

Supplementary material

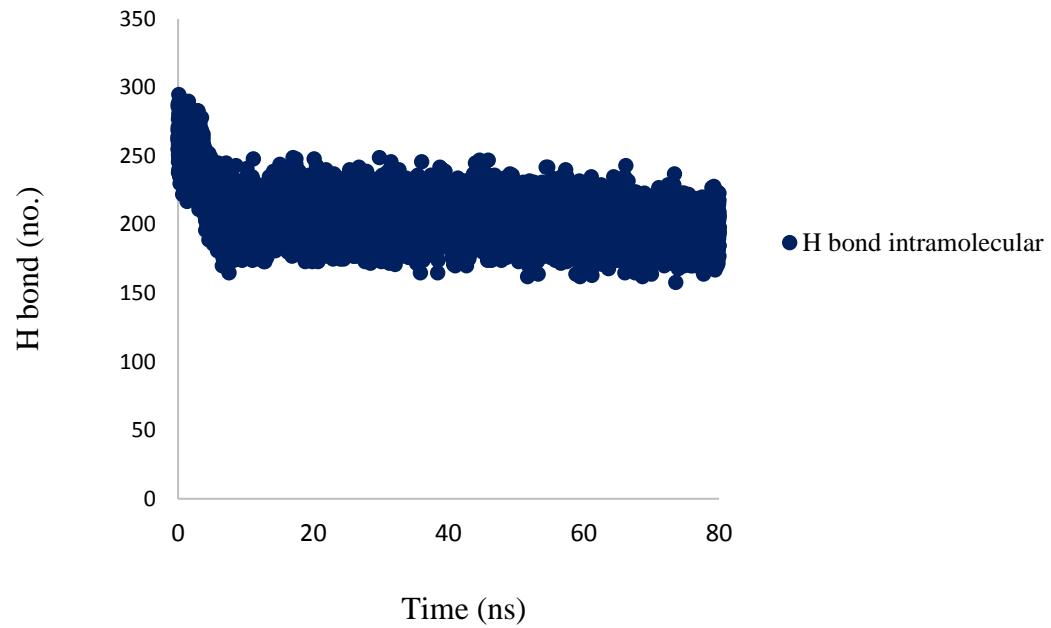


Figure S1. Number of intramolecular hydrogen bonds of protein in time scale.

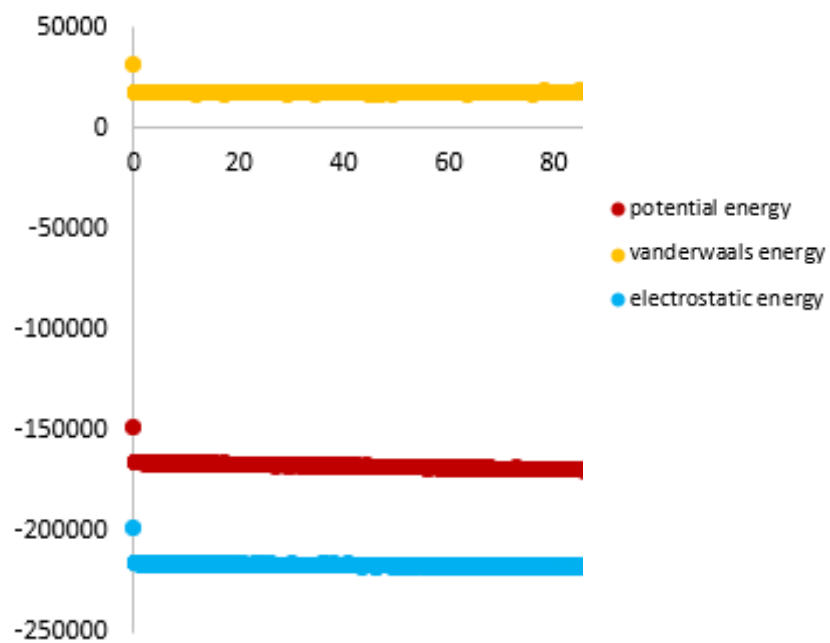
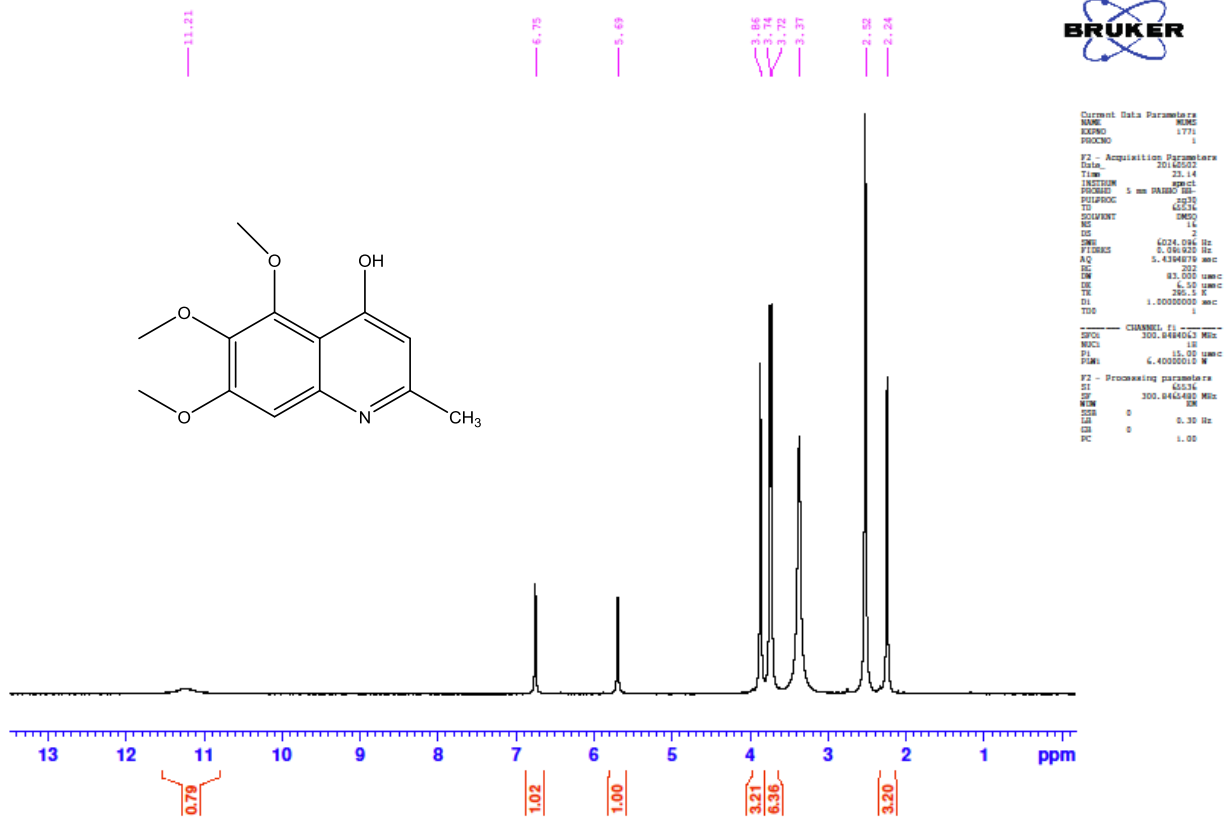


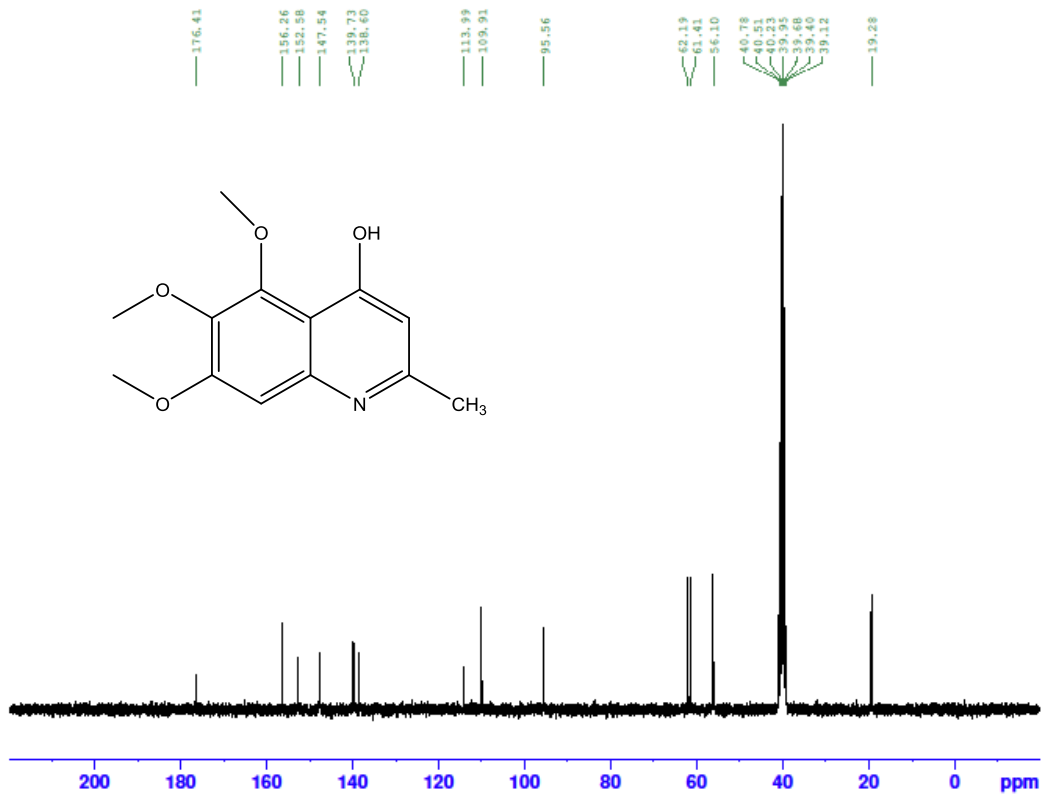
Figure S2. Potential energy, vanderwaals and electrostatic energy vs. simulation time plot of protein in complex with ligand.

Dr. Ghodsi- code T1-



2-methylquinolin-4-ol (4)

Dr. Ghodsi- code T1-Repeat

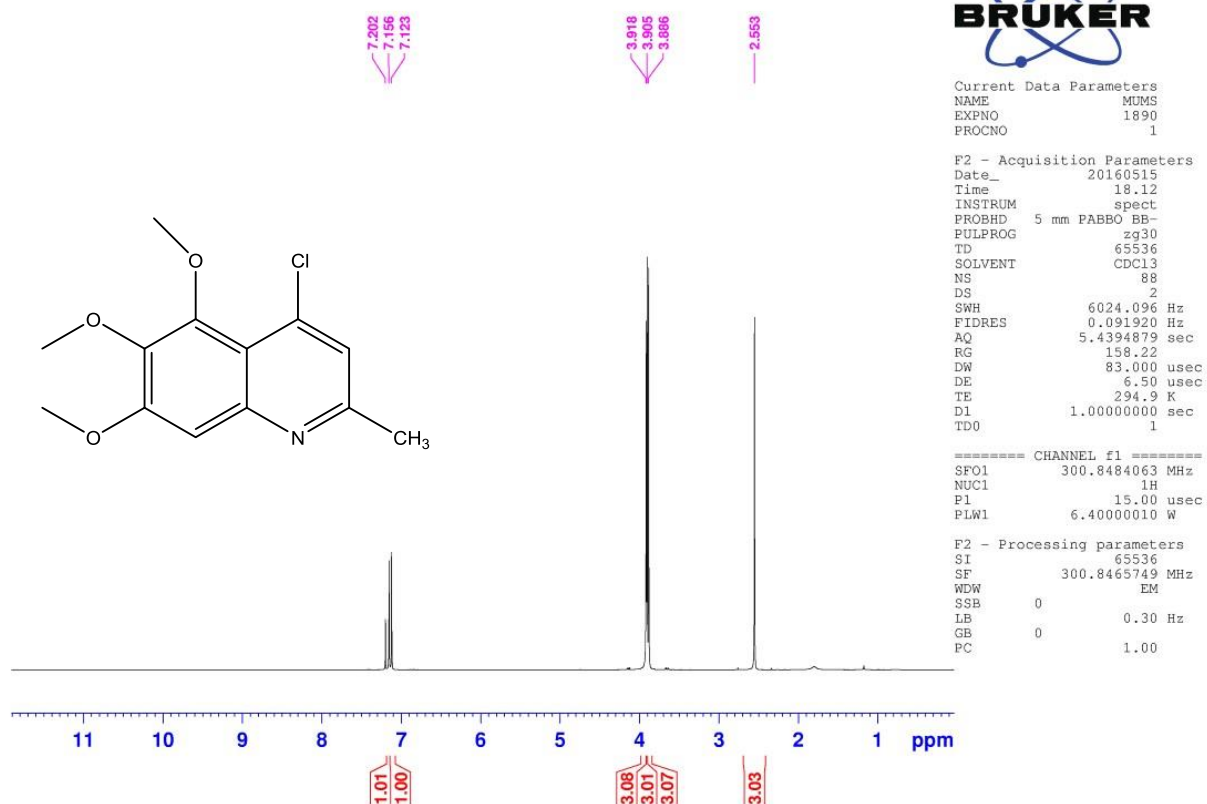


```
Current Data Parameters
NAME      404
EXPNO    1773
PROCNO    0

F2 - Acquisition Parameters
Date_     20160203
Time      11:29
INSTRUM   spect
PROBHD    5 mm HXBOB-90
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        350
DS        4
SWH        18114.942 Hz
FIDRES    0.235027 Hz
AQ        1.3027930 sec
RG        383
DE        27.500 mm
TE        300.2 K
SI        2.0000000 sec
SFO       125.761 MHz
===== CHANNEL f1 =====
NUC1      13C
P1        12.00
PL1       0.0000000 W
===== CHANNEL f2 =====
NUC2      13C
P2        12.00
PL2       0.0000000 W
===== CHANNEL f3 =====
NUC3      13C
P3        12.00
PL3       0.0000000 W
===== CHANNEL f4 =====
NUC4      13C
P4        12.00
PL4       0.0000000 W
F2 - Processing parameters
SI        65536
SF        125.761 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

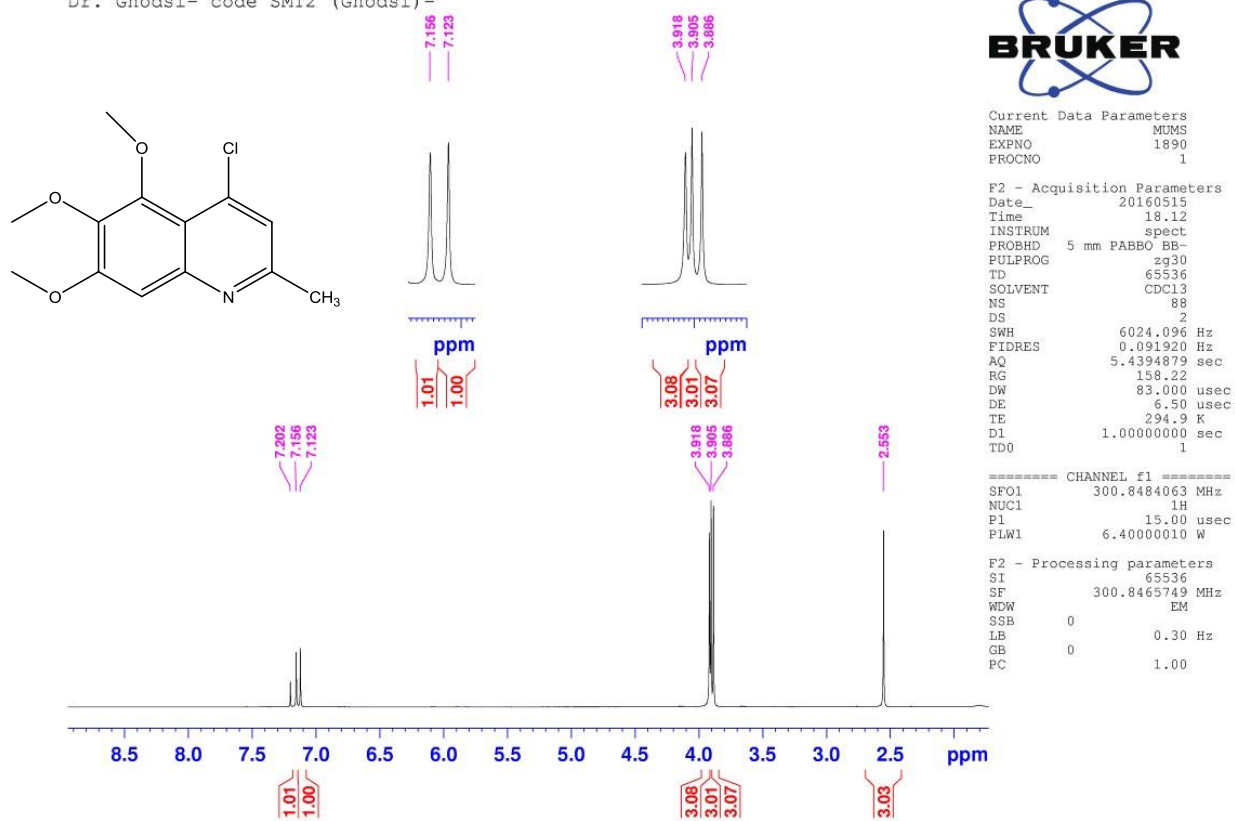
2-methylquinolin-4-ol (4)

Dr. Ghodsi- code SMT2 (Ghodsi)-



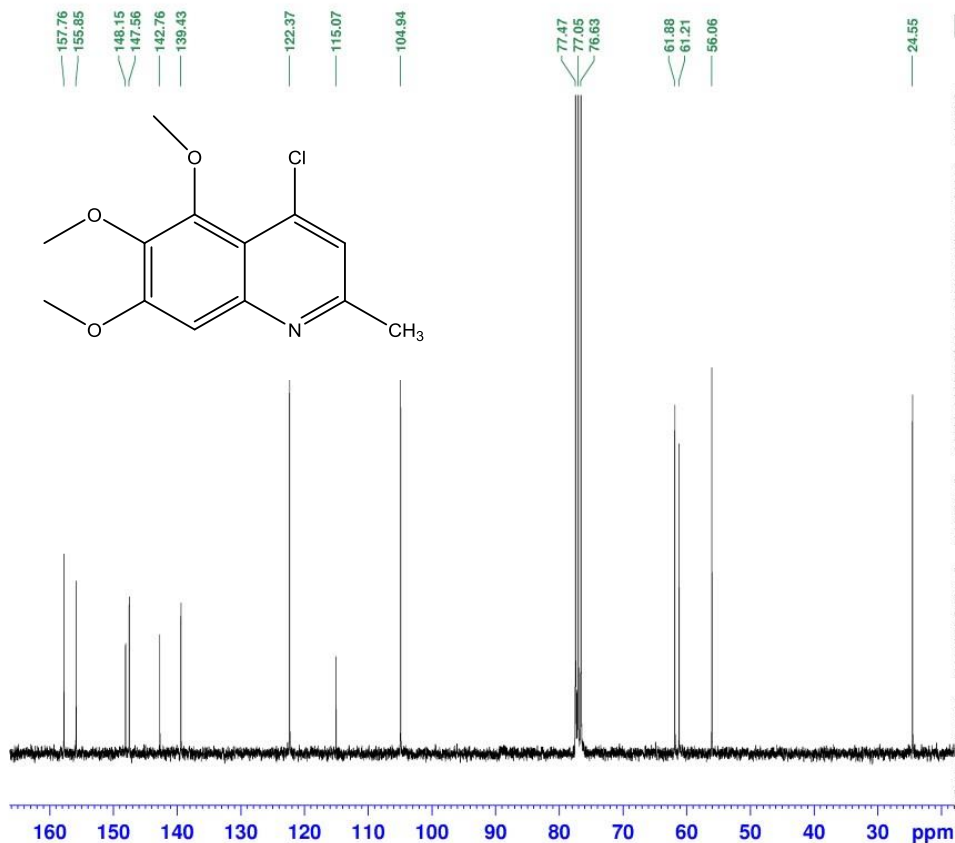
5.1.2. 4-chloro-2-methylquinoline (5)

Dr. Ghodsi- code SMT2 (Ghodsi)-



5.1.2. 4-chloro-2-methylquinoline (5)

C13CPD-Dr. Ghodsi- code SMT2 (Ghodsi)-



Current Data Parameters
NAME MUMS
EXPNO 1891
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160515
Time 19.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 908
