

## **Supporting Information**

**for**

### **Identification and synthesis of impurities formed during sertindole preparation**

I. V. Sunil Kumar<sup>\*1</sup>, G. S. R. Anjaneyulu<sup>1</sup> and V. Hima Bindu<sup>2</sup>

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Email: I. V. Sunil Kumar - sunil.indukuri@aptuitlaurus.com

\*Corresponding author

### **Supporting Information File 2:**

**<sup>1</sup>H and <sup>13</sup>C NMR spectral data and HPLC chromatograms for all new compounds**

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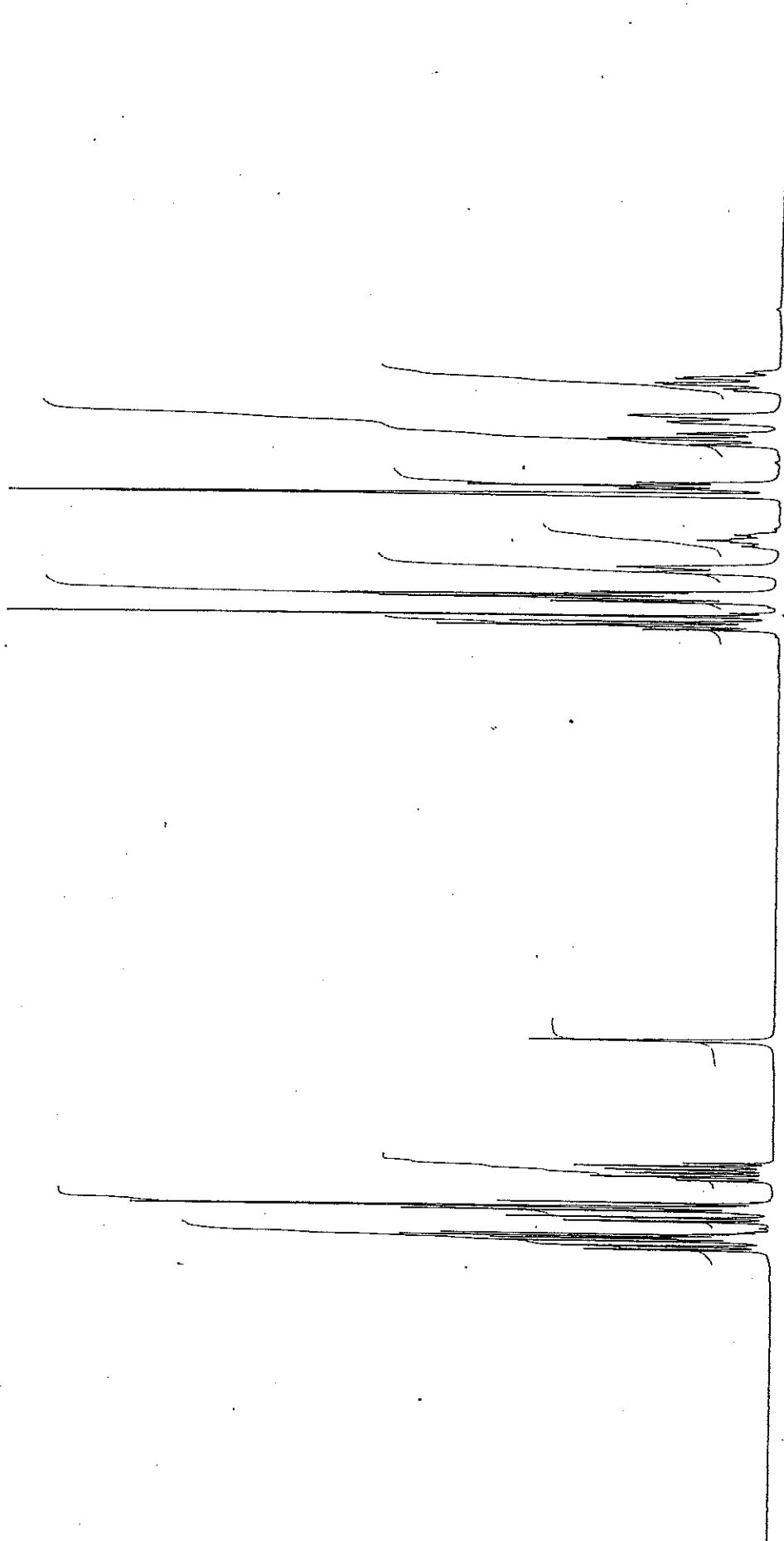
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1H NMR of Q080/2059/003 in DMSO-d6  
 Date:- 02/06/09 ARNO : SE0509/027  
 {C:/LKT/Structure elucidation/May2009/94/1}

Des-chloro 2

7.654  
7.630  
7.598  
7.582  
7.568  
7.552  
7.461  
7.434  
7.393  
7.370  
7.364  
7.335  
7.180  
7.176  
7.157  
7.153  
7.130  
7.126  
7.107  
7.104  
7.081  
7.058  
7.055  
6.214

3.397  
3.373  
3.364  
3.345  
3.209  
3.183  
3.162  
3.140  
3.005  
2.967  
2.819  
2.792  
2.780  
2.769  
2.741  
2.485  
2.479  
2.473  
2.467  
2.461  
2.433  
2.411  
2.388  
2.125  
2.087  
2.053  
1.971  
1.934  
1.718  
1.708  
1.677  
1.667



9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

3.213  
3.957  
2.000  
0.984  
2.036  
4.083  
2.080  
1.080  
1.990  
4.112  
2.070

2.166109

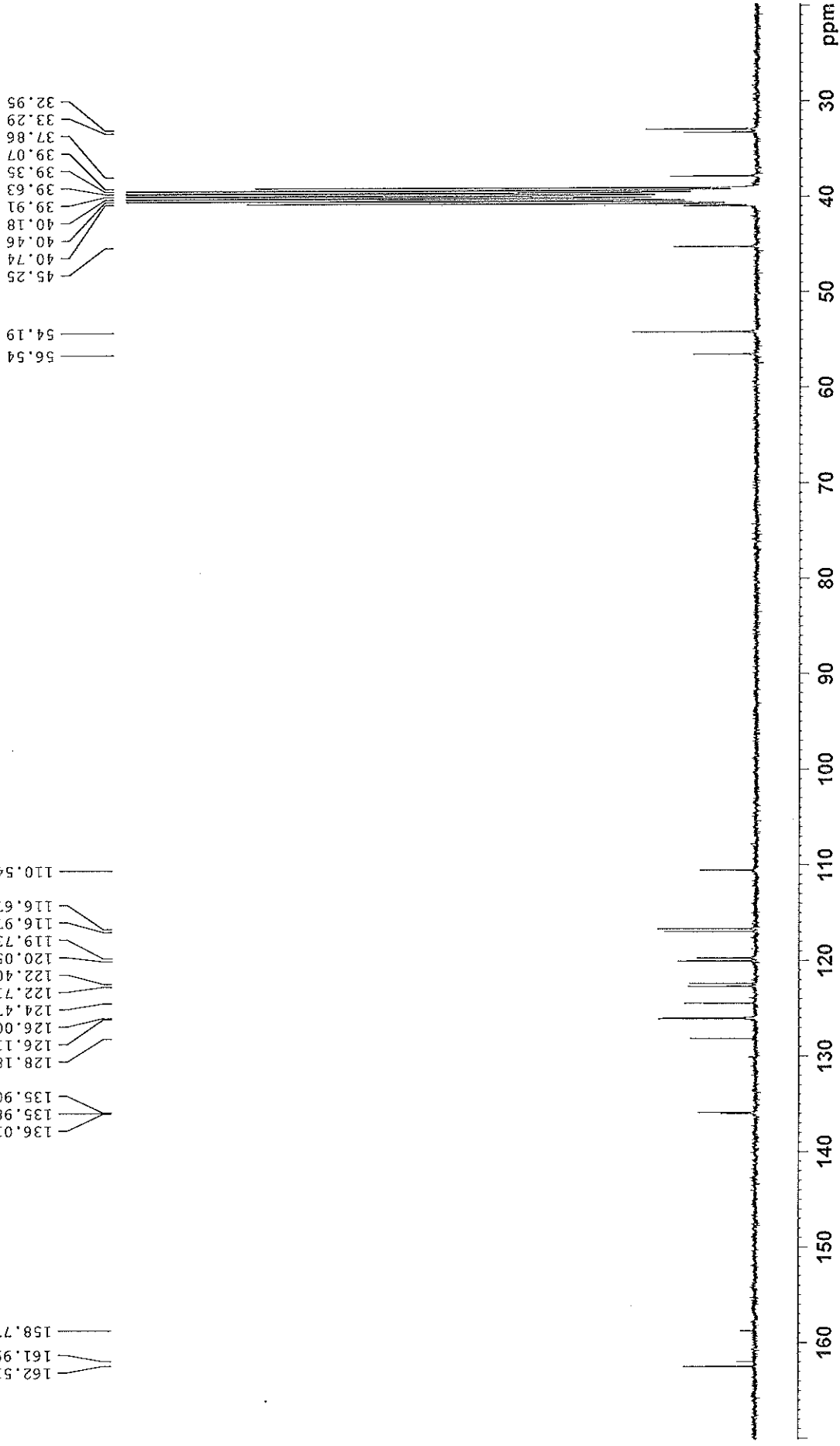
13C NMR of 0080/2059/003 in DMSO-d6  
Date:- 02/06/09 ARNo :SE0509/027  
{C:/LKT/Structure elucidation/May2009/98/1}

aptuit laurus

Des-chloro 2

162.51  
161.99  
158.77  
136.01  
135.98  
135.90  
128.18  
126.11  
126.00  
124.47  
122.71  
122.40  
120.05  
119.73  
116.97  
116.67  
110.54

56.54  
54.19  
45.25  
40.74  
40.46  
40.18  
39.91  
39.63  
39.35  
39.07  
37.86  
33.29  
32.95

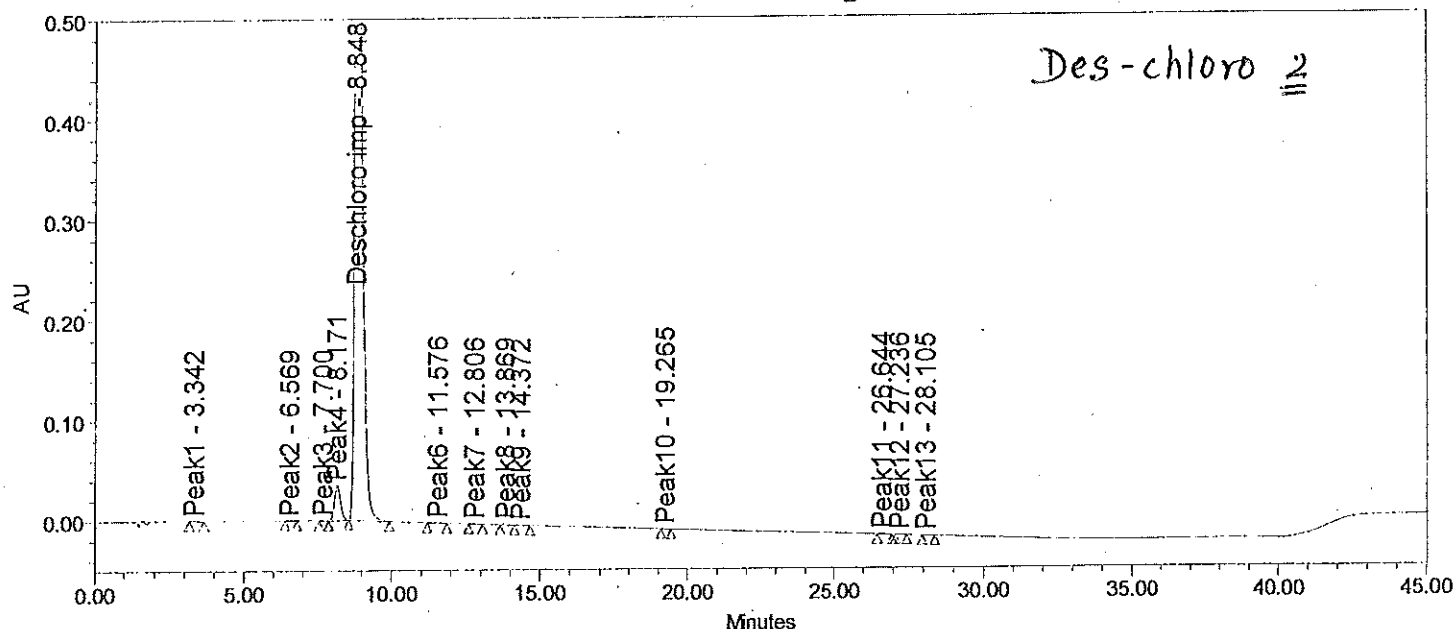


Analyst: Lakshmi Kumar.Tatini

## SAMPLE INFORMATION

Sample Name:	0080/AST-imp/2059/003 pre-1	Instrument Method Id	4820
Sample Type:	Unknown	Acquired By:	Analyst
Vial:	58	Date Acquired:	7/31/2009 2:33:26 AM IST
Injection #:	1	Date Processed:	7/31/2009 9:49:56 AM IST
Injection Volume:	10.00 ul	Processing Method:	0080_RS
Sample Set Id	5596	Processing Method Id	5731
Sample Set Name:	300709 01	Proc. Chnl. Descr.:	VWD AU On nm
Project Name:	Sertindole_July_09	System Name	LL_AD_LC_SYS011
Result Id	5746	Result Set Id	
		Software:	Empower 2 Software Build 2154

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area ( $\mu\text{V}\cdot\text{sec}$ )	% Area	RT Ratio	USP Resolution	USP Tailing	USP Plate Count
1	Peak1	3.34	6067.41	0.04	0.38		1.34	1214
2	Peak2	6.57	1798.65	0.01	0.74	8.46	1.02	2302
3	Peak3	7.70	1917.25	0.01	0.87	3.24	1.04	15365
4	Peak4	8.17	501604.51	3.45	0.92	1.32	1.19	7448
5	Deschloro imp	8.85	13956027.74	96.11	1.00	1.66	1.65	7064
6	Peak6	11.58	9009.57	0.06	1.31	5.56	0.87	6036
7	Peak7	12.81	4204.26	0.03	1.45	2.93	1.04	20843
8	Peak8	13.87	16011.02	0.11	1.57	3.14	1.15	19867
9	Peak9	14.37	6659.43	0.05	1.62	1.30	1.14	25101
10	Peak10	19.27	3827.95	0.03	2.18	14.28	0.94	76063
11	Peak11	26.64	8441.21	0.06	3.01	19.79	1.32	48031
12	Peak12	27.24	2521.73	0.02	3.08	1.44	1.07	121292

SampleName 0080/AST-imp/2059/003 pre-1

Date Acquired 7/31/2009 2:33:26 AM IST

Signature / Date: *[Signature]* 7/31/09

Page: 1 of 2

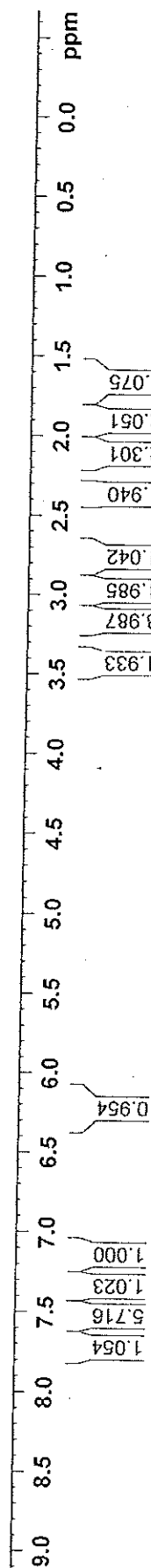
<sup>1</sup>H NMR of 0080/2198/164 in DMSO-d<sub>6</sub>  
 Date:- 06/08/09 ARNO :SE0809/06  
 {C:/LKT/Structure elucidation/Aug-2009/20/1

