

Supplementary Material

On the Ionizing Properties of Supercritical Carbon Dioxide: Uncatalyzed Electrophilic Bromination of Aromatics

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

General. Reagents and solvents were purified by standard procedures¹ and distilled before use. 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 CO₂, and a set of high-pressure valves, pressure and temperature probes, and rupture discs, suitably placed to control the flow of CO₂ along the system (Scheme S1). The reservoir was filled with Drierite.

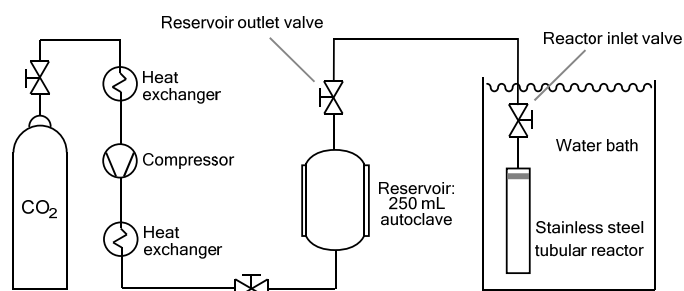
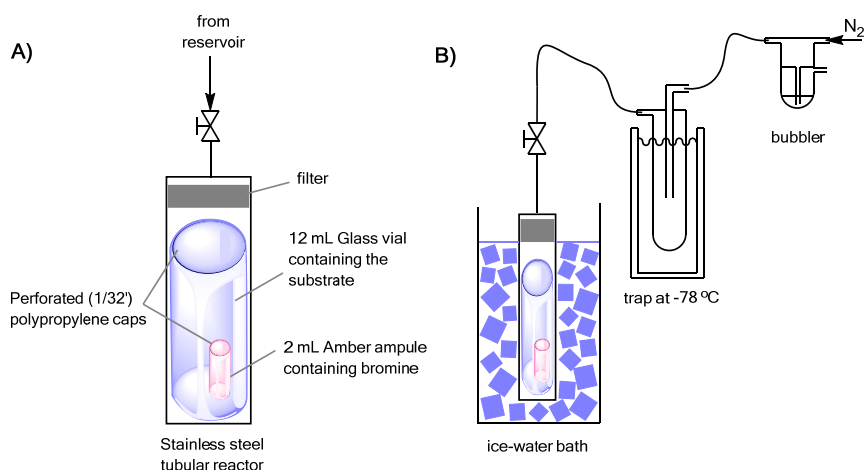


Figure S1. Schematic setup for standard experiments. Rupture discs, manometers, temperature probes, and fittings are not shown.

Reactions of bromine with aromatics 1 in scCO₂. General procedure. A 2 mL amber glass vial charged with bromine (0.123 mL, 2.4 mmol) and capped with a pierced (1/32') polypropylene top was placed inside a 12 mL glass vial containing toluene (0.763 mL, 7.2 mmol). The glass vial was then fitted with a drilled (1/32') polypropylene cap and inserted into a 33 mL stainless

steel tubular reactor (Scheme S2A). The system was closed and connected to the reservoir through a high pressure valve. The reactor was tightly closed with a stainless steel filter placed on the upper end of the column, and connected through a high-pressure valve to the 250 mL autoclave outlet valve. The reactor remained in a vertical position throughout all these operations to prevent mixing the reaction components prior to pressurization. The reservoir was charged with CO₂ and pressurized. When the reservoir reached *ca.* 170 bar, the reactor was placed in a water bath heated to 40°C, and was then connected to the reservoir by opening the valve. The system was then allowed to pressurize to 250 bar. After closing the valves and venting the line, the reactor inlet valve was disconnected from the line and the high pressure reactor was allowed to stand at 40°C for 2 h. Afterward, 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 (Scheme S2B). The internal walls of the glass vial and the ampule were washed with 20 mL of either a 1:1 mixture of dichloromethane and acetone, or a 0.84 M dichloromethane solution of cyclohexene, as bromine quenchers. A 0.5 mL aliquot of the resulting solution was diluted with 2.5 mL of dichloromethane. The samples for gas chromatography and mass spectrometry analysis were prepared by mixing 0.5 mL of the latter solution with 0.5 mL of a 0.02 M dichloromethane solution of adamantane as an external standard. The analysis to determine substrate conversion and products distribution was performed after treating the sample with sodium bicarbonate and sodium sulfate. The reaction products were identified by comparison with authentic commercial samples. The external walls of the glass vial, the stainless steel reactor, the outlet valve and the cold trap were washed separately with 20 mL of the dichloromethane solutions of bromine quenchers. The resulting solutions were treated as described above, and were then analyzed by gas chromatography and mass spectrometry to determine the organic material lost from the glass vial under the reaction conditions. Mass balances were found to be >95 % in all cases.

Control experiments in liquid carbon dioxide were performed as described above until the pressurization stage was completed. After closing the valves and venting the line, the reactor inlet valve was disconnected from the line, and the high pressure reactor was cooled to 0°C and maintained at this temperature for 2 h. Afterward, the reactor was depressurized and the reaction mixture was analyzed following the procedures described above.



Scheme S2. Schematic setup for (A) the bromination of aromatics **1** in scCO₂ and (B) the depressurization stage.

Reactions of bromine with aromatics 1 in conventional solvents. General procedure. Bromine (12.1 μ L, 0.24 mmol) was added to 1.2 mL of a 0.6 M solution of substrate **1** in the selected solvent (glacial acetic acid, trifluoroacetic acid, carbon tetrachloride, 85% v/v aqueous acetic acid, 85% v/v aqueous trifluoroacetic acid) contained in an amber glass reactor thermostatted at 40°C. The reactor was tightly closed, stirred and placed inside a water bath at 40°C for 2 h. The reaction mixture was treated with 10.56 mL of either a 1:1 mixture of dichloromethane and acetone, or a 0.84 M dichloromethane solution of cyclohexene, as bromine quenchers. A 0.5 mL aliquot of the resulting solution was mixed with 0.5 mL of a 0.02 dichloromethane solution of adamantane as an external standard. The gas chromatography and mass spectrometry analyses to determine the substrate conversion and products distribution were performed after treating the sample with sodium bicarbonate and sodium sulfate. For the reactions performed in acetic and trifluoroacetic acids, samples were cooled to 0°C before the neutralization step.

Bromobenzene (2a) [108-86-1]. EM (EI+, 70ev): m/z (rel abund) 51 (29), 62 (2), 74 (14), 77 (100), 93 (1), 106 (1), 117 (1), 129 (1), 141 (1), 156 (73).

2-Bromotoluene (2b_o) [95-46-5]. EM (EI+, 70ev): m/z (rel abund) 39 (7), 45 (1), 50 (5), 65 (14), 74 (2), 81 (1), 86 (2), 89 (23), 91 (100), 117 (1), 143 (1), 170 (45), 172 (44).

4-Bromotoluene (2b_p) [106-38-7]. EM (EI+, 70ev): m/z (rel abund) 39 (5), 45 (1), 50 (6), 65 (17), 74 (2), 81 (1), 86 (2), 89 (14), 91 (100), 117 (1), 143 (1), 170 (50), 172 (47).

(Bromomethyl)benzene (2b_a) [100-39-0]. EM (EI+, 70ev): m/z (rel abund) 39 (5), 45 (1), 51 (5), 65 (18), 74 (1), 81 (1), 86 (1), 91 (100), 170 (17), 172 (15).

1-Bromoethylbenzene (2c_a) [585-71-7]. EM (EI+, 70ev): m/z (rel abund) 51 (11), 63 (5), 74 (2), 79 (34), 89 (2), 105 (100), 169 (1), 184 (1), 186 (1).

2-Bromoethylbenzene (2c_o) [9173-22-4]. EM (EI+, 70ev): m/z (rel abund) 15 (3), 27 (6), 39 (11), 51 (35), 63 (23), 77 (42), 89 (23), 105 (100), 169 (64), 171 (62), 184 (37), 186 (36).

4-Bromoethylbenzene (2c_p) [1585-07-5]. EM (EI+, 70ev): m/z (rel abund) 39 (4), 51 (12), 63 (9), 77 (17), 90 (18), 105 (68), 169 (100), 171 (97), 184 (54), 186 (53).

1-Bromo-2-isopropylbenzene (2d_o) [7073-94-1]. EM (EI+, 70ev): m/z (rel abund) 39 (10), 51 (18), 63 (10), 77 (32), 104 (88), 115 (10), 169 (3), 183 (100), 185 (96), 198 (37), 200 (36).

1-Bromo-4-isopropylbenzene (2d_p) [586-61-8]. EM (EI+, 70ev): m/z (rel abund) 39 (6), 51 (14), 63 (6), 77 (22), 91 (14), 104 (90), 115 (5), 119 (18), 143 (1), 145 (1), 156 (1), 169 (2), 171 (2), 183 (100), 185 (96), 198 (37), 200 (36).

4-Bromo-tert-butylbenzene (2e_p) [3972-65-4]. EM (EI+, 70ev): m/z (rel abund) 41 (10), 51 (6), 58 (5), 77 (8), 91 (8), 102 (11), 118 (29), 133 (1), 157 (2), 159 (1), 169 (25), 171 (24), 181 (2), 183 (2), 197 (100), 199 (95), 212 (23), 214 (22).

4-Bromo-1,2-dimethylbenzene (2f₄) [583-71-1]. EM (EI+, 70ev): m/z (rel abund) 39 (6), 51 (12), 63 (10), 77 (22), 89 (6), 105 (100), 169 (11), 171 (11), 184 (52), 186 (49).

4,5-Dibromo-1,2-dimethylbenzene (2f_{4,5}) [24932-48-7]. EM (EI+, 70ev): m/z (rel abund) 39 (17), 44 (6), 51 (40), 63 (23), 69 (1), 77 (48), 89 (7), 104 (43), 117 (1), 131 (3), 143 (1), 168 (1), 185 (51), 249 (9), 264 (100).

1,2-bis(Bromomethyl)benzene (2f_{αα}) [91-13-4]. EM (EI+, 70ev): m/z (rel abund) 39 (4), 51 (12), 63 (6), 78 (17), 91 (1), 104 (90), 160 (1), 171 (1), 183 (100), 185 (98), 264 (15).

2-Bromo-1,4-dimethylbenzene (2g₂) [553-94-6]. EM (EI+, 70ev): m/z (rel abund) 15 (2), 27 (5), 39 (10), 51 (28), 63 (14), 74 (7), 77 (30), 89 (6), 105 (100), 169 (5), 171 (5), 184 (41), 186 (40).

2,5-Dibromo-1,4-dimethylbenzene (2g_{2,5}) [1074-24-4]. EM (EI+, 70ev): m/z (rel abund) 39 (3), 51 (22), 63 (10), 77 (26), 87 (4), 103 (34), 117 (1), 131 (2), 143 (1), 183 (63), 185 (60), 249 (1), 264 (100).

1-(Bromomethyl)-4-methylbenzene (2g_α) [104-81-4]. EM (EI+, 70ev): m/z (rel abund) 27 (3), 39 (4), 51 (7), 63 (10), 77 (10), 91 (2), 105 (100), 119 (1), 169 (1), 184 (7), 186 (7).

4-Bromobiphenyl (2h_p) [92-66-0]. EM (EI+, 70ev): m/z (rel abund) 27 (1), 39 (3), 50 (7), 63 (12), 76 (30), 87 (3), 102 (4), 116 (4), 126 (7), 152 (93), 232 (100).

4,4'-Dibromobiphenyl (2h_{p,p}) [92-86-4]. EM (EI+, 70ev): m/z (rel abund) 39 (1), 50 (3), 63 (3), 76 (12), 87 (1), 101 (2), 113 (1), 126 (6), 152 (63), 180 (1), 204 (1), 232 (1), 312 (100).

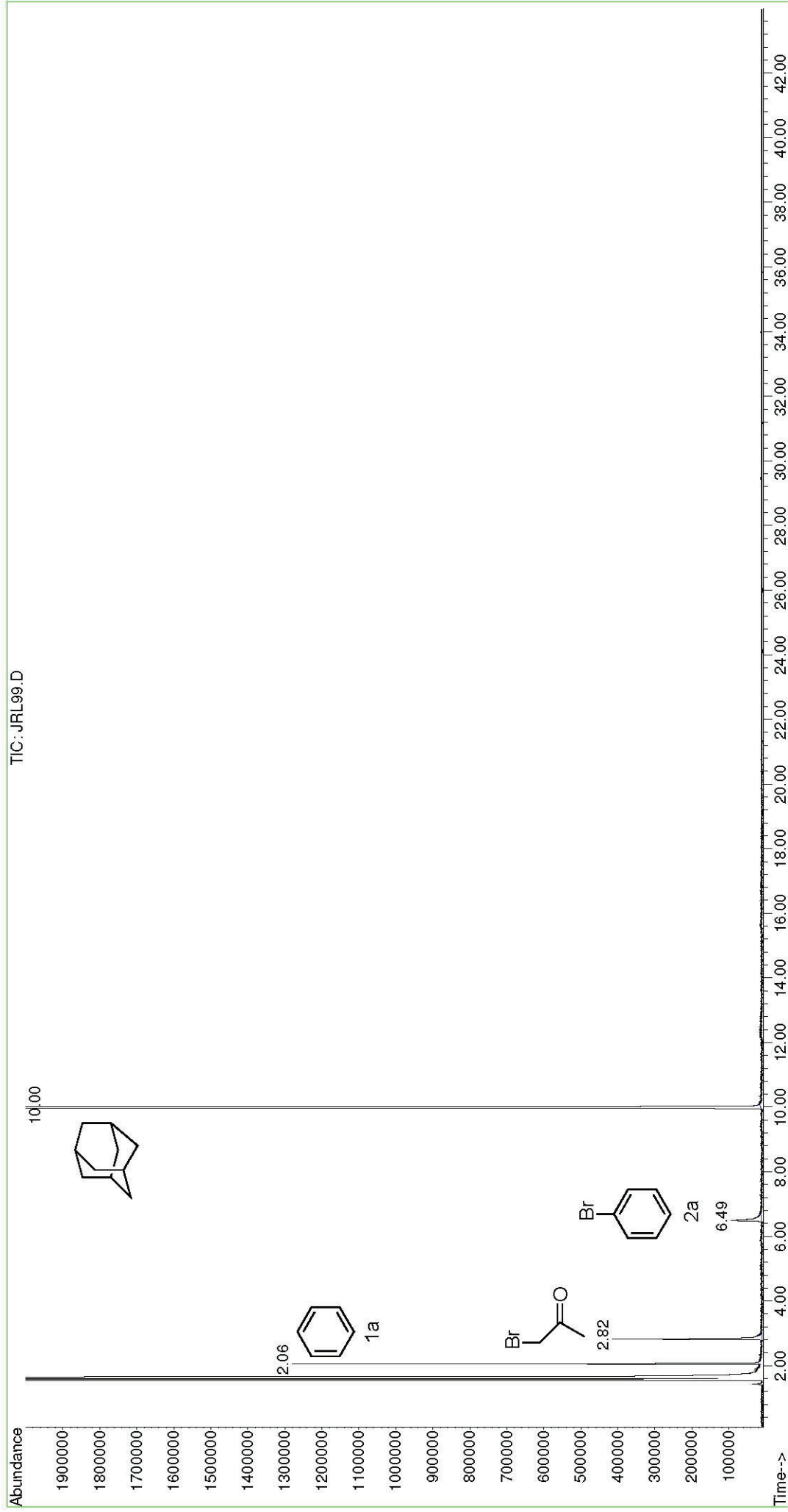
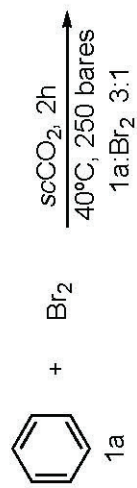
4-Bromo-1-fluorobenzene (2i_p) [460-00-4]. EM (EI+, 70ev): m/z (rel abund) 31 (1), 37 (2), 50 (13), 62 (4), 68 (7), 75 (41), 81 (1), 87 (4), 95 (90), 104 (1), 117 (1), 128 (1), 143 (1), 155 (1), 174 (100), 176 (97).

References

1. Perrin, D. D. & Armarego, W. L. F. *Purification of Laboratory Chemicals*, 3rd Edition, Pergamon Press, New York, **1988**.

GC-MS spectra are shown in pages S5-S197

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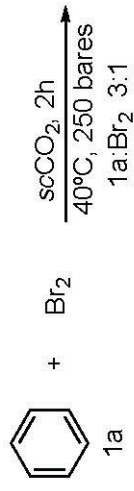
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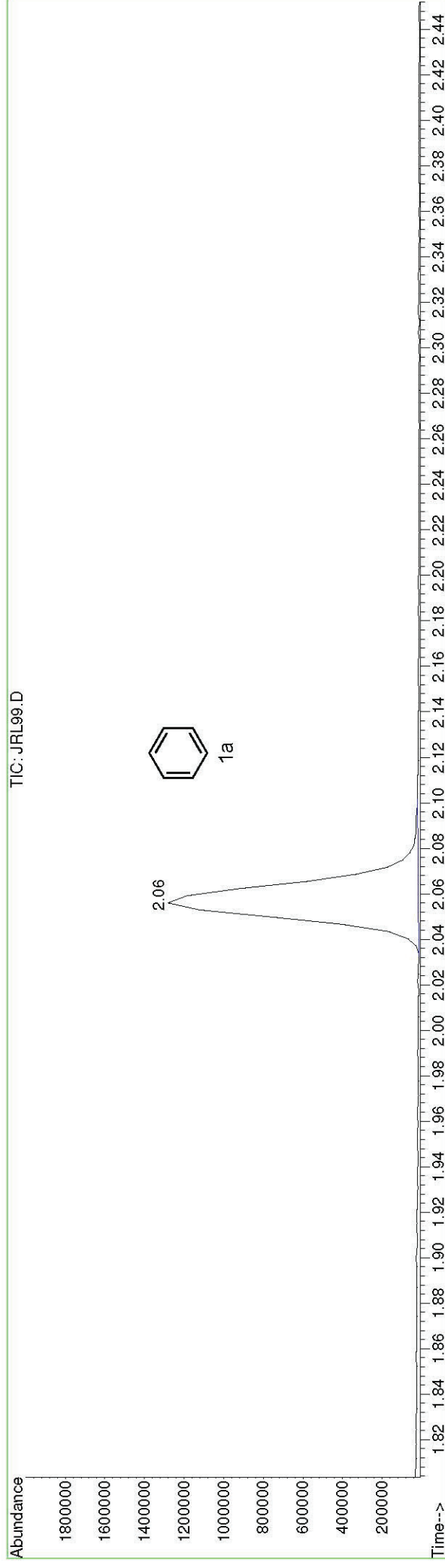
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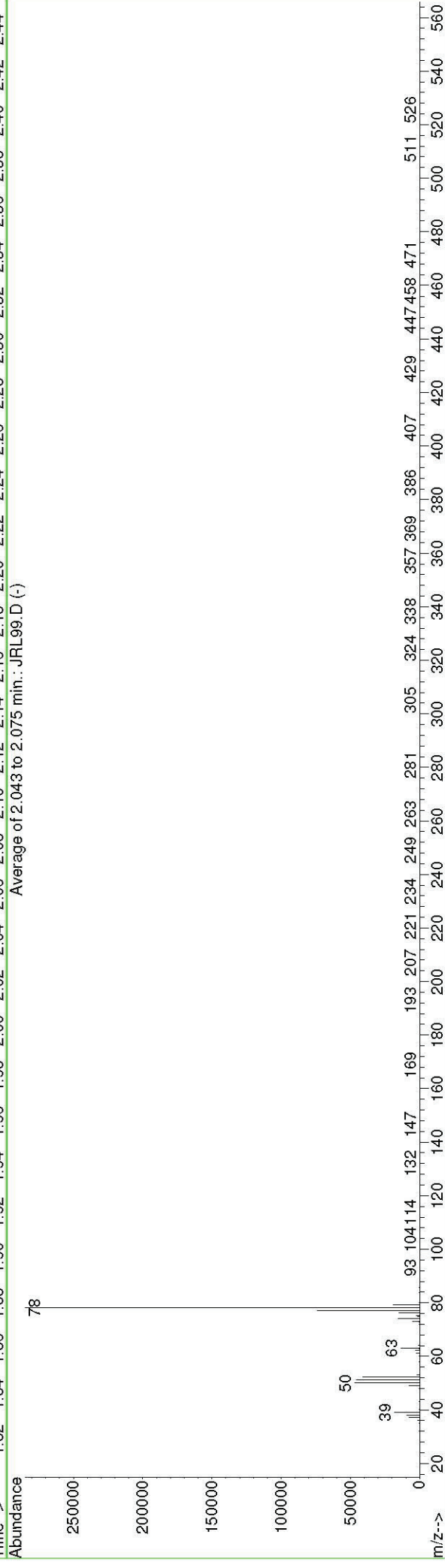
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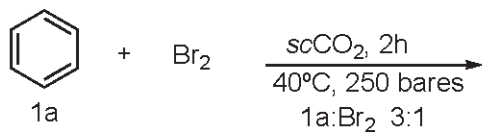


