

# Supporting Information

for

## **Synthesis of novel 5-alkyl/aryl/heteroaryl substituted diethyl 2*H*-pyrrole-4,4(3*H*)-dicarboxylates by aziridine ring expansion of 2-[(aziridin-1-yl)-1-alkyl/aryl/heteroaryl-methylene]malonic acid diethyl esters**

Satish S. More<sup>\*1</sup>, T. Krishna Mohan<sup>1</sup>, Y. Sateesh Kumar<sup>1</sup>, U. K. Syam Kumar<sup>1</sup> and Navin B. Patel<sup>2</sup>

Address: <sup>1</sup>Technology Development centre, Custom Pharmaceutical Services, Dr. Reddy's Laboratories Ltd., Miyapur, Hyderabad -500 049, India and <sup>2</sup>Department of Chemistry, Veer Narmad South Gujarat University, Surat, India

Email: Satish S. More\* - satishsm@drreddys.com

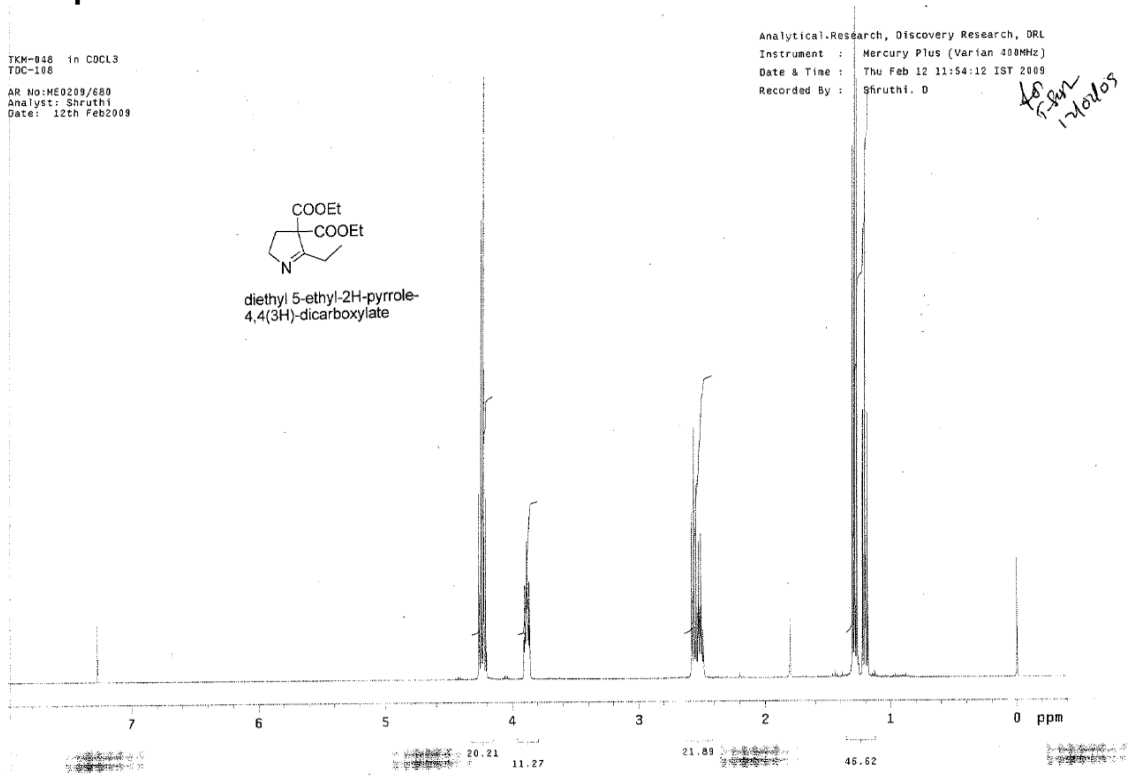
\* Corresponding author

<sup>1</sup>H NMR, <sup>13</sup>C NMR, IR, and mass spectra of **21b**, **21d**, **21g**, **21h**, **21i**, **21j**, **23**, **24**, **28**, **29**, **31**, **32** and HRMS spectra of **21a–21j**, **23**, **24**, **29**, and **32**.

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## $^1\text{H}$ NMR spectrum of 21b

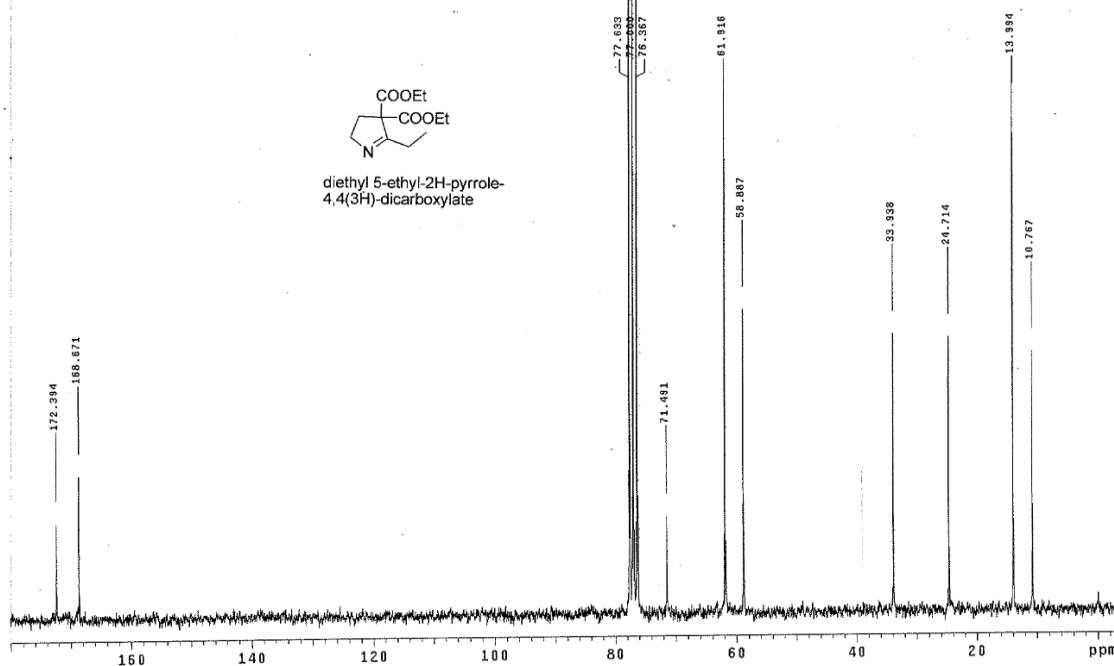


### <sup>13</sup>C NMR spectrum of 21b

TKM-048 in CDCl<sub>3</sub>  
TDC-108  
AR.No: GE0209/49  
Analyst: Srikanth.A  
Date: 20th Feb 2009

Analytical Research, Discovery Research; UKR  
Instrument : Gemini 2000 (Varian 200MHz)  
Date & Time : Fri Feb 20 11:01:00 GMT 2009  
Recorded By : Shruthi.D

*SR*  
20/2/09



### Mass spectrum of 21b

CPS,MIYAPUR

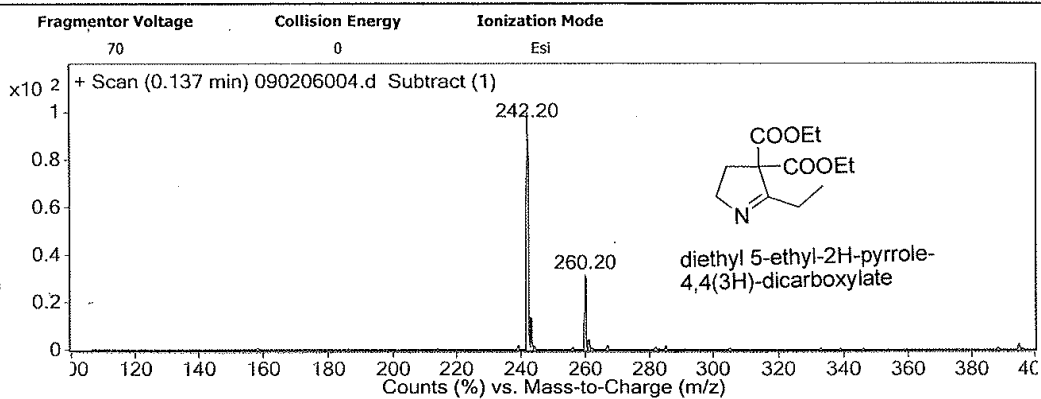
### Mass Analysis Report

DR. RIDDY'S

Data Filename 090206004.d  
Sample Type Sample  
Instrument Name Instrument 1  
Acq Method  
DA Method DA.m

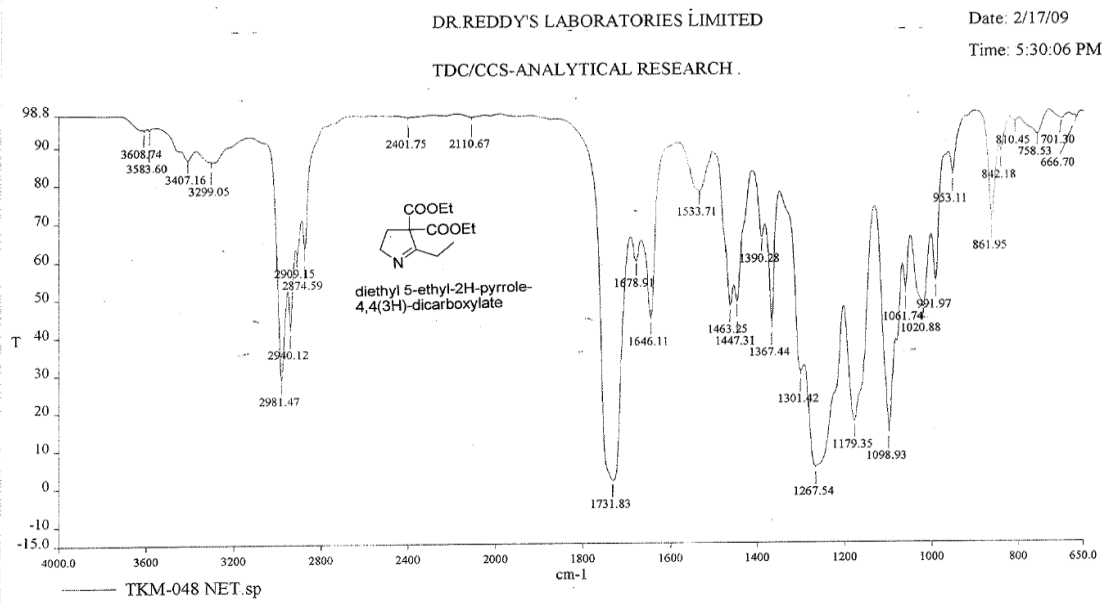
Sample Name TKM-048  
Position Vial 74  
User Name  
IRM Calibration Status **Success**  
Comment

#### User Spectra



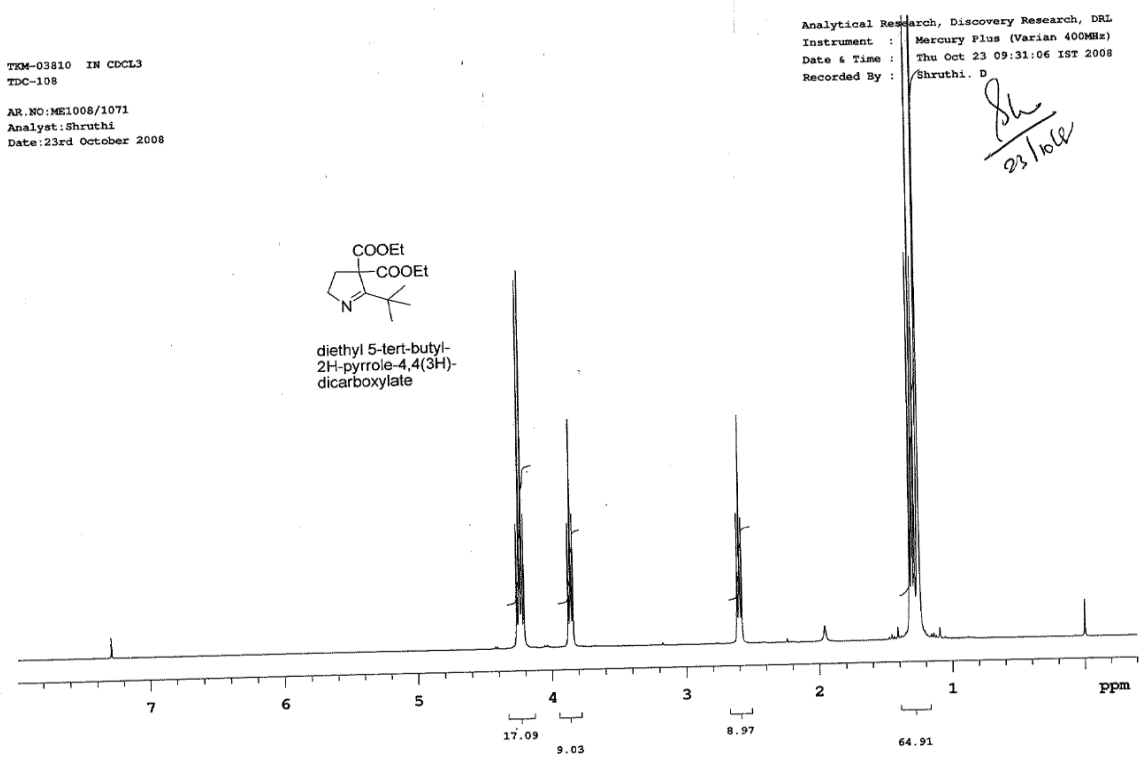
--- End Of Report ---

# IR spectrum of 21b



ARD09052/AP/084  
Analyst: APARNA  
SIGN: *[Signature]*  
17/02/09

# <sup>1</sup>H NMR spectrum of 21d

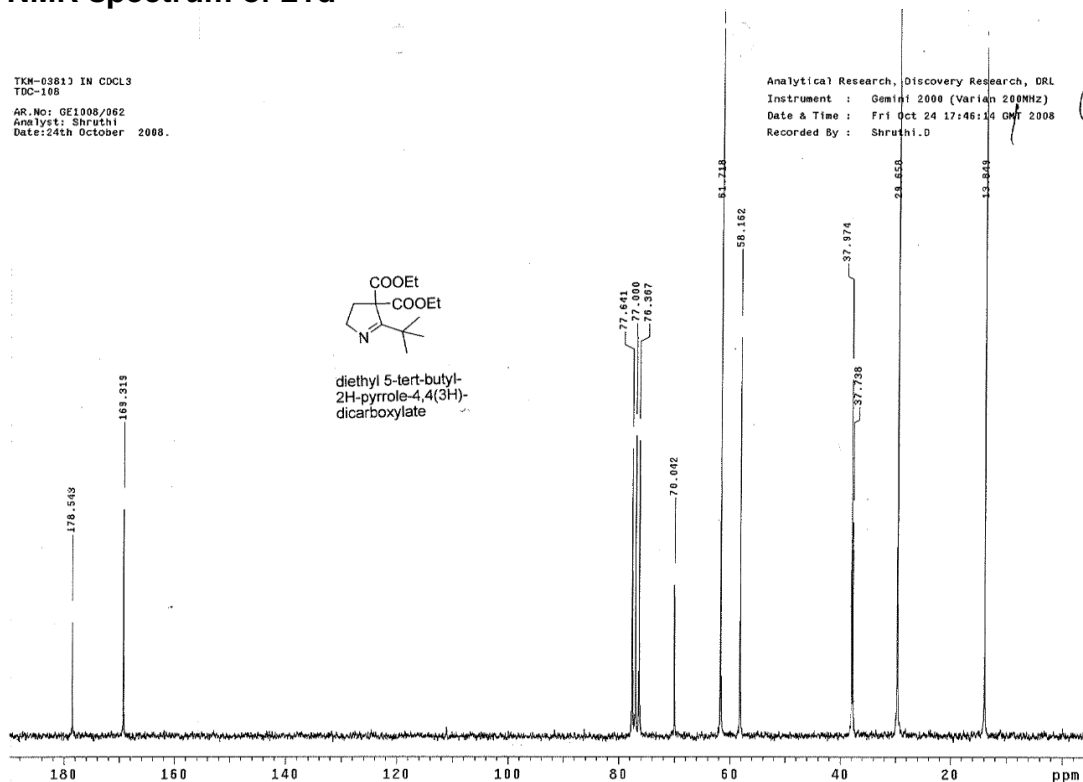


# <sup>13</sup>C NMR spectrum of 21d

TKM-03810 IN CDCL3  
TDC-108  
AR.No: GE1908/062  
Analyst: Shruthi  
Date: 24th October 2008.

