

# Supporting Information

## Photoinduced C-C cross-coupling of aryl chlorides and inert arenes

Lele Wang, Wenzhao Qiu, Hongge Shao and Rusheng Yuan\*

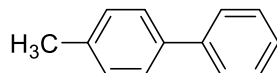
Research Institute of Photocatalysis, State Key Laboratory of Photocatalysis on Energy and Environment, Fuzhou University, Fuzhou, 350002, P. R. China

\*E-mail: yuanrs@fzu.edu.cn

|   |       |
|---|-------|
| NMR Spectra of the Isolated Cross-Coupling Products.....  | 1-11  |
| GC-MS Spectra of the Products Generated from Direct Cross-Coupling of Chlorobenzene with Cyclohexane (Figure S1)..... | 12    |
| <sup>1</sup> H NMR Spectrum of 4-Methylbiphenyl and 4-Methylbiphenyl-2',3',4',5',6'-d5 (Figure S2).....               | 13    |
| GC-MS Spectra of the Products for Different Reactions.....  | 14-39 |
| References.....   | 40    |

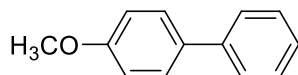
## Characterization of Products in Details:

### (3a) 4-Methylbiphenyl



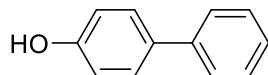
The title compound was prepared according to the general procedure using 4-chlorotoluene with benzene, and purified by silica gel column chromatography as white solid (7.9 mg, 47%). The observed characterization data ( $^1\text{H}$ ) was consistent with that previously reported in the literature [1].  **$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**  $\delta$  = 2.49 (s, 3H), 7.34 (d,  $J$ = 8.1 Hz, 2H), 7.41 (t,  $J$ = 7.3 Hz, 1H), 7.52 (t,  $J$ = 7.5 Hz, 2H), 7.59 (d,  $J$ = 8.0 Hz, 2H), 7.68 (d,  $J$ = 7.6 Hz, 2H).  **$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**  $\delta$  = 21.1, 127.0, 128.8, 129.6, 137.0, 138.4, 141.2.

### (3b) 4-Methoxybiphenyl



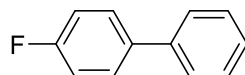
The title compound was prepared according to the general procedure using 4-chloroanisole with benzene, and purified by silica gel column chromatography as white solid (10.1 mg, 55%). The observed characterization data ( $^1\text{H}$ ) was consistent with that previously reported in the literature [1].  **$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**  $\delta$  = 3.90 (s, 3H), 7.03 (d,  $J$ =8.5 Hz, 2H), 7.27-7.39 (m, 1H), 7.47 (t,  $J$ = 7.6 Hz, 2H), 7.59 (t,  $J$ = 8.1 Hz, 4H).  **$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**  $\delta$  =55.4, 114.2, 126.7, 128.2, 128.7, 133.8, 140.8, 159.2.

### (3c) 4-Phenylphenol



The title compound was prepared according to the general procedure using 4-chlorophenol with benzene, and purified by silica gel column chromatography as white solid (7.5 mg, 44%).  **$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**  $\delta$  = 6.71 (d,  $J$ =8.6 Hz, 2H), 6.93 (s, 1H) 7.09 (t,  $J$ = 7.2 Hz, 1H), 7.21 (t,  $J$ =7.6 Hz, 2H), 7.28 (d,  $J$ =8.4 Hz, 2H), 7.35 (d,  $J$ =7.6 Hz, 2H).  **$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**  $\delta$  =115.5, 116.9, 126.3, 127.9, 128.6, 132.4, 140.6, 156.4.

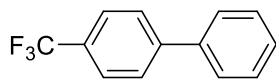
### (3d) 4-Fluorobiphenyl



The title compound was prepared according to the general procedure using 1-chloro-4-fluorobenzene with benzene, and purified by silica gel column chromatography as white solid (7.8 mg, 45.3%). The observed characterization data ( $^1\text{H}$ ) was consistent with that previously reported in the literature [1].  **$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**  $\delta$  = 7.18 (t,  $J$ =8.5 Hz, 2H), 7.41 (t,  $J$ =7.5 Hz, 1H), 7.49 (t,  $J$ =7.4 Hz, 2H),

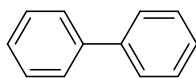
7.56-7.64 (m, 4H). **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):** δ = 115.6, 115.7, 127.1, 127.3, 128.7, 128.8, 128.9, 137.4, 137.5, 140.3, 161.3, 163.7.

### (3e) 4-Trifluoromethylbiphenyl



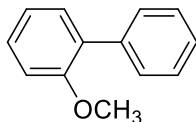
The title compound was prepared according to the general procedure using 4-chlorobenzotrifluoride with benzene, and purified by silica gel column chromatography as white solid (8.0 mg, 36%). The observed characterization data (<sup>1</sup>H) was consistent with that previously reported in the literature [2]. **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)** δ = 7.44 (t, J=7.3 Hz, 1H), 7.51 (t, J=7.3 Hz, 2H), 7.64 (d, J=7.3 Hz, 2H), 7.73 (s, 4H). **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):** δ = 120.2, 123.0, 125.7 (q, J= 3.7, CF<sub>3</sub>), 127.3, 127.4, 128.2, 129.0, 129.5, 139.8, 144.8.

### (3g) Biphenyl



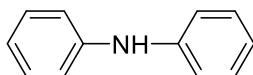
The title compound was prepared according to the general procedure using chlorobenzene with benzene, and purified by silica gel column chromatography as white solid (5.8 mg, 37.5%). The observed characterization data (<sup>1</sup>H) was consistent with that previously reported in the literature [1]. **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):** δ = 7.49 (t, J=7.3 Hz, 2H), 7.59 (t, J=7.6 Hz, 4H), 7.75 (d, J=7.2 Hz, 4H). **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):** δ = 127.3, 127.4, 128.9, 141.4.

### (3i) 2-Methoxybiphenyl



The title compound was prepared according to the general procedure using 2-chloroanisole with benzene, and purified by silica gel column chromatography as white solid (5.9 mg, 32%). The observed characterization data (<sup>1</sup>H) was consistent with that previously reported in the literature [1]. **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):** δ = 3.87 (s, 3H), 7.03-7.13 (m, 2H), 7.39 (t, J=7.3 Hz, 3H), 7.47 (t, J=7.5 Hz, 2H), 7.60 (d, J=7.5 Hz, 2H). **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):** δ = 55.6, 111.3, 120.9, 126.9, 128.0, 128.6, 130.8, 130.9, 138.6, 156.5.

### (3l) Diphenylamine

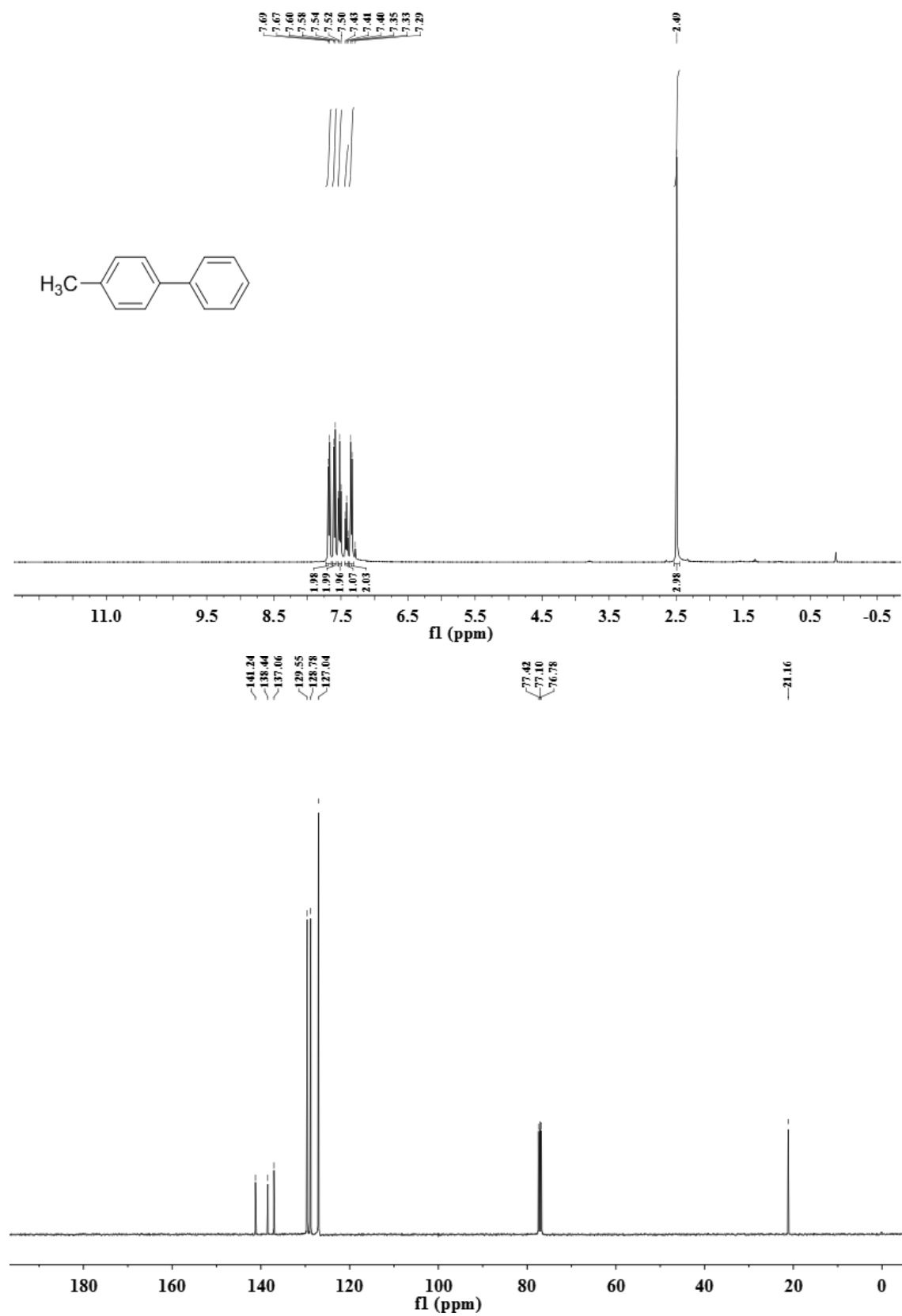


The title compound was prepared according to the general procedure using chlorobenzene with aniline, and purified by silica gel column chromatography as white solid (7.4 mg, 44%). **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):** δ = 7.04 (t, J=7.3 Hz 2H), 7.17 (d,

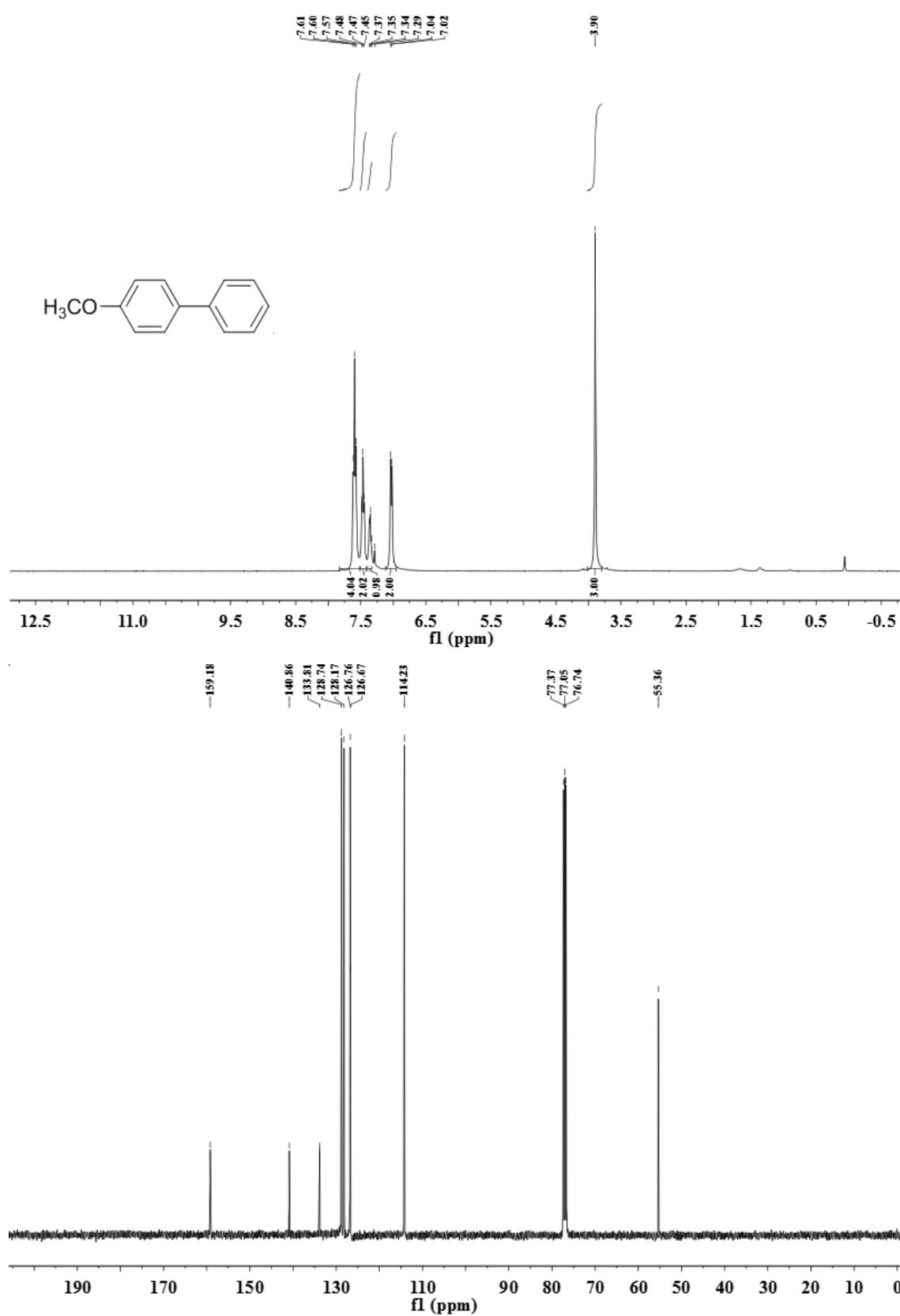
J= 7.6 Hz, 4H), 7.37 (t, J= 7.9 Hz 4H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  =117.9, 121.1, 129.4, 143.2.

