Electronic Supplementary Material (ESI) for RSC Advances.

Novel edaravone-based azo dyes: Efficient synthesis, characterization, antibacterial activity, DFT calculations and comprehensive investigation of the solvent effect on the absorption spectra

Mohammad Amin Davasaz Rabbani, Behzad Khalili, Hamid Saeidian

^{1}H NMR, and ^{13}C NMR spectra of Novel edaravone-based azo dyes D1-D10

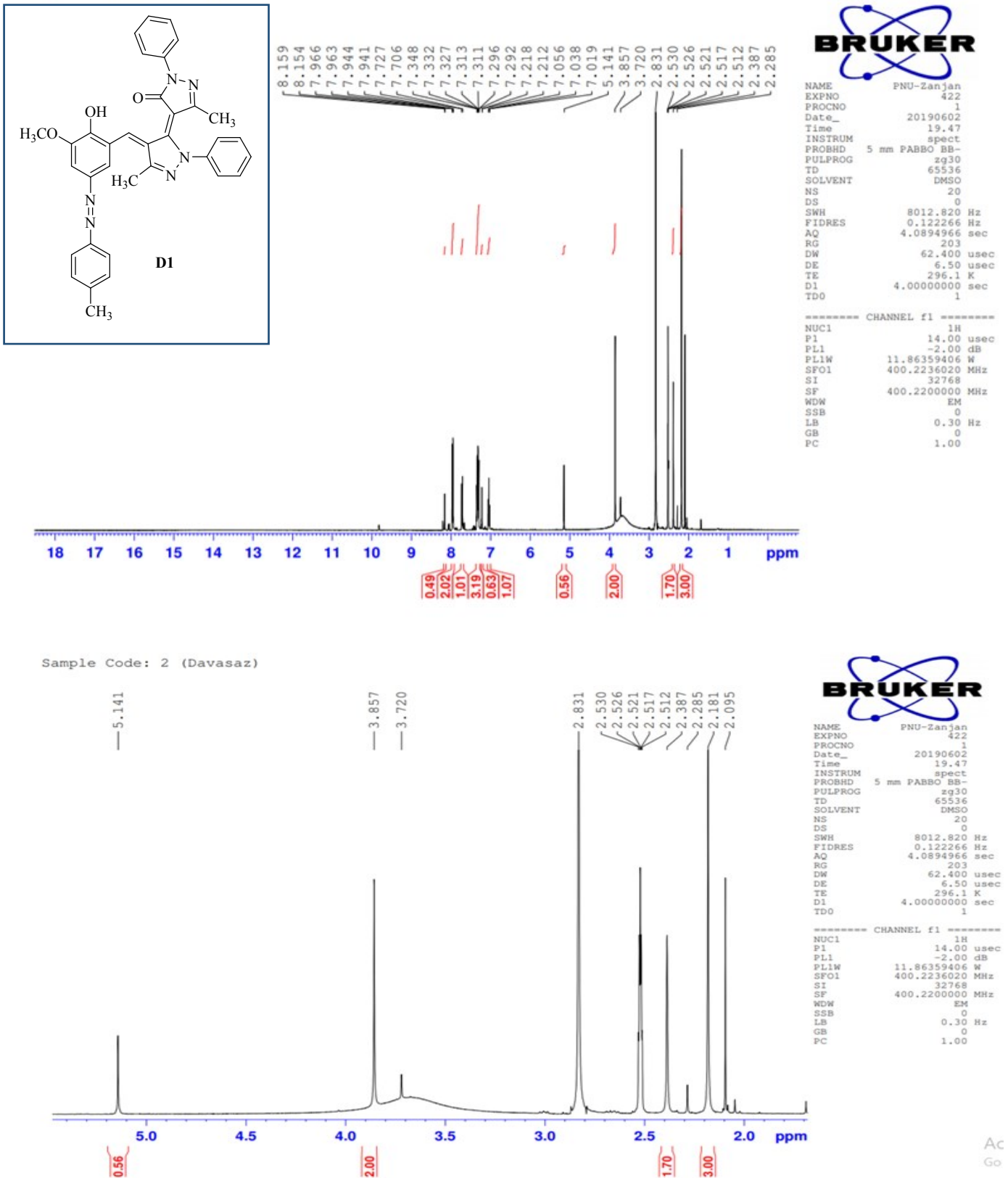


Fig ^{1}H NMR of **D1**

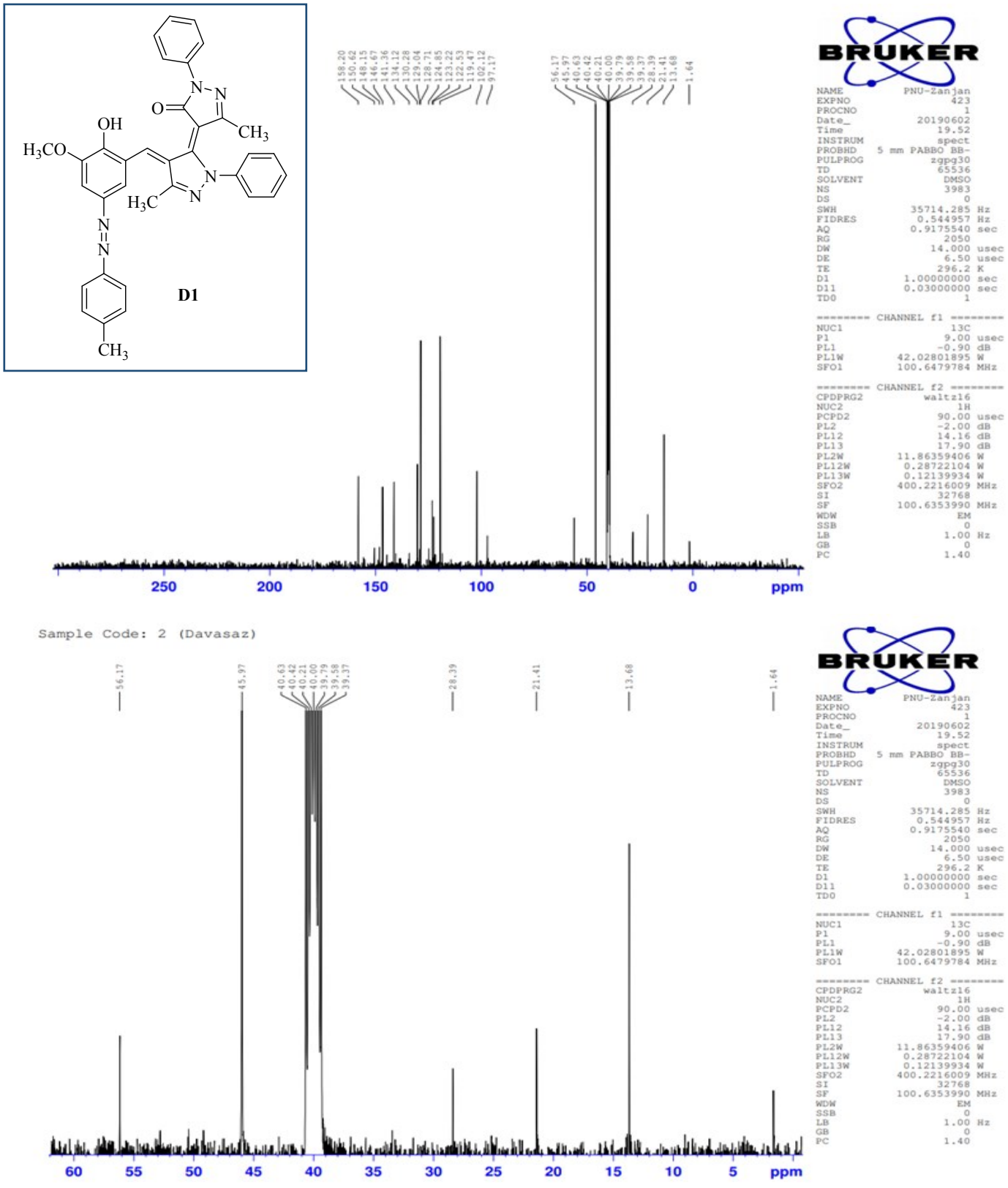
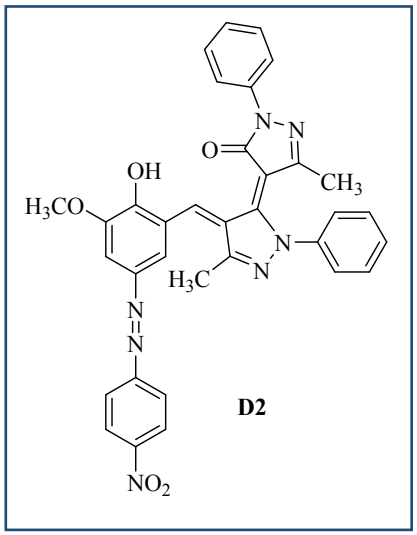
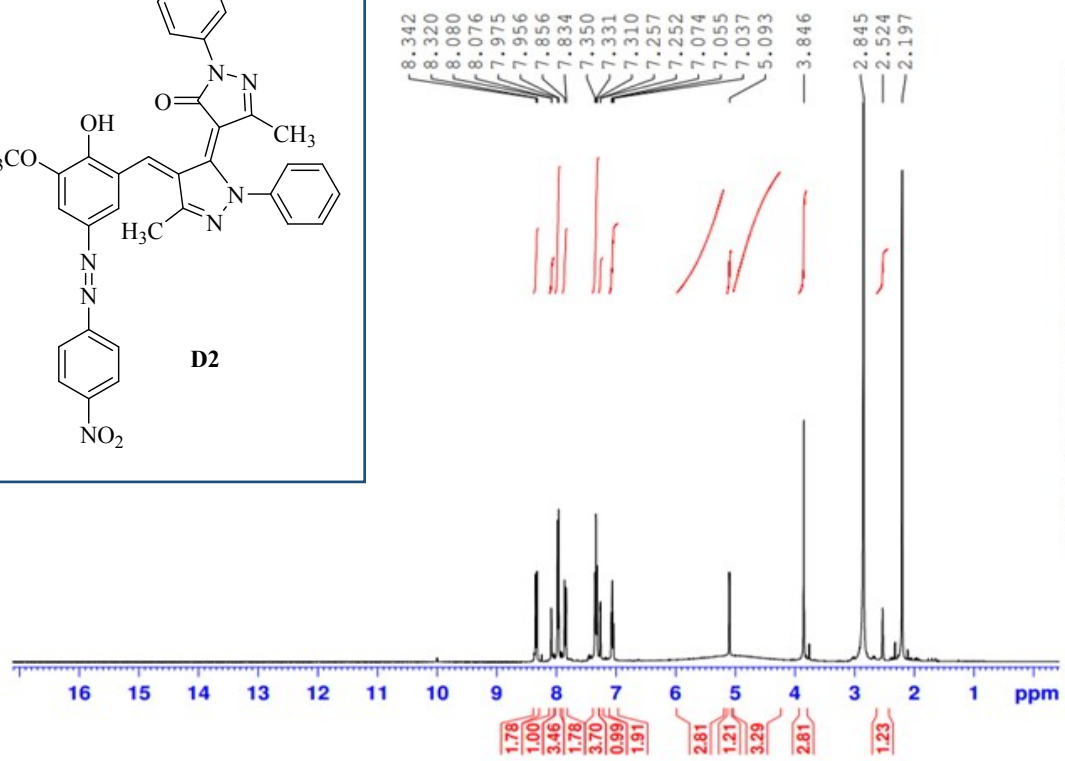


Fig ^{13}C NMR of **D1**.





