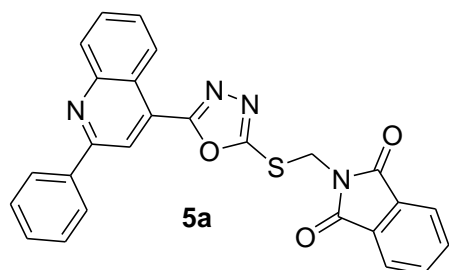


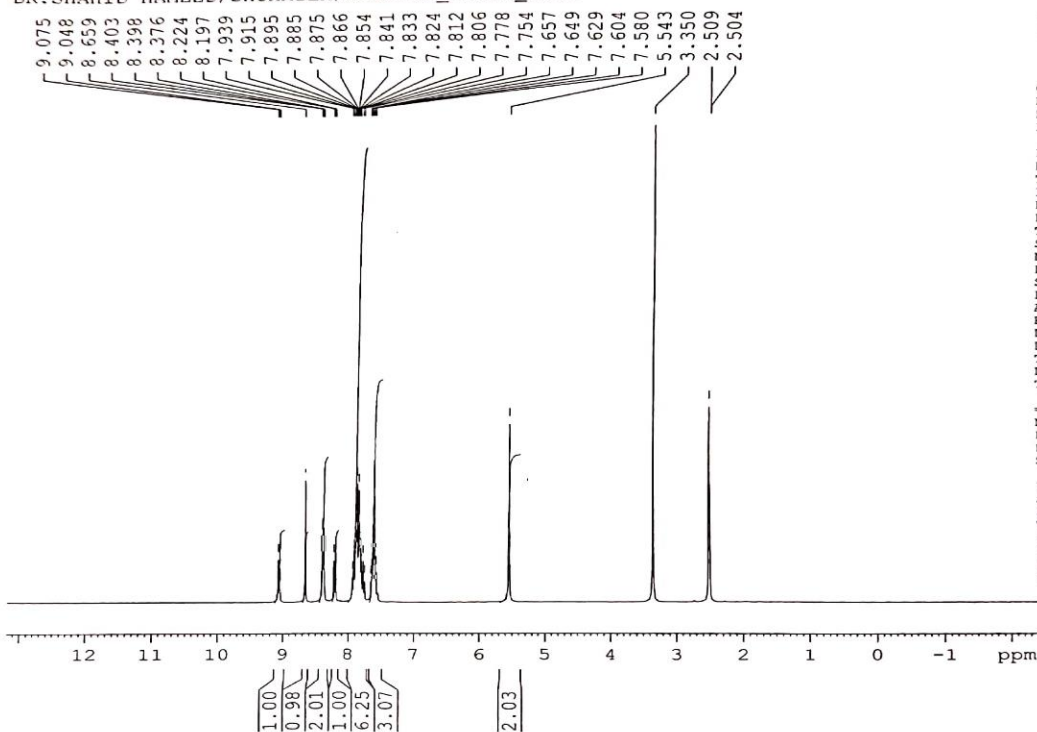
## **Supplementary Material**

# <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and FT-IR Spectra of compounds 5a-f and 6a-d

## <sup>1</sup>H-NMR Spectra of 5a



DR.SHAHID HAMEED/SHUMAILA/OX2PHME\_1HNMR\_DMSO



Current Data Parameters  
NAME OX2PHME\_1HNMR\_DMSO  
EXPNO 1  
PROCNO 1

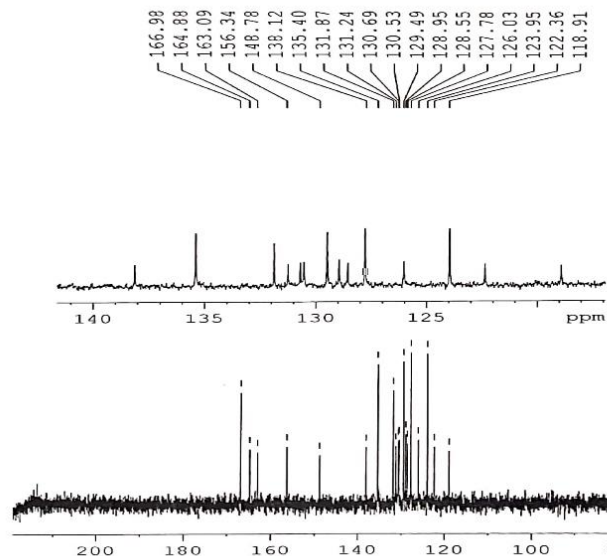
F2 - Acquisition Parameters  
Date\_ 20171122  
Time 15.05  
INSTRUM spect  
PROBHD 5 == BBO BB-1H  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 8  
DS 0  
SWH 5172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 512  
DW 81.000 usec  
DE 6.00 usec  
TE 294.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.00 usec  
PL1 2.00 dB  
SFO1 300.1316534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

# <sup>13</sup>C-NMR Spectra of 5a

DR.SHAHID HAMEED/SHUMAILA/OX2PHME\_13CNMR\_DMSO



Current Data Parameters  
NAME OX2PHME\_13CNMR\_DMSO  
EXPNO 1  
PROCNO 1

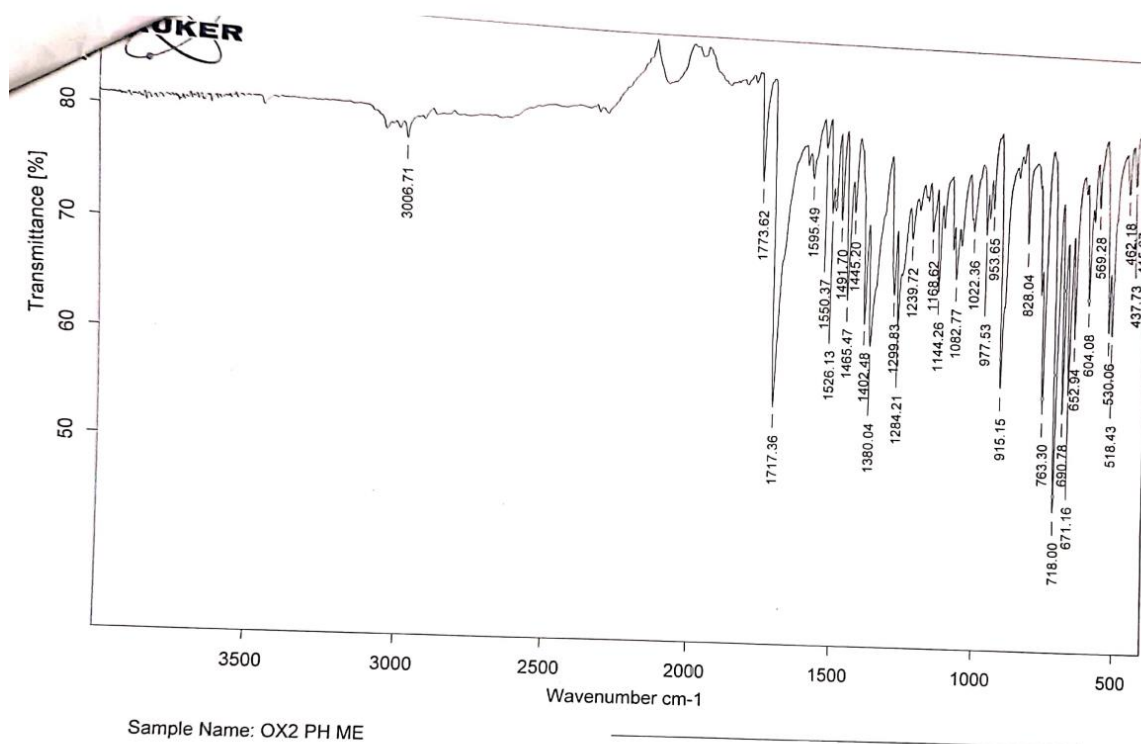
F2 - Acquisition Parameters  
Date\_ 20171122  
Time 15.03  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 35568  
SOLVENT DMSO  
NS 861  
DS 0  
SWH 17985.611 Hz  
FIDRES 0.500045 Hz  
AQ 0.9999604 sec  
RG 11585.2  
DM 27.800 usec  
DE 6.00 usec  
TE 294.5 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 6.00 usec  
PL1 -5.00 dB  
SFO1 75.4752953 MHz

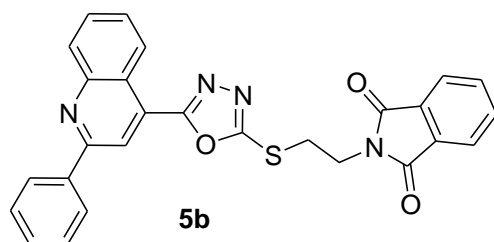
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 20.98 dB  
PL13 20.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

