

Supporting Information

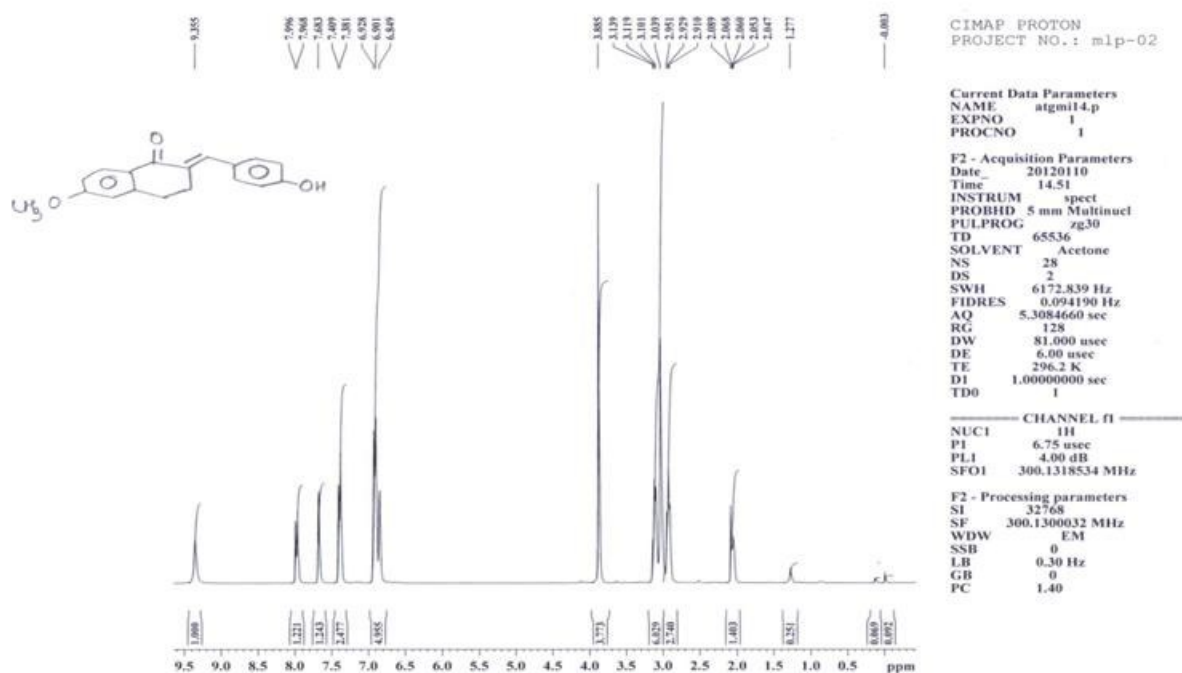
Synthesis of 4-phenyl-5,6-dihydrobenzo[*h*]quinazolines and their evaluation as growth inhibitors of carcinoma cells

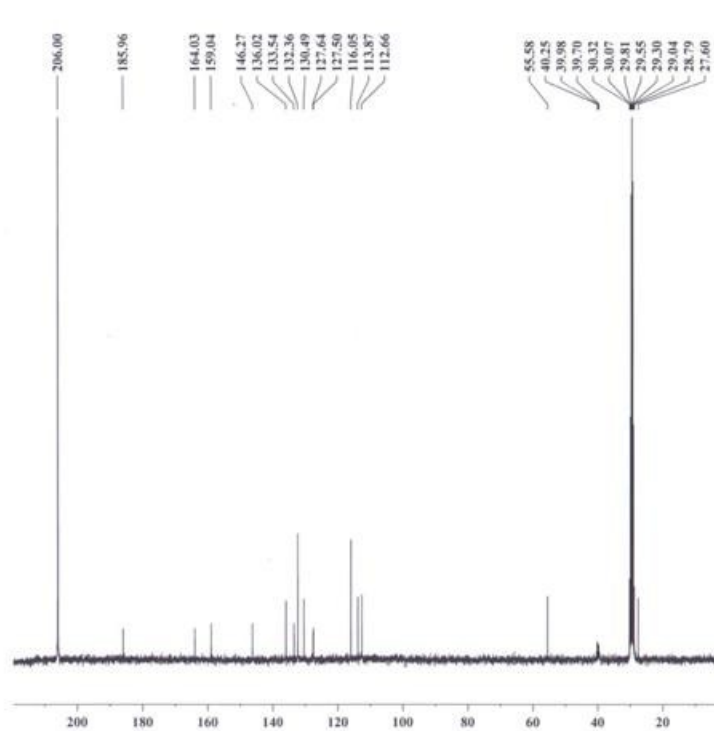
Hardesh K Maurya^a, Mohammad Hasanain^d, Sarita Singh^a, Jayanta Sarkar^d, Vijaya Dubey^b,
Aparna Shukla^c, Suaib Luqman^b, Feroz Khan,^c Atul Gupta^{a,*}

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(*E*)-2-(4-hydroxybenzylidene)-6-methoxy-3,4-dihydronaphthalen-1(2*H*)-one (3a).





CIMAP-CARBON
PROJECT NO.: MLP-04

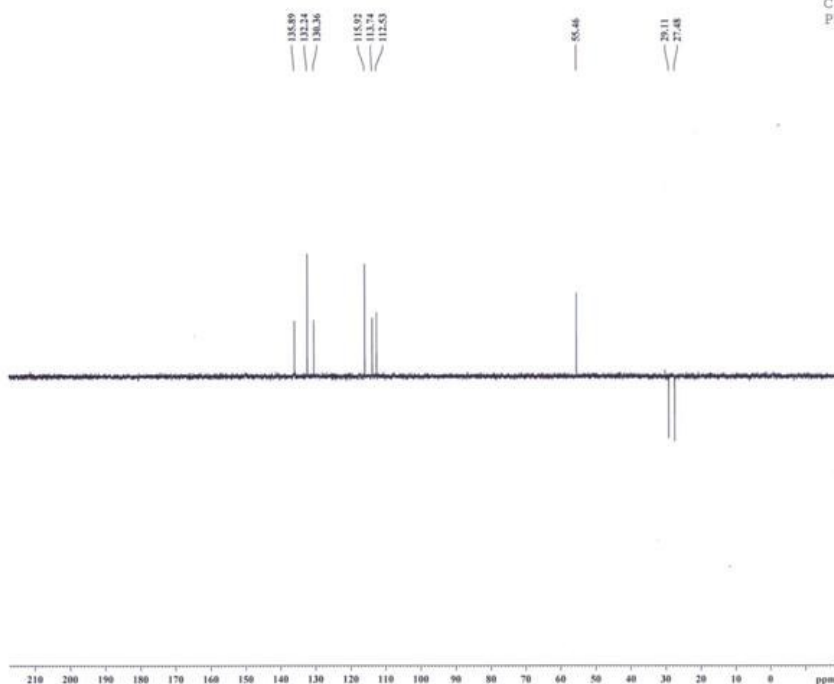
Current Data Parameters
NAME: atgm14.p
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20120110
Time: 14.54
INSTRUM: spect
PROBHD: 5 mm Multinuc1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 550
DS: 4
SWH: 17985.611 Hz
FIDRES: 0.274439 Hz
AQ: 1.8219508 sec
RG: 32768
DW: 27.800 usec
DE: 6.00 usec
TE: 296.2 K
D1: 2.00000000 sec
d11: 0.83000000 sec
DELTA: 1.89999998 sec
TD0: 1

CHANNEL f1
NUC1: 13C
P1: 11.50 usec
PL1: -6.00 dB
SFO1: 75.4752950 MHz

CHANNEL f2
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 120.00 usec
PL2: 4.00 dB
PL12: 29.00 dB
PL13: 33.00 dB
SFO2: 300.1312000 MHz

F2 - Processing parameters
SI: 32768
SF: 75.4677993 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40



CIMAP-DEPT 135
PROJECT NO.: ILP-13

Current Data Parameters
NAME: atgm14.p
EXPNO: 3
PROCNO: 1

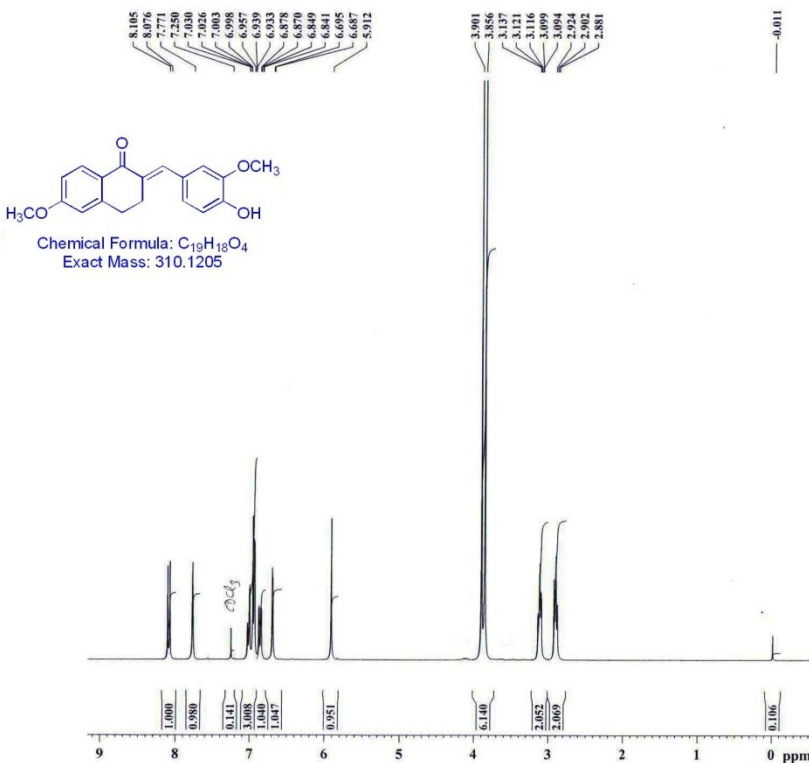
F2 - Acquisition Parameters
Date_: 20120110
Time: 15.56
INSTRUM: spect
PROBHD: 5 mm Multinuc1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 450
DS: 4
SWH: 17985.611 Hz
FIDRES: 0.274439 Hz
AQ: 1.8219508 sec
RG: 16384
DW: 27.800 usec
DE: 6.00 usec
TE: 296.2 K
CNS12: 145.0000000
D1: 2.00000000 sec
d1: 0.80344828 sec
d12: 0.00002000 sec
DELTA: 0.00001464 sec
TD0: 1

CHANNEL f1
NUC1: 13C
P1: 11.50 usec
PL1: -6.00 dB
SFO1: 75.4752950 MHz

CHANNEL f2
CPDPRG2: waltz16
NUC2: 1H
P2: 6.75 usec
PL2: 13.50 usec
PCPD2: 120.00 usec
PL12: 29.00 dB
PL13: 33.00 dB
SFO2: 300.1312000 MHz

F2 - Processing parameters
SI: 32768
SF: 75.4677196 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

(E)-2-(4-hydroxy-3-methoxybenzylidene)-6-methoxy-3,4-dihydronaphthalen-1(2H)-one (3b).



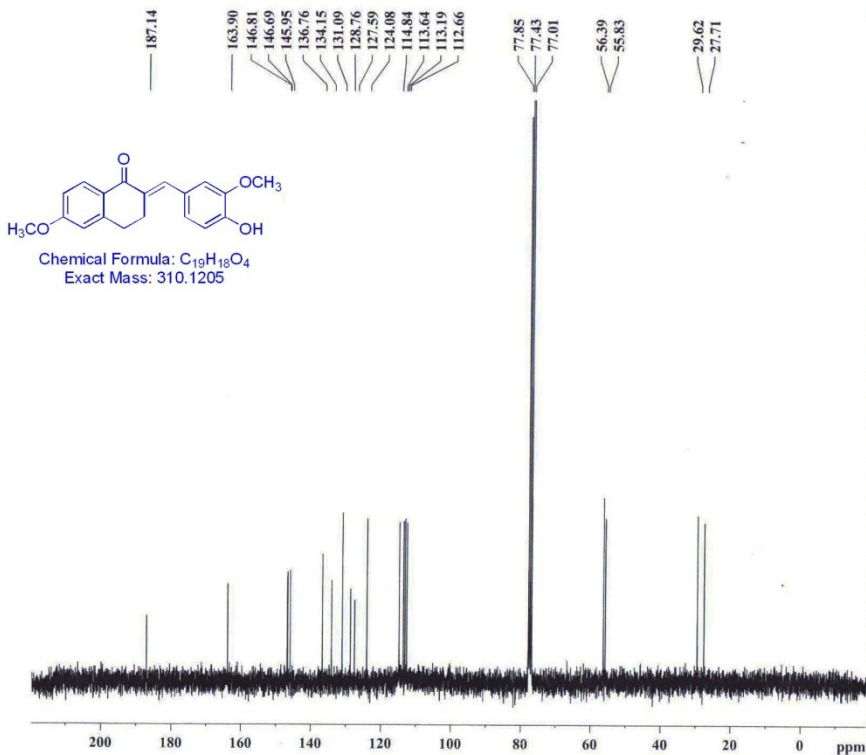
CIMAP-PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk248.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140724
Time 15.30
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 181
DW 55.600 usec
DE 6.00 usec
TE 300.3 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



CIMAP-CARBON
PROJECT NO.: MLP-04

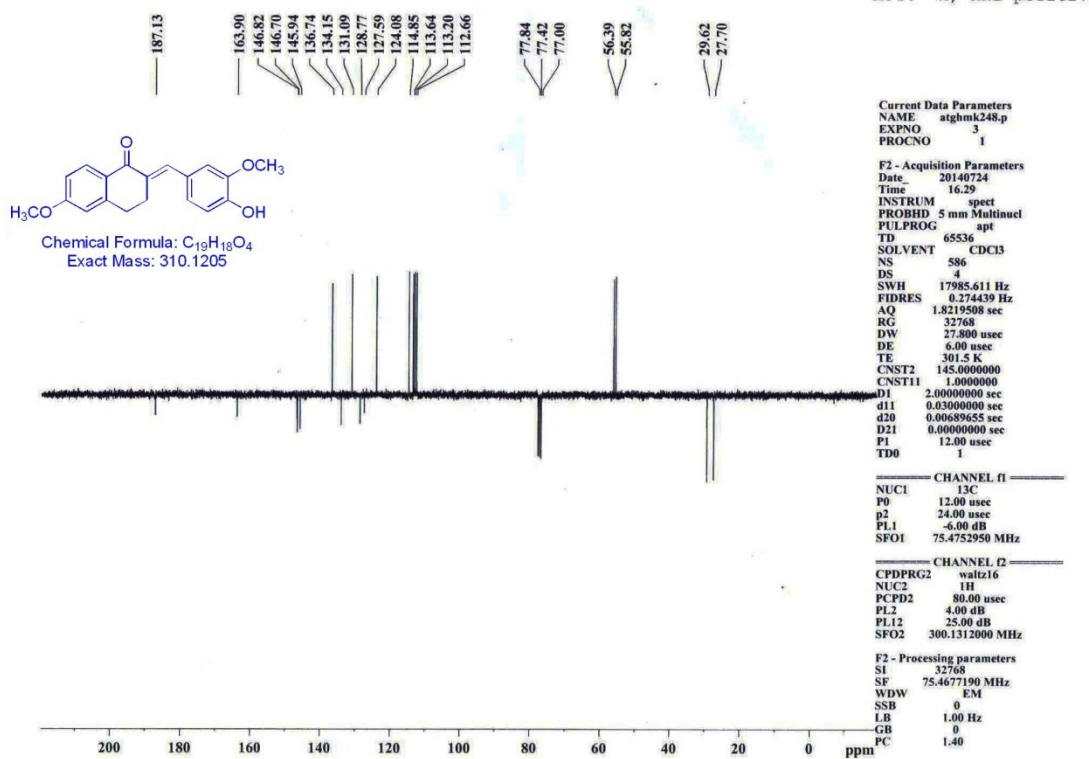
Current Data Parameters
NAME atghmk248.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140724
Time 15.32
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.4 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

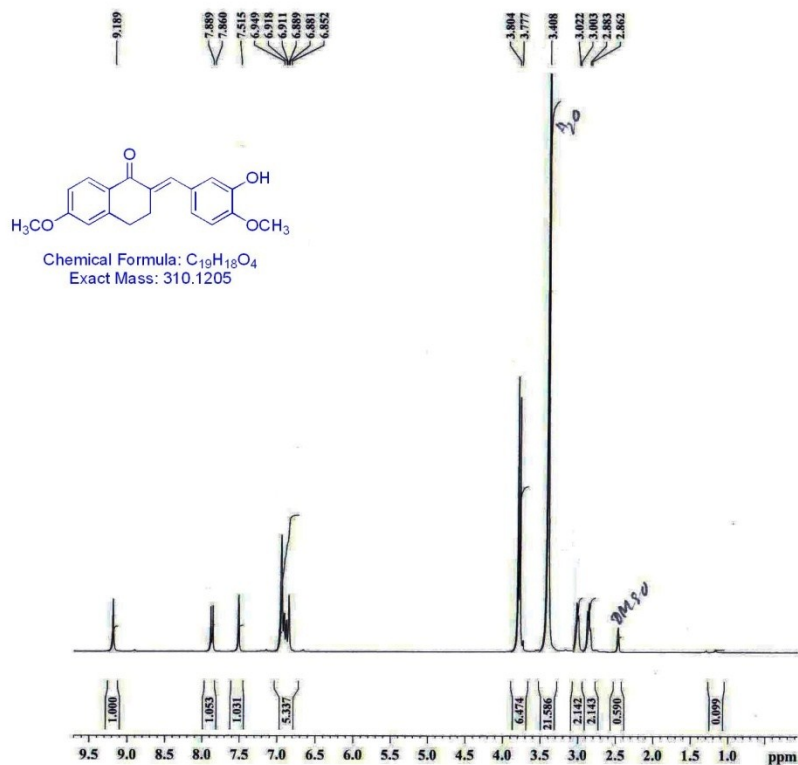
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
PL13 29.00 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



(E)-2-(3-hydroxy-4-methoxybenzylidene)-6-methoxy-3,4-dihydronaphthalen-1(2H)-one (3c).