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NAME                PNU-Zanjan
EXPNO                      412
PROCNO                       1
Date_               20190305
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PROBHD     5 mm PABBO BB-
PULPROG                 zg30
TD                      65536
SOLVENT                 DMSO
NS                         20
DS                          0
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894966 sec
RG                       90.5
DW                    62.400 usec
DE                     6.50 usec
TE                    293.0 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
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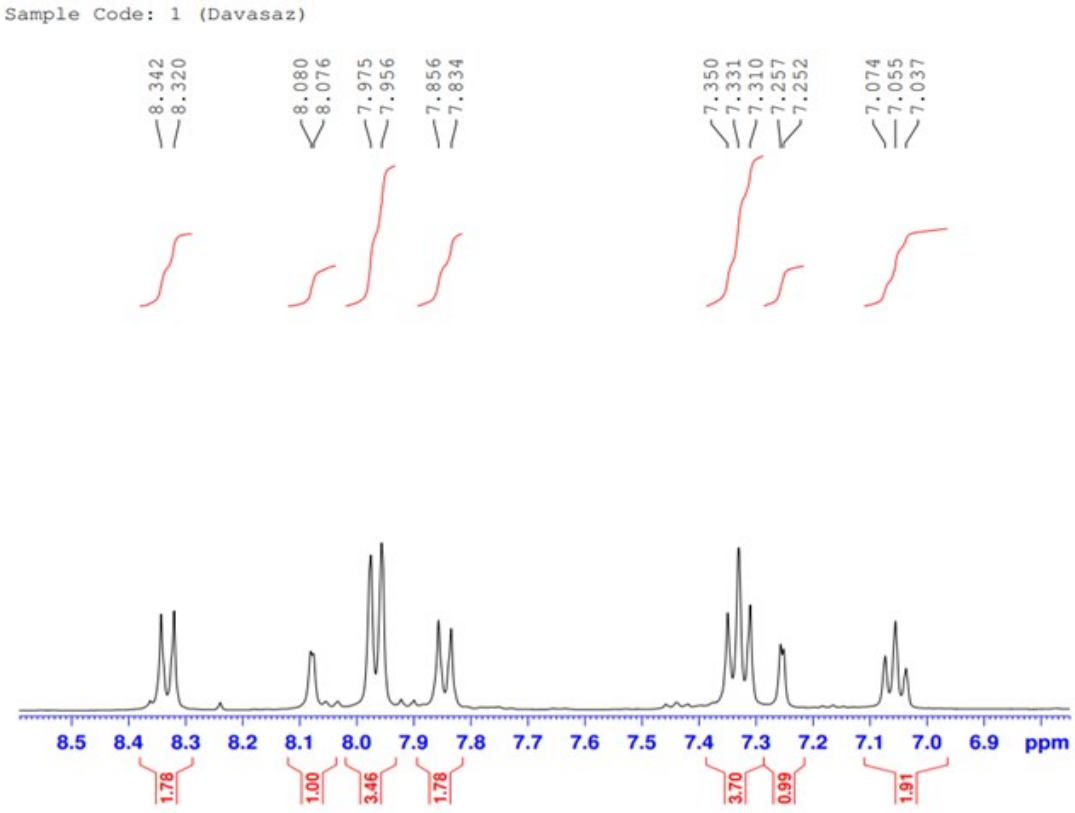

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EXPNO                      412
PROCNO                       1
Date_               20190305
Time                    13.13
INSTRUM                 spect
PROBHD     5 mm PABBO BB-
PULPROG                 zg30
TD                      65536
SOLVENT                 DMSO
NS                         20
DS                          0
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894966 sec
RG                       90.5
DW                    62.400 usec
DE                     6.50 usec
TE                    293.0 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
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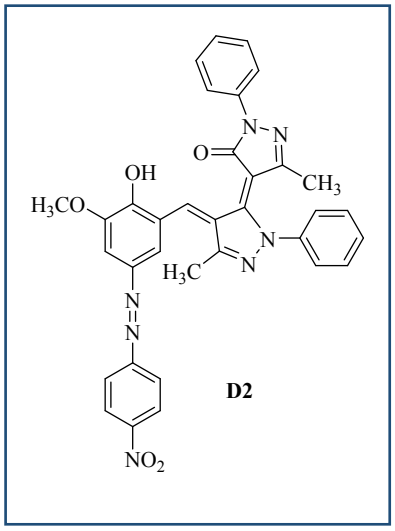
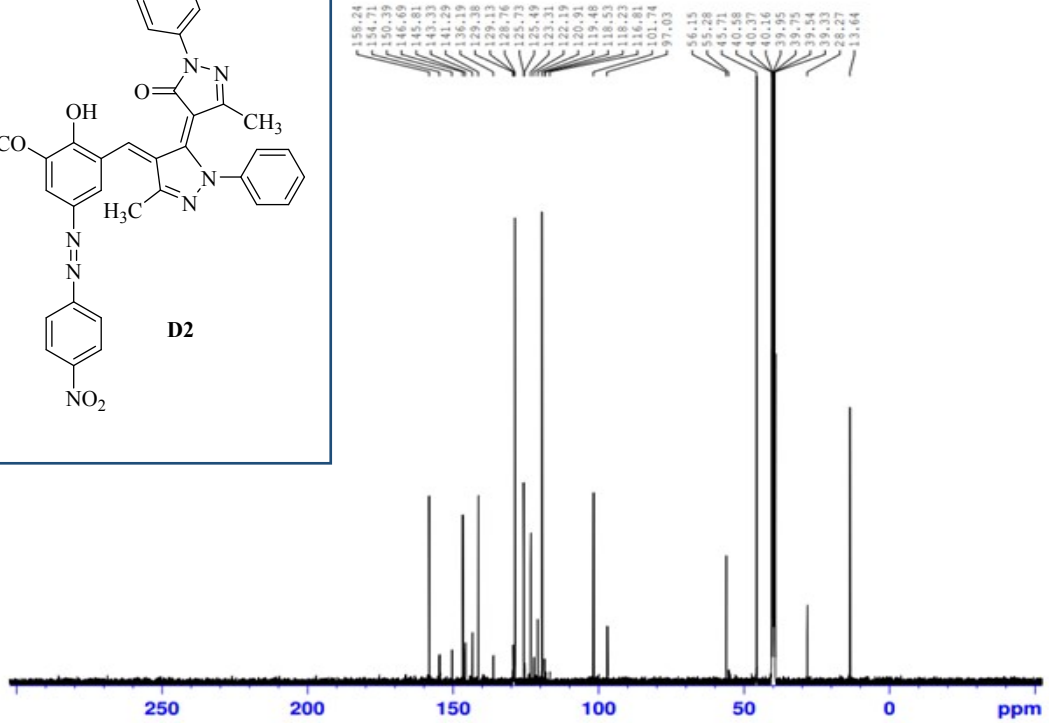
Fig ^{1}H NMR of **D2**





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PROCNO                       1
Date_                 20190309
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TD                      65536
SOLVENT                  DMSO
NS                       3856
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                    293.0 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
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SF            100.6353990 MHz
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SSB                          0
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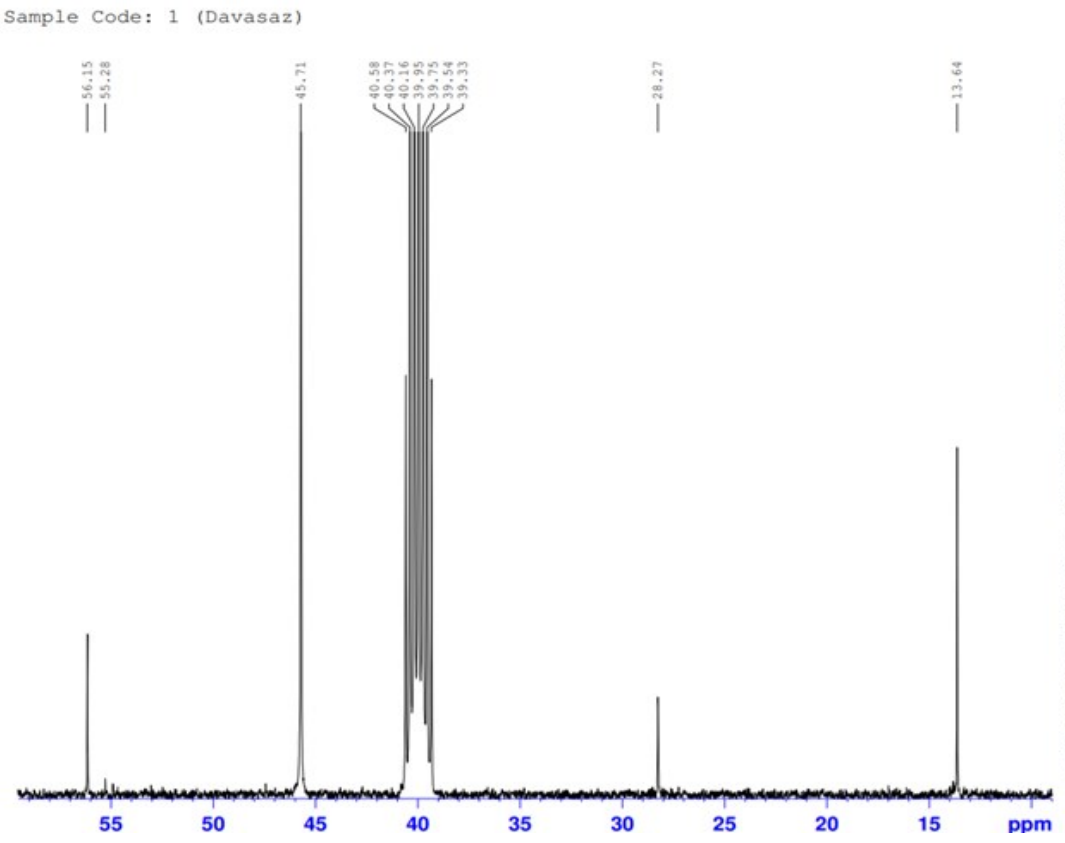

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```
NAME                PNU-Zanjan
EXPNO                      417
PROCNO                       1
Date_                 20190309
Time                     18.54
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       3856
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                    293.0 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
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Fig ^{13}C NMR of **D2**.

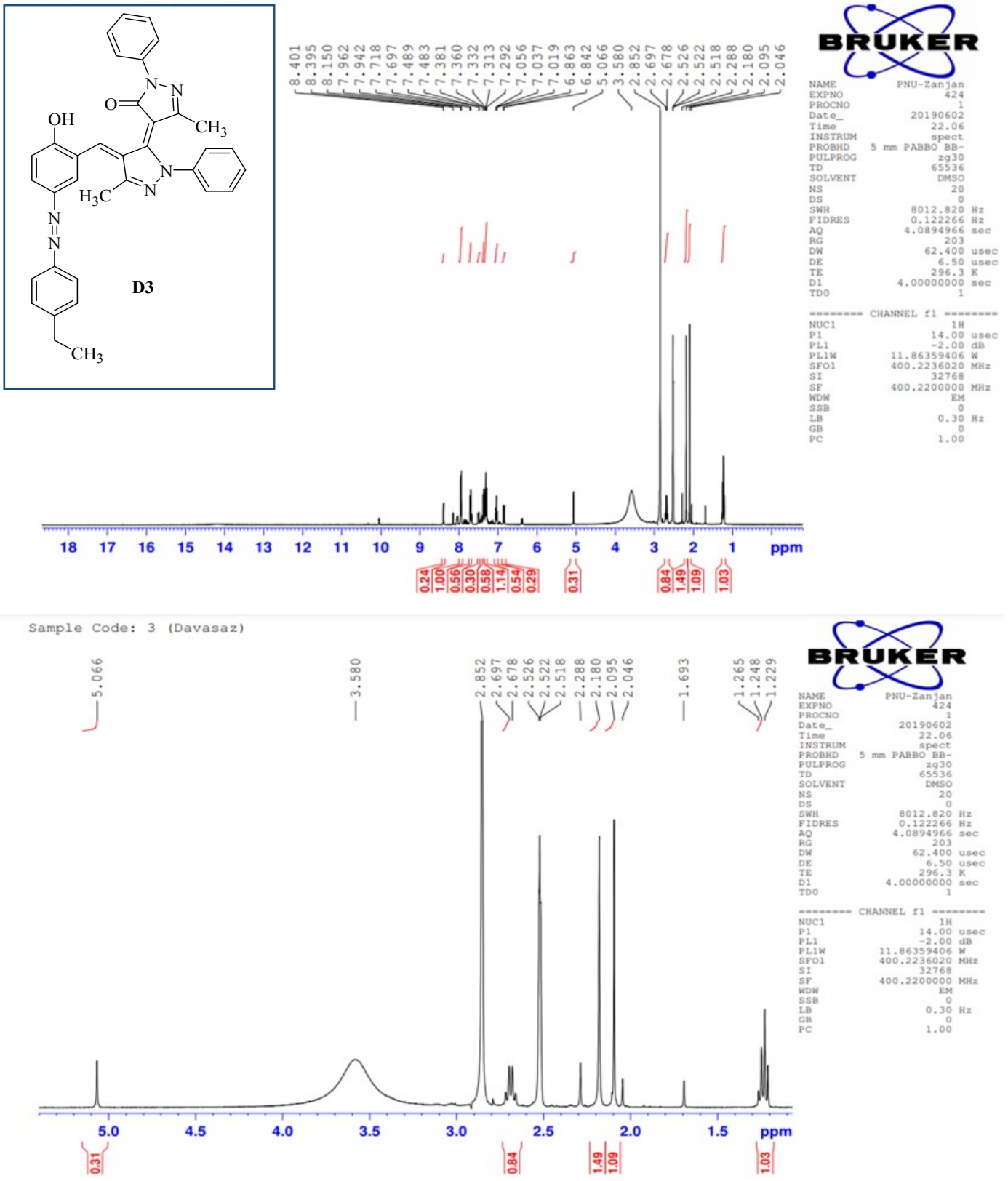


Fig ^{1}H NMR of **D3**.