Des-fluoro 3

7.690  
 7.684  
 7.540  
 7.526  
 7.514  
 7.485  
 7.385  
 7.370  
 7.355  
 7.341  
 7.164  
 7.157  
 7.135  
 7.128

6.210

3.393  
 3.368  
 3.360  
 3.340  
 3.308  
 3.308  
 3.208  
 3.181  
 3.159  
 3.136  
 2.989  
 2.951  
 2.814  
 2.774  
 2.735  
 2.485  
 2.479  
 2.473  
 2.467  
 2.462  
 2.426  
 2.404  
 2.381  
 2.120  
 2.083  
 2.057  
 2.048  
 1.950  
 1.914  
 1.722  
 1.691  
 1.682  
 1.651  
 1.642  
 1.611  
 1.601



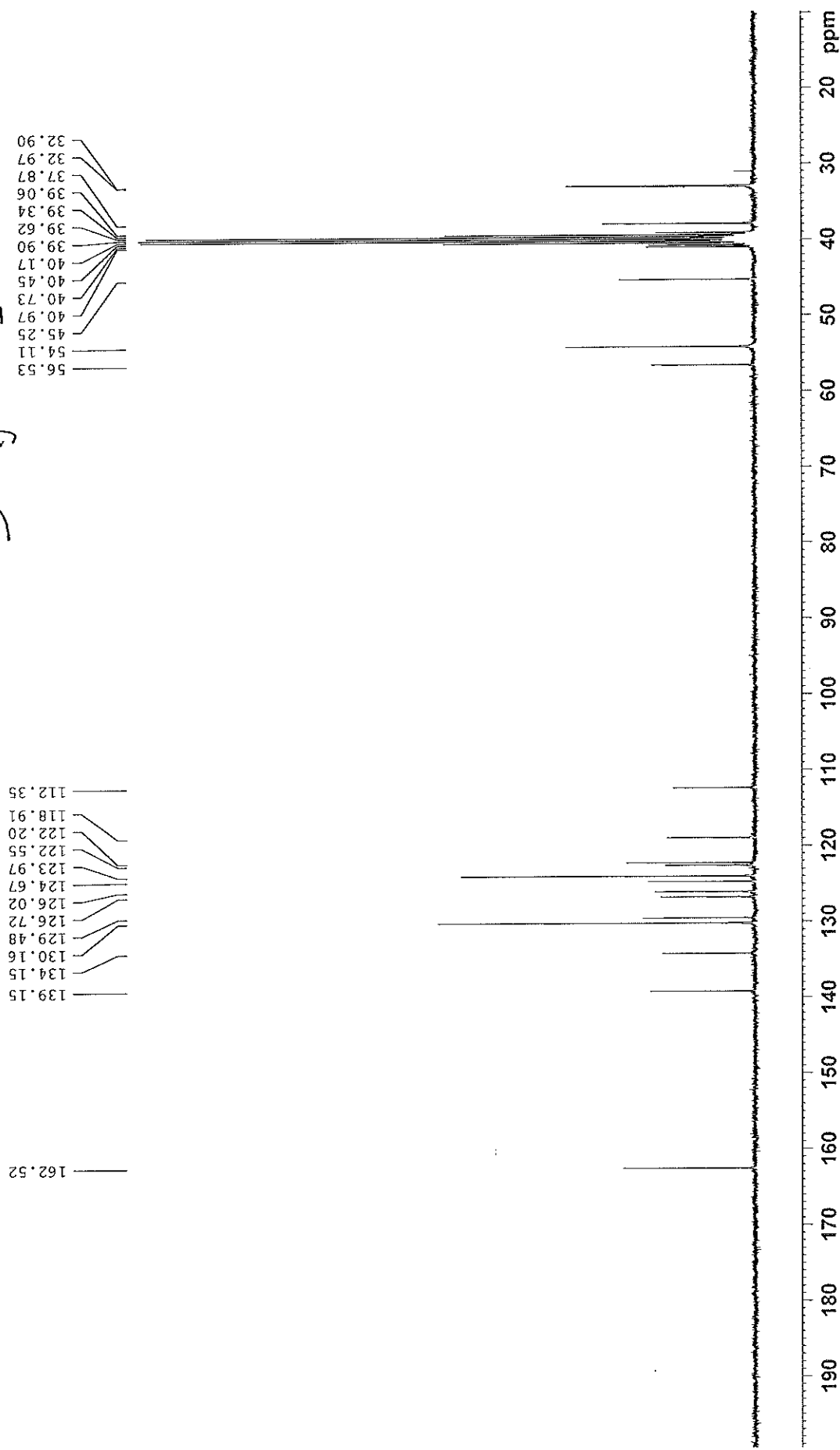
Analyst: Suresh Kumar.K

06/08/09

13C NMR of 0080/A-imp/2198/164 in DMSO-d6  
Date:- 14/09/10  
{D:/LKT/aptit laurus/September-2010/178/1}

aptit laurus

Des-fluoro 3



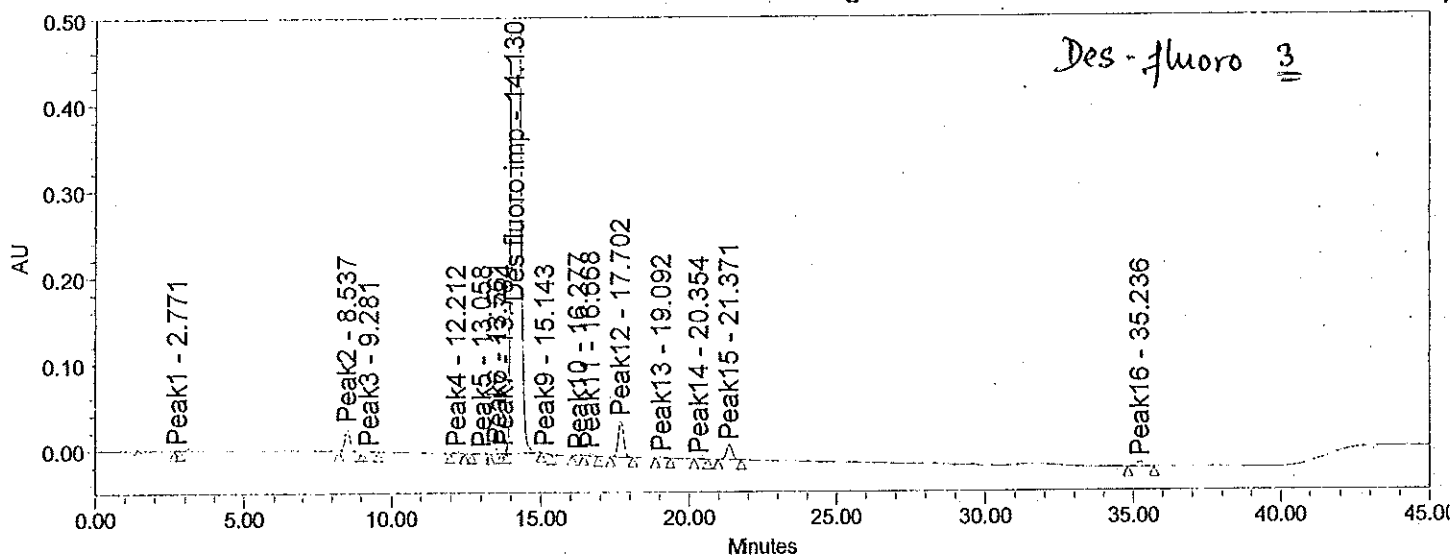
Analyst: Srikanth.M

## SAMPLE INFORMATION

Sample Name: 0080/2198/164(Desfluoro)Pre-1  
Sample Type: Unknown  
Vial: 59  
Injection #: 1  
Injection Volume: 10.00 ul  
Sample Set Id 6733  
Sample Set Name: 040809\_01  
Project Name: Sertindole\_July\_09  
Result Id 7014 Result Set Id

Instrument Method Id 6729  
Acquired By: Analyst  
Date Acquired: 8/5/2009 10:32:10 AM IST  
Date Processed: 8/5/2009 11:55:47 AM IST  
Processing Method: 0080\_Stage123\_RS  
Processing Method Id 6996  
Proc. Chnl. Descr.:  
System Name LL\_AD\_LC\_SYS006  
Software: Empower 2 Software Build 2154

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area ( $\mu\text{V}\cdot\text{sec}$ )	% Area	RT Ratio	USP Resolution	USP Tailing	USP Plate Count
1	Peak1	2.77	9367.56	0.03	0.20		0.97	6270
2	Peak2	8.54	315026.63	1.09	0.60	25.76	1.12	12987
3	Peak3	9.28	8431.83	0.03	0.66	2.26	1.41	11458
4	Peak4	12.21	23863.12	0.08	0.86	8.66	1.12	23397
5	Peak5	13.06	29652.15	0.10	0.92	2.05	0.85	12827
6	Peak6	13.56	61613.31	0.21	0.96	1.22		33573
7	Peak7	13.78	23970.56	0.08	0.98			
8	Des fluoro imp	14.13	27411722.68	94.96	1.00		1.35	22506
9	Peak9	15.14	23009.95	0.08	1.07	3.10	1.45	50407
10	Peak10	16.28	16785.55	0.06	1.15	4.05	0.92	51175
11	Peak11	16.67	41175.82	0.14	1.18	1.19	1.15	33289
12	Peak12	17.70	543571.51	1.88	1.25	2.90	1.10	43760
13	Peak13	19.09	24241.61	0.08	1.35	4.03	1.17	50389
14	Peak14	20.35	4448.94	0.02	1.44	3.61	1.39	53655
15	Peak15	21.37	232405.96	0.81	1.51	2.83	1.09	57013

SampleName 0080/2198/164(Desfluoro)Pre-1

Date Acquired 8/5/2009 10:32:10 AM IST

Signature / Date: *VGO* / 05/08/09

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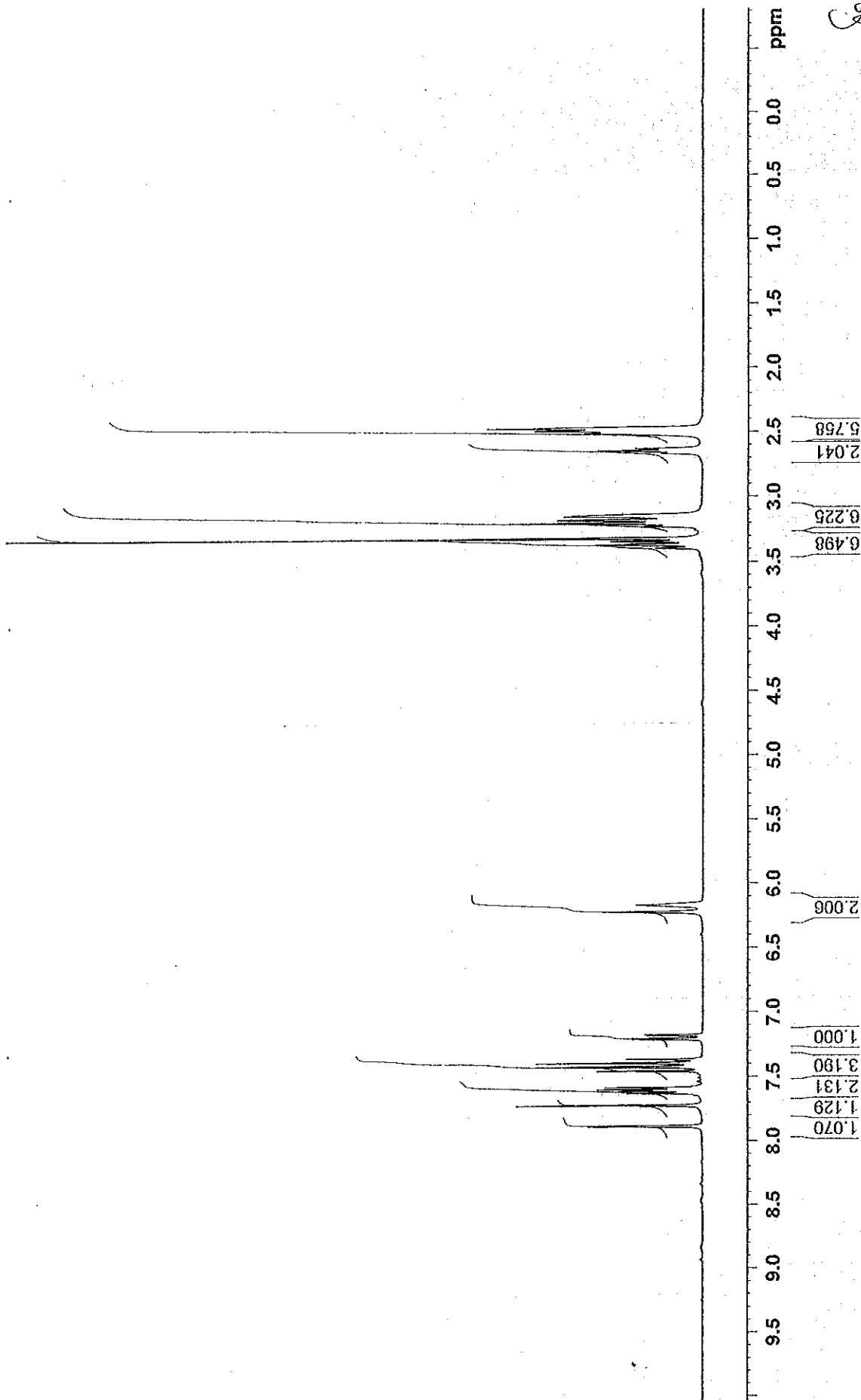
Anhydro S

1H NMR of 0080/1847/031 in DMSO-d6  
 Date: 07/04/09 AR.No: SE0409/01  
 {C:/LKT/apruit Laurus/April 2009/21/1}

7.890  
7.883  
7.723  
7.630  
7.614  
7.600  
7.584  
7.458  
7.428  
7.395  
7.366  
7.214  
7.207  
7.184  
7.178

6.225  
6.170

3.395  
3.371  
3.364  
3.344  
3.321  
3.227  
3.206  
3.181  
3.153  
2.666  
2.648  
2.630  
2.515  
2.494  
2.486  
2.479  
2.473  
2.468



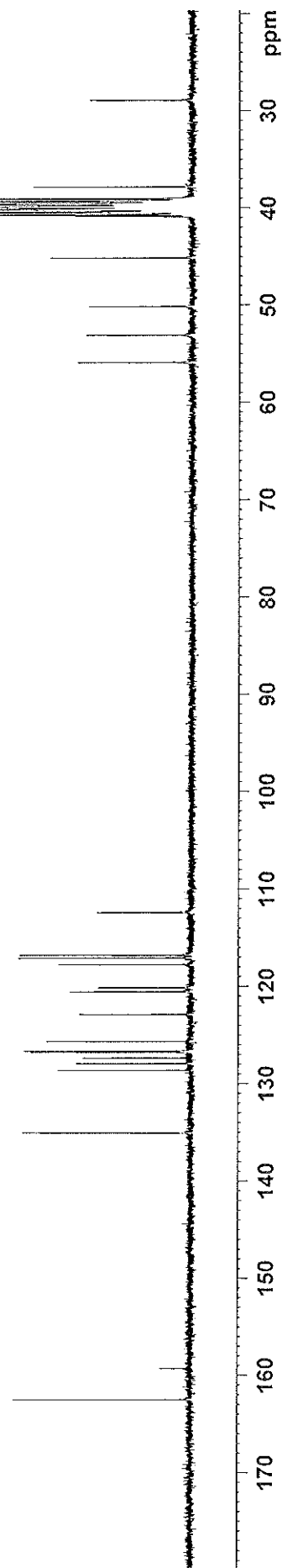
07/04/09

13C NMR of 0080/1847/031 in DMSO-d6  
Date:04/04/09 AR.No:SE0409/01  
{C:/LKT/aptuit Laurus/April 2009/11/1}

aptuit laurus  
Anhydro

162.53  
159.32  
135.11  
135.07  
128.65  
127.96  
127.39  
126.79  
126.68  
125.68  
122.92  
120.58  
120.16  
117.80  
117.12  
116.81  
112.44

