

**Supporting Information:**

**Design and synthesis of 3-arylbenzopyran based non-steroidal  
vitamin-D<sub>3</sub> mimics as osteogenic agents**

**Mohd. Imran Ahmad,<sup>a‡</sup> Dushyant Singh Raghuvanshi,<sup>a‡</sup> Sarita Singh,<sup>a</sup> Aijaz A. John,<sup>c</sup> Ravi  
Prakash,<sup>c</sup> Kripa Shankar Nainawat,<sup>a</sup> Divya Singh,<sup>c</sup> Shubhendra Tripathi,<sup>b</sup> Ashok Sharma,<sup>b</sup> Atul  
Gupta<sup>\*#a</sup>**

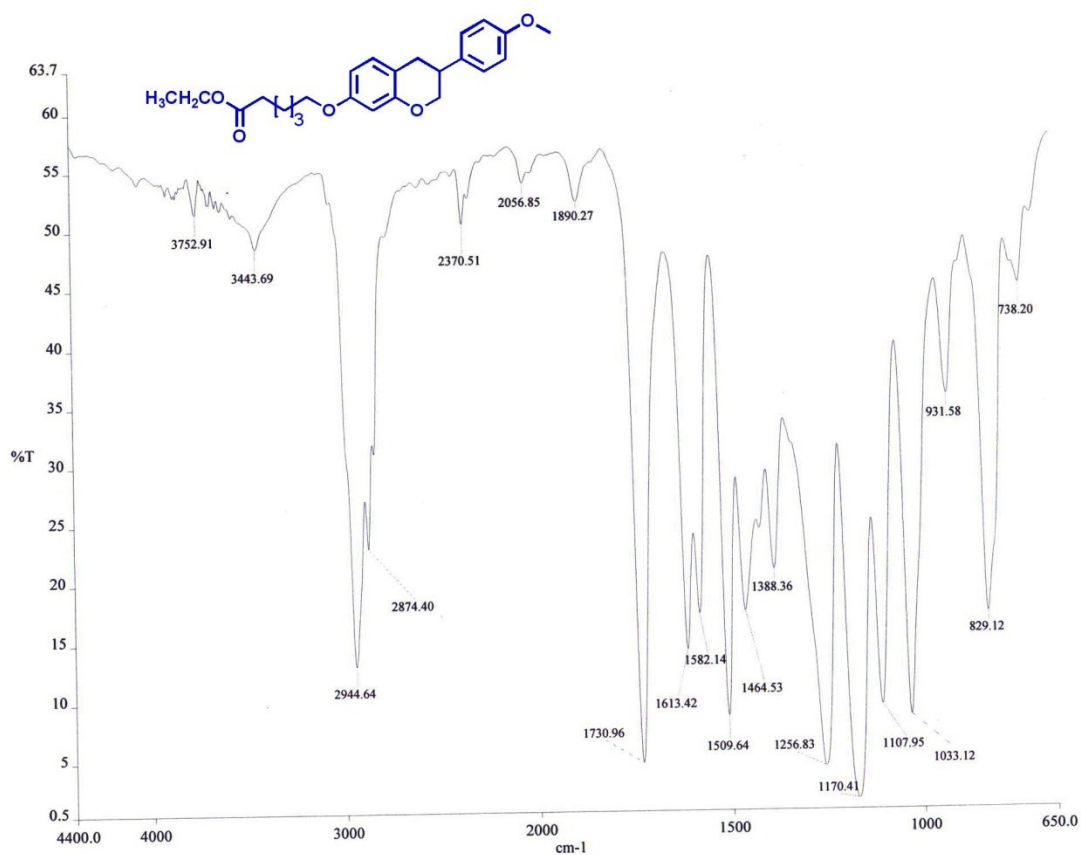
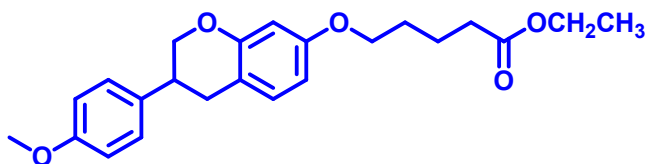
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Medicinal and aromatic Plants, Lucknow-226015, <sup>c</sup>Division of Endocrinology, CSIR-Central Drug  
Research Institute, Sec-10, Jankipuram Extension, Lucknow, India,*

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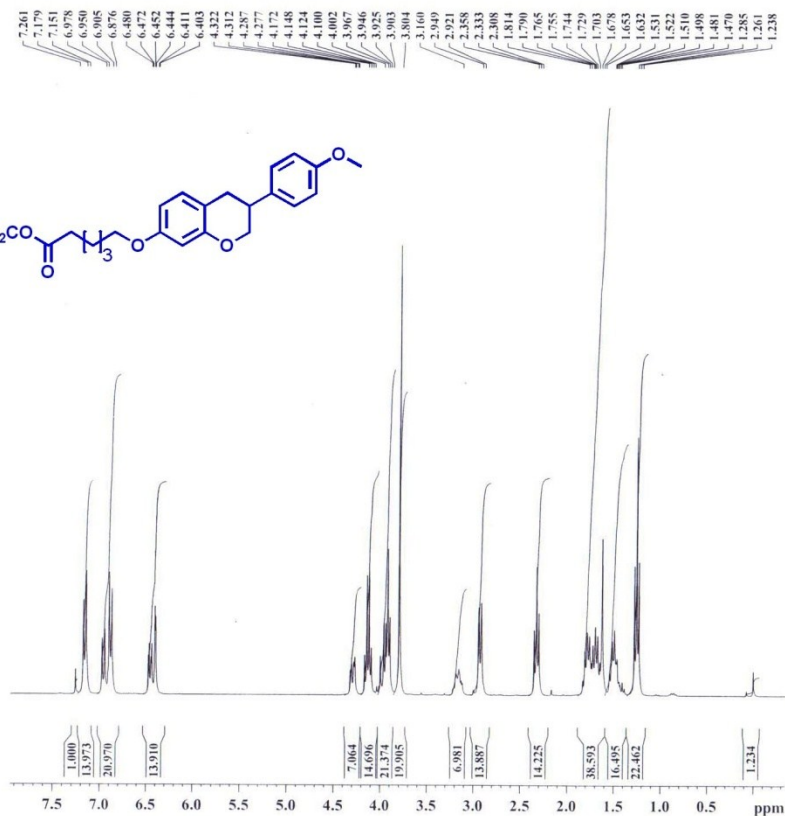
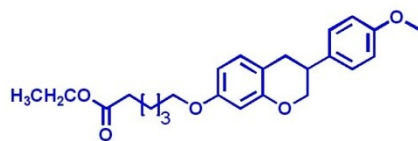
Corresponding Address: Email:atisky2001@yahoo.co.in (A. G.), Tel.: 915222718556,

