

# Design, Synthesis, and Biological Evaluation of novel trifluoromethyl Indole derivatives as Potent HIV-1 Non-nucleoside Reverse Transcriptase Inhibitors with an Improved Drug Resistance Profile

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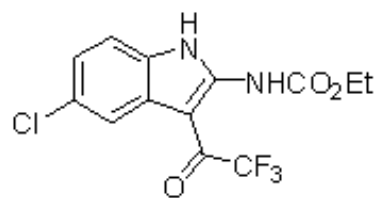
## 1. General Methods:

All reactions were carried out under air atmosphere. All commercially available reagents and solvents were used without further purification. Column chromatography was carried out on silica gel. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded on a Varian instrument (300 MHz, 75 MHz and 282 MHz, respectively) or Bruker instrument (400 MHz and 100 MHz, respectively) and internally referenced to tetramethylsilane signal. Data for <sup>1</sup>H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet or unresolved, coupling

constant(s) in Hz, integration). Data for  $^{13}\text{C}$  NMR is reported in terms of chemical shift ( $\delta$ , ppm). IR spectra were taken on a Nicolet AV-330 spectrophotometer and only major peaks were reported in  $\text{cm}^{-1}$ . Low resolution mass spectra (LRMS) were taken on a Agilent 592N spectrometer and a Shimadzu LCMS-2010EV. HPLC spectra were taken on a Shimadzu (SPD20A LC-20AT) with Reversed-phase column of Kromasil (5u 100A C18 150\*4.6mm). Gradient conditions: 1) solvent A (acetonitrile) and solvent B (water): 0–20.00 min, 10/90 (A/B)–100/0 (A/B) (linear gradient); 20.00–30.00 min, 100% A. Eluting products were detected by UV at 254 nm 2) solvent A (acetonitrile) and solvent B (water): 0–20.00 min, 80/20 (A/B). Eluting products were detected by UV at 214 nm.

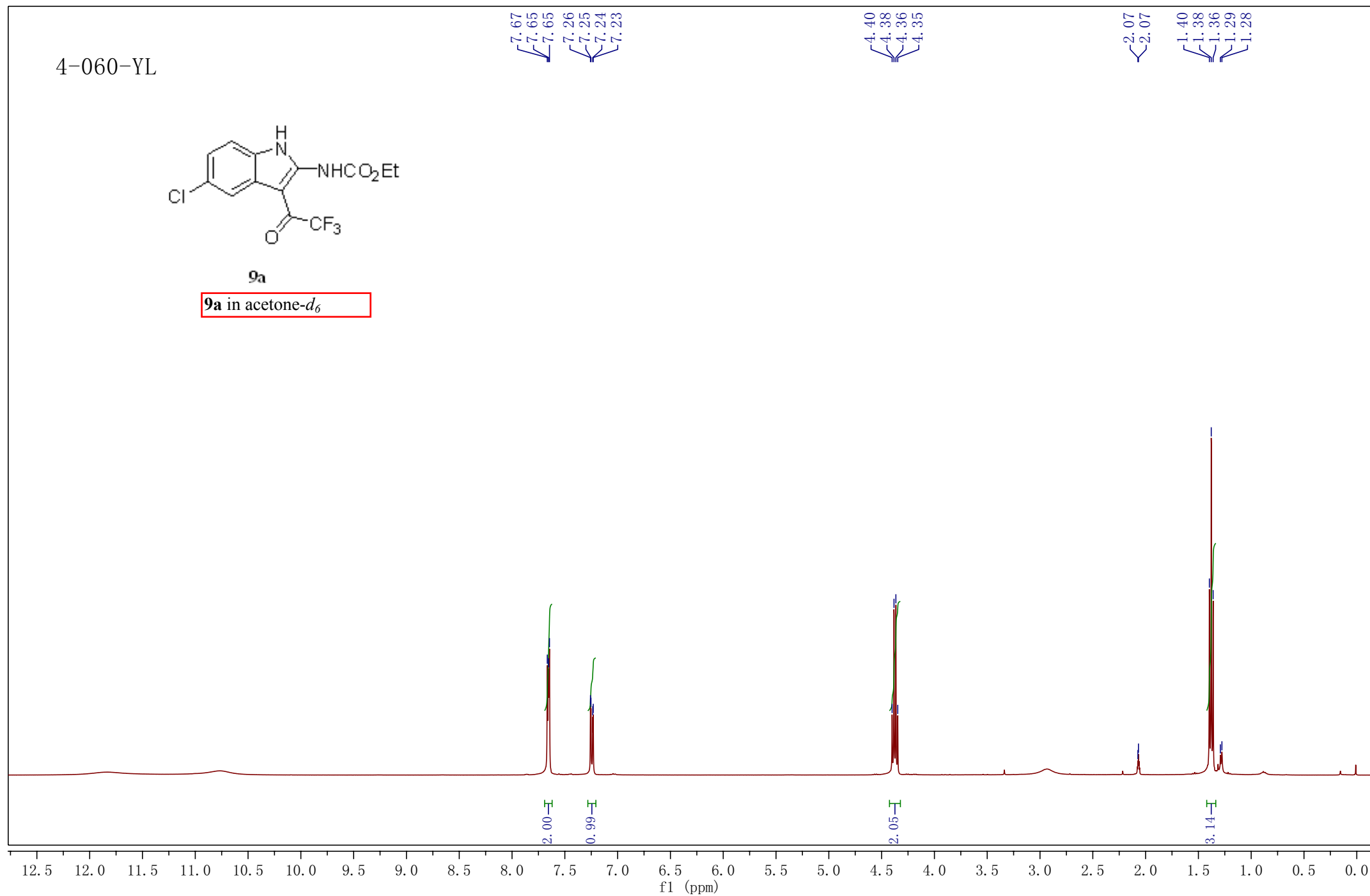
2.  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, MS and HPLC Spectra of Compounds **9a–9e** and **10a–10q**:

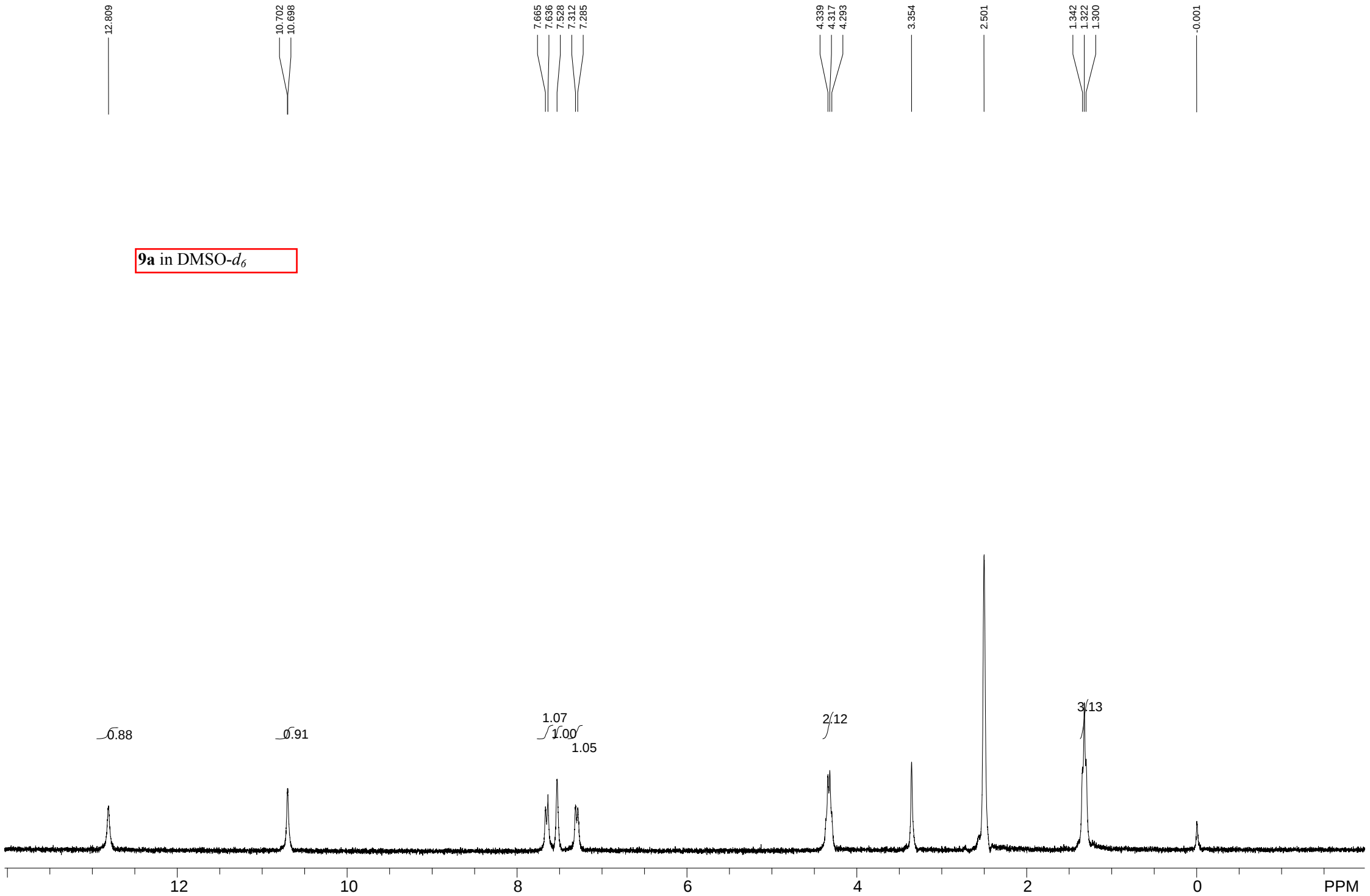
4-060-YL



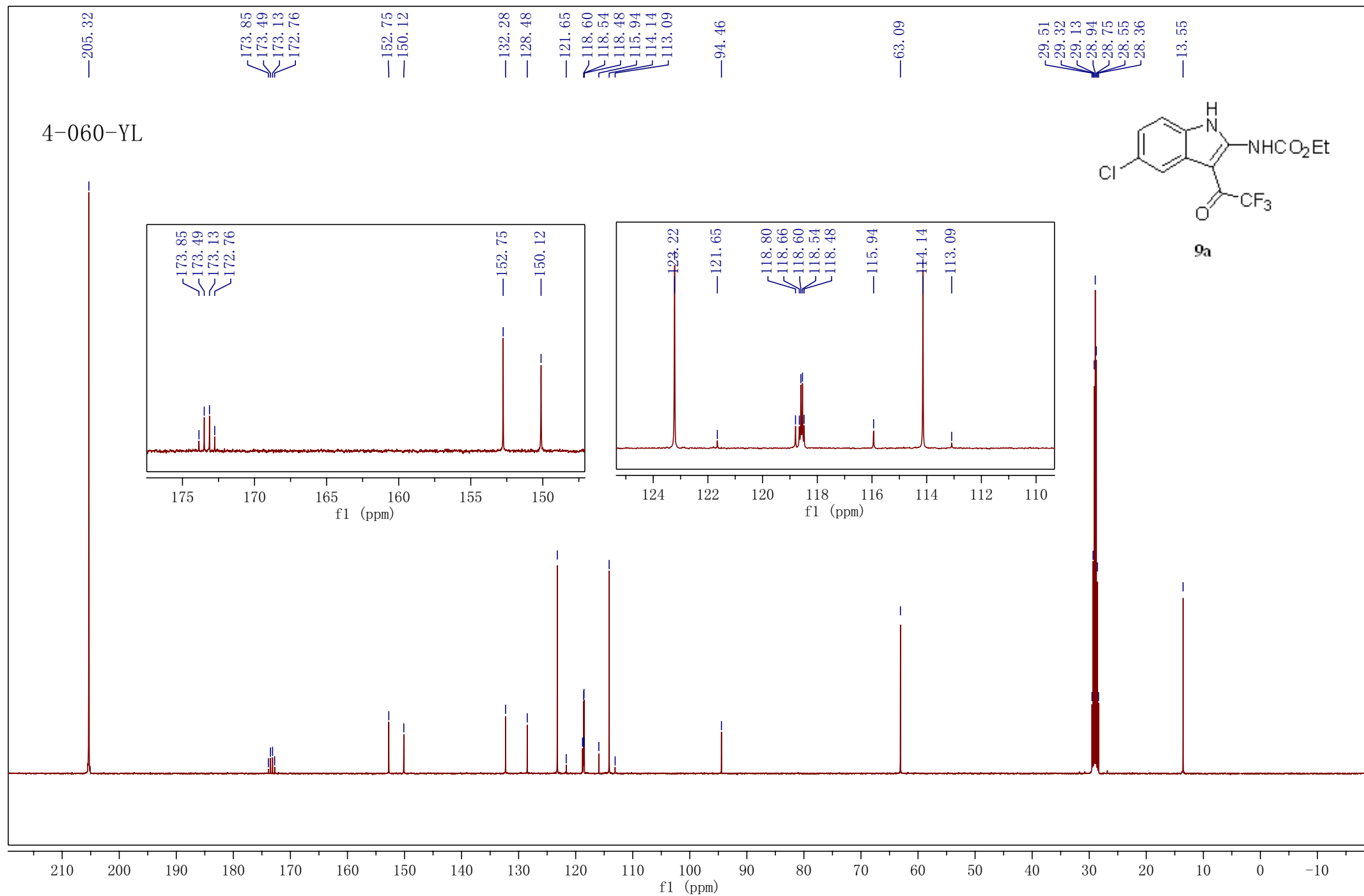
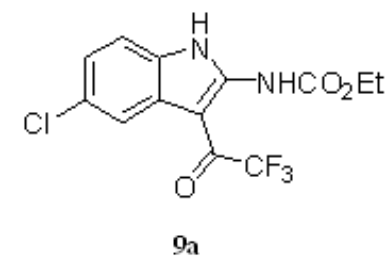
**9a**

9a in acetone-*d*<sub>6</sub>





4-060-YL

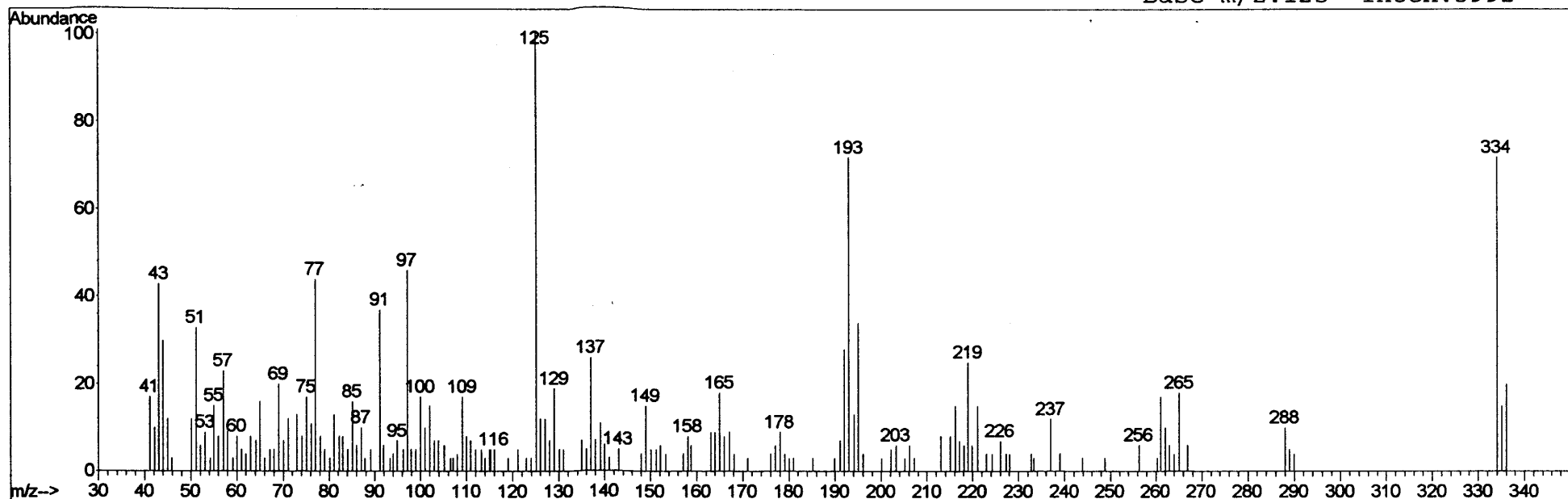


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Shanghai Institute of Organic Chemistry

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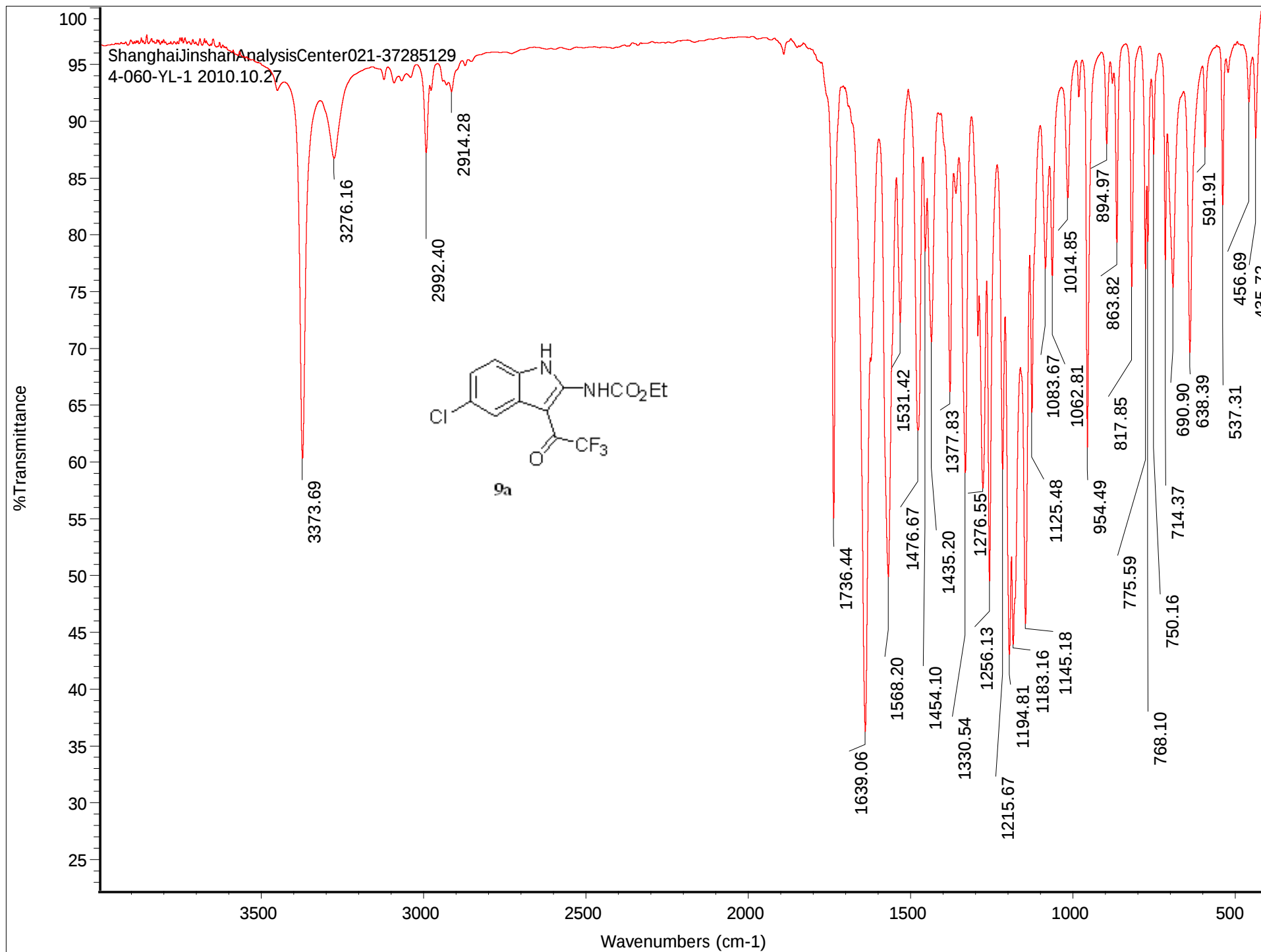
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| 41  | 16.87 | 61  | 5.17  | 78  | 8.03  | 98  | 5.01  | 115 | 4.66   | 143 | 4.62  | 192 | 27.37 |
| 42  | 9.73  | 63  | 7.74  | 81  | 12.97 | 99  | 5.37  | 125 | 100.00 | 149 | 14.45 | 193 | 71.31 |
| 43  | 42.12 | 64  | 6.96  | 82  | 7.69  | 100 | 16.51 | 126 | 11.93  | 150 | 5.01  | 194 | 13.08 |
| 44  | 29.89 | 65  | 15.69 | 83  | 7.46  | 101 | 10.36 | 127 | 12.13  | 152 | 5.97  | 195 | 33.59 |
| 45  | 11.88 | 67  | 4.84  | 84  | 5.37  | 102 | 14.55 | 128 | 6.59   | 158 | 8.21  | 202 | 5.31  |
| 50  | 12.07 | 68  | 5.16  | 85  | 15.45 | 103 | 7.41  | 129 | 18.51  | 159 | 5.84  | 203 | 5.66  |
| 51  | 33.09 | 69  | 20.26 | 86  | 5.77  | 104 | 6.78  | 130 | 5.29   | 163 | 8.90  | 206 | 5.69  |
| 52  | 6.17  | 70  | 7.03  | 87  | 9.86  | 105 | 5.81  | 131 | 5.36   | 164 | 9.10  | 213 | 7.76  |
| 53  | 9.28  | 71  | 12.15 | 89  | 5.44  | 109 | 17.12 | 135 | 6.96   | 165 | 18.11 | 215 | 8.31  |
| 55  | 14.60 | 73  | 12.93 | 91  | 36.50 | 110 | 8.01  | 136 | 5.24   | 166 | 7.66  | 216 | 14.45 |
| 56  | 7.91  | 74  | 7.54  | 92  | 5.52  | 111 | 6.96  | 137 | 26.13  | 167 | 8.98  | 217 | 7.24  |
| 57  | 22.90 | 75  | 17.22 | 95  | 6.61  | 112 | 4.94  | 138 | 6.88   | 177 | 5.46  | 218 | 5.47  |
| 58  | 8.73  | 76  | 10.90 | 96  | 5.32  | 113 | 4.97  | 139 | 10.66  | 178 | 8.83  | 219 | 24.45 |
| 60  | 7.53  | 77  | 43.31 | 97  | 45.43 | 115 | 4.71  | 140 | 5.97   | 191 | 7.38  | 220 | 5.99  |

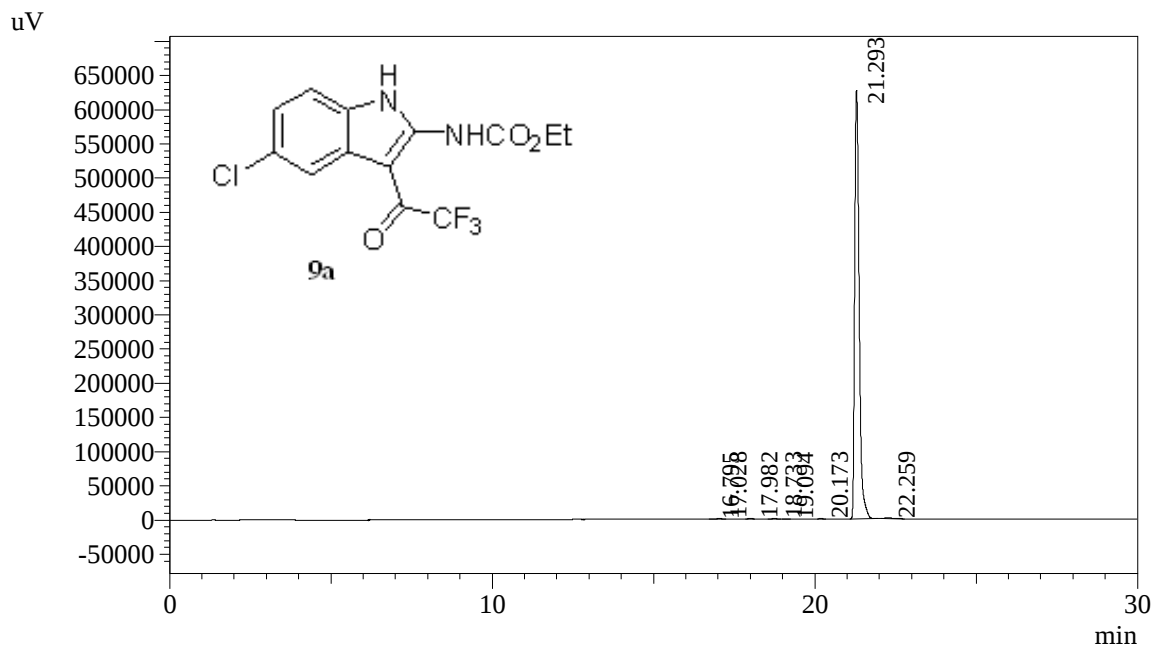
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| 125 | 100.00 | 193 | 71.31 | 334 | 71.19 | 97 | 45.43 | 77 | 43.31 | 43 | 42.12 | 91 | 36.50 | 195 | 33.59 |
|-----|--------|-----|-------|-----|-------|----|-------|----|-------|----|-------|----|-------|-----|-------|



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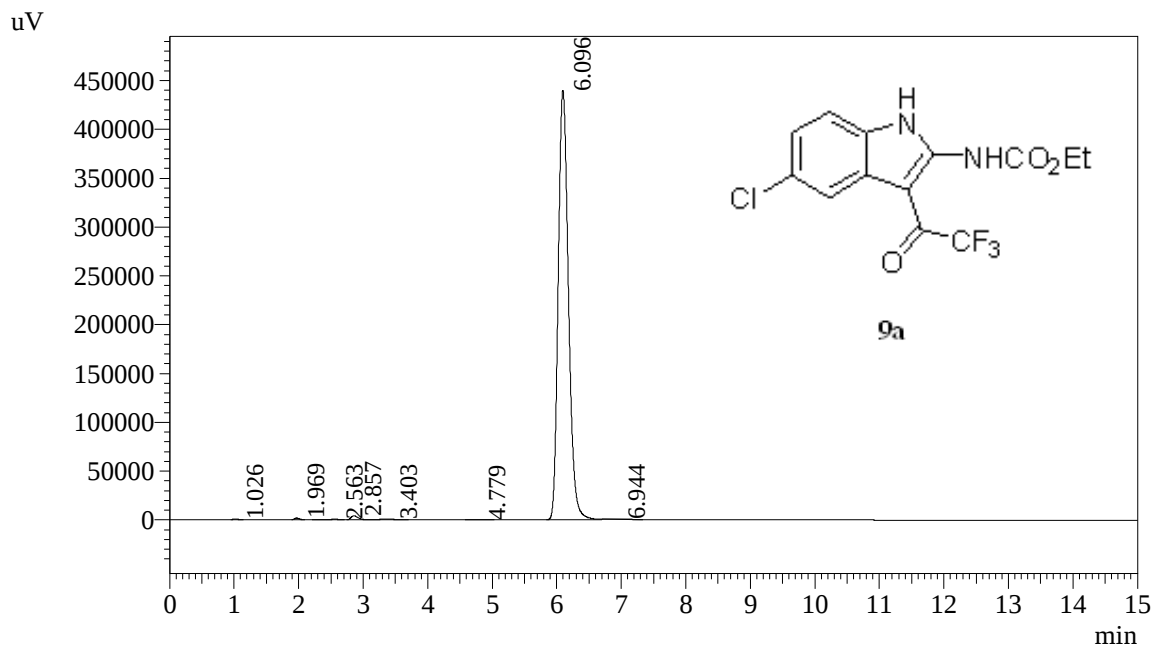
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| 1     | 16.795   | 1514    | 176    | 8.595  | 0.0246   |
| 2     | 17.028   | 10451   | 1103   | 9.476  | 0.1700   |
| 3     | 17.982   | 8392    | 1043   | 8.044  | 0.1365   |
| 4     | 18.733   | 8195    | 815    | 10.056 | 0.1333   |
| 5     | 19.094   | 3045    | 369    | 8.248  | 0.0495   |
| 6     | 20.173   | 2704    | 316    | 8.561  | 0.0440   |
| 7     | 21.293   | 6090944 | 626256 | 9.726  | 99.0765  |
| 8     | 22.259   | 22476   | 1591   | 14.131 | 0.3656   |
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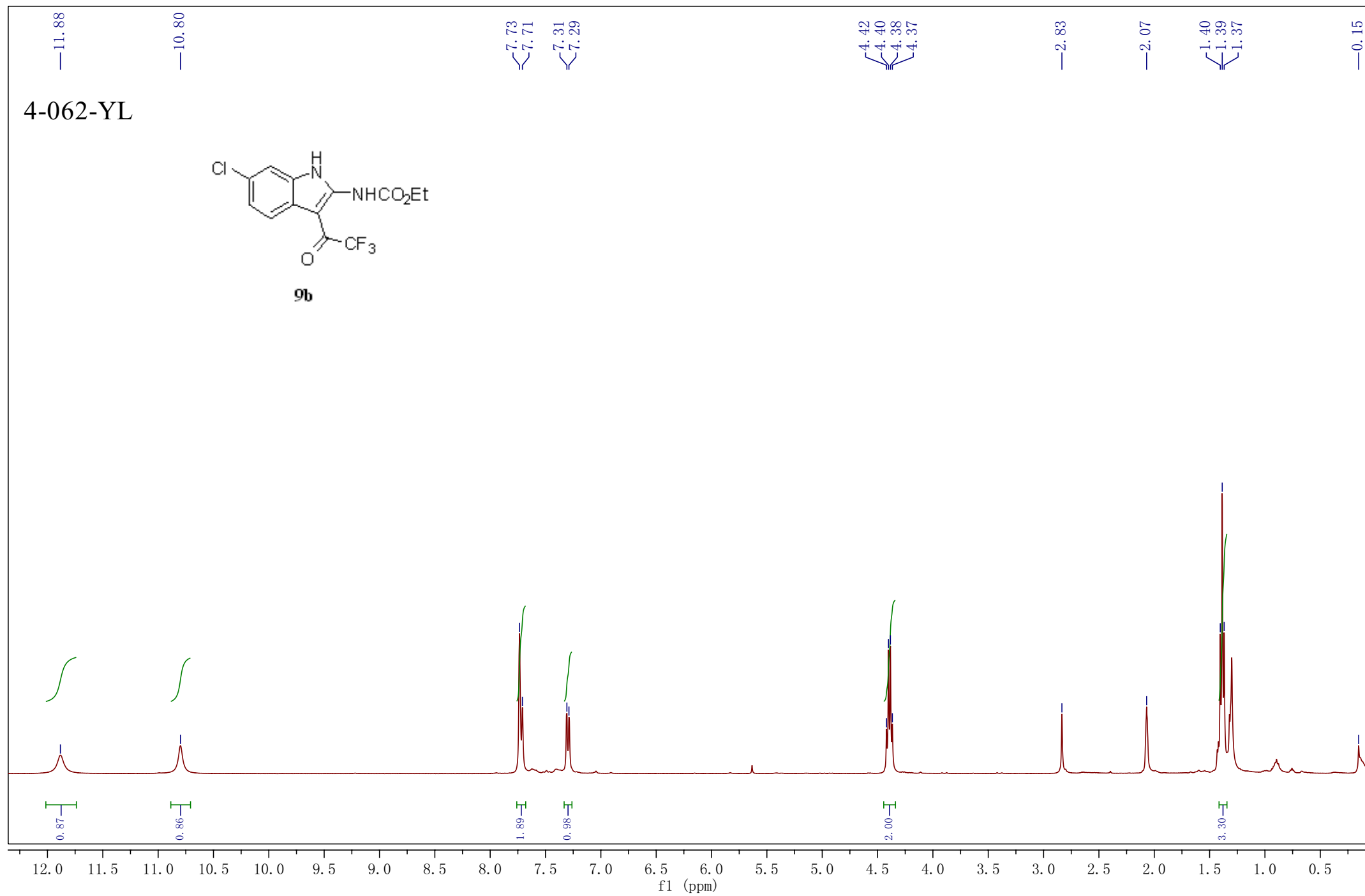
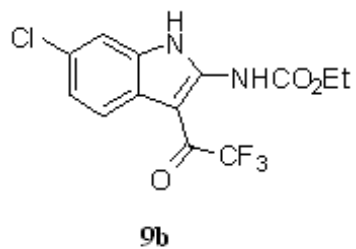
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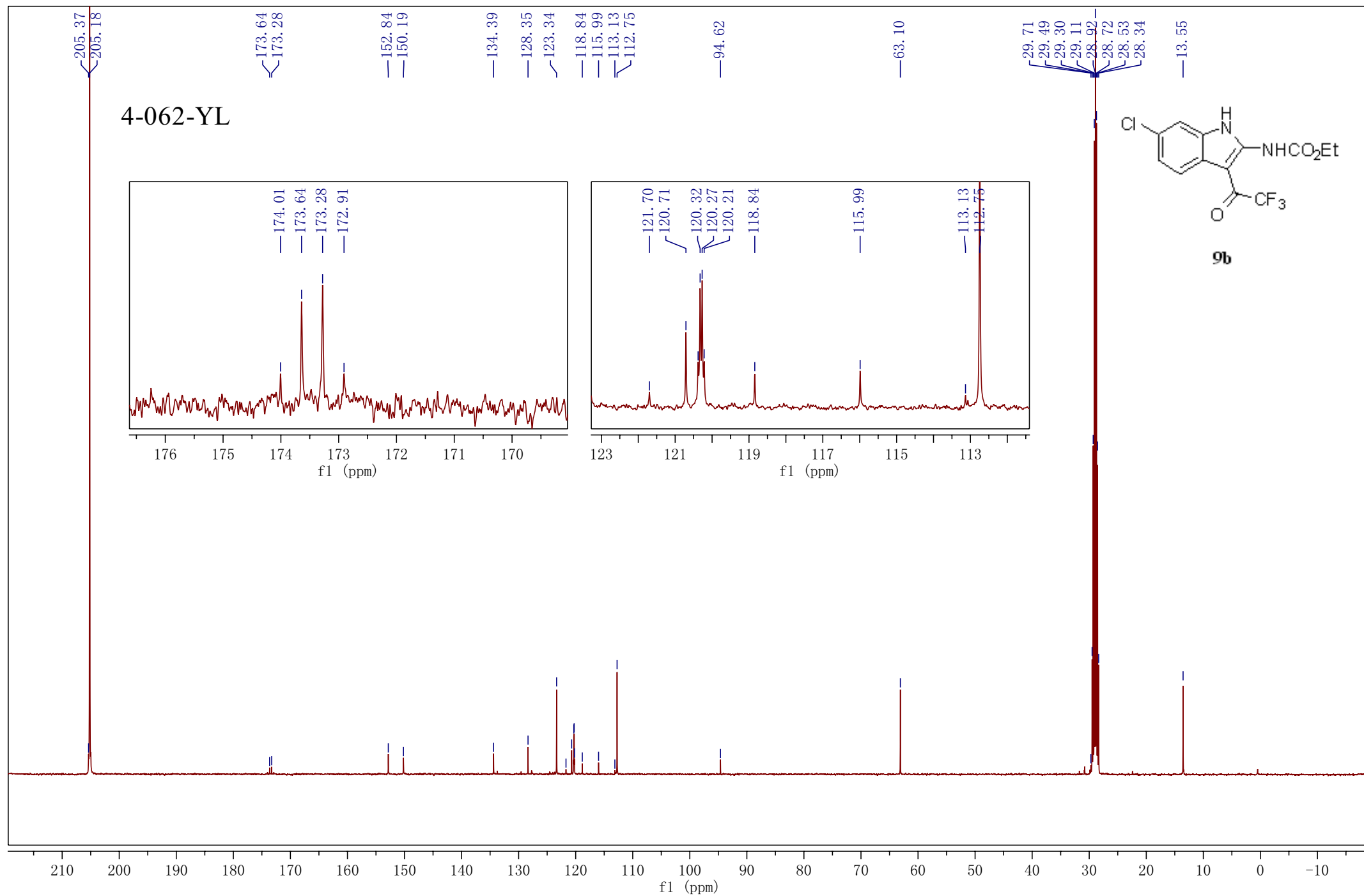
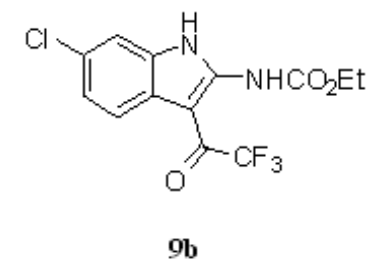


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|-------|----------|---------|--------|--------|----------|
| 1     | 1.026    | 3944    | 807    | 4.888  | 0.0801   |
| 2     | 1.969    | 7398    | 1597   | 4.631  | 0.1502   |
| 3     | 2.563    | 5541    | 551    | 10.062 | 0.1125   |
| 4     | 2.857    | 29397   | 4033   | 7.289  | 0.5968   |
| 5     | 3.403    | 11394   | 903    | 12.622 | 0.2313   |
| 6     | 4.779    | 3178    | 326    | 9.735  | 0.0645   |
| 7     | 6.096    | 4854311 | 439587 | 11.043 | 98.5479  |
| 8     | 6.944    | 10678   | 657    | 16.241 | 0.2168   |
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4-062-YL



4-062-YL



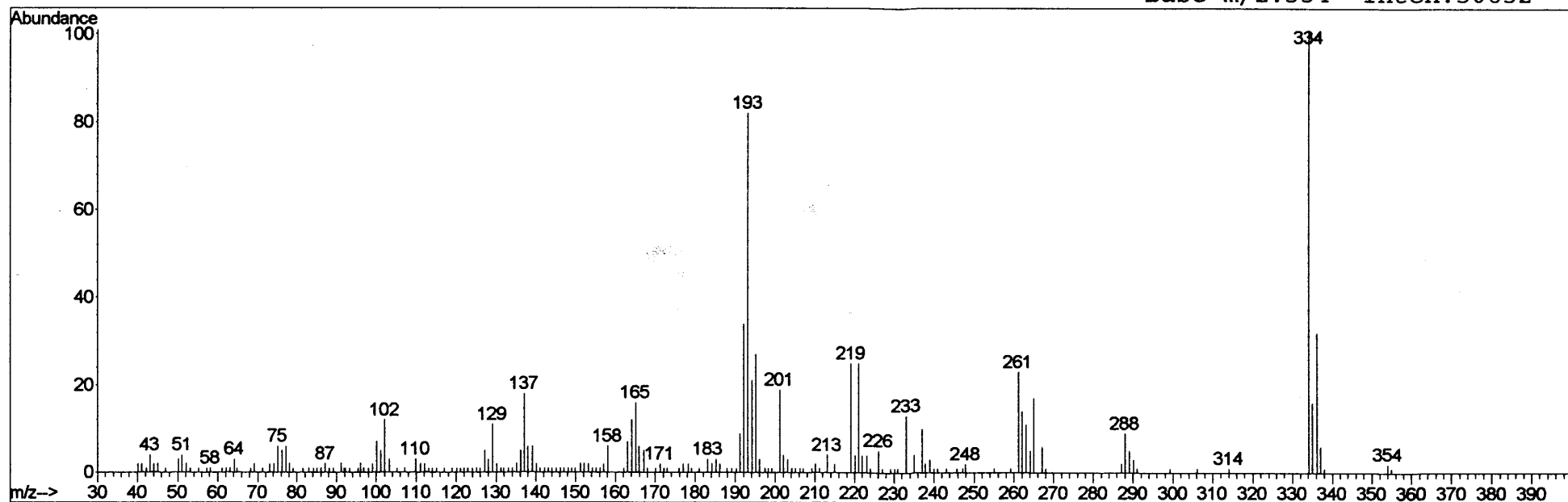
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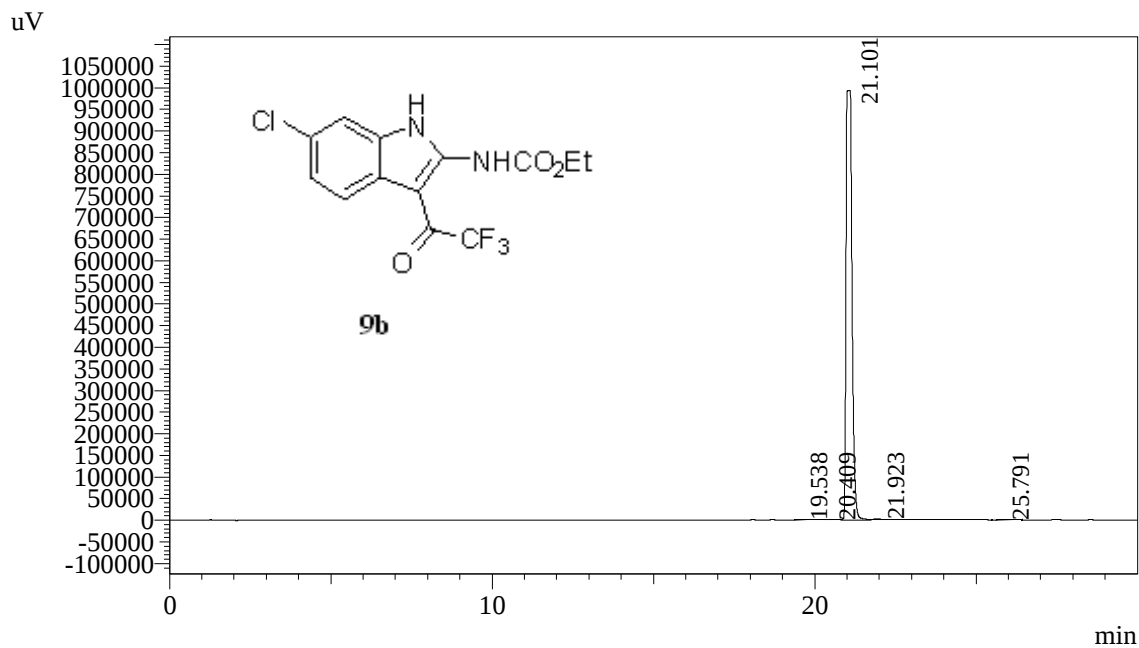
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| 40  | 1.74 | 75  | 5.93  | 103 | 3.29  | 136 | 5.14  | 165 | 15.74 | 194 | 20.88 | 224 | 1.27  |
| 41  | 1.79 | 76  | 4.53  | 105 | 1.48  | 137 | 18.02 | 166 | 5.63  | 195 | 26.52 | 226 | 5.11  |
| 43  | 3.73 | 77  | 5.92  | 110 | 2.72  | 138 | 5.88  | 167 | 4.82  | 196 | 2.86  | 231 | 1.29  |
| 44  | 1.82 | 78  | 1.94  | 111 | 2.00  | 139 | 6.43  | 171 | 1.58  | 201 | 18.66 | 233 | 12.56 |
| 45  | 1.52 | 81  | 1.27  | 112 | 1.61  | 140 | 1.62  | 177 | 1.90  | 202 | 3.62  | 235 | 3.78  |
| 50  | 2.80 | 85  | 1.30  | 113 | 1.25  | 149 | 1.42  | 178 | 1.91  | 203 | 2.55  | 237 | 9.99  |
| 51  | 3.72 | 87  | 1.61  | 114 | 1.47  | 151 | 2.38  | 179 | 1.25  | 210 | 2.34  | 238 | 2.18  |
| 52  | 1.56 | 91  | 2.05  | 115 | 1.38  | 152 | 2.08  | 183 | 3.20  | 213 | 4.40  | 239 | 3.13  |
| 55  | 1.34 | 95  | 1.46  | 125 | 1.44  | 153 | 1.54  | 184 | 1.67  | 215 | 1.77  | 248 | 1.87  |
| 57  | 1.24 | 96  | 2.23  | 127 | 4.53  | 157 | 2.41  | 185 | 3.31  | 219 | 24.36 | 261 | 22.97 |
| 64  | 2.67 | 99  | 1.92  | 128 | 2.88  | 158 | 5.48  | 186 | 2.06  | 220 | 3.71  | 262 | 13.68 |
| 69  | 2.44 | 100 | 6.54  | 129 | 10.92 | 162 | 1.42  | 191 | 8.50  | 221 | 24.54 | 263 | 10.97 |
| 73  | 1.58 | 101 | 4.63  | 130 | 2.35  | 163 | 6.91  | 192 | 33.61 | 222 | 3.65  | 264 | 5.35  |
| 74  | 2.29 | 102 | 11.54 | 135 | 2.28  | 164 | 11.51 | 193 | 80.90 | 223 | 4.06  | 265 | 16.73 |

8 Peak Value:

|     |        |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
|-----|--------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|
| 334 | 100.00 | 193 | 80.90 | 192 | 33.61 | 336 | 31.38 | 195 | 26.52 | 221 | 24.54 | 219 | 24.36 | 261 | 22.97 |
|-----|--------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|

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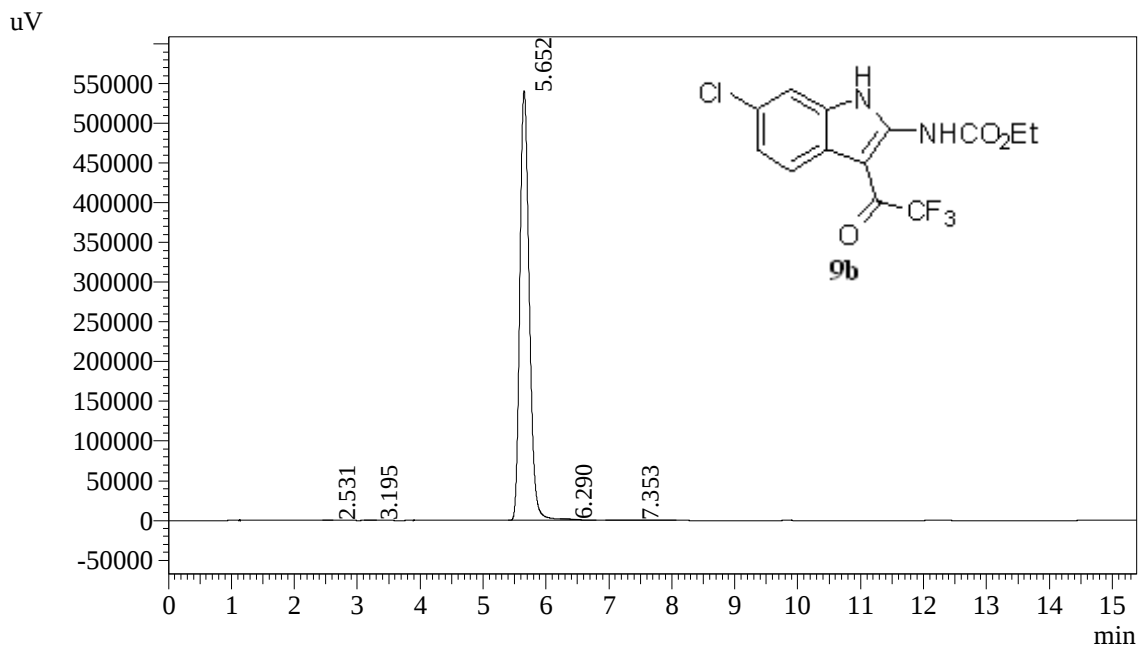
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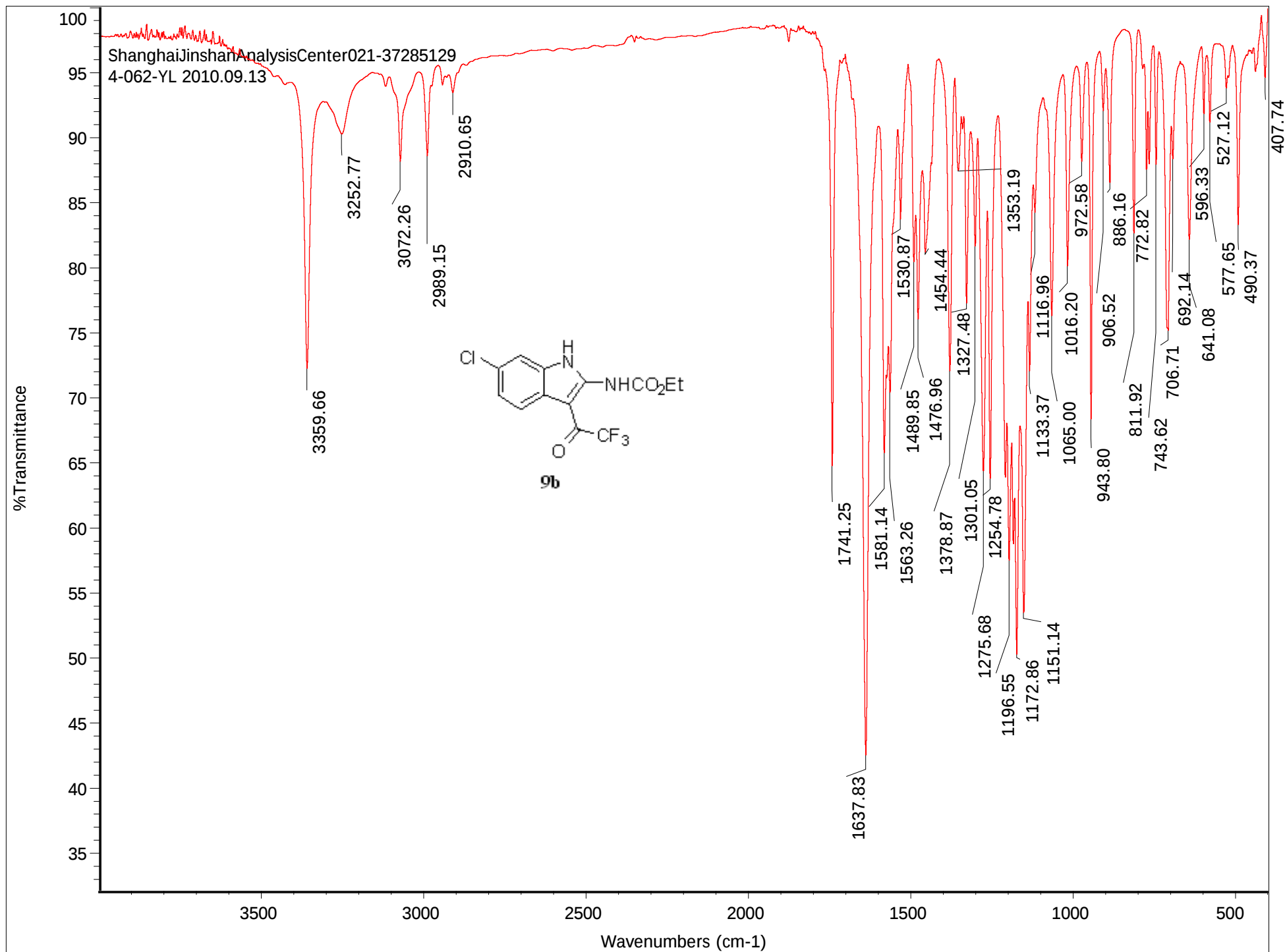
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| 2     | 20.409   | 3357     | 398    | 8.434  | 0.0263   |
| 3     | 21.101   | 12732347 | 992920 | 12.823 | 99.7522  |
| 4     | 21.923   | 19522    | 1742   | 11.206 | 0.1529   |
| 5     | 25.791   | 6211     | 486    | 12.779 | 0.0487   |
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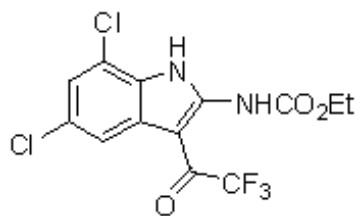
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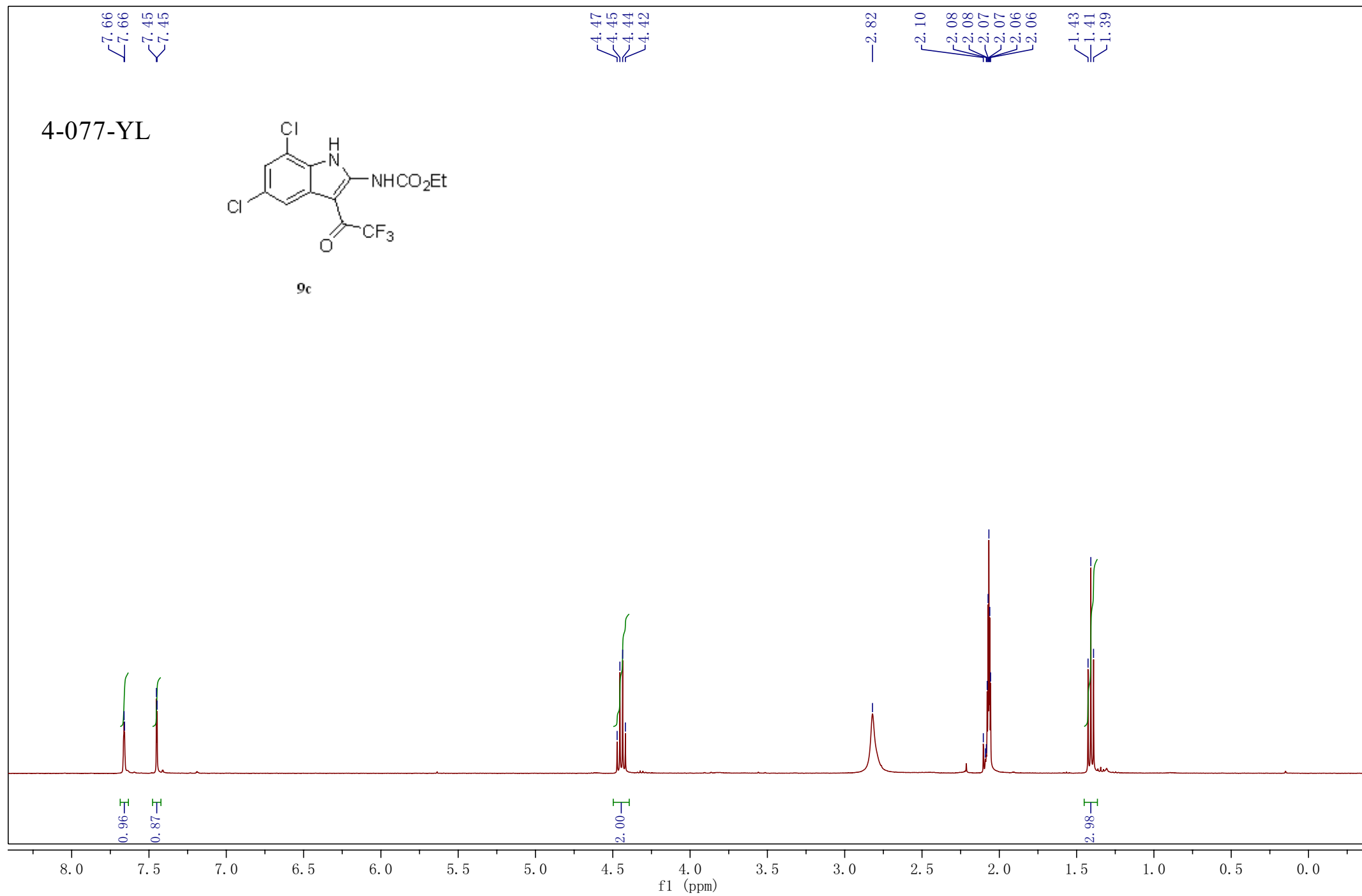
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| 1     | 2.531    | 1185    | 238    | 4.968  | 0.0210   |
| 2     | 3.195    | 1567    | 272    | 5.757  | 0.0277   |
| 3     | 5.652    | 5638372 | 540633 | 10.429 | 99.7972  |
| 4     | 6.290    | 1886    | 225    | 8.403  | 0.0334   |
| 5     | 7.353    | 6817    | 203    | 33.621 | 0.1207   |
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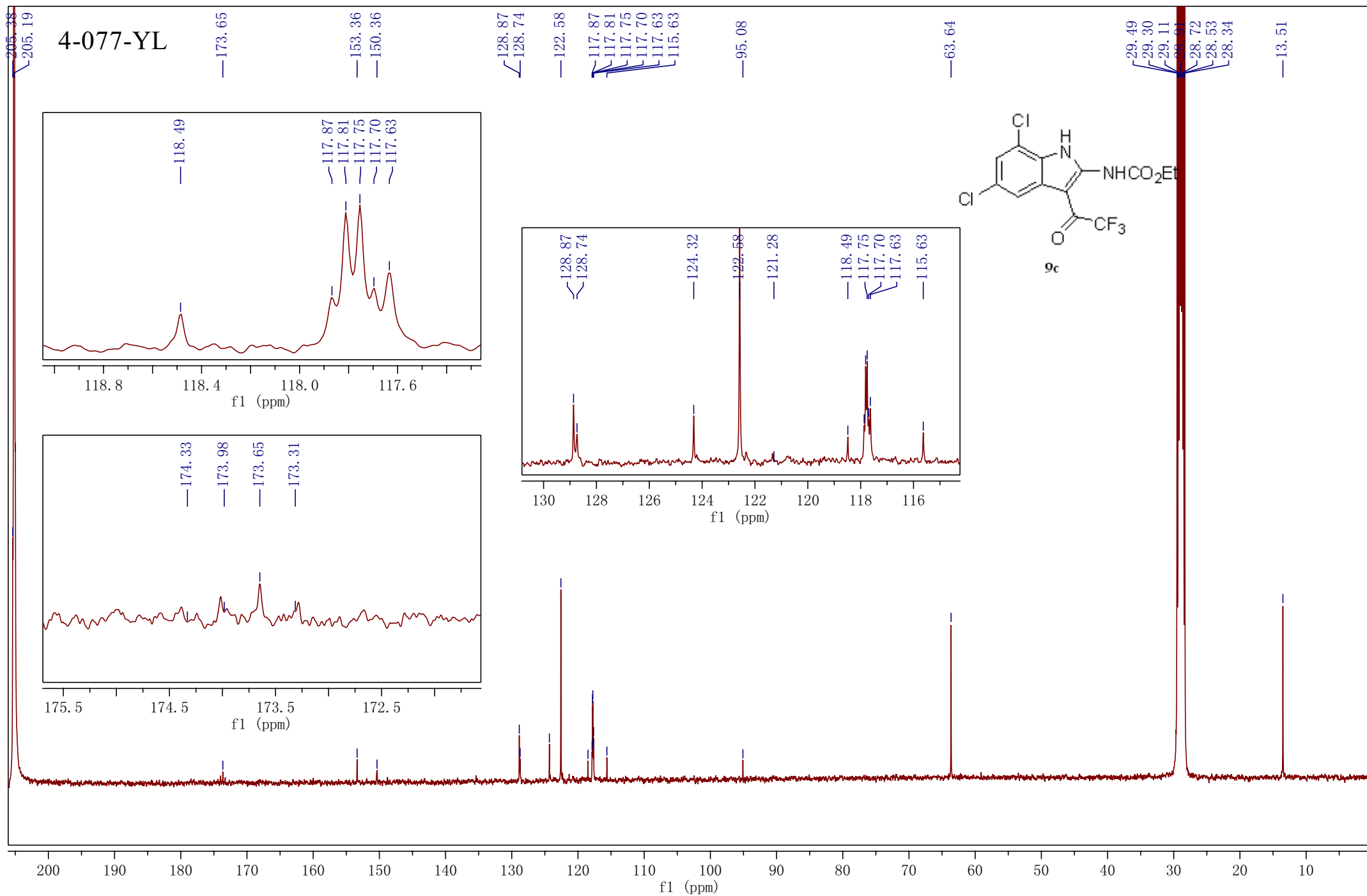


4-077-YL



9c



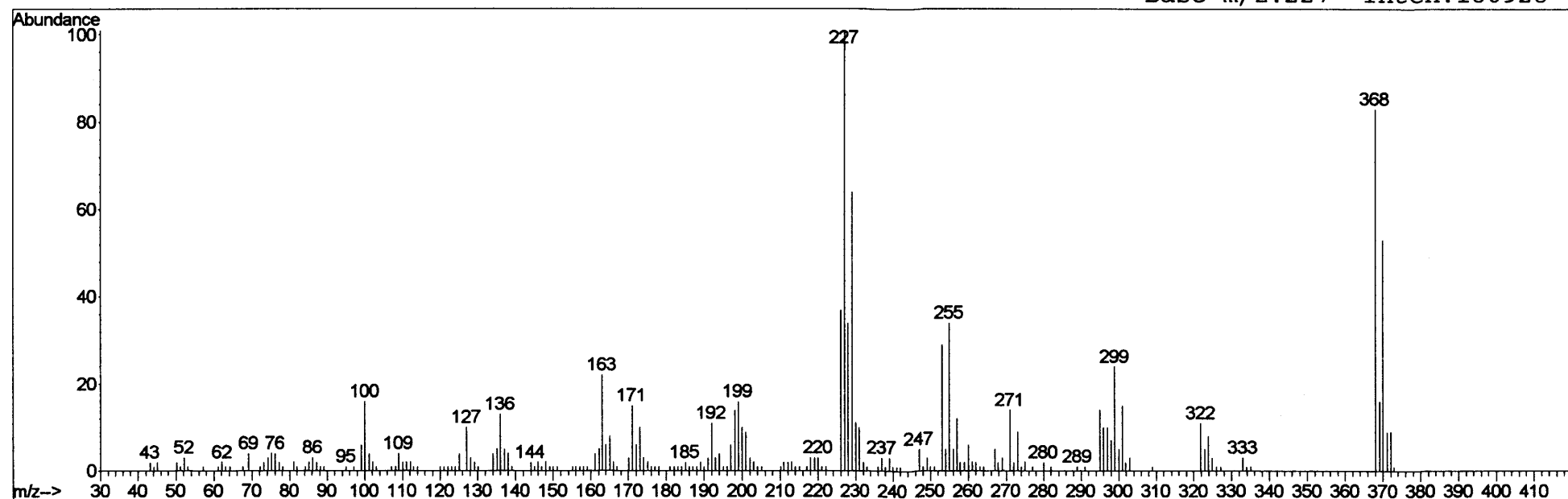


4-OTF-YL

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b

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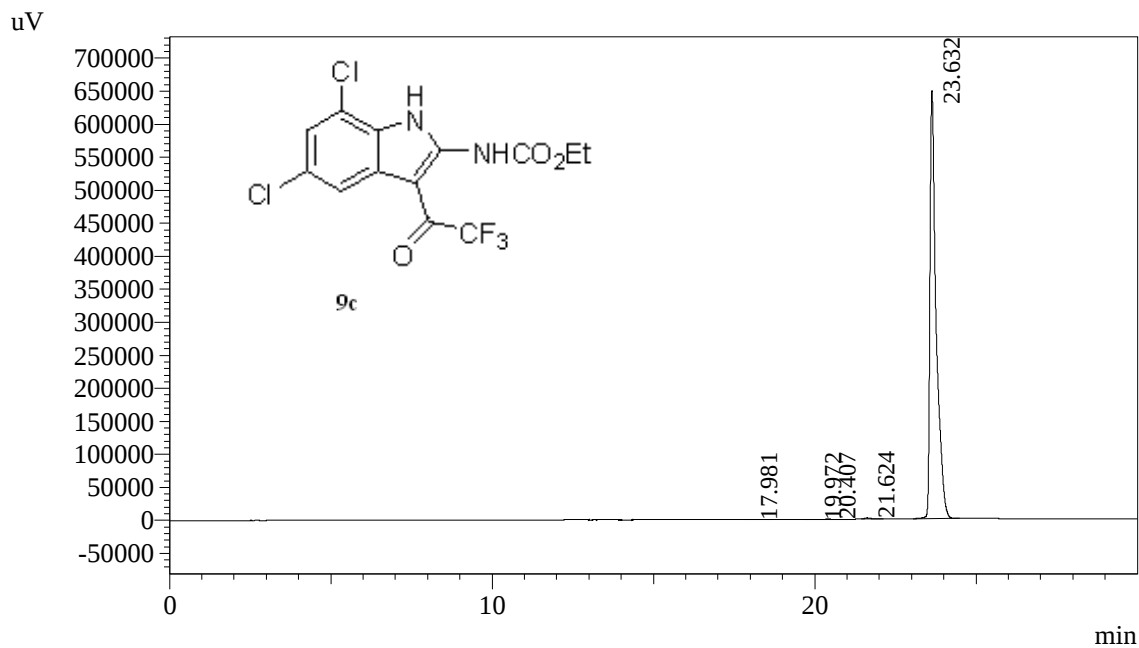
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| 43  | 2.16 | 100 | 15.76 | 137 | 5.20  | 174 | 3.10  | 211 | 2.25   | 247 | 4.91  | 269 | 3.27  | 303 | 2.49  |
| 50  | 1.80 | 101 | 4.26  | 138 | 4.12  | 175 | 2.13  | 213 | 2.15   | 249 | 3.19  | 271 | 13.85 | 322 | 10.82 |
| 52  | 2.58 | 102 | 1.87  | 144 | 2.07  | 189 | 1.70  | 218 | 3.38   | 253 | 29.04 | 272 | 2.30  | 323 | 5.21  |
| 62  | 1.71 | 109 | 3.86  | 148 | 1.87  | 191 | 3.43  | 219 | 2.83   | 254 | 5.29  | 273 | 8.49  | 324 | 7.62  |
| 69  | 3.75 | 110 | 2.19  | 161 | 4.14  | 192 | 11.18 | 220 | 3.38   | 255 | 33.25 | 275 | 2.25  | 325 | 3.04  |
| 74  | 3.03 | 111 | 2.41  | 162 | 4.72  | 193 | 2.51  | 226 | 37.06  | 256 | 4.79  | 280 | 2.04  | 333 | 3.35  |
| 75  | 3.85 | 112 | 2.13  | 163 | 22.07 | 194 | 3.56  | 227 | 100.00 | 257 | 12.21 | 295 | 13.93 | 368 | 81.89 |
| 76  | 4.32 | 125 | 3.70  | 164 | 5.45  | 197 | 5.64  | 228 | 33.45  | 258 | 1.89  | 296 | 9.84  | 369 | 15.58 |
| 77  | 2.12 | 127 | 10.21 | 165 | 7.44  | 198 | 13.67 | 229 | 63.12  | 259 | 1.94  | 297 | 10.00 | 370 | 52.13 |
| 81  | 1.80 | 128 | 3.42  | 166 | 1.77  | 199 | 15.42 | 230 | 10.62  | 260 | 6.29  | 298 | 6.64  | 371 | 8.74  |
| 85  | 2.15 | 129 | 2.01  | 170 | 3.17  | 200 | 10.23 | 231 | 10.16  | 261 | 1.82  | 299 | 23.69 | 372 | 8.74  |
| 86  | 2.73 | 134 | 4.34  | 171 | 14.78 | 201 | 8.64  | 232 | 1.86   | 262 | 2.19  | 300 | 4.55  |     |       |
| 87  | 1.78 | 135 | 5.20  | 172 | 5.64  | 202 | 3.04  | 237 | 3.36   | 267 | 5.03  | 301 | 14.52 |     |       |
| 99  | 5.47 | 136 | 13.03 | 173 | 9.94  | 203 | 1.76  | 239 | 2.49   | 268 | 2.46  | 302 | 2.09  |     |       |