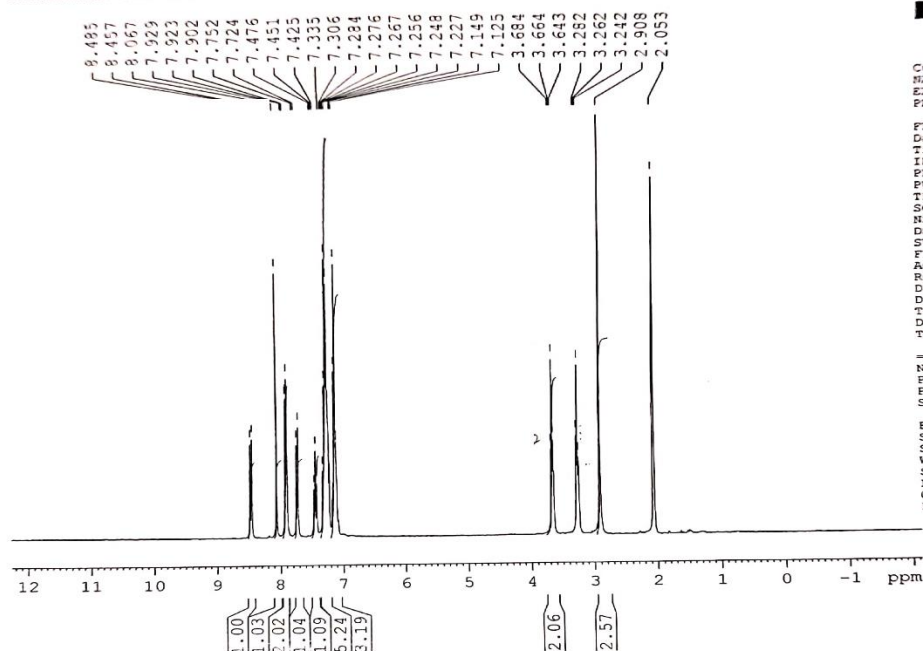
## FT-IR Spectra of 5a



# <sup>1</sup>H-NMR Spectra of 5b



DR.SHAHID HAMEED/SHUMAILA/OX2PHET\_1HNMR\_DMSO



Current Data Parameters  
NAME OX2PHET\_1HNMR\_DMSO  
EXPNO 1  
PROCNO 1

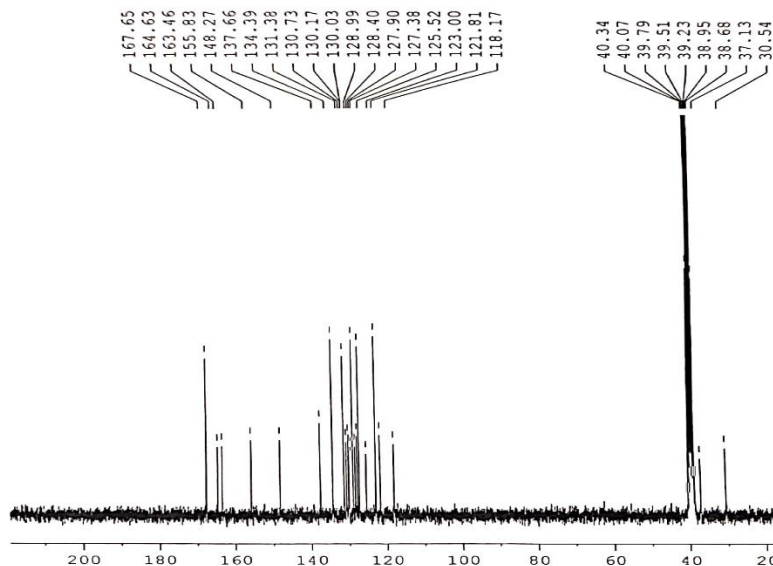
F2 - Acquisition Parameters  
Date\_ 20171122  
Time 13.12  
INSTRUM spect  
PROBHD 5 mm BBO SS-1H  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 8  
DS 4  
SWH 6172.83 Hz  
FIDRES 0.094150 Hz  
AQ 5.3084800 sec  
RG 400  
DW 81.000 usec  
DE 6.000 usec  
TE 300.2 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.00 usec  
PL1 2.00 dB  
SFO1 300.1319534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
FC 1.00

# <sup>13</sup>C-NMR Spectra of 5b

DR.SHAHID HAMEED/SHUMAILA/OX2PHET\_13CNMR\_DMSO



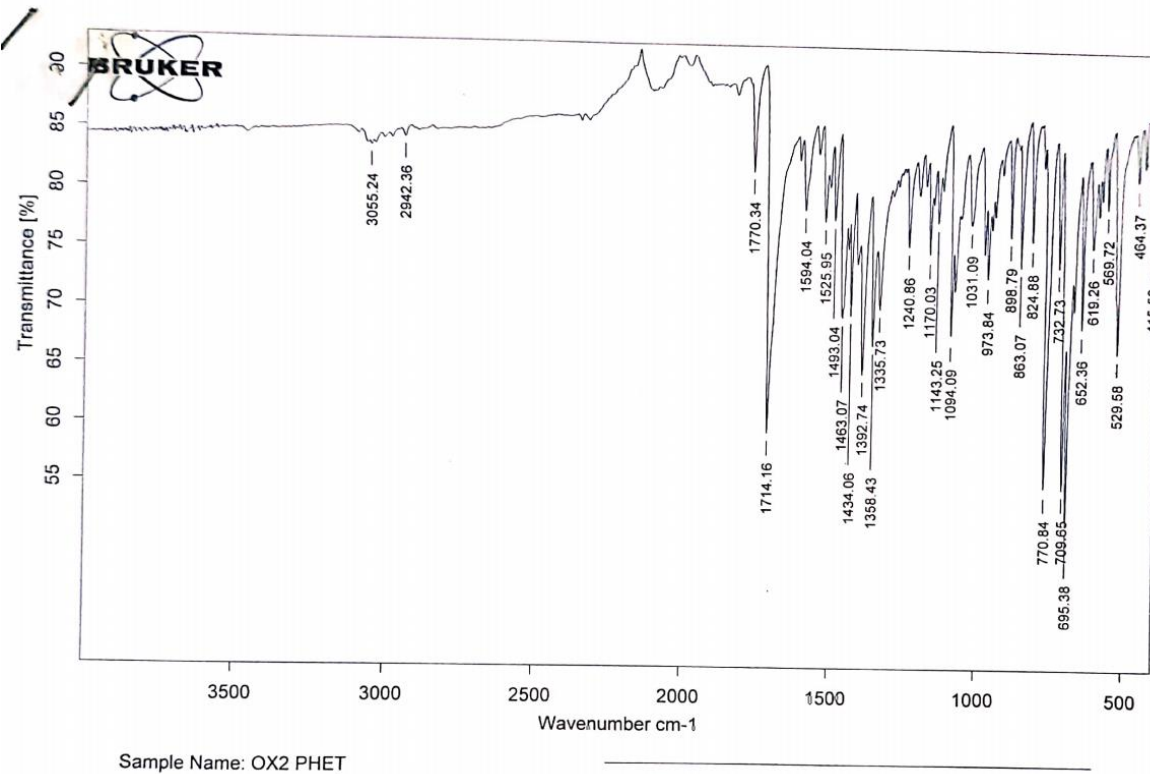
Current Data Parameters  
NAME OX2PHET\_13CNMR\_DMSO  
EXPTNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171122  
Time 14.03  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 35968  
SOLVENT DMSO  
NS 1024  
DS 0  
SWH 17995.611 Hz  
FIDRES 0.500045 Hz  
AQ 0.999904 sec  
RG 26008  
DW 27.8000 usec  
DE 6.00 usec  
TE 294.1 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

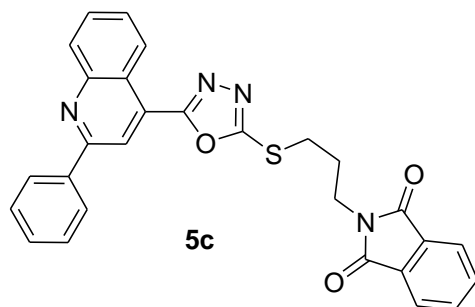
----- CHANNEL f1 -----  
NUC1 13C  
P1 6.00 usec  
PL1 5.00 dB  
SFO1 75.4752853 MHz  
----- CHANNEL f2 -----  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 20.98 dB  
PL13 20.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