Analytical Research, Discovery Research, ORL  
Instrument : Gemini 2000 (Varian 200MHz)  
Date & Time : Fri Oct 24 17:46:14 GMT 2008  
Recorded By : Shruthi.D

*Shruthi*  
*24/10/08*



## Mass Spectra of 21d

CPS,MIYAPUR

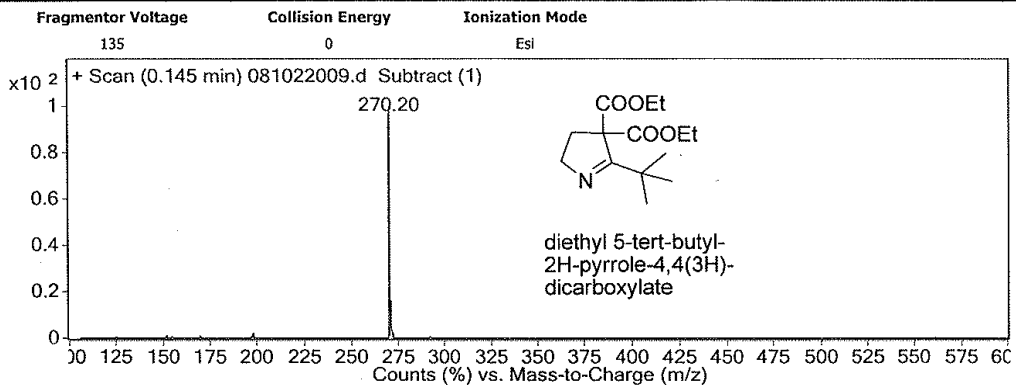
## Mass Analysis Report

DR. REDDY'S

Data Filename: 081022009.d  
Sample Type: Sample  
Instrument Name: Instrument 1  
Acq Method: DA.m  
DA Method: DA.m

Sample Name: TKM-03810  
Position: Vial 9  
User Name:  
IRM Calibration Status: **Success**  
Comment:

### User Spectra



--- End Of Report ---

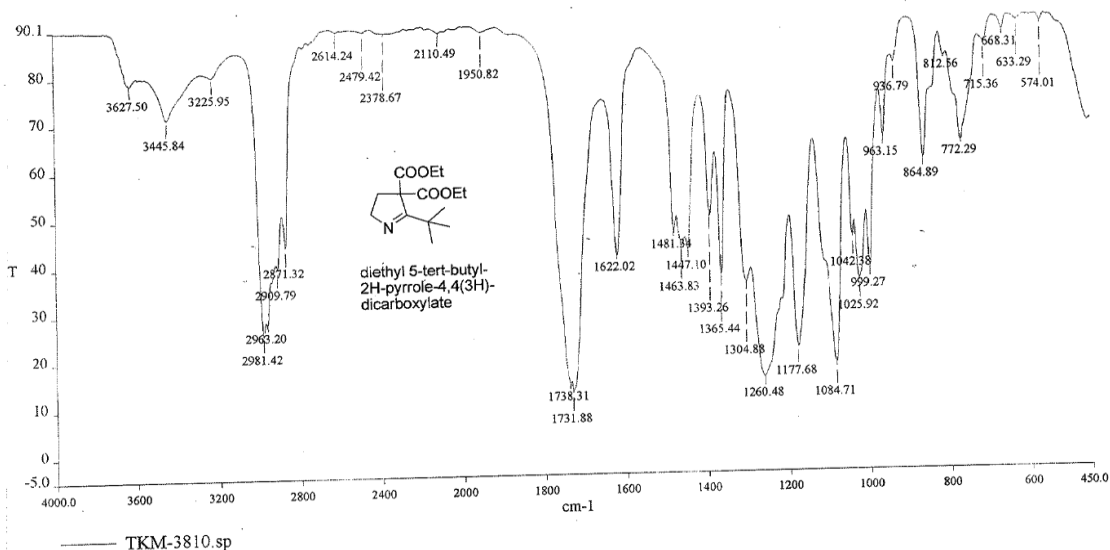
# IR spectrum of 21d

DR.REDDY'S LABORATORIES LIMITED

Date: 1/19/09

Time: 12:48:33 PM

TDC/CCS-ANALYTICAL RESEARCH.



AR09052/19/018  
 Analyst: APARNA  
 SIGN: *[Signature]*  
 19/01/09

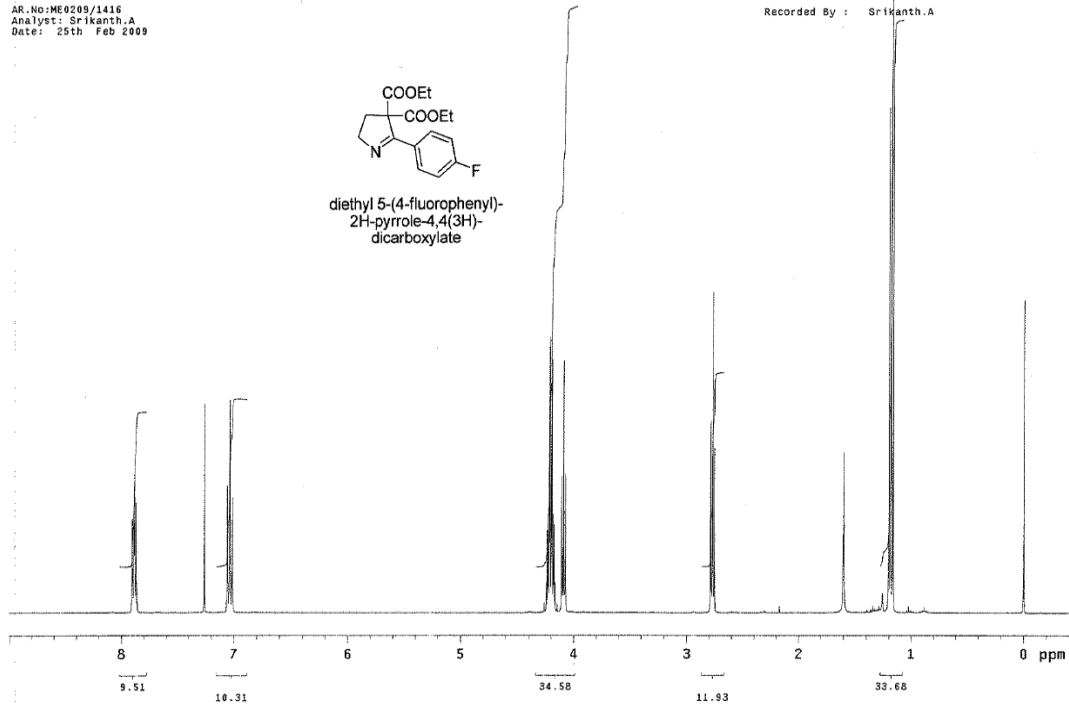
# <sup>1</sup>H NMR spectrum of 21g

TKM-852 in CDCl3  
 TDC-108

AR.No:ME0209/1416  
 Analyst: Srikanth.A  
 Date: 25th Feb 2009

Analytical Research, Discovery Research, DRL  
 Instrument : Mercury Plus (Varian 400MHz)  
 Date & Time : Wed Feb 25 16:33:05 IST 2009  
 Recorded By : Srikanth.A

*[Handwritten Signature]*  
 25/2/09



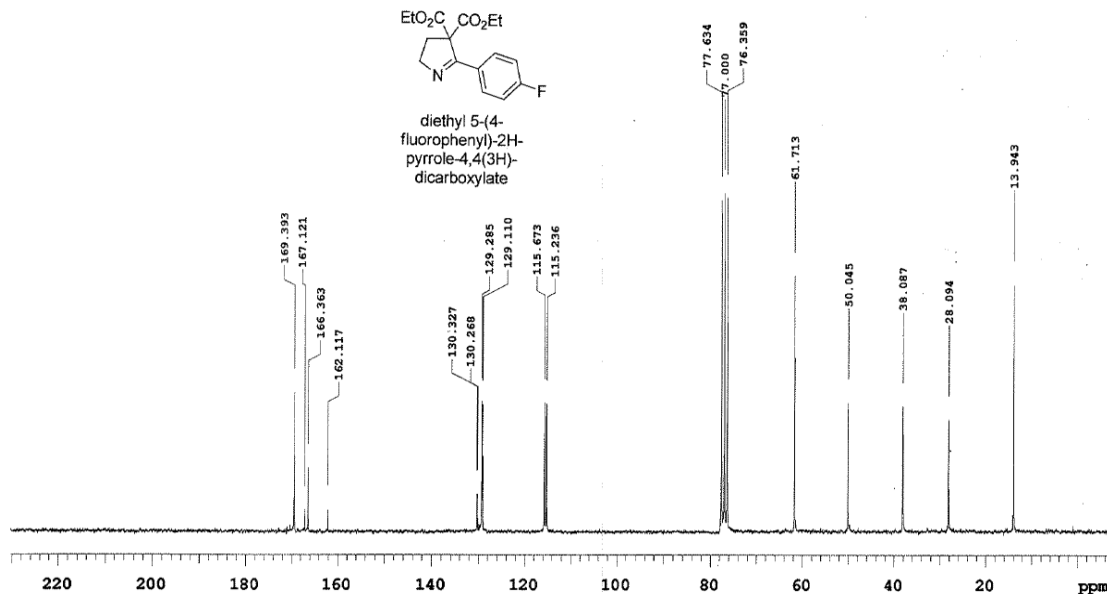
# <sup>13</sup>C NMR spectrum of 21g

TKM05208 in CDCl<sub>3</sub>  
TDC-219

AR NO: GE0810/70  
Analyst: Haribabu.R  
Date: 26 th Aug. 2010

AR&D, Aurigene Discovery Technologies Ltd, Hyderabad  
Instrument : Mercury Plus (Varian 400MHz)  
Date & Time : Fri Aug 27 17:03:09 IST 2010  
Recorded By : Haribabu.R

21g



## Mass spectrum of 21g

CPS,MIYAPUR

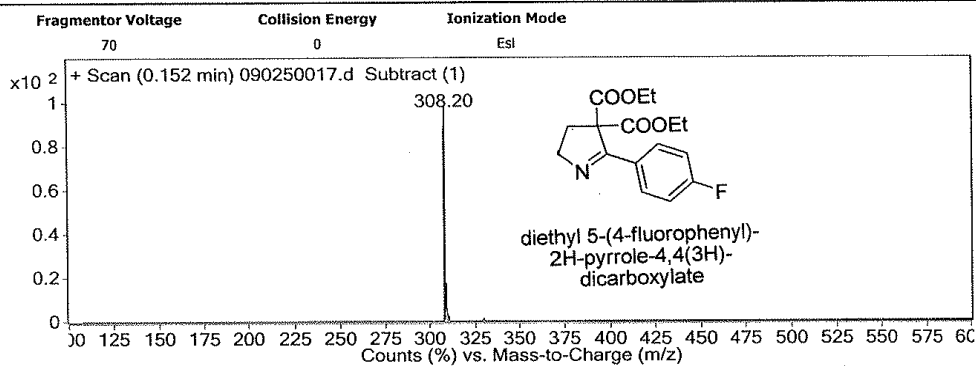
## Mass Analysis Report

Dr. REDDY'S

Data Filename: 090250017.d  
Sample Type: Sample  
Instrument Name: Instrument 1  
Acq Method: ESI.m  
DA Method: DA.m

Sample Name: TKM-052  
Position: Vial 39  
User Name:  
IRM Calibration Status: Success  
Comment:

### User Spectra



--- End Of Report ---

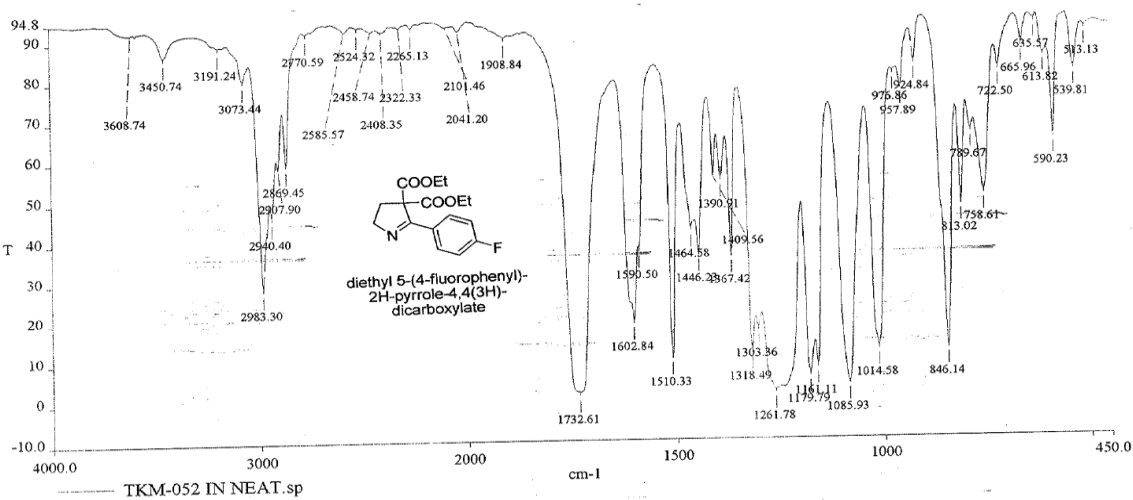
# IR spectrum of 21g

DR. REDDY'S LABORATORIES LIMITED

Date: 3/3/09

Time: 5:20:29 PM

TDC/CCS-ANALYTICAL RESEARCH



Analyst: SHYAM

SIGN: *[Signature]*

03/03/09

ARO0906918Am1004

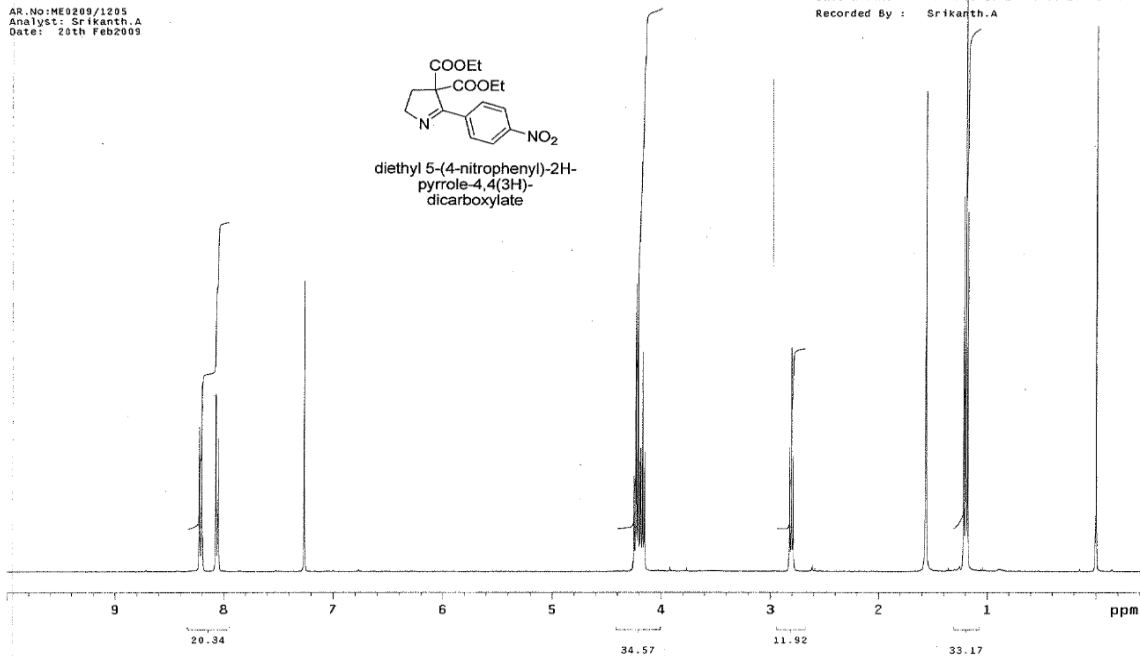
# <sup>1</sup>H NMR spectrum of 21h

TKM-055 IN CDCl3  
TDC-108

AR.No:ME0209/1205  
Analyst: Srikanth.A  
Date: 23th Feb2009

Analytical Research, Discovery Research, DRL  
Instrument : Mercury Plus (Varian 400MHz)  
Date & Time : Fri Feb 20 14:45:33 IST 2009  
Recorded By : Srikanth.A

