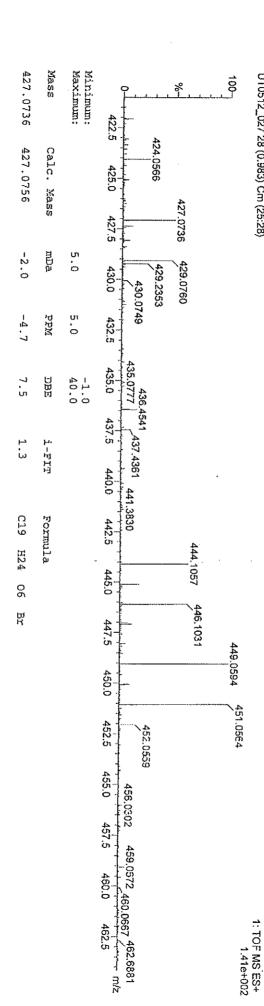


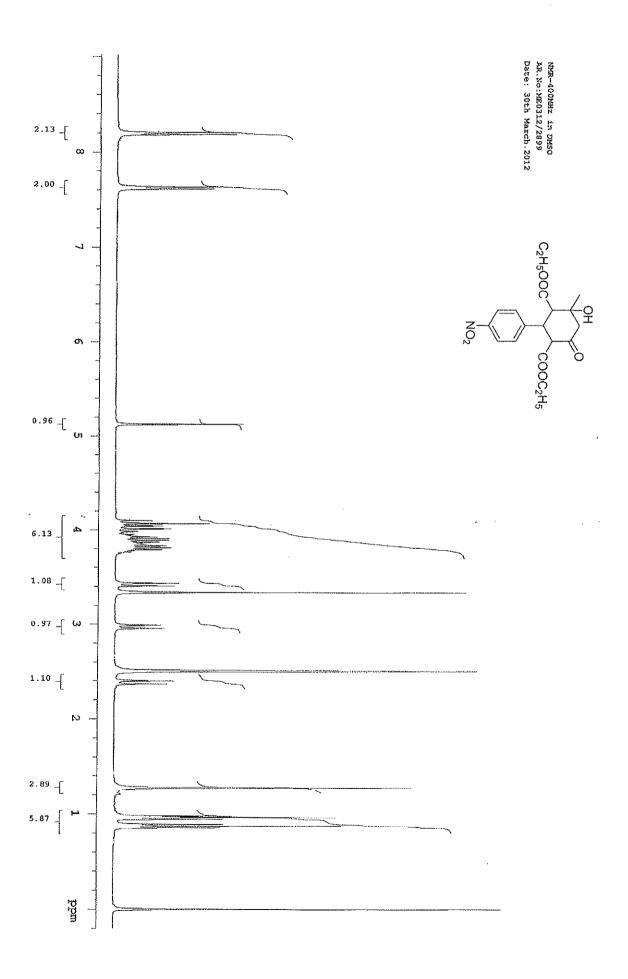
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 40.0 Element prediction: Off

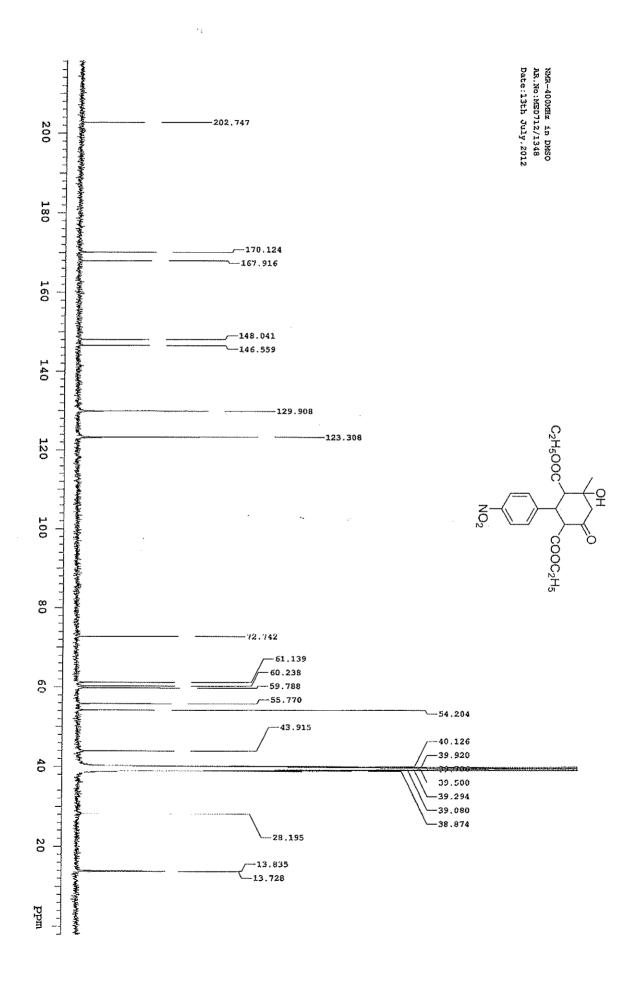
Number of isotope peaks used for i-FIT = 2

Elements Used: C: 0-35 H: 0-35 O: 0-10 Br: 0-1 Monoisotopic Mass, Even Electron lons 69 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

UT0512\_027 28 (0.983) Cm (25:28)







Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 40.0 Element prediction: Off

Number of isotope peaks used for i-FIT = 2

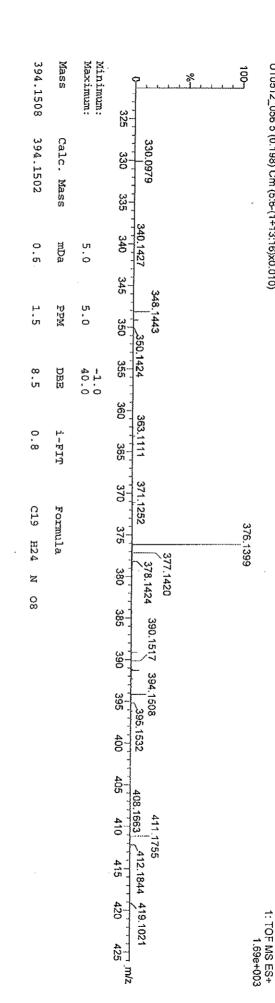
Monoisotopic Mass, Even Electron lons

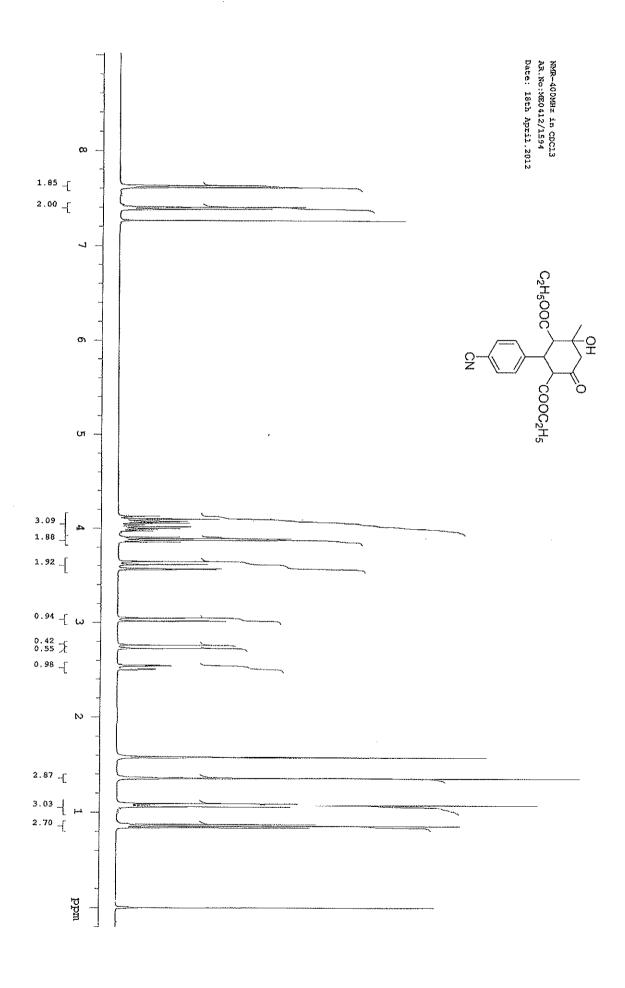
22 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

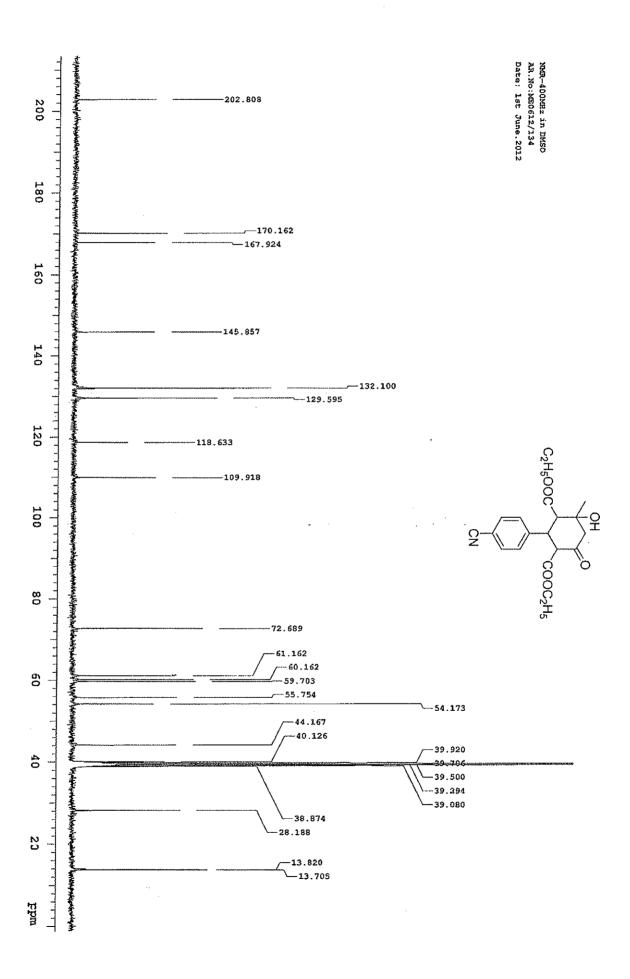
Elements Used:

C: 0-25 H: 0-35 N: 0-1 O: 0-8

UT0512\_056 5 (0.198) Cm (5:6-(1+13:16)x0.010)







Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 40.0 Number of isotope peaks used for i-FIT = 2 Element prediction: Off

Monoisotopic Mass, Even Electron Ions
37 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used: C: 0-30 H: 0-30 N: 0-1 O: 0-6

UT0512\_049 4 (0.138) Cm (4:5)

Š

356,1480

Dr.Reddy's Laboratories Ltd, ARD, TDC-1

1: TOF MS ES+ 6.08e+002

Minimum: Mass 374.1618 0 ... 349.1199 374.1604 Calc. Mass 351,1367 352.1324 352.0 354.0 5.0 1.4 mDa 355,7994 356.0 Mdd 5.0 357,1561 358,1521 358.0 9.5 -1.0 40.0 DBE 360.1605,360.8491 362.8584 365.5411 368.4137 369.1440 371.3039 360.0 0.3 i-FIT 362.0 364.0 C20 H24 N Formula 366.0 1.0 368.0 370.0 37 90 372.0 374.0

374,1618 375.1727<sub>376,5206</sub>

376.0

378.0

COOC<sub>2</sub>H<sub>5</sub>

## SAMPLE INFORMATION

Sampel\_Type : Unknown Acquired By : System

Injection Volume : 63 Date Acquired : 10/3/2012 7:15:37 PM

Vial no: 10.00 ulChannel Name: PDA 254.0 nmRun Time: 40.00 MinutesAcq Method Set: CHIRAL

 System Name
 :
 HPLC\_005\_PDA
 Date Processed
 :
 10/4/2012 11:58:05 AM

 Sample Set Name
 :
 12100302
 Project Name
 :
 Alliance\_005\_OCT\_2012

Injection # : 1 Processing Method : H

## HPLC CONDITIONS

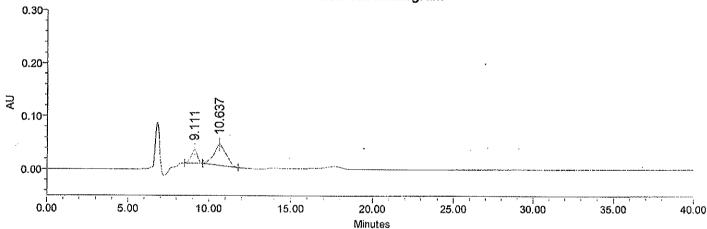
Wavelength

Column : chiral pak AD-H(250\*4.6)mmδμm Mobile\_phase : Ethanoi:MeOH:DEA(800:200:1)

: 254.0 nm

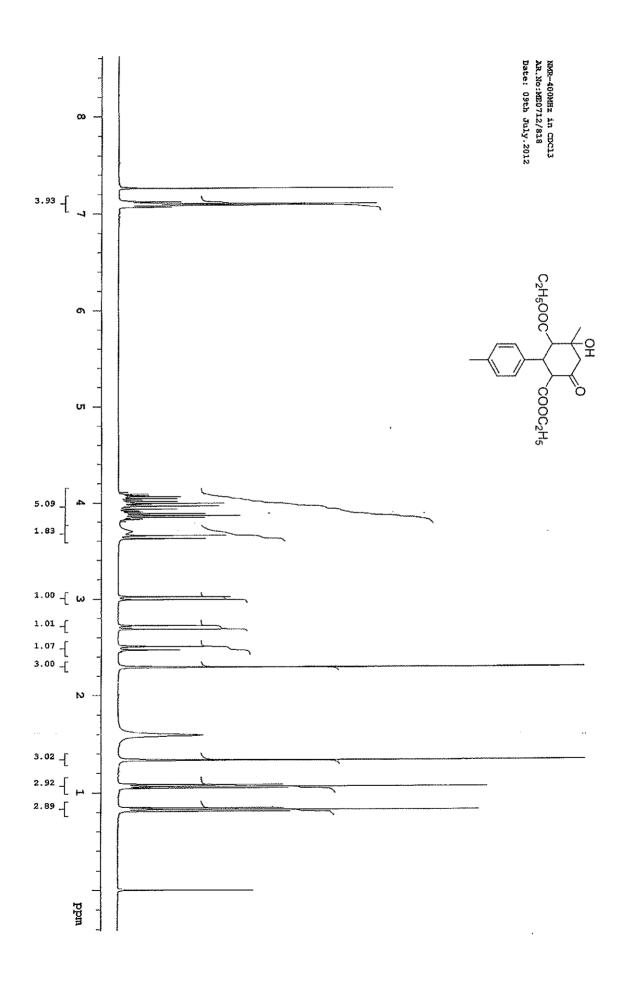
Diluent : DCM Flow rate :0.5 mL/min, Column temp :27 °C, Inj vol:5µl  $C_2H_5OOC$   $COOC_2H_5$  CN