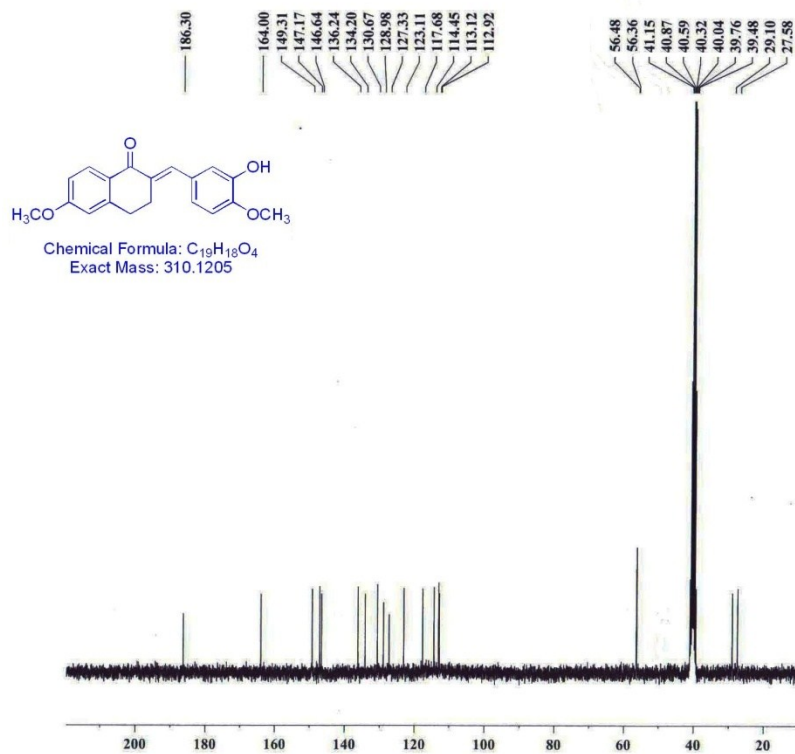
CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk251.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140721
Time 14.24
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 18
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 80.6
DW 55.600 usec
DE 6.00 usec
TE 299.7 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



CIMAP-CARBON
PROJECT NO.: MLP-04

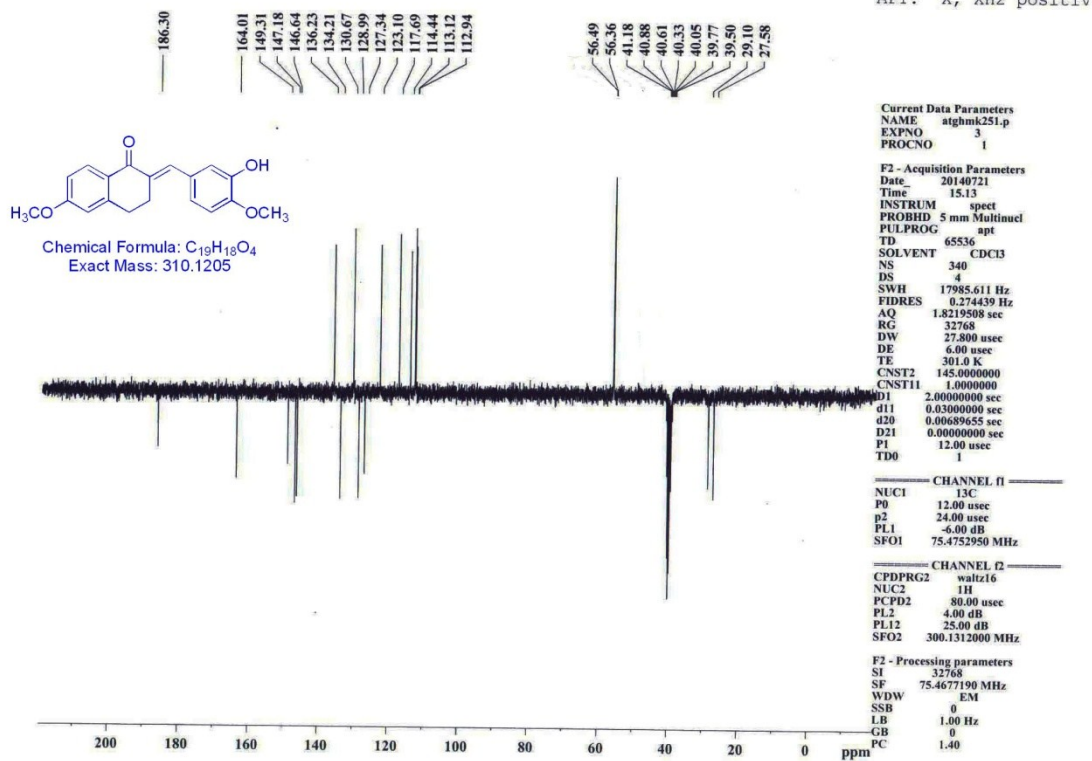
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NAME atghmk251.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140721
Time 14.25
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 412
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 299.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

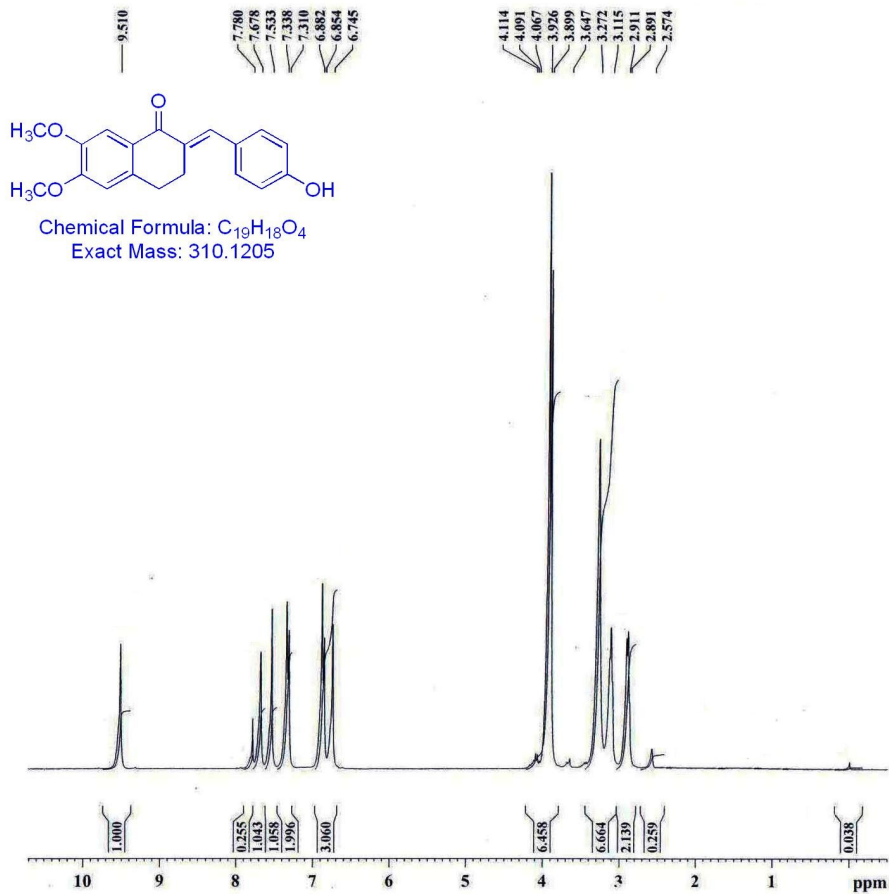
CHANNEL f1
NUC1 13C
P1 12.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
PL13 29.00 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



(*E*)-2-(4-hydroxybenzylidene)-6,7-dimethoxy-3,4-dihydronaphthalen-1(2*H*)-one (3d).



CIMAP PROTON
PROJECT NO.: mlp-02

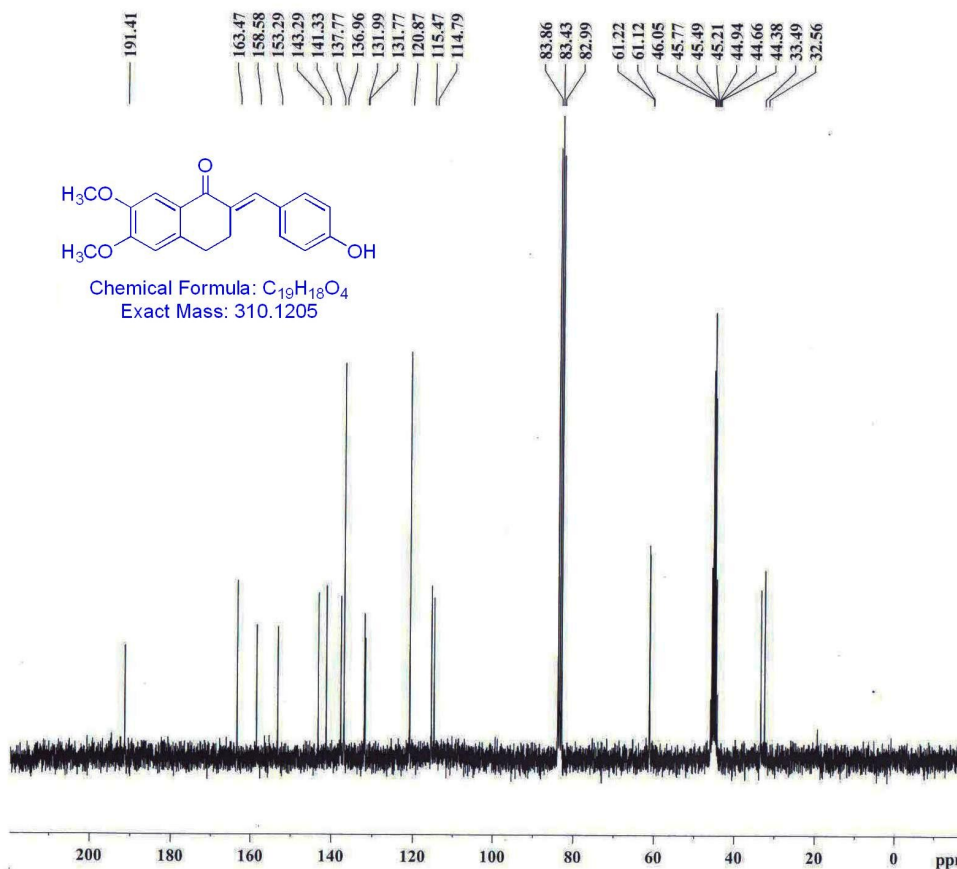
Current Data Parameters
NAME atgvp189.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140728
Time 13.57
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 322.5
DW 55.600 usec
DE 6.00 usec
TE 301.0 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1314046 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

CIMAP-CARBON
PROJECT NO.:MLP-04

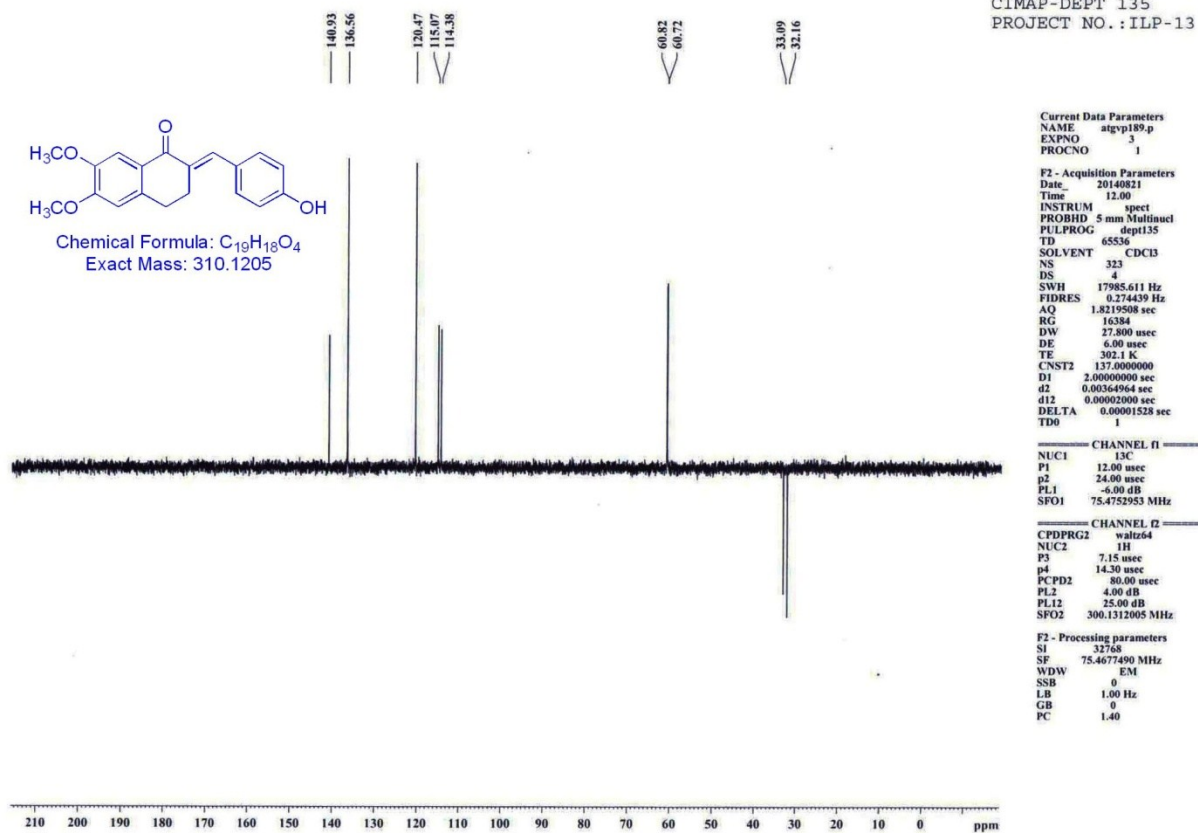


Current Data Parameters
NAME afgyp189.p
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date 20140821
Time 11.49
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 302.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

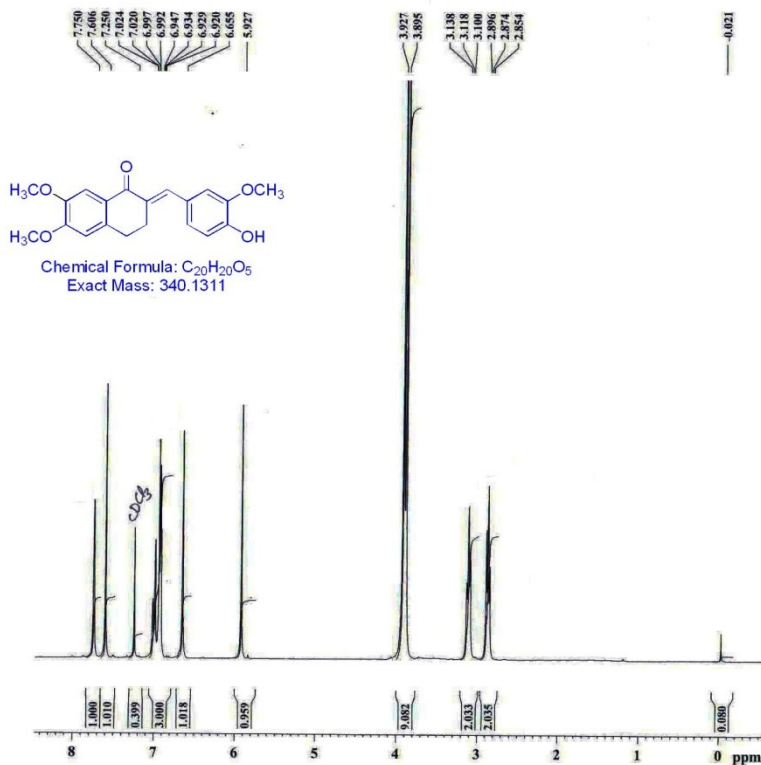
===== CHANNEL f1 =====
NUC1 13C
PI 12.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
PL13 29.00 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



(*E*)-2-(4-hydroxy-3-methoxybenzylidene)-6,7-dimethoxy-3,4-dihydronaphthalen-1(2*H*)-one (3e).