*[Signature]*  
03/03/09



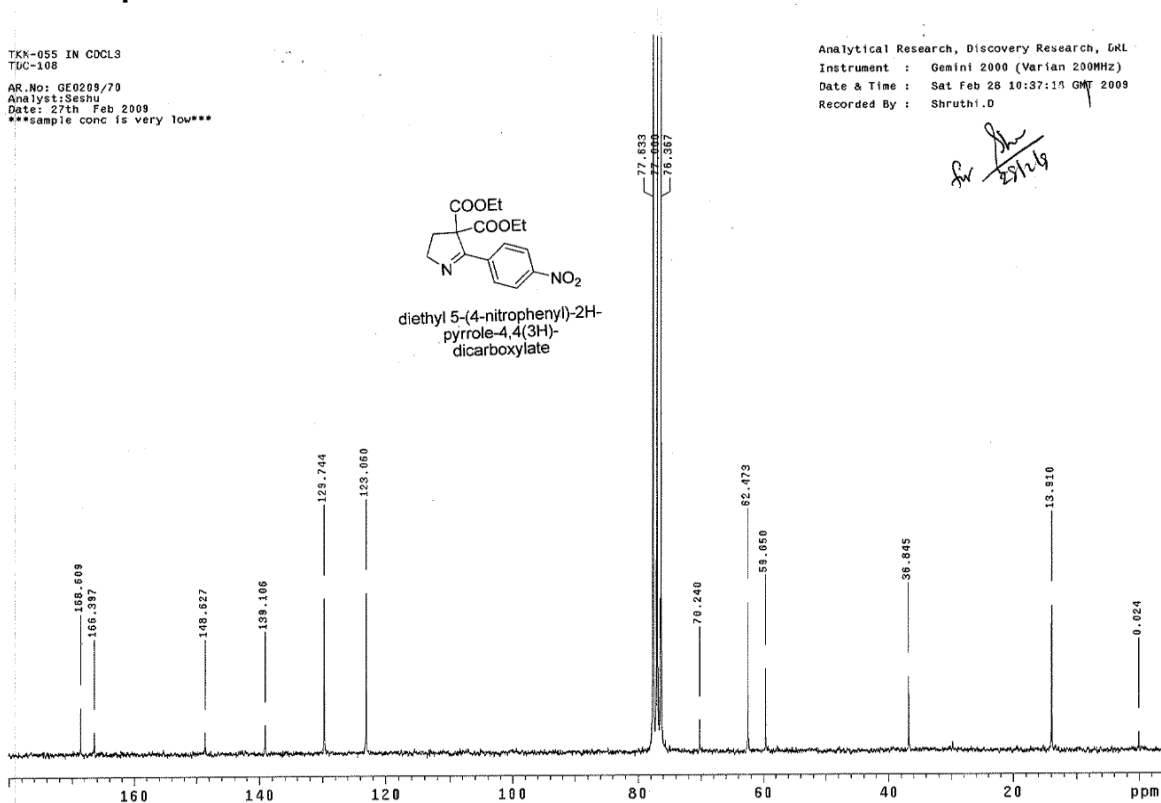


# <sup>13</sup>C NMR spectrum of 21h

TKM-055 IN CDCL3  
TDC-108  
AR.No: GE0209/70  
Analyst: Seshu  
Date: 27th Feb 2009  
\*\*\*sample conc is very low\*\*\*

Analytical Research, Discovery Research, GRL  
Instrument : Gemini 2000 (Varian 200MHz)  
Date & Time : Sat Feb 28 10:37:10 GMT 2009  
Recorded By : Shruthi.D

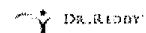
*for Seshu*  
25/2/09



# Mass spectrum of 21h

CPS,MIYAPUR

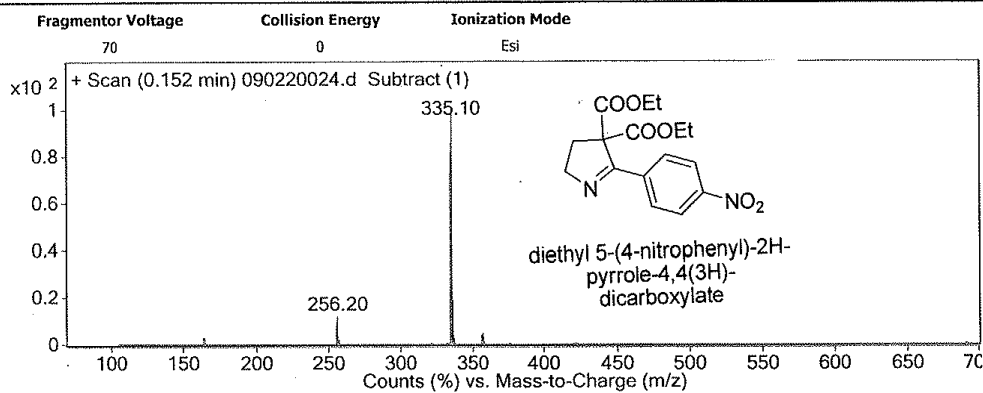
## Mass Analysis Report



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Sample Type Sample  
Instrument Name Instrument 1  
Acq Method ESI.m  
DA Method DA.m

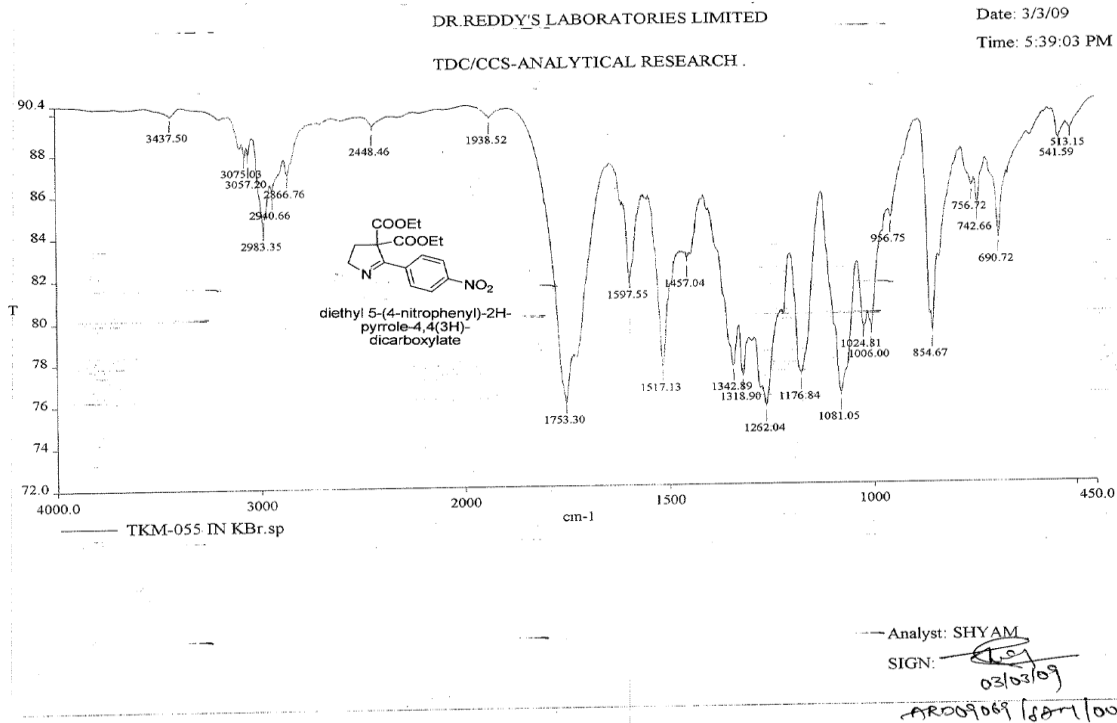
Sample Name TKM-055  
Position Vial 22  
User Name  
IRM Calibration Status Success  
Comment

### User Spectra

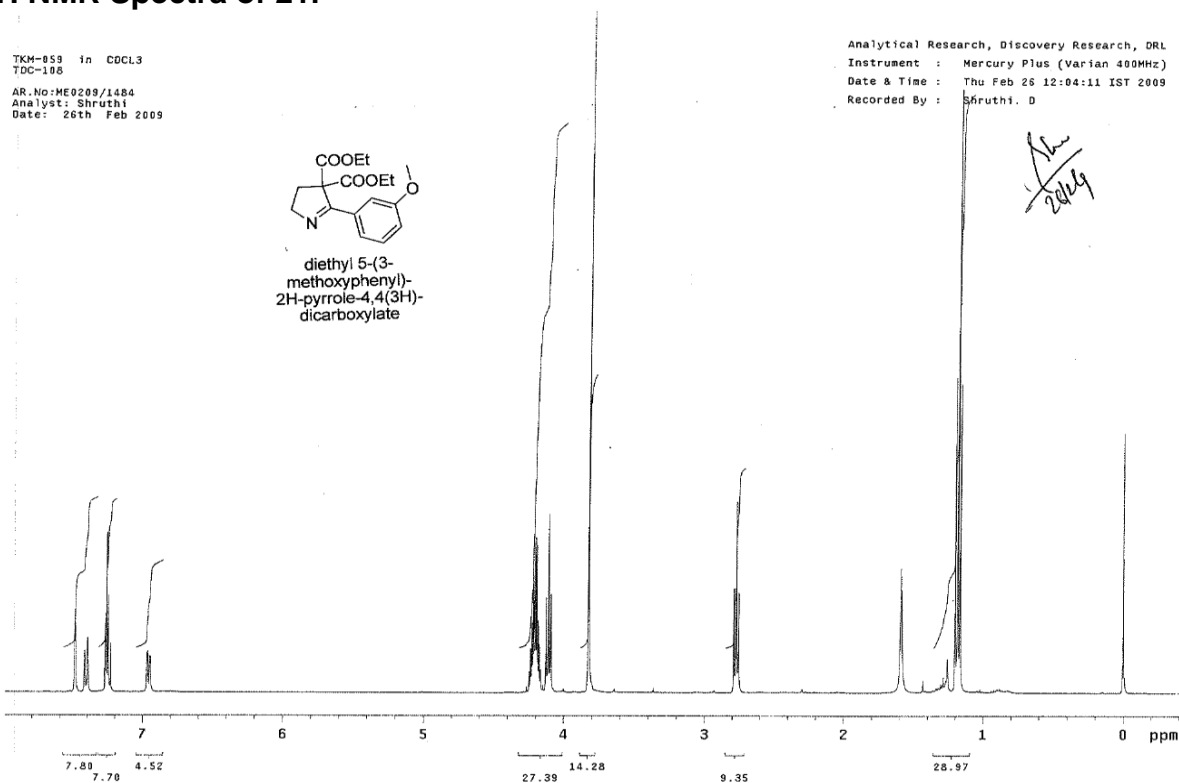


--- End Of Report ---

# IR spectrum of 21h



# <sup>1</sup>H NMR Spectra of 21i



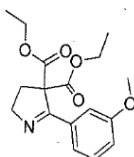
# <sup>13</sup>C NMR spectrum of 21i

TKM05908 in CDC13  
TDC-219

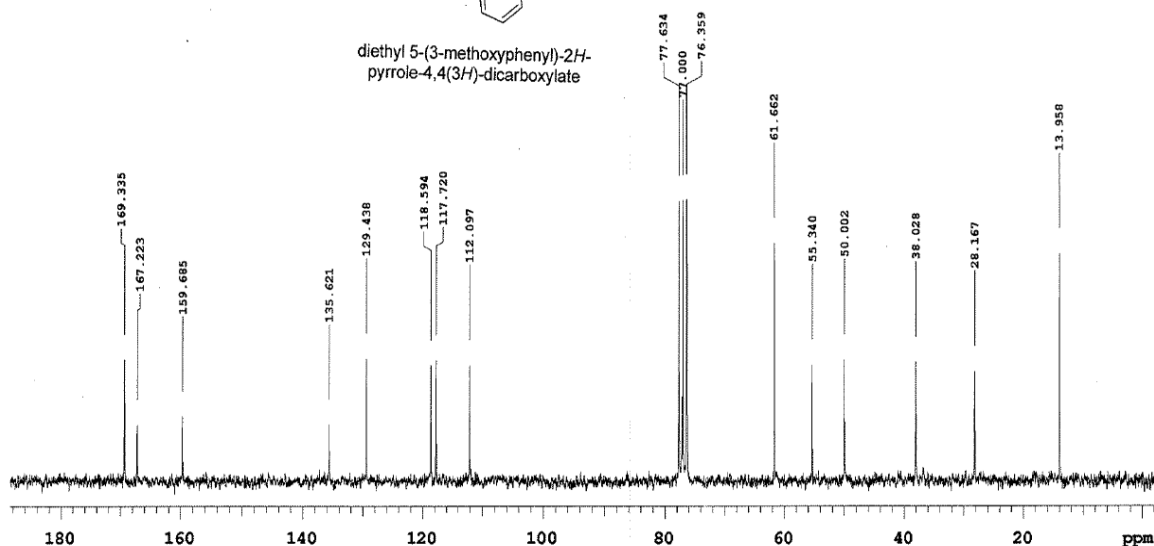
AR NO: GR0810/72  
Analyst: Haribabu.R  
Date: 27 th Aug.2010

AR&D, Aurigene Discovery Technologies Ltd, Hyderabad  
Instrument : Mercury Plus (Varian 400MHz)  
Date & Time : Fri Aug 27 17:03:59 IST 2010  
Recorded By : Haribabu.R

5K



diethyl 5-(3-methoxyphenyl)-2H-pyrrole-4,4(3H)-dicarboxylate



## Mass spectrum of 21i

CPS,MIYAPUR

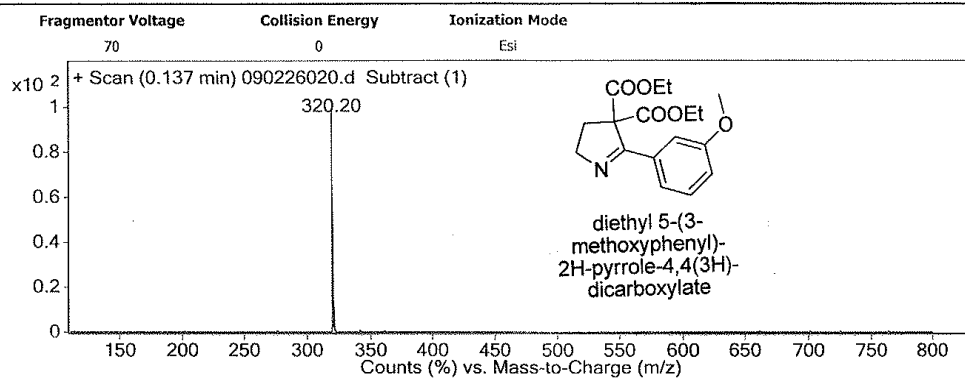
## Mass Analysis Report

DR. REDDY'S

Data Filename: 090226020.d  
Sample Type: Sample  
Instrument Name: Instrument 1  
Acq Method: ESI.m  
DA Method: Amcscine.m

Sample Name: TKM-059  
Position: Vial 30  
User Name:  
IRM Calibration Status: Success  
Comment:

### User Spectra



--- End Of Report ---

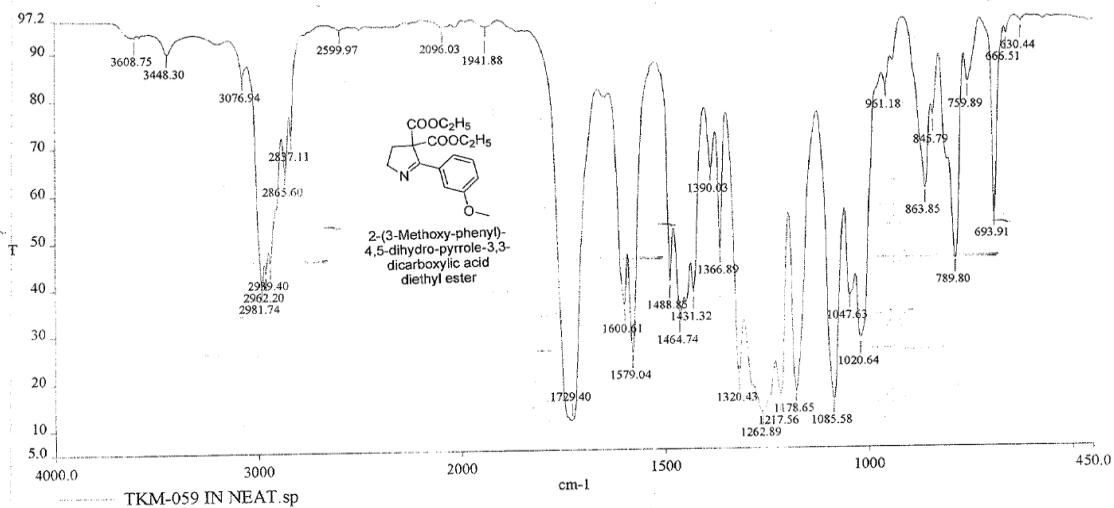
# IR spectrum of 21i

DR REDDY'S LABORATORIES LIMITED

Date: 3/3/09

Time: 5:12:09 PM

TDC/CCS-ANALYTICAL RESEARCH



Analyst: RAMANJANEYULU

SIGN: *[Signature]*

03/03/09

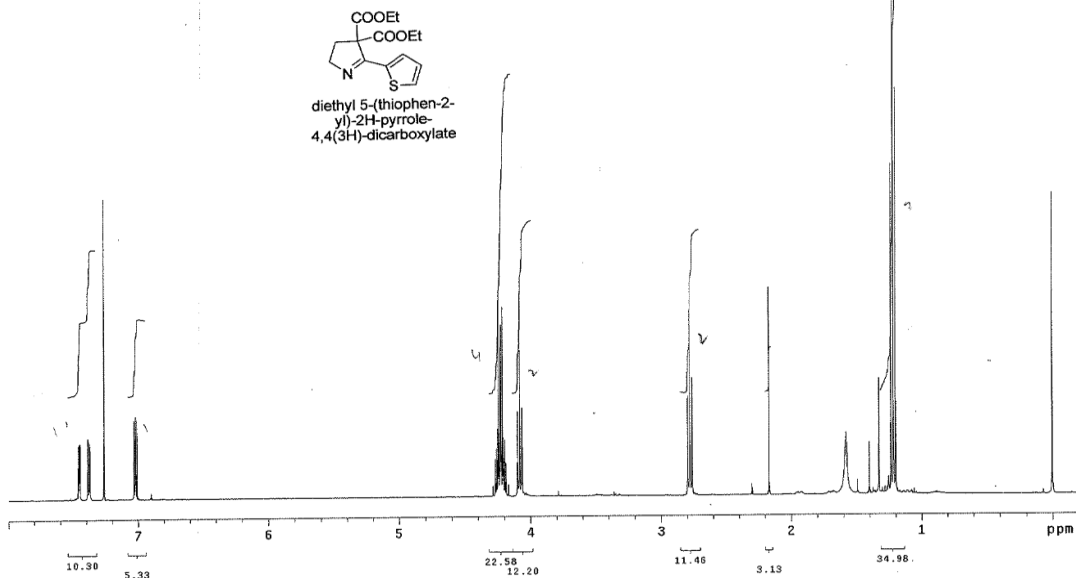
ARD0906R/DA-1/004

# <sup>1</sup>H NMR spectrum of 21j

TKM-01308 IN CDCl3  
TDC-108  
AR.No:ME0806/508  
Date: 8th August 2008.  
Analyst: Srikanth.A

Analytical Research, Discovery Research, DRL  
Instrument : Mercury Plus (Varian 400MHz)  
Date & Time : Fri Aug 8 18:11:50 IST 2008  
Recorded By : Srikanth.A

*[Signature]*  
8/8/08

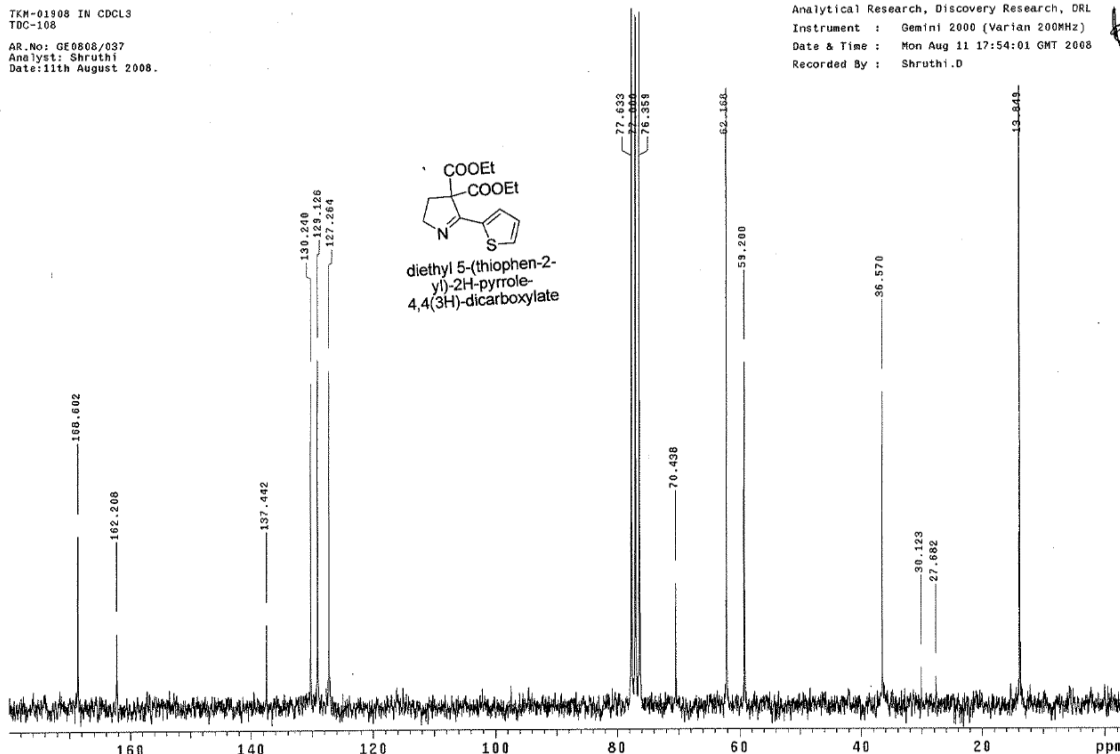


# <sup>13</sup>CNMR spectrum of 21j

TKM-01908 IN CDCL3  
TDC-108  
AR.No: GE0808/037  
Analyst: Shruthi  
Date: 11th August 2008.

Analytical Research, Discovery Research, DRL  
Instrument : Gemini 2000 (Varian 200MHz)  
Date & Time : Mon Aug 11 17:54:01 GMT 2008  
Recorded By : Shruthi.D

*Handwritten signature*



# Mass spectrum of 21j

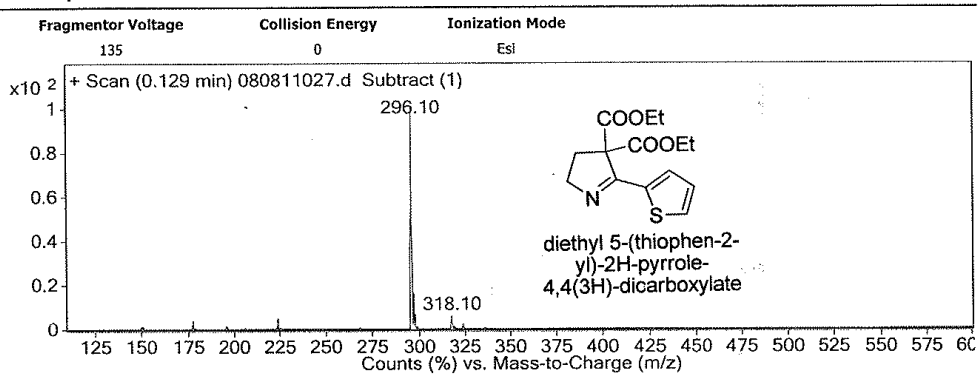
CPS,MIYAPUR

## Mass Analysis Report

EXTRADEPT

<b>Data Filename</b>	080811027.d	<b>Sample Name</b>	TKM-019-08
<b>Sample Type</b>	Sample	<b>Position</b>	Vial 86
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>		<b>IRM Calibration Status</b>	Success
<b>DA Method</b>	DA.m	<b>Comment</b>	

### User Spectra



--- End Of Report ---

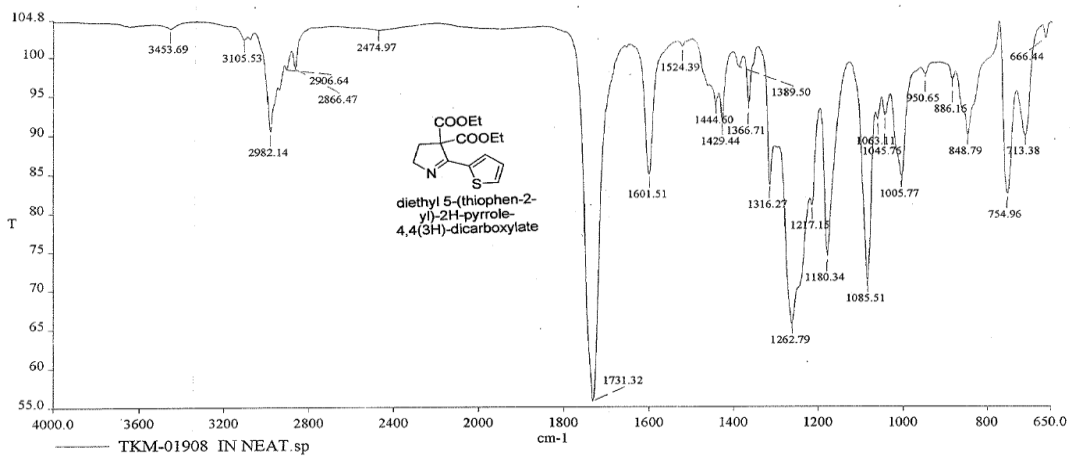
# IR spectrum of 21j

DR.REDDY'S LABORATORIES LIMITED

Date: 8/8/08

TDC/CCS-ANALYTICAL RESEARCH

Time: 6:02:15 PM



Analyst: ANUSHA

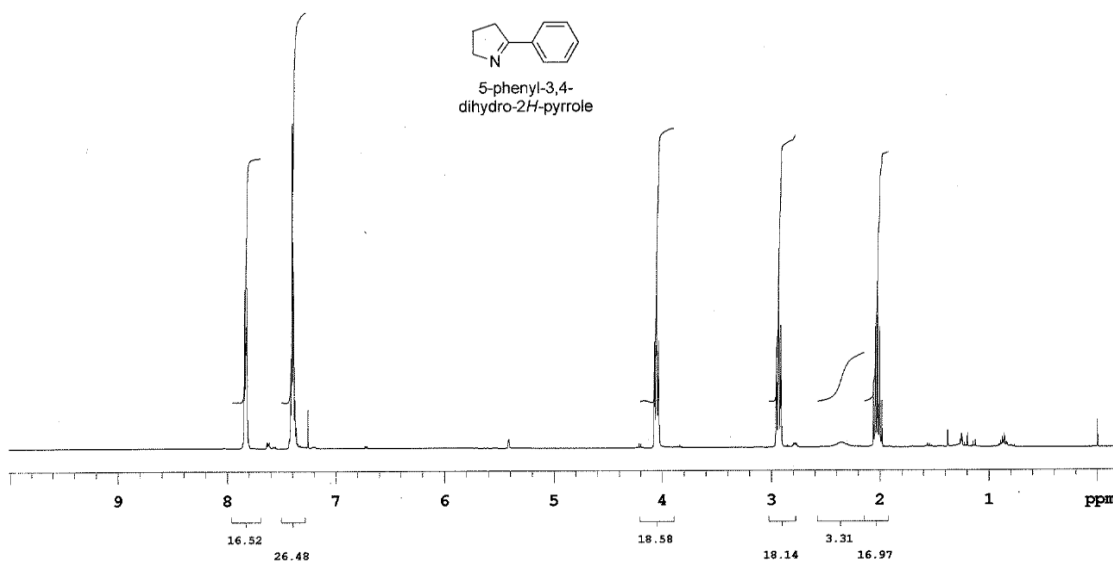
SIGN: *[Signature]*

# <sup>1</sup>H NMR spectrum of 23

TDC-219 2-SSM-105 in CDCl<sub>3</sub>

AR.No:ME0810/900  
 Analyst:Haribabu.R  
 Date:11th Aug 2010.

AR&D, Aurigene Discovery Technologies Ltd, Hyderabad  
 Instrument : Mercury Plus (Varian 400MHz)  
 Date & Time : Thu Aug 12 12:18:51 IST 2010  
 Recorded By : Haribabu.R

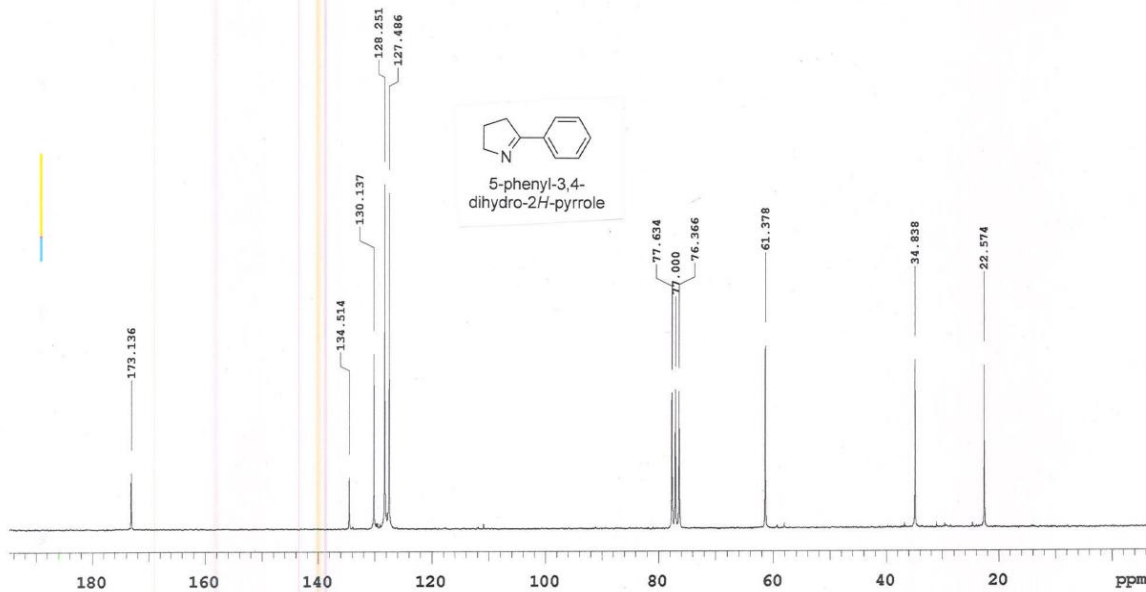


# <sup>13</sup>C NMR spectrum of 23

2-SSM-105 in CDCl<sub>3</sub>  
TDC-219

AR NO:GE0810/26  
Analyst:Haribabu.R  
Date: 13 th Aug.2010

AR&D, Aurigene Discovery Technologies Ltd, Hyderabad  
Instrument : Mercury Plus (Varian 400MHz)  
Date & Time : Mon Aug 16 09:50:08 IST 2010  
Recorded By : Haribabu.R



# Mass spectrum of 23

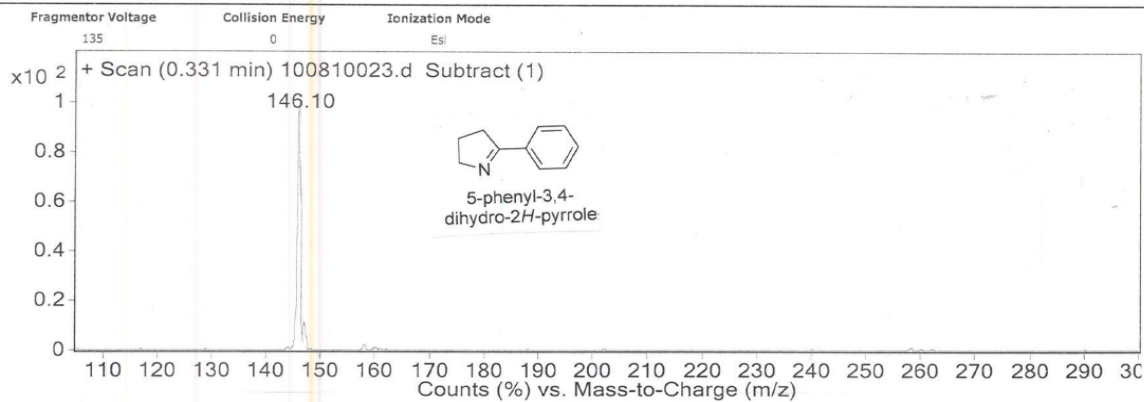
CPS,MIYAPUR

## Mass Analysis Report

Data Filename 100810023.d  
Sample Type Sample  
Instrument Name Instrument 1  
Acq Method ESI.m  
DA Method default.m