## NMR Spectra of Products:

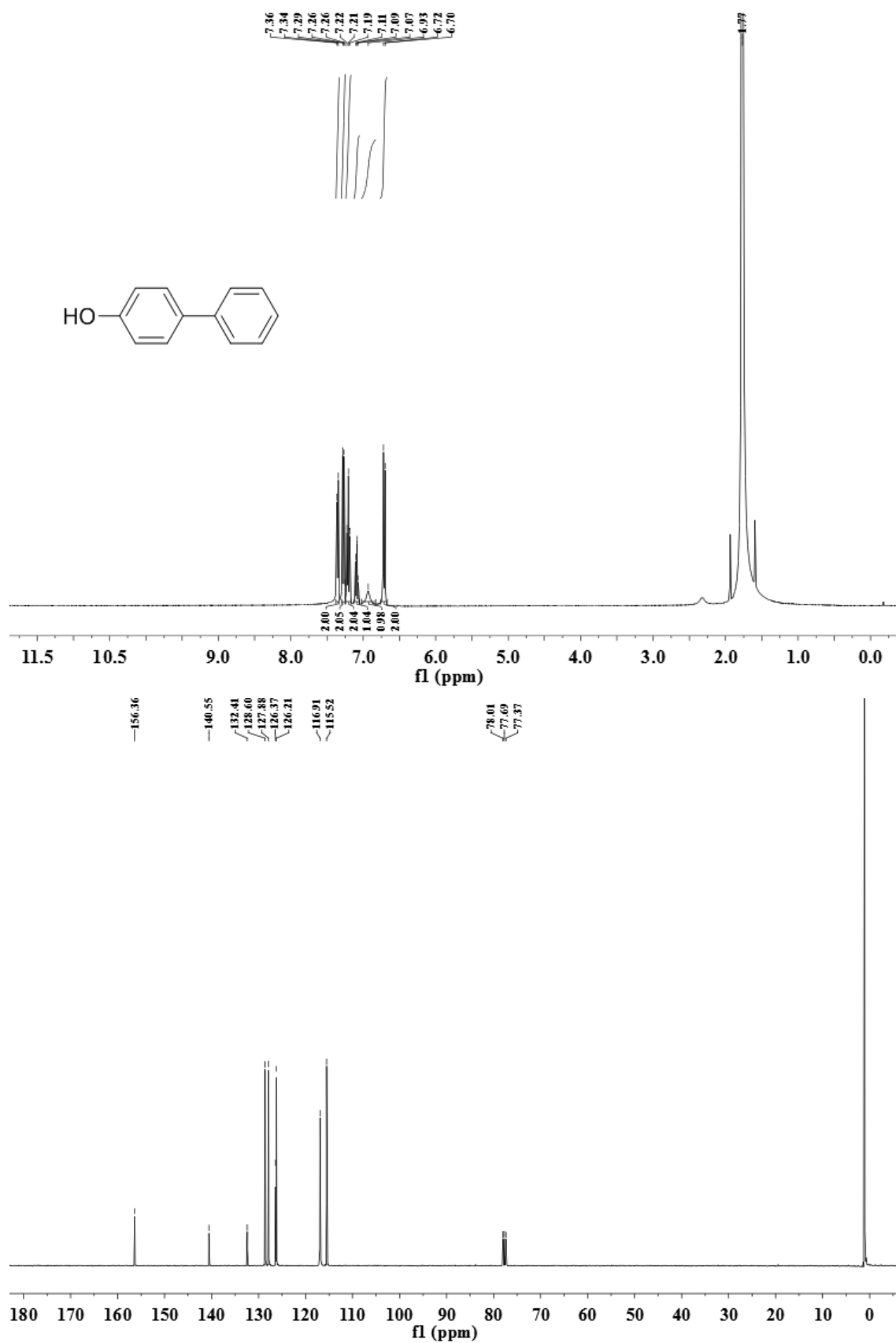
### (3a) 4-Methylbiphenyl



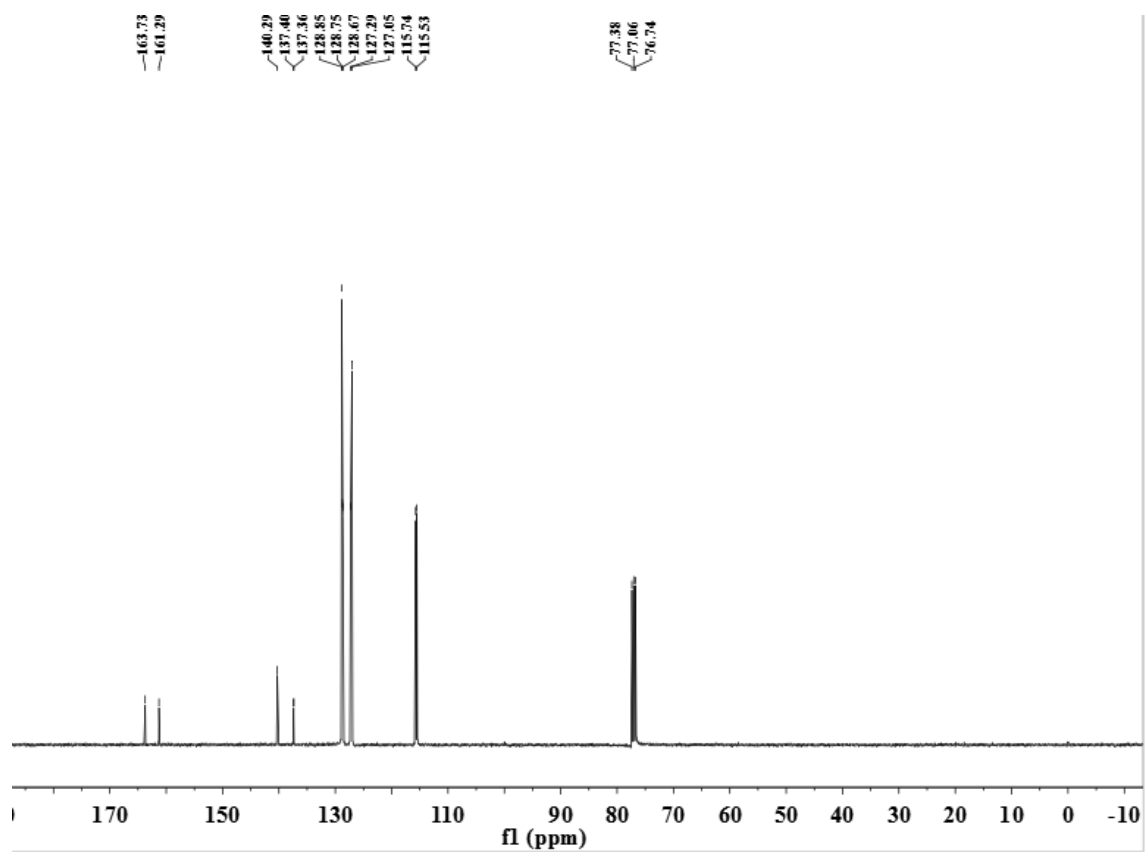
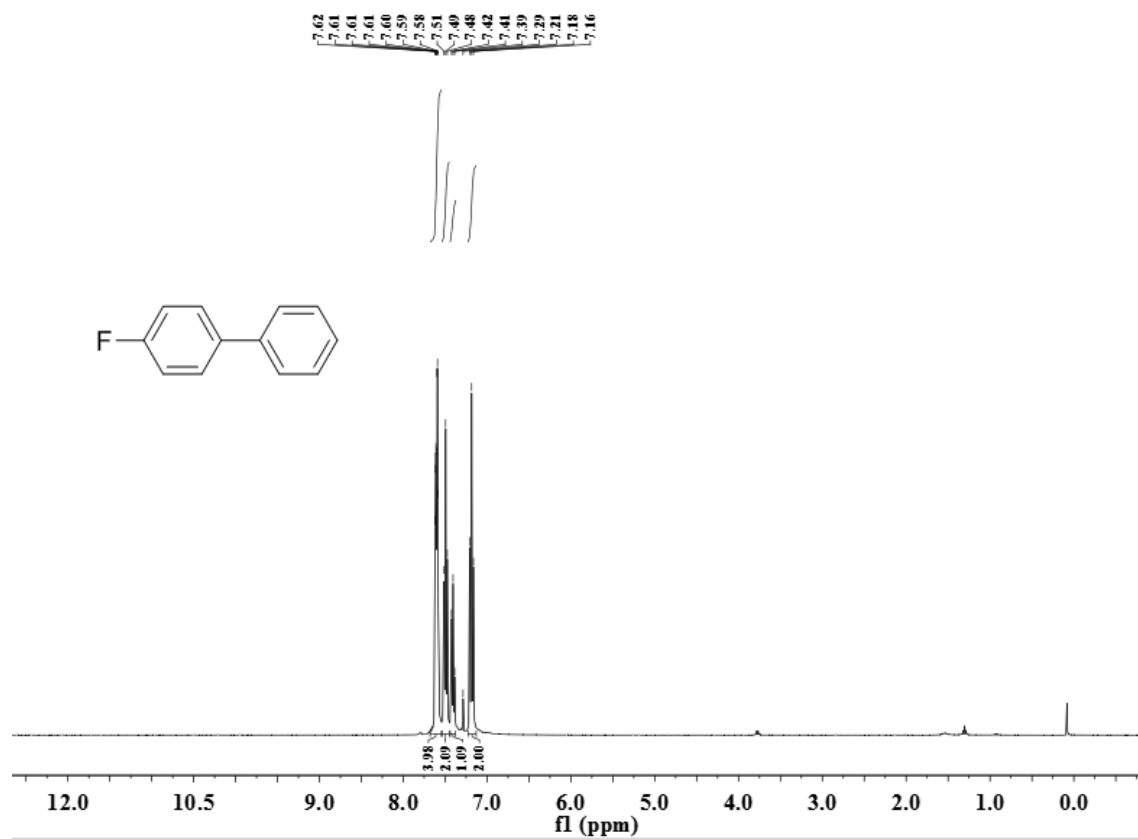
(3b) 4-Methoxybiphenyl