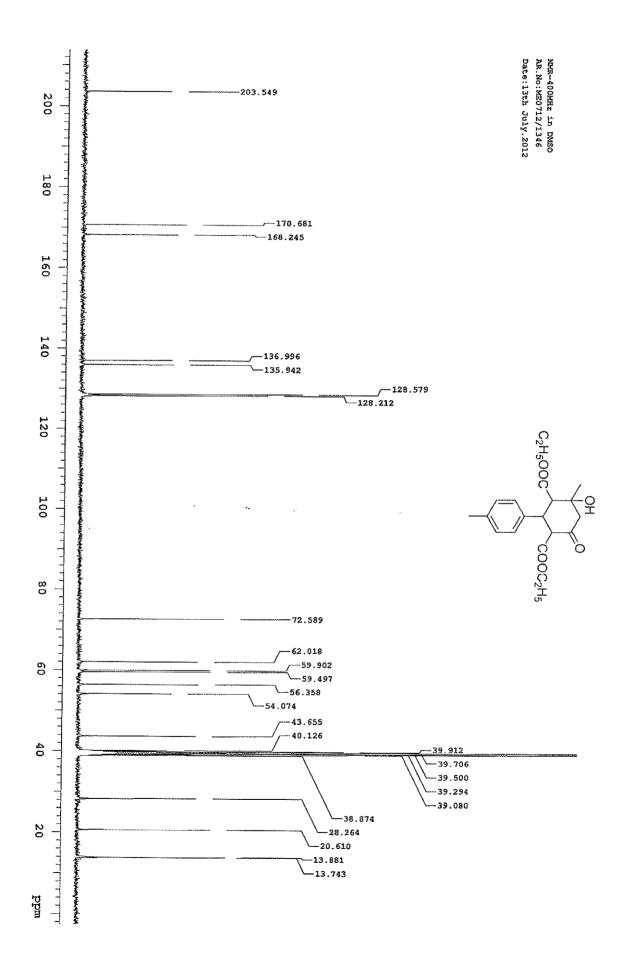
## Auto-Scaled Chromatogram



## Peak Results

	Name	RT	Area	% Area
1		9.111	· 653062	23.96
2		10.637	2072206	76.04





Single Mass Analysis
Tolerance = 5.0 PPM / DBE; min = -1.0, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

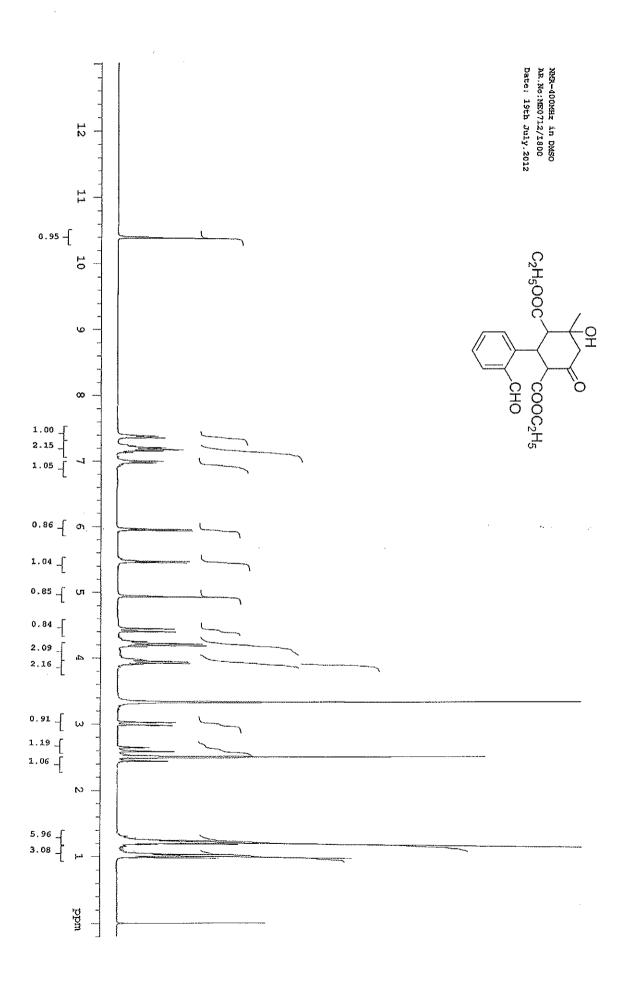
Monoisotopic Mass, Even Electron Ions 28 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

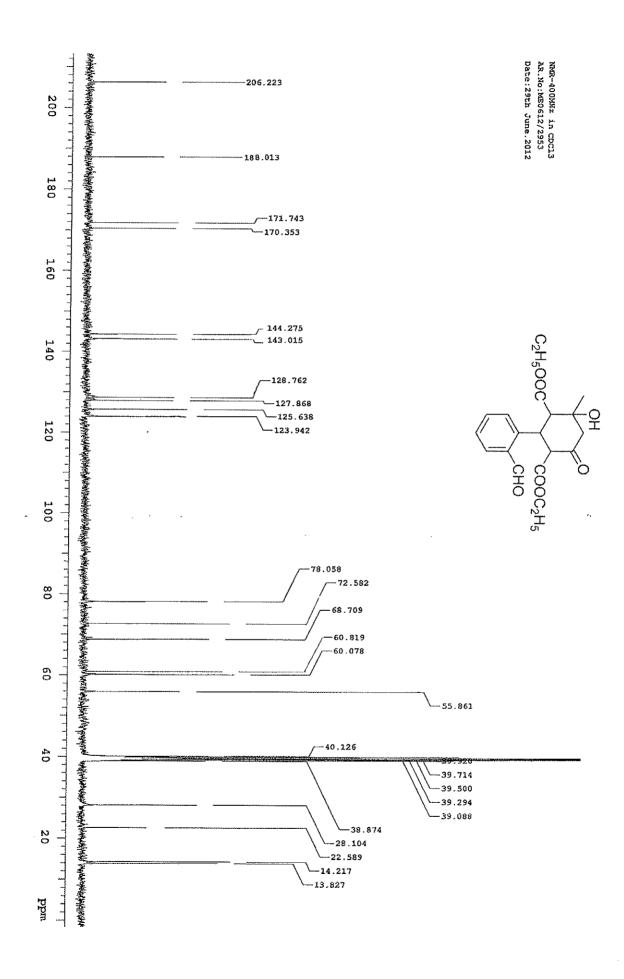
Elements Used: C: 0-25 H: 0-35 O: 0-10

Dr.Reddy's Laboratories Ltd, ARD,TDC-1

UT0512\_021 21 (0.762) Cm (17:27-2:8x0.010)

Minimum: Maximum: Mass 363.1819 3 360.0 359.1776 363.1808 Calc. Mass 363,1819 365.0 364,1848 ۍ. 0 mDa 370.0 371 3174 3.0 Mdd 5.0 375.0 375.2063 378.1575 7.5 40.0 DBE 380,2083 380.0 ر... ق i-FIT 385.1632 382.1510 C20 H27 O6 Formula 386,1662 390.0 391,2868 393,2883 395.0 400.7614 400.0 401,1373 402.1411 ,403,1400 405.0 408.2394 410.0 Transfer m/z 412,2500 1: TOF MS ES+ 2.03e+004





Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 40.0 Element prediction: Off

Monoisotopic Mass, Even Electron lons
22 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Number of isotope peaks used for i-FIT = 2

Elements Used: C: 0-25 H: 0-35 O: 0-10

UT0512\_024 24 (0.841) Cm (21:29-5:13x0.010)

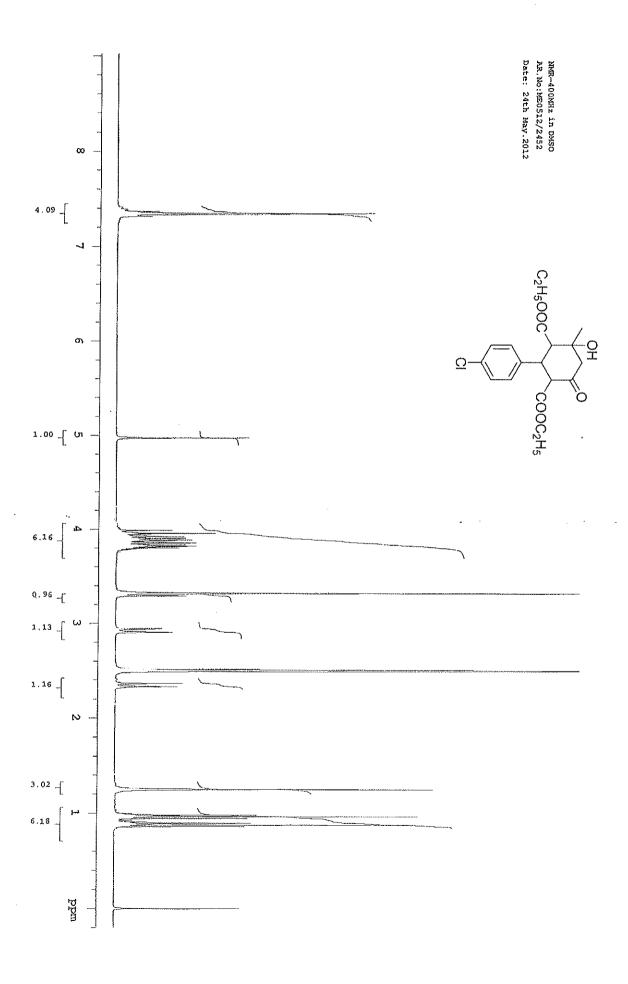
371,3162

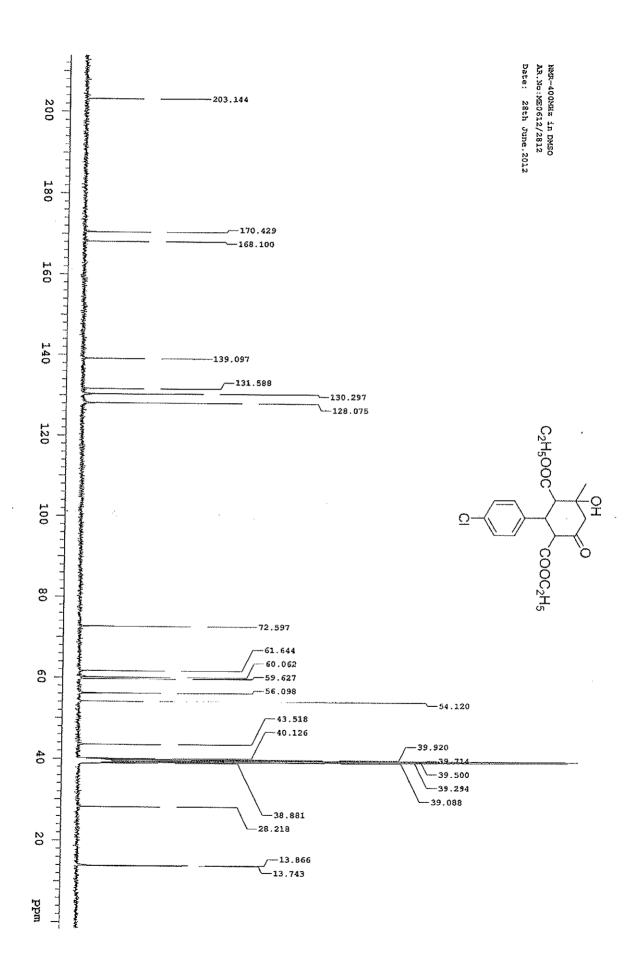
Dr.Reddy's Laboratories Ltd, ARD,TDC-1

1: TOF MS ES+ 5.94e+002

Minimum: Maximum: Mass 377.1611 Š 369,3566 377.1600 Calc. Mass 370.0 370.3424 5.0 щDа 371.4089 372.0 5. O 2.9 PPM 373.0 ω . . -1.0 40.0373,3176 374 0 374,1591 0.5 1-FIT 375.0 375.1439 C20 H25 O7 Formula 376.0372 376.0 377.1611 378.0 378,1585 379.0 379,1768 380,1975 381.1196 381.3918 miz

$$C_2H_5OOC$$
 $CH_5$ 
 $CHO$ 





Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0 Element prediction: Off

Number of isotope peaks used for i-FIT = 3

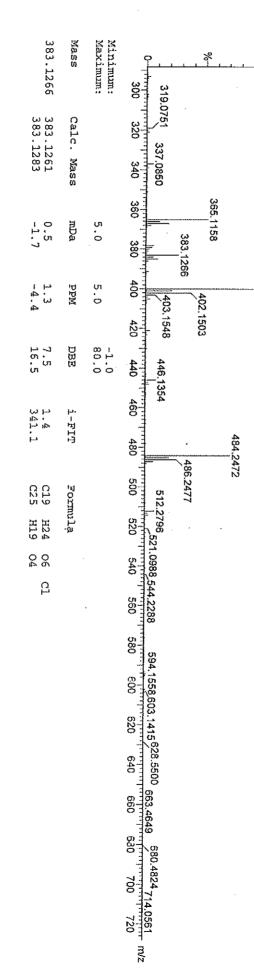
<u>ફ</u>

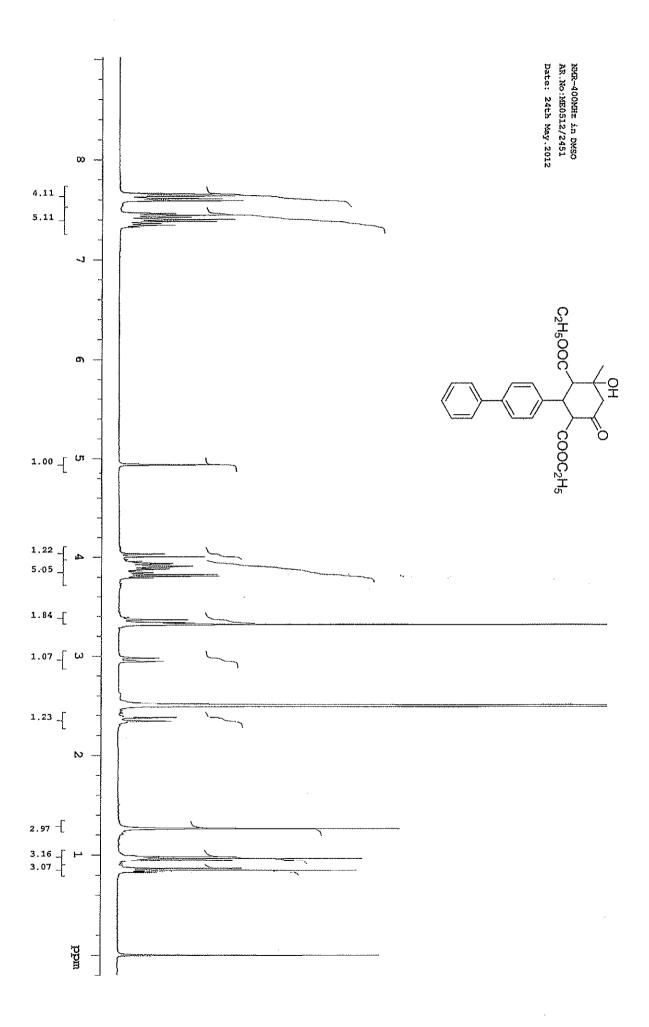
400,1523

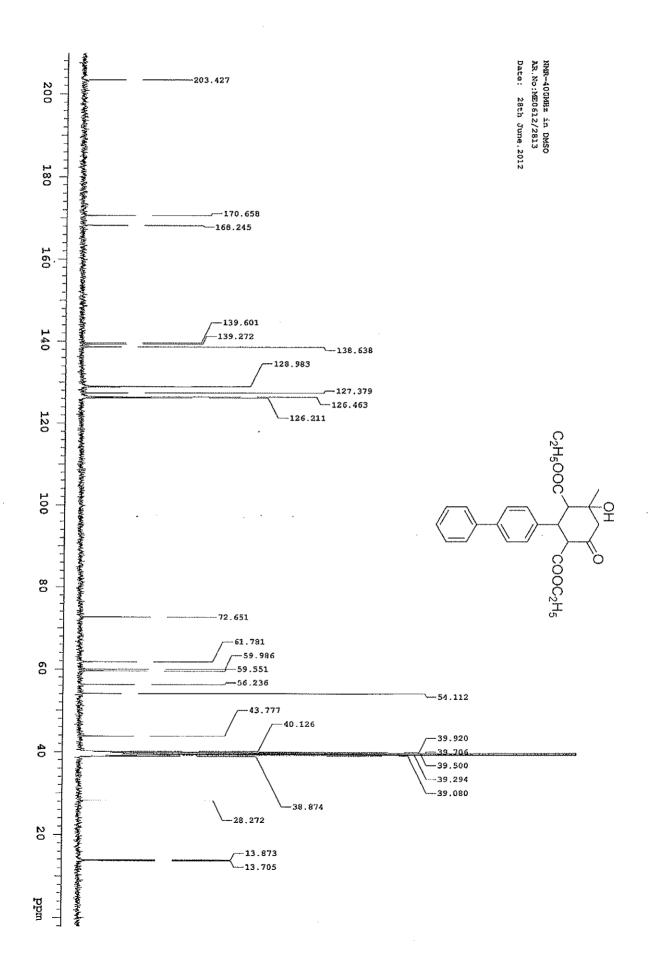
A786/CSAT1/063 UT0712\_41 16 (0.293) Cm (16:20)