8 Peak Value:

|     |        |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
|-----|--------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|
| 227 | 100.00 | 368 | 81.89 | 229 | 63.12 | 370 | 52.13 | 226 | 37.06 | 228 | 33.45 | 255 | 33.25 | 253 | 29.04 |
|-----|--------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|

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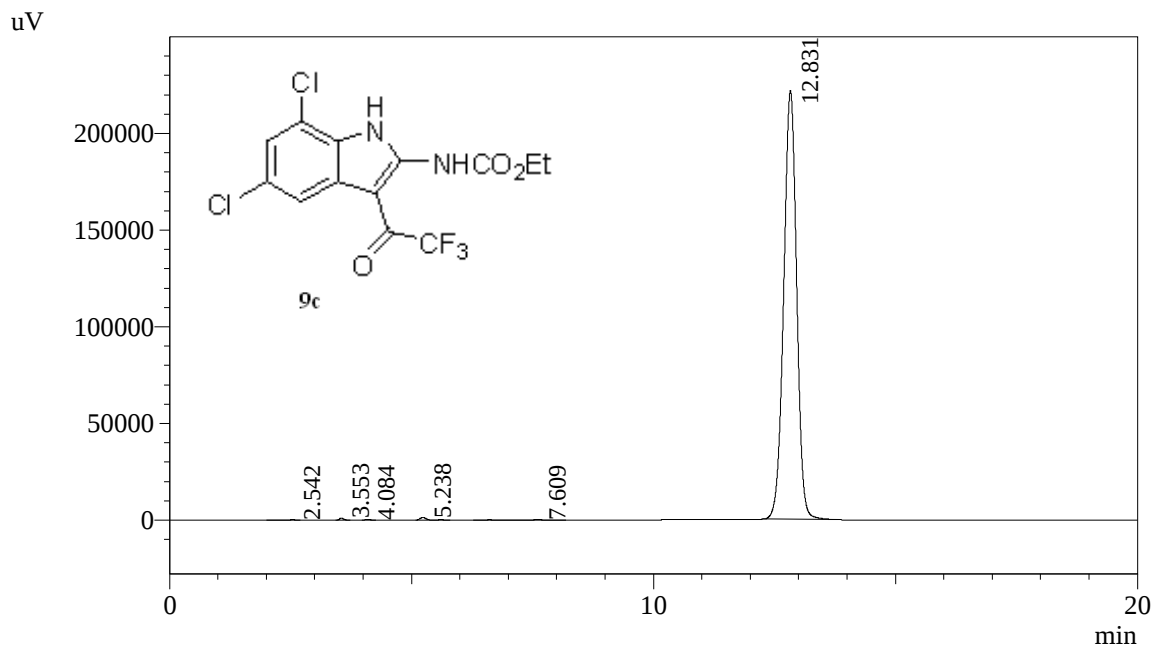
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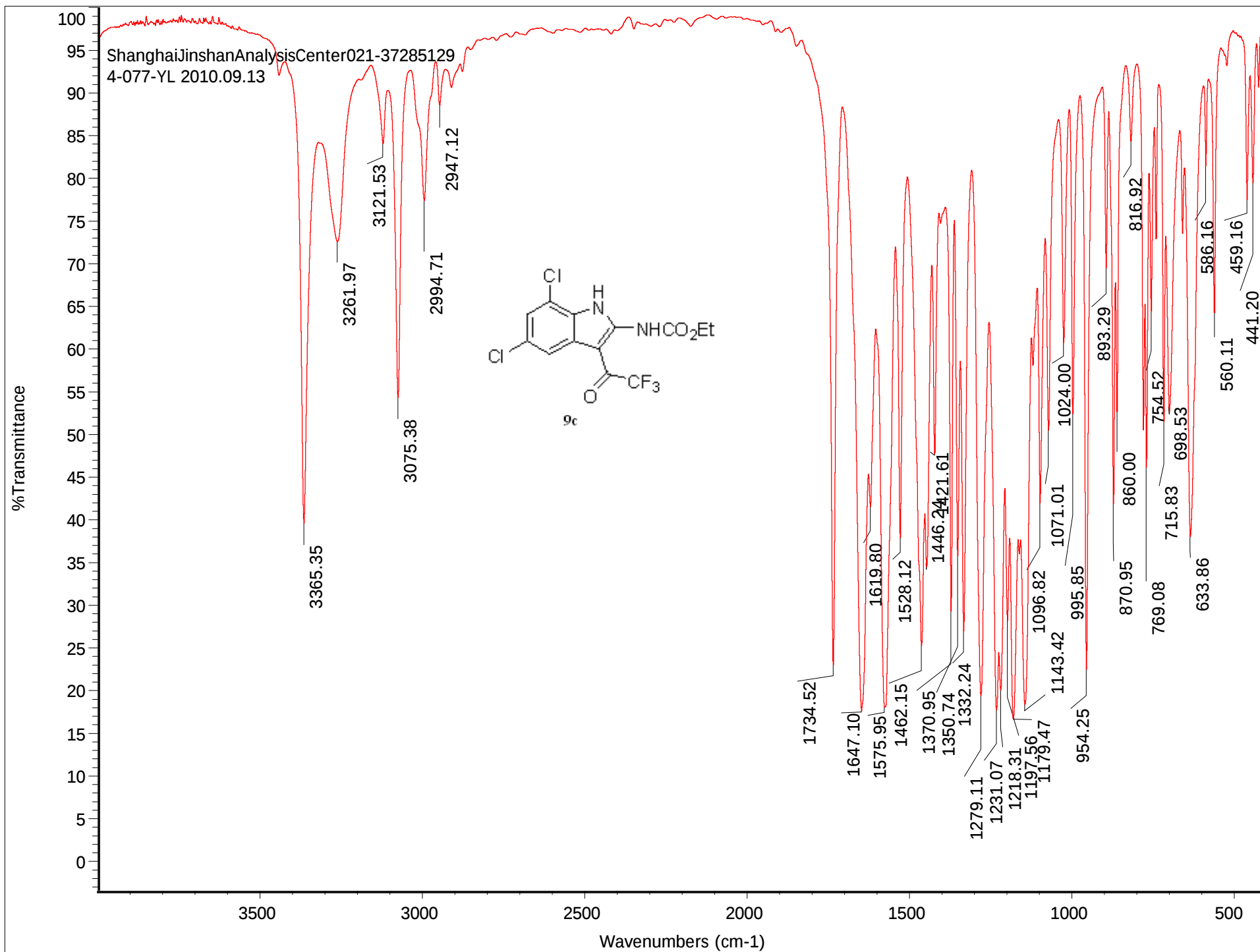
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| 2     | 19.972   | 2439    | 210    | 11.611 | 0.0278   |
| 3     | 20.407   | 11868   | 751    | 15.792 | 0.1350   |
| 4     | 21.624   | 27485   | 1959   | 14.030 | 0.3127   |
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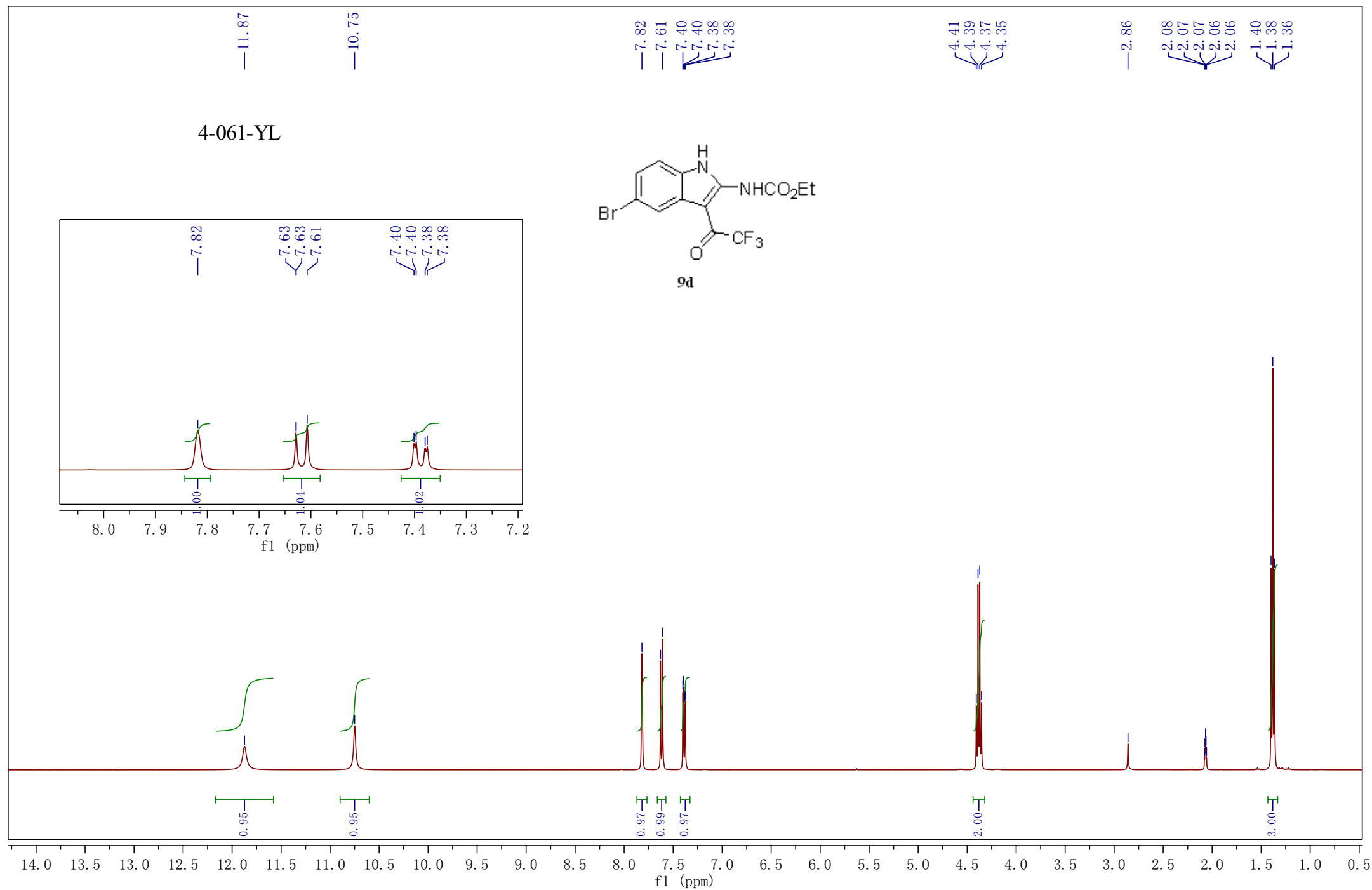
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 Sample Name : 4-077-YL  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6206.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/09 15:31:01

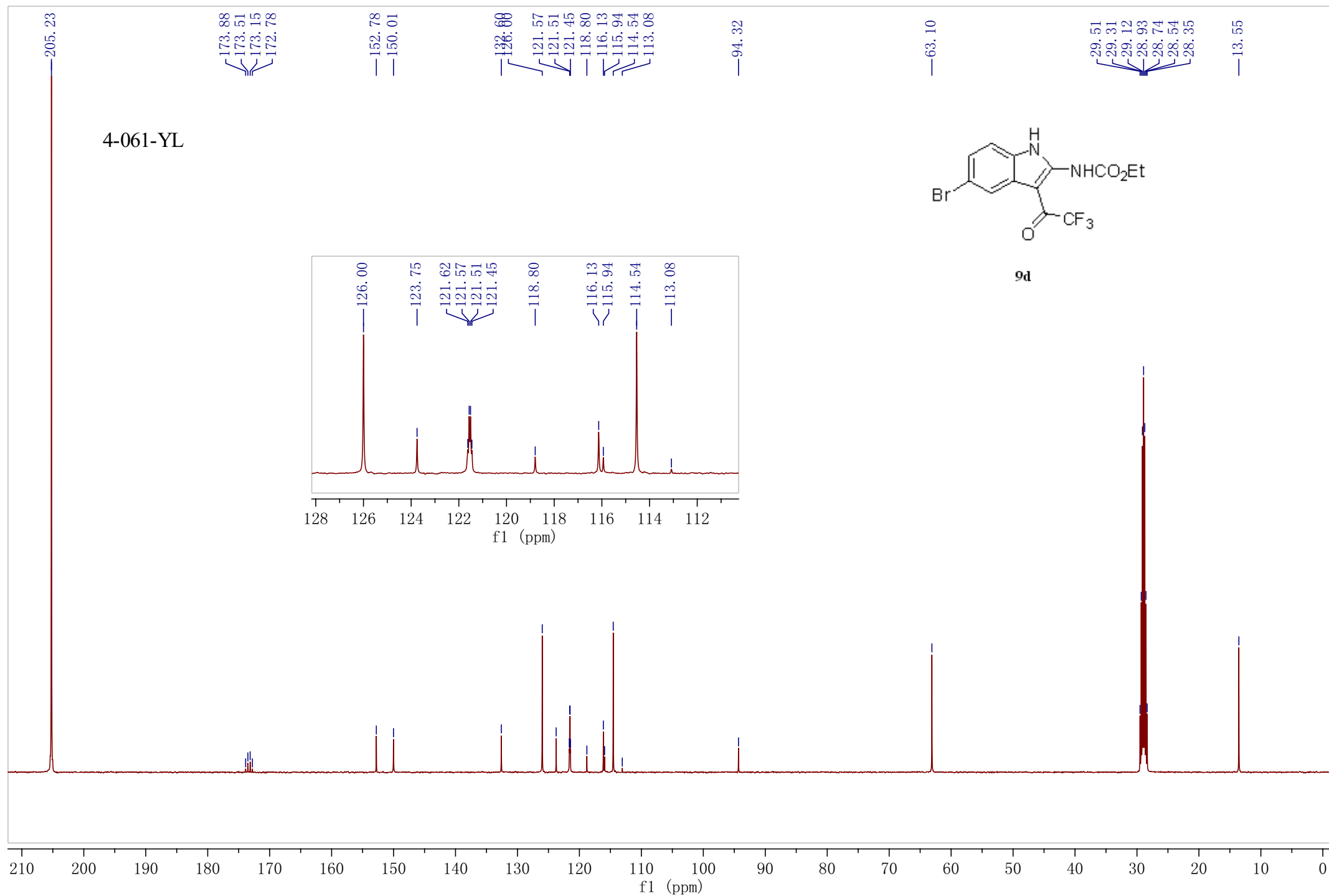
# HPLC



| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 2.542    | 2679    | 413    | 6.489  | 0.0644   |
| 2     | 3.553    | 6738    | 1065   | 6.325  | 0.1619   |
| 3     | 4.084    | 2832    | 308    | 9.196  | 0.0681   |
| 4     | 5.238    | 14897   | 1356   | 10.985 | 0.3580   |
| 5     | 7.609    | 6375    | 278    | 22.910 | 0.1532   |
| 6     | 12.831   | 4128104 | 221572 | 18.631 | 99.1945  |
| 全部    |          | 4161625 | 224992 |        | 100.0000 |





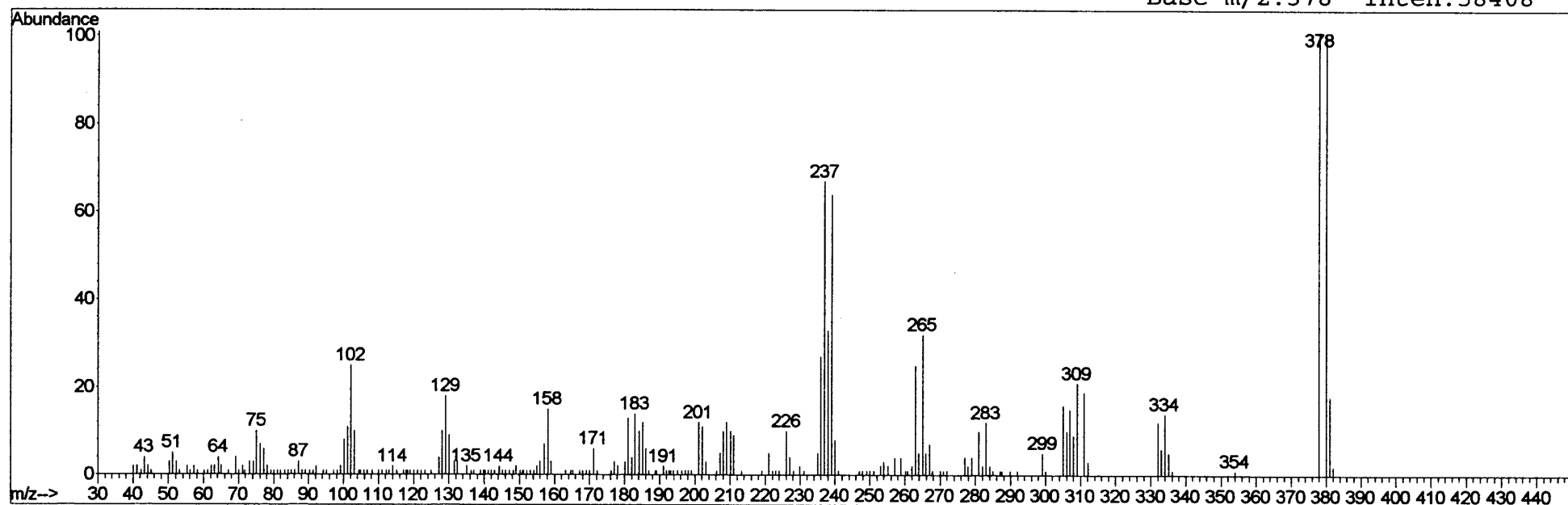


4-061-YL

File : C:\MSDCHEM\1\DATA\Snapshot\09010927.D #231(2.039 min)  
Acquired : 9 Jan 2009 4:35 pm  
Sample Name : 494087  
Misc Info : Agilent 5973N MSD EI 70eV  
Shanghai Institute of Organic Chemistry

李海泉

Base m/z:378 Inten:58408



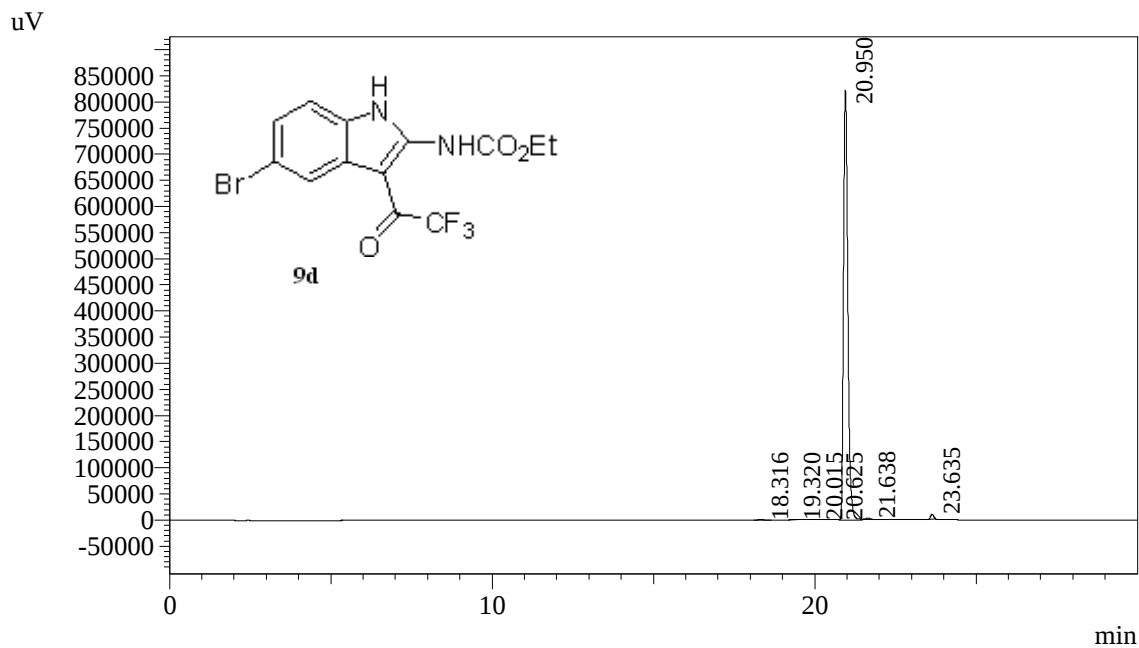
| m/z | %RA  | m/z | %RA   | m/z | %RA   | m/z | %RA   | m/z | %RA   | m/z | %RA   | m/z | %RA   |
|-----|------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|
| 40  | 1.79 | 69  | 3.64  | 102 | 24.52 | 156 | 2.54  | 191 | 2.06  | 236 | 26.71 | 266 | 4.67  |
| 41  | 2.14 | 71  | 1.59  | 103 | 9.99  | 157 | 6.44  | 201 | 11.88 | 237 | 66.66 | 267 | 7.32  |
| 43  | 4.45 | 73  | 2.54  | 104 | 1.44  | 158 | 15.07 | 202 | 10.83 | 238 | 32.43 | 268 | 1.43  |
| 44  | 1.75 | 74  | 3.43  | 114 | 1.99  | 159 | 2.56  | 203 | 2.64  | 239 | 63.85 | 277 | 4.00  |
| 50  | 3.06 | 75  | 10.10 | 127 | 4.28  | 171 | 5.47  | 207 | 4.50  | 240 | 7.43  | 278 | 2.44  |
| 51  | 4.78 | 76  | 6.68  | 128 | 9.48  | 177 | 2.70  | 208 | 9.95  | 253 | 1.77  | 279 | 3.55  |
| 52  | 2.64 | 77  | 5.50  | 129 | 17.86 | 178 | 1.80  | 209 | 11.97 | 254 | 2.78  | 281 | 9.51  |
| 55  | 2.17 | 78  | 2.14  | 130 | 8.62  | 180 | 3.16  | 210 | 10.10 | 255 | 2.16  | 282 | 1.79  |
| 57  | 1.90 | 79  | 1.43  | 131 | 3.10  | 181 | 12.69 | 211 | 8.79  | 257 | 4.34  | 283 | 11.61 |
| 61  | 1.46 | 87  | 2.96  | 132 | 2.82  | 182 | 4.17  | 221 | 4.48  | 259 | 3.72  | 284 | 1.94  |
| 62  | 1.82 | 92  | 1.80  | 135 | 1.80  | 183 | 13.60 | 226 | 10.24 | 262 | 1.83  | 299 | 5.00  |
| 63  | 1.80 | 99  | 2.35  | 144 | 1.89  | 184 | 10.24 | 227 | 4.18  | 263 | 24.37 | 305 | 15.99 |
| 64  | 4.22 | 100 | 7.89  | 149 | 1.57  | 185 | 12.30 | 230 | 2.25  | 264 | 4.71  | 306 | 9.43  |
| 65  | 1.94 | 101 | 10.65 | 155 | 1.88  | 186 | 5.55  | 235 | 4.50  | 265 | 31.71 | 307 | 14.93 |

8 Peak Value:

|     |        |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
|-----|--------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|
| 378 | 100.00 | 380 | 99.36 | 237 | 66.66 | 239 | 63.85 | 238 | 32.43 | 265 | 31.71 | 236 | 26.71 | 102 | 24.52 |
|-----|--------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|

User Name : CJK  
 Sample ID :  
 Sample Name : 4-061-YL  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6200.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/09 13:15:23

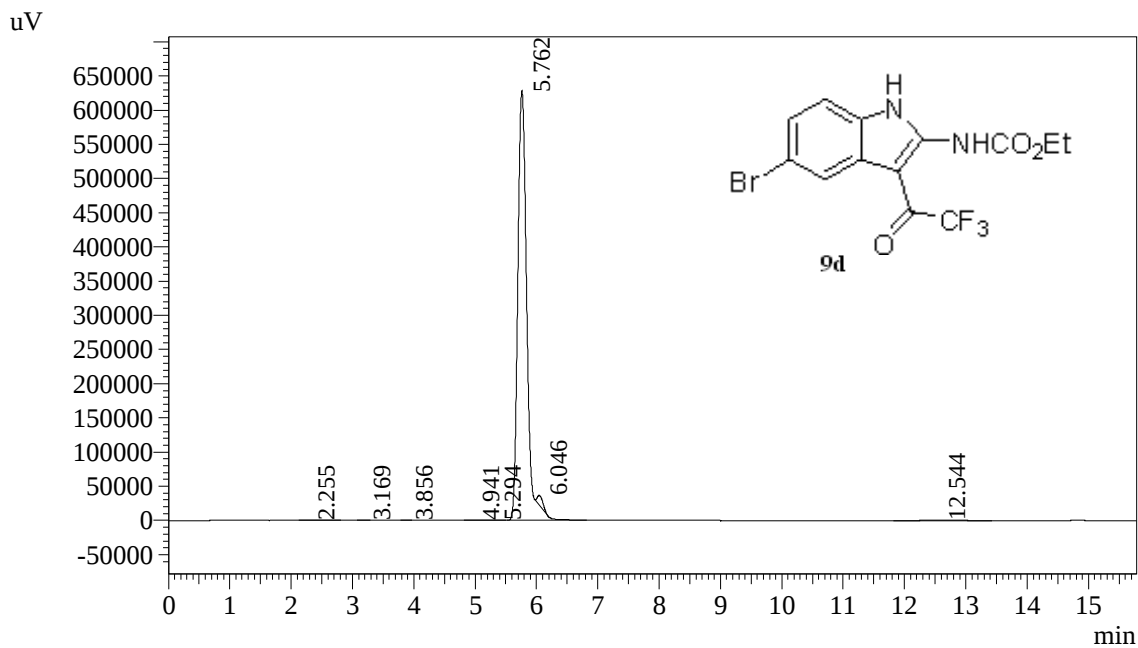
# HPLC



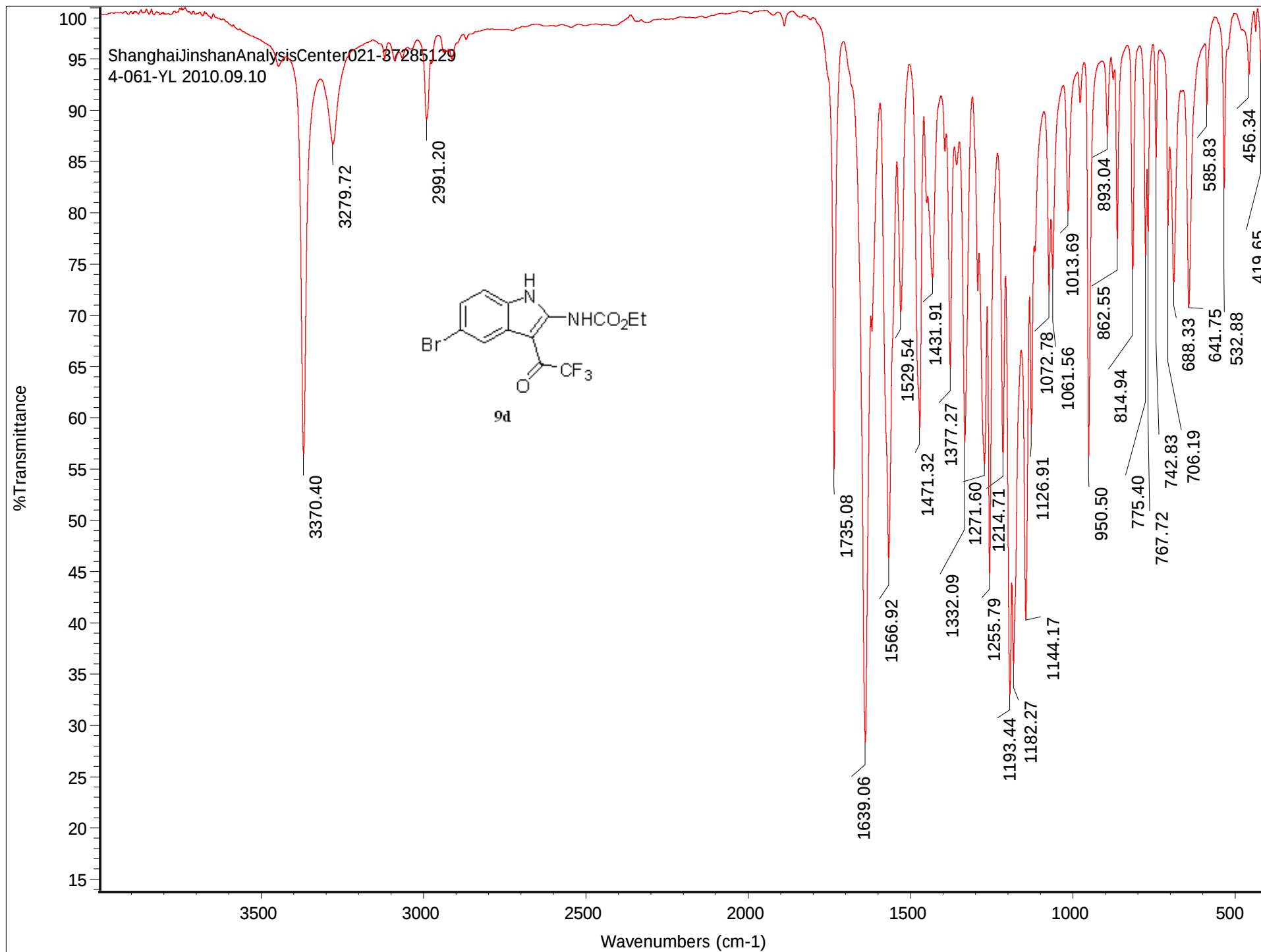
| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 18.316   | 3816    | 329    | 11.608 | 0.0494   |
| 2     | 19.320   | 3334    | 358    | 9.309  | 0.0432   |
| 3     | 20.015   | 2002    | 204    | 9.819  | 0.0259   |
| 4     | 20.625   | 4956    | 427    | 11.616 | 0.0642   |
| 5     | 20.950   | 7618805 | 820269 | 9.288  | 98.6981  |
| 6     | 21.638   | 22015   | 1981   | 11.112 | 0.2852   |
| 7     | 23.635   | 64375   | 9658   | 6.666  | 0.8340   |
| 全部    |          | 7719303 | 833226 |        | 100.0000 |

User Name : CJK  
 Sample ID :  
 Sample Name : 4-061-YL  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6207.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/09 15:54:49

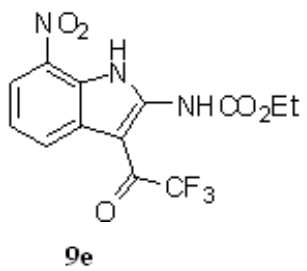
# HPLC



| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 2.255    | 2700    | 273    | 9.875  | 0.0413   |
| 2     | 3.169    | 1358    | 231    | 5.886  | 0.0208   |
| 3     | 3.856    | 987     | 182    | 5.433  | 0.0151   |
| 4     | 4.941    | 2938    | 373    | 7.882  | 0.0450   |
| 5     | 5.294    | 5963    | 517    | 11.525 | 0.0913   |
| 6     | 5.762    | 6417475 | 627939 | 10.220 | 98.2497  |
| 7     | 6.046    | 89901   | 13885  | 6.475  | 1.3764   |
| 8     | 12.544   | 10484   | 306    | 34.299 | 0.1605   |
| 全部    |          | 6531806 | 643706 |        | 100.0000 |



4-078-YL



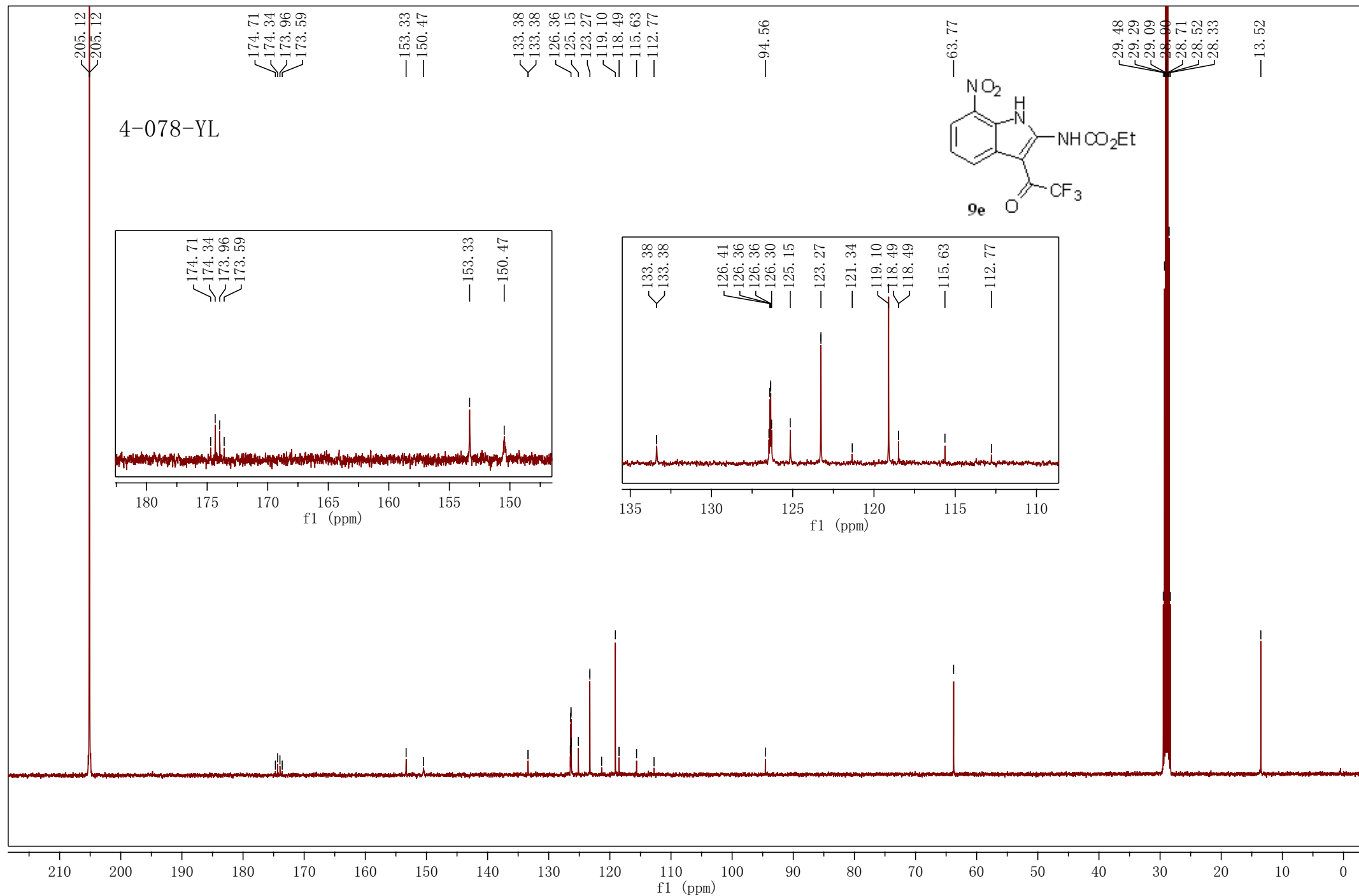
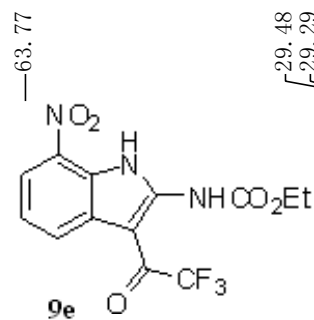
12.26  
10.67  
8.18  
8.15  
8.13  
7.43  
7.40  
7.37  
7.27  
4.46  
4.44  
4.42  
4.39  
1.61  
1.45  
1.42  
1.40  
1.25  
0.88  
0.07  
0.00

0.67  
0.86  
1.91  
1.02  
2.00  
3.10

14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1

f1 (ppm)

4-078-YL

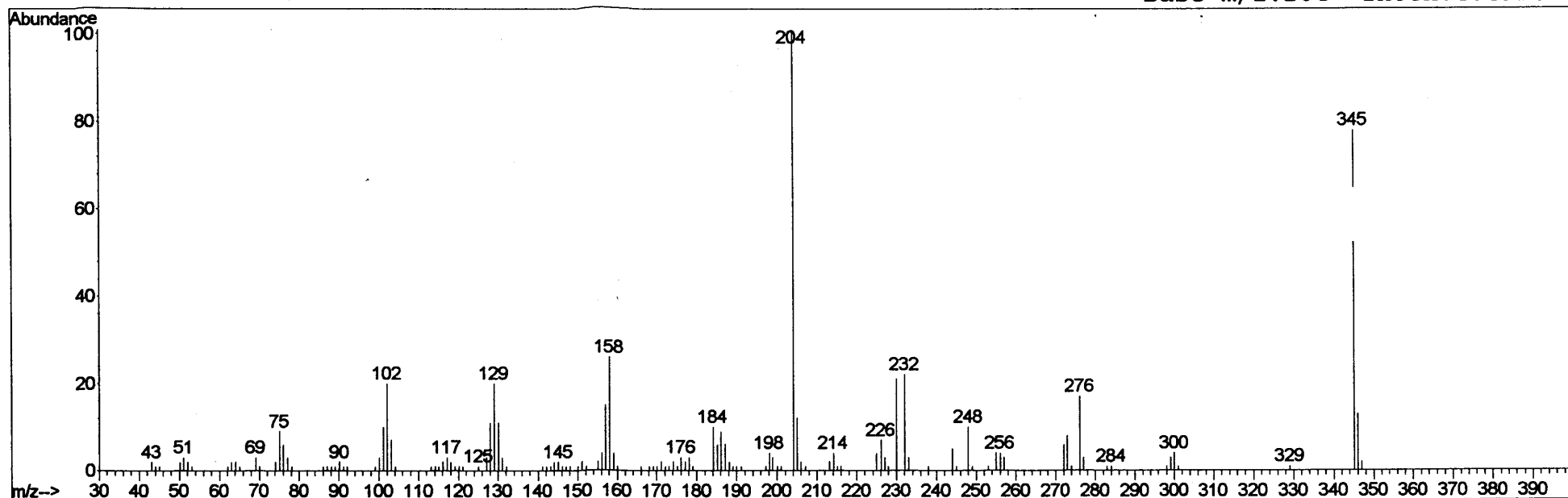


4078-YL

File : C:\MSDCHEM\1\DATA\Snapshot\09060228.D #193 (1.716 min)  
Acquired : 2 Jun 2009 4:39 pm  
Sample Name : 4941611 MW.345  
Misc Info : Agilent 5973N MSD EI 70eV  
Shanghai Institute of Organic Chemistry

芳  
星  
⑥

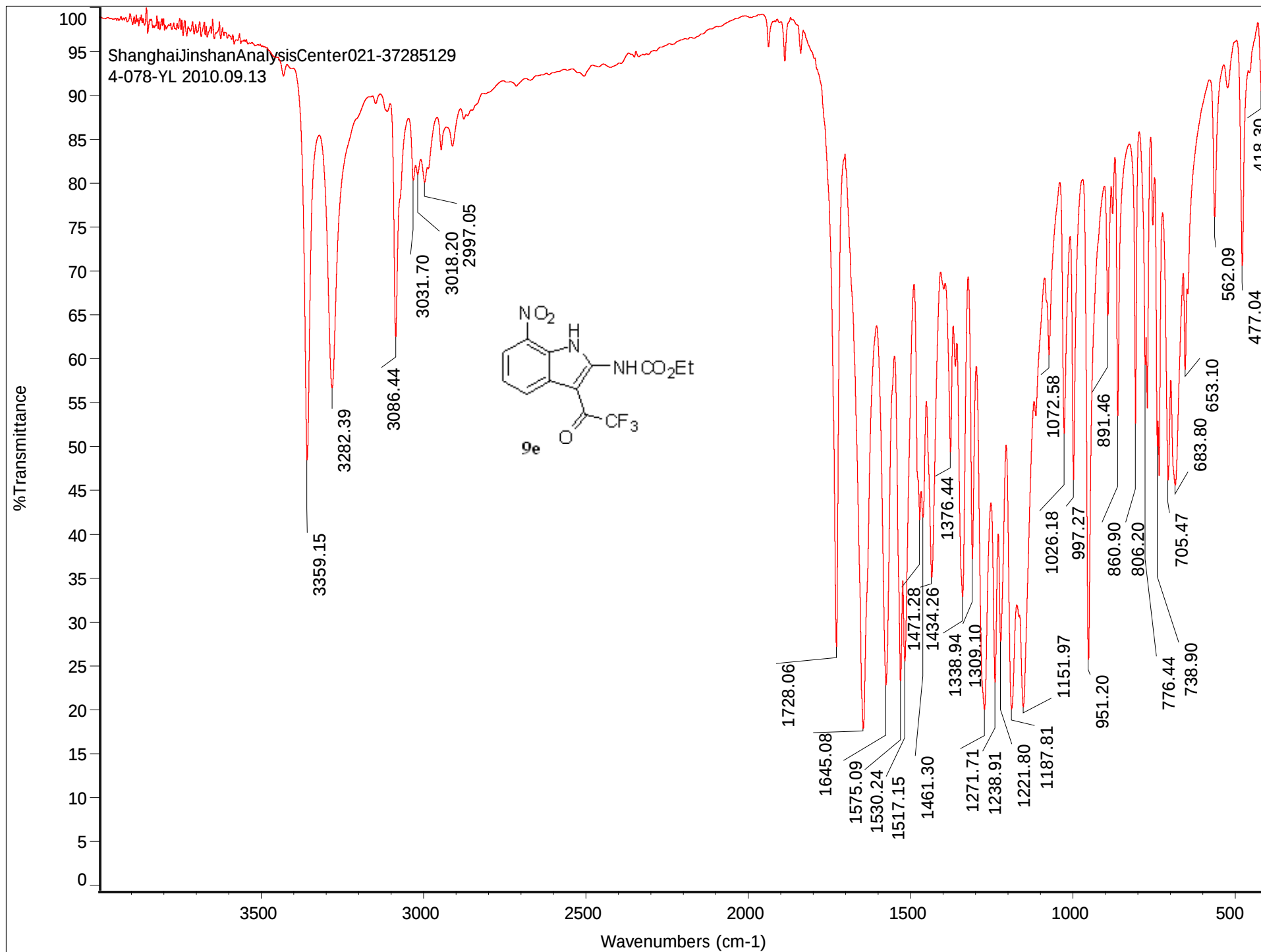
Base m/z:204 Inten:404928



| m/z | %RA  | m/z | %RA   | m/z | %RA   | m/z | %RA   | m/z | %RA   | m/z | %RA    | m/z | %RA   | m/z | %RA   |
|-----|------|-----|-------|-----|-------|-----|-------|-----|-------|-----|--------|-----|-------|-----|-------|
| 43  | 1.64 | 76  | 6.34  | 104 | 1.22  | 141 | 0.75  | 158 | 25.88 | 186 | 8.56   | 215 | 1.19  | 256 | 3.89  |
| 44  | 1.24 | 77  | 2.87  | 114 | 0.91  | 142 | 1.04  | 159 | 3.48  | 187 | 5.76   | 216 | 0.72  | 257 | 3.30  |
| 45  | 1.10 | 78  | 1.15  | 115 | 1.43  | 143 | 1.04  | 168 | 0.78  | 188 | 2.35   | 225 | 3.92  | 272 | 5.76  |
| 50  | 2.19 | 87  | 1.29  | 116 | 1.62  | 144 | 1.74  | 170 | 1.31  | 191 | 0.84   | 226 | 6.61  | 273 | 8.17  |
| 51  | 2.59 | 88  | 1.42  | 117 | 2.53  | 145 | 1.79  | 171 | 1.95  | 197 | 0.95   | 227 | 3.24  | 274 | 1.22  |
| 52  | 2.46 | 89  | 1.23  | 118 | 1.63  | 146 | 0.88  | 172 | 0.93  | 198 | 4.25   | 228 | 0.75  | 276 | 17.32 |
| 53  | 0.82 | 90  | 2.04  | 121 | 0.76  | 147 | 0.71  | 173 | 1.27  | 199 | 3.03   | 230 | 21.04 | 277 | 2.79  |
| 62  | 0.97 | 91  | 0.88  | 125 | 0.78  | 148 | 0.92  | 174 | 1.66  | 200 | 1.11   | 232 | 22.01 | 298 | 0.97  |
| 63  | 1.49 | 92  | 0.71  | 127 | 3.37  | 150 | 0.82  | 175 | 1.06  | 201 | 0.73   | 233 | 3.07  | 299 | 3.42  |
| 64  | 2.06 | 99  | 0.95  | 128 | 10.87 | 151 | 2.06  | 176 | 2.59  | 204 | 100.00 | 238 | 0.89  | 300 | 3.63  |
| 65  | 0.76 | 100 | 3.19  | 129 | 20.02 | 152 | 1.09  | 177 | 1.77  | 205 | 11.83  | 244 | 5.06  | 329 | 1.10  |
| 69  | 3.02 | 101 | 10.02 | 130 | 10.99 | 155 | 2.12  | 178 | 2.48  | 206 | 1.88   | 248 | 10.24 | 345 | 76.94 |
| 74  | 1.77 | 102 | 19.76 | 131 | 3.25  | 156 | 3.77  | 184 | 9.47  | 213 | 1.83   | 249 | 1.31  | 346 | 13.10 |
| 75  | 9.12 | 103 | 6.99  | 132 | 1.12  | 157 | 15.10 | 185 | 5.87  | 214 | 3.51   | 255 | 3.74  | 347 | 1.84  |

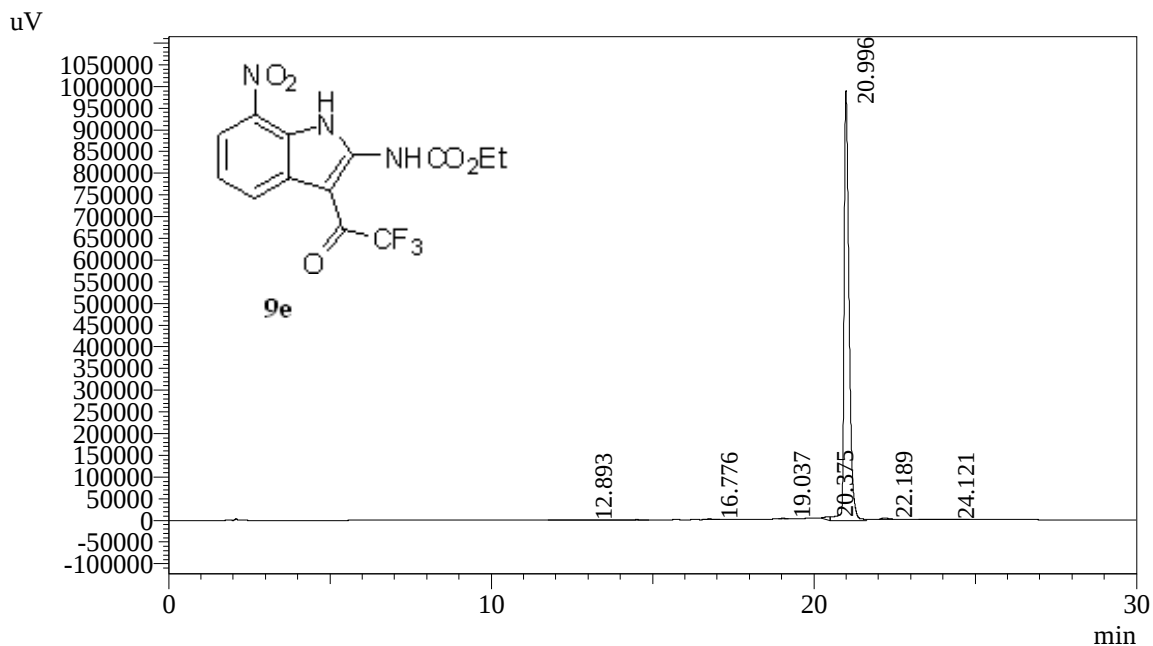
8 Peak Value:

|     |        |     |       |     |       |     |       |     |       |     |       |     |       |     |       |
|-----|--------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|
| 204 | 100.00 | 345 | 76.94 | 158 | 25.88 | 232 | 22.01 | 230 | 21.04 | 129 | 20.02 | 102 | 19.76 | 276 | 17.32 |
|-----|--------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|-----|-------|



User Name : CJK  
 Sample ID :  
 Sample Name : 4-078-yl  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6505.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/11/08 13:20:58

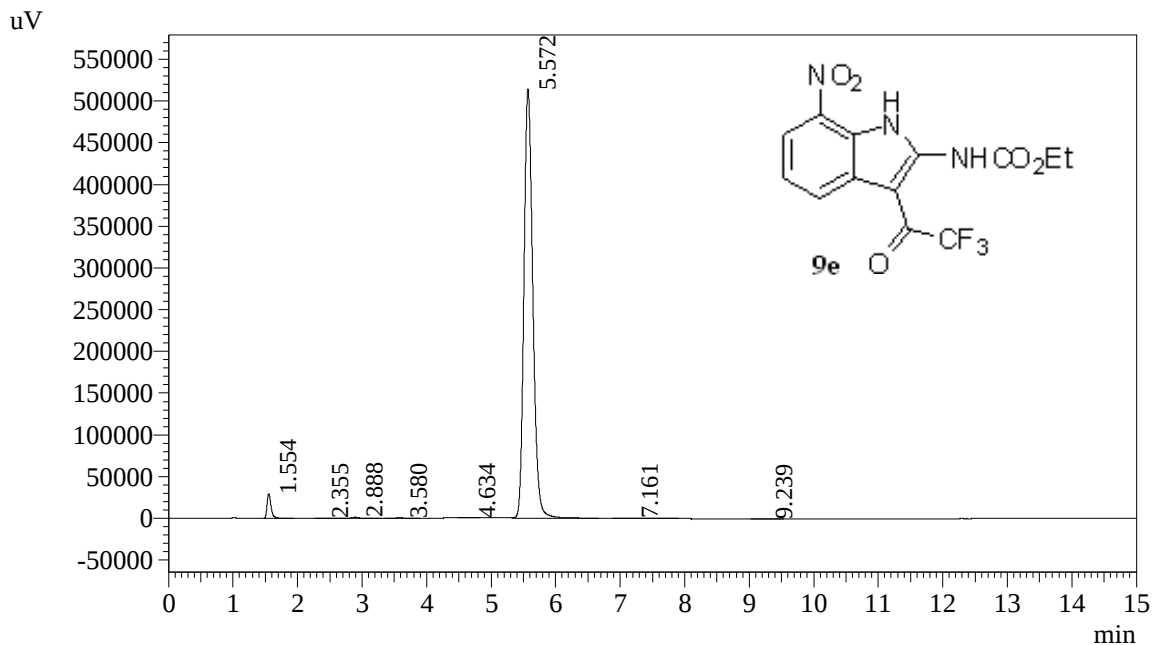
# HPLC



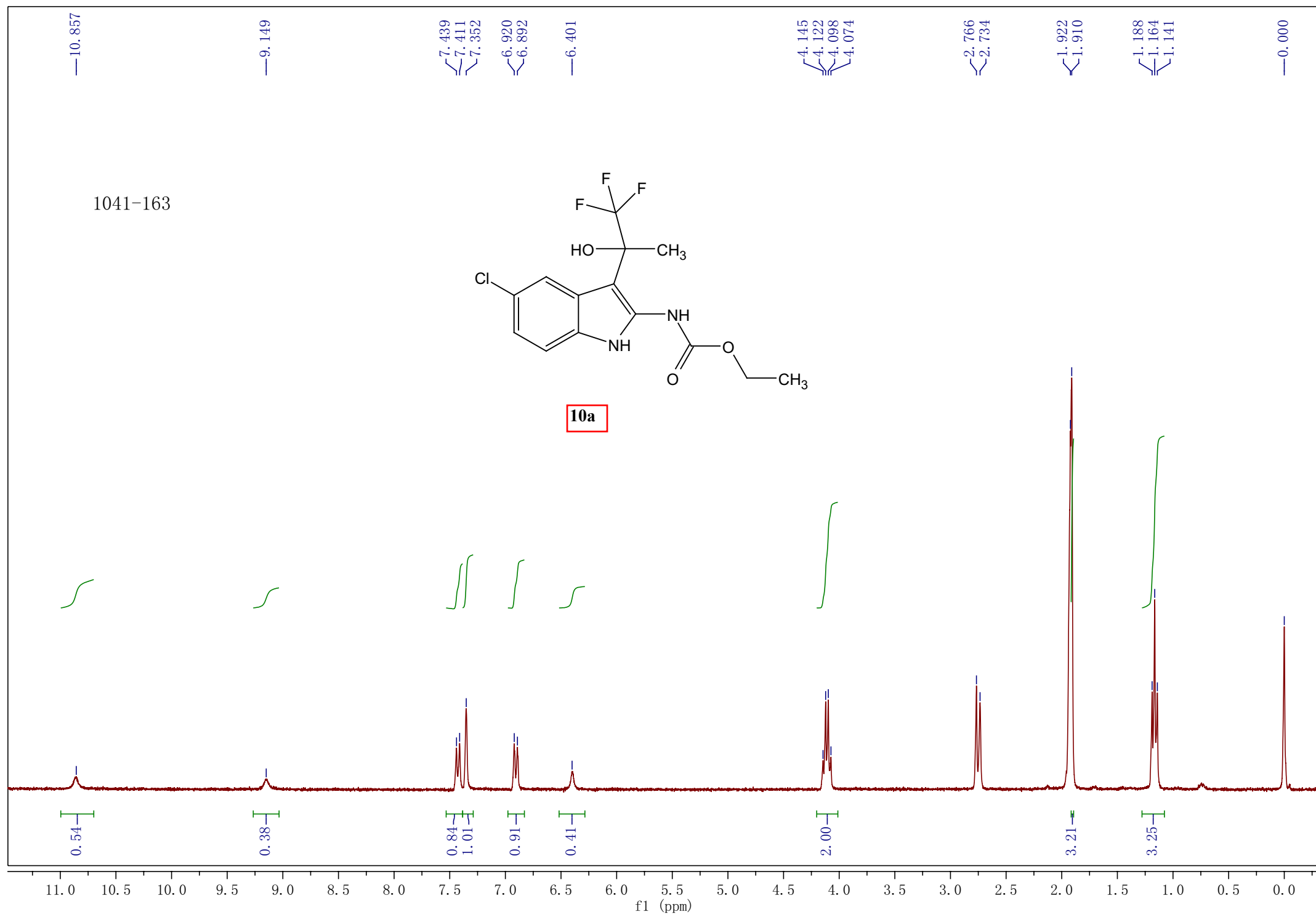
| Peak# | Ret.Time | Area     | Height  | A/H    | Area%    |
|-------|----------|----------|---------|--------|----------|
| 1     | 12.893   | 37783    | 579     | 65.278 | 0.3487   |
| 2     | 16.776   | 22478    | 1433    | 15.681 | 0.2074   |
| 3     | 19.037   | 12363    | 1350    | 9.160  | 0.1141   |
| 4     | 20.375   | 71320    | 5098    | 13.991 | 0.6582   |
| 5     | 20.996   | 10635737 | 989421  | 10.749 | 98.1501  |
| 6     | 22.189   | 33967    | 2949    | 11.517 | 0.3135   |
| 7     | 24.121   | 22550    | 761     | 29.627 | 0.2081   |
| 全部    |          | 10836198 | 1001591 |        | 100.0000 |

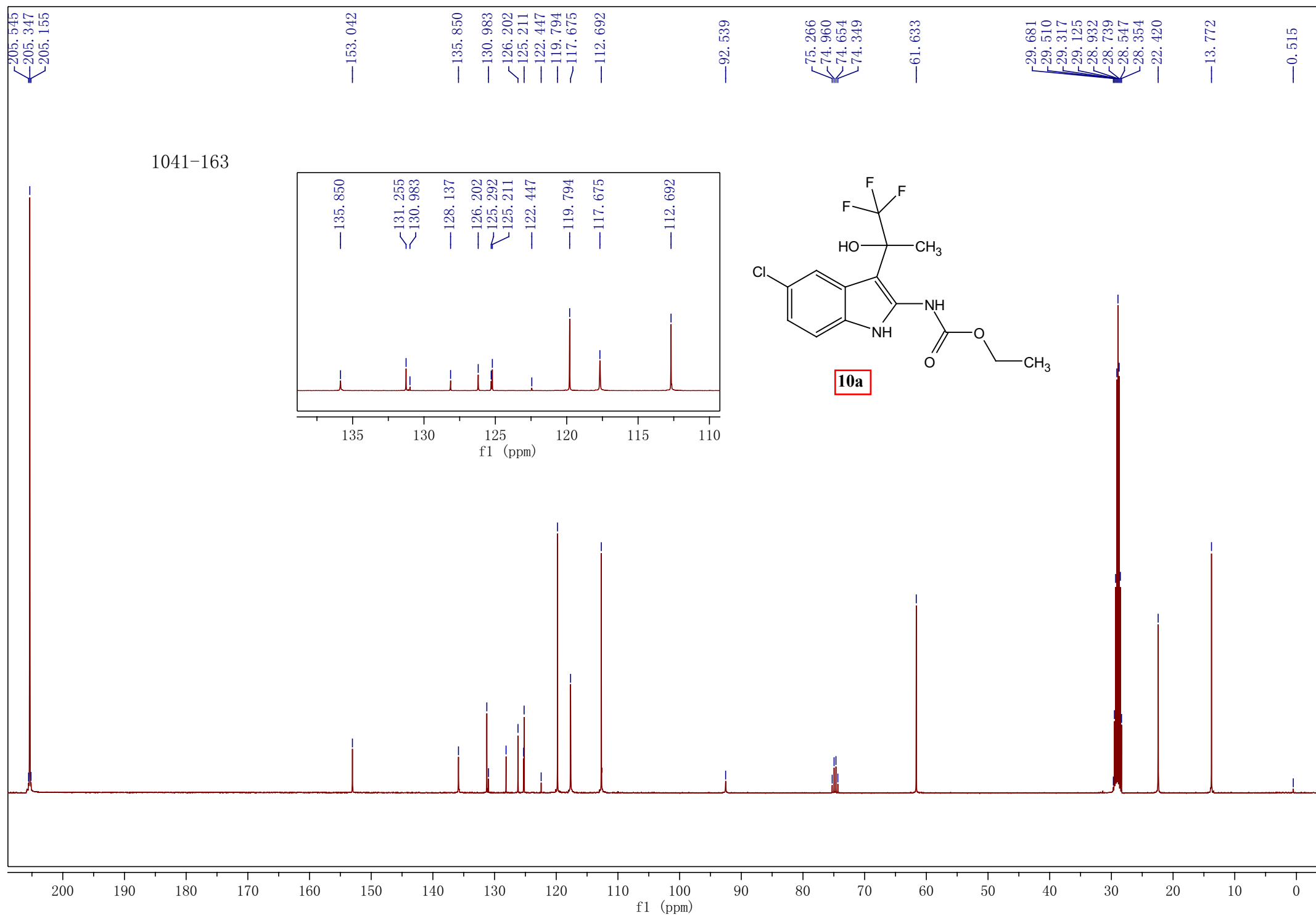
User Name : CJK  
 Sample ID :  
 Sample Name : 4-078-yl  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6507.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/11/08 14:45:06

# HPLC



| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 1.554    | 130528  | 29672  | 4.399  | 2.5620   |
| 2     | 2.355    | 6016    | 444    | 13.544 | 0.1181   |
| 3     | 2.888    | 7802    | 1116   | 6.993  | 0.1531   |
| 4     | 3.580    | 3334    | 385    | 8.661  | 0.0654   |
| 5     | 4.634    | 3617    | 416    | 8.702  | 0.0710   |
| 6     | 5.572    | 4936167 | 514265 | 9.598  | 96.8883  |
| 7     | 7.161    | 6690    | 258    | 25.922 | 0.1313   |
| 8     | 9.239    | 544     | 26     | 20.779 | 0.0107   |
| 全部    |          | 5094698 | 546582 |        | 100.0000 |