(3c) 4-Phenylphenol

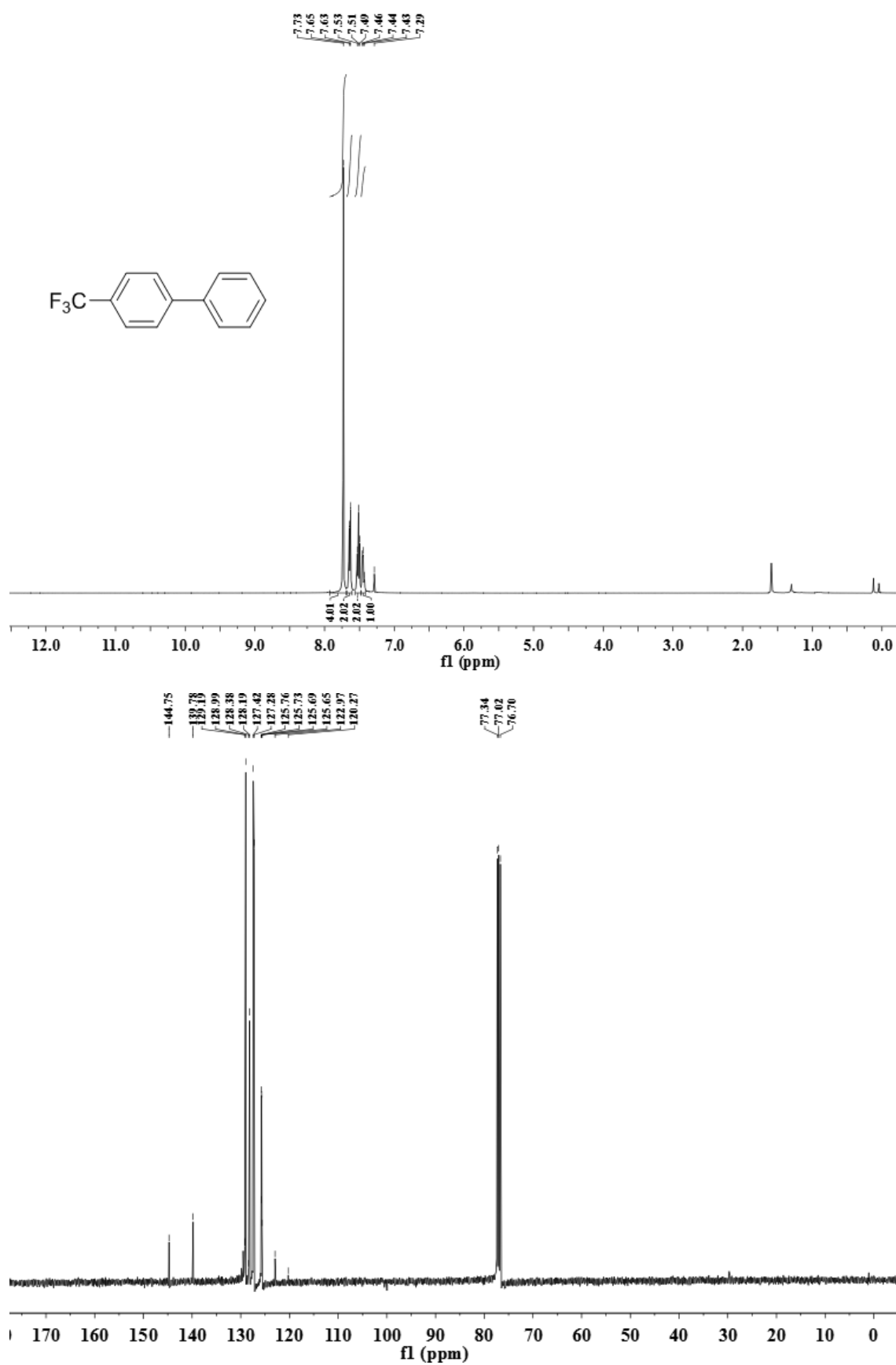


### 3(d) 4-Fluorobiphenyl

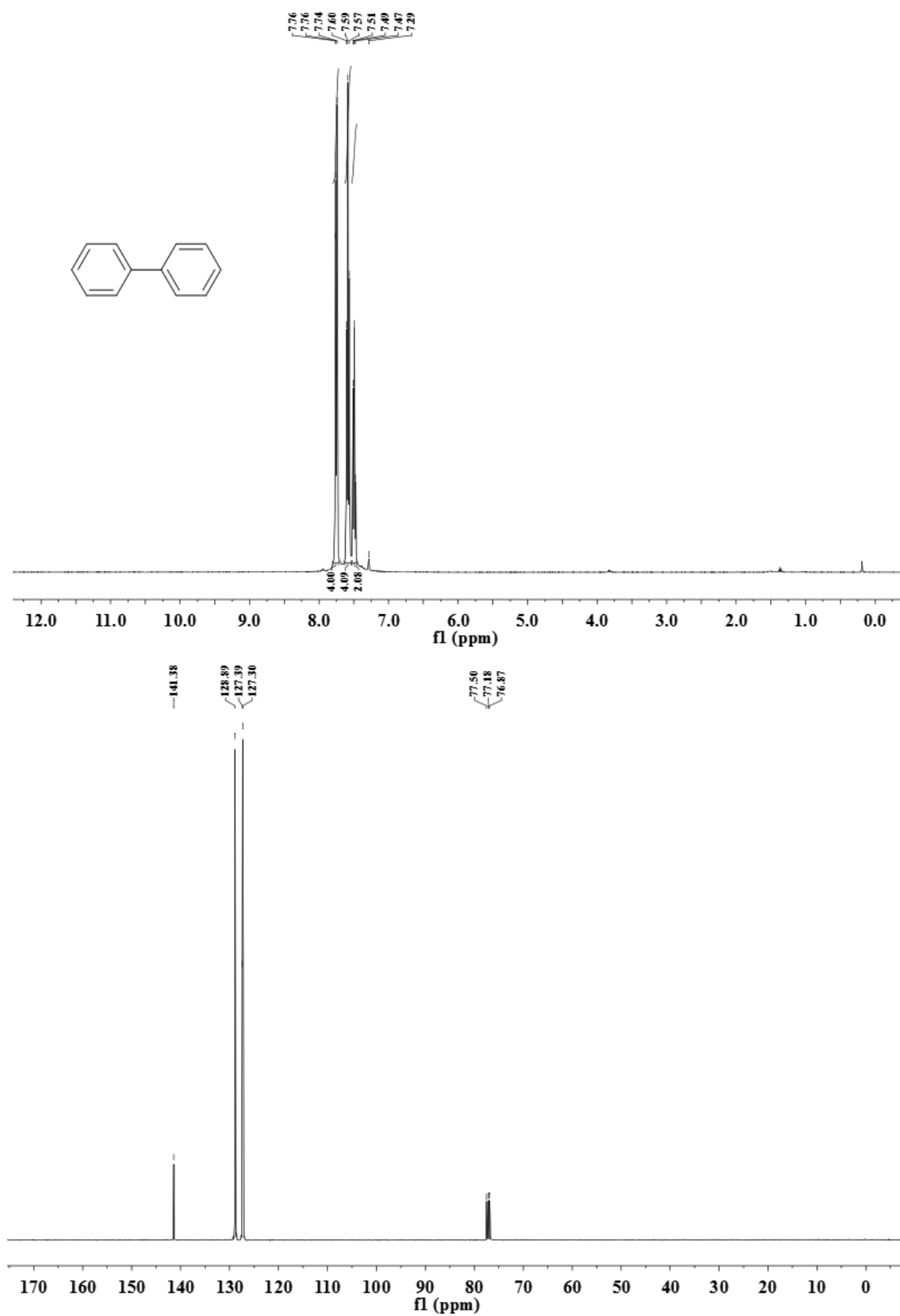




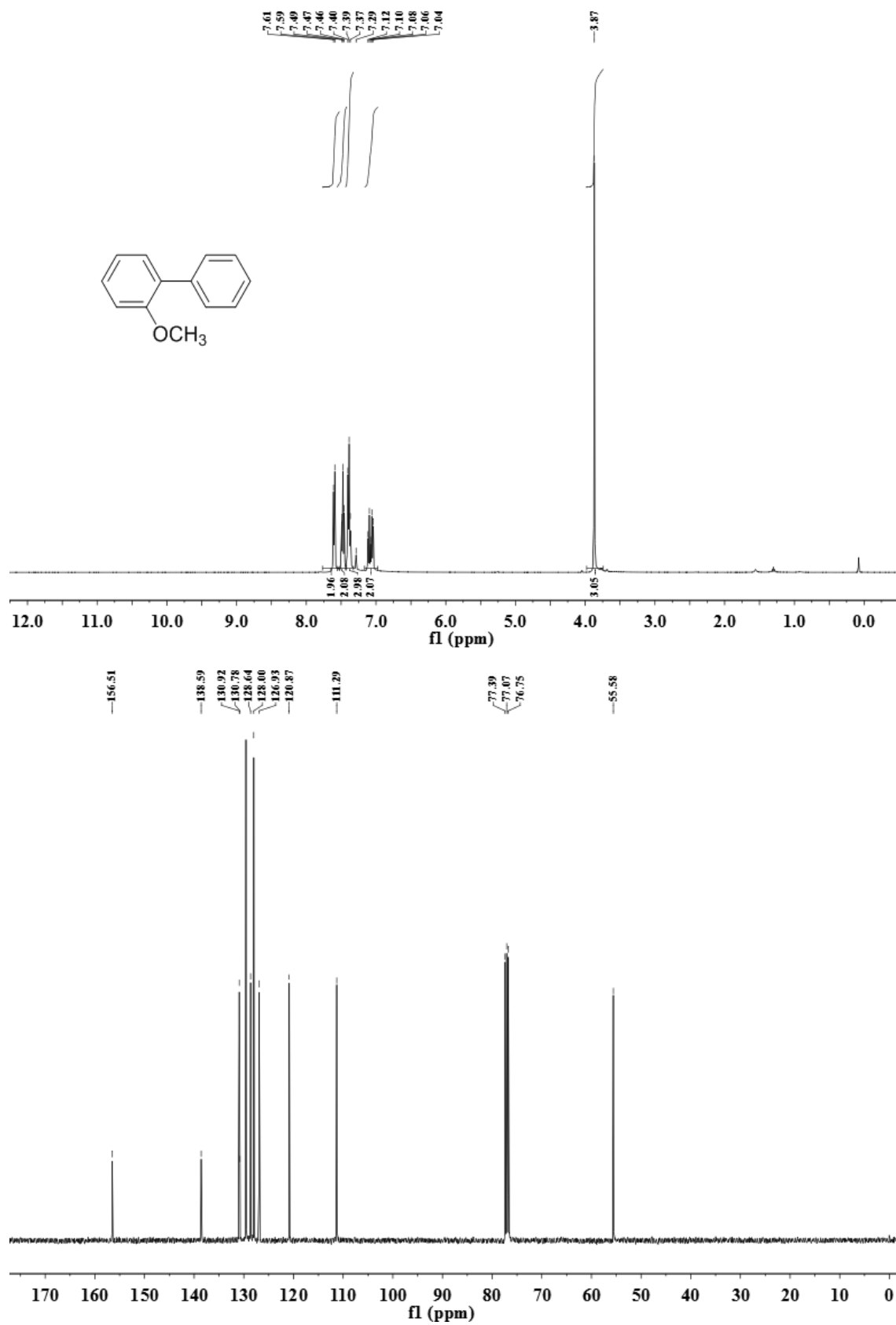
### 3(e) 4-Trifluoromethylbiphenyl



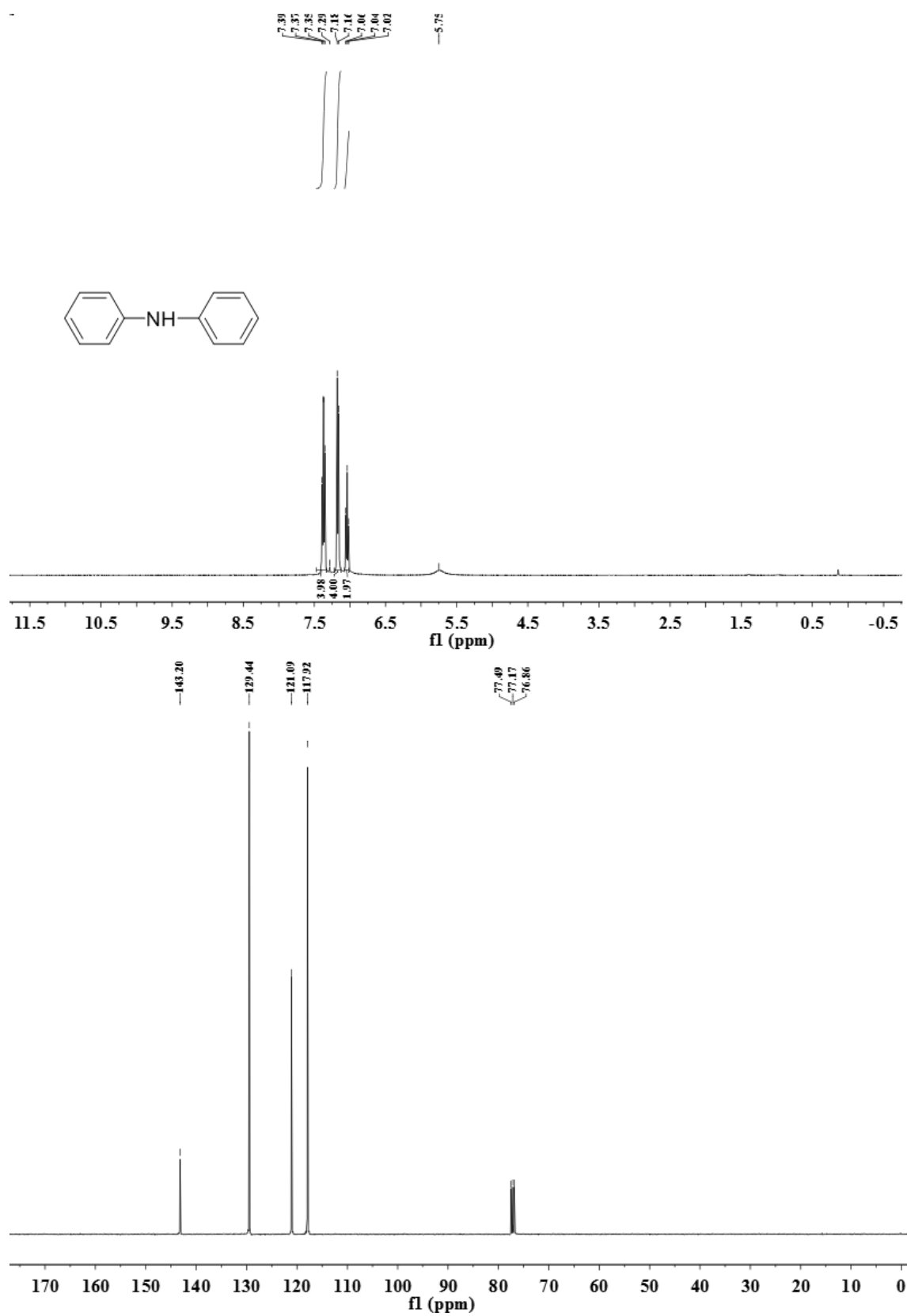
### 3(g) Biphenyl

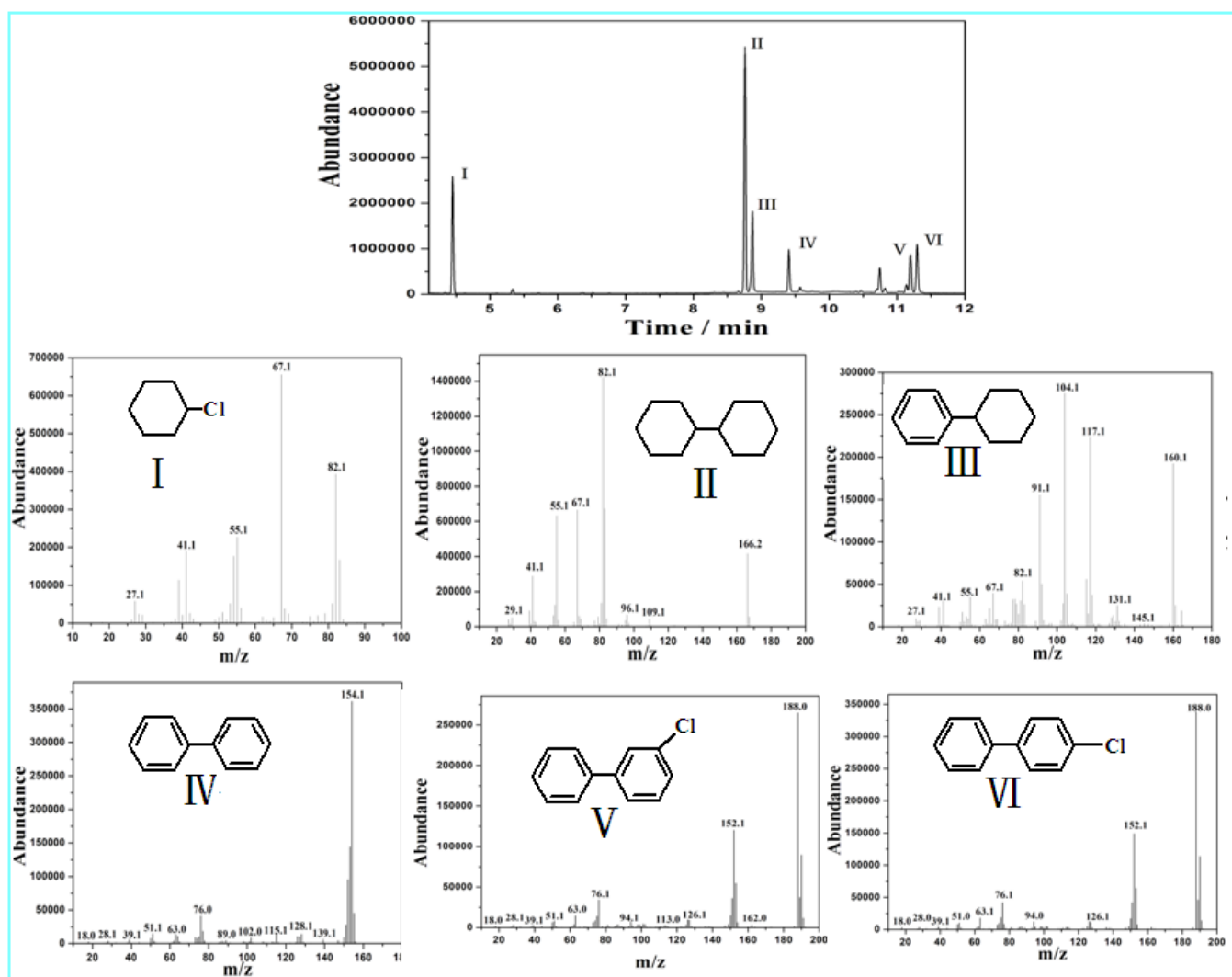


### 3(i) 2-Methoxybiphenyl



### 3(l) Diphenylamine





**Figure S1. GC-MS spectra of the products generated from direct cross-coupling of chlorobenzene with cyclohexane.**

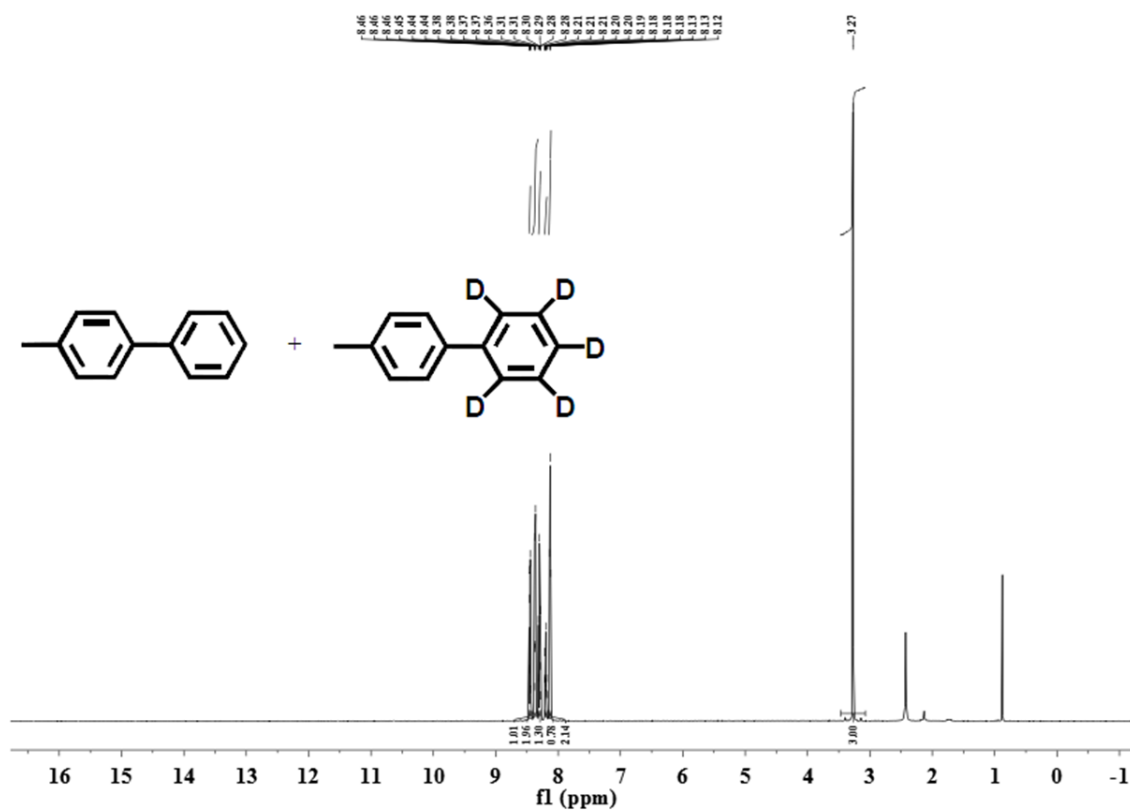
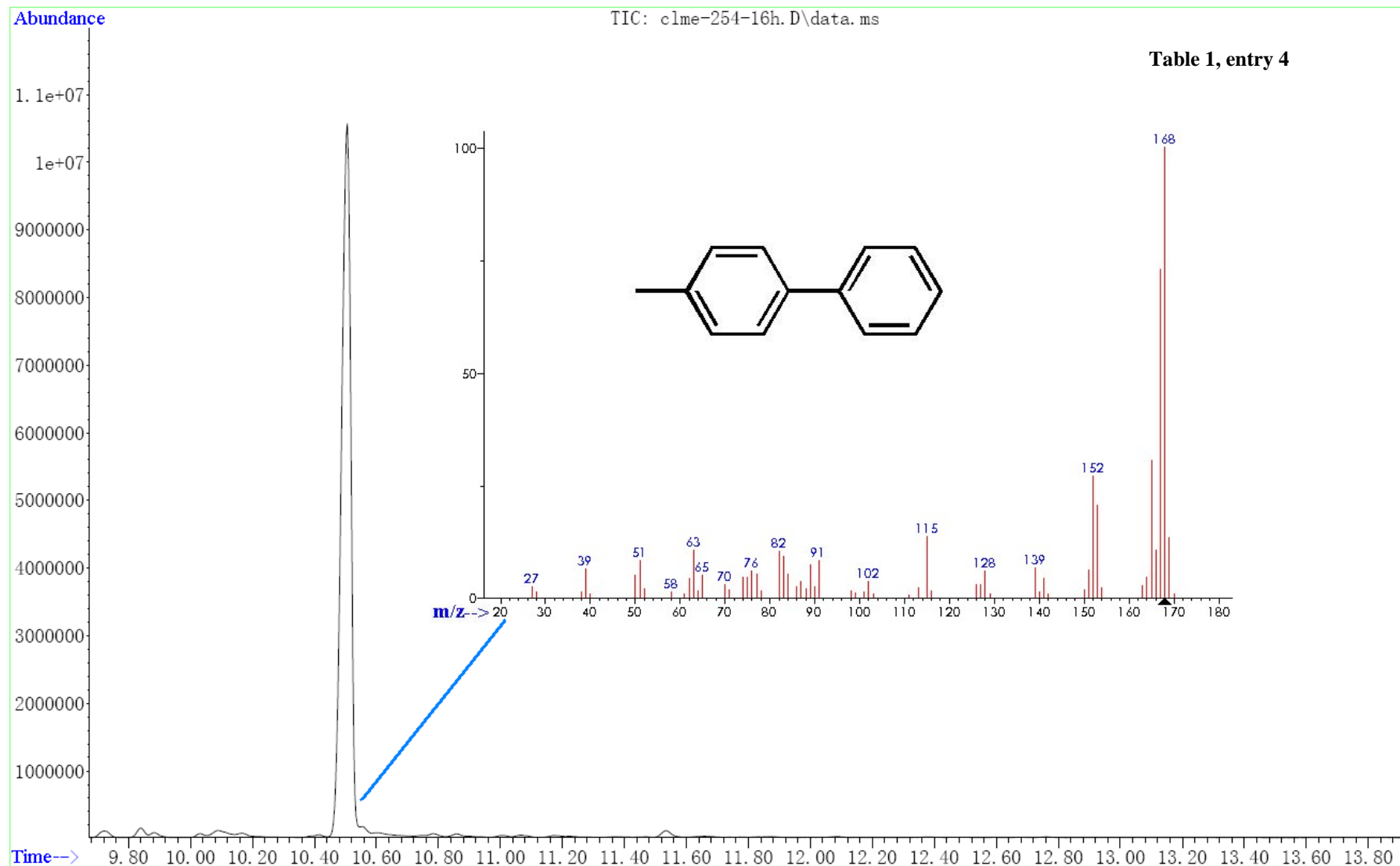
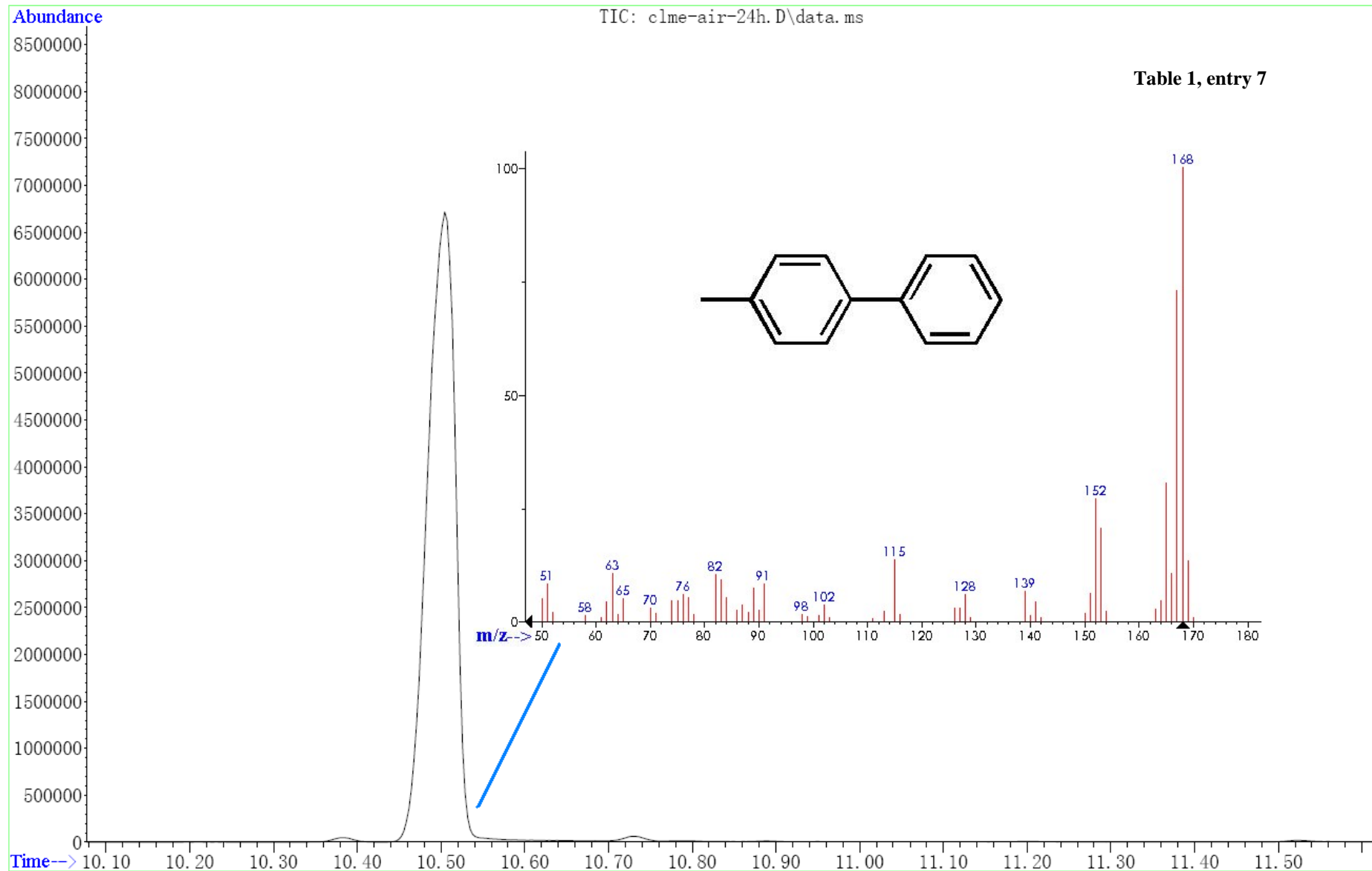
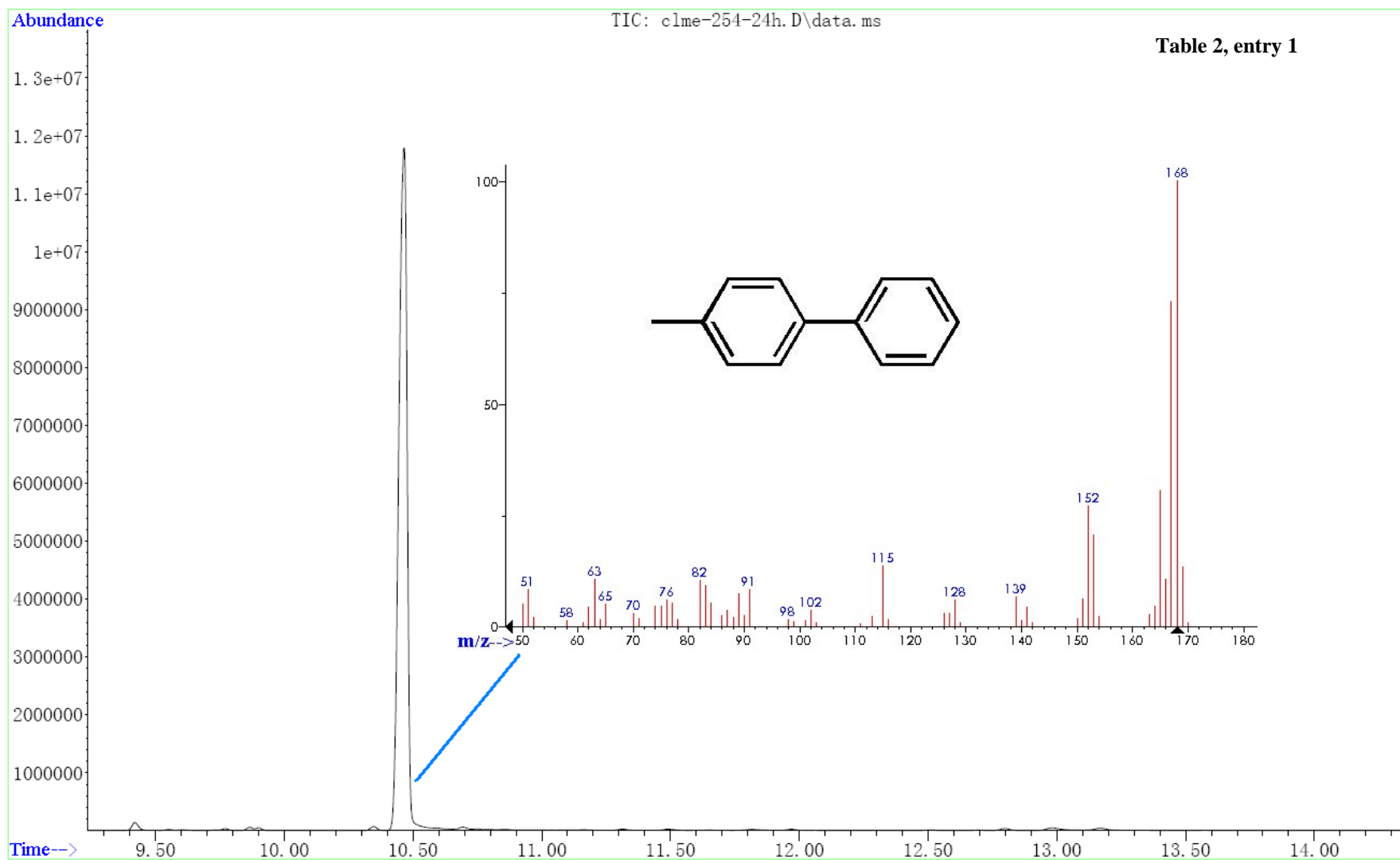