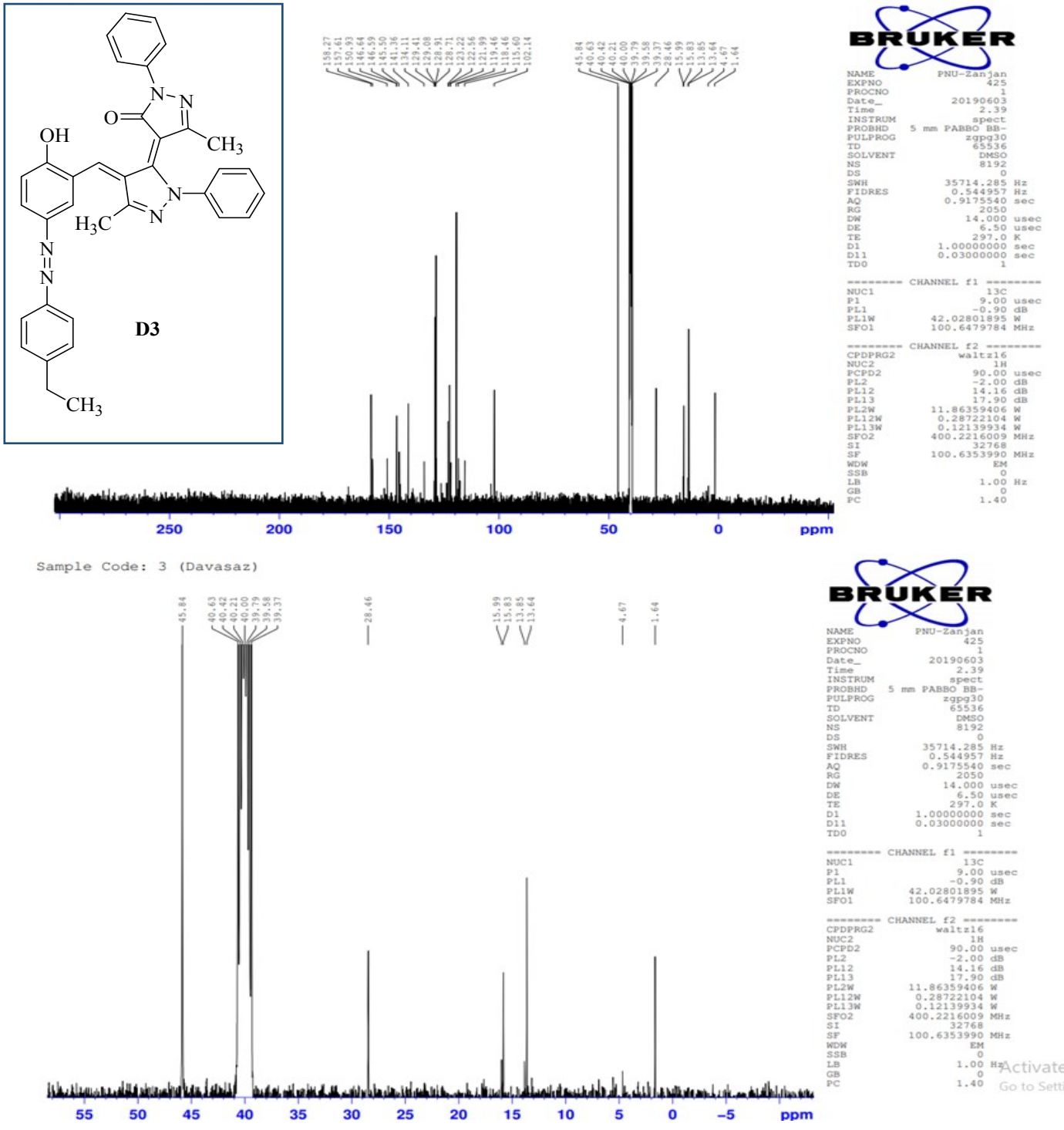


Fig ^{13}C NMR of **D3**.

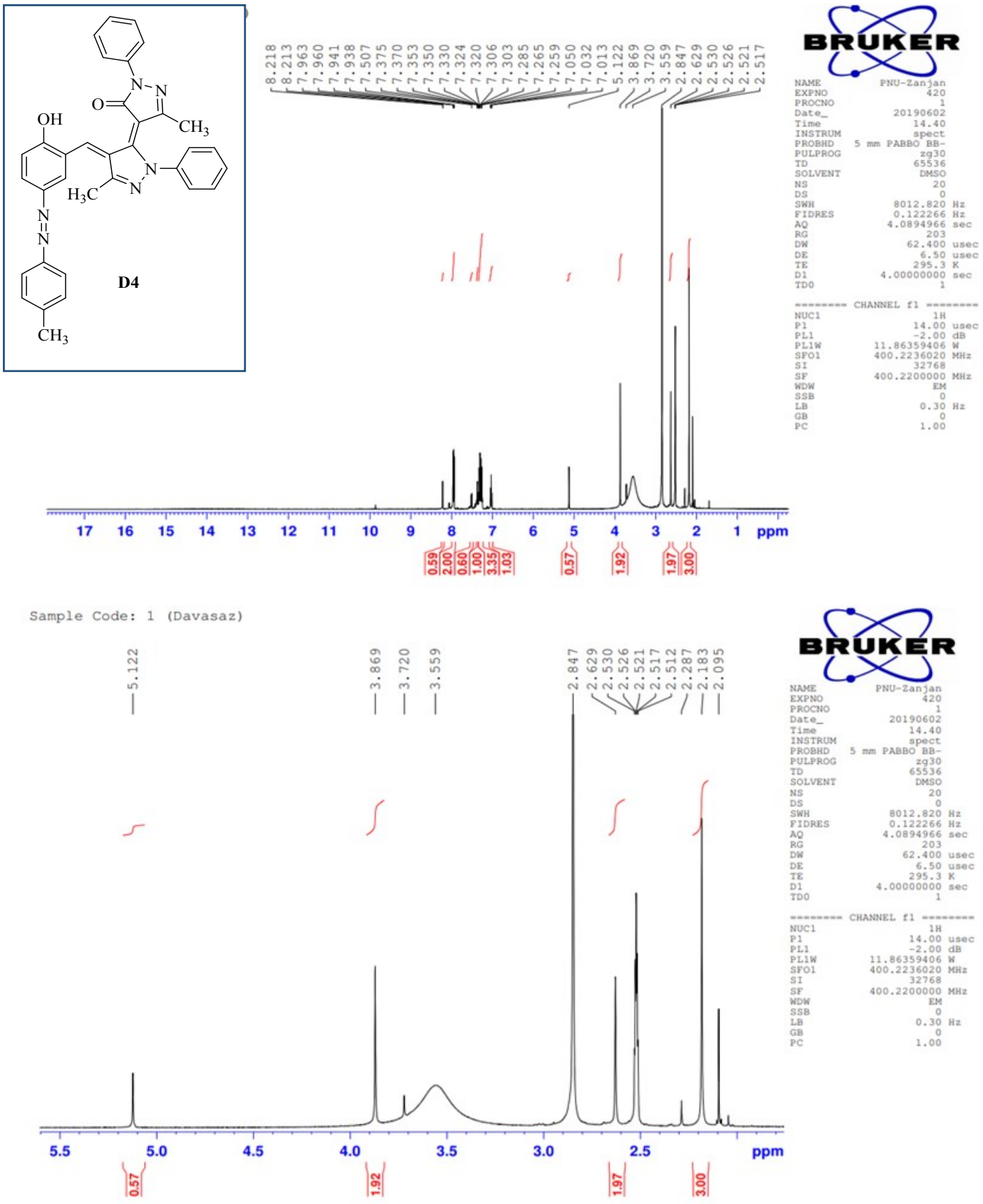


Fig ^{1}H NMR of **D4**.

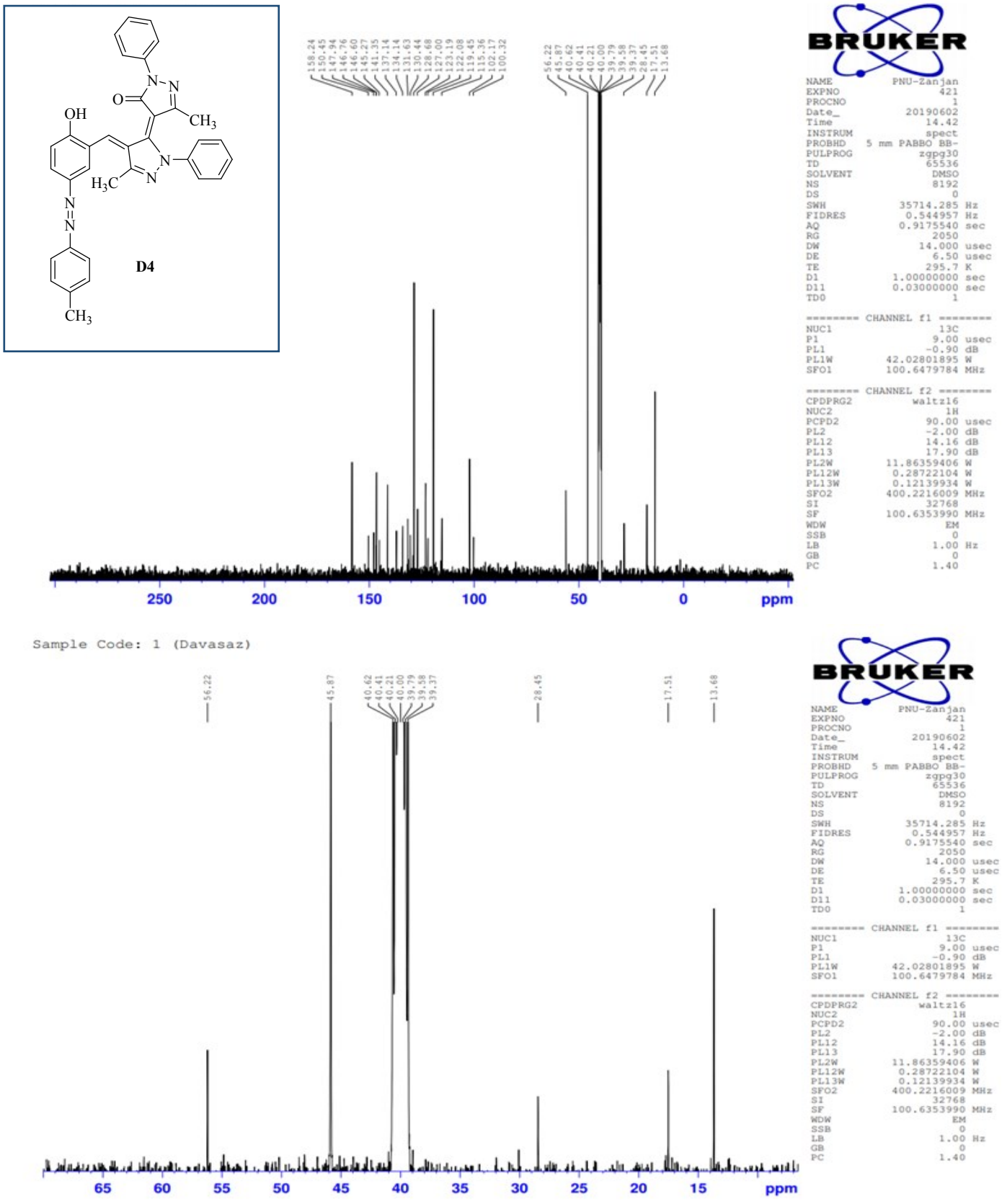


Fig ^{13}C NMR of **D4**.

