

## **Supplementary Material**

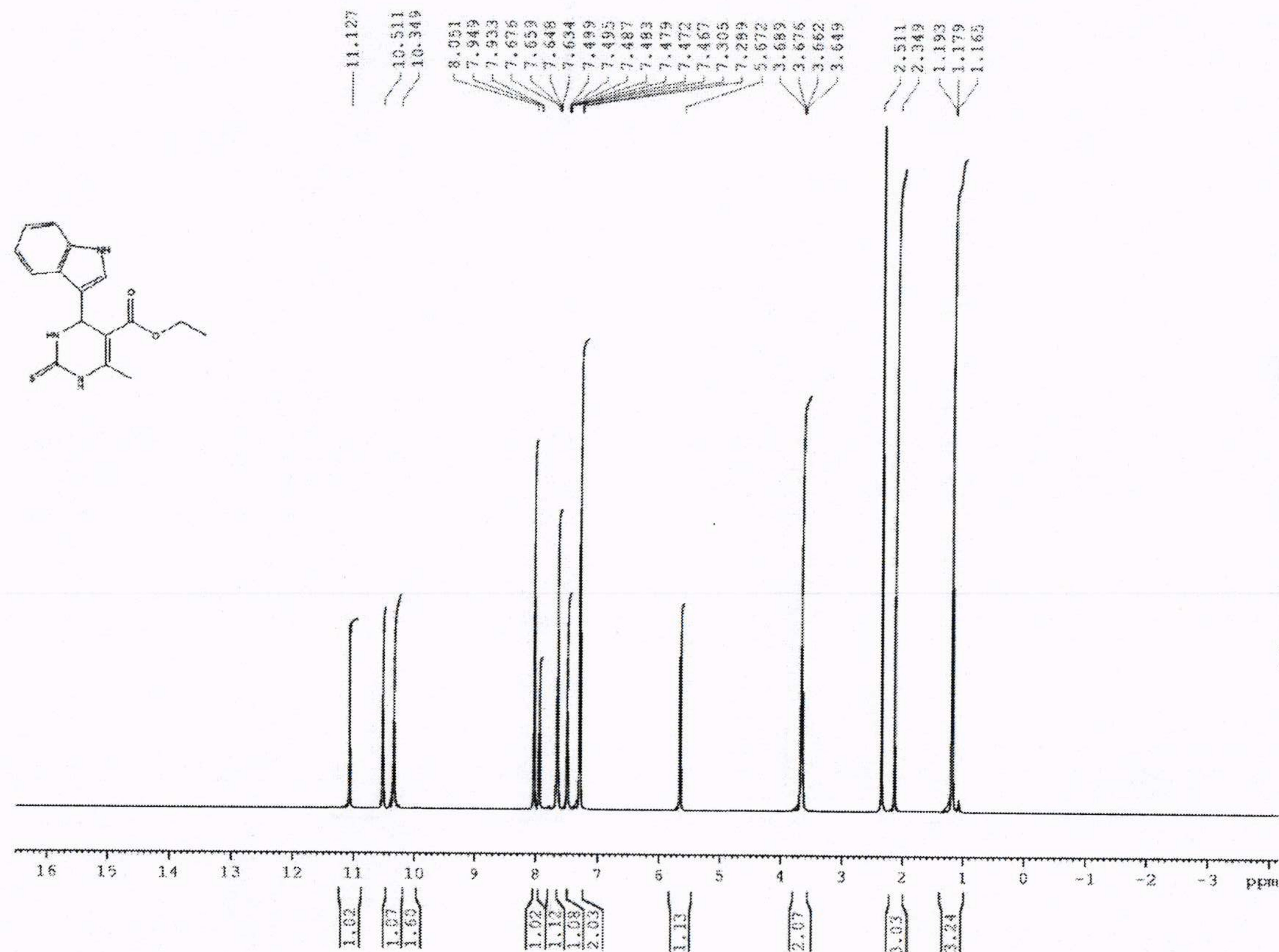
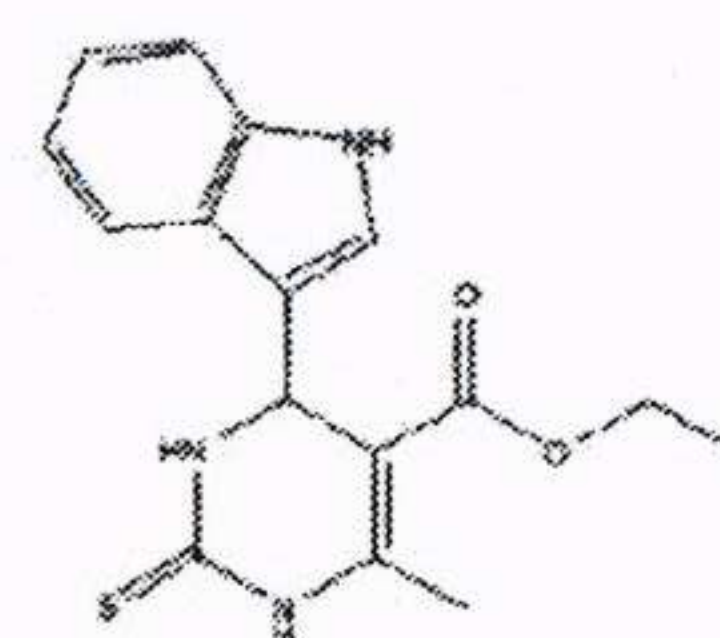
### **Table of Contents**

**$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra copies**



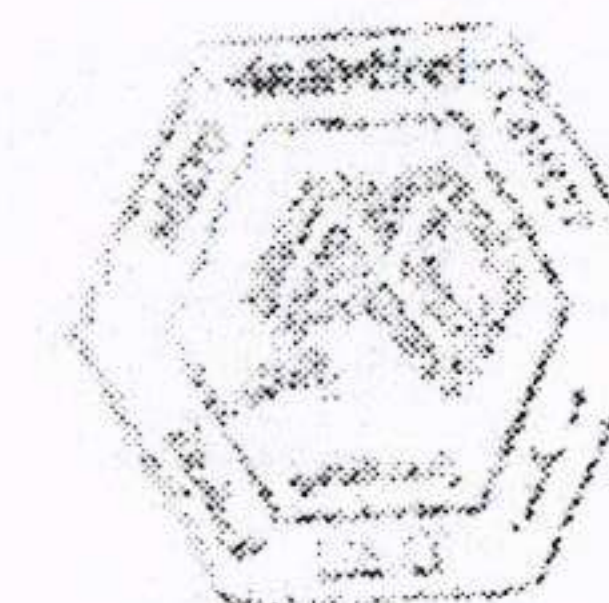
Ethyl 4-(1H-indol-3-yl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate **4a**

DN DMSO D:\ abar



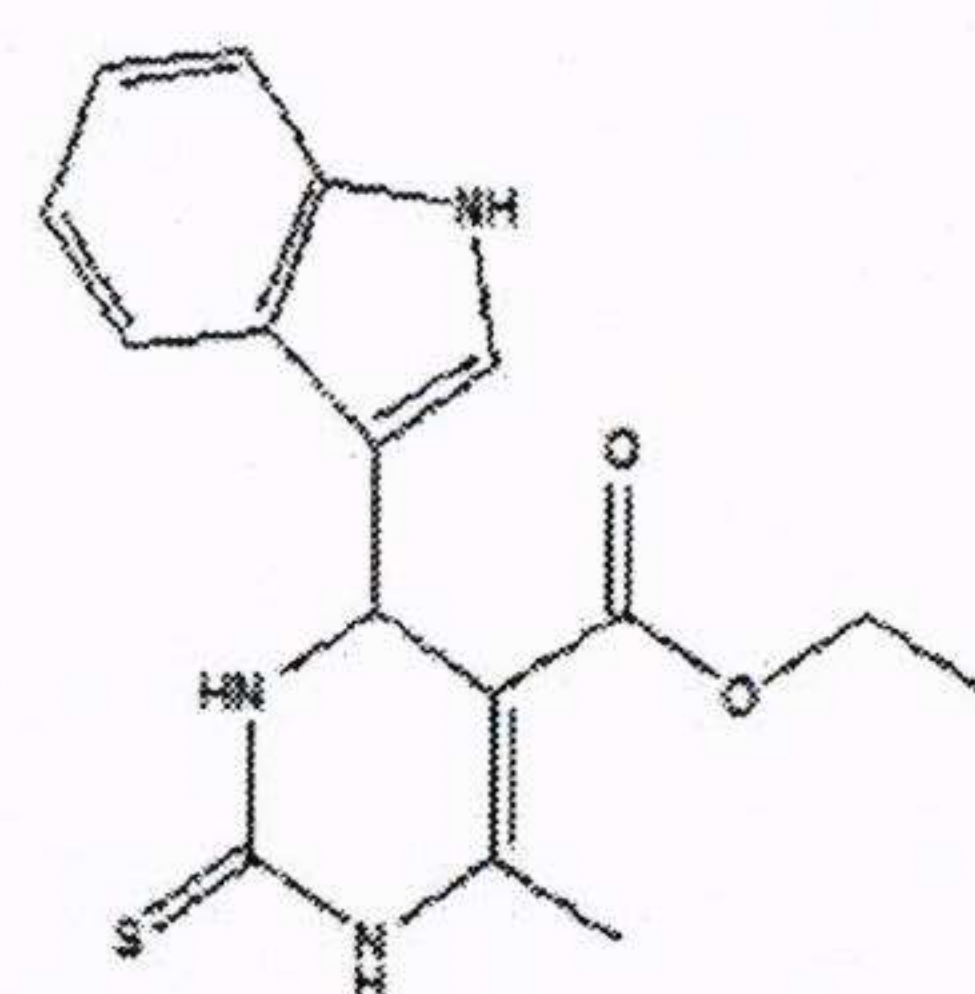
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PROCNO 1  
Date\_ 20210624  
Time 12.45  
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PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1720407 sec  
RG 35.9  
DW 48.400 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.70 usec  
PL1 -1.10 dB  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

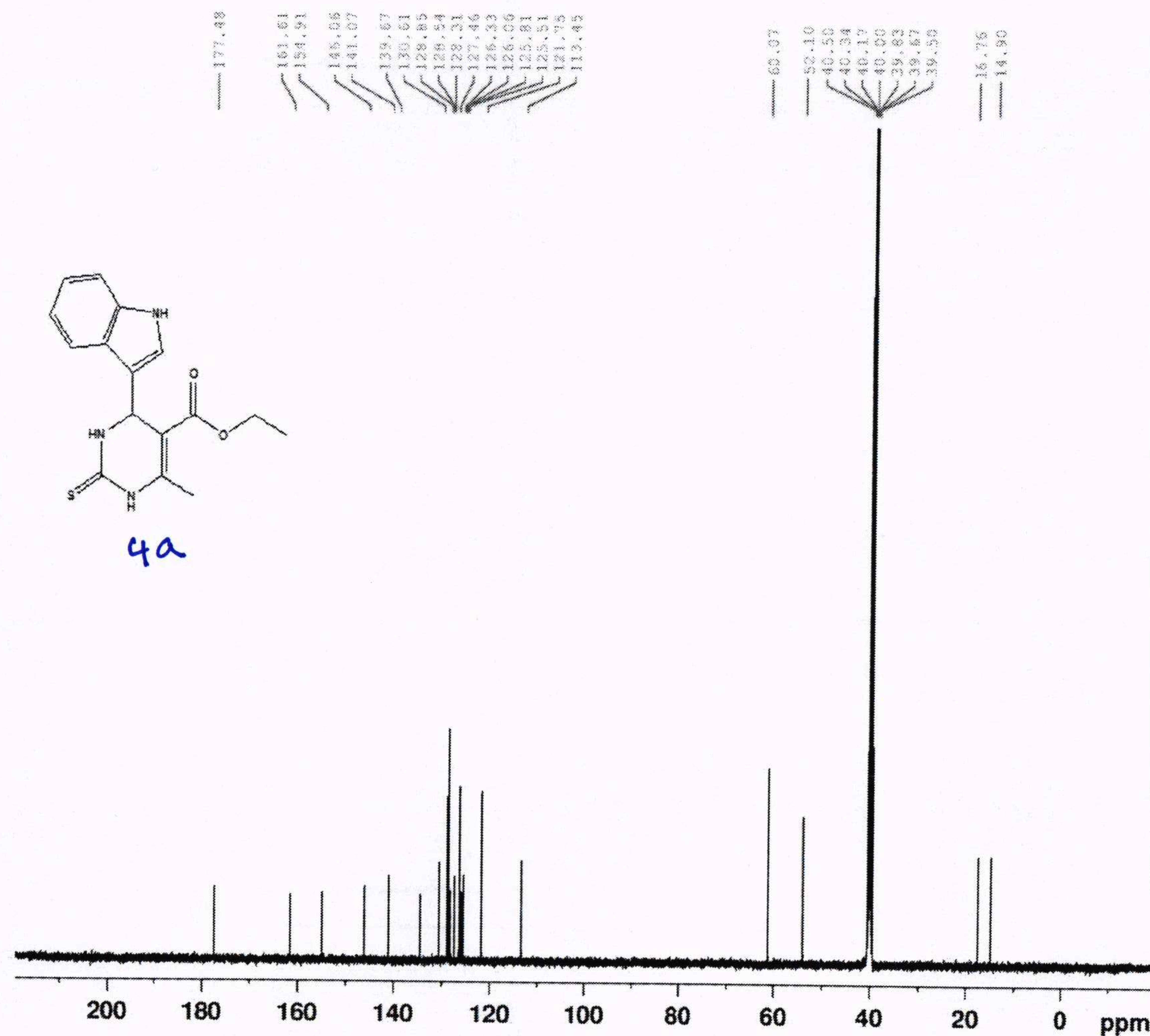




C13CPD32 DMSO D:\ abari 46



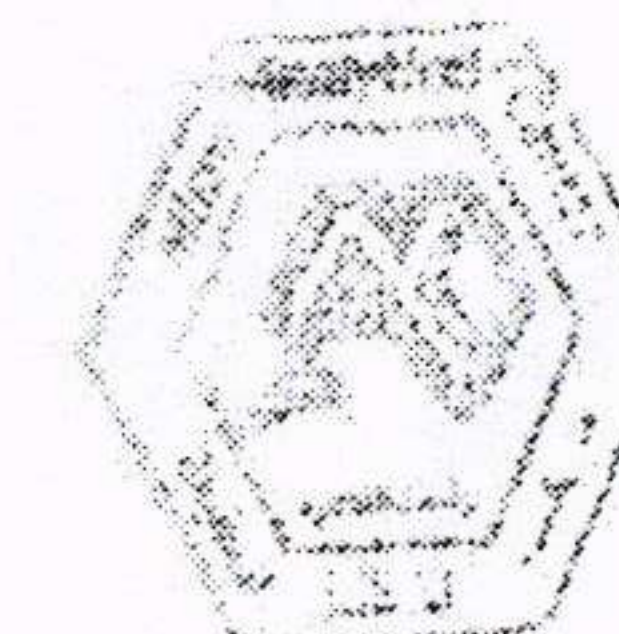
4a



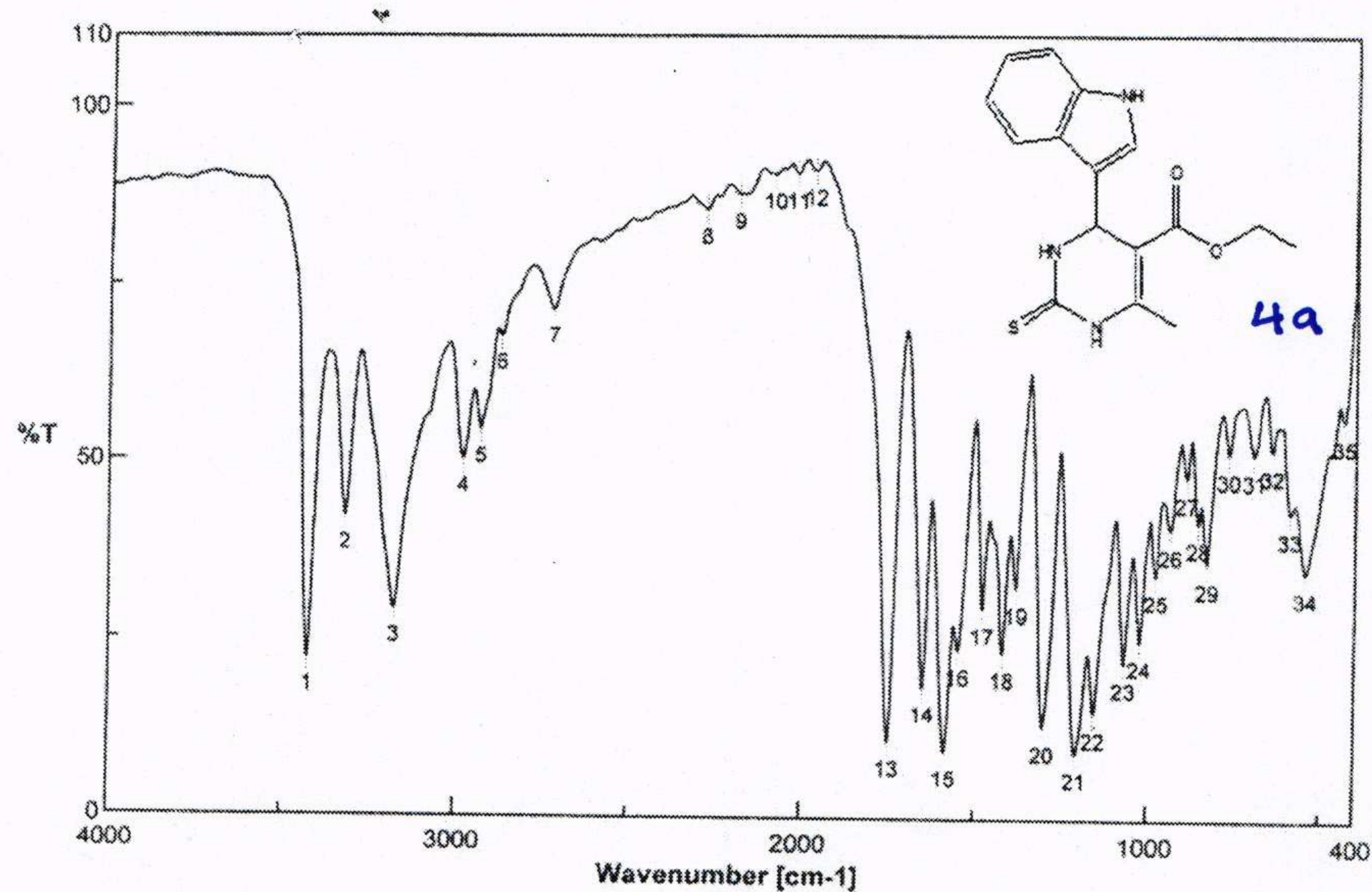
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TD 65536  
SOLVENT DMSO  
NS 2000  
DS 2  
SWH 30030.029 Hz  
FIDRES 0.458222 Hz  
AQ 1.0912410 sec  
RG 14596.5  
DW 16.650 usec  
DE 6.50 usec  
TE 299.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 20.00 usec  
PL1 -6.00 dB  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.10 dB  
PL12 13.44 dB  
PL13 16.40 dB  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7577890 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

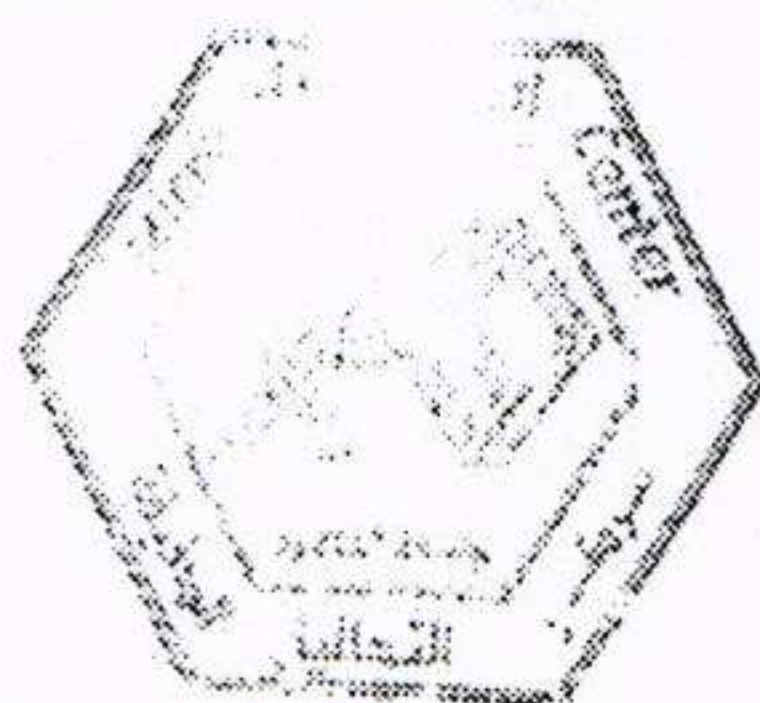






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 Zero Filling ON  
 Apodization Cosine  
 Gain Auto (4)  
 Scanning Speed Auto (2 mm/sec)  
 Date/Time 15/06/21 8:44  
 Update 15/06/21 8:45  
 Operator  
 File Name Memory#27  
 Sample Name 1  
 Comment

No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3425.92	22.2424	2	3319.86	42.1963	3	3178.11	29.2658
4	2980.45	50.2125	5	2930.31	54.382	6	2872.45	67.6564
7	2723	71.4615	8	2285.23	85.5904	9	2188.81	87.8301
10	2090.46	90.6215	11	2023.93	90.6816	12	1971.86	91.0892
13	1749.12	10.9233	14	1650.77	18.535	15	1586.16	9.60047
16	1549.52	23.6982	17	1480.1	29.5846	18	1422.24	23.3596
19	1383.68	32.5285	20	1302.68	13.0578	21	1207.22	9.40387
22	1155.15	14.9925	23	1070.3	21.991	24	1024.98	25.0683
25	978.697	34.4013	26	937.235	40.6767	27	891.916	47.9657
28	858.168	41.6919	29	831.169	35.9772	30	771.387	51.2849
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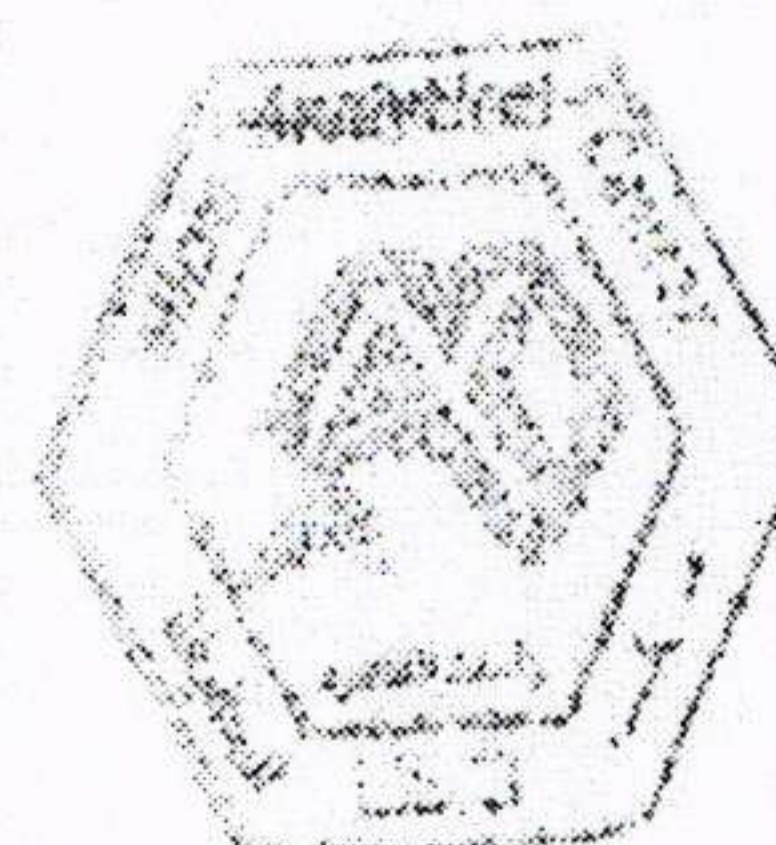


**Cairo University  
Micro Analytical Center**

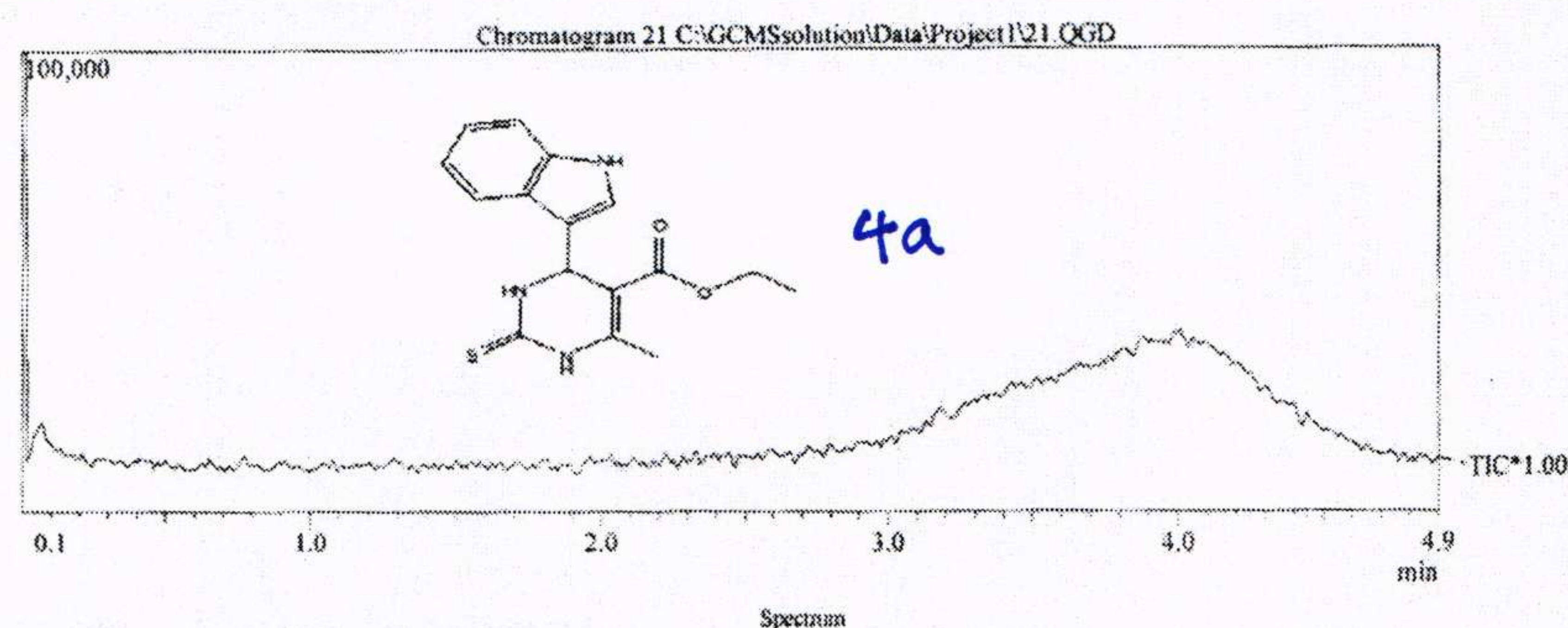
**DI Analysis  
Shimadzu Qp-2010 Plus**

Sample Information  
Analyzed by : Mai Younis  
Analyzed : 22/06/2021 02:44:23  
Sample Name : 2  
Sample ID :  
Customer Name : Dr. Moh F  
Data File : C:\GCMSolution\Data\Project1\21.QGD  
Org Data File : C:\GCMSolution\Data\Project1\21.QGD  
Method File : C:\GCMSolution\Data\Project1\Mai.qgm  
Org Method File : C:\GCMSolution\Data\Project1\Mai.qgm  
Report File :  
Tuning File : C:\GCMSolution\System1\Tune1\_default1.qgt  
SendIfModified by : Mai Younis  
Modified : 22/06/2021 02:49:22

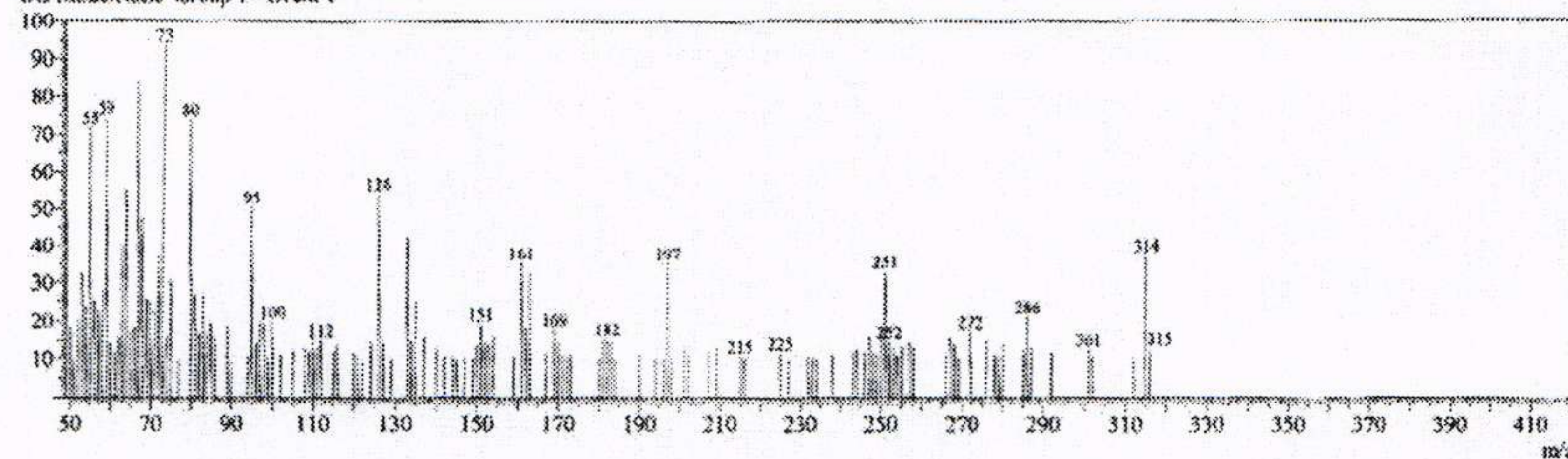
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End Time : 10.00min  
ACQ Mode : Scan  
Event Time : 0.50sec  
Scan Speed : 1000  
Start m/z : 50.00  
End m/z : 500.00  
  
Electron Voltage : 70 eV  
Ionization Mode : EI



C:\GCMSolution\Data\Project1\21.QGD



Line#:1 R.Time:3.1(Scan#:370)  
MassPeaks: 315  
RawMode:Single 3.1(370) BasePeak: 73(537)  
BG Mode:None Group 1 - Event 1



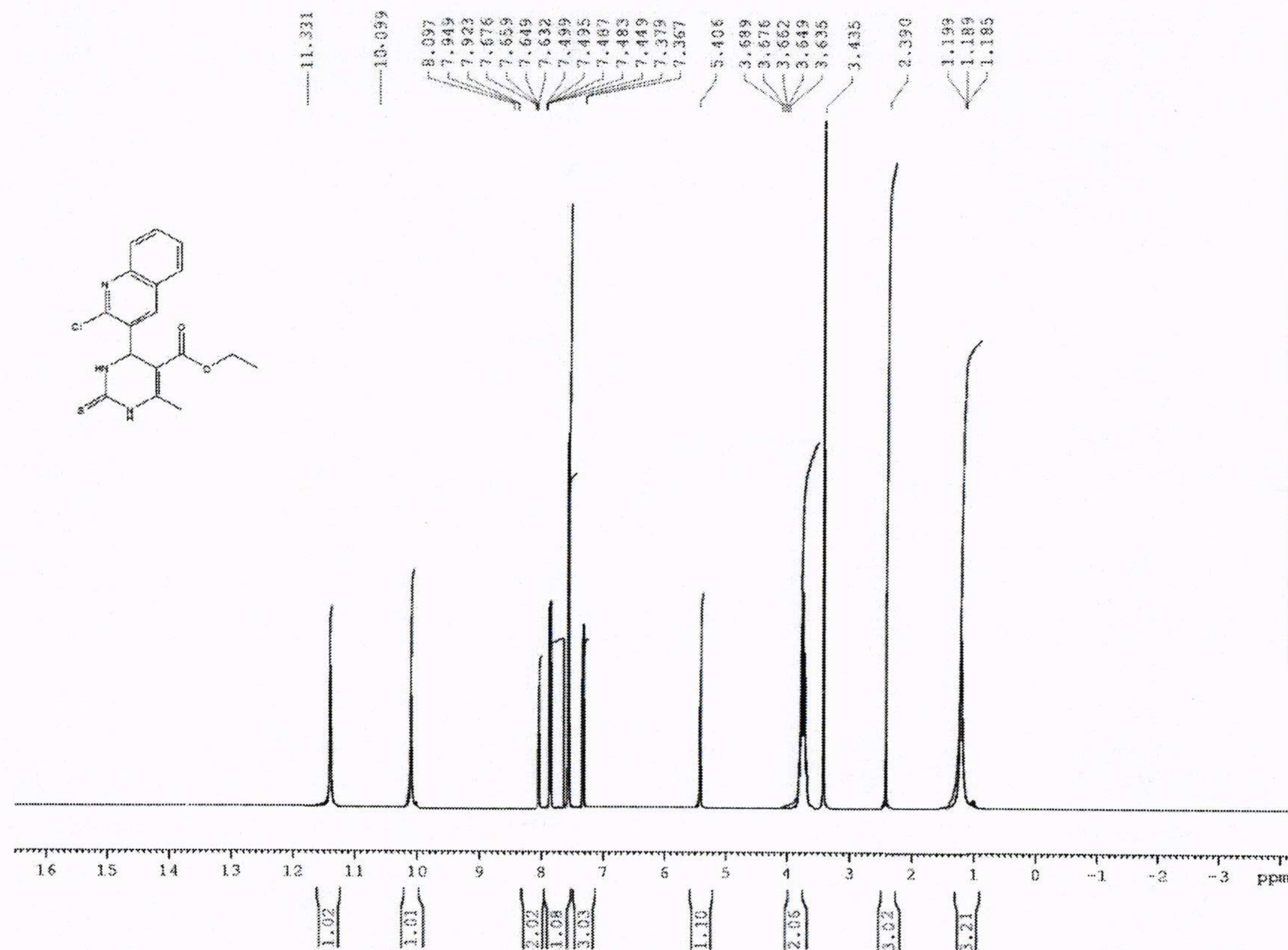
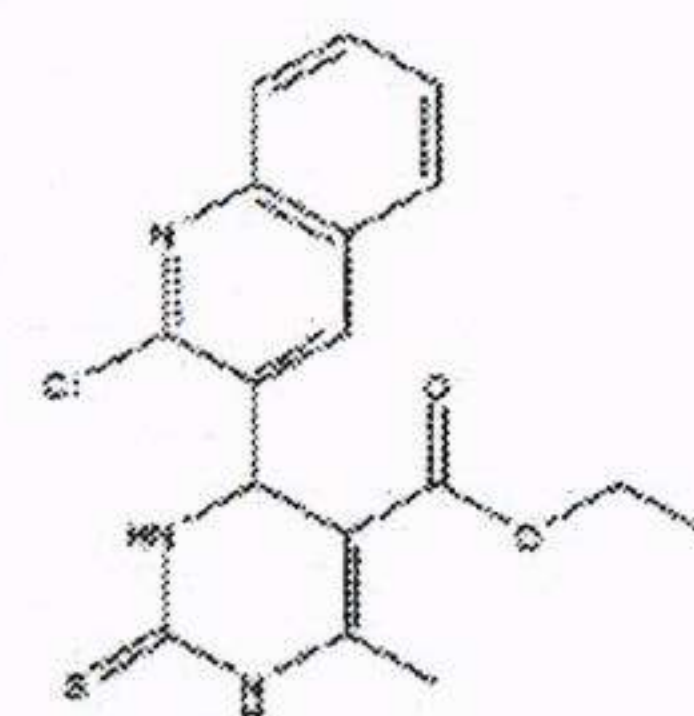
Mass Table  
Line#:1 R.Time:3.1(Scan#:370)  
MassPeaks: 315  
RawMode:Single 3.1(370) BasePeak:73(537)  
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	97	18.06	4	53.00	177	32.96	7	56.00	135	25.14
2	51.00	52	9.68	5	54.00	127	23.65	8	57.00	122	22.72
3	52.00	110	20.48	6	55.00	386	71.88	9	58.00	154	28.68



