

# Pd-catalyzed site selective C-H acetoxylation of aryl/ heteroaryl/ thiophenyl tethered dihydroquinolinones.

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## Supporting Information

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Table of Contents	Pages
1. General experimental method. -----	: S2-S3
2. Synthesis and experimental data of <b>3a-m</b> , <b>4a-m</b> , <b>5a-m</b>	: S4-S7
4. X-ray Crystallography and References	: S8-S8
5. <sup>1</sup> H NMR, <sup>13</sup> C NMR and HRMS spectra of all new substrates	: S9-S59
6. <sup>1</sup> H NMR, <sup>13</sup> C NMR and HRMS spectra of all the products 6a-m, 7a-m, 8a-m, 10 and 11	: S60—S185
7. 1D NOE spectra of 7j, 7l and 8k	: S186-S189

**General method:** Appropriate names for all the new compounds were given with the help of ChemBioOffice 2012. All reactions were performed under nitrogen. Melting points were measured in open capillary tubes and are uncorrected. IR spectra were recorded as neat liquids or KBr pellets and absorptions are reported in  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (300 MHz, 400 MHz and 500 MHz) and  $^{13}\text{C}$  NMR (75 MHz) spectra were recorded in  $\text{CDCl}_3$  using TMS as internal standard or the solvent signals as secondary standards and the chemical shifts are shown in  $\delta$  scales. High-resolution mass spectra were obtained by using ESI-QTOF and ORBITOF mass spectrometries. All of the yields reported in the experimental data are of isolated and purified products. 3-Dimethylamino-1-(phenyl)prop-2-enone (**1a**), 3-Dimethylamino-1-(4-methyl phenyl)prop-2-enone (**1b**), 3-Dimethylamino-1-(4-methoxyphenyl)prop-2-enone (**1c**), 3-Di methylamino-1-(4-chlorophenyl)prop-2-enone (**1d**), 1-(6-(biphenyl-4-yl)pyridin-3-yl)-3-(dimethylamino)prop-2-enone (**1e**), 3-Dimethyl amino-1-(3-methoxyphenyl)prop-2-enone (**1f**), 3-Dimethylamino-1-(3-chlorophenyl)prop-2-enone (**1g**), 3-Dimethylamino-1-naphthalen-2-yl-propenone (**1h**), 3-(dimethylamino)-1-(6-methoxynaphthalen-2-yl)prop-2-en-1-one(**1i**), 6-(3-Dimethylaminoacryloyl)-4-methyl-4*H*-benzo[1,4]oxazin-3-one (**1j**) 3-Di methylaminothio phen-2-yl-propenone (**1k**), 1-(5-Chlorothiophen-2-yl)-3-dimethyl aminopropenone (**1l**), 1-(5-Bromo thiophen-2-yl)-3-dimethyl aminopropenone (**1m**) were synthesized by previously reported<sup>1</sup> procedures and were fully characterized by spectral analysis.

**General procedure for the preparation of dihydroisoquinolinones (3a-m, 4a-m and 5a-m):**

To a mixture of  $\beta$ - enaminones **2a-m** (1.0 mmol), 1,3-cyclohexanedione (or) 5,5-dimethyl-1,3-cyclohexanedione (or) 4,4-dimethyl-1,3-cyclohexanedione (1.2 mmol), ammonium acetate (2.0 mmol) in 2-propanol (5 mL) were added  $\text{CeCl}_3 \cdot 7\text{H}_2\text{O}$  (0.2 mmol), NaI (0.2 mmol) and refluxed for 4h (monitored by TLC). The reaction mixture was cooled to room temperature; solid precipitate was filtered and washed with ice cold 2-propanol. The combined solvent was evaporated, and crude residue thus obtained was subjected to column chromatography (silica gel; hexane: ethyl acetate, 9:1) to give dihydroisoquinolinones **3a-m**, **4a-m** and **5a-m**. 2-(4-methoxy phenyl)-7,7-dimethyl-7,8-dihydroquinolin-5(6*H*)-one (**4c**), 2-(4-chlorophenyl)-7,7-dimethyl-7,8-dihydroquinolin-5(6*H*)-one (**4d**), 2-(4-chlorophenyl)-6,6-dimethyl-7,8-dihydroquinolin-5(6*H*)-one (**5d**), 2-(naphthalen-2-yl)- 7,7-dimethyl-7,8-dihydroquinolin-5(6*H*)-one (**4h**), 2-(naphthalen-2-yl)-6,6-dimethyl-7,8-dihydro quinolin-5(6*H*)-one (**5h**), 4-methyl-6-(7,7-dimethyl-5-oxo-5,6,7, 8-tetrahydroquinolin-2-yl)-2*H*-benzo[b][1,4]oxazin-3(4*H*)-one (**4j**), 4-methyl-6-(6,6-dimethyl-5-oxo-5,6, 7,8-tetrahydroquinolin-2-yl)-2*H*-benzo[b][1,4]oxazin-3(4*H*)-one (**5j**), 2-thiophen-2-yl-7,8-dihydro-6*H*-quinolin-5-one (**3k**), 7,7-Dimethyl-2-thiophen-2-yl-7,8-dihydro-6*H*-quinolin-5-one (**4k**), 6,6-Dimethyl-2-thio phen-2-yl-7,8-dihydro-6*H*-quinolin-5-one (**5k**), 2-(5-Chloro thio phen-2-yl)-7,8-dihydro-6*H*-quinolin-5-one (**3l**) 2-(5-Chloro thio phen-2-yl)-7,7-dimethyl-7,8-dihydro-6*H*-quinolin-5-one (**4l**), 2-(5-Chloro thiophen-2-yl)-6,6-dimethyl-7,8-dihydro-6*H*-

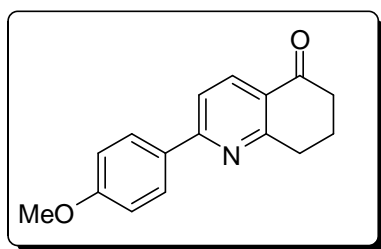
quinolin-5-one (**5l**), 2-(5-Bromothiophen-2-yl)-7,8-dihydro-6H-quinolin-5-one (**3m**), 2-(5-Bromothiophen-2-yl)-7,7-dimethyl-7,8-dihydro-6H-quinolin-5-one (**4m**) 2-(5-Chlorothiophen-2-yl)-6,6-dimethyl-7,8-dihydro-6H-quinolin-5-one (**5m**) were fully characterized by spectral analysis and compared with our previously reported data.<sup>1</sup>

## Experimental data:

### General procedure for the synthesis of dihydroisoquinolinones 3a-m, 4a-m and 5a-m.

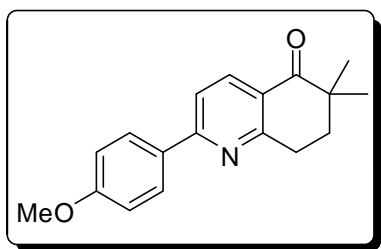
To a mixture of  $\beta$ - enaminones **2a-m** (1.0 mmol), 1,3-cyclohexanedione (or) 5,5-dimethyl-1,3-cyclohexanedione (or) 4,4-dimethyl-1,3-cyclohexanedione (1.2 mmol), ammonium acetate (2.0 mmol) in 2-propanol (5 mL) were added  $\text{CeCl}_3 \cdot 7\text{H}_2\text{O}$  (0.2 mmol), NaI (0.2 mmol) and refluxed for 4 h (monitored by TLC). The reaction mixture was cooled to room temperature; a solid precipitate was filtered and washed with cold 2-propanol. The combined solvent was evaporated, and the crude residue obtained was subjected to column chromatography (silica gel; hexane: ethyl acetate, 9:1) to obtain dihydroisoquinolinones **3a-m**, **4a-m** and **5a-m**.

### **2-(4-methoxyphenyl)-7,8-dihydroquinolin-5(6H)-one (3c)**



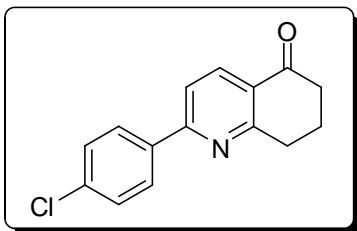
Yield:71%; MP:135 °C.<sup>1</sup>H NMR ( $\text{CDCl}_3$ , 300MHz)  $\delta$  8.28(d, J=8.3Hz, 1H), 8.04(d, J=8.8Hz, 2H), 7.64(d, J=8.3Hz, 1H), 7.01(d, J=8.8Hz, 2H), 3.88(s, 3H), 3.19(t, J=6.2Hz, 2H), 2.70(t, J=6.9Hz, 2H), 2.22(qt, J=6.2Hz, 2H).IR (KBr) 2951, 1669, 1579, 1558, 1454, 1422, 1346, 1250, 1190, 1172, 1025  $\text{cm}^{-1}$ . MS(ESI) m/z: 254 (M+H)<sup>+</sup>; HRMS (ESI) Calcd for  $\text{C}_{16}\text{H}_{16}\text{NO}_2$  (M+H)<sup>+</sup>: 254.11756, found: 254.11665.

### **2-(4-methoxyphenyl)-6,6-dimethyl-7,8-dihydroquinolin-5(6H)-one (5c)**



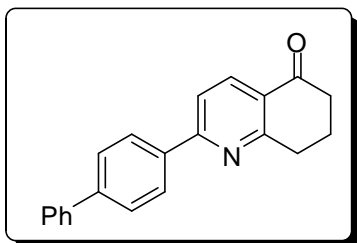
Yield:73%; MP:112 °C.<sup>1</sup>H NMR ( $\text{CDCl}_3$ , 300MHz)  $\delta$  8.30(d, J=8.3Hz, 1H), 8.03(d, J=8.8Hz, 2H), 7.64(d, J=8.3Hz, 1H), 7.00(d, J=8.8Hz, 2H), 3.87(s, 3H), 3.21(t, J=6.4Hz, 2H), 2.05(t, J=6.4Hz, 2H), 1.25(s, 6H).<sup>13</sup>C NMR ( $\text{CDCl}_3$ , 75MHz)  $\delta$  202.1, 162.4, 161.1, 159.9, 136.4, 130.8, 130.4, 128.7, 117.9, 114.0, 55.2, 41.2, 35.2, 29.0, 24.0. IR(KBr) 2961, 1671, 1579, 1512, 1453, 1281, 1251, 1177, 1023  $\text{cm}^{-1}$ . MS(ESI) m/z 282 (M+H)<sup>+</sup>; HRMS (ESI) Calcd for  $\text{C}_{18}\text{H}_{20}\text{NO}_2$  (M+H)<sup>+</sup>: 282.14886, found: 282.14867.

### **2-(4-chlorophenyl)-7,8-dihydroquinolin-5(6H)-one (3d)**



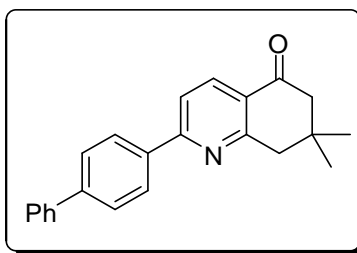
Yield:70%; MP:115 °C.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300MHz)  $\delta$  8.33(d,  $J=8.1\text{Hz}$ , 1H), 8.08-7.95(m, 2H), 7.69(d,  $J=8.1\text{Hz}$ , 1H), 7.55-7.41(m, 2H), 3.21(t,  $J=6.2\text{Hz}$ , 2H), 2.73(t,  $J=6.0\text{Hz}$ , 2H), 2.24(qt,  $J=6.2\text{Hz}$ , 2H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75MHz)  $\delta$  197.6, 163.7, 159.3, 136.7, 136.2, 135.9, 129.0, 128.6, 126.6, 118.5, 38.5, 32.8, 21.8. IR(KBr) 2948, 1680, 1573, 1416, 1328, 1279, 1088, 1008, 820 $\text{cm}^{-1}$ . MS (ESI)  $m/z$  258 ( $\text{M}+\text{H}^+$ ); HRMS(ESI) Calcd for  $\text{C}_{15}\text{H}_{13}\text{ClNO}$  ( $\text{M}+\text{H}^+$ ): 258.06802, found : 258.06772.

### 2-(biphenyl-4-yl)-7,8-dihydroquinolin-5(6H)-one (3e)



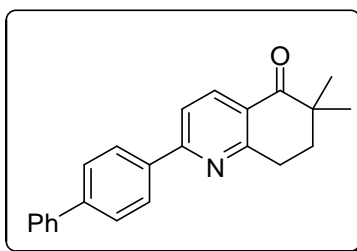
Yield:74%; MP:170 °C.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300MHz)  $\delta$  8.35(d,  $J=8.1\text{Hz}$ , 1H), 8.24-8.10(m, 2H), 7.82-7.16(m, 5H), 7.54-7.33(m, 3H), 3.24(t,  $J=6.2\text{Hz}$ , 2H), 2.73(t,  $J=6.0\text{Hz}$ , 2H), 2.24(qt,  $J=6.2\text{Hz}$ , 2H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75MHz)  $\delta$  197.8, 163.8, 160.2, 142.6, 140.2, 137.2, 135.7, 128.8, 127.8, 127.7, 127.4, 127.0, 126.4, 118.7, 38.5, 32.8, 21.9. IR (KBr) 2951, 1668, 1579, 1449, 1417, 1348, 1284, 1192  $\text{cm}^{-1}$ . MS(ESI)  $m/z$  300 ( $\text{M}+\text{H}^+$ ); HRMS (ESI) Calcd for  $\text{C}_{21}\text{H}_{18}\text{NO}$  ( $\text{M}+\text{H}^+$ ): 300.13829, found: 300.13798.

### 2-(biphenyl-4-yl)-7,7-dimethyl-7,8-dihydroquinolin-5(6H)-one (4e)



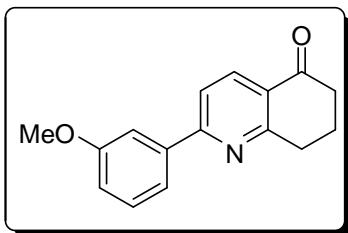
Yield:78%; MP:148 °C.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300MHz)  $\delta$  8.33(d,  $J=7.9\text{Hz}$ , 1H), 8.18-8.13(m, 2H), 7.79-7.71(m, 3H), 7.69-7.63(m, 2H), 7.47(t,  $J=7.4\text{Hz}$ , 2H), 7.42-7.35(m, 1H), 3.12(s, 2H), 2.58(s, 2H), 1.15(s, 6H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75MHz)  $\delta$  197.8, 162.4, 160.6, 142.6, 140.3, 137.2, 135.3, 128.8, 127.8, 127.7, 127.5, 127.0, 125.5, 118.6, 52.1, 46.7, 32.9, 28.3. IR(KBr) 2958, 1676, 1578, 1468, 1447, 1413, 1307  $\text{cm}^{-1}$ . MS(EI)  $m/z$  328 ( $\text{M}+\text{H}^+$ ); HRMS(ESI) Calcd for  $\text{C}_{23}\text{H}_{22}\text{NO}$  ( $\text{M}+\text{H}^+$ ): 328.16959, found: 328.16944.

### 2-(biphenyl-4-yl)-6,6-dimethyl-7,8-dihydroquinolin-5(6H)-one (5e)



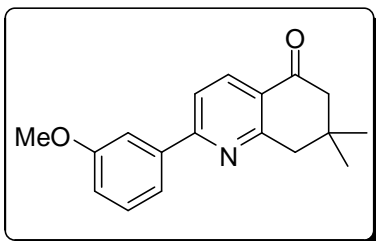
Yield:72%; MP:144 °C.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.37(d,  $J=8.1\text{Hz}$ , 1H), 8.20-8.10(m, 2H), 7.79-7.70(m, 3H), 7.70-7.62(m, 2H), 7.54-7.34(m, 3H), 3.25(t,  $J=6.4\text{Hz}$ , 2H), 2.08(t,  $J=6.4\text{Hz}$ , 2H), 1.27(s, 6H).  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  202.2, 162.6, 160.0, 142.6, 140.3, 137.3, 136.6, 128.8, 127.8, 127.6, 127.4, 127.0, 125.2, 118.7, 41.4, 35.3, 29.1, 24.1. IR(KBr) 2963, 1679, 1578, 1468, 1448, 1379, 1329, 1237  $\text{cm}^{-1}$ . MS(ESI)  $m/z$  328 ( $\text{M}+\text{H}^+$ ); HRMS(ESI) Calcd for  $\text{C}_{23}\text{H}_{22}\text{NO}$  ( $\text{M}+\text{H}^+$ ): 328.16959, found: 328.16939.

### 2-(3-methoxyphenyl)-7,8-dihydroquinolin-5(6H)-one (3f)



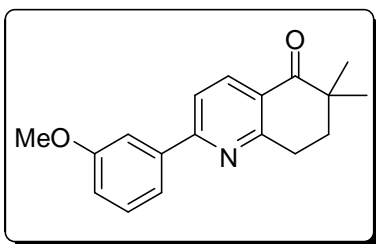
Yield:77%; MP:90 °C.<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300MHz) δ 8.32(d, J=8.3Hz, 1H), 7.69(d, J=8.3Hz, 1H), 7.66-7.56(m, 2H), 7.40(t, J=7.9Hz, 1H), 7.06-6.96(m, 1H), 3.90(s, 3H), 3.21(t, J=6.2Hz, 2H), 2.71(t, J=6.2Hz, 2H), 2.22(qt, J=6.4Hz, 2H).<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75MHz) δ 197.7, 163.5, 160.2, 159.9, 139.6, 135.6, 129.7, 126.4, 119.6, 118.8, 115.6, 112.5, 55.2, 38.4, 32.6, 21.7. IR(KBr) 2920, 1675, 1567, 1393, 1284, 1034, 765 cm<sup>-1</sup>. MS(ESI) m/z 254 (M+H)<sup>+</sup>; HRMS(ESI) Calcd for C<sub>16</sub>H<sub>16</sub>NO<sub>2</sub> (M+H)<sup>+</sup>: 254.11756, found: 254.11754.

#### 2-(3-methoxyphenyl)-7,7-dimethyl-7,8-dihydroquinolin-5(6H)-one (4f)



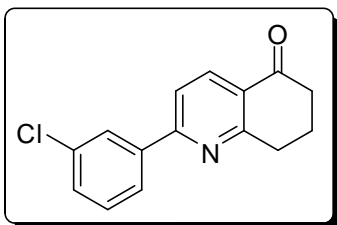
Yield:80%; MP:81 °C.<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300MHz) δ 8.31(d, J=8.1Hz, 1H), 7.70(d, J=8.1Hz, 1H), 7.76-7.57(m, 2H), 7.40(t, J=7.9Hz, 1H), 7.06-6.97(m, 1H), 3.91(s, 3H), 3.11(s, 2H), 2.57(s, 2H), 1.14(s, 6H).<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75MHz) δ 197.7, 162.2, 160.7, 159.9, 139.7, 135.1, 129.7, 125.5, 119.7, 118.8, 115.7, 112.5, 55.2, 51.9, 46.5, 32.8, 28.2. IR(KBr) 2958, 1676, 1548, 1492, 1388, 1304, 1122, 1044 cm<sup>-1</sup>. MS(ESI) m/z 282 (M+H)<sup>+</sup>; HRMS(ESI) Calcd for C<sub>18</sub>H<sub>20</sub>NO<sub>2</sub> (M+H)<sup>+</sup>: 282.14886, found: 282.14866.

#### 2-(3-methoxyphenyl)-6,6-dimethyl-7,8-dihydroquinolin-5(6H)-one (5f)



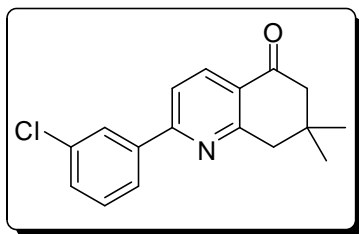
Yield:73%; MP:99 °C;<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.34(dd, J=1.8Hz & 8.3Hz, 1H), 7.68(dd, J=1.7Hz & 8.3Hz, 1H), 7.66-7.56(m, 2H), 7.40(td, J=1.7Hz & 7.7Hz, 1H), 7.06-6.96(m, 1H), 3.09(s, 3H), 3.23(t, J=6.2Hz, 2H), 2.06(t, J=6.2Hz, 2H), 1.26(s, 6H).<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 202.1, 162.4, 160.1, 159.9, 139.8, 136.5, 129.7, 125.2, 119.7, 118.9, 115.6, 112.5, 55.2, 41.3, 35.2, 29.0, 24.0. IR(KBr) 2929, 1669, 1607, 1578, 1494, 1347, 1108, 1046 cm<sup>-1</sup>. MS(ESI) m/z 282 (M+H)<sup>+</sup>; HRMS(ESI) Calcd for C<sub>18</sub>H<sub>20</sub>NO<sub>2</sub> (M+H)<sup>+</sup>: 282.14886, found: 282.14866.

#### 2-(3-chlorophenyl)-7,8-dihydroquinolin-5(6H)-one (3g)



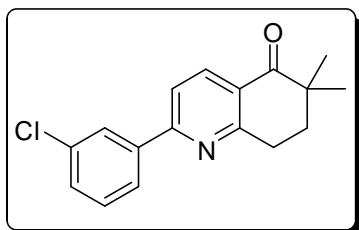
Yield:74%, MP:85 °C.<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.34(d, J=8.1Hz, 1H), 8.12-8.06(m, 1H), 7.97-7.88(m, 1H), 7.69(d, J=8.1Hz, 1H), 7.47-7.39(m, 2H), 3.22(t, J=6.2Hz, 2H), 2.73(t, J=6.9Hz, 2H), 2.24(qt, J=6.2Hz, 2H).<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 197.6, 163.7, 158.9, 140.0, 135.8, 134.8, 129.9, 129.8, 127.5, 126.8, 125.3, 118.8, 38.4, 32.6, 21.7. IR(KBr) 2960, 1667, 1557, 1479, 1389, 1329, 1280, 1182 cm<sup>-1</sup>. MS(ESI) m/z: 258 (M+H)<sup>+</sup>; HR MS(ESI) Calcd for C<sub>15</sub>H<sub>13</sub>ClNO (M+H)<sup>+</sup>: 258.06802, found: 258.06766.

### 2-(3-chlorophenyl)-7,7-dimethyl-7,8-dihydroquinolin-5(6H)-one (4g)



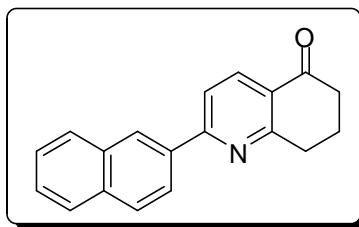
Yield:79%; MP:87 °C.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300MHz)  $\delta$  8.32(d,  $J=8.3\text{Hz}$ , 1H), 8.12-8.06(m, 1H), 7.97-7.87(m, 1H), 7.69(d,  $J=8.3\text{Hz}$ , 1H), 7.47-7.39(m, 2H), 3.11(s, 2H), 2.58(s, 2H), 1.15(s, 6H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75MHz)  $\delta$  197.7, 162.3, 159.3, 140.0, 135.4, 134.9, 129.9, 129.8, 127.5, 125.8, 125.3, 118.7, 51.9, 46.5, 32.9, 28.2. IR(KBr) 2957, 1681, 1557, 1424, 1386, 1286, 1117  $\text{cm}^{-1}$ . MS(ESI)  $m/z$  286 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS(ESI) Calcd for  $\text{C}_{17}\text{H}_{17}\text{ClNO}$  ( $\text{M}+\text{H}$ ) $^+$ : 286.09932, found: 286.09911.

### 2-(3-chlorophenyl)-6,6-dimethyl-7,8-dihydroquinolin-5(6H)-one (5g)



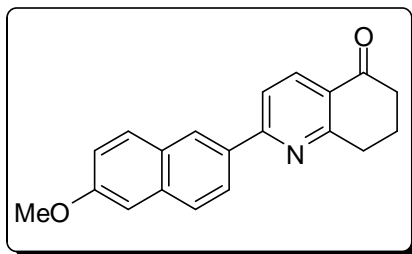
Yield:75%; MP:89 °C.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.36(d,  $J=8.3\text{Hz}$ , 1H), 8.12-8.05(m, 1H), 7.98-7.86(m, 1H), 7.68(d,  $J=8.3\text{Hz}$ , 1H), 7.48-7.38(m, 2H), 3.23(t,  $J=6.4\text{Hz}$ , 2H), 1.26(s, 6H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75MHz)  $\delta$  201.9, 162.6, 158.7, 140.1, 136.7, 134.9, 129.9, 129.7, 127.5, 125.6, 125.3, 118.8, 41.3, 35.2, 29.0, 24.0. IR(KBr) 2930, 1673, 1558, 1480, 1451, 1382, 1325, 1234, 1081  $\text{cm}^{-1}$ . MS(ESI)  $m/z$  286 ( $\text{M}+\text{H}$ ) $^+$ ; HRMS(ESI) Calcd for  $\text{C}_{17}\text{H}_{17}\text{ClNO}$  ( $\text{M}+\text{H}$ ) $^+$ : 286.09932, found: 286.09905.

### 2-(naphthalen-2-yl)-7,8-dihydroquinolin-5(6H)-one (3h)



Yield:68%; MP:140 °C.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300MHz)  $\delta$  8.56(d,  $J=1.1\text{Hz}$ , 1H), 8.36(d,  $J=8.3\text{Hz}$ , 1H), 8.19(dd,  $J=1.7\text{Hz}$  & 8.4Hz, 1H), 8.02-7.92(m, 2H), 7.91-7.82(m, 2H), 7.60-7.49(m, 2H), 3.26(t,  $J=6.2\text{Hz}$ , 2H), 2.73(t,  $J=7.1\text{Hz}$ , 2H), 2.25(qt,  $J=6.2\text{Hz}$ , 2H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75MHz)  $\delta$  197.7, 163.7, 160.4, 135.7, 135.6, 134.0, 133.2, 128.8, 128.5, 127.6, 127.3, 126.9, 126.4, 126.3, 124.5, 119.0, 38.5, 32.8, 21.8. IR(KBr) 2951, 1676, 1581, 1403, 1331, 1273, 1126, 821  $\text{cm}^{-1}$ . MS(ESI)  $m/z$  274 ( $\text{M}+\text{H}$ ) $^+$  Calcd for  $\text{C}_{19}\text{H}_{16}\text{NO}$  ( $\text{M}+\text{H}$ ) $^+$ : 274.12264, found: 274.12213.

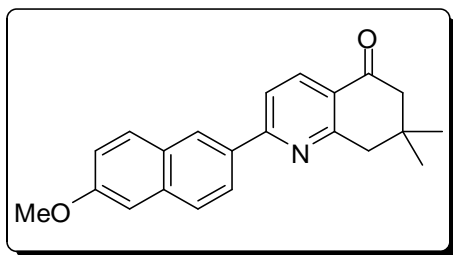
### 2-(6-methoxynaphthalen-2-yl)-7,8-dihydroquinolin-5(6H)-one (3i)



Yield:70%; MP:180 °C.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300MHz)  $\delta$  8.49(s, 1H), 8.34(d,  $J=8.1\text{Hz}$ , 1H), 8.16(dd,  $J=1.5\text{Hz}$  & 8.6Hz, 1H), 7.91-7.77(m, 3H), 7.24-7.13(m, 2H), 3.94(s, 3H), 3.25(t,  $J=6.2\text{Hz}$ , 2H), 2.73(t,  $J=6.4\text{Hz}$ , 2H), 2.24(qt,  $J=6.2\text{Hz}$ , 2H).  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  197.7, 163.7, 160.5, 158.6, 135.6, 135.4, 133.4, 130.4, 128.7, 127.3, 127.1, 126.2, 125.0, 119.3, 118.6, 105.6, 55.2, 38.5, 32.8, 21.9. IR(KBr) 2945, 1671, 1626, 1581, 1483,

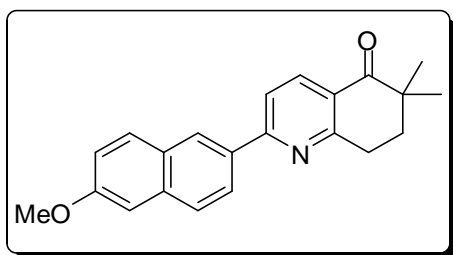
1421, 1280, 1208  $\text{cm}^{-1}$ .MS(ESI)  $m/z$  304 (M+H)<sup>+</sup>: HRMS (ESI) Calcd for  $\text{C}_{20}\text{H}_{18}\text{NO}_2$  (M+H)<sup>+</sup>: 304.13321, found: 304.13293.

### 2-(6-methoxynaphthalen-2-yl)-7,7-dimethyl-7,8-dihydroquinolin-5(6H)-one (4i)



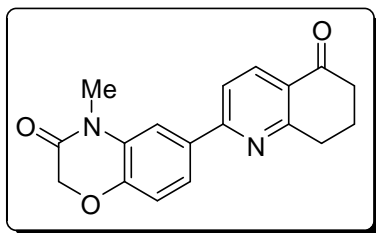
Yield:72%; MP:178 °C. <sup>1</sup>H NMR ( $\text{CDCl}_3$ , 300MHz)  $\delta$  8.51(d, J=1.5Hz, 1H), 8.34(d, J=7.5Hz, 1H), 8.17(dd, J=1.5Hz & 9.0Hz, 1H), 7.93-7.79(m, 3H), 7.24-7.13(m, 2H), 3.96(s, 3H), 3.15(s, 2H), 2.59(s, 2H), 1.16(s, 6H).<sup>13</sup>C NMR ( $\text{CDCl}_3$ , 75MHz)  $\delta$  197.9, 162.4, 161.0, 158.6, 135.5, 135.2, 133.5, 130.4, 128.8, 127.3, 127.2, 125.3, 125.0, 119.3, 118.6, 105.6, 55.3, 52.1, 46.8, 32.9, 29.6, 28.3.IR(KBr) 2934, 1675, 1625, 1580, 1481, 1422, 1389, 1303, 1211, 1165  $\text{cm}^{-1}$ .MS(ESI)  $m/z$  332 (M+H)<sup>+</sup>; HRMS(ESI) Calcd for  $\text{C}_{22}\text{H}_{22}\text{NO}_2$  (M+H)<sup>+</sup>: 332.16451, found: 332.16442.

### 2-(6-methoxynaphthalen-2-yl)-6,6-dimethyl-7,8-dihydroquinolin-5(6H)-one (5i)



Yield:76%; MP:175 °C.<sup>1</sup>H NMR ( $\text{CDCl}_3$ , 300MHz)  $\delta$  8.49(d, J=1.5Hz, 1H), 8.37(d, J=8.3Hz, 1H), 8.16(dd, J=1.8Hz & 8.6Hz, 1H), 7.92-7.79(m, 3H), 7.24-7.15(m, 2H), 3.95(s, 3H), 3.27(t, J=6.4Hz, 2H), 2.08(t, J=6.4Hz, 2H), 1.27(s, 6H).<sup>13</sup>C NMR ( $\text{CDCl}_3$ , 75MHz)  $\delta$  221.7, 182.1, 179.9, 178.1, 156.1, 154.9, 153.1, 149.9, 148.3, 146.8, 146.6, 144.5, 144.4, 138.8, 138.2, 125.1, 74.8, 60.9, 54.9, 48.7, 43.6.IR(KBr) 2930, 1671, 1577, 1423, 1383, 1208, 1164, 1021, 894  $\text{cm}^{-1}$ .MS(ESI)  $m/z$  332 (M+H)<sup>+</sup>; HRMS(ESI) Calcd for  $\text{C}_{22}\text{H}_{22}\text{NO}_2$  (M+H)<sup>+</sup>: 332.16451, found: 332.16446.

### 4-methyl-6-(5-oxo-5,6,7,8-tetrahydroquinolin-2-yl)-2H-benzo[b][1,4]oxazin-3(4H)-one (3j)



Yield:62%; MP:185 °C.<sup>1</sup>H NMR ( $\text{CDCl}_3$ , 300MHz)  $\delta$  8.33(d, J=8.3Hz, 1H), 7.82(d, J=1.8Hz, 1H), 7.67(d, J=8.3Hz, 1H), 7.66(d, J=8.4Hz, 1H), 7.08(d, J=8.4Hz, 1H), 4.69(s, 2H), 3.49(s, 3H), 3.22(t, J=6.2Hz, 2H), 2.72(t, J=6.0Hz, 2H), 2.24(qt, J=6.2Hz, 2H).<sup>13</sup>C NMR ( $\text{CDCl}_3$ , 75MHz)  $\delta$  197.7, 164.0, 163.7, 159.4, 146.6, 135.8, 133.1, 129.8, 126.3, 123.0, 118.3, 116.9, 114.0, 67.4, 38.5, 32.7, 28.1, 21.8.IR(KBr) 2932, 1688, 1579, 1475, 1266, 1134, 869, 827  $\text{cm}^{-1}$ .MS(ESI)  $m/z$  309 (M+H)<sup>+</sup>; HRMS(ESI) Calcd for  $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_3$  (M+H)<sup>+</sup>: 309.12337, found: 309.12322.

**X-ray Crystallography:** X-ray data for the compounds were collected at room temperature using a Bruker Smart Apex CCD diffractometer with graphite monochromated MoK $\alpha$  radiation ( $\lambda=0.71073\text{\AA}$ ) with  $\omega$ -scan method.<sup>2</sup> Preliminary lattice parameters and orientation matrices were obtained from four sets of frames. Integration and scaling of intensity data were accomplished using SAINT program.<sup>13</sup> The structure was solved by direct methods using SHELXS97 and refinement was carried out by full-matrix least-squares technique using SHELXL97.<sup>2</sup> Anisotropic displacement parameters were included for all non-hydrogen atoms. The atoms C4A and C4B of AM97 are disordered over two sites (C4A/C4A' and C4B/C4B') and the site-occupation factors refined to 0.576(6) and 0.424(6). EADP and DFIX constraints were applied to the disordered atoms. All H atoms were located in difference Fourier maps and subsequently geometrically optimized and allowed for as riding atoms, with C-H = 0.93- 0.97  $\text{\AA}$ , with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl H or  $1.2U_{\text{eq}}(\text{C},\text{N})$ . The methyl groups were allowed to rotate but not to tip.

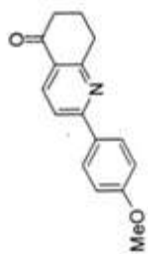
Crystal data for 6k: C<sub>15</sub>H<sub>13</sub>NO<sub>3</sub>S,  $M = 287.32$ , colorless needle,  $0.21 \times 0.13 \times 0.09 \text{ mm}^3$ , monoclinic, space group  $P2_1/c$  (No. 14),  $a = 12.5933(11)$ ,  $b = 15.1264(13)$ ,  $c = 15.0649(13) \text{\AA}$ ,  $\beta = 111.798(1)^\circ$ ,  $V = 2664.5(4) \text{\AA}^3$ ,  $Z = 8$ ,  $D_c = 1.432 \text{ g/cm}^3$ ,  $F_{000} = 1200$ , CCD Area Detector, MoK $\alpha$  radiation,  $\lambda = 0.71073 \text{\AA}$ ,  $T = 294(2)\text{K}$ ,  $2\theta_{\text{max}} = 50.0^\circ$ , 24988 reflections collected, 4682 unique ( $R_{\text{int}} = 0.0257$ ). Final  $Goof = 1.187$ ,  $RI = 0.0563$ ,  $wR2 = 0.1625$ ,  $R$  indices based on 3740 reflections with  $I > 2\sigma(I)$  (refinement on  $F^2$ ), 358 parameters, 8 restraints,  $\mu = 0.249 \text{ mm}^{-1}$ .

Crystal data for 7e: C<sub>25</sub>H<sub>23</sub>NO<sub>3</sub>,  $M = 385.44$ , colourless block,  $0.18 \times 0.16 \times 0.12 \text{ mm}^3$ , monoclinic, space group  $P2_1/c$  (No. 14),  $a = 16.2313(10)$ ,  $b = 15.4503(10)$ ,  $c = 8.0772(5) \text{\AA}$ ,  $\beta = 96.738(1)^\circ$ ,  $V = 2011.6(2) \text{\AA}^3$ ,  $Z = 4$ ,  $D_c = 1.273 \text{ g/cm}^3$ ,  $F_{000} = 816$ , CCD Area Detector, MoK $\alpha$  radiation,  $\lambda = 0.71073 \text{\AA}$ ,  $T = 294(2)\text{K}$ ,  $2\theta_{\text{max}} = 50.0^\circ$ , 19132 reflections collected, 3554 unique ( $R_{\text{int}} = 0.0217$ ). Final  $Goof = 1.030$ ,  $RI = 0.0377$ ,  $wR2 = 0.1021$ ,  $R$  indices based on 3043 reflections with  $I > 2\sigma(I)$  (refinement on  $F^2$ ), 265 parameters, 0 restraints,  $\mu = 0.083 \text{ mm}^{-1}$ .

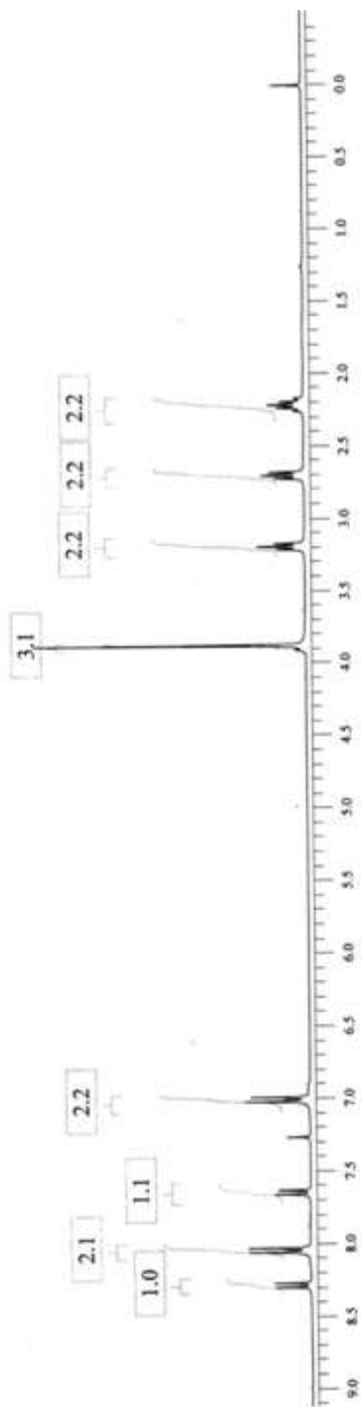
## References:

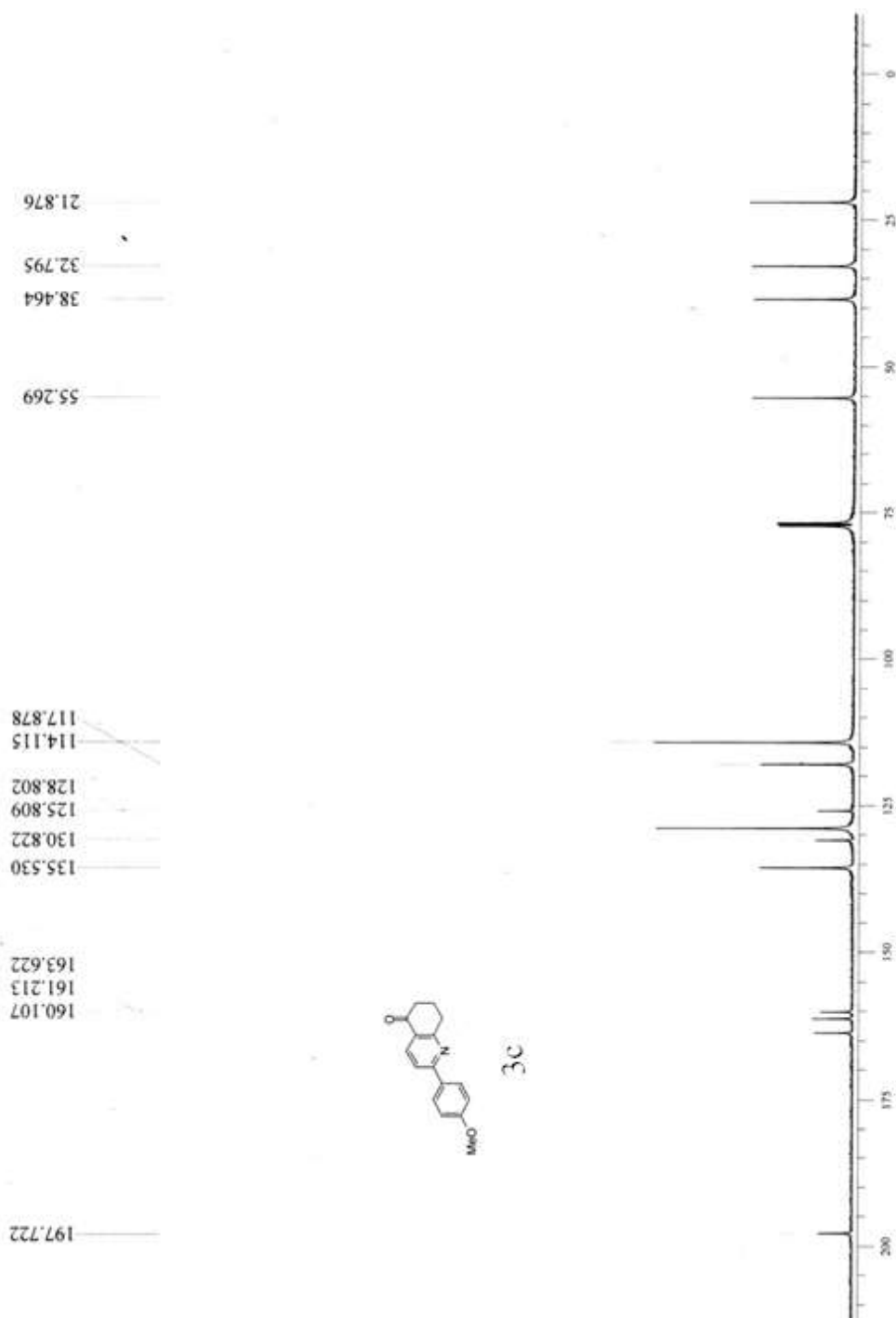
- 1) (a) S. kantevari, S. R. Patpi, D. Addla, S. R. Putapatri, B. Sreedhar, P. Yogeewari and D. Sriram, *ACS Comb. Sci.*, 2011, **13**, 427-435; (b) S. kantevari, S. R. Patpi, B. Sreedhar, P. Yogeewari and D. Sriram, *Bioorg. Med. Chem. Lett.*, 2011, **21**, 1214-1218; (c) S. kantevari, D. Addla and B. Sreedhar, *Synthesis*, 2010, 3745-3754; (d) S. Kantevari and S. R. Putapatri, *SynLett.* 2010, 2251-2256; (e) S. kantevari, M. V. Chary and S. V. N. Vuppalapati, *Tetrahedron*, 2007, **63**, 13024-13031.
- 2) (a) Bruker SAINT (Version 6.28a) & SMART (Version 5.625). Bruker AXS Inc., Madison, Wisconsin, USA; 2001 (b) G.M. Sheldrick, *Acta Crystallogr.*, 2008, **A64**, 112-122.





3c



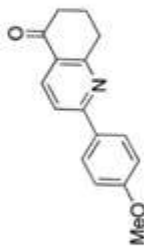


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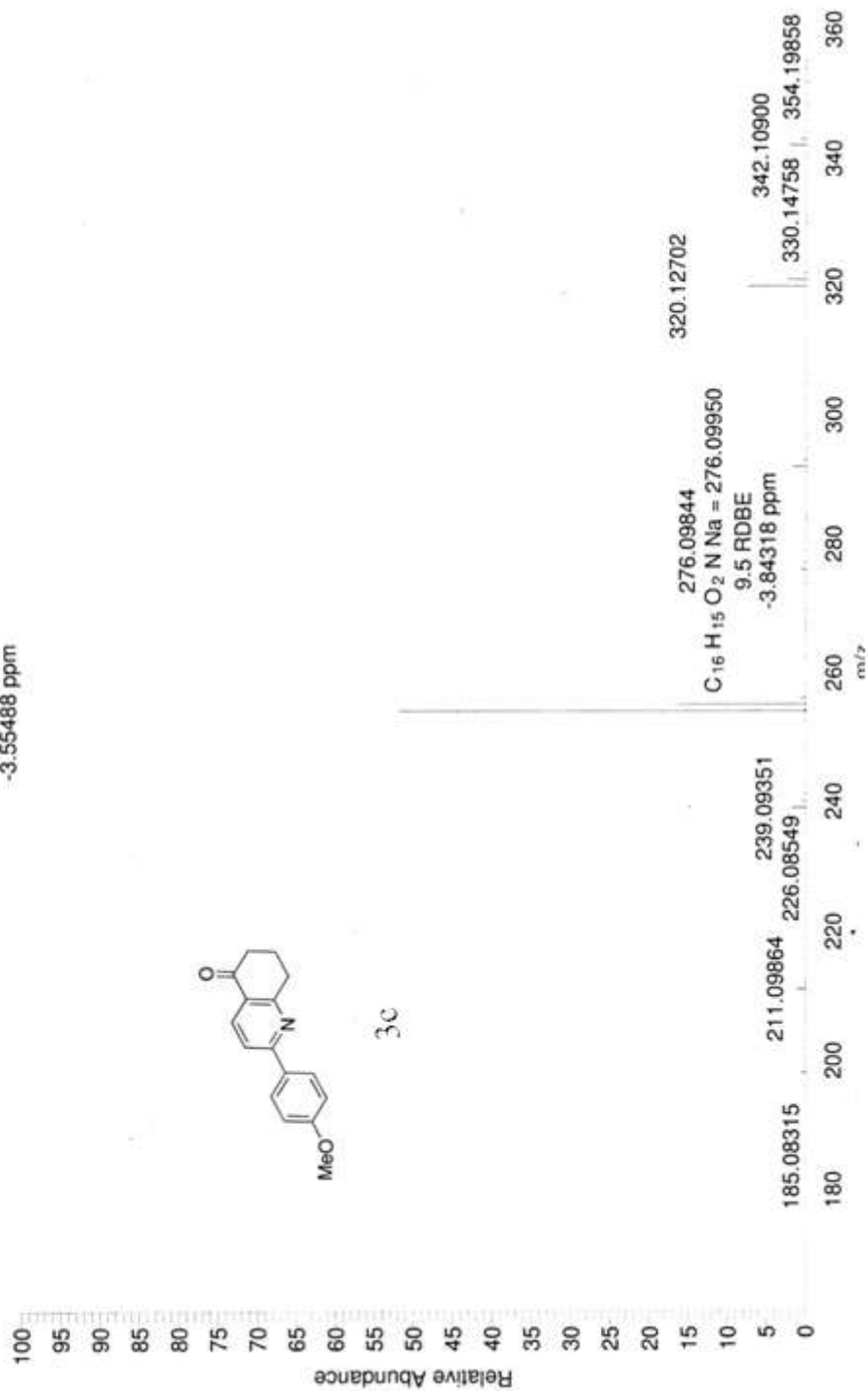
INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY  
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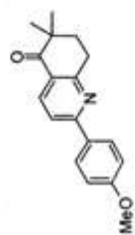
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9.5 RDBE  
-3.55488 ppm



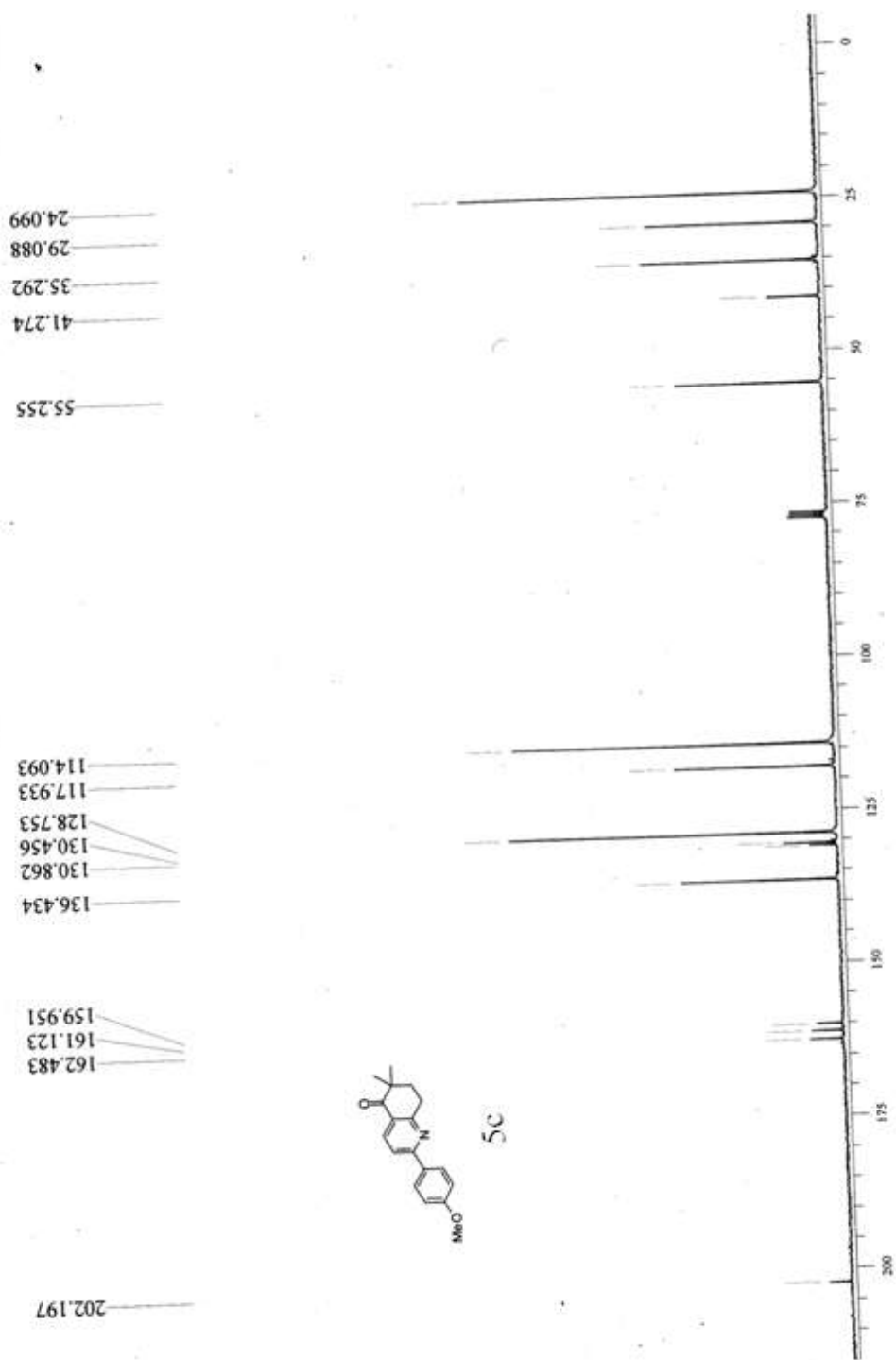
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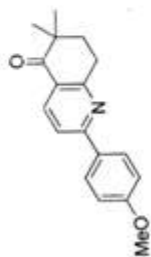
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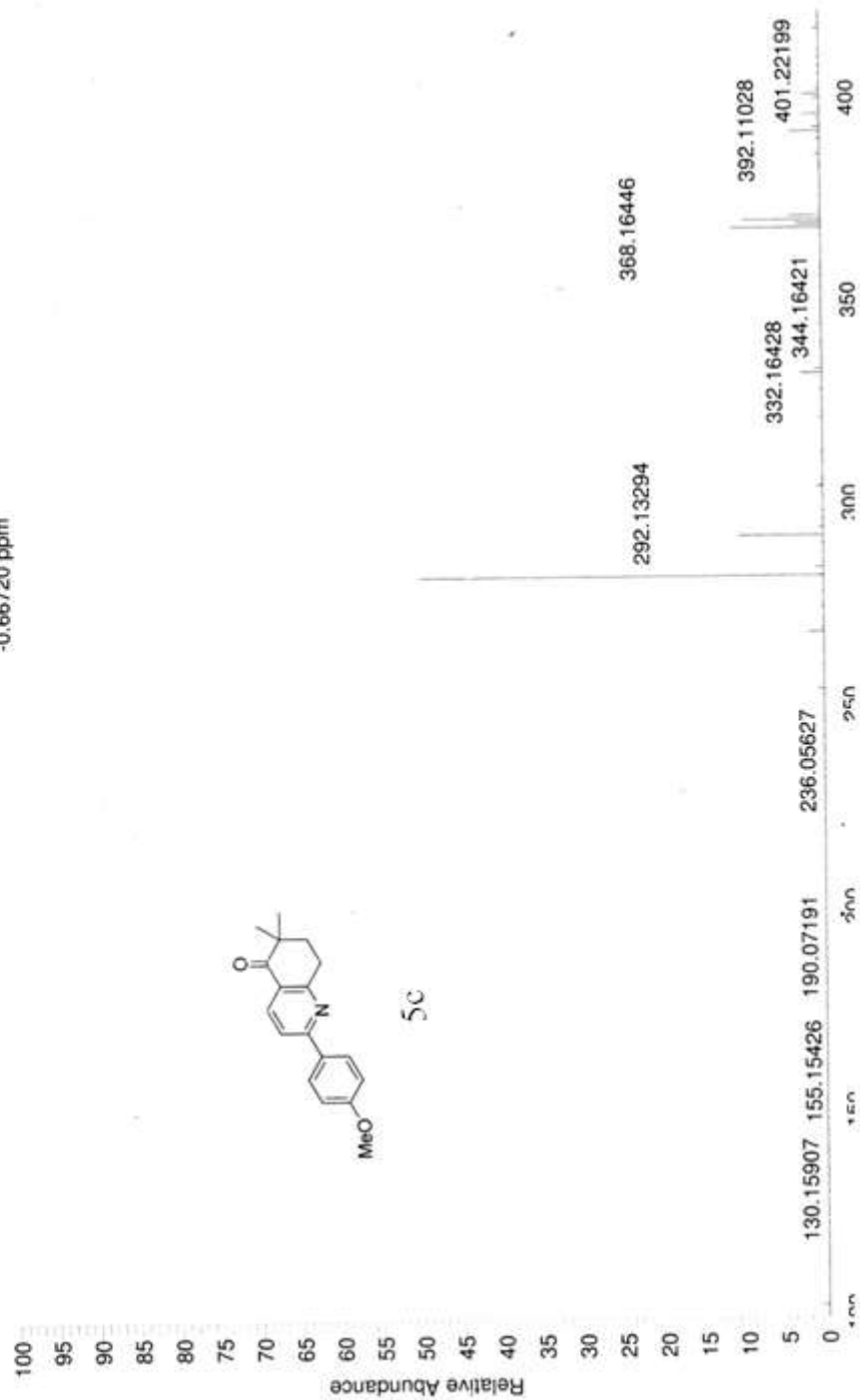


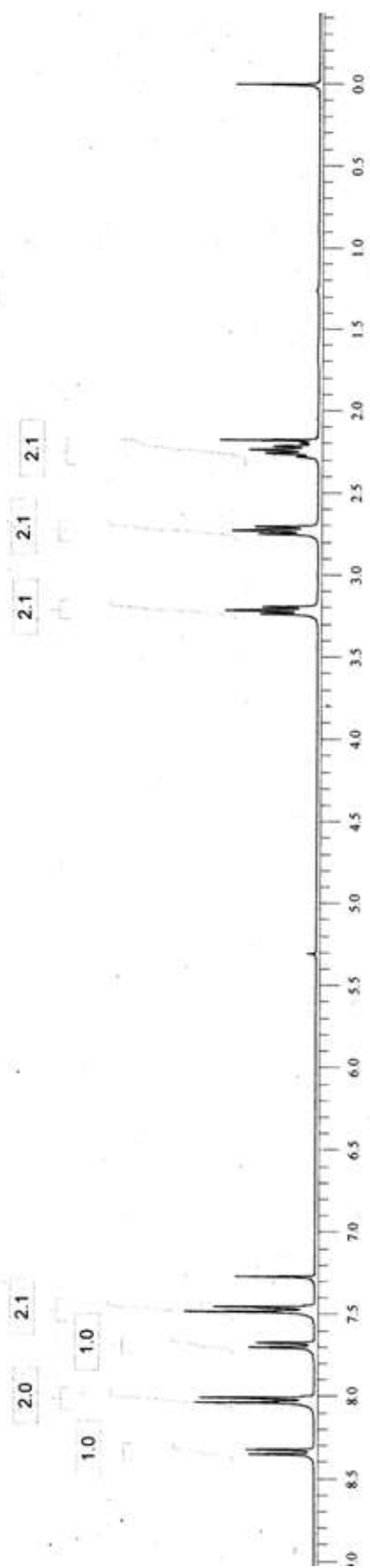
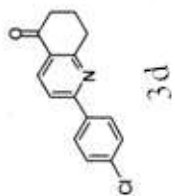
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INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY  
NATIONAL CENTRE FOR MASS SPECTROMETRY  
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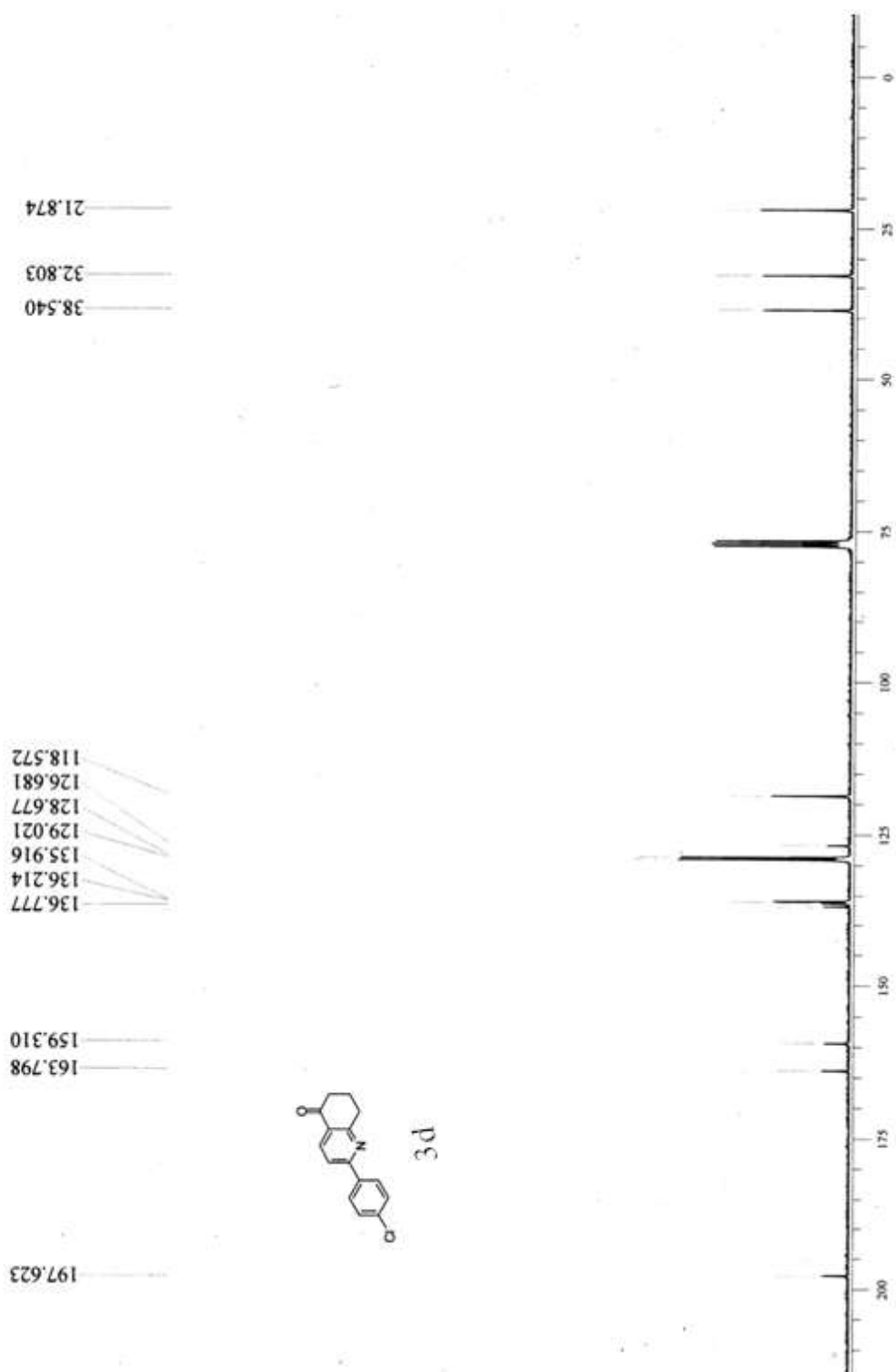
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C<sub>18</sub> H<sub>20</sub> O<sub>2</sub> N = 282.14886  
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-0.66720 ppm



5c





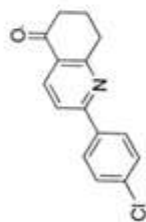




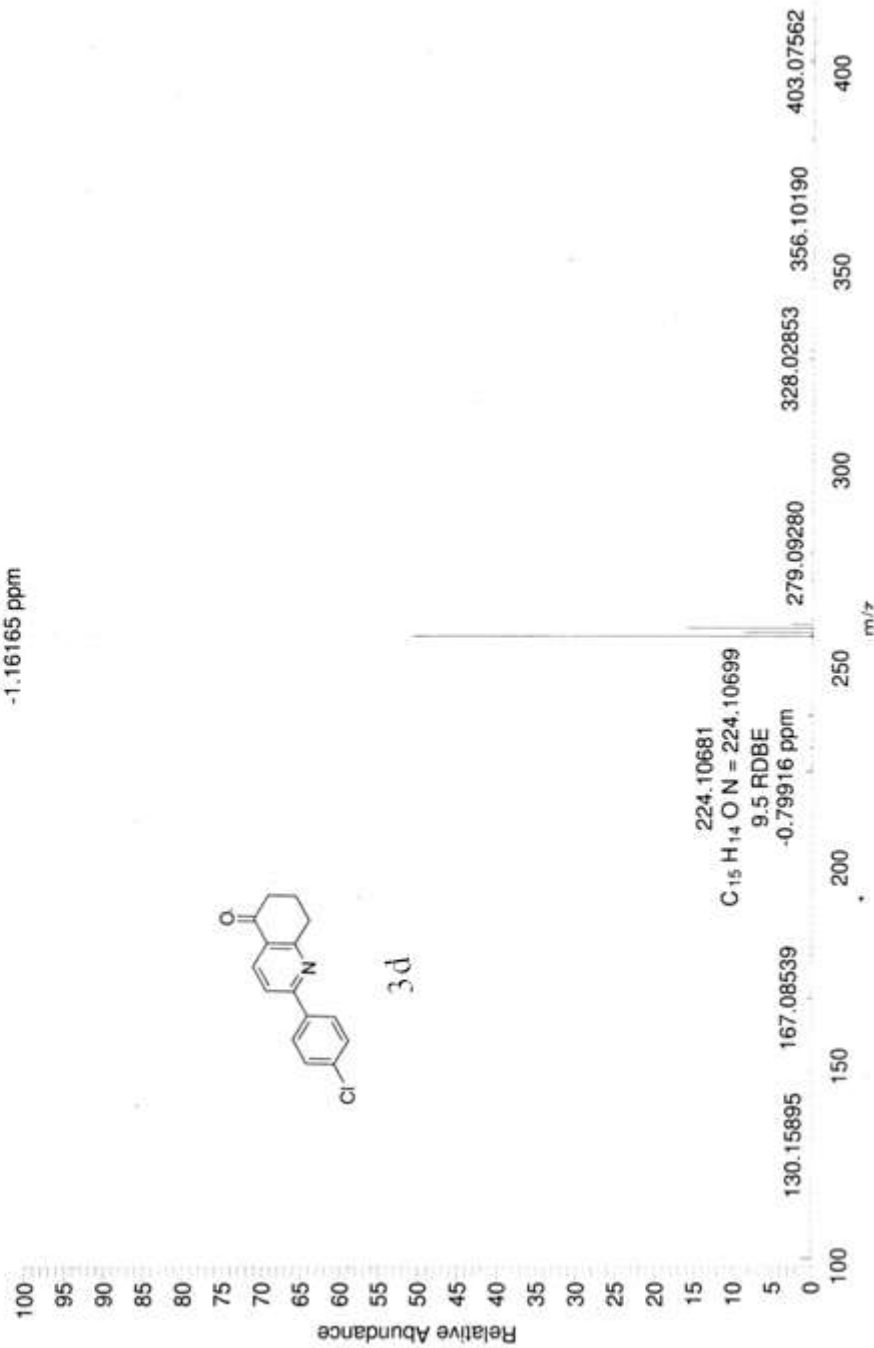
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INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY  
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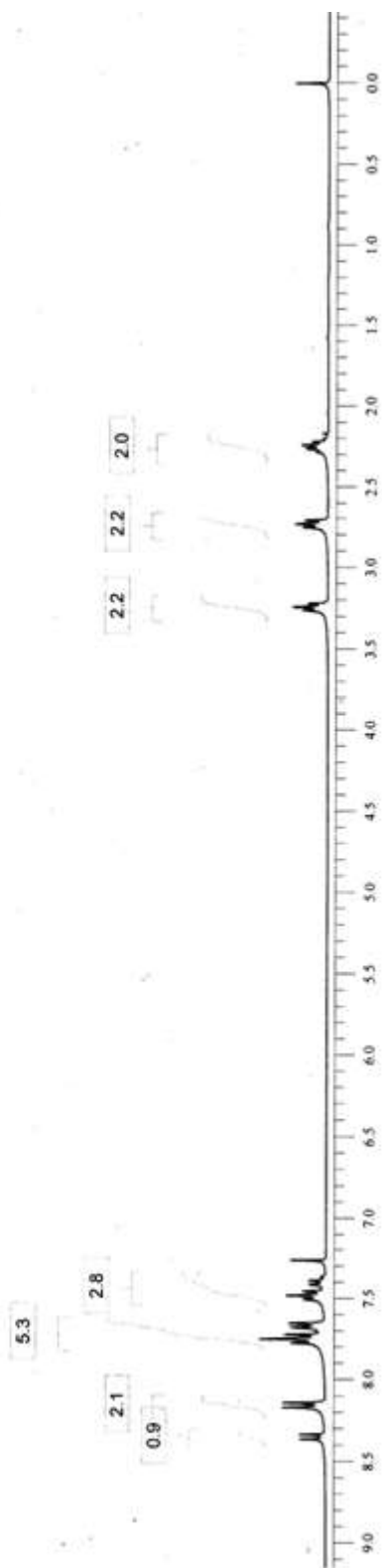
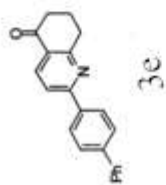
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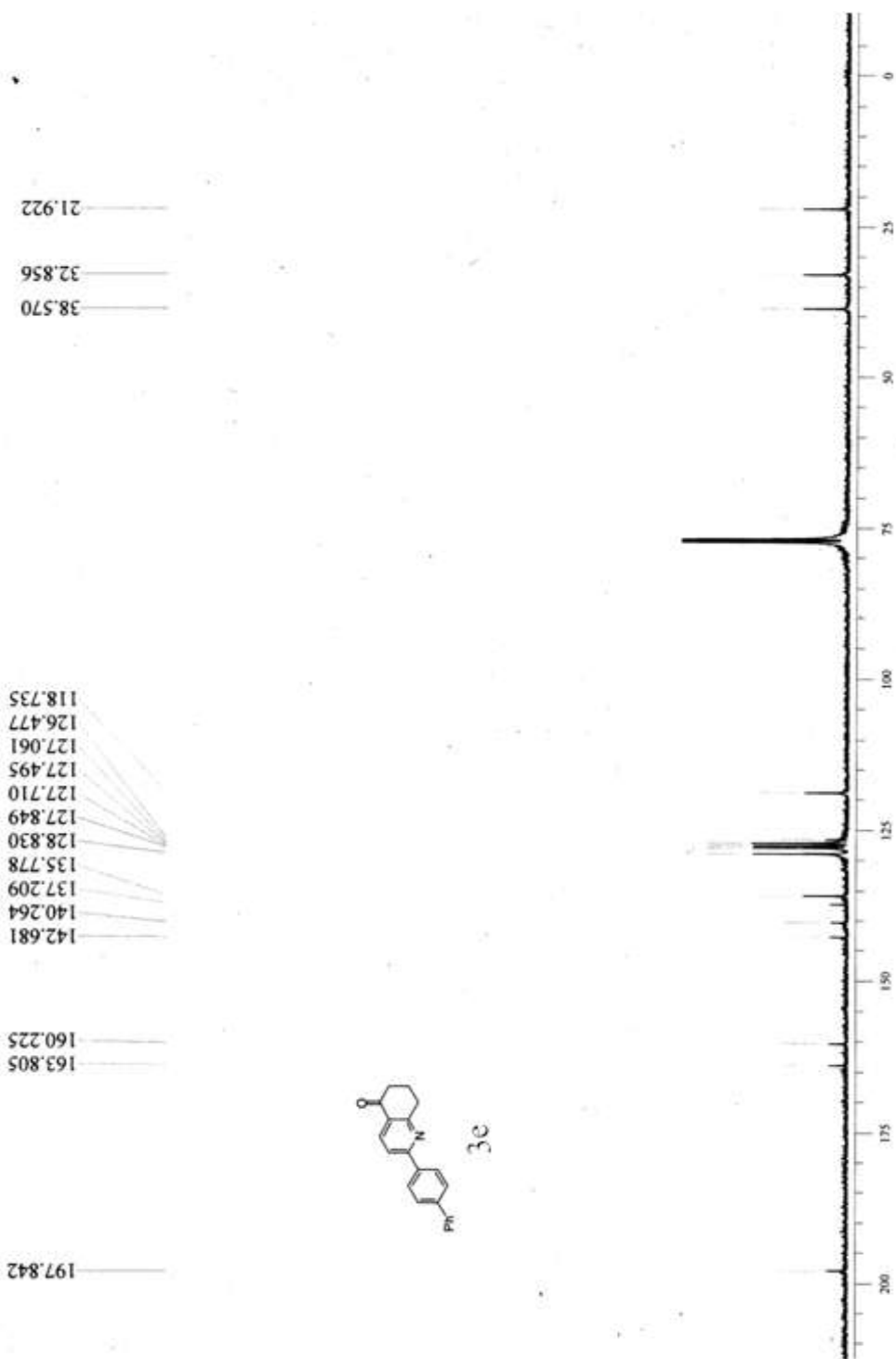
258.06772  
C<sub>15</sub> H<sub>13</sub> O N Cl = 258.06802  
9.5 RDBE  
-1.16165 ppm



3d



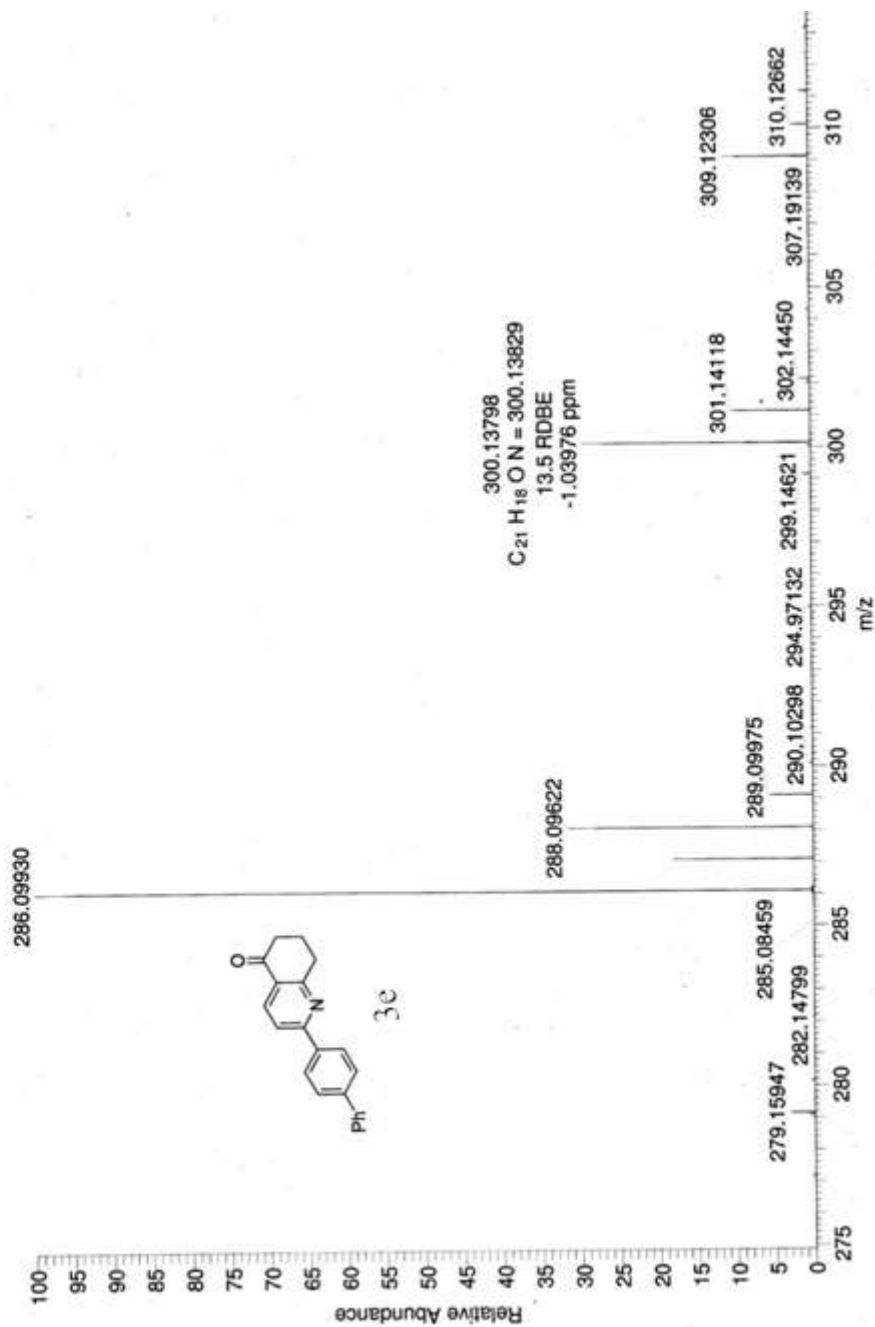


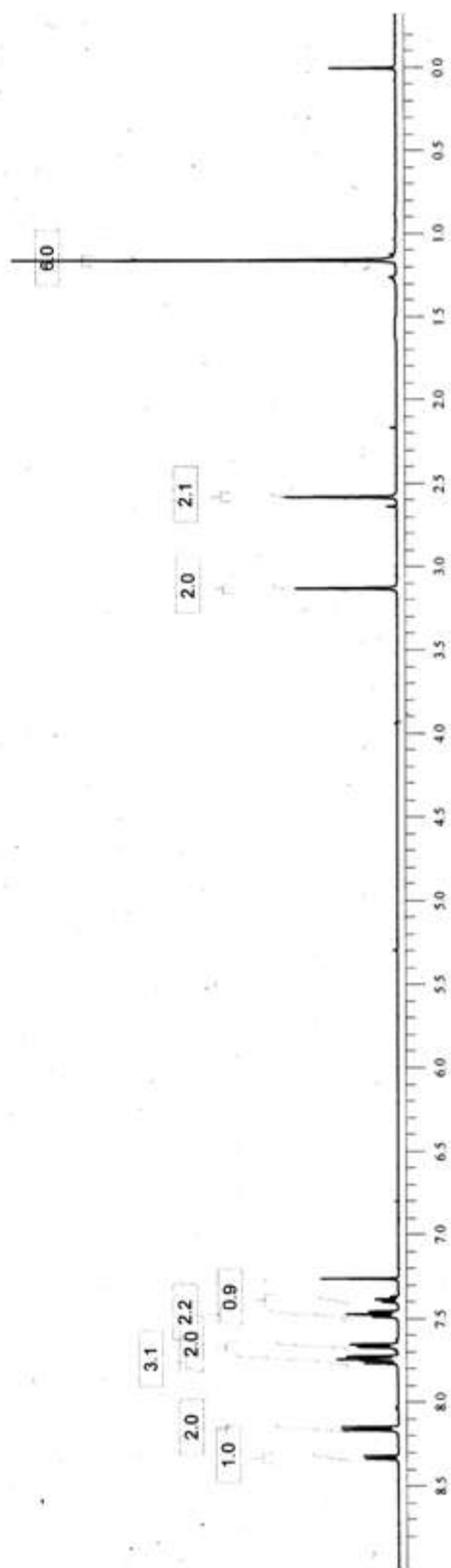
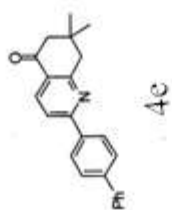


