Supporting Information

for

An oxidative amidation and heterocyclization approach for the synthesis of β-carbolines and dihydroeudistomin Y

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Experimental and analytical data

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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. TLC plates were visualized by ultraviolet light or by treatment with a spray of Pancaldi reagent {$(NH4)_6MoO_4$, $Ce(SO_4)_2$, H_2SO_4, H_2O}. Chromatographic purification of products was carried out by flash column chromatography on silica gel (60–120mesh). Melting points were determined either on DSC-60A, Schimadzu or on an electro thermal melting point apparatus and are uncorrected. NMR spectra were measured in $CDCl_3$, and DMSO-d_6 (all with TMS as internal standard) on a Varian Gemini 400 MHz FT and 500 MHz FT magnetic resonance spectrometers. 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 quadrapole mass spectrometer.

Section B: Experimental section:

Analytical data of *α*-keto-amides (9f–9j).

***N*-(2-(1*H*-Indol-3-yl)ethyl)-2-(4-methoxyphenyl)-2-oxoacetamide (9f):**

55% Yield mp 130-132.4 °C. IR (cm^{-1}): 3246, 2935, 2842, 1668, 1650, 1621, 1598, 1568, 1315, 1264, 1173, 1029, 841, 764, 741. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.40 (d, 2H, J = 9.2 Hz), 8.04 (1H, s, NH), 7.65 (d, 1H, J = 7.6 Hz), 7.39 (d, 1H, J = 8 Hz), 7.23 to 7.09 (3H ArH), 6.94 (d, 2H, J = 8.8 Hz), 3.88 (s, 3H), 3.73 (d, 2H, J = 6.8 Hz), 3.09 (t, 2H, J = 6.8 Hz). ^{13}C NMR (100 MHz, DMSO d^6): δ_c 188.7, 165.0, 164.0, 136.1, 132.2

(2C), 127.1, 125.7, 122.7, 120.8, 118.2 (2C), 114.1 (2C), 111.3 (2C), 55.6, 39.2 and 24.7. Ms, *m/z* (%) = 323.2 (M+1), 345.2 (M+23).

***N*-(2-(1*H*-Indol-3-yl)ethyl)-2-(2,4-dichlorophenyl)-2-oxoacetamide (9g):**

50% Yield. ^{1}H NMR (400 MHz, DMSO d^{6}): δ_H 10.84 (s, 1H, NH), 9.14 (s, 1H, NH), 7.77 (s, 1H), 7.62 to 7.53 (3H, ArH), 7.36 (d, 1H, *J* = 2.0 Hz), 7.19 (s, 1H), 6.98 (dd, 1H, *J* = 7.6 Hz), 7.09 (dd, 1H, *J* = 7.6 Hz), 3.52 (d, 2H, *J* = 6.8 Hz), 2.95 (t, 2H, *J* = 7.2 Hz). ^{13}C NMR (100 MHz, DMSO d^{6}): δ_c 189.5, 162.3, 137.5, 136.2, 132.8, 132.6, 129.8 (2C), 127.4, 127.1, 122.7, 120.9, 118.2 (2C), 111.3 (2C), 55.7 and 24.5. Ms, *m/z* (%) = 361.1 (M+1), 363.1 (M+3), 383.1 (M+23).

***N*-(2-(1*H*-Indol-3-yl)ethyl)-2-(4-(benzyloxy)phenyl)-2-oxoacetamide (9h)**:

52% Yield. mp 137.1-138.2 °C. IR (cm^{-1}): 3439, 3251, 3091, 2902, 1681, 1643, 1598, 1568, 1456, 1258, 1225, 1173, 995, 850, 741. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.39 (d, 2H, *J* = 9.2 Hz), 8.06 (s, 1H, NH), 7.64 (d, 1H, *J* = 7.6 Hz), 7.43- 7.34 (m, 5 ArH), 7.23 – 7.13 (m, 3ArH), 7.11 (s, 1H), 7.02 (d, 2H, *J* = 9.2 Hz), 5.25 (s, 2H), 3.72 (d, 2H, *J* = 6.6 Hz), 3.07 (t, 2H, *J* = 6.8 Hz). ^{13}C NMR (100 MHz, DMSO d^{6}): δ_c 188.6, 164.9, 163.0, 136.1 (2C), 132.1 (2C), 128.3 (2C), 127.9, 127.6 (2C), 127.0, 125.9, 122.6, 120.8, 118.1 (2C), 114.8 (2C), 111.3, 111.2, 69.5, 39.2 and 24.6. Ms, *m/z* (%) = 399.4 (M+1).

***N*-(2-(1*H*-Indol-3-yl)ethyl)-2-([1,1'-biphenyl]-4-yl)-2-oxoacetamide (9i)**:

60% Yield. mp 175.1-177.1 °C. IR (cm^{-1}): 3436, 3239, 3089, 1684, 1645, 1599, 1485, 1457, 1202, 1100, 857, 762, 743. ^{1}H NMR: (400 MHz, $CDCl_3$): δ_H 8.41 (d, 2H, *J* = 6.6 Hz), 8.06 (s, 1H, NH), 7.70 - 7.63 (m, 5 ArH), 7.47- 7.38 (m, 4 ArH), 7.22 – 7.10 (m, 3 ArH), 3.76 (d, 2H, *J* = 6.6 Hz), 3.10 (t, 2H, *J* = 6.8 Hz). ^{13}C NMR (100 MHz, DMSO d^{6}):

δ_c 189.9, 164.8, 145.6, 138.6, 136.2, 131.6, 130.4 (2C), 129.1 (2C), 128.6, 127.1 (2C), 127.0 (2C), 126.9, 122.9, 120.9, 118.2 (2C), 111.3 (2C), 39.2 and 24.8. Ms, *m/z* (%) = 369.2 (M+1), 391.2 (M+23).

***N*-(2-(1*H*-Indol-3-yl)ethyl)-2-oxo-2-(thiophen-2-yl)acetamide (9j):**

42% Yield. mp 147.7-149.9 °C. IR (cm^{-1}): 3394, 3354, 2936, 2916, 2859, 1685, 1654, 1567, 1500, 1404, 1357, 1287, 1093, 1023, 844, 817, 743, 725. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.38 (d, 1H, *J* = 4 Hz), 8.08 (s, 1H, NH), 7.81 (d, 1H, *J* = 5.5 Hz), 7.63 (d, 1H, *J* = 8.0 Hz), 7.39 (d, 2H, *J* = 8.4 Hz), 7.23 – 7.11 (m, 2 ArH), 7.06 (d, 1H, *J* = 2 Hz), 3.73 (d, 2H, *J* = 6.6 Hz), 3.07 (t, 2H, *J* = 7.2 Hz). ^{13}C NMR (100 MHz, DMSO d^6): δ_c 179.8, 161.8, 138.8, 137.2, 137.2, 136.2, 128.5, 127.1, 122.6, 120.9, 118.2 (2C), 111.3 (2C), 39.2 and 24.6. Ms, *m/z* (%) = 299.4 (M+1), 321.4 (M+23).

Analytical data of dihydro-eudistomin (7e–7j).

(2,9-Dihydro-1*H*-pyrido[3,4-*b*]indol-1-yl)(3-nitrophenyl)methanone (7e):

20% Yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.33 (s, 1H), 8.14 (d, 1H, *J* = 8.0 Hz), 8.06 (s, 1H), 7.68 (d, 1H, *J* = 8.0 Hz), 7.53 (d, 1H, *J* = Hz), 7.48 (t, 1H, *J* = 8.0 Hz), 7.41 (d, 1H, *J* = 8.0 Hz), 7.30 - 7.17 (m, 3 ArH), 6.52 (d, 1H, *J* = 8.4 Hz), 5.91 (dd, 1H, *J* = 3.2 & 5.4 Hz), 5.28 (s, 1H), 3.78 (s, 3H). Ms, *m/z* (%) = 320 (M+1).

(2,9-Dihydro-1*H*-pyrido[3,4-*b*]indol-1-yl)(4-methoxyphenyl)methanone (7f):

38% Yield. IR (cm^{-1}): 3222, 3185, 3042, 2937, 2835, 1657, 1624, 1509, 1456, 1249, 1177, 1055, 1032, 848, 810, 770, 742. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.17 (s, 1H), 7.67 (d, 1H, *J* = 7.2 Hz), 7.35 (t, 2H, *J* = 8.0 Hz), 7.23 (d, 1H, *J* = 7.2 Hz), 7.20 (d, 3H, *J* = 8.0 Hz), 6.86 (d, 2H, *J* = 7.6 Hz), 6.48 (d, 1H, *J* = 8.8 Hz), 5.94 (dd, 1H, *J* = 3.6 & 5.6 Hz), 5.02 (s, 1H), 3.78 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO d^6): δ_c 166.8, 157.3,

135.4, 130.1, 129.4, 127.0, 126.7, 124.9, 120.6, 118.4, 117.3, 116.9, 112.5, 110.6, 109.0, 108.8, 105.0, 53.9, 51.5. Ms, *m/z* (%) = 305 (M+1), 327 (M+23).

(2,4-Dichlorophenyl)(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-yl)methanone (8g):

45% Yield. mp 281.1-284.2 °C. IR (cm^{-1}): 3356, 3211, 3086, 2834, 1678, 1581, 1556, 1469, 1385, 1337, 1184, 1110, 1073, 1052, 906, 822, 800, 745. ^{1}H NMR (400 MHz, DMSO d^{6}): δ_H 10.95 (s, 1H), 8.50 (t, 1H, *J* = 6.8 Hz), 7.64 (s, 1H), 7.43 (d, 2H, *J* = 8.4 Hz), 7.34 (dd, 1H, *J* = 2.0, 6.4 Hz) 7.12 (t, 1H, *J* = 7.6 Hz), 7.02 (t, 1H, *J* = 7.6 Hz), 6.77 (d, 1H, *J* = 8.8 Hz), 6.15 (s, 1H), 3.20 (m, 1H), 3.01 (m, 1H), 2.81 (m, 2H). ^{13}C NMR (100 MHz, DMSO d^{6}): δ_c 171.9, 139.7, 135.1, 133.4, 132.4, 131.6, 130.5, 130.2, 127.9, 127.1, 121.7, 118.7, 118.1, 111.7, 108.6, 74.8, 38.2 and 25.2. Ms, *m/z* (%) = 343.1 (M+1), 321.4 (M+23). HRMS (EI): calcd. *m/z* for $C_{18}H_{13}N_2OCl_2$ $[M]^+$ 343.0405, found 343.0101.

(4-(Benzyloxy)phenyl)(2,9-dihydro-1*H*-pyrido[3,4-*b*]indol-1-yl)methanone (7h):

46% Yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.04 (s, 1H), 7.65 (d, 1H, *J* = 8.8 Hz), 7. 40-7.32 (m, 5 ArH), 7.23-7.11 (m, 4 ArH), 6.95 (d, 2H, *J* = 8.8 Hz), 6.51 (d, 1H, *J* = 8.4 Hz), 5.95 (dd, 1H, *J* = 5.6 & 3.6 Hz), 5.04 (s, 2H), 5.00 (s, 1H). Ms, *m/z* (%) = 381.2 (M+1), 403 (M+23). HRMS (EI): calcd. *m/z* for $C_{25}H_{21}N_2O_2$ $[M]^+$ 381.1603, found 381.1583.

[1,1'-Biphenyl]-4-yl(2,9-dihydro-1*H*-pyrido[3,4-*b*]indol-1-yl)methanone (7i):

35% Yield. mp 224-226 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.12 (s, 1H), 7.69 (d, 1H, *J* = 8.0 Hz), 7.64 - 7.21 (m, 12 ArH), 6.54 (d, 1H, *J* = 8.4 Hz), 5.97 (dd, 1H, *J* = 3.6 & 4.8 Hz), 5.13 (s, 1H). ^{13}C NMR (100 MHz, DMSO d^{6}): δ_c 173.7, 166.8, 143.0, 139.5, 138.9,

136.2, 135.2, 130.7, 128.8, 127.8, 127.3, 126.9, 126.6, 125.7, 121.8, 119.4, 118.6, 118.0, 111.5, 109.7, 108.5, 105.4, 75.4, 52.8, 25.2 Ms, *m/z* (%) = 351.2 (M+1).

[1,1'-Biphenyl]-4-yl(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-yl)methanone (8i):

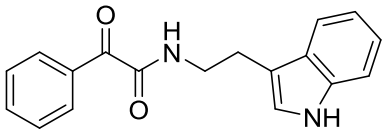
20% Yield. mp 271.1-273.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.81 (*s*, 1H), 7.55 - 7.27 (m, 11 ArH), 6.31 (t, 1H, *J* = 7.0 Hz, NH), 5.77 (s, 1H, OH), 3.49 (m, 1H), 3.27 (m, 1H), 3.00 (m, 2H). ^{13}C NMR (100 MHz, DMSO d^6): δ_c. 173.7, 143.0, 139.5, 139.4, 135.0, 130.9, 128.8 (3C), 127.7, 127.5, 126.6 (5), 121.3, 118.4, 117.9, 111.5, 108.5, 75.3,38.2 and 25.2. Ms, *m/z* (%) = 351.2 (M+1).

(1-Hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indol-1-yl)(thiophen-2-yl)methanone (8j):

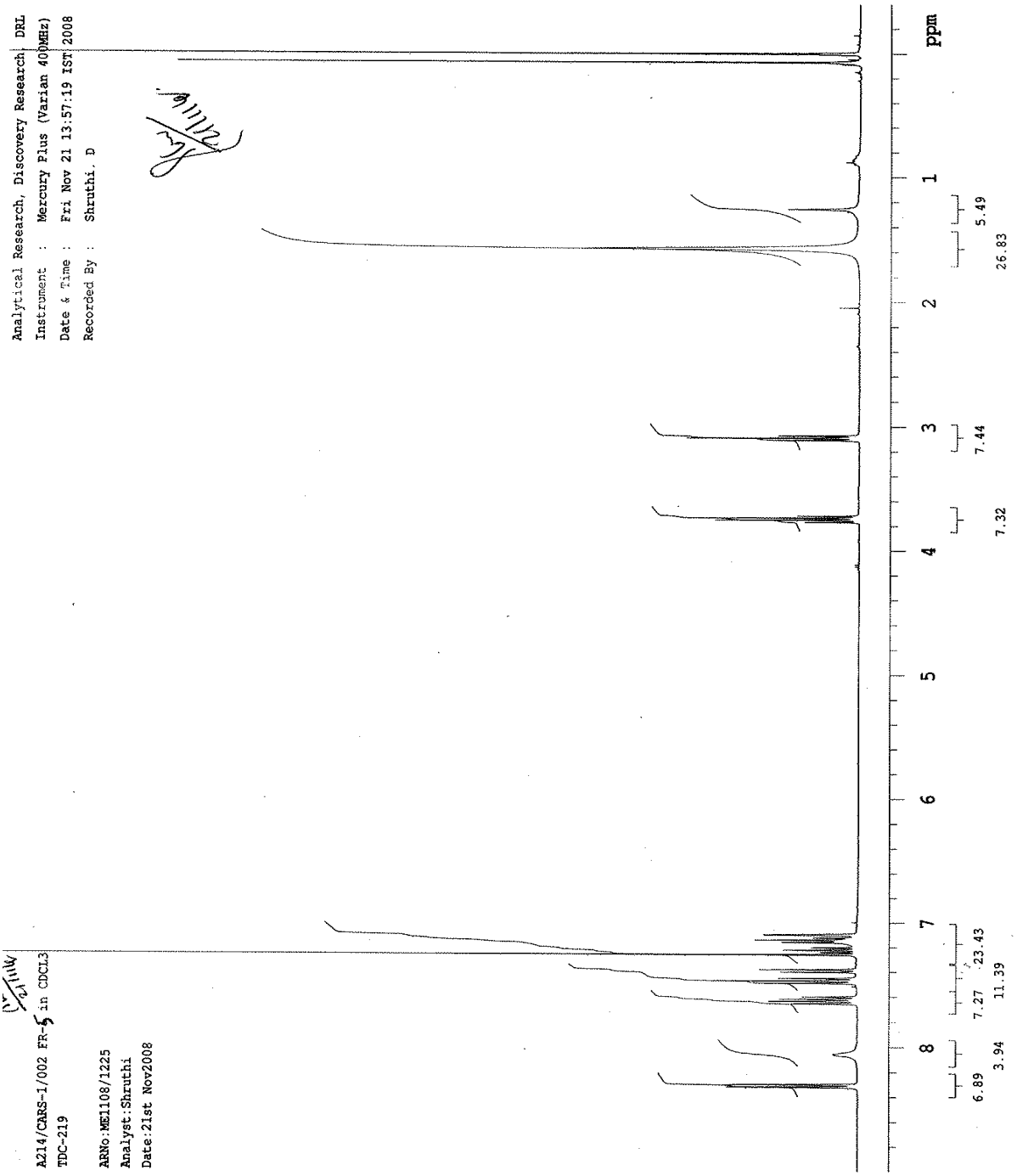
42% Yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.77 (s, 1H), 7.52 (d, 1H, *J* = 8.0 Hz), 7.44 (m, 2H), 7.17 (t, 2H, *J* = 7.6 Hz), 7.05 (d, 1H, *J* = 8.8 Hz), 6.84 (d, 1H, *J* = 8.8 Hz), 6.15 (brs, 1H, NH), 5.84 (s, 1H, OH), 3.36 – 3.29 (m, 2H), 3.02 (m, 1H), 2.89 (m, 1H). ^{13}C NMR (100 MHz, DMSO d^6): δ_c 171.8, 139.6, 135.1, 133.4, 132.4, 131.5, 130.5, 127.8, 127.0, 121.6, 118.0, 111.6, 108.6, 74.7, 38.2 and 25.1. Ms, *m/z* (%) = 281 (M+1).

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

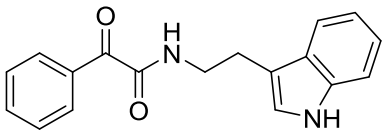
^{1}H NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-phenylacetamide (**9a**):



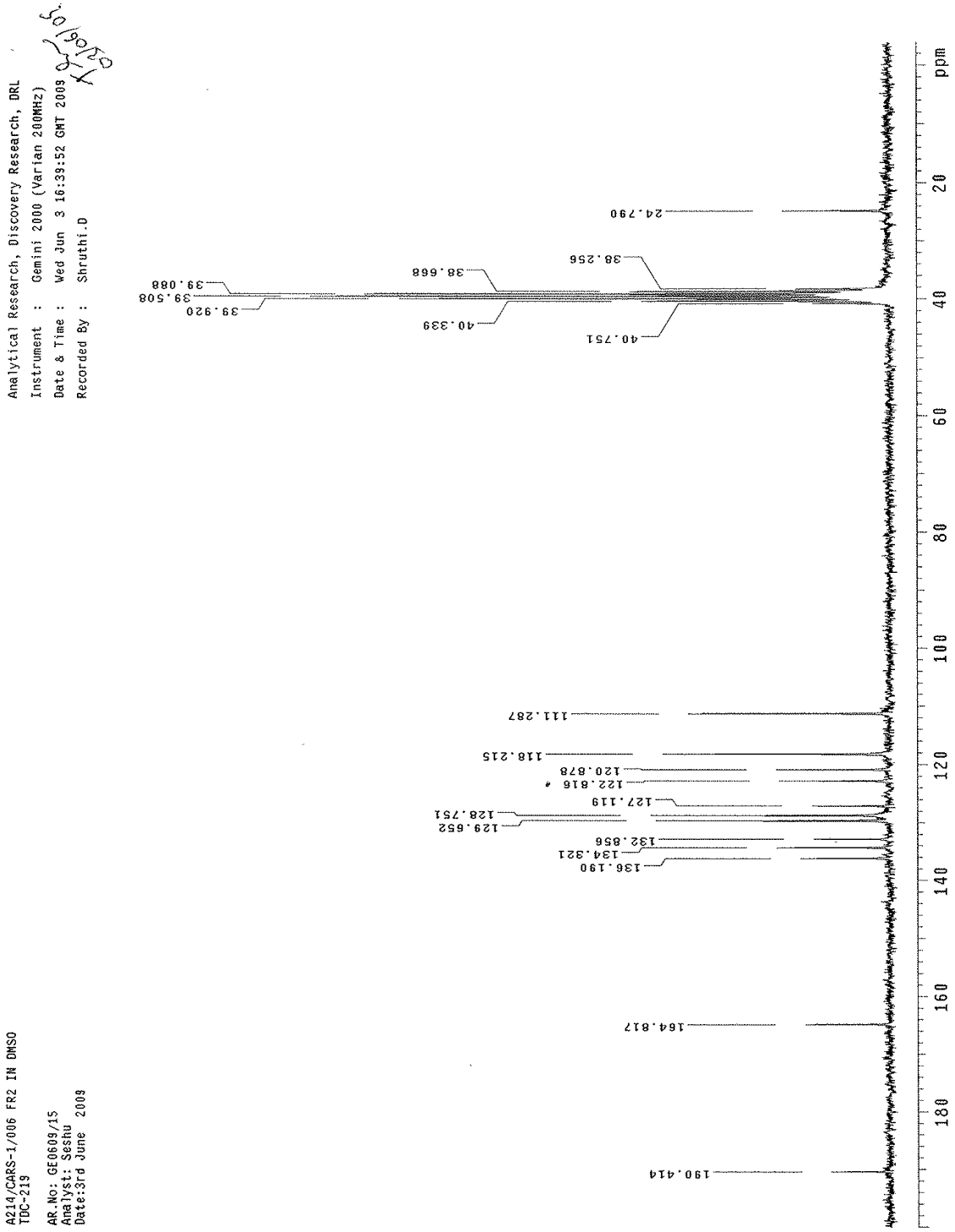
9a



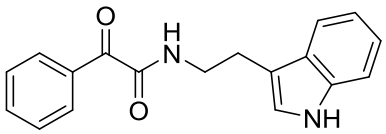
^{13}C NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-phenylacetamide (**9a**):



9a



Mass spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-phenylacetamide (**9a**):



9a

CPS,MIYAPUR

Mass Analysis Report

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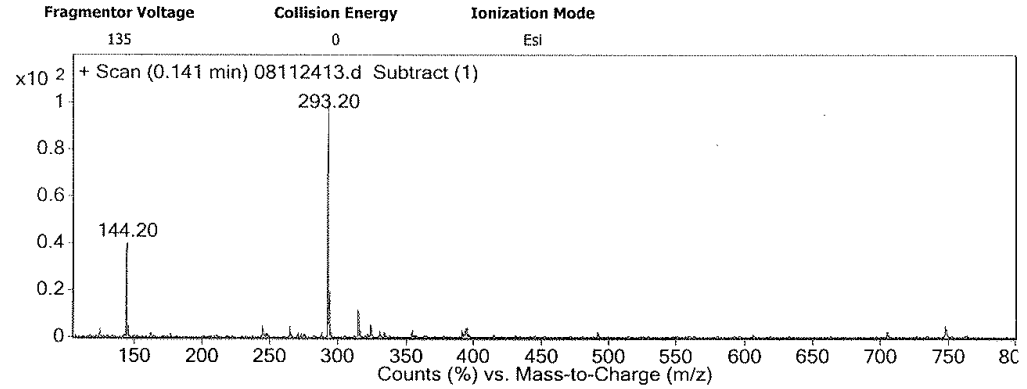
DA Method	DA.m	**Comment**	

User Spectra



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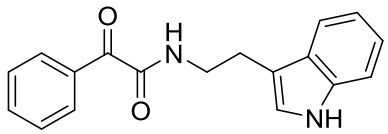
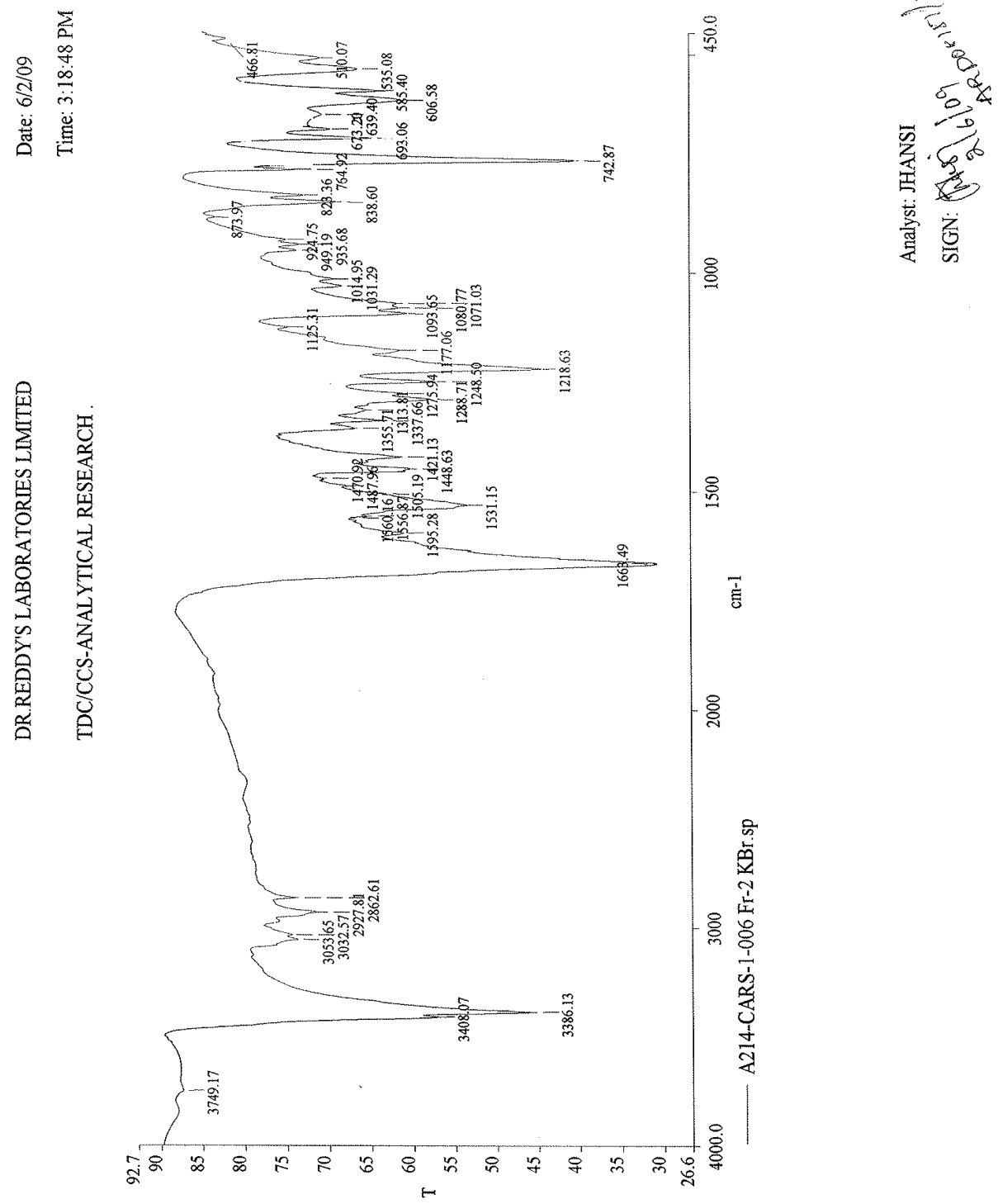
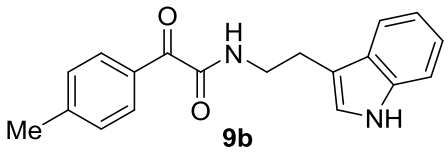
IR spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-phenylacetamide (**9a**):



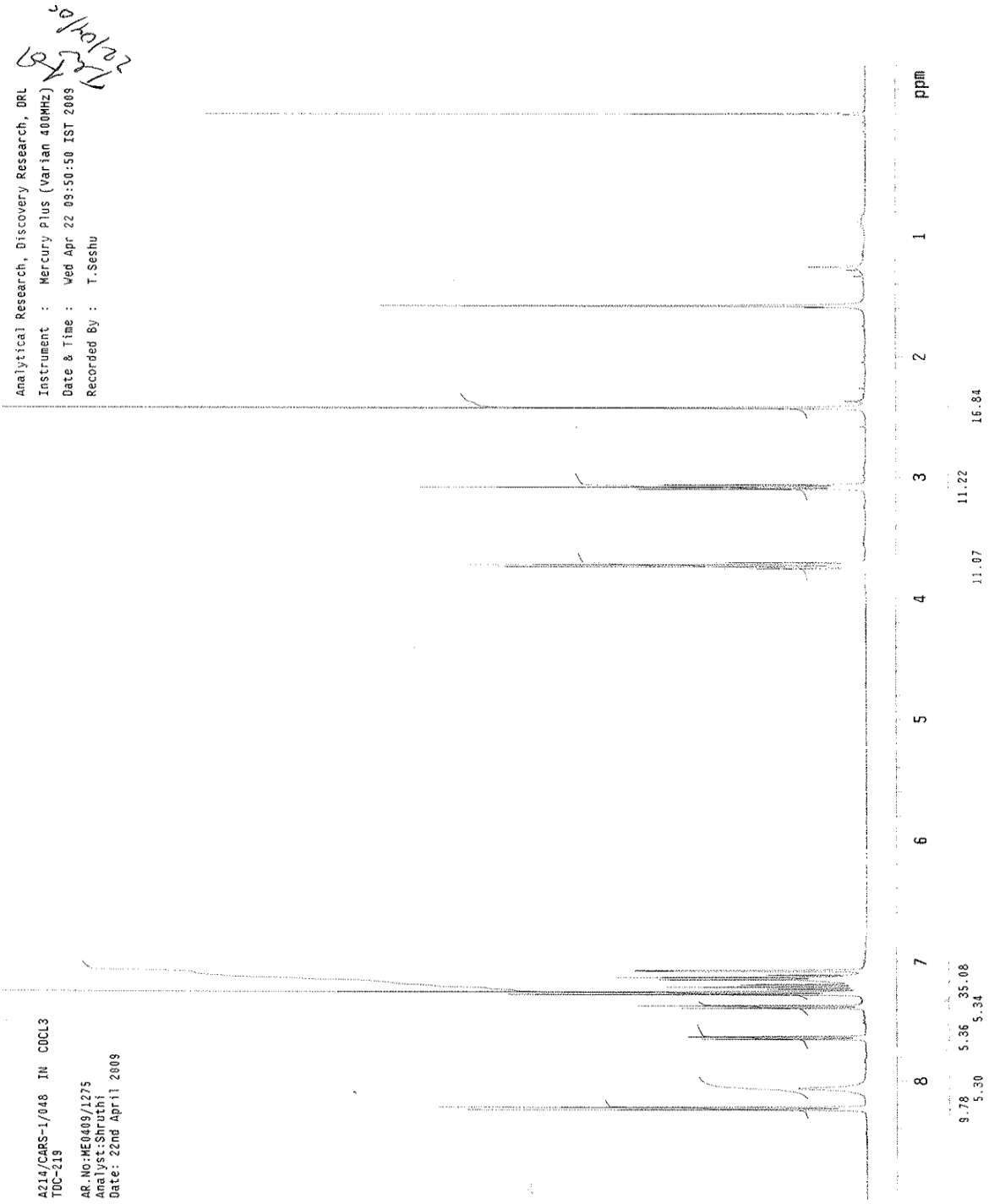
9a



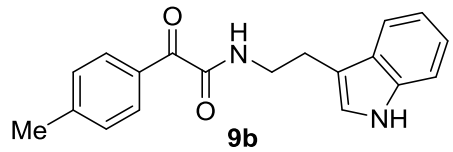
^{1}H NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-(*p*-tolyl)acetamide (**9b**):



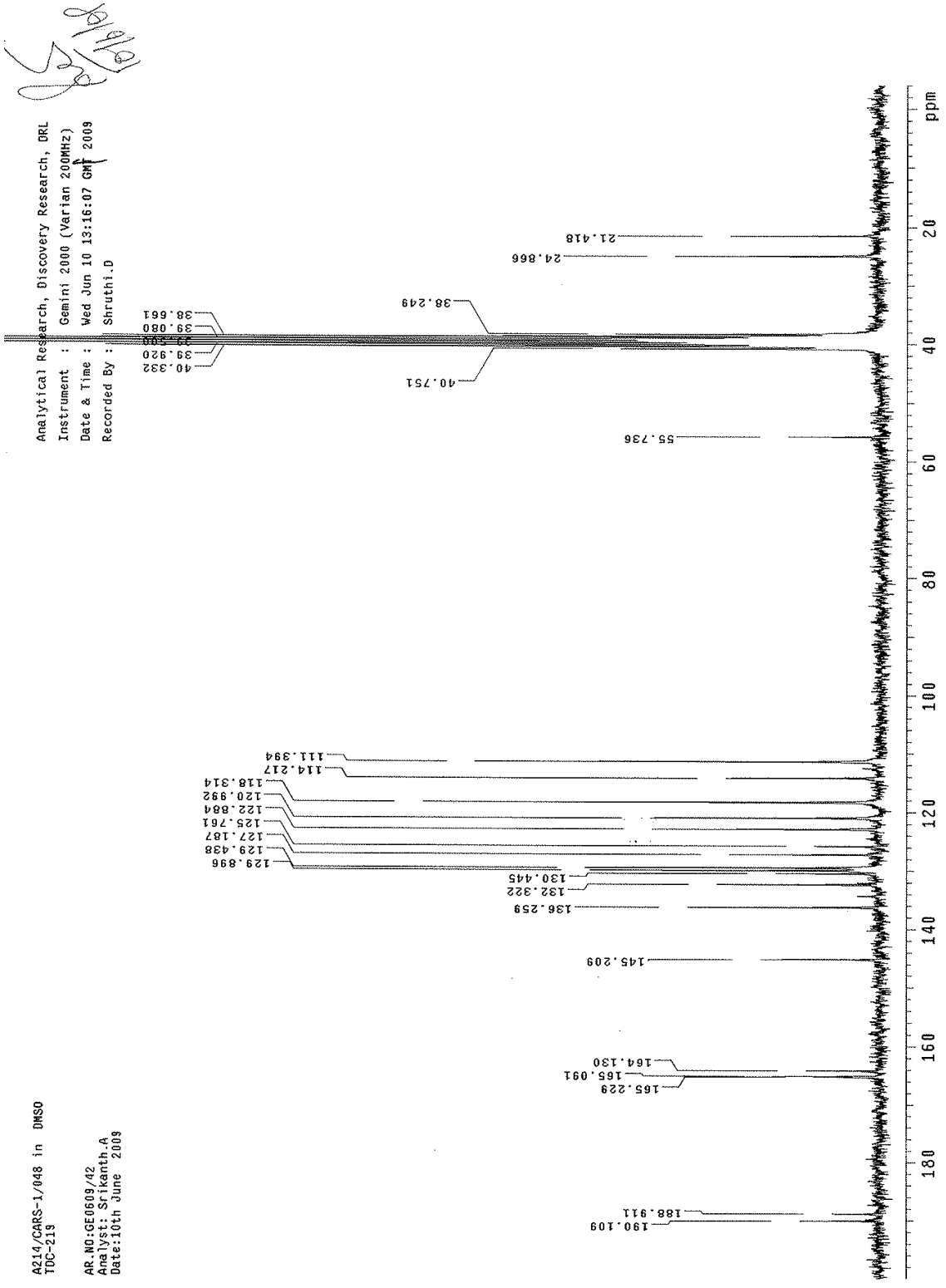
9b



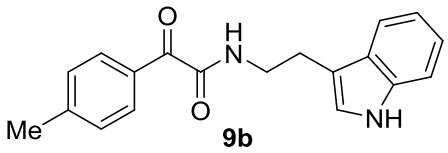
^{13}C NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-(*p*-tolyl)acetamide (**9b**):



9b



Mass spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-(*p*-tolyl)acetamide (**9b**):



9b

CPS,MIYAPUR

Mass Analysis Report

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Sample Type	Sample	**Position**	Vial 54
Instrument Name	Instrument 1	**User Name**	
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DA Method	Quant Process.m	**Comment**	

User Spectra

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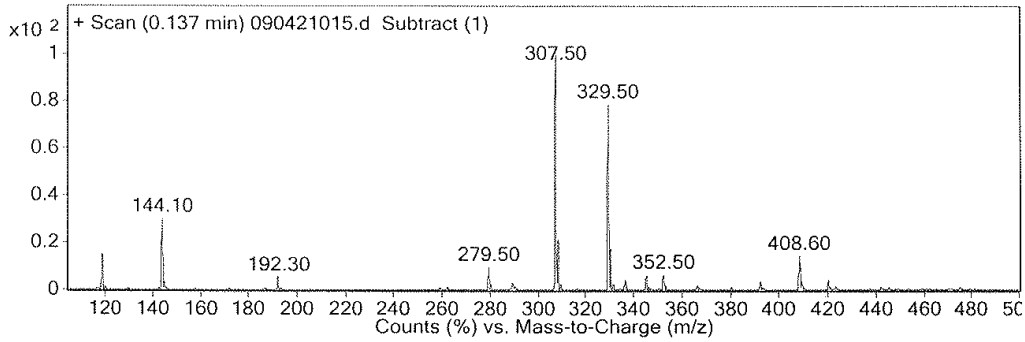

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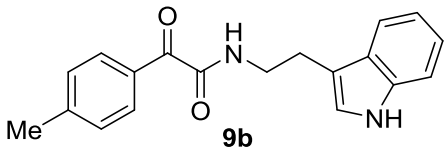
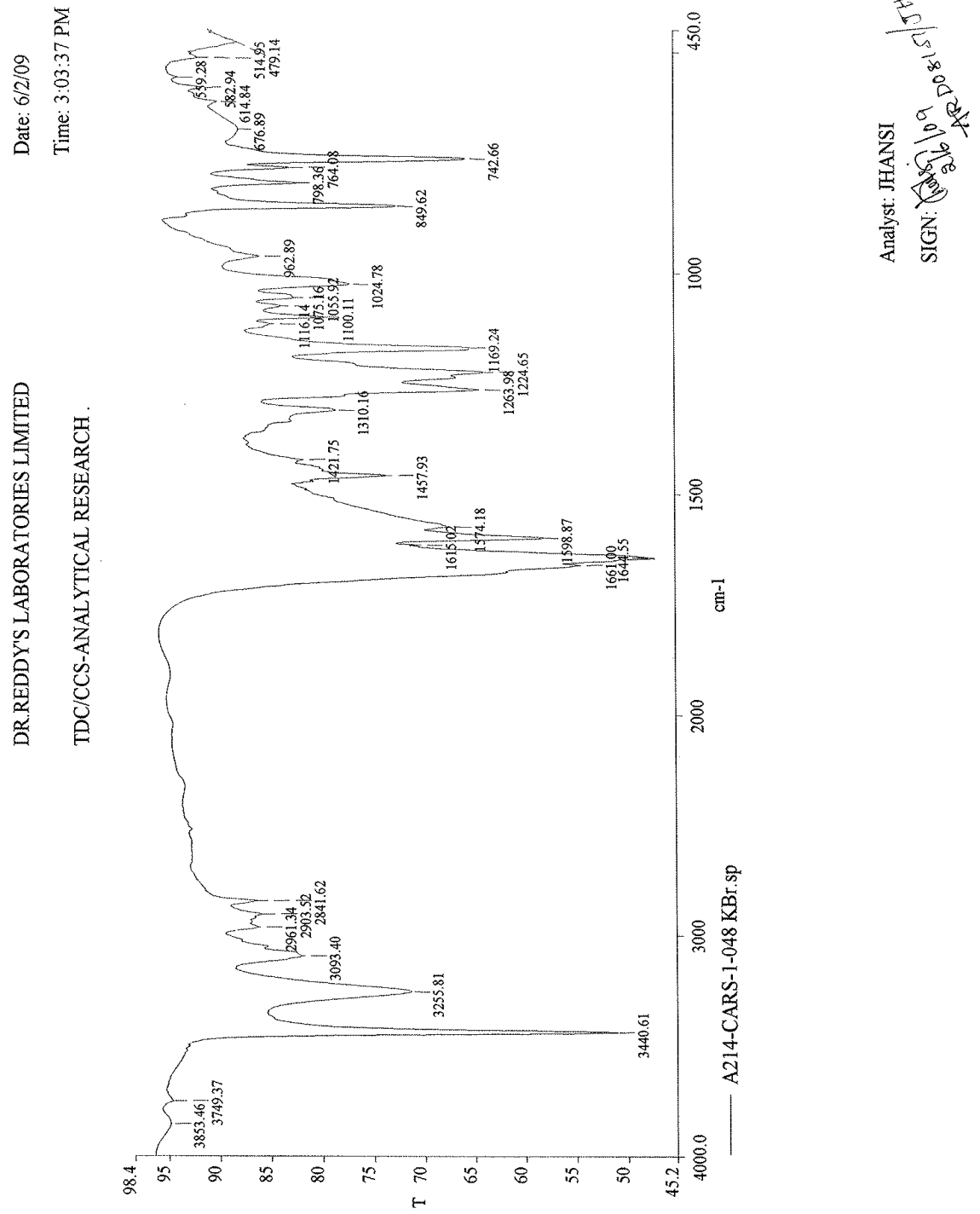
29/04/09