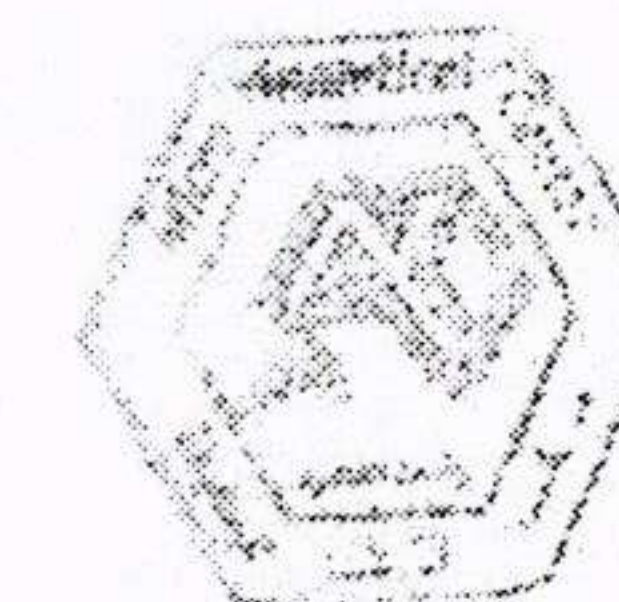
Ethyl 4-(2-chloroquinolin-3-yl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate 4b

DN DMSO D:\ abar



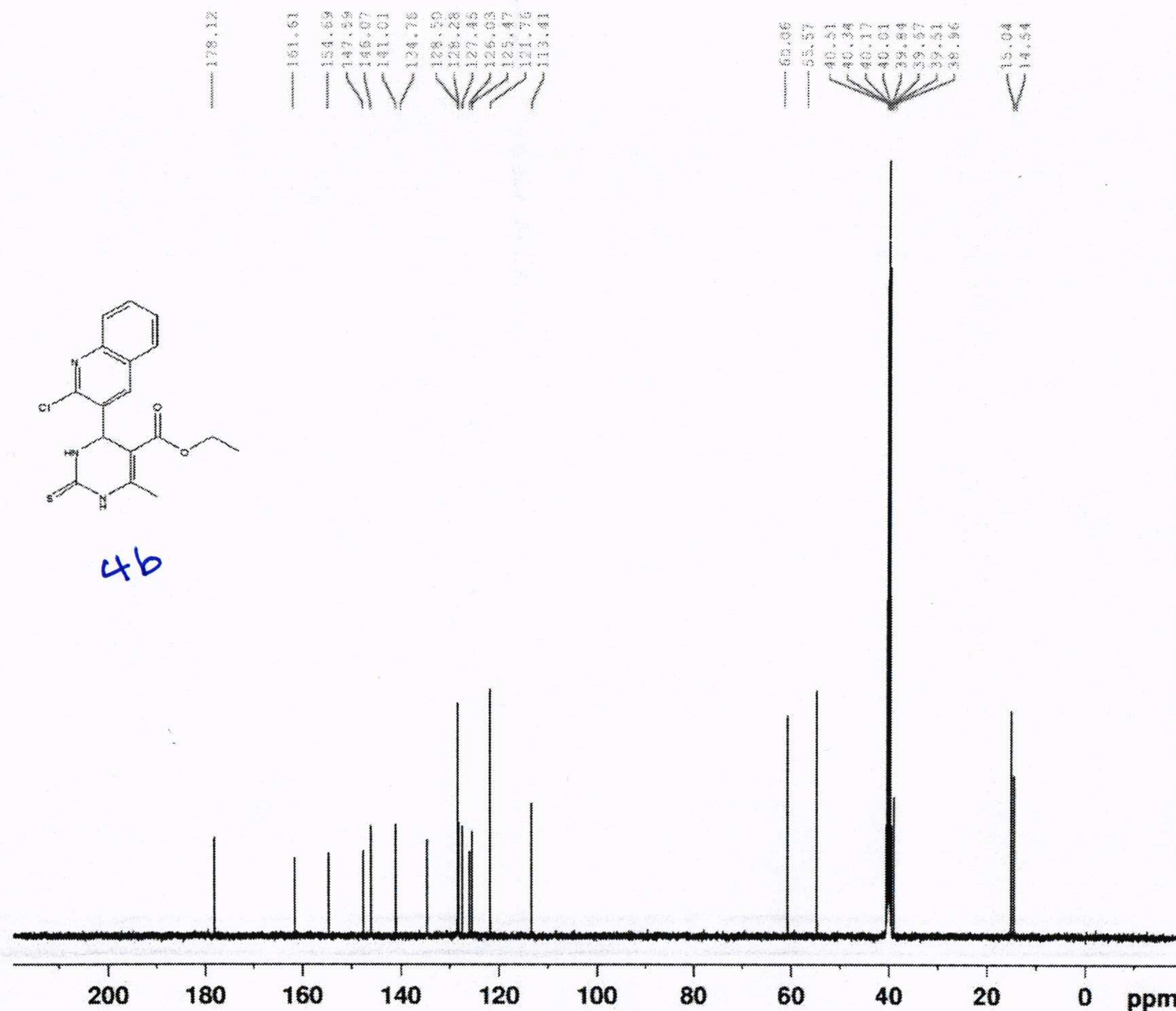
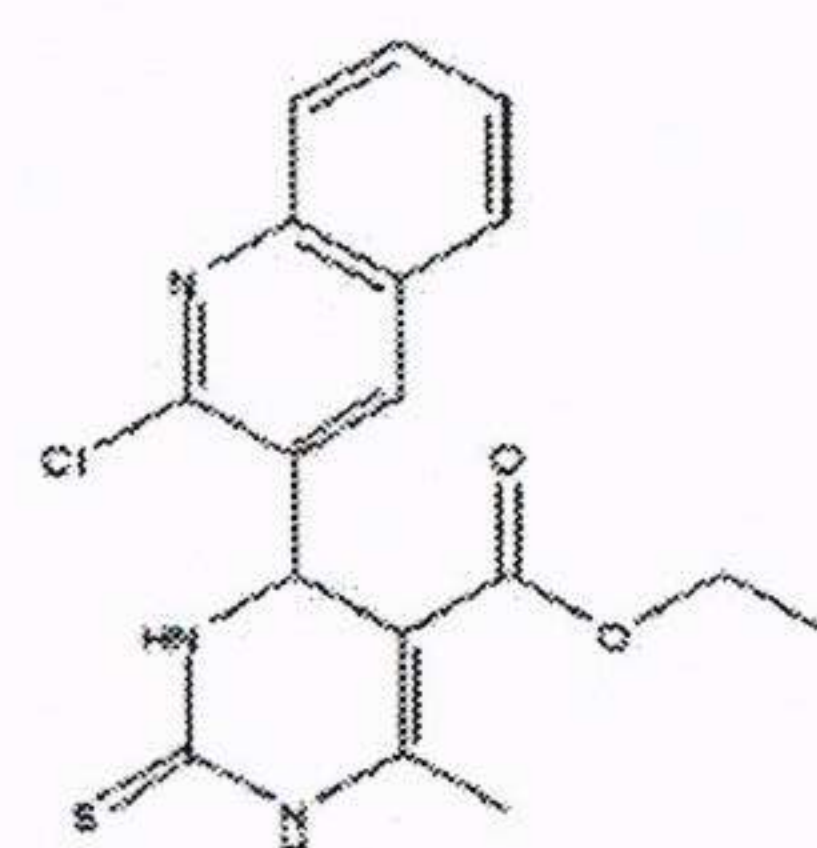
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PROCNO 1  
Date\_ 20210624  
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PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1720407 sec  
RG 90.5  
DW 48.400 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.70 usec  
PL1 -1.10 dB  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





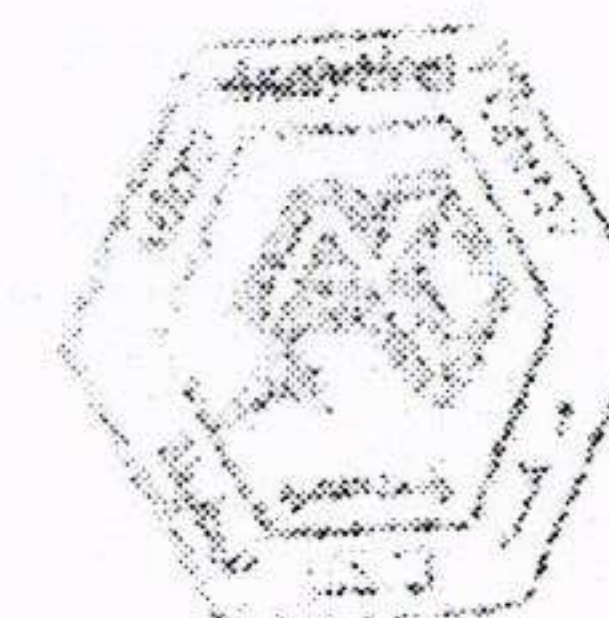
C13CPD32 DMSO D:\ abari 45



NAME drshahat-1  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20210624  
 Time 13.45  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1104  
 DS 2  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912410 sec  
 RG 2048  
 DW 16.650 usec  
 DE 6.50 usec  
 TE 299.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 20.00 usec  
 PL1 -6.00 dB  
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.10 dB  
 PL12 13.44 dB  
 PL13 16.40 dB  
 SFO2 500.1320005 MHz  
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 SF 125.7577890 MHz  
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 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

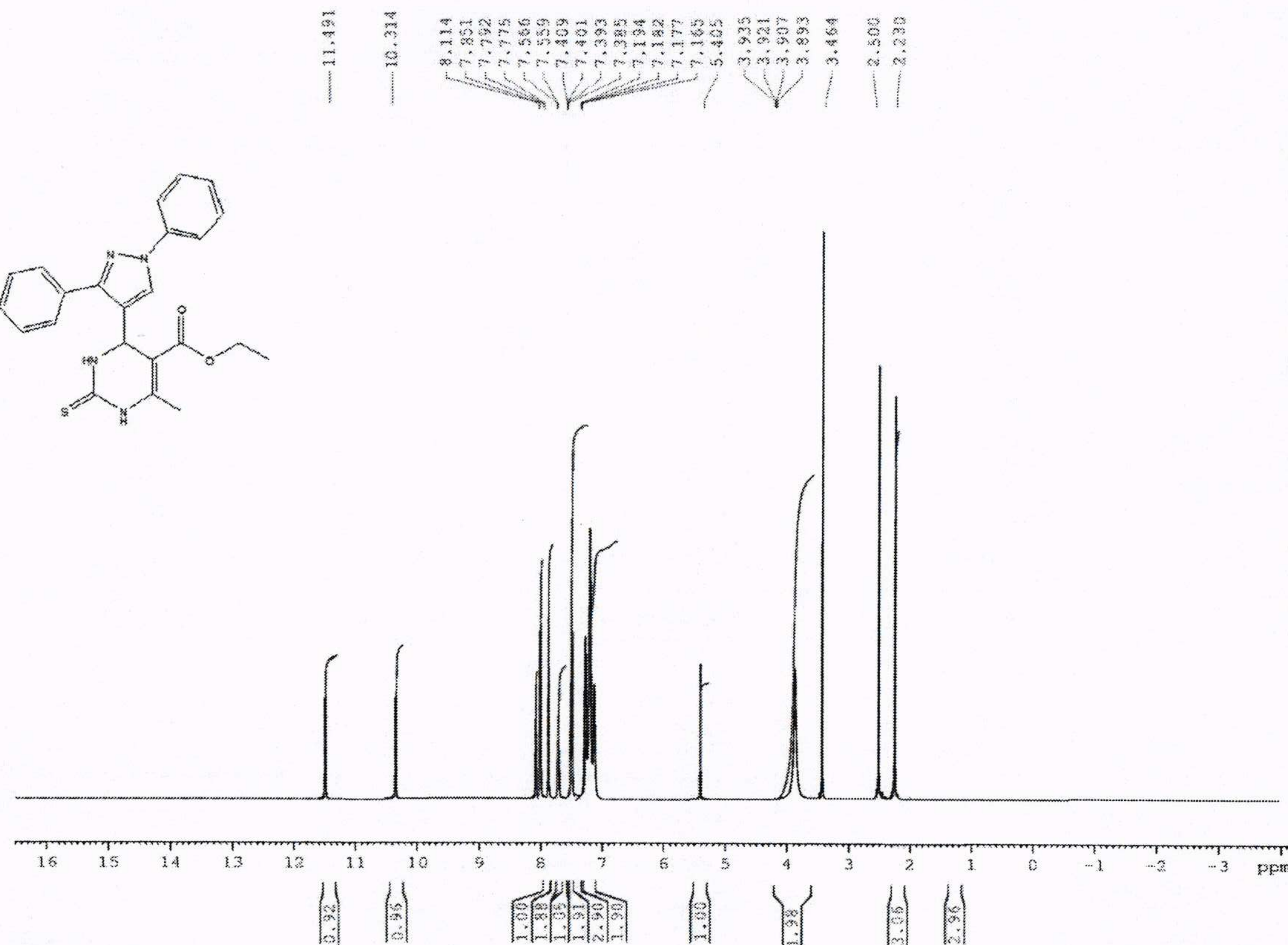
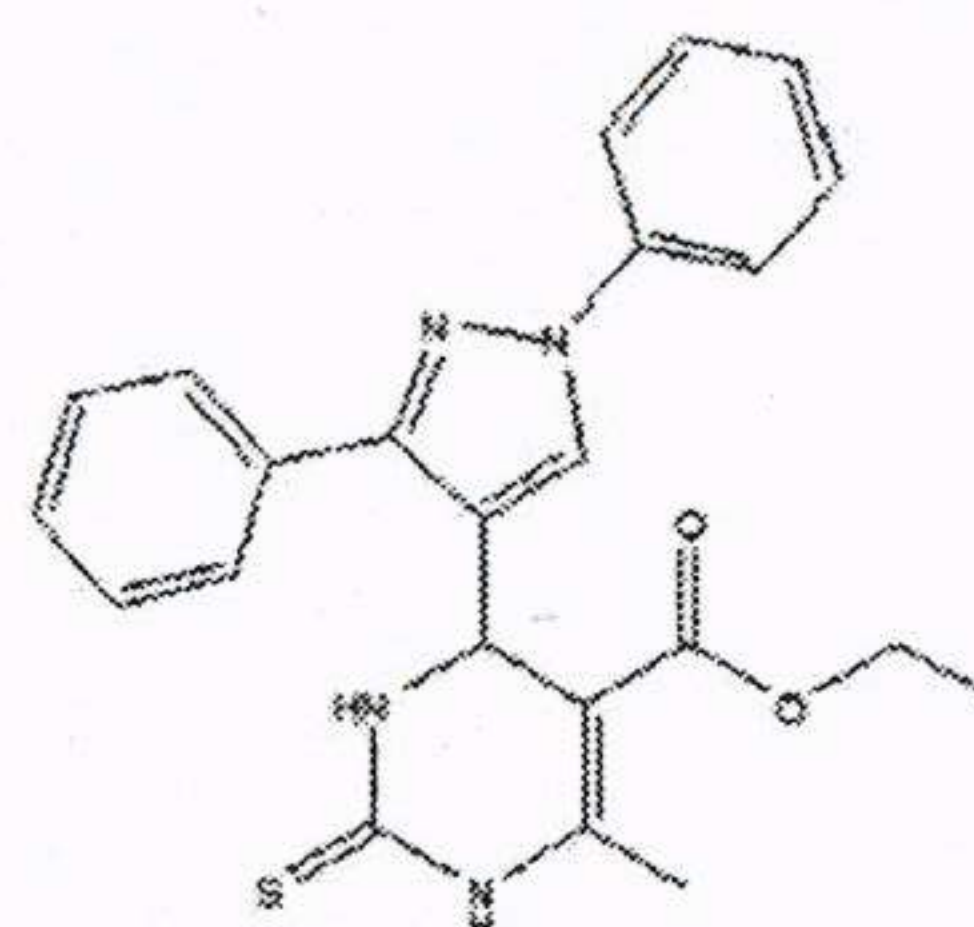




Ethyl 4-(1,3-diphenyl-1H-pyrazol-4-yl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

4c

ON DMSO D:\ abar



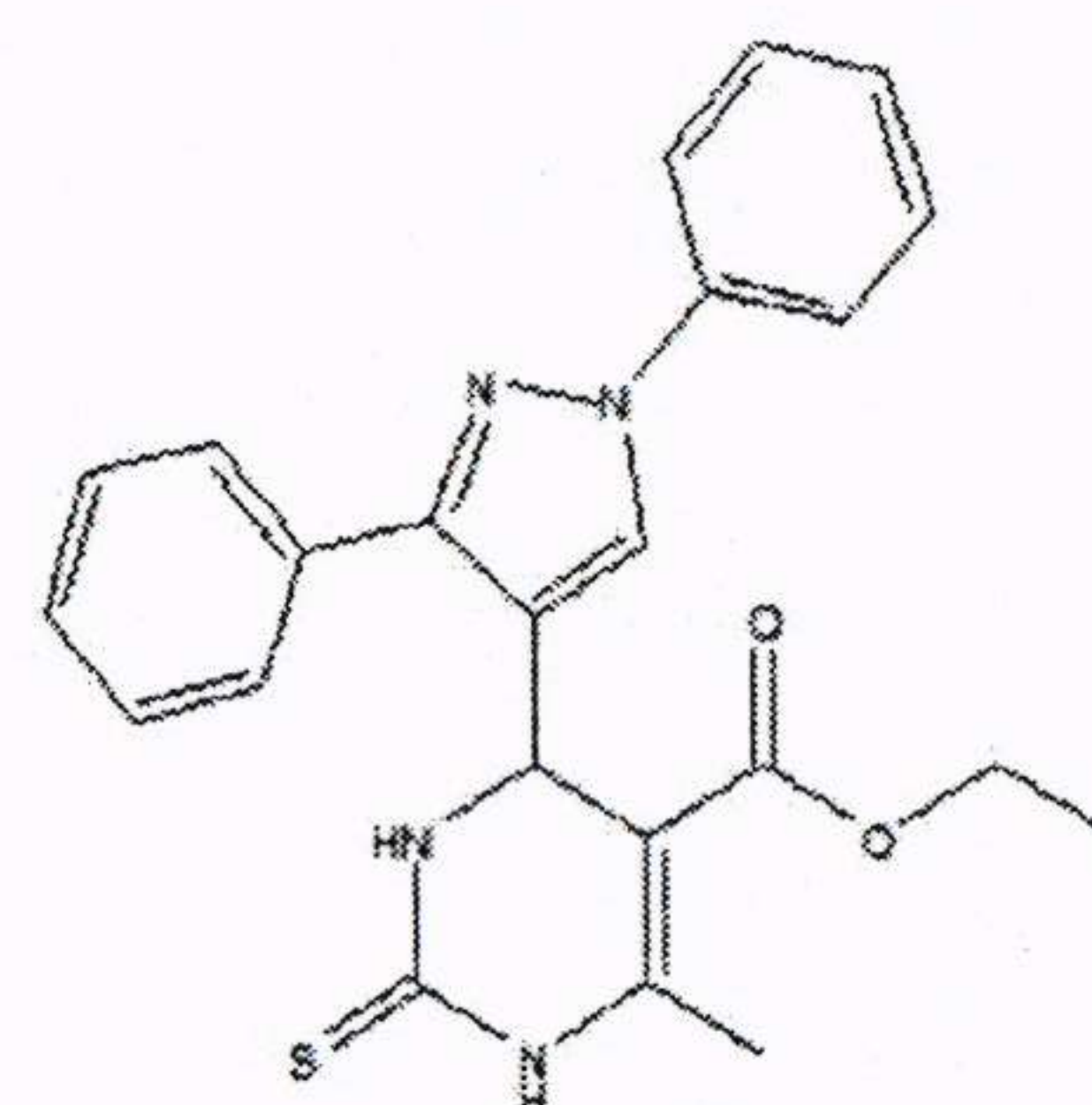
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 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 128  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.70 usec  
 PL1 -1.10 dB  
 SFO1 500.1330885 MHz  
 SI 32768  
 SF 500.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

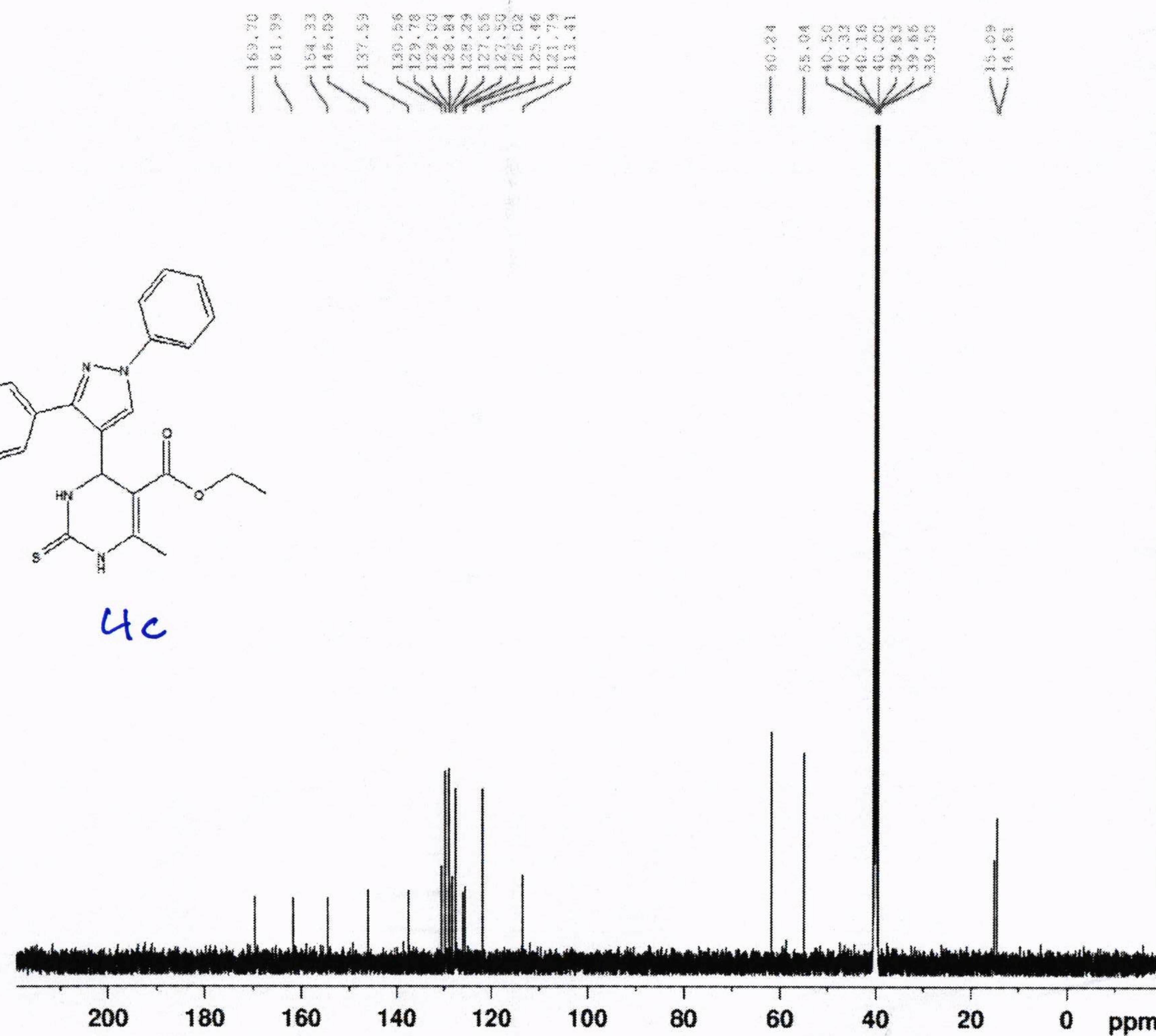




C13CPD32 DMSO D:\\ abari 44



4c



NAME drshahat-3  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20210624  
 Time 12.07  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1165  
 DS 2  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912410 sec  
 RG 4597.6  
 DW 16.650 usec  
 DE 6.50 usec  
 TE 299.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 20.00 usec  
 PL1 -6.00 dB  
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.10 dB  
 PL12 13.44 dB  
 PL13 16.40 dB  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7577890 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

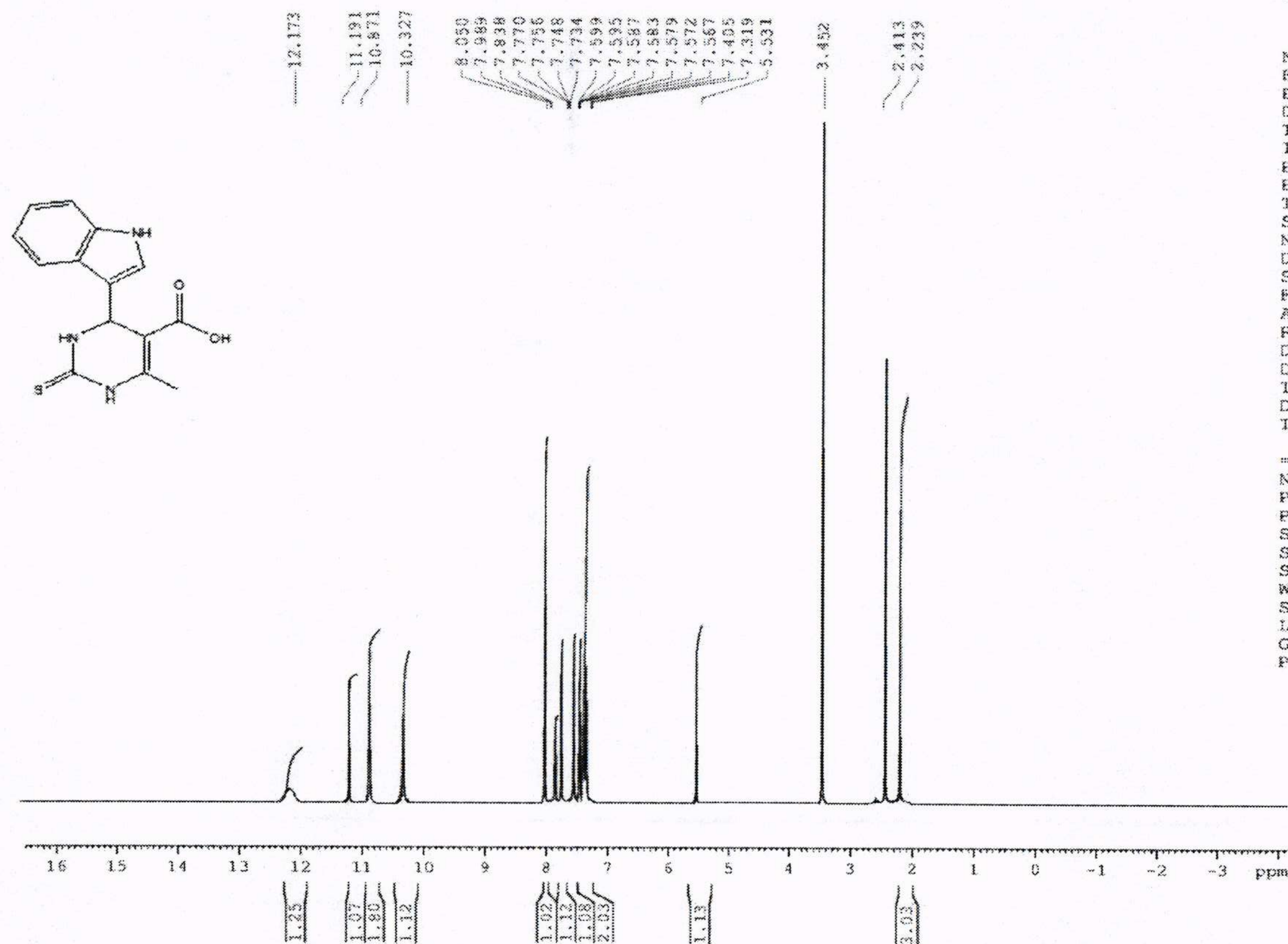




4-(1H-Indol-3-yl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylic acid

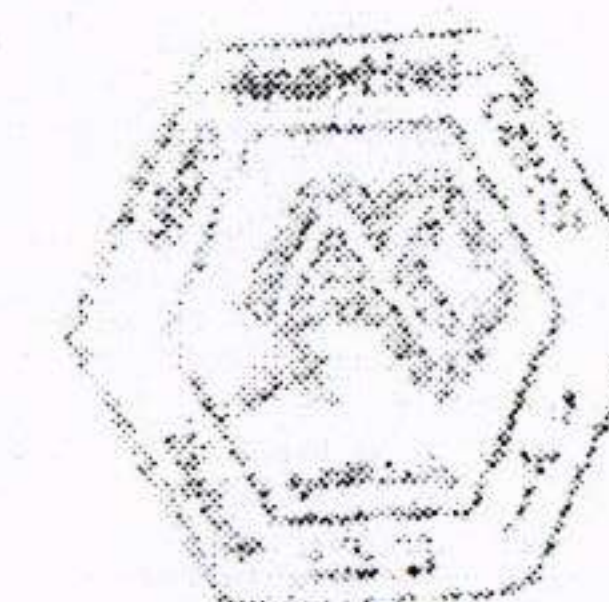
5a

ON DMSO D:\ abar



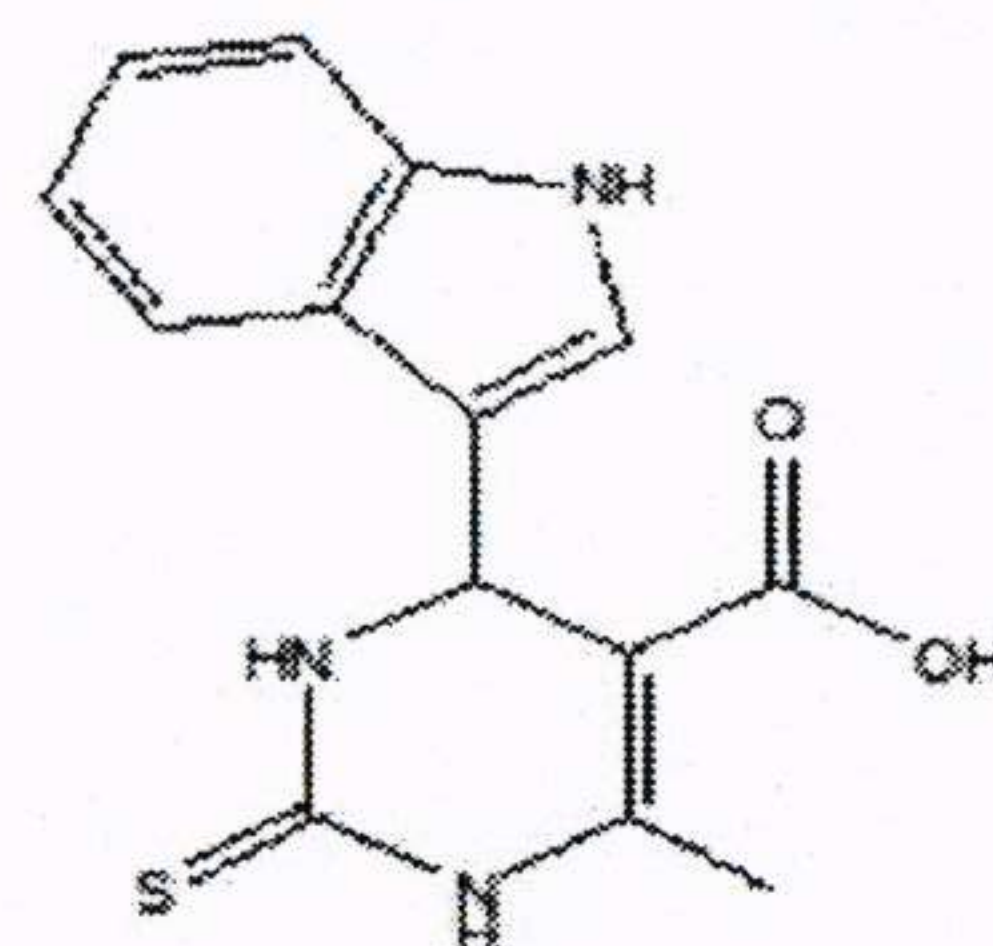
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 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 90.5  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.70 usec  
 PL1 -1.10 dB  
 SFO1 500.1330885 MHz  
 SI 32768  
 SF 500.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