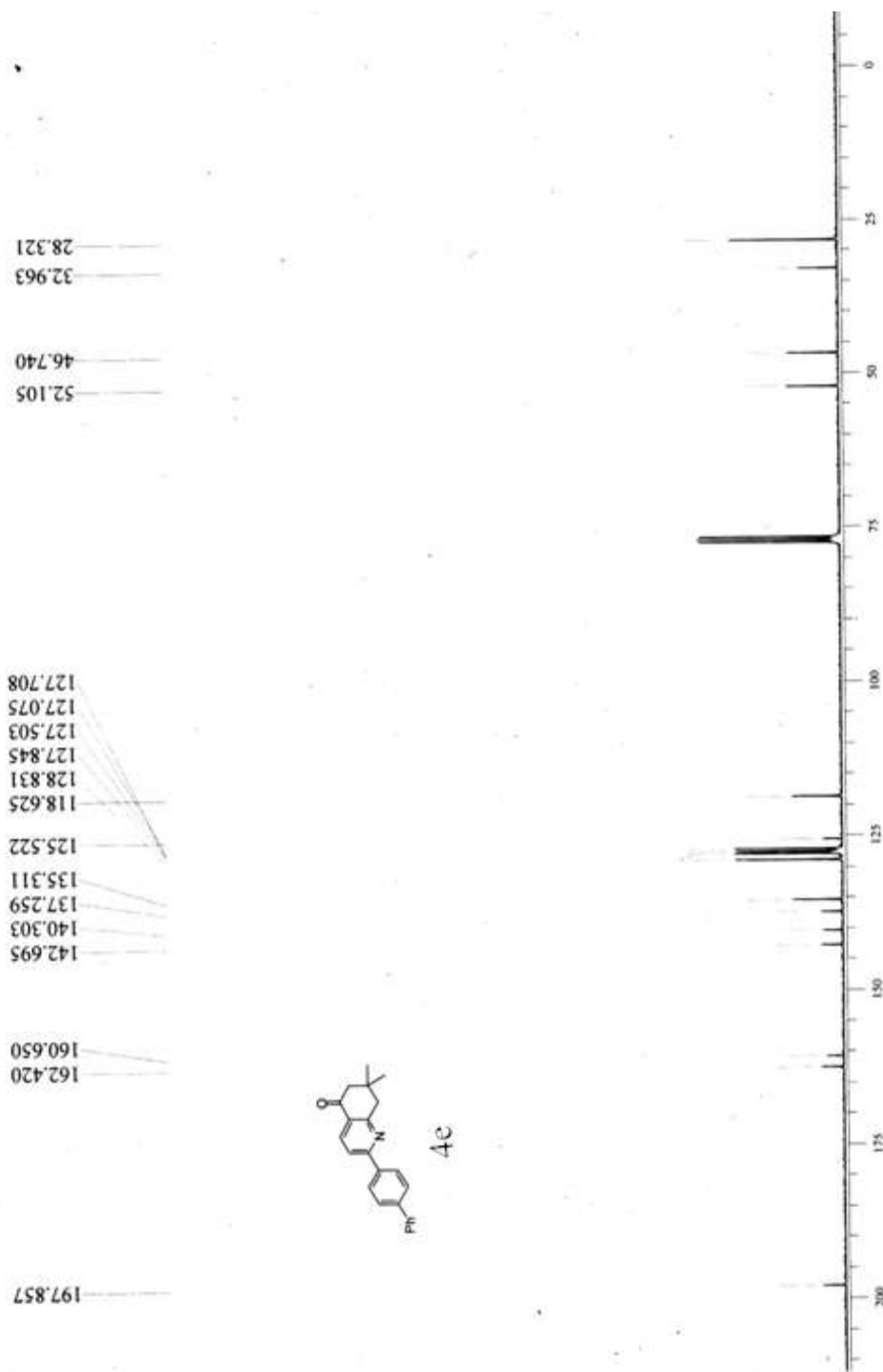
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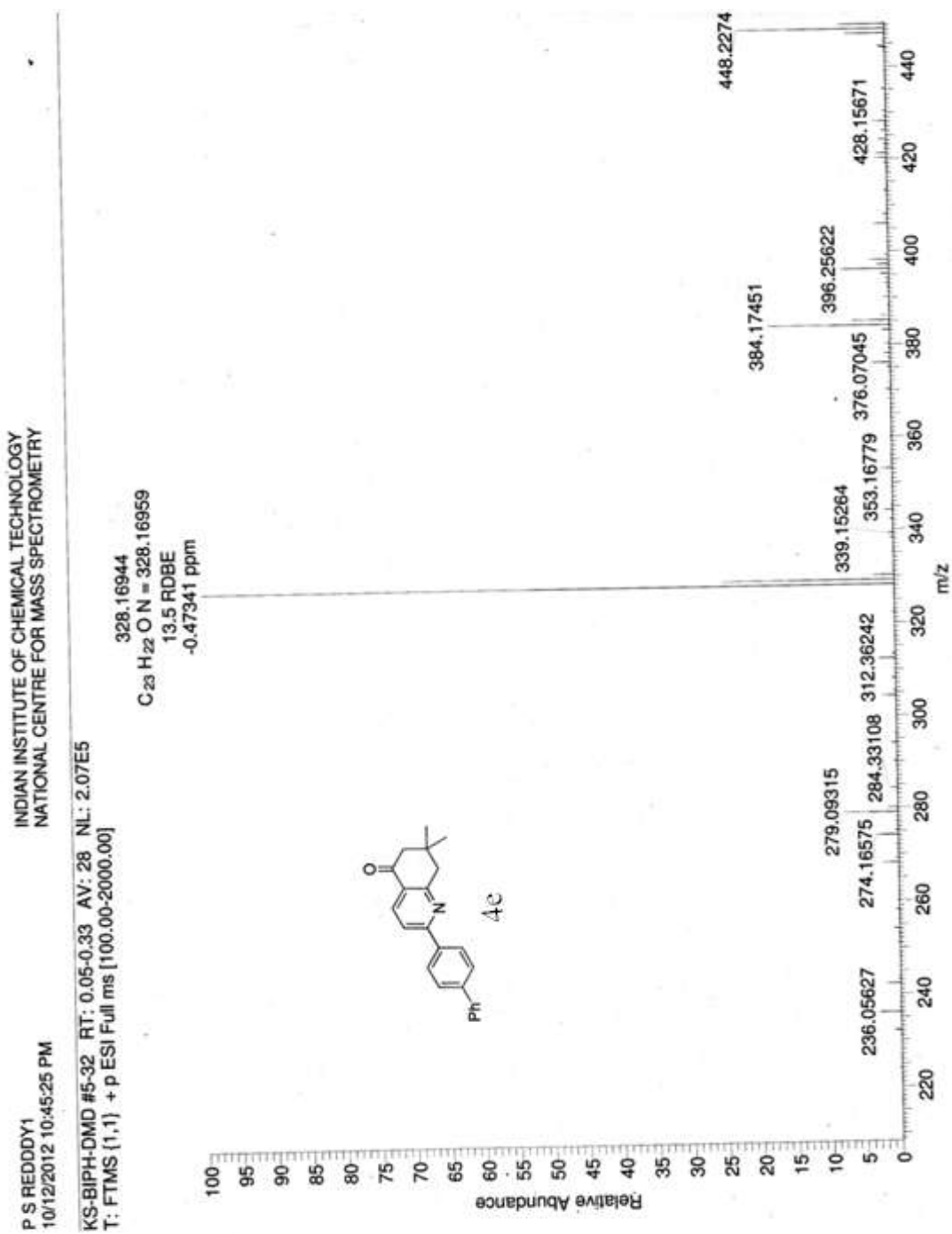
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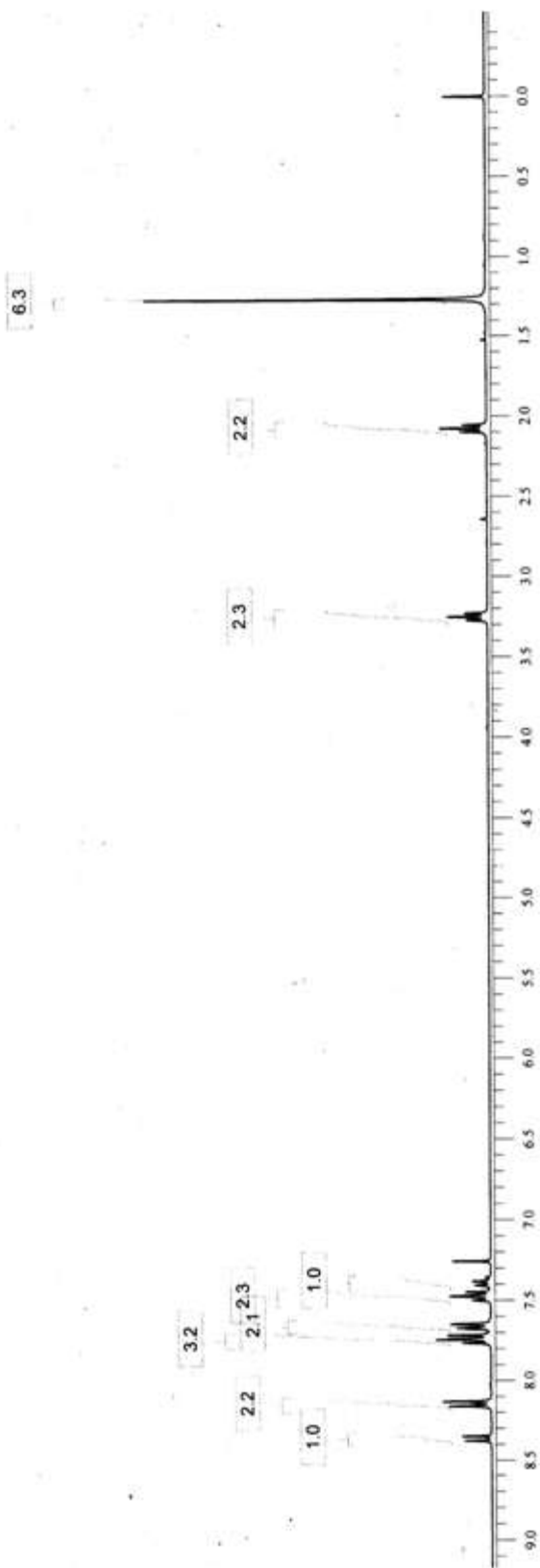
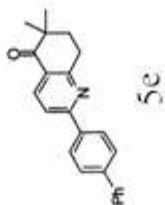
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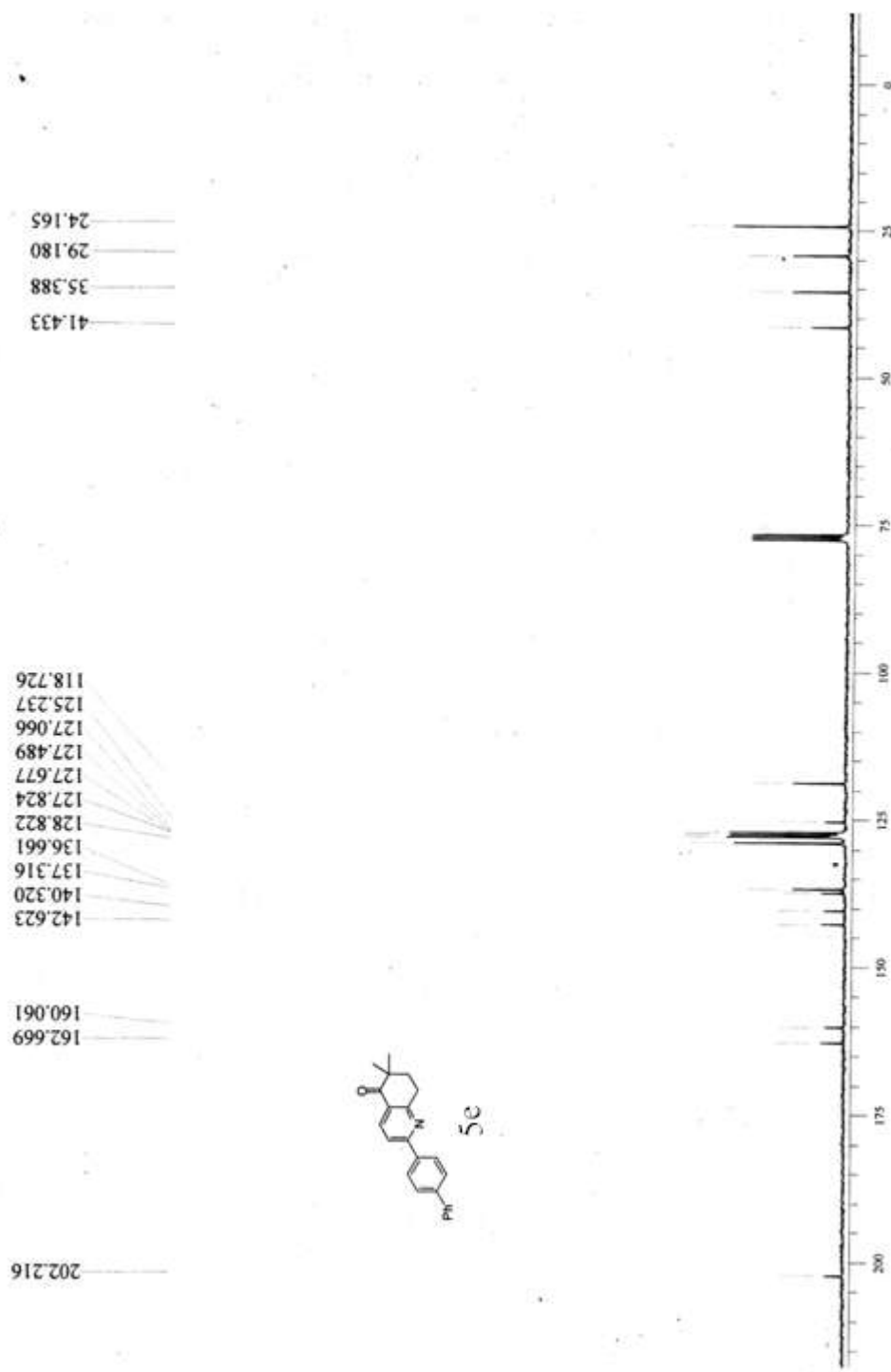


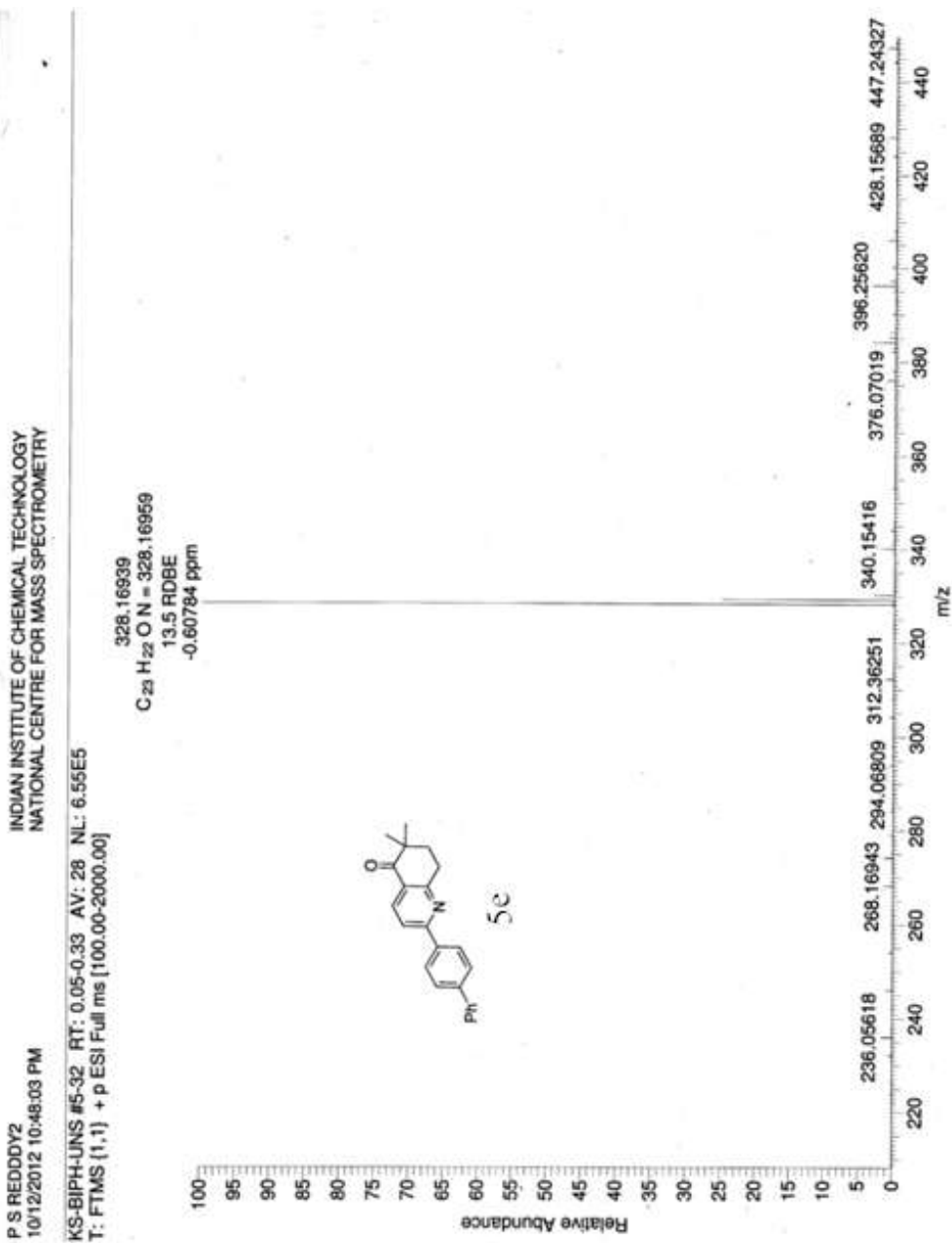


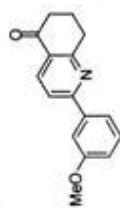






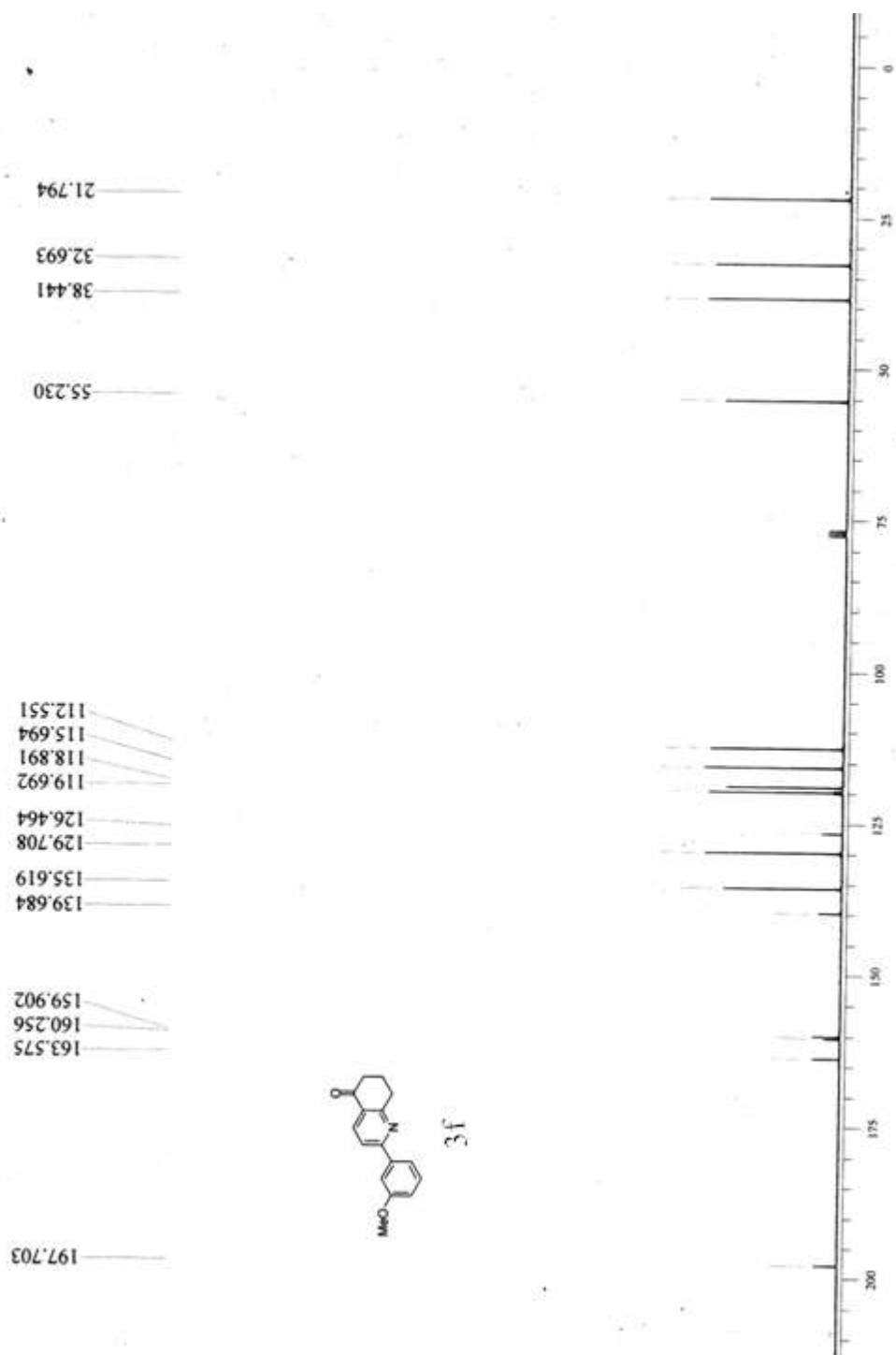


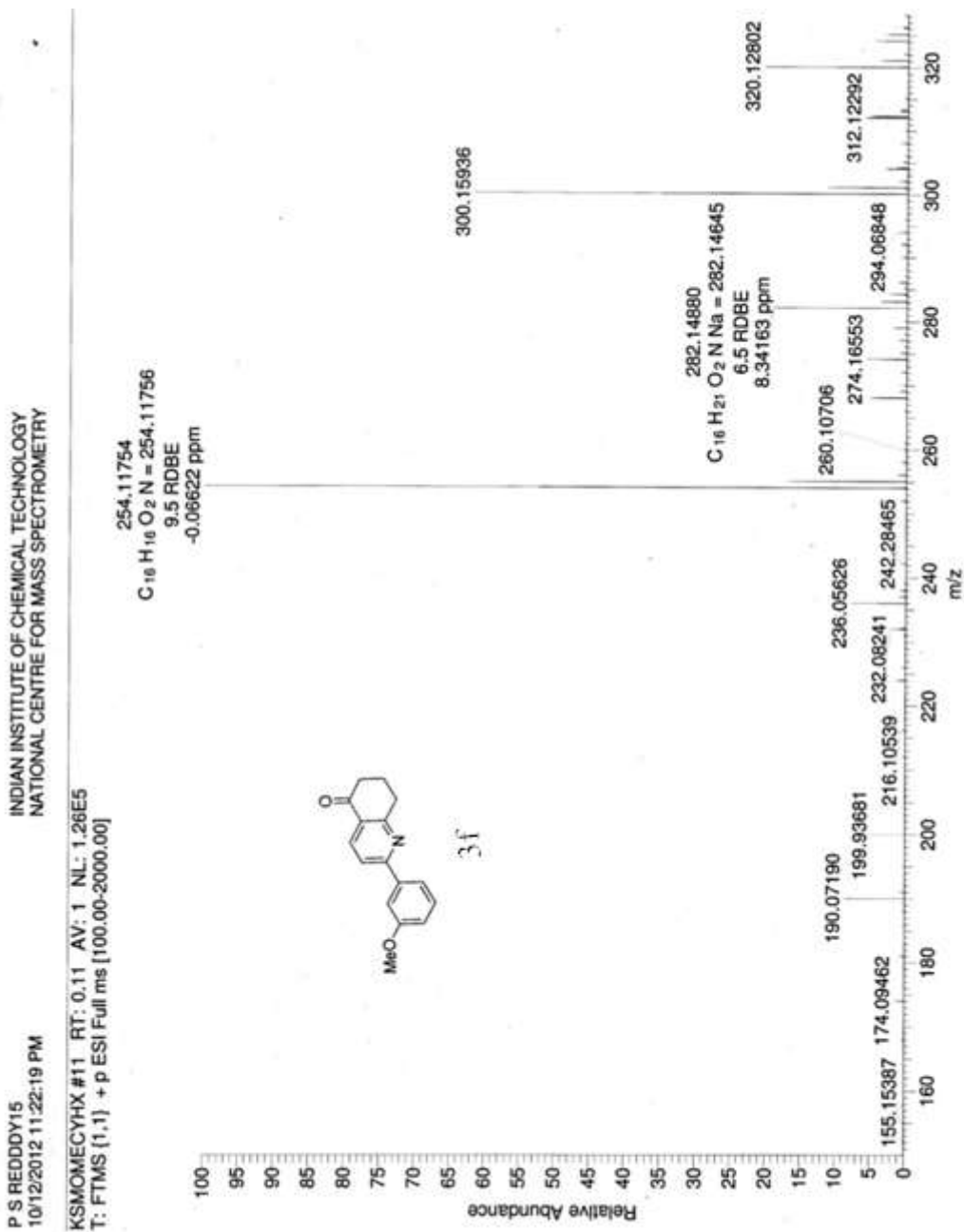


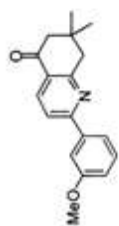


3f

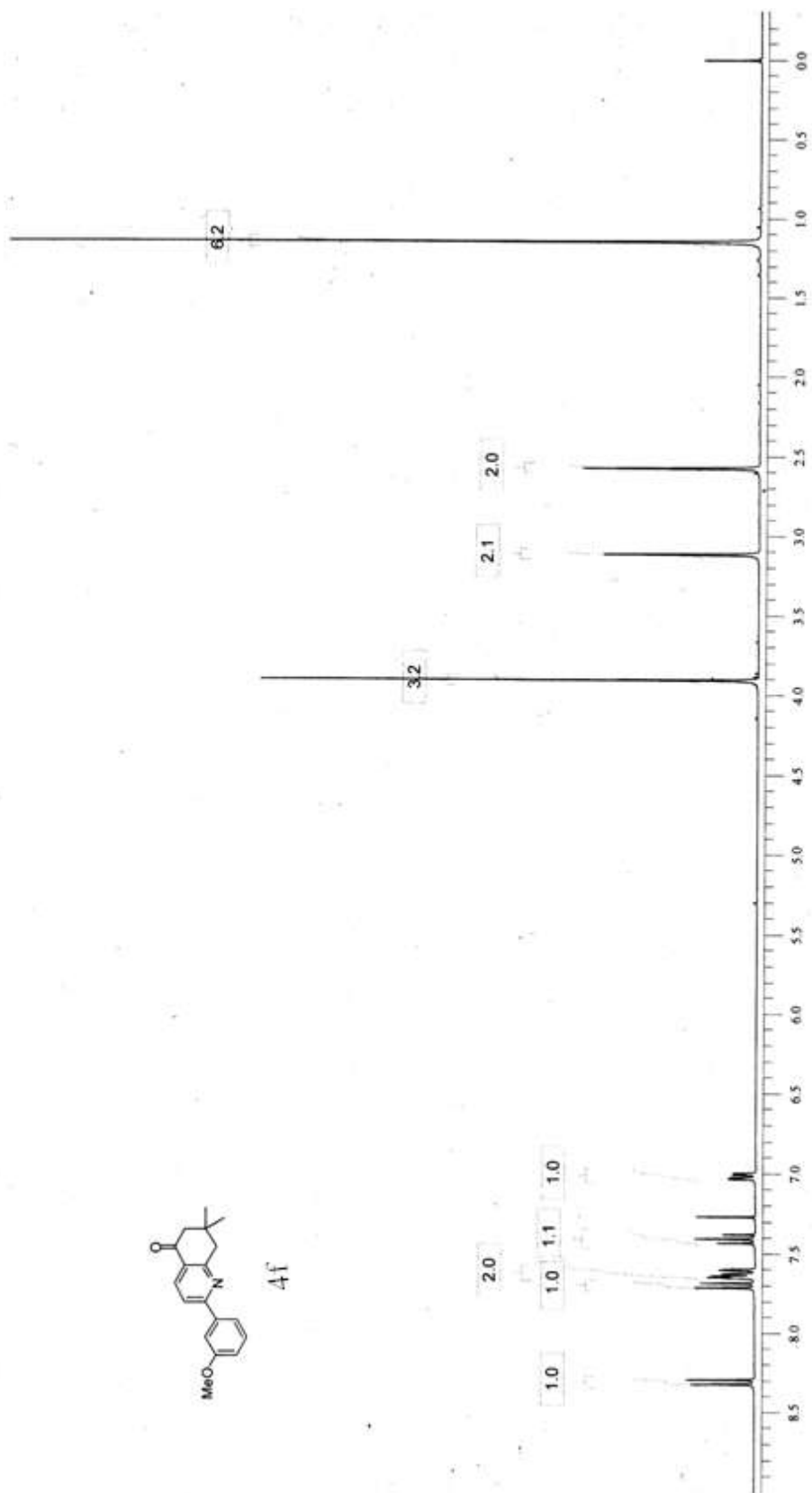


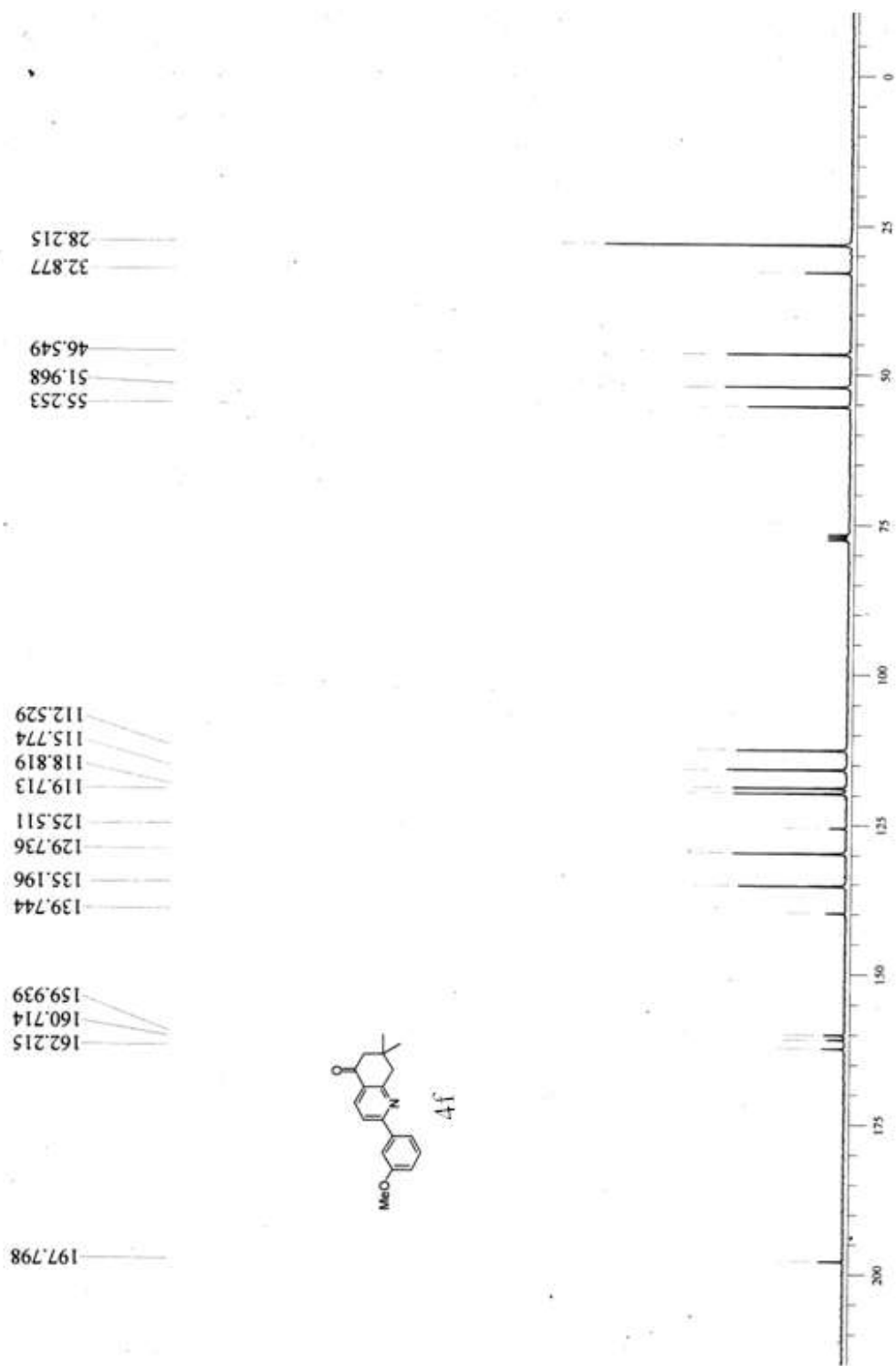






4f



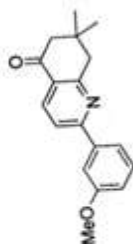


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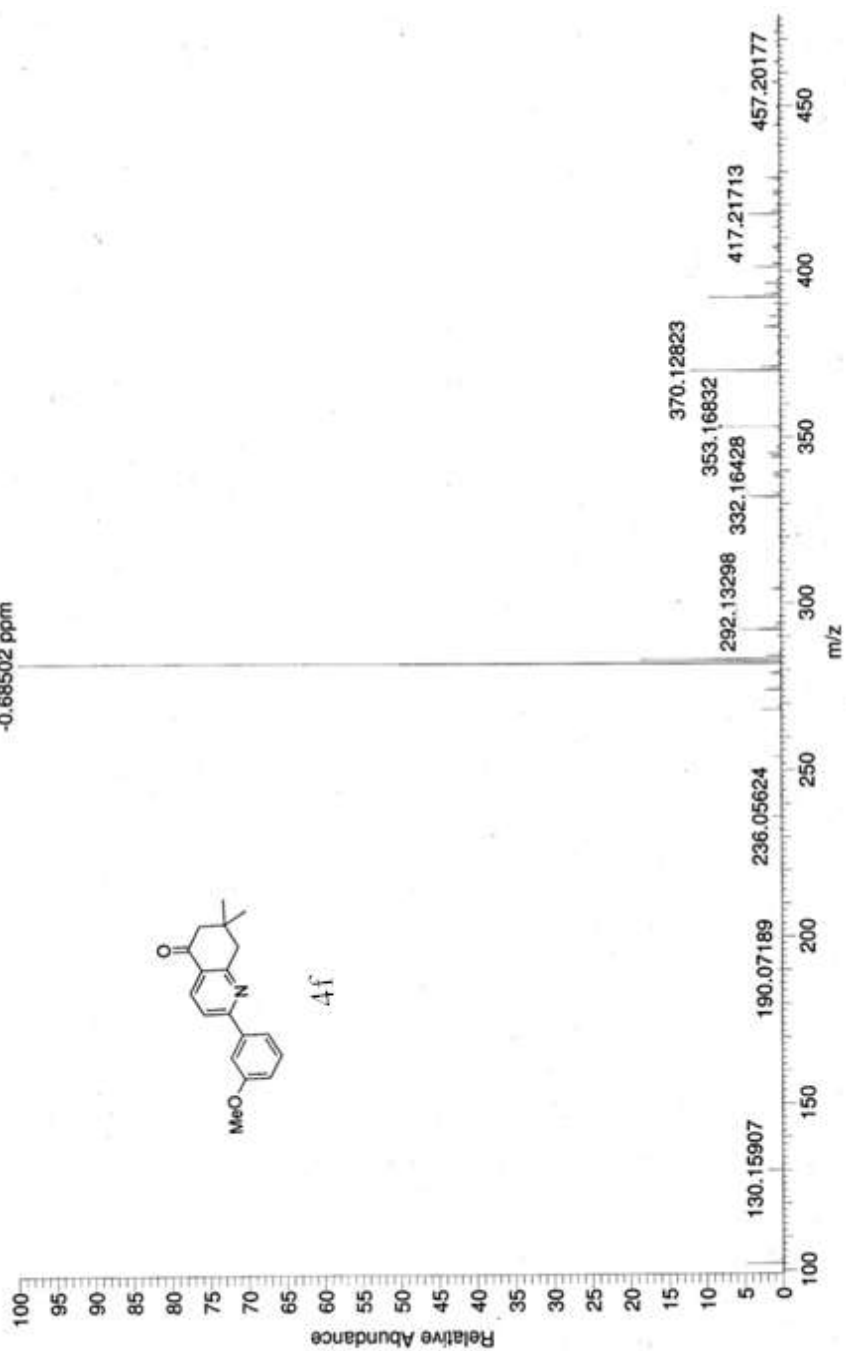
INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY  
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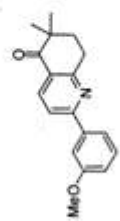
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9.5 FIDBE  
-0.68502 ppm



4f

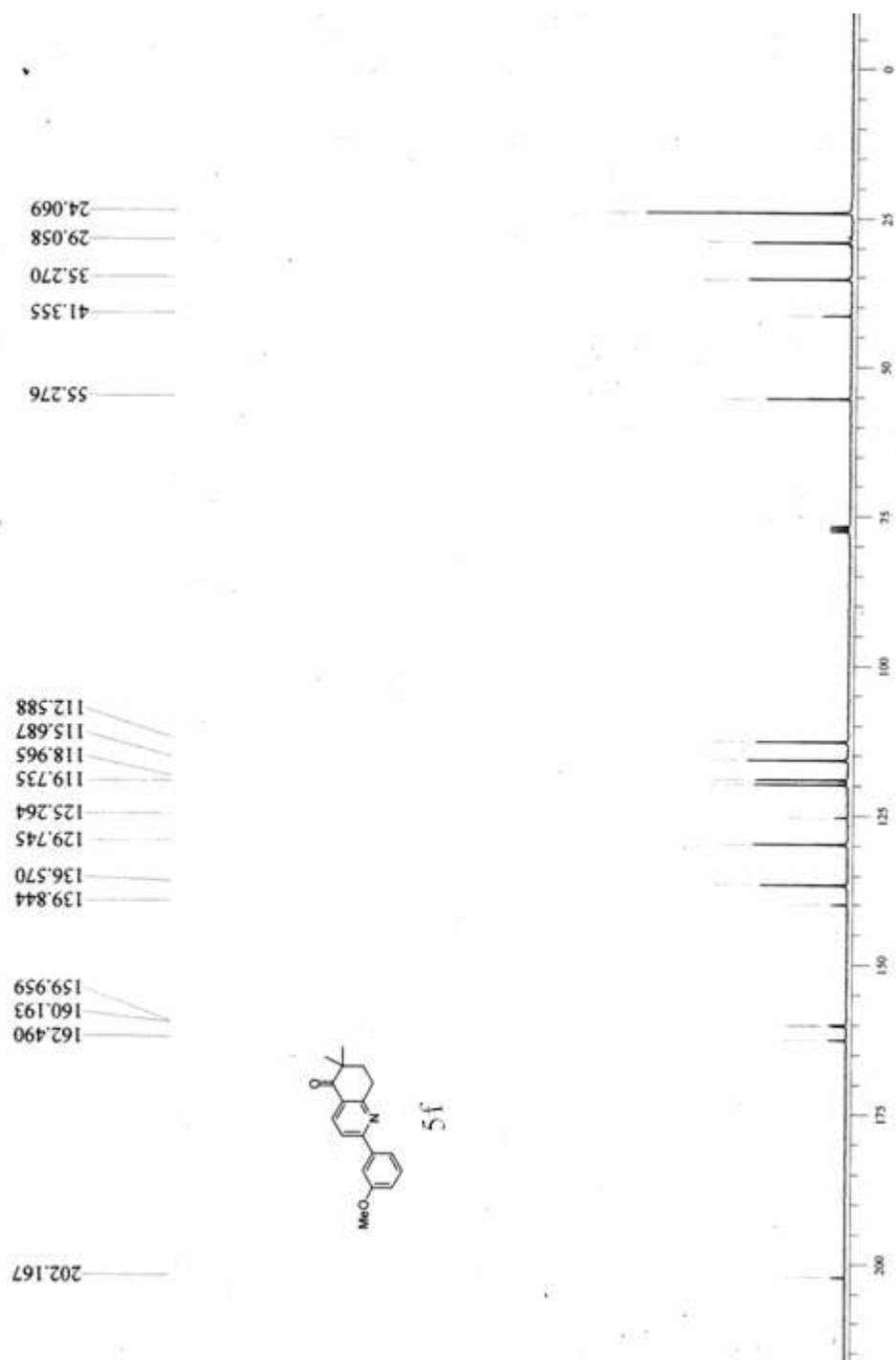


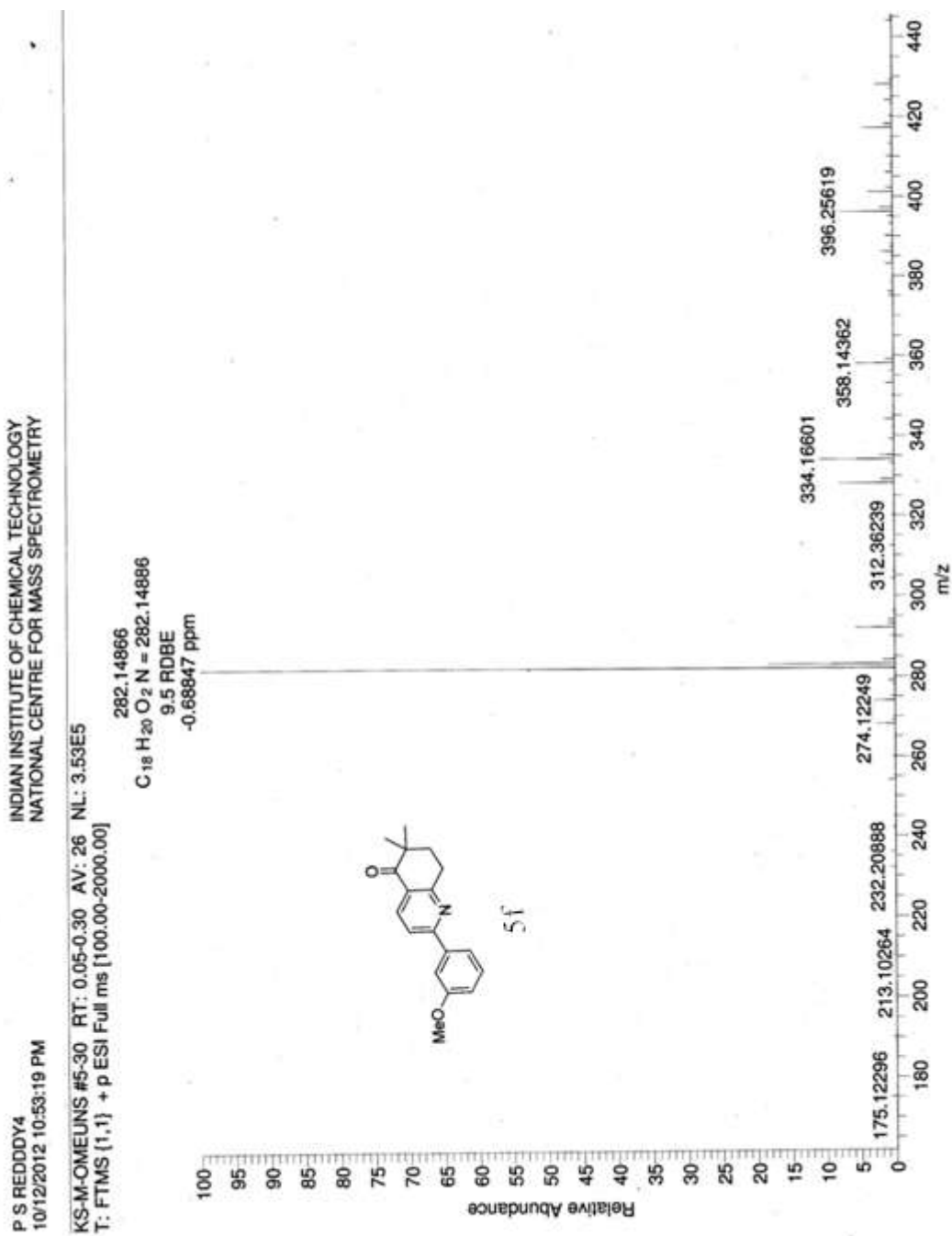


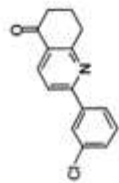


5f

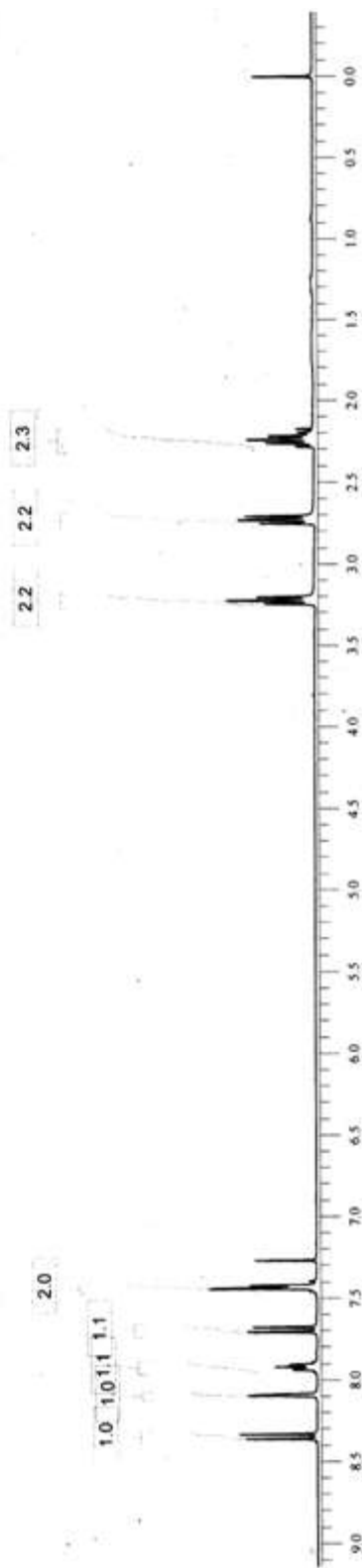


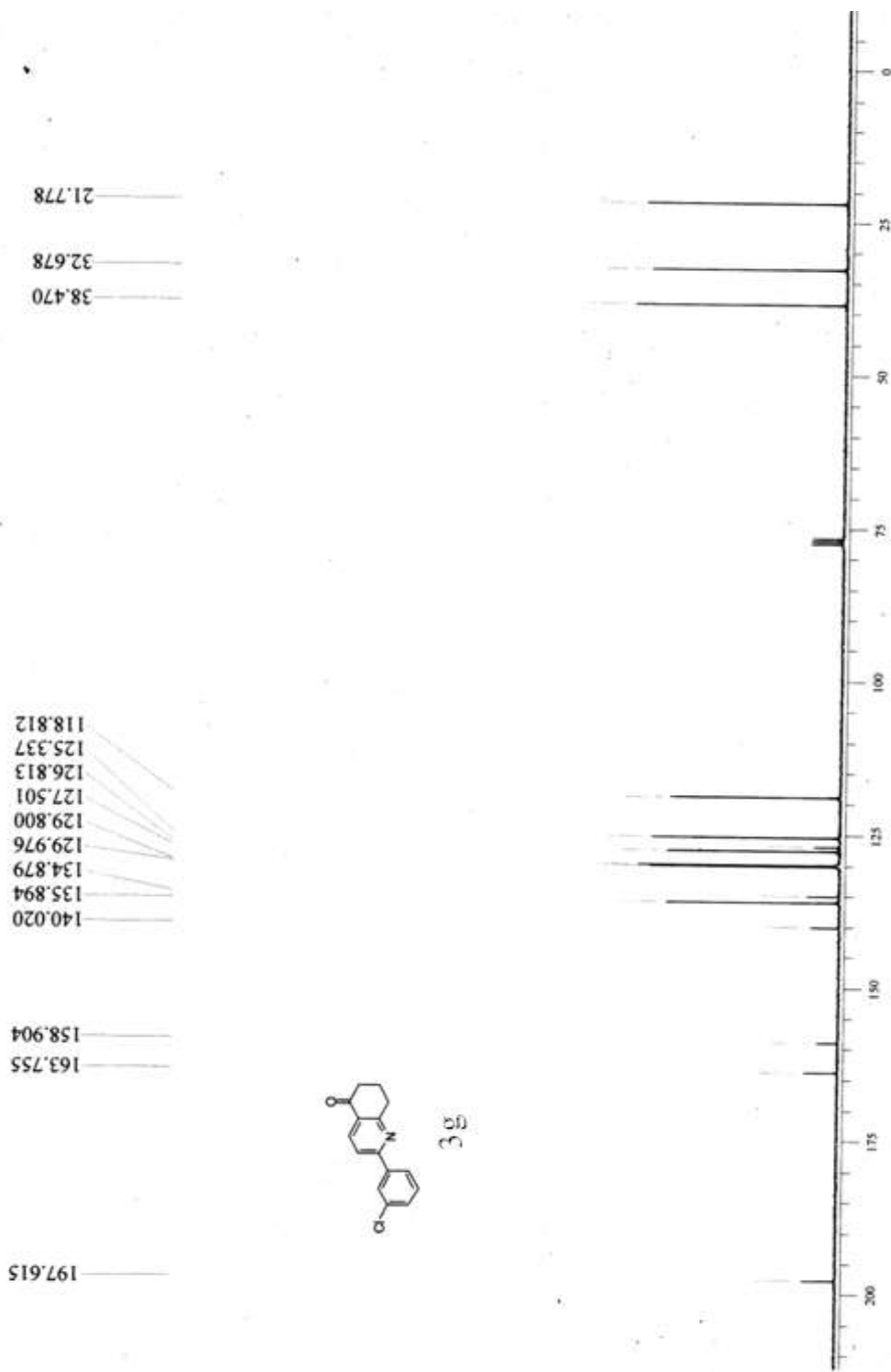


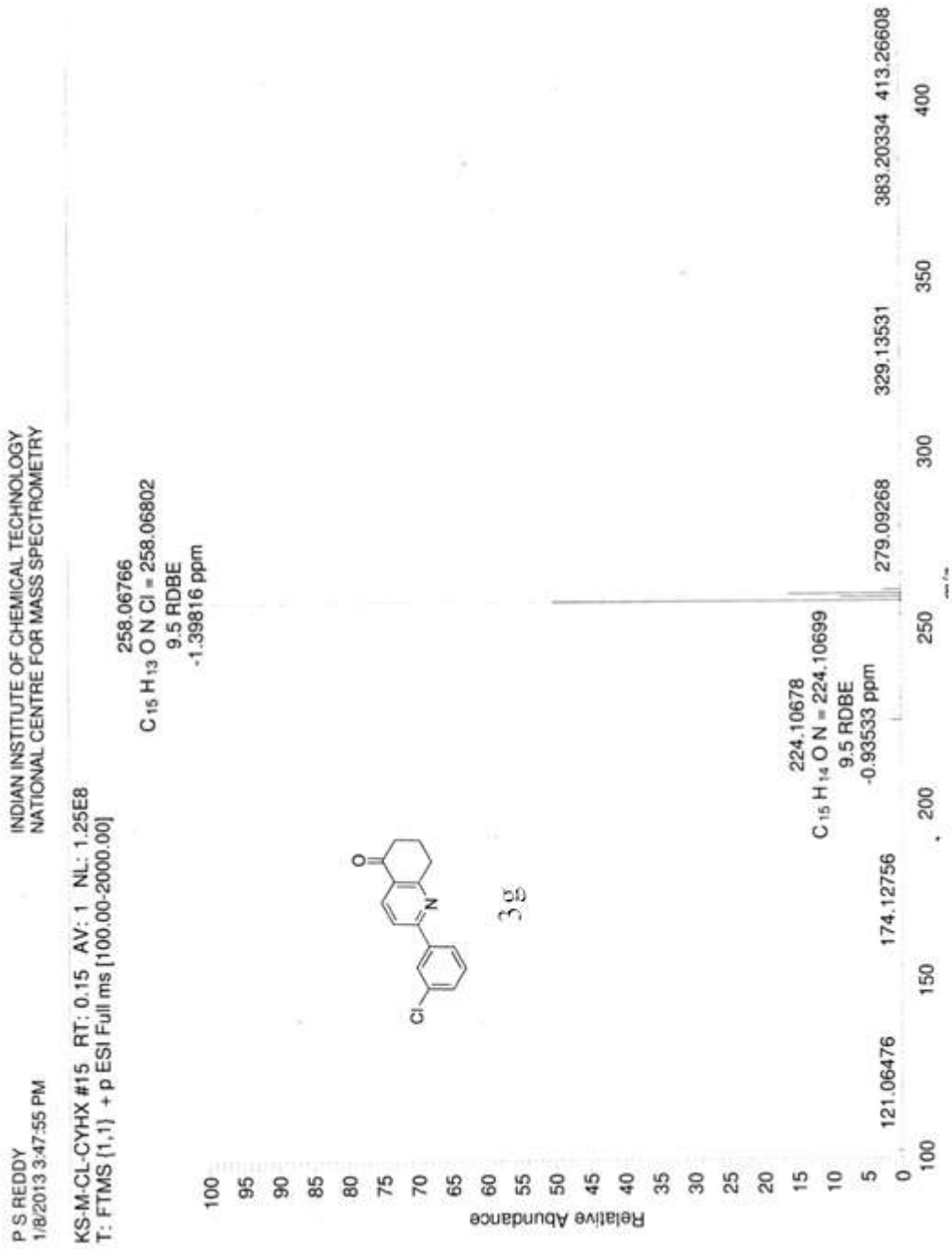


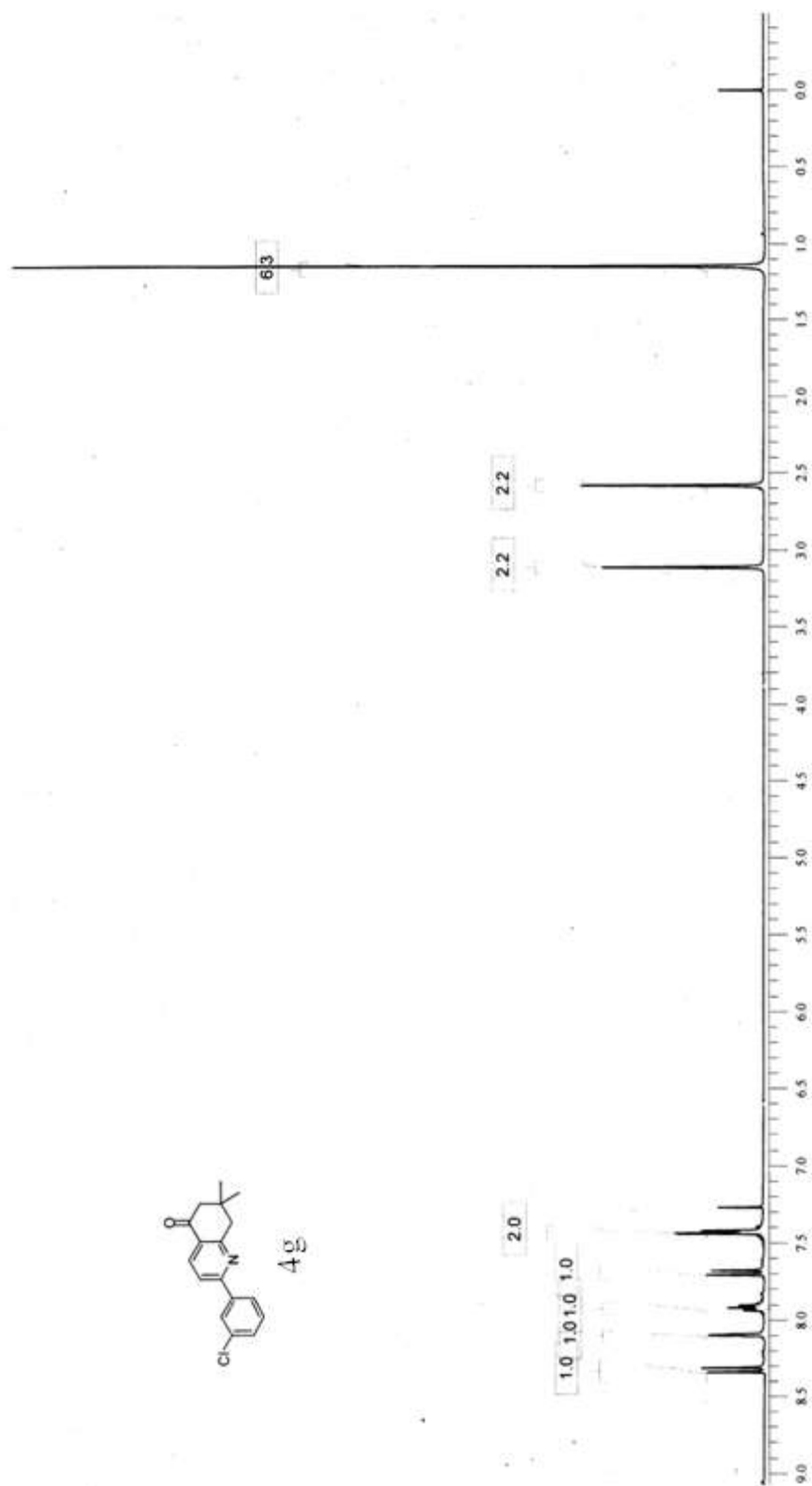


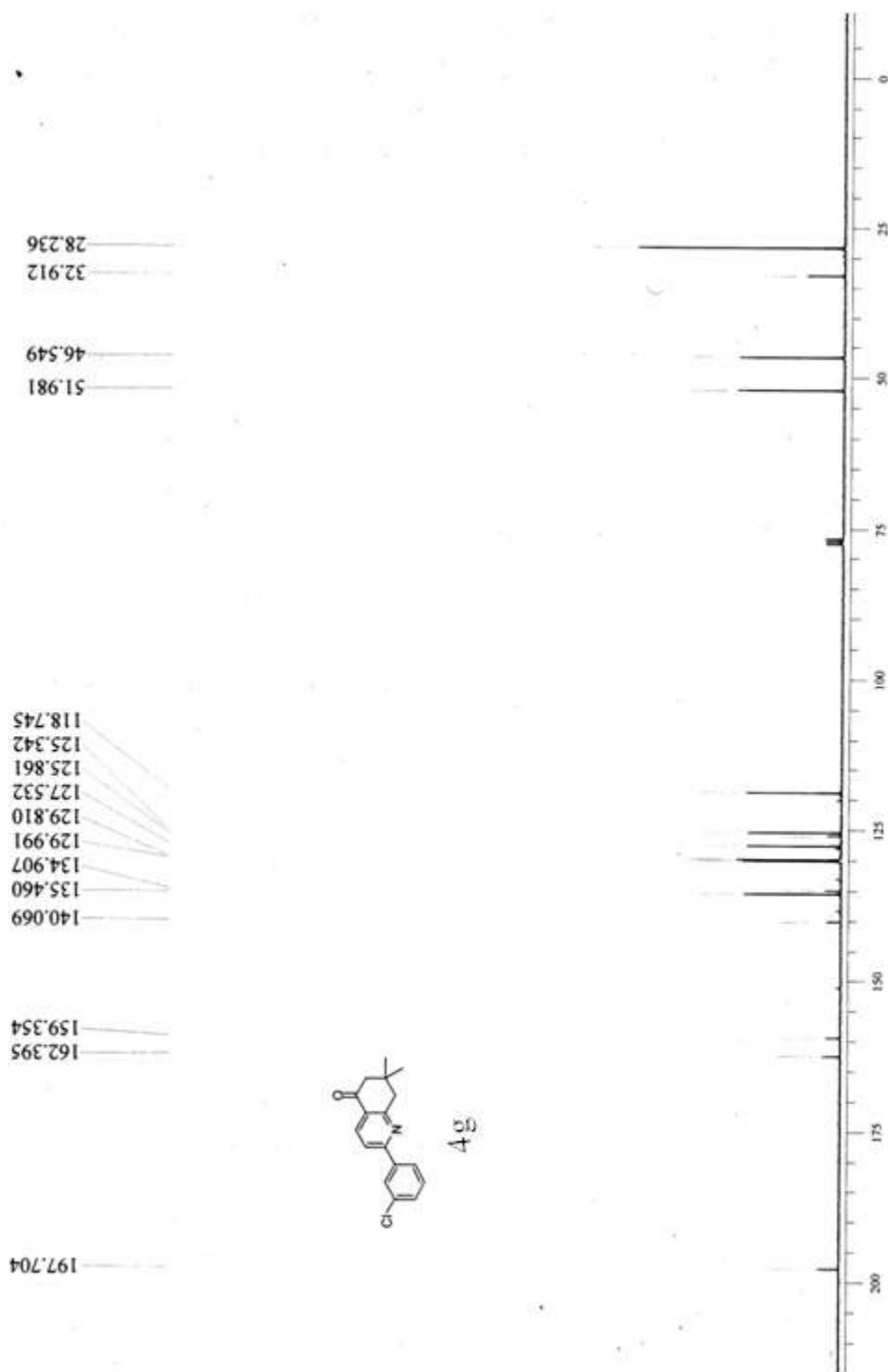
3.99



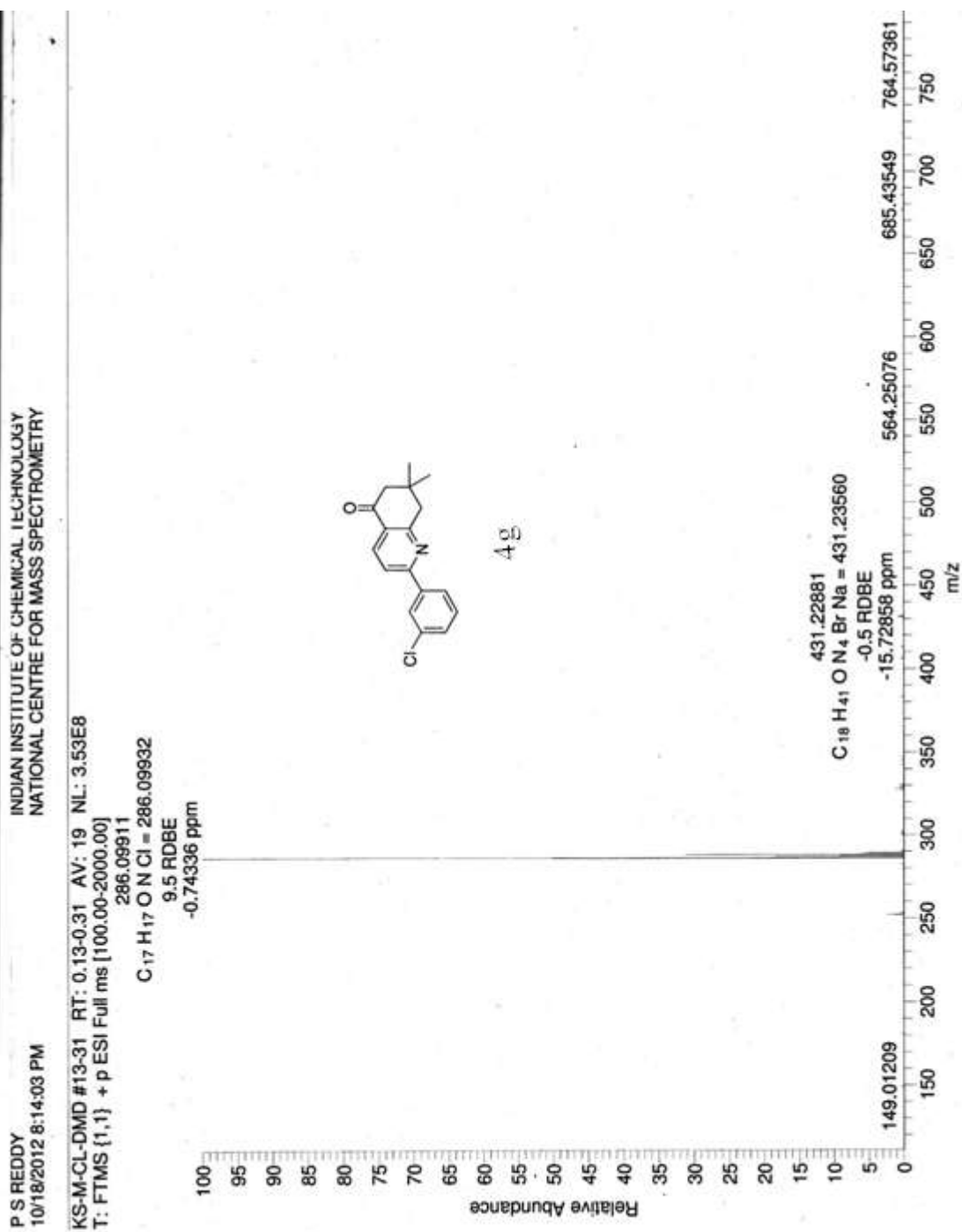


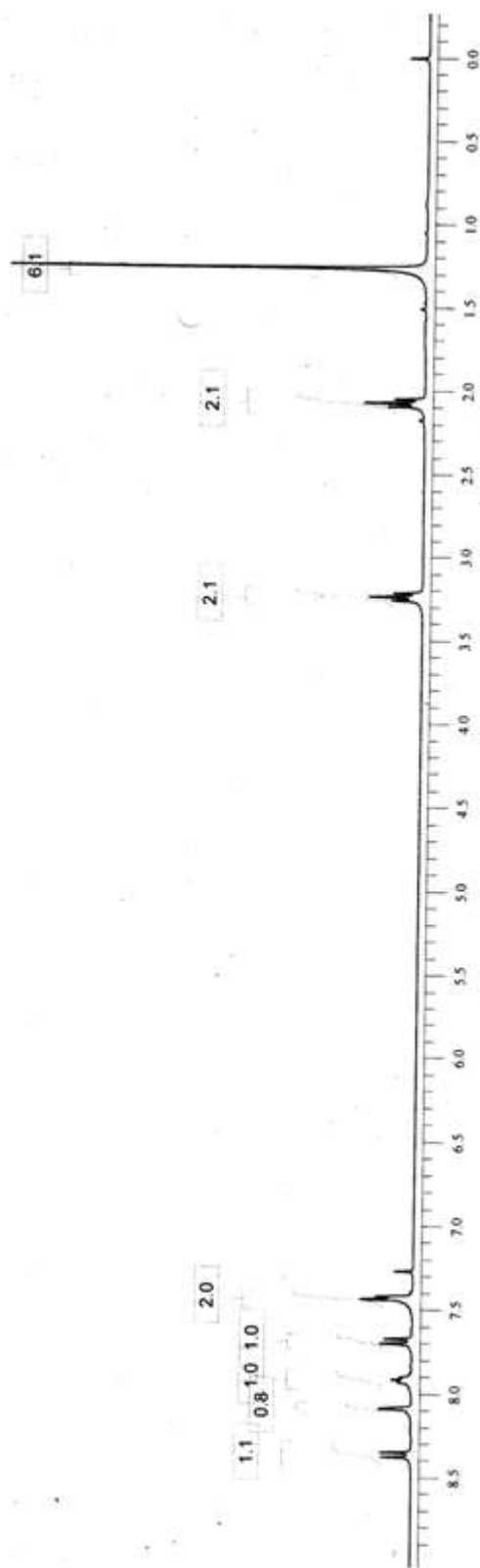
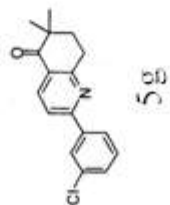


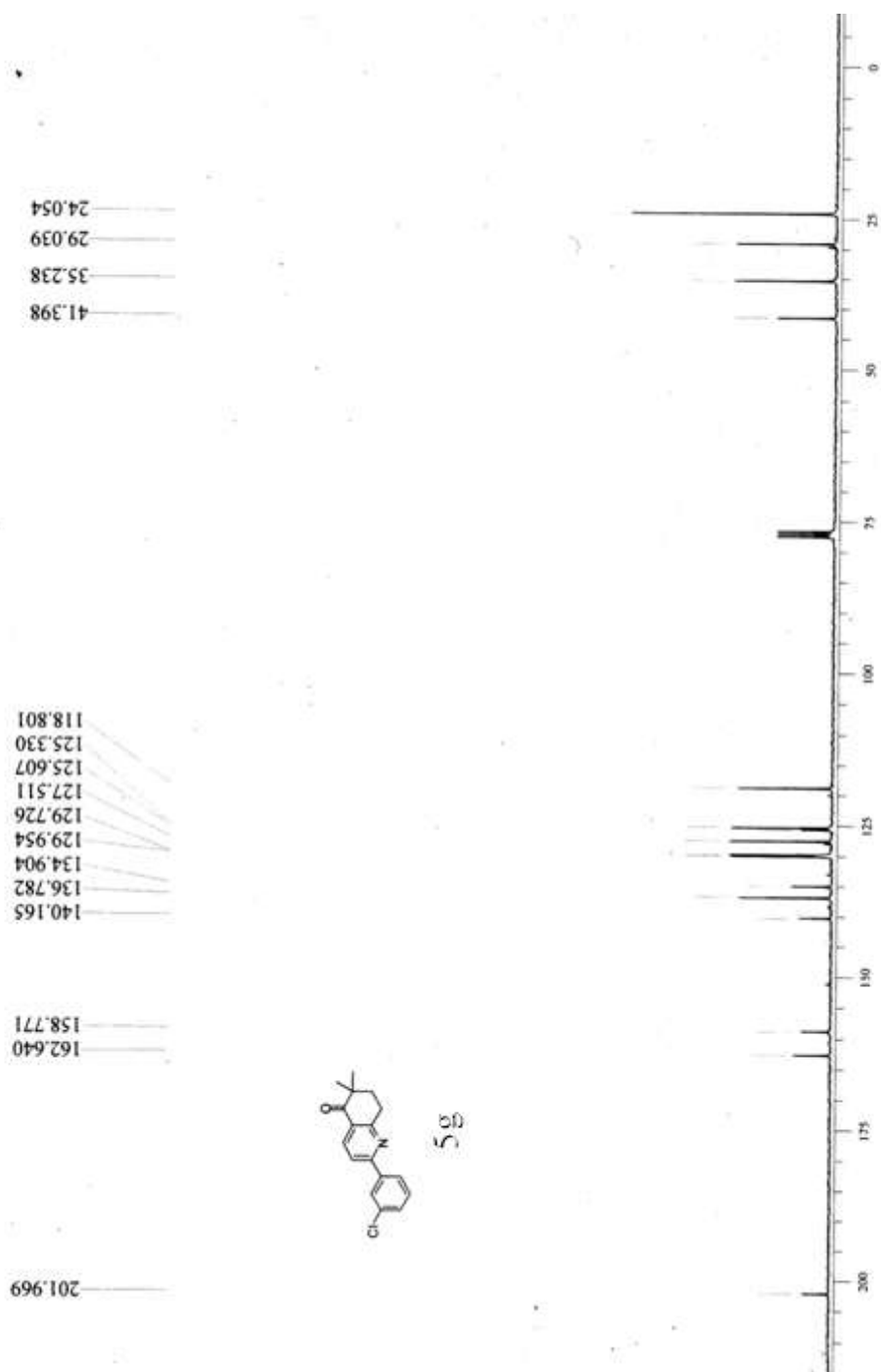


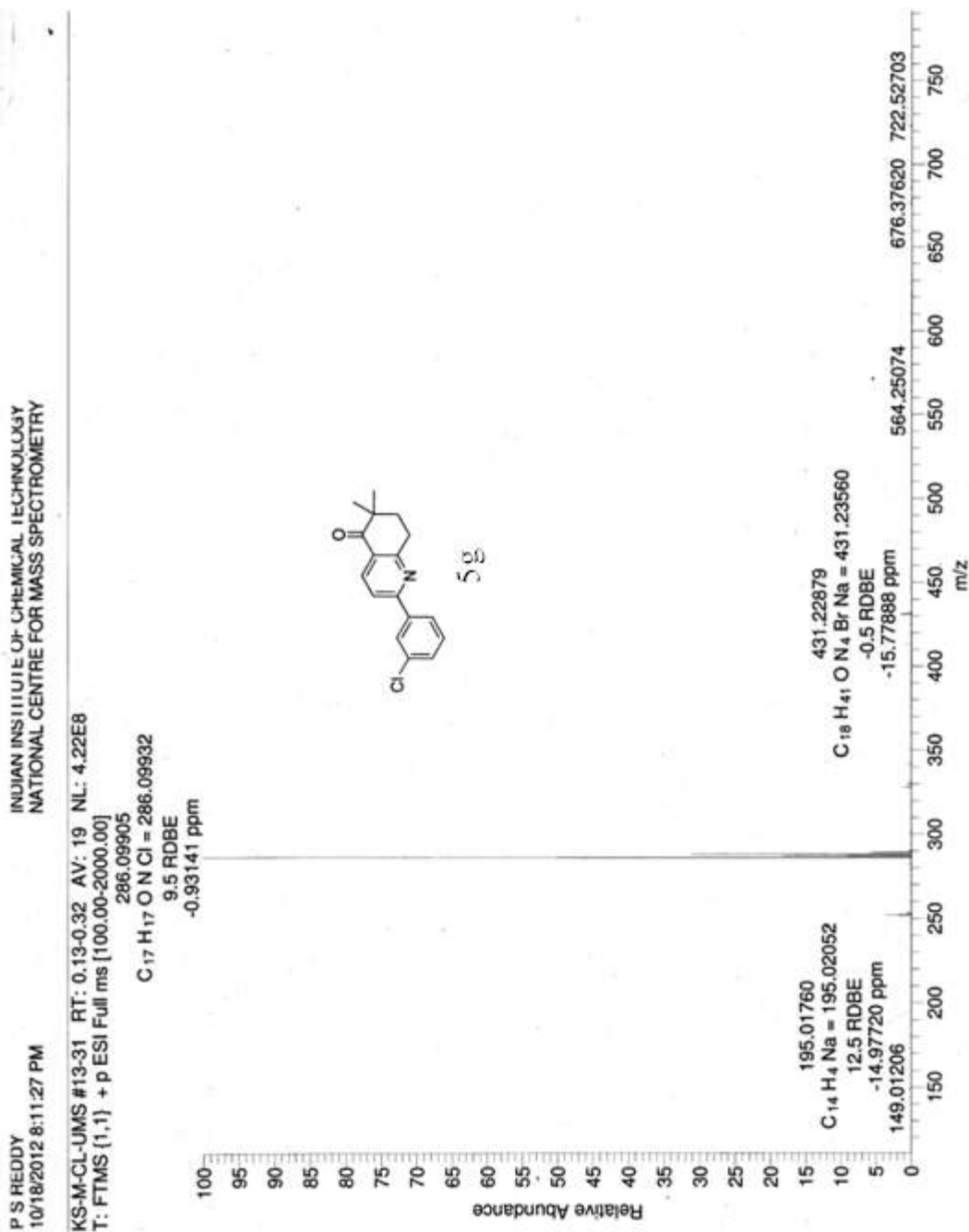


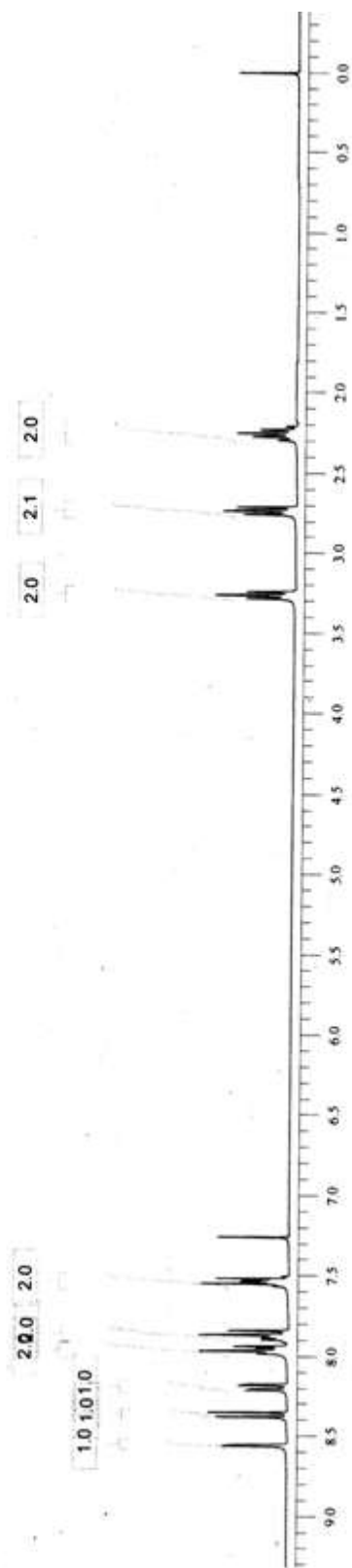
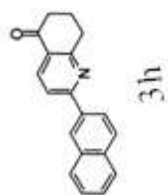