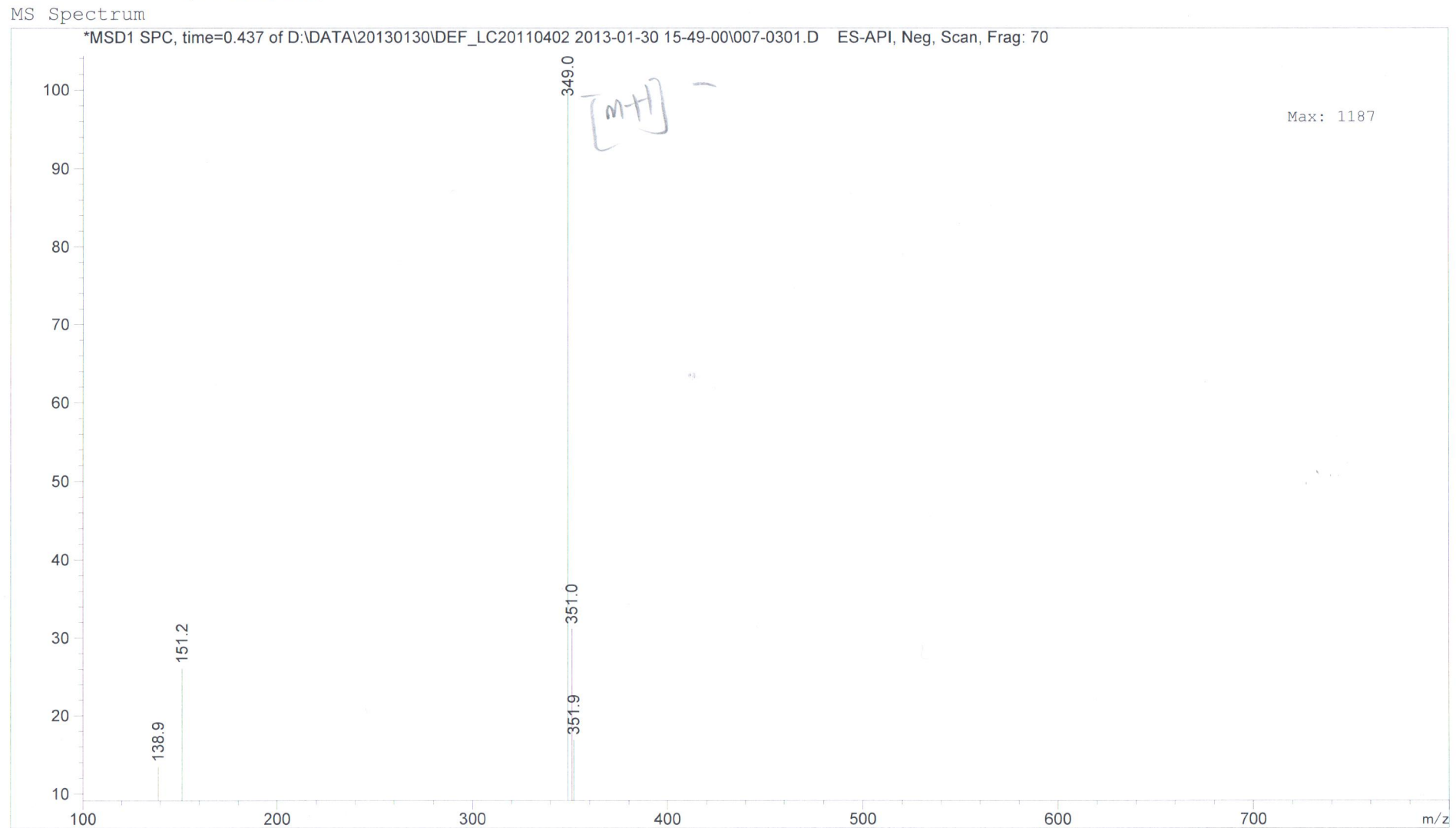


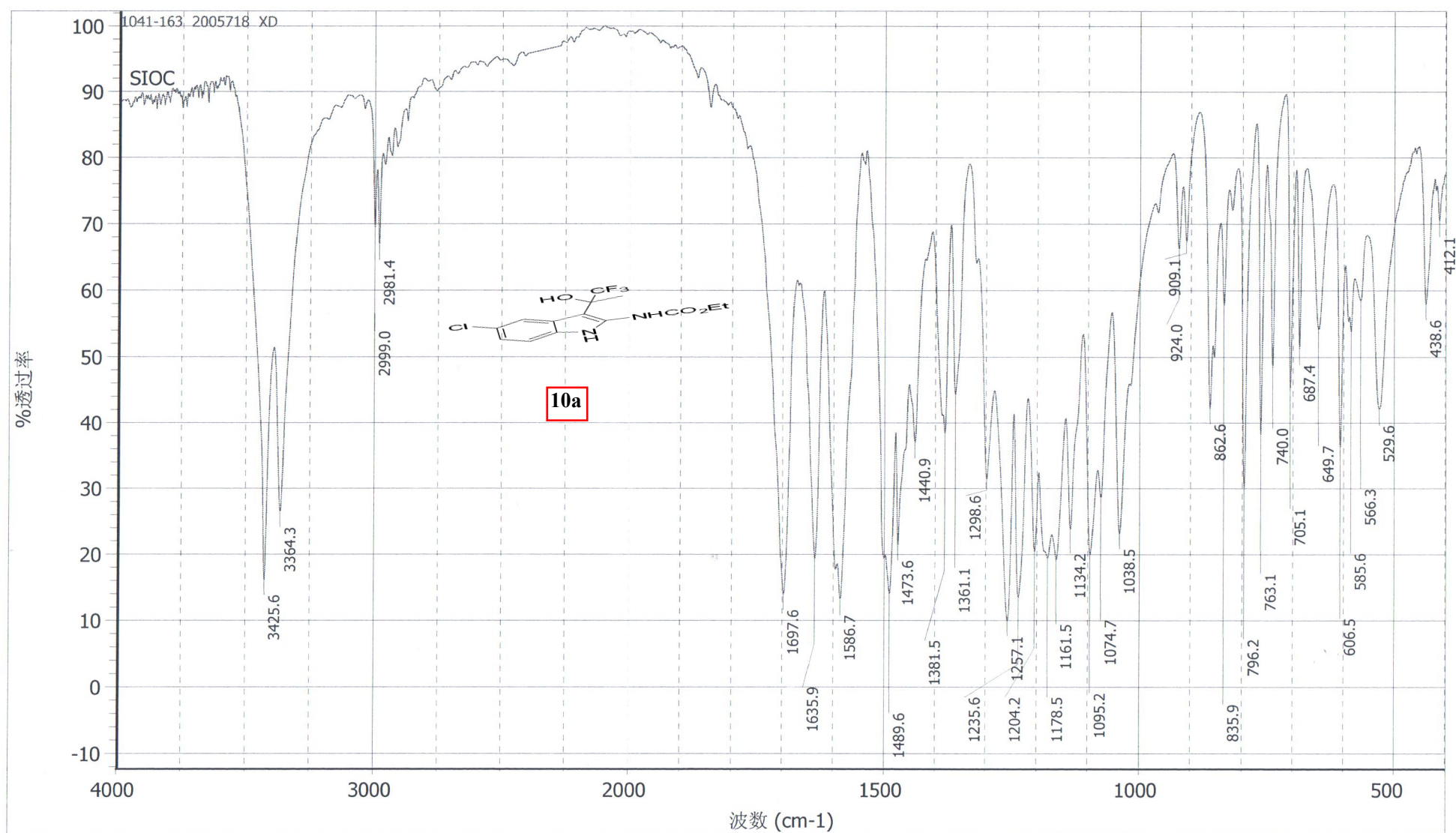
打印窗口 80: MS Spectrum  
数据文件: : D:\DATA\20130130\DEF\_LC20110402 2013-01-30 15-49-00\007-0301.D  
样品名称 : 1041-163

=====

|      |   |                                                                      |      |   |        |
|------|---|----------------------------------------------------------------------|------|---|--------|
| 操作者  | : |                                                                      | 序列行  | : | 3      |
| 仪器   | : | 仪器 1                                                                 | 位置   | : | 样品瓶 7  |
| 进样日期 | : | 2013-1-30 15:57:38                                                   | 进样次数 | : | 1      |
|      |   |                                                                      | 进样量  | : | 0.2 µl |
| 采集方法 | : | D:\DATA\20130130\DEF_LC20110402 2013-01-30 15-49-00\DEF_LC20110310.M |      |   |        |
| 最后修改 | : | 2013-1-30 15:48:28                                                   |      |   |        |
| 分析方法 | : | C:\CHEM32\1\METHODS\DEF_LC20110310.M                                 |      |   |        |
| 最后修改 | : | 2013-1-30 9:25:21                                                    |      |   |        |

(调用后修改)





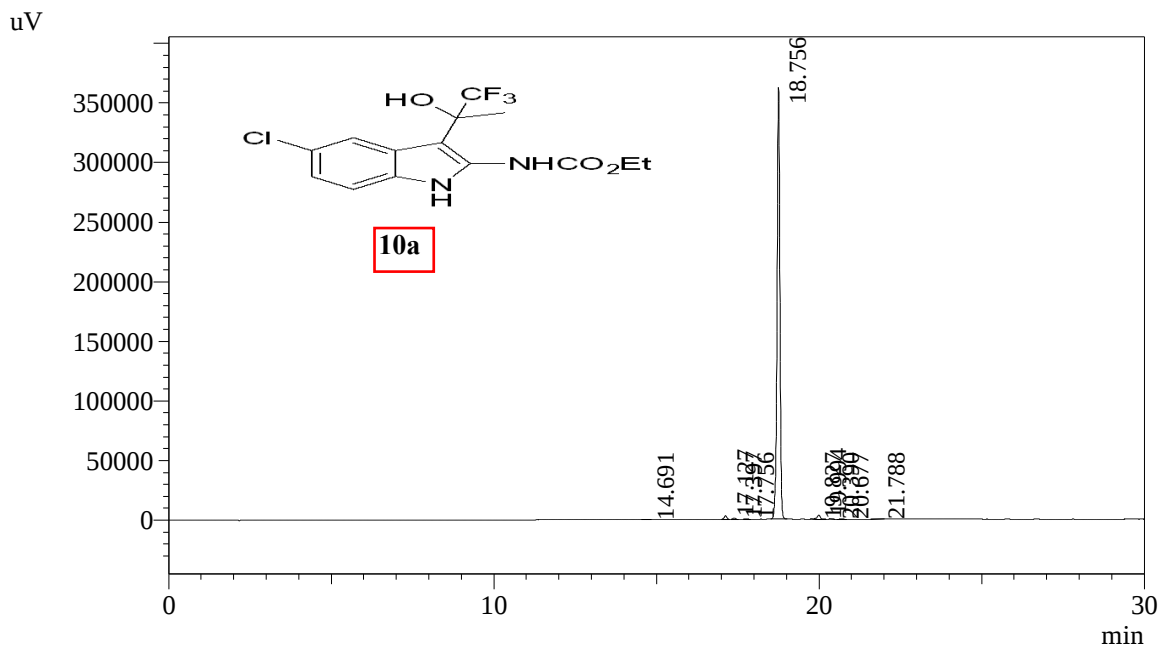
1041-163 2005718 XD

样品扫描次数: 32  
背景扫描次数: 32  
分辨率: 4.000  
采样增益: 1.0  
动镜速度: 0.6329

10c

User Name : CJK  
 Sample ID :  
 Sample Name : 1041-163  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-10982.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2013/01/31 9:32:15

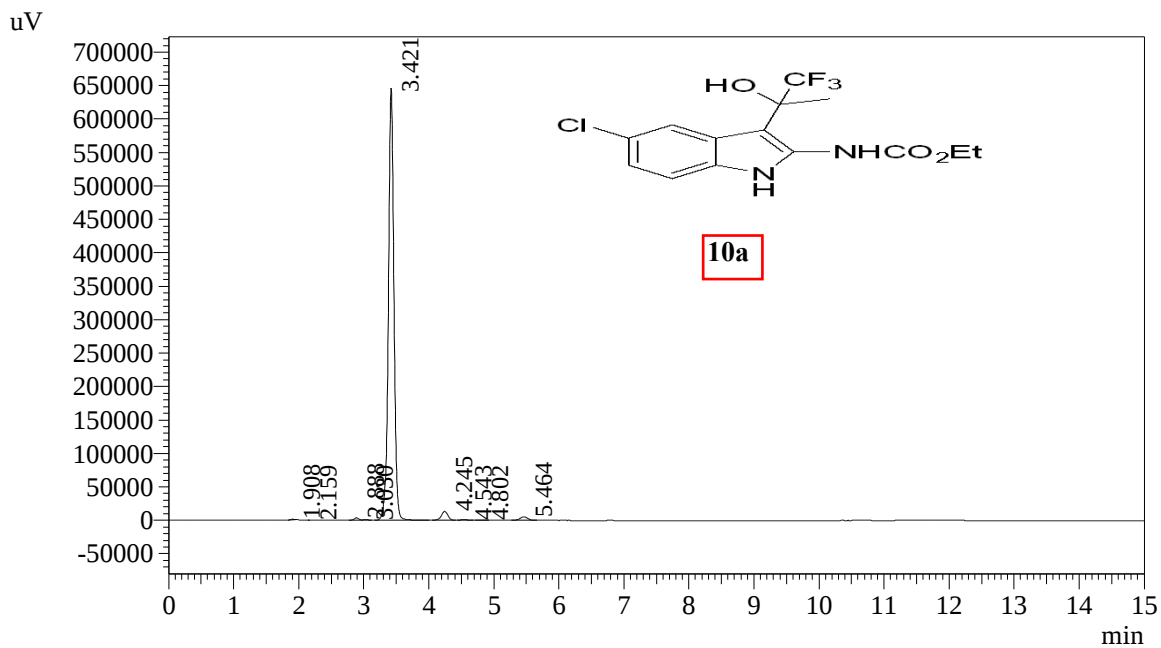
# HPLC



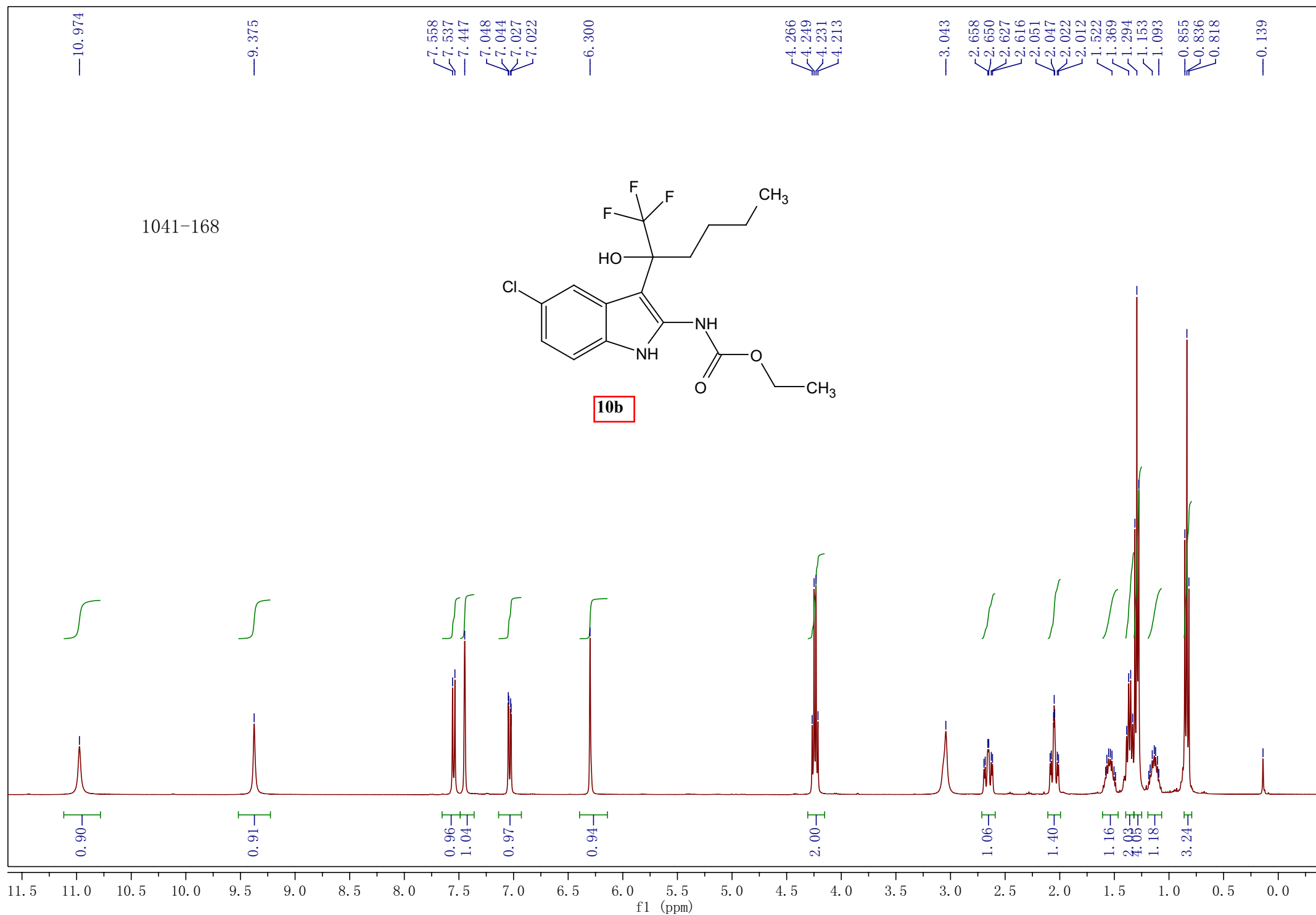
| Peak# | Ret.Time | Area    | Height | A/H   | Area%    |
|-------|----------|---------|--------|-------|----------|
| 1     | 14.691   | 1225    | 201    | 6.083 | 0.0543   |
| 2     | 17.127   | 16186   | 2829   | 5.722 | 0.7173   |
| 3     | 17.397   | 6478    | 1153   | 5.619 | 0.2870   |
| 4     | 17.756   | 3641    | 579    | 6.287 | 0.1613   |
| 5     | 18.756   | 2197213 | 362051 | 6.069 | 97.3642  |
| 6     | 19.827   | 2829    | 447    | 6.335 | 0.1254   |
| 7     | 19.994   | 23660   | 3497   | 6.765 | 1.0485   |
| 8     | 20.390   | 1991    | 377    | 5.277 | 0.0882   |
| 9     | 20.677   | 1073    | 150    | 7.130 | 0.0475   |
| 10    | 21.788   | 2398    | 386    | 6.213 | 0.1063   |
| 全部    |          | 2256694 | 371670 |       | 100.0000 |

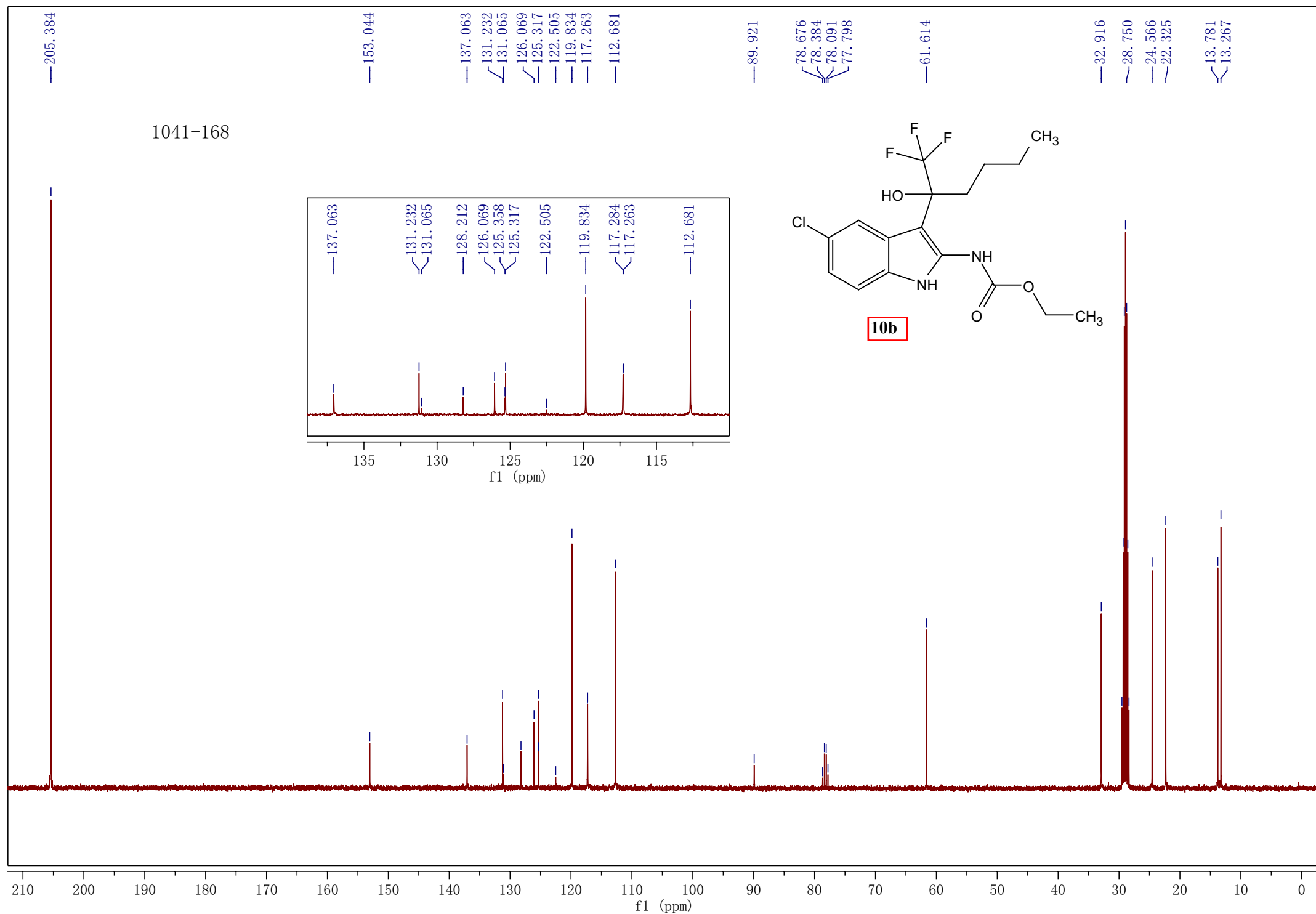
User Name : CJK  
 Sample ID :  
 Sample Name : 1041-163  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-10988.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2013/01/31 12:34:14

# HPLC



| Peak# | Ret.Time | Area    | Height | A/H   | Area%    |
|-------|----------|---------|--------|-------|----------|
| 1     | 1.908    | 5469    | 1067   | 5.127 | 0.1364   |
| 2     | 2.159    | 32      | 19     | 1.643 | 0.0008   |
| 3     | 2.888    | 15551   | 3280   | 4.741 | 0.3879   |
| 4     | 3.030    | 3945    | 932    | 4.232 | 0.0984   |
| 5     | 3.421    | 3842196 | 638701 | 6.016 | 95.8412  |
| 6     | 4.245    | 88142   | 13151  | 6.702 | 2.1986   |
| 7     | 4.543    | 7951    | 1278   | 6.221 | 0.1983   |
| 8     | 4.802    | 811     | 119    | 6.834 | 0.0202   |
| 9     | 5.464    | 44825   | 5486   | 8.171 | 1.1181   |
| 全部    |          | 4008922 | 664033 |       | 100.0000 |



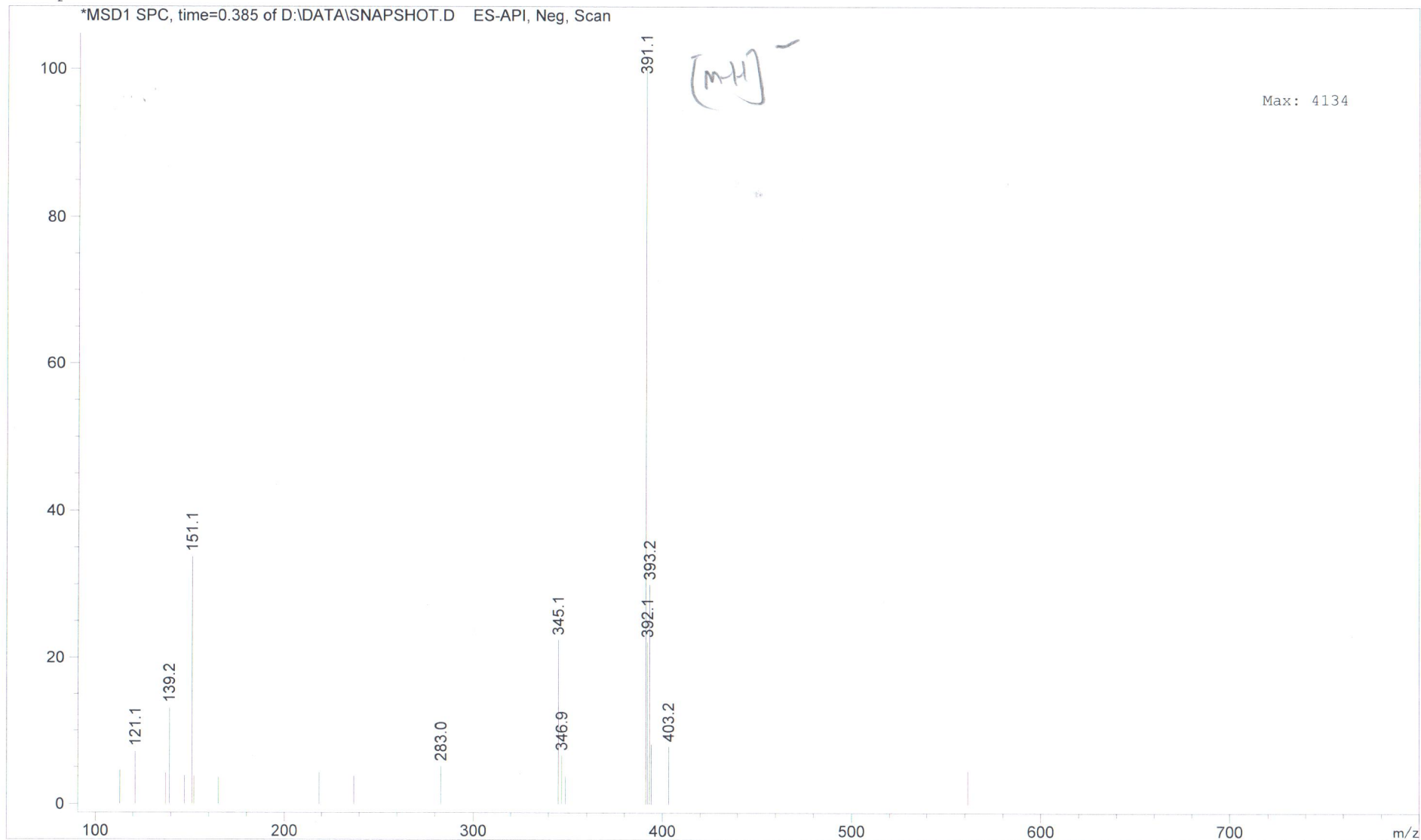


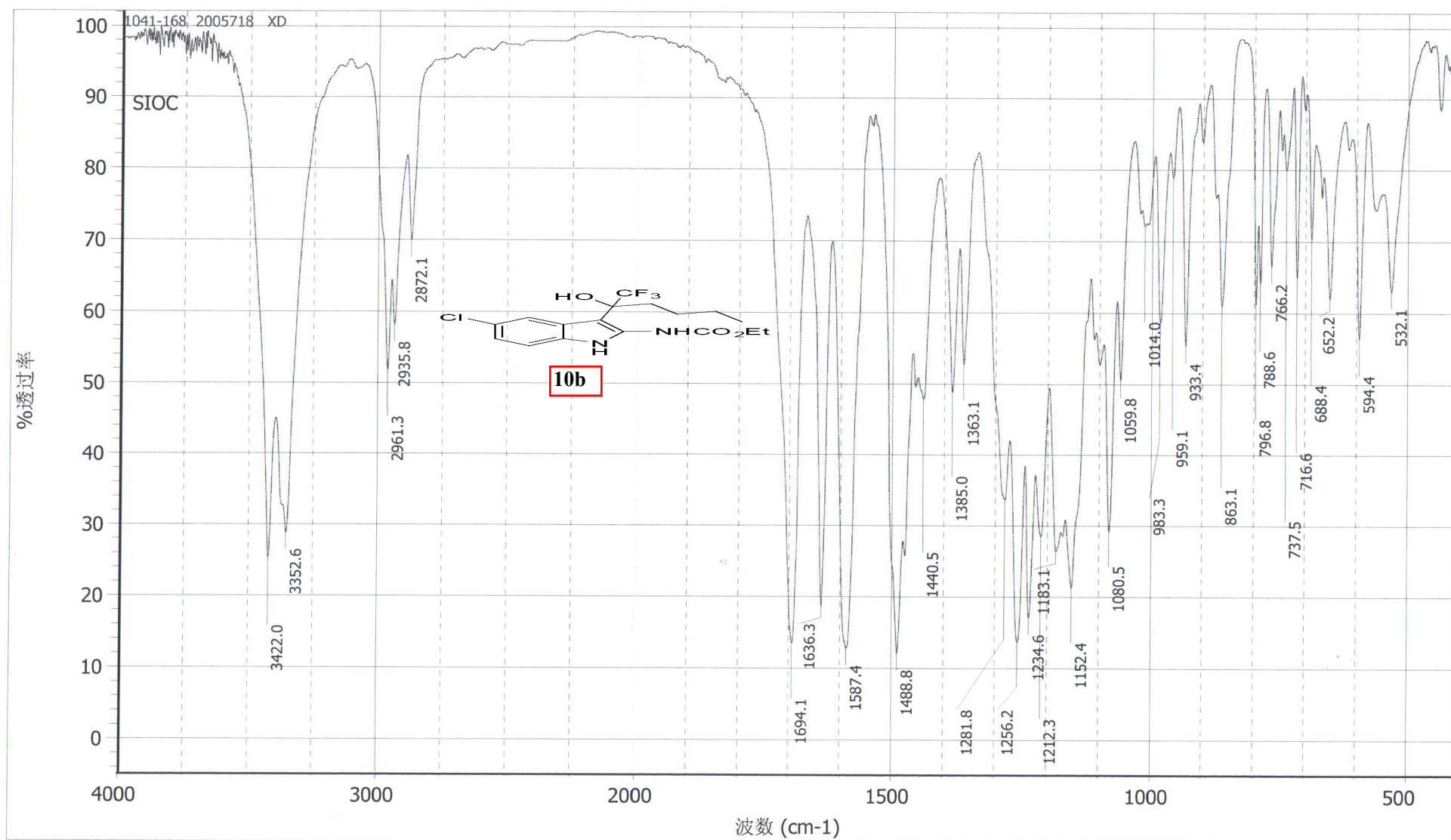
□ 80: MS Spectrum  
件: : D:\DATA\SNAPSHOT.D  
称 : 1041-168

期  
法  
改

位置 : 样品瓶 18  
进样次数 : 1  
: 22 Feb 13 4:21 pm +0800  
: DEF\_LC20110310.M  
: C:\CHEM32\1\METHODS\DEF\_LC20110310.M  
: 2013-2-22 16:07:09  
(调用后修改)

MS Spectrum



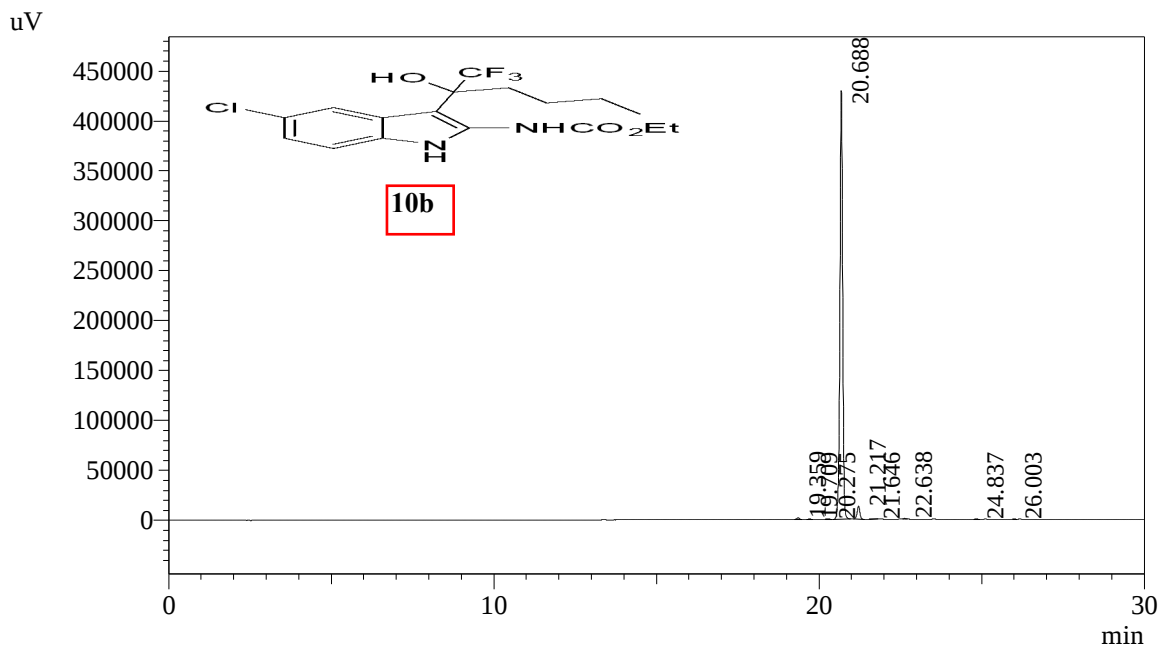


1041-168 2005718 XD

样品扫描次数: 32  
背景扫描次数: 32  
分辨率: 4.000  
采样增益: 1.0  
动镜速度: 0.6329

User Name : CJK  
 Sample ID :  
 Sample Name : 1041-168  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-11039.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2013/02/25 13:37:14

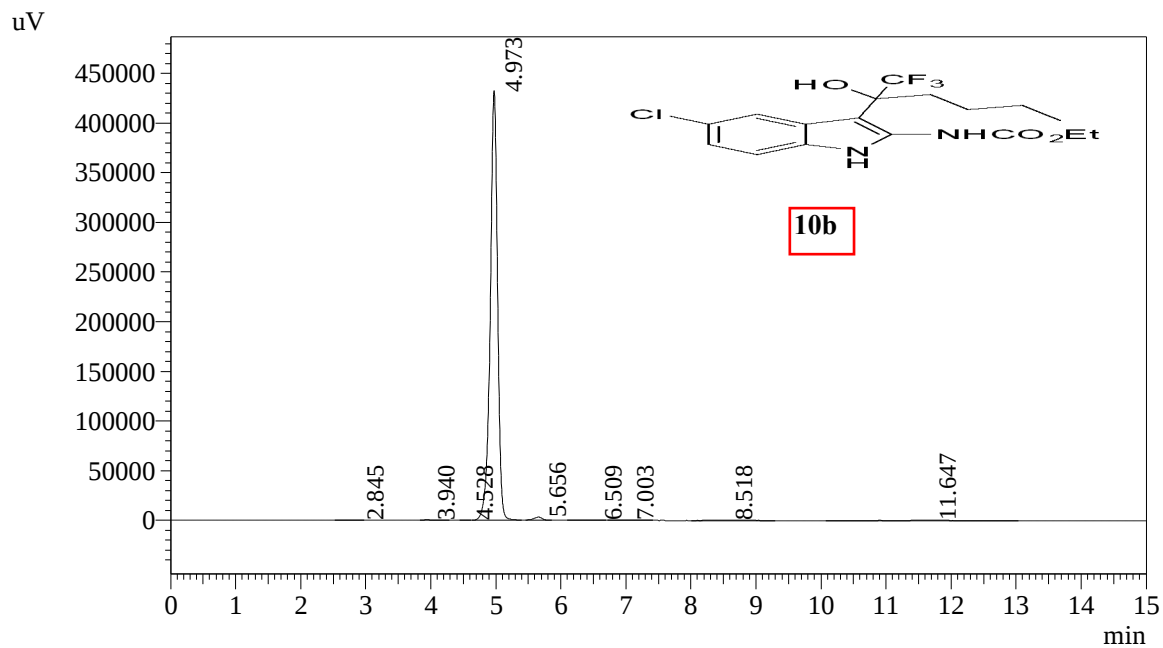
# HPLC



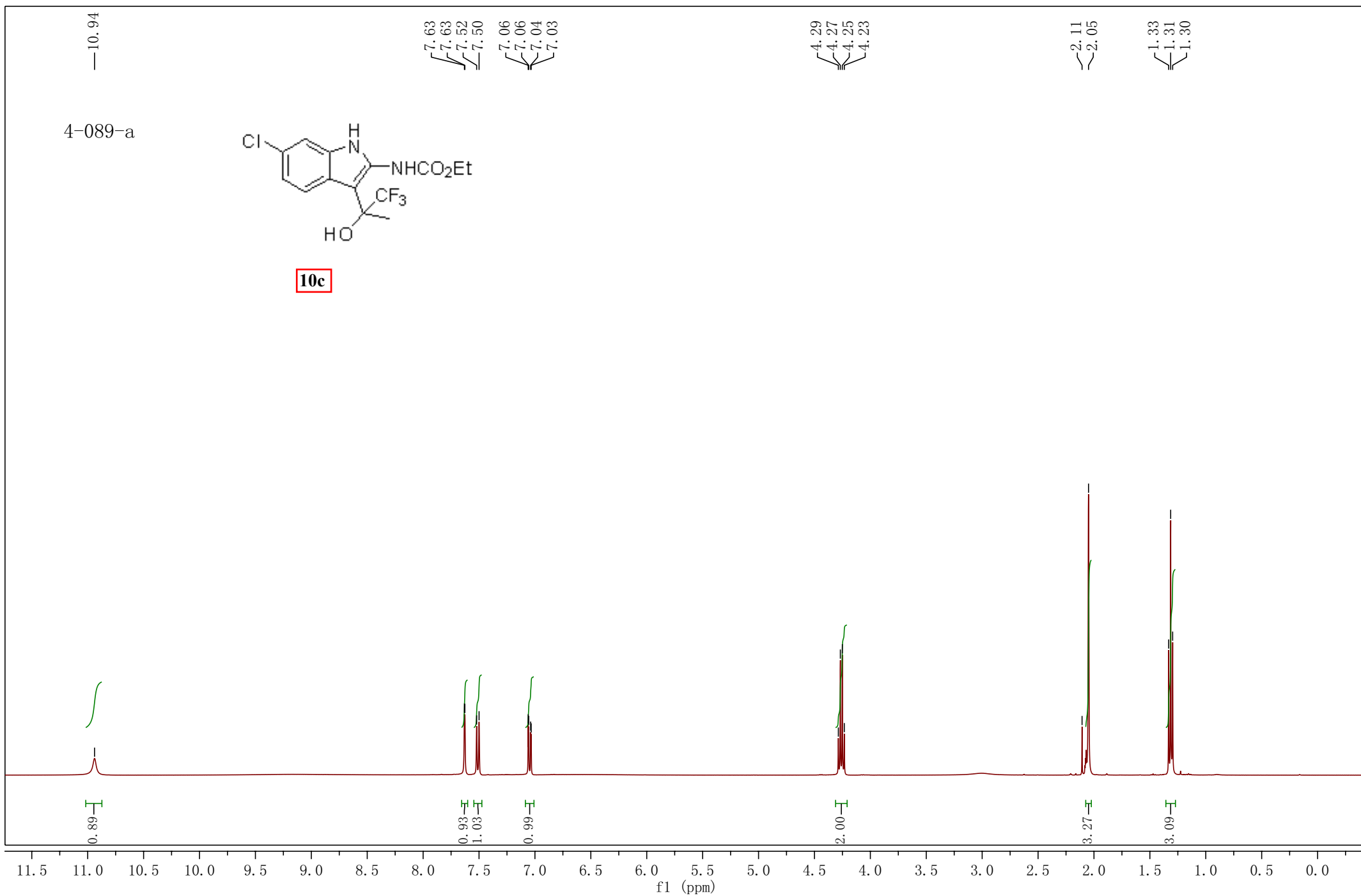
| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 19.359   | 8867    | 1608   | 5.515  | 0.3341   |
| 2     | 19.709   | 2384    | 401    | 5.947  | 0.0898   |
| 3     | 20.275   | 3290    | 641    | 5.133  | 0.1240   |
| 4     | 20.688   | 2552928 | 428997 | 5.951  | 96.1949  |
| 5     | 21.217   | 75583   | 13214  | 5.720  | 2.8480   |
| 6     | 21.646   | 4408    | 413    | 10.661 | 0.1661   |
| 7     | 22.638   | 2355    | 553    | 4.260  | 0.0887   |
| 8     | 24.837   | 2022    | 388    | 5.217  | 0.0762   |
| 9     | 26.003   | 2073    | 175    | 11.811 | 0.0781   |
| 全部    |          | 2653910 | 446390 |        | 100.0000 |

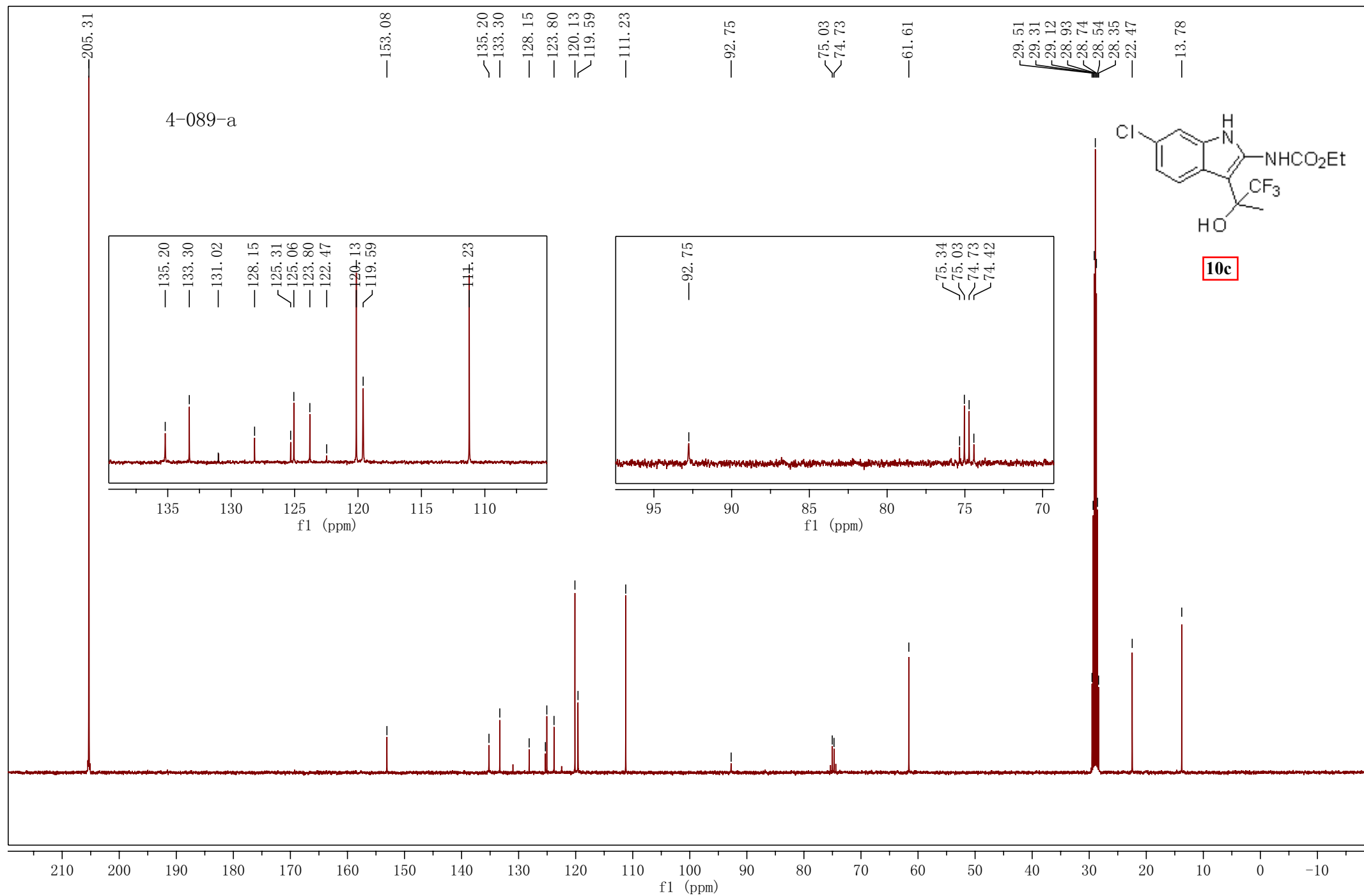
User Name : CJK  
 Sample ID :  
 Sample Name : 1041-168  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-11041.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2013/02/25 14:34:23

# HPLC



| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 2.845    | 879     | 125    | 7.014  | 0.0255   |
| 2     | 3.940    | 6777    | 751    | 9.029  | 0.1966   |
| 3     | 4.528    | 2047    | 370    | 5.535  | 0.0594   |
| 4     | 4.973    | 3398985 | 432226 | 7.864  | 98.6325  |
| 5     | 5.656    | 27303   | 3083   | 8.857  | 0.7923   |
| 6     | 6.509    | 2070    | 230    | 9.003  | 0.0601   |
| 7     | 7.003    | 811     | 39     | 20.846 | 0.0235   |
| 8     | 8.518    | 2837    | 103    | 27.421 | 0.0823   |
| 9     | 11.647   | 4403    | 102    | 43.300 | 0.1278   |
| 全部    |          | 3446112 | 437029 |        | 100.0000 |





姜海波

## Sample Information

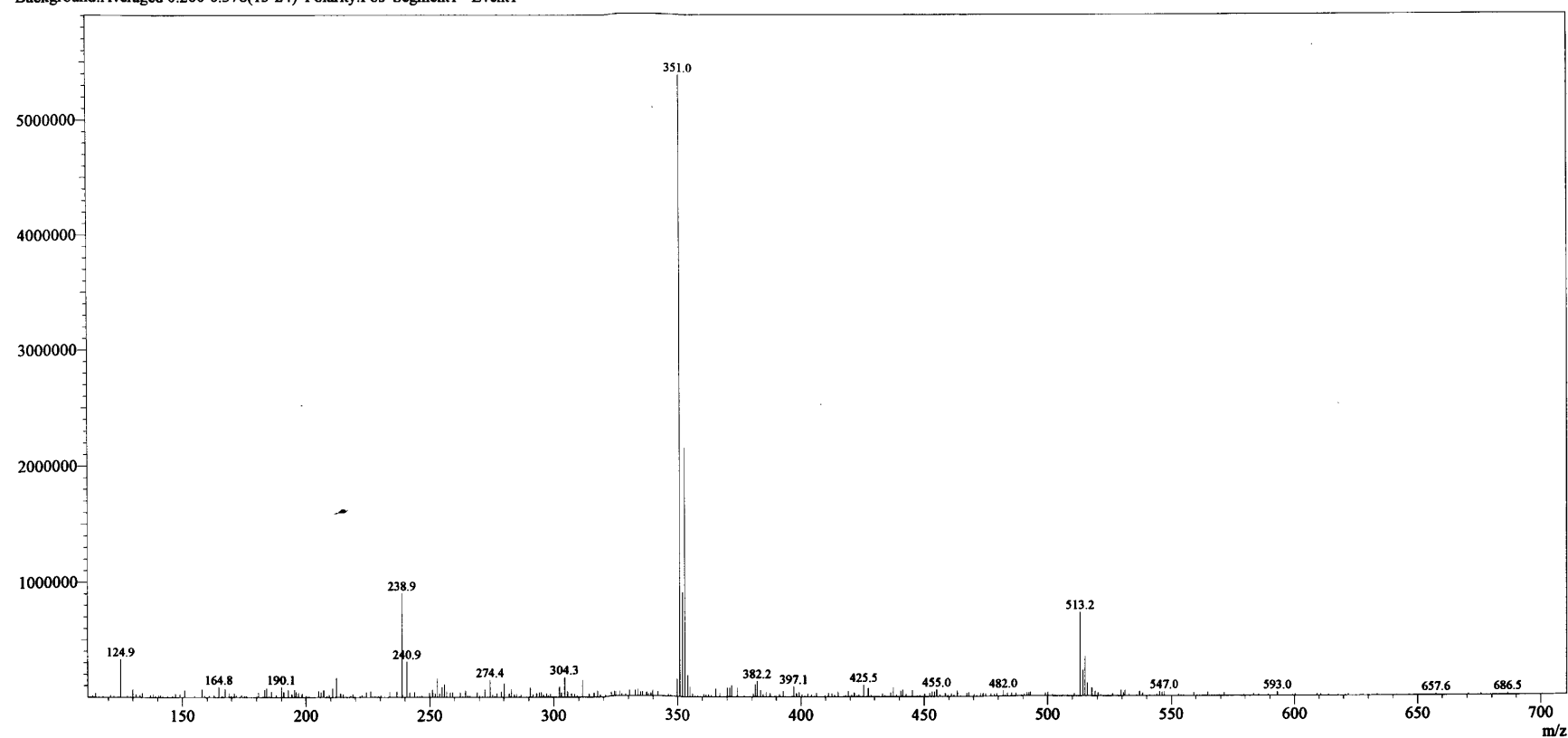
Date Acquired : 10/26/2010 2:20:04 PM  
Sample Name : jhx  
Sample ID : 4-089-2-a  
Data File : 4-089-2-a-002.lcd  
Method File : HPLC-smyj30.lcm  
Original Data File : D:\DATA\jiangbiao-group\4-089-2-a-002.lcd  
Original Method : D:\DATA\HPLC-smyj30.lcm  
Modified Date : 10/26/2010 2:22:09 PM  
Instrument : Shimadzu LCMS-2010EV

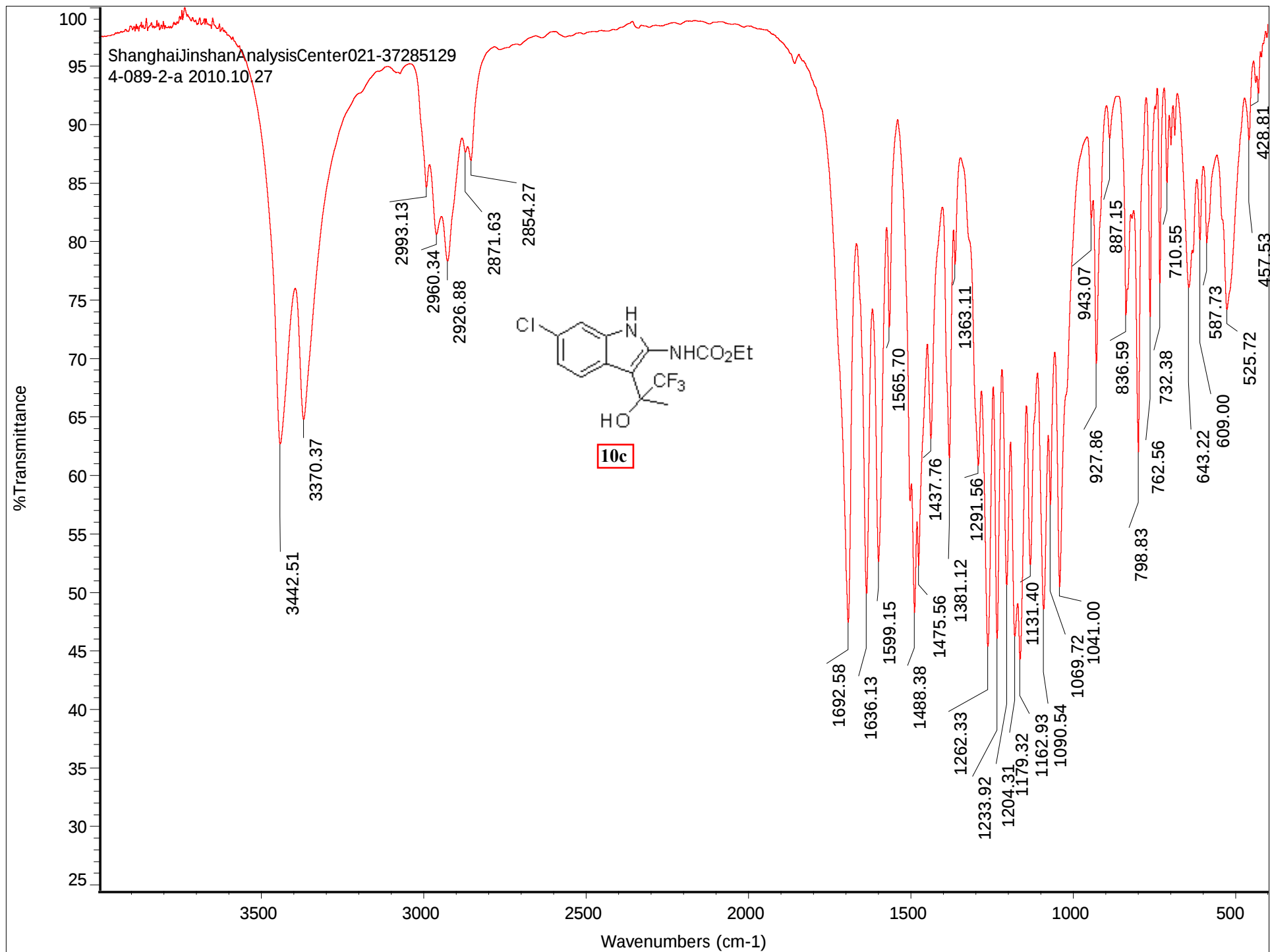
Retention Time: 0.600 (Scan#: 37)

Max Peak: 640 Base Peak: 351.00 (5383159)

Spectrum: Single 0.600 (37)

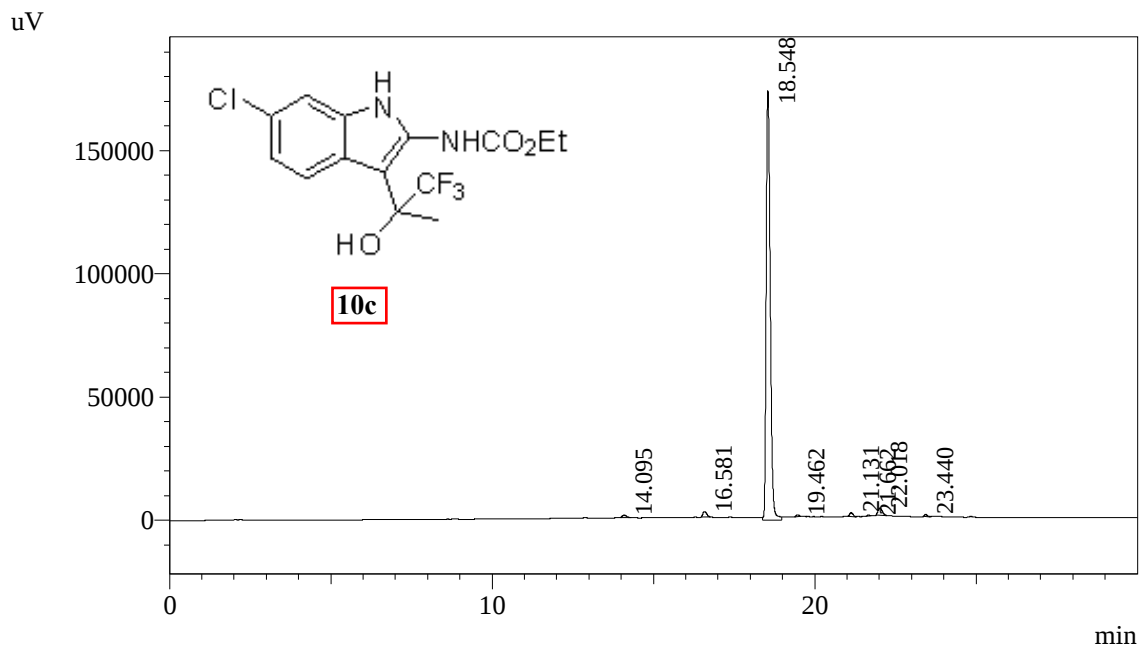
Background: Averaged 0.200-0.378 (13-24) Polarity: Pos Segment 1 - Event 1





User Name : CJK  
 Sample ID :  
 Sample Name : 4-089  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6229.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/16 11:59:15

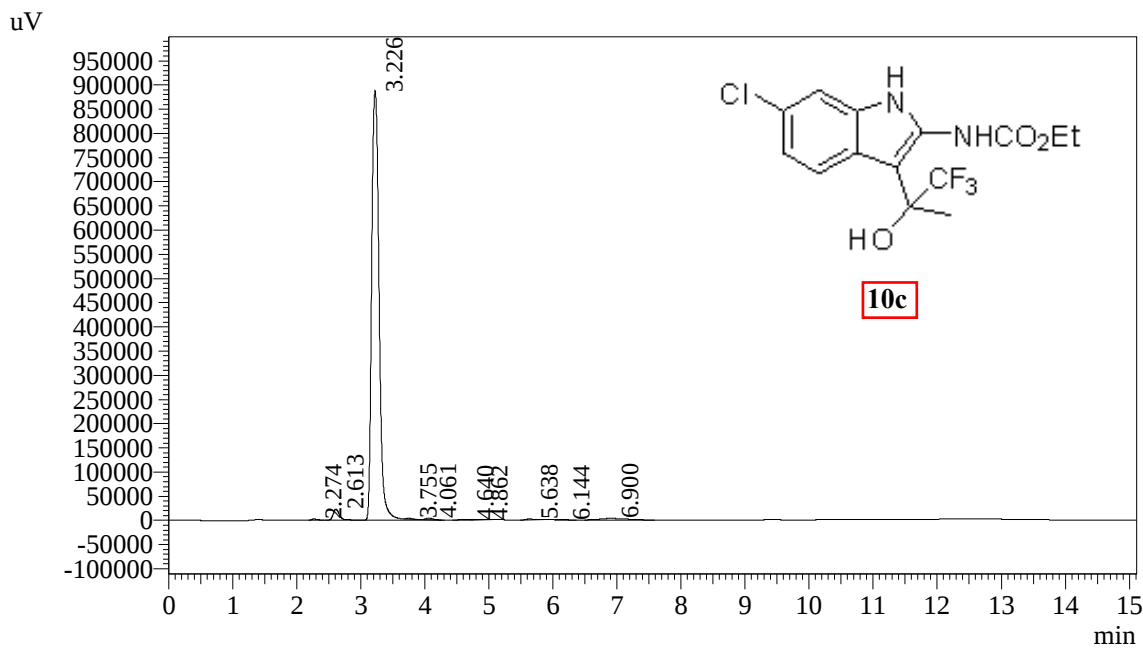
# HPLC



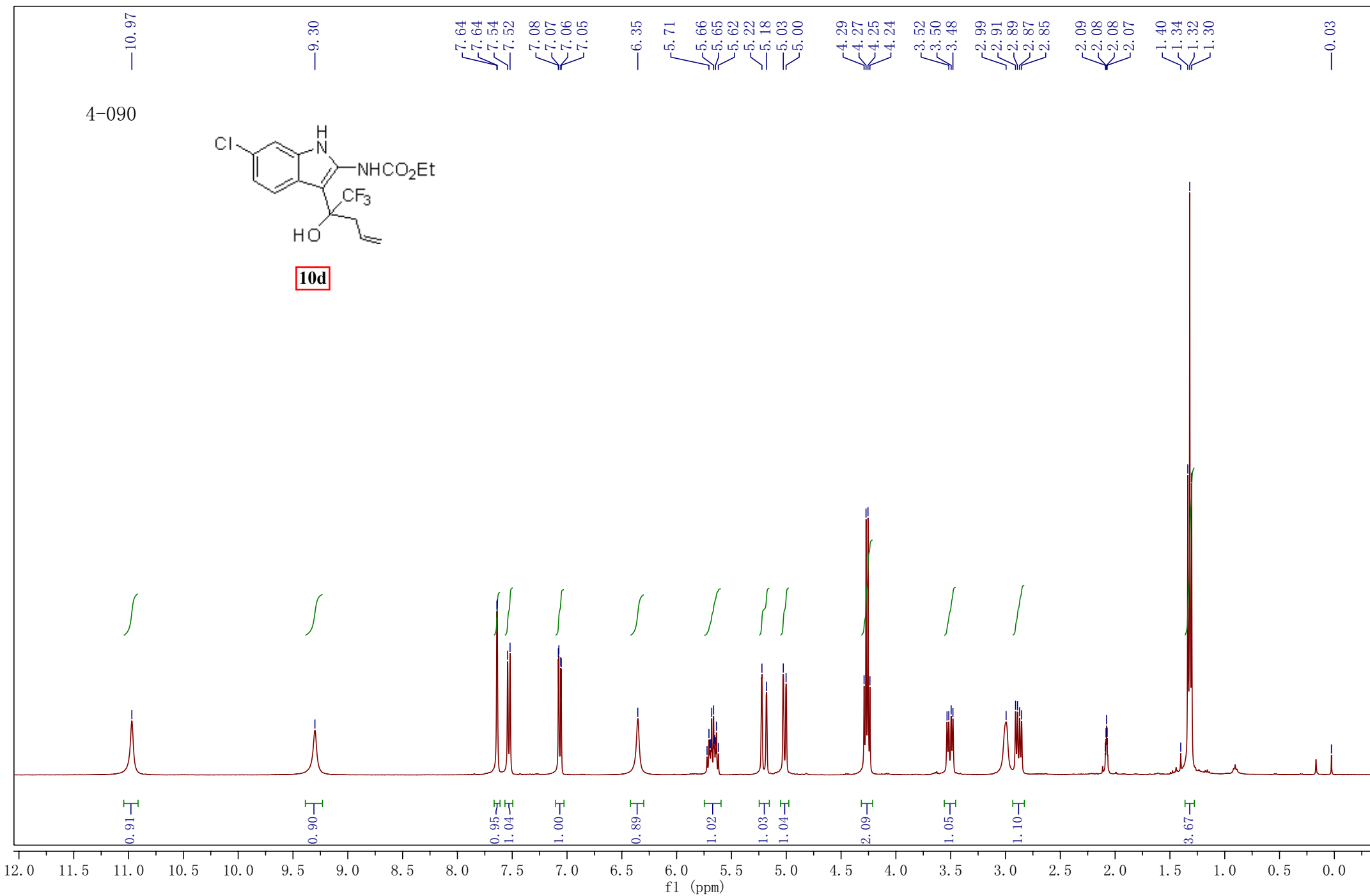
| Peak# | Ret.Time | Area    | Height | A/H   | Area%    |
|-------|----------|---------|--------|-------|----------|
| 1     | 14.095   | 8153    | 902    | 9.043 | 0.5069   |
| 2     | 16.581   | 17639   | 2184   | 8.078 | 1.0967   |
| 3     | 18.548   | 1533729 | 173528 | 8.839 | 95.3594  |
| 4     | 19.462   | 5221    | 813    | 6.425 | 0.3246   |
| 5     | 21.131   | 10523   | 1501   | 7.013 | 0.6543   |
| 6     | 21.662   | 2177    | 400    | 5.441 | 0.1354   |
| 7     | 22.018   | 26107   | 2806   | 9.303 | 1.6232   |
| 8     | 23.440   | 4818    | 795    | 6.059 | 0.2996   |
| 全部    |          | 1608367 | 182929 |       | 100.0000 |

User Name : CJK  
 Sample ID :  
 Sample Name : 4-089  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6233.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/16 13:45:15

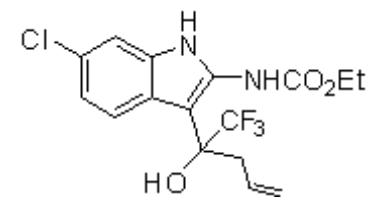
# HPLC



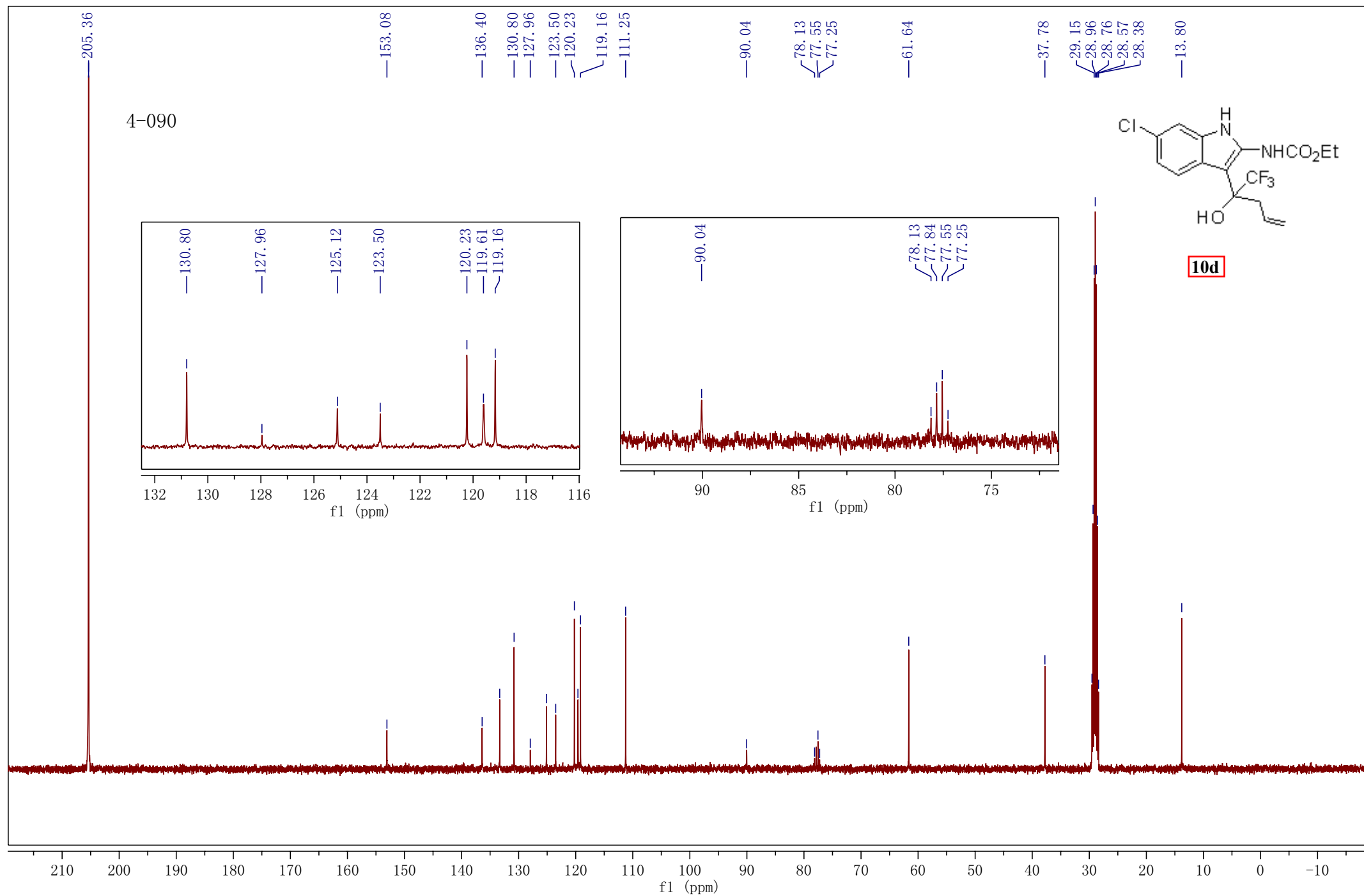
| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 2.274    | 13499   | 2155   | 6.265  | 0.1803   |
| 2     | 2.613    | 158858  | 22657  | 7.011  | 2.1217   |
| 3     | 3.226    | 7158365 | 886807 | 8.072  | 95.6064  |
| 4     | 3.755    | 8963    | 1493   | 6.002  | 0.1197   |
| 5     | 4.061    | 23629   | 3081   | 7.670  | 0.3156   |
| 6     | 4.640    | 5196    | 521    | 9.965  | 0.0694   |
| 7     | 4.862    | 10433   | 1286   | 8.113  | 0.1393   |
| 8     | 5.638    | 17547   | 1969   | 8.913  | 0.2344   |
| 9     | 6.144    | 3253    | 427    | 7.621  | 0.0434   |
| 10    | 6.900    | 87587   | 3026   | 28.946 | 1.1698   |
| 全部    |          | 7487330 | 923422 |        | 100.0000 |