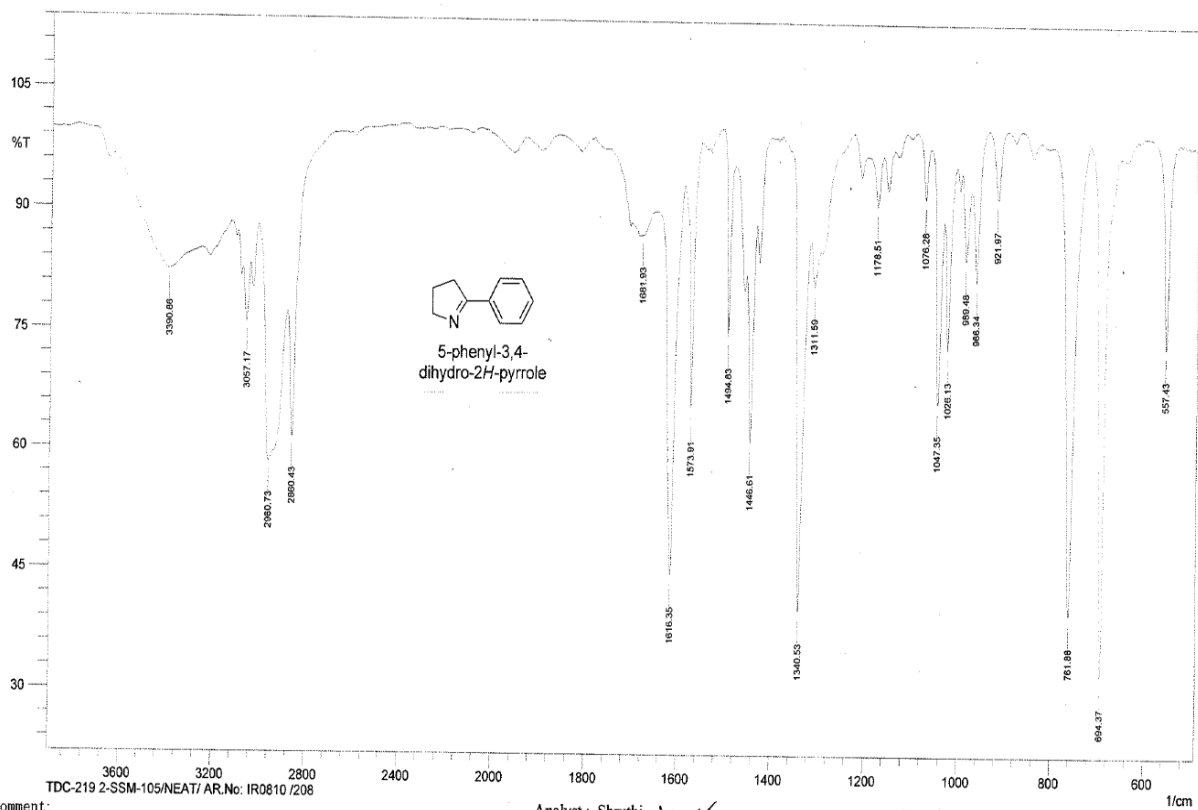
Sample Name 2/SSM/105  
Position Vial 73  
User Name  
IRM Calibration Status Success  
Comment

### User Spectra

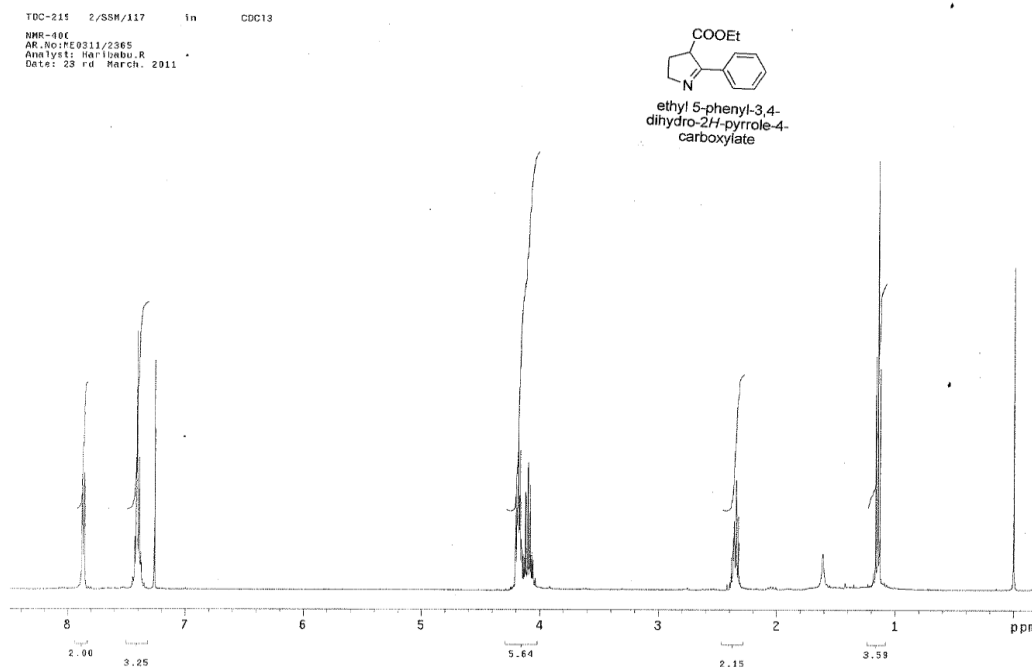


--- End Of Report ---

# IR spectrum of 23



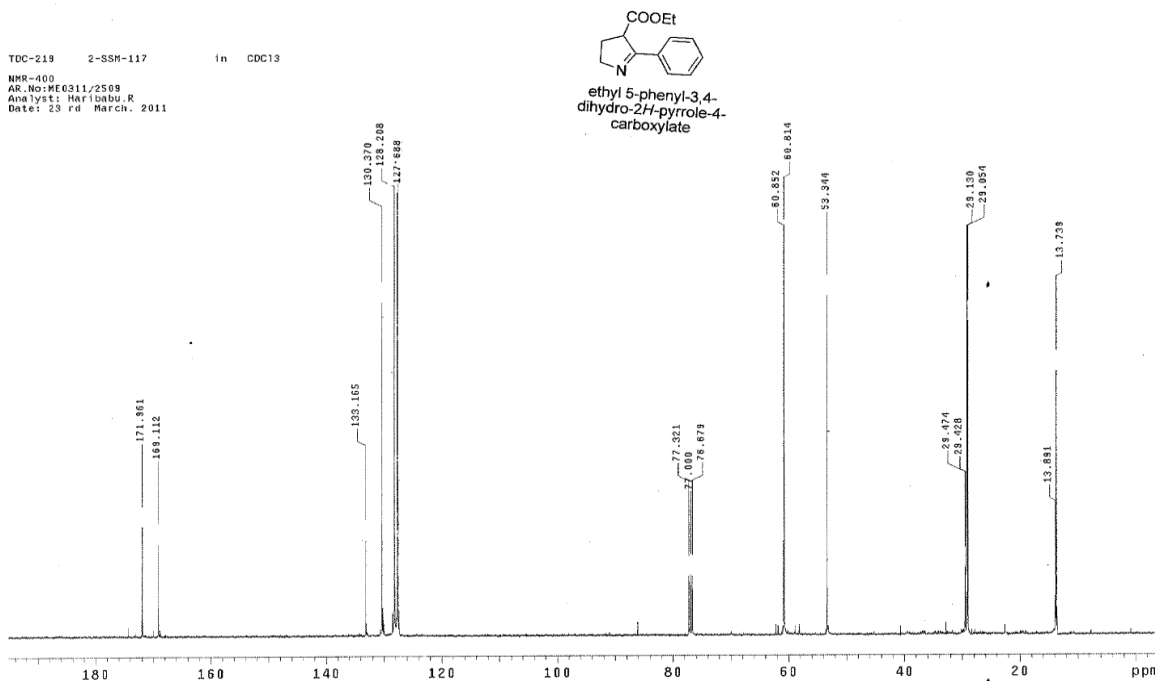
# <sup>1</sup>H NMR spectrum of 24





# <sup>13</sup>C NMR spectrum of 24

Handwritten mark



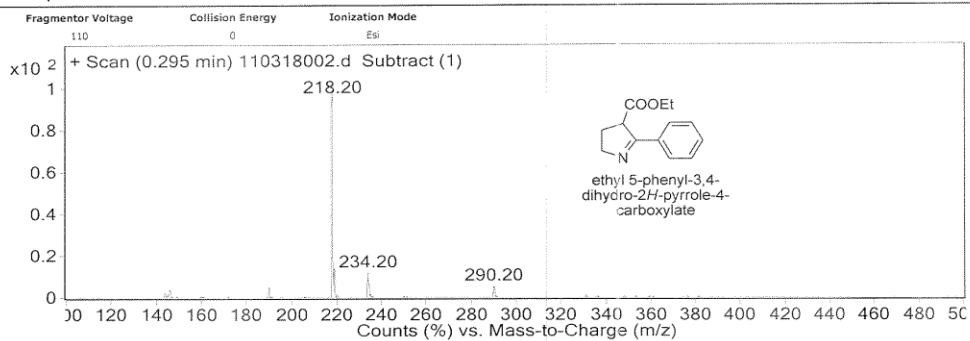
## Mass spectrum of 24

CPS,MIYAPUR

## Mass Analysis Report

Data Filename	110318002.d	Sample Name	SSM/116
Sample Type	Sample	Position	Vial 31
Instrument Name	Instrument 1	User Name	
Acq Method	ESI.m	IRM Calibration Status	Success
DA Method	CEST1_QUANT.m	Comment	

### User Spectra



--- End Of Report ---

Handwritten signature and date: 18/03/2011

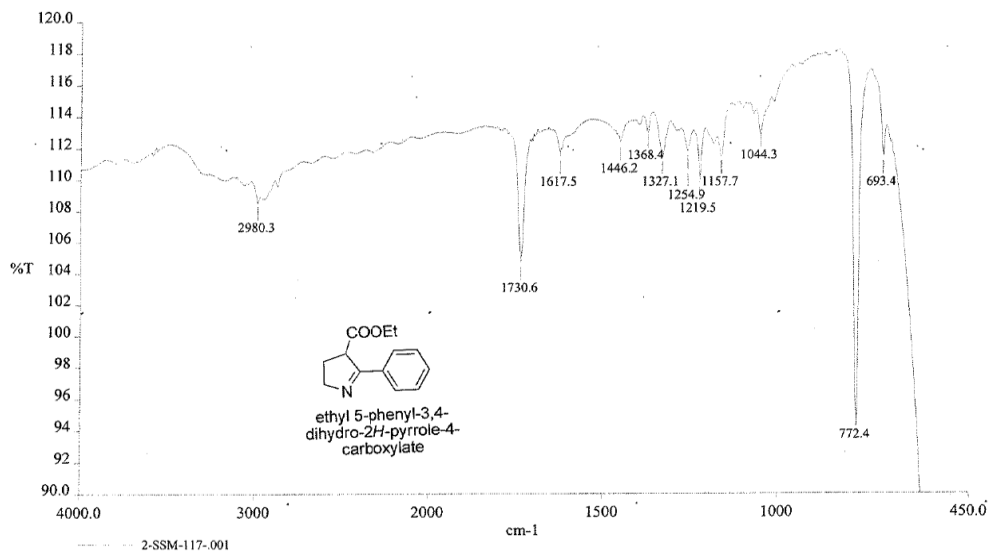
# IR spectrum of 24

software version: Report Builder, Rev. 2.01

CUSTOM PHARMACEUTICAL SERVICES

date: 3/23/2011

time: 3:38:08 PM



spectrum pathname: C:\pel\_data\spectra\2-SSM-117-.001

date created: wed mar 23 15:36:30 2011

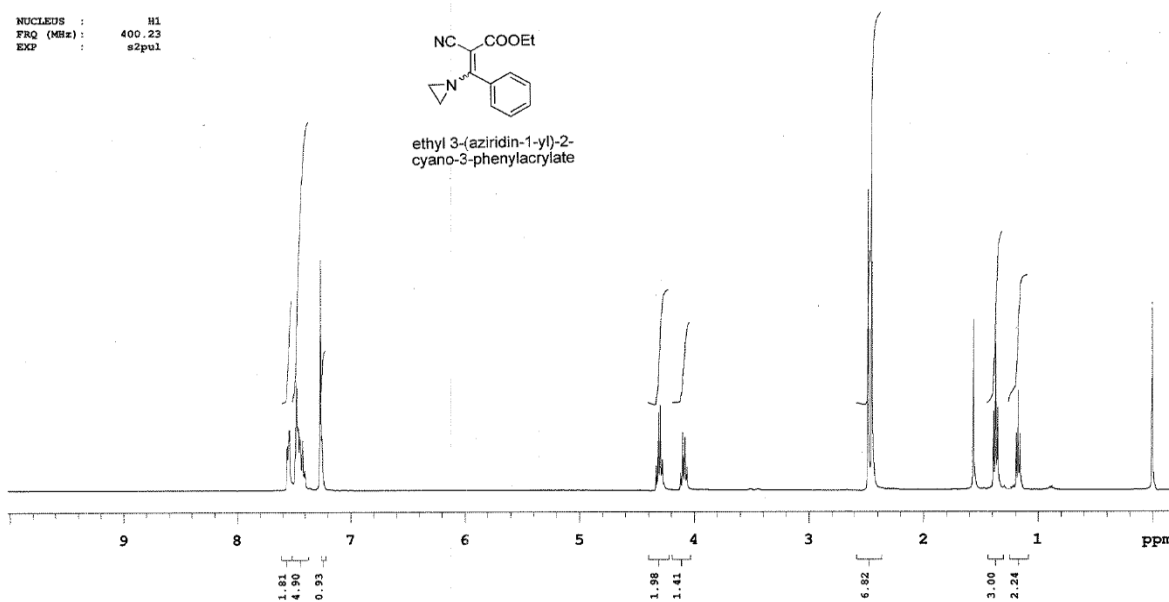
*Handwritten signature and date: 23 24/03/2011*

# <sup>1</sup>H NMR spectrum of 28

TDC-219 2-SSM-112-F CDC13

NMR-400  
AR.No:ME0211/2849  
Analyst: Ganesh  
Date: 28th Feb. 2011

NUCLEUS : H1  
FRQ (MHz): 400.23  
EXP : s2pul

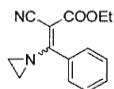


het.

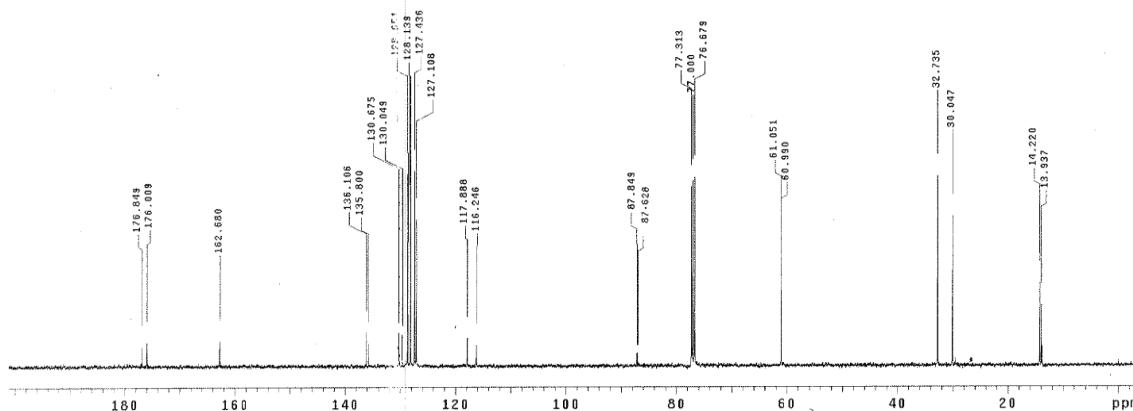
# <sup>13</sup>C NMR spectrum of 28

TDC-218 2-SSM-113 in CDC13

NMR-490  
AR\_NO:REG011/494  
Analyst: Haribabu.R  
Date: 4th March, 2011



ethyl 3-(aziridin-1-yl)-2-cyano-3-phenylacrylate



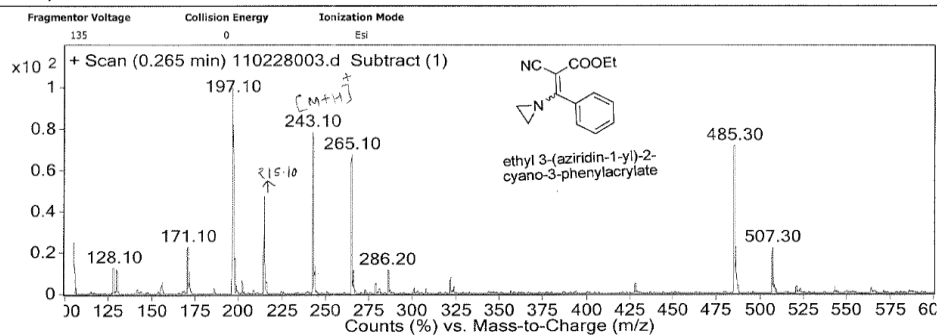
# Mass spectrum of 28

CPS.MIYAPUR

## Mass Analysis Report

<b>Data Filename</b>	110228003.d	<b>Sample Name</b>	2/SSM/112-Crude
<b>Sample Type</b>	Sample	<b>Position</b>	Vial 53
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	ESL.m	<b>IRM Calibration Status</b>	Success
<b>DA Method</b>	CDD-MRM.m	<b>Comment</b>	