## Spectra of compounds 25c, 26b, 27b and 27c

### Ethyl 5-(3-(4-methoxyphenyl)chroman-7-yloxy)pentanoate (25c);



c:\pel\_data\spectra\atgmi85\_300813.002 - DR ATUL GUPTA



CIMAP PROTON  
PROJECT NO.: mlp-02

# Current Data Parameters

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EXPNO 1  
PROCNO 1

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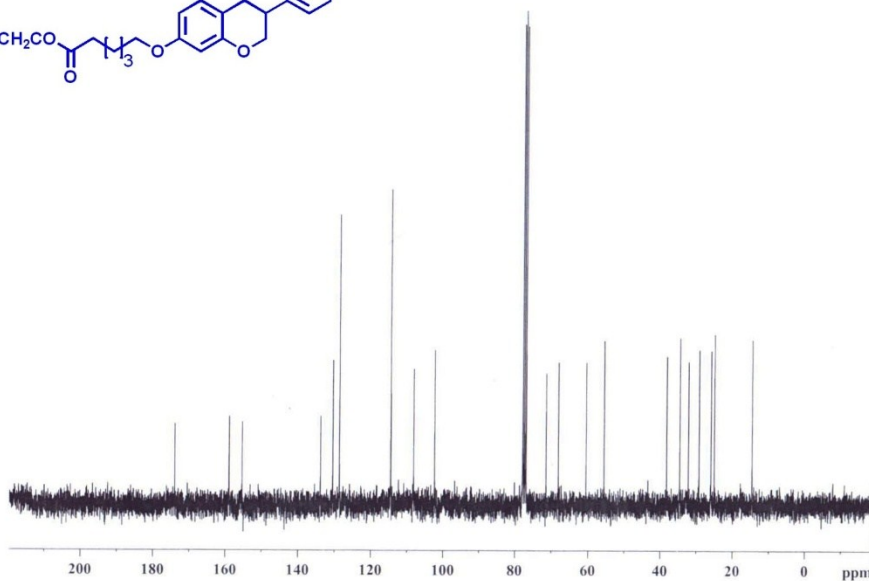
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SOLVENT CDCl3  
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DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 161.3  
DW 81.000 usec  
DE 6.00 usec  
TE 302.3 K  
D1 1.00000000 sec  
TD0 1

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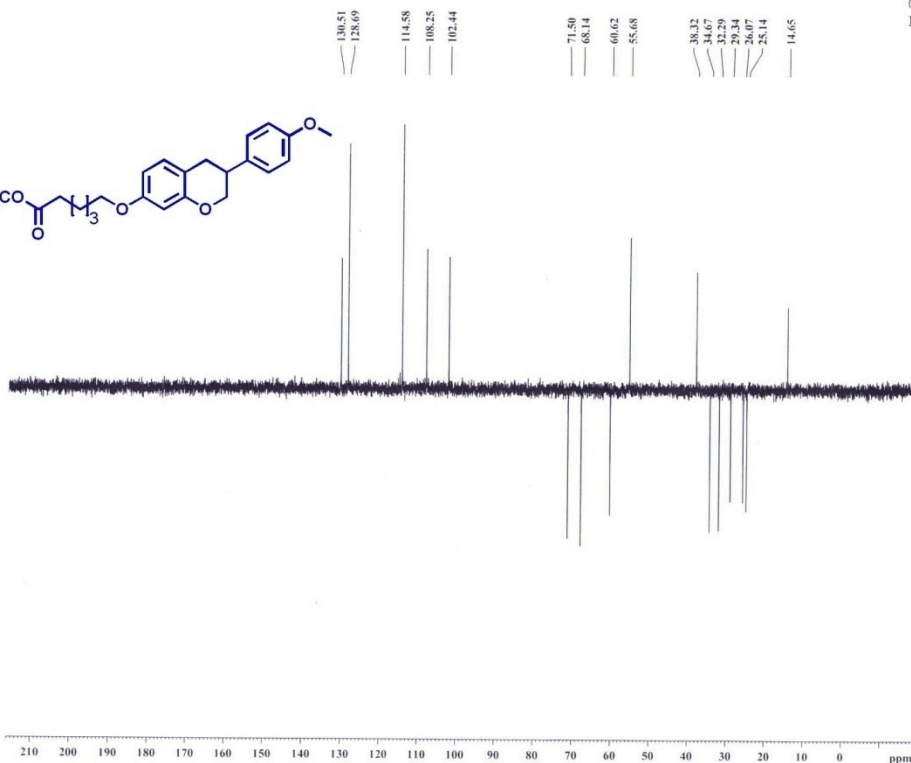
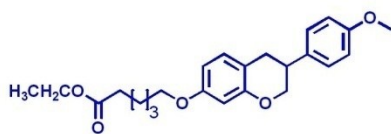
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P1 6.78 usec  
PL1 4.00 dB  
SFO1 300.1318534 MHz

## F2 - Processing parameters

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



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 atgm85.p  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130723  
Time 15.02  
INSTRUM spect  
PROBHD 5 mm Multinucl  
PULPROG dept135  
TD 65536  
SOLVENT CDCl3  
NS 277  
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 301.4 K  
CNST2 145.0000000  
D1 2.00000000 sec  
d2 0.00344828 sec  
d12 0.00002000 sec  
DELTA 0.00001604 sec  
TD0 1

CHANNEL f1  
NUC1 13C  
P1 12.60 usec  
p2 25.20 usec  
PL1 -6.00 dB  
SFO1 75.4752950 MHz

CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
P3 6.78 usec  
p4 13.56 usec  
PCPD2 80.00 usec  
PL2 4.00 dB  
PL12 25.44 dB  
SFO2 300.1312090 MHz

F2 - Processing parameters  
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GB 0  
PC 1.40

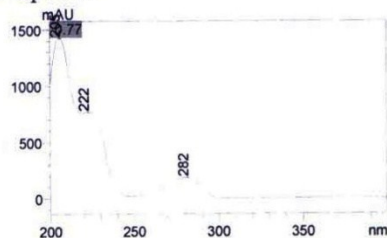
ANALYTICAL TEST REPORT  
[HPLC-PDA-MS]

Sample Information for Direct Mass Analysis of Isolates/synthetic molecule  
Sample Code : ATG-MI-85  
Name of the Scientist : Dr. Atul Gupta  
Project Code: MLP-02  
Mass Range: 150-550

