

Supporting Information

for

Synthesis of enantiomerically pure *N*-(2,3-dihydroxypropyl)arylamides via oxidative esterification

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Analytical data and NMR, MS and IR spectra

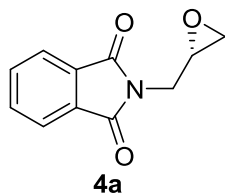
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Section A: General Information

All reagents were used as received from commercial sources without further purification or prepared as described in the literature. Reactions were stirred using Teflon-coated magnetic stirring bars. Spots on TLC plates were visualized by ultraviolet light or by treatment with a spray of Pancaldi reagent $\{(\text{NH}_4)_6\text{MoO}_4, \text{Ce}(\text{SO}_4)_2, \text{H}_2\text{SO}_4, \text{H}_2\text{O}\}$. Chromatographic purification of products was carried out by flash column chromatography on silica gel (60–120 mesh). Melting points were determined using an electrothermal melting point apparatus and are uncorrected. Infrared spectra were recorded on a Perkin-Elmer 1650 Fourier transform spectrometer. NMR spectra were measured in CDCl_3 or methanol- d_4 (with TMS as internal standard) on a Varian Gemini 400 MHz FT NMR spectrometer magnetic resonance spectrometer. Chemical shifts (δ) are reported in ppm, and coupling constants (J) are in Hz. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Mass spectra were recorded on an HP-5989A quadrupole mass spectrometer

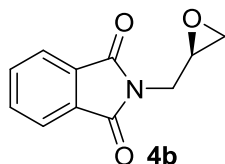
Section B: Analytical

(S)-2-(oxiran-2-ylmethyl)isoindoline-1,3-dione (4a):



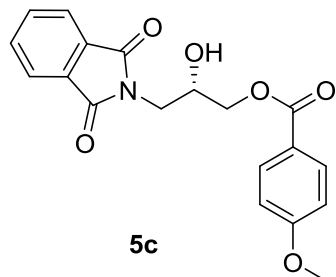
Crystalline solid, Mp. 102-103.5°C, IR (KBr): 3460, 3007, 1769, 1713, 1396, 1308, 1049, 961, 724. ¹H NMR (400 MHz, CDCl₃) δ: 2.68-2.70 (m, 1H), 2.80-2.82 (m, 1H), 3.22-3.26 (m, 1H), 3.78-3.83 (m, 1H), 3.94-3.99 (m, 1H), 7.75 (dd, *J* = 2.8 Hz, 2H), 7.86 (dd, *J* = 3.2 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃): 39.5, 46.0, 48.9, 123.3, 131.8, 134.0 and 167.8. HPLC: (Chiral PAK-1A (250x4.6mm, column 5.0u), 1.0 ml/min, 220 nm, *n*-hexane/IPA 80:20, Ambient, 5 μL, retention times: 22.35 min, 99.2% ee. Specific Optical Rotation: [α]_D²⁵ = 9.0° (c 2.241, Methanol)

(R)-2-(oxiran-2-ylmethyl)isoindoline-1,3-dione (4b):



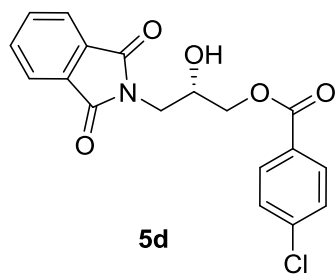
Crystalline solid, Mp. 101.7-103.5 °C, IR (KBr): 3461, 3006, 1770, 1714, 1398, 1398, 1041, 910, 724, ¹H NMR (400 MHz, CDCl₃) δ: 2.68-2.70 (m, 1H), 2.80-2.82 (m, 1H), 3.22-3.26 (m, 1H), 3.78-3.80 (m, 1H), 3.94-3.99 (m, 1H), 7.75 (dd, *J* = 2.8 Hz, 2H), 7.86 (dd, *J* = 3.2 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃): 39.5, 46.0, 48.9, 123.3, 131.8, 134.0 and 167.8. HPLC: (Chiral PAK-1A (250x4.6mm, column 5.0u), 1.0 ml/min, 220 nm, *n*-hexane/IPA 80:20, Ambient, 5 μL, retention times: 22.35 min, 99.6% ee. Specific Optical Rotation: [α]_D²⁵ = -9.1° (c 2.241, Methanol)

(S)-3-(1,3-dioxoisindolin-2-yl)-2-hydroxypropyl 4-methoxybenzoate (5c):



Viscous liquid. yield: (63%). IR (KBr): 756, 1031, 1261, 1395, 1606, 1718, 1774, 3019, cm^{-1} . ^1H NMR (400 MHz, CDCl_3) δ : 3.28 (s, 1H, OH), 3.75 (s, 3H, CH_3), 3.84-3.87 (m, 2H, CH_2), 4.21-4.25 (m, 1H, CH), 4.27-4.29 (m, 2H, CH_2), 6.82 (d, $J = 9.2$ Hz, 2H, ArH), 7.60-7.61 (m, 2H, ArH), 7.72-7.73 (m, 2H, ArH), 7.90 (d, $J = 8.8$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl_3) = 41.2, 55.3, 66.0, 68.3, 113.6, 121.9, 133.3, 131.6, 131.8, 134.0, 163.4, 166.1, 168.5. MS: $m/z = 356$ [$M + 1$], HRMS: Calc. Mass: 356.1570, found 356.1574, Molecular Formula. $\text{C}_{19}\text{H}_{18}\text{NO}_6$, HPLC: (Chiral PAK-1A (250x4.6mm, column 5.0u), 1.0 ml/min, 220 nm, *n*-hexane/IPA 80:20, Ambient, 5 μL , retention times: 22.35 min, 96.6% ee. Specific Optical Rotation: $[\alpha]_{\text{D}}^{25} = -10.54^\circ$ (c 1.04, Methanol)

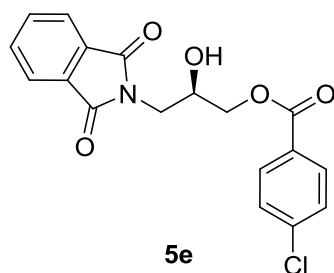
(S)-3-(1,3-dioxoisindolin-2-yl)-2-hydroxypropyl 4-chlorobenzoate (5d):



Crystalline solid. yield: (65%). IR (KBr): 722, 760, 1013, 1090, 1271, 1398, 1593, 1699, 1772, 2934, 3474 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) δ : 2.9 (s, 1H, OH), 3.9 (d, $J = 5.6$ Hz, 2H, CH_2), 4.30-4.32 (m, 1H, CH), 4.39 (d, $J = 4.8$ Hz, 2H, CH_2), 7.42 (d, $J = 4.8$ Hz, 2H,

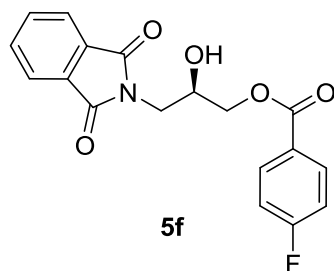
ArH), 7.74-7.75 (m, 2H, ArH), 7.85-7.86 (m, 2H, ArH), 7.99 (d, $J = 8.8$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl_3) = 41.3, 66.3, 68.5, 123.5, 128.0, 128.8, 131.1, 131.8, 134.3, 139.7, 165.6, 168.7. MS: $m/z = 360$ [$M + 1$], HRMS: Calc. Mass: 360.0639, found : 360.0635, Molecular Formula. $\text{C}_{18}\text{H}_{15}\text{NO}_5\text{Cl}$, HPLC: (Chiral PAK-1A (250x4.6mm, column 5.0u), 1.0 ml/min, 220 nm, n -hexane: IPA:: 80:20, Ambient, 5 μL , retention times: 23.05 min, 98.2% ee. Specific Optical Rotation: $[\alpha]_{\text{D}}^{25} = -0.05^\circ$ (c 1.00, Methanol)

(R)-3-(1,3-dioxoisindolin-2-yl)-2-hydroxypropyl 4-chlorobenzoate (5e):



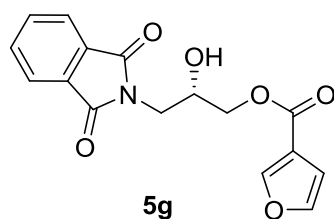
Crystalline solid: yield: (65%). IR (KBr): 721, 755, 1014, 1090, 1272, 1392, 1710, 1731, 1777, 2911, 3503 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) δ : 2.9 (s, 1H, OH), 3.9 (d, $J = 5.6$ Hz, 2H, CH_2), 4.30-4.32 (m, 1H, CH), 4.39 (d, $J = 4.8$ Hz, 2H, CH_2), 7.42 (d, $J = 4.8$ Hz, 2H, ArH), 7.74-7.75 (m, 2H, ArH), 7.85-7.86 (m, 2H, ArH), 8.0 (d, $J = 8.8$ Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl_3) = 41.4, 66.4, 68.5, 123.5, 128.1, 128.7, 131.1, 131.8, 134.2, 139.7, 165.5, 168.6. MS: $m/z = 360$ [$M + 1$] HRMS: Calc. Mass: 360.0639, found : 360.0635, Molecular Formula. $\text{C}_{18}\text{H}_{15}\text{NO}_5\text{Cl}$, HPLC: (Chiral PAK-1A (250x4.6mm, column 5.0u), 1.0 ml/min, 220 nm, n -hexane/IPA 80:20, Ambient,: 5 μL , retention times: 21.72 min, 99% ee Specific Optical Rotation: $[\alpha]_{\text{D}}^{25} = +0.05$ (c 1.00, Methanol).

(R)-3-(1,3-dioxisoindolin-2-yl)-2-hydroxypropyl 4-fluorobenzoate (5f):



Crystalline solid: yield: (64%). IR (KBr): 951, 1071, 1274, 1604, 1700, 1718, 2997, 3478 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) δ : 2.96 (d, J = 5.2 Hz, 1H, OH), 3.97 (d, J = 5.6 Hz, 2H, CH_2), 4.29-4.33 (m, 1H, CH_2), 4.39 (d, J = 4.8 Hz, 2H, CH_2), 7.09-7.12 (m, 2H, ArH), 7.73-7.75 (m, 2H, ArH), 7.85-7.87 (m, 2H, ArH), 8.09 (d, J = 5.6 Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl_3) = 41.3, 66.2, 68.5, 115.5, 115.7, 123.5, 131.8, 132.2, 132.3, 134.2, 165.4, 168.7. MS: m/z = 344 [$M + 1$]. HRMS: Calc. Mass: 344.0934, found : 344.0928. Molecular Formula. $\text{C}_{18}\text{H}_{15}\text{NO}_5\text{F}$. HPLC: (Chiral PAK-1A (250x4.6mm, column 5.0u), 1.0 ml/min, 220 nm, *n*-hexane/IPA 80:20, Ambient,: 5 μL , retention times: 22.63 min, 98.1% ee Specific Optical Rotation: $[\alpha]_{\text{D}}^{25} = +4.08^\circ$ (c 1.02, Methanol).

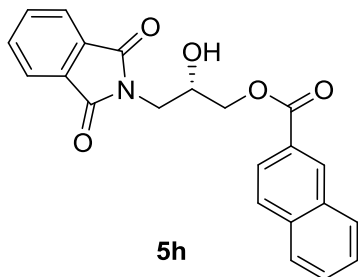
(S)-3-(1,3-dioxisoindolin-2-yl)-2-hydroxypropyl furan-3-carboxylate (5g):



Crystalline solid: yield: (60%). IR (KBr): 761, 1030, 1173, 1309, 1431, 1576, 1706, 1763, 3143, 3384 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) δ : 3.09 (s, 1H, OH), 3.93-3.94 (m, 2H, CH_2), 4.27-4.29 (m, 1H, CH), 4.33-4.34 (m, 2H, CH_2), 6.75 (d, 1H, ArH), 7.42 (s, 1H, ArH), 7.72-7.73 (m, 2H, ArH), 7.85-7.87 (m, 2H, ArH), 8.09 (d, 1H, ArH). ^{13}C NMR (100 MHz, CDCl_3) = 41.2, 65.7, 68.4, 109.7, 118.7, 123.4, 131.7, 134.2, 143.7, 148.1, 162.8,

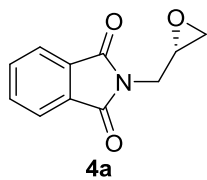
168.6. MS: $m/z = 316$ $[M + 1]$, HRMS: Calc. Mass: 316.0821, found :344.0826, Molecular Formula. $C_{16}H_{14}NO_6$. HPLC: (Chiral PAK-1A (250x4.6 mm, column 5.0u), 1.0 ml/min, 220 nm, *n*-hexane/IPA 80:20, Ambient,: 5 μ L, retention times: 19.99 min, 99.2% ee Specific Optical Rotation: $[\alpha]_D^{25} = -9.49^\circ$ (c 1.02, Methanol).

(S)-3-(1,3-dioxisoindolin-2-yl)-2-hydroxypropyl 2-naphthoate (5h):



Viscous liquid: yield: (59%). IR (KBr): 780.2, 1096, 1282, 1394, 1467, 1712, 1772, 3467, cm^{-1} . 1H NMR (400 MHz, $CDCl_3$) δ : 3.12 (d, $J = 4.4$ Hz, 1H, OH), 4.02 (d, $J = 4.4$ Hz, 2H, CH_2), 4.37-4.39 (m, 1H, CH), 4.48 (d, $J = 4.8$ Hz, 2H, CH_2), 7.54-7.59 (m, 2H, ArH), 7.70-7.71 (m, 2H, ArH), 7.83-7.87 (m, 4H, ArH), 7.95 (d, $J = 8$ Hz, 1H, ArH), 8.06 (d, $J = 8.8$ Hz, 1H, ArH), 8.61 (s, 1H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$) = 41.1, 66.4, 68.1, 123.2, 125.0, 126.4, 126.7, 127.5, 128.0, 128.2, 129.2, 131.1, 131.6, 132.2, 133.9, 135.4, 166.4, 168.5. MS: $m/z = 376$ $[M + 1]$, HRMS: Calc. Mass :376.1185, found: 376.1167, Molecular Formula. $C_{22}H_{18}NO_5$

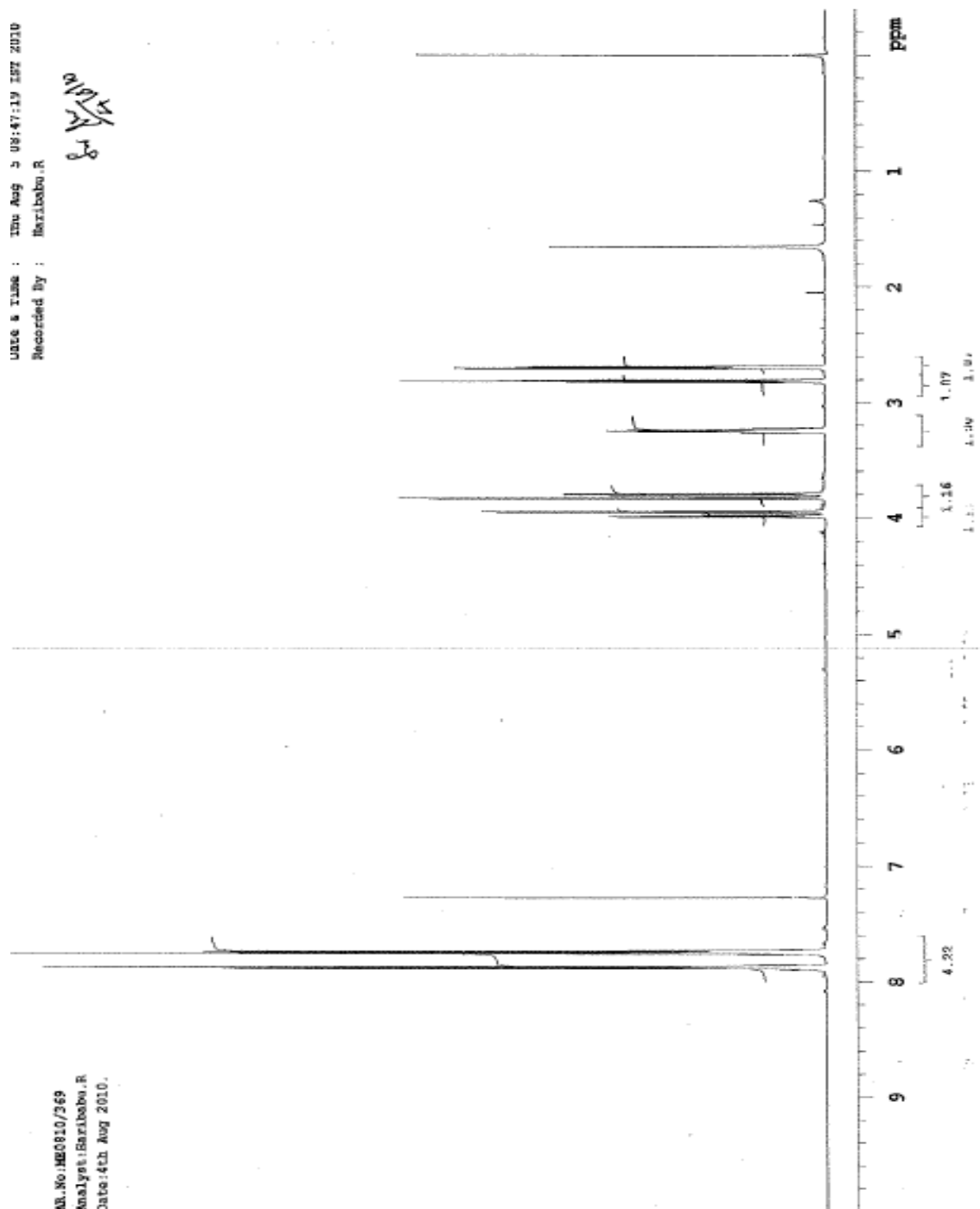
Section C: ^1H , ^{13}C NMR, Mass and IR spectra

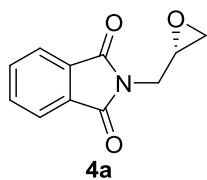


DATE & TIME : Thu Aug 5 08:47:19 EST 2010
Recorded by : Baribabu.R

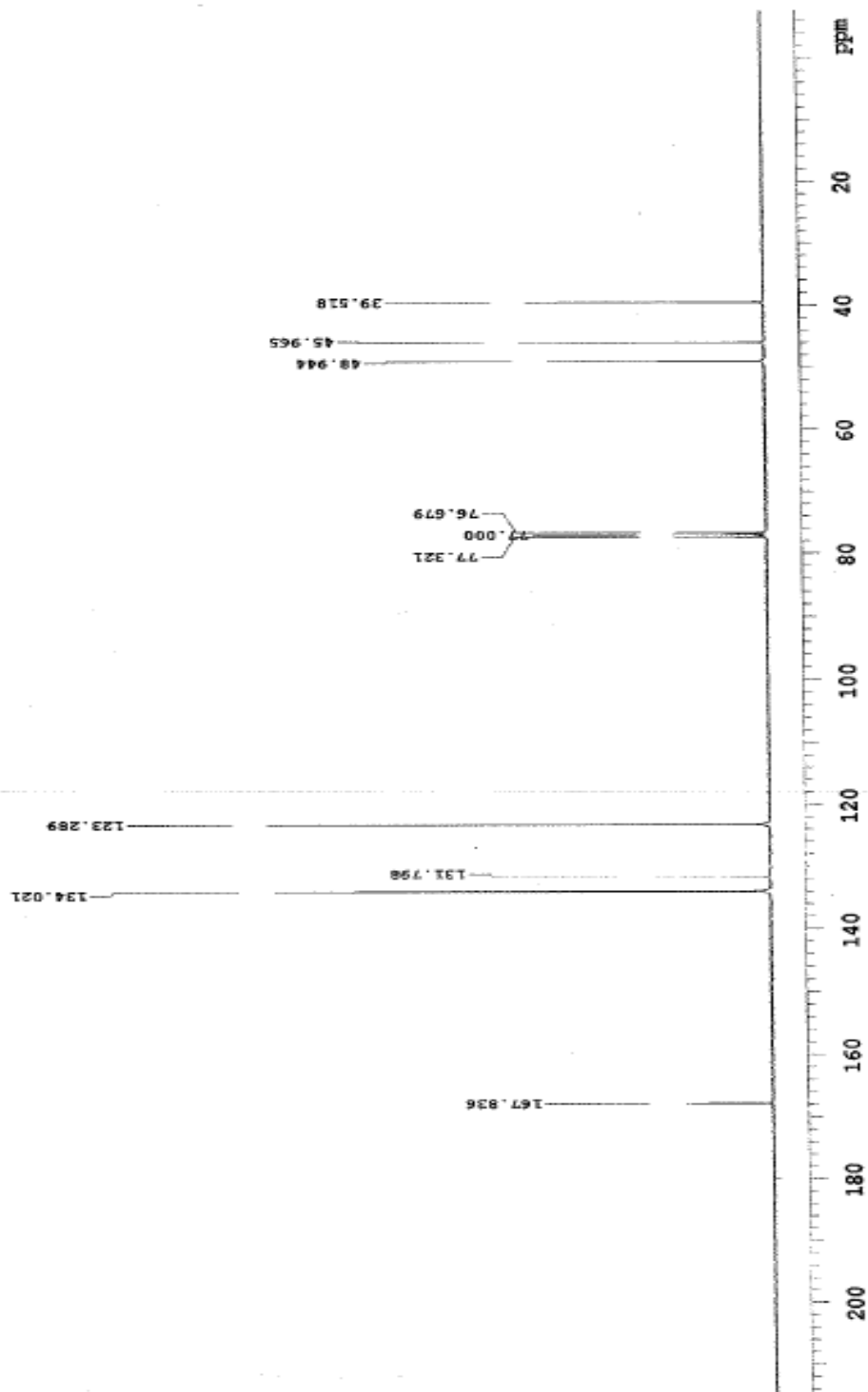
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JR

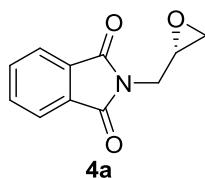
AN.No:HE0810/369
Analyst:Baribabu.R
Date:4th Aug 2010.