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 202
DW 27.600 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

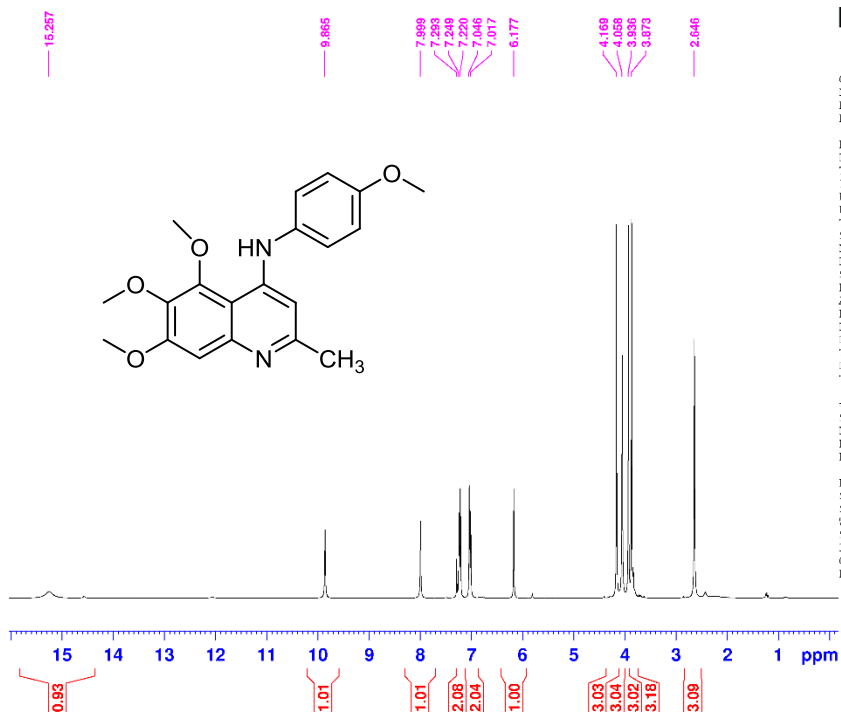
===== CHANNEL f1 =====
SFO1 75.6554892 MHz
NUC1 13C
P1 10.00 usec
PLW1 30.00000000 W

===== CHANNEL f2 =====
SFO2 300.8477518 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 6.40000010 W
PLW12 0.1778000 W
PLW13 0.143999999 W

F2 - Processing parameters
SI 32768
SF 75.6479250 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
EC 1.40

5.1.2. 4-chloro-2-methylquinoline (5)

Dr. Ghodsi- code ST5 (Mirzaei)-



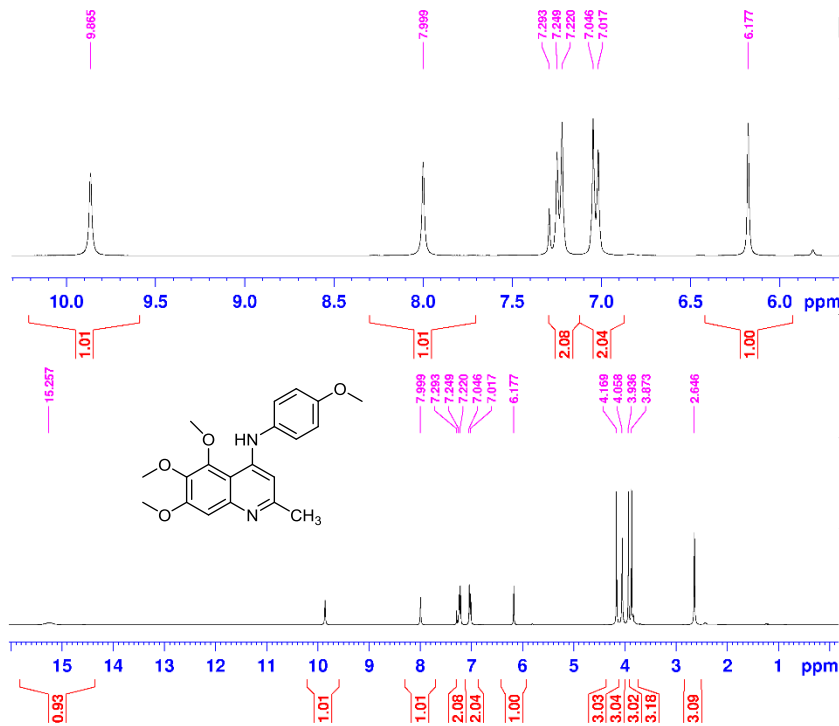
Current Data Parameters
NAME MUMS
EXPNO 857
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161114
Time 14.40
INSTRUM spect
PROBHD 5 mm FATHO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 48
DS 2
SWH 6024.096 Hz
FIDRES 0.091920 Hz
AQ 5.4394879 sec
RG 158.22
DW 83.000 usec
DE 6.50 usec
TE 295.2 K
D1 1.0000000 sec
TD0 1

----- CHANNEL f1 -----
SF01 300.8484063 MHz
NUC1 1H
P1 15.00 usec
PLW1 6.40000010 W

F2 - Processing parameters
SI 65536
SF 300.846480 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dr. Ghodsi- code ST5 (Mirzaei)-



Current Data Parameters
NAME MUMS
EXPNO 857
PROCNO 1

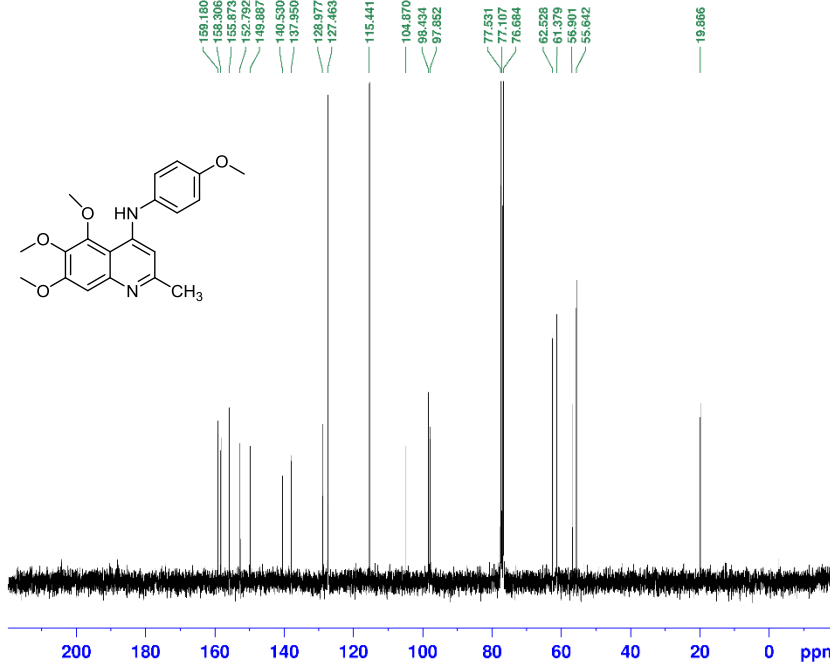
F2 - Acquisition Parameters
Date_ 20161114
Time 14.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 48
DS 2
SWH 6024.096 Hz
FIDRES 0.091920 Hz
AQ 5.7394879 sec
RG 158.22
CW 83.000 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 300.6484063 MHz
NUC1 1H
P1 15.00 usec
PLW1 6.40000010 W

F2 - Processing parameters
SI 65536
SF 300.8465480 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4a

C13-Dr.ghodsi- code S15(mirzaei)-

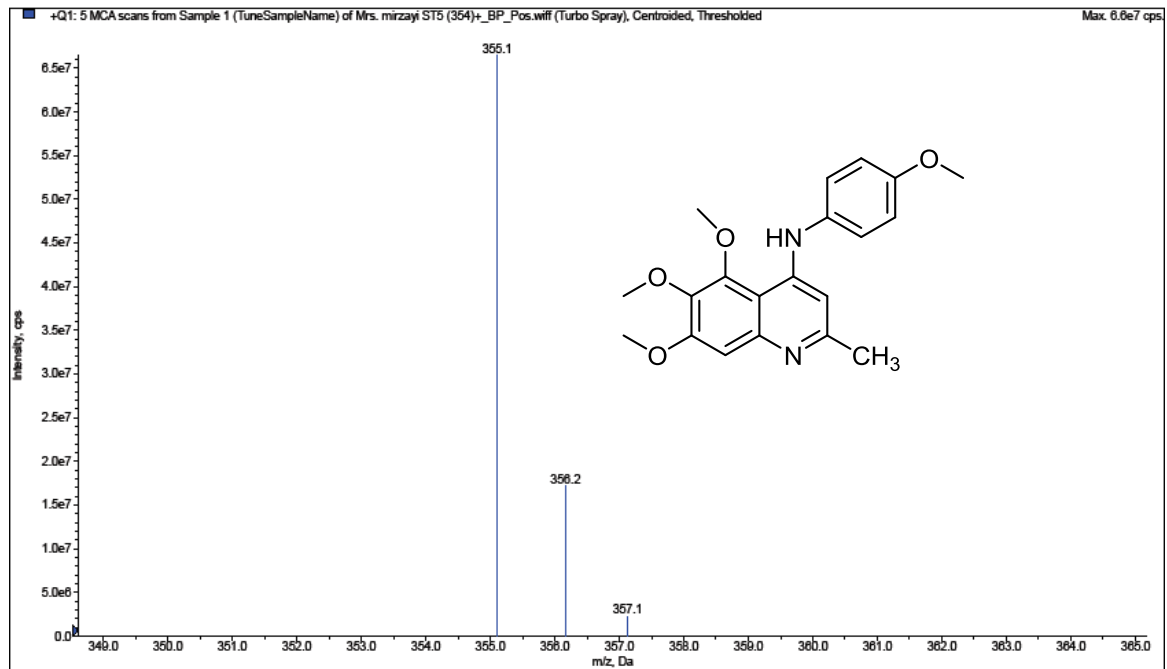


Current Data Parameters
NAME MUMS
EXPNO 964