Monoisotopic Mass, Even Electron lons
35 formula(e) evaluated with 2 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-25 H: 0-25 O: 0-6 CI: 0-2









Element prediction: Off

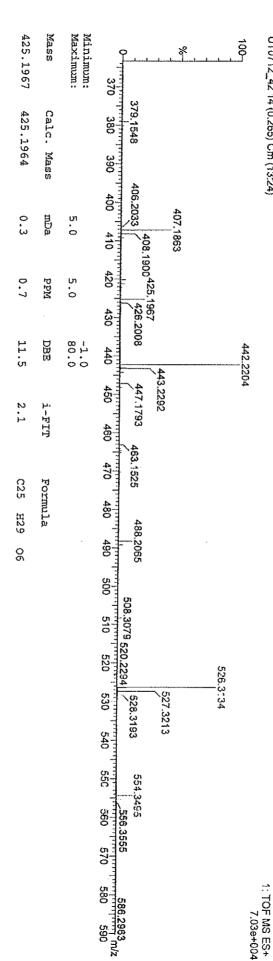
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)

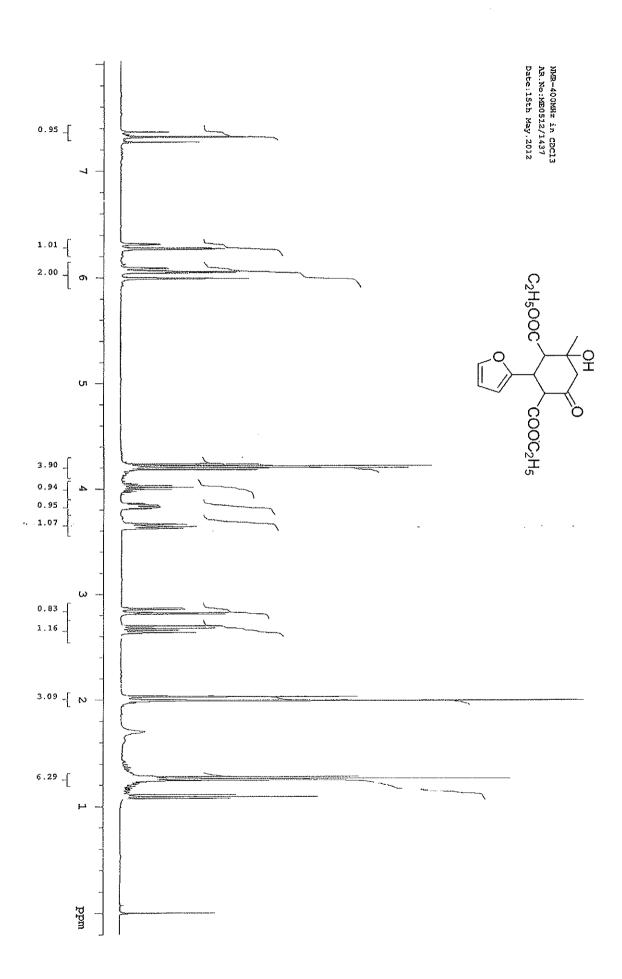
Elements Used: C: 0-30 H: 0-30 O: 0-6

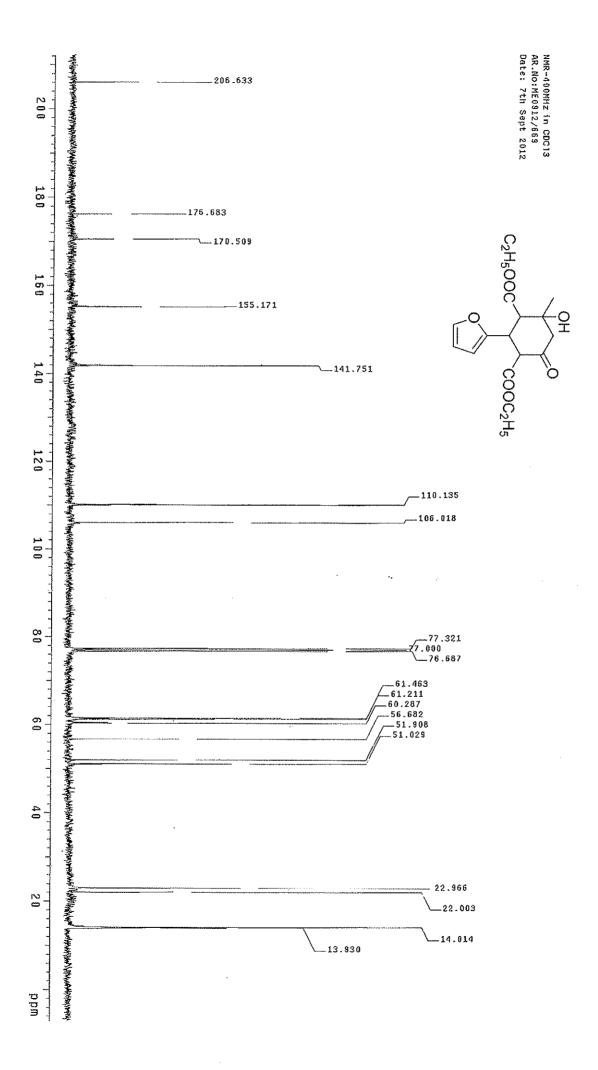
UT0712\_42 14 (0.265) Cm (13:24)

Dr.Reddy's Laboratories Ltd, ARD, TDC-1



C<sub>2</sub>H<sub>5</sub>OOC COOC<sub>2</sub>H<sub>5</sub>





Single Wass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 40.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Elements Used: C: 0-30 H: 0-30 O: 0-7

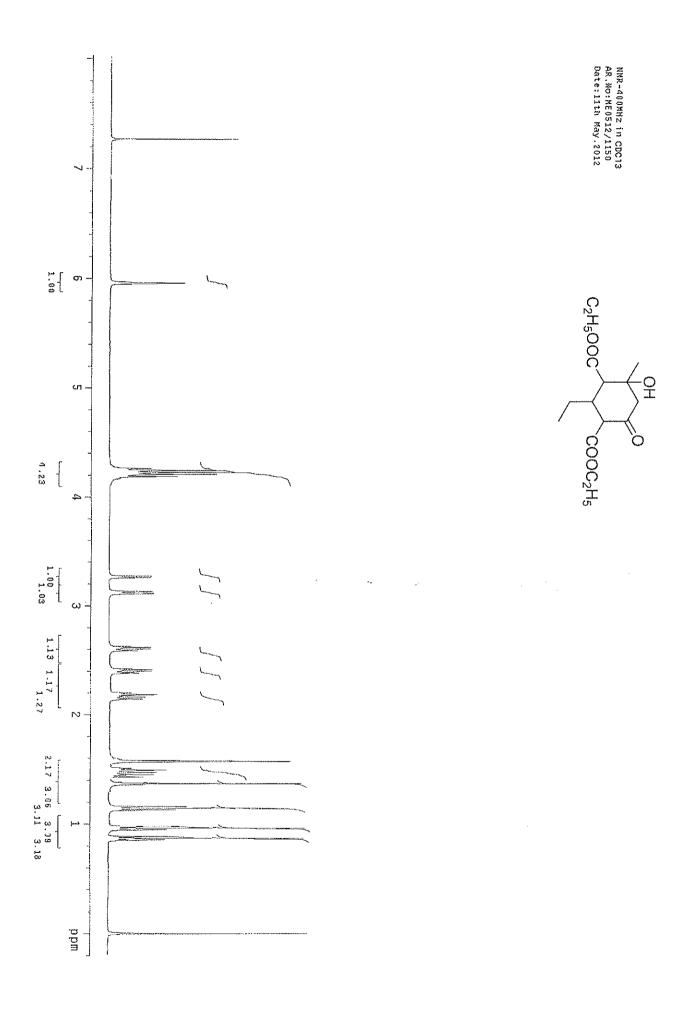
Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

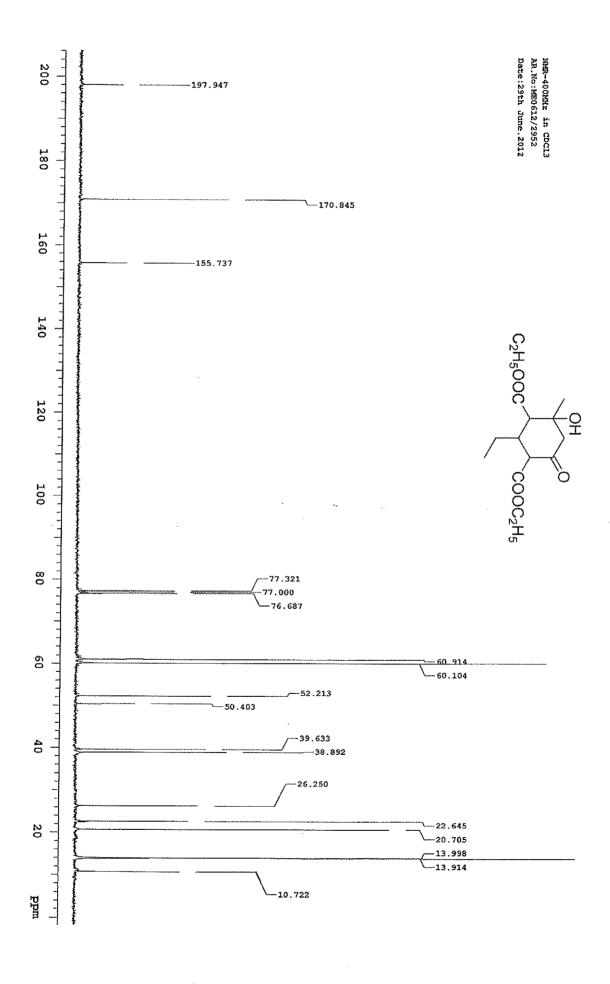
UT0512\_053 6 (0.225) Cm (6:8)

Dr.Reddy's Laboratories Ltd, ARD, TDC-1

1: TOF MS ES+ 2.01e+004

Minimum: Maximum: 339.1447 Mass 8 280 279.1596 290.1393 293.1030 285 339.1444 Calc. Mass 290 295 0.3 mDa 5.0 303.1247 300 305 307,1190 0.9 5-0 Medd 310 6.5 40.0 DBE 31. 55. 316.1196 320 321.1332 <u>,</u>, i-FIT 323.1396 334.1299 325 330 C17 H23 Formula 335 9 340 345 353,1021 356,1708 350 355 360 361.1263 365 370 375 377.1026379.1083 m/z 380





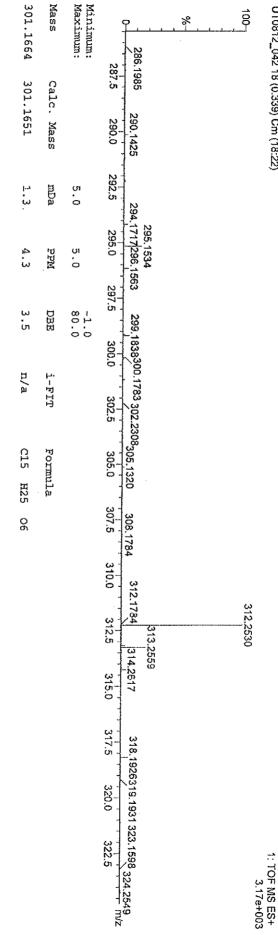
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0 Element prediction: Off

Number of isotope peaks used for i-FIT = 3

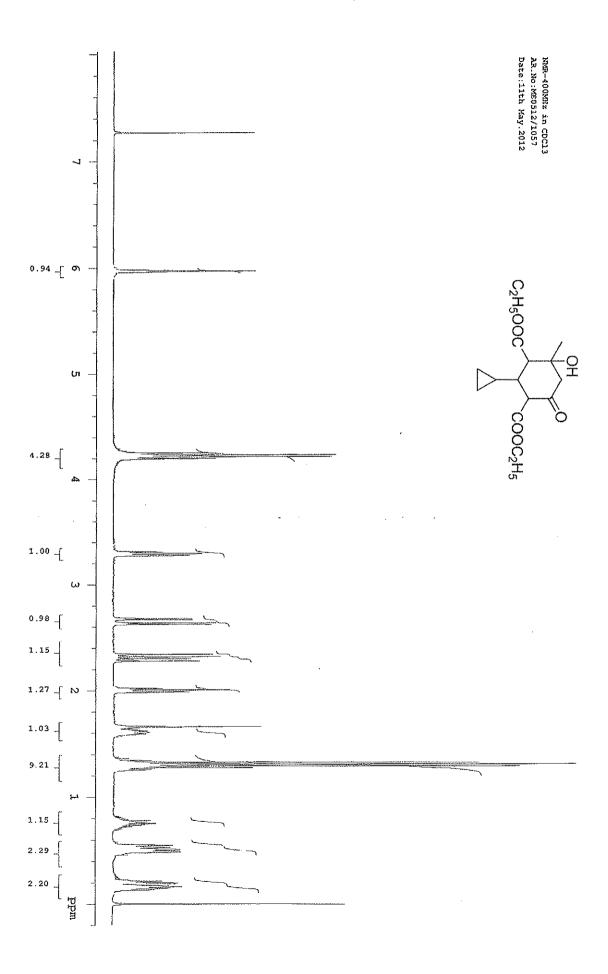
Monoisotopic Mass, Even Electron Ions
39 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)