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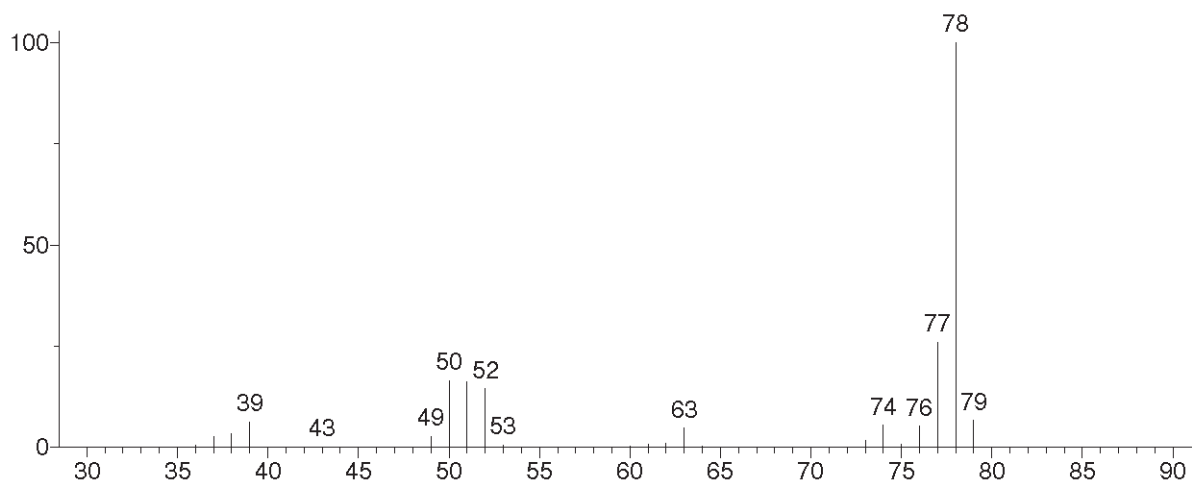
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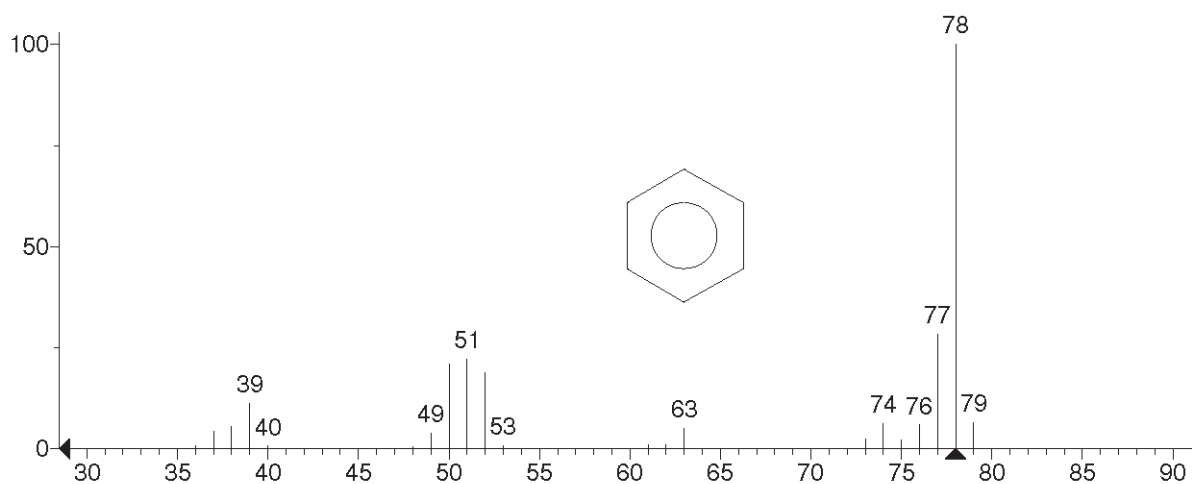


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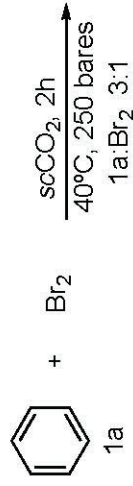
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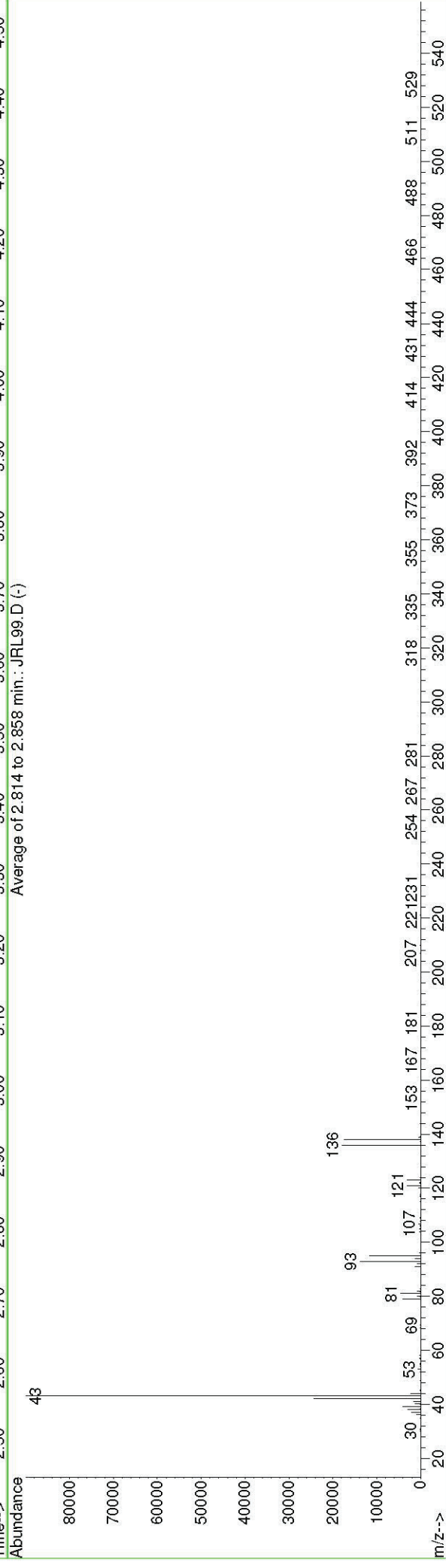
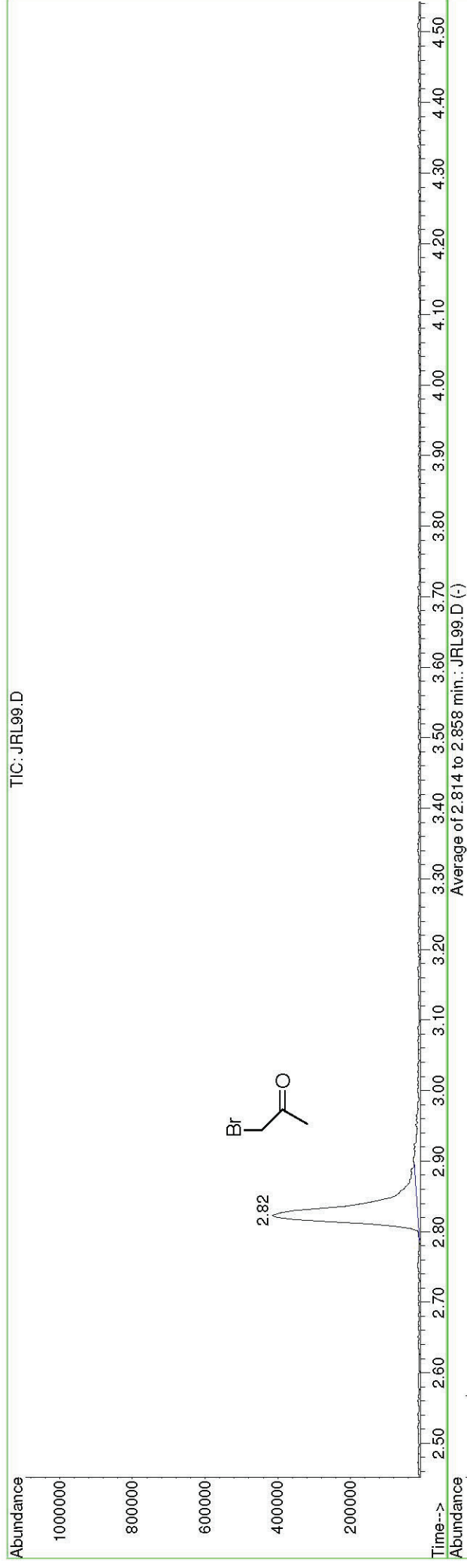
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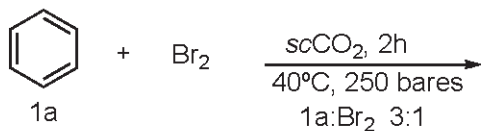
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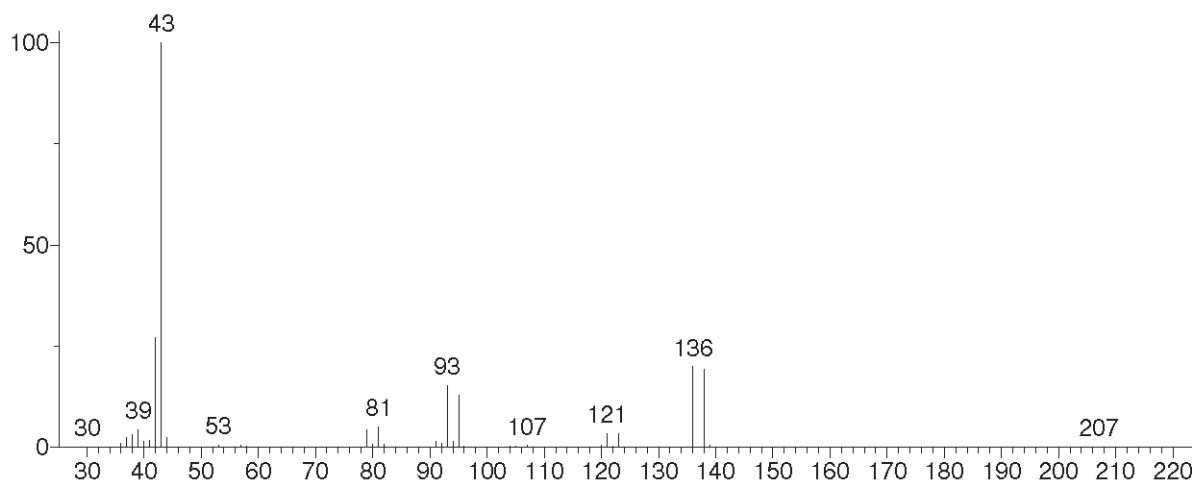
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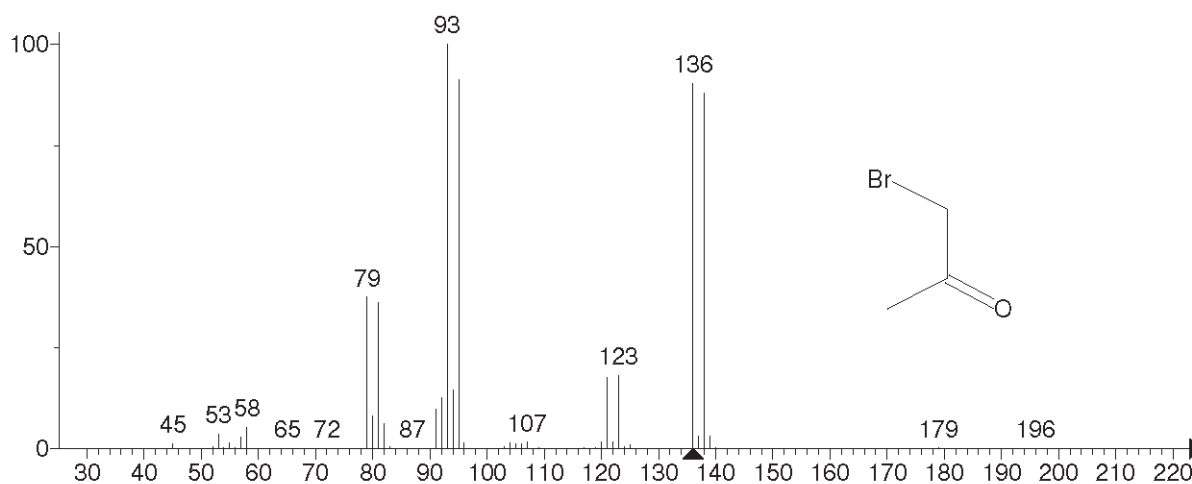


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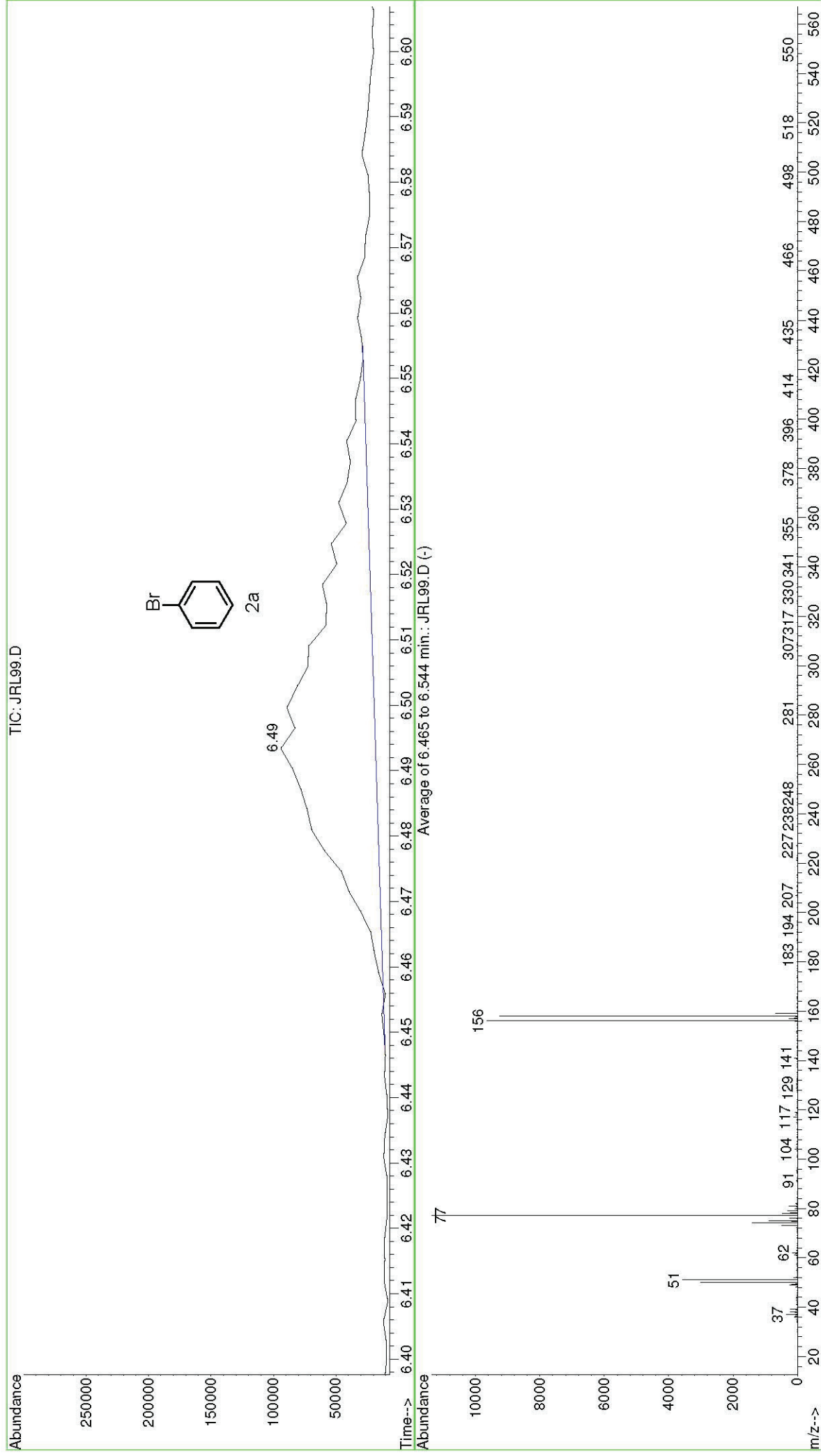
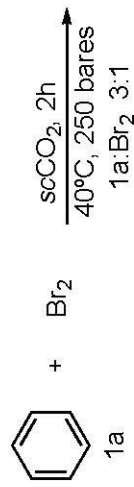
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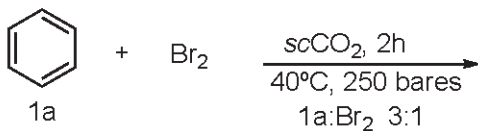


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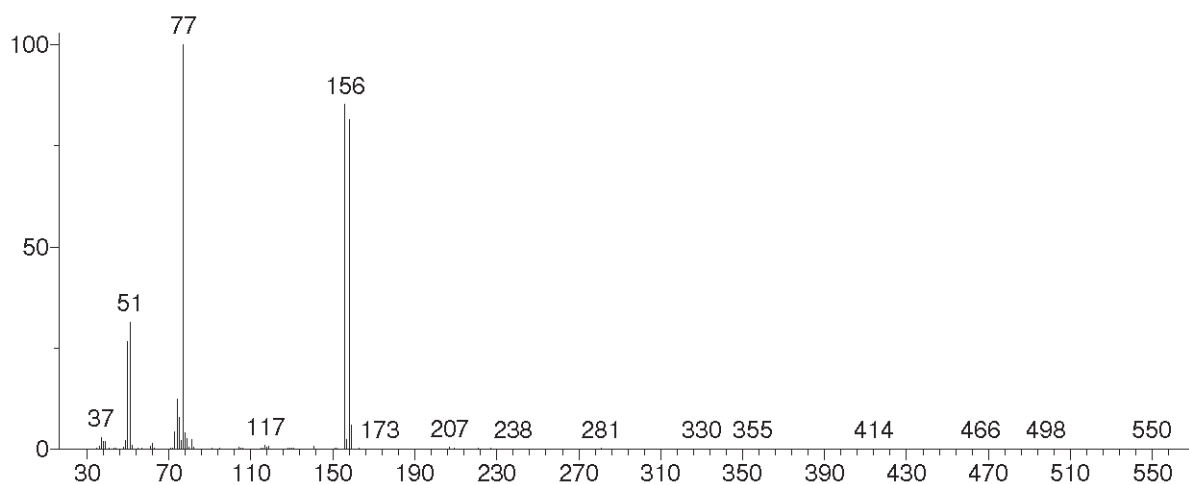