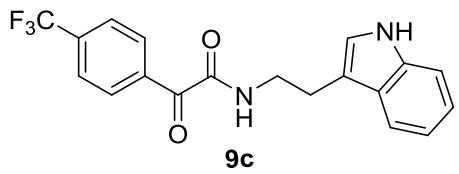
IR spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-(*p*-tolyl)acetamide (**9b**):



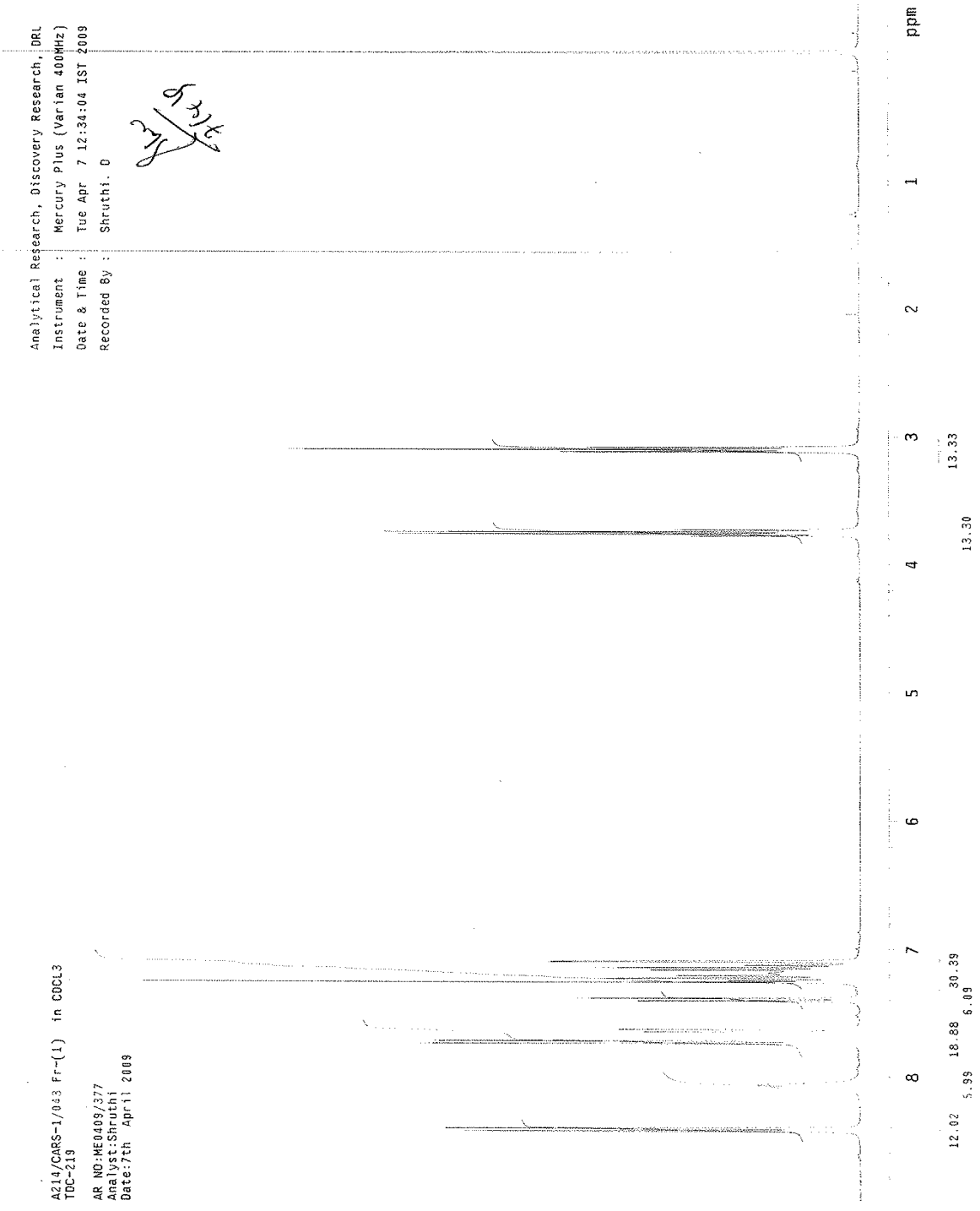
9b



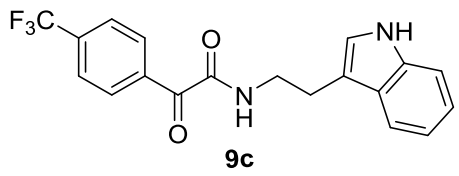
^{1}H NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-(4-(trifluoromethyl)phenyl)acetamide (**9c**):



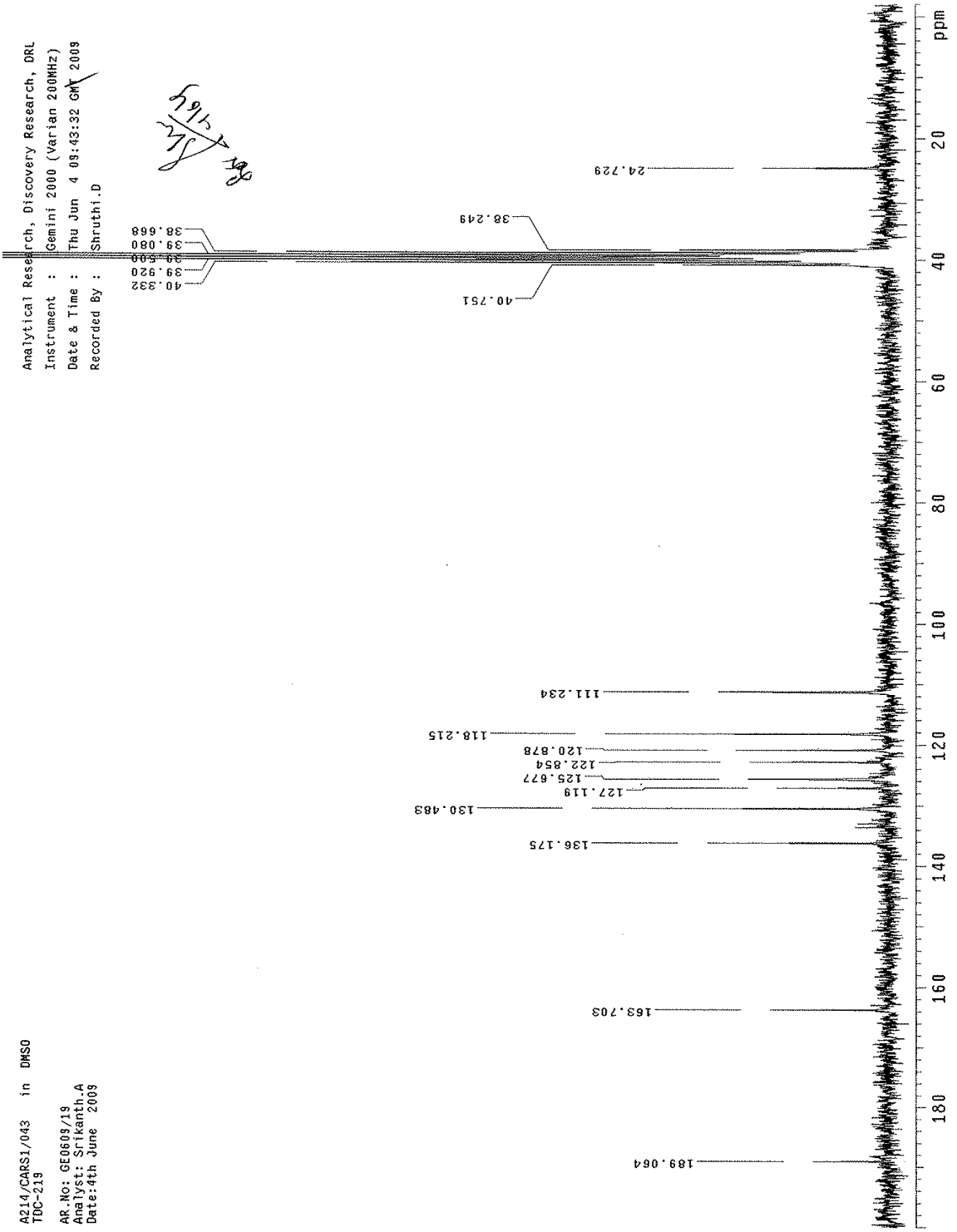
9c



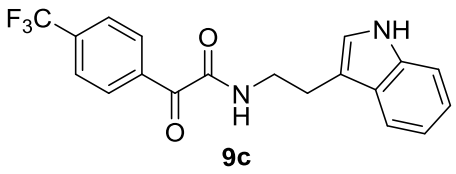
^{13}C NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-(4-(trifluoromethyl)phenyl)acetamide (**9c**):



9c



Mass spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-(4-(trifluoromethyl)phenyl)acetamide (**9c**):



9c

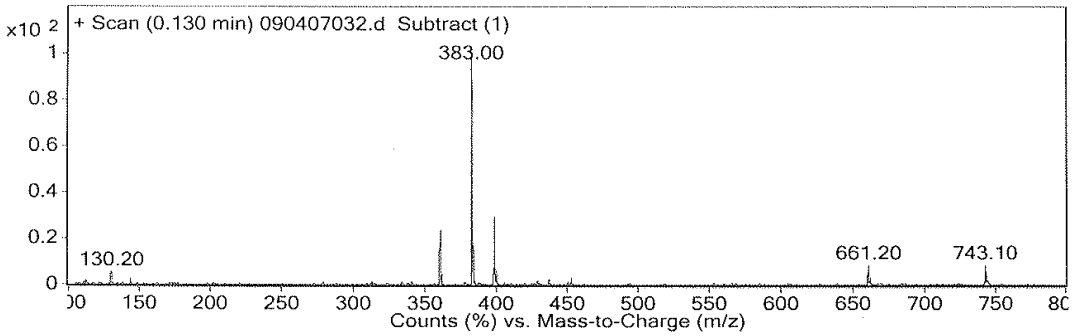
CPS,MIYAPUR

Mass Analysis Report

Data Filename	090407032.d	**Sample Name**	A214/CARS-1/043 FR-1
Sample Type	Sample	**Position**	Vial 78
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	ESMS.m	**Comment**	

User Spectra

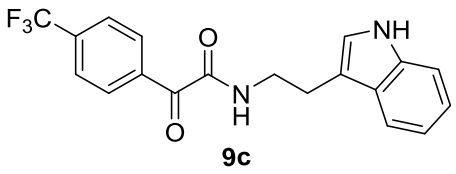
Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	Esi



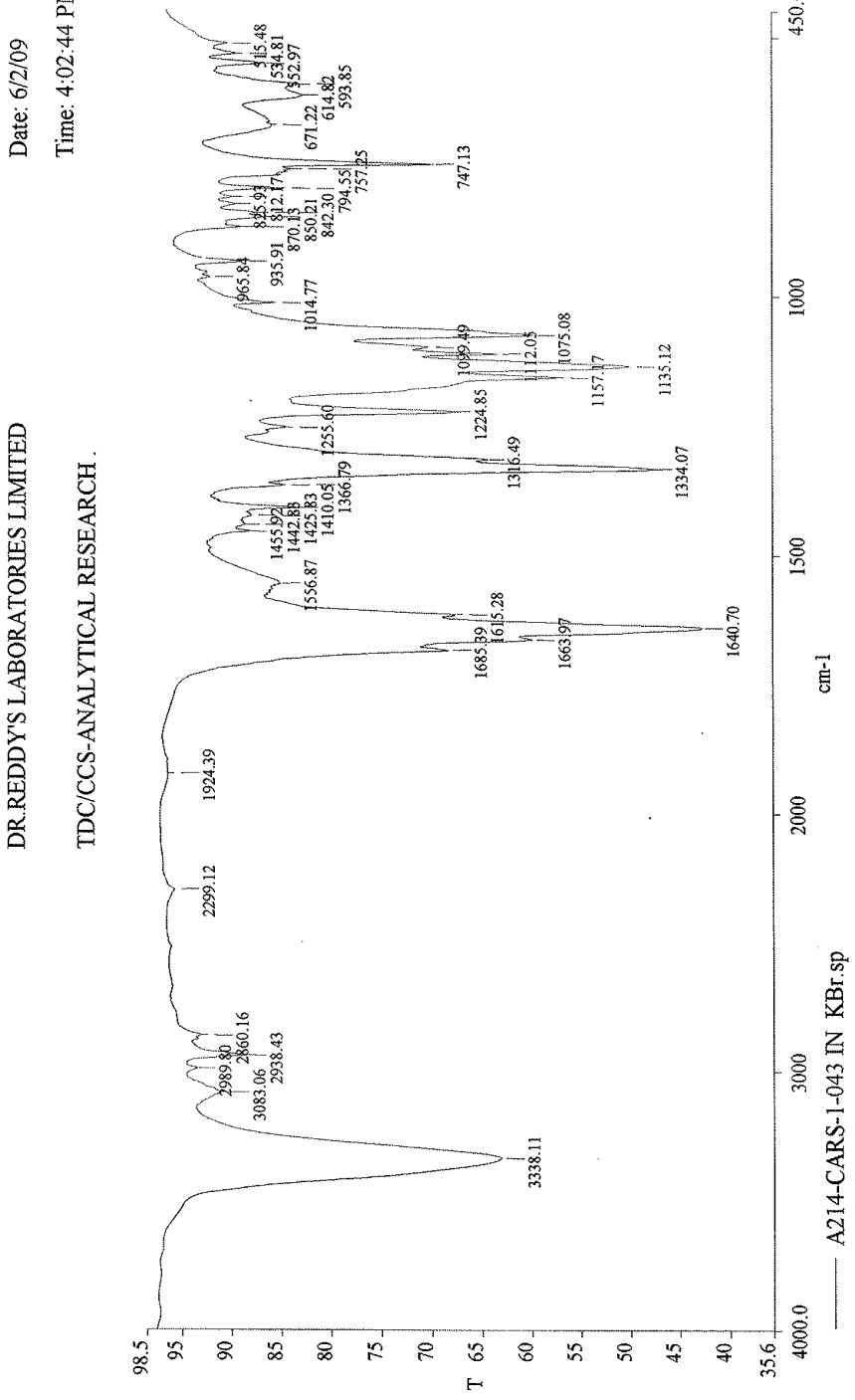
--- End Of Report ---

07/04/09

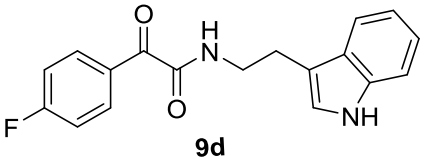
IR spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-(4-(trifluoromethyl)phenyl)acetamide (**9c**):



9c

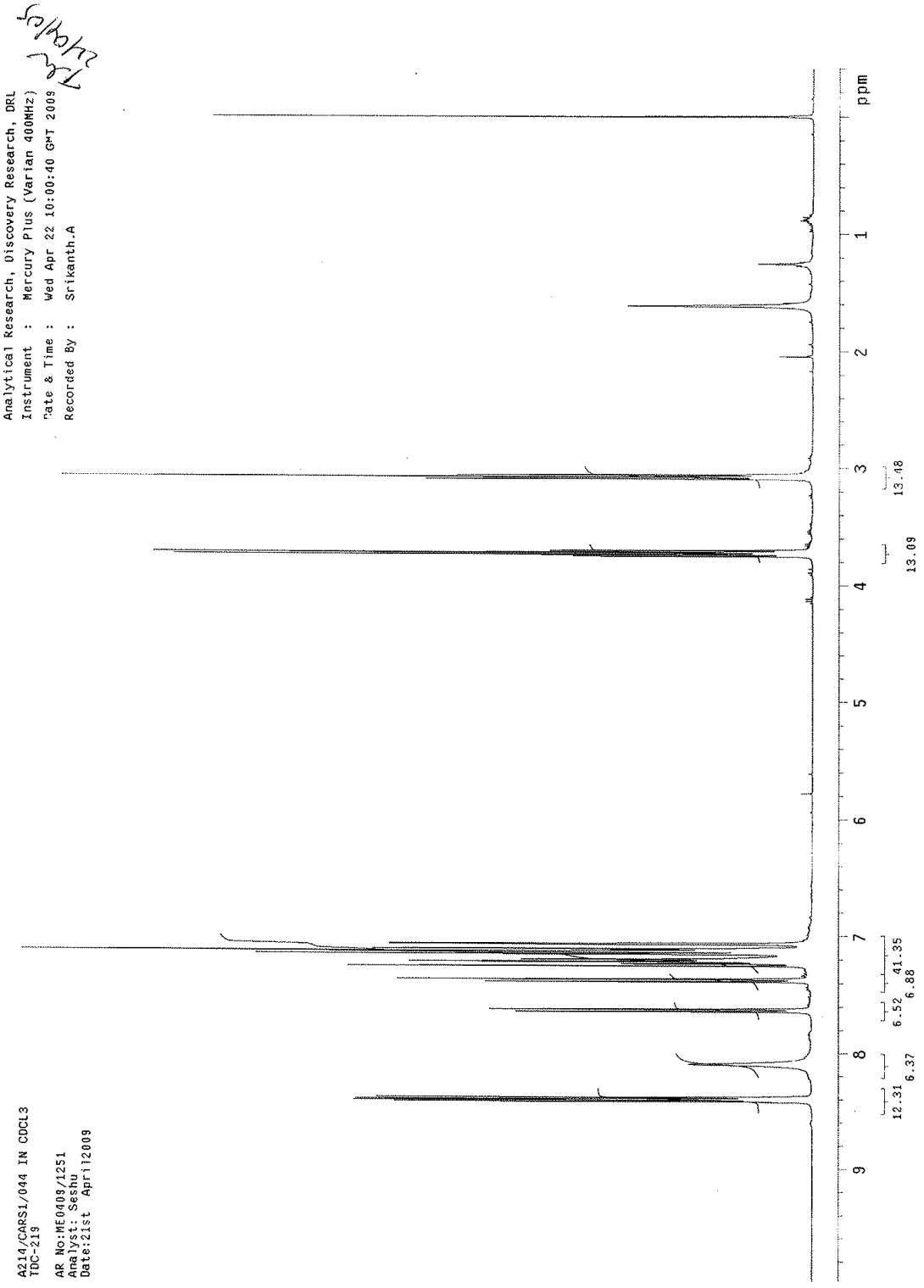


^{1}H NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(4-fluorophenyl)-2-oxoacetamide

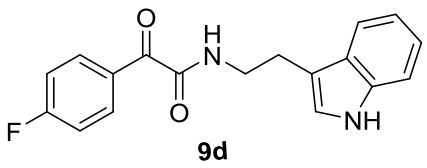


9d

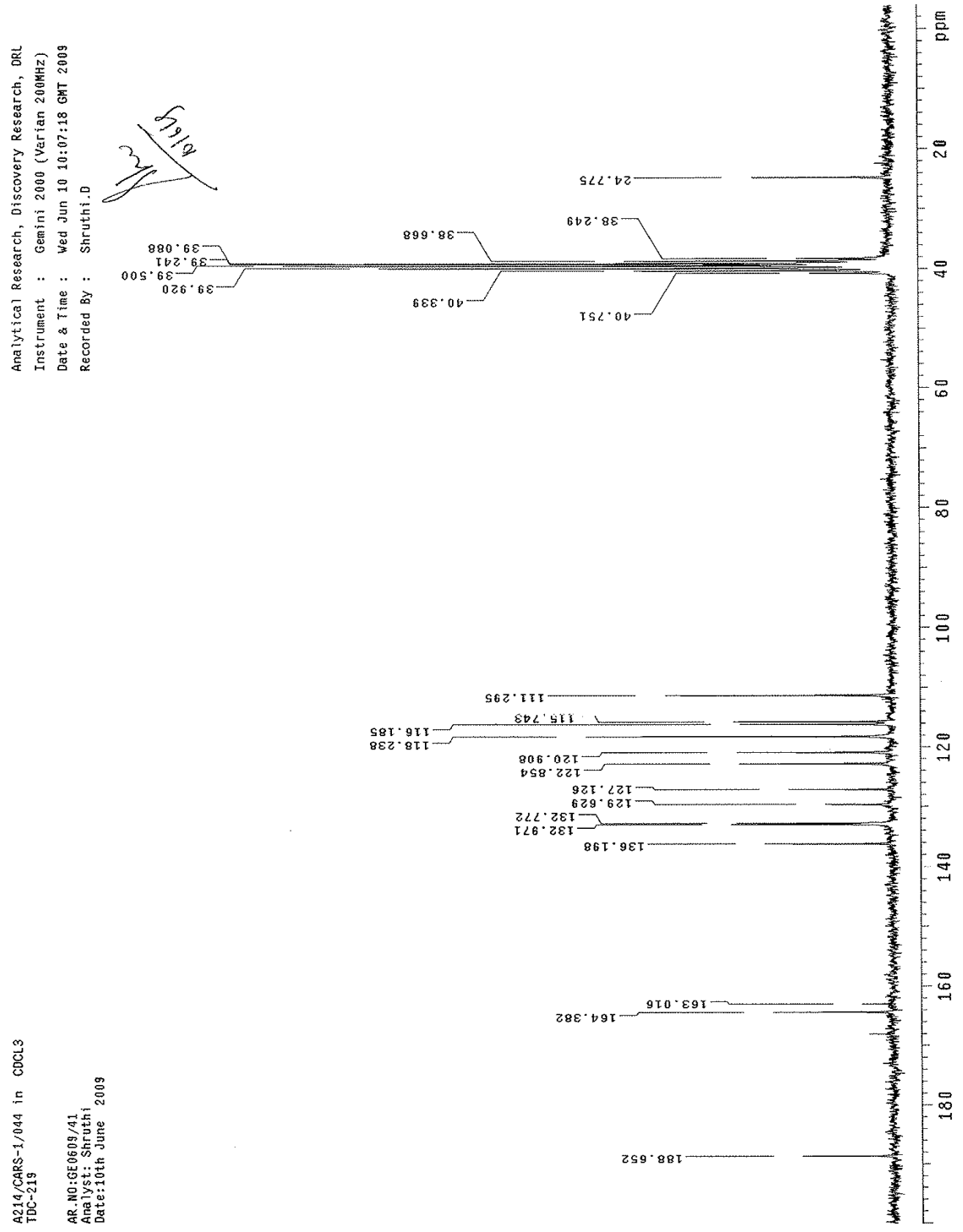
(**9d**):



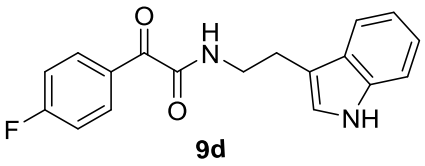
^{13}C NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(4-fluorophenyl)-2-oxoacetamide (**9d**):



9d



Mass spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(4-fluorophenyl)-2-oxoacetamide (**9d**):



9d

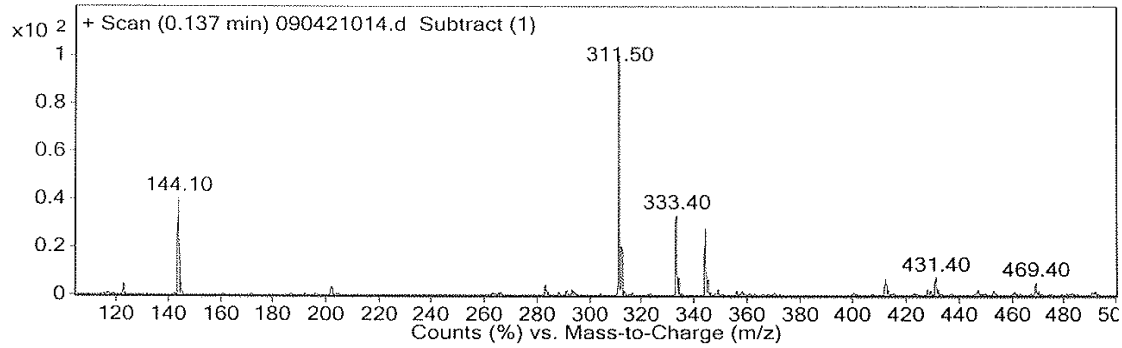
CPS,MIYAPUR

Mass Analysis Report

Data Filename	090421014.d	**Sample Name**	A214/CARS-1/044
Sample Type	Sample	**Position**	Vial 53
Instrument Name	Instrument 1	**User Name**	
Acq Method		**IRM Calibration Status**	Success
DA Method	Quant Process.m	**Comment**	

User Spectra

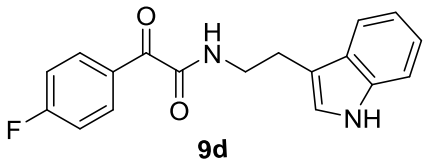
Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	Esi



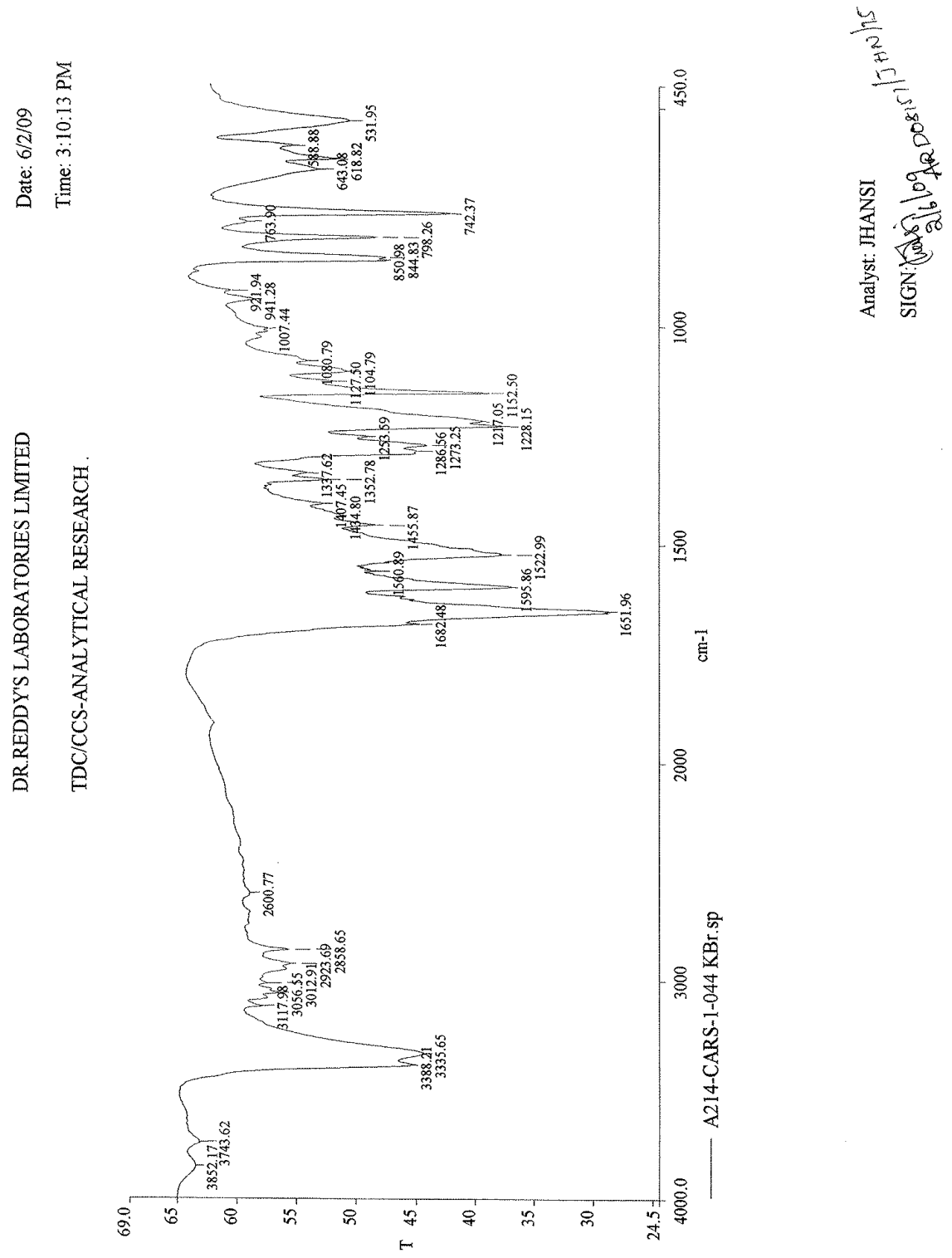
--- End Of Report ---

21/04/09

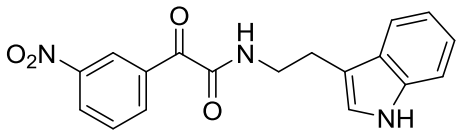
IR spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(4-fluorophenyl)-2-oxoacetamide (**9d**):



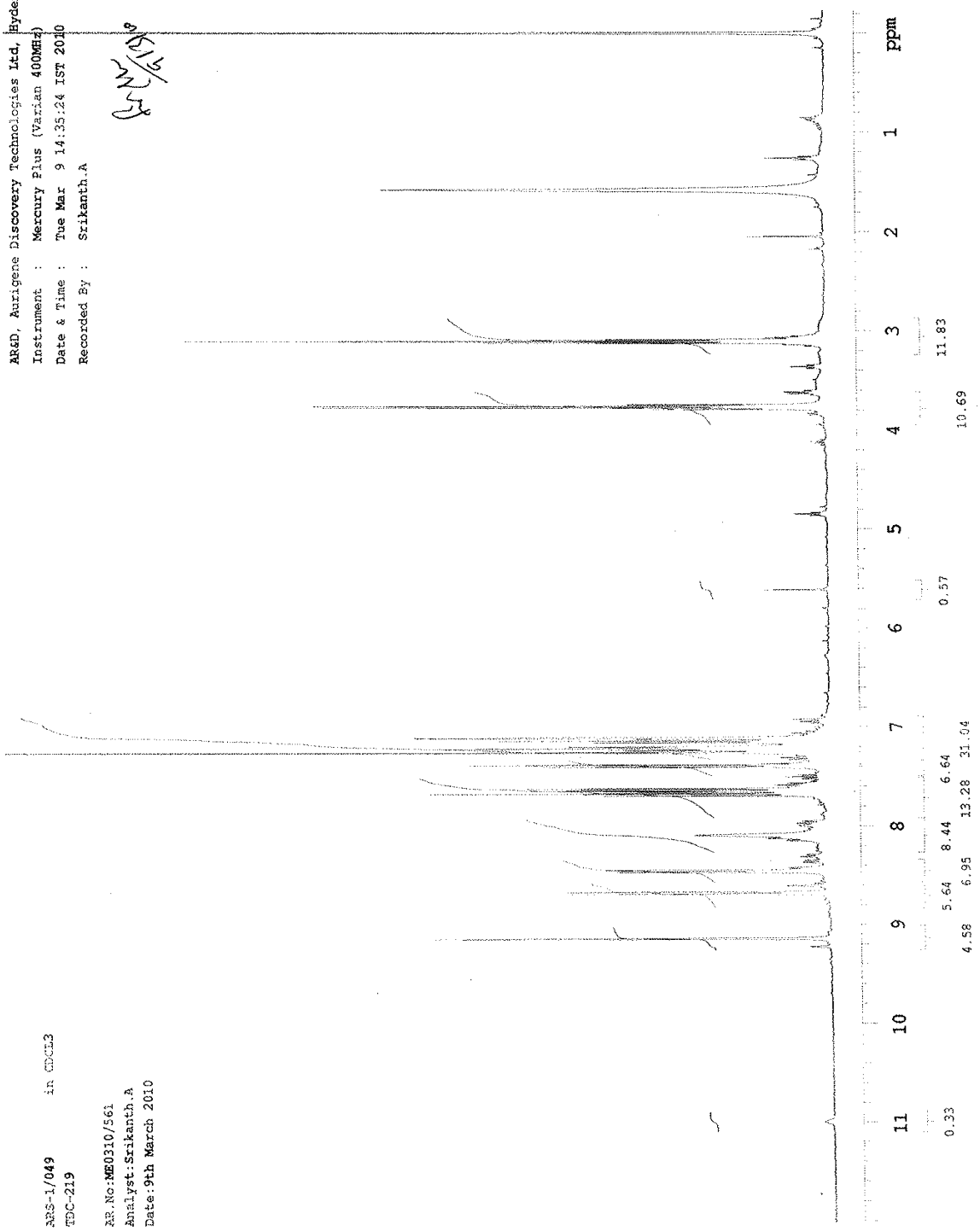
9d



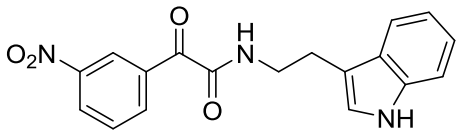
^{1}H NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(3-nitrophenyl)-2-oxoacetamide (**9e**):



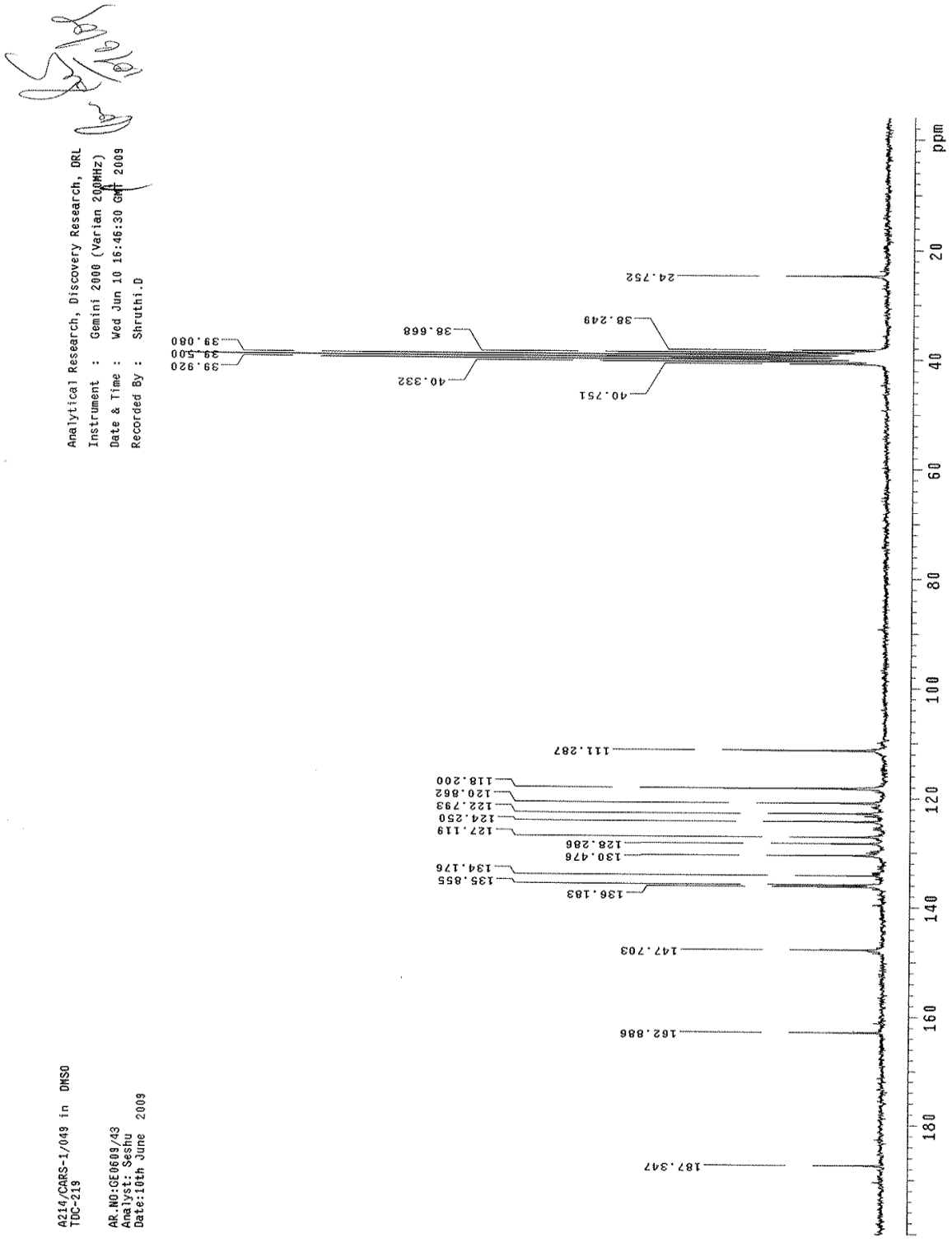
9e



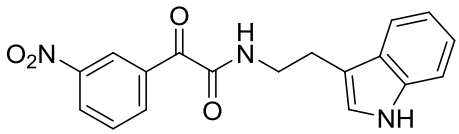
^{13}C NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(3-nitrophenyl)-2-oxoacetamide (**9e**):



9e



Mass spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(3-nitrophenyl)-2-oxoacetamide (**9e**):



9e

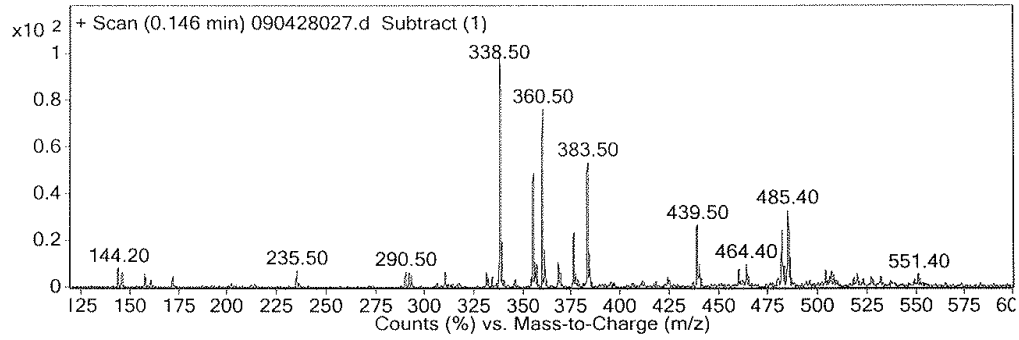
CPS,MIYAPUR

Mass Analysis Report

Data Filename	090428027.d	**Sample Name**	A214/CARS-1/049
Sample Type	Sample	**Position**	Vial 82
Instrument Name	Instrument 1	**User Name**	
Acq Method		**IRM Calibration Status**	Success
DA Method	Quant Process.m	**Comment**	

User Spectra

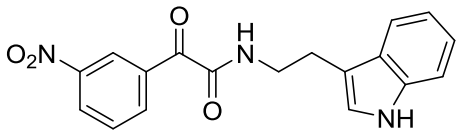
Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	Esi