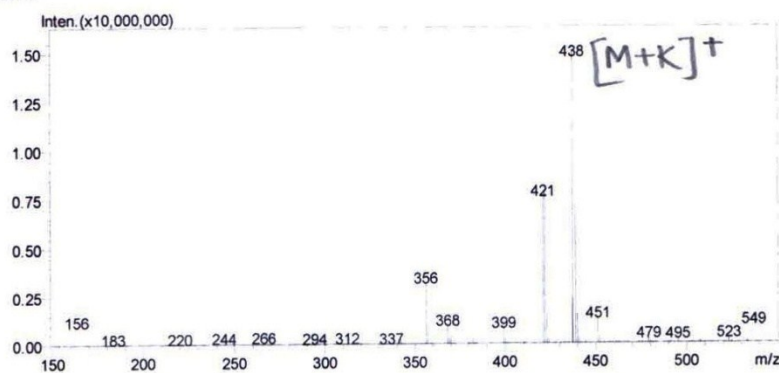
Mass TIC Chromatogram



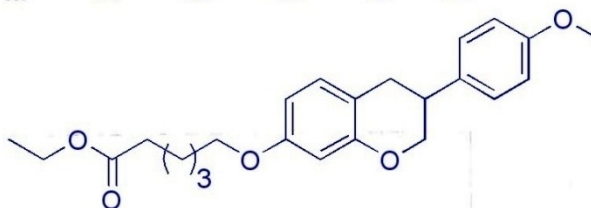
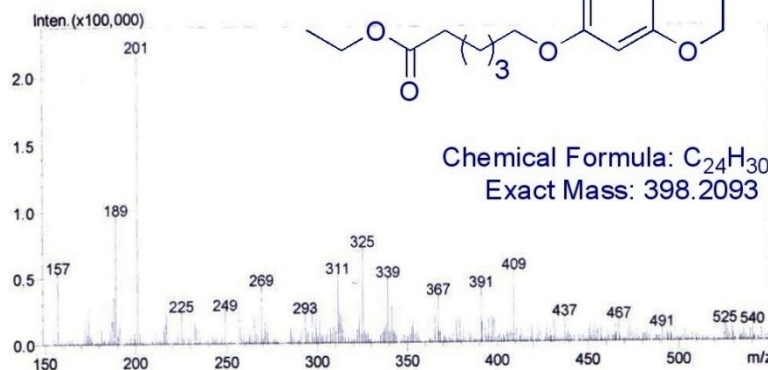
UV-Spectra



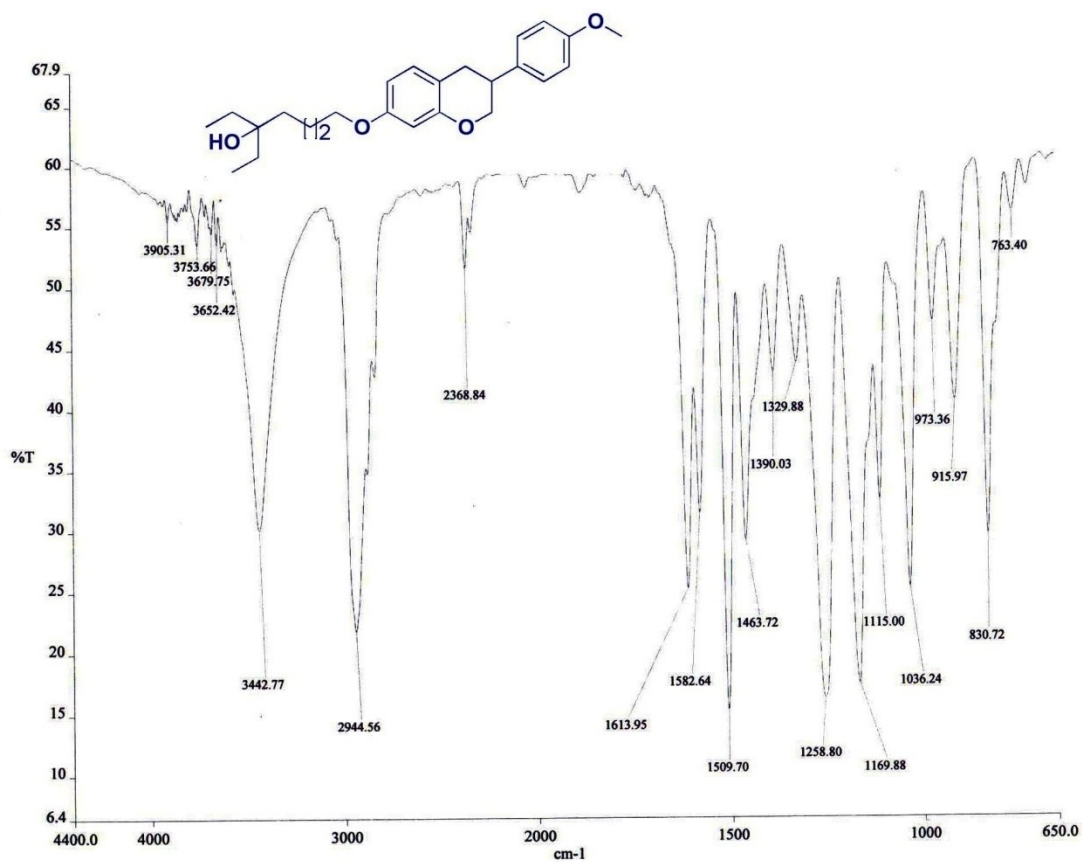
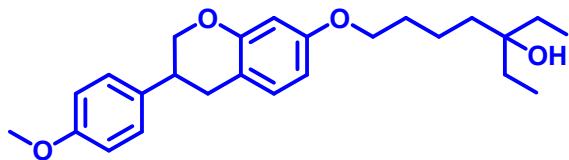
ESI+



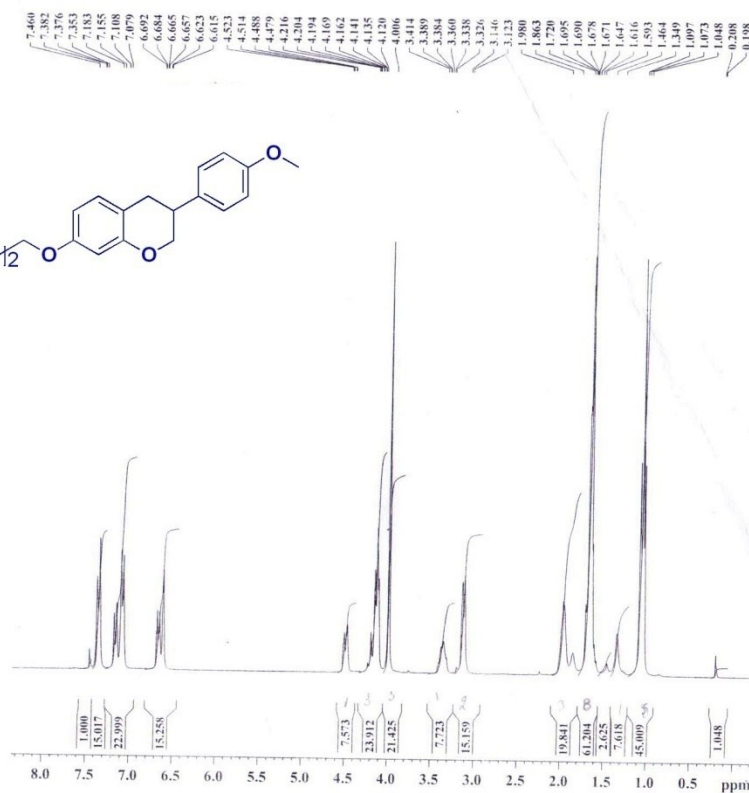
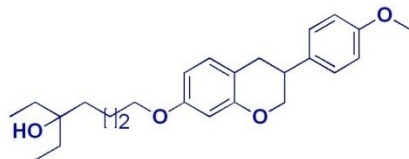
ESI-