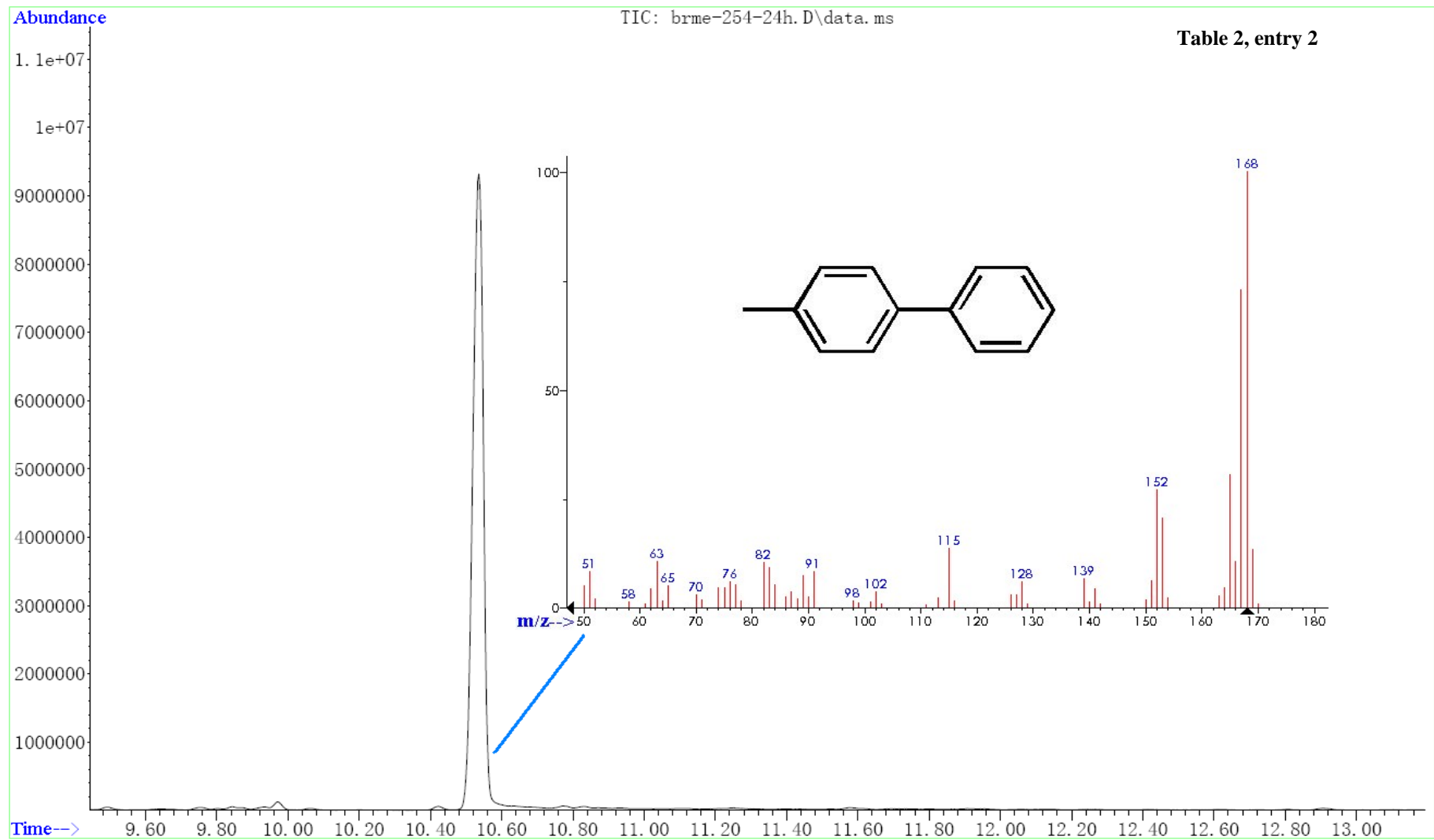
Figure S2.  $^1\text{H}$  NMR spectrum of 4-methylbiphenyl and 4-methylbiphenyl-2',3',4',5',6'-d<sub>5</sub>