1905-400
 AR No: NML1010/2086
 Analyst: Shrutika
 Date: 25th Oct. 2010





cira2 Report

Reported by User: System

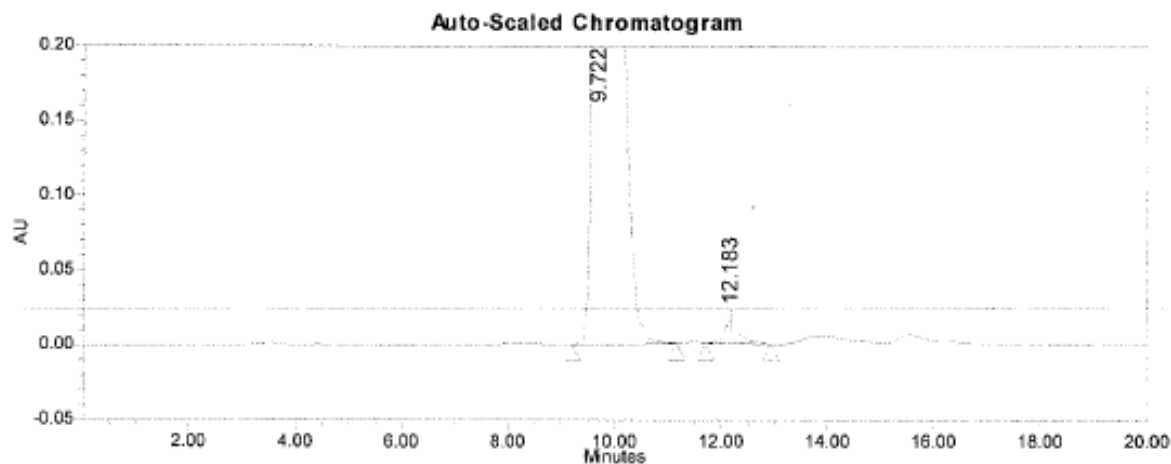
Project Name: HPLC_007_AUG_2010

SAMPLE INFORMATION

Sample Name: S-EPOXIDE PURE
Sample Type: Unknown
Vial: 95
Injection #: 1
Injection Volume: 5.00 ul
Run Time: 20.0 Minutes
Sample Set Name 10081201

Acquired By: System
Date Acquired: 8/12/2010 9:46:56 PM
Acq. Method Set: CIRA2
Date Processed: 8/13/2010 11:47:44 AM
Processing Method: cira2
Channel Name: WvIn Ch2
Proc. Chnl. Descr: PDA 220.0 nm

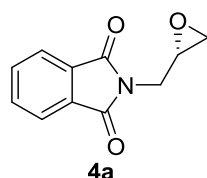
Column: ChiralPAK-IA(250x4.6mm,5.0u)
Mobile Phase: n-Hexane:ipa:80:20
Flow:1.0ml/min,Wave Length:220nm,
Column Temperature:Ambient,Inj Vol:5ul,
Runtime:25min, Dilut: mp, Conc:0.5mg/mL



Peak Results

Name	RT	Area	%Area
1	9.722	47051685	99.32
2	12.183	324028	0.68

AKD
P.D.
13108110



S-Epoxyde

[Comment]

Sample name

Comment

User swapna

Workgroup ARND

Division

Company DRL

[Data Information]

Creation Date 8/17/2010 2:40 PM

[Measurement Information]

Instrument Name PL/118/002

Model Name P-2000

Serial No. A035861232

Polarizer Glan-Taylor Prism

Faraday Cell Flint Glass

Accessory PTC-203

Accessory S/N A014261234

Path Length 100 mm

Light Source Na

Monitor wavelength 589 nm

D.I.T. 5 sec

No. of cycle 5

Cycle interval 0 sec

Temp. Monitor Cell

Temp. Corr. Factor None

Aperture(S) 3.0mm

Aperture(L) Auto

Mode Specific O.R.

Path Length 100 mm

Concentration 2.242 w/v

Factor 1

	No.	Sample No.	Mode	Calc. Data	Meas. Data	Monitor(deg)	Temperature(C)	Blank	
1	*	1	S-EPOXIDE-1	Specific O.R.	9.3256	0.2091	0.2092	24.83	0.0001
2	*	2	S-EPOXIDE-2	Specific O.R.	9.2409	0.2072	0.2073	24.85	0.0001
3	*	3	S-EPOXIDE-3	Specific O.R.	9.2899	0.2083	0.2084	24.88	0.0001
4	*	4	S-EPOXIDE-4	Specific O.R.	9.2988	0.2085	0.2086	24.91	0.0001
5	*	5	S-EPOXIDE-5	Specific O.R.	9.1873	0.2060	0.2081	24.95	0.0001
6	*	6	Avg.		9.2685				
7		7	S.D		0.0548				
8		8	C.V		0.5908				

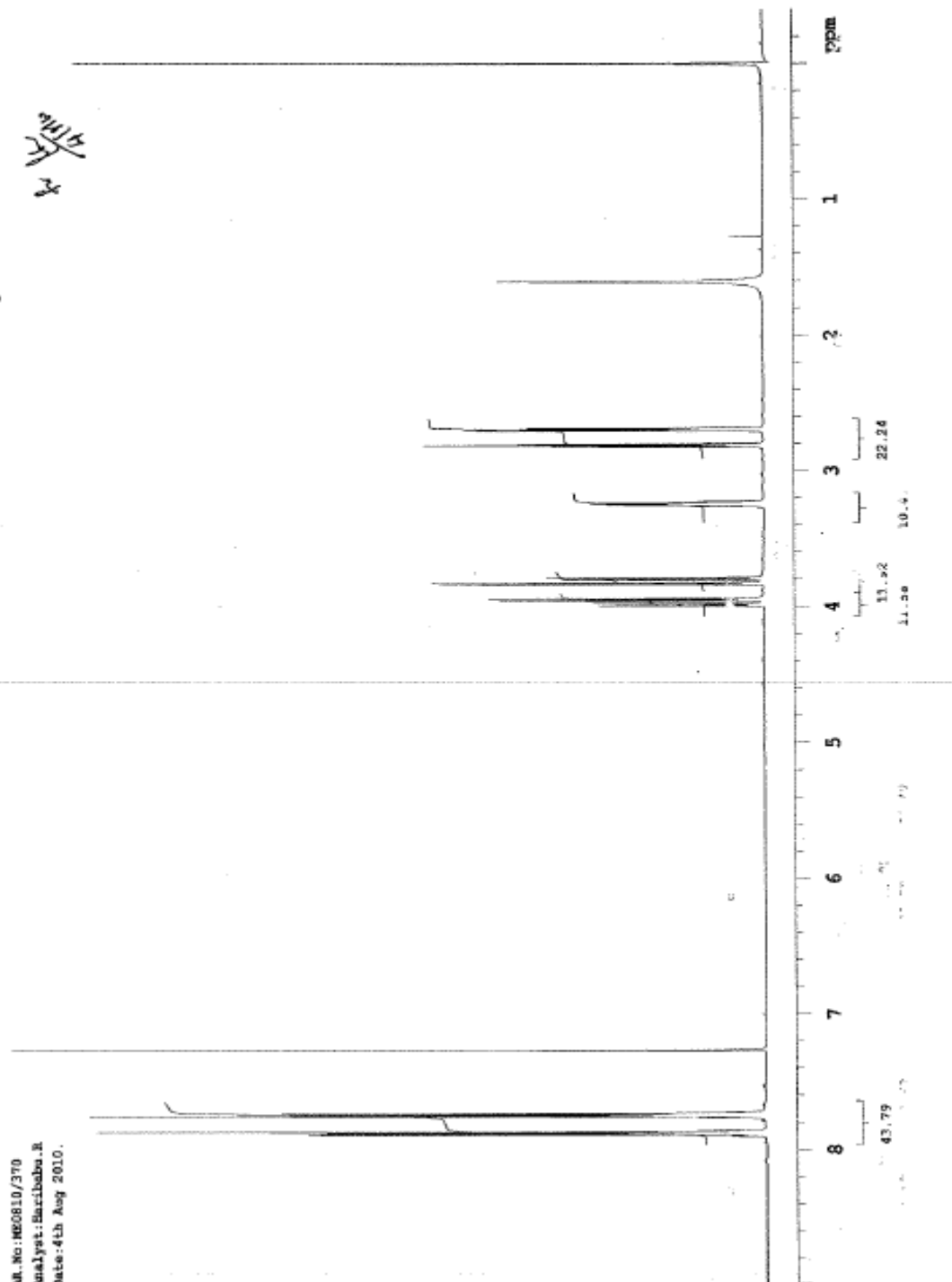
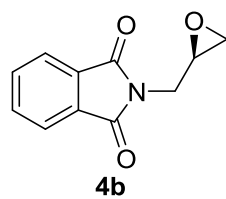
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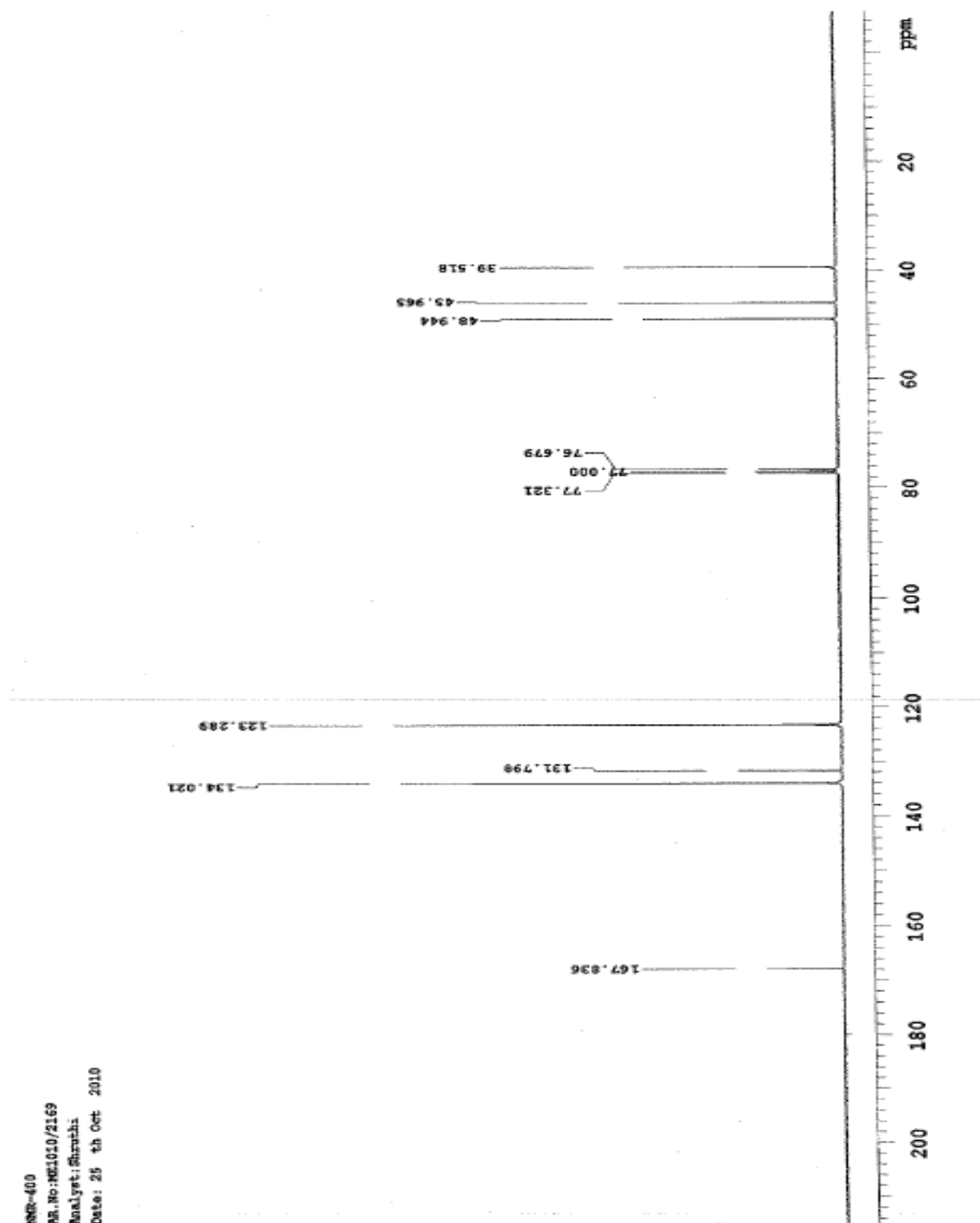
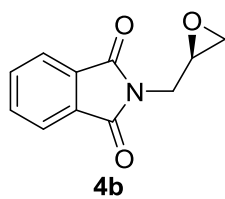
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MR. No: ME0810/370
Analyst: Haribabu.R
Date: 4th Aug 2010.

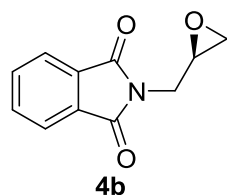
Date & Time : Thu Aug 5 08:48:34 IST 2010
Recorded By : Haribabu.R

4/10
2





NMR-400
 AR.No:ME1010/2163
 Analyst: Shreshth
 Date: 25th Oct 2010

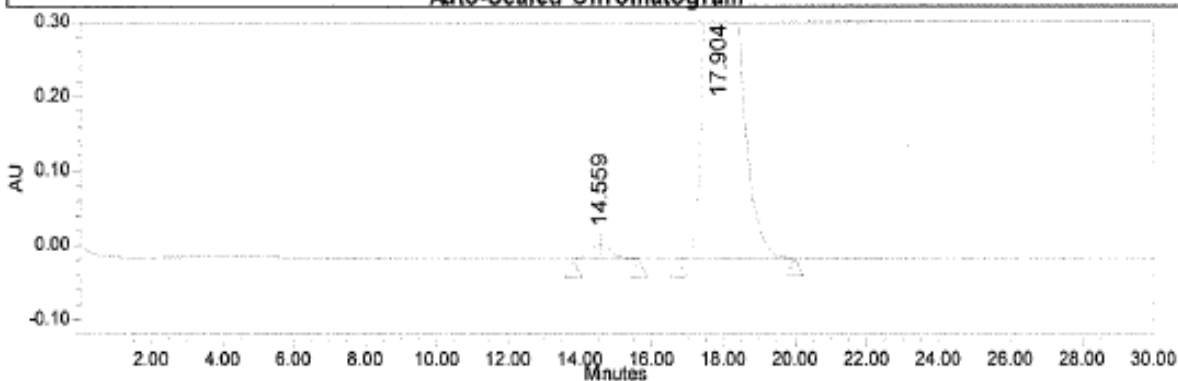


SAMPLE INFORMATION

Sample Name: CIRA2-EPOXIDE2
 Sample Type: Unknown
 Vial: 13
 Injection #: 1
 Injection Volume: 5.00 ul
 Run Time: 30.0 Minutes
 Sample Set Name: 10070501

Acquired By: System
 Date Acquired: 7/5/2010 2:46:50 PM
 Acq. Method Set: cira2
 Date Processed: 7/5/2010 4:50:03 PM
 Processing Method: CIRA2
 Channel Name: W2996 220.0nm-4.8
 Proc. Chnl. Descr: W2996 PDA 220.0 nm at 4.8

Auto-Scaled Chromatogram



Column: chiral pak IA(250*4.6mm)5μ

Mobile Phase:HEXANE:IA(8:2)

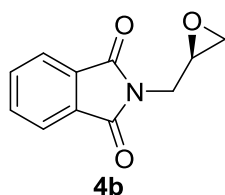
Flow:1.0ml/min, Wave Length:220nm,

Column Temperature:Ambient, Inj Vol:5ul,

Conc: 0.5 mg/ml, Diluent : MP

Peak Results

	Name	RT	Area	% Area
1		14.559	865573	1.92
2		17.904	44264795	98.08



R-Epoxyde

[Comment]

Sample name

Comment

User

swapna

Workgroup

ARND

Division

Company

DRL

[Data Information]

Creation Date 8/12/2010 4:50 PM

[Measurement Information]

Instrument Name PL/118/002

Model Name P-2000

Serial No. A035861232

Polarizer Glan-Taylor Prism

Faraday Cell Flint Glass

Accessory PTC-203

Accessory S/N A014261234

Path Length 100 mm

Light Source Na

Monitor wavelength 589 nm

D.I.T. 5 sec

No. of cycle 5

Cycle interval 0 sec

Temp. Monitor Cell

Temp. Corr. Factor None

Aperture(S) 3.0mm

Aperture(L) Auto

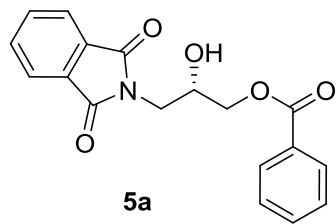
Mode Specific O.R.

