

## Supplementary Material

### $S_N1$ Reactions in Supercritical Carbon Dioxide in the Presence of Alcohols: the Role of Preferential Solvation

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Page S1-3: Experimental procedures and Table S1

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Page S7-66: GC-MS spectra of the reaction mixtures.

**CAUTION!** *Some of the experiments described in this paper involve the use of relatively high pressures and require equipment with the appropriate pressure rating.*

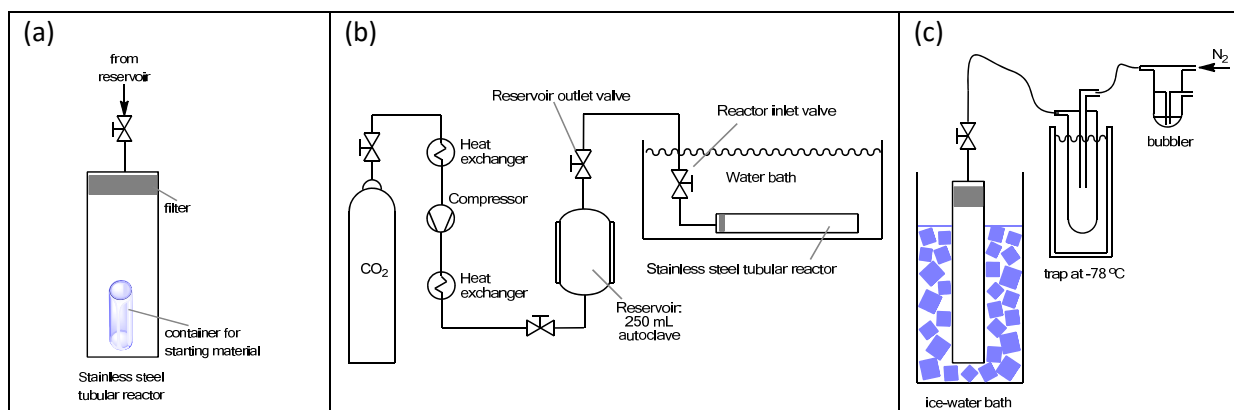
#### Experimental procedures

**General.** Solvents were purified by standard procedures<sup>1</sup> and distilled before use. Dichloromethane was treated with sodium hydrogencarbonate for 4 h at room temperature before use. 1-Chloro-1-phenylethane (**1a**), 1-chloro-1-deutero-1-phenylethane (**1d-1a**), and 1-deutero-1-phenylethanol (**1d-3a**) were prepared following reported procedures.<sup>2</sup>

The high-pressure equipment consisted of a 250-mL AISI 316 stainless-steel jacketed autoclave set at 40 °C which was used as a reservoir, a diaphragm pump (Orlita MHS 30/8) with a maximum theoretical flow of 8.44 L/h of liquid  $CO_2$ , and a set of high-pressure valves, pressure and temperature probes, and rupture-discs, suitably placed to control the flow of  $CO_2$  along the system. The reservoir was filled with activated alumina or Drierite which were exchanged on a weekly basis. *Carbon monoxide and basic organic compounds must be carefully excluded from the system in order to obtain reproducible results.*

**Reactions of alkyl halide **1** with 1,3-dimethoxybenzene (**2**) in supercritical carbon dioxide in the presence of alcohols **3**. General procedure.**<sup>2</sup> A suitable glass or polypropylene tube containing alkyl halide **1** (0.23 mmol) was placed into a 7.5 mL stainless steel reactor charged with 1,3-dimethoxybenzene, and alcohol **3**, under air atmosphere. After placing a stainless steel filter on the upper end of the column, the reactor was tightly closed and connected through a high-pressure valve to the 250 mL autoclave outlet valve. The reservoir was pressurized with  $CO_2$  up to the desired pressure, the reactor was placed into a water bath at 60 °C and allowed to pressurize by carefully opening the connecting valves. After closing the valves and venting the line, the reactor inlet valve was disconnected from the line, and the reactor was allowed to stand at 60 °C for the desired reaction time (Figures S1a,b). Afterwards, the reactor was placed in an ice bath, the valve was connected through a 1/8' Teflon-tube to a trap cooled with a dry-ice bath and equilibrated with a

flow of nitrogen, and the system was allowed to carefully depressurize (Figure S1c). Reactor, valve, tubing and trap were washed with 20 mL of diethyl ether, and the solution was treated with  $\text{NaHCO}_3$  prior to analysis with the aid of GC and GC-MS techniques. Substrate conversions were determined by using adamantane as external standard. The reaction products were identified with authentic samples, prepared following reported procedures.<sup>2</sup> Control experiments performed in a 25 mL view cell confirmed that the reaction mixtures were homogeneous under the working conditions. Further experimental details are collected in the third section of this Supplementary Material.



**Figure S1.** Schematic illustration of: (a) tubular reactor used in the experiments; (b) standard experiment set up (rupture discs, manometers, temperature probes, and fittings are not shown); and (c) depressurization set up.<sup>2</sup>

**1-Chloro-1-deutero-1-phenylethane (1d-1a) [41203-27-4].**  $^1\text{H}$  RMN (300MHz,  $\text{CDCl}_3$ ):  $\delta$  1.7 (t, 3H), 7.1-7.3 (m, 5H);  $^{13}\text{C}$  RMN (75MHz,  $\text{CDCl}_3$ ):  $\delta$  26.3, 58.1, 126.4, 128.2, 128.6, 142.7; EM (EI+, 70ev): m/z (rel. abund.) 51 (7), 63 (3), 78 (9), 90 (3), 106 (100), 126 (9), 128 (3), 141 (17), 143 (5).

**1-Chloro-1-phenylethane (1a) [672-65-1].**  $^1\text{H}$  RMN (300MHz,  $\text{CDCl}_3$ ):  $\delta$  1.8 (d, 3H,  $J$  = 6.9Hz), 5.1 (q, 1H,  $J$  = 6.9Hz), 7.2-7.4 (m, 5H);  $^{13}\text{C}$  RMN (75MHz,  $\text{CDCl}_3$ ):  $\delta$  26.9, 59.2, 126.9, 128.6, 129.0, 143.2; EM (EI+, 70ev): m/z (rel. Abund.) 51 (7), 63 (3), 77 (15), 89 (4), 105 (100), 125 (9), 140 (17), 142 (5).

**1-Deutero-1-phenylethanol (1d-3a) [3101-96-0].**  $^1\text{H}$  RMN (300MHz,  $\text{CDCl}_3$ ):  $\delta$  1.5 (s, 3H), 1.8 (s, 1H), 7.28-7.39 (m, 5H);  $^{13}\text{C}$  RMN (75MHz,  $\text{CDCl}_3$ ):  $\delta$  24.9, 69.9 ( $J$  = 21.9Hz), 125.3, 127.4, 128.4, 145.7; EM (EI+, 70ev): m/z (rel. Abund.) 51 (25), 63 (3), 77 (25), 78 (37), 79 (17), 80 (88), 108 (100).

**2,4-Dimethoxy-1-(1-phenylethyl)benzene (4a<sub>o,p</sub>) [54459-34-6].**  $^1\text{H}$  RMN (300MHz,  $\text{CDCl}_3$ ):  $\delta$  1.5 (d, 3H,  $J$  = 3Hz), 3.6 (s, 3H), 3.7 (s, 3H), 4.4 (q, 1H,  $J$  = 7.2 Hz), 6.34-6.38 (m, 2H), 6.9 (d, 1H,  $J$  = 9Hz), 7.03-7.09 (m, 1H), 7.1-7.2 (m, 4H);  $^{13}\text{C}$  RMN (75MHz,  $\text{CDCl}_3$ ):  $\delta$  21.0, 36.9, 55.3, 55.4, 98.6, 103.9, 125.6, 127.6, 127.9, 128.0, 146.7, 157.7, 159.0. EM (EI+, 70ev): m/z (rel. abund.) 77 (9), 91 (82), 105 (7), 115 (6), 152 (11), 165 (28), 181 (5), 195 (15), 211 (7), 227 (100), 242 (94).

**1,3-Dimethoxy-2-(1-phenylethyl)benzene (4a<sub>o,o</sub>) [672-65-1].**  $^1\text{H}$  RMN (300MHz,  $\text{CDCl}_3$ ):  $\delta$  1.6 (d, 3H,  $J$  = 7.2Hz), 3.6 (s, 6H), 4.7 (q, 1H,  $J$  = 7.2 Hz), 6.4 (d, 2H,  $J$  = 8.1Hz), 6.9-7.2 (m, 7H);  $^{13}\text{C}$  RMN (75MHz,  $\text{CDCl}_3$ ):  $\delta$  17.4, 33.2, 55.7, 104.7, 123.2, 124.8, 127.4, 146.2, 158.4. EM (EI+, 70ev): m/z (rel. abund.) 91 (100), 105 (6), 115 (6), 131 (3), 152 (12), 165 (27), 211 (7), 227 (91), 242 (82).

**1-Benzyl-2,4-dimethoxybenzene (4c<sub>o,p</sub>) [32565-33-6].**  $^1\text{H}$  RMN (300MHz,  $\text{CDCl}_3$ ):  $\delta$  3.71 (s, 6H), 3.8 (s, 2H), 6.39 (d, 1H,  $J$  = 2.4 Hz), 6.8 (d, 1H,  $J$  = 8.4Hz), 7.0-7.2 (m, 6H);  $^{13}\text{C}$  RMN (75MHz,  $\text{CDCl}_3$ ):  $\delta$  35.2, 55.3; 55.7, 98.5, 103.7, 125.6, 127.9, 128.1, 128.5, 128.7, 130.5, 141.4, 158.1, 158.2, 159.3. EM (EI+, 70ev): m/z (rel. abund.) 77 (4), 91 (17), 121 (7), 141 (6), 151 (26), 165 (10), 181 (7), 197 (28), 213 (22), 228 (100).

**2-Benzyl-1,3-dimethoxybenzene (4c<sub>o,o</sub>) [32565-76-7].**  $^1\text{H}$  RMN (300MHz,  $\text{CDCl}_3$ ):  $\delta$  3.72 (s, 6H), 3.9 (s, 2H), 6.32 (1H, d,  $J$  = 2.4 Hz), 6.34 (1H, d,  $J$  = 2.4 Hz), 6.48 (d, 1H,  $J$  = 8.4Hz), 7.0-7.2 (m, 6H);  $^{13}\text{C}$  RMN (75MHz,  $\text{CDCl}_3$ ):  $\delta$  28.5, 55.7, 103.8, 122.1, 127.9, 128.1, 128.5, 128.7, 141.4, 158.1, 158.2, 159.3; EM (EI+, 70ev): m/z (rel. abund.) 77 (4), 91 (56), 115 (6), 137 (7), 152 (19), 165 (19), 181 (10), 197 (28), 213 (10), 228 (100).

Table S1. PhCHCH<sub>3</sub>- and PhCDCH<sub>3</sub>-distributions for reactions in Figures 1 and 2.

## 1a-1d + 3a (1:1) [Entry 1, Figure 1]

| sin-6aa |    | PhCHCH <sub>3</sub>     | 133 |
|---------|----|-------------------------|-----|
| % HH    | 50 | PhCDCH <sub>3</sub>     | 67  |
| % HD    | 33 |                         | 200 |
| % DD    | 17 | PhCHCH <sub>3</sub> (%) | 67  |
|         |    | PhCDCH <sub>3</sub> (%) | 34  |

| anti-6aa |    | PhCHCH <sub>3</sub>     | 120 |
|----------|----|-------------------------|-----|
| % HH     | 41 | PhCDCH <sub>3</sub>     | 80  |
| % HD     | 38 |                         | 200 |
| % DD     | 21 | PhCHCH <sub>3</sub> (%) | 60  |
|          |    | PhCDCH <sub>3</sub> (%) | 40  |

| t0 | Product (%) | PhCH(D)CH <sub>3</sub> | PhCH(D)CH <sub>3</sub> (%) | PhCHCH <sub>3</sub> (%) | PhCDCH <sub>3</sub> (%) | PhCHCH <sub>3</sub> | PhCDCH <sub>3</sub> |
|----|-------------|------------------------|----------------------------|-------------------------|-------------------------|---------------------|---------------------|
|    |             | PhEtCl                 | 100                        | 50                      | 0,2                     | 0,8                 | 10                  |
| tf | PhEtOH      | 100                    | 50                         | 0,9                     | 0,1                     | 45                  | 5                   |
|    |             | 200                    |                            | 1,1                     | 0,9                     | 55                  | 45                  |
| tf | PhEtCl      | 51                     | 51                         | 0,23                    | 0,77                    | 9                   | 29                  |
|    | PhEtOH      | 13                     | 13                         | 0,84                    | 0,16                    | 8                   | 2                   |
|    | sin 6aa     | 20                     | 40                         | 0,67                    | 0,34                    | 20                  | 10                  |
|    | anti 6aa    | 16                     | 32                         | 0,6                     | 0,4                     | 14                  | 9                   |
|    |             | 100                    | 136                        | 100                     | 2                       | 2                   | 50                  |

| 1d-1a | PhCHCH <sub>3</sub> | PhCDCH <sub>3</sub> |
|-------|---------------------|---------------------|
| t0    | 20                  | 80                  |
| tf    | 23                  | 77                  |

conv %

25

81

| 3a | PhCHOHCH <sub>3</sub> | PhCDOHCH <sub>3</sub> |
|----|-----------------------|-----------------------|
| t0 | 90                    | 10                    |
| tf | 84                    | 16                    |

Isotopic dilution %

7

## 1a + 3a-1d (1:2) [Entry 2, Figure 1]

| 6aa sin |    | PhCHCH <sub>3</sub>     | 46  |
|---------|----|-------------------------|-----|
| % HH    | 3  | PhCDCH <sub>3</sub>     | 154 |
| % HD    | 40 |                         | 200 |
| % DD    | 57 | PhCHCH <sub>3</sub> (%) | 23  |
|         |    | PhCDCH <sub>3</sub> (%) | 77  |

| 6aa anti |      | PhCHCH <sub>3</sub>     | 39  |
|----------|------|-------------------------|-----|
| % HH     | 0,24 | PhCDCH <sub>3</sub>     | 161 |
| % HD     | 39   |                         | 200 |
| % DD     | 61   | PhCHCH <sub>3</sub> (%) | 20  |
|          |      | PhCDCH <sub>3</sub> (%) | 80  |

| t0 | Product (%) | PhCH(D)CH <sub>3</sub> | PhCH(D)CH <sub>3</sub> (%) | PhCHCH <sub>3</sub> (%) | PhCDCH <sub>3</sub> (%) | PhCHCH <sub>3</sub> | PhCDCH <sub>3</sub> |
|----|-------------|------------------------|----------------------------|-------------------------|-------------------------|---------------------|---------------------|
|    |             | PhEtCl                 | 100                        | 33                      | 0,91                    | 0,09                | 30                  |
| tf | PhEtOH      | 200                    | 67                         | 0,12                    | 0,88                    | 8                   | 59                  |
|    |             | 300                    |                            | 1,03                    | 0,97                    | 38                  | 62                  |
| tf | PhEtCl      | 37                     | 37                         | 0,79                    | 0,21                    | 24                  | 6                   |
|    | PhEtOH      | 42                     | 42                         | 0,12                    | 0,88                    | 4                   | 31                  |
|    | sin 6aa     | 11                     | 22                         | 0,23                    | 0,77                    | 4                   | 14                  |
|    | anti 6aa    | 10                     | 20                         | 0,2                     | 0,8                     | 3                   | 13                  |
|    |             | 100                    | 121                        | 100                     | 1                       | 3                   | 36                  |

| 1a | PhCHCH <sub>3</sub> | PhCDCH <sub>3</sub> |
|----|---------------------|---------------------|
| t0 | 91                  | 9                   |
| tf | 79                  | 21                  |

conv %

8

48

| 1d-3a | PhCHOHCH <sub>3</sub> | PhCDOHCH <sub>3</sub> |
|-------|-----------------------|-----------------------|
| t0    | 12                    | 88                    |
| tf    | 12                    | 88                    |

Isotopic dilution %

0

## 1a-1d + 3a + 2 (1:1:4) [Entry 2, Figure 2]

| 4op |     | 4oo |                         | 5   |                         | 5'  |                         | 6aa sin |                         | 6aa anti |  |
|-----|-----|-----|-------------------------|-----|-------------------------|-----|-------------------------|---------|-------------------------|----------|--|
| % H | 56  | 53  | % HH                    | 30  | % HH                    | 32  | % HH                    | 50      | % HH                    | 50       |  |
| % D | 44  | 47  | % HD                    | 47  | % HD                    | 40  | % HD                    | 38      | % HD                    | 45       |  |
|     | 100 | 100 | % DD                    | 23  | % DD                    | 28  | % DD                    | 12      | % DD                    | 5        |  |
|     |     |     | PhCHCH <sub>3</sub>     | 107 | PhCHCH <sub>3</sub>     | 104 | PhCHCH <sub>3</sub>     | 138     | PhCHCH <sub>3</sub>     | 145      |  |
|     |     |     | PhCDCH <sub>3</sub>     | 93  | PhCDCH <sub>3</sub>     | 96  | PhCDCH <sub>3</sub>     | 62      | PhCDCH <sub>3</sub>     | 55       |  |
|     |     |     |                         | 200 |                         | 200 |                         | 200     |                         | 200      |  |
|     |     |     | PhCHCH <sub>3</sub> (%) | 54  | PhCHCH <sub>3</sub> (%) | 52  | PhCHCH <sub>3</sub> (%) | 69      | PhCHCH <sub>3</sub> (%) | 73       |  |
|     |     |     | PhCDCH <sub>3</sub> (%) | 47  | PhCDCH <sub>3</sub> (%) | 48  | PhCDCH <sub>3</sub> (%) | 31      | PhCDCH <sub>3</sub> (%) | 28       |  |

| t0 | Product (%) | PhCH(D)CH <sub>3</sub> | PhCH(D)CH <sub>3</sub> (%) | PhCHCH <sub>3</sub> (%) | PhCDCH <sub>3</sub> (%) | PhCHCH <sub>3</sub> | PhCDCH <sub>3</sub> |
|----|-------------|------------------------|----------------------------|-------------------------|-------------------------|---------------------|---------------------|
|    |             | PhEtCl                 | 100                        | 50                      | 0,2                     | 0,8                 | 10                  |
| tf | PhEtOH      | 100                    | 50                         | 0,9                     | 0,1                     | 45                  | 5                   |
|    |             | 200                    |                            | 1,1                     | 0,9                     | 55                  | 45                  |
| tf | PhEtCl      | 33                     | 33                         | 0,23                    | 0,77                    | 7                   | 22                  |
|    | PhEtOH      | 16                     | 16                         | 0,9                     | 0,1                     | 13                  | 1                   |
|    | 4 o,p       | 32                     | 32                         | 0,56                    | 0,44                    | 16                  | 12                  |
|    | 4 o,o       | 6                      | 6                          | 0,53                    | 0,47                    | 3                   | 2                   |
|    | 5           | 3                      | 6                          | 0,54                    | 0,47                    | 3                   | 2                   |
|    | 5'          | 3                      | 6                          | 0,52                    | 0,48                    | 3                   | 3                   |
|    | sin 6aa     | 4                      | 8                          | 0,69                    | 0,31                    | 5                   | 2                   |
|    | anti 6aa    | 3                      | 6                          | 0,73                    | 0,28                    | 4                   | 1                   |
|    |             | 100                    | 113                        | 100                     | 5                       | 3                   | 53                  |
|    |             |                        |                            |                         |                         |                     | 48                  |

| 1d-1a | PhCHCH <sub>3</sub> | PhCDCH <sub>3</sub> |
|-------|---------------------|---------------------|
| t0    | 20                  | 80                  |
| tf    | 23                  | 77                  |

conv %

42

72

| 3a | PhCHOHCH <sub>3</sub> | PhCDOHCH <sub>3</sub> |
|----|-----------------------|-----------------------|
| t0 | 90                    | 10                    |
| tf | 90                    | 10                    |

Isotopic dilution %

0

## 1a-1d + 3a + 2 (1:1:1) [Entry 3, Figure 2]

| 4op |     | 4oo |                         | 5   |                         | 5'  |                         | 6aa sin |                         | 6aa anti |  |
|-----|-----|-----|-------------------------|-----|-------------------------|-----|-------------------------|---------|-------------------------|----------|--|
| % H | 63  | 65  | % HH                    | 41  | % HH                    | 41  | % HH                    | 50      | % HH                    | 52       |  |
| % D | 37  | 35  | % HD                    | 42  | % HD                    | 42  | % HD                    | 33      | % HD                    | 35       |  |
|     | 100 | 100 | % DD                    | 17  | % DD                    | 17  | % DD                    | 17      | % DD                    | 13       |  |
|     |     |     | PhCHCH <sub>3</sub>     | 124 | PhCHCH <sub>3</sub>     | 124 | PhCHCH <sub>3</sub>     | 133     | PhCHCH <sub>3</sub>     | 139      |  |
|     |     |     | PhCDCH <sub>3</sub>     | 76  | PhCDCH <sub>3</sub>     | 76  | PhCDCH <sub>3</sub>     | 67      | PhCDCH <sub>3</sub>     | 61       |  |
|     |     |     |                         | 200 |                         | 200 |                         | 200     |                         | 200      |  |
|     |     |     | PhCHCH <sub>3</sub> (%) | 62  | PhCHCH <sub>3</sub> (%) | 62  | PhCHCH <sub>3</sub> (%) | 67      | PhCHCH <sub>3</sub> (%) | 70       |  |
|     |     |     | PhCDCH <sub>3</sub> (%) | 38  | PhCDCH <sub>3</sub> (%) | 38  | PhCDCH <sub>3</sub> (%) | 34      | PhCDCH <sub>3</sub> (%) | 31       |  |

| t0 | Product (%) | PhCH(D)CH <sub>3</sub> | PhCH(D)CH <sub>3</sub> (%) | PhCHCH <sub>3</sub> (%) | PhCDCH <sub>3</sub> (%) | PhCHCH <sub>3</sub> | PhCDCH <sub>3</sub> |
|----|-------------|------------------------|----------------------------|-------------------------|-------------------------|---------------------|---------------------|
|    |             | PhEtCl                 | 100                        | 50                      | 0,2                     | 0,8                 | 10                  |
| tf | PhEtOH      | 100                    | 50                         | 0,9                     | 0,1                     | 45                  | 5                   |
|    |             | 200                    |                            | 1,1                     | 0,9                     | 55                  | 45                  |
| tf | PhEtCl      | 40                     | 40                         | 0,3                     | 0,7                     | 9                   | 21                  |
|    | PhEtOH      | 3                      | 3                          | 0,9                     | 0,1                     | 2                   | 0                   |
|    | 4 o,p       | 20                     | 20                         | 0,63                    | 0,37                    | 9                   | 6                   |
|    | 4 o,o       | 4                      | 4                          | 0,65                    | 0,35                    | 2                   | 1                   |
|    | 5           | 10                     | 20                         | 0,62                    | 0,38                    | 9                   | 6                   |
|    | 5'          | 10                     | 20                         | 0,62                    | 0,38                    | 9                   | 6                   |
|    | sin 6aa     | 10                     | 20                         | 0,67                    | 0,33                    | 10                  | 5                   |
|    | anti 6aa    | 3                      | 6                          | 0,7                     | 0,31                    | 3                   | 1                   |
|    |             | 100                    | 133                        | 100                     | 5                       | 3                   | 54                  |
|    |             |                        |                            |                         |                         |                     | 46                  |

| 1d-1a | PhCHCH <sub>3</sub> | PhCDCH <sub>3</sub> |
|-------|---------------------|---------------------|
| t0    | 20                  | 80                  |
| tf    | 30                  | 70                  |

conv %

40

95

| 3a | PhCHOHCH <sub>3</sub> | PhCDOHCH <sub>3</sub> |
|----|-----------------------|-----------------------|
| t0 | 90                    | 10                    |
| tf | 90                    | 10                    |

Isotopic dilution %

0

## Detailed experimental protocols for performing $S_N1$ reactions in $scCO_2$

The experimental details and observations described herein are related to our particular experimental conditions and should be properly adapted to the different procedures and equipment used by other researchers. The product numbers, schemes, figures, tables and pages mentioned in the following text refer to those described in our previous report and its Supplementary Material.<sup>2</sup>

**Placing the reagents in the reactor.** The reactions described in our report<sup>2</sup> were initially performed by placing alkyl halide **1** and 1,3-dimethoxybenzene (**2**) at the bottom of a stainless steel tubular reactor, and then pressurizing up to 250 bar as described below (General Procedure on page S4 of the Supplementary Material). In order to prevent possible solventless reactions prior to reaching an homogeneous  $scCO_2$  solution, the reactions were performed by placing reagents in separate containers: alkyl halide **1** was placed inside a suitable polypropylene container, and 1,3-dimethoxybenzene (**2**) was placed at the bottom of the tubular reactor (Control Experiment 1 and Figure S2B on pages S5 and S6 of the Supplementary Material). The containers for alkyl halide **1** were made by welding one end of a *ca.* 2 cm piece of 1/8' polypropylene tubing, and were tested for leaks prior to use. Actually, all the reactions described in our report<sup>2</sup> (Table 1, Scheme 2) were performed in both ways with the same results. Alternatively, alkyl halide **1** was added to the reactor that contained 1,3-dimethoxybenzene (**2**) through a Rheodyne valve in the pressurization step (Control Experiment 2 on page S6 of the Supplementary Material). This control experiment was performed for some representative substrates with results similar to those shown in Table 1.

**Pressurization.** Pressurization of the tubular reactor that contained the reagents (Scheme S1, on page S5 of the Supplementary Material) was done by first pressurizing up to *ca.* 200 bar the stainless-steel jacketed 250-mL reservoir set at 40 °C, placing the reactor into a water bath at the desired temperature, opening the connecting valves, and then continuing the compressor operation until the desired pressure was reached. After closing the valves, the reactor was disconnected from the line and allowed to stand horizontally in the water bath. The compressor was continuously operating during the pressurization process, and the reactor was maintained in a proper position to avoid the mixing of reagents prior to  $CO_2$  intake. Given the different volumes of the reservoir (250 mL) and the tubular reactor (7-8 mL), the time interval in which the reagents were at the bath temperature before reaching a  $scCO_2$  solution at *ca.* 180 bar lasted a few seconds. The reactions performed by pressurizing the tubular reactor prior to immersion in the water bath gave the same results. The reactor was disconnected from the line to prevent the reaction mixture from occupying the dead volume of the line in the event that the reactor's high pressure valve was not properly sealed.

**Control experiments in conventional solvents.** The control experiments done in conventional solvents were performed in a stainless steel tubular reactor. As we found that testing the reactions in  $scCO_2$  by rigorously excluding stainless steel surfaces from the reaction medium was difficult, we decided to include this factor in the reactions performed under conventional conditions reasoning that any catalysis by the metallic surface should also be evident under these conditions. The reactions done in conventional solvents, with the same substrate concentrations and temperature as for the experiments in  $scCO_2$ , and performed in sealed stainless steel tubular reactors, gave no Friedel-Crafts products. These control experiments are described in the main text (page 13300) and the Supplementary Material (Control Experiment 5, page S8) of our previous report.<sup>2</sup>

**Preventing contaminants.**  $S_N1$  reactions in  $scCO_2$  are extremely sensitive to presence of water and organic contaminants in the reaction medium. This was explicitly stated in the main text (first paragraph on page 13300), in reference 18, and in the Supplementary Material (page S1, and control experiment 7 in page S9) of our initial report<sup>2</sup> and explained now. We specifically tested water, ethanol, acetone, ethyl acetate, trimethylsilanol, 2,6-lutidine and triphenylphosphine. Organic



compounds carrying any of these functional groups, and atoms with lone electron pairs in general, inhibited the reactions in more or less extension depending on the sensitivity of alkyl halide **1** to ionization and the ability of the additive to interact with carbon dioxide. Occasionally we found that the reactions performed when the CO<sub>2</sub>-cylinder had less than *ca.* 30% of its initial contents, or when room temperature came close to 30 °C, did not properly work. We attributed this to carbon monoxide being present in the cylinder (Supplementary Material, page S1),<sup>2</sup> although no specific tests that addressed the impact of carbon monoxide on our reactions were performed. In order to prevent adventitious water condensed in the lines from reaching the reaction mixture, the reservoir was filled with alumina beads or Drierite, which were exchanged on a weekly basis (Supplementary Material, page S1). Alternatively, a stainless steel column filled with Drierite as desiccant and thermostated at 40 °C was placed prior to the outlet valve of the reservoir; in this case Drierite was exchanged when the indicator showed that it was exhausted. The operations associated with introducing reagents into the reactor were always done very carefully to avoid contaminating the system. Finally, it should be noticed that *sc*CO<sub>2</sub>-promoted S<sub>N</sub>1 reactions which lead to products with Lewis basic sites are expected to auto-inhibit.

Apart from water and ethanol, we found that amines and triphenylphosphine were strong inhibitors of S<sub>N</sub>1 reactions in *sc*CO<sub>2</sub>. For instance, after a series of experiments done to explore the E1/E2 reactions of alkyl halides **1** with 2,6-lutidine as a base in *sc*CO<sub>2</sub>, the reactions of alkyl halides **1** with aromatic **2** in *sc*CO<sub>2</sub> failed to give any Friedel-Crafts products. The usual performance of our system was recovered after extensive thorough washings of the tubular reactor and the line (see below for details), and purging of the reservoir and its outlet valve with *sc*CO<sub>2</sub> through a series of pressurization/ depressurization steps. Similar problems arose when the reservoir and the line were used for pressurizing other reaction mixtures from different research topics. After this experience, the reservoir and the line were used exclusively for the S<sub>N</sub>1 reactions in *sc*CO<sub>2</sub>, and were purged with CO<sub>2</sub> prior to each experiment as a standard experimental protocol. We also selected one of the reported Friedel-Crafts reactions (Entry 3, Table 1) to regularly prove our system's performance. We attributed the cross-contamination to transport of organic material from the reactor to the line in the pressurization stage, which occurs even when positive CO<sub>2</sub> pressure is maintained during the process. We should note that the sensitivity to contamination of S<sub>N</sub>1 reactions promoted by *sc*CO<sub>2</sub> allowed this non insignificant detail to be observed.

**Stainless steel reactor.** The tubular reactor used in our experiments was homemade by sealing 3/8' stainless steel tubing with a standard cap and connecting the other end to a high pressure valve through 1/16' tubing and suitable fittings (Figure S2B of Supplementary Material, page S5). A stainless steel filter was placed on top of the reactor to protect the 1/16' tubing and the valve from any solid material which may be ejected from the reactor in the pressurization or depressurization stages. The working pressure of these materials was *ca.* 500 bar. These reactors were exclusively used for the S<sub>N</sub>1 reactions in *sc*CO<sub>2</sub>. The reactor was accessed through either the top, by dismantling the fitting and removing the filter, or from the bottom, by disconnecting the plug.

No P/T probes, stirrer, manometer, rupture discs, additional purge or sample valve was connected to the tubular reactor (Figure S2B of Supplementary Material, page S5). These components complicate the reactor's internal geometry by introducing nooks, crevices, threads, and gaskets, which become deposits of organic materials from the reaction mixtures. *sc*CO<sub>2</sub> is an ideal medium for transporting organic solutes to all the interstices in the reactor, and for depositing them there upon depressurization. Conventional solvents, and even *sc*CO<sub>2</sub>, fail to efficiently remove tars from these stagnant regions. Given the sensitivity of S<sub>N</sub>1 reactions in *sc*CO<sub>2</sub> to even trace amounts of certain organic compounds, particularly amines and phosphines, the use of reactors with complex internal geometries, which have been previously used for other chemical reactions, is not recommended.

**Products isolation.** The reaction products were collected as described in the General Procedure of our report (page S5, and Figure S2A on page S6 of the Supplementary Material).<sup>2</sup> The tubular reactor was placed in a water bath at 0 °C. Then it was carefully depressurized into a trap cooled at -78 °C and equilibrated with a flow of nitrogen. After removing the plug, diethyl ether was added to the tubular reactor and allowed to flow at ambient pressure through the tubing and valve into a glass vial. The plug, the polypropylene container and the trap were washed with diethyl ether separately. All the solutions were combined, and the external standard was added in this stage. The volume of diethyl ether used was that required to achieve a suitable concentration for the gas chromatography analysis. Occasionally, solutions were treated with sodium bicarbonate and magnesium sulfate prior to the gas chromatography analysis, and the same results were obtained. Product isolation, performed by flowing *sc*CO<sub>2</sub> through the tubular reactor for 3 h under the reaction conditions (Control Experiment 3 and Figure S4, page S7 of the Supplementary Material), led to the same results. These control experiments were performed only for some representative substrates.

**Cleaning.** Standard reactor cleaning was performed by disconnecting the plug and then successively flowing through the reactor, tubing and valve aqueous sodium hydrogen carbonate, distilled water and then acetone, in both directions, with a water aspirator. The stainless steel 1/8' line that connected the reservoir's outlet valve to the tubular reactor (Scheme S1, Supplementary Material) was washed in the same way. The plug and container used for alkyl halide **1** were washed successively with aqueous sodium hydrogen carbonate, distilled water and then acetone in an ultrasound bath. The reactor was cleaned regularly by disassembling its elements (plug, fittings, tubing and valve) and washing them in this way. All the reactor components were dried under vacuum (0.1 mbar) for a minimum of 4 h at room temperature before use. Access to the vacuum line by other users was prevented during this operation. The stainless steel filter and plug were inspected with a magnifying glass, and discarded when signs of tars or deformation were detected.

**Concluding remarks.** The experimental details described herein are addressed to prevent basic compounds from reaching the reaction mixture in the different experimental setup stages. Experimental conditions are critical for the success of S<sub>N</sub>1 reactions promoted by *sc*CO<sub>2</sub>, which is a common feature for many organic reactions of synthetic relevance; for instance, organolithium reactions,<sup>3</sup> Sharpless epoxidation,<sup>4</sup> reactions mediated by samarium (II) iodide,<sup>5</sup> and some transition-metal catalyzed reactions.<sup>6</sup> The impact of Lewis bases on S<sub>N</sub>1 reactions promoted by *sc*CO<sub>2</sub> may have been concealing this chemistry for a rather long time, so it should not be surprising that this chemistry can be revealed only under rigorous experimental conditions. Hopefully, the experimental procedures in our original paper<sup>2</sup> with the additional comments reported herein will suffice to make crystal clear what the words “[basic contaminants] must be carefully excluded from the system in order to obtain reproducible results”, stated in page S1 of the Supplementary Material,<sup>2</sup> stand for.

## References

- 1) D. D. Perrin, and W. L. F. Armarego, *Purification of Laboratory Chemicals*, 3rd Edition, Pergamon Press, New York, **1988**.
- 2) T. Delgado-Abad, J. Martínez-Ferrer, A. Caballero, A. Olmos, R. Mello, M. E. González-Núñez, P. J. Pérez, and G. Asensio, *Angew. Chem.* **2013**, *125*, 13540-13543; *Angew. Chem. Int. Ed.* **2013**, *52*, 13298-13301.
- 3) L. Degennaro, A. Glovine, L. Carroccia, and R. Luisi “Practical aspects of organolithium chemistry” in *Lithium Compounds in Organic Synthesis*, eds. R. Luisi and V. Capriati, Wiley-VCH, Weinheim, 2014, p.513.
- 4) T. Katsuki, and V. Martin, *Organic Reactions* 1995, **48**, 1-299.
- 5) D. Procter, R. A. Flowers II, and T. Skrydstrup, “Organic Synthesis using Samarium Diiodide. A Practical Guide”, RSC Publishing, Cambridge, **2010**.
- 6) D. F. Shriver, “The Manipulation of Air-Sensitive Compounds” McGraw-Hill, New York, **1969**.