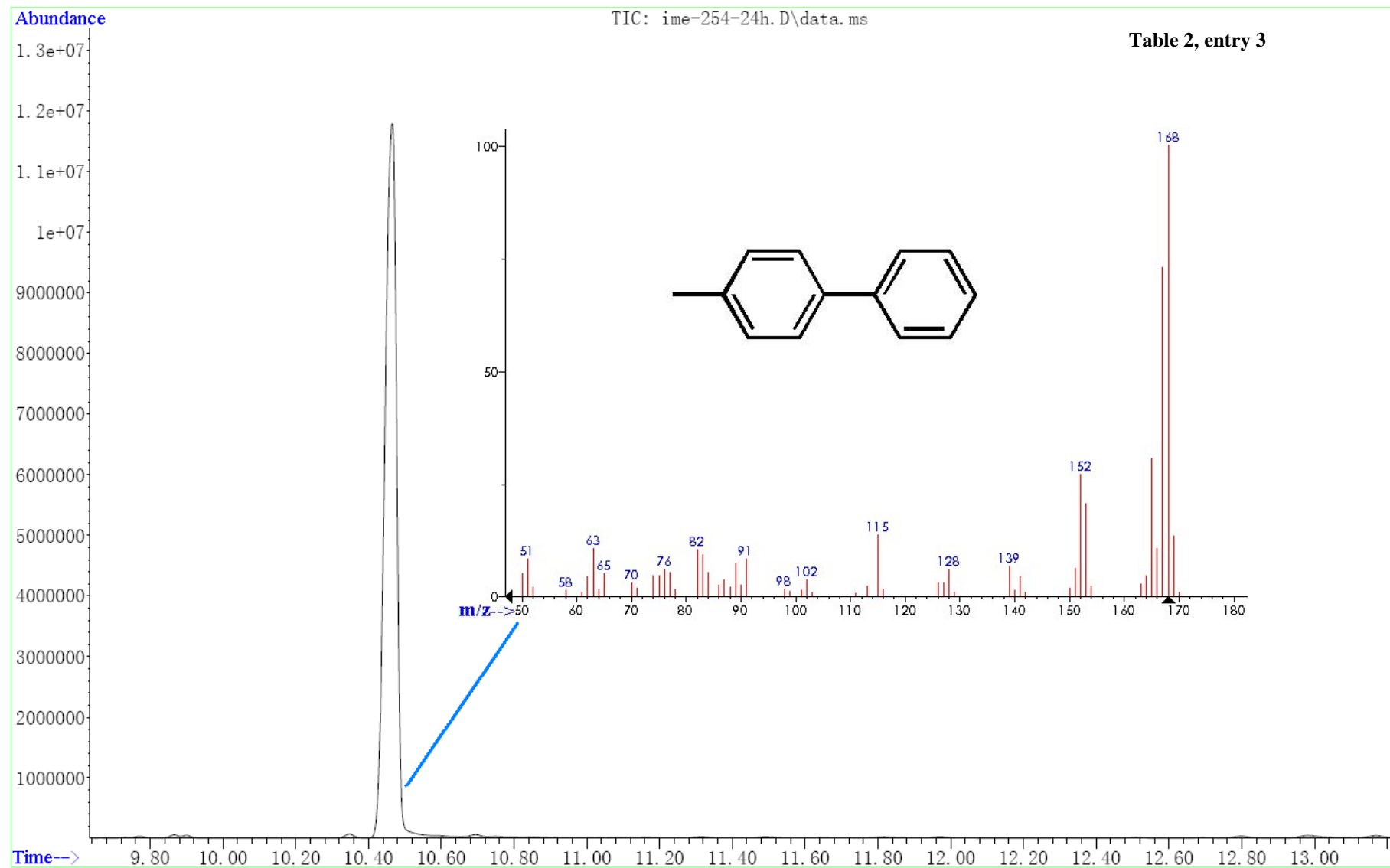


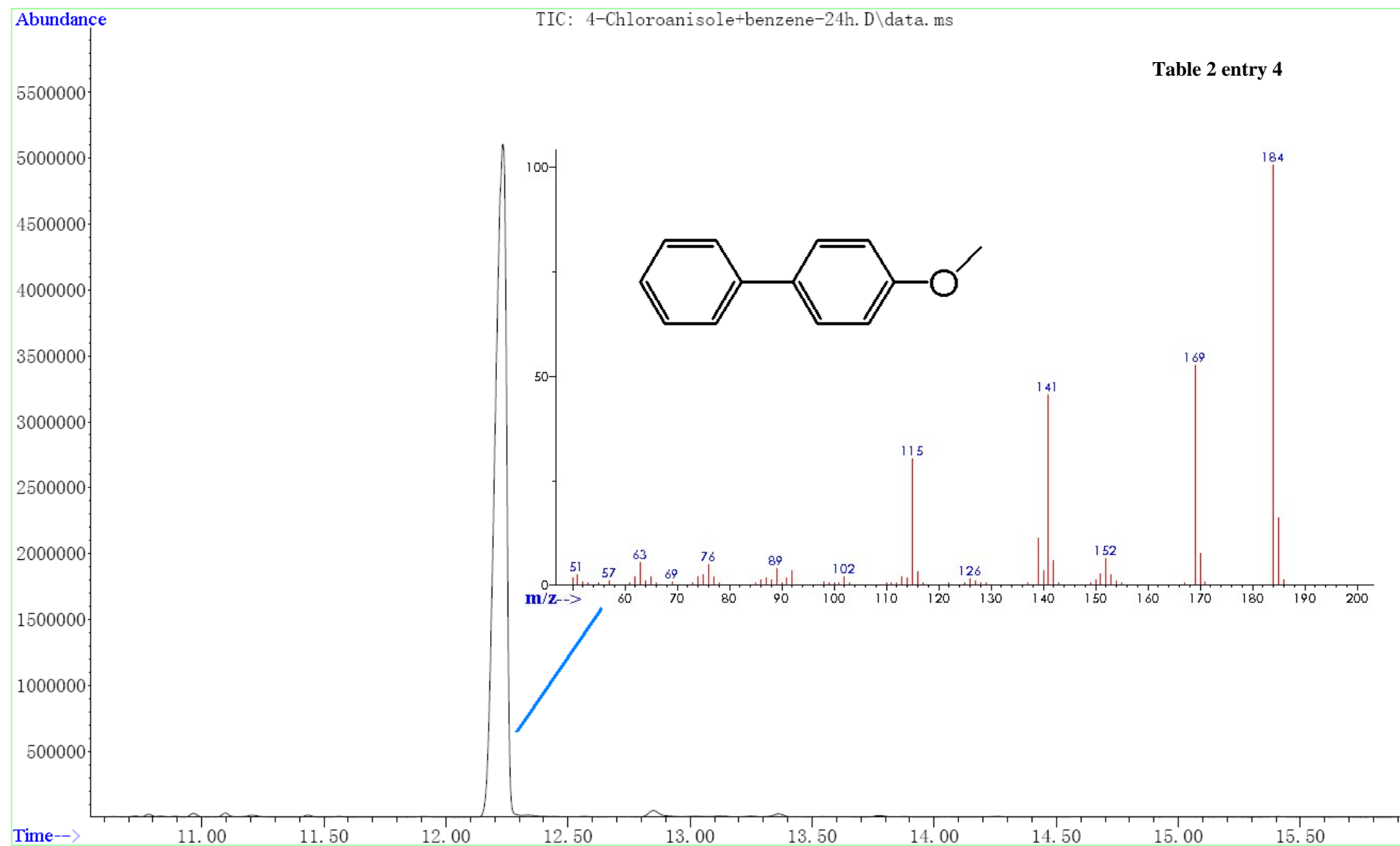


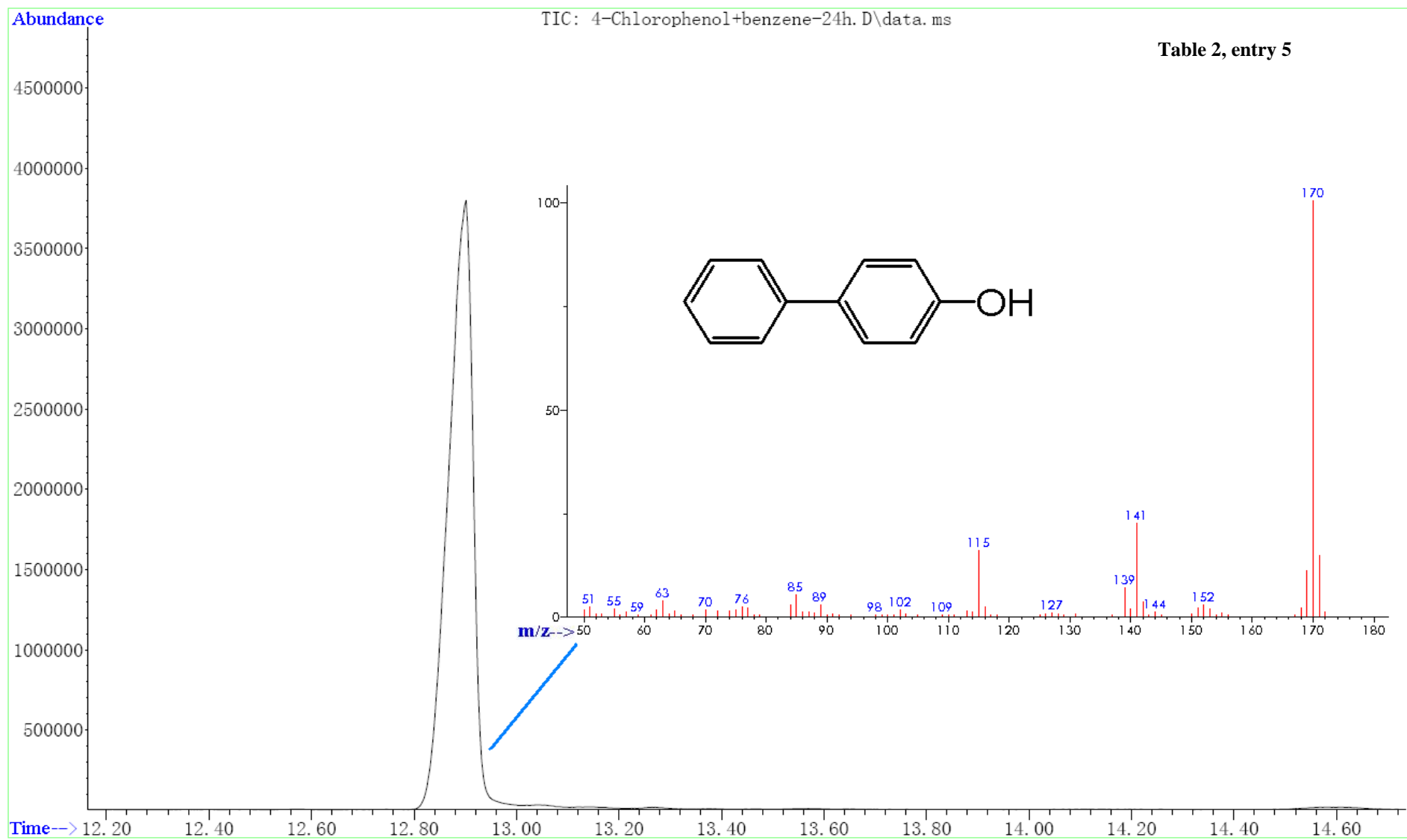


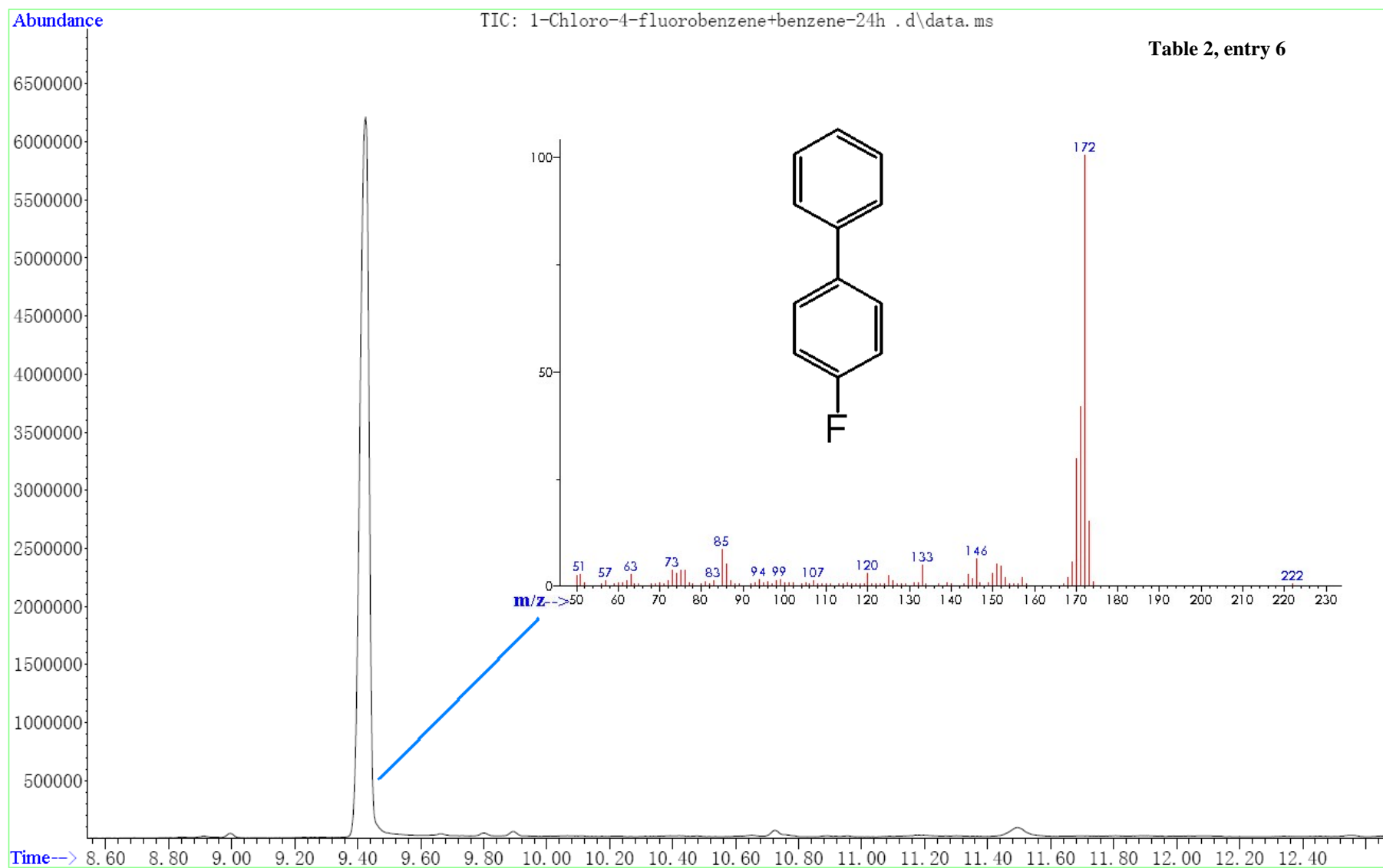


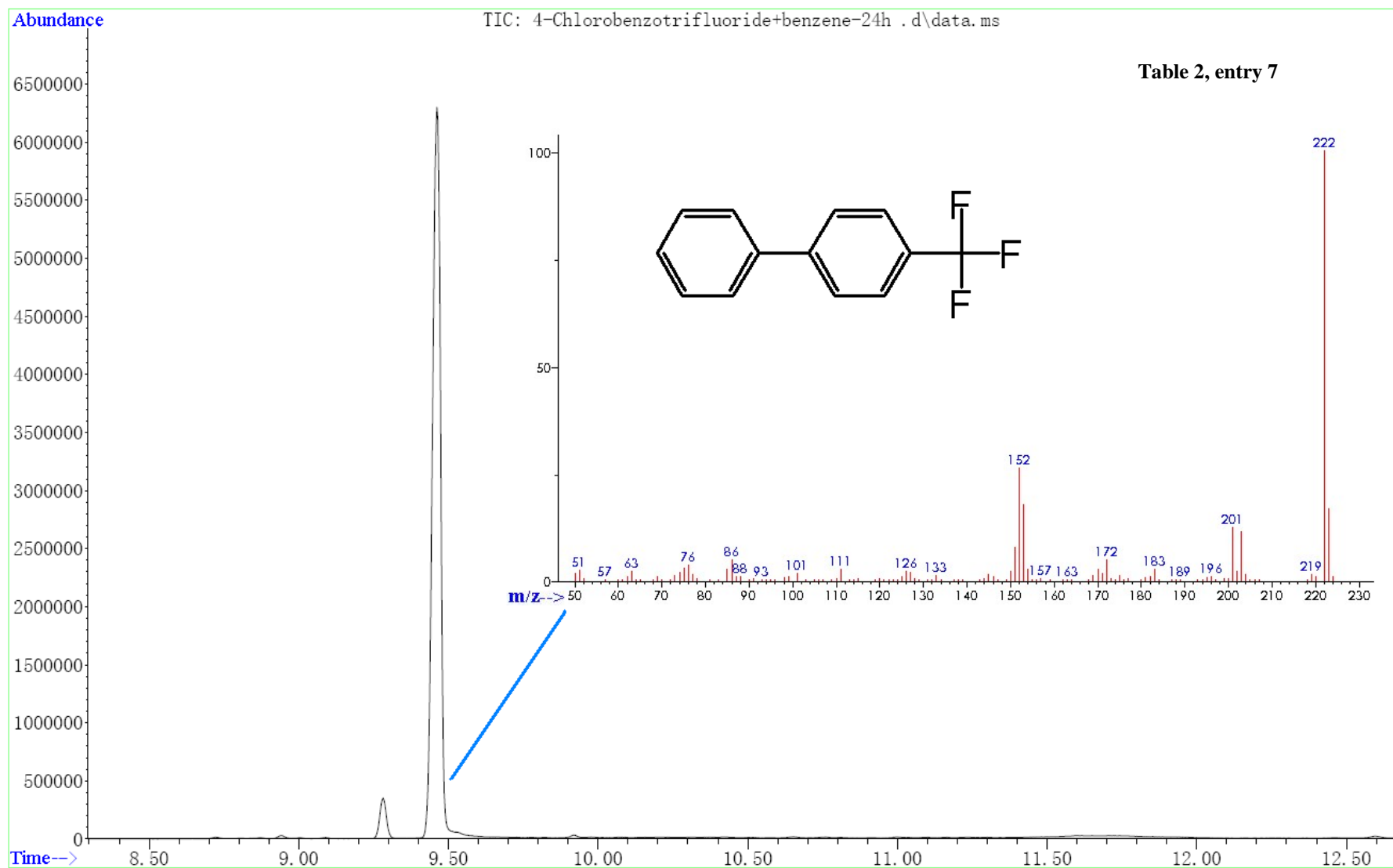


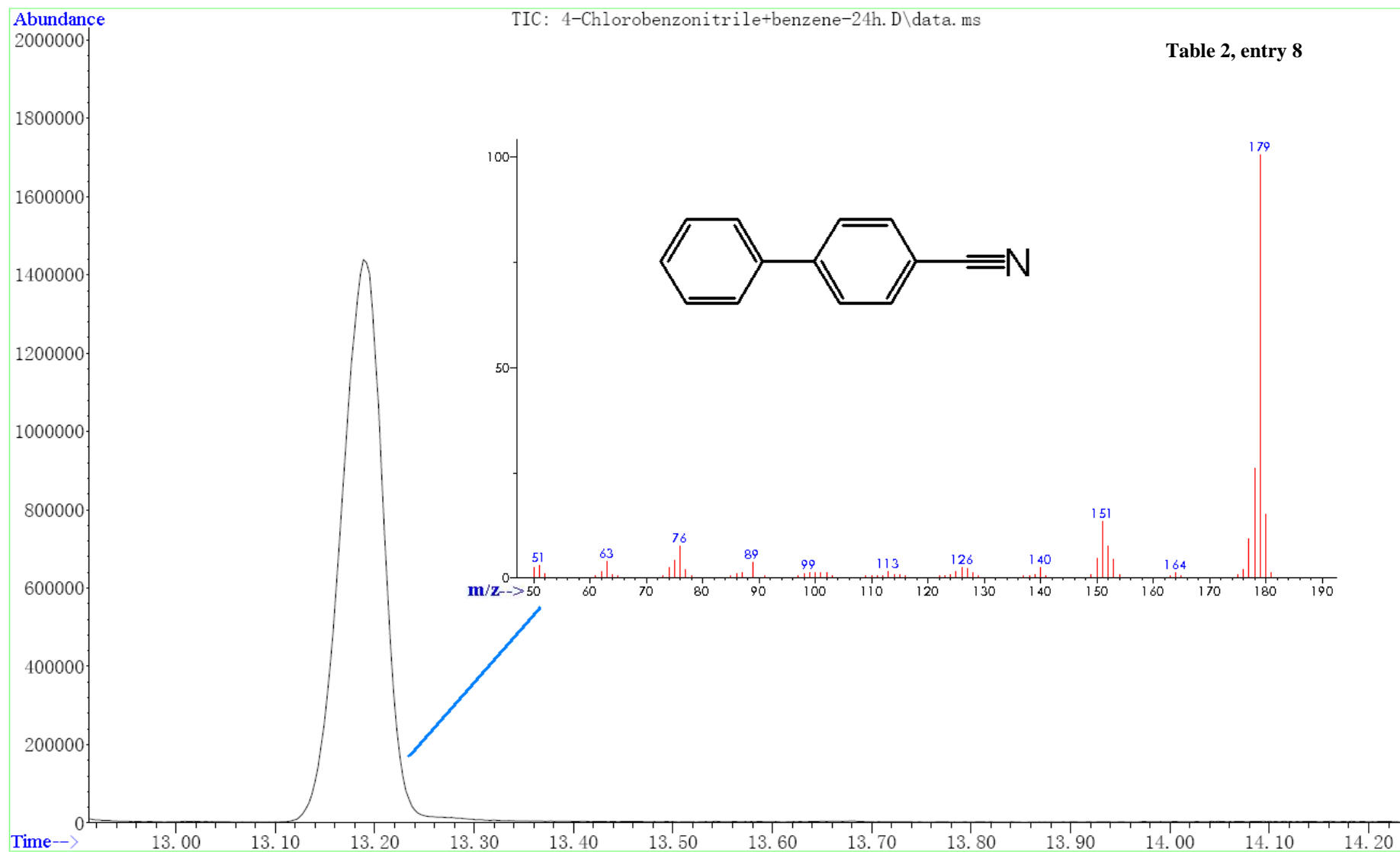




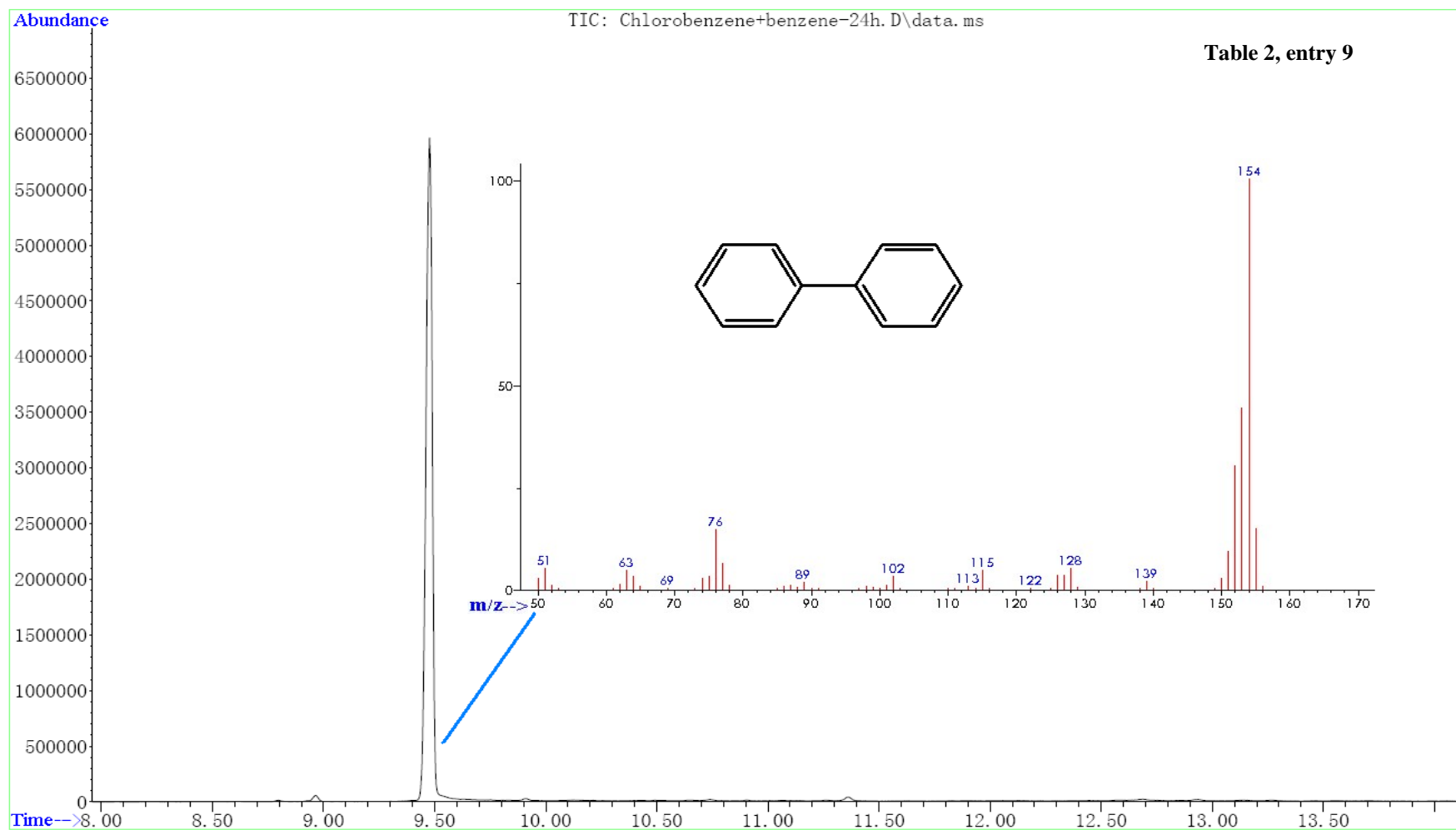