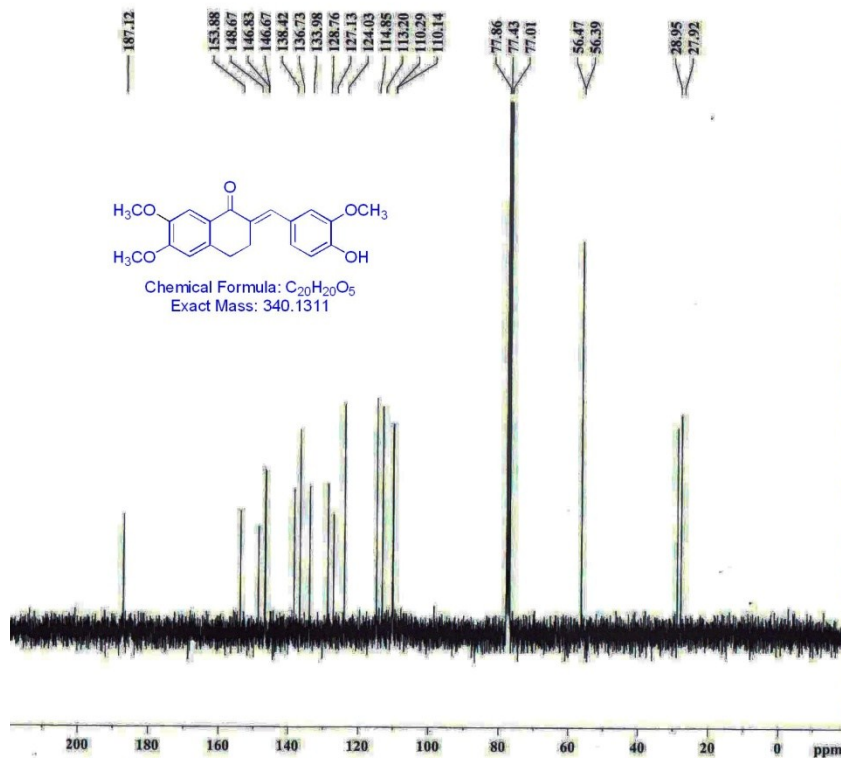
CIMAP-PROTON
 PROJECT NO.: mlp-02

Current Data Parameters
 NAME atghmk254.p
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20140811
 Time 15.30
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 12
 DS 2
 SWH 8992.806 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 161.3
 DW 55.600 usec
 DE 6.00 usec
 TE 301.1 K
 D1 1.00000000 sec
 TD0 1

CHANNEL f1
 NUC1 1H
 P1 7.15 usec
 PL1 4.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40



CIMAP-CARBON
 PROJECT NO.: MLP-04

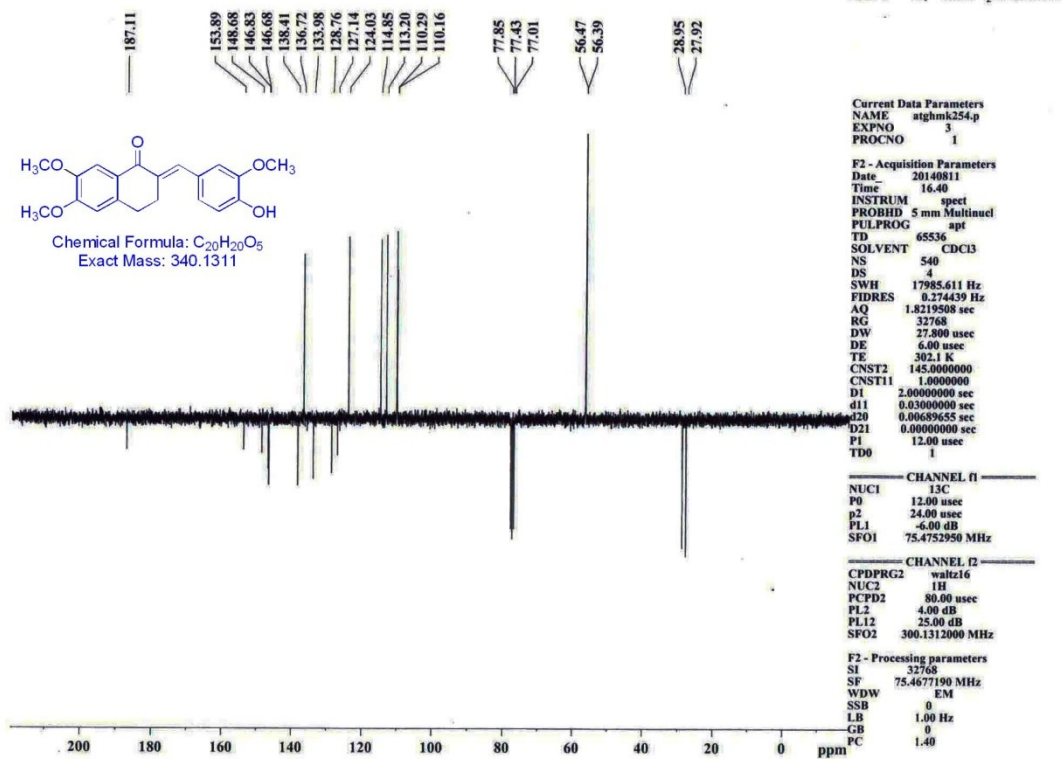
Current Data Parameters
 NAME atghmk254.p
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20140811
 Time 16.04
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 32768
 DW 27.800 usec
 DE 6.00 usec
 TE 301.7 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

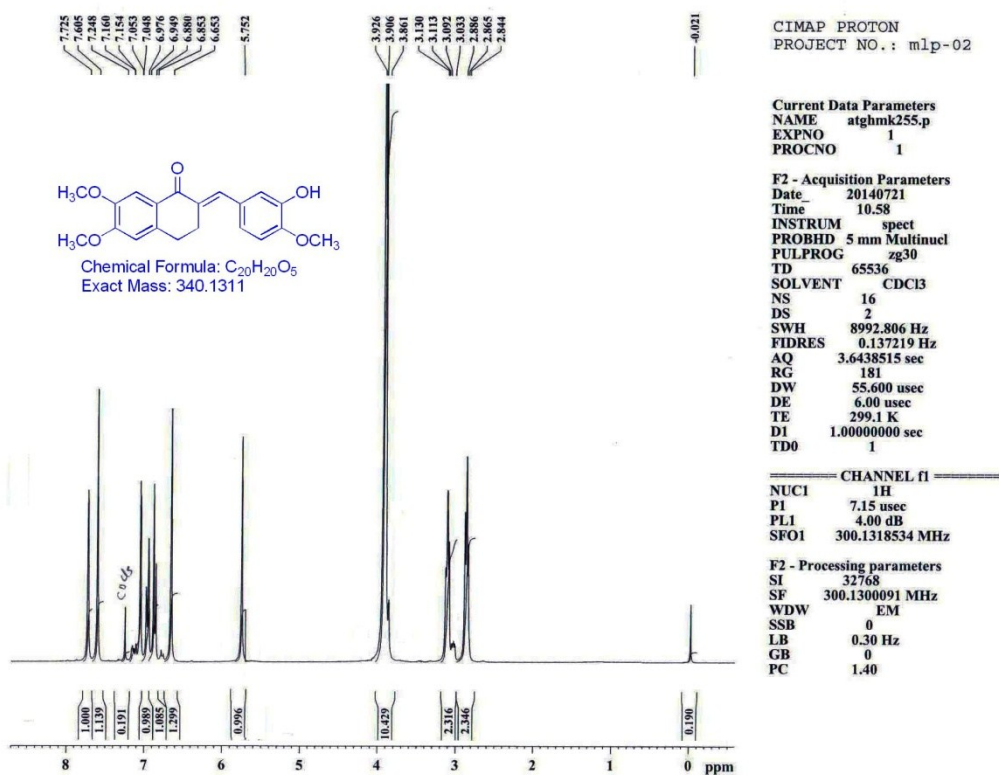
CHANNEL f1
 NUC1 13C
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 75.4752950 MHz

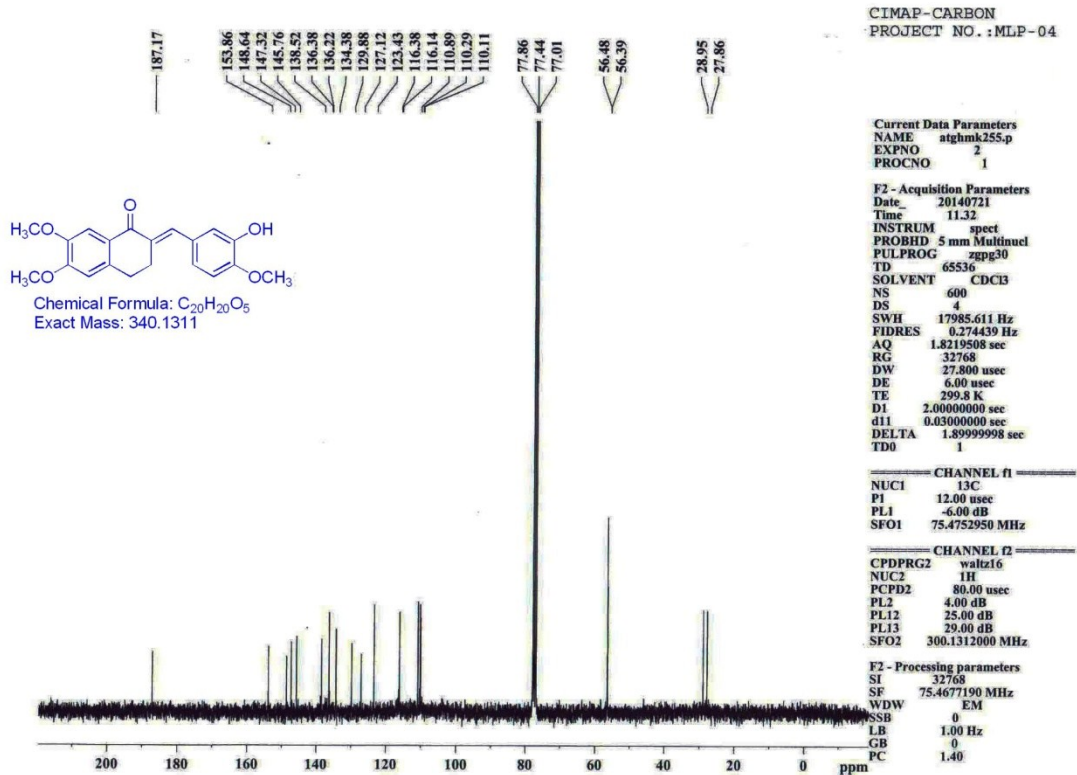
CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 4.00 dB
 PL12 25.00 dB
 PL13 29.00 dB
 SFO2 300.1312000 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677190 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

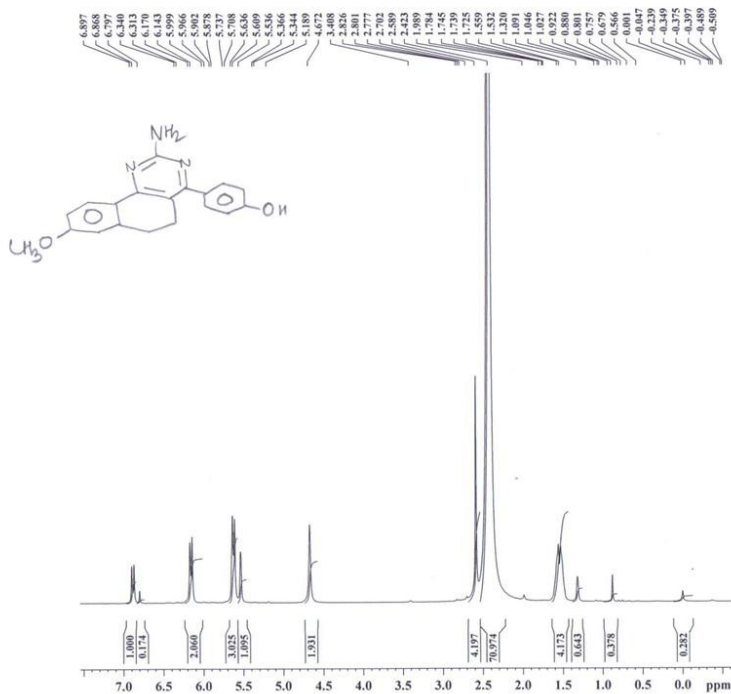


(E)-2-(3-hydroxy-4-methoxybenzylidene)-6,7-dimethoxy-3,4-dihydronaphthalen-1(2H)-one (3f).





8-Methoxy-4-(4-hydroxyphenyl)-5,6-dihydrobenzo[*h*]quinazolin-2-amine (4a).

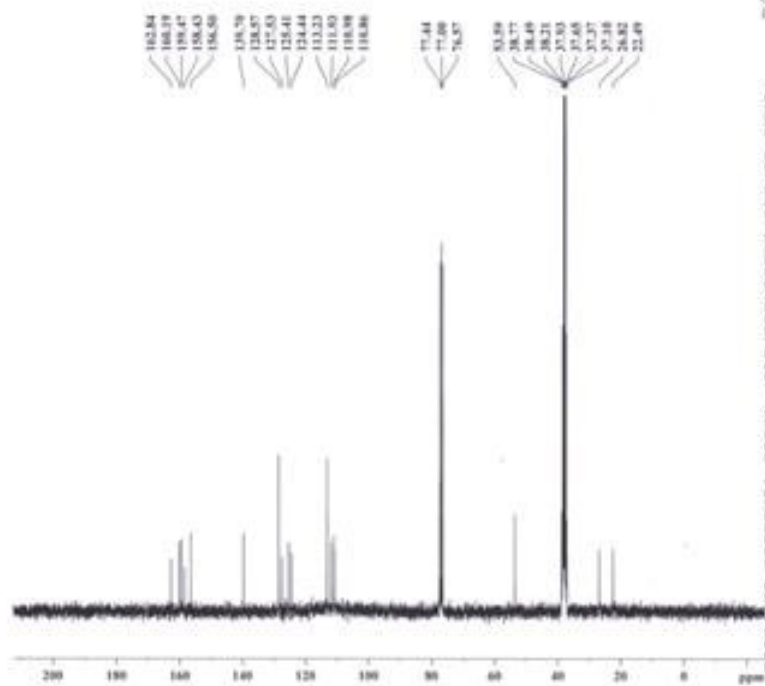


CIMAP-PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atgsa5a.p
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160104
Time 14.21
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 57
DW 81.000 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1317813 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