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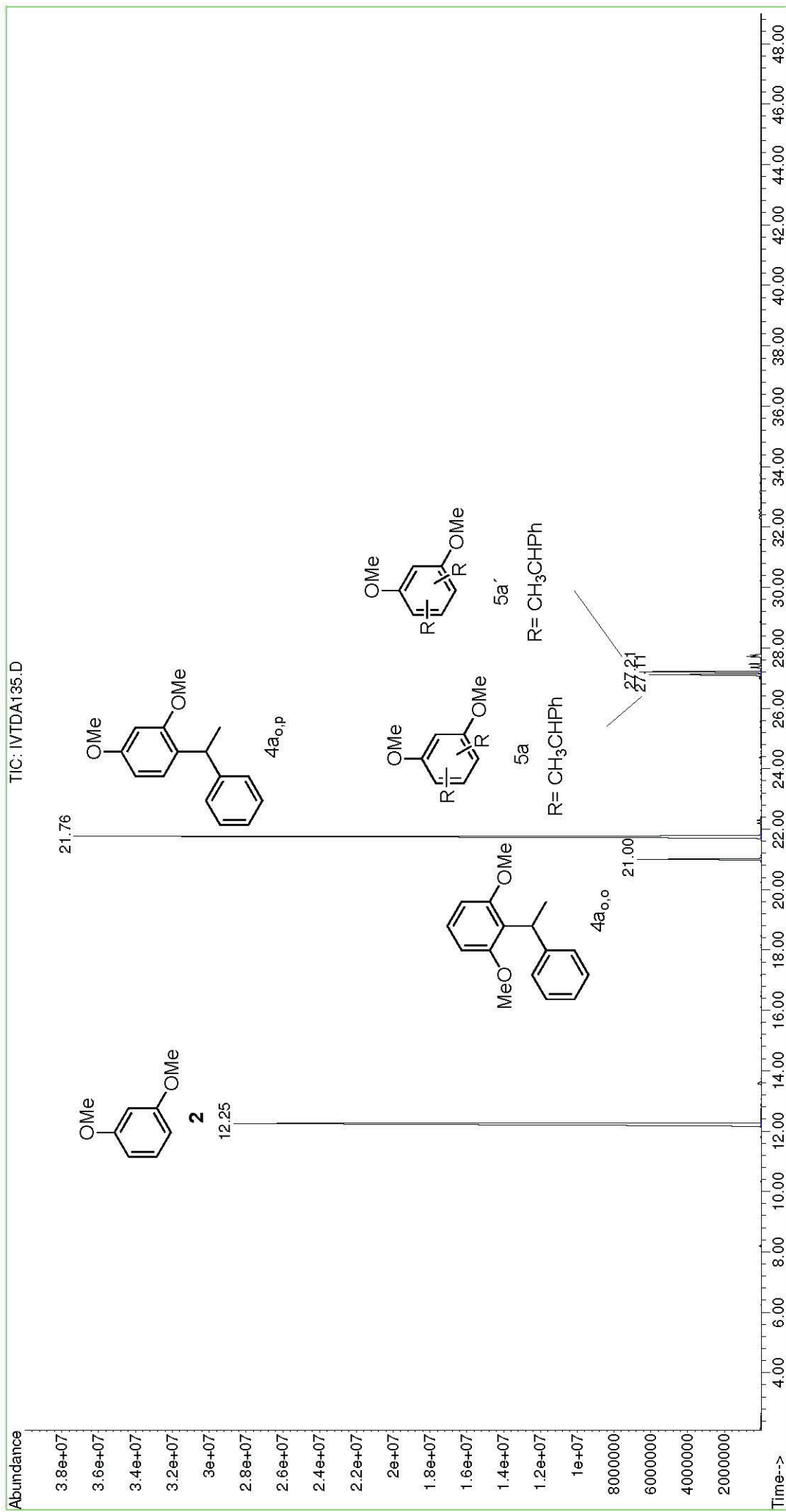
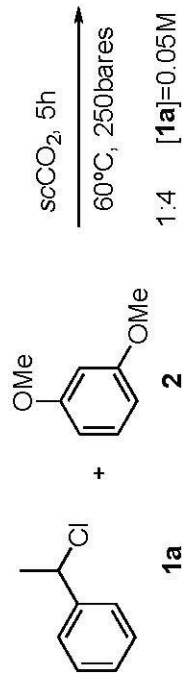
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Instrument : Instrument

Sample Name:

Misc Info :

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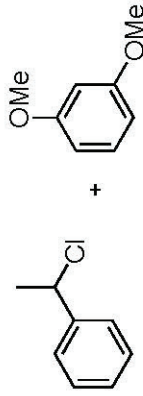
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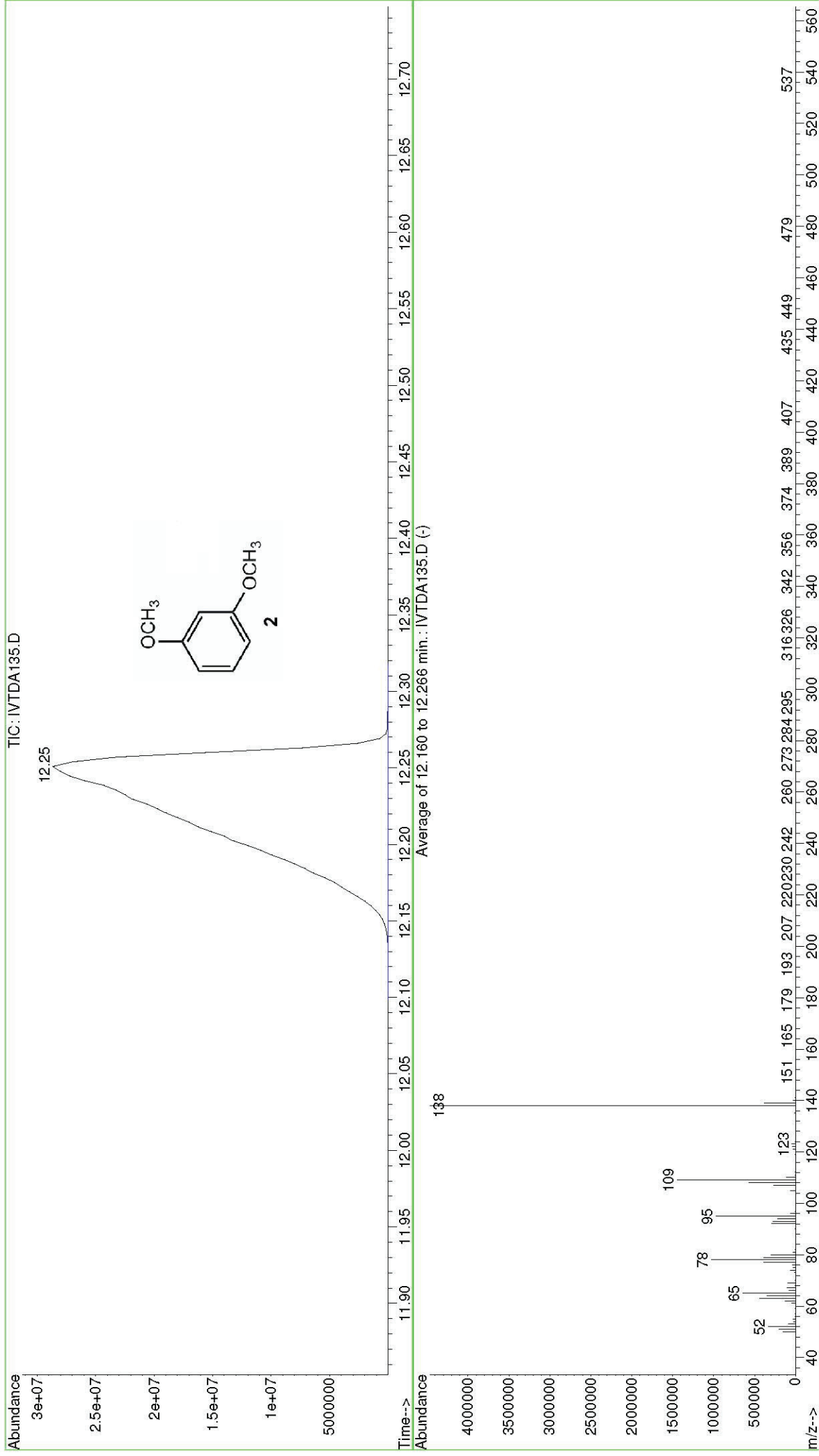
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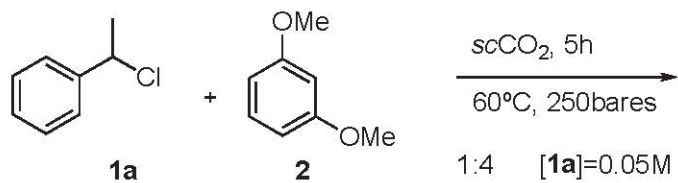


scCO<sub>2</sub>, 5h

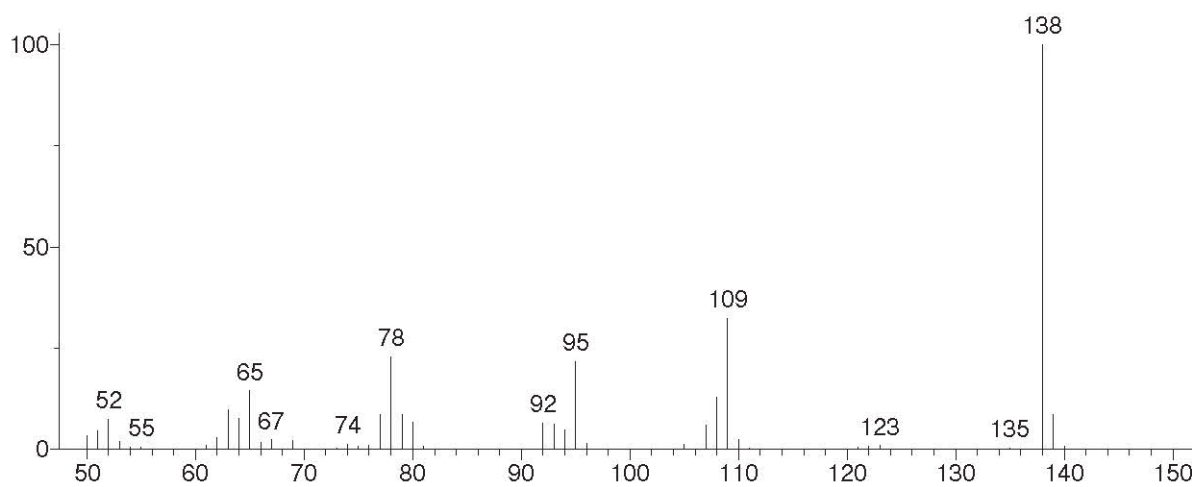
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1:4 [1a]=0.05M

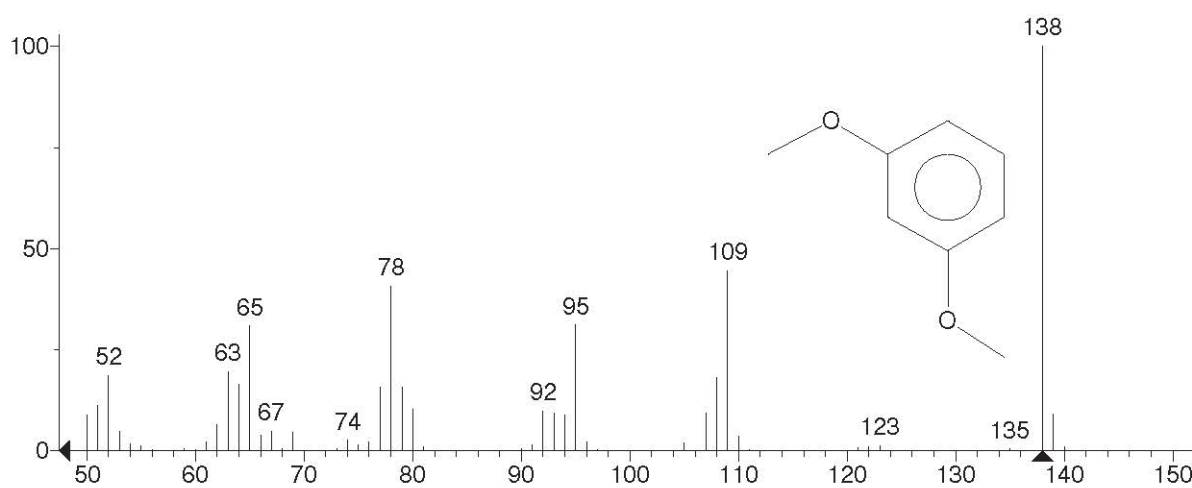




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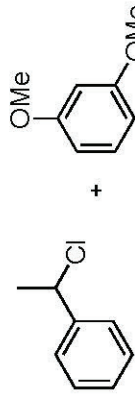
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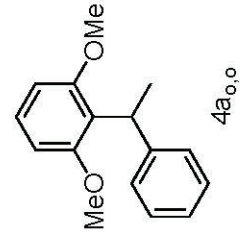


**1a**

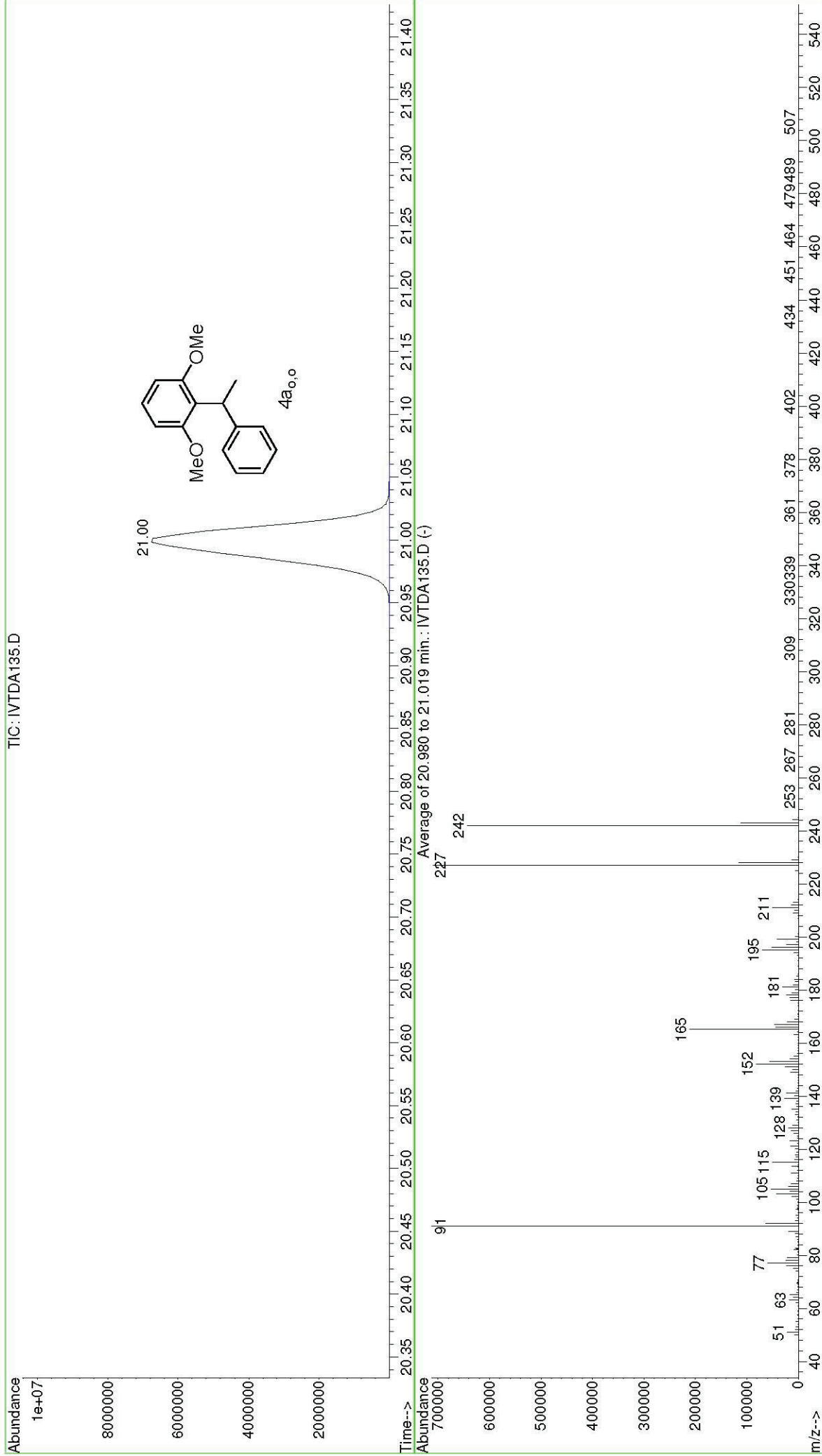
**2**

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1:4 [1a]=0.05M



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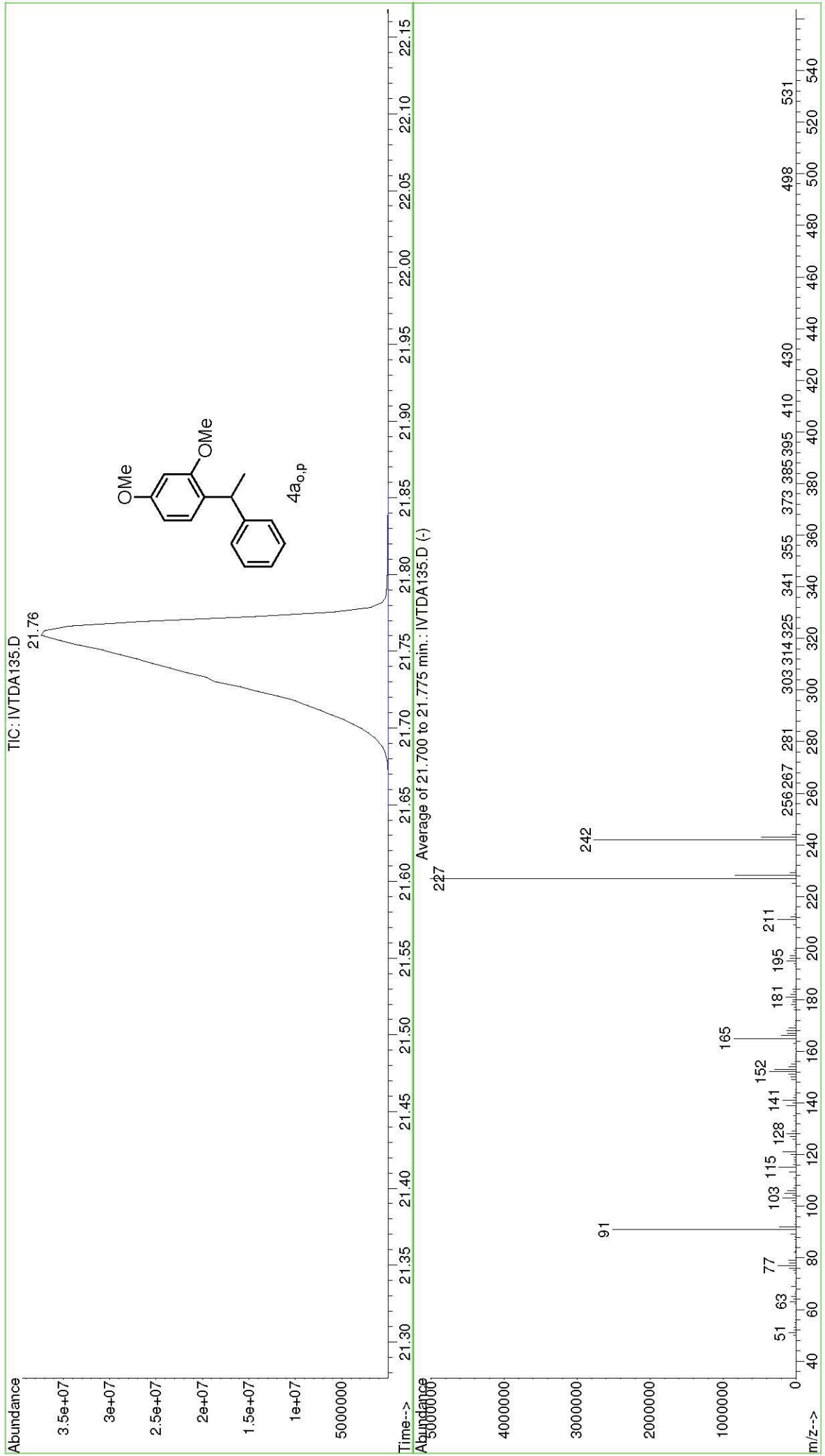
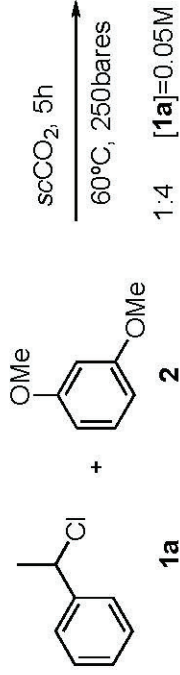
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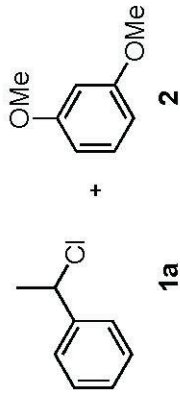
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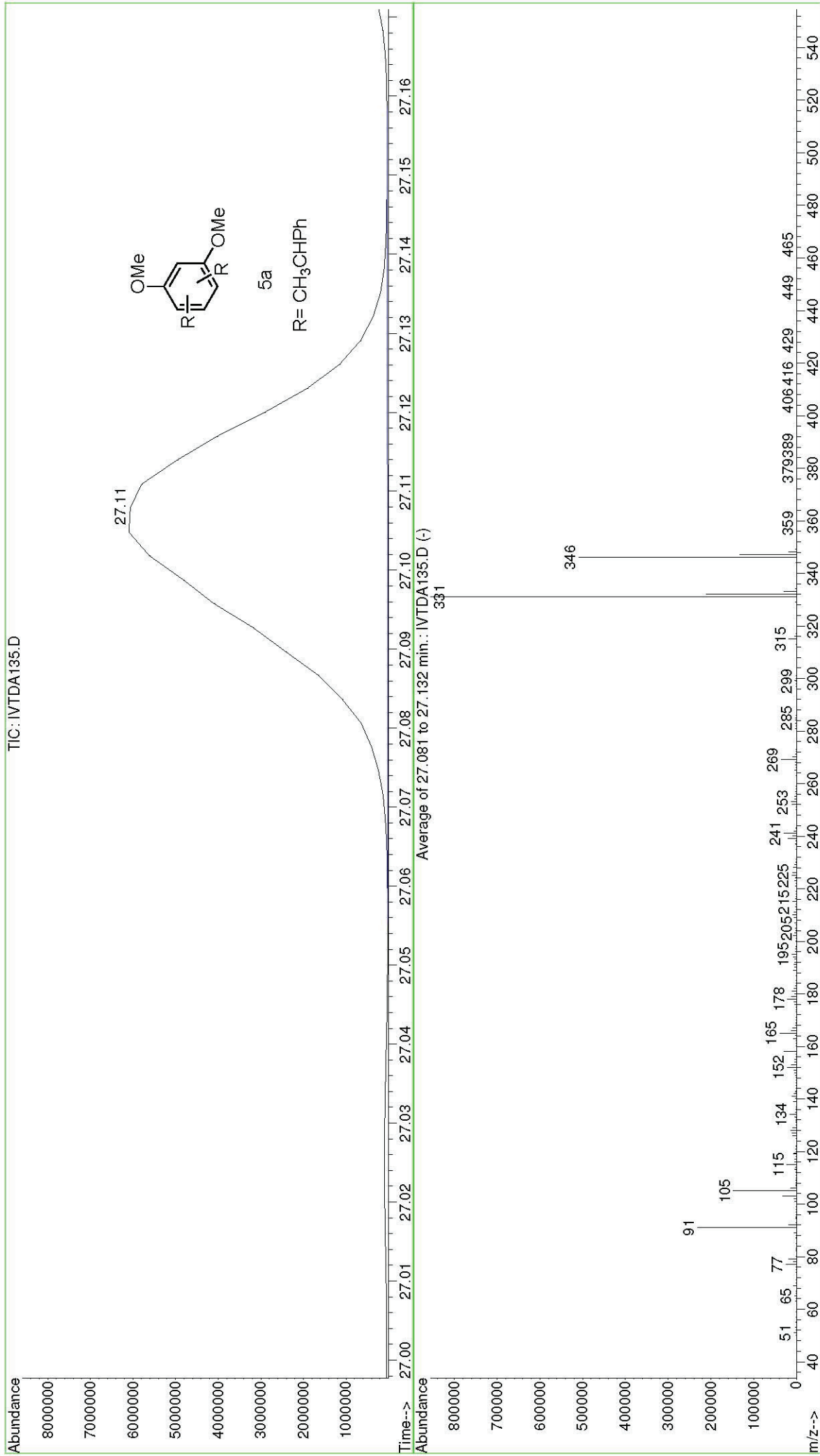
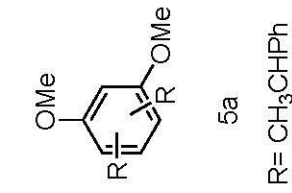
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scCO<sub>2</sub>, 5h  
60°C, 250bares

1:4 [1a]=0.05M





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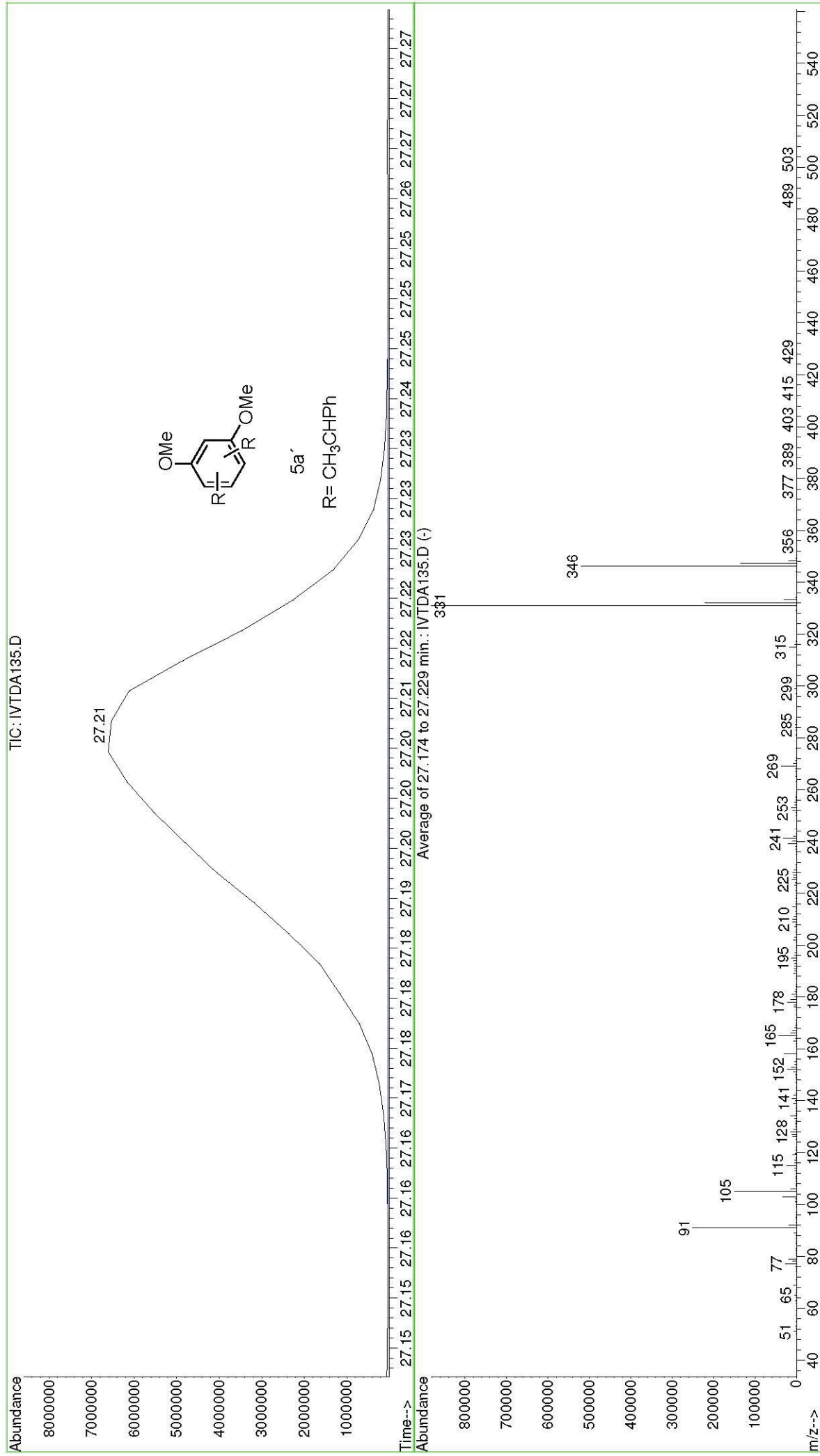
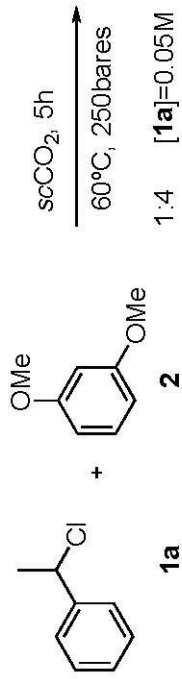
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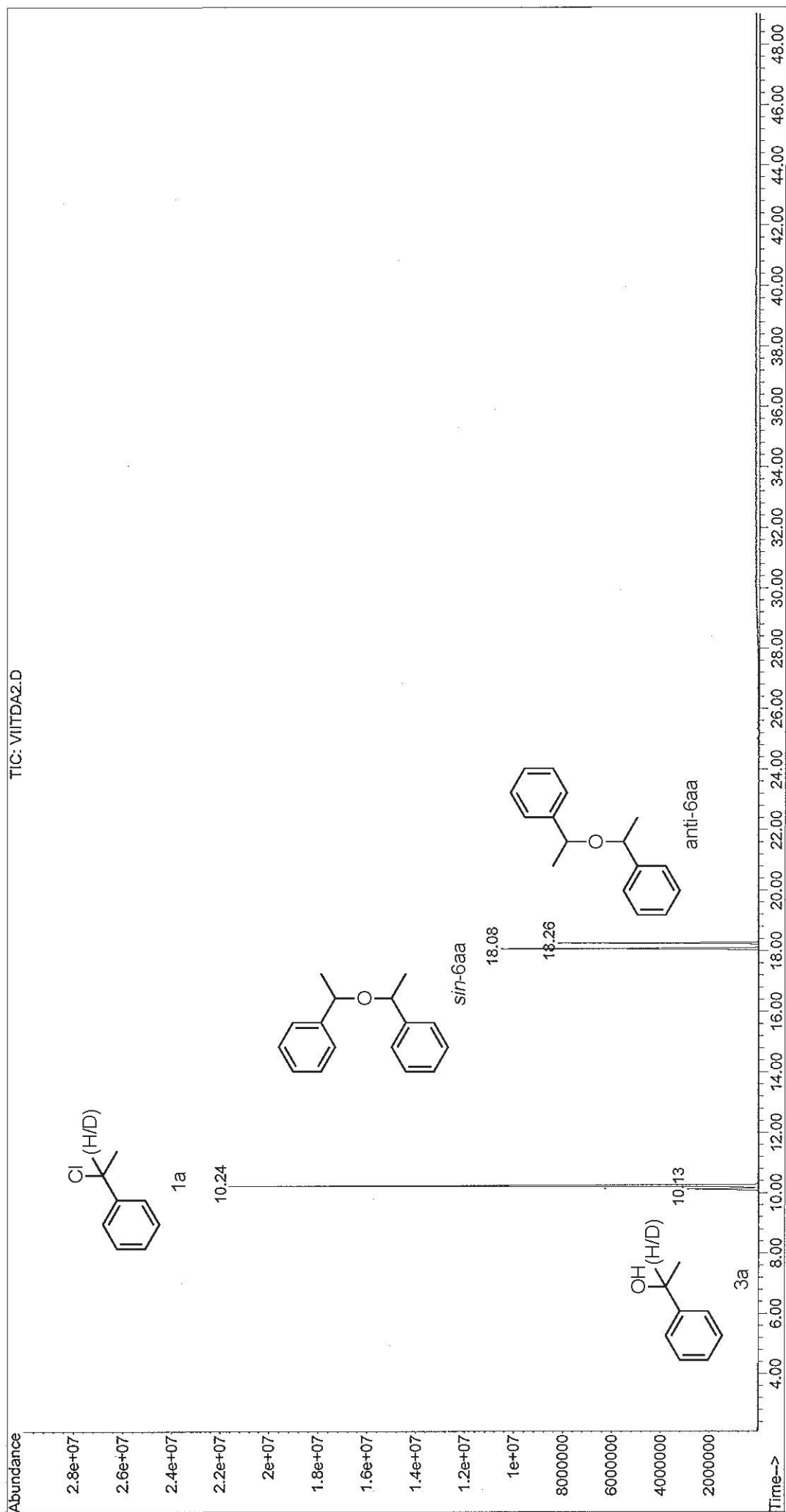
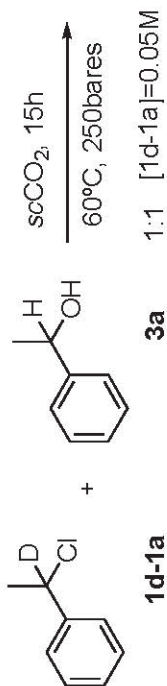
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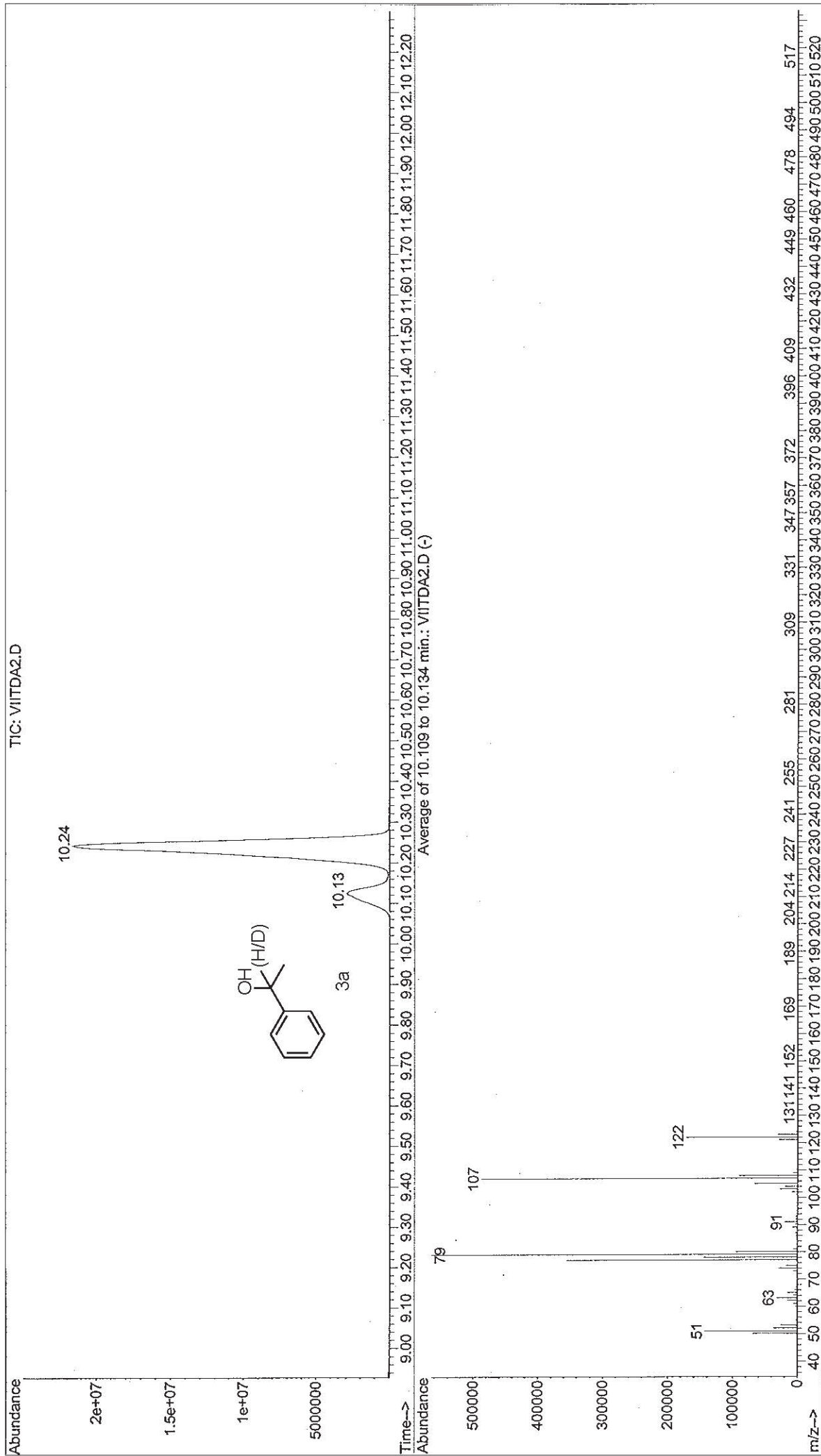
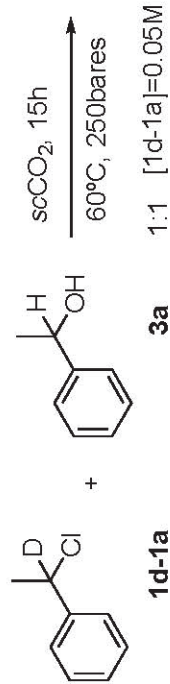
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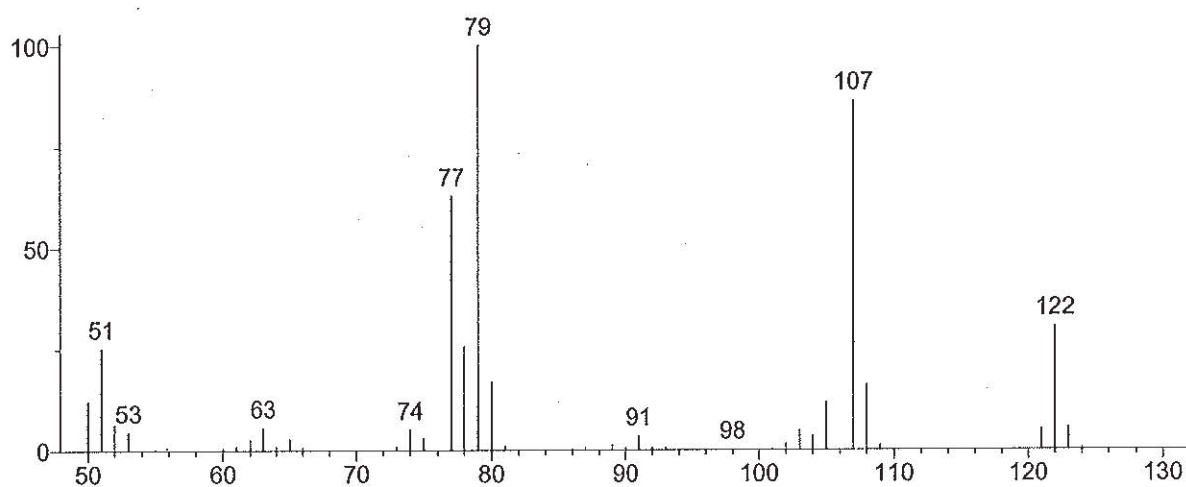
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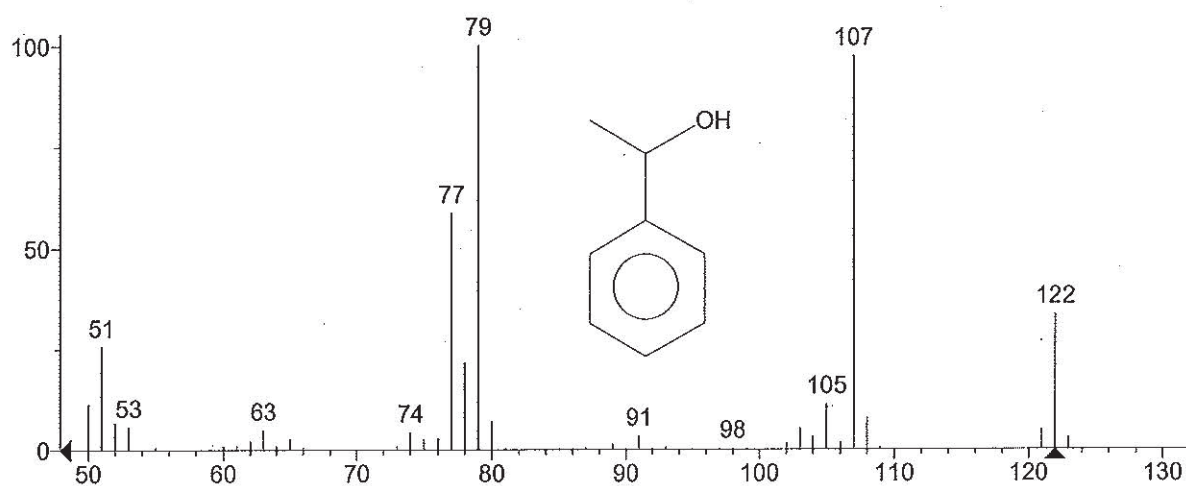