55.92  
53.10  
50.14  
45.13  
40.87  
40.70  
40.42  
40.14  
39.86  
39.58  
39.31  
39.03  
37.83  
28.91



Analyst: Lakshmi Kumar.Tatini

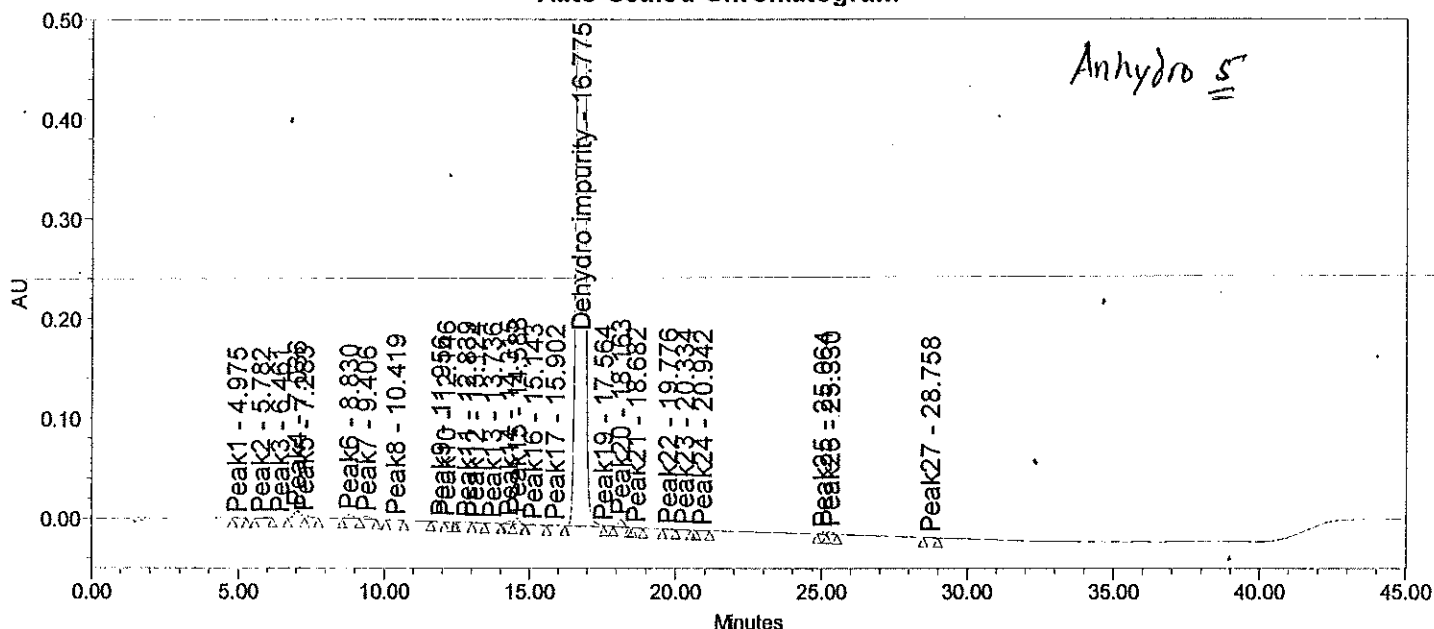
## SAMPLE INFORMATION

Sample Name: 0080/AST-imp/1847/031pre-1  
 Sample Type: Unknown  
 Vial: 56  
 Injection #: 1  
 Injection Volume: 10.00 ul  
 Sample Set Id 5596  
 Sample Set Name: 300709 01  
 Project Name: Sertindole\_July\_09  
 Result Id 5729 Result Set Id

Instrument Method Id 4820

Acquired By: Analyst  
 Date Acquired: 7/31/2009 12:59:11 AM IST  
 Date Processed: 7/31/2009 9:40:50 AM IST  
 Processing Method: 0080\_RS  
 Processing Method Id 5700  
 Proc. Chnl. Descr.: VWD AU On nm  
 System Name LL\_AD\_LC\_SYS011  
 Software: Empower 2 Software Build 2154

## Auto-Scaled Chromatogram



## Peak Results

	Name	RT	Area ( $\mu\text{V}\cdot\text{sec}$ )	% Area	RT Ratio	USP Resolution	USP Tailing	USP Plate Count
1	Peak1	4.97	4235.71	0.01	0.30		1.12	3159
2	Peak2	5.78	4677.11	0.02	0.34	2.14	1.09	2329
3	Peak3	6.46	3155.47	0.01	0.39	1.59	0.85	2132
4	Peak4	7.04	105617.05	0.37	0.42	1.35		4212
5	Peak5	7.28	25931.05	0.09	0.43			
6	Peak6	8.83	60238.89	0.21	0.53		1.18	7101
7	Peak7	9.41	36308.64	0.13	0.56	1.39	1.21	8564
8	Peak8	10.42	12944.27	0.05	0.62	2.16	0.84	7135
9	Peak9	11.96	12461.13	0.04	0.71			
10	Peak10	12.15	9117.20	0.03	0.72			
11	Peak11	12.84	15091.42	0.05	0.77			
12	Peak12	13.12	7469.25	0.03	0.78			

SampleName 0080/AST-imp/1847/031pre-1

Date Acquired 7/31/2009 12:59:11 AM IST

Signature / Date: *Voo*  
21/07/09

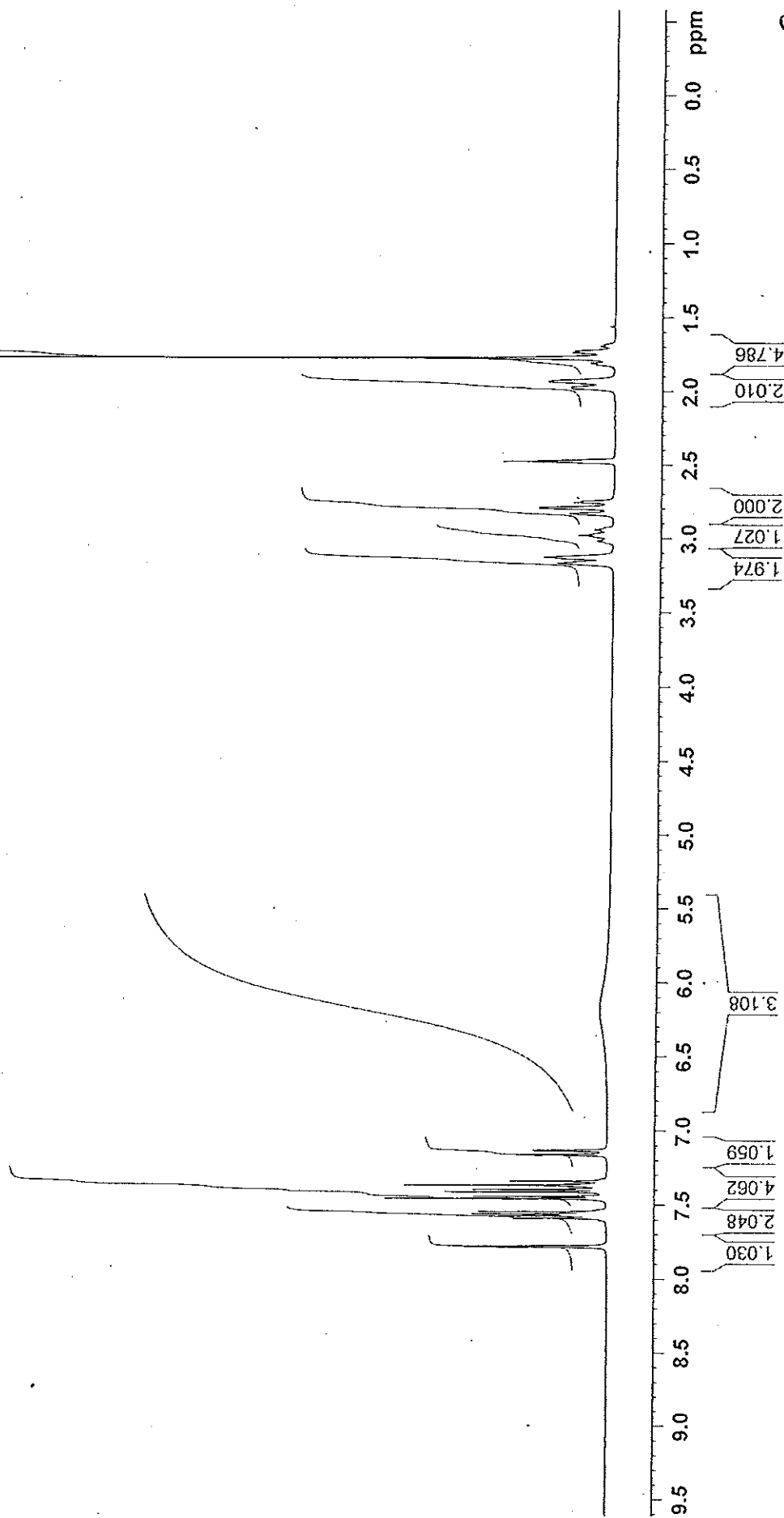
Page: 1 of 2

<sup>1</sup>H NMR of 0080/Ast-2/2198/121 in DMSO-d6  
 Date:- 31/07/09 ARNo : SE0709/024  
 {C:/LKT/Structure elucidation/July2009/59/1

Nor-Sertmole 9

7.783  
 7.777  
 7.591  
 7.575  
 7.568  
 7.561  
 7.545  
 7.458  
 7.442  
 7.413  
 7.397  
 7.368  
 7.338  
 7.166  
 7.159  
 7.136  
 7.130

3.167  
 3.126  
 3.017  
 2.989  
 2.978  
 2.967  
 2.938  
 2.835  
 2.828  
 2.795  
 2.786  
 2.754  
 2.746  
 2.486  
 2.480  
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 1.932  
 1.772  
 1.735  
 1.724



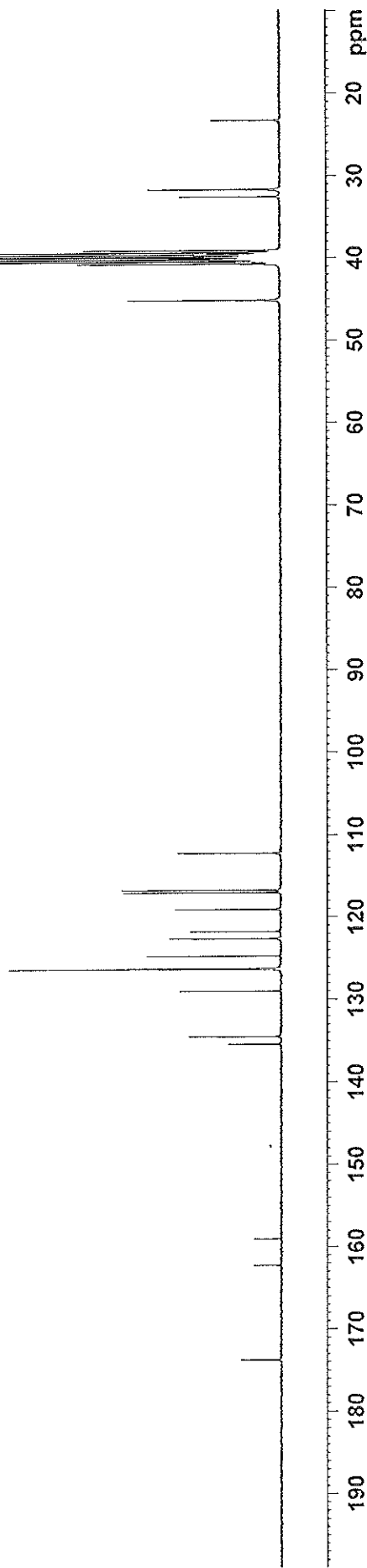
Analyst: Suresh Kumar.K

13C NMR of 0080/Ast-2/2198/121 in DMSO-d6  
Date:- 31/07/09 ARNo :SE0709/024  
{C:/LKT/Structure elucidation/July2009/62/1}

aptut laurus  
Nor-Sentindol g

173.78  
162.30  
159.07  
135.46  
135.43  
134.52  
129.01  
126.37  
126.26  
124.75  
122.66  
121.78  
119.08  
117.05  
116.75  
112.27

45.15  
40.73  
40.46  
40.18  
39.90  
39.62  
39.34  
39.07  
32.54  
31.67  
23.25

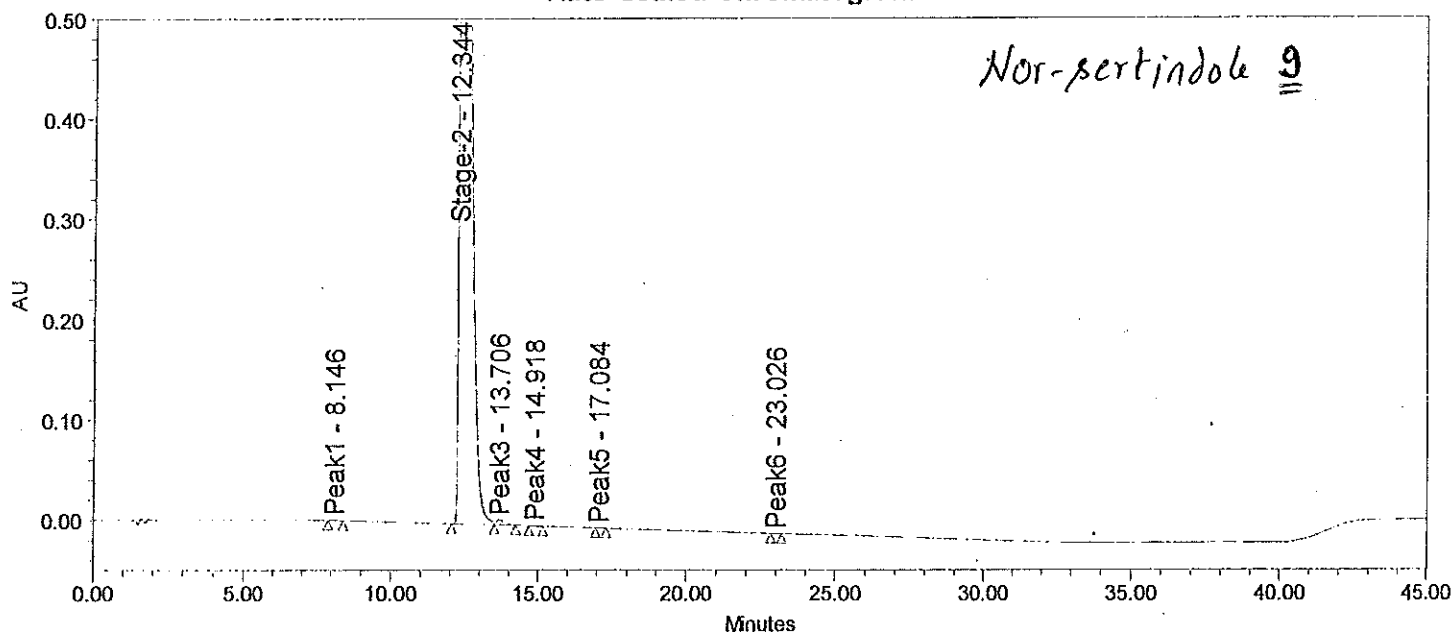


Analyst: Lakshmi Kumar.Tatini

## SAMPLE INFORMATION

Sample Name: 0080/A St-2/2198/121 pre-1 Sample Type: Unknown Vial: 54 Injection #: 1 Injection Volume: 10.00 ul Sample Set Id 5596 Sample Set Name: 300709 01 Project Name: Sertindole_July_09 Result Id 5694      Result Set Id	Instrument Method Id 4820 Acquired By: Analyst Date Acquired: 7/30/2009 11:25:07 PM IST Date Processed: 7/31/2009 9:37:05 AM IST Processing Method: 0080_RS Processing Method Id 5686 Proc. Chnl. Descr.: VWD AU On nm System Name LL_AD_LC_SYS011 Software: Empower 2 Software Build 2154
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### Auto-Scaled Chromatogram