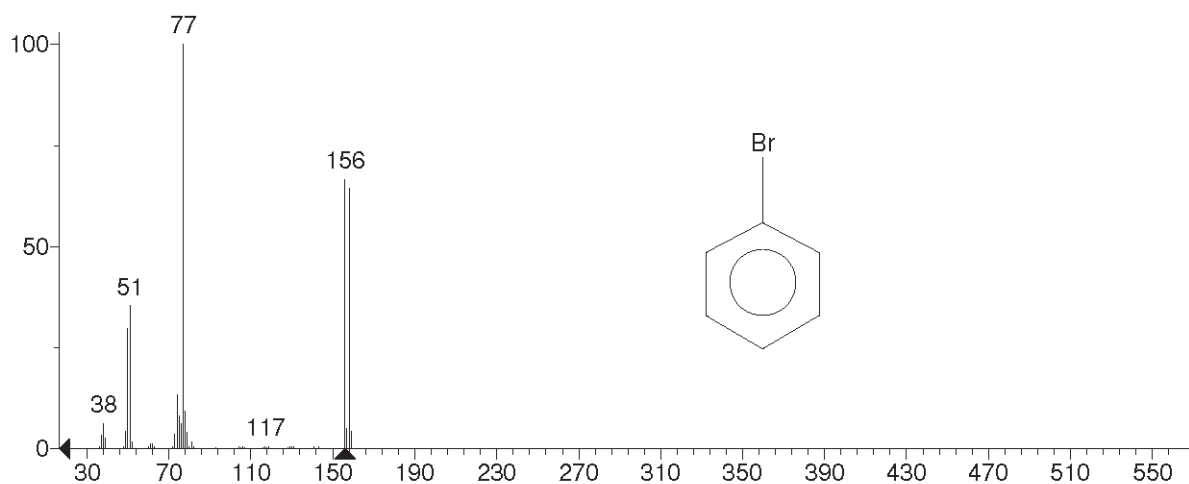
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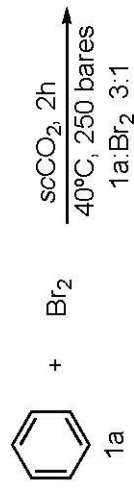
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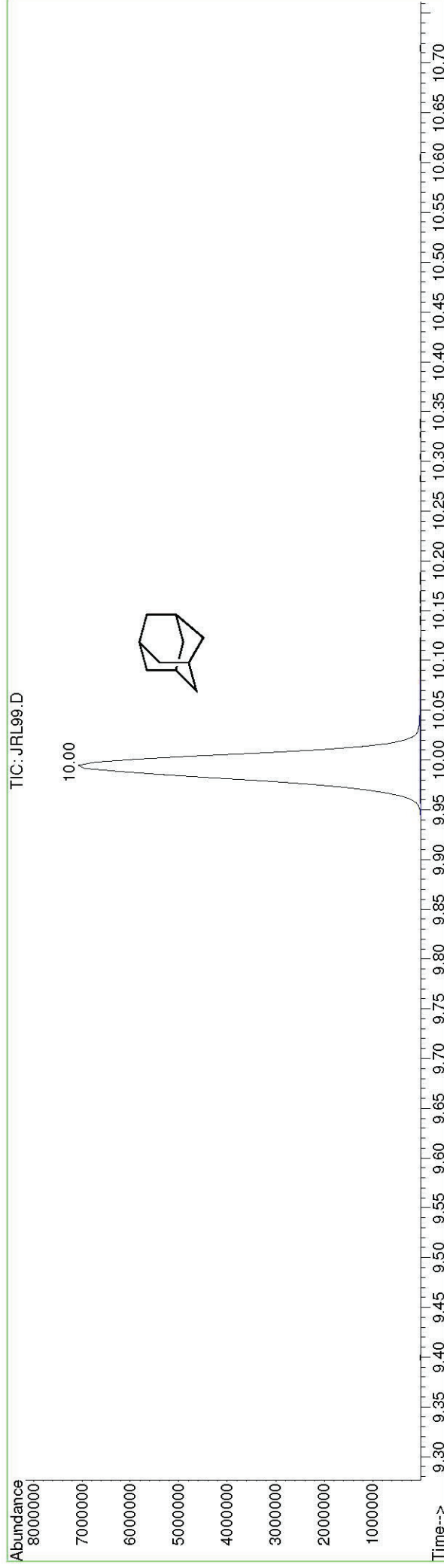
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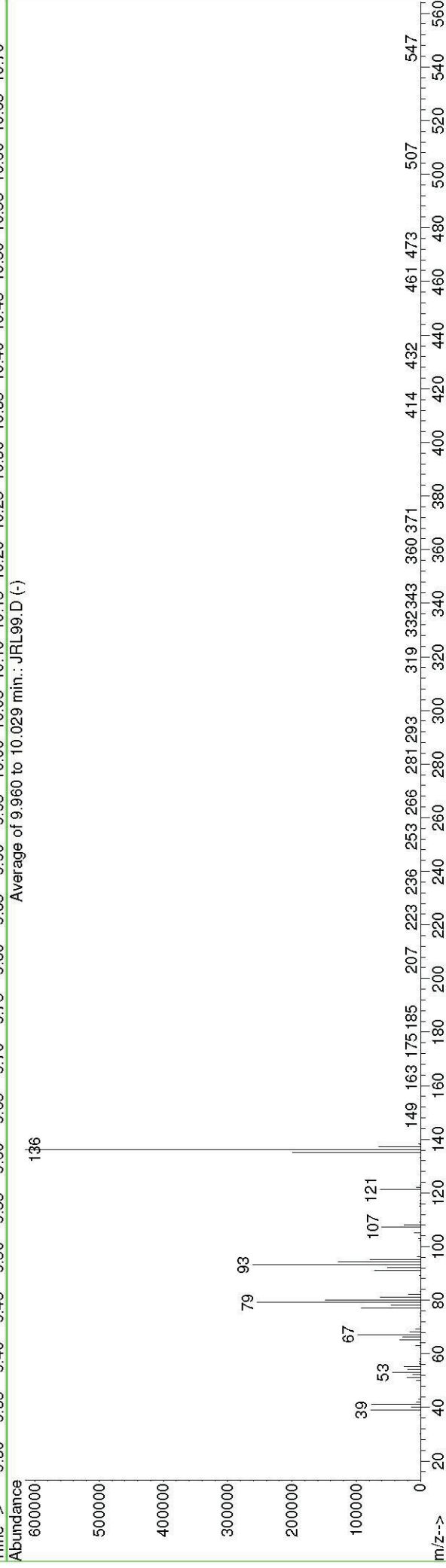
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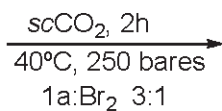


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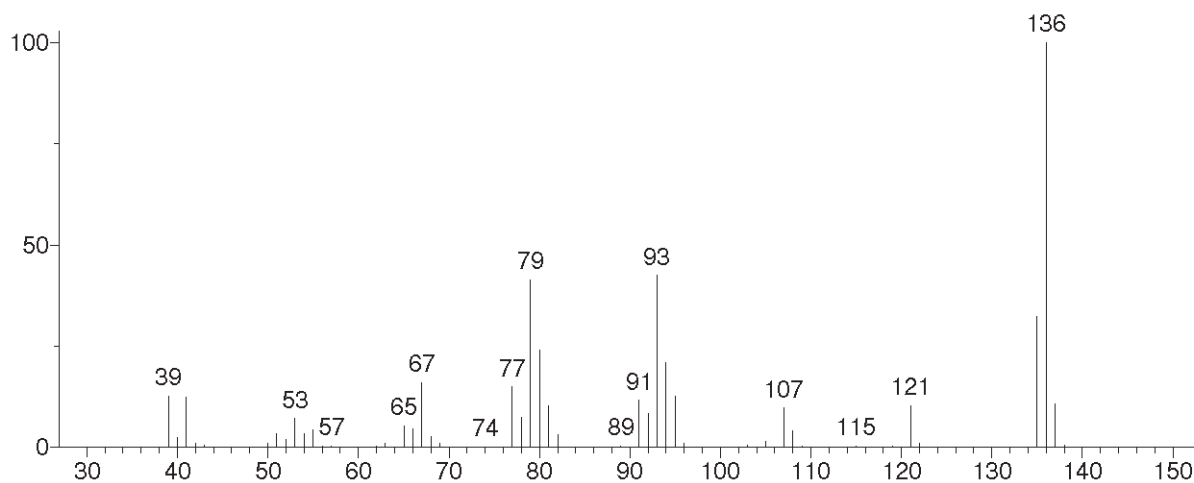
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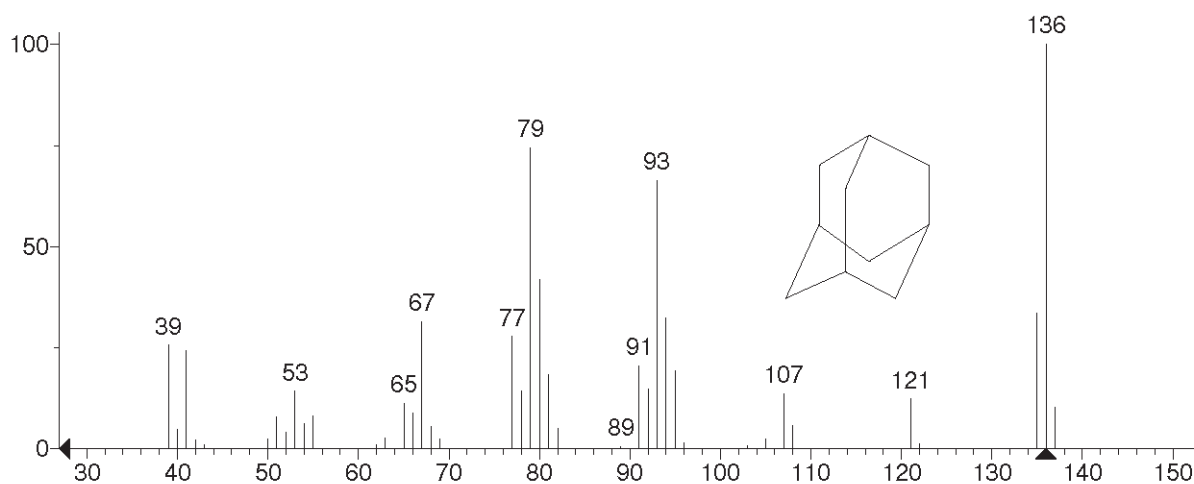
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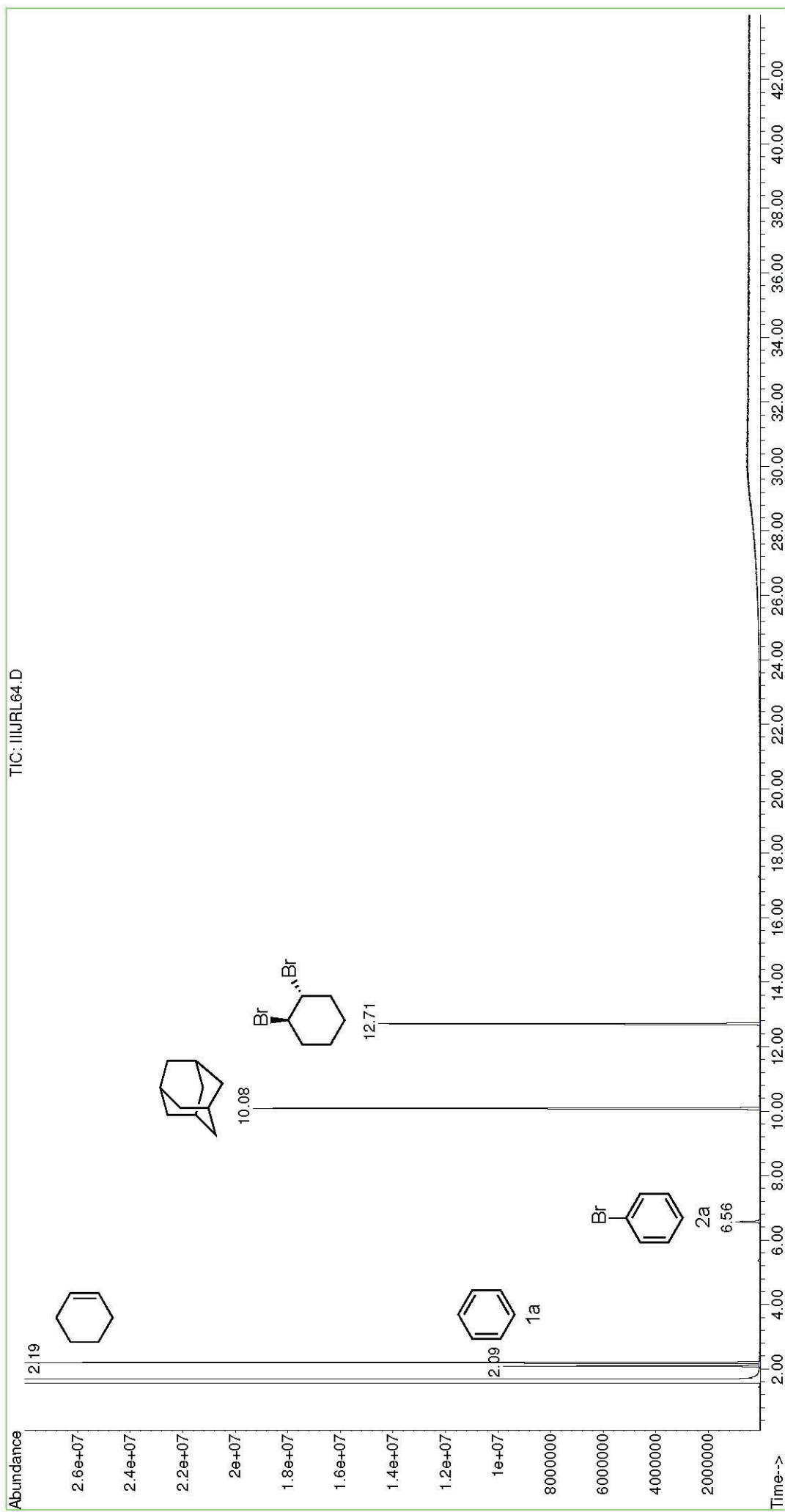
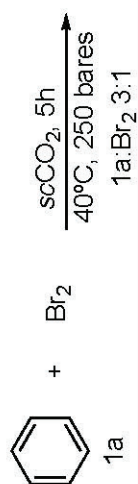
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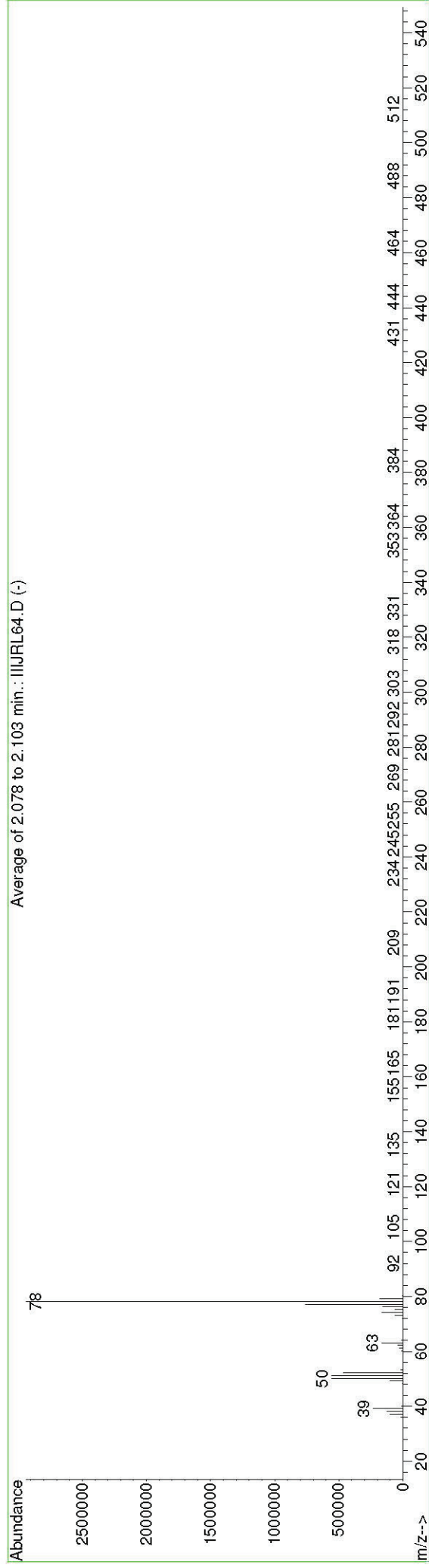
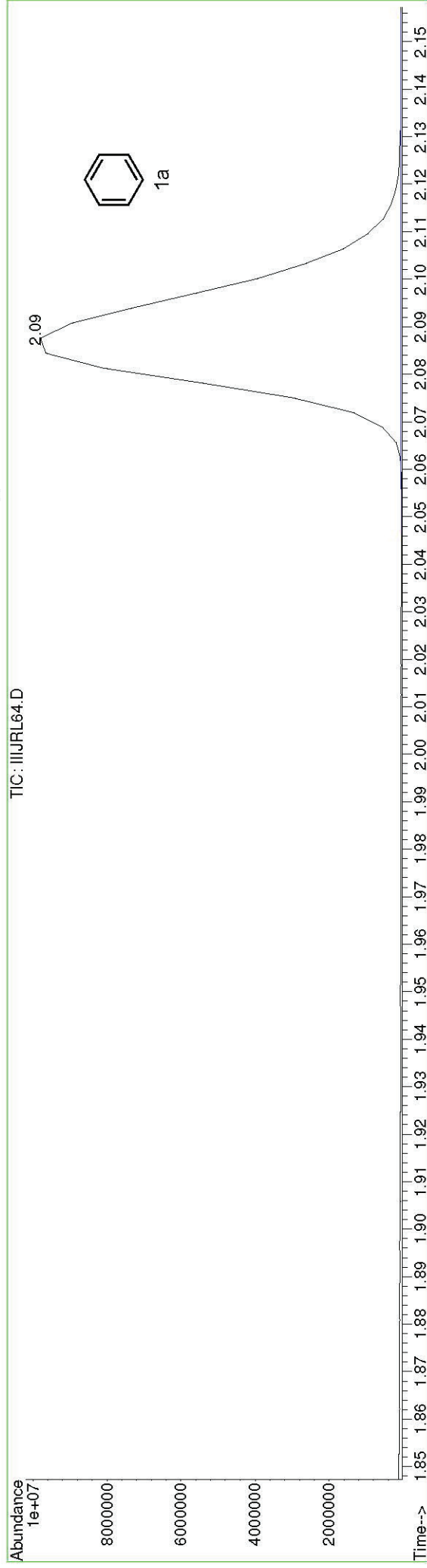
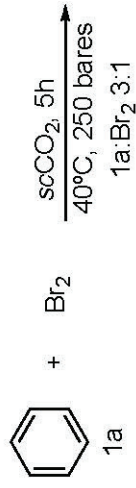
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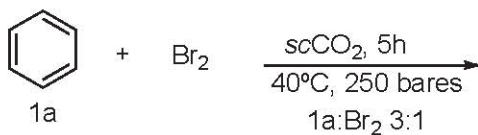
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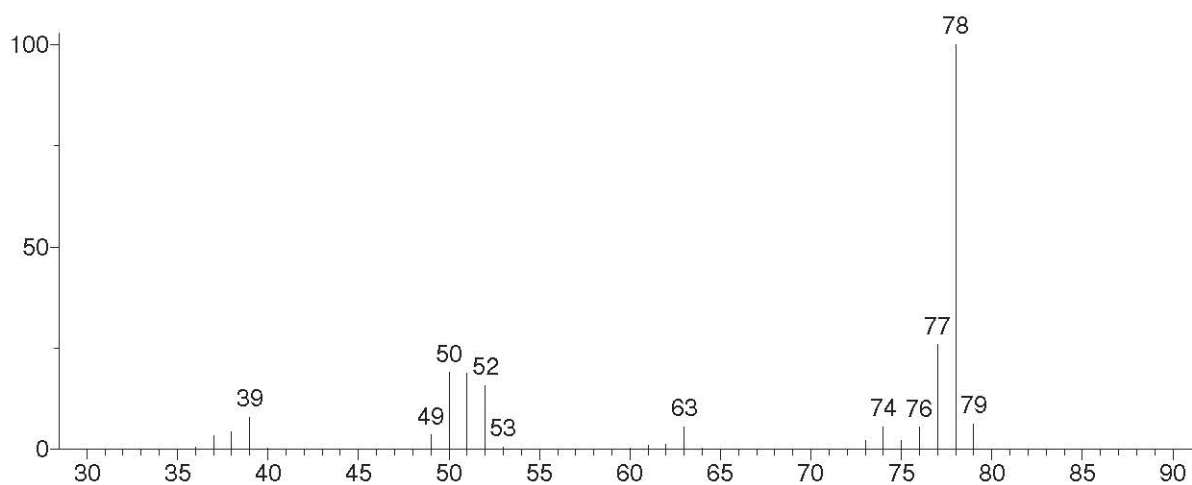
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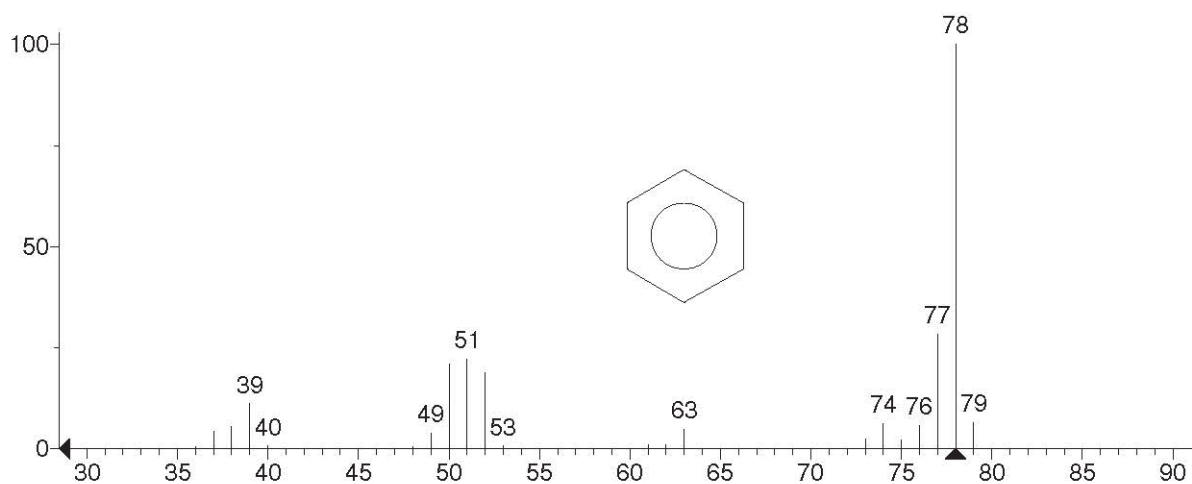