### User Spectra



--- End Of Report ---

*Handwritten signature:* B. S. S. S.  
28/02/2011

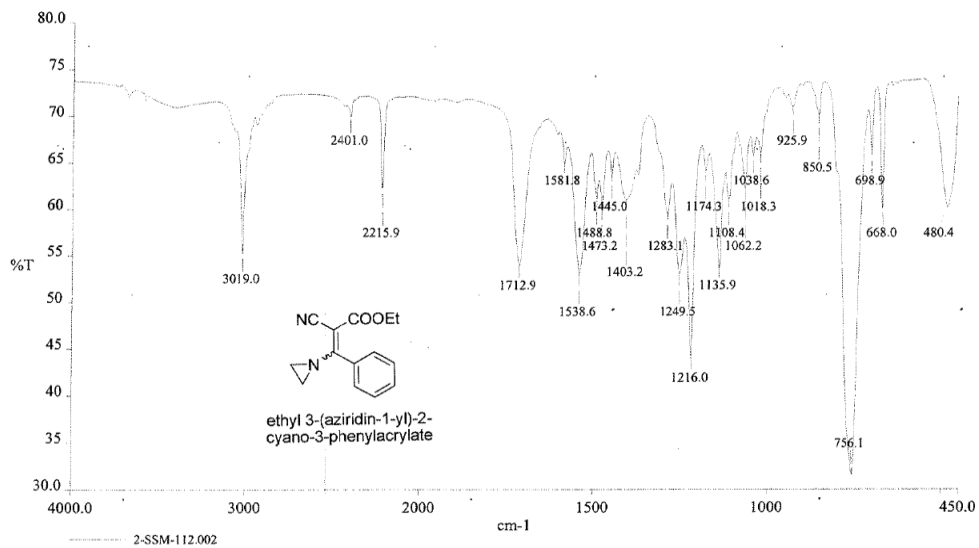
# IR spectrum of 28

software version: Report Builder, Rev. 2.01

CUSTOM PHARMACEUTICAL SERVICES

date: 3/2/2011

time: 7:04:41 PM



spectrum pathname: C:\pel\_data\spectra\2-SSM-112.002

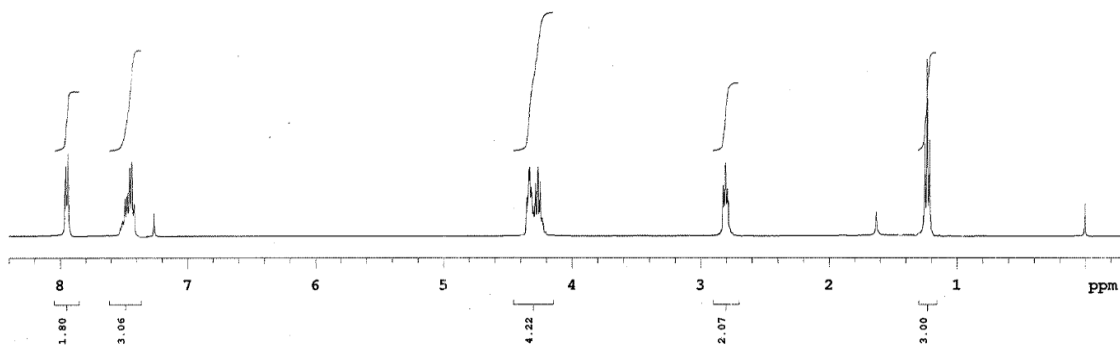
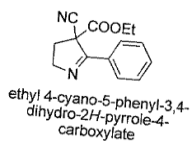
date created: wed mar 02 19:03:53 2011

# <sup>1</sup>H NMR spectrum of 29

TDC-219 2-SSM-113 in CDCl<sub>3</sub>

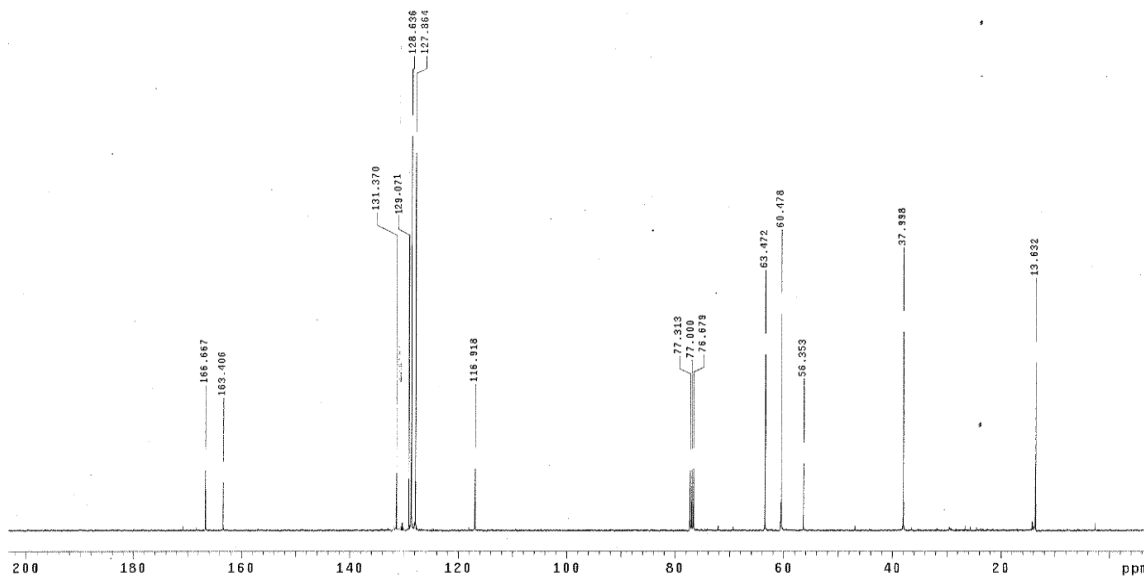
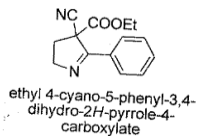
NMR-400  
AR.No:ME0311/156  
Analyst: Ganesh  
Date: 2nd March, 2011

NUCLEUS : H1  
FREQ (MHz): 400.23  
EXP : s2pul



# <sup>13</sup>C NMR spectrum of 29

TDC-004 CRR-DK-03 in CDC13  
 NMR-400  
 AR\_No:ME0311/492  
 Analyst: Naribabu.3  
 Date: 4th March, 2011



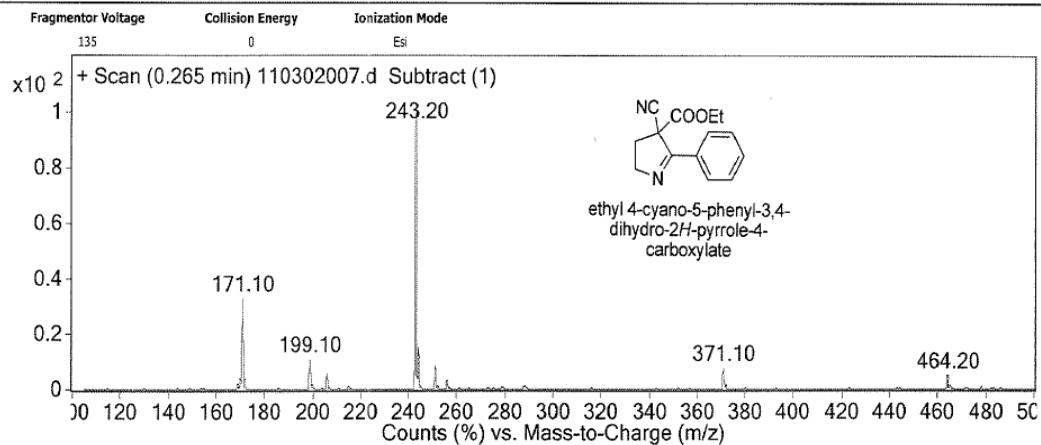
## Mass spectrum of 29

CPS,MIYAPUR

## Mass Analysis Report

<b>Data Filename</b>	110302007.d	<b>Sample Name</b>	Z/SSM/113
<b>Sample Type</b>	Sample	<b>Position</b>	Vial 36
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	ESI.m	<b>IRM Calibration Status</b>	Success
<b>DA Method</b>	CDD-MRM.m	<b>Comment</b>	

### User Spectra



--- End Of Report ---

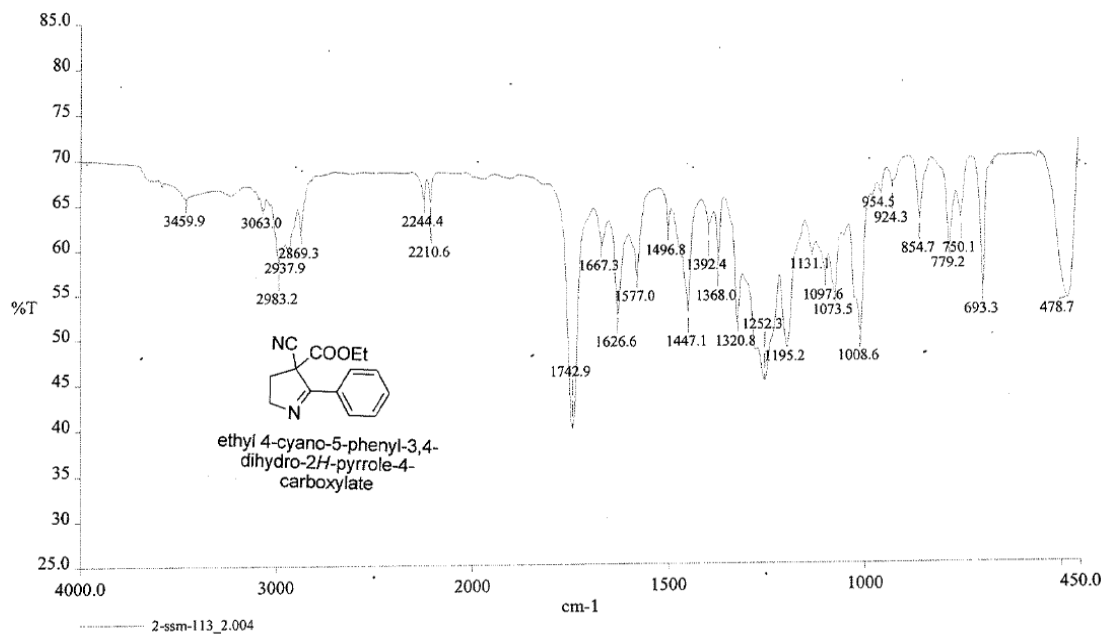
# IR spectrum of 29

software version: Report Builder, Rev. 2.01

CUSTOM PHARMACEUTICAL SERVICES

date: 3/26/2011

time: 4:32:02 PM



# <sup>1</sup>H NMR spectrum of 31

TDC-108 ERM-0109 1.0 CDCl<sub>3</sub>

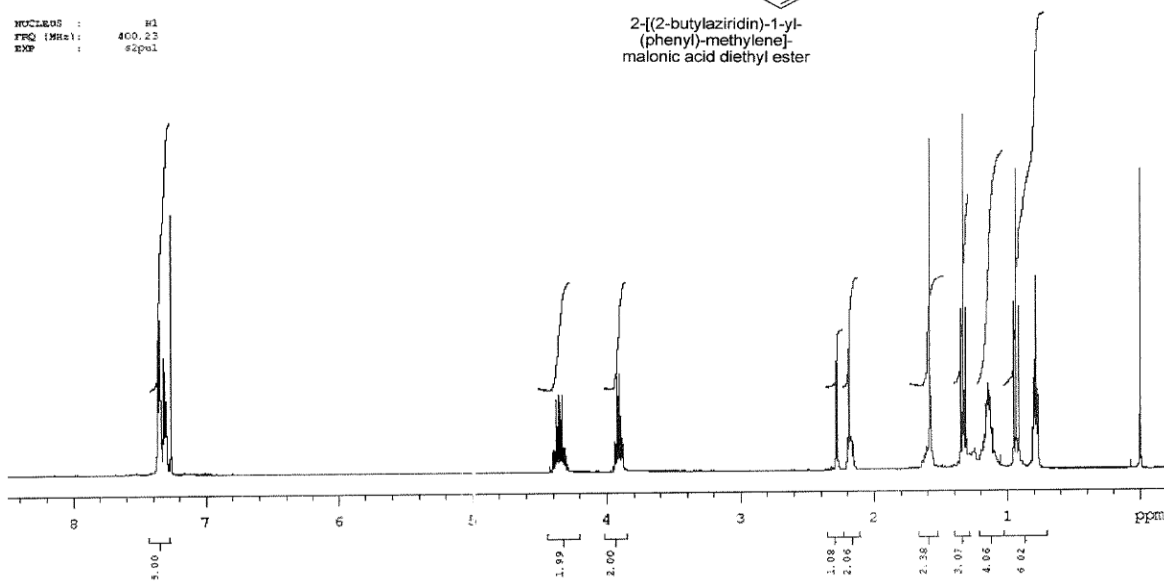
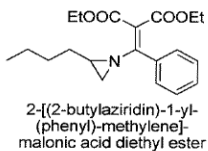
NMR-400

AP.No:ME0311/2621

Analyst: Haridiba.R

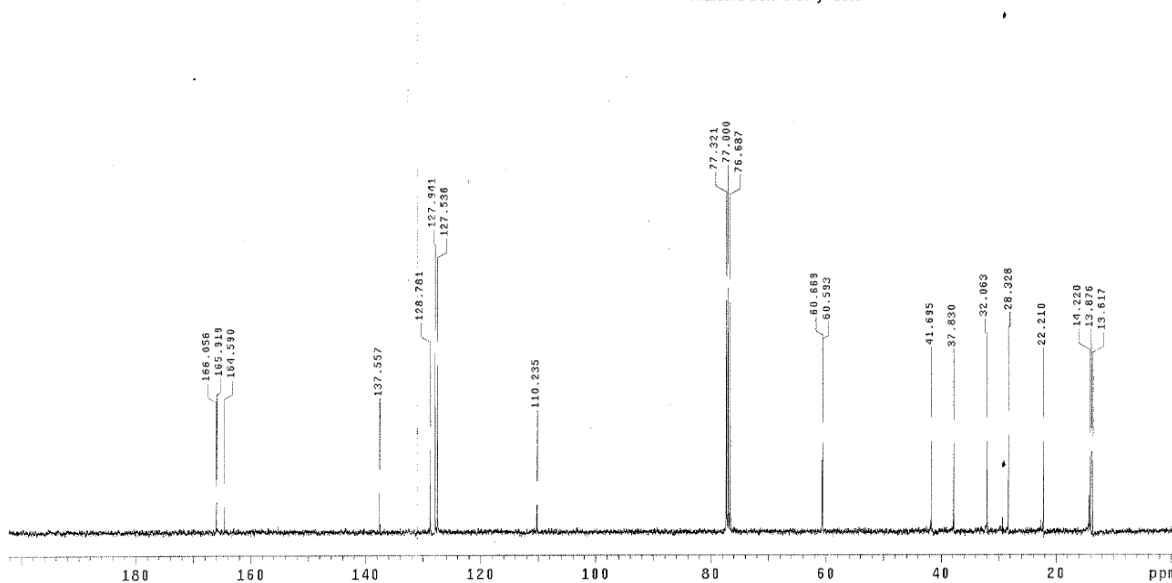
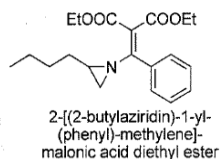
Date: 24 th March, 2011

NUCLEUS : H1  
 FREQ (MHz): 400.23  
 EXP : sgpul



# <sup>13</sup>C NMR spectrum of 31

TDC-108 TKM-0109 in CDCl<sub>3</sub>  
 NMR-400  
 AR.No:ME0311/2764  
 Analyst: Ganesh  
 Date: 25 th March. 2011