**3-ethyl-7-(3-(4-methoxyphenyl)chroman-7-yloxy)heptan-3-ol (26b);**



c:\pel\_data\spectra\tatgm\95\_300813.002 - DR ATUL GUPTA



CIMAP PROTON  
PROJECT NO.: mlp-02

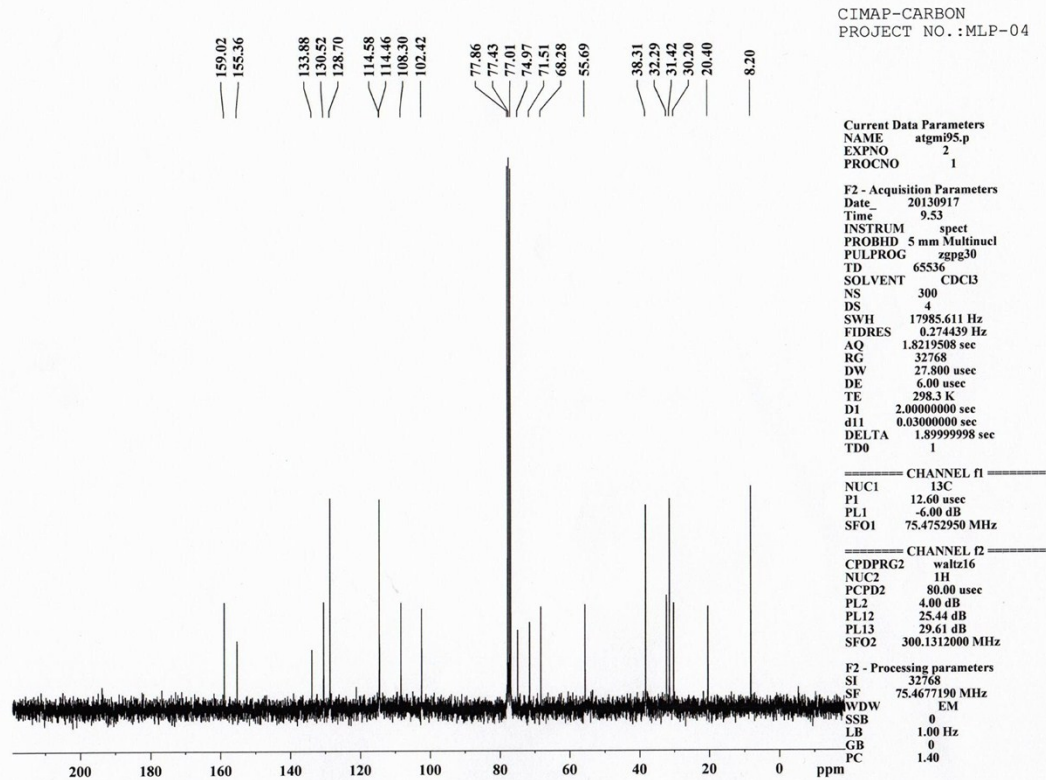
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EXPNO 1  
PROCNO 1

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PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 114  
DW 81.000 usec  
DE 6.00 usec  
TE 297.6 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  
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SF 300.1299467 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.40





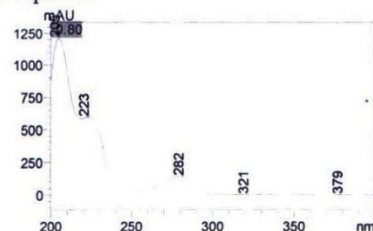
ANALYTICAL TEST REPORT  
[HPLC-PDA-MS]

Sample Information for Direct Mass Analysis of Isolates/synthetic molecule  
Sample Code : ATG-MI-95  
Name of the Scientist : Dr. Atul Gupta  
Project Code: MLP-02  
Mass Range: 150-550

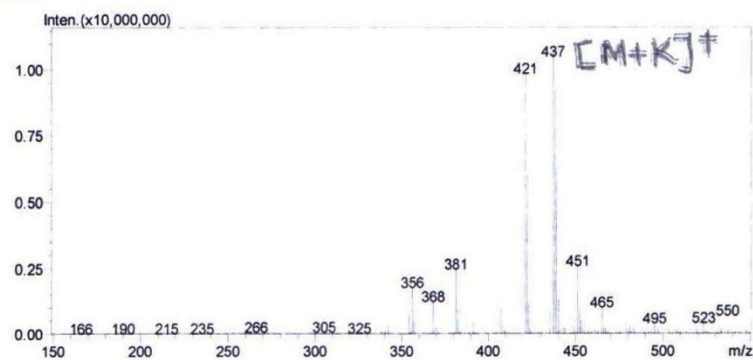
Mass TIC Chromatogram



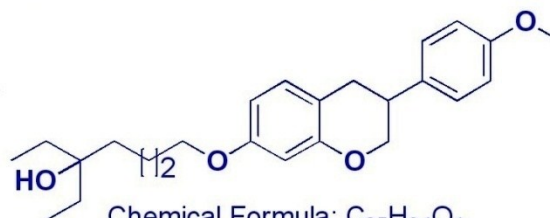
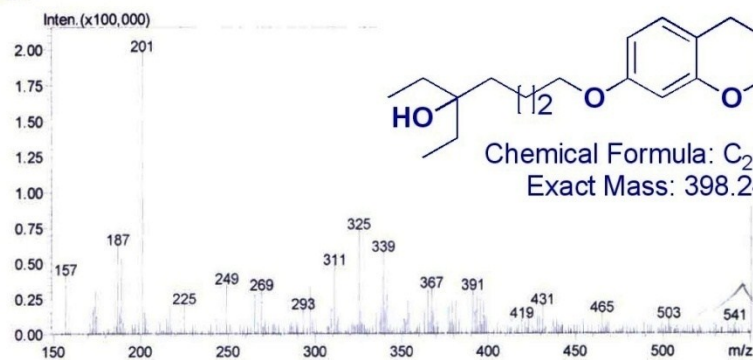
UV-Spectra