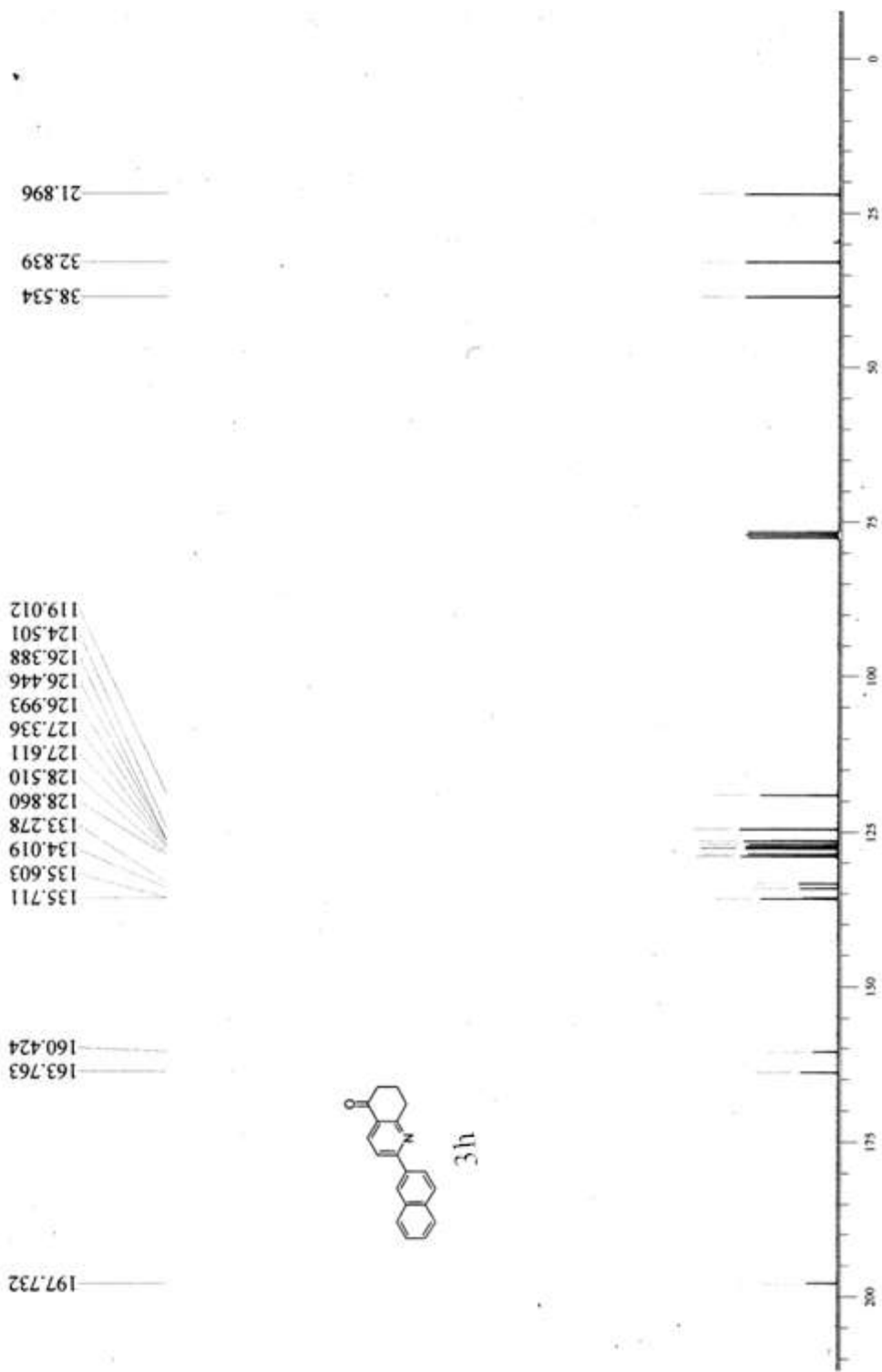


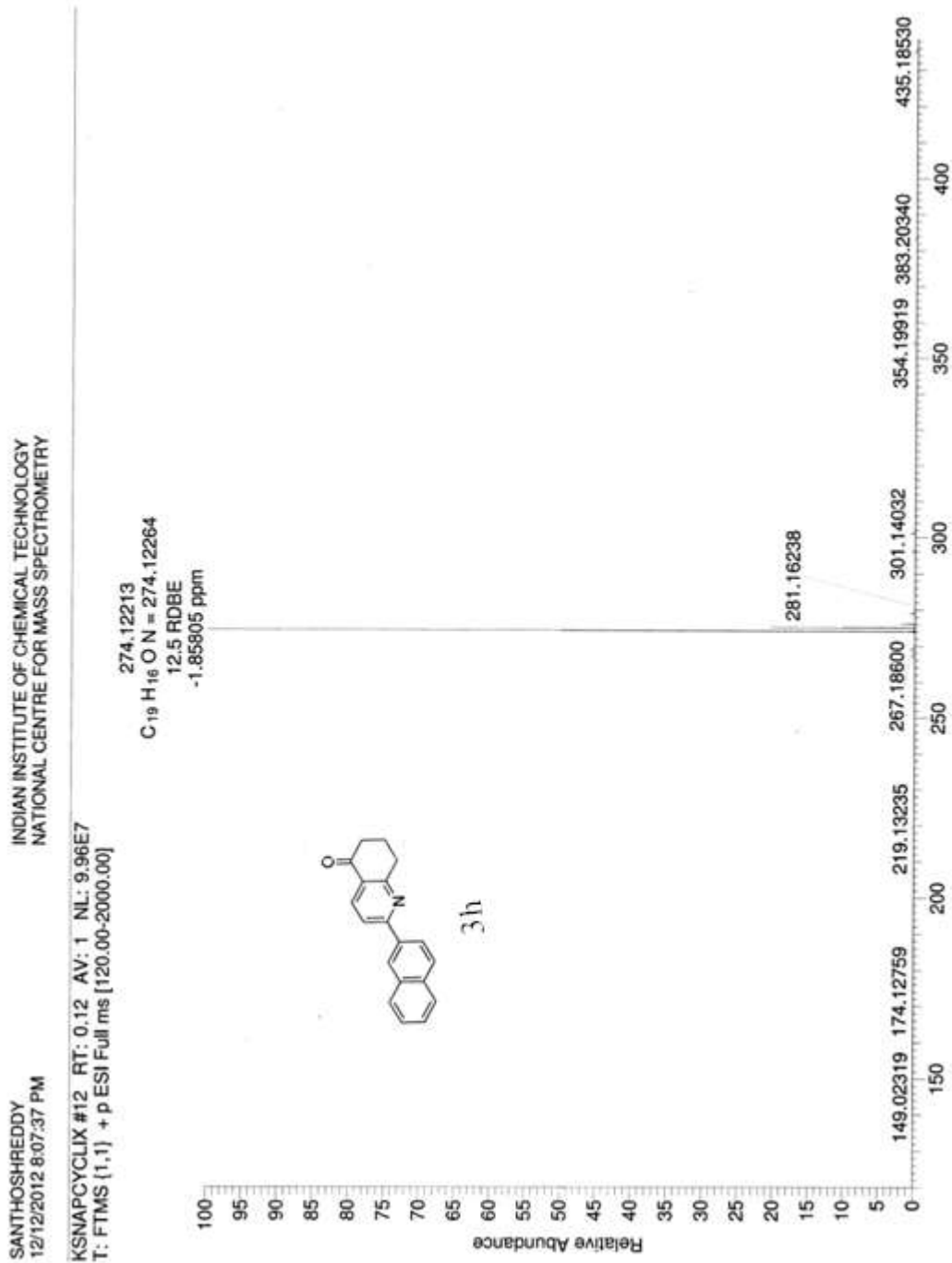


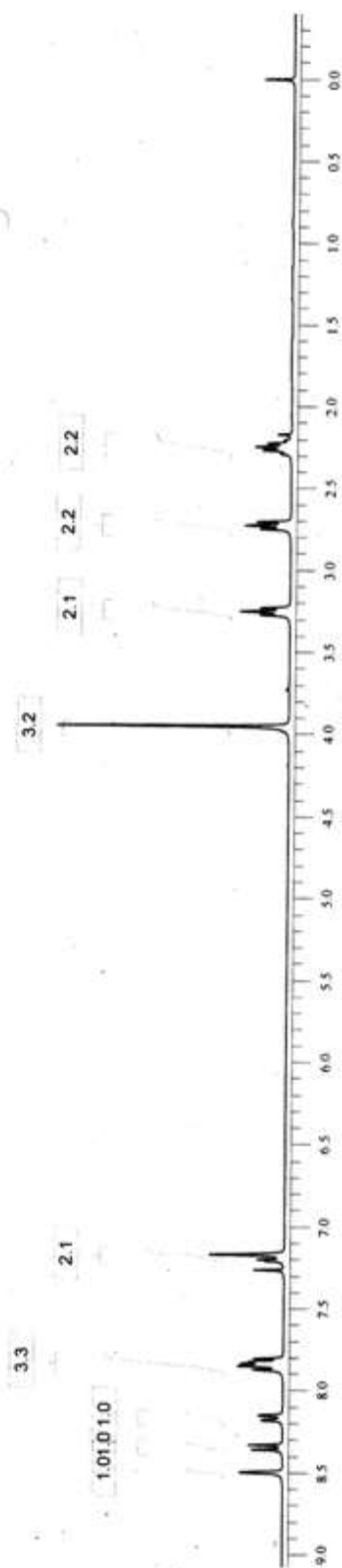
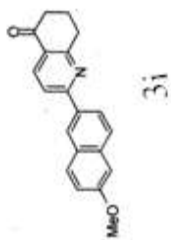




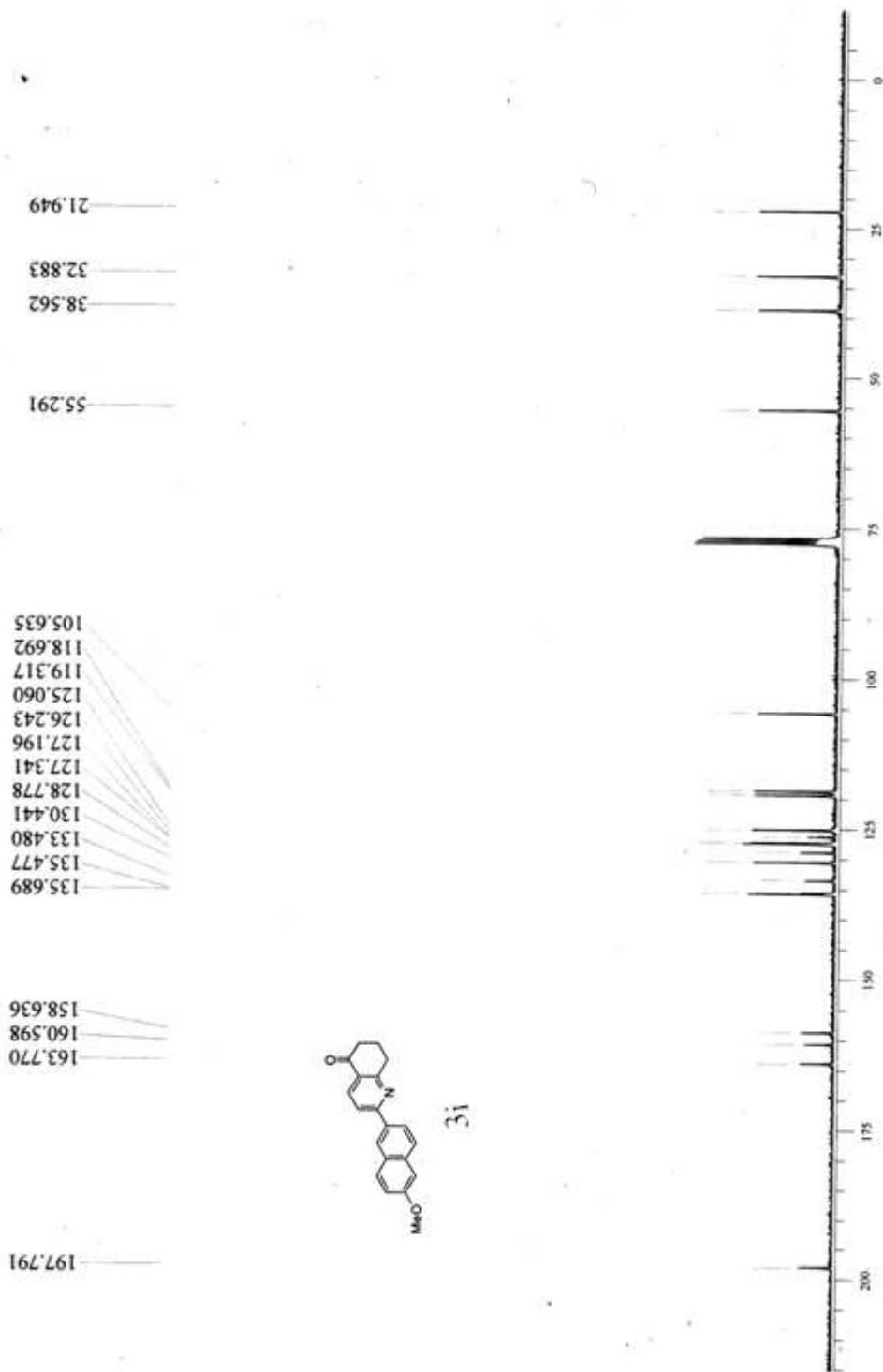


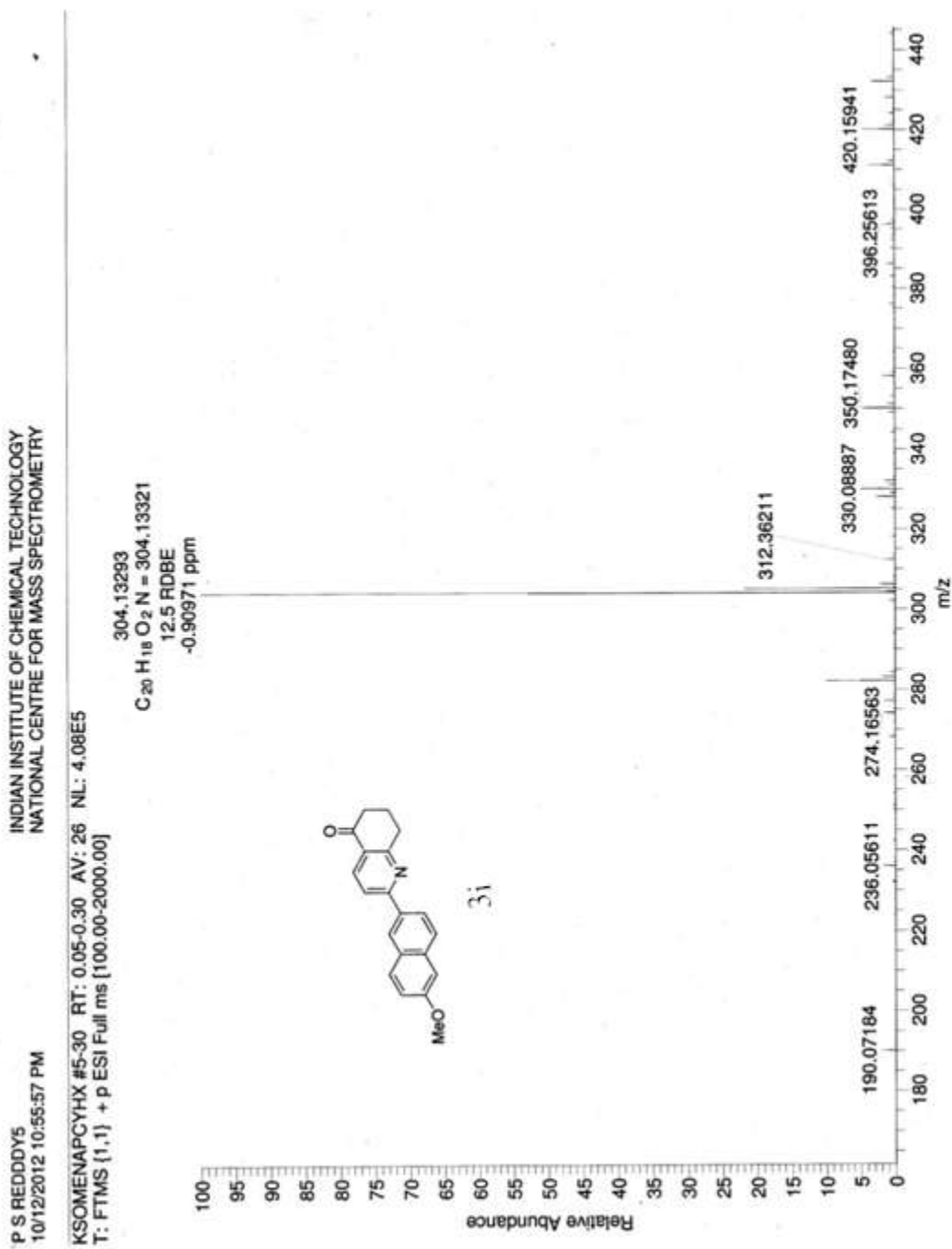


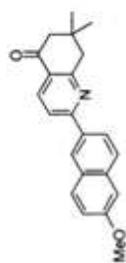






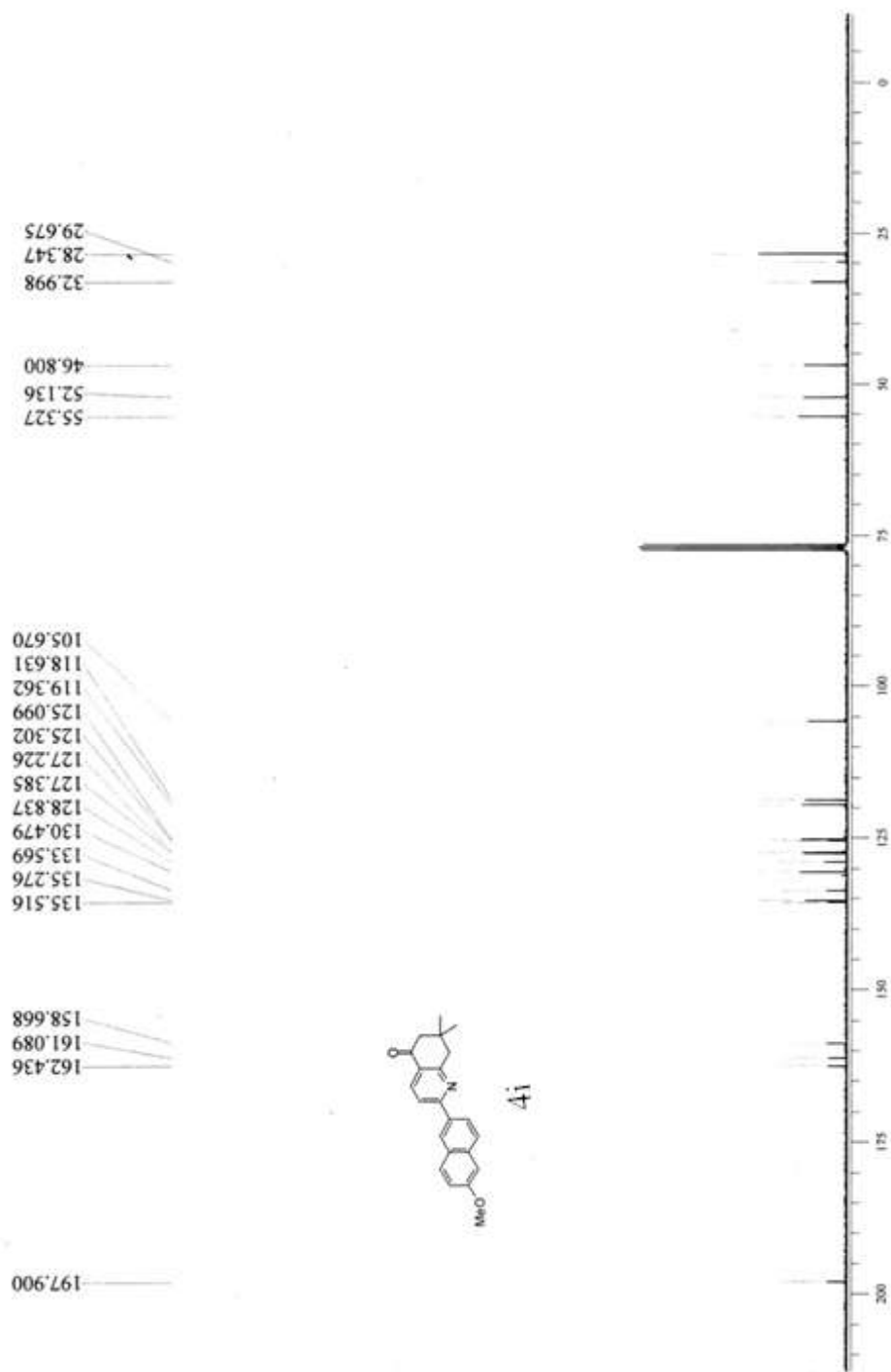






4i

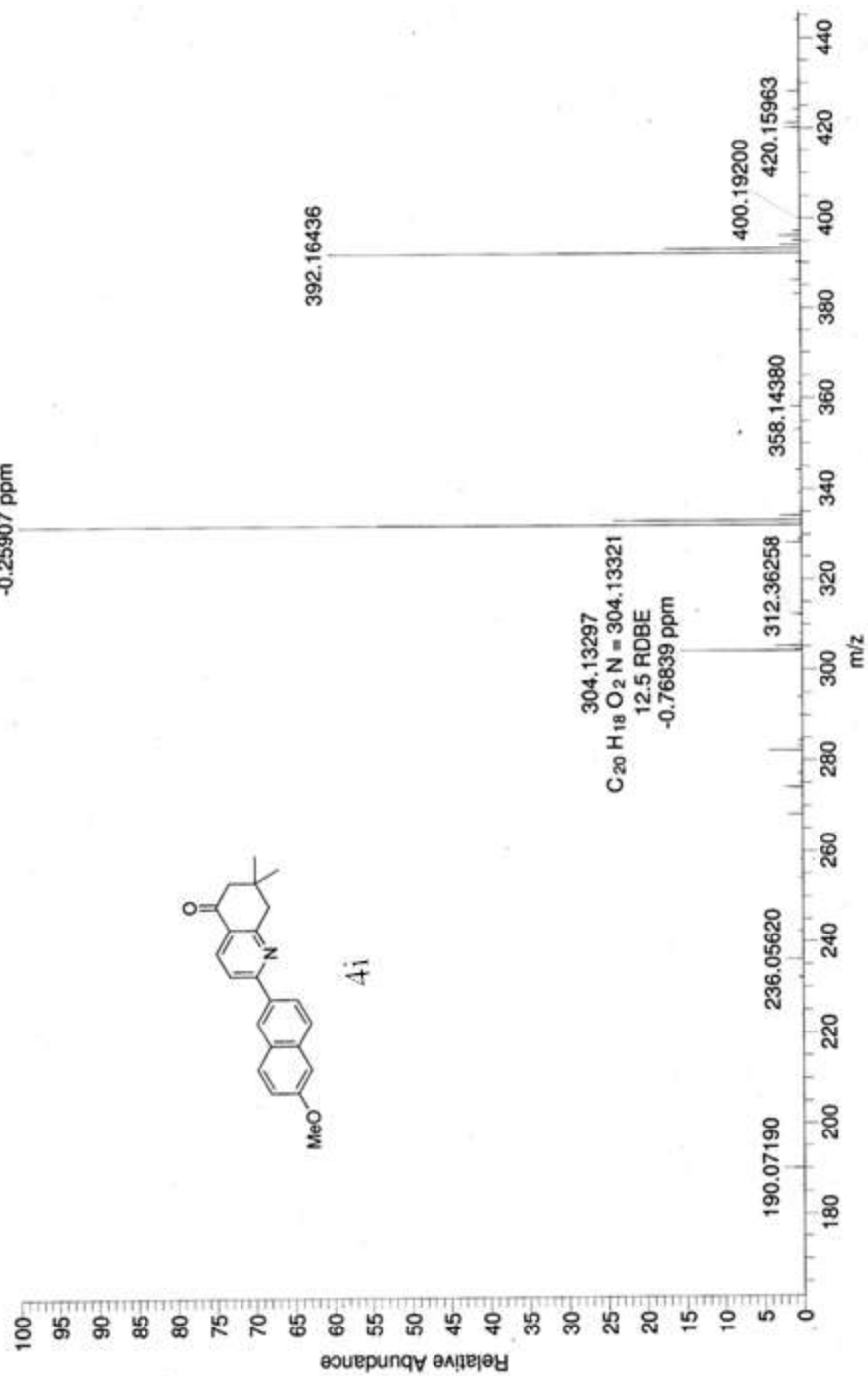


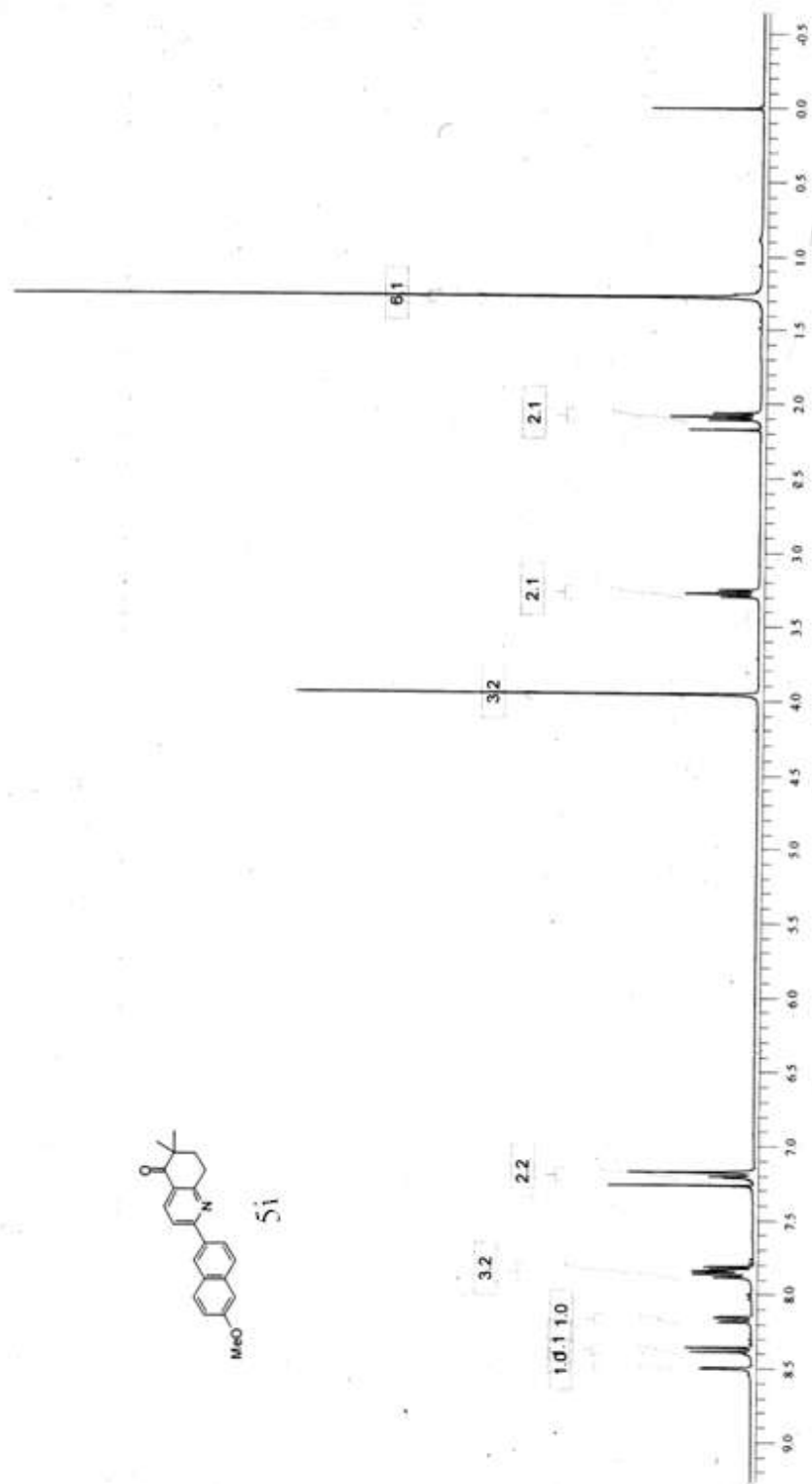


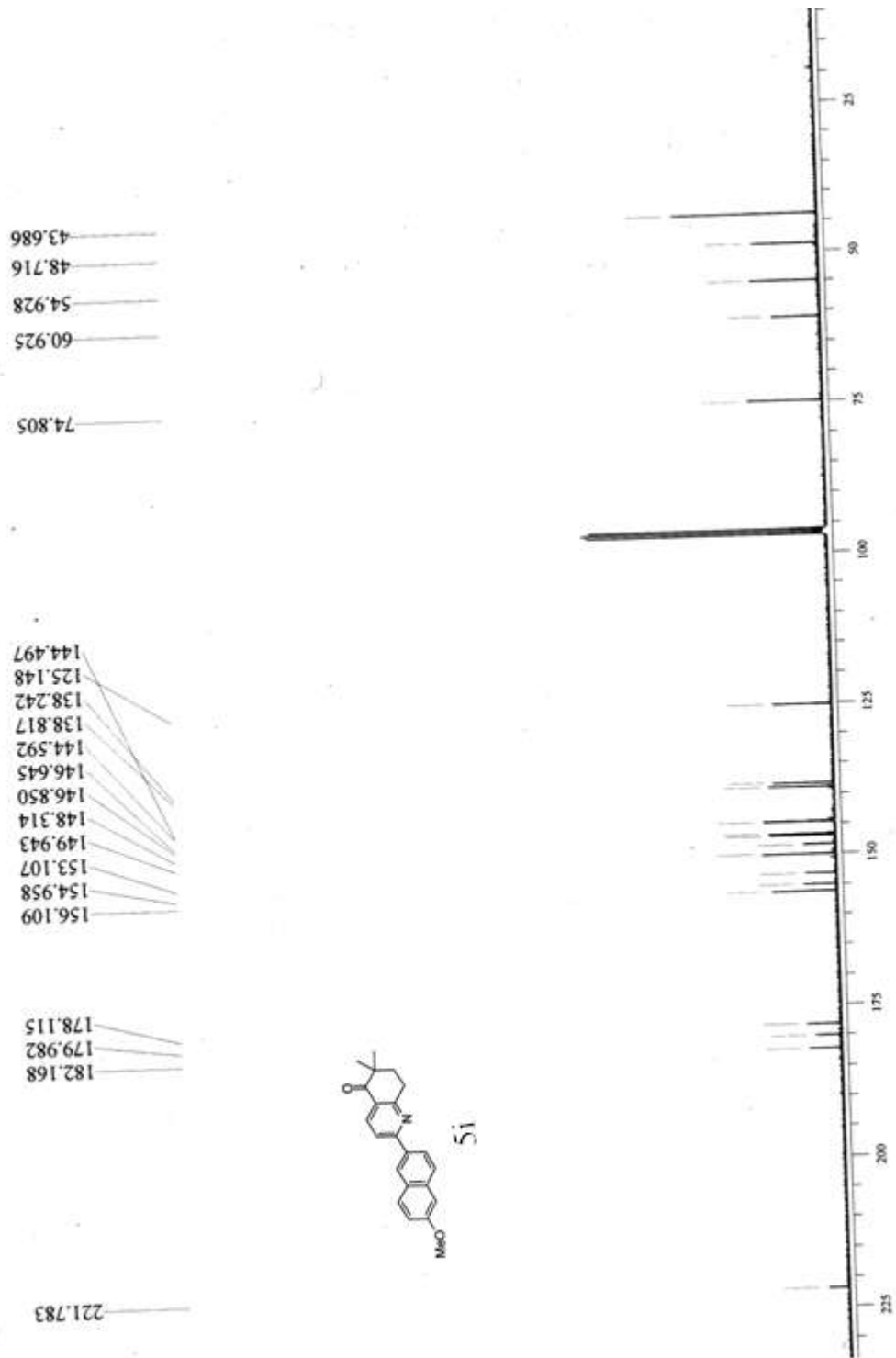
P S REDDYY6  
10/12/2012 10:58:35 PM

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KSOMENAPDMD #5-30 RT: 0.05-0.30 AV: 26 NL: 2.62E5  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]



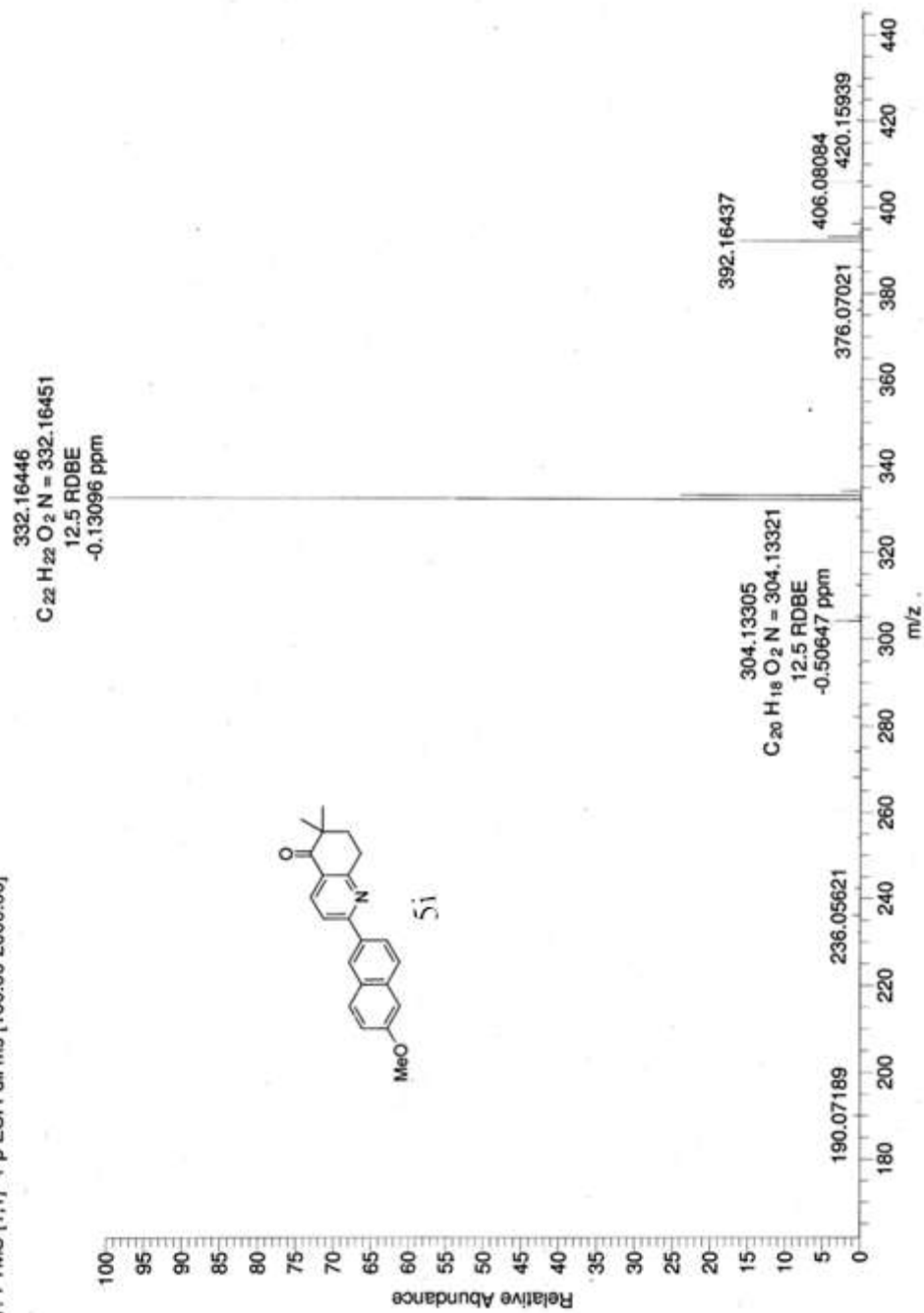




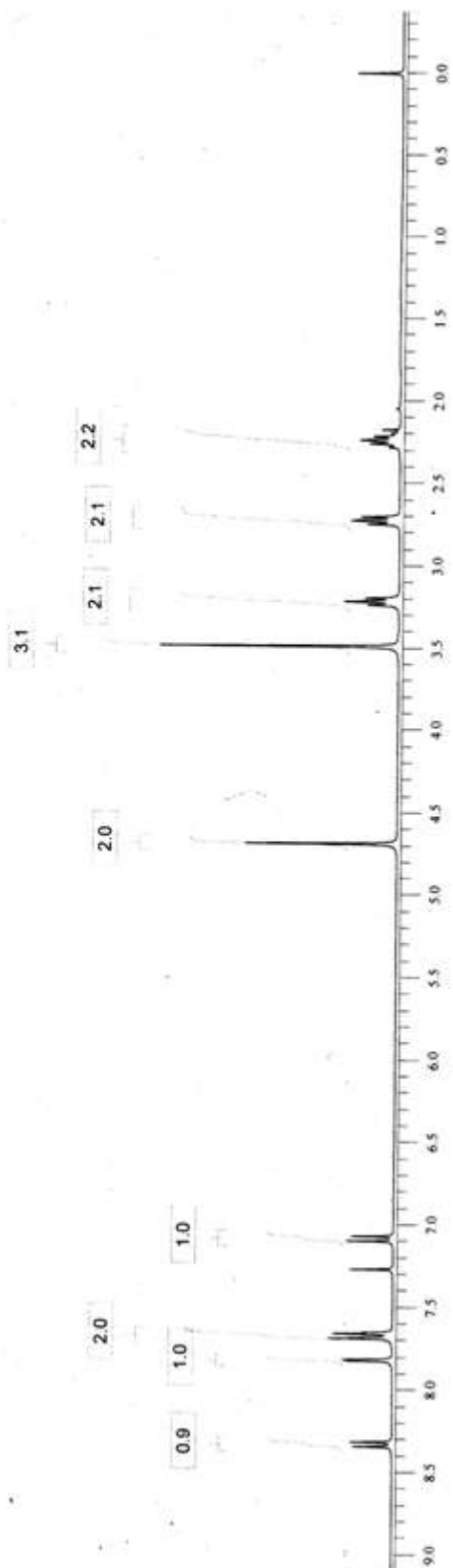
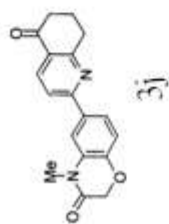
P S REDDDY  
10/12/2012 11:01:13 PM

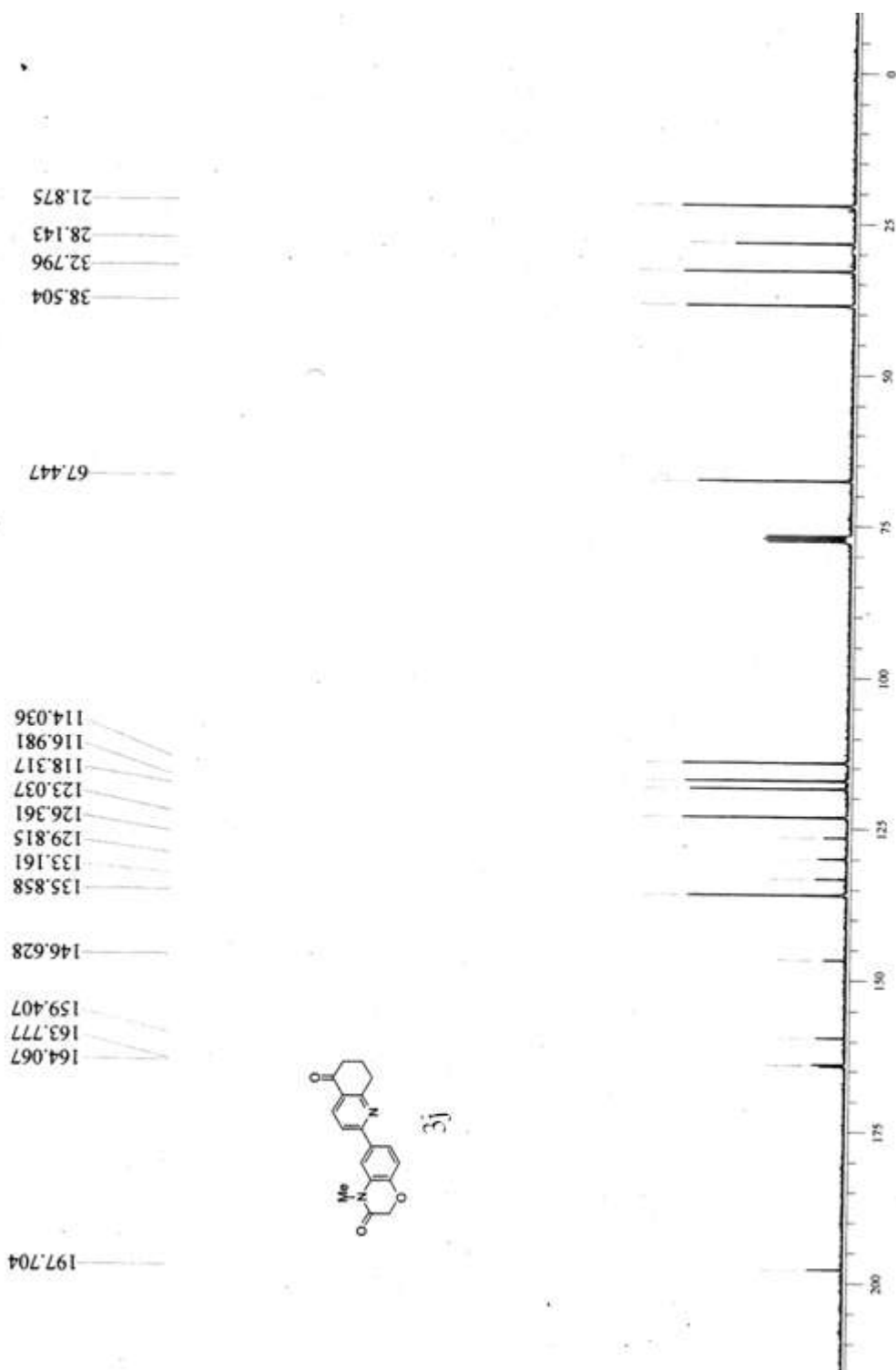
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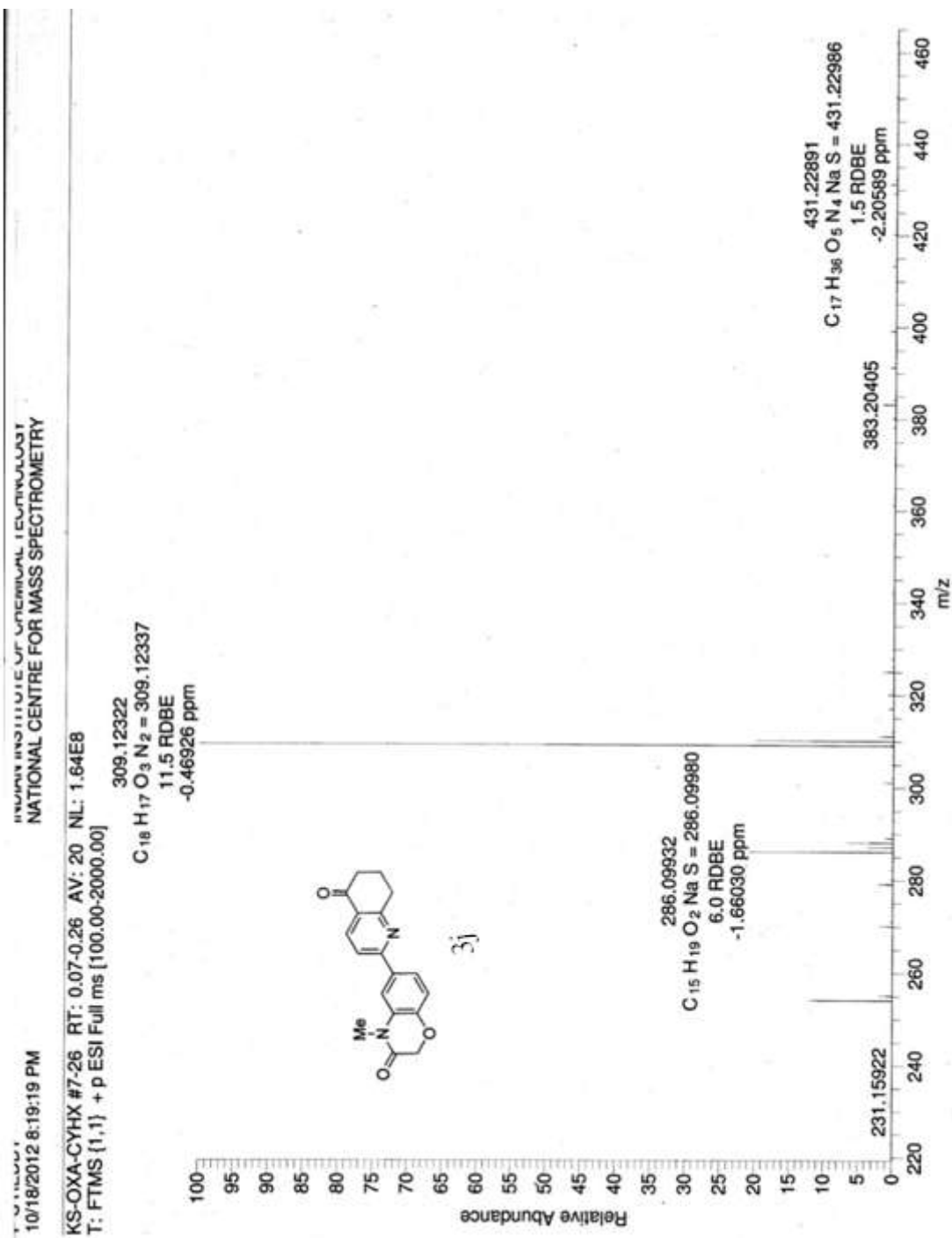
KSOMENAPUNUS #5-29 RT: 0.05-0.29 AV: 25 NL: 8.72E5  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

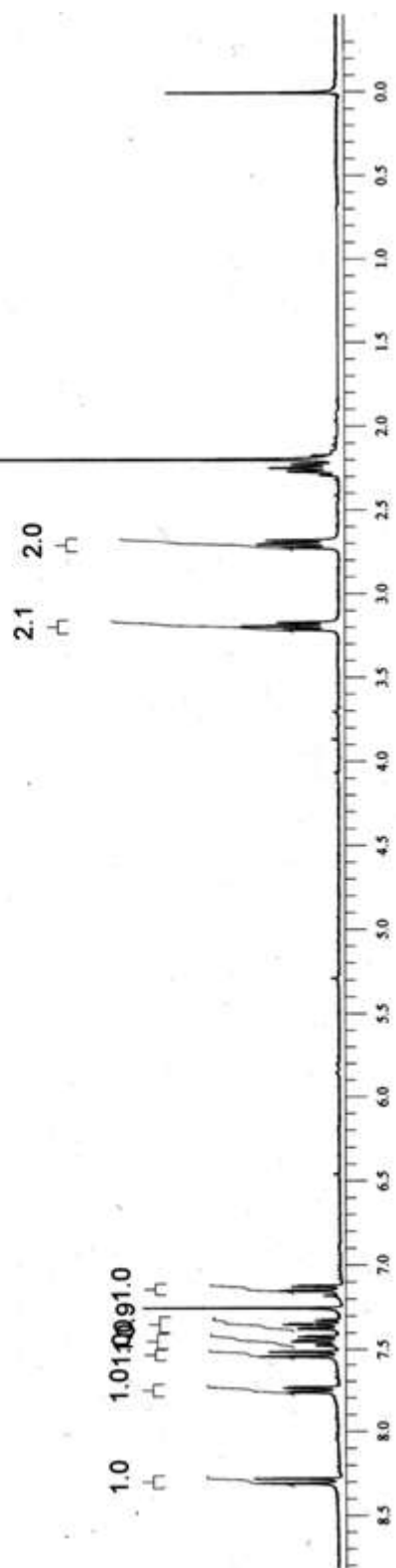
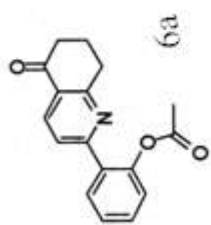


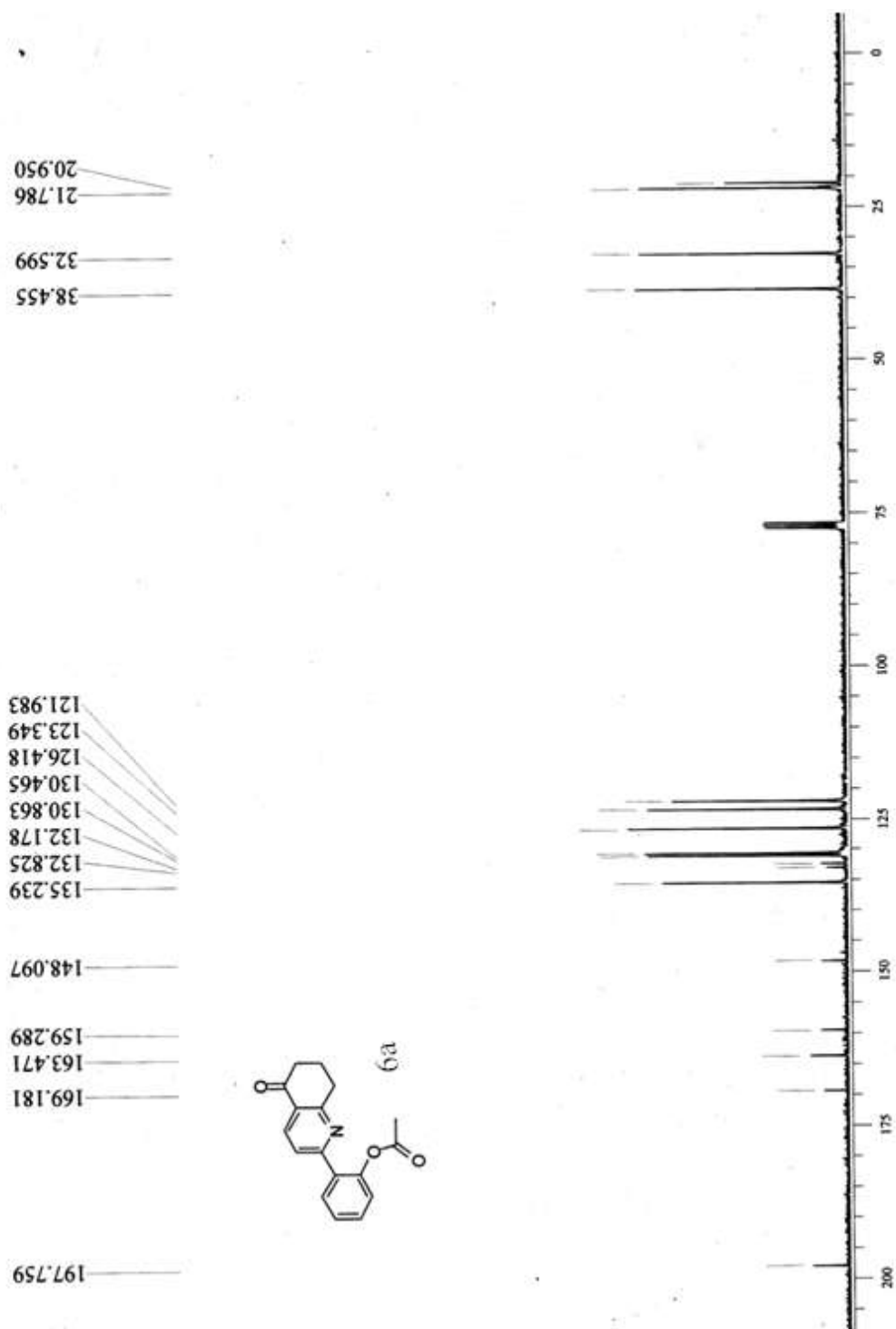








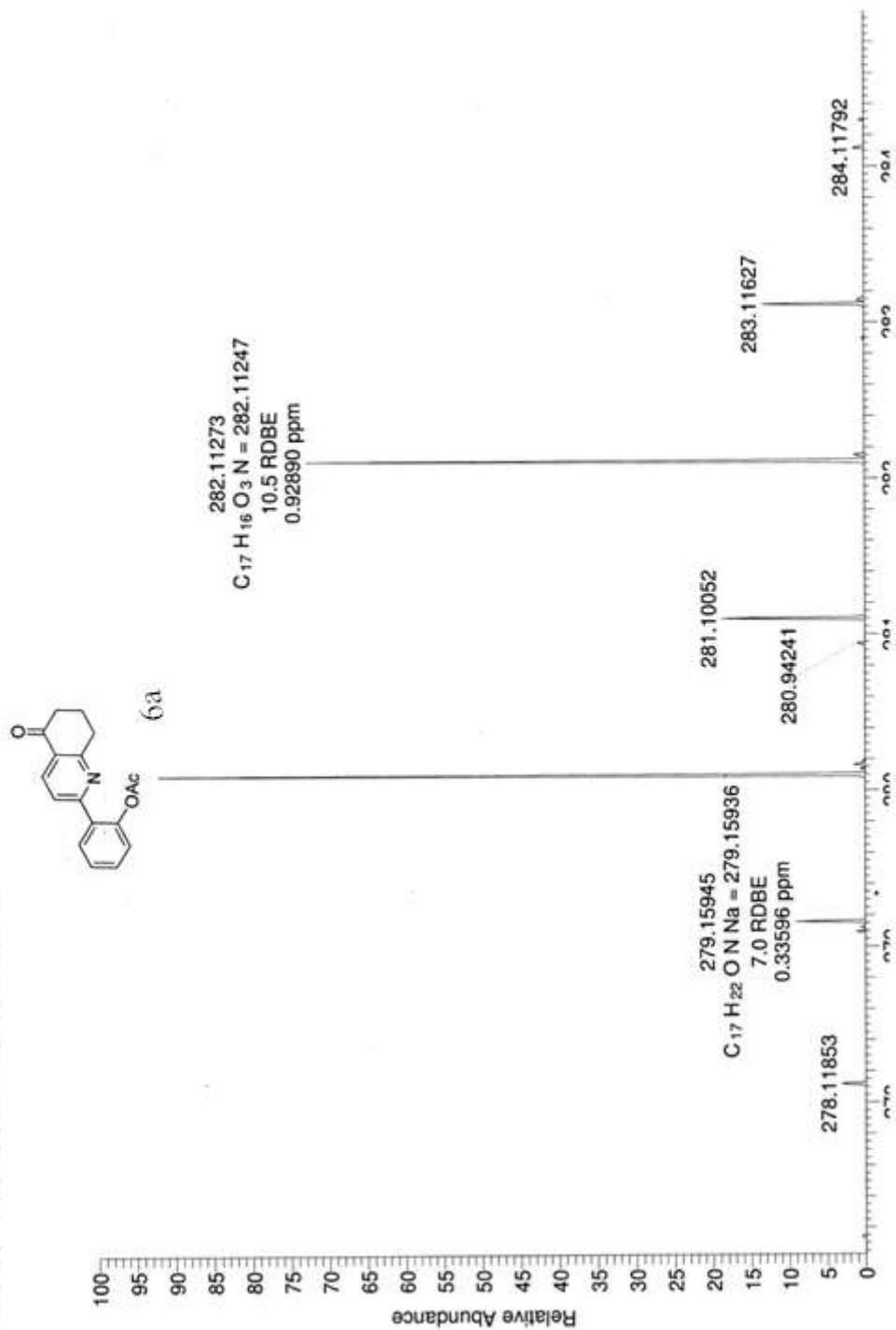


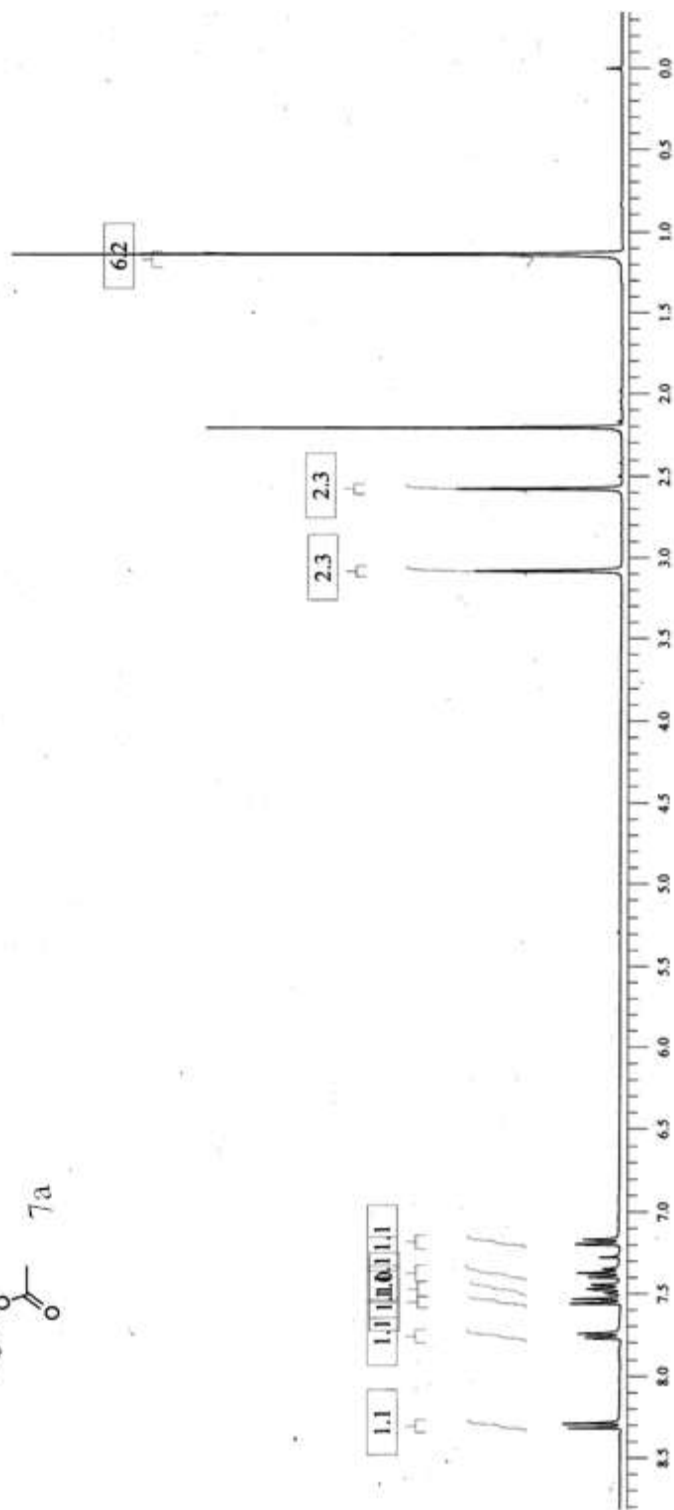
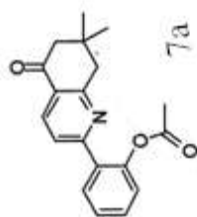


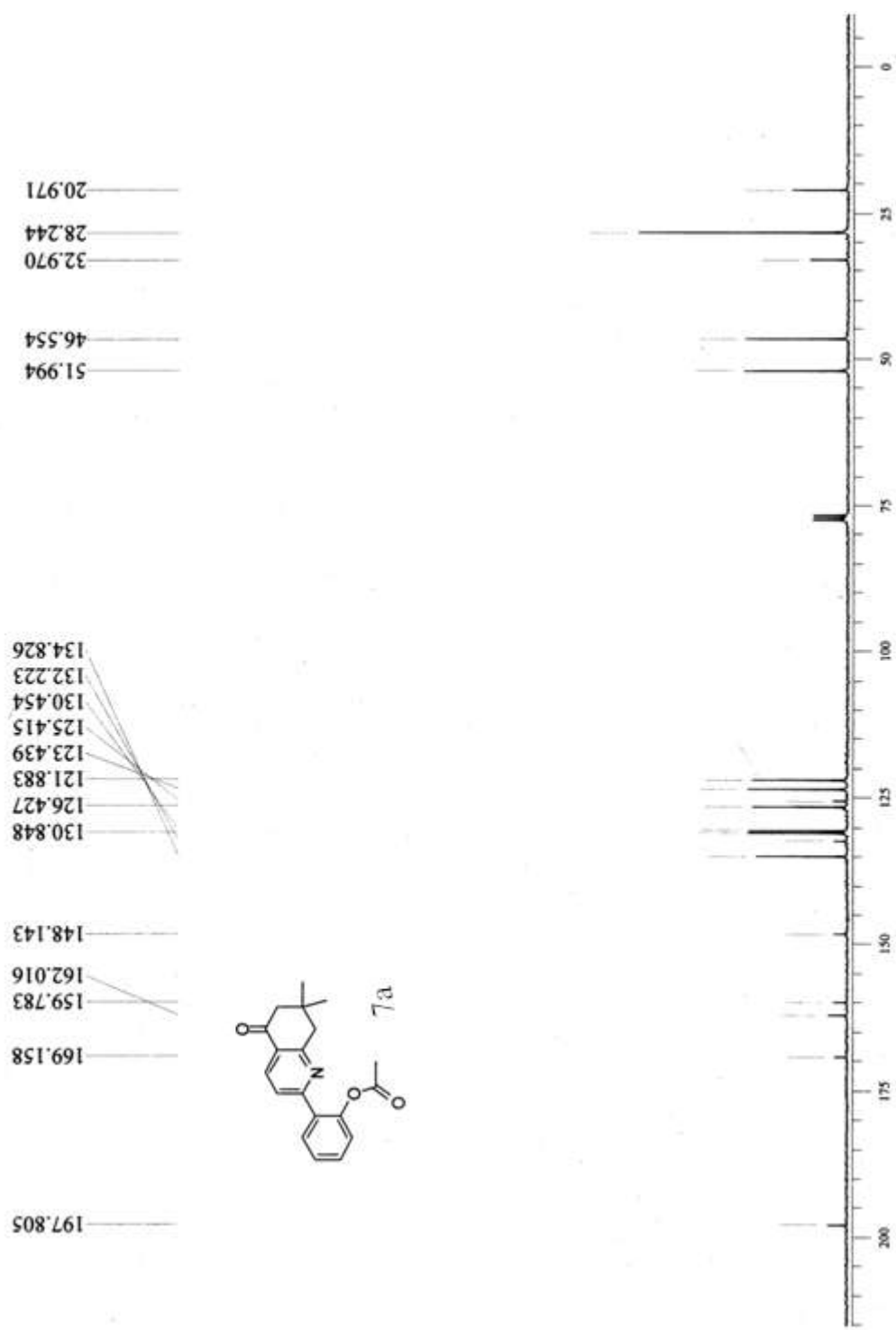
K SRINIVAS  
2/6/2013 2:41:50 PM

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KS-PH-CYHX-OAC-II #30 RT: 0.30 AV: 1 NL: 2.67E6  
T: FTMS [1,1] + p ESI Full ms [100.00-2000.00]







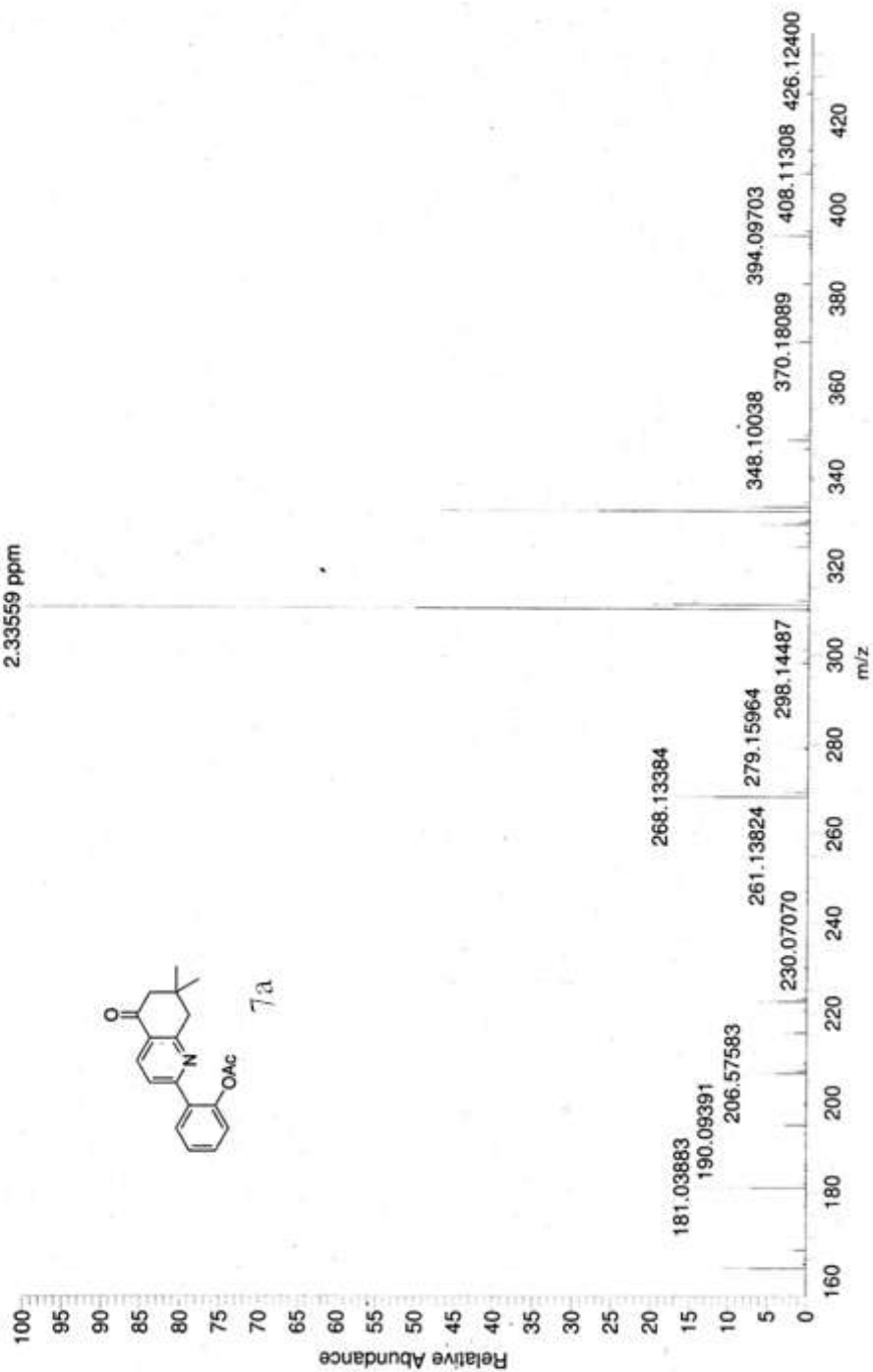
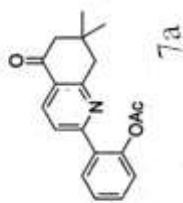


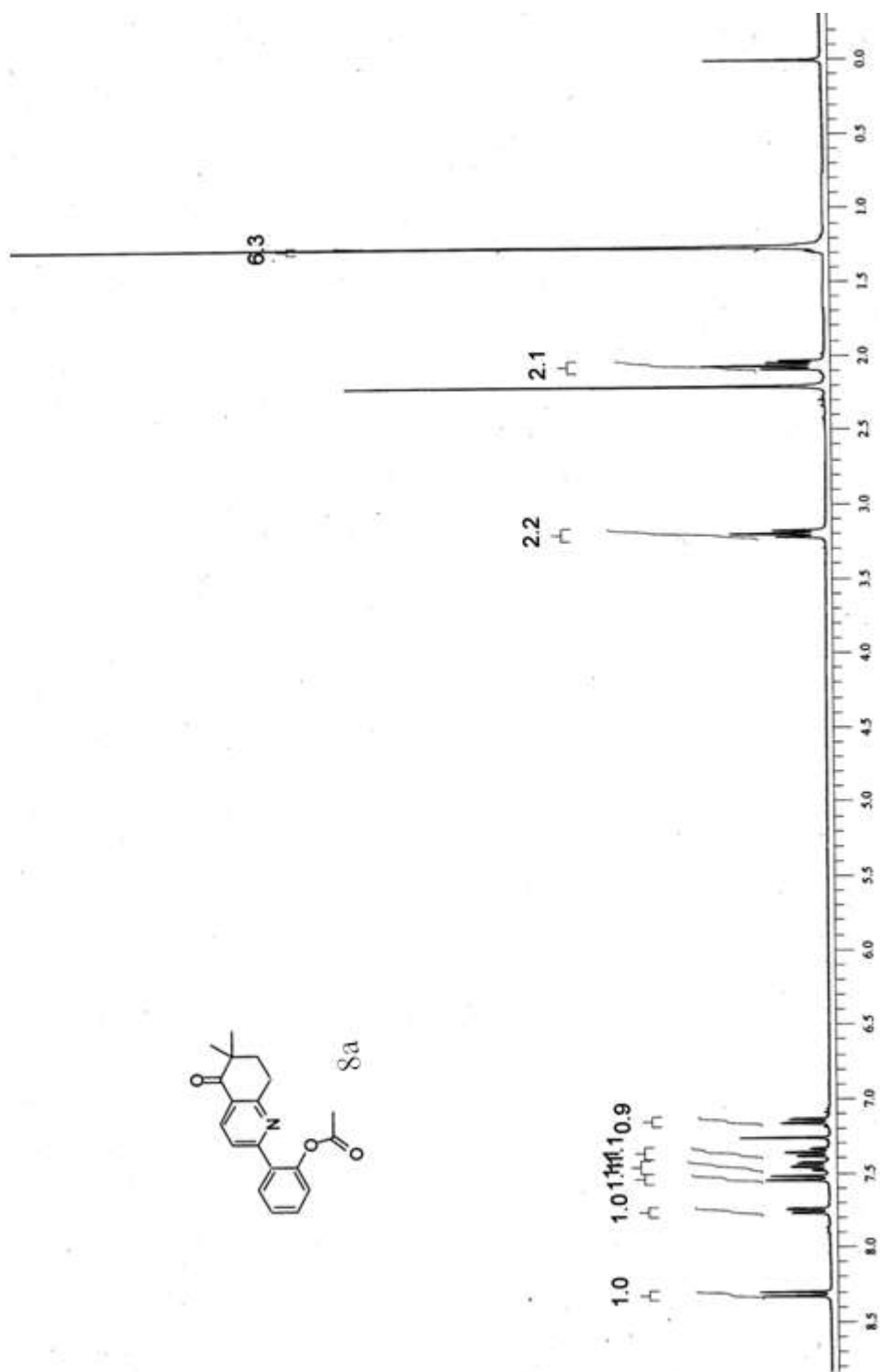
P.S.REDDY  
9/21/2012 4:12:49 PM

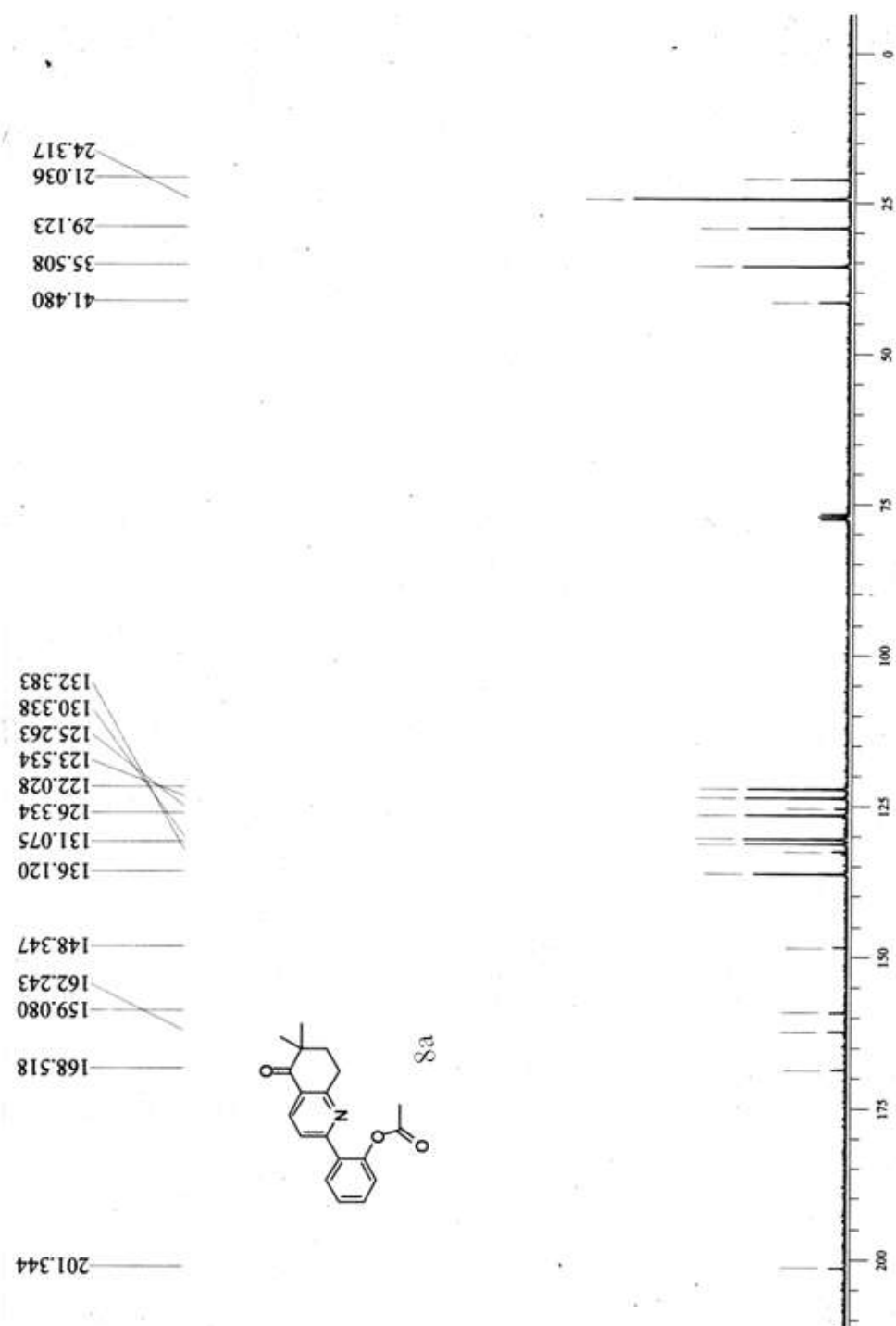
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KSPHNMDOAC #7-26 RT: 0.07-0.26 AV: 20 NL: 4.65E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

310.14449  
C<sub>19</sub>H<sub>20</sub>O<sub>3</sub> N = 310.14377  
10.5 RDBE  
2.33559 ppm



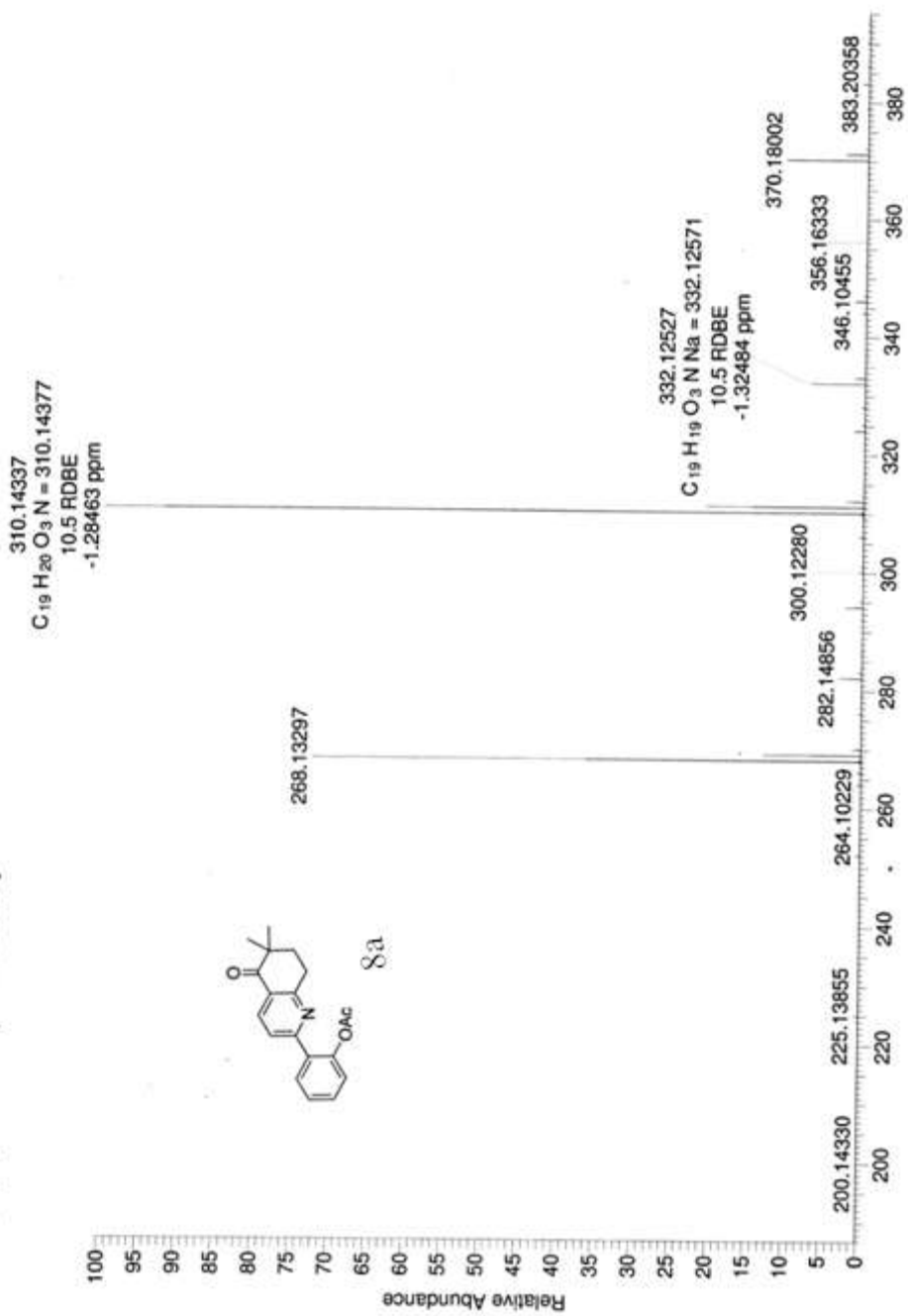


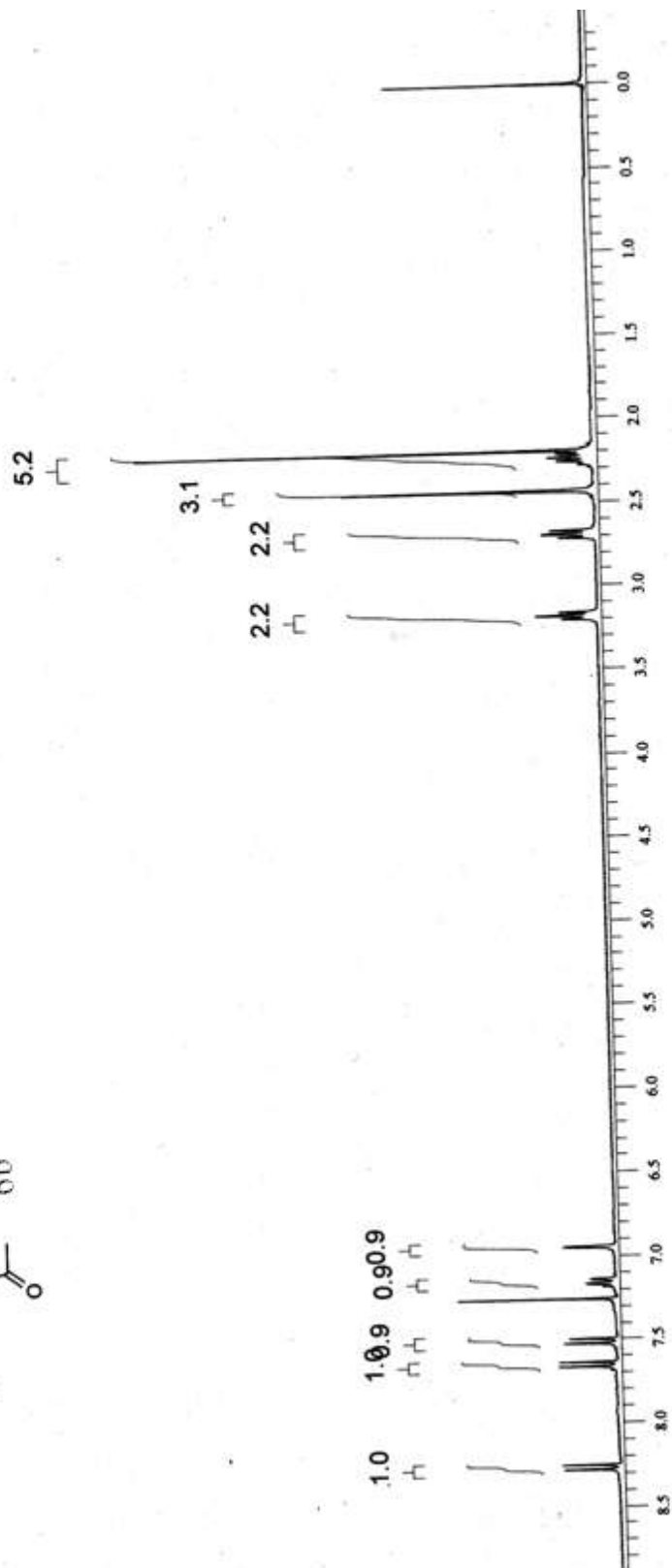
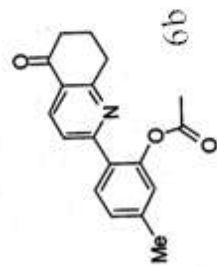