### Peak Results

	Name	RT	Area ( $\mu\text{V}\cdot\text{sec}$ )	%Area	RT Ratio	USP Resolution	USP Tailing	USP Plate Count
1	Peak1	8.15	6350.47	0.02	0.66		1.01	7002
2	Stage-2	12.34	28374700.77	99.61	1.00	8.07	3.15	6914
3	Peak3	13.71	94258.59	0.33	1.11			
4	Peak4	14.92	5302.13	0.02	1.21		1.04	30829
5	Peak5	17.08	2242.89	0.01	1.38	6.89	1.21	184174
6	Peak6	23.03	1774.47	0.01	1.87	19.19	0.86	75973

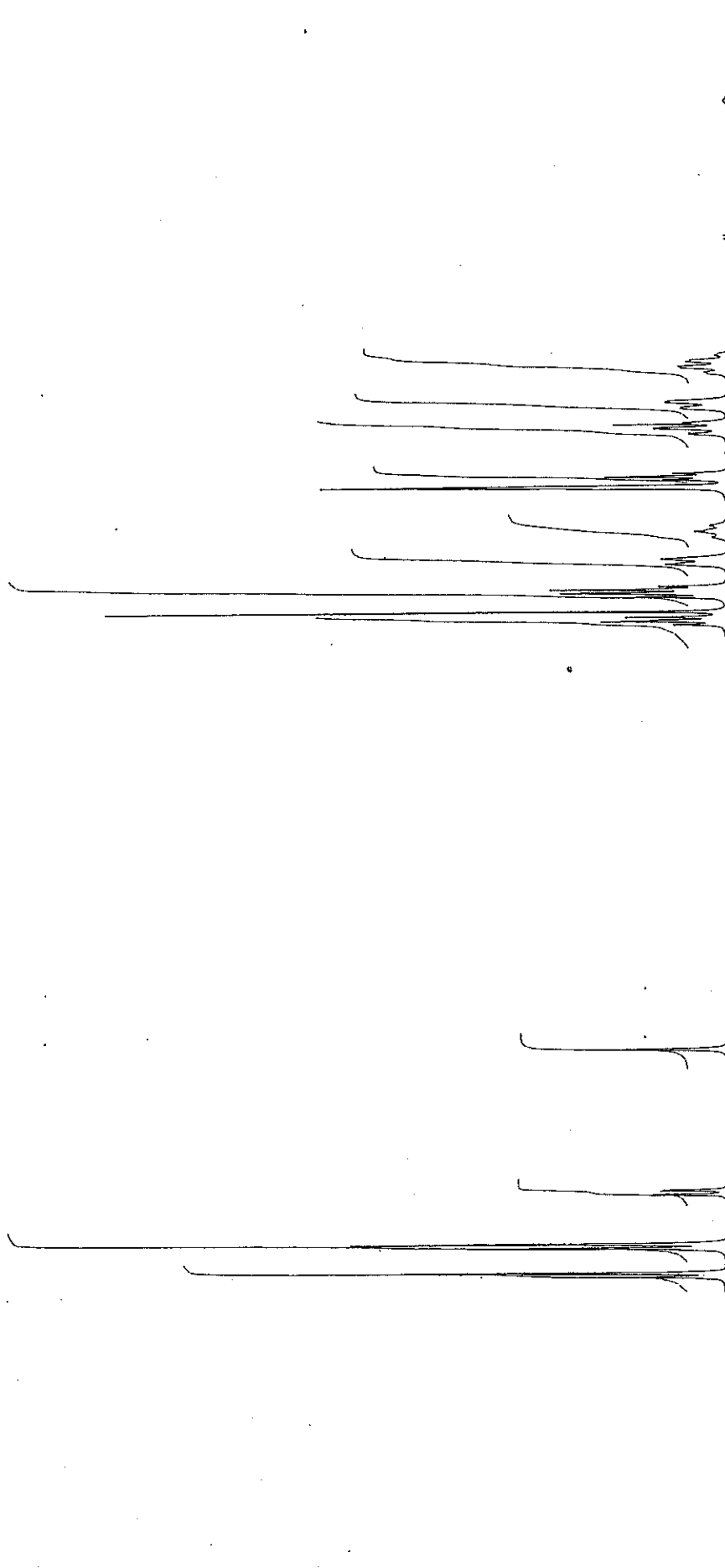
1H NMR of 0080/2246/117 in DMSO-d6  
 Date:- 28/08/09 ARNO :SE0809/033  
 (C:/LKT/Structure elucidation/Aug-2009/72/1

1-(4-Bromophenyl) 21

7.722  
7.716  
7.698  
7.693  
7.543  
7.533  
7.529  
7.503  
7.181  
7.174  
7.152  
7.145

3.393  
3.369  
3.360  
3.341  
3.304  
3.208  
3.181  
3.158  
3.136  
2.989  
2.952  
2.809  
2.770  
2.731  
2.485  
2.480  
2.474  
2.468  
2.462  
2.426  
2.404  
2.382  
2.120  
2.084  
2.057  
2.047  
1.947  
1.907  
1.680  
1.671  
1.640  
1.631

6.209



9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

3.028  
4.076  
1.000  
0.989  
2.232  
4.067  
2.010  
1.067  
1.877  
2.220  
1.987  
1.931

Analyst: Suresh Kumar.K

28/08/09

<sup>13</sup>C NMR of 0080/2246/117 in DMSO-d6  
 Date:- 28/08/09 ARNO : SE0809/033  
 {C:/LKT/Structure elucidation/Aug-2009/75/1}

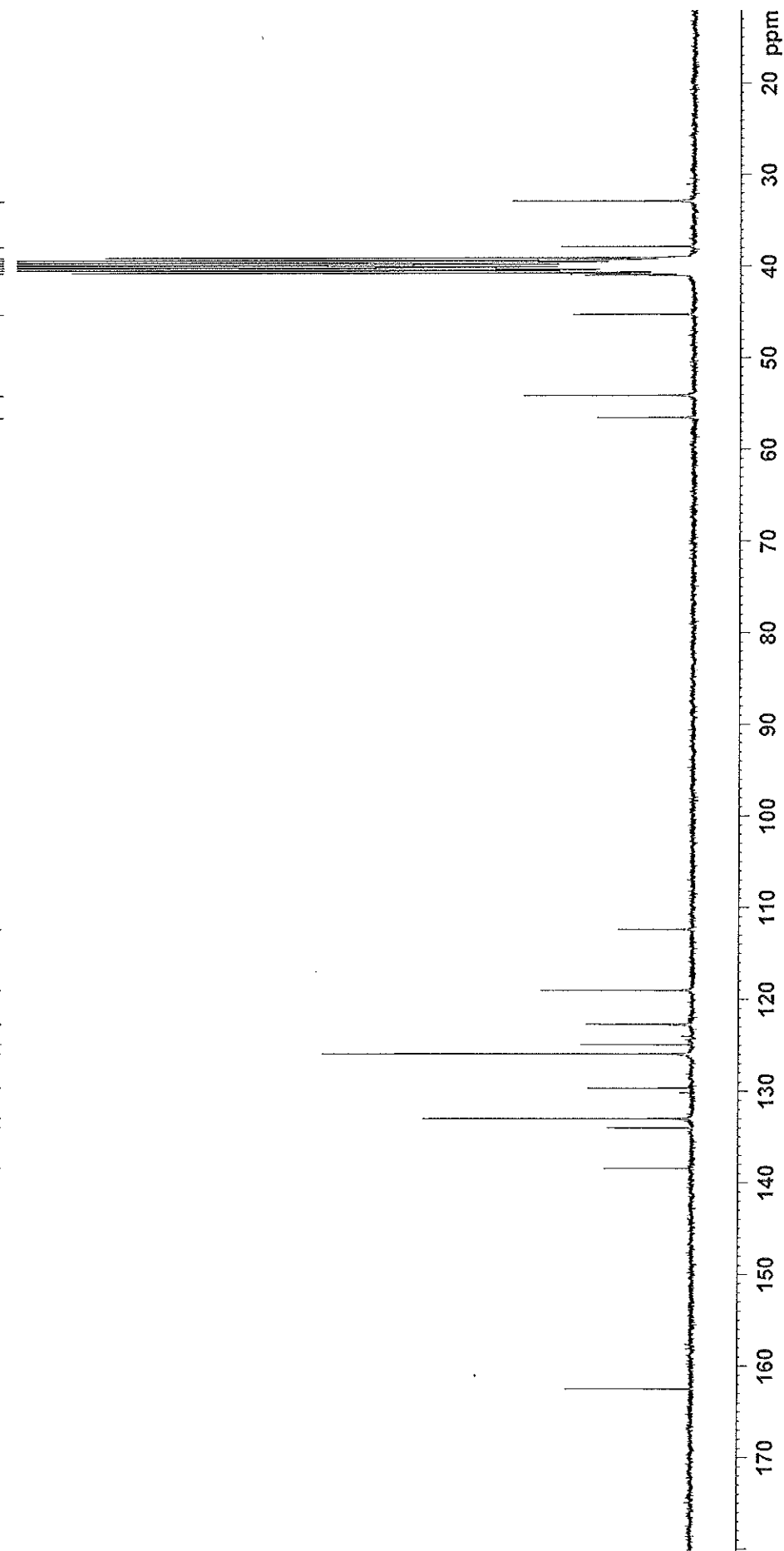
aptut laurus

i-(4-Bromophenyl)

21

162.51  
 138.43  
 134.01  
 133.00  
 129.66  
 125.93  
 124.93  
 122.76  
 122.68  
 119.02  
 112.39

45.25  
 40.75  
 40.47  
 40.19  
 39.91  
 39.63  
 39.36  
 39.08  
 37.86  
 32.90  
 32.86



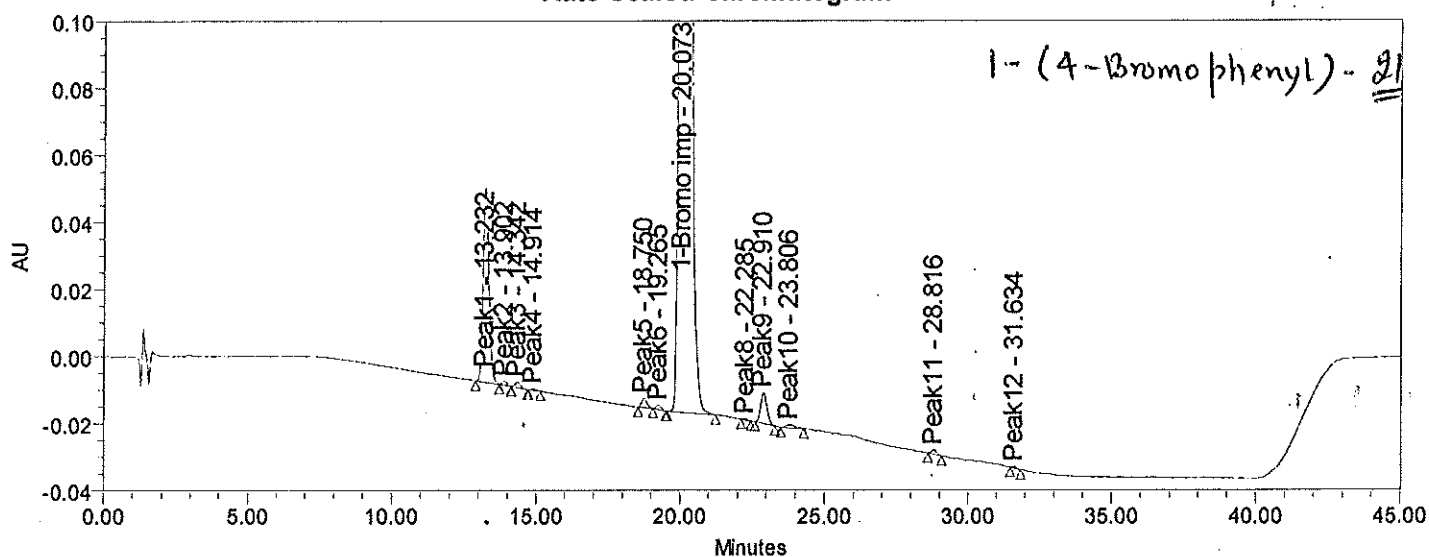
Analyst: Lakshmi Kumar.Tatini



SAMPLE INFORMATION

Sample Name: 0080/2246/117(1-Bromo imp) Pre-1 Instrument Method Id 2893  
Sample Type: Unknown Acquired By: Analyst  
Vial: 25 Date Acquired: 9/8/2009 2:24:33 PM IST  
Injection #: 1 Date Processed: 9/8/2009 5:05:41 PM IST  
Injection Volume: 10.00 ul Processing Method: 0080\_Stage123\_RS  
Sample Set Id 11609 Processing Method Id 11621  
Sample Set Name: 080909\_01 Proc. Chnl. Descr.: VWD AU On nm  
Project Name: Sertindole\_July\_09 System Name LL\_AD\_LC\_SYS012  
Result Id 11635 Result Set Id Software: Empower 2 Software Build 2154

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Area ( $\mu V \cdot sec$ )	% Area	RT Ratio	USP Tailing	USP Plate Count	USP Resolution
1	Peak1	13.23	805021.53	2.83	0.659	1.23	21240	
2	Peak2	13.90	12461.86	0.04	0.693	1.15	34128	1.95
3	Peak3	14.34	20947.52	0.07	0.714	1.45	28039	1.32
4	Peak4	14.91	4943.95	0.02	0.743	1.39	42461	1.77
5	Peak5	18.75	36363.78	0.13	0.934	1.24	44034	11.81
6	Peak6	19.27	14998.50	0.05	0.960	1.23	54606	1.50
7	1-Bromo imp	20.07	27356173.03	96.19	1.000	1.39	32044	2.06
8	Peak8	22.29	3448.03	0.01	1.110	1.00	82094	5.82
9	Peak9	22.91	138750.59	0.49	1.141	1.17	51773	1.74
10	Peak10	23.81	22591.38	0.08	1.186	1.40	26437	1.64
11	Peak11	28.82	17632.31	0.06	1.436	1.10	112881	9.62
12	Peak12	31.63	5890.80	0.02	1.576	1.18	205970	8.69