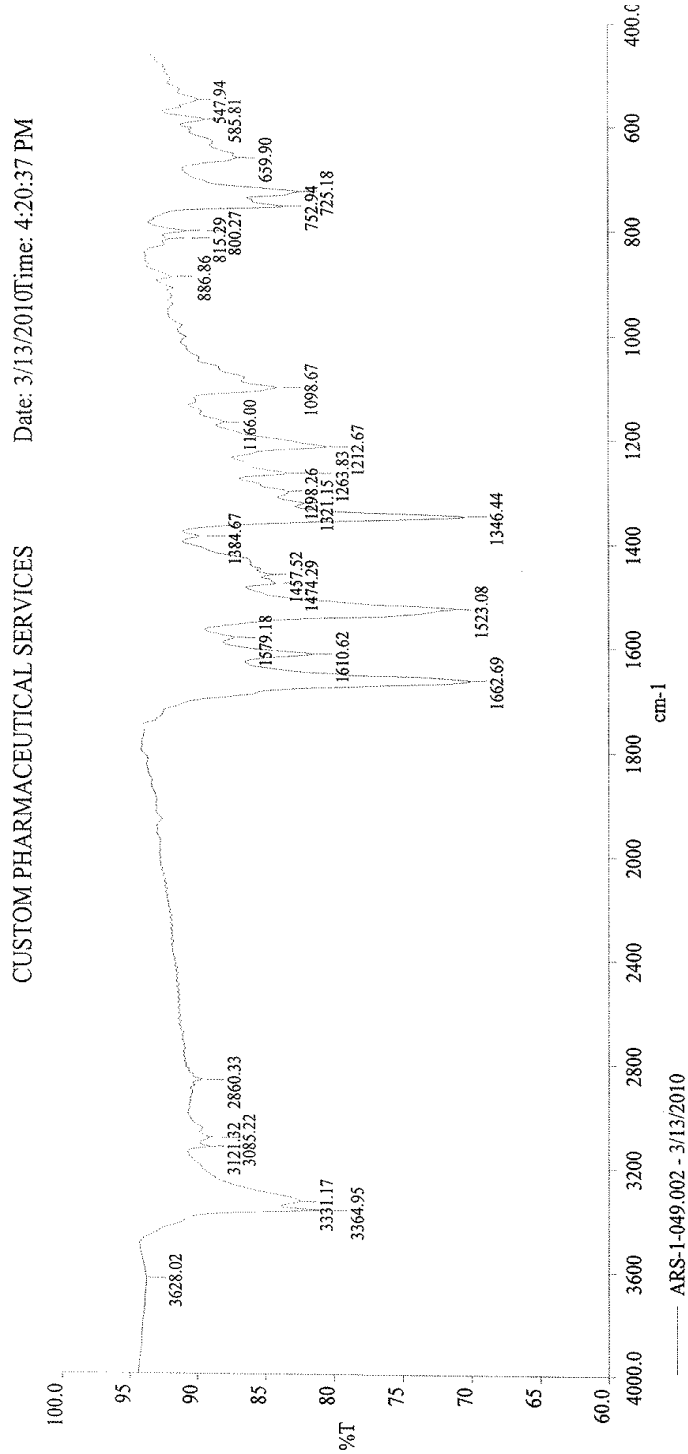
--- End Of Report ---

DA4-28/04/09

IR spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(3-nitrophenyl)-2-oxoacetamide (**9e**):

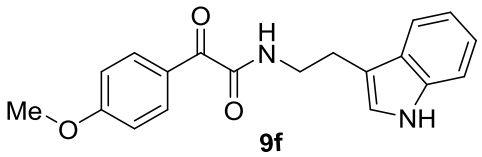


9e

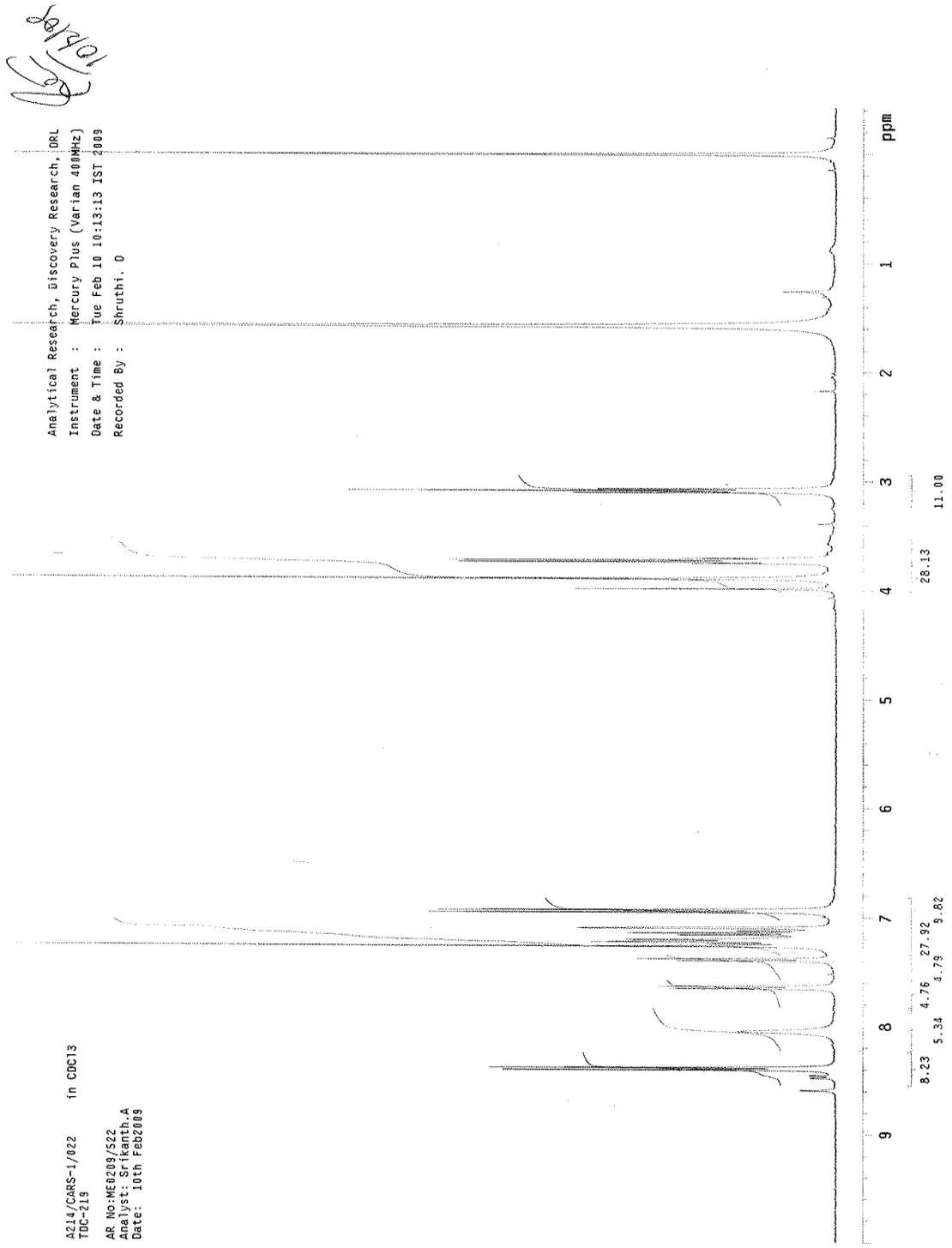


analyst

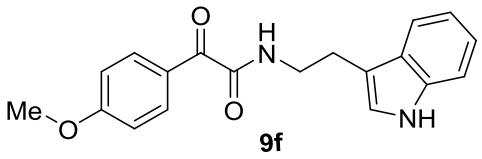
^{1}H NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(4-methoxyphenyl)-2-oxoacetamide (**9f**):



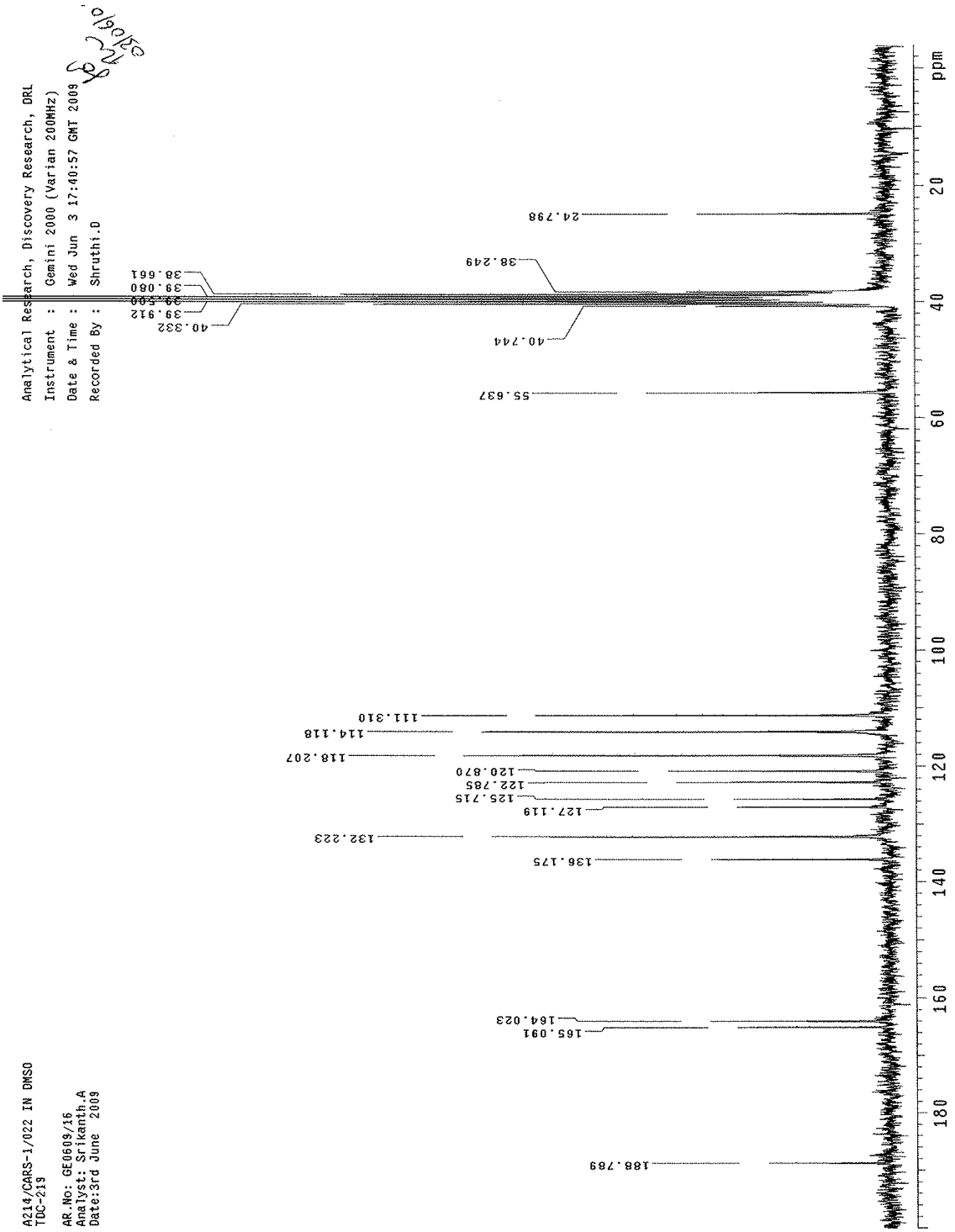
9f



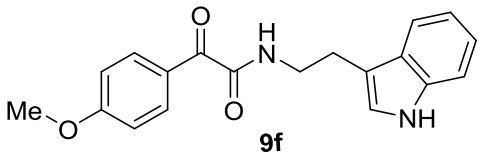
^{13}C NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(4-methoxyphenyl)-2-oxoacetamide (**9f**):



9f



Mass spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(4-methoxyphenyl)-2-oxoacetamide (**9f**):



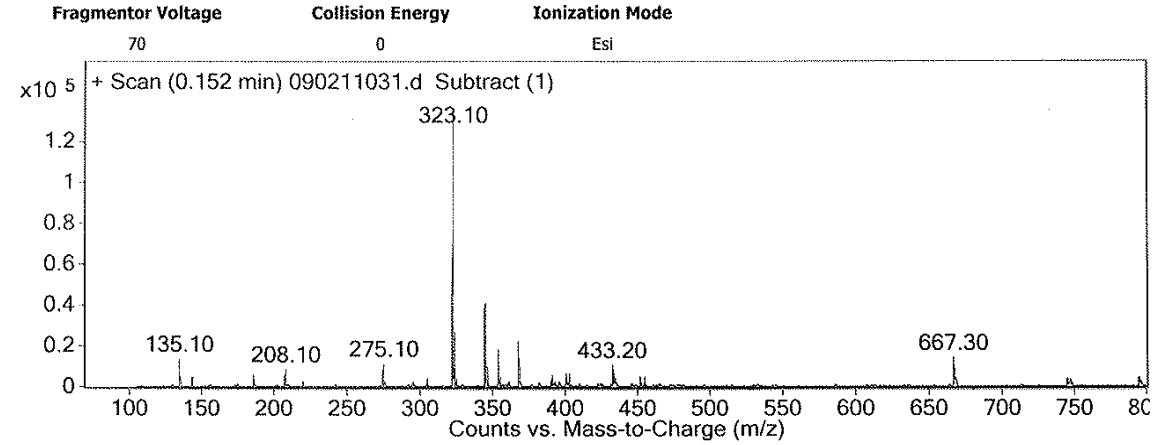
9f

CPS,MIYAPUR

Mass Analysis Report

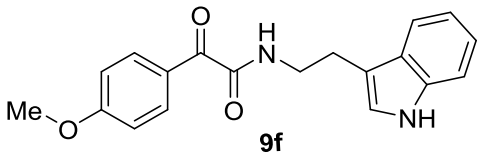
Data Filename	090211031.d	**Sample Name**	A214/CARS/022
Sample Type	Sample	**Position**	Vial 30
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	DA.m	**Comment**	

User Spectra

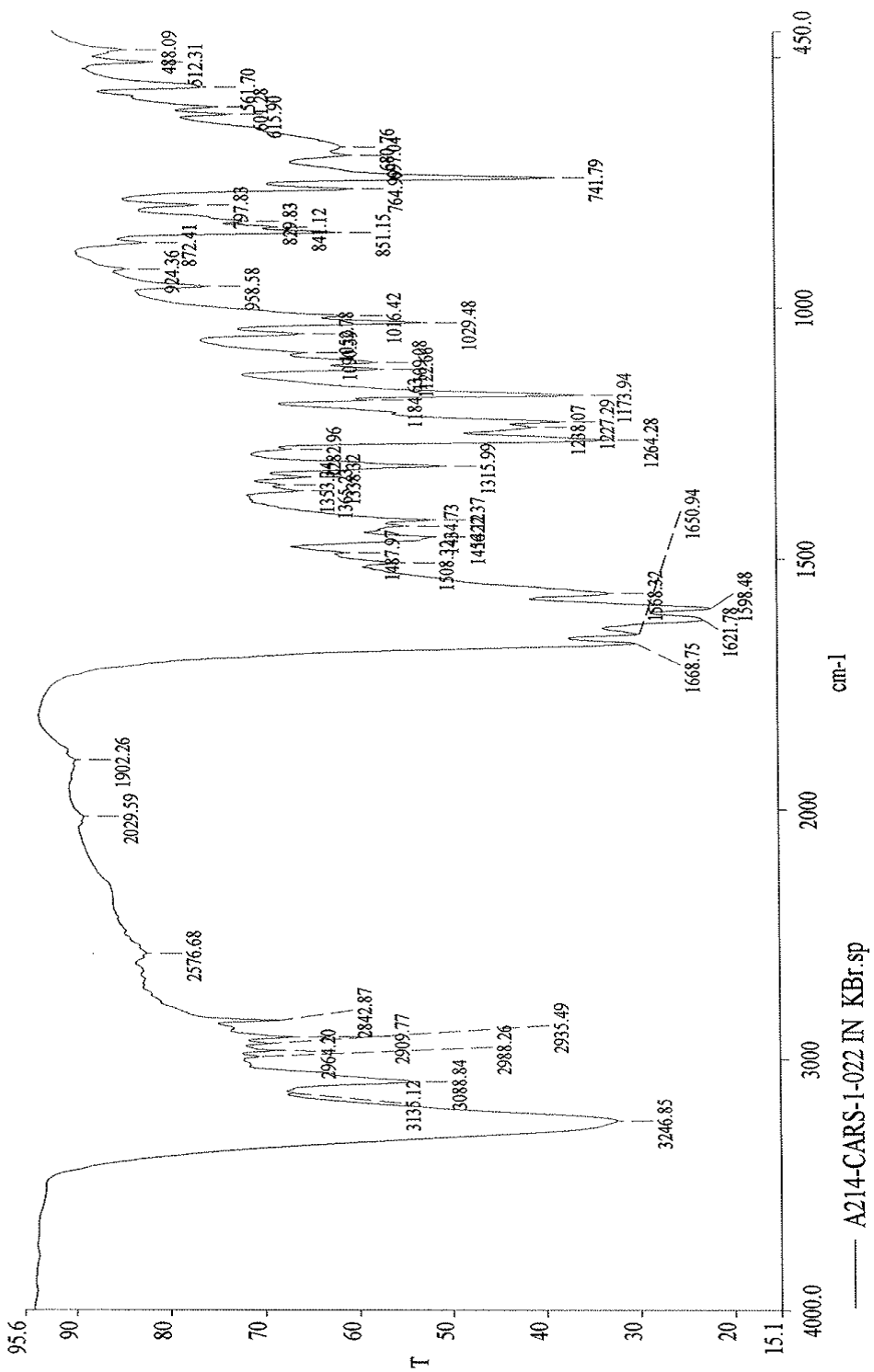


--- End Of Report ---

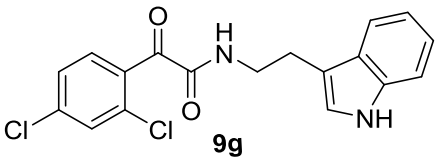
IR spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(4-methoxyphenyl)-2-oxoacetamide (**9f**):



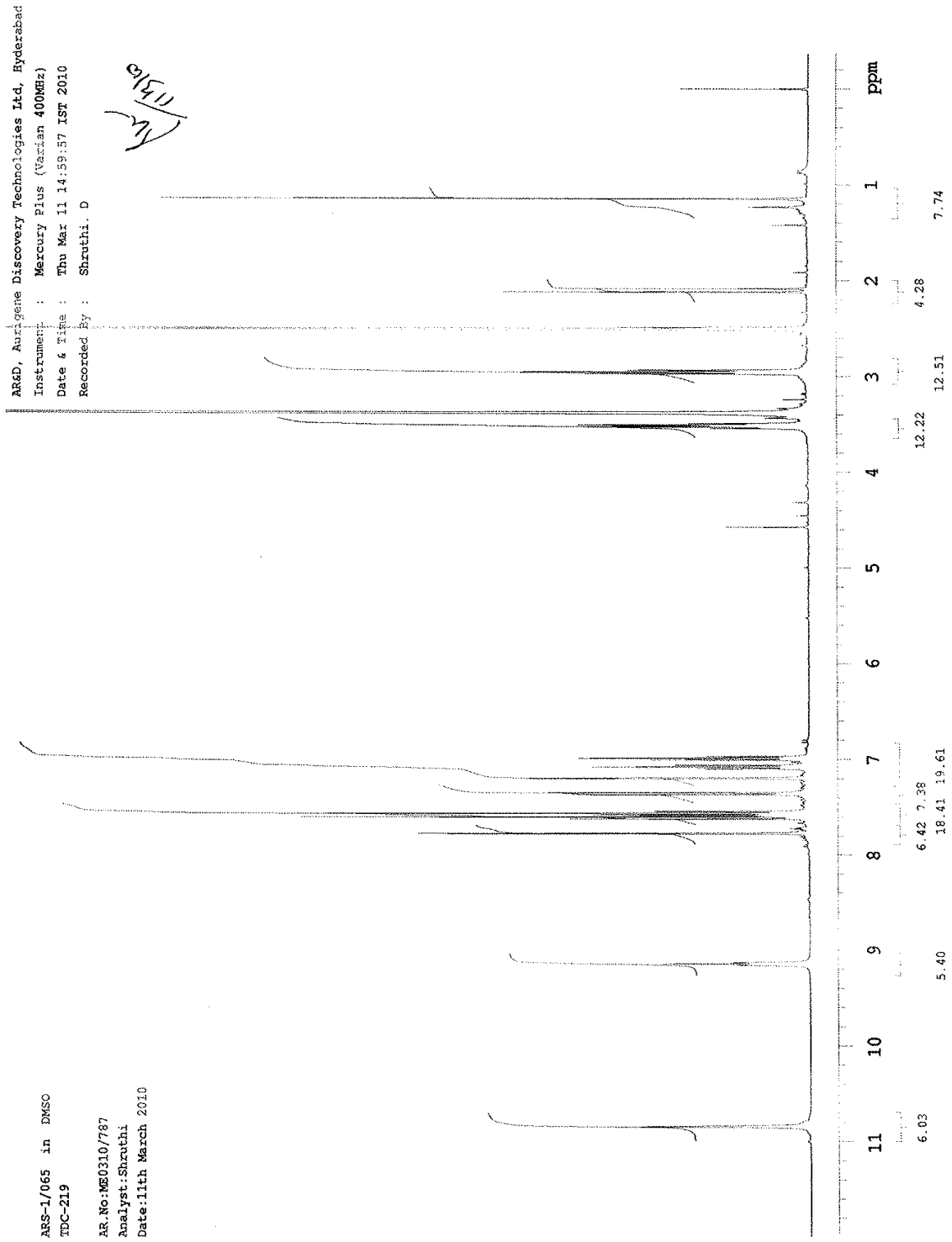
9f



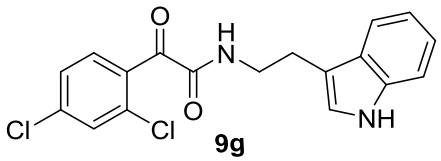
^{1}H NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(2,4-dichlorophenyl)-2-oxoacetamide (**9g**):



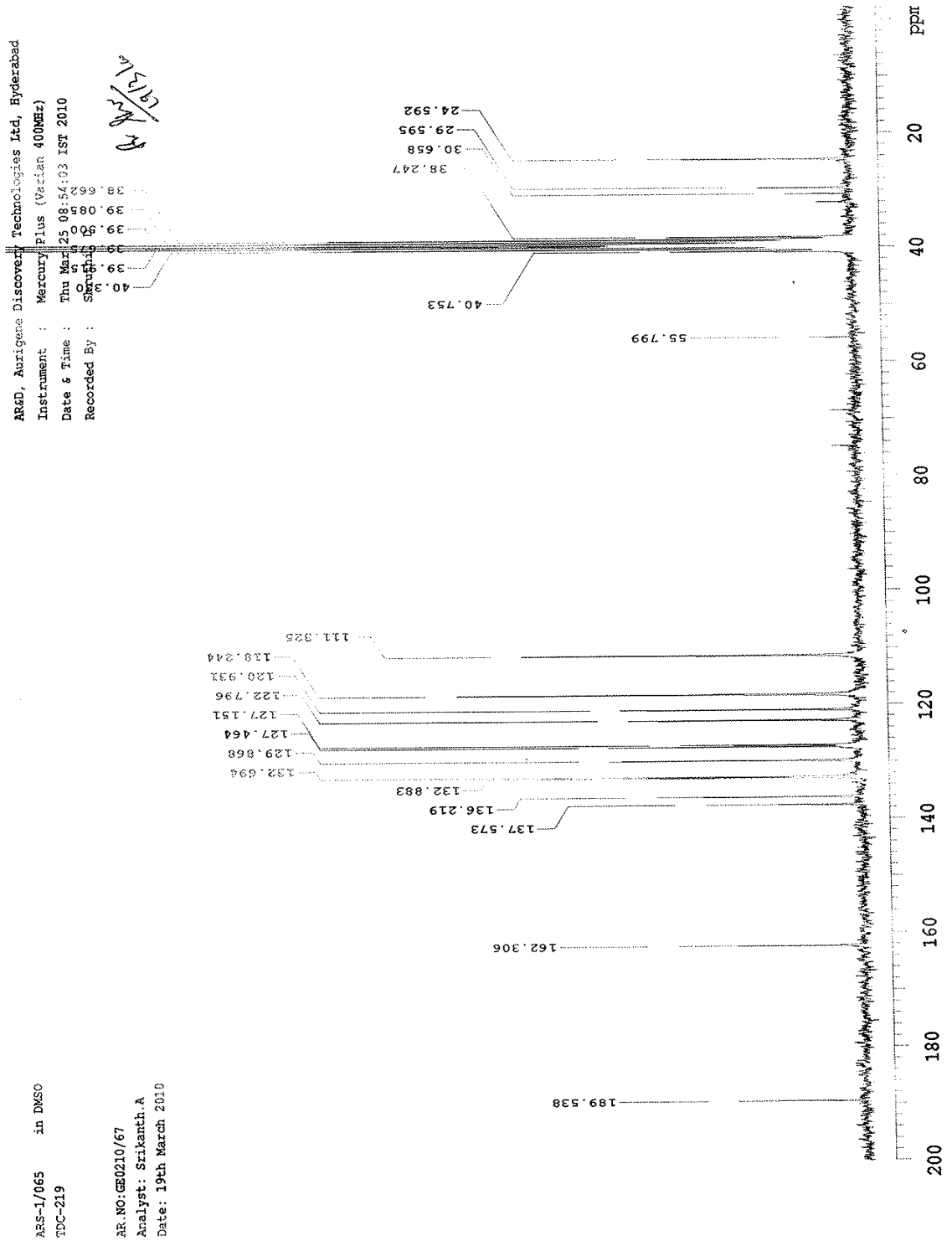
9g



^{13}C NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(2,4-dichlorophenyl)-2-oxoacetamide (**9g**):



9g



Mass spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(2,4-dichlorophenyl)-2-oxoacetamide (**9g**):

9g

CPS.MIYAPUR

Mass Analysis Report

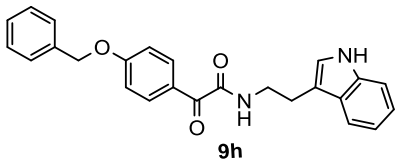
Data Filename	100308022.d	**Sample Name**	ARS-1/065
Sample Type	Sample	**Position**	Vial 62
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	default.m	**Comment**	

User Spectra

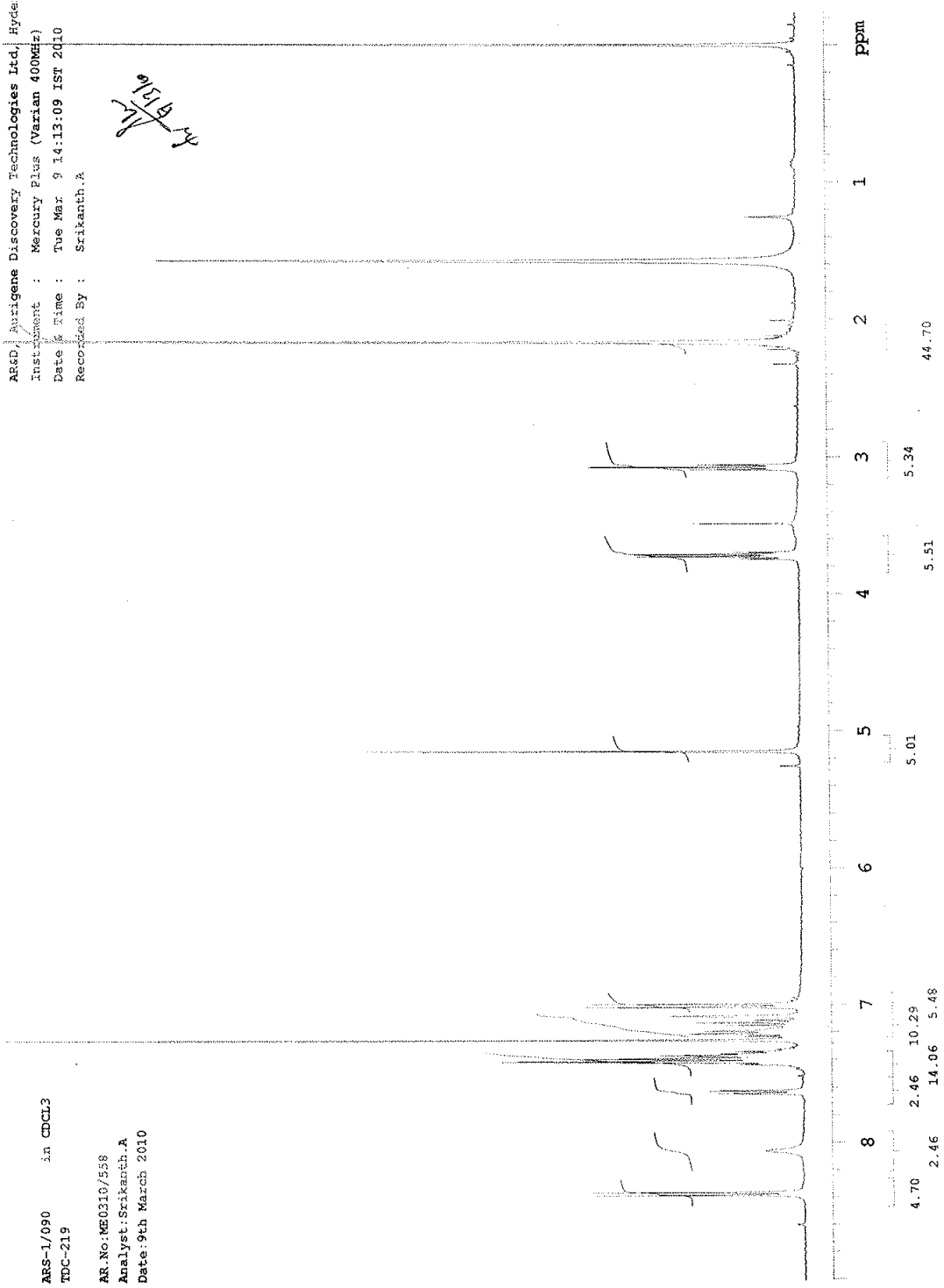
Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	Esi

--- End Of Report ---

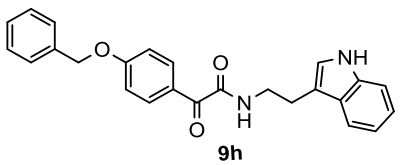
^{1}H NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(4-(benzyloxy)phenyl-2-oxoacetamide (**9h**):



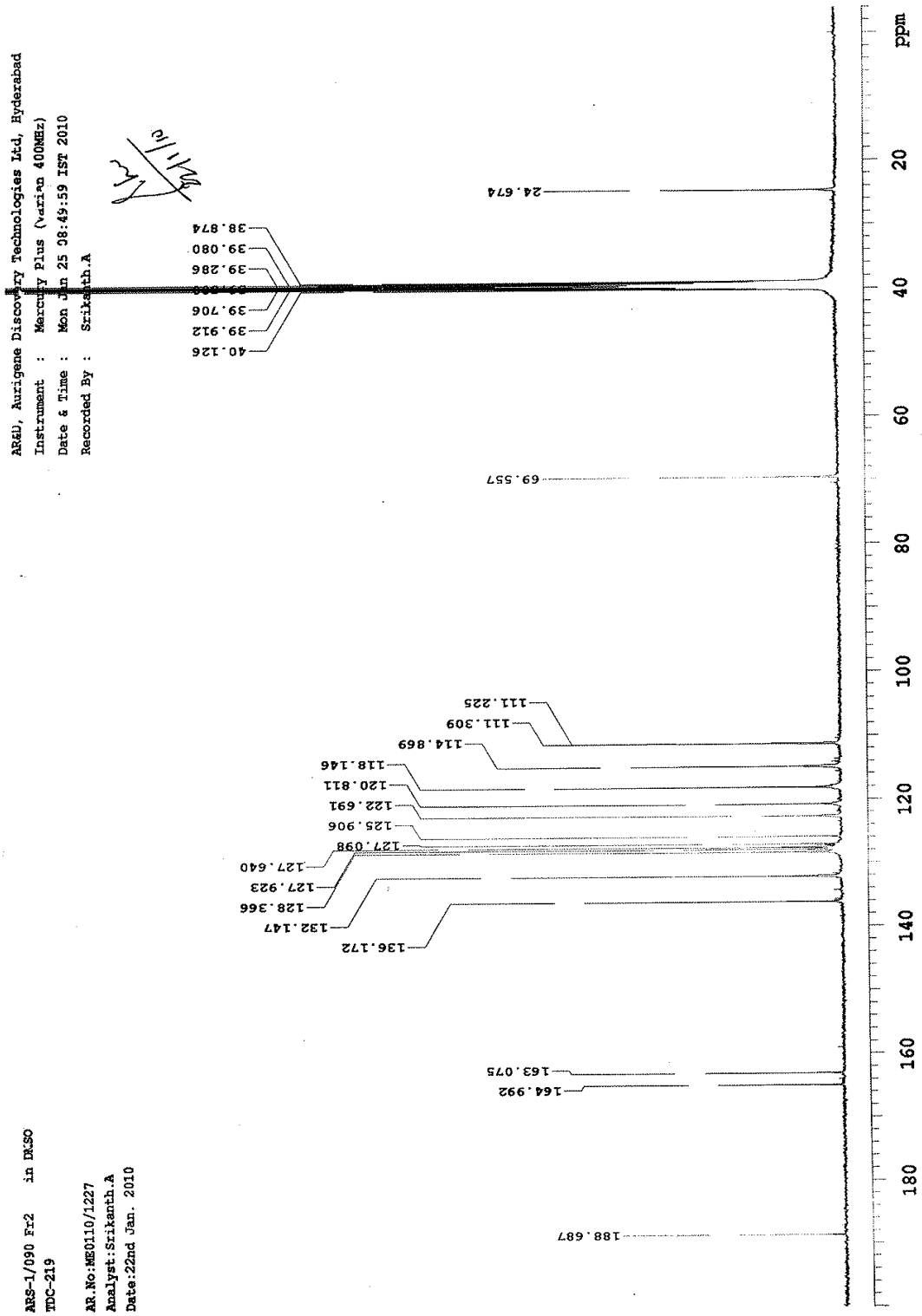
9h



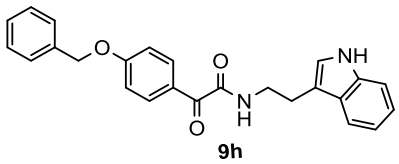
^{13}C NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(4-(benzyloxy)phenyl)-2-oxoacetamide (**9h**):



9h



Mass spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(4-(benzyloxy)phenyl)-2-oxoacetamide (**9h**):



9h

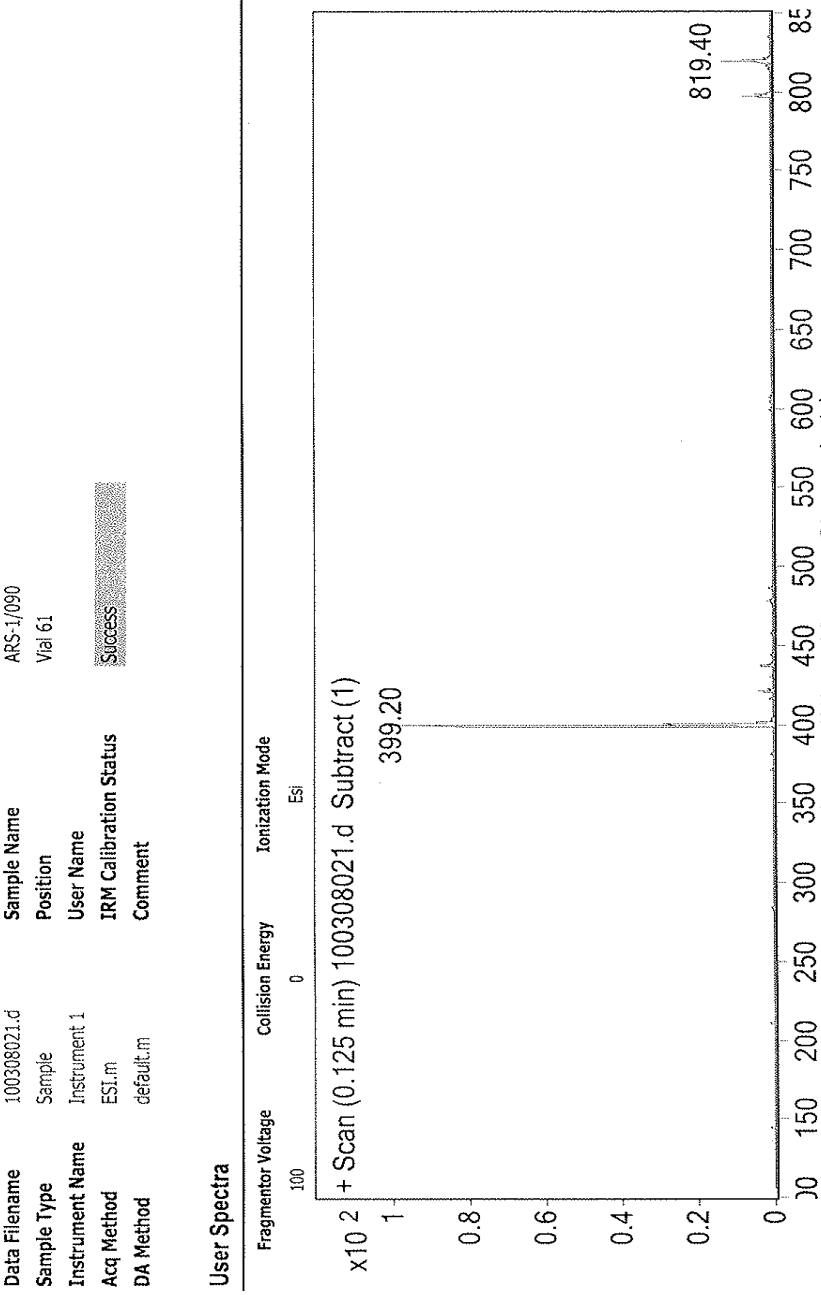
CPS,MIYAPUR

Mass Analysis Report

Data Filename	100308021.d	**Sample Name**	ARS-1/090
Sample Type	Sample	**Position**	Vial 61
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	default.m	**Comment**	

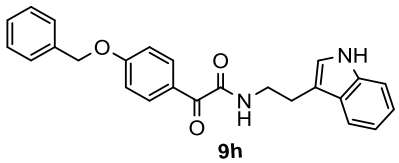
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	Esi

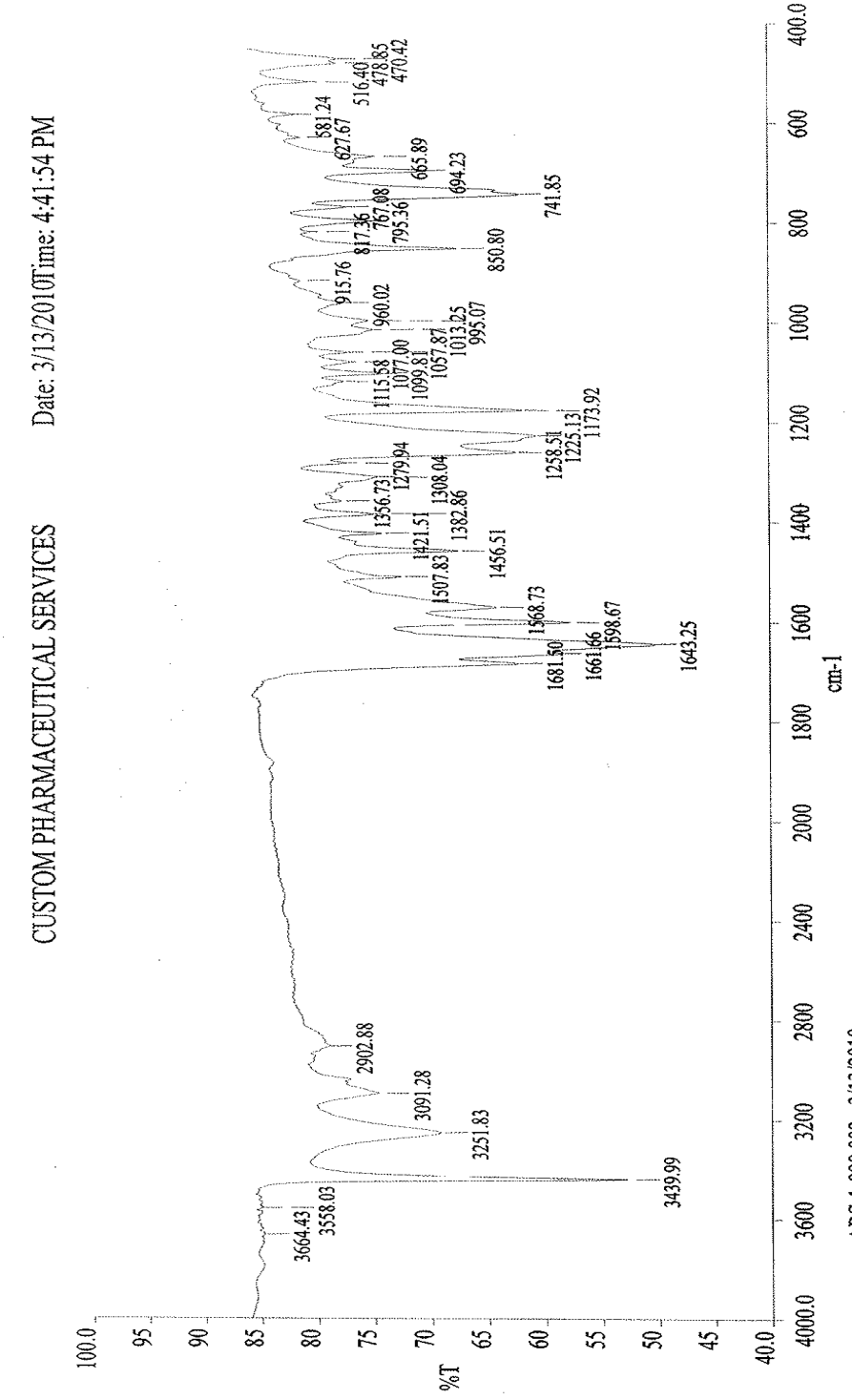


--- End Of Report ---

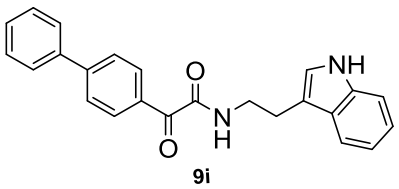
IR spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-(4-(benzyloxy)phenyl)-2-oxoacetamide (**9h**):