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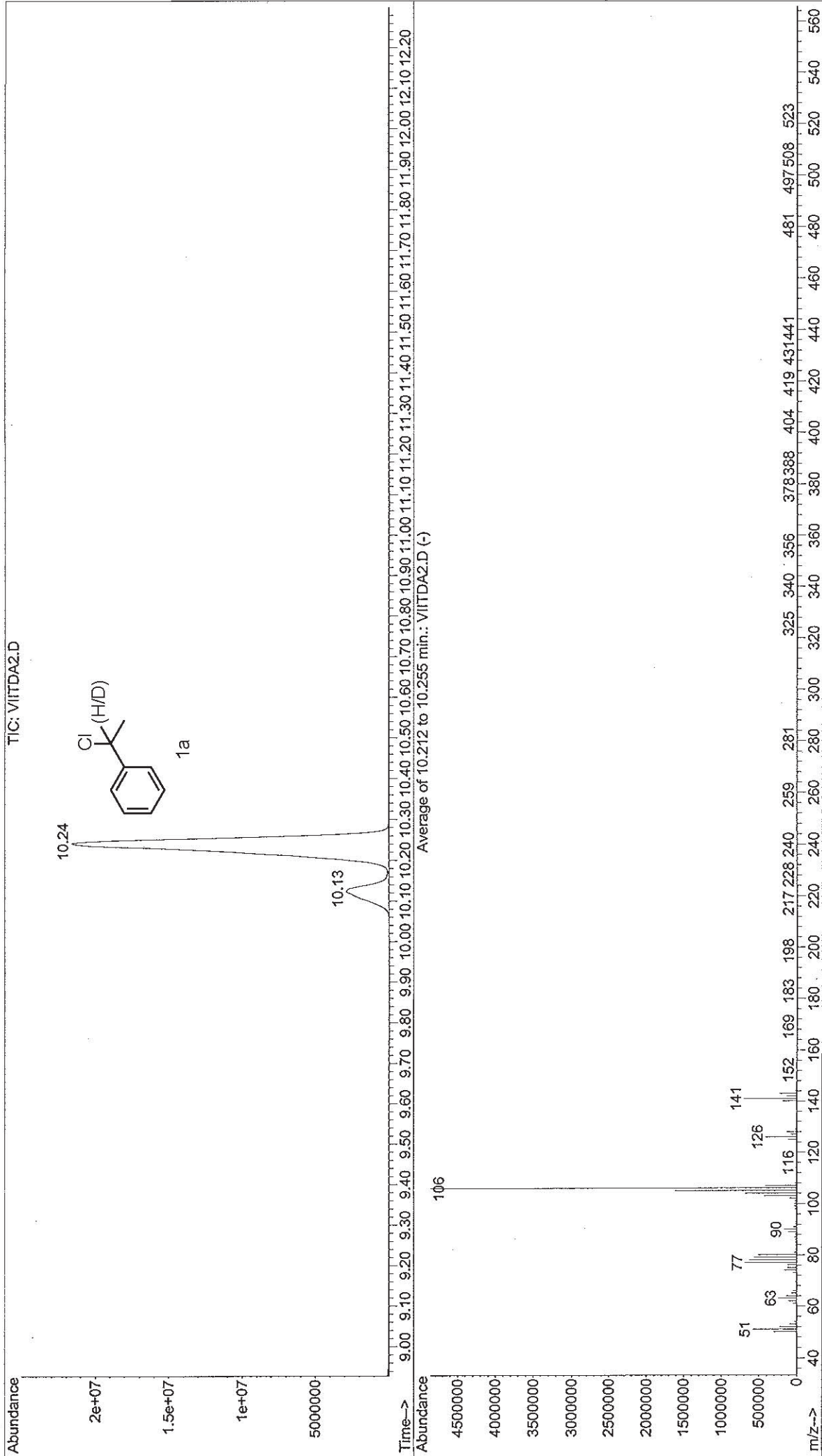
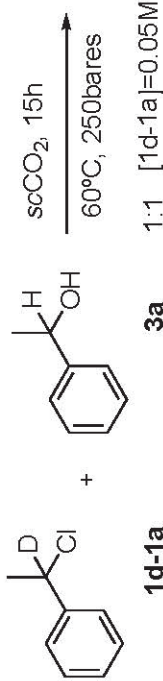
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Sample Name:

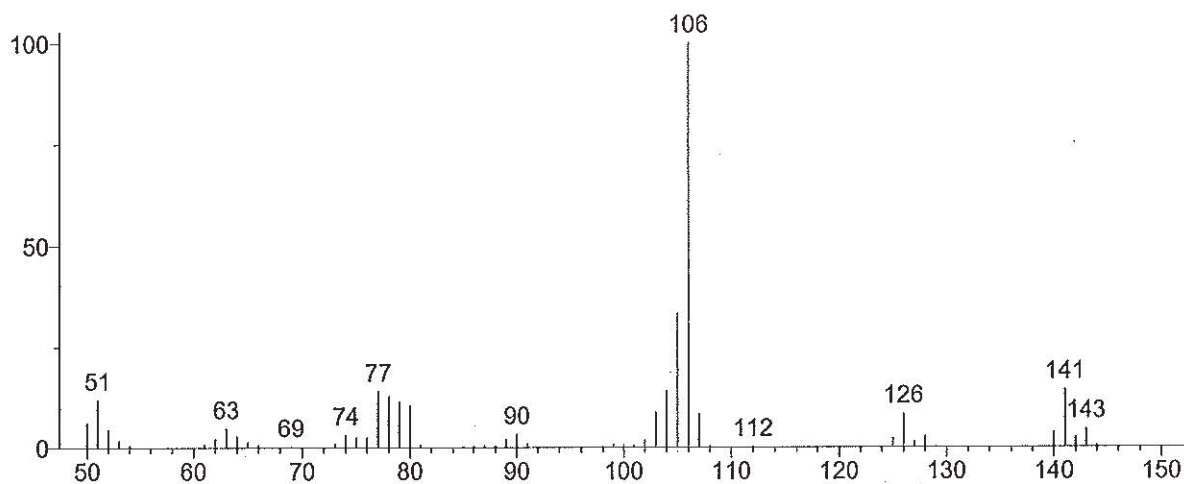
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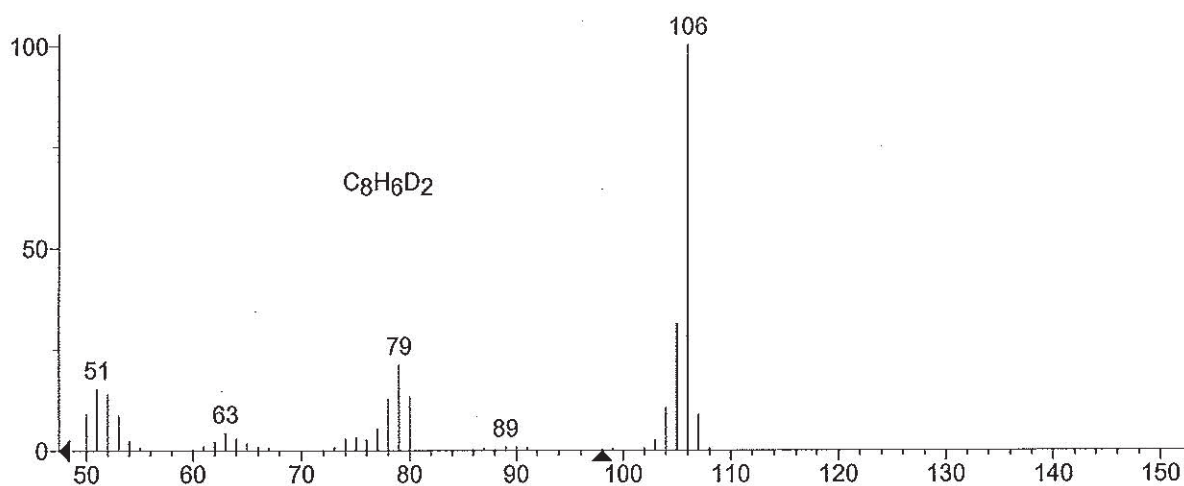




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Compound in Library Factor = -324



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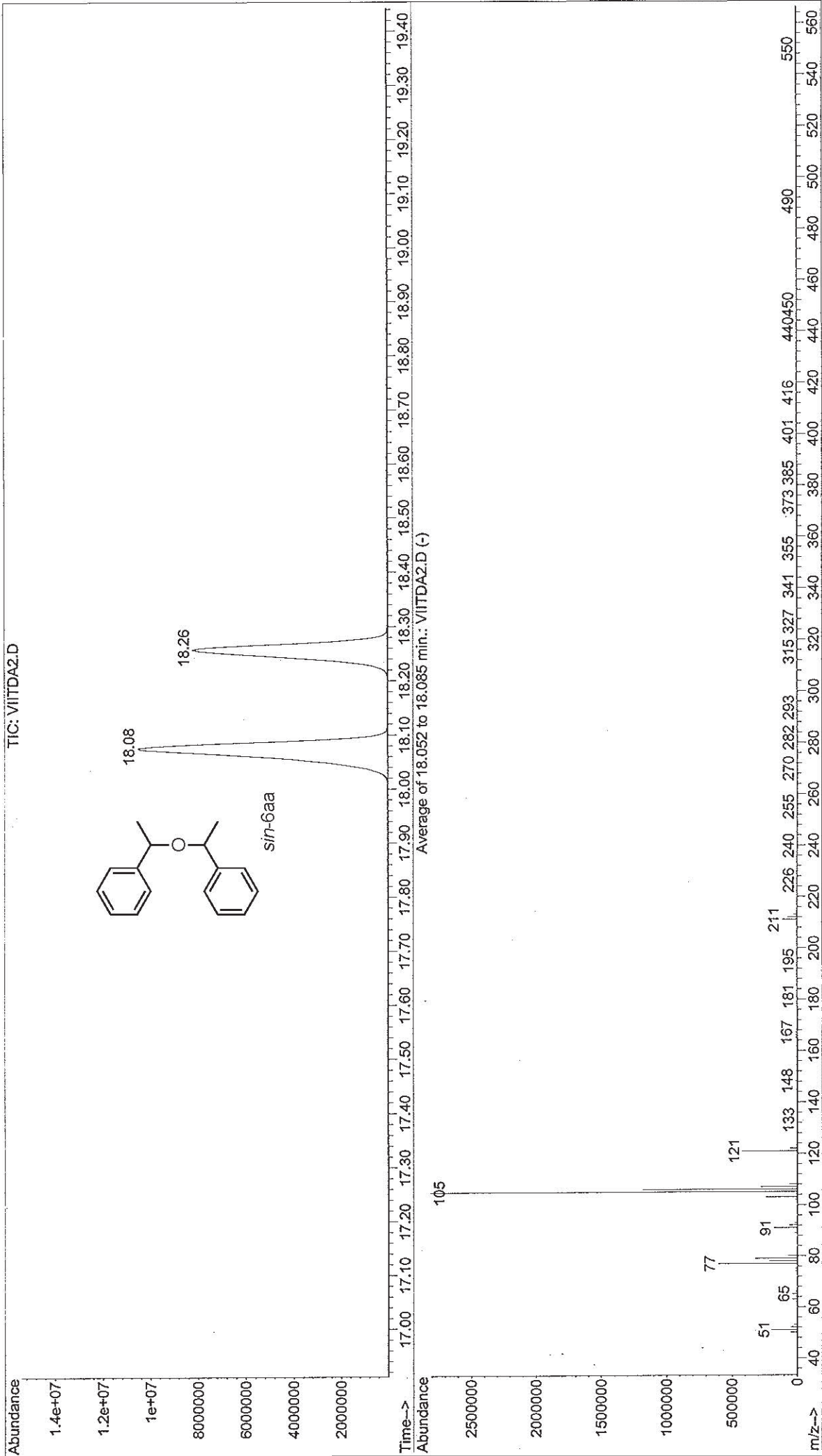
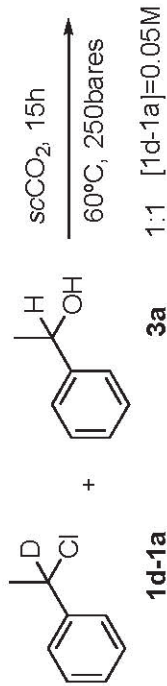
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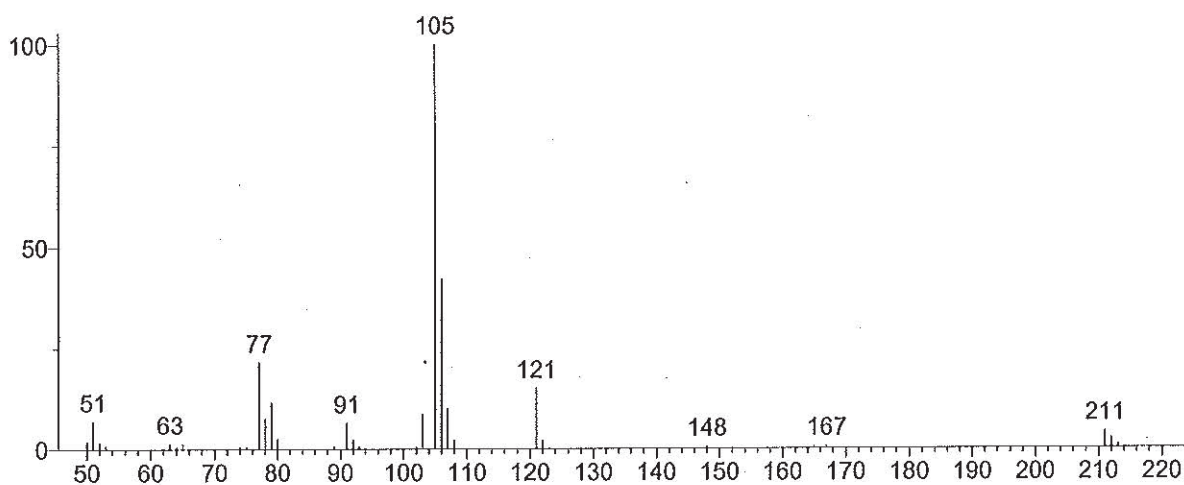
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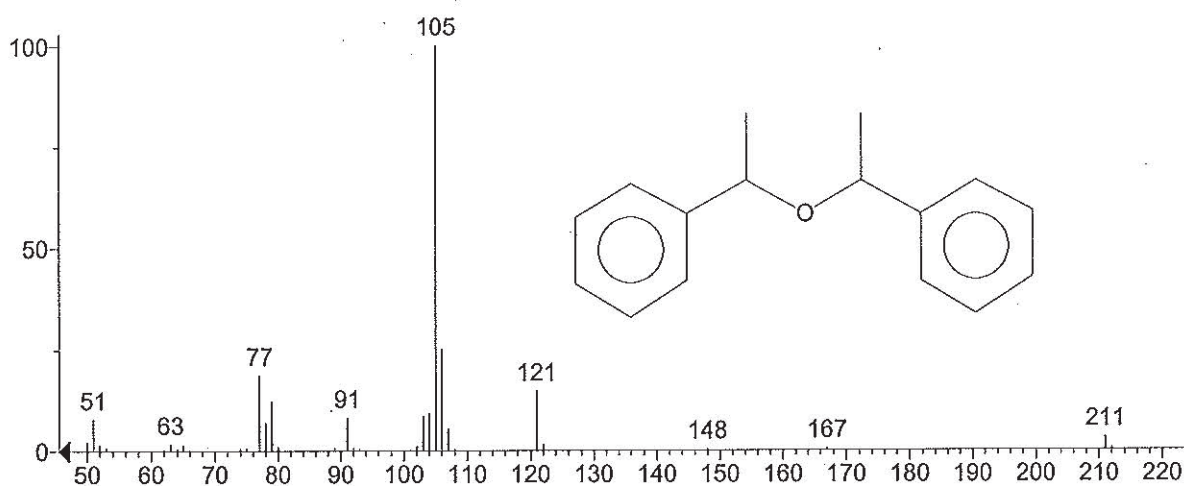




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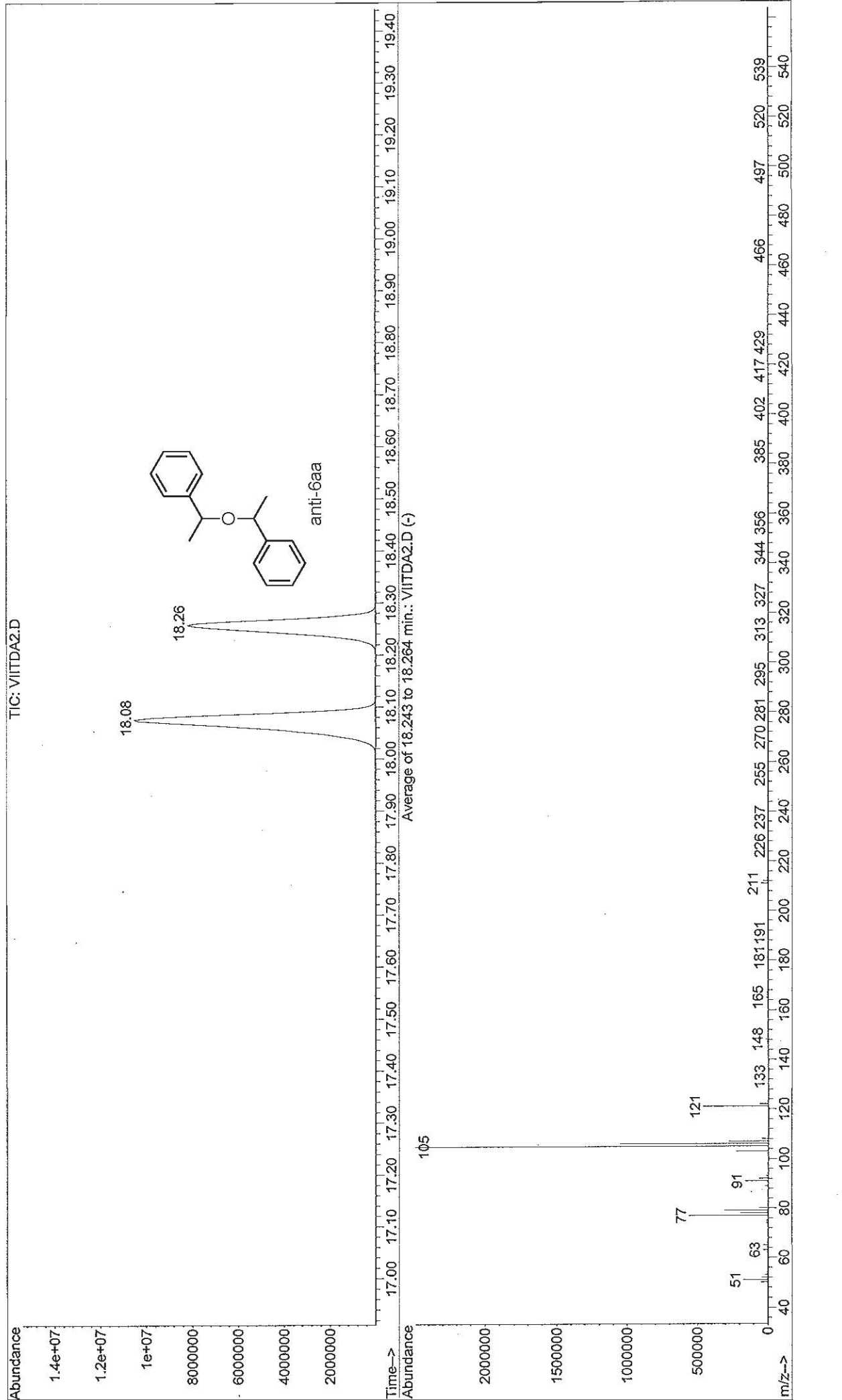
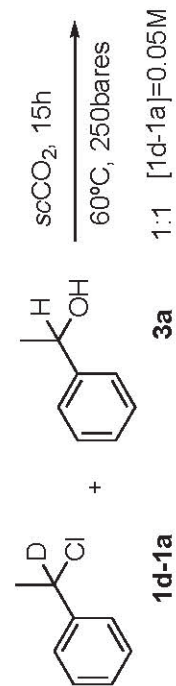
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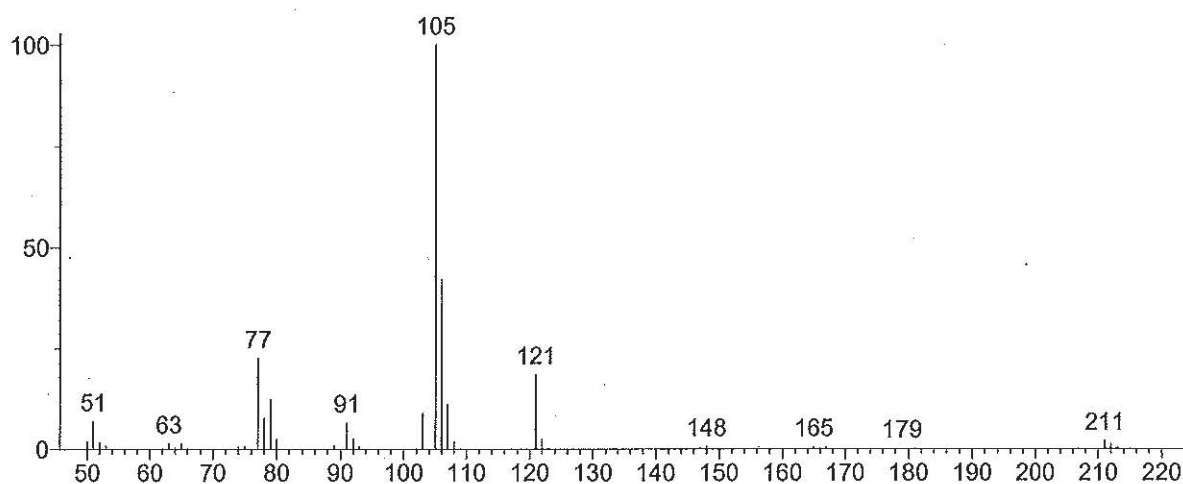
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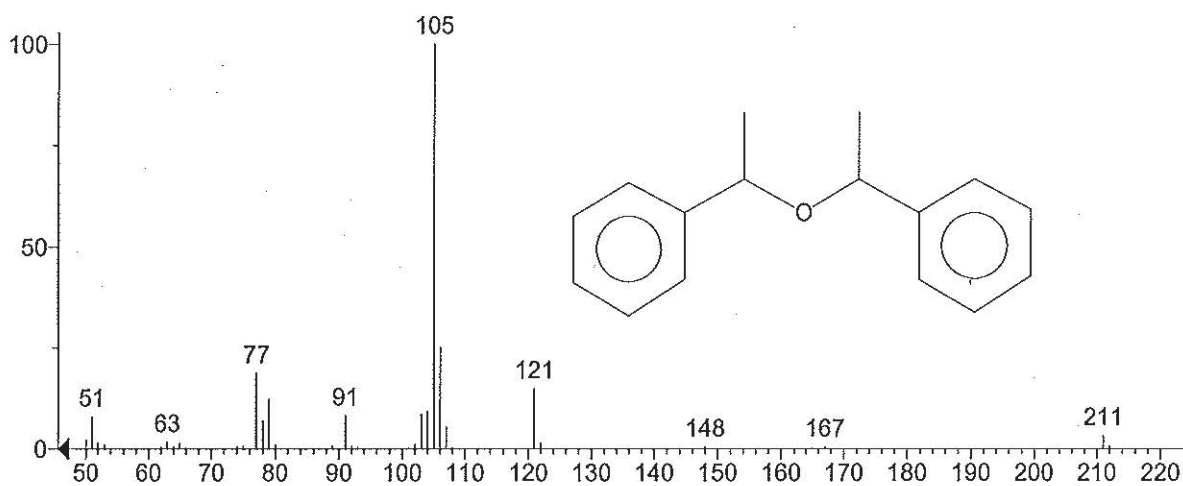




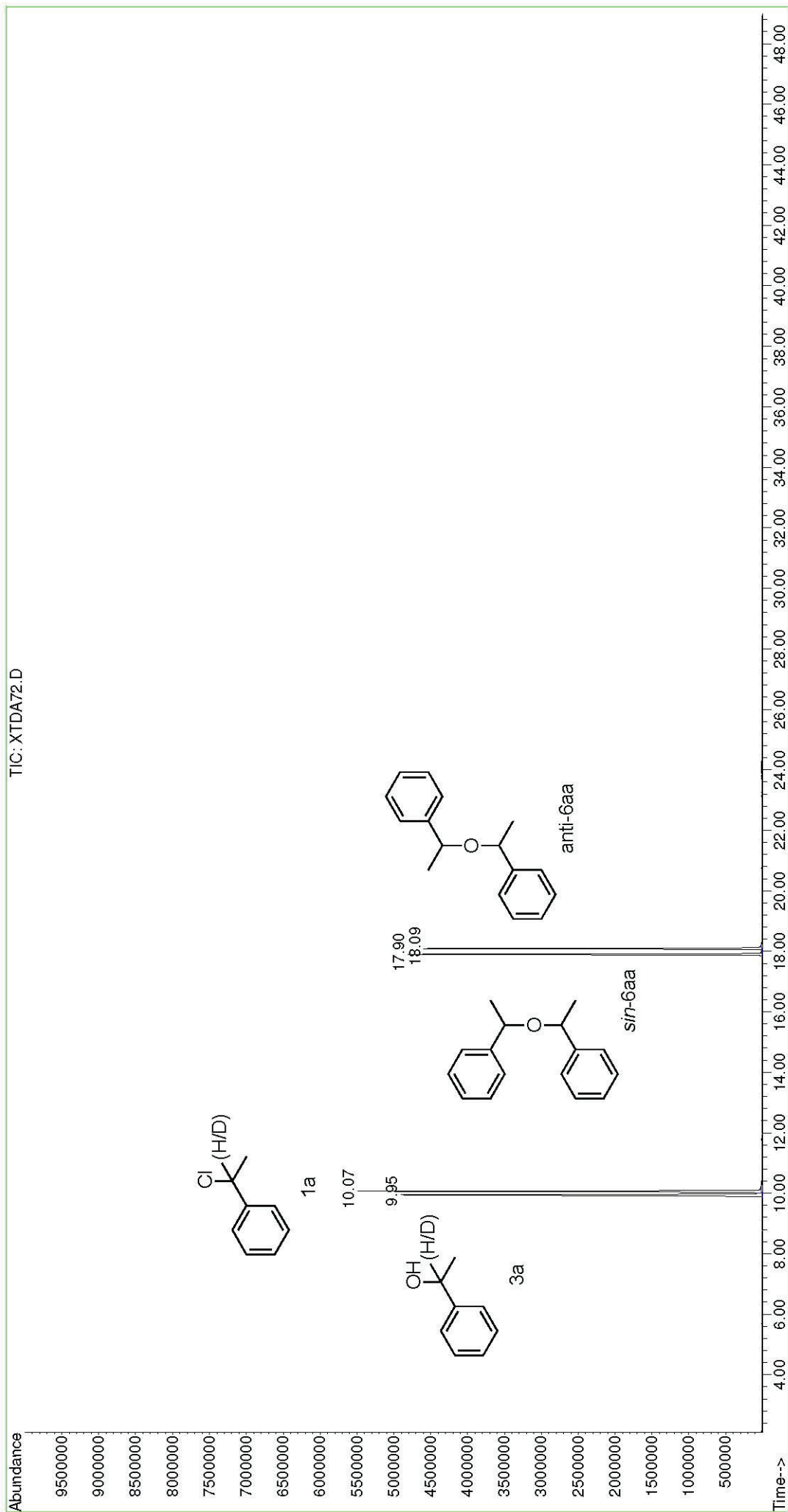
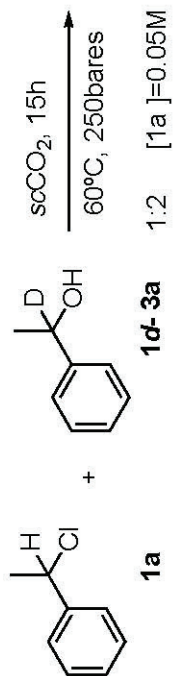
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Compound in Library Factor = -122



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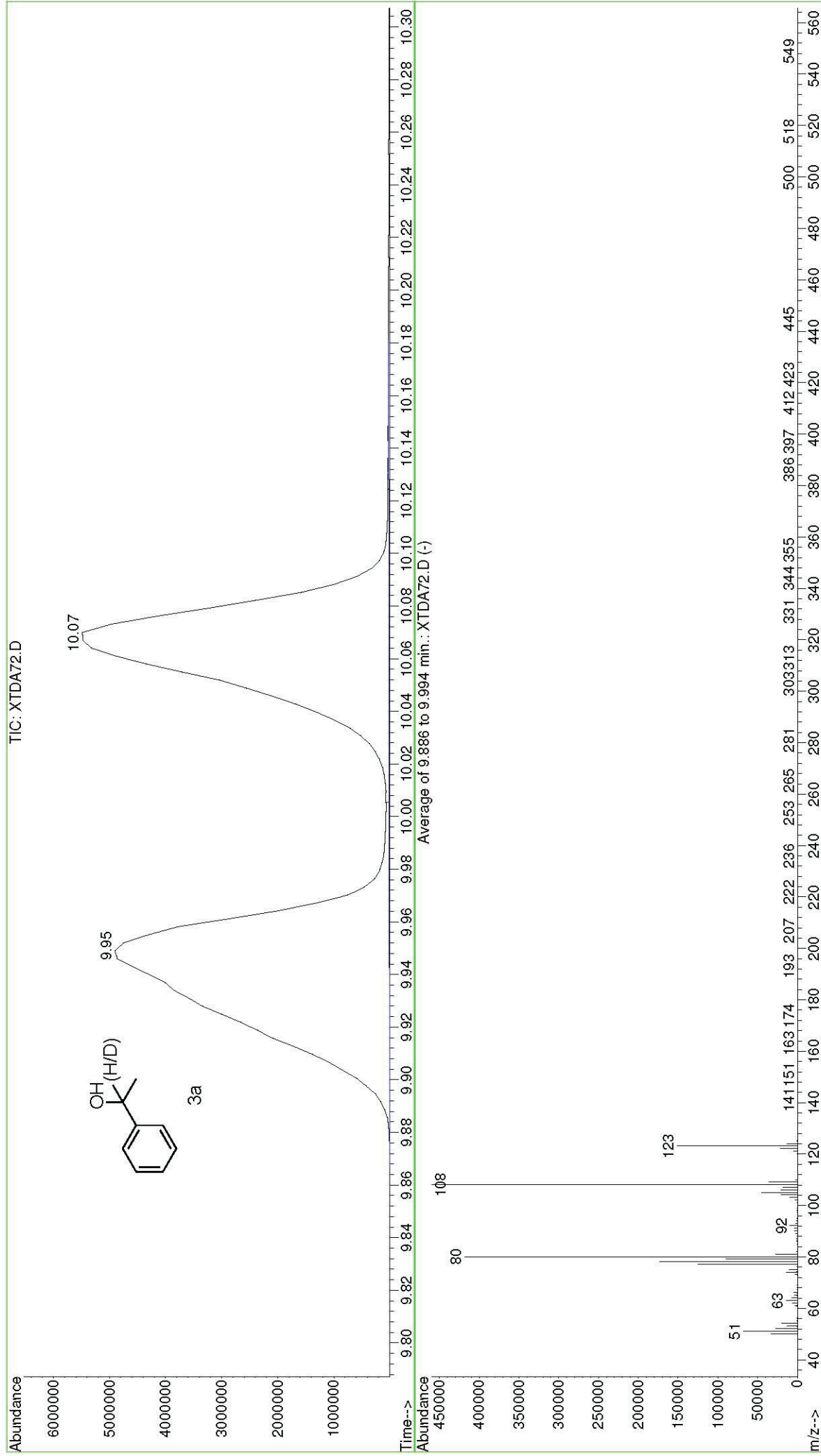
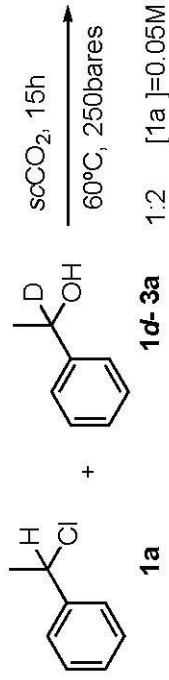
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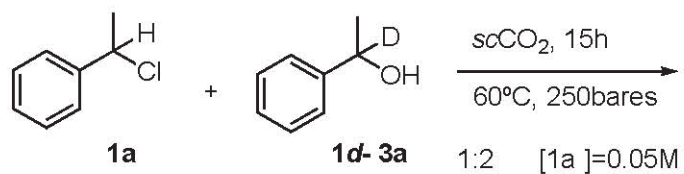
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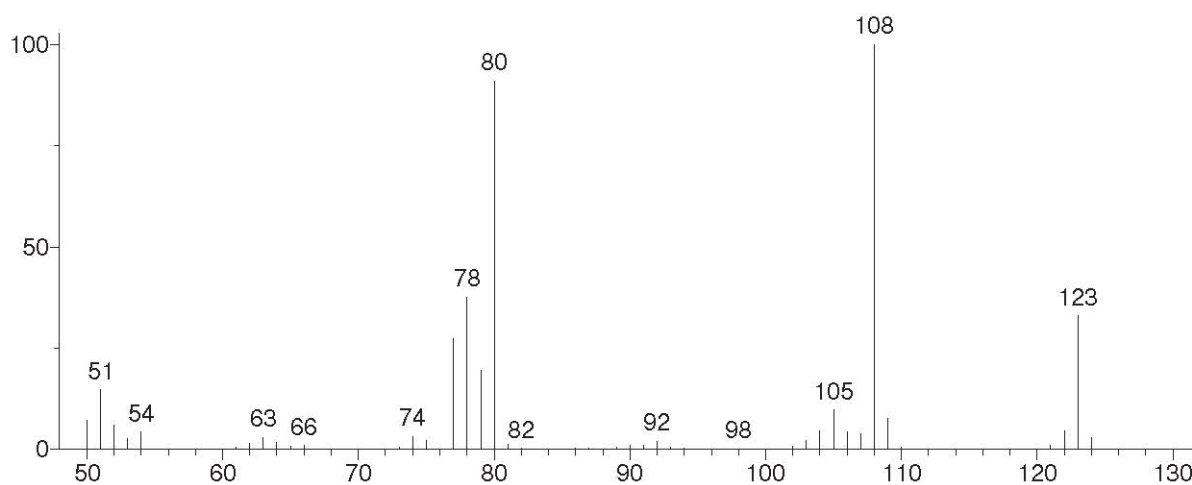
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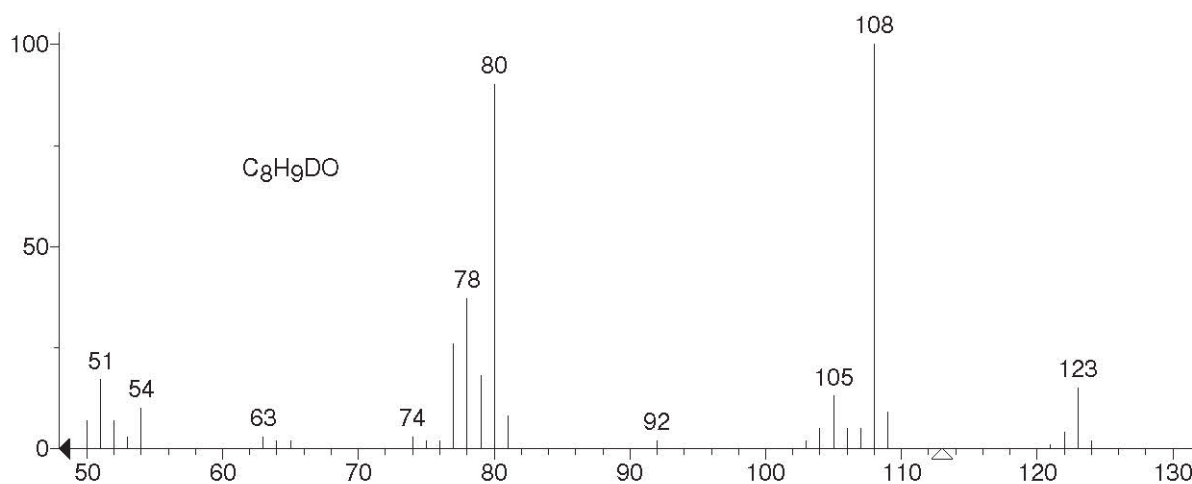