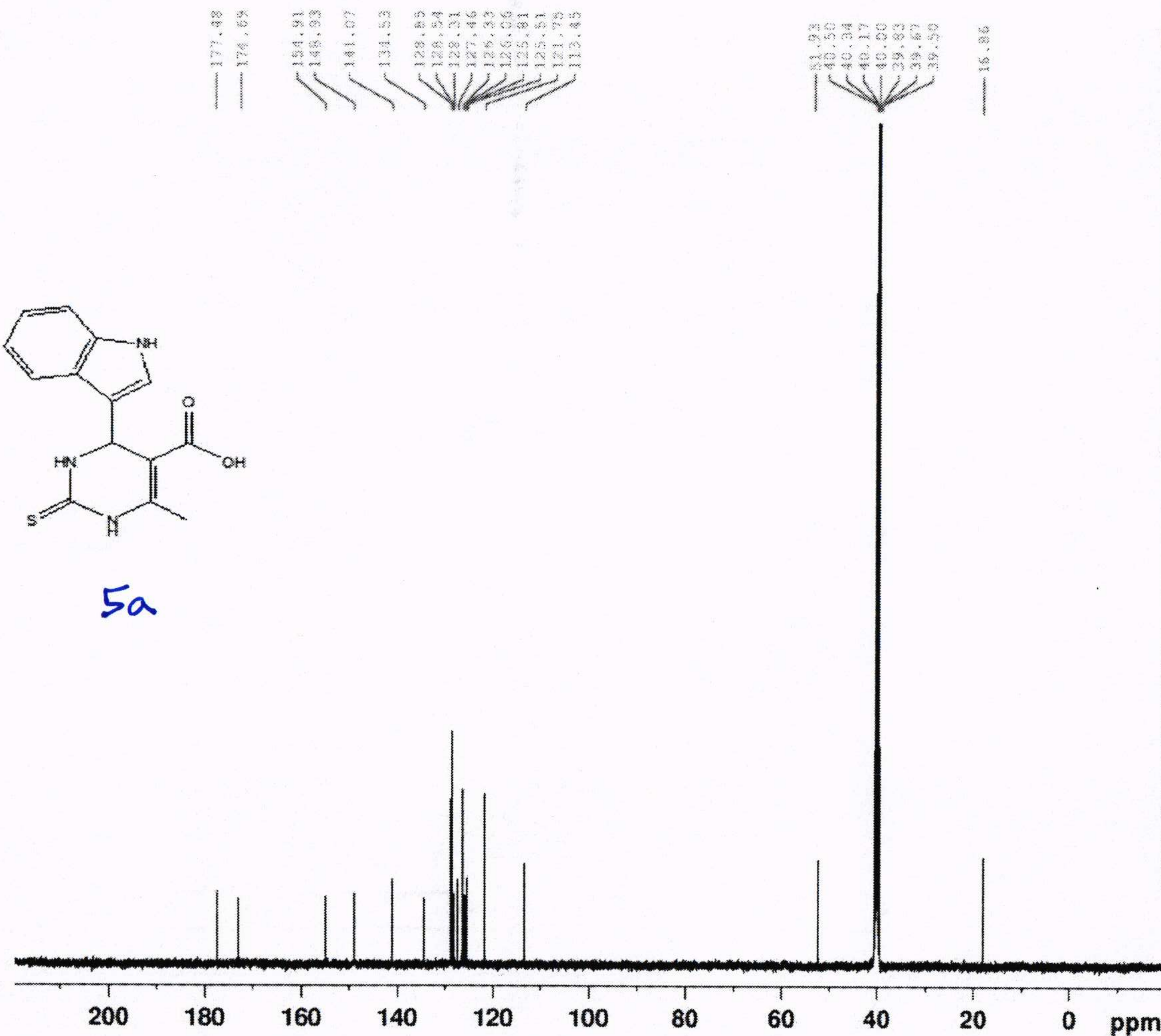




C13CPD32 DMSO D:\\ abari 46



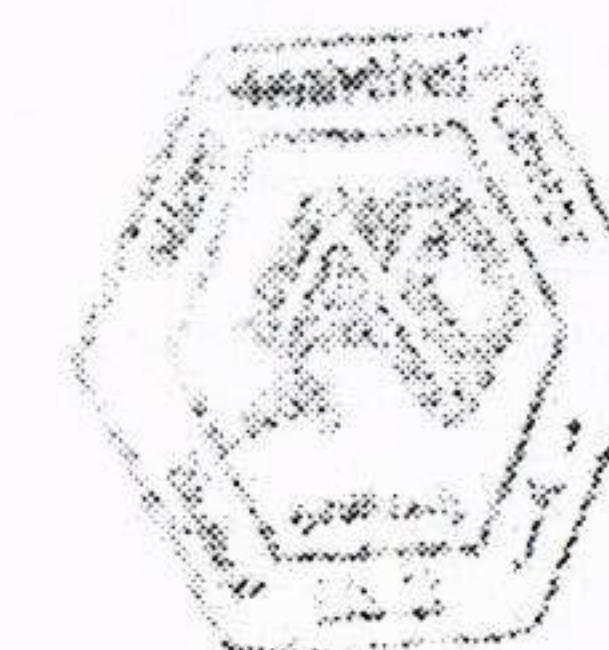
5a



NAME drshahat-5  
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 PROCNO 1  
 Date\_ 20210624  
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 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2000  
 DS 2  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912410 sec  
 RG 14596.5  
 DW 16.650 usec  
 DE 6.50 usec  
 TE 299.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 20.00 usec  
 PL1 -6.00 dB  
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.10 dB  
 PL12 13.44 dB  
 PL13 16.40 dB  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7577890 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 1.40

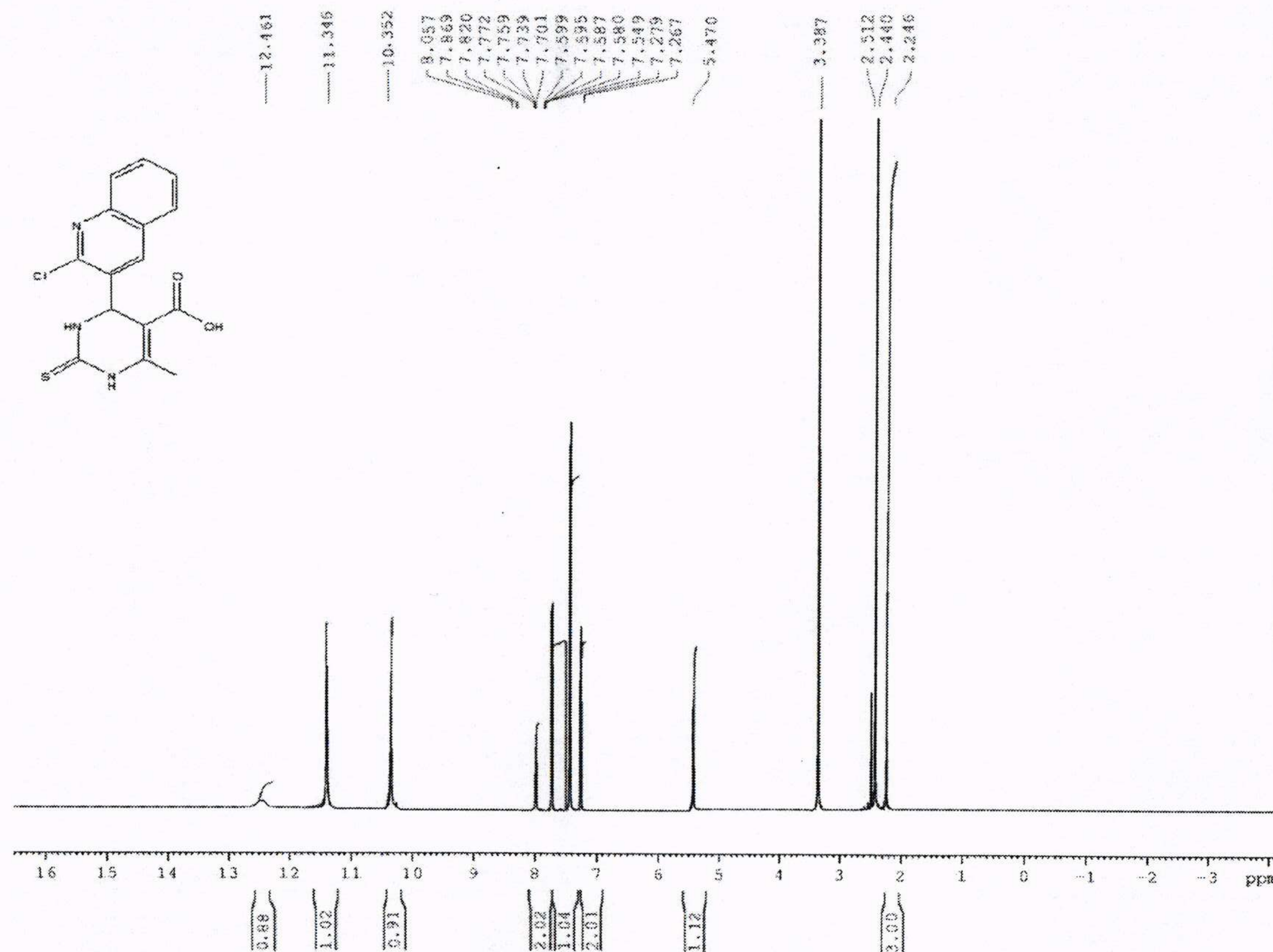
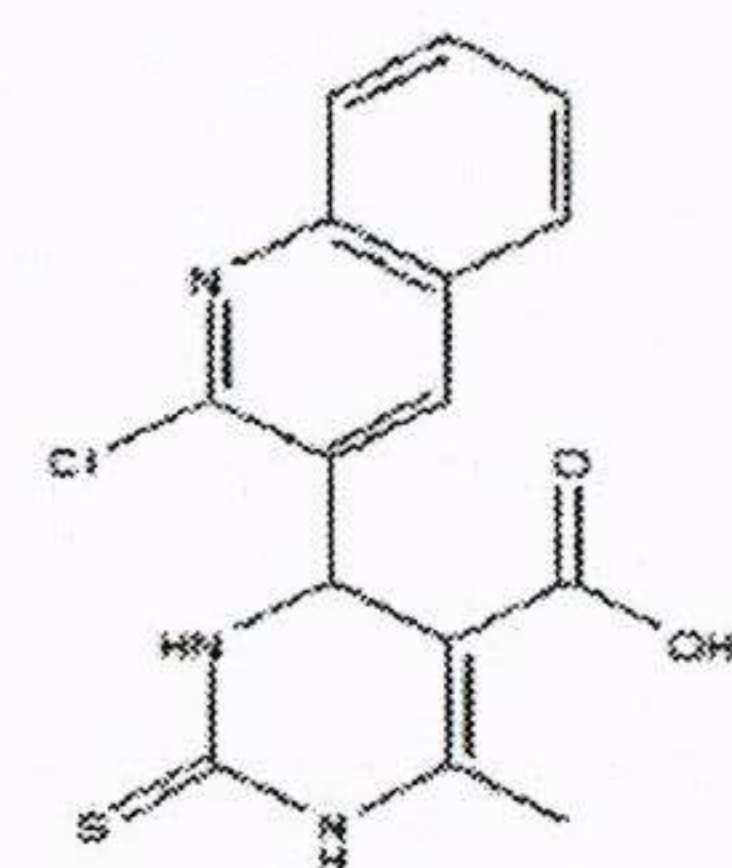




4-(2-Chloroquinolin-3-yl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylic acid

5b

ON DMSO D:\ abar



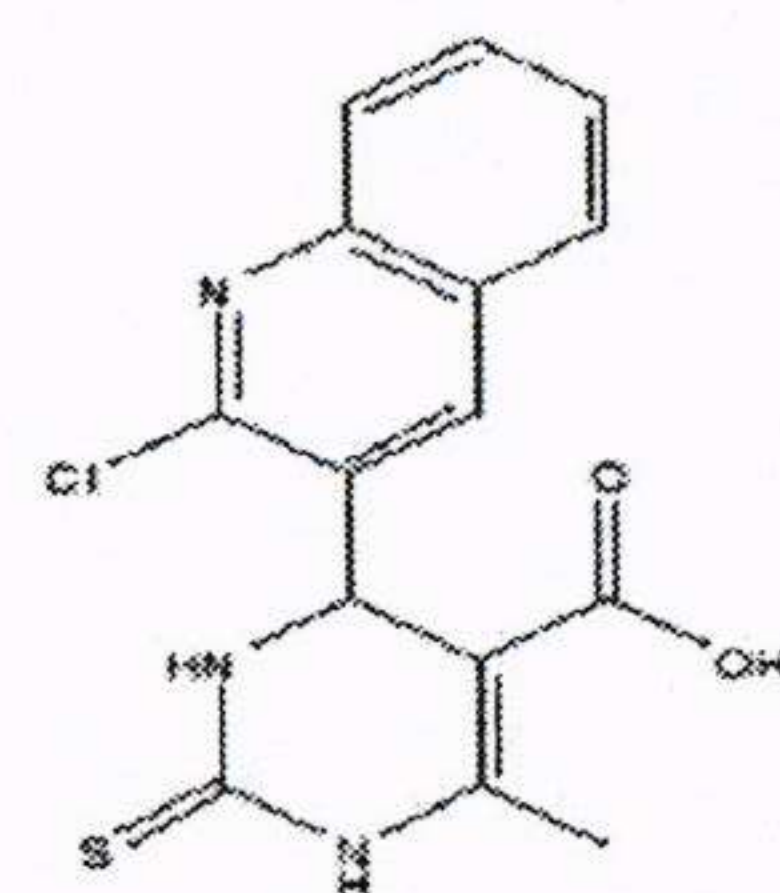
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Date\_ 20210624  
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PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1720407 sec  
RG 90.5  
DW 48.400 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
TD0 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 14.70 usec  
PL1 -1.10 dB  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

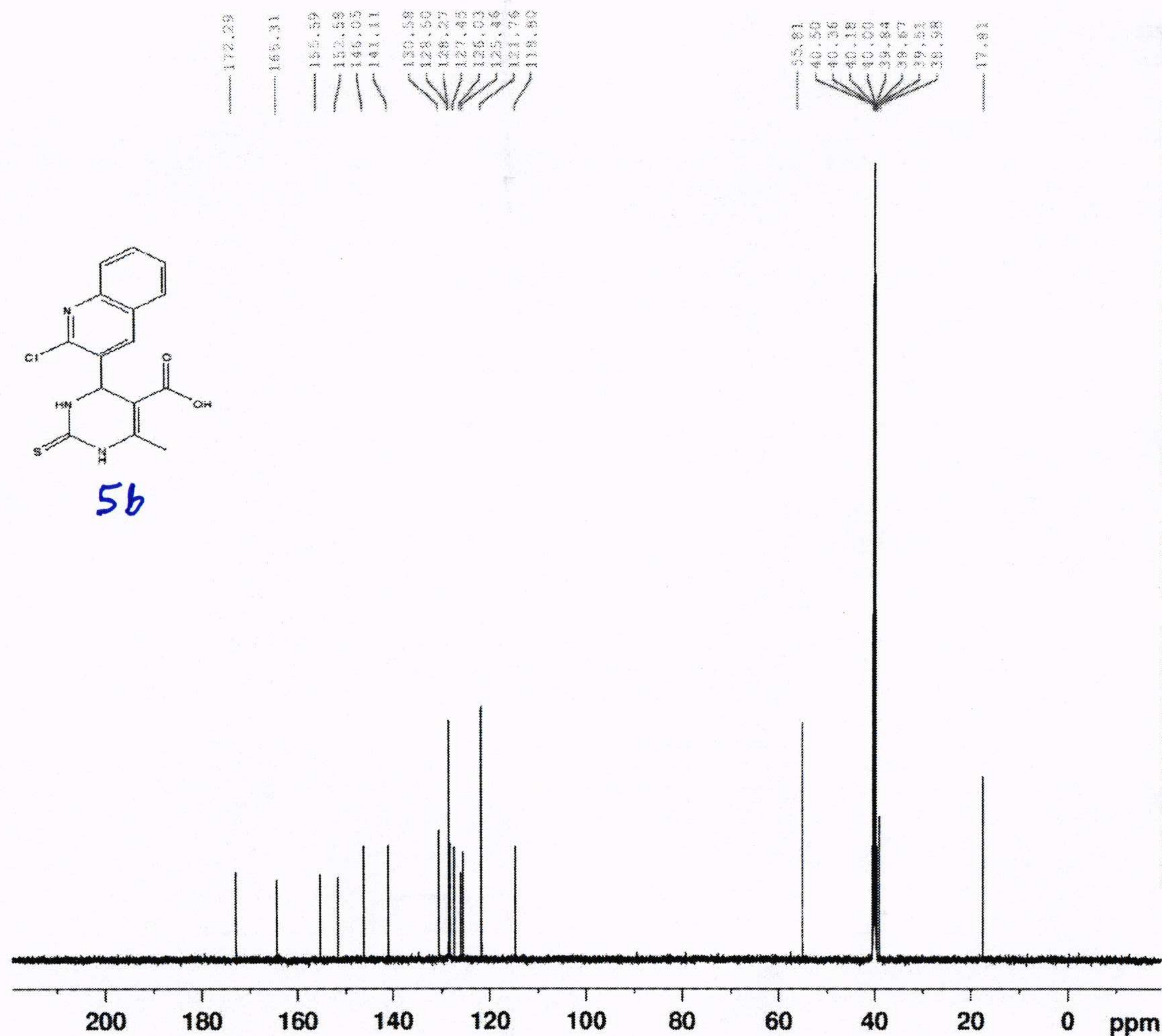




C13CPD32 DMSO D:\\ abari 45



5b



NAME drshahat-4  
 EXPNO 11  
 PROCNO 1  
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 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1104  
 DS 2  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912410 sec  
 RG 2048  
 DW 16.650 usec  
 DE 6.50 usec  
 TE 299.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 20.00 usec  
 PL1 -6.00 dB  
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.10 dB  
 PL12 13.44 dB  
 PL13 16.40 dB  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7577890 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

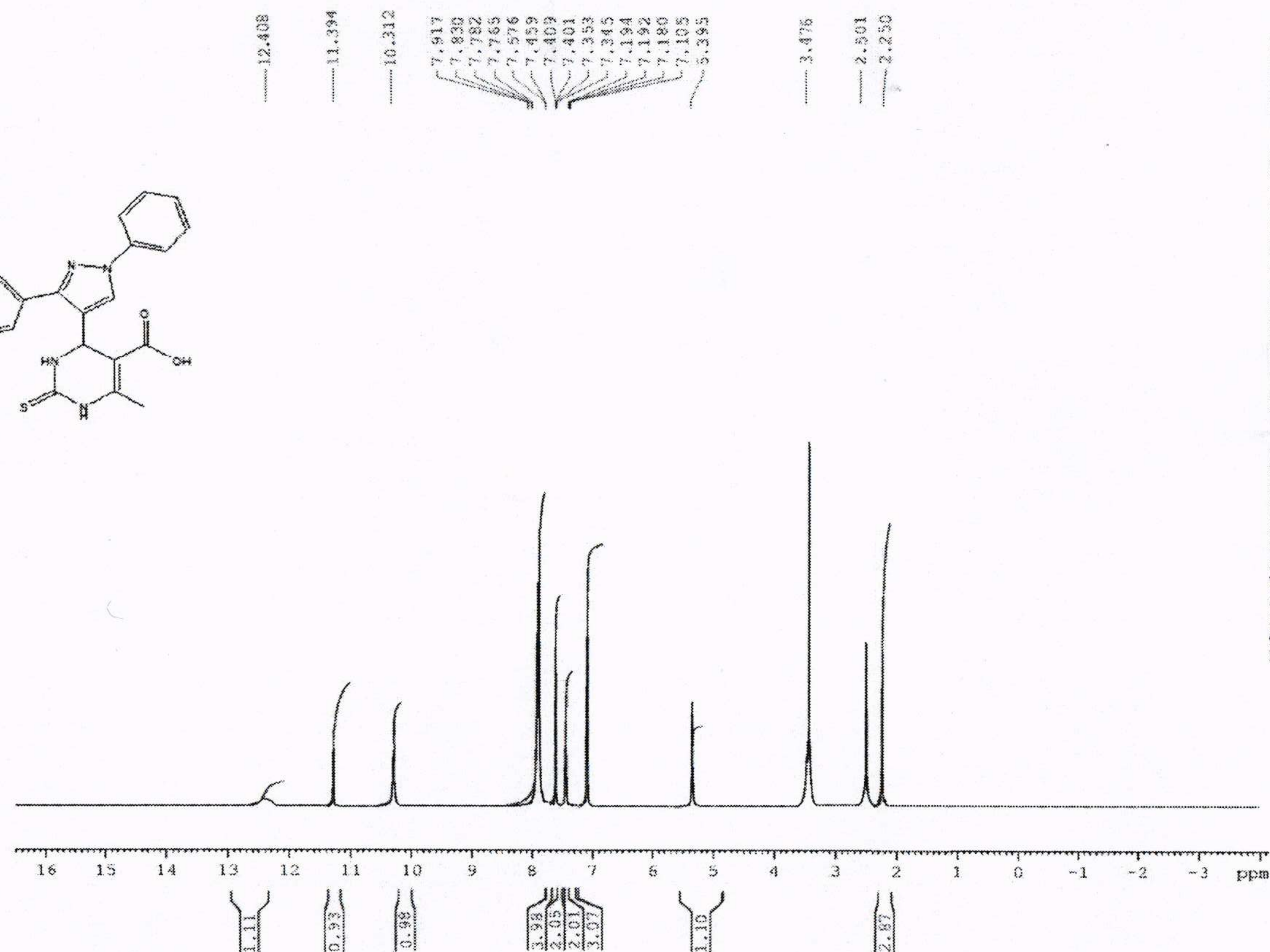
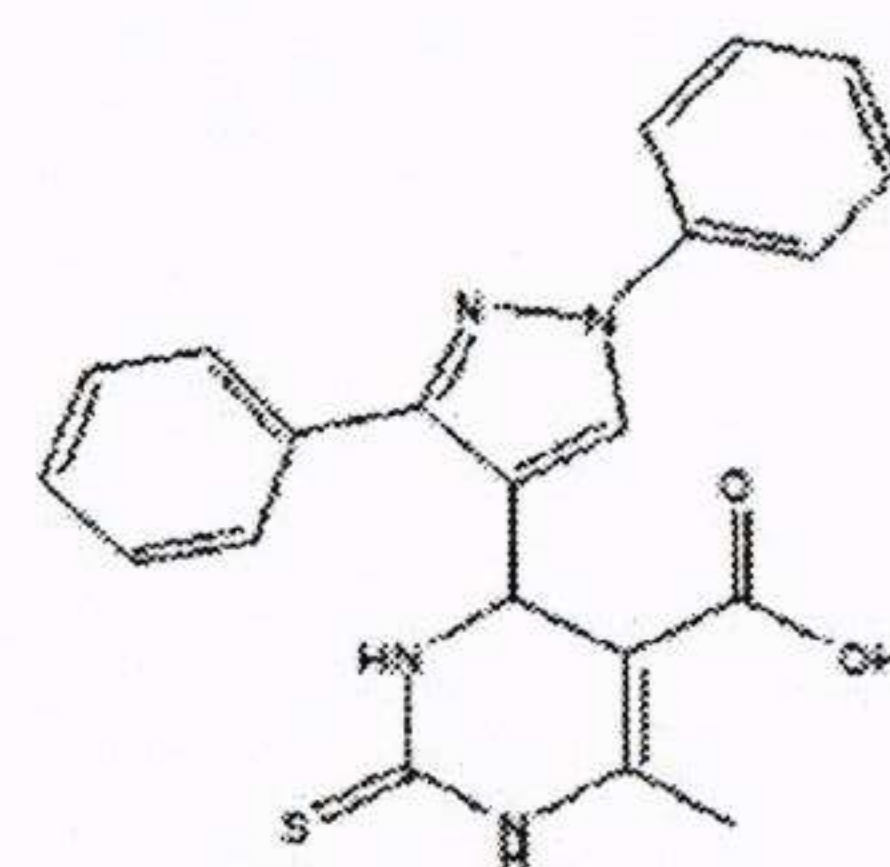




4-(1,3-Diphenyl-1H-pyrazol-4-yl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylic acid

5c

ON DMSO D:\ abar



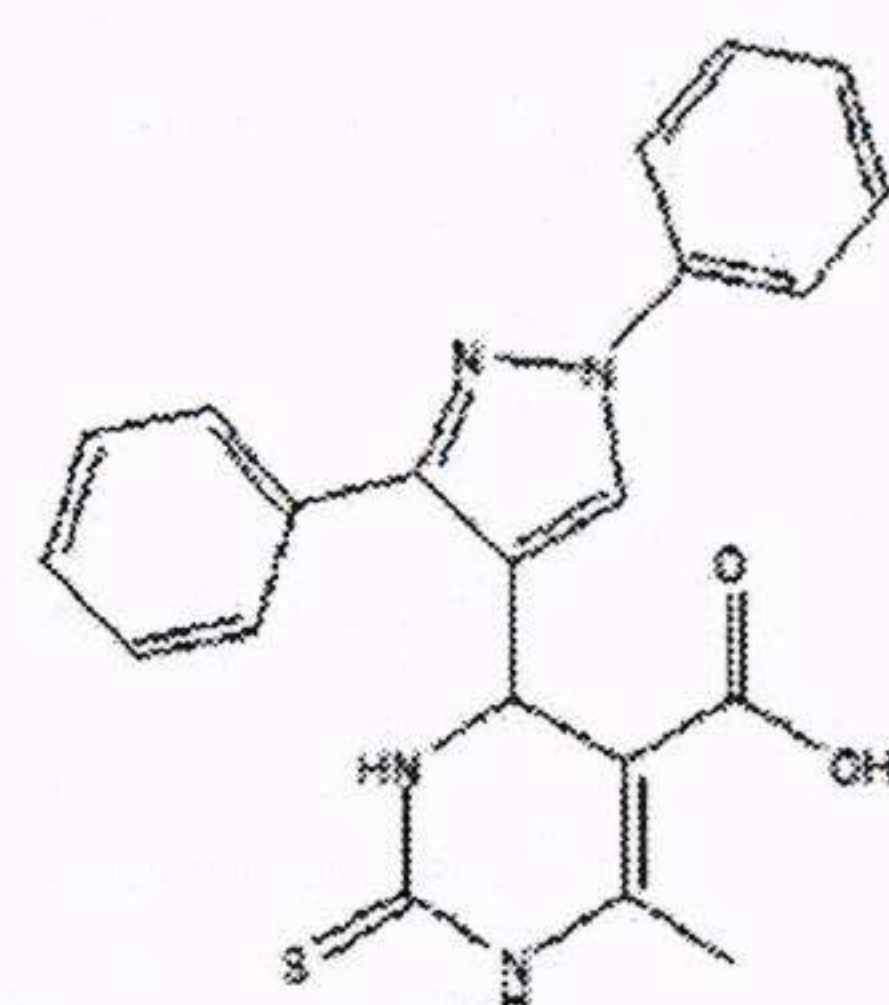
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PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1720407 sec  
RG 128  
DW 48.400 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.70 usec  
PL1 -1.10 dB  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

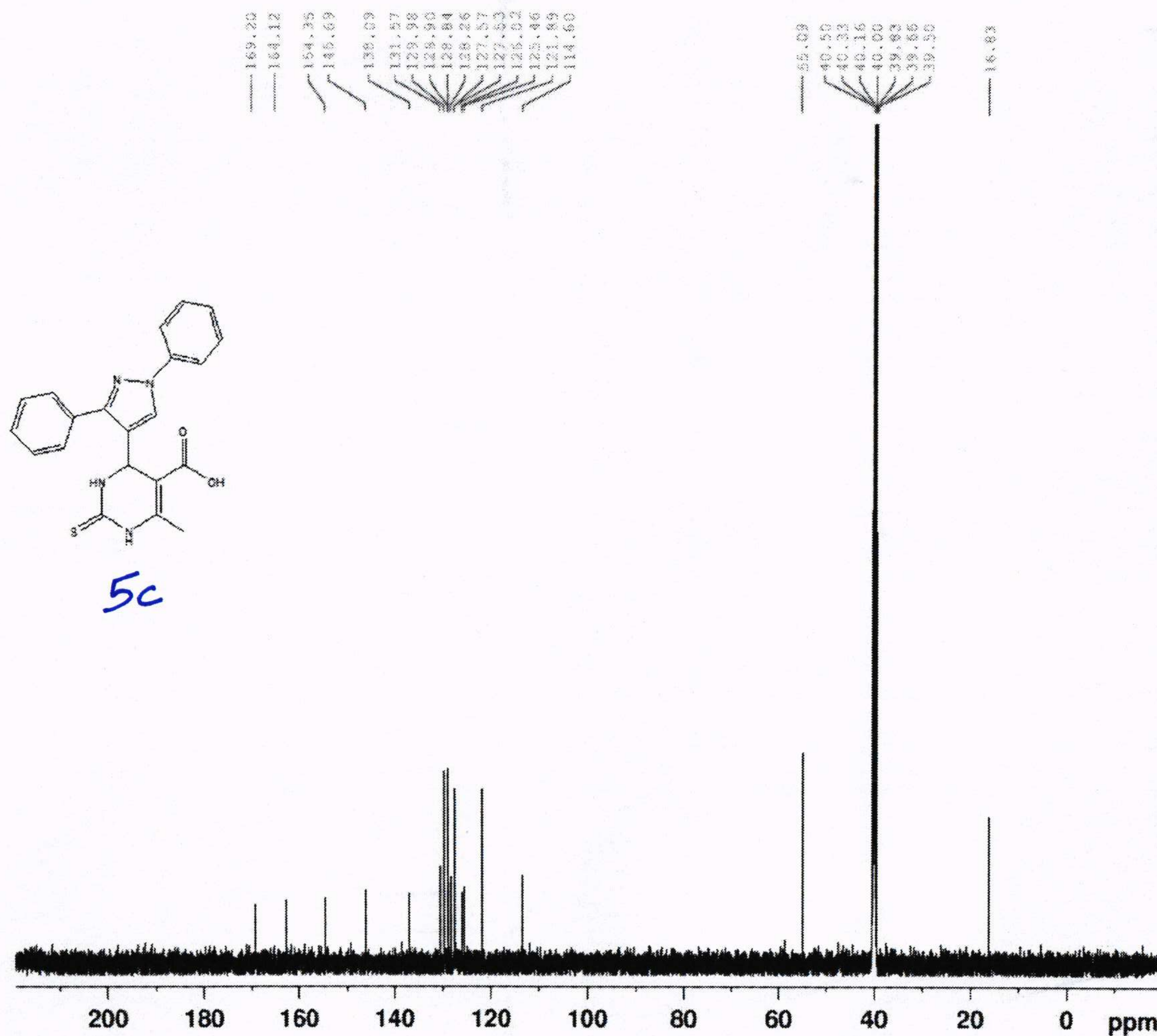




C13CPD32 DMSO D:\\ abari 44



5c



NAME drshahat-6  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20210624  
 Time 12.07  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1165  
 DS 2  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912410 sec  
 RG 4597.6  
 DW 16.650 usec  
 DE 6.50 usec  
 TE 299.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 20.00 usec  
 PL1 -6.00 dB  
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.10 dB  
 PL12 13.44 dB  
 PL13 16.40 dB  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7577890 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

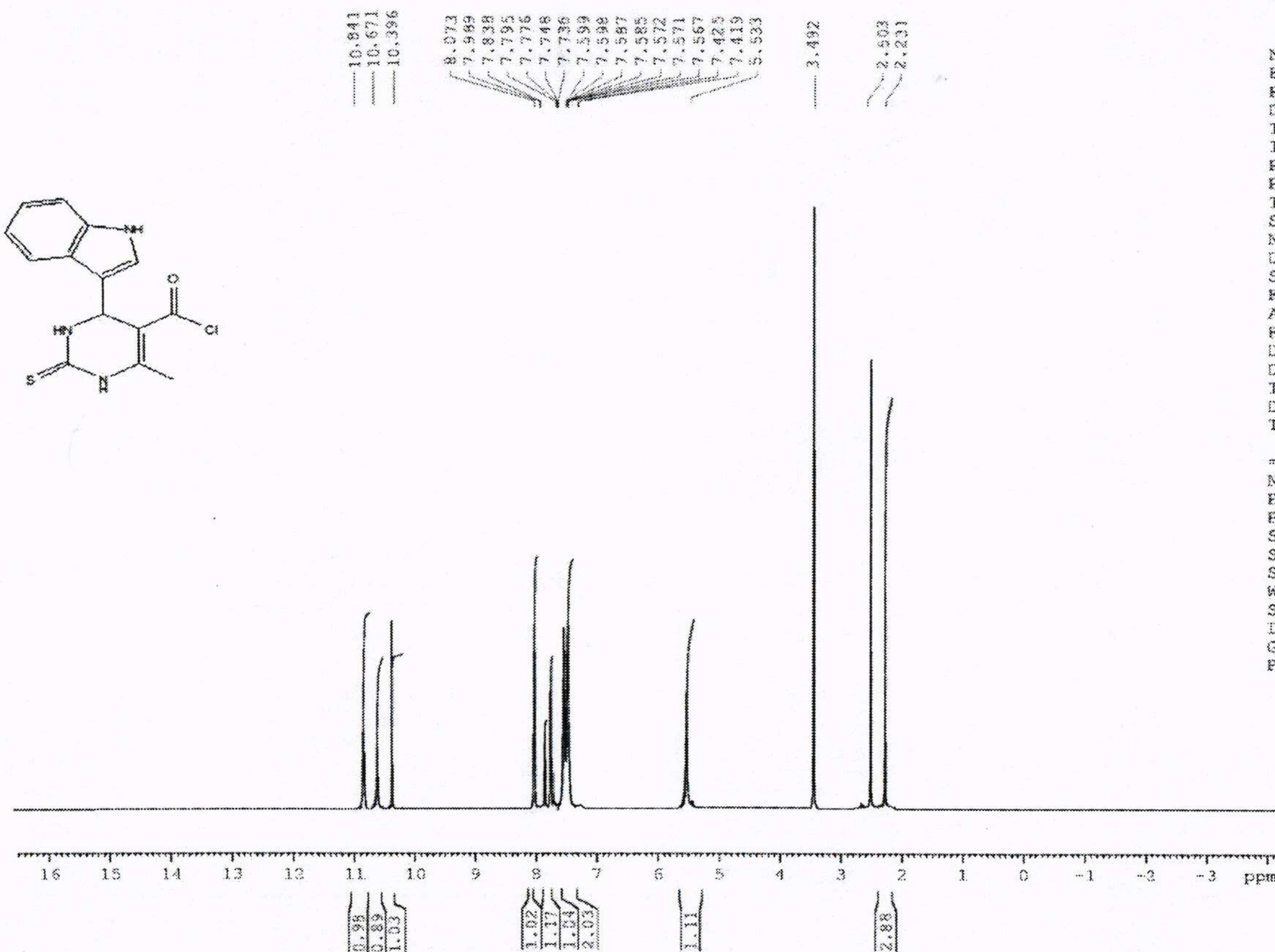
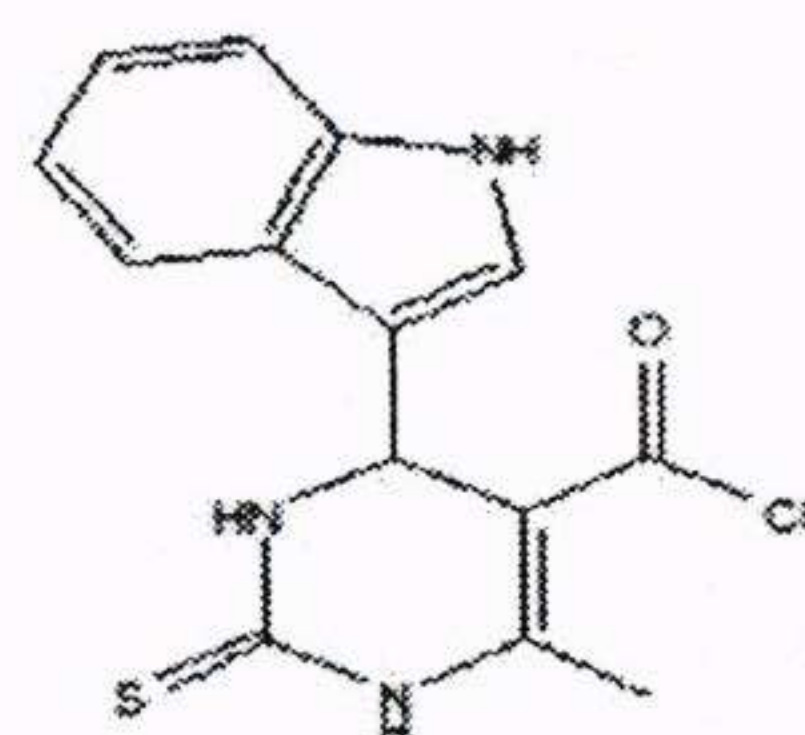