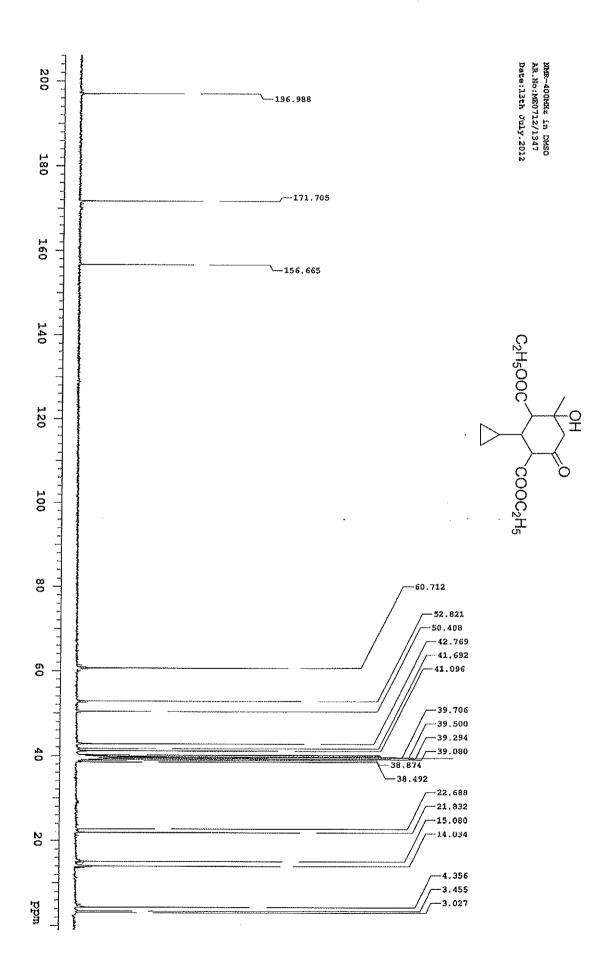
Elements Used: C: 0-50 H: 0-60 O: 0-10

UT0812\_042 18 (0.339) Cm (18:22)



$$C_2H_5OOC$$
  $C0OC_2H_5$ 





Single Mass Analysis
Tolerance = 5.0 PPM / DBE; min = -1.0, max = 40.0
Element prediction: Off

Number of isotope peaks used for i-FIT = 2

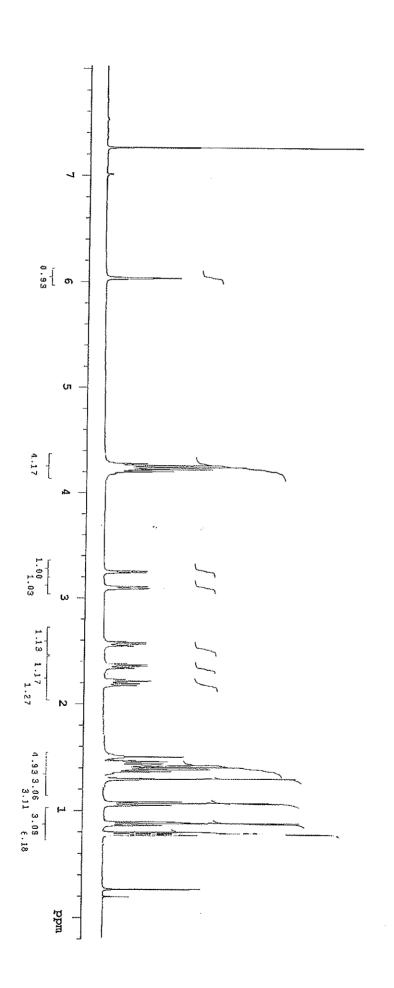
Monoisotopic Mass, Even Electron lons
31 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used: C: 0-25 H: 0-35 O: 0-10

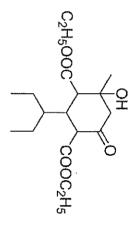
Dr.Reddy's Laboratories Ltd, ARD, TDC-1

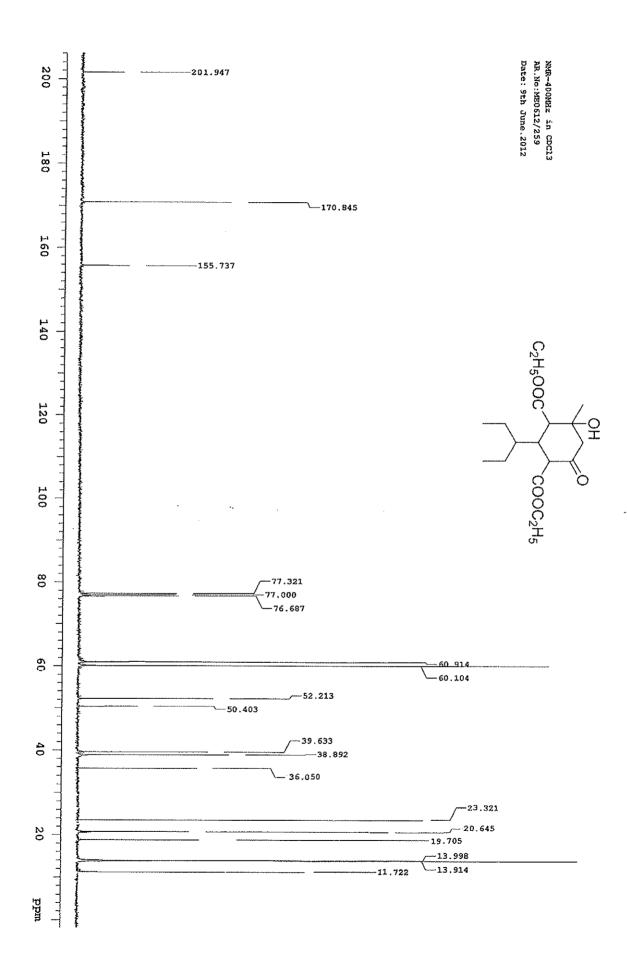
Minimum: Maximum: 313.1650 Mass UT0512\_022 25 (0.902) Cm (25:34-6:10x0.010) 6 306.2124307.1862309.1388.311.1506 313.1651 Calc. Mass 310.0 m Edm 5.0 -0.1 312.5 313,1650 314,1675,315.1898,318.1355,319.1389,321.2086,324,1800,325.2905,328,1497,330.2010 Mad -0.3 5.0 315.0 . 5 -1.0 40.0 317,1338 DBE 317.5 1.0 i-FIT 320.0 322.5 C16 H25 Formula 325.0 8 327.5 330.0 332.5 333,1109 334,1133335,1090 337.5 338.3404 340.1707 340.0 1: TOF MS ES+ 2.41e+003 z/m r

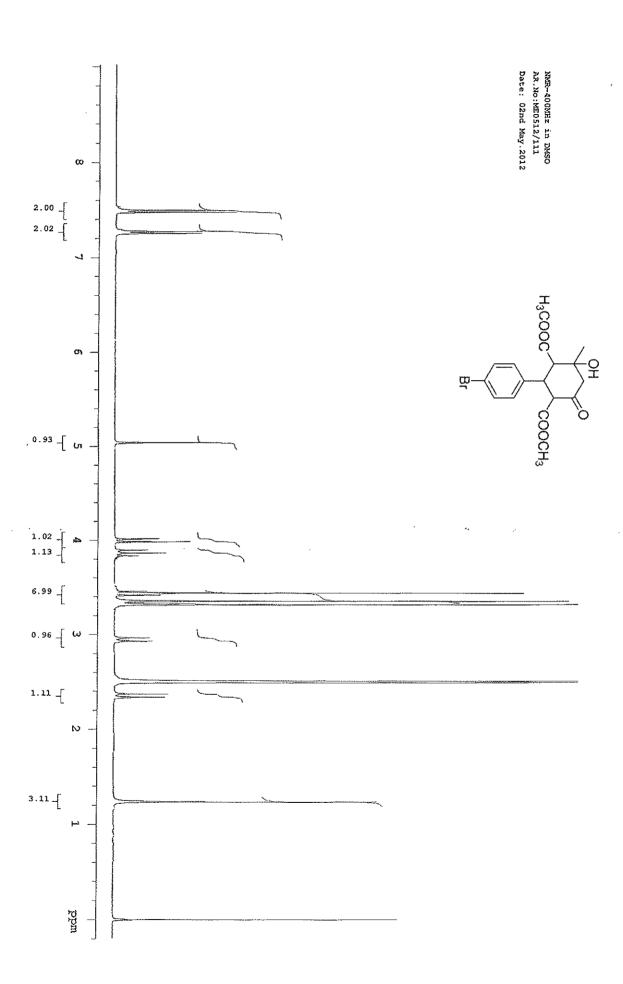
$$C_2H_5OOC$$
 $C_2H_5OOC_2H_5$ 

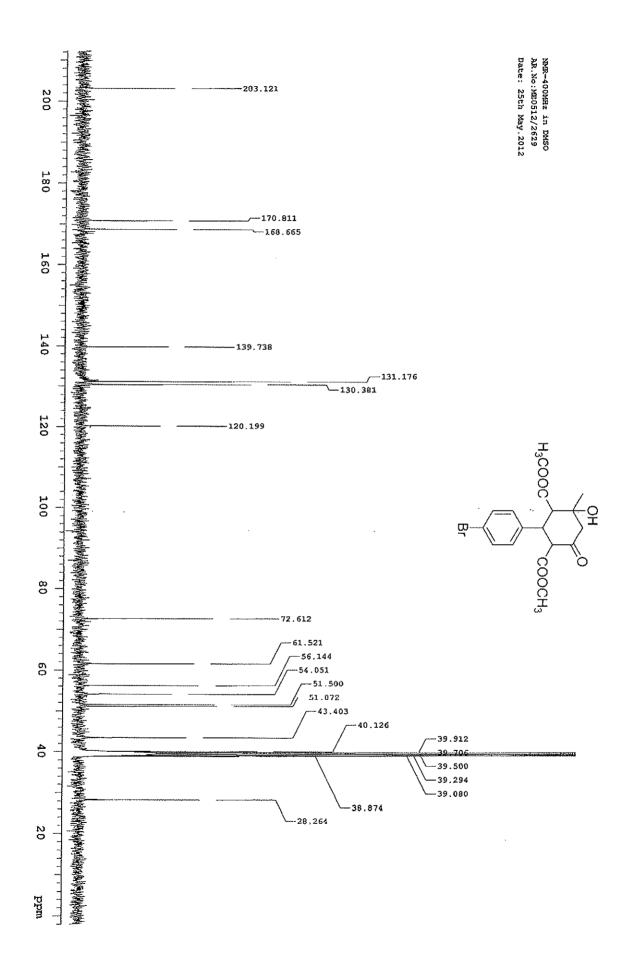


NMR-400MHz in CDC13 AR.No:ME0812/465 Date: 6th Sept 2012









Mass

5.0 mDa -0.3

5 0

399.0440

399.0443 Calc. Mass

-0.8 Mad

7.5 DBE

υτ 00

C17 H20

8

뫄

i-FIT

Formula

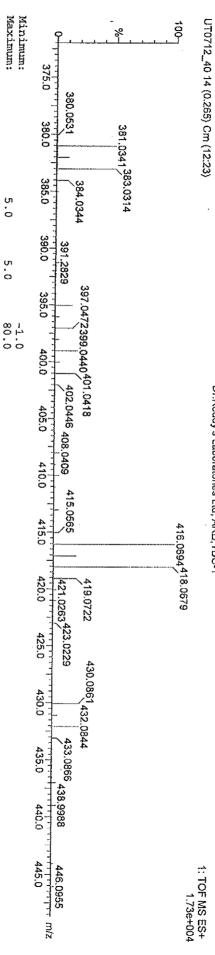
# **Elemental Composition Report**

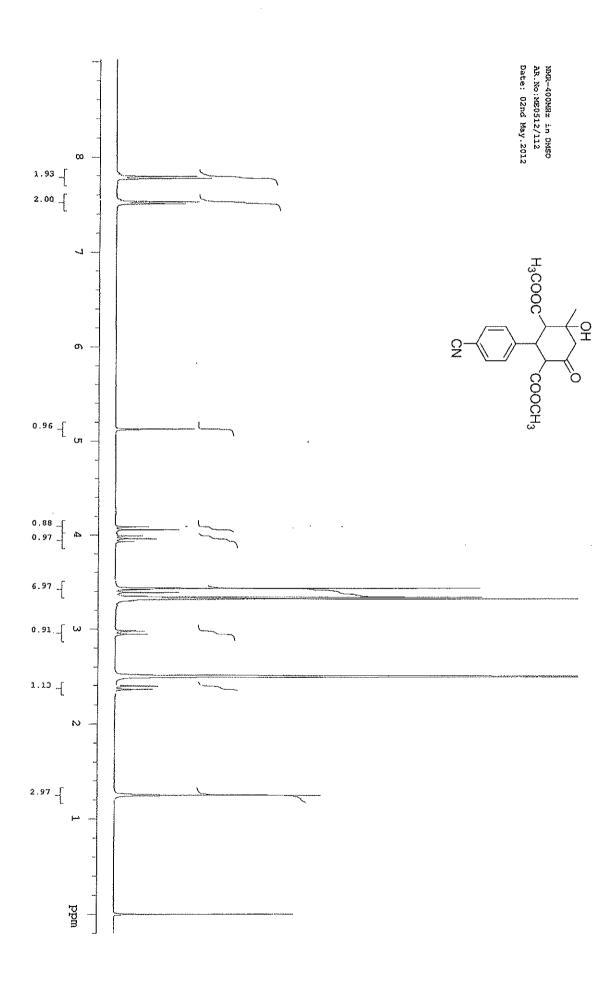
Element prediction: Off Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0 Number of isotope peaks used for i-FIT = 3

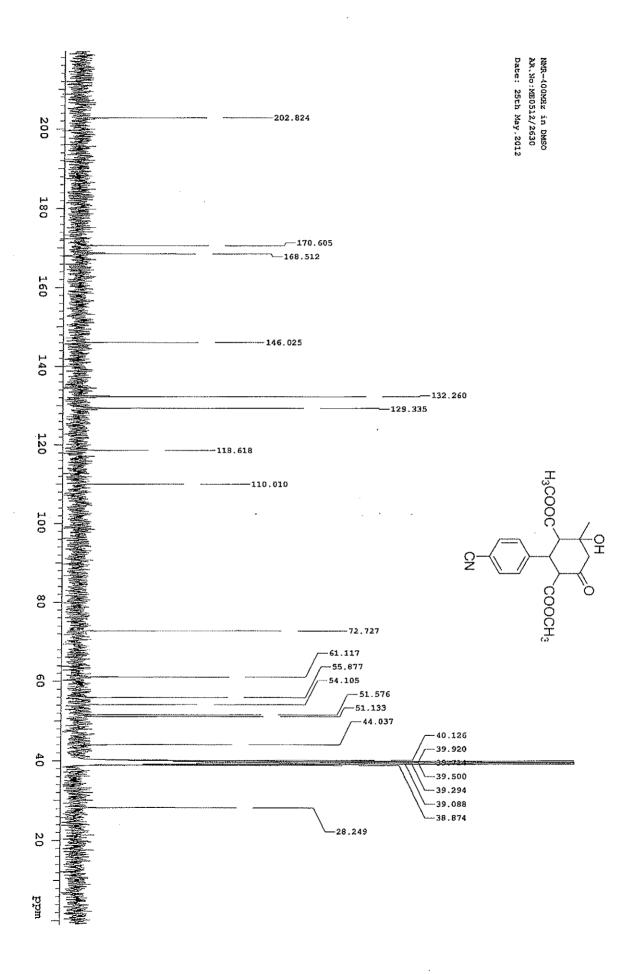
Monoisotopic Mass, Even Electron Ions 38 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)