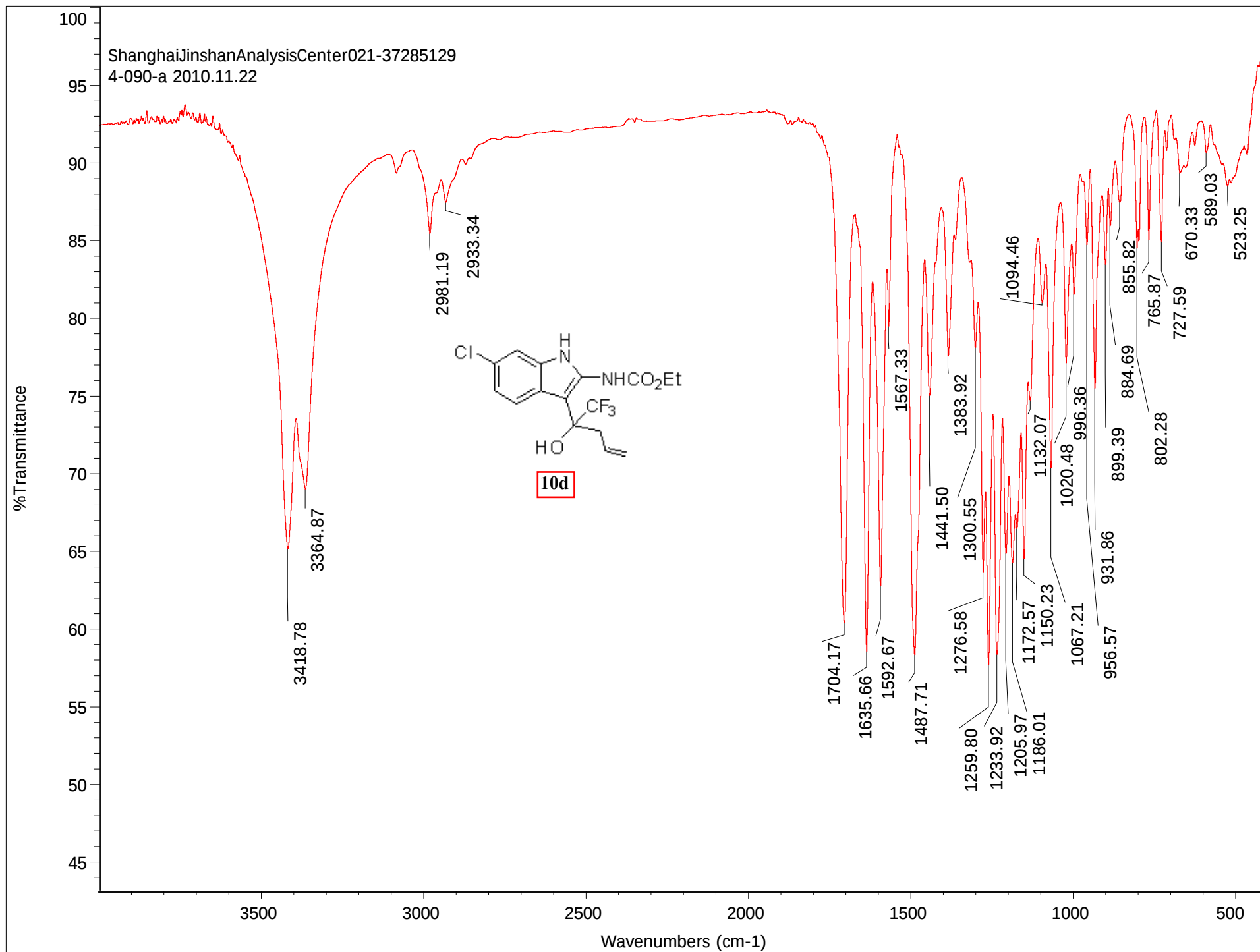


4-090



**10d**





# Mass Spectrometer Report TEL:021-37285047

## Analysis Info

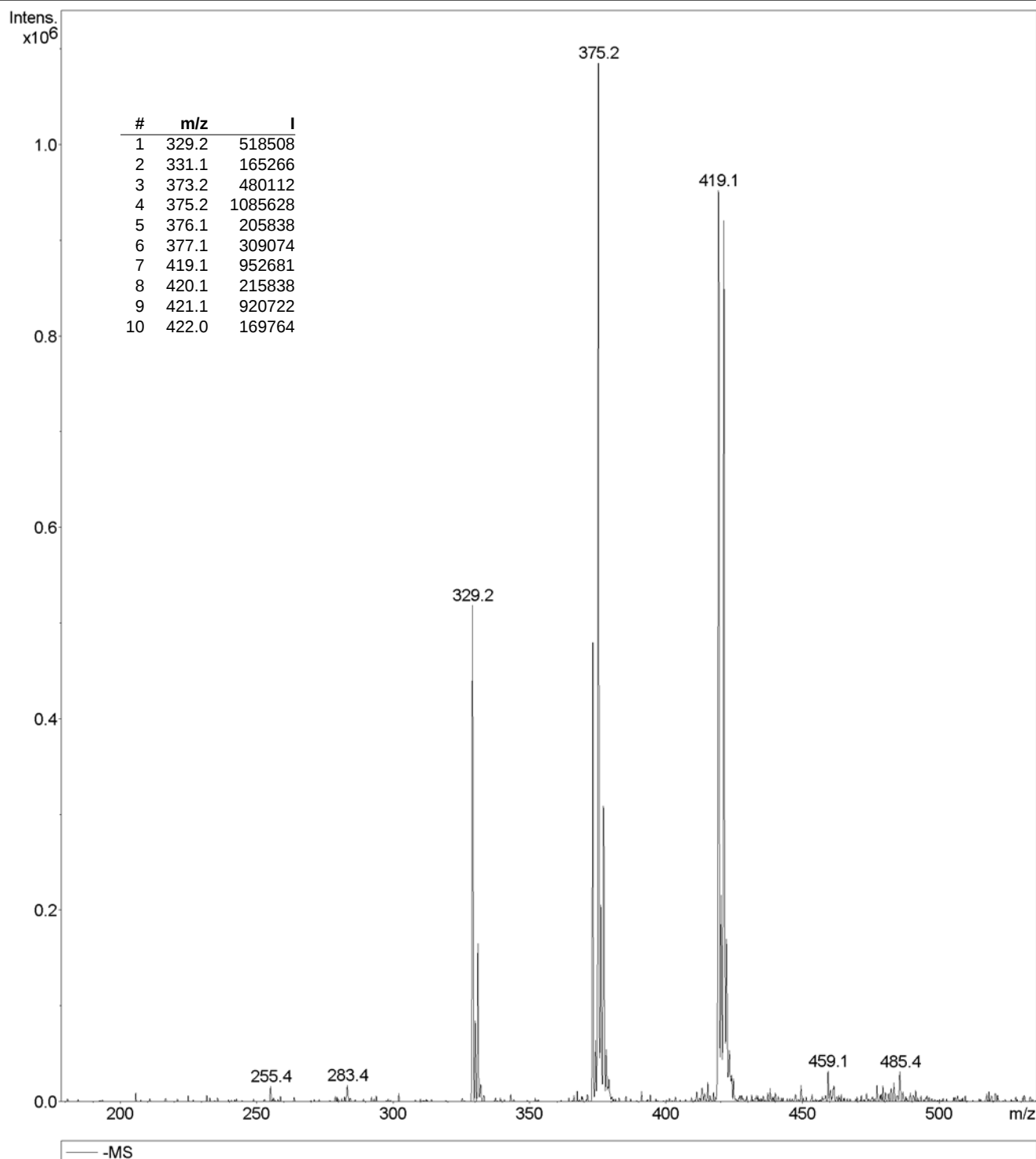
Analysis Name D:\Data\User\SIOC1122MS01.d  
Method MS1000.m  
Sample Name 4-090-a  
Comment

Acquisition Date 11/22/2010 8:47:58 AM

Operator Dai  
Instrument esquire6000

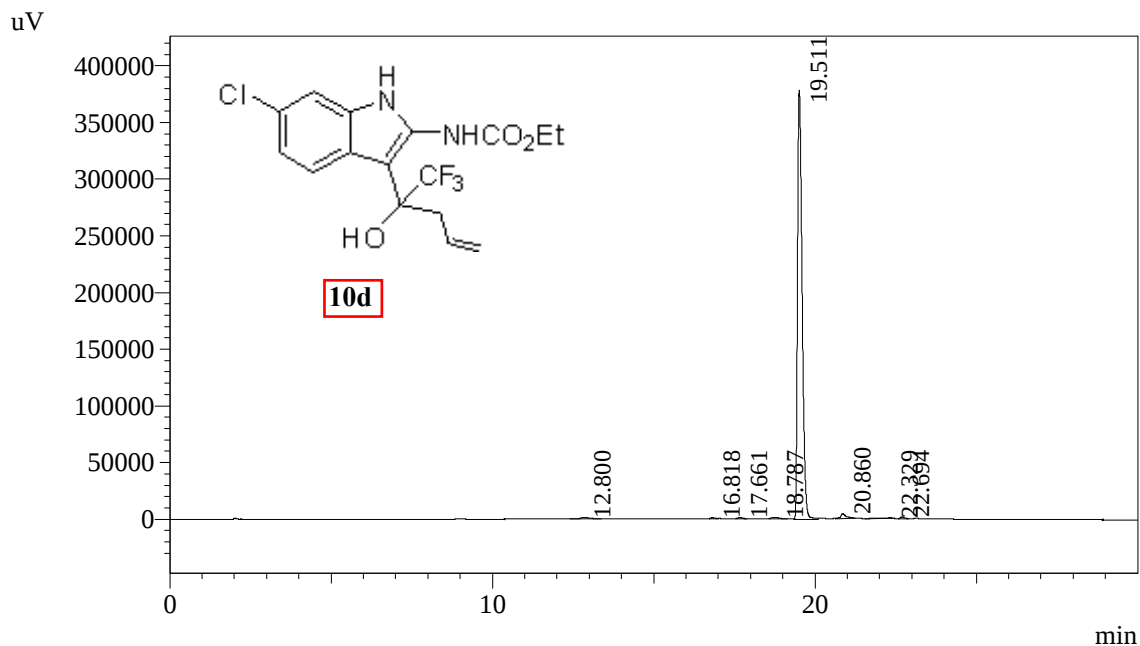
## Acquisition Parameter

|                   |             |              |            |                          |          |
|-------------------|-------------|--------------|------------|--------------------------|----------|
| Ion Source Type   | ESI         | Ion Polarity | Negative   | Alternating Ion Polarity | off      |
| Mass Range Mode   | Std/Normal  | Scan Begin   | 50 m/z     | Scan End                 | 1000 m/z |
| Capillary Exit    | -115.0 Volt | Skimmer      | -40.0 Volt | Trap Drive               | 54.2     |
| Accumulation Time | 315 $\mu$ s | Averages     | 20 Spectra | Auto MS/MS               | off      |



User Name : CJK  
 Sample ID :  
 Sample Name : 4-090  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6571.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/11/16 8:59:08

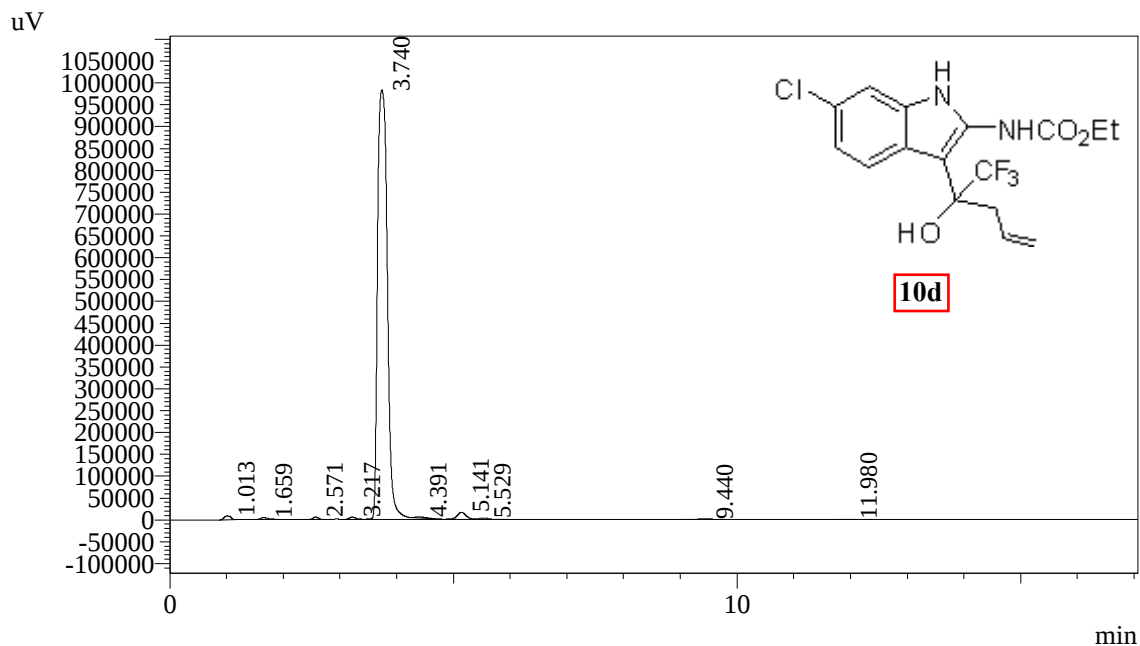
# HPLC



| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 12.800   | 23563   | 1163   | 20.262 | 0.6050   |
| 2     | 16.818   | 6005    | 750    | 8.004  | 0.1542   |
| 3     | 17.661   | 10145   | 1013   | 10.019 | 0.2605   |
| 4     | 18.787   | 15947   | 995    | 16.025 | 0.4094   |
| 5     | 19.511   | 3757784 | 378189 | 9.936  | 96.4796  |
| 6     | 20.860   | 51142   | 4453   | 11.486 | 1.3131   |
| 7     | 22.329   | 16925   | 689    | 24.576 | 0.4346   |
| 8     | 22.694   | 13387   | 1621   | 8.256  | 0.3437   |
| 全部    |          | 3894898 | 388873 |        | 100.0000 |

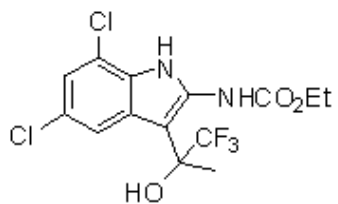
User Name : CJK  
 Sample ID :  
 Sample Name : 4-090  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6573.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/11/16 10:16:35

# HPLC

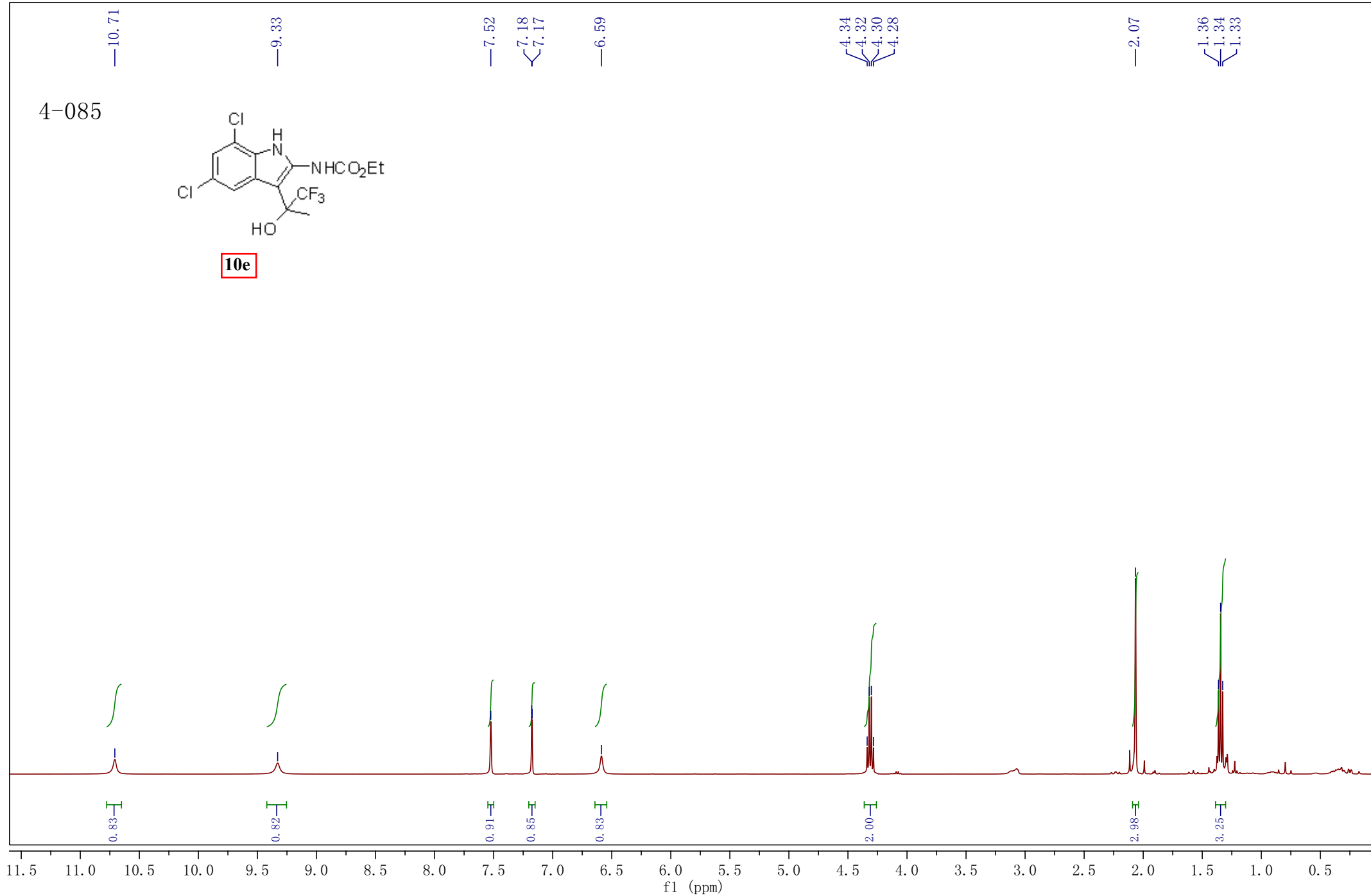


| Peak# | Ret.Time | Area     | Height  | A/H    | Area%    |
|-------|----------|----------|---------|--------|----------|
| 1     | 1.013    | 72404    | 8822    | 8.207  | 0.5864   |
| 2     | 1.659    | 48524    | 4897    | 9.909  | 0.3930   |
| 3     | 2.571    | 37840    | 5891    | 6.423  | 0.3065   |
| 4     | 3.217    | 45036    | 5461    | 8.247  | 0.3648   |
| 5     | 3.740    | 11839872 | 982244  | 12.054 | 95.8920  |
| 6     | 4.391    | 34903    | 2771    | 12.595 | 0.2827   |
| 7     | 5.141    | 176654   | 16093   | 10.977 | 1.4307   |
| 8     | 5.529    | 39531    | 3219    | 12.282 | 0.3202   |
| 9     | 9.440    | 42708    | 2401    | 17.787 | 0.3459   |
| 10    | 11.980   | 9616     | 518     | 18.548 | 0.0779   |
| 全部    |          | 12347088 | 1032317 |        | 100.0000 |

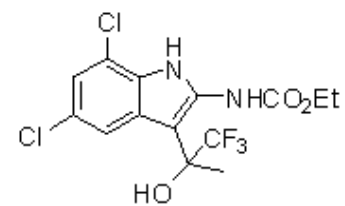
4-085



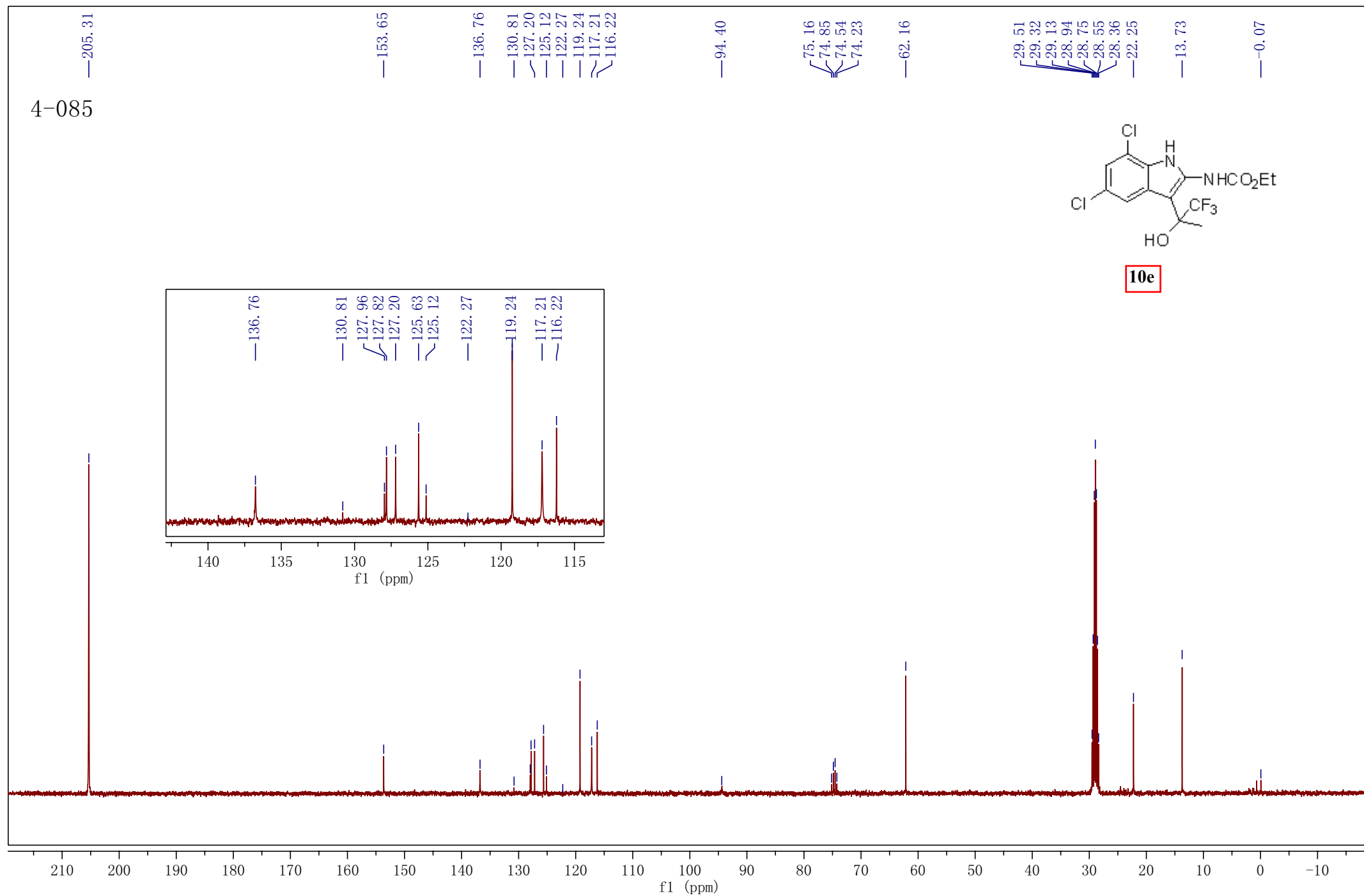
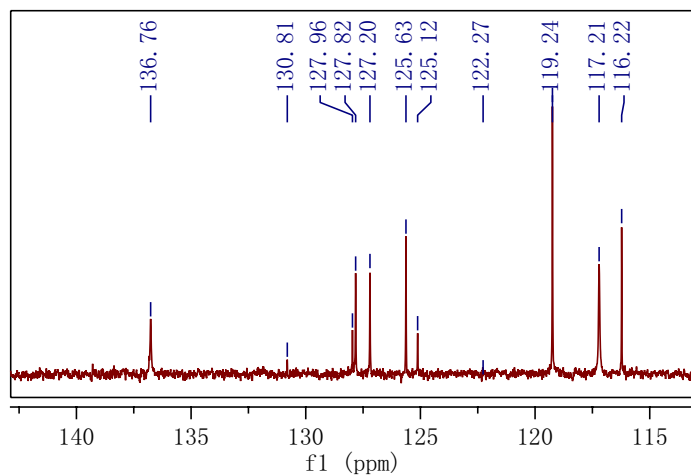
**10e**



4-085



10e

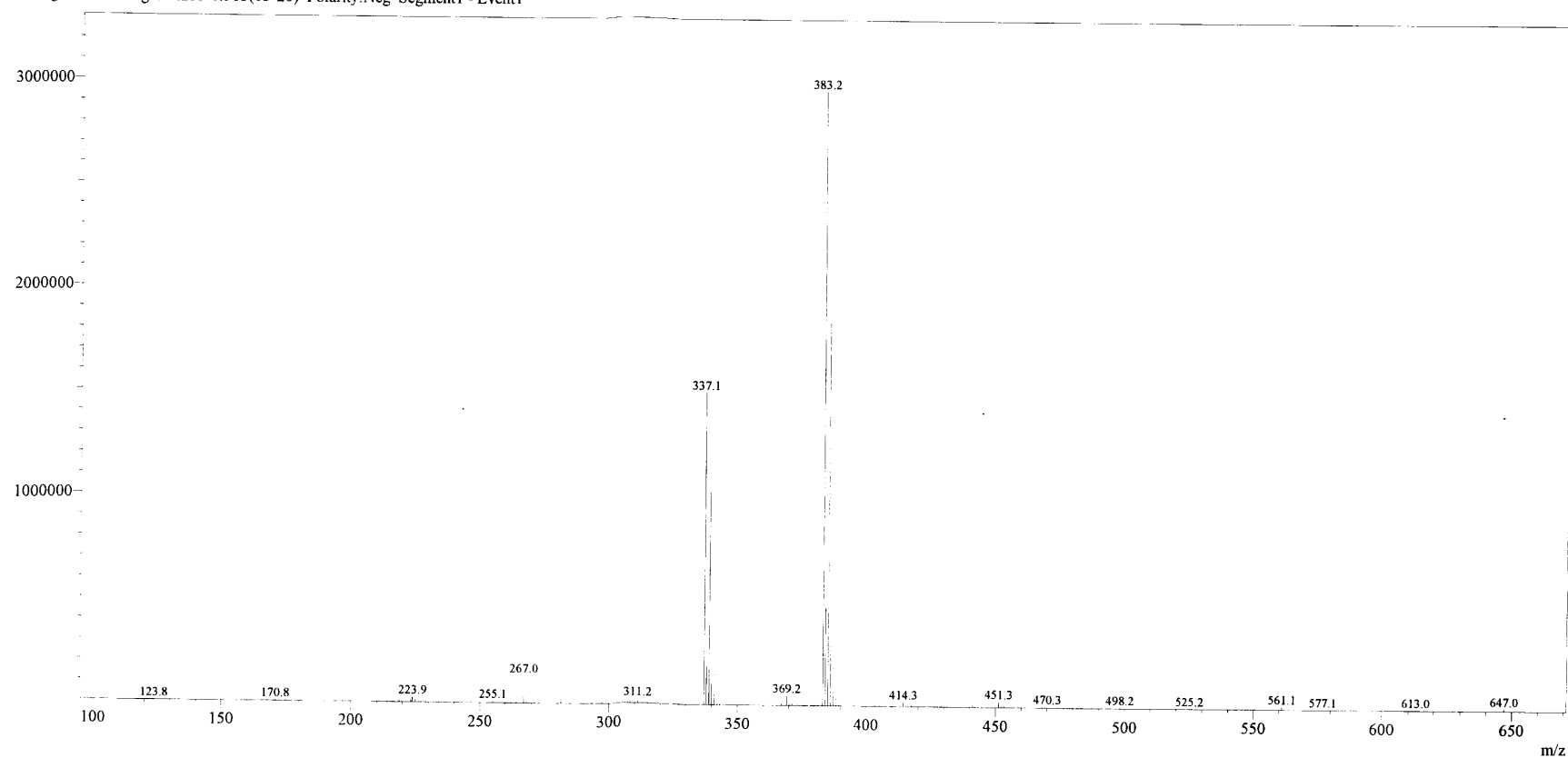


2010-09-14 11:23:51  
4-085

# Sample Information

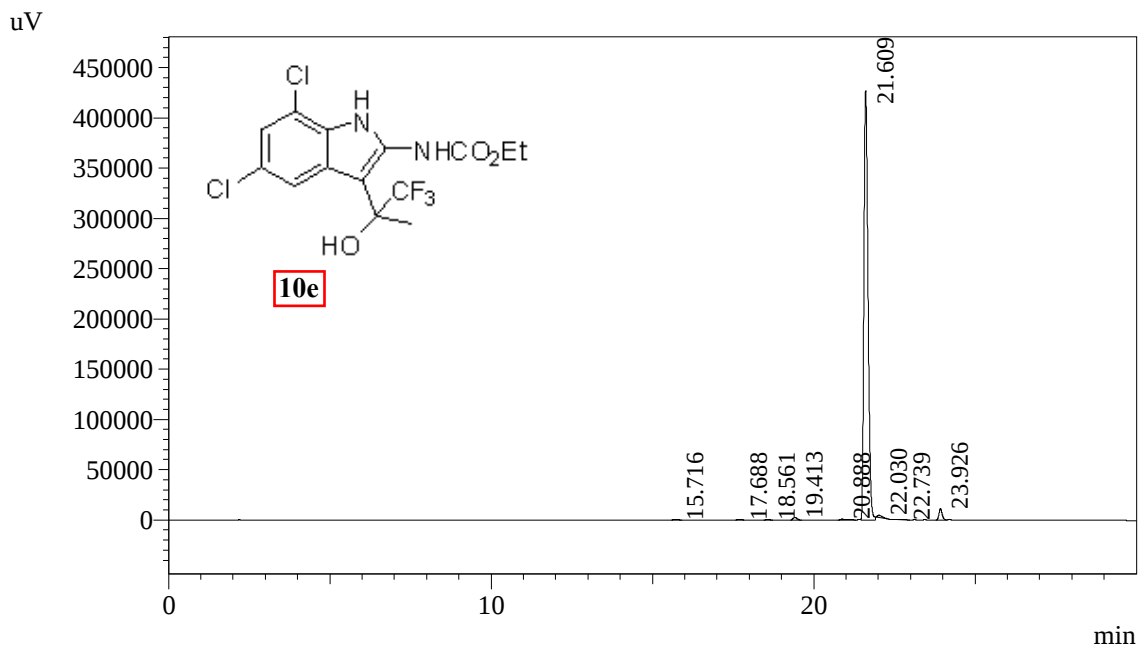
Date Acquired : 9/14/2010 11:21:50 AM  
Sample Name : 4-085  
Sample ID :  
Data File : 4-085-001.lcd  
Method File : HPLC-smyj1.lcm  
Original Data File : D:\DATA\jiangbiao-group\4-085-001.lcd  
Original Method : D:\DATA\HPLC-smyj1.lcm  
Modified Date : 9/14/2010 11:23:51 AM  
Instrument : Shimadzu LCMS-2010EV

Retention Time: 0.600(Scan#:37)  
Max Peak: 546 Base Peak: 383.15(2966884)  
Spectrum: Single 0.600(37)  
Background: Averaged 0.233-0.313(15-20) Polarity: Neg Segment1 - Event1



User Name : CJK  
 Sample ID :  
 Sample Name : 4-085  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6221.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/14 11:54:02

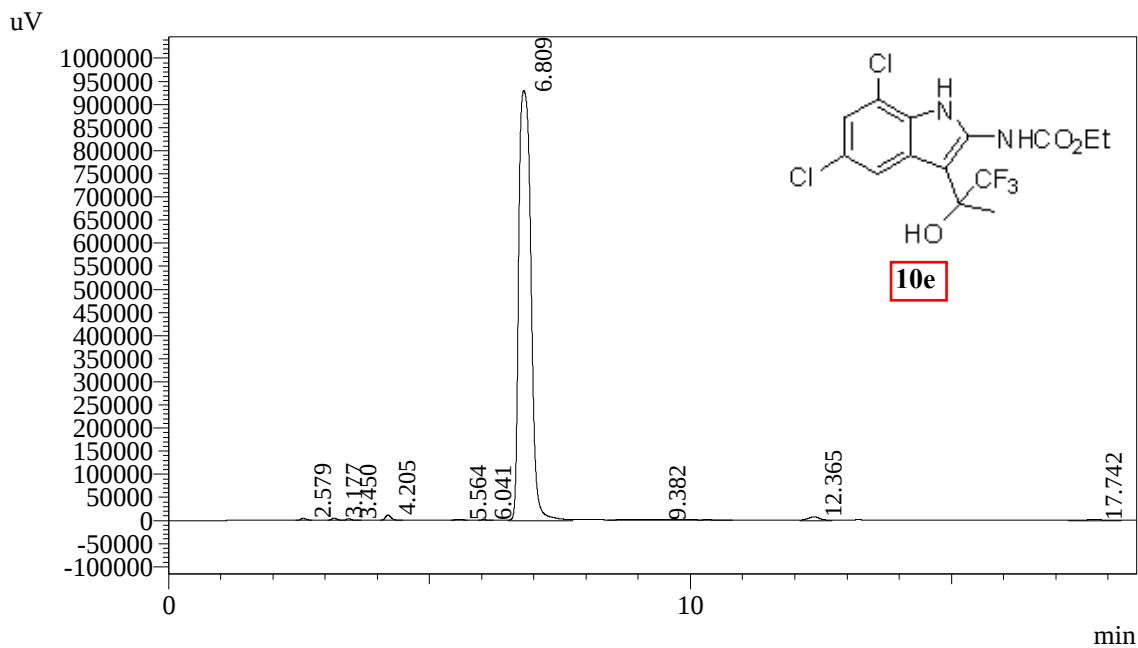
# HPLC



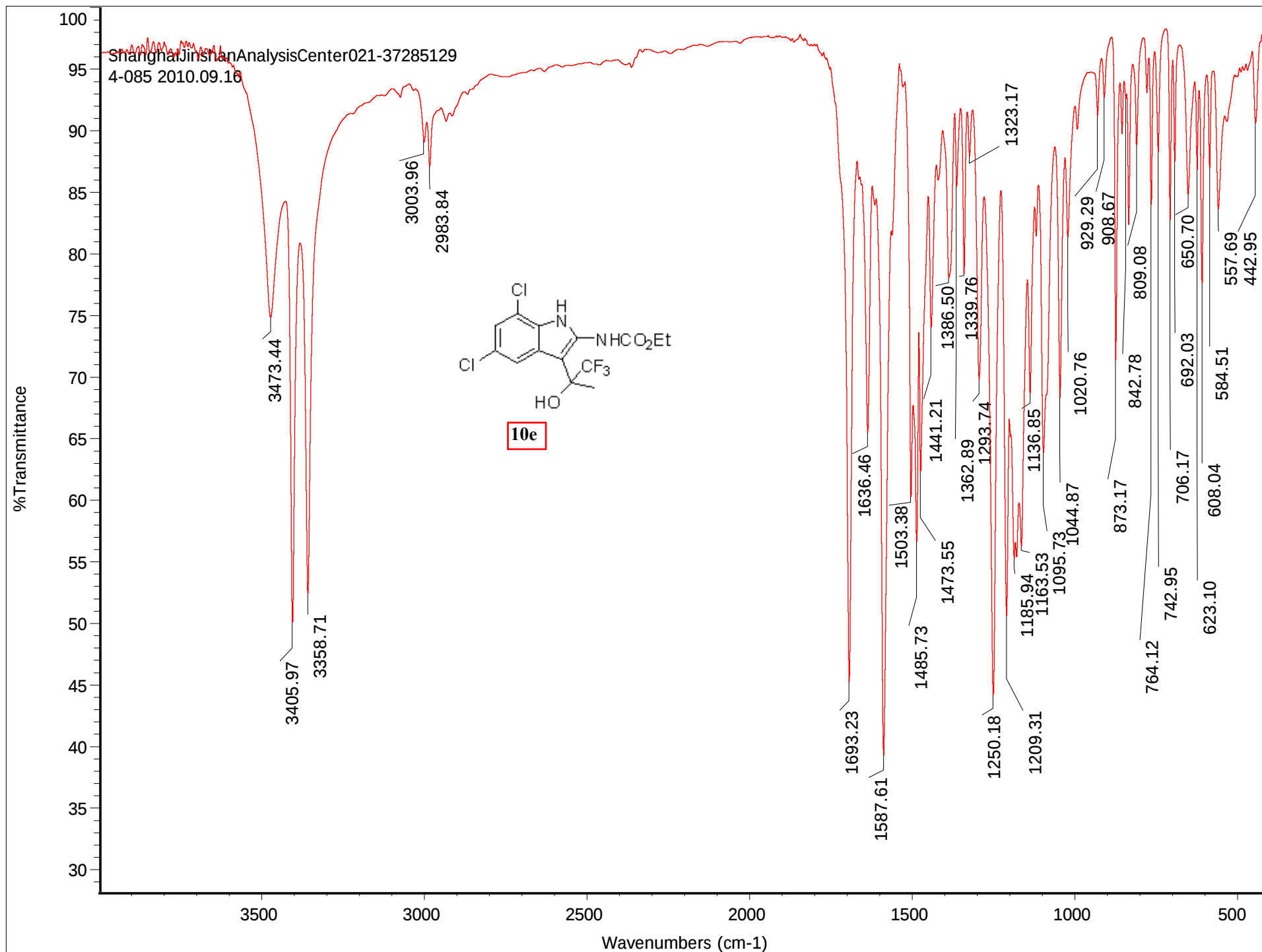
| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 15.716   | 7627    | 786    | 9.701  | 0.1930   |
| 2     | 17.688   | 5260    | 597    | 8.804  | 0.1331   |
| 3     | 18.561   | 6588    | 771    | 8.539  | 0.1667   |
| 4     | 19.413   | 23312   | 2505   | 9.305  | 0.5898   |
| 5     | 20.888   | 14733   | 920    | 16.011 | 0.3728   |
| 6     | 21.609   | 3793105 | 425667 | 8.911  | 95.9674  |
| 7     | 22.030   | 24940   | 2418   | 10.315 | 0.6310   |
| 8     | 22.739   | 2805    | 325    | 8.635  | 0.0710   |
| 9     | 23.926   | 74123   | 11050  | 6.708  | 1.8753   |
| 全部    |          | 3952493 | 445039 |        | 100.0000 |

User Name : CJK  
 Sample ID :  
 Sample Name : 4-085  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6223.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/14 13:07:49

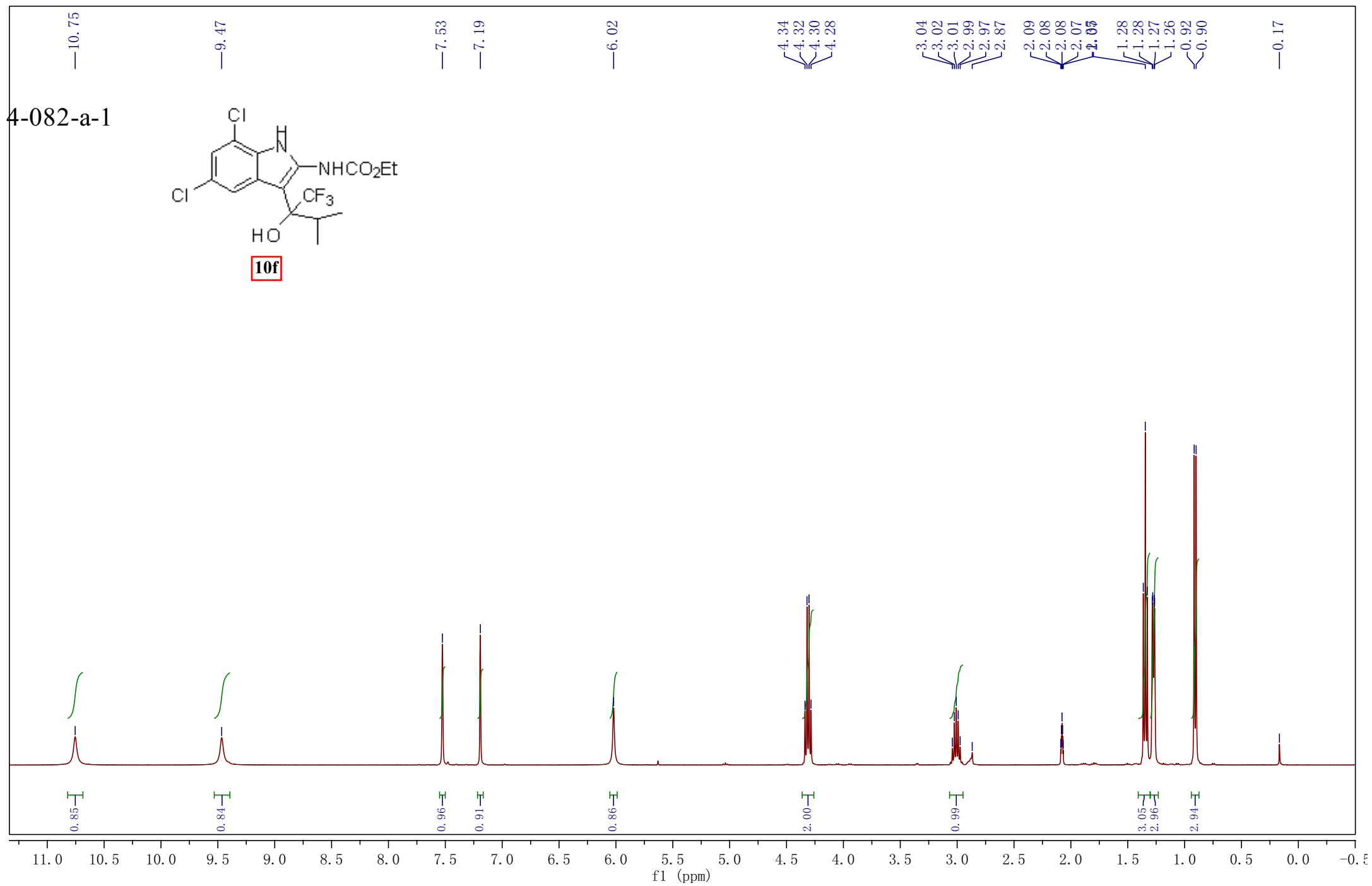
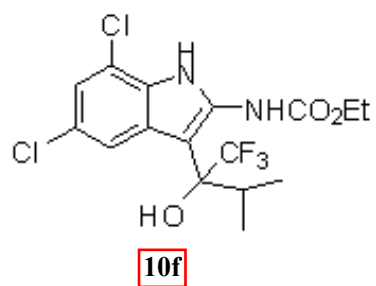
# HPLC



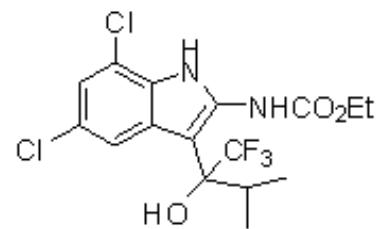
| Peak# | Ret.Time | Area     | Height | A/H    | Area%    |
|-------|----------|----------|--------|--------|----------|
| 1     | 2.579    | 30223    | 4235   | 7.137  | 0.1945   |
| 2     | 3.177    | 30789    | 4709   | 6.538  | 0.1982   |
| 3     | 3.450    | 22159    | 3288   | 6.739  | 0.1426   |
| 4     | 4.205    | 83045    | 11074  | 7.499  | 0.5345   |
| 5     | 5.564    | 15034    | 1784   | 8.428  | 0.0968   |
| 6     | 6.041    | 5922     | 711    | 8.324  | 0.0381   |
| 7     | 6.809    | 15092096 | 929208 | 16.242 | 97.1365  |
| 8     | 9.382    | 53783    | 1397   | 38.493 | 0.3462   |
| 9     | 12.365   | 135012   | 7808   | 17.291 | 0.8690   |
| 10    | 17.742   | 68941    | 1855   | 37.171 | 0.4437   |
| 全部    |          | 15537004 | 966069 |        | 100.0000 |



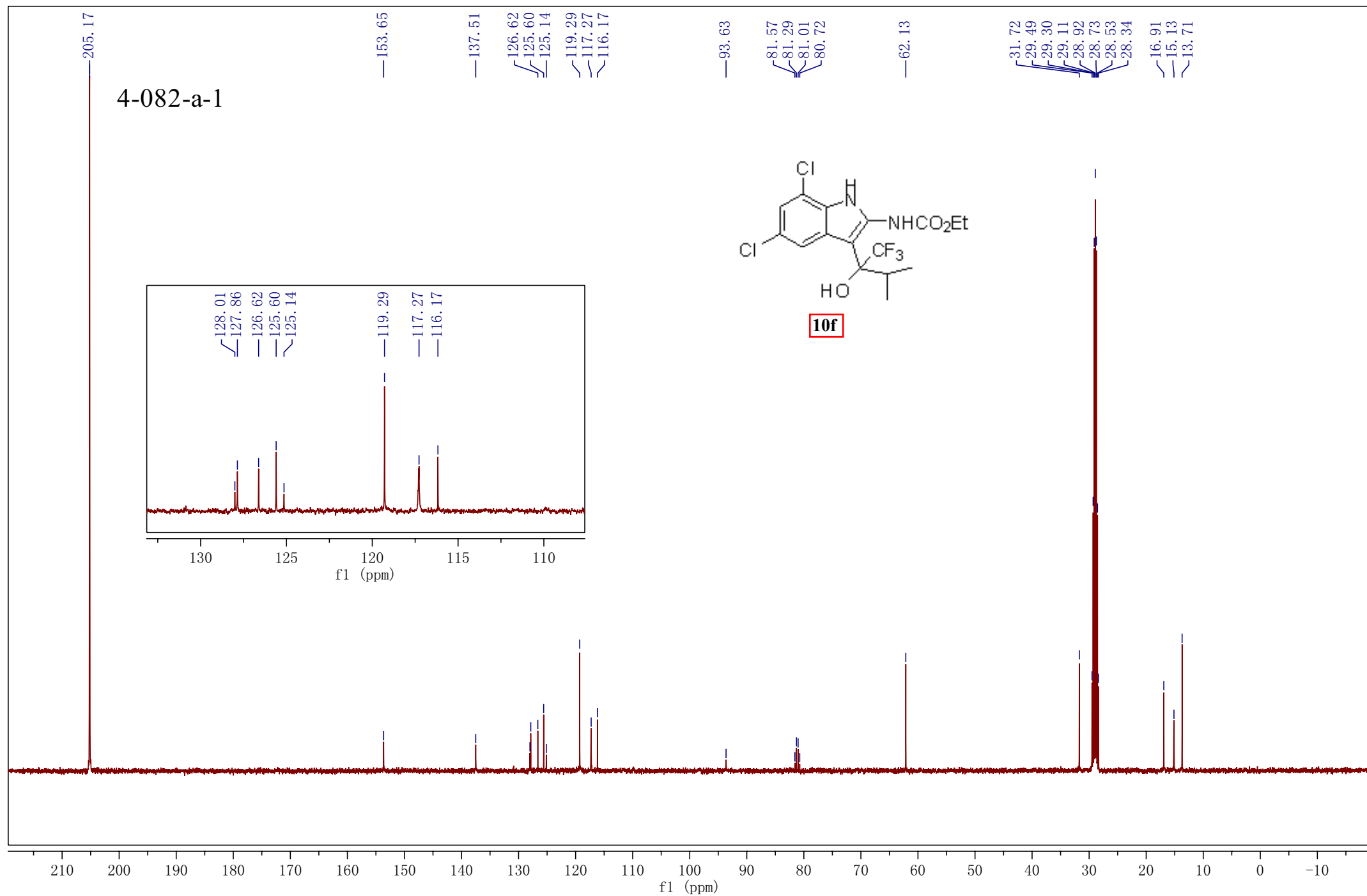
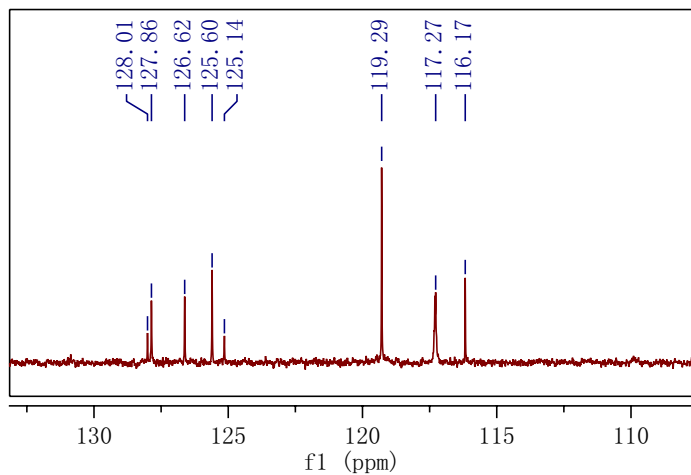
4-082-a-1



4-082-a-1



**10f**



# Sample Information

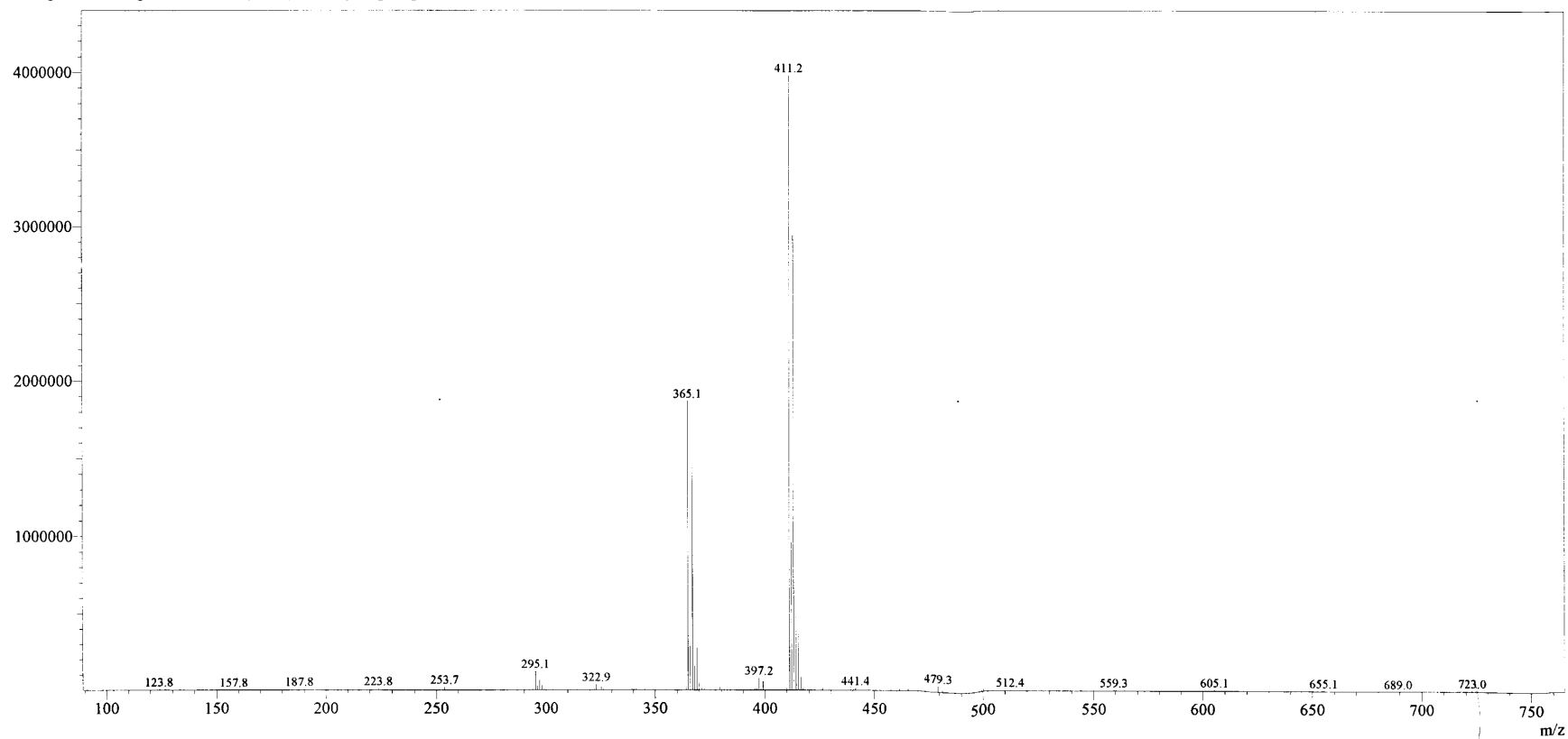
Date Acquired : 9/8/2010 3:53:55 PM  
Sample Name : jhx  
Sample ID : 4-082-2  
Data File : 4-082-2-002.lcd  
Method File : HPLC-smyj1.lcm  
Original Data File : D:\DATA\jiangbiao-group\4-082-2-002.lcd  
Original Method : D:\DATA\HPLC-smyj1.lcm  
Modified Date : 9/8/2010 3:56:03 PM  
Instrument : Shimadzu LCMS-2010EV

Retention Time:0.633(Scan#:39)

Max Peak:819 Base Peak:411.20(3983821)

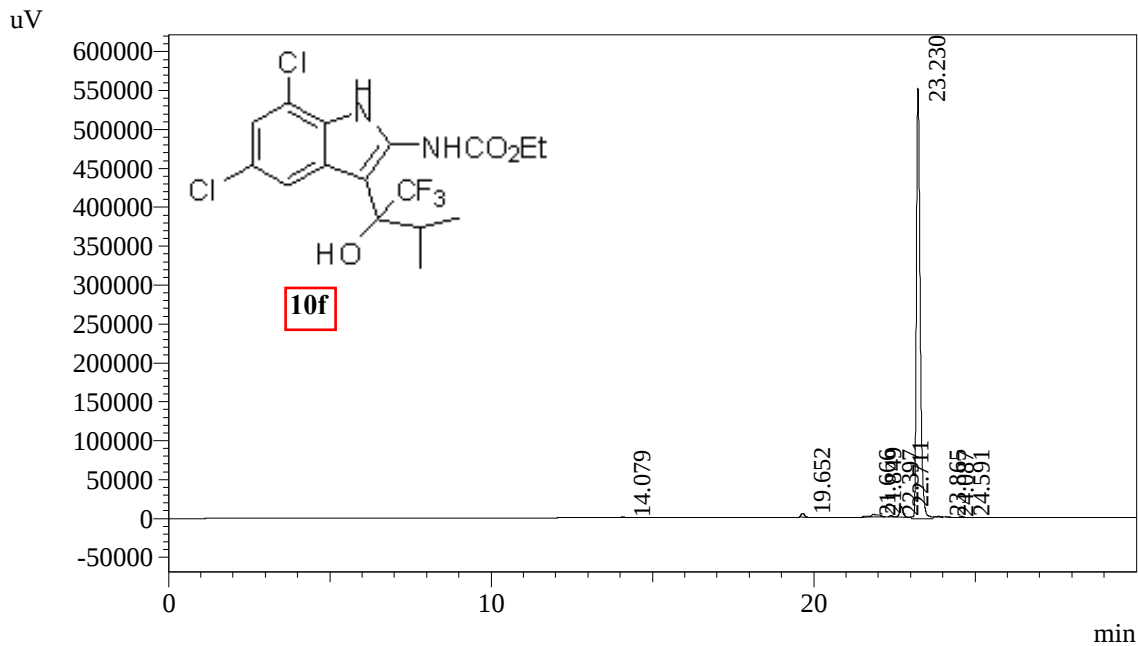
Spectrum:Single 0.633(39)

Background:Averaged 0.267-0.333(17-21) Polarity:Neg Segment1 - Event1



User Name : CJK  
 Sample ID :  
 Sample Name : 4-082-a-1  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6230.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/16 12:35:54

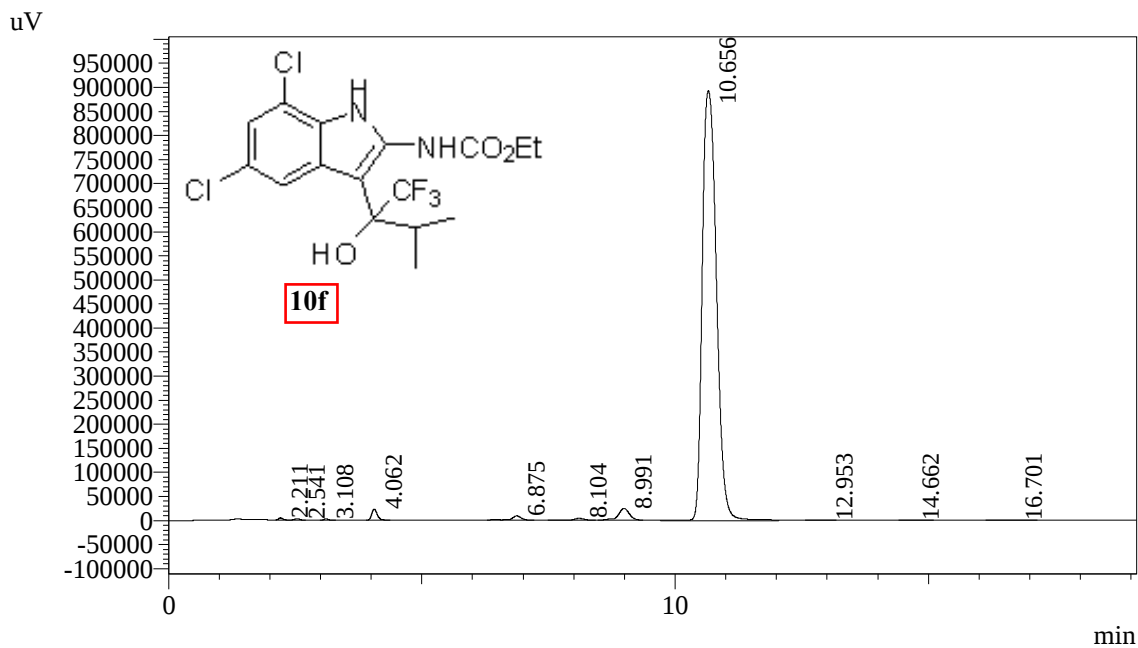
# HPLC



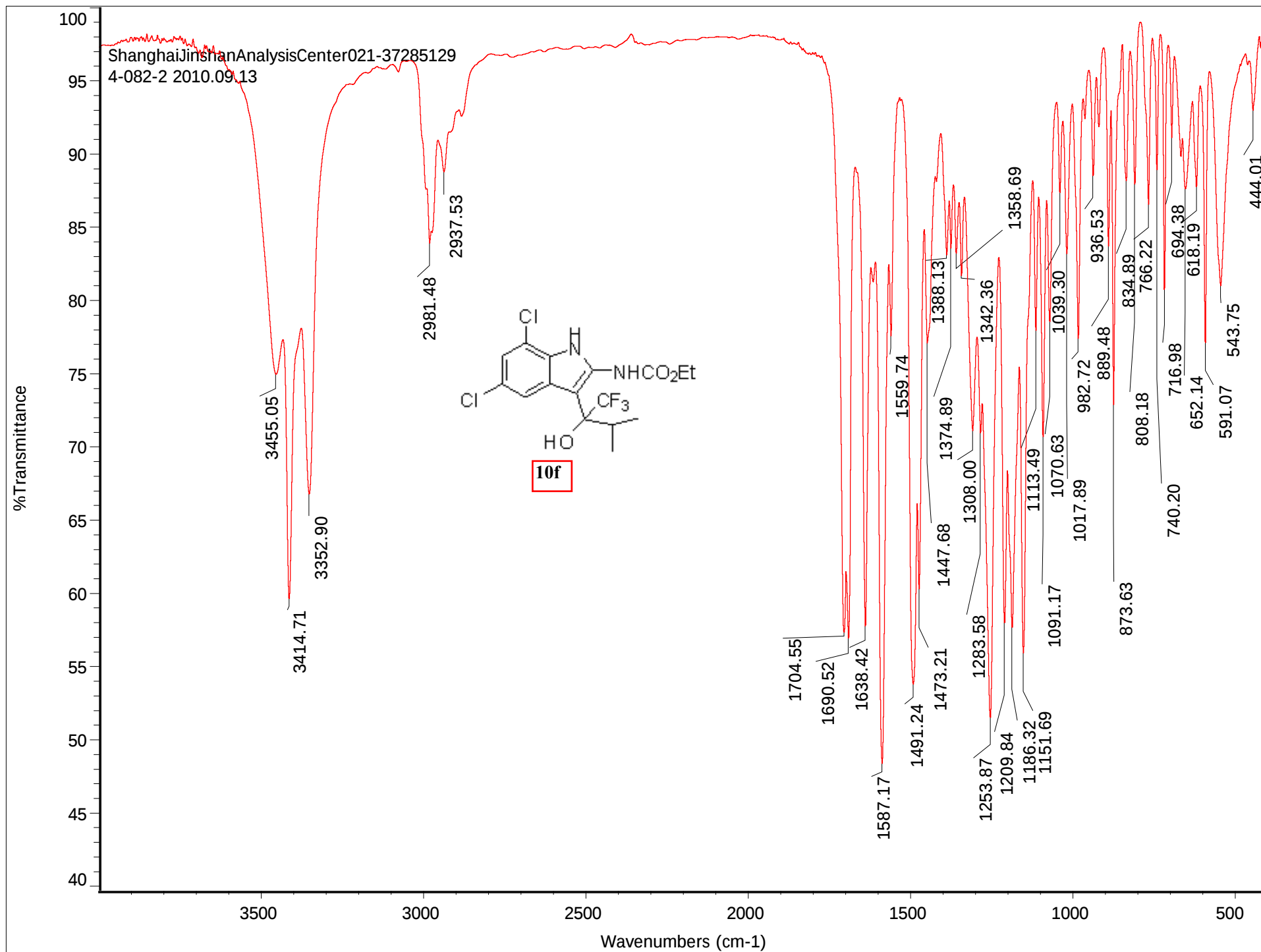
| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 14.079   | 9154    | 959    | 9.542  | 0.1947   |
| 2     | 19.652   | 32857   | 4584   | 7.168  | 0.6989   |
| 3     | 21.666   | 10746   | 960    | 11.190 | 0.2286   |
| 4     | 21.849   | 42500   | 3195   | 13.303 | 0.9040   |
| 5     | 22.397   | 10991   | 1749   | 6.284  | 0.2338   |
| 6     | 22.711   | 101332  | 13348  | 7.591  | 2.1554   |
| 7     | 23.230   | 4477914 | 551085 | 8.126  | 95.2488  |
| 8     | 23.865   | 4018    | 747    | 5.378  | 0.0855   |
| 9     | 24.087   | 3192    | 93     | 34.403 | 0.0679   |
| 10    | 24.591   | 8579    | 1255   | 6.834  | 0.1825   |
| 全部    |          | 4701283 | 577975 |        | 100.0000 |

User Name : CJK  
 Sample ID :  
 Sample Name : 4-082-a-1  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6234.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/16 14:07:01

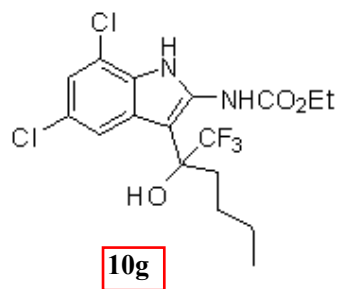
# HPLC



| Peak# | Ret.Time | Area     | Height | A/H    | Area%    |
|-------|----------|----------|--------|--------|----------|
| 1     | 2.211    | 24688    | 4288   | 5.757  | 0.1359   |
| 2     | 2.541    | 21483    | 3164   | 6.789  | 0.1183   |
| 3     | 3.108    | 19631    | 3135   | 6.261  | 0.1081   |
| 4     | 4.062    | 177691   | 23330  | 7.616  | 0.9781   |
| 5     | 6.875    | 127382   | 8884   | 14.338 | 0.7012   |
| 6     | 8.104    | 58316    | 3761   | 15.504 | 0.3210   |
| 7     | 8.991    | 366931   | 24515  | 14.968 | 2.0198   |
| 8     | 10.656   | 17345048 | 892813 | 19.427 | 95.4791  |
| 9     | 12.953   | 3394     | 226    | 15.049 | 0.0187   |
| 10    | 14.662   | 11663    | 602    | 19.383 | 0.0642   |
| 11    | 16.701   | 10113    | 451    | 22.412 | 0.0557   |
| 全部    |          | 18166340 | 965169 |        | 100.0000 |