4-(1H-Indol-3-yl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carbonyl chloride

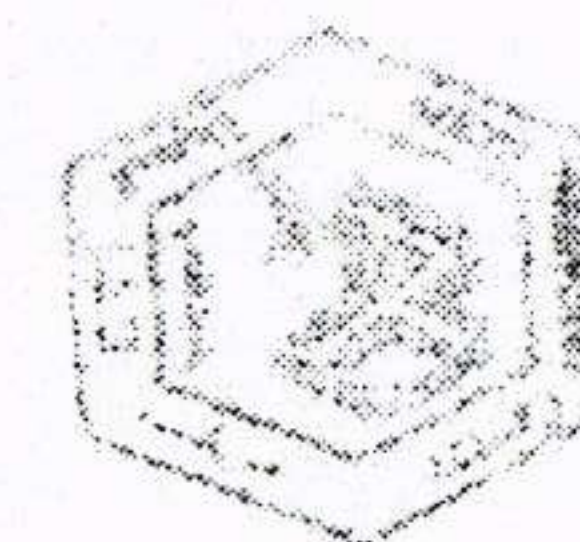
6a

DN DMSO D:\ abar



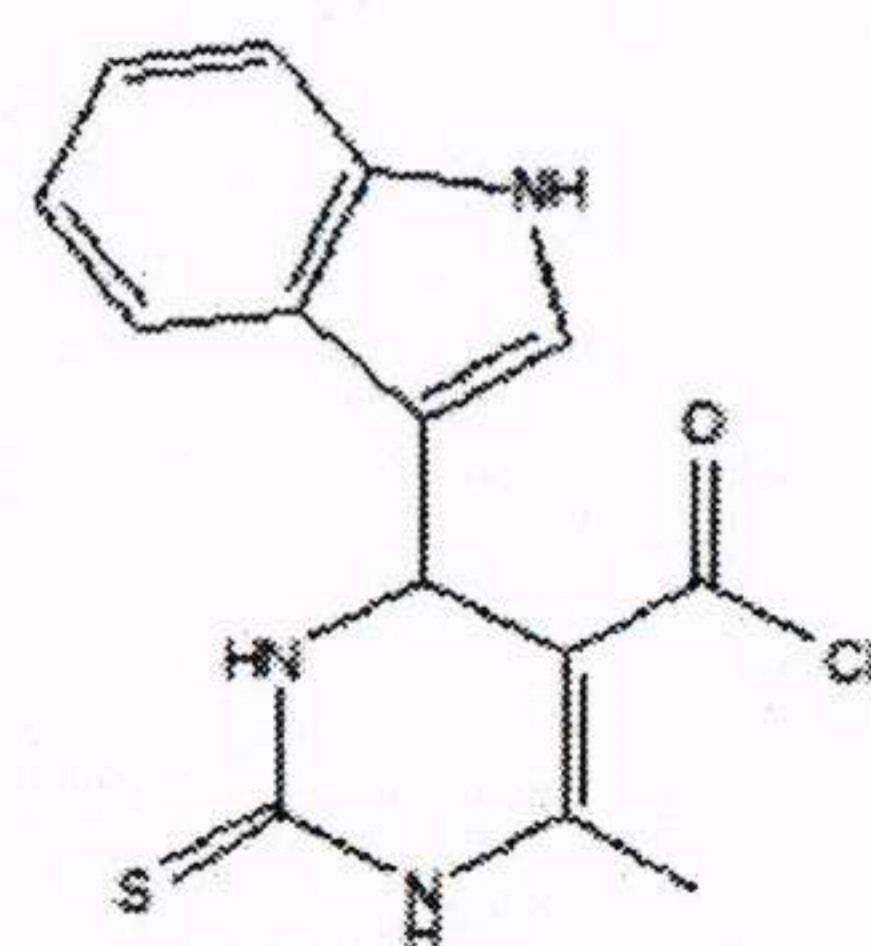
NAME drshahat-8  
EXPNO 10  
PROCNO 1  
Date\_ 20210625  
Time 18.59  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1720407 sec  
RG 90.5  
DW 48.400 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.70 usec  
PL1 -1.10 dB  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

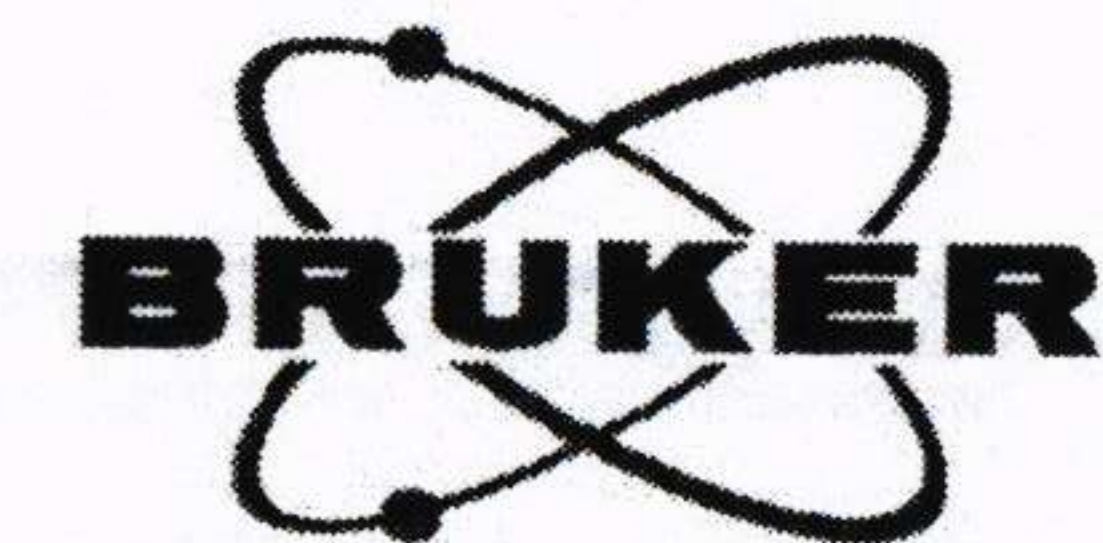
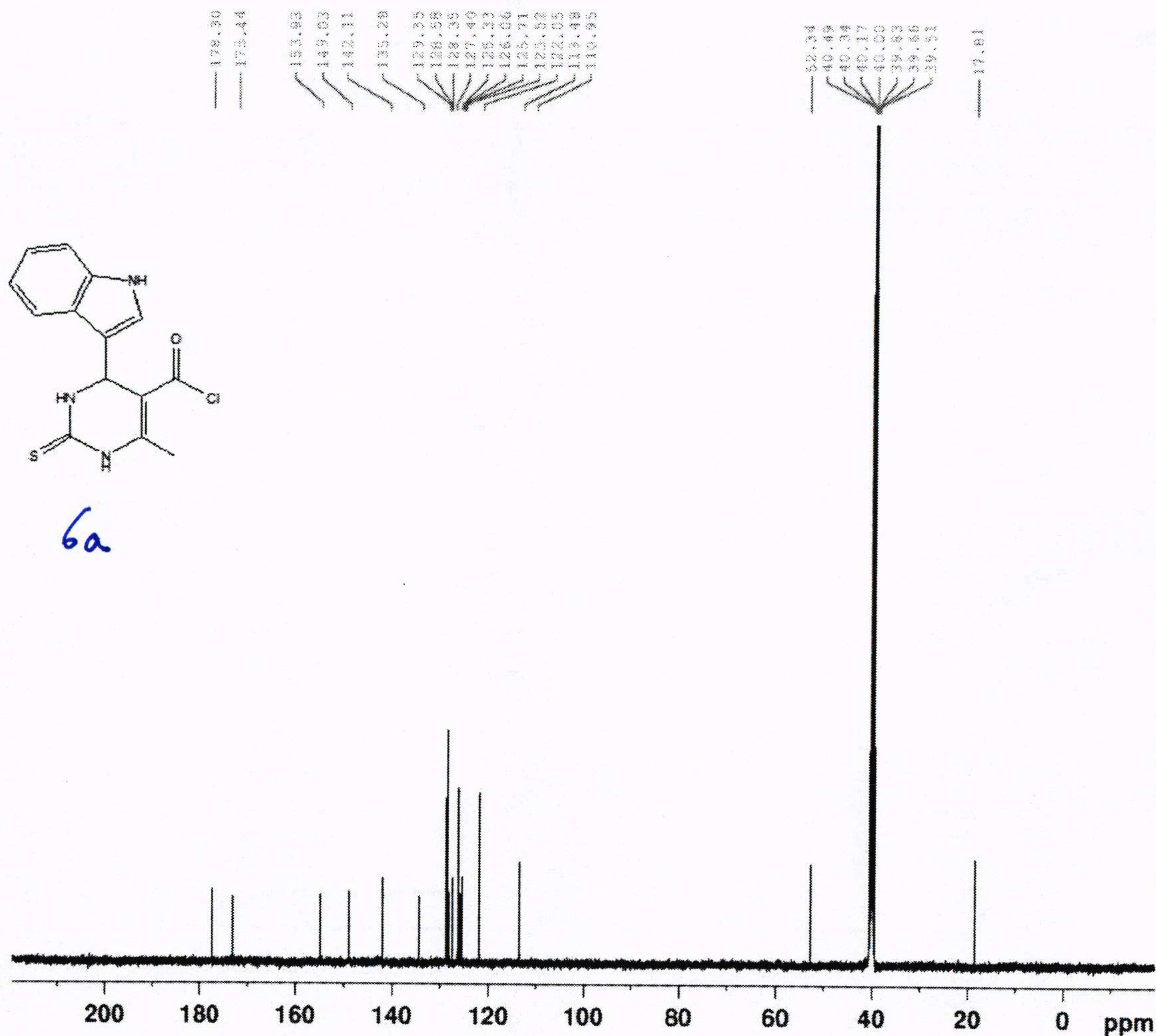




C13CPD32 DMSO D:\\ abari 46



6a



NAME drshahat-8  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20210625  
 Time 20.47  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2000  
 DS 2  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912410 sec  
 RG 14596.5  
 DW 16.650 usec  
 DE 6.50 usec  
 TE 299.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 20.00 usec  
 PL1 -6.00 dB  
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.10 dB  
 PL12 13.44 dB  
 PL13 16.40 dB  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7577890 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

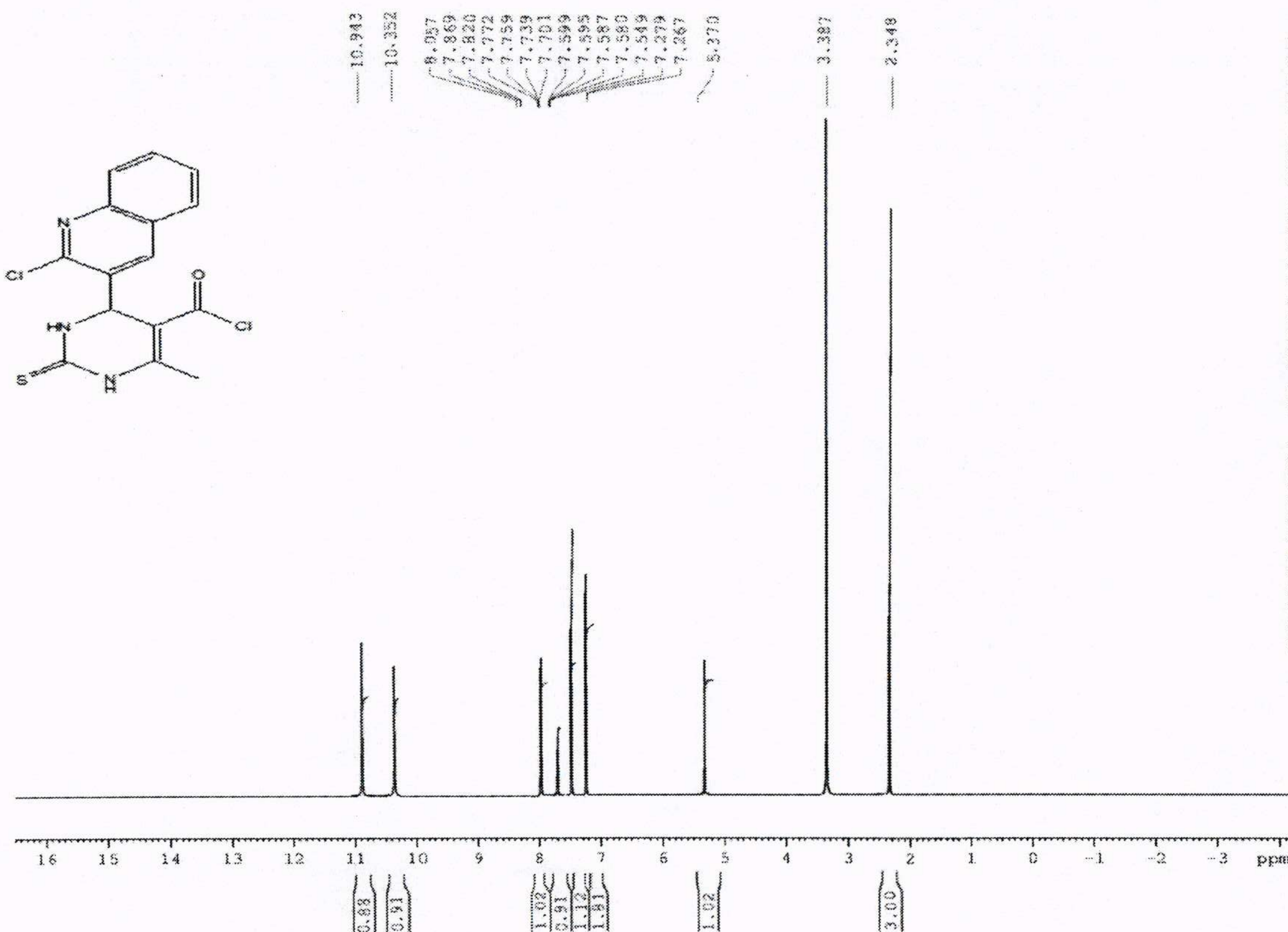
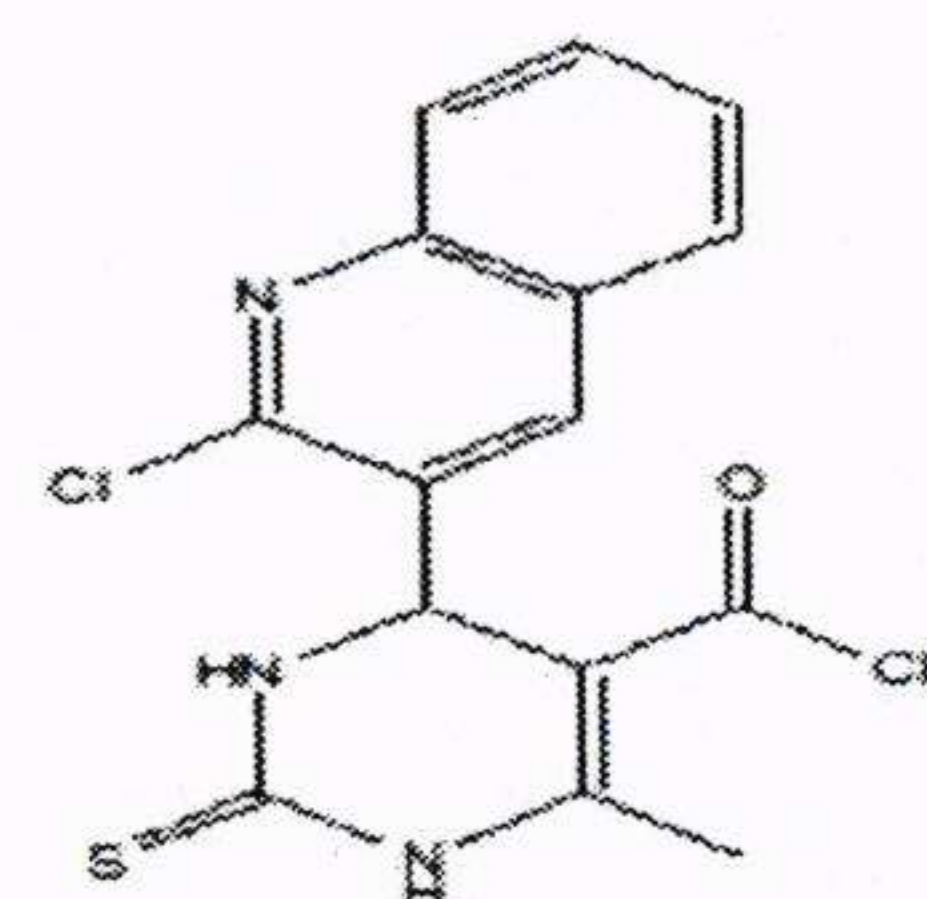




4-(2-Chloroquinolin-3-yl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carbonyl chloride

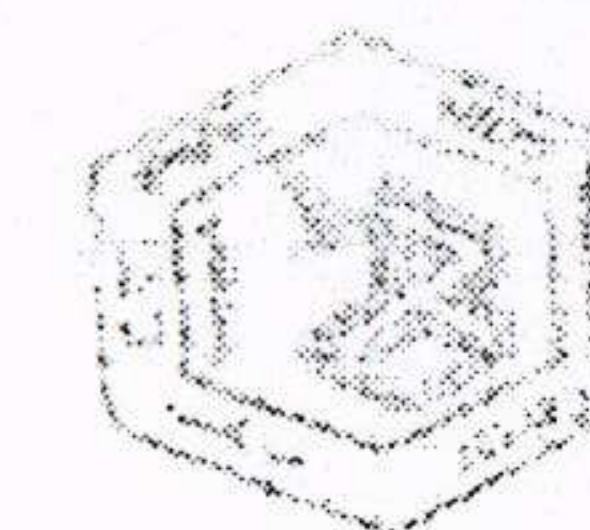
66

ON DMSO D:\ abar



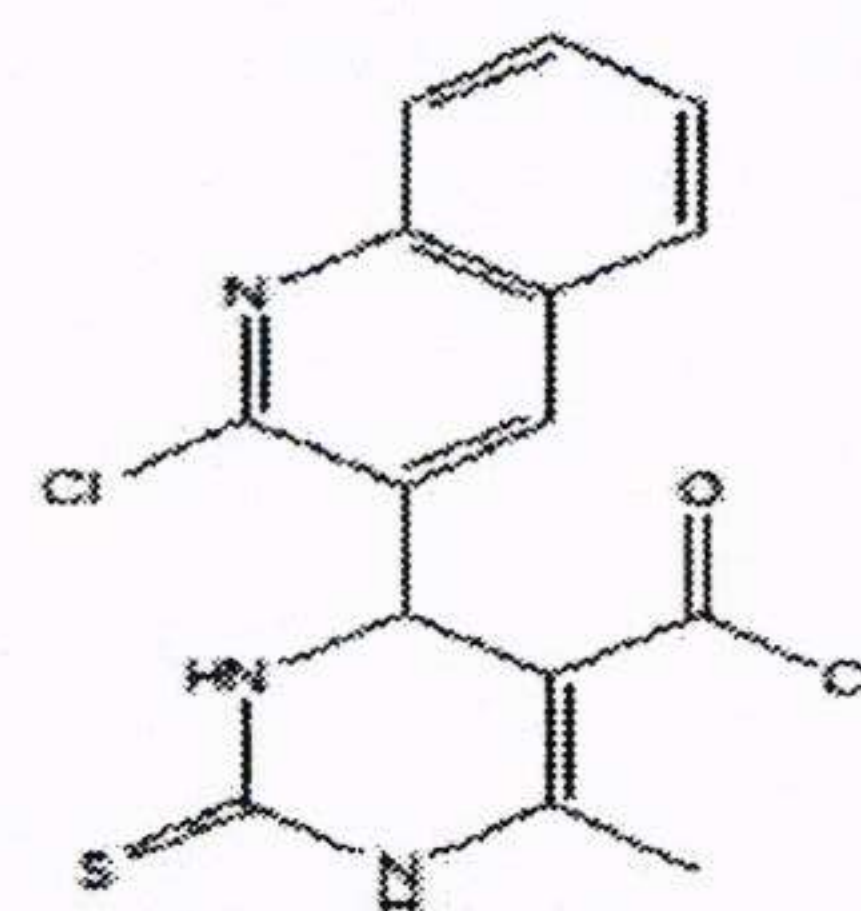
NAME drshahat-7  
EXPNO 10  
PROCNO 1  
Date\_ 20210624  
Time 18.59  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1720407 sec  
RG 90.5  
DW 48.400 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
TD0 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P1 14.70 usec  
PL1 -1.10 dB  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

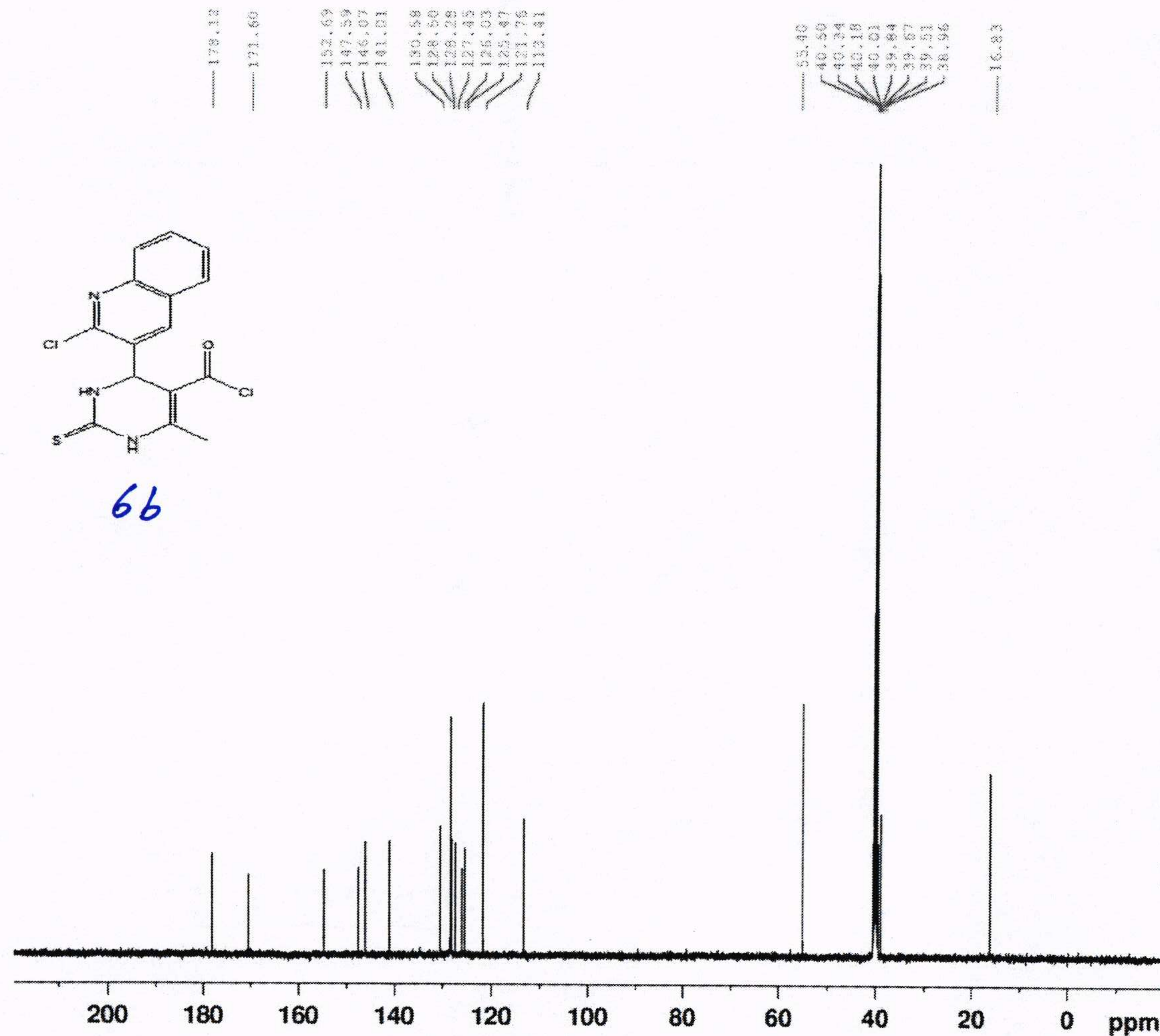




C13CPD32 DMSO D:\\ abari 45



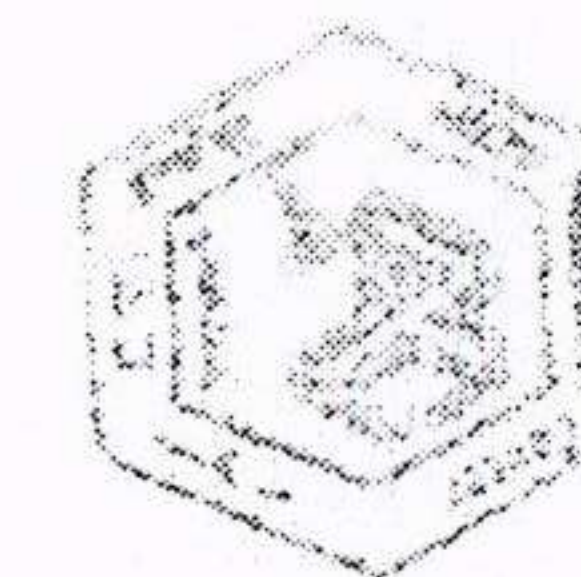
66



NAME drshahat-7  
EXPNO 11  
PROCNO 1  
Date\_ 20210624  
Time 13.45  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 1104  
DS 2  
SWH 30030.029 Hz  
FIDRES 0.458222 Hz  
AQ 1.0912410 sec  
RG 2048  
DW 16.650 usec  
DE 6.50 usec  
TE 299.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 20.00 usec  
PL1 -6.00 dB  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.10 dB  
PL12 13.44 dB  
PL13 16.40 dB  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7577890 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

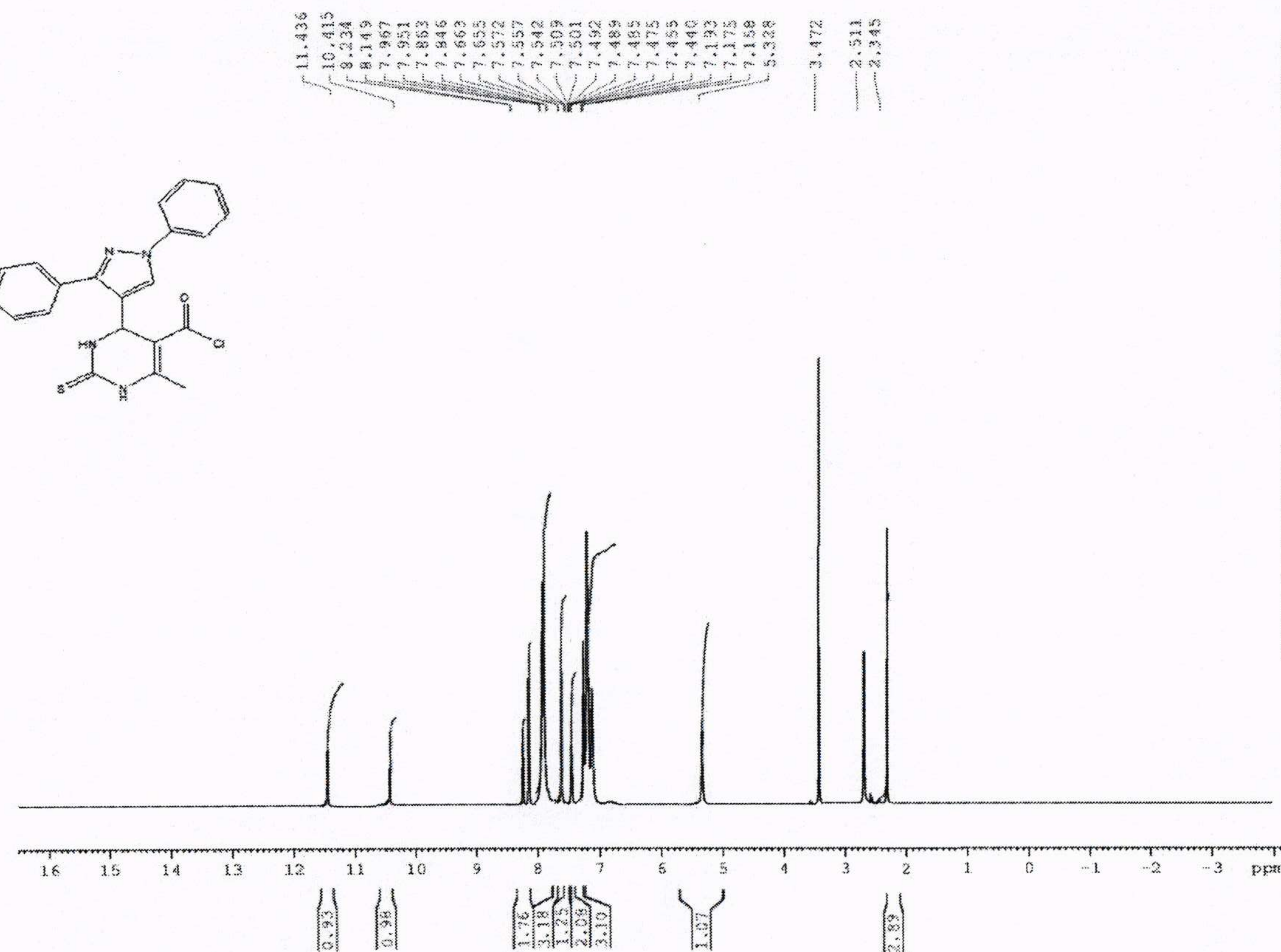
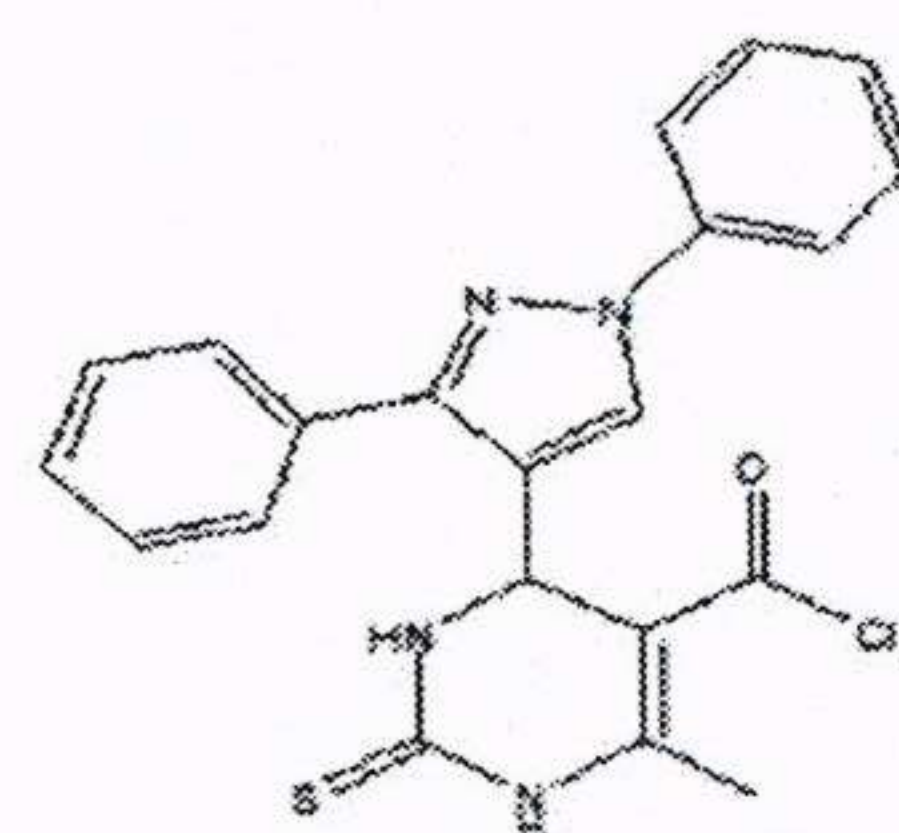