Elements Used: C: 0-25 H: 0-25 O: 0-6 Br: 0-2

Dr.Reddy's Laboratories Ltd, ARD, TDC-1







Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron lons
11 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used: C: 0-20 H: 0-20 N: 0-1 O: 0-6

UT0512\_050 3 (0.110) Cm (3:8)

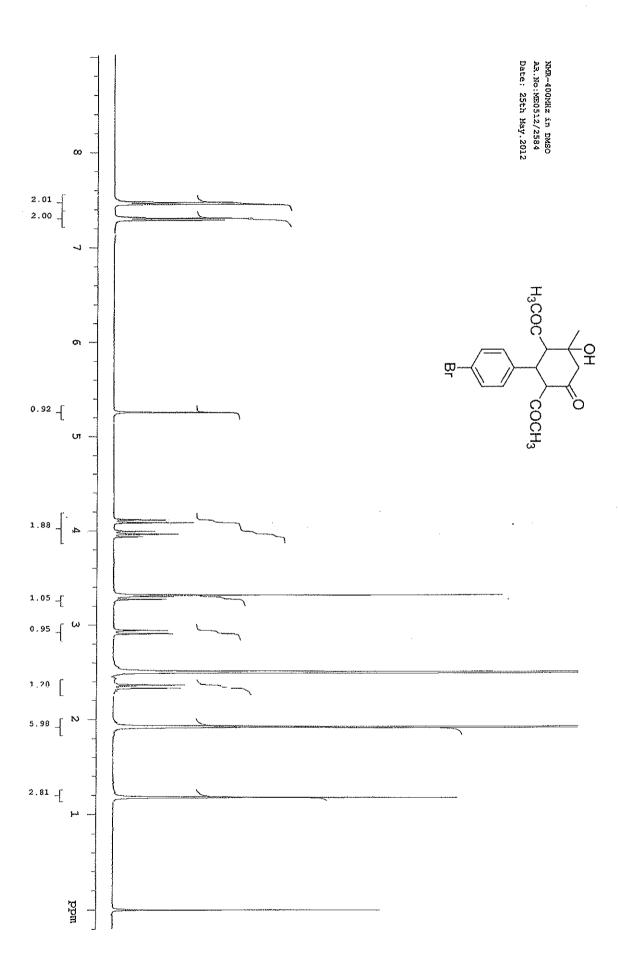
**100** 

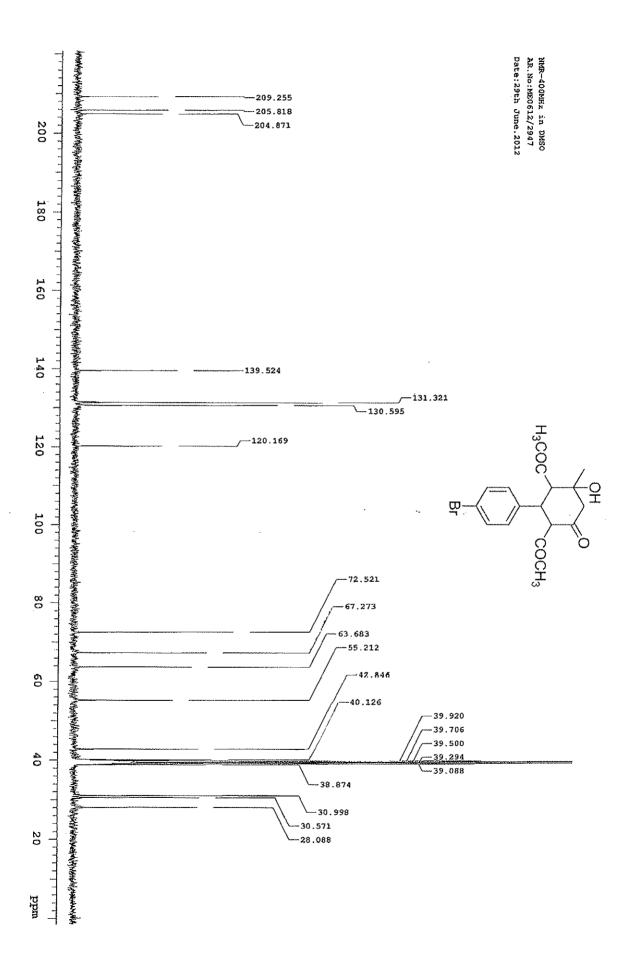
328,1193

Dr.Reddy's Laboratories Ltd, ARD, TDC-1

1: TOF MS ES+ 3.05e+003

Minimum: Maximum: 346.1292 Mass 310.0 314,1033 346.1291 Calc. Mass 315.0 317.0567 320.0 0.1 ្រ. 0 mDa 324.3156 325.05.0 0.3 Mdď 330.0 329,1215 335.0 9 5 -1.0 40.0DBE 337.1213 0.2 i-FIT 338,3428 340.0 342,1339 346,1292 348,1310 C18 H20 Formula 345.0 z 350.0 90 355,1299 355.0 360.1449 360.0 363,1577 365.0 370 



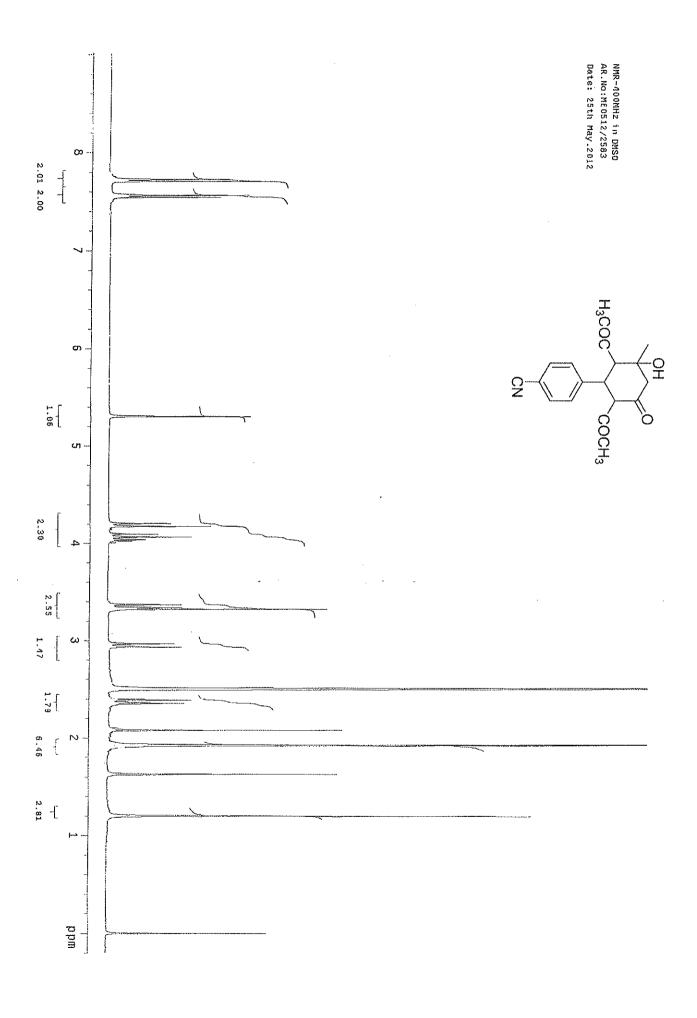


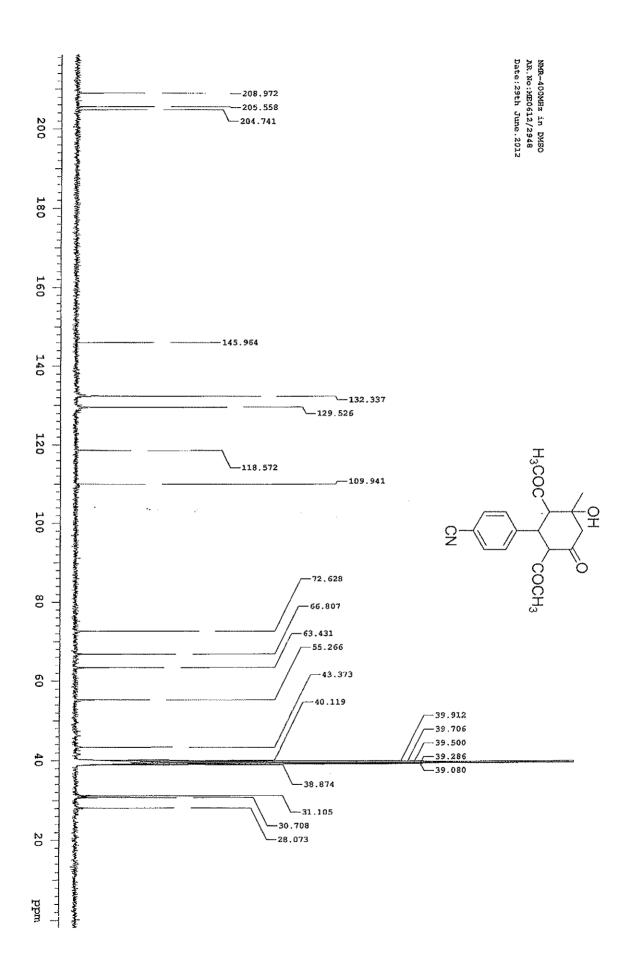
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0 Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Minimum: Maximum: Mass 367.0554 C: 0-25 H: 0-25 O: 0-6 Br: 0-2 Monoisotopic Mass, Even Electron lons
42 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used: UT0712\_38 20 (0.367) Cm (20:25) 340.0 340.1497 367.0545 Calc. Mass 345.0 348.0587 349.0458 351,0435 350.0 0.9 шDа 5.0 352.0462 353.0496 2.5 5.0 Maa 355.0 7.5 DBE -1.0 80.0 360.0 363.0606 2.0 i~FIT Dr.Reddy's Laboratories Ltd, ARD, TDC-1 367.0554 369.0569 C17 Formula H20 371.3174 04 375.0 ä 378.3906 380.0 381.0384 384.0835 386,0810 390.0725 390.0

1: TOF MS ES+ 1.44e+003





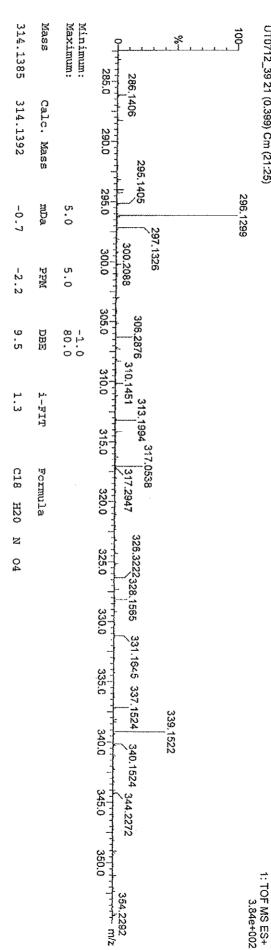
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0 Element prediction: Off

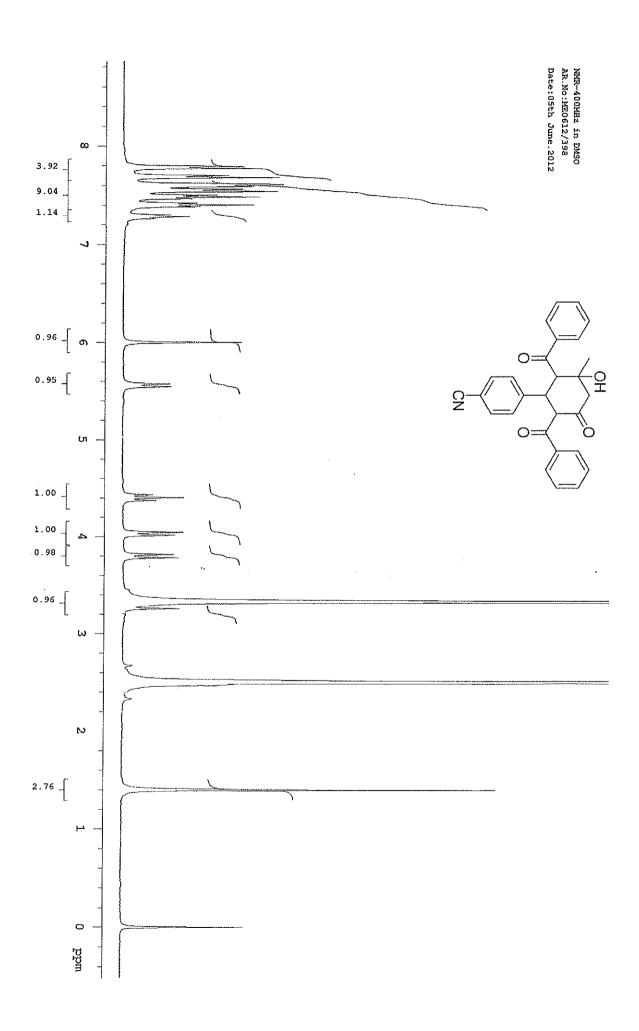
Monoisotopic Mass, Even Electron Ions 56 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass) Number of isotope peaks used for i-FIT = 3

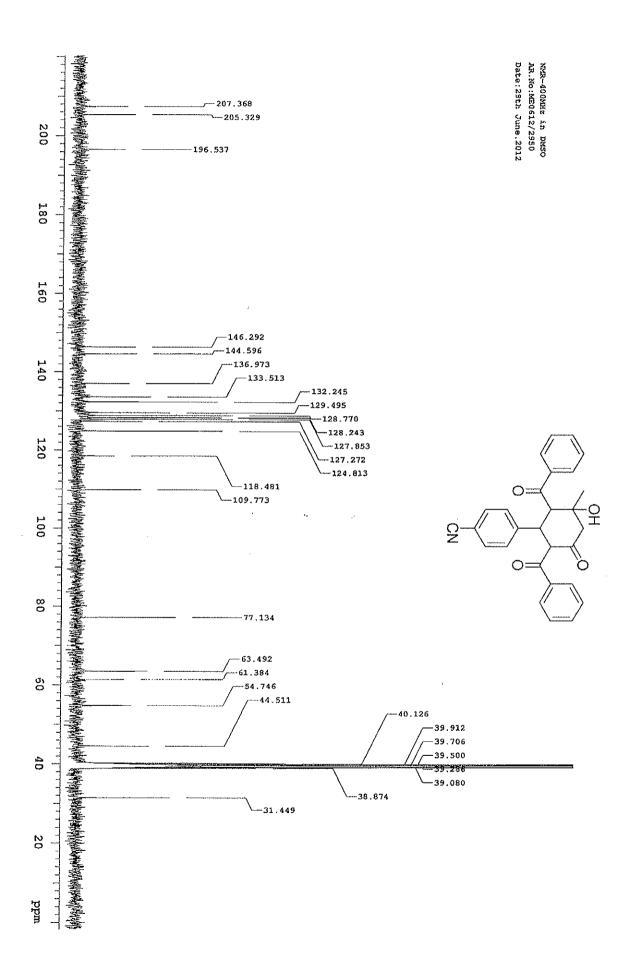
Elements Used: C: 0-30 H: 0-20 N: 0-5 C A786/CSAT1/066 UT0712\_39 21 (0.399) Cm (21:25)