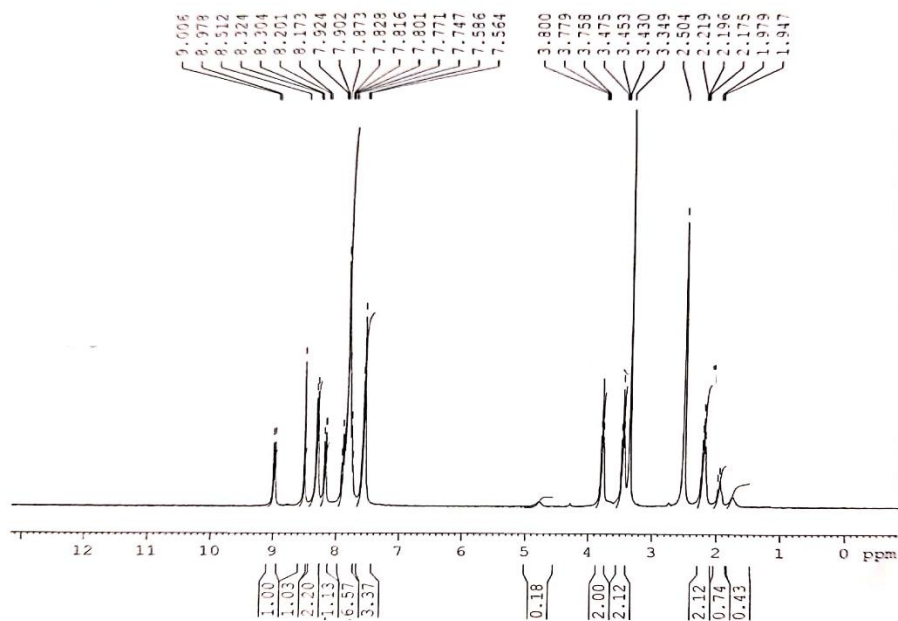
## FT-IR Spectra of 5b



# <sup>1</sup>H-NMR Spectra of 5c



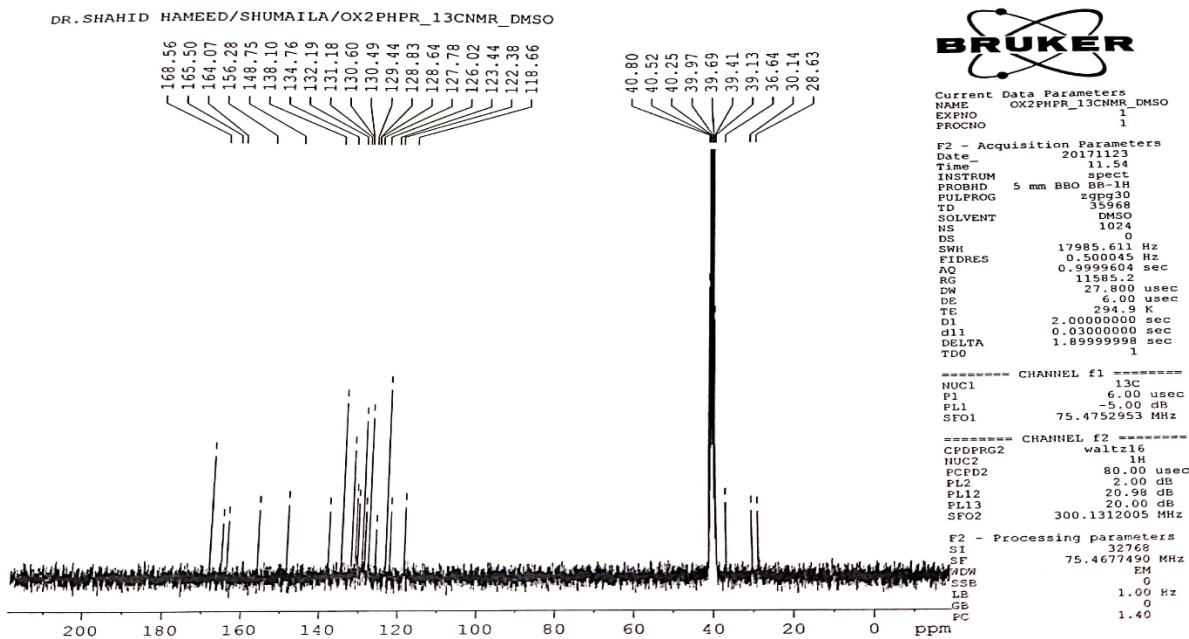
DR.SHAHID NAMEED/SHUMAILA/OX2FHFR\_1HNMR\_DMSO



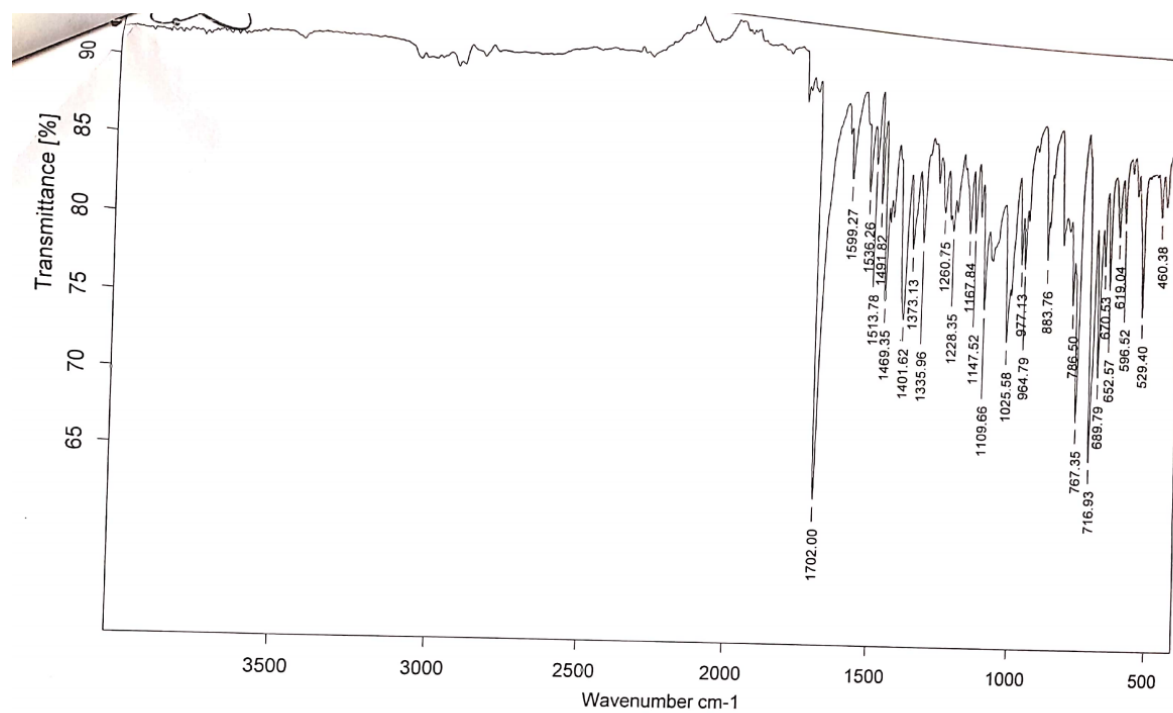
Current Data Parameters  
NAME OX2FHFR\_1HNMR\_DMSO  
EXPNO 1  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20171123  
Time 12.09  
INSTRUM spect  
PROBHD 5 mm BBO  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 8  
DS 8  
SWH 4170.83 Hz  
FIDRES 0.0041900 Hz  
AQ 0.30845600 sec  
RG 4096  
DM 81.000000 sec  
DE 4.000000 sec  
TE 300.2 K  
D1 1.00000000 sec  
TD0 1  
----- CHANNEL f1 -----  
NUC1 1H  
P1 12.00000000 sec  
PL1 0.00000000 dB  
SFO1 300.1360534 MHz  
F2 - Processing parameters  
SI 32768  
SF 300.1360534 MHz  
WDW EM  
SSB 0  
LB 0.300000 Hz  
GB 0  
PC 1.00000000



# <sup>13</sup>C-NMR Spectra of 5c

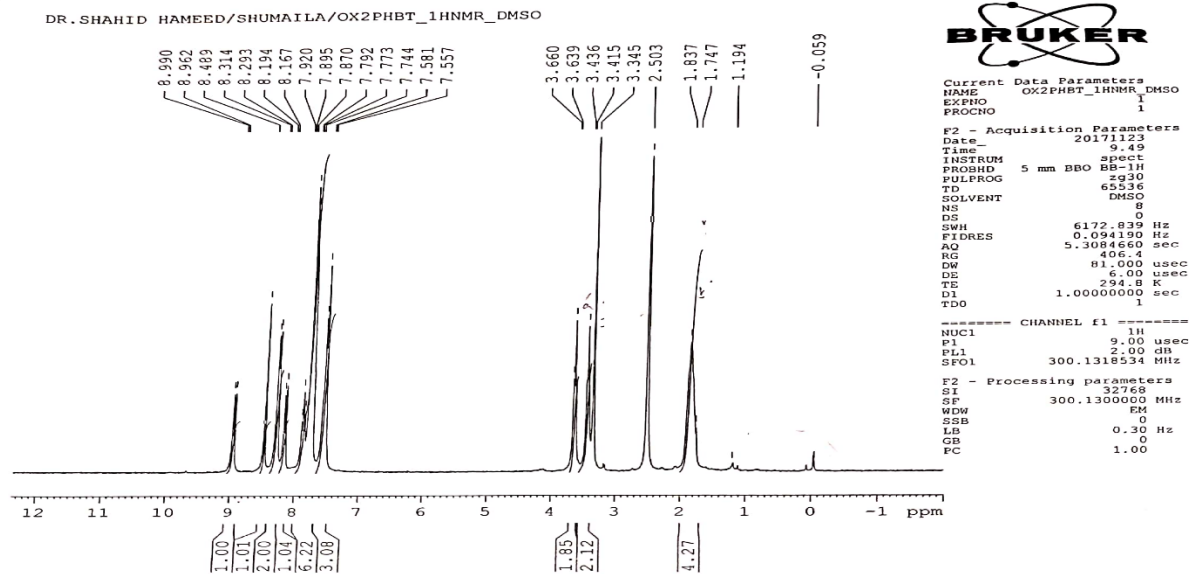
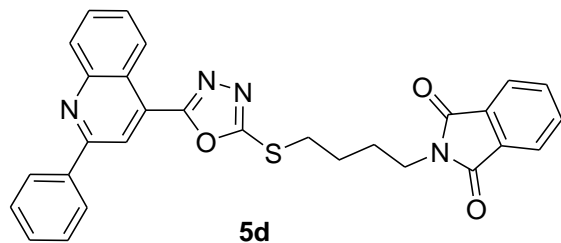