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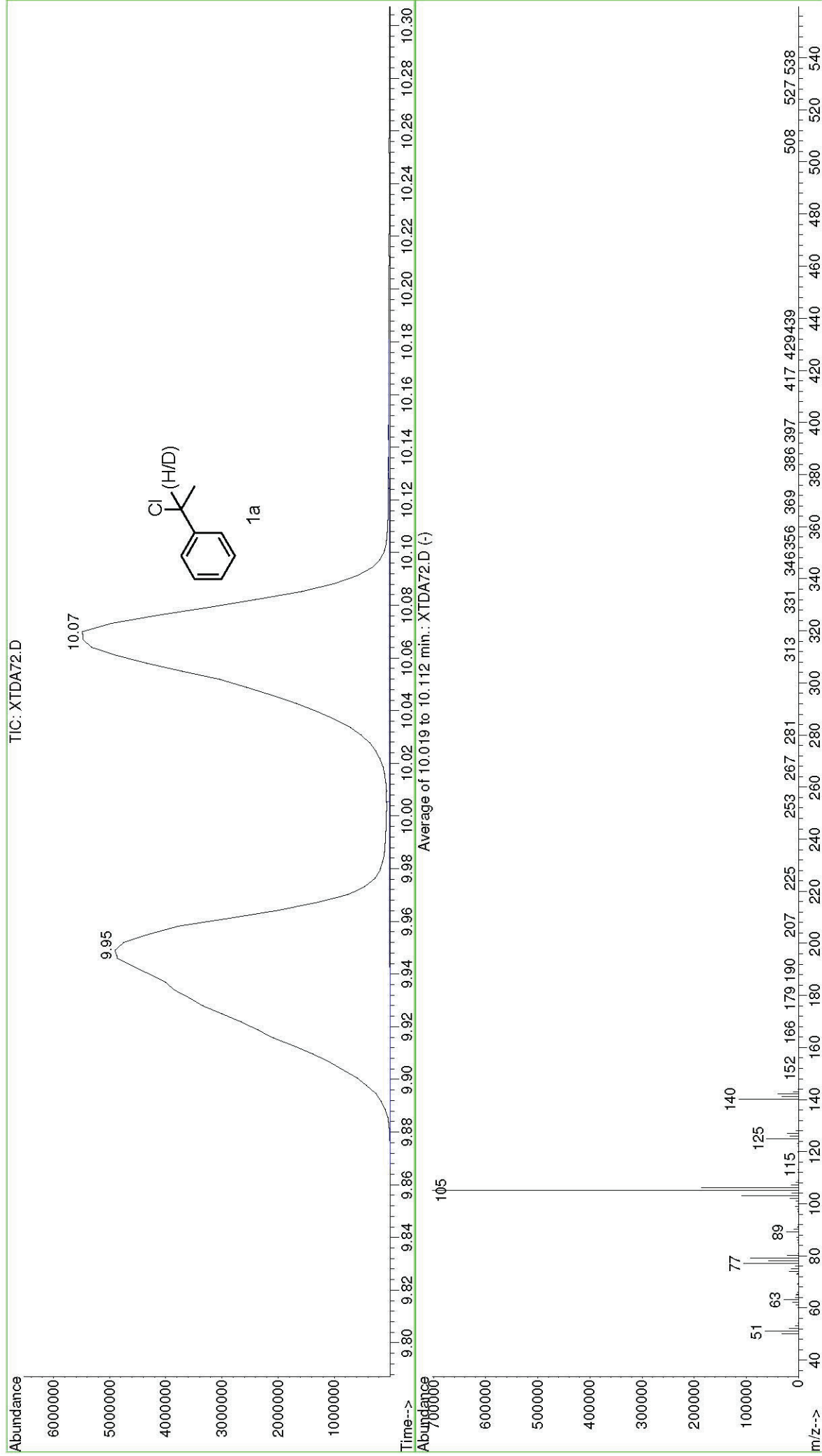
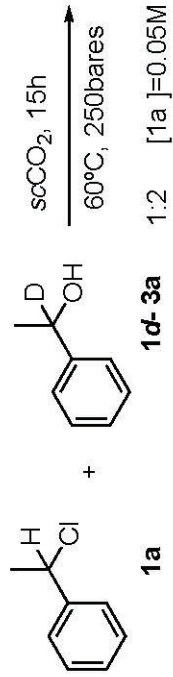
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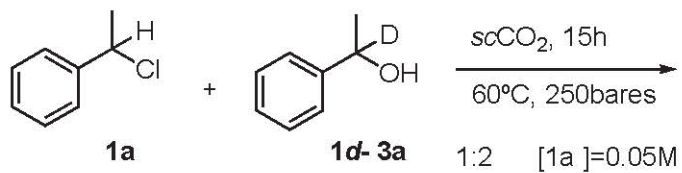
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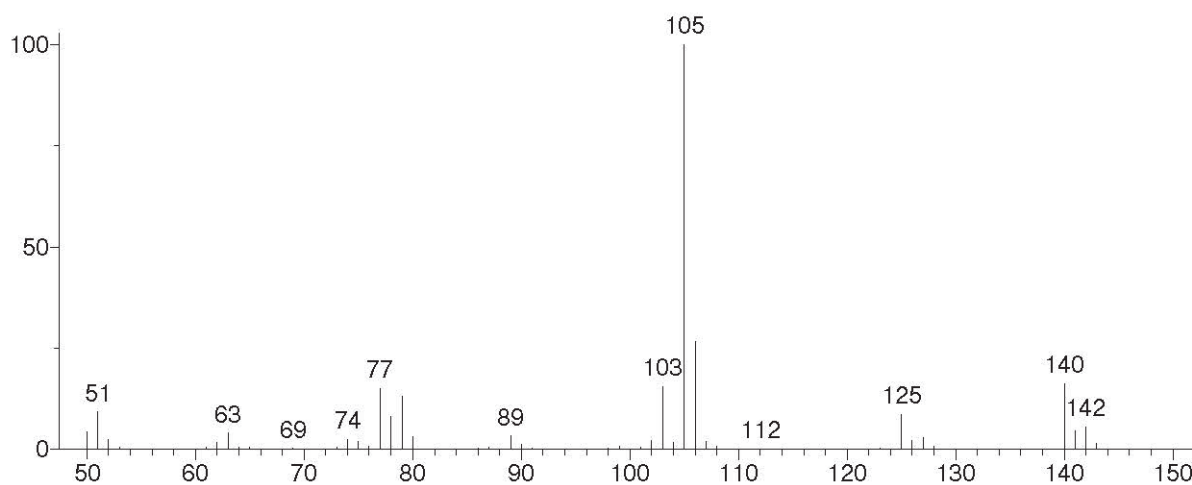
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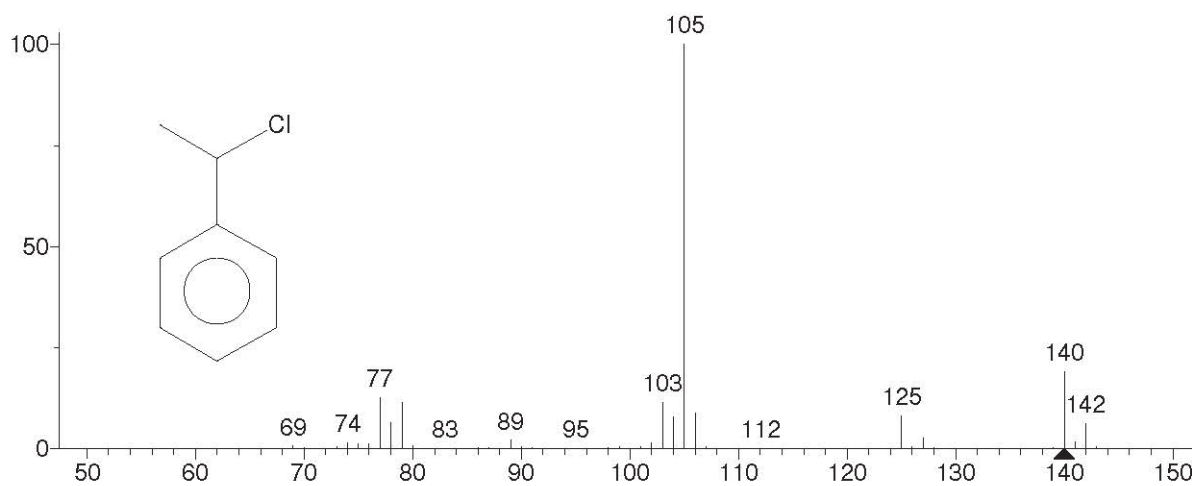




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Compound in Library Factor = -229

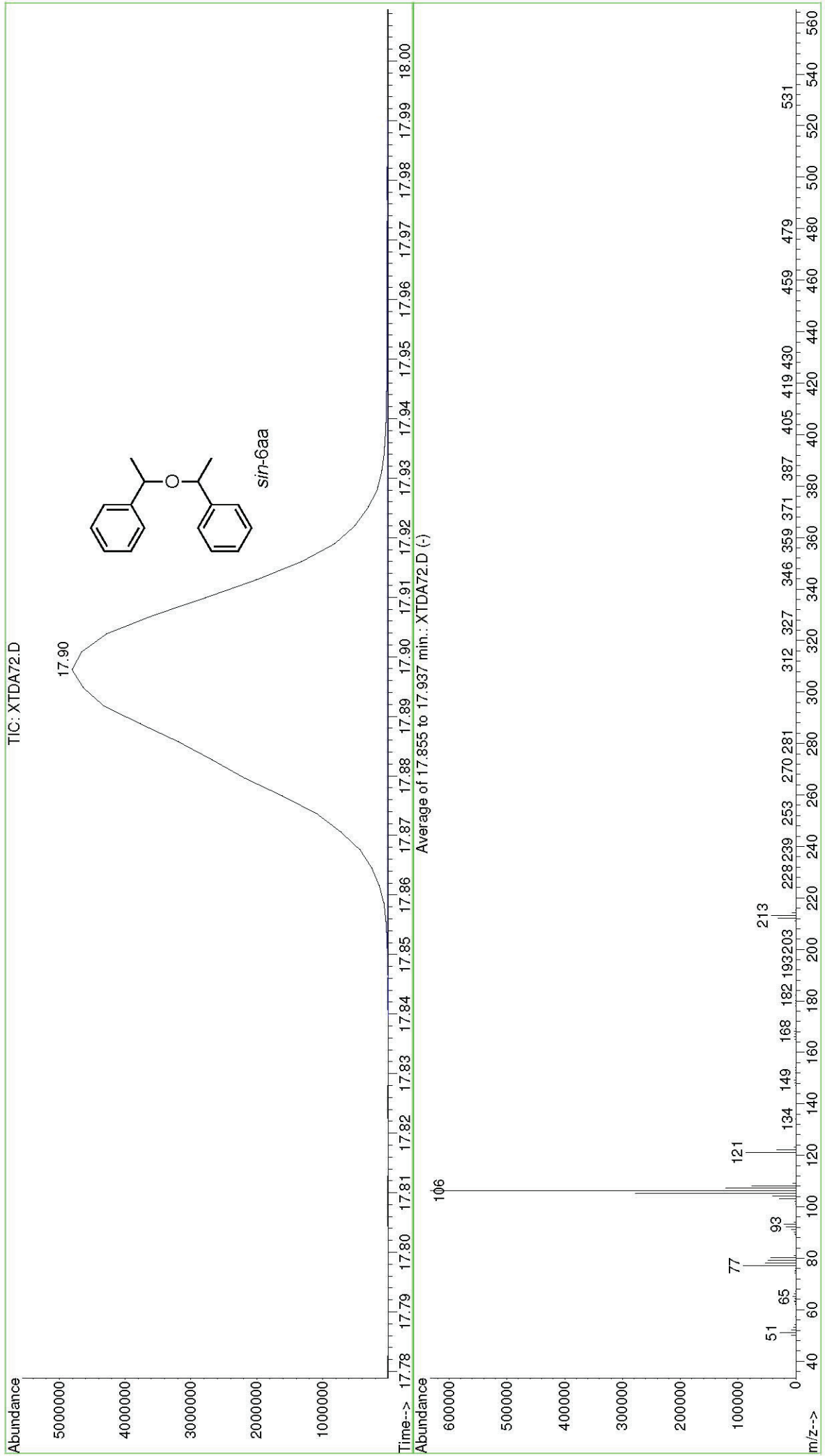
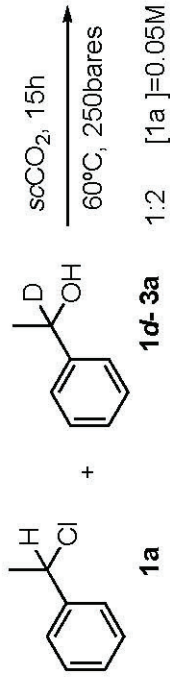


Hit 1 : Benzene, (1-chloroethyl)-  
C<sub>8</sub>H<sub>9</sub>Cl; MF: 835; RMF: 837; Prob 21.3%; CAS: 672-65-1; Lib: wiley7n; ID: 35469.

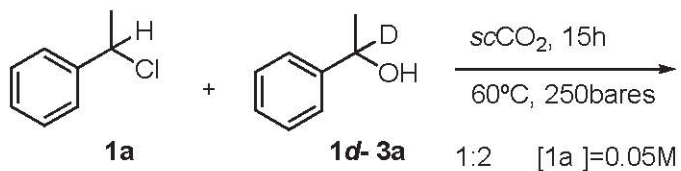


File : D:\ASENSIO\THAIS\XTDA72.D

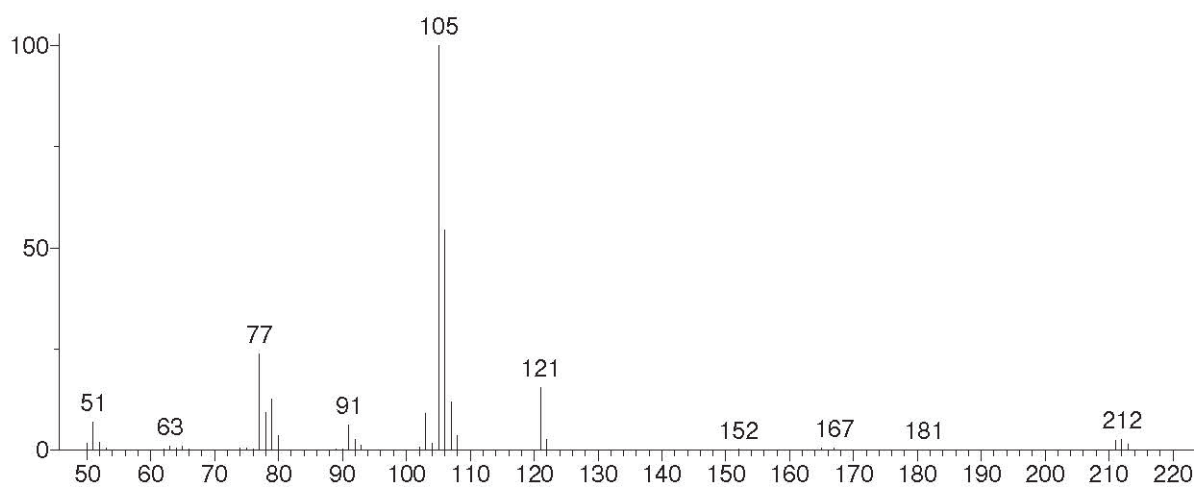
Operator :  
Acquired : 29 Jan 2014 14:26 using AcqMethod THAIS  
Instrument : Instrumenten  
Sample Name :  
Misc Info :  
Vial Number: 8



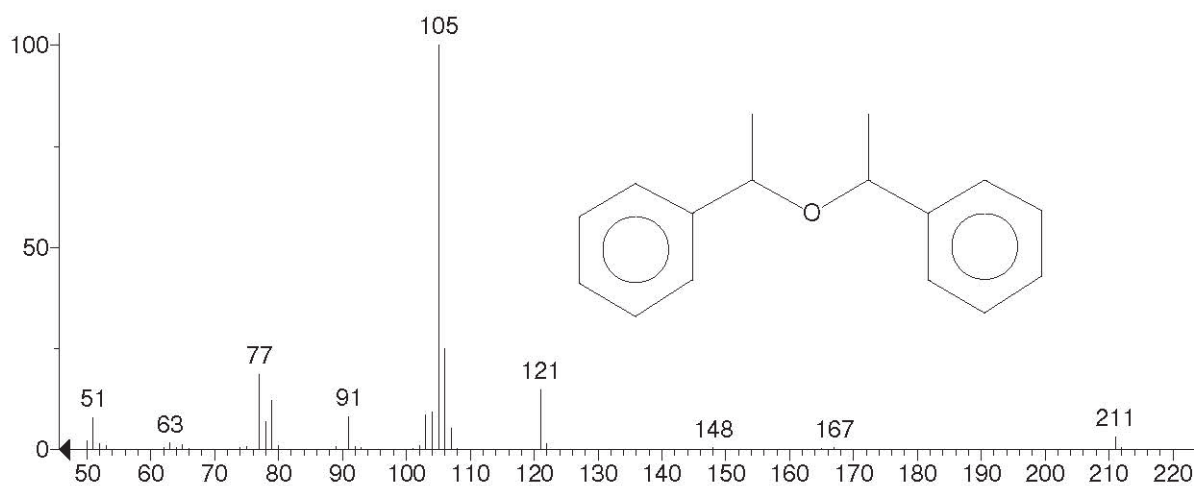




Unknown: Average of 17.862 to 17.928 min.: XTDA72.D  
Compound in Library Factor = -898



Hit 1 : Benzene, 1,1'-(oxydiethylidene)bis-  
C<sub>16</sub>H<sub>18</sub>O; MF: 810; RMF: 817; Prob 51.1%; CAS: 93-96-9; Lib: wiley7n; ID: 154842.



File : D:\ASENSIO\THAIS\XTDA72.D

Operator :

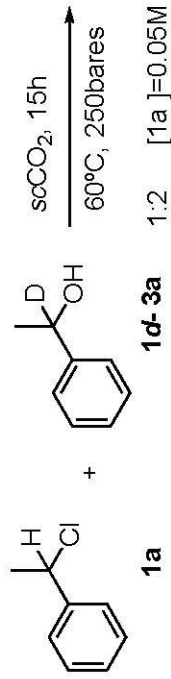
Acquired : 29 Jan 2014 14:26 using AcqMethod THAIS

Instrument : Instrument

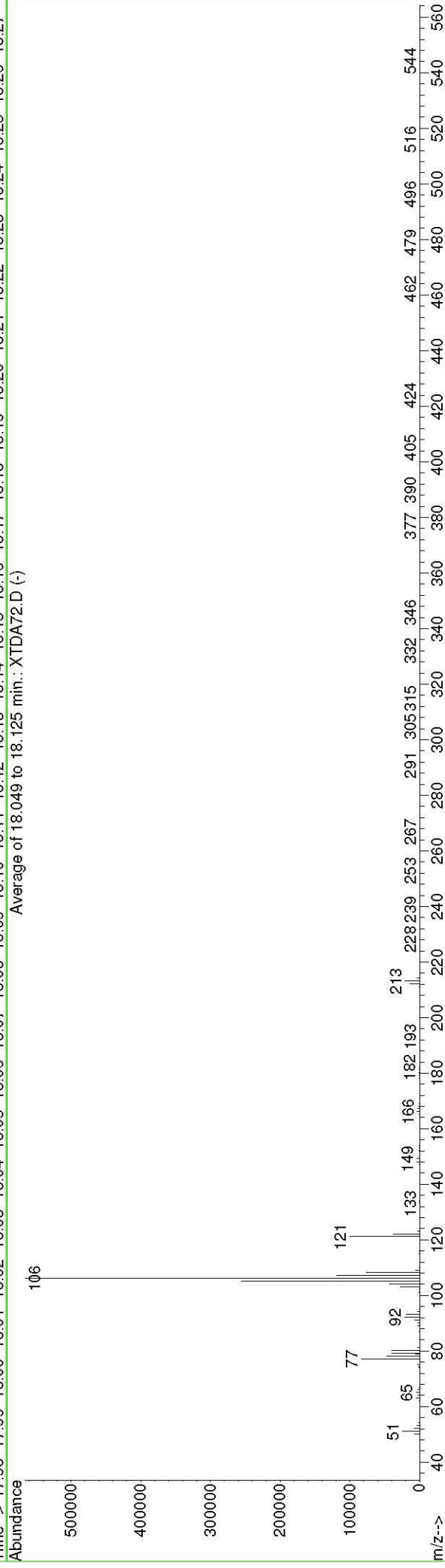
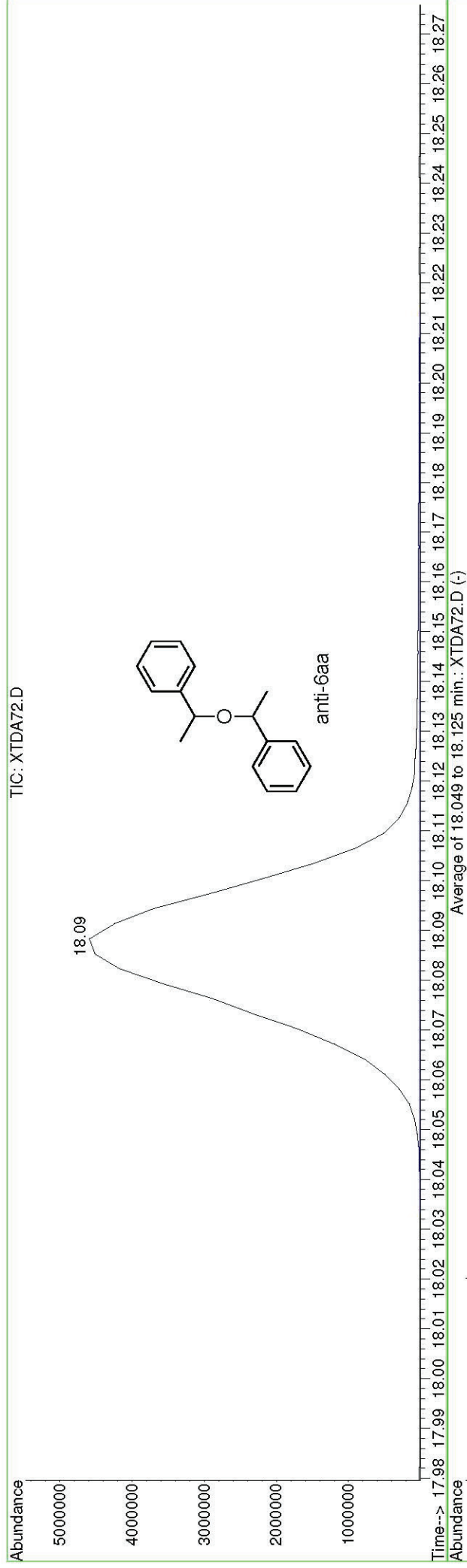
Sample Name:

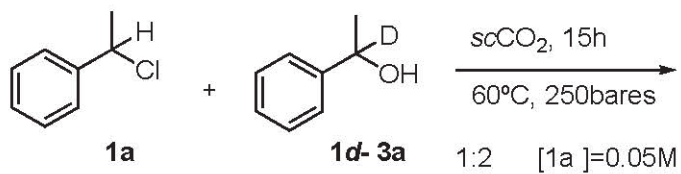
Misc Info :

Vial Number: 8

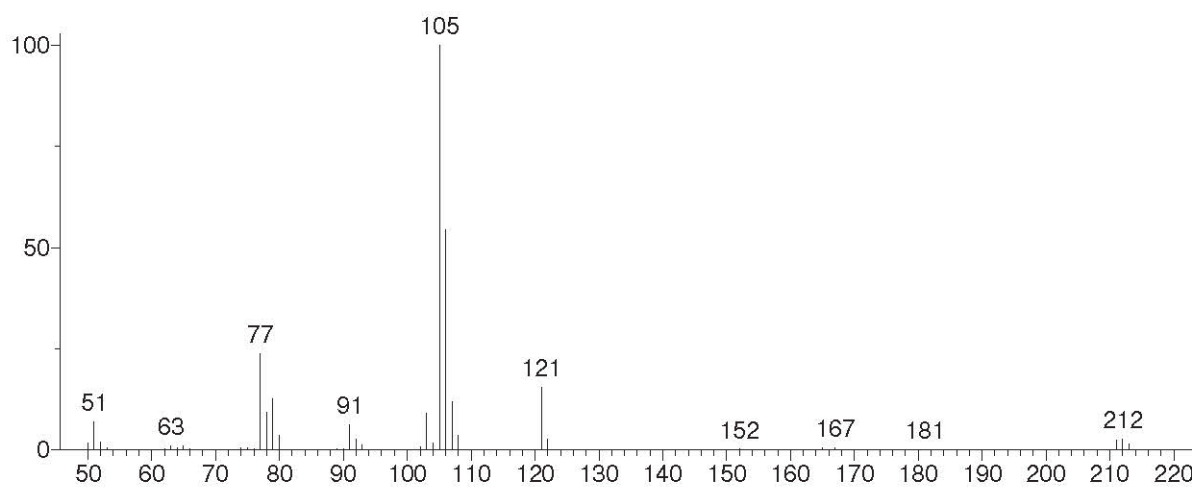


TIC: XTDA72.D

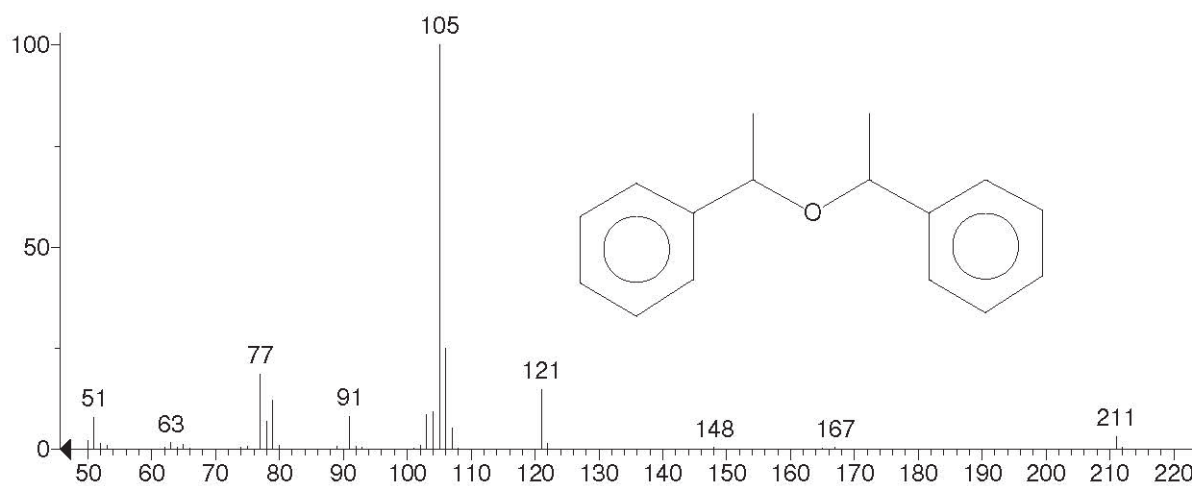




Unknown: Average of 18.055 to 18.128 min.: XTDA72.D  
Compound in Library Factor = -819



Hit 1 : Benzene, 1,1'-(oxydiethylidene)bis-  
C<sub>16</sub>H<sub>18</sub>O; MF: 810; RMF: 817; Prob 51.1%; CAS: 93-96-9; Lib: wiley7n; ID: 154842.



File : F:\THAIS\VTIDA198A.D

Operator :

Acquired : 21 May 2013 14:55

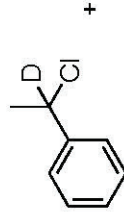
Instrument : Instrument

Sample Name:

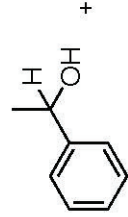
Misc Info :

Vial Number: 12

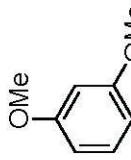
using AcqMethod THAIS



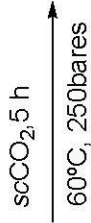
**1d-1a**



**3a**

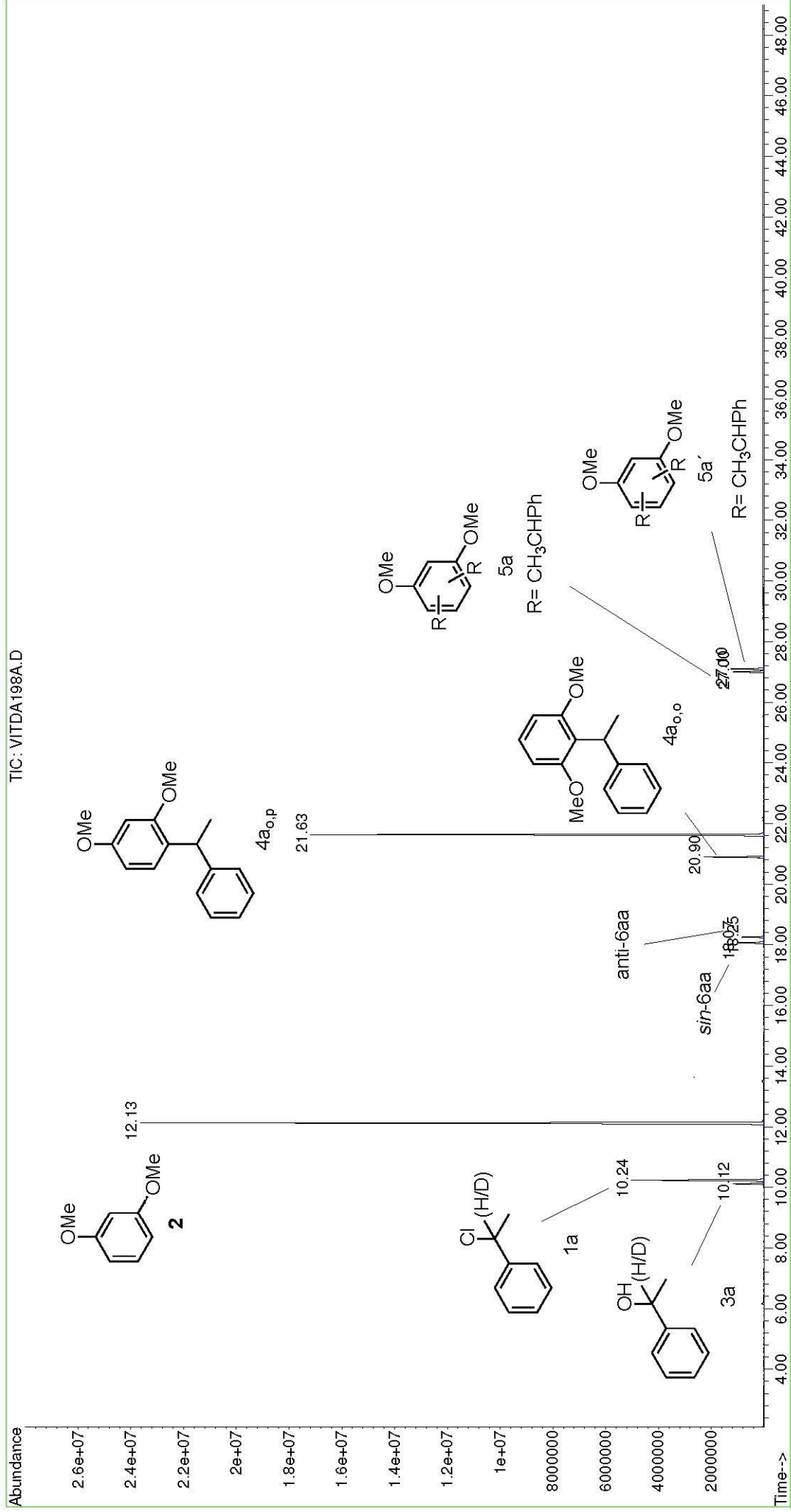


**2**



1:1:4 [1d-1a]=0.05M

TIC: VTIDA198A.D



File : F:\THAIS\VITDA198A.D

Operator :

Acquired : 21 May 2013 14:55

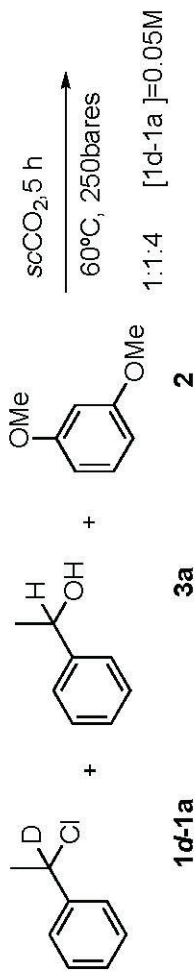
using AcqMethod THAIS

Instrument : Instrument

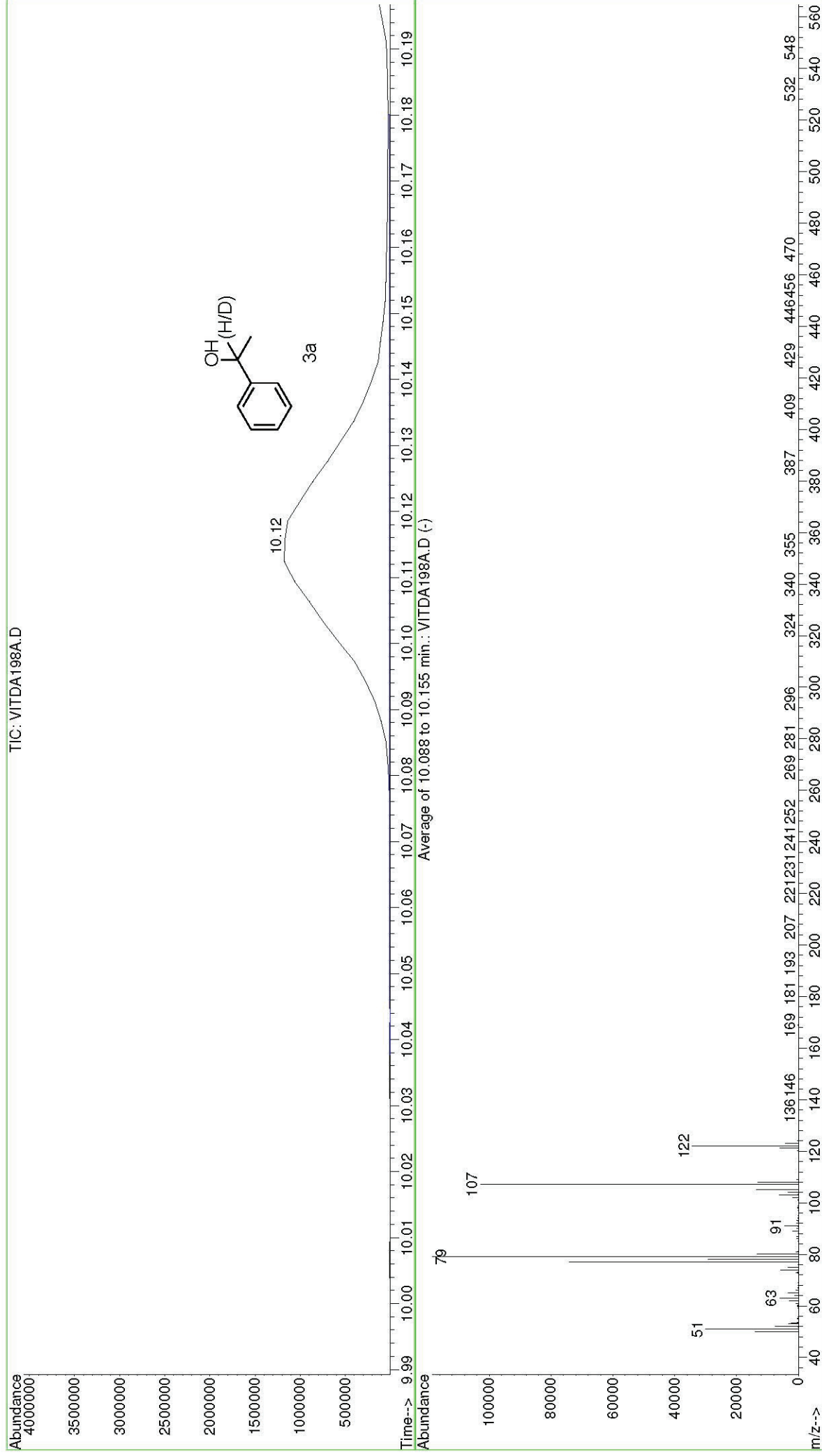
Sample Name:

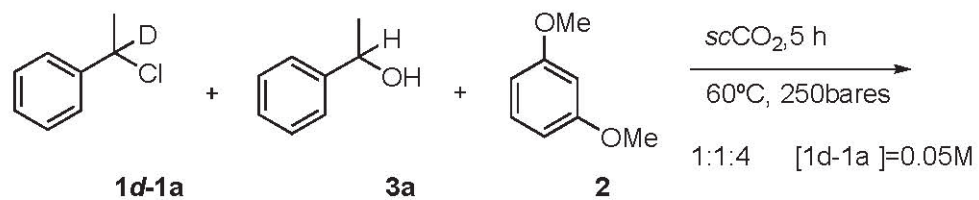
Misc Info :

Vial Number: 12

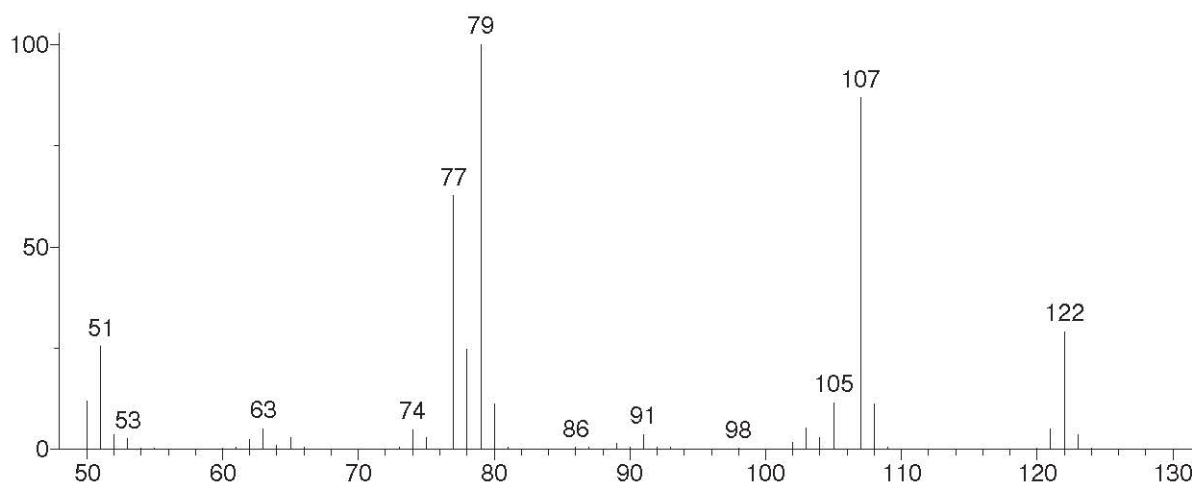


TIC: VITDA198A.D

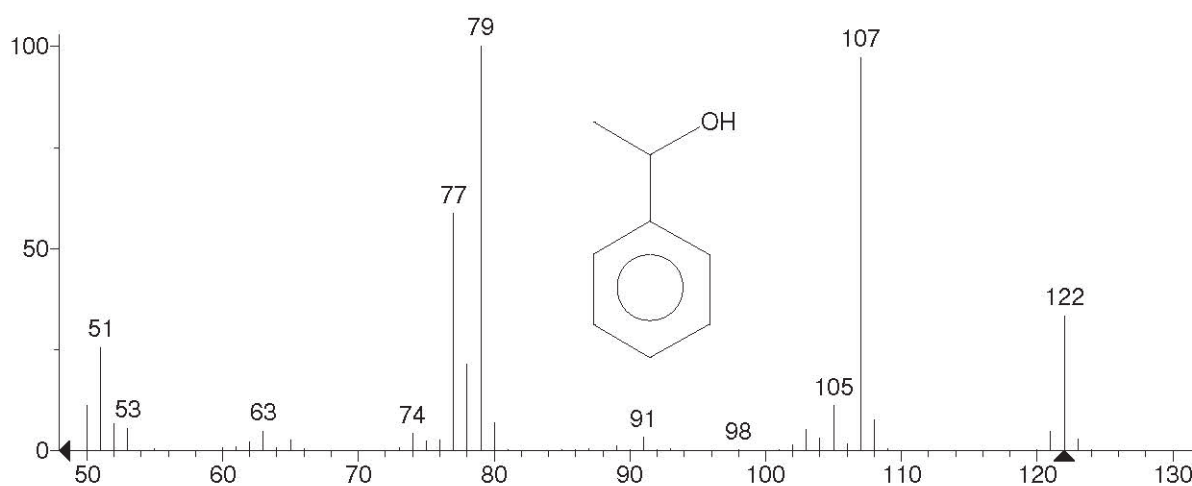




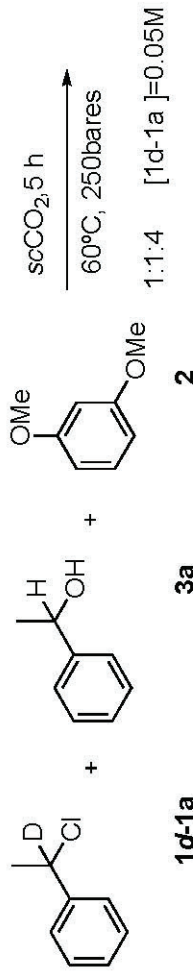
Unknown: Average of 10.088 to 10.155 min.: VITDA198A.D  
Compound in Library Factor = 116