0.05

Dr.Reddy's Laboratories Ltd, ARD,TDC-1







Mass

mDa ა. ი

Mad 5.0

438.1699

438.1705 Calc. Mass

-0.6

-1.4

17.5 DBE

Ω Ω i-FIT

C28 H24 Formula

z 04

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

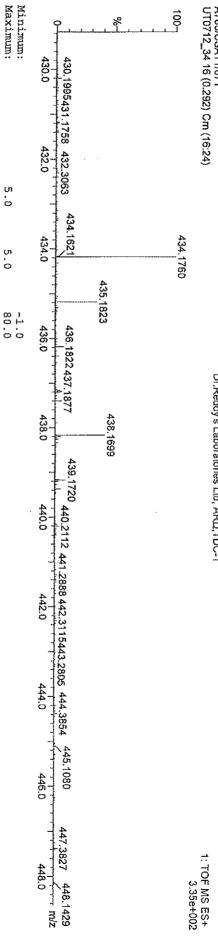
Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used: C: 0-30 H: 0-30 N: 0-2

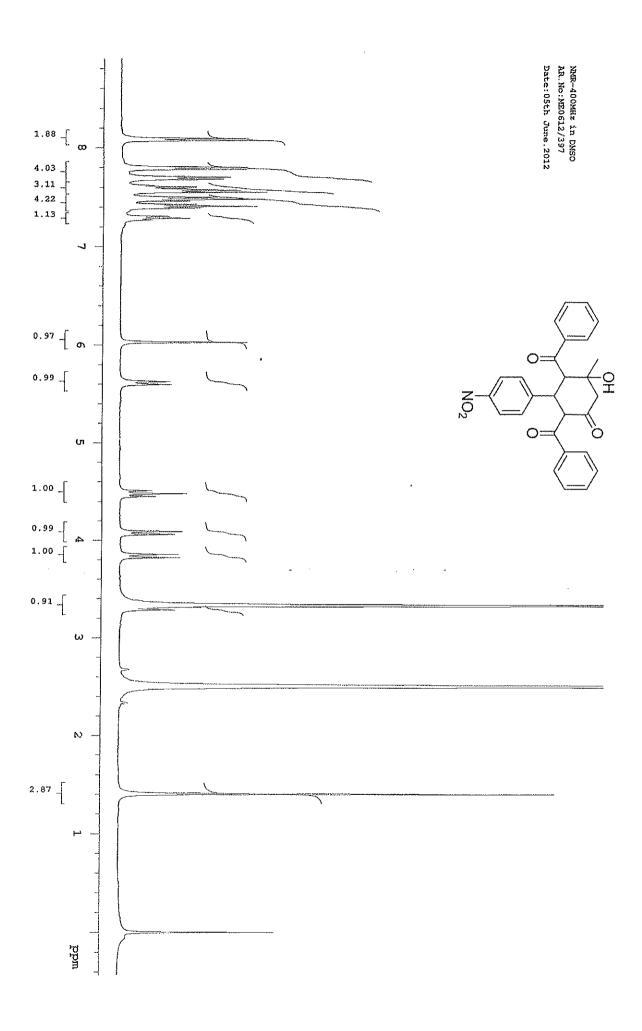
A786/CSAT1/071

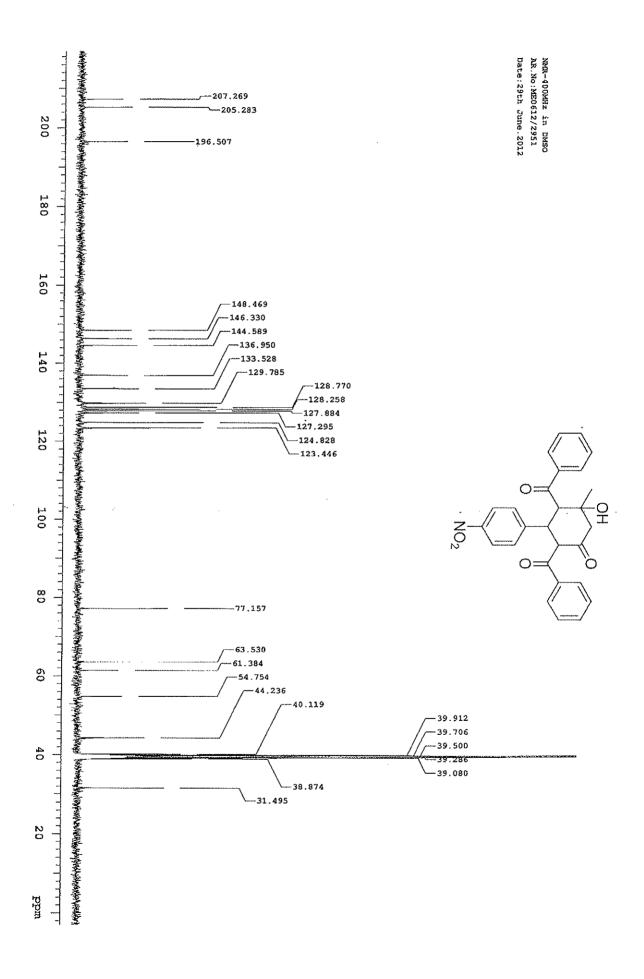
0:04

Dr.Reddy's Laboratories Ltd, ARD, TDC-1



Page 1





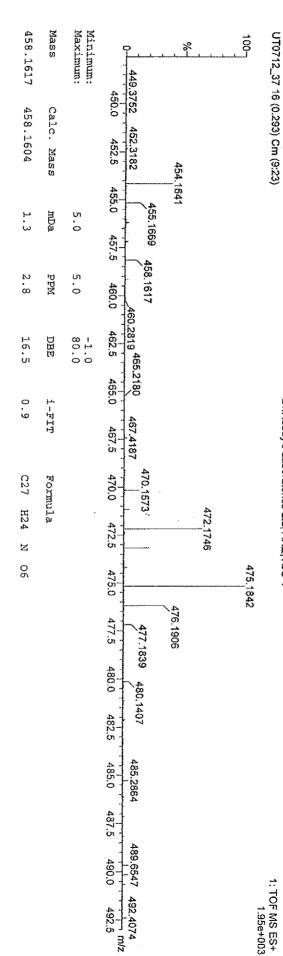
Element prediction: Off Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0

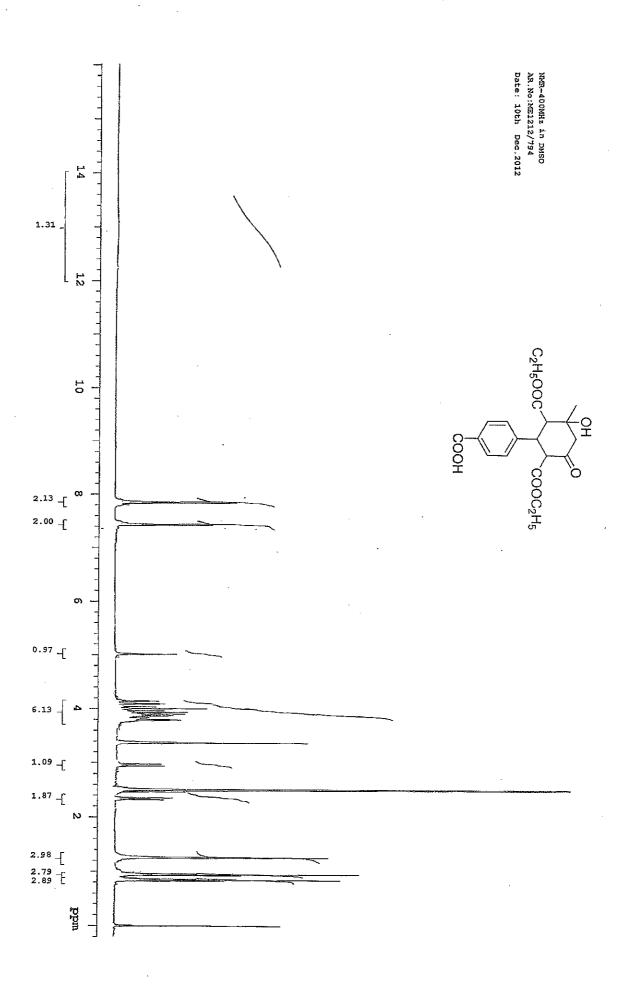
Number of isotope peaks used for i-FIT = 3

Elements Used: C: 0-30 H: 0-30 Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

N: 0-2 0:0-8

Dr.Reddy's Laboratories Ltd, ARD, TDC-1





Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

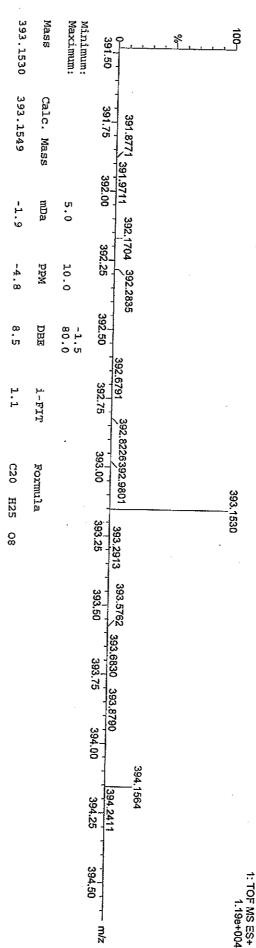
Number of isotope peaks used for i-FIT = 2

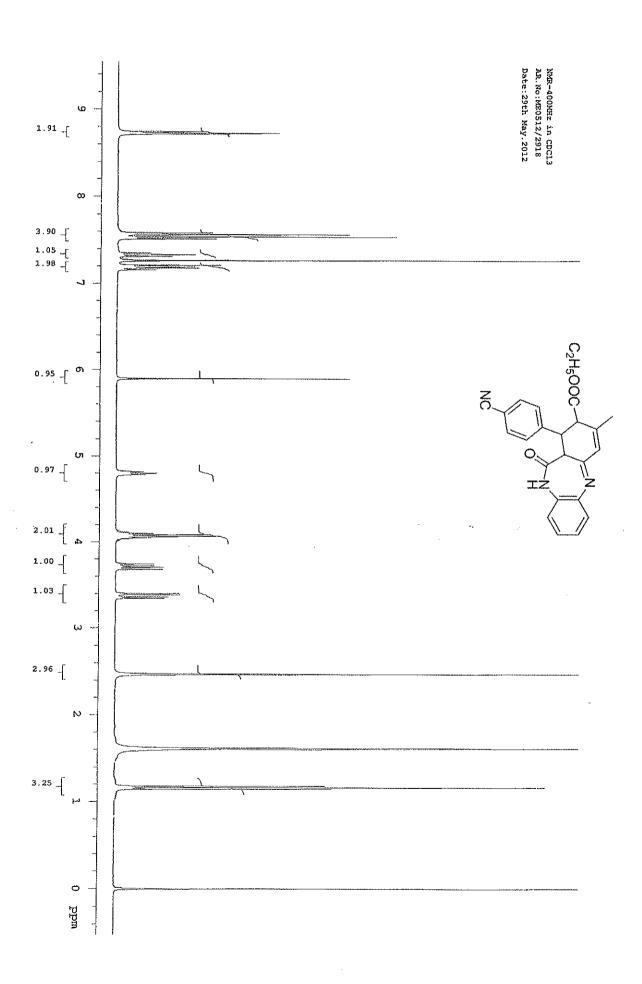
Monoisotopic Mass, Even Electron lons 29 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)

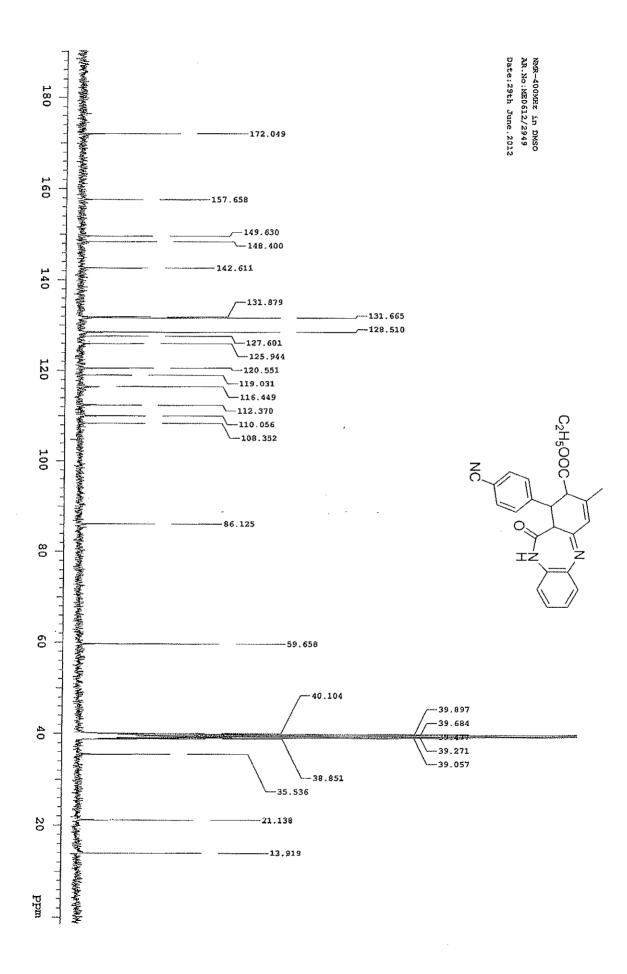
Elements Used: C: 0-22 H: 0-27 N: 0-1

0: 0-10

UT1212\_073 12 (0.420) Cm (12:17-48:52x0.010)







Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0 Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron lons 126 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used: C: 0-35 H: 0-40 N: 0-5

0:0-5

UT0712\_67 19 (0.353) Cm (19:22)

Dr.Reddy's Laboratories Ltd, ARD, TDC-1

Minimum: Maximum: Mass 400.1665 ş 171.1870 208.0404 175 400.1661 Calc. Mass 80 252,2441 250 0.4 mDa 5. O 275 276.0286308.2789 300 ڻ. 0 Mďď 325 350 354.1227 15.5 -1.0 DBE 375 400,1665 400 401.1713 402.1729 182.2 i-FIT 425 450 C24 H22 N3 Formula 475 5 501.2857 500 529,3183 525 င္သ 550 575 586.4118 621.1136 600 625 650 675 700 725 750 1: TOF MS ES+ 2.09e+004 z/m m/z

# SAMPLE INFORMATION

Sampel Type Unknow n System Acquired By

61 Date Acquired 10/3/2012 5:53:59 PM Injection Volume

10.00 uf Vial no Channel Name PDA 254.0 nm Run Time 40.00 Minutes Acq Method Set CHIRAL

HPLC 005 PDA System Name Date Processed 10/4/2012 11:57:20 AM 12100302 Sample Set Name Alliance\_005\_OCT\_2012

Project Name Injection# **Processing Method** Α

# HPLC CONDITIONS

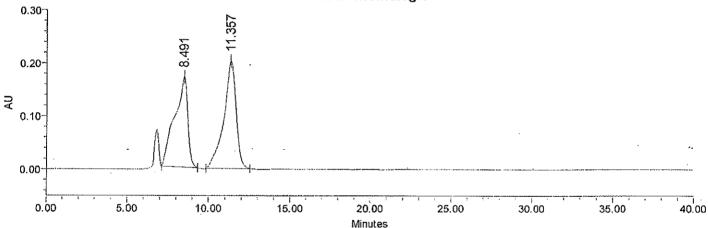
: chiral pak AD-H(250\*4.6)mm5µm Column : Ethanol:MeOH:DEA(800:200:1) Mobile phase