## FT-IR Spectra of 5c



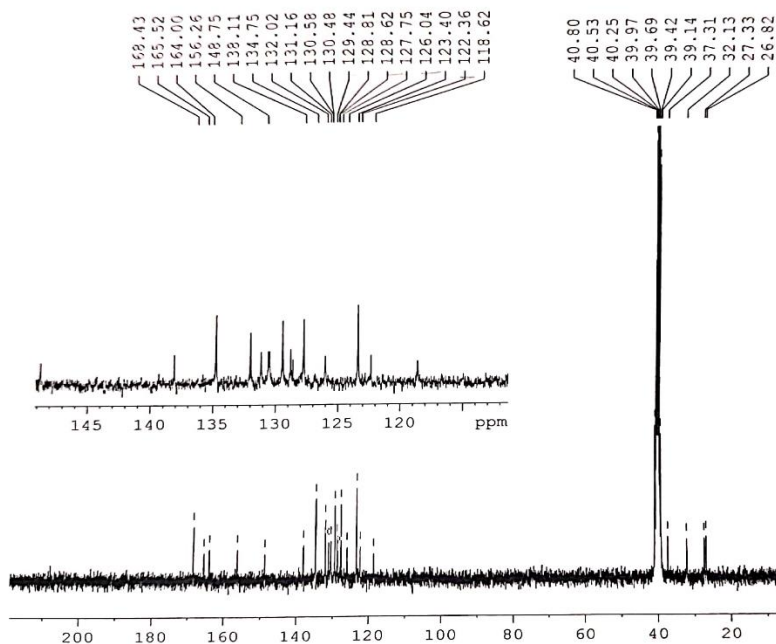
Sample Name: OX2 PH PR

# <sup>1</sup>H-NMR Spectra of 5d



# <sup>13</sup>C-NMR Spectra of 5d

DR.SHAHID HAMEED/SHUMAILA/OX2PHBT\_13CNMR\_DMSO



Current Data Parameters  
NAME OX2PHBT\_13CNMR\_DMSO  
EXPNO 1  
PROCNO 1

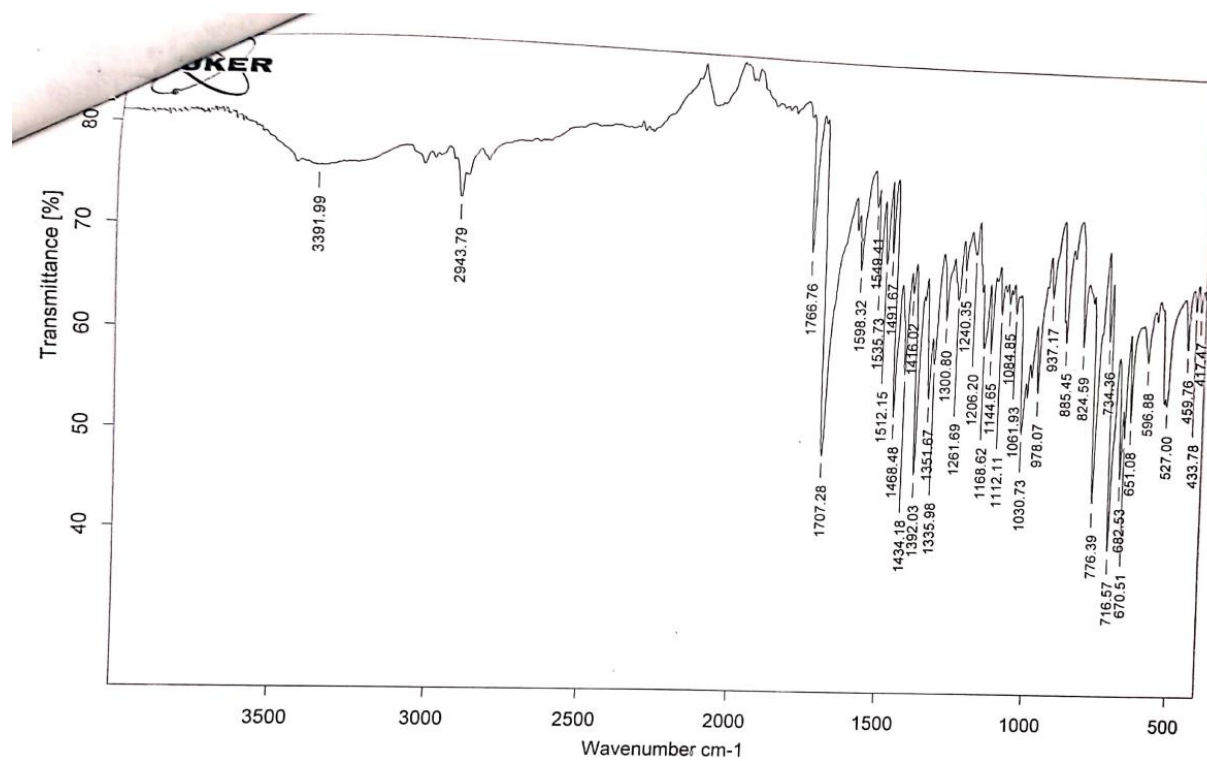
F2 - Acquisition Parameters  
Date\_ 20171123  
Time 10.46  
INSTRUM spect  
PROBHD 5 mm BBO BB-LH  
PULPROG zgpg30  
TD 32768  
SOLVENT DMSO  
NS 1024  
DS 0  
SWH 17985.611 Hz  
FIDRES 0.500045 Hz  
AQ 0.999924 sec  
RG 32768  
DW 27.800 usec  
DE 8.00 usec  
TE 284.2 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDD 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 6.00 usec  
PL1 -5.00 dB  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 20.98 dB  
PL13 20.00 dB  
SFO2 300.1312005 MHz

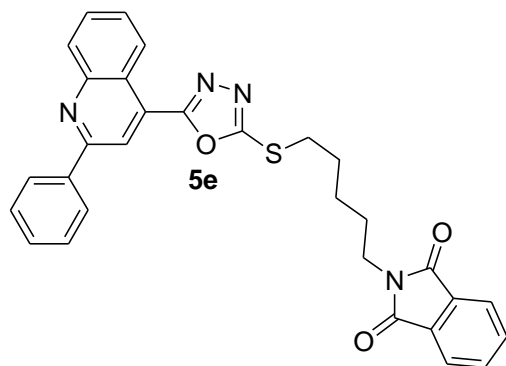
F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

## FT-IR Spectra of 5d

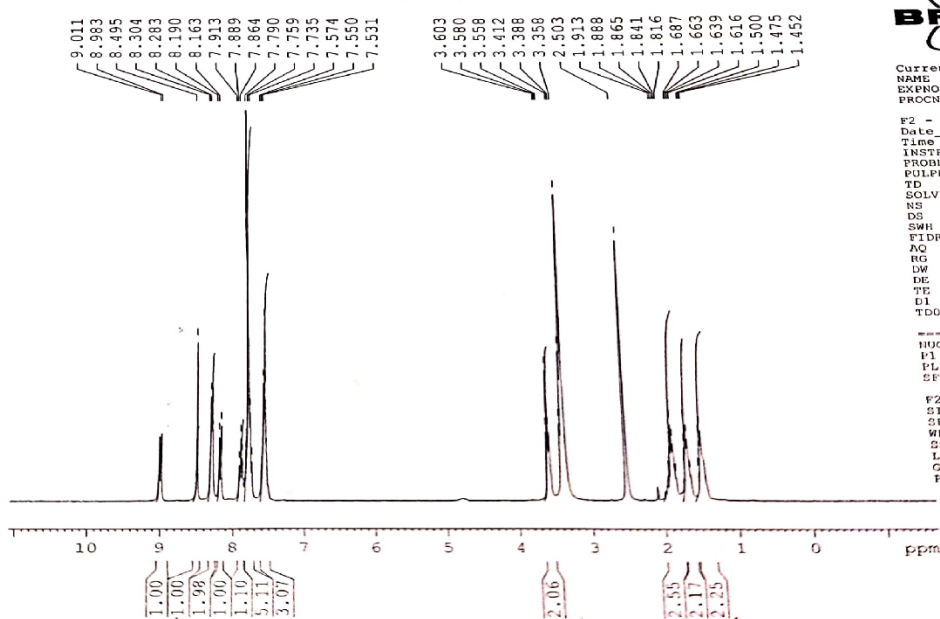


Sample Name: OX2 PH BT

# <sup>1</sup>H-NMR Spectra of 5e



DR.SHAHID HAMEED/SHUMAILA/OX2PHNT\_1HNMR\_DMSO



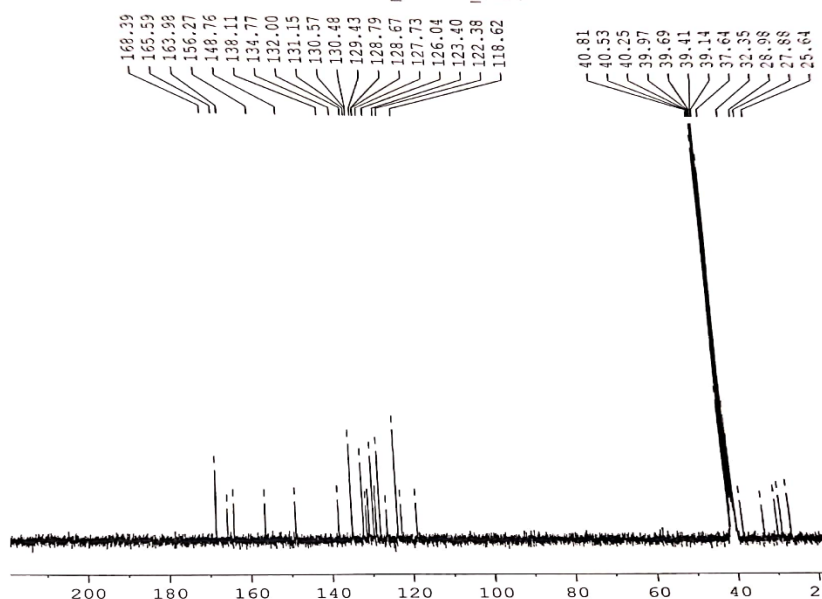
Current Data Parameters  
NAME OX2PHNT\_1HNMR\_DMSO  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171121  
Time 16.36  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
DS 8  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 362  
DW 81.000 usec  
DE 6.00 usec  
TE 295.0 K  
D1 1.00000000 sec  
TDO 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 9.00 usec  
PL1 2.00 dB  
SFO1 300.1318534 MHz  
  
F2 - Processing parameters  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.39 Hz  
GB 0  
PC 1.00

# <sup>13</sup>C-NMR Spectra of 5e

DR. SHAHID HAMEED/SHUMAILA/OX2PHNT\_13CNMR\_DMSO



Current Data Parameters  
NAME OX2PHNT\_13CNMR\_D  
EXPHO 1  
PROCNO 1

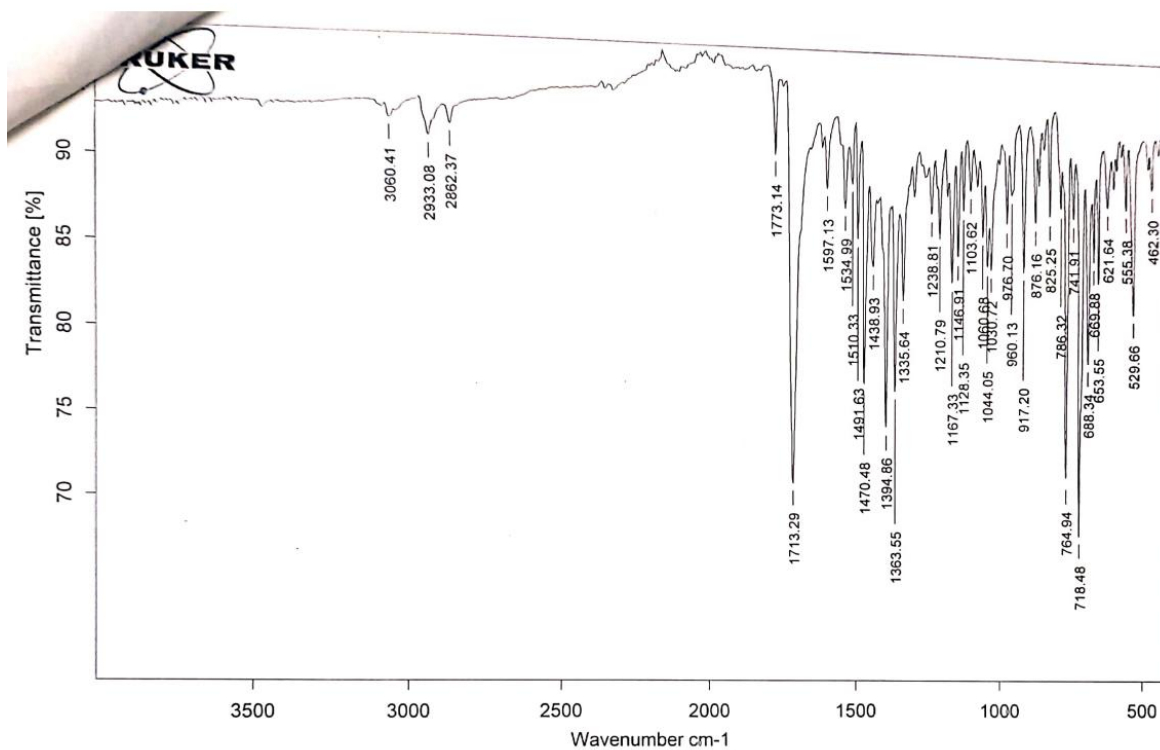
F2 - Acquisition Parameters  
Date 20171121  
Time 17.07  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 35868  
SOLVENT DMSO  
NS 586  
DS 0  
SWH 17985.611  
FIDRES 0.500045  
FQ 0.9999604  
PC 9195.2  
DM 27.800  
DE 6.00  
TE 295.1  
D1 2.0000000  
d11 0.0300000  
DELTA 1.8999999  
TD0