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161116
Time 14.13
INSTRUM spect
PROBHD 5 mm F40X 3B-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 240
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 202
DW 27.600 usec
DE 6.30 usec
TE 0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 75.6554892 MHz
NUC1 13C
P1 10.00 usec
PLW1 30.0000000 W
----- CHANNEL f2 -----
SFO2 300.8477518 MHz
NUC2 1H
CPOBPRG2 waltz16
PCPD2 98.00 usec
PLW2 6.4000010 W
PLW12 0.17778000 W
PLW13 0.14399999 W

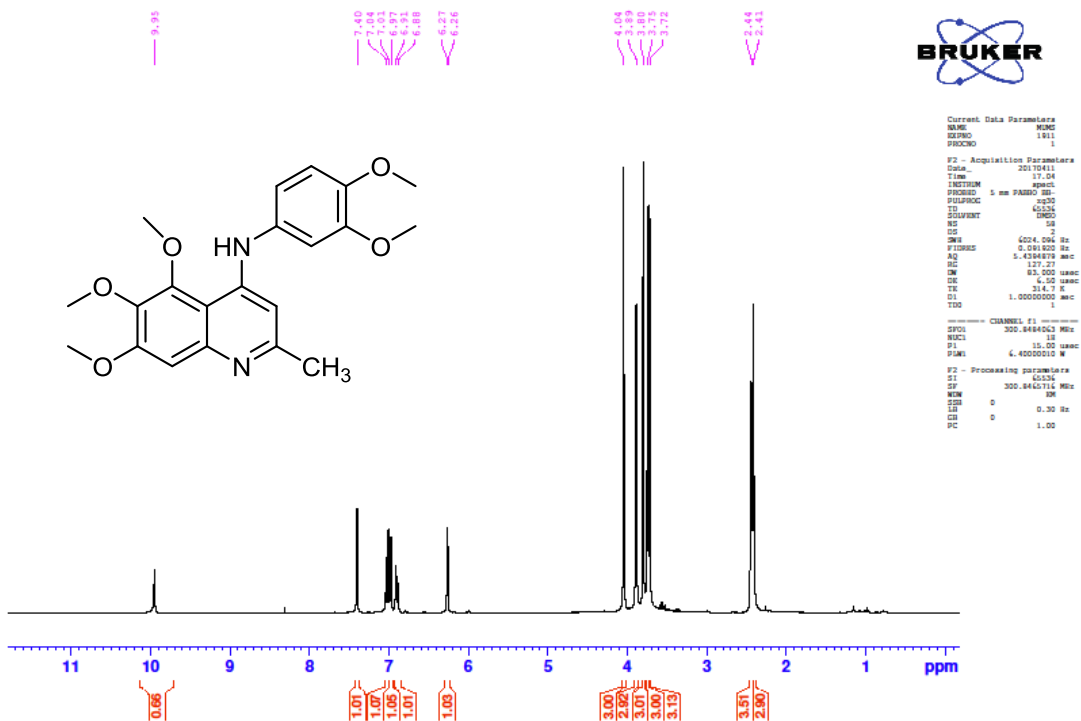
F2 - Processing parameters
SI 32768
SF 75.6479250 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



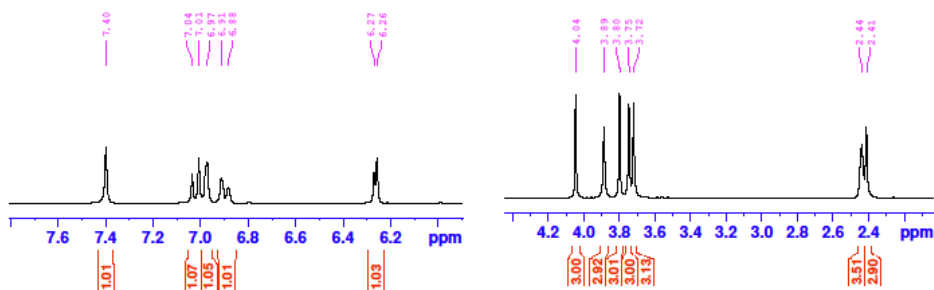
*Bu-Ali Research Center, Mashhad University of Medical Sciences, Mashhad, Iran.

4a

Dr. Ghodsi- code ST59 (Mirzaei)-

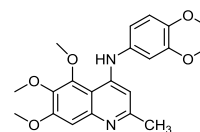
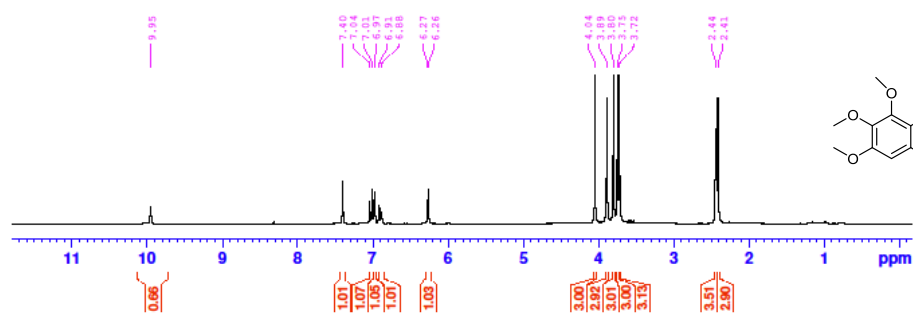


4b

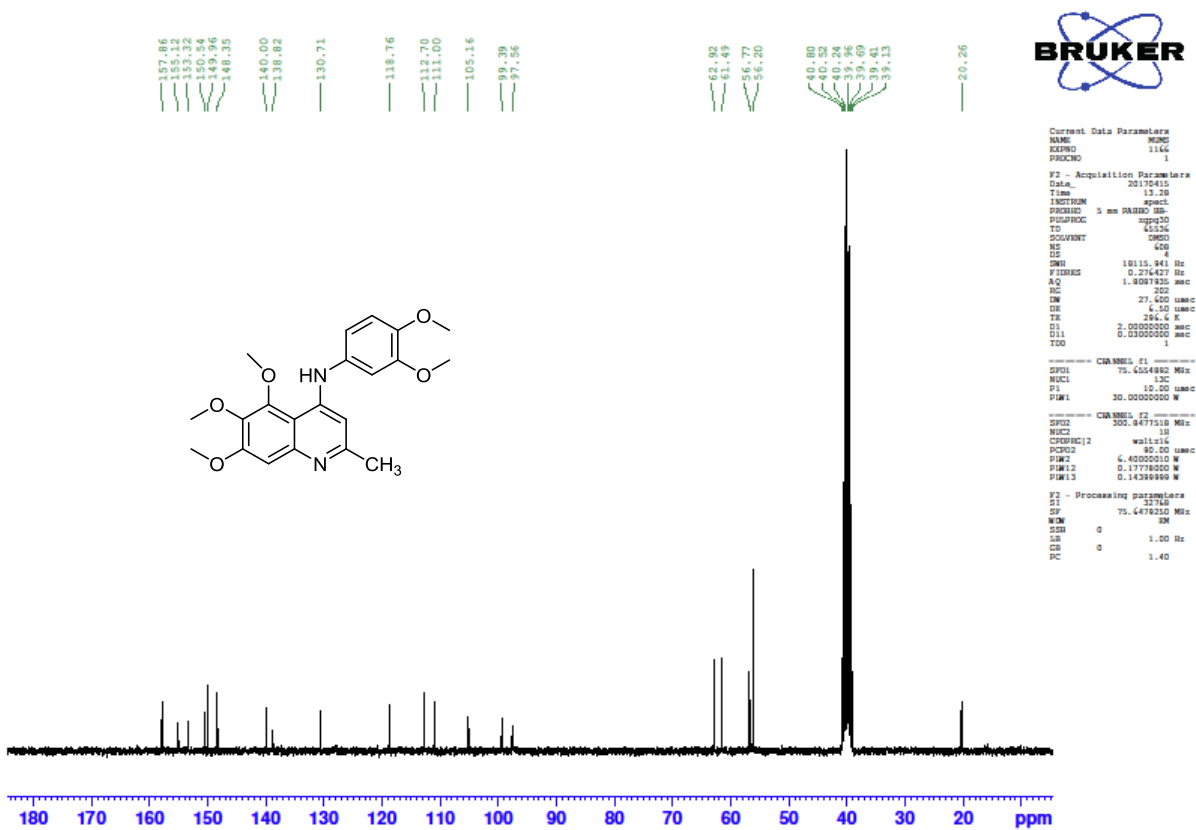


Current Data Parameters
 NAME MNS
 DATE 1911
 PROCNO 1

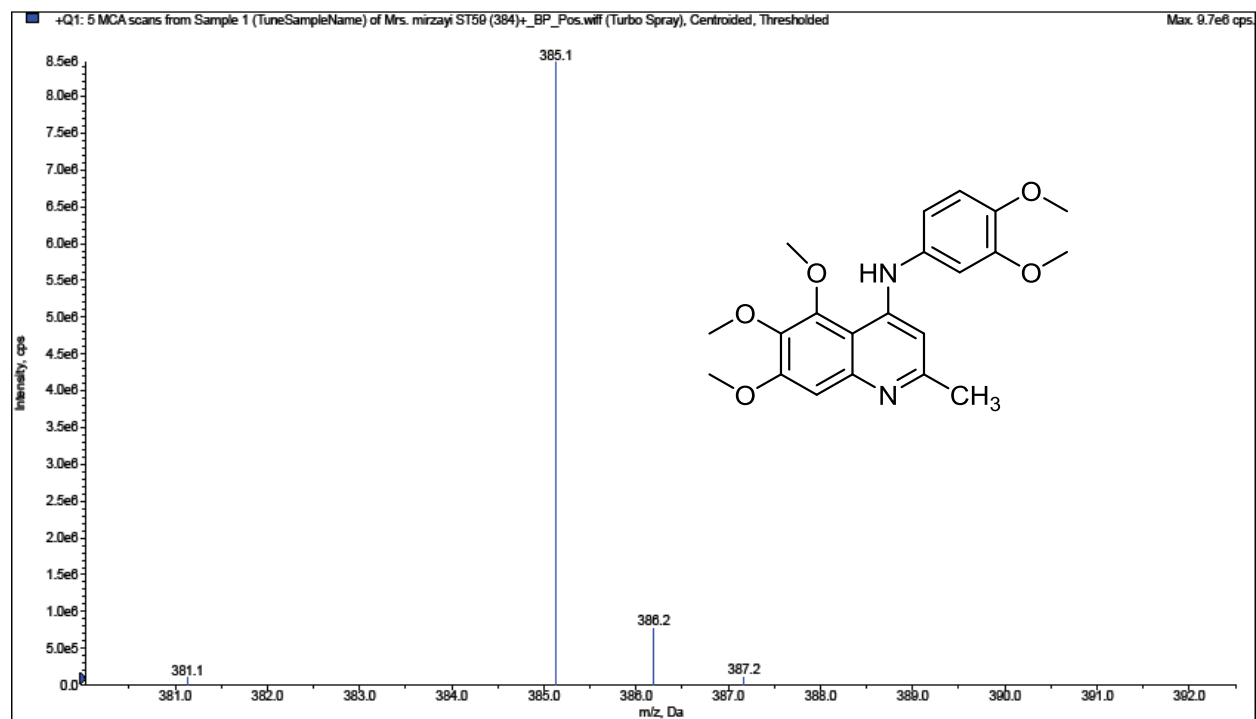
F2 - Acquisition Parameters
 Date_ 20170411
 Time 17:04
 INSTRUM spect
 PROCNO 5
 PULPROG zgpg30
 F2 - Processing parameters
 CHAN1 300.844043 MHz
 NUC1 13C
 P1 13.00 usec
 PL1 0.0000015 E



C13-Dr.ghodsi- code ST59(mirzaei)-test



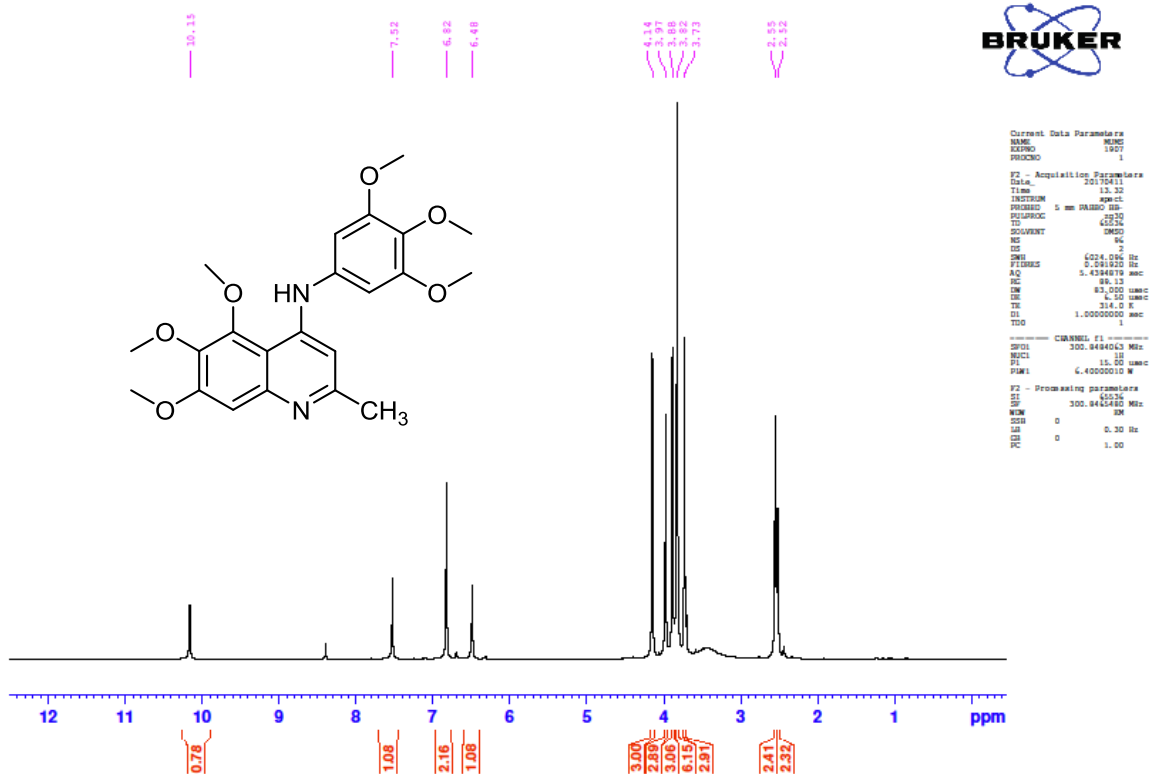
4b



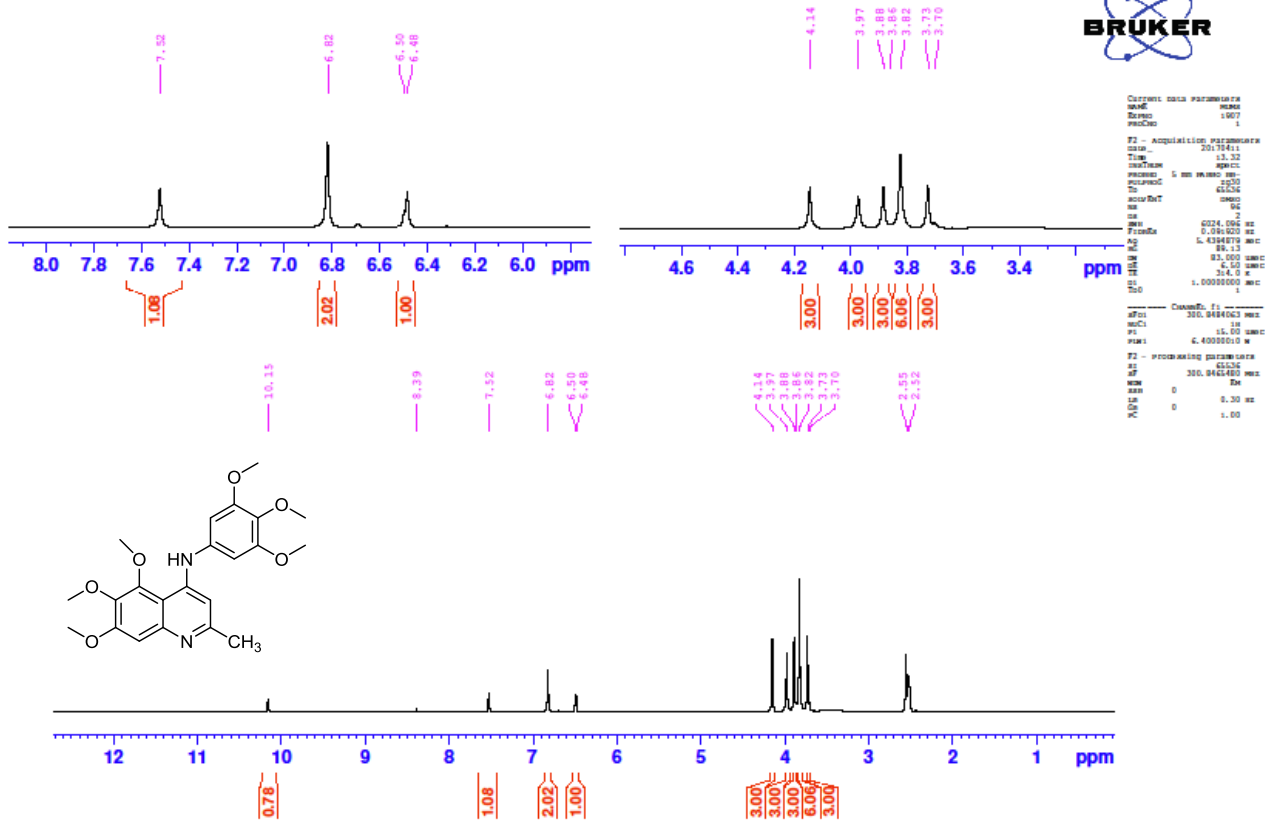
*Bu-Ali Research Center, Mashhad University of Medical Sciences, Mashhad, Iran.

4b

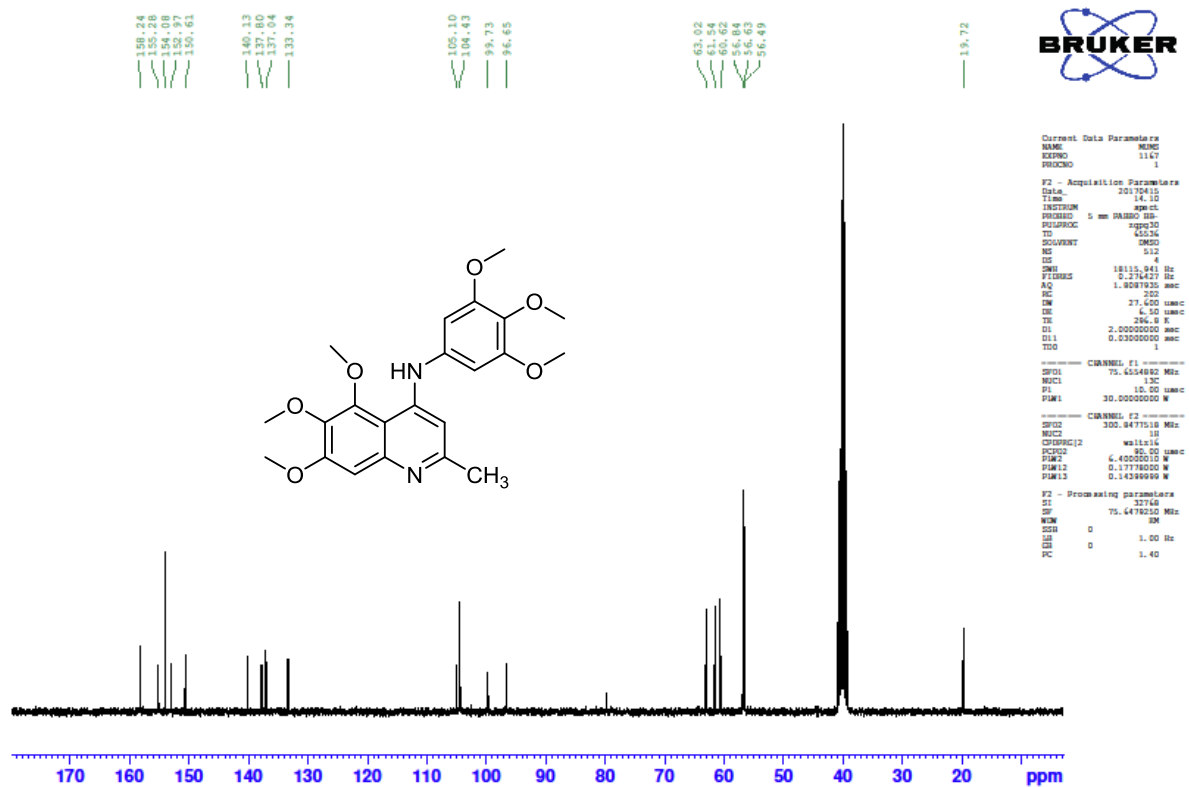
Dr. Ghodsi- code ST60 (Mirzaei)-



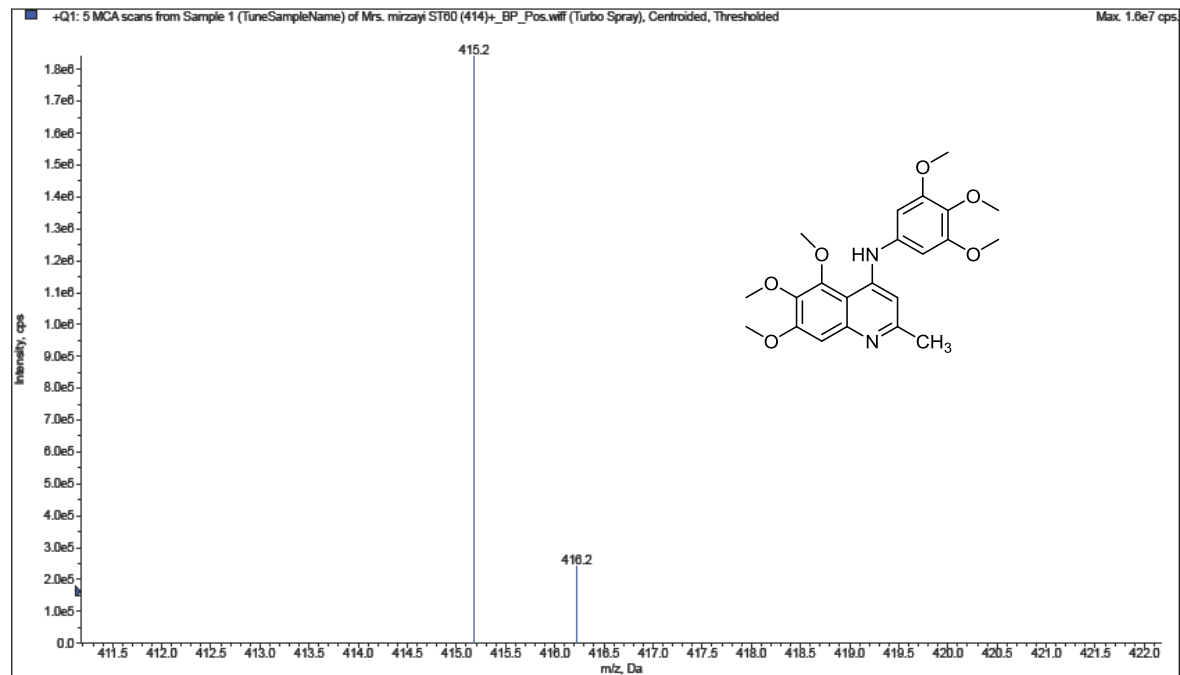
4c



C13-Dr.ghodsi- code ST60(mirzaei)-test

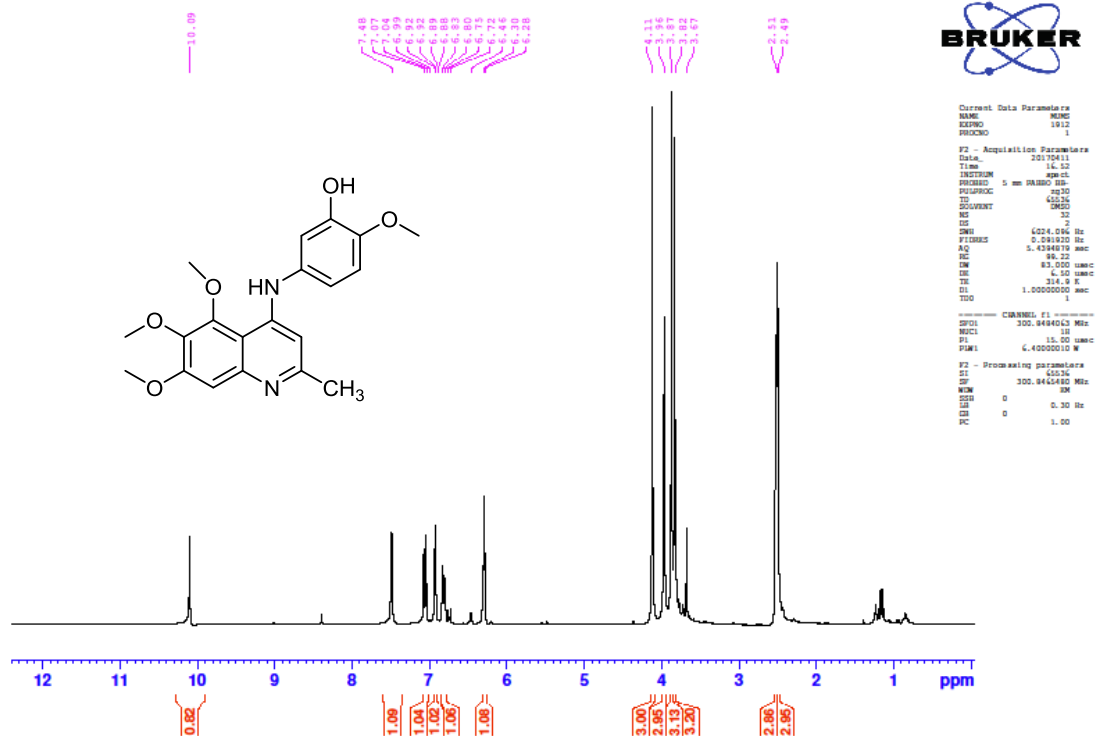


4c



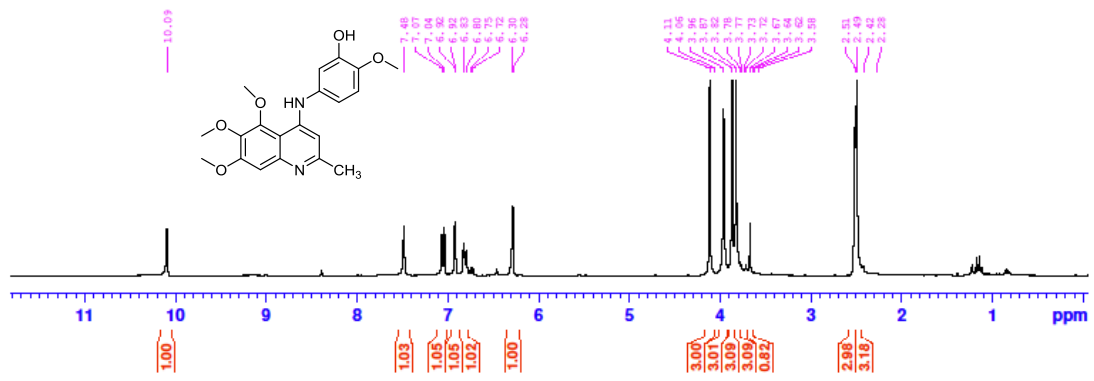
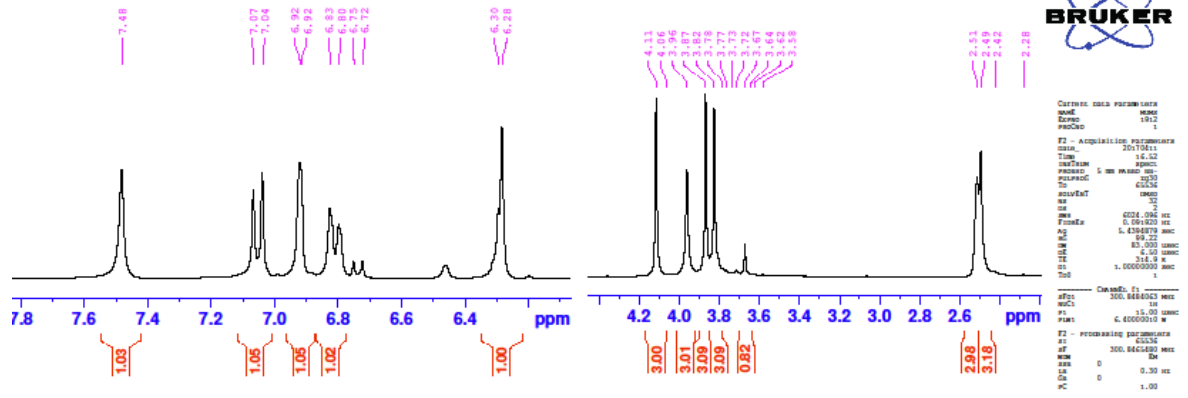
*Bu-Ali Research Center, Mashhad University of Medical Sciences, Mashhad, Iran.