ESI+

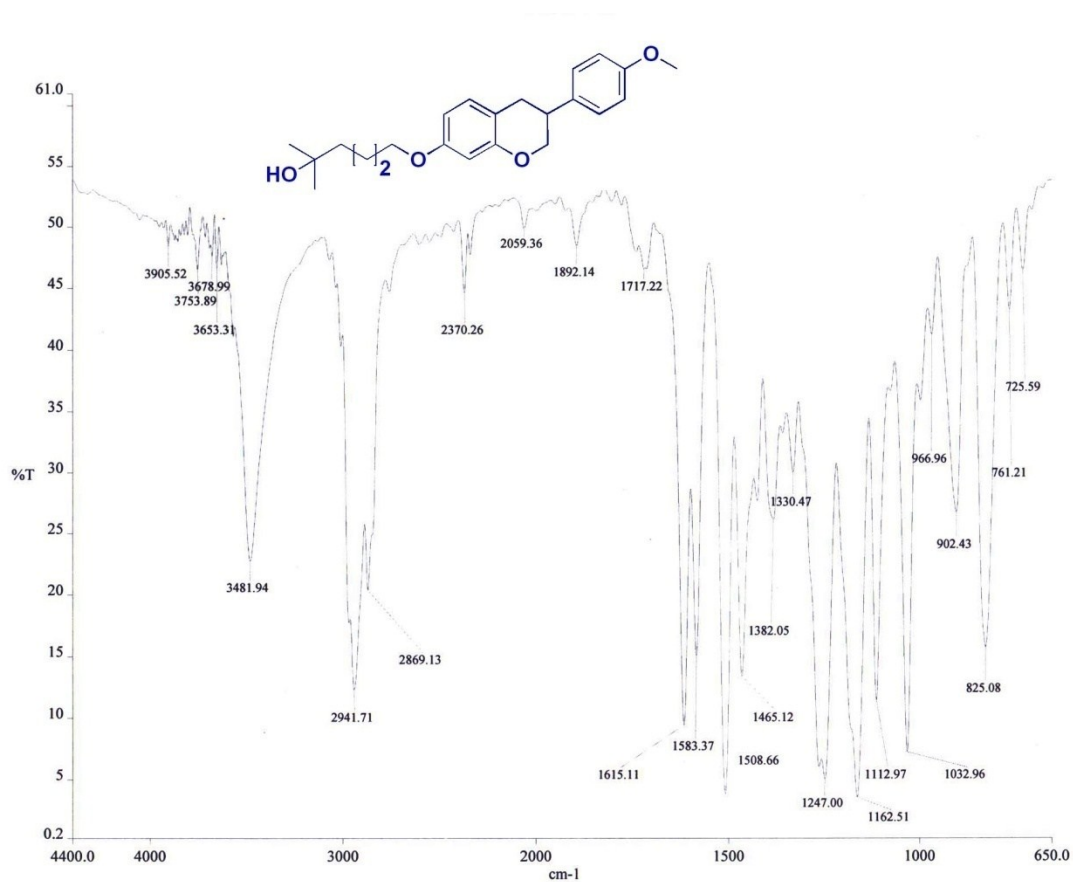
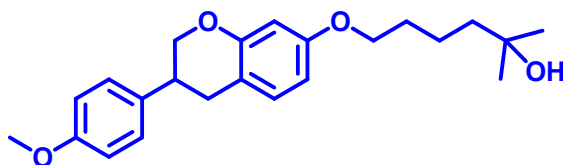


ESI-

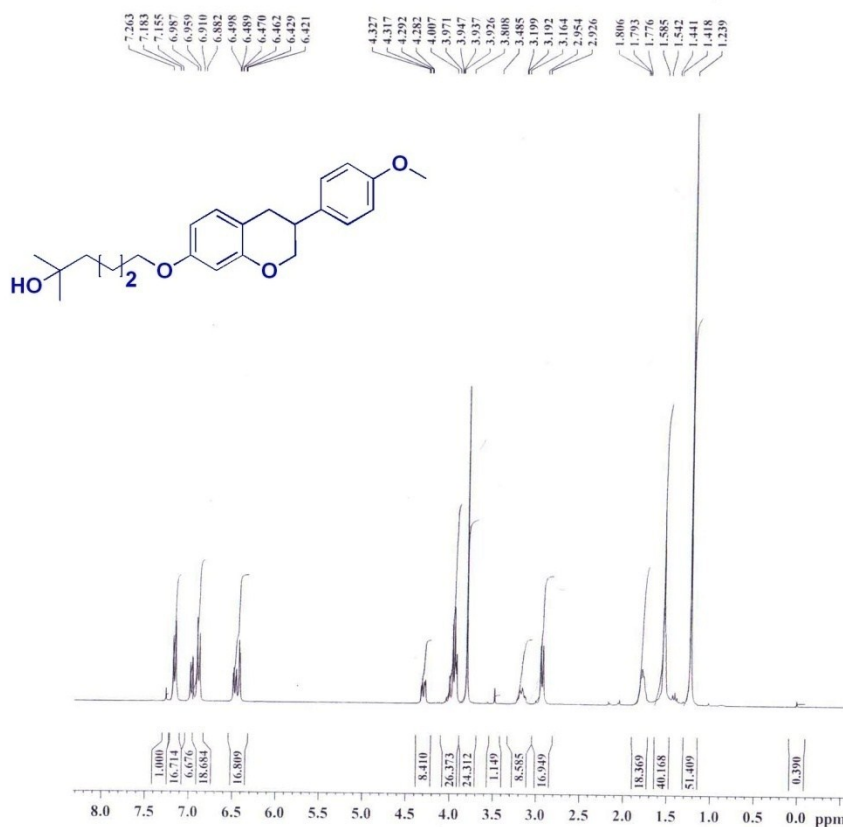


Chemical Formula:  $C_{25}H_{34}O_4$   
Exact Mass: 398.2457

**6-(3-(4-methoxyphenyl)chroman-7-yloxy)-2-methylhexan-2-ol (27b);**



c:\pel\_data\spectra\atgmi91\_300813.002 - DR ATUL GUPTA



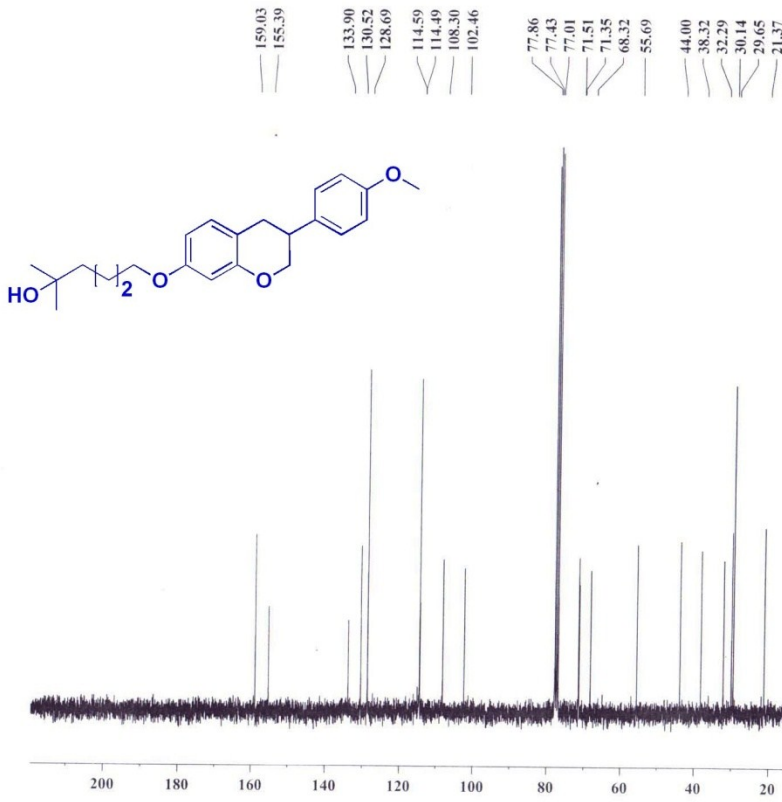
CIMAP PROTON  
PROJECT NO.: mlp-02

Current Data Parameters  
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EXPNO 1  
PROCNO 1