SAVITHRISHREEDY  
12/12/2012 8:15:15 PM

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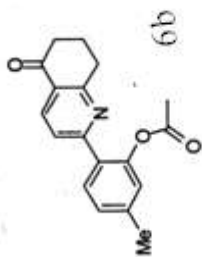
KSPHUUSOAC #12 RT: 0.12 AV: 1 NL: 7.12E7  
T: FTMS (1,1) + p ESI Full ms [120.00-2000.00]





21.664  
20.933  
20.795  
32.504  
38.292

129.115  
127.080  
123.719  
121.571  
126.044  
130.493  
134.955  
140.966  
147.930  
163.239  
159.164  
169.041  
197.469

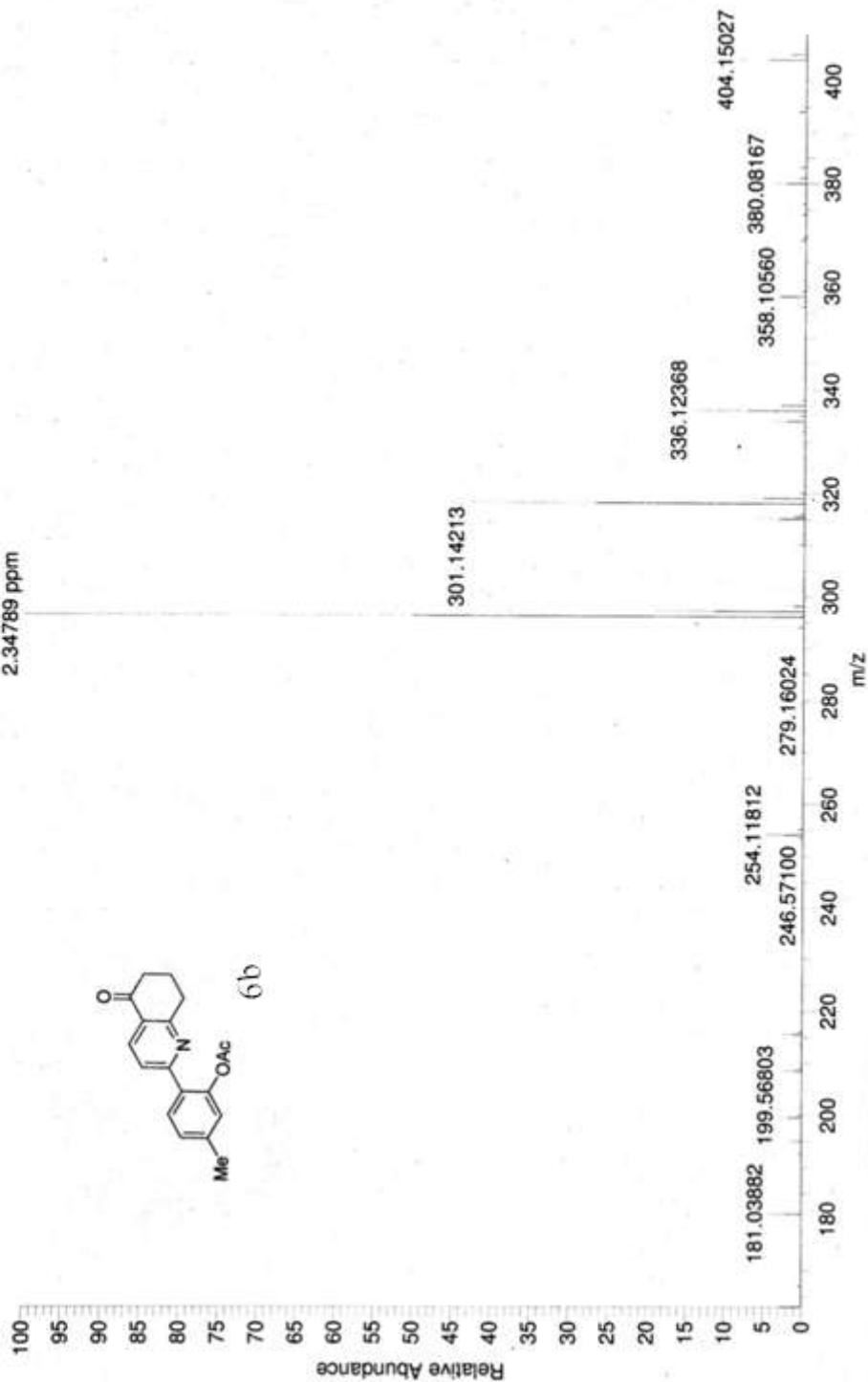
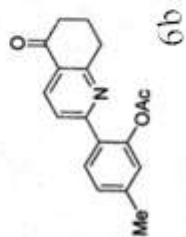


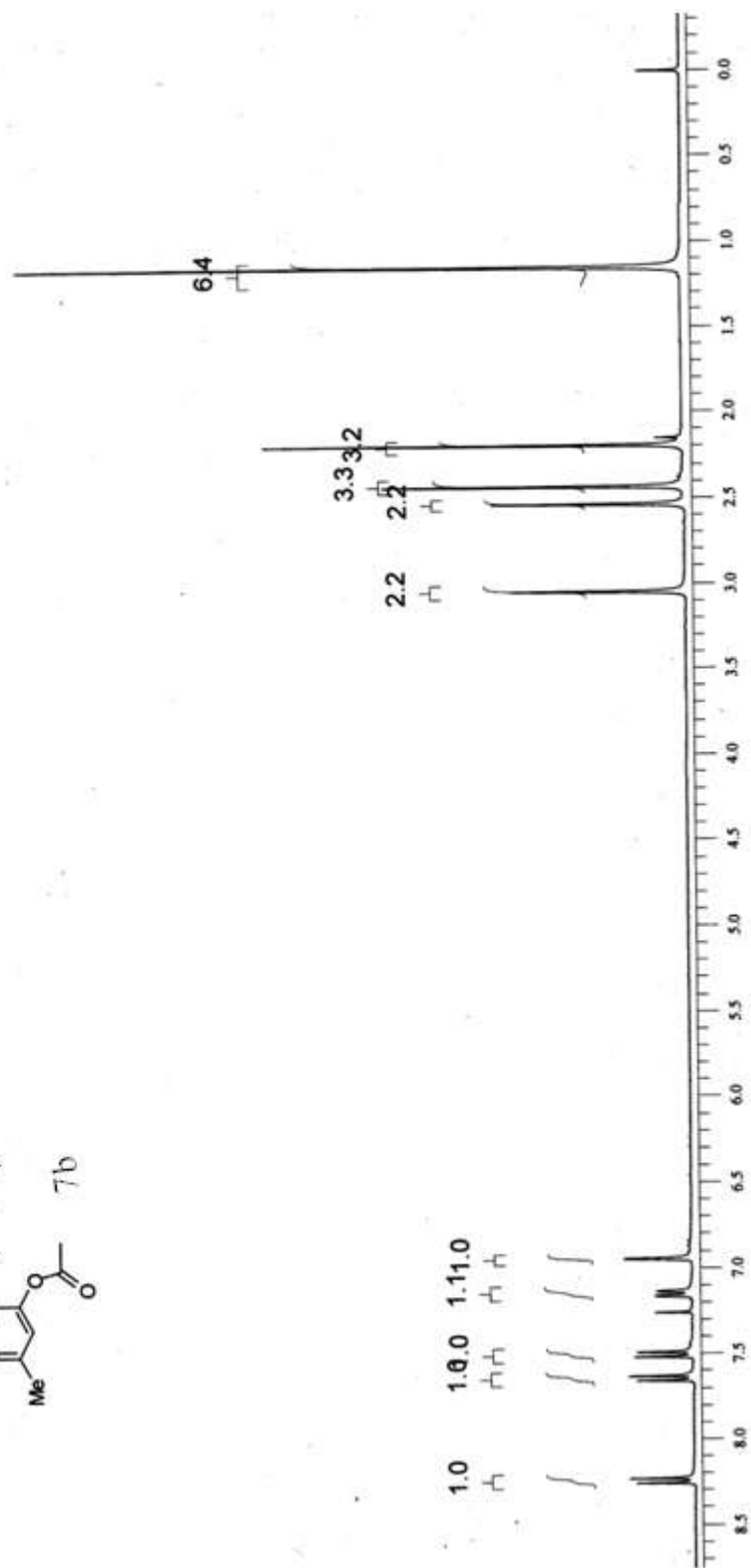
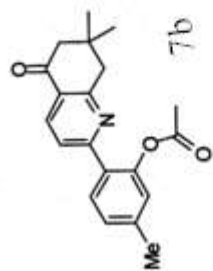
P.S.REDDY  
9/21/2012 4:15:27 PM

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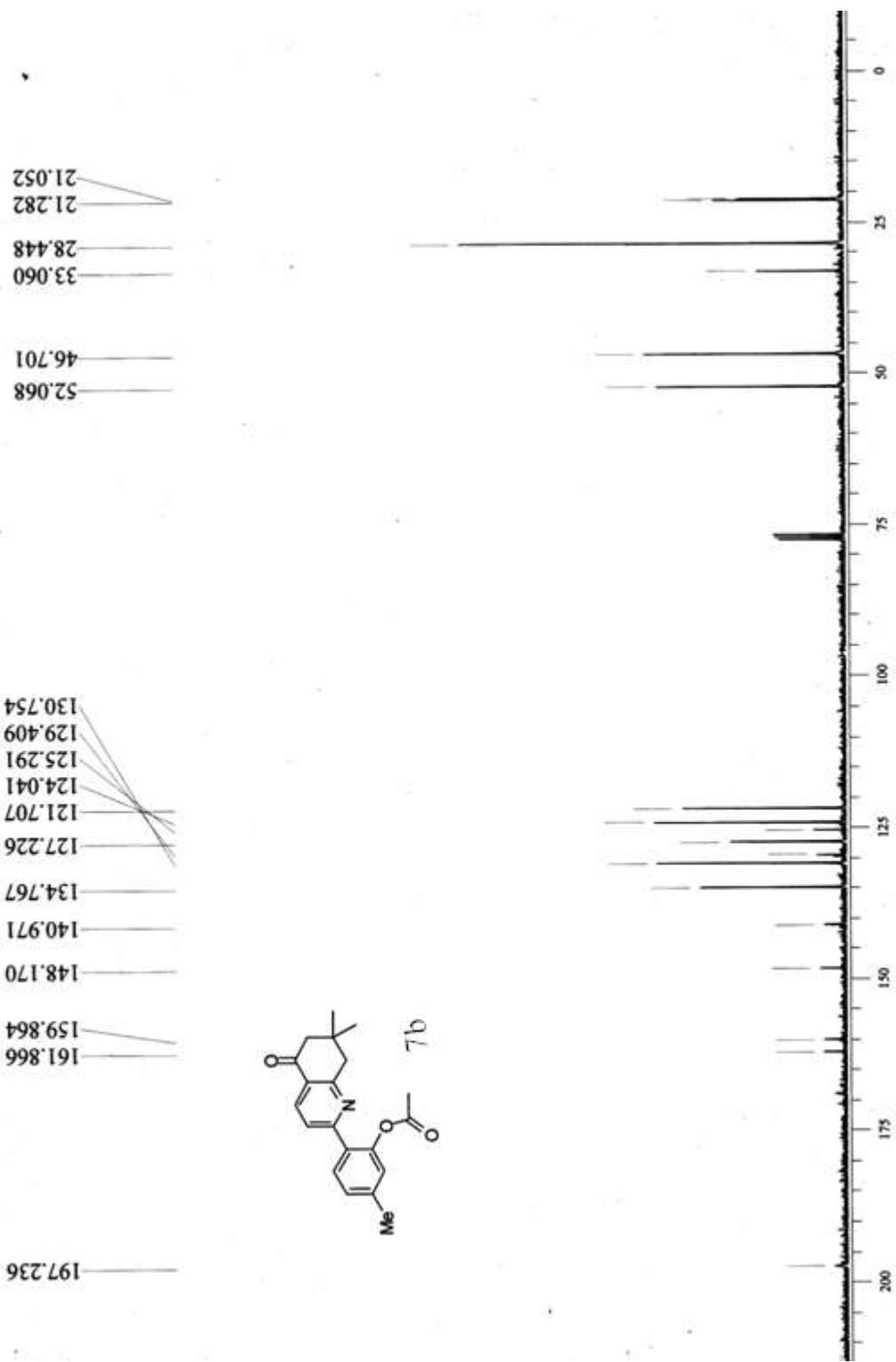
KSMECYHXOAC #6-25 RT: 0.06-0.25 AV: 20 NL: 8.17E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

296.12882  
C<sub>18</sub>H<sub>18</sub>O<sub>3</sub> N = 296.12812  
10.5 RDBE  
2.34789 ppm







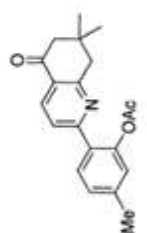


KSPHIJSOAC  
12/12/2012 8:17:49 PM

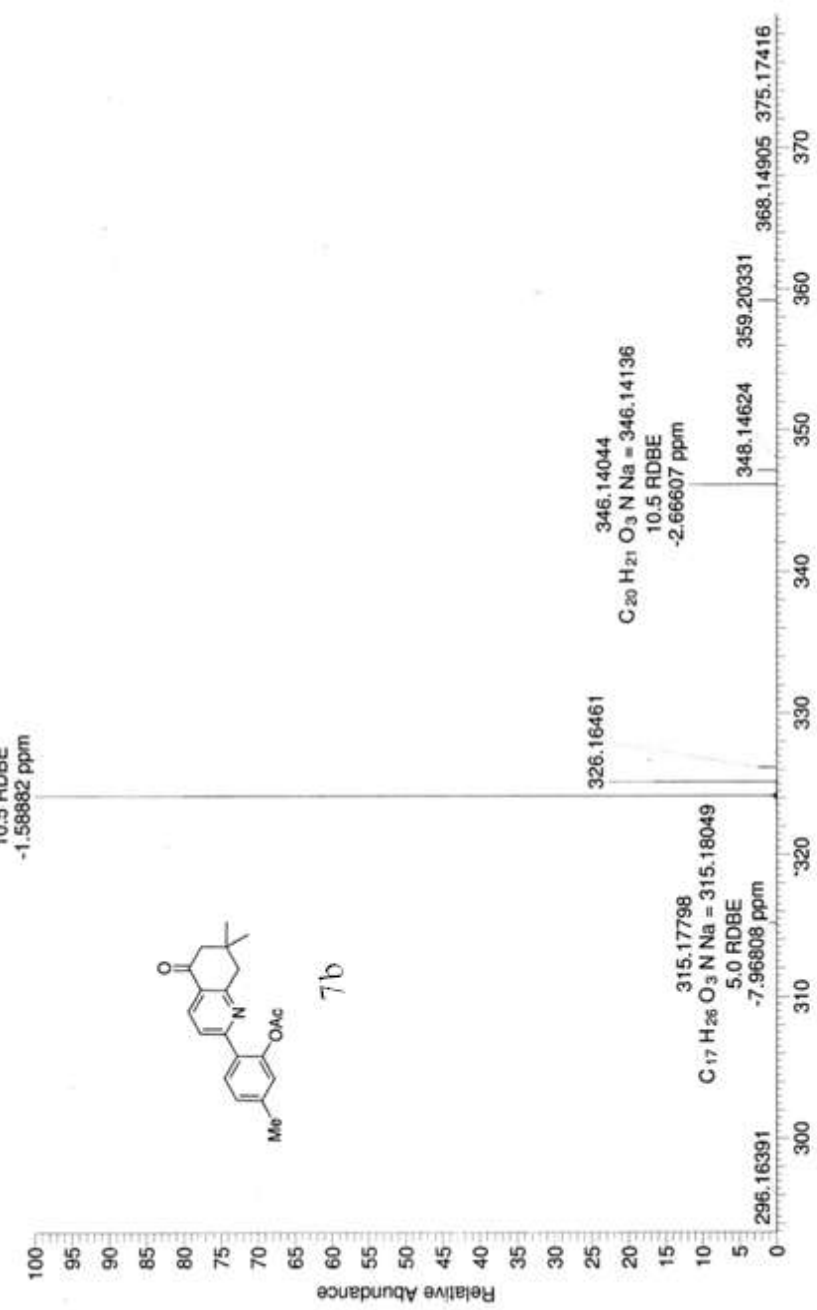
INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY  
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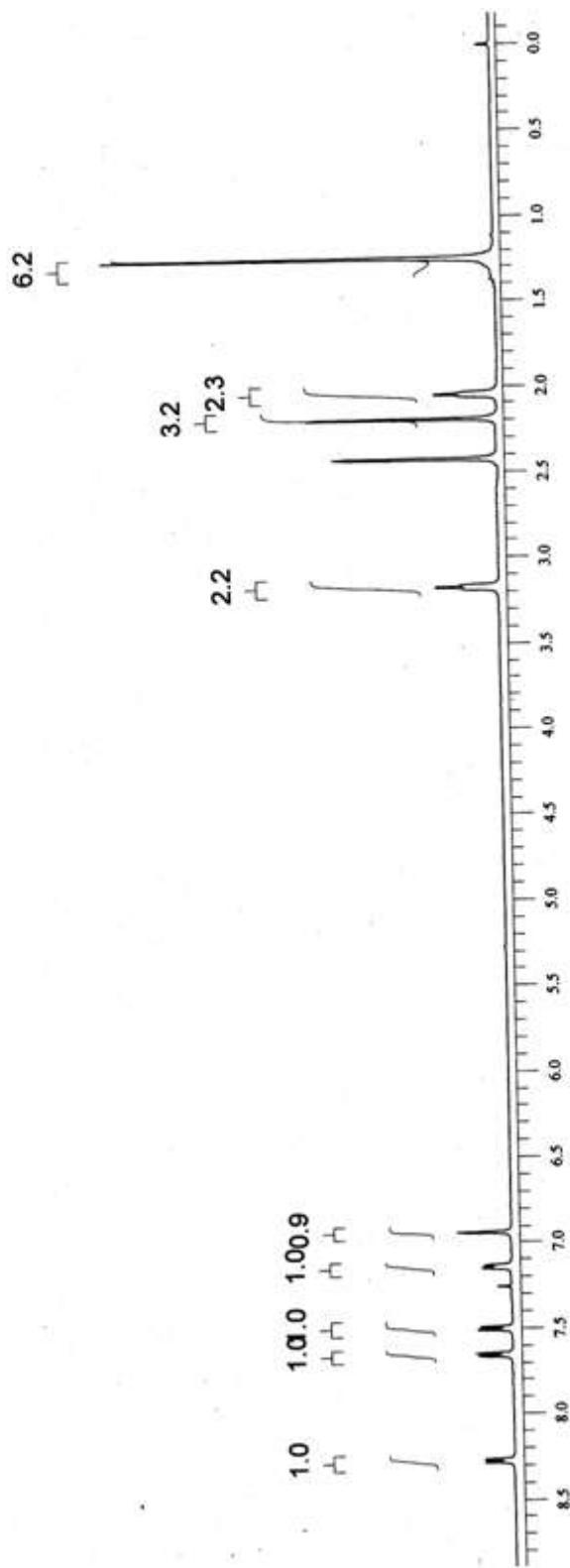
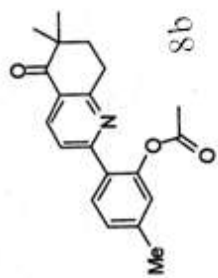
KSMEDMOAC #12 RT: 0.12 AV: 1 NL: 1.30E8  
T: FTMS (1,1) + p ESI Full ms [120.00-2000.00]

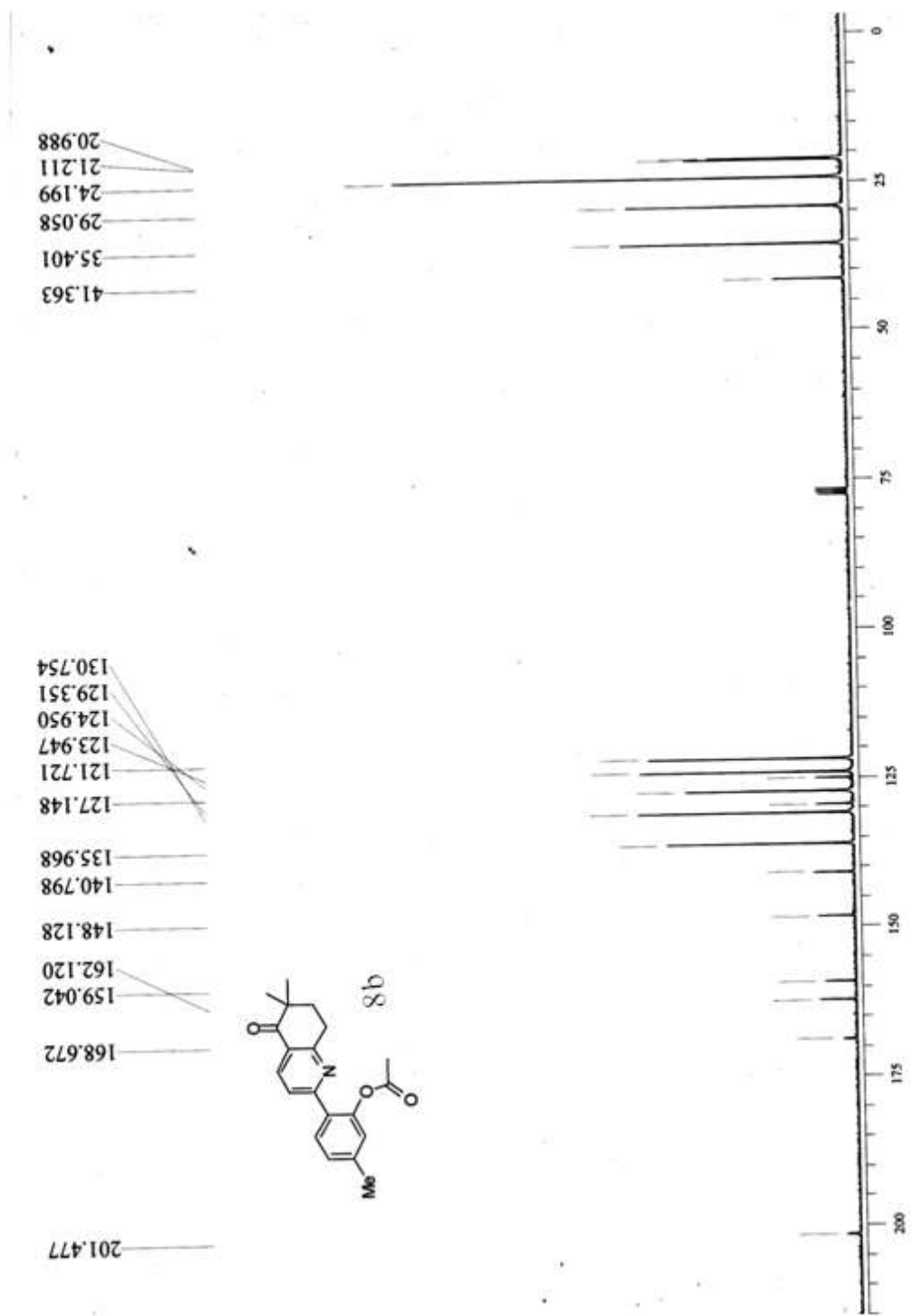
324.15891  
C<sub>20</sub> H<sub>22</sub> O<sub>3</sub> N = 324.15942  
10.5 RDBE  
-1.58882 ppm



7b



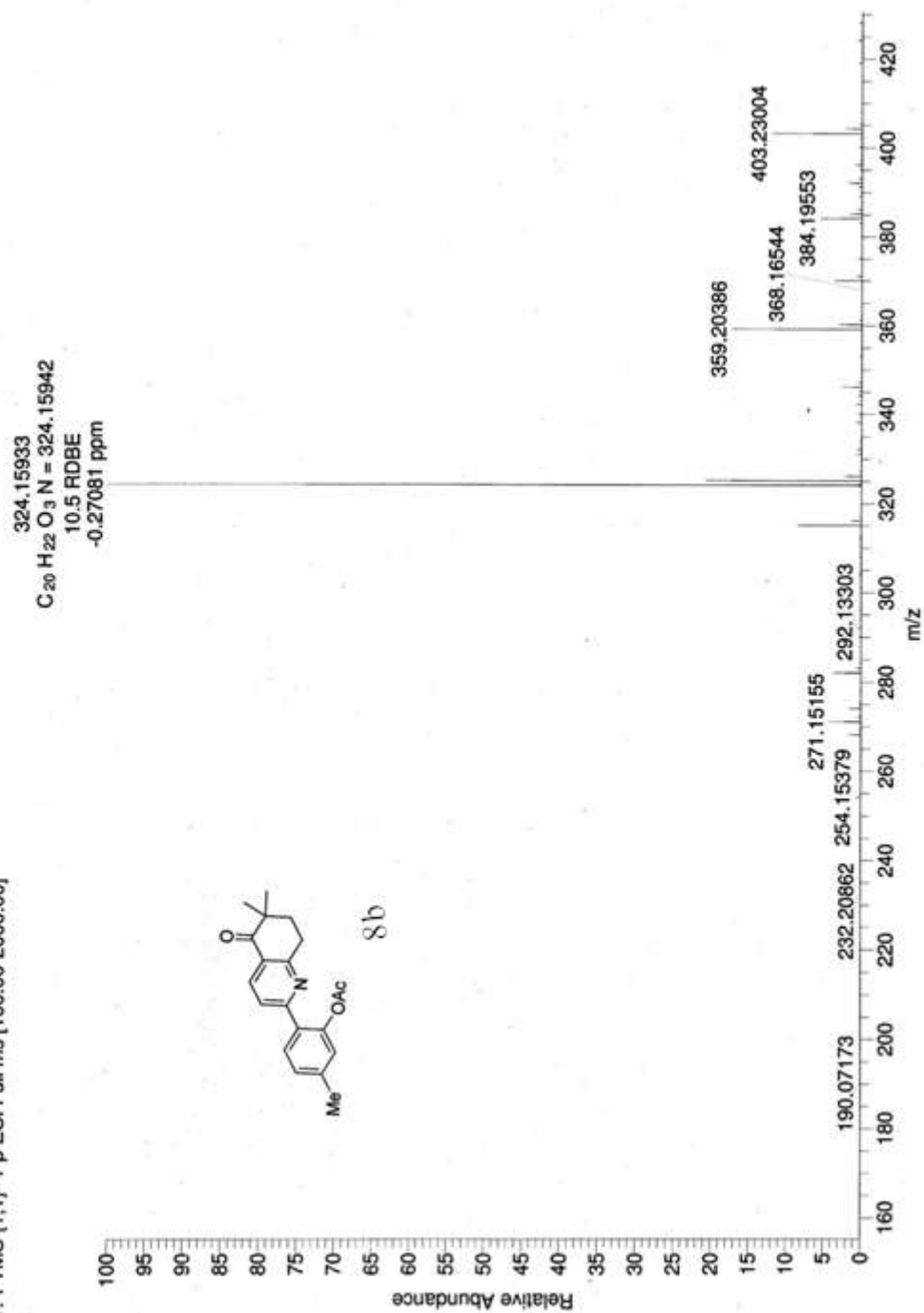


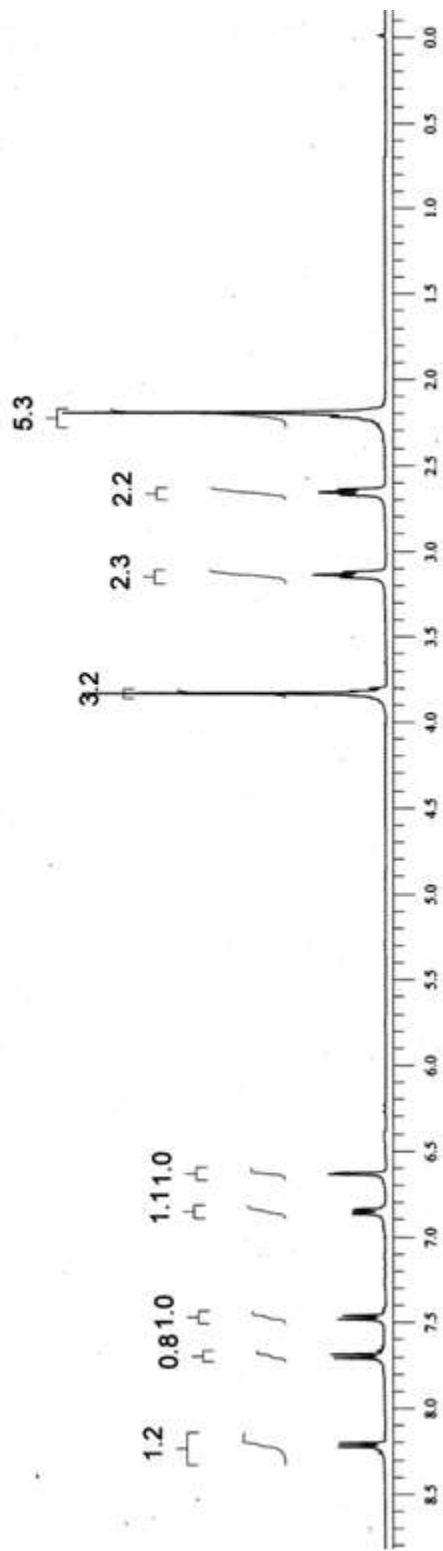
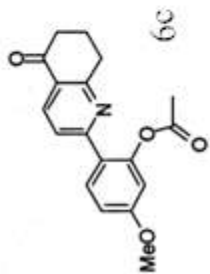


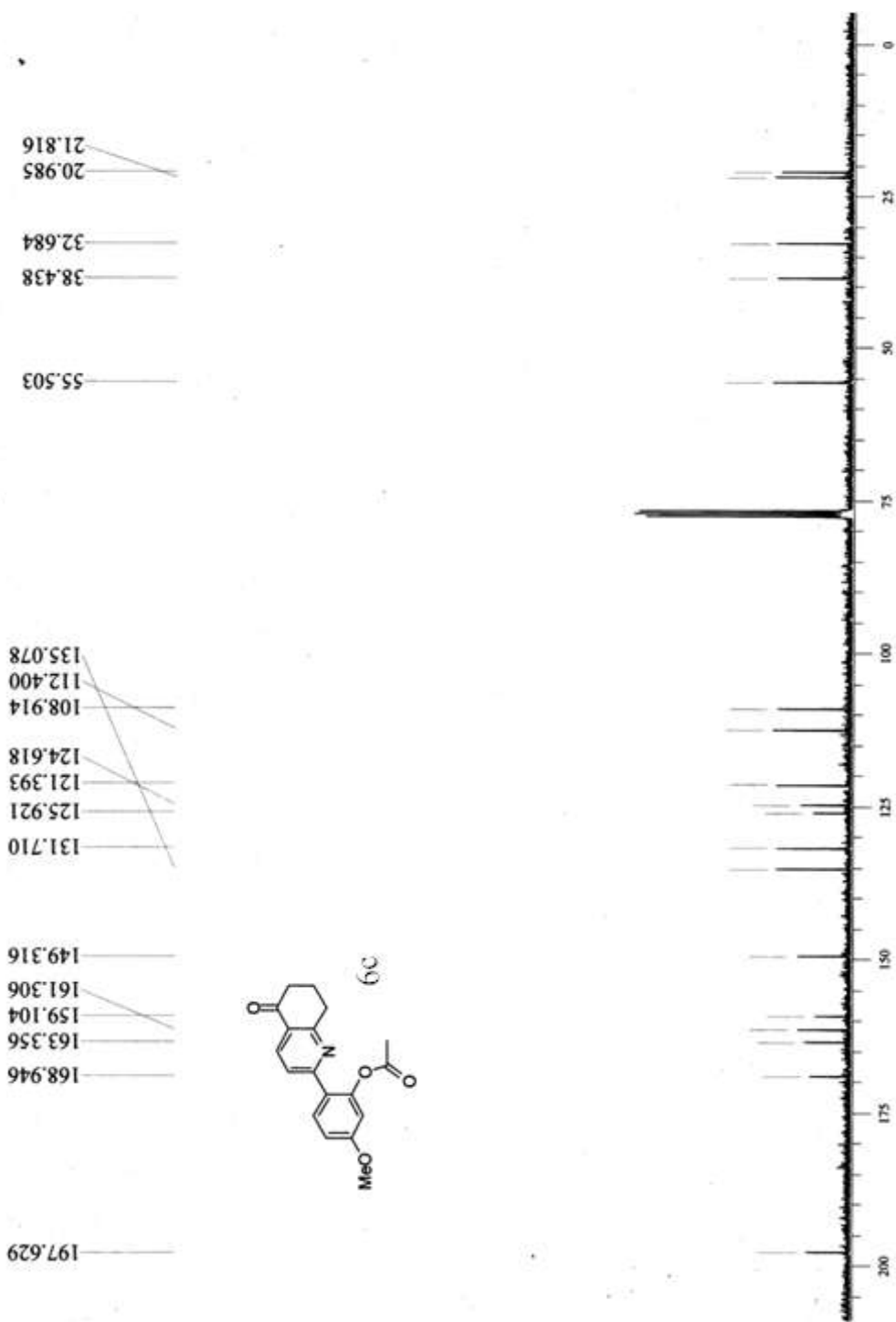
P S REDDYY12  
10/12/2012 11:14:25 PM

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KSMEUNSOAC #22 RT: 0.22 AV: 1 NL: 4.82E5  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]





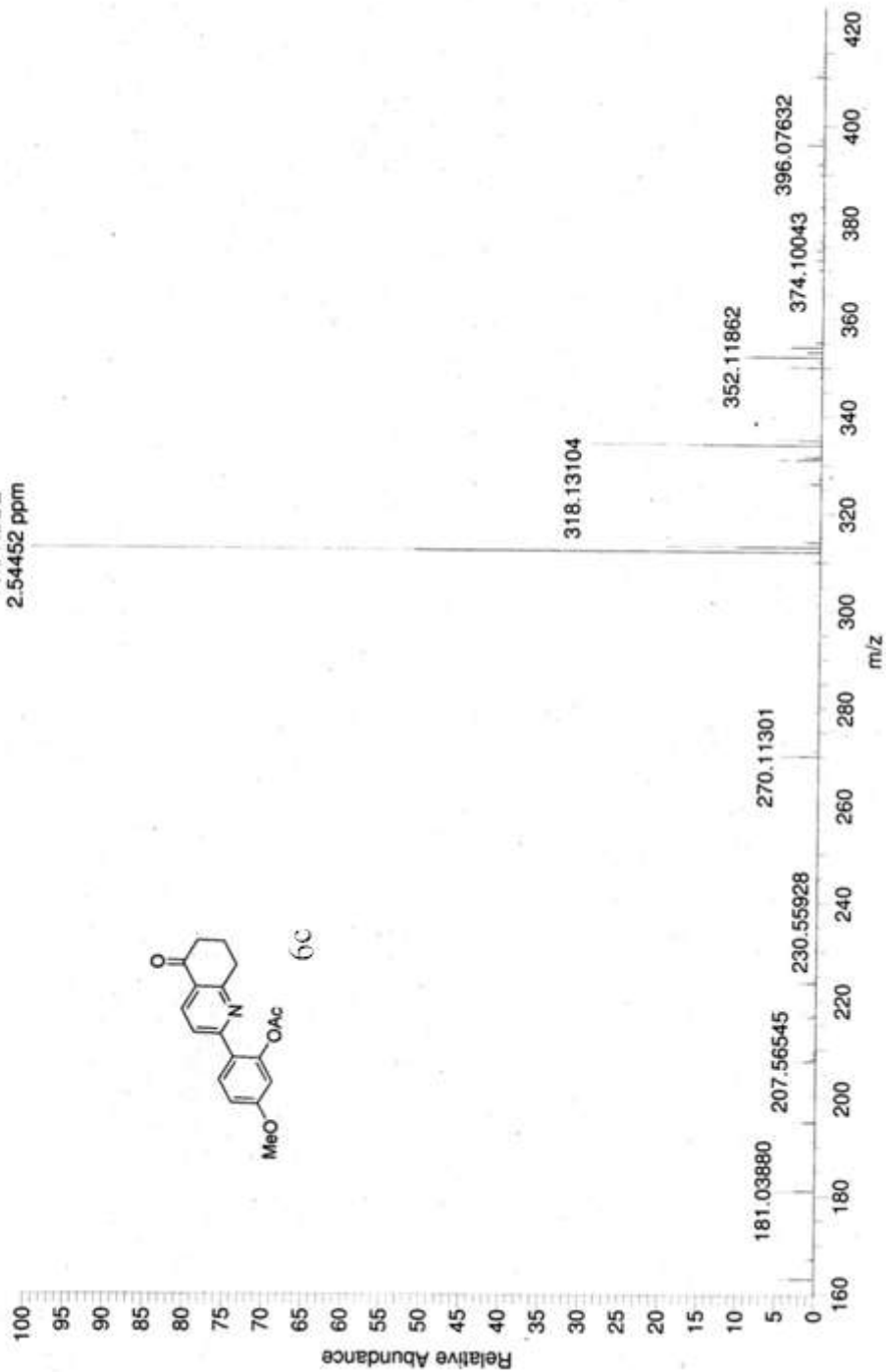


P.S REDDY  
9/21/2012 3:25:25 PM

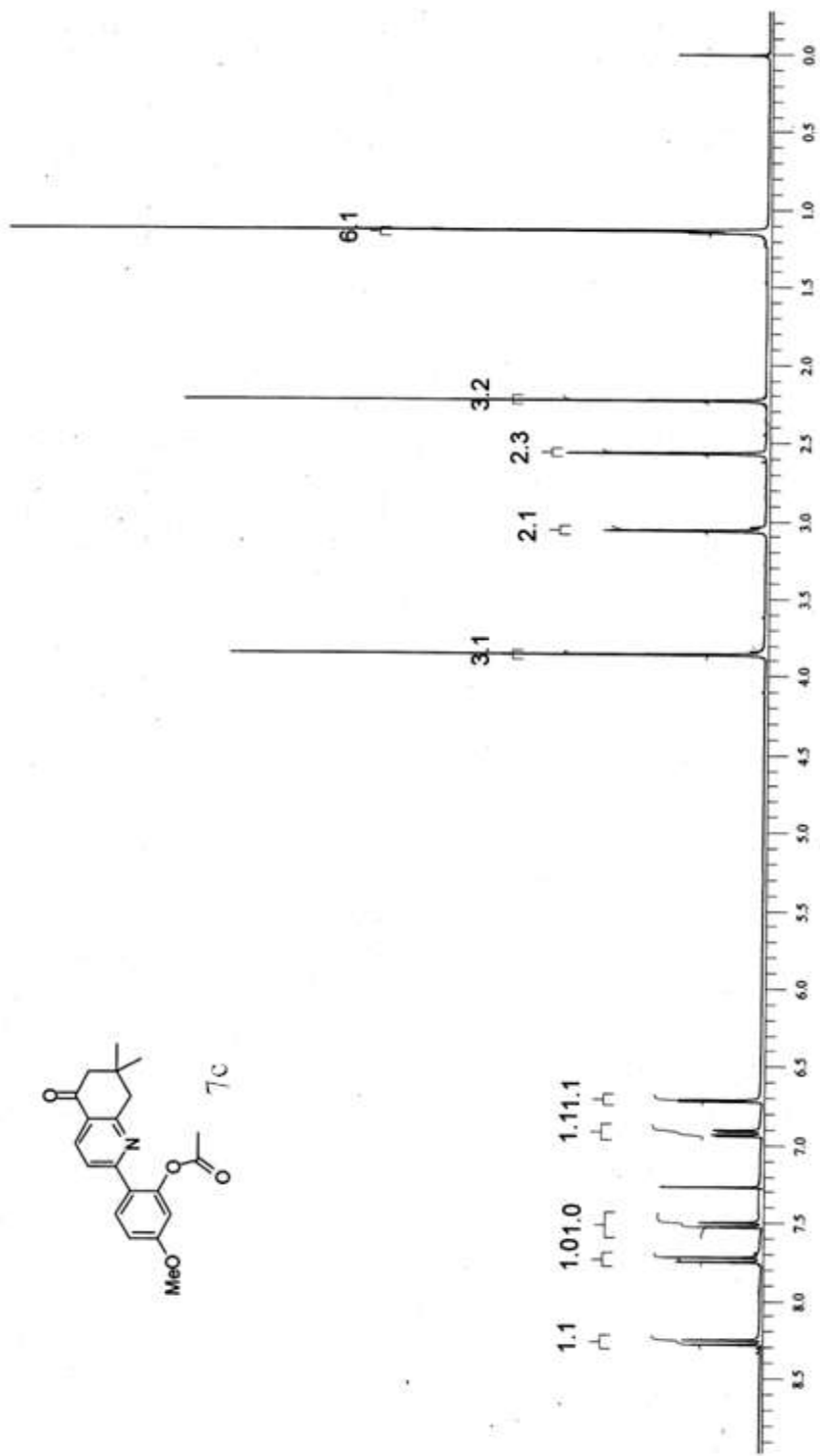
INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY  
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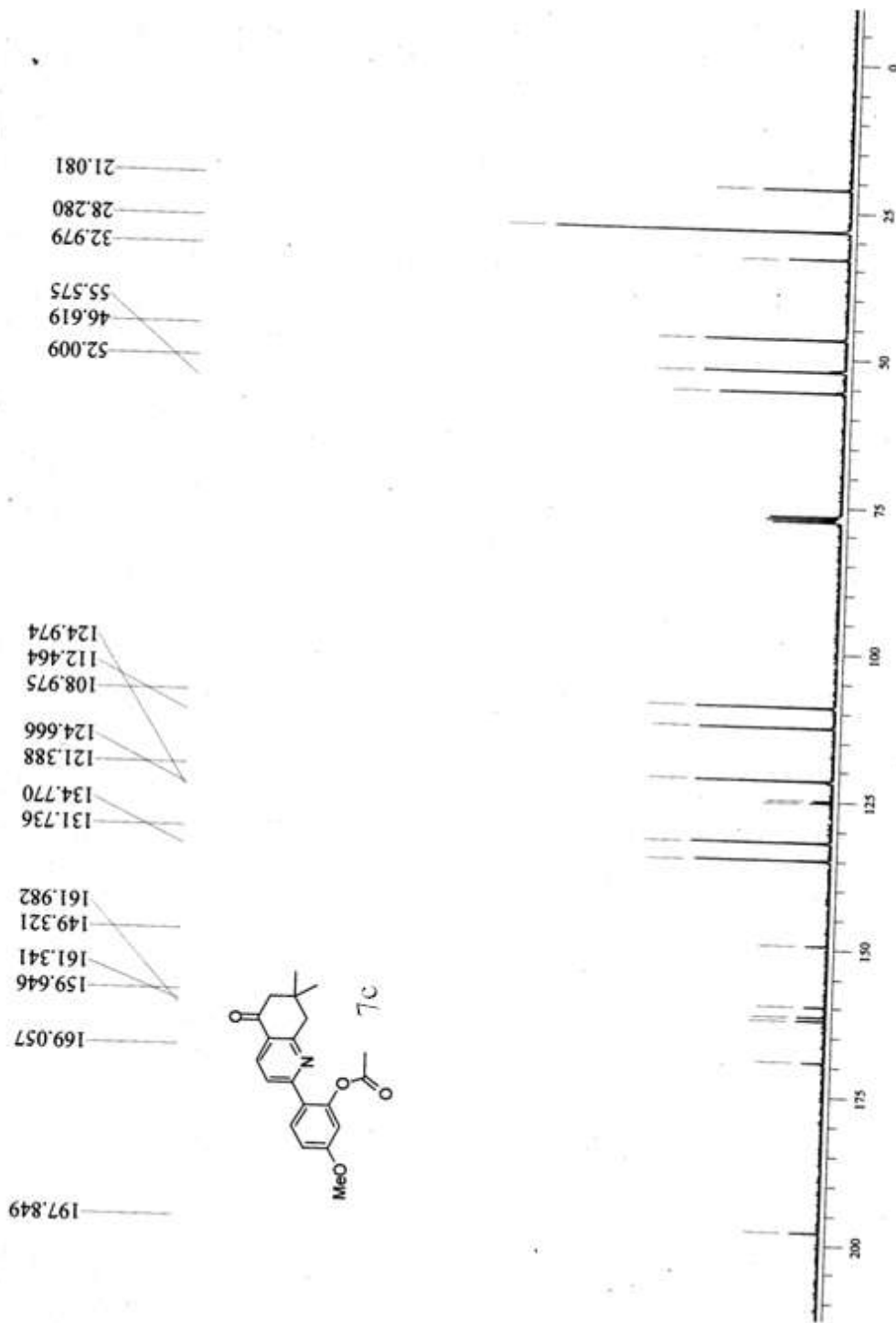
KSOMECHYOAC #6-25 RT: 0.06-0.25 AV: 20 NL: 7.42E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

312.12383  
C<sub>18</sub>H<sub>18</sub>O<sub>4</sub>N = 312.12303  
10.5 RDBE  
2.54452 ppm







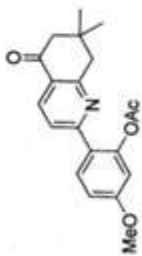
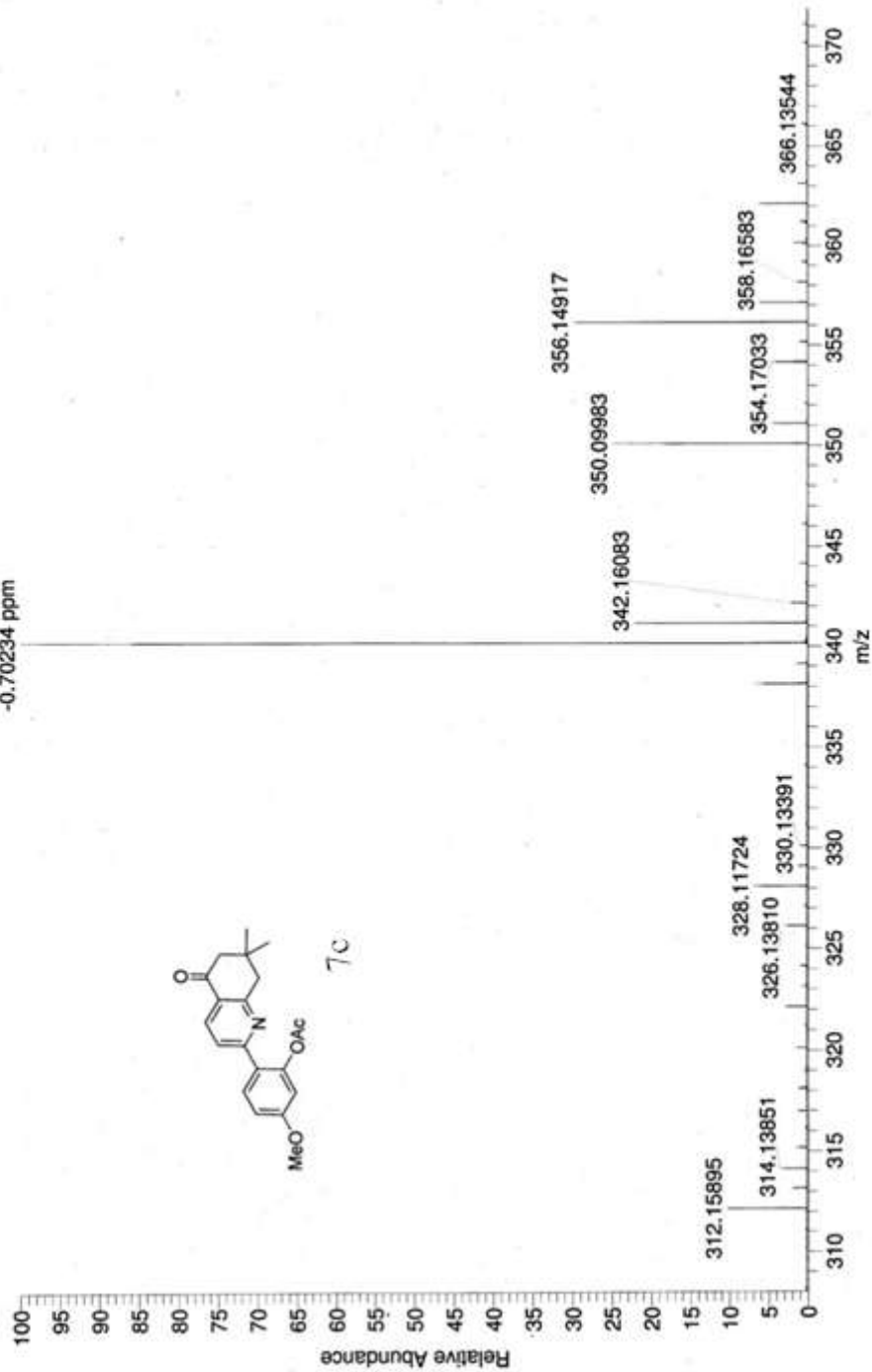


P S REDDY  
10/9/2012 9:51:30 PM

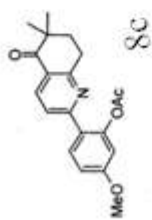
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KS-OME-DMD-OAC #9-28 RT: 0.09-0.28 AV: 20 NL: 2.13E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

340.15410  
C<sub>20</sub>H<sub>22</sub>O<sub>4</sub> N = 340.15433  
10.5 RDBE  
-0.70234 ppm



7c



20.920  
23.959  
28.759  
35.115  
41.245

55.400

108.779

112.290

124.607

121.468

127.977

131.654

136.006

149.160

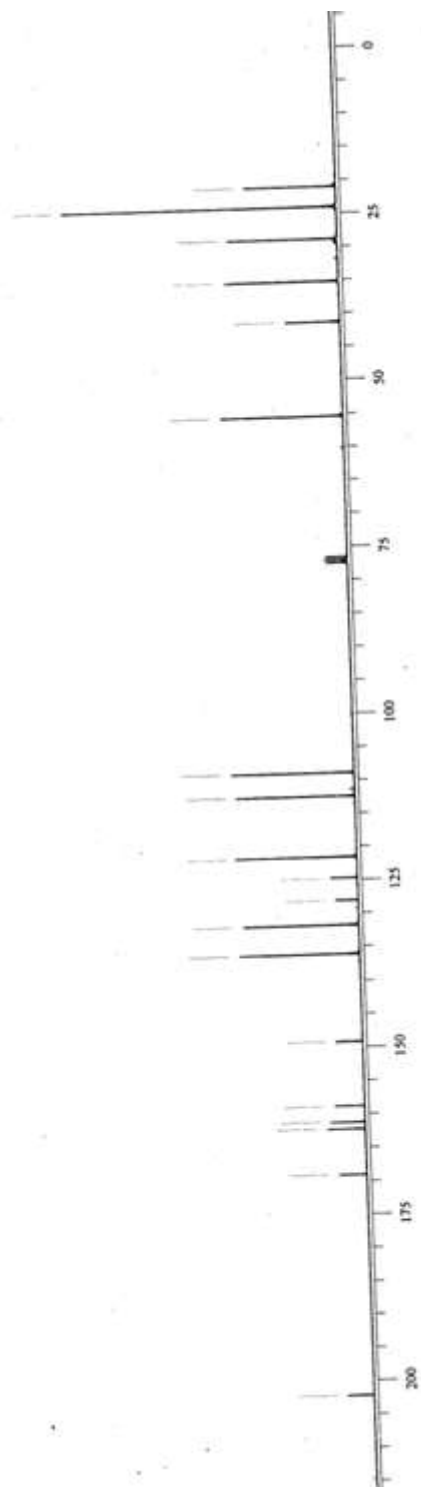
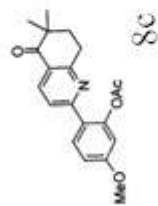
158.753

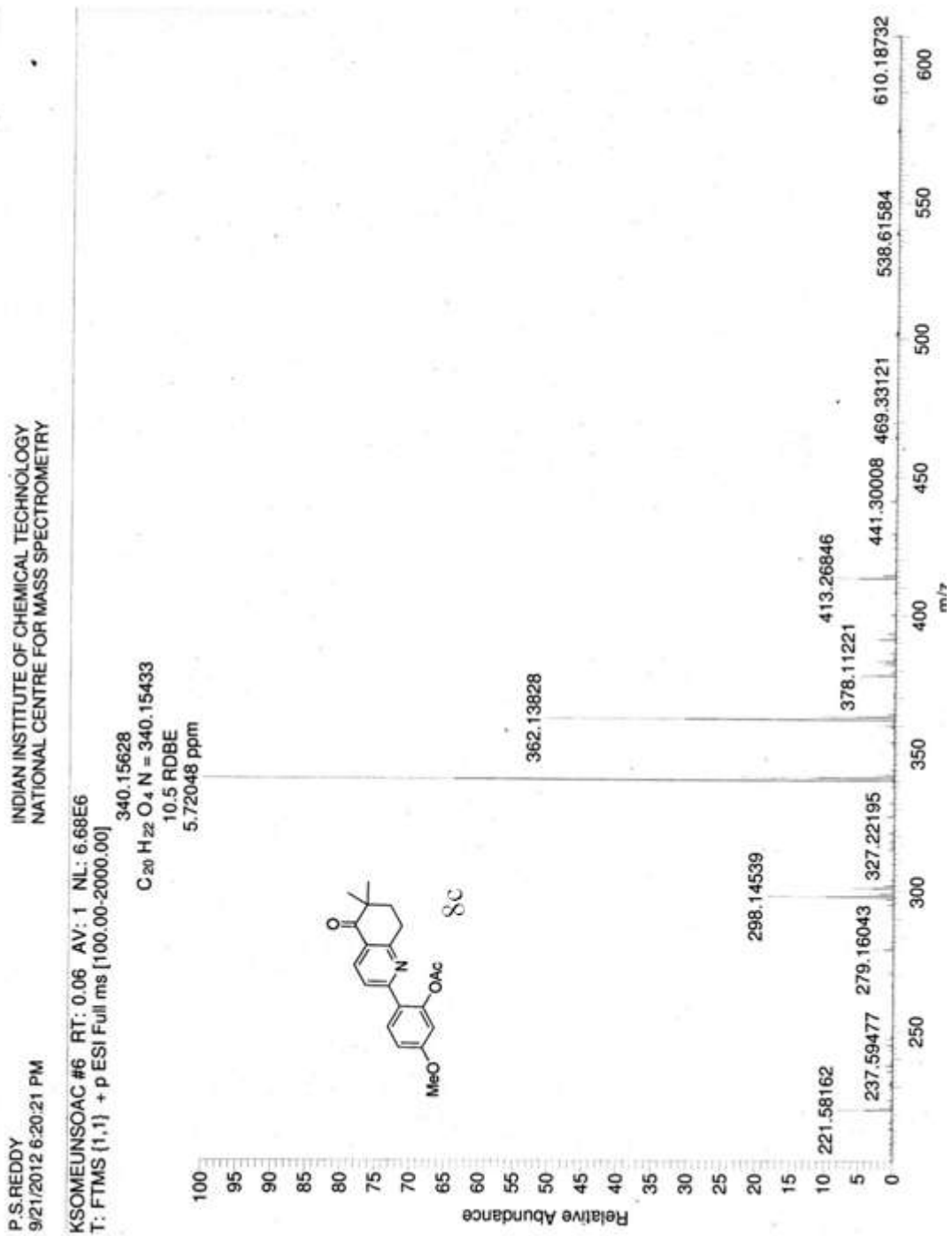
161.173

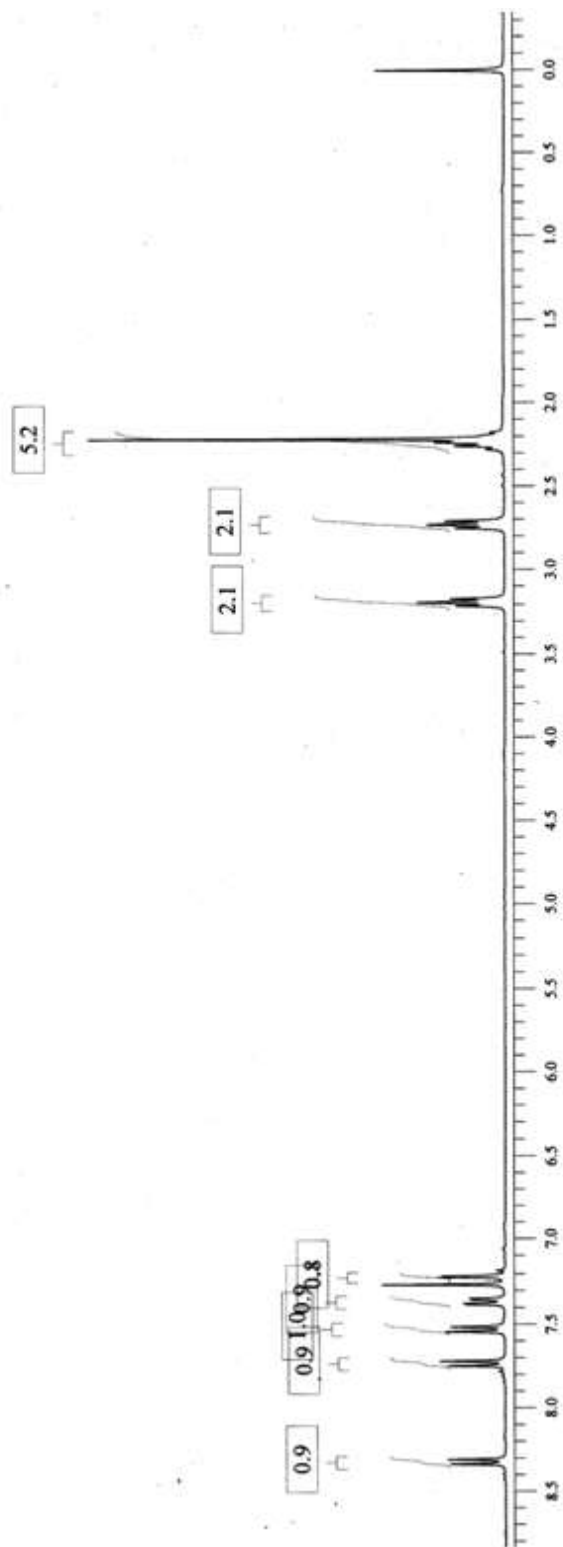
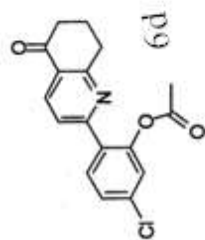
162.179

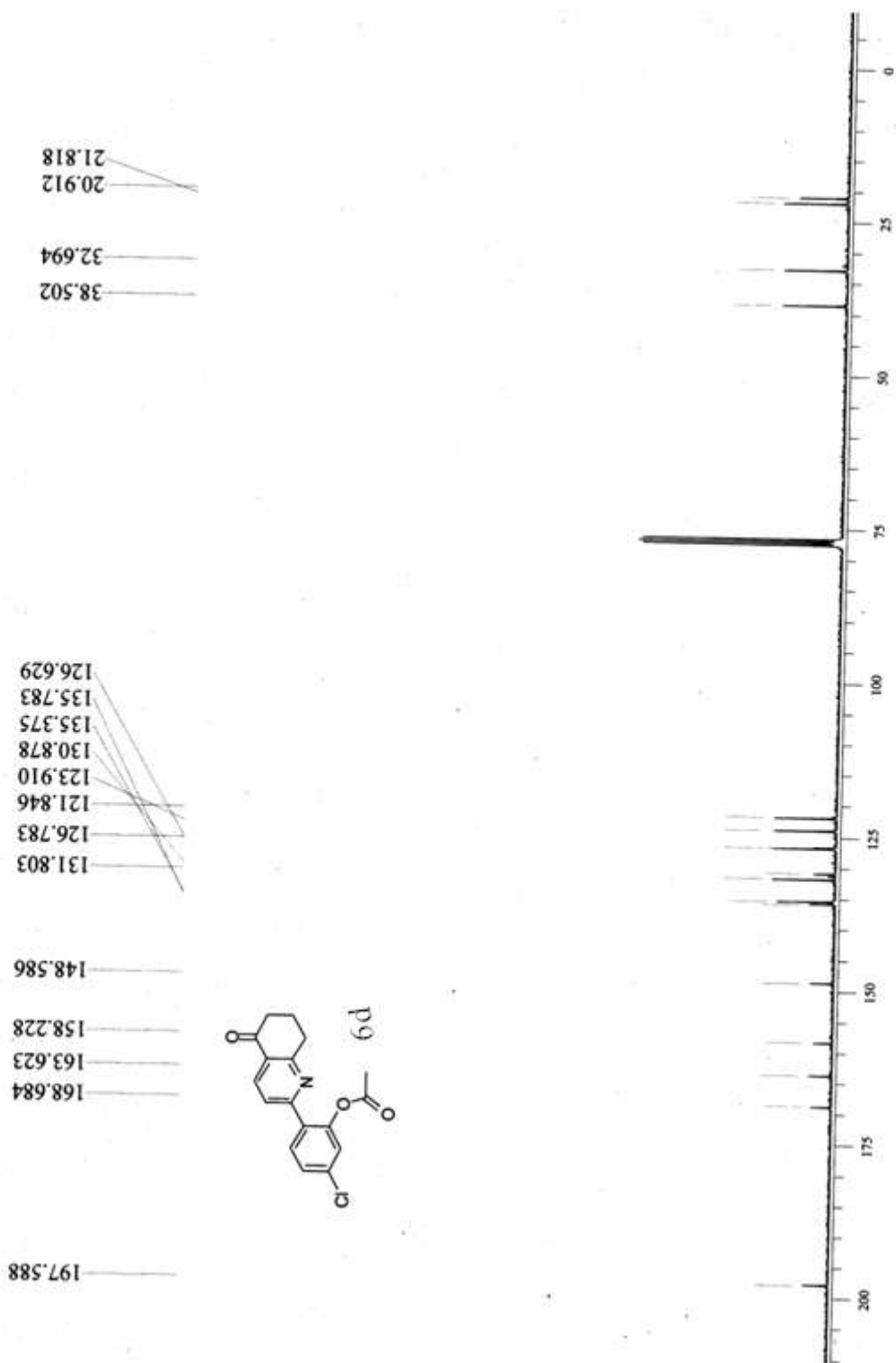
169.008

202.080







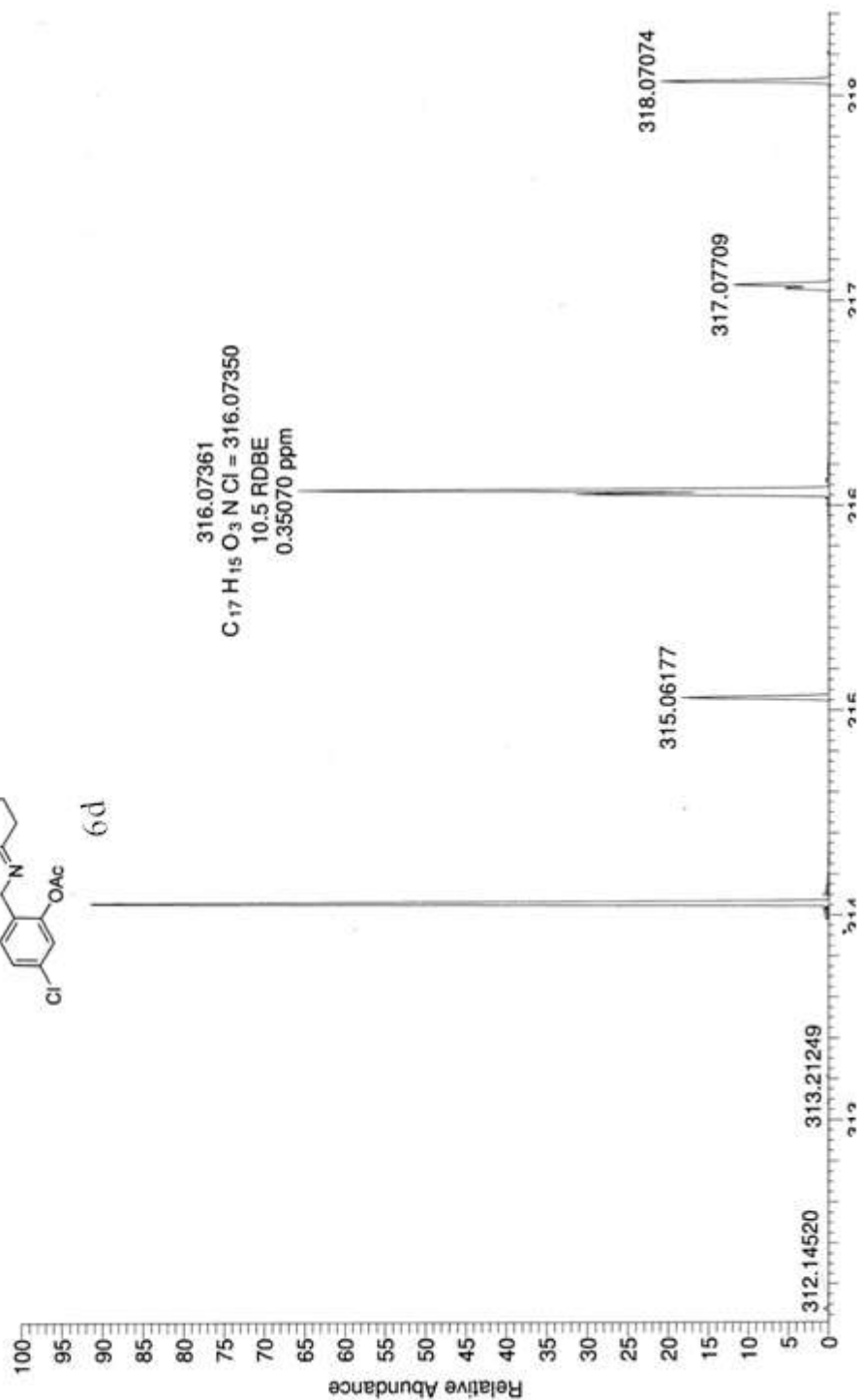
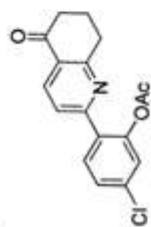


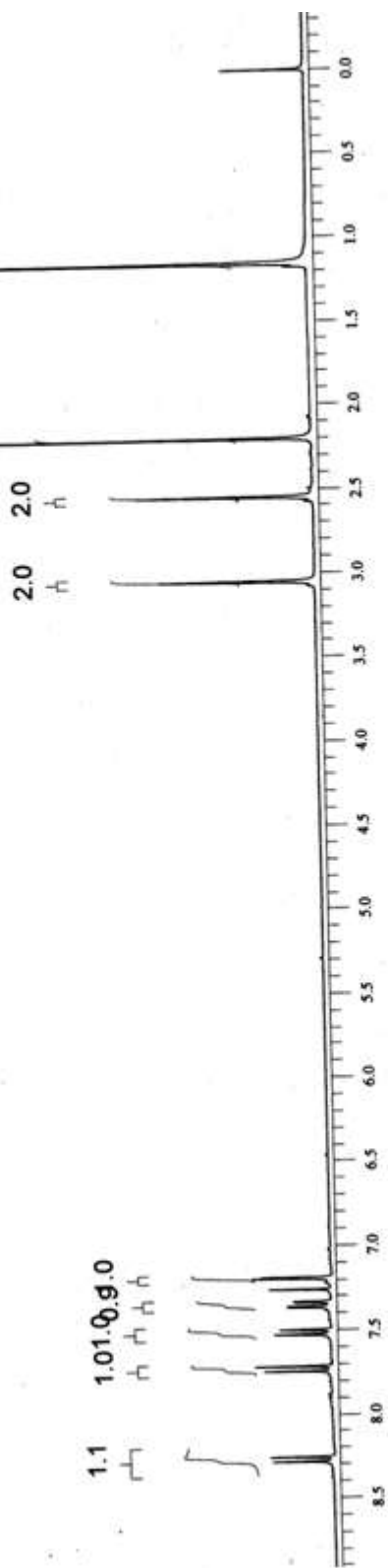
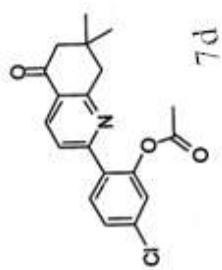


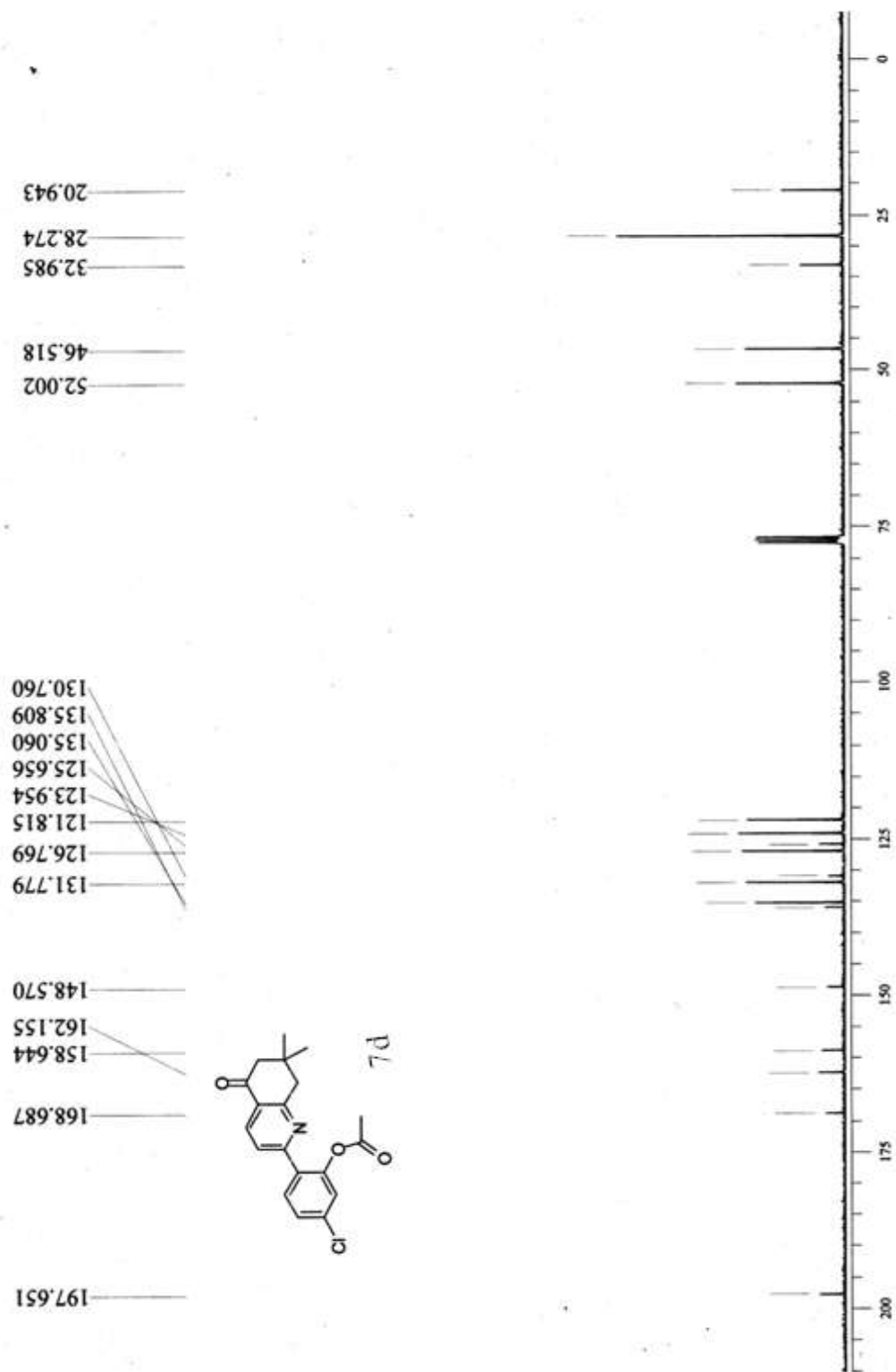
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2/6/2013 2:32:32 PM

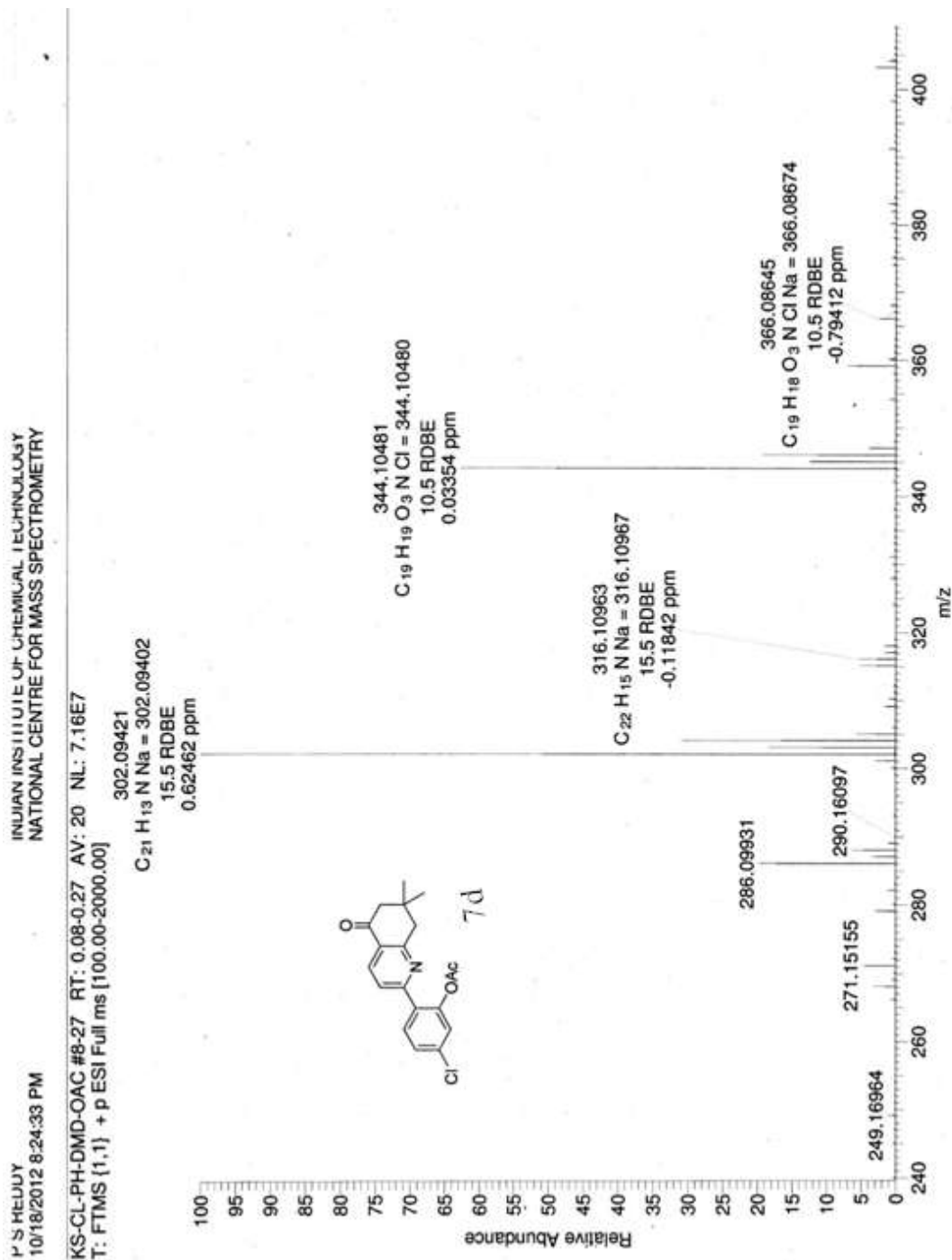
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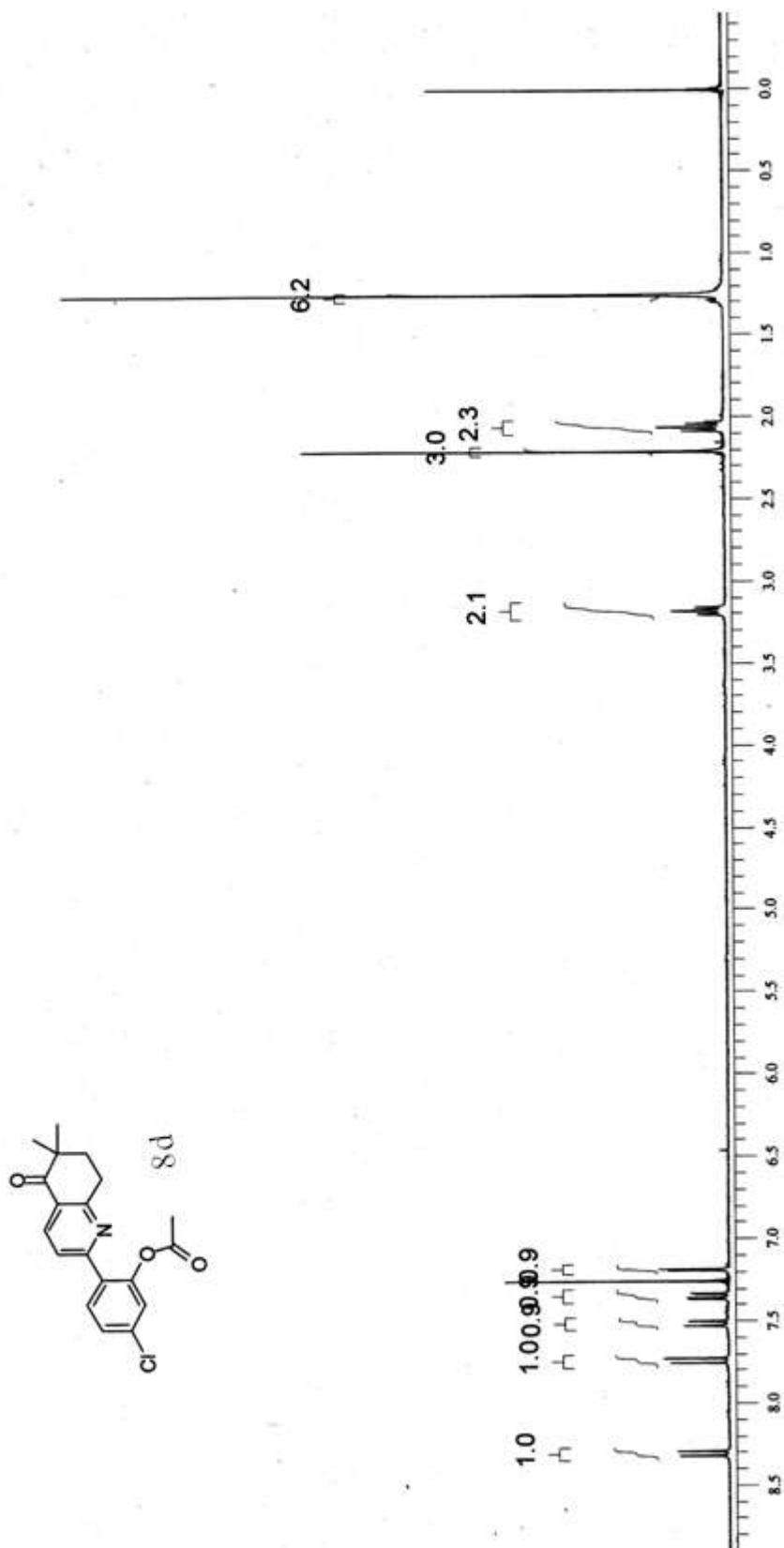
KS-P-CL-Ph-Cyhx-OAc #14 RT: 0.14 AV: 1 NL: 1.60E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000 nnt]