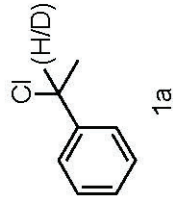
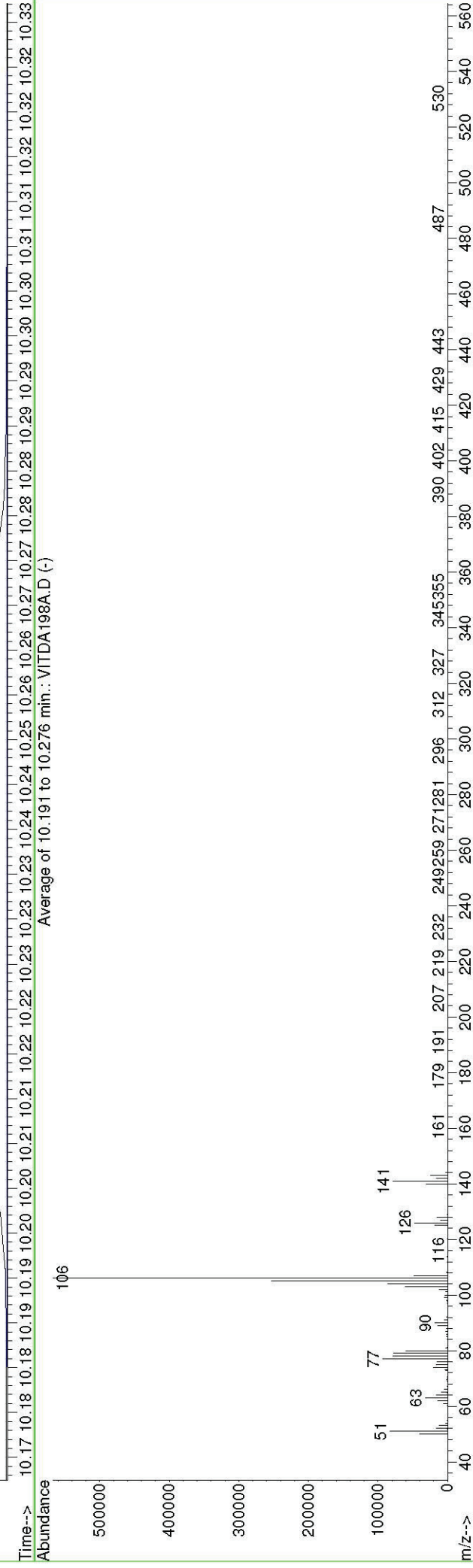
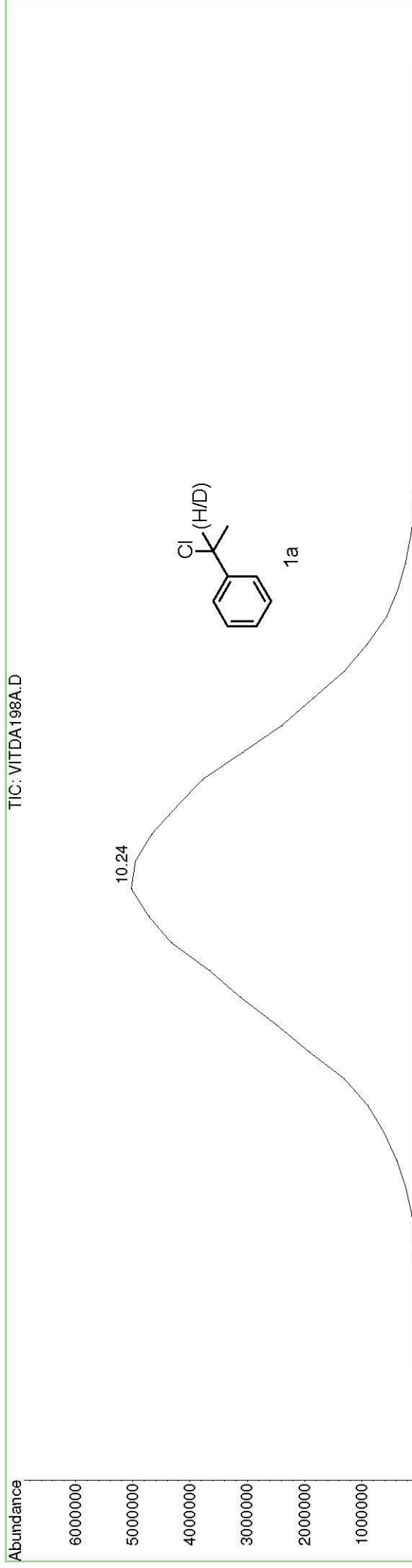
Hit 1 : Benzenemethanol, .alpha.-methyl-  
C<sub>8</sub>H<sub>10</sub>O; MF: 903; RMF: 903; Prob 49.9%; CAS: 98-85-1; Lib: replib; ID: 9674.



File : F:\THAIS\VITDA198A.D  
 Operator :  
 Acquired : 21 May 2013 14:55  
 Instrument : using AcqMethod THAIS  
 Sample Name : Instrument  
 Misc Info :  
 Vial Number: 12

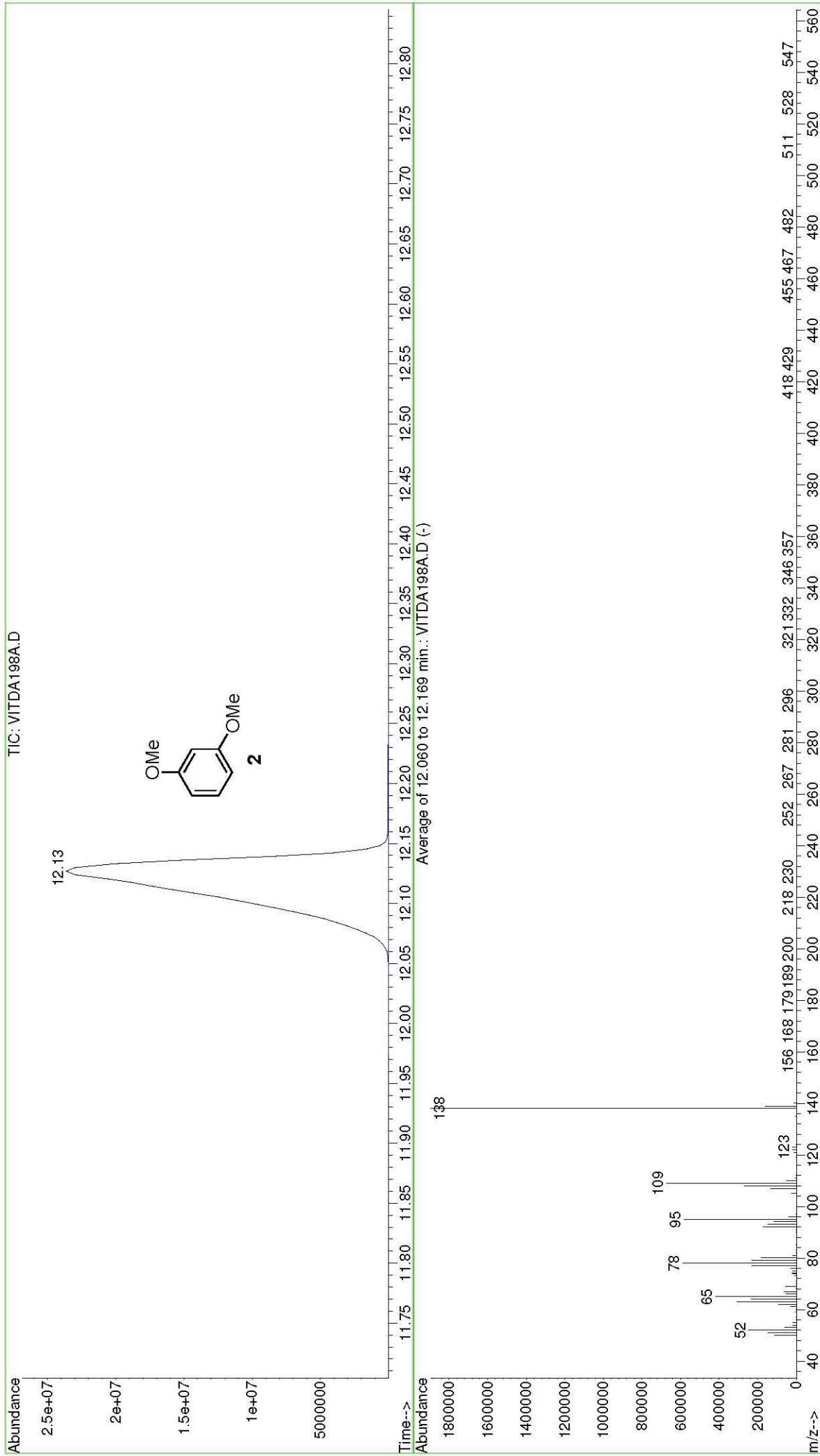
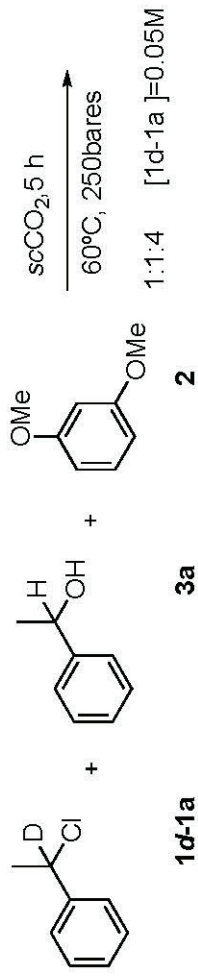


TIC: VITDA198A.D

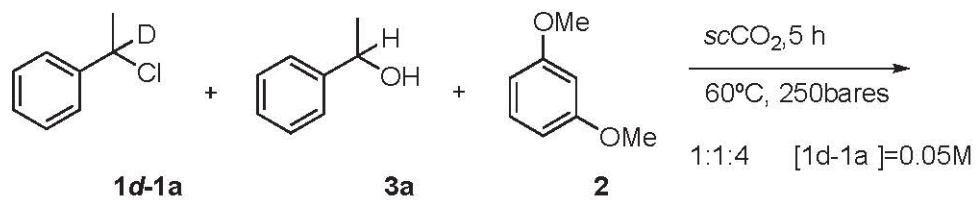




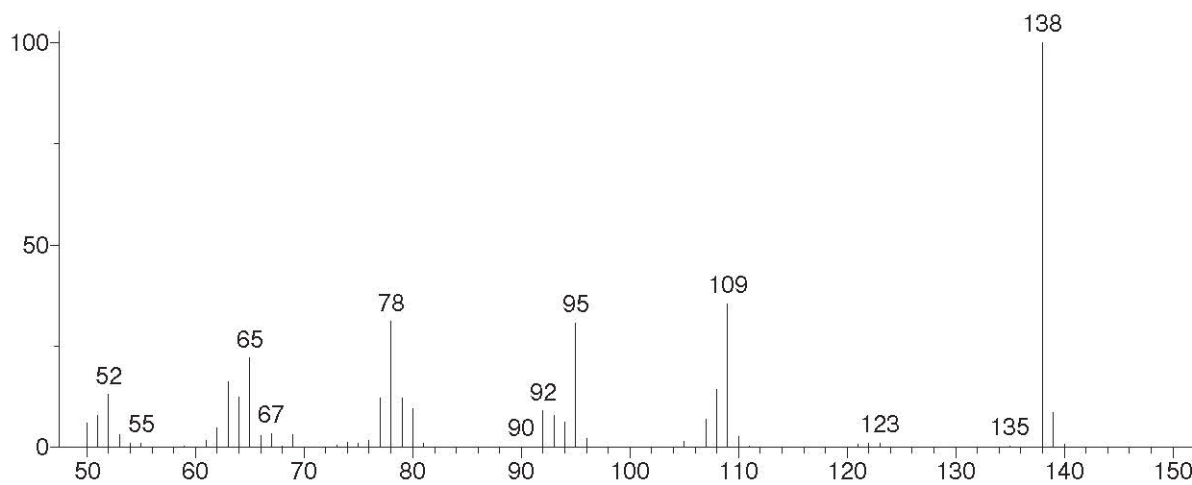
File : F:\THAIS\VITDA198A.D  
Operator :  
Acquired : 21 May 2013 14:55  
Instrument : using AcqMethod THAIS  
Sample Name : Instrument  
Misc Info :  
Vial Number: 12



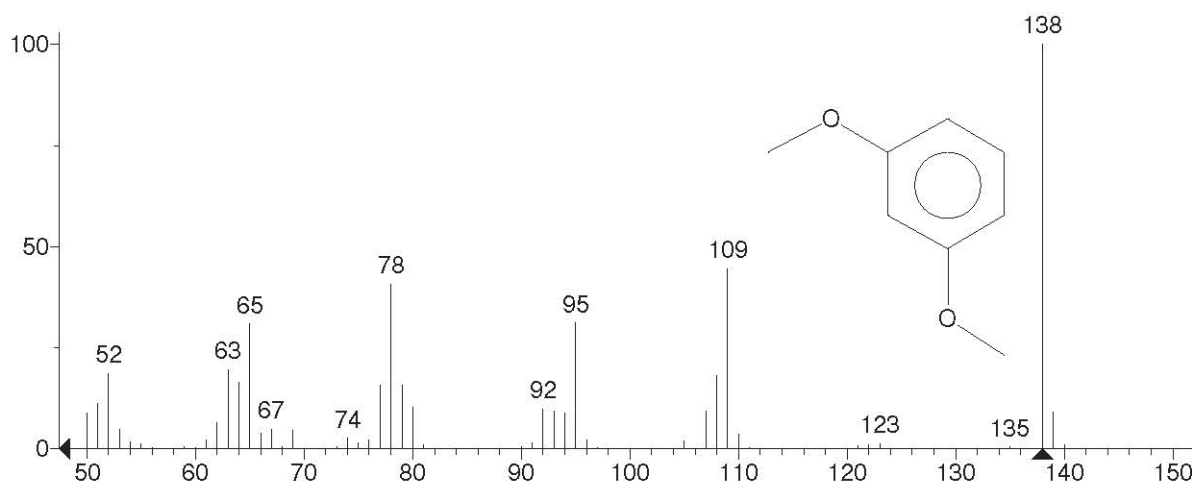




Unknown: Average of 12.060 to 12.169 min.: VITDA198A.D  
Compound in Library Factor = 513



Hit 1 : Benzene, 1,3-dimethoxy-  
C<sub>8</sub>H<sub>10</sub>O<sub>2</sub>; MF: 954; RMF: 954; Prob 57.6%; CAS: 151-10-0; Lib: replib; ID: 18631.



File : F:\THAIS\VITDA198A.D

Operator :

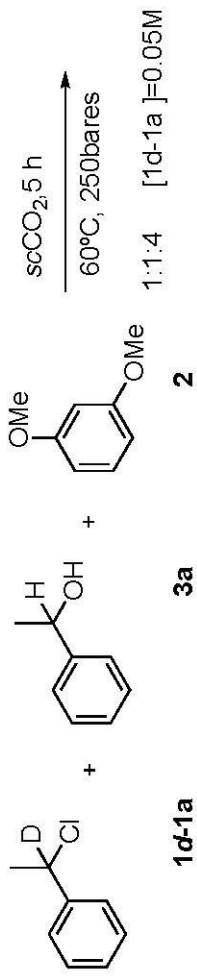
Acquired : 21 May 2013 14:55

Instrument : using AcqMethod THAIS

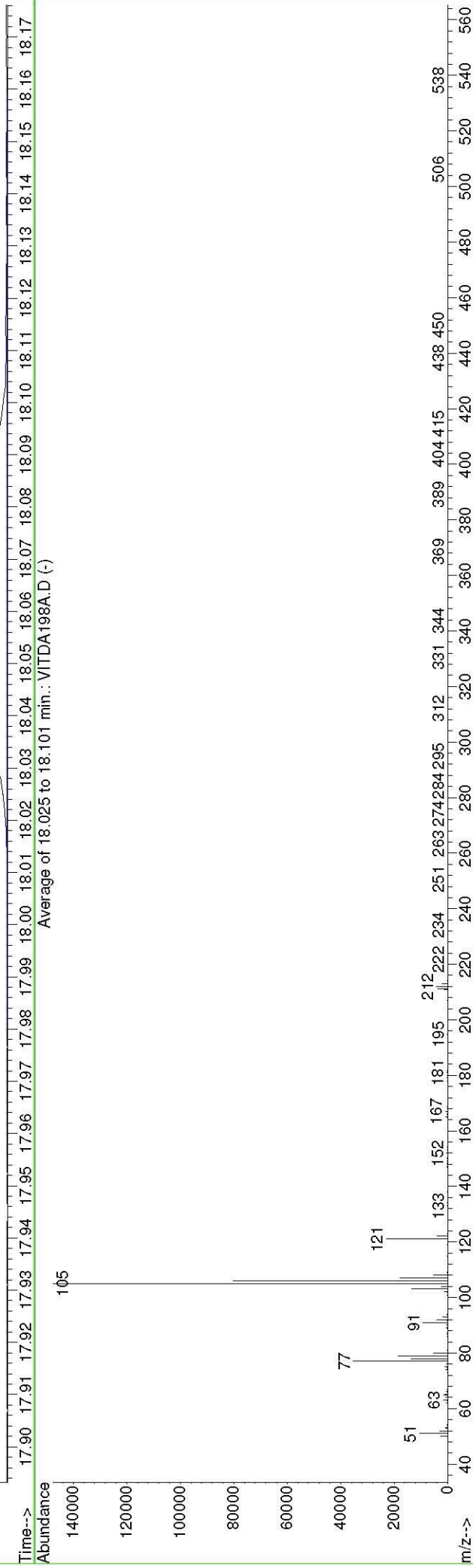
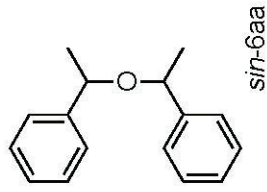
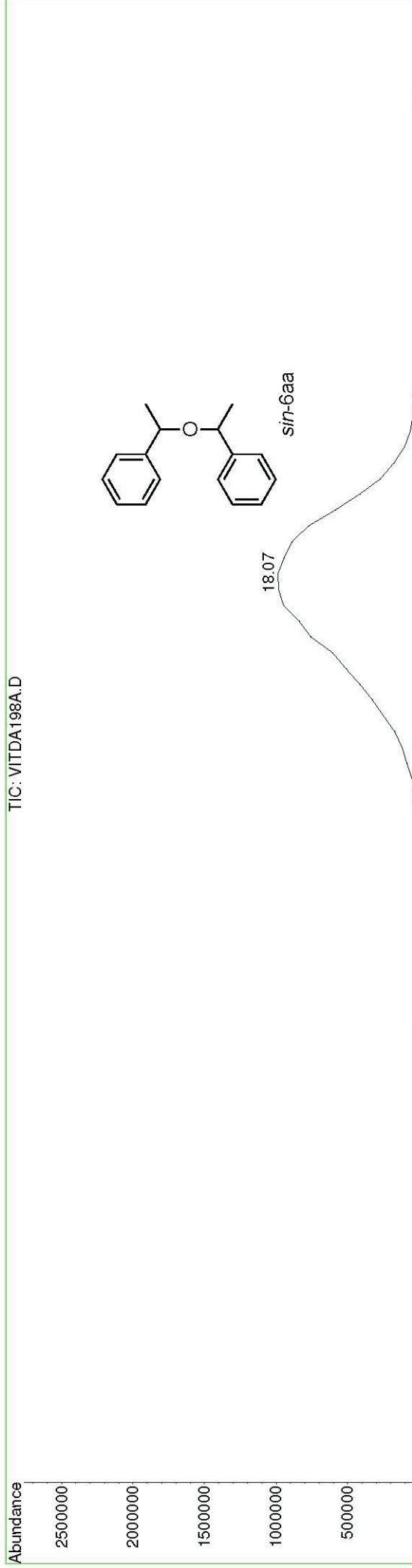
Sample Name:

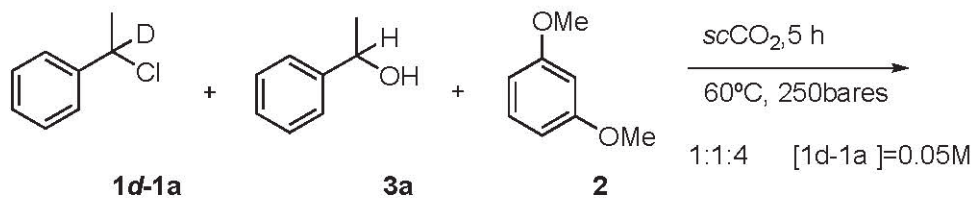
Misc Info :

Vial Number: 12

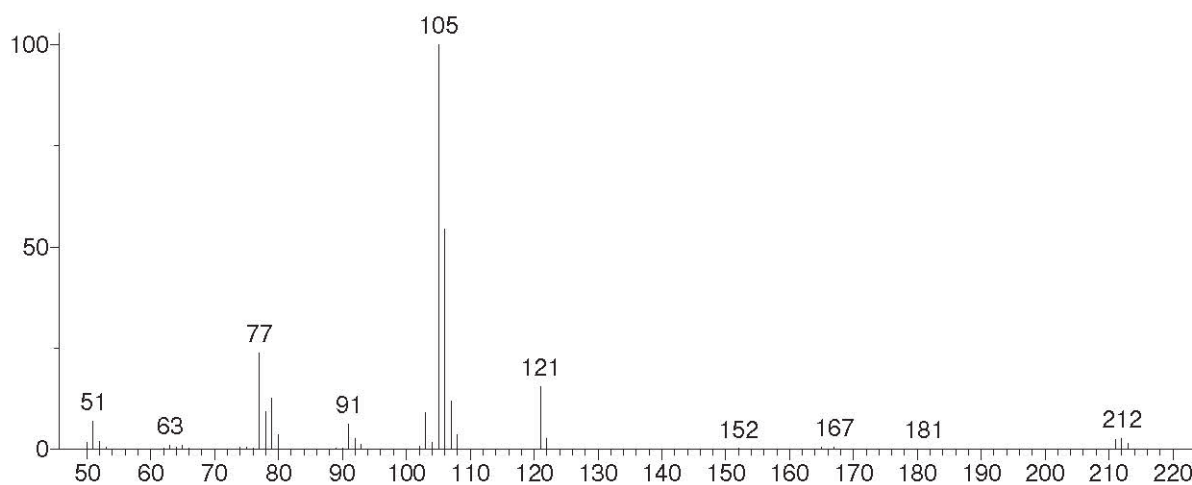


TIC: VITDA198A.D

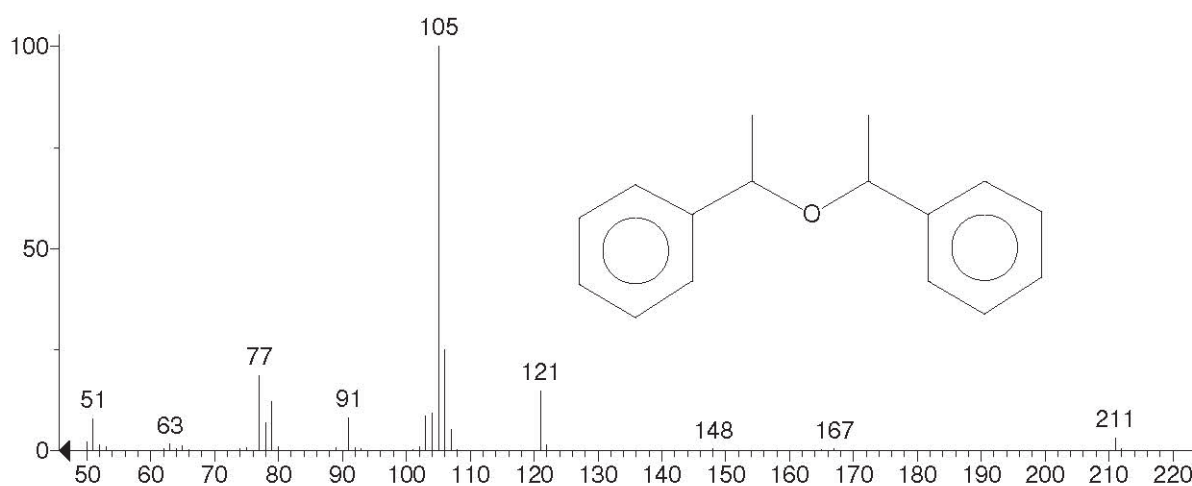




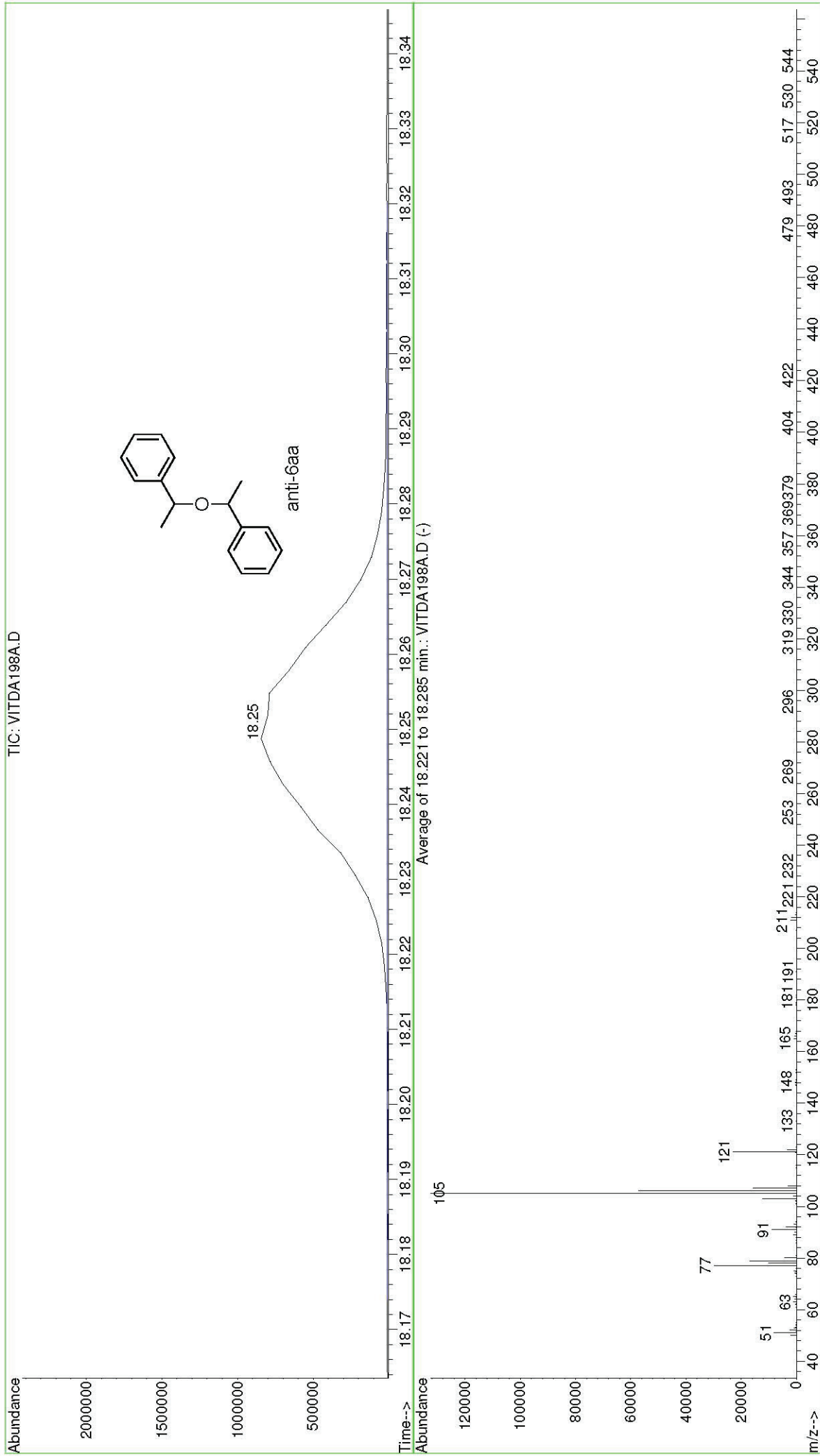
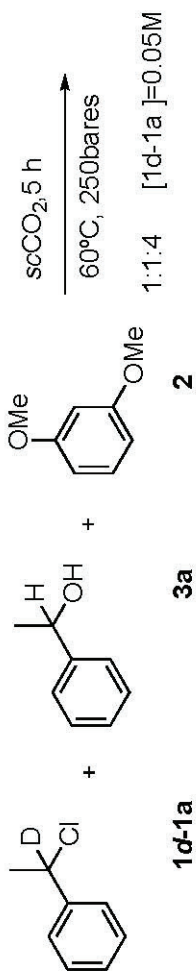
Unknown: Average of 18.025 to 18.101 min.: VITDA198A.D  
Compound in Library Factor = -240

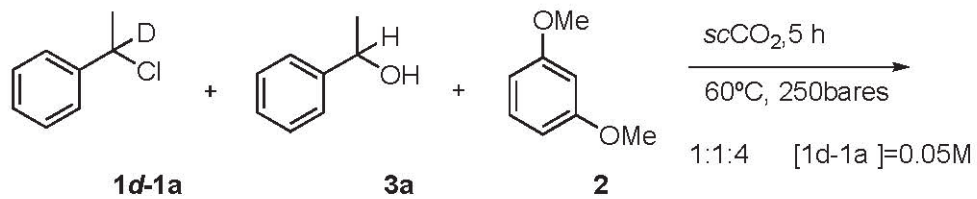


Hit 1 : Benzene, 1,1'-(oxydiethylidene)bis-  
C<sub>16</sub>H<sub>18</sub>O; MF: 810; RMF: 817; Prob 51.1%; CAS: 93-96-9; Lib: wiley7n; ID: 154842.

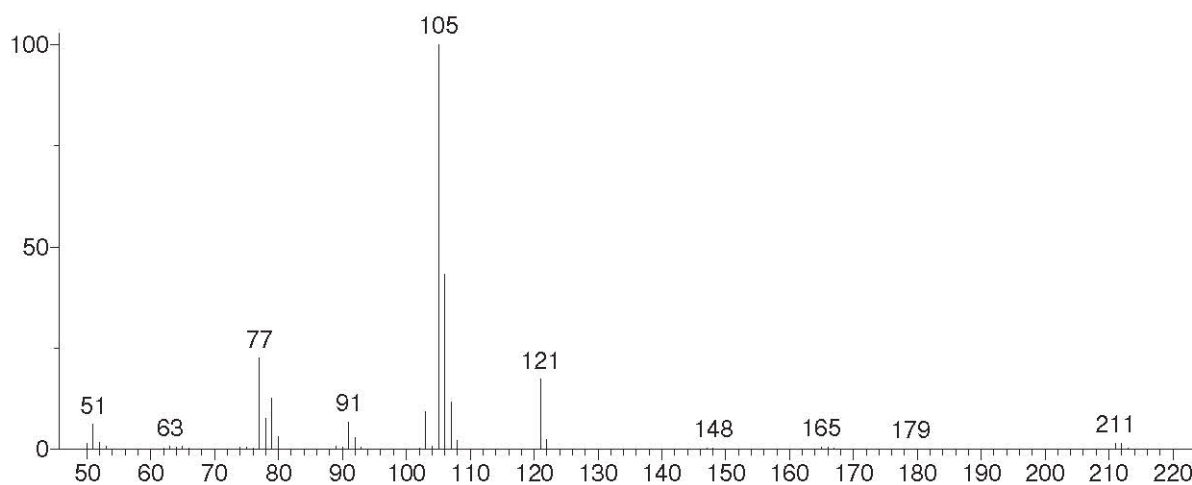


File : F:\THAIS\VITDA198A.D  
Operator :  
Acquired : 21 May 2013 14:55  
Instrument : using AcqMethod THAIS  
Sample Name : Instrument  
Misc Info :  
Vial Number: 12

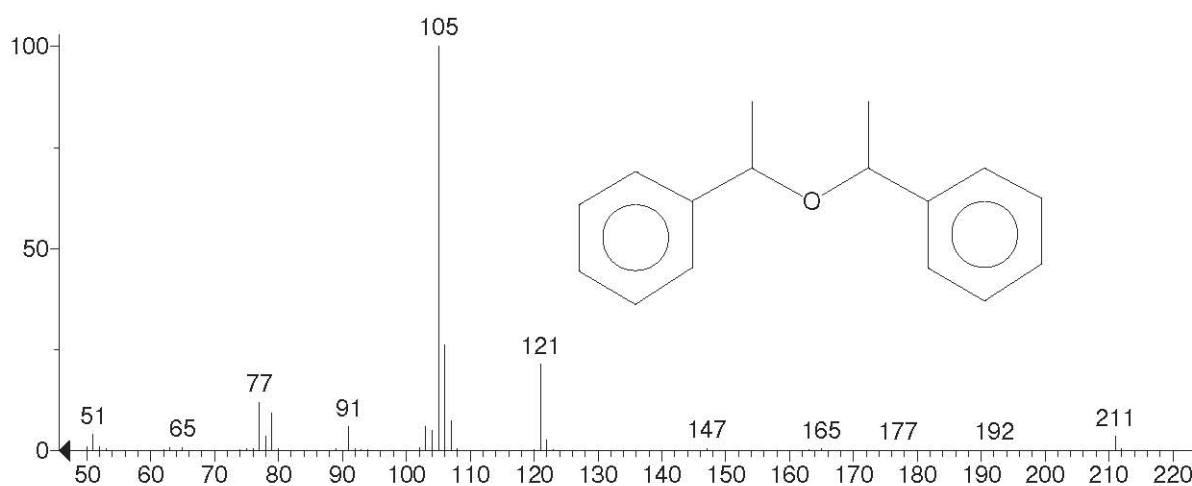




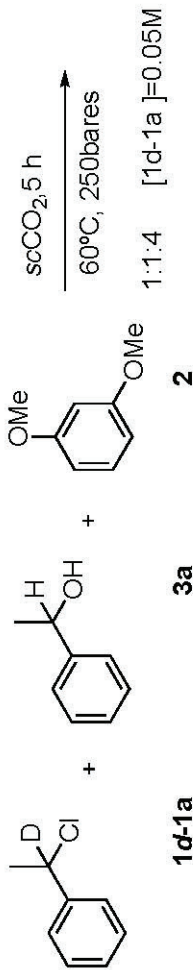
Unknown: Average of 18.221 to 18.285 min.: VITDA198A.D  
Compound in Library Factor = -194



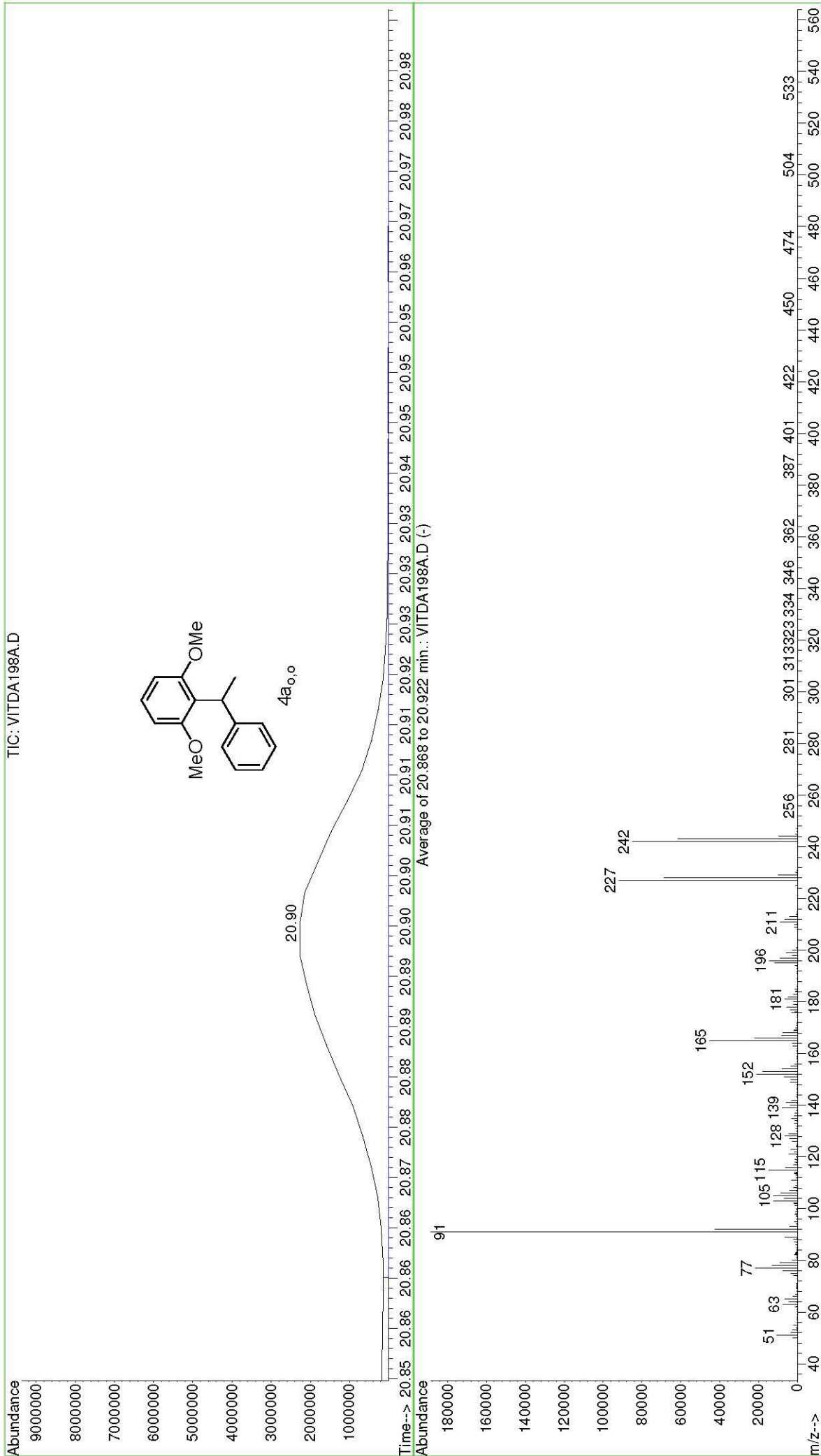
Hit 1 : Benzene, 1,1'-(oxydiethylidene)bis-  
C<sub>16</sub>H<sub>18</sub>O; MF: 814; RMF: 816; Prob 40.3%; CAS: 93-96-9; Lib: replib; ID: 13889.