4-083



—10.75

—9.43

—7.49

7.18  
7.18

—6.35

4.33  
4.32  
4.30  
4.28

—3.14

2.66  
2.66  
2.63

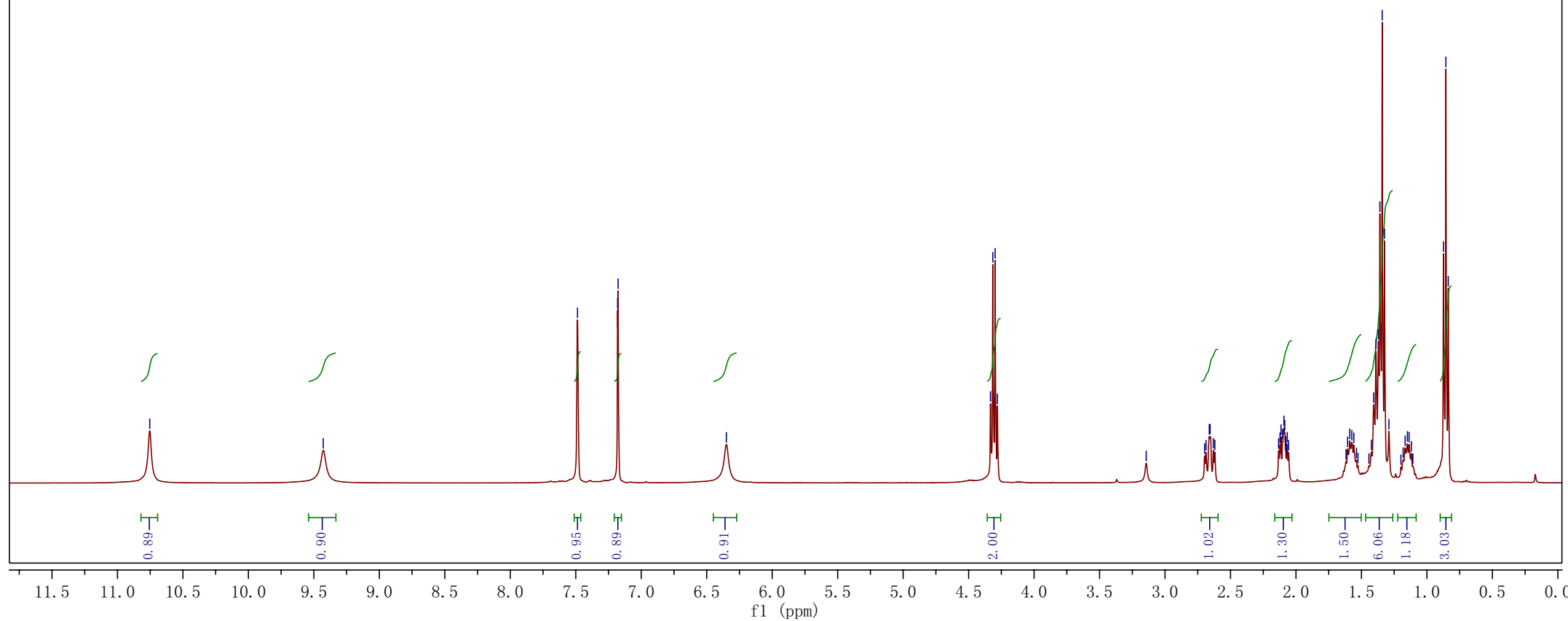
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2.10  
2.09

2.06  
2.06  
1.39

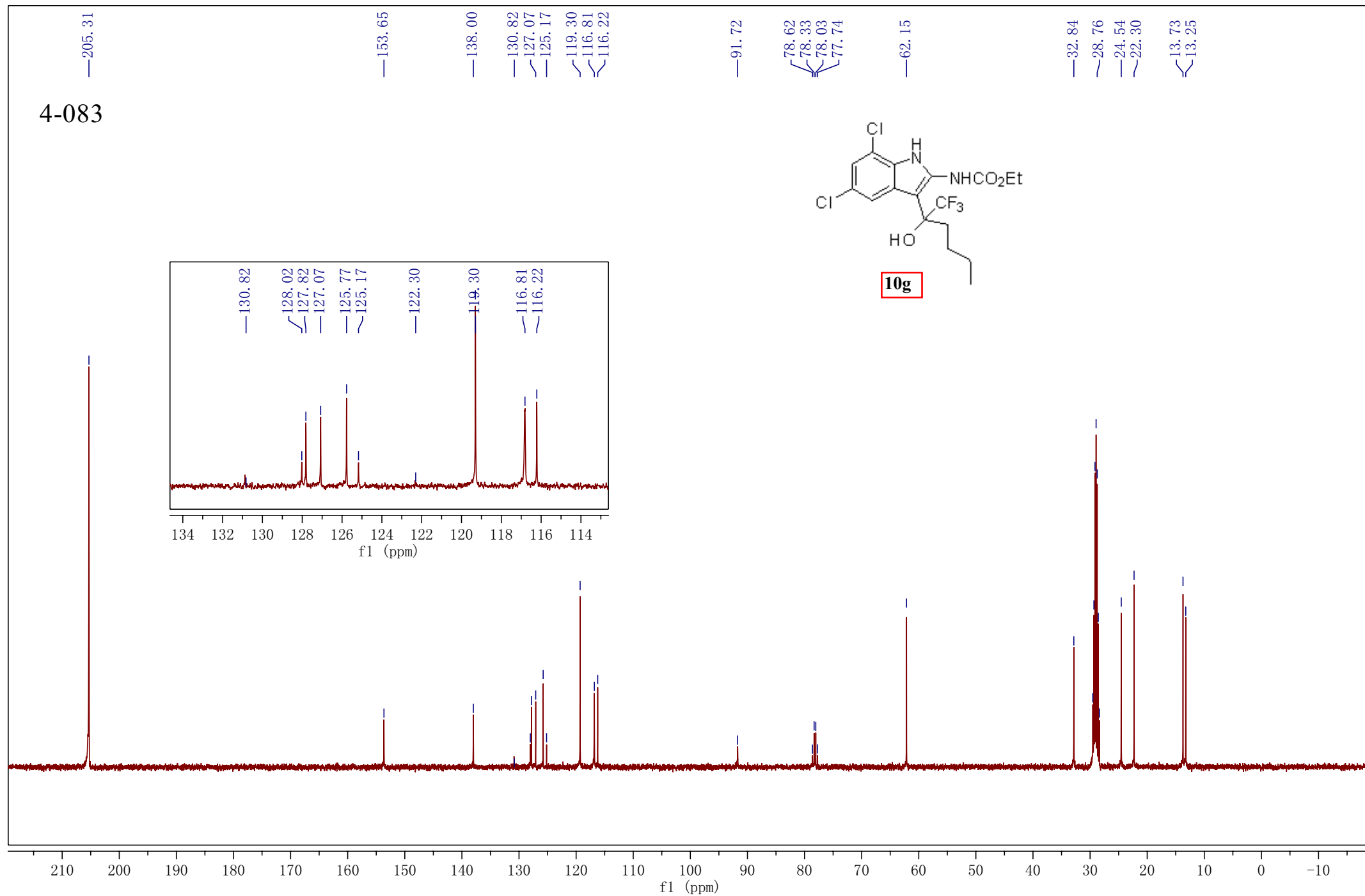
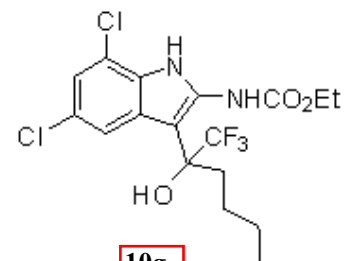
1.34  
1.20  
1.15

1.11  
0.87  
0.86

0.84



4-083



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## Sample Information

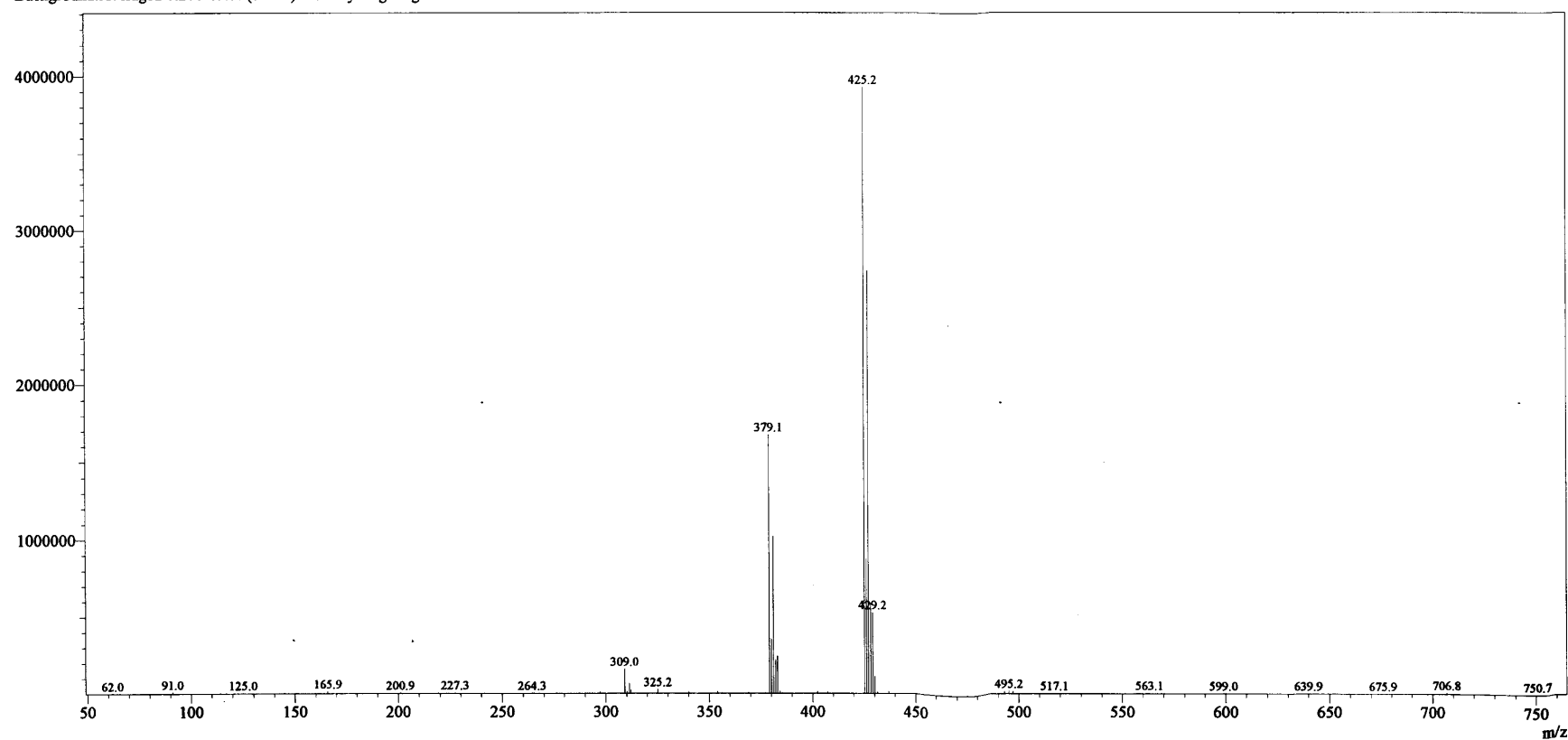
Date Acquired : 9/8/2010 3:51:28 PM  
Sample Name : jhx  
Sample ID : 4-083  
Data File : 4-083-002.lcd  
Method File : HPLC-smyj1.lcm  
Original Data File : D:\DATA\jiangbiao-group\4-083-002.lcd  
Original Method : D:\DATA\HPLC-smyj1.lcm  
Modified Date : 9/8/2010 3:53:34 PM  
Instrument : Shimadzu LCMS-2010EV

Retention Time: 0.767(Scan#: 47)

Max Peak: 749 Base Peak: 425.20(3929545)

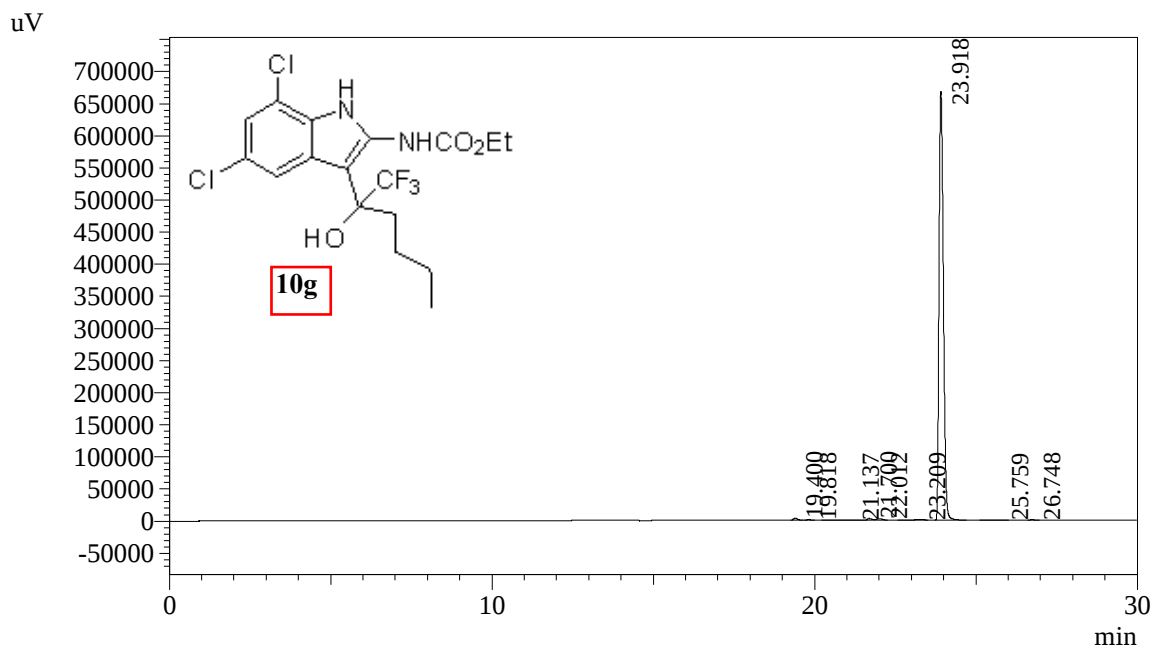
Spectrum: Single 0.767(47)

Background: Averaged 0.200-0.439(13-27) Polarity: Neg Segment1 - Event1



User Name : CJK  
 Sample ID :  
 Sample Name : 4-083  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6186.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/08 13:26:33

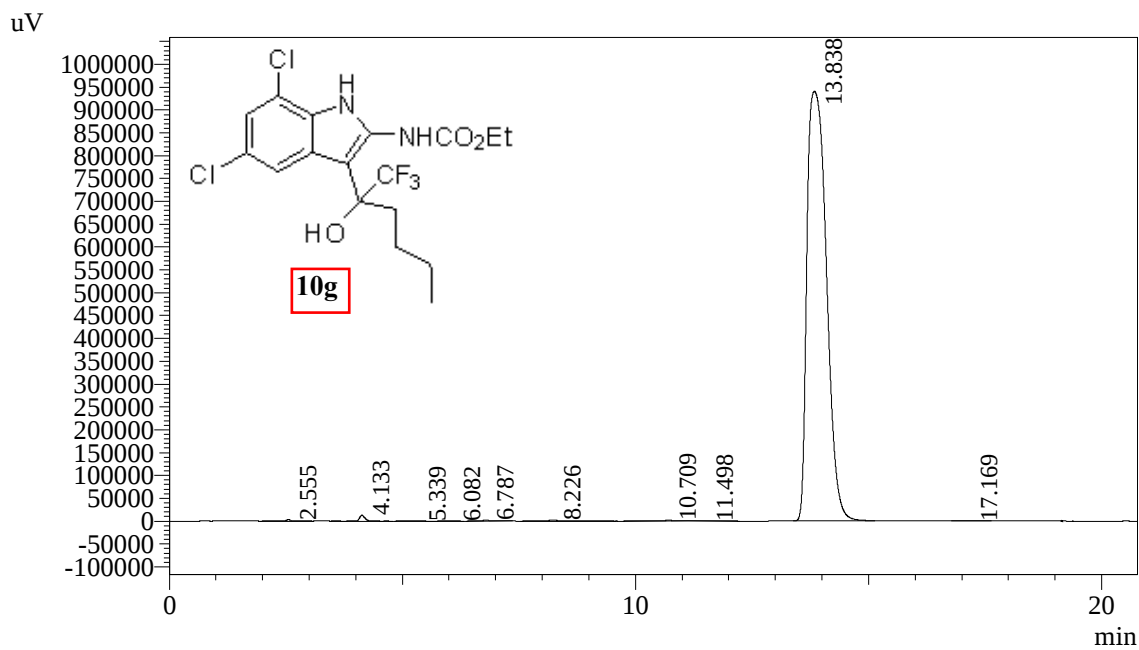
# HPLC



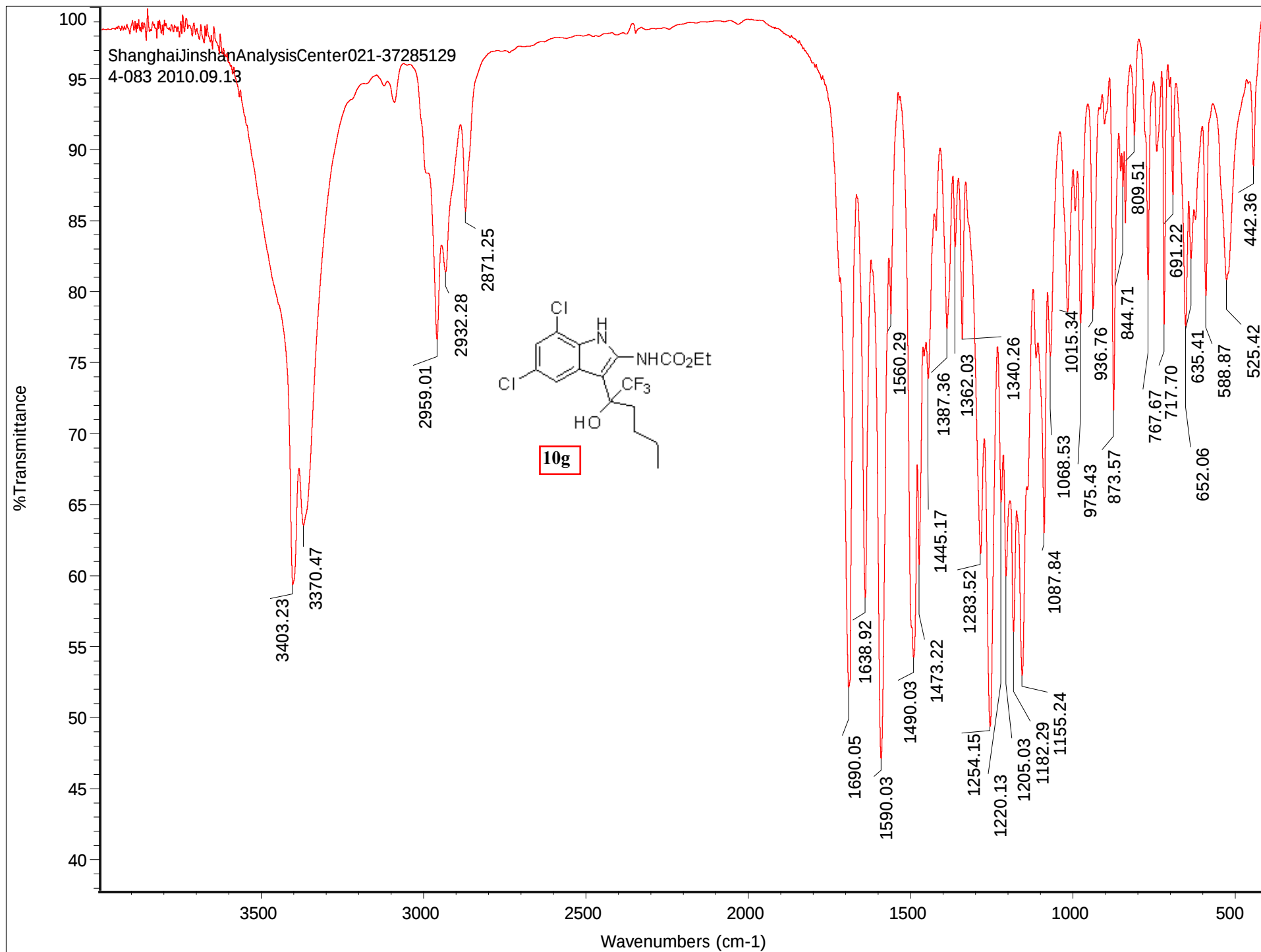
| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 19.400   | 29470   | 2926   | 10.071 | 0.4602   |
| 2     | 19.818   | 7532    | 798    | 9.441  | 0.1176   |
| 3     | 21.137   | 11108   | 374    | 29.717 | 0.1735   |
| 4     | 21.700   | 24550   | 2517   | 9.754  | 0.3834   |
| 5     | 22.012   | 25974   | 2024   | 12.831 | 0.4056   |
| 6     | 23.209   | 25147   | 1336   | 18.823 | 0.3927   |
| 7     | 23.918   | 6262332 | 667456 | 9.382  | 97.7950  |
| 8     | 25.759   | 7769    | 511    | 15.198 | 0.1213   |
| 9     | 26.748   | 9650    | 968    | 9.964  | 0.1507   |
| 全部    |          | 6403532 | 678910 |        | 100.0000 |

User Name : CJK  
 Sample ID :  
 Sample Name : 4-083  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6190.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/08 15:37:16

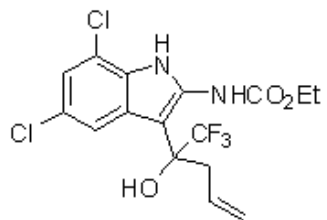
# HPLC



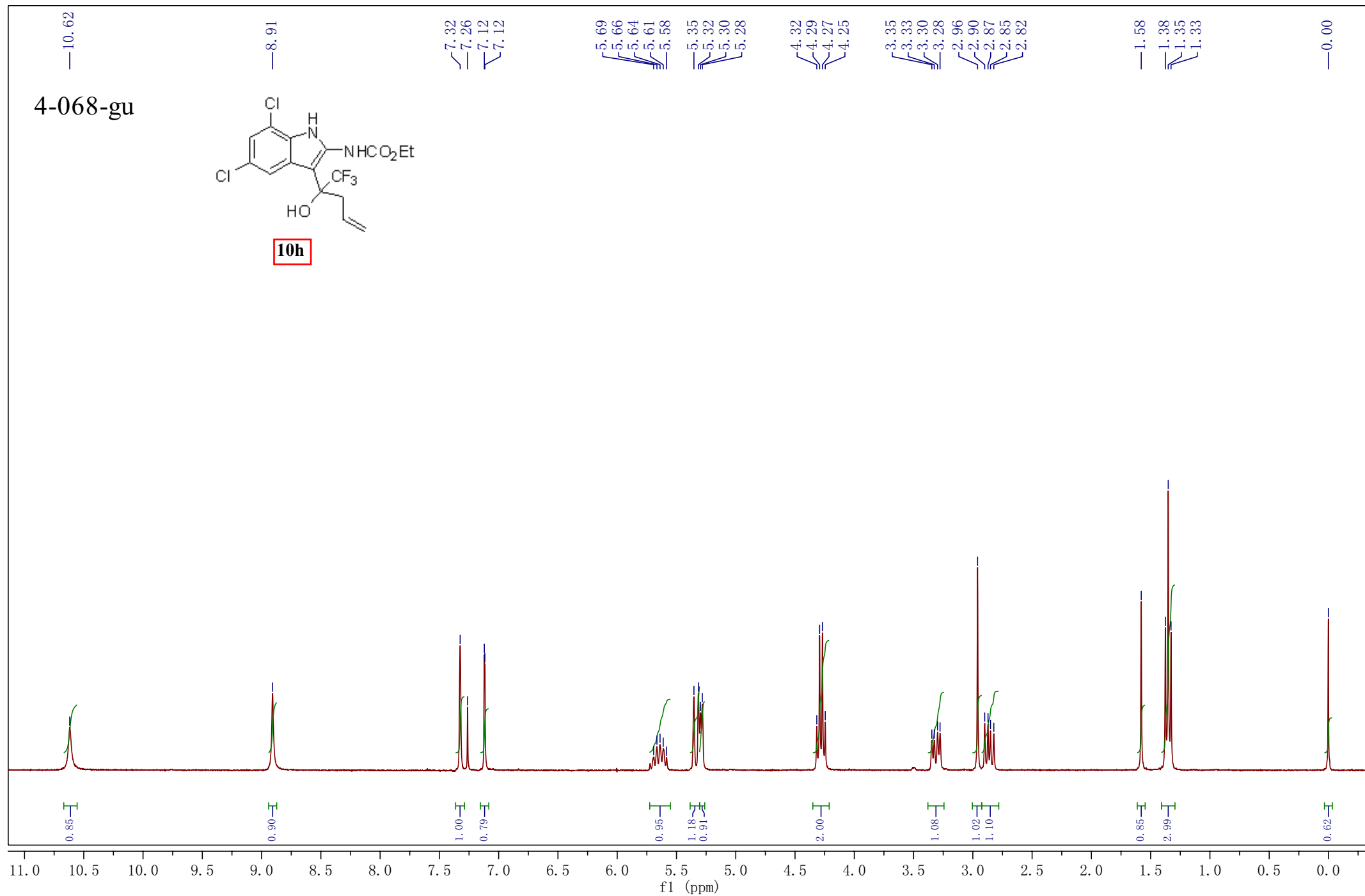
| Peak# | Ret.Time | Area     | Height | A/H    | Area%    |
|-------|----------|----------|--------|--------|----------|
| 1     | 2.555    | 37246    | 3196   | 11.655 | 0.1351   |
| 2     | 4.133    | 107677   | 13013  | 8.275  | 0.3907   |
| 3     | 5.339    | 13425    | 791    | 16.963 | 0.0487   |
| 4     | 6.082    | 12615    | 782    | 16.135 | 0.0458   |
| 5     | 6.787    | 36962    | 2010   | 18.385 | 0.1341   |
| 6     | 8.226    | 41618    | 2182   | 19.070 | 0.1510   |
| 7     | 10.709   | 45037    | 1594   | 28.254 | 0.1634   |
| 8     | 11.498   | 13387    | 596    | 22.458 | 0.0486   |
| 9     | 13.838   | 27252194 | 940244 | 28.984 | 98.8706  |
| 10    | 17.169   | 3324     | 138    | 24.010 | 0.0121   |
| 全部    |          | 27563485 | 964546 |        | 100.0000 |



4-068-gu



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## Sample Information

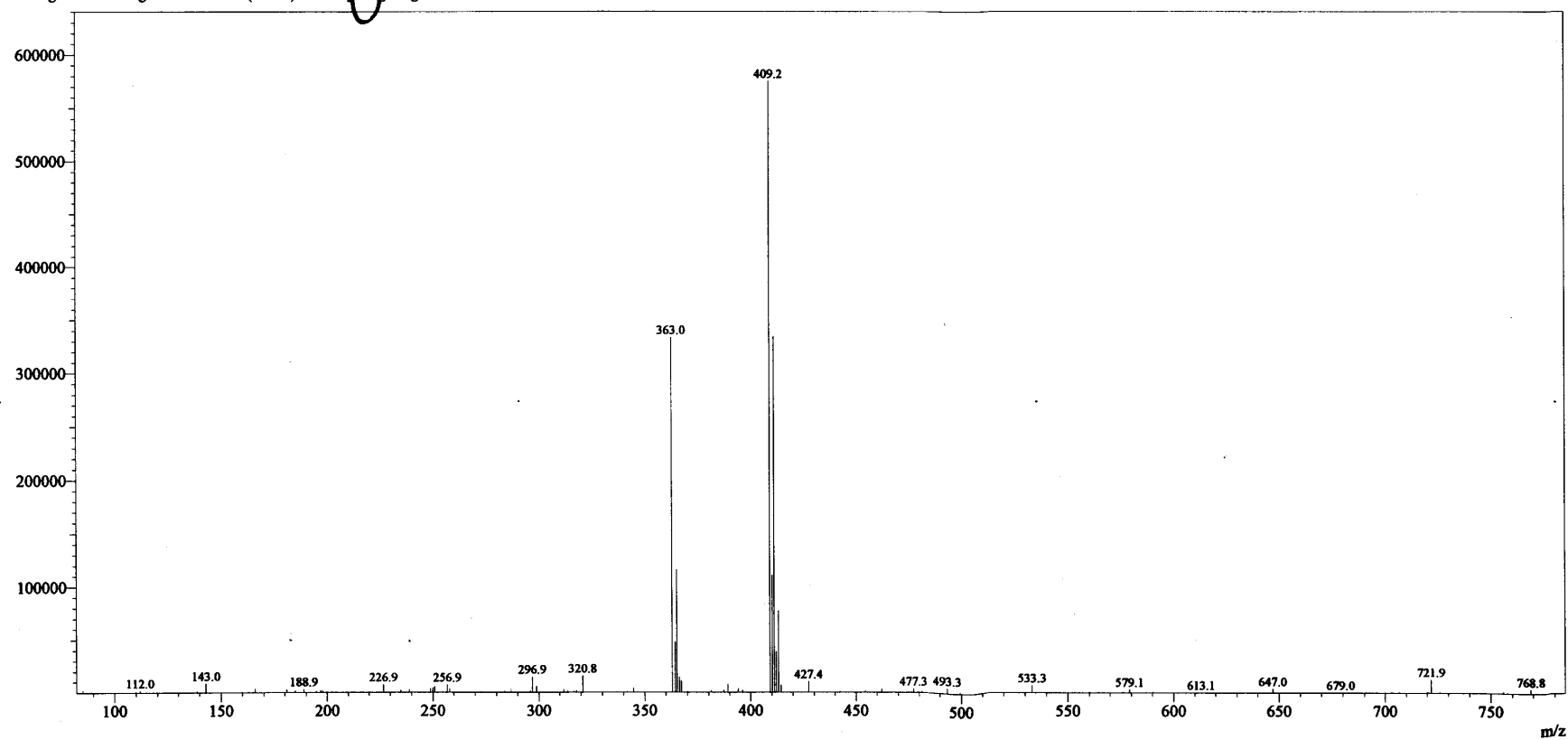
Date Acquired : 9/8/2010 3:49:00 PM  
Sample Name : jhx  
Sample ID : 4-068  
Data File : 4-068-002.lcd  
Method File : HPLC-smyj1.lcm  
Original Data File : D:\DATA\jiangbiao-group\4-068-002.lcd  
Original Method : D:\DATA\HPLC-smyj1.lcm  
Modified Date : 9/8/2010 3:51:07 PM  
Instrument : Shimadzu LCMS-2010EV

Retention Time: 1.067(Scan#:65)

Max Peak: 751 Base Peak: 409.15(575195)

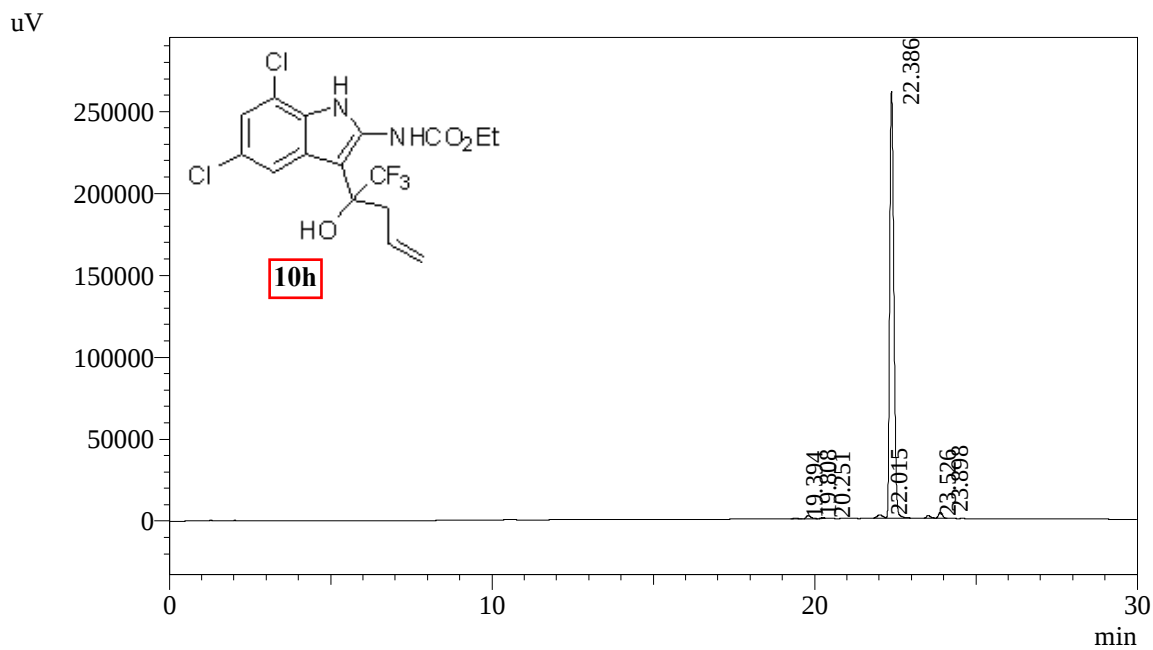
Spectrum: Single 1.067(65)

Background: Averaged 0.283-0.360(18-23) Polarity: Neg Segment1 - Event1



User Name : CJK  
 Sample ID :  
 Sample Name : 4-068  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6183.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/08 11:37:39

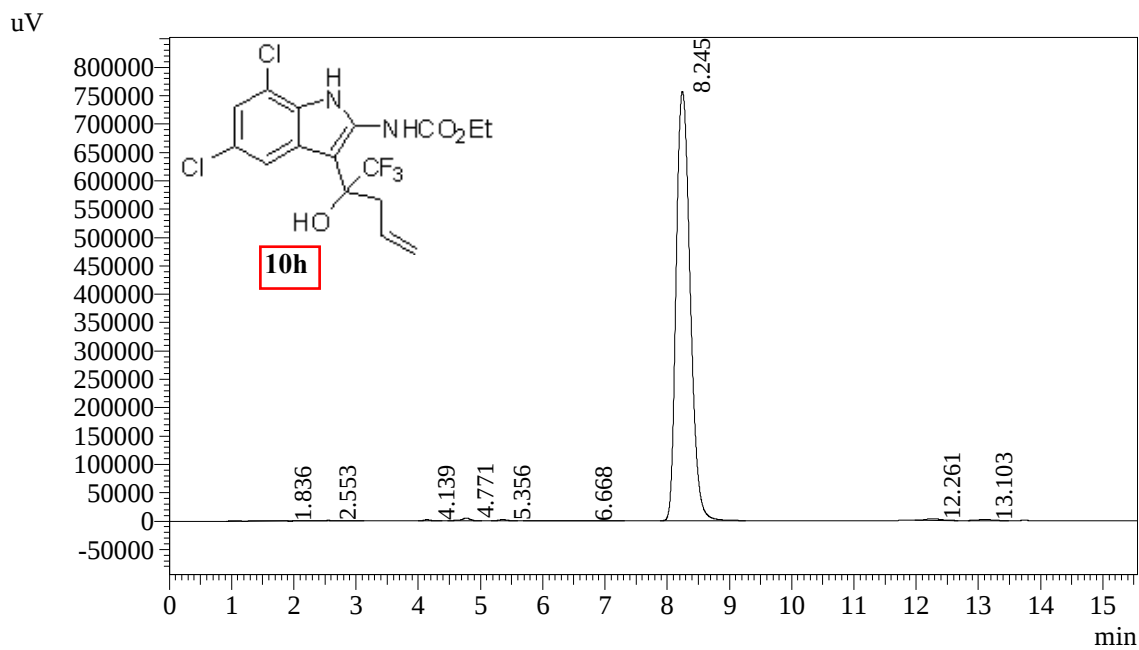
# HPLC



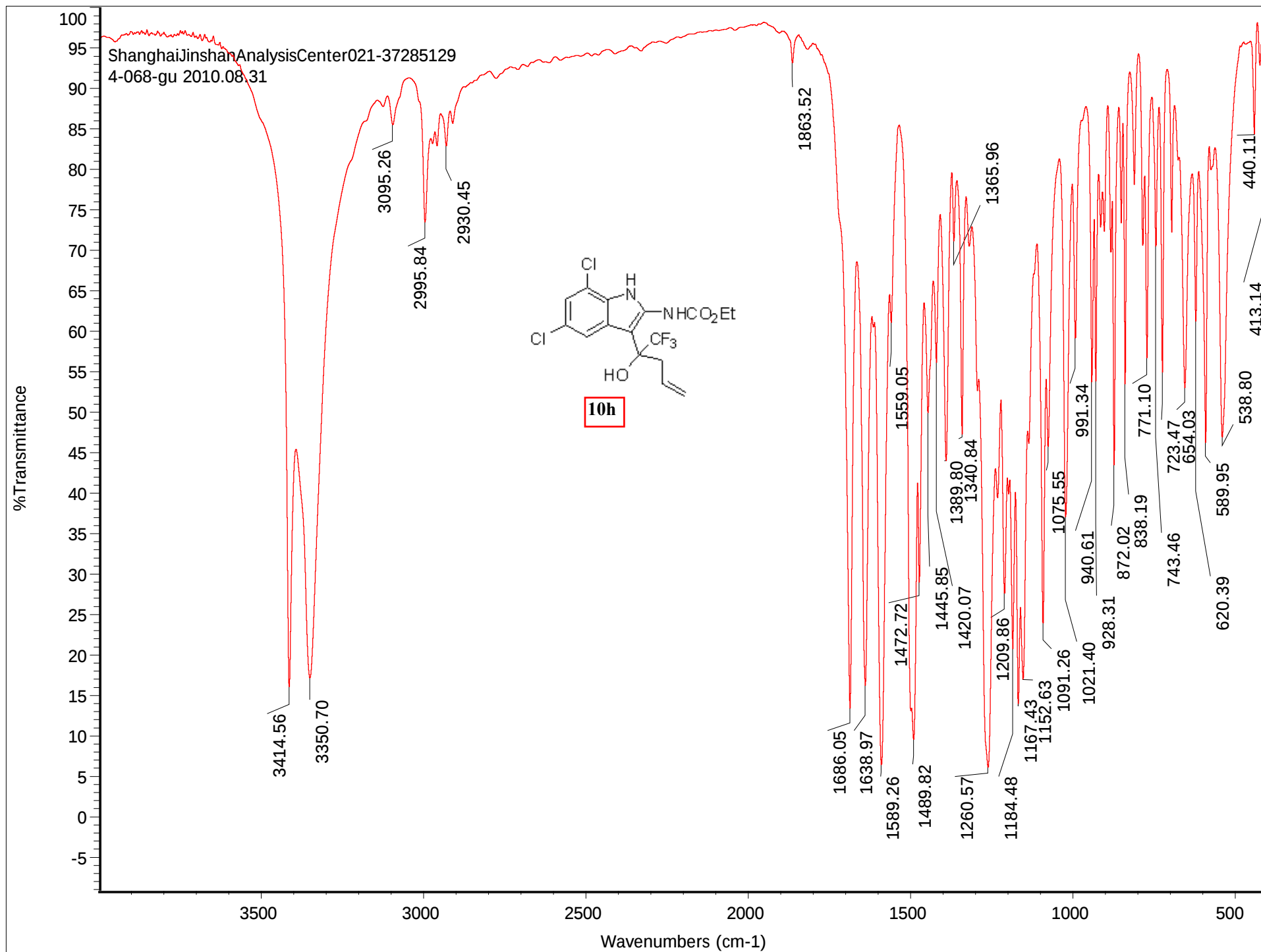
| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 19.394   | 4706    | 431    | 10.922 | 0.1953   |
| 2     | 19.808   | 19125   | 1892   | 10.110 | 0.7938   |
| 3     | 20.251   | 2801    | 402    | 6.975  | 0.1163   |
| 4     | 22.015   | 23237   | 2002   | 11.607 | 0.9644   |
| 5     | 22.386   | 2317006 | 260140 | 8.907  | 96.1645  |
| 6     | 23.526   | 13450   | 1670   | 8.054  | 0.5582   |
| 7     | 23.898   | 29094   | 3689   | 7.887  | 1.2075   |
| 全部    |          | 2409419 | 270226 |        | 100.0000 |

User Name : CJK  
 Sample ID :  
 Sample Name : 4-068  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6189.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/08 15:20:12

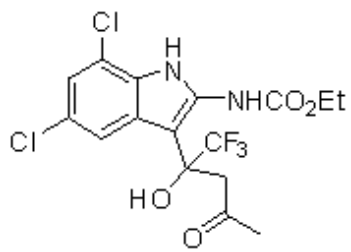
# HPLC



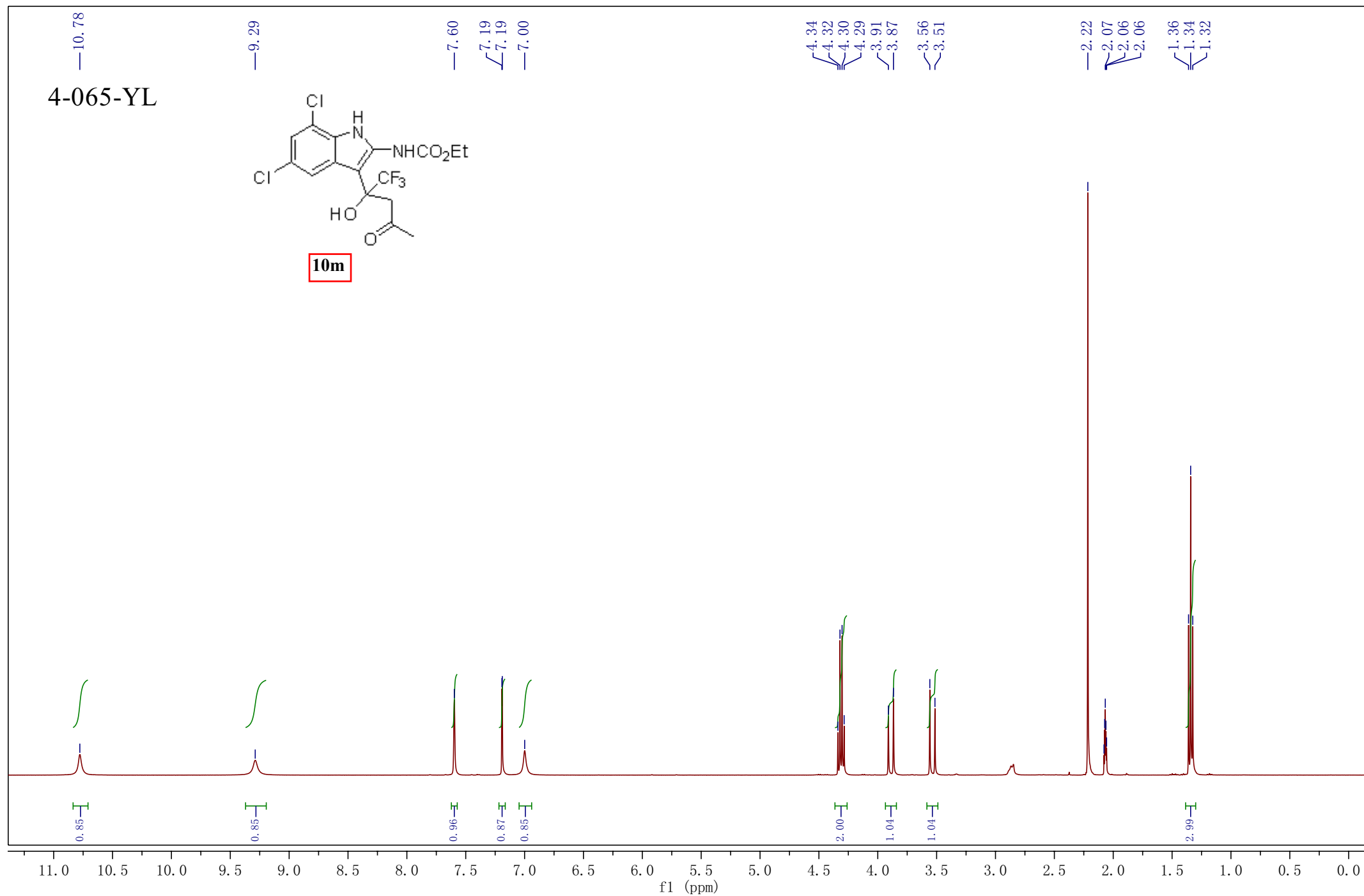
| Peak# | Ret.Time | Area     | Height | A/H    | Area%    |
|-------|----------|----------|--------|--------|----------|
| 1     | 1.836    | 13633    | 859    | 15.869 | 0.1130   |
| 2     | 2.553    | 14934    | 1195   | 12.494 | 0.1238   |
| 3     | 4.139    | 16417    | 2111   | 7.779  | 0.1361   |
| 4     | 4.771    | 52540    | 4947   | 10.621 | 0.4354   |
| 5     | 5.356    | 20869    | 2151   | 9.701  | 0.1730   |
| 6     | 6.668    | 16965    | 624    | 27.185 | 0.1406   |
| 7     | 8.245    | 11850595 | 756701 | 15.661 | 98.2119  |
| 8     | 12.261   | 50594    | 3113   | 16.250 | 0.4193   |
| 9     | 13.103   | 29800    | 1741   | 17.115 | 0.2470   |
| 全部    |          | 12066347 | 773442 |        | 100.0000 |



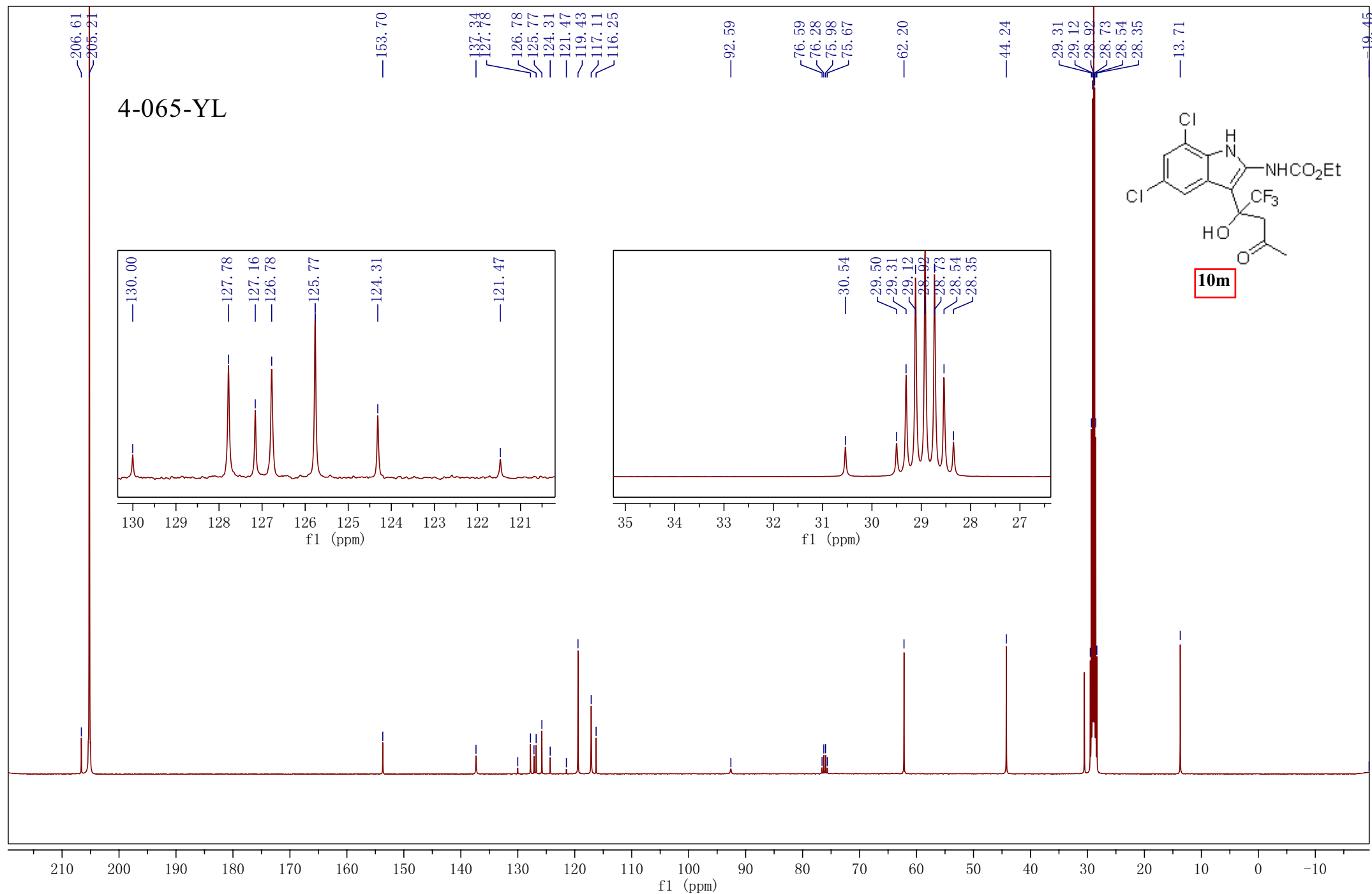
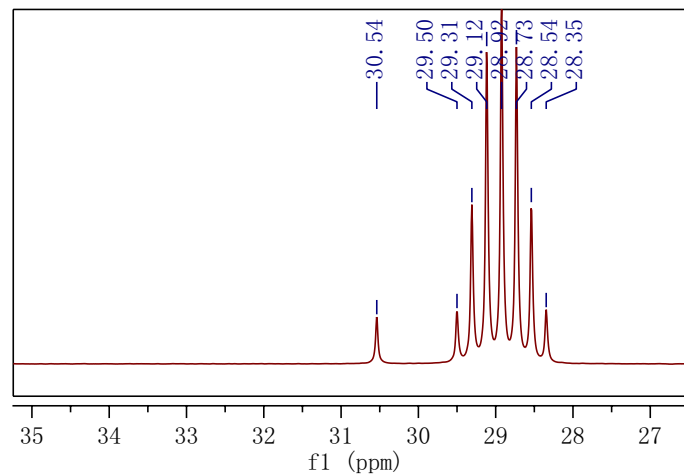
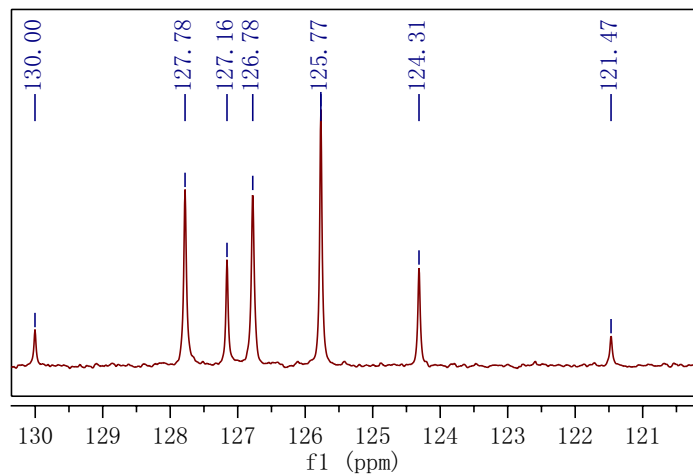
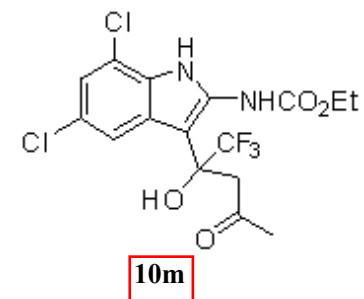
4-065-YL



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4-065-YL



4-05-YL-

新皮

## Sample Information

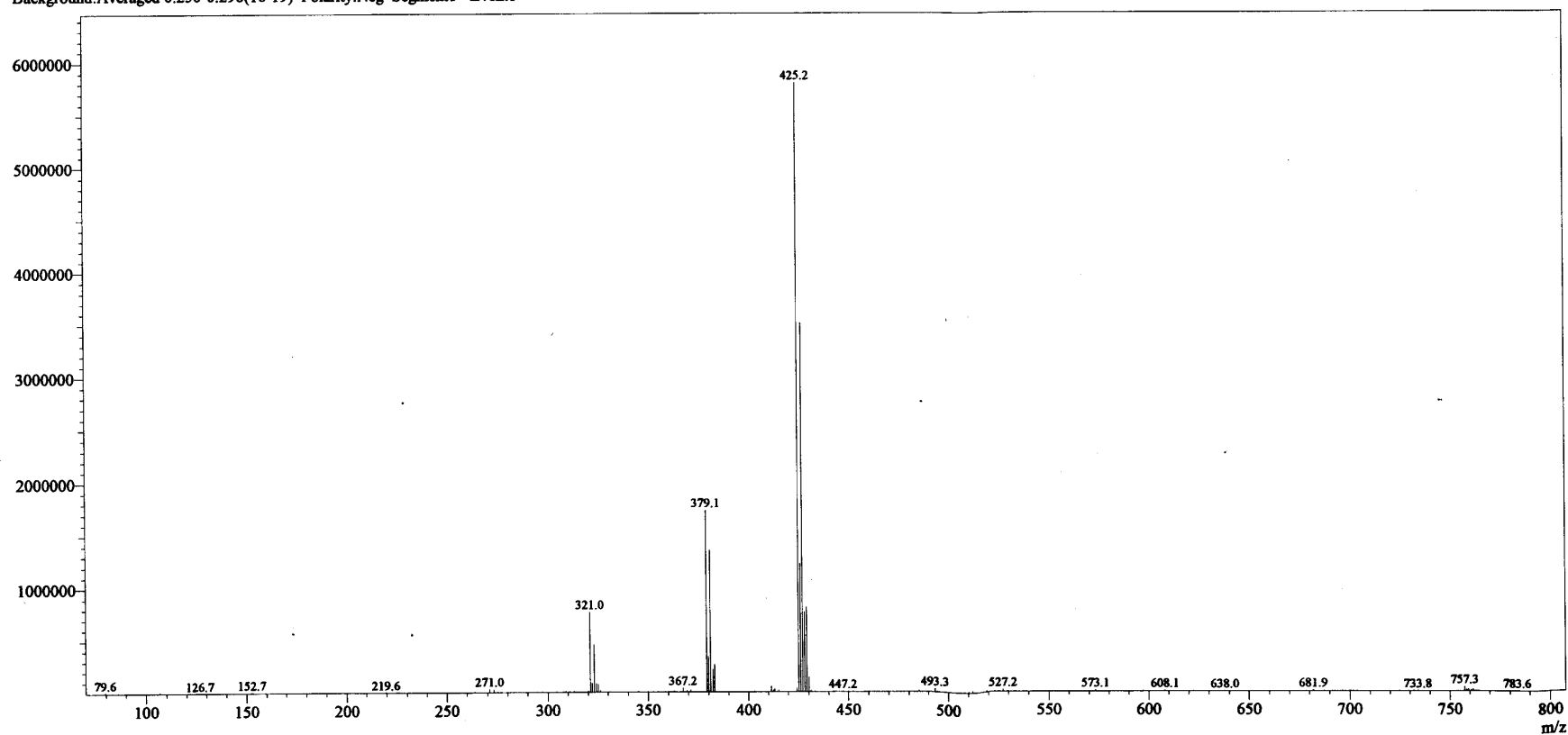
Date Acquired : 9/8/2010 3:56:22 PM  
Sample Name : jhx  
Sample ID : cx-85-hou  
Data File : cx-85-hou-002.lcd  
Method File : HPLC-smyj1.lcm  
Original Data File : D:\DATA\jiangbiao-group\cx-85-hou-002.lcd  
Original Method : D:\DATA\HPLC-smyj1.lcm  
Modified Date : 9/8/2010 3:58:26 PM  
Instrument : Shimadzu LCMS-2010EV

Retention Time:0.617(Scan#:38)

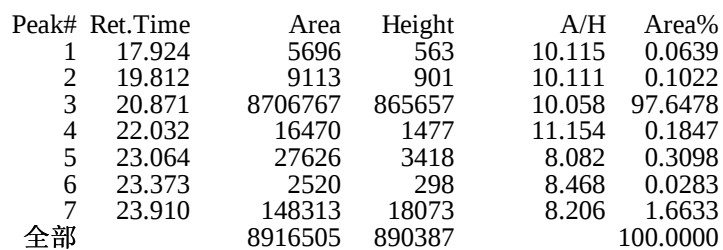
Max Peak:817 Base Peak:425.15(5806971)

Spectrum:Single 0.617(38)

Background:Averaged 0.250-0.296(16-19) Polarity:Neg Segment1 - Event1

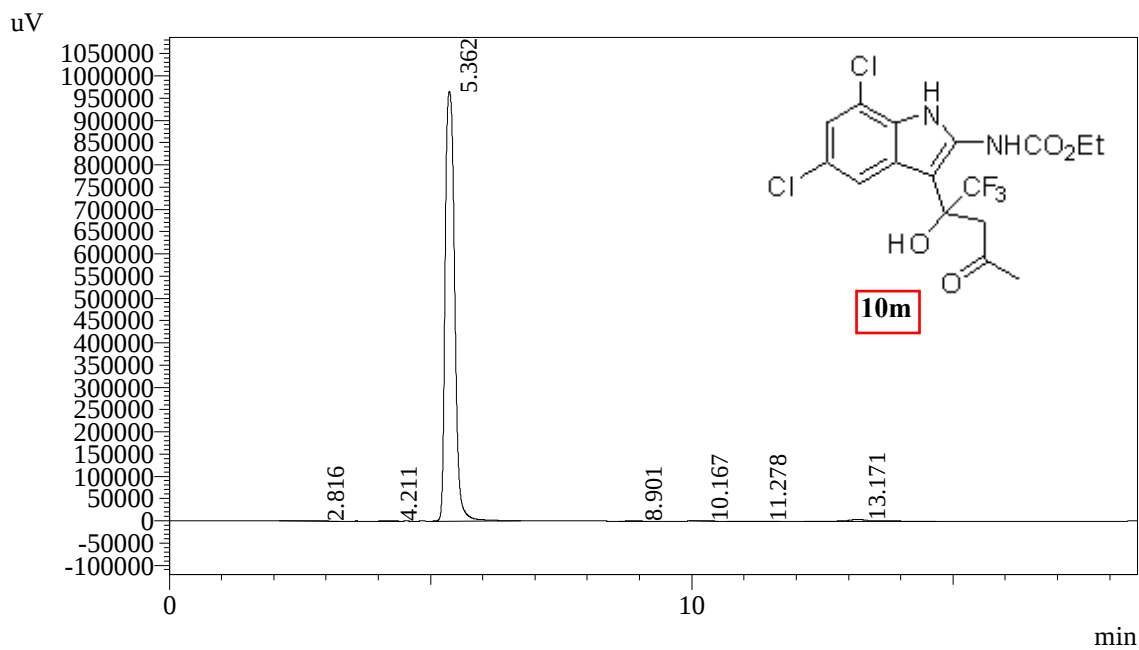


HPLC

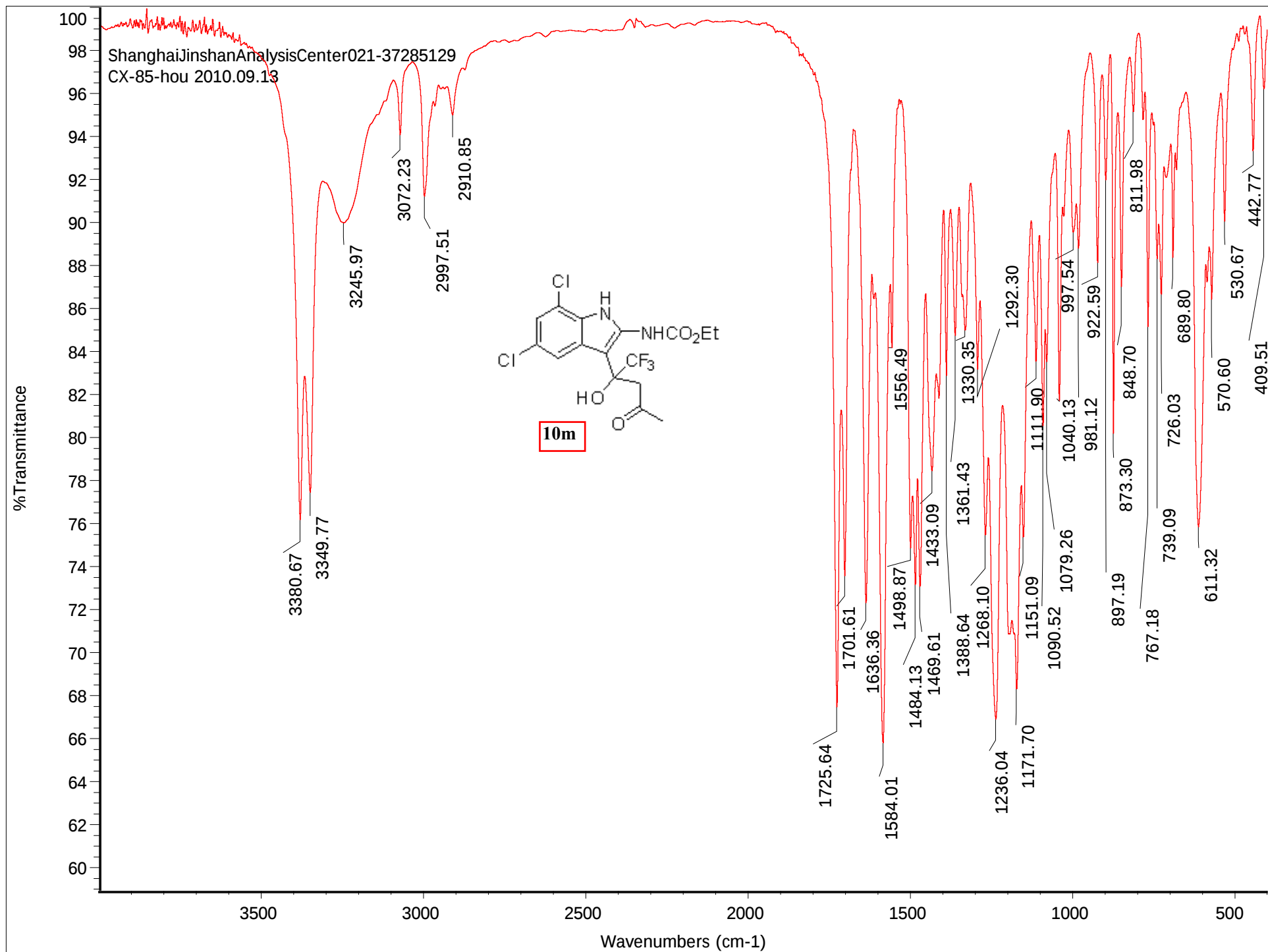


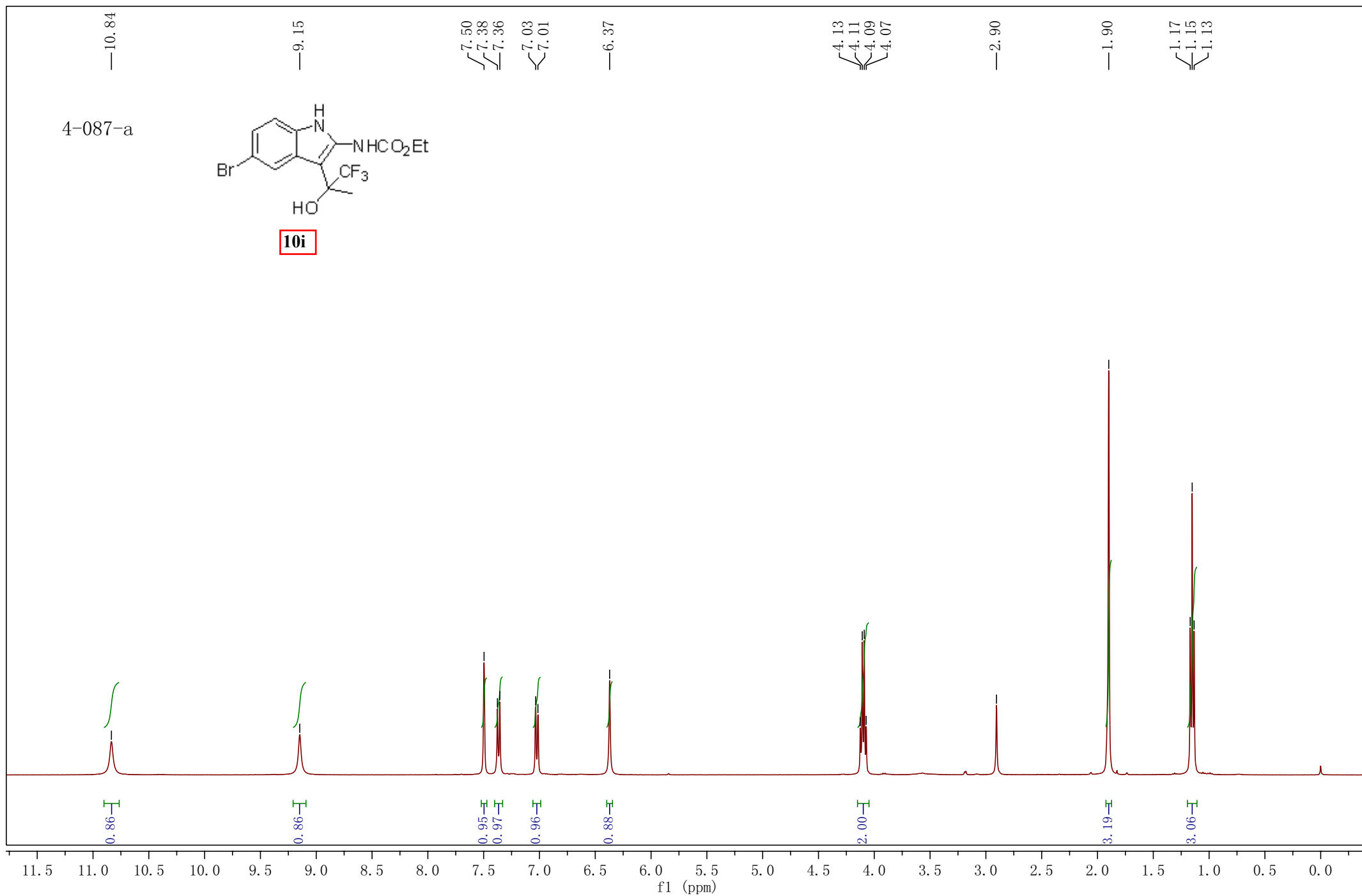
User Name : CJK  
 Sample ID :  
 Sample Name : CX-85-hou  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6191.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/08 15:58:16