===== CHANNEL f1 =====  
NUC1 1  
P1 6.  
PL1 -5.  
SFO1 75.47521

===== CHANNEL f2 =====  
CPDPRG2 walt  
NUC2  
PCPD2 8  
PL2  
PL12 2  
PL13  
SFO2 300.13

F2 - Processing pa  
SI  
SF 75.47  
WDW  
SSB  
LB  
GB  
PC

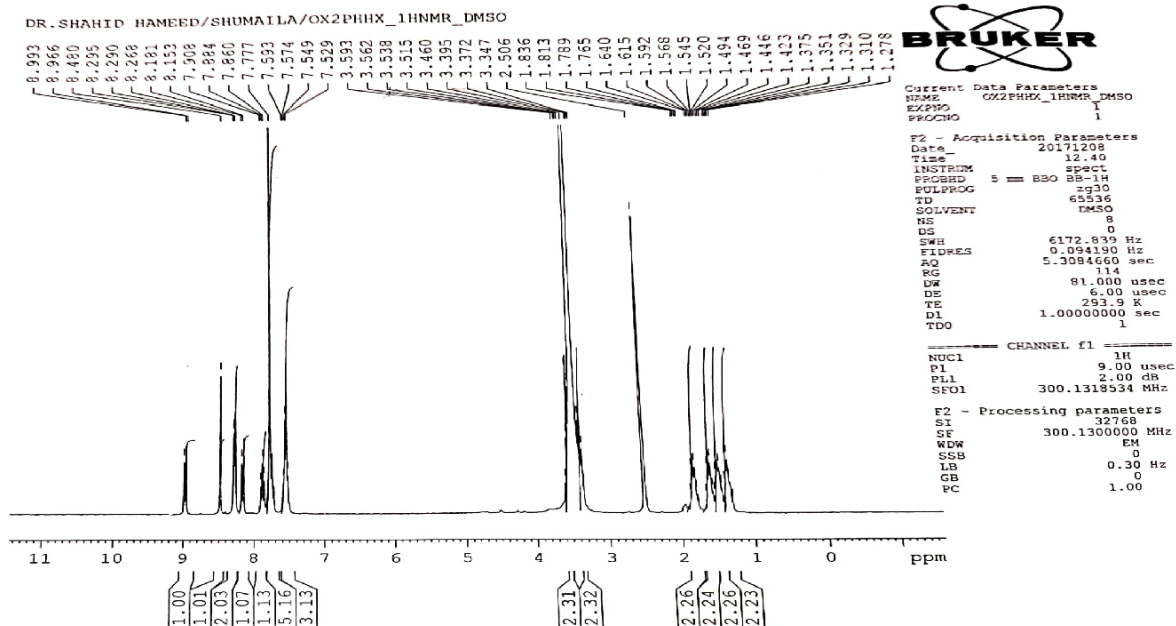
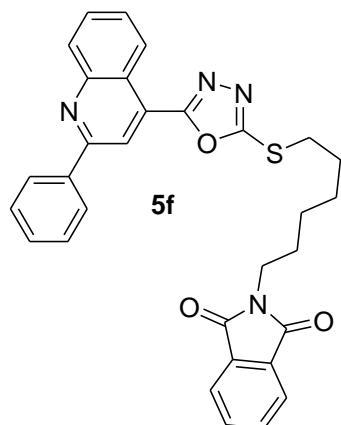
## FT-IR Spectra of 5e



