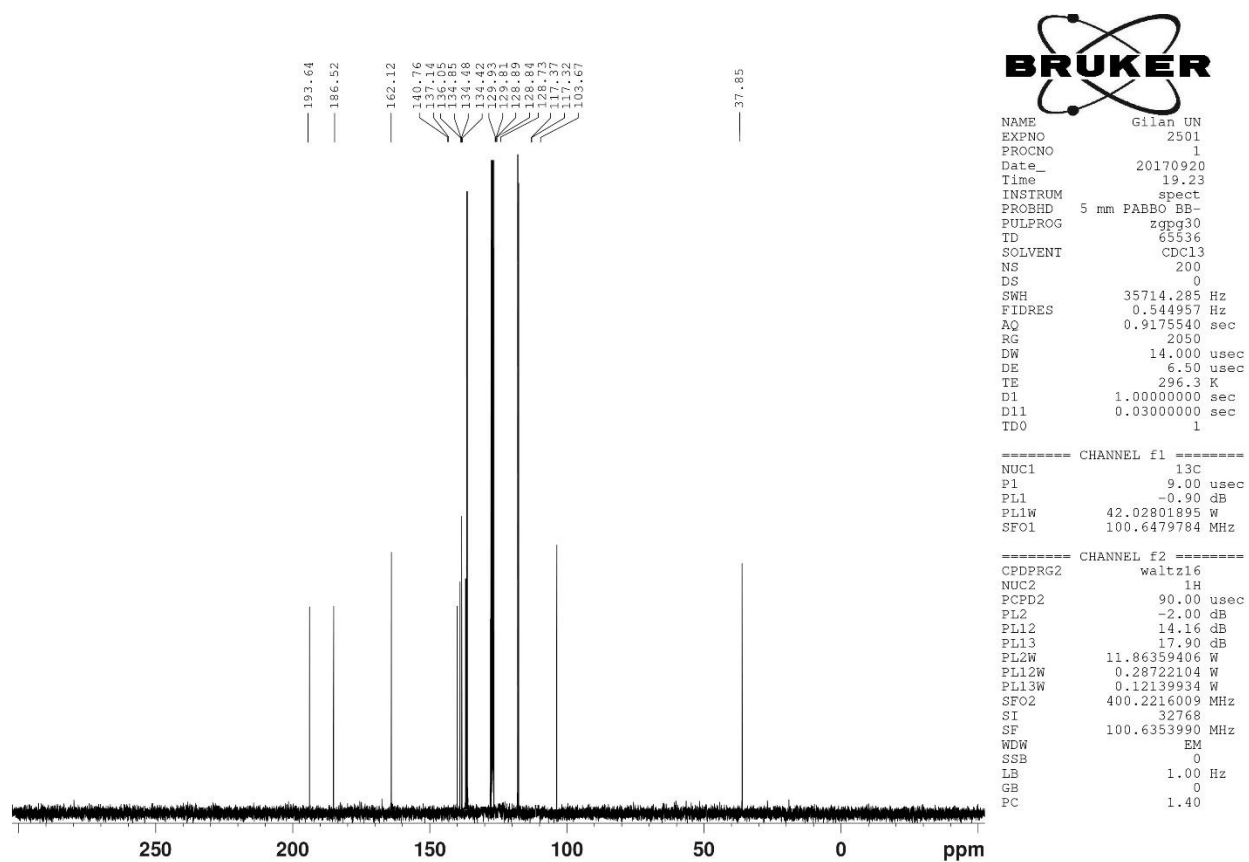
```

NAME          Gilan UN
EXPNO         2409
PROCNO        1
Date_         20170909
Time          10.26
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            20
DS            0
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            181
DW            62.400 usec
DE            6.50 usec
TE            296.8 K
D1            4.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.00 usec
PL1           -2.00 dB
PL1W          11.86359406 W
SFO1          400.2236020 MHz
SI            32768
SF            400.2200000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

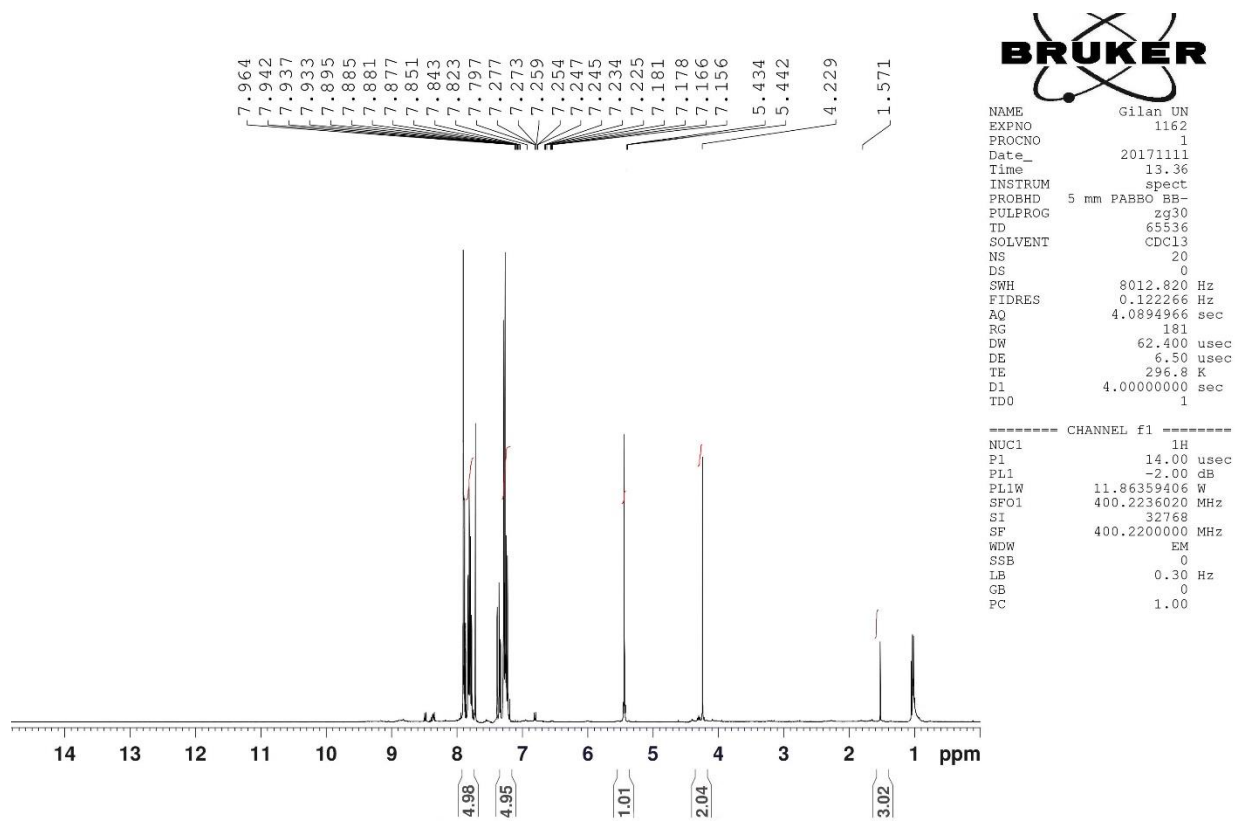
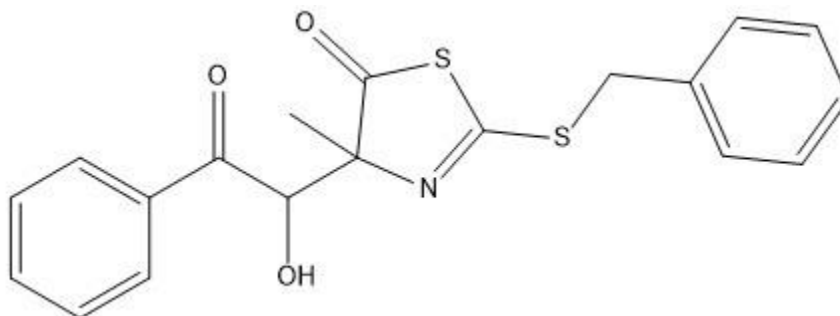
For

O=[N+]([O-])c1ccc(cc1)C(=O)C=C2C(=O)SC(C2)SCc3ccccc3

¹H NMR

For

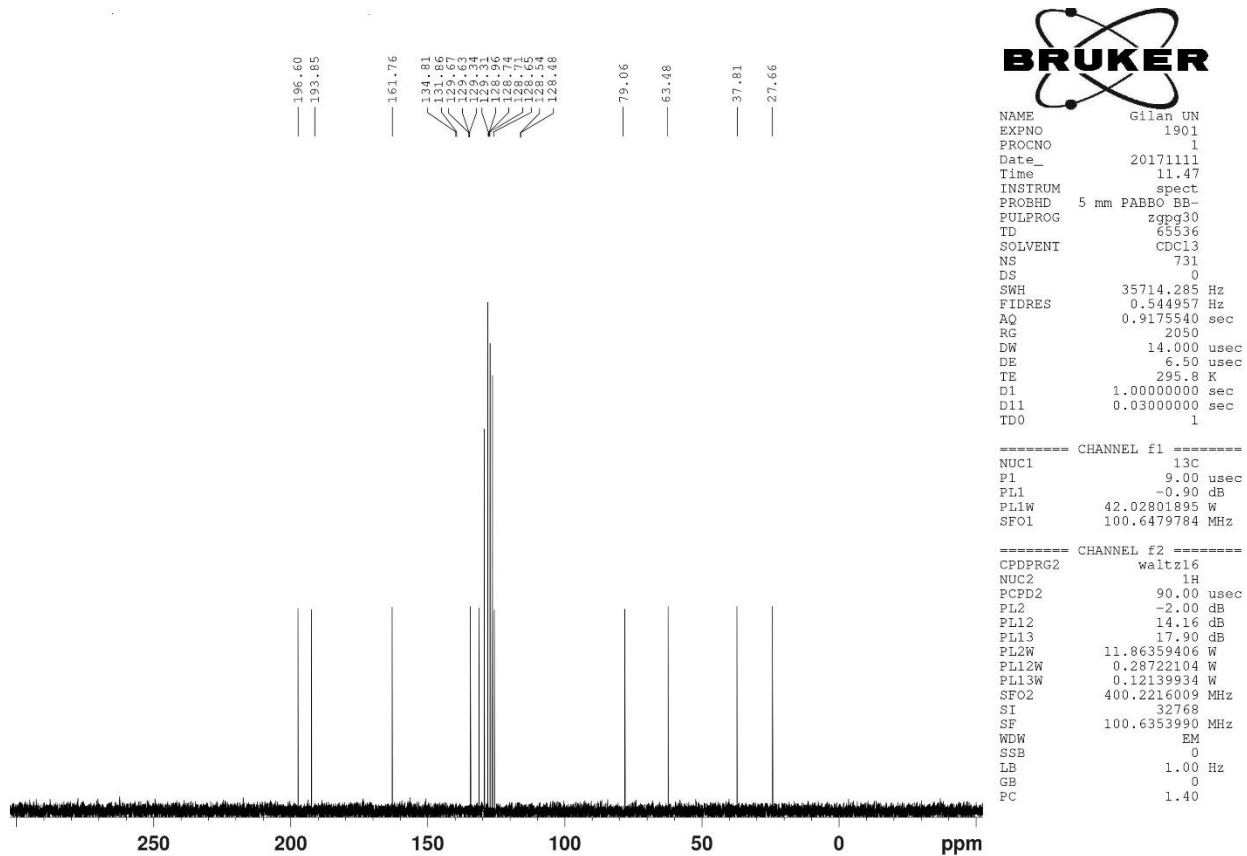
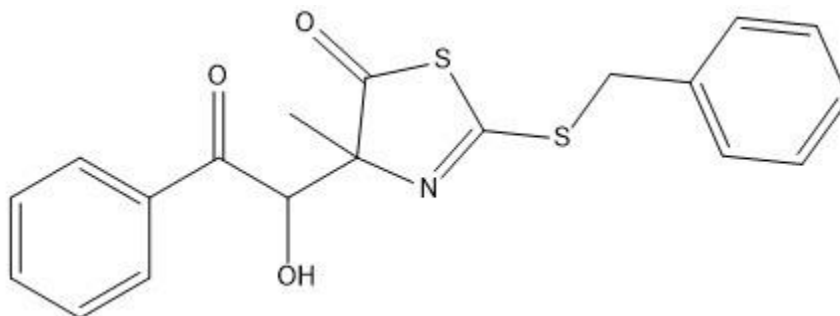
2-(benzylthio)-4-(1-hydroxy-2-oxo-2-phenylethyl)-4-methylthiazol-5(4H)-one(4H-Ala):



¹³C NMR

For

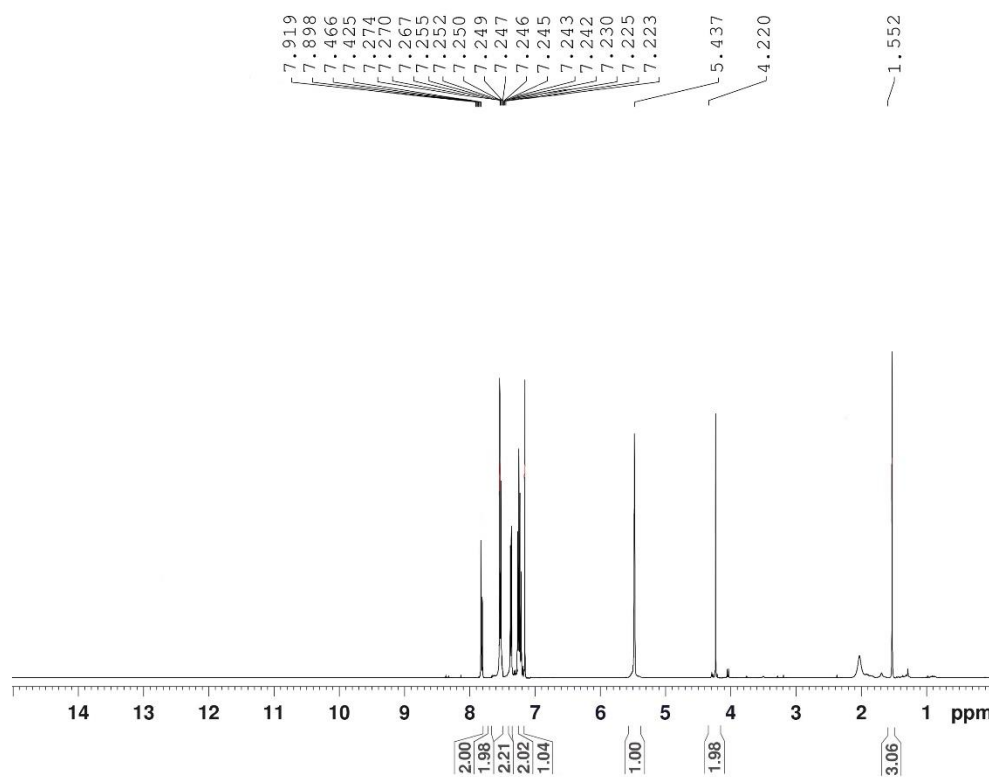
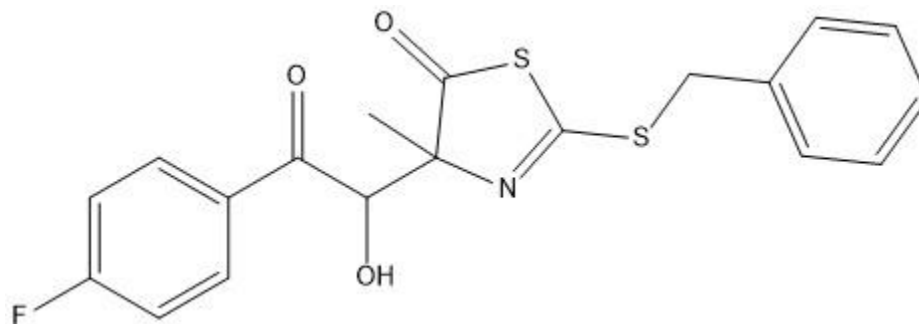
2-(benzylthio)-4-(1-hydroxy-2-oxo-2-phenylethyl)-4-methylthiazol-5(4H)-one(4H-Ala):



¹H NMR

For

2-(benzylthio)-4-(2-(4-fluorophenyl)-1-hydroxy-2-oxoethyl)-4-methylthiazol-5(4H)-one(4F-Ala):



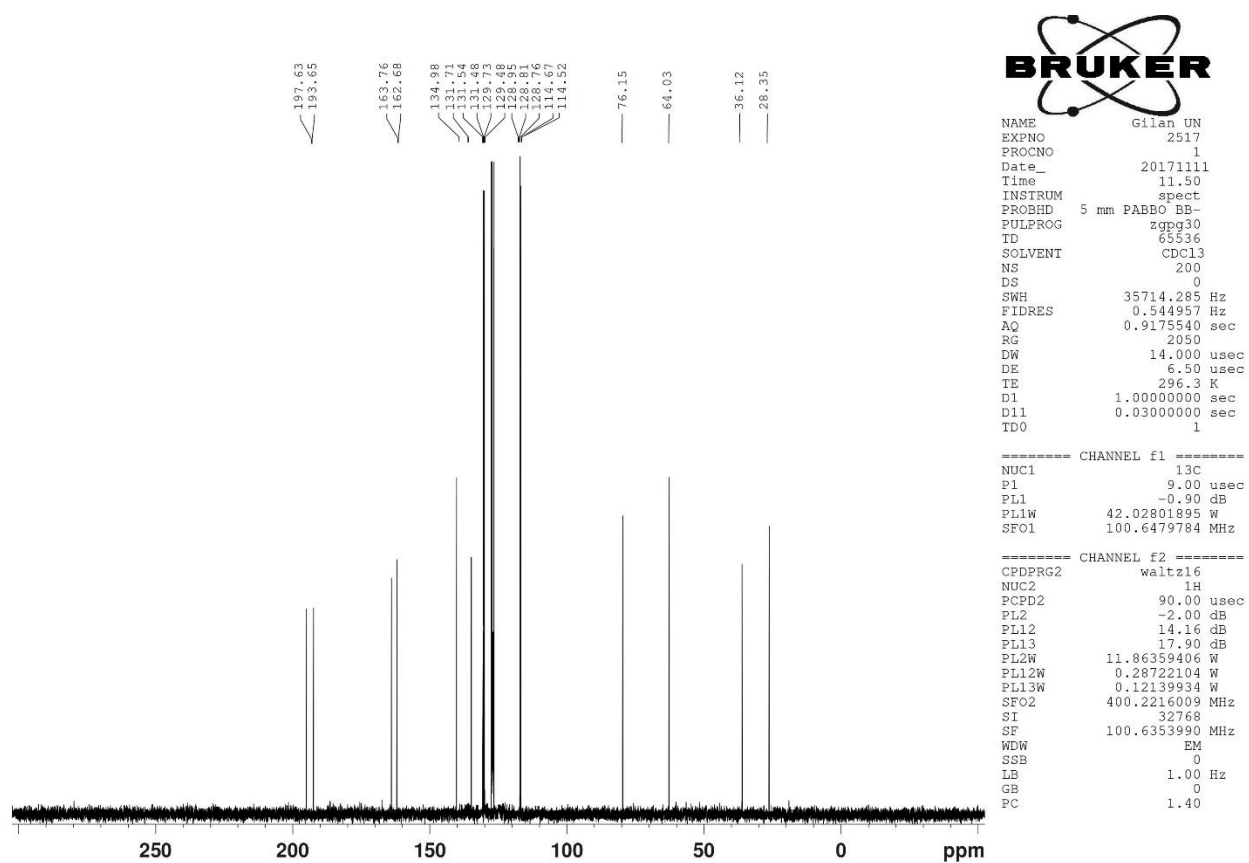
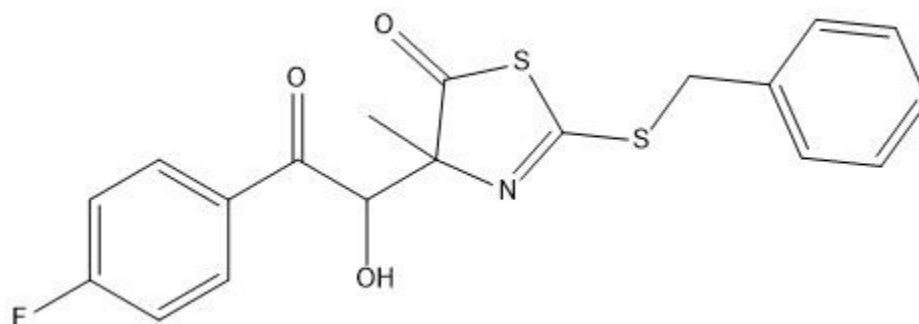
```
NAME      Gilan UN
EXPNO     1635
PROCNO    1
Date_     20171111
Time      11.50
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         20
DS         0
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894966 sec
RG         203
DW         62.400 usec
DE         6.50 usec
TE         295.3 K
D1         4.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.00 usec
PL1        -2.00 dB
PL1W       11.86359406 W
SFO1       400.2236020 MHz
SI         32768
SF         400.2200000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