Path Length 100 mm

Concentration 1.006 w/v

Factor 1

	No.	Sample No.	Mode	Calc. Data	Meas. Data	Monitor(deg)	Temperature(C)	Blank
1	1	1-1	Specific O.R.	-7.8330	-0.0768	-0.0966	23.90	-0.0178
2	2	1-2	Specific O.R.	-7.7833	-0.0783	-0.0961	23.93	-0.0178
3	3	1-3	Specific O.R.	-7.8429	-0.0789	-0.0967	23.95	-0.0178
4	4	1-4	Specific O.R.	-7.7833	-0.0783	-0.0961	23.95	-0.0178
5	5	1-5	Specific O.R.	-8.3002	-0.0835	-0.1013	23.96	-0.0178
6	6	Avg.		-7.9085				
7	7	S.D		0.2207				
8	8	C.V		2.7902				
9	9	R EPOXIDE 1a-1	Specific O.R.	-8.8668	-0.0882	-0.1070	23.86	-0.0178
10	10	R EPOXIDE 1a-2	Specific O.R.	-9.2346	-0.0929	-0.1107	23.86	-0.0178
11	11	R EPOXIDE 1a-3	Specific O.R.	-9.0457	-0.0910	-0.1088	23.86	-0.0178
12	12	R EPOXIDE 1a-4	Specific O.R.	-9.0557	-0.0911	-0.1089	23.86	-0.0178



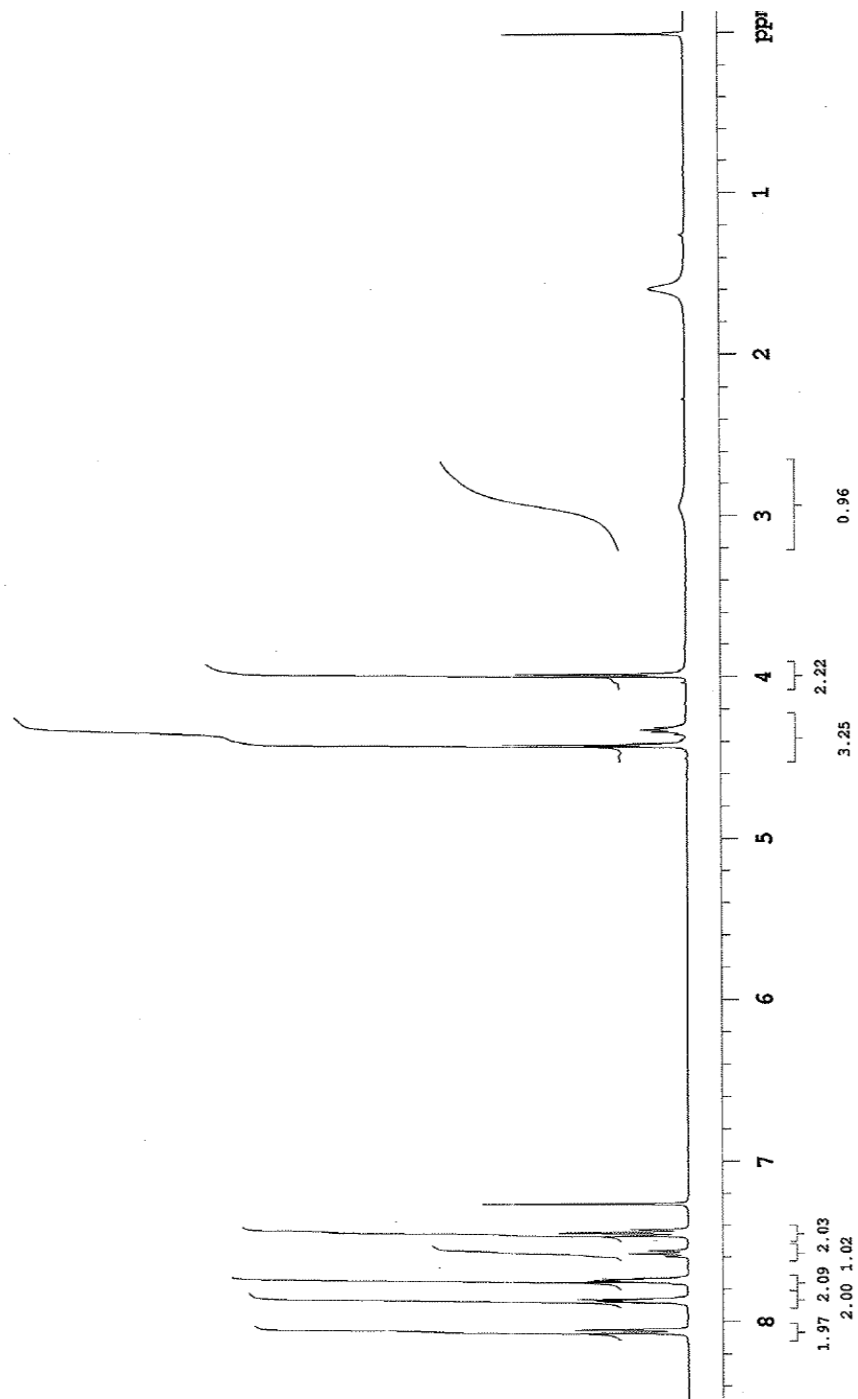
TDC-219 2/HGR/064 1D CDCL₃

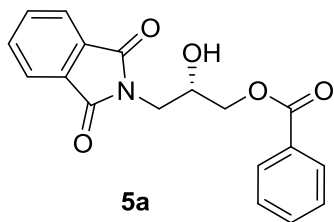
NMR-400

AR.No:ME1010/05

Analyst:Haribabu.R

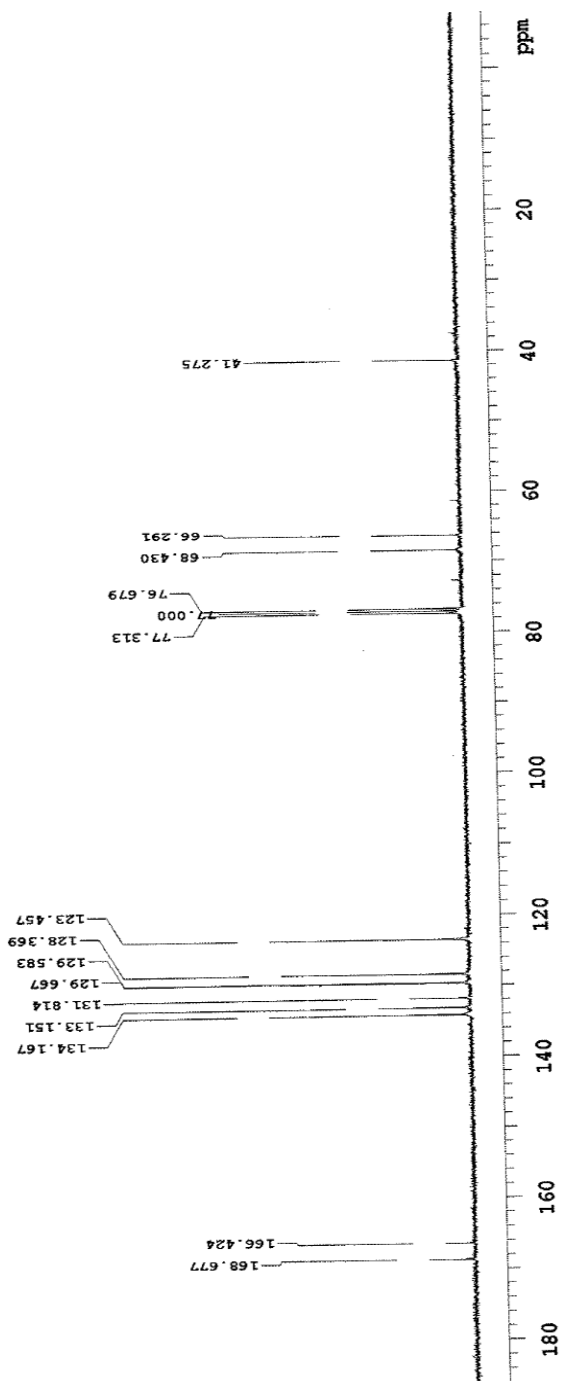
Date: 01 st Oct 2010

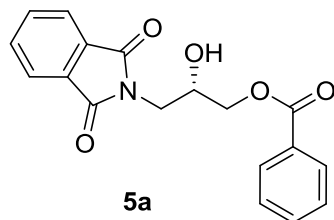




ARSD, Aurigene Discovery Technologies Ltd, Hyderabad
 Instrument : Mercury Plus (Varian 400MHz)
 Date & Time : Fri May 28 14:29:04 IST 2010
 Recorded By : Srikanth.A

2-RGK-050 in CDCl₃
 CWO-219
 AR.No:ME0510/2036
 Analyst:Srikanth.A
 Date:27th May 2010





2-RGK-064.p1d

[Comment]

Sample name

Comment

User ramanjaneyulu

Workgroup ARND

Division

Company DRL

[Data Information]

Creation Date 10/1/2010 11:06 AM

[Measurement Information]

Instrument Name PL/118/002

Model Name P-2000

Serial No. A035861232

Polarizer Glan-Taylor Prism

Faraday Cell Flint Glass

Accessory PTC-203

Accessory S/N A014261234

Path Length 100 mm

Light Source Na

Monitor wavelength 589 nm

D.I.T. 5 sec

No. of cycle 5

Cycle interval 0 sec

Temp. Monitor Cell

Temp. Corr. Factor None

Aperture(S) 3.0mm

Aperture(L) Auto

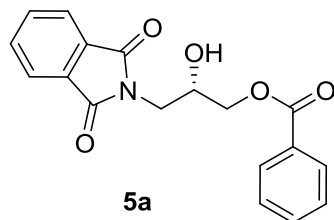
Mode Specific O.R.

Path Length 100 mm

Concentration 1.0123 w/v

Factor 1

		No.	Sample No.	Mode	Calc. Data	Meas. Data	Monitor(deg)	Temperature(C)	Blank
1	*	1	12-RGK-064-1	Specific O.R.	-7.6045	-0.0770	-0.0815	23.63	-0.0045
2	*	2	12-RGK-064-2	Specific O.R.	-7.2587	-0.0735	-0.0780	23.71	-0.0045
3	*	3	12-RGK-064-3	Specific O.R.	-7.5946	-0.0769	-0.0814	23.78	-0.0045
4	*	4	12-RGK-064-4	Specific O.R.	-7.6440	-0.0774	-0.0819	23.83	-0.0045
5	*	5	12-RGK-064-5	Specific O.R.	-7.4464	-0.0754	-0.0799	23.89	-0.0045
6	*	6	Avg.		-7.5096				
7		7	S.D		0.1591				
8		8	C.V		2.1182				



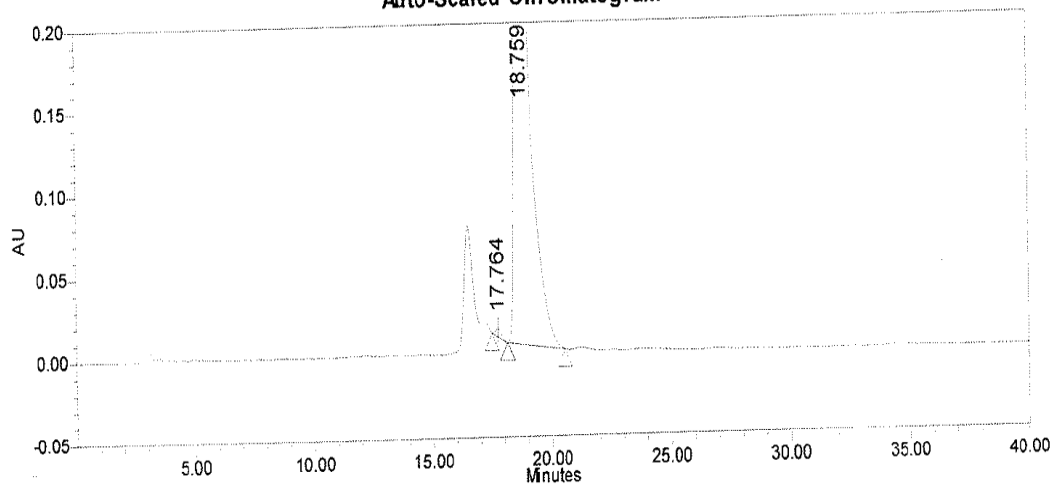
SAMPLE INFORMATION

Sample Name: S-related aldehyde
 Sample Type: Unknown
 Vial: 89
 Injection #: 1
 Injection Volume: 5.00 μ l
 Run Time: 40.0 Minutes
 Sample Set Name 10081201

Acquired By: System
 Date Acquired: 8/12/2010 7:21:26 PM
 Acq. Method Set: CIRA2
 Date Processed: 8/13/2010 11:45:45 AM
 Processing Method: cira2
 Channel Name: WvIn Ch2
 Proc. Chnl. Descr: PDA 220.0 nm

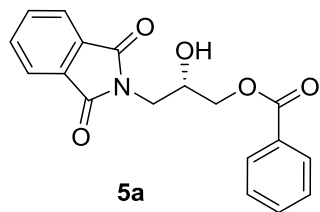
Column: ChiralPAK-IA(250x4.6mm,5.0 μ)
 Mobile Phase: n-Hexane:ipa::80:20
 Flow:1.0ml/min,Wave Length:220nm,
 Column Temperature:Ambient,Inj Vol:5 μ l,
 Runtime:25min, Dilut: mp, Conc:0.5mg/mL

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area
1		17.764	84596	0.48
2		18.759	17568524	99.52



Page 1

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

112 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-30 N: 0-5 O: 0-6

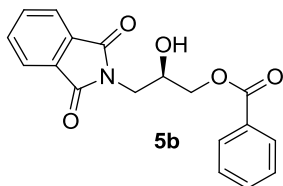
2/RGK0087

LT1211_030 18 (0.339) Cm (18.23)

11 TQF MS ES+
6.48e+003



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
326.1021	326.1029	0.3	0.9	11.5	0.9	C19 H16 N O5
326.1042		-1.1	-3.4	16.5	3.1	C19 H12 N5 O

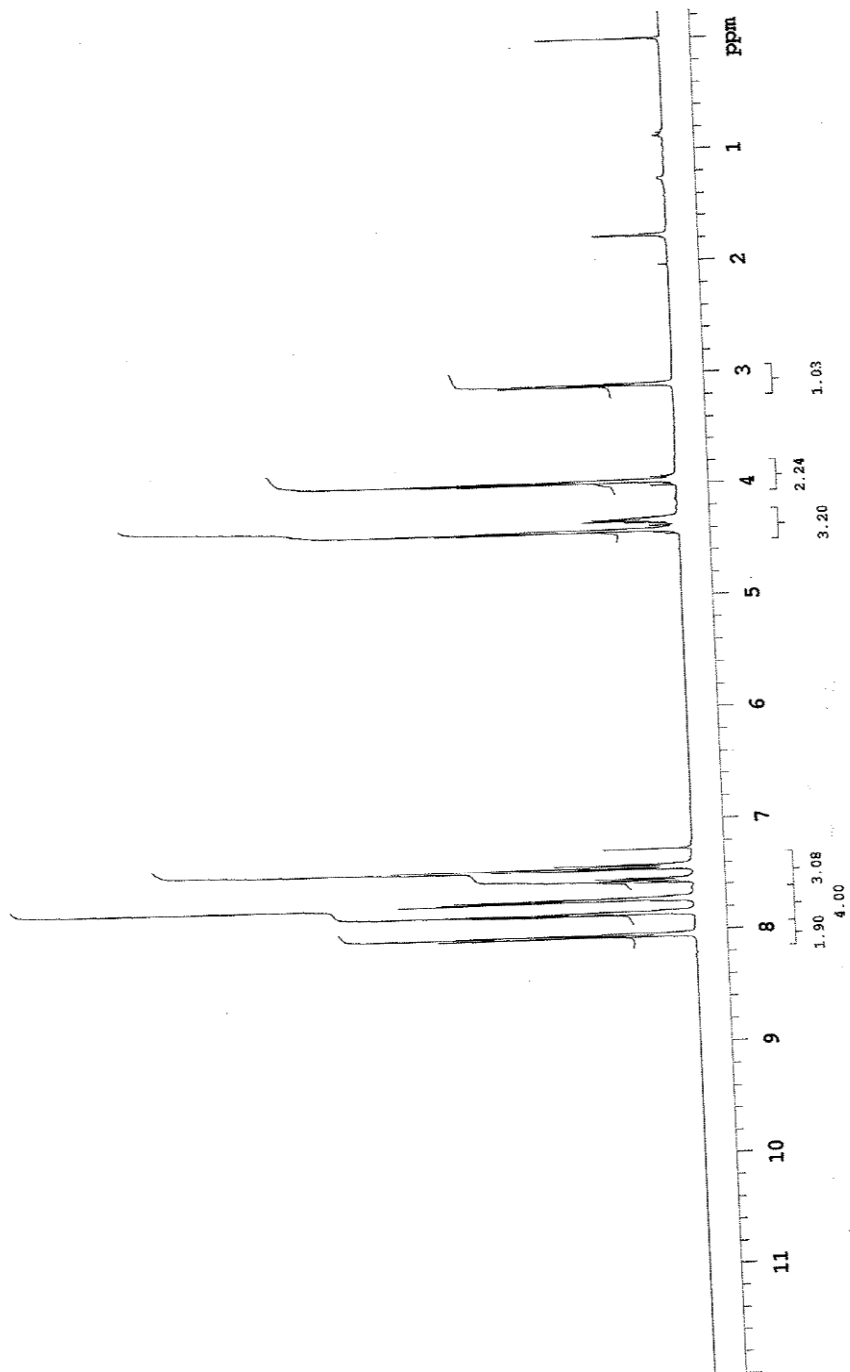


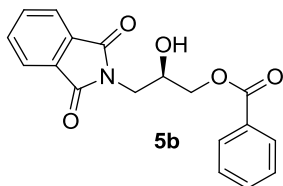
ARED, Aurigene Discovery Technologies Ltd, Hyderabad
 Instrument : Mercury Plus (Varian 400MHz)
 Date & Time : Mon Aug 2 16:17:28 IST 2010
 Recorded By : Haribabu.R

2-RGR-067
 TDC-219
 CDCl₃

AR.No:ME0810/55
 Analyst:Haribabu.R
 Date:2nd Aug. 2010.

rw
 248

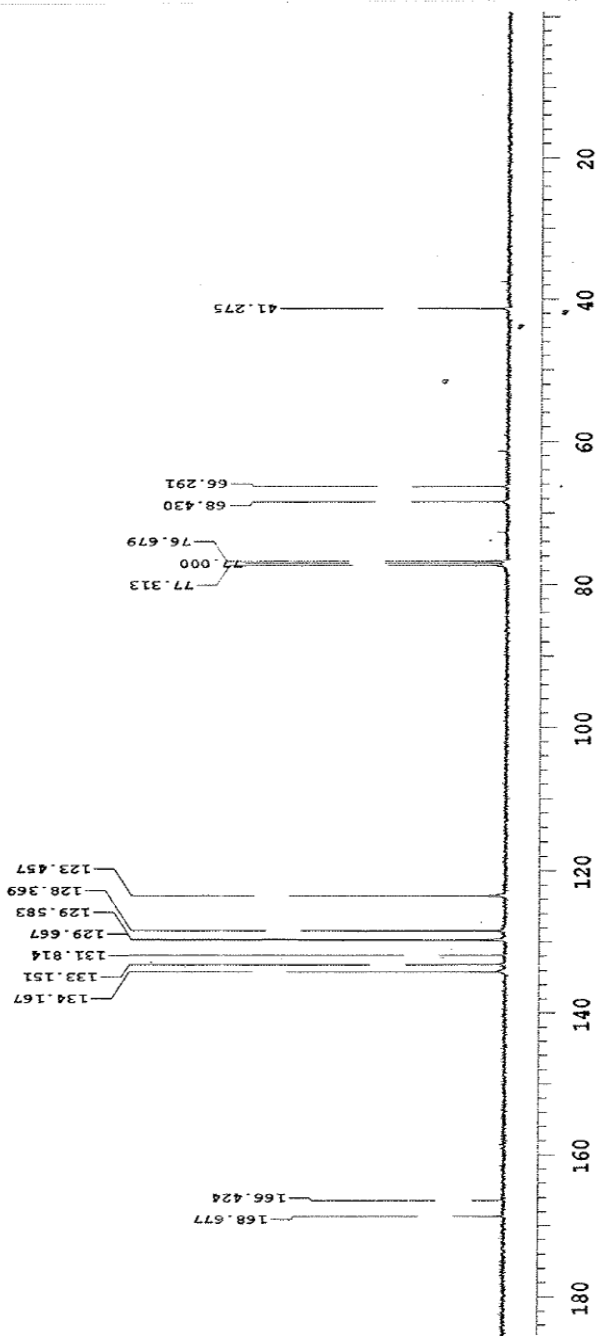


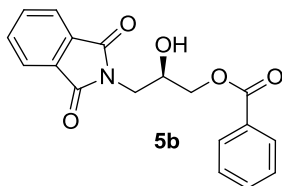


ARAD, Aurigene Discovery Technologies Ltd., Hydera
 Instrument : Gemini 2000 (Varian 200MHz)
 Date & Time : Thu Aug 5 14:11:11 05/2010
 Recorded By : Haribabu.R

TMO-219-2-RGK-067
 In CDCl₃

AR NO:GE0810/06
 Analyst:Haribabu.R
 Date:4 th Aug,2010





2-RGK-067.p1d

[Comment]

Sample name

Comment

User ramanjaneyulu

Workgroup ARND

Division

Company DRL

[Data Information]

Creation Date 10/1/2010 11:15 AM

[Measurement Information]

Instrument Name PL/118/002

Model Name P-2000

Serial No. A035861232

Polarizer Glan-Taylor Prism

Faraday Cell Flint Glass

Accessory PTC-203

Accessory S/N A014261234

Path Length 100 mm

Light Source Na

Monitor wavelength 589 nm

D.I.T. 5 sec

No. of cycle 5

Cycle interval 0 sec

Temp. Monitor Cell

Temp. Corr. Factor None

Aperture(S) 3.0mm

Aperture(L) Auto

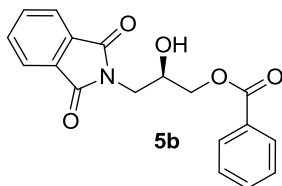
Mode Specific O.R.