Dr. Ghodsi- code ST61 (Mirzaei)-



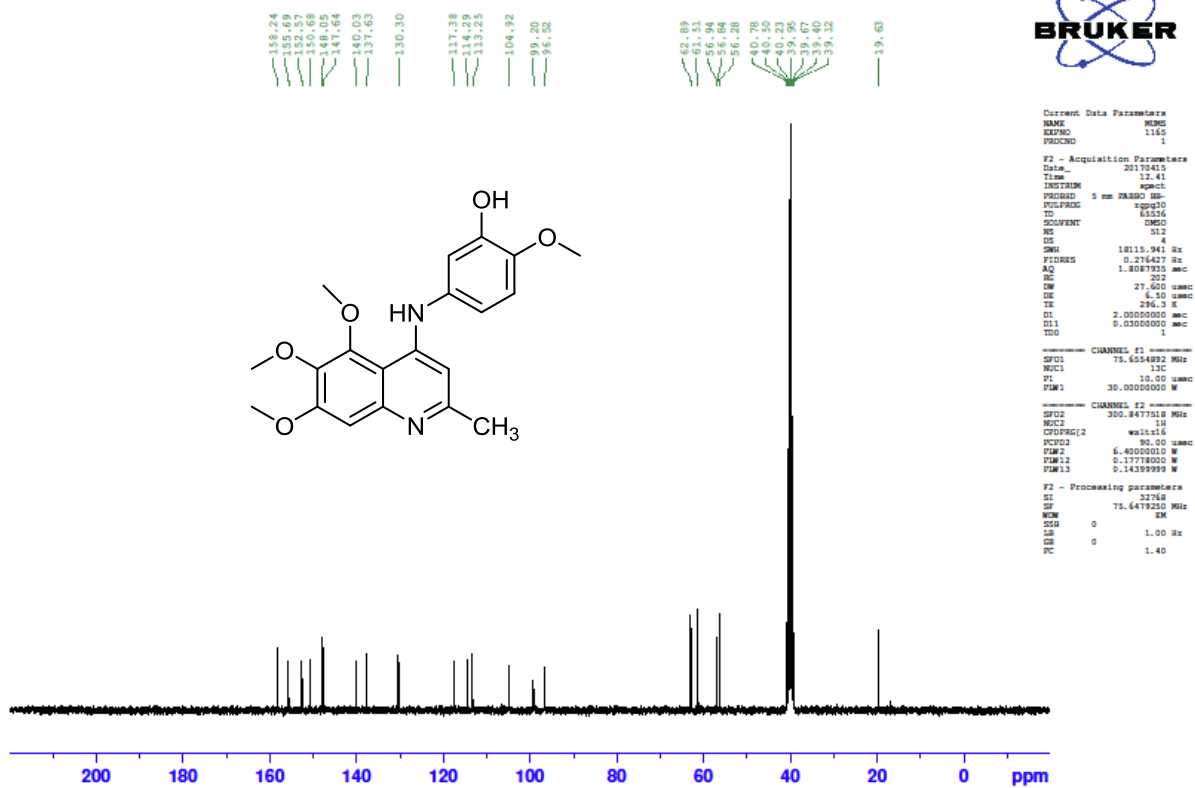
4d

Dr. Ghodsi- code ST61 (Mirzaei)-

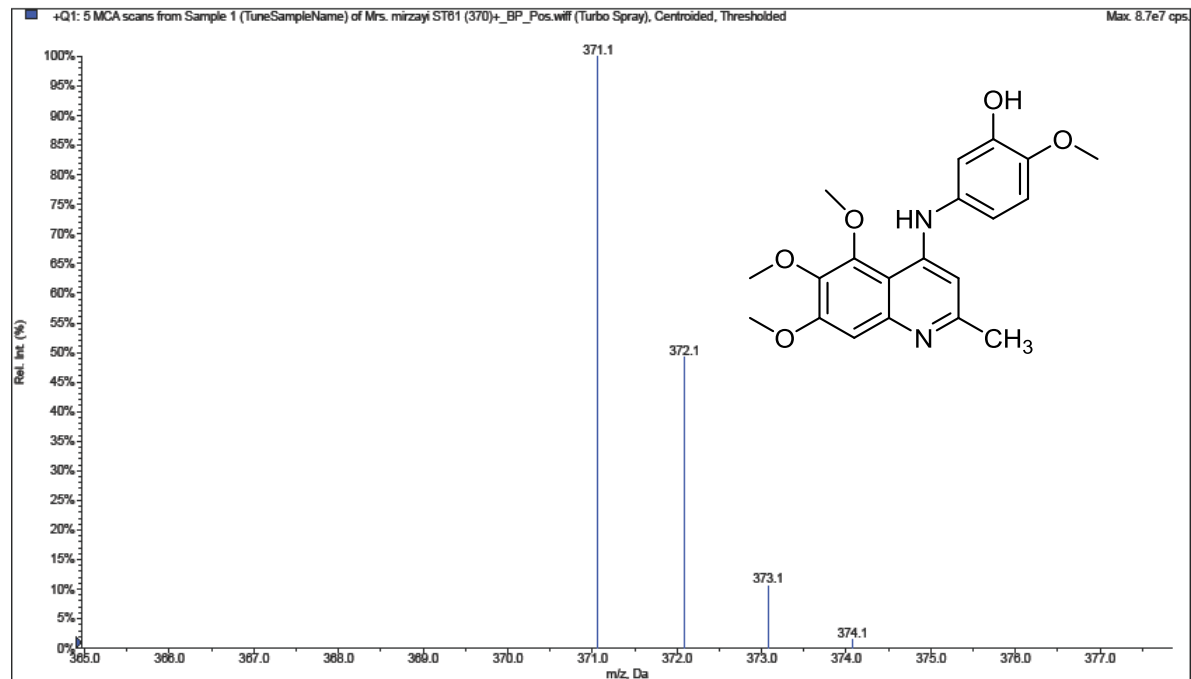


4d

C13-Dr.ghodsi- code ST61(mirzaei)-test

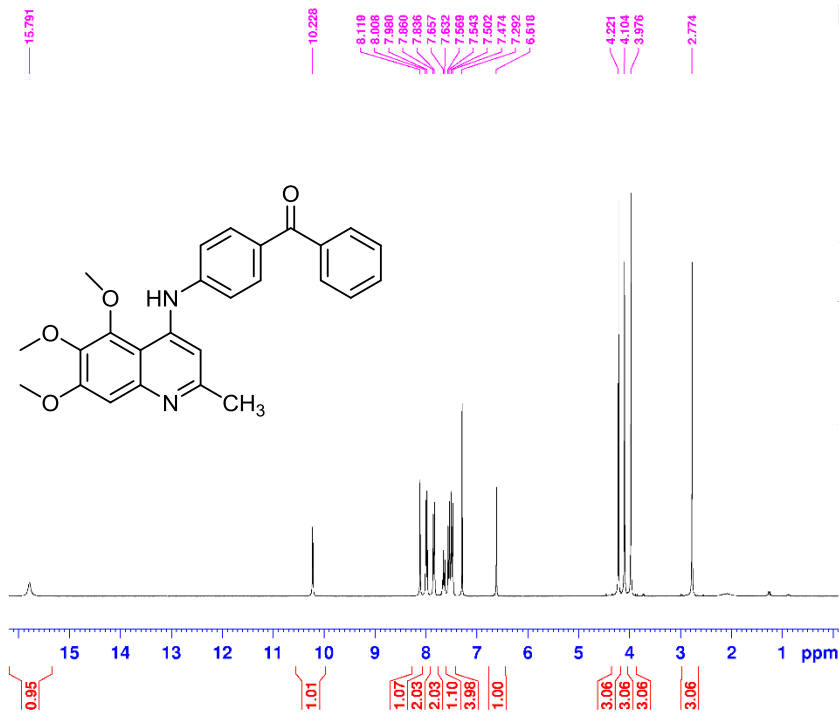


4d



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Dr. Ghodsi- code ST4 (Mirzaei)-



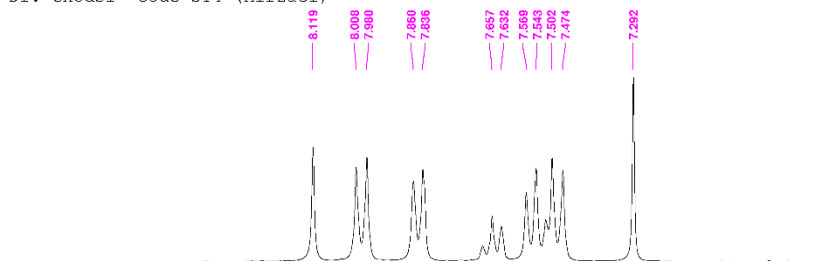
Current: Data Parameters
NAME MUMS
EXPNO 858
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161114
Time 15.16
INSTRUM spect
PROBHD 5 mm FAPBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 48
DS 2
SWH 6024.096 Hz
FIDRES 0.091920 Hz
AQ 5.7394879 sec
RG 202
CW 83.000 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 300.6404063 MHz
NUC1 1H
P1 15.00 usec
PLW1 6.40000010 W

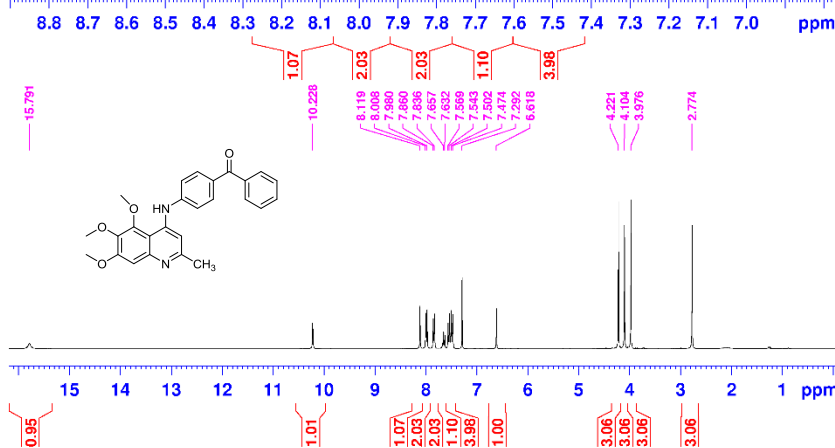
F2 - Processing parameters
SI 65536
SF 300.6465480 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dr. Ghodsi- code ST4 (Mirzaei)-



Current: Data Parameters
NAME MUMS
EXPNO 858
PROCNO 1

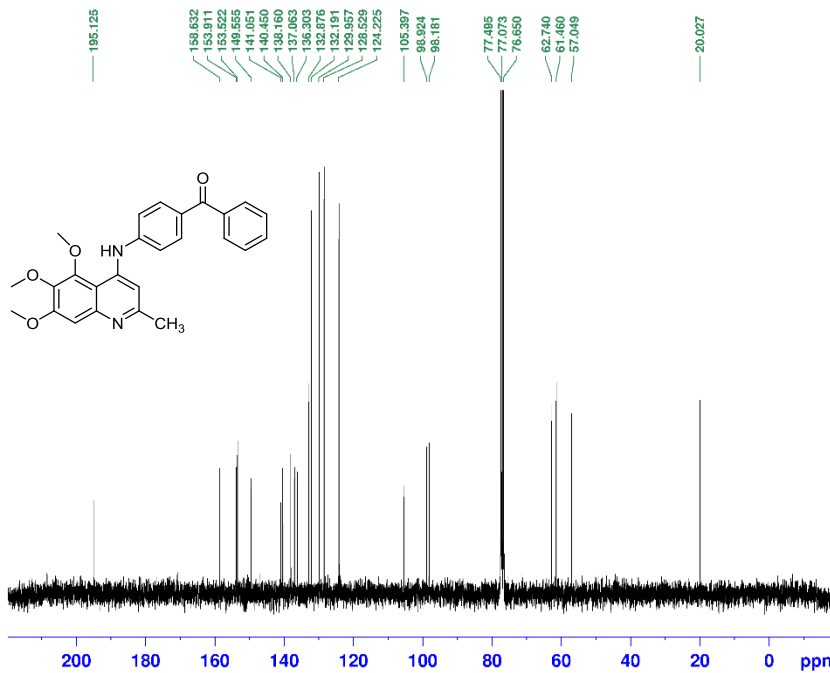
F2 - Acquisition Parameters
Date_ 20161114
Time 15.16
INSTRUM spect
PROBHD 5 mm FAPBBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 48
DS 2
SWH 6024.096 Hz
FIDRES 0.091920 Hz
AQ 5.7394879 sec
RG 202
CW 83.000 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1



----- CHANNEL f1 -----
SFO1 300.6484063 MHz
NUC1 1H
P1 15.00 usec
PLW1 6.40000010 W

F2 - Processing parameters
SI 65536
SF 300.8465480 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C13-Dr.ghodsi- code ST4(mirzaei)-



195.125
 158.632
 153.911
 153.522
 149.555
 146.161
 146.160
 138.160
 137.063
 136.303
 132.876
 132.191
 129.957
 126.529
 124.225
 106.397
 98.924
 98.181
 77.095
 77.073
 76.650
 62.740
 61.460
 57.049
 20.027



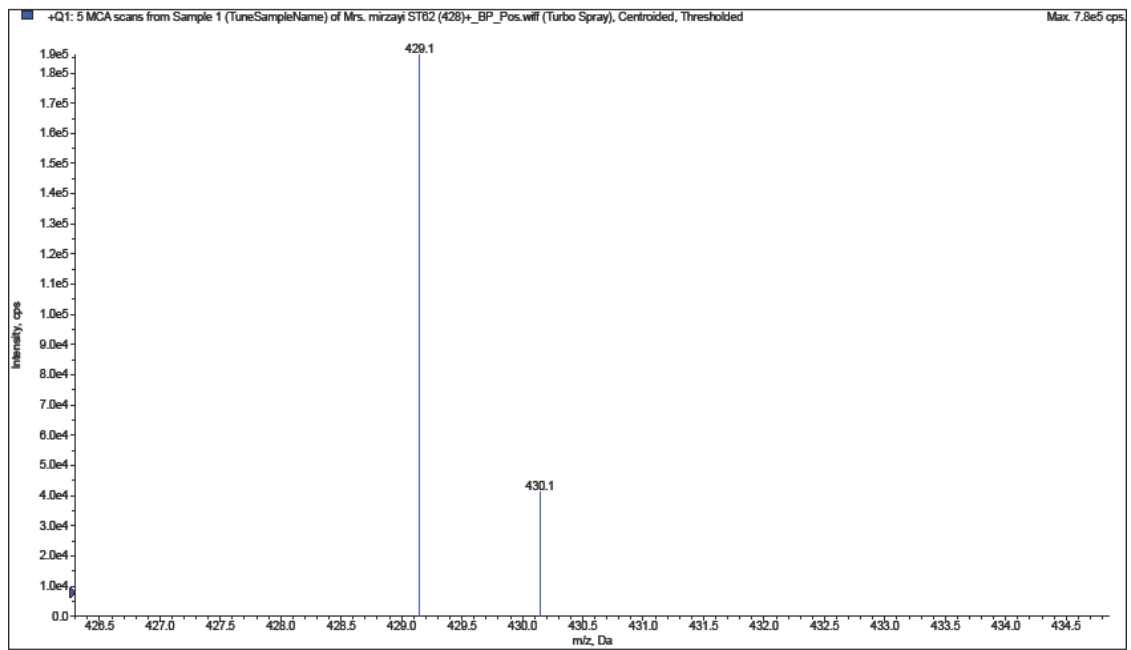
Current Data Parameters
 NAME MUMS
 EXPNO 961
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20161116
 Time 13.51
 INSTRUM spect
 PROBHD 5 mm FAPBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 18115.941 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 202
 DW 27.600 usec
 DE 6.50 usec
 TE 0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

----- CHANNEL f1 -----
 SF01 75.6554892 MHz