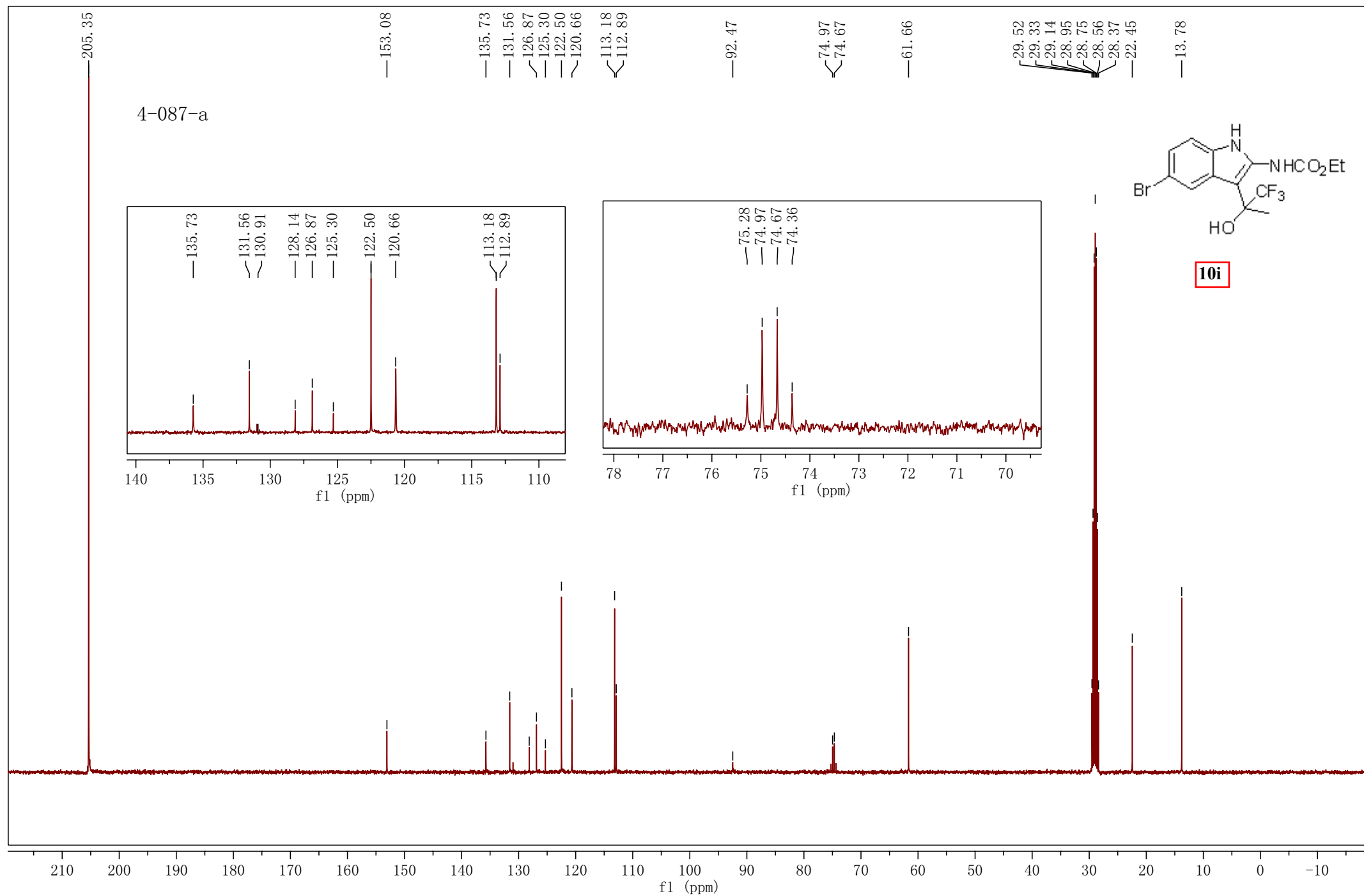
# HPLC



| Peak# | Ret.Time | Area     | Height | A/H    | Area%    |
|-------|----------|----------|--------|--------|----------|
| 1     | 2.816    | 12146    | 891    | 13.639 | 0.0989   |
| 2     | 4.211    | 8148     | 702    | 11.614 | 0.0663   |
| 3     | 5.362    | 12160575 | 965403 | 12.596 | 98.9712  |
| 4     | 8.901    | 1123     | 78     | 14.420 | 0.0091   |
| 5     | 10.167   | 13515    | 884    | 15.291 | 0.1100   |
| 6     | 11.278   | 2215     | 69     | 32.233 | 0.0180   |
| 7     | 13.171   | 89267    | 3851   | 23.179 | 0.7265   |
| 全部    |          | 12286989 | 971878 |        | 100.0000 |







# Mass Spectrometer Report TEL:021-37285047

## Analysis Info

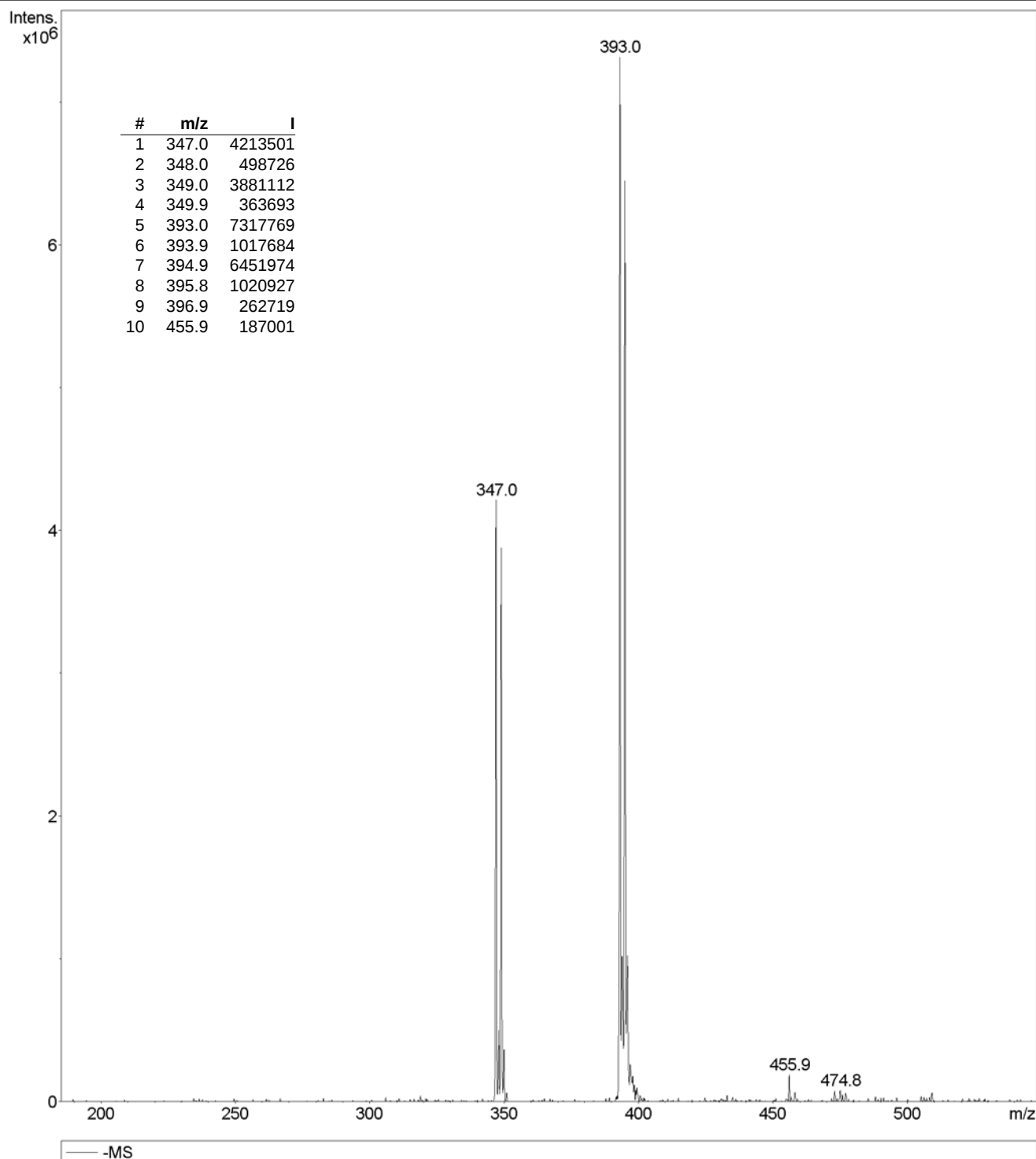
Analysis Name D:\Data\User\SIOC0930MS01.d  
Method MS800.m  
Sample Name 4-087-a  
Comment

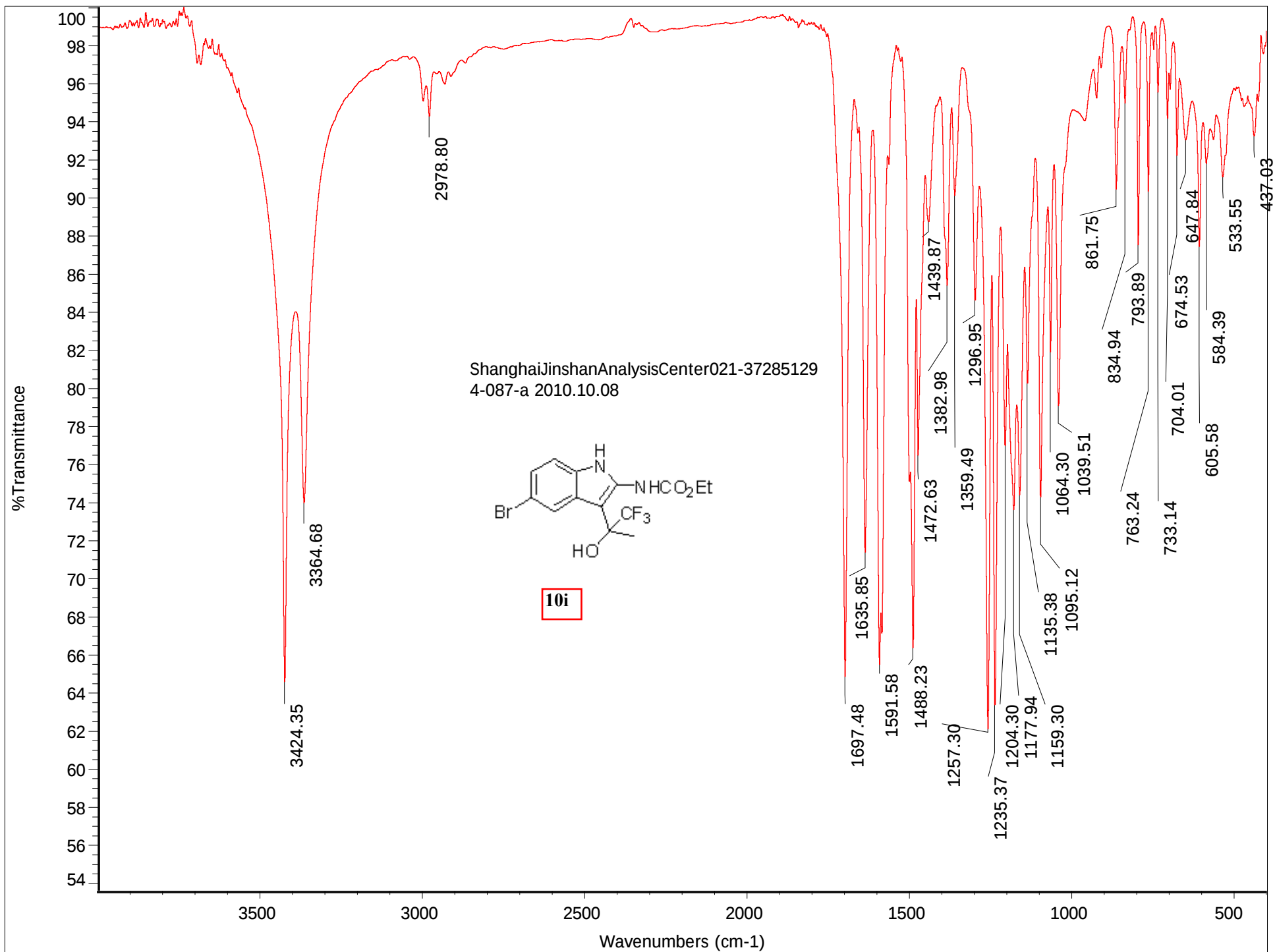
Acquisition Date 10/8/2010 11:44:19 AM

Operator Dai  
Instrument esquire6000

## Acquisition Parameter

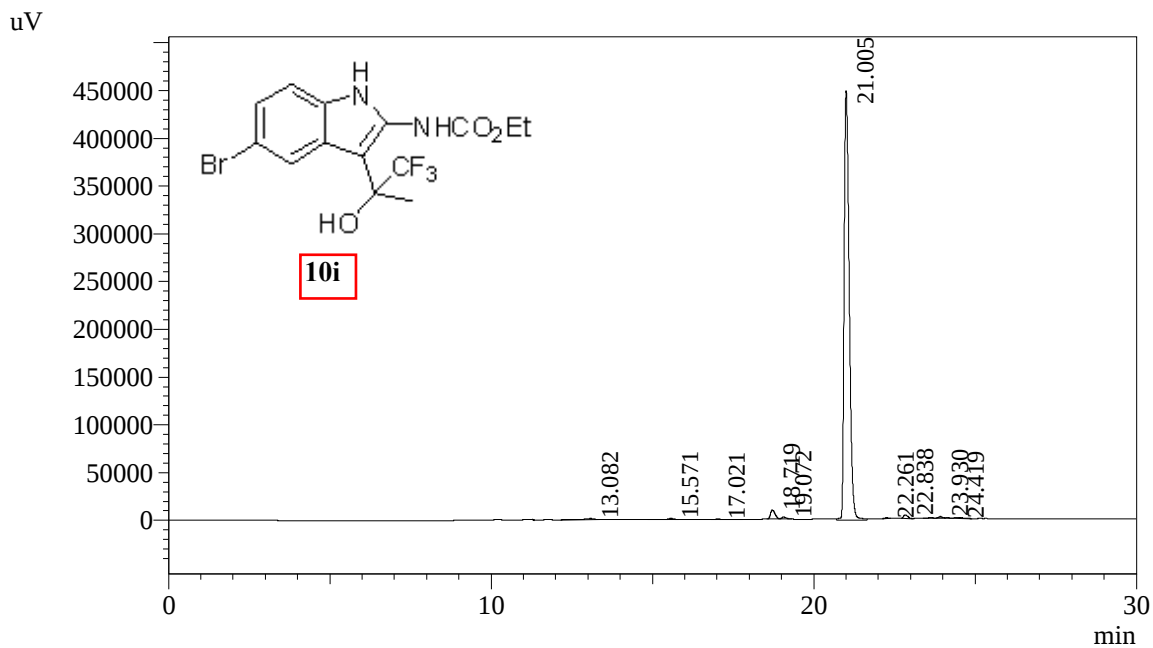
|                   |             |              |            |                          |         |
|-------------------|-------------|--------------|------------|--------------------------|---------|
| Ion Source Type   | ESI         | Ion Polarity | Negative   | Alternating Ion Polarity | off     |
| Mass Range Mode   | Std/Normal  | Scan Begin   | 50 m/z     | Scan End                 | 800 m/z |
| Capillary Exit    | -109.0 Volt | Skimmer      | -40.0 Volt | Trap Drive               | 45.7    |
| Accumulation Time | 77 $\mu$ s  | Averages     | 20 Spectra | Auto MS/MS               | off     |





User Name : CJK  
 Sample ID :  
 Sample Name : 4-087-a  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6306.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/25 15:46:35

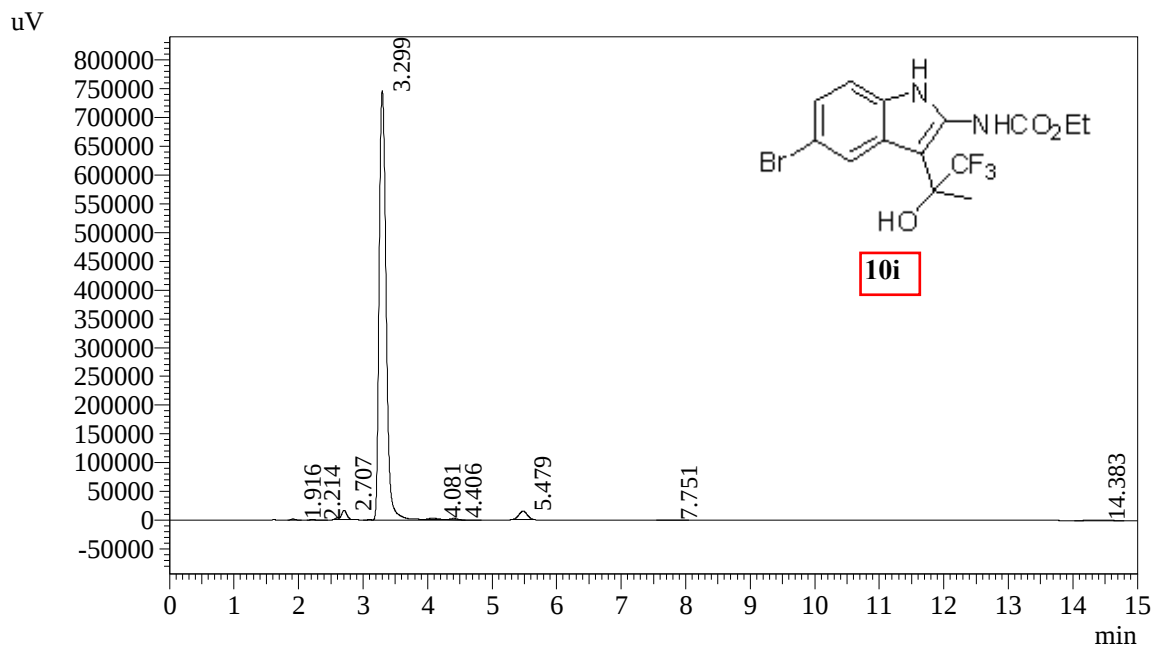
# HPLC



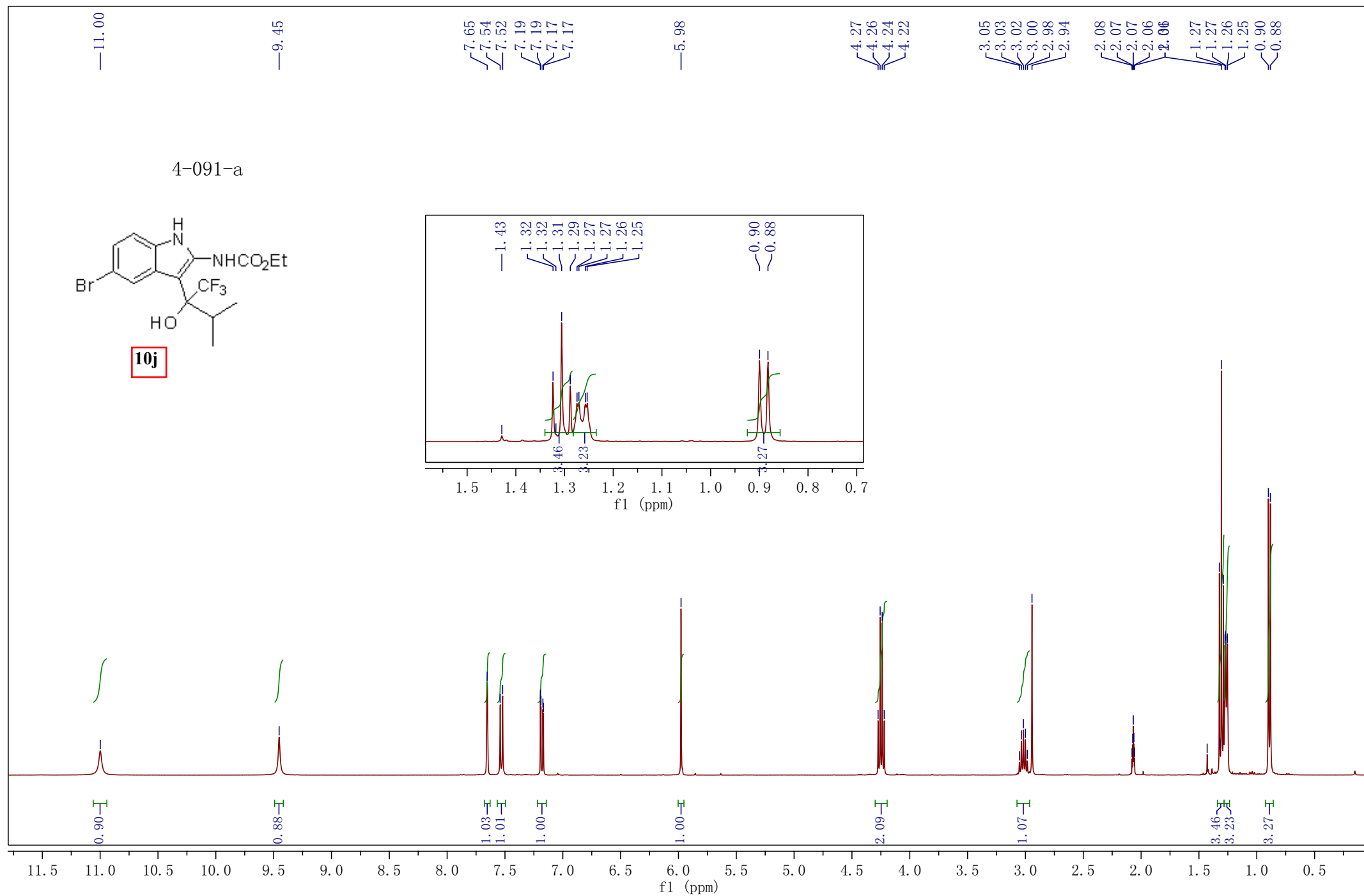
| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 13.082   | 27904   | 1206   | 23.141 | 0.5353   |
| 2     | 15.571   | 22722   | 1200   | 18.936 | 0.4359   |
| 3     | 17.021   | 6930    | 511    | 13.553 | 0.1329   |
| 4     | 18.719   | 97684   | 9505   | 10.277 | 1.8741   |
| 5     | 19.072   | 22417   | 2190   | 10.236 | 0.4301   |
| 6     | 21.005   | 4958715 | 449283 | 11.037 | 95.1331  |
| 7     | 22.261   | 5344    | 737    | 7.252  | 0.1025   |
| 8     | 22.838   | 34313   | 3917   | 8.761  | 0.6583   |
| 9     | 23.930   | 25553   | 1714   | 14.910 | 0.4902   |
| 10    | 24.419   | 10813   | 752    | 14.382 | 0.2074   |
| 全部    |          | 5212395 | 471015 |        | 100.0000 |

User Name : CJK  
 Sample ID :  
 Sample Name : 4-087-a  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6311.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/26 9:50:08

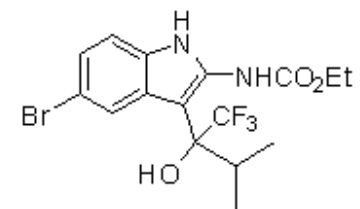
# HPLC



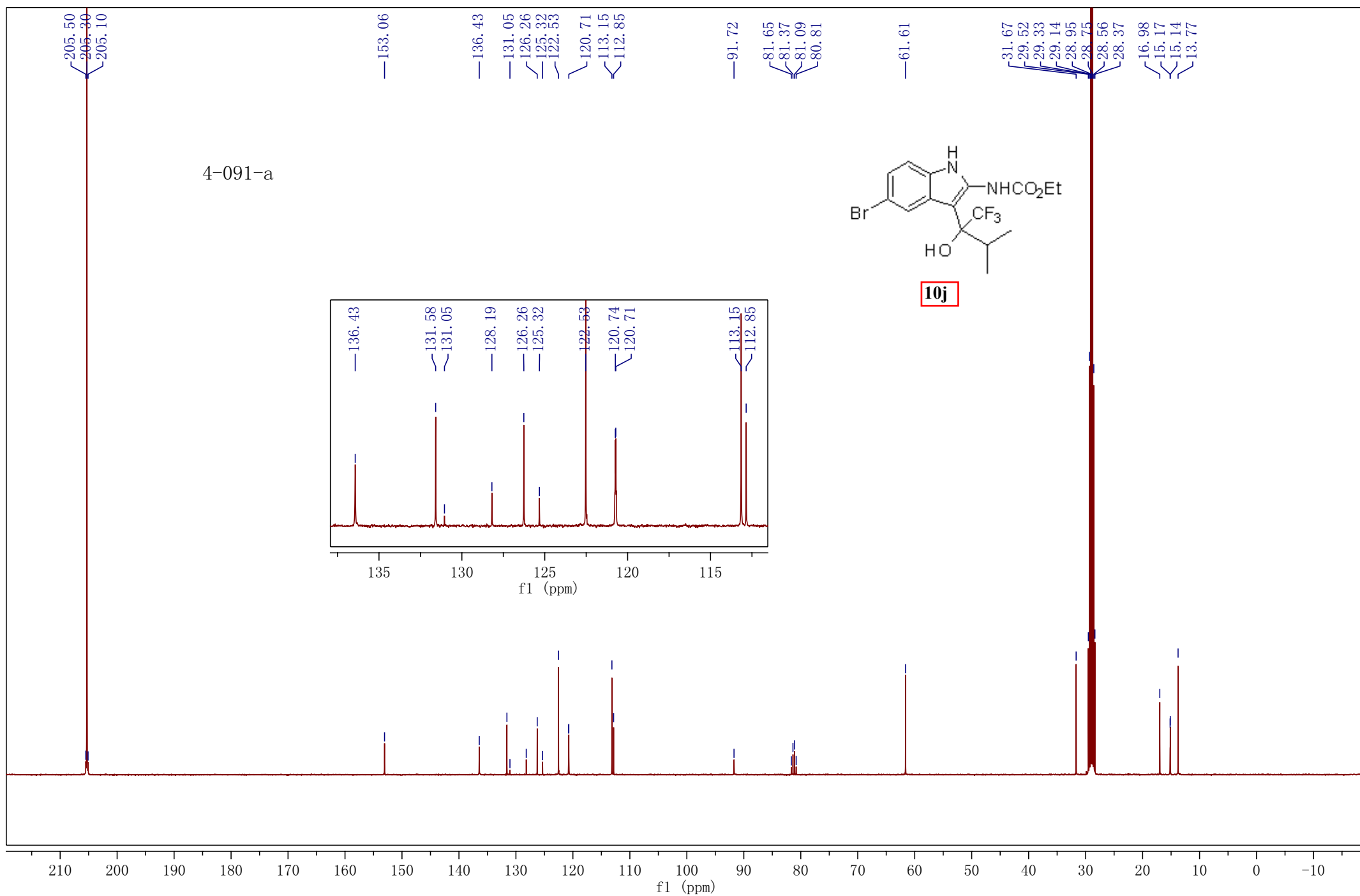
| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 1.916    | 7940    | 1688   | 4.705  | 0.1323   |
| 2     | 2.214    | 5495    | 1042   | 5.272  | 0.0916   |
| 3     | 2.707    | 96761   | 15745  | 6.145  | 1.6126   |
| 4     | 3.299    | 5713505 | 743277 | 7.687  | 95.2174  |
| 5     | 4.081    | 24327   | 2535   | 9.597  | 0.4054   |
| 6     | 4.406    | 18977   | 2496   | 7.602  | 0.3163   |
| 7     | 5.479    | 125104  | 14437  | 8.665  | 2.0849   |
| 8     | 7.751    | 3595    | 266    | 13.504 | 0.0599   |
| 9     | 14.383   | 4776    | 226    | 21.117 | 0.0796   |
| 全部    |          | 6000480 | 781712 |        | 100.0000 |



4-091-a



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# Mass Spectrometer Report TEL:021-37285047

## Analysis Info

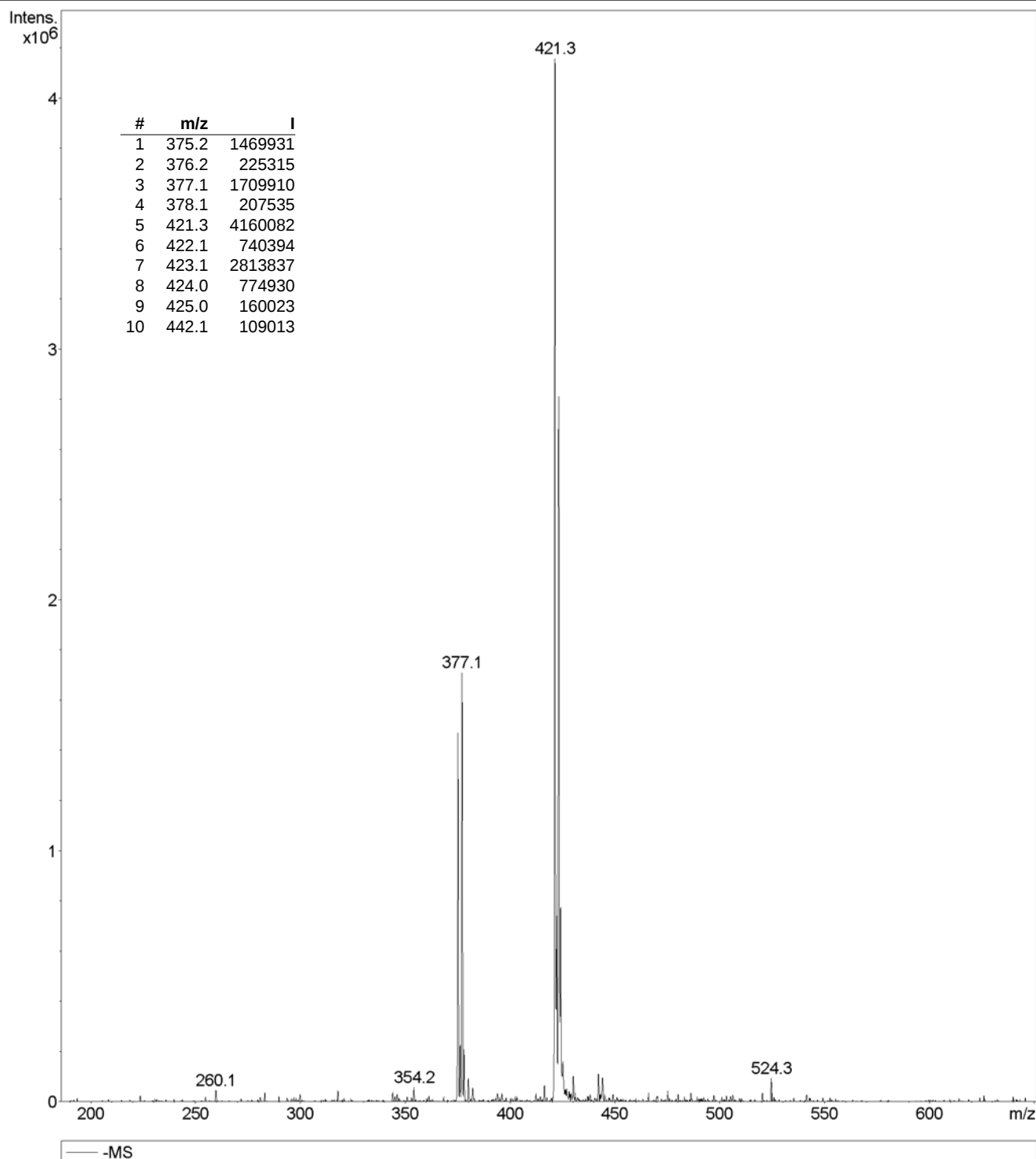
Analysis Name D:\Data\User\SIOC1103MS01.d  
Method MS1000.m  
Sample Name 4-091  
Comment

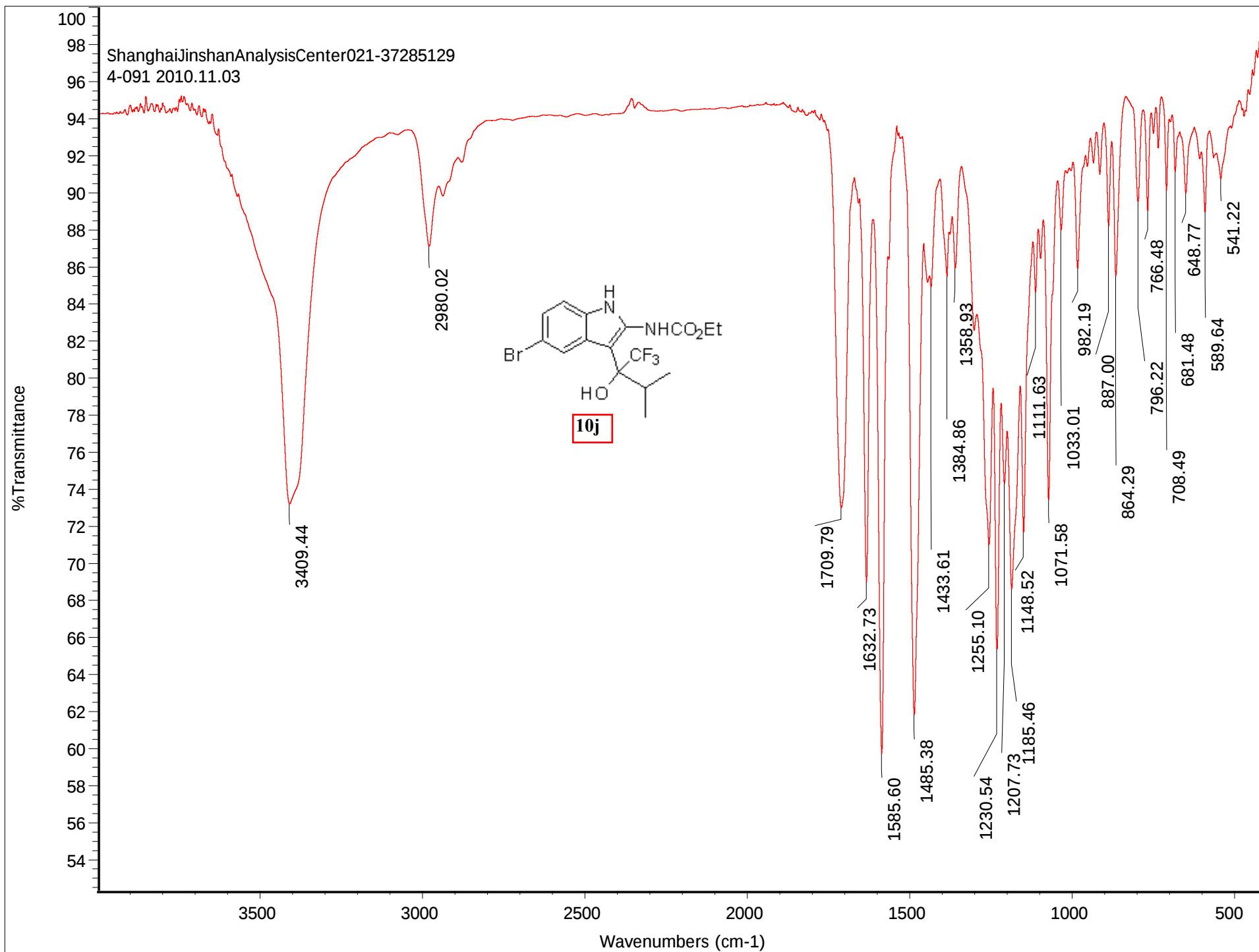
Acquisition Date 11/3/2010 4:36:53 PM

Operator Dai  
Instrument esquire6000

## Acquisition Parameter

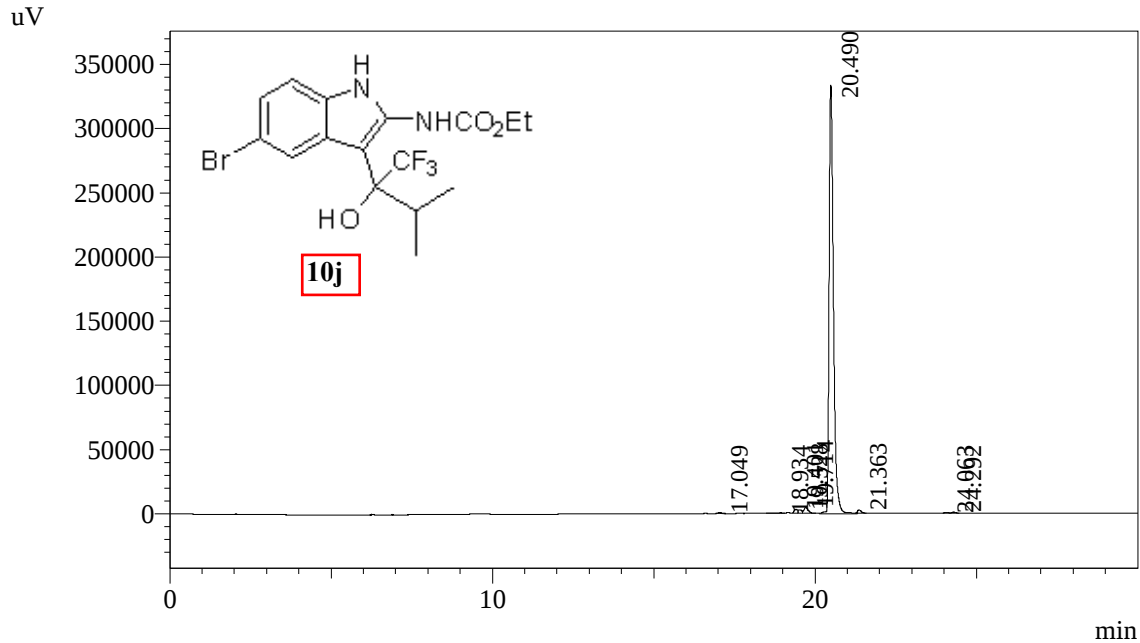
|                   |             |              |            |                          |          |
|-------------------|-------------|--------------|------------|--------------------------|----------|
| Ion Source Type   | ESI         | Ion Polarity | Negative   | Alternating Ion Polarity | off      |
| Mass Range Mode   | Std/Normal  | Scan Begin   | 50 m/z     | Scan End                 | 1000 m/z |
| Capillary Exit    | -115.0 Volt | Skimmer      | -40.0 Volt | Trap Drive               | 54.2     |
| Accumulation Time | 136 $\mu$ s | Averages     | 20 Spectra | Auto MS/MS               | off      |





User Name : CJK  
Sample ID :  
Sample Name : 4-091-a  
Data Name : D:\Chromato Solution-Light\Data\Project1\test-6537.gcd  
Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
2010/11/10 14:18:42

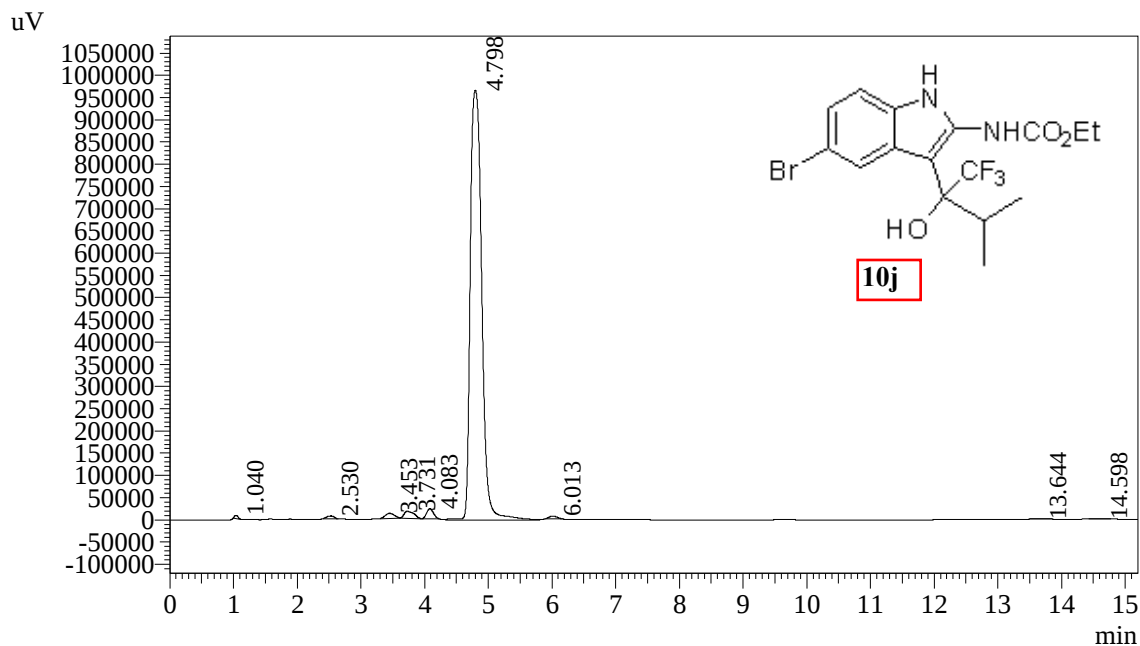
HPLC



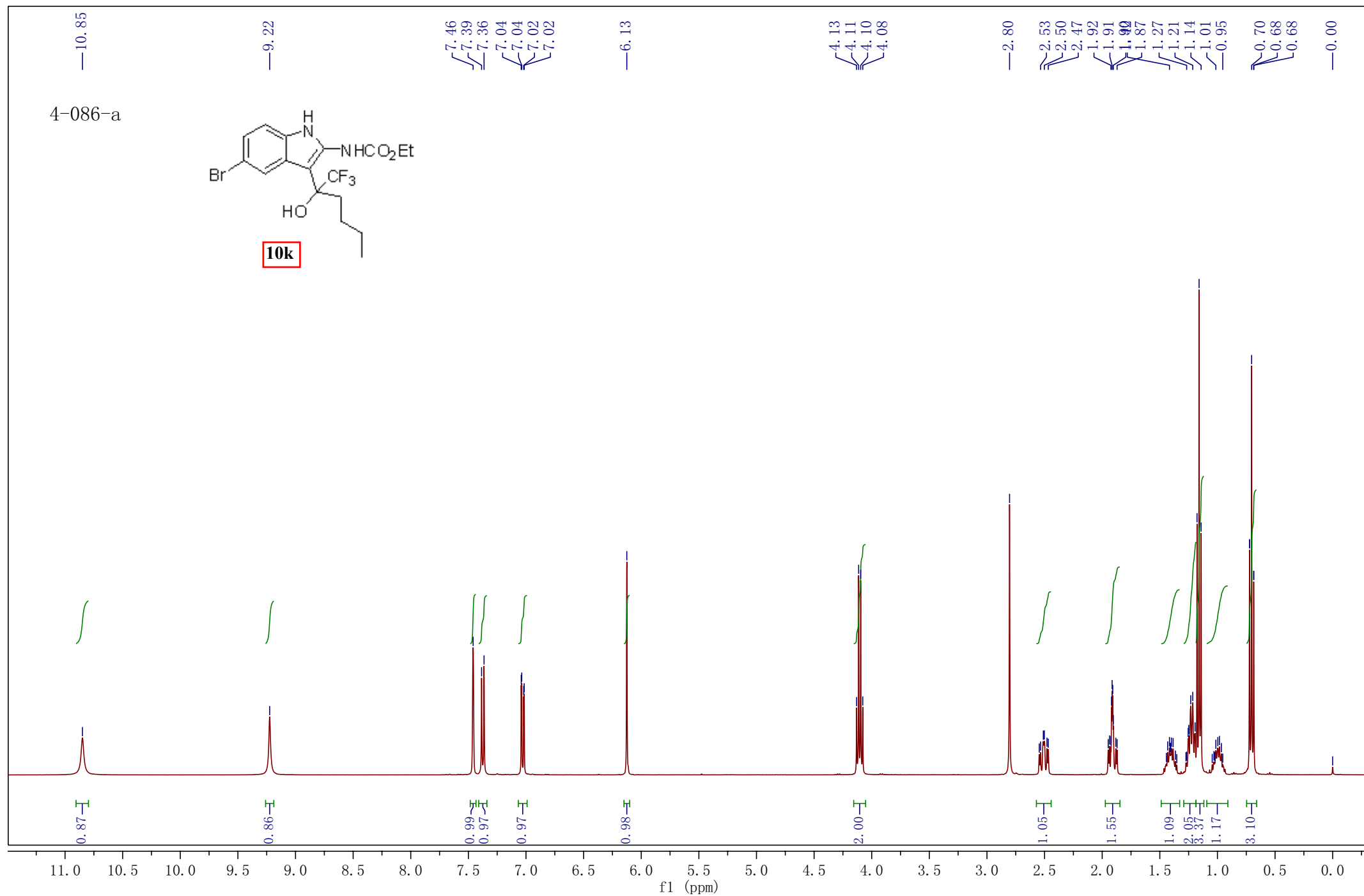
| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 17.049   | 5367    | 673    | 7.970  | 0.1665   |
| 2     | 18.934   | 4846    | 325    | 14.893 | 0.1504   |
| 3     | 19.401   | 21955   | 3080   | 7.129  | 0.6812   |
| 4     | 19.528   | 19227   | 2608   | 7.373  | 0.5965   |
| 5     | 19.714   | 40254   | 4477   | 8.992  | 1.2489   |
| 6     | 20.490   | 3101958 | 333144 | 9.311  | 96.2431  |
| 7     | 21.363   | 18762   | 2369   | 7.919  | 0.5821   |
| 8     | 24.063   | 4469    | 581    | 7.691  | 0.1386   |
| 9     | 24.292   | 6208    | 741    | 8.379  | 0.1926   |
| 全部    |          | 3223046 | 347998 |        | 100.0000 |

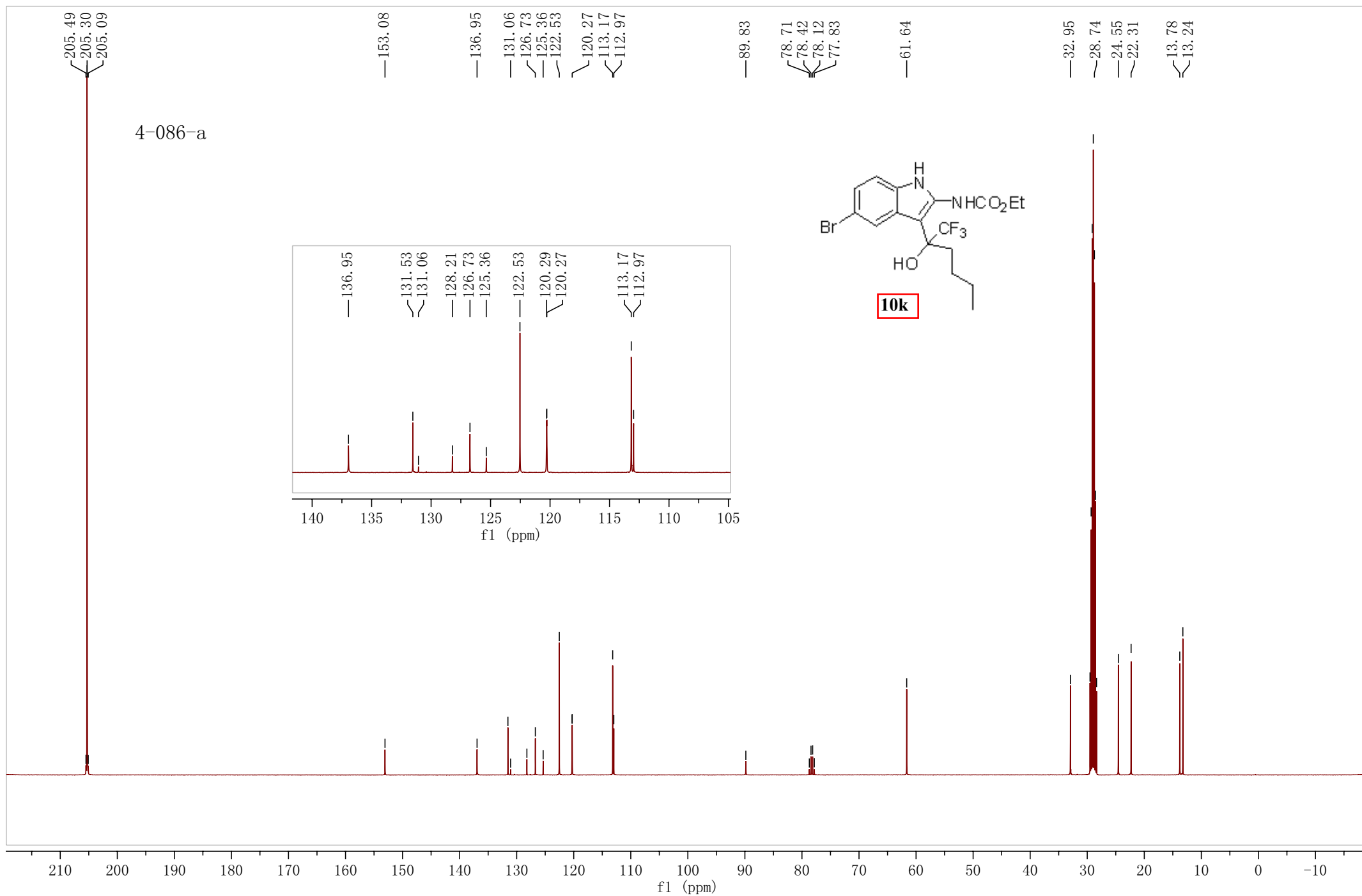
User Name : CJK  
 Sample ID :  
 Sample Name : 4-091-a  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6538.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/11/10 14:58:52

# HPLC



| Peak# | Ret.Time | Area     | Height  | A/H    | Area%    |
|-------|----------|----------|---------|--------|----------|
| 1     | 1.040    | 30802    | 7806    | 3.946  | 0.2430   |
| 2     | 2.530    | 50837    | 6301    | 8.068  | 0.4010   |
| 3     | 3.453    | 110128   | 11247   | 9.792  | 0.8688   |
| 4     | 3.731    | 169629   | 15619   | 10.861 | 1.3382   |
| 5     | 4.083    | 173687   | 22642   | 7.671  | 1.3702   |
| 6     | 4.798    | 12060021 | 966584  | 12.477 | 95.1401  |
| 7     | 6.013    | 60564    | 6640    | 9.122  | 0.4778   |
| 8     | 13.644   | 10357    | 814     | 12.718 | 0.0817   |
| 9     | 14.598   | 10037    | 788     | 12.745 | 0.0792   |
| 全部    |          | 12676062 | 1038441 |        | 100.0000 |





# Mass Spectrometer Report TEL:021-37285047

## Analysis Info

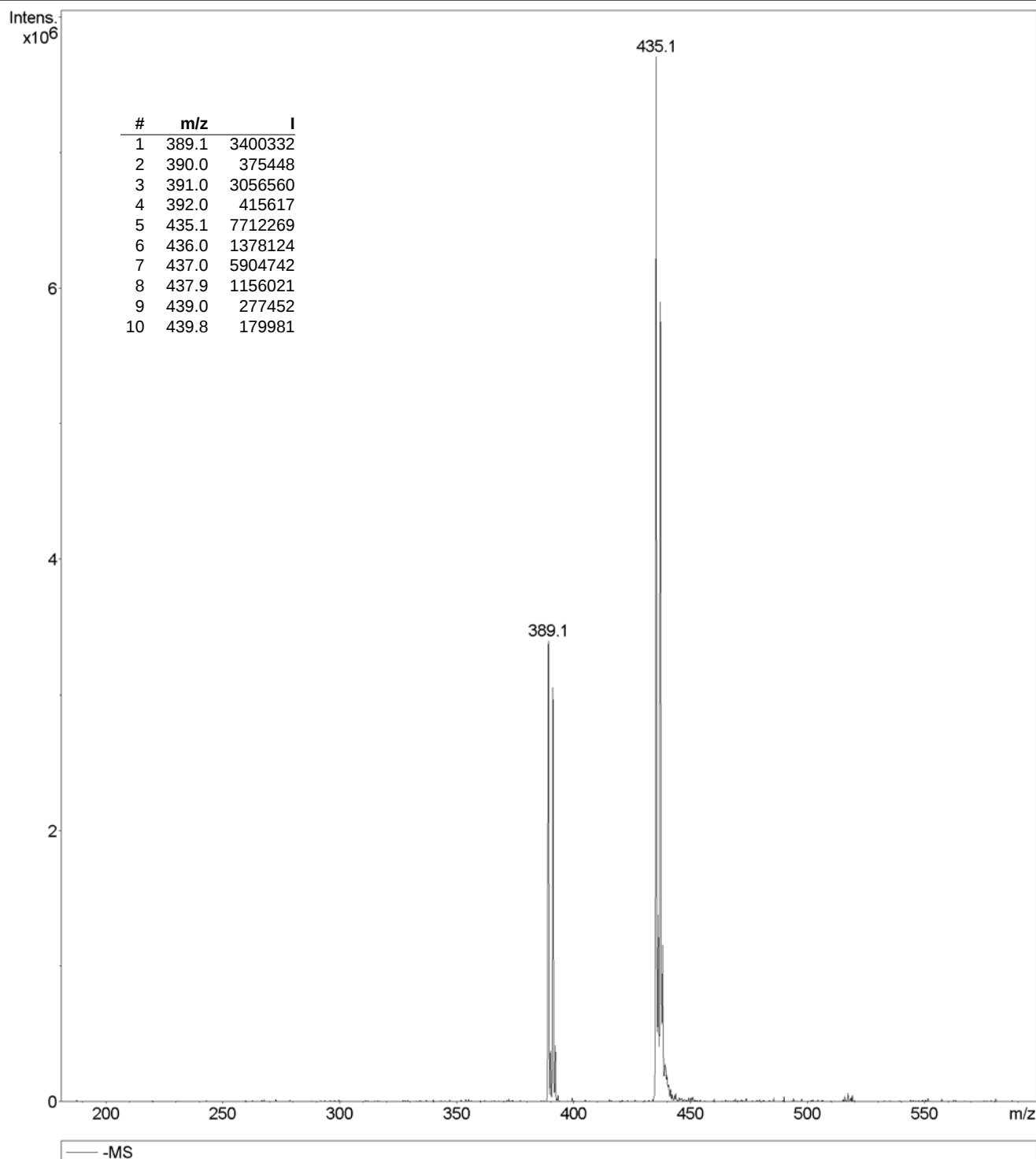
Analysis Name D:\Data\User\SIOC0930MS00.d  
Method MS800.m  
Sample Name 4-086-a  
Comment

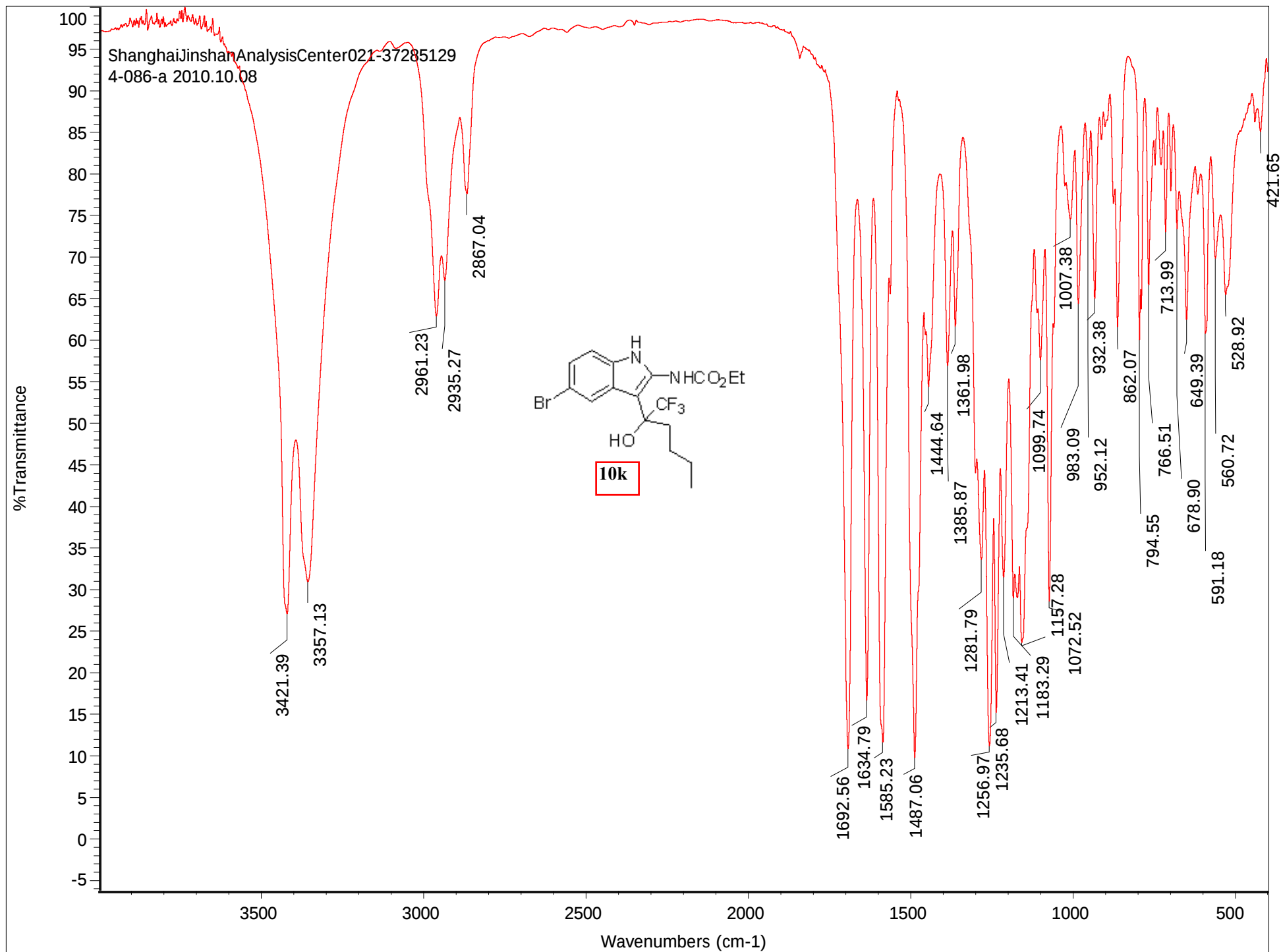
Acquisition Date 10/8/2010 11:41:07 AM

Operator Dai  
Instrument esquire6000

## Acquisition Parameter

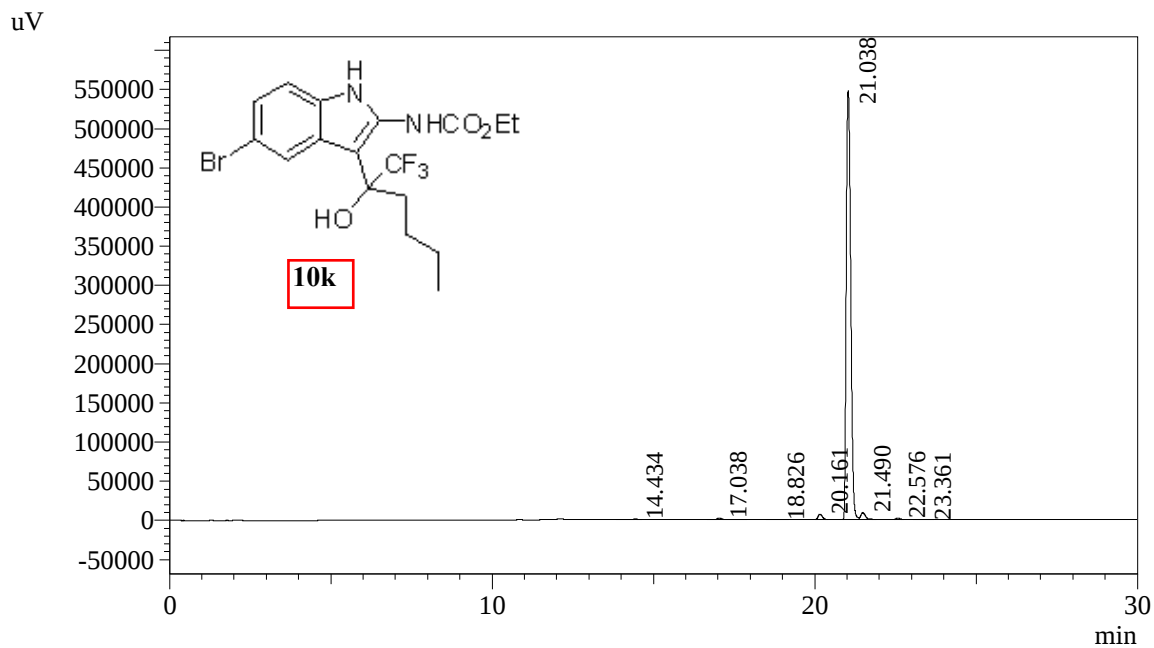
|                   |             |              |            |                          |         |
|-------------------|-------------|--------------|------------|--------------------------|---------|
| Ion Source Type   | ESI         | Ion Polarity | Negative   | Alternating Ion Polarity | off     |
| Mass Range Mode   | Std/Normal  | Scan Begin   | 50 m/z     | Scan End                 | 800 m/z |
| Capillary Exit    | -109.0 Volt | Skimmer      | -40.0 Volt | Trap Drive               | 45.7    |
| Accumulation Time | 86 $\mu$ s  | Averages     | 20 Spectra | Auto MS/MS               | off     |





User Name : CJK  
 Sample ID :  
 Sample Name : 4-086-2  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6304.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/25 14:35:34

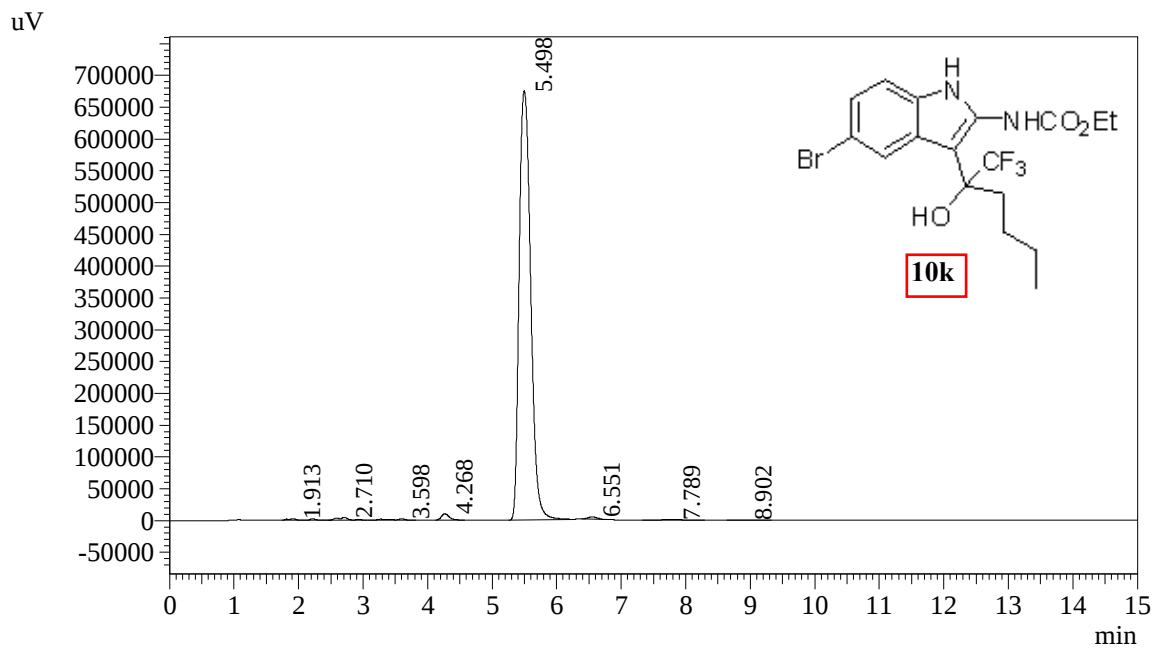
# HPLC



| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 14.434   | 16106   | 842    | 19.117 | 0.2952   |
| 2     | 17.038   | 25088   | 1745   | 14.378 | 0.4598   |
| 3     | 18.826   | 5330    | 257    | 20.771 | 0.0977   |
| 4     | 20.161   | 59138   | 6539   | 9.044  | 1.0838   |
| 5     | 21.038   | 5252717 | 546899 | 9.605  | 96.2676  |
| 6     | 21.490   | 85437   | 8421   | 10.146 | 1.5658   |
| 7     | 22.576   | 11199   | 1321   | 8.476  | 0.2052   |
| 8     | 23.361   | 1354    | 121    | 11.181 | 0.0248   |
| 全部    |          | 5456369 | 566145 |        | 100.0000 |