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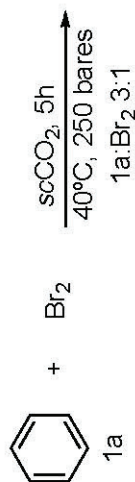
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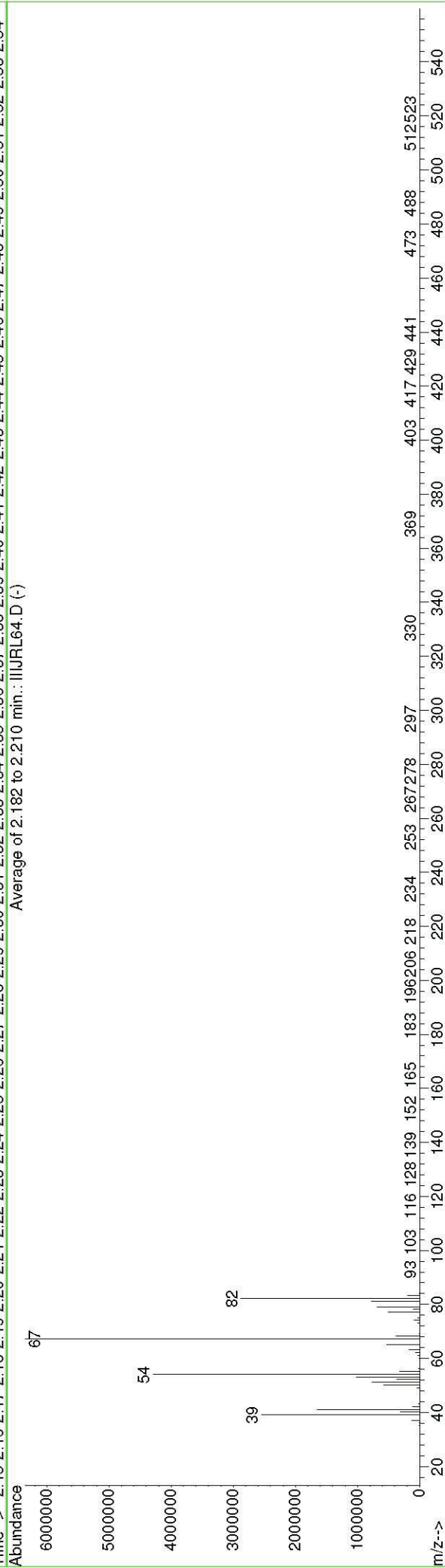
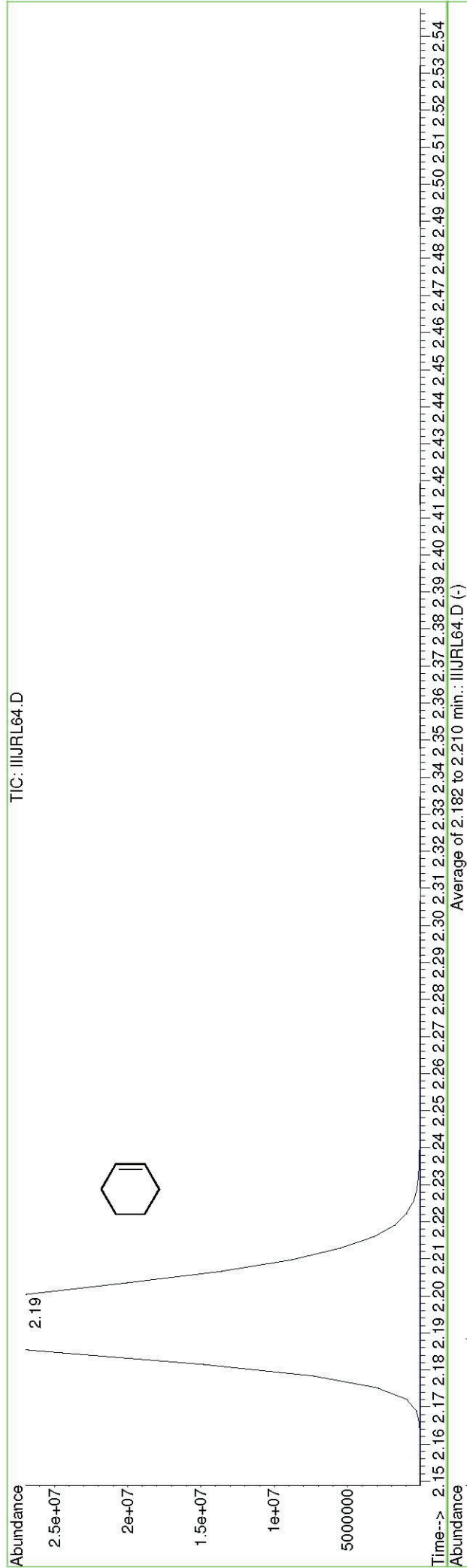
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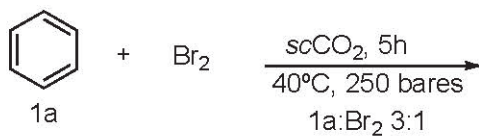


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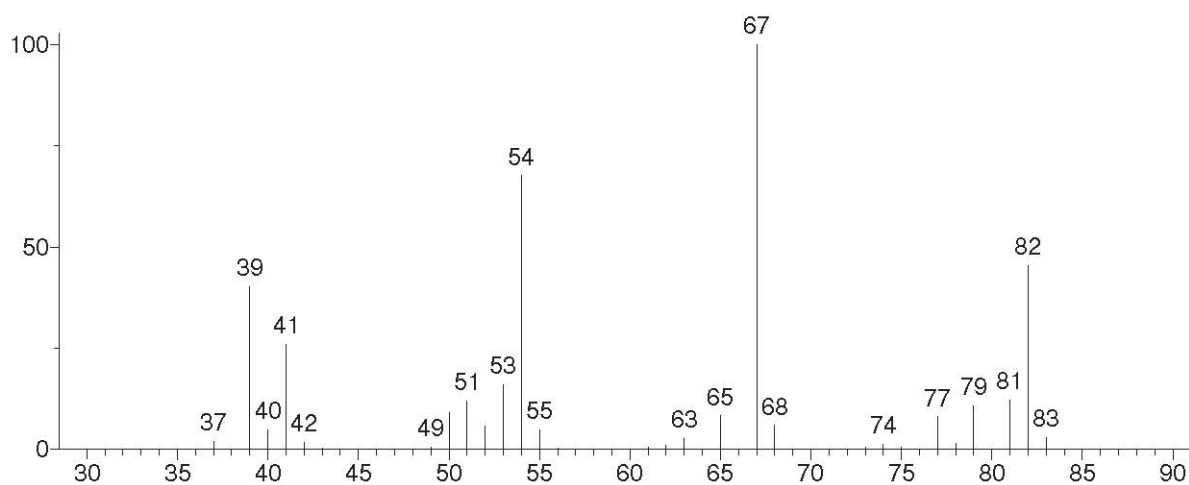
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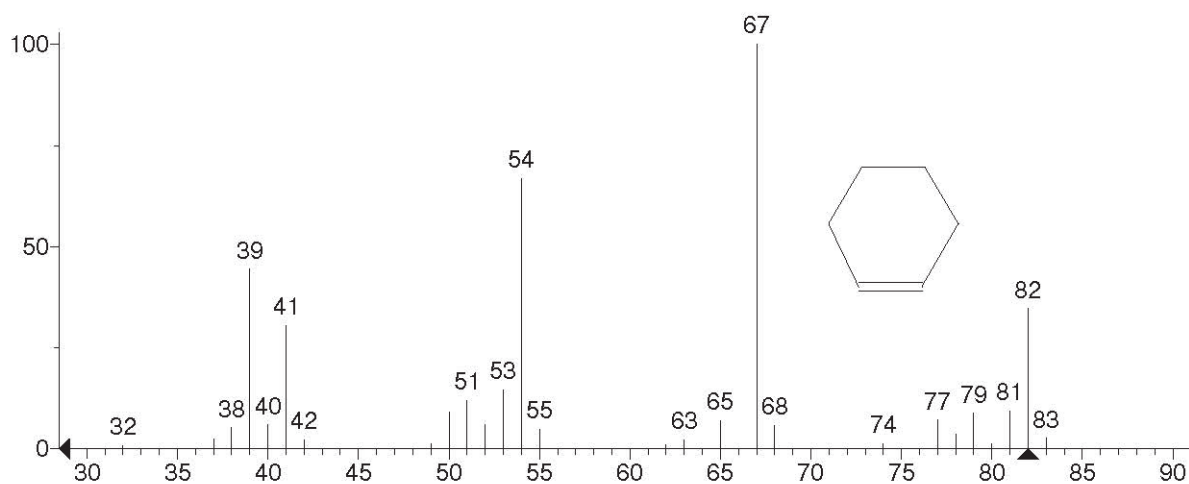


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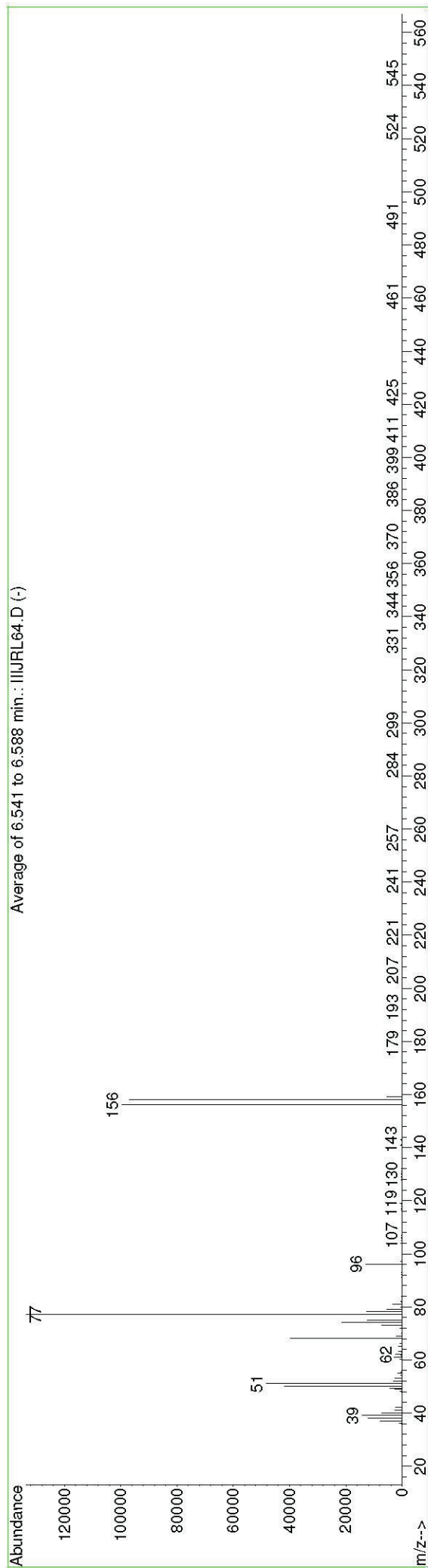
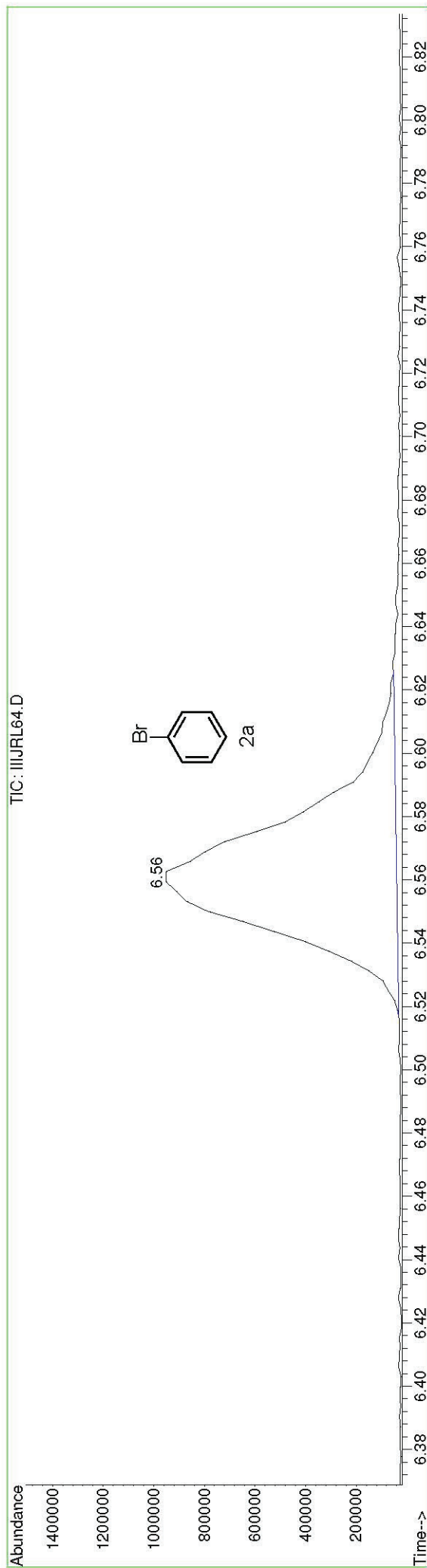
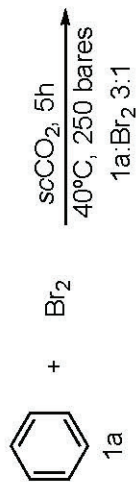
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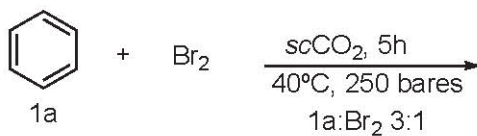
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Sample Name: VIDRIO

Misc Info :

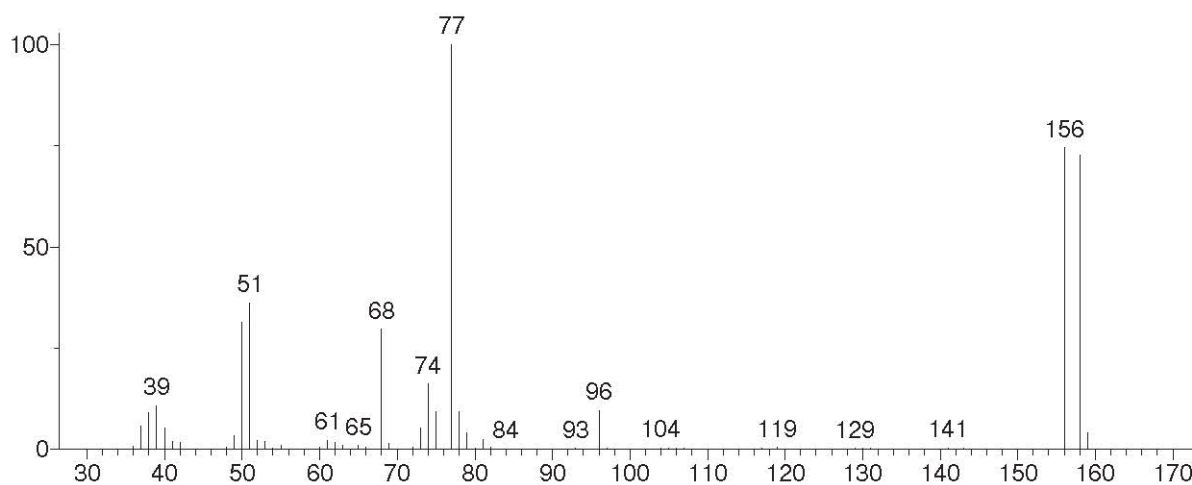
Vial Number: 20



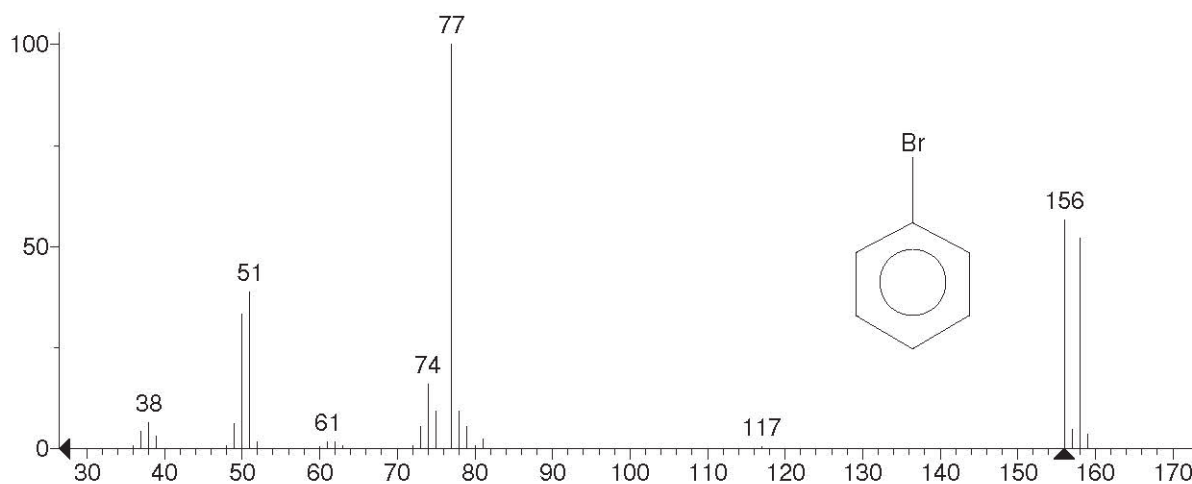


** Search Report Page 1 of 1 **

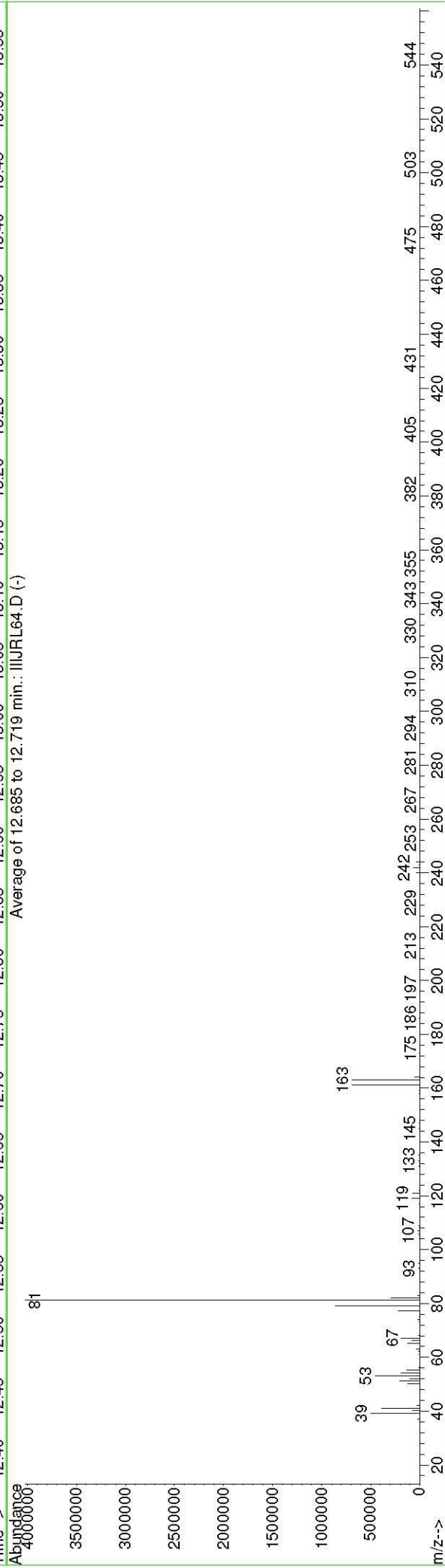
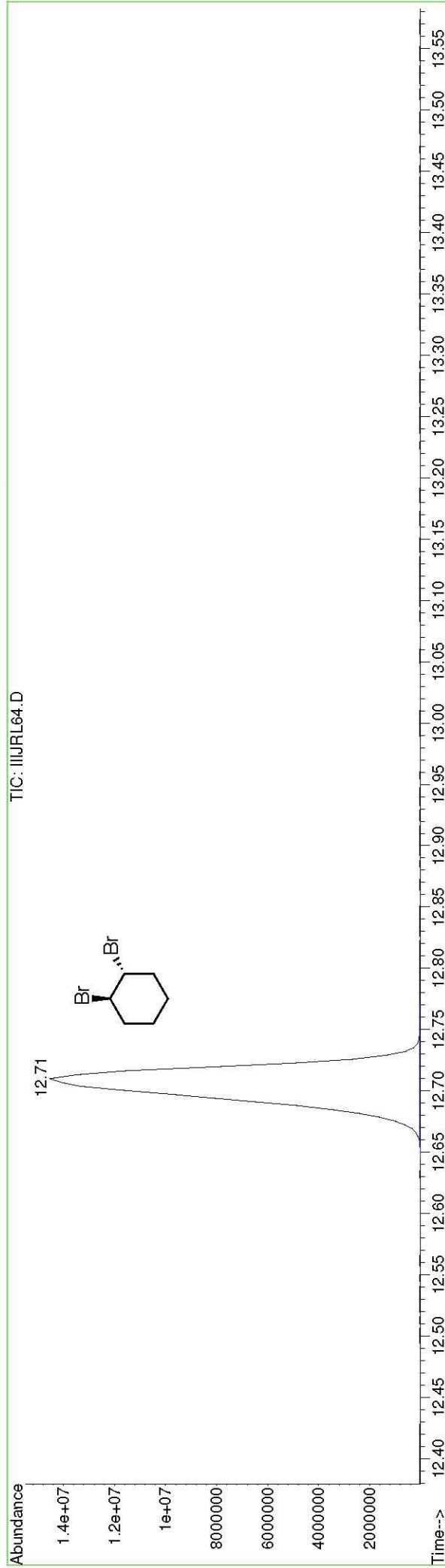
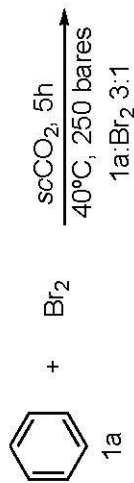
Unknown: Average of 6.541 to 6.588 min.: IIIJRL64.D
Compound in Library Factor = 400

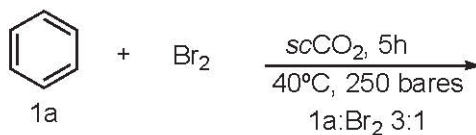


Hit 1 : Benzene, bromo-
C₆H₅Br; MF: 881; RMF: 932; Prob 97.5%; CAS: 108-86-1; Lib: wiley7n; ID: 54585.