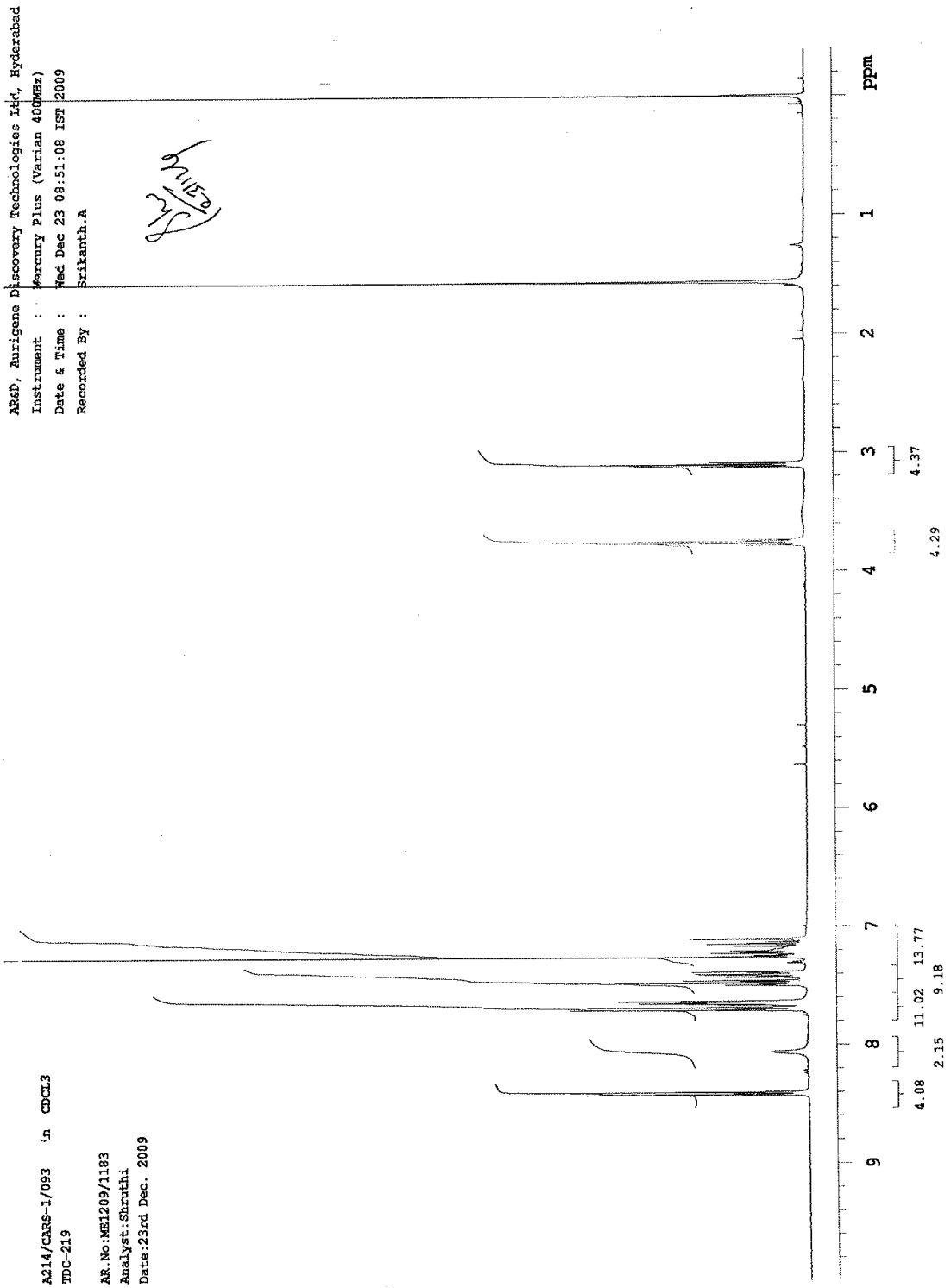
9h



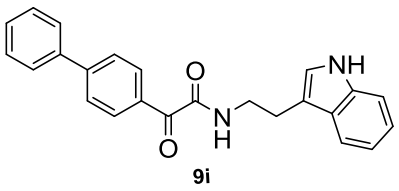
^{1}H NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-([1,1'-biphenyl]-4-yl)-2-oxoacetamide (**9i**):



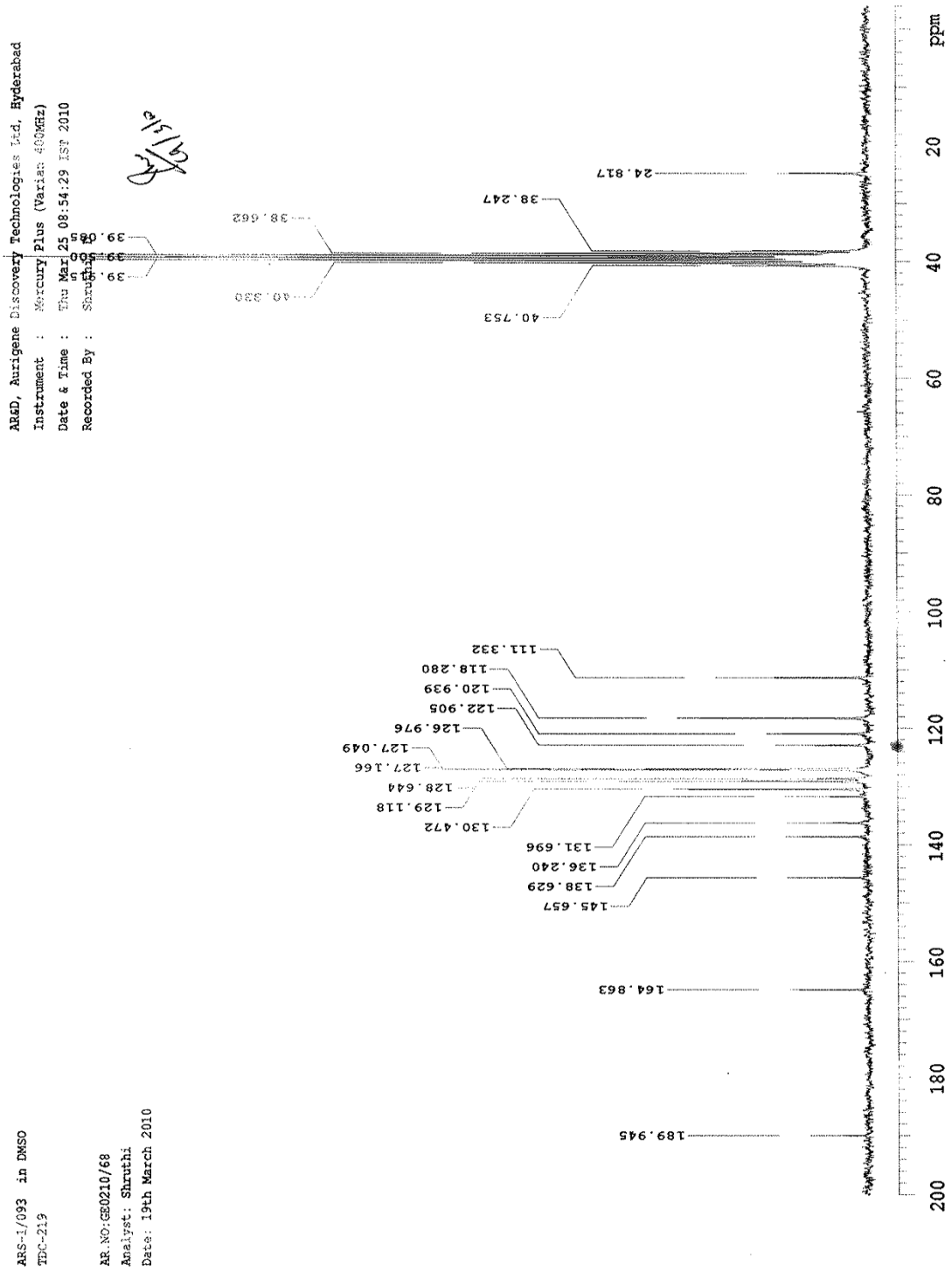
9i



^{13}C NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-([1,1'-biphenyl]-4-yl)-2-oxoacetamide (**9i**):



9i



Mass spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-([1,1'-biphenyl]-4-yl)-2-oxoacetamide (**9i**):

9i

CPS,MIYAPUR

Mass Analysis Report

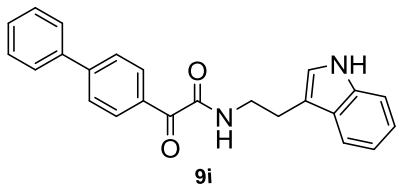
Data Filename	091222014.d	**Sample Name**	A214/CARS-1/093
Sample Type	Sample	**Position**	Vial 44
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	default.m	**Comment**	

User Spectra

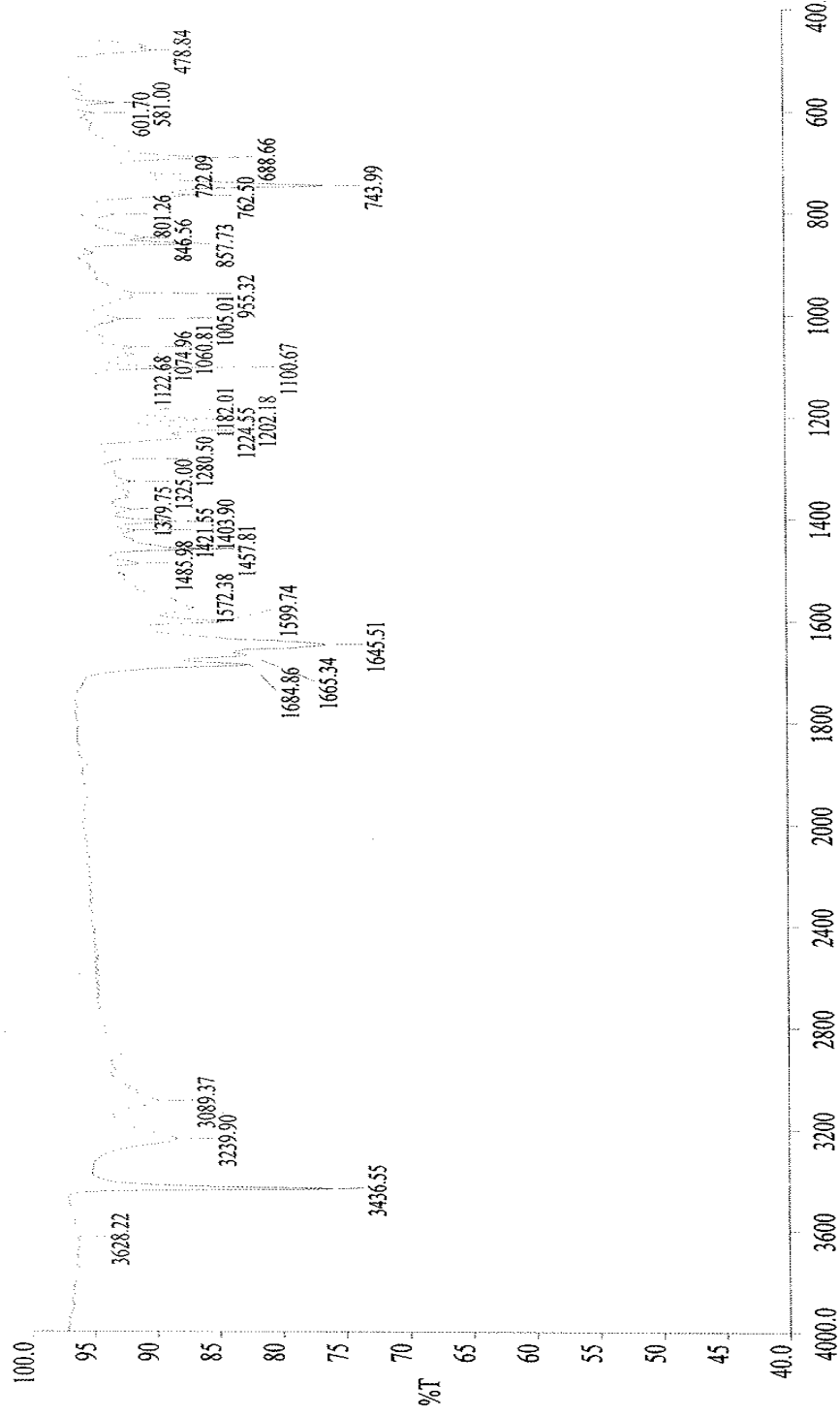
Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	Esi

--- End Of Report ---

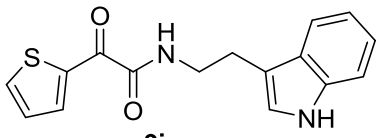
IR spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-([1,1'-biphenyl]-4-yl)-2-oxoacetamide (**9i**):



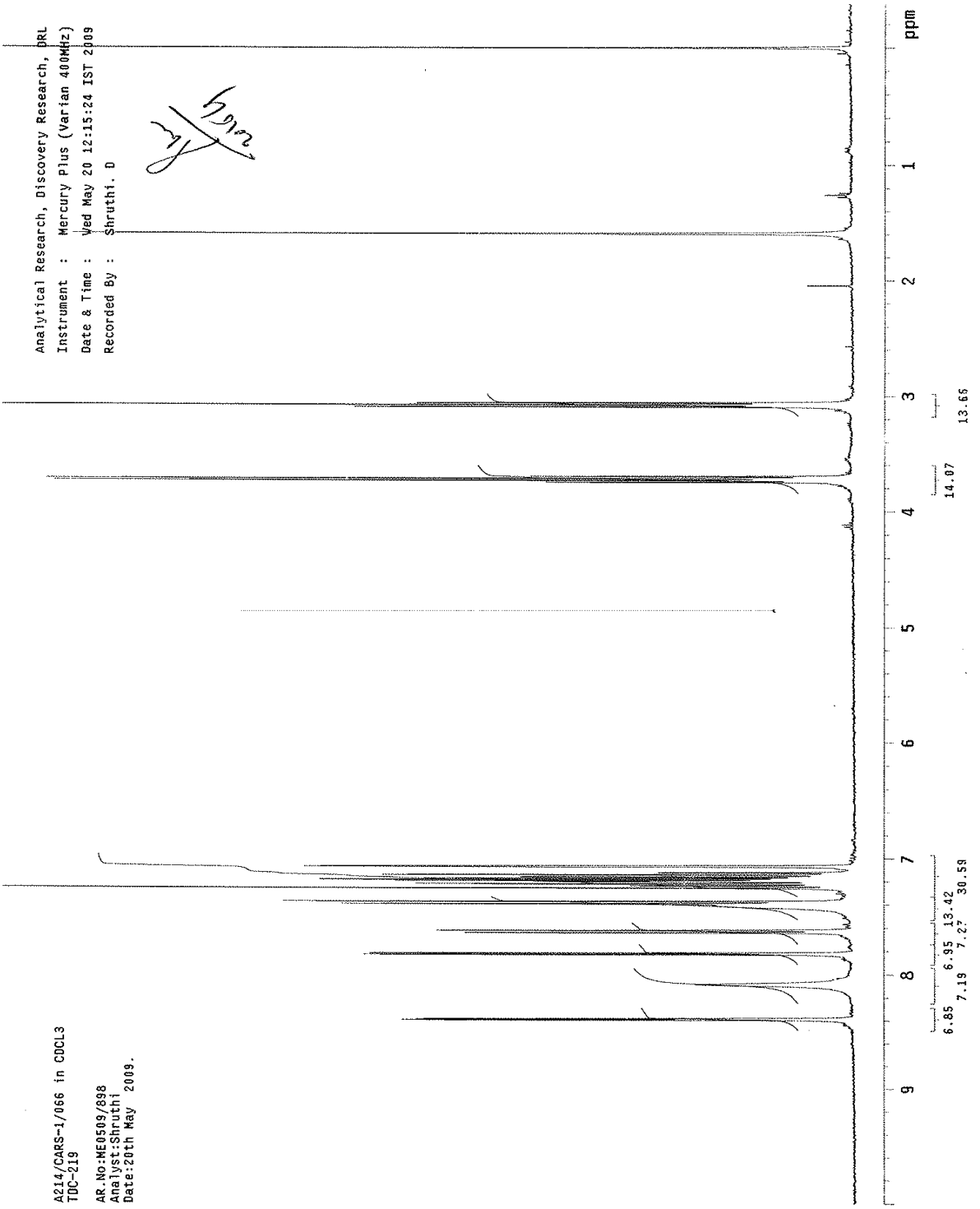
9i



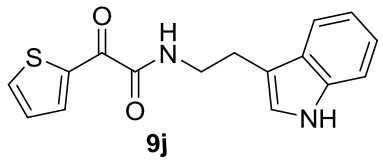
^{1}H NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-(thiophen-2-yl)acetamide (**9j**):



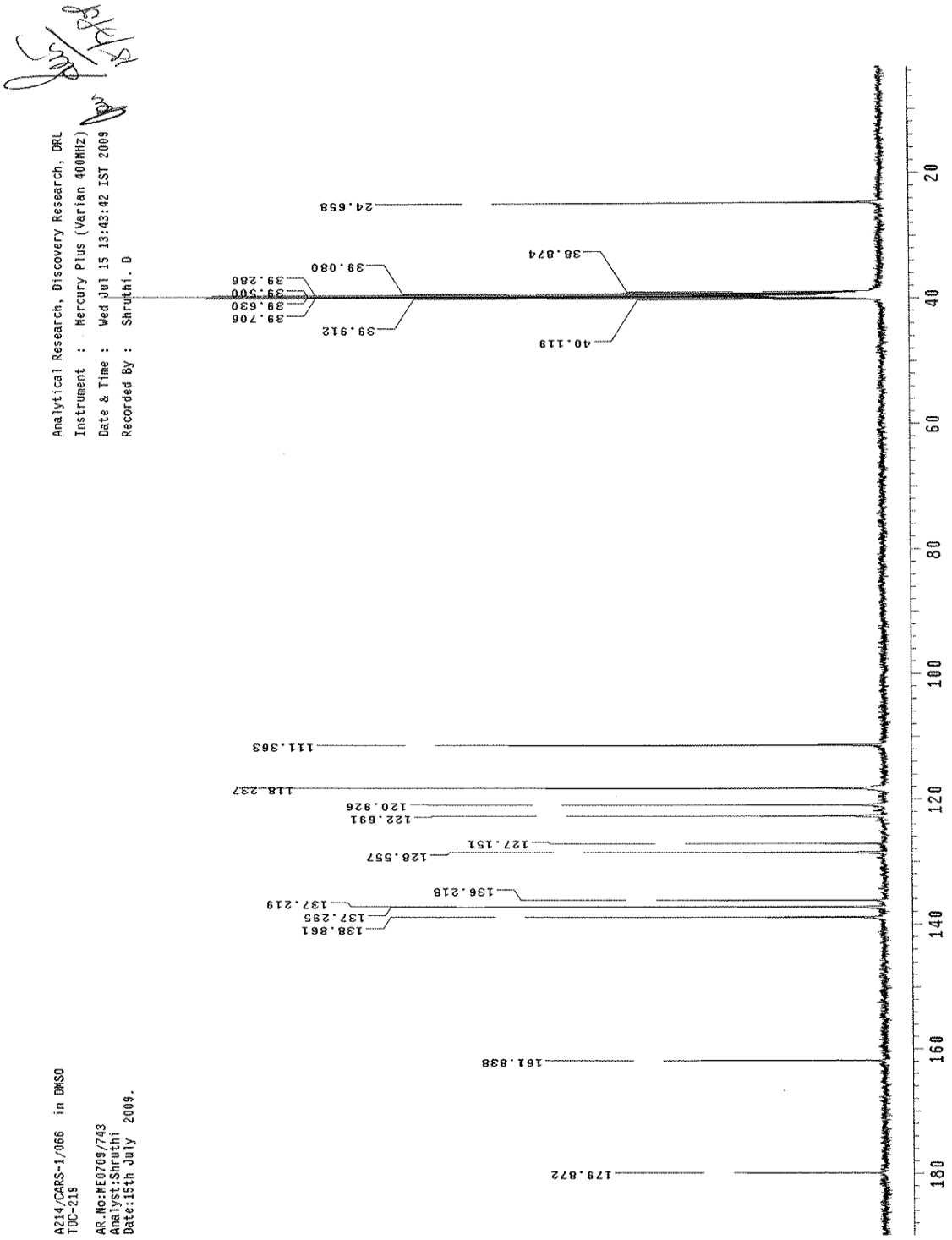
9j



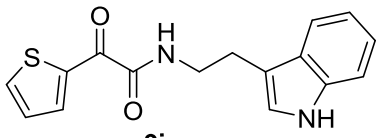
^{13}C NMR of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-(thiophen-2-yl)acetamide (**9j**):



9j



Mass spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-(thiophen-2-yl)acetamide (**9j**):



9j

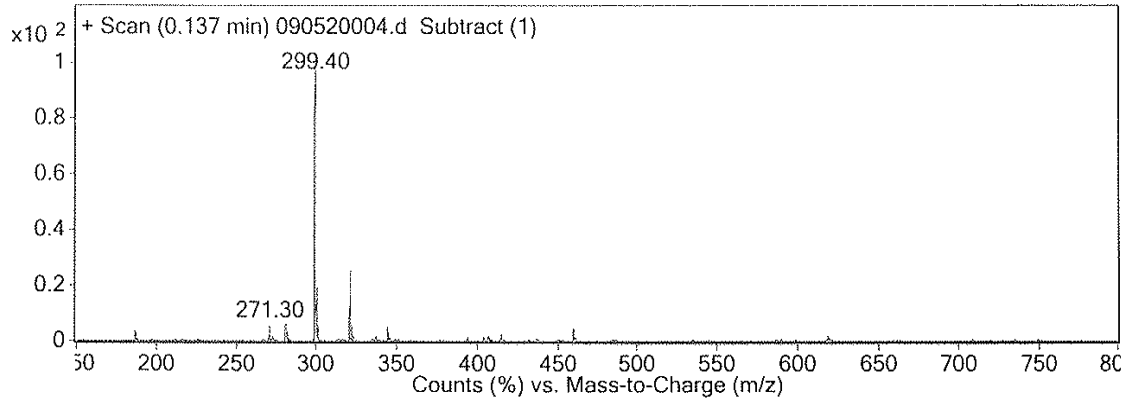
CPS,MIYAPUR

Mass Analysis Report

Data Filename	090520004.d	**Sample Name**	A214/CARS-1/066 FR-1
Sample Type	Sample	**Position**	Vial 54
Instrument Name	Instrument 1	**User Name**	
Acq Method		**IRM Calibration Status**	Success
DA Method	Quant Process.m	**Comment**	

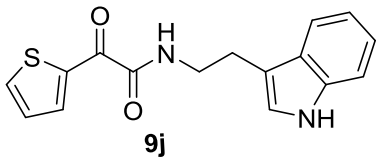
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	Esi

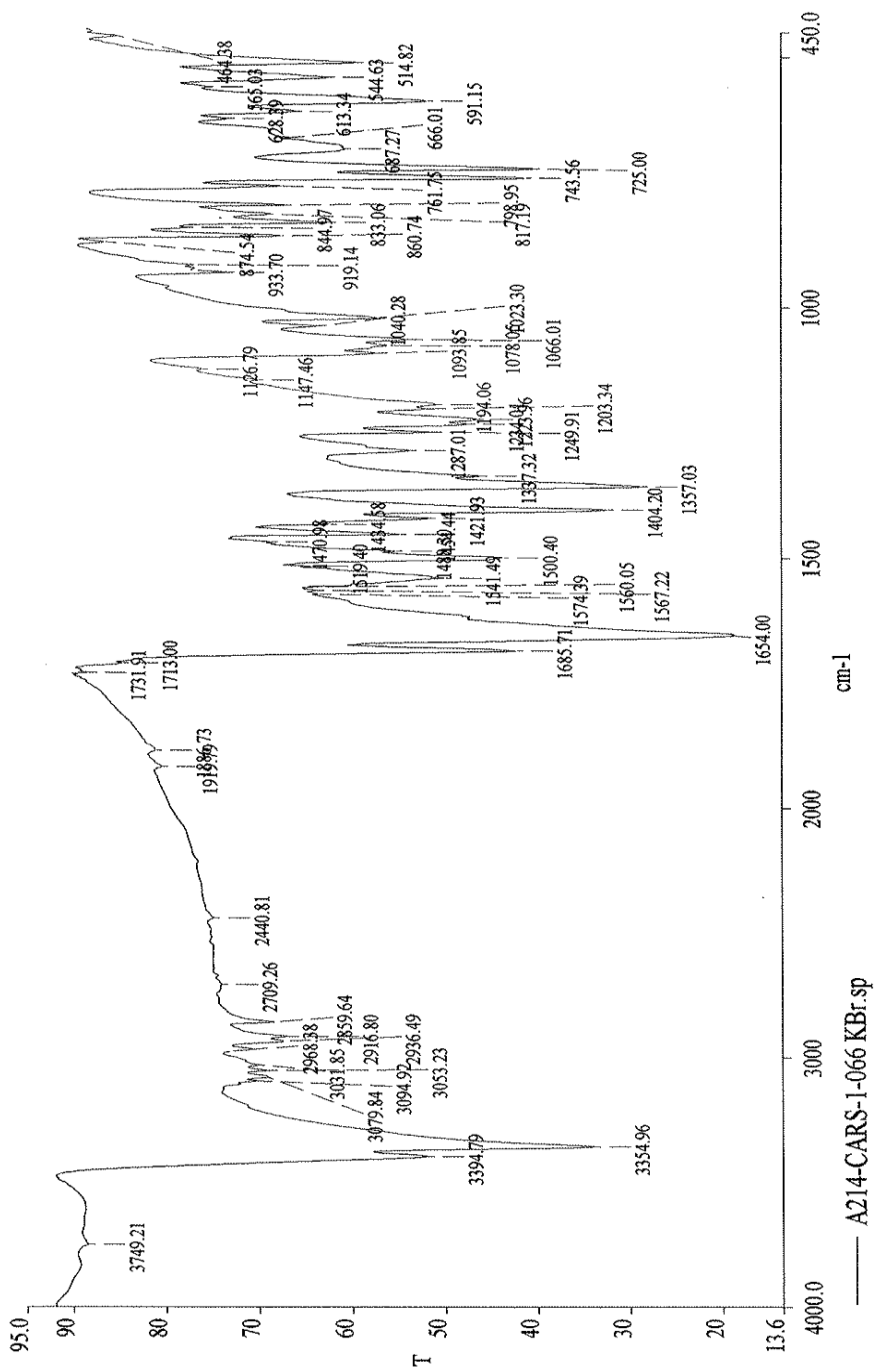


--- End Of Report ---

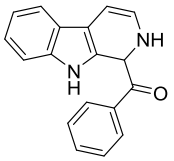
IR spectrum of *N*-(2-(1*H*-indol-3-yl)ethyl)-2-oxo-2-(thiophen-2-yl)acetamide (**9j**):



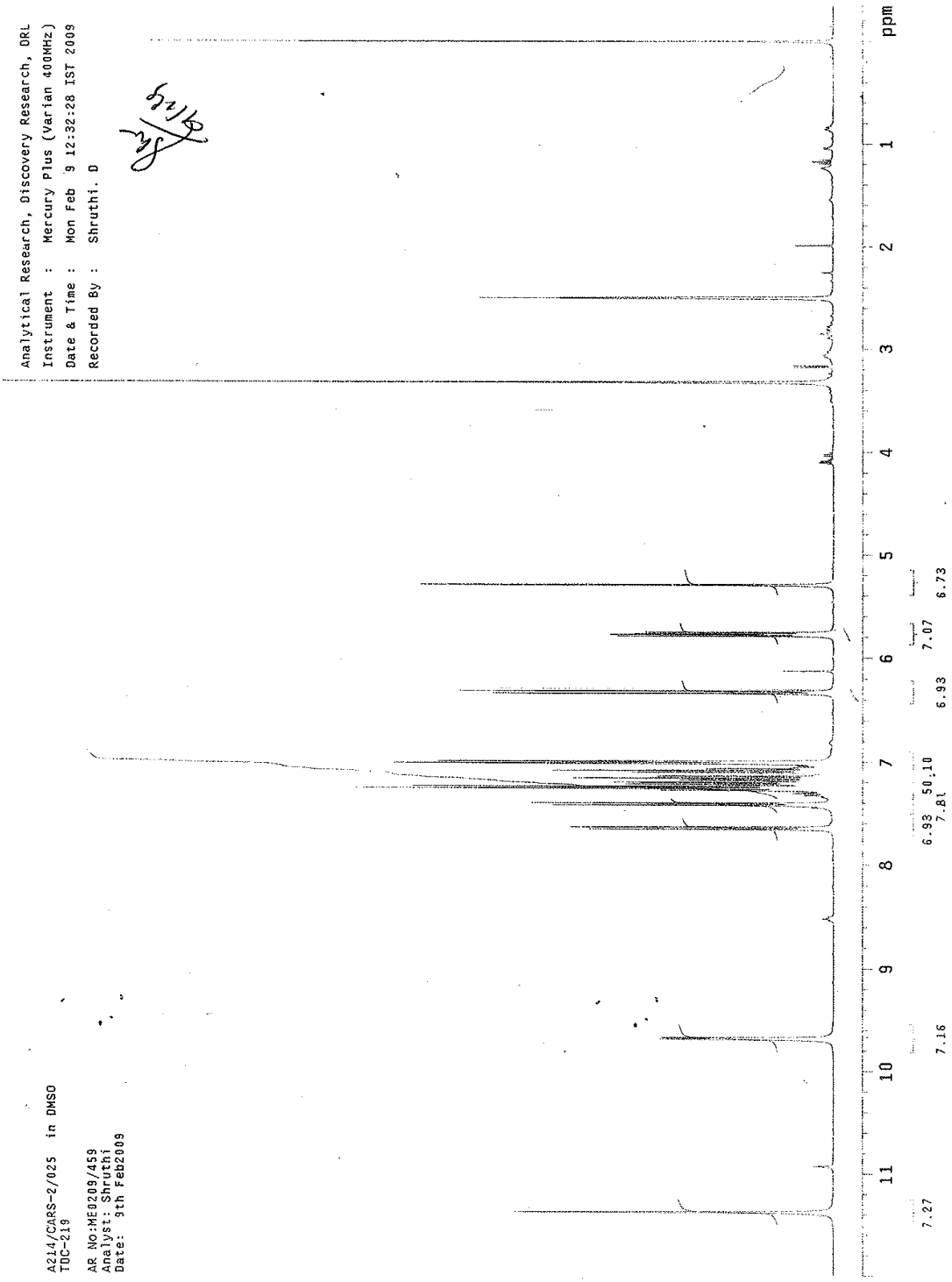
9j



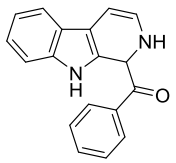
^{1}H NMR of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(phenyl)methanone (**7a**):



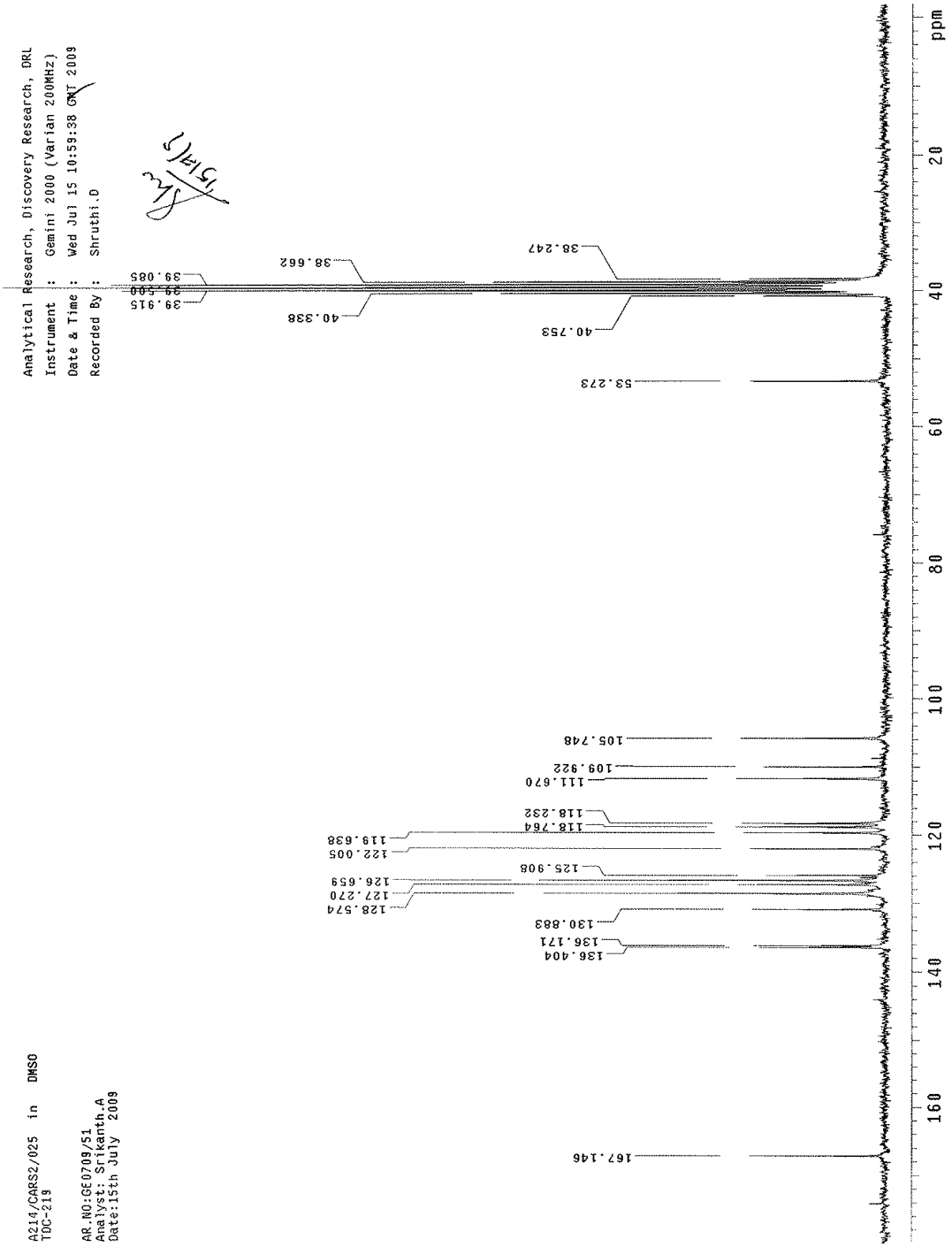
7a



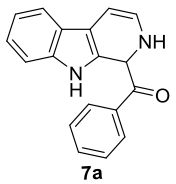
^{13}C NMR of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(phenyl)methanone (**7a**):



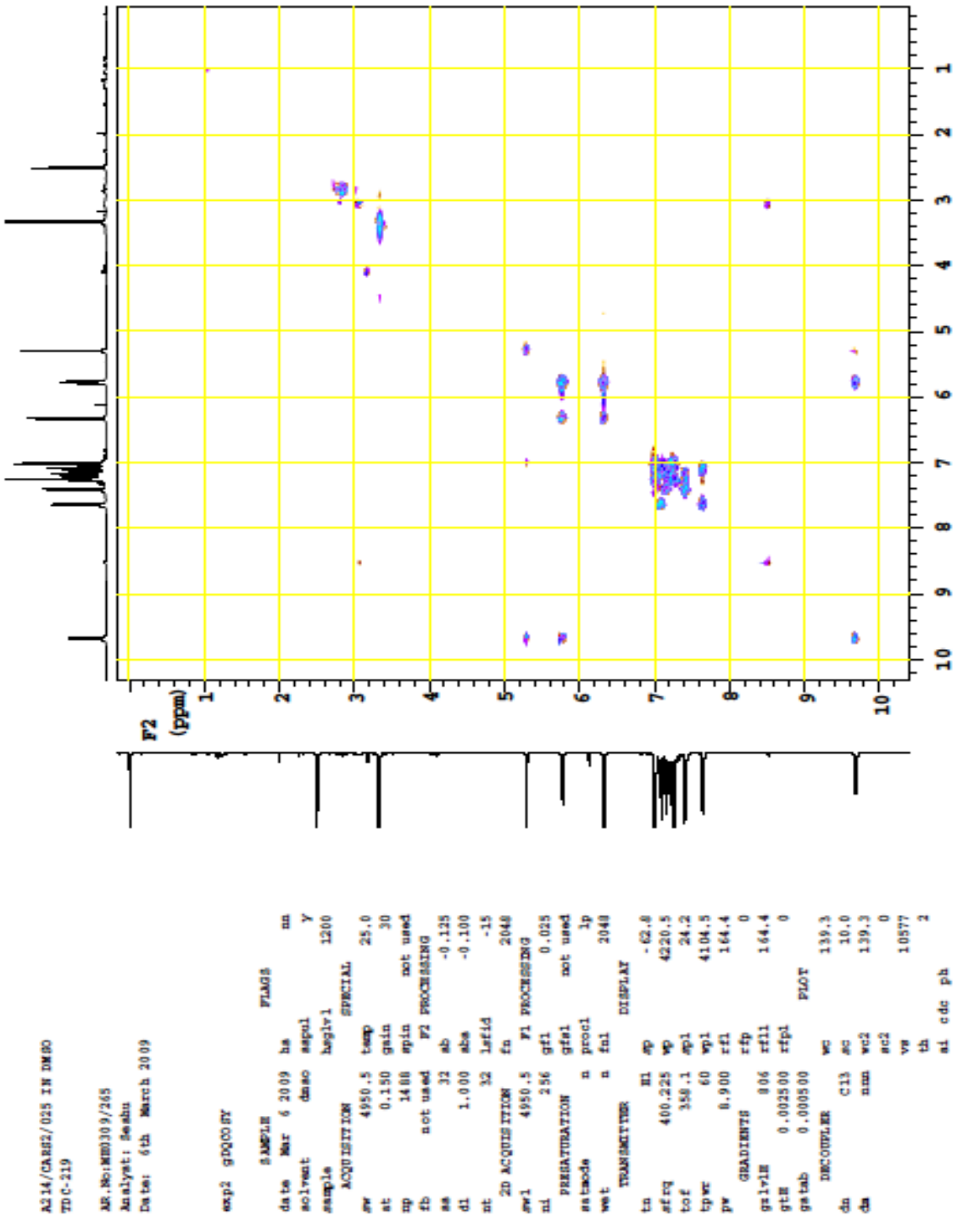
7a



COSY spectrum of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(phenyl)methanone (**7a**):