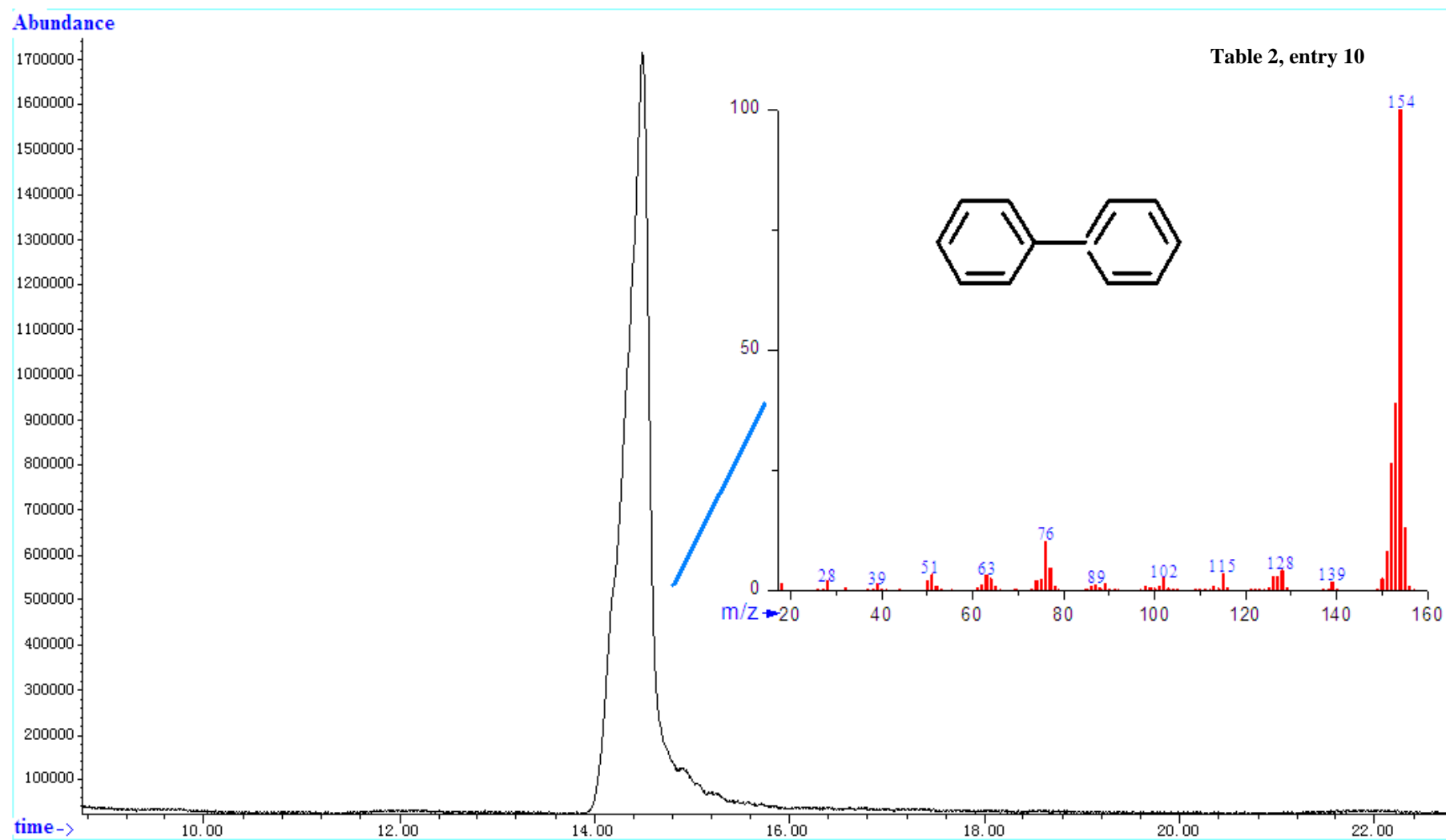


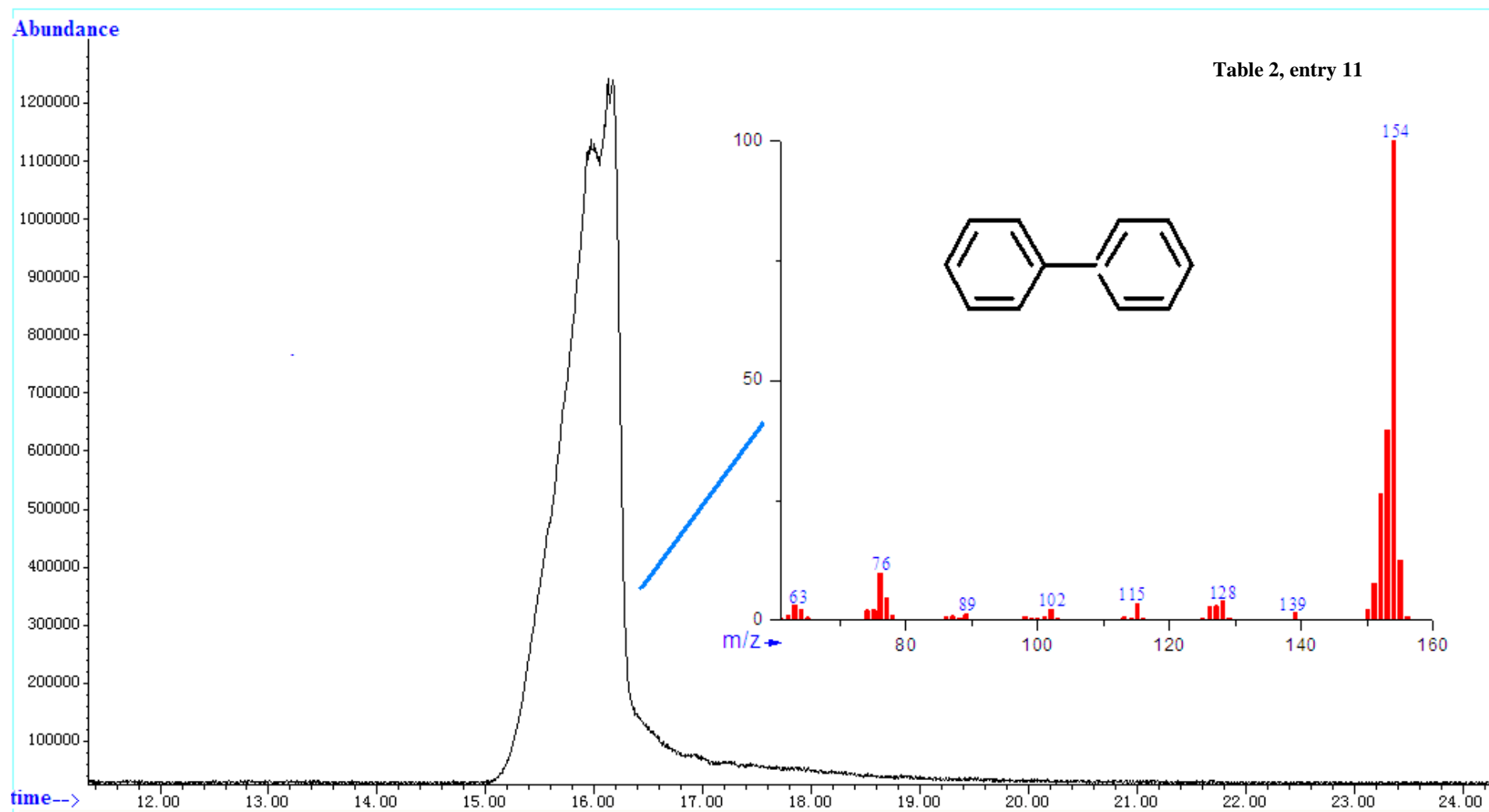


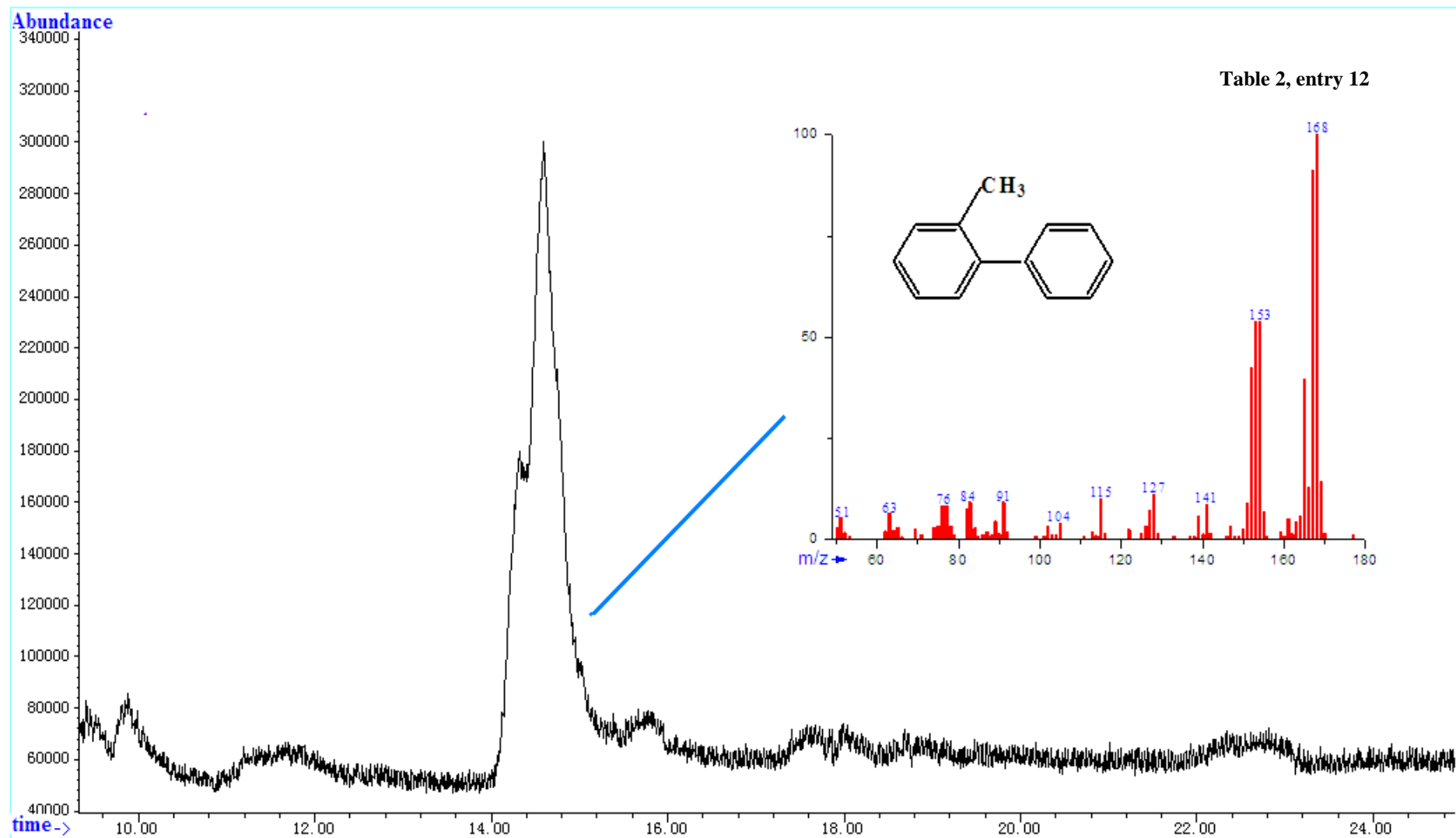


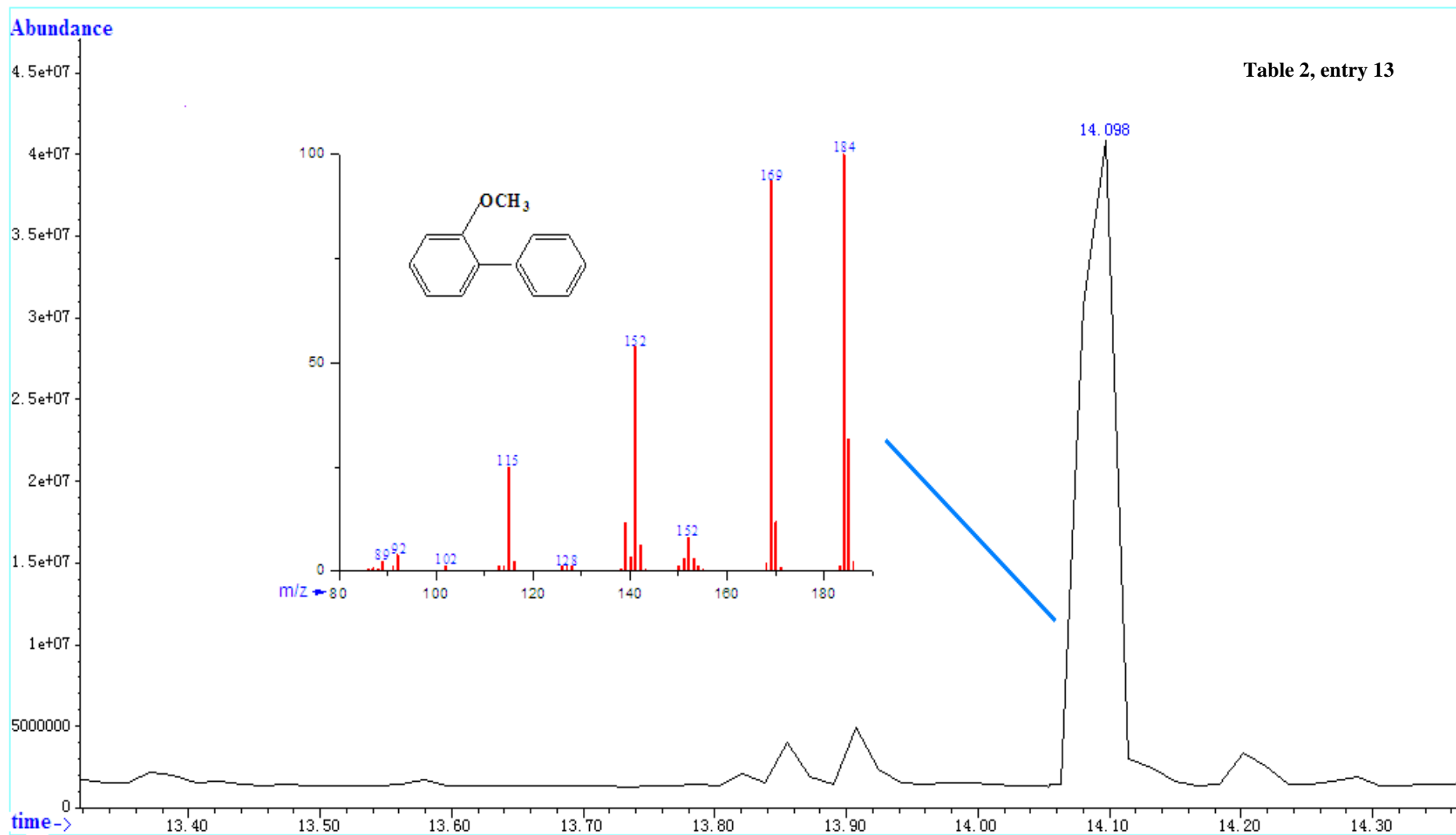


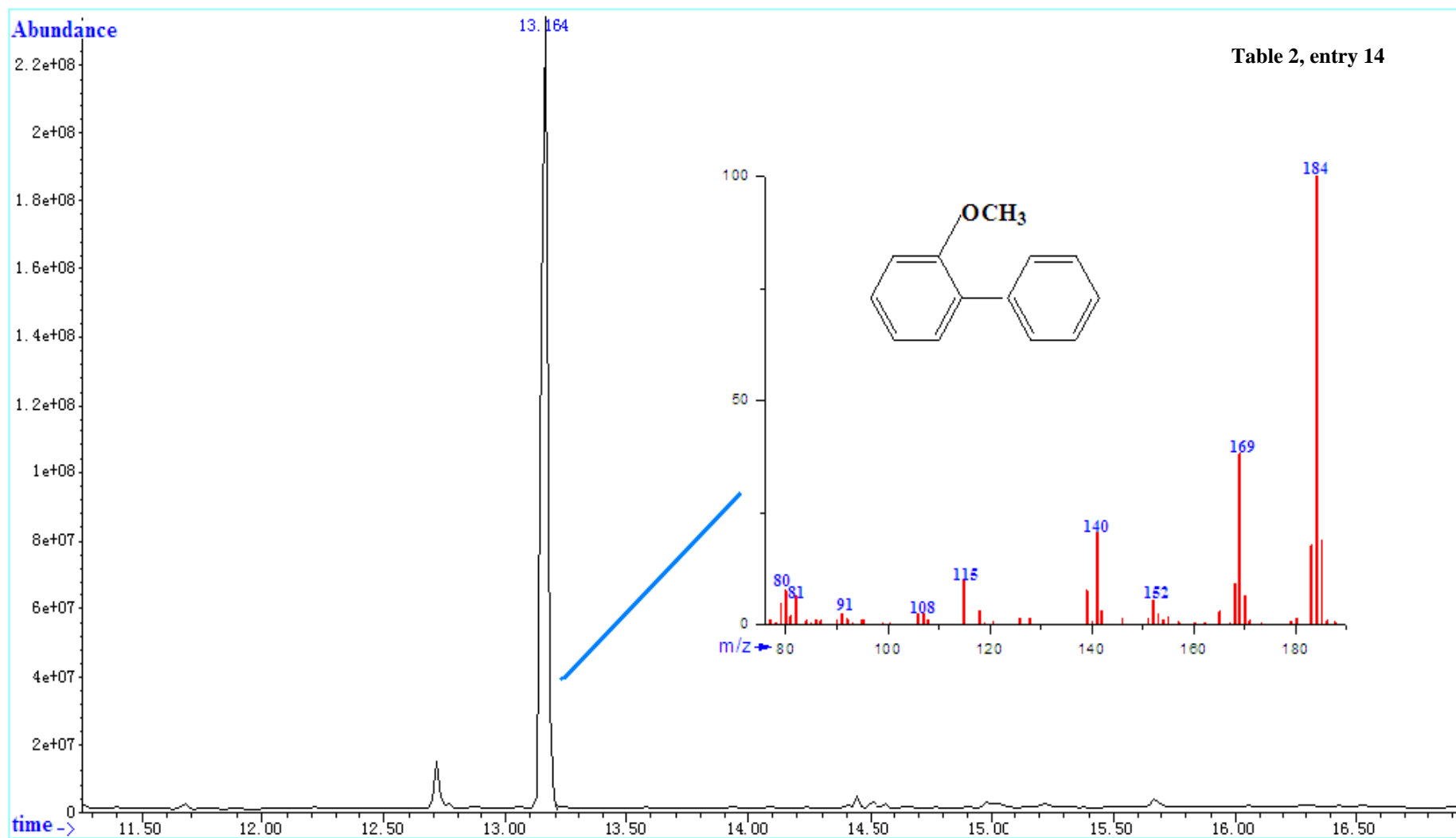


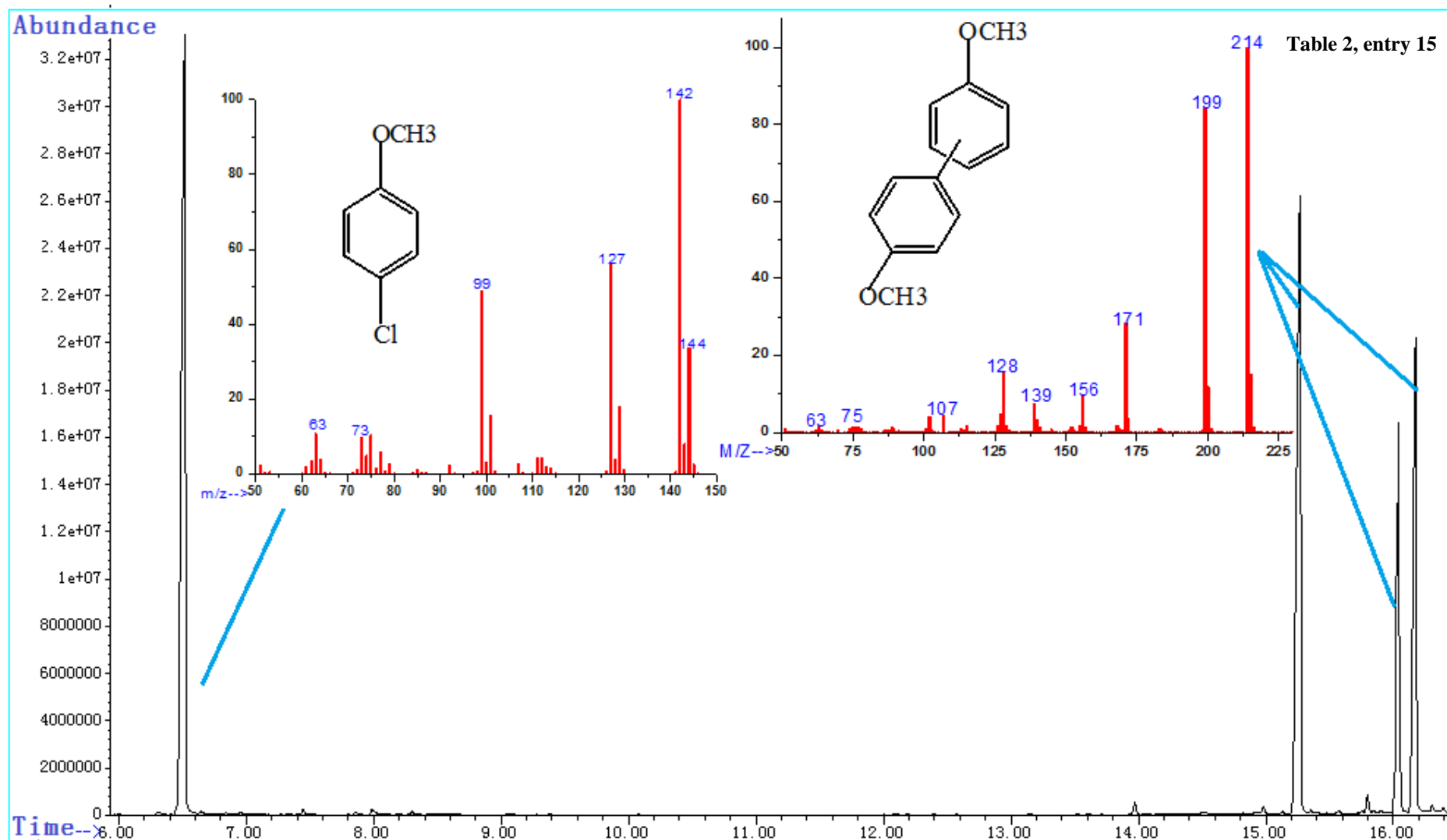


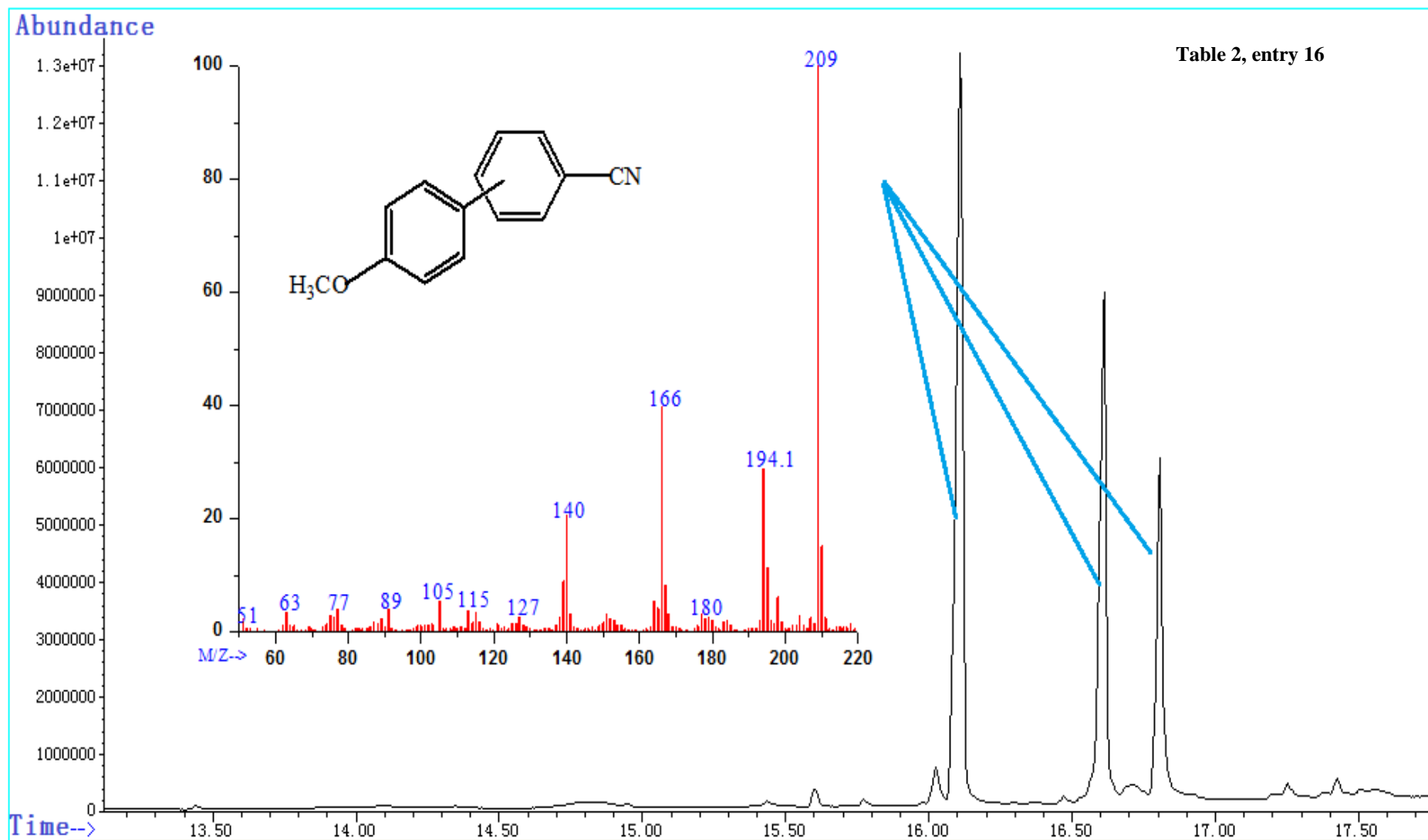