¹³C NMR

For

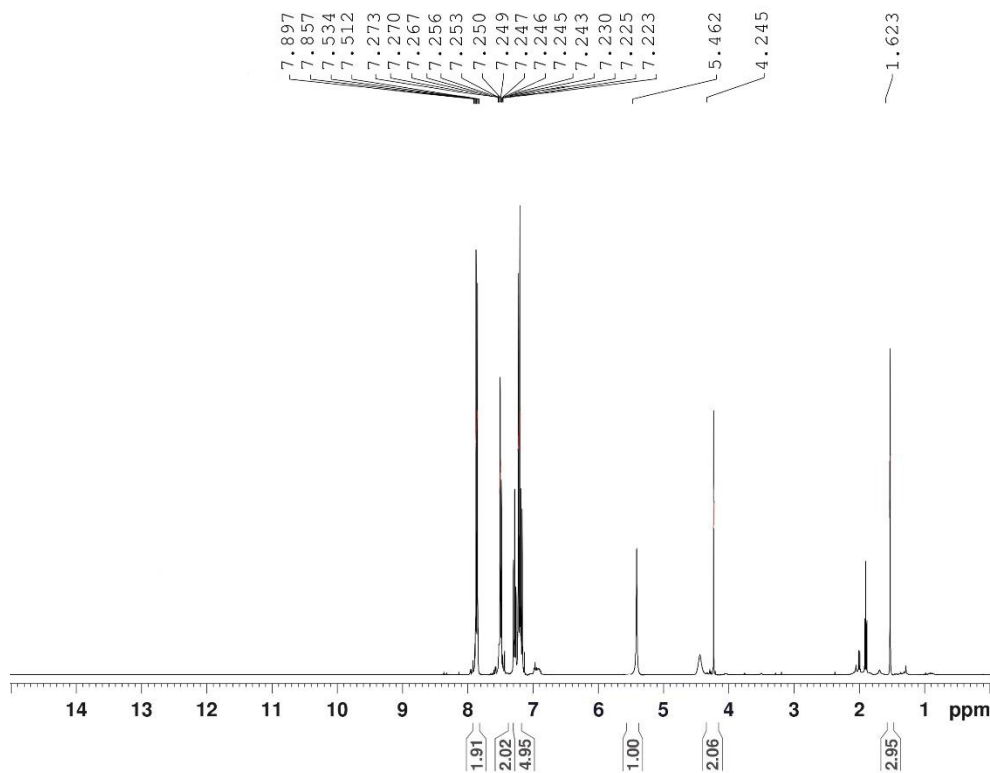
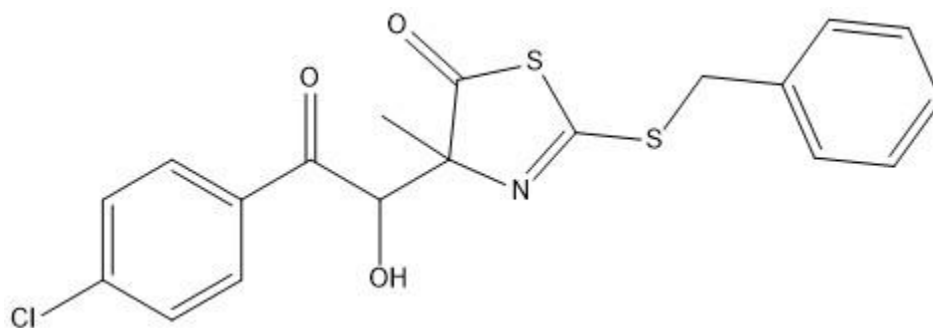
2-(benzylthio)-4-(2-(4-fluorophenyl)-1-hydroxy-2-oxoethyl)-4-methylthiazol-5(4H)-one(4F-Ala):