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Time 16.29  
INSTRUM spect  
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PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 114  
DW 81.000 usec  
DE 6.00 usec  
TE 300.8 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  
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SF 300.1300052 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.40



CIMAP-CARBON  
PROJECT NO.: MLP-04

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EXPNO 2  
PROCNO 1

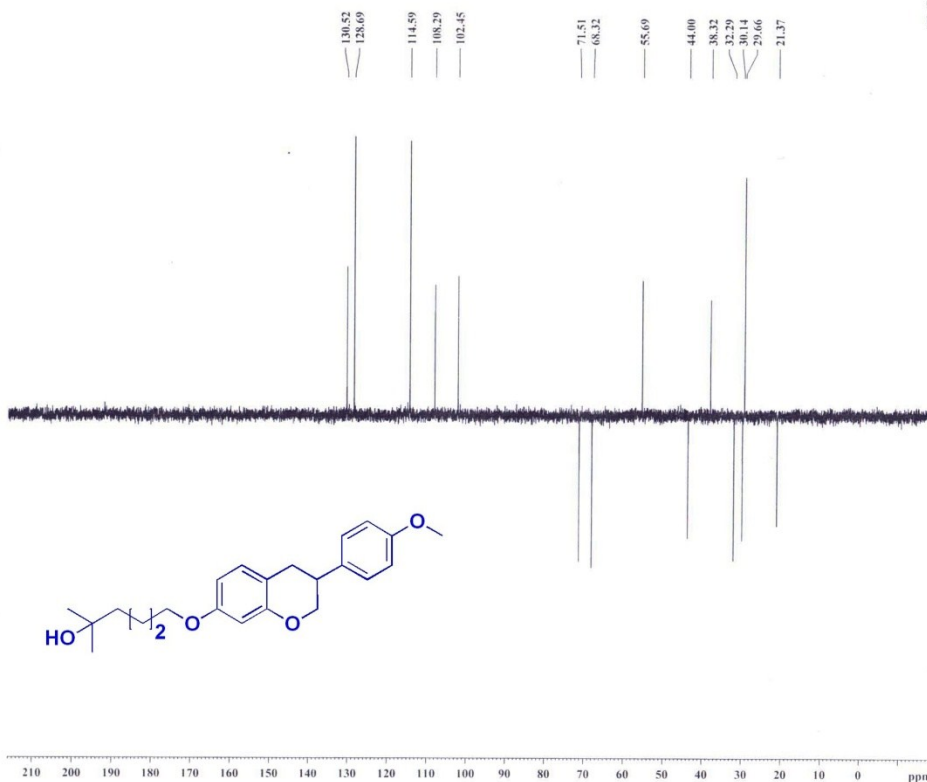
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PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 370  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 32768  
DW 27.800 usec  
DE 6.00 usec  
TE 301.5 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== 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

CIMAP-DEPT 135  
PROJECT NO.:LIP-13



Current Data Parameters  
NAME atgm91.p  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date 20130812  
Time 17.03  
INSTRUM spect  
PROBHD 5 mm Multinuc1  
PULPROG dept135  
TD 65536  
SOLVENT CDCl3  
NS 208  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 16384  
DW 27.800 usec  
DE 0.00 usec  
TE 301.2 K  
CNST2 145.0000000  
D1 2.00000000 sec  
d2 0.00344828 sec  
d12 0.00002000 sec  
DELTA 0.00001604 sec  
TD0 1

CHANNEL f1  
NUC1 13C  
P1 12.60 usec  
p2 25.20 usec  
PL1 -6.00 dB  
SFO1 75.4752950 MHz

CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
P3 6.78 usec  
p4 13.56 usec  
PC PD2 80.00 usec  
PL2 4.00 dB  
PL12 25.44 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

ANALYTICAL TEST REPORT

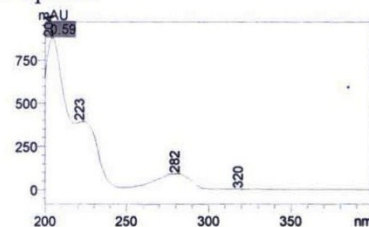
[HPLC-PDA-MS]

Sample Information for Direct Mass Analysis of Isolates/synthetic molecule  
Sample Code : ATG-MI-91  
Name of the Scientist : Dr. Atul Gupta  
Project Code: MLP-02  
Mass Range: 150-550

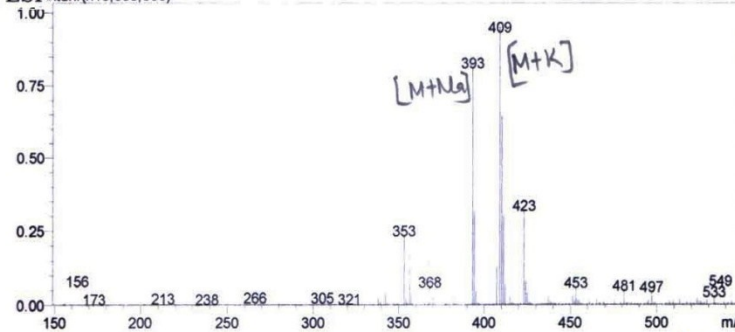
Mass TIC Chromatogram



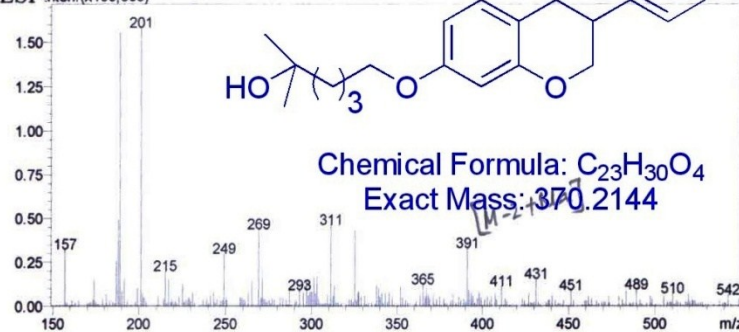
UV-Spectra



ESI-<sup>+</sup>Inten. (x10,000,000)