7a



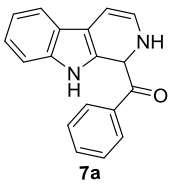
A214/CAB82/025 IN DMSO
TDC-219

AR.Mo:MM0309/245
Analyst: Sambu
Date: 6th March 2009

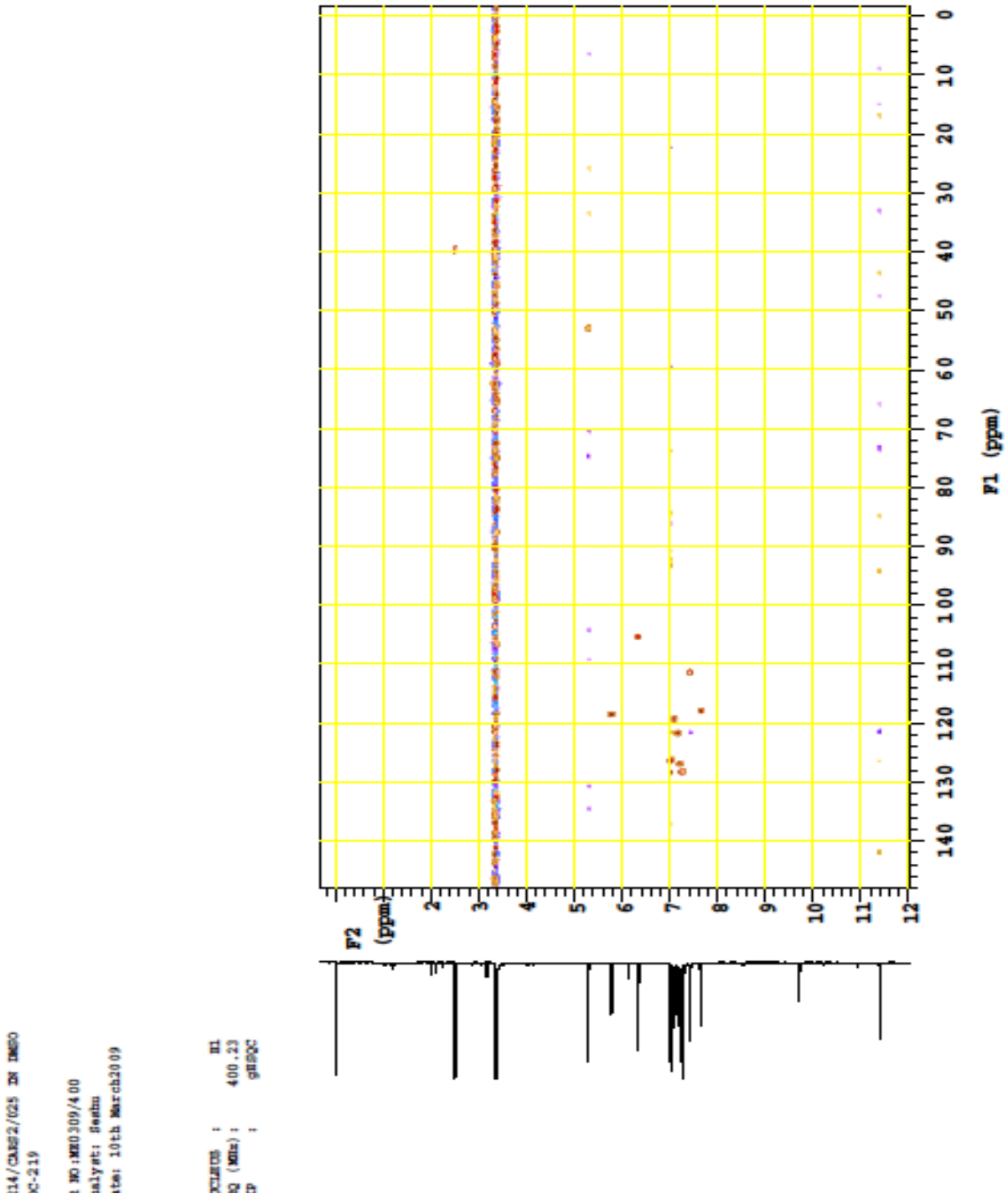
exp2 gDQCOSY

SAMPLE FLAGS
date Mar 6 2009 ha nm
solvent dmso sspul y
sample hg1v1 1200
ACQUISITION SPECIAL
sw 4950.5 temp 25.0
at 0.150 gain 30
np 1488 spin not used
fb not used F2 PROCESSING
ss 32 ab -0.125
d1 1.000 abs -0.100
nt 32 lsfid -15
2D ACQUISITION fn 2048
sw1 4950.5 F1 PROCESSING
ni 256 gf1 0.025
PREPARATION gfs1 not used
sstmode n proc1 lp
wet n fn1 2048
TRANSMITTER DISPLAY
tn H1 sp -62.8
sfrq 400.225 wp 4220.5
tof 350.1 sp1 24.2
tpwr 60 vp1 4104.5
pw 8.900 rf1 164.4
GRADIENTS rfp 0
gt1v1E 806 rfl1 164.4
gtE 0.002500 rfp1 0
gstab 0.000500 PLOT
DECOUPLER ws 139.3
dn C13 as 10.0
dm nnn wc2 139.3
sc2 0
vs 10577
th 2
ai cdc ph

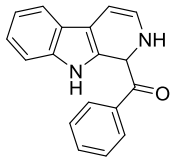
HSQC spectrum of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(phenyl)methanone (**7a**):



7a



Mass spectrum of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(phenyl)methanone (**7a**):



7a

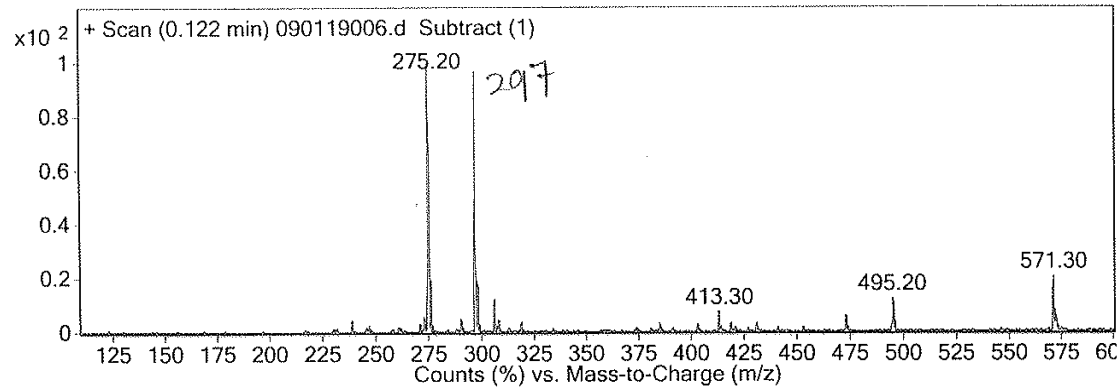
CPS,MIYAPUR

Mass Analysis Report

Data Filename	090119006.d	**Sample Name**	A214/CARS-2/016 RC
Sample Type	Sample	**Position**	Vial 5
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	DA.m	**Comment**	

User Spectra

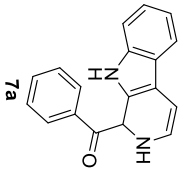
Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	Esi



--- End Of Report ---

HRMS of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(phenyl)methanone (**7a**):

Elemental Composition Report



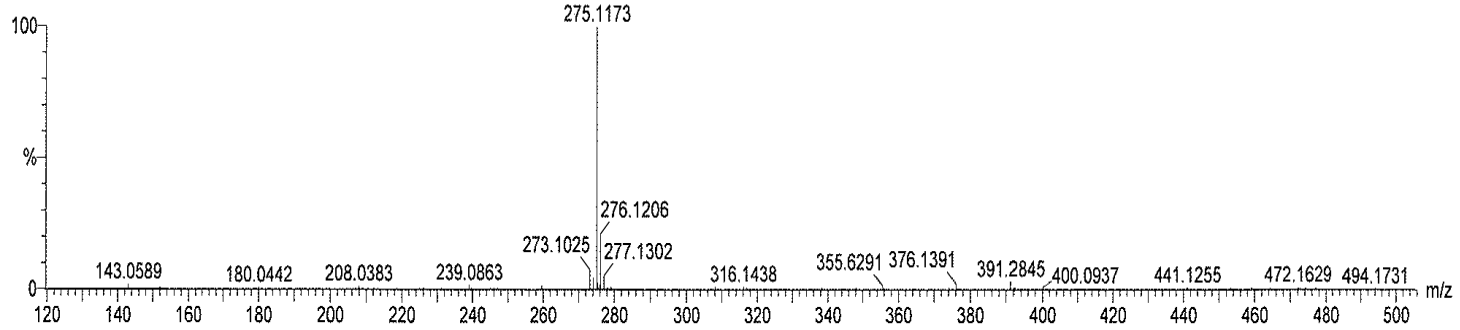
Single Mass Analysis

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
96 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: 0-5

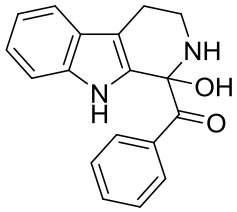
9a
UT1212_148 10 (0.366) Cm (10:13-(1:4+22:28)x0.010)

Gajanan
1: TOF MS ES+
7.37e+003

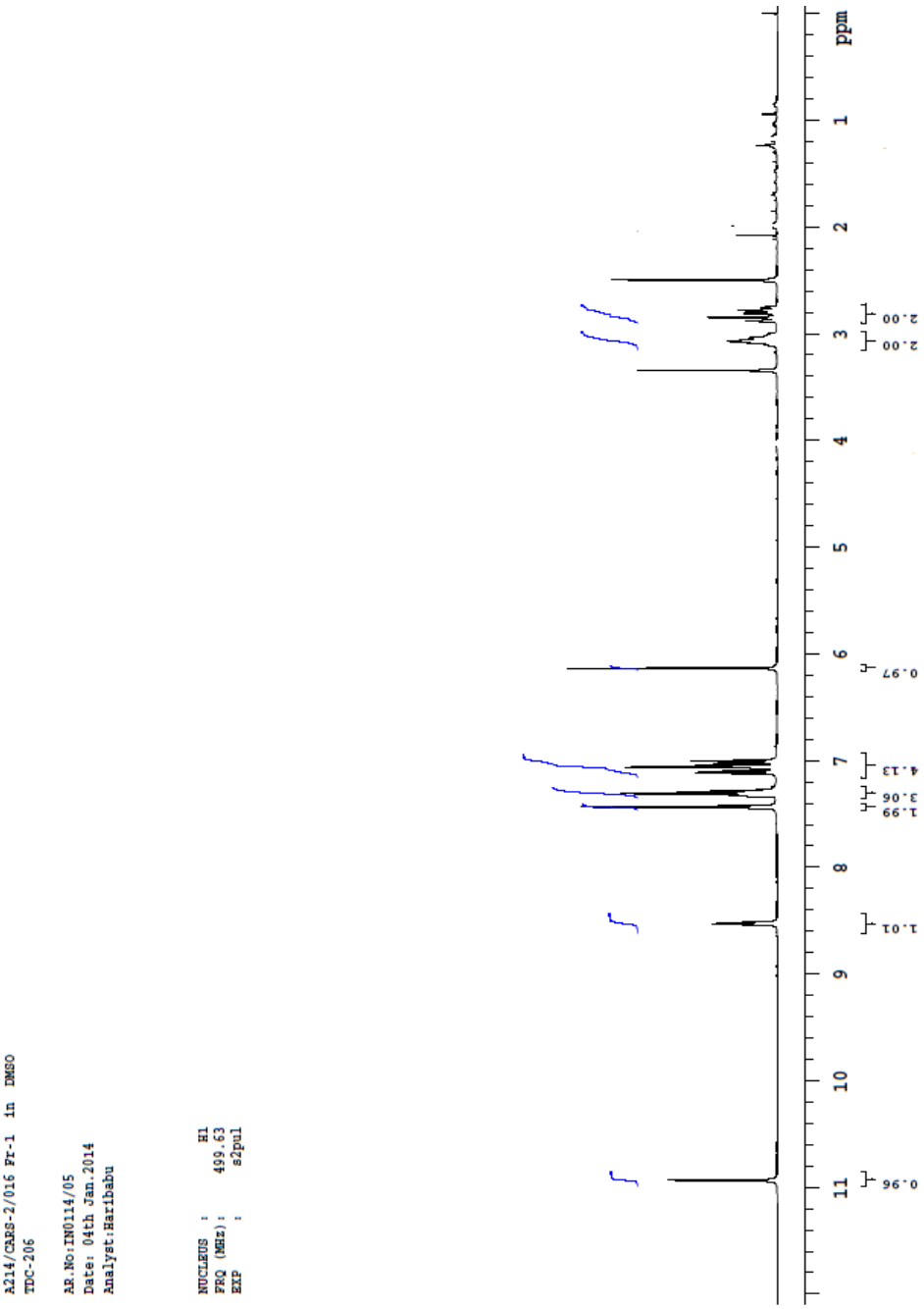


Minimum:				-1.5		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
275.1173	275.1184	-1.1	-4.0	12.5	54.7	C18 H15 N2 O

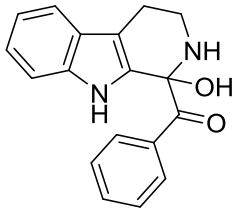
^{1}H NMR of (1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)(phenyl)methanone (**8a**):



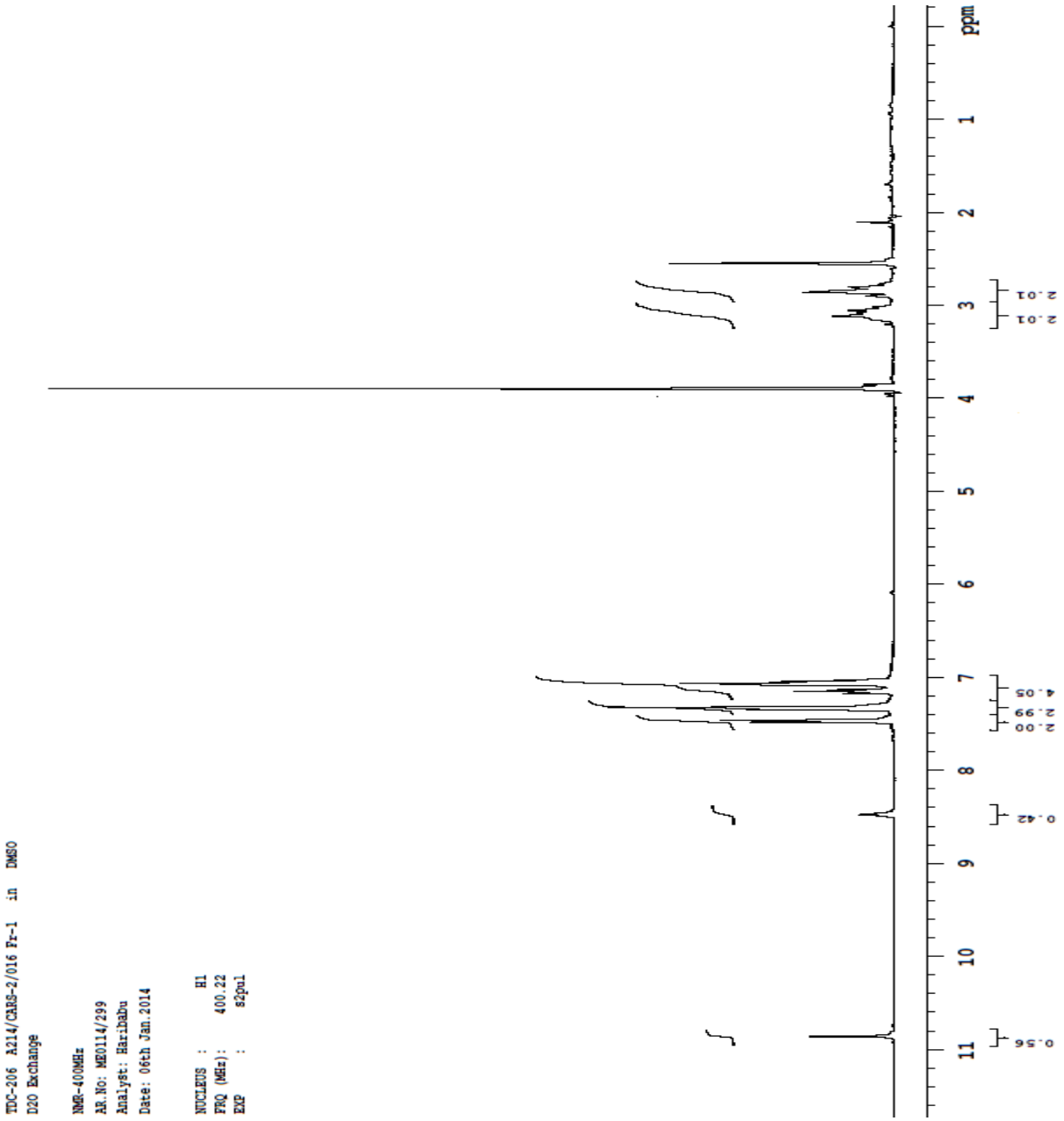
8a



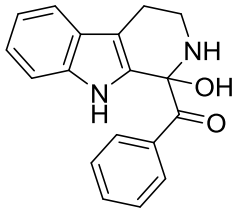
^{1}H NMR D_2O exchange of (1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)(phenyl)methanone (**8a**):



8a

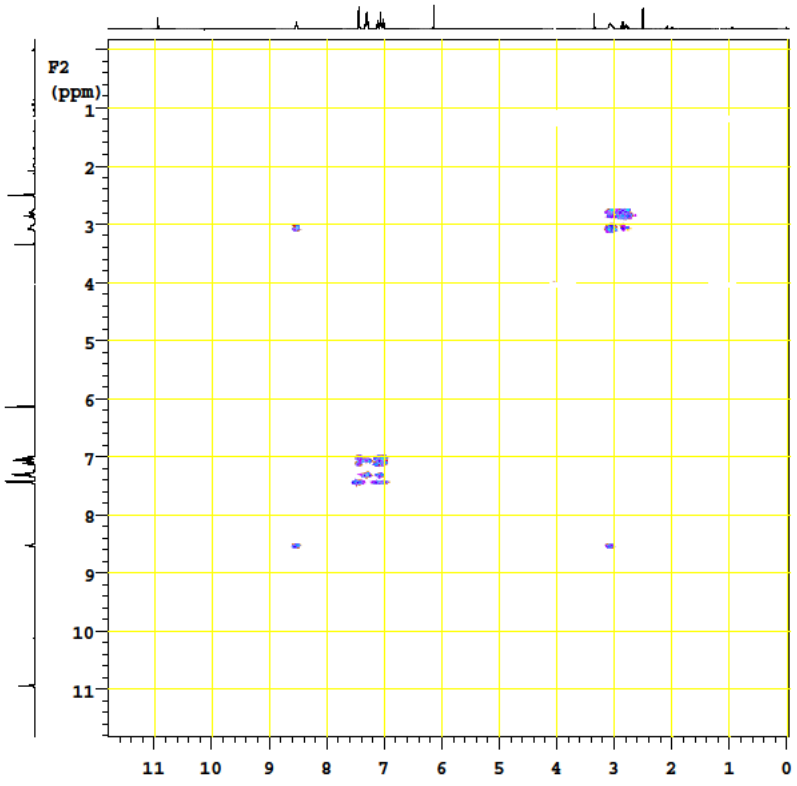


COSY spectrum of(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)(phenyl)methanone (**8a**):

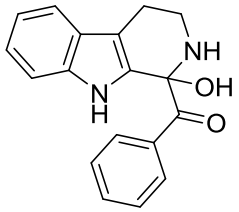


8a

```
A214/CARS-2/016 Fr-1  in  DMSO
TDC-206

AR.No:IN0114/06
Date: 04th Jan.2014
Analyst:Haribabu


exp2  gDQCOSY

      SAMPLE              FLAGS
date   Jan  4 2014  hs              nn
solvent       DMSO  sspul           y
sample              hsglvl       4237
   ACQUISITION          SPECIAL
sw          7107.3  temp         25.0
at           0.144  gain           16
np            2048  spin      not used
fb        not used    F2 PROCESSING
ss              32  sb         -0.108
d1           1.000  sbs        -0.072
nt               8  lsfid         -22
  2D ACQUISITION    fn            2048
sw1         7107.3    F1 PROCESSING
n1             400  sb1        -0.056
   TRANSMITTER      sbs1       -0.025
tn              H1  gf1         0.024
sfrq       499.629  gfs1      not used
tof          530.1  proc1          lp
tpwr            58  fn1           2048
pw           7.200       DISPLAY
    GRADIENTS        sp          -90.5
gzlvl1      3177.5  wp         5989.9
gt1       0.002500  sp1         -21.1
gzlvl2       6355  wp1        5913.5
gt2       0.002500  rfl        1776.8
gstab     0.000500  rfp        1249.1
    DECOUPLER       rfl1       1776.8
dn              C13 rfp1       1249.1
dm              nnn         PLOT
                    wc          138.9
                    sc           10.0
                    wc2         138.9
                    sc2             0
                    vs             66
                    th              2
                    a1  cdc  nh
```



HSQC spectrum of(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)(phenyl)methanone (**8a**):

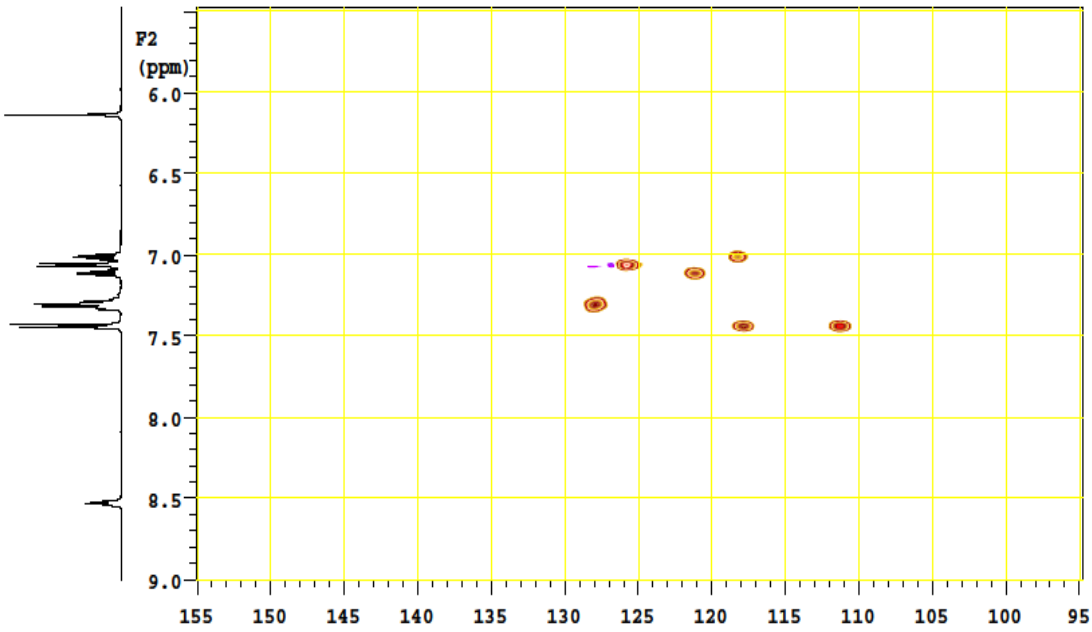


8a

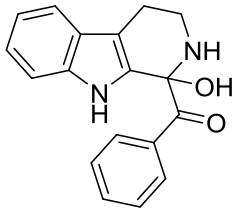
A214/CARS-2/016 Fr-1 in DMSO
TDC-206

AR.No:IN0114/07
Date: 04th Jan.2014
Analyst:Haribabu

NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHSQC



NOESY spectrum of(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)(phenyl)methanone (**8a**):



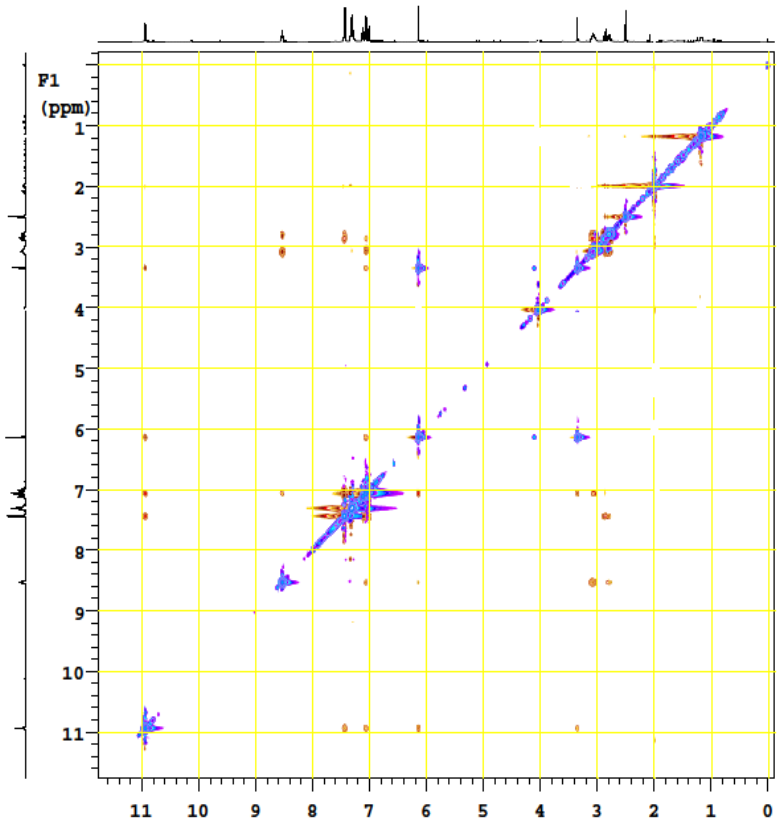
8a

A214/CARS-2/016 Fr-1 in DMSO
TDC-206

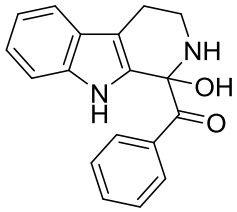
AR.No:IN0114/09
Date: 04th Jan.2014
Analyst:Haribabu

exp2 NOESY

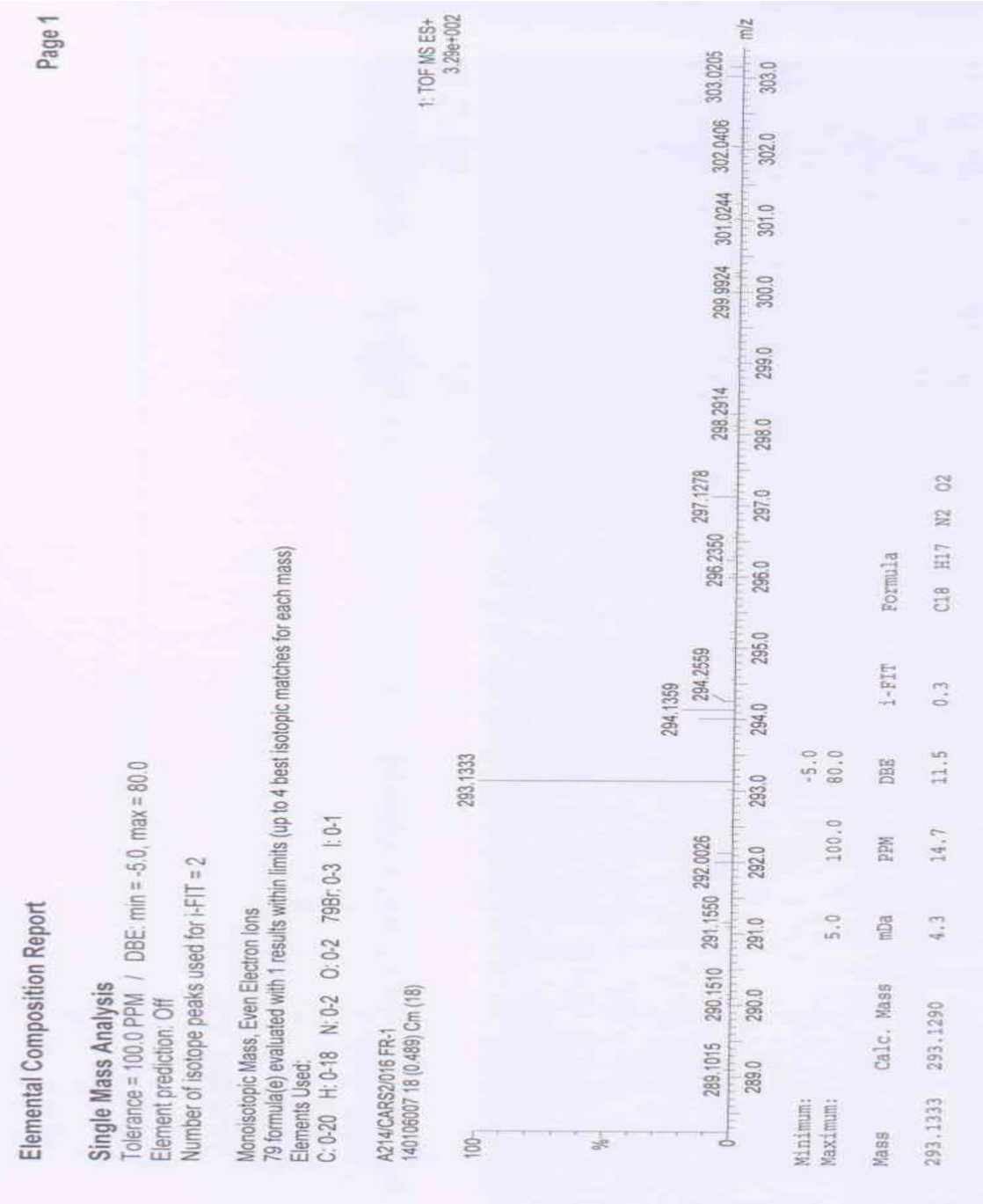
SAMPLE		FLAGS	
date	Jan 4 2014	hs	n
solvent	DMSO	sspul	y
sample		PFGflg	y
ACQUISITION		hsglvl	4237
sw	7107.3	SPECIAL	
at	0.144	temp	25.0
np	2048	gain	14
fb	not used	spin	not used
ss	32	F2 PROCESSING	
d1	1.000	gf	0.067
nt	16	gfs	not used
2D ACQUISITION		fn	2048
sw1	7107.3	F1 PROCESSING	
ni	400	gf1	0.024
TRANSMITTER		gfs1	not used
tn	H1	proc1	lp
sfrq	499.629	fn1	2048
tof	530.1	DISPLAY	
tpwr	58	sp	-55.8
pw	7.200	wp	5934.3
NOESY		sp1	-104.4
mix	0.600	wp1	5976.0
PRESATURATION		rf1	1776.8
satmode	nnnn	rfp	1249.1
satpwr	0	rfl1	1776.8
satdly	0	rfp1	1249.1
satfrq	0	PLOT	
DECOUPLER		wc	139.3
dn	C13	sc	10.0
dm	nnn	wc2	139.3
		sc2	0
		vs	4913
		th	2
		ai	ph



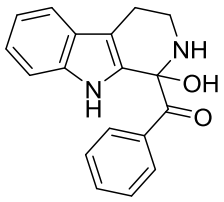
HRMS spectrum of of(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)(phenyl)methanone (**8a**):



8a



Mass spectrum of (1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)(phenyl)methanone (**8a**):



8a

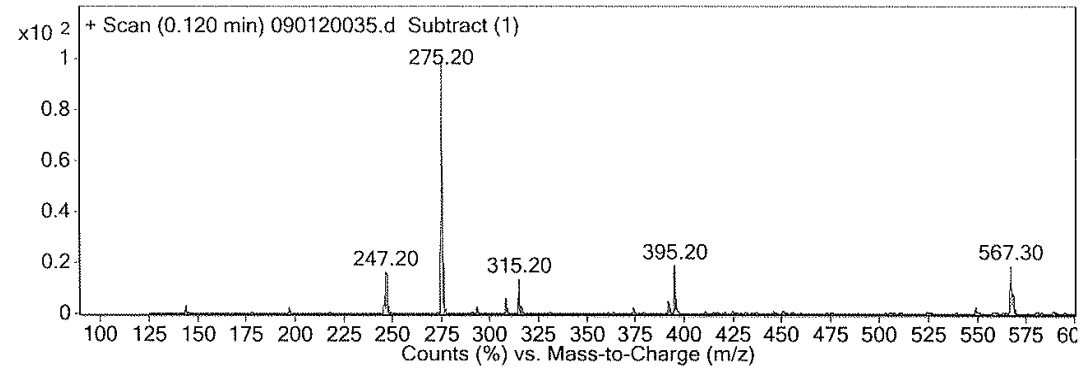
CPS,MIYAPUR

Mass Analysis Report

Data Filename	090120035.d	**Sample Name**	A214/CARS-2/017 C
Sample Type	Sample	**Position**	Vial 88
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	DA.m	**Comment**	

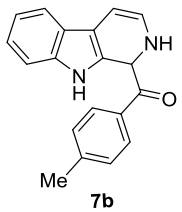
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	Esi

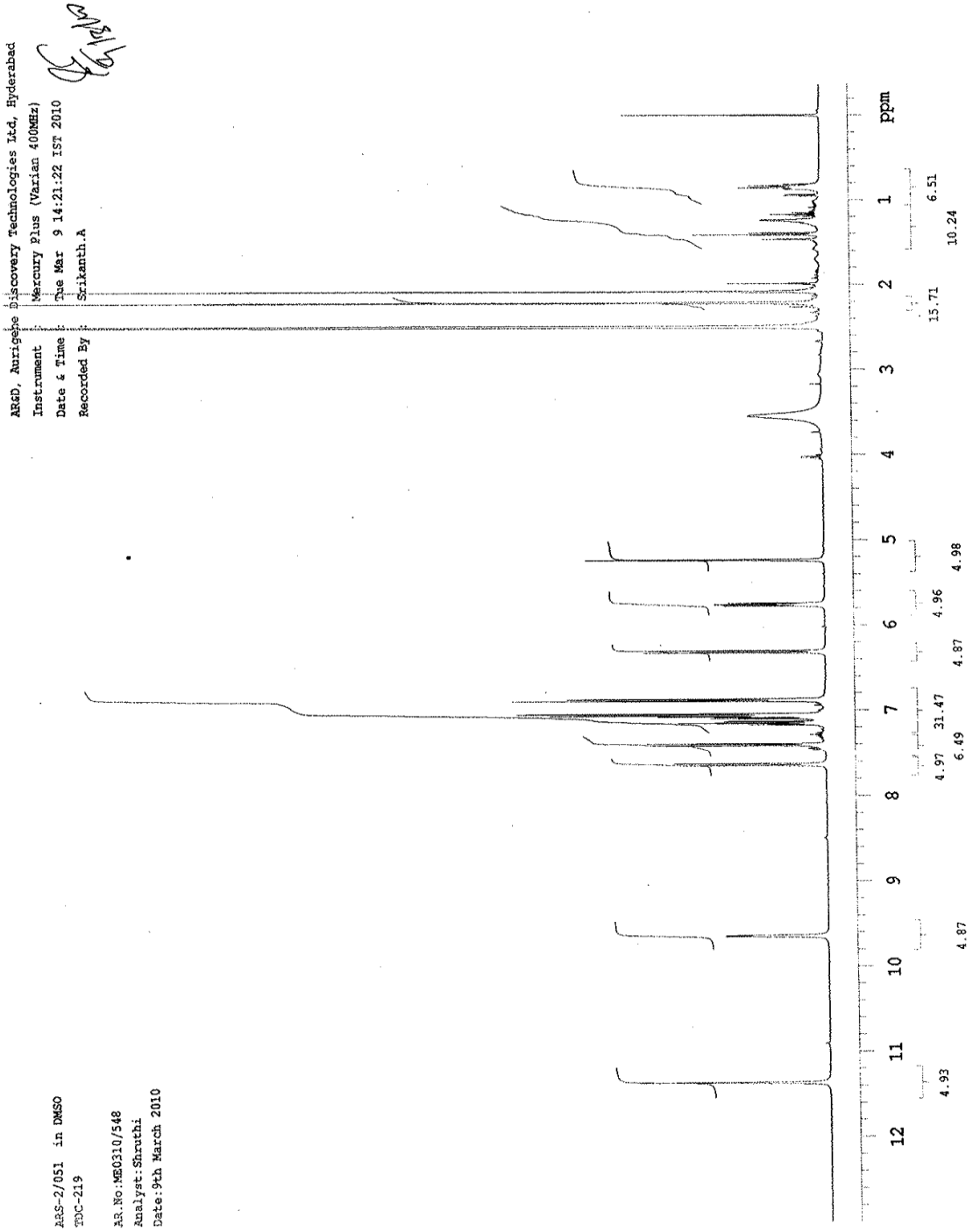


--- End Of Report ---

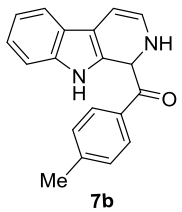
^{1}H NMR of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(*p*-tolyl)methanone (**7b**):



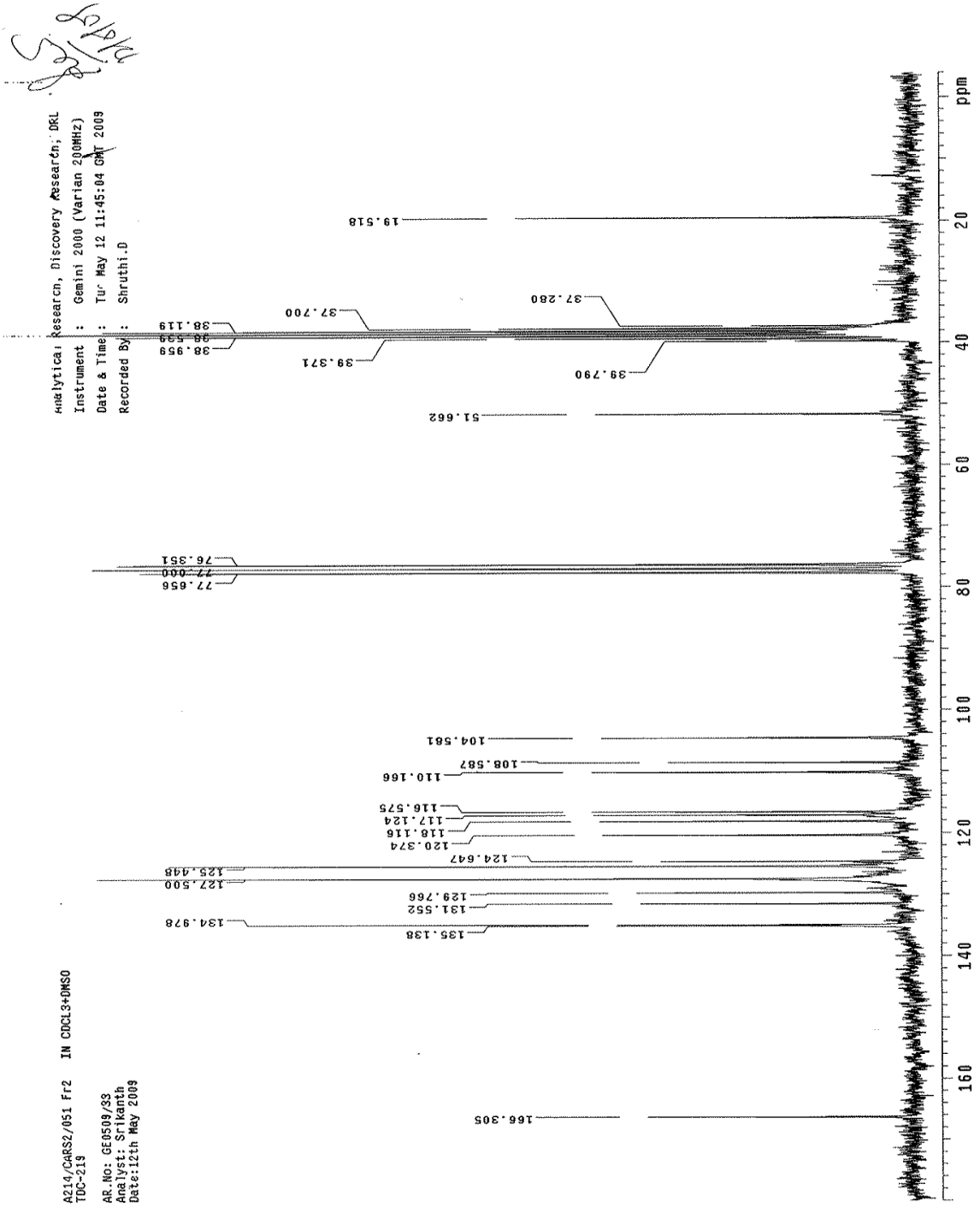
7b



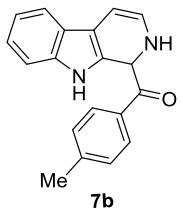
^{13}C NMR of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(*p*-tolyl)methanone (**7b**):



7b



Mass spectrum of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(*p*-tolyl)methanone (**7b**):



7b

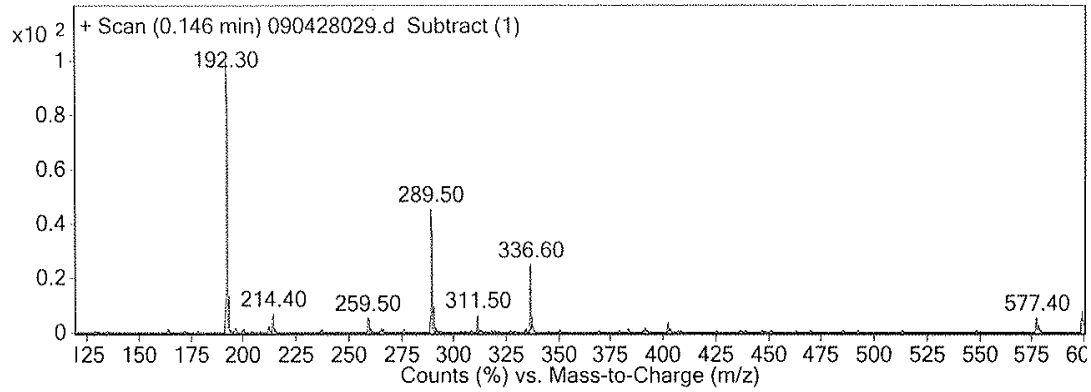
CPS,MIYAPUR

Mass Analysis Report

Data Filename	090428029.d	**Sample Name**	A214/CARS-2/051 FR-2
Sample Type	Sample	**Position**	Vial 84
Instrument Name	Instrument 1	**User Name**	
Acq Method		**IRM Calibration Status**	Success
DA Method	Quant Process.m	**Comment**	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	Esi