^1H NMR

For

2-(benzylthio)-4-(2-(4-chlorophenyl)-1-hydroxy-2-oxoethyl)-4-methylthiazol-5(4H)-one(4Cl-Ala):



BRUKER

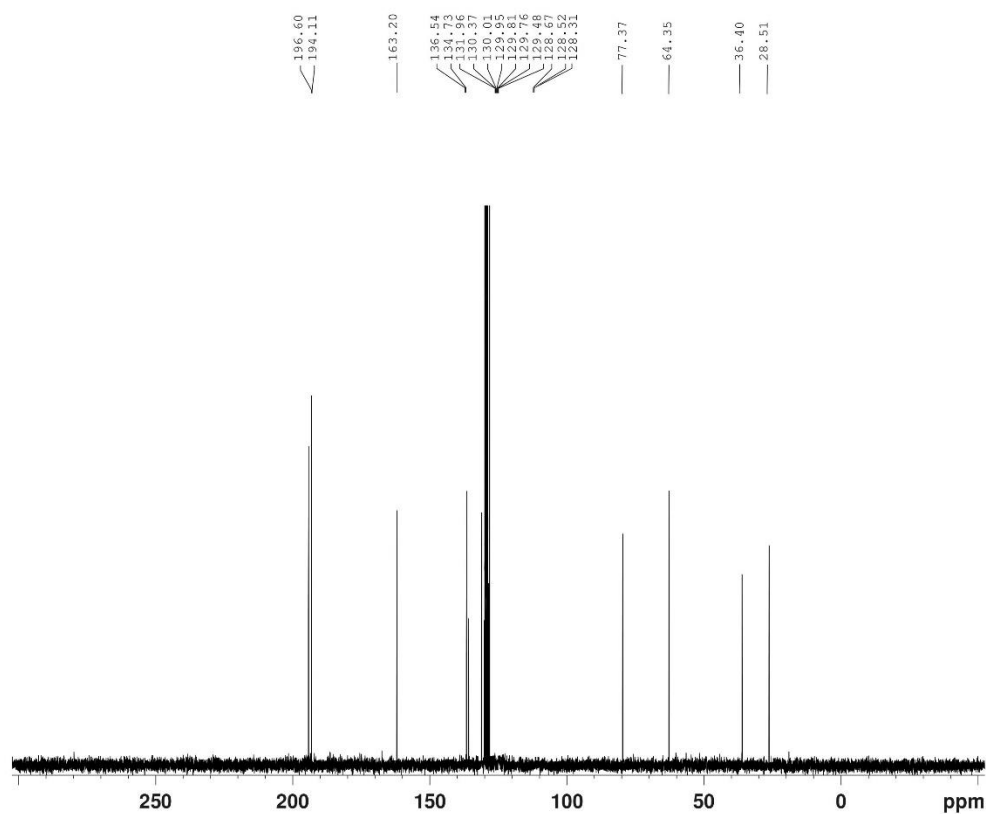
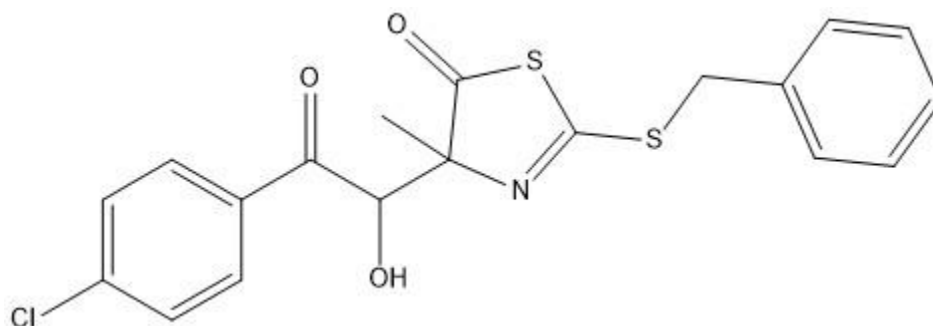
```
NAME      Gilan UN
EXPNO     1820
PROCNO    1
Date_     20171111
Time      14.30
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         20
DS         0
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ          4.0894966 sec
RG          203
DW          62.400 usec
DE           6.50 usec
TE          295.3 K
D1          4.0000000 sec
TD0         1

===== CHANNEL f1 =====
NUC1       1H
P1          14.00 usec
PL1         -2.00 dB
PL1W       11.86359406 W
SF01       400.2236020 MHz
SI          32768
SF          400.2200000 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00
```


¹³C NMR

For

2-(benzylthio)-4-(2-(4-chlorophenyl)-1-hydroxy-2-oxoethyl)-4-methylthiazol-5(4H)-one(4Cl-Ala):



NAME Gilan UN
EXPNO 2718
PROCNO 1
Date_ 20171111
Time 12.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 200
DS 0
SWH 35714.285 Hz
FIDRES 0.544957 Hz
AQ 0.9175540 sec
RG 2050
DW 14.000 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

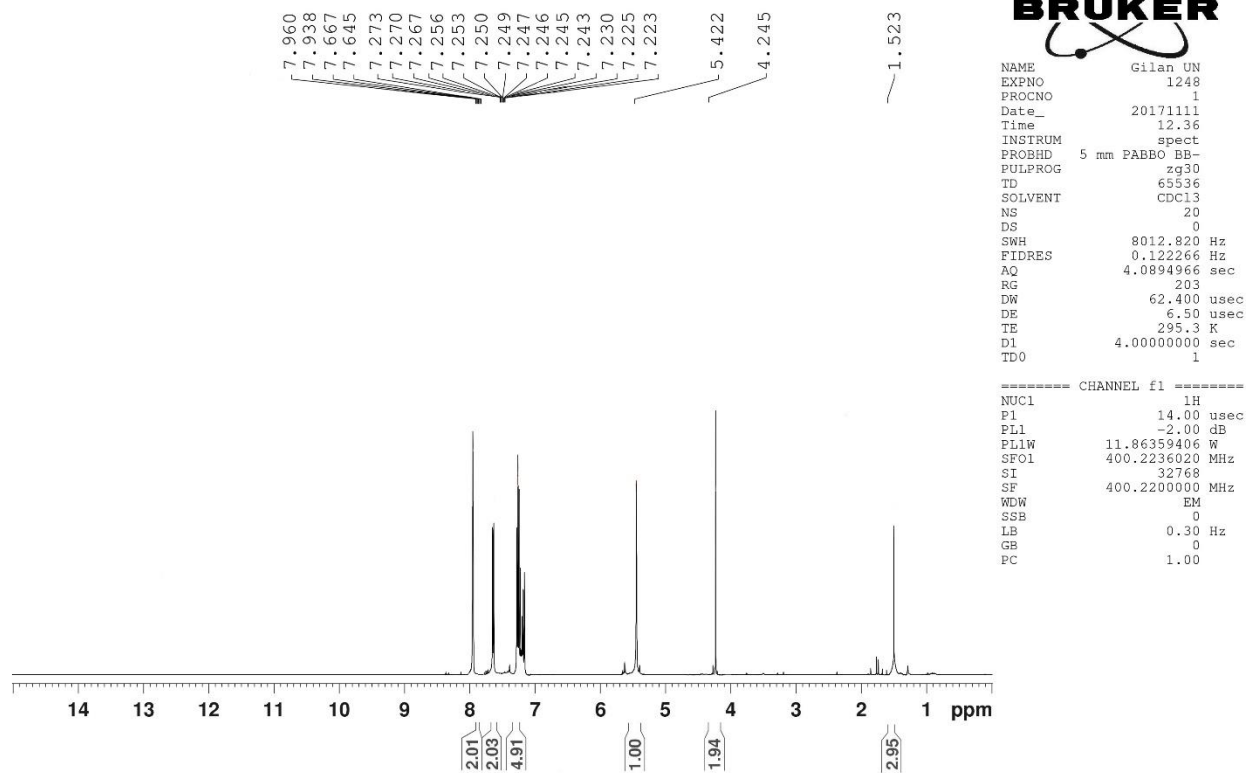
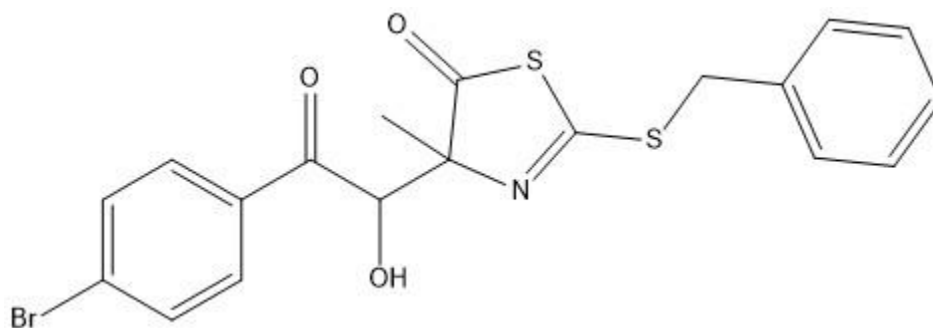
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^1H NMR

For

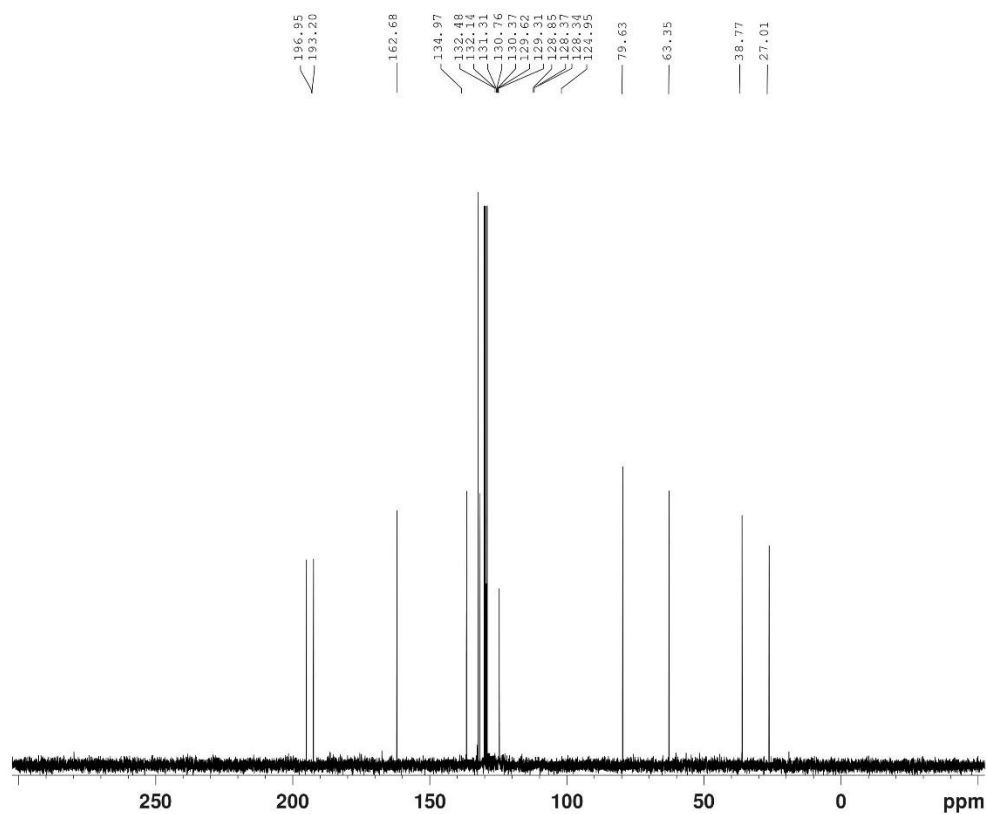
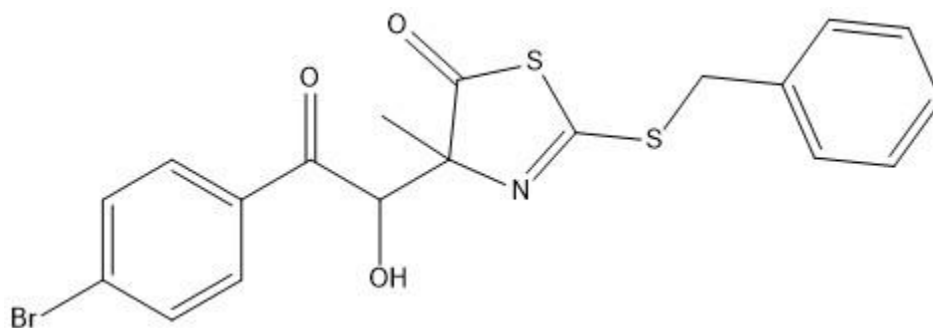
2-(benzylthio)-4-(2-(4-bromophenyl)-1-hydroxy-2-oxoethyl)-4-methylthiazol-5(4H)-one(4Br-Ala):