File : F:\THAIS\VITDA198A.D  
 Operator :  
 Acquired : 21 May 2013 14:55  
 Instrument : using AcqMethod THAIS  
 Sample Name :  
 Misc Info :  
 Vial Number : 12



TIC: VITDA198A.D



File : F:\THAIS\VITDA198A.D

Operator :

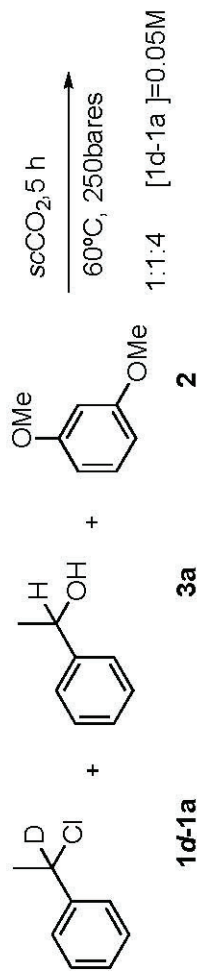
Acquired : 21 May 2013 14:55 using AcqMethod THAIS

Instrument : Instrument

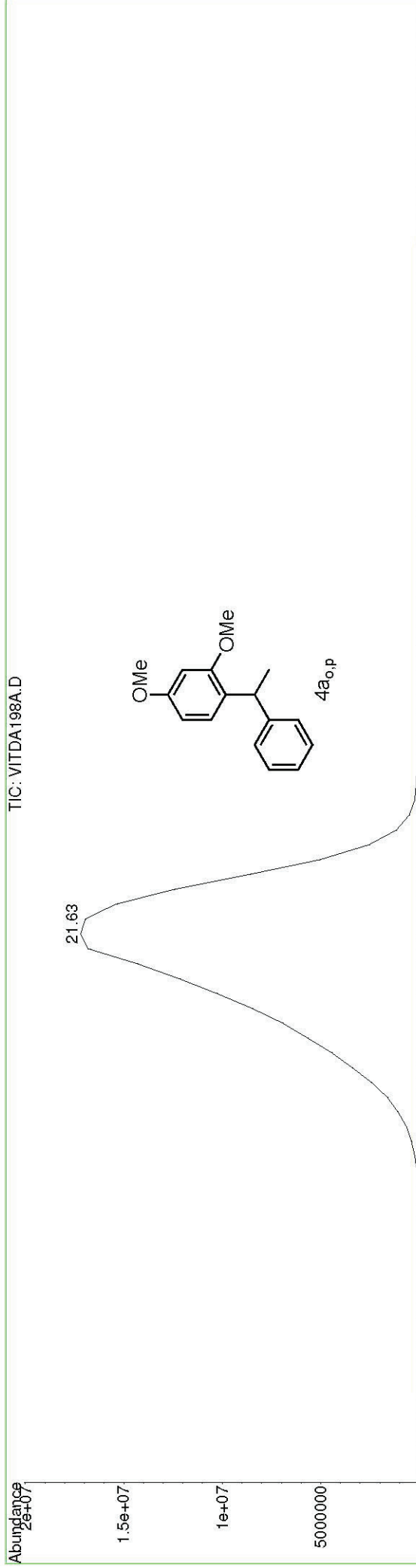
Sample Name:

Misc Info :

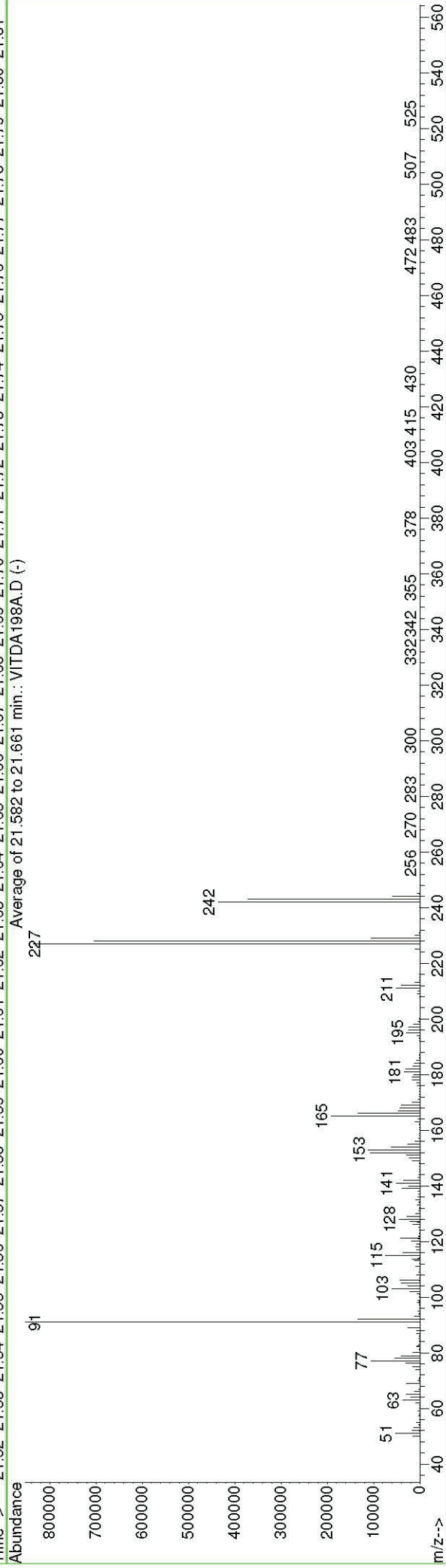
Vial Number: 12



TIC: VITDA198A.D

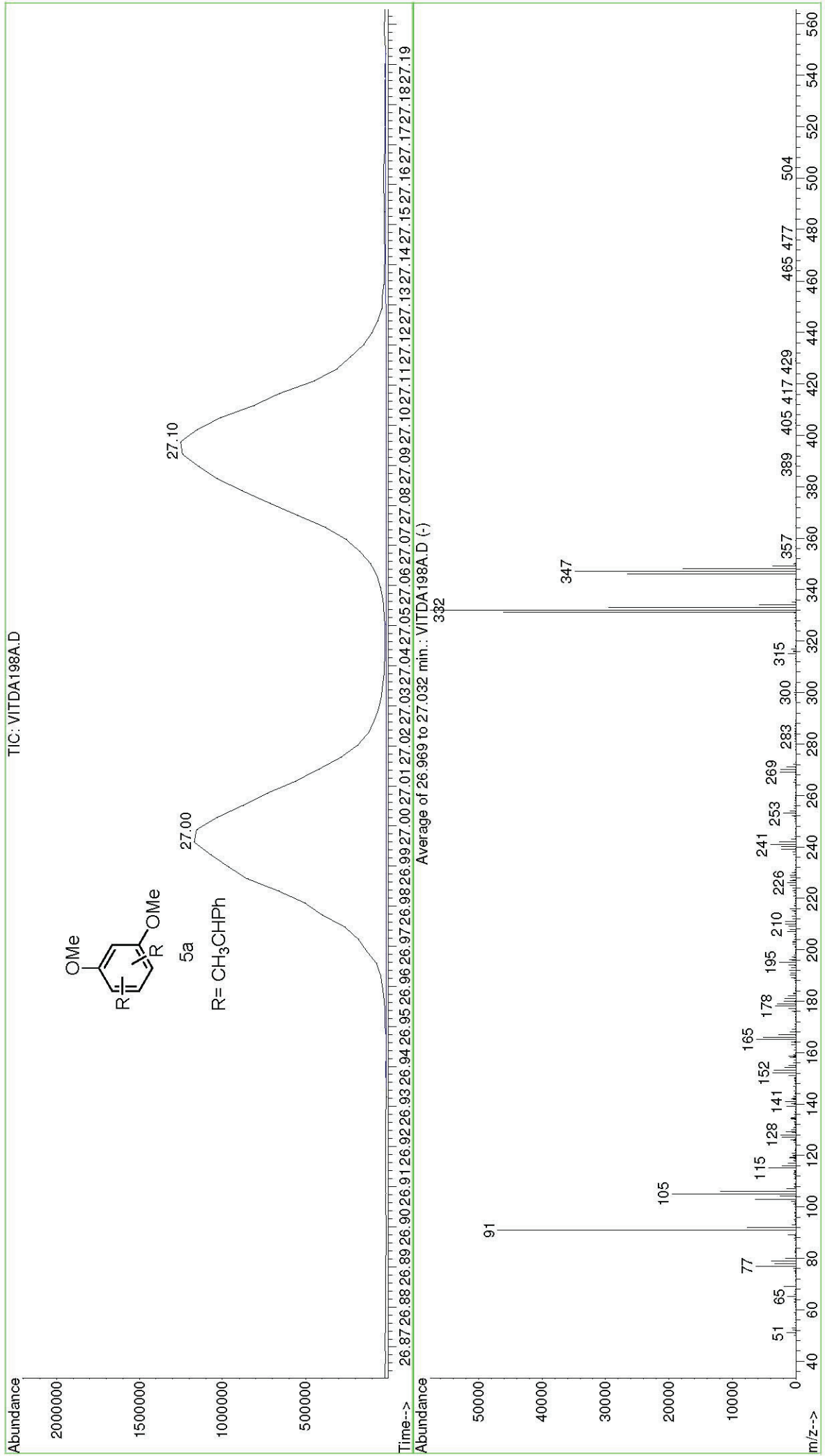
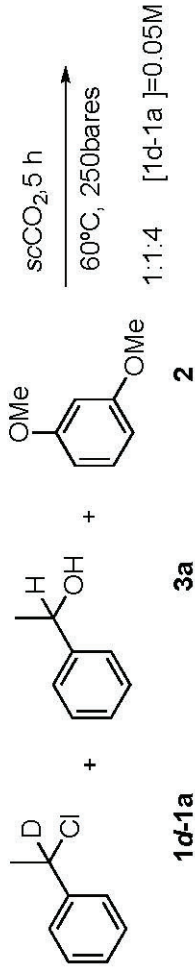


Average of 21.582 to 21.661 min.: VITDA198A.D (-)



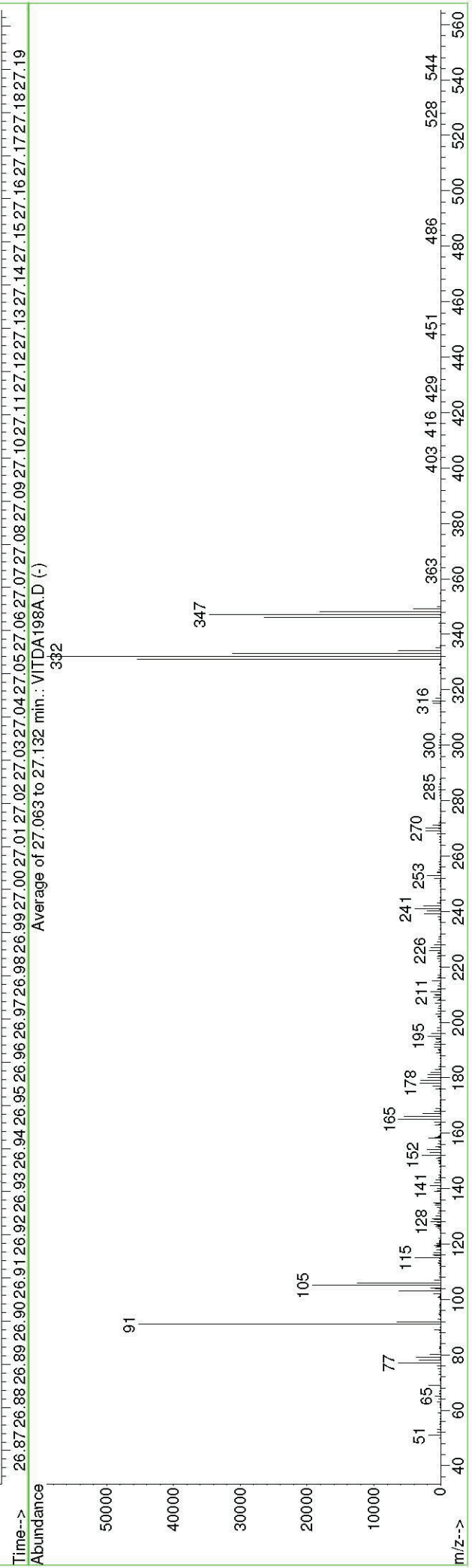
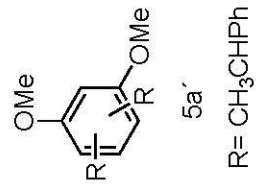
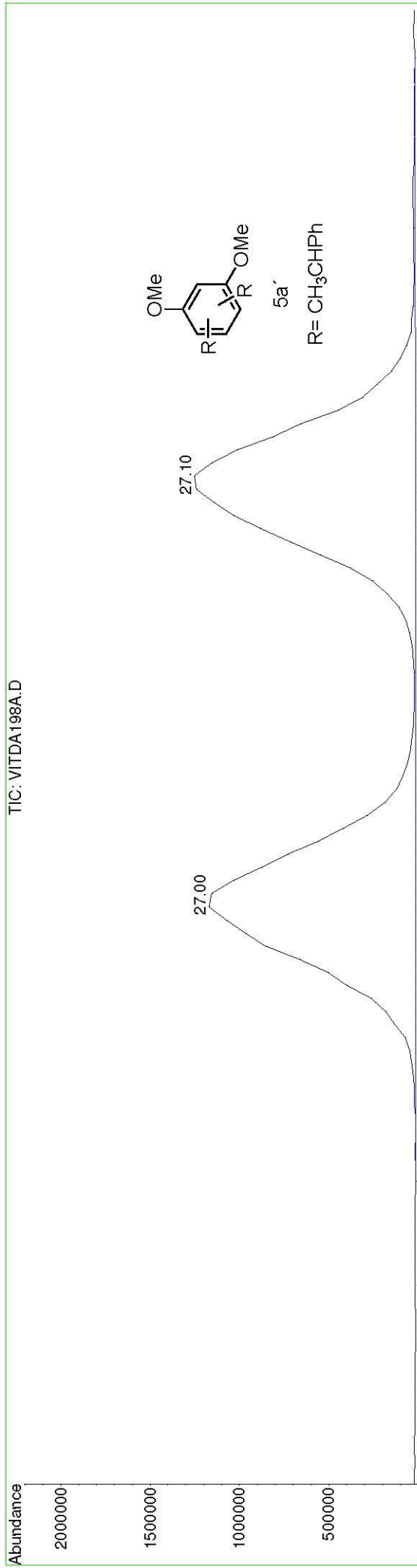
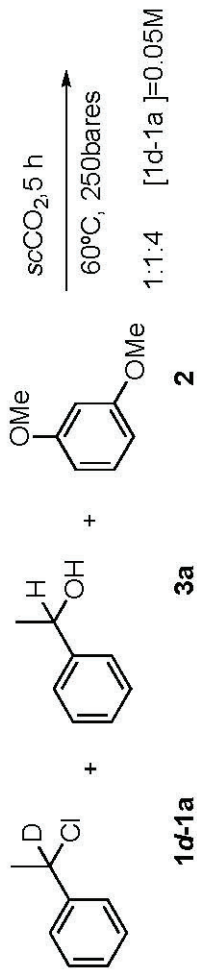


File : F:\THAIS\VITDA198A.D  
 Operator :  
 Acquired : 21 May 2013 14:55  
 Instrument : using AcqMethod THAIS  
 Sample Name :  
 Misc Info :  
 Vial Number: 12



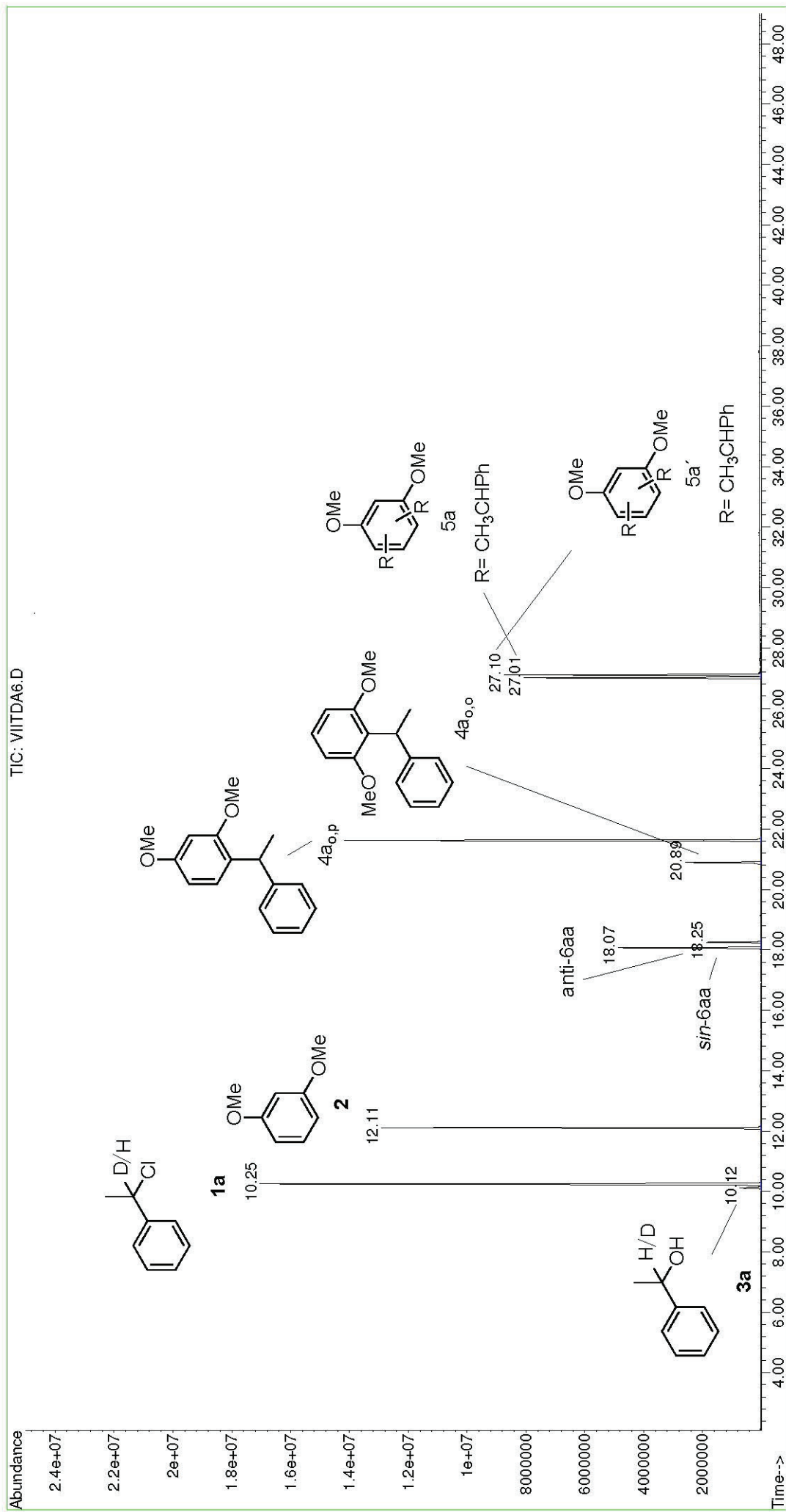
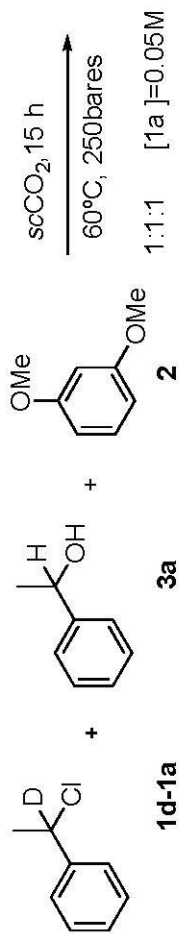


File : F:\THAIS\VITDA198A.D  
 Operator :  
 Acquired : 21 May 2013 14:55  
 Instrument : using AcqMethod THAIS  
 Sample Name :  
 Misc Info :  
 Vial Number: 12

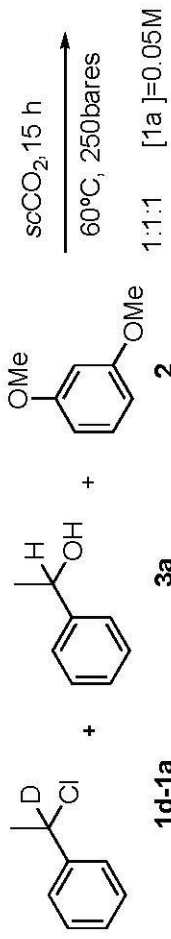


File : E:\THAIS\VIITDA6.D  
 Operator :  
 Acquired : 24 May 2013 14:49  
 Instrument : Instrument  
 Sample Name :  
 Misc Info :  
 Vial Number : 17

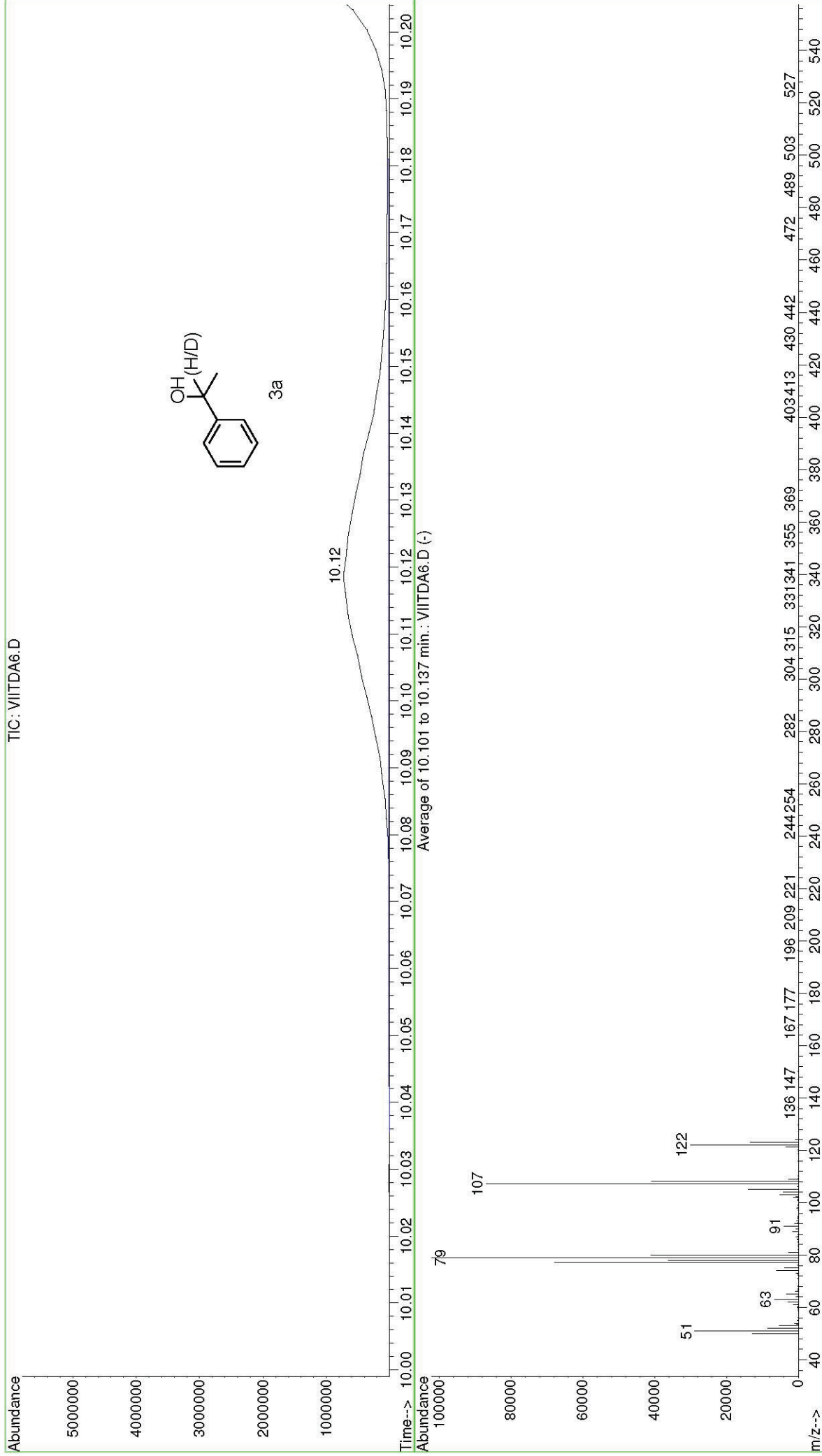
using AcqMethod THAIS

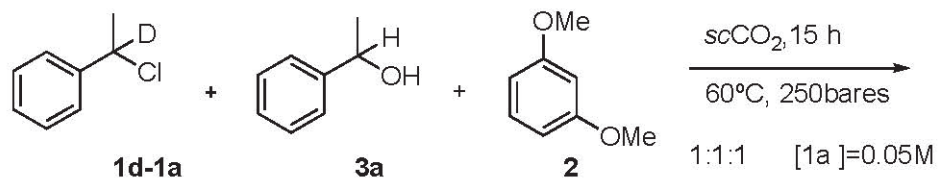


File : E:\THAIS\VIITDA6.D  
Operator :  
Acquired : 24 May 2013 14:49  
Instrument : using AcqMethod THAIS  
Sample Name : Instrument  
Misc Info :  
Vial Number: 17

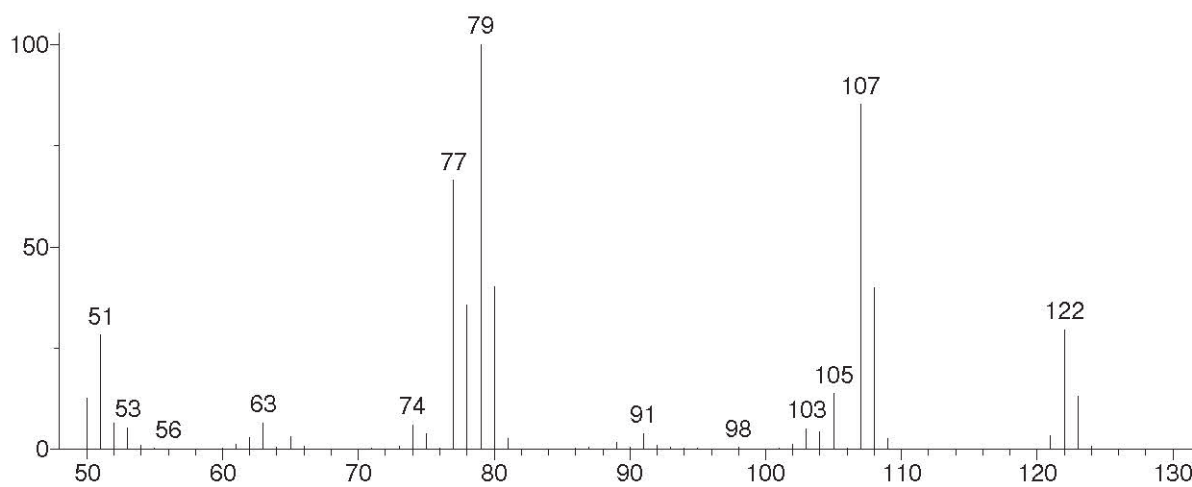


TIC: VIITDA6.D

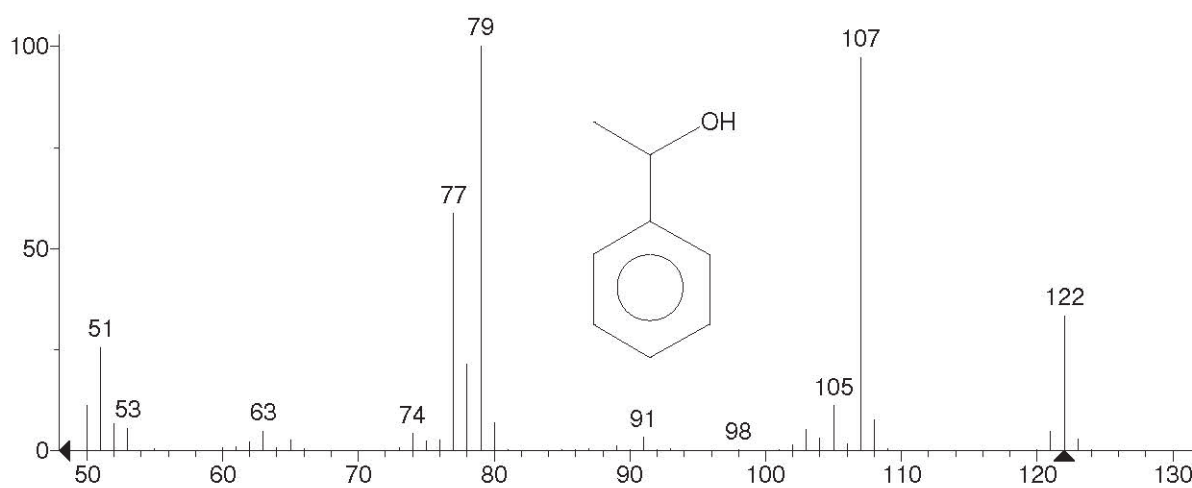




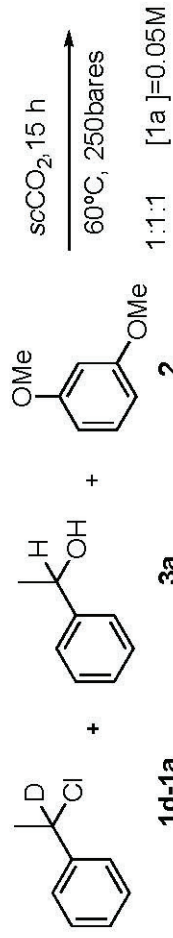
Unknown: Average of 10.101 to 10.137 min.: VIITDA6.D  
Compound in Library Factor = -334



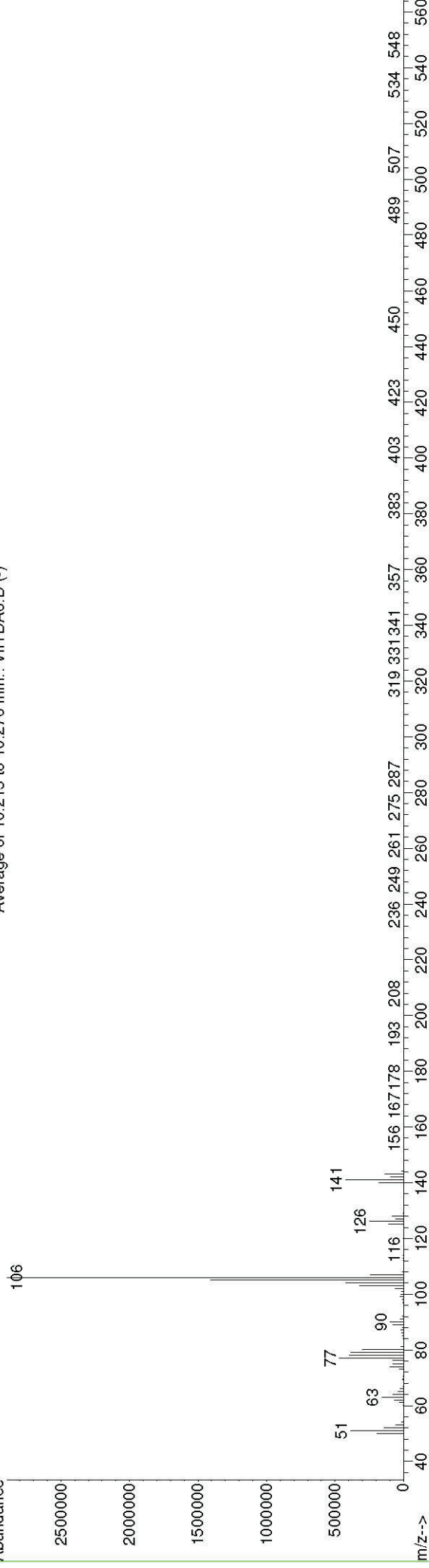
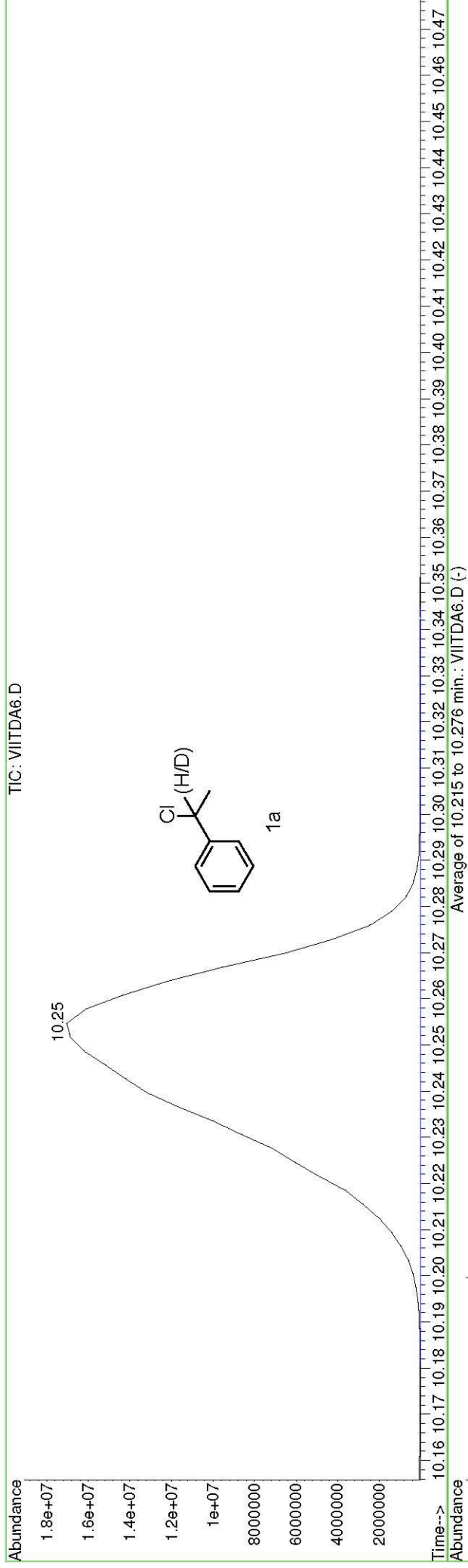
Hit 1 : Benzenemethanol, .alpha.-methyl-  
C<sub>8</sub>H<sub>10</sub>O; MF: 829; RMF: 829; Prob 50.5%; CAS: 98-85-1; Lib: replib; ID: 9674.