CIMAP-CARBON
PROJECT NO.: MLP-04

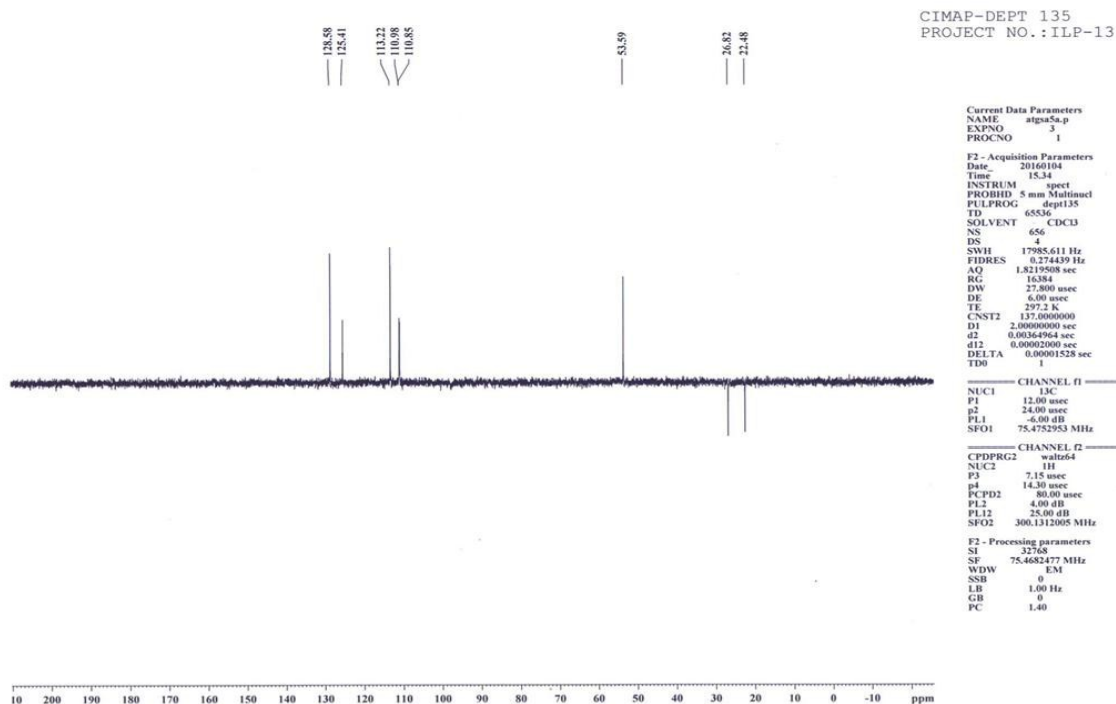
Current Data Parameters
NAME atgsa5a.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160104
Time 15.31
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 17905.611 Hz
FIDRES 0.274639 Hz
AQ 3.8219500 sec
RG 32768
DW 17.800 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
D11 0.05000000 sec
DELTA 1.89999999 sec
TD0 1

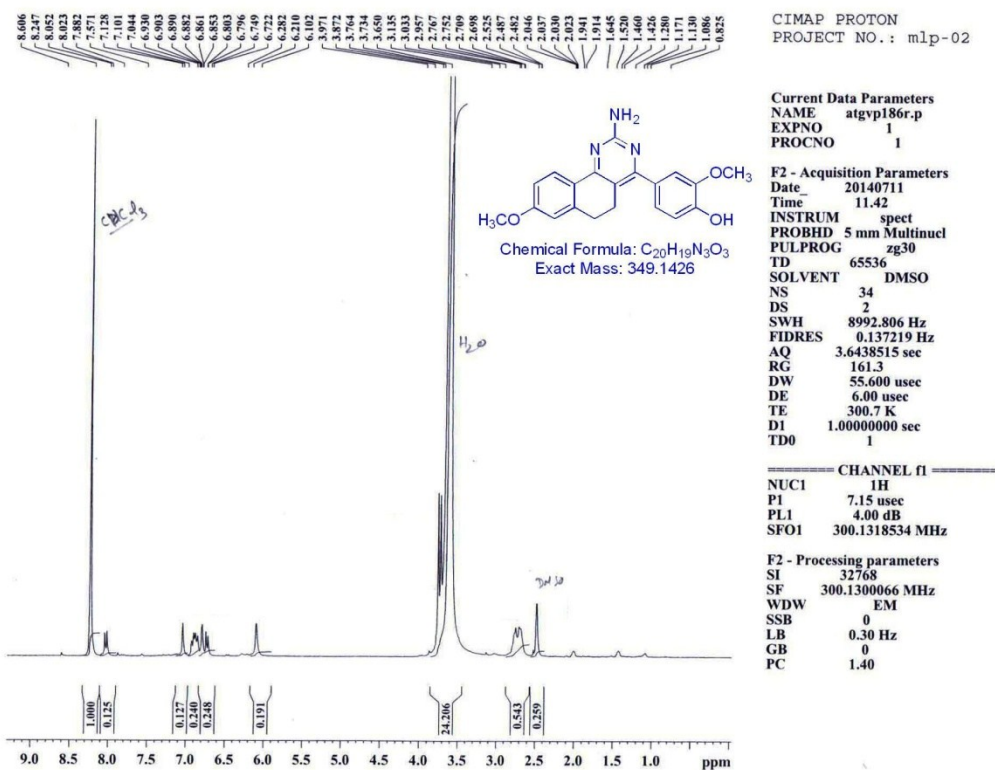
CHANNEL f1
NUC1 13C
P1 12.00 usec
PL1 4.00 dB
SFO1 75.4752904 MHz

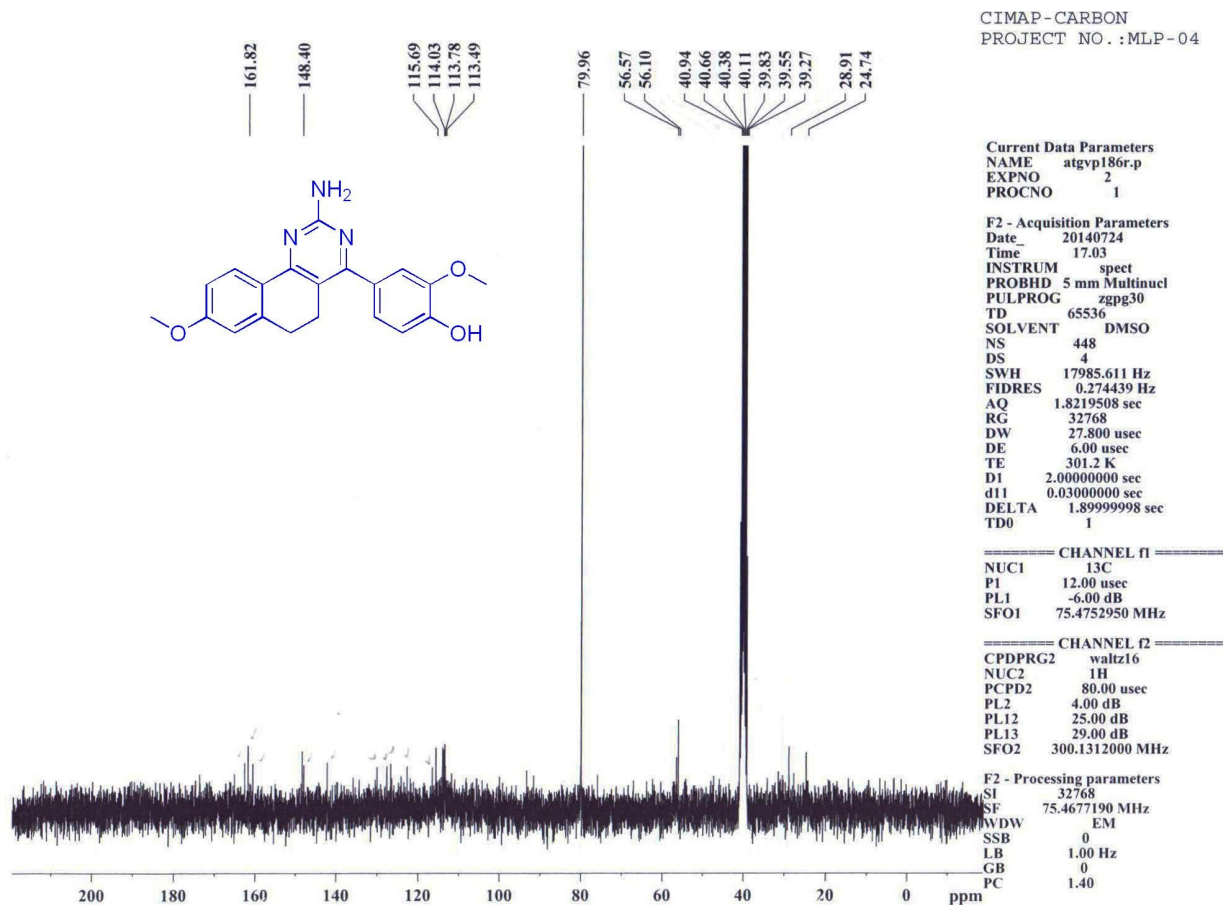
CHANNEL f2
NUC2 1H
PCFPG2 waltz16
PL1 00.00 usec
PL2 4.00 dB
PL3 25.00 dB
PL4 25.00 dB
SFO2 300.1317800 MHz

F2 - Processing parameters
SI 32768
SF 75.462474 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

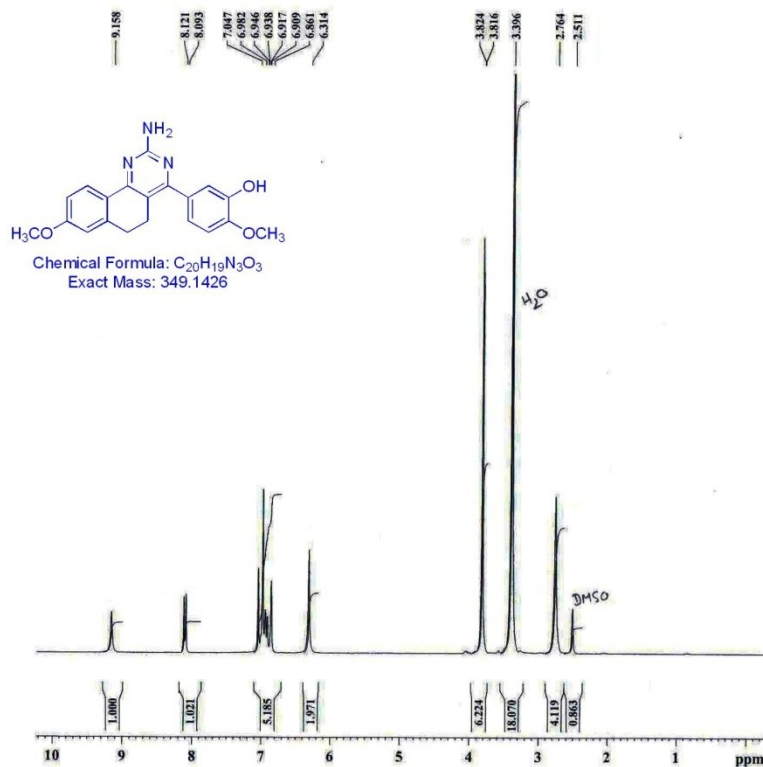


4-(2-amino-8-methoxy-5,6-dihydrobenzo[h]quinazolin-4-yl)-2-methoxyphenol (4b)





4-(2-amino-8-methoxy-5,6-dihydrobenzo[h]quinazolin-4-yl)-2-methoxyphenol (4c)



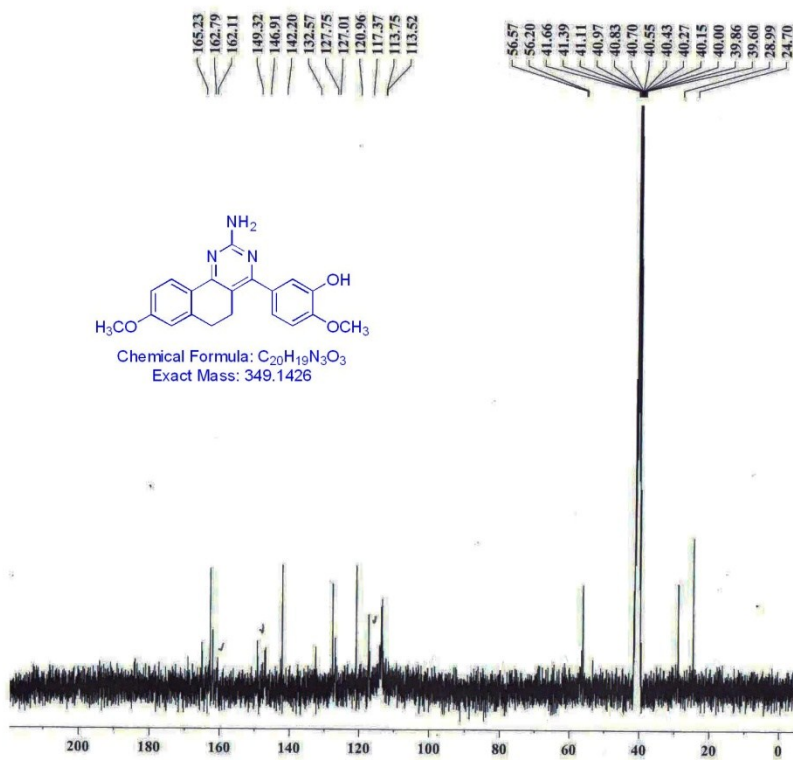
CIMAP-PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atgvp190.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20140820
Time 14.15
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 128
DW 55.600 usec
DE 6.00 usec
TE 301.5 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



CIMAP-CARBON
PROJECT NO.: MLP-04

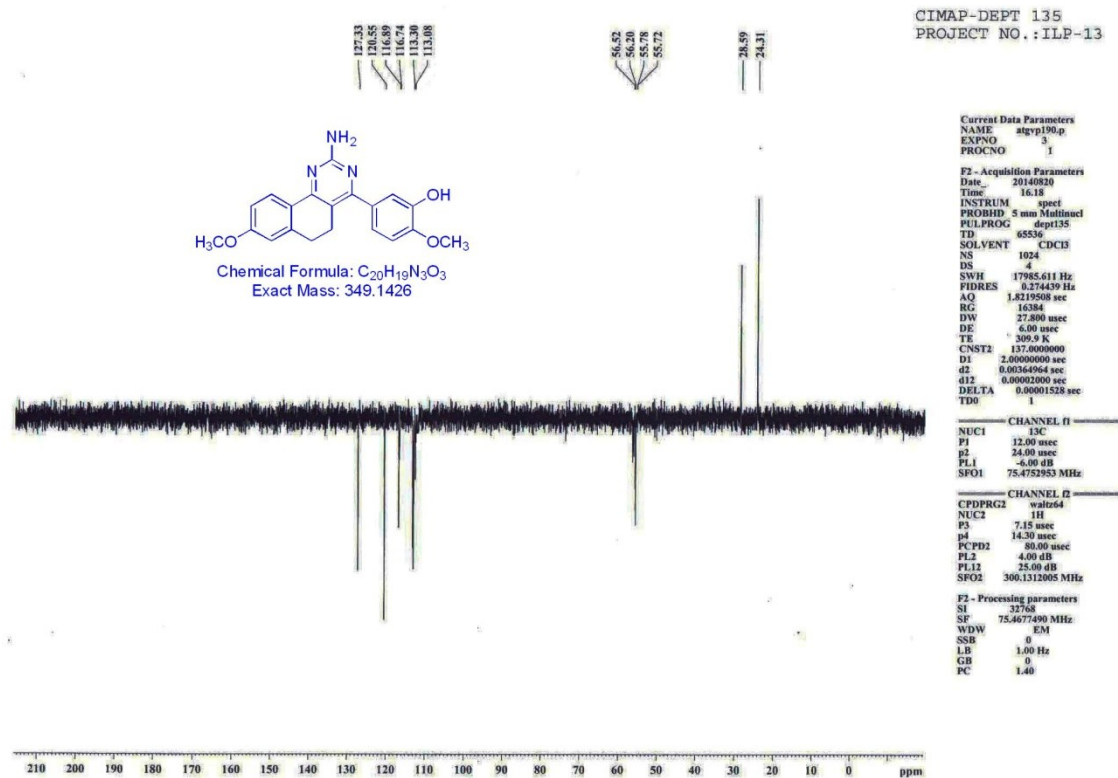
Current Data Parameters
NAME atgvp190.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20140820
Time 14.40
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1012
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 304.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