¹³C NMR

For

2-(benzylthio)-4-(2-(4-bromophenyl)-1-hydroxy-2-oxoethyl)-4-methylthiazol-5(4H)-one(4Br-Ala):



```
NAME          Gilan UN
EXPNO          2510
PROCNO         1
Date_          20171111
Time           11.47
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zgpg30
TD             65536
SOLVENT        CDC13
NS             200
DS             0
SWH            35714.285 Hz
FIDRES         0.544957 Hz
AQ            0.9175540 sec
RG            2050
DW            14.000 usec
DE            6.50 usec
TE            296.3 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0           1

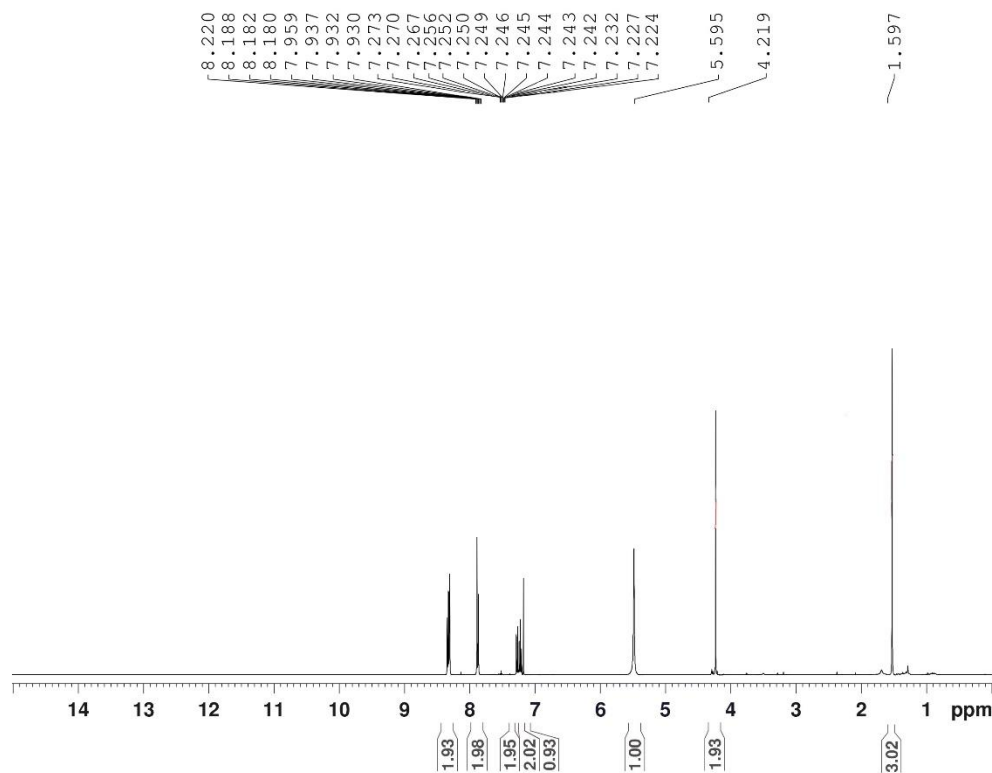
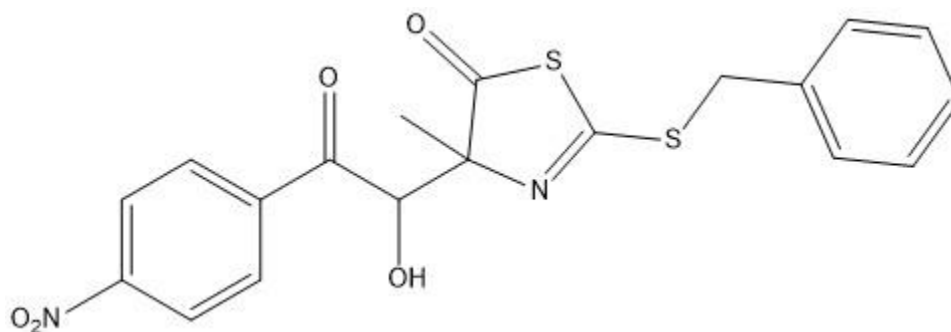
===== CHANNEL f1 =====
NUC1           13C
P1            9.00 usec
PL1           -0.90 dB
PL1W          42.02801895 W
SFO1          100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         90.00 usec
PL2           -2.00 dB
PL12          14.16 dB
PL13          17.90 dB
PL2W          11.86359406 W
PL12W         0.28722104 W
PL13W         0.12139934 W
SFO2          400.2216009 MHz
SI            32768
SF            100.6353990 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB           0
PC            1.40
```

^1H NMR

For

2-(benzylthio)-4-(1-hydroxy-2-(4-nitrophenyl)-2-oxoethyl)-4-methylthiazol-5(4H)-one(4NO₂-Ala):



BRUKER

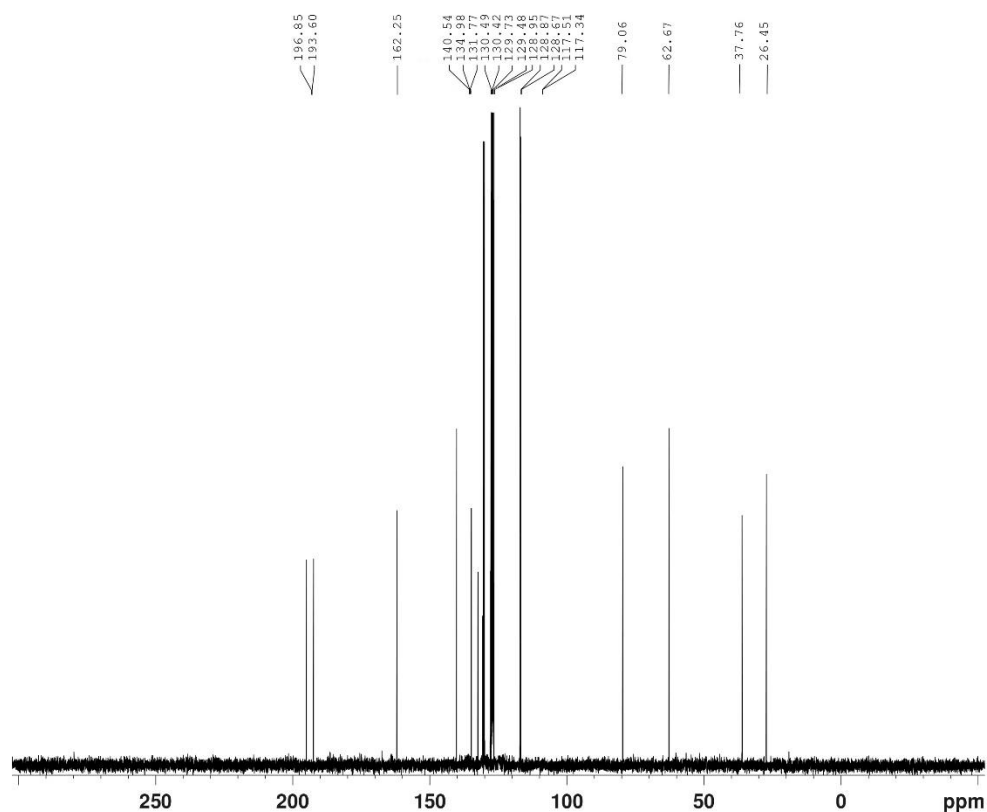
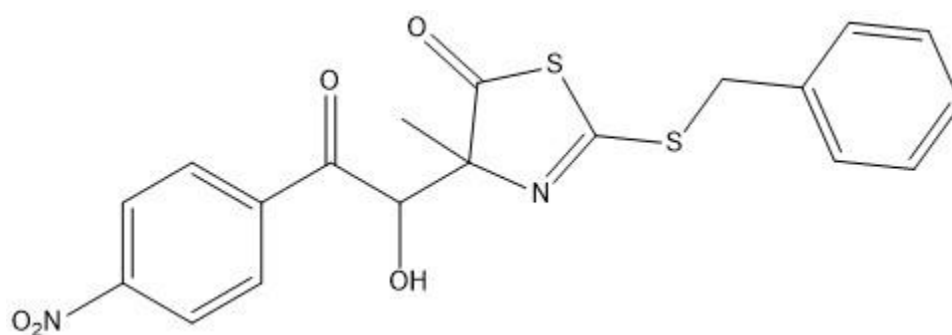
```
NAME      Gilan UN
EXPNO     1309
PROCNO    1
Date_     20171111
Time      13.20
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        65536
SOLVENT   CDC13
NS         20
DS         0
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894966 sec
RG         203
DW         62.400 usec
DE         6.50 usec
TE         295.3 K
D1         4.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.00 usec
PL1        -2.00 dB
PL1W       11.96359406 W
SF01       400.2236020 MHz
SI         32768
SF         400.2200000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

¹³C NMR

For

2-(benzylthio)-4-(1-hydroxy-2-(4-nitrophenyl)-2-oxoethyl)-4-methylthiazol-5(4H)-one(4NO₂-Ala):



```
NAME          Gilan UN
EXPNO          2501
PROCNO         1
Date_          20170909
Time           10.56
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zgpg30
TD             65536
SOLVENT        CDCl3
NS             200
DS             0
SWH            35714.285 Hz
FIDRES         0.544957 Hz
AQ            0.9175540 sec
RG            2050
DW            14.000 usec
DE            6.50 usec
TE            296.3 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0           1