4-(1,3-Diphenyl-1H-pyrazol-4-yl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carbonyl chloride

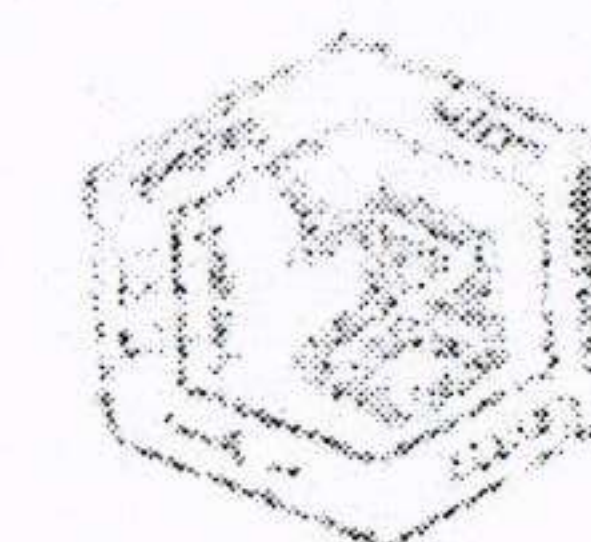
6c

DN DMSO D:\ abar



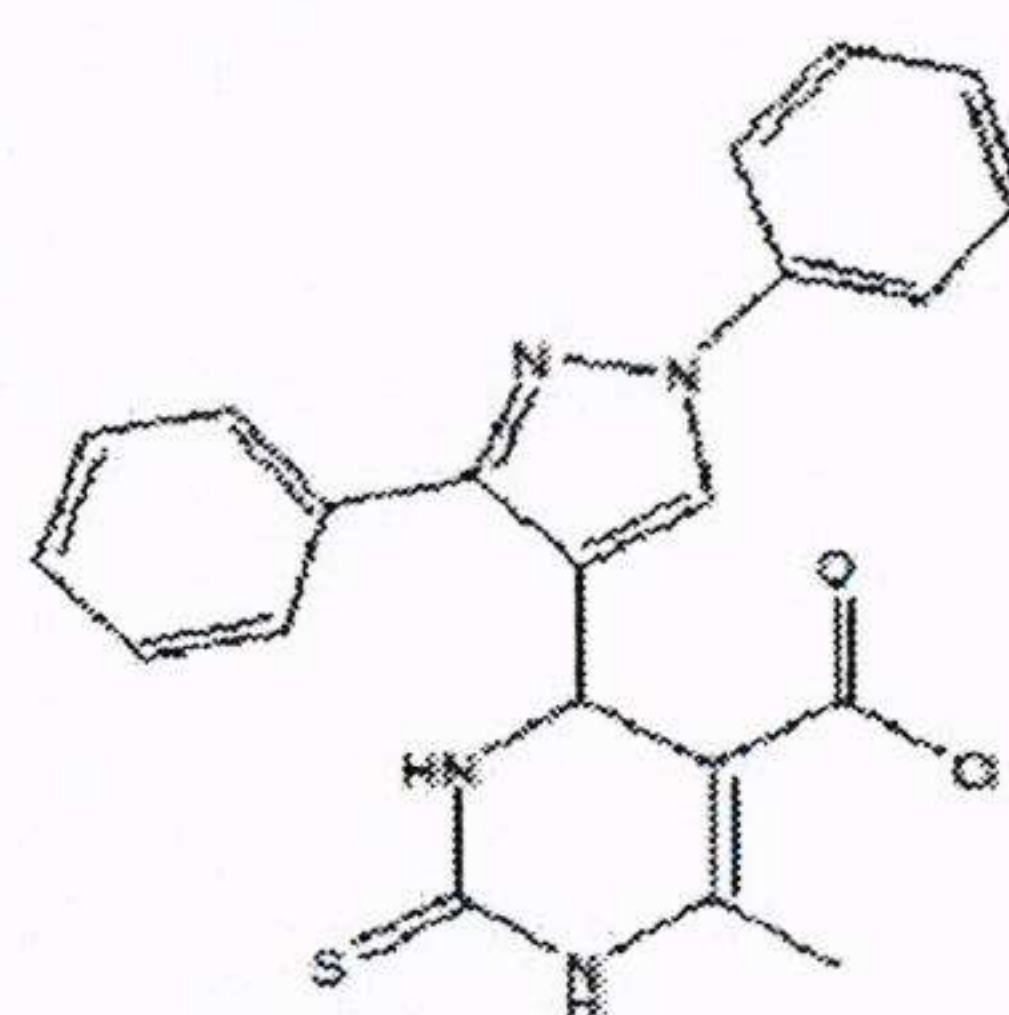
NAME drshahat-9  
EXPNO 10  
PROCNO 1  
Date\_ 20210622  
Time 11.17  
INSTRUM spect  
PROBHD 5 mm F4BBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1720407 sec  
RG 128  
DW 48.400 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.70 usec  
PL1 -1.10 dB  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

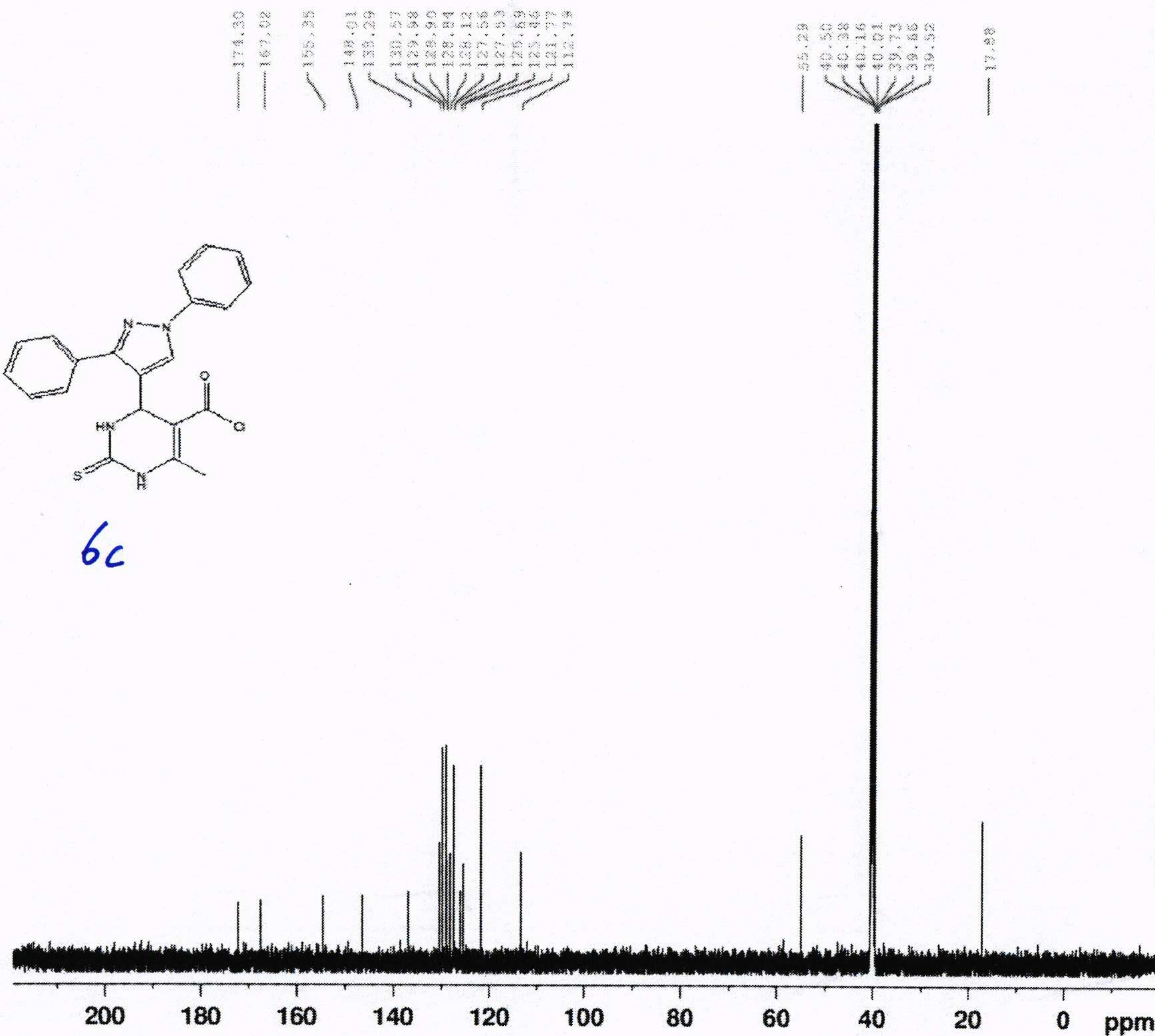




C13CPD32 DMSO D:\\ abari 44



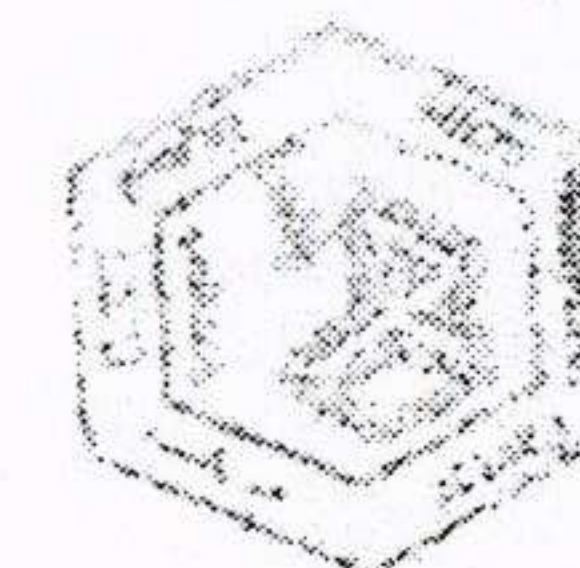
6c



NAME drshahat-9  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20210622  
 Time 12.07  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1165  
 DS 2  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912410 sec  
 RG 4597.6  
 DW 16.650 usec  
 DE 6.50 usec  
 TE 299.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 20.00 usec  
 PL1 -6.00 dB  
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.10 dB  
 PL12 13.44 dB  
 PL13 16.40 dB  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7577890 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

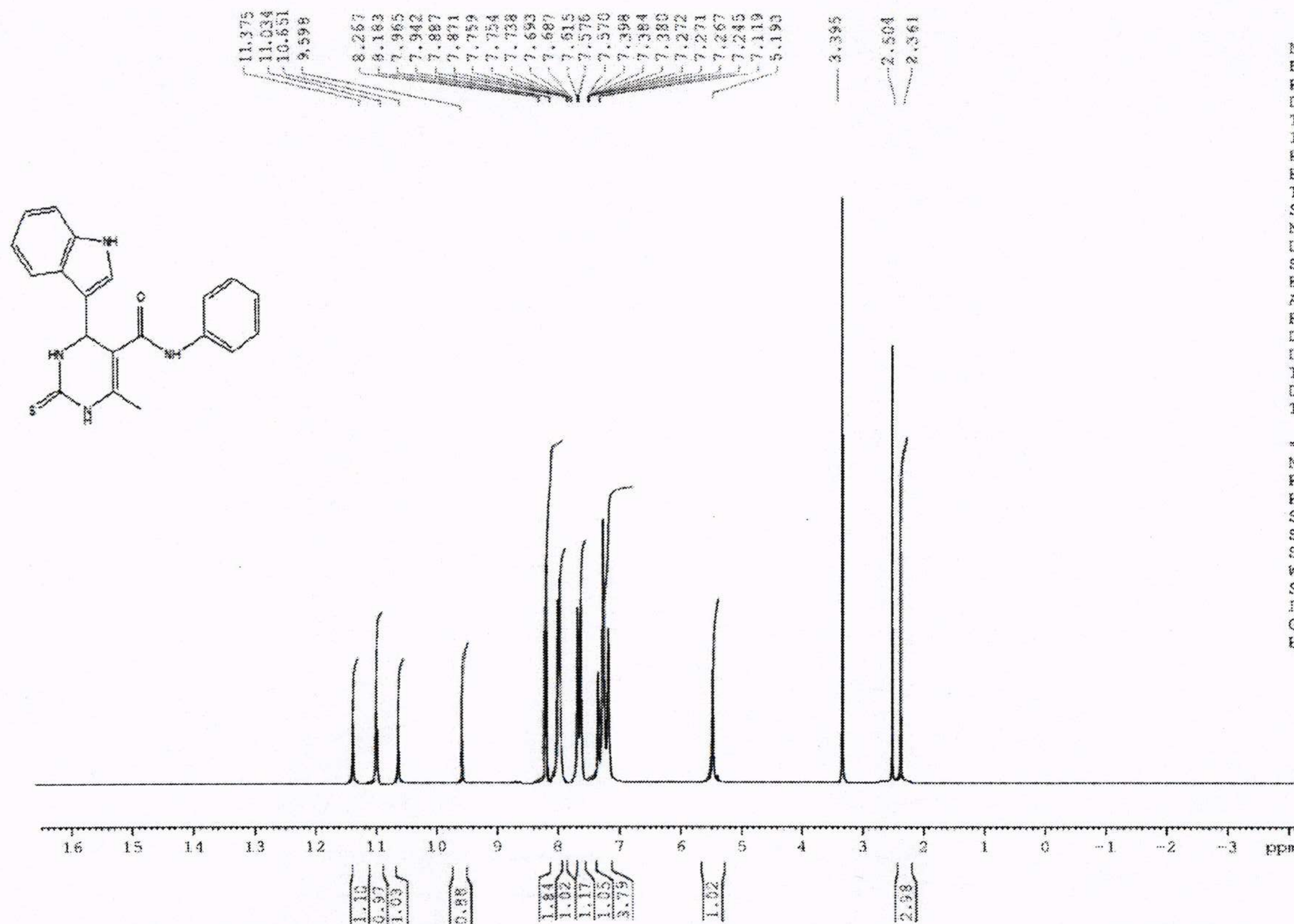




4-(1H-Indol-3-yl)-6-methyl-N-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxamide

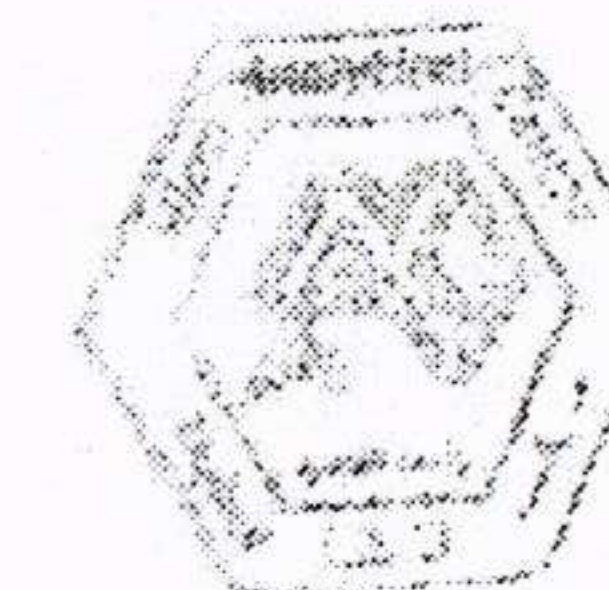
7a

ON DMSO D:\ abar



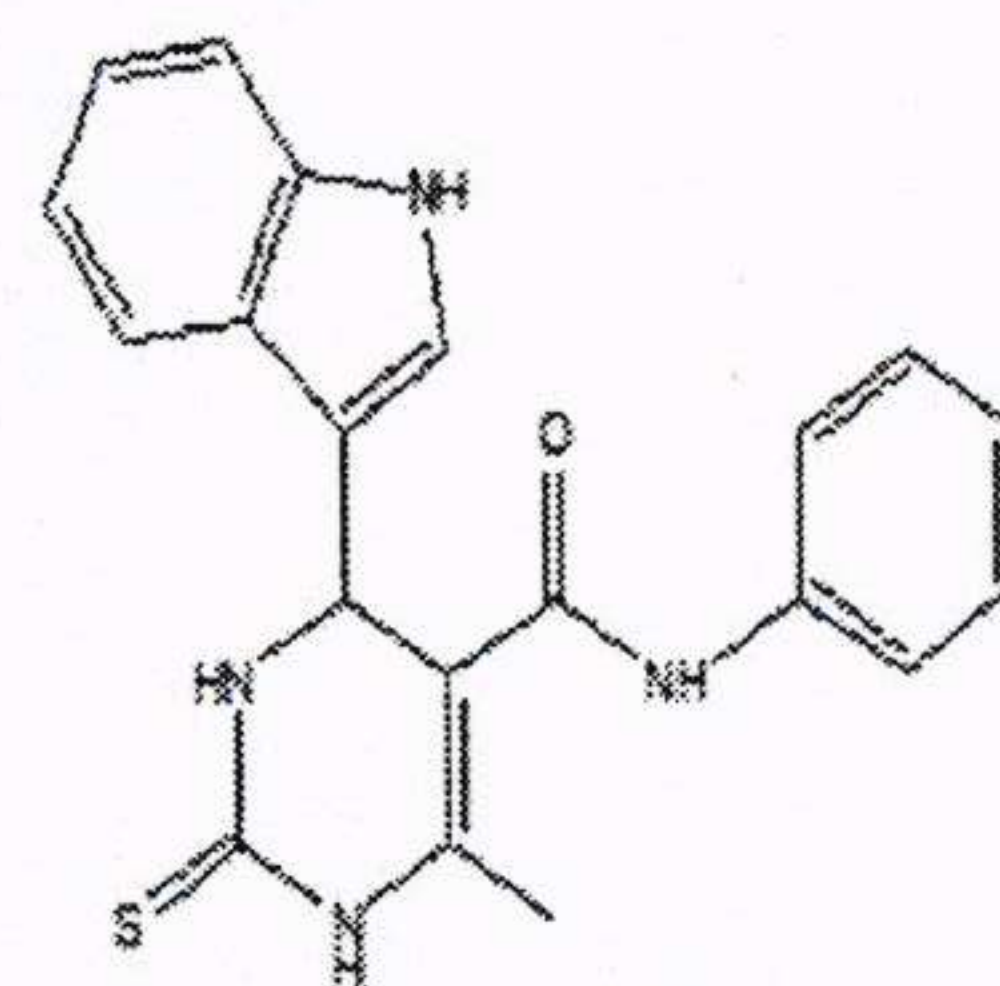
NAME drshahat-11  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20210624  
 Time 18.59  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 90.5  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.70 usec  
 PL1 -1.10 dB  
 SFO1 500.1330885 MHz  
 SI 32768  
 SF 500.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

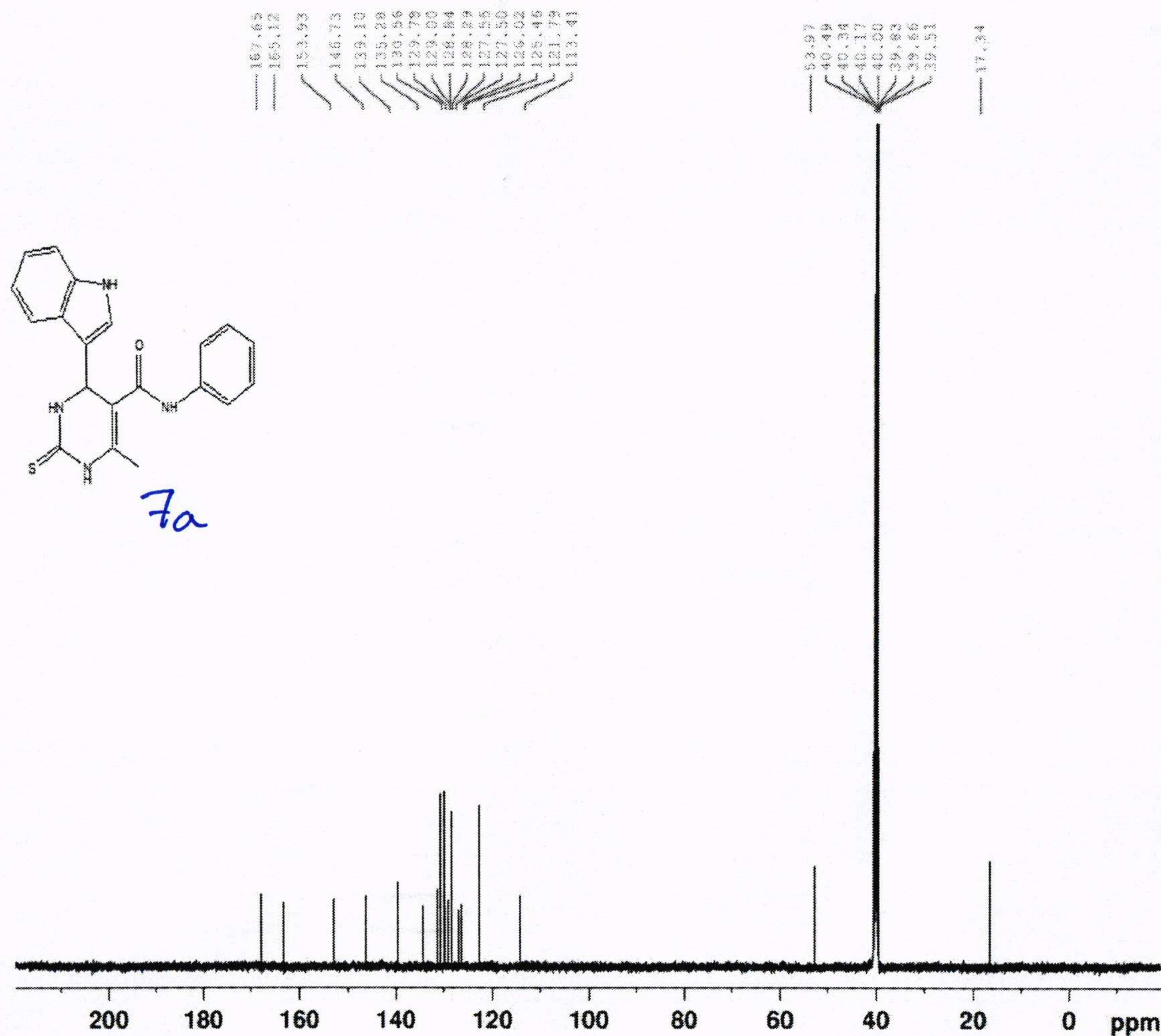




C13CPD32 DMSO D:\\ abari 46



7a



NAME drshahat-11  
EXPNO 11  
PROCNO 1  
Date\_ 20210624  
Time 20.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 2000  
DS 2  
SWH 30030.029 Hz  
FIDRES 0.458222 Hz  
AQ 1.0912410 sec  
RG 14596.5  
DW 16.650 usec  
DE 6.50 usec  
TE 299.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 20.00 usec  
PL1 -6.00 dB  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.10 dB  
PL12 13.44 dB  
PL13 16.40 dB  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7577890 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

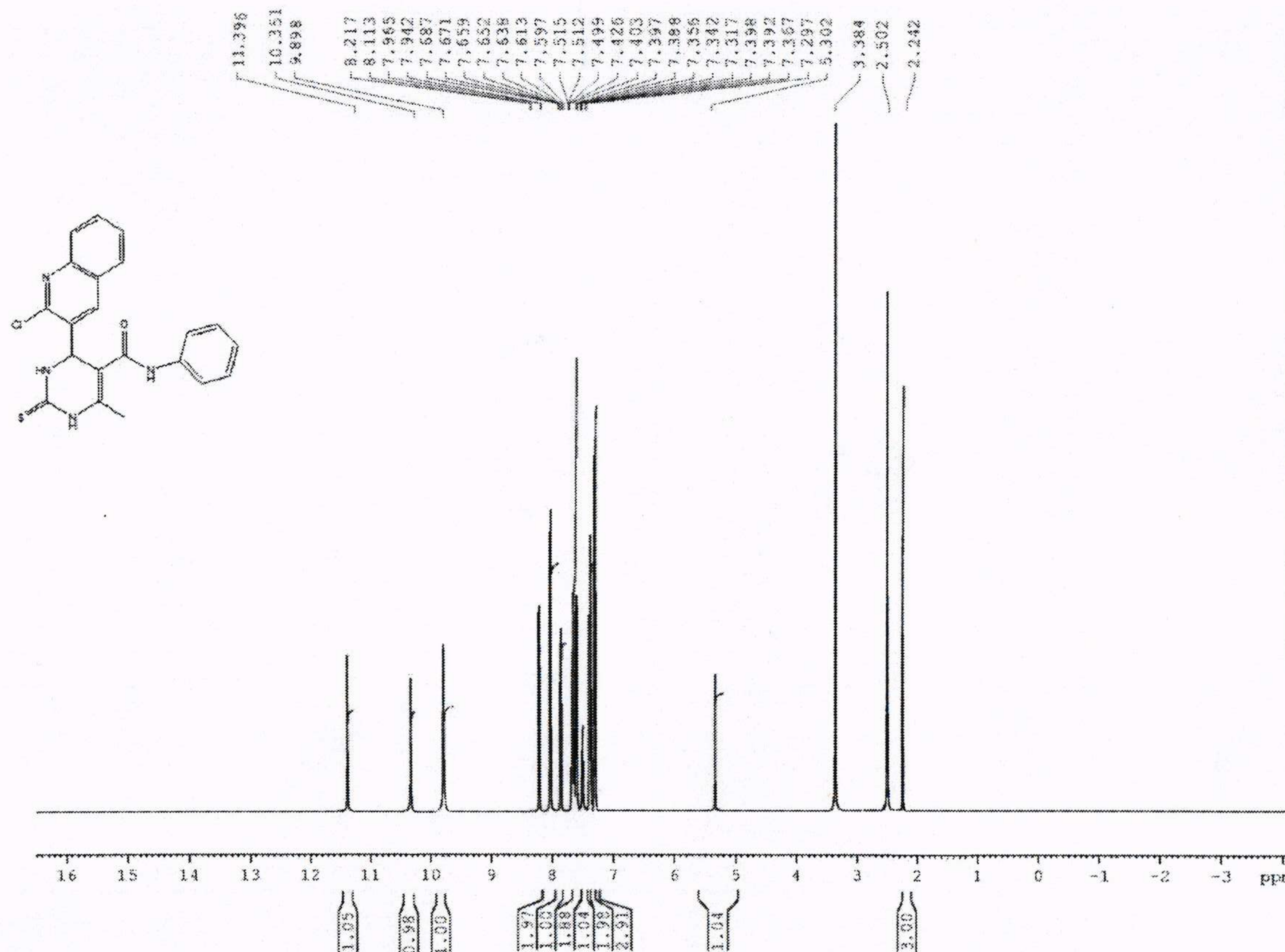




4-(2-Chloroquinolin-3-yl)-6-methyl-N-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxamide

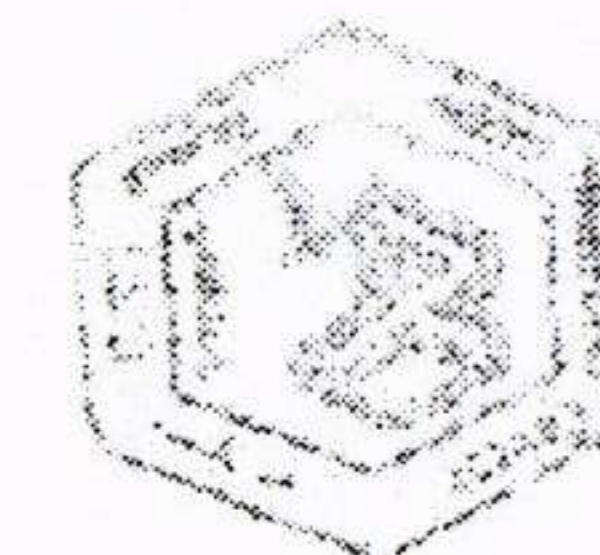
76

DN DMSO D:\ abar



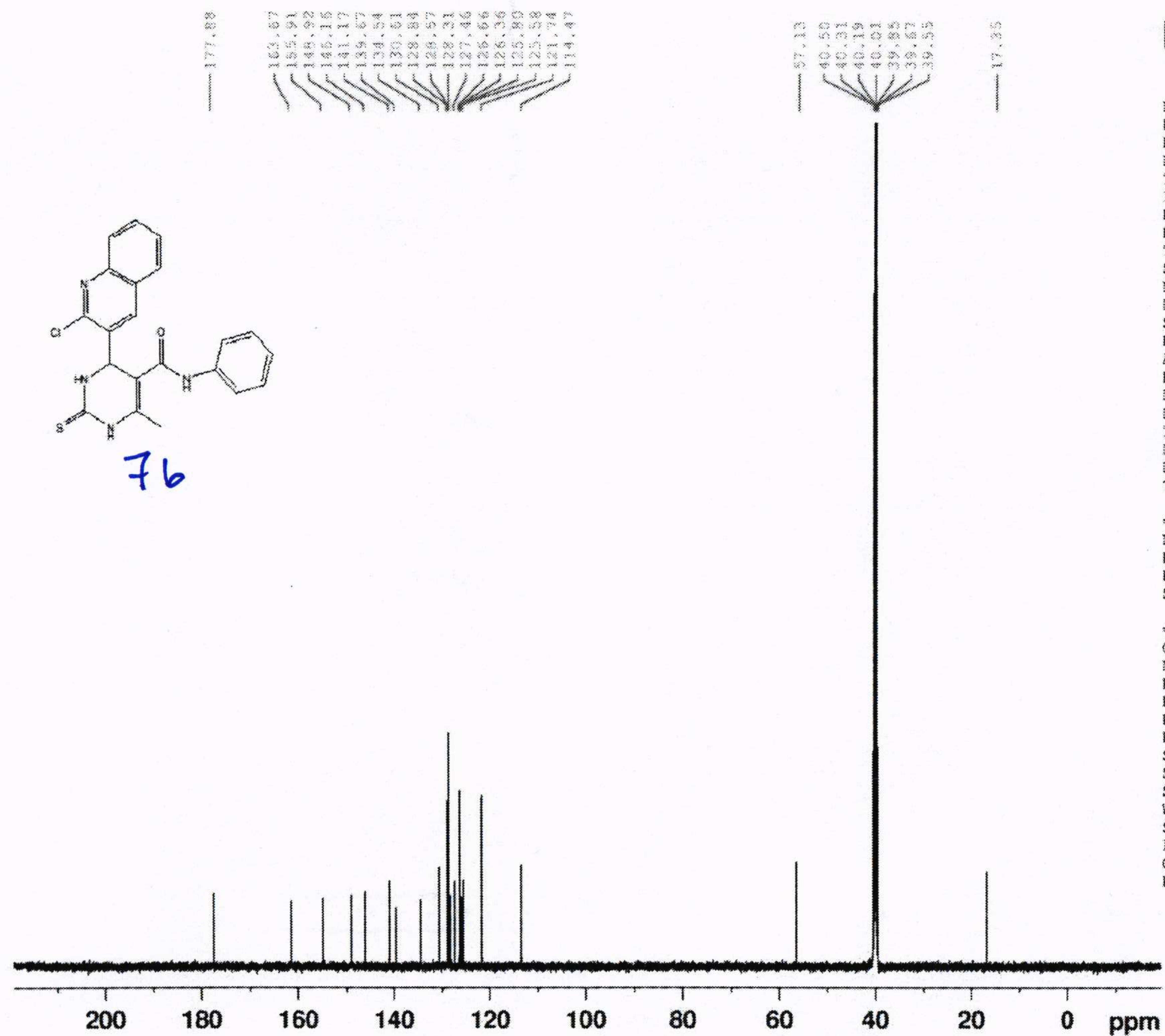
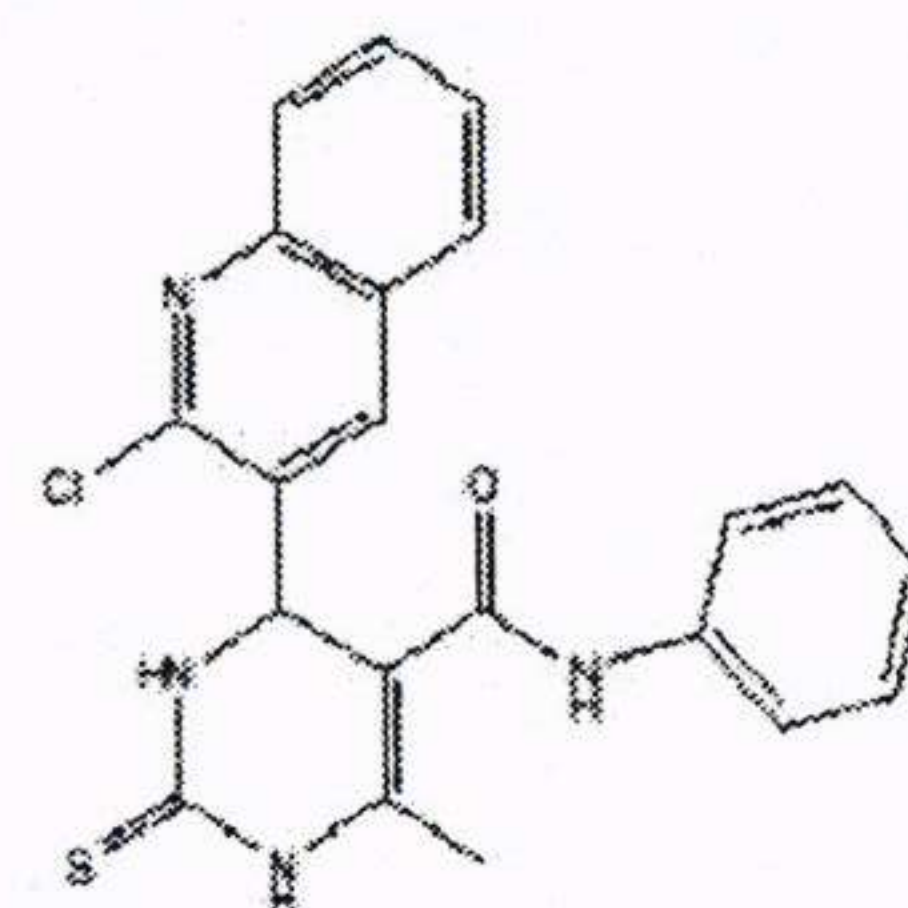
NAME drshahat-10  
EXPNO 10  
PROCNO 1  
Date\_ 20210624  
Time 18.59  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1720407 sec  
RG 90.5  
DW 48.400 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.70 usec  
PL1 -1.10 dB  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