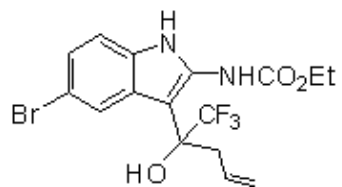
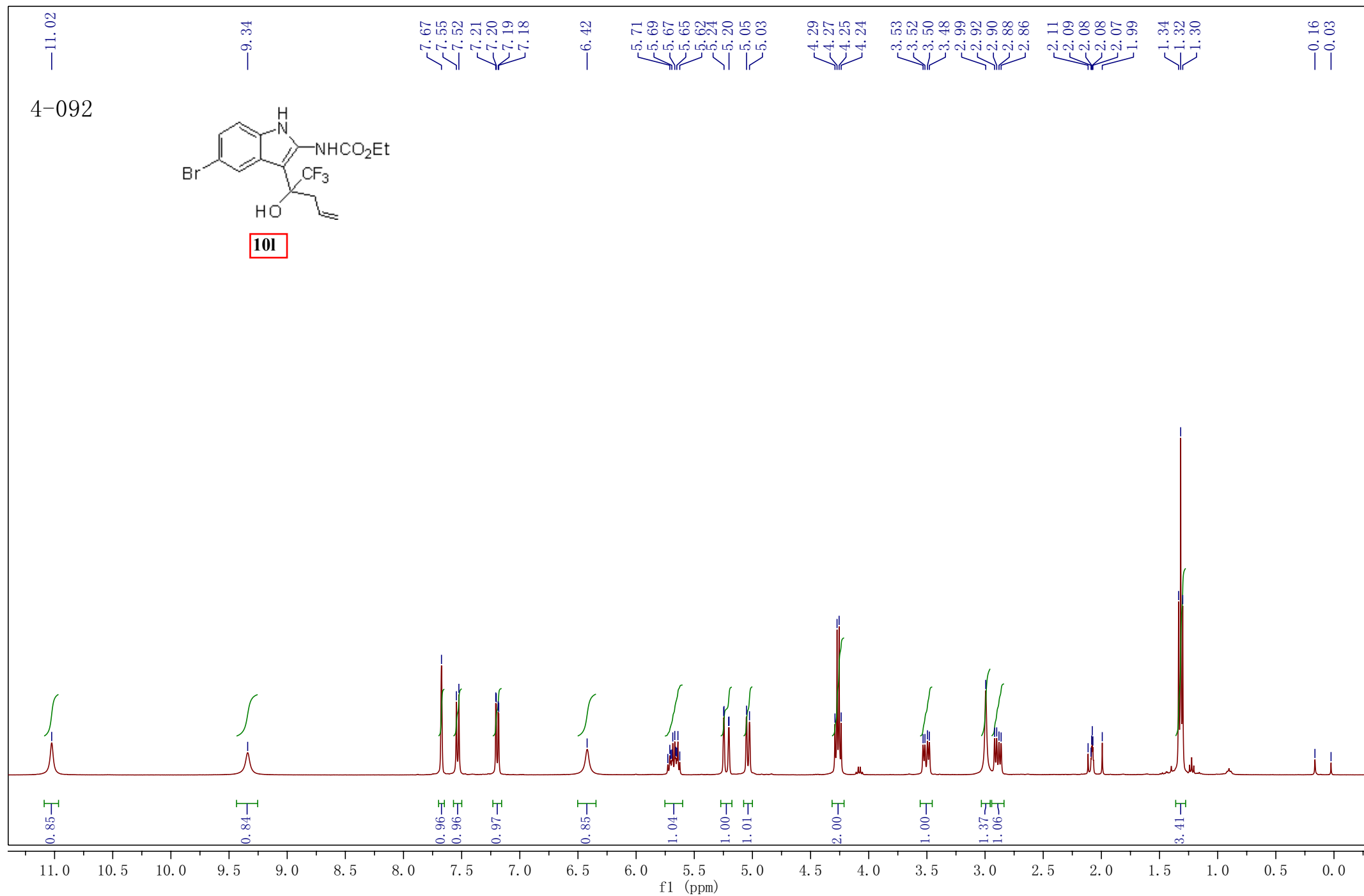
User Name : CJK  
 Sample ID :  
 Sample Name : 4-086-2  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6308.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/09/26 8:59:07

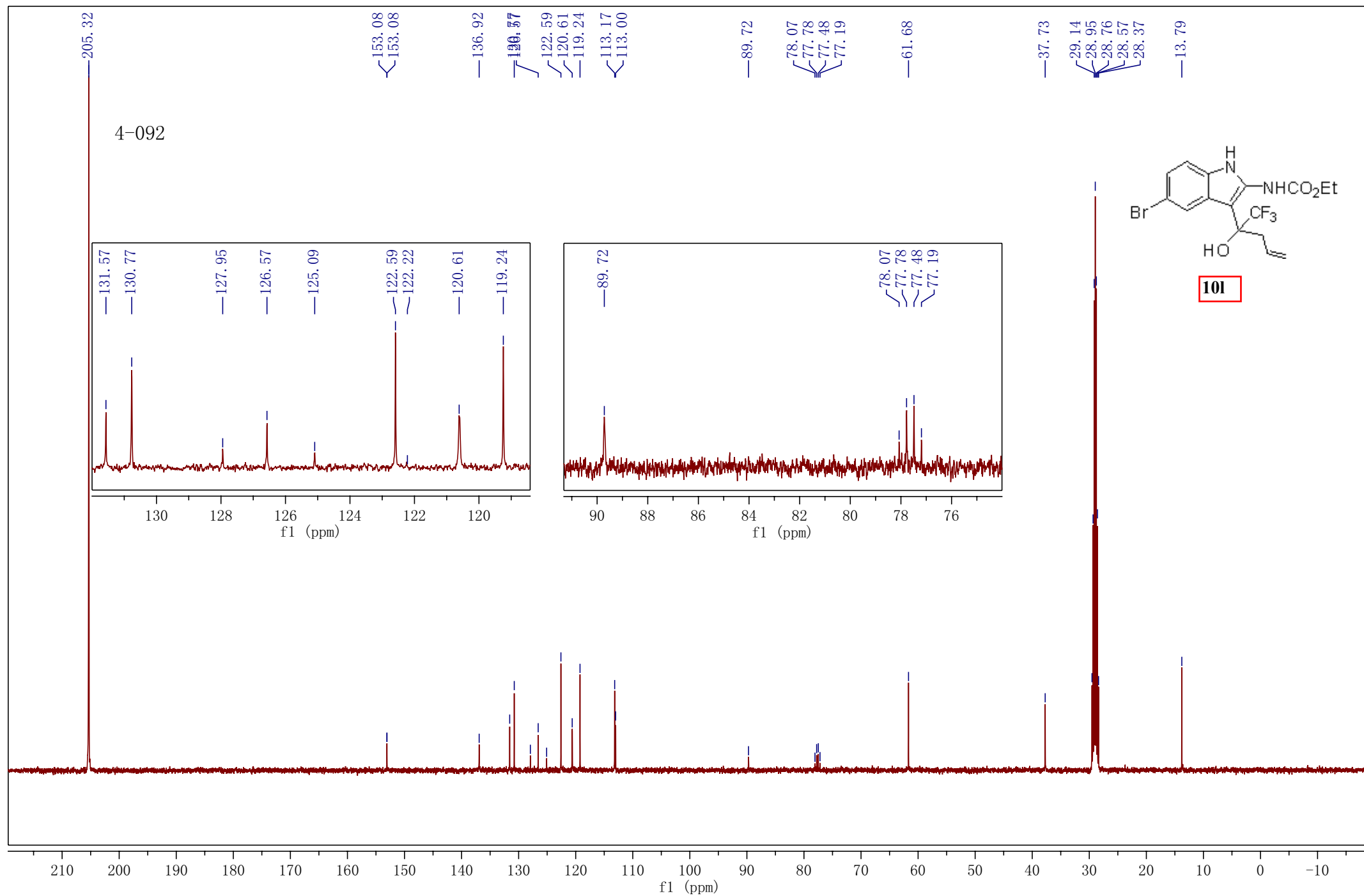
# HPLC

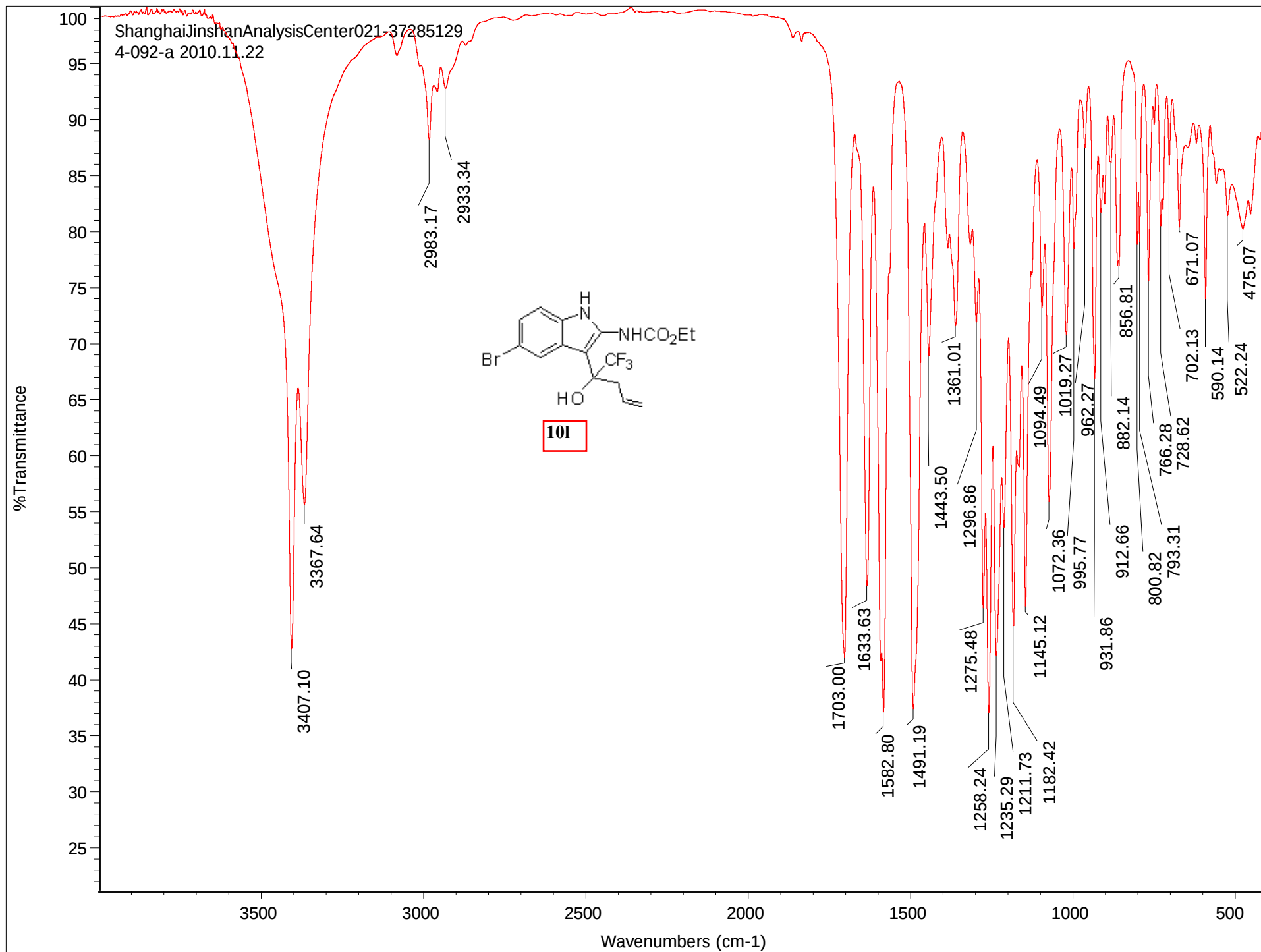


| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 1.913    | 23393   | 2360   | 9.912  | 0.2707   |
| 2     | 2.710    | 56192   | 4511   | 12.457 | 0.6503   |
| 3     | 3.598    | 35259   | 2207   | 15.978 | 0.4081   |
| 4     | 4.268    | 83249   | 9828   | 8.471  | 0.9634   |
| 5     | 5.498    | 8380963 | 674859 | 12.419 | 96.9918  |
| 6     | 6.551    | 40688   | 3815   | 10.665 | 0.4709   |
| 7     | 7.789    | 14892   | 736    | 20.245 | 0.1723   |
| 8     | 8.902    | 6262    | 449    | 13.963 | 0.0725   |
| 全部    |          | 8640898 | 698765 |        | 100.0000 |

4-092

**101**





# Mass Spectrometer Report TEL:021-37285047

## Analysis Info

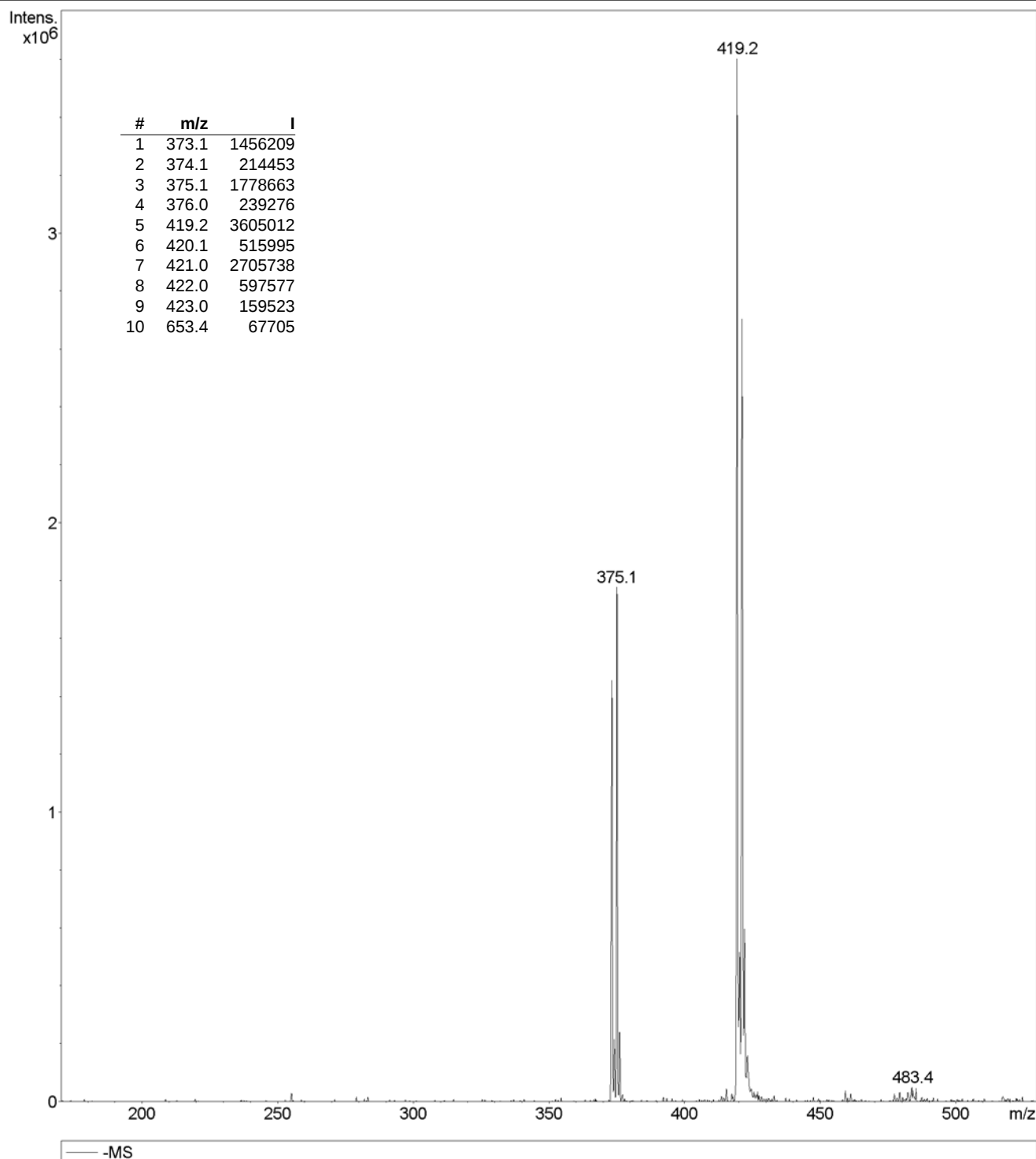
Analysis Name D:\Data\User\SIOC1122MS03.d  
Method MS1000.m  
Sample Name 4-092-a  
Comment

Acquisition Date 11/22/2010 8:54:48 AM

Operator Dai  
Instrument esquire6000

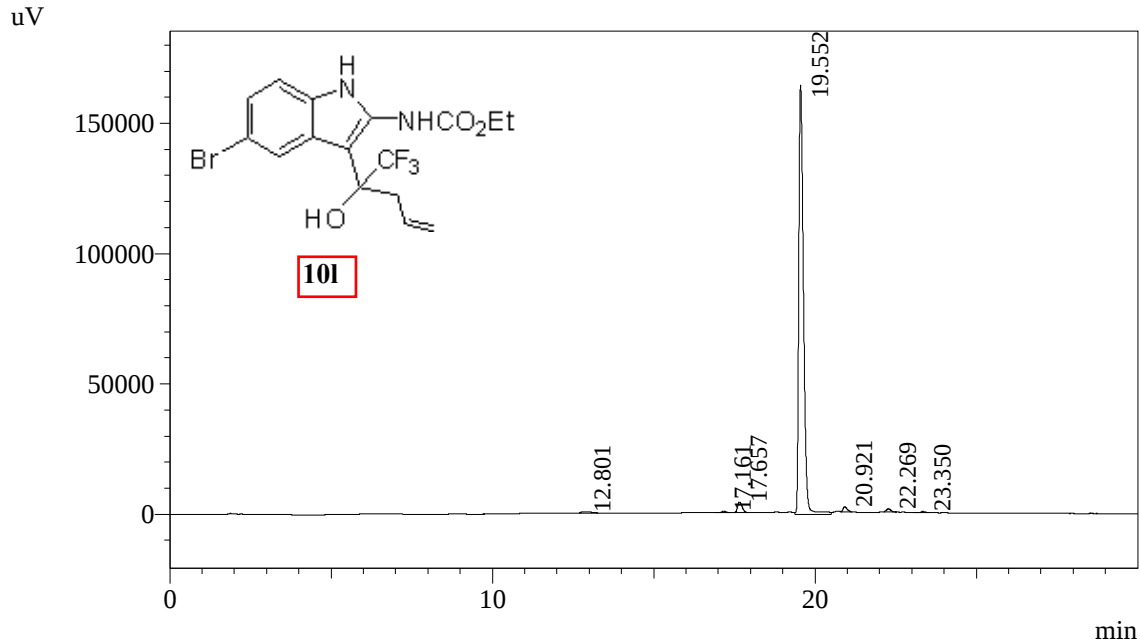
## Acquisition Parameter

|                   |             |              |            |                          |          |
|-------------------|-------------|--------------|------------|--------------------------|----------|
| Ion Source Type   | ESI         | Ion Polarity | Negative   | Alternating Ion Polarity | off      |
| Mass Range Mode   | Std/Normal  | Scan Begin   | 50 m/z     | Scan End                 | 1000 m/z |
| Capillary Exit    | -115.0 Volt | Skimmer      | -40.0 Volt | Trap Drive               | 54.2     |
| Accumulation Time | 167 $\mu$ s | Averages     | 20 Spectra | Auto MS/MS               | off      |



User Name : CJK  
Sample ID :  
Sample Name : 4-092  
Data Name : D:\Chromato Solution-Light\Data\Project1\test-6572.gcd  
Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
2010/11/16 9:38:09

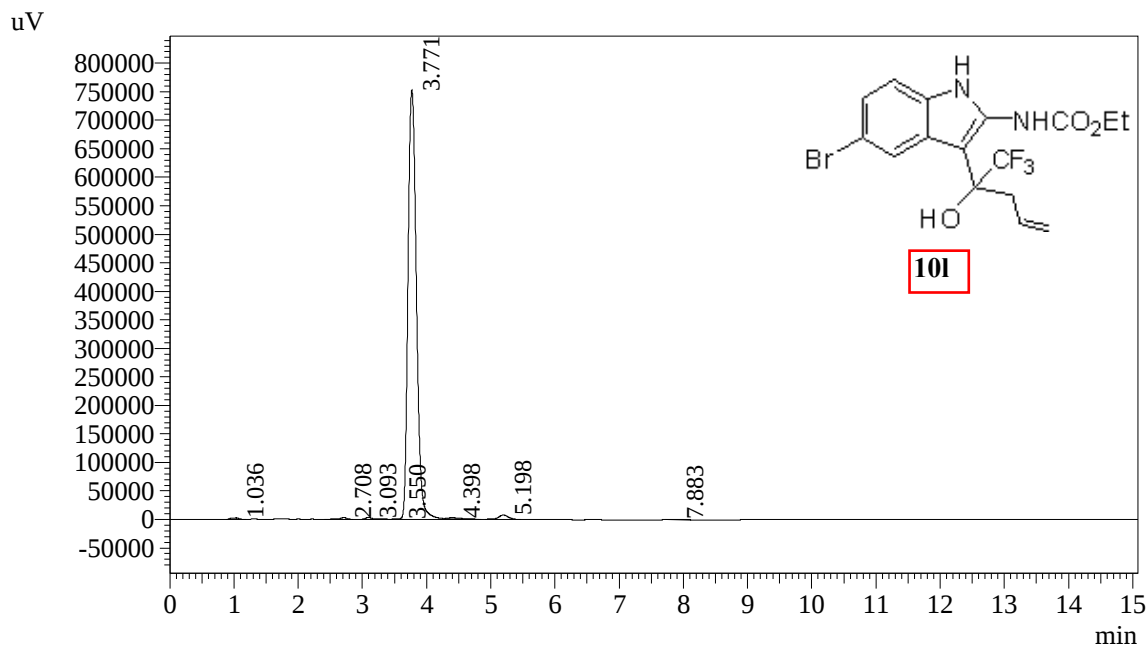
HPLC



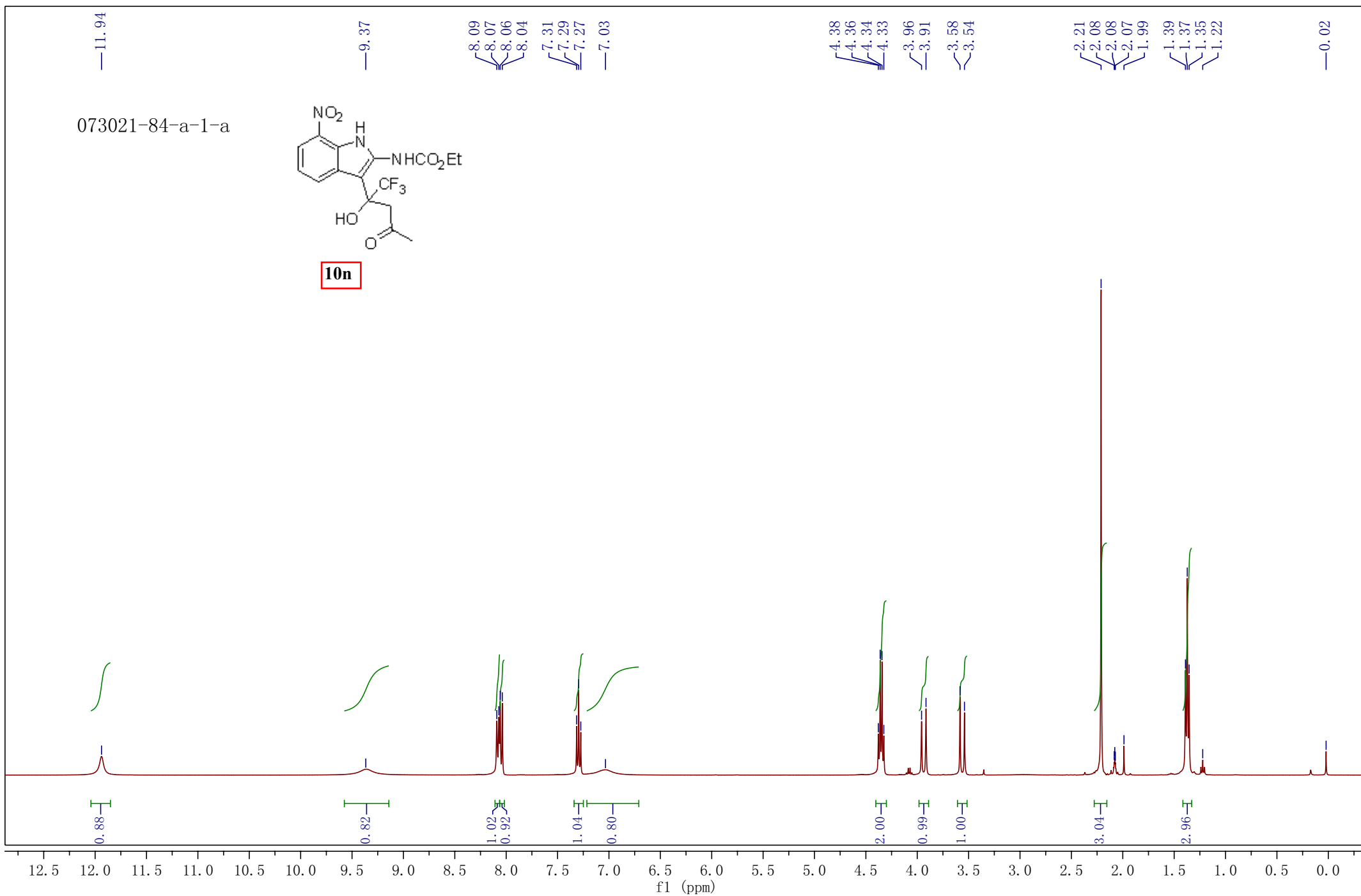
| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 12.801   | 9930    | 520    | 19.103 | 0.5664   |
| 2     | 17.161   | 4985    | 522    | 9.555  | 0.2844   |
| 3     | 17.657   | 40252   | 4049   | 9.941  | 2.2959   |
| 4     | 19.552   | 1666569 | 164557 | 10.128 | 95.0591  |
| 5     | 20.921   | 16145   | 1838   | 8.785  | 0.9209   |
| 6     | 22.269   | 12159   | 1233   | 9.857  | 0.6935   |
| 7     | 23.350   | 3153    | 436    | 7.225  | 0.1798   |
| 全部    |          | 1753193 | 173155 |        | 100.0000 |

User Name : CJK  
 Sample ID :  
 Sample Name : 4-092  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-6574.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2010/11/16 10:34:27

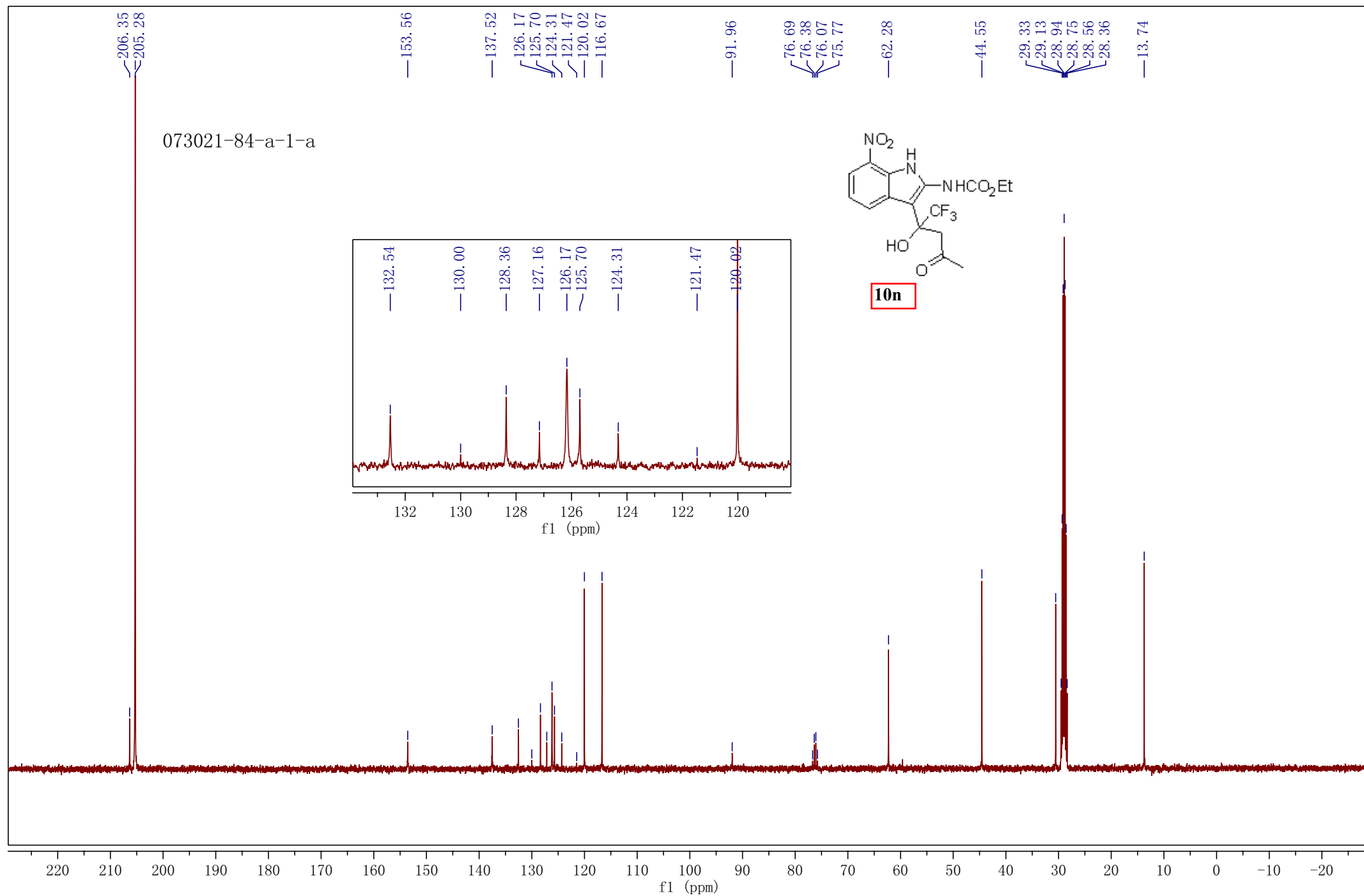
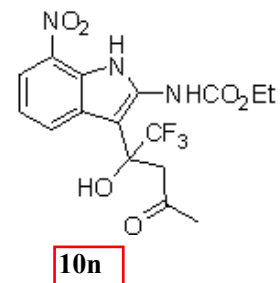
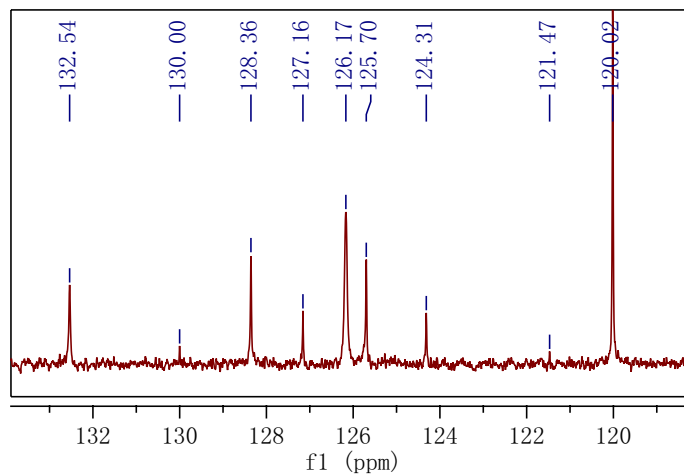
# HPLC

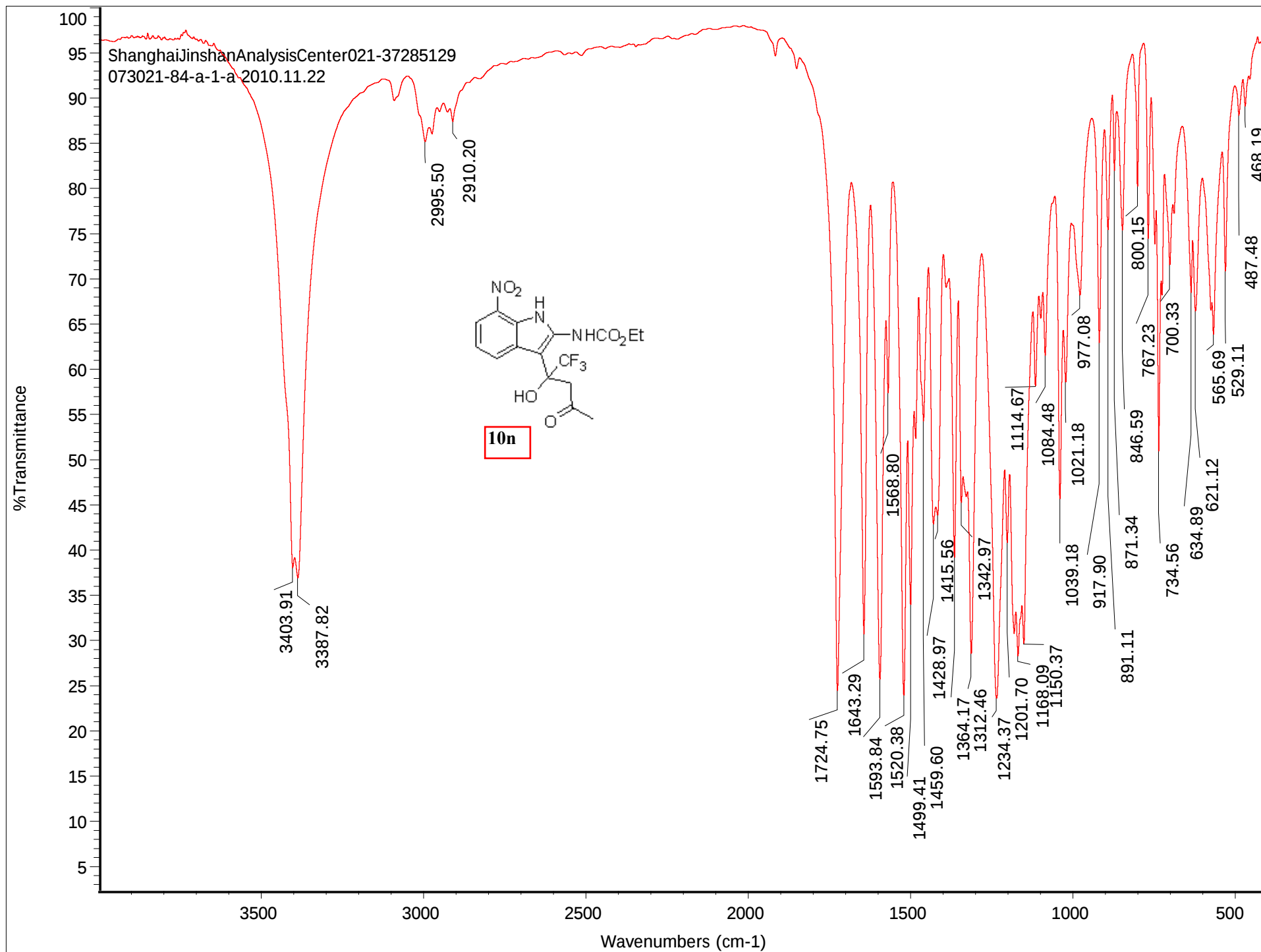


| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 1.036    | 21170   | 2515   | 8.416  | 0.2996   |
| 2     | 2.708    | 23239   | 3014   | 7.709  | 0.3288   |
| 3     | 3.093    | 27244   | 3095   | 8.804  | 0.3855   |
| 4     | 3.550    | 5866    | 1097   | 5.349  | 0.0830   |
| 5     | 3.771    | 6877367 | 751950 | 9.146  | 97.3158  |
| 6     | 4.398    | 21921   | 1696   | 12.924 | 0.3102   |
| 7     | 5.198    | 79663   | 7484   | 10.645 | 1.1272   |
| 8     | 7.883    | 10590   | 898    | 11.788 | 0.1499   |
| 全部    |          | 7067060 | 771749 |        | 100.0000 |



073021-84-a-1-a





## Sample Information

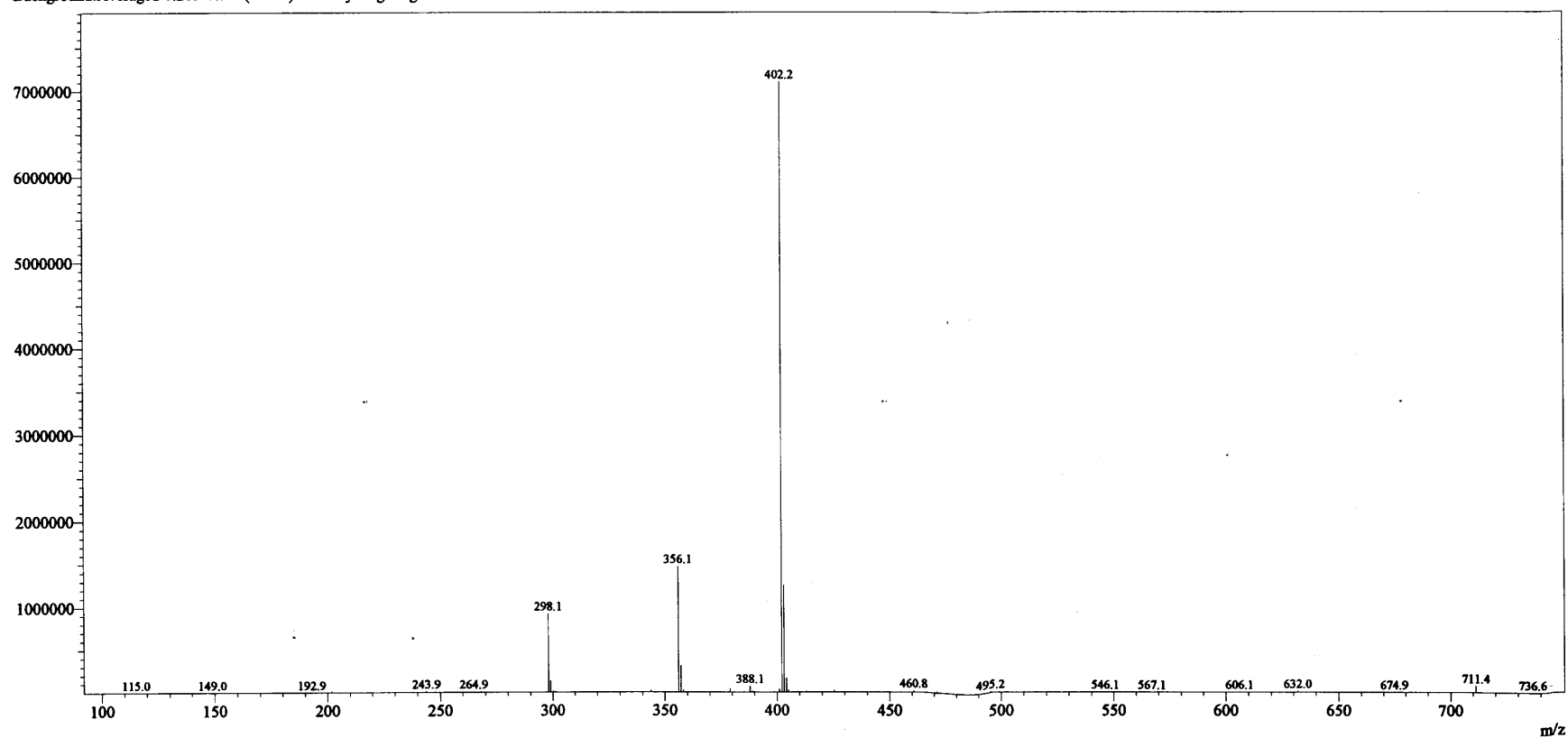
Date Acquired : 9/8/2010 3:58:50 PM  
Sample Name : jhx  
Sample ID : 073021-84-a-2  
Data File : 073021-84-a-2-002.lcd  
Method File : HPLC-smyj1.lcm  
Original Data File : D:\DATA\jiangbiao-group\073021-84-a-2-002.lcd  
Original Method : D:\DATA\HPLC-smyj1.lcm  
Modified Date : 9/8/2010 4:00:11 PM  
Instrument : Shimadzu LCMS-2010EV

Retention Time: 0.617(Scan#:38)

Max Peak: 762 Base Peak: 402.15(7104354)

Spectrum: Single 0.617(38)

Background: Averaged 0.283-0.371(18-23) Polarity: Neg Segment1 - Event1



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## Sample Information

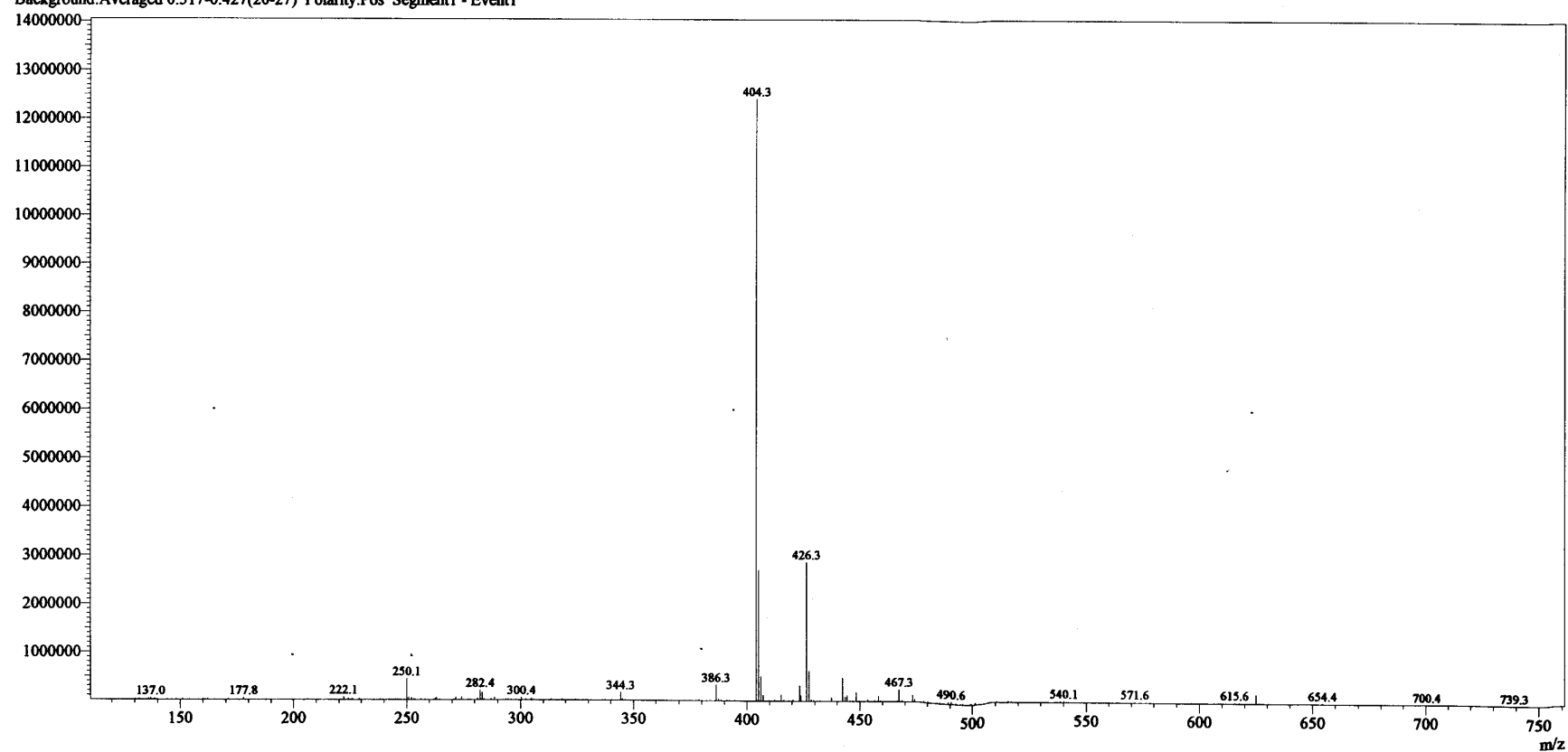
Date Acquired : 9/8/2010 2:15:27 PM  
Sample Name : jhx  
Sample ID : 073021-84-a-2  
Data File : 073021-84-a-2-001.lcd  
Method File : HPLC-smjy30.lcm  
Original Data File : D:\DATA\jiangbiao-group\073021-84-a-2-001.lcd  
Original Method : D:\DATA\HPLC-smjy30.lcm  
Modified Date : 9/8/2010 2:17:32 PM  
Instrument : Shimadzu LCMS-2010EV

Retention Time: 0.617(Scan#: 38)

Max Peak: 625 Base Peak: 404.25(12423164)

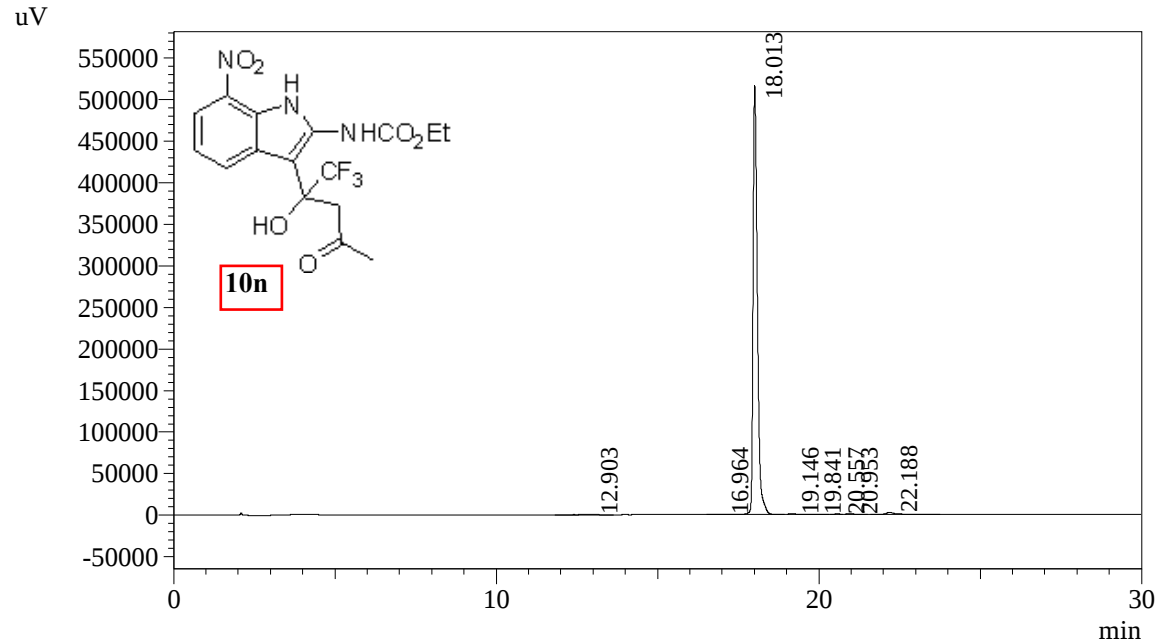
Spectrum: Single 0.617(38)

Background: Averaged 0.317-0.427(20-27) Polarity: Pos Segment1 - Event1



User Name : CJK  
Sample ID :  
Sample Name : 073021-84-a-1-a  
Data Name : D:\Chromato Solution-Light\Data\Project1\test-6506.gcd  
Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
2010/11/08 14:06:50

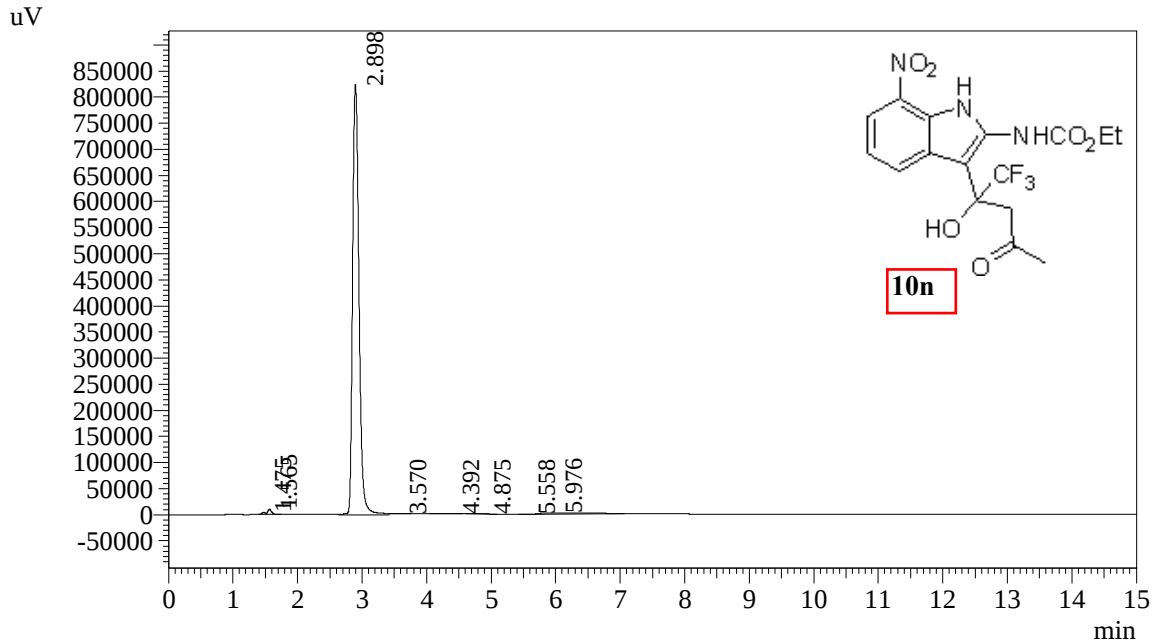
HPLC



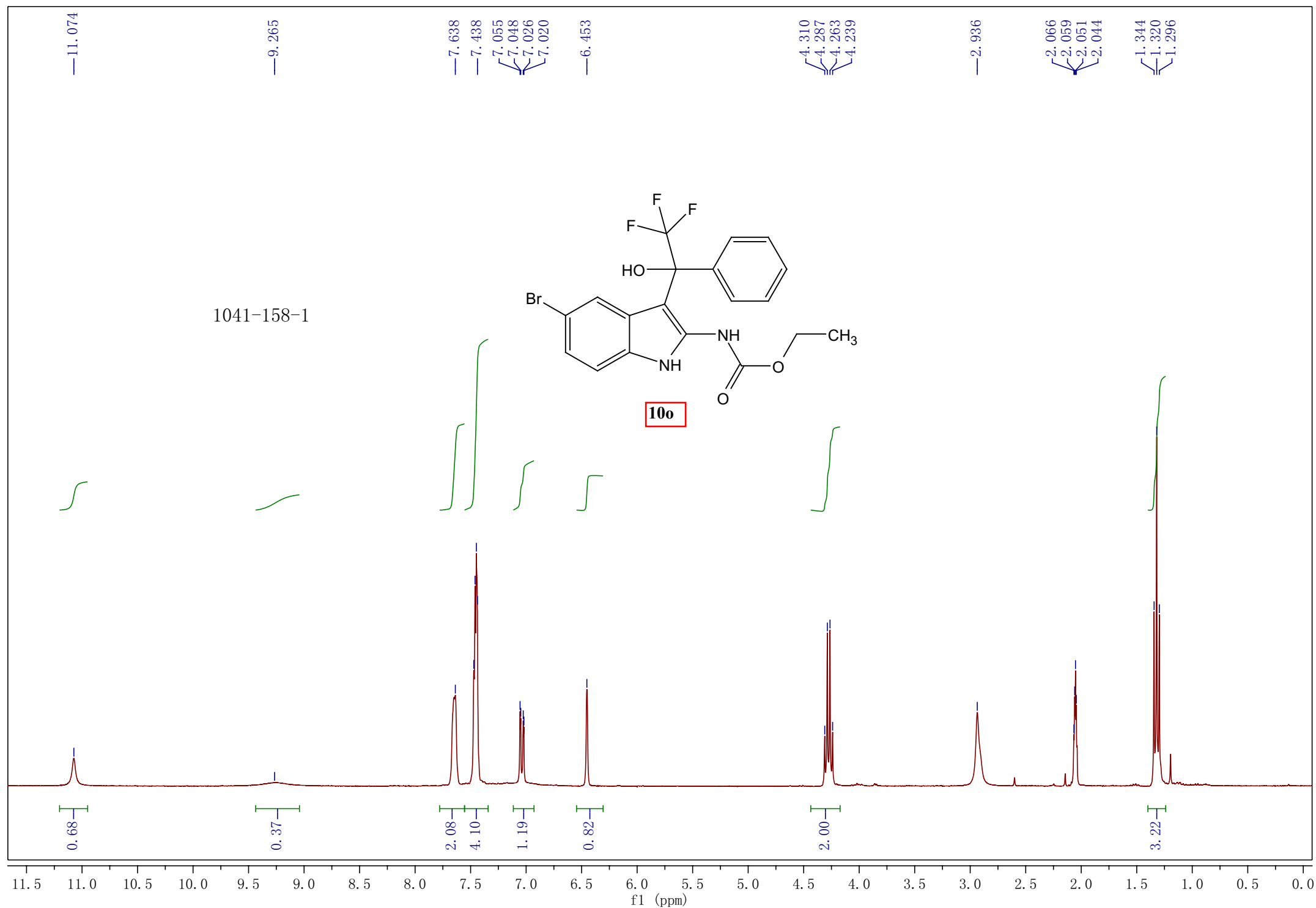
| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 12.903   | 12558   | 372    | 33.800 | 0.2557   |
| 2     | 16.964   | 6248    | 326    | 19.151 | 0.1272   |
| 3     | 18.013   | 4808466 | 515423 | 9.329  | 97.8978  |
| 4     | 19.146   | 11865   | 924    | 12.844 | 0.2416   |
| 5     | 19.841   | 5749    | 356    | 16.141 | 0.1170   |
| 6     | 20.557   | 6158    | 661    | 9.309  | 0.1254   |
| 7     | 20.953   | 12037   | 918    | 13.109 | 0.2451   |
| 8     | 22.188   | 48638   | 2533   | 19.201 | 0.9903   |
| 全部    |          | 4911719 | 521513 |        | 100.0000 |

User Name : CJK  
Sample ID :  
Sample Name : 073021-84-a-1-a  
Data Name : D:\Chromato Solution-Light\Data\Project1\test-6508.gcd  
Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
2010/11/08 15:04:55

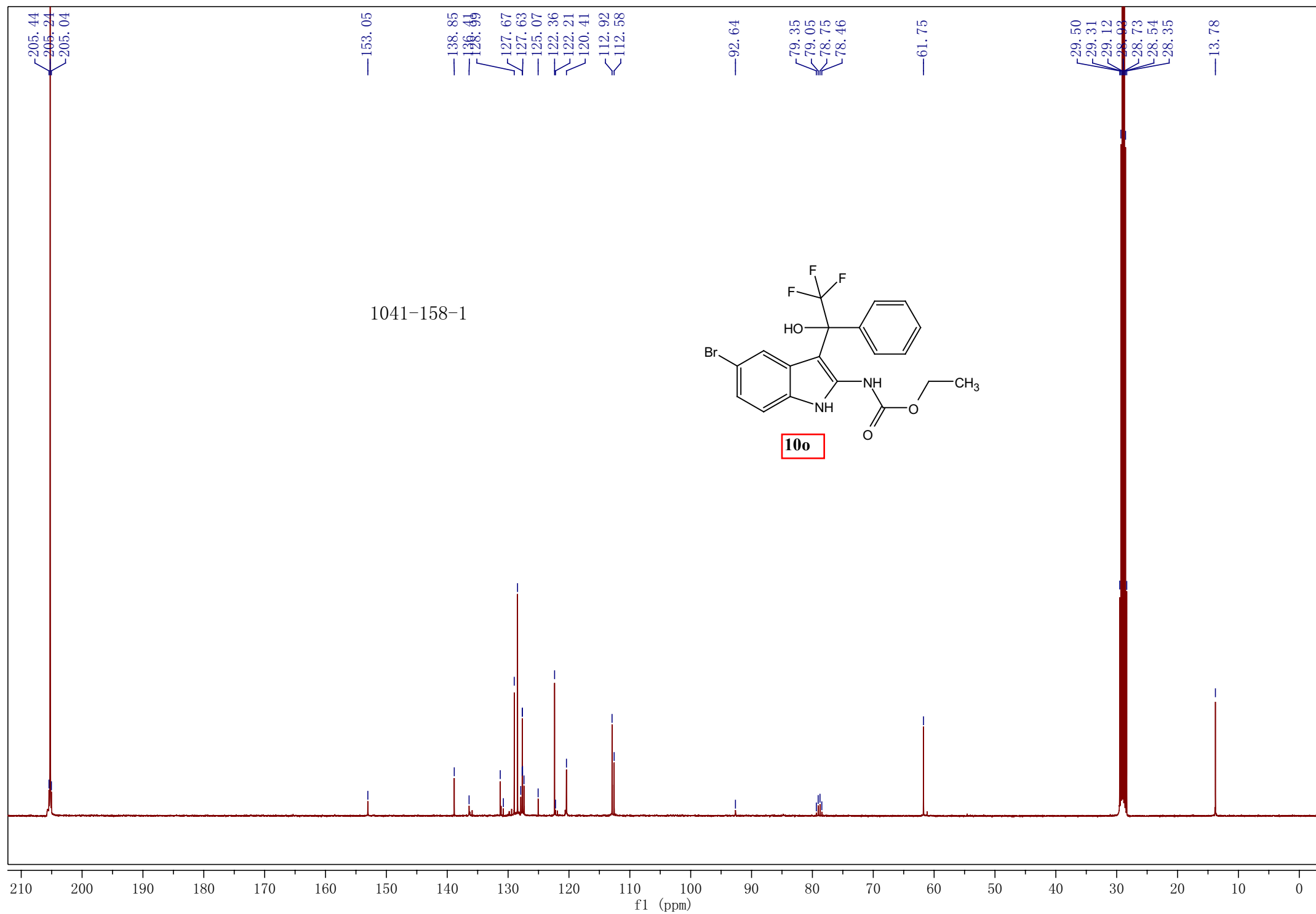
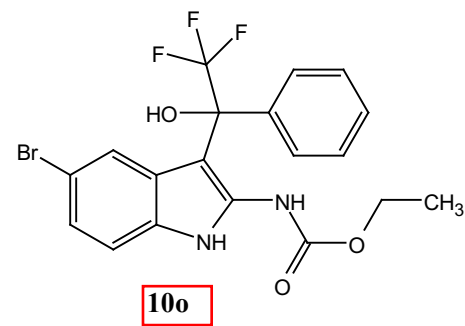
HPLC



| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 1.475    | 16263   | 4138   | 3.930  | 0.2784   |
| 2     | 1.565    | 42592   | 9791   | 4.350  | 0.7291   |
| 3     | 2.898    | 5644490 | 818520 | 6.896  | 96.6196  |
| 4     | 3.570    | 6290    | 682    | 9.224  | 0.1077   |
| 5     | 4.392    | 8381    | 845    | 9.917  | 0.1435   |
| 6     | 4.875    | 8173    | 687    | 11.895 | 0.1399   |
| 7     | 5.558    | 1301    | 212    | 6.131  | 0.0223   |
| 8     | 5.976    | 114482  | 2465   | 46.447 | 1.9597   |
| 全部    |          | 5841972 | 837340 |        | 100.0000 |



1041-158-1



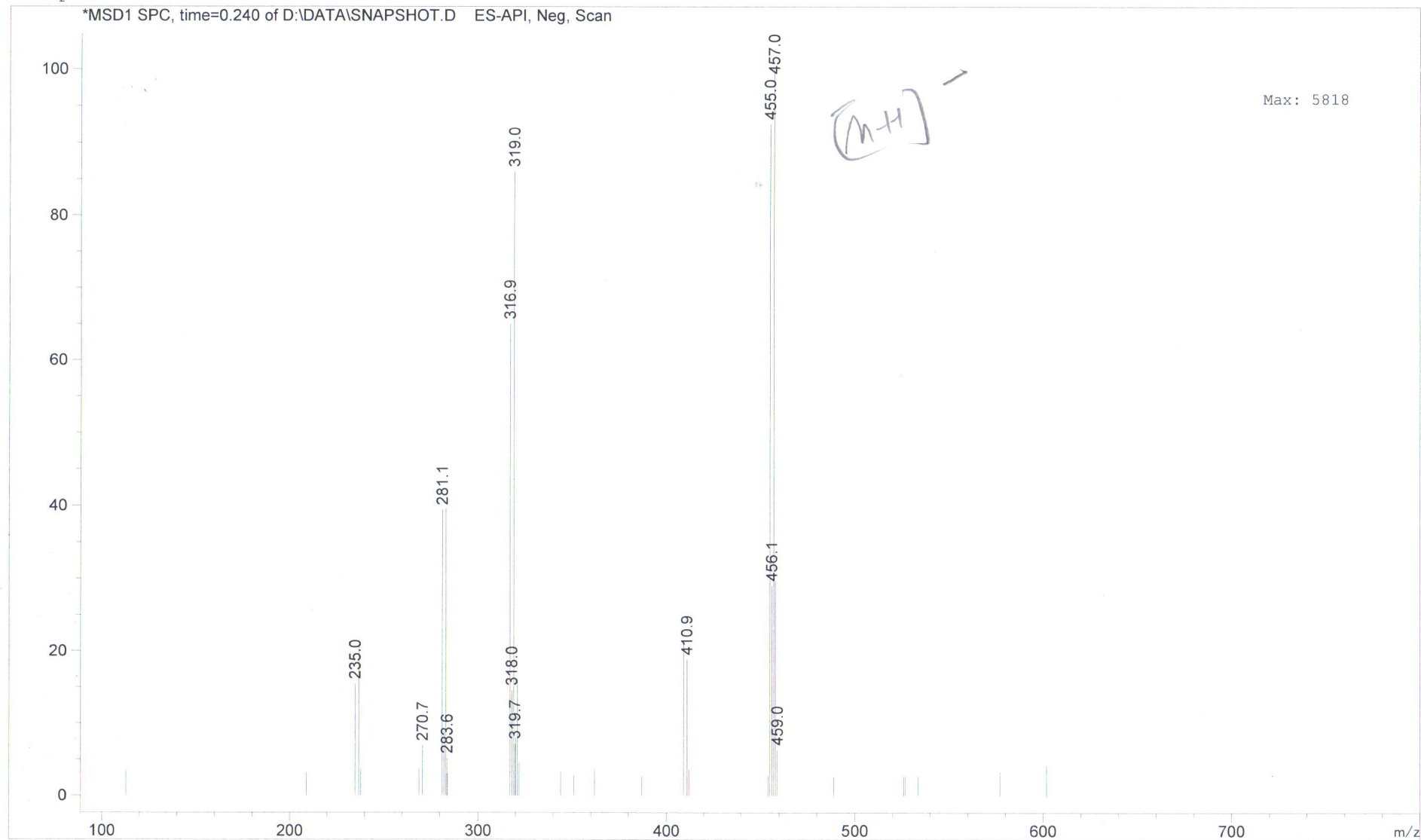
口 80: MS Spectrum  
件: : D:\DATA\SNAPSHOT.D  
称 : 1041-158