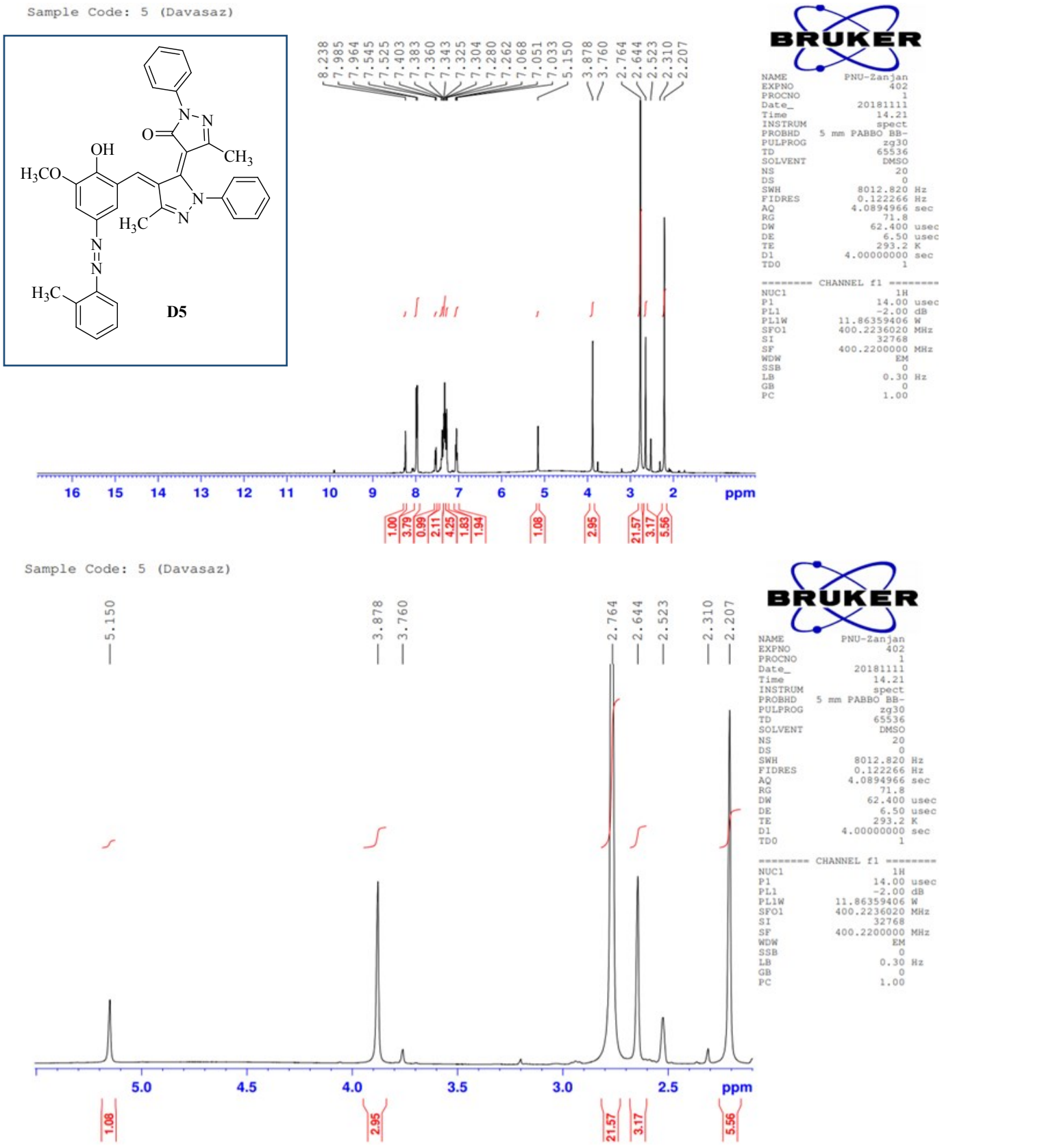
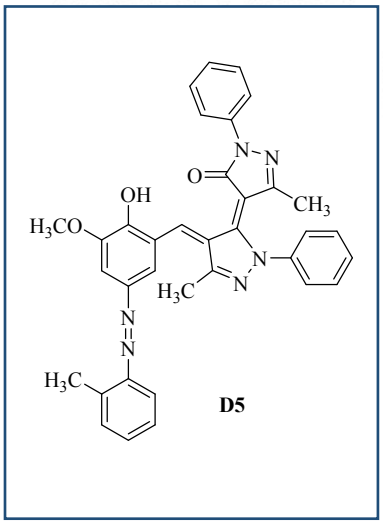
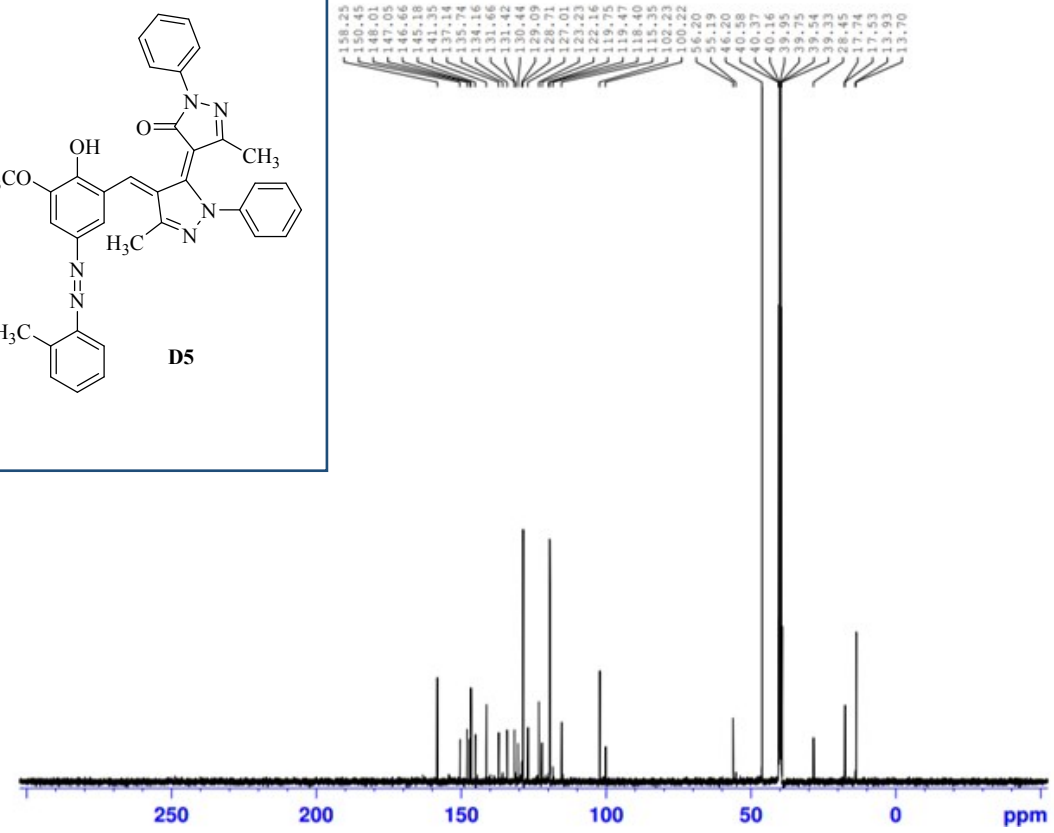


Fig ^{1}H NMR of **D5**





BRUKER

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EXPNO                      411
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PROBHD     5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       1724
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                     292.4 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
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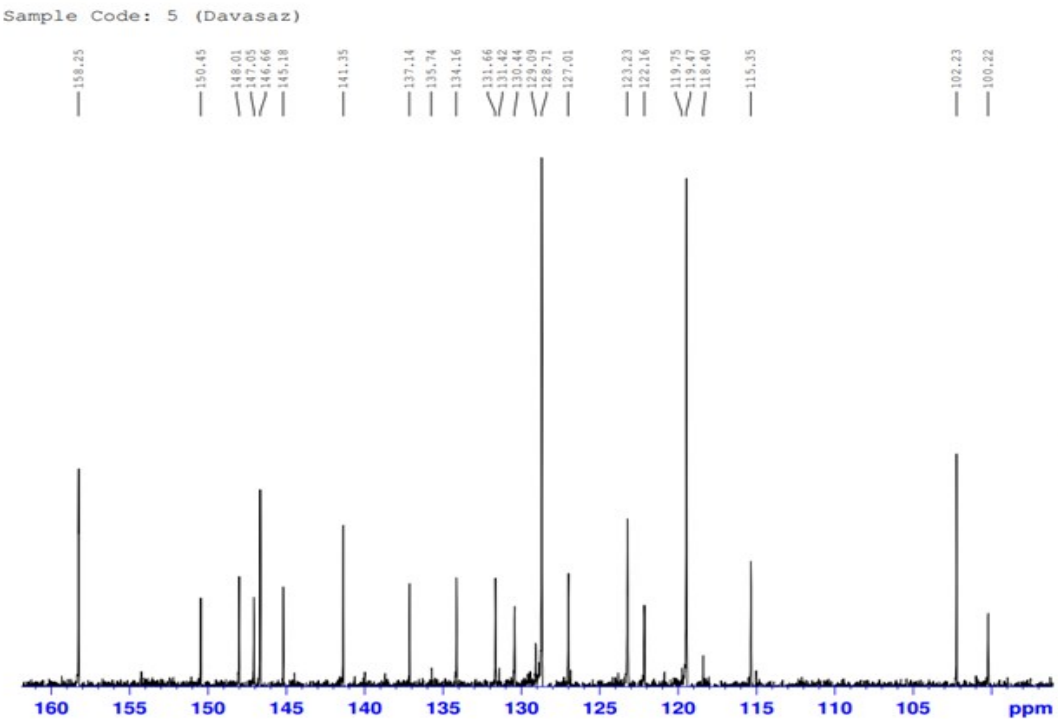

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NAME                PNU-Zanjan
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PROCNO                       1
Date_                 20181117
Time                     12.41
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       1724
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                     292.4 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
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PC                        1.40
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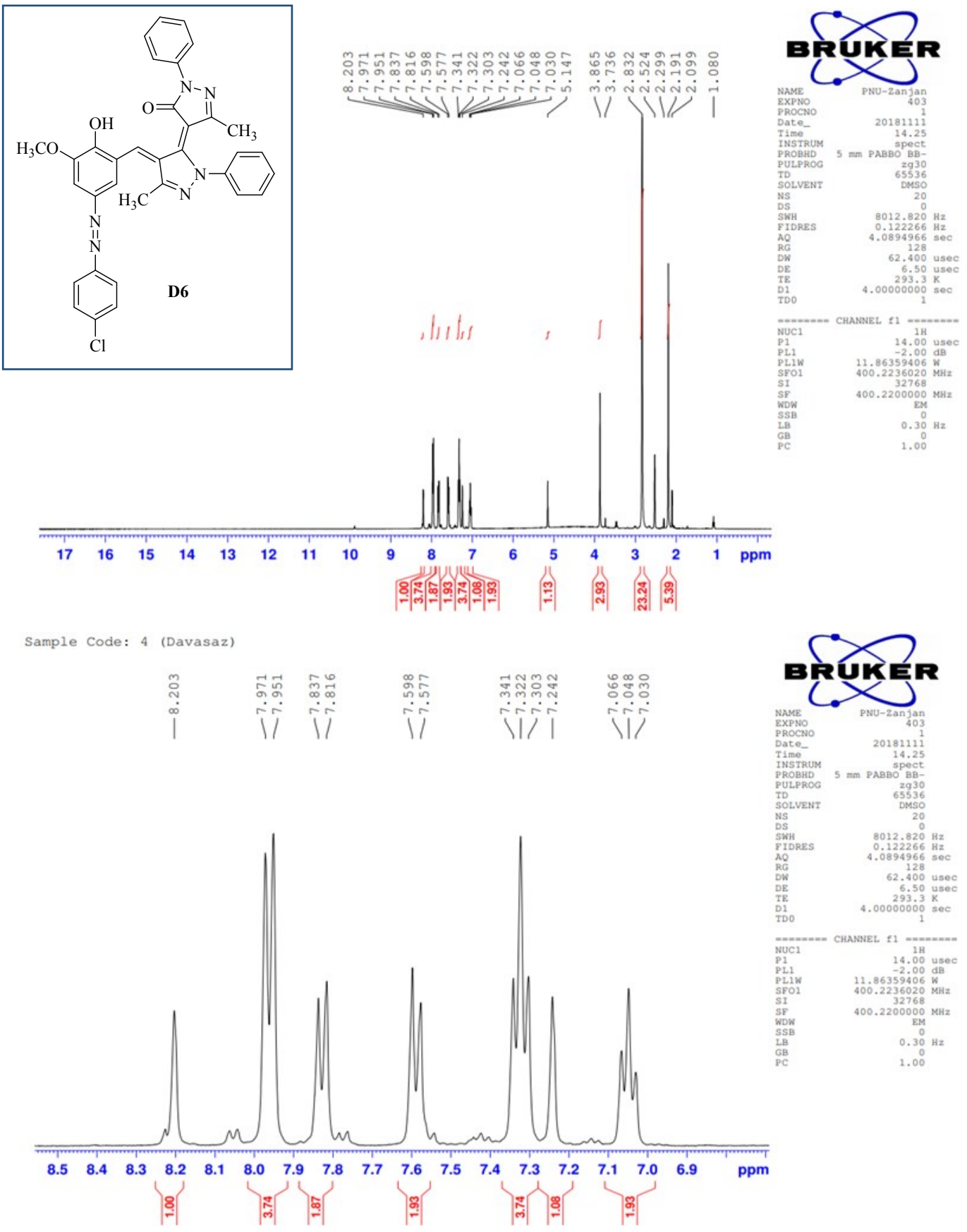
Fig ^{13}C NMR of **D5**.