File : E:\THAIS\VIITDA6.D  
Operator :  
Acquired : 24 May 2013 14:49  
Instrument : using AcqMethod THAIS  
Sample Name : Instrument  
Misc Info :  
Vial Number : 17

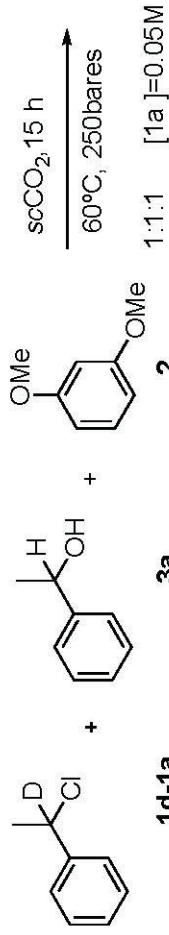


TIC: VIITDA6.D

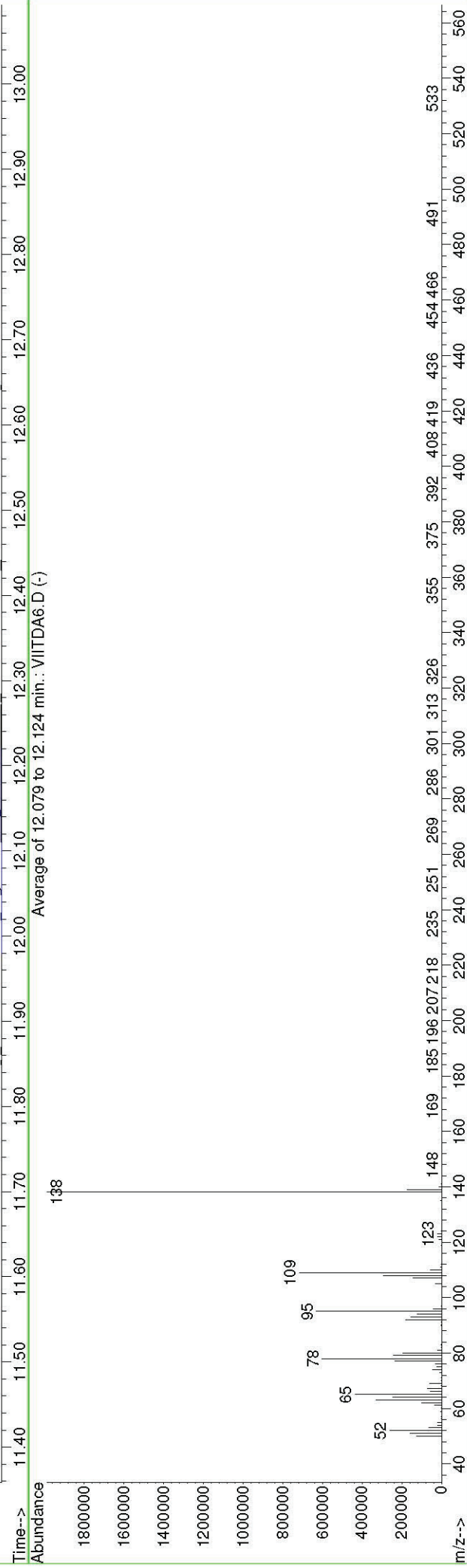
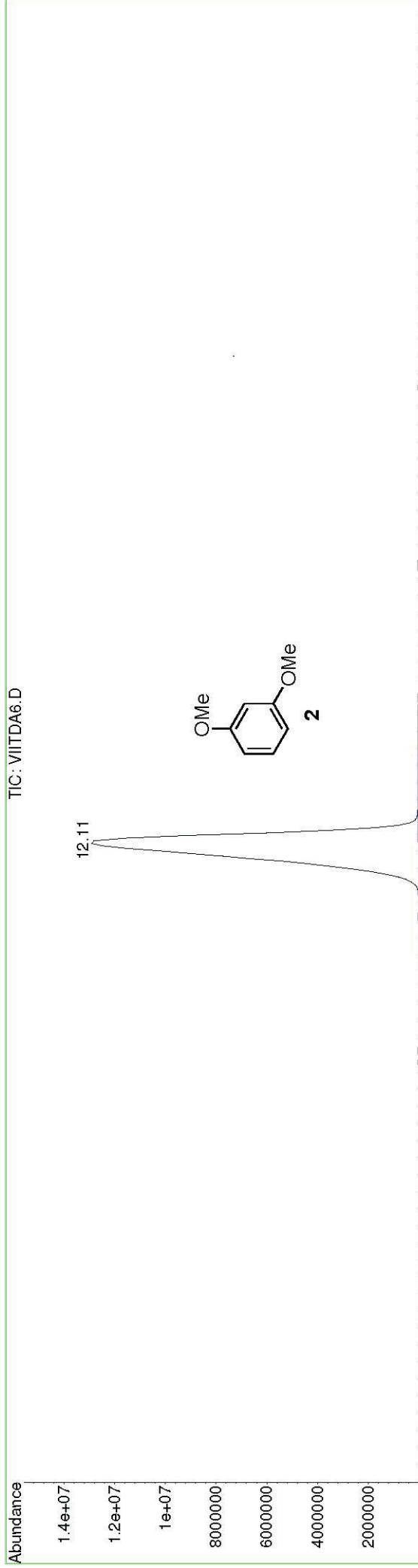


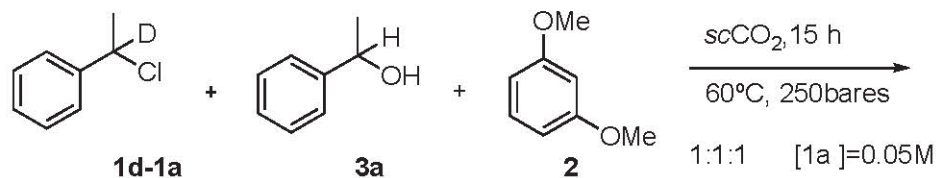
File : E:\THAIS\VIITDA6.D  
Operator :  
Acquired : 24 May 2013 14:49  
Instrument : Instrument  
Sample Name :  
Misc Info :  
Vial Number: 17

using AcqMethod THAIS

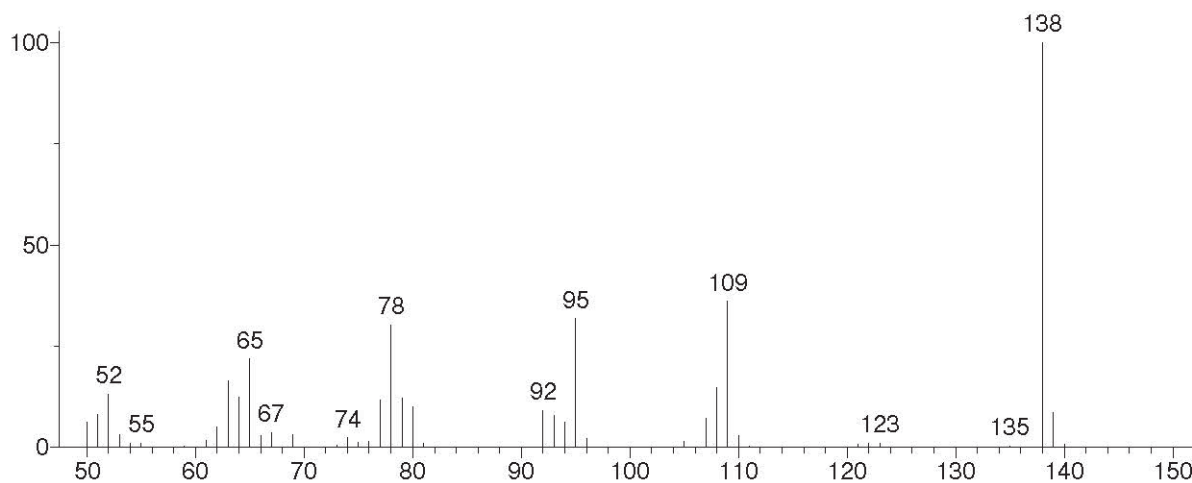


TIC: VIITDA6.D

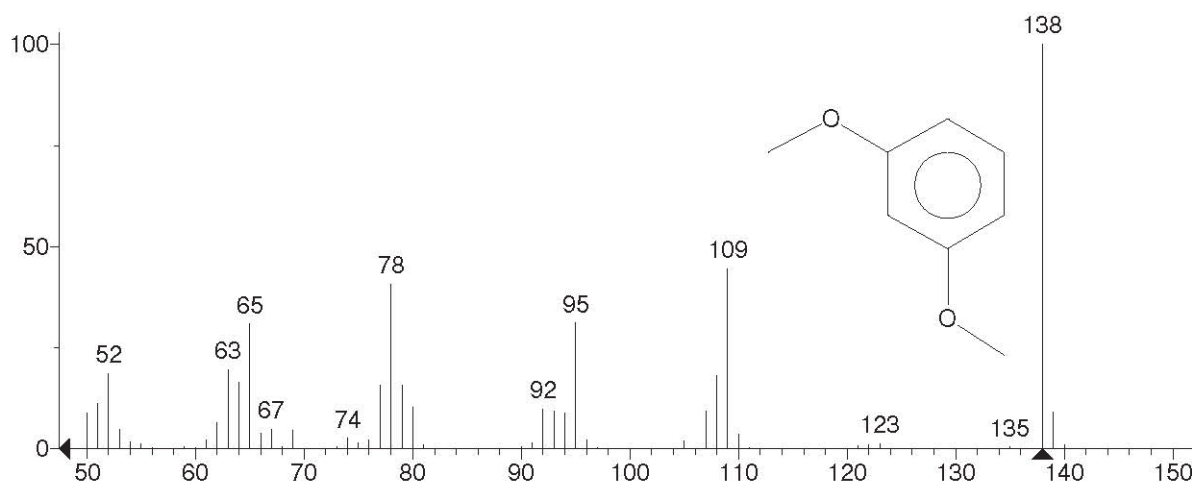




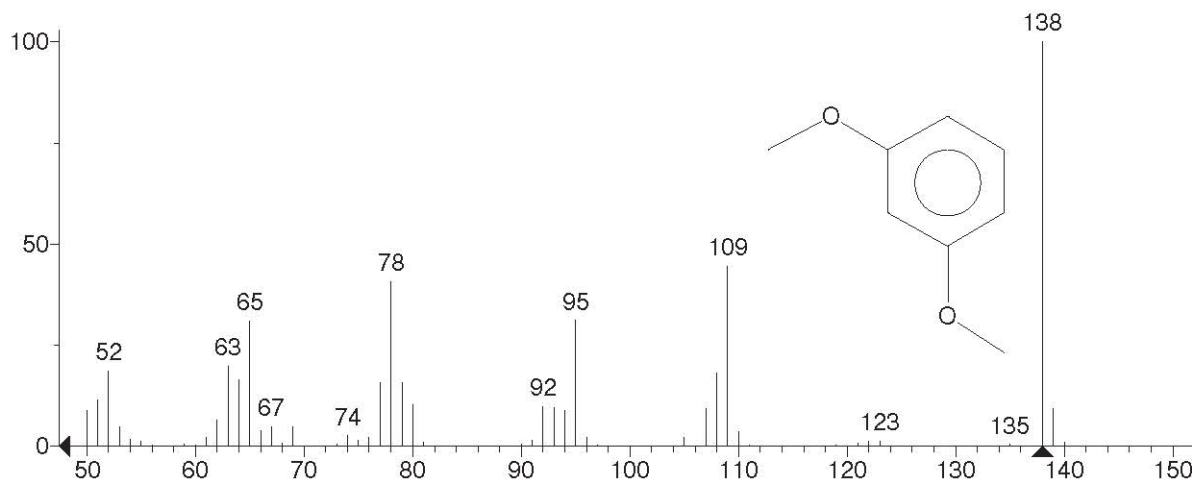
Unknown: Average of 12.079 to 12.124 min.: VIITDA6.D  
 Compound in Library Factor = 504



Hit 1 : Benzene, 1,3-dimethoxy-  
 C<sub>8</sub>H<sub>10</sub>O<sub>2</sub>; MF: 948; RMF: 948; Prob 74.8%; CAS: 151-10-0; Lib: replib; ID: 18631.

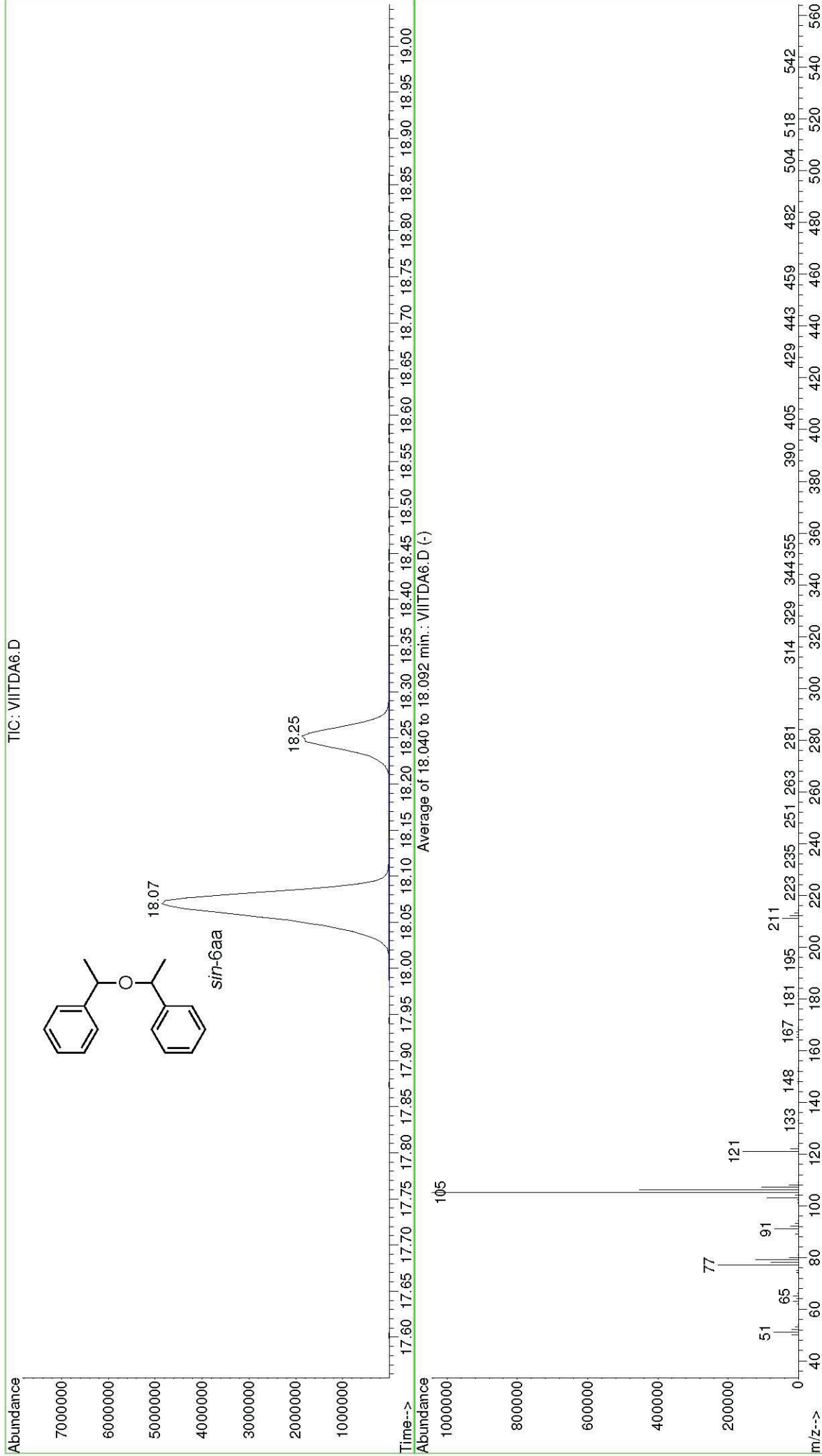
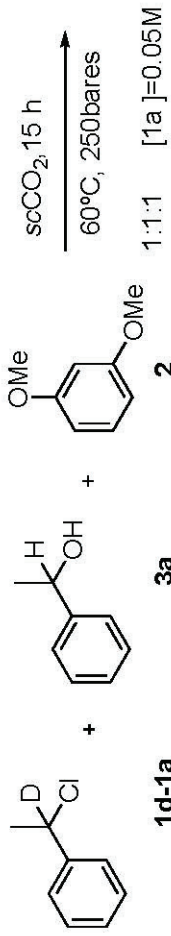


Hit 2 : Benzene, 1,3-dimethoxy-  
 C<sub>8</sub>H<sub>10</sub>O<sub>2</sub>; MF: 943; RMF: 943; Prob 74.8%; CAS: 151-10-0; Lib: wiley7n; ID: 33461.

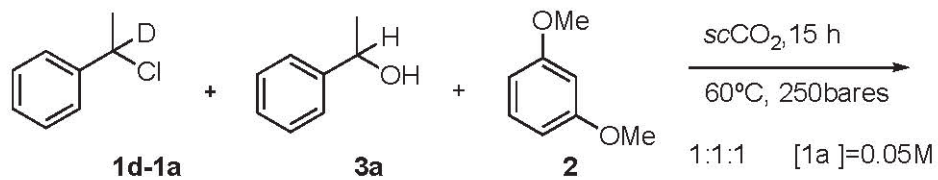




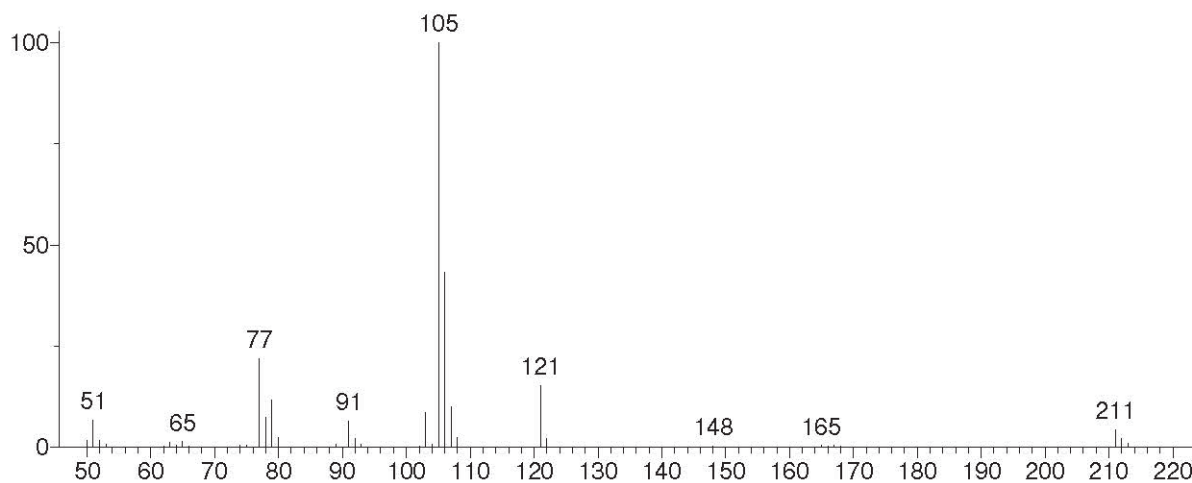
File : E:\THAIS\VIITDA6.D  
 Operator :  
 Acquired : 24 May 2013 14:49  
 Instrument : using AcqMethod THAIS  
 Sample Name :  
 Misc Info :  
 Vial Number : 17



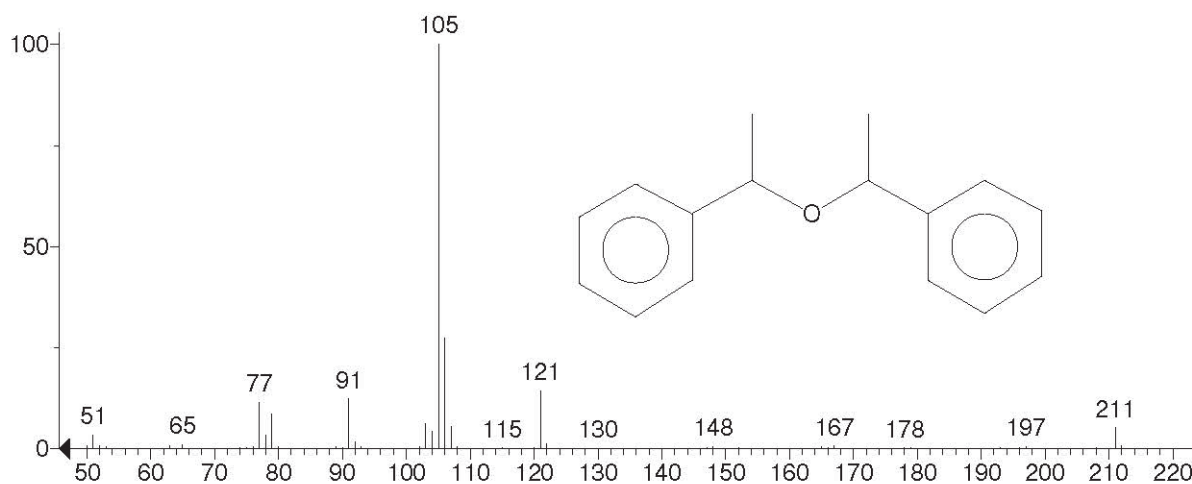




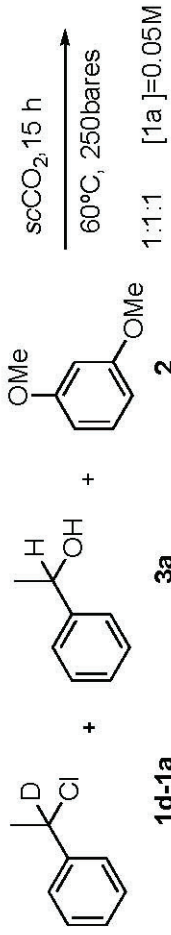
Unknown: Average of 18.040 to 18.092 min.: VIITDA6.D  
Compound in Library Factor = -119



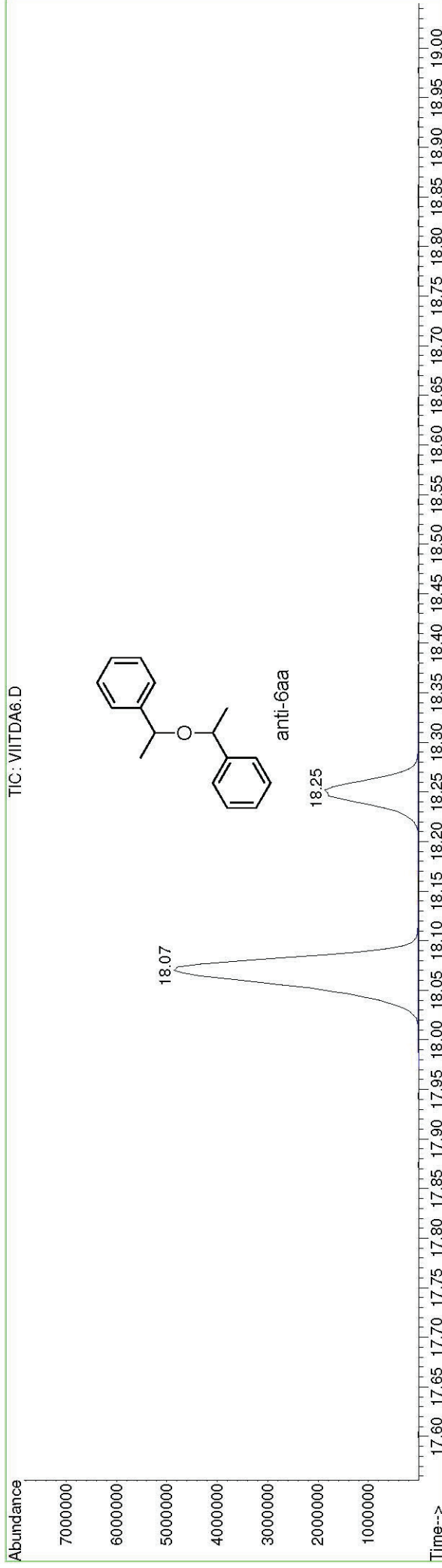
Hit 1 : Benzene, 1,1'-(oxydiethylidene)bis-  
C<sub>16</sub>H<sub>18</sub>O; MF: 834; RMF: 838; Prob 52.6%; CAS: 93-96-9; Lib: replib; ID: 13891.



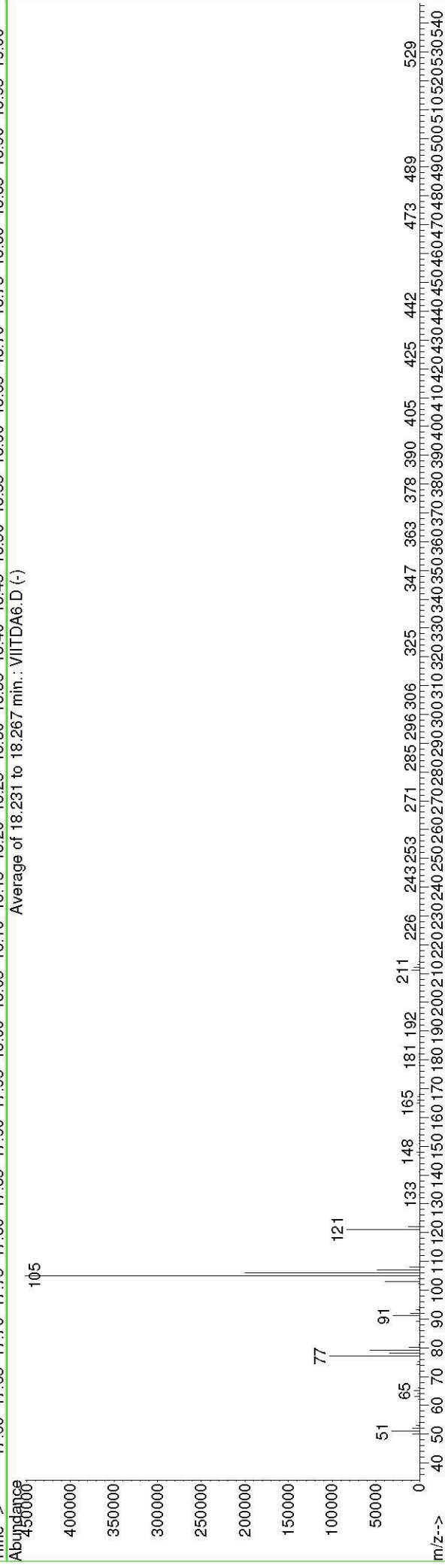
File : E:\THAIS\VIITDA6.D  
 Operator :  
 Acquired : 24 May 2013 14:49  
 Instrument : using AcqMethod THAIS  
 Sample Name : Instrument  
 Misc Info :  
 Vial Number: 17

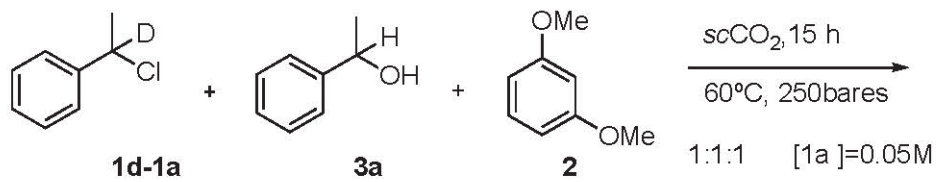


TIC: VIITDA6.D

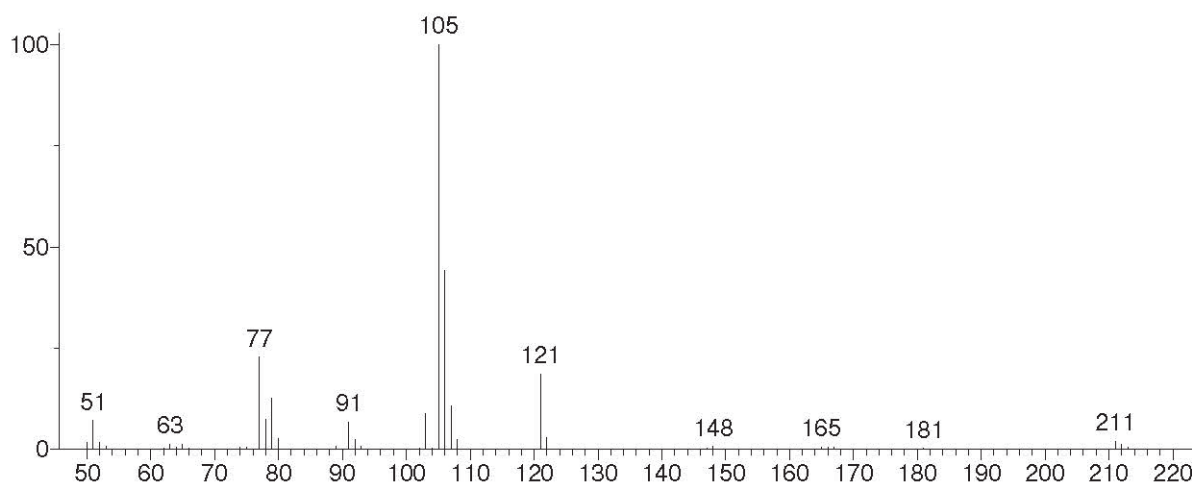


Average of 18.231 to 18.267 min.: VIITDA6.D (-)

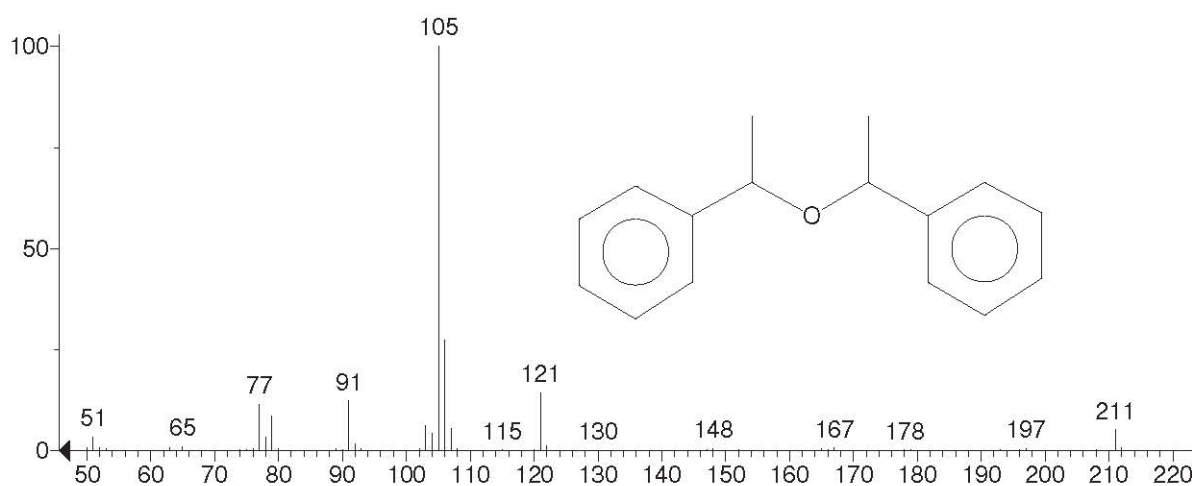




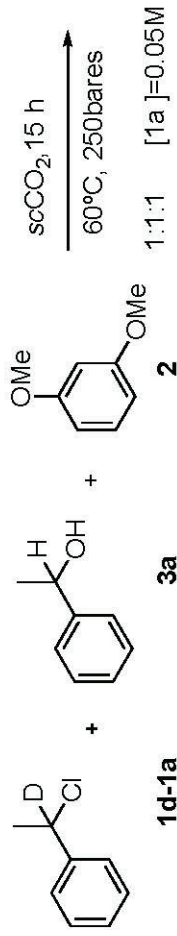
Unknown: Average of 18.231 to 18.267 min.: VIITDA6.D  
Compound in Library Factor = -121



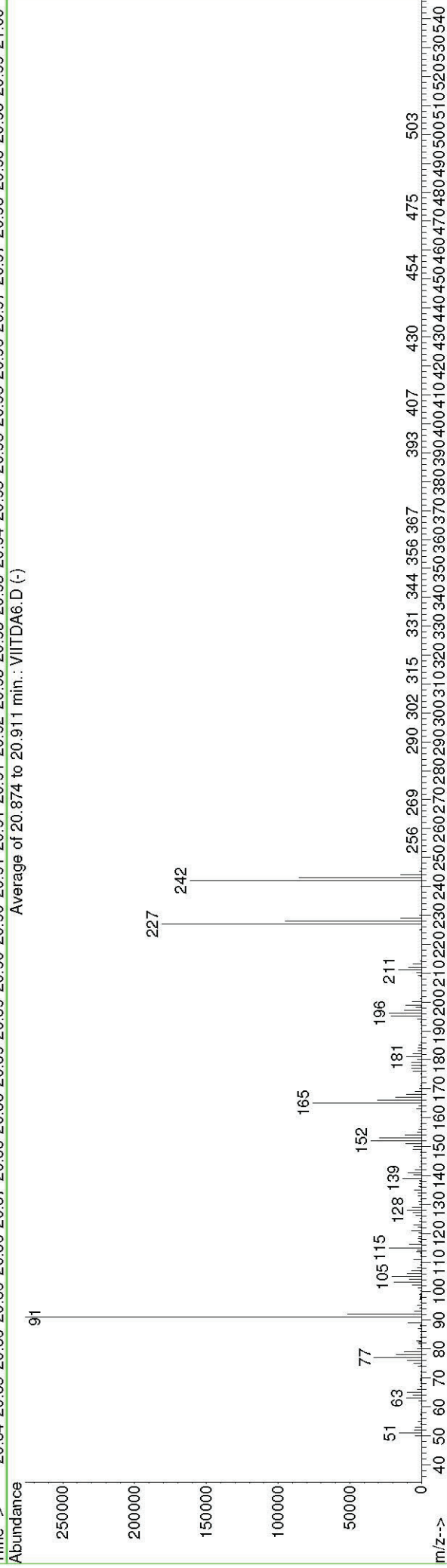
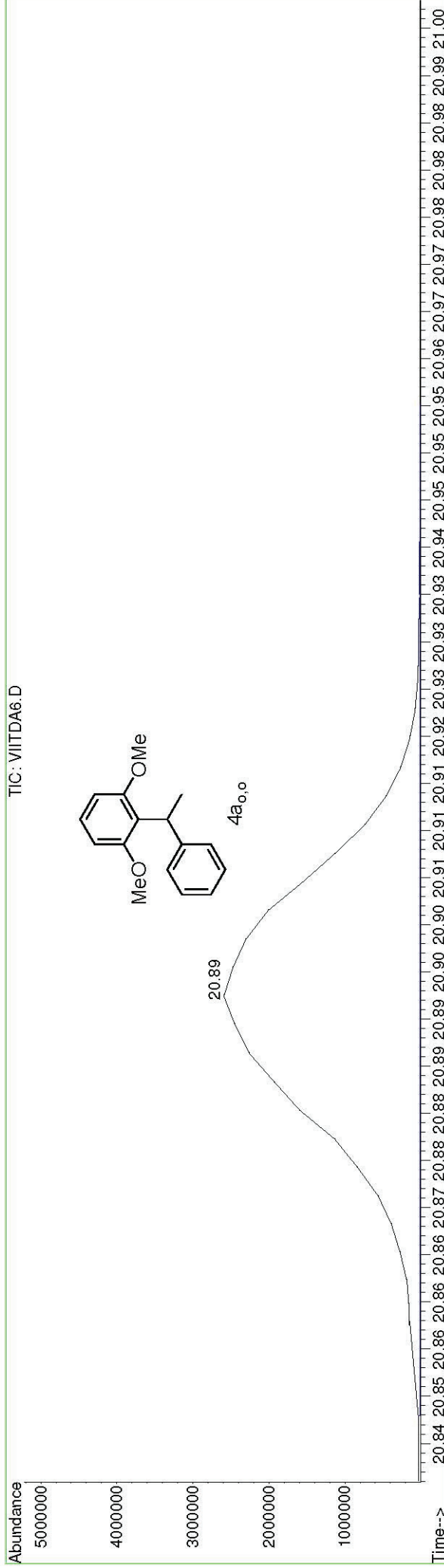
Hit 1 : Benzene, 1,1'-(oxydiethylidene)bis-  
C<sub>16</sub>H<sub>18</sub>O; MF: 827; RMF: 828; Prob 50.2%; CAS: 93-96-9; Lib: replib; ID: 13891.