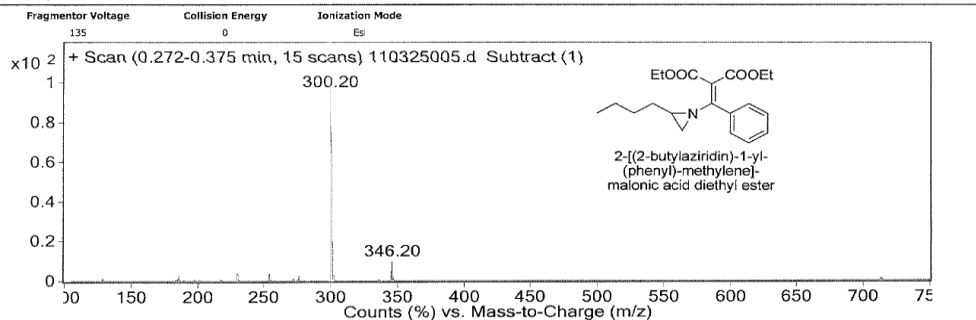
# Mass spectrum of 31

CPS,MIYAPUR

## Mass Analysis Report

<b>Data Filename</b>	110325005.d	<b>Sample Name</b>	TKM-0109
<b>Sample Type</b>	Sample	<b>Position</b>	Vial 18
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	ESL.m	<b>IRM Calibration Status</b>	Success
<b>DA Method</b>	CEST1_QUANT.m	<b>Comment</b>	

### User Spectra

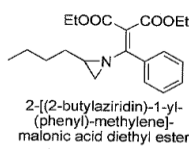
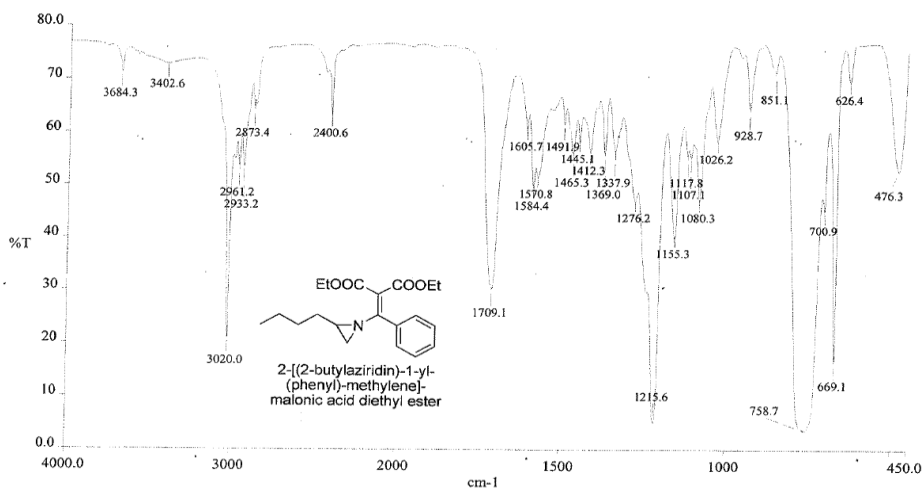


# IR spectrum of 31

software version: Report Builder, Rev. 2.01

CUSTOM PHARMACEUTICAL SERVICES

date: 3/25/2011 time: 4:04:44 PM



TKM-0109.sp

spectrum pathname: C:\pel\_data\spectra\RAMYA\TKM-0109.sp

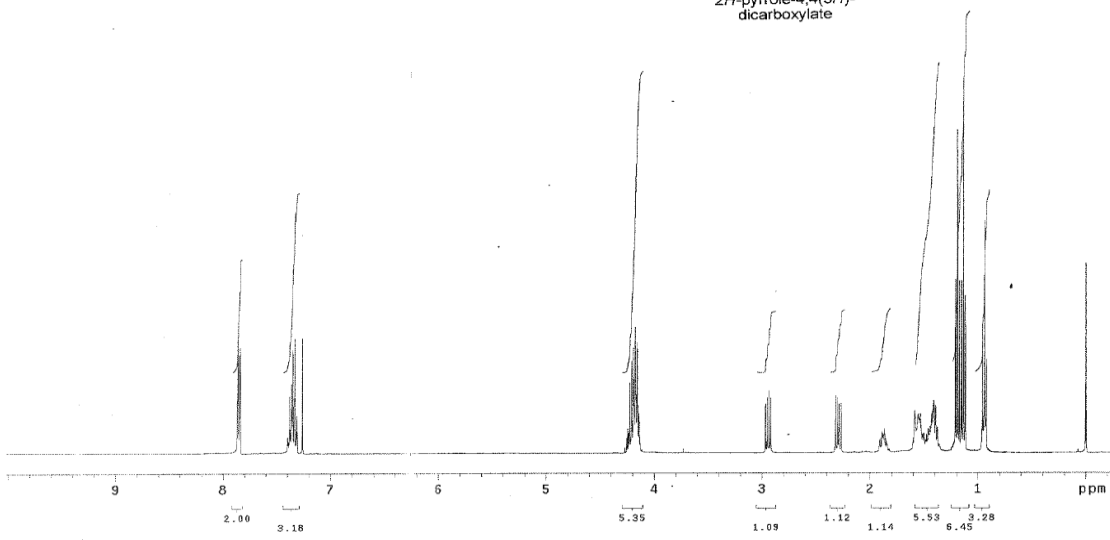
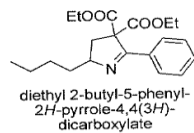
date created: fri mar 25 16:04:10 2011

*ARD11008/AR/187*  
*Ramya*  
*25/03/2011*

# <sup>1</sup>H NMR spectrum of 32

*Her*

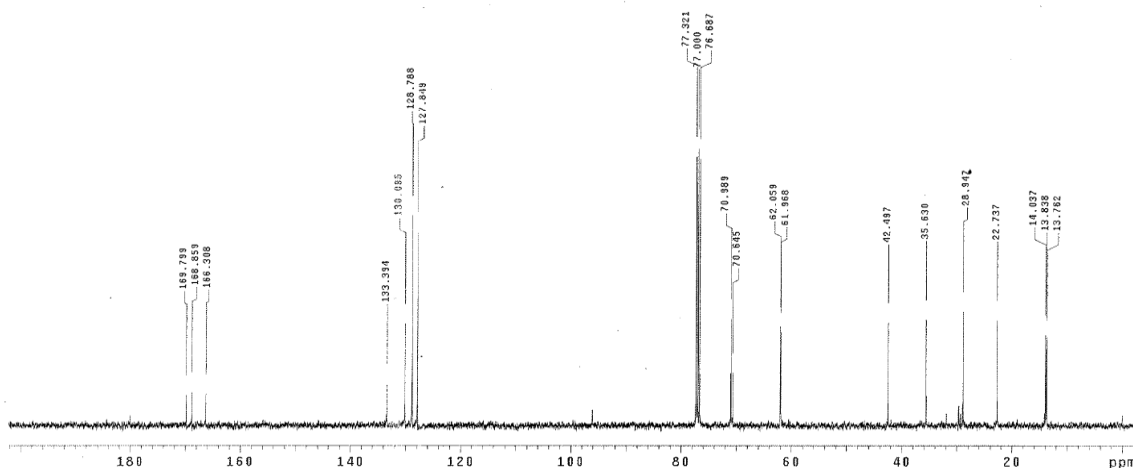
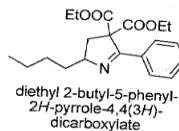
TDC-198 TKM-0104-Fr-1 in CDCl3  
 NMR-400  
 AR.No: NE0311/1172  
 Analyst: Ganesh  
 Date: 11th March, 2011





# <sup>13</sup>C NMR spectrum of 32

TDC-108 TKM-0104 in CDC13  
 NMR-400  
 AR No: ME0811/1608  
 Analyst: Haribabu R  
 Date: 15th March, 2011



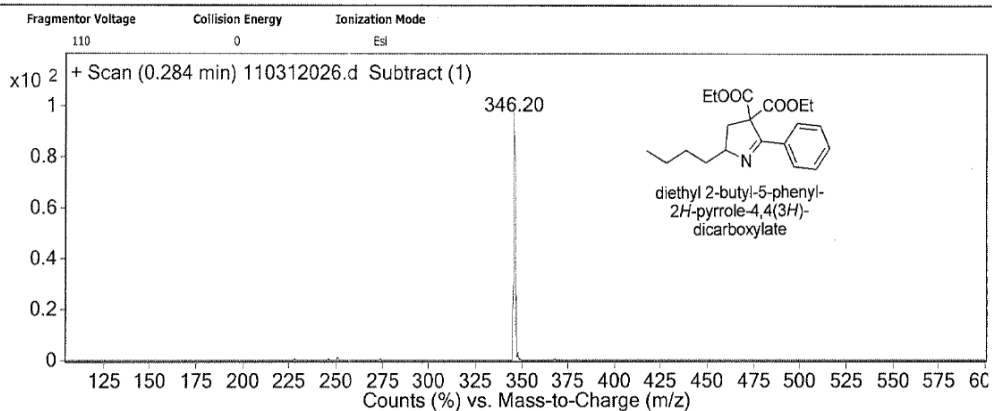
# Mass spectrum of 32

CPS,MIYAPUR

## Mass Analysis Report

<b>Data Filename</b>	110312026.d	<b>Sample Name</b>	TKM-0104/Fr1
<b>Sample Type</b>	Sample	<b>Position</b>	Vial 2
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	ESI.m	<b>IRM Calibration Status</b>	Success
<b>DA Method</b>	CEST1_QUANT.m	<b>Comment</b>	

### User Spectra



--- End Of Report ---

Har  
12/03/2011

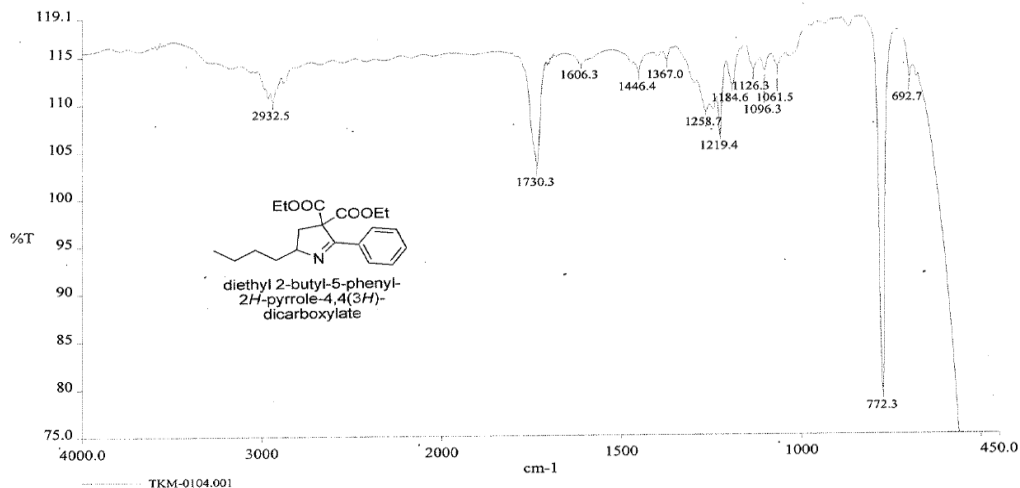
# IR spectrum of 32

software version: Report Builder, Rev. 2.01

CUSTOM PHARMACEUTICAL SERVICES

date: 3/23/2011

time: 3:43:01 PM



spectrum pathname: C:\pel\_data\spectra\TKM-0104.001

date created: wed mar 23 15:41:53 2011

*Handwritten signature and date: 23/03/11*

# HRMS of 21a

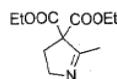
## Elemental Composition Report

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 15.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions  
 52 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)  
 Elements Used:  
 C: 0-25 H: 0-25 N: 0-3 O: 0-5  
 TKM-070 TDC-108

Aurigene Discovery Technologies, Hyderabad



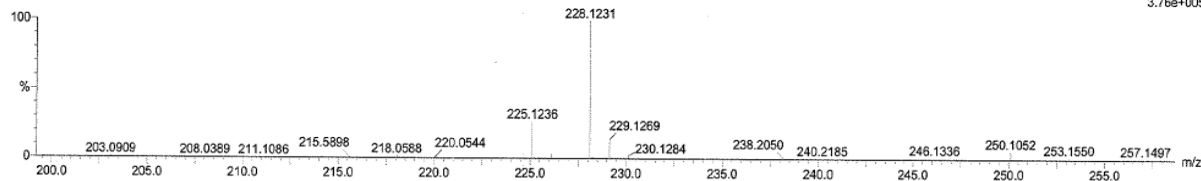
diethyl 5-methyl-2H-pyrrole-4,4(3H)-dicarboxylate

Page 1

*Handwritten date: 02/03/11*

UT0311\_014 22 (0.411) Cm (22:49-88:99x0.010)

02-Mar-2011  
 Lakshminanth  
 1: TOF MS ES+  
 3.76e+005



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
228.1231	228.1236	-0.5	-2.2	3.5	102.7	C11 H18 N O4

# HRMS of 21b

## Elemental Composition Report

### Single Mass Analysis

Tolerance = 8.0 PPM / DBE: min = -1.0, max = 15.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

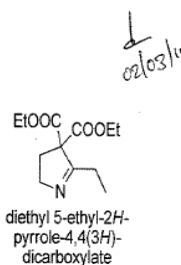
28 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-13 H: 0-30 N: 0-2 O: 0-5

TKM-046 TDC-108

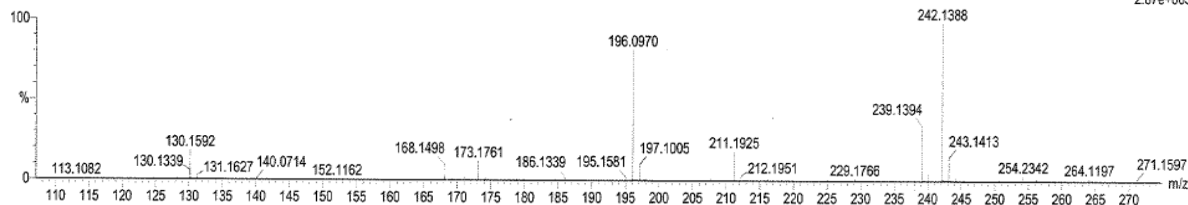
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Page 1

UT0311\_015 15 (0.278) Cm (15:35-89:100x0.010)

02-Mar-2011  
 Lakshminanth  
 1: TOF MS ES+  
 2.87e+005



Minimum: -1.0  
 Maximum: 5.0 8.0 15.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
242.1388	242.1392	-0.4	-1.7	3.5	148.4	C12 H20 N O4

# HRMS of 21c

## Elemental Composition Report

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 15.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

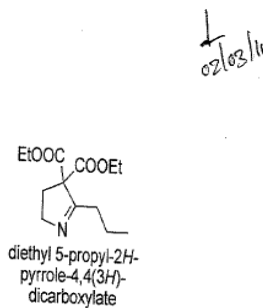
62 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-18 H: 0-30 N: 0-2 O: 0-8

TKM-031 TDC-108

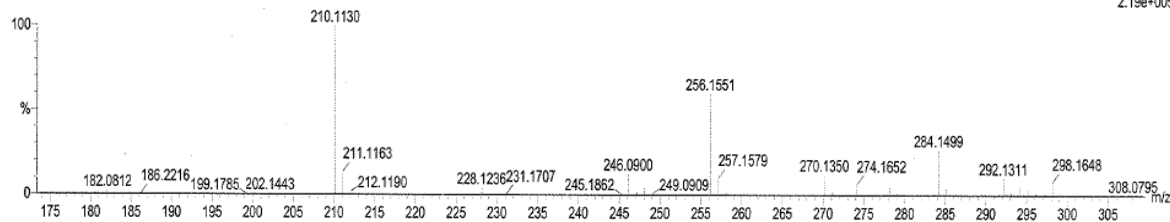
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Page 1

UT0311\_012 19 (0.351) Cm (19:31-80:88x0.010)

02-Mar-2011  
 Lakshminanth  
 1: TOF MS ES+  
 2.19e+005



Minimum: -1.0  
 Maximum: 5.0 5.0 15.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
256.1551	256.1549	0.2	0.8	3.5	139.4	C13 H22 N O4

# HRMS of 21d

## Elemental Composition Report

Page 1

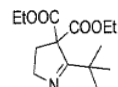
### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 15.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions  
 58 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)  
 Elements Used:  
 C: 0-18 H: 0-30 N: 0-2 O: 0-8  
 TKM-037 TDC-108