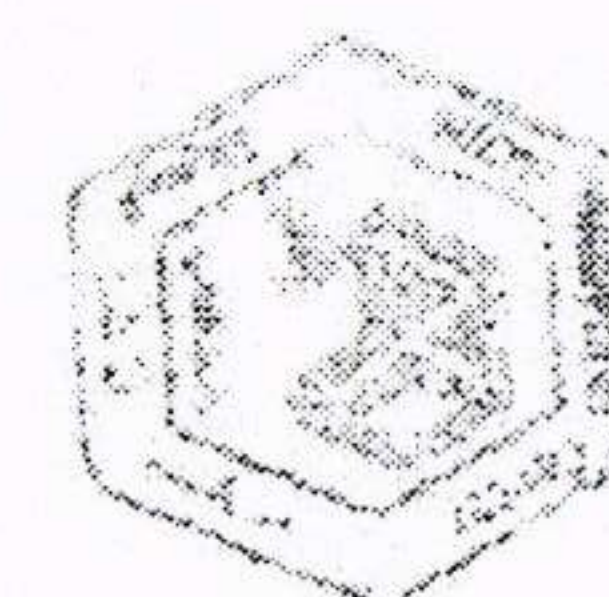
C13CPD32 DMSO D:\\ abari 46



NAME drshahat-10  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20210624  
 Time 20.47  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2000  
 DS 2  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912410 sec  
 RG 14596.5  
 DW 16.650 usec  
 DE 6.50 usec  
 TE 299.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 20.00 usec  
 PL1 -6.00 dB  
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.10 dB  
 PL12 13.44 dB  
 PL13 16.40 dB  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7577890 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





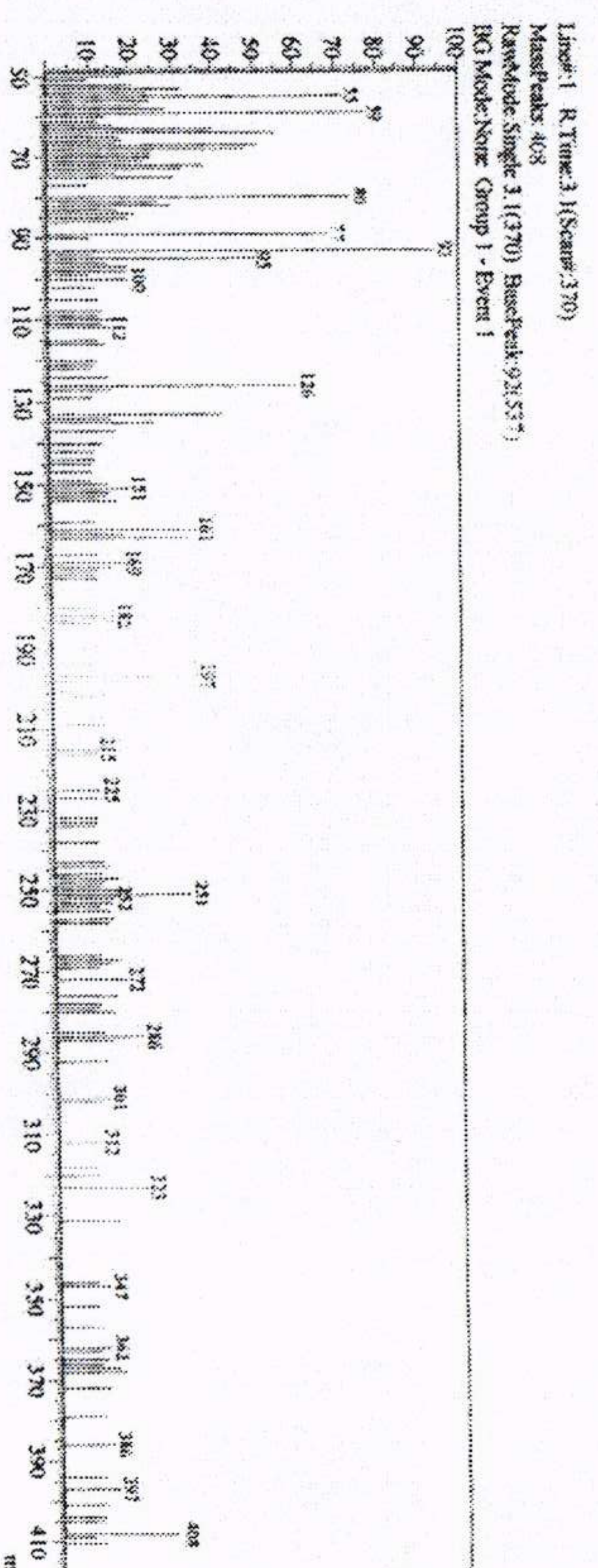
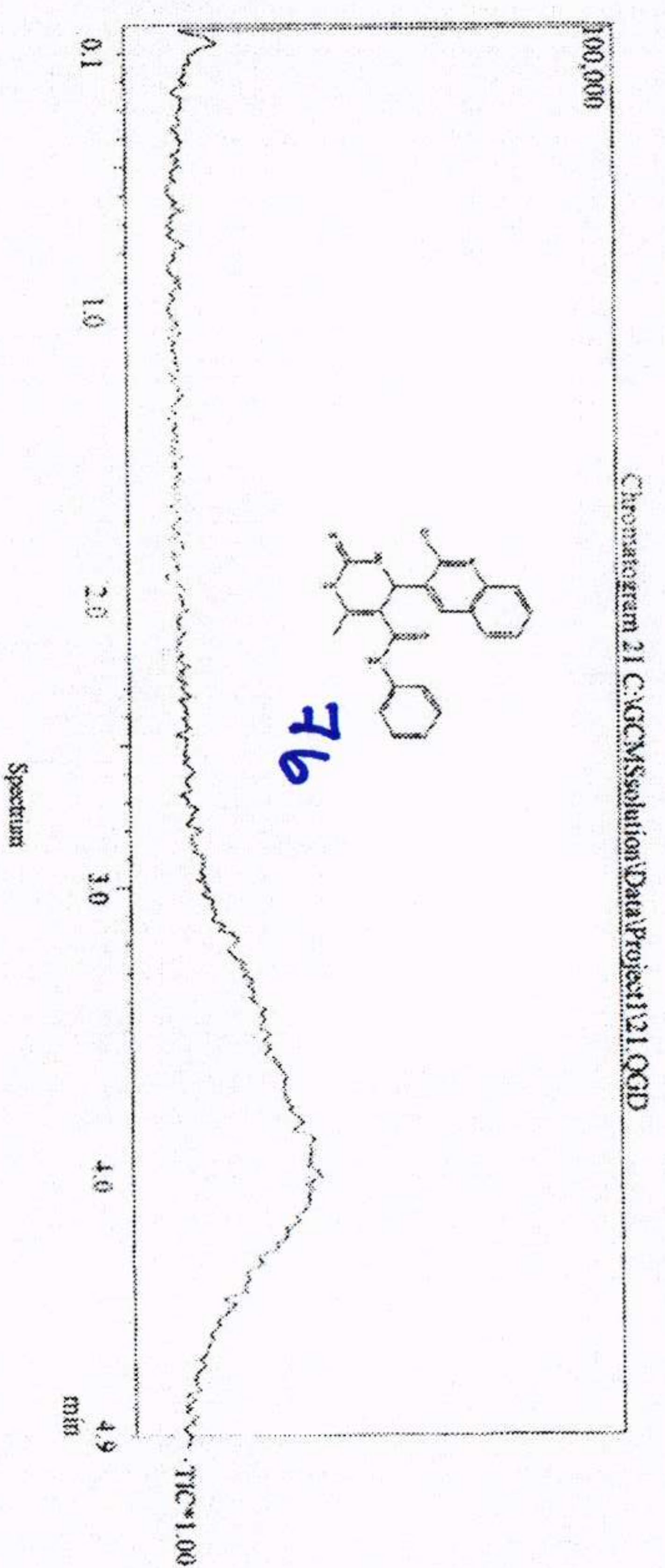
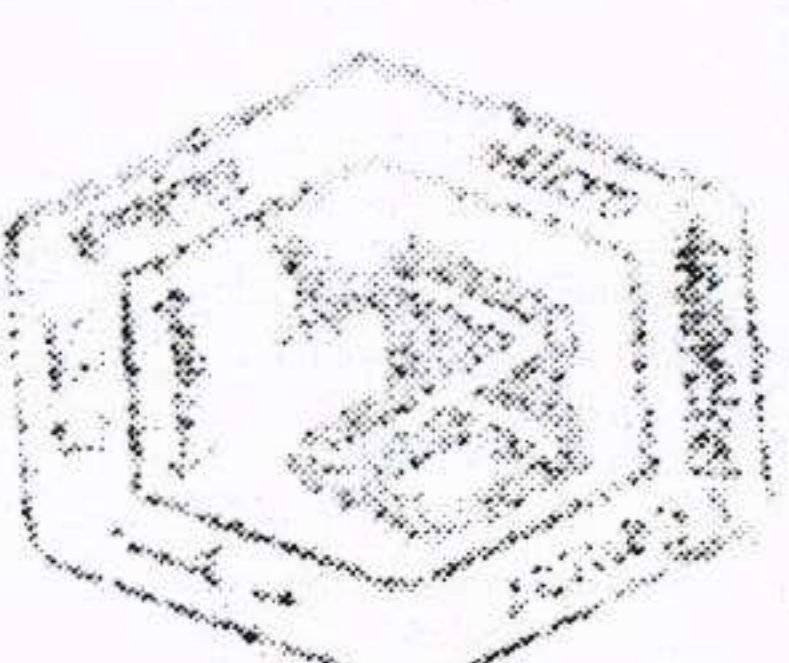
**Cairo University  
Micro Analytical Center**

**DI Analysis  
Shimadzu Qp-2010 Plus**

**Sample Information**  
 Analyzed by : Mai Younis  
 Analyzed : 22/05/2021 02:44:23 +  
 Sample Name : 10  
 Sample ID :  
 Customer Name : Dr. Moh P  
 Data File : C:\COMS\Solution\Data Project\21\QCD  
 Org Data File : C:\COMS\Solution\Data Project\21\QCD  
 Method File : C:\COMS\Solution\Data Project\21\QCD  
 Org Method File : C:\COMS\Solution\Data Project\21\QCD  
 Report File :  
 Tuning File : C:\COMS\Solution\System Tune1 \_default1.agr  
 Standard/Modified by : Mai Younis  
 Modified : 22/05/2021 02:49:22 +

**Method**  
 Analytical Line 1  
 IonSourceTemp : 250.00 °C  
 [MS Table]  
 -Group 1 - Event 1-  
 Start Time : 0.00min  
 End Time : 10.00min  
 ACQ Mode : Scan  
 Event Time : 0.50sec  
 Scan Speed : 1000  
 Start m/z : 50.00  
 End m/z : 500.00

**Electron Voltage** : 70 eV  
**Ionization Mode** : EI



**Mass Table**  
 Line# 1 R Time:3.11(Scan#370)  
 MassPeaks: 408  
 RawMode: Single 3.1(370) BasePeak: 92(537)  
 BG Mode: None (Group 1 - Event 1)

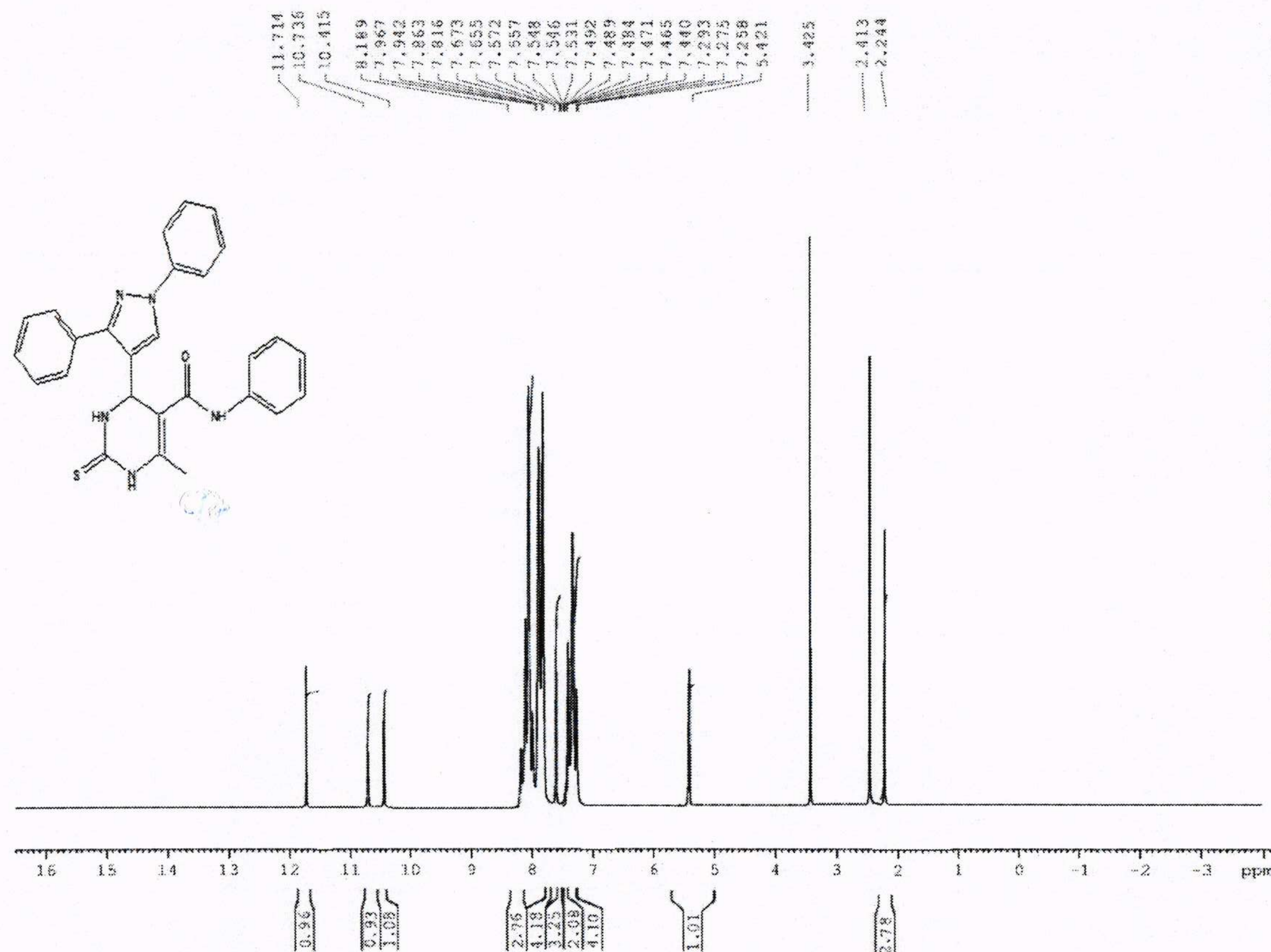
#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	97	18.06	4	53.00	177	32.96	7	56.00	135	25.14
2	51.00	52	9.68	5	54.00	127	23.65	8	57.00	122	22.72
3	52.00	110	20.48	6	55.00	386	71.88	9	58.00	154	28.68



4-(1,3-Diphenyl-1H-pyrazol-4-yl)-6-methyl-N-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxamide

7c

DN DMSO D:\ abar



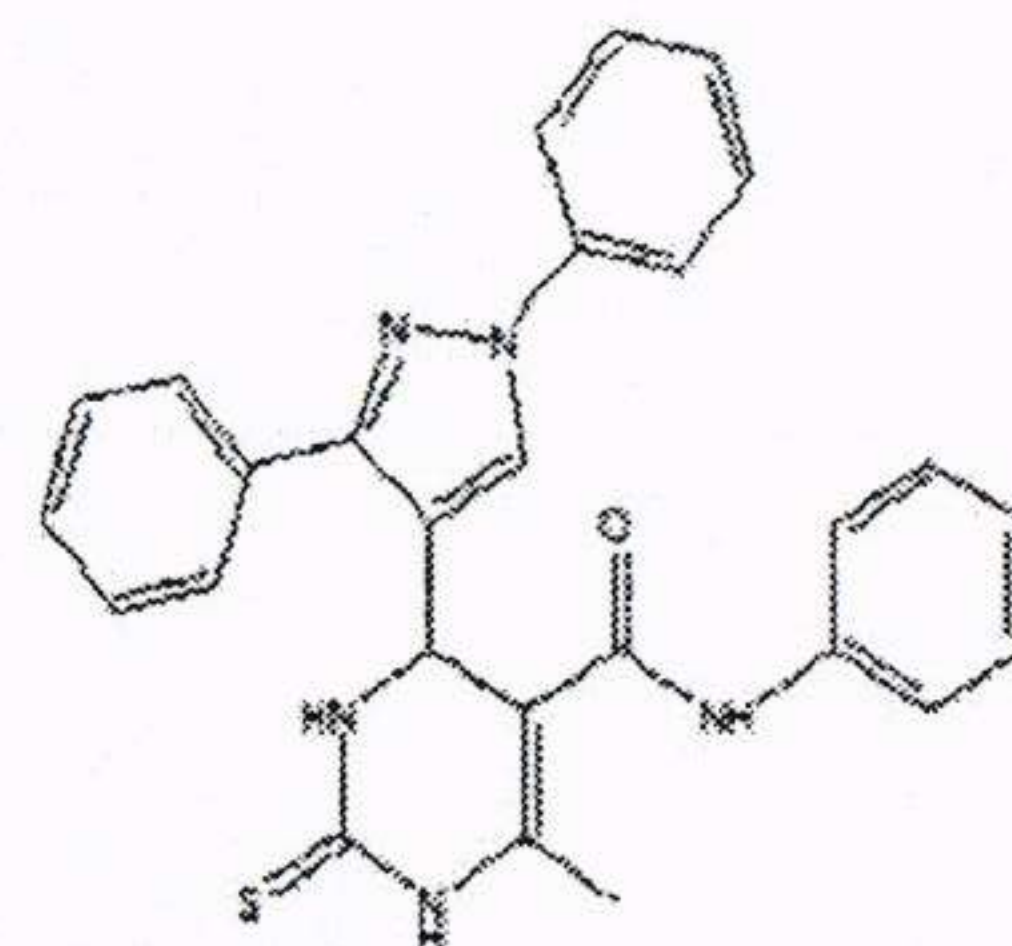
NAME drshahat-12  
EXPNO 10  
PROCNO 1  
Date\_ 20210624  
Time 11.17  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1720407 sec  
RG 128  
DW 48.400 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.70 usec  
PL1 -1.10 dB  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

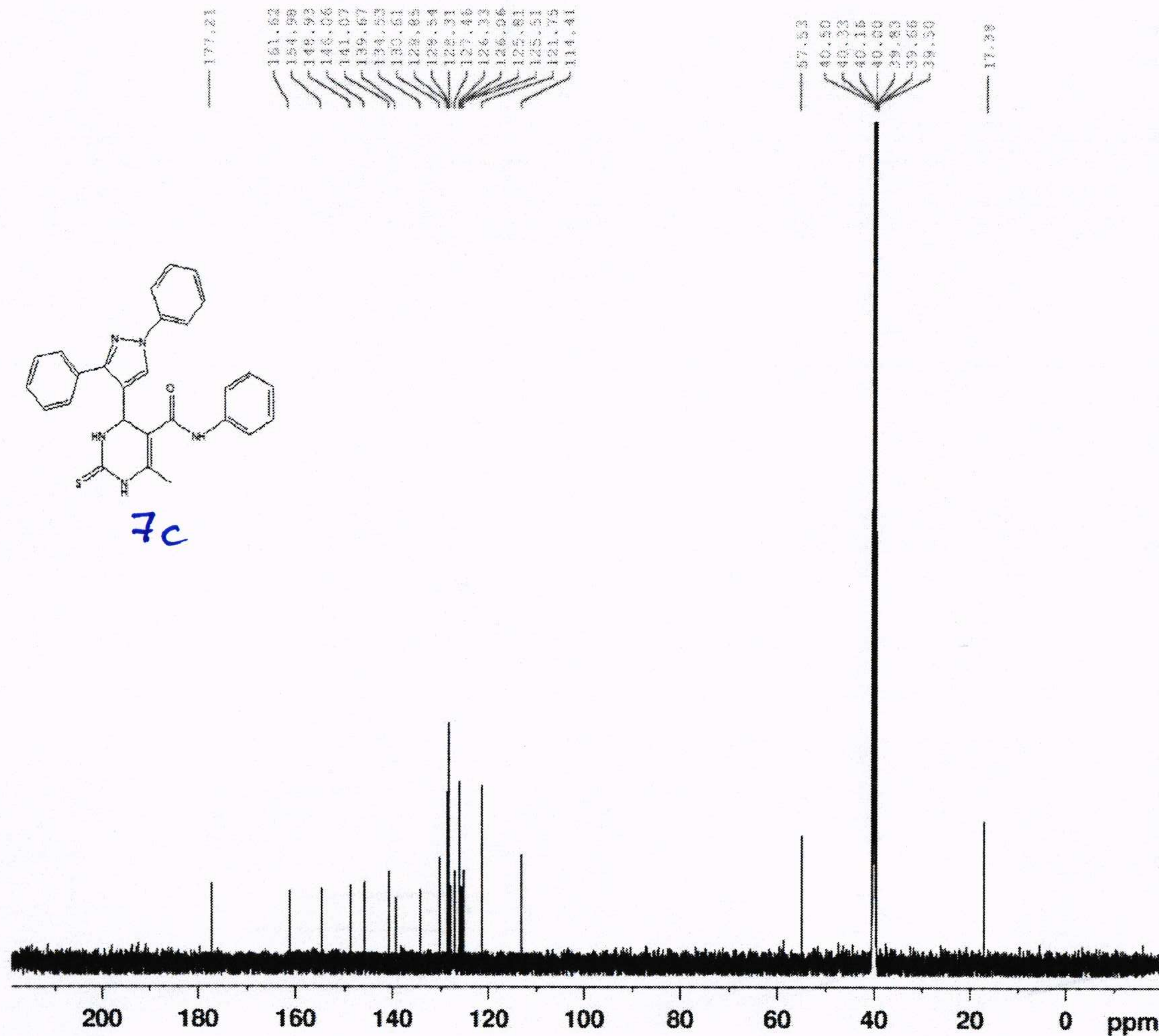




C13CPD32 DMSO D:\\ abari 44



7c



NAME drshahat-12  
EXPNO 11  
PROCNO 1  
Date\_ 20210624  
Time 12.07  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 1165  
DS 2  
SWH 30030.029 Hz  
FIDRES 0.458222 Hz  
AQ 1.0912410 sec  
RG 4597.6  
DW 16.650 usec  
DE 6.50 usec  
TE 299.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 20.00 usec  
PL1 -6.00 dB  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.10 dB  
PL12 13.44 dB  
PL13 16.40 dB  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7577890 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





4-(1H-Indol-3-yl)-6-methyl-2-thioxo-N-p-tolyl-1,2,3,4-tetrahydropyrimidine-5-carboxamide

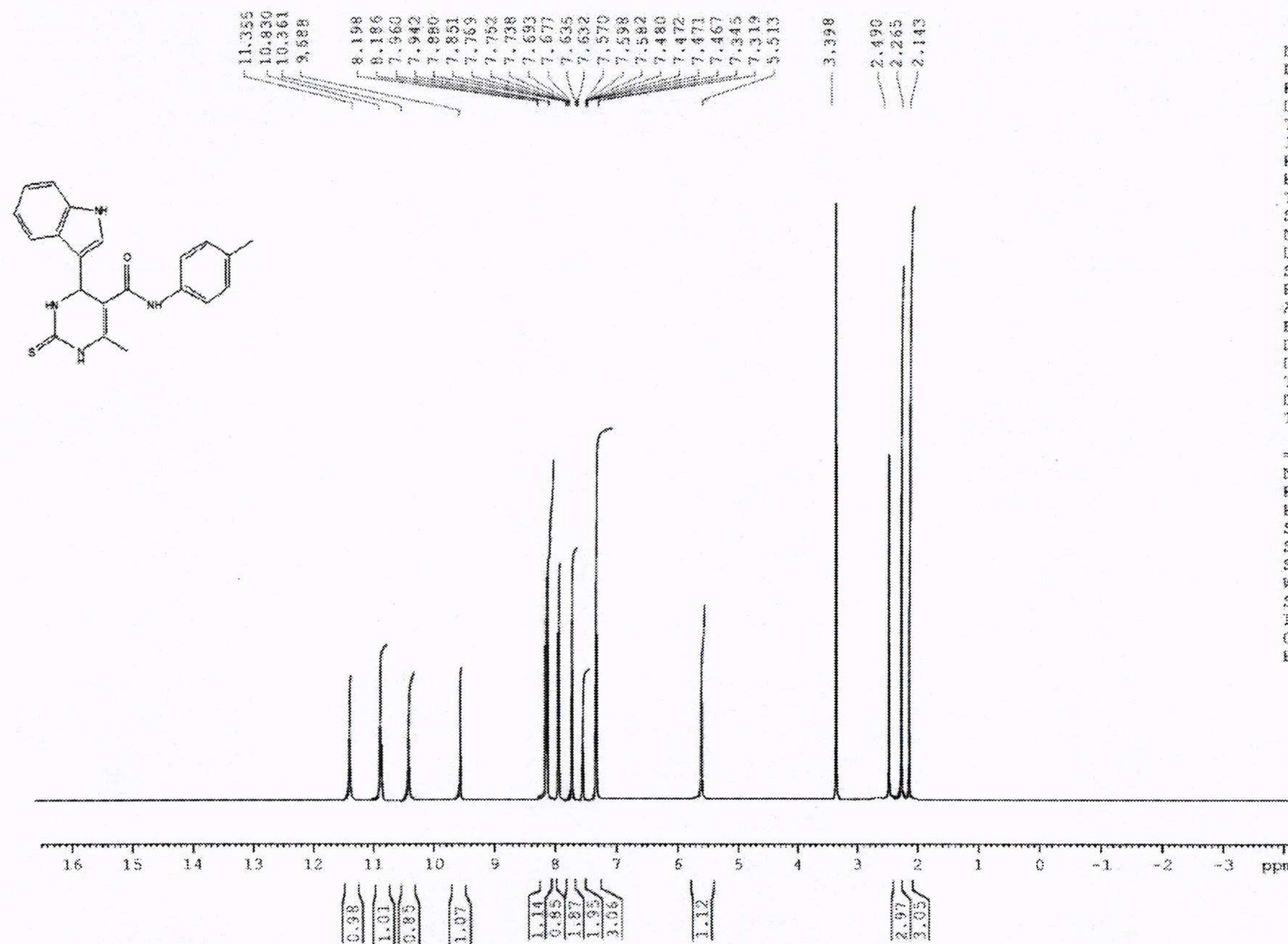
8a

DN DMSO D:\ abar



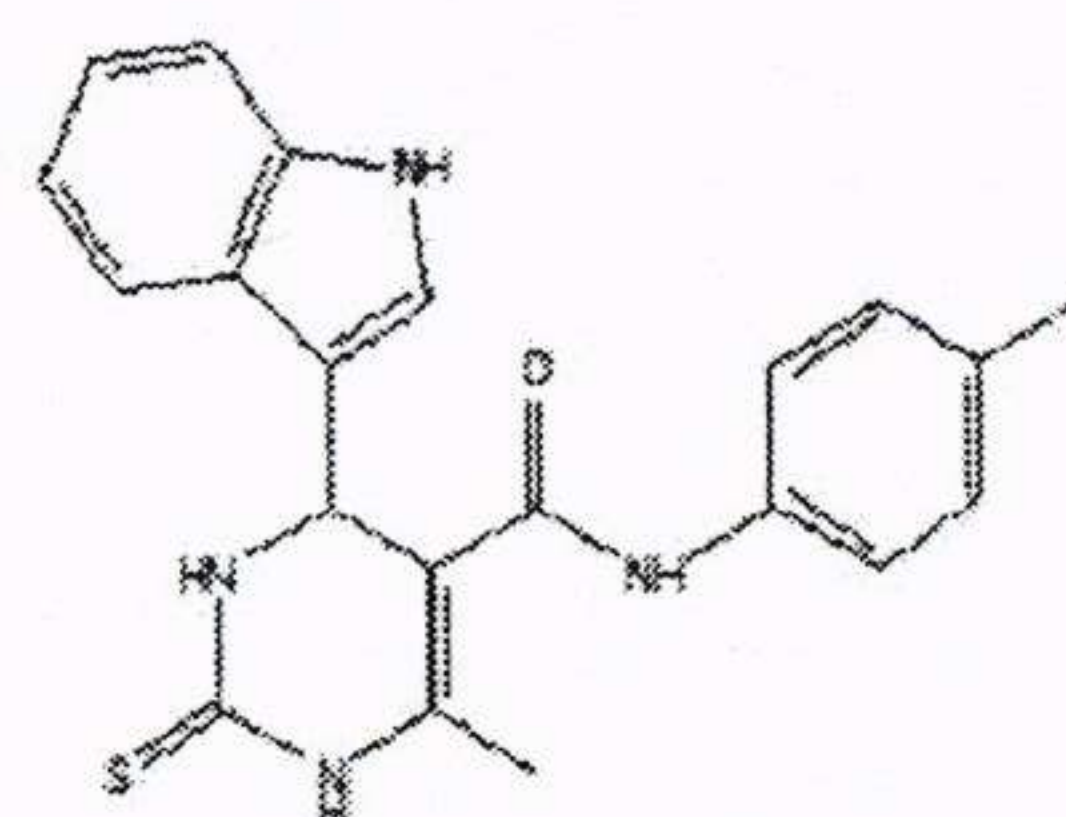
NAME drshahat-14  
EXPNO 10  
PROCNO 1  
Date\_ 20210624  
Time 18.59  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1720407 sec  
RG 90.5  
DW 48.400 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.70 usec  
PL1 -1.10 dB  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

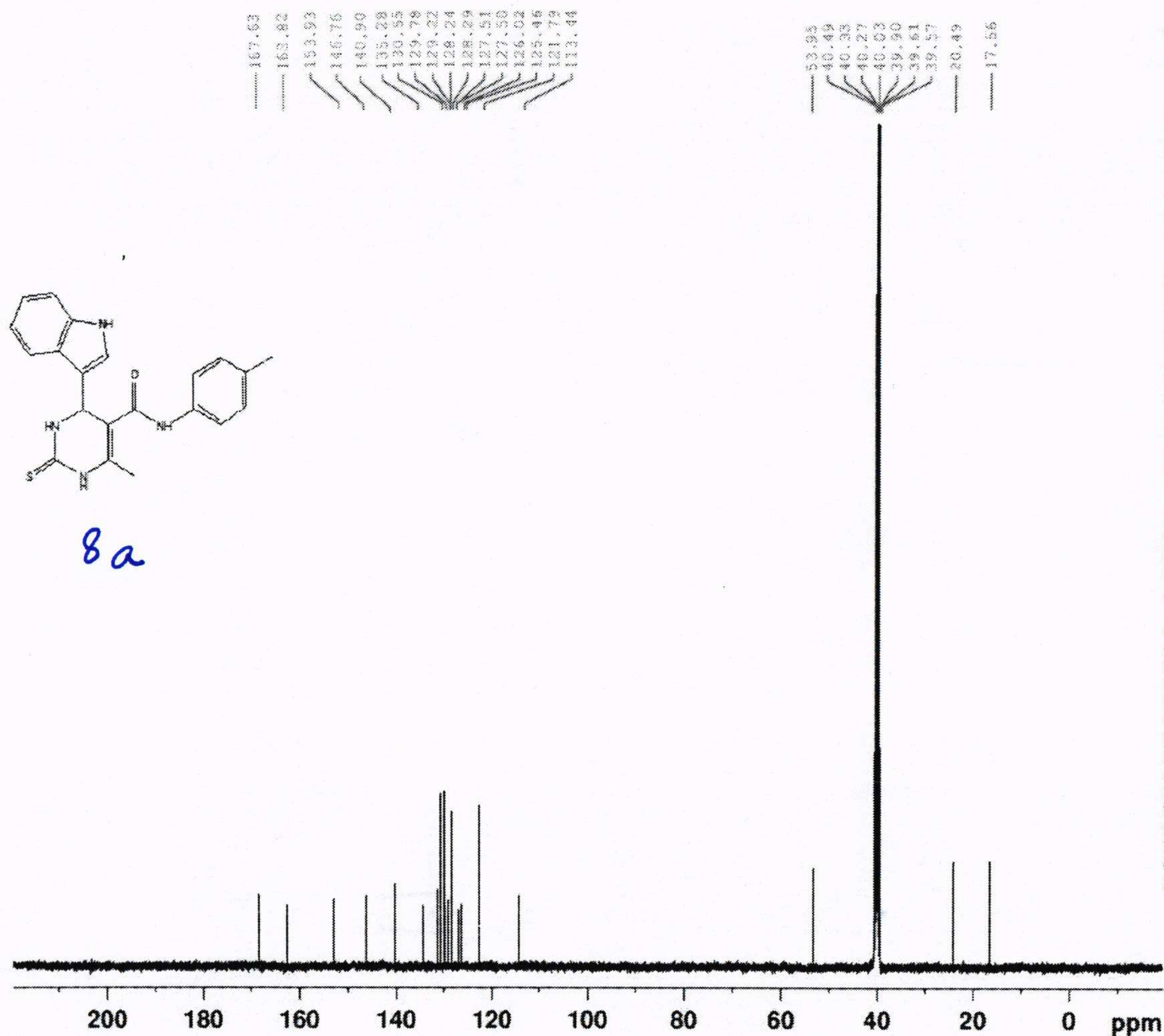




C13CPD32 DMSO D:\\ abari 46



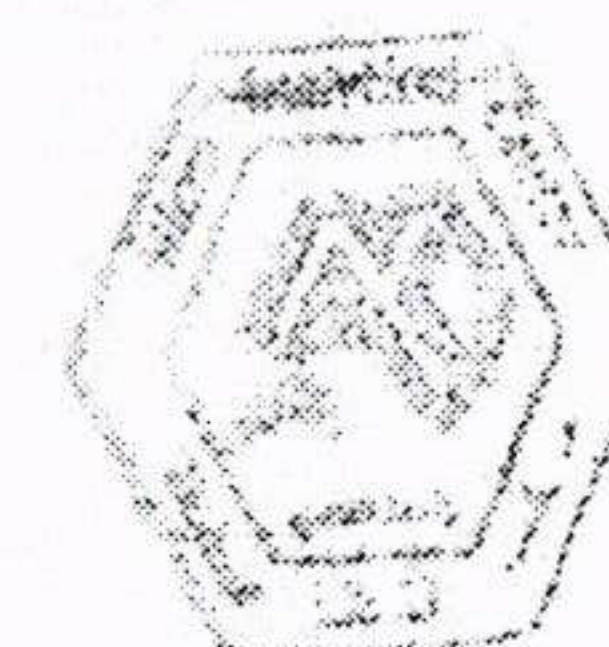
8a



NAME drshahat-14  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20210624  
 Time 20.47  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2000  
 DS 2  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912410 sec  
 RG 14596.5  
 DW 16.650 usec  
 DE 6.50 usec  
 TE 299.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 20.00 usec  
 PL1 -6.00 dB  
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.10 dB  
 PL12 13.44 dB  
 PL13 16.40 dB  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7577890 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