: 254.0 nm

Diluent : DCM Flow rate :0.5 mL/min, :27 °C, Inj vol:5µl Column temp Wavelength

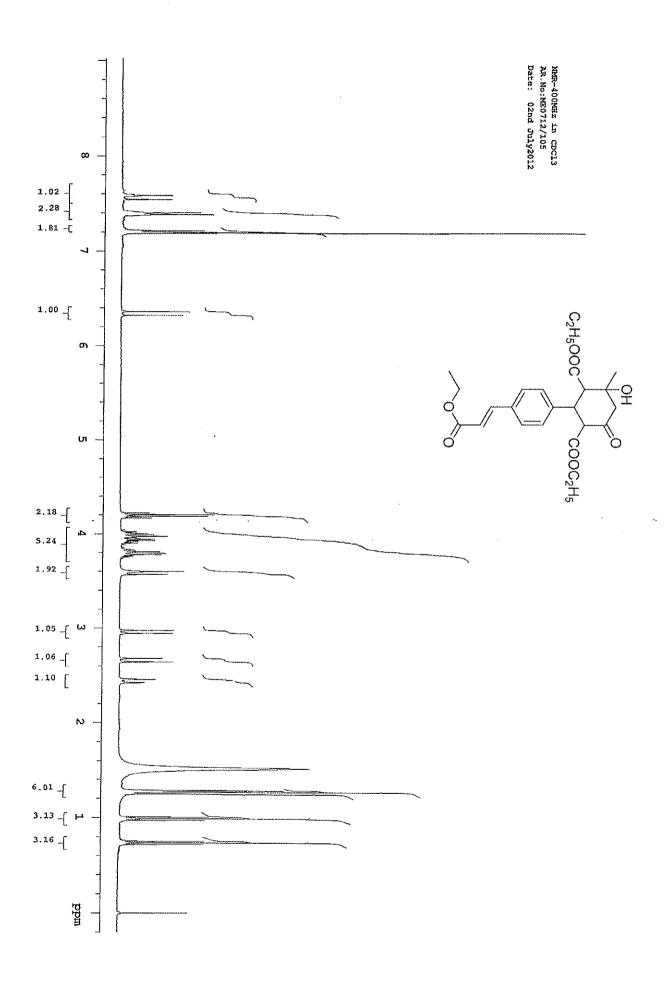
C<sub>2</sub>H<sub>5</sub>OOC

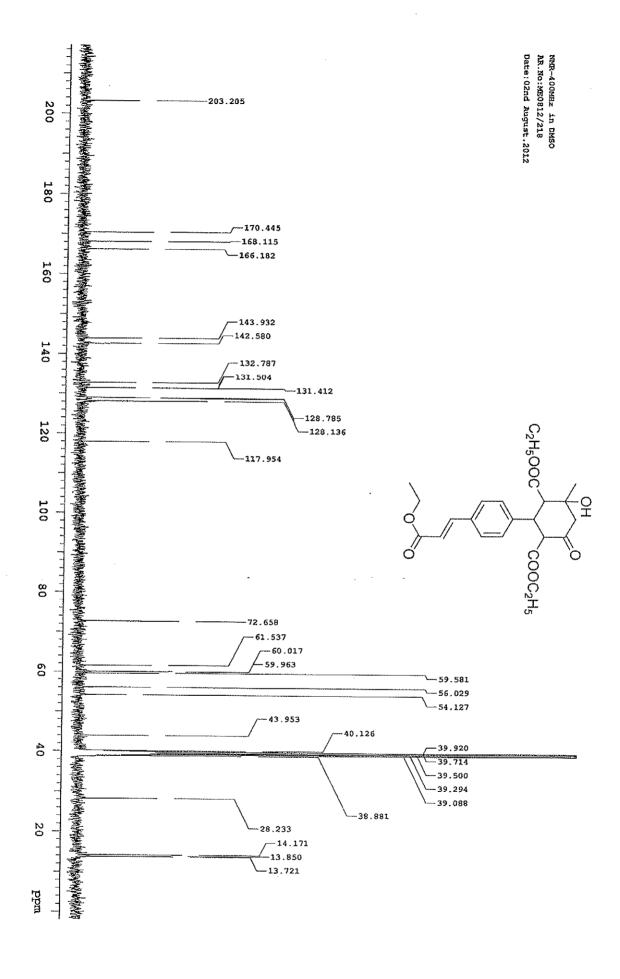
# **Auto-Scaled Chromatogram**



# Peak Results

	Name	RT	Area	% Area
1		8.491	9556836	47.57
2		11.357	10532450	52.43





Element prediction: Off

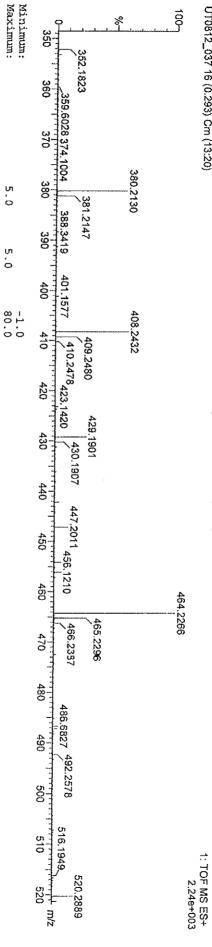
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron lons 57 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)

Elements Used: C: 0-50 H: 0-60 0:0-10

UT0812\_037 16 (0.293) Cm (13:20)

Dr.Reddy's Laboratories Ltd, ARD, TDC-1



Mass

Calc. Mass

mDa 0.8

447.2011

447.2019

-1.8 PPM

9.5 DBE

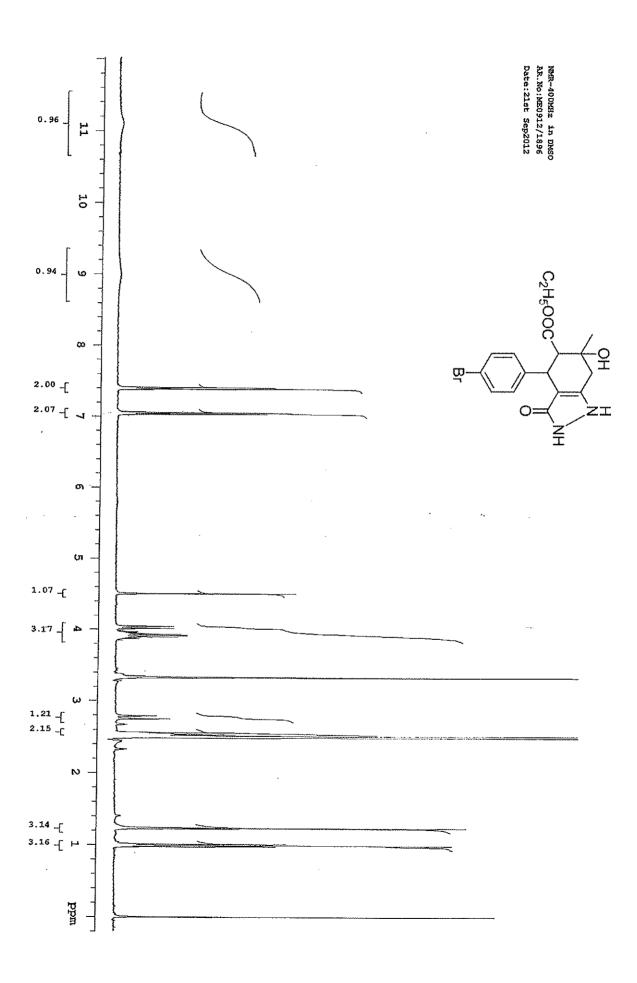
15.4 i-FIT

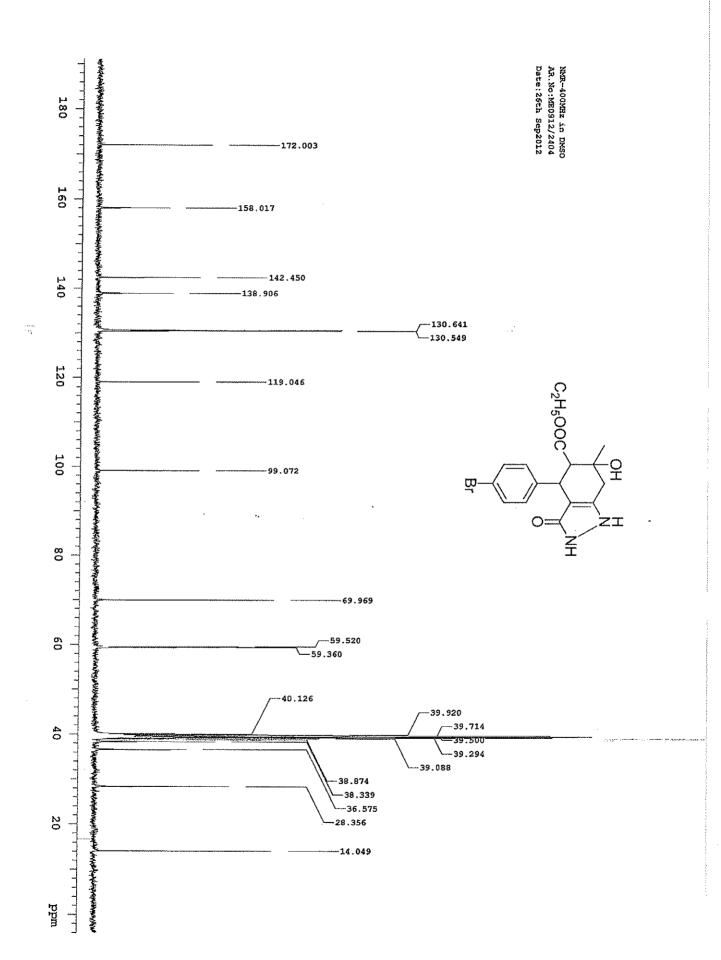
C24 H31 08

Formula

$$C_2H_5OOC$$
 $COOC_2H_5$ 

Page 1





395.0598

395,0606 Calc. Mass

-0.8 mDa

-2.0 PPM

& . . . DBE

0.8 i-FIT

C17 H20 Formula

z

Q 4

В

Mass

# **Elemental Composition Report**

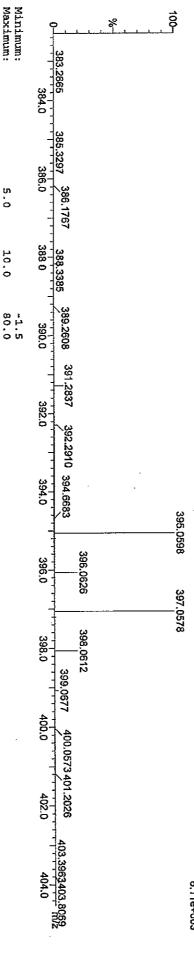
# Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 80.0 Element prediction: Off

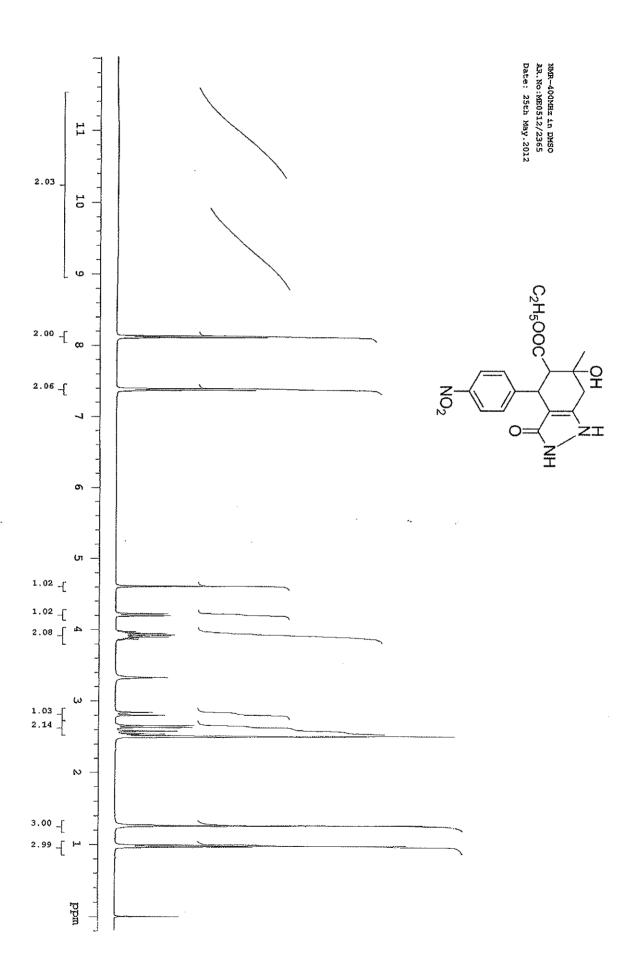
Number of isotope peaks used for i-FIT = 3

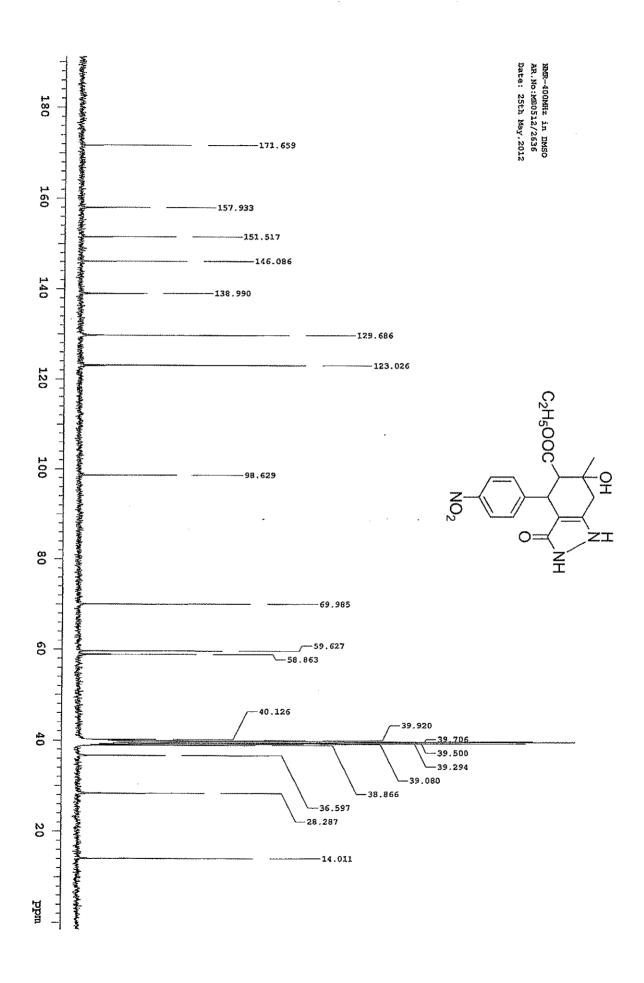
Monoisotopic Mass, Even Electron Ions 61 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass). Elements Used:
C: 0-20 H: 0-20 N: 0-4 O: 0-5 Br: 0-1