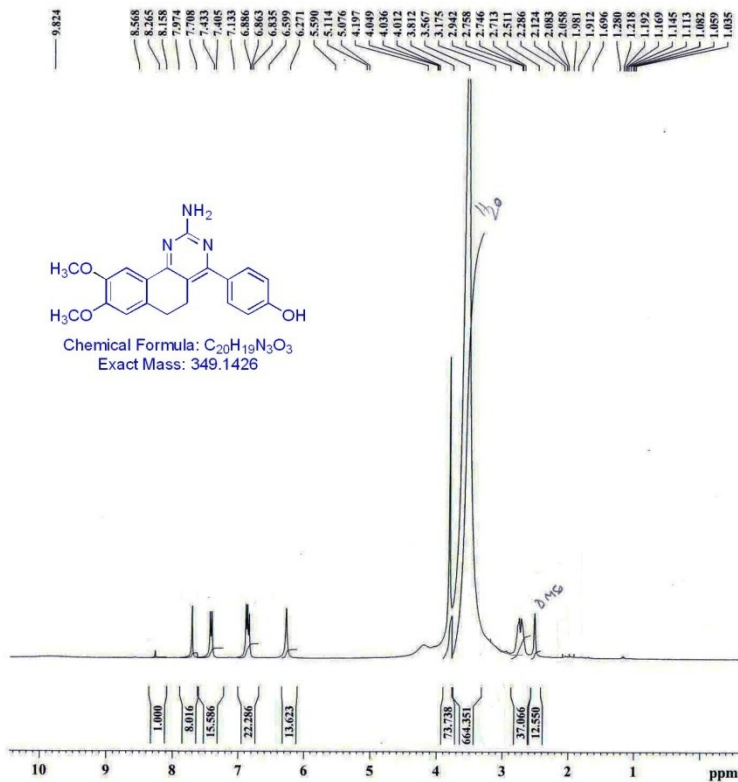
CHANNEL f1
NUC1 13C
P1 12.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
PL13 29.00 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4-(2-amino-8-methoxy-5,6-dihydrobenzo[h]quinazolin-4-yl)-2-methoxyphenol (4d)



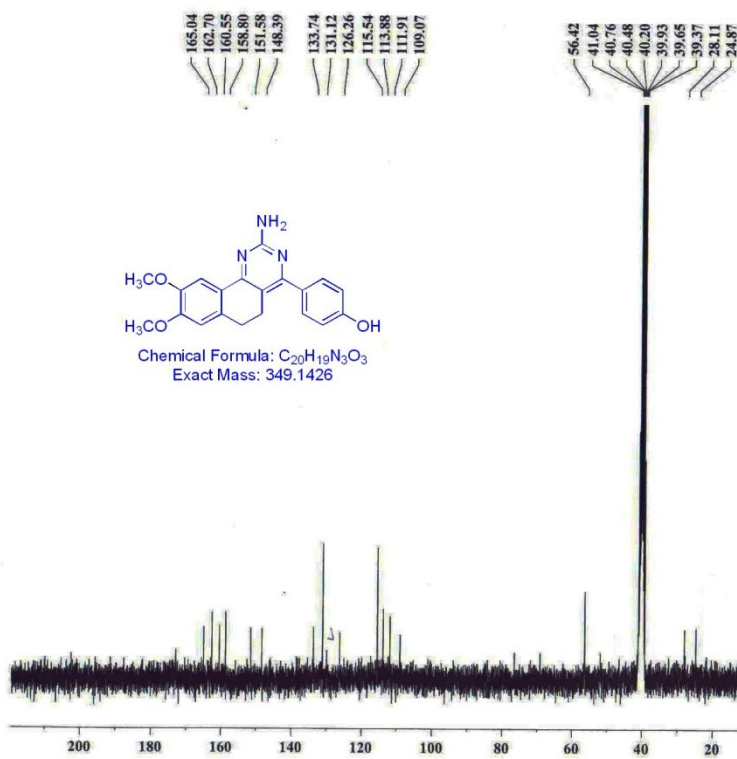
CIMAP-PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk265.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141008
Time 10.20
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 20
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 57
DW 55.600 usec
DE 6.00 usec
TE 300.3 K
D1 1.0000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



CIMAP-CARBON
PROJECT NO.: MLP-04

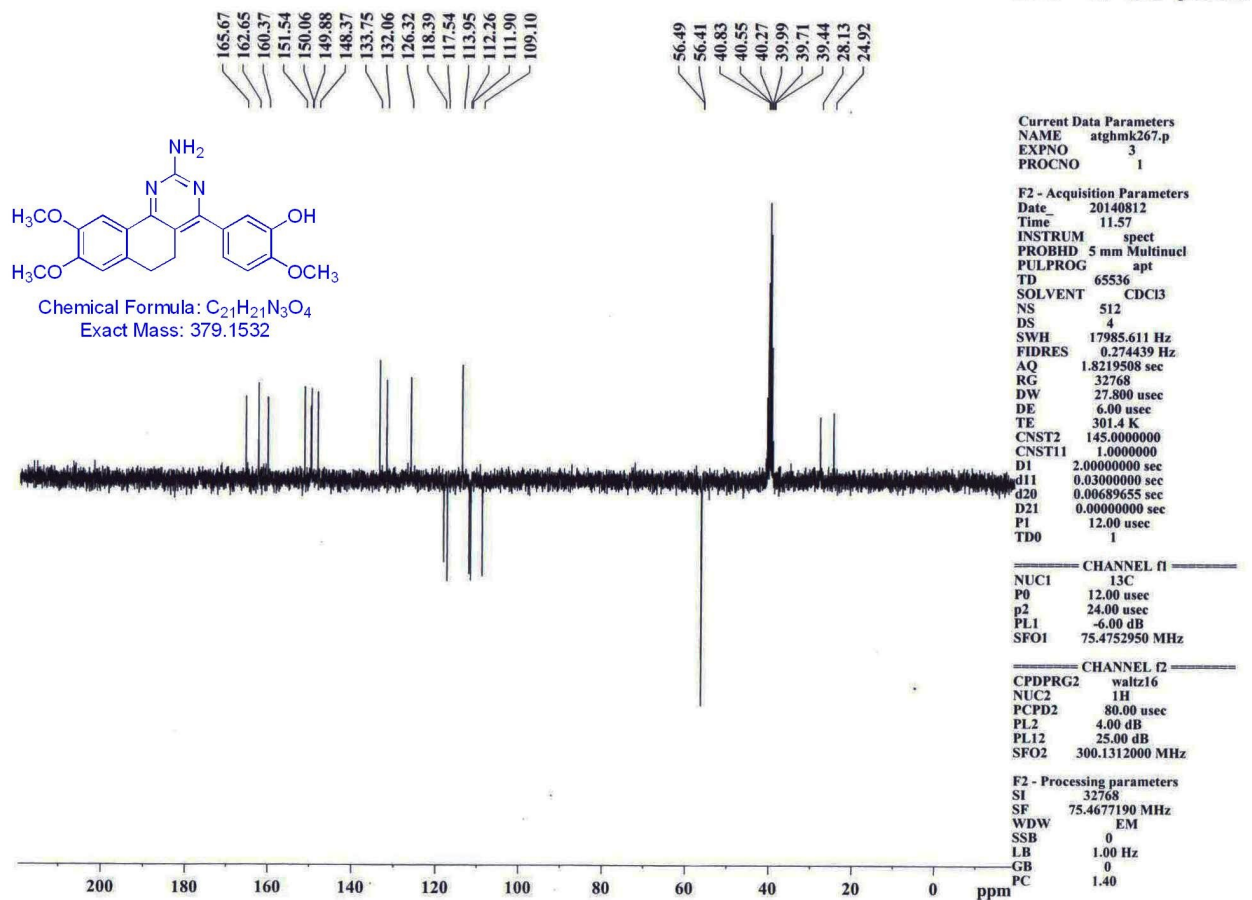
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NAME atghmk265.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141008
Time 11.04
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 660
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 301.3 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

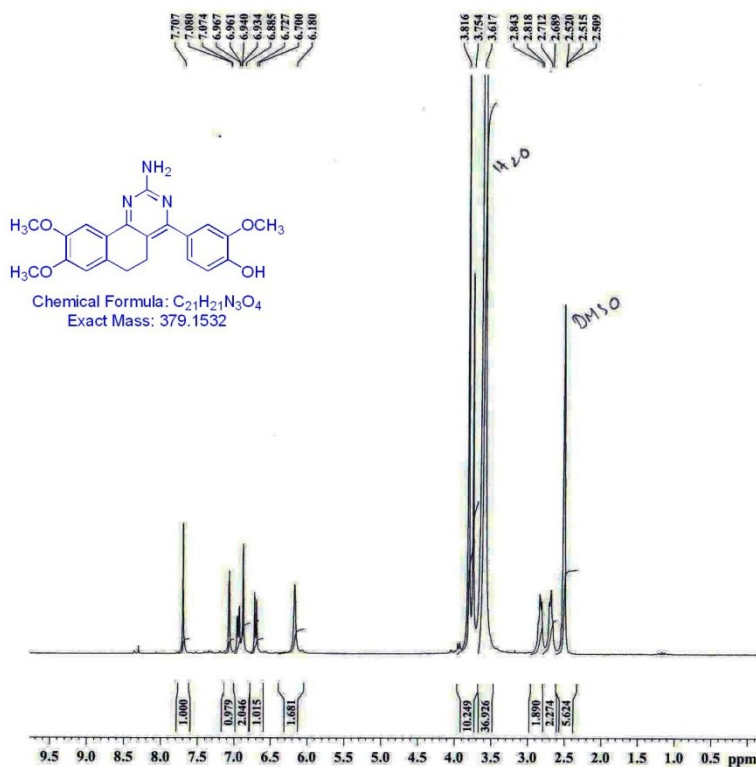
CHANNEL f1
NUC1 13C
P1 12.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
PL13 29.00 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4-(2-amino-8-methoxy-5,6-dihydrobenzo[h]quinazolin-4-yl)-2-methoxyphenol (4e)



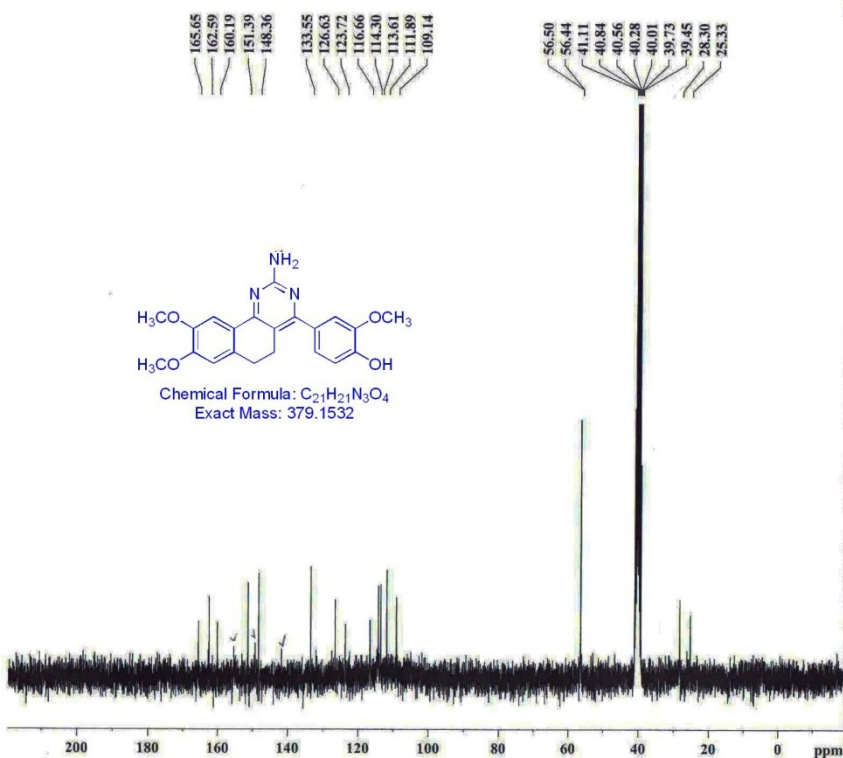
CIMAP-PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk269.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140821
Time 12.20
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 114
DW 55.600 usec
DE 6.00 usec
TE 301.6 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



CIMAP-CARBON
PROJECT NO.: MLP-04

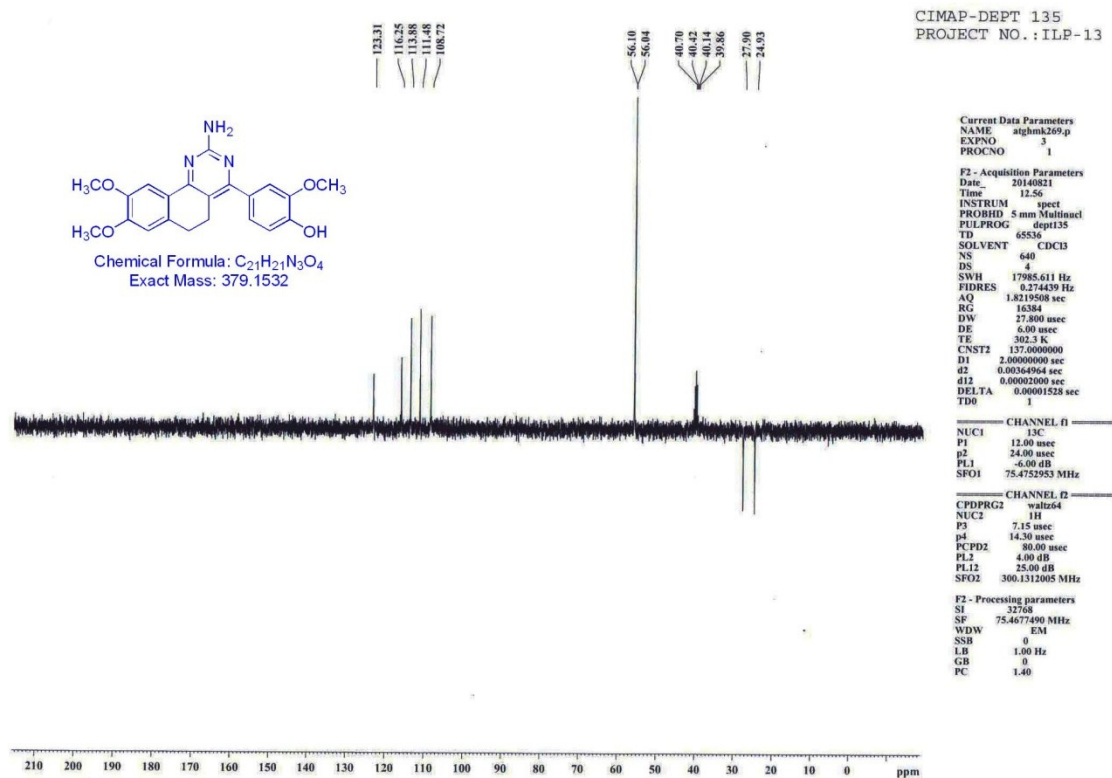
Current Data Parameters
NAME atghmk269.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140821
Time 12.37
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 662
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 302.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

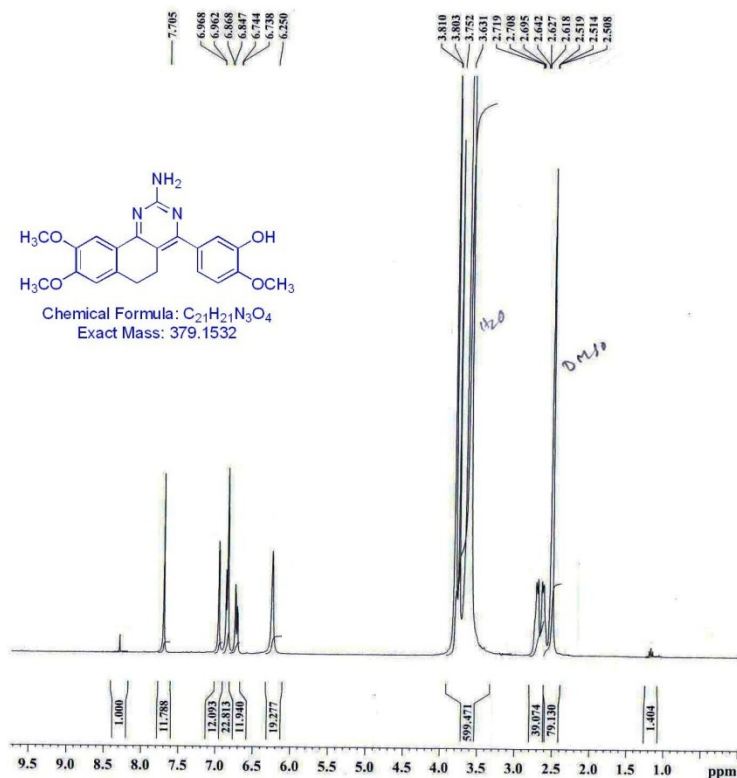
CHANNEL f1
NUC1 13C
P1 12.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.00 dB
PL13 29.00 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4-(2-amino-8-methoxy-5,6-dihydrobenzo[h]quinazolin-4-yl)-2-methoxyphenol (4f)