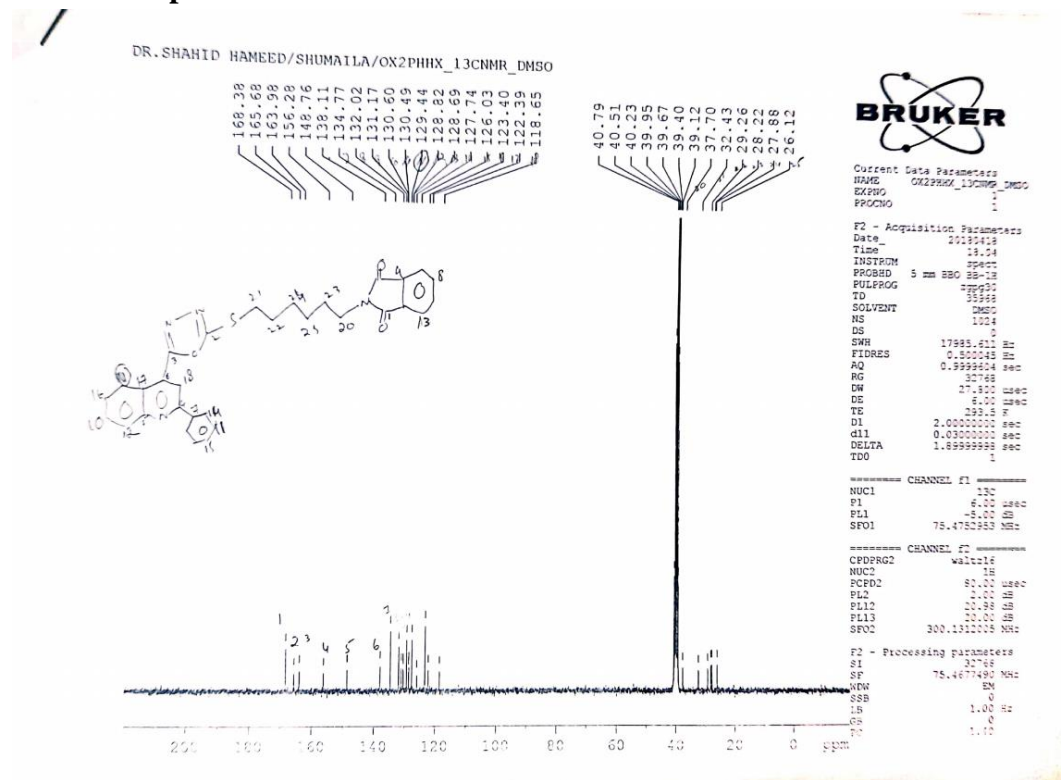
Sample Name: OX2 PH PNT



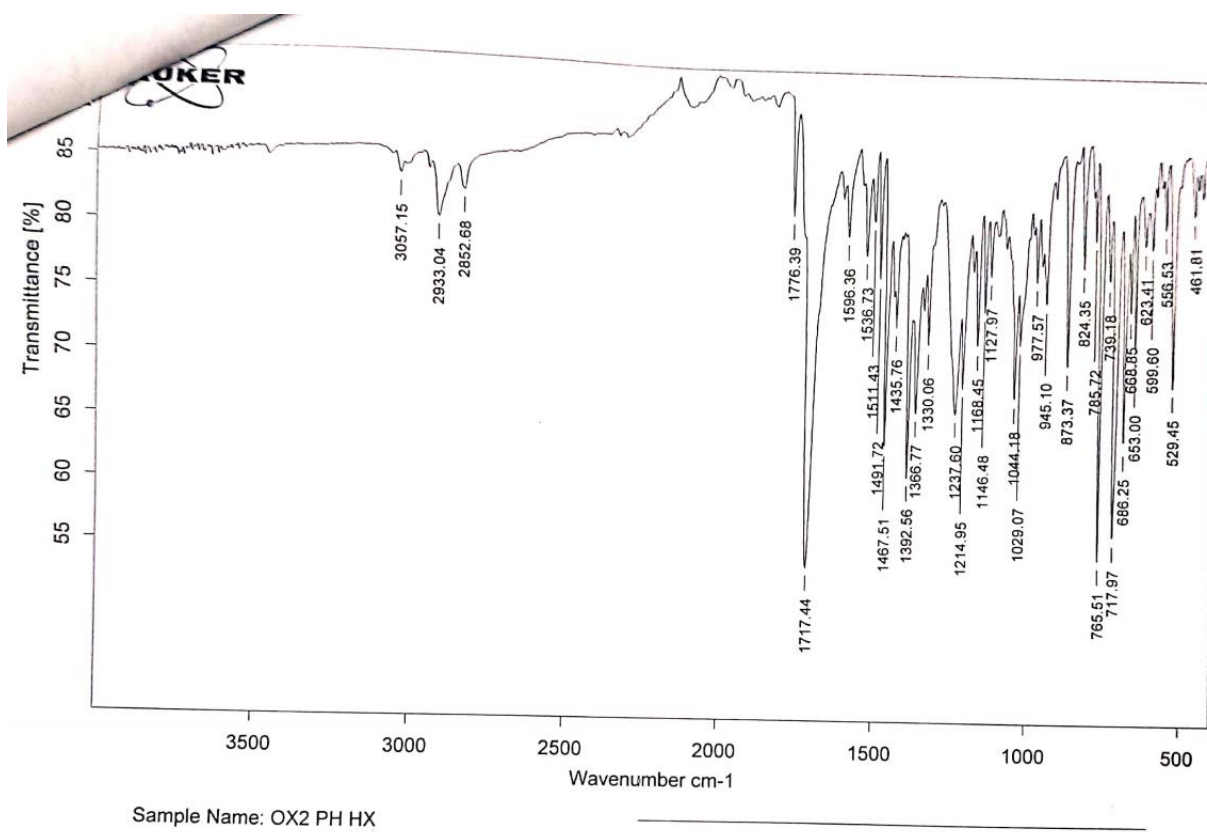
# <sup>1</sup>H-NMR Spectra of 5f



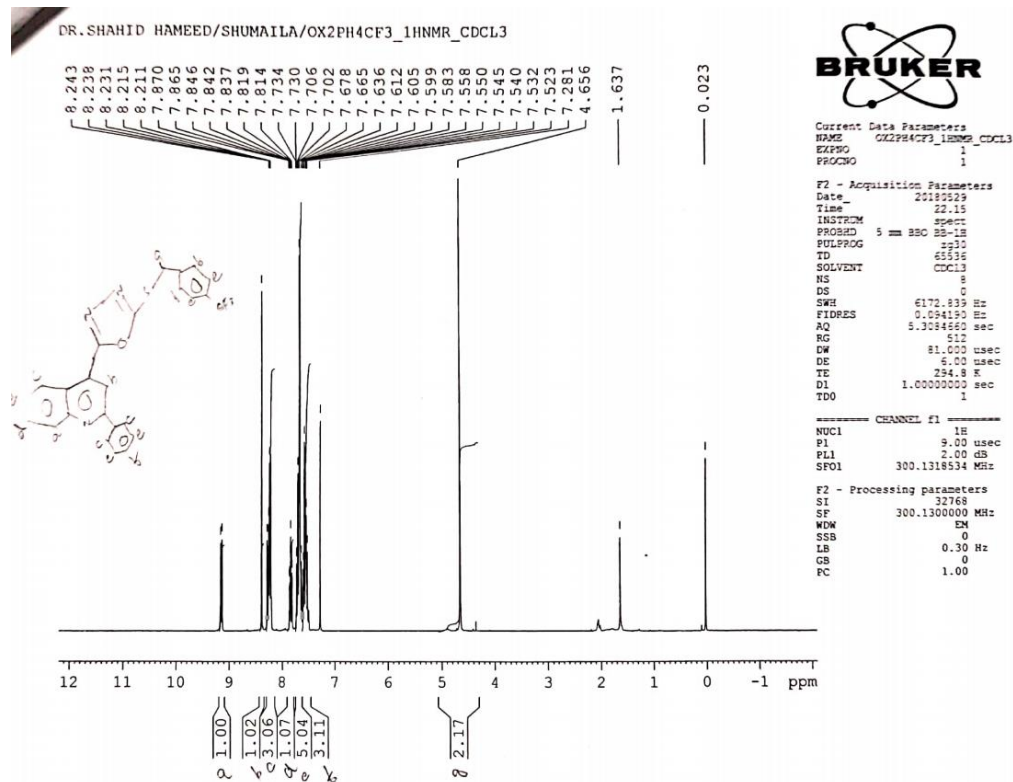
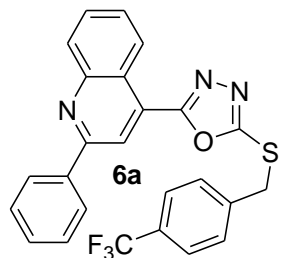
# <sup>13</sup>C-NMR Spectra of 5f



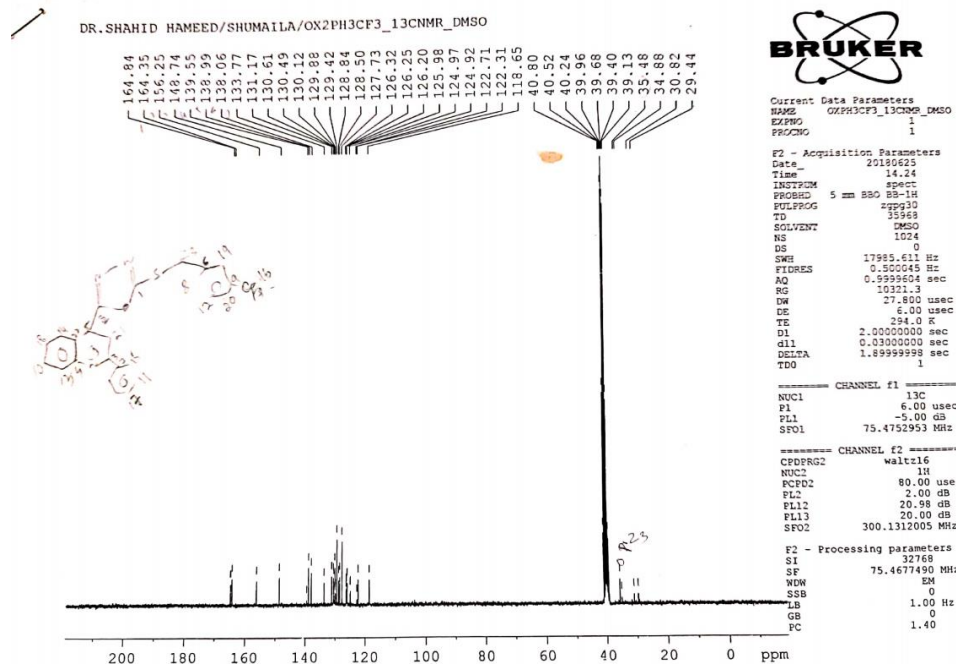
# FT-IR Spectra of 5f



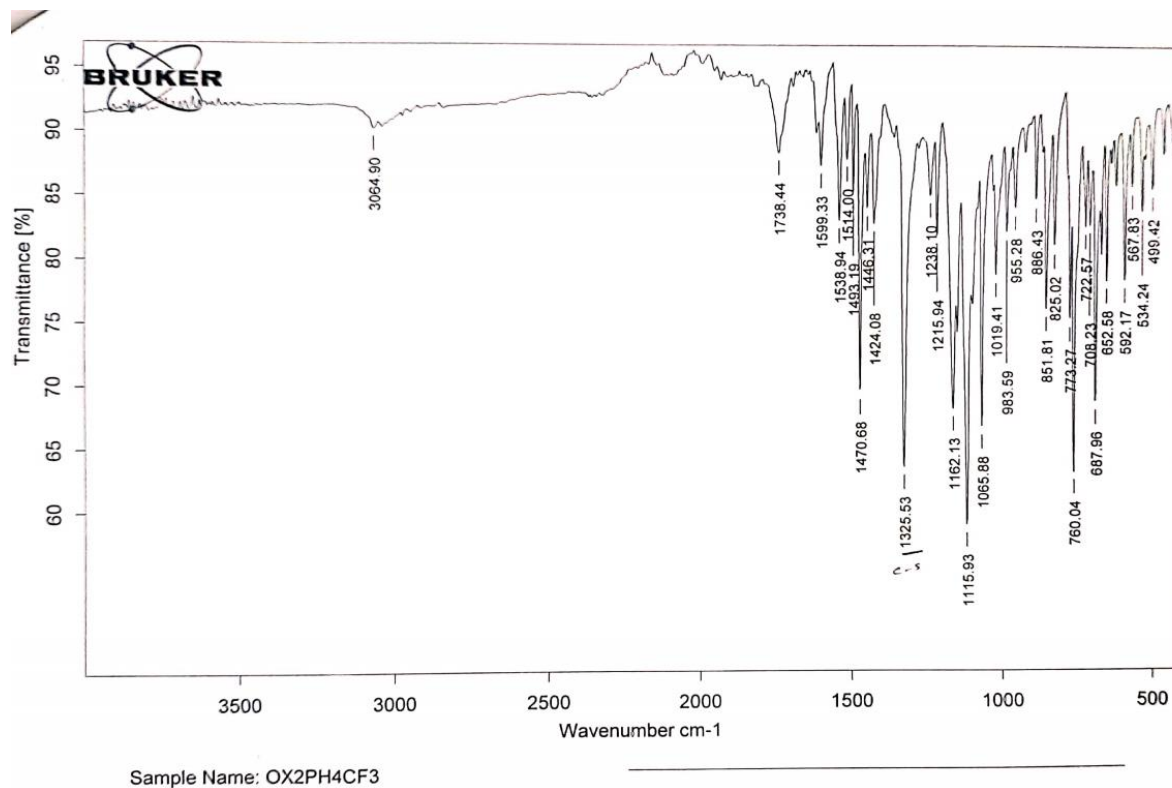
# **<sup>1</sup>H-NMR Spectra of 6a**



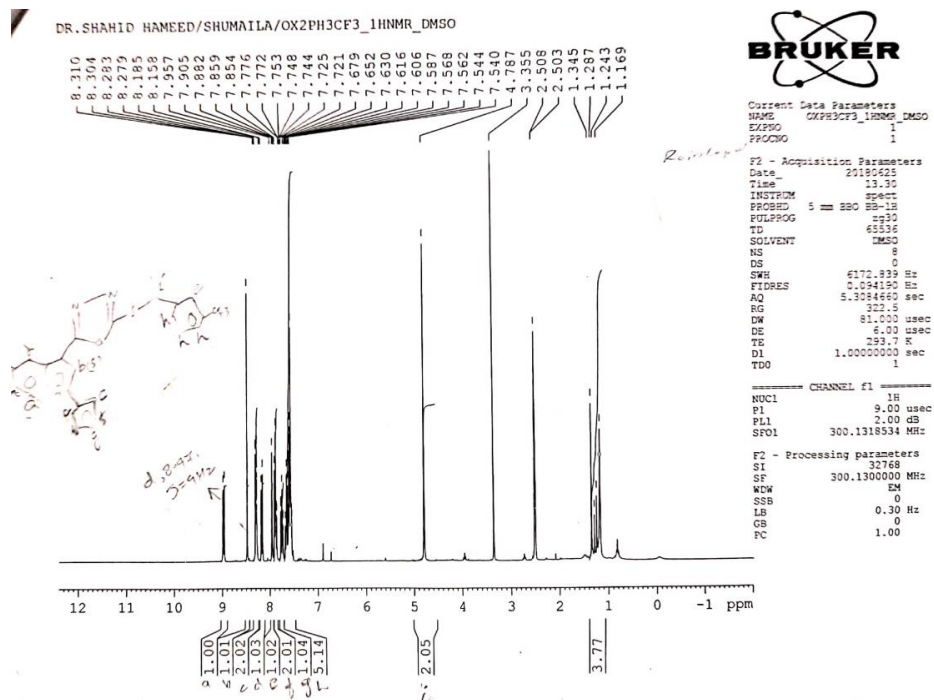
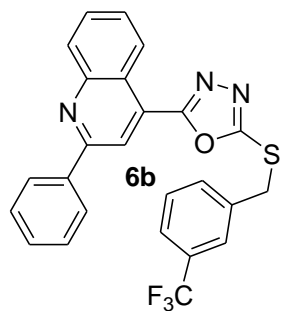
## 13C-NMR Spectra of 6a