File : E:\THAIS\VIITDA6.D  
 Operator :  
 Acquired : 24 May 2013 14:49  
 Instrument : using AcqMethod THAIS  
 Sample Name : Instrument  
 Misc Info :  
 Vial Number : 17

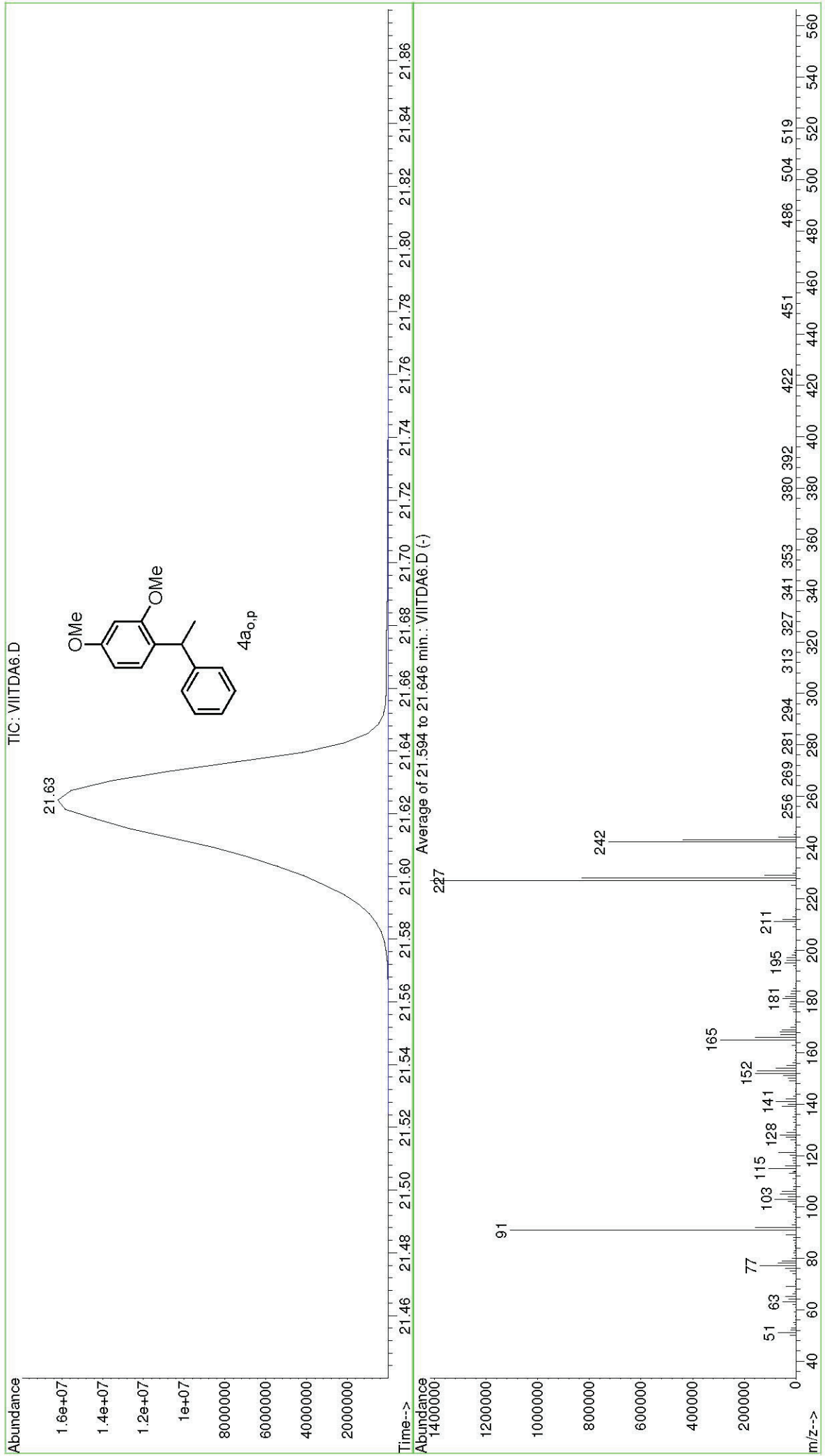
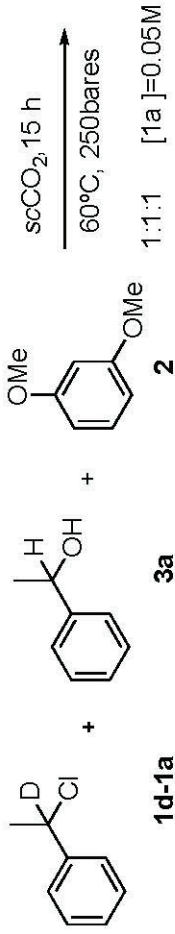


TIC: VIITDA6.D

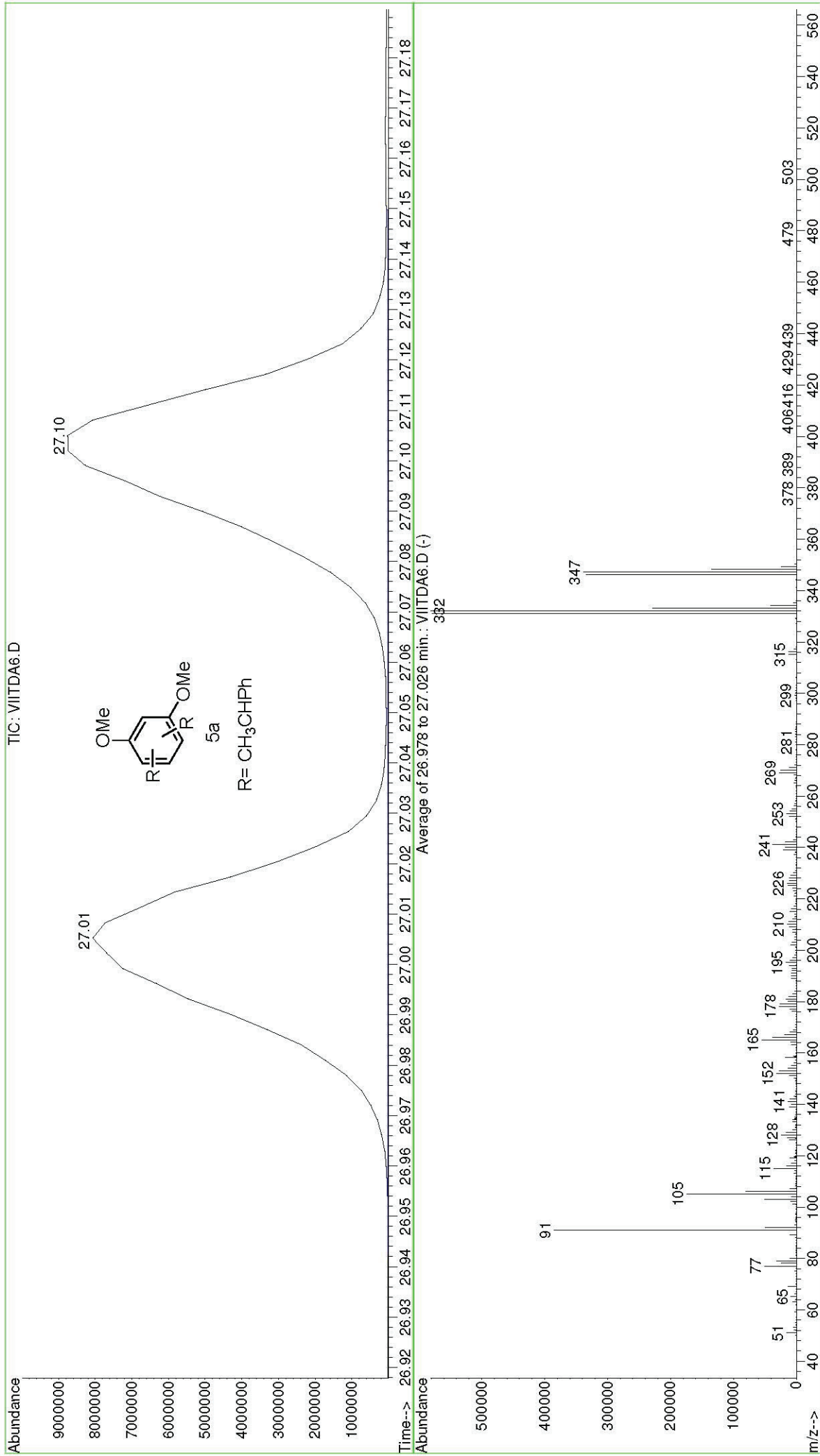
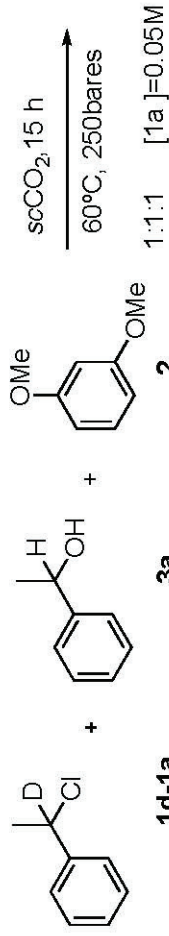


File : E:\THAIS\VIITDA6.D  
 Operator :  
 Acquired : 24 May 2013 14:49  
 Instrument : Instrument  
 Sample Name :  
 Misc Info :  
 Vial Number: 17

using AcqMethod THAIS

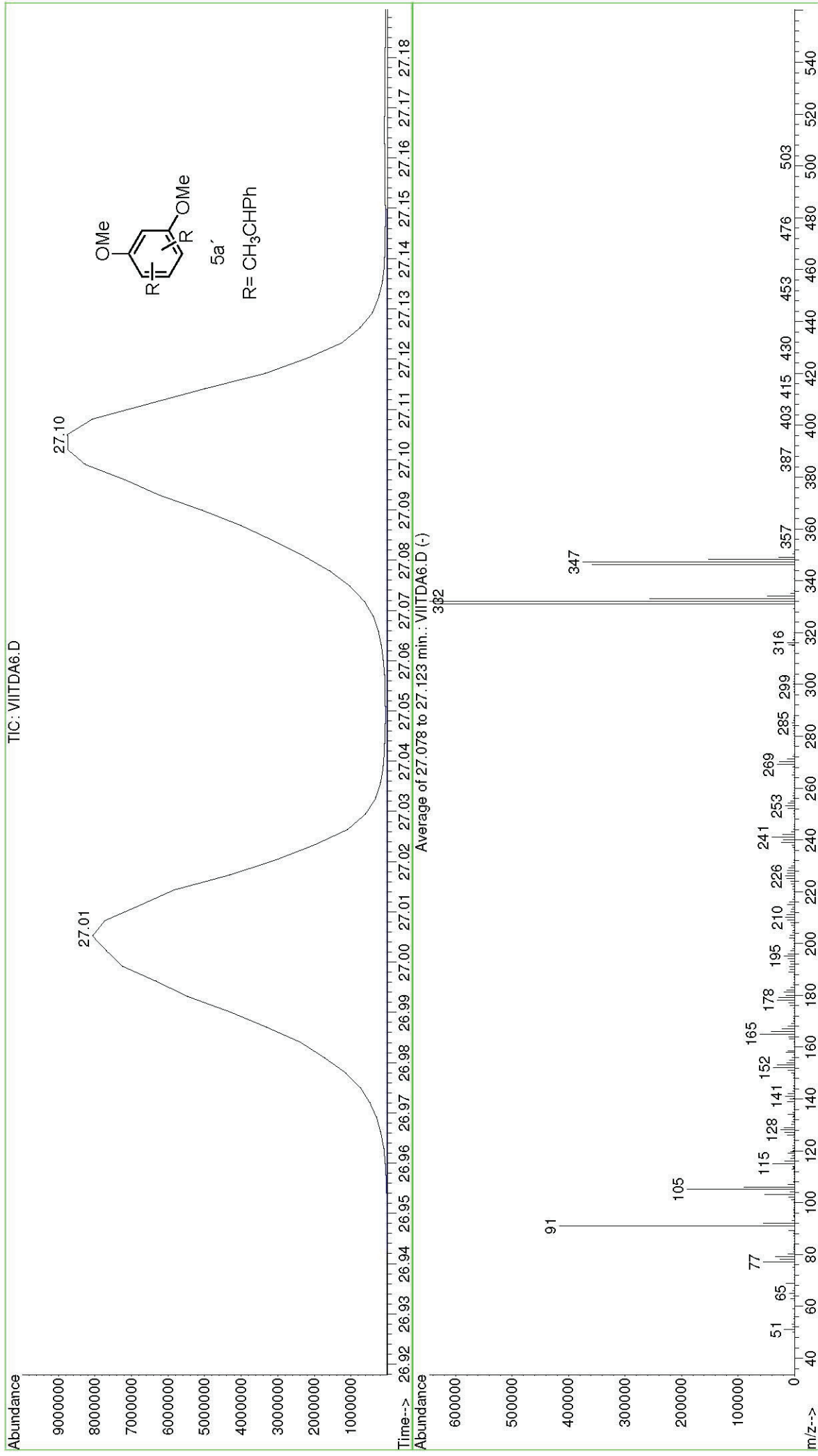
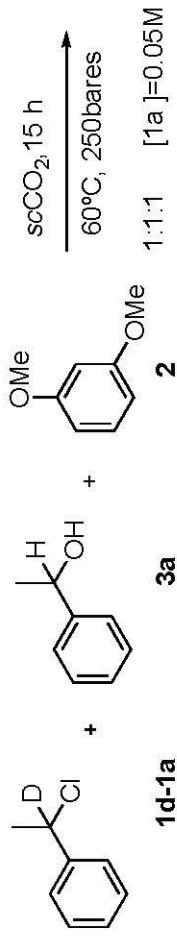


File : E:\THAIS\VIITDA6.D  
 Operator :  
 Acquired : 24 May 2013 14:49  
 Instrument : using AcqMethod THAIS  
 Sample Name : Instrument  
 Misc Info :  
 Vial Number: 17





File : E:\THAIS\VIITDA6.D  
 Operator :  
 Acquired : 24 May 2013 14:49  
 Instrument : using AcqMethod THAIS  
 Sample Name : Instrument  
 Misc Info :  
 Vial Number: 17



File : D:\ASENSIO\JAUME\JMF61.D

Operator :

Acquired : 21 May 2012 22:49

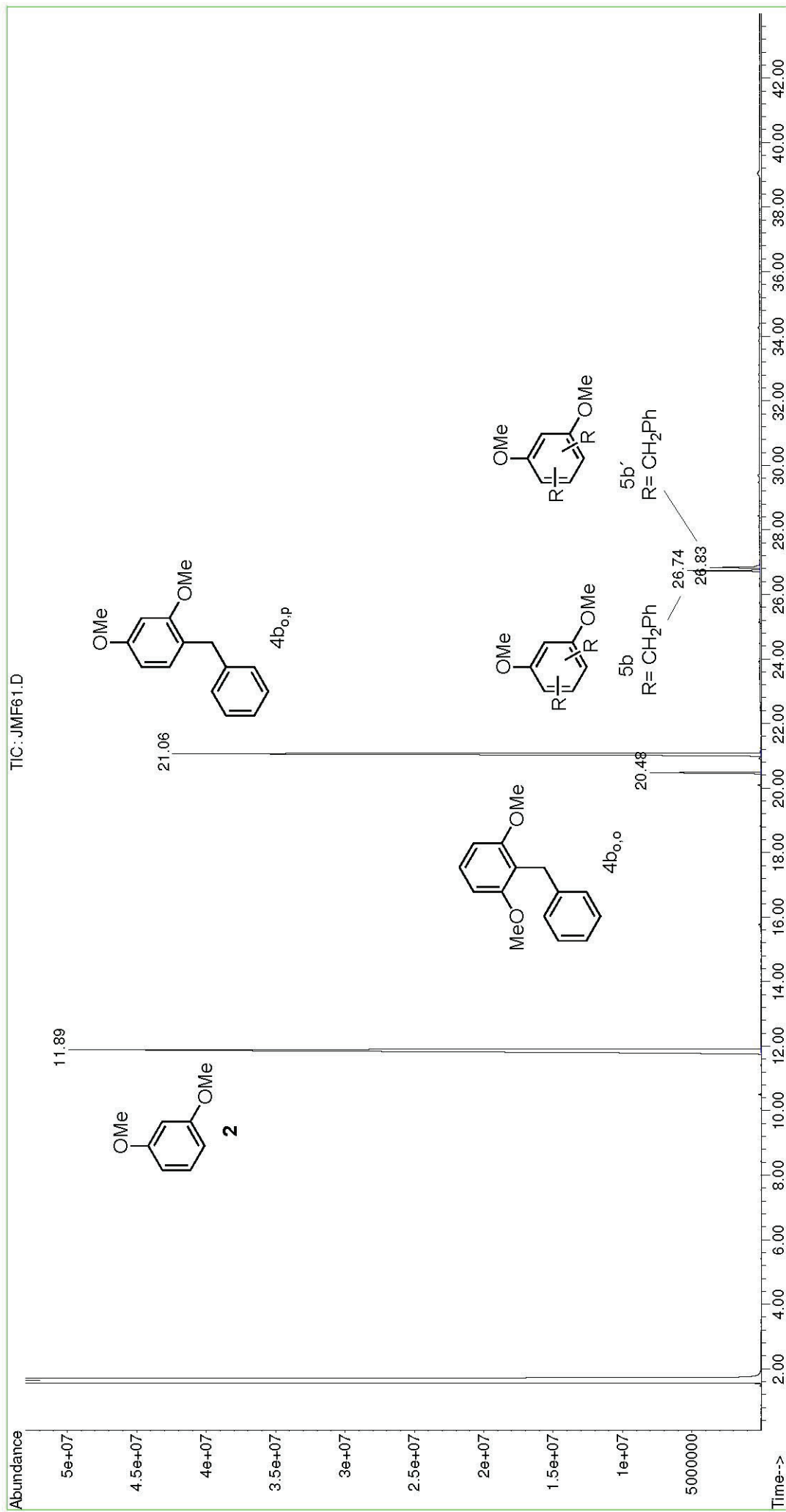
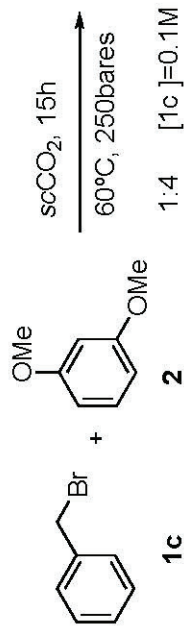
Instrument : Instrument

Sample Name:

Misc Info :

Vial Number: 18

using AcqMethod JMF60





File : D:\ASENSIO\JAUME\JMF61.D

Operator :

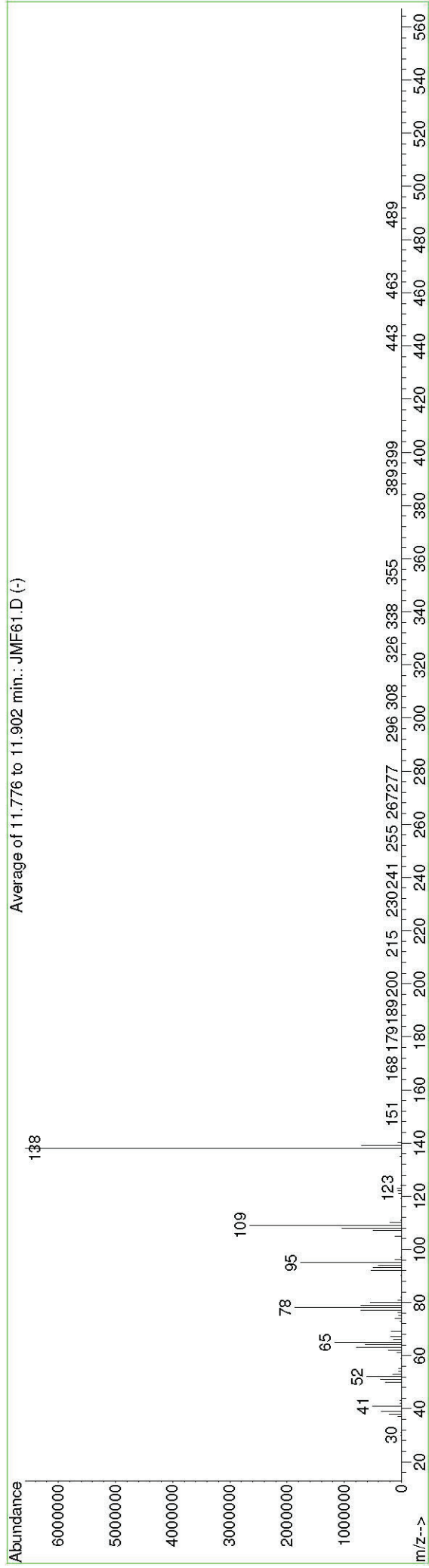
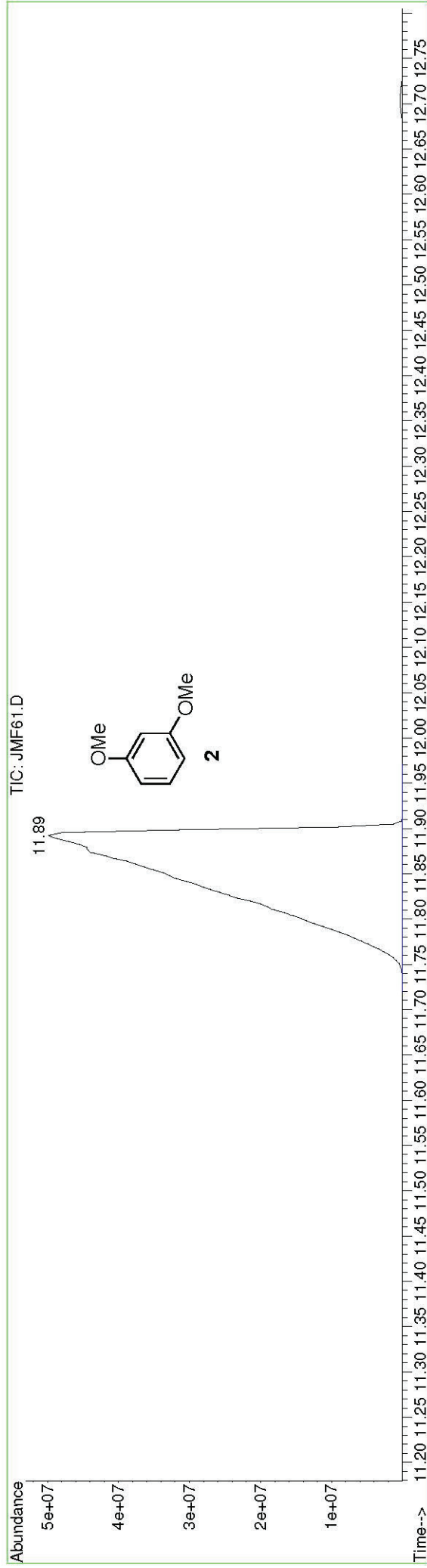
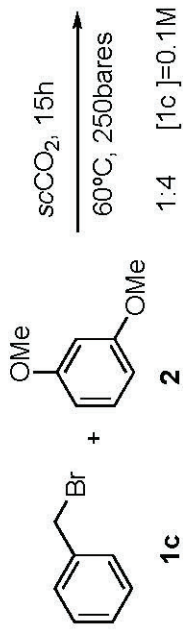
Acquired : 21 May 2012 22:49 using AcqMethod JMF60

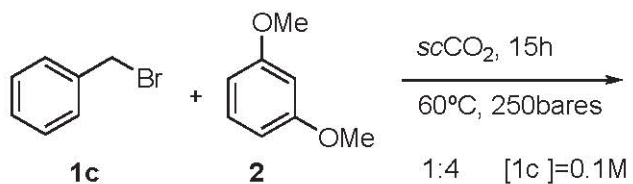
Instrument : Instrument

Sample Name:

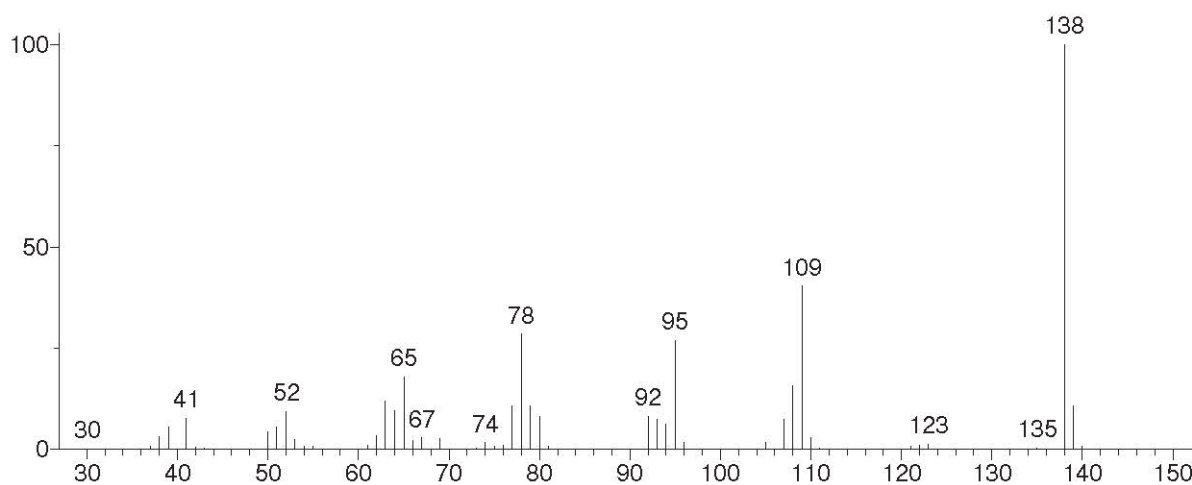
Misc Info :

Vial Number: 18

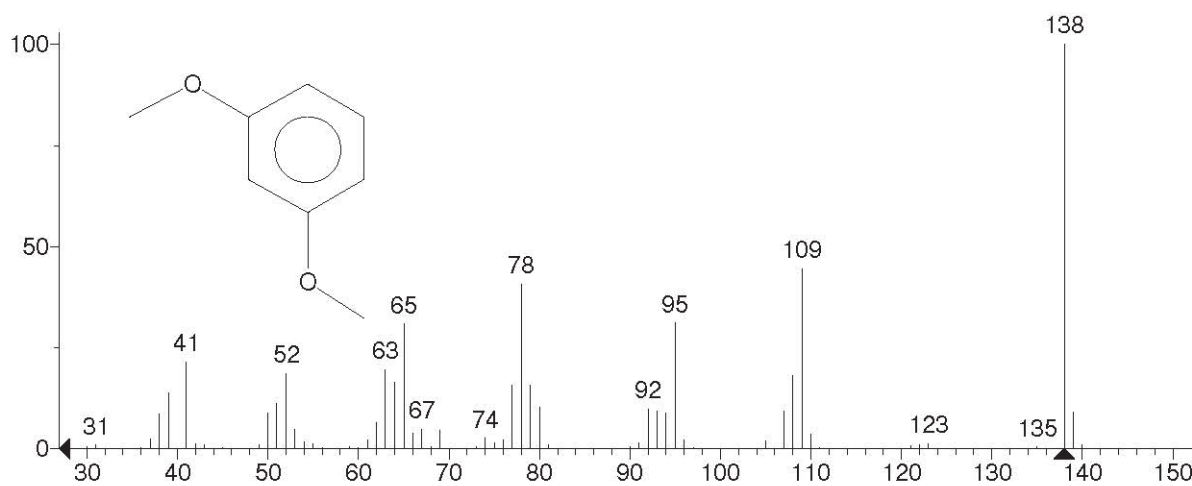




Unknown: Average of 11.776 to 11.902 min.: JMF61.D  
Compound in Library Factor = 515



Hit 1 : Benzene, 1,3-dimethoxy-  
C<sub>8</sub>H<sub>10</sub>O<sub>2</sub>; MF: 951; RMF: 951; Prob 68.1%; CAS: 151-10-0; Lib: replib; ID: 18631.



File : D:\ASENSIO\JAUME\JMF61.D

Operator :

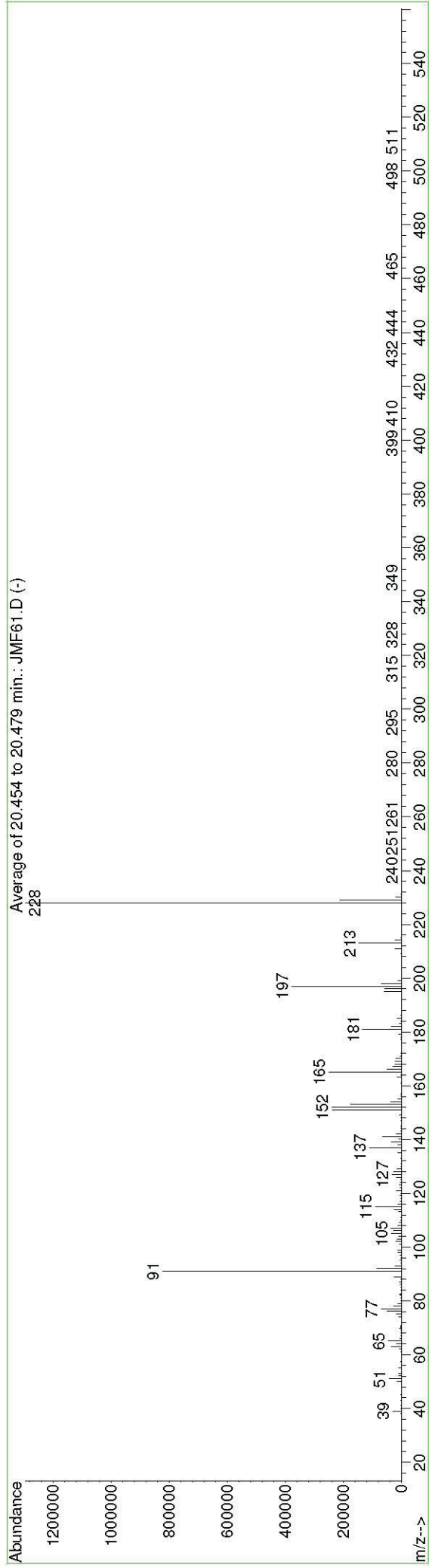
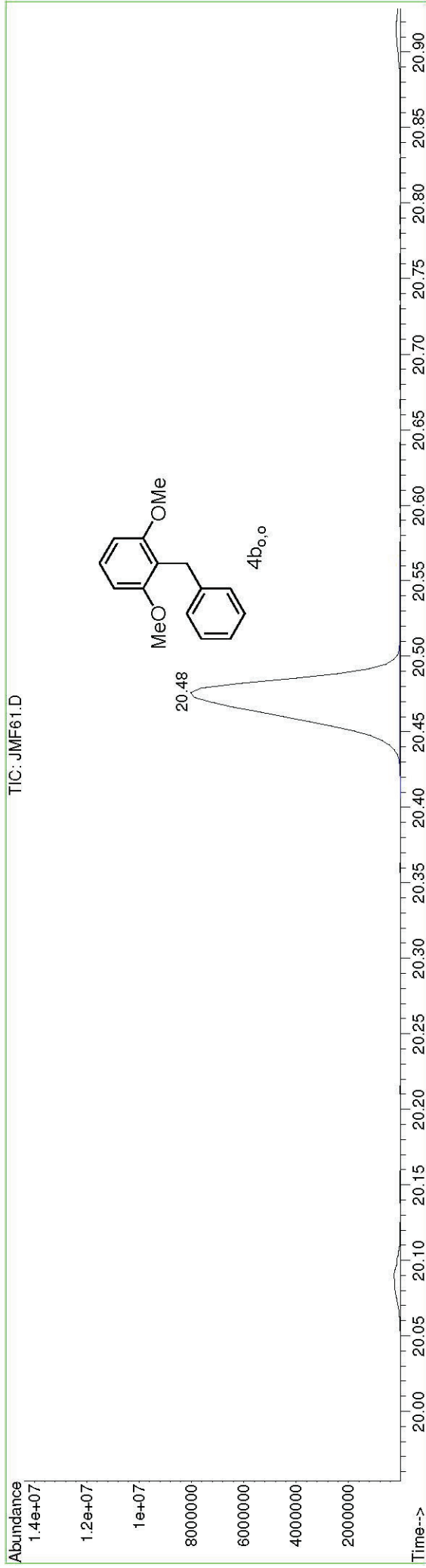
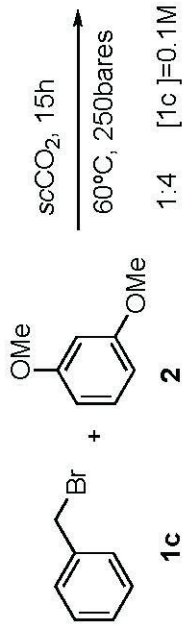
Acquired : 21 May 2012 22:49

Instrument : using AcqMethod JMF60

Sample Name :

Misc Info :

Vial Number: 18



File : D:\ASENSIO\JAUME\JMF61.D

Operator :

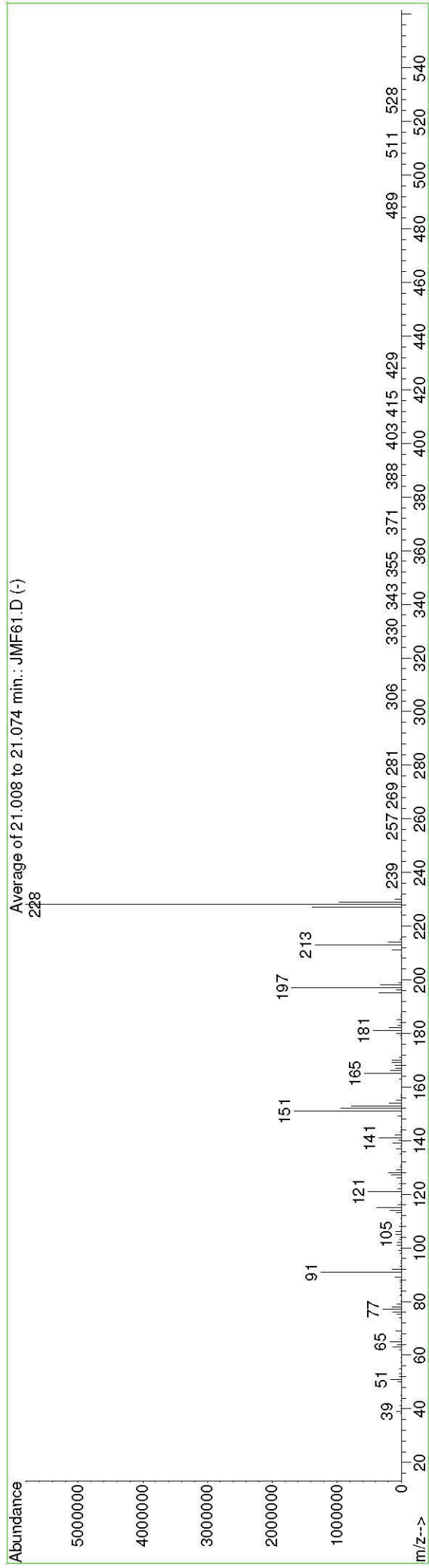
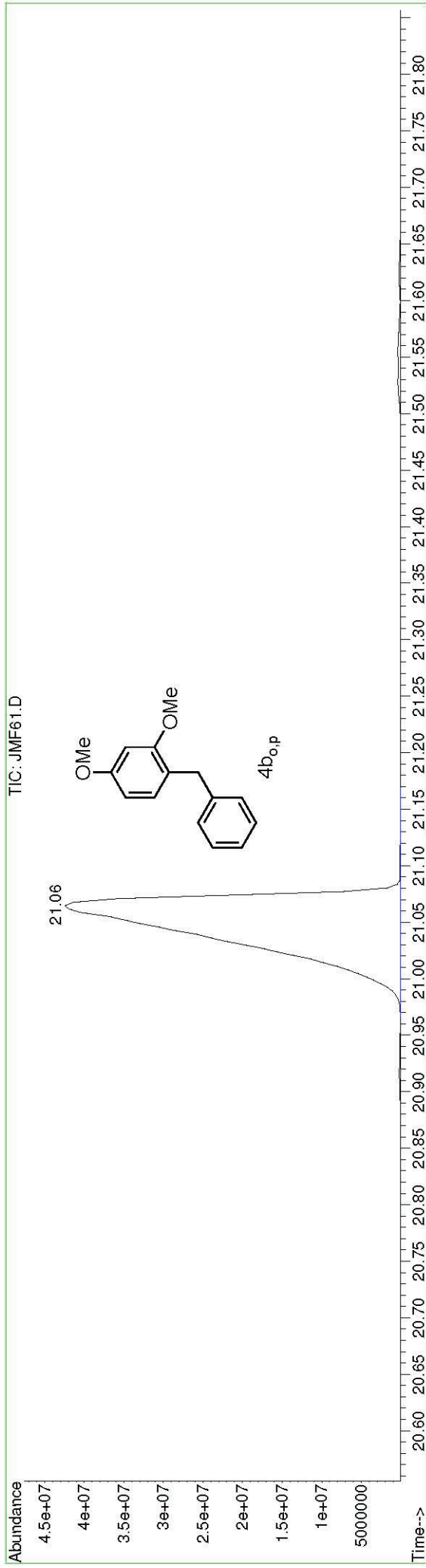
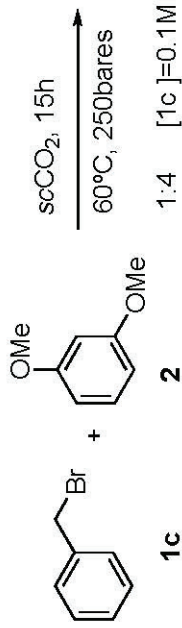
Acquired : 21 May 2012 22:49 using AcqMethod JMF60

Instrument : Instrumenten

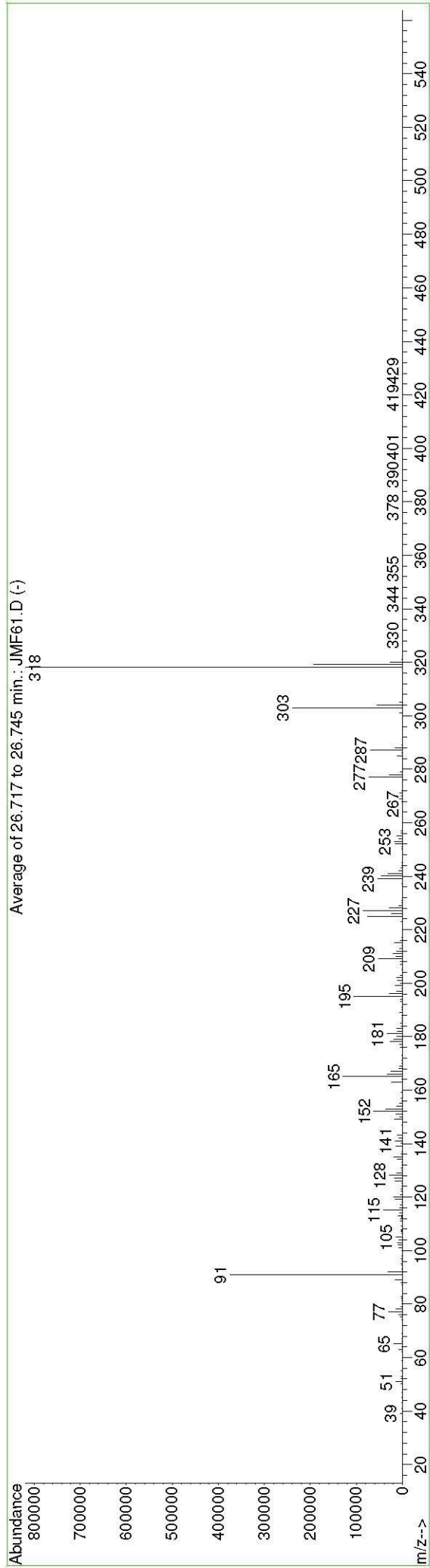
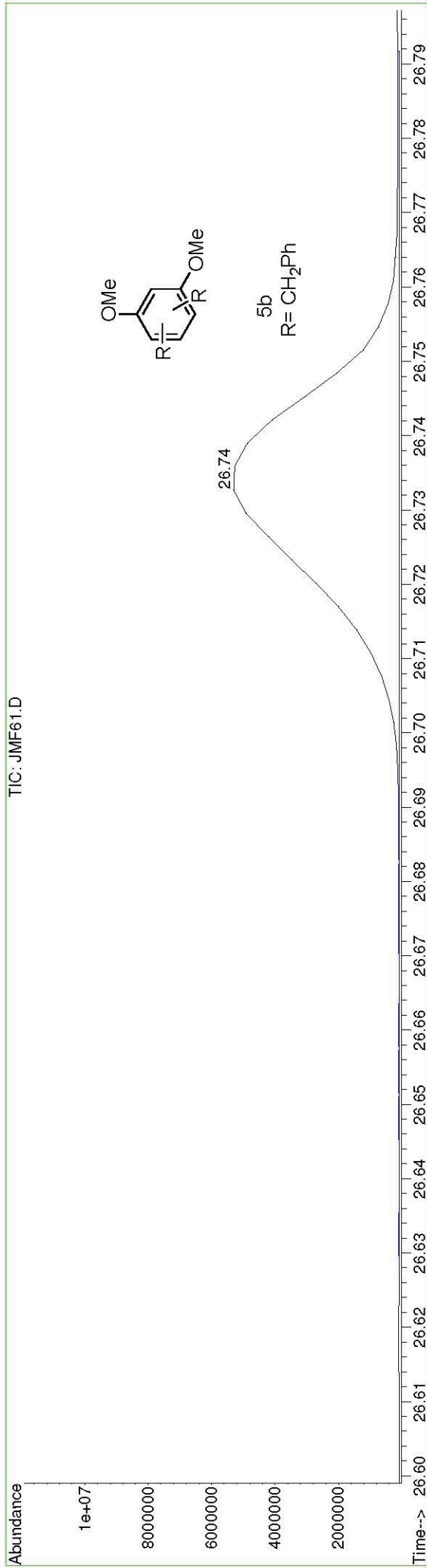
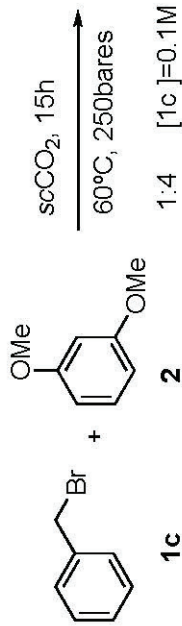
Sample Name:

Misc Info :

Vial Number: 18



File : D:\ASENSIO\JAUME\JMF61.D  
Operator :  
Acquired : 21 May 2012 22:49 using AcqMethod JMF60  
Instrument : Instrumenten  
Sample Name :  
Misc Info :  
Vial Number: 18



File : D:\ASENSIO\JAUME\JMF61.D

Operator :

Acquired : 21 May 2012 22:49

Instrument : using AcqMethod JMF60

Sample Name:

Misc Info :

Vial Number: 18