--- End Of Report ---

HRMS of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(*p*-tolyl)methanone (**7b**):

7b

Page 1

Elemental Composition Report

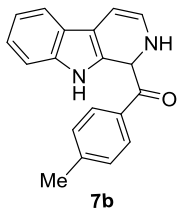
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
58 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 N: 0-4 O: 0-4
9b
UT1212_150 8 (0.278) Cm (8:10)

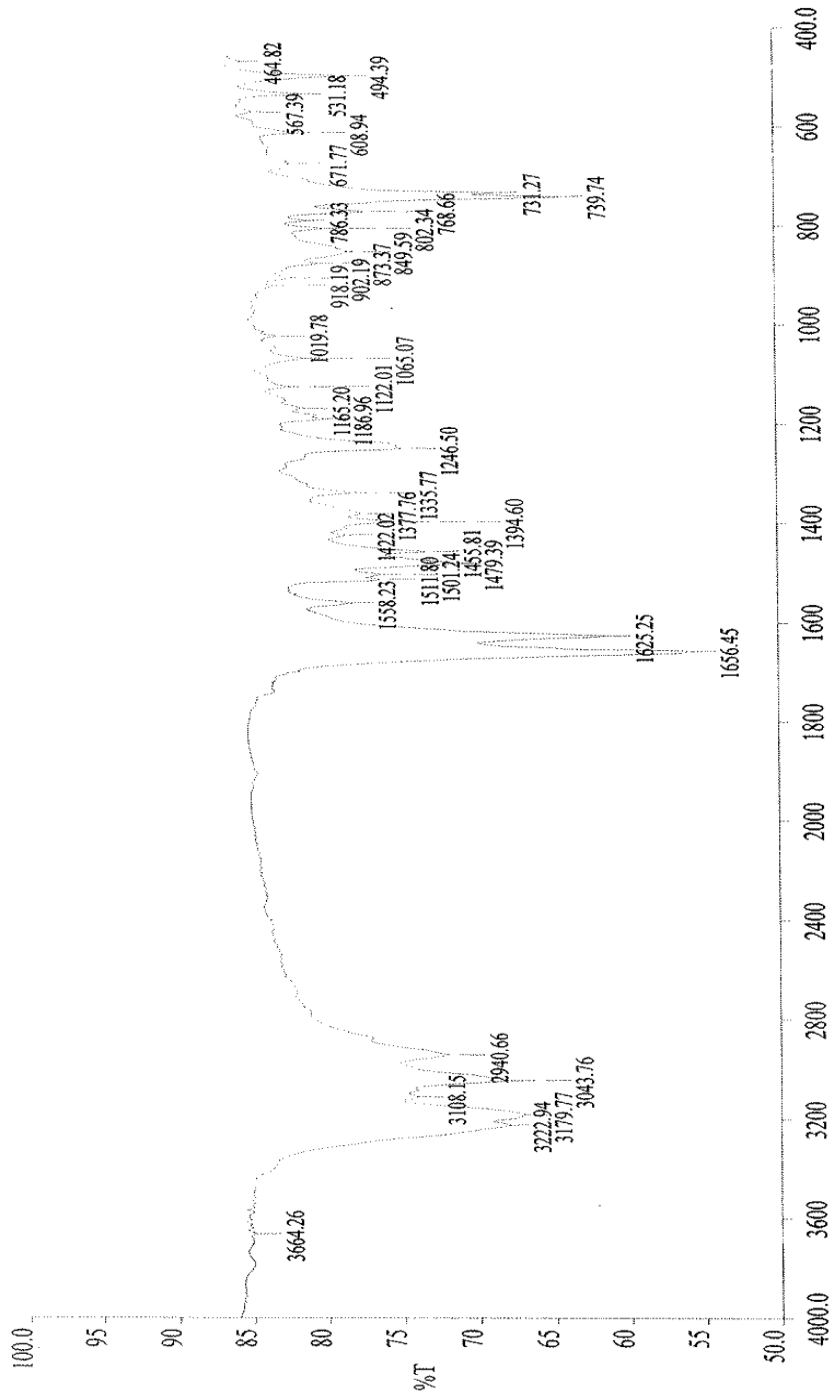
Gajanan
1: TOF MS ES+
8.86e+003

Minimum:			-1.5				
Maximum:		5.0	5.0	80.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
289.1349	289.1341	0.8	2.8	12.5	5.4	C19 H17 N2 O	

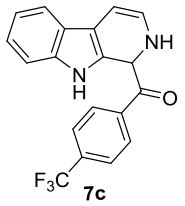
IR spectrum of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(*p*-tolyl)methanone (**7b**):



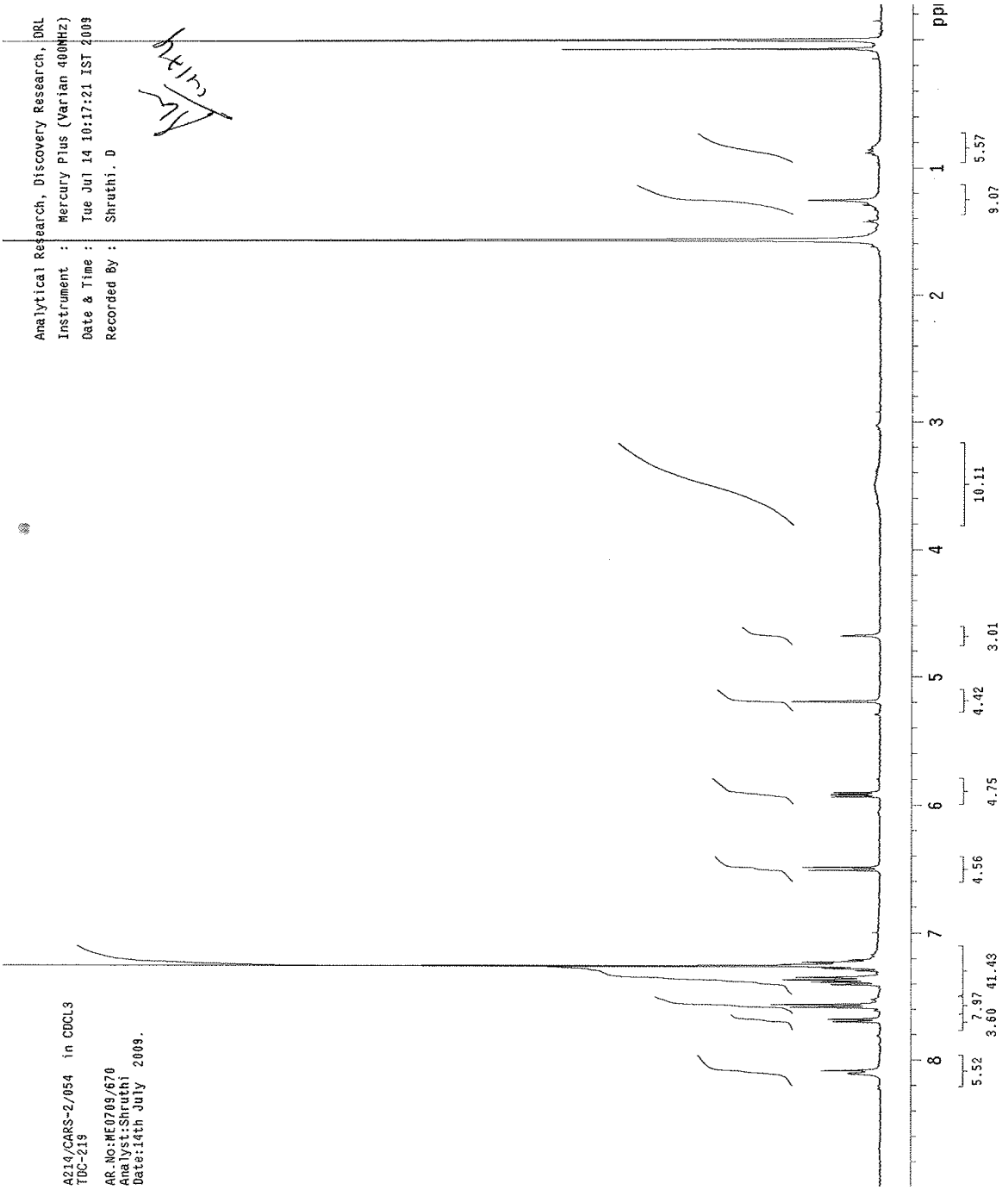
7b



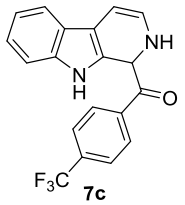
^{1}H NMR of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-(trifluoromethyl)phenyl)methanone (**7c**):



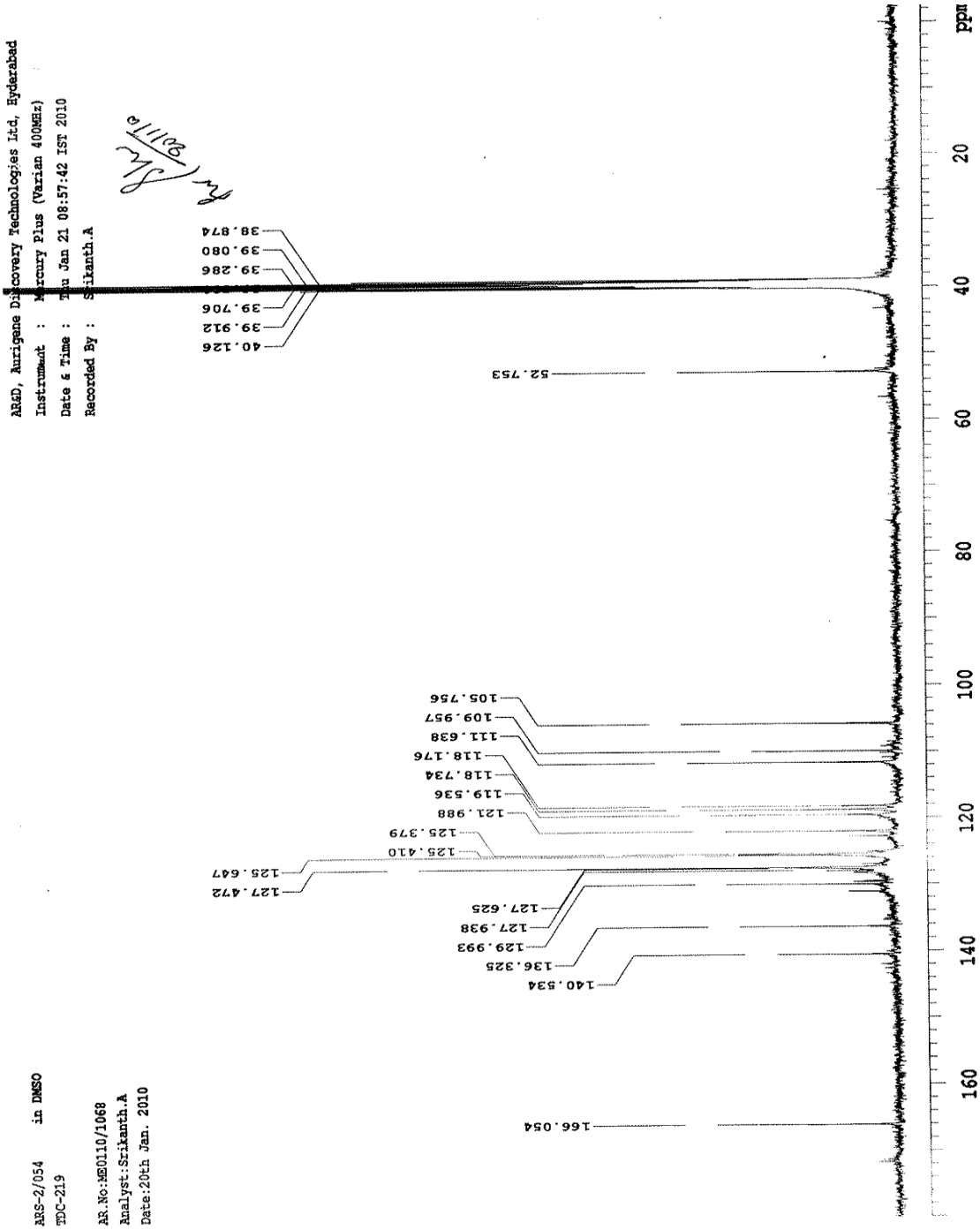
7c



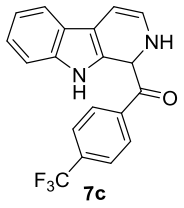
^{13}C NMR of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-(trifluoromethyl)phenyl)methanone (**7c**):



7c



Mass spectrum of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-(trifluoromethyl)phenyl)methanone (**7c**):



7c

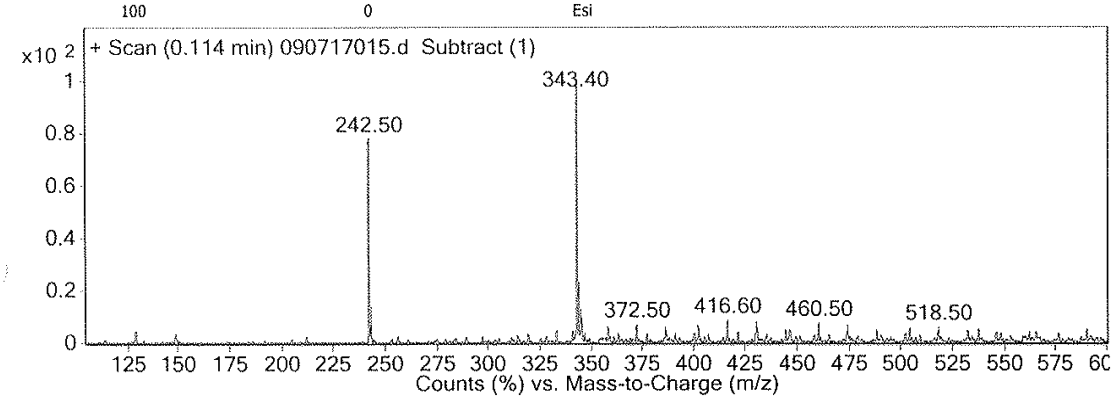
CPS,MIYAPUR

Mass Analysis Report

Data Filename	090717015.d	**Sample Name**	CARS2/054
Sample Type	Sample	**Position**	Vial 14
Instrument Name	Instrument 1	**User Name**	
Acq Method		**IRM Calibration Status**	Success
DA Method	Quant Process.m	**Comment**	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	Esi



--- End Of Report ---

HRMS of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-(trifluoromethyl)phenyl)methanone (**7c**):

Page 1

Elemental Composition Report

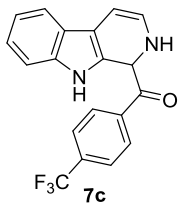
Single Mass Analysis
Tolerance = 6.0 PPM / DBE: min = -1.5, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
26 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: 0-2 O: 0-2 F: 0-3
9c
UT1212_179 9 (0.337) Cm (9:10)

Gajanan
1: TOF MS ES+
2.27e+002

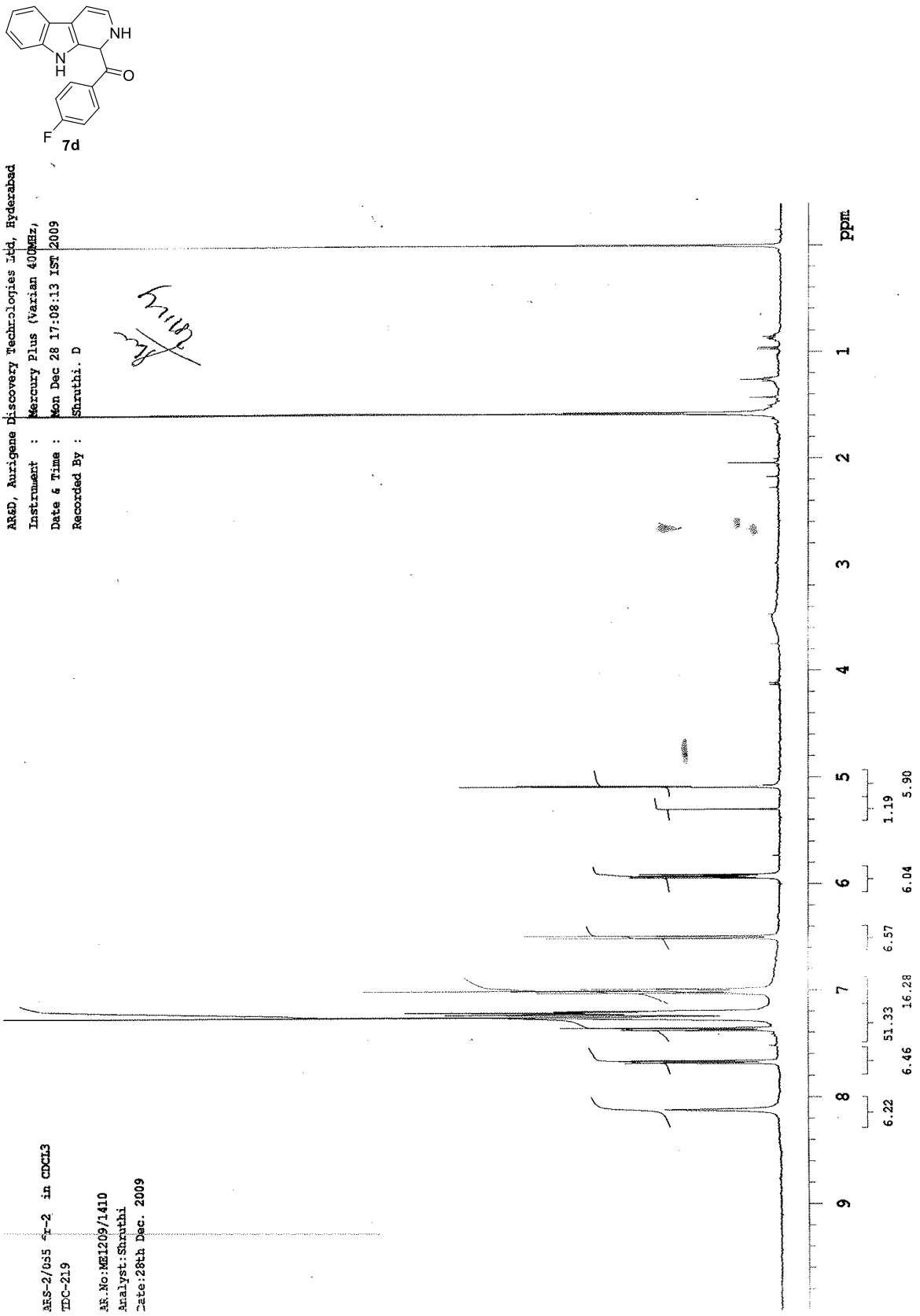
Minimum:			-1.5				
Maximum:		5.0	6.0	80.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
343.1038	343.1058	-2.0	-5.8	12.5	11.6	C19 H14 N2 O F3	

IR spectrum of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-(trifluoromethyl)phenyl)methanone (**7c**):

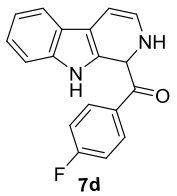


7c

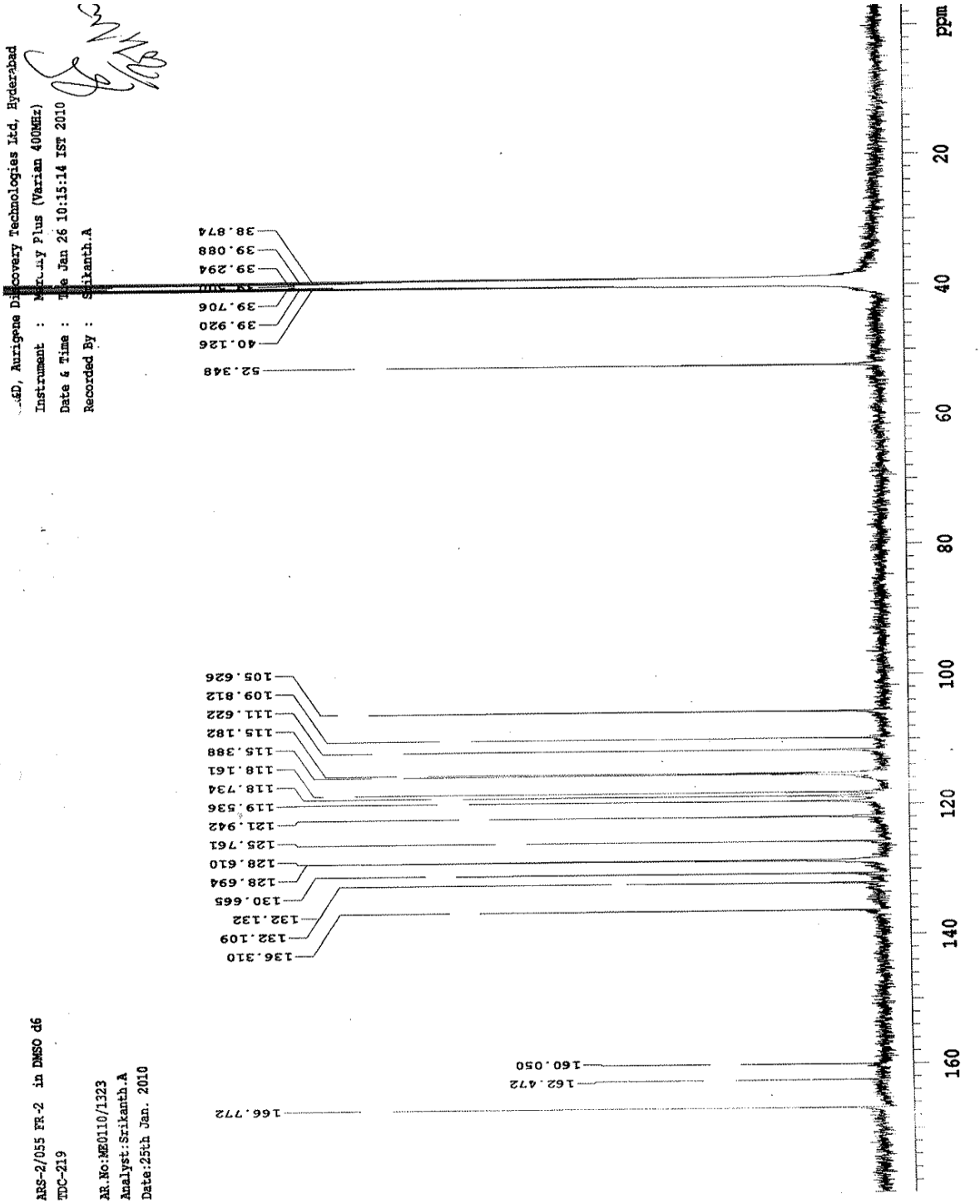
^{1}H NMR of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-fluorophenyl)methanone (**7d**):



^{13}C NMR of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-fluorophenyl)methanone (**7d**):



7d



Mass spectrum of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-fluorophenyl)methanone (**7d**):

7d

CPS,MIYAPUR

Mass Analysis Report

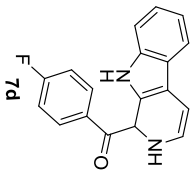
Data Filename	091228020.d	**Sample Name**	ARS-2/055 FR-2
Sample Type	Sample	**Position**	Vial 5
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	default.m	**Comment**	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
125	0	Esi

--- End Of Report ---

HRMS of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-fluorophenyl)methanone (**7d**):



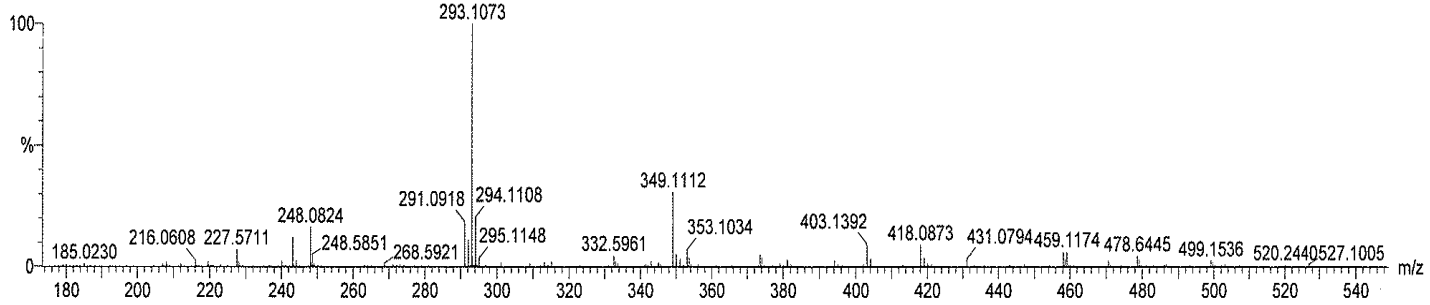
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 6.0 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
62 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: 0-6 O: 0-2 F: 0-1

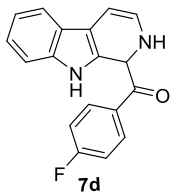
9d
UT1212_181 7 (0.252) Cm (7:8)

Gajanan
1: TOF MS ES+
2.03e+003

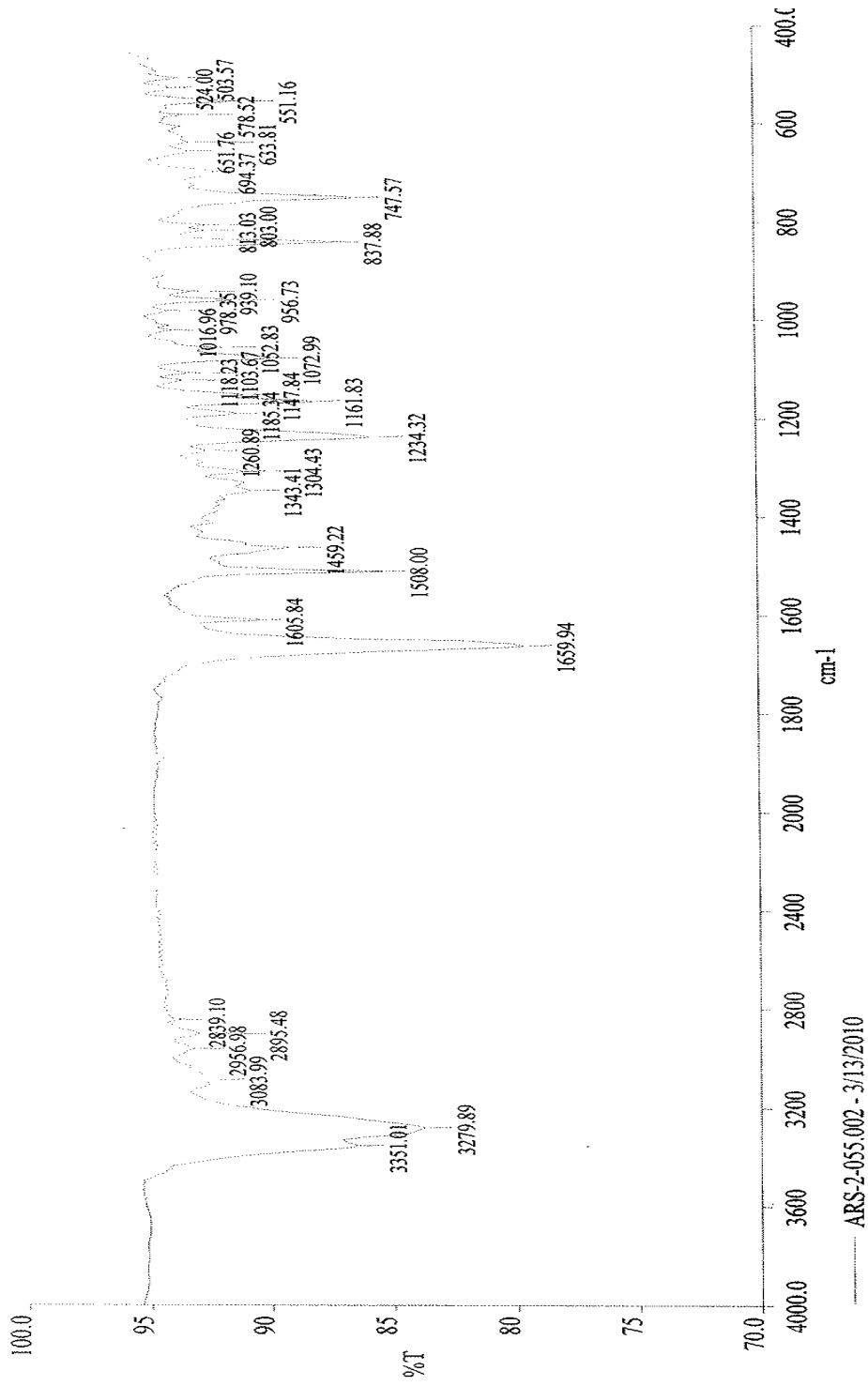


Minimum:				-1.5		
Maximum:		5.0	6.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
293.1073	293.1090	-1.7	-5.8	12.5	3.9	C18 H14 N2 O F

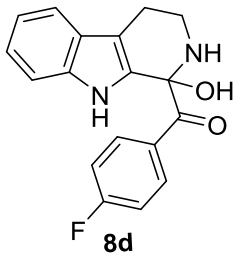
IR spectrum of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-fluorophenyl)methanone (**7d**):



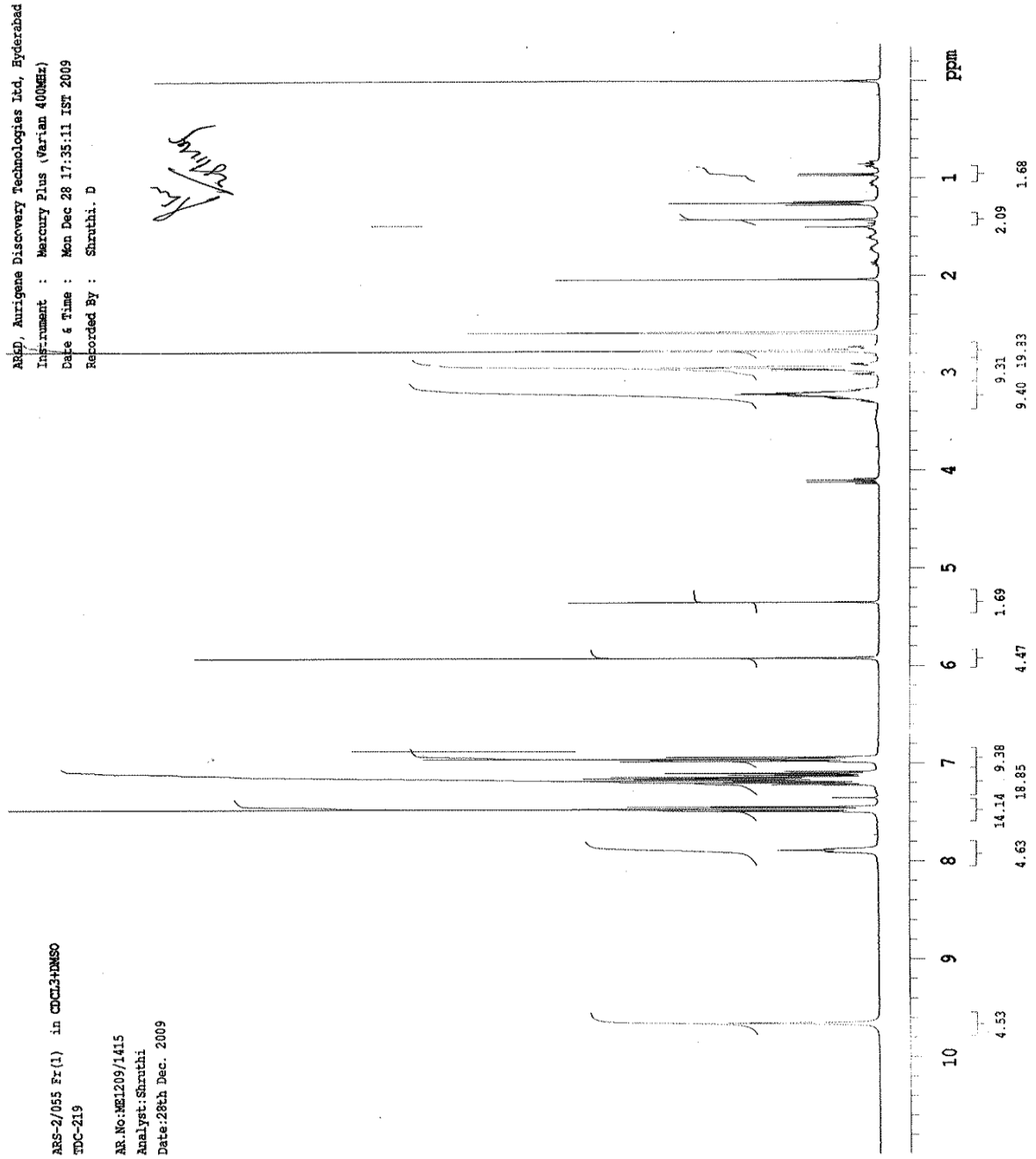
7d



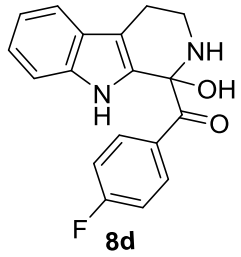
^{1}H NMR of (4-fluorophenyl)(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**8d**):



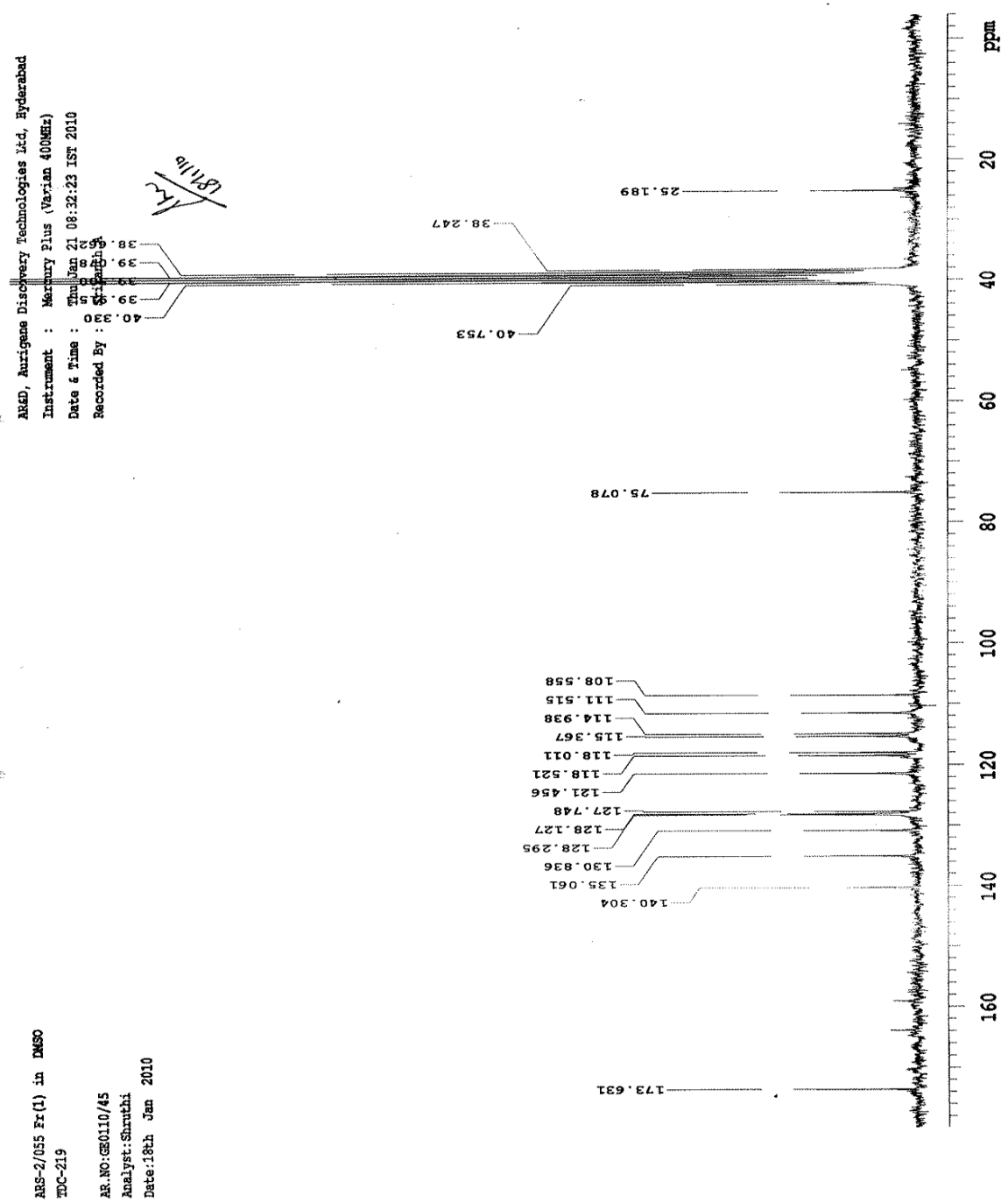
8d



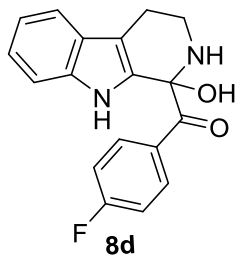
^{13}C NMR of (4-fluorophenyl)(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**8d**):



8d



Mass spectrum of (4-fluorophenyl)(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**8d**):



8d

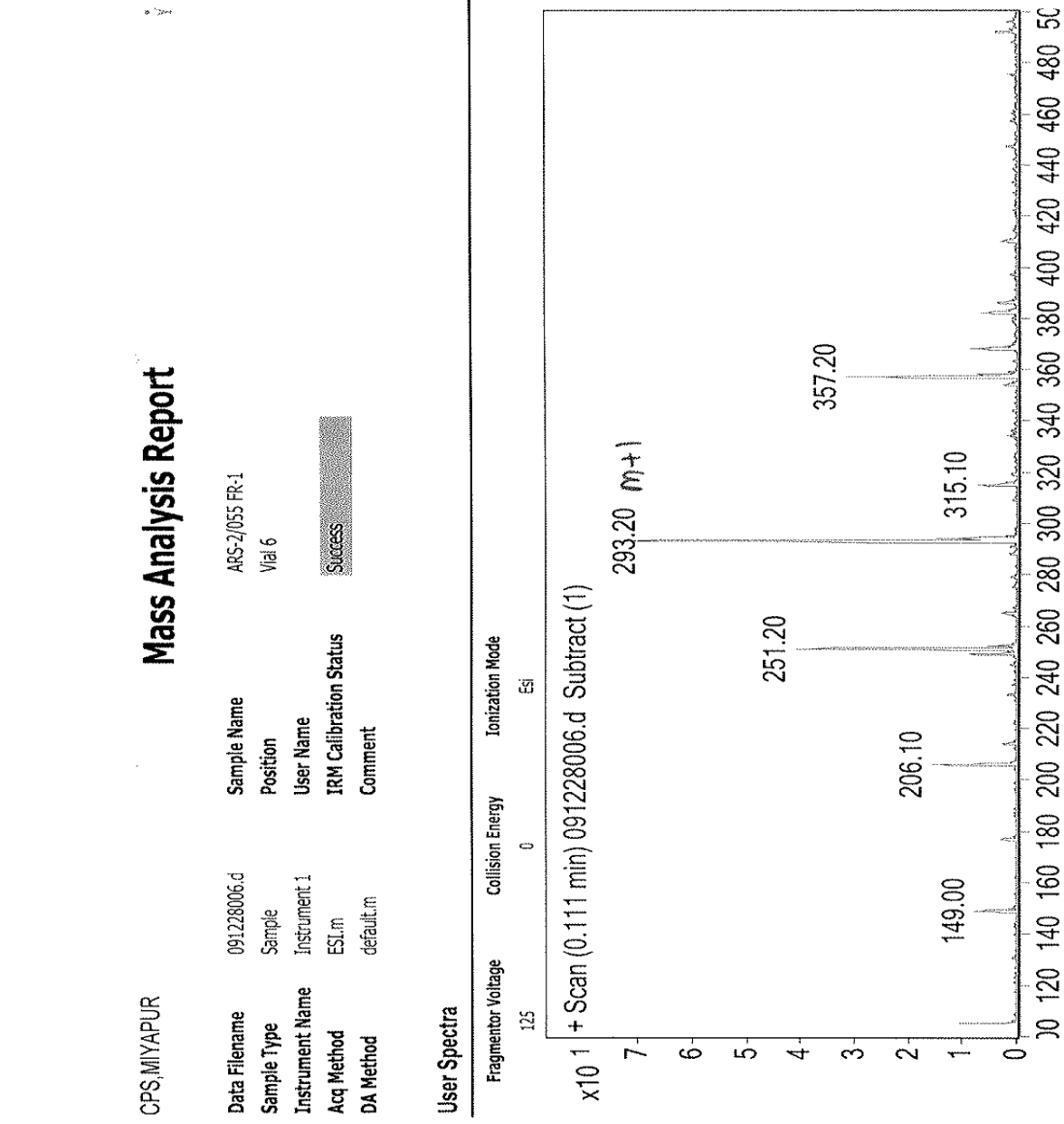
CPS,MIYAPUR

Mass Analysis Report

Data Filename	091228006.d	**Sample Name**	ARS-2/055 FR-1
Sample Type	Sample	**Position**	Vial 6
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	default.m	**Comment**	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
125	0	Esi