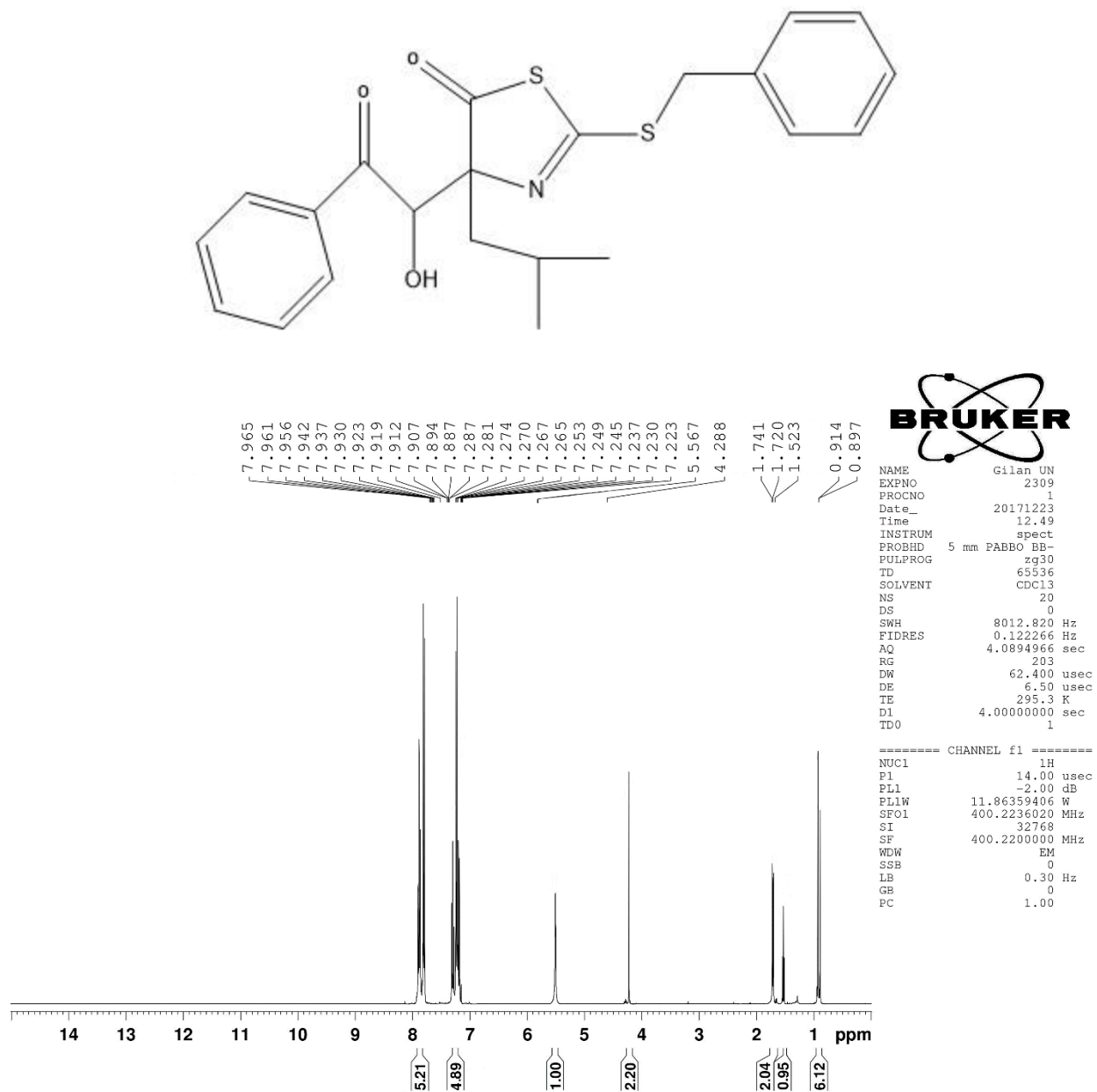
===== CHANNEL f1 =====
NUC1           13C
P1            9.00 usec
PL1           -0.90 dB
PL1W          42.02801895 W
SFO1          100.6479784 MHz

===== CHANNEL F2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         90.00 usec
PL2           -2.00 dB
PL12          14.16 dB
PL13          17.90 dB
PL2W          11.86359406 W
PL12W         0.28722104 W
PL13W         0.12139934 W
SFO2          400.2216009 MHz
SI            32768
SF            100.6353990 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

^1H NMR

For

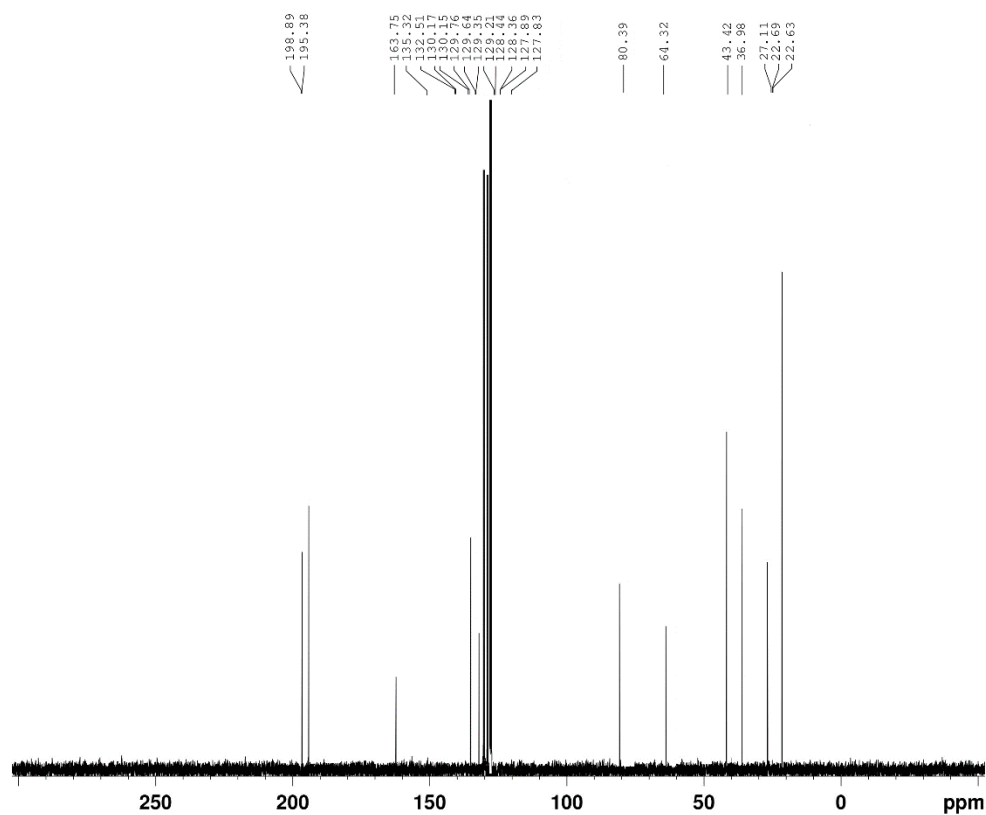
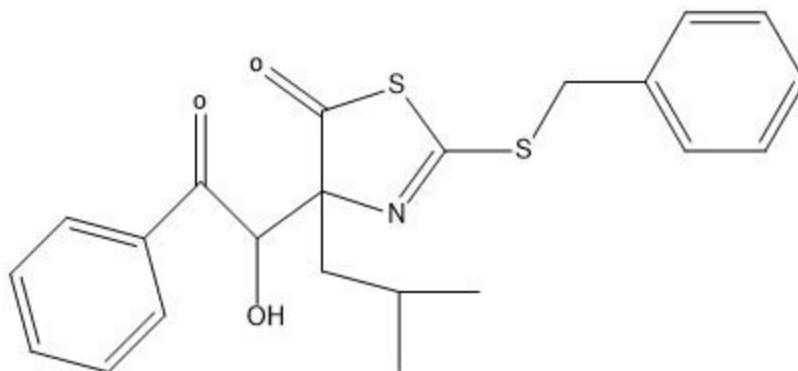
2-(benzylthio)-4-(1-hydroxy-2-oxo-2-phenylethyl)-4-isobutylthiazol-5(4H)-one(4H-Leu):



¹³C NMR

For

2-(benzylthio)-4-(1-hydroxy-2-oxo-2-phenylethyl)-4-isobutylthiazol-5(4H)-one(4H-Leu):



```
NAME      Gilan UN
EXPNO     2119
PROCNO    1
Date_     20171223
Time      17.12
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         731
DS         0
SWH        35714.285 Hz
FIDRES     0.544957 Hz
AQ         0.9175540 sec
RG         2050
DW         14.000 usec
DE         6.50 usec
TE         295.8 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

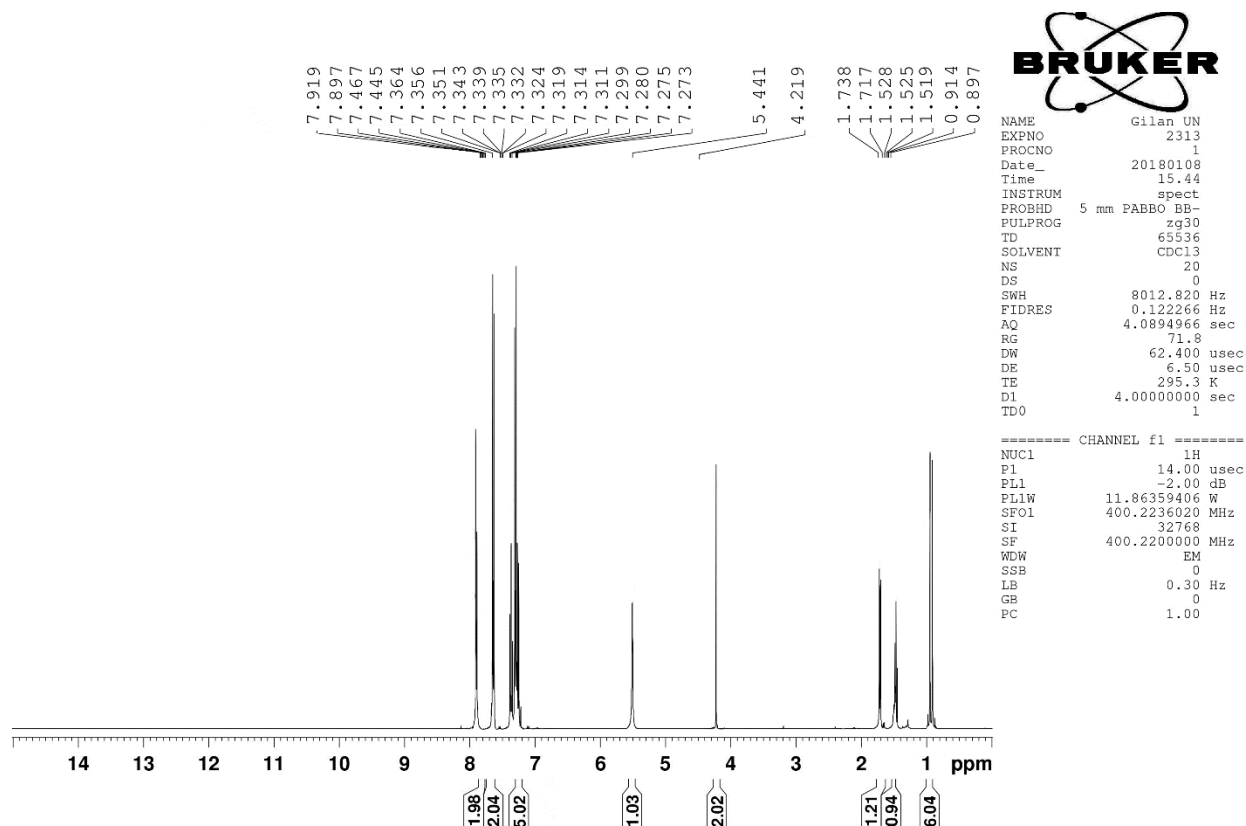
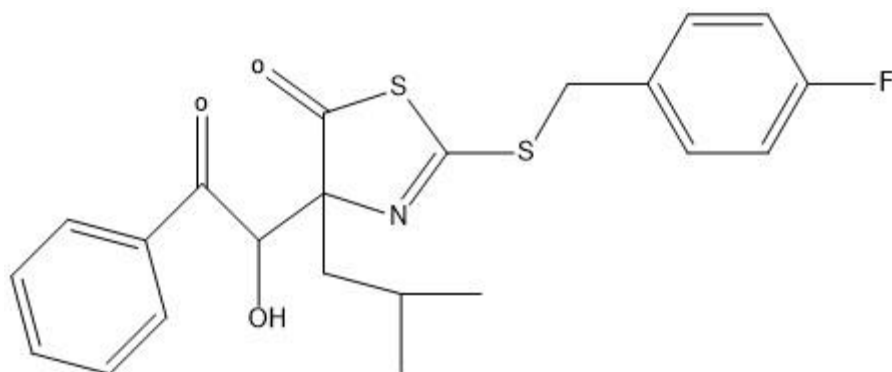
----- CHANNEL f1 -----
NUC1       13C
P1         9.00 usec
PL1        -0.90 dB
PL1W       42.02801895 W
SFO1       100.6479784 MHz

----- CHANNEL f2 -----
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.00 dB
PL12       14.16 dB
PL13       17.90 dB
PL2W       11.86359406 W
PL12W      0.28722104 W
PL13W      0.12139934 W
SFO2       400.2216009 MHz
SI         32768
SF         100.6353990 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

¹H NMR

For

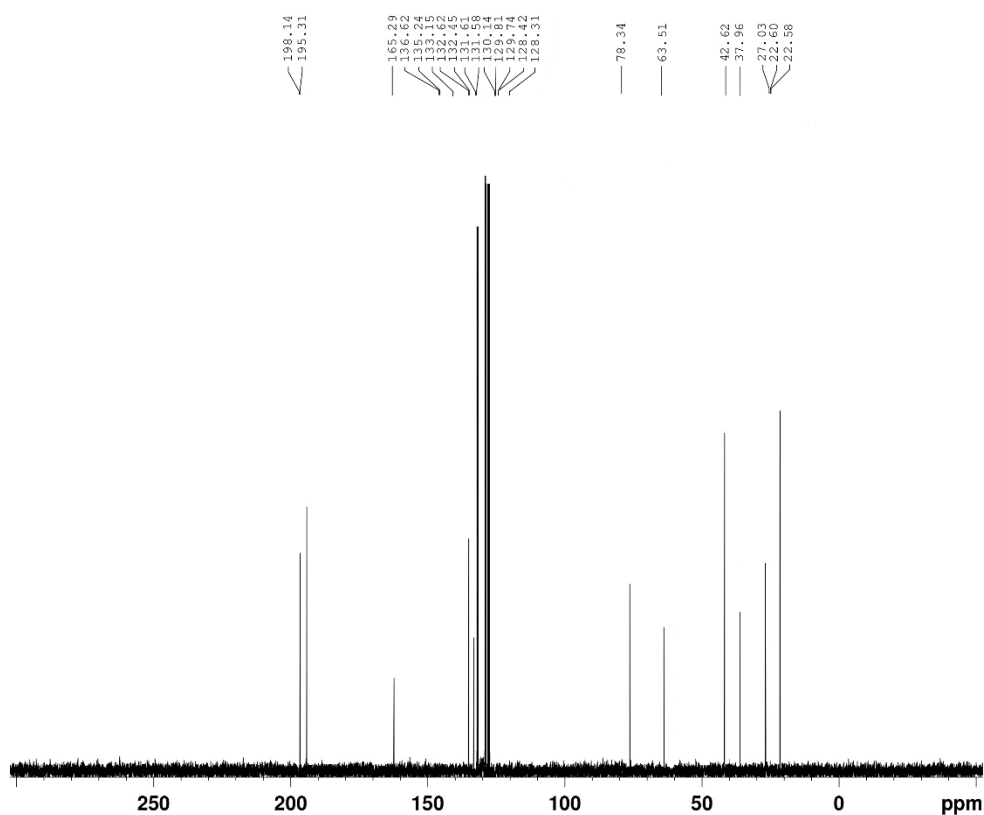
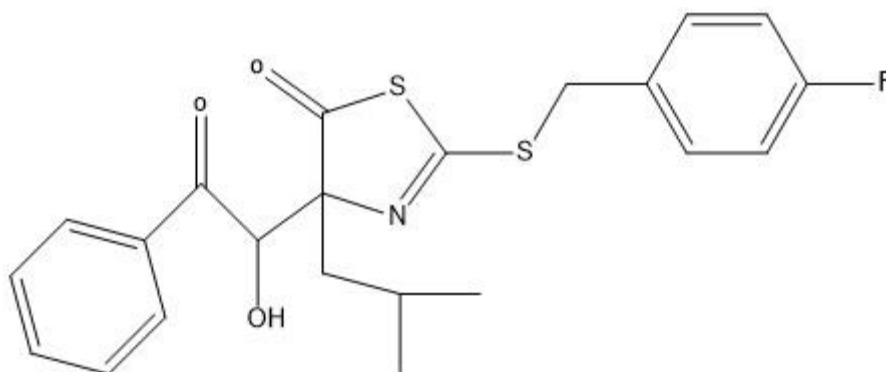
2-(benzylthio)-4-(2-(4-fluorophenyl)-1-hydroxy-2-oxoethyl)-4-isobutylthiazol-5(4H)-one(4F-Leu):



¹³C NMR

For

2-(benzylthio)-4-(2-(4-fluorophenyl)-1-hydroxy-2-oxoethyl)-4-isobutylthiazol-5(4H)-one(4F-Leu):