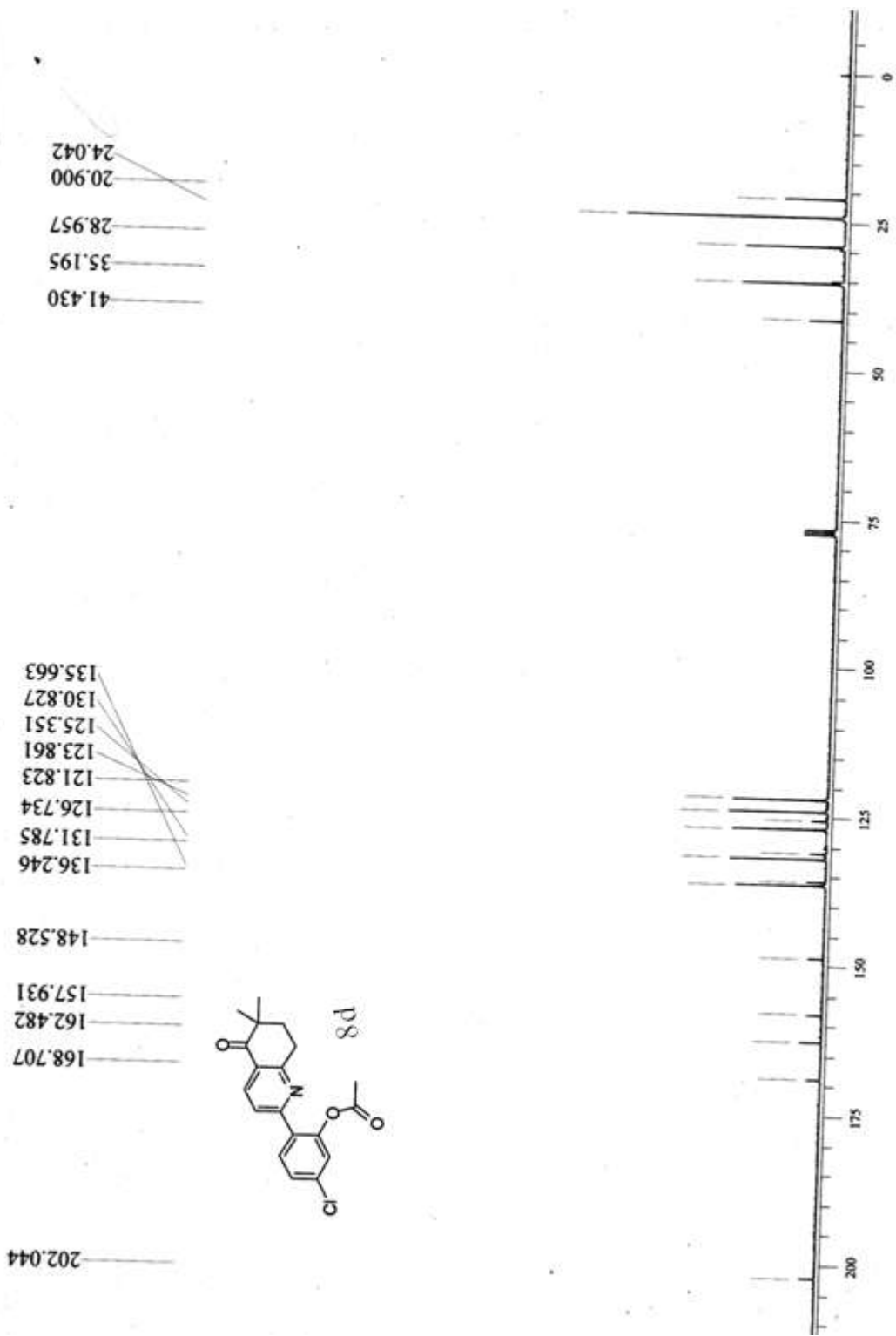


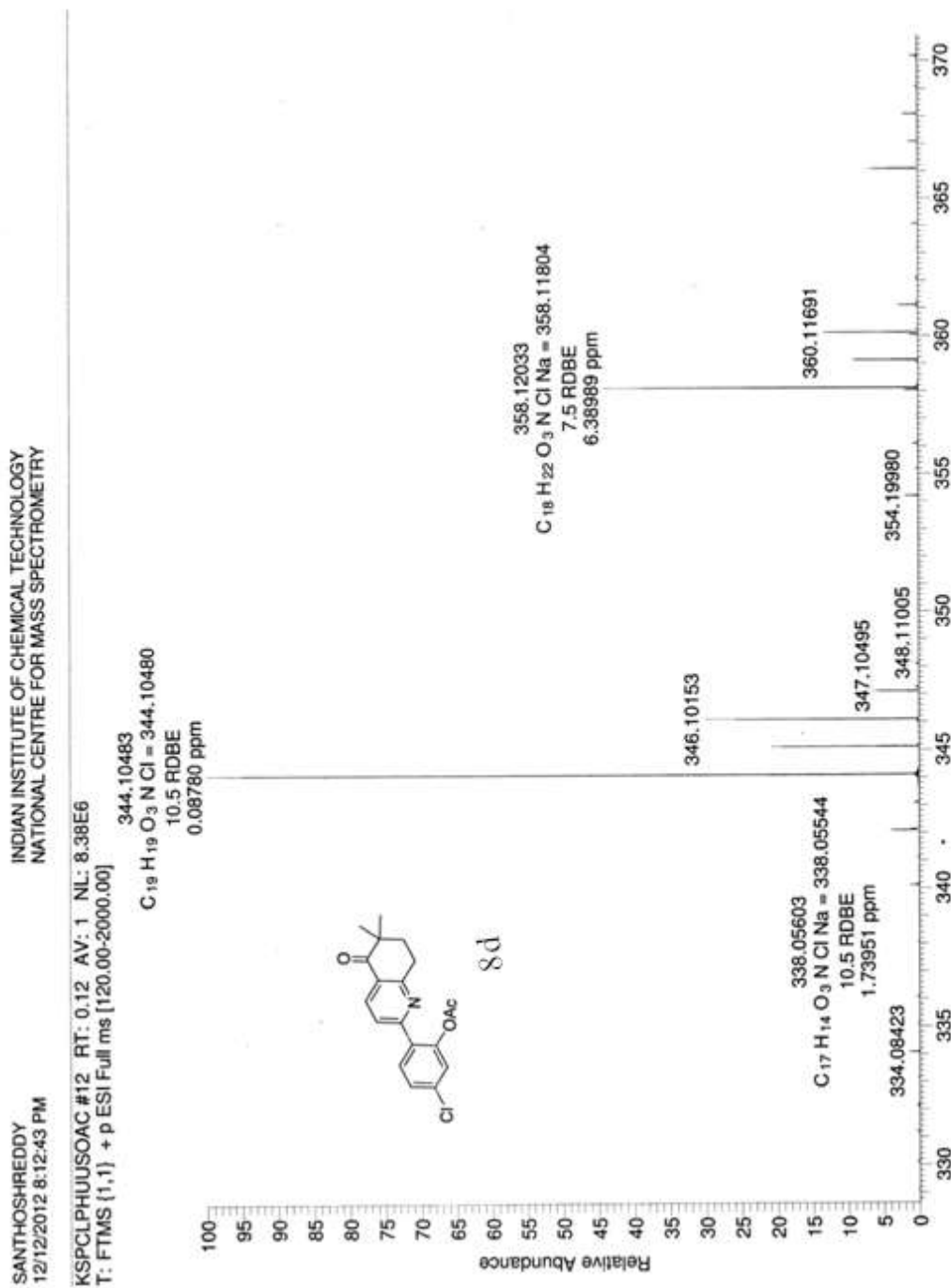


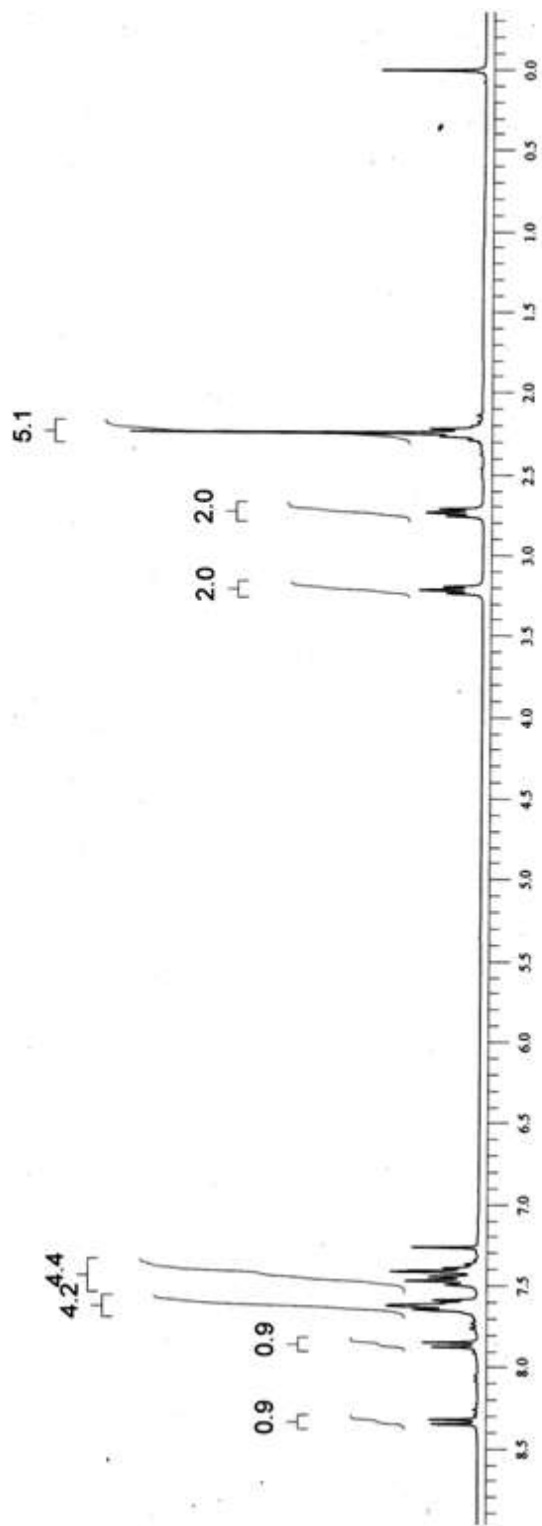
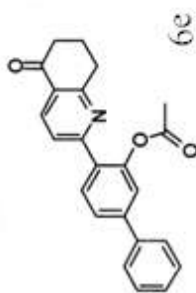




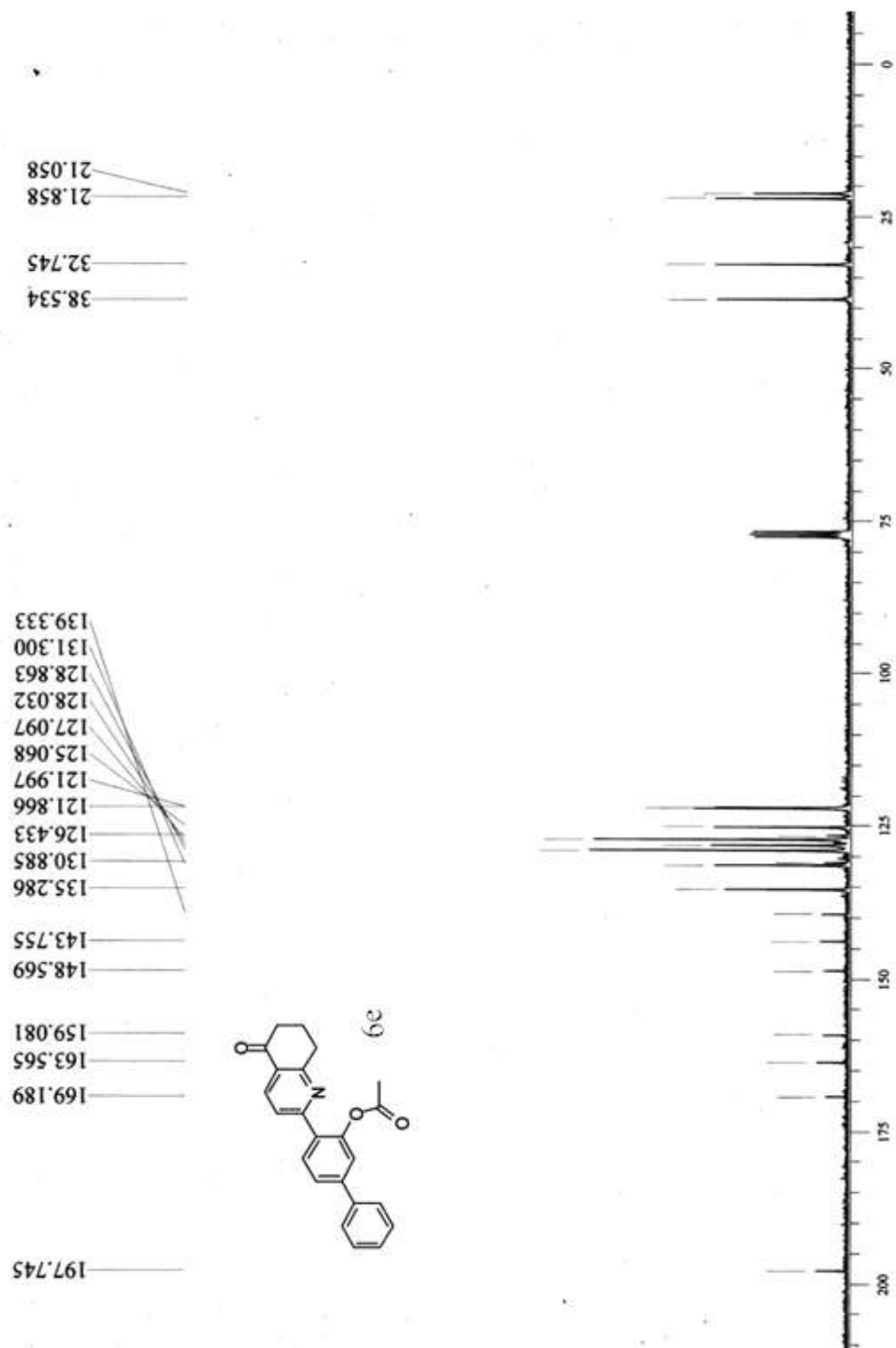










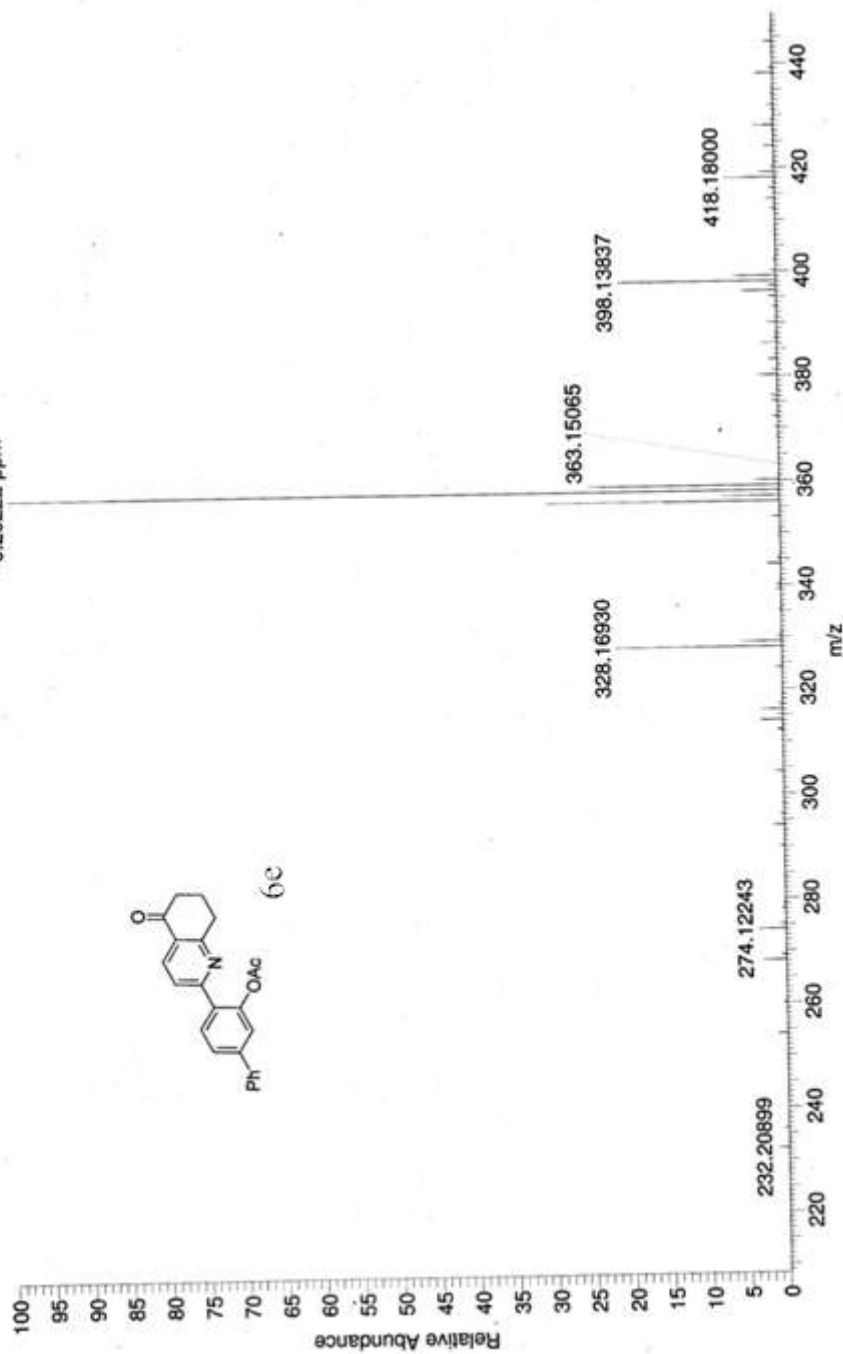
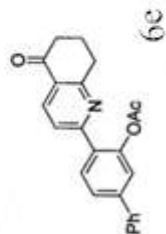


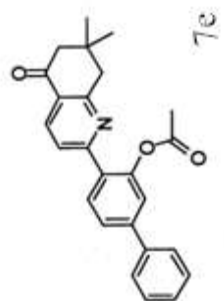
P. S. REDDDY  
10/12/2012 10:50:41 PM

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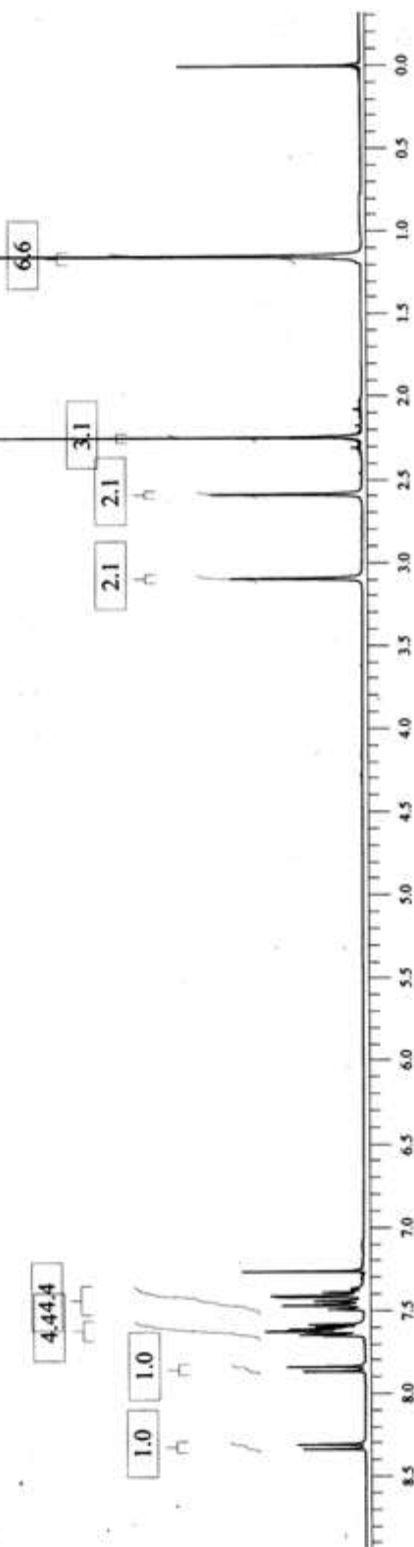
KS-BIPH-CYHX-OAC #8-56 RT: 0.08-0.57 AV: 49 NL: 2.62E5  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

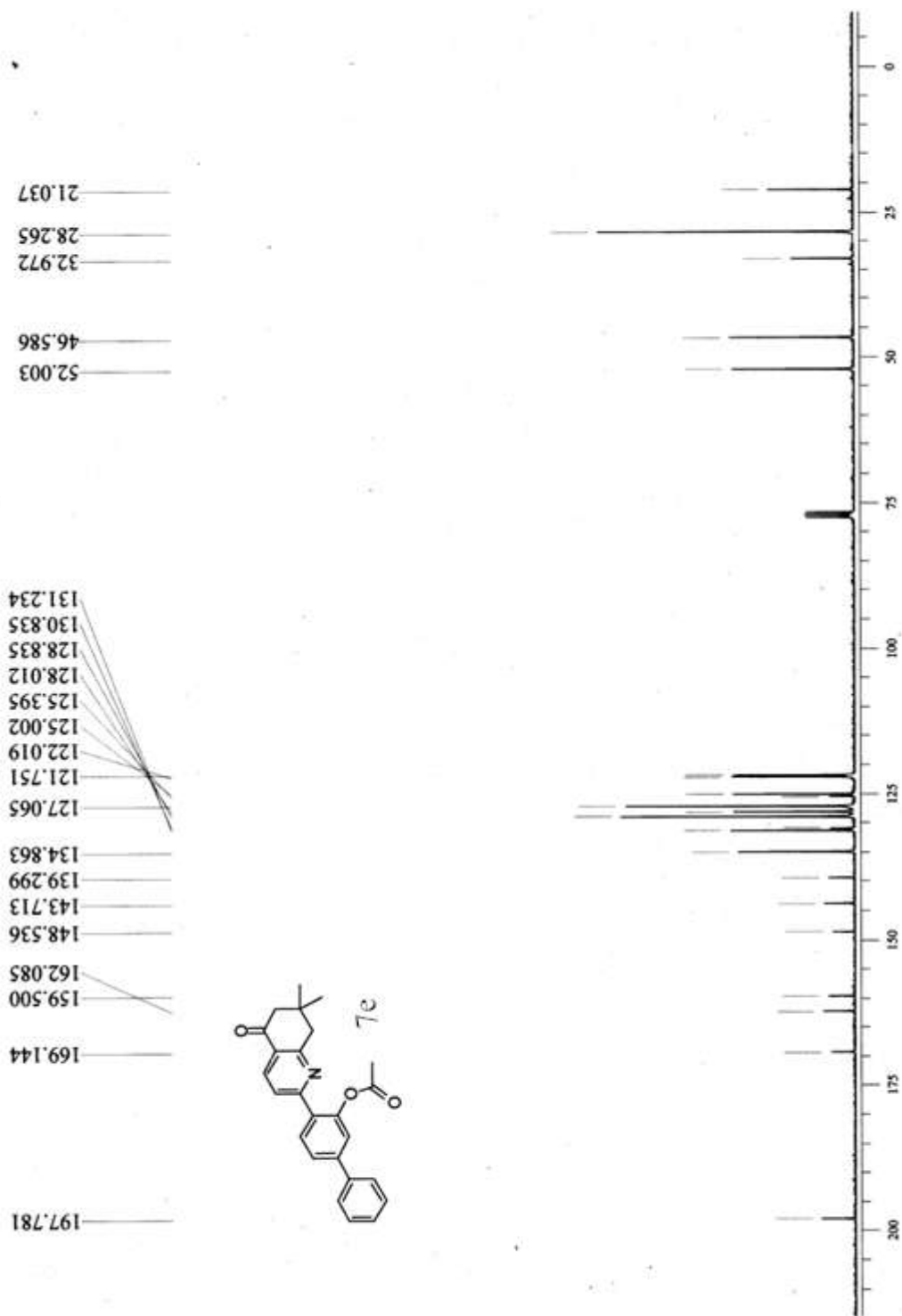
358.14370  
C<sub>23</sub>H<sub>20</sub>O<sub>3</sub>N = 358.14377  
14.5 FIDBE  
-0.20222 ppm





7e



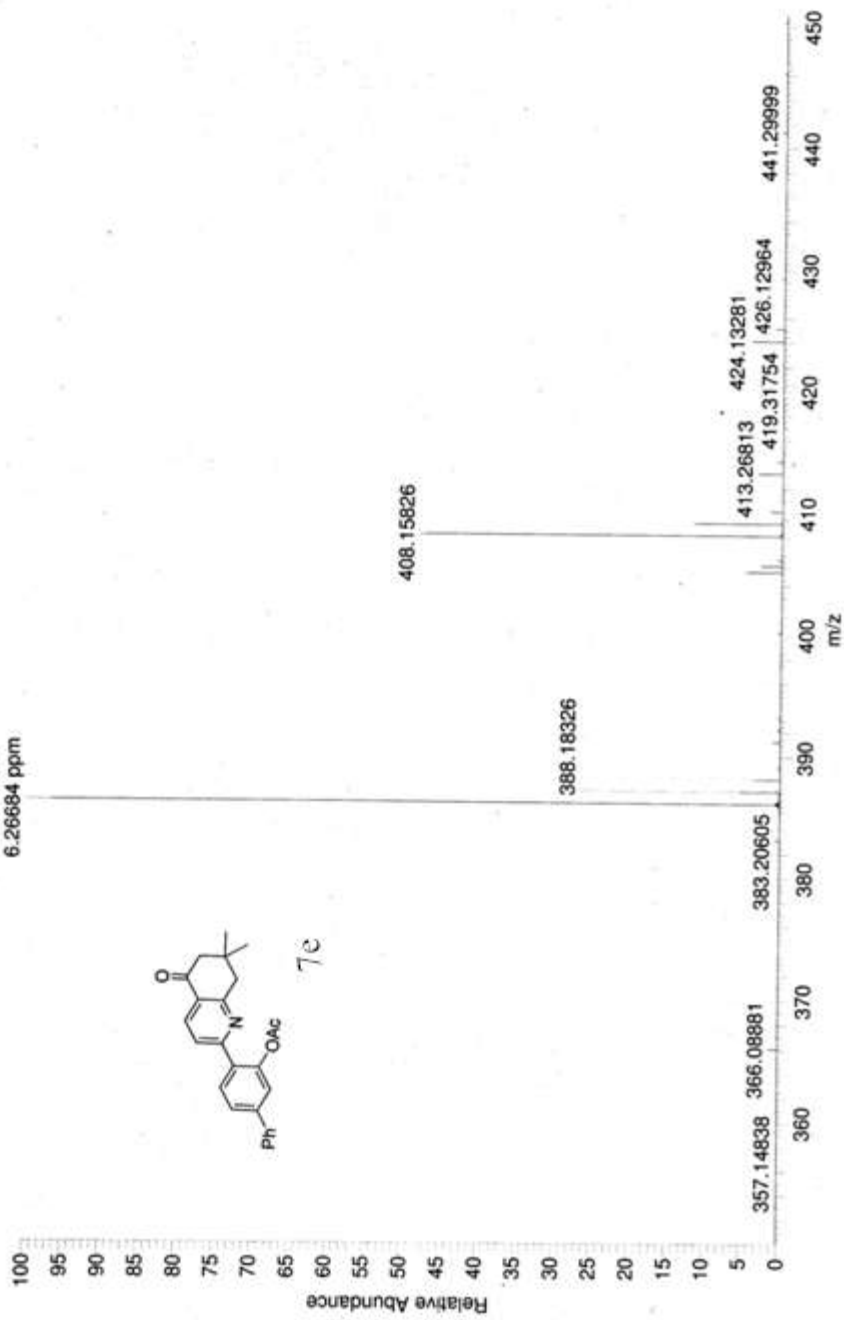


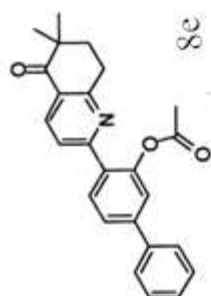
P.S.REDDY  
9/21/2012 6:08:25 PM

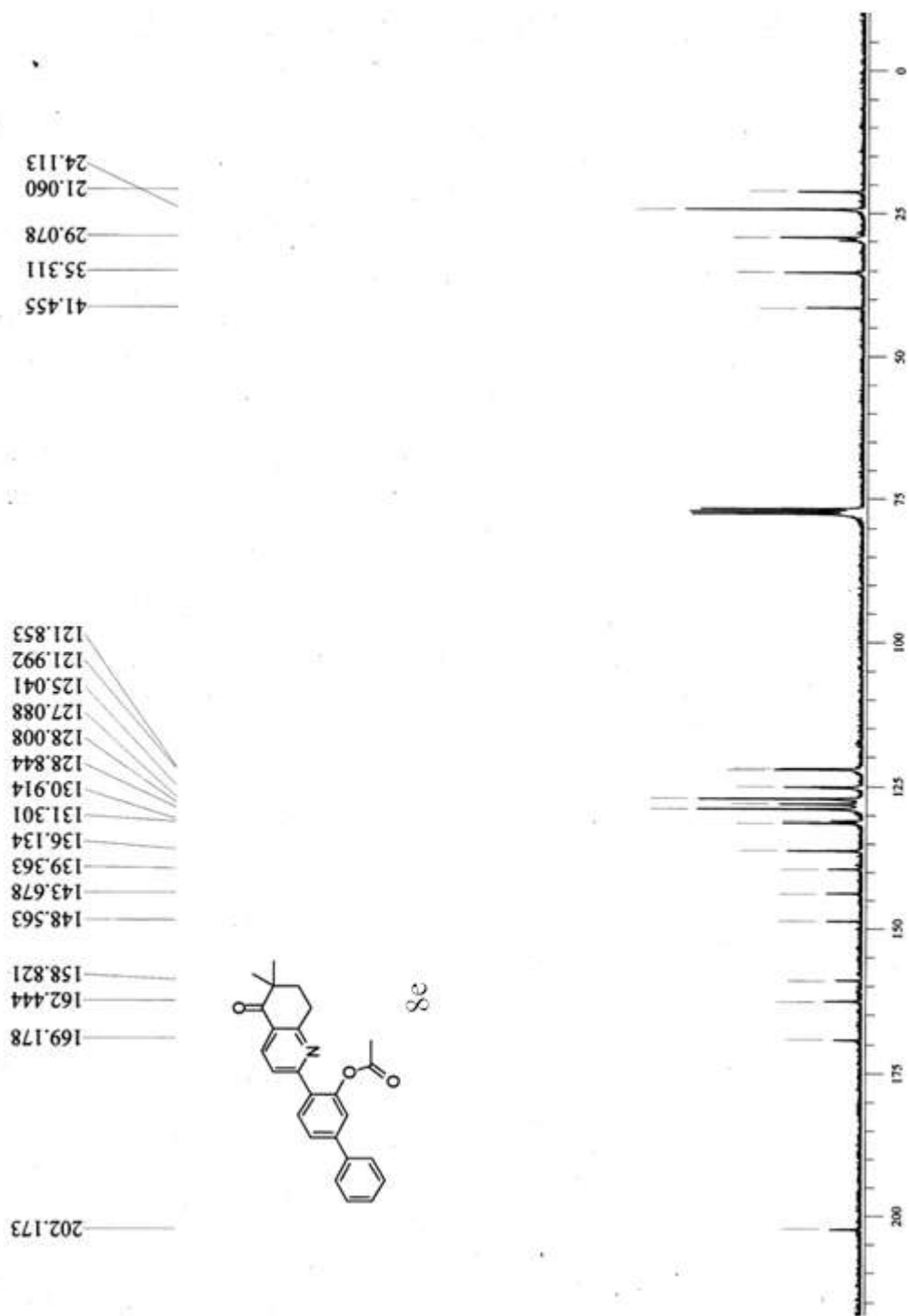
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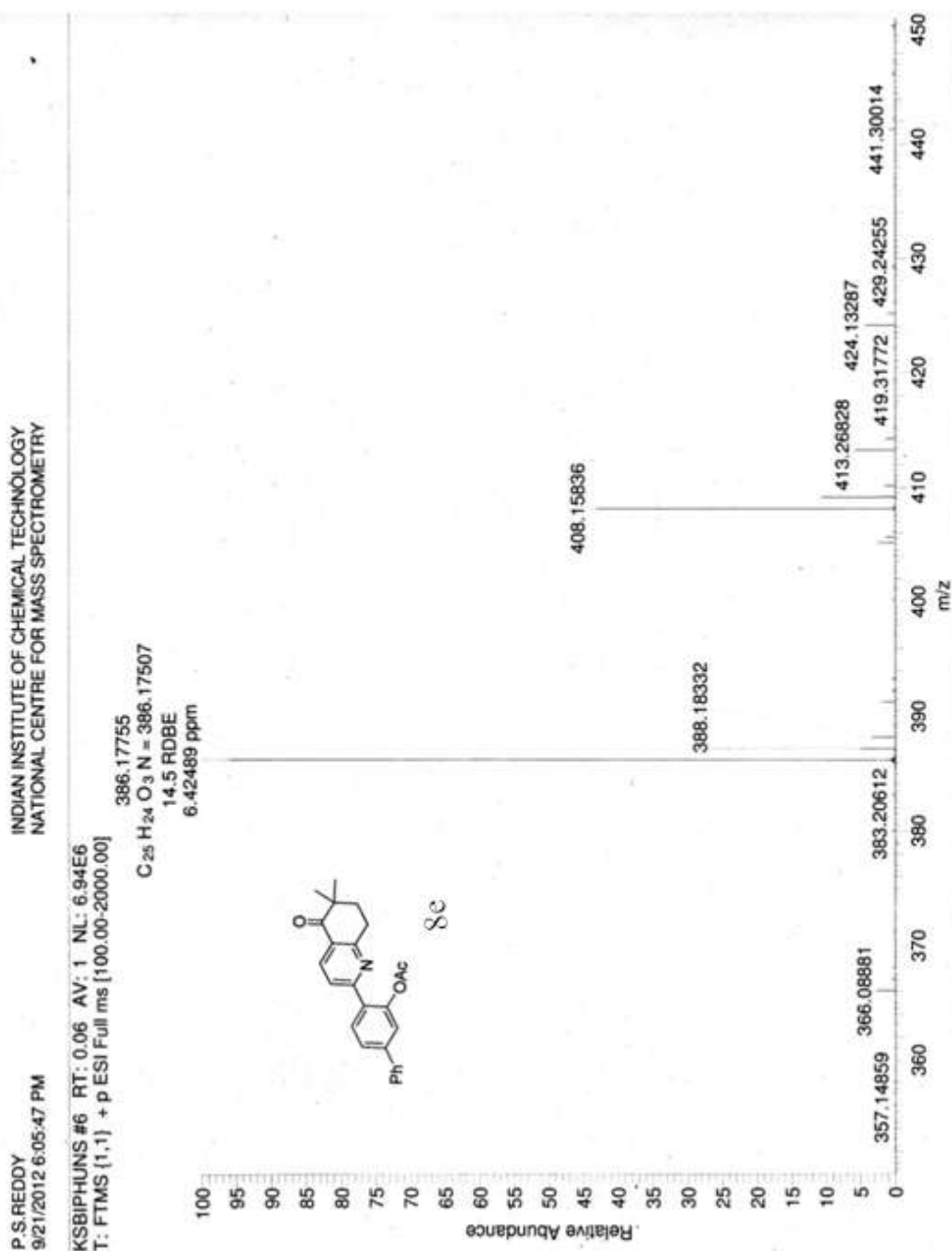
KSBIPHMDOAC #6 RT: 0.06 AV: 1 NL: 9.81E6  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

396.17749  
C<sub>25</sub>H<sub>24</sub>O<sub>3</sub>N = 386.17507  
14.5 RDBE  
6.26684 ppm

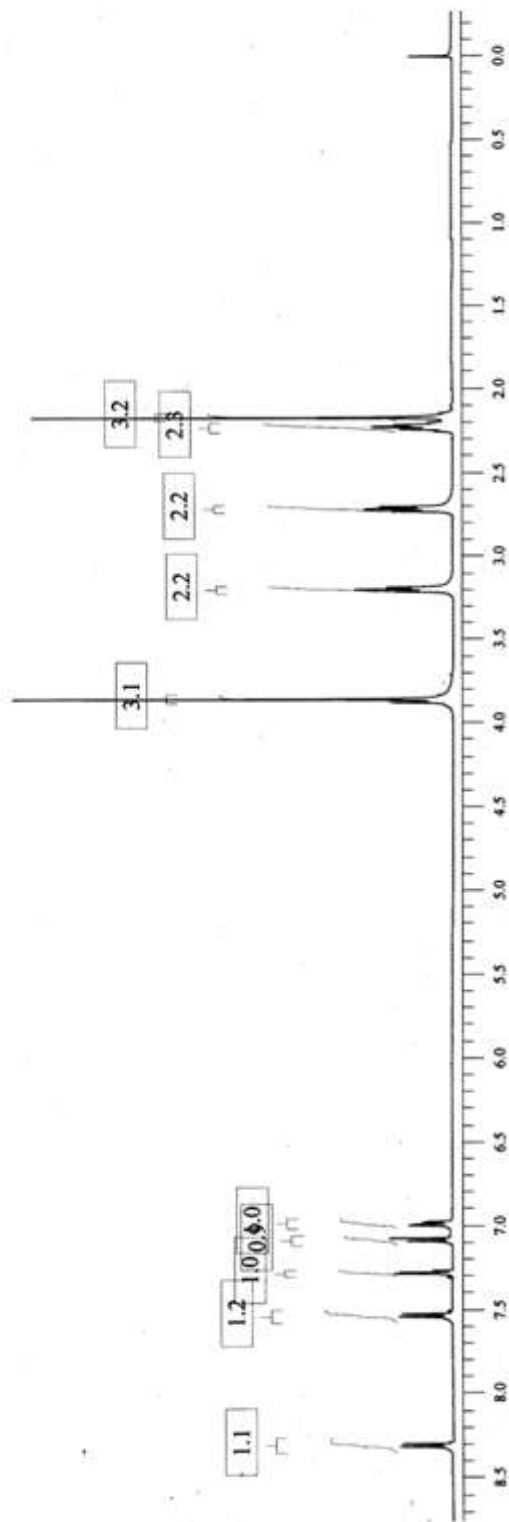
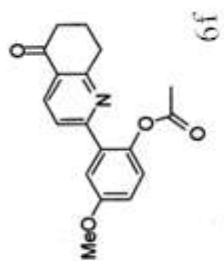


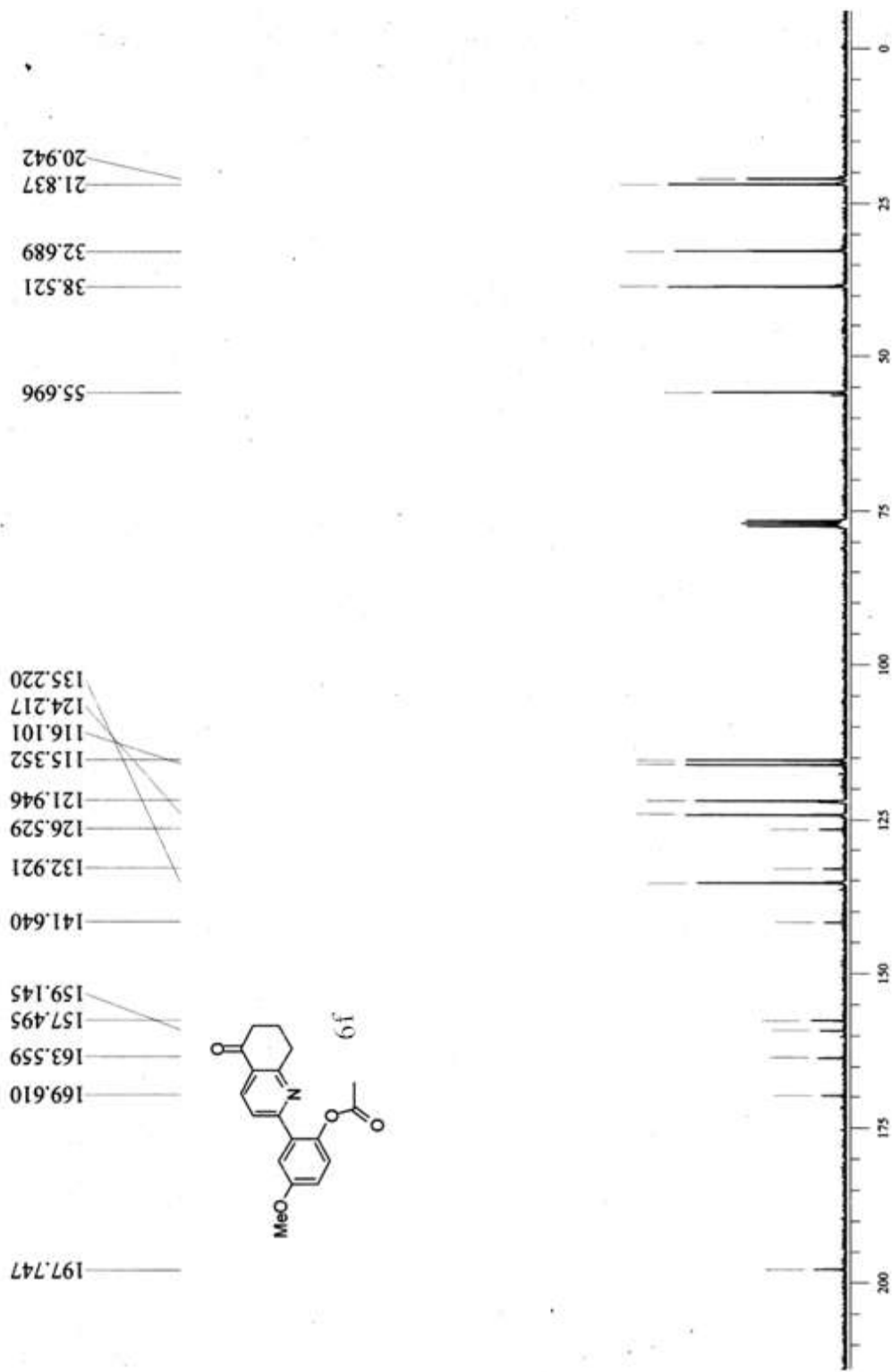










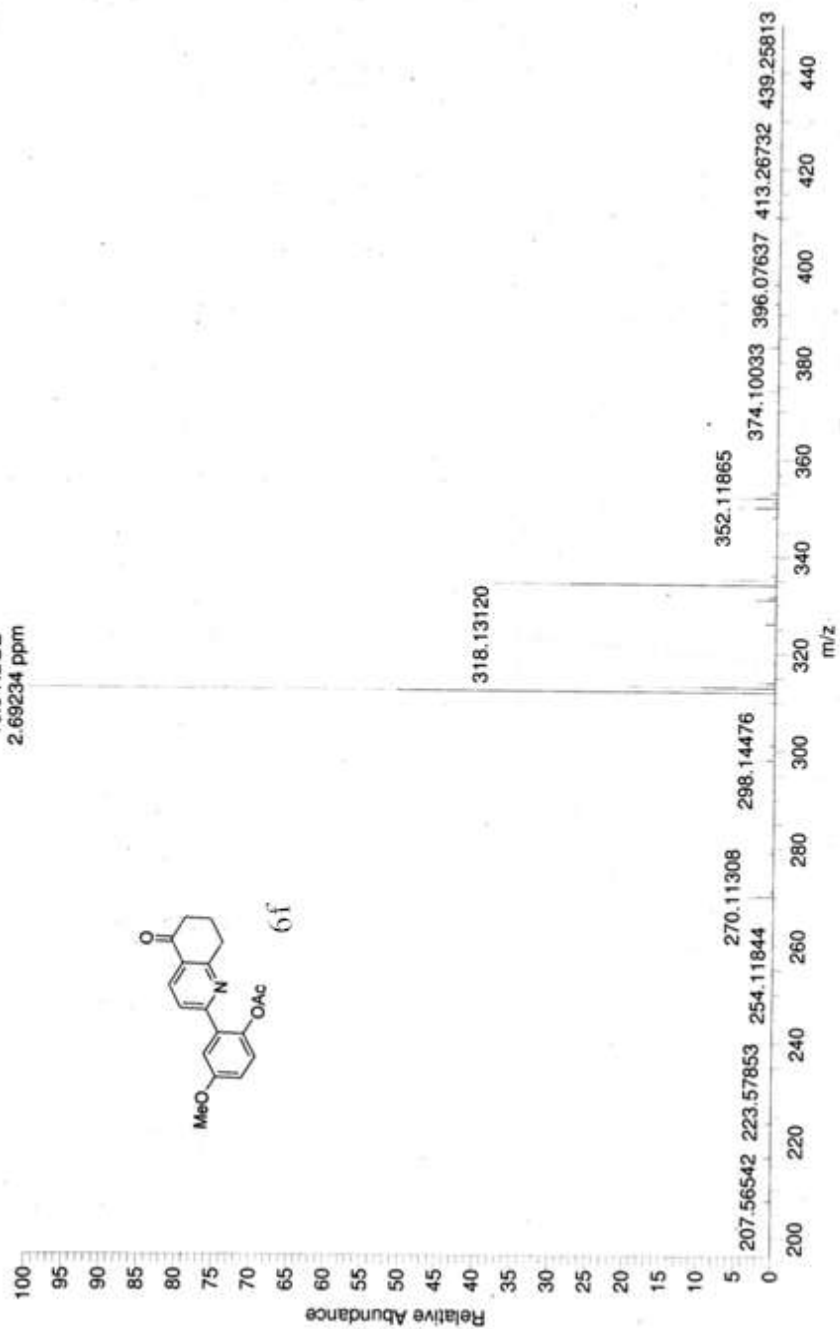
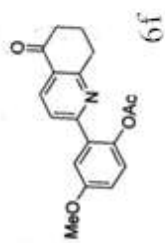


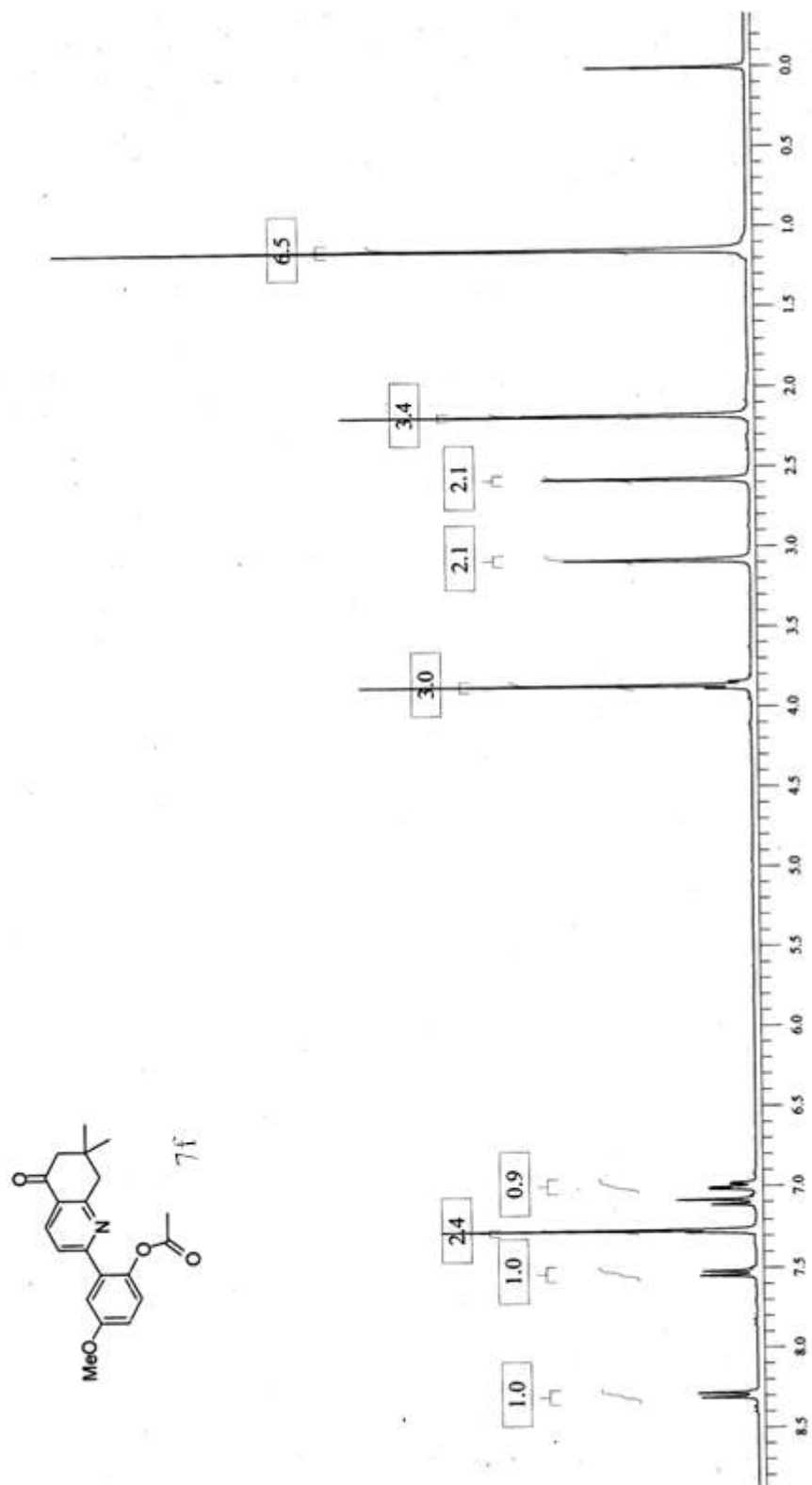
P.S.REDDY  
9/21/2012 3:49:07 PM

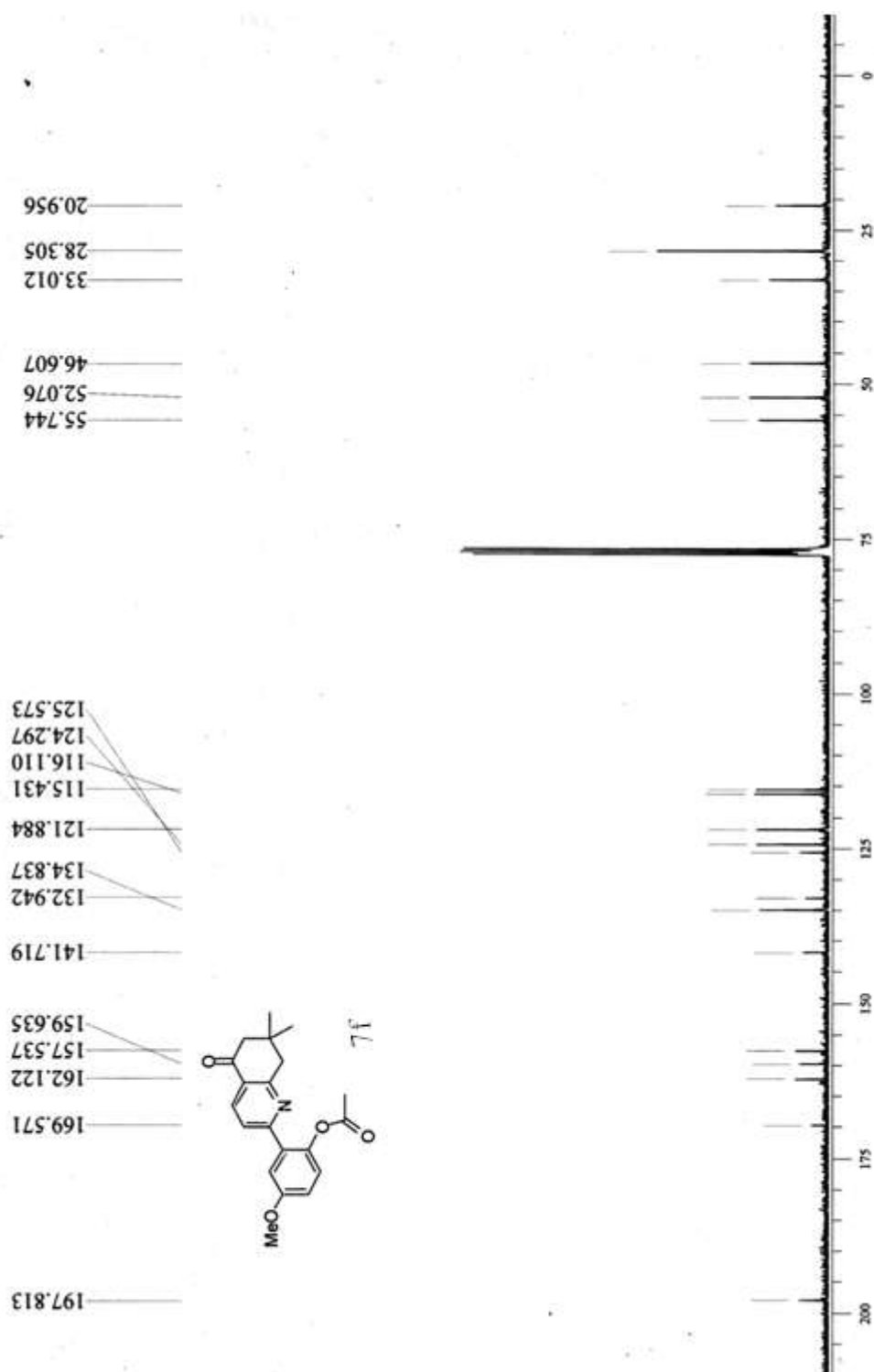
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KSMOMECHYOAC #10-39 RT: 0.10-0.40 AV: 30 NL: 6.71E7  
T: FTMS (1.1) + p ESI Full ms [100.00-2000.00]

312.12387  
C<sub>18</sub>H<sub>16</sub>O<sub>4</sub> N = 312.12303  
10.5 RDBE  
2.69234 ppm





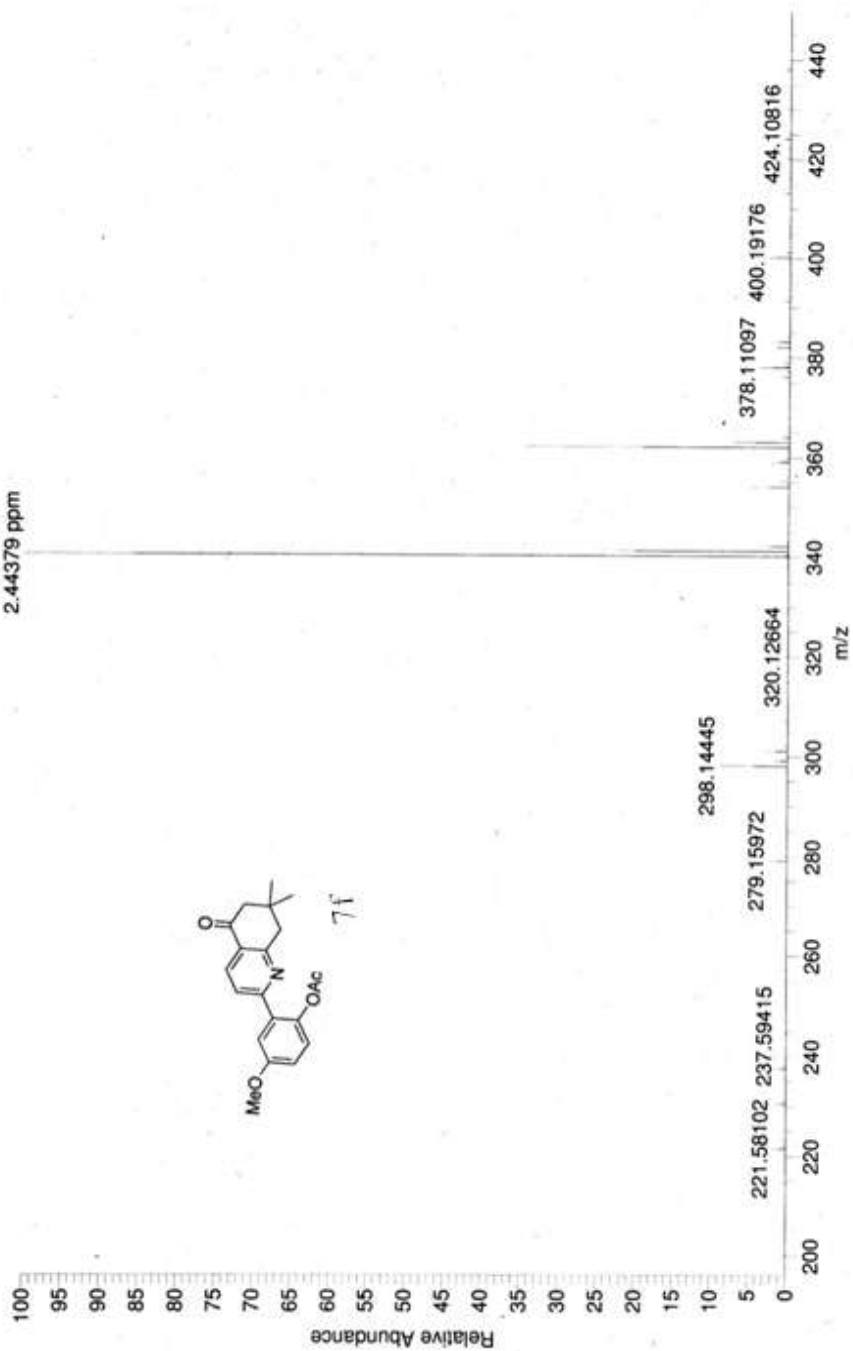


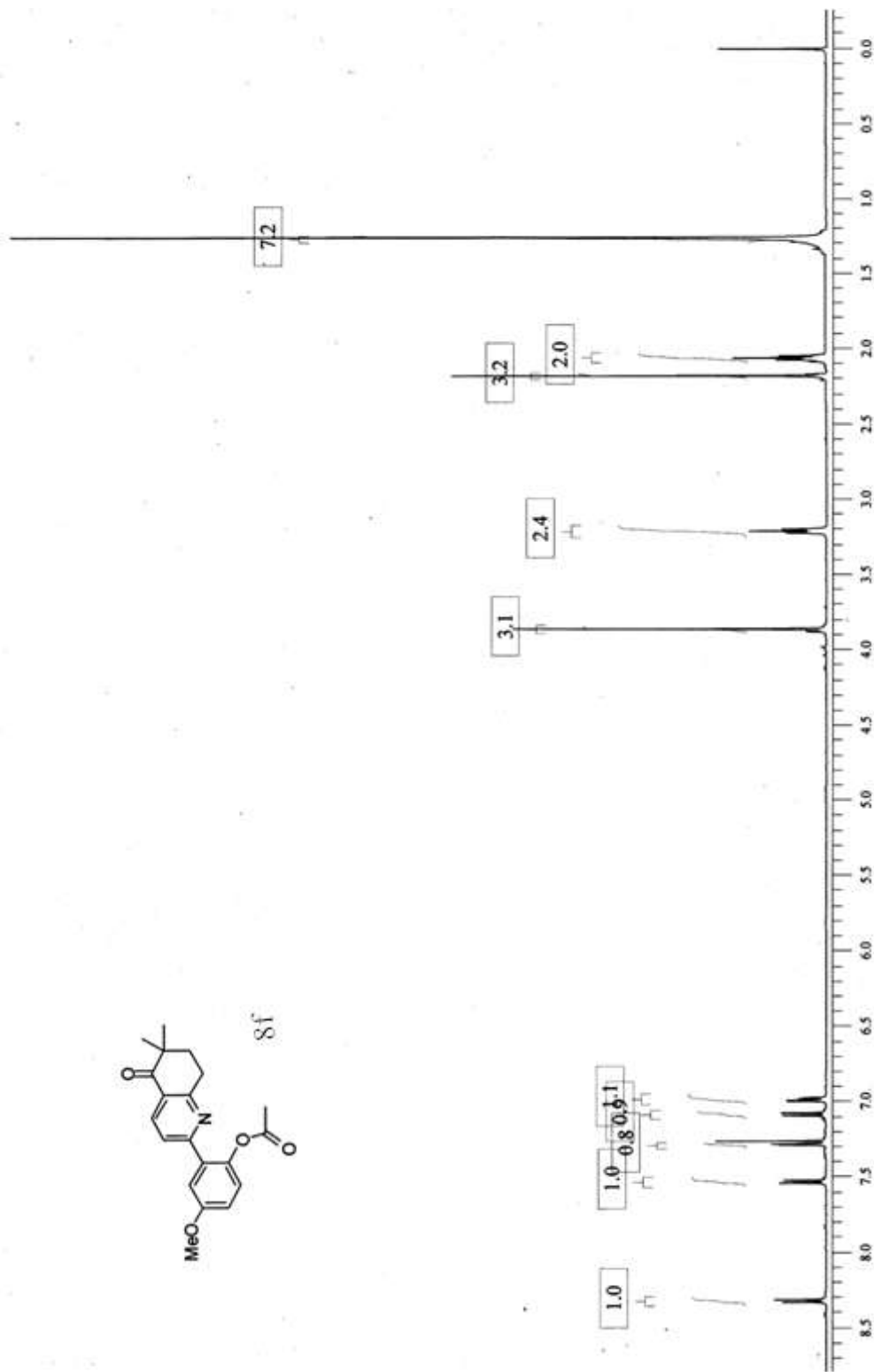
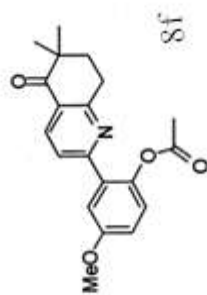
P.S.REDDY  
9/21/2012 3:46:29 PM

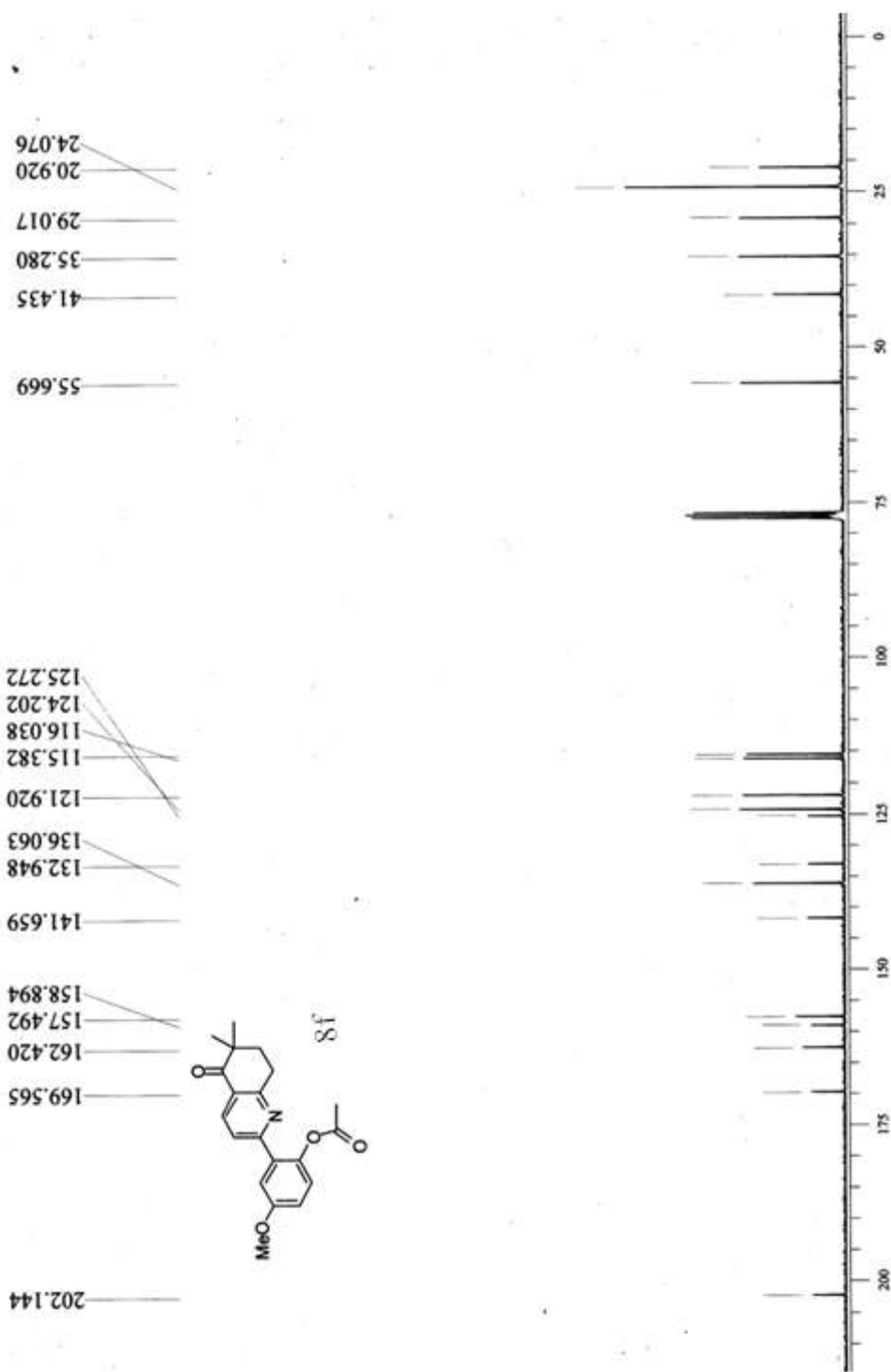
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KSMOMEDMOAC #8-27 RT: 0.08-0.27 AV: 20 NL: 6.44E7  
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

340.15517  
C<sub>20</sub>H<sub>22</sub>O<sub>4</sub> N = 340.15433  
10.5 RDBE  
2.44379 ppm



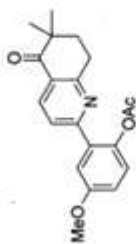
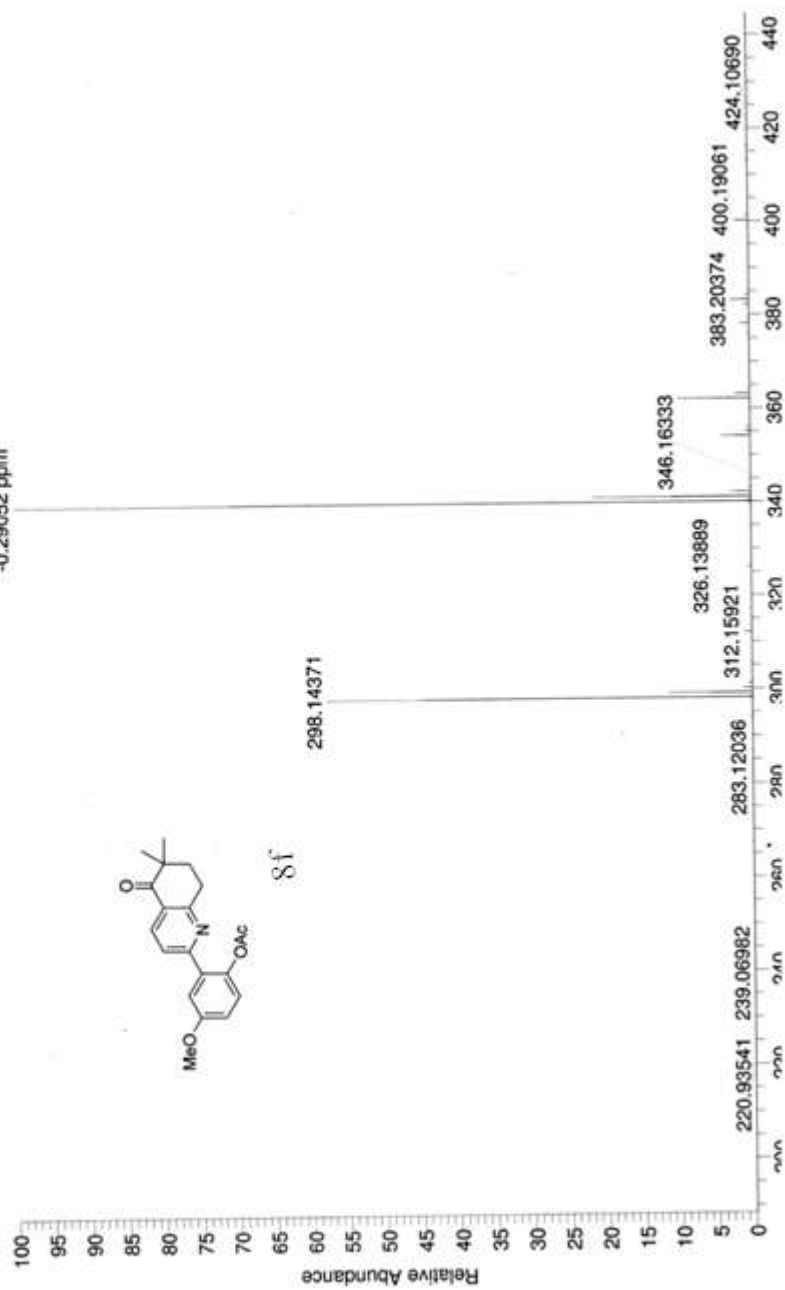




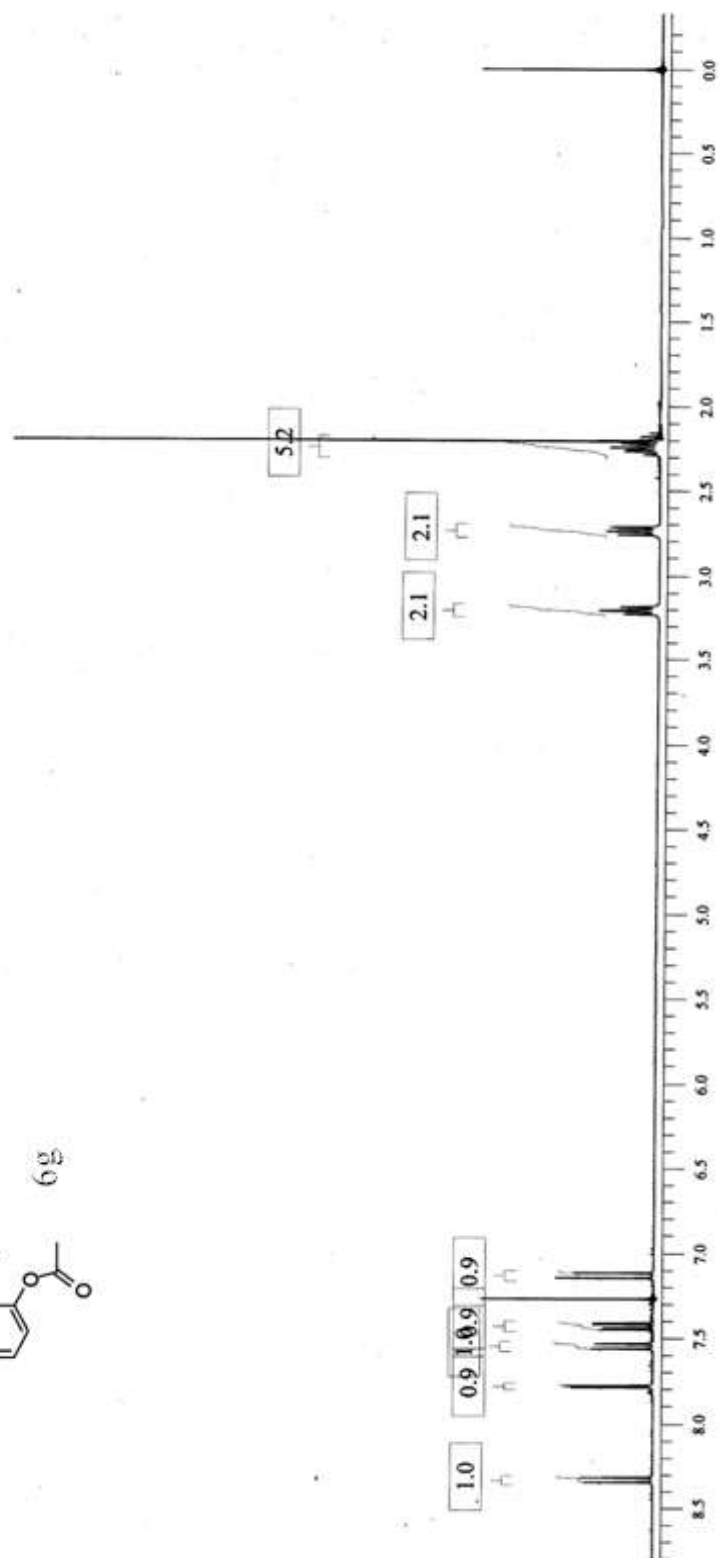
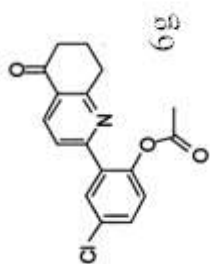


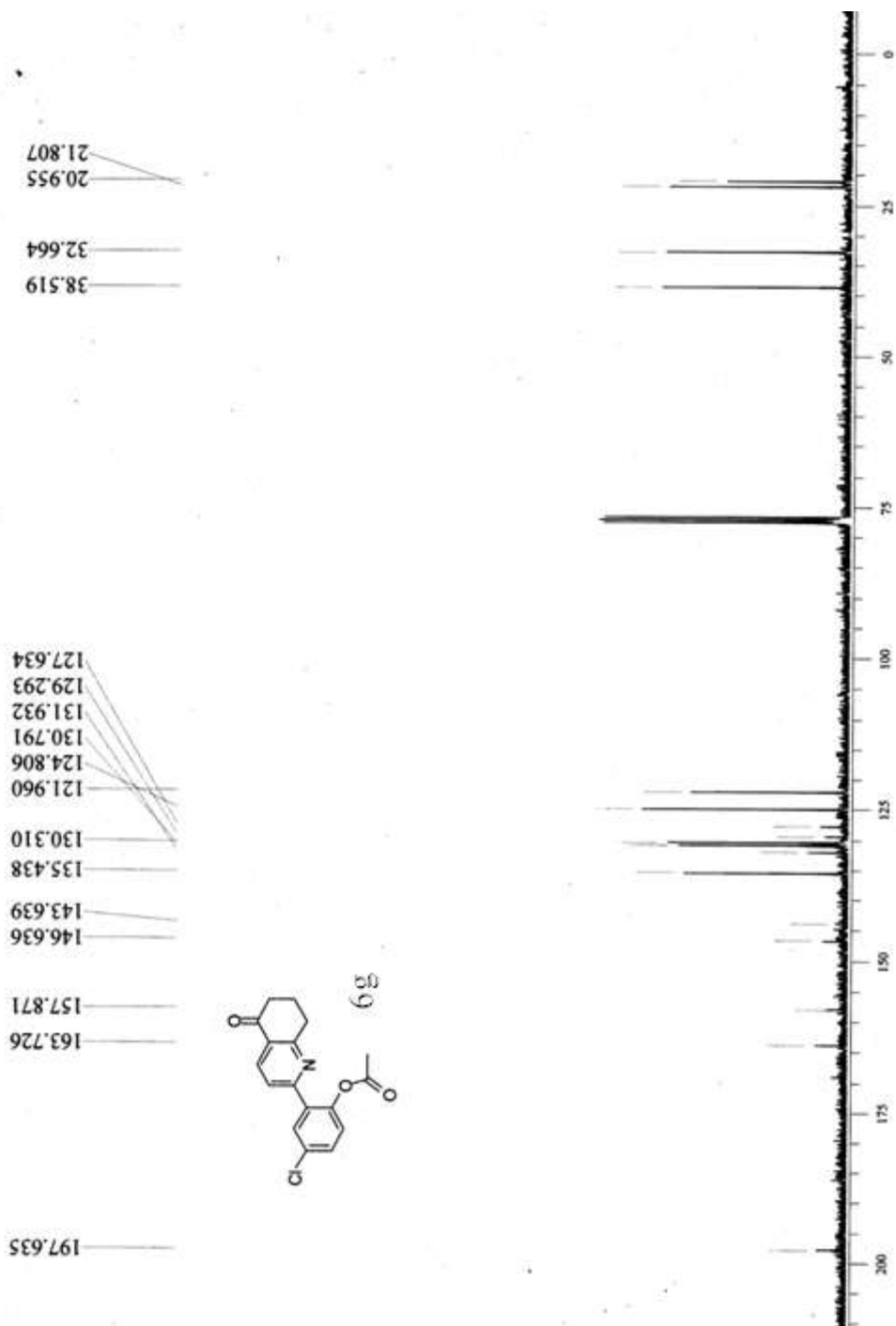
SANTHOSHREDDY  
12/12/2012 8:05:03 PM  
INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY  
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KSMOMEIUSOAC #12 RT: 0.12 AV: 1 NL: 4.15E7  
T: FTMS (1.1) + p ESI Full ms [120.00-2000.00]