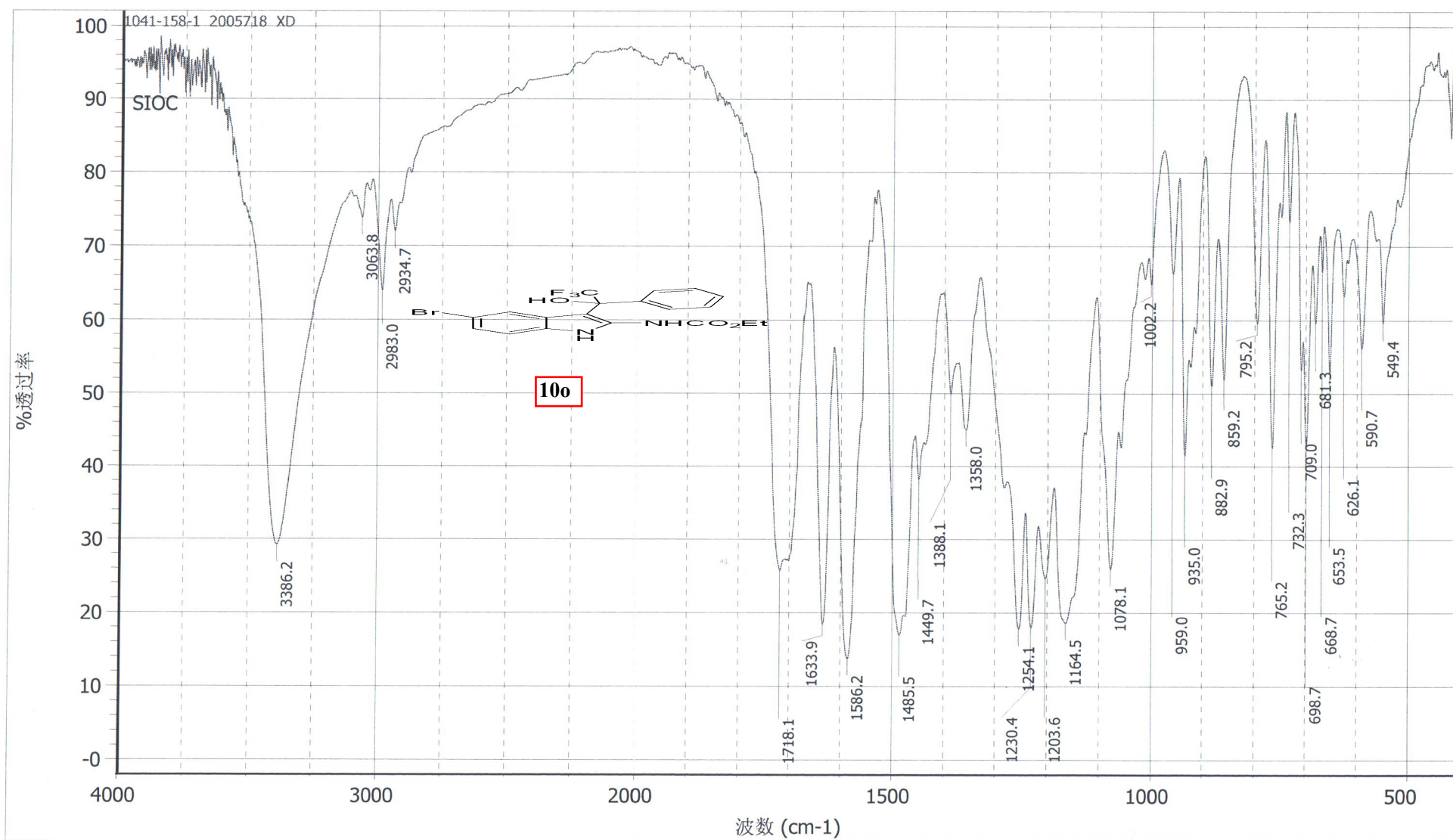
期  
法  
法  
改

序列行 : 2  
位置 : 样品瓶 49  
进样次数 : 1  
: 11 Jan 13 2:23 pm +0800  
: DEF\_LC20110310.M  
: C:\CHEM32\1\METHODS\DEF\_LC20110310.M  
: 2013-1-11 14:26:03  
(调用后修改)

姜海荣

MS Spectrum



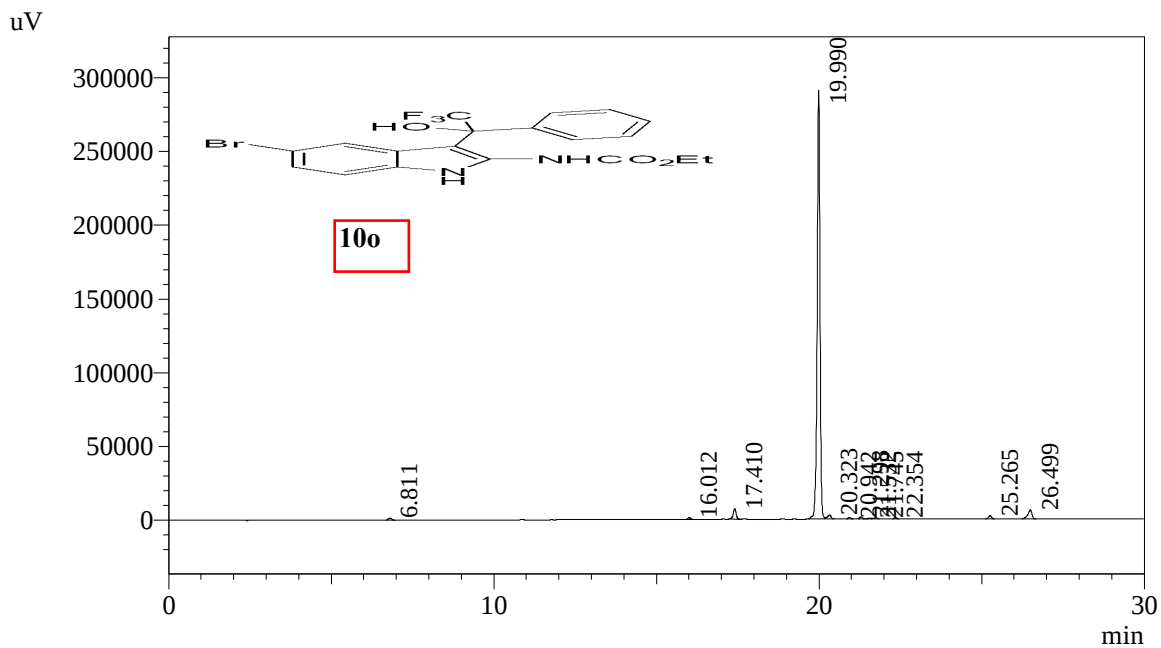


1041-158-1 2005718 XD

样品扫描次数: 32  
背景扫描次数: 32  
分辨率: 4.000  
采样增益: 1.0  
动镜速度: 0.6329

User Name : CJK  
 Sample ID :  
 Sample Name : 1041-158-1  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-11044.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2013/02/25 16:30:22

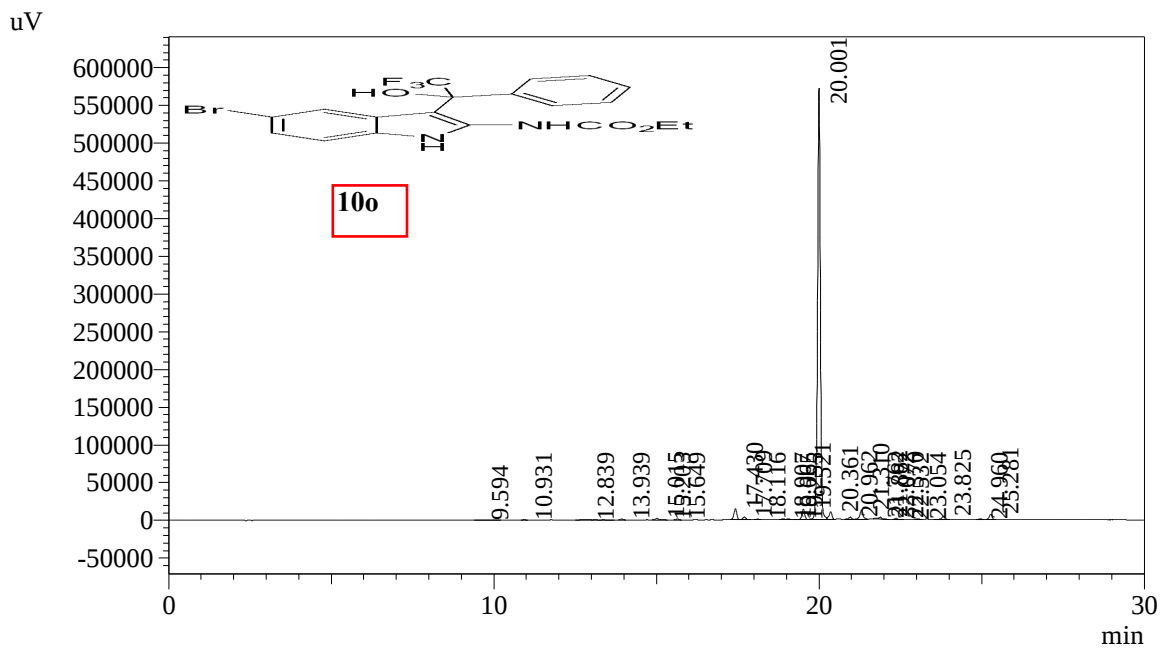
# HPLC



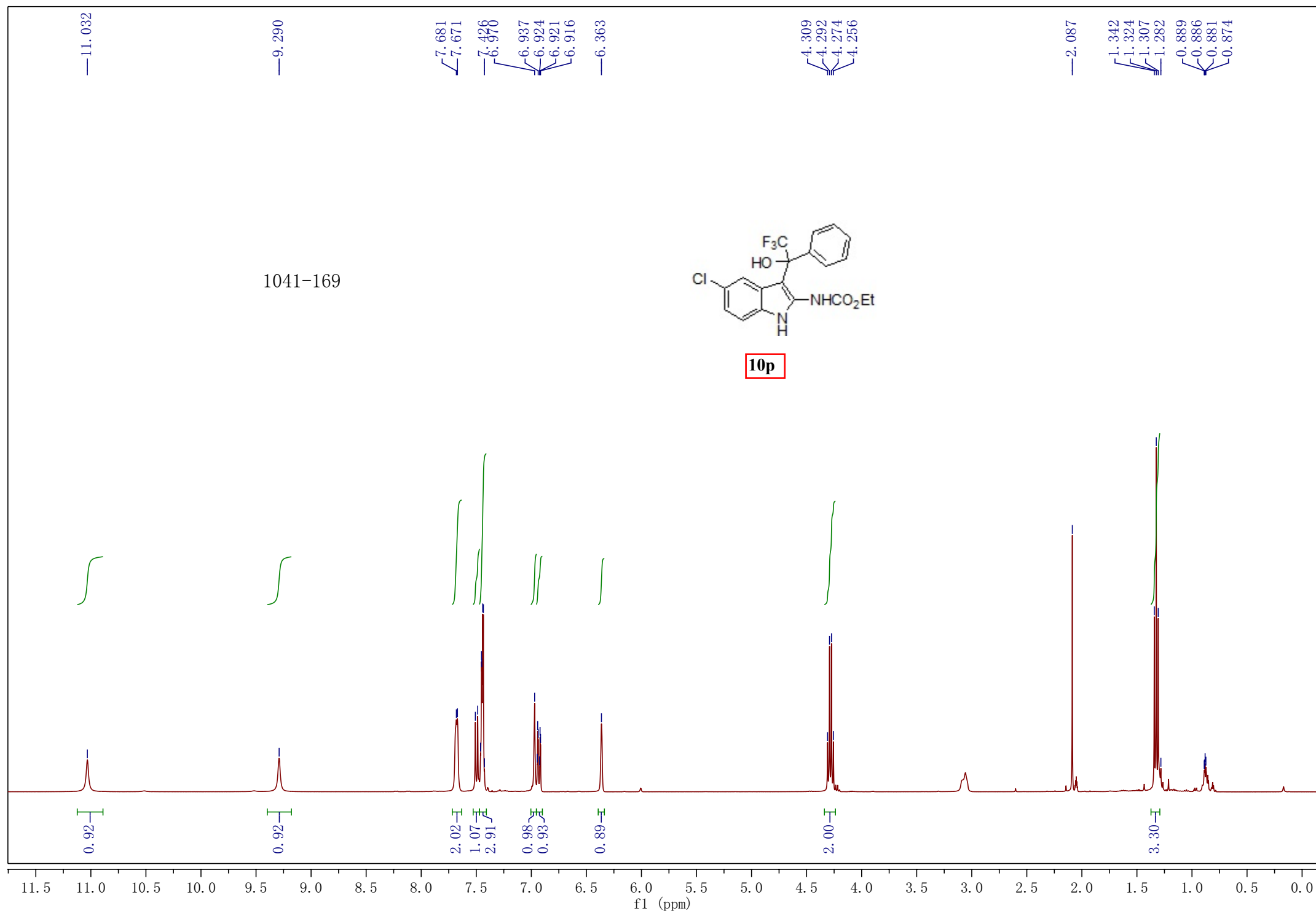
| Peak# | Ret.Time | Area    | Height | A/H   | Area%    |
|-------|----------|---------|--------|-------|----------|
| 1     | 6.811    | 10218   | 1412   | 7.235 | 0.5307   |
| 2     | 16.012   | 6484    | 1047   | 6.191 | 0.3368   |
| 3     | 17.410   | 43225   | 7180   | 6.020 | 2.2451   |
| 4     | 19.990   | 1750596 | 290954 | 6.017 | 90.9245  |
| 5     | 20.323   | 21800   | 2930   | 7.441 | 1.1323   |
| 6     | 20.942   | 5065    | 860    | 5.889 | 0.2630   |
| 7     | 21.298   | 7818    | 1344   | 5.815 | 0.4060   |
| 8     | 21.532   | 3351    | 393    | 8.530 | 0.1741   |
| 9     | 21.745   | 5012    | 726    | 6.899 | 0.2603   |
| 10    | 22.354   | 4419    | 827    | 5.346 | 0.2295   |
| 11    | 25.265   | 14040   | 2213   | 6.344 | 0.7292   |
| 12    | 26.499   | 53303   | 6052   | 8.808 | 2.7685   |
| 全部    |          | 1925331 | 315938 |       | 100.0000 |

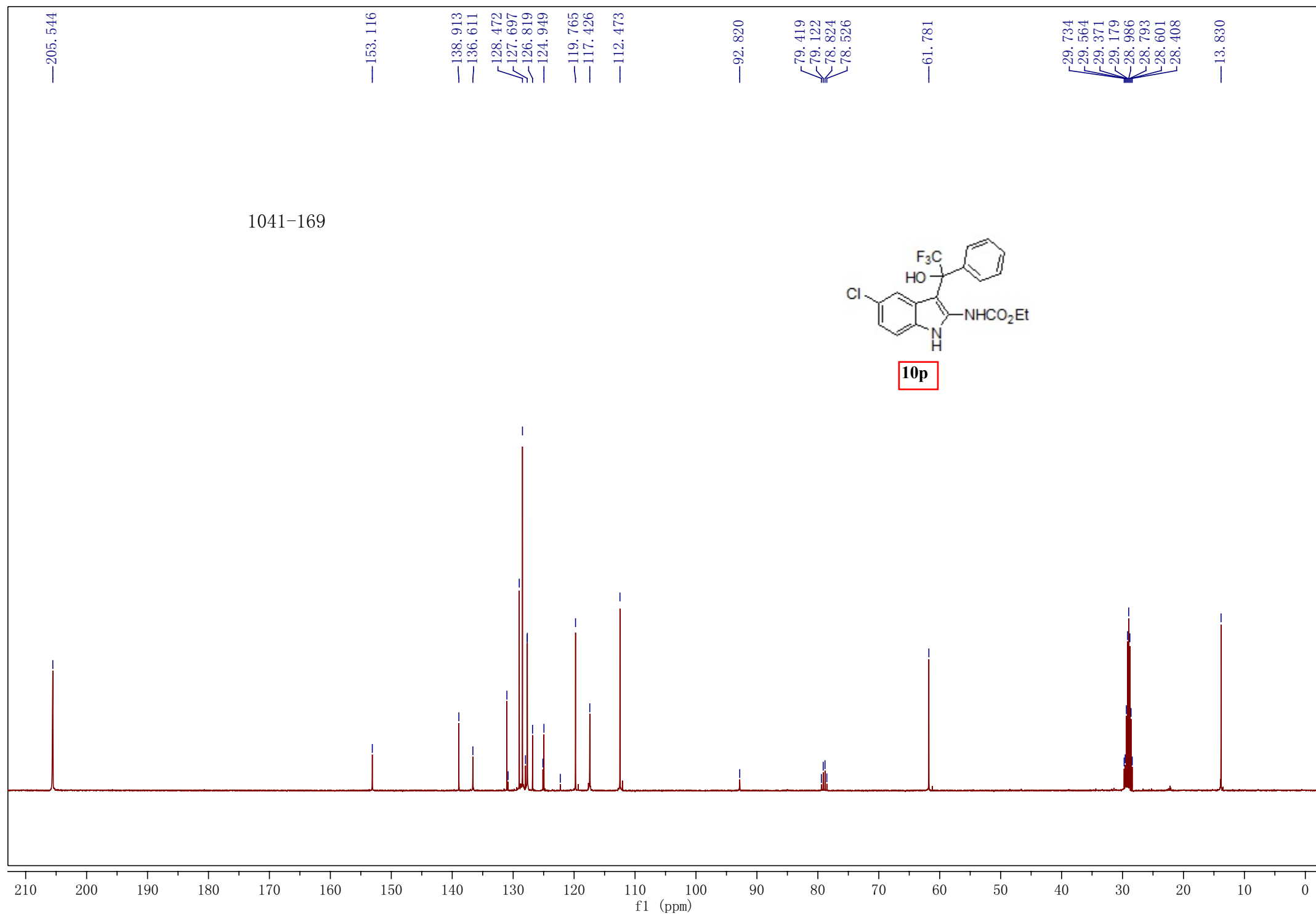
User Name : CJK  
 Sample ID :  
 Sample Name : 1041-158-1(11036)  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-11051.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2013/02/26 12:00:07

# HPLC



| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 9.594    | 2132    | 138    | 15.459 | 0.0532   |
| 2     | 10.931   | 3794    | 624    | 6.082  | 0.0947   |
| 3     | 12.839   | 12819   | 559    | 22.940 | 0.3201   |
| 4     | 13.939   | 5966    | 1053   | 5.663  | 0.1490   |
| 5     | 15.015   | 12744   | 1895   | 6.724  | 0.3182   |
| 6     | 15.203   | 3467    | 550    | 6.304  | 0.0866   |
| 7     | 15.649   | 8327    | 1396   | 5.966  | 0.2079   |
| 8     | 17.430   | 89402   | 14728  | 6.070  | 2.2323   |
| 9     | 17.709   | 25207   | 3836   | 6.571  | 0.6294   |
| 10    | 18.116   | 4824    | 834    | 5.784  | 0.1204   |
| 11    | 18.907   | 5437    | 747    | 7.274  | 0.1358   |
| 12    | 19.065   | 7880    | 1340   | 5.882  | 0.1968   |
| 13    | 19.255   | 1983    | 406    | 4.883  | 0.0495   |
| 14    | 19.521   | 81430   | 13995  | 5.819  | 2.0333   |
| 15    | 20.001   | 3442805 | 571563 | 6.023  | 85.9647  |
| 16    | 20.361   | 66839   | 10145  | 6.589  | 1.6689   |
| 17    | 20.962   | 19630   | 2848   | 6.892  | 0.4901   |
| 18    | 21.310   | 87257   | 12515  | 6.972  | 2.1788   |
| 19    | 21.762   | 6934    | 1189   | 5.833  | 0.1731   |
| 20    | 21.882   | 14797   | 2514   | 5.885  | 0.3695   |
| 21    | 22.072   | 1211    | 294    | 4.124  | 0.0302   |
| 22    | 22.370   | 9719    | 1619   | 6.003  | 0.2427   |
| 23    | 22.532   | 1941    | 350    | 5.543  | 0.0485   |
| 24    | 23.054   | 5559    | 1043   | 5.332  | 0.1388   |
| 25    | 23.825   | 30301   | 4086   | 7.417  | 0.7566   |
| 26    | 24.960   | 6388    | 951    | 6.714  | 0.1595   |
| 27    | 25.281   | 46113   | 7348   | 6.275  | 1.1514   |
| 全部    |          | 4004906 | 658566 |        | 100.0000 |



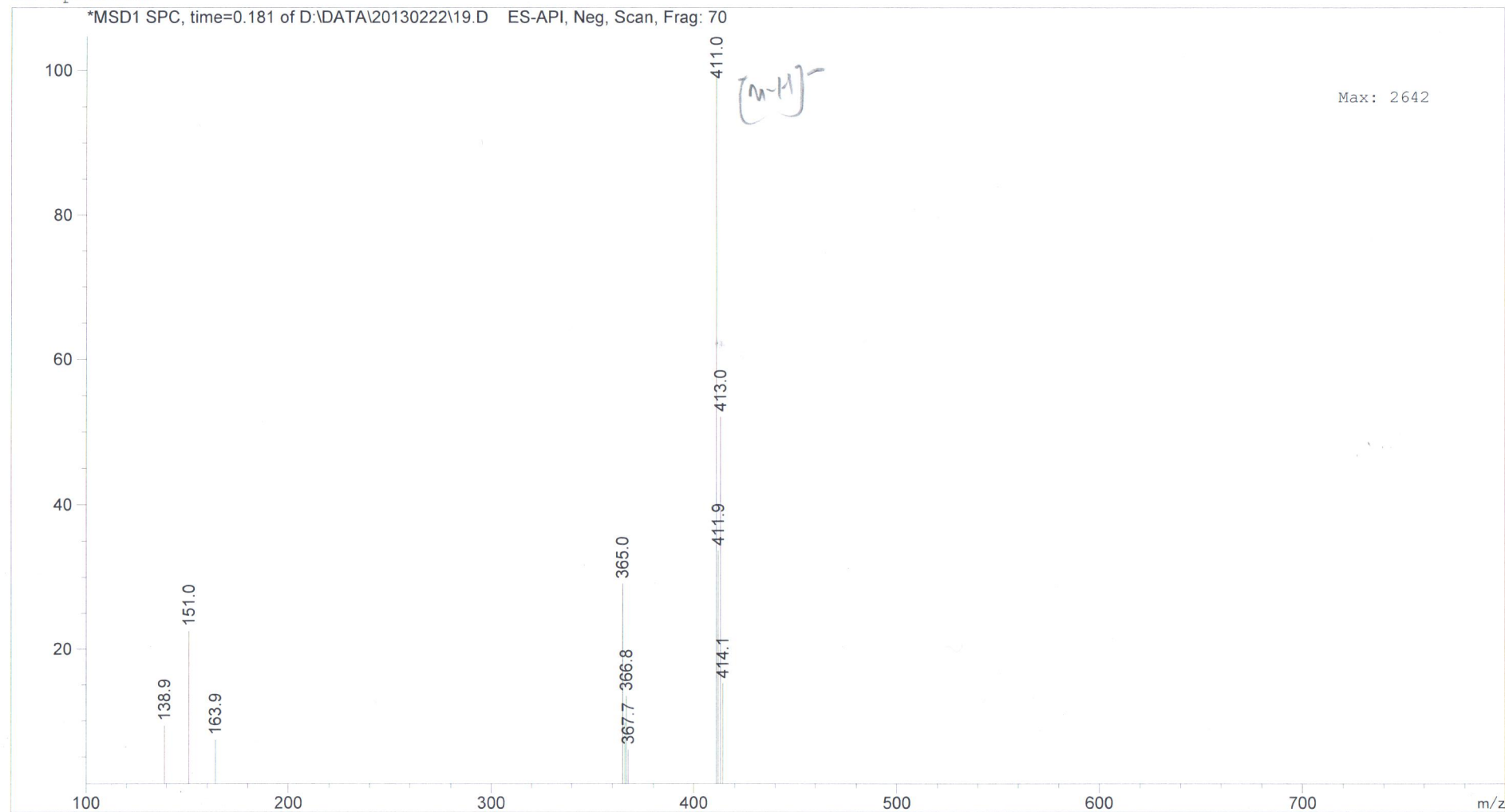


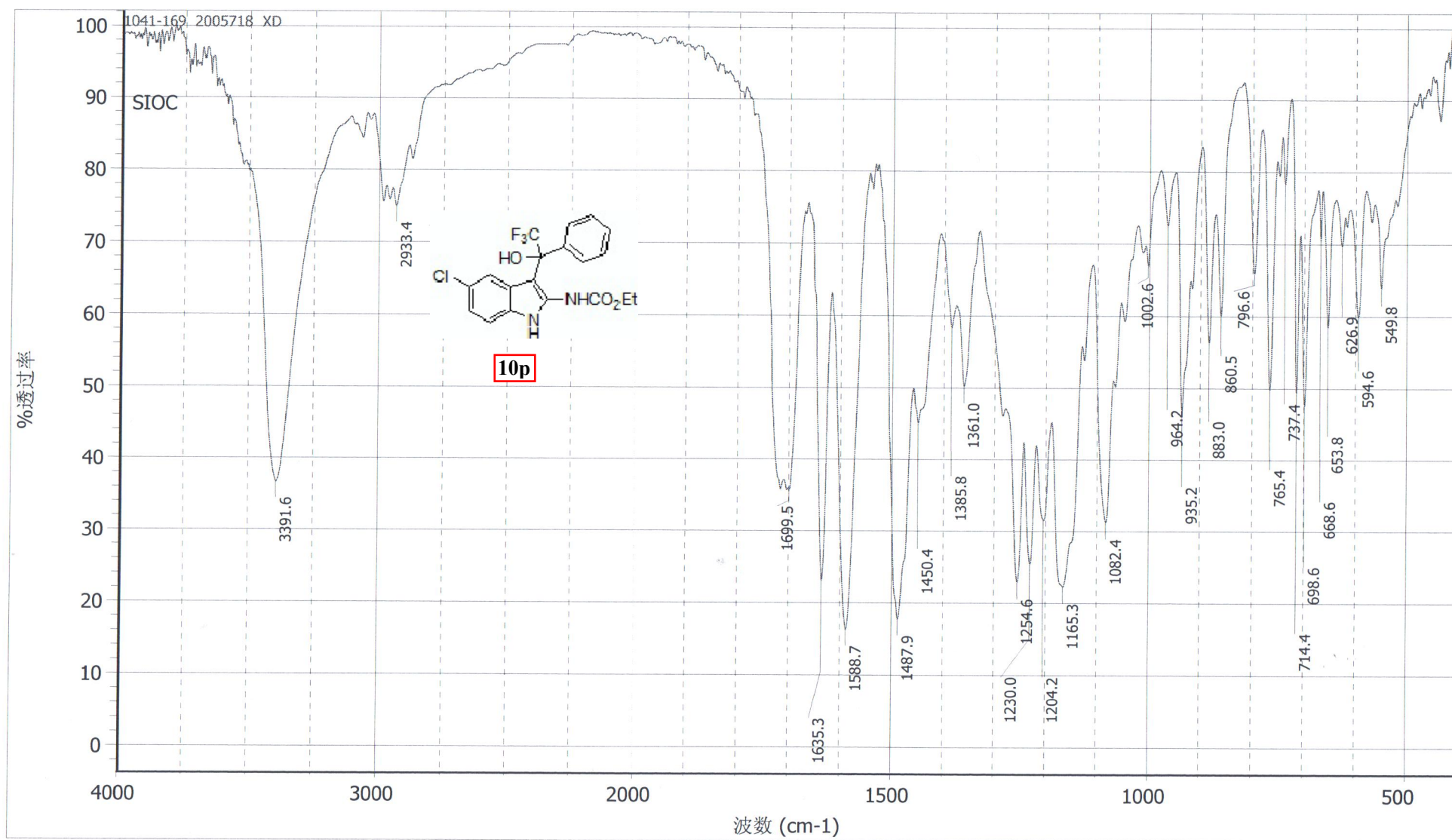
打印窗口 80: MS Spectrum  
数据文件: : D:\DATA\20130222\19.D  
样品名称 : 1041-169

=====

|      |   |                                      |      |          |
|------|---|--------------------------------------|------|----------|
| 操作者  | : |                                      | 位置   | : 样品瓶 19 |
| 仪器   | : | 仪器 1                                 | 进样次数 | : 1      |
| 进样日期 | : | 2013-2-22 16:26:03                   | 进样量  | : 0.2 µl |
| 采集方法 | : | C:\CHEM32\1\METHODS\DEF_LC20110310.M |      |          |
| 最后修改 | : | 2013-2-22 16:25:03<br>(调用后修改)        |      |          |
| 分析方法 | : | C:\CHEM32\1\METHODS\DEF_LC20110310.M |      |          |
| 最后修改 | : | 2013-2-22 16:07:09<br>(调用后修改)        |      |          |

MS Spectrum



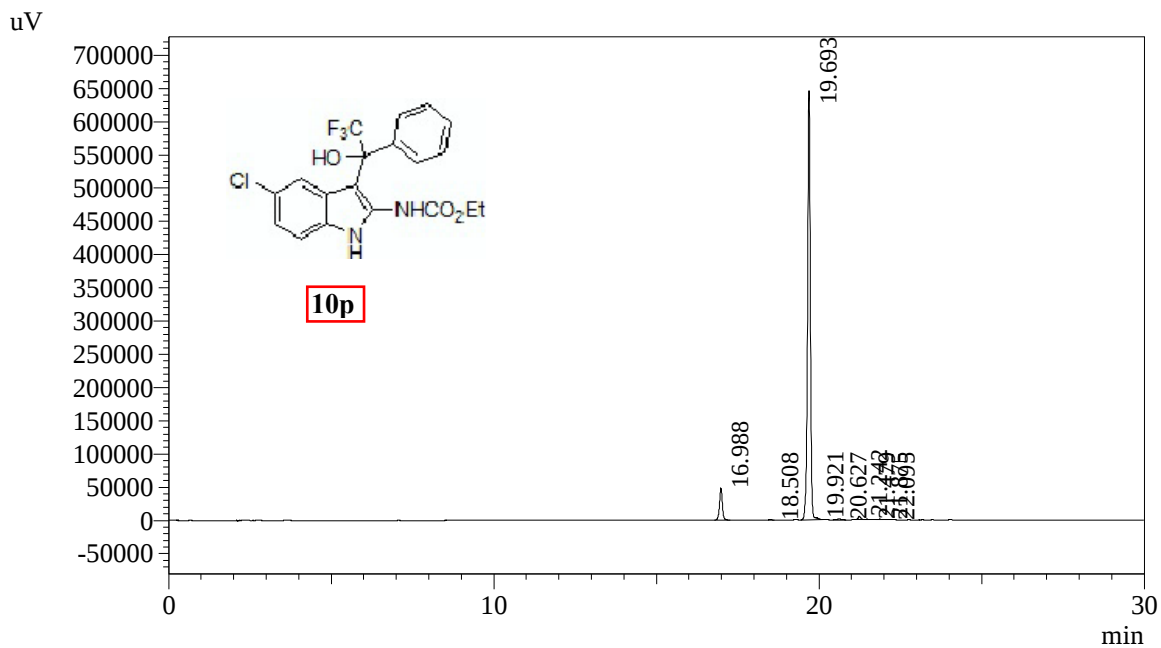


1041-169 2005718 XD

样品扫描次数: 32  
背景扫描次数: 32  
分辨率: 4.000  
采样增益: 1.0  
动镜速度: 0.6329

User Name : CJK  
 Sample ID :  
 Sample Name : 1041-169-3  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-11042.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2013/02/25 15:24:11

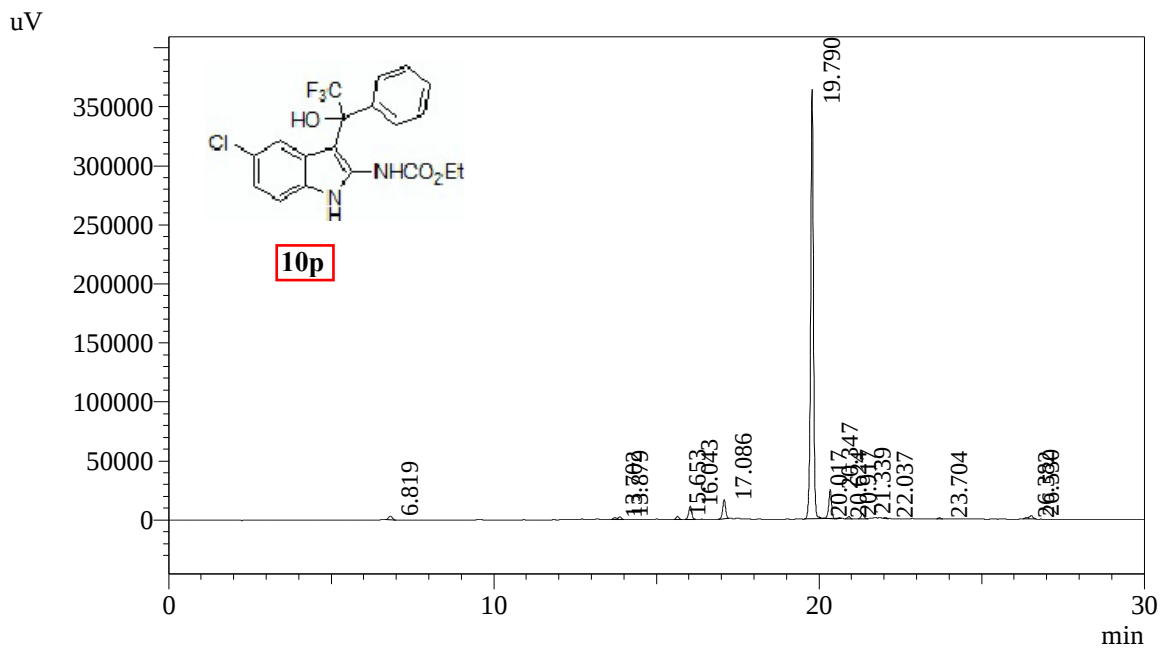
# HPLC



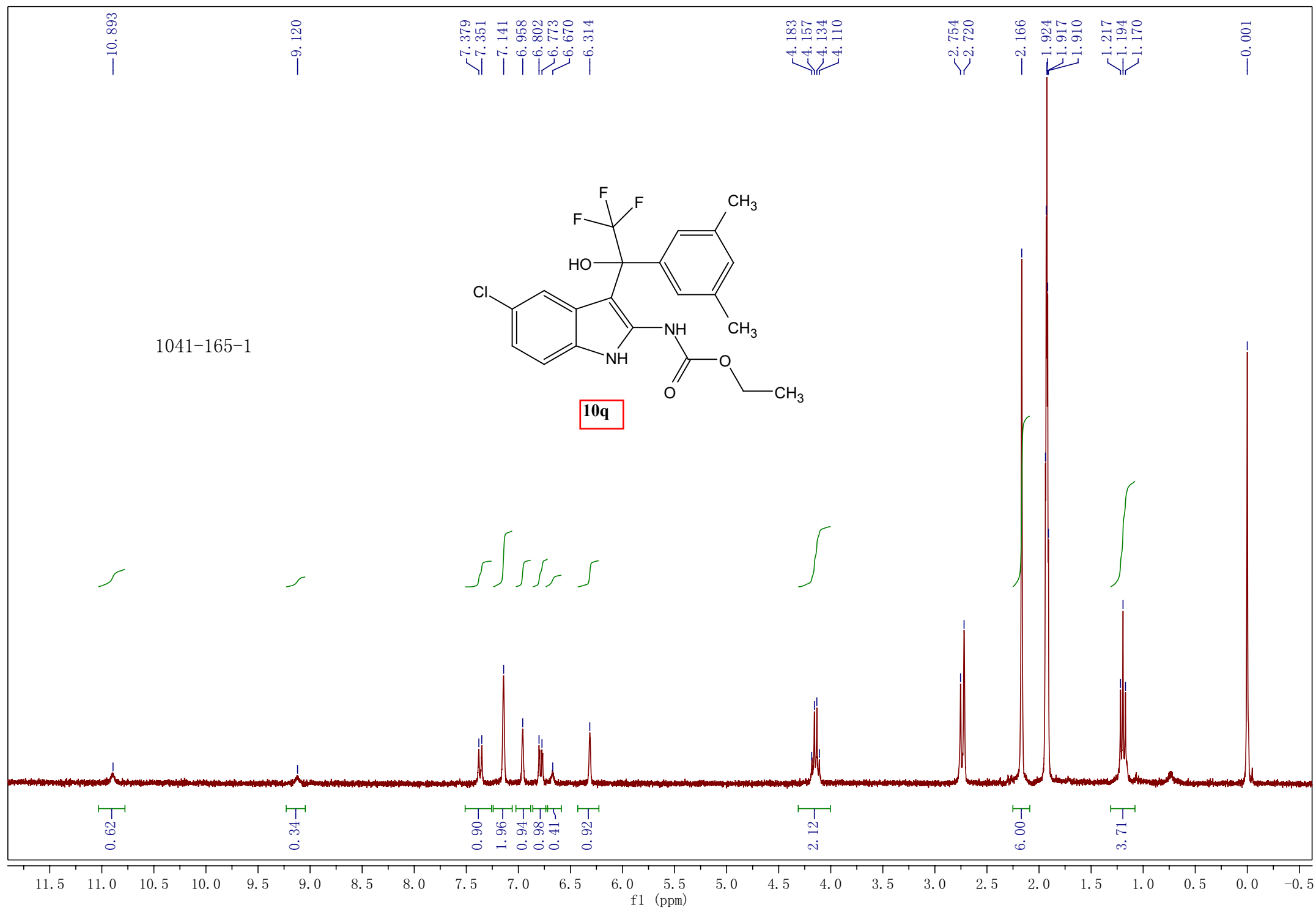
| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 16.988   | 290102  | 47593  | 6.095  | 6.8484   |
| 2     | 18.508   | 2128    | 368    | 5.780  | 0.0502   |
| 3     | 19.693   | 3884518 | 645506 | 6.018  | 91.7014  |
| 4     | 19.921   | 4115    | 1199   | 3.433  | 0.0971   |
| 5     | 20.627   | 12537   | 1171   | 10.708 | 0.2960   |
| 6     | 21.242   | 31086   | 5121   | 6.071  | 0.7338   |
| 7     | 21.479   | 3731    | 767    | 4.863  | 0.0881   |
| 8     | 21.875   | 5363    | 829    | 6.467  | 0.1266   |
| 9     | 22.095   | 2470    | 392    | 6.307  | 0.0583   |
| 全部    |          | 4236050 | 702946 |        | 100.0000 |

User Name : CJK  
 Sample ID :  
 Sample Name : 1041-169  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-11047.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2013/02/26 10:01:06

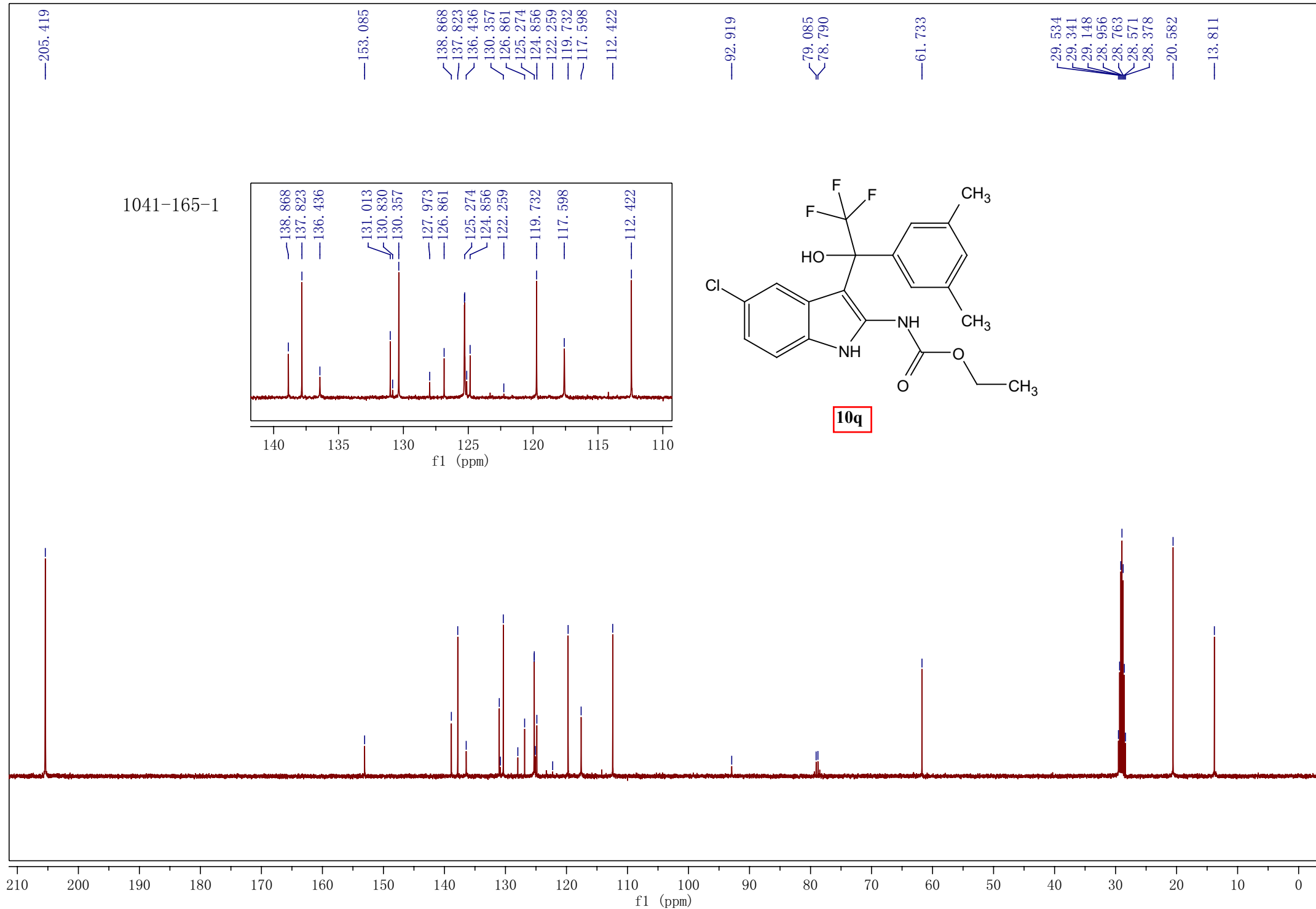
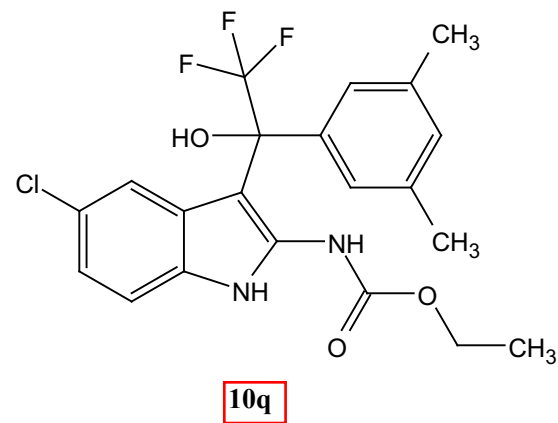
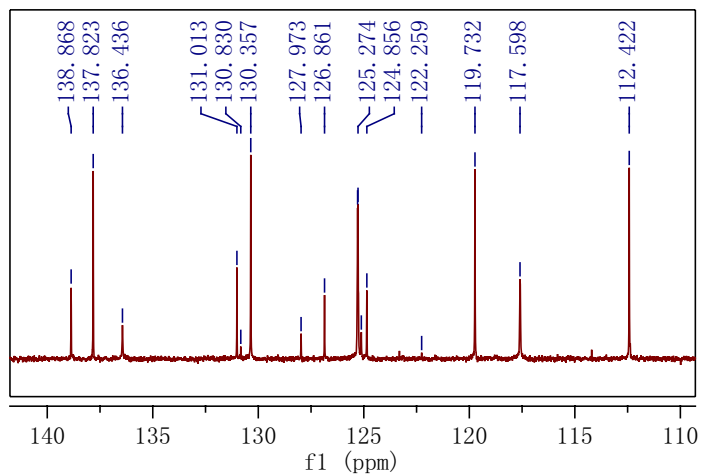
# HPLC



| Peak# | Ret.Time | Area    | Height | A/H   | Area%    |
|-------|----------|---------|--------|-------|----------|
| 1     | 6.819    | 26957   | 3326   | 8.104 | 1.0190   |
| 2     | 13.702   | 10052   | 1233   | 8.151 | 0.3800   |
| 3     | 13.879   | 12967   | 2125   | 6.103 | 0.4902   |
| 4     | 15.653   | 15024   | 2490   | 6.033 | 0.5679   |
| 5     | 16.043   | 73340   | 10992  | 6.672 | 2.7723   |
| 6     | 17.086   | 100628  | 16457  | 6.115 | 3.8039   |
| 7     | 19.790   | 2176921 | 363960 | 5.981 | 82.2901  |
| 8     | 20.017   | 972     | 362    | 2.686 | 0.0367   |
| 9     | 20.347   | 152818  | 24641  | 6.202 | 5.7767   |
| 10    | 20.624   | 2863    | 599    | 4.775 | 0.1082   |
| 11    | 20.917   | 11236   | 1939   | 5.796 | 0.4247   |
| 12    | 21.339   | 24056   | 3995   | 6.021 | 0.9093   |
| 13    | 22.037   | 3016    | 692    | 4.358 | 0.1140   |
| 14    | 23.704   | 5040    | 995    | 5.066 | 0.1905   |
| 15    | 26.382   | 8384    | 1118   | 7.499 | 0.3169   |
| 16    | 26.530   | 21151   | 2994   | 7.065 | 0.7995   |
| 全部    |          | 2645425 | 437918 |       | 100.0000 |



1041-165-1

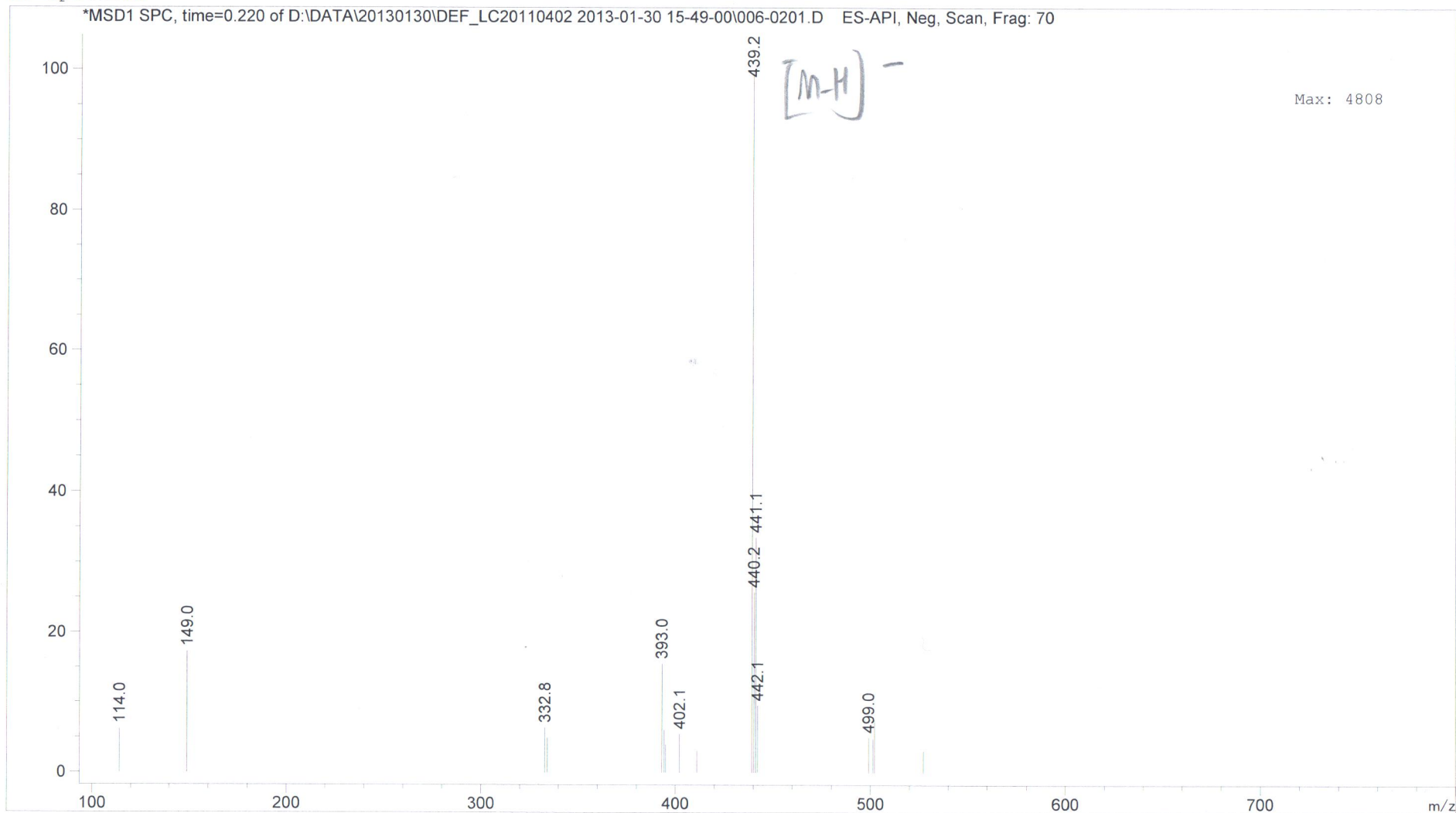


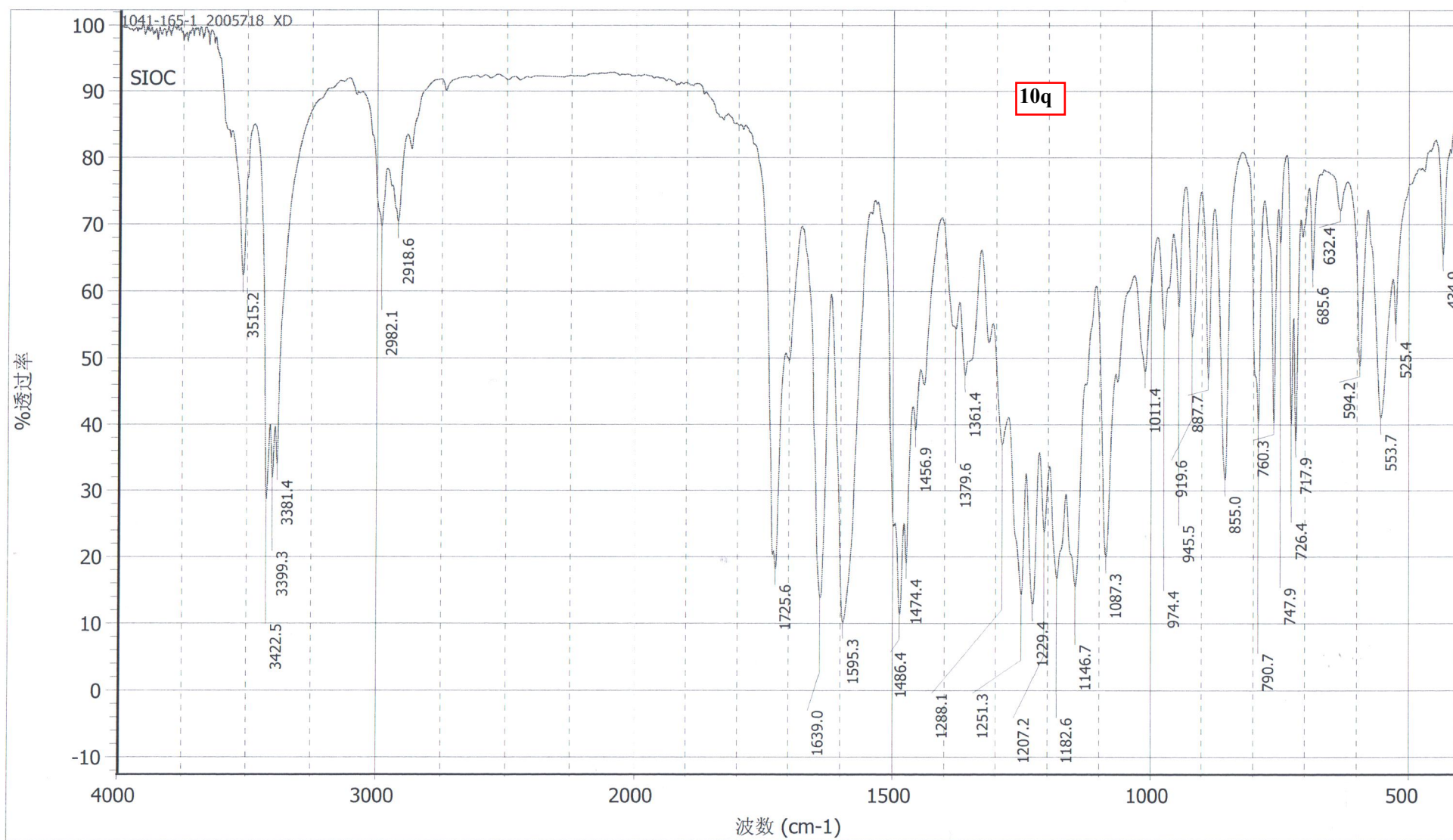
打印窗口 80: MS Spectrum  
数据文件: : D:\DATA\20130130\DEF\_LC20110402 2013-01-30 15-49-00\006-0201.D  
样品名称 : 1041-165-1

=====

|      |   |                                                                      |      |   |        |
|------|---|----------------------------------------------------------------------|------|---|--------|
| 操作者  | : |                                                                      | 序列行  | : | 2      |
| 仪器   | : | 仪器 1                                                                 | 位置   | : | 样品瓶 6  |
| 进样日期 | : | 2013-1-30 15:53:41                                                   | 进样次数 | : | 1      |
|      |   |                                                                      | 进样量  | : | 0.2 µl |
| 采集方法 | : | D:\DATA\20130130\DEF_LC20110402 2013-01-30 15-49-00\DEF_LC20110310.M |      |   |        |
| 最后修改 | : | 2013-1-30 15:48:28                                                   |      |   |        |
| 分析方法 | : | C:\CHEM32\1\METHODS\DEF_LC20110310.M                                 |      |   |        |
| 最后修改 | : | 2013-1-30 9:25:21                                                    |      |   |        |
|      |   | (调用后修改)                                                              |      |   |        |

MS Spectrum



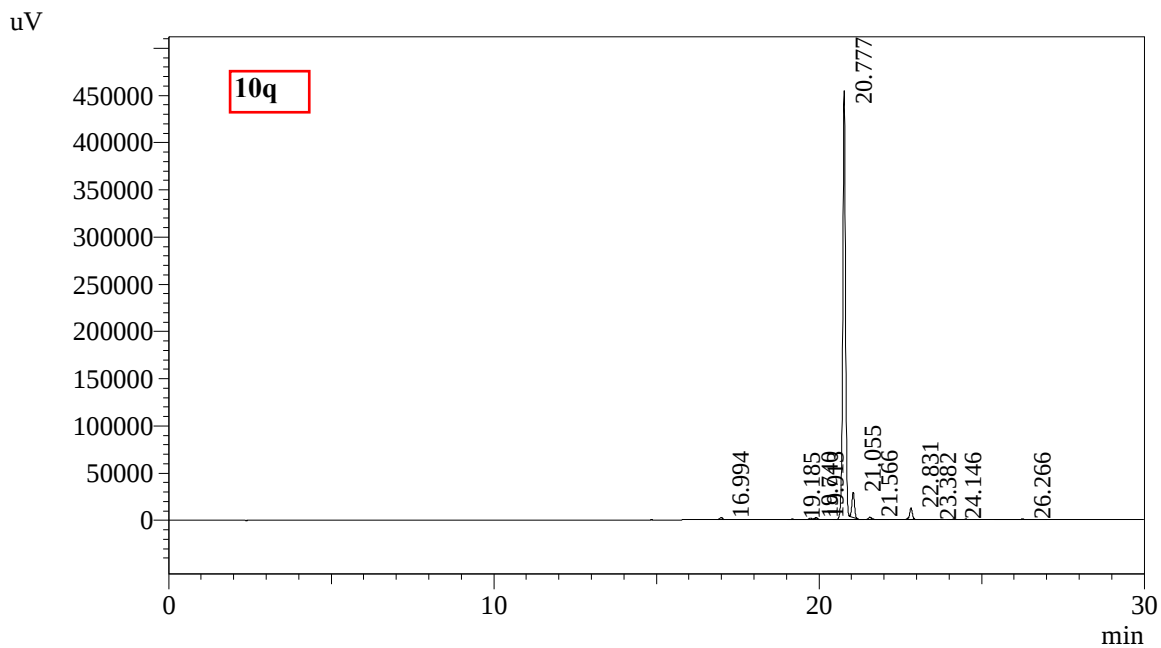


1041-165-1 2005718 XD

样品扫描次数: 32  
背景扫描次数: 32  
分辨率: 4.000  
采样增益: 1.0  
动镜速度: 0.6329

User Name : CJK  
 Sample ID :  
 Sample Name : 1041-165-1  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-11037.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2013/02/25 12:31:44

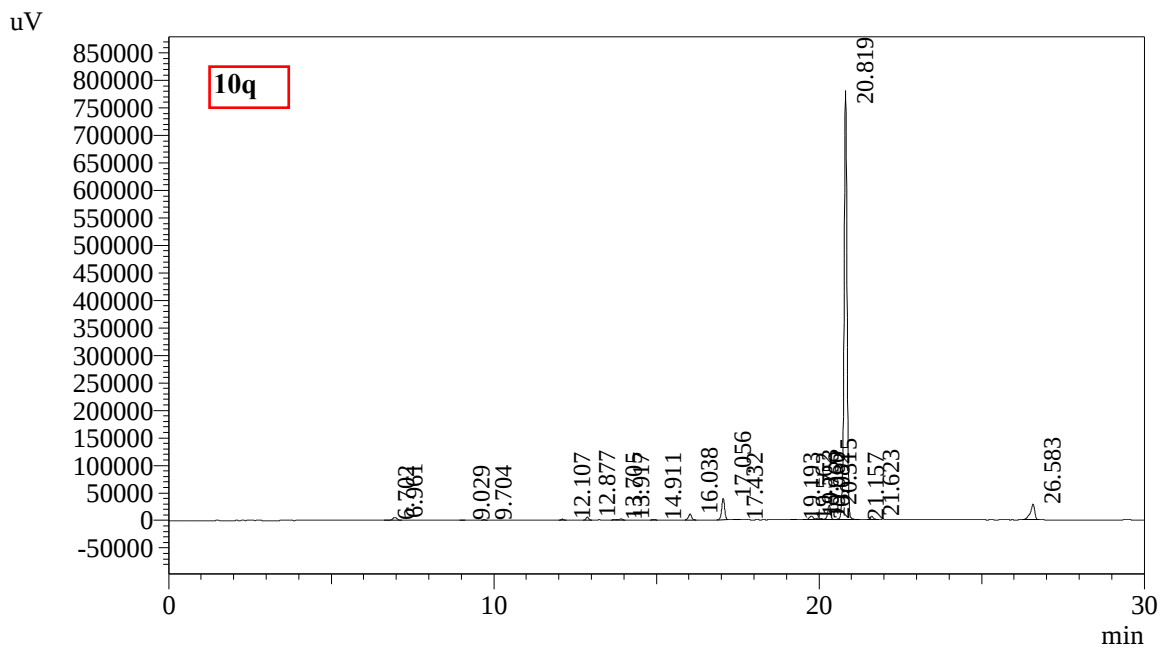
# HPLC



| Peak# | Ret.Time | Area    | Height | A/H    | Area%    |
|-------|----------|---------|--------|--------|----------|
| 1     | 16.994   | 11607   | 2134   | 5.438  | 0.3730   |
| 2     | 19.185   | 3280    | 518    | 6.335  | 0.1054   |
| 3     | 19.740   | 8859    | 1616   | 5.481  | 0.2847   |
| 4     | 19.913   | 11109   | 1995   | 5.570  | 0.3570   |
| 5     | 20.777   | 2821057 | 449642 | 6.274  | 90.6602  |
| 6     | 21.055   | 147583  | 26206  | 5.632  | 4.7429   |
| 7     | 21.566   | 17289   | 2277   | 7.592  | 0.5556   |
| 8     | 22.831   | 70658   | 12199  | 5.792  | 2.2707   |
| 9     | 23.382   | 3412    | 282    | 12.102 | 0.1097   |
| 10    | 24.146   | 7479    | 423    | 17.688 | 0.2403   |
| 11    | 26.266   | 9349    | 555    | 16.848 | 0.3005   |
| 全部    |          | 3111682 | 497847 |        | 100.0000 |

User Name : CJK  
 Sample ID :  
 Sample Name : 1041-165-1  
 Data Name : D:\Chromato Solution-Light\Data\Project1\test-11045.gcd  
 Method Name : D:\Chromato Solution-Light\Data\Project1\070417.gcm  
 2013/02/26 8:56:22

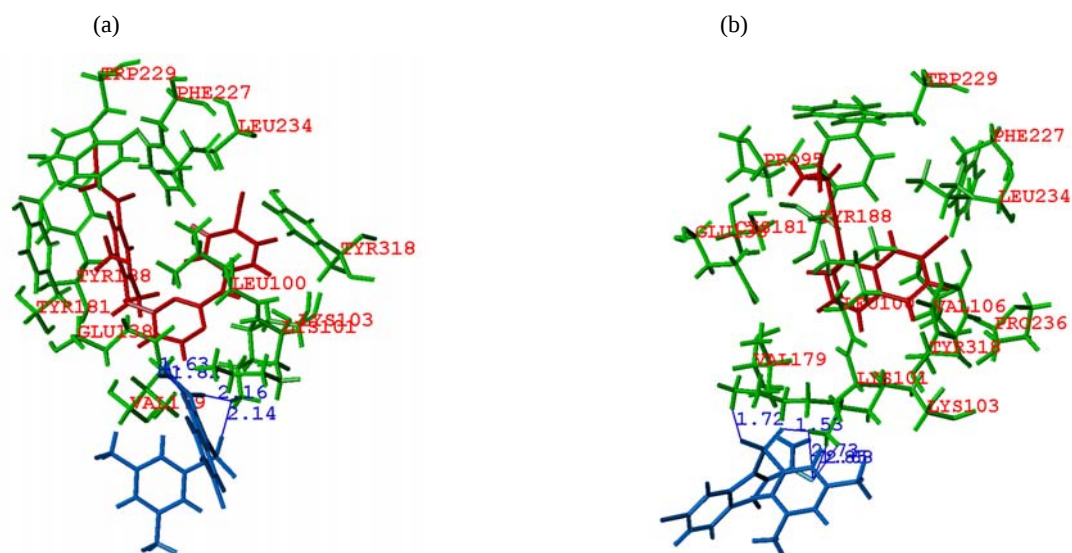
# HPLC



| Peak# | Ret.Time | Area    | Height | A/H   | Area%    |
|-------|----------|---------|--------|-------|----------|
| 1     | 6.702    | 5786    | 620    | 9.333 | 0.1000   |
| 2     | 6.961    | 49091   | 5229   | 9.389 | 0.8486   |
| 3     | 9.029    | 3303    | 608    | 5.430 | 0.0571   |
| 4     | 9.704    | 6318    | 1125   | 5.615 | 0.1092   |
| 5     | 12.107   | 10175   | 1862   | 5.463 | 0.1759   |
| 6     | 12.877   | 31070   | 5575   | 5.573 | 0.5371   |
| 7     | 13.705   | 7812    | 1319   | 5.922 | 0.1350   |
| 8     | 13.917   | 15565   | 2338   | 6.658 | 0.2690   |
| 9     | 14.911   | 7430    | 1280   | 5.806 | 0.1284   |
| 10    | 16.038   | 72120   | 10850  | 6.647 | 1.2466   |
| 11    | 17.056   | 233834  | 38901  | 6.011 | 4.0419   |
| 12    | 17.432   | 3477    | 604    | 5.756 | 0.0601   |
| 13    | 19.193   | 3331    | 617    | 5.398 | 0.0576   |
| 14    | 19.562   | 4389    | 666    | 6.587 | 0.0759   |
| 15    | 19.753   | 56849   | 6202   | 9.166 | 0.9827   |
| 16    | 19.960   | 19960   | 3175   | 6.287 | 0.3450   |
| 17    | 20.082   | 13305   | 2149   | 6.190 | 0.2300   |
| 18    | 20.315   | 165035  | 26279  | 6.280 | 2.8527   |
| 19    | 20.819   | 4762404 | 780353 | 6.103 | 82.3206  |
| 20    | 21.157   | 4104    | 583    | 7.034 | 0.0709   |
| 21    | 21.623   | 38267   | 5603   | 6.830 | 0.6615   |
| 22    | 26.583   | 271565  | 28699  | 9.463 | 4.6941   |
| 全部    |          | 5785190 | 924637 |       | 100.0000 |

### 3. Interaction between IAS 2 and WT / Y181C mutant:

As shown in Figure 1, IAS 2 is not in the active site of TMC278 and EFV.



**Fig. 1** (a) Interaction between HIV-1 RT WT (PDB: 2ZD1) and TMC278 (red, cry.), IAS 2 (blue, docking result); (b) Interaction between Y181C mutant HIV-1 RT (PDB: 1JKH) and EFV (red, cry.), IAS 2 (blue, docking result).