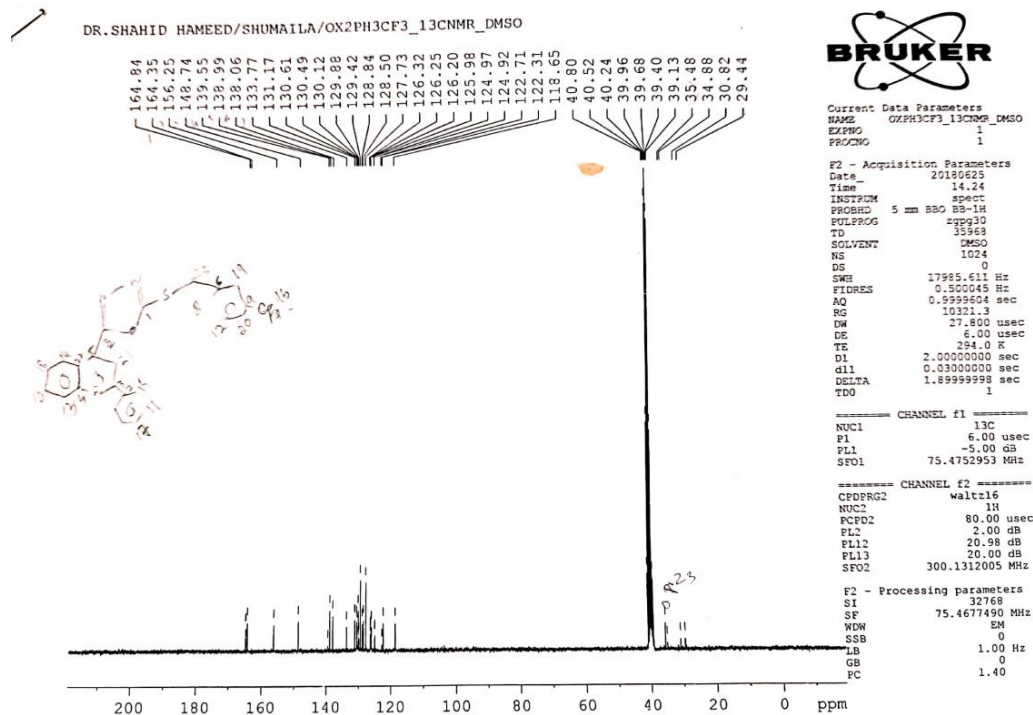
## FT-IR Spectrum of 6a



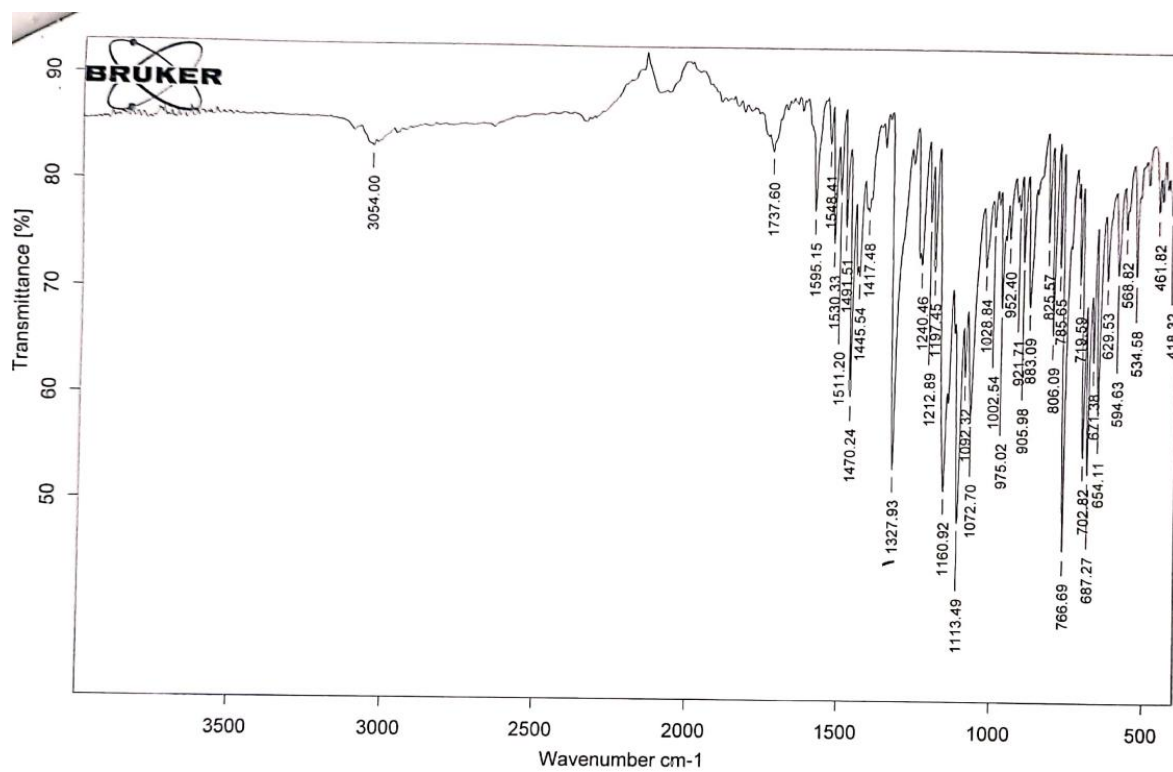
# **<sup>1</sup>H-NMR Spectra of 6b**



# **<sup>13</sup>C-NMR Spectra of 6b**



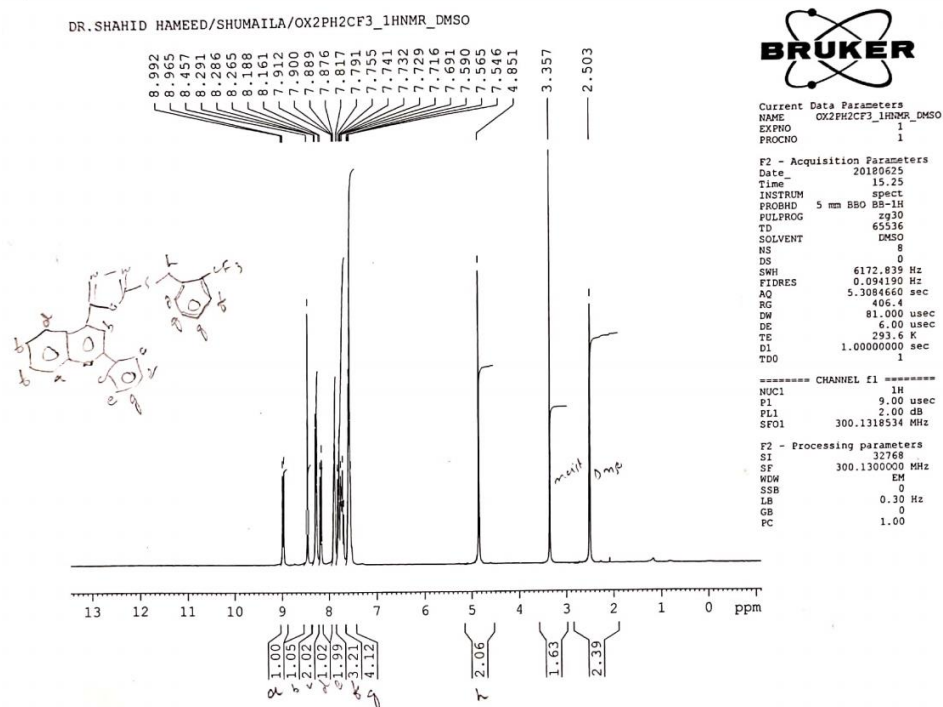
## FT-IR Spectra of 6b



Sample Name: OX2PH3CF3

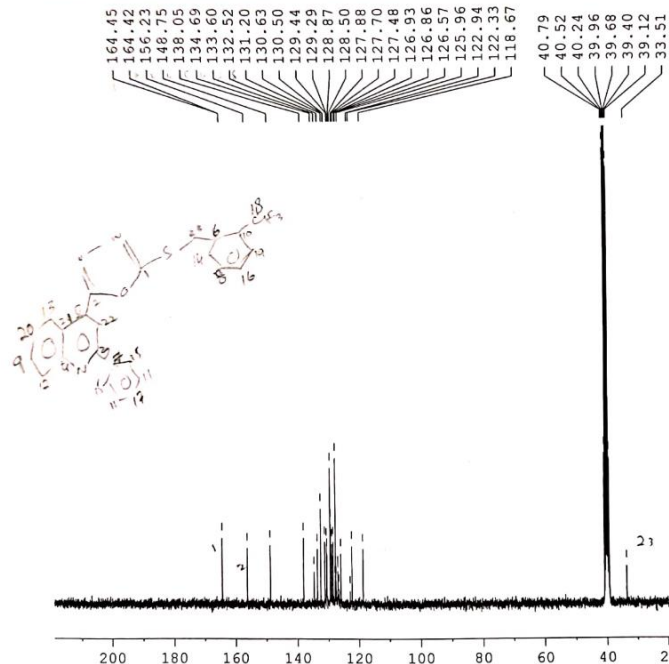


Chemical structure of compound **6c** is shown, which is a quinoline derivative. It features a phenyl group at position 2 and a 1,3,4-oxadiazole ring at position 3. The 1,3,4-oxadiazole ring is further substituted with a (2-(trifluoromethyl)phenyl)methylthio group at position 5.