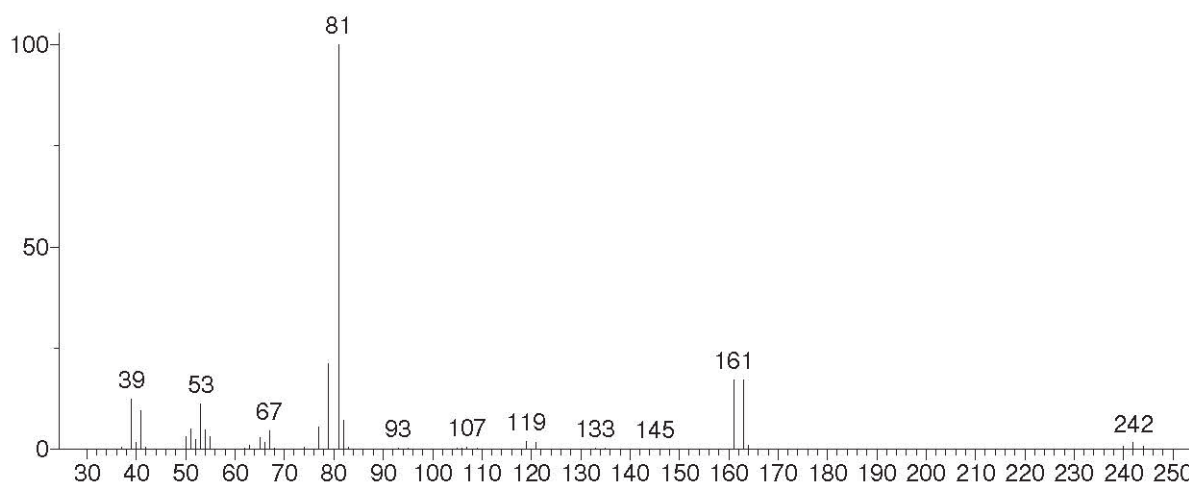
File : D:\ASENSIO\MATEO\IIIJRL64.D
Operator :
Acquired : 16 Jun 2014 22:37 using AcqMethod JMF60
Instrument : Instrument
Sample Name : VIDRIO
Misc Info :
Vial Number: 20



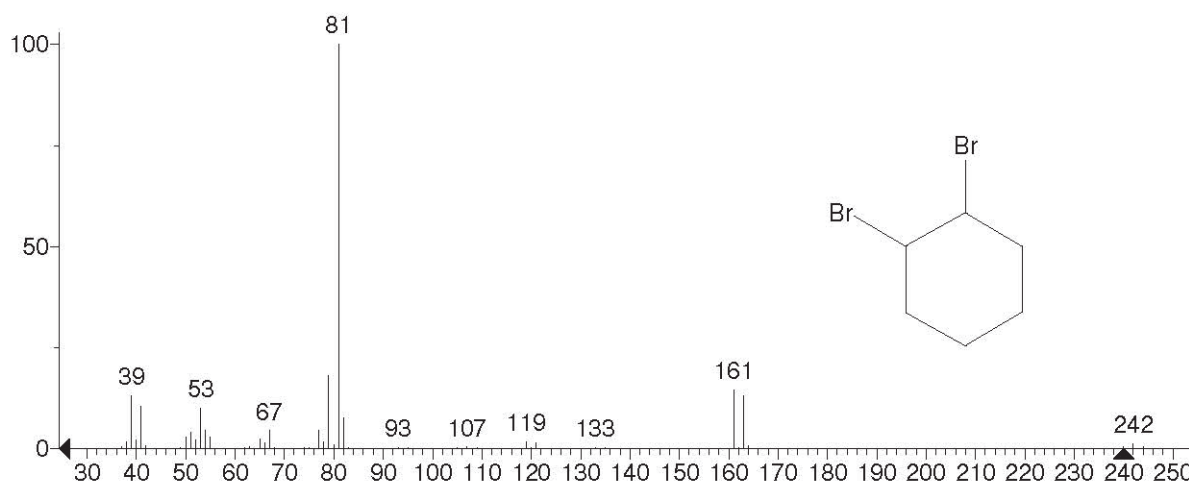


** Search Report Page 1 of 1 **

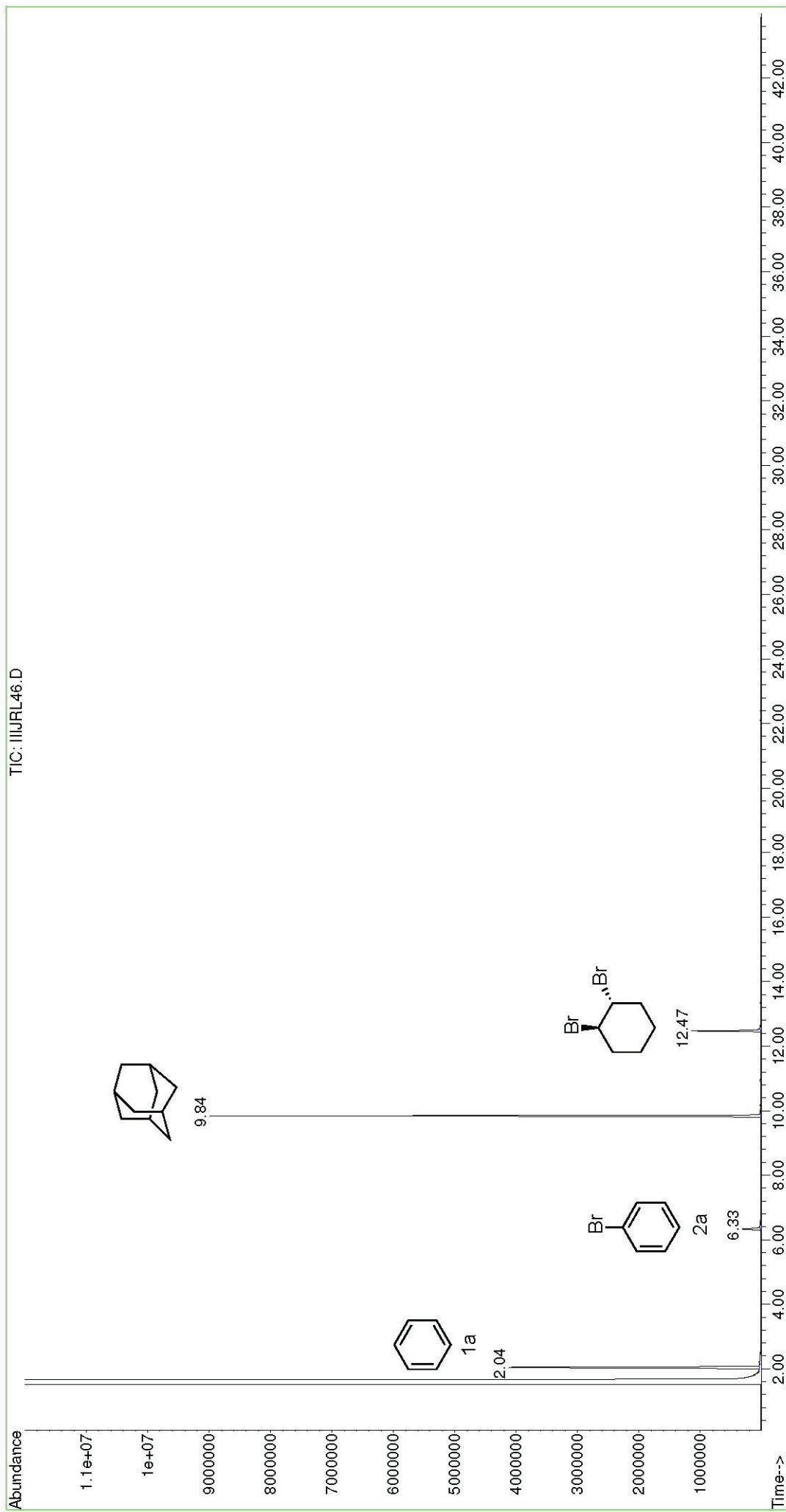
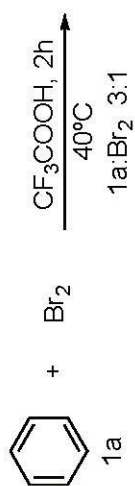
Unknown: Average of 12.685 to 12.719 min.: IIIJRL64.D
Compound in Library Factor = 168



Hit 1 : Cyclohexane, 1,2-dibromo-
C₆H₁₀Br₂; MF: 955; RMF: 956; Prob 38.8%; CAS: 5401-62-7; Lib: replib; ID: 9912.



File : D:\ASENSIO\JAVI\IIIJRL46.D
Operator :
Acquired : 25 Feb 2014 20:49 using AcqMethod JMF60
Instrument : Instrumenten
Sample Name: IIIJRL46
Misc Info :
Vial Number: 16



File : D:\ASENSIO\JAVI\IIJRL46.D

Operator :

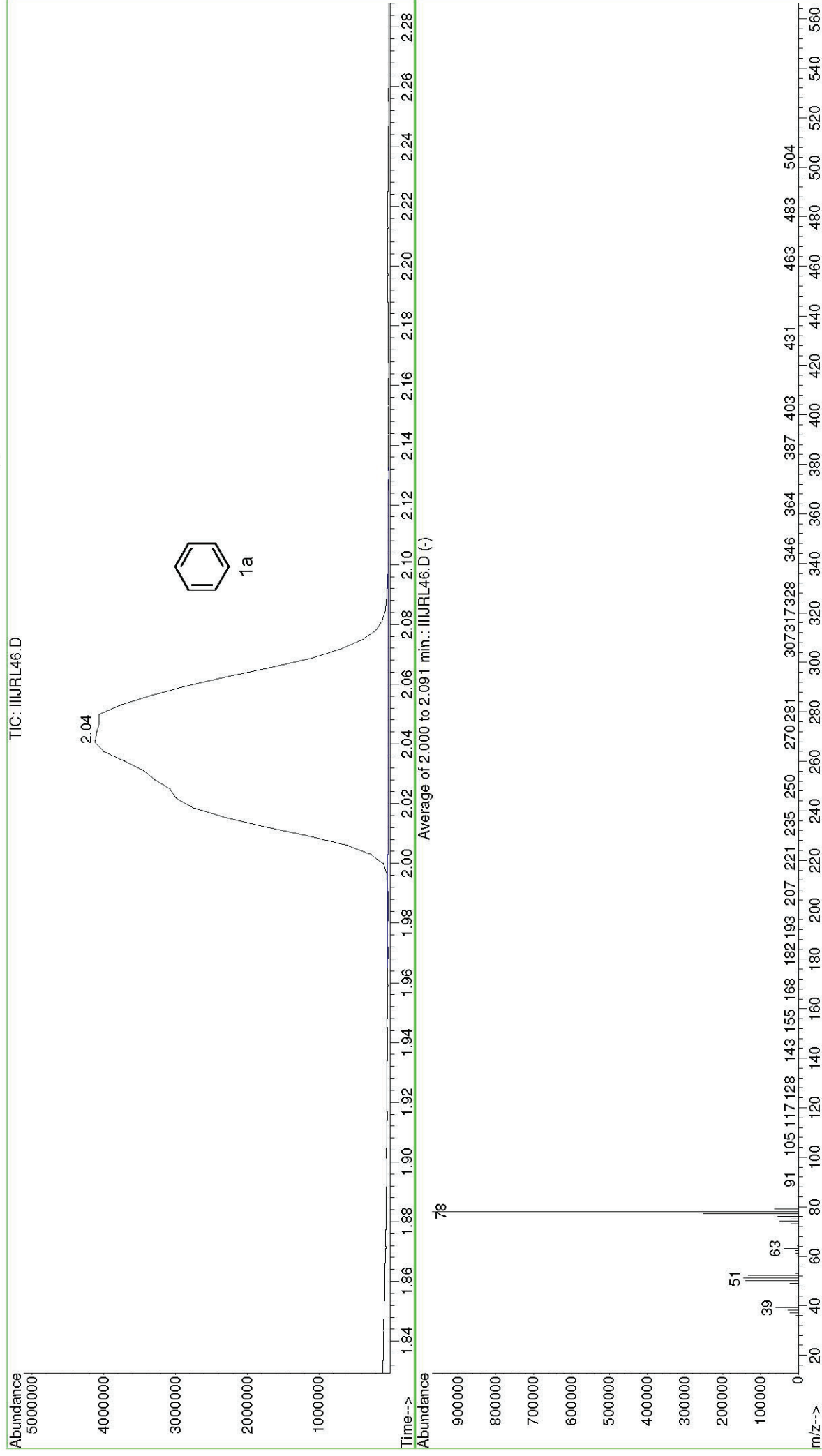
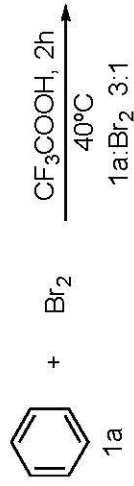
Acquired : 25 Feb 2014 20:49 using AcqMethod JMF60

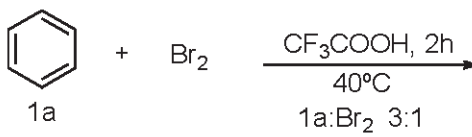
Instrument : Instrument

Sample Name: IIJRL46

Misc Info :

Vial Number: 16

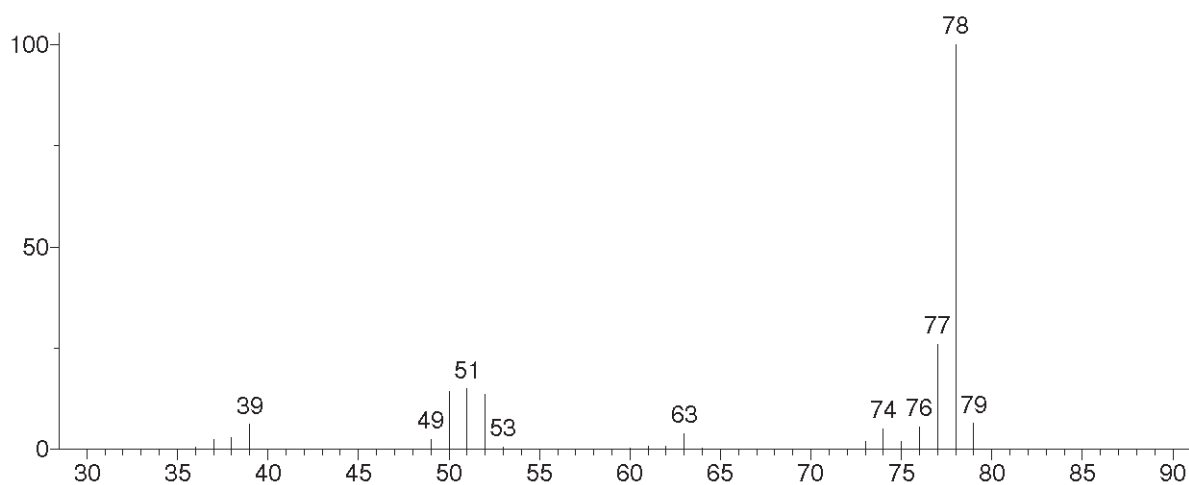




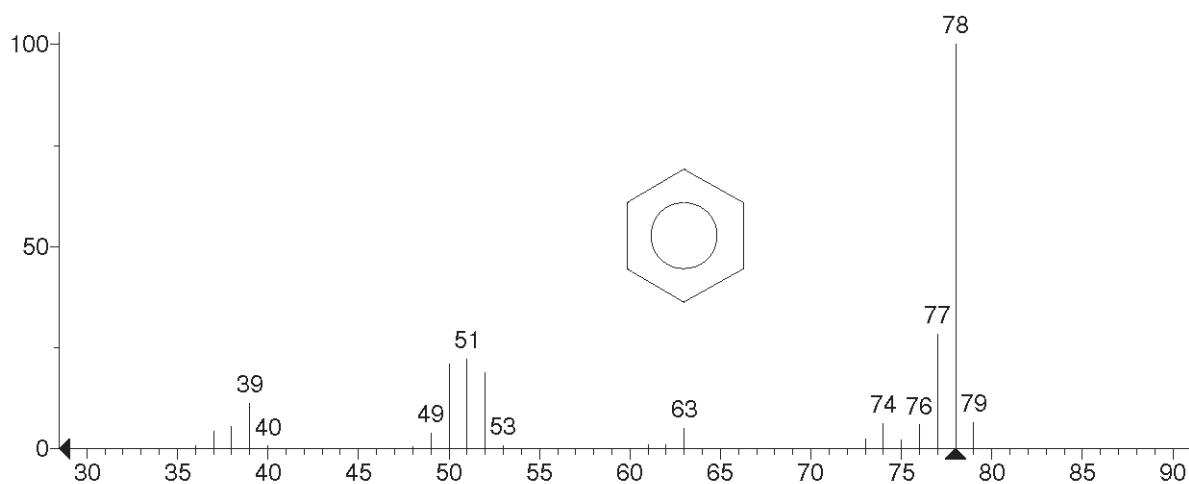
S 25

** Search Report Page 1 of 1 **

Unknown: Average of 2.000 to 2.091 min.: IIIJRL46.D
 Compound in Library Factor = 192



Hit 1 : Benzene
 C₆H₆; MF: 960; RMF: 961; Prob 65.3%; CAS: 71-43-2; Lib: wiley7n; ID: 2493.