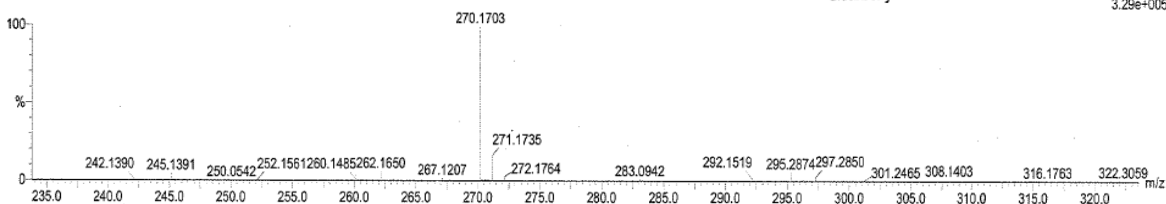
UT0311\_011 29 (0.545) Cm (29:42-93:100x0.010)

Aurigene Discovery Technologies, Hyderabad



diethyl 5-tert-butyl-2H-pyrrole-4,4(3H)-dicarboxylate

02-Mar-2011  
 Lakshminanth  
 1: TOF MS ES+  
 3.29e+005



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
270.1703	270.1705	-0.2	-0.7	3.5	149.3	C14 H24 N O4

# HRMS of 21e

## Elemental Composition Report

Page 1

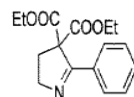
### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 15.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions  
 28 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)  
 Elements Used:  
 C: 0-18 H: 0-30 N: 0-2 O: 0-5  
 TKM-014 3 Amino piperidine CNOP

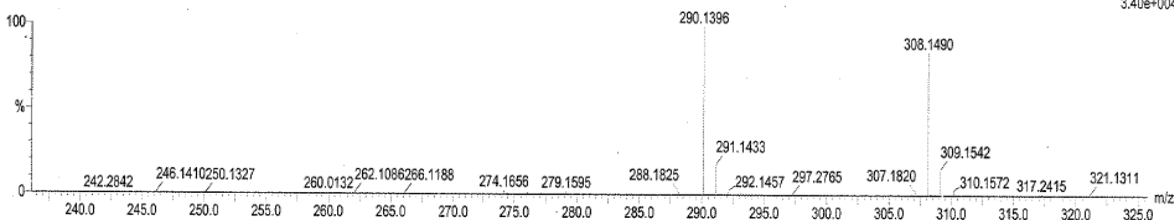
UT0211\_183 16 (0.292) Cm (16:24-49:51x0.010)

Aurigene Discovery Technologies, Hyderabad



diethyl 5-phenyl-2H-pyrrole-4,4(3H)-dicarboxylate

24-Feb-2011  
 Lakshminanth  
 1: TOF MS ES+  
 3.40e+004



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
290.1396	290.1392	0.4	1.4	7.5	3.2	C16 H20 N O4

# HRMS of 21f

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 15.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

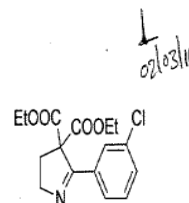
38 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-18 H: 0-30 N: 0-1 O: 0-6 Cl: 0-1

.TKM-023 TDC-108

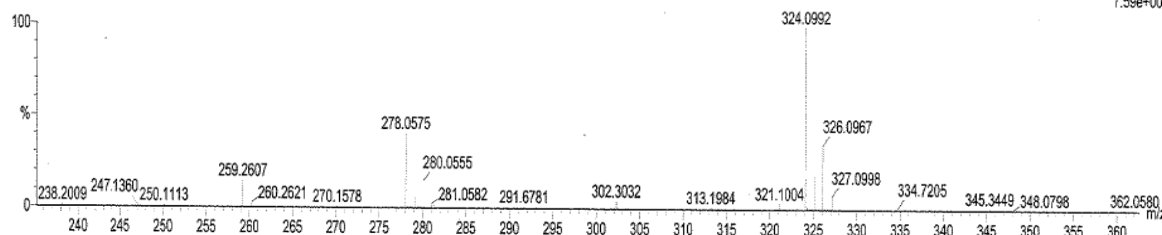
Aurigene Discovery Technologies, Hyderabad



diethyl 5-(3-chlorophenyl)-2H-pyrrole-4,4(3H)-dicarboxylate

02-Mar-2011  
Lakshmikanth  
1: TOF MS ES+  
7.59e+005

UT0311\_016 25 (0.472) Cm (25:40-93:100x0.010)



Minimum: -1.0  
Maximum: 5.0 5.0 15.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
324.0992	324.1003	-1.1	-3.4	7.5	75.0	C16 H19 N O4 Cl

# HRMS of 21g

## Elemental Composition Report

Page 1

### 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 = 4

Monoisotopic Mass, Even Electron Ions

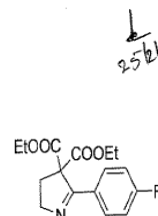
34 formula(e) evaluated with 1 results within limits (up to 15 closest results for each mass)

Elements Used:

C: 0-18 H: 0-25 N: 0-1 O: 0-6 F: 0-1

.TKM-052 3 Amino piperidine CNOP

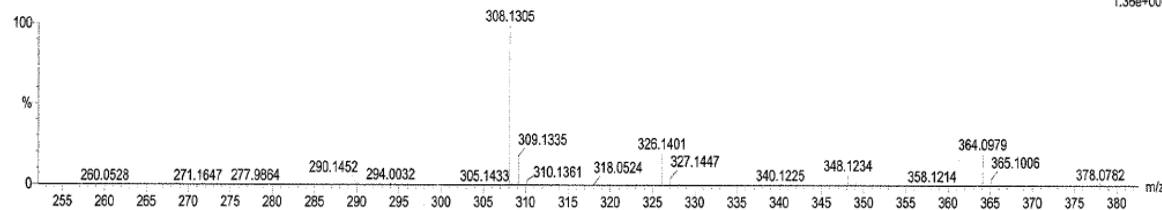
Aurigene Discovery Technologies, Hyderabad



diethyl 5-(4-fluorophenyl)-2H-pyrrole-4,4(3H)-dicarboxylate

24-Feb-2011  
Lakshmikanth  
1: TOF MS ES+  
1.36e+004

UT0211\_179 22 (0.412) Cm (21:28-86:100)



Minimum: -1.0  
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
308.1305	308.1298	0.7	2.3	7.5	5.2	C16 H19 N O4 F

# HRMS of 21h

## Elemental Composition Report

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 15.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

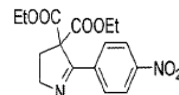
38 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-18 H: 0-30 N: 0-2 O: 0-8

TKM-055 3-Amino piperidine CNOP

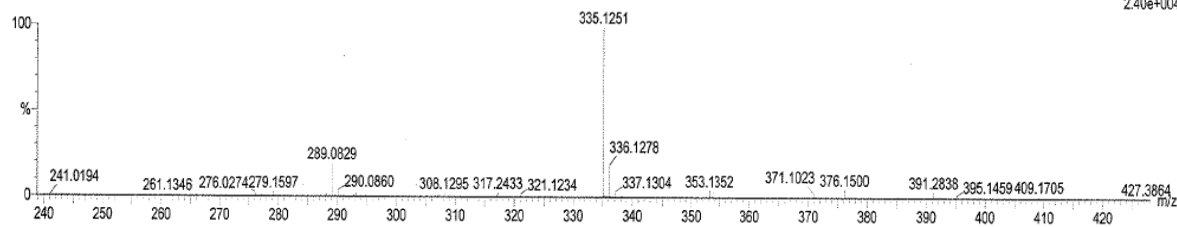
Aurigene Discovery Technologies, Hyderabad



diethyl 5-(4-nitrophenyl)-2H-pyrrole-4,4(3H)-dicarboxylate

24-Feb-2011  
Lakshminanth  
1: TOF MS ES+  
2.40e+004

UT0211\_180 17 (0.325) Cm (17:24-82:90x0.010)



Minimum: -1.0  
Maximum: 5.0 5.0 15.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
335.1251	335.1243	0.8	2.4	8.5	4.5	C16 H19 N2 O6

# HRMS of 21i

## Elemental Composition Report

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 15.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

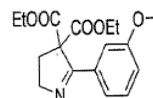
42 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-18 H: 0-30 N: 0-2 O: 0-8

TKM-058 TDC-108

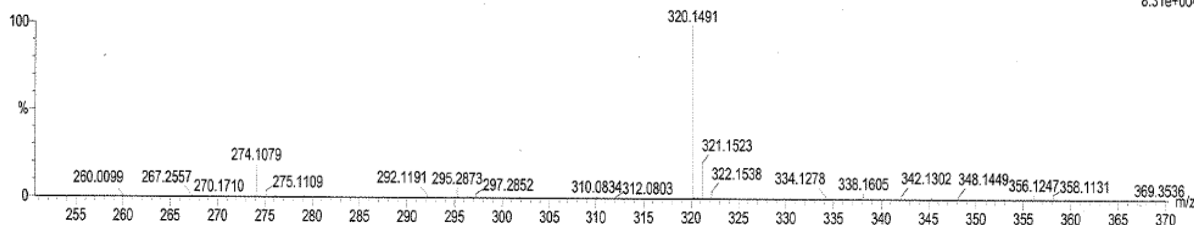
Aurigene Discovery Technologies, Hyderabad



diethyl 5-(3-methoxyphenyl)-2H-pyrrole-4,4(3H)-dicarboxylate

02-Mar-2011  
Lakshminanth  
1: TOF MS ES+  
8.31e+004

UT0311\_013 23 (0.426) Cm (23:28-89:93x0.010)



Minimum: -1.0  
Maximum: 5.0 5.0 15.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
320.1491	320.1498	-0.7	-2.2	7.5	90.1	C17 H22 N O5

# HRMS of 21j

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 15.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

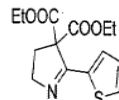
42 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-15 H: 0-30 N: 0-2 O: 0-5 S: 0-1

TKM-017 TDC-108

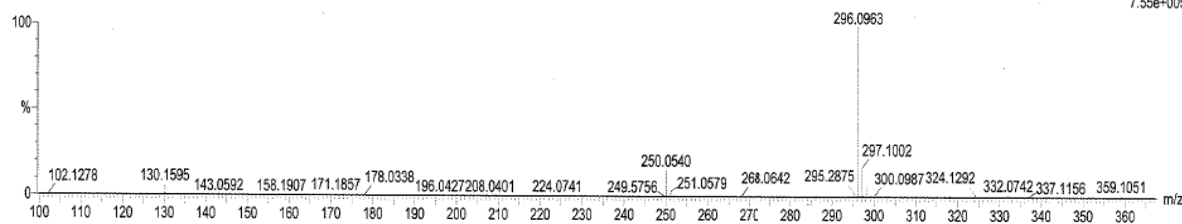
Aurigene Discovery Technologies, Hyderabad



diethyl 5-(thiophen-2-yl)-  
2H-pyrrole-4,4(3H)-  
dicarboxylate

02-Mar-2011  
Lakshminanth  
1: TOF MS ES+  
7.55e+005

UT0311\_010 19 (0.352) Cm (19:28-73:84x0.010)



Minimum: -1.0  
Maximum: 5.0 5.0 15.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
296.0963	296.0957	0.6	2.0	6.5	125.1	C14 H18 N O4 S

# HRMS of 23

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 15.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

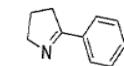
32 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-22 H: 0-35 N: 0-2 O: 0-5

2/SSM1

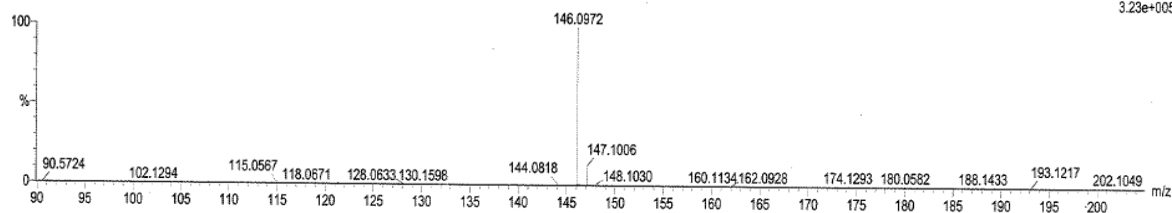
Aurigene Discovery Technologies, Hyderabad



5-phenyl-3,4-  
dihydro-2H-pyrrole

25-Mar-2011  
Lakshminanth  
1: TOF MS ES+  
3.23e+005

UT0311\_137 7 (0.251) Cm (5:9-47:50x0.010)



Minimum: 0.0  
Maximum: 5.0 5.0 15.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
146.0972	146.0970	0.2	1.4	5.5	62.5	C10 H12 N

# HRMS of 24

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 8.0 PPM / DBE: min = 0.0, max = 15.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

21 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

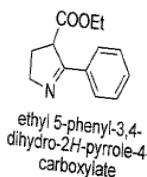
Elements Used:

C: 0-15 H: 0-25 N: 0-2 O: 0-3

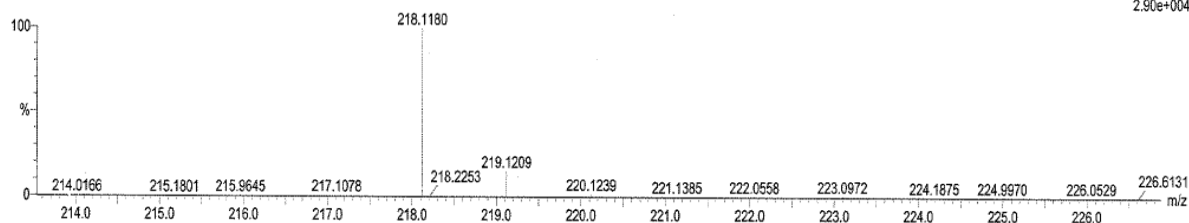
2/SSM117

Aurigene Discovery Technologies, Hyderabad

UT0311\_135 23 (0.620) Cm (23:28-53:55x0.010)



23-Mar-2011  
Lakshminanth  
1: TOF MS ES+  
2.90e+004



Minimum: 0.0  
Maximum: 5.0 8.0 15.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
218.1180	218.1181	-0.1	-0.5	6.5	1.6	C13 H16 N O2

# HRMS of 29

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 15.0

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 (all results (up to 1000) for each mass)

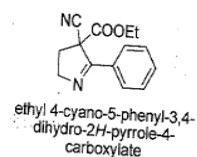
Elements Used:

C: 0-15 H: 0-30 N: 0-3 O: 0-2

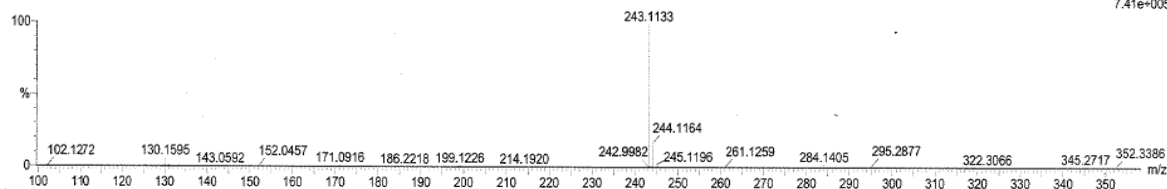
2/SSM113 CATO

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UT0311\_037 21 (0.397) Cm (21:31-89:94x0.010)



02-Mar-2011  
Lakshminanth  
1: TOF MS ES+  
7.41e+005



Minimum: -1.0  
Maximum: 5.0 5.0 15.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
243.1133	243.1134	-0.1	-0.4	8.5	71.1	C14 H15 N2 O2



# HRMS of 32

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 15.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

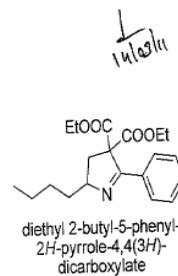
178 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-25 H: 0-35 N: 0-2 O: 0-6 S: 0-2

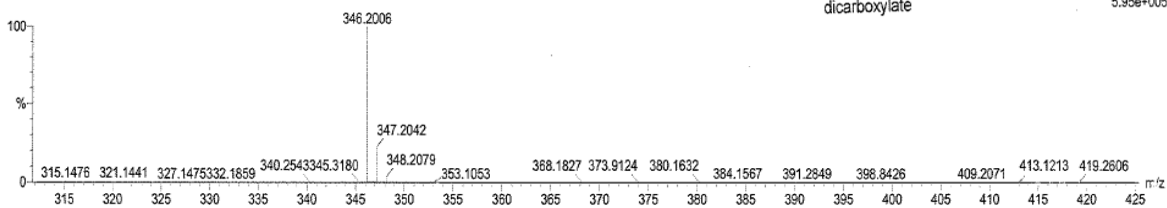
TKM-0104

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14-Mar-2011  
Lakshminanth  
1: TOF MS ES+  
5.95e+005

UT0311\_082 21 (0.489) Cm (21:31-64:72x0.010)



Minimum:

Maximum:

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
346.2006	346.2018	-1.2	-3.5	7.5	162.1	C20 H28 N O4