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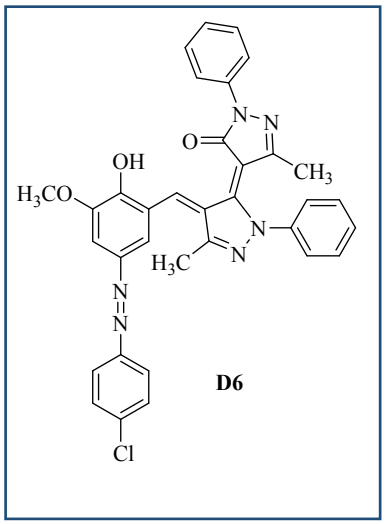
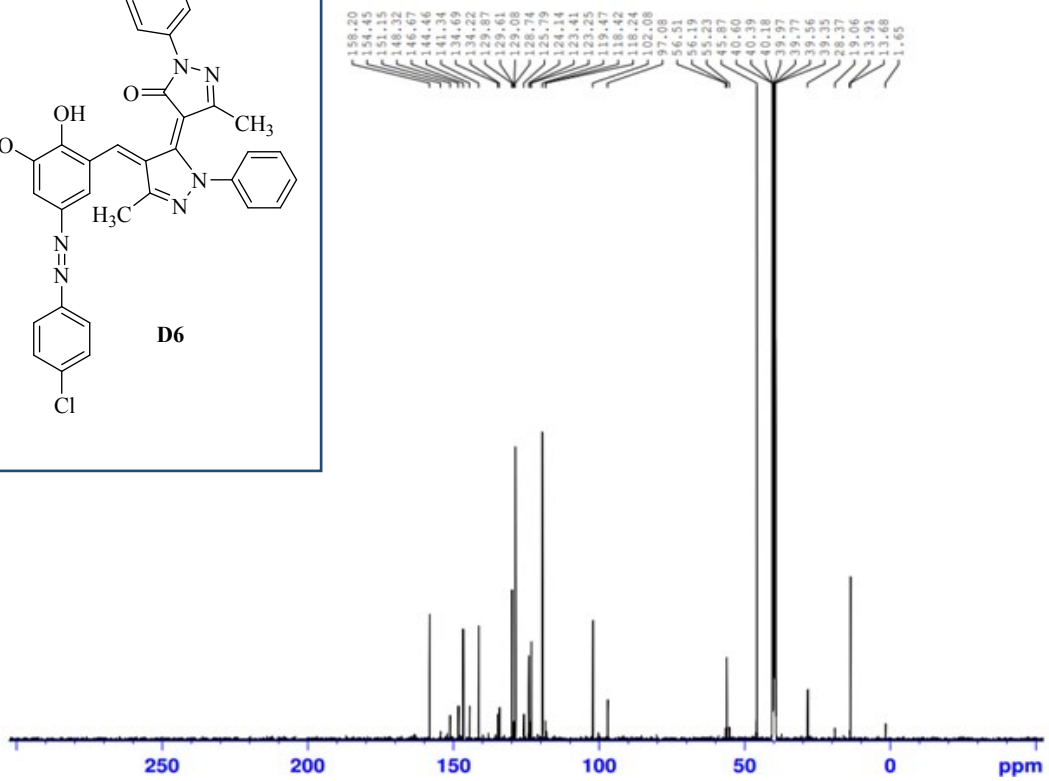


D6



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TD                       65536
SOLVENT                  DMSO
NS                       8192
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FIDRES             0.544957 Hz
AQ                 0.9175540 sec
RG                       2050
DW                     14.000 usec
DE                      6.50 usec
TE                     293.3 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
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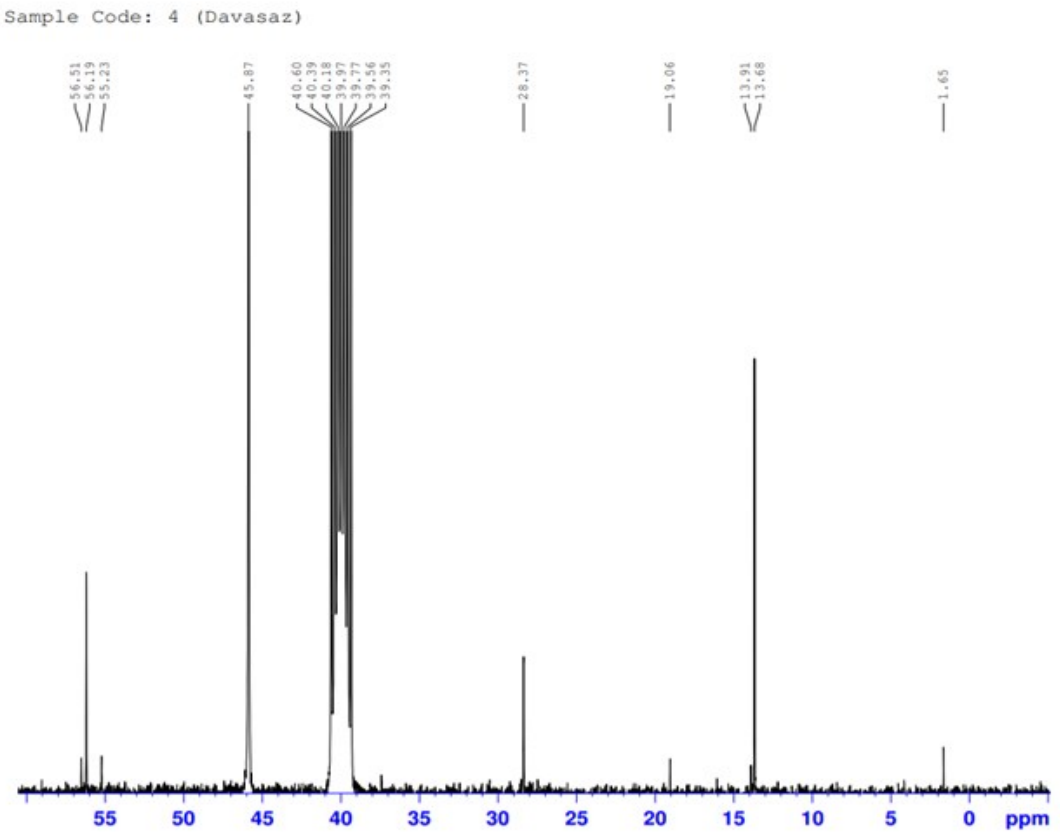

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NAME                PNU-Zanjan
EXPNO                      409
PROCNO                       1
Date_               20181116
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PULPROG                 zgpg30
TD                       65536
SOLVENT                  DMSO
NS                       8192
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                     293.3 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
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Fig ^{13}C NMR of D6.

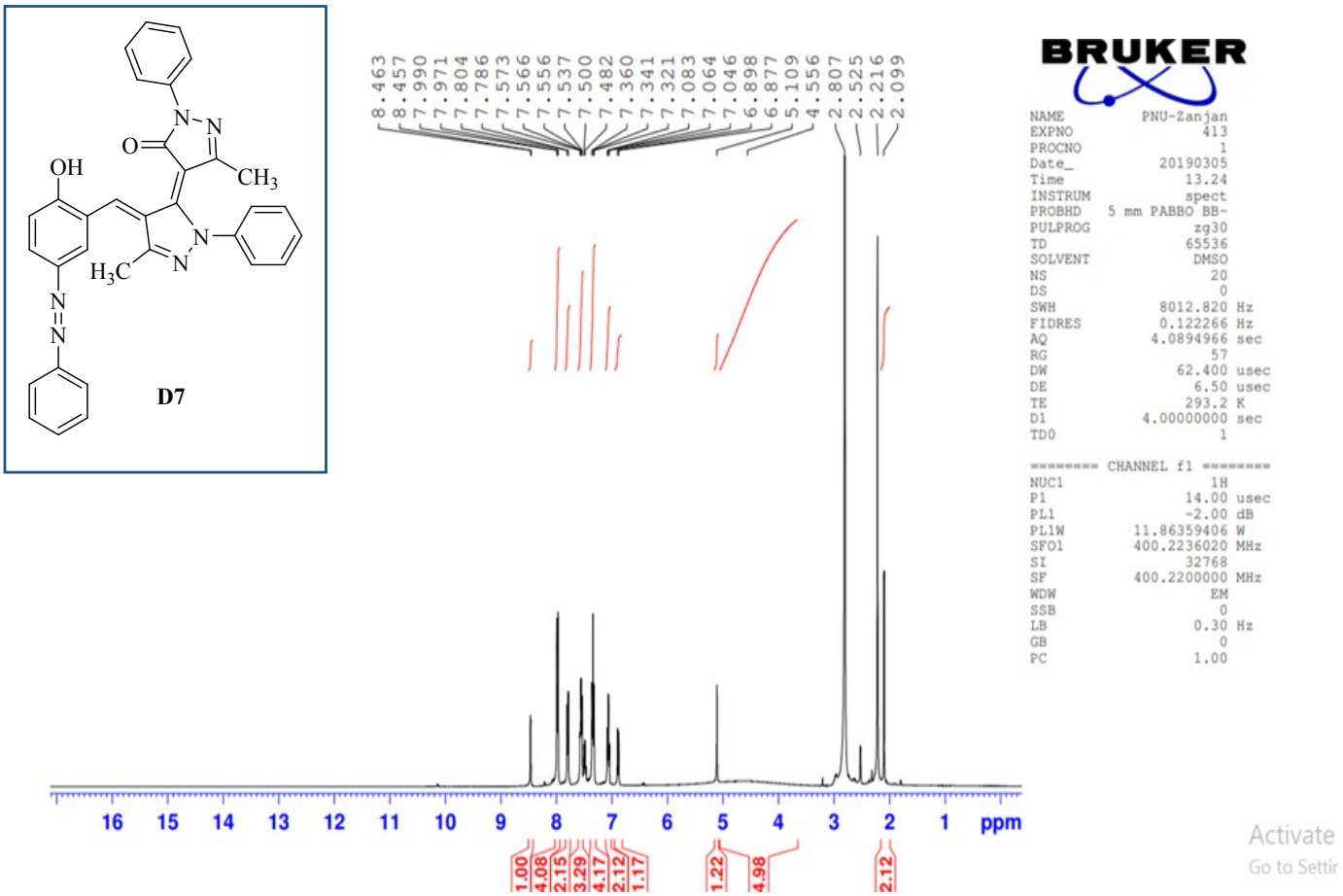


Fig ^{1}H NMR of D7.