File : D:\ASENSIO\JAVI\IIIJRL46.D

Operator :

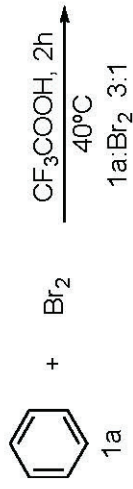
Acquired : 25 Feb 2014 20:49 using AcqMethod JMF60

Instrument : Instrument

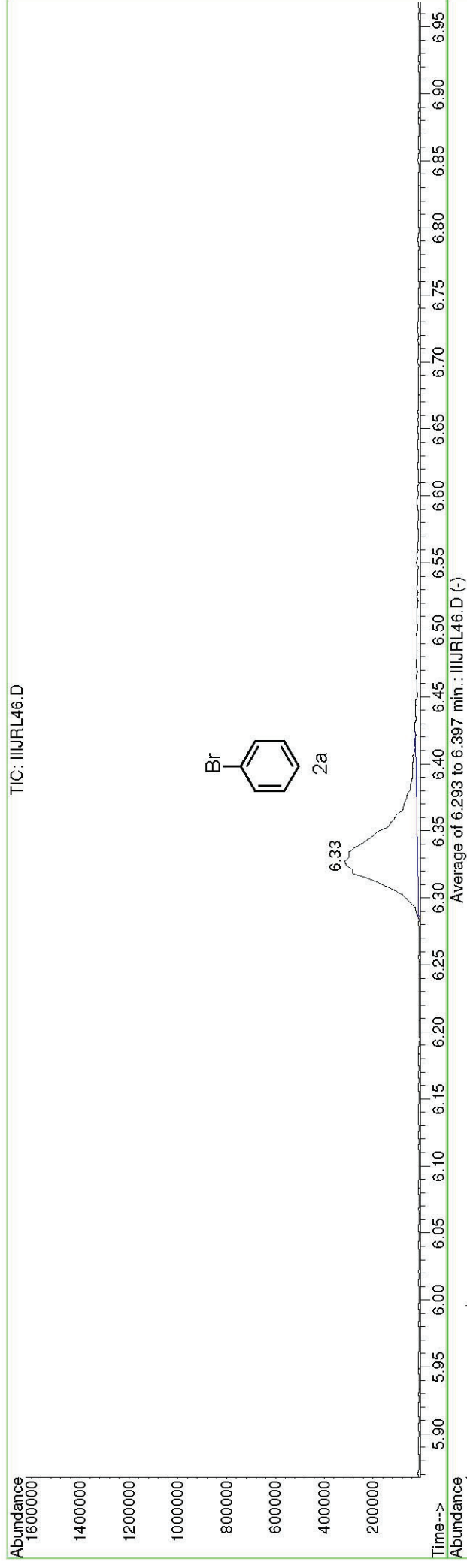
Sample Name : IIIJRL46

Misc Info :

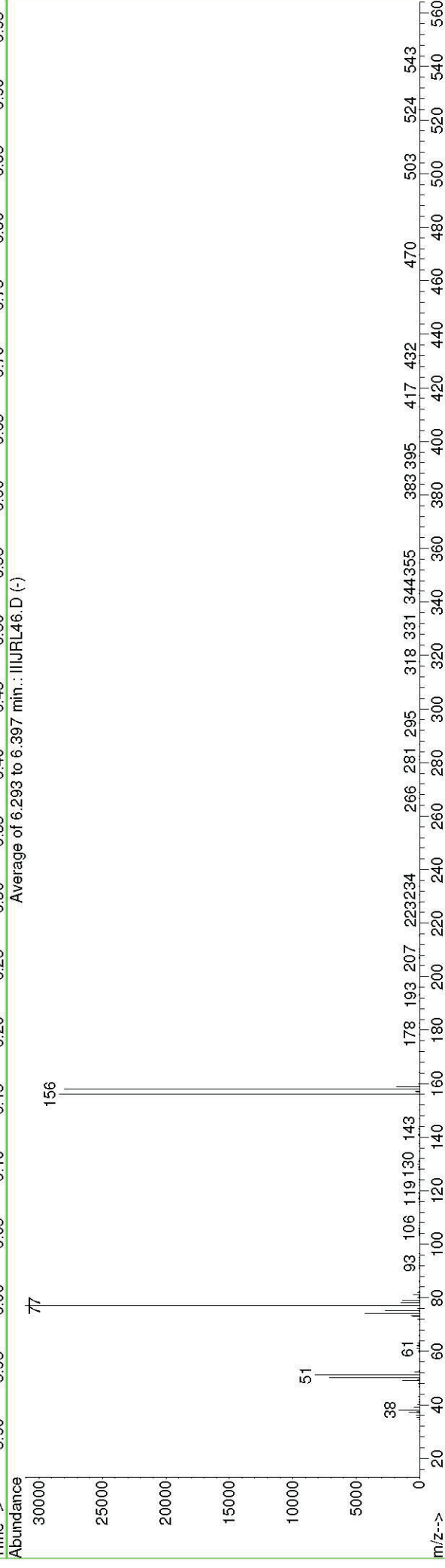
Vial Number: 16



TIC: IIIJRL46.D



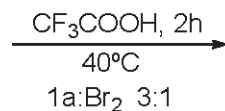
Average of 6.293 to 6.397 min.: IIIJRL46.D (-)





1a

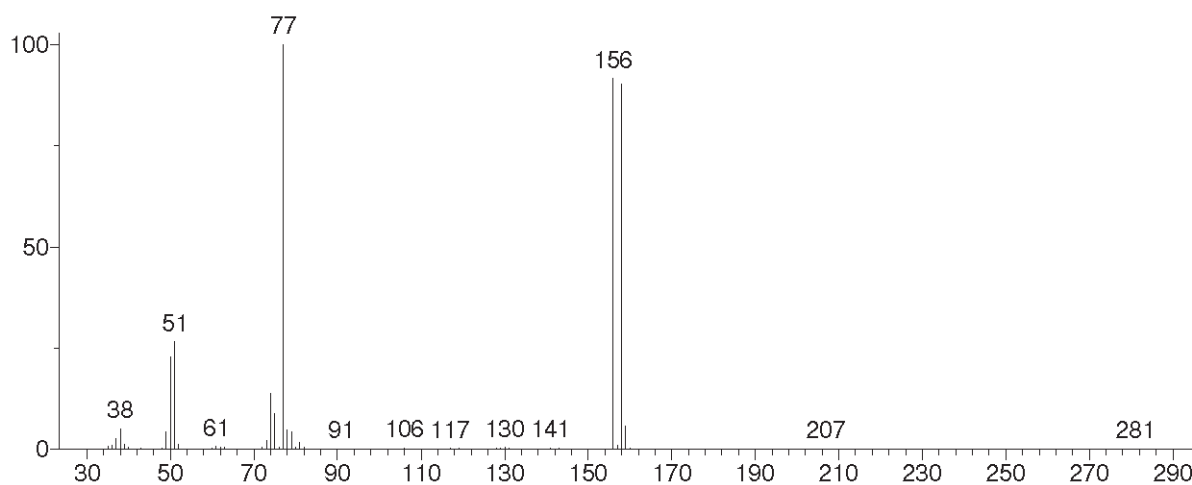
+



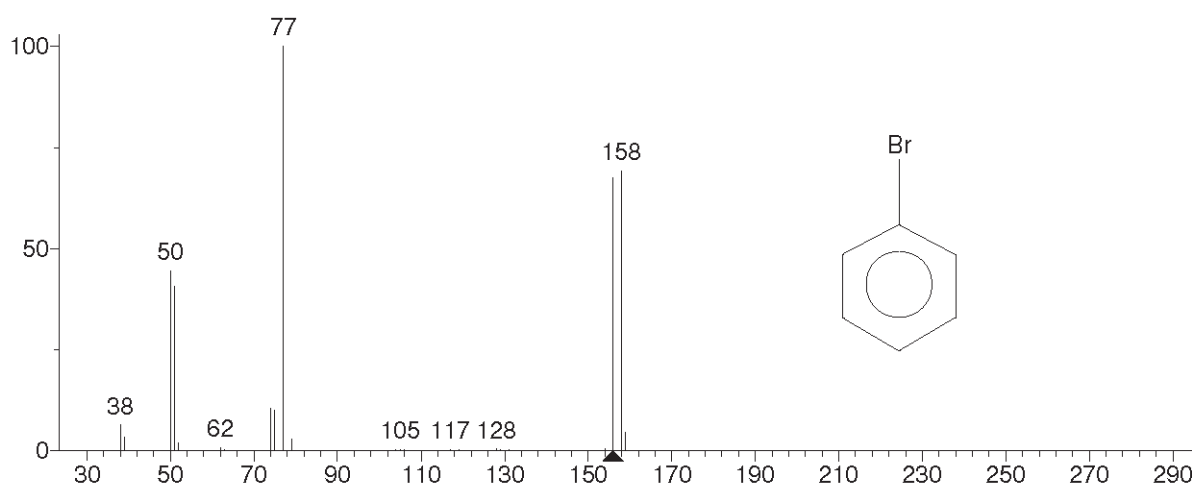
S 27

** Search Report Page 1 of 1 **

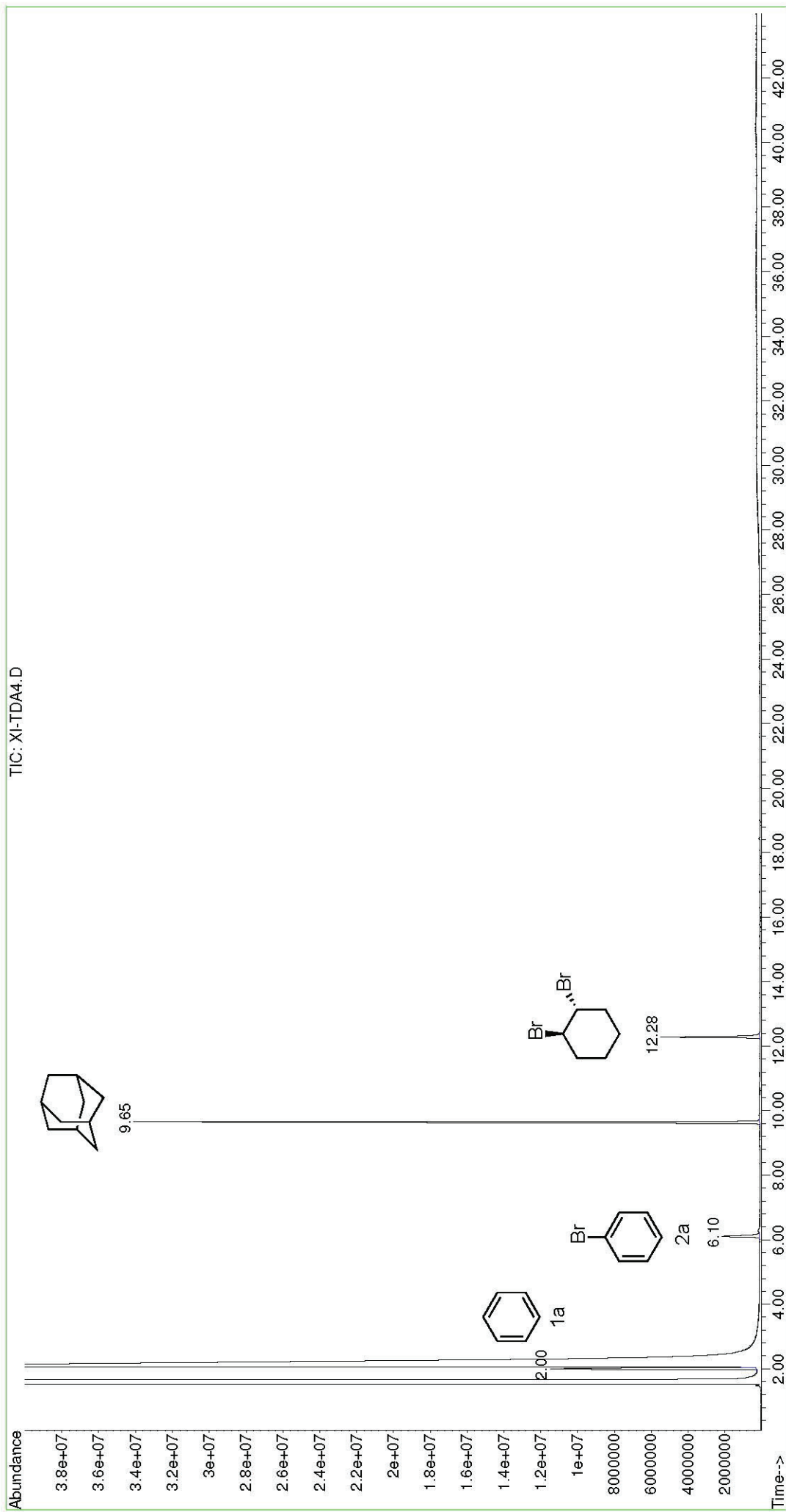
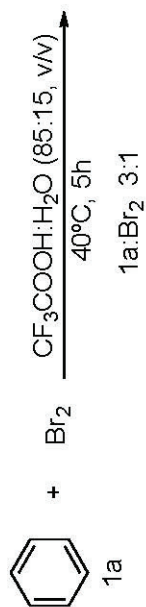
Unknown: Average of 6.293 to 6.397 min.: IIIJRL46.D
Compound in Library Factor = 454



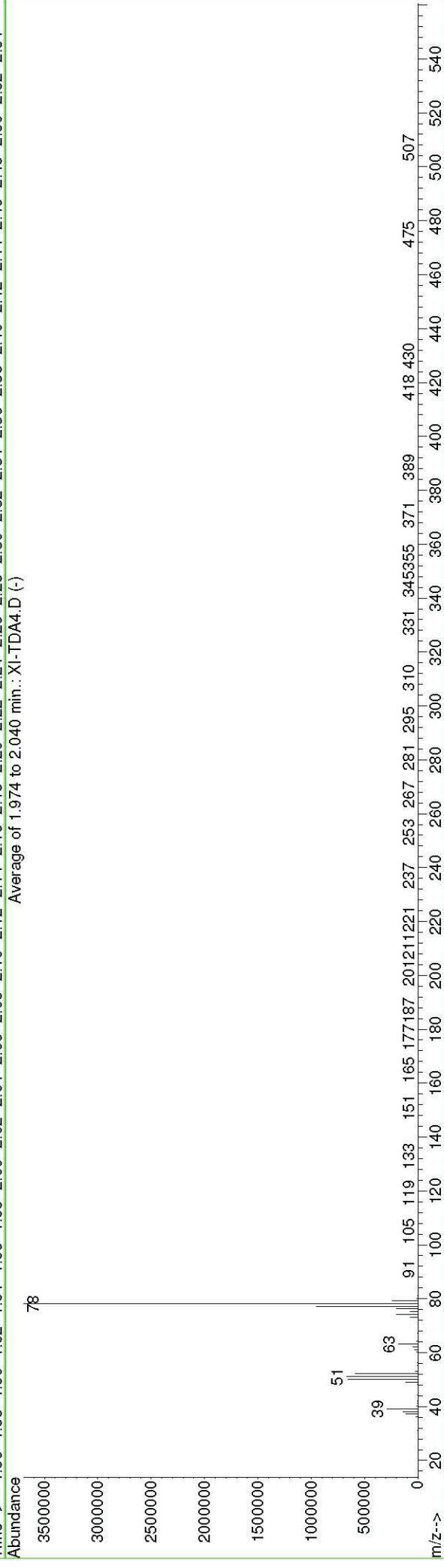
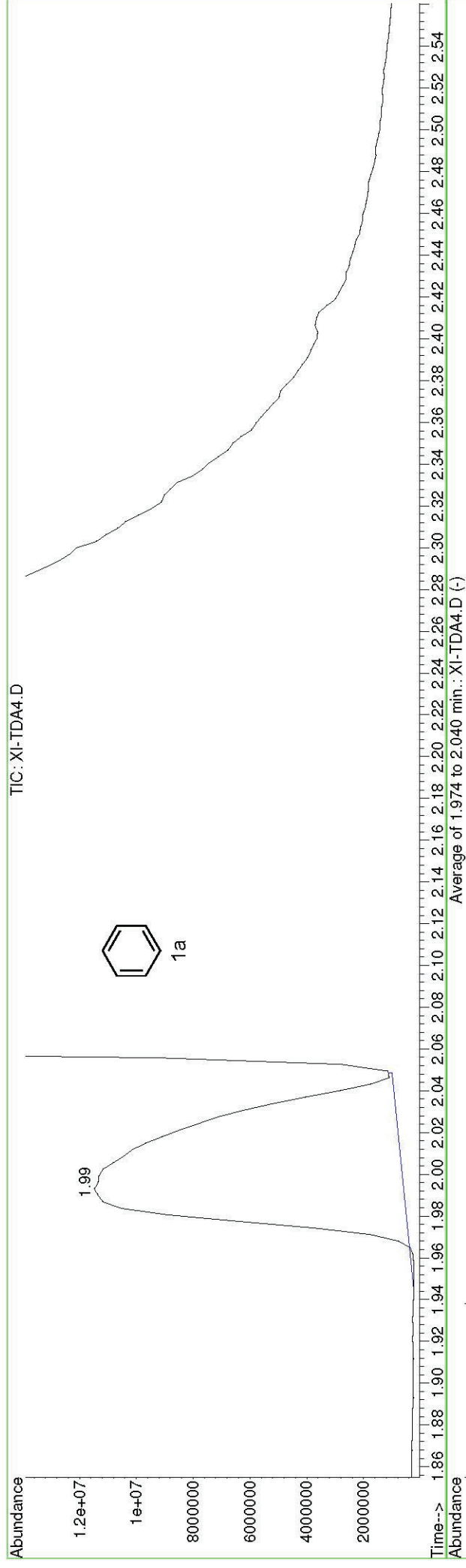
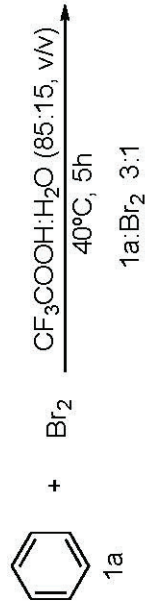
Hit 1 : Benzene, bromo-
C₆H₅Br; MF: 885; RMF: 906; Prob 97.9%; CAS: 108-86-1; Lib: wiley7n; ID: 54587.



File : D:\ASENSIO\THAIS\MAY014\XI-TDA4.D
 Operator :
 Acquired : 12 May 2014 16:53 using AcqMethod JMF60
 Instrument : Instrument
 Sample Name :
 Misc Info :
 Vial Number: 12

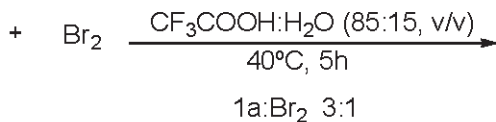


File : C:\MSDCHEM\1\DATA\ASENSIO\THAIS\XI-TDA4.D
 Operator :
 Acquired : 12 May 2014 16:53 using AcqMethod JMF60
 Instrument : Instrument
 Sample Name :
 Misc Info :
 Vial Number: 12