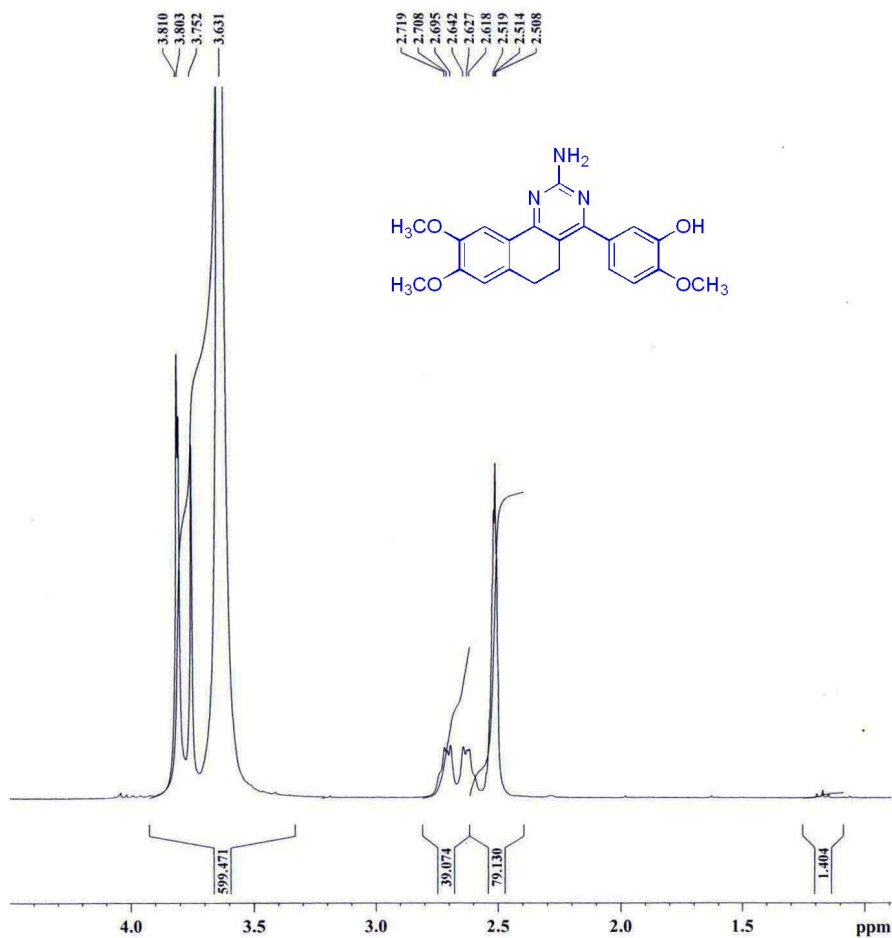
CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk267.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20140804
Time 15.33
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 228.1
DW 55.600 usec
DE 6.00 usec
TE 301.7 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



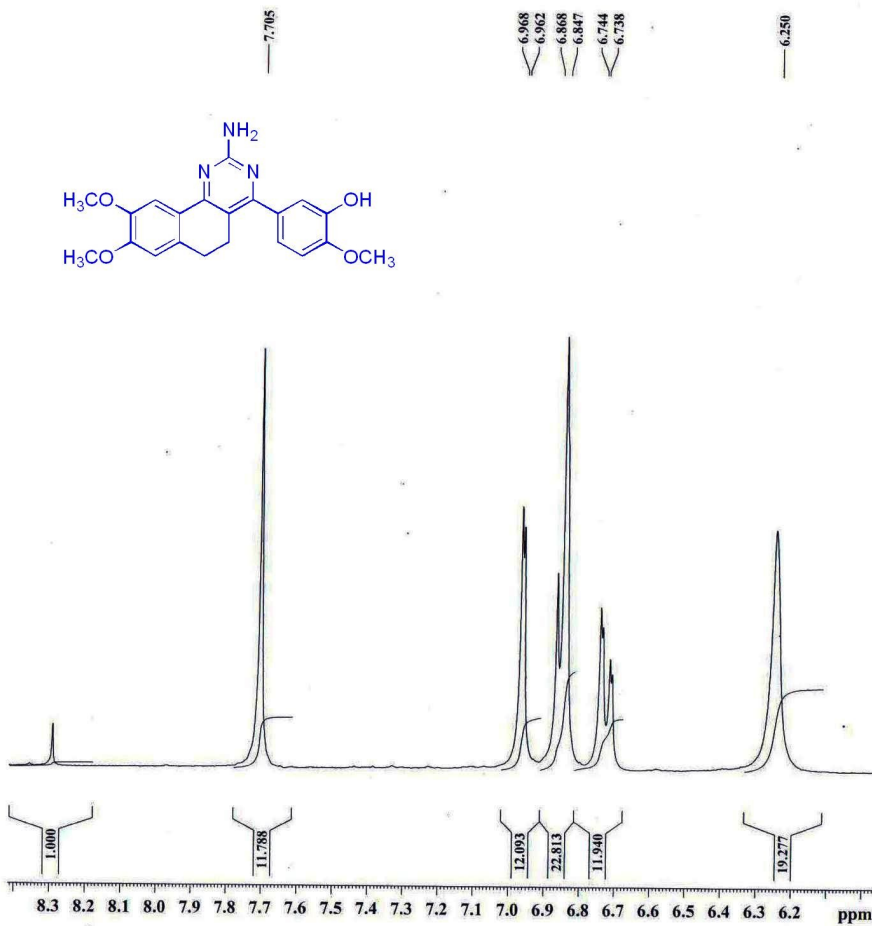
CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk267.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140804
Time 15.33
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 228.1
DW 55.600 usec
DE 6.00 usec
TE 301.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



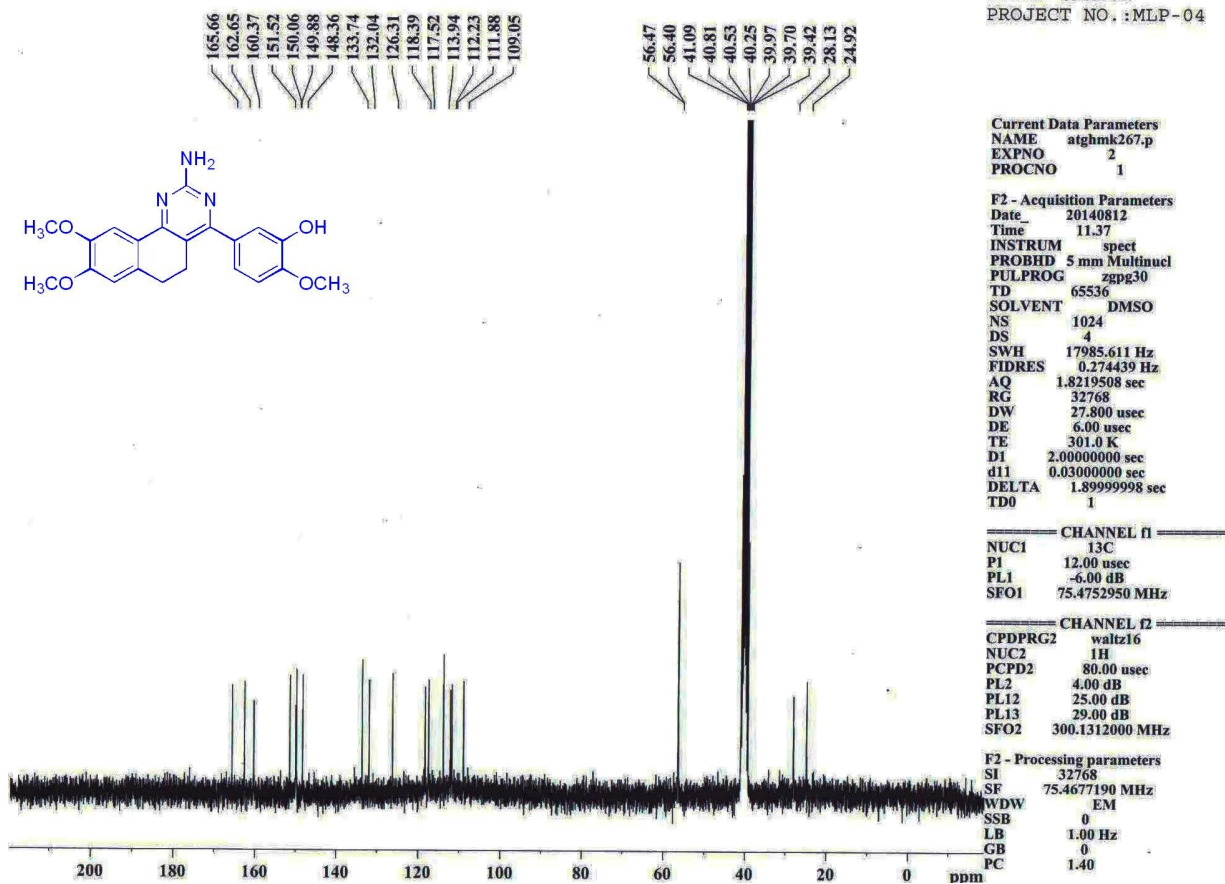
CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atghmk267.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140804
Time 15.33
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 228.1
DW 55.600 usec
DE 6.00 usec
TE 301.7 K
D1 1.00000000 sec
TD0 1

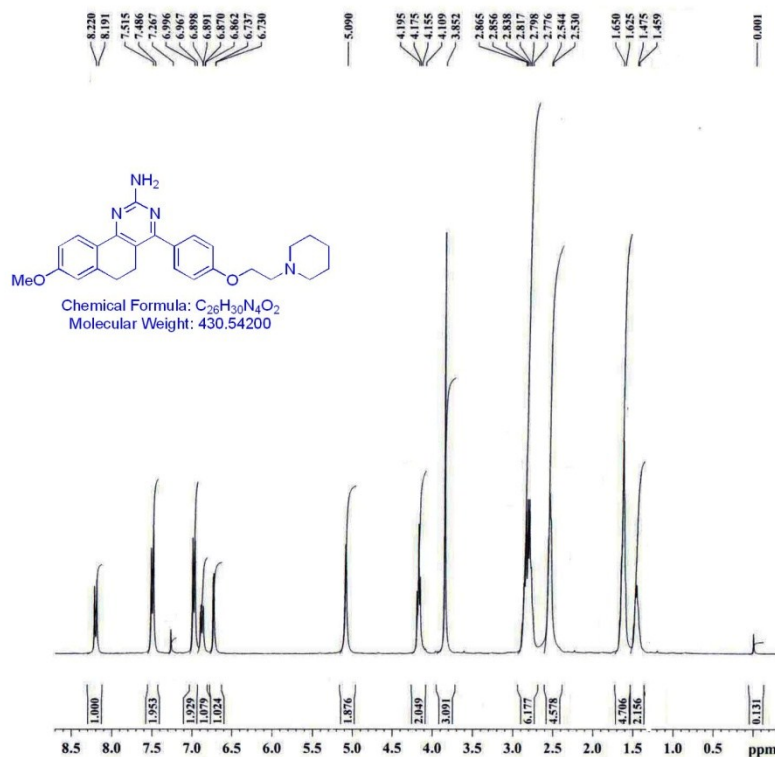
===== CHANNEL f1 =====
NUC1 1H
P1 7.15 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40





4-(4-(2-(piperidin-1-yl)ethoxy)phenyl)-5,6-dihydro-8-methoxybenzo[h] quinazolin-2-amine (6a):



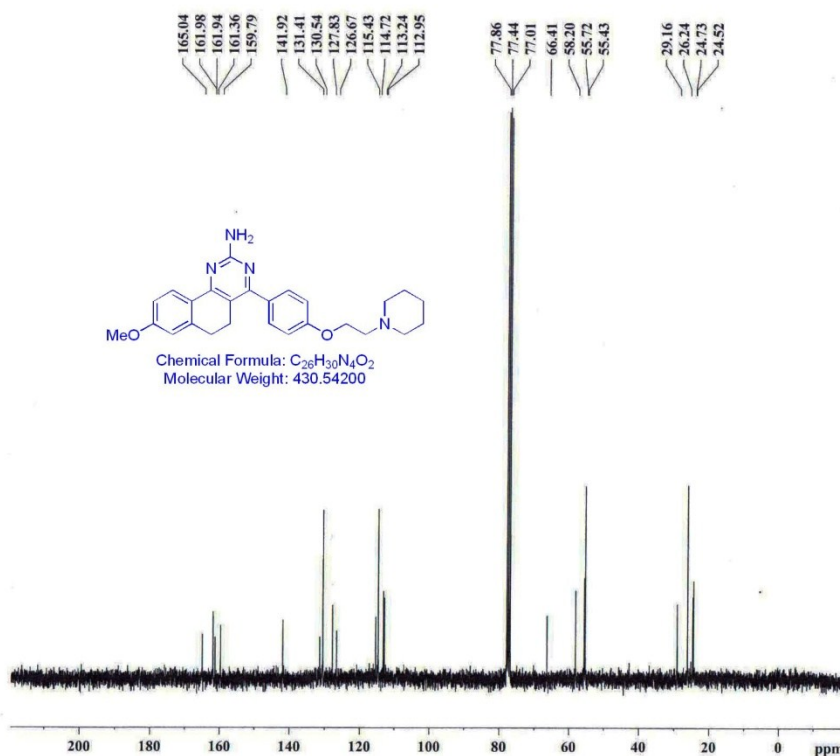
CIMAP-PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atgsa20.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130313
Time 11.22
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 17
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 181
DW 81.000 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 6.78 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



CIMAP-CARBON
PROJECT NO.: MLP-04

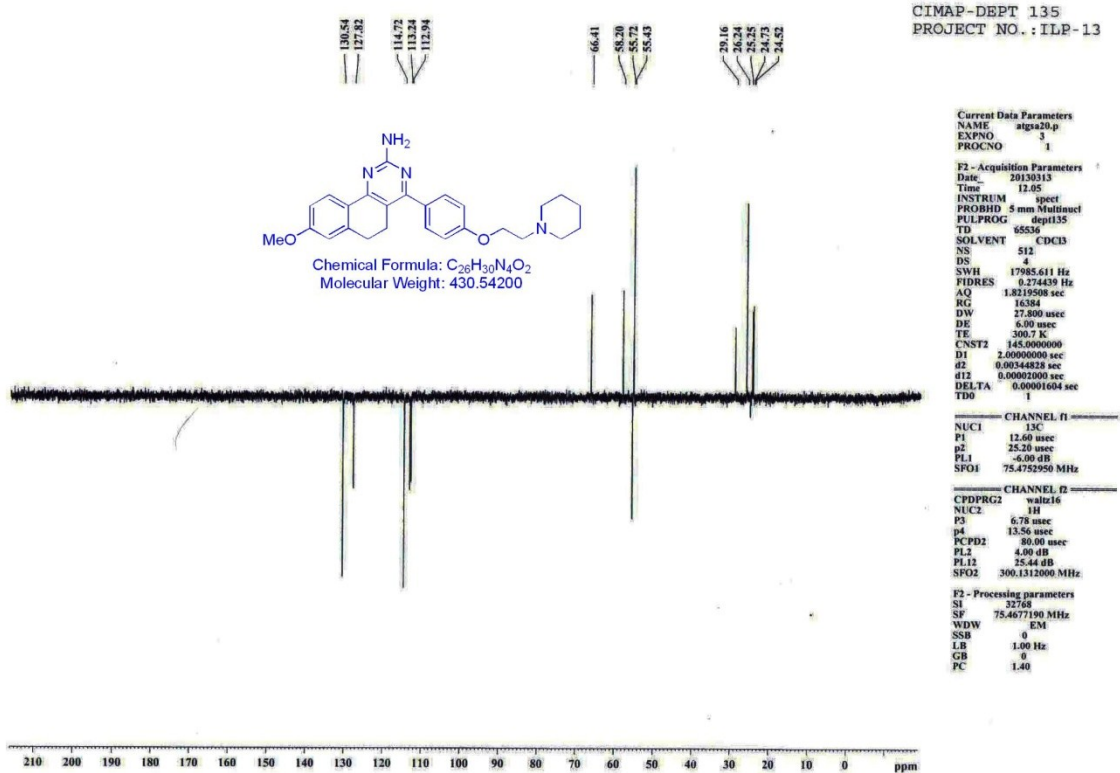
Current Data Parameters
NAME atgsa20.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130313
Time 11.40
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