```
NAME          Gilan UN
EXPNO          1165
PROCNO         1
Date_          20171223
Time           10.53
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zgpg30
TD             65536
SOLVENT        CDCl3
NS             731
DS             0
SWH            35714.285 Hz
FIDRES         0.544957 Hz
AQ            0.9175540 sec
RG            2050
DW            14.000 usec
DE            6.50 usec
TE            295.2 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0           1

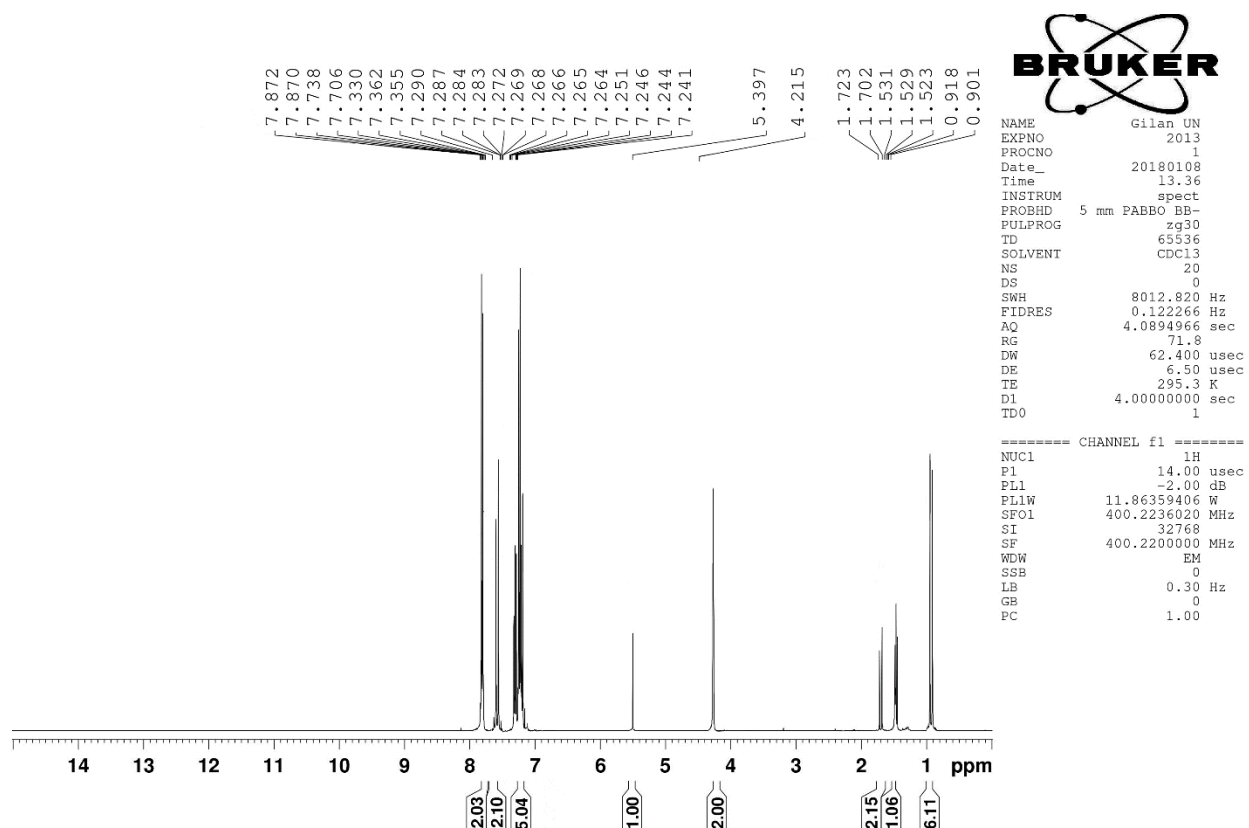
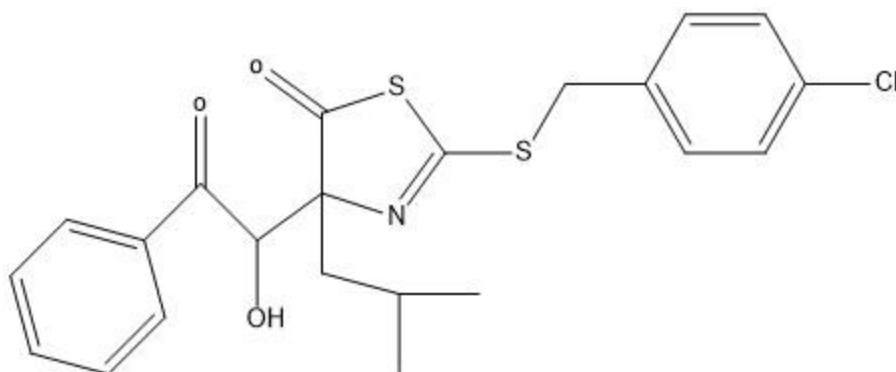
===== CHANNEL f1 =====
NUC1           13C
P1            9.00 usec
PL1           -0.90 dB
PL1W          42.02801895 W
SFO1          100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         90.00 usec
PL2           -2.00 dB
PL12          14.16 dB
PL13          17.90 dB
PL2W          11.86359406 W
PL12W         0.28722104 W
PL13W         0.12139934 W
SFO2          400.2216009 MHz
SI            32768
SF            100.6353990 MHz
WDW            EM
SSB            0
LB            1.00 Hz
GB            0
PC            1.40
```

¹H NMR

For

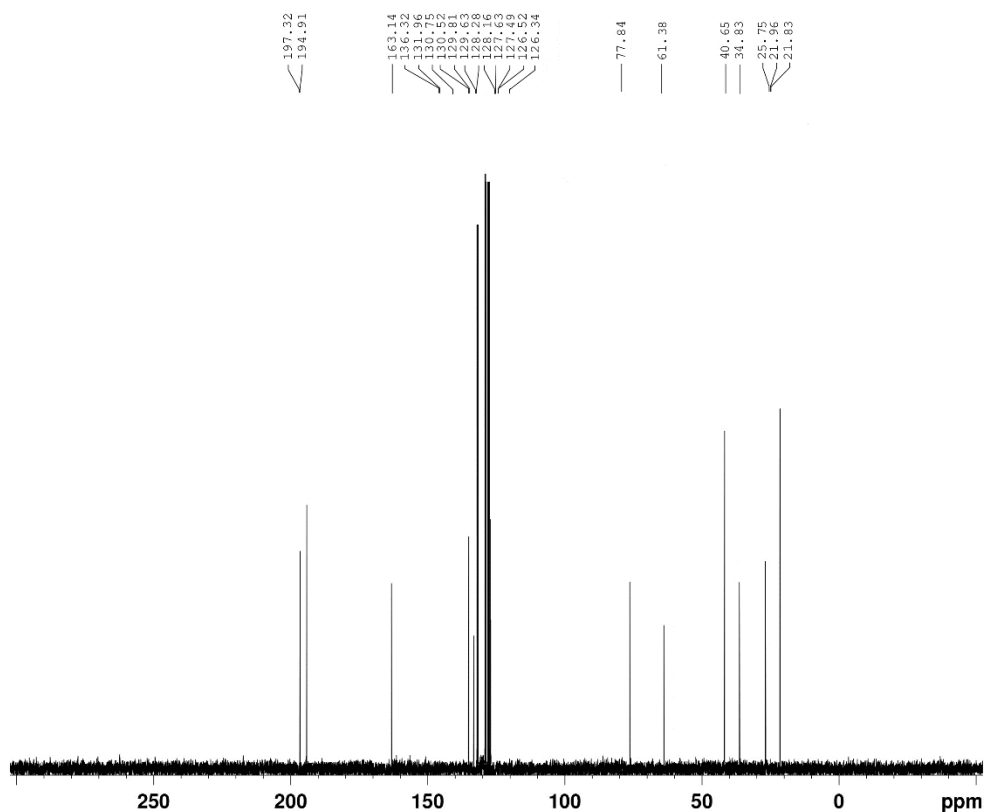
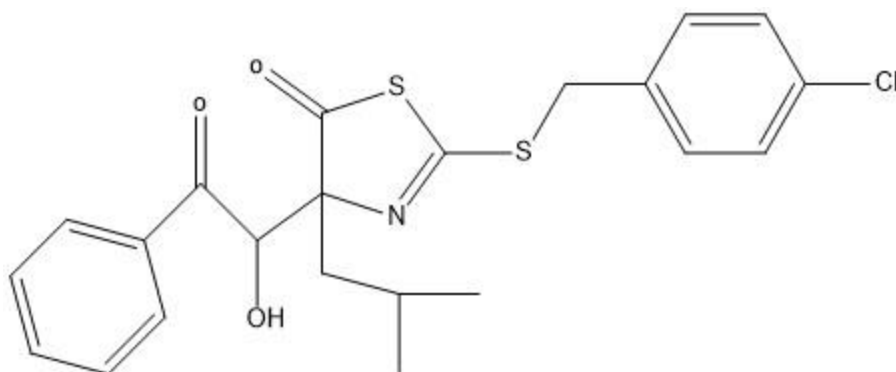
2-(benzylthio)-4-(2-(4-chlorophenyl)-1-hydroxy-2-oxoethyl)-4-isobutylthiazol-5(4H)-one(4CI-Leu):



¹³C NMR

For

2-(benzylthio)-4-(2-(4-chlorophenyl)-1-hydroxy-2-oxoethyl)-4-isobutylthiazol-5(4H)-one(4Cl-Leu):