8f



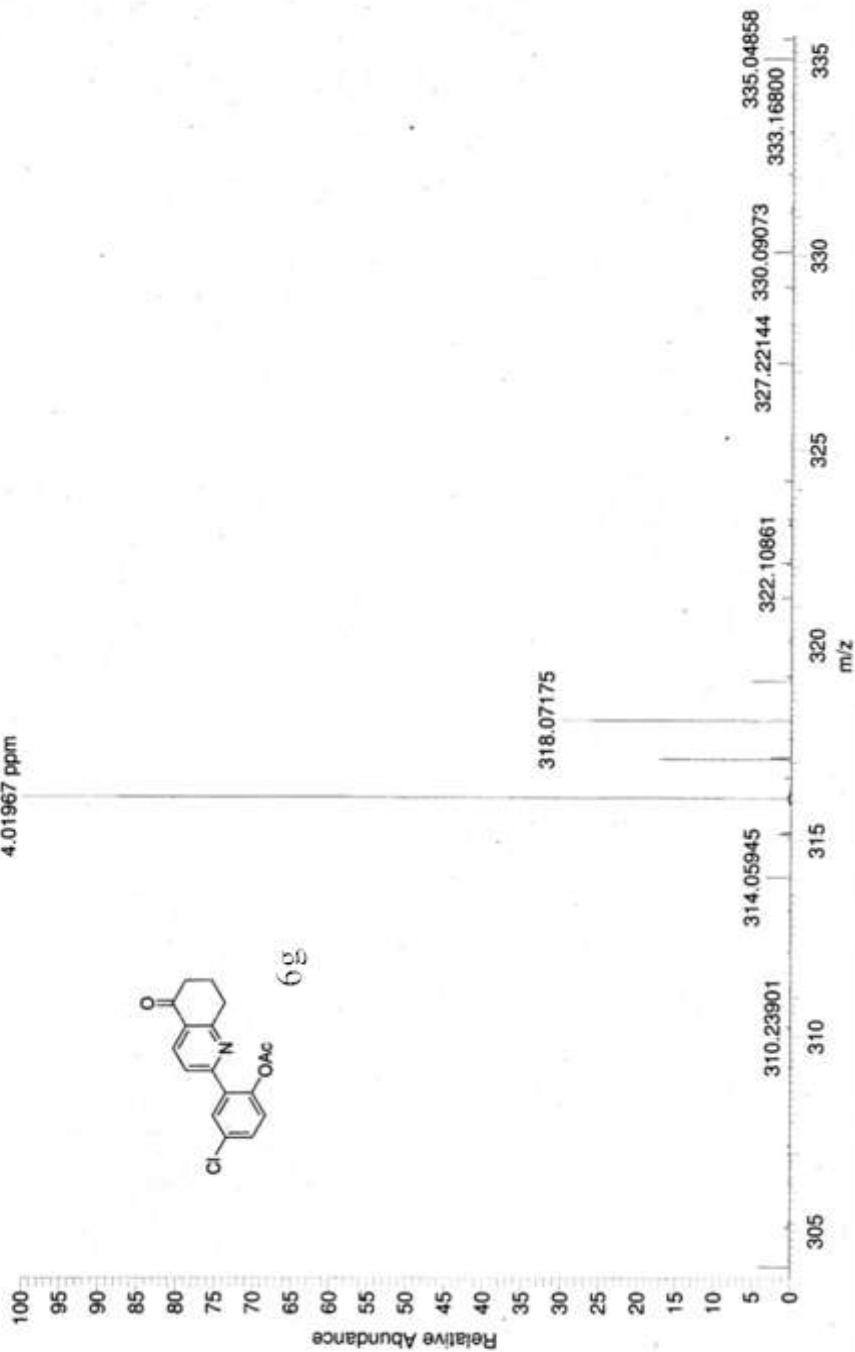
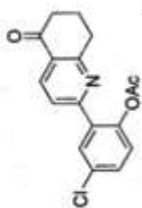


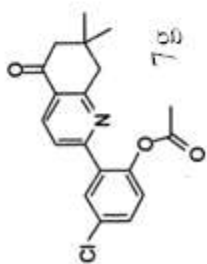
P.S.REDDY  
9/21/2012 6:03:11 PM

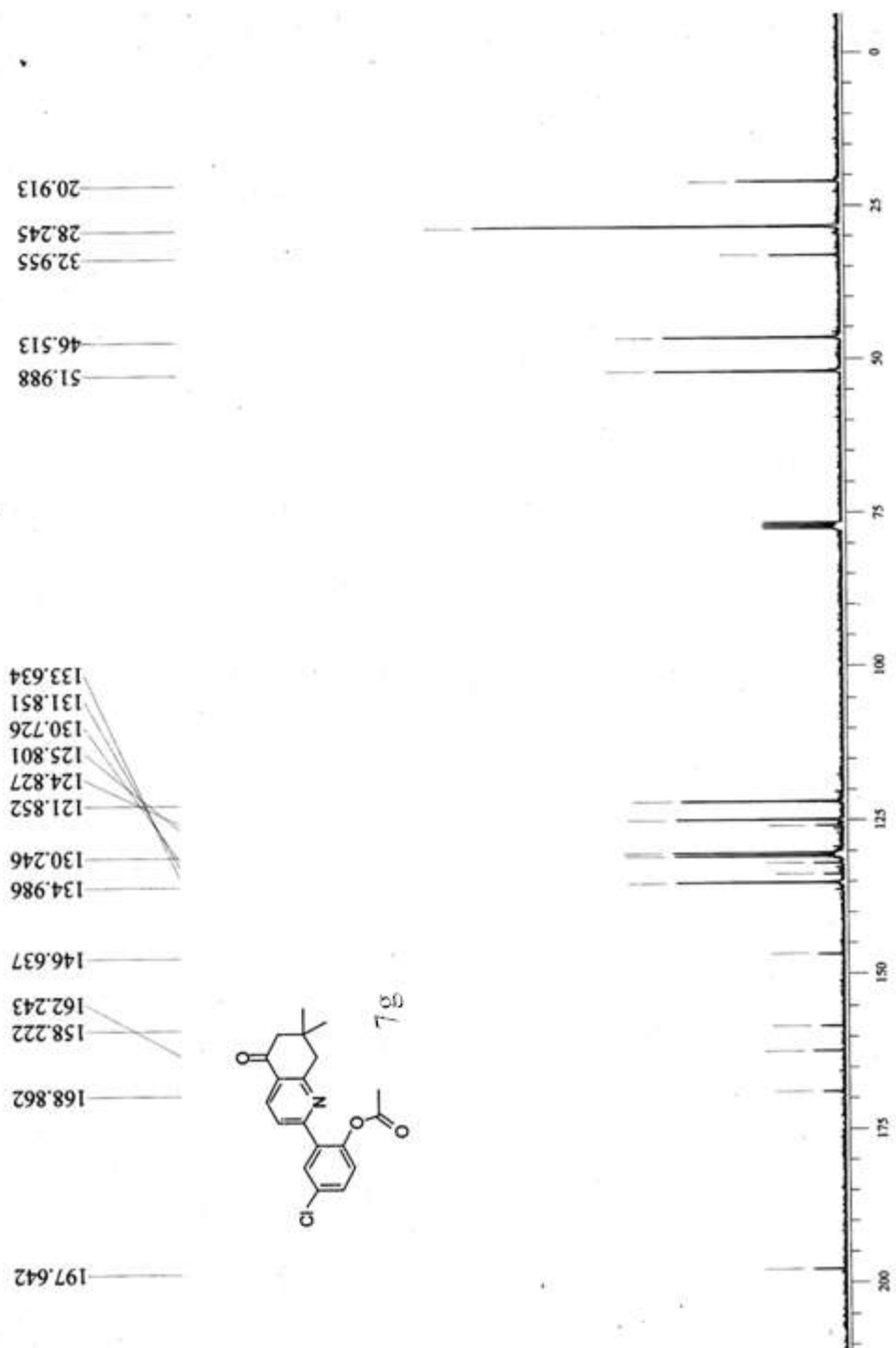
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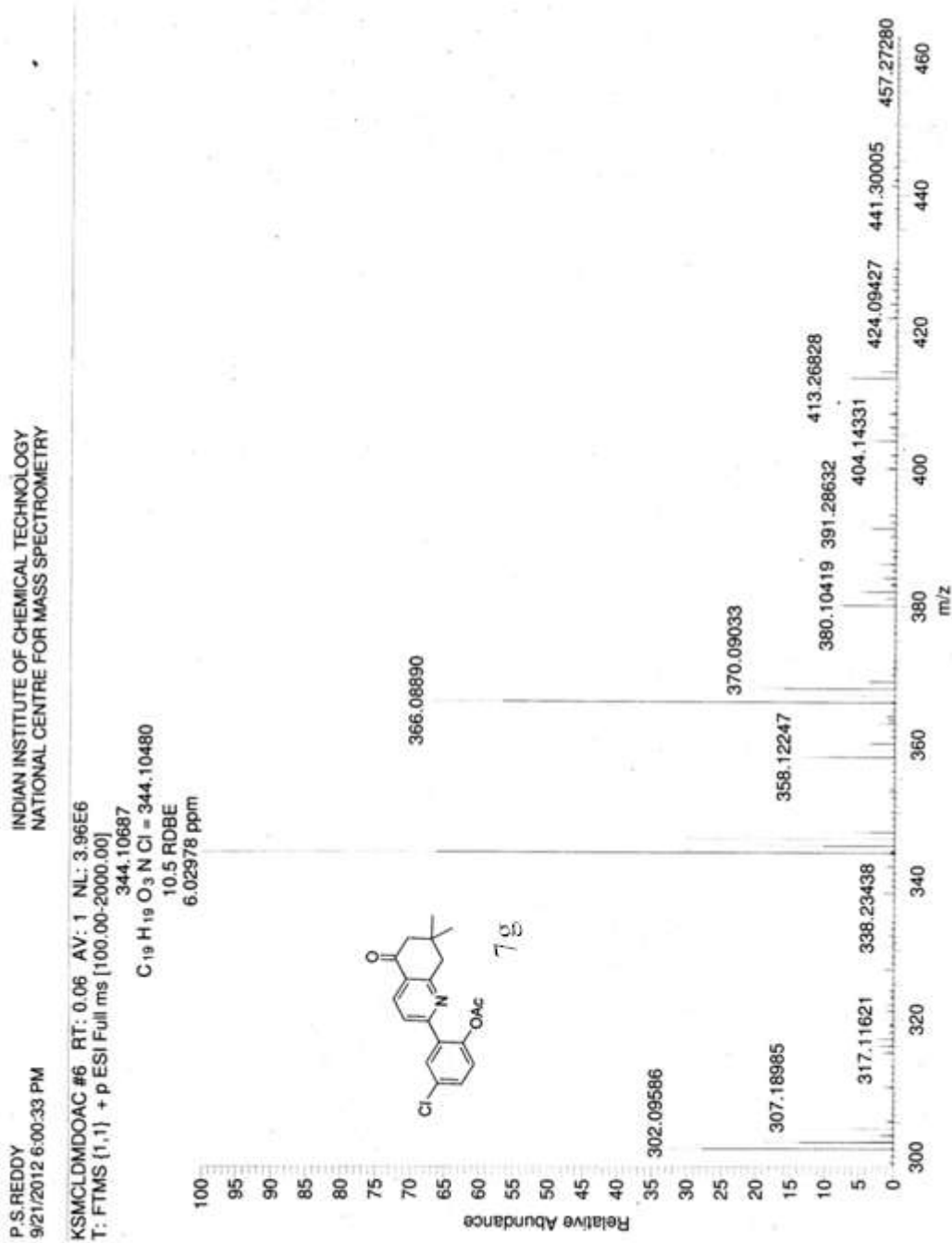
KSMCLCYHXOAC #6 RT: 0.06 AV: 1 NL: 2.84E6  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

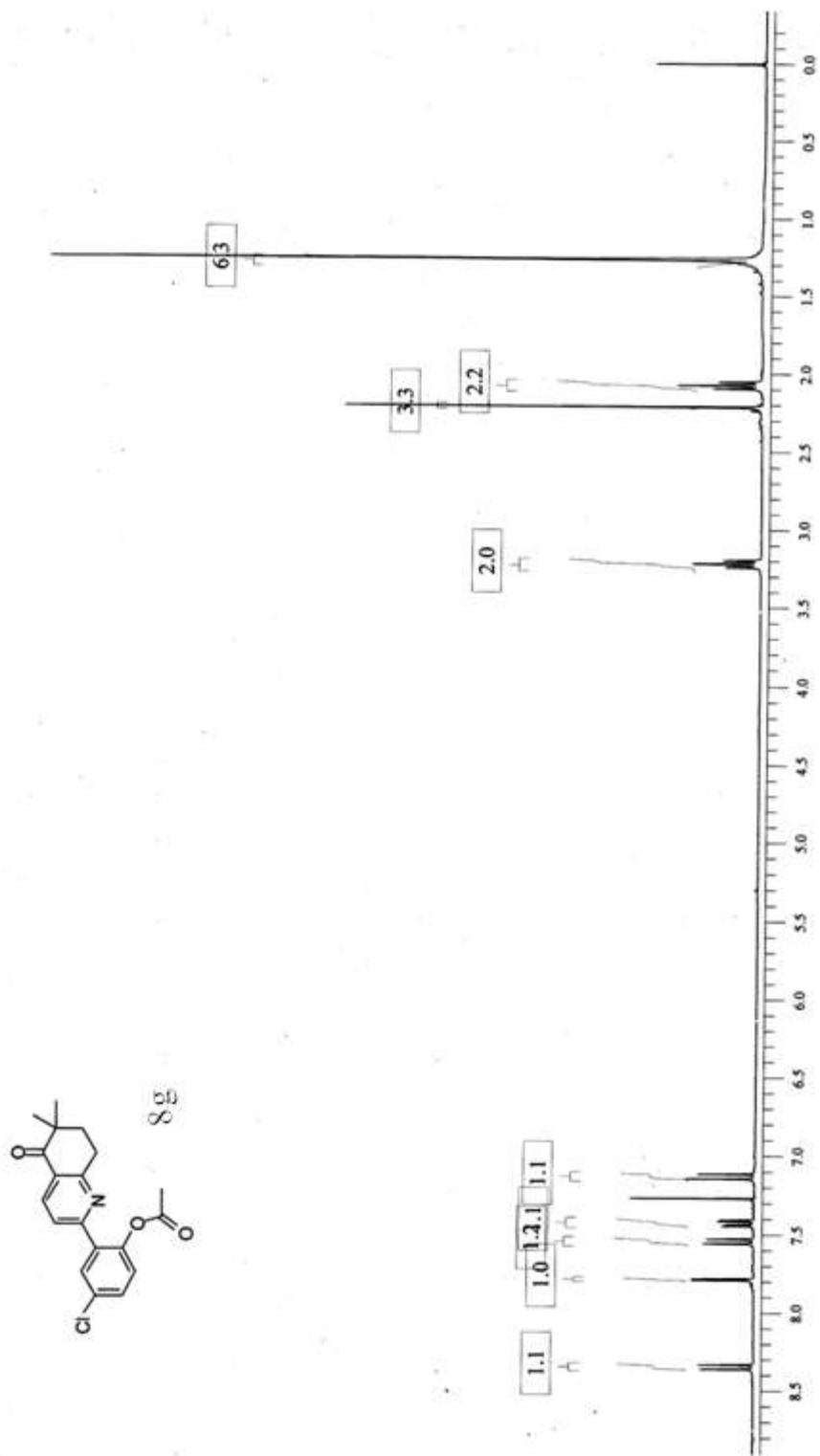
316.07477  
C<sub>17</sub>H<sub>15</sub>O<sub>3</sub>N Cl = 316.07350  
10.5 RDBE  
4.01967 ppm



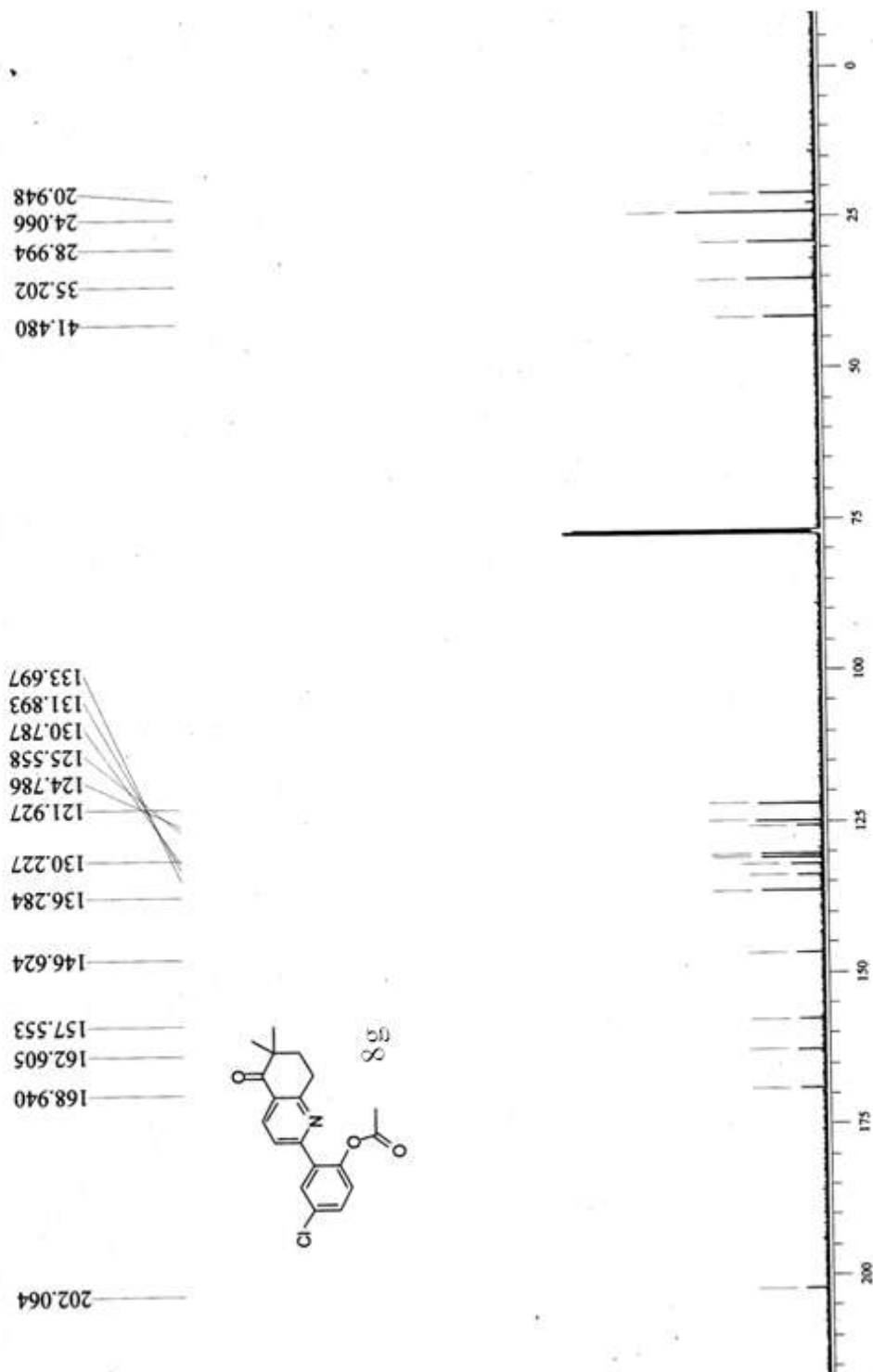










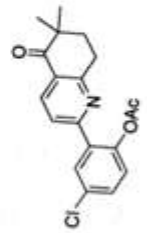


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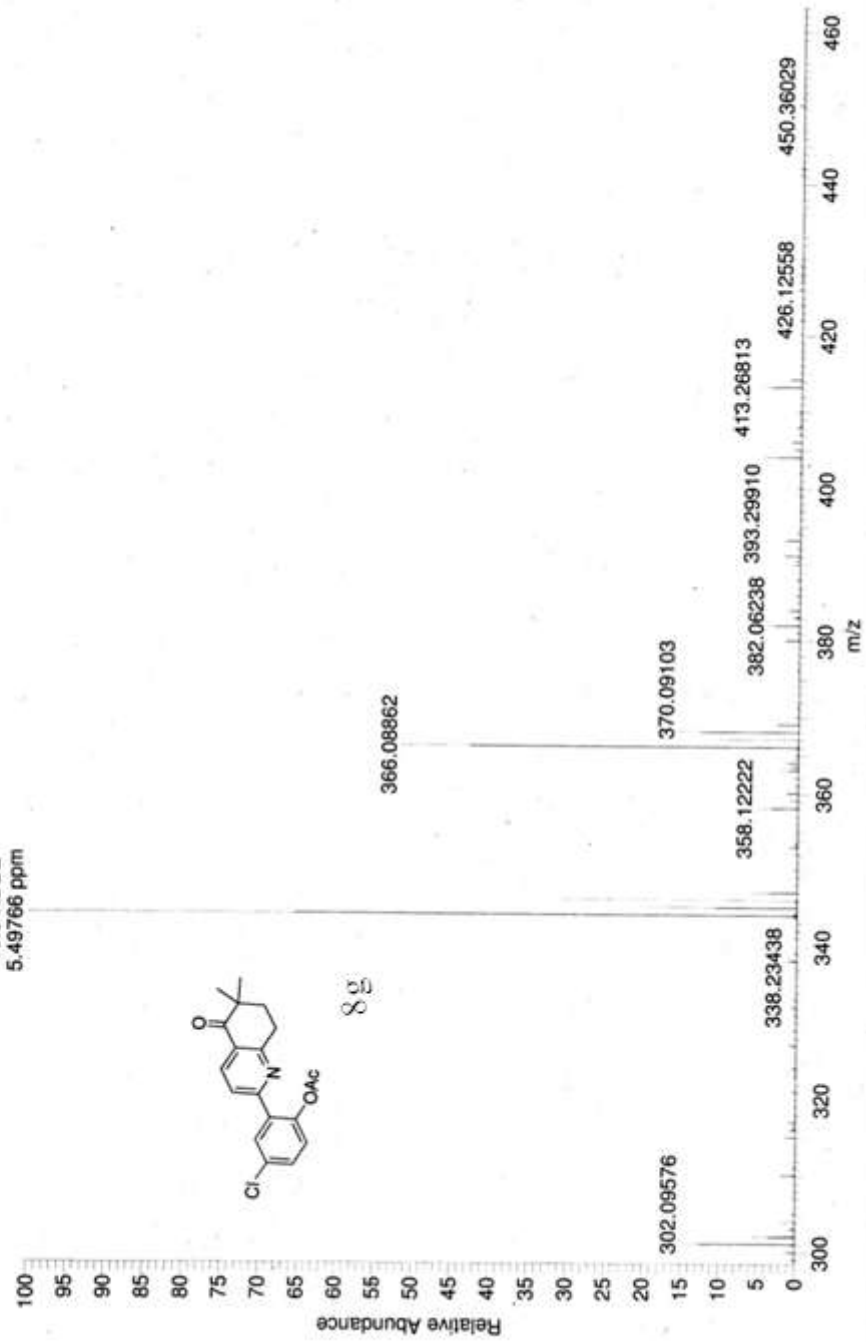
P.S.REDDY  
9/21/2012 5:57:55 PM

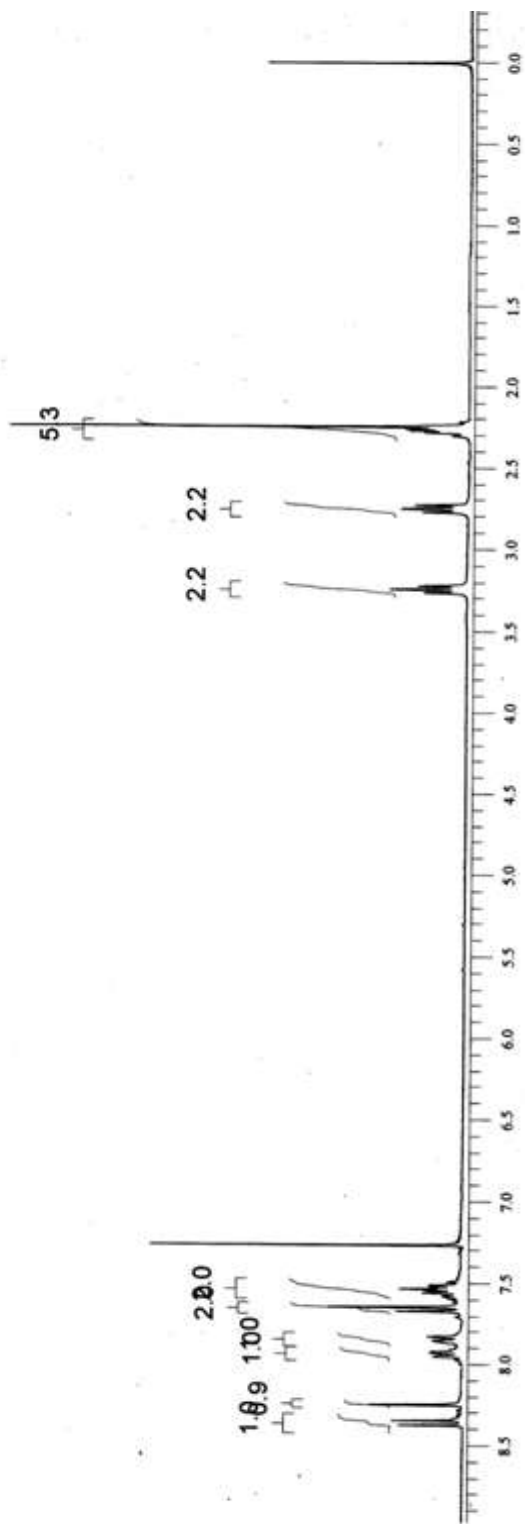
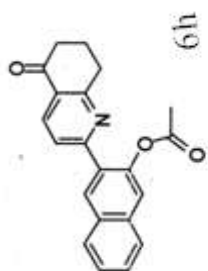
KSMCLUNSOAC #6 RT: 0.06 AV: 1 NL: 8.26E6  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

344.10669  
C<sub>19</sub>H<sub>19</sub>O<sub>3</sub>N Cl = 344.10480  
10.5 RDBE  
5.49766 ppm



8.5





21.830  
20.993

32.701  
38.495

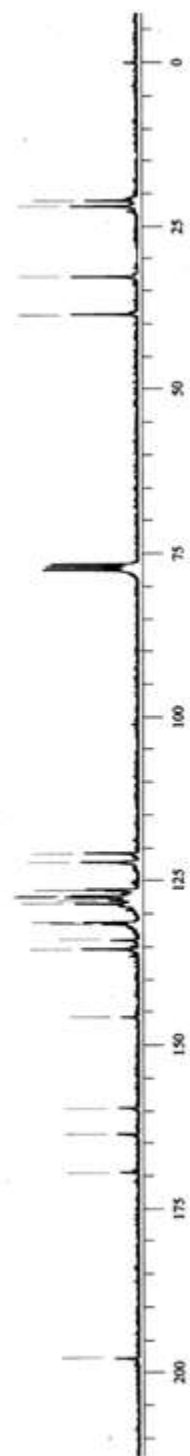
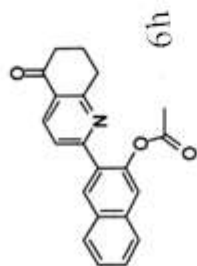
135.274  
133.926  
131.448  
128.378  
127.884  
127.430  
127.234  
126.438  
122.117  
120.733  
126.242  
131.214

145.677

163.508  
159.492

169.341

197.698



P.S.REDDY  
9/21/2012 6:17:45 PM

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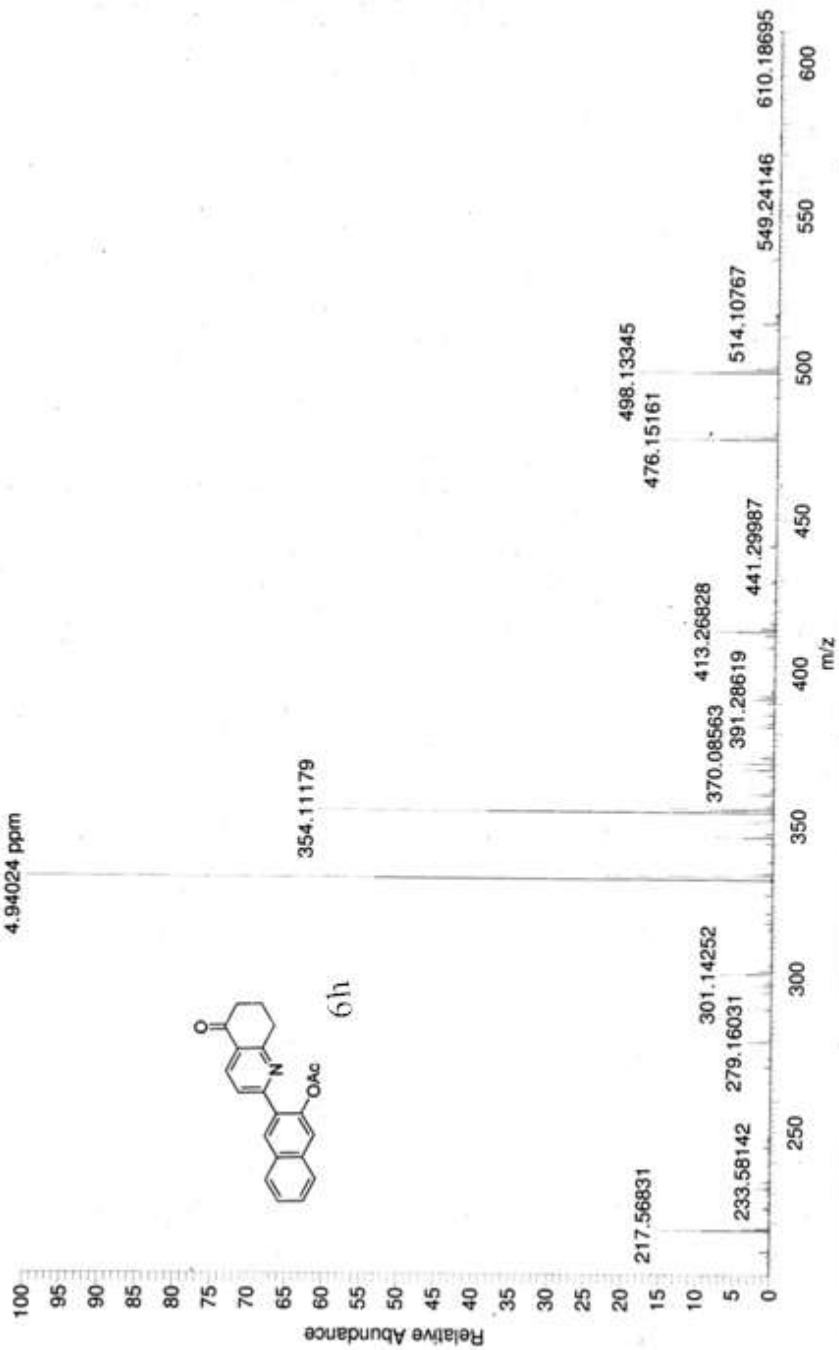
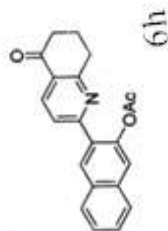
KSNAPCYHXOAC #6 RT: 0.06 AV: 1 NL: 5.84E6  
T: FTMS [1,1] + p ESI Full ms [100.00-2000.00]

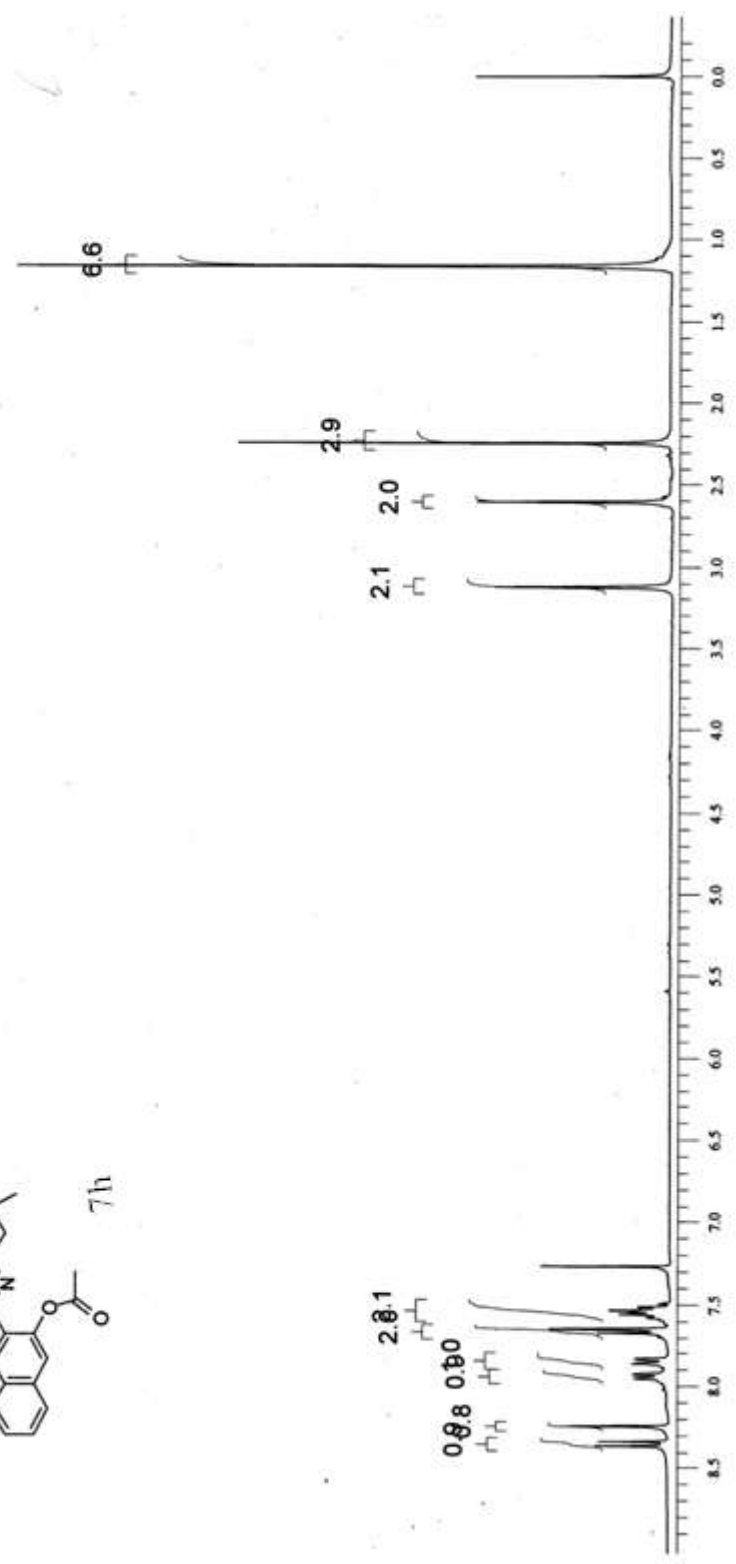
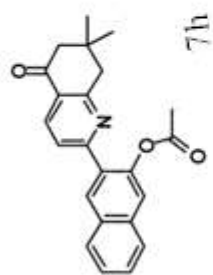
332.12976

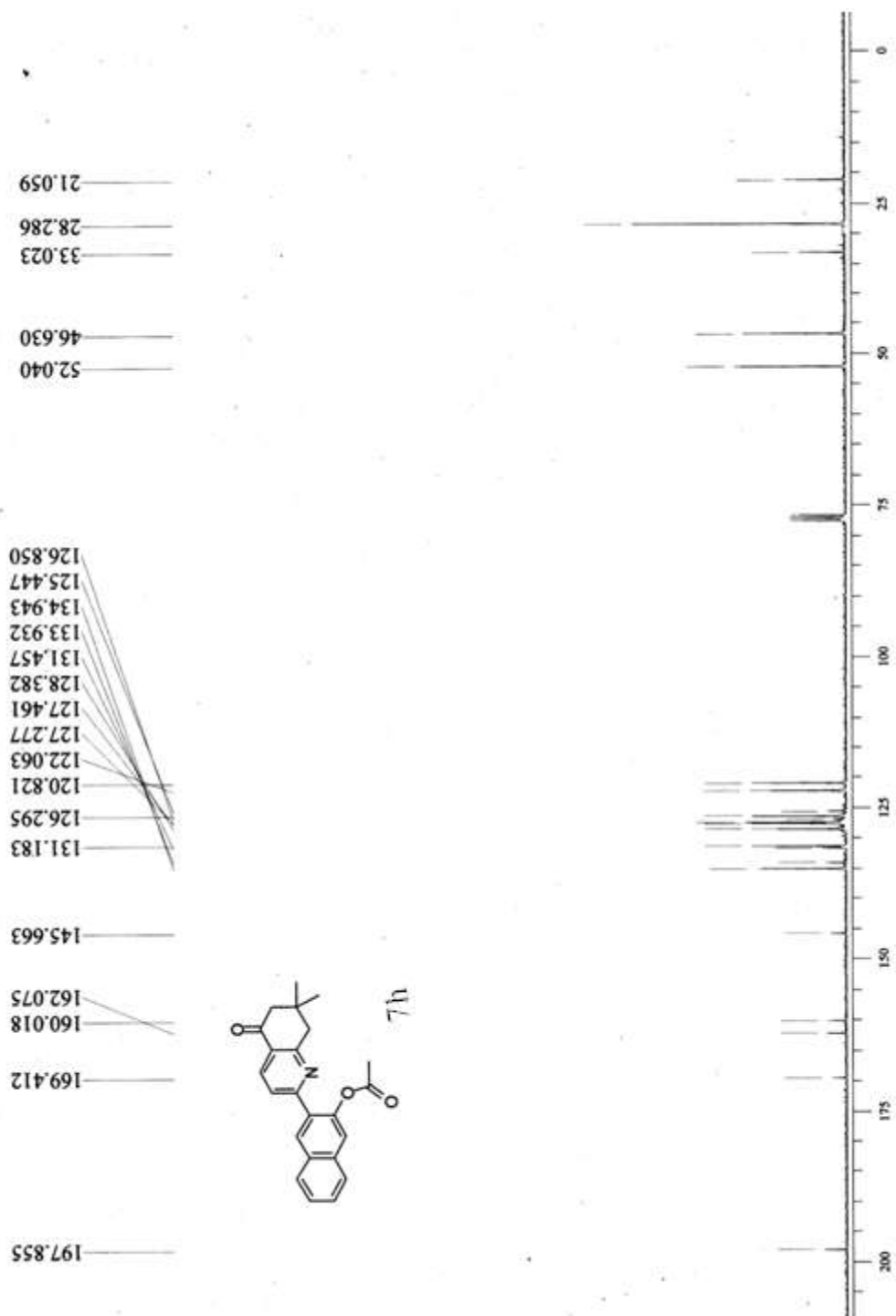
C<sub>21</sub>H<sub>18</sub>O<sub>3</sub>N = 332.12812

13.5 RDBE

4.94024 ppm





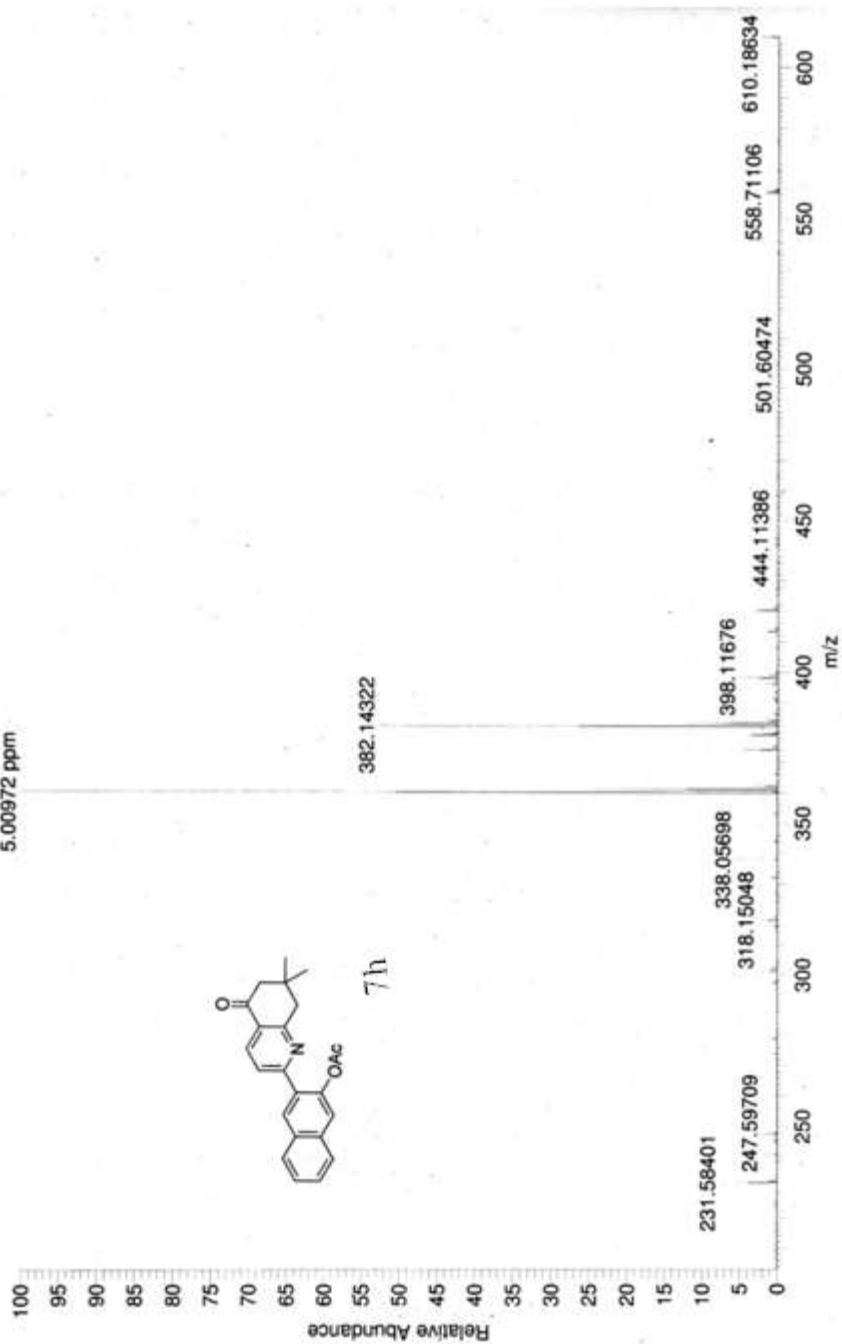


P.S.REDDY  
9/21/2012 6:15:08 PM

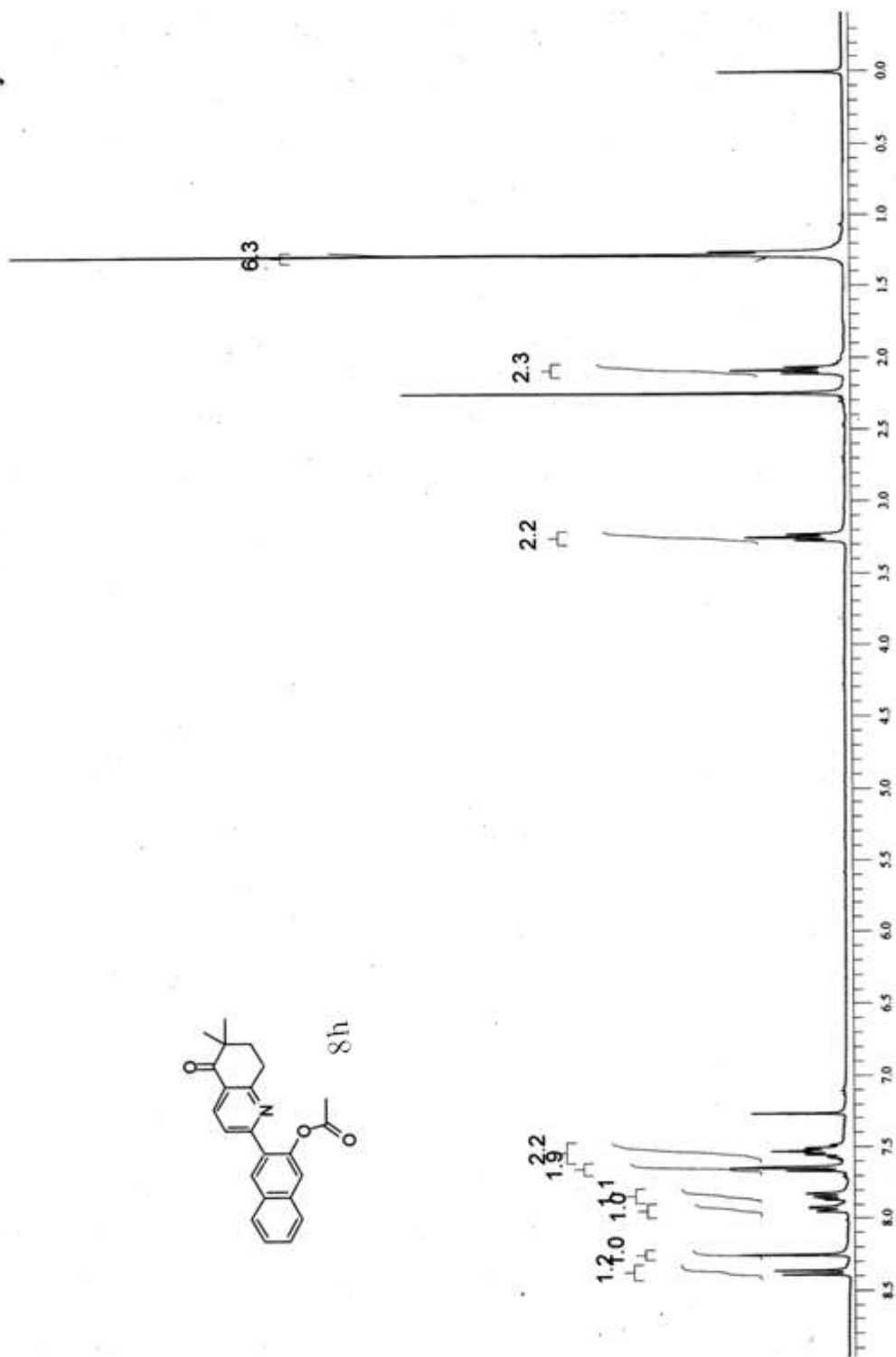
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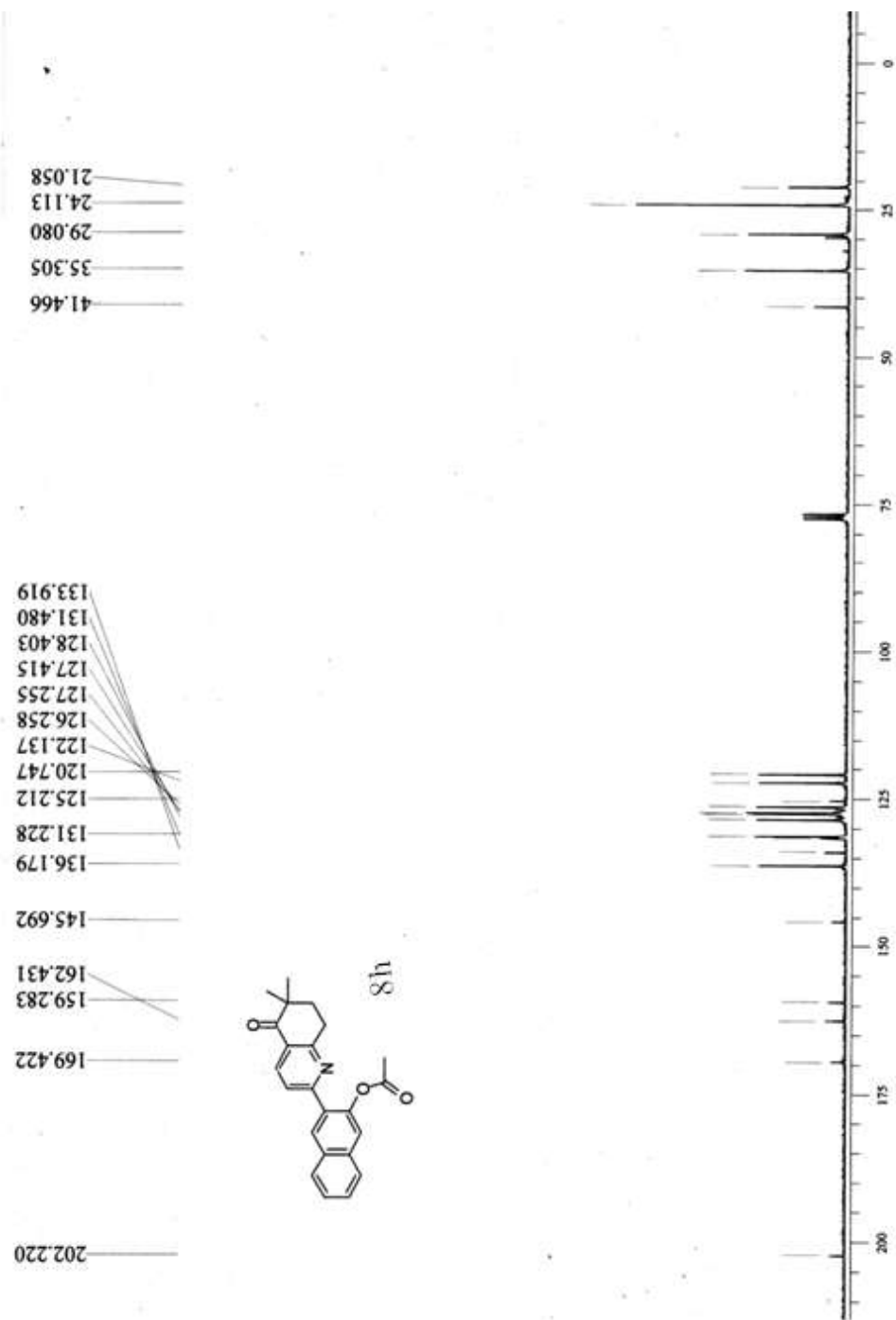
KSNAPDMDOAC #6 RT: 0.06 AV: 1 NL: 1.61E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

360.16122  
C<sub>23</sub>H<sub>22</sub>O<sub>3</sub>N = 360.15942  
13.5 RDBE  
5.00972 ppm







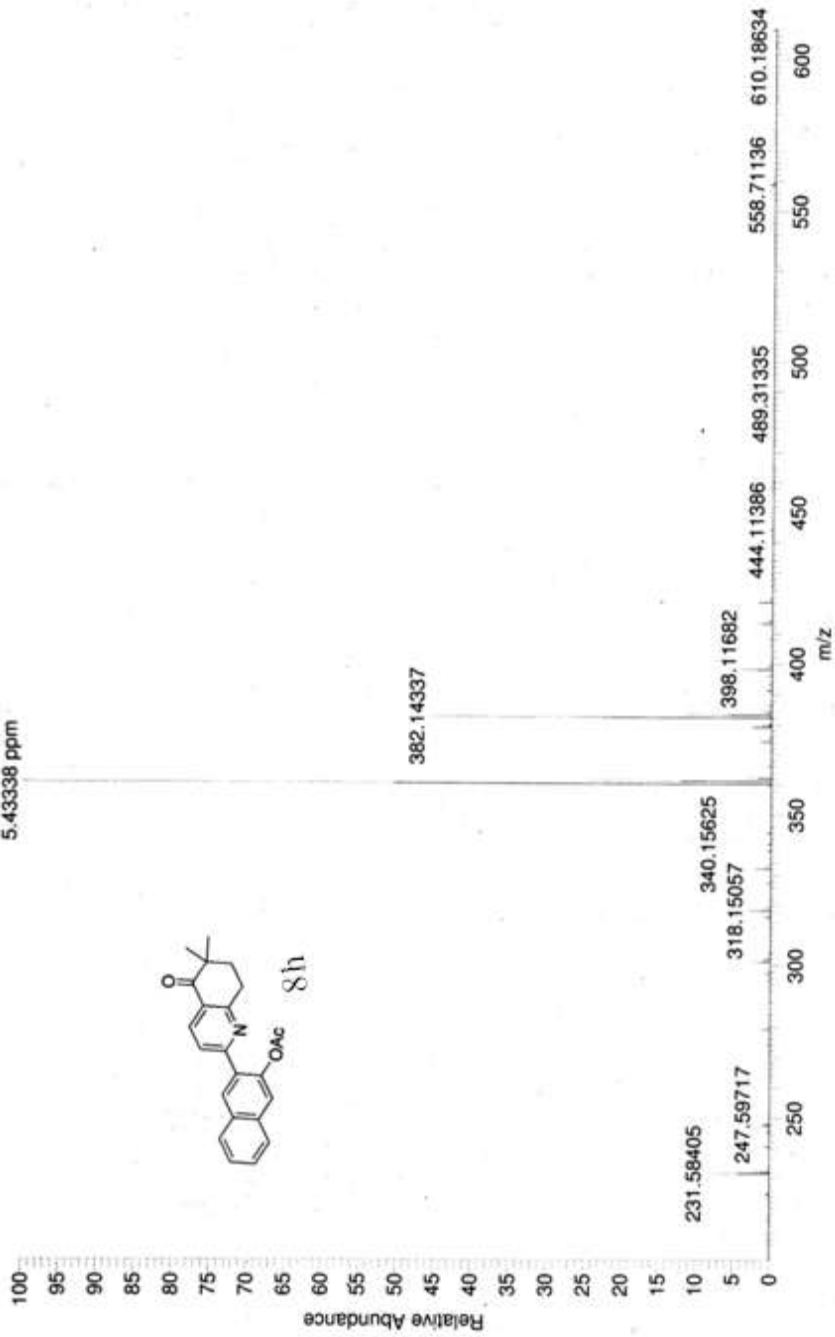


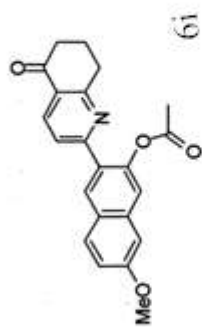
P.S.REDDY  
9/21/2012 6:11:05 PM

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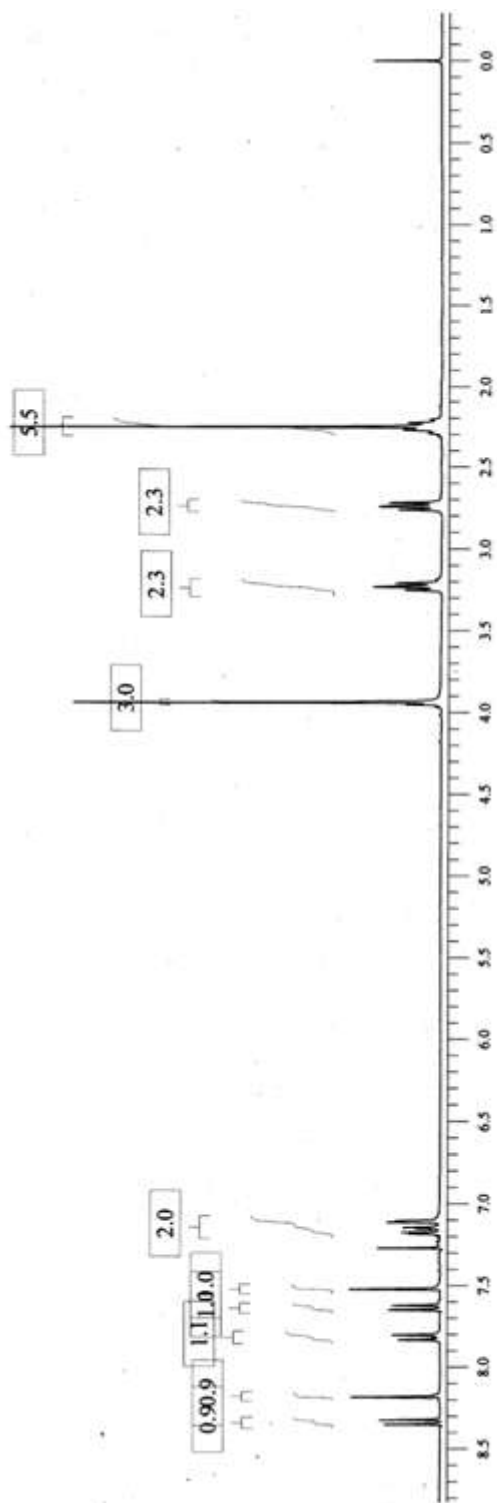
KSNAPUNSOAC #6 RT: 0.06 AV: 1 NL: 1.60E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

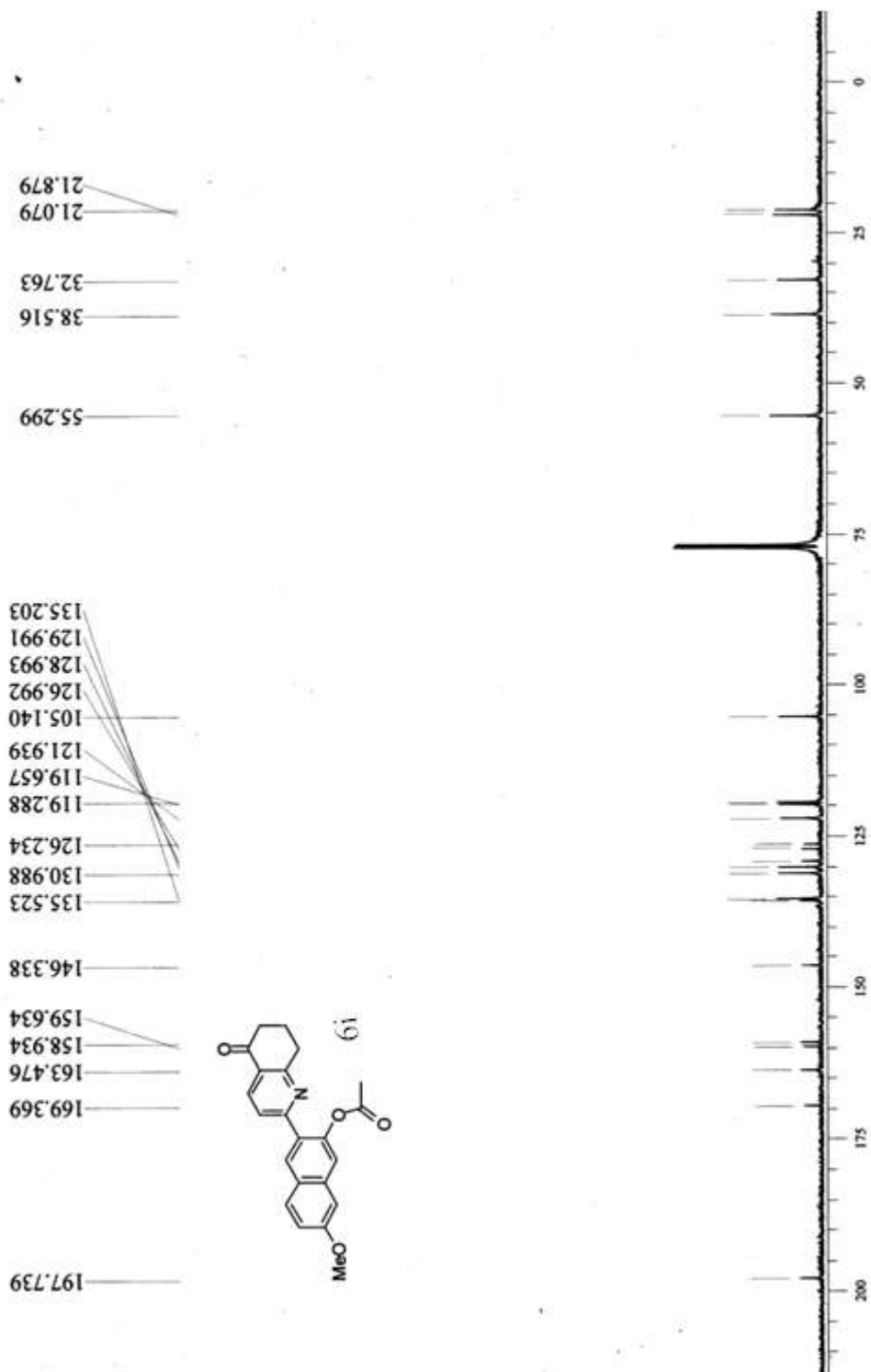
360.16138  
C<sub>23</sub>H<sub>22</sub>O<sub>3</sub>N = 360.15942  
13.5 RDBE  
5.43338 ppm





6i



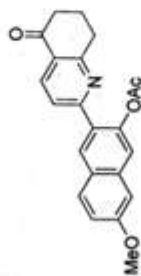
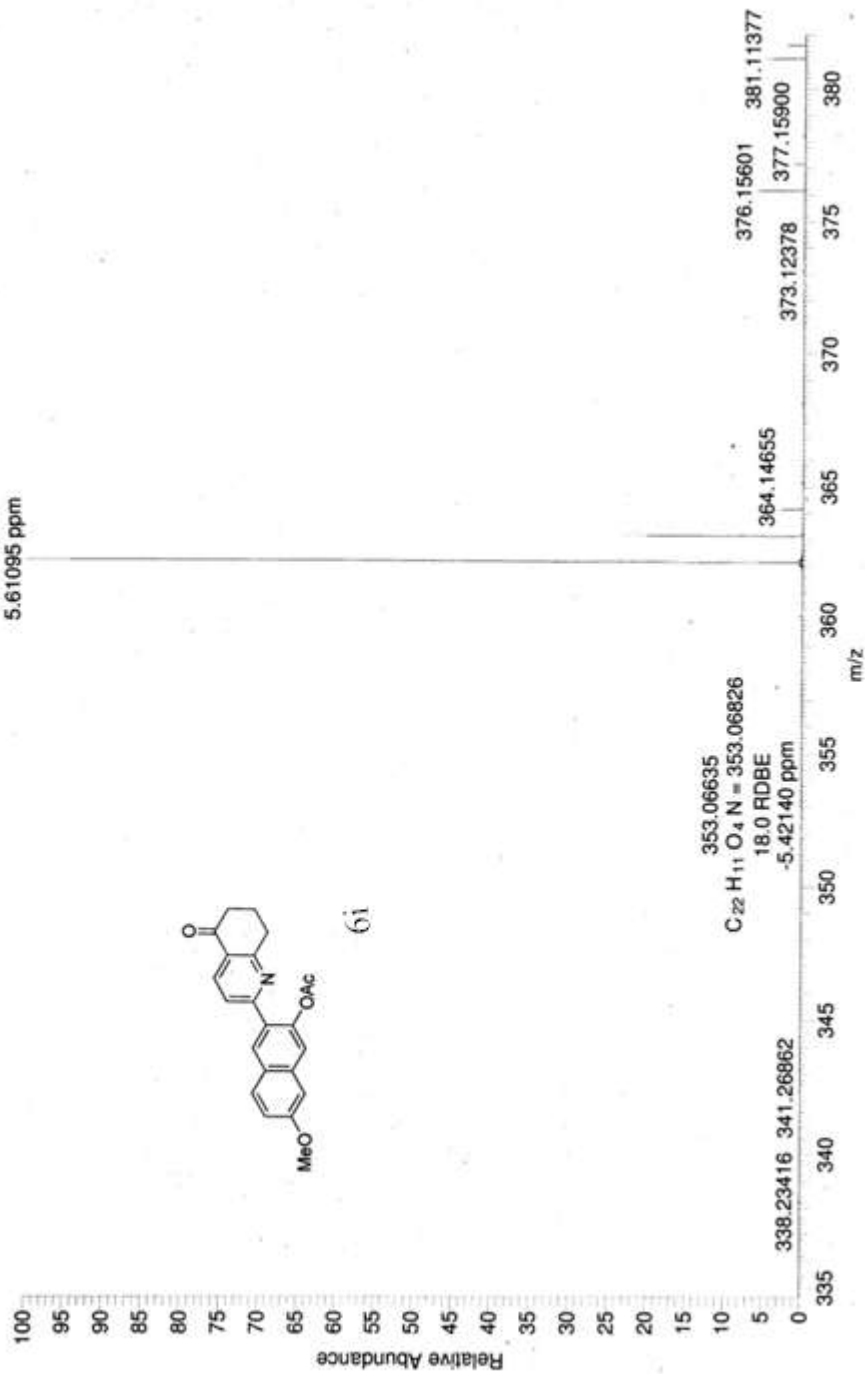


P.S.REDDY  
9/21/2012 5:55:17 PM

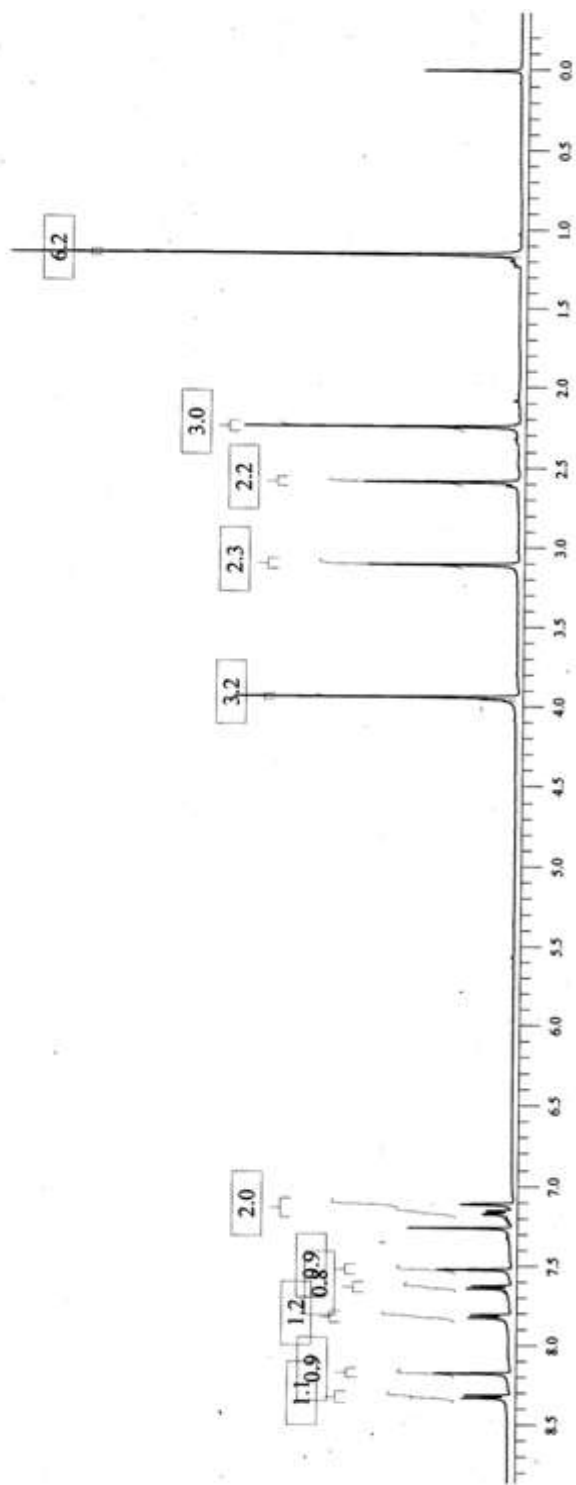
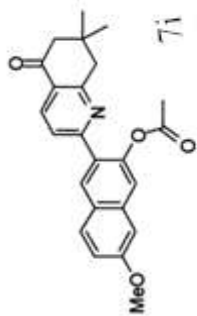
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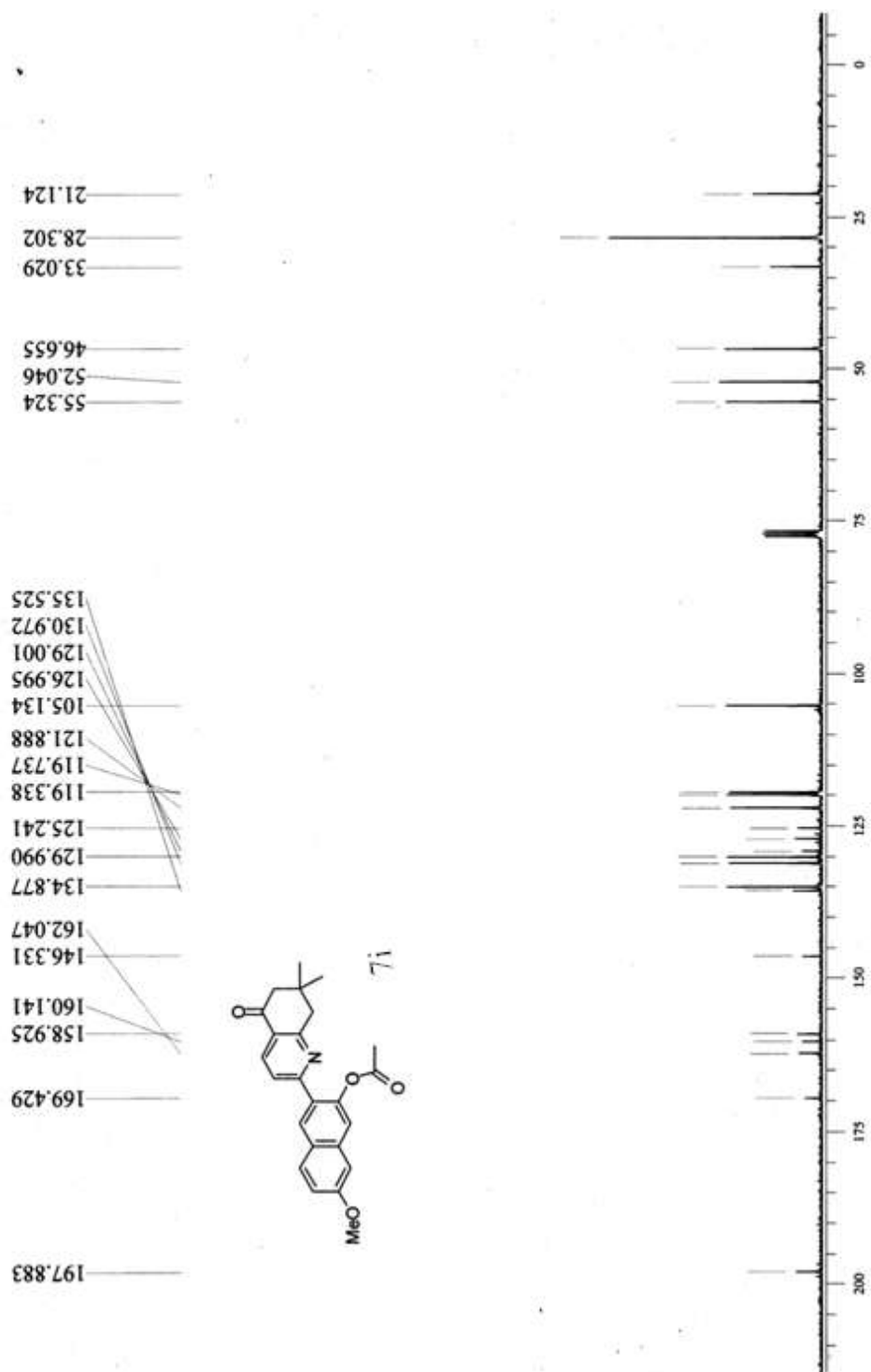
KSOMENAPCYHXOAC #6 RT: 0.06 AV: 1 NL: 8.00E6  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

362.14072  
C<sub>22</sub>H<sub>20</sub>O<sub>4</sub> N = 362.13868  
13.5 RDBE  
5.61095 ppm



6i





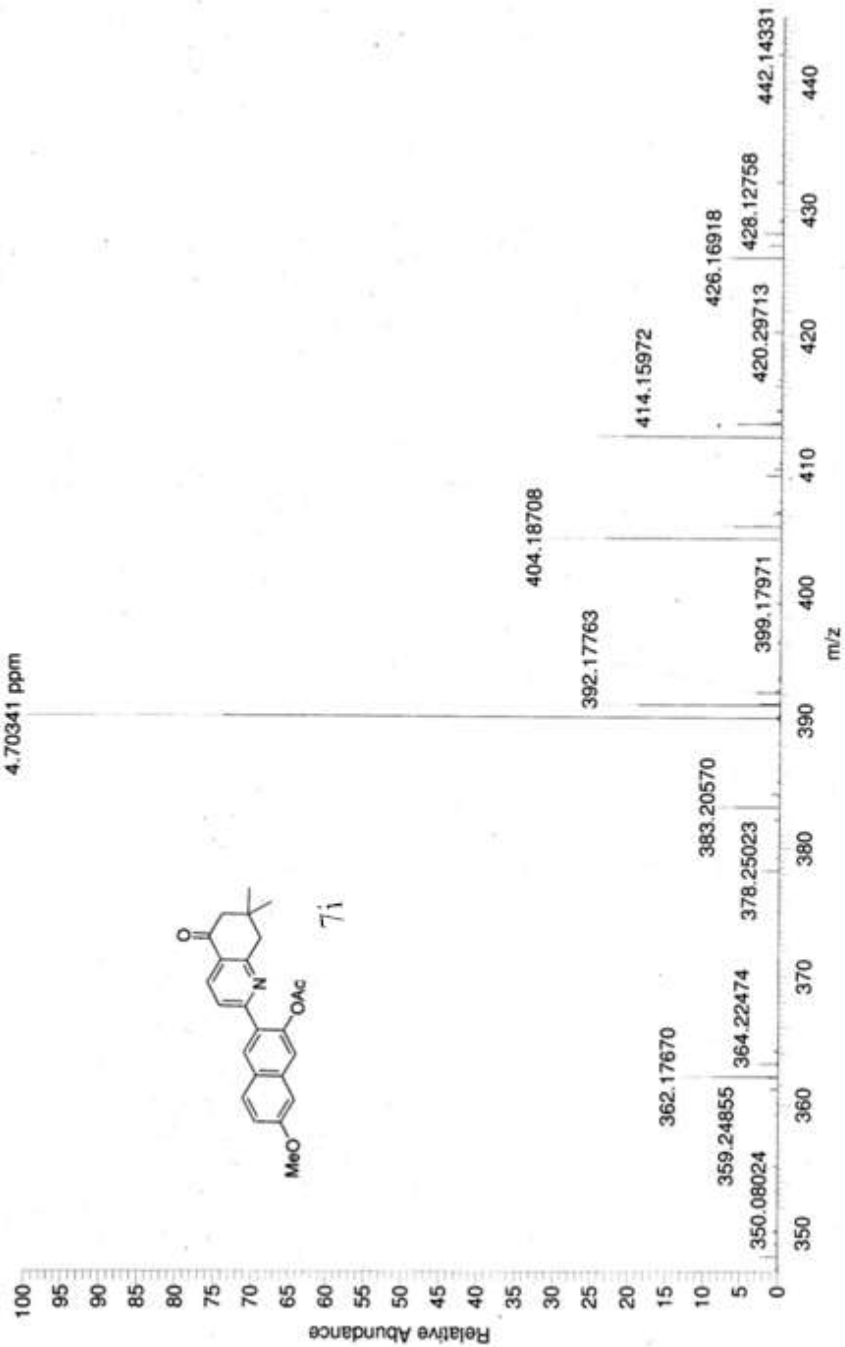


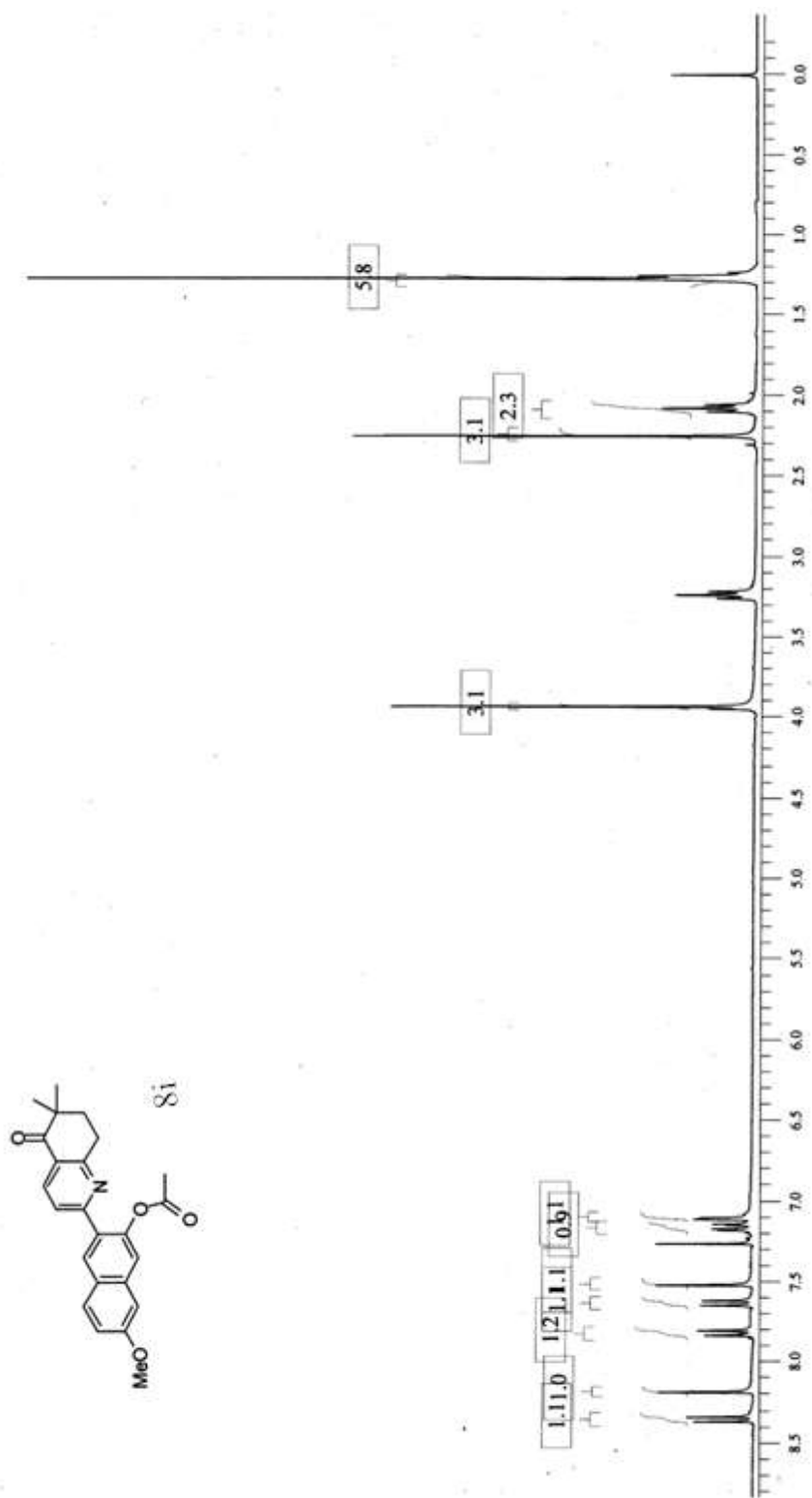
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9/21/2012 3:51:45 PM