Path Length 100 mm

Concentration 0.9912 w/v

Factor 1

	No.	Sample No.	Mode	Calc. Data	Meas. Data	Monitor(deg)	Temperature(C)	Blank	
1	*	1	2-RGK-067-1	Specific O.R.	7.6634	0.0760	0.0719	23.37	-0.0041
2	*	2	2-RGK-067-2	Specific O.R.	7.6433	0.0758	0.0717	23.43	-0.0041
3	*	3	2-RGK-067-3	Specific O.R.	7.5121	0.0745	0.0704	23.50	-0.0041
4	*	4	2-RGK-067-4	Specific O.R.	7.5626	0.0750	0.0709	23.56	-0.0041
5	*	5	2-RGK-067-5	Specific O.R.	7.5928	0.0753	0.0712	23.61	-0.0041
6	*	6	Avg.		7.5948				
7		7	S.D		0.0611				
8		8	C.V		0.8047				

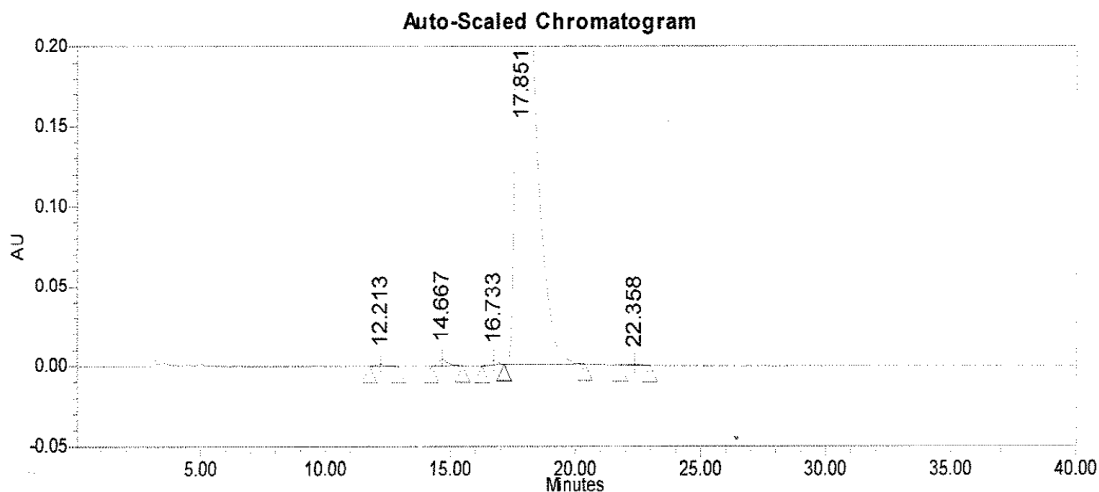


SAMPLE INFORMATION

Sample Name: R-related aldehyde
 Sample Type: Unknown
 Vial: 88
 Injection #: 1
 Injection Volume: 5.00 ul
 Run Time: 40.0 Minutes
 Sample Set Name 10081201

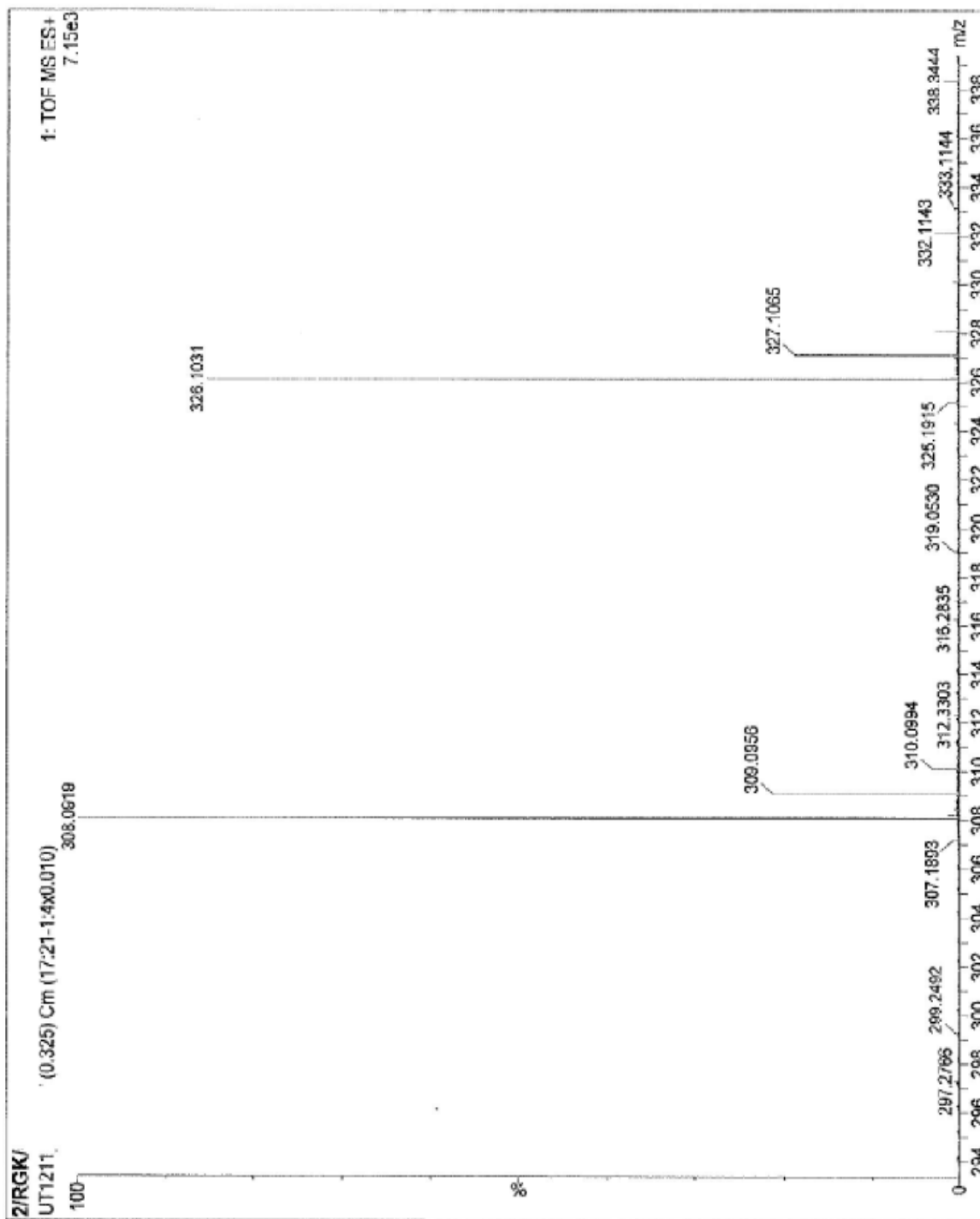
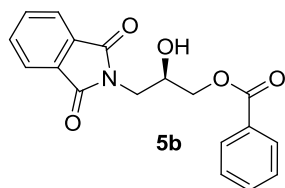
Acquired By: System
 Date Acquired: 8/12/2010 6:40:20 PM
 Acq. Method Set: CIRA2
 Date Processed: 8/13/2010 11:28:23 AM
 Processing Method: cira2
 Channel Name: WvIn Ch2
 Proc. Chnl. Descr: PDA 220.0 nm

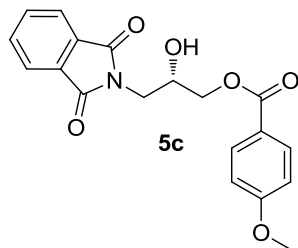
Column: ChiralPAK-IA(250x4.6mm,5.0u)
 Mobile Phase: n-Hexane:ipa::80:20
 Flow: 1.0ml/min, Wave Length: 220nm,
 Column Temperature: Ambient, Inj Vol: 5ul,
 Runtime: 25min, Dilut: mp, Conc: 0.5mg/mL



Peak Results

	Name	RT	Area	% Area
1		12.213	35169	0.13
2		14.667	102253	0.38
3		16.733	60435	0.22
4		17.851	26881191	99.21
5		22.358	15693	0.06

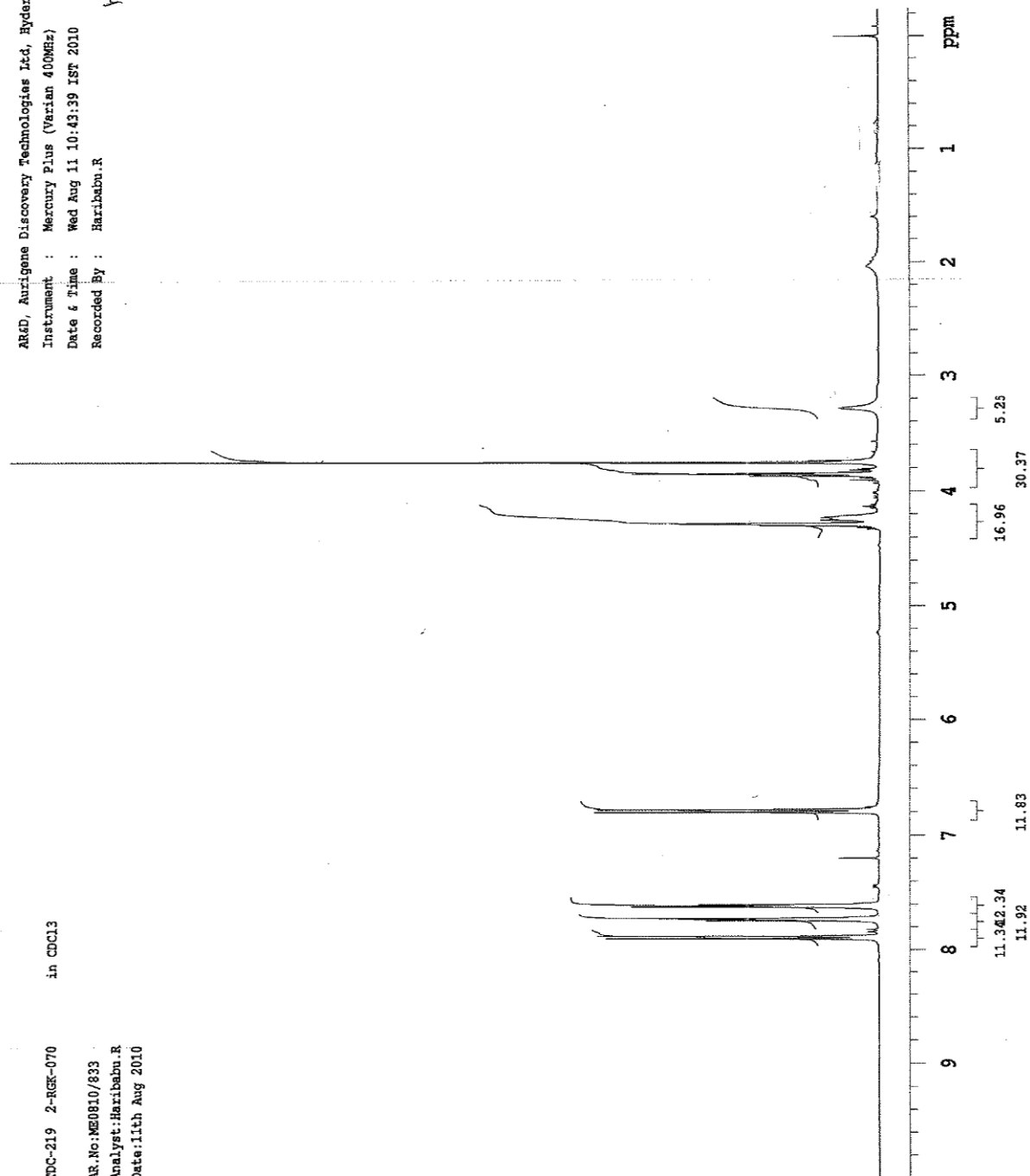


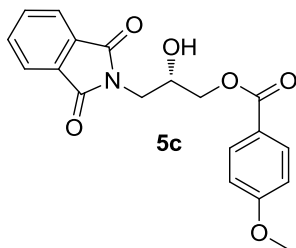


AR&D, Aurigene Discovery Technologies Ltd, Hyderabad
 Instrument : Mercury Plus (Varian 400MHz)
 Date & Time : Wed Aug 11 10:43:39 IST 2010
 Recorded By : Haribabu.R

in CDCl₃

TDC-219 2-RGR-070
 AR.No:ME0810/833
 Analyst:Haribabu.R
 Date:11th Aug 2010





ARdD, Aurigene Discovery Technologies Ltd, Hyderabad

Instrument : Mercury Plus (Varian 400MHz)

Date & Time : Fri Aug 13 15:18:52 IST 2010

Recorded By : Haribabu.R

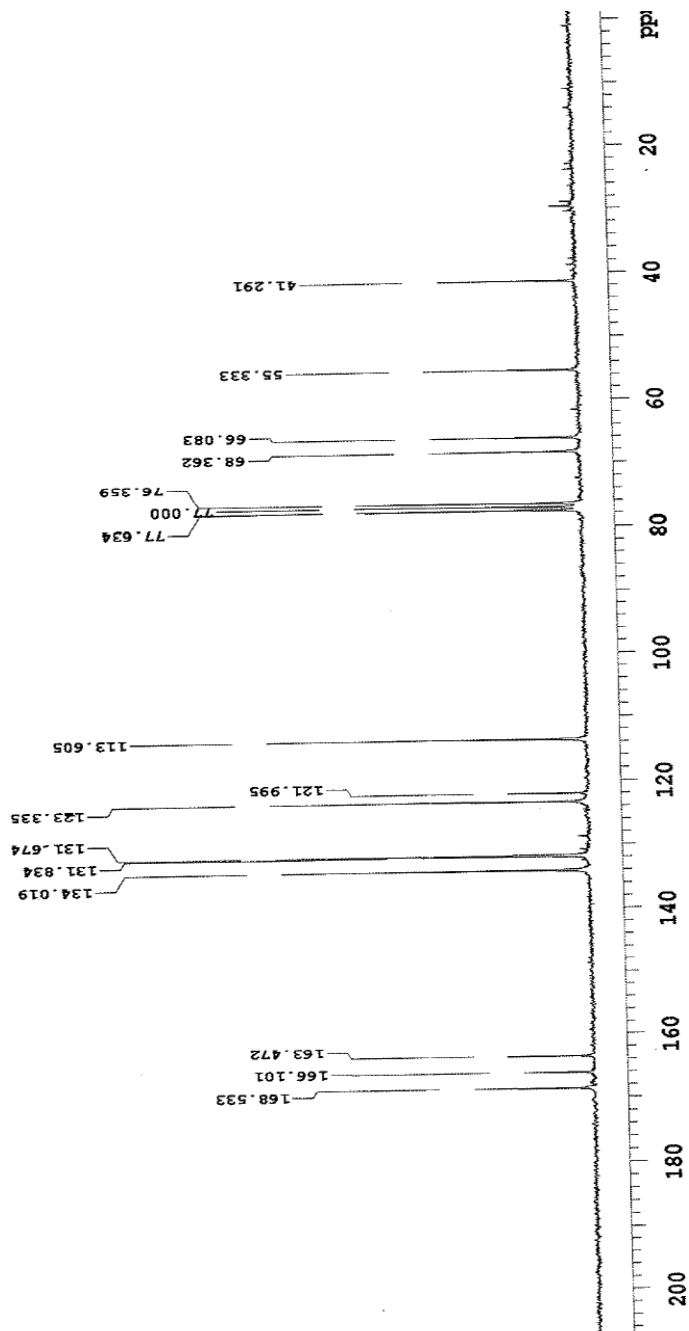
2-RGN-070 in CDCl₃

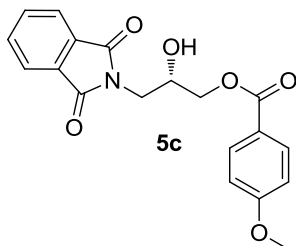
TDC-219

AR NO:GE0810/24

Analyst:Haribabu.R

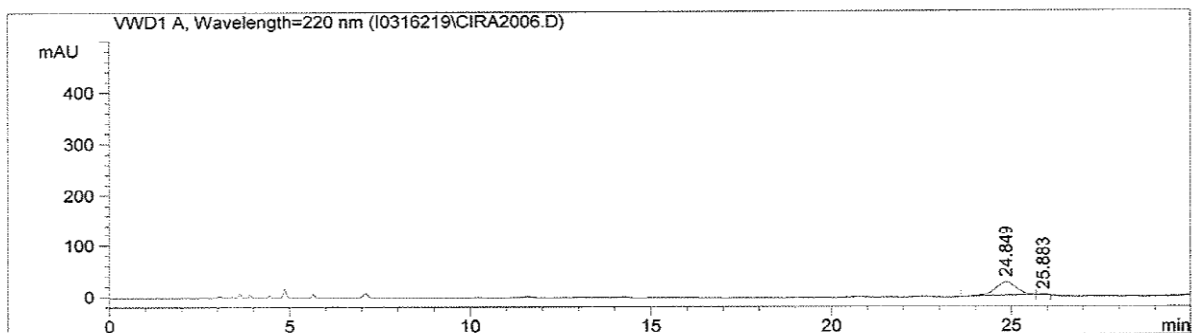
Date: 12 th Aug.2010





2/RGK/072-S PURE-4OME

```
=====
Injection Date   : 9/16/2010 5:40:25 PM           Seq. Line :    6
Sample Name      : 2/RGK/073                     Location  : Vial 6
Acq. Operator    : Ashok                          Inj       :    1
Acq. Instrument  : CPS1/ARD/HPLC/003              Inj Volume: 5 µl
Acq. Method      : C:\HPCHEM\1\METHODS\CIRA2CH.M
Last changed     : 9/16/2010 5:32:47 PM by Ashok
                  (modified after loading)
Analysis Method  : C:\HPCHEM\1\METHODS\CIRA2CH.M
Last changed     : 9/17/2010 8:33:52 AM by RAMANJANEYULU
                  (modified after loading)
Column:          CHIRAL PAK IA(250*4.6)5µm
Mobile Phase     : n-Hexane:IPA:8:2
Flow:            1.0mL/min, Wavelength: 220nm,
Run time:        25min
=====
```