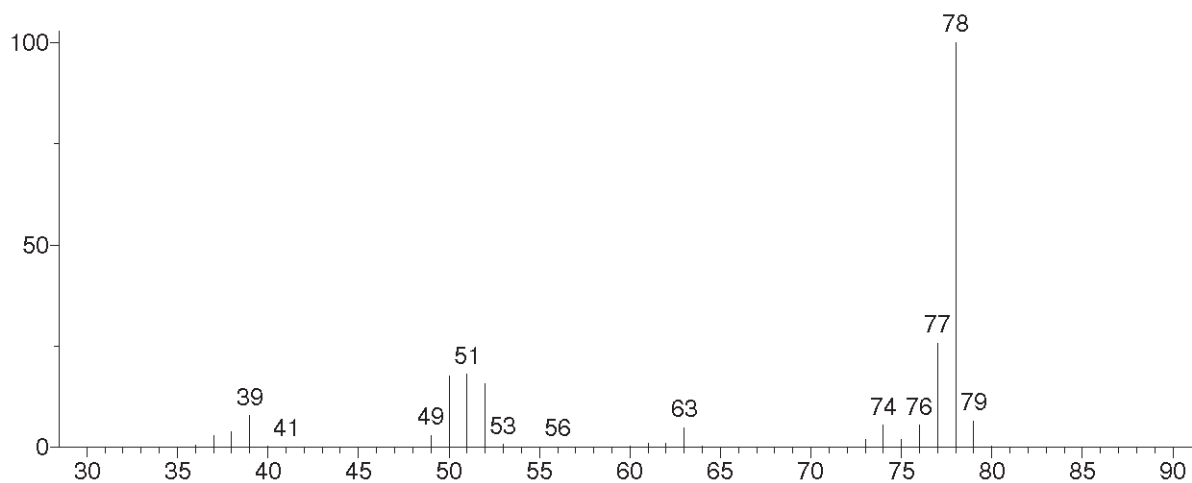
1a



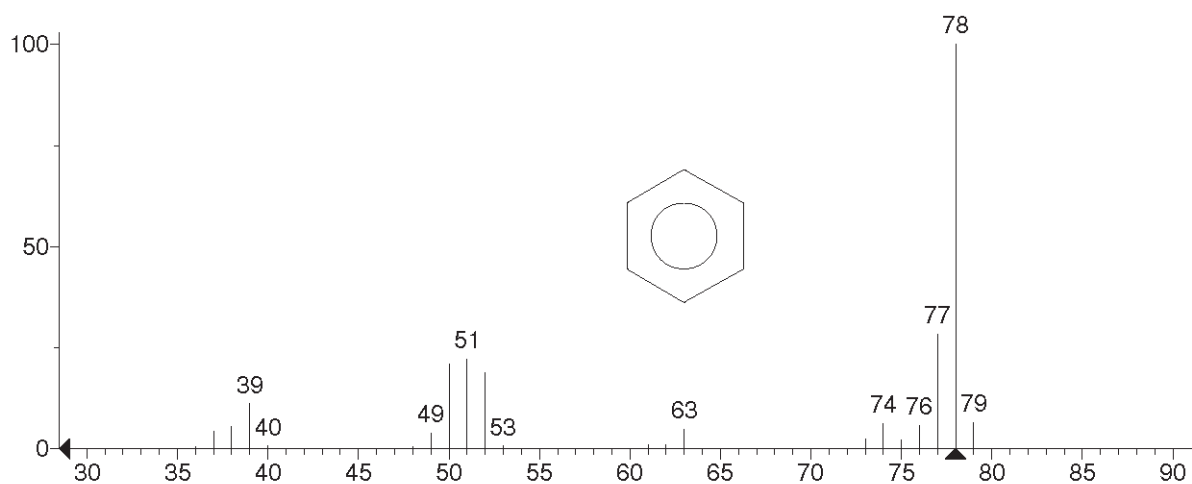
S 30

** Search Report Page 1 of 1 **

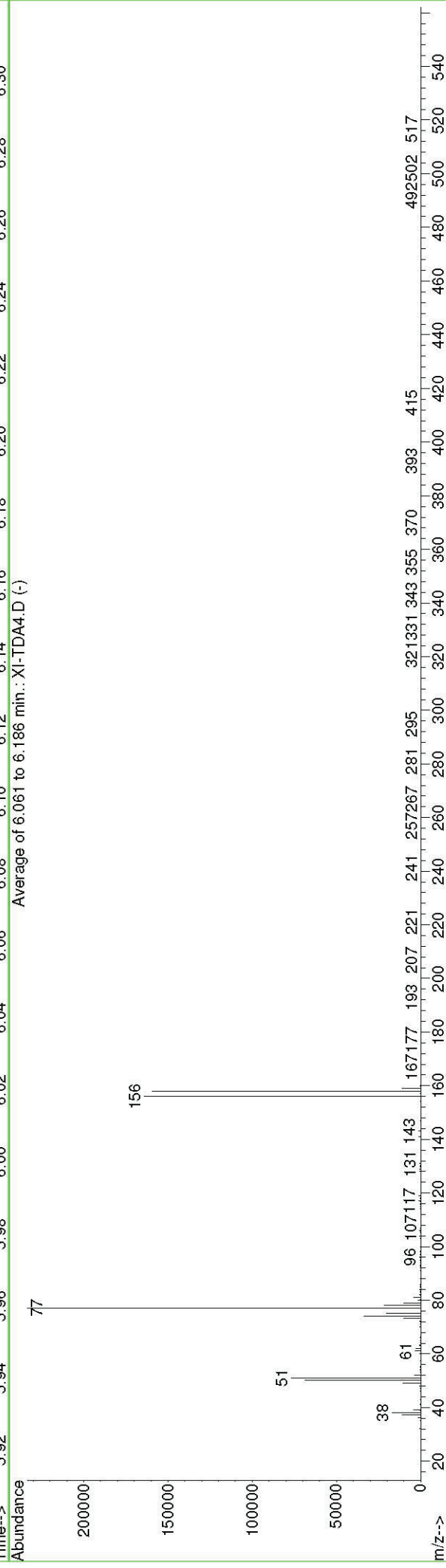
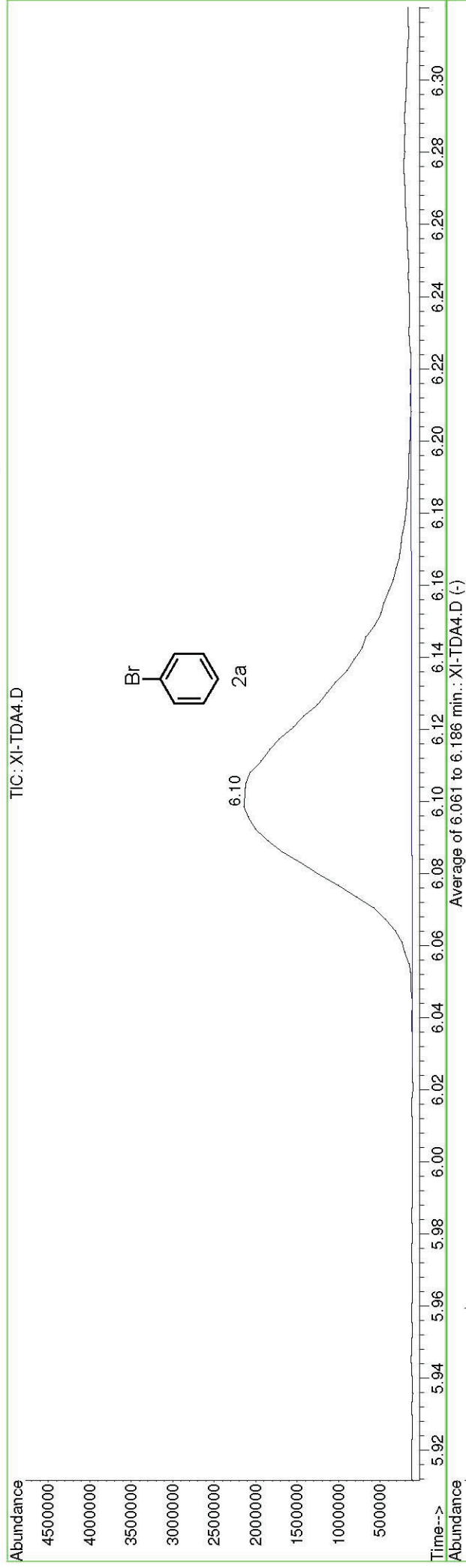
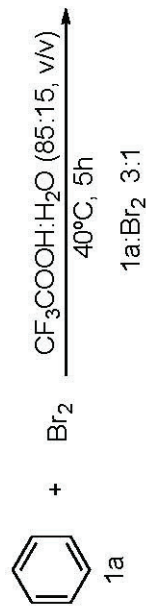
Unknown: Average of 1.974 to 2.040 min.: XI-TDA4.D
Compound in Library Factor = 170

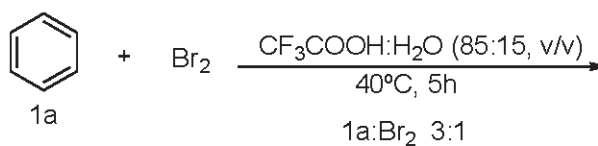


Hit 1 : Benzene
C₆H₆; MF: 968; RMF: 969; Prob 65.4%; CAS: 71-43-2; Lib: mainlib; ID: 37960.



File : C:\MSDCHEM\1\DATA\ASENSIO\THAIS\XI-TDA4.D
 Operator :
 Acquired : 12 May 2014 16:53 using AcqMethod JMF60
 Instrument : Instrument
 Sample Name :
 Misc Info :
 Vial Number: 12

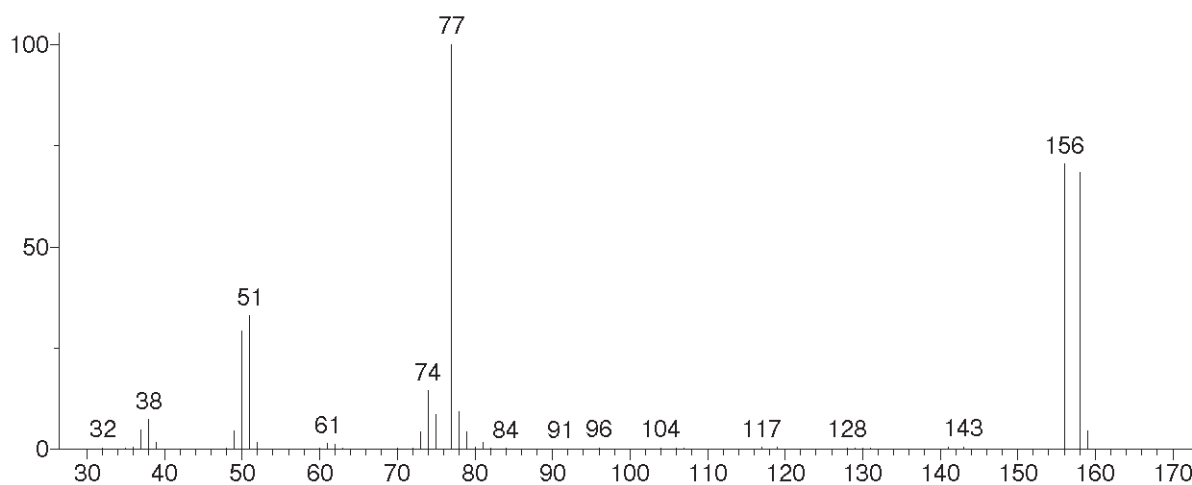




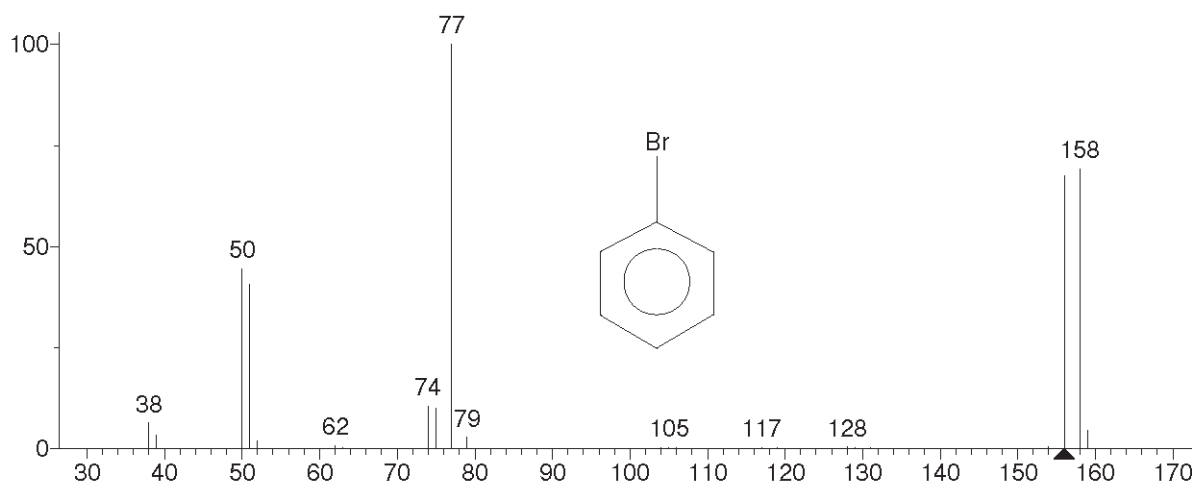
S 32

** Search Report Page 1 of 1 **

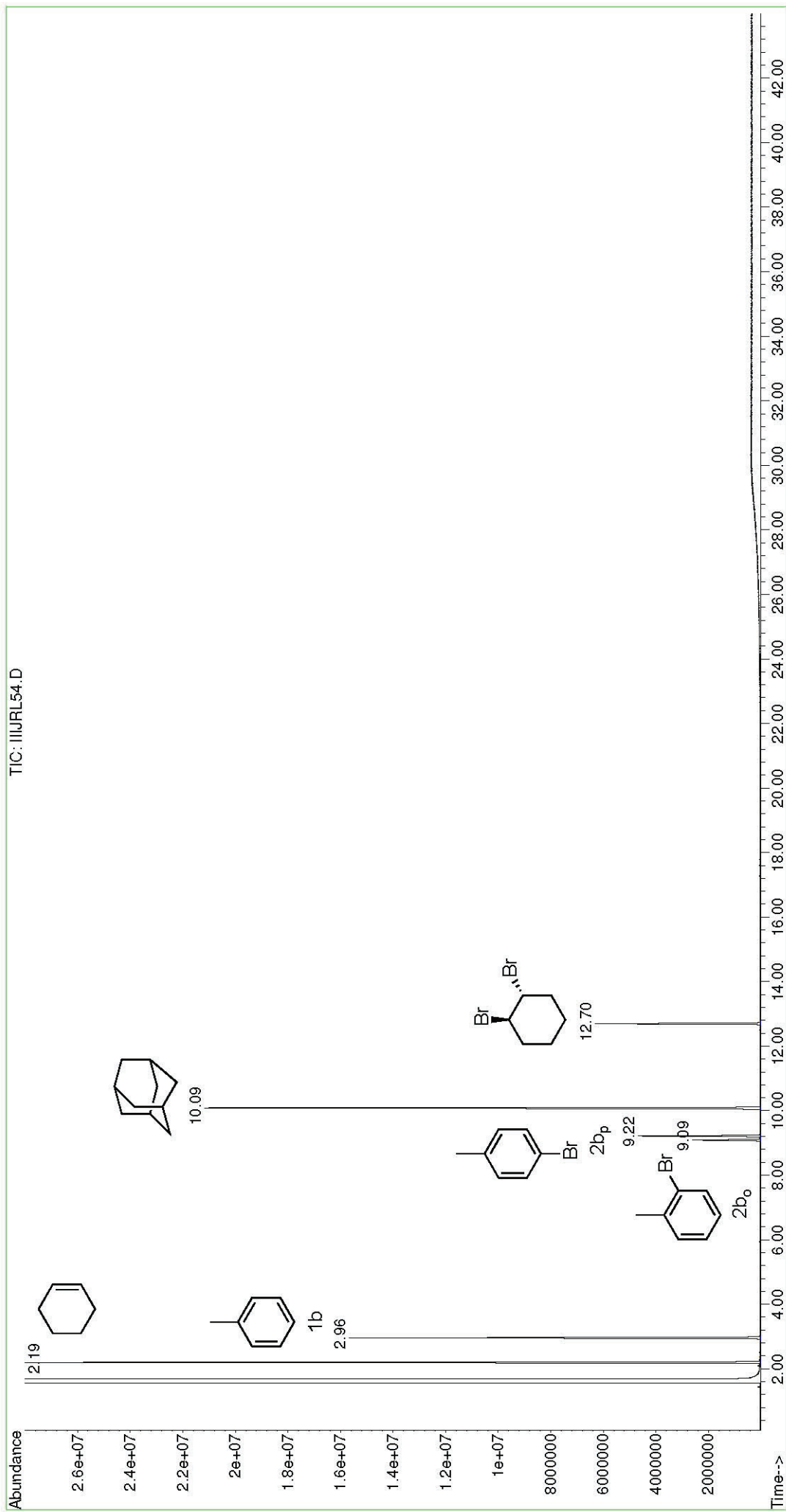
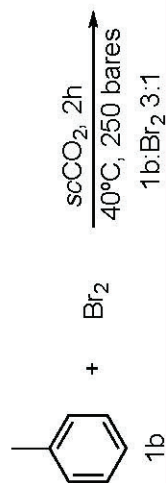
Unknown: Average of 6.061 to 6.186 min.: XI-TDA4.D
Compound in Library Factor = 711



Hit 1 : Benzene, bromo-
C₆H₅Br; MF: 918; RMF: 949; Prob 97.2%; CAS: 108-86-1; Lib: wiley7n; ID: 54587.



File : D:\ASENSIO\MATEO\IIJURL54.D
 Operator :
 Acquired : 17 Jun 2014 1:09 using AcqMethod JMF60
 Instrument : Instrumen
 Sample Name: VIDRIO
 Misc Info :
 Vial Number: 23



File : D:\ASENSIO\MATEO\IIIJRL54.D

Operator :

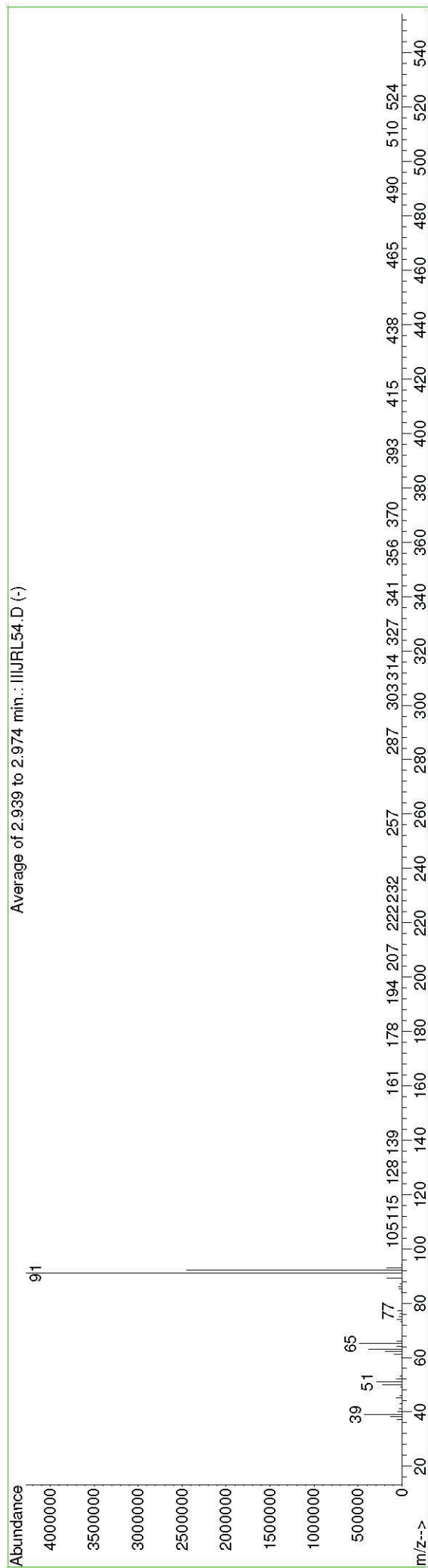
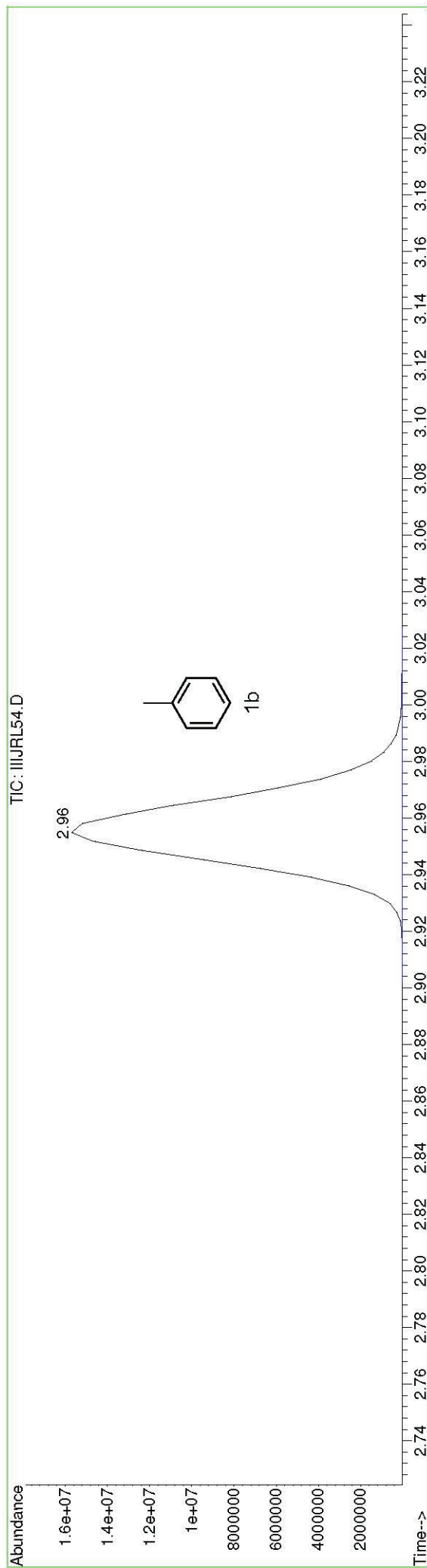
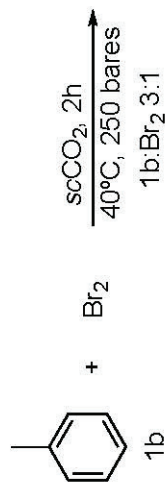
Acquired : 17 Jun 2014 1:09 using AcqMethod JMF60