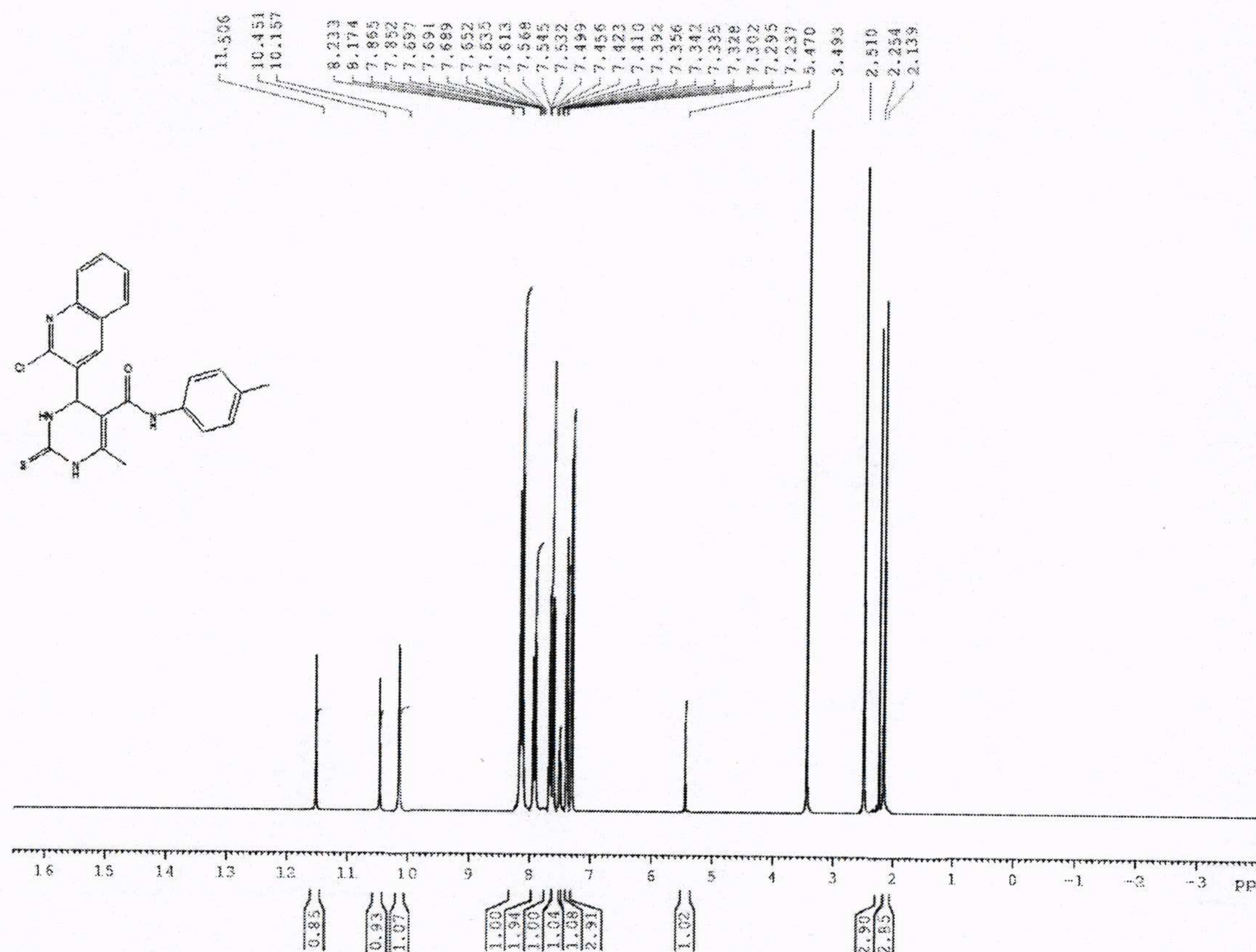




4-(2-Chloroquinolin-3-yl)-6-methyl-2-thioxo-N-p-tolyl-1,2,3,4-tetrahydropyrimidine-5-carboxamide

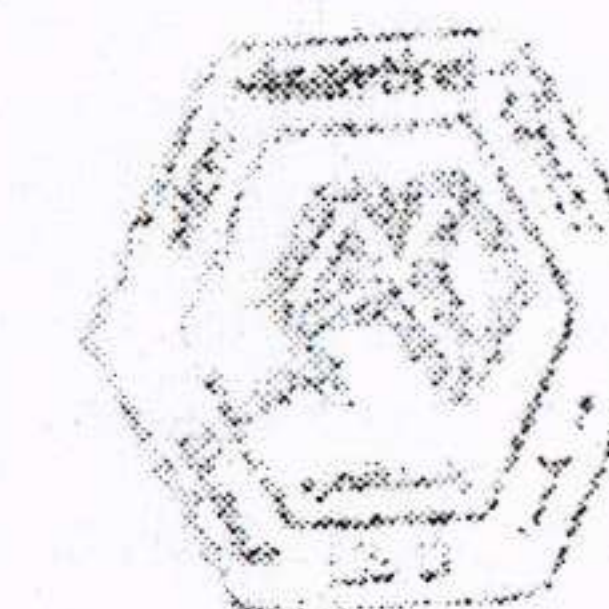
86

DN DMSO D:\ abar



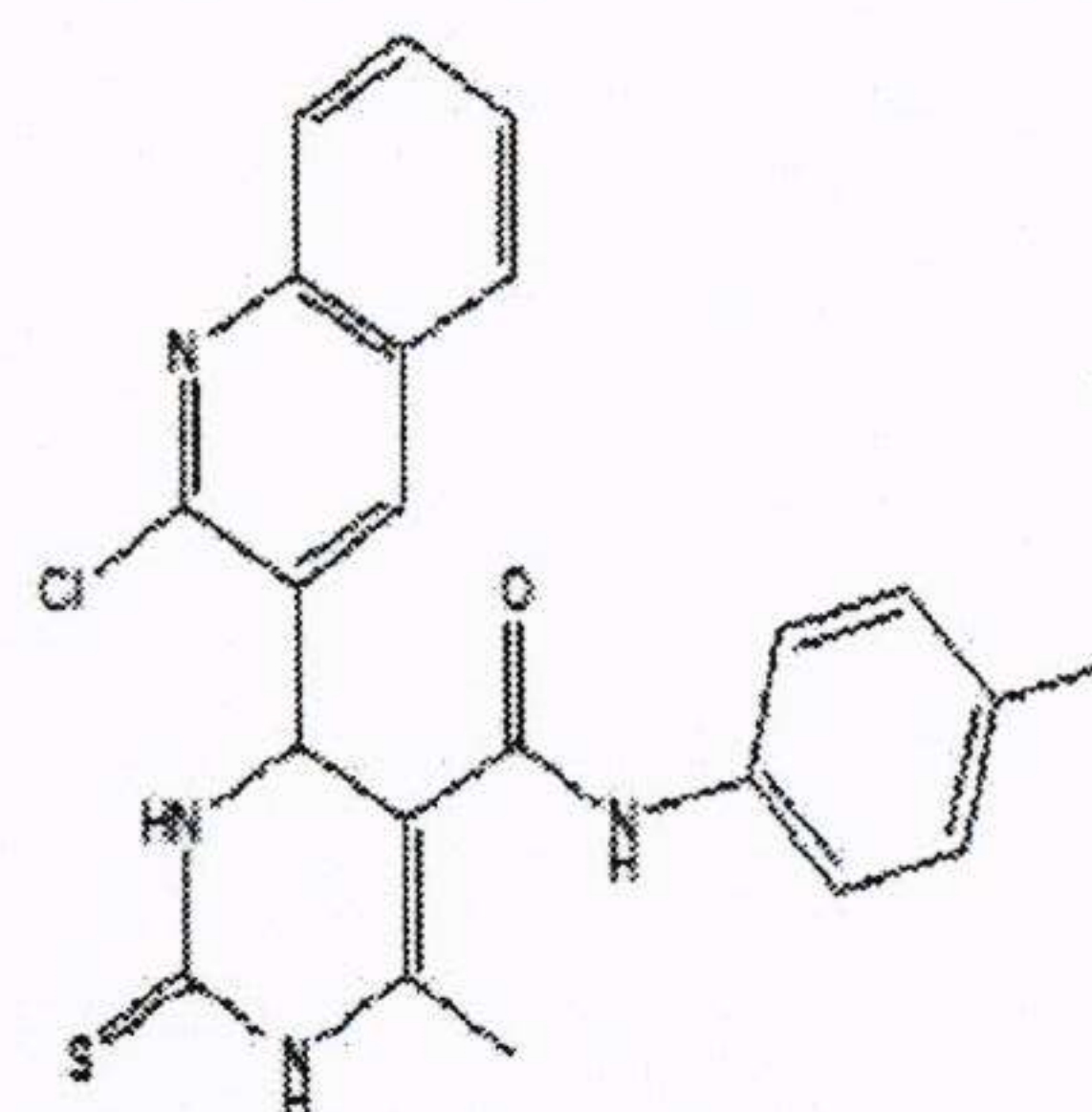
NAME dirshahat-13  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20210623  
 Time 18.59  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 90.5  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 1.00000000 sec  
 ID0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.70 usec  
 PL1 -1.10 dB  
 SFO1 500.1330885 MHz  
 SI 32768  
 SF 500.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

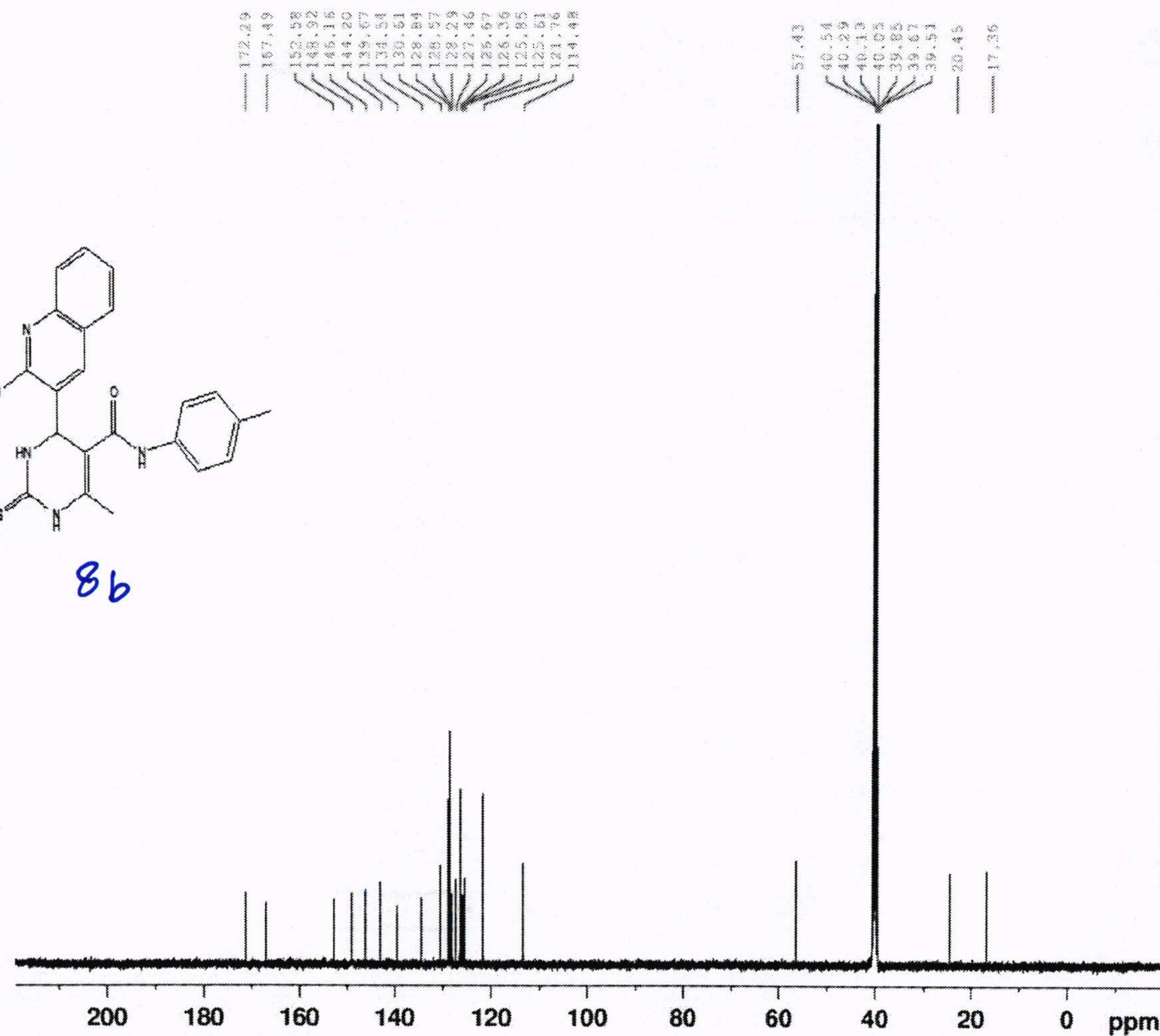




C13CPD32 DMSO D:\\ abari 46



8b



NAME drshahat-13  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20210623  
 Time 20.47  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2000  
 DS 2  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912410 sec  
 RG 14596.5  
 DW 16.650 usec  
 DE 6.50 usec  
 TE 299.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 20.00 usec  
 PL1 -6.00 dB  
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.10 dB  
 PL12 13.44 dB  
 PL13 16.40 dB  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7577890 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

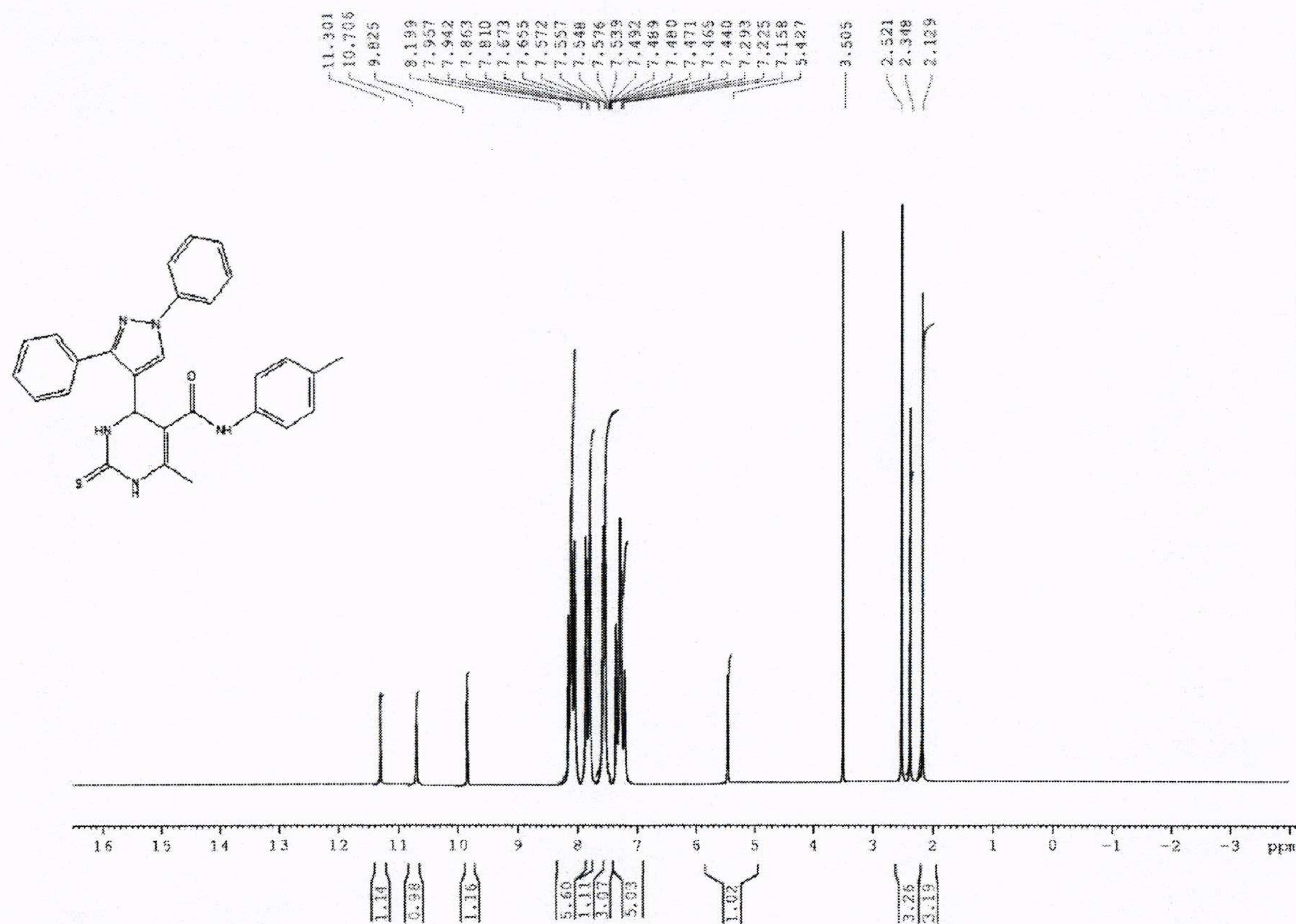




4-(1,3-Diphenyl-1H-pyrazol-4-yl)-6-methyl-2-thioxo-N-p-tolyl-1,2,3,4-tetrahydropyrimidine-5-carboxamide

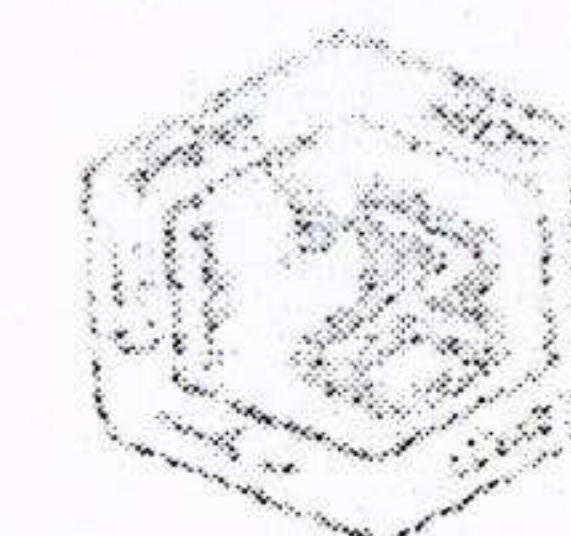
8c

DN DMSO D:\ abar



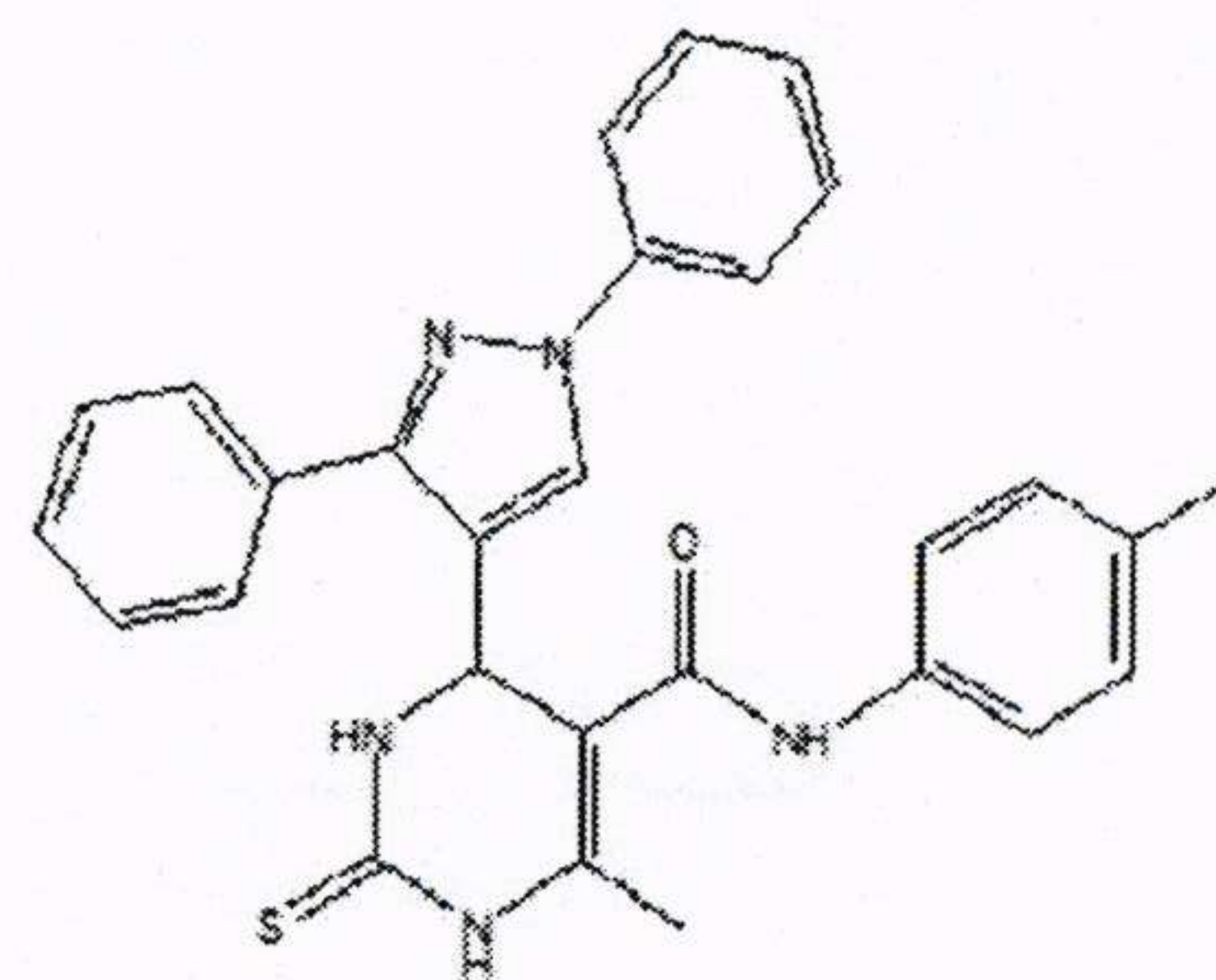
NAME drshahat-15  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20210622  
 Time 11.17  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 128  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.70 usec  
 PL1 -1.10 dB  
 SFO1 500.1330885 MHz  
 SI 32768  
 SF 500.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



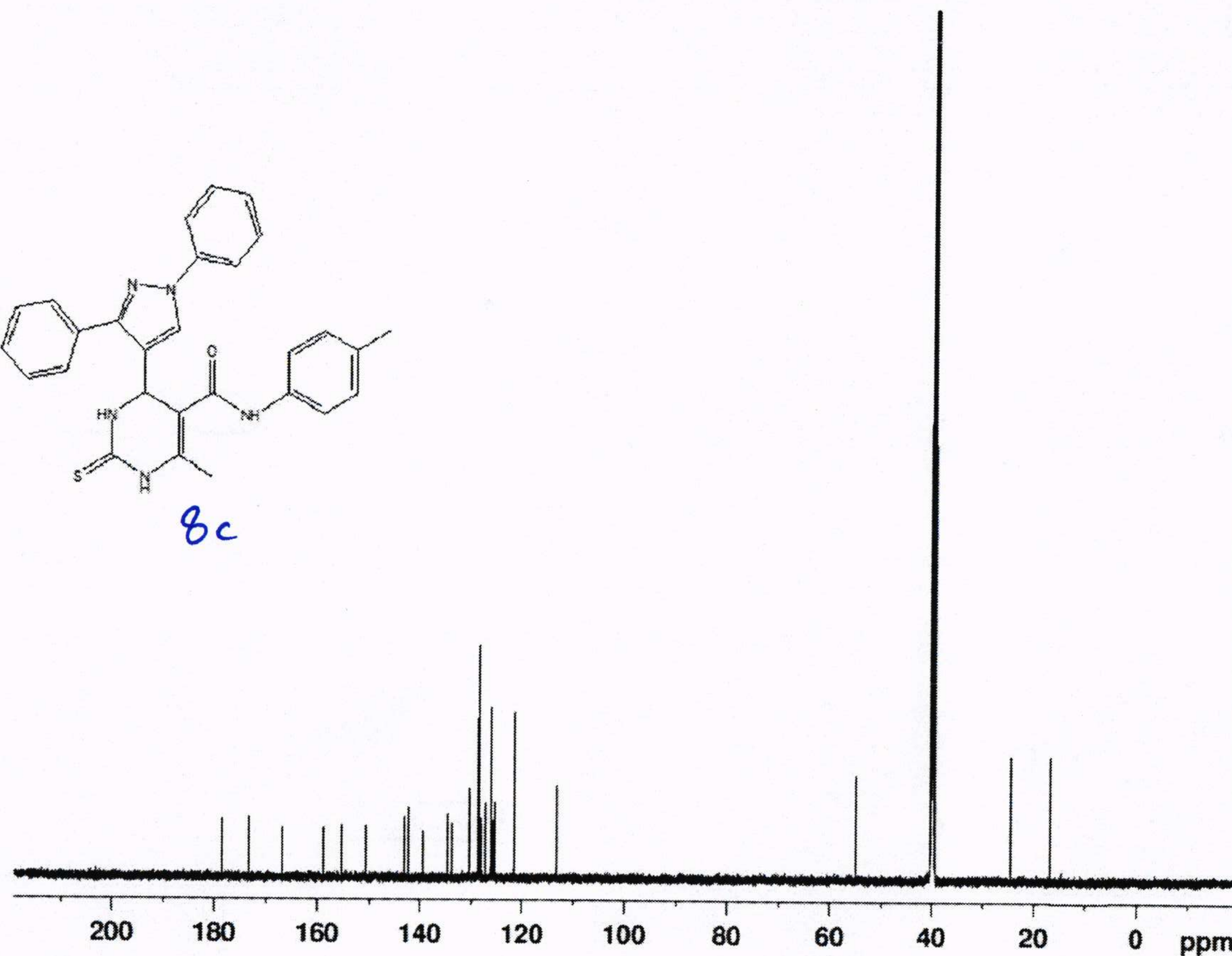


C13CPD32 DMSO D:\\ abari 44



178.69  
174.12  
168.11  
159.90  
155.16  
151.07  
143.67  
142.06  
141.17  
139.67  
138.53  
138.51  
128.82  
128.58  
128.35  
127.47  
126.23  
126.18  
125.94  
125.52  
121.77  
113.15

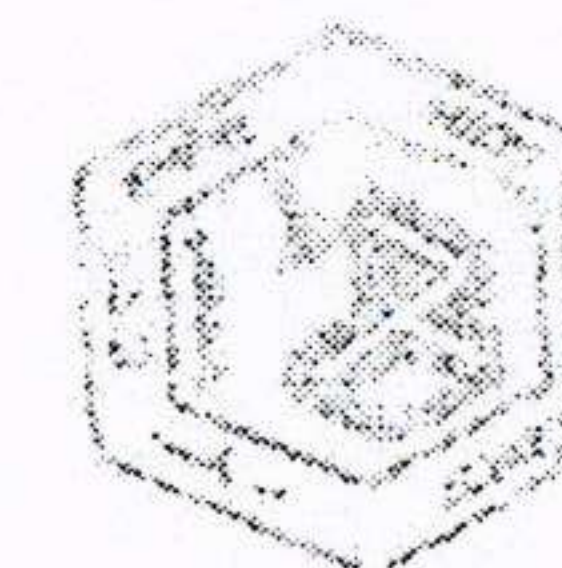
57.87  
40.48  
40.43  
40.18  
40.01  
39.83  
39.35  
39.25  
23.55  
17.96



NAME drshahat-15  
EXPNO 11  
PROCNO 1  
Date\_ 20210622  
Time 12.07  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 1165  
DS 2  
SWH 30030.029 Hz  
FIDRES 0.458222 Hz  
AQ 1.0912410 sec  
RG 4597.6  
DW 16.650 usec  
DE 6.50 usec  
TE 299.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 20.00 usec  
PL1 -6.00 dB  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.10 dB  
PL12 13.44 dB  
PL13 16.40 dB  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7577890 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

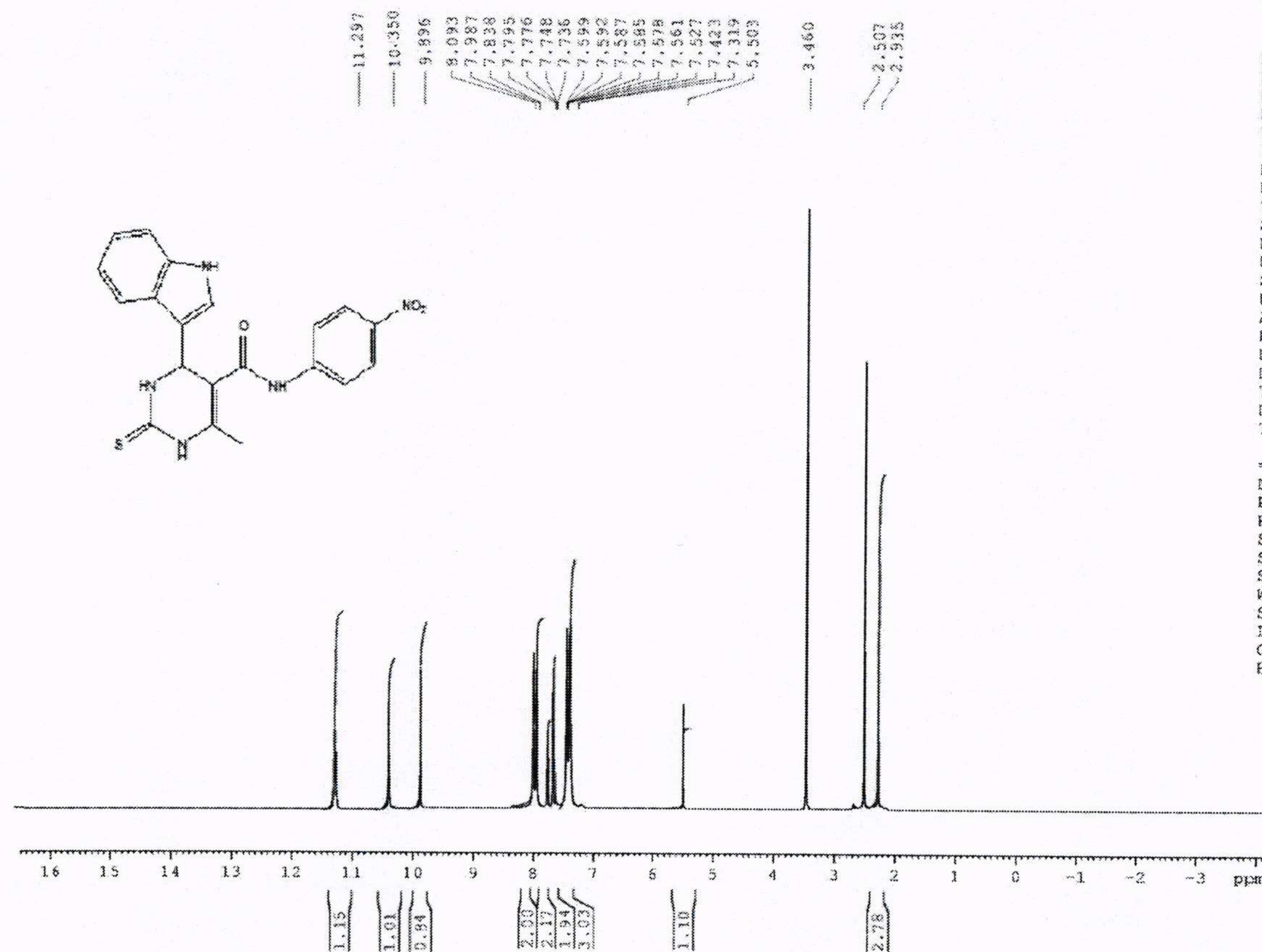




4-(1H-Indol-3-yl)-6-methyl-N-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxamide

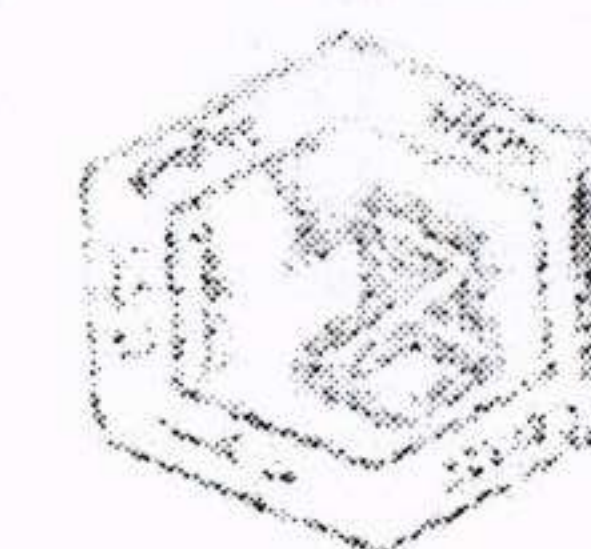
9a

ON DMSO D:\ abar



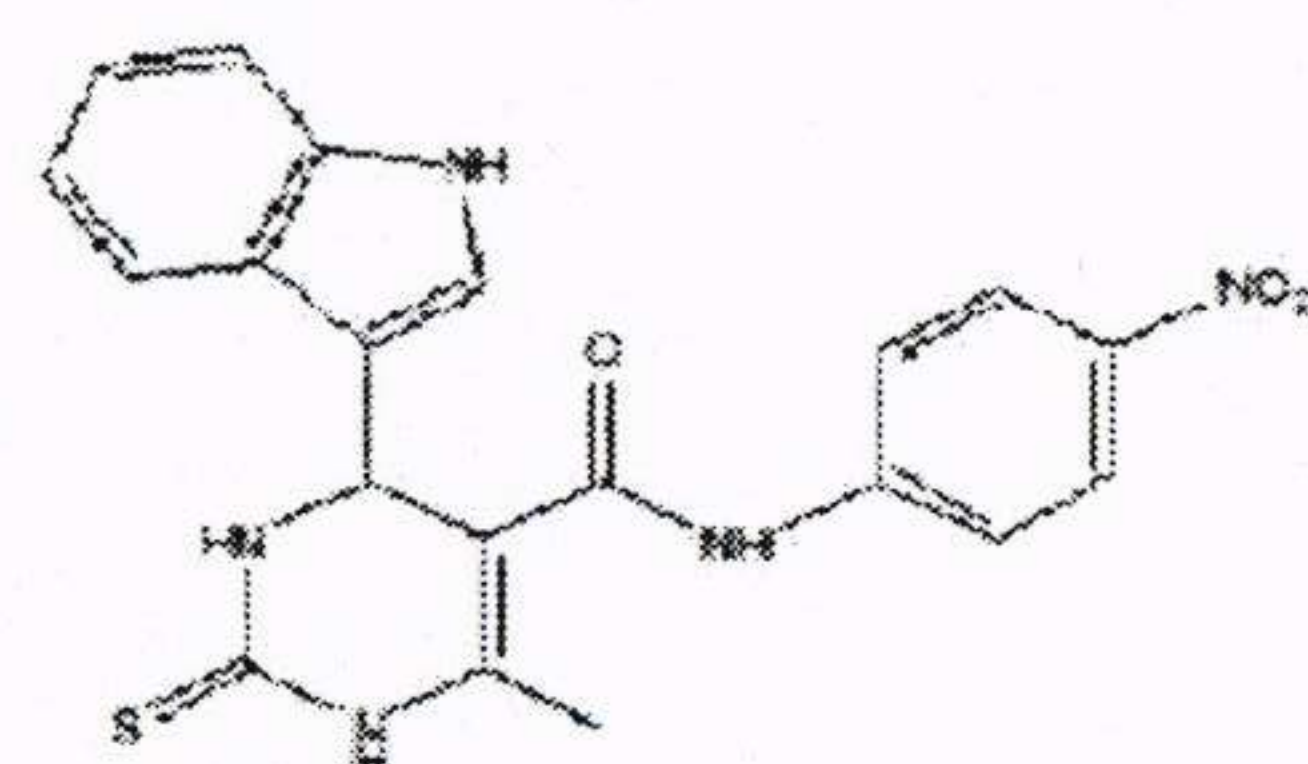
NAME drshahat-17  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20210622  
 Time 18.59  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 90.5  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.70 usec  
 PL1 -1.10 dB  
 SFO1 500.1330885 MHz  
 SI 32768  
 SF 500.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

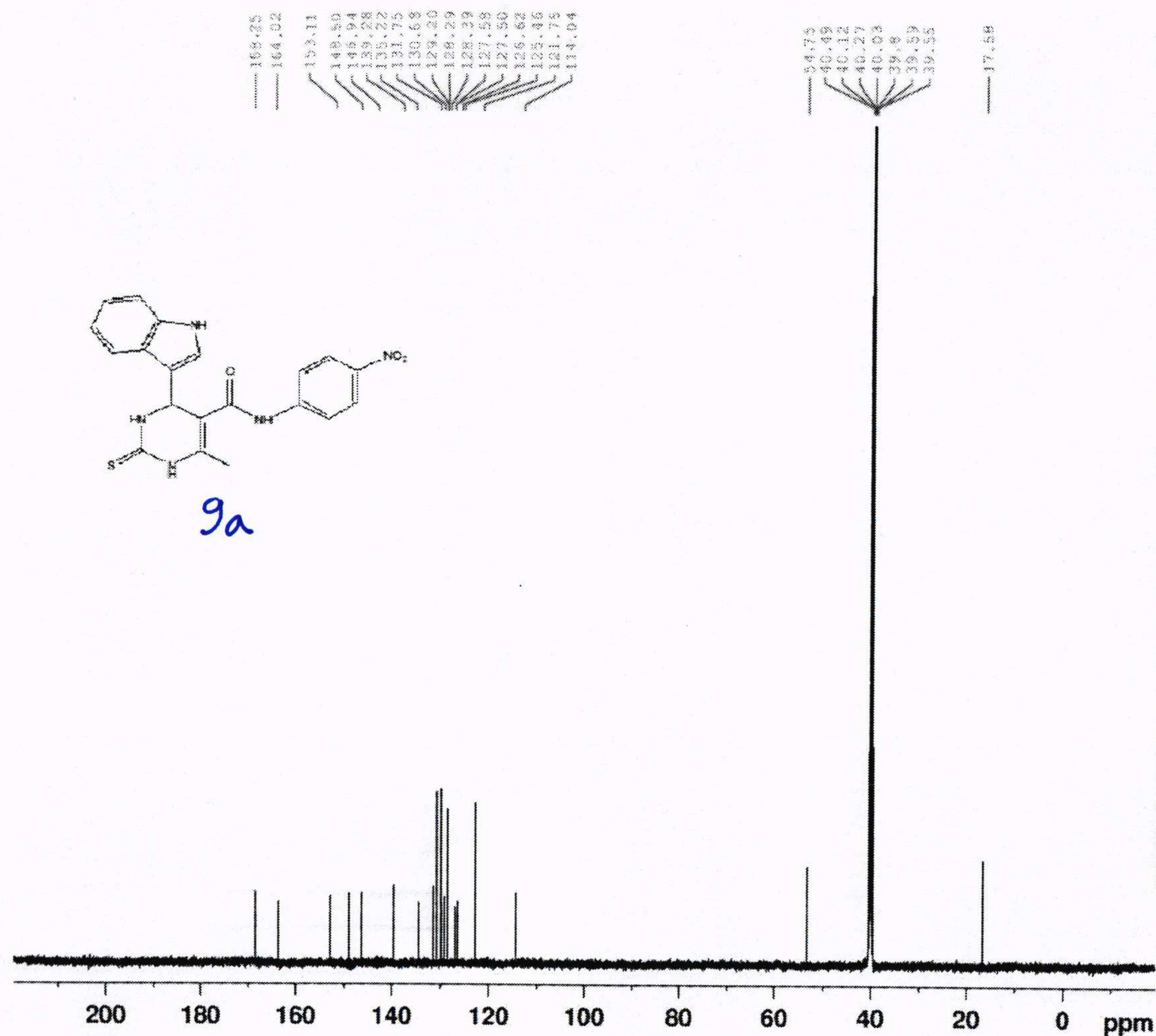




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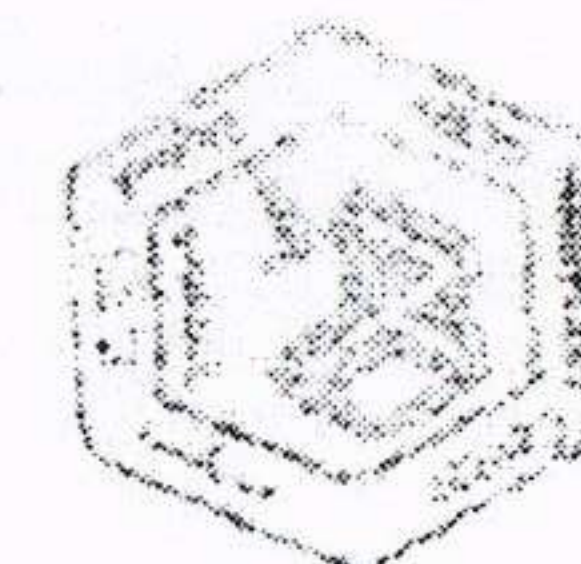
9a



NAME drshahat-17  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20210622  
 Time 20.47  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2000  
 DS 2  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912410 sec  
 RG 14596.5  
 DW 16.650 usec  
 DE 6.50 usec  
 TE 299.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 20.00 usec  
 PL1 -6.00 dB  
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.10 dB  
 PL12 13.44 dB  
 PL13 16.40 dB  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7577890 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

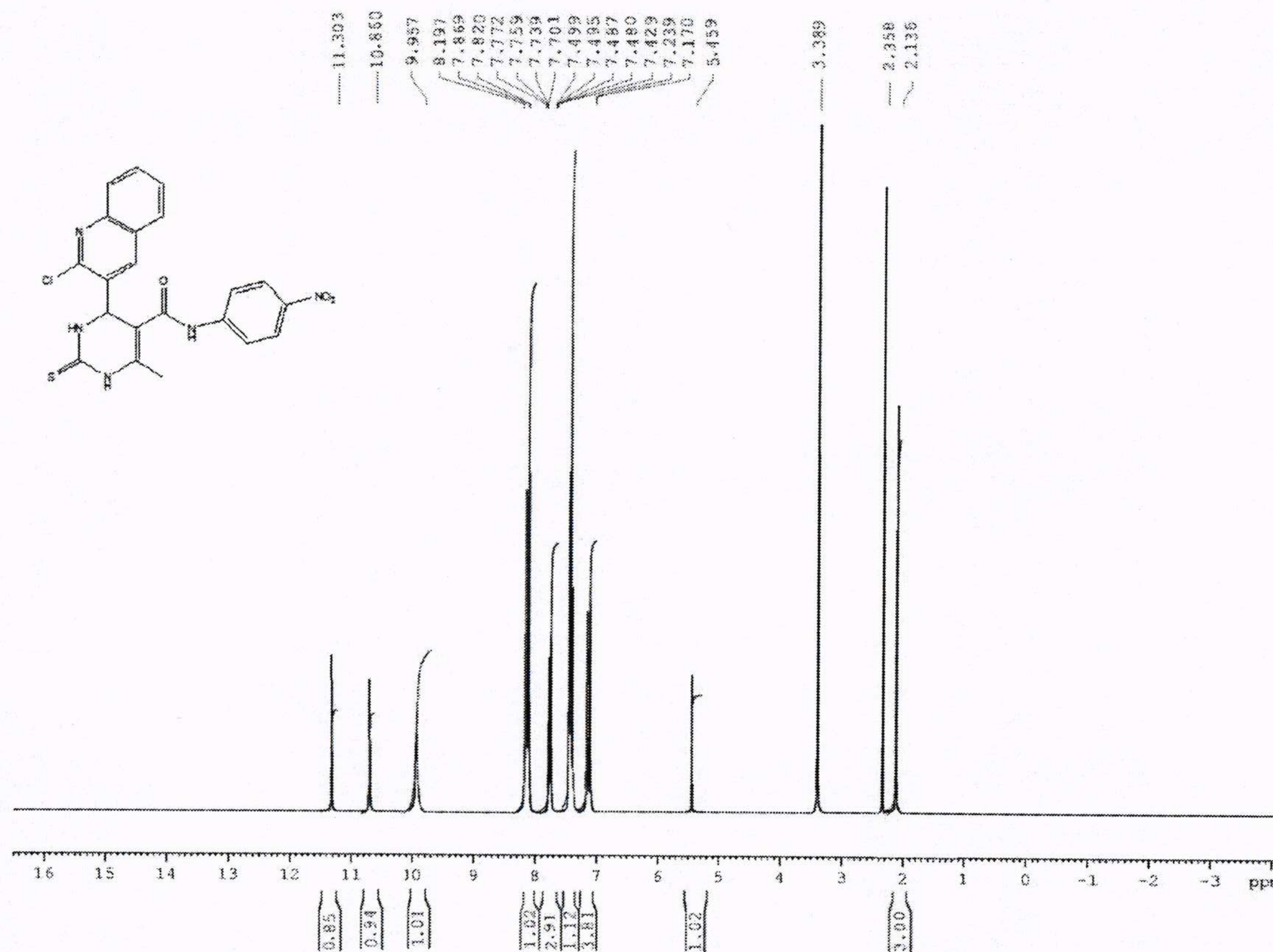




4-(2-Chloroquinolin-3-yl)-6-methyl-N-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxamide

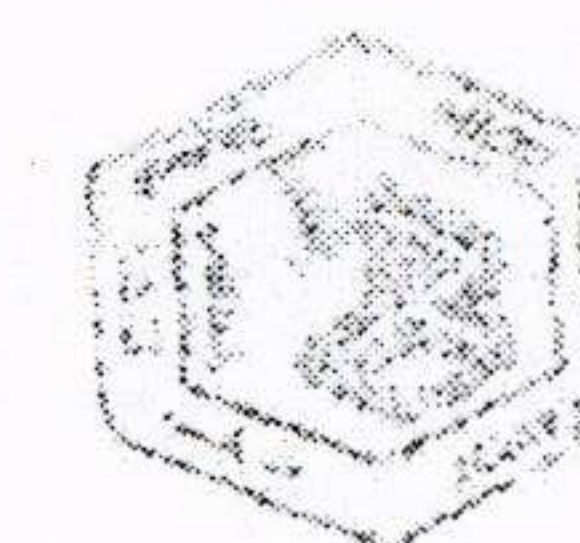
96

ON DMSO D:\ abar



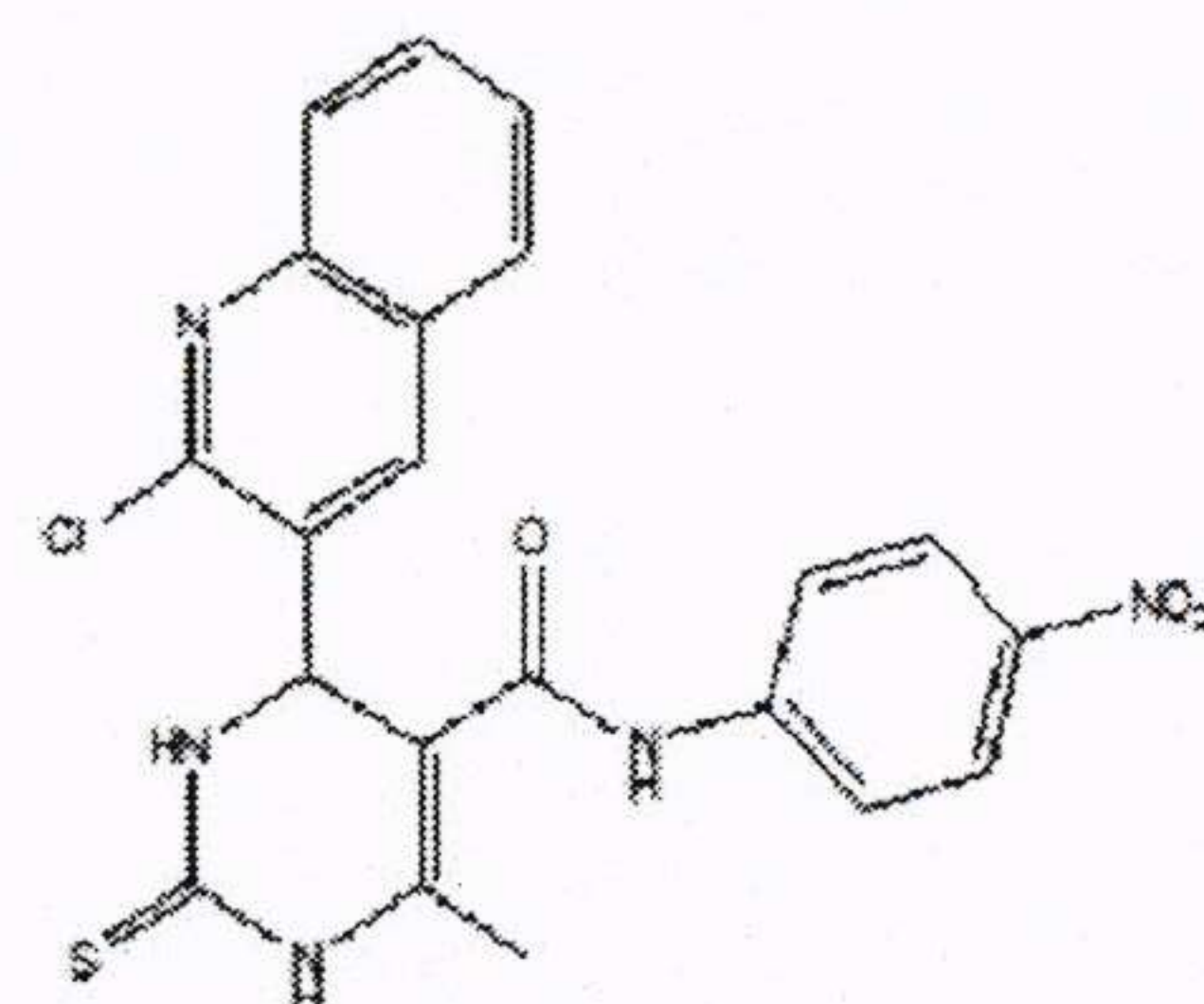
NAME drshahat-16  
EXPNO 10  
PROCNO 1  
Date\_ 20210622  
Time 18.59  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1720407 sec  
RG 90.5  
DW 48.400 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
TDO 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 14.70 usec  
PL1 -1.10 dB  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

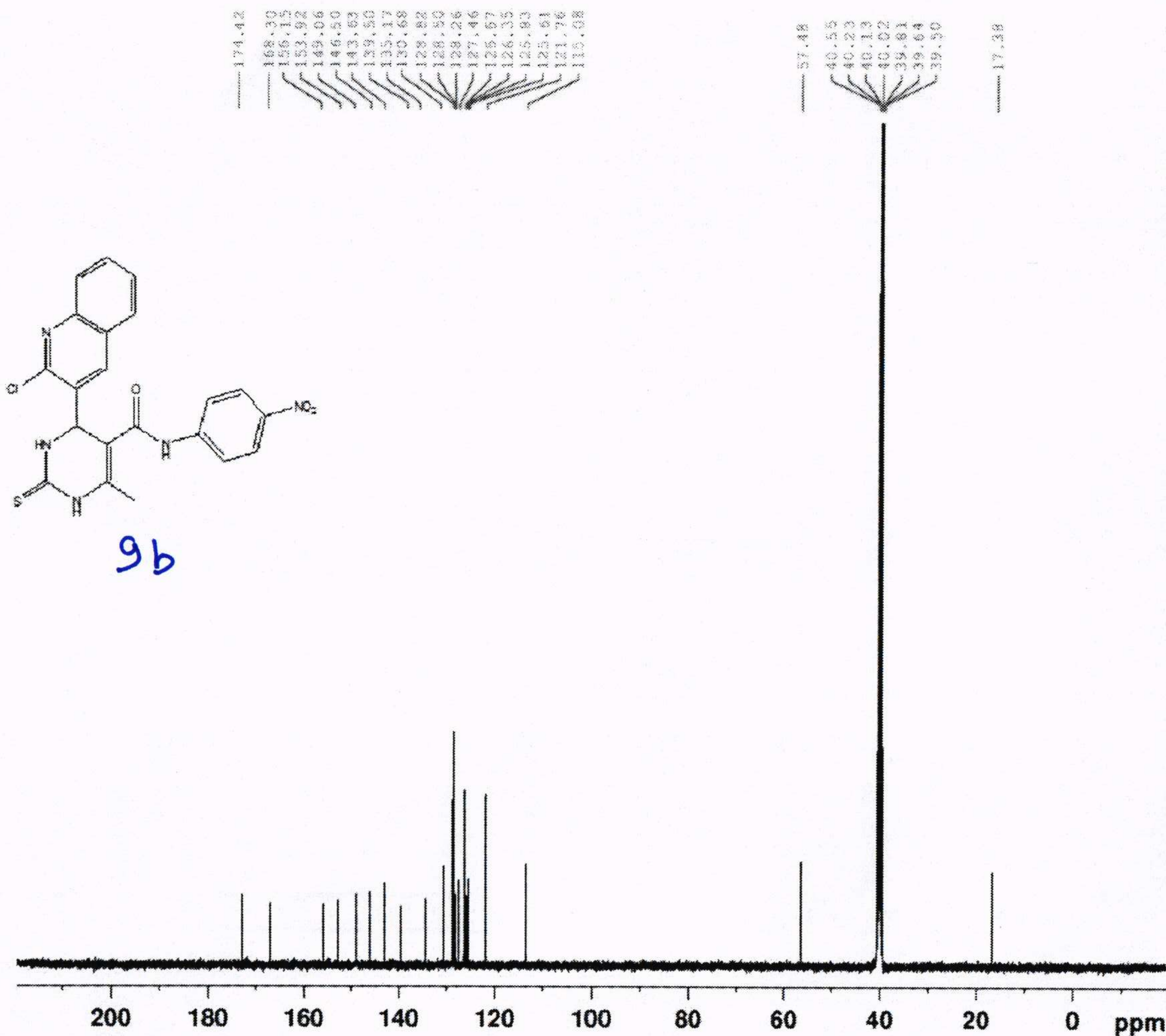




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9b



NAME drshahat-16  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20210622  
 Time 20.47  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2000  
 DS 2  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912410 sec  
 RG 14596.5  
 DW 16.650 usec  
 DE 6.50 usec  
 TE 299.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

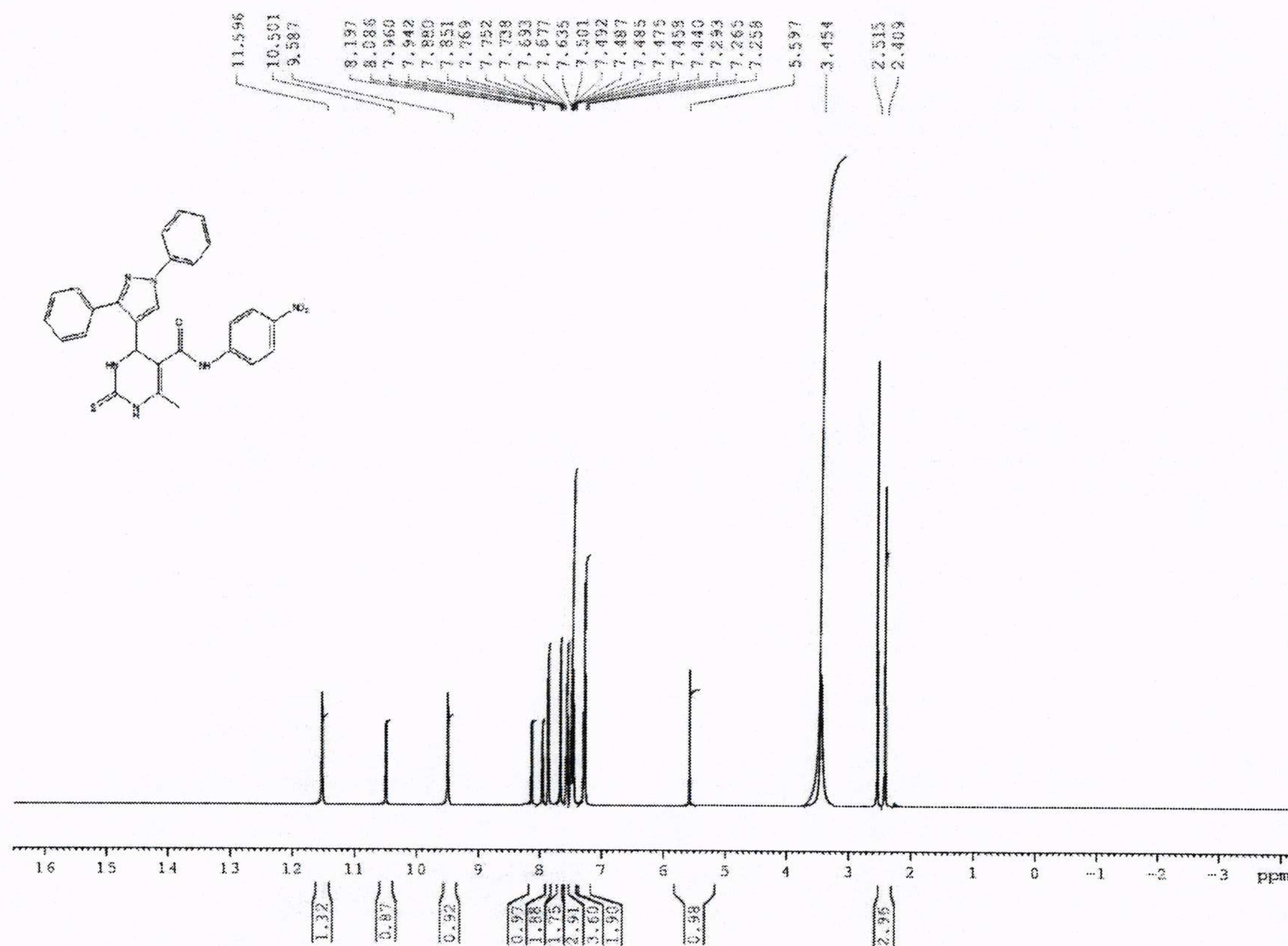
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 20.00 usec  
 PL1 -6.00 dB  
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.10 dB  
 PL12 13.44 dB  
 PL13 16.40 dB  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7577890 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



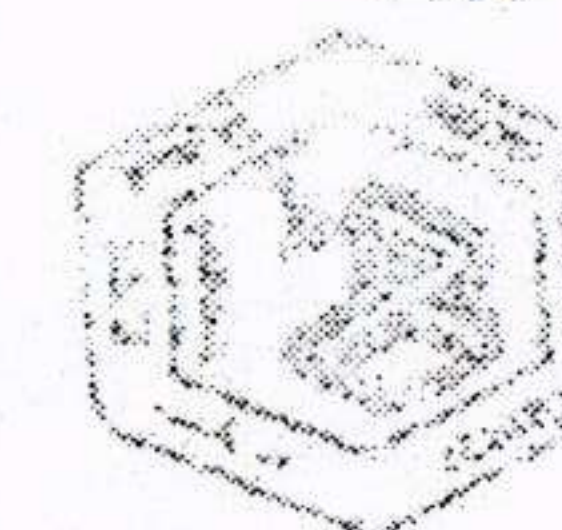


4-(1,3-Diphenyl-1H-pyrazol-4-yl)-6-methyl-N-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxamide 9c



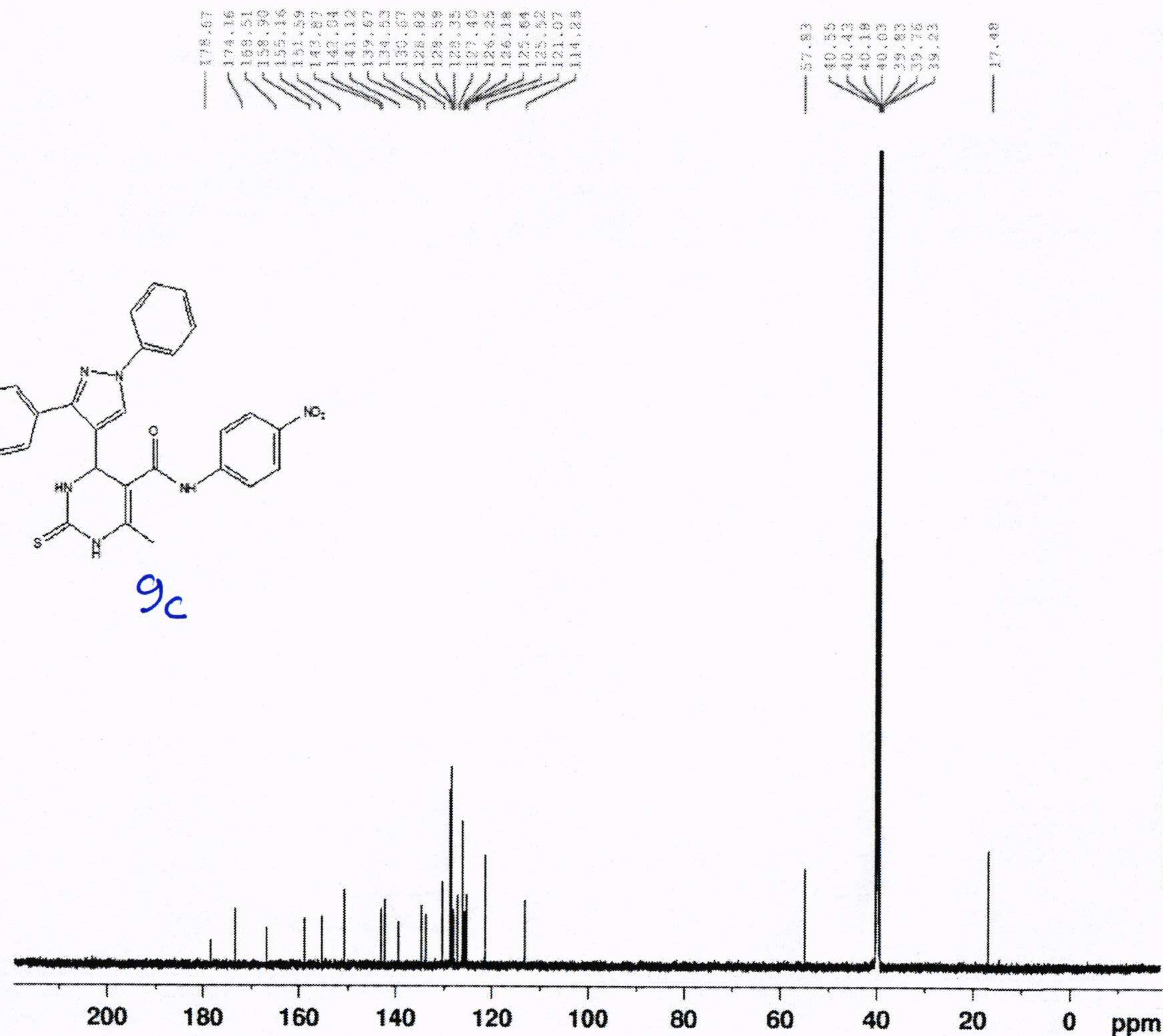
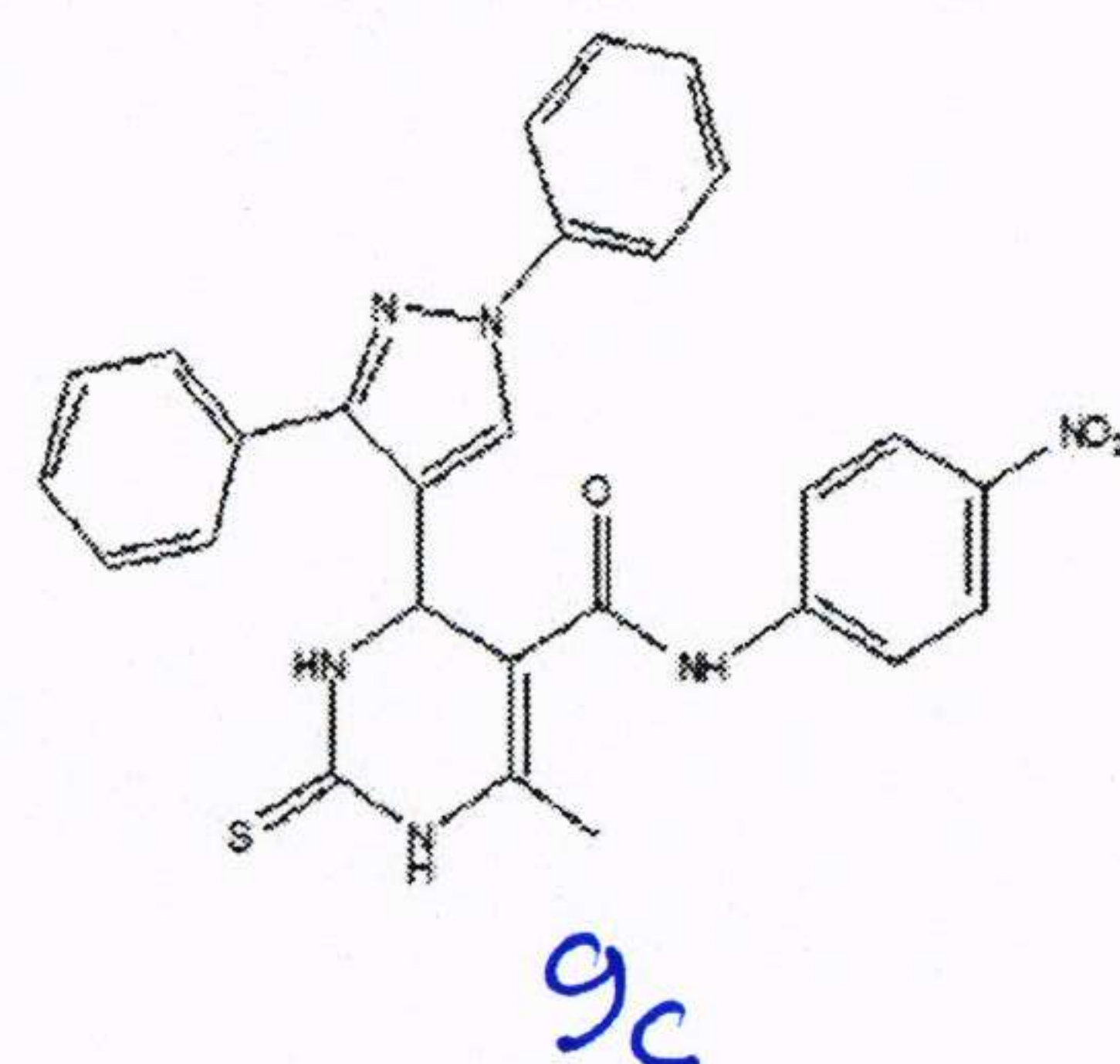
NAME drshahat-18  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20210622  
 Time 11.17  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1720407 sec  
 RG 128  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 1.00000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 14.70 usec  
 PL1 -1.10 dB  
 SFO1 500.1330885 MHz  
 SI 32768  
 SF 500.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





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NAME drshahat-18  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20210622  
 Time 12.07  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1165  
 DS 2  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912410 sec  
 RG 4597.6  
 DW 16.650 usec  
 DE 6.50 usec  
 TE 299.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 20.00 usec  
 PL1 -6.00 dB  
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.10 dB  
 PL12 13.44 dB  
 PL13 16.40 dB  
 SFO2 500.1320005 MHz  
 SI 32768  
 SF 125.7577890 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