<sup>1</sup>H NMR of 0080/2198/177 in DMSO-d<sub>6</sub>

Date:- 05/08/09 ARNO : SE0809/05

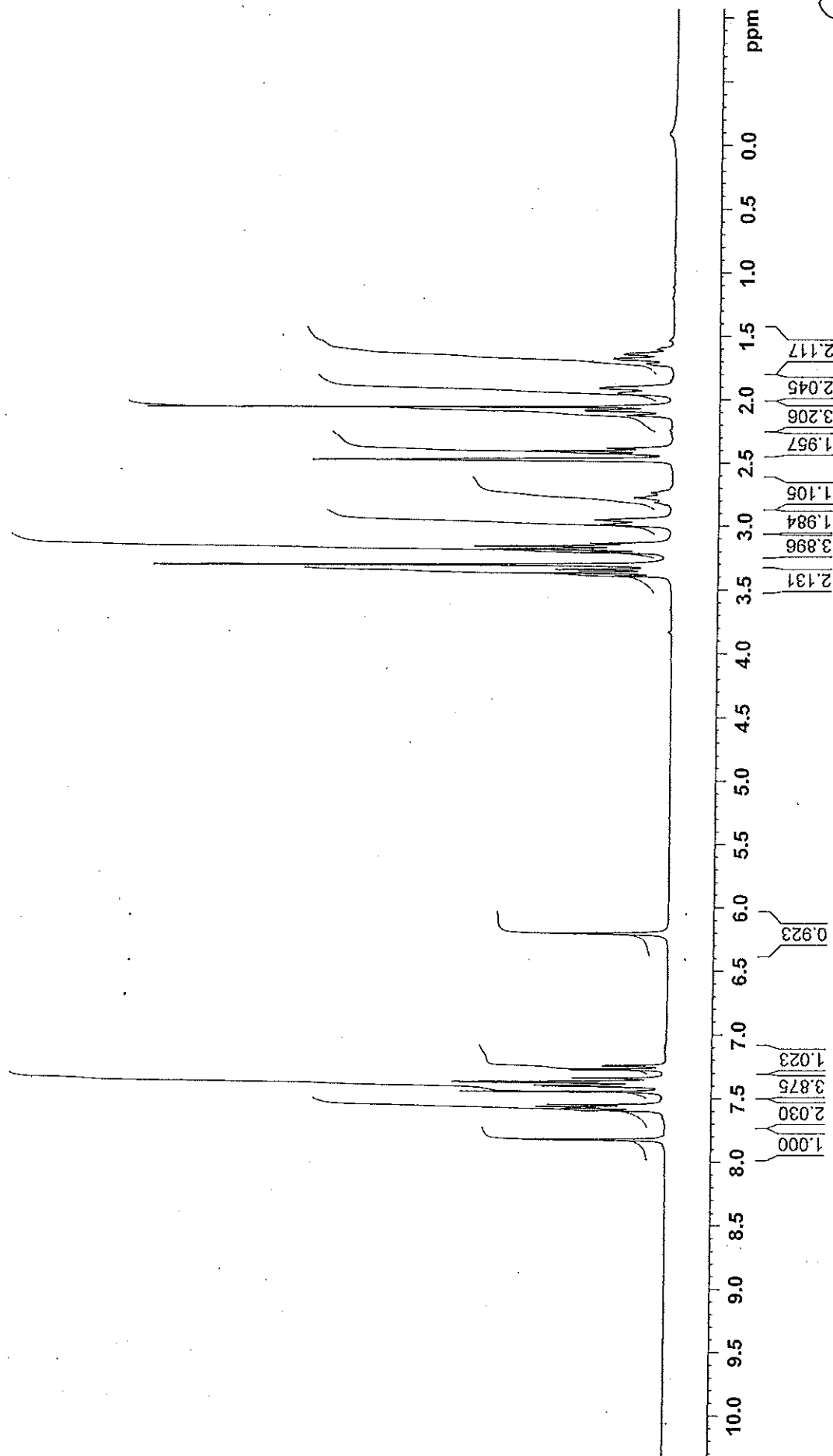
{C:/LKT/Structure elucidation/Aug-2009/16/1

5-Bromo

27

7.828  
7.822  
7.596  
7.580  
7.566  
7.550  
7.447  
7.407  
7.399  
7.377  
7.370  
7.340  
7.276  
7.270  
7.247  
7.240  
6.206

3.394  
3.369  
3.361  
3.341  
3.304  
3.208  
3.180  
3.158  
3.136  
2.988  
2.951  
2.813  
2.774  
2.745  
2.735  
2.479  
2.473  
2.467  
2.426  
2.404  
2.382  
2.121  
2.084  
2.057  
1.945  
1.908  
1.713  
1.682  
1.673  
1.642  
1.633  
1.602



Analyst: Suresh Kumar.K

05/08/09

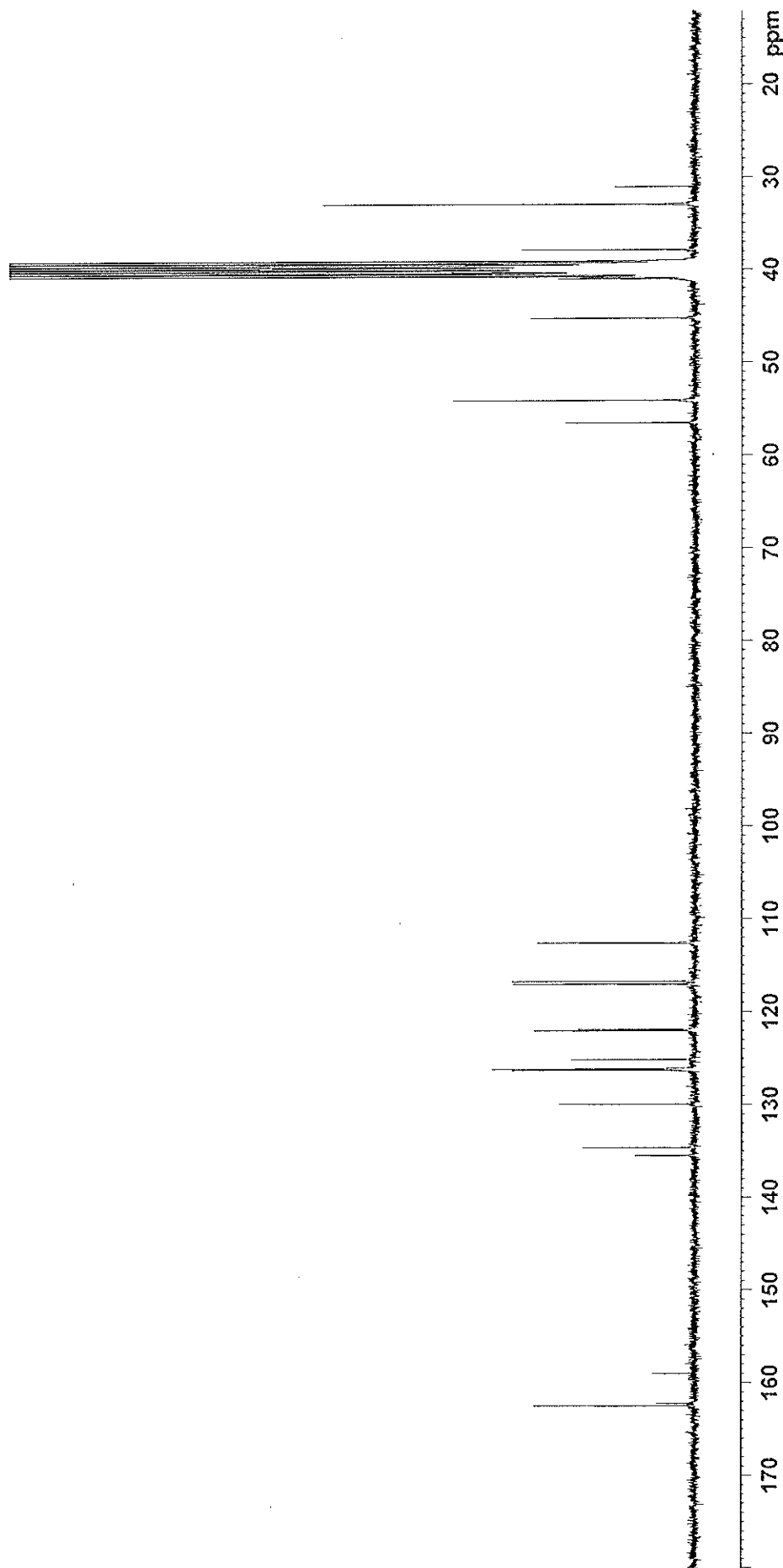
13C NMR of 0080/2198/177 in DMSO-d6  
Date:- 05/08/09 ARNO :SE0809/05  
{C:/LKT/Structure elucidation/Aug-2009/19/1}

5-bromo 27

aptut laurus

162.51  
162.26  
159.04  
  
135.51  
135.48  
134.65  
129.97  
126.32  
126.21  
126.15  
125.15  
122.06  
121.91  
117.05  
116.75  
112.67  
112.60

56.52  
54.10  
  
45.25  
40.98  
40.74  
40.46  
40.19  
39.91  
39.63  
39.35  
39.07  
37.85  
32.92



Analyst: Lakshmi Kumar.Tatini

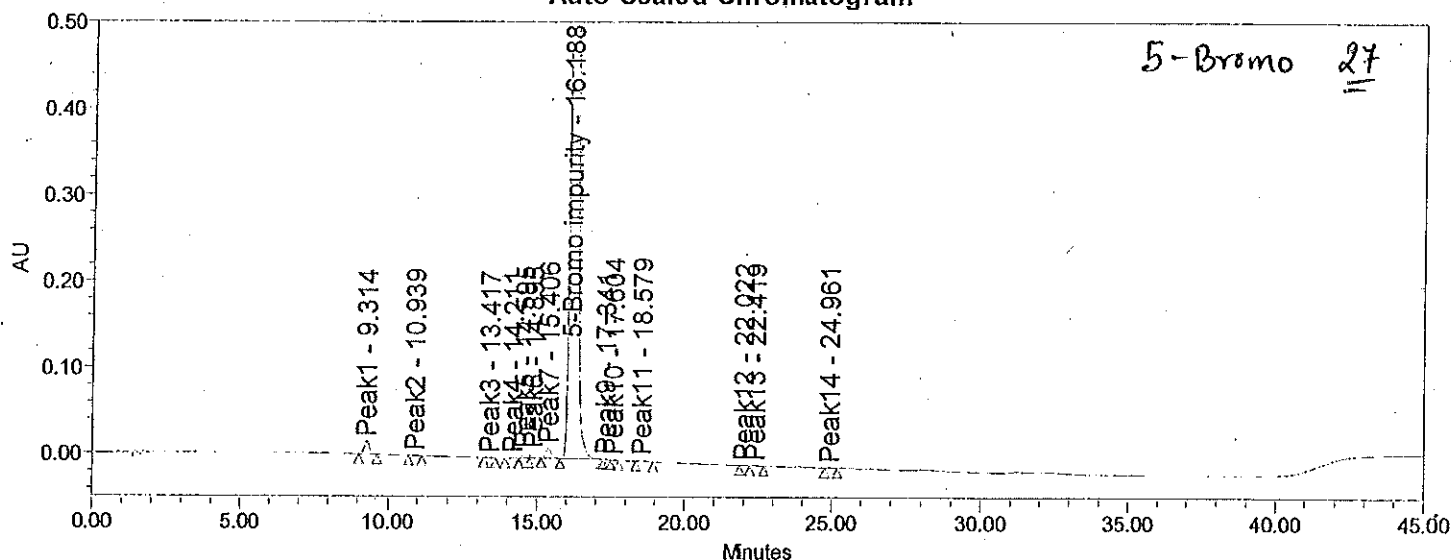
## SAMPLE INFORMATION

Sample Name: 0080/2198/177(5-Bromo)Pre-1  
 Sample Type: Unknown  
 Vial: 57  
 Injection #: 1  
 Injection Volume: 10.00 ul  
 Sample Set Id 6733  
 Sample Set Name: 040809\_01  
 Project Name: Sertindole\_July\_09  
 Result Id 6994 Result Set Id

Instrument Method Id 6729

Acquired By: Analyst  
 Date Acquired: 8/5/2009 9:00:15 AM IST  
 Date Processed: 8/5/2009 11:52:43 AM IST  
 Processing Method: 0080\_Stage123\_RS  
 Processing Method Id 6978  
 Proc. Chnl. Descr.:  
 System Name LL\_AD\_LC\_SYS006  
 Software: Empower 2: Software Build 2154

## Auto-Scaled Chromatogram



## Peak Results

	Name	RT	Area ( $\mu\text{V}\cdot\text{sec}$ )	% Area	RT Ratio	USP Resolution	USP Tailing	USP Plate Count
1	Peak1	9.31	169853.55	0.82	0.58		1.11	15386
2	Peak2	10.94	6288.65	0.03	0.68	5.10	1.36	18075
3	Peak3	13.42	1289.42	0.01	0.83	7.63	0.93	29975
4	Peak4	14.21	9390.67	0.05	0.88	2.58	0.94	37378
5	Peak5	14.60	68669.33	0.33	0.90			25965
6	Peak6	14.89	71981.76	0.35	0.92			19277
7	Peak7	15.41	140468.91	0.68	0.95		1.34	39381
8	5-Bromo impurity	16.19	20124412.85	97.52	1.00	2.29	1.25	32573
9	Peak9	17.34	2364.73	0.01	1.07	4.03	1.26	103152
10	Peak10	17.60	2355.05	0.01	1.09	1.15	1.24	76840
11	Peak11	18.58	25197.58	0.12	1.15	3.09	1.44	40669
12	Peak12	22.02	3613.92	0.02	1.36	10.36	1.18	96388
13	Peak13	22.42	6470.13	0.03	1.38	1.27	1.36	68778
14	Peak14	24.96	3719.33	0.02	1.54	7.97	1.33	114360

SampleName 0080/2198/177(5-Bromo)Pre-1

Date Acquired 8/5/2009 9:00:15 AM IST

Signature / Date: *[Signature]*  
05/03/09

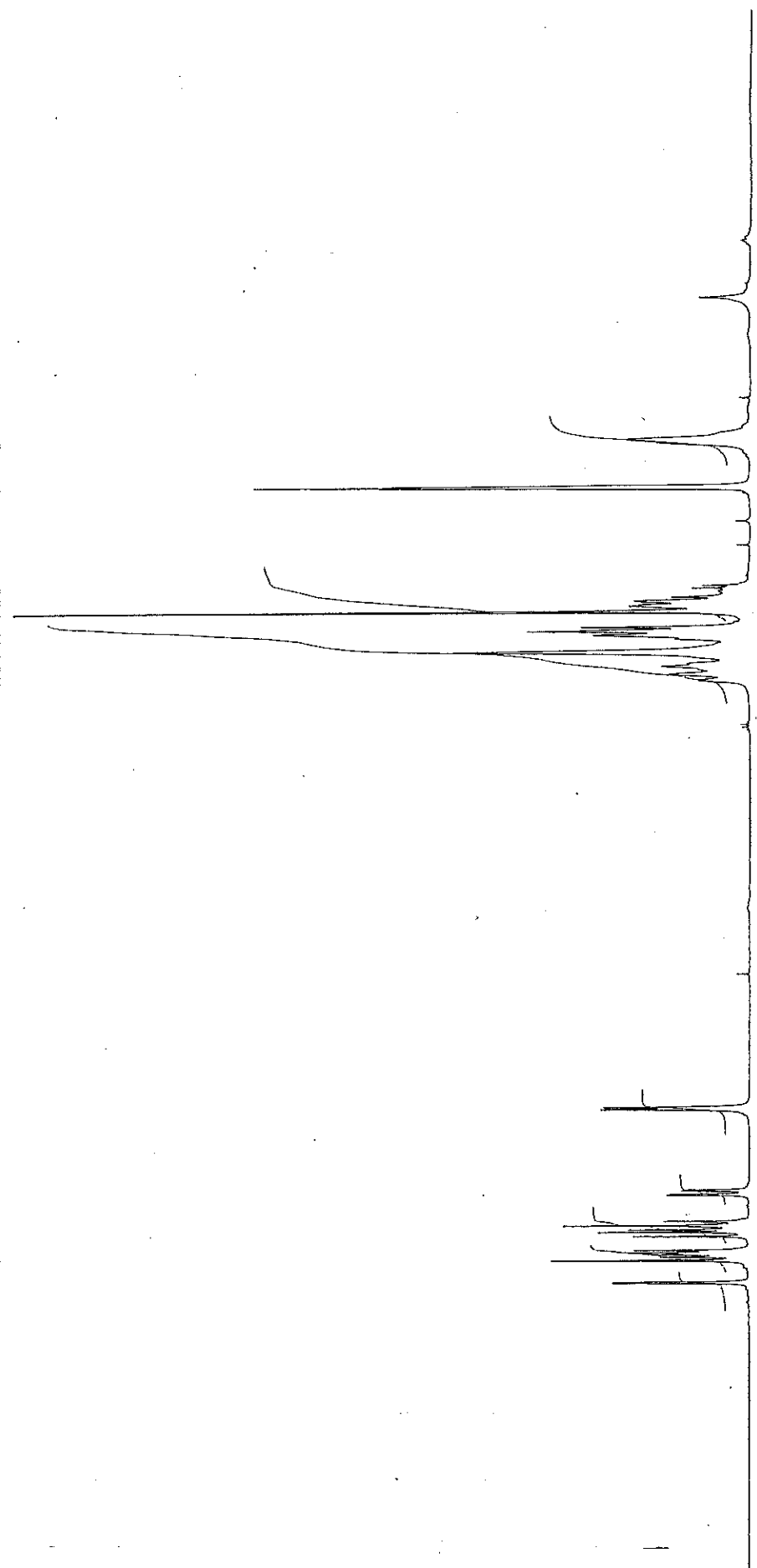
Page: 1 of 1

<sup>1</sup>H NMR of 0080/2154/200 in DMSO-d6  
 Date:- 29/07/09 ARNo : SE0709/022  
 {C:/IKT/Structure elucidation/July2009/54/1