Area Percent Report

```
=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

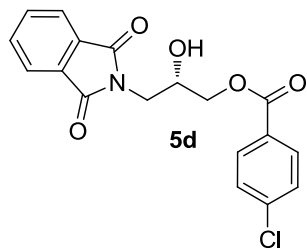
Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	24.849	MM R	0.9344	1084.80518	25.97355	98.3181
2	25.883	MM R	0.2241	18.55733	1.37995	1.6819

Totals : 1103.36251 27.35351

Results obtained with enhanced integrator!

*** End of Report ***



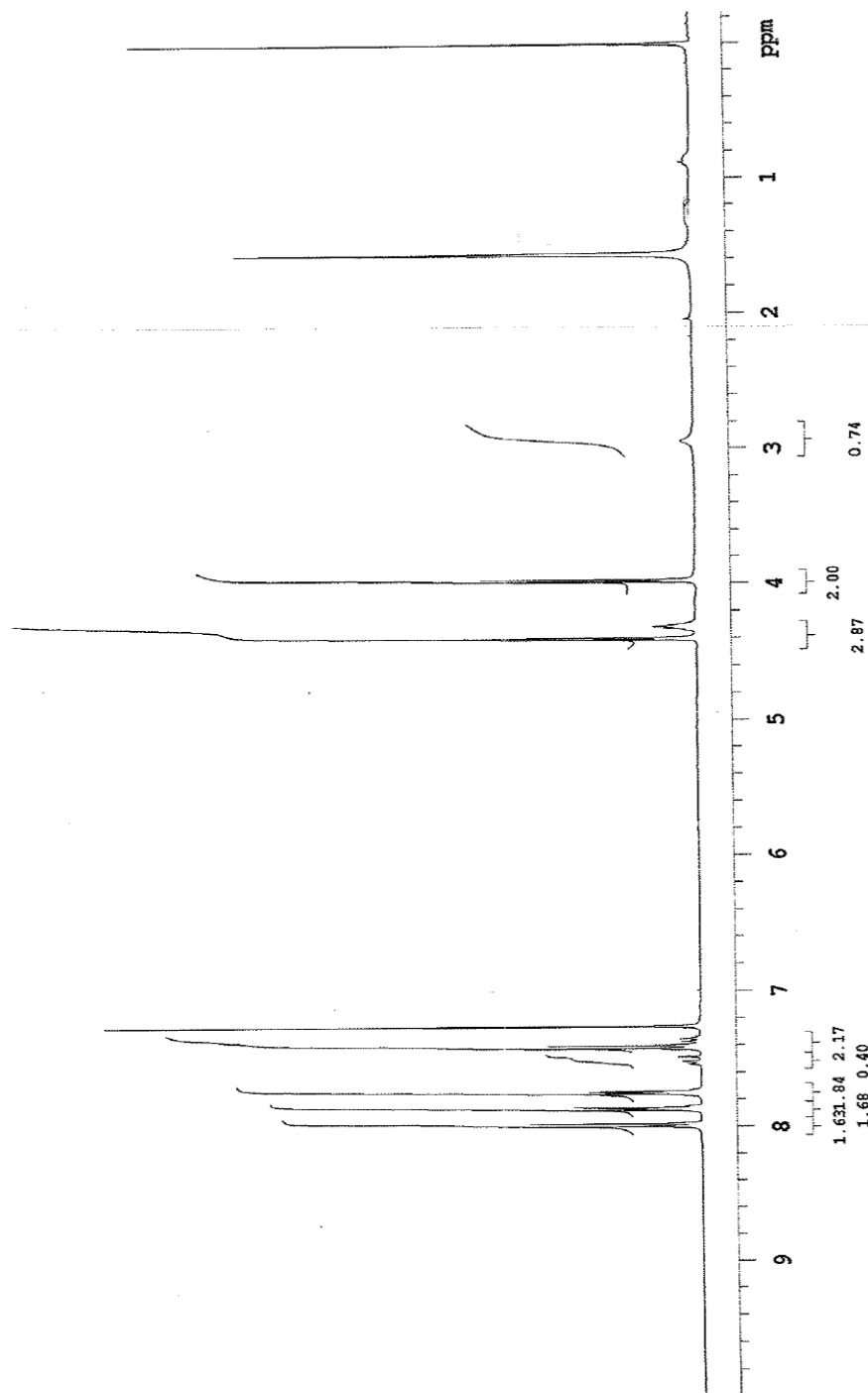
TDC-219 2-RGX-069 in CDCl₃

NMR-400

AR.No:ME1010/1968

Analyst:Haribabu.R

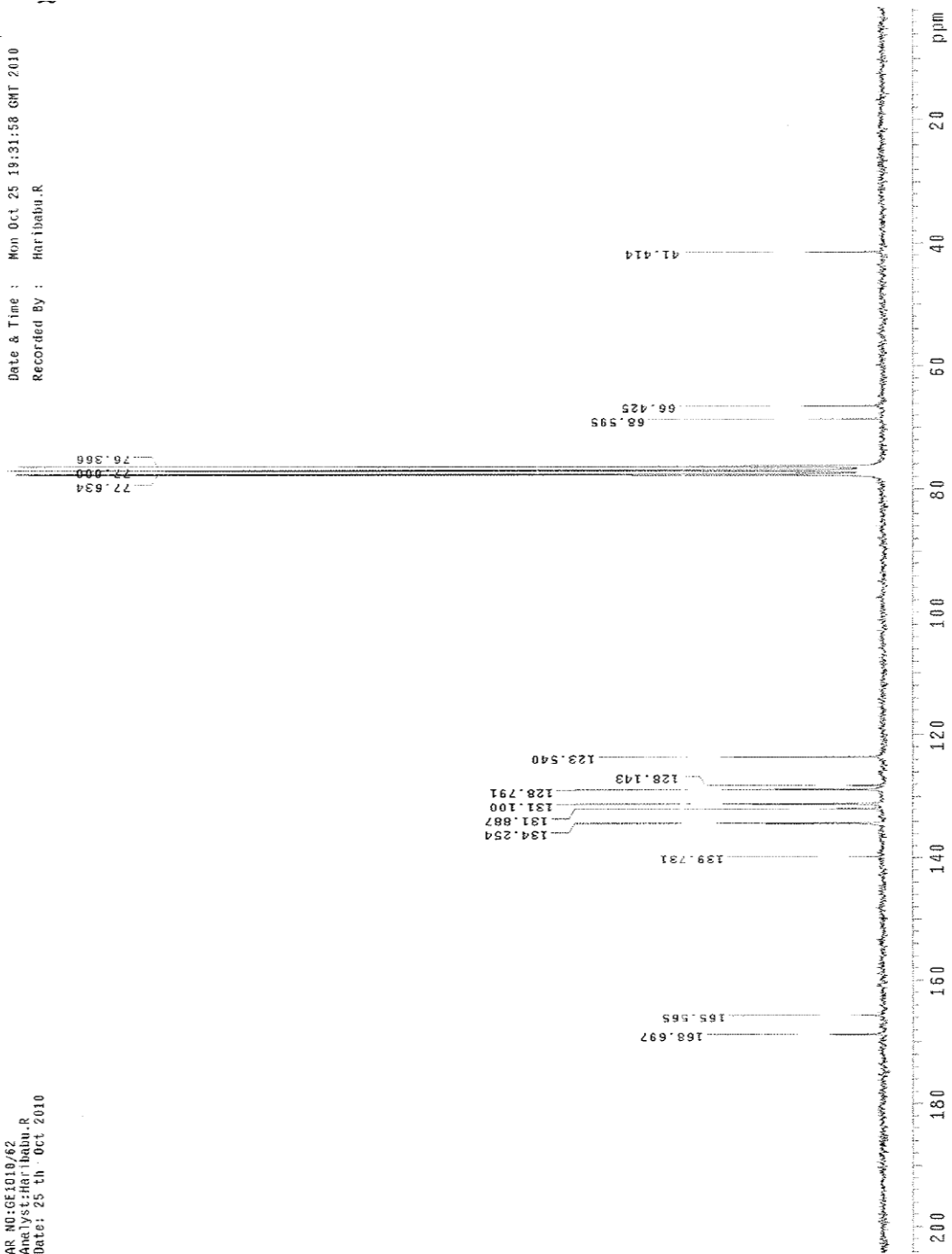
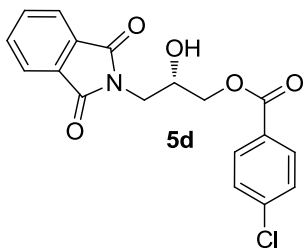
Date: 25 th Oct 2010

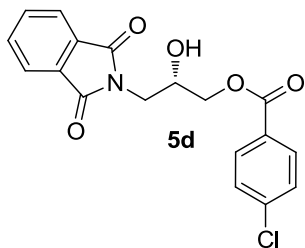


2/RGK/069 in CDCl3
T0C-219

AR NO:GE1010/62
Analyst:Haribabu.R
Date: 25 th Oct 2010

AR&D, Aurigene Discovery Technologies Ltd, Hyderabad
Instrument : Gemini 2000 (Varian 200MHz)
Date & Time : Mon Oct 25 19:31:58 GMT 2010
Recorded By : Haribabu.R

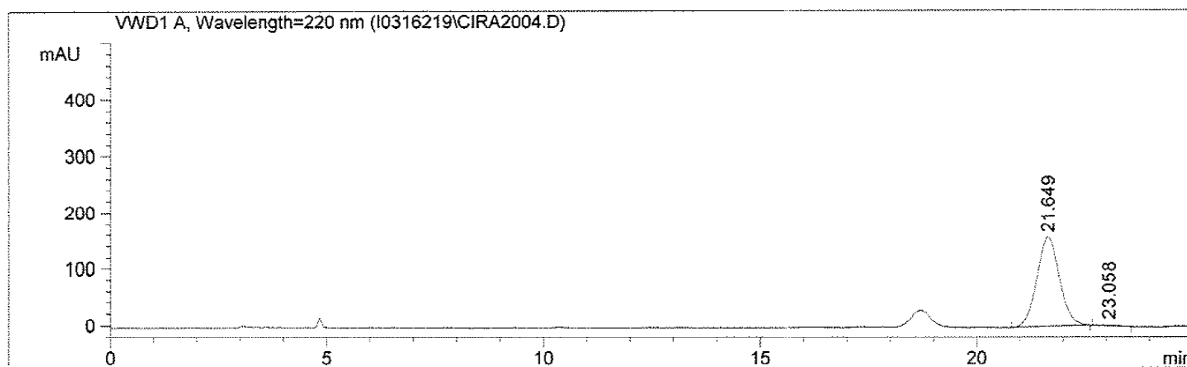




```

=====
Injection Date   : 9/16/2010 4:42:07 PM           Seq. Line :    4
Sample Name     : 2/RGK/069                     Location  : Vial 4
Acq. Operator   : Ashok                          Inj       :    1
Acq. Instrument : CPS1/ARD/HPLC/003              Inj Volume: 5 µl
Acq. Method     : C:\HPCHEM\1\METHODS\CIRA2CH.M
Last changed    : 9/14/2010 8:10:18 PM by Muralikrishna Ch
Analysis Method : C:\HPCHEM\1\METHODS\CIRA2CH.M
Last changed    : 9/17/2010 8:33:52 AM by RAMANJANEYULU
                  (modified after loading)
Column: CHIRAL PAK IA(250*4.6)5µm
Mobile Phase : n-Hexane:IPA:8:2
Flow: 1.0mL/min, Wavelength: 220nm,
Run time:25min

```



=====
Area Percent Report
=====

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	21.649	BB	0.5515	5608.70752	156.16954	99.5308
2	23.058	MM R	0.4677	26.44208	9.42218e-1	0.4692

Totals : 5635.14960 157.11176

Results obtained with enhanced integrator!

=====
*** End of Report ***

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 ppm / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotopic peaks used for $\pm H11 = 3$

Mass/Charge Ratio: Even Electron Ion

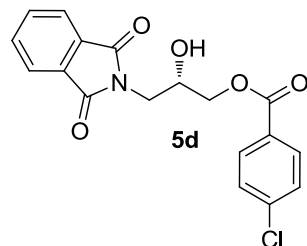
38 formulae calculated with 1 result within limits (up to at least isotopic resolution for each result)

Percent Error

C: 0.20 H: 0.20 N: 0.2 C: 0.6 Cl: 0.1

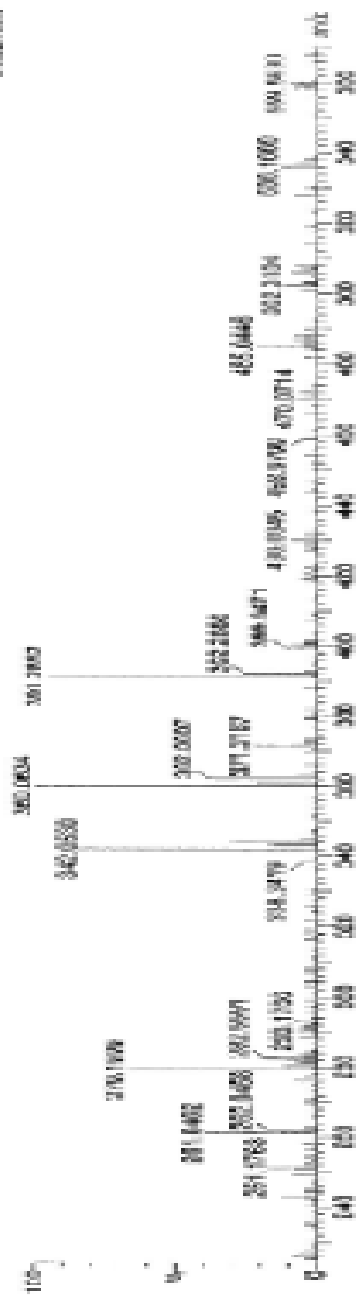
380.0000

1000000.0000 1000000.0000 1000000.0000



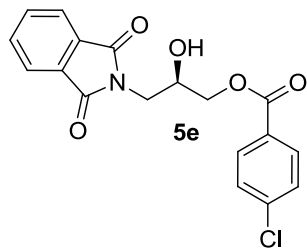
Page 1

1. TOP MD (2.0)
3. Mass (2.0)



Kindness: -1.5
Mass Ratio: 8.0 8.0 80.0

Mass	Calc.	Mass	Calc.	Mass	Calc.	Mass	Calc.
380.0000	380.0000	380.0000	380.0000	380.0000	380.0000	380.0000	380.0000



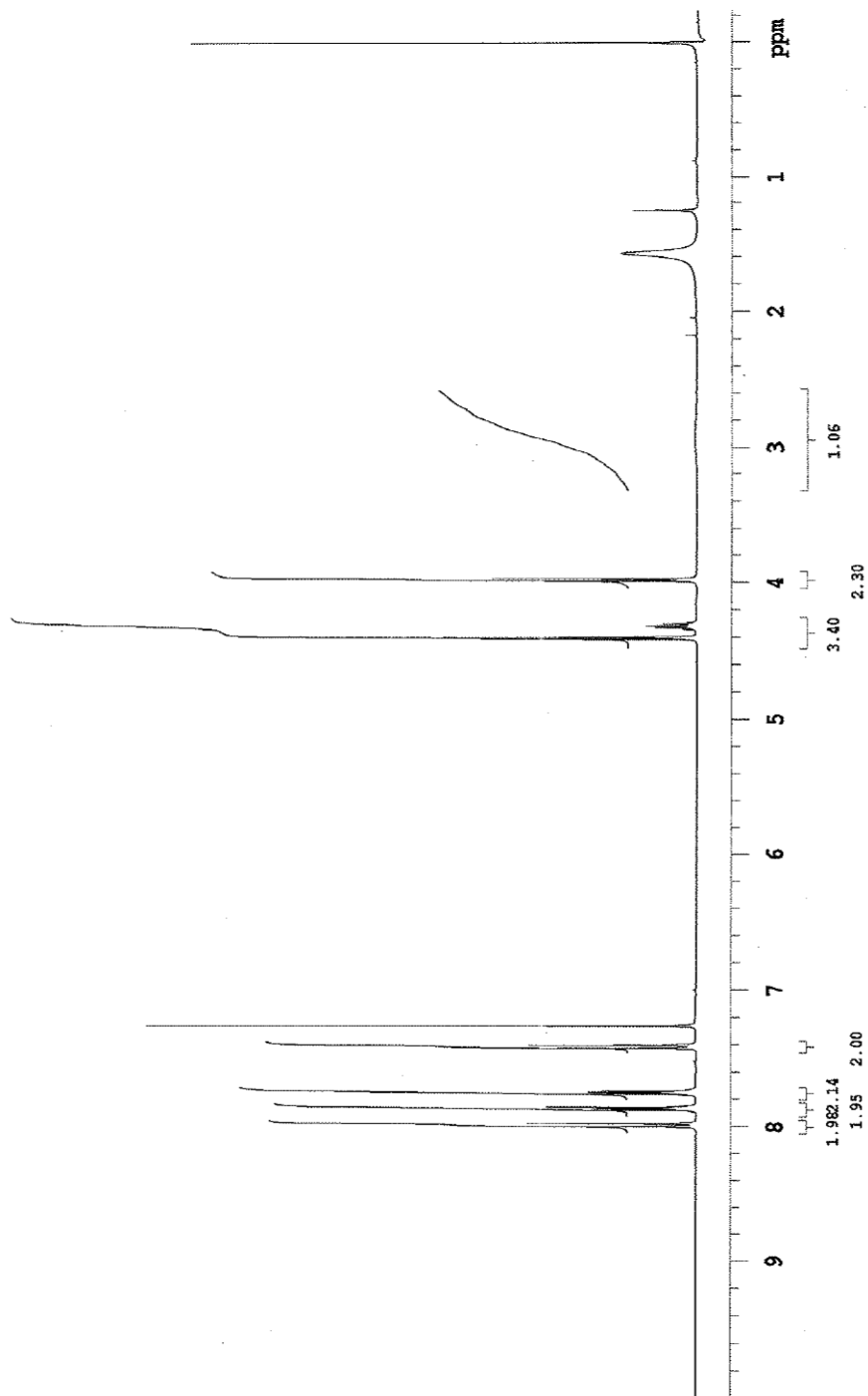
TDC-219 2-RGR-072 in CDCl₃

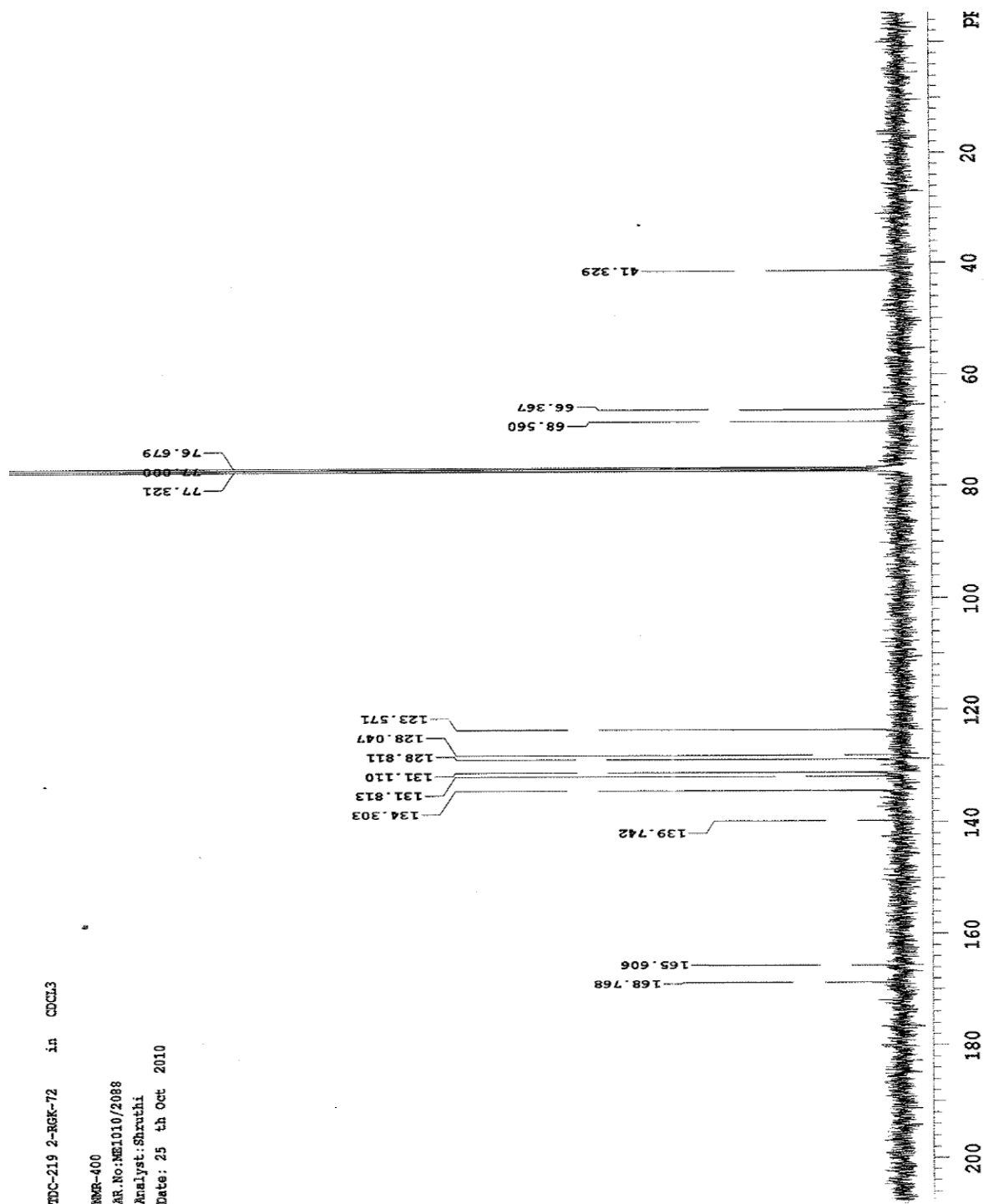
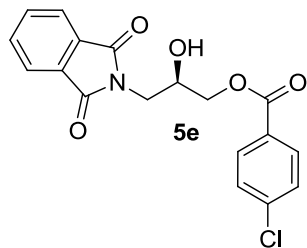
NMR-400

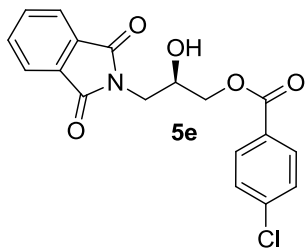
AS.No:ME1010/1964

Analyst:Haribabu.R

Date: 25 th Oct 2010



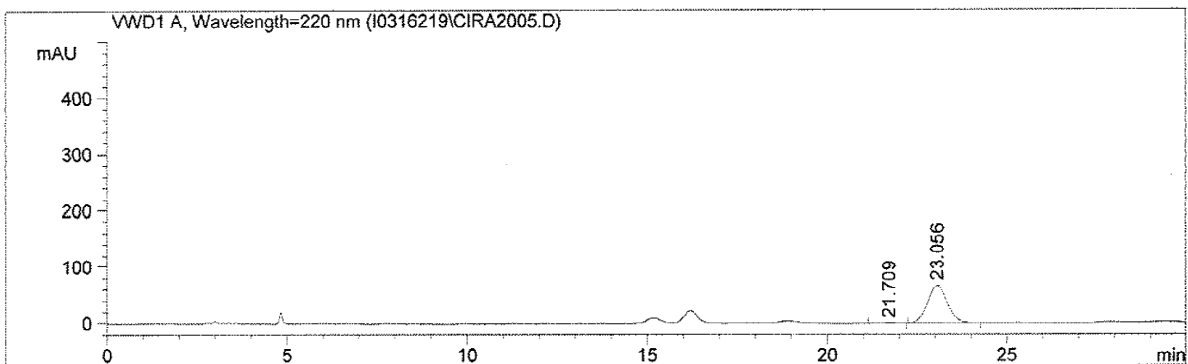




```

=====
Injection Date   : 9/16/2010 5:08:47 PM          Seq. Line :    5
Sample Name     : 2/RGK/072                    Location  : Vial 5
Acq. Operator   : Ashok                        Inj       :    1
Acq. Instrument : CPS1/ARD/HPLC/003            Inj Volume: 5 µl
Acq. Method     : C:\HPCHEM\1\METHODS\CIRA2CH.M
Last changed    : 9/16/2010 5:32:47 PM by Ashok
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CIRA2CH.M
Last changed    : 9/17/2010 8:33:52 AM by RAMANJANEYULU
                  (modified after loading)
Column: CHIRAL PAK IA(250*4.6)5µm
Mobile Phase : n-Hexane:IPA:8:2
Flow: 1.0mL/min, Wavelength: 220nm,
Run time:25min

```



Area Percent Report

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs

```

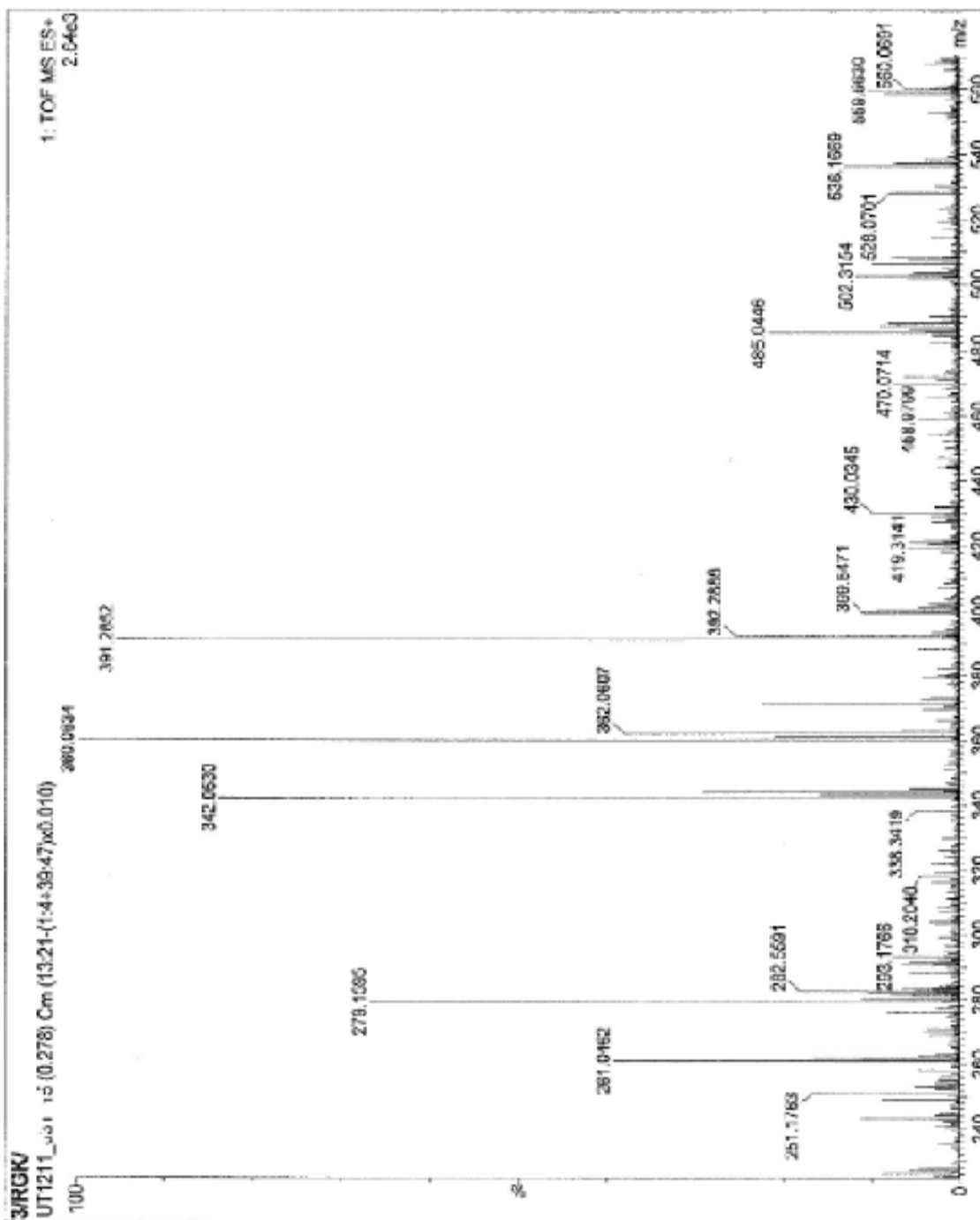
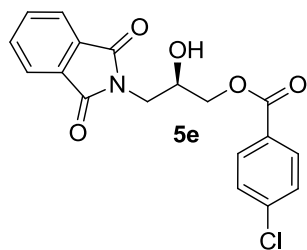
Signal 1: VWD1 A, Wavelength=220 nm

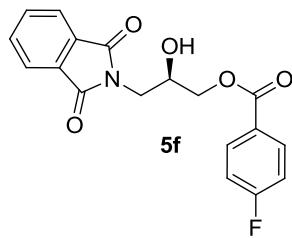
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	21.709	MM R	0.5429	21.54136	6.61289e-1	0.8460
2	23.056	MM R	0.6389	2524.79077	65.86342	99.1540

Totals : 2546.33213 66.52471

Results obtained with enhanced integrator!

*** End of Report ***





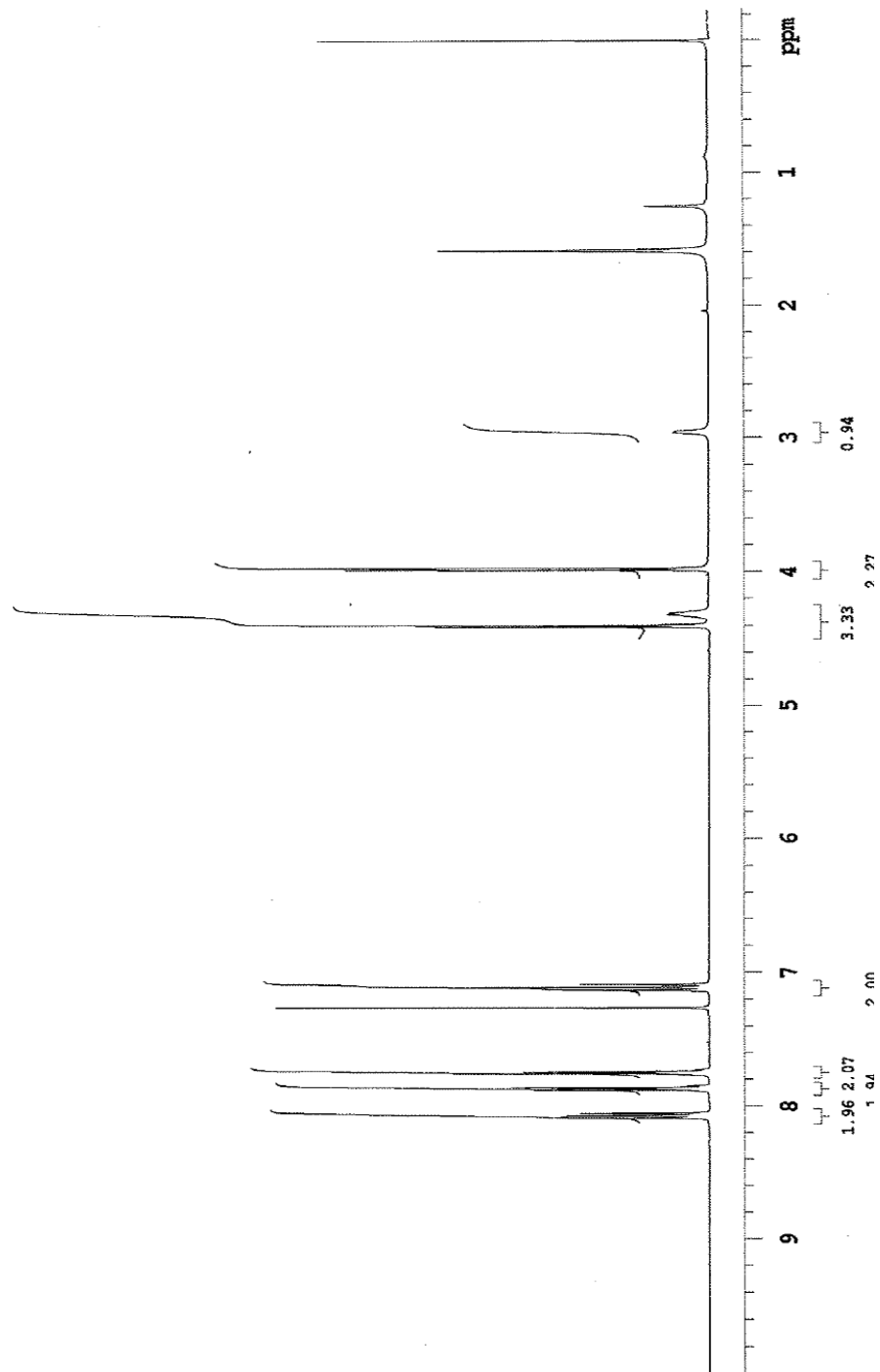
TDC-219 2-RGK-054 in CDCl₃

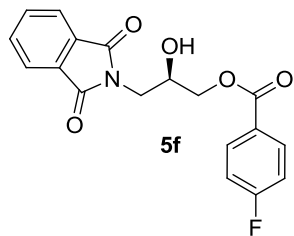
NMR-400

AS.No:ME1010/1966

Analyst:Haribabu.R

Date: 25 th Oct 2010





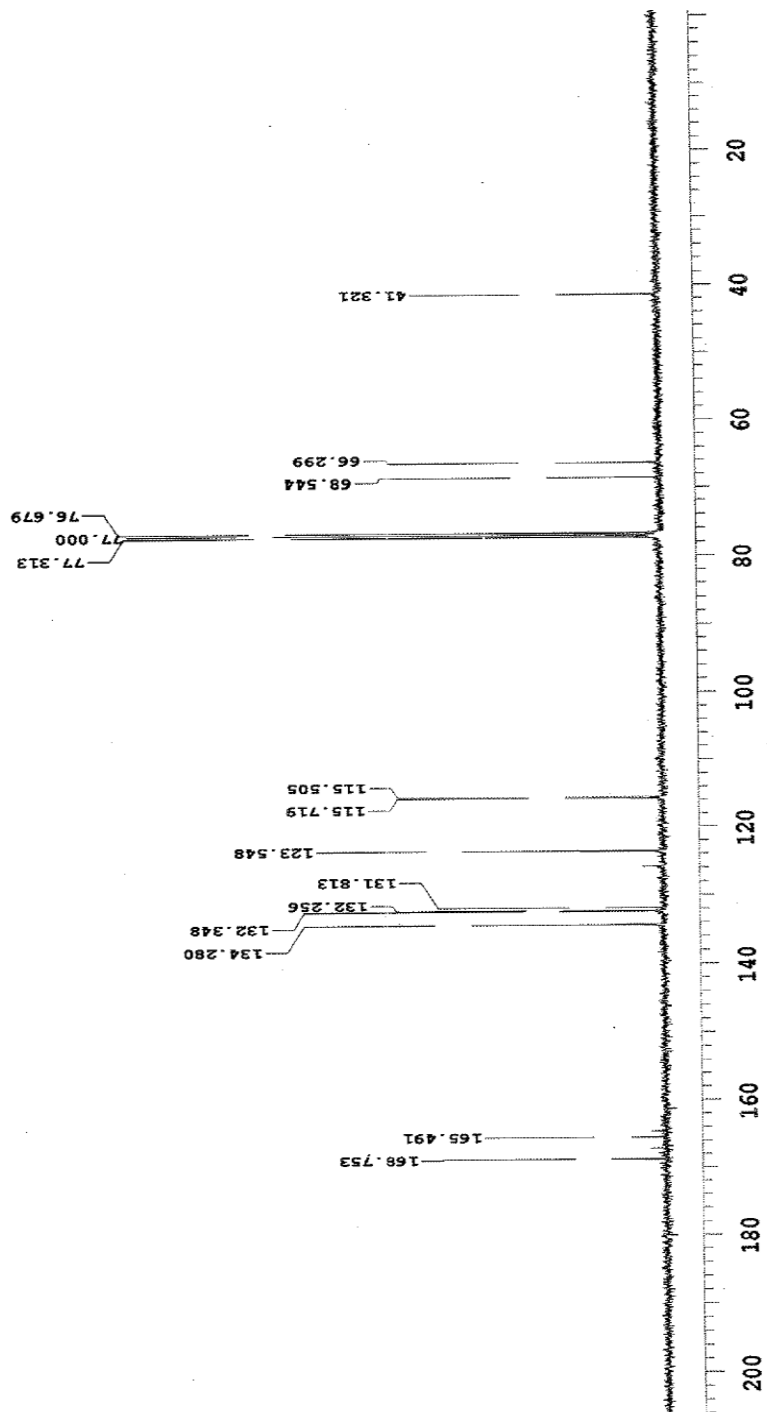
TDC-219 2-RGK-54 in CDCl₃

NMR-400

AR No: ME1010/2087

Analyst: Shruthi

Date: 25 th Oct 2010



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for iFIT = 3

Monoisotopic Mass, Even Electron Ions

75 formula(s) 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: 0-6 F: 0-1

38624004

011211_020 1s (0.277) Cm (18.20)

1: TOP MS ES+
4.54e+03



Minimum: -1.5
Maximum: 80.0

mass	Calc. Mass	DBE	DBE	i-FIT	Formula	
344.0928	344.0934	-0.6	1.7	11.5	3.0	C10 H15 N O5 F

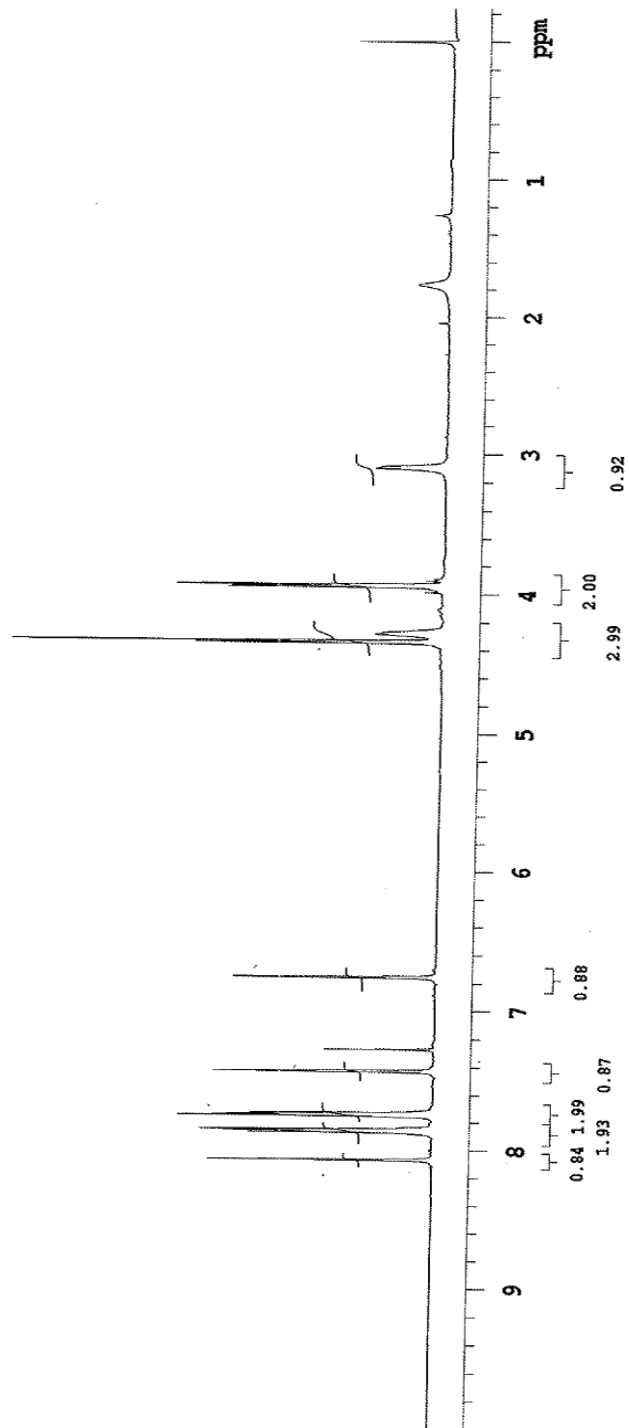
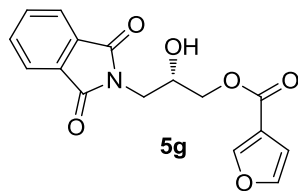
TDC-219 2-RGR-076 in CDCl₃

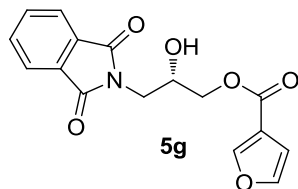
AR.No:ME0810/1812

NMR:400MHz

Analyst:Haribabu.R

Date:23rd Aug 2010





AR&D, Aurigene Discovery Technologies Ltd, Hyderabad

Instrument : Mercury Plus (Varian 400MHz)

Date & Time : Wed Aug 25 20:19:42 IST 2010

Recorded By : Haribabu.R

151
251

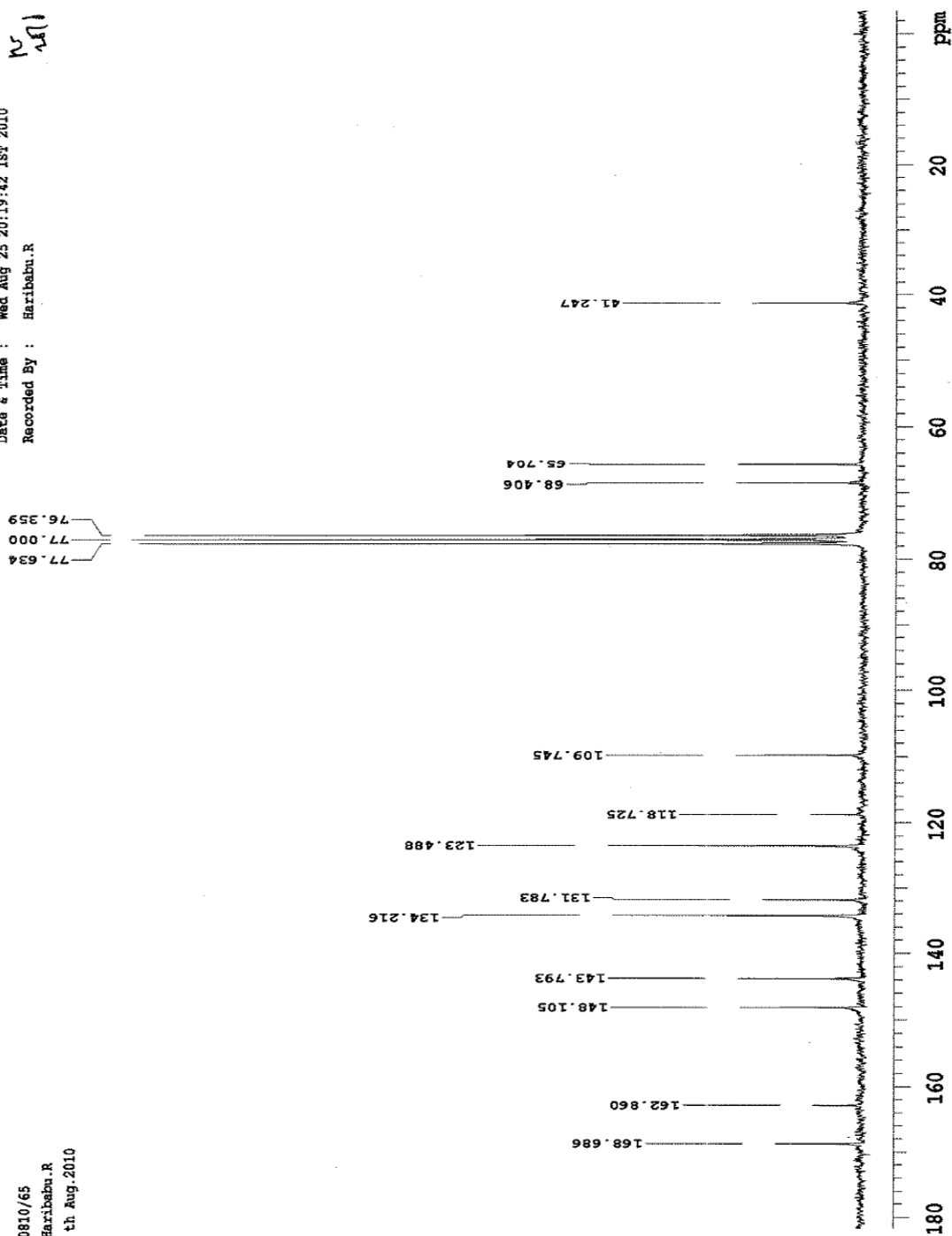
2/RSG/076 in CDCl₃

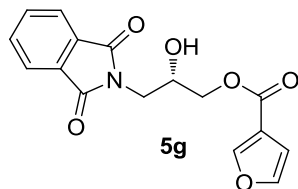
TDC-219

AR NO:GE0810/65

Analyst: Haribabu.R

Date: 24 th Aug.2010

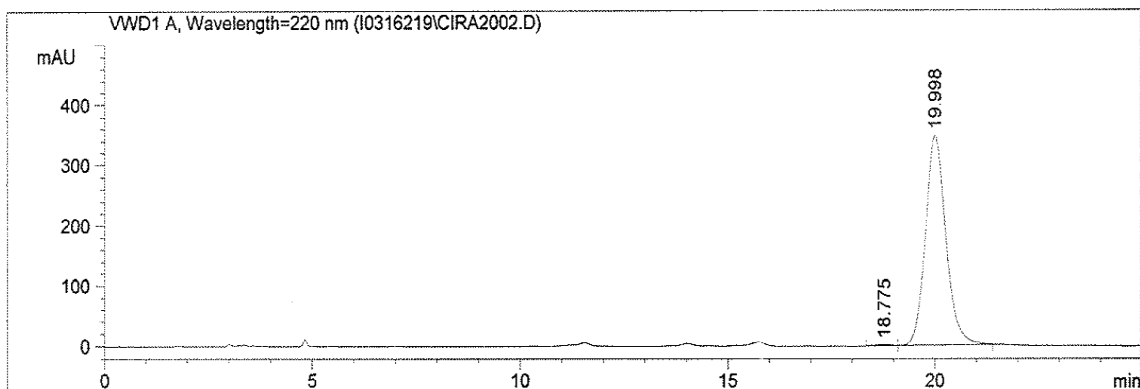




```

=====
Injection Date   : 9/16/2010 3:48:43 PM          Seq. Line :    2
Sample Name      : 2/RGK/076 FURAN              Location  : Vial 2
Acq. Operator    : Ashok                        Inj       :    1
Acq. Instrument  : CPS1/ARD/HPLC/003            Inj Volume: 5 µl
Acq. Method      : C:\HPCHEM\1\METHODS\CIRA2CH.M
Last changed     : 9/14/2010 8:10:18 PM by Muralikrishna Ch
Analysis Method  : C:\HPCHEM\1\METHODS\CIRA2CH.M
Last changed     : 9/17/2010 8:33:52 AM by RAMANJANEYULU
                  (modified after loading)
Column: CHIRAL PAK IA(250*4.6)5µm
Mobile Phase : n-Hexane:IPA:8:2
Flow: 1.0mL/min, Wavelength: 220nm,
Run time:25min

```



Area Percent Report

```

Sorted By       : Signal
Multiplier      : 1.0000
Dilution        : 1.0000
Use Multiplier & Dilution Factor with ISTDs

```

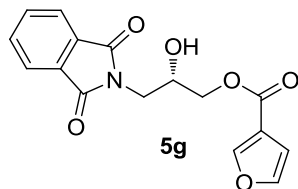
Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.775	BV	0.3991	44.23079	1.66289	0.3706
2	19.998	VB	0.5186	1.18905e4	347.51443	99.6294

Totals : 1.19347e4 349.17732

Results obtained with enhanced integrator!