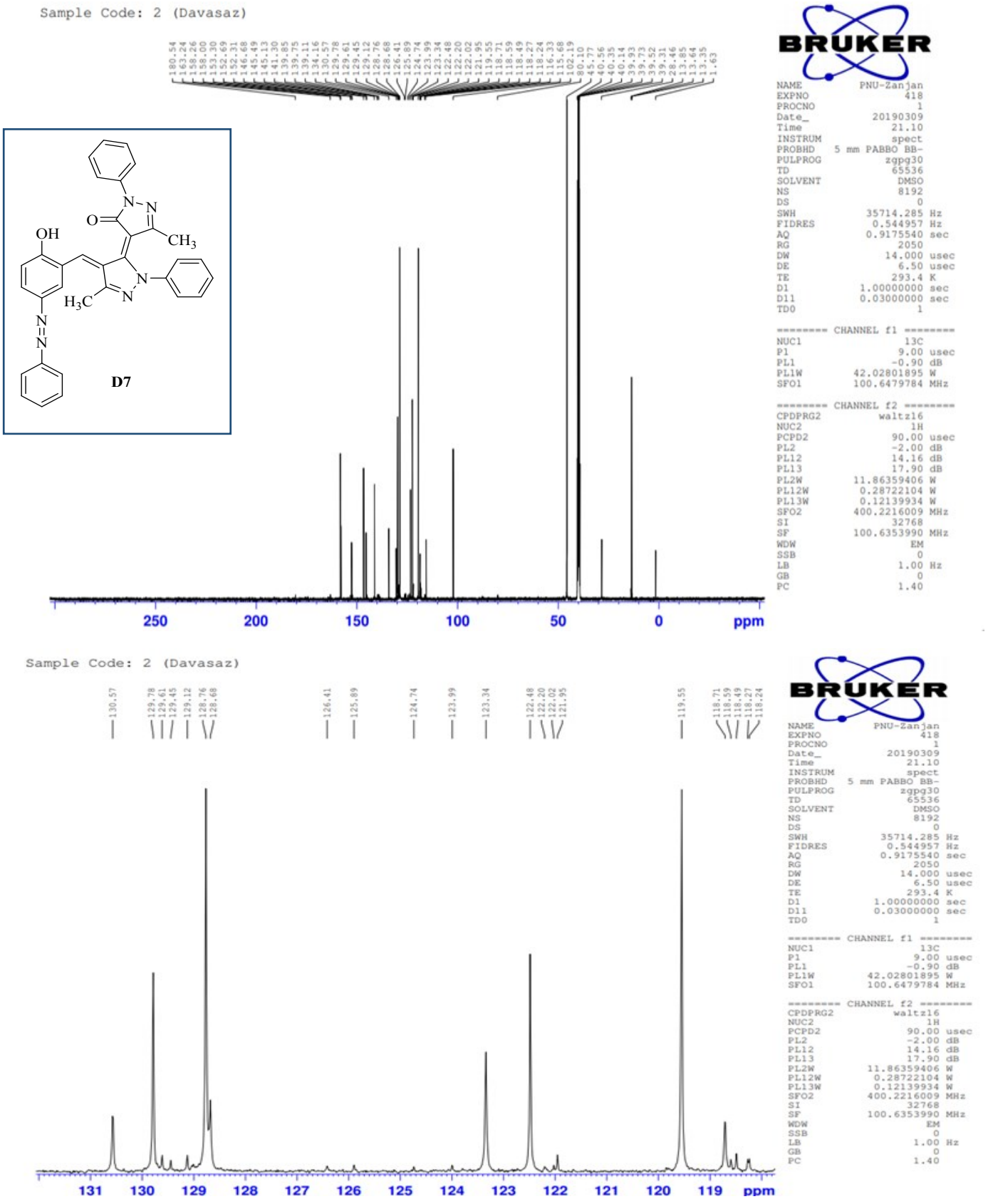
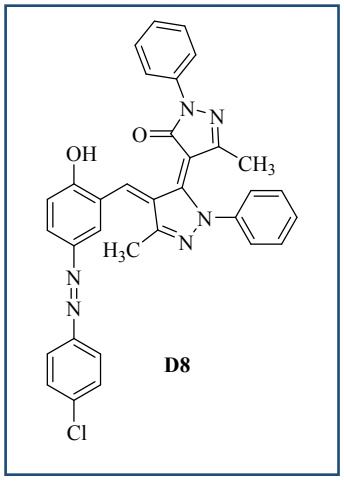
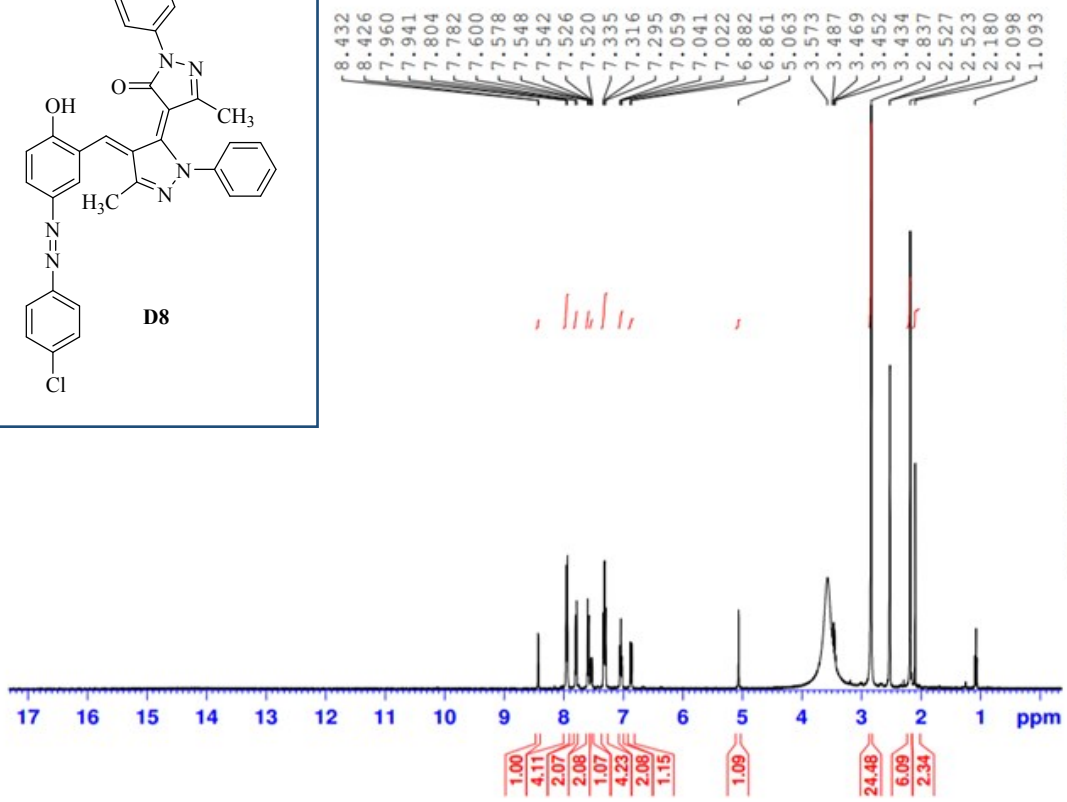


Fig ^{13}C NMR of D7.





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TD                      65536
SOLVENT                  DMSO
NS                         20
DS                          0
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894966 sec
RG                         228
DW                    62.400 usec
DE                     6.50 usec
TE                     293.3 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                          no
SSB                           0
LB                     0.00 Hz
GB                            0
PC                         1.00
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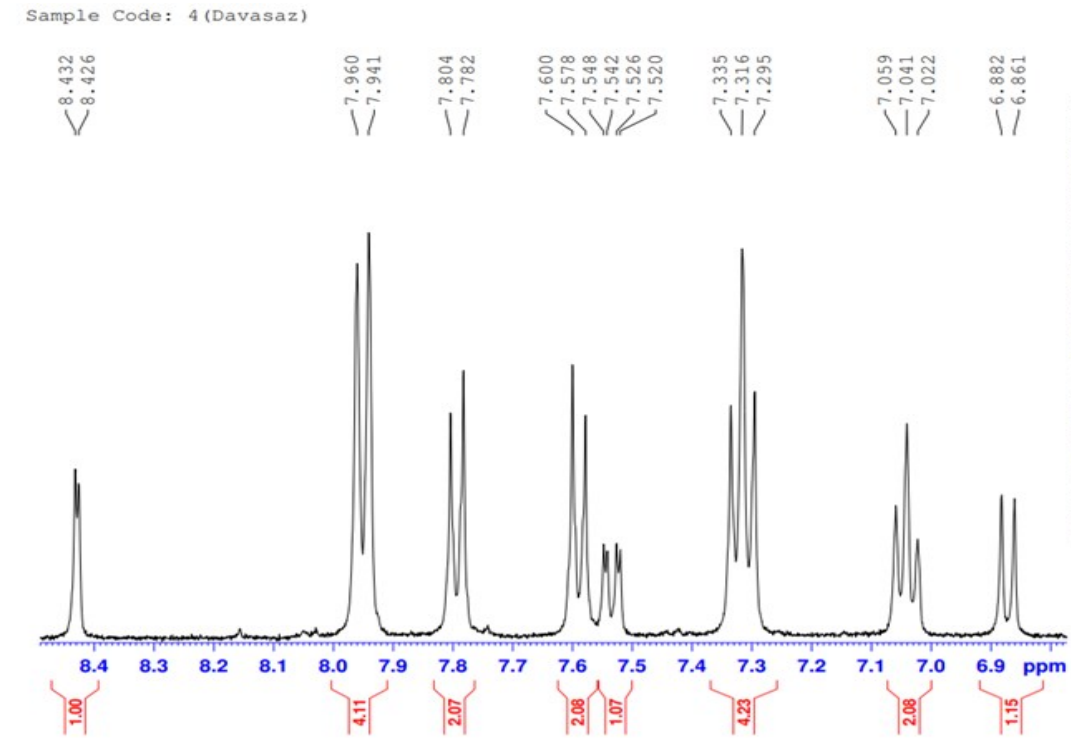

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PULPROG                  zg30
TD                      65536
SOLVENT                  DMSO
NS                         20
DS                          0
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894966 sec
RG                         228
DW                    62.400 usec
DE                     6.50 usec
TE                     293.3 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                          no
SSB                           0
LB                     0.00 Hz
GB                            0
PC                         1.00
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Fig ^{1}H NMR of **D8**.