Bis-alkylated 28

7.796  
7.790  
7.645  
7.622  
7.606  
7.599  
7.592  
7.576  
7.485  
7.455  
7.440  
7.411  
7.382  
7.207  
7.201  
7.178  
7.171  
6.633  
6.619

3.764  
3.723  
3.671  
3.650  
3.575  
3.487  
3.461  
3.435  
3.408  
3.307  
3.267  
3.258  
3.231  
3.207  
3.147  
3.130  
2.479  
2.474  
2.468  
2.176  
2.156



9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

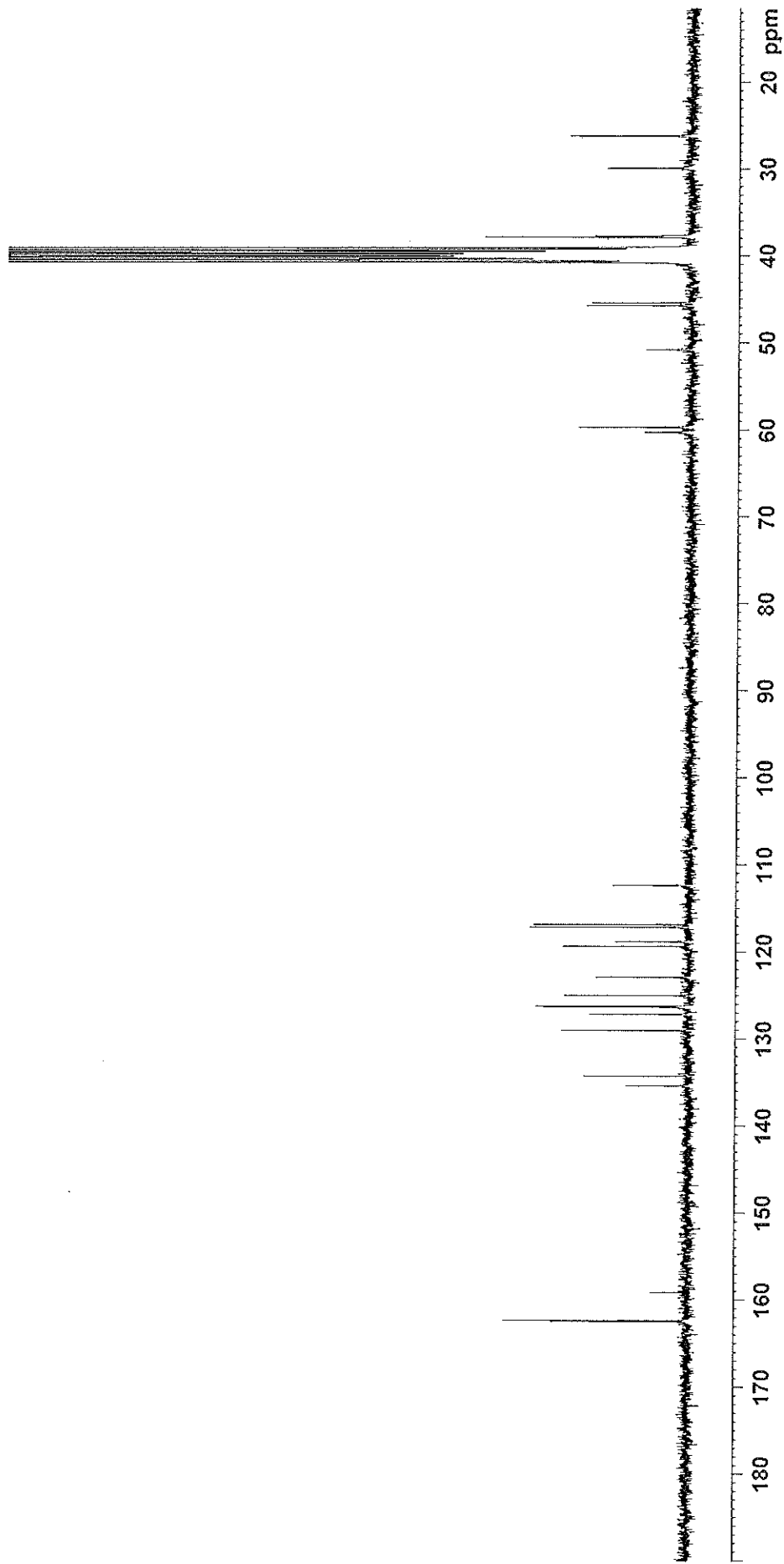
Analyst: Suresh Kumar.K  
 29/07/09

<sup>13</sup>C NMR of 0080/2154/200 in DMSO-d6  
 Date:- 29/07/09 ARNo :SE0709/022  
 {C:/IKT/Structure elucidation/July2009/57/1}

Bis-alkylated 28  
 aptuit laurus

162.51  
 162.38  
 159.16  
 135.42  
 135.39  
 134.30  
 129.04  
 127.19  
 126.36  
 126.25  
 125.03  
 122.91  
 119.38  
 118.84  
 117.18  
 116.88  
 112.38

59.69  
 45.75  
 45.43  
 40.74  
 40.46  
 40.19  
 39.91  
 39.63  
 39.35  
 39.07  
 37.84  
 37.71  
 29.91  
 26.19



Analyst: Lakshmi Kumar.Tatini

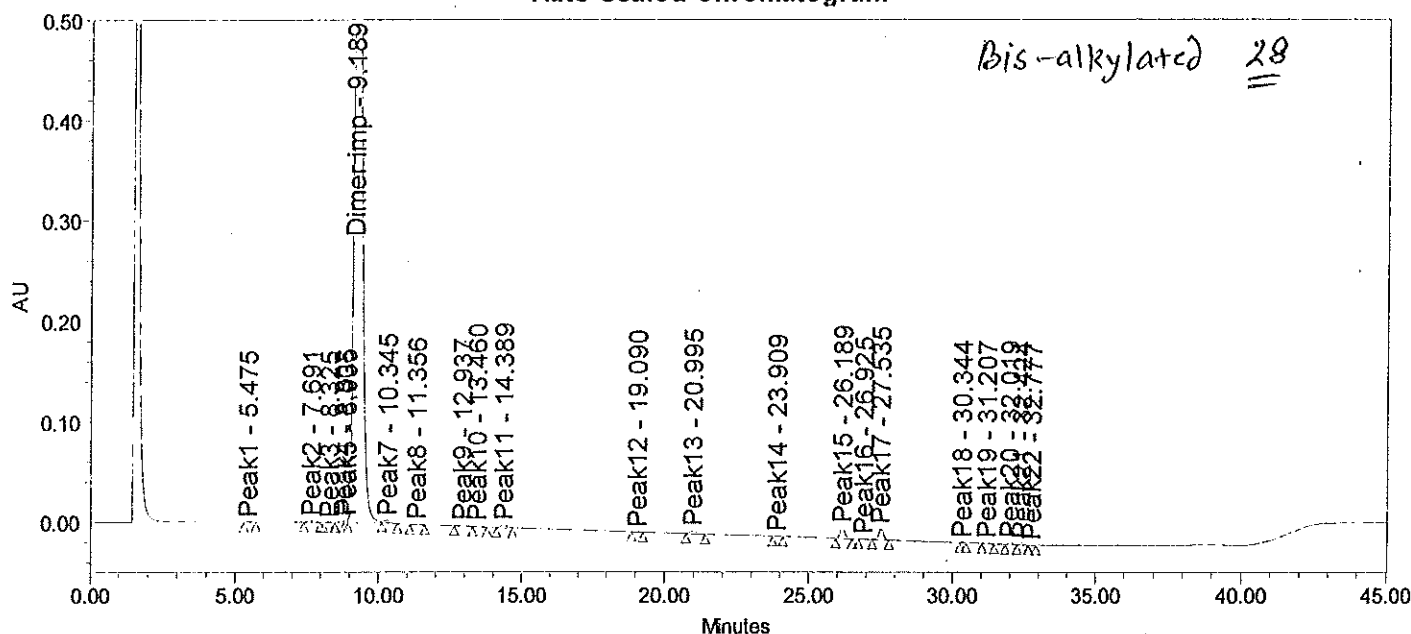
## SAMPLE INFORMATION

Sample Name: 0080/2154/200(dimer) pre-1  
 Sample Type: Unknown  
 Vial: 62  
 Injection #: 1  
 Injection Volume: 10.00 ul  
 Sample Set Id 5596  
 Sample Set Name: 300709 01  
 Project Name: Sertindole\_July\_09  
 Result Id 5791 Result Set Id

Instrument Method Id 4820

Acquired By: Analyst  
 Date Acquired: 7/31/2009 5:41:41 AM IST  
 Date Processed: 7/31/2009 10:00:23 AM IST  
 Processing Method: 0080\_RS  
 Processing Method Id 5767  
 Proc. Chnl. Descr.: VWD AU On nm  
 System Name LL\_AD\_LC\_SYS011  
 Software: Empower 2 Software Build 2154

## Auto-Scaled Chromatogram



## Peak Results

	Name	RT	Area ( $\mu$ V $\cdot$ sec)	% Area	RT Ratio	USP Resolution	USP Tailing	USP Plate Count
1	Peak1	5.47	2896.68	0.02	0.60		1.23	3663
2	Peak2	7.69	14796.54	0.10	0.84	5.94	1.10	7305
3	Peak3	8.33	2672.10	0.02	0.91	1.83	0.84	10900
4	Peak4	8.81	9477.23	0.06	0.96			
5	Peak5	8.94	14247.40	0.10	0.97			
6	Dimer imp	9.19	14262222.61	96.67	1.00		1.90	6663
7	Peak7	10.35	32588.51	0.22	1.13	2.81	1.28	13121
8	Peak8	11.36	7449.18	0.05	1.24	2.80	0.93	13919
9	Peak9	12.94	19684.40	0.13	1.41	3.63	1.19	9482
10	Peak10	13.46	12459.01	0.08	1.46	1.17	1.46	22709
11	Peak11	14.39	33203.96	0.23	1.57	2.55	1.10	29855
12	Peak12	19.09	1939.73	0.01	2.08	13.90	0.84	63712

SampleName 0080/2154/200(dimer) pre-1

Date Acquired 7/31/2009 5:41:41 AM IST

Signature / Date: VGO  
31/07/09

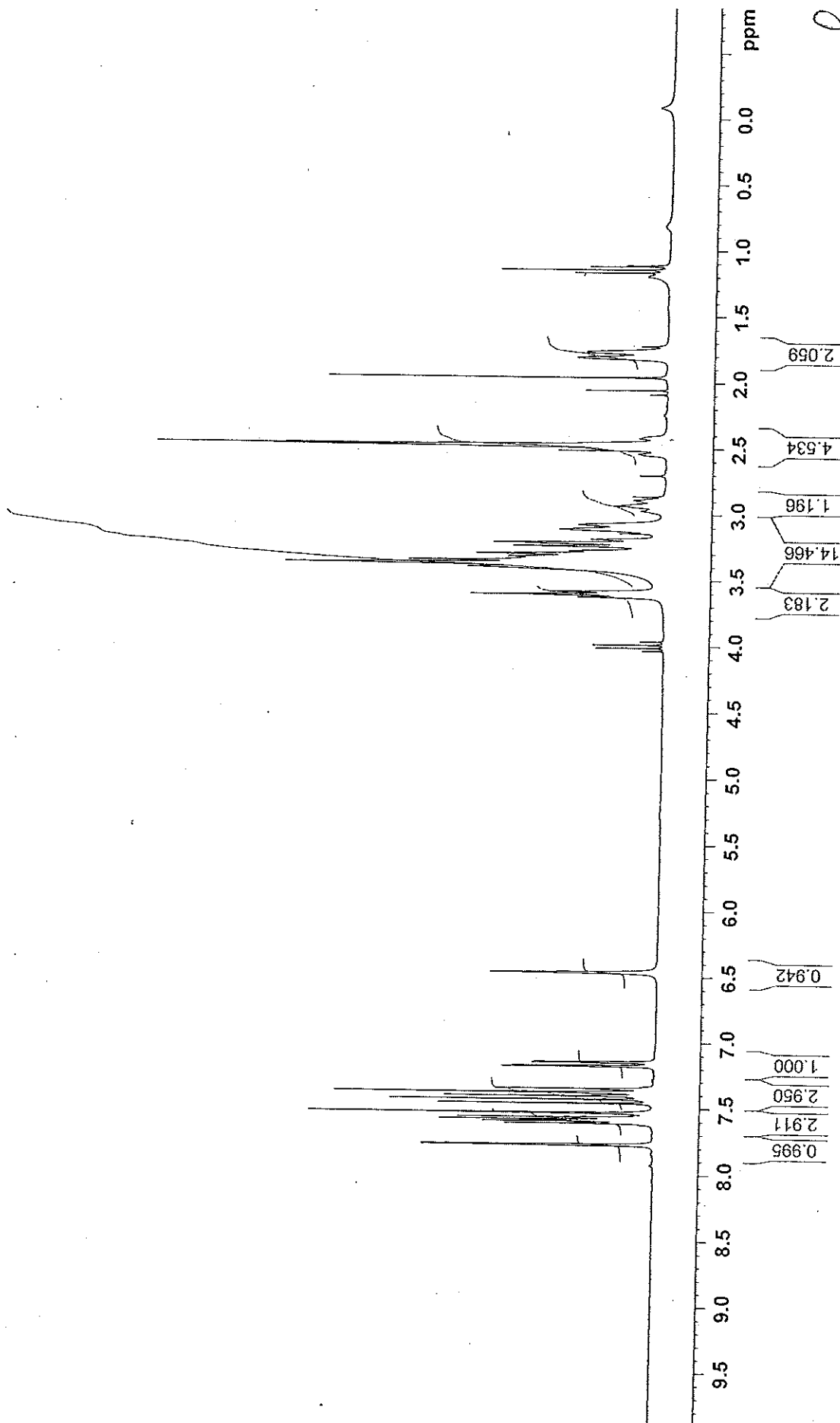
Page: 1 of 2

<sup>1</sup>H NMR of 0080/2198/090 in DMSO-d<sub>6</sub>  
 Date:- 29/07/09 ARNO :SE0709/023  
 {C:/LKT/Structure elucidation/July2009/51/1

N-wide 29

7.773  
 7.766  
 7.609  
 7.593  
 7.586  
 7.579  
 7.563  
 7.529  
 7.458  
 7.428  
 7.404  
 7.375  
 7.346  
 7.179  
 7.173  
 7.150  
 7.143  
 6.462

3.626  
 3.603  
 3.582  
 3.399  
 3.374  
 3.366  
 3.347  
 3.295  
 3.273  
 3.237  
 3.210  
 3.110  
 3.074  
 2.971  
 2.930  
 2.889  
 2.860  
 2.537  
 2.513  
 2.486  
 2.480  
 2.474  
 2.467  
 2.462  
 2.419  
 1.808  
 1.766



Analyst: Suresh Kumar.K



<sup>13</sup>C NMR of 0080/2198/090 in DMSO-d<sub>6</sub>  
 Date:- 30/07/09 ARNo : SE0709/023  
 {C:/LKT/Structure elucidation/July2009/58/1}