 NU01 13C
 P1 10.00 usec
 PLW1 30.00000000 W

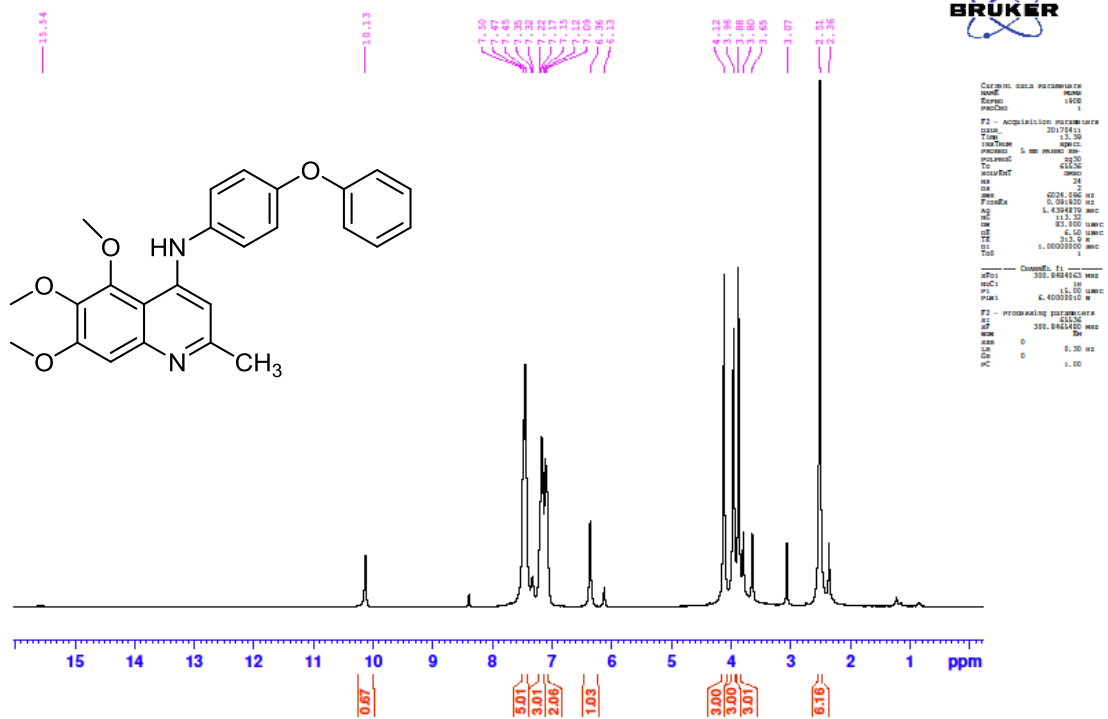
----- CHANNEL f2 -----
 SF02 300.8477518 MHz
 NU02 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 6.40000016 W
 PLW12 0.17778000 W
 PLW13 0.14399999 W

F2 - Processing parameters
 SI 32768
 SF 75.6479200 MHz
 BW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

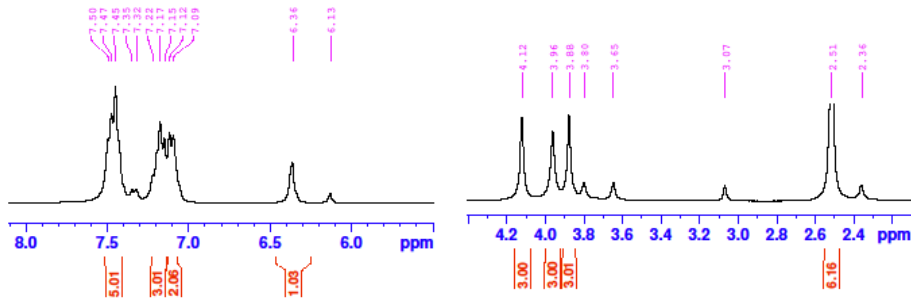


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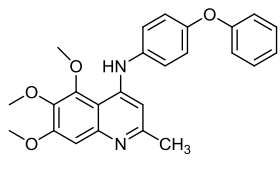
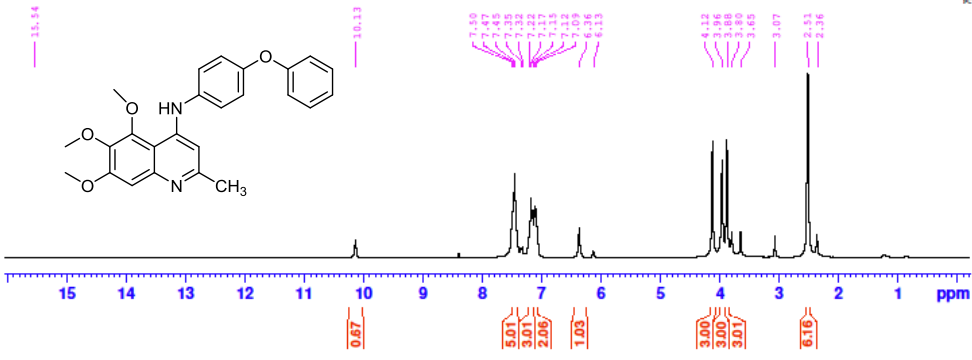
Dr. Ghodsi- code ST57 (Mirzaei)-



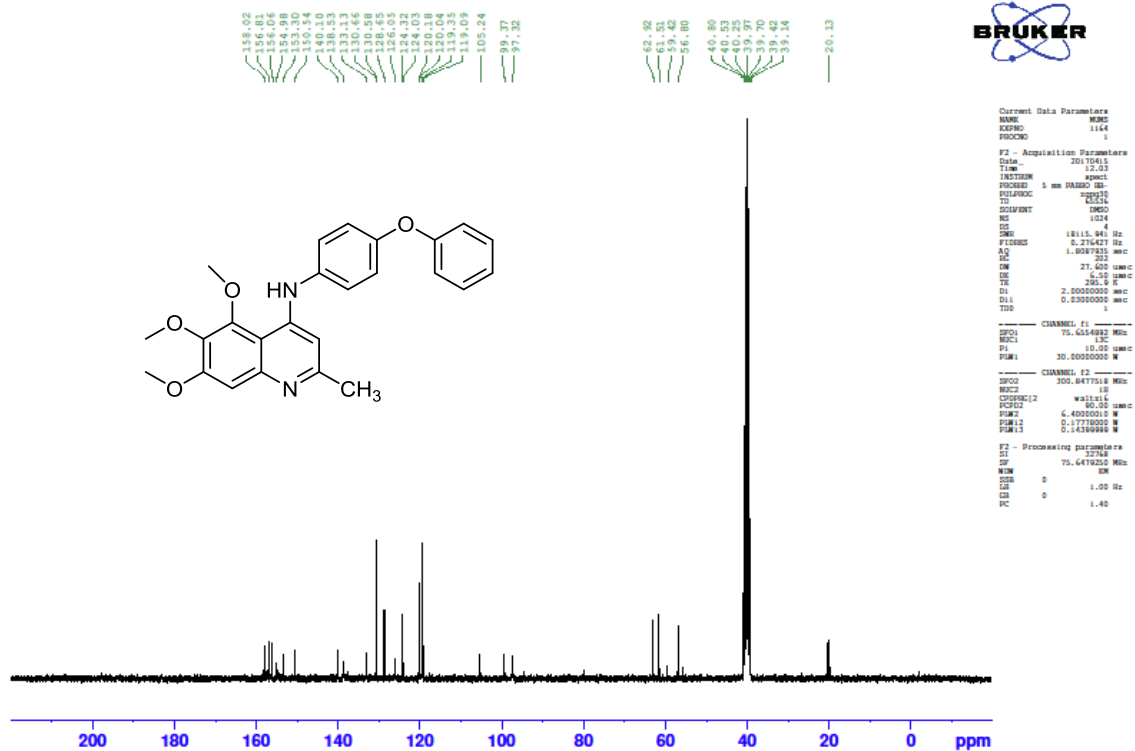
Dr. Ghodsi- code ST57 (Mirzaei)-



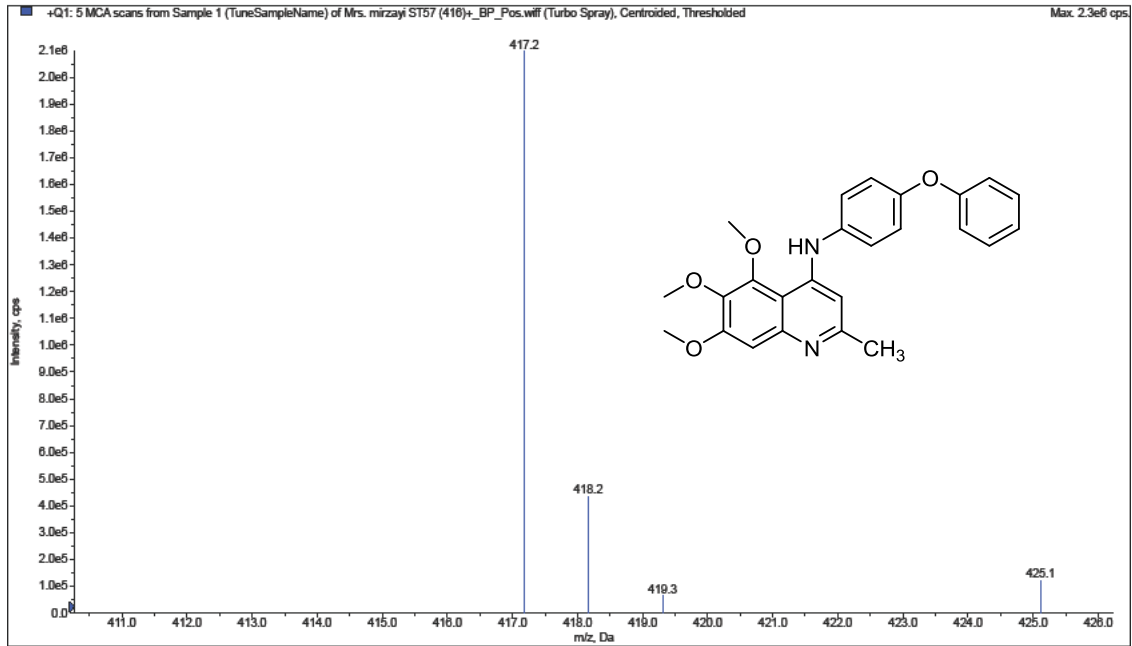
```
Current data parameters
NAME: ST57
EXPNO: 1
PROCNO: 1
F2 - Acquisition parameters
Date_ : 20170411
Time: 11.30
Instrum: spect
Probnam: 1 mm Hahn
Pulprog: zgpg30
TD: 65536
SFO: 400
AQ: 0.02000000
RG: 327.500
WDW: EM
SSB: 0
LB: 3.15000000
GB: 0
PC: 1.00000000
=====
Compound 1
aPoi: 300.8464833 MHz
nuC1: 15.0000000 MHz
nuH1: 4.000000000 MHz
F2 - Processing parameters
SI: 32768
SF: 300.8464833 MHz
WDW: EM
SSB: 0
LB: 3.15000000
GB: 0
PC: 1.00
```



C13-Dr.ghodsi- code ST57(mirzaei)-test

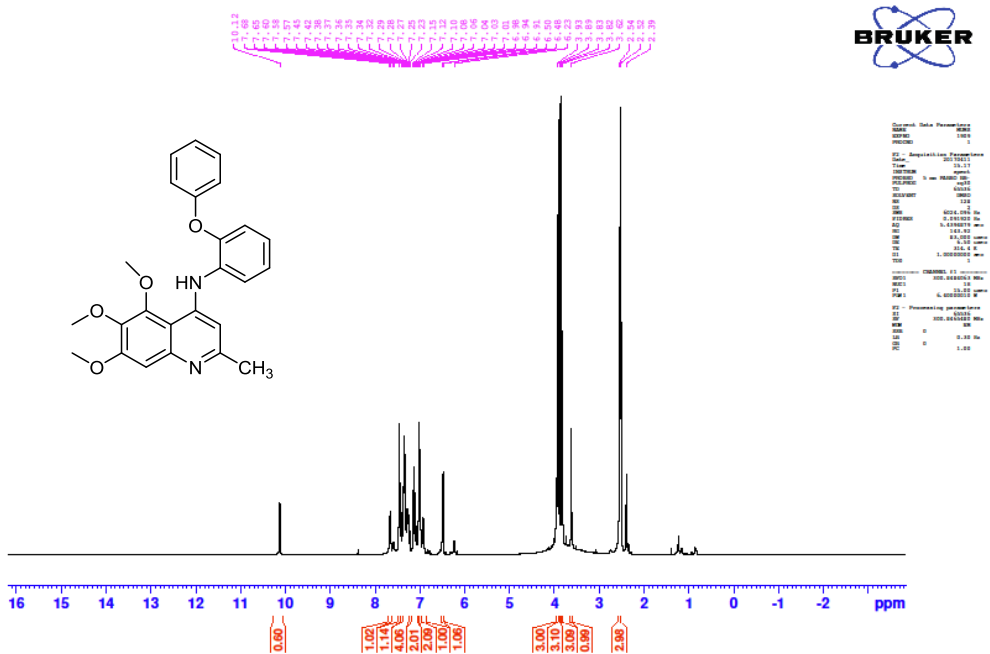


4f



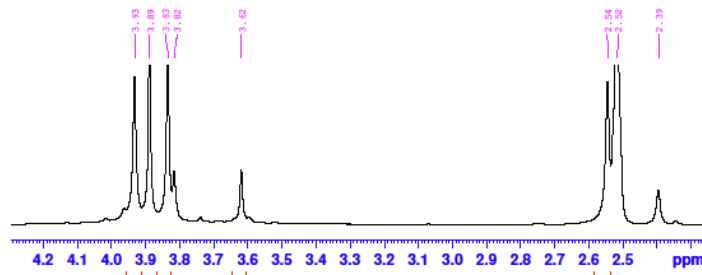
*Bu-Ali Research Center, Mashhad University of Medical Sciences, Mashhad, Iran.

Dr. Ghodsi- code ST58 (Mirzaei)-

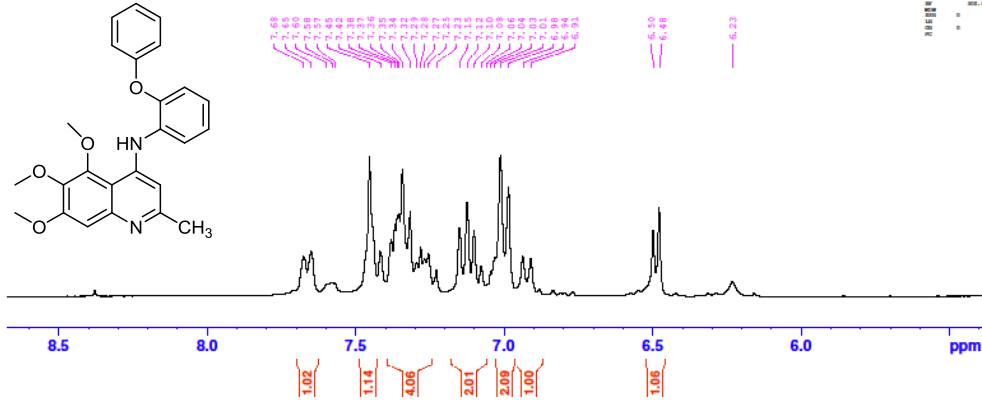
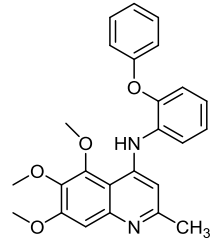


4g

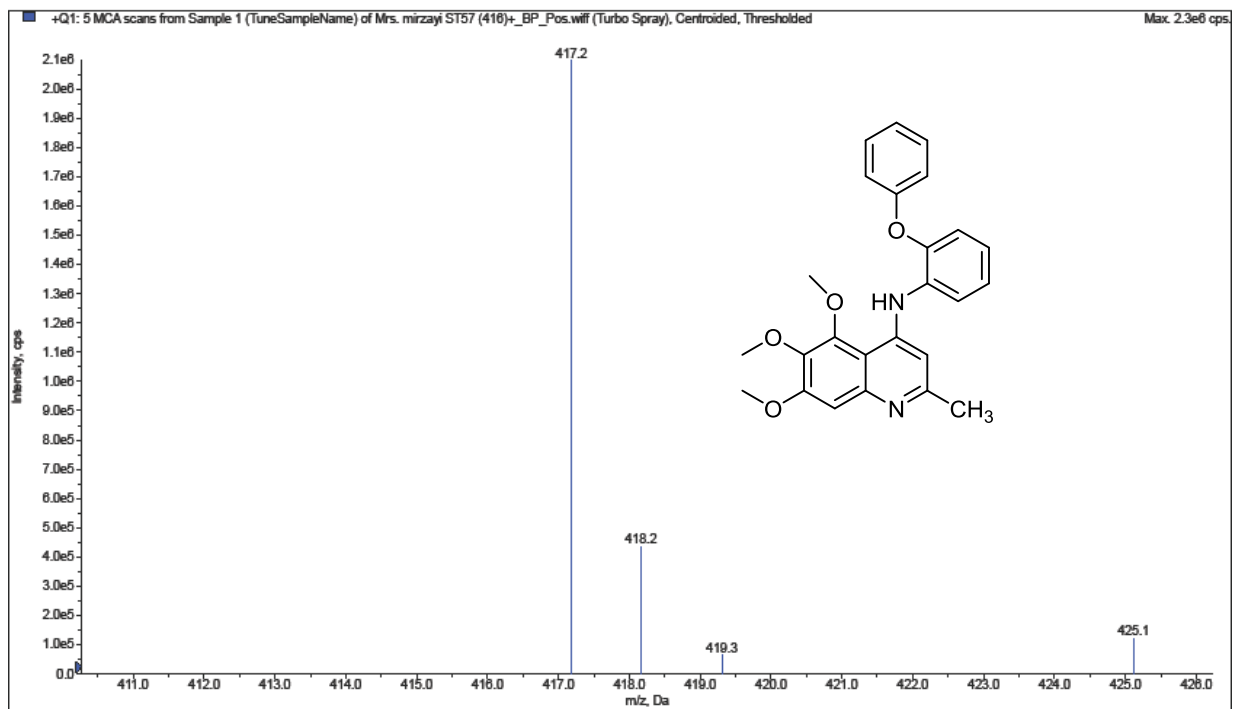
Dr. Ghodsi- code ST58 (Mirzaei)-



===== CHANNEL DATA =====
NAME: ST58
EXPNO: 2
PROCNO: 1
F1 - Acquisition Parameters
Date_ : 20161113
Time : 15:12
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
PROBHD2: zgpg30
PCPDPRG2: waltz16
SFO: 400
AQ: 1.19
RG: 655.000 Hz
FIDRES: 0.000100 Hz
AQRES: 0.000100 Hz
AQ: 0.100000 sec
RG: 655.000 Hz
SFO2: 125.761 MHz
PCPDPRG2: zgpg30
SFO3: 125.761 MHz
PCPDPRG3: zgpg30
===== CHANNEL PARAMETERS =====
NAME: ST58
EXPNO: 2
PROCNO: 1
F1 - Processing parameters
SI: 32768
SF: 400.146400 MHz
WDW: EM
SSB: 0
GB: 0
PC: 1.00



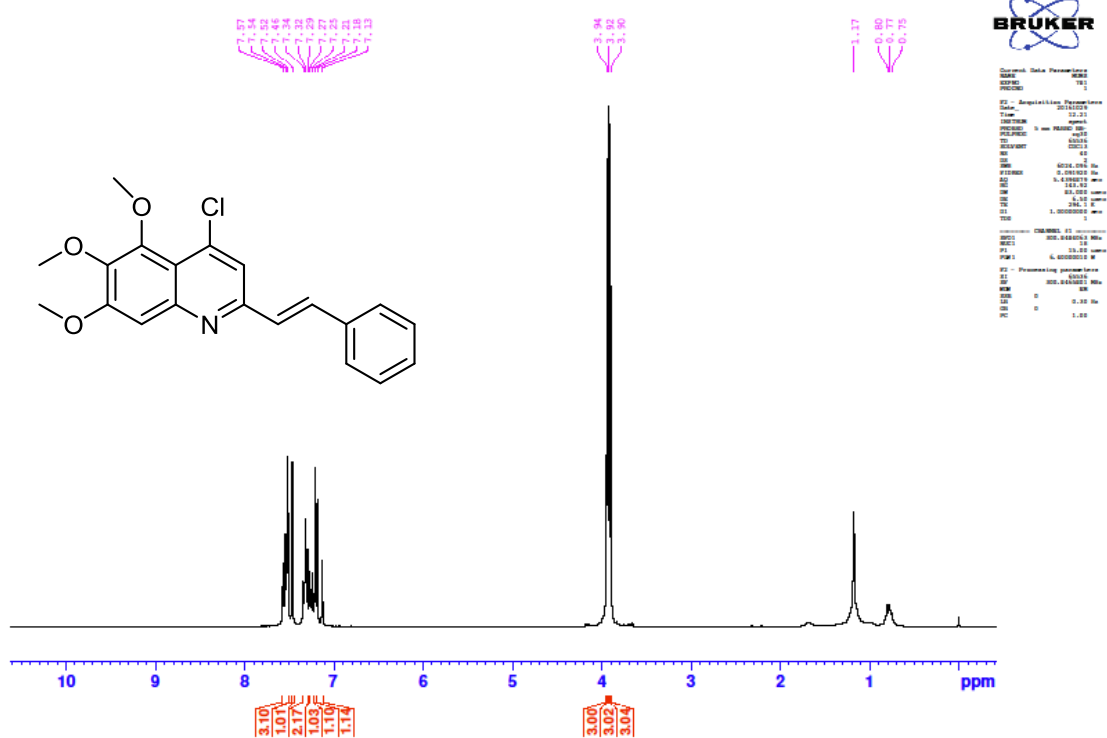
4g



*Bu-Ali Research Center, Mashhad University of Medical Sciences, Mashhad, Iran.