# **<sup>13</sup>C-NMR Spectra of 6c**

DR.SHAHID HAMEED/SHUMAILA/OX2PH2CF3\_13CNMR\_DMSO



Current Data Parameters  
NAME OX2PH2CF3\_13CNMR\_DMSO  
EXPNO 1  
PROCNO 1

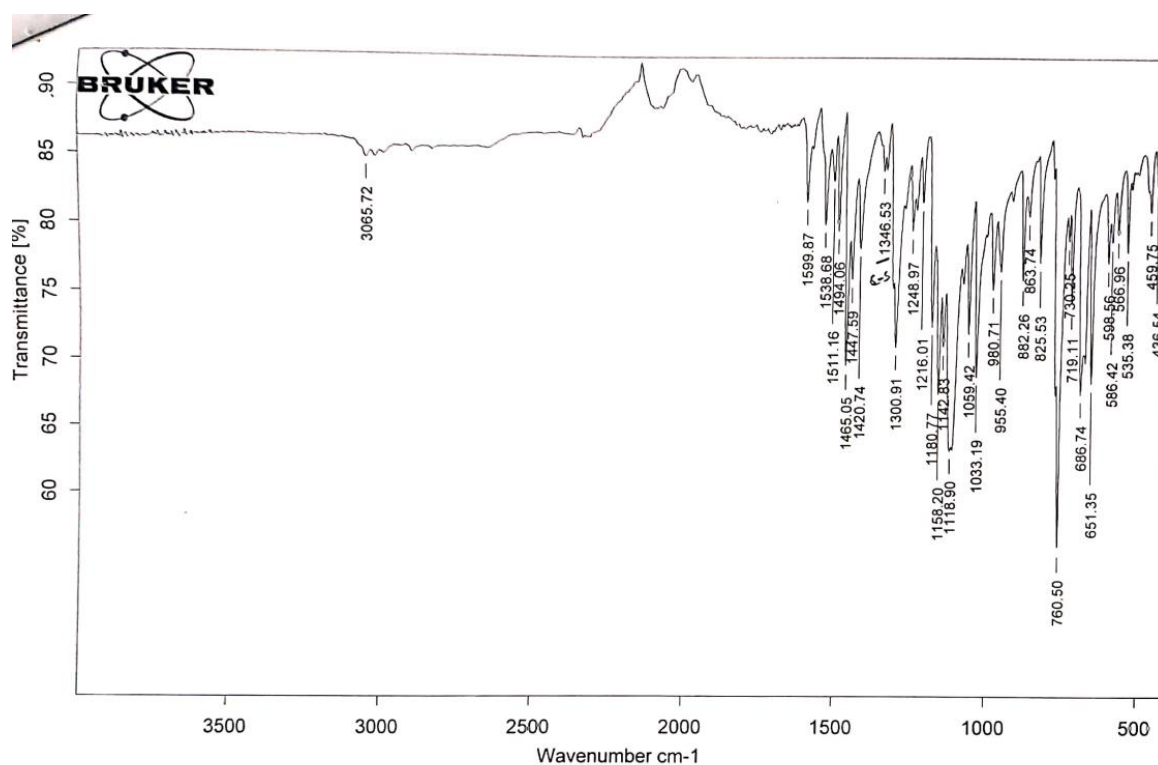
F2 - Acquisition Parameters  
Date\_ 20180625  
Time 15.19  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 35968  
SOLVENT DMSO  
NS 1024  
DS 0  
SWH 17985.611 Hz  
FIDRES 0.500045 Hz  
AQ 0.9999604 sec  
RG 32768  
DW 27.800 usec  
DE 6.00 usec  
TE 294.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 6.00 usec  
PL1 -5.00 dB  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 20.98 dB  
PL13 20.00 dB  
SFO2 300.1312005 MHz

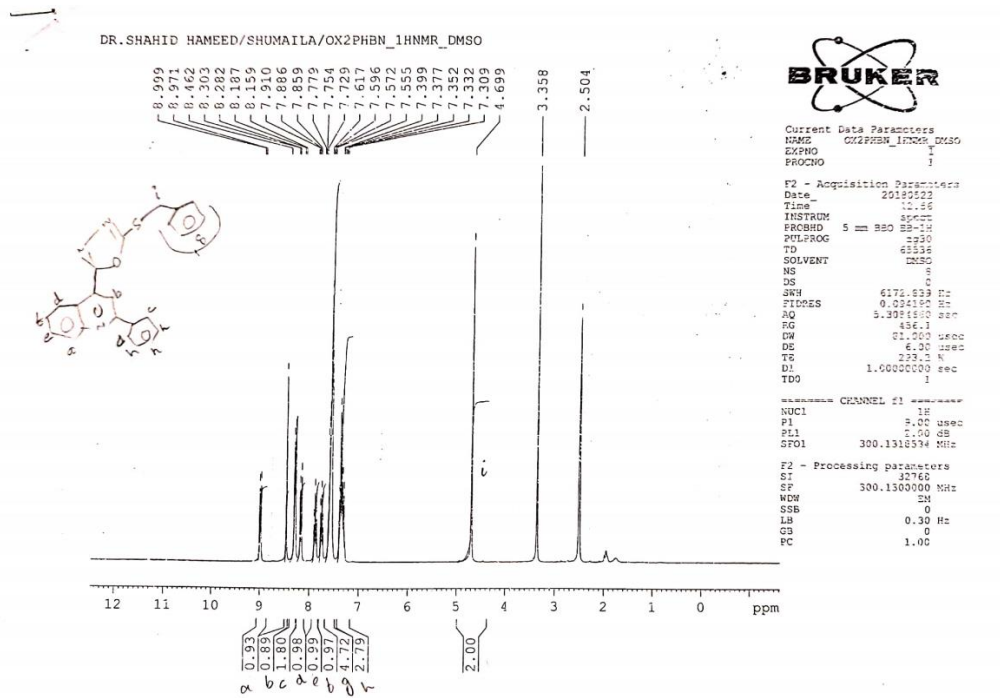
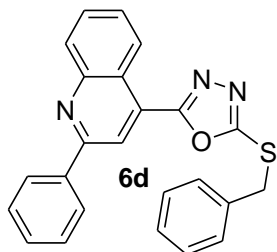
F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

## FT-IR Spectra of 6c



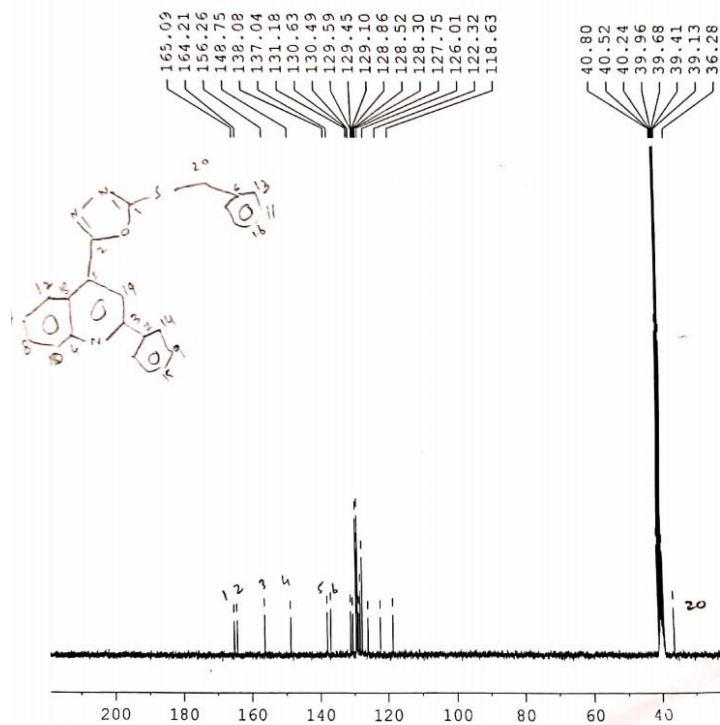
Sample Name: OX2PH2CF3

# **<sup>1</sup>H-NMR Spectra of 6d**



# **<sup>13</sup>C-NMR Spectra of 6d**

DR.SHAHID HAMEED/SHUMAILA/OX2PHBN\_13CNMR\_DMSO



Current Data Parameters  
NAME OX2PHBN\_13CNMR\_DMSO  
EXPNO 1  
PROCNO 1

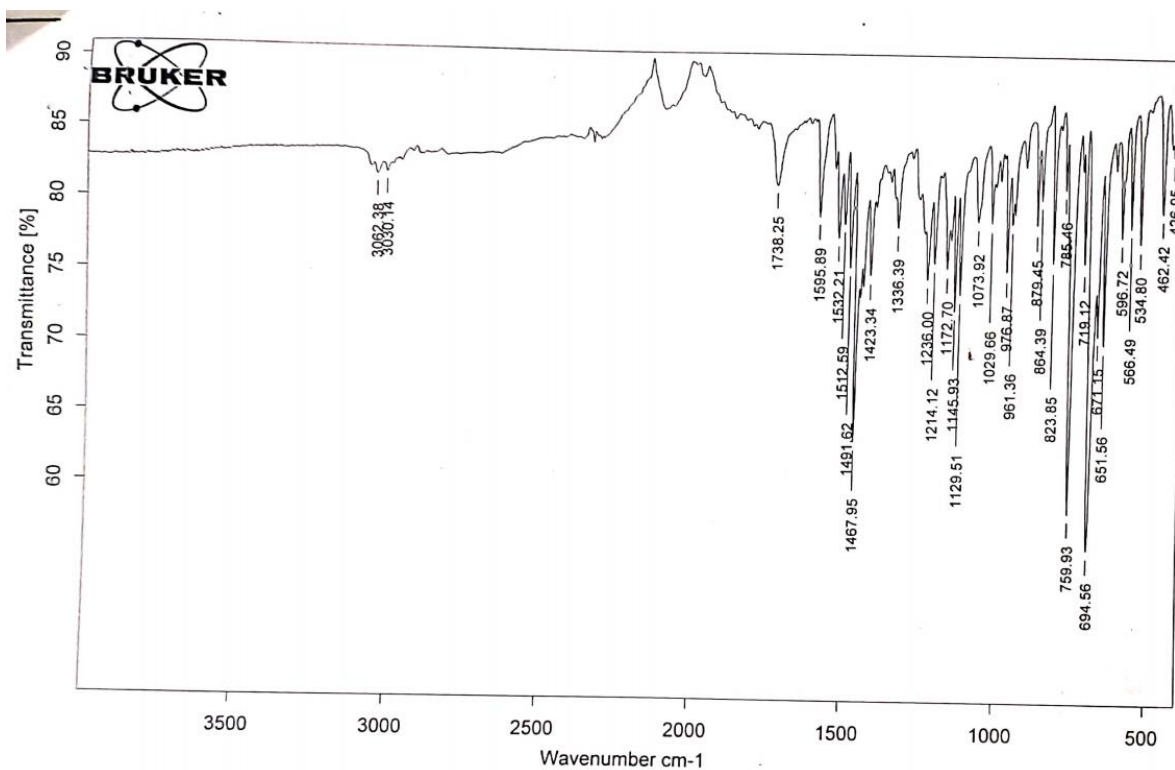
F2 - Acquisition Parameters  
Date\_ 20180522  
Time 12.53  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 35968  
SOLVENT DMSO  
NS 1011  
DS 0  
SWH 17985.611 Hz  
FIDRES 0.500045 Hz  
AQ 0.9999604 sec  
RG 3251  
DW 27.800 usec  
DE 6.00 usec  
TE 293.6 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 6.00 usec  
PL1 -5.00 dB  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 20.98 dB  
PL13 20.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
S1 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

# FT-IR Spectra of 6d



Sample Name: OX2PH BN