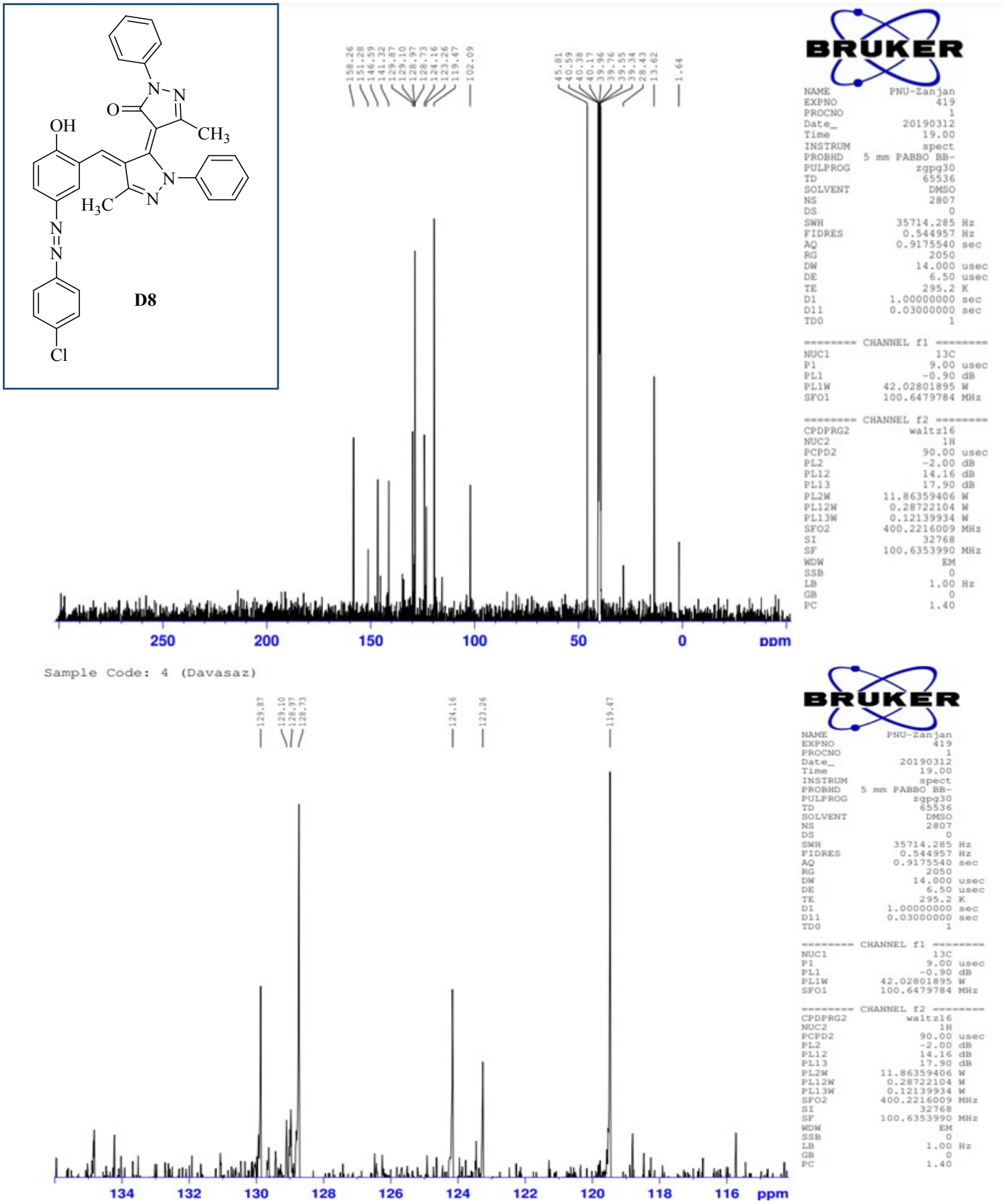
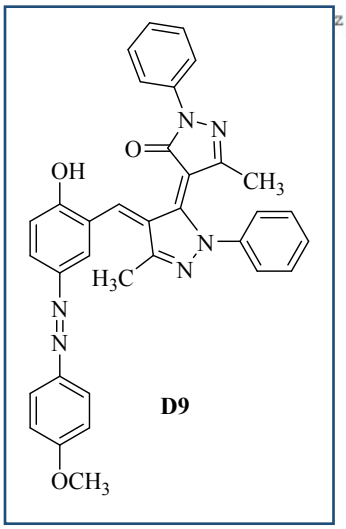
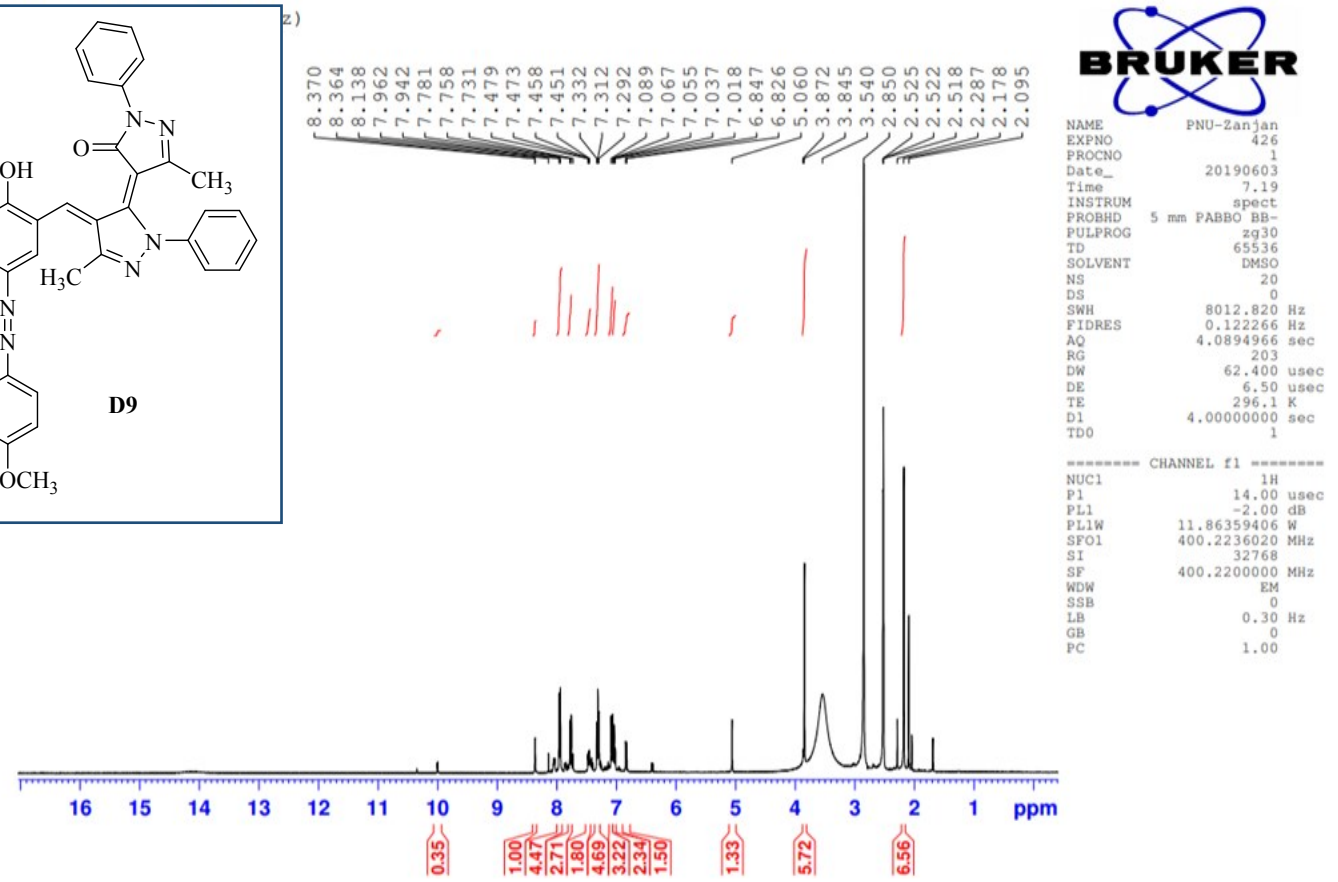


Fig ^{13}C NMR of **D8**.





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TD                      65536
SOLVENT                  DMSO
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                    296.1 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
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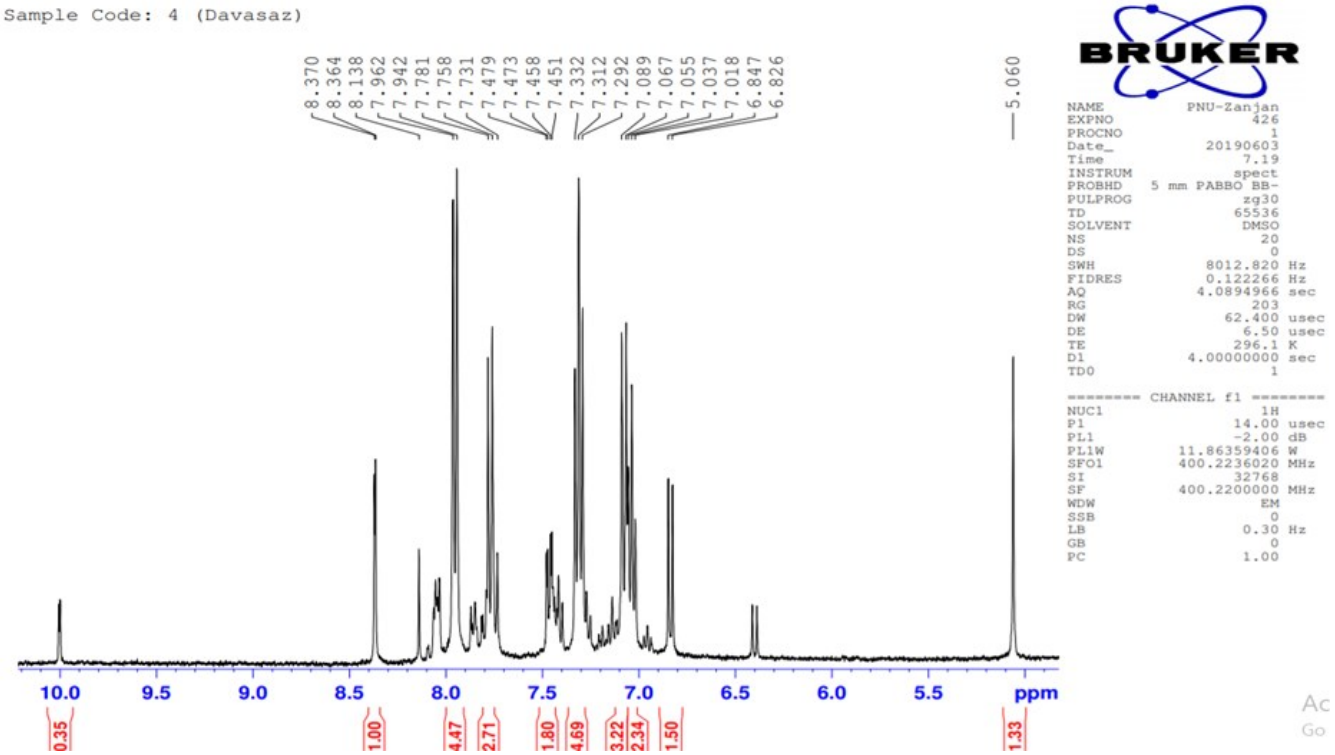