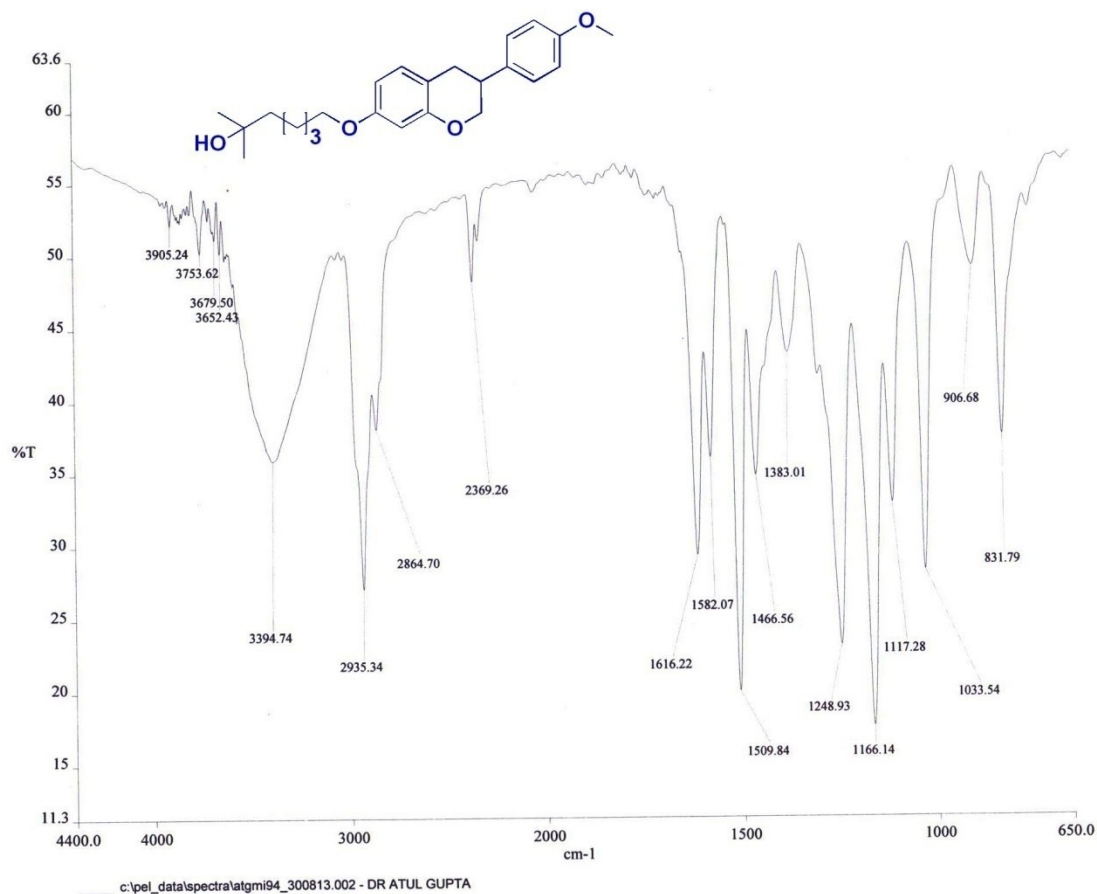
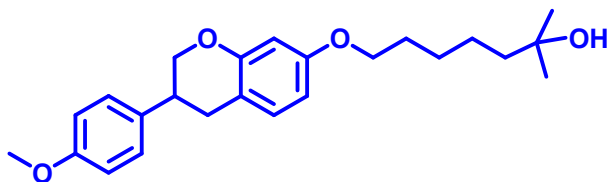
ESI-Inten. (x100,000)



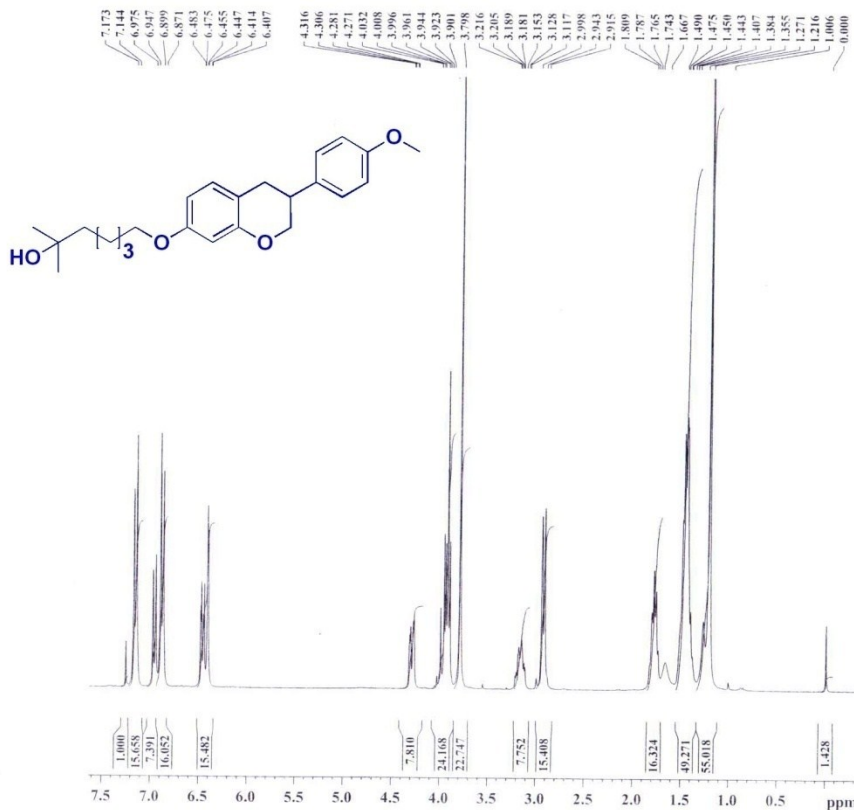
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**7-(3-(4-methoxyphenyl)chroman-7-yloxy)-2-methylheptan-2-ol (27c);**







CIMAP PROTON  
PROJECT NO.: mlp-02

Current Data Parameters

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EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

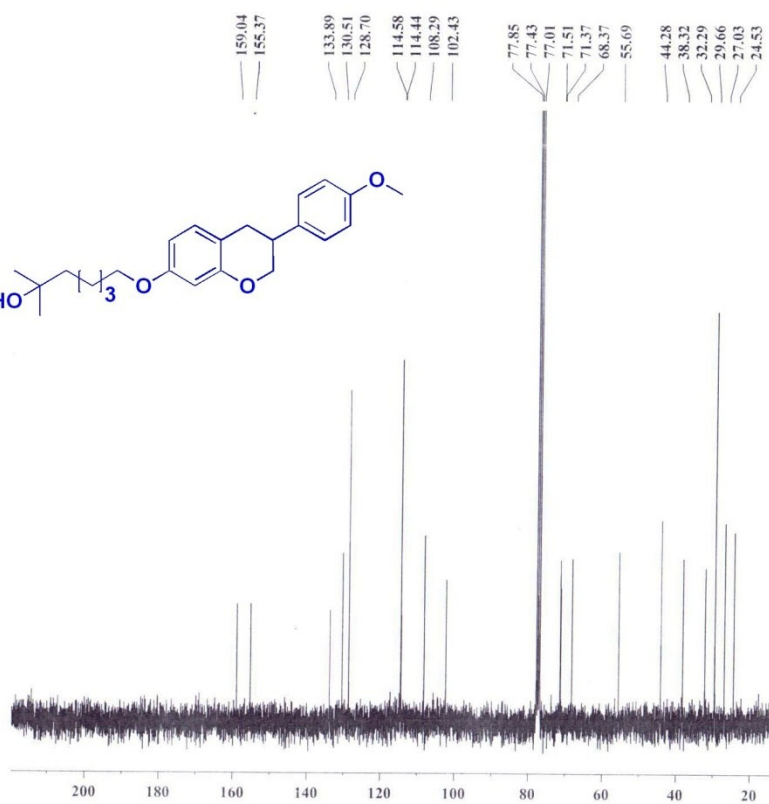
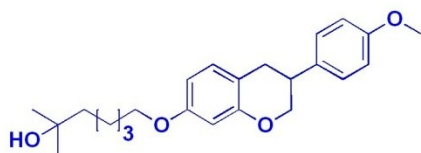
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PROBHD 5 mm Multinucl  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 128  
DW 81.000 usec  
DE 6.00 usec  
TE 299.7 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====