A786/CSAT2/084 UT1211\_036 25 (0.472) Cm (25:26-77:84x0.010) 주 주



₽-	- O=	C <sub>2</sub> H <sub>5</sub> OOC		2
	0=	≓ - ₹	Ž	1





Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 40.0
Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron lons 129 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used: C: 0-25 H: 0-30 N: 0-4 O: 0-10

UT0512\_031 37 (1.322) Cm (37:49)

9

362, 1356

Dr.Reddy's Laboratories Ltd, ARD, TDC-1

1: TOF MS ES+ 4.41e+003

Minimum: Maximum: Mass 362.1356 205,0862 223.0978 362.1352 Calc. Mass 279,1604 293.1767 шDа 5. O 0.4 بر 1 Mad 5.0 352,3398 9.5 40.0 DBE 360 380 391.2856 |392.2876 2.0 i-FTT 400 420 C17 H20 N3 Formula 429.2430454.2800 494.8012 536.0615 552.0587 567.3123.593.1442 440 460 480 90 500 520 E 540

560

580 600 62

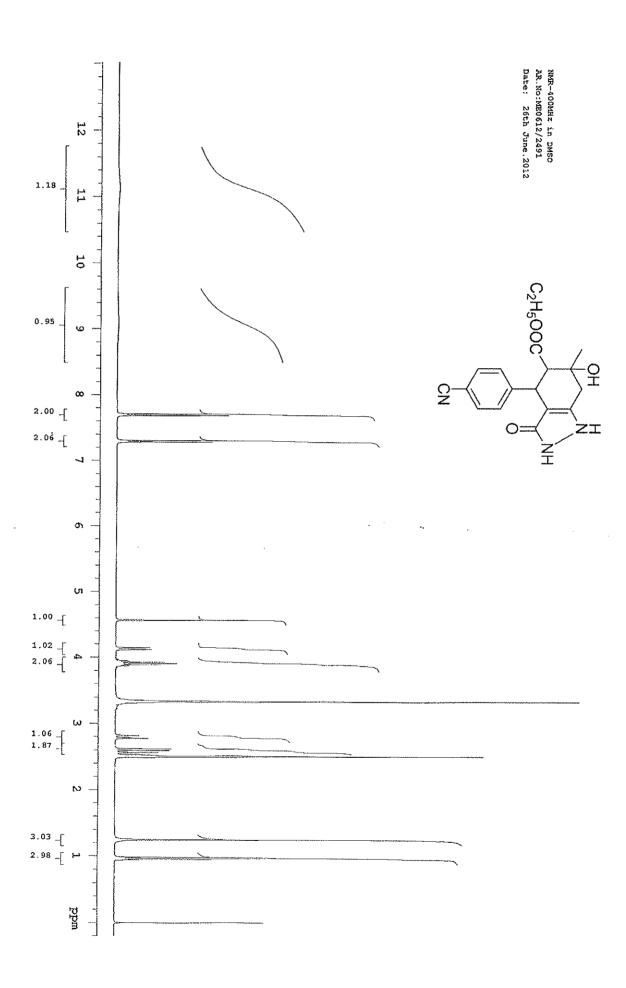
620

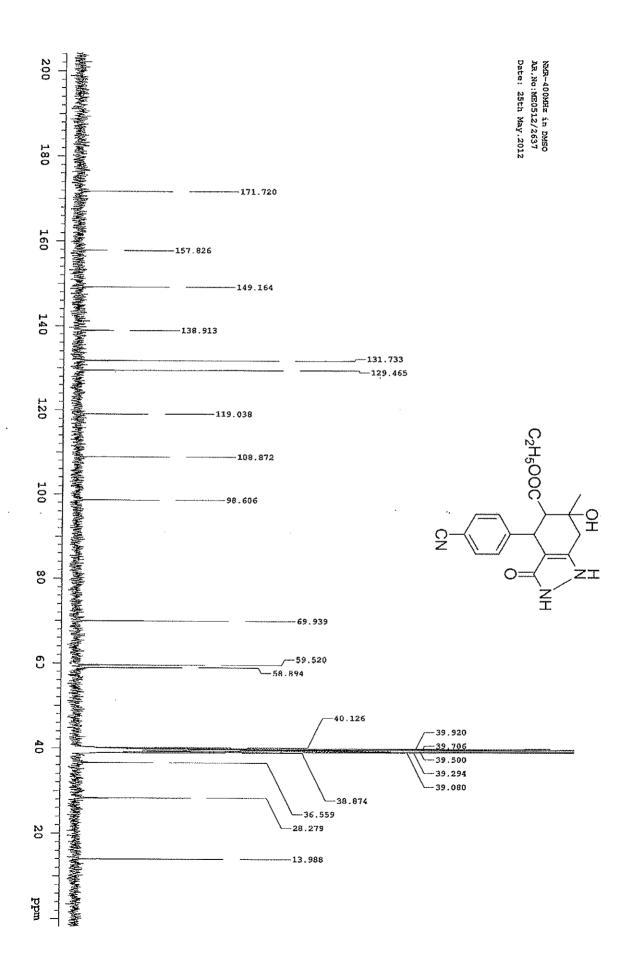
640

660

677.4978 m/z

Page 1





Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 40.0 Element prediction; Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
138 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used: C: 0-25 H: 0-30 N: 0-4 O: 0-10

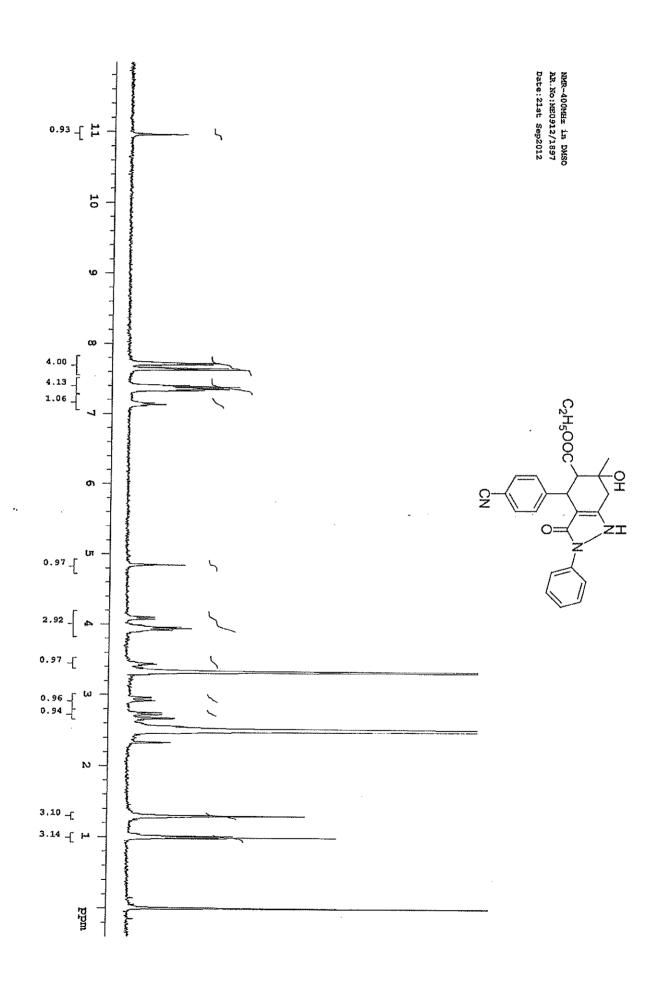
UT0512\_030 32 (1.123) Cm (29:38)

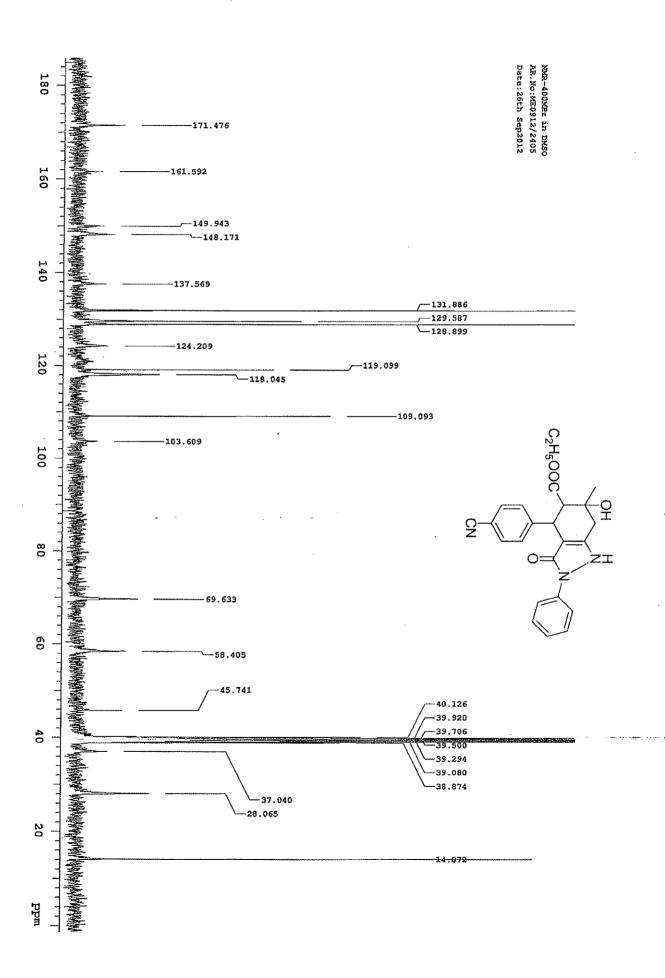
Dr.Reddy's Laboratories Ltd, ARD, TDC-1

1: TOF MS ES+ 7.00e+003

342.1448

Minimum: Maximum: Mass 342.1448 <u>5</u> 205,0863 342.1454 Calc. Mass 220 223.0947 240 260 276.0251 mDa ຫ • -0.6 279,1602 280 280,1638 300 Mad 5.0 321 1328 320 10.5 DBE -1.0 40.0 340 343.1487 0.1 360 J-FIT 380 391.2858 392.2888 C18 H20 N3 Formula 429.2387.437.4311.473.4105.484.0758 400 420 440 460 480 500 04 520,4247 532,0528 520 540 58 560 900 4.1. ut.:. u/z





Number of isotope peaks used for i-FIT = 3 Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5 max = 80.0
Element prediction: Off

Monoisotopic Mass, Even Electron Ions
27 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-26 H: 0-26 N: 0-4 O: 0-5

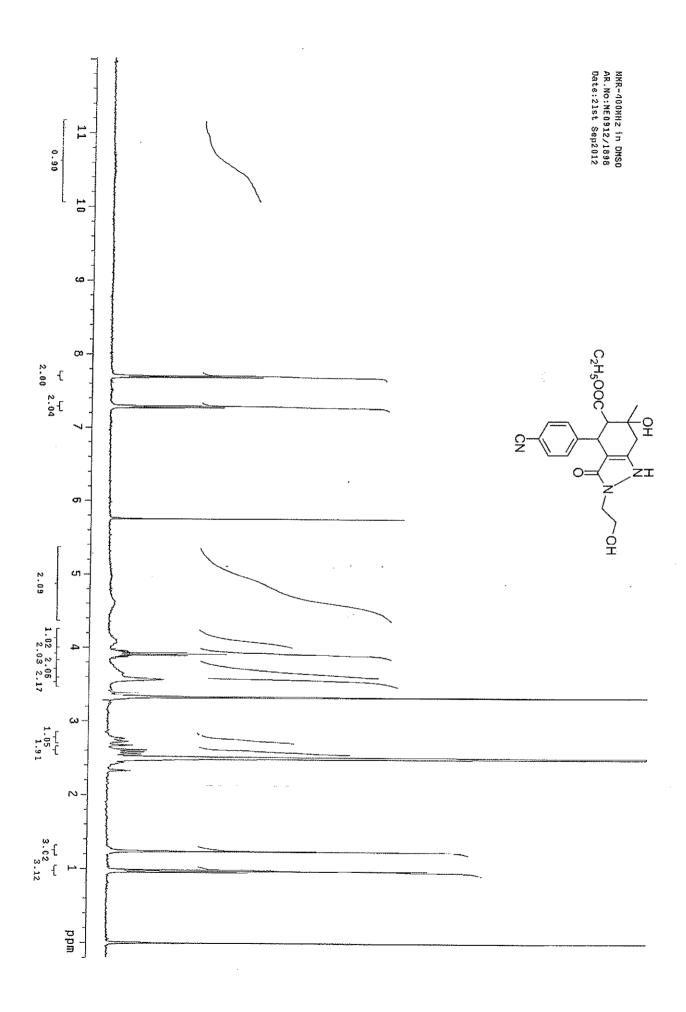
UT1211\_037 16 (0.292) Cm (14:18-49:56x0.010)

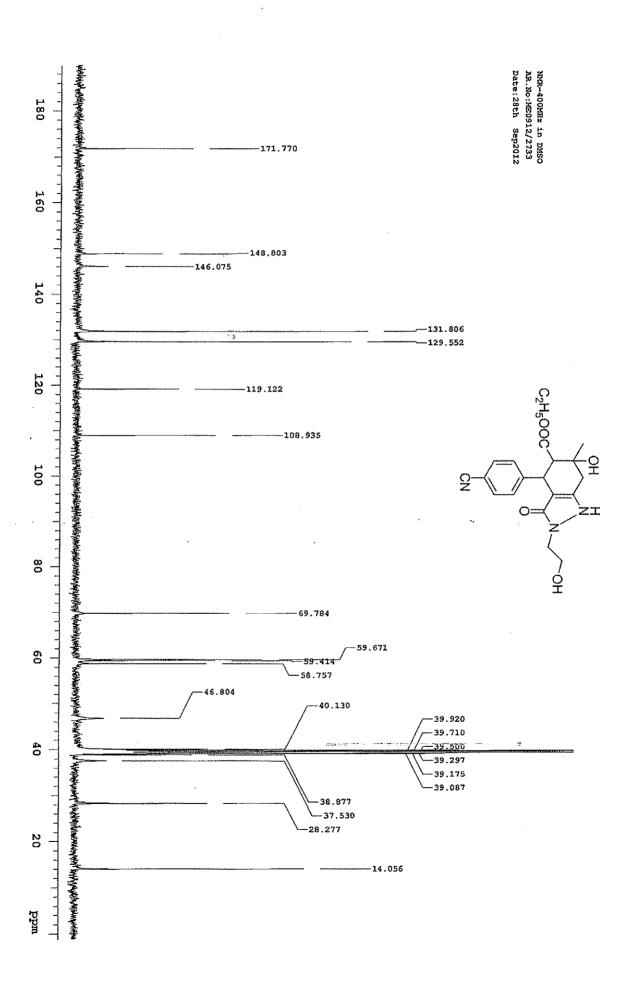
418.1752

Minimum: Maximum: Mass 418.1752 8 400.0 400.1665 403.1991 .0 405.0 418.1767 Calc. Mass 410.0 -1.5 m Da 5.0 415.2148 417.7182 MAA <u>-3</u>.6 20.0 -1.5 80.0 14.5 DBE 418.2180 420.0 419.2253 419,1812 420.2230,423.387 26.9 i-FIT 425.0 Formula C24 H24 N3 O4 430.0 440,0 444.3331 447.3558 445.0

454.3011

1: TOF MS ES+ 1.12e+005





C<sub>2</sub>H<sub>5</sub>OOC

# **Elemental Composition Report**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
45 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-26 H: 0-26 N: 0-4 O: 0-5

UT1211\_038 18 (0.340) Cm (18:22-52:76x0.010)