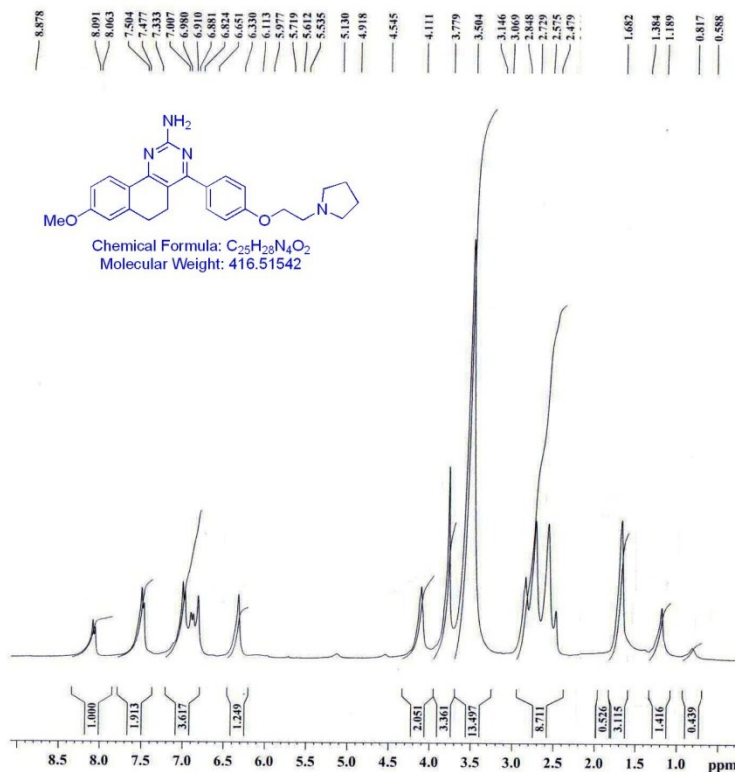
CHANNEL f1
NUC1 13C
P1 12.60 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.44 dB
PL13 29.61 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4-(4-(2-(pyrrolidin-1-yl)ethoxy)phenyl)-5,6-dihydro-8-methoxybenzo[h]quinazolin-2-amine (6b):



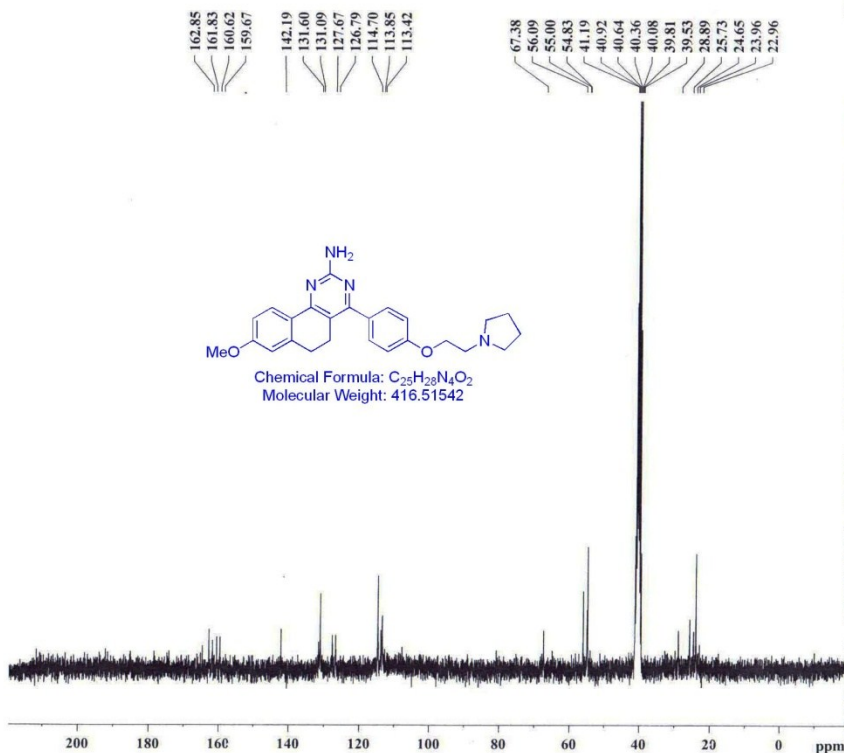
CIMAP-PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atgsal3.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130101
Time 15.28
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 46
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 90.5
DW 81.000 usec
DE 6.00 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 6.85 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



CIMAP-CARBON
PROJECT NO.: MLP-04

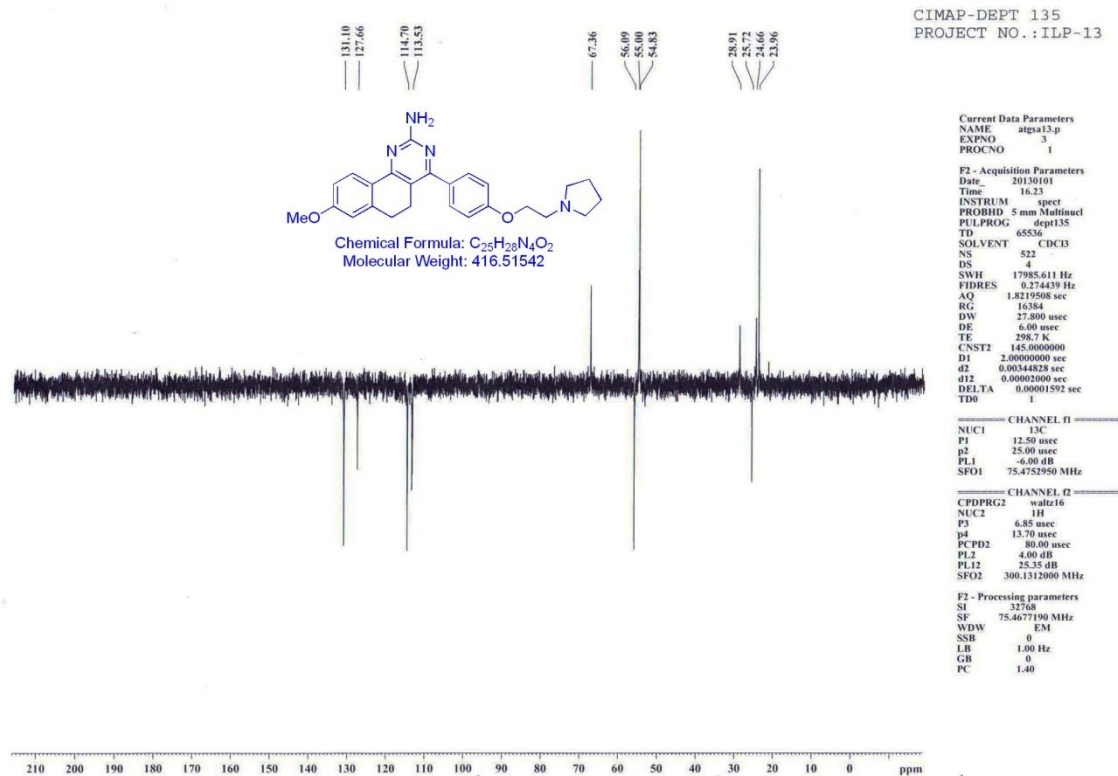
Current Data Parameters
NAME atgsal3.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130101
Time 16.03
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 689
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 298.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

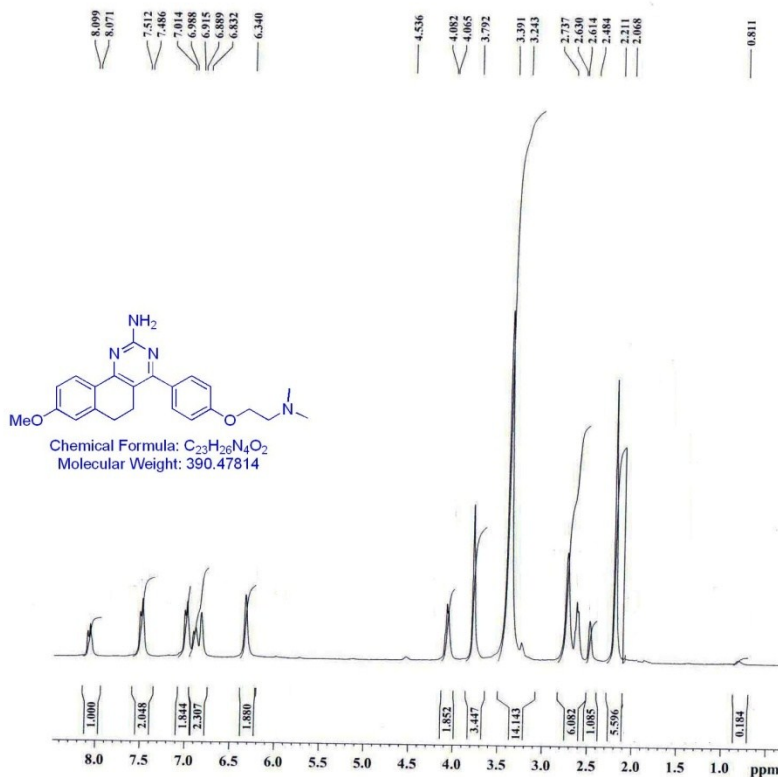
CHANNEL f1
NUC1 13C
P1 12.50 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.35 dB
PL13 29.61 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4-(4-(2-(dimethylamino)ethoxy)phenyl)-5,6-dihydro-8-methoxybenzo[h]quinazolin-2-amine (6c):



CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters

NAME atgsa14.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

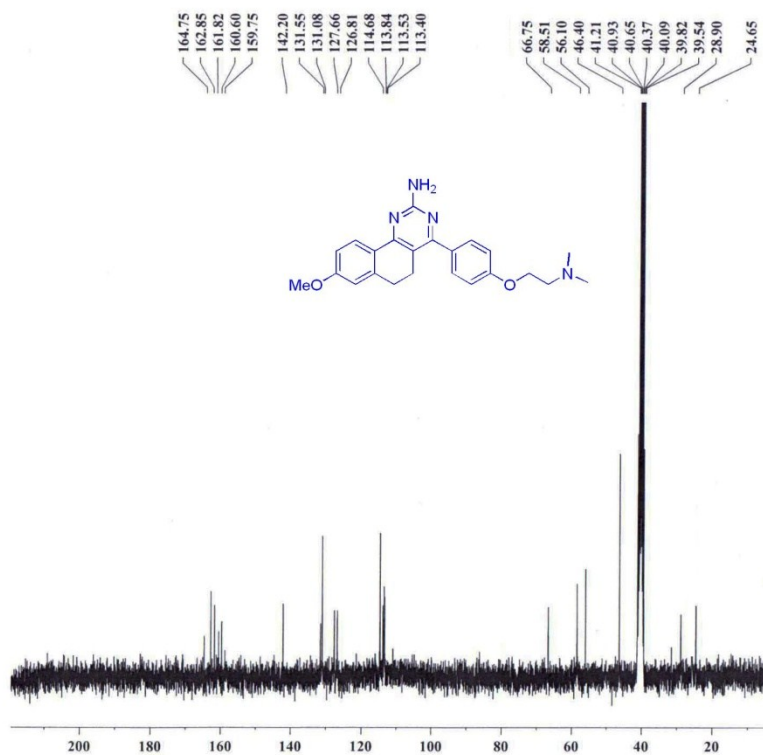
Date_ 20130103
Time 15.04
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 19
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 114
DW 55.600 usec
DE 6.00 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1

CHANNEL f1

NUC1 1H
P1 6.85 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters

SI 32768
SF 300.1300071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



CIMAP-CARBON
PROJECT NO.:MLP-04

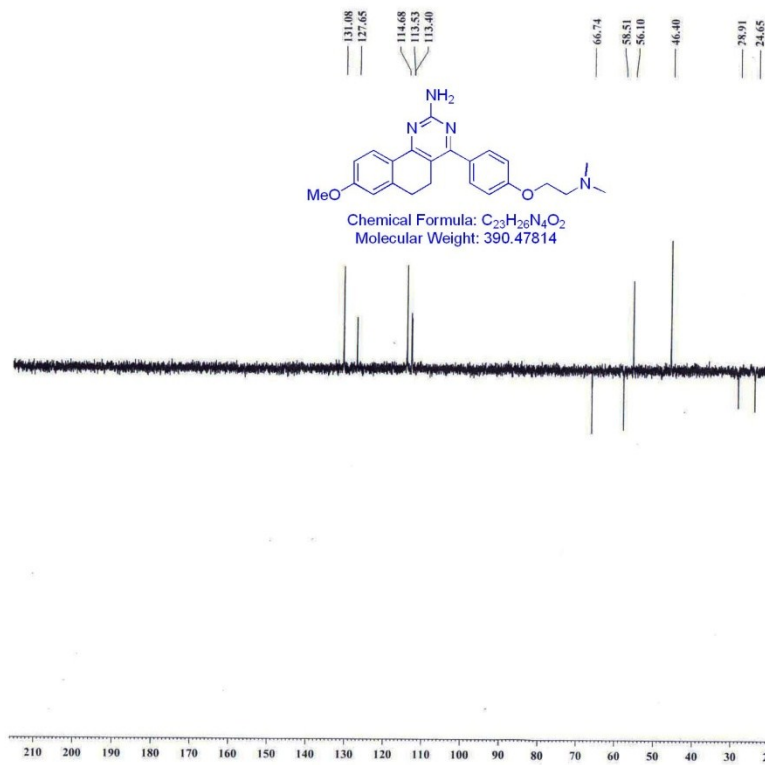
Current Data Parameters
NAME atgsa14.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130103
Time 15.39
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 803
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 12.50 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.35 dB
PL13 29.61 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



CIMAP-DEPT 135
PROJECT NO.:ILP-13

Current Data Parameters
NAME atgsa14.p
EXPNO 3
PROCNO 1

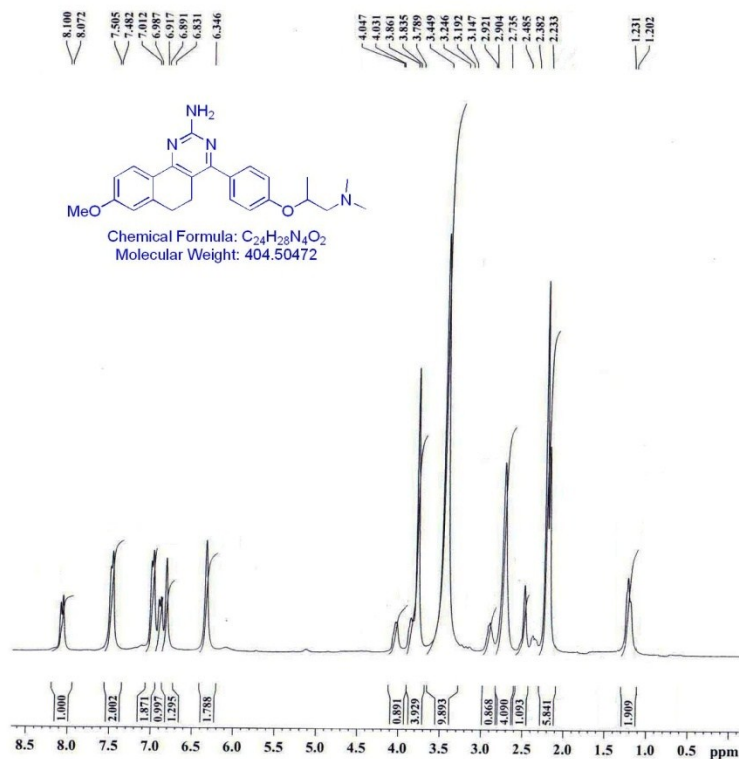
F2 - Acquisition Parameters
Date_ 20130103
Time 15.49
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 611
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344823 sec
d12 0.00002000 sec
DELTA 0.00001592 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 12.50 usec
P2 25.00 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 6.85 usec
P4 13.70 usec
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.35 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