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

F2 - Processing parameters

SF 32768  
SF 300.1300084 MHz  
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LB 0.30 Hz  
GB 0  
PC 1.40



CIMAP-CARBON  
PROJECT NO.:MLP-04

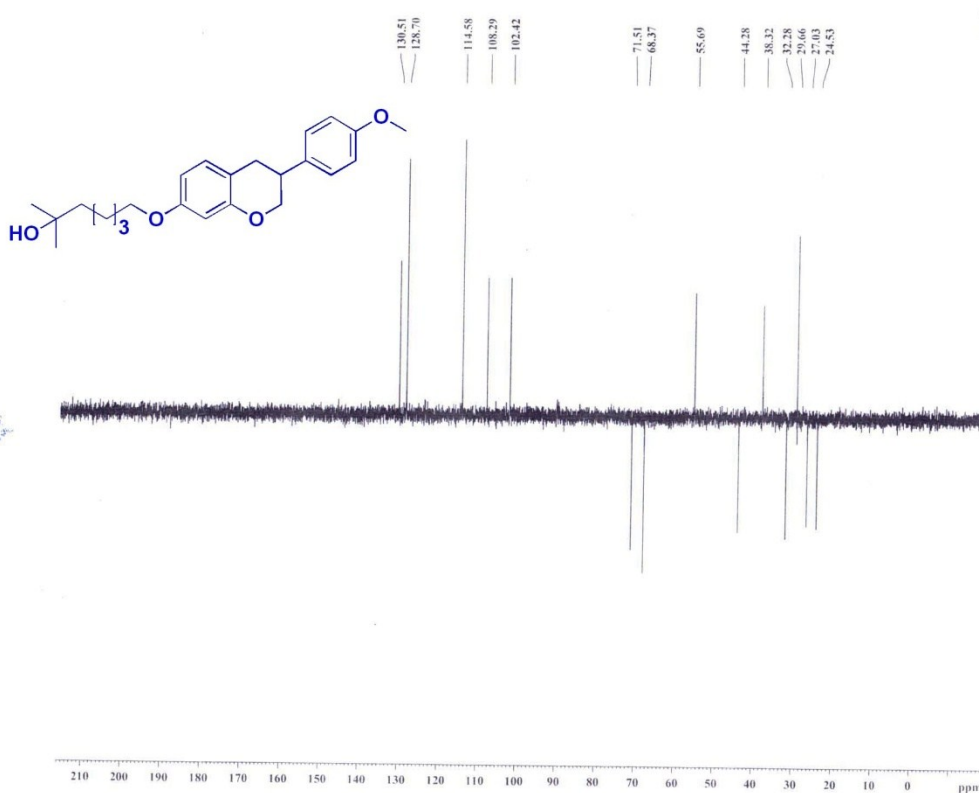
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EXPNO 2  
PROCNO 1

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PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 256  
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 2.00000000 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 25.44 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



CIMAP-DEPT 135  
PROJECT NO.: ILP-13

Current Data Parameters  
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EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130917  
Time 13.53  
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PULPROG dept135  
TD 65536  
SOLVENT CDCl3  
NS 216  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 16384  
DW 27.800 usec  
DE 6.09 usec  
TE 300.3 K  
CNST2 145.0000000  
D1 2.00000000 sec  
d2 0.00344828 sec  
d12 0.00002000 sec  
DELTA 0.00001604 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.60 usec  
p2 25.20 usec  
PL1 -6.00 dB  
SFO1 75.4752950 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
P3 6.78 usec  
p4 13.50 usec  
PCPD2 80.00 usec  
PL2 4.00 dB  
PL12 25.44 dB  
SFO2 300.1312000 MHz

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

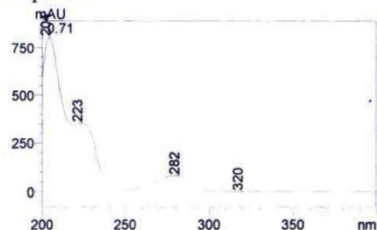
ANALYTICAL TEST REPORT  
[HPLC-PDA-MS]

Sample Information for Direct Mass Analysis of Isolates/synthetic molecule  
Sample Code : ATG-MI-94  
Name of the Scientist : Dr. Atul Gupta  
Project Code: MLP-02  
Mass Range: 150-550

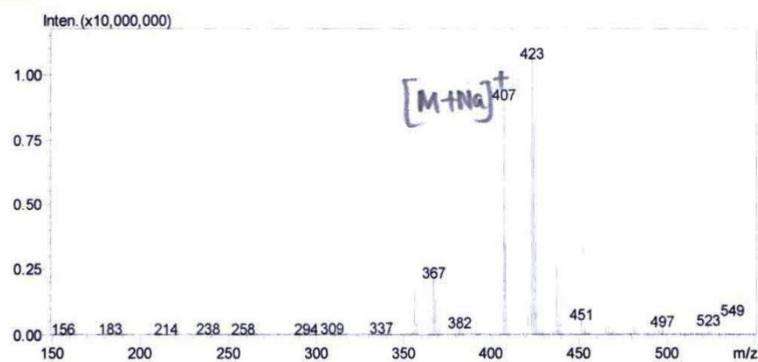
Mass TIC Chromatogram



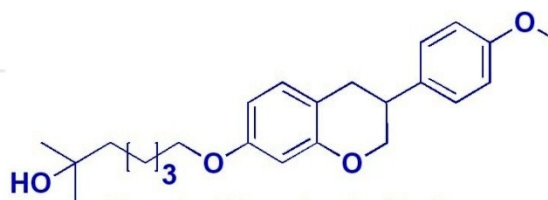
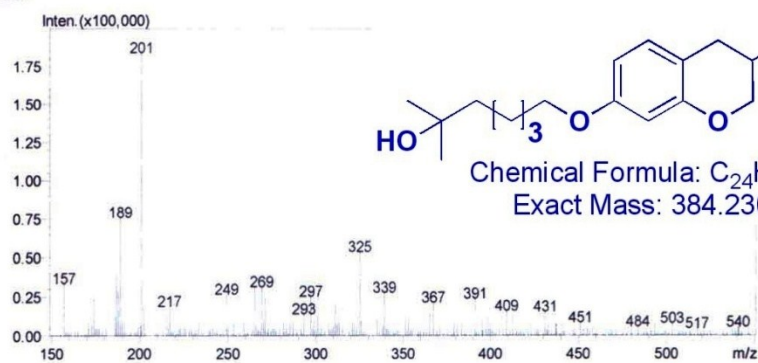
UV-Spectra



ESI+



ESI-



Chemical Formula:  $C_{24}H_{32}O_4$   
Exact Mass: 384.2301