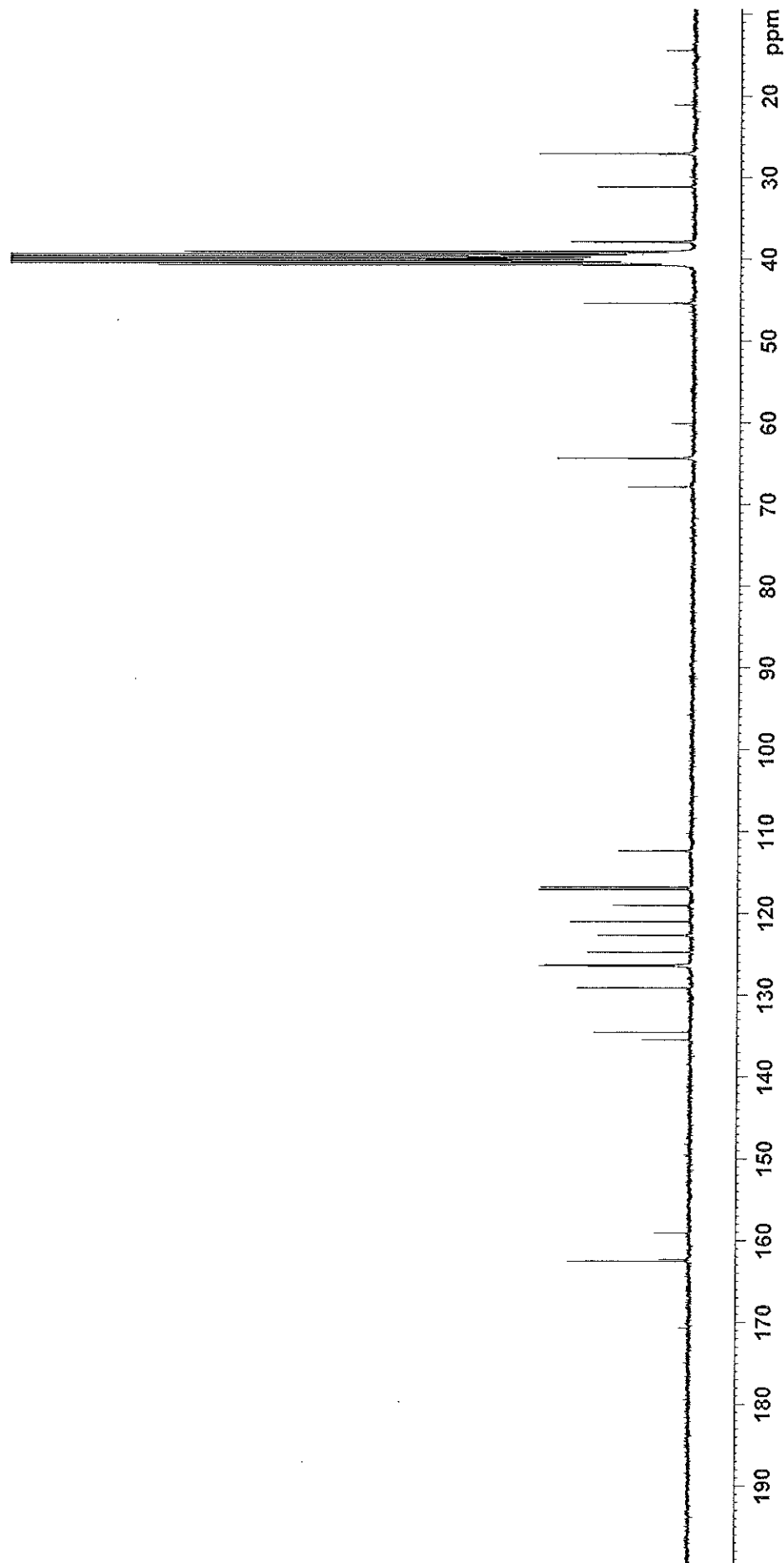
aptul laurus

*N-oxide* 29

159.08  
 162.31  
 162.54  
 135.46  
 135.42  
 134.54  
 129.11  
 126.50  
 126.39  
 126.27  
 124.76  
 122.69  
 121.00  
 119.01  
 117.06  
 116.76  
 112.34

67.86  
 64.34

45.42  
 40.74  
 40.46  
 40.18  
 39.90  
 39.62  
 39.35  
 39.07  
 37.95  
 37.86  
 31.15  
 27.06



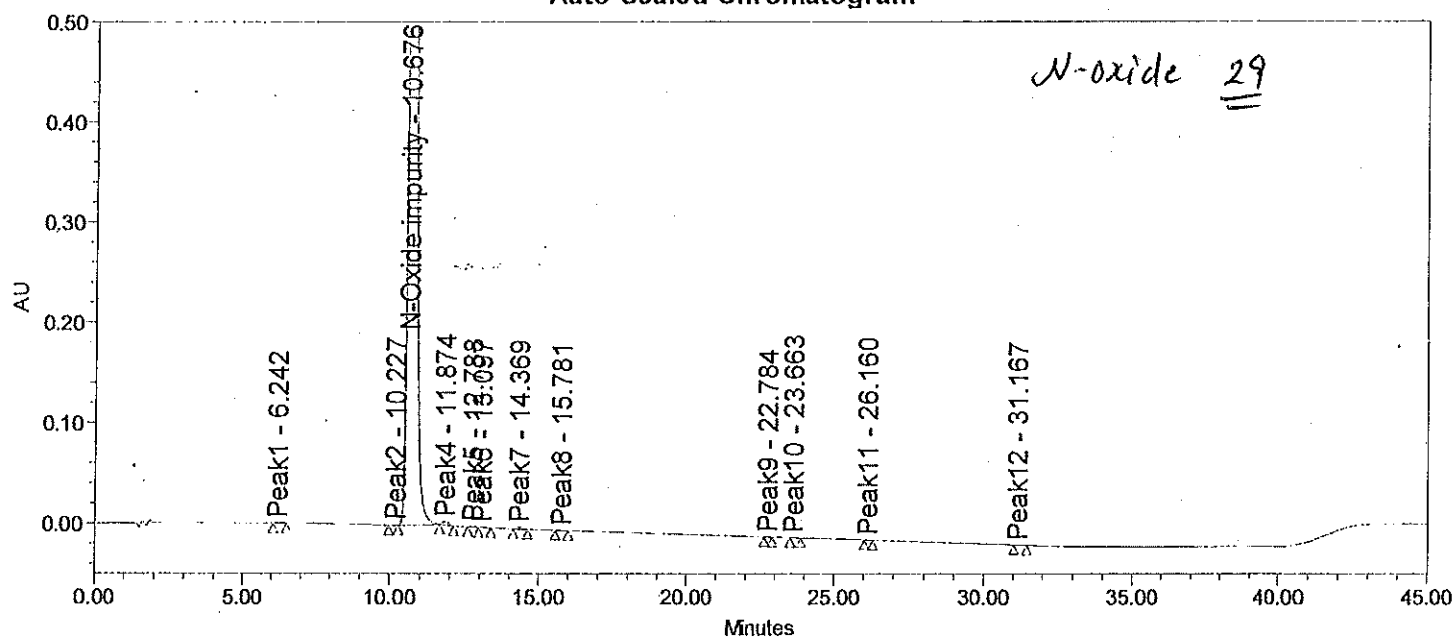
Analyst: Lakshmi Kumar.Tatini

## SAMPLE INFORMATION

Sample Name: 0080/2198/090(N-Oxide)pre-1  
Sample Type: Unknown  
Vial: 60  
Injection #: 1  
Injection Volume: 10.00 ul  
Sample Set Id 5596  
Sample Set Name: 300709 01  
Project Name: Sertindole\_July\_09  
Result Id 5762 Result Set Id

Instrument Method Id 4820  
Acquired By: Analyst  
Date Acquired: 7/31/2009 4:07:35 AM IST  
Date Processed: 7/31/2009 9:53:06 AM IST  
Processing Method: 0080\_RS  
Processing Method Id 5748  
Proc. Chnl. Descr.: VWD AU On nm  
System Name LL\_AD\_LC\_SYS011  
Software: Empower 2 Software Build 2154

## Auto-Scaled Chromatogram



## Peak Results

	Name	RT	Area ( $\mu\text{V}\cdot\text{sec}$ )	% Area	RT Ratio	USP Resolution	USP Tailing	USP Plate Count
1	Peak1	6.24	3592.17	0.02	0.58		1.09	4024
2	Peak2	10.23	5303.52	0.02	0.96			
3	N-Oxide Impurity	10.68	23008159.93	99.51	1.00		1.26	12833
4	Peak4	11.87	44388.07	0.19	1.11	3.24	1.19	18072
5	Peak5	12.79	14219.19	0.06	1.20	2.51		20467
6	Peak6	13.10	8240.95	0.04	1.23			
7	Peak7	14.37	24744.88	0.11	1.35		1.11	27527
8	Peak8	15.78	3249.25	0.01	1.48	4.54	0.98	29353
9	Peak9	22.78	1289.54	0.01	2.13	27.23	0.91	86436
10	Peak10	23.66	3557.38	0.02	2.22	3.38	1.12	170517
11	Peak11	26.16	1693.83	0.01	2.45	8.43	1.06	189542
12	Peak12	31.17	3847.68	0.02	2.92	14.84	1.41	169601

SampleName 0080/2198/090(N-Oxide)pre-1

Date Acquired 7/31/2009 4:07:35 AM IST

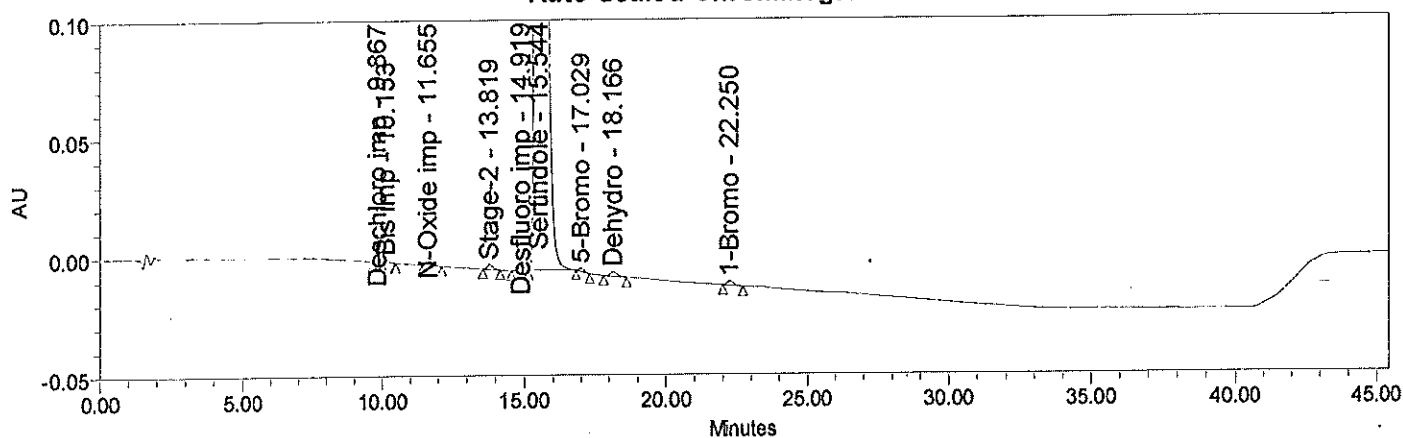
Signature / Date:  3/6 7/09

Page: 1 of 1

## SAMPLE INFORMATION

Sample Name:	0.1%(Solution)Accuracy	Instrument Method Id	12617
Sample Type:	Unknown	Acquired By:	Analyst
Vial:	60	Date Acquired:	9/17/2009 6:13:52 AM IST
Injection #:	1	Date Processed:	9/17/2009 9:36:25 AM IST
Injection Volume:	10.00 ul	Processing Method:	0080_Stage 4_RS
Sample Set Id	12704	Processing Method Id	12819
Sample Set Name:	160909_02	Proc. Chnl. Descr.:	VWD AU On nm
Project Name:	Sertindole_July_09	System Name	LL_AD_LC_SYS011
Result Id	12832	Result Set Id	
		Software:	Empower 2 Software Build 2154

## Auto-Scaled Chromatogram



## Peak Results

	Name	RT	Area ( $\mu\text{V}\cdot\text{sec}$ )	%Area	RT Ratio	USP Resolution	USP Tailing	USP Plate Count	s/n
1	Deschloro imp	9.87	12966.78	0.05	0.63				21.62
2	Bis imp	10.15	14725.13	0.05	0.65				21.67
3	N-Oxide imp	11.66	22585.48	0.08	0.75		1.54	11568	31.81
4	Stage-2	13.82	29223.62	0.11	0.89	5.12	1.26	20203	46.26
5	Desfluoro imp	14.92	32837.84	0.12	0.96	2.50	0.84	16831	45.99
6	Sertindole	15.54	26807667.48	99.30		1.31	1.40	17973	34756.09
7	5-Bromo	17.03	19482.56	0.07	1.10	3.48	1.31	32746	32.30
8	Dehydro	18.17	30939.38	0.11	1.17	2.71	1.41	27197	42.44
9	1-Bromo	22.25	27398.08	0.10	1.43	9.17	1.39	44192	39.70

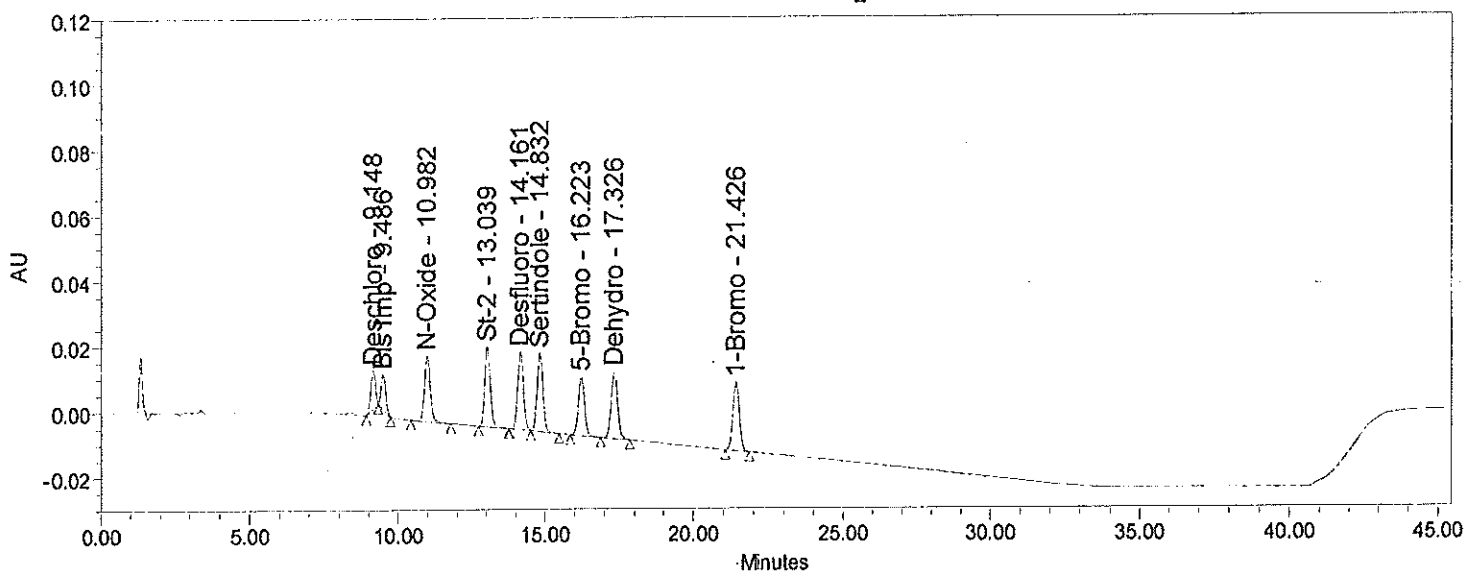
Base line noise : 0.044

## SAMPLE INFORMATION

Sample Name: 0080 sst solution  
Sample Type: Unknown  
Vial: 14  
Injection #: 1  
Injection Volume: 10.00 ul  
Sample Set Id 2253  
Sample Set Name: 241009\_01  
Project Name: Sertindole\_OCT\_09  
Result Id 2330 Result Set Id

Instrument Method Id 1302  
Acquired By: Analyst  
Date Acquired: 10/24/2009 1:37:43 PM IST  
Date Processed: 10/25/2009 9:03:50 AM IST  
Processing Method: 0080\_Stage4\_RS  
Processing Method Id 2319  
Proc. Chnl. Descr.: VWD AU On nm  
System Name LL\_AD\_LC\_SYS012  
Software: Empower 2 Software Build 2154