--- End Of Report ---

HRMS of (4-fluorophenyl)(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**8d**):

8d

Page 1

Elemental Composition Report

Single Mass Analysis
Tolerance = 7.0 PPM / DBE: min = -1.5, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

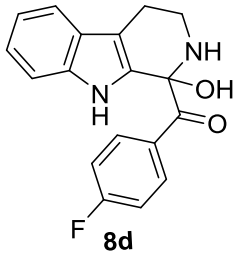
Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 N: 0-2 O: 0-2 F: 0-1
8d
UT1212_175 5 (0.198) Cm (5)

Gajanan
1: TOF MS ES+
8.04e+003

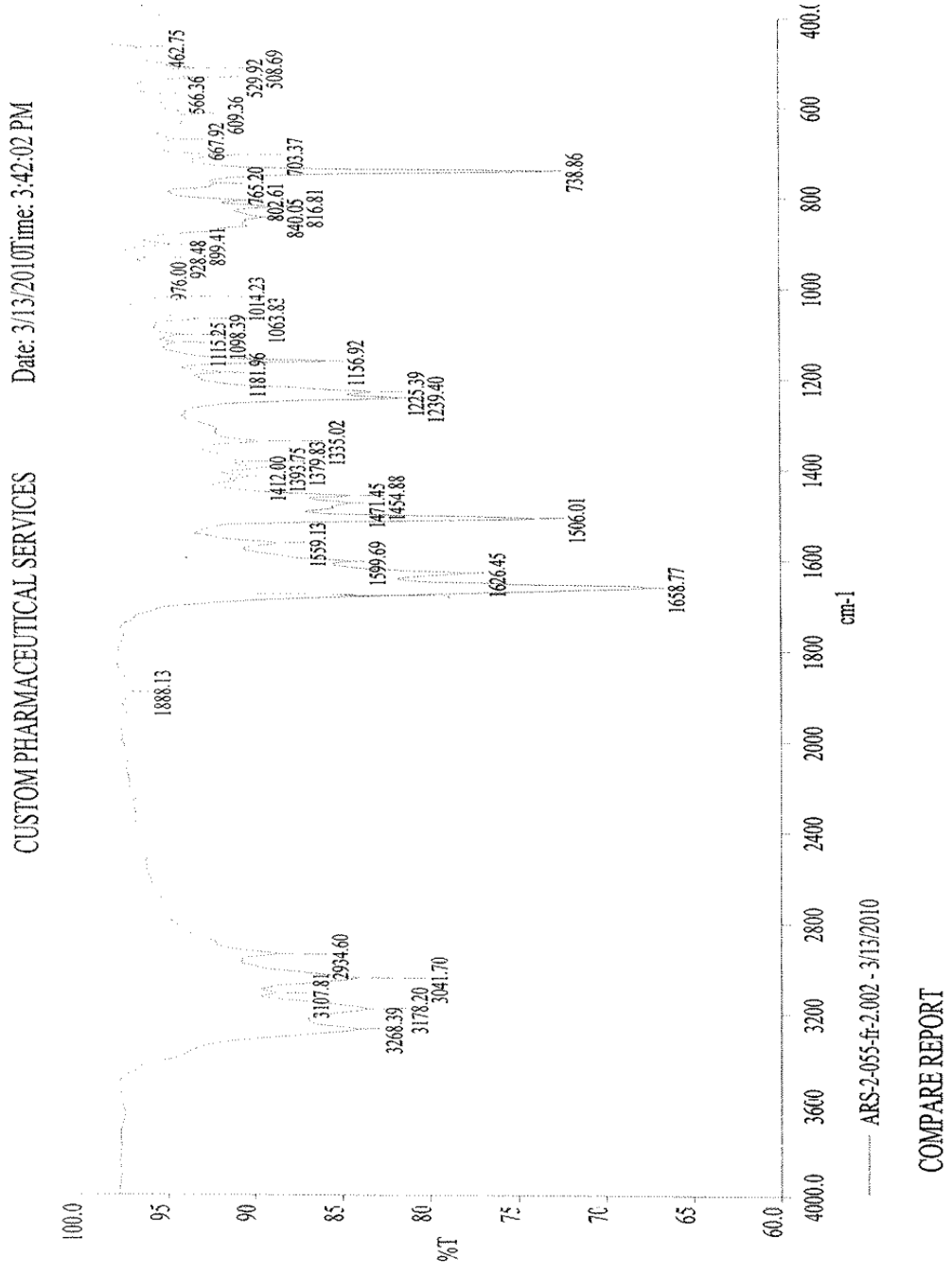
Minimum:			-1.5	
Maximum:	5.0	7.0	80.0	

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
293.1070	293.1079	-0.9	-3.1	16.5	6.4	C21 H13 N2
	293.1090	-2.0	-6.8	12.5	7.0	C18 H14 N2 O F

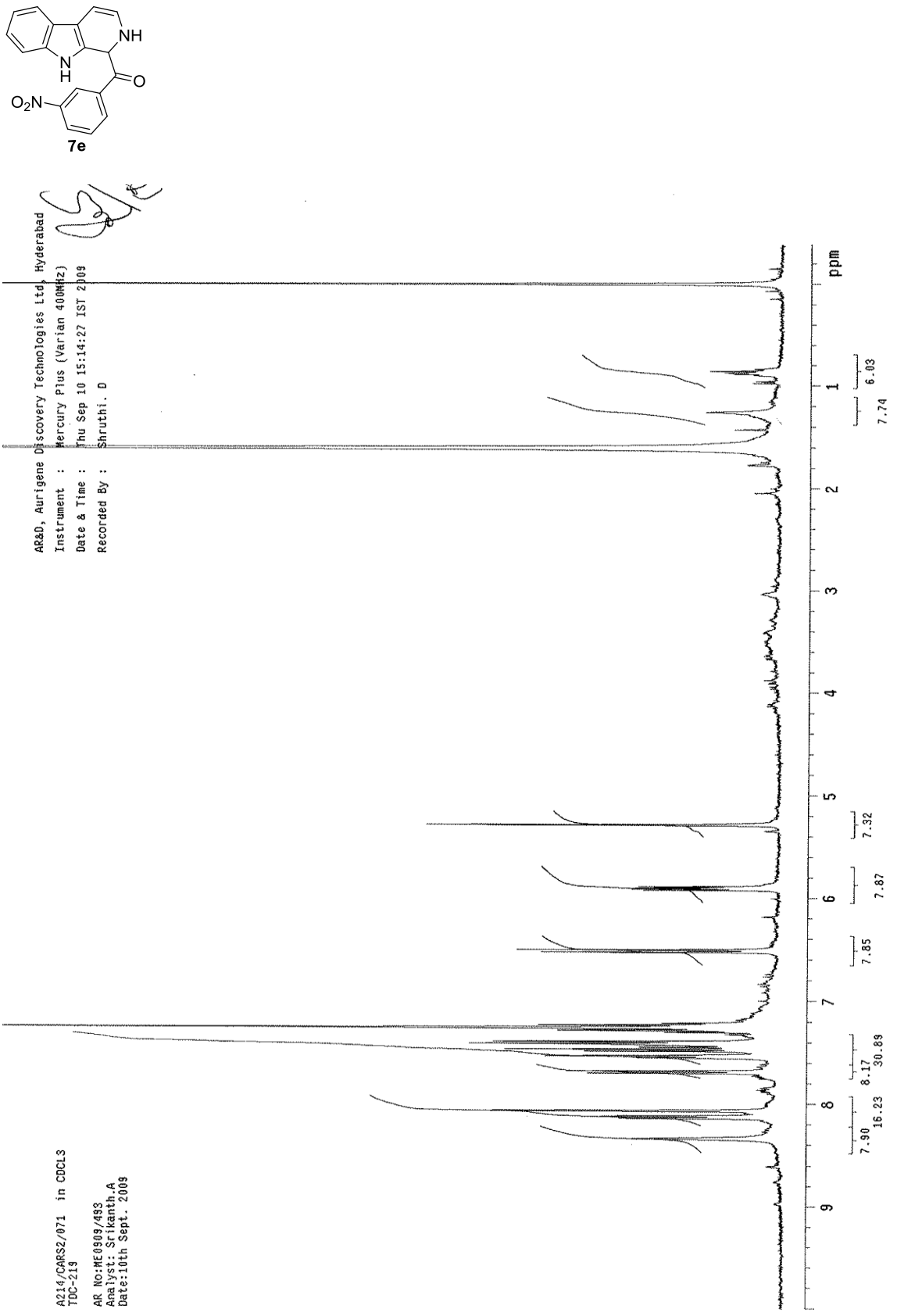
IR spectrum (4-fluorophenyl)(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**8d**):



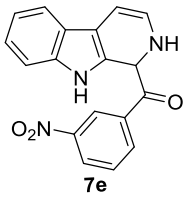
8d



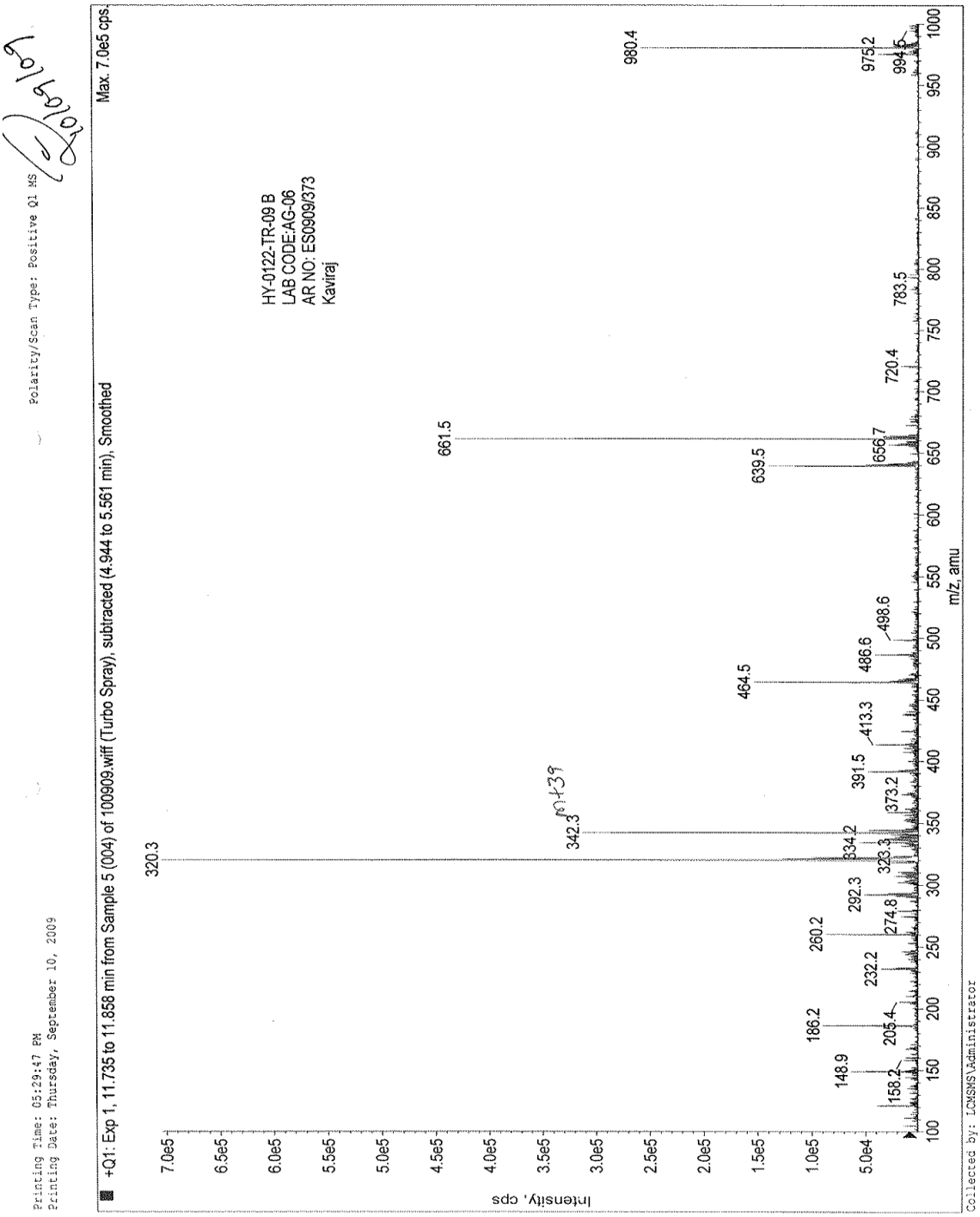
^{1}H NMR of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(3-nitrophenyl)methanone (**7e**):



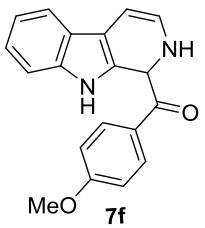
Mass spectrum of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(3-nitrophenyl)methanone (**7e**):



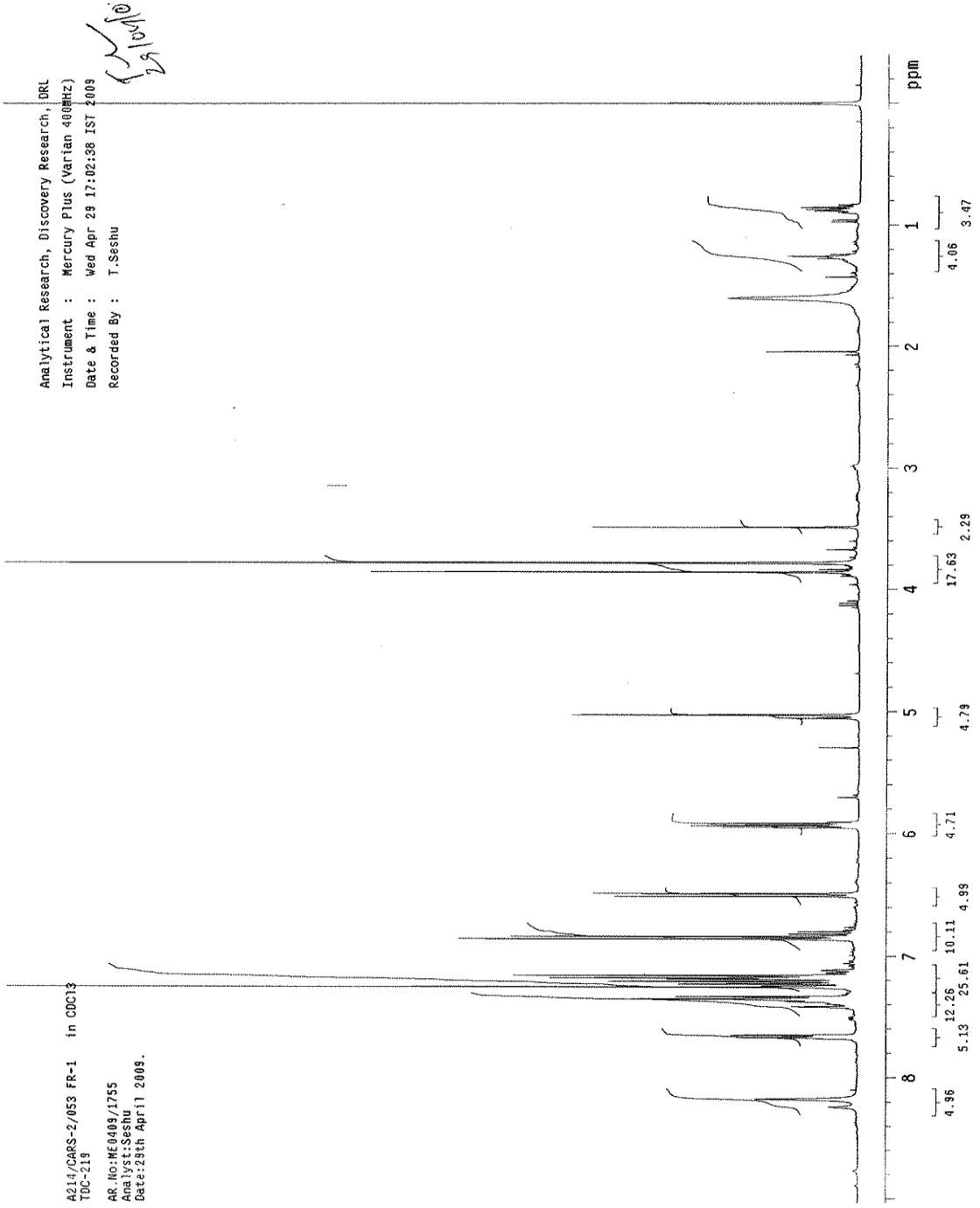
7e



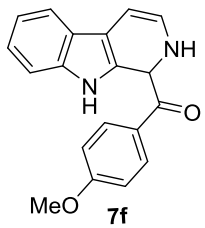
^{1}H NMR of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-methoxyphenyl)methanone (**7f**):



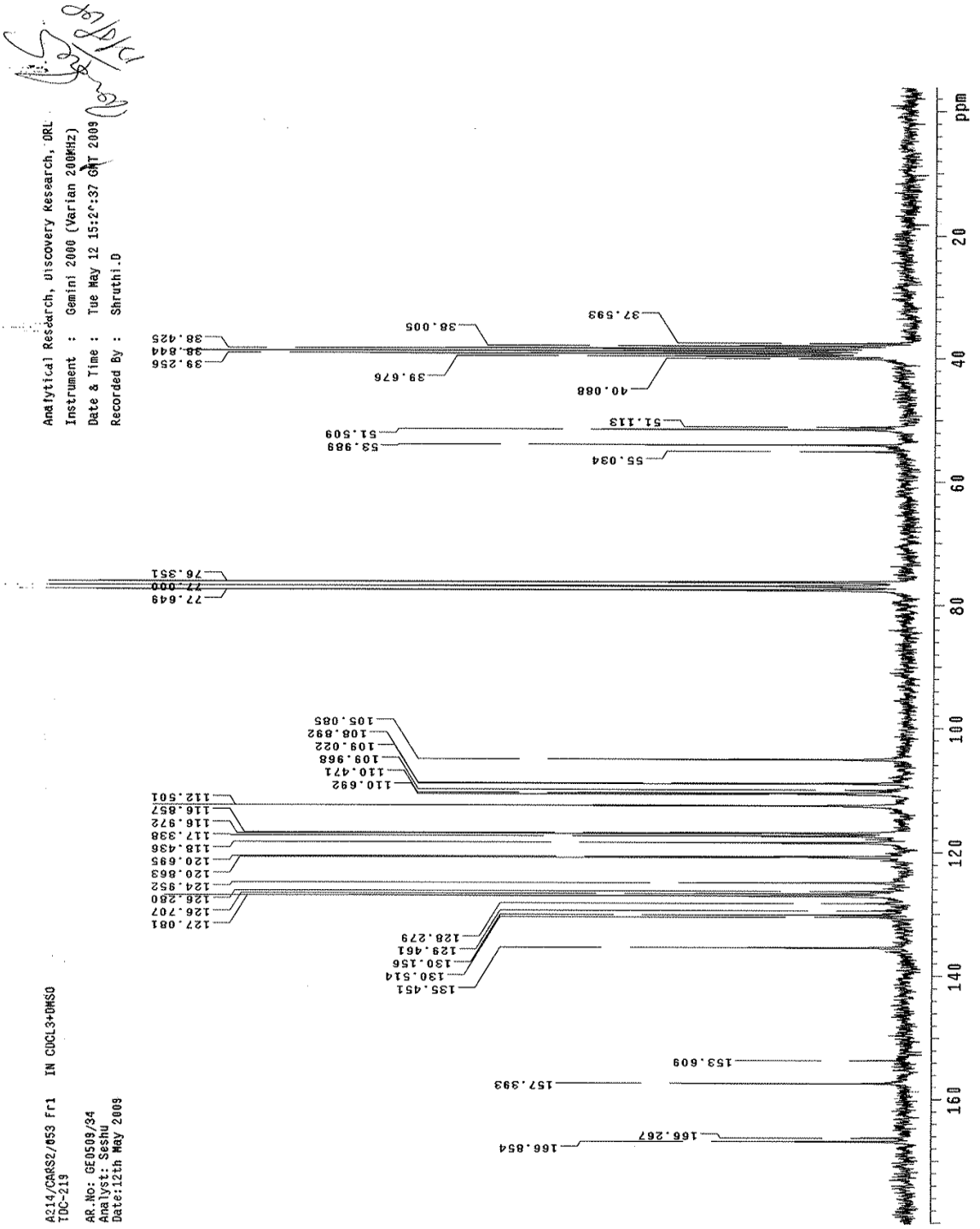
7f



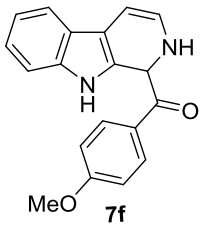
^{13}C NMR of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-methoxyphenyl)methanone (**7f**):



7f



Mass spectrum of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-methoxyphenyl)methanone (**7f**):



7f

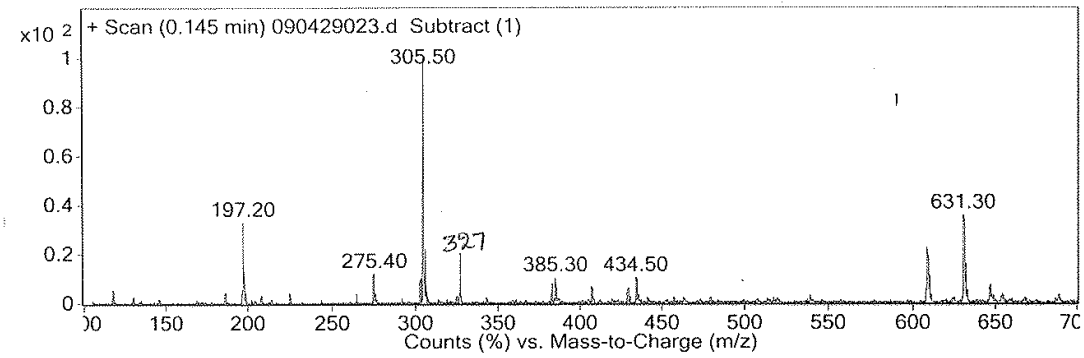
CPS,MIYAPUR

Mass Analysis Report

Data Filename	090429023.d	**Sample Name**	A214/CARS-2/053 FR-1
Sample Type	Sample	**Position**	Vial 42
Instrument Name	Instrument 1	**User Name**	
Acq Method		**IRM Calibration Status**	Success
DA Method	Quant Process.m	**Comment**	

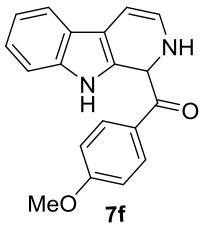
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	Esi

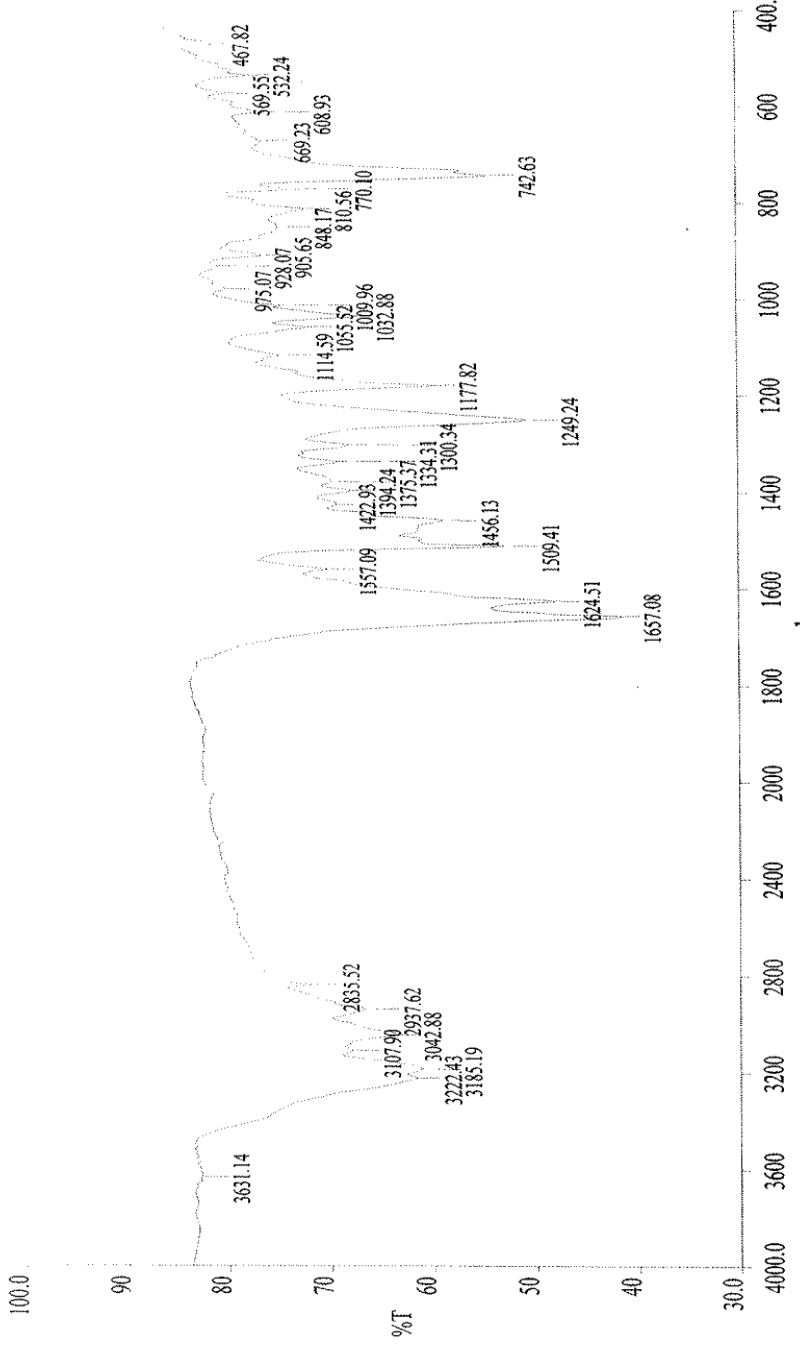


--- End Of Report ---

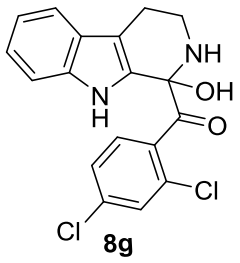
IR spectrum of (2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)(4-methoxyphenyl)methanone (**7f**):



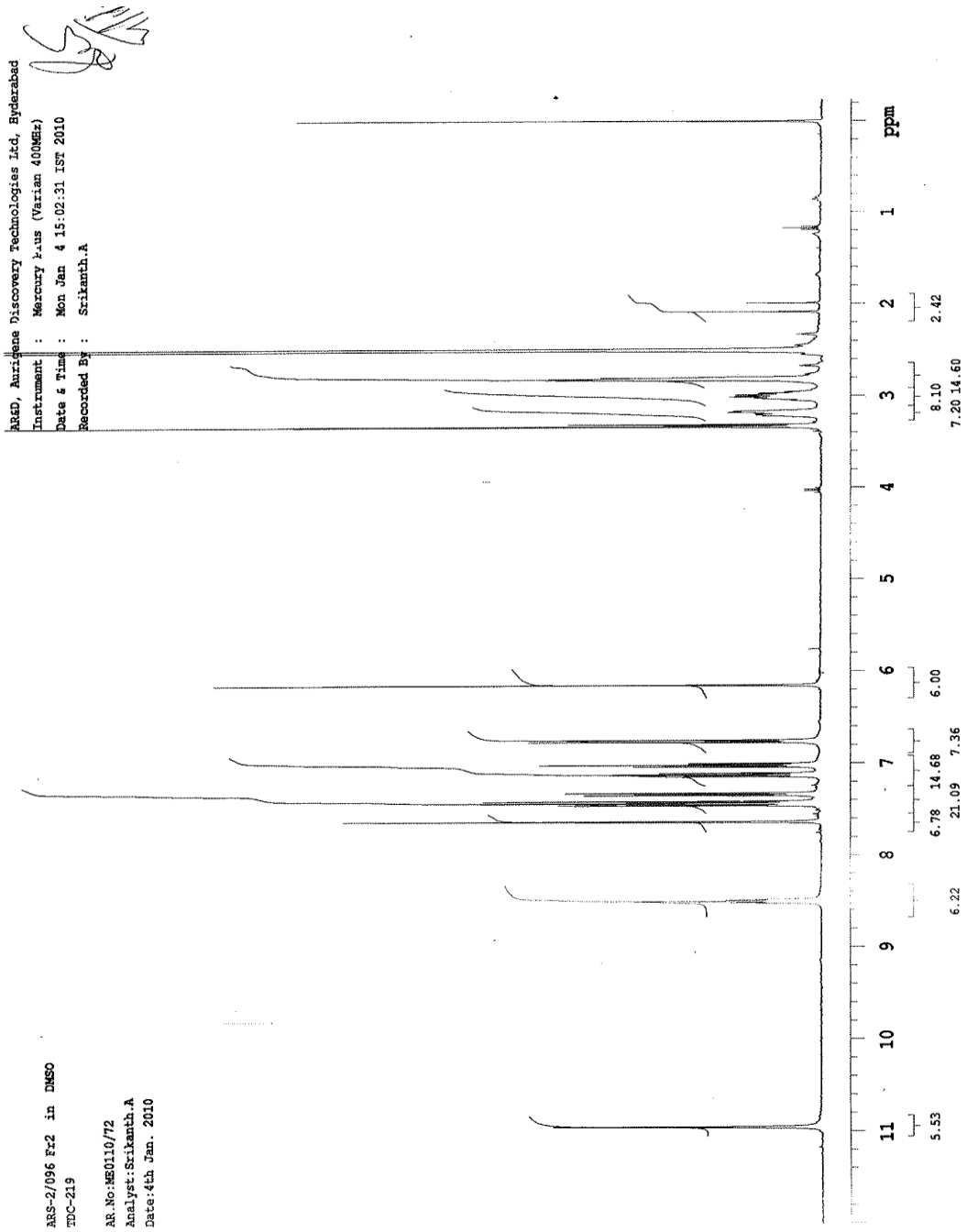
7f



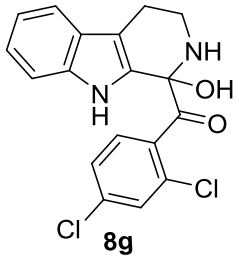
^{1}H NMR of (2,4-dichlorophenyl)(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**8g**):



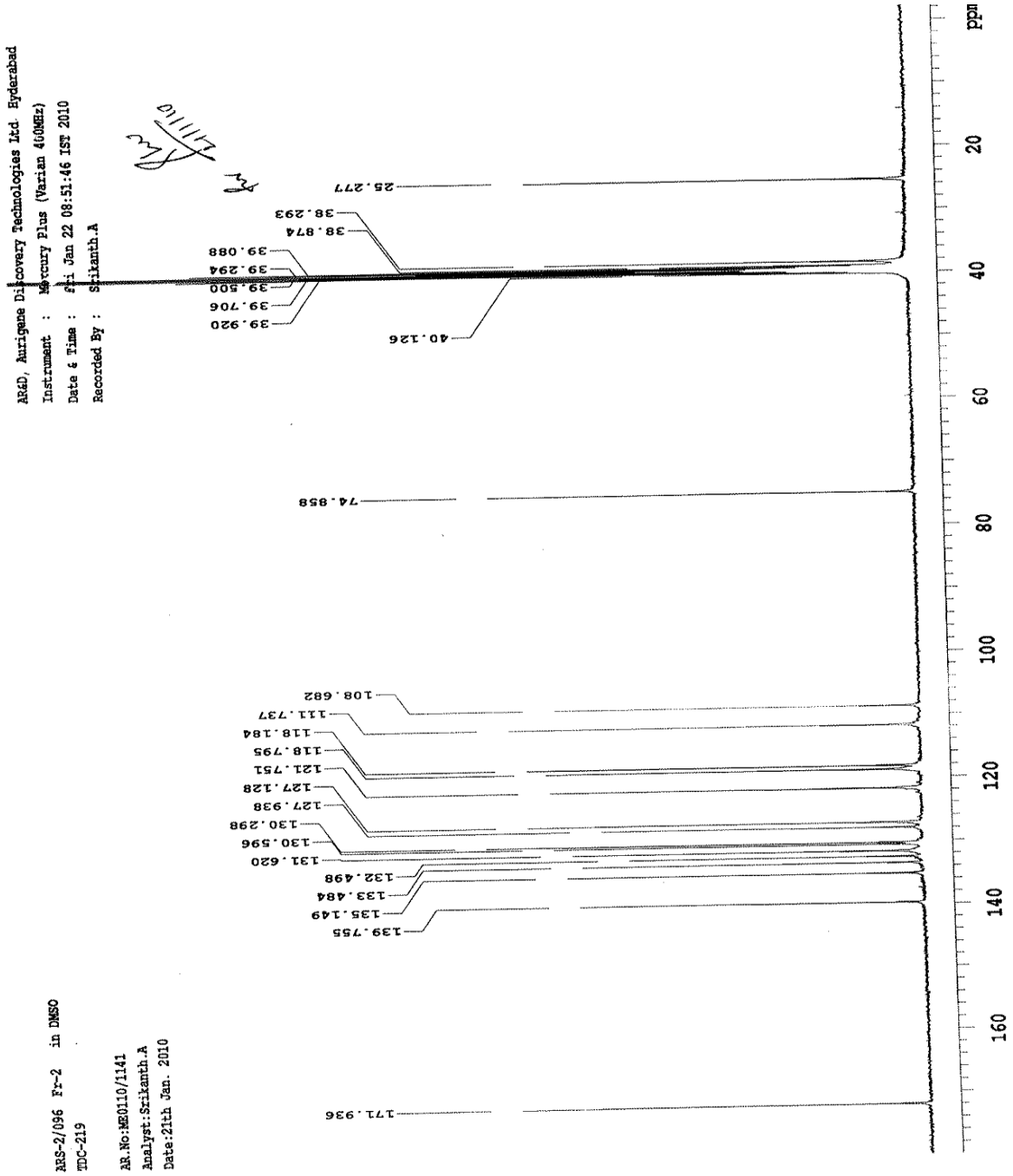
8g



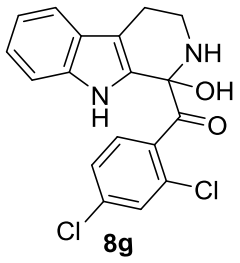
^{13}C NMR of (2,4-dichlorophenyl)(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**8g**):



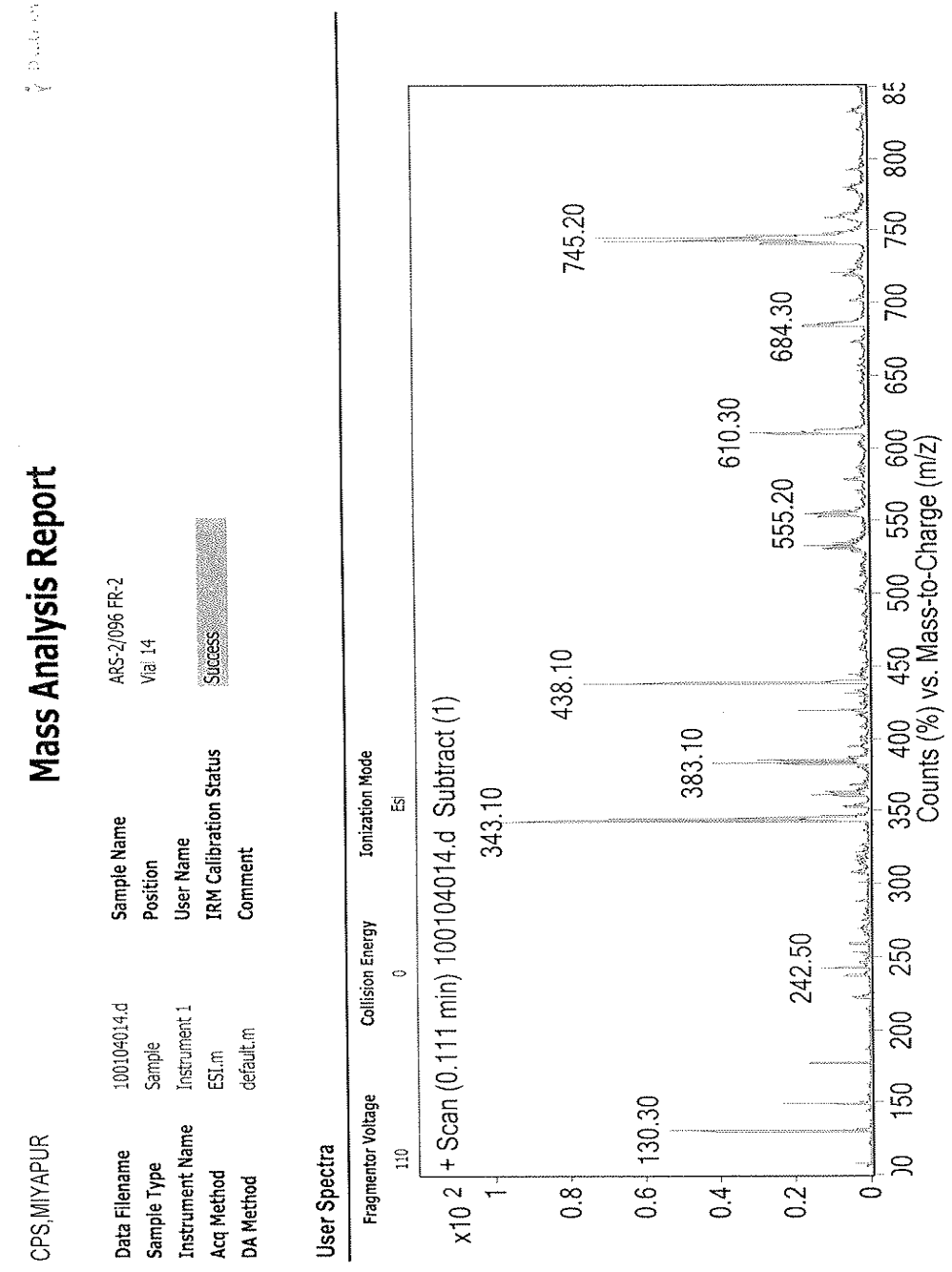
8g



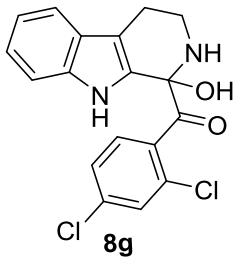
Mass spectrum (2,4-dichlorophenyl)(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**8g**):