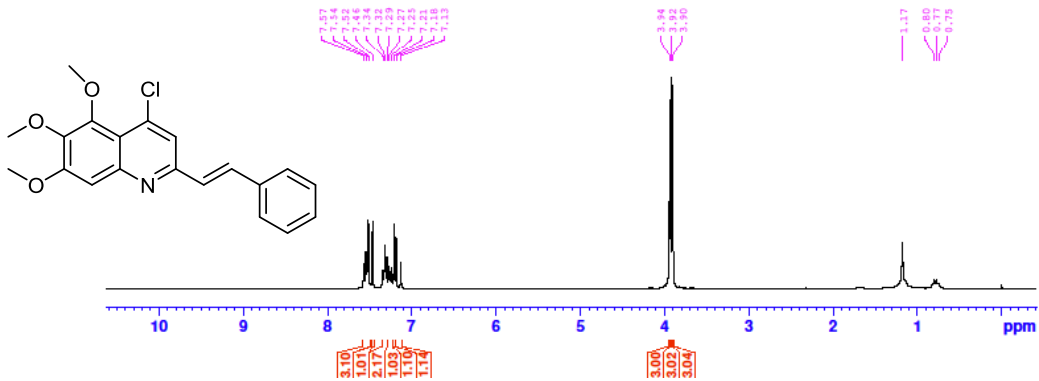
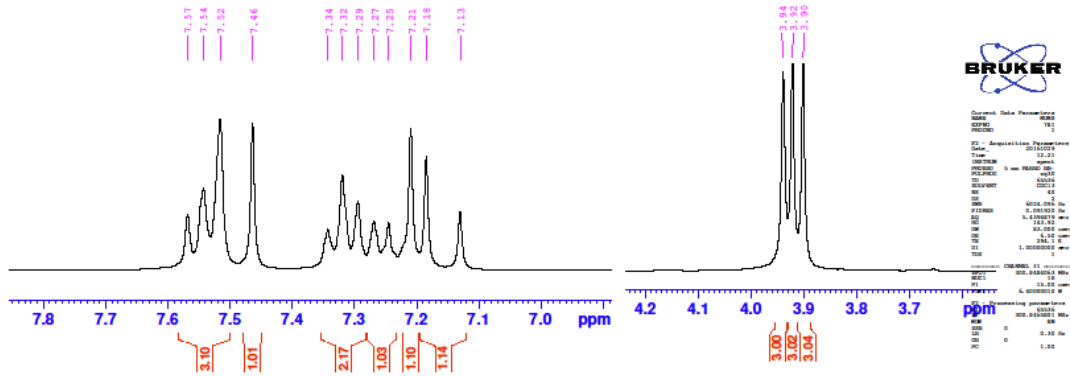
4g

Dr.ghodsi- code ST3(mirzaei)-



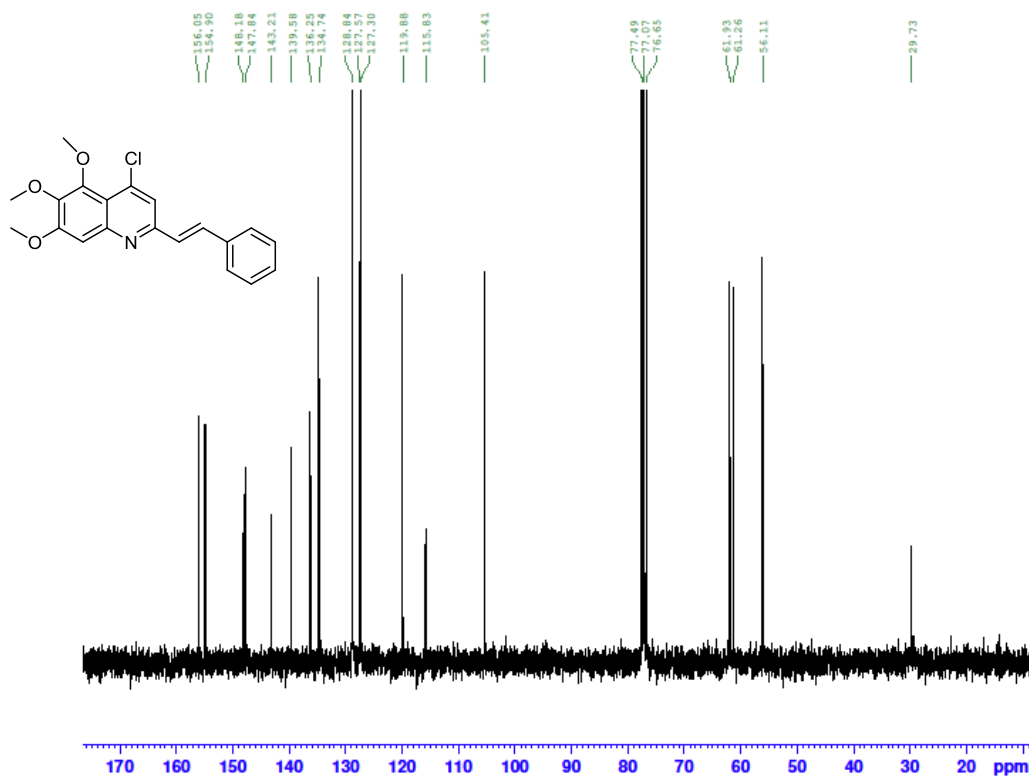
5a

Dr.ghodsi- code ST3(mirzaei)-



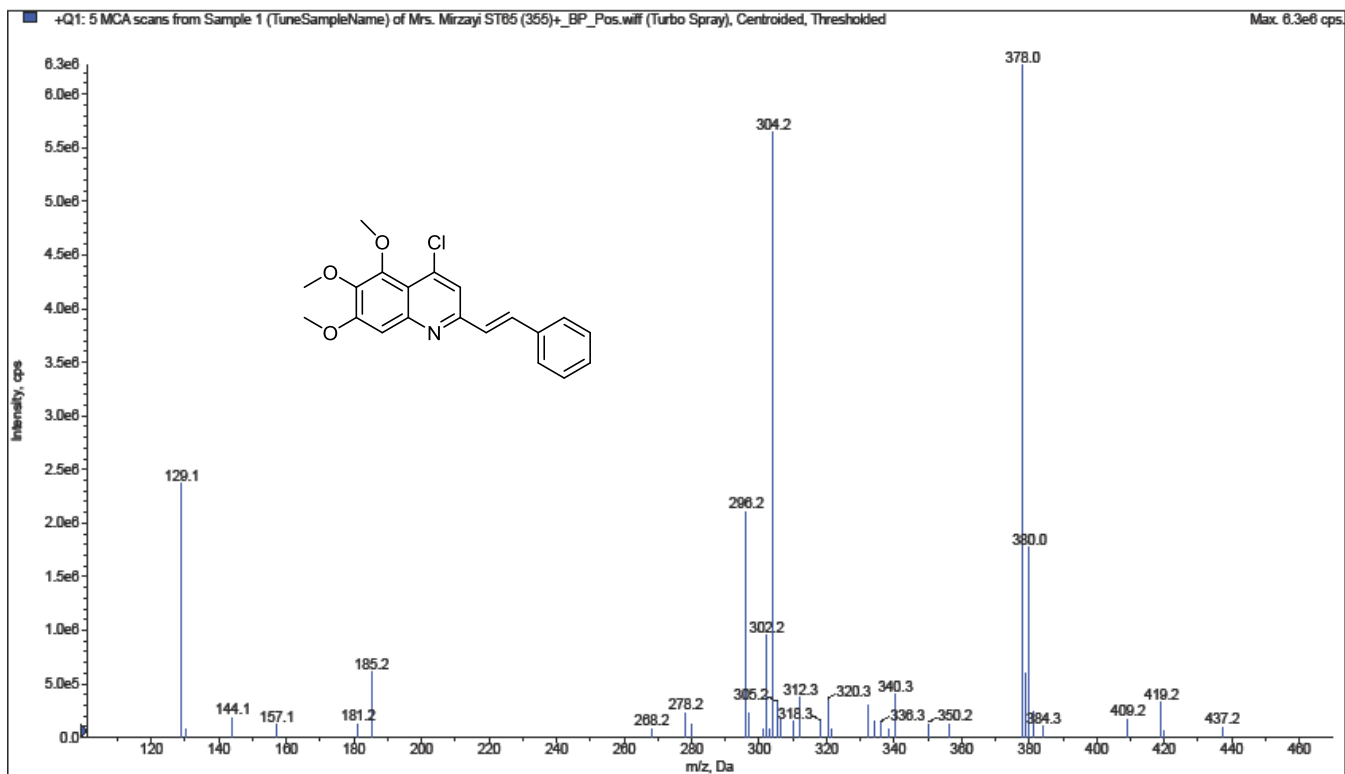
5a

C13-Dr.ghodsi- code ST3(mirzaei) -



```
Current Data Parameters
NAME      M002
EXPNO    1
PROCNO   1
F2 - Acquisition Parameters
Date_    20161203
Time     12.14
INSTRUM  spect
PROBHD   5 mm HNPQ 1H/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        2048
DS        4
SWH       18119.941 Hz
FIDRES    0.37627 Hz
AQ         1.509753 sec
RG         320
SQ         27.100000 sec
RG2        28.11
SI         0.0000000 sec
SI1        0.0000000 sec
TSD        1
===== CHANNEL f1 =====
NUC1       13C
P1         12.00
PL1        0.0000000 Hz
===== CHANNEL f2 =====
NUC2       13C
P2         12.00
PL2        0.0000000 Hz
===== CHANNEL f3 =====
NAME      M002
EXPNO    1
PROCNO   1
F2 - Processing parameters
SI         0.0000000 sec
SI1        0.0000000 sec
TSD        1
===== CHANNEL f1 =====
NUC1       13C
P1         12.00
PL1        0.0000000 Hz
===== CHANNEL f2 =====
NUC2       13C
P2         12.00
PL2        0.0000000 Hz
```

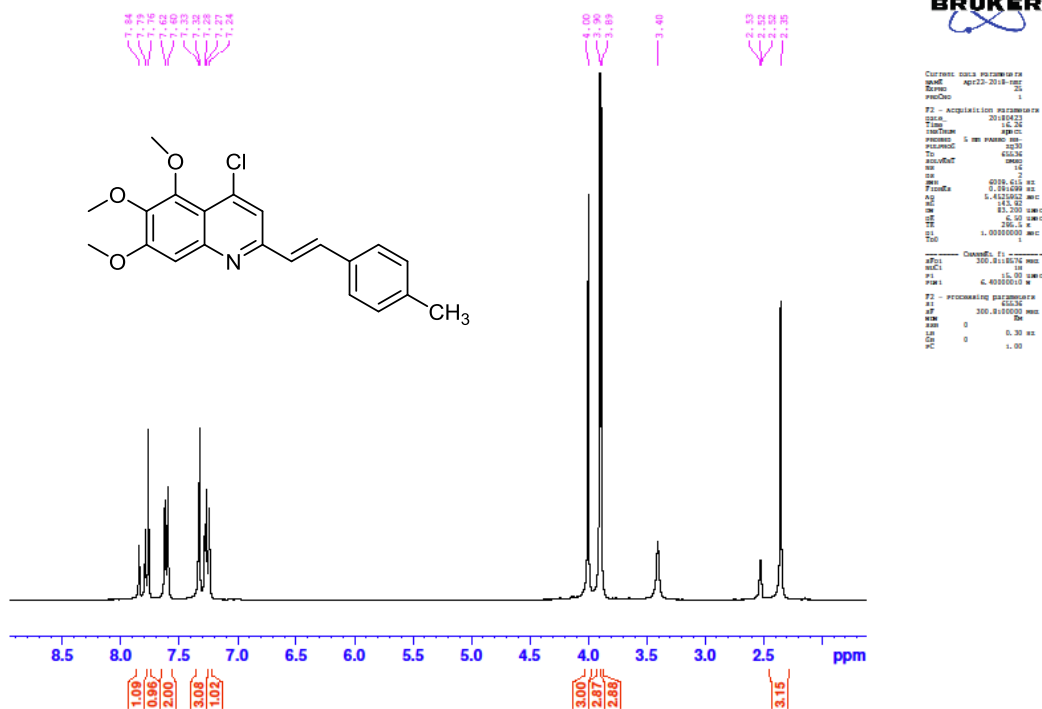
5a



*Bu-Ali Research Center, Mashhad University of Medical Sciences, Mashhad, Iran.

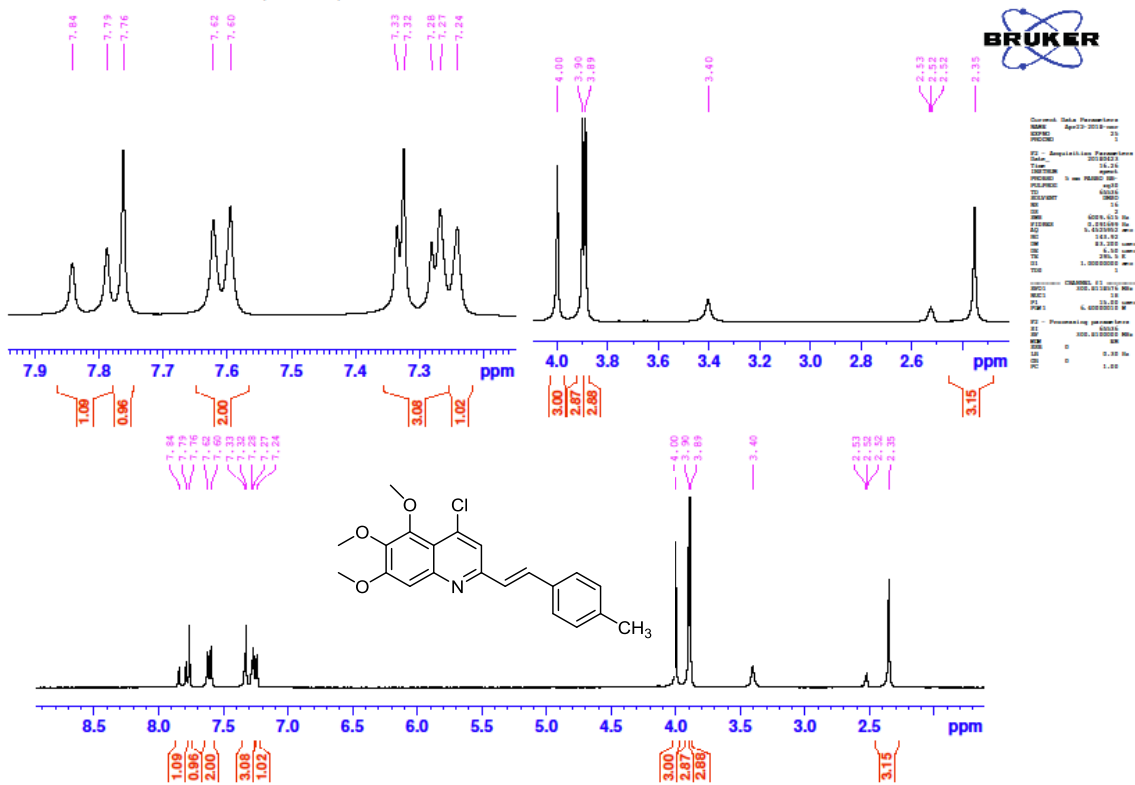
5a

Dr. Ghodsi- code st68 (Mirzaei)-

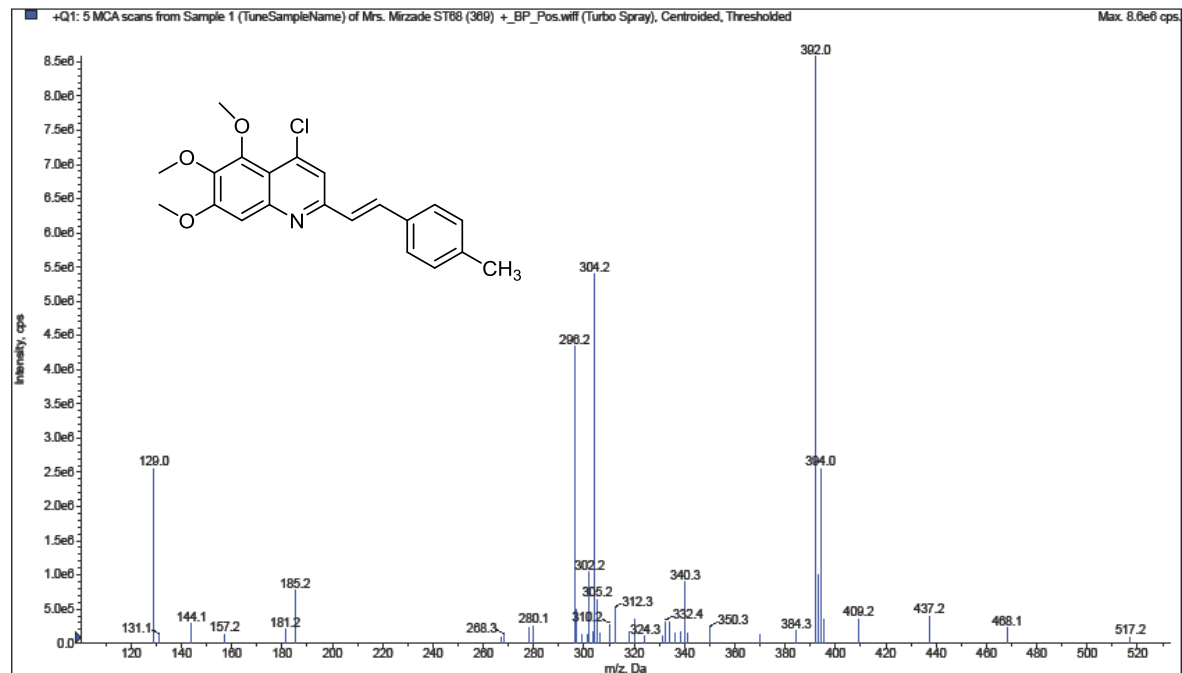


5b

Dr. Ghodsi- code st68 (Mirzaei)-

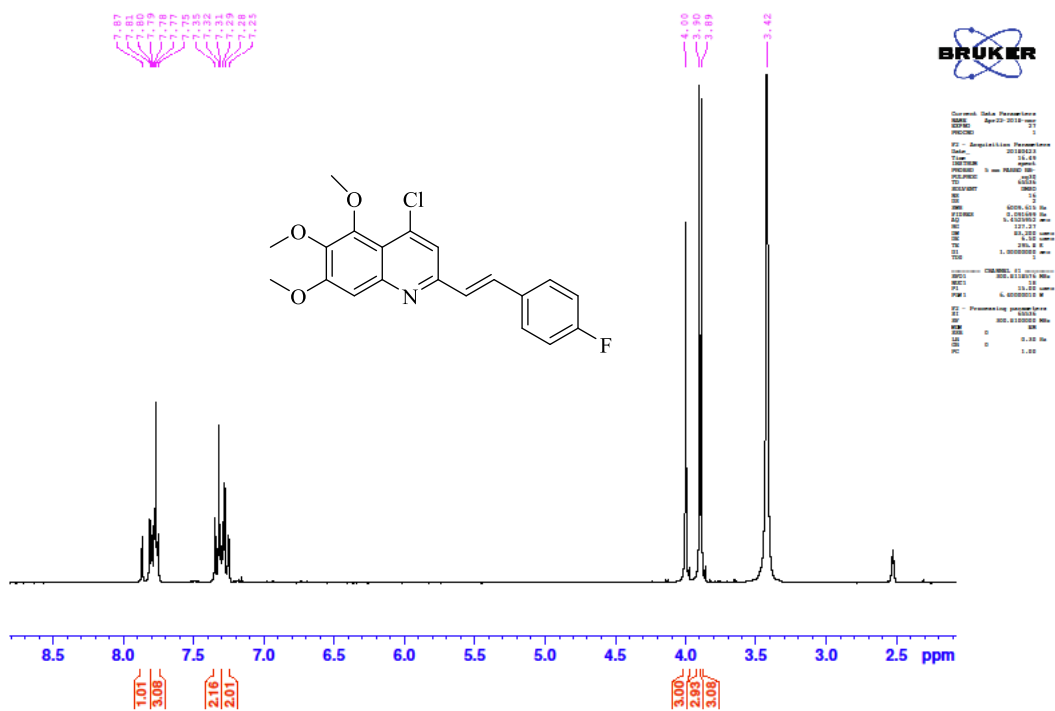


5b



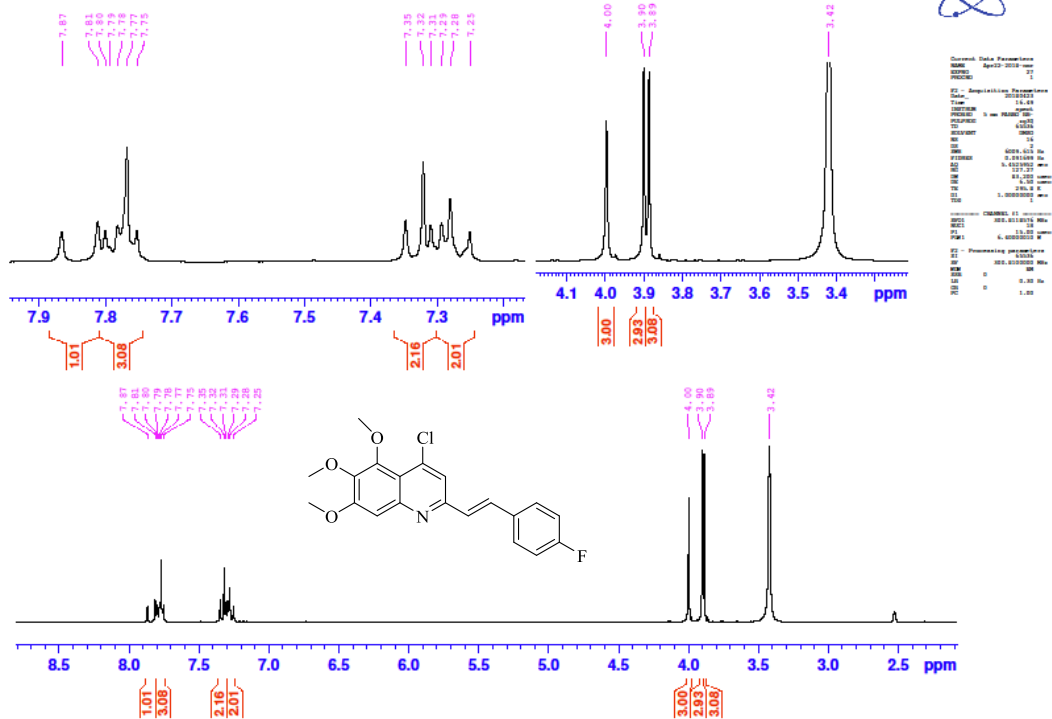
*Bu-Ali Research Center, Mashhad University of Medical Sciences, Mashhad, Iran.