## Auto-Scaled Chromatogram



## Peak Results

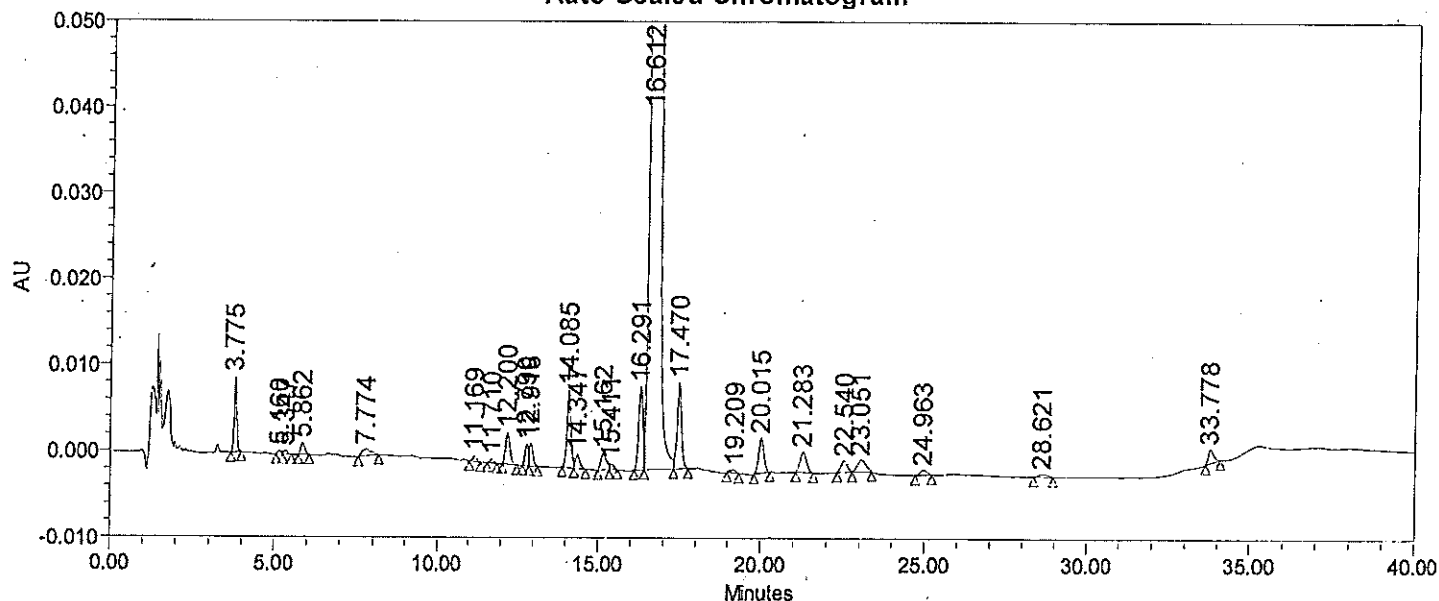
	Name	RT	Area ( $\mu\text{V}\cdot\text{sec}$ )	% Area	RT Ratio
1	Deschloro	9.15	126531.33	5.32	0.62
2	Bis Imp	9.49	118654.03	4.99	0.64
3	N-Oxide	10.98	279757.64	11.77	0.74
4	St-2	13.04	324819.57	13.66	0.88
5	Desfluoro	14.16	327803.19	13.79	0.95
6	Sertindole	14.83	329496.88	13.86	1.00
7	5-Bromo	16.22	255223.59	10.73	1.09
8	Dehydro	17.33	304297.36	12.80	1.17
9	1-Bromo	21.43	310908.94	13.08	1.44

# SAMPLE INFORMATION

Sample Name: 0080/st 4/1974/130  
Sample Type: Unknown  
Vial: 34  
Injection #: 1  
Injection Volume: 20.00 ul  
Sample Set Id 6145  
Sample Set Name: 120509\_01  
Project Name: Sertindole\_FD\_April\_09  
Result Id 6345 Result Set Id

Instrument Method Id 5847  
Acquired By: Analyst  
Date Acquired: 5/12/2009 3:07:37 PM IST  
Date Processed: 5/13/2009 10:49:32 AM IST  
Processing Method: 0080\_Stage4\_RS  
Processing Method Id 6318  
Proc. Chnl. Descr.: VWD AU On nm  
System Name LL\_AD\_LC\_SYS012  
Software: Empower 2 Software Build 2154

## Auto-Scaled Chromatogram



## Peak Results

	Name	RT	Area	% Area	RT Ratio	USP Resolution	USP Tailing	USP Plate Count
1	Peak1	3.77	51020	0.20	0.227		1.15	9954
	Peak2	5.16	2835	0.01	0.311			
3	Peak3	5.35	3486	0.01	0.322			5138
4	Peak4	5.86	11636	0.04	0.353		1.11	9400
5	Peak5	7.77	14786	0.06	0.468	4.48	1.25	5562
6	Peak6	11.17	5532	0.02	0.672	8.05	0.98	51195
7	Peak7	11.71	3589	0.01	0.705	2.31	1.02	60372
8	Peak8	12.20	34378	0.13	0.734	2.02	1.25	37223
9	Peak9	12.79	18673	0.07	0.770			
10	Peak10	12.92	20651	0.08	0.778			
11	Peak11	14.09	77792	0.30	0.848			62500
12	Peak12	14.35	15043	0.06	0.864	0.90		47349
13	Peak13	15.16	24259	0.09	0.913	2.27		31865
14	Peak14	15.41	5877	0.02	0.928			
15	Peak15	16.29	81829	0.32	0.981			70687

SampleName 0080/st 4/1974/130

Date Acquired 5/12/2009 3:07:37 PM IST

Signature / Date: *[Signature]*  
13/05/09  
Page: 1 of 2

# Peak Results

	Name	RT	Area	% Area	RT Ratio	USP Resolution	USP Tailing	USP Plate Count
16	Stage-4	16.61	25307712	97.59	1.000	1.30	1.13	80645
17	Peak17	17.47	97279	0.38	1.052	3.47		77537
18	Peak18	19.21	4581	0.02	1.156	5.96	0.75	65531
19	Peak19	20.02	45778	0.18	1.205	2.56	1.03	70197
20	Peak20	21.28	32395	0.12	1.281	3.73	1.12	53336
21	Peak21	22.54	17330	0.07	1.357	3.35	0.98	59651
22	Peak22	23.05	24793	0.10	1.388	1.17	1.08	34474
23	Peak23	24.96	8064	0.03	1.503	4.28	1.00	49134
24	Peak24	28.62	5340	0.02	1.723	8.17	1.11	44386
25	Peak25	33.78	18313	0.07	2.033	12.45	1.32	171446

LC-MS of Sertindole

LCMS\_Nov\_10\_039 168 (7.866) Cm (168:169-(146:159+179:194))

1: Scan ES+  
3.00e6

407

Des-chloro 2

%

0 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 m/z

LC-MS of Sertindole

LCMS\_Nov\_10\_039 165 (7.725) Cm (165-(125:154+175:199))

1: Scan ES+  
7.67e5

Bis-aryl 28

553

100

%

m/z

775

750

725

700

675

650

625

600

575

550

525

500

475

450

425

400

375

350

325



LC-MS of Sertindole

LCMS\_Nov\_10\_039 259 (12.146) Cm (259-(215:248+263:298))

1: Scan ES+  
9.15e6

*N*-oxide 29

457

100

%

0 250 300 350 400 450 500 550 600 650 700 750 800 m/z

LC-MS of Sertindole

LCMS\_Nov\_10\_039 248 (11.629)

1: Scan ES+  
2.60e7

Nor-Sertindole 9

329

%

0 100 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 m/z

LC-MS of Sertindole

LCMS\_Nov\_10\_039 291 (13.651) Cm (291-(270:289+295:304))

1: Scan ES+  
2.63e6

423

Des-fluoro 3

%

m/z

675

650

625

600

575

550

525

500

475

450

425

400

375

350

325

300

275

250

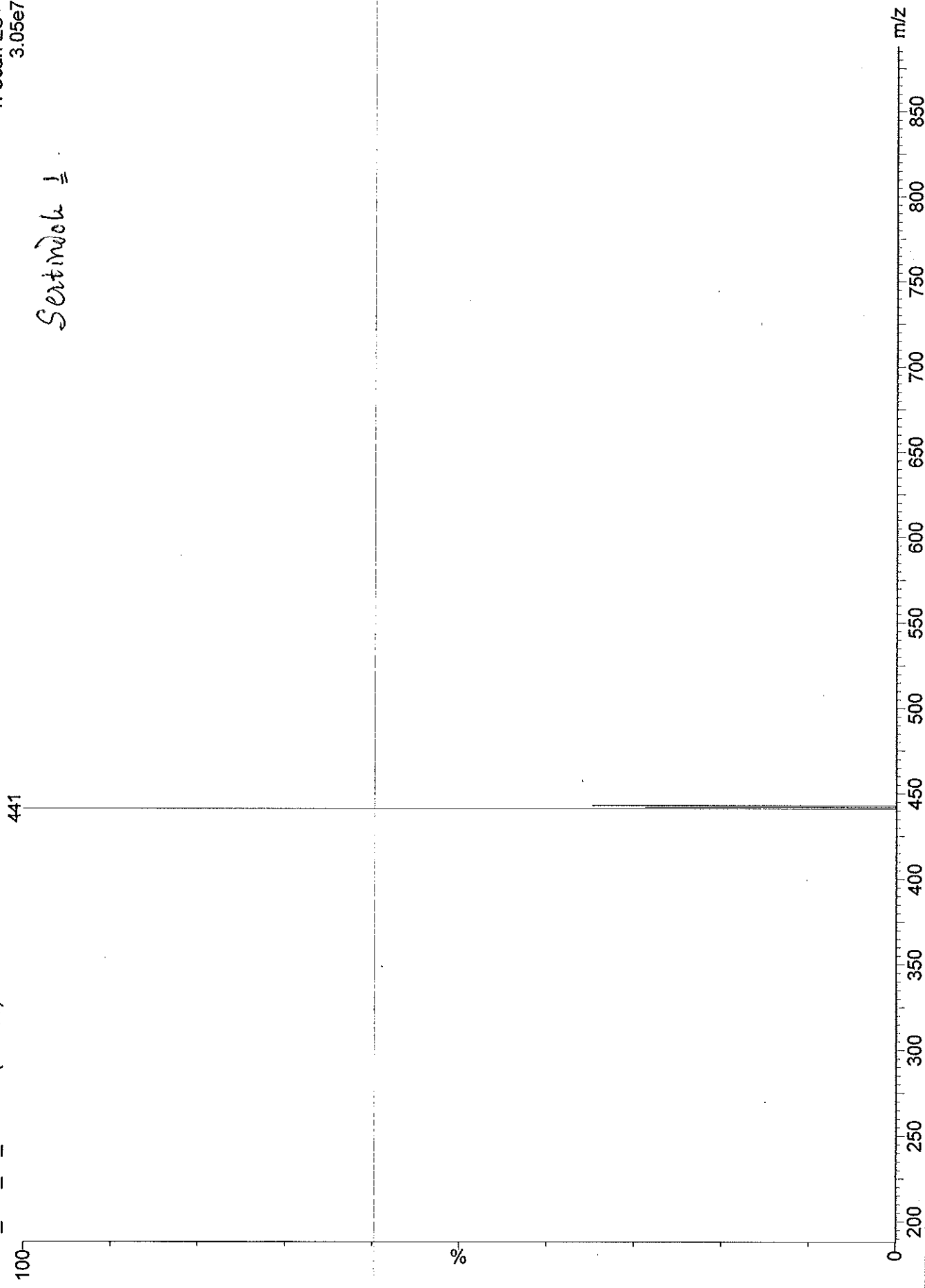
225

200

LC-MS of Serindole  
LCMS\_Nov\_10\_039 309 (14.498)

1: Scan ES+  
3.05e7

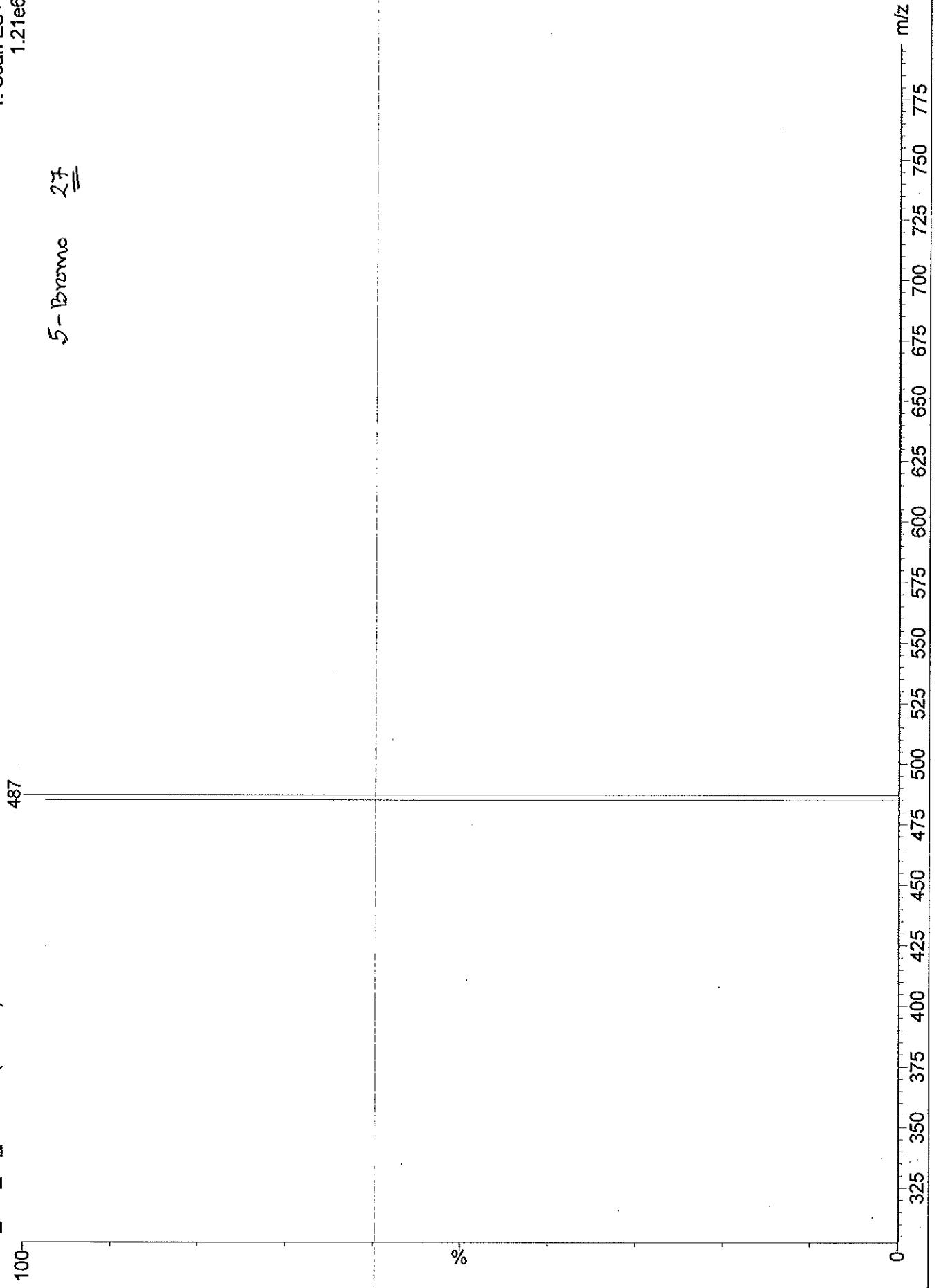
Serindole !



LC-MS of Sertindole

LCMS\_Nov\_10\_039 355 (16.662)

1: Scan ES+  
1.21e6



5-Bromo 27

LC-MS of Sertindole

LCMS\_Nov\_10\_039 401 (18.825)

1: Scan ES+  
6.61e6

Anhydro 5

439

%

m/z

260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680

LC-MS of Sertindole  
LCMS\_Nov\_10\_039 528 (24.798)

1: Scan ES+  
7.04e5

1- (4-Bromo phenyl) 21