```
NAME      Gilan UN
EXPNO     2295
PROCNO    1
Date_     20171223
Time      14.28
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         731
DS         0
SWH        35714.285 Hz
FIDRES     0.544957 Hz
AQ         0.9175540 sec
RG         2050
DW         14.000 usec
DE         6.50 usec
TE         295.8 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1
```

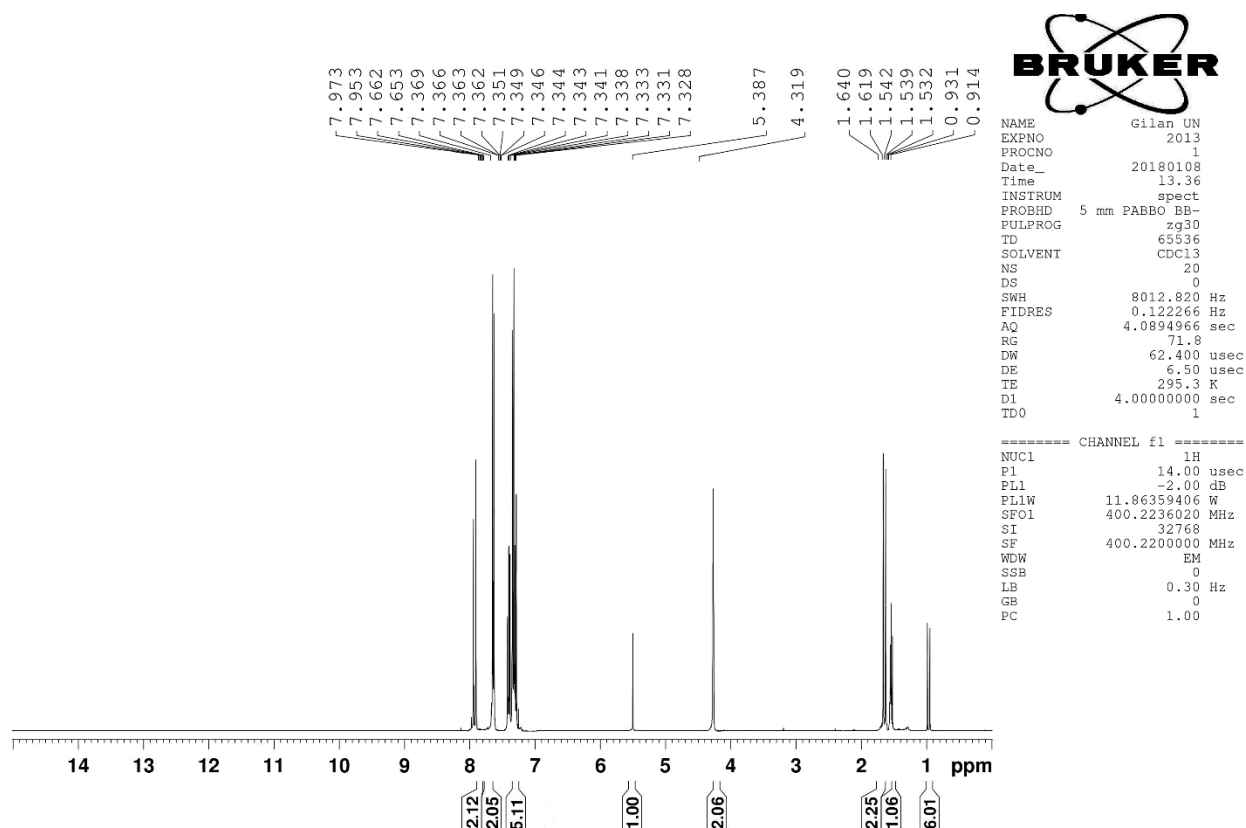
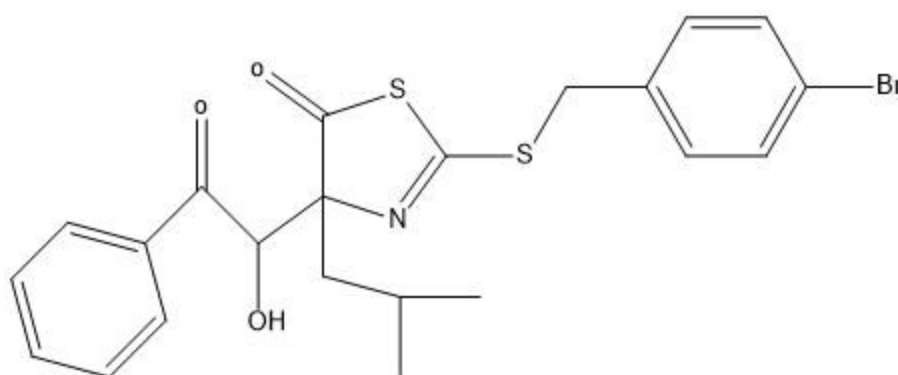
```
----- CHANNEL f1 -----
NUC1       13C
P1         9.00 usec
PL1        -0.90 dB
PL1W       42.02801895 W
SFO1       100.6479784 MHz
```

```
----- CHANNEL f2 -----
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.00 dB
PL12       14.16 dB
PL13       17.90 dB
PL2W       11.86359406 W
PL12W      0.28722104 W
PL13W      0.12139934 W
SFO2       400.2216009 MHz
SI         32768
SF         100.6353990 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

¹H NMR

For

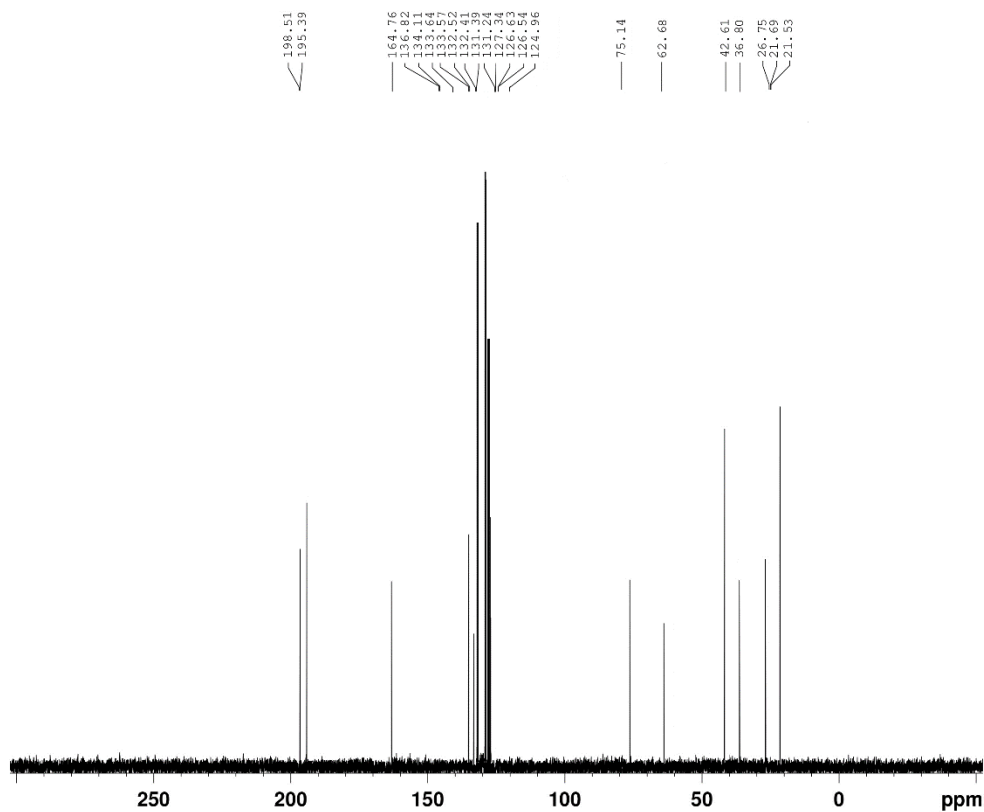
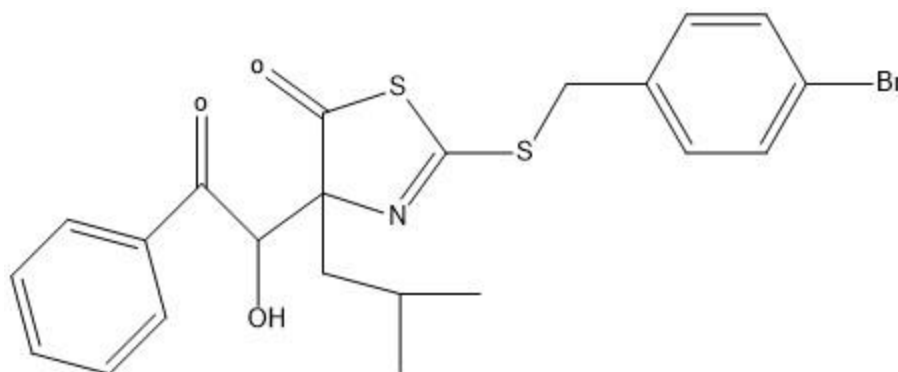
2-(benzylthio)-4-(2-(4-bromophenyl)-1-hydroxy-2-oxoethyl)-4-isobutylthiazol-5(4H)-one(4Br-Leu):



¹³C NMR

For

2-(benzylthio)-4-(2-(4-bromophenyl)-1-hydroxy-2-oxoethyl)-4-isobutylthiazol-5(4H)-one(**4Br-Leu**):



```
NAME      Gilan UN
EXPNO     1895
PROCNO    1
Date_     20171223
Time      15.31
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         731
DS         0
SWH        35714.285 Hz
FIDRES     0.544957 Hz
AQ         0.9175540 sec
RG         2050
DW         14.000 usec
DE         6.50 usec
TE         295.8 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1
```