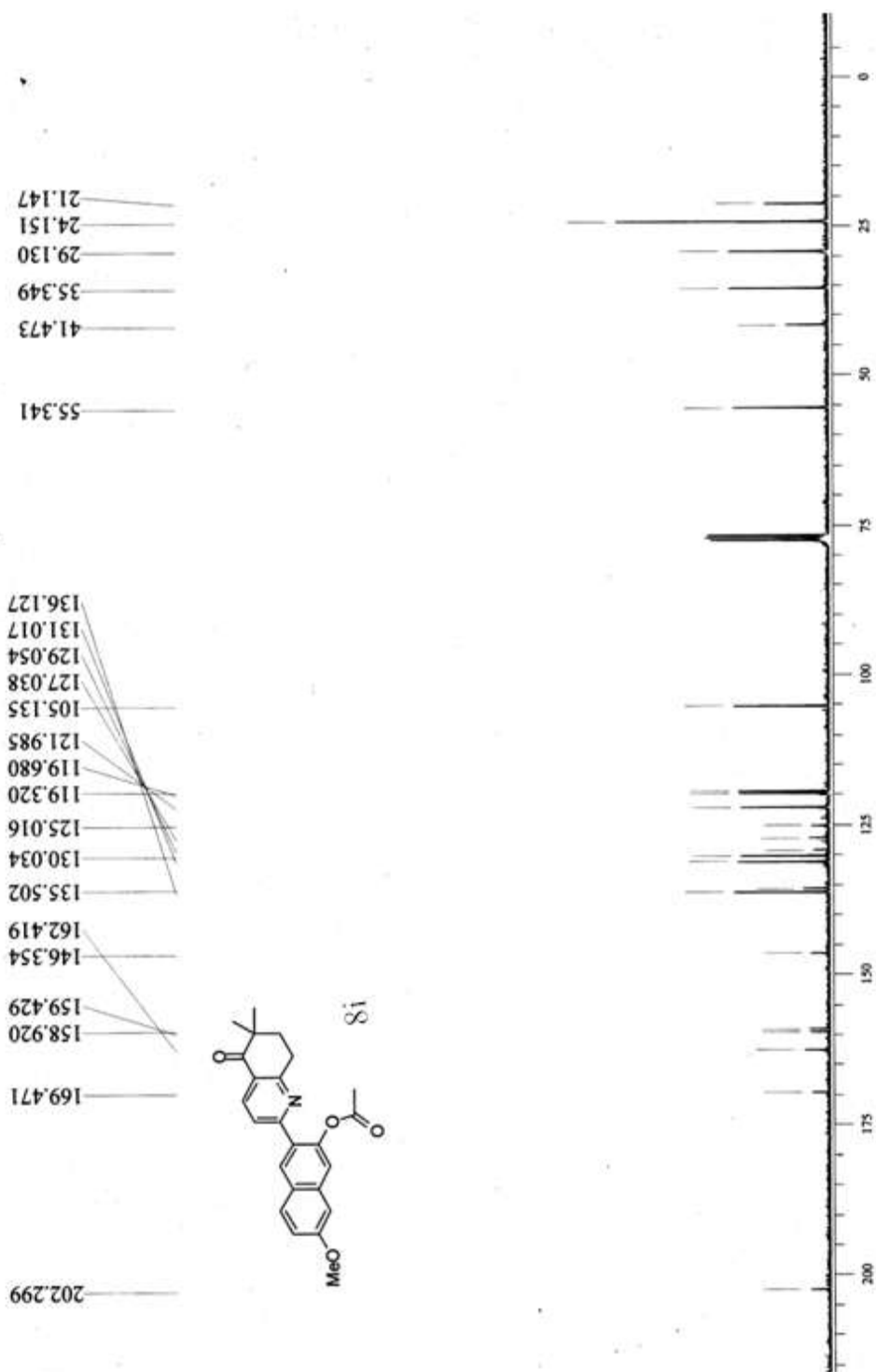
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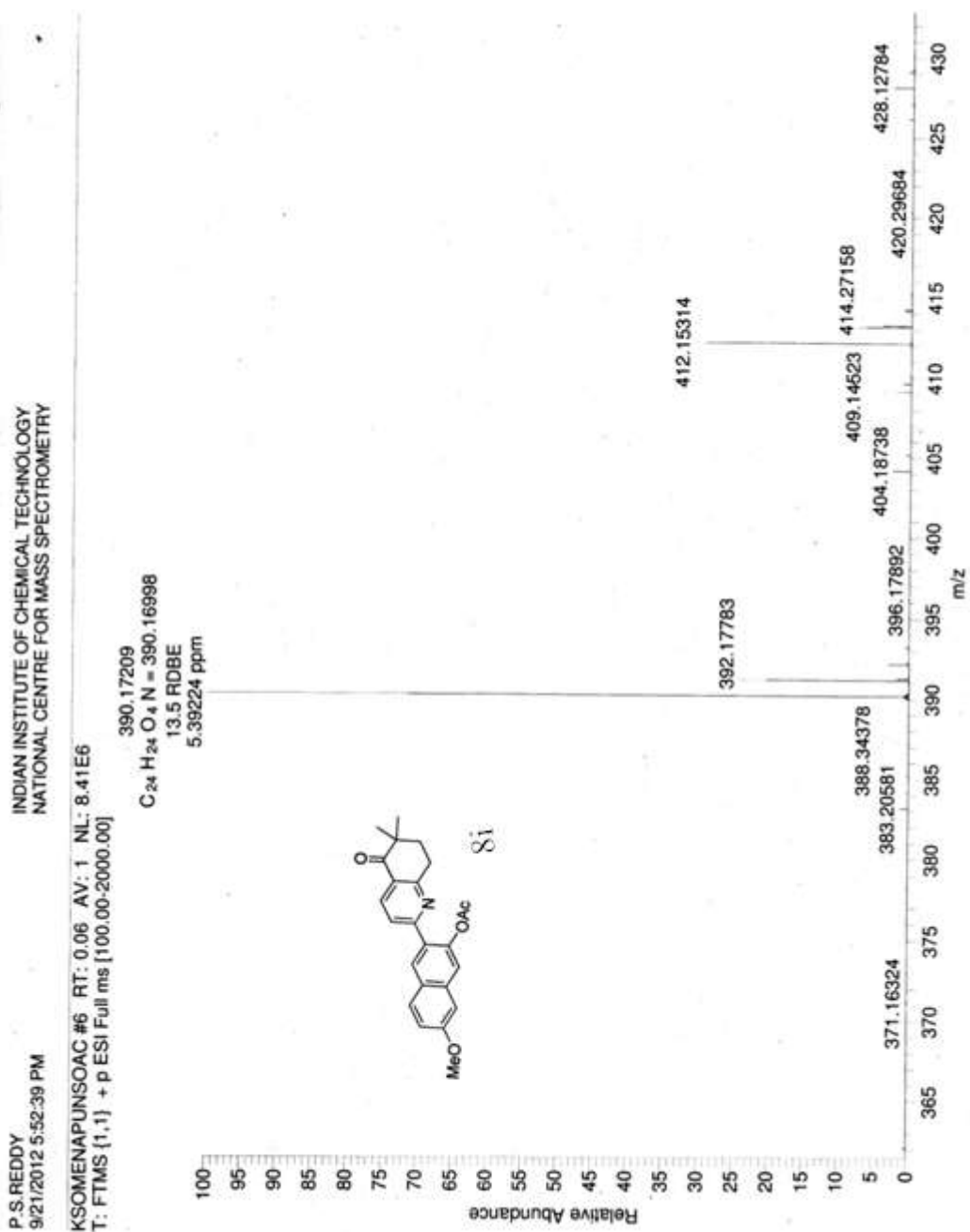
KSOMENACDMDOAC #10-39 RT: 0.10-0.40 AV: 30 NL: 8.66E6  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

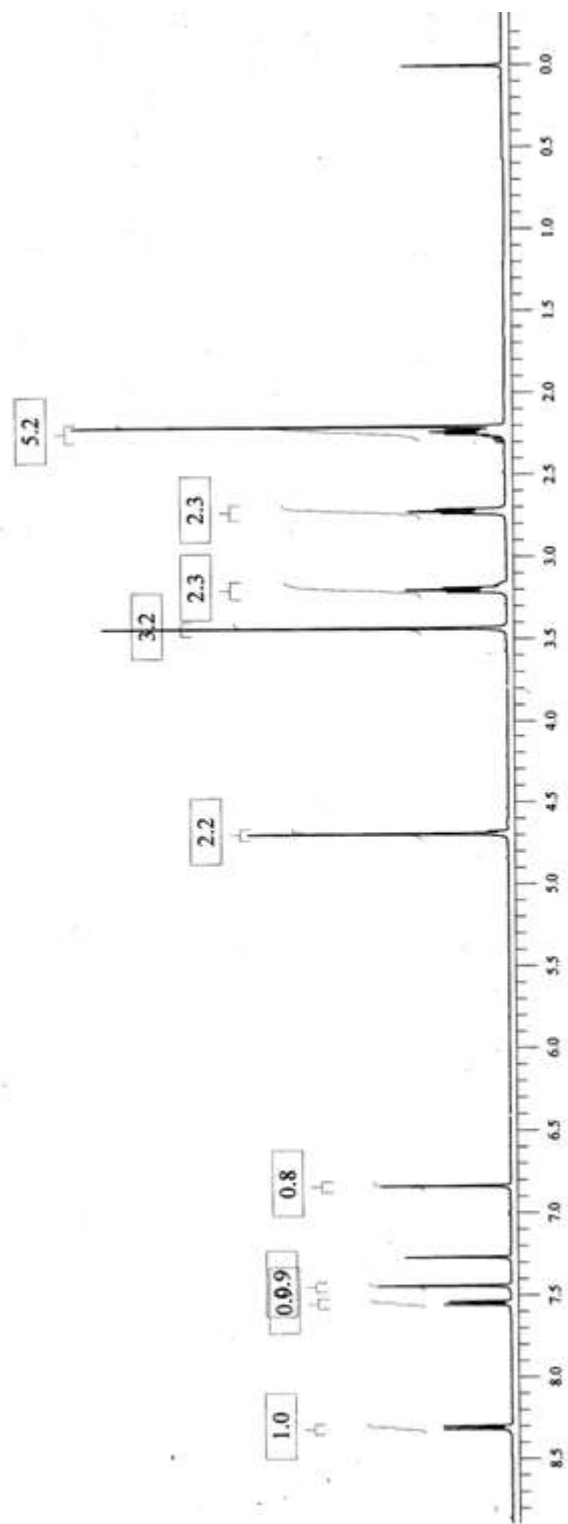
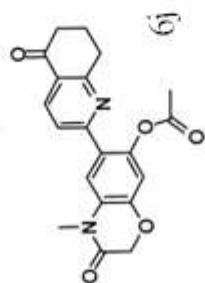
390.17182  
C<sub>24</sub>H<sub>24</sub>O<sub>4</sub>N = 390.16998  
13.5 RDBE  
4.70341 ppm

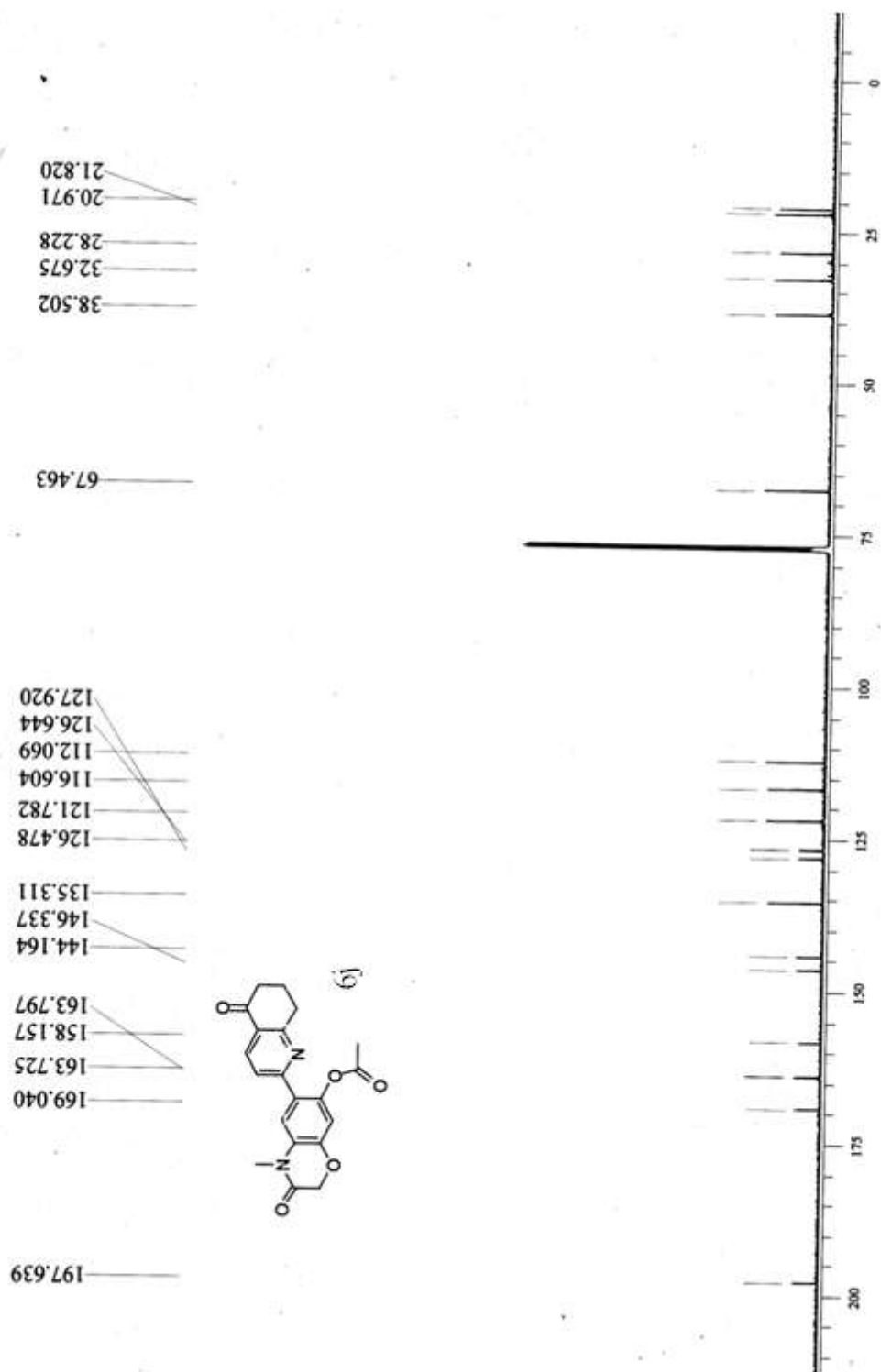


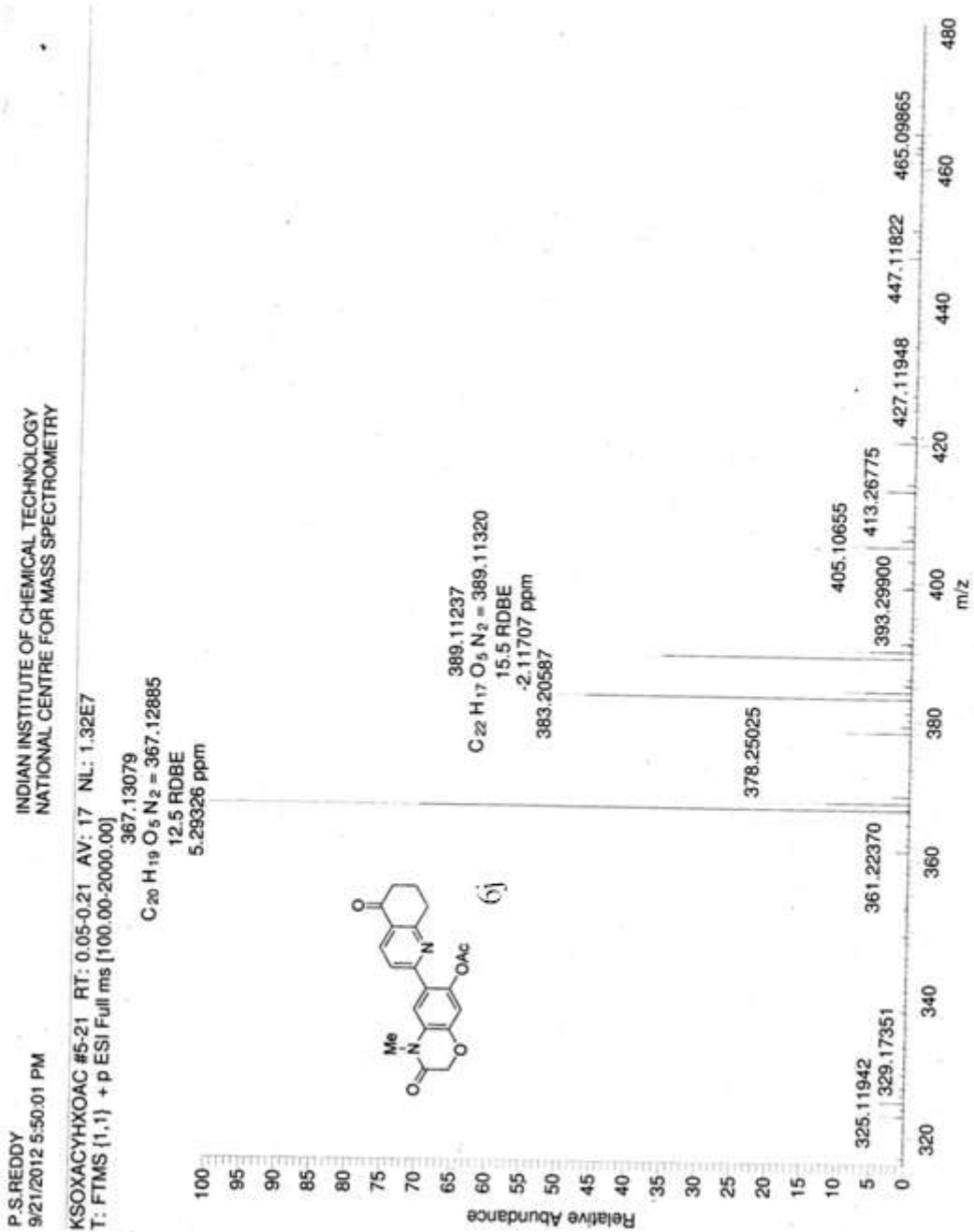


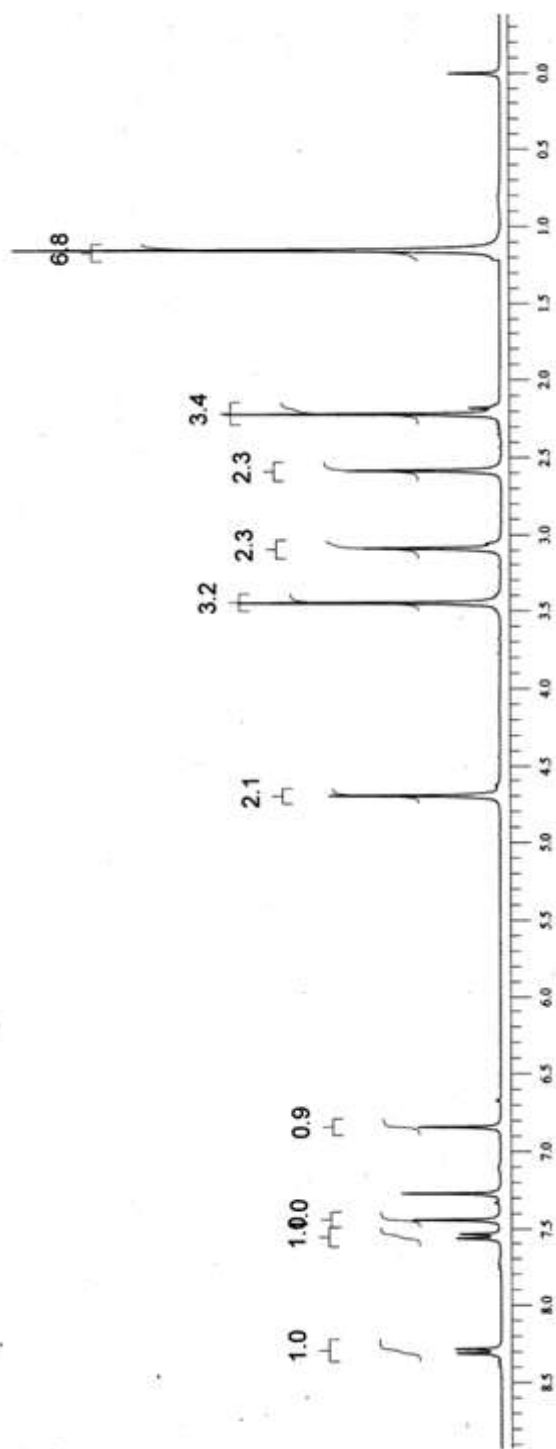
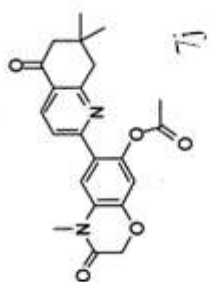




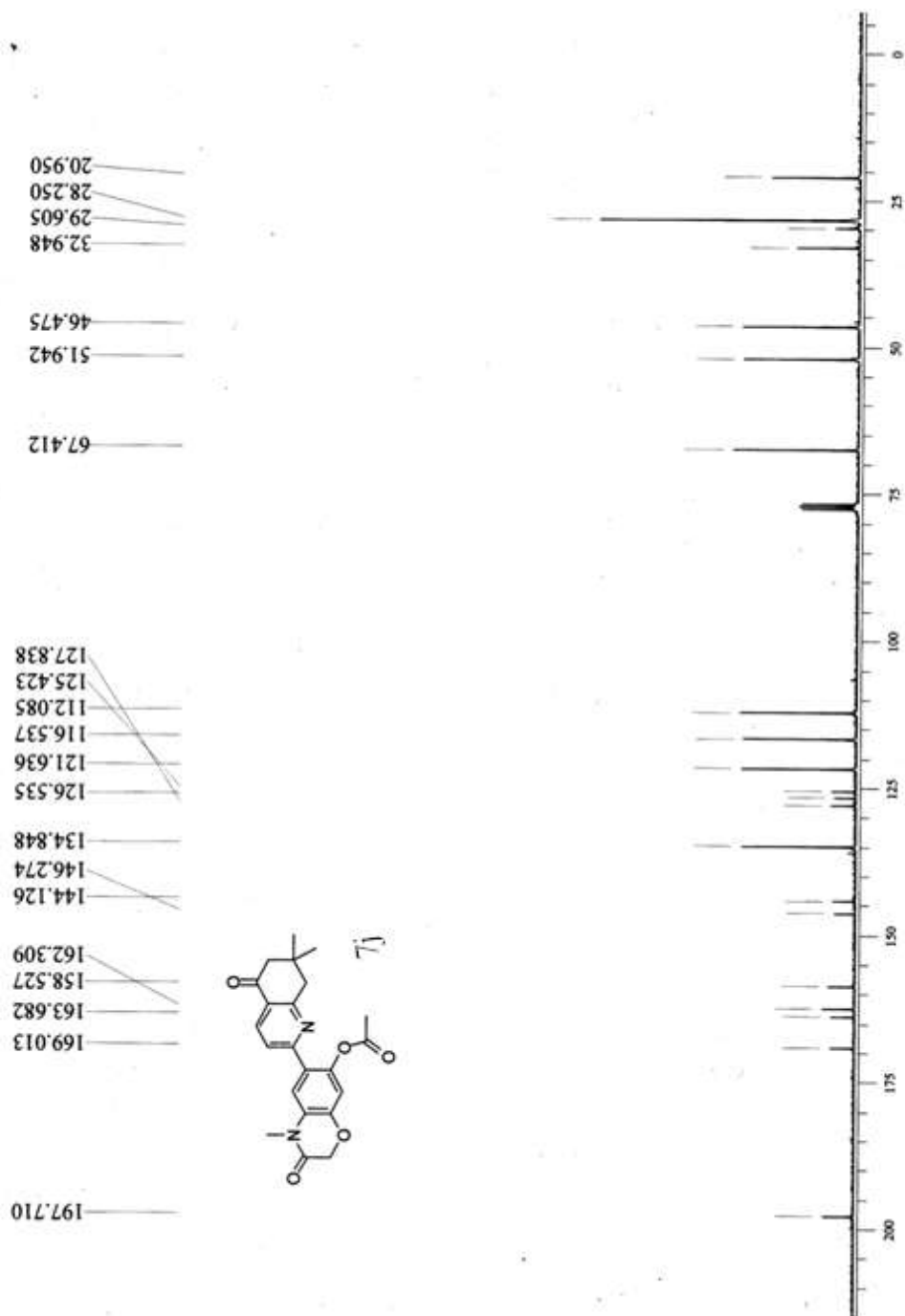








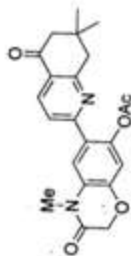
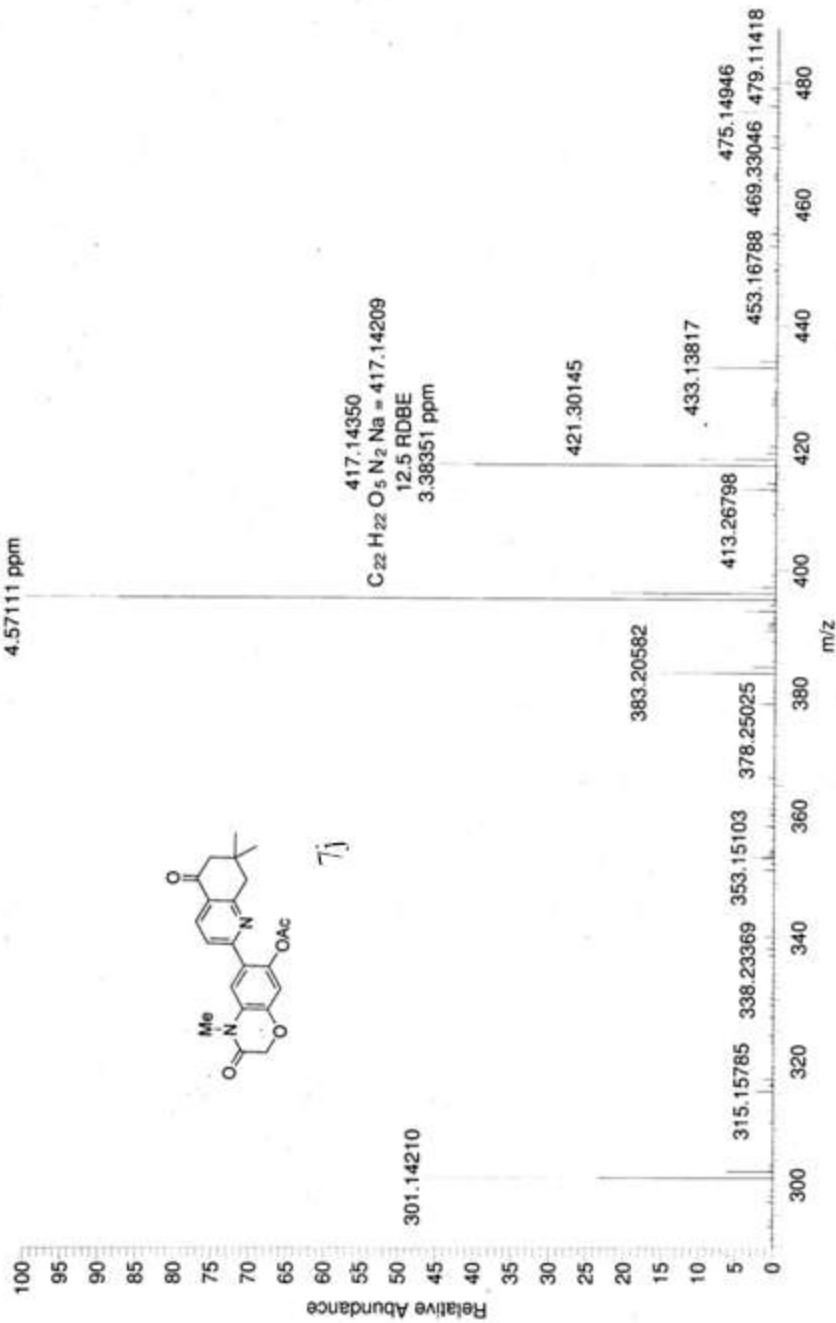




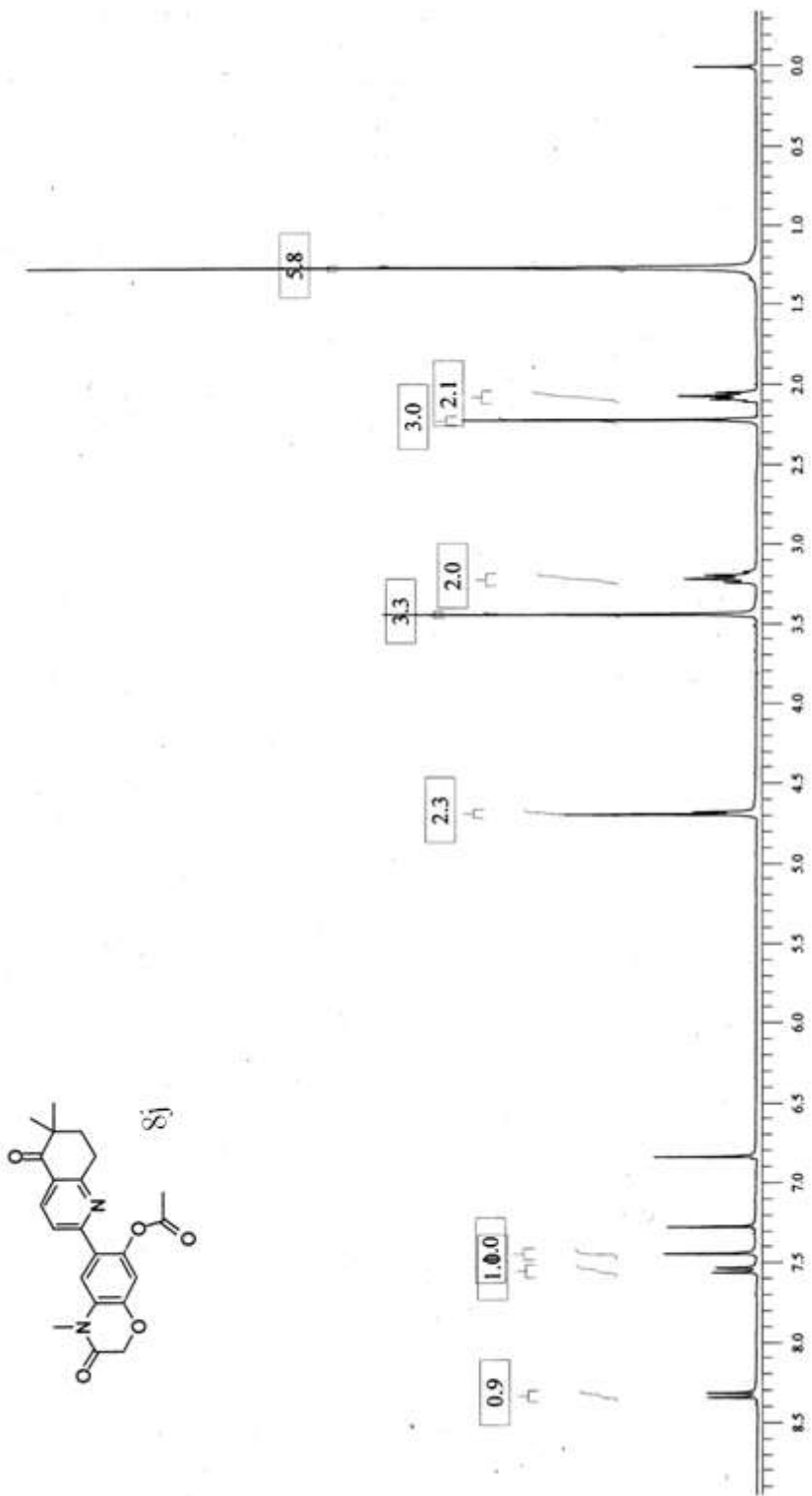
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9/21/2012 5:47:28 PM

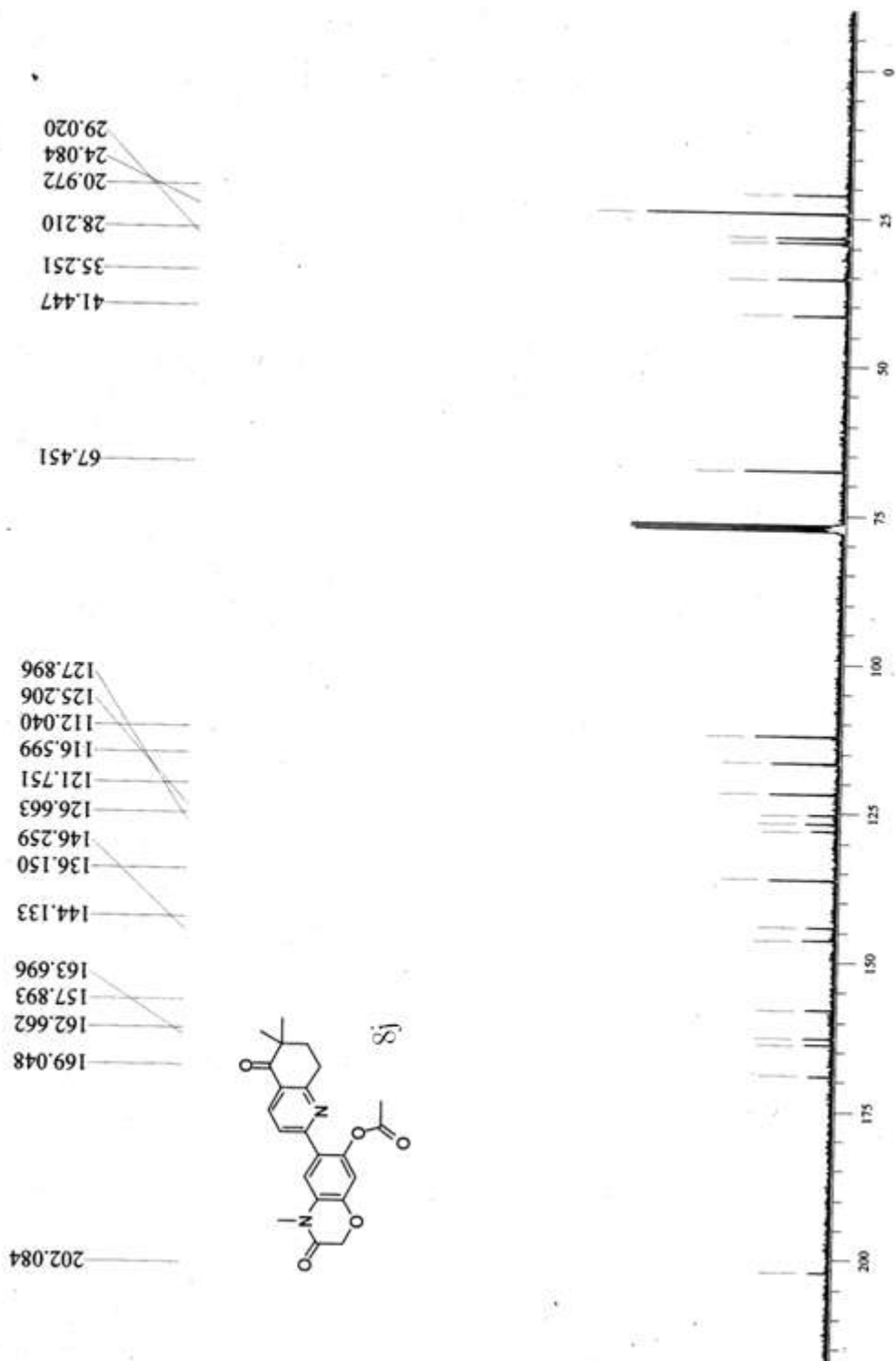
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KSOXADMDOAC #6-27 RT: 0.06-0.27 AV: 22 NL: 1.11E7  
T: FTMS (1.1) + p ESI Full ms [100.00-2000.00]



7j

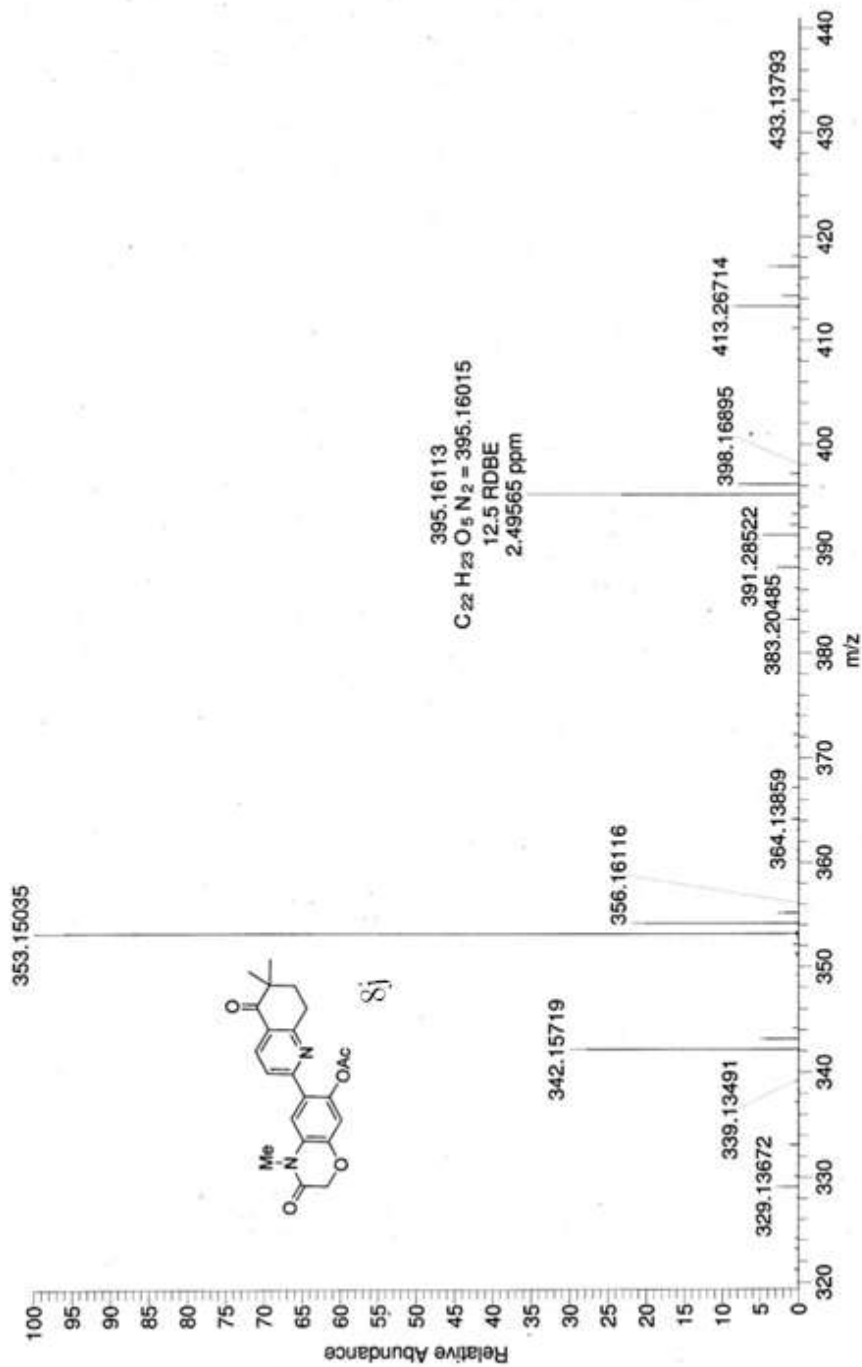


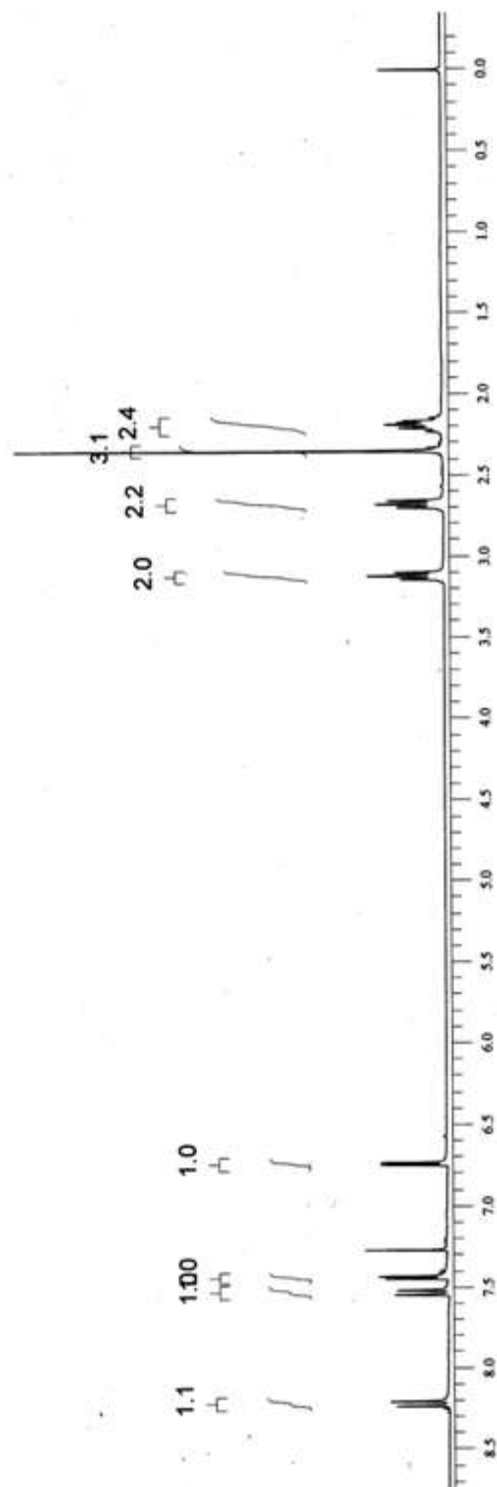
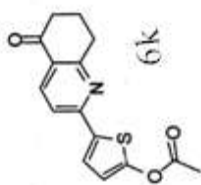


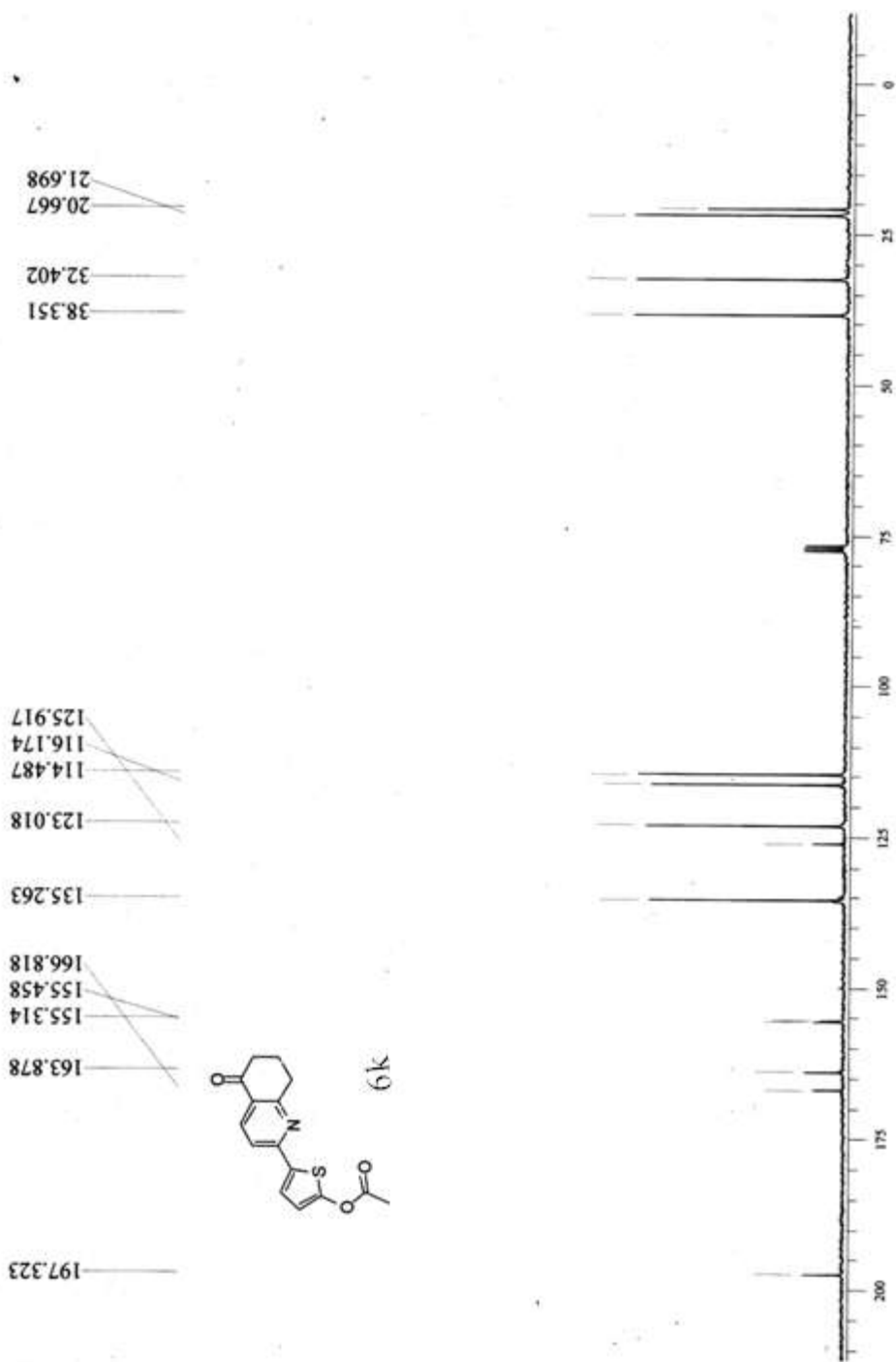
P S REDDY  
10/9/2012 9:48:52 PM

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KS-OXA-UNS-OAC #6-23 RT: 0.06-0.23 AV: 18 NL: 1.85E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]





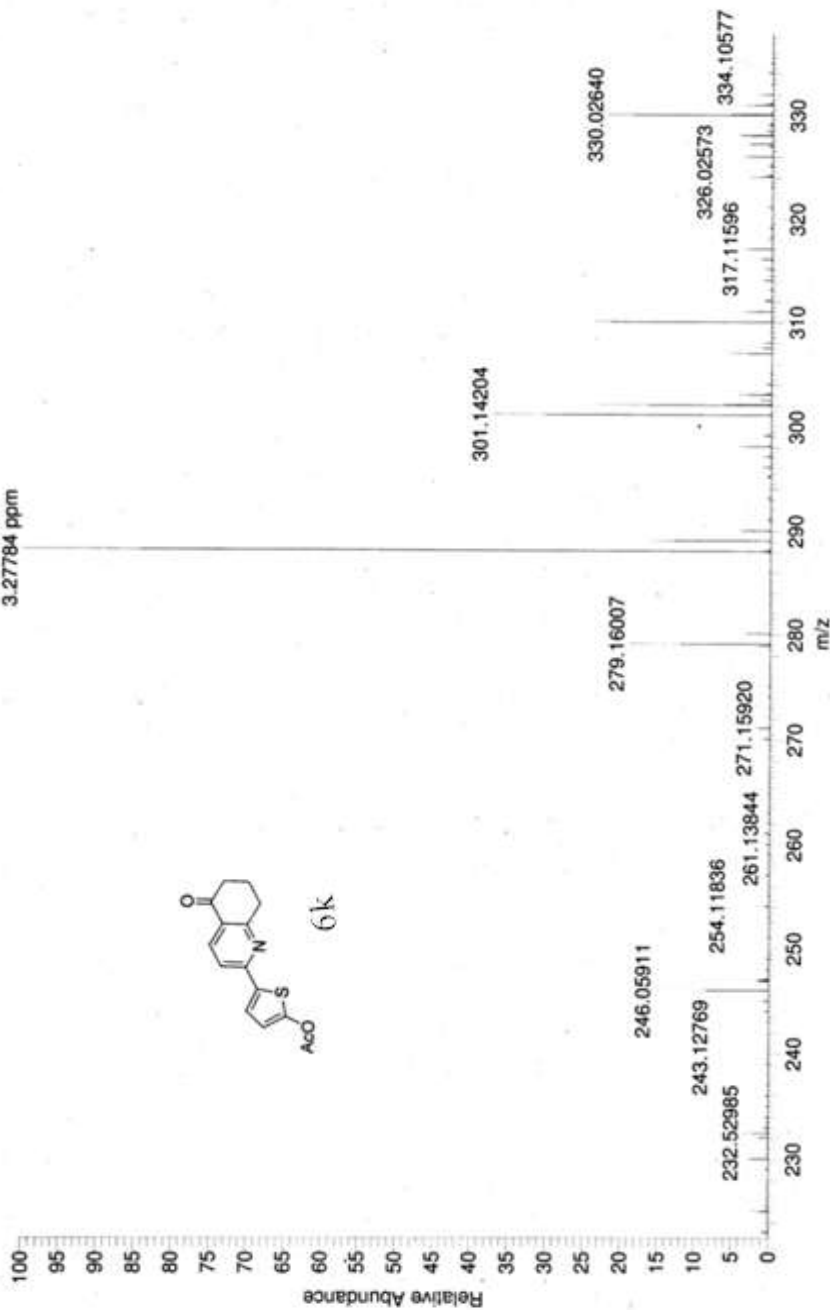
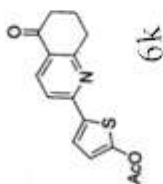


P.S.REDDY  
9/21/2012 4:39:09 PM

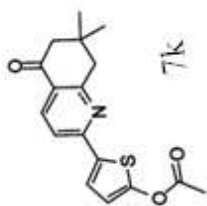
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KSTHCYHXOAC #8-21 RT: 0.06-0.21 AV: 14 NL: 1.08E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

288.06983  
C<sub>15</sub>H<sub>14</sub>O<sub>3</sub>N S = 288.06889  
9.5 RDBE  
3.27784 ppm





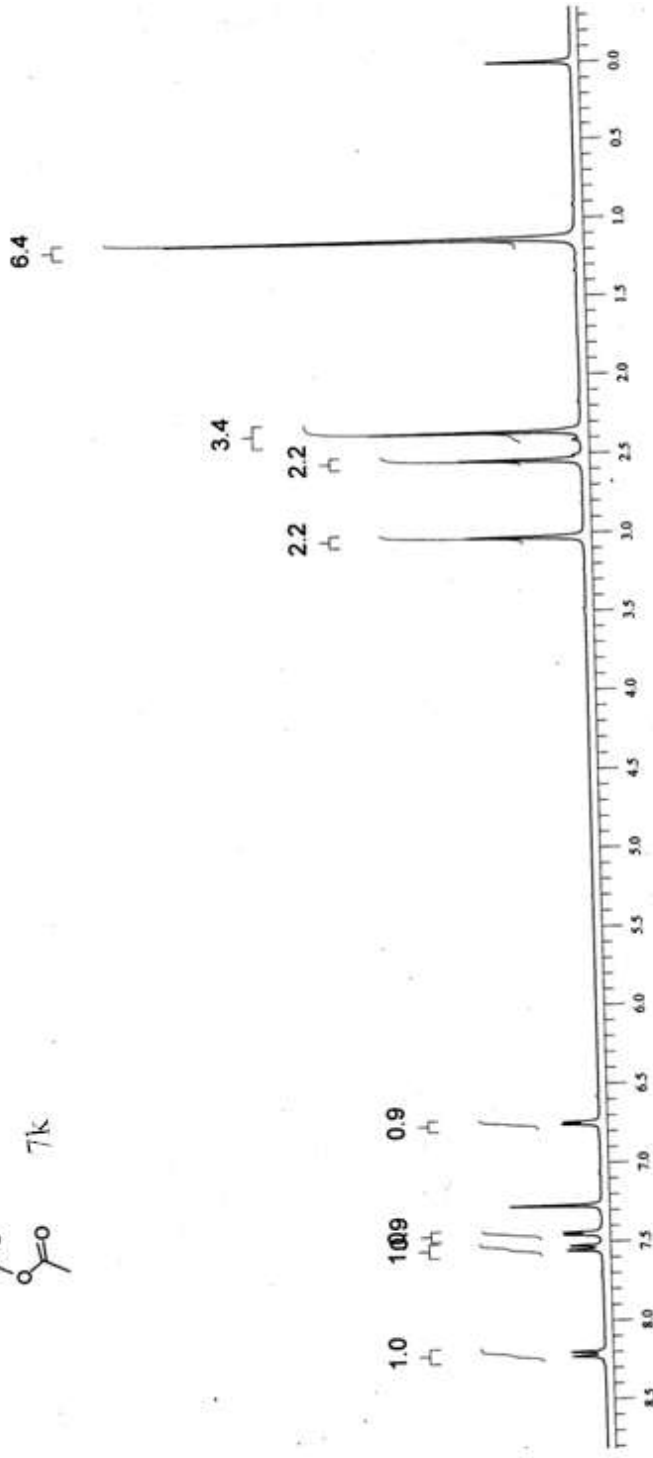


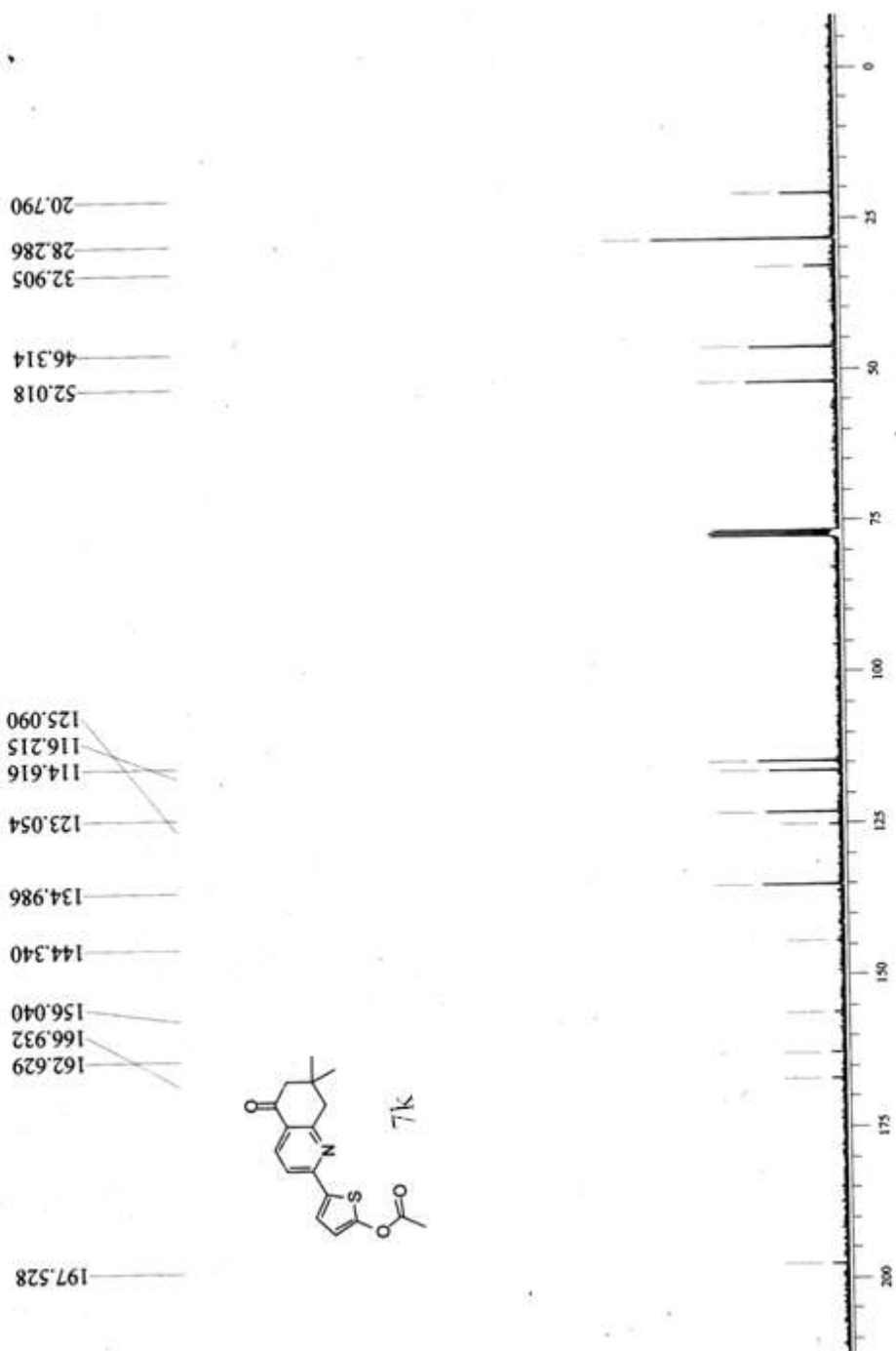
6.4

3.4

2.2 2.2

1.0 1.0 0.9

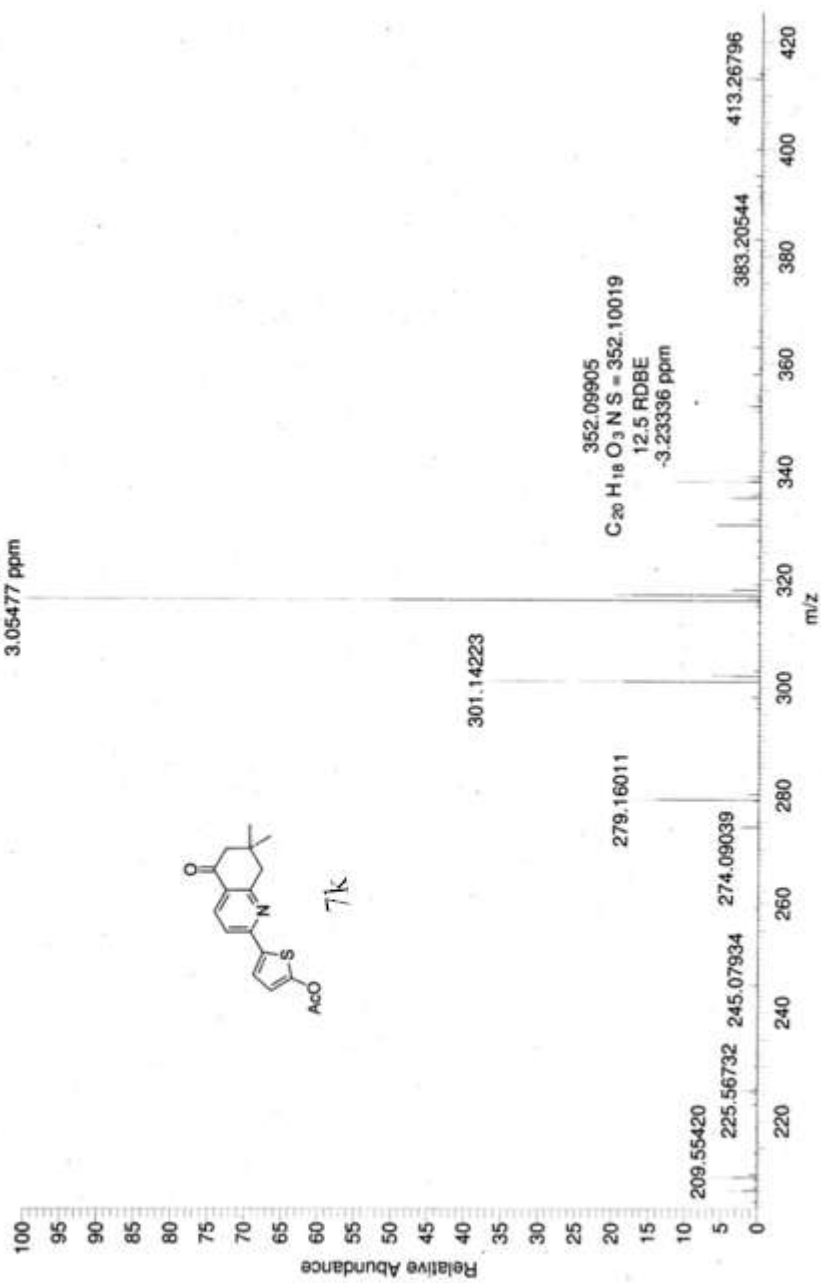
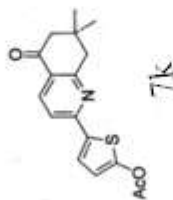


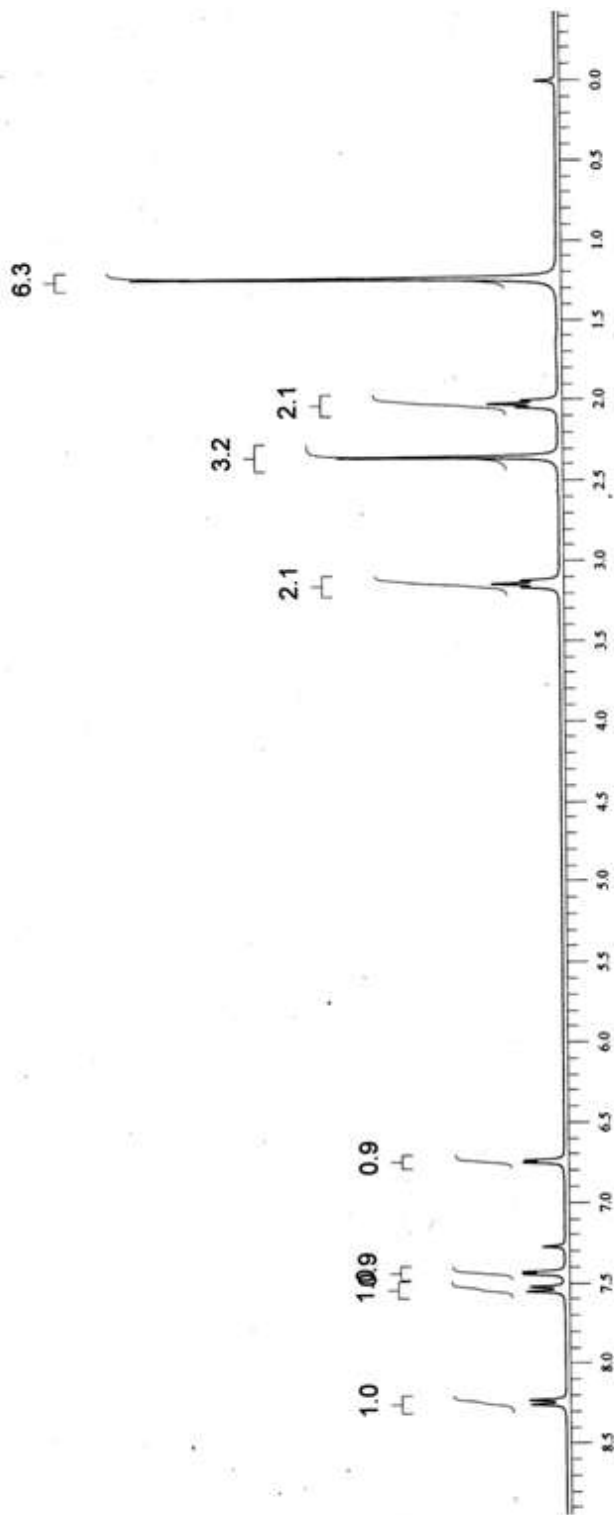
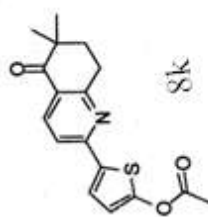


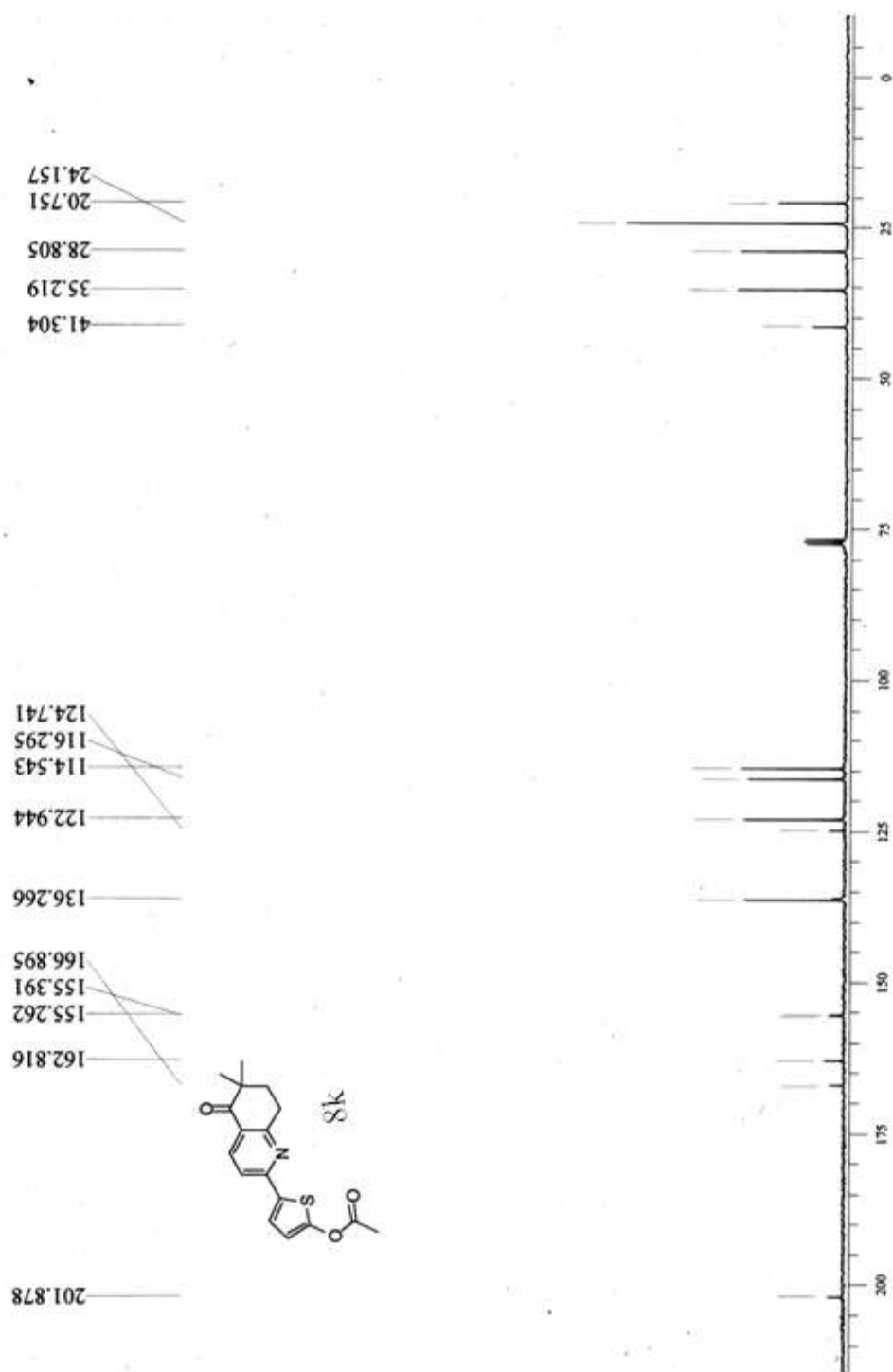
P.S.REDDY  
9/21/2012 4:36:31 PM  
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KSTHDMDOAC #6-22 RT: 0.06-0.22 AV: 17 NL: 3.12E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

316.10116  
C<sub>17</sub>H<sub>18</sub>O<sub>3</sub> N S = 316.10019  
9.5 RDBE  
3.05477 ppm





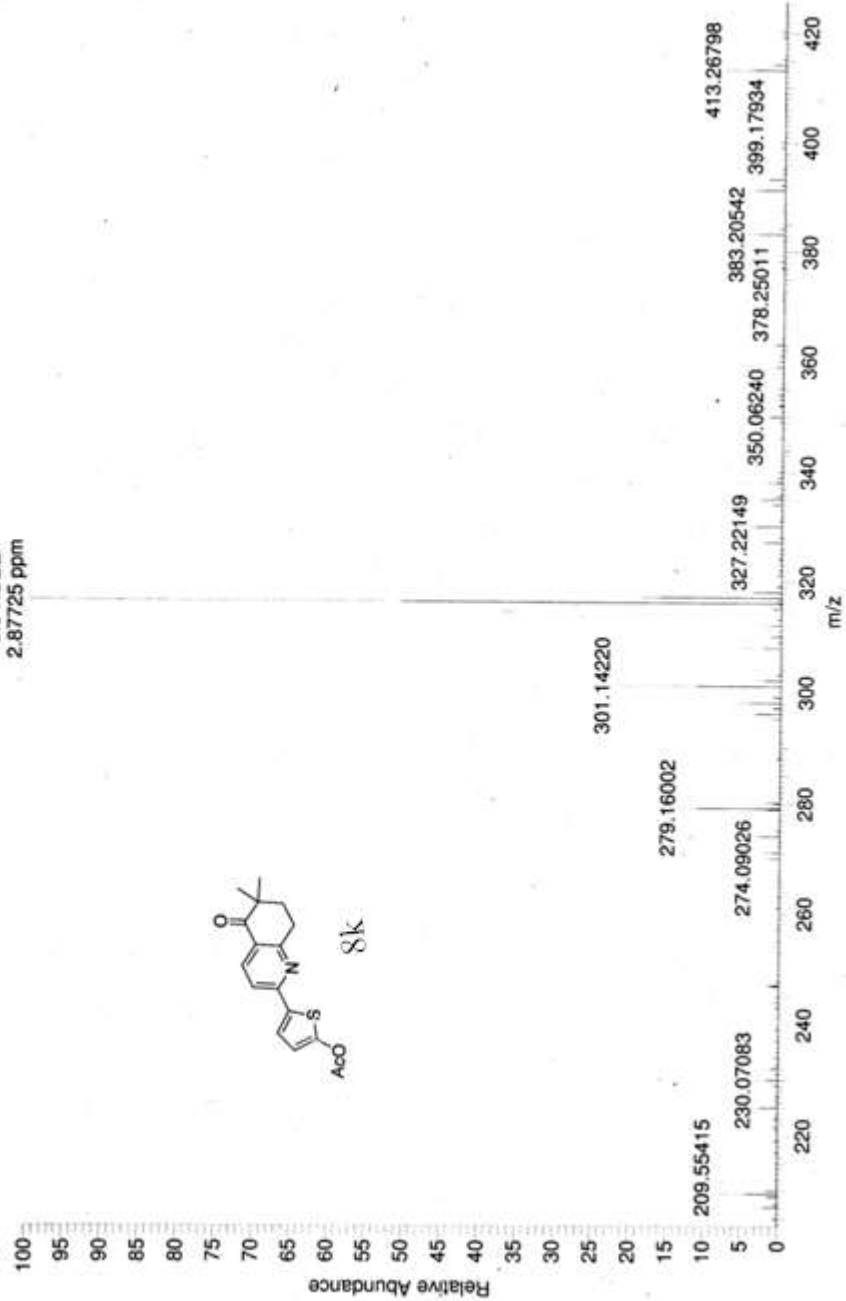
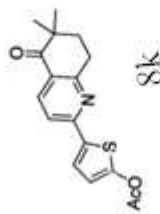


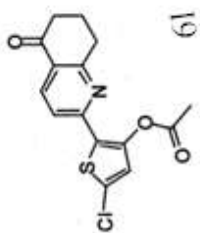
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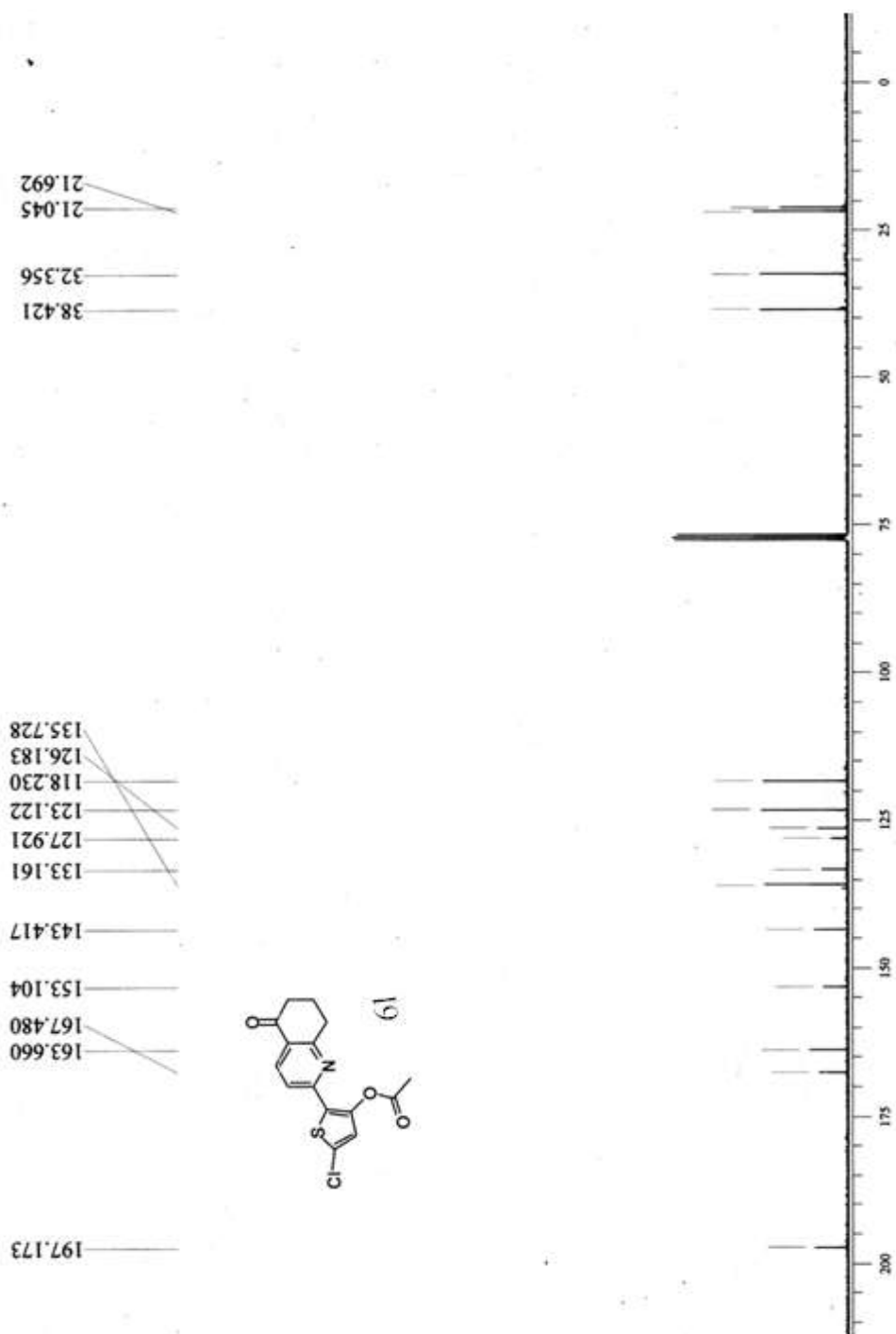
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KSTHUNSOAC #5-26 RT: 0.05-0.26 AV: 22 NL: 8.78E6  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