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NAME                PNU-Zanjan
EXPNO                      426
PROCNO                       1
Date_                 20190603
Time                      7.19
INSTRUM                  spect
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PULPROG                  zg30
TD                      65536
SOLVENT                  DMSO
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                    296.1 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
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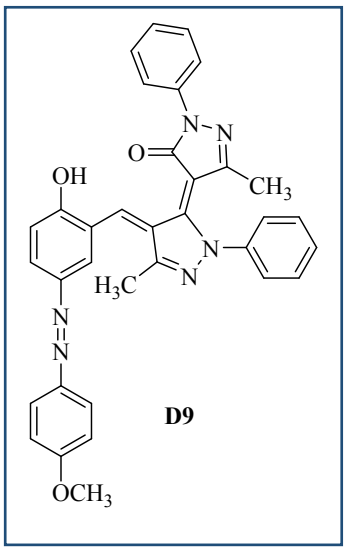
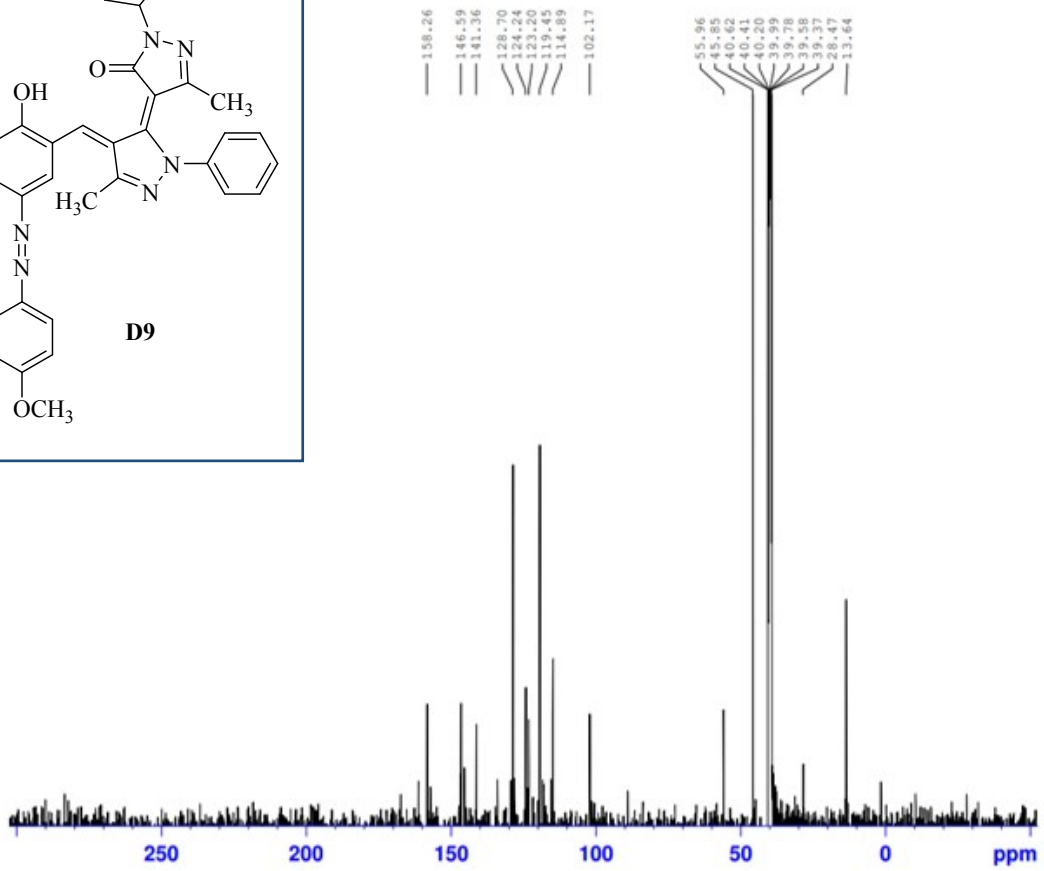
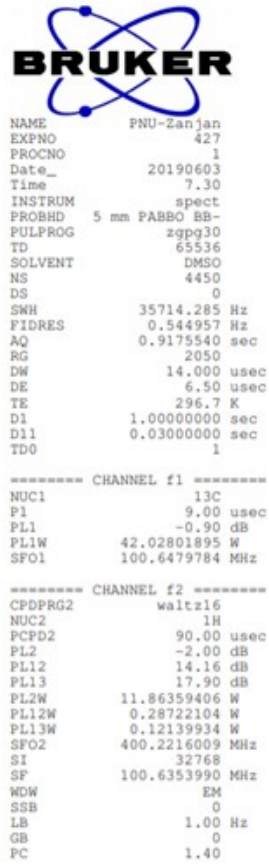
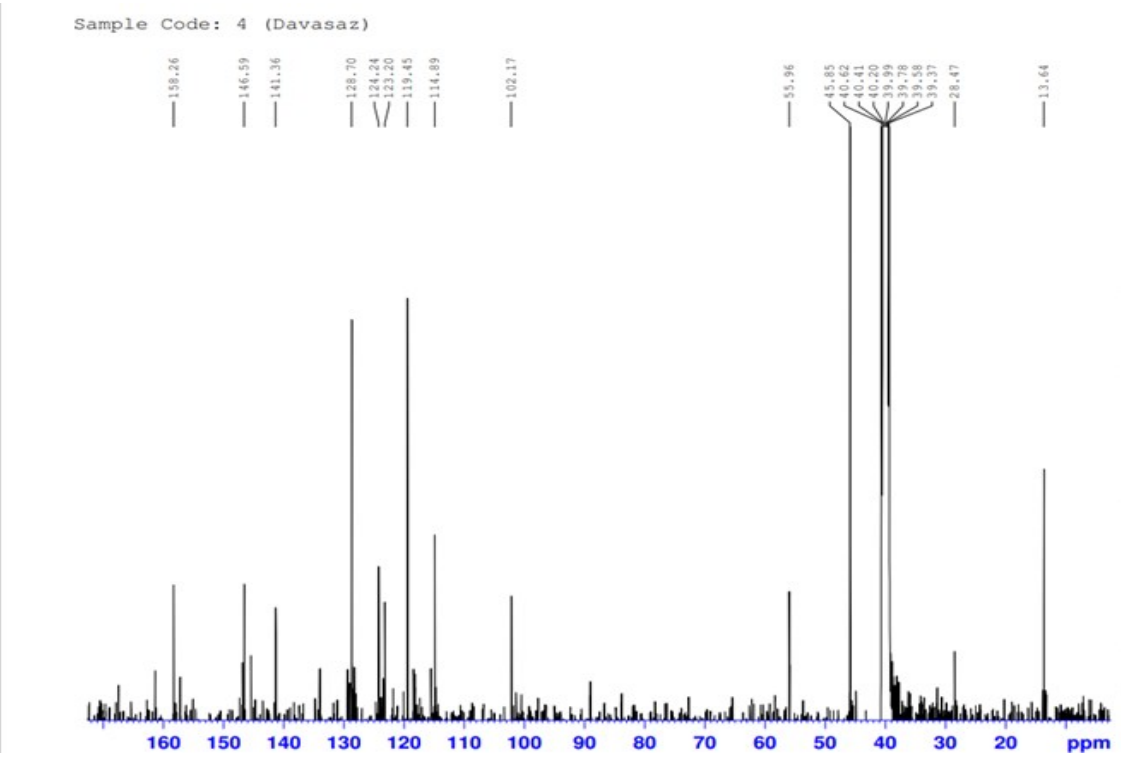
Fig ^{1}H NMR of **D9**.









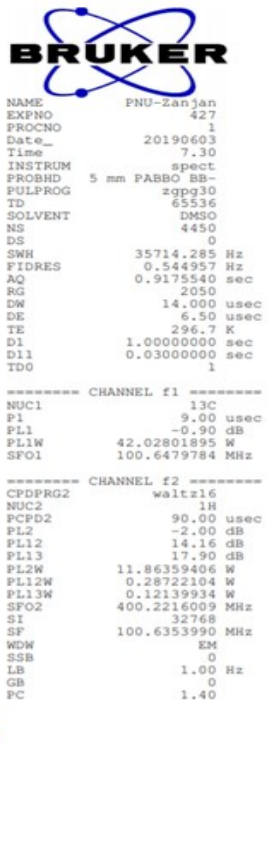


Fig ^{13}C NMR of **D9**.

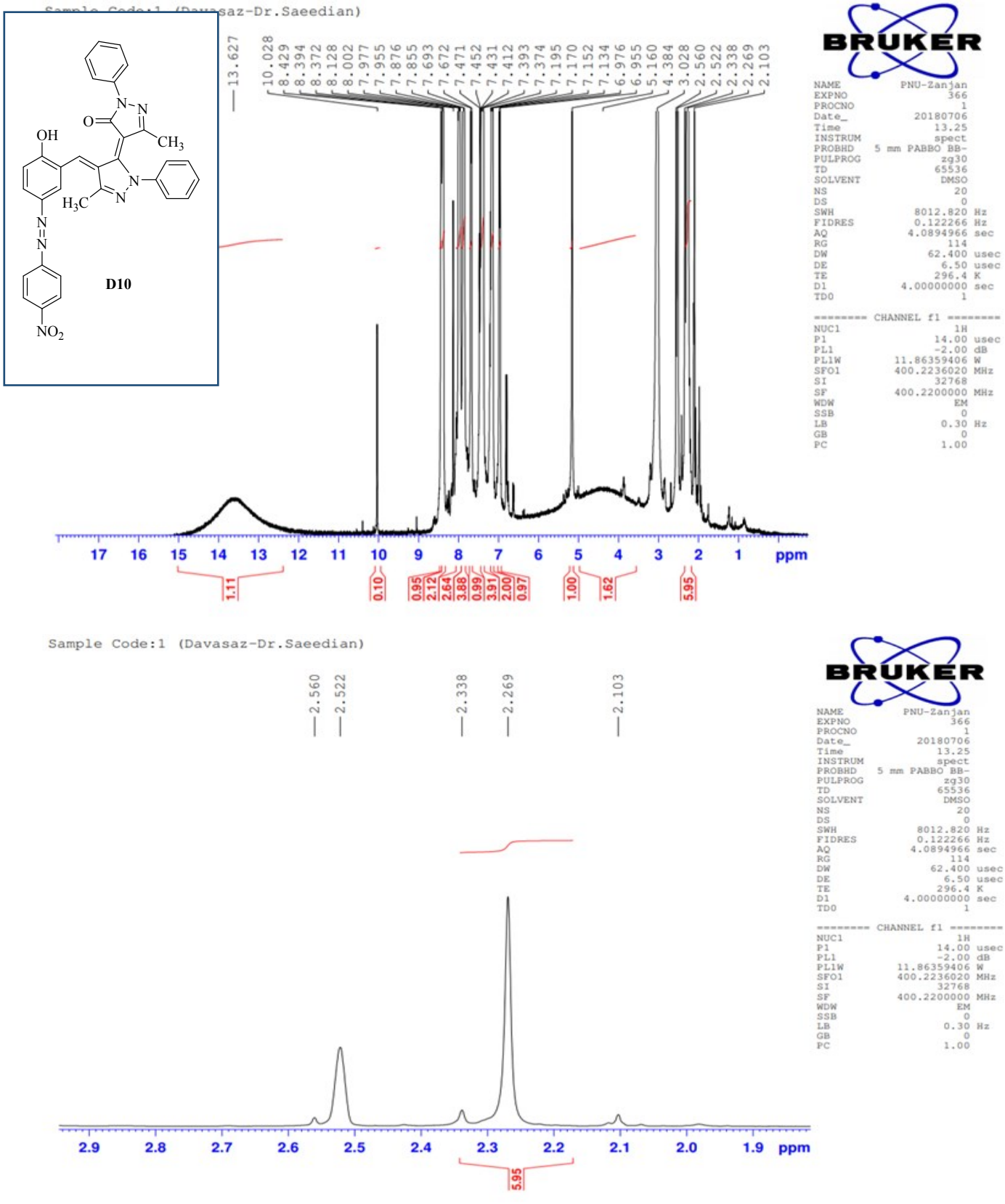


Fig ^{1}H NMR of **D10**

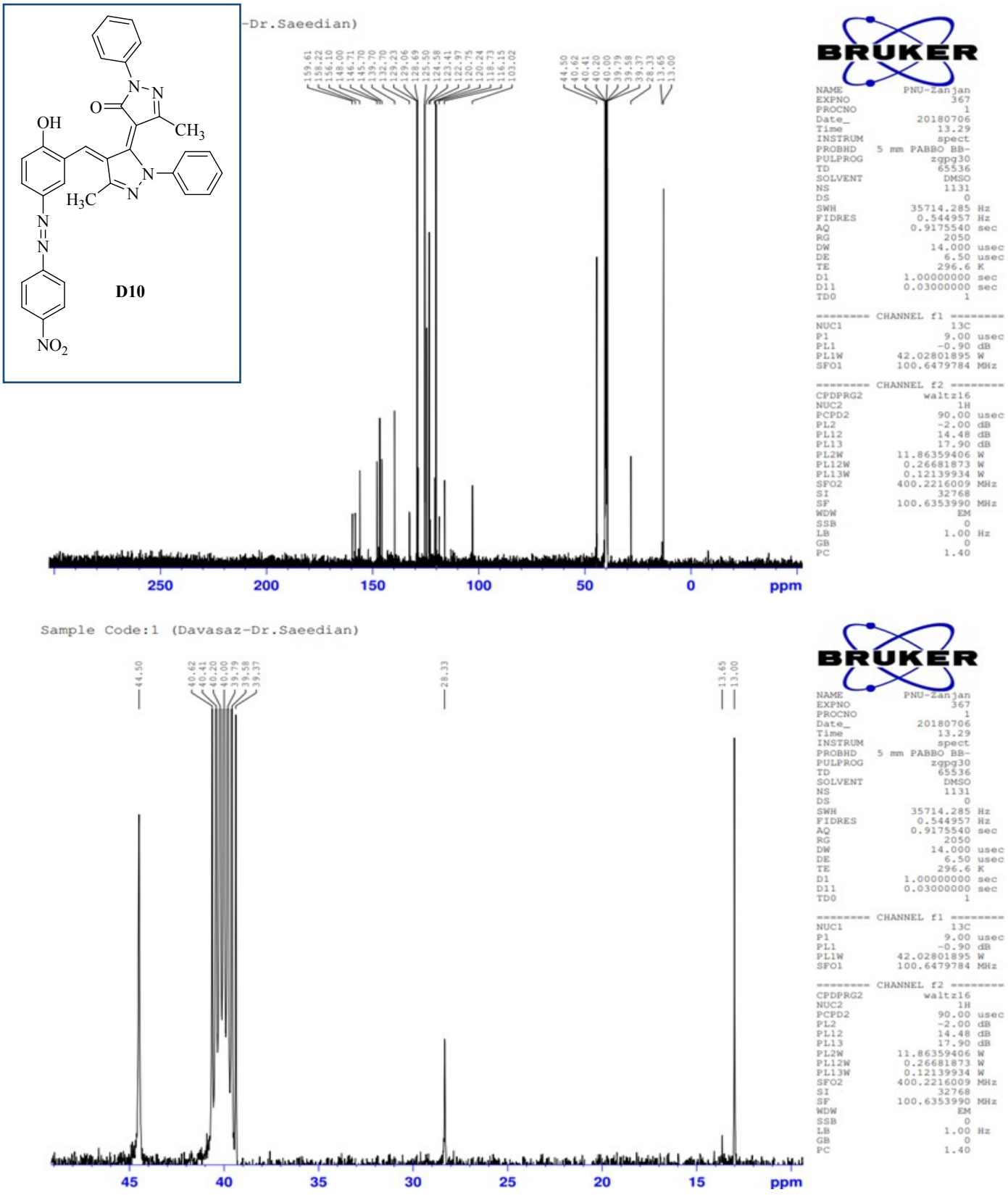


Fig ^{13}C NMR of D10.