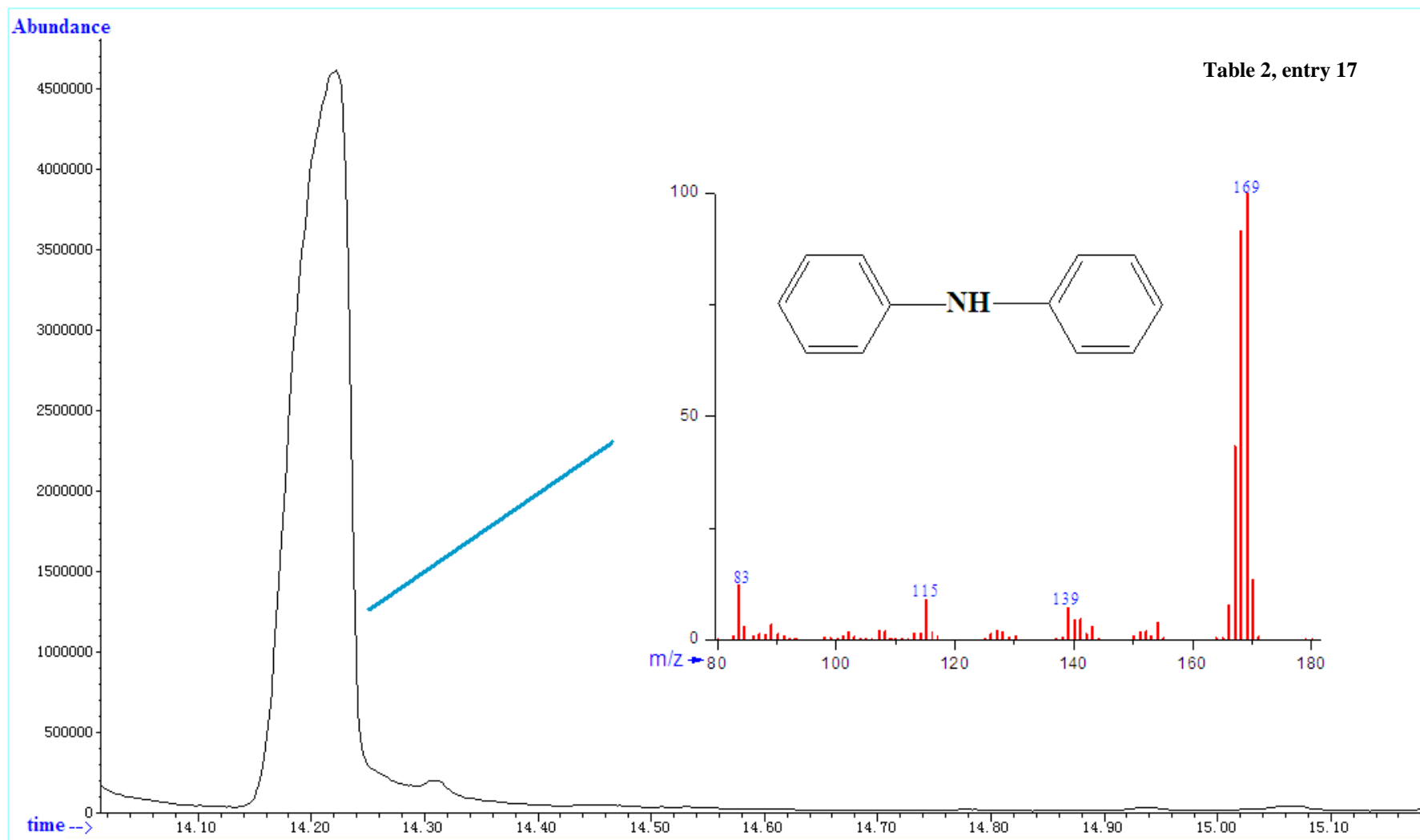


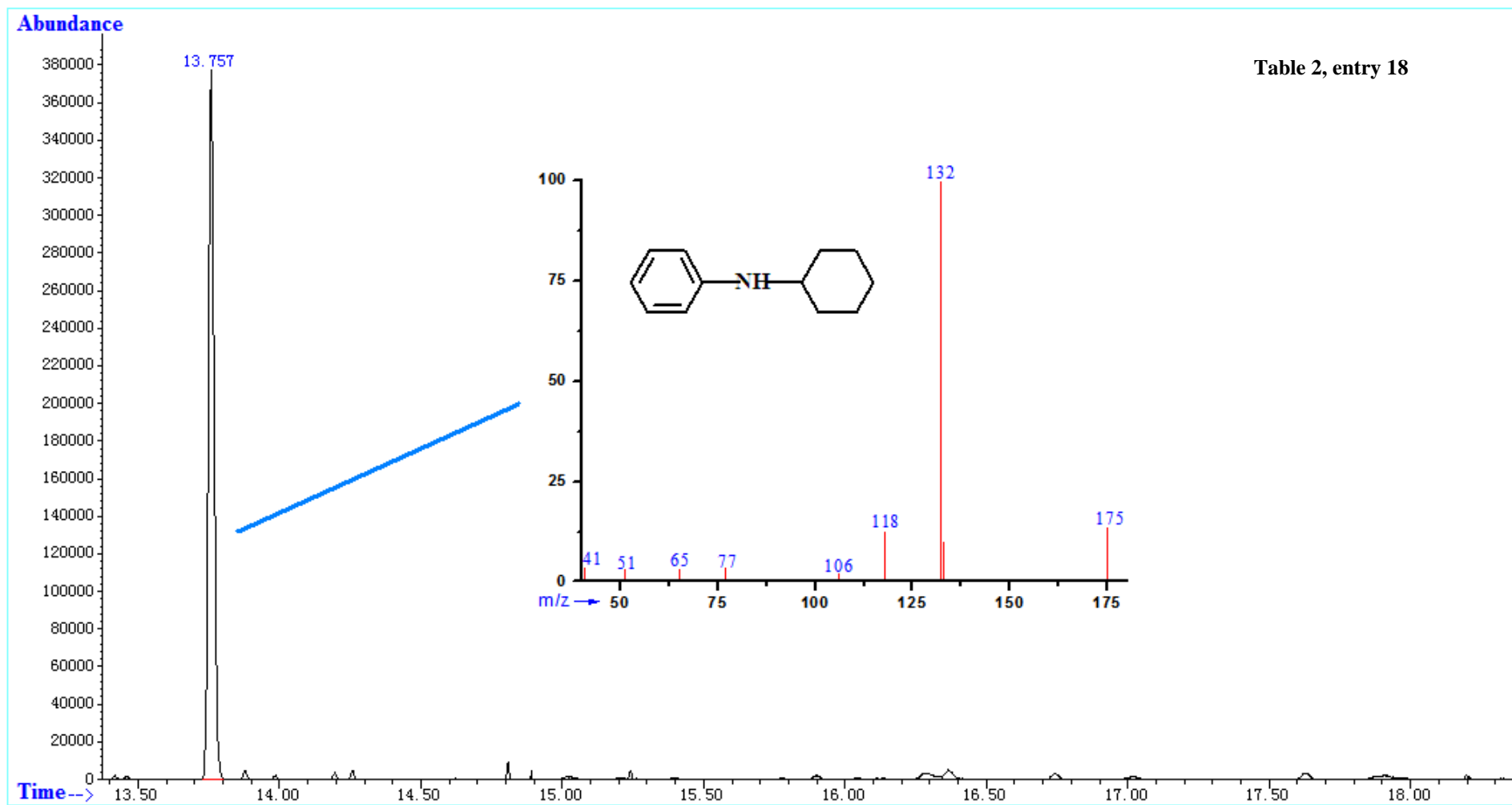


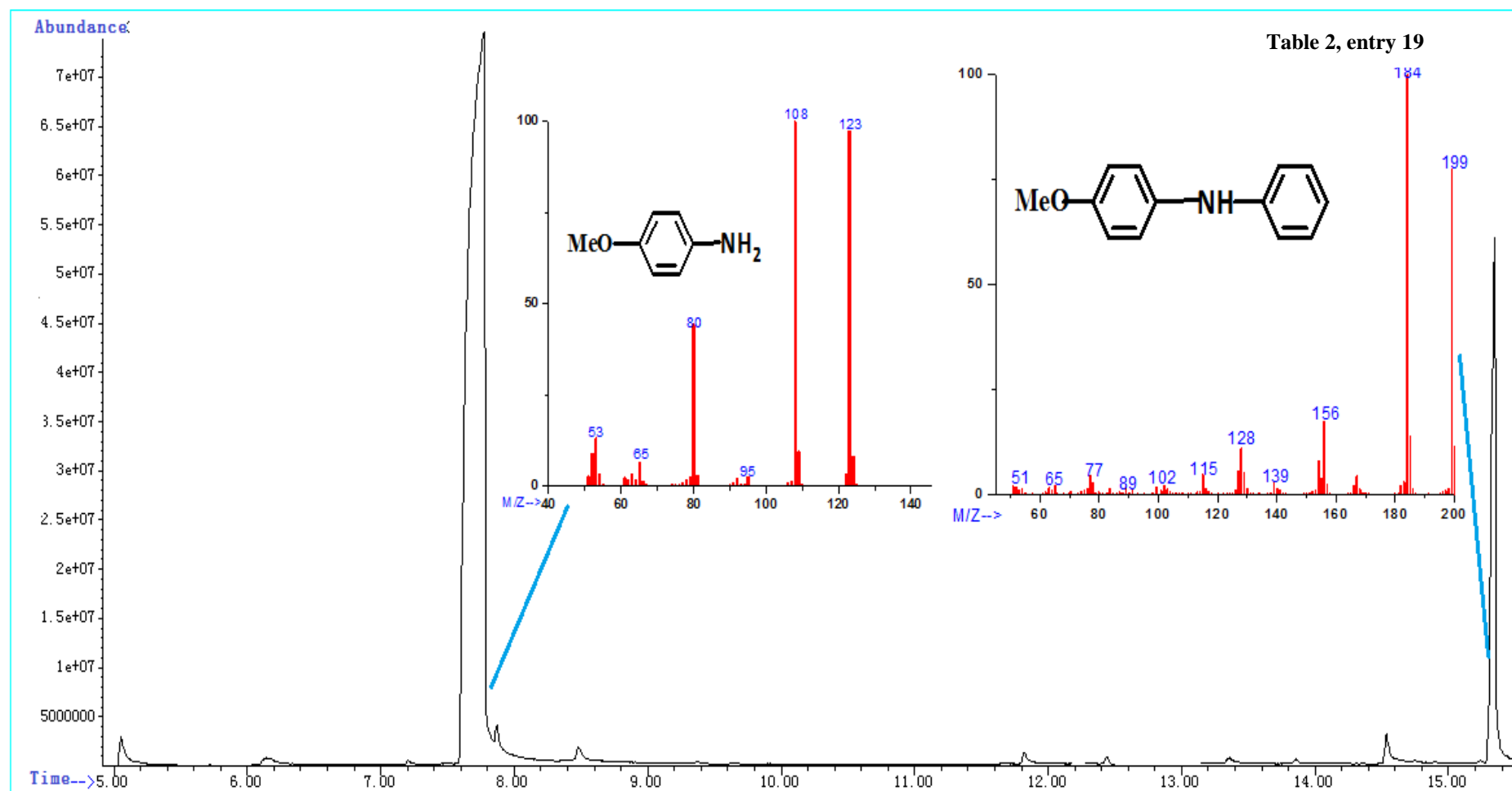


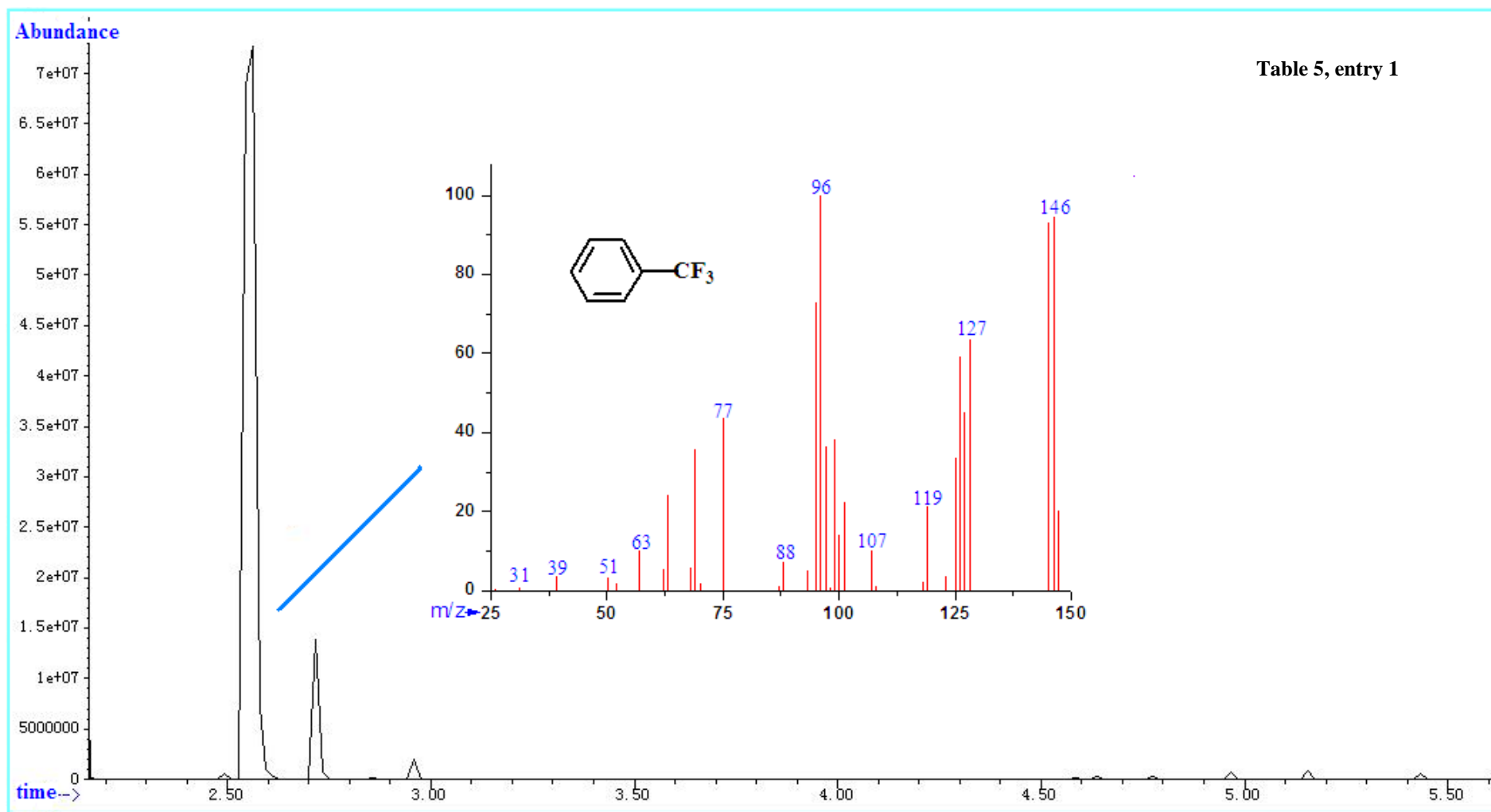


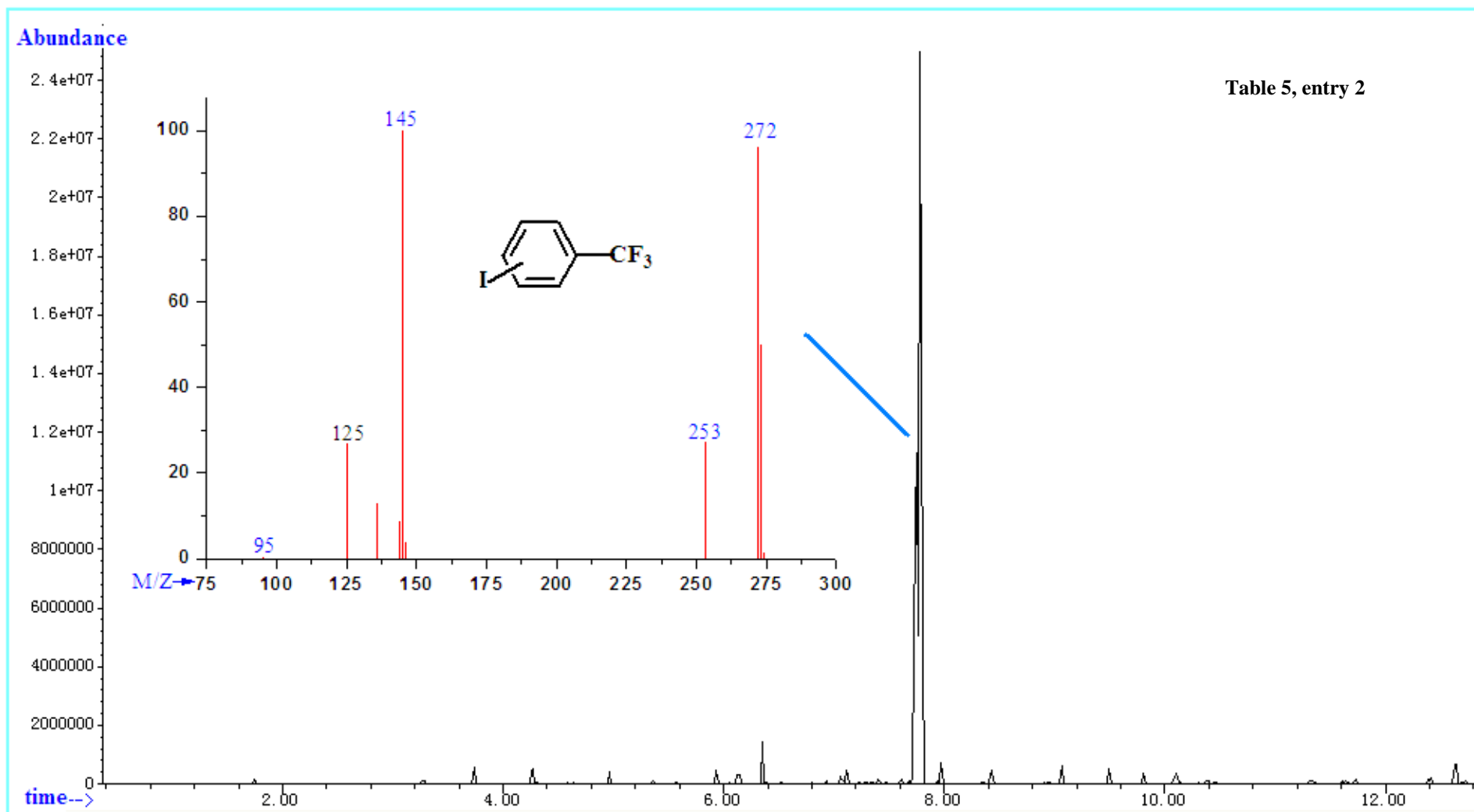


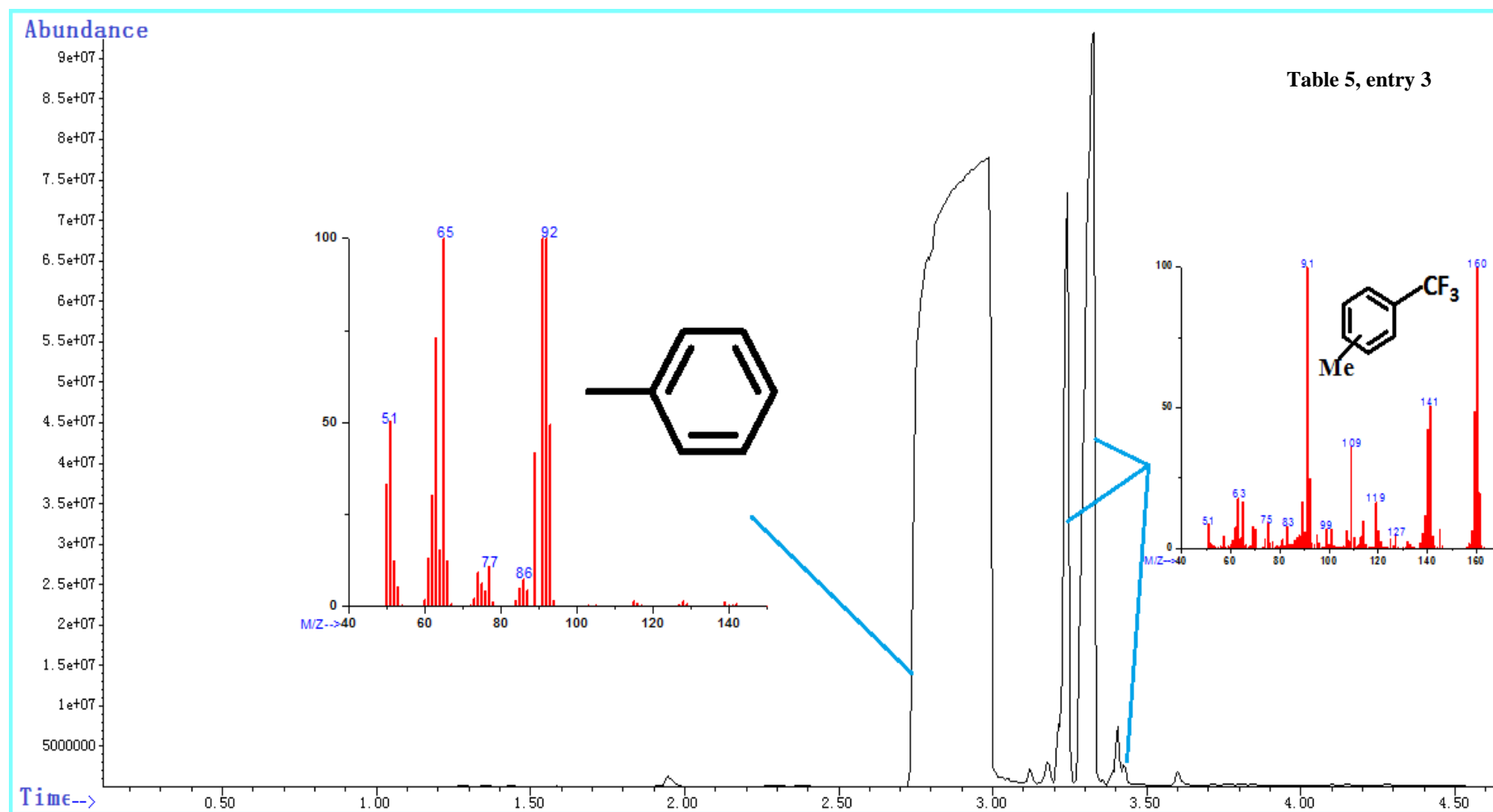


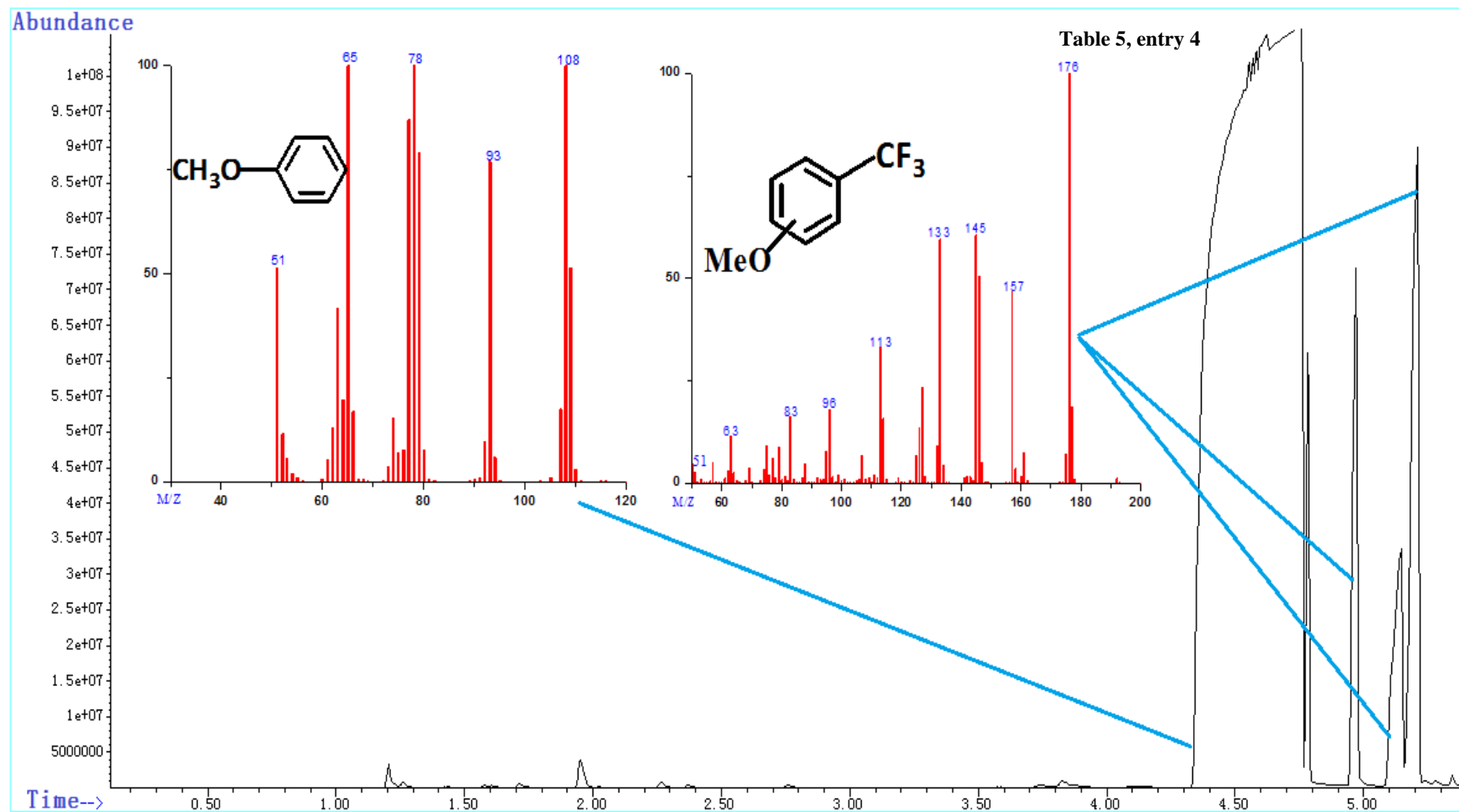