Dr. Ghodsi- code st69 (Mirzaei)-69-

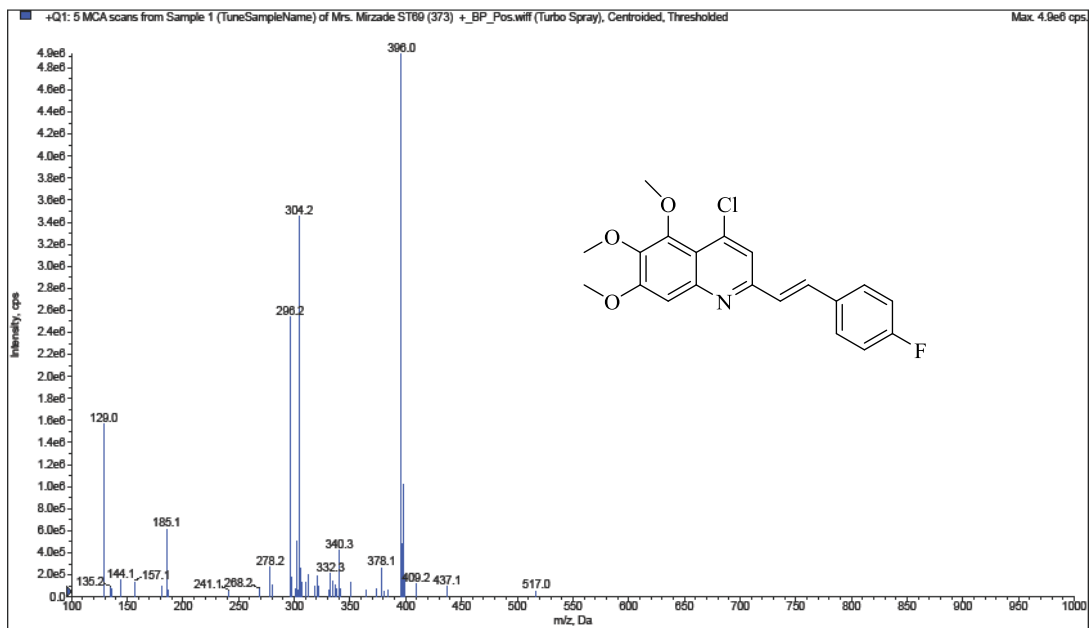


5c

Dr. Ghodsi- code st69 (Mirzaei)-69-

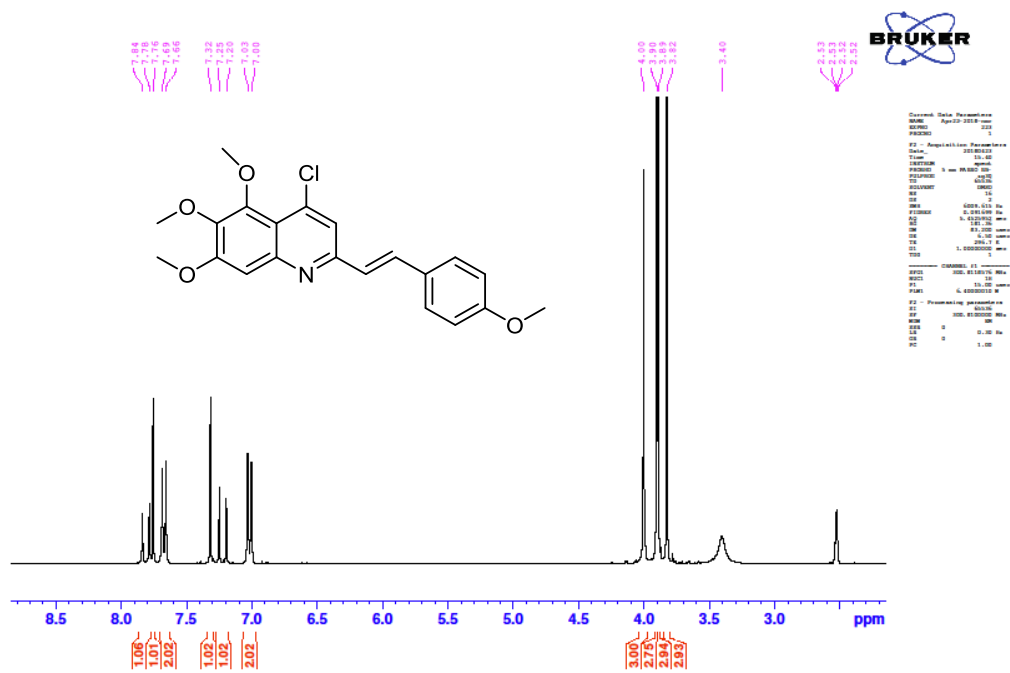


5c



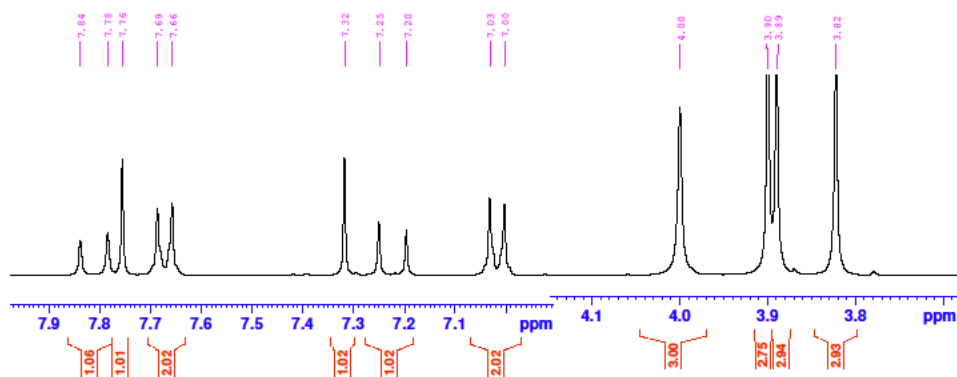
*Bu-Ali Research Center, Mashhad University of Medical Sciences, Mashhad, Iran.

Dr. Ghodsi- code st66 (Mirzaei)-

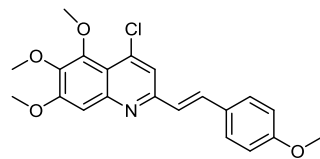
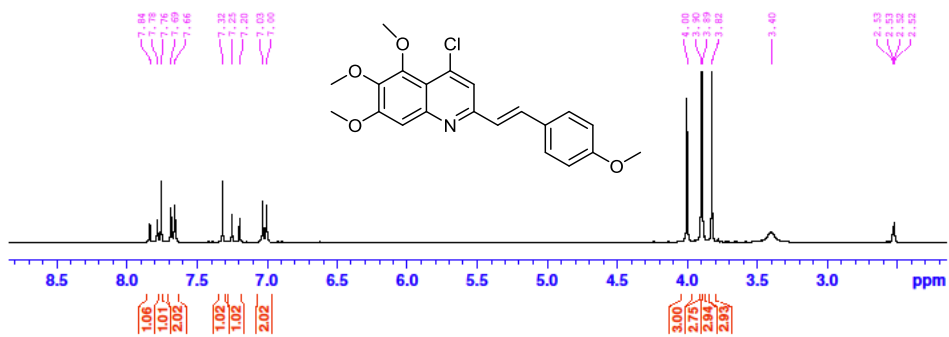


5d

Dr. Ghodsi- code st66 (Mirzaei)-

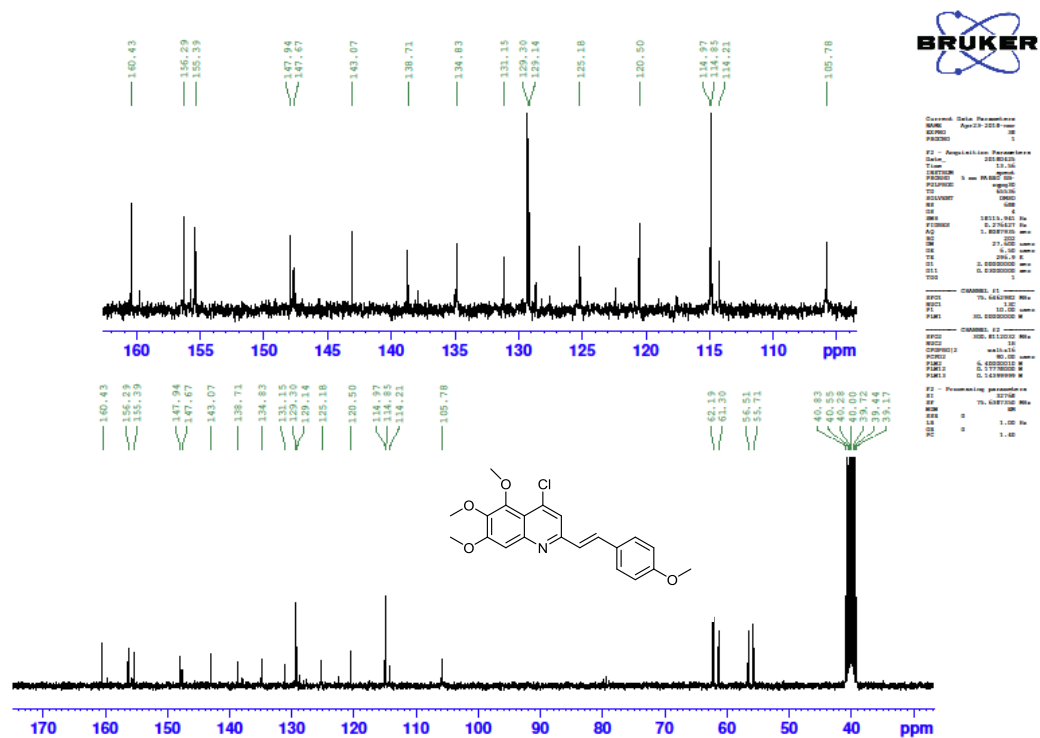


===== Data Parameters =====
NAME: April20-2018-022
EXPNO: 2
PROCNO: 1
F2 - Acquisition Parameters
Date_ 20180220
Time: 12.00
INSTRUM: spect
PROBHD: 5 mm BBOBO-500
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 1024
DS: 4
SWH: 6000.000 MHz
FIDRES: 0.0012490 MHz
AQ: 0.12000000 sec
RG: 655.36
SF: 500.136000 MHz
WDW: EM
SSB: 0
LB: 3.00 Hz
GB: 0
PC: 1.00000000 sec
===== Processing parameters =====
SI: 32768
SF: 500.136000 MHz
WDW: EM
SSB: 0
LB: 3.00 Hz
GB: 0
PC: 1.00

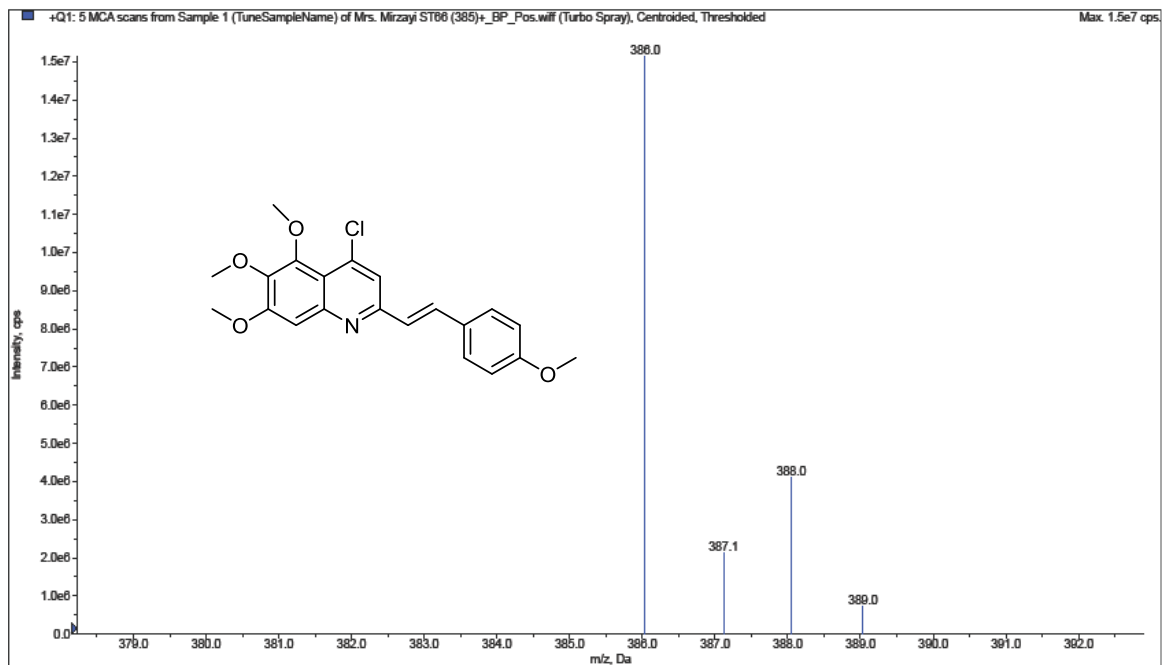


5d

C13-Dr.ghodai- code ST66(mirzaei)-

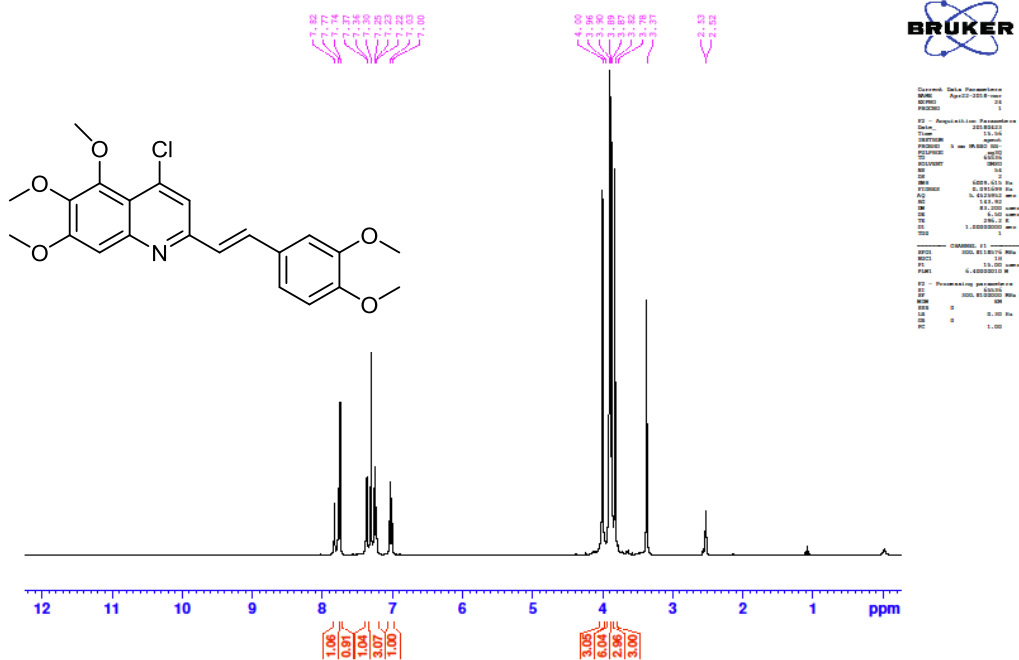


5d



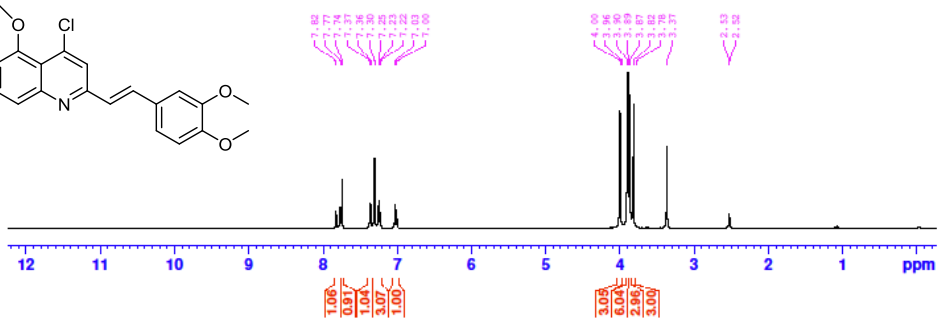
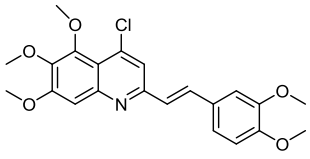
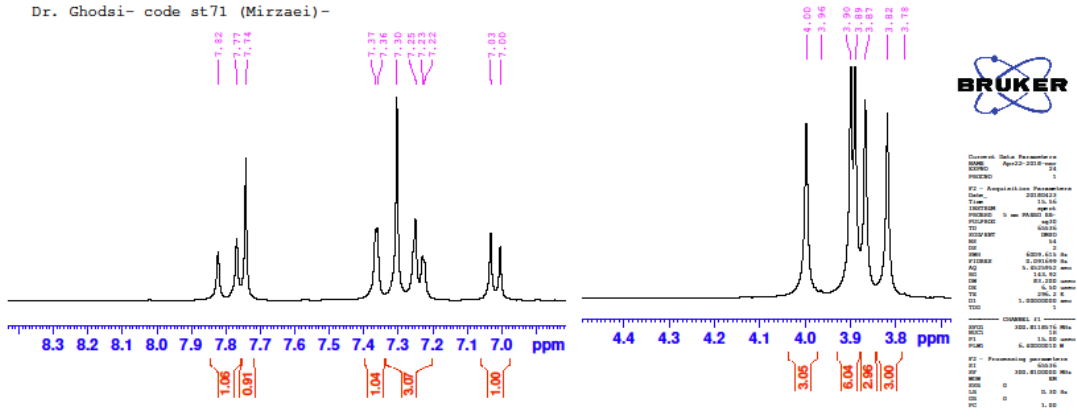
*Bu-Ali Research Center, Mashhad University of Medical Sciences, Mashhad, Iran.

Dr. Ghodsi- code st71 (Mirzaei)-

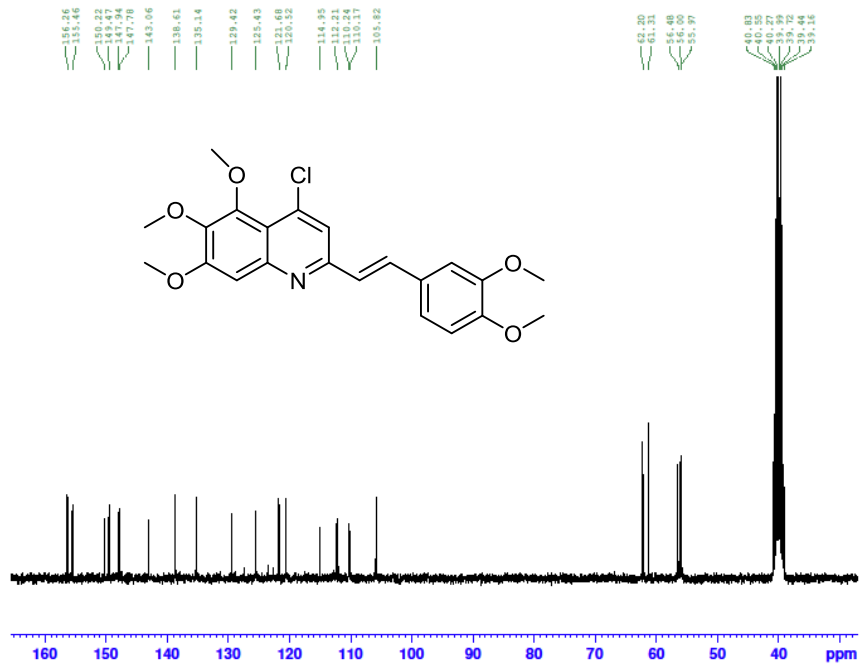


5e

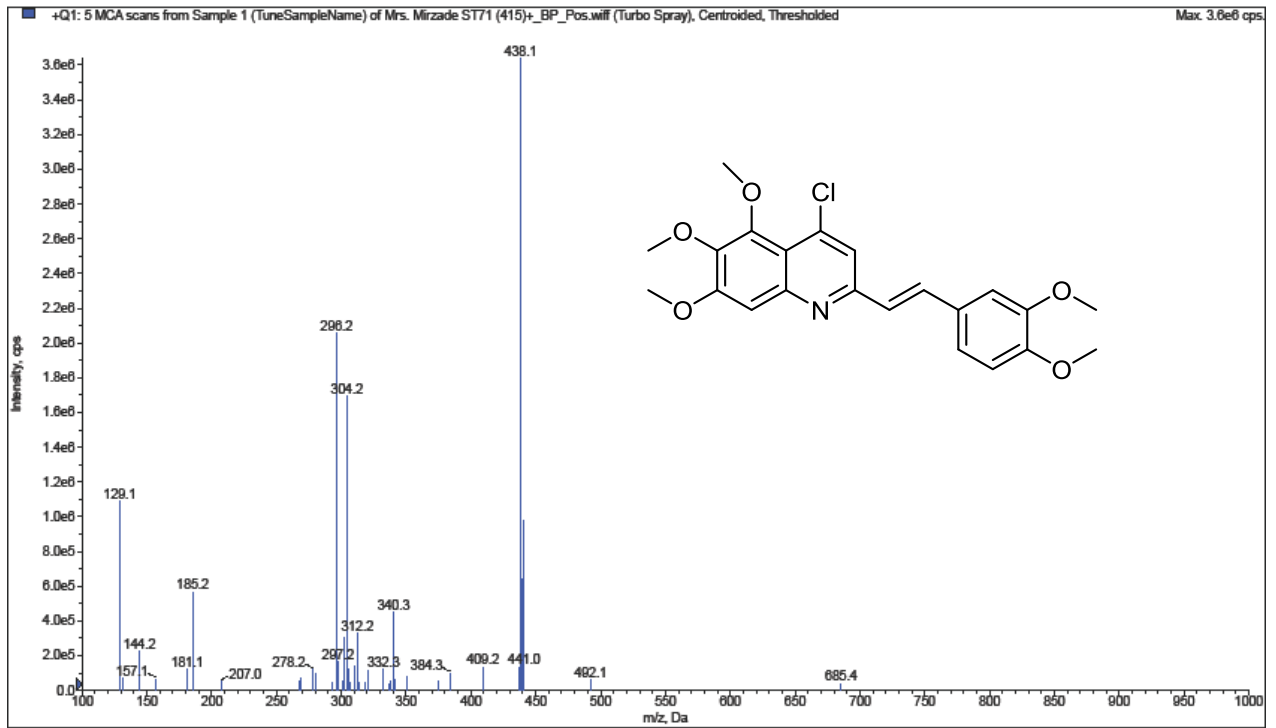
Dr. Ghodsi- code st71 (Mirzaei)-



C13-Dr.ghodsi- code ST71(mirzaei)-

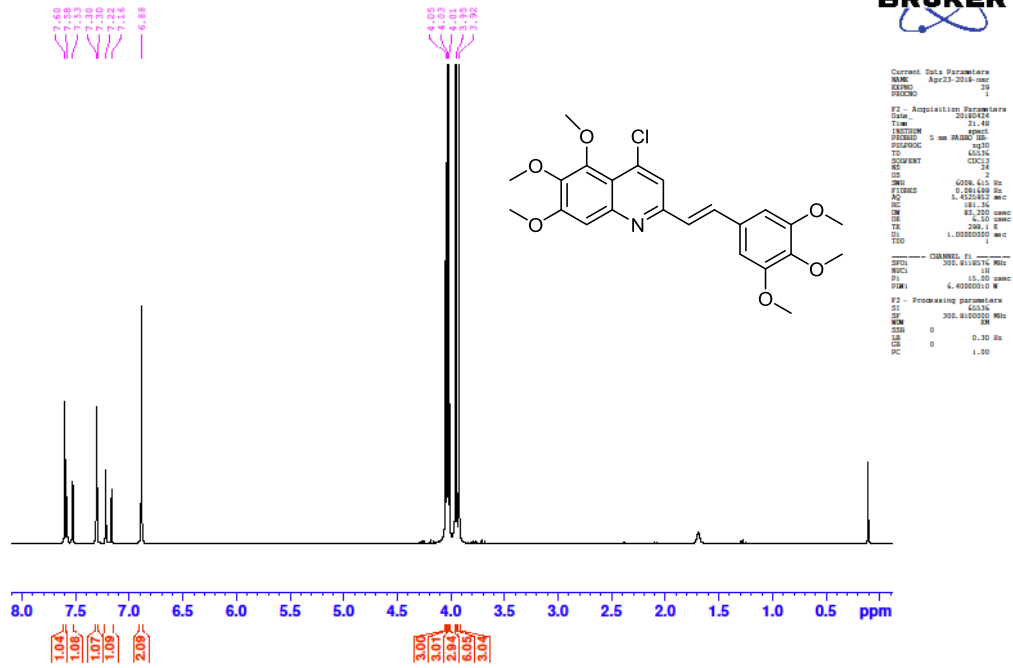


5e

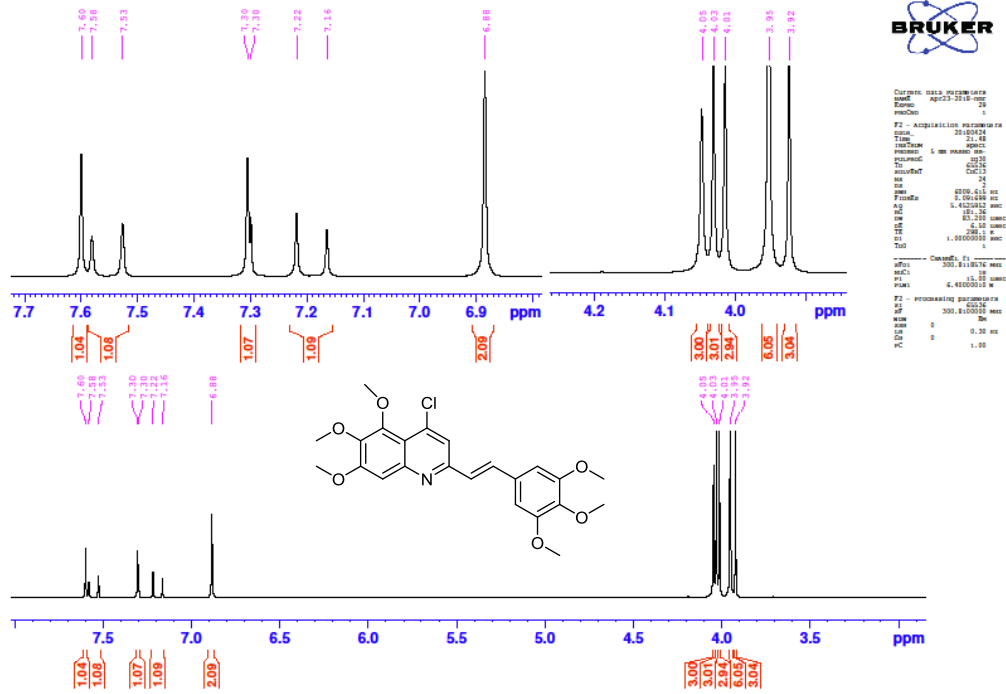


*Bu-Ali Research Center, Mashhad University of Medical Sciences, Mashhad, Iran.