*** End of Report ***



2-RGK-076.p1d

[Comment]

Sample name

Comment

User ramanjaneyulu

Workgroup ARND

Division

Company DRL

[Data Information]

Creation Date 10/1/2010 12:25 PM

[Measurement Information]

Instrument Name PL/118/002

Model Name P-2000

Serial No. A035861232

Polarizer Glan-Taylor Prism

Faraday Cell Flint Glass

Accessory PTC-203

Accessory S/N A014261234

Path Length 100 mm

Light Source Na

Monitor wavelength 589 nm

D.I.T. 5 sec

No. of cycle 5

Cycle interval 0 sec

Temp. Monitor Cell

Temp. Corr. Factor None

Aperture(S) 3.0mm

Aperture(L) Auto

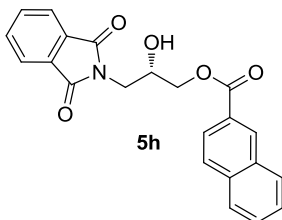
Mode Specific O.R.

Path Length 100 mm

Concentration 0.6139 w/v

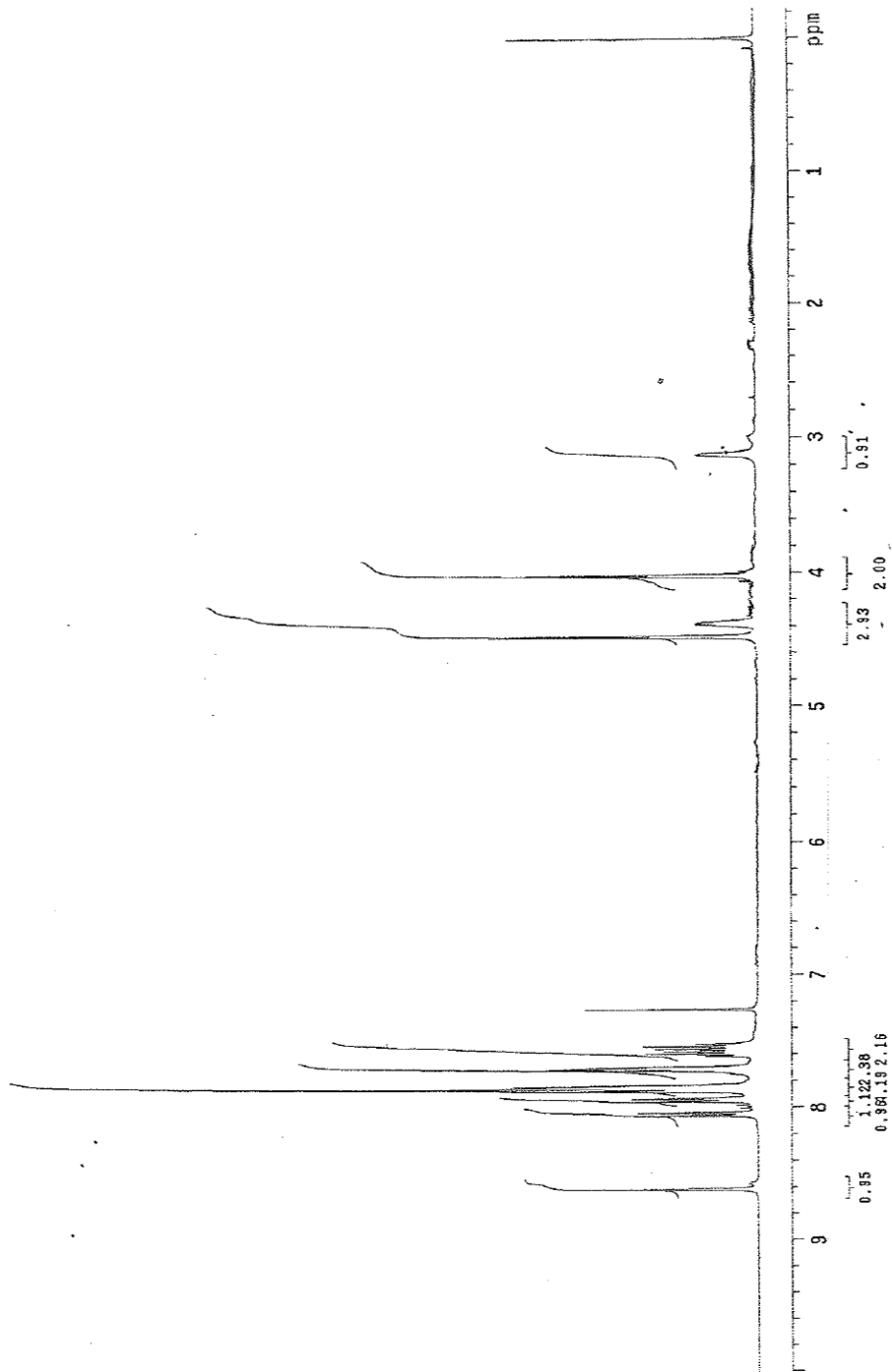
Factor 1

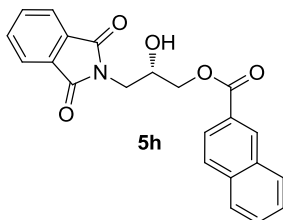
		No.	Sample No.	Mode	Calc. Data	Meas. Data	Monitor(deg)	Temperature(C)	Blank
1	*	1	2-RGK-076-1	Specific O.R.	-10.1515	-0.0623	-0.0538	24.66	0.0085
2	*	2	2-RGK-076-2	Specific O.R.	-9.4836	-0.0582	-0.0497	24.65	0.0085
3	*	3	2-RGK-076-3	Specific O.R.	-9.3370	-0.0573	-0.0488	24.64	0.0085
4	*	4	2-RGK-076-4	Specific O.R.	-9.3859	-0.0576	-0.0491	24.64	0.0085
5	*	5	2-RGK-076-5	Specific O.R.	-9.0927	-0.0558	-0.0473	24.63	0.0085
6	*	6	Avg.		-9.4901				
7		7	S.D		0.3968				
8		8	C.V		4.1809				



AR&D, Aurigene Discovery Technologies Ltd.
 Instrument : Mercury Plus (Varian 400MHz)
 Date & Time : Fri Sep 3 19:02:30 GMT 2010
 Recorded By : Haribabu.R

TDC-219 2/RGK/082 in CDCl3
 AR-NO:ME0910/148
 Date: 3rd Sept 2010
 Analyst:Haribabu.R





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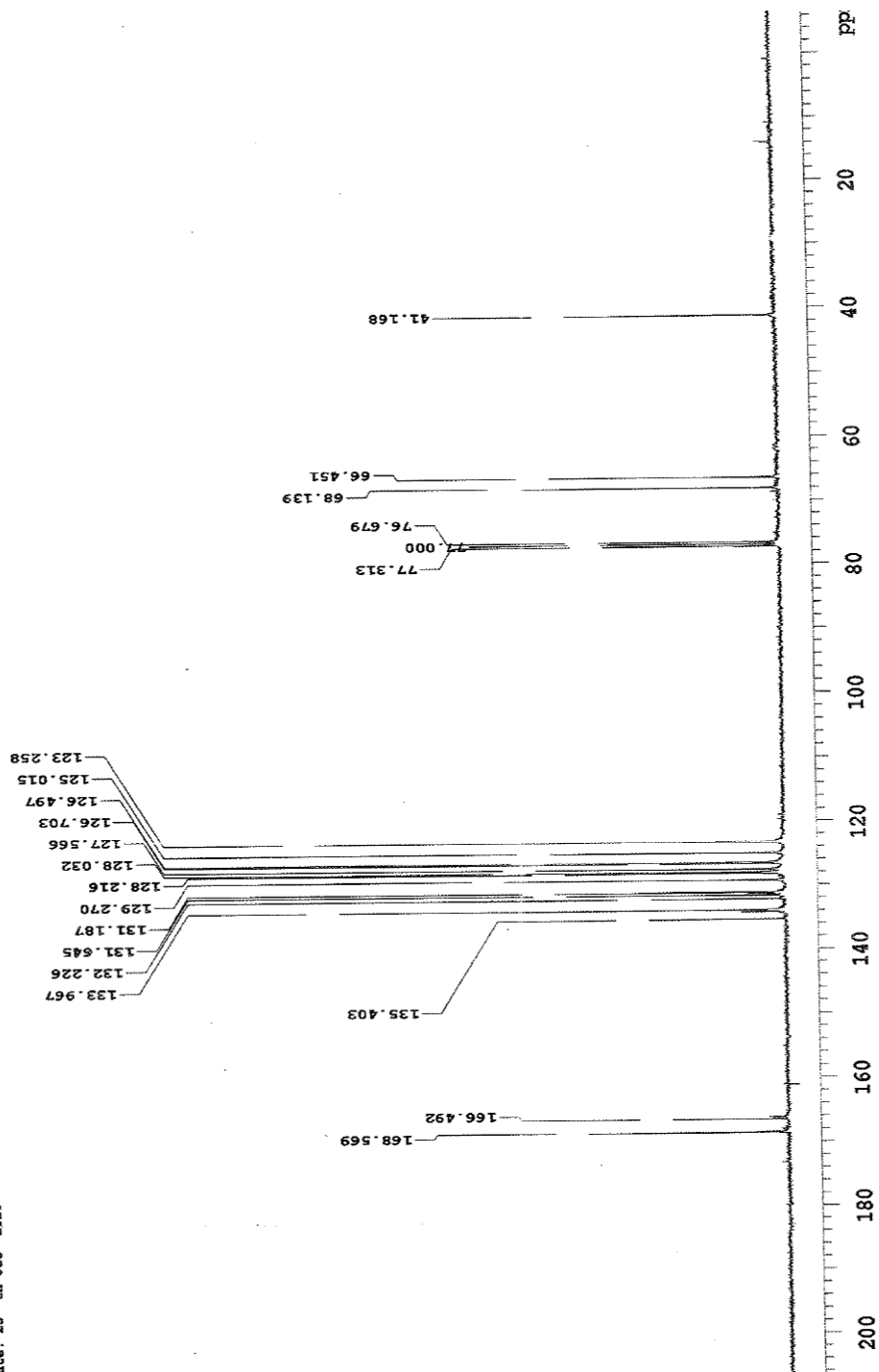
1DC-219 2-RGR-82 in CDCl₃

MMR-400

AR.No:ME1010/2086

Analyst: Shruthi

Date: 25 th Oct 2010



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

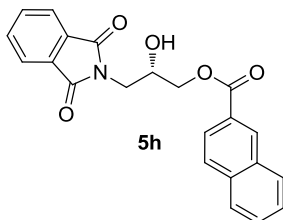
130 formulae evaluated with 1 result within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-30 N: 0-6 O: 6

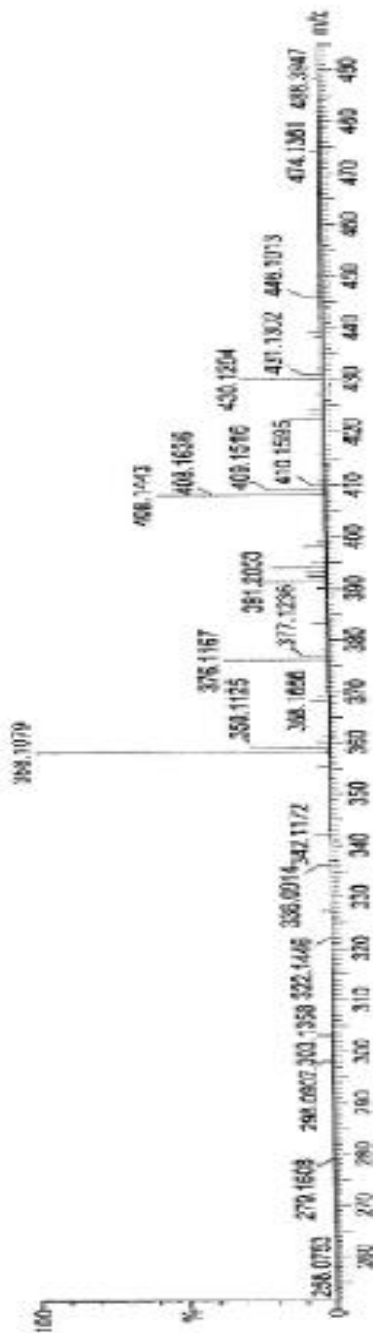
376X382

UTY211_08113 (0.289) Cm (13.218-14.010)

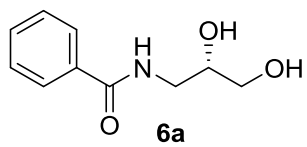


Page 1

1: TOF MS ES+
3.62e+004



Minimum:	5.0	5.0	-2.5			
Maximum:	5.0	5.0	80.0			
Mass	Calc. Mass	MEV	FORM	UNIT	I-FIT	Formula
376.1167	376.1165	-2.0	-4.0	14.5	3.0	C22 H19 N O5



3/6/10

TDC-219-2-RGX-090-1 in CD300

IR.No: M20910/748

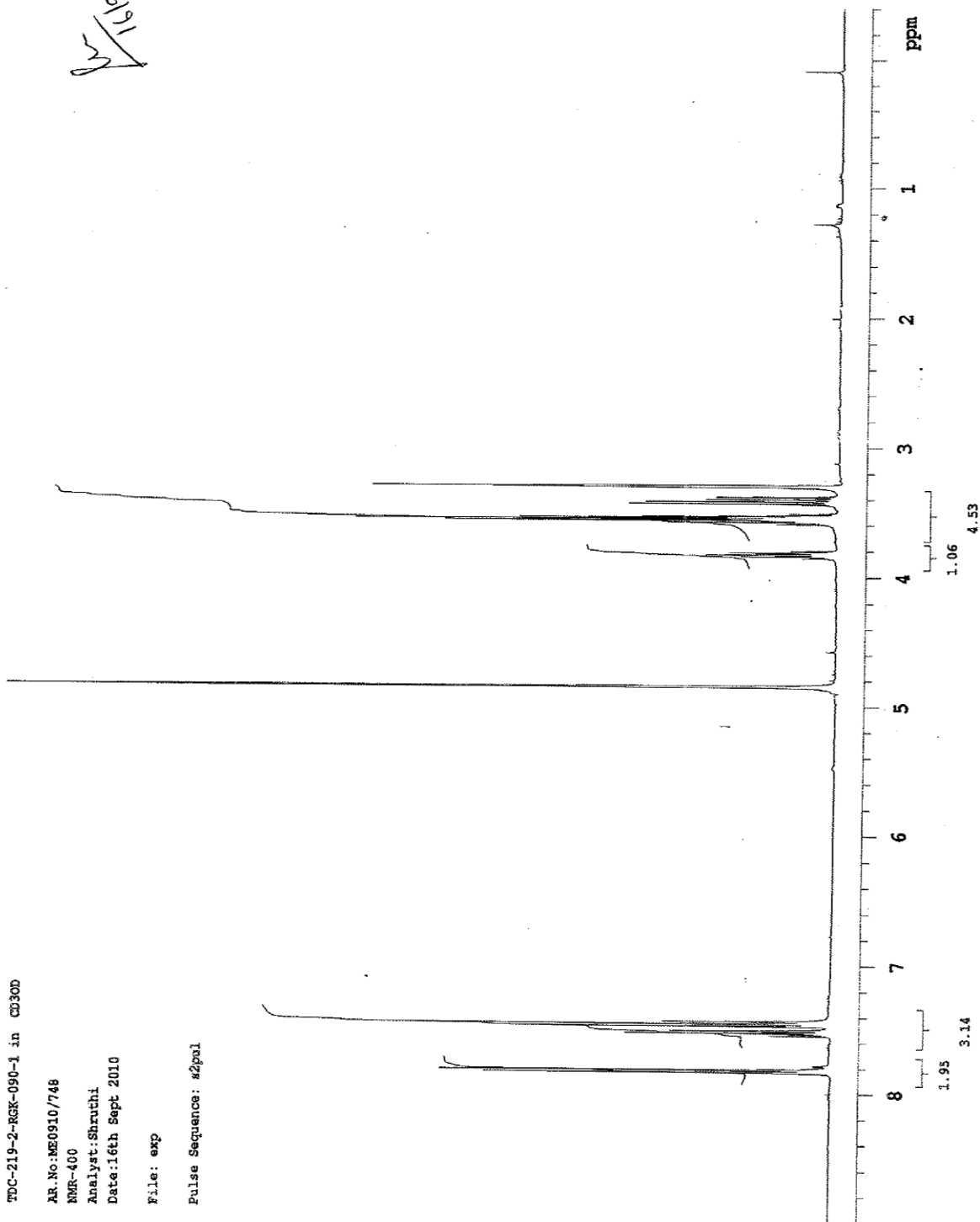
NMR-400

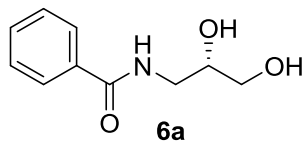
Analyst: Shruthi

Date: 16th Sept 2010

File: exp

Pulse Sequence: #2pul





AR&D, Aurigene Discovery Technologies Ltd, Hyderabad

Instrument : Gemini 2000 (Varian 200MHz)