**4-(4-(1-(dimethylamino)propan-2-yloxy)phenyl)-5,6-dihydro-8-methoxybenzo[h]quinazolin-2-amine
(6d):**



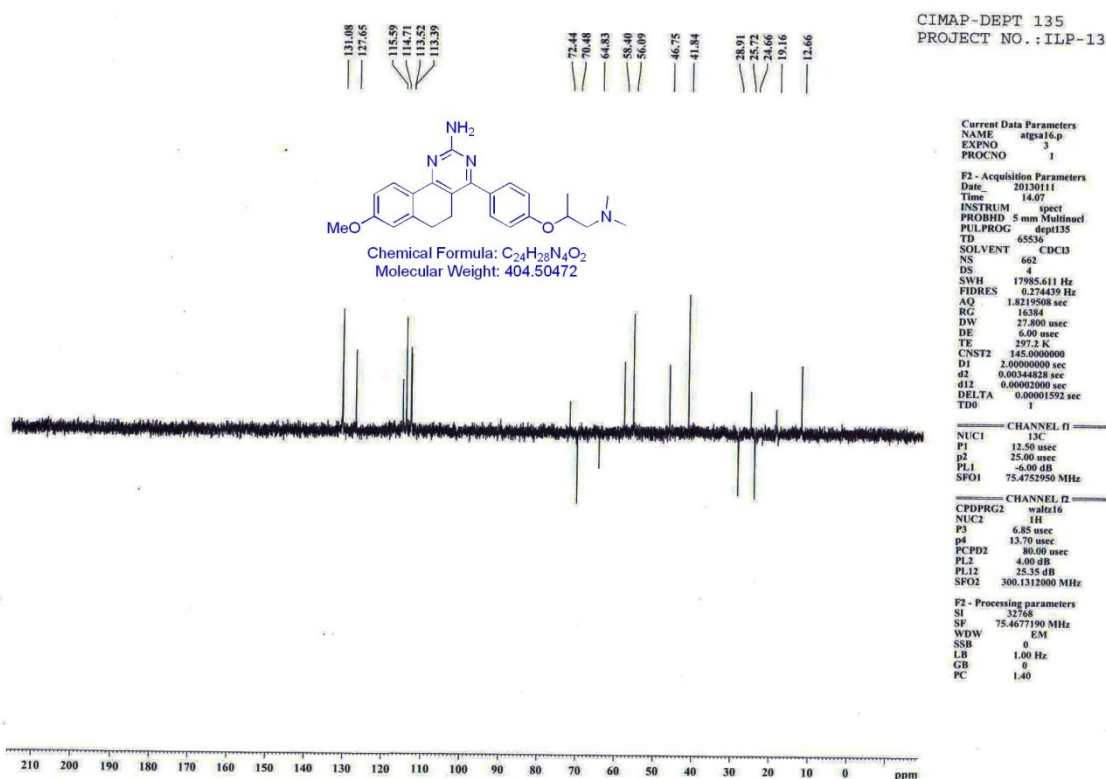
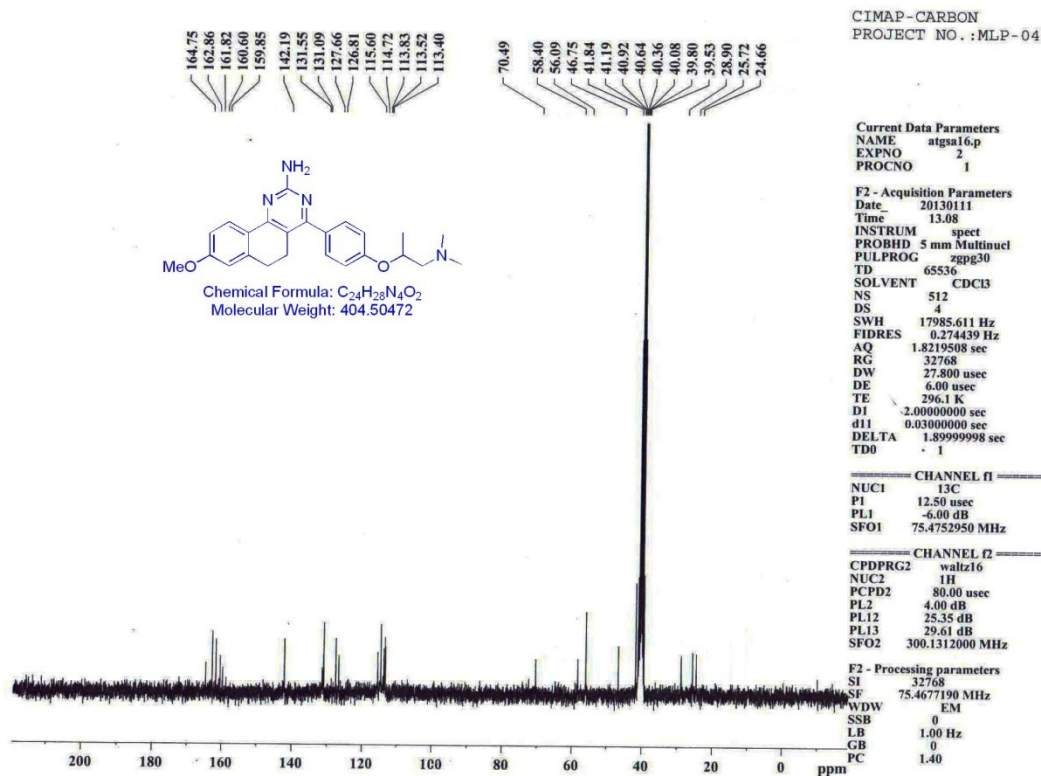
CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atgsa16.p
EXPNO 1
PROCNO 1

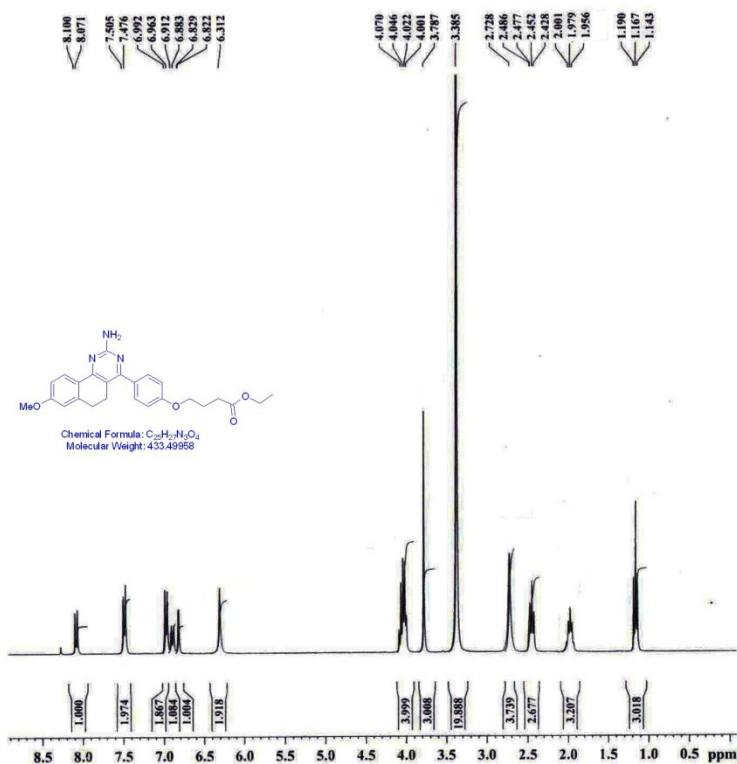
F2 - Acquisition Parameters
Date_ 20130111
Time 13.07
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 101.6
DW 55.600 usec
DE 6.00 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 6.85 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300064 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



Ethyl 4-(4-(2-amino-8-methoxy-5,6-dihydrobenzo[h]quinazolin-4-yl)phenoxy)butanoate (8a):



CIMAP-PROTON
PROJECT NO.: mlp-02

Current Data Parameters

NAME atgru103.p
EXPNO 1
PROCNO 1

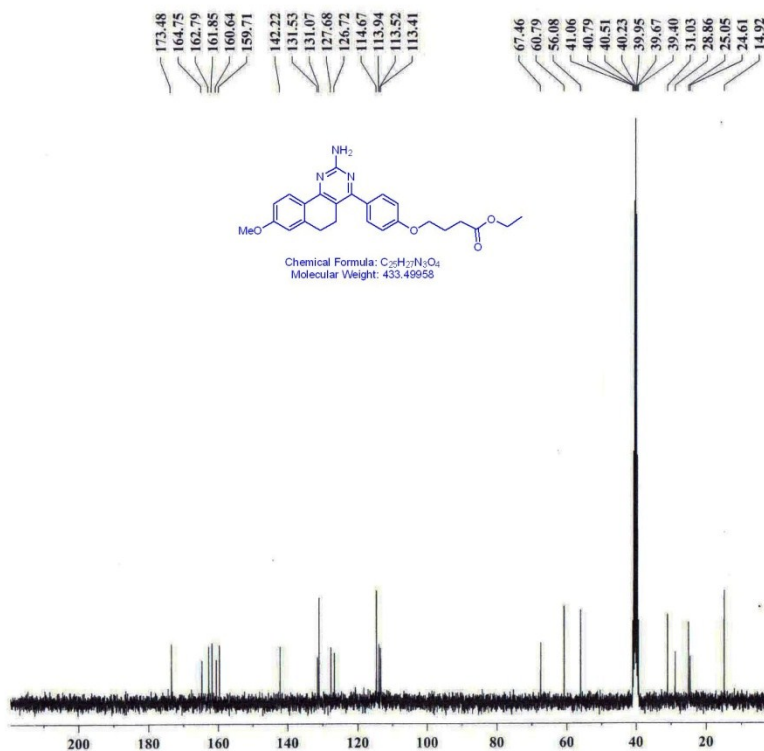
F2 - Acquisition Parameters

Date 20130705
Time 16.37
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 39
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 90.5
DW 81.000 usec
DE 6.00 usec
TE 300.4 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 6.78 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters

SI 32768
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



CIMAP-CARBON
PROJECT NO.: MLP-04

Current Data Parameters

NAME atgru103.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date 20130718
Time 12.19
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 401
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

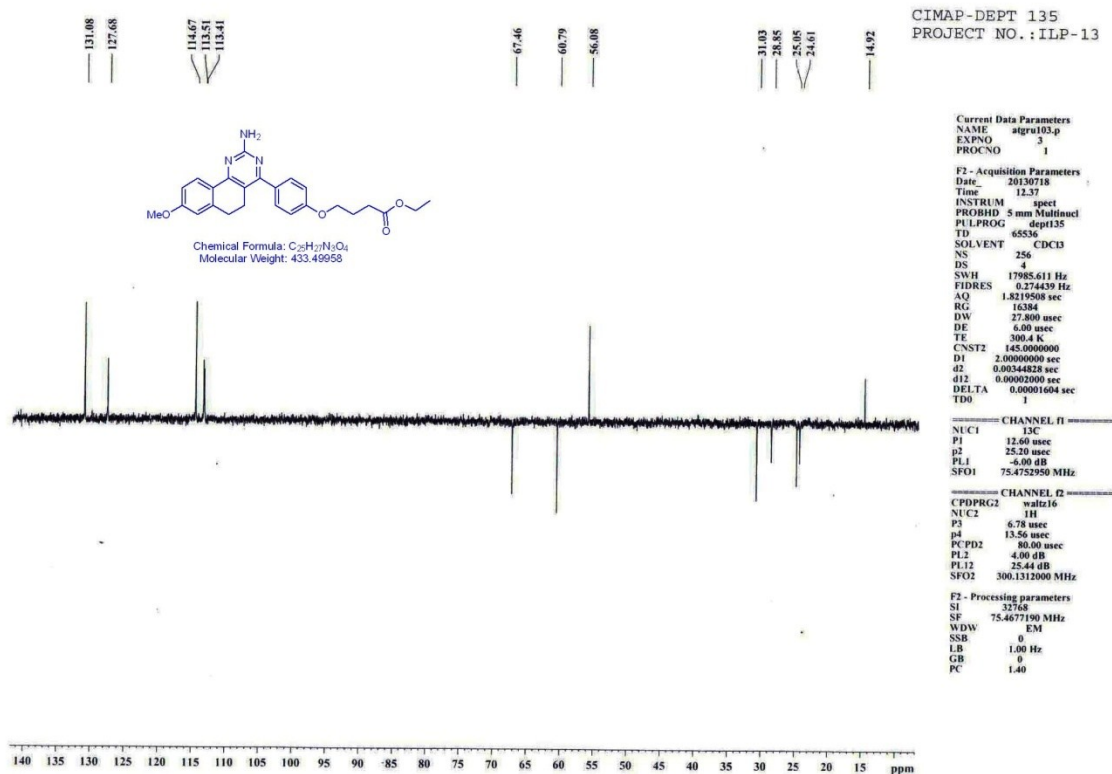
CHANNEL f1
NUC1 13C
P1 12.60 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2

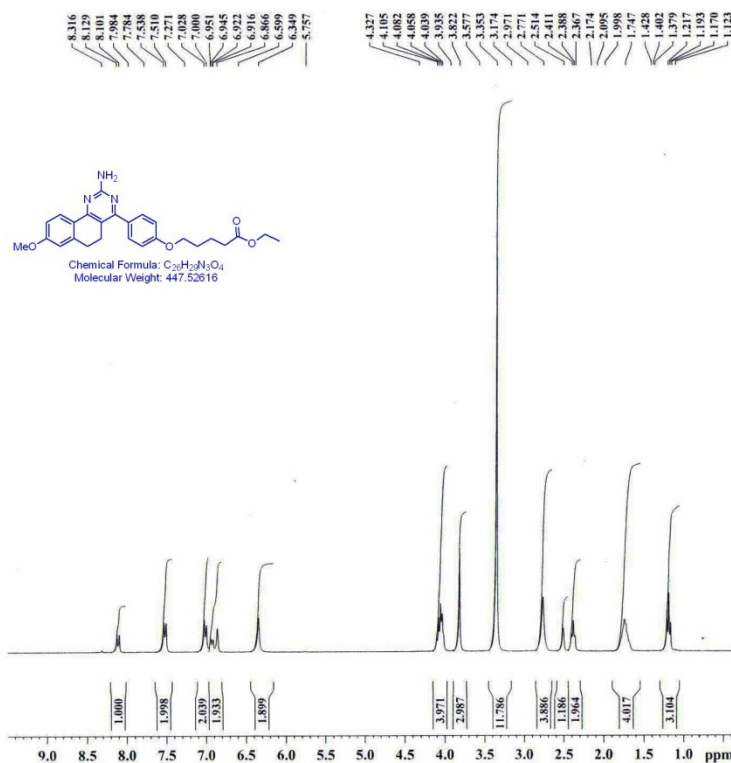
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.44 dB
PL13 29.61 dB
SFO2 300.1312000 MHz

F2 - Processing parameters

SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Ethyl 5-(4-(2-amino-8-methoxy-5,6-dihydrobenzo[h]quinazolin-4-yl)phenoxy)pentanoate (8b):



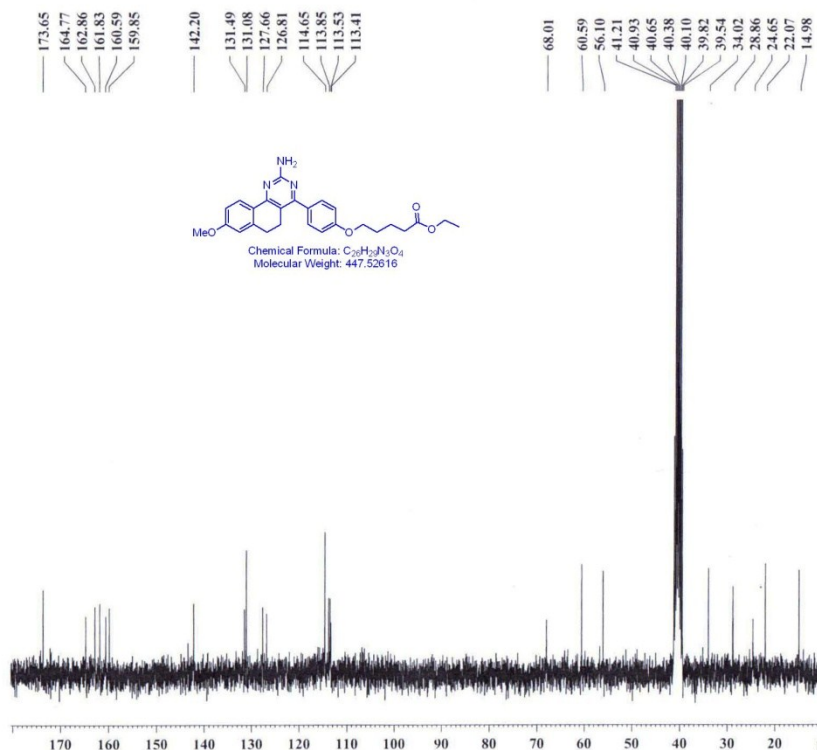
CIMAP PROTON
PROJECT NO.: mlp-02

Current Data Parameters
NAME atgru104.p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20130522
Time 16.24
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 17
DS 2
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 406.4
DW 55.600 usec
DE 6.00 usec
TE 301.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 6.78 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299972 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



CIMAP-CARBON
PROJECT NO.: MLP-04

Current Data Parameters
NAME atgru104.p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20130606
Time 14.36
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 531
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 12.60 usec
PL1 -6.00 dB
SFO1 75.4752950 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 25.44 dB
PL13 29.61 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40