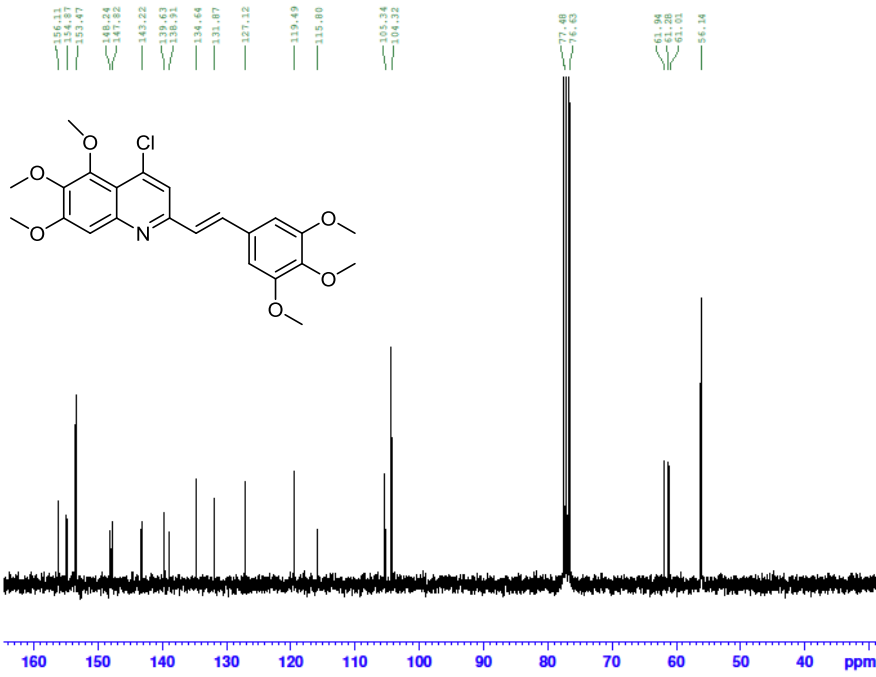
Dr. Ghodsi- code st67 (Mirzaei)-

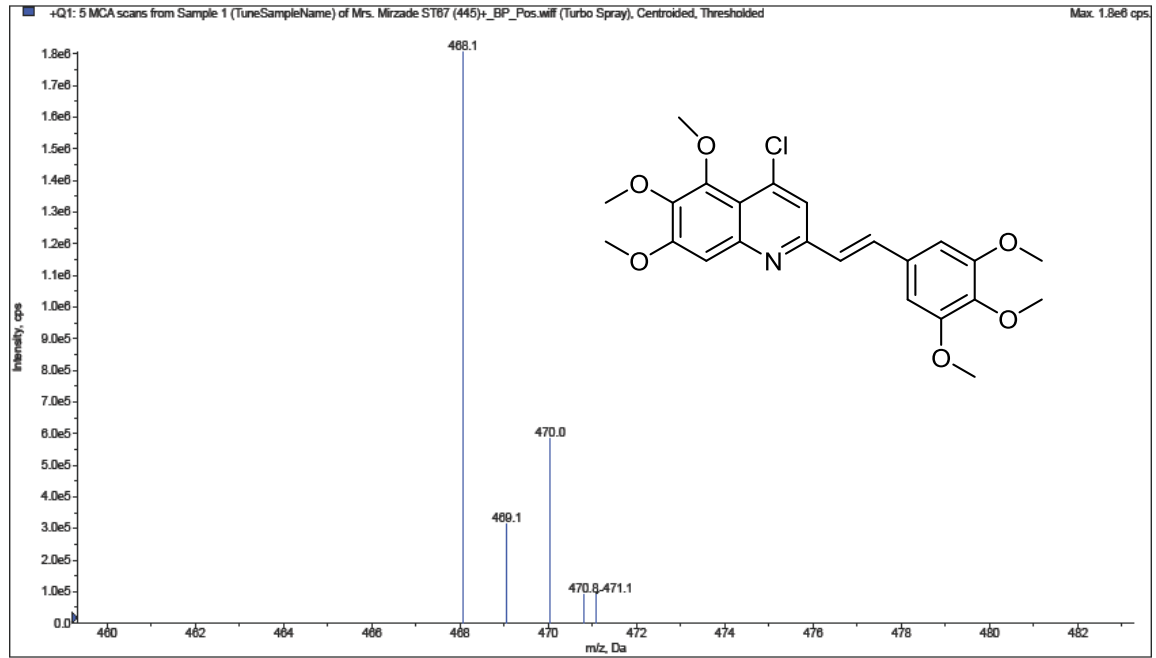


Dr. Ghodsi- code st67 (Mirzaei)-



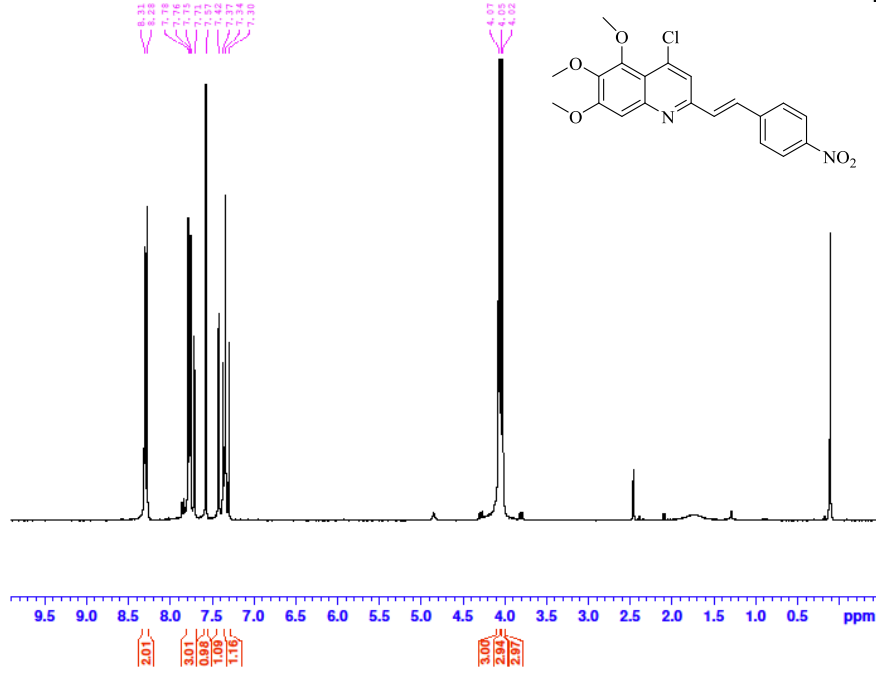
C13-Dr.ghodsi- code ST67(mirzaei)-





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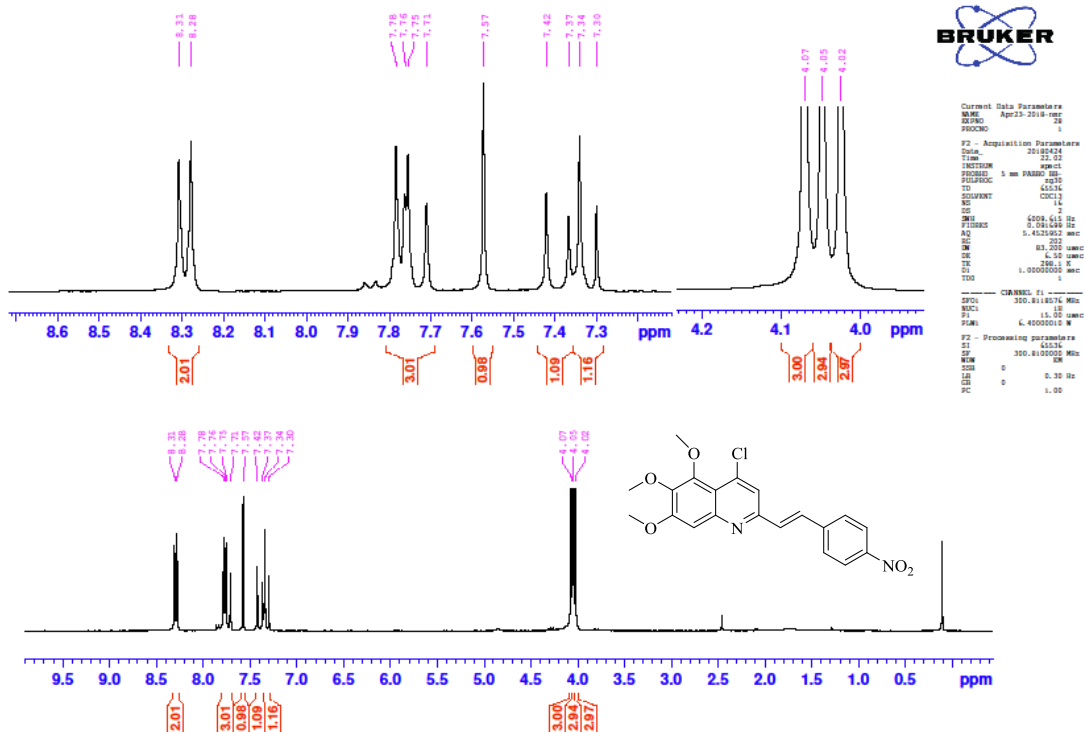
Dr. Ghodsi- code st70 (Mirzaei)-



Current Data Parameters
Date: Apr 23 2018 09:28
PROCNO: 1
F2 - Acquisition Parameters
Date: 20180424
Time: 11:21
INSTRUM: spect
PROBHD: 5 mm HANNUM QNP
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 1
DS: 4
SWH: 4008.613 Hz
FIDRES: 0.081448 Hz
AQ: 5.4521862 sec
RG: 320
IN: 83.300 umec
DE: 6.20 umec
TE: 298.2 K
SI: 1.00000000 sec
SFO: 1
----- CHANNEL f1 -----
SFO1: 300.811876 MHz
NUC1: 13C
P1: 15.00 umec
PULSE: C40000010.0 W
F2 - Processing parameters
SI: 65536
SF: 300.8100000 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

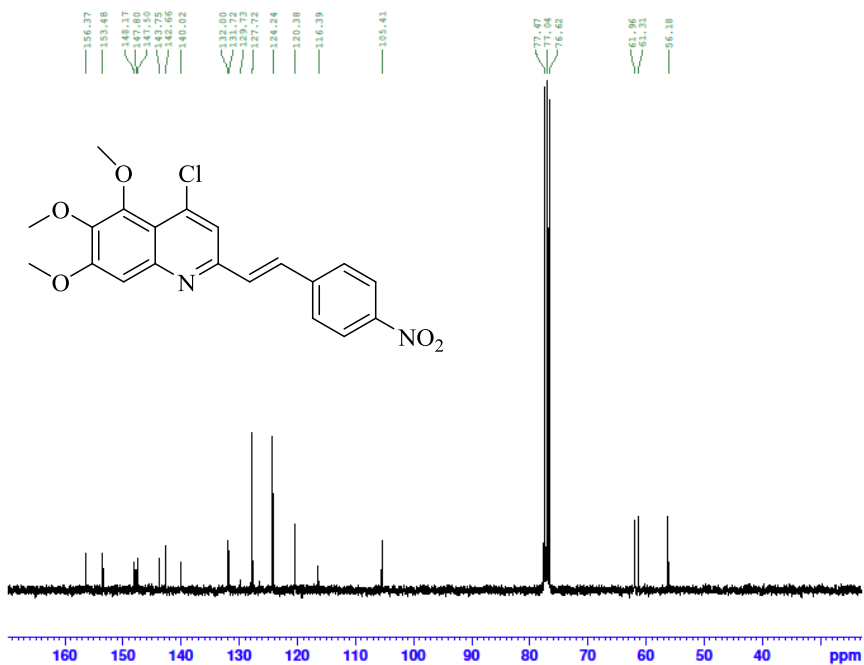
5g

Dr. Ghodsi- code st70 (Mirzaei)-



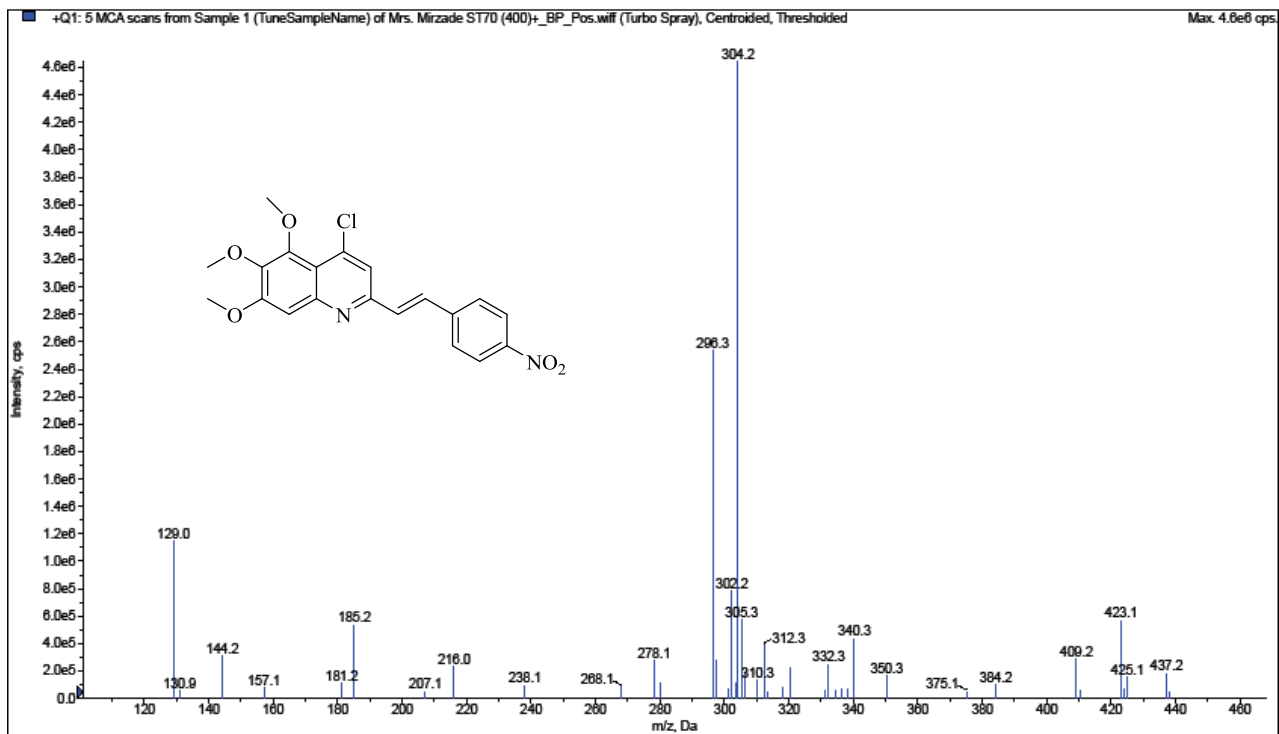
5g

C13-Dr.ghodsi- code ST70(mirzaei)-



```
Current data parameters
NAME: Apr23-2018-001
EXPNO: 01
PROCNO: 1
F2 - acquisition parameters
NAME:
DATE_:
TIME: 15.14
PULPROG: zgpg30
PROBHD: 5 mm PABBO-1
P1: 0.00100000
PRGPHC: zgpg30
TD: 65536
AQ: 0.03125000
RG: 327.50
SI: 327.50
SF: 125.760361
WDW: EM
SSB: 0
GB: 0
PC: 1.00
FIDRES: 0.272471
AQ: 1.897933
RG: 327.50
SI: 327.50
SF: 125.760361
WDW: EM
SSB: 0
GB: 0
PC: 1.00
F2 - processing parameters
SI: 327.50
SF: 125.760361
WDW: EM
SSB: 0
GB: 0
PC: 1.00
```

5g



*Bu-Ali Research Center, Mashhad University of Medical Sciences, Mashhad, Iran.

5g