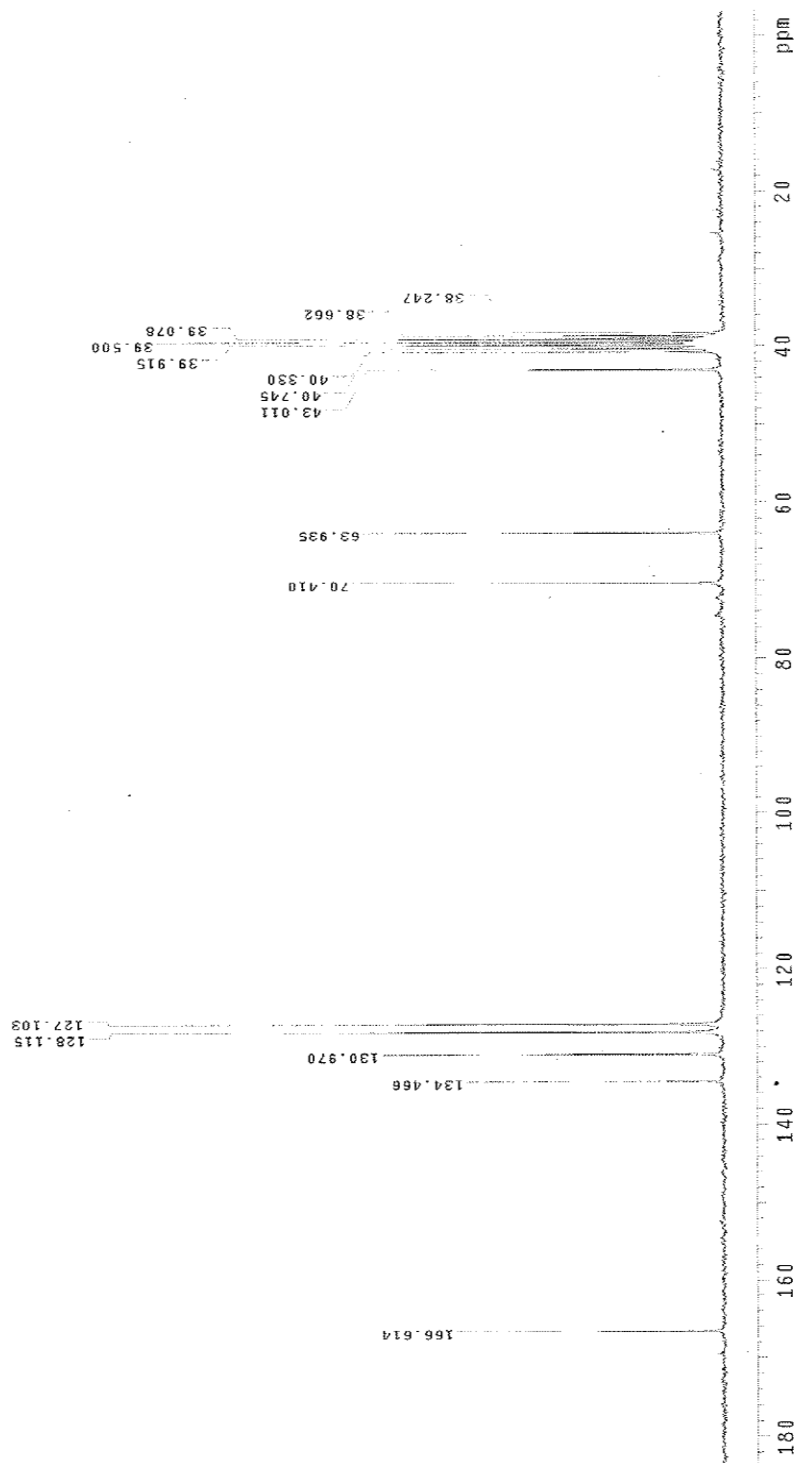
Date & Time : Fri Sep 3 11:55:08 GMT 2010

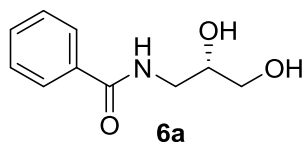
Recorded By : Haribabu.R

2-RGX-084 in DMSO
TDC-219

AR NO:GE0910/04
Analyst:Haribabu.R
Date: 03 rd Aug.2010

3/9





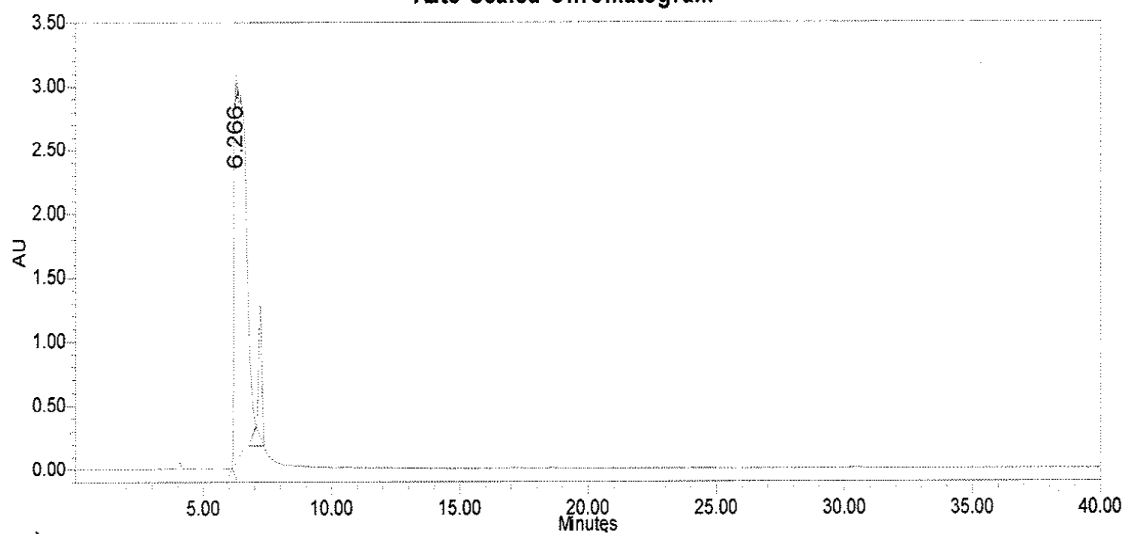
SAMPLE INFORMATION

Sample Name: 2/RGK/090
 Sample Type: Unknown
 Vial: 27
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 40.0 Minutes
 Sample Set Name: 10100101

Acquired By: System
 Date Acquired: 10/1/2010 1:21:38 PM
 Acq. Method Set: CIRA2
 Date Processed: 10/11/2010 5:11:16 PM
 Processing Method: cira2
 Channel Name: WvIn Ch2
 Proc. Chnl. Descr: PDA 220.0 nm

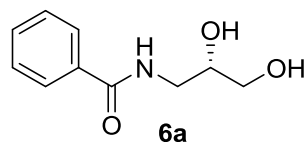
Column: Chiral pak IA(250x4.6mm,5μ)
 Mobile Phase:N-HEXANE:IPA(8:2)
 Flow:1.0ml/min,Wave Length:220nm,
 Column Temperature:40°C,Inj Vol:10ul,
 Runtime:25min,Dilut:mp

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area	% Area	Purity1 Angle	Purity1 Threshold	Purity1 Flag	USP Resolution	USP Tailing	% Height	RT Ratio
1		6.266	92918333	100.00					3.344986e+000	100.00	



2-RGK-064-.p1d

[Comment]

Sample name

Comment

User swapna

Workgroup ARND

Division

Company DRL

[Data Information]

Creation Date 10/25/2010 11:03 AM

[Measurement Information]

Instrument Name PL/118/002

Model Name P-2000

Serial No. A035861232

Polarizer Glan-Taylor Prism

Faraday Cell Flint Glass

Accessory PTC-203

Accessory S/N A014261234

Path Length 100 mm

Light Source Na

Monitor wavelength 589 nm

D.I.T. 5 sec

No. of cycle 5

Cycle interval 0 sec

Temp. Monitor Cell

Temp. Corr. Factor None

Aperture(S) 3.0mm

Aperture(L) Auto

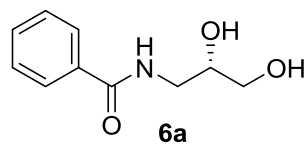
Mode Specific O.R.

Path Length 100 mm

Concentration 0.759 w/v

Factor 1

		No.	Mode	Calc. Data	Meas. Data	Monitor(deg)	Temperature(C)	Blank
1	*	1	Specific O.R.	-12.4401	-0.0944	-0.0869	23.88	0.0075
2	*	2	Specific O.R.	-12.4532	-0.0945	-0.0870	23.96	0.0075
3	*	3	Specific O.R.	-12.2688	-0.0931	-0.0856	24.02	0.0075
4	*	4	Specific O.R.	-12.4928	-0.0948	-0.0873	24.07	0.0075
5	*	5	Specific O.R.	-12.5455	-0.0952	-0.0877	24.11	0.0075
6	*	6		-12.4401				
7		7		0.1042				
8		8		0.8373				



Page 1

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: C₉H₁₁N

Number of isotope peaks used for FIT = 3

Monoisotopic Mass, Even Electron Ions

97 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: 0-5 O: 0-6

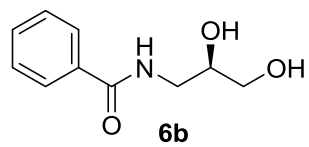
355K004

1.01211_003_25 (0.413) Cm (21.2%)

1: TOF MS ES+
1.42e+004



Minimum:	-1.5		
Maximum:	80.0		
Mass	Calc. Mass	MSA	PPM
186.0967	186.0976	-0.7	-3.6
		DBE	1-FIT
		4.5	2.5
		C10	H14 N O3
			Formula



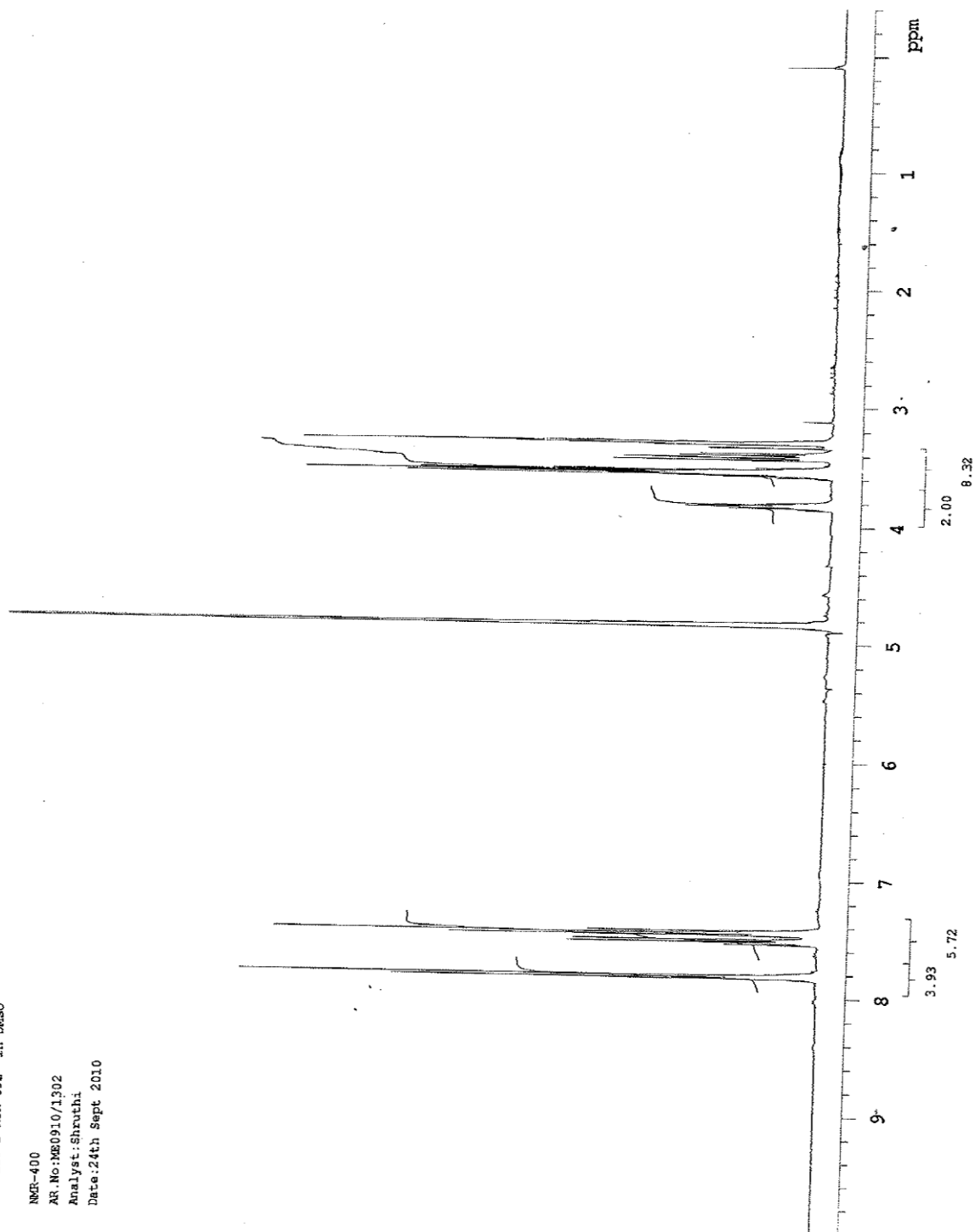
TDC-219-2-RGR-092 in DMSO

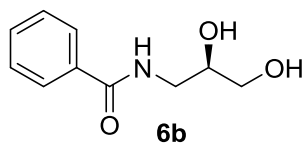
NMR-400

AN.No:ME0910/1302

Analyst: Shruthi

Date: 24th Sept 2010





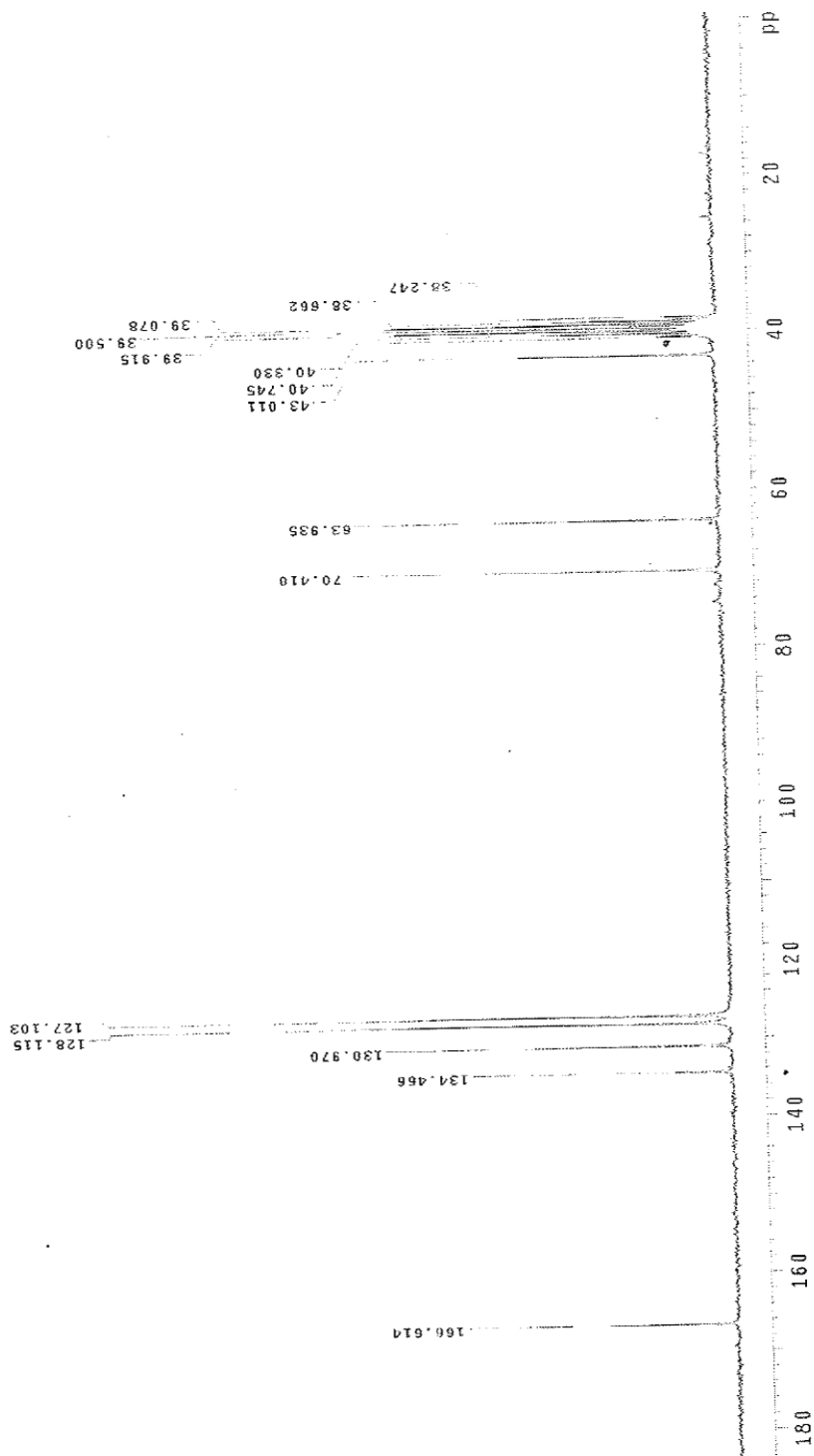
TDC-219-2-RGK-093 in DMSO

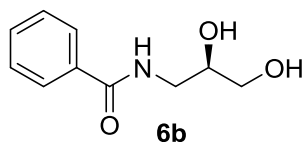
NMR-400

AR.No:ME0910/1303

Analyst:Shruthi

Date:24th Sept 2010



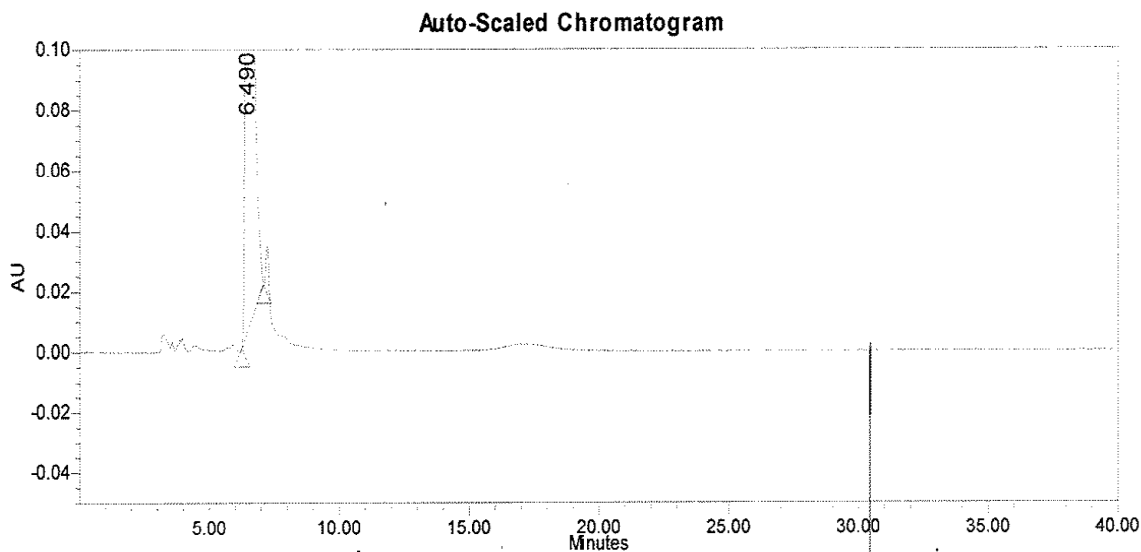


SAMPLE INFORMATION

Sample Name: 2/RGK/092
 Sample Type: Unknown
 Vial: 25
 Injection #: 1
 Injection Volume: 10.00 ul
 Run Time: 40.0 Minutes
 Sample Set Name 10100101

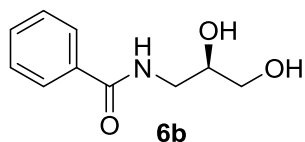
Acquired By: System
 Date Acquired: 10/1/2010 11:59:23 AM
 Acq. Method Set: CIRA2
 Date Processed: 10/11/2010 5:10:43 PM
 Processing Method: cira2
 Channel Name: WvIn Ch9
 Proc. Chnl. Descr. PDA 220.0 nm

Column: Chiral pak IA(250x4.6mm,5μ)
 Mobile Phase:N-HEXANE:IPA(8:2)
 Flow:1.0ml/min,Wave Length:220nm,
 Column Temperature:40°C,Inj Vol:10ul,
 Runtime:25min,Dilut: mp



Peak Results

	Name	RT	Area	% Area	Purity1 Angle	Purity1 Threshold	Purity1 Flag	USP Resolution	USP Tailing	% Height	RT Ratio
1		6.490	5921473	100.00					1.790058e+000	100.00	



2-RGK-092 - RIIsomer.p1d

[Comment]

Sample name

Comment

User

ramanjaneyulu

Workgroup

ARND

Division

Company

DRL

[Data Information]

Creation Date

10/19/2010 3:34 PM

[Measurement Information]

Instrument Name PL/118/002

Model Name P-2000

Serial No. A035861232

Polarizer Glan-Taylor Prism

Faraday Cell Flint Glass

Accessory PTC-203

Accessory S/N A014261234

Path Length 100 mm

Light Source Na

Monitor wavelength 589 nm

D.I.T. 5 sec

No. of cycle 5

Cycle interval 0 sec

Temp. Monitor Cell

Temp. Corr. Factor None

Aperture(S) 3.0mm

Aperture(L) Auto

Mode Specific O.R.

Path Length 100 mm

Concentration 0.88 w/v

Factor 1

		No.	Mode	Calc. Data	Meas. Data	Monitor(deg)	Temperature(C)	Blank
1	*	1	Specific O.R.	12.3341	0.1085	0.1085	23.40	-0.0000
2	*	2	Specific O.R.	11.9818	0.1054	0.1054	23.47	-0.0000
3	*	3	Specific O.R.	12.0841	0.1063	0.1063	23.51	-0.0000
4	*	4	Specific O.R.	12.3341	0.1085	0.1085	23.54	-0.0000
5	*	5	Specific O.R.	12.2432	0.1077	0.1077	23.56	-0.0000
6	*	6		12.1955				
7		7		0.1571				
8		8		1.2884				