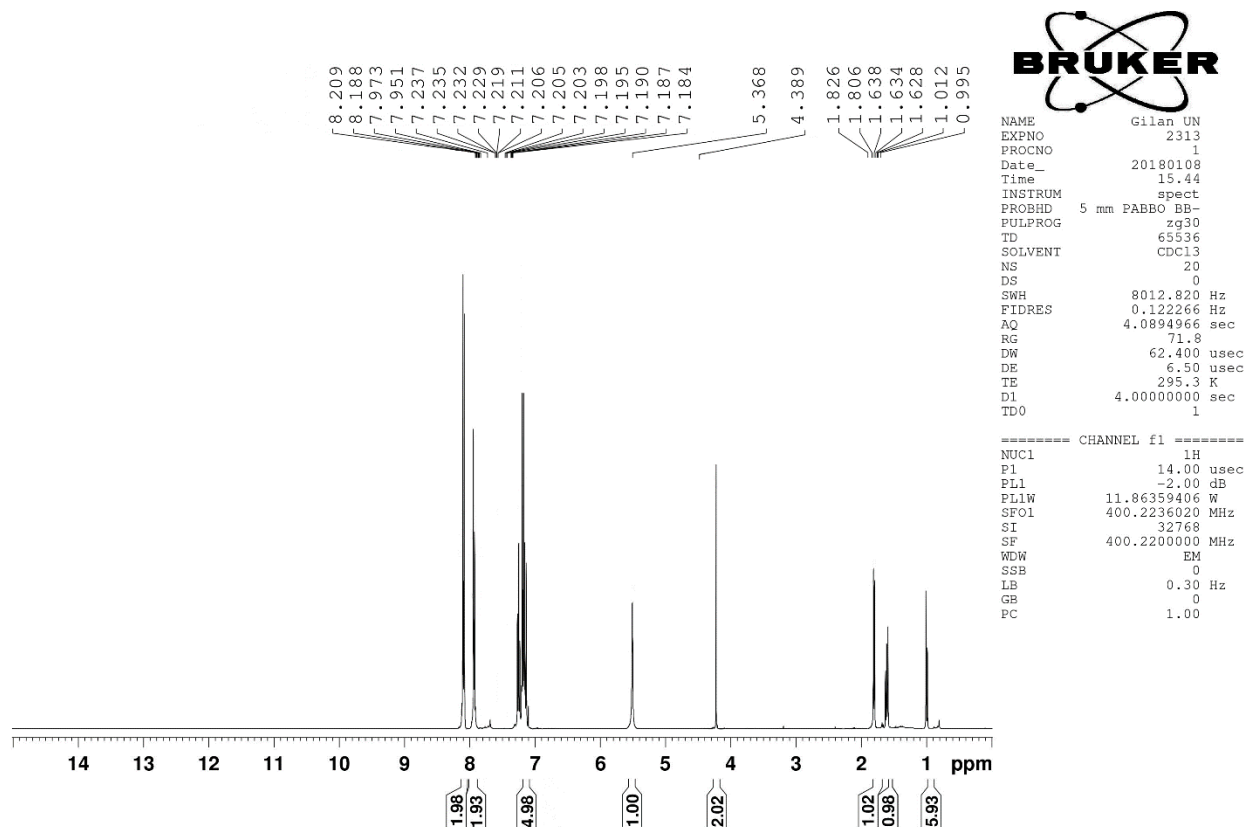
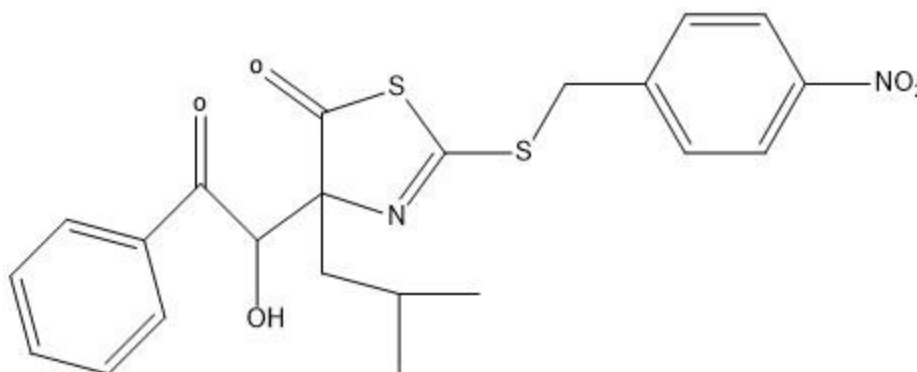
```
----- CHANNEL f1 -----
NUC1       13C
P1         9.00 usec
PL1        -0.90 dB
PL1W       42.02801895 W
SFO1       100.6479784 MHz
```

```
----- CHANNEL f2 -----
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.00 dB
PL12       14.16 dB
PL13       17.90 dB
PL2W       11.86359406 W
PL12W      0.28722104 W
PL13W      0.12139934 W
SFO2       400.2216009 MHz
SI         32768
SF         100.6353990 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

¹H NMR

For

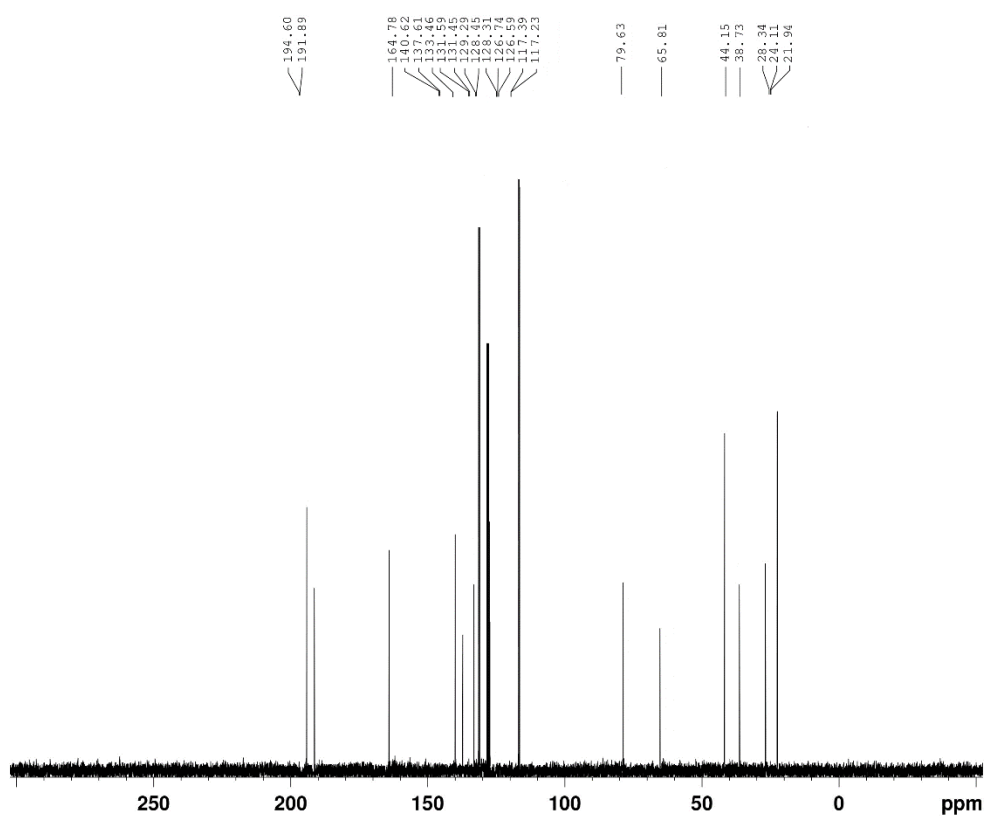
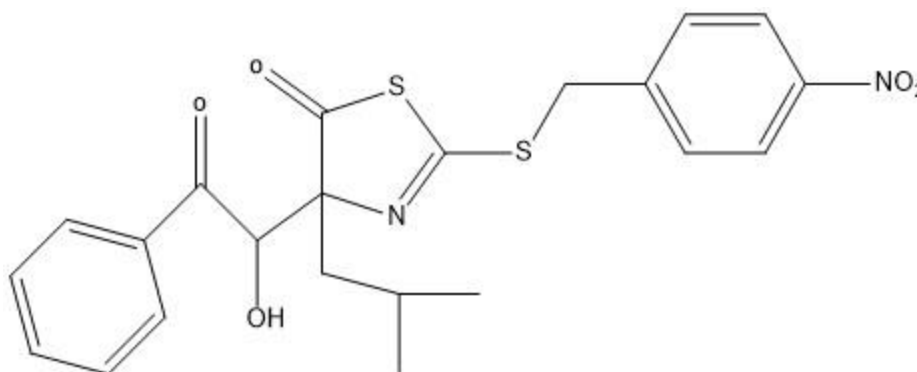
2-(benzylthio)-4-(1-hydroxy-2-(4-nitrophenyl)-2-oxoethyl)-4-isobutylthiazol-5(4H)-one(4NO₂-
Leu):



¹³C NMR

For

2-(benzylthio)-4-(1-hydroxy-2-(4-nitrophenyl)-2-oxoethyl)-4-isobutylthiazol-5(4H)-one(4NO₂-
Leu):



NAME Gilan UN
EXPNO 1349
PROCNO 1
Date_ 20171223
Time 12.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 731
DS 0
SWH 35714.285 Hz
FIDRES 0.544957 Hz
AQ 0.9175540 sec
RG 2050
DW 14.000 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

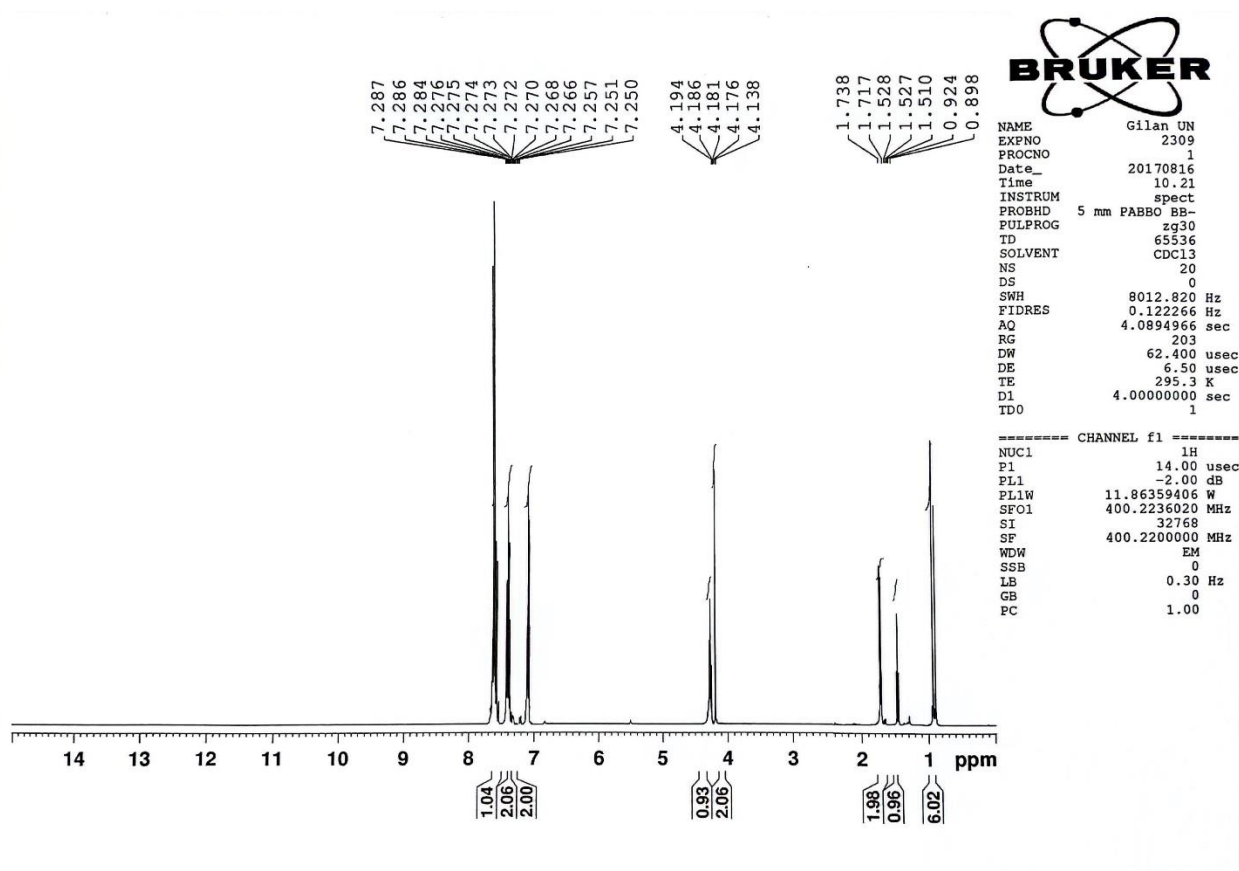
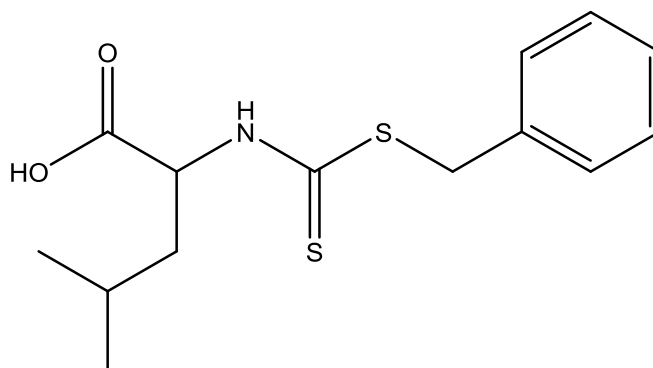
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^1H NMR

For

((benzylthio)carbonothioyl)leucine



¹³C NMR

For

((benzylthio)carbonothioyl)leucine