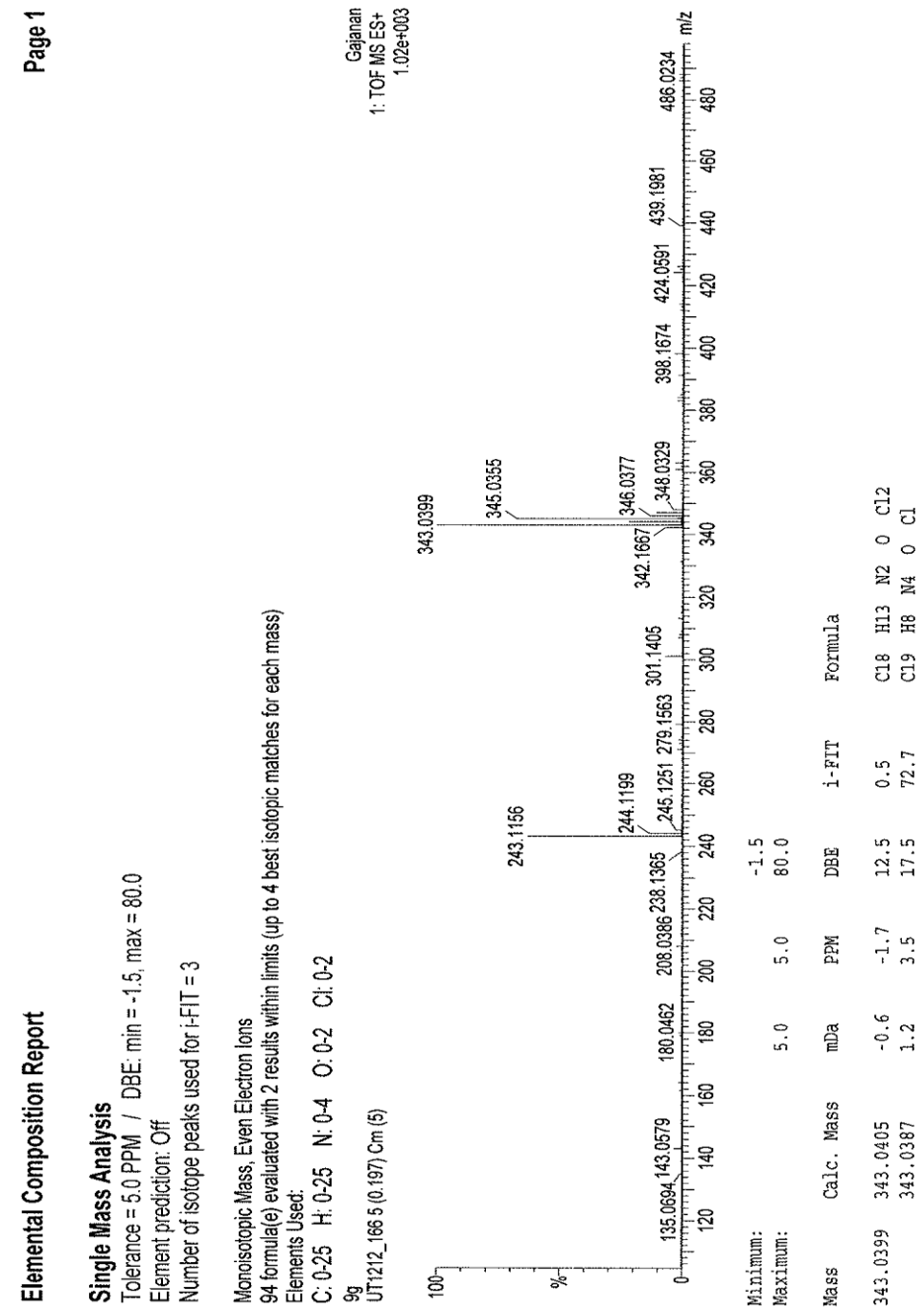
8g



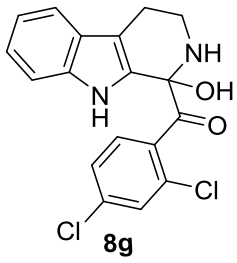
HRMS of (2,4-dichlorophenyl)(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**8g**):



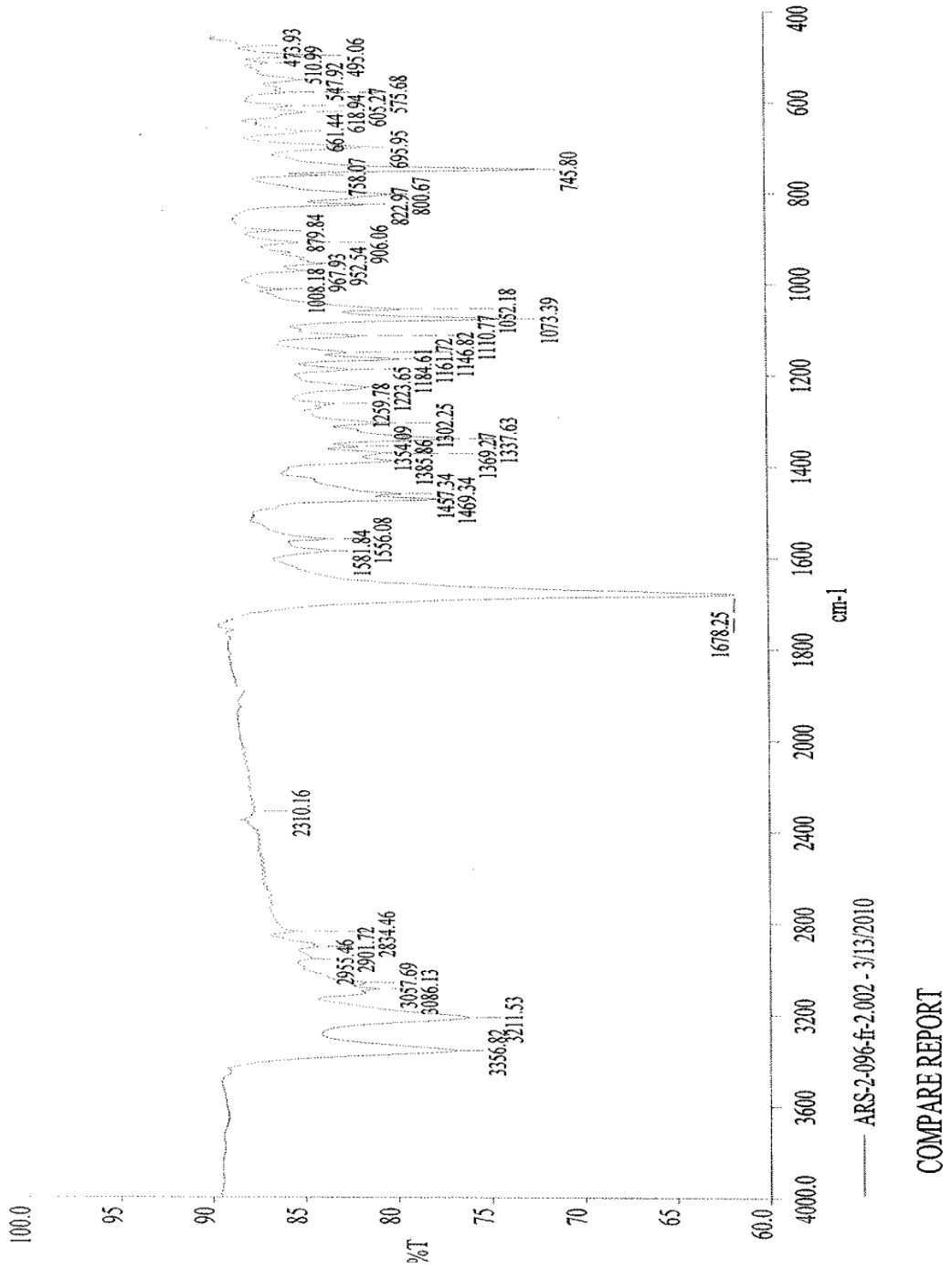
8g



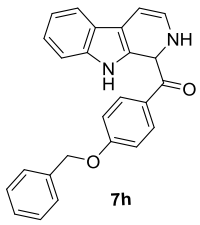
IR spectrum of (2,4-dichlorophenyl)(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**8g**):



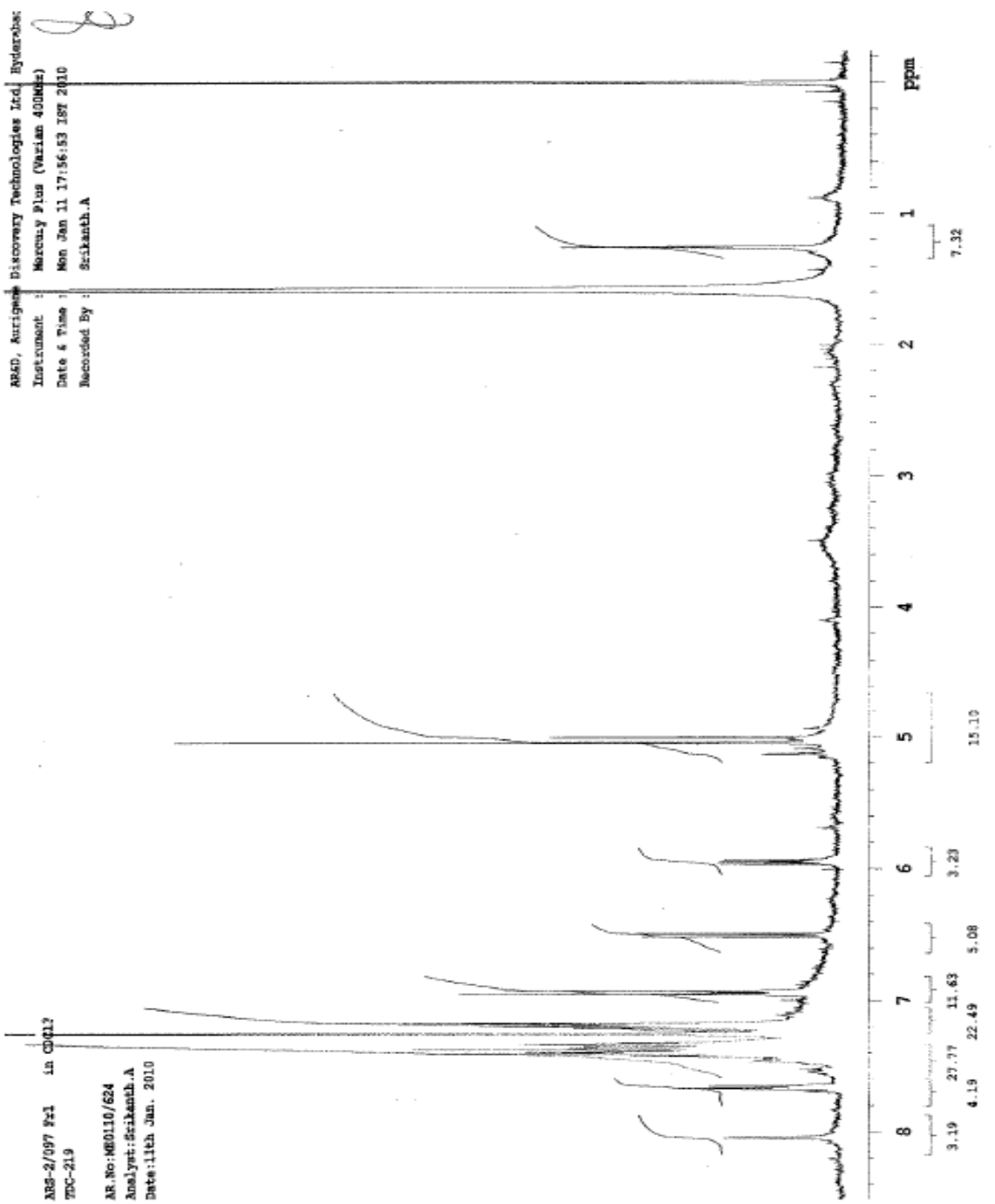
8g



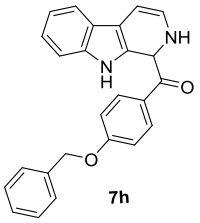
^{1}H NMR of (4-(benzyloxy)phenyl)(2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**7h**):



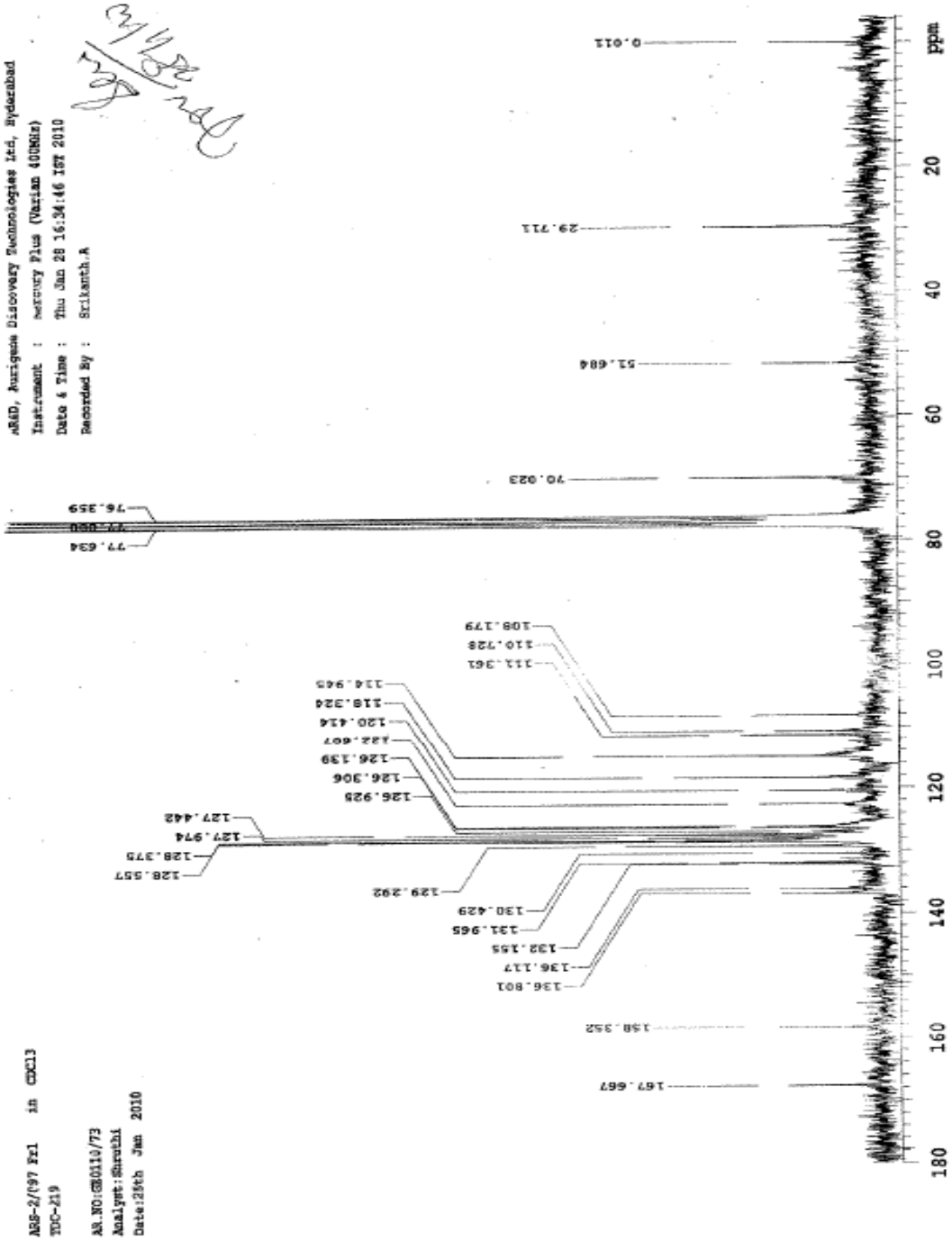
7h



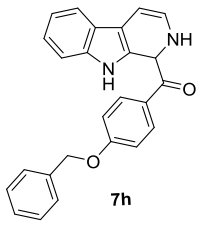
^{13}C NMR of (4-(benzyloxy)phenyl)(2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**7h**):



7h



Mass spectrum of (4-(benzyloxy)phenyl)(2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**7h**):



7h

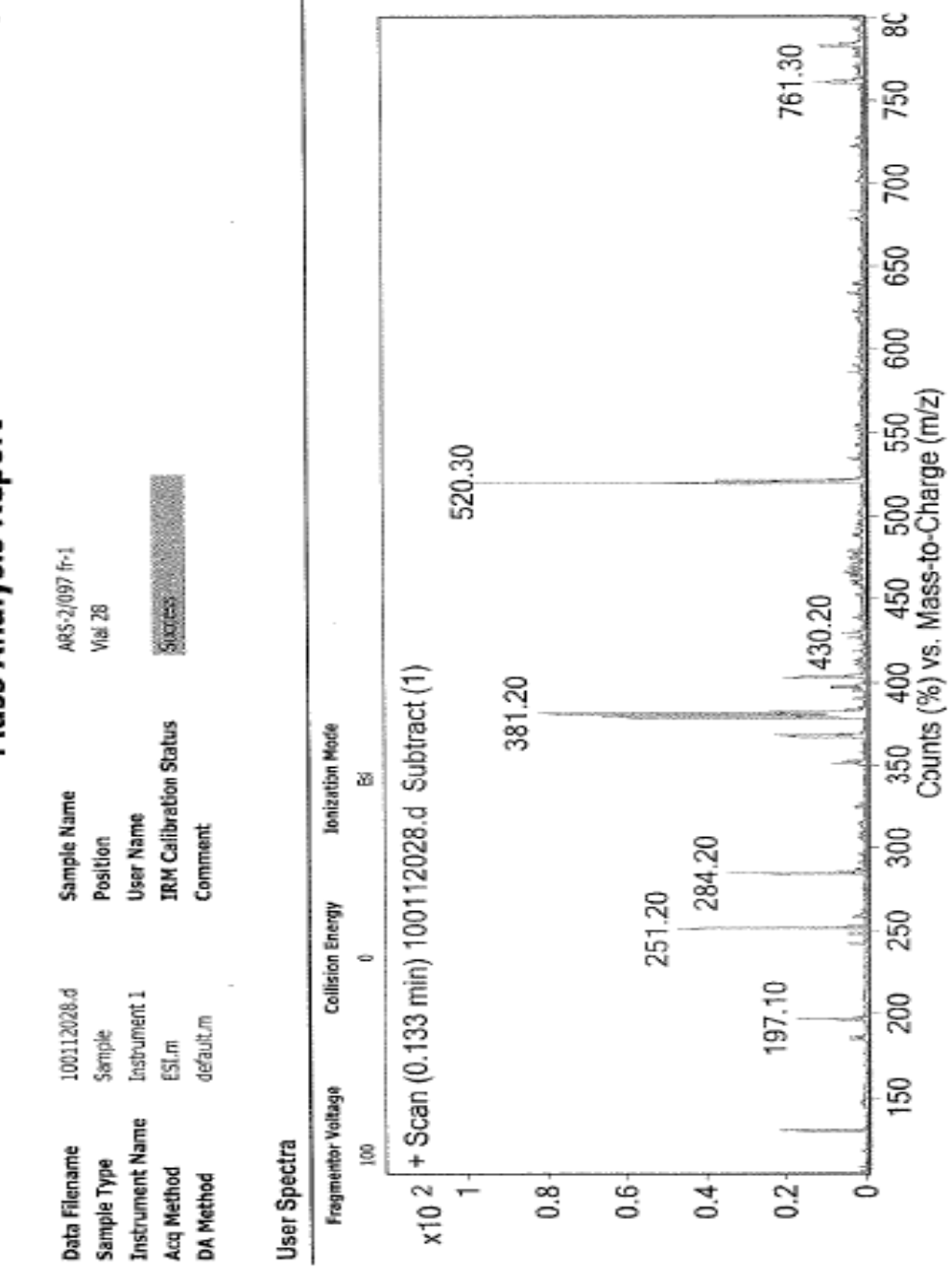
CPS,MIYAPUR

Mass Analysis Report

Data Filename	100112028.d	**Sample Name**	ARS-2/097 fr-1
Sample Type	Sample	**Position**	Vial 28
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	default.m	**Comment**	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	Esi



--- End Of Report ---

HRMS of (4-(benzyloxy)phenyl)(2,9-dihydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**7h**):

7h

Elemental Composition Report

Page 1

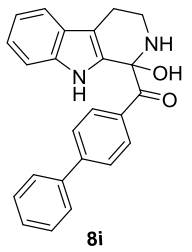
Single Mass Analysis
Tolerance = 6.0 PPM / DBE: min = -1.5, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-25 N: 0-2 O: 0-2
9h
UT1212_178 6 (0.224) Cm (6:8)

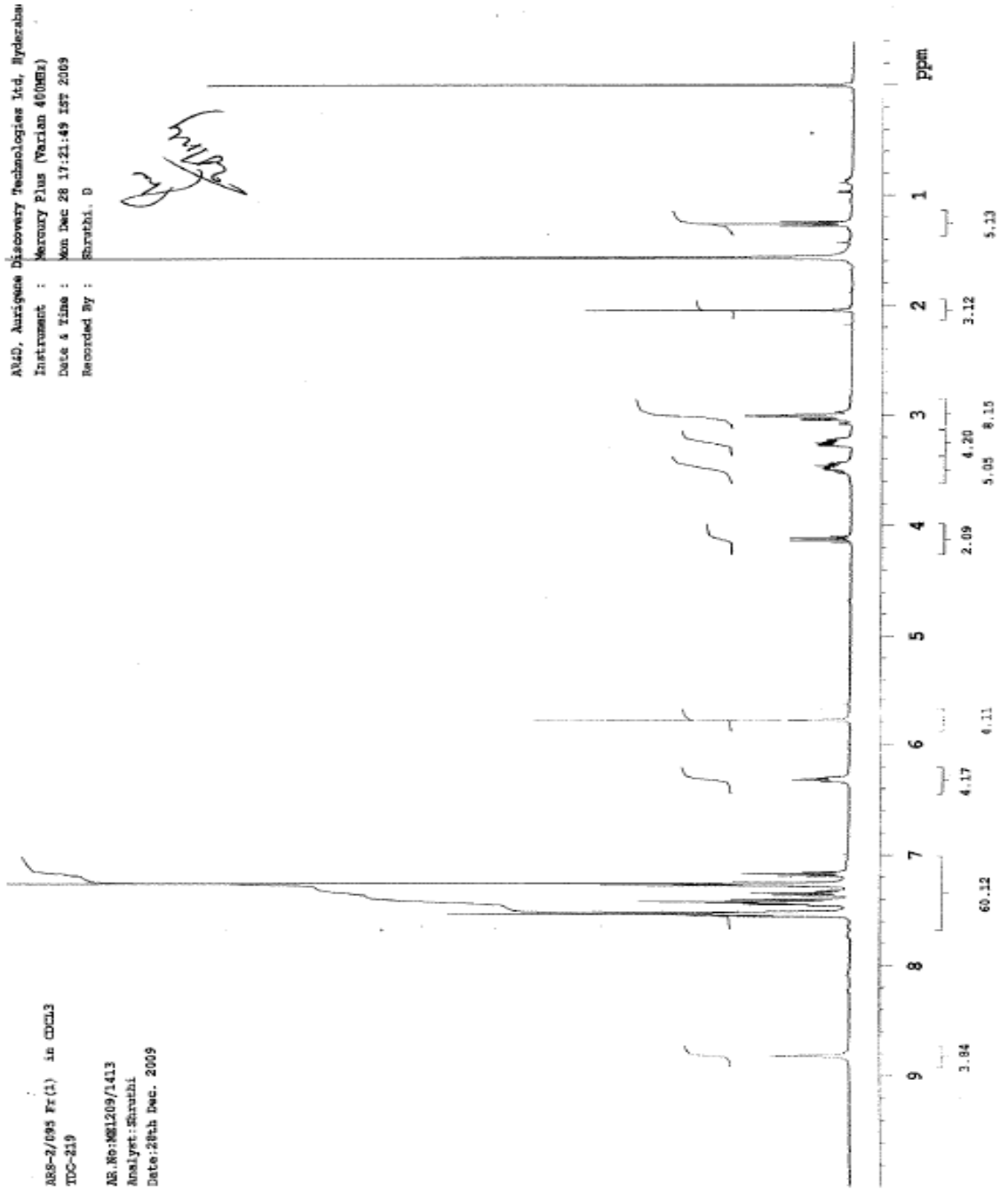
Gajanan
1: TOF MS ES+
2.61e+003

Minimum:			-1.5		
Maximum:		5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
381.1583	381.1603	-2.0	-5.2	16.5	6.5	C25 H21 N2 O2

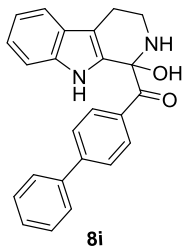
^{1}H NMR of [1,1'-biphenyl]-4-yl(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**8i**):



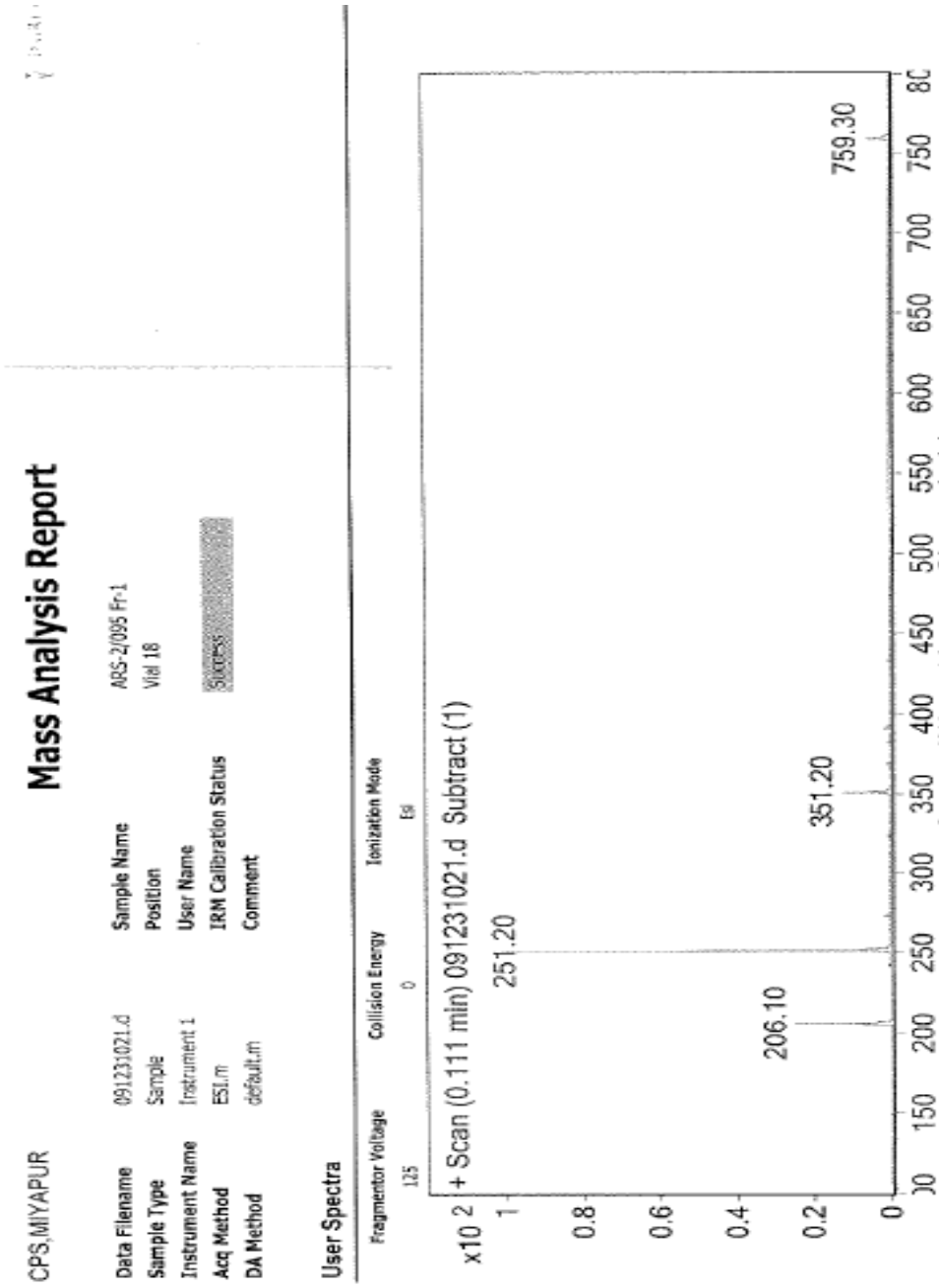
8i



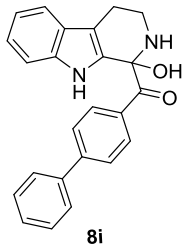
Mass spectrum of [1,1'-biphenyl]-4-yl(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**8i**):



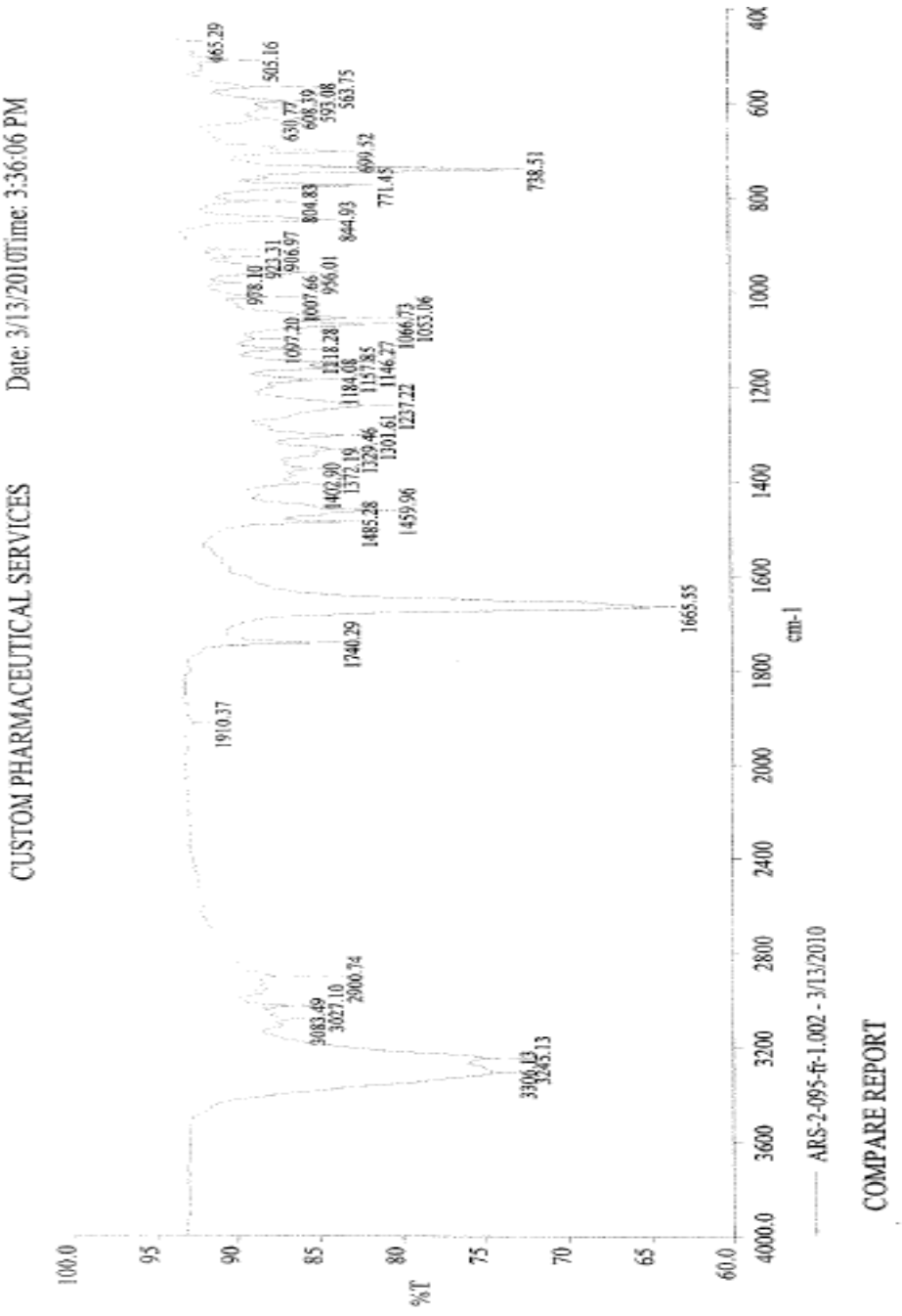
8i



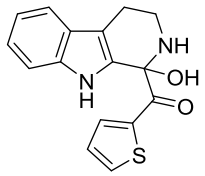
IR spectrum of [1,1'-biphenyl]-4-yl(1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)methanone (**8i**):



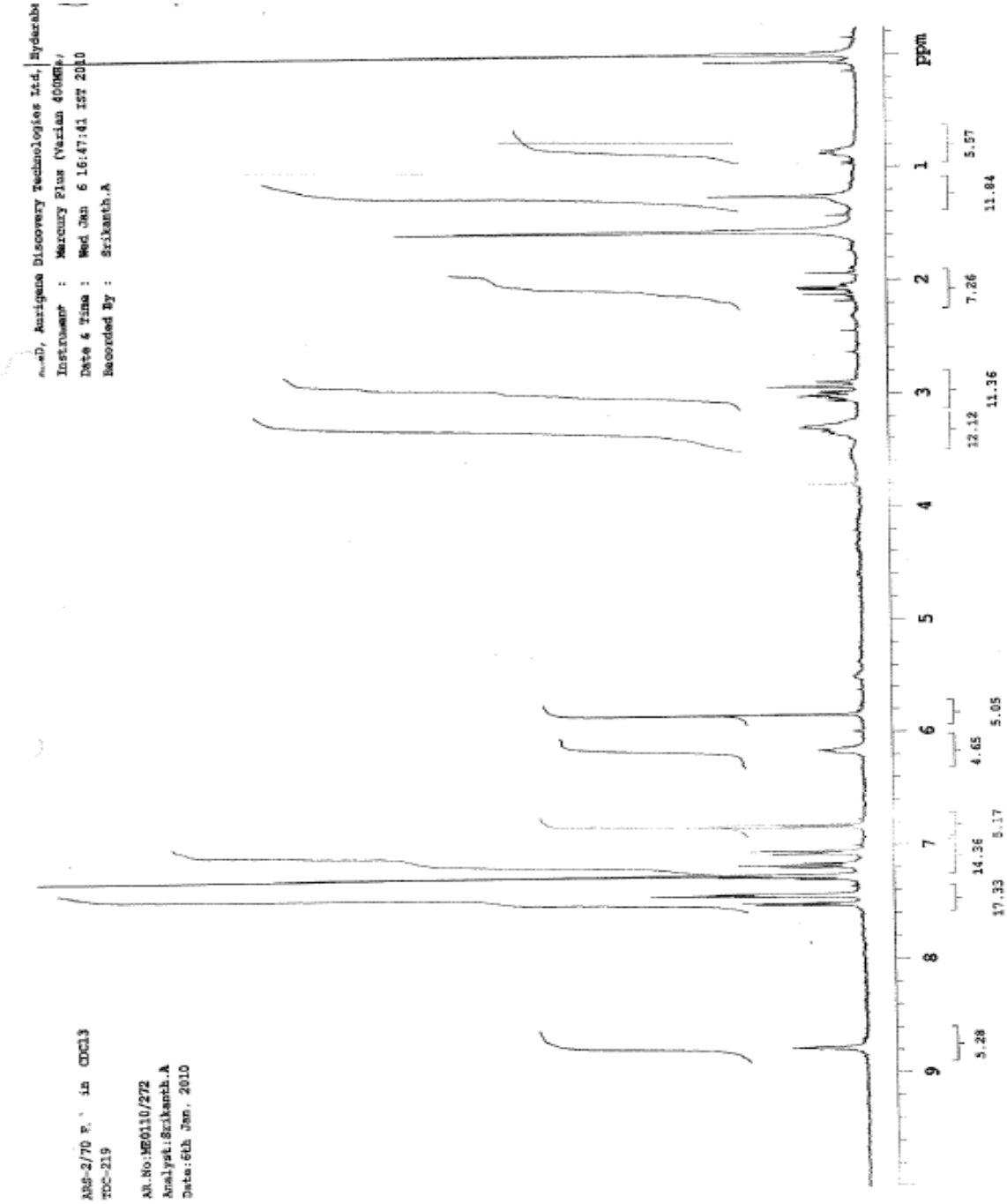
8i



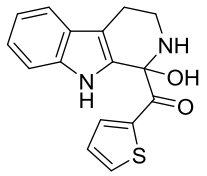
^{1}H NMR of (1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)(thiophen-2-yl)methanone (**8j**):



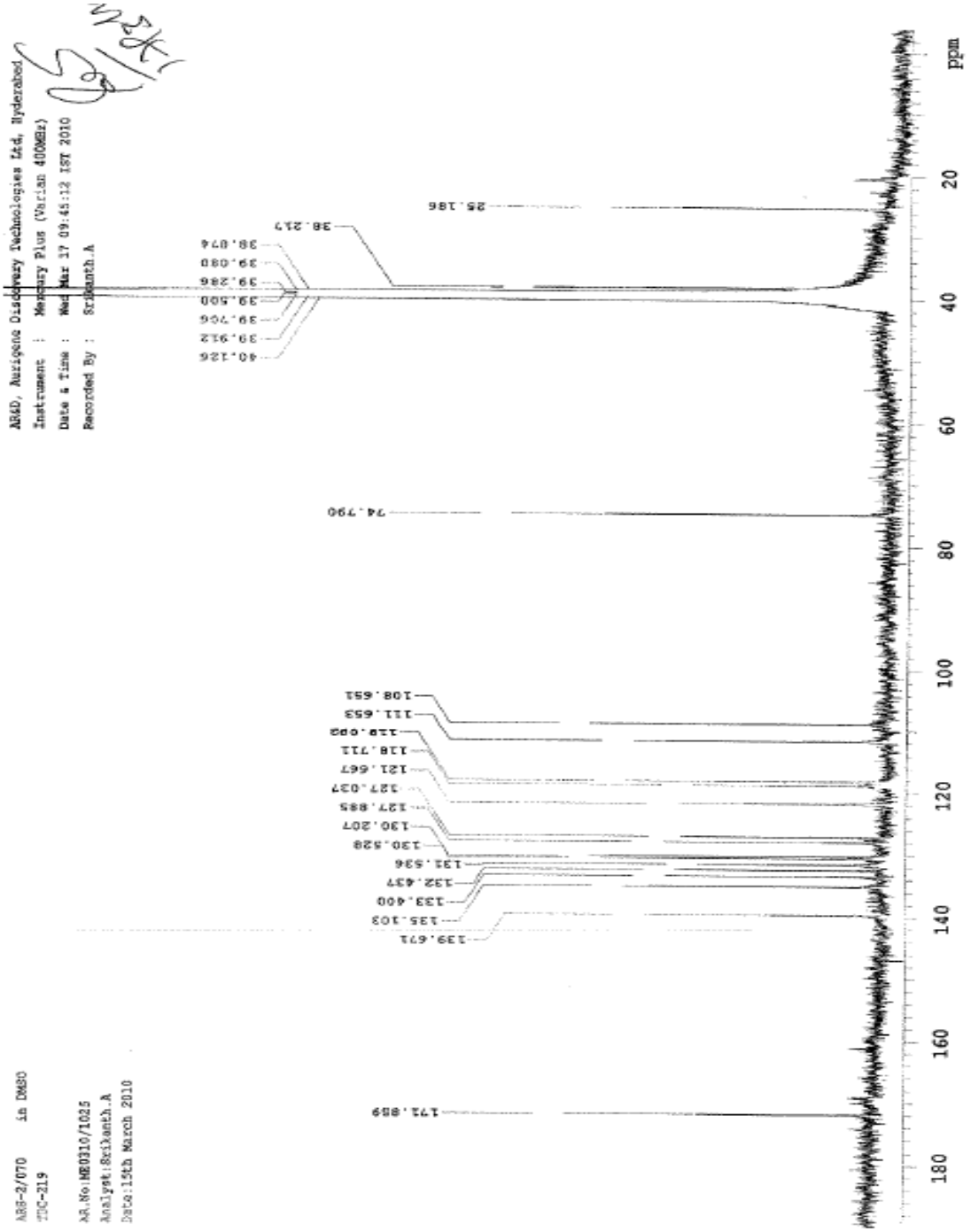
8j



^{13}C NMR of (1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)(thiophen-2-yl)methanone (**8j**):



8j



Mass spectrum of (1-hydroxy-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-b]indol-1-yl)(thiophen-2-yl)methanone (**8j**):

8j

CPS,MIYAPUR

Mass Analysis Report

Data Filename	100104024.d	**Sample Name**	ARS-2/070
Sample Type	Sample	**Position**	Vial 21
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	default.m	**Comment**	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
110	0	Esi

--- End Of Report ---