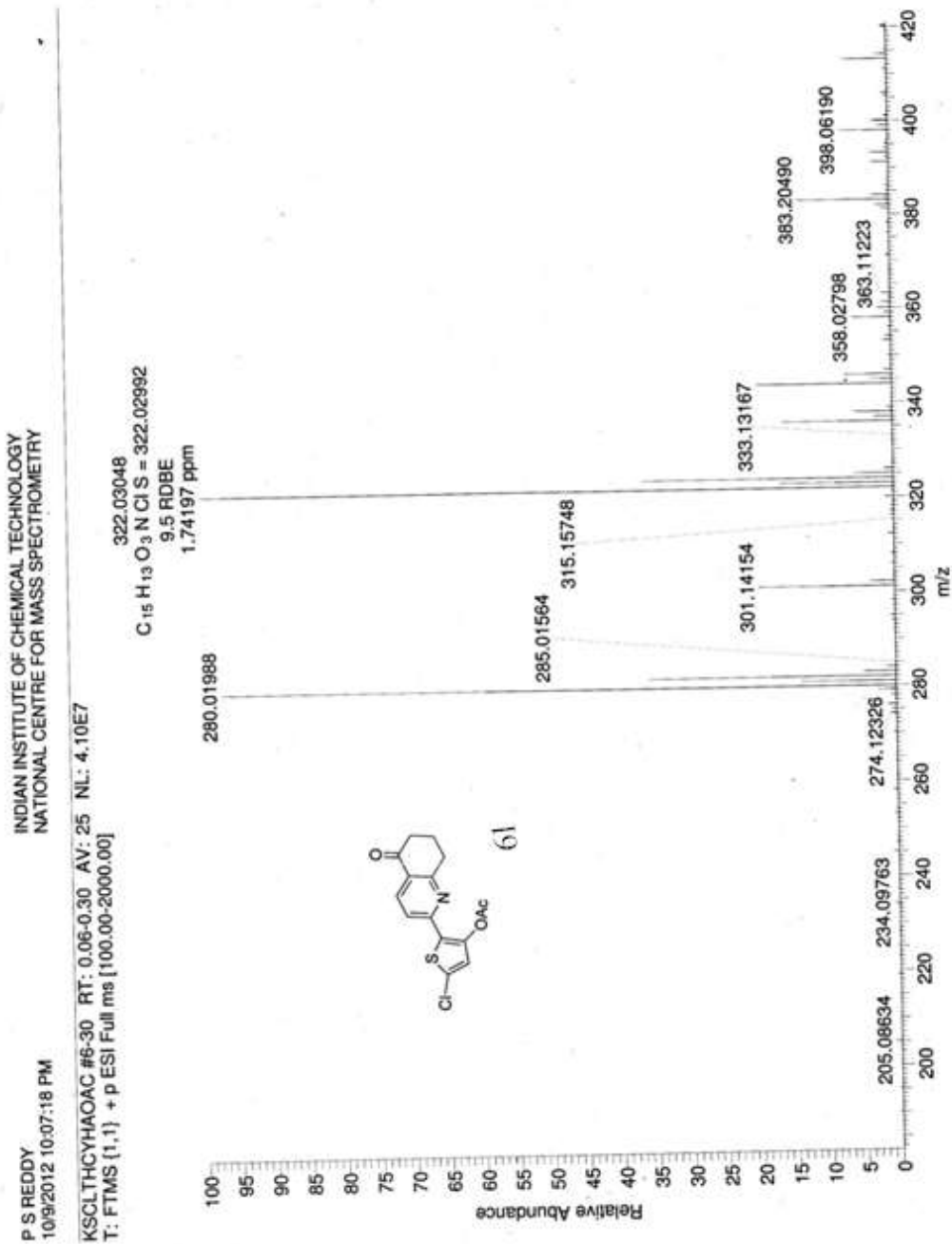
316.10110  
C<sub>17</sub>H<sub>18</sub>O<sub>3</sub>N S = 316.10019  
9.5 RDBE  
2.87725 ppm

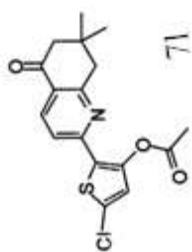


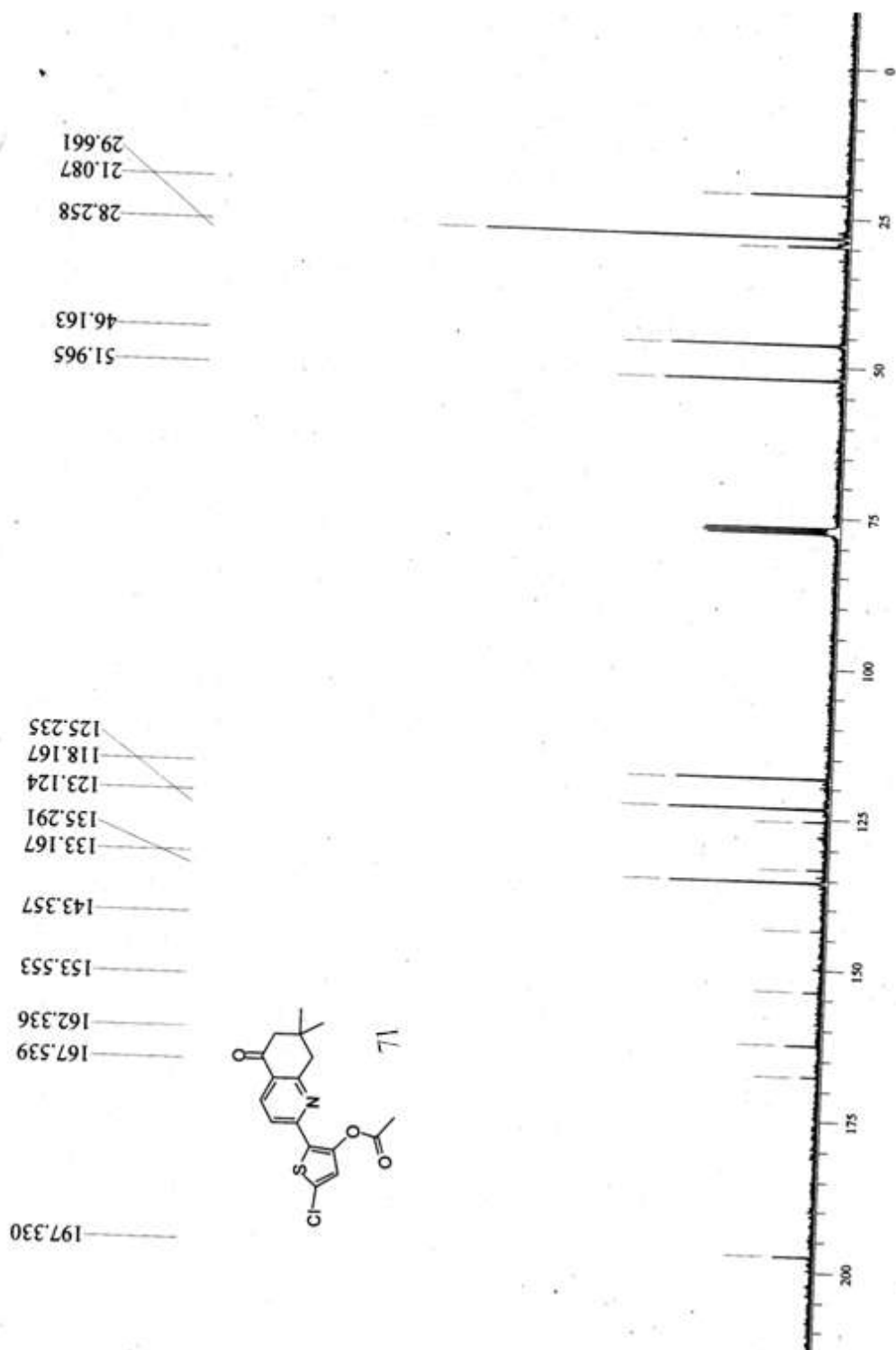












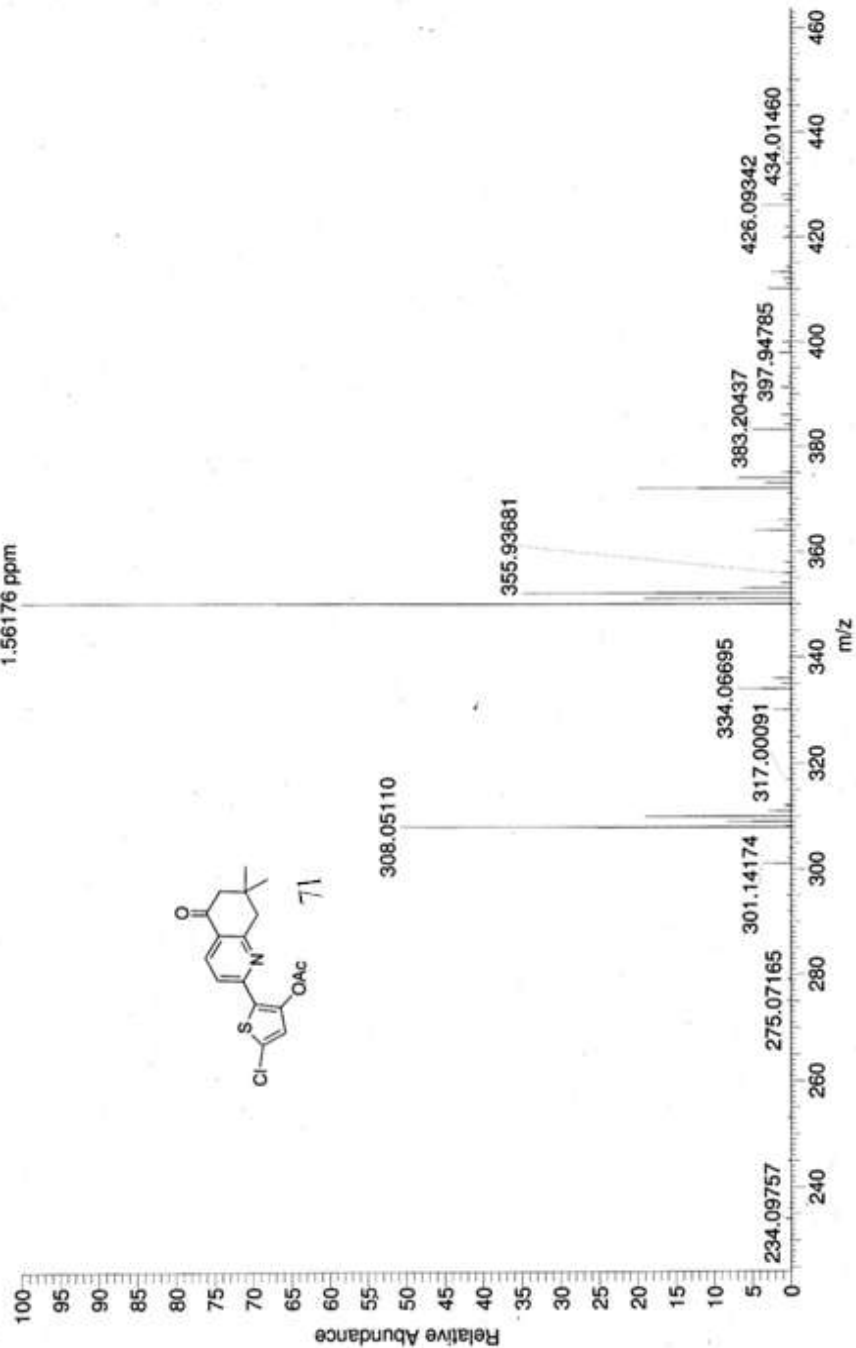
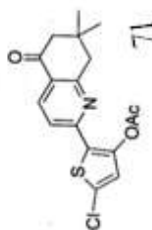
P S REDDY  
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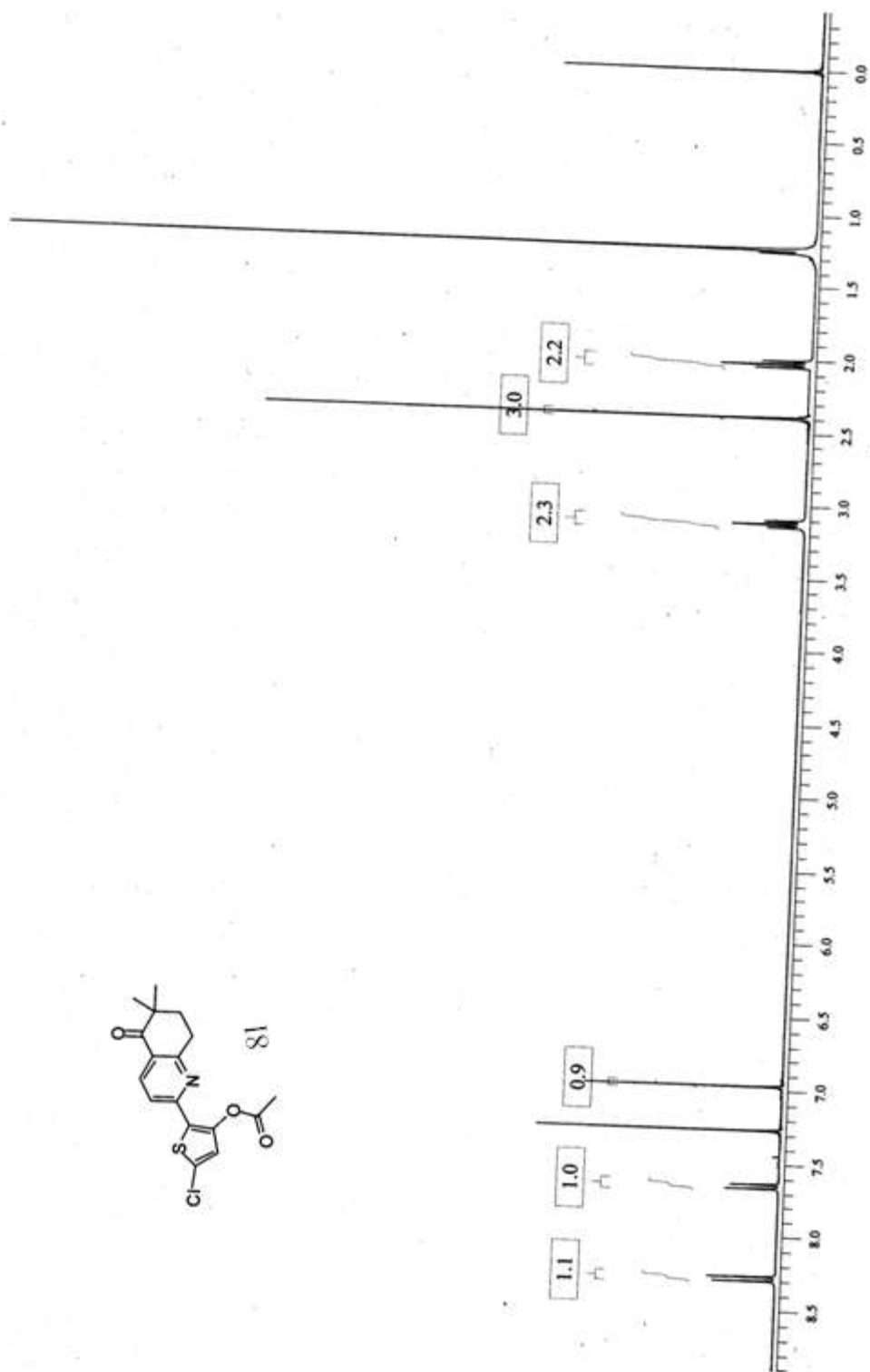
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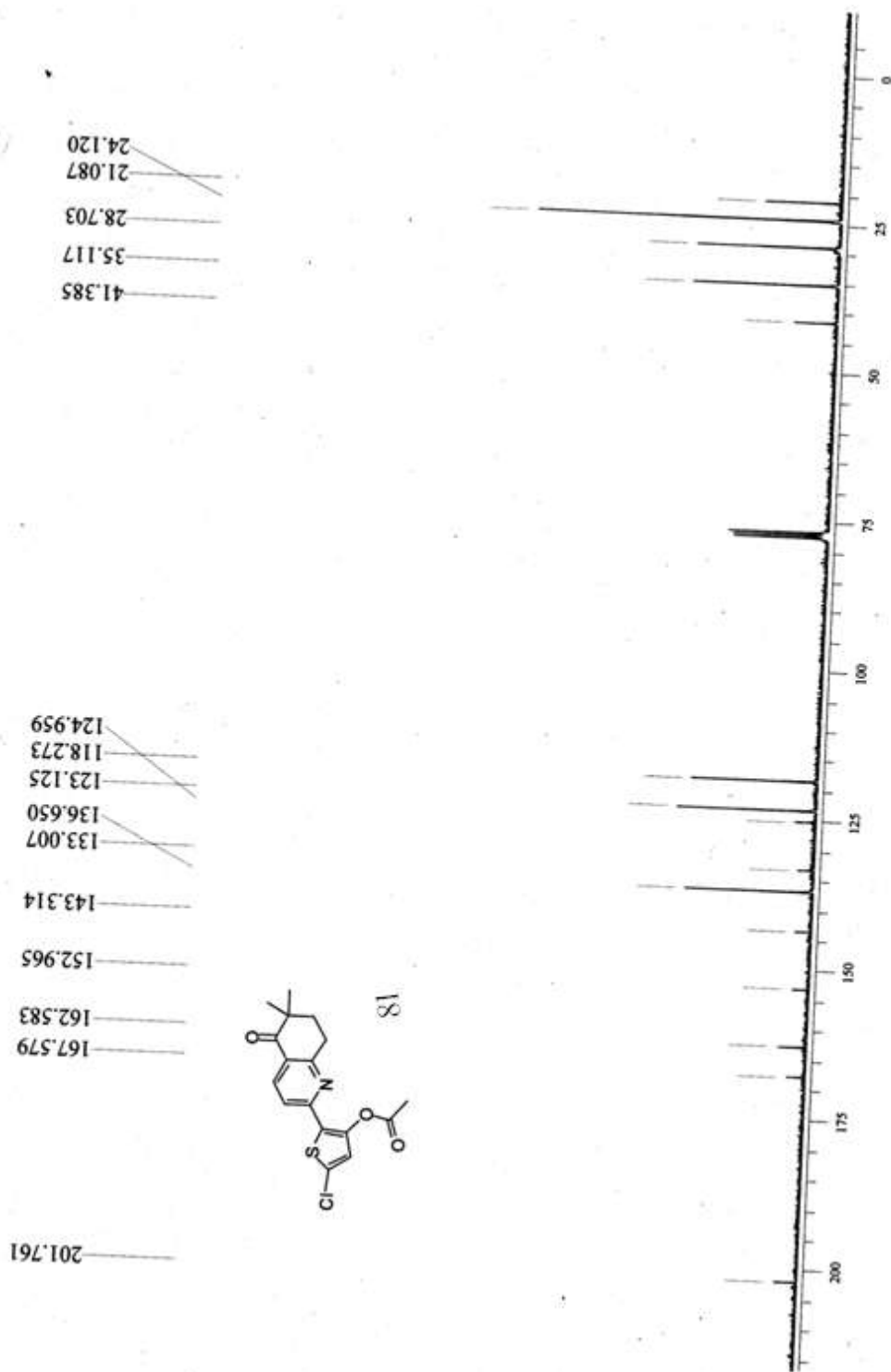
KSCLTHDMDOAC #5-42 RT: 0.05-0.43 AV: 38 NL: 6.00E7

T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

350.06177  
C<sub>17</sub>H<sub>17</sub>O<sub>3</sub>NClS = 350.06122  
9.5 RDBE  
1.56176 ppm



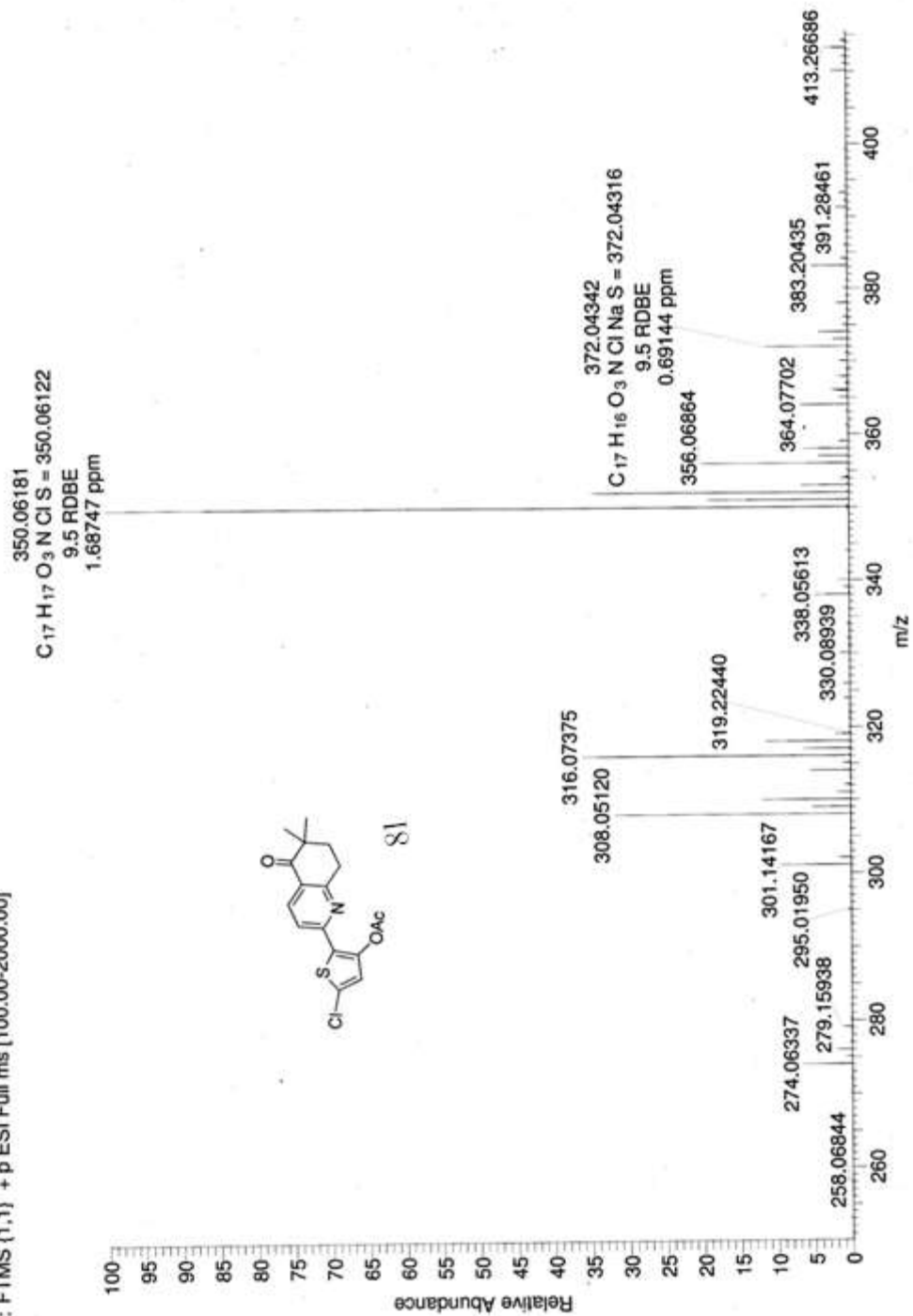


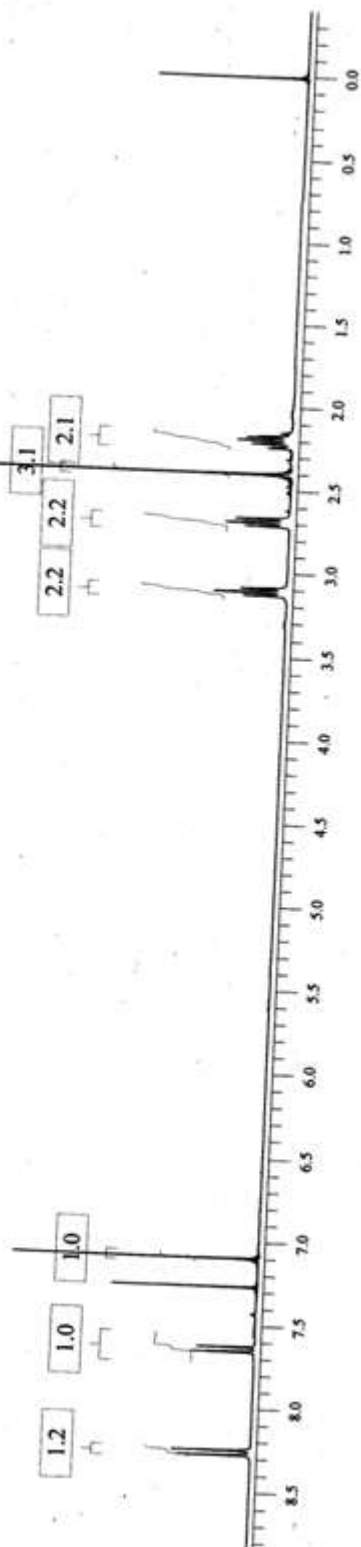
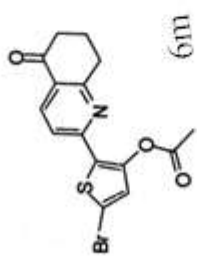


P S REDDY  
10/9/2012 10:02:02 PM

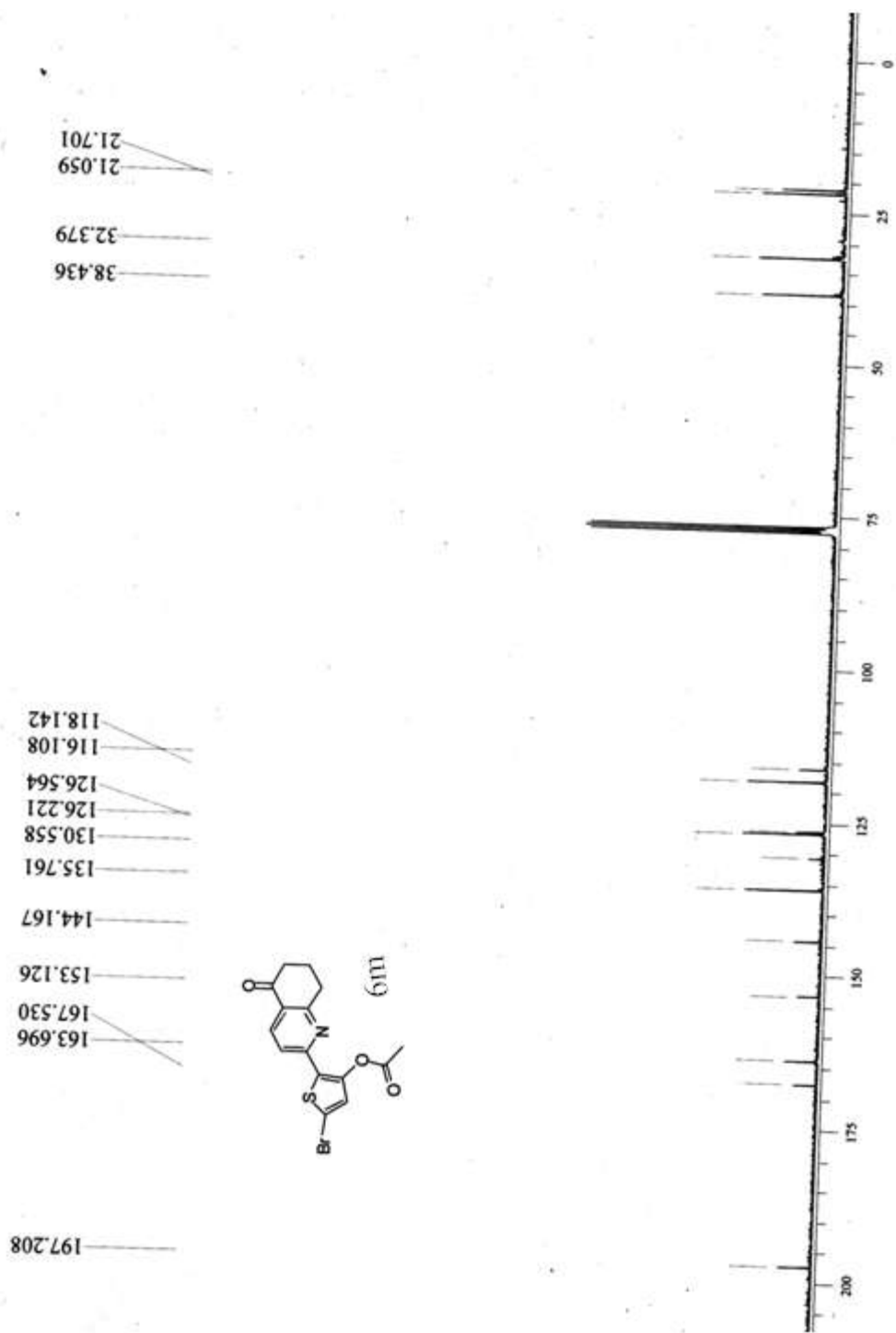
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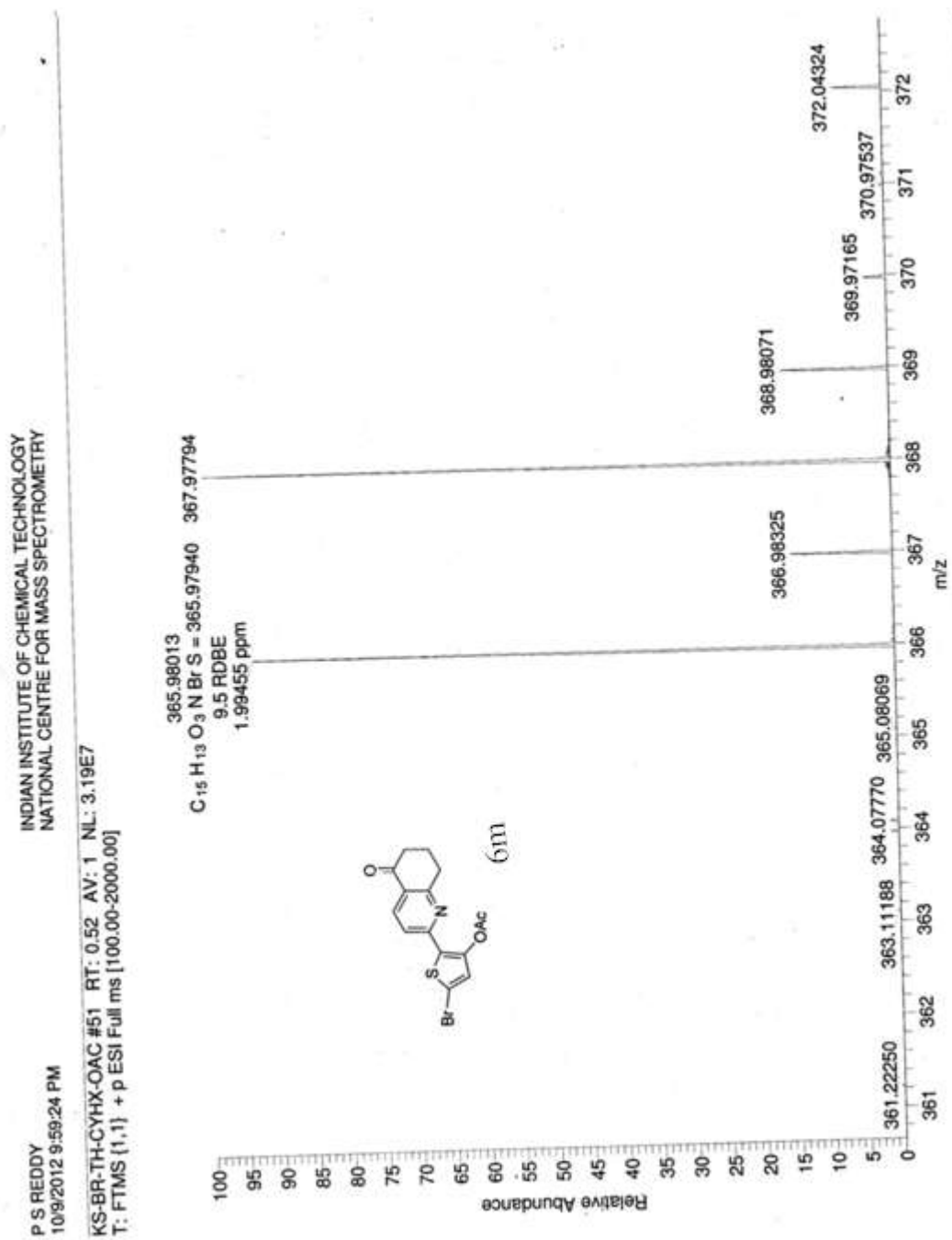
KS-KS-CL-TH-UNSOAC #4-32 RT: 0.04-0.32 AV: 29 NL: 5.99E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

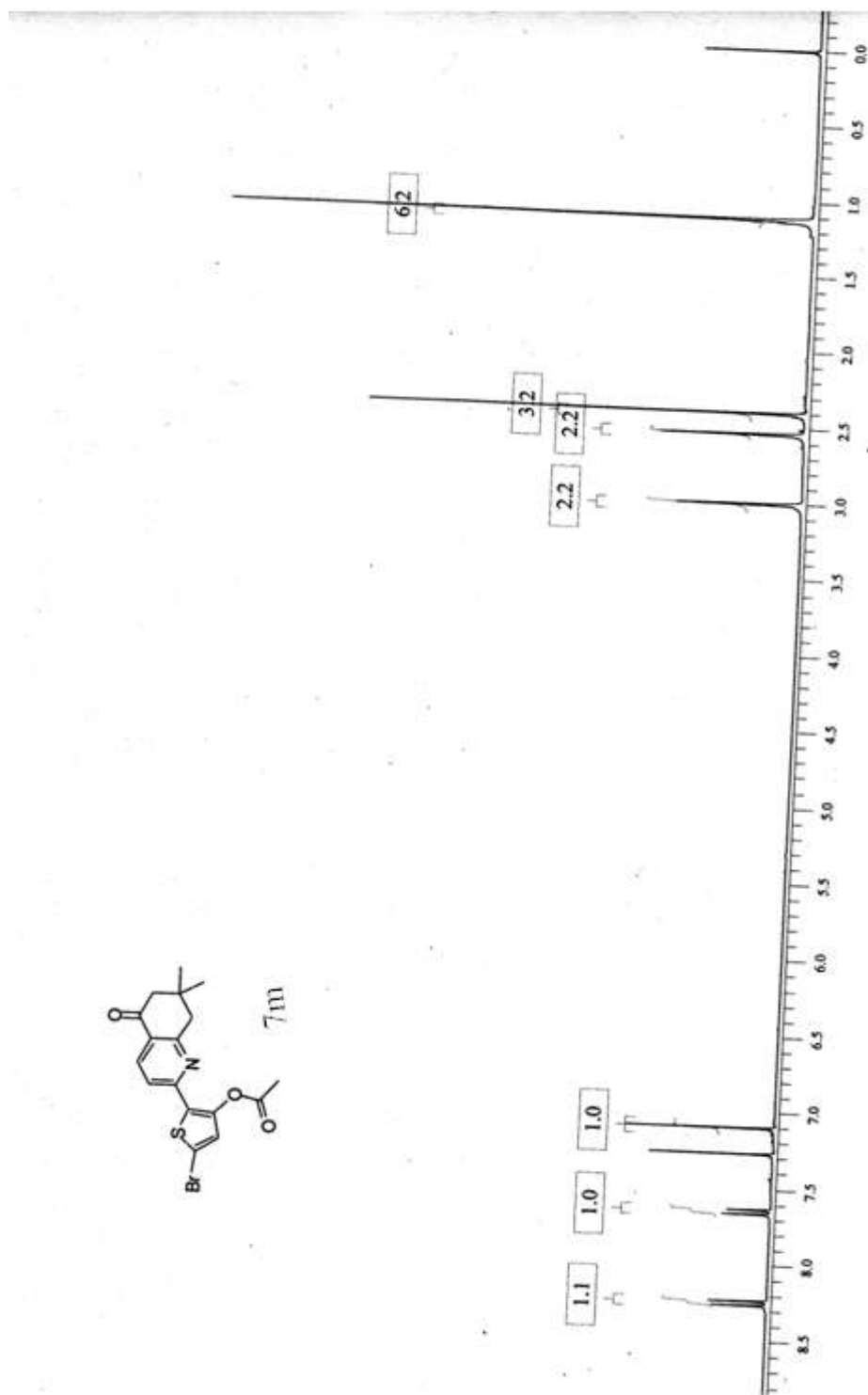
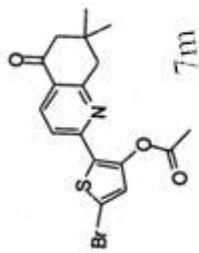


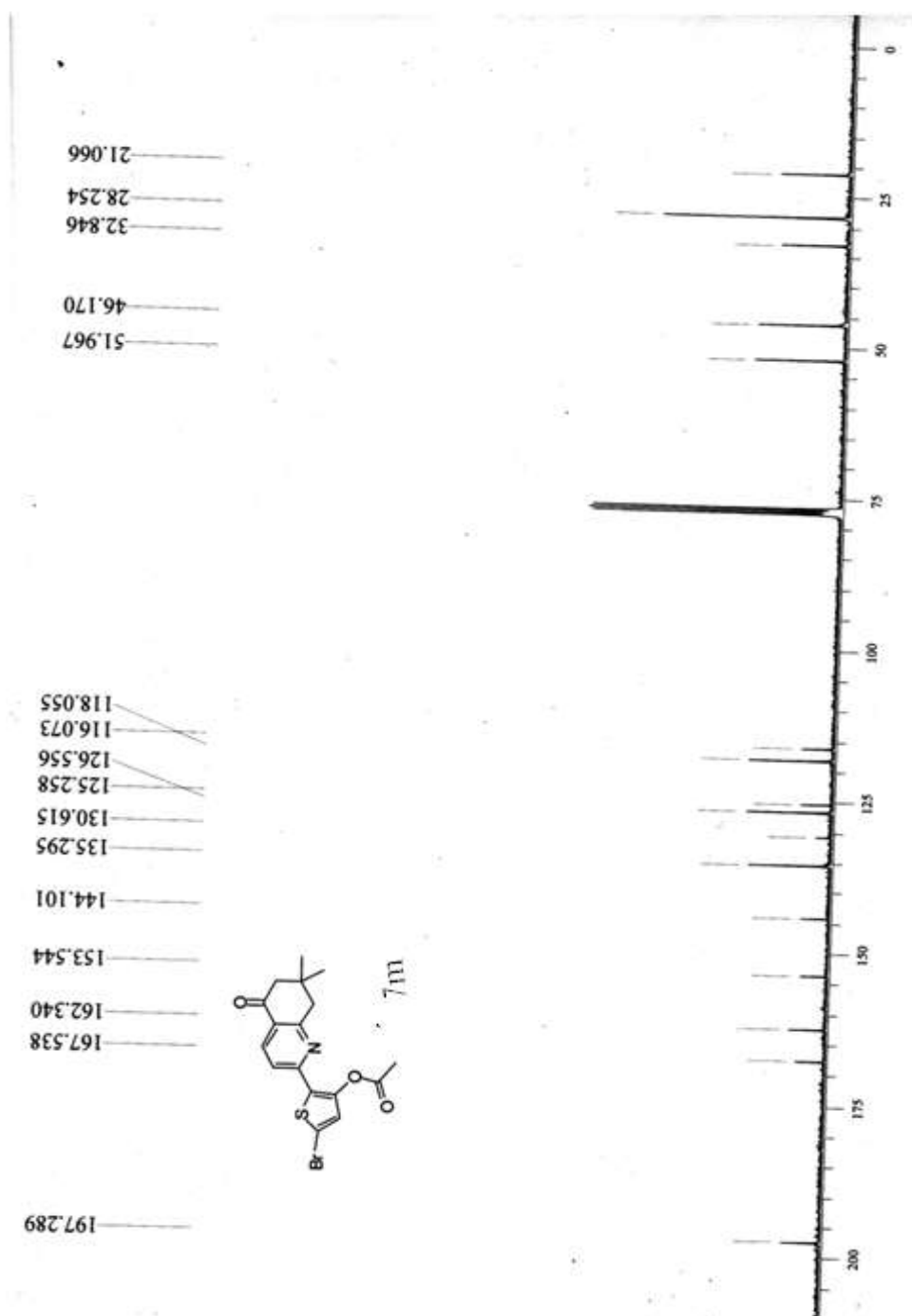


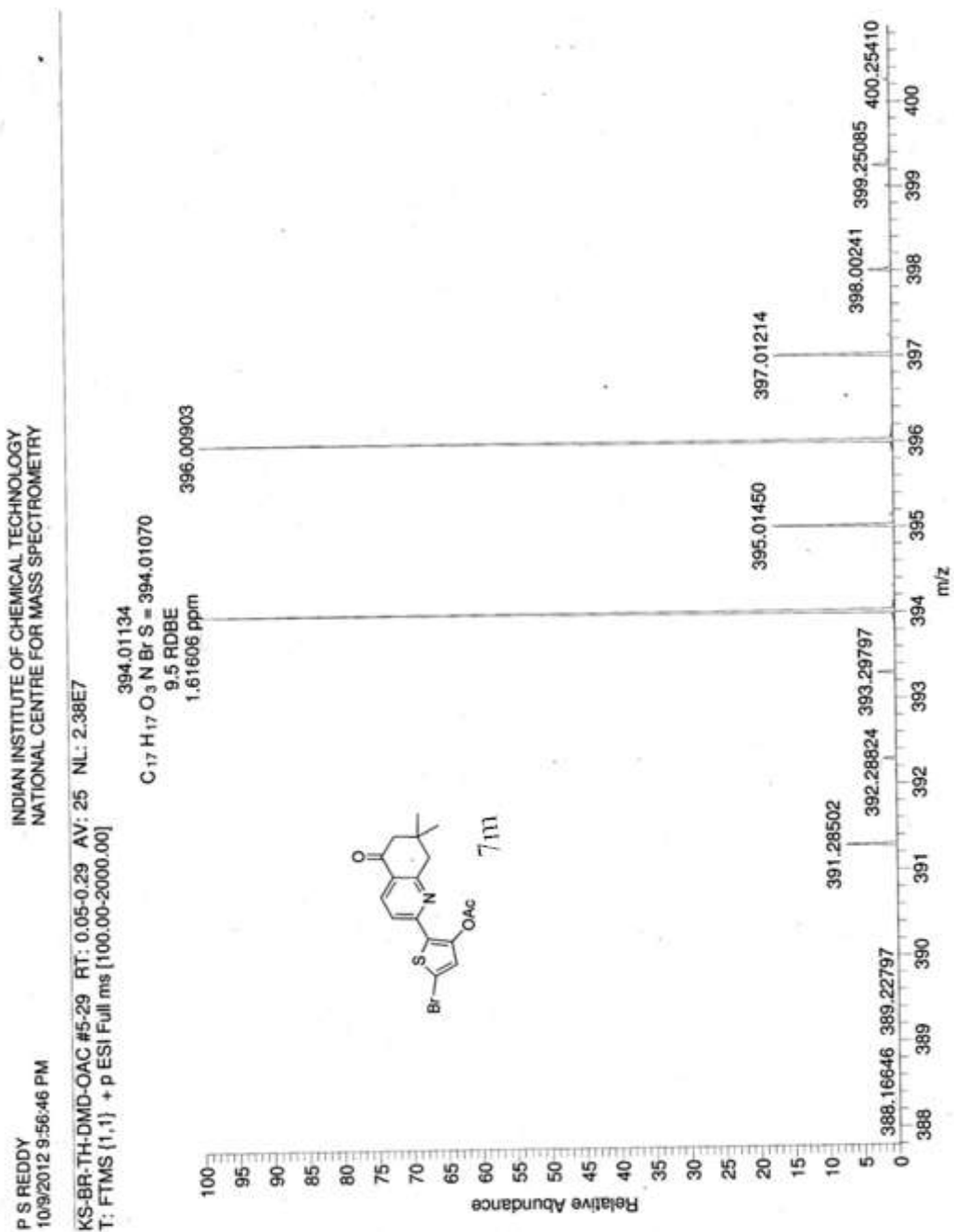


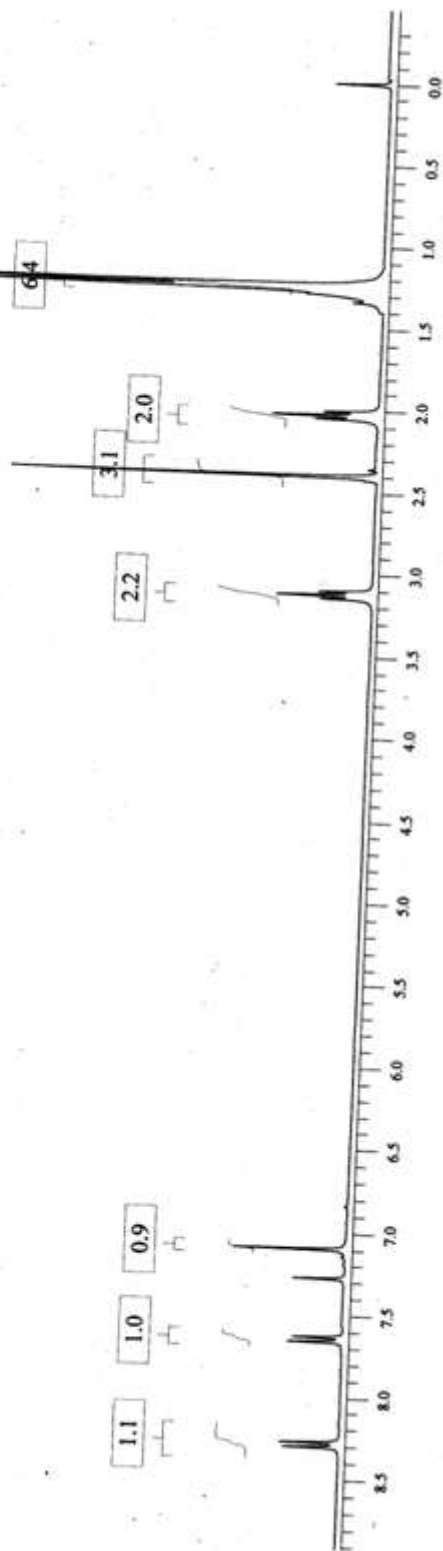
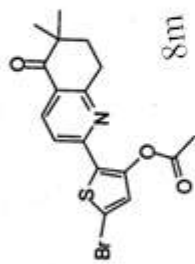


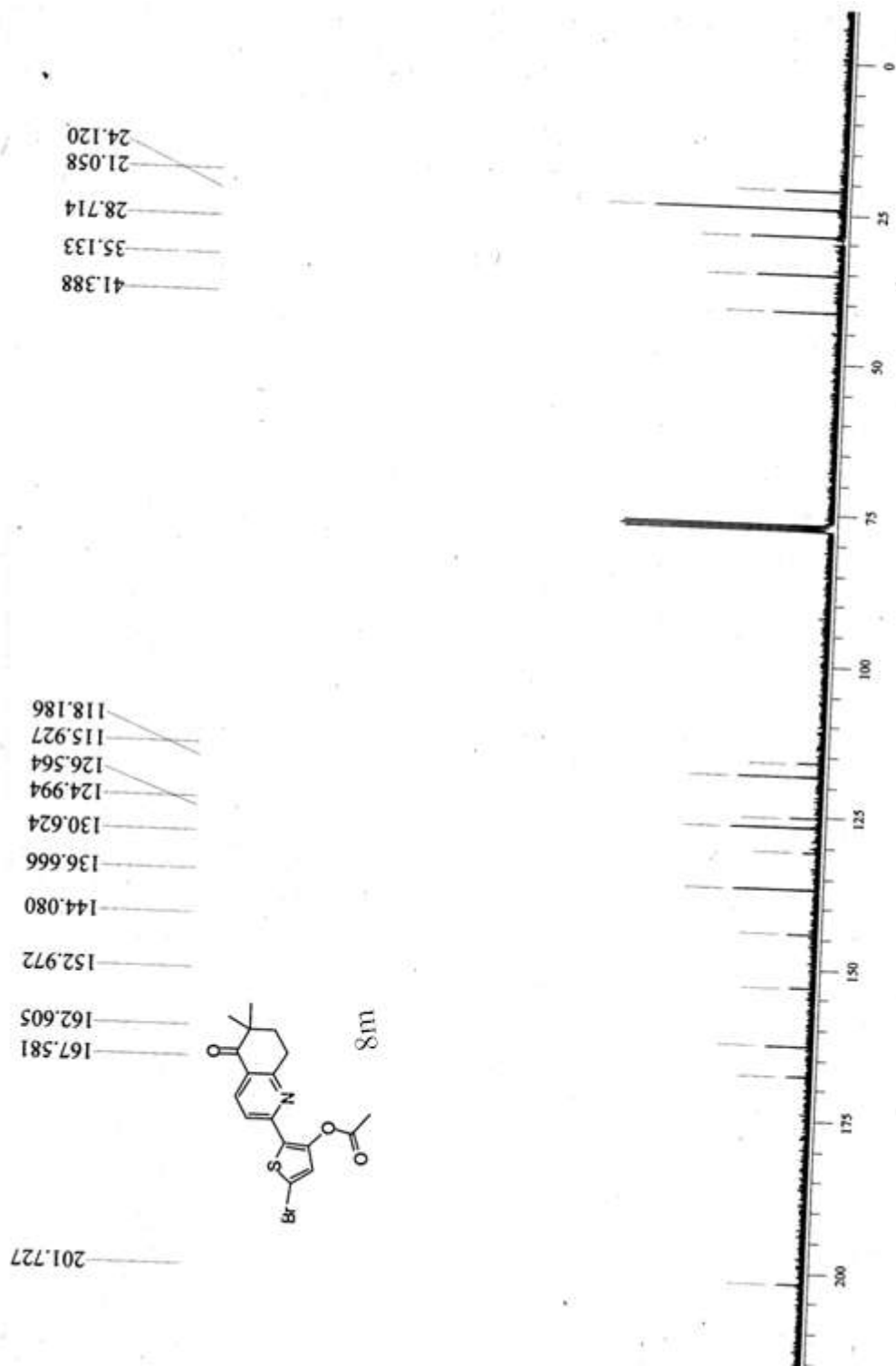


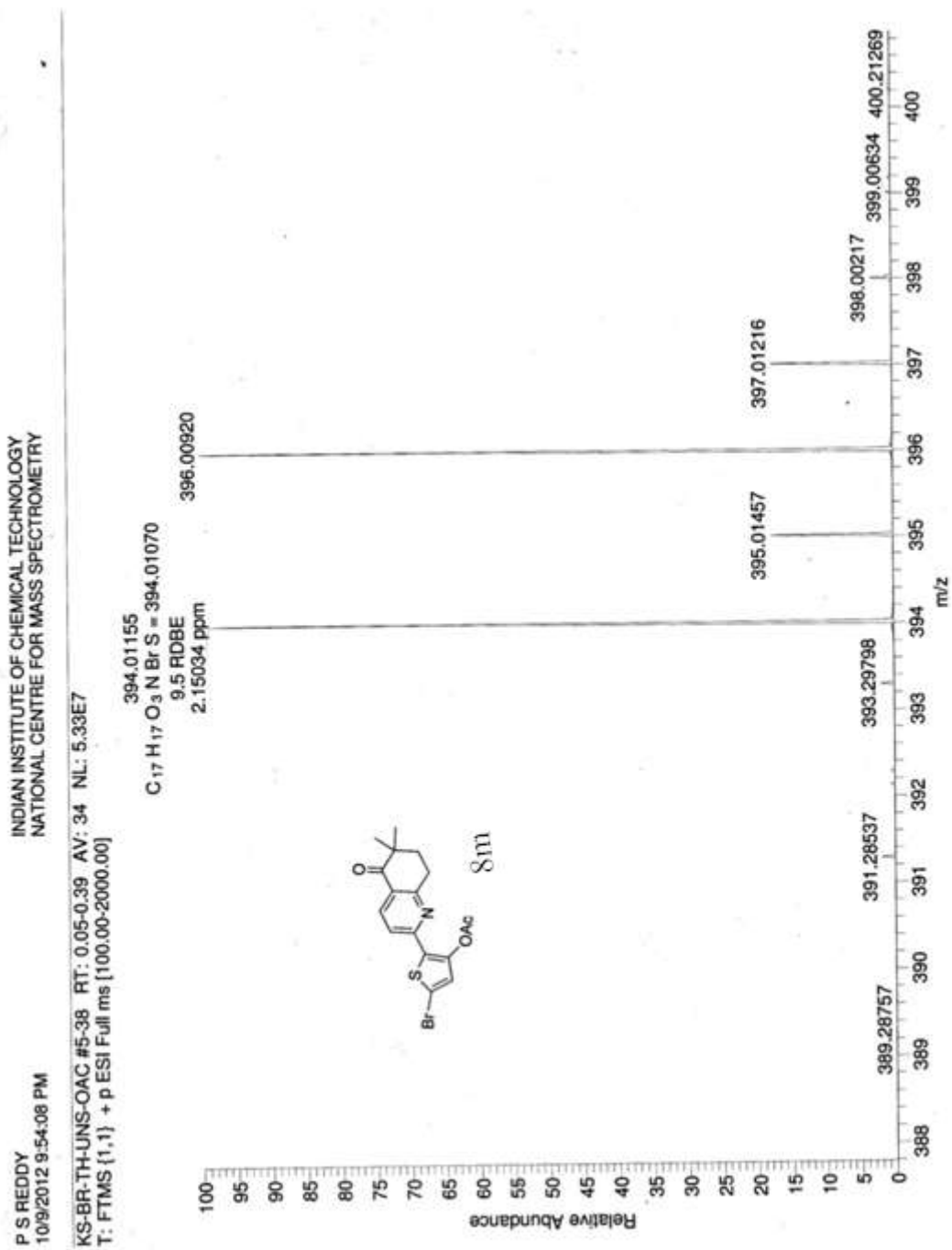




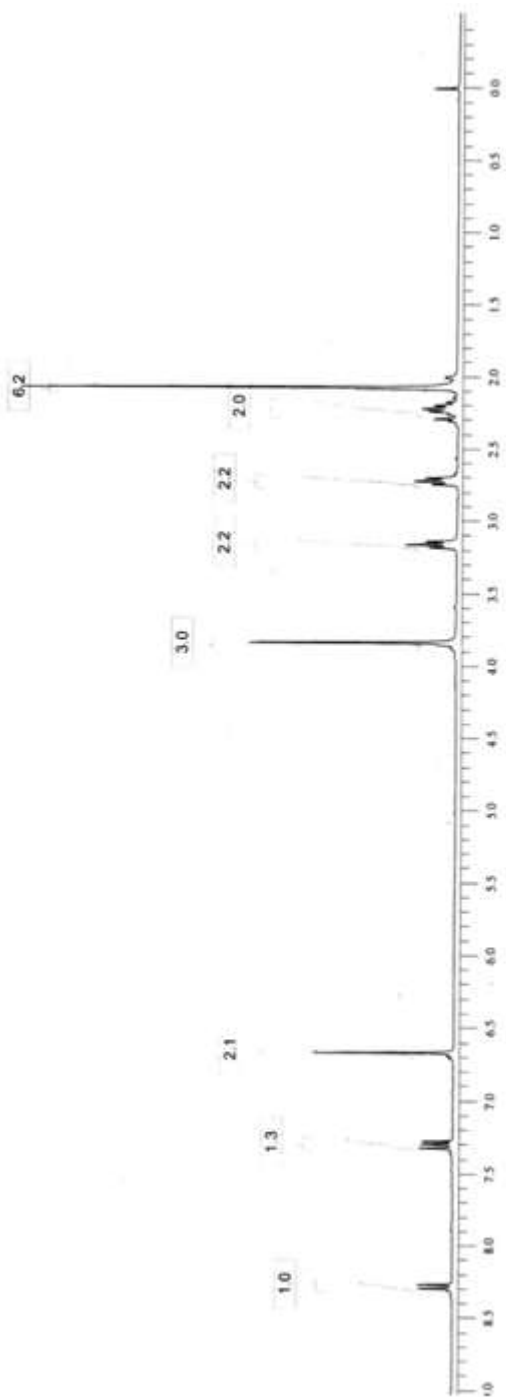
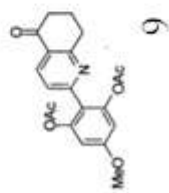


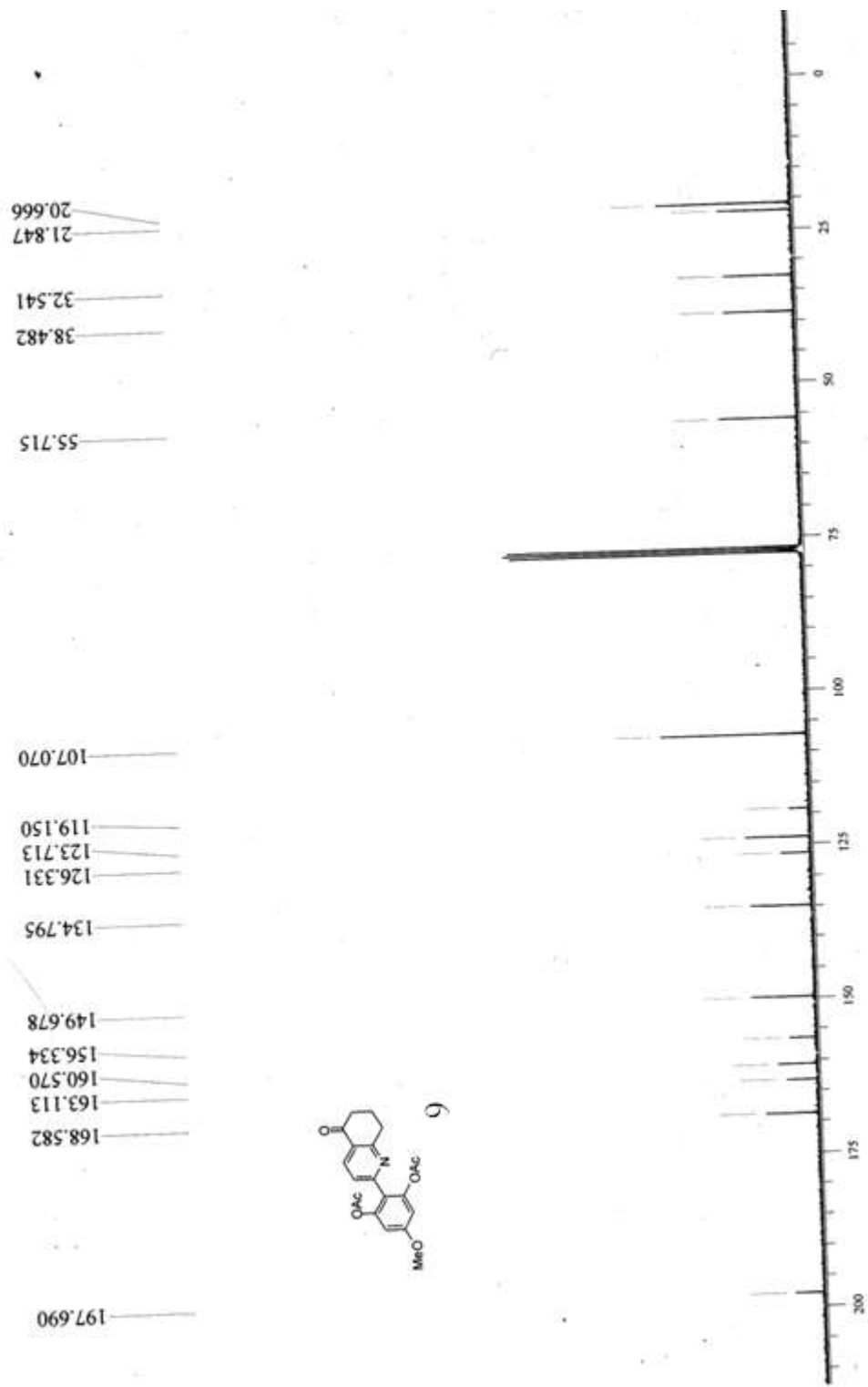








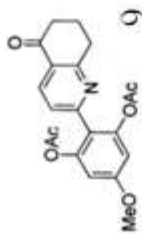
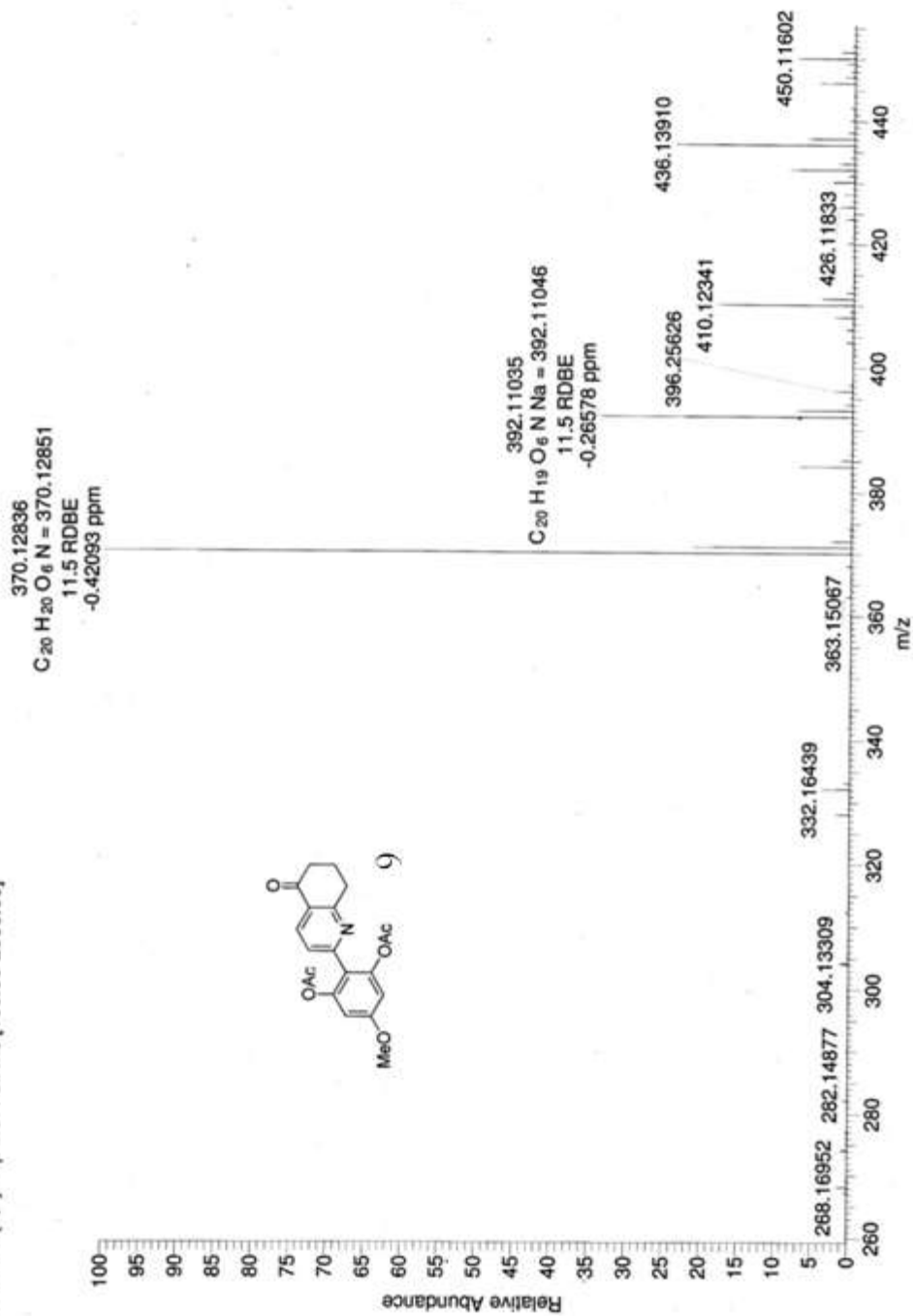


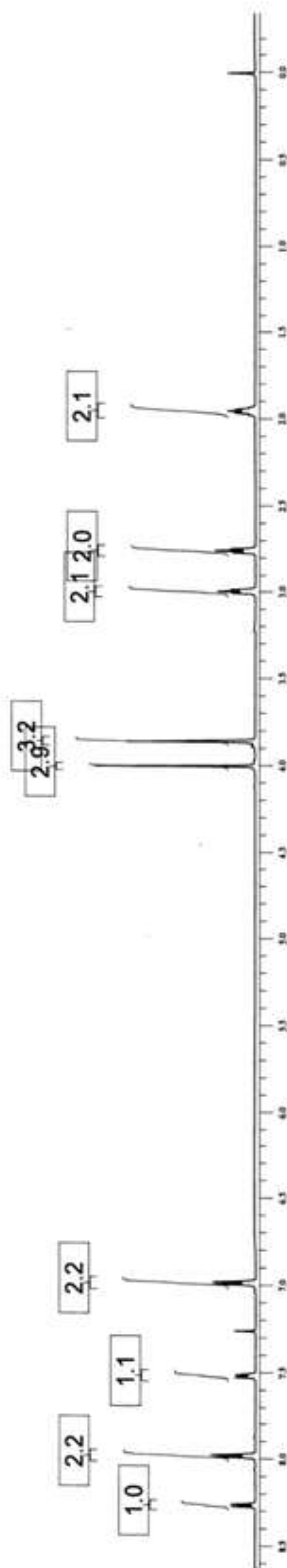
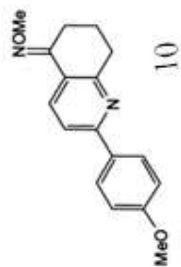


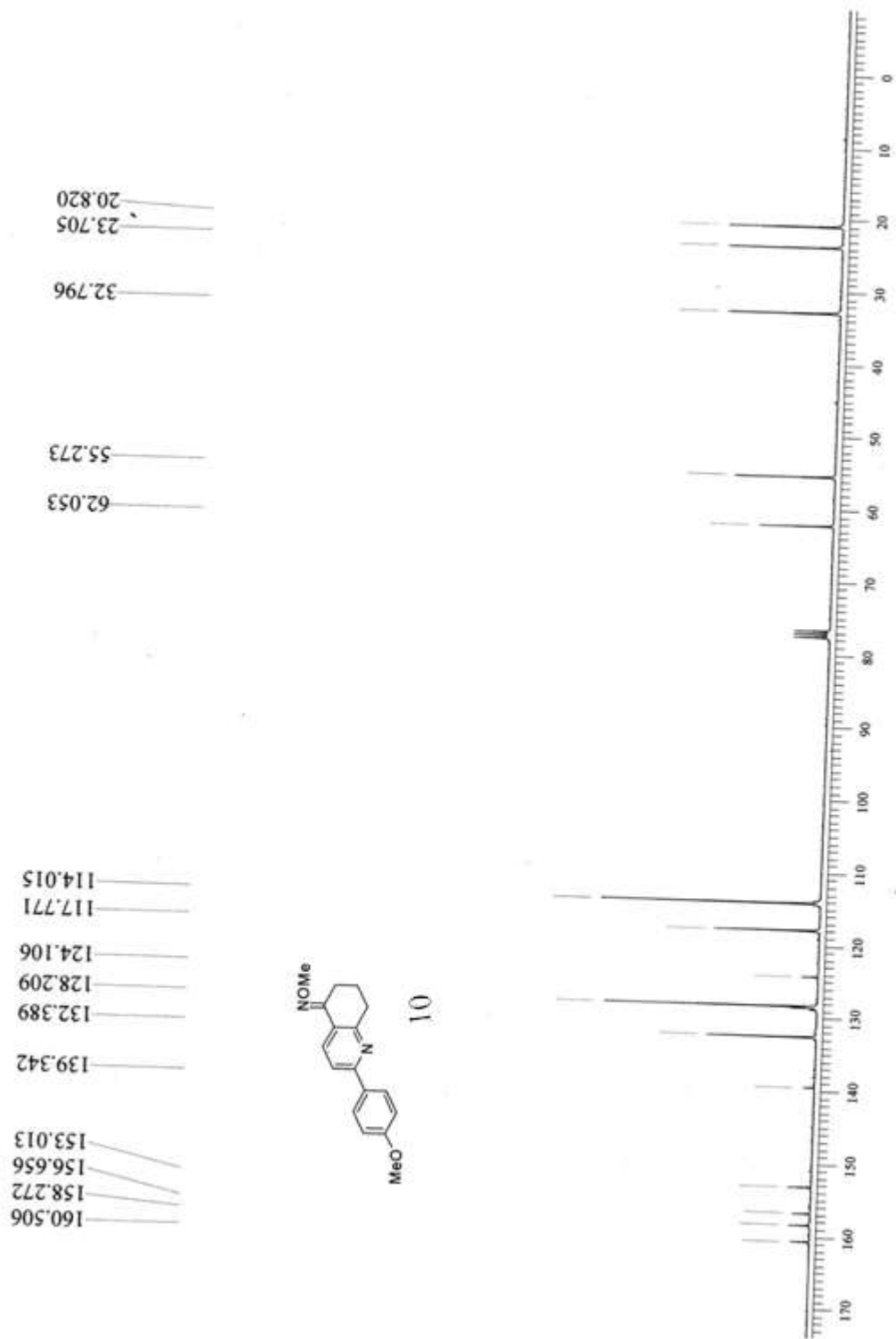
P S REDDYY9  
10/12/2012 11:06:31 PM

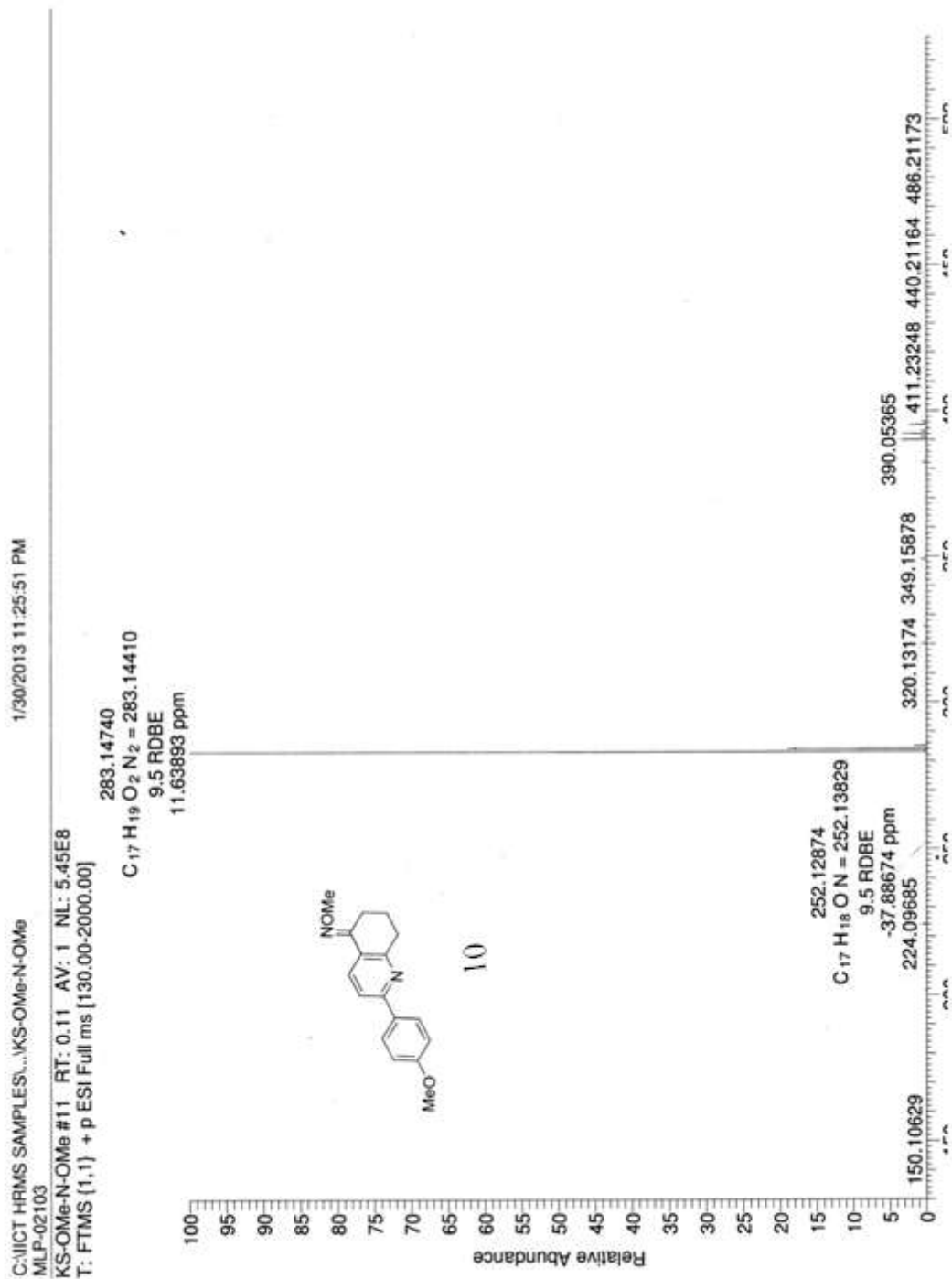
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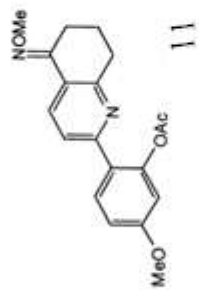
KSPOMECYHXDIOAC #7-30 RT: 0.07-0.30 AV: 24 NL: 1.73E5  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]



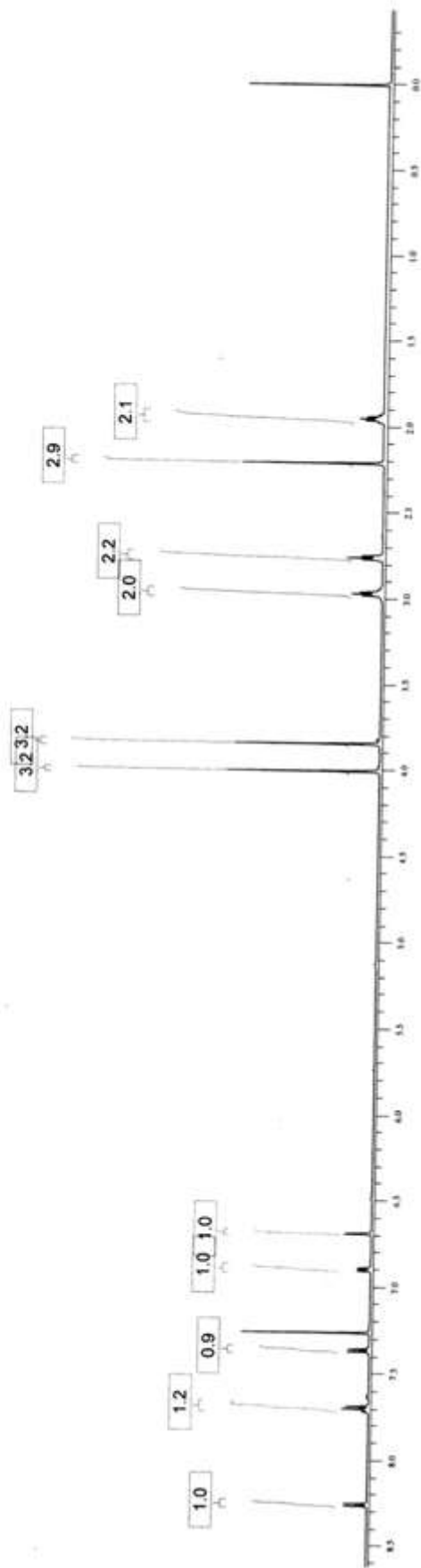


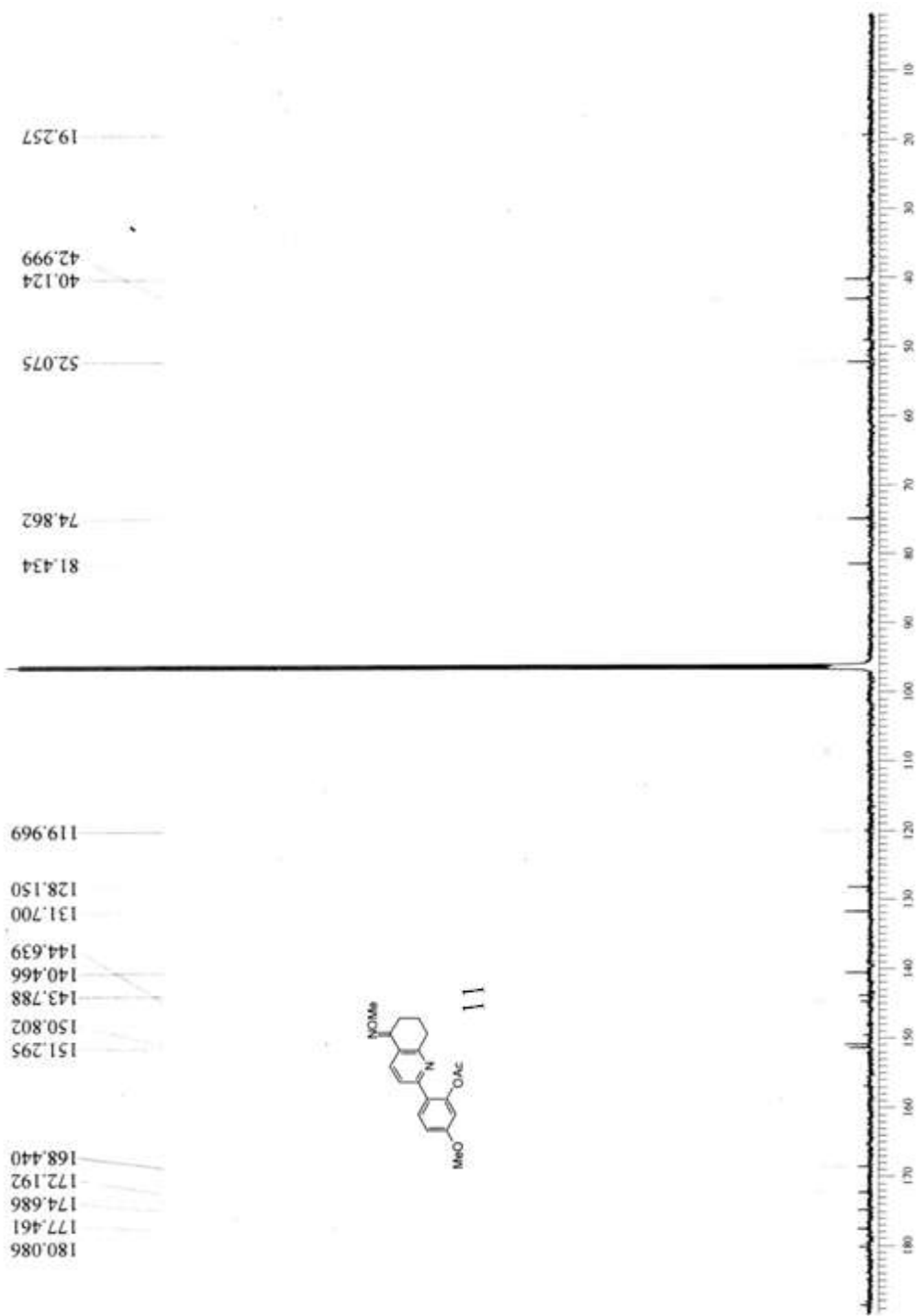






11







K SRINIVAS  
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KS-Ph-CYHX-OAC\_130206144532 #4-30 RT: 0.04-0.30 AV: 27 NL: 1.81E8  
T: FTMS [1,1] + p ESI Full ms [100.00-2000.00]

341.14959  
C<sub>19</sub>H<sub>21</sub>O<sub>4</sub>N<sub>2</sub> = 341.14958  
10.5 RDBE  
0.01857 ppm