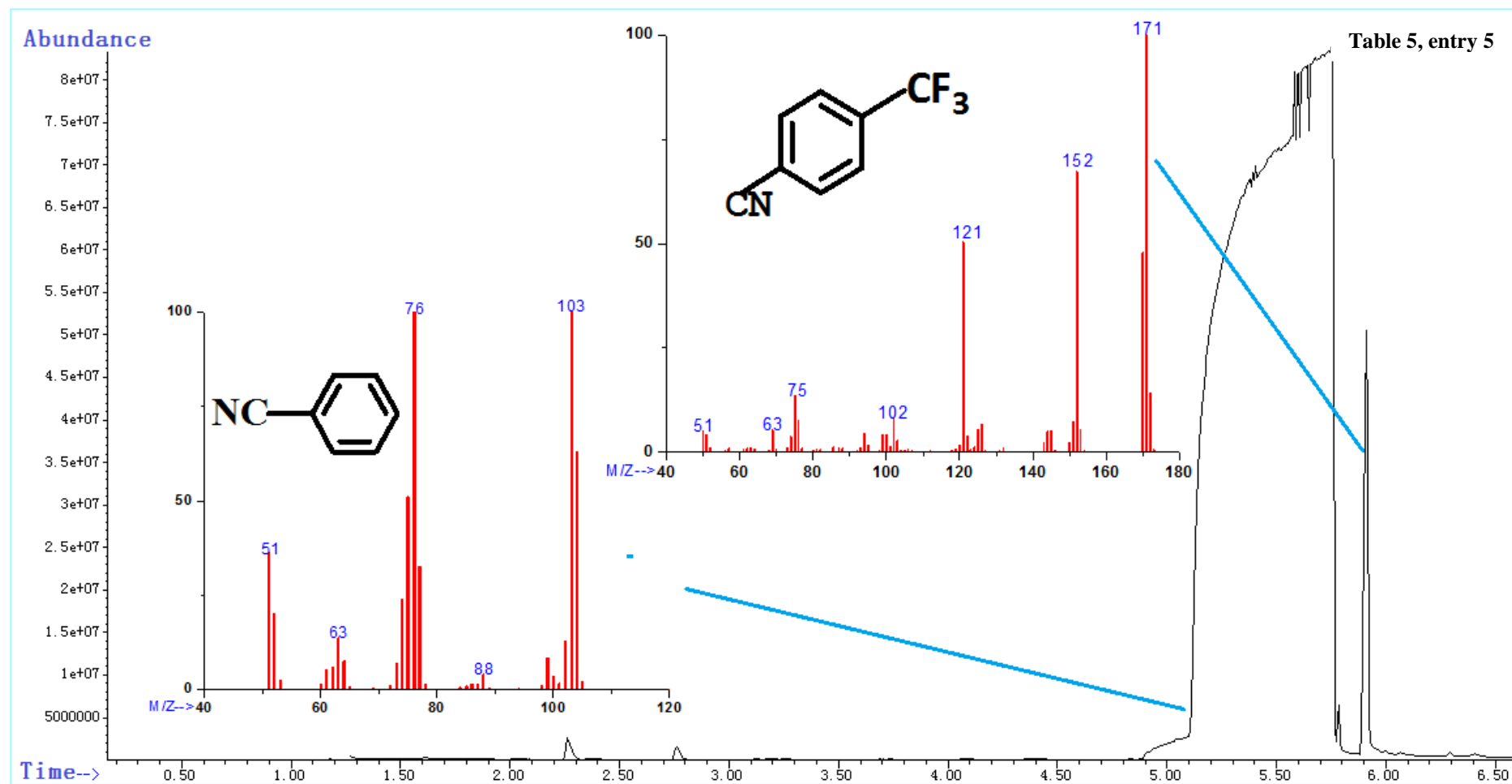














**References:**

- [1] C. L. Sun, H. Li, D. G. Yu, M. Yu, X. Zhou, X. Y. Lu, K. Huang, S. F. Zheng, B. J. Li, and Z. J. Shi, *Nature chemistry*, 2 (2010), 1044.
- [2] Z. Xu, L. Gao, L. L. Wang, M. W. Gong, W. F. Wang and R. S. Yuan, *ACS Catal.*, 5 (2015), 45.