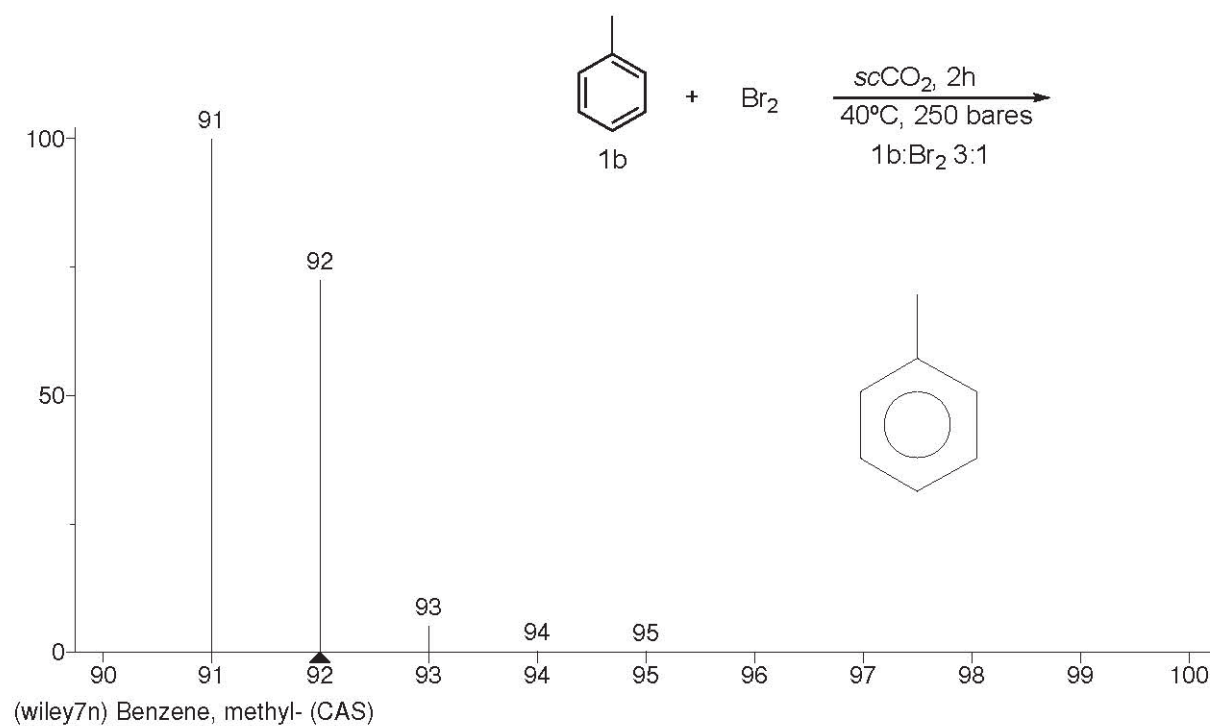
Instrument : Instrument

Sample Name: VIDRIO

Misc Info :

Vial Number: 23





File : D:\ASENSIO\MATEO\IIIJRL54.D

Operator :

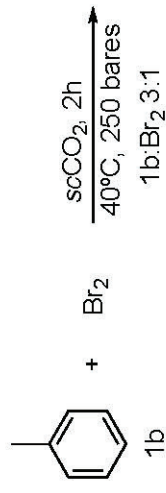
Acquired : 17 Jun 2014 1:09 using AcqMethod JMF60

Instrument : Instrumen

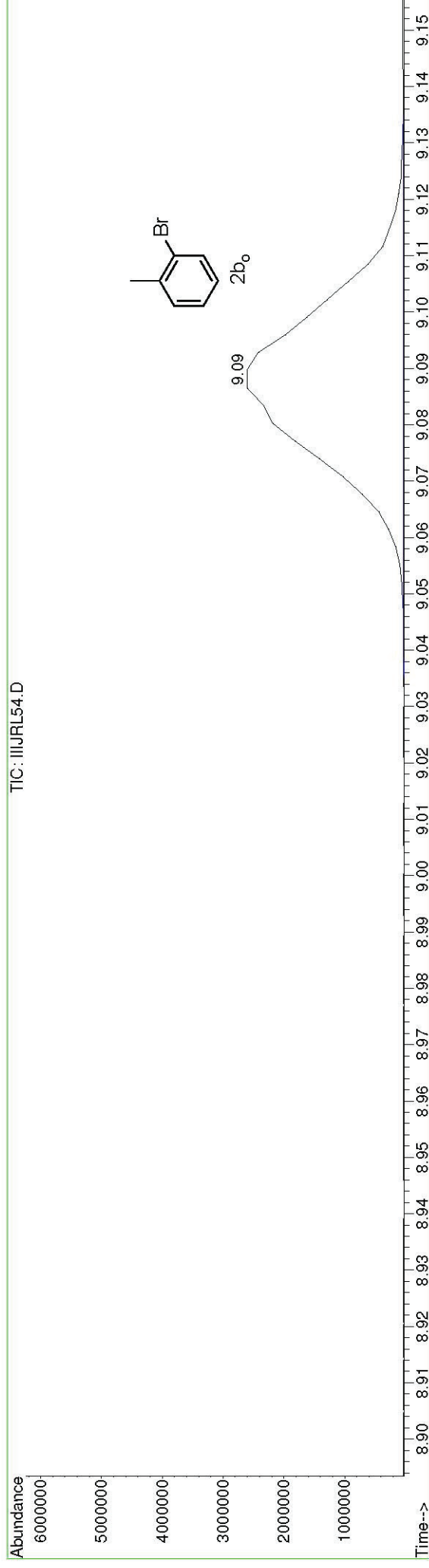
Sample Name: VIDRIO

Misc Info :

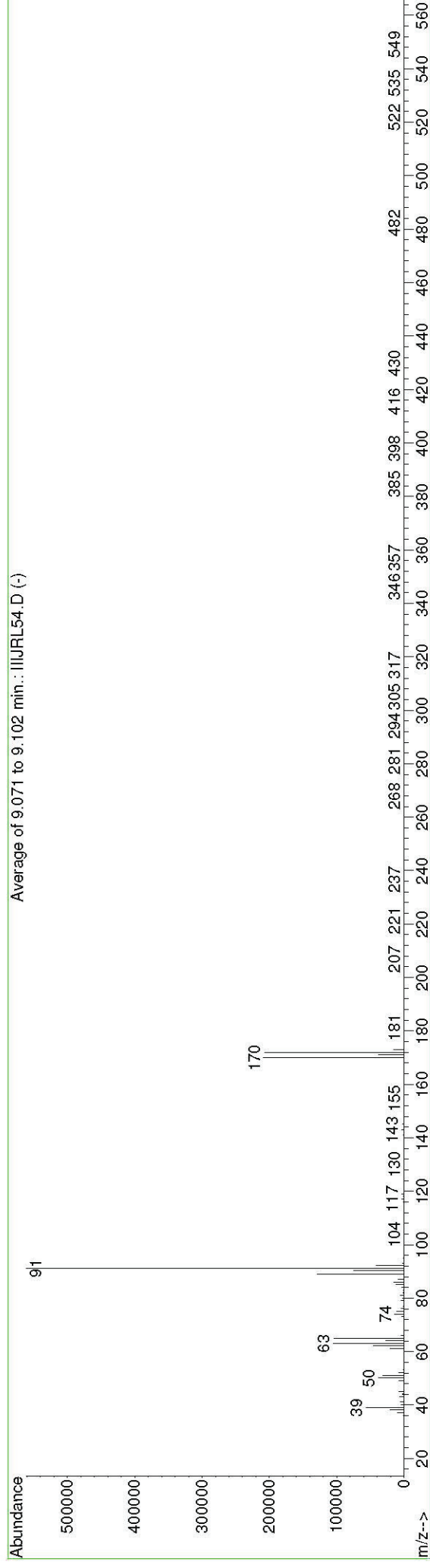
Vial Number: 23

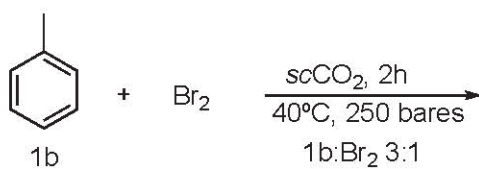


TIC: IIJJRL54.D



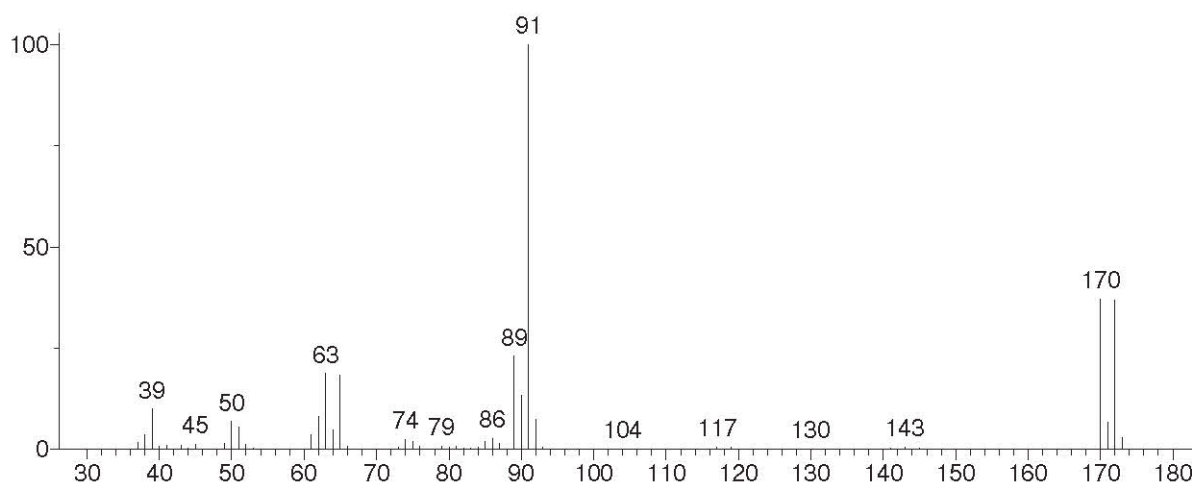
Average of 9.071 to 9.102 min.: IIJJRL54.D (-)



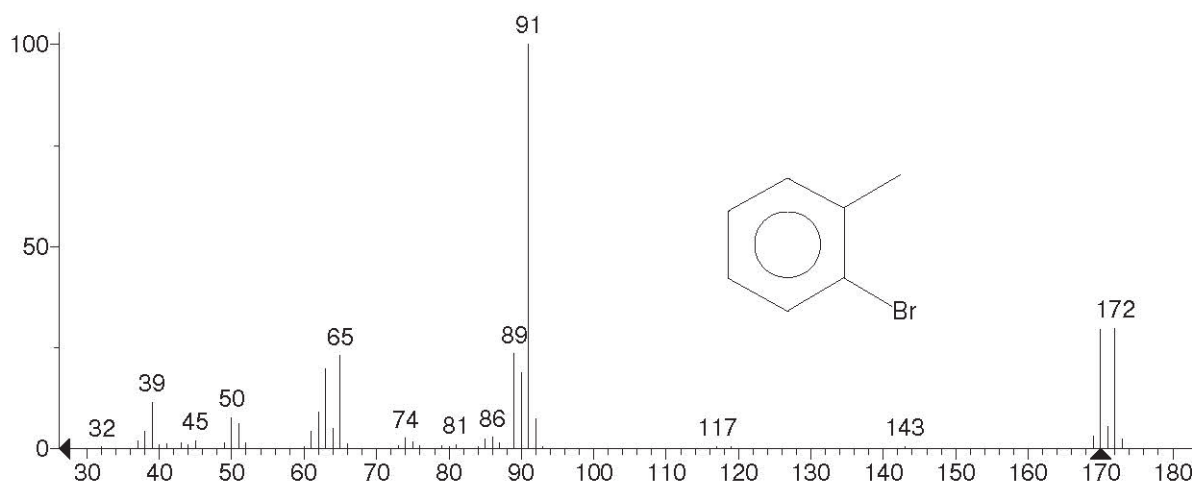


** Search Report Page 1 of 1 **

Unknown: Average of 9.071 to 9.102 min.: IIIJRL54.D
 Compound in Library Factor = 326



Hit 1 : Benzene, 1-bromo-2-methyl-
 C₇H₇Br; MF: 955; RMF: 957; Prob 43.0%; CAS: 95-46-5; Lib: wiley7n; ID: 72508.



File : D:\ASENSIO\MATEO\IIIJRL54.D

Operator :

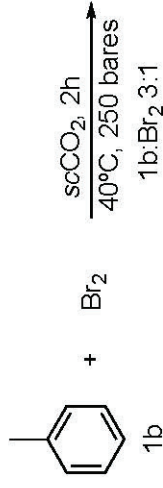
Acquired : 17 Jun 2014 1:09 using AcqMethod JMF60

Instrument : Instrument

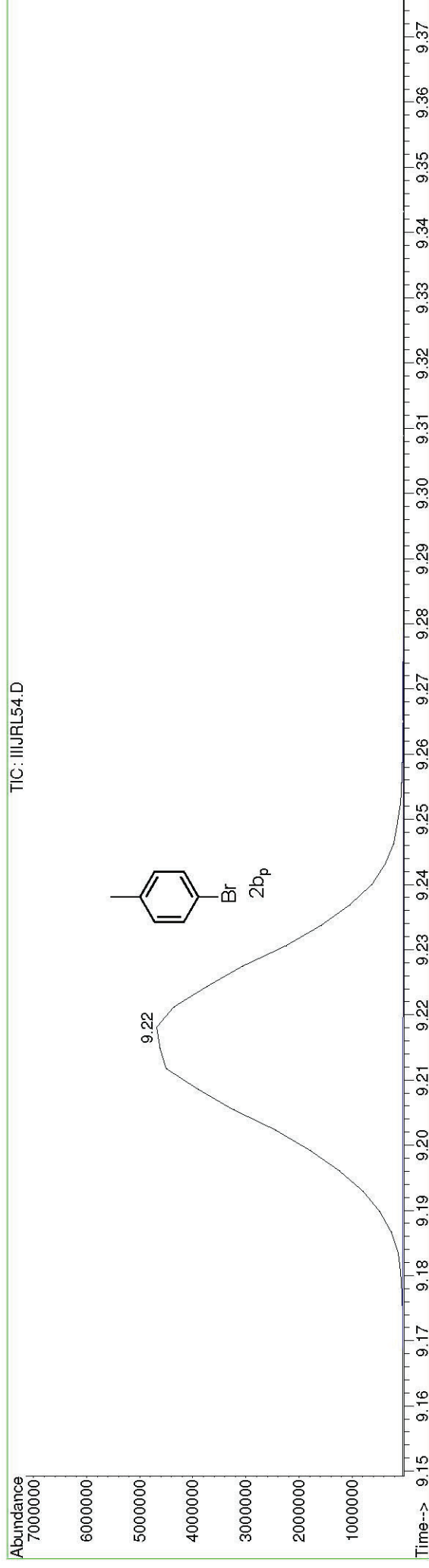
Sample Name: VIDRIO

Misc Info :

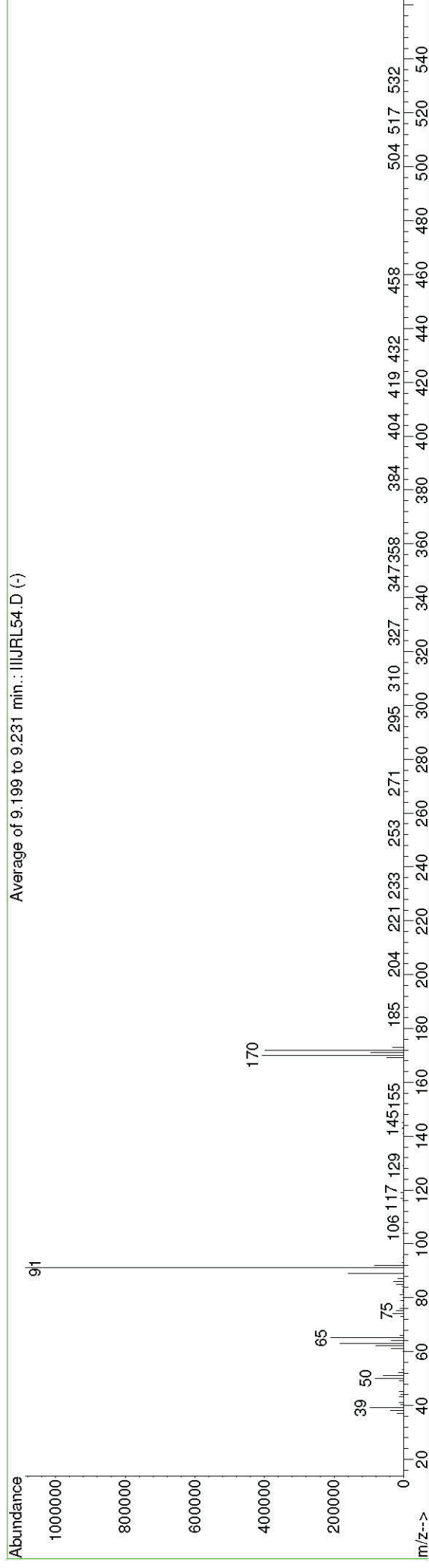
Vial Number: 23

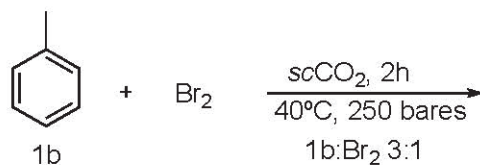


TIC: IIJJRL54.D



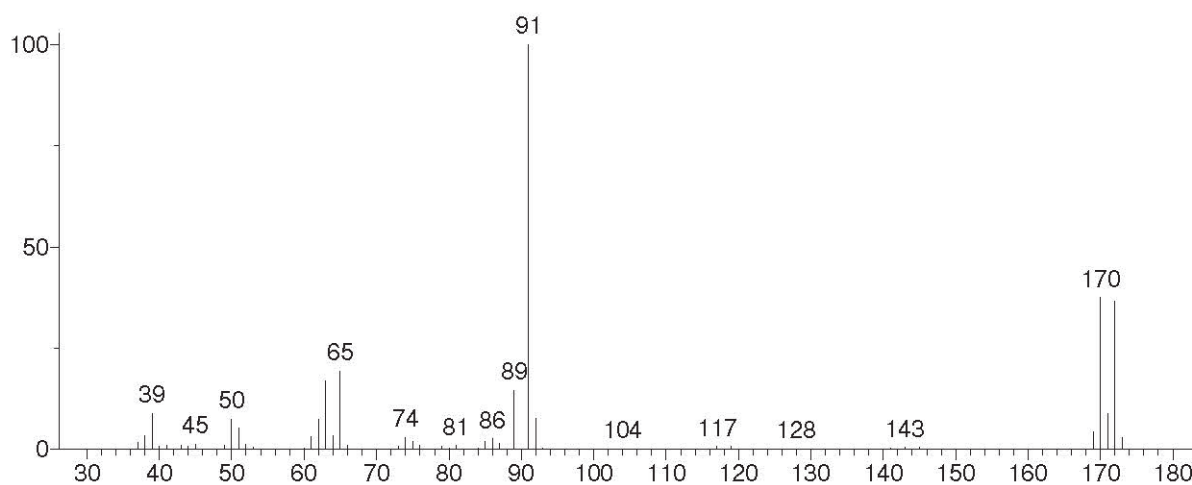
Average of 9.199 to 9.231 min.: IIJJRL54.D (-)



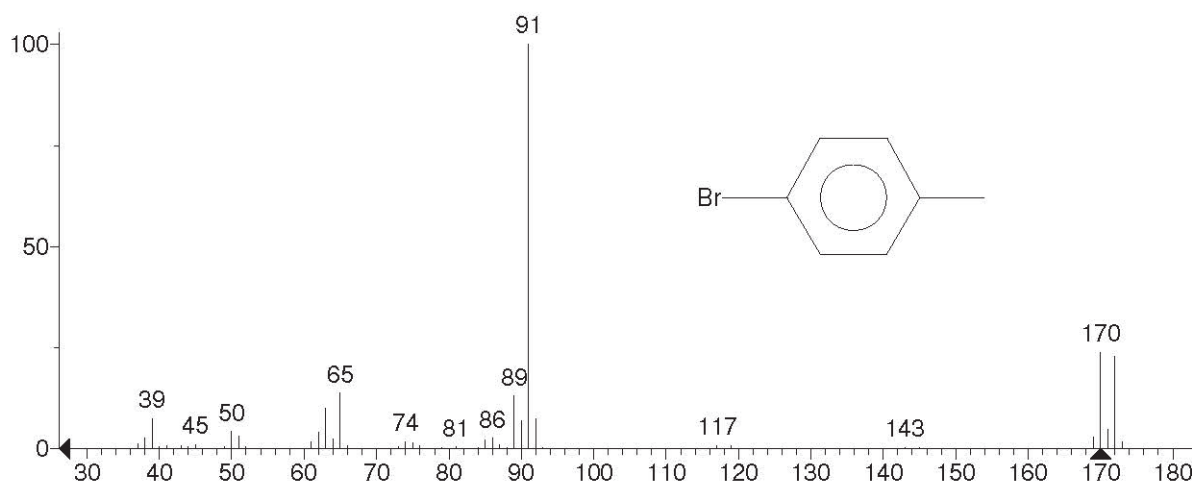


** Search Report Page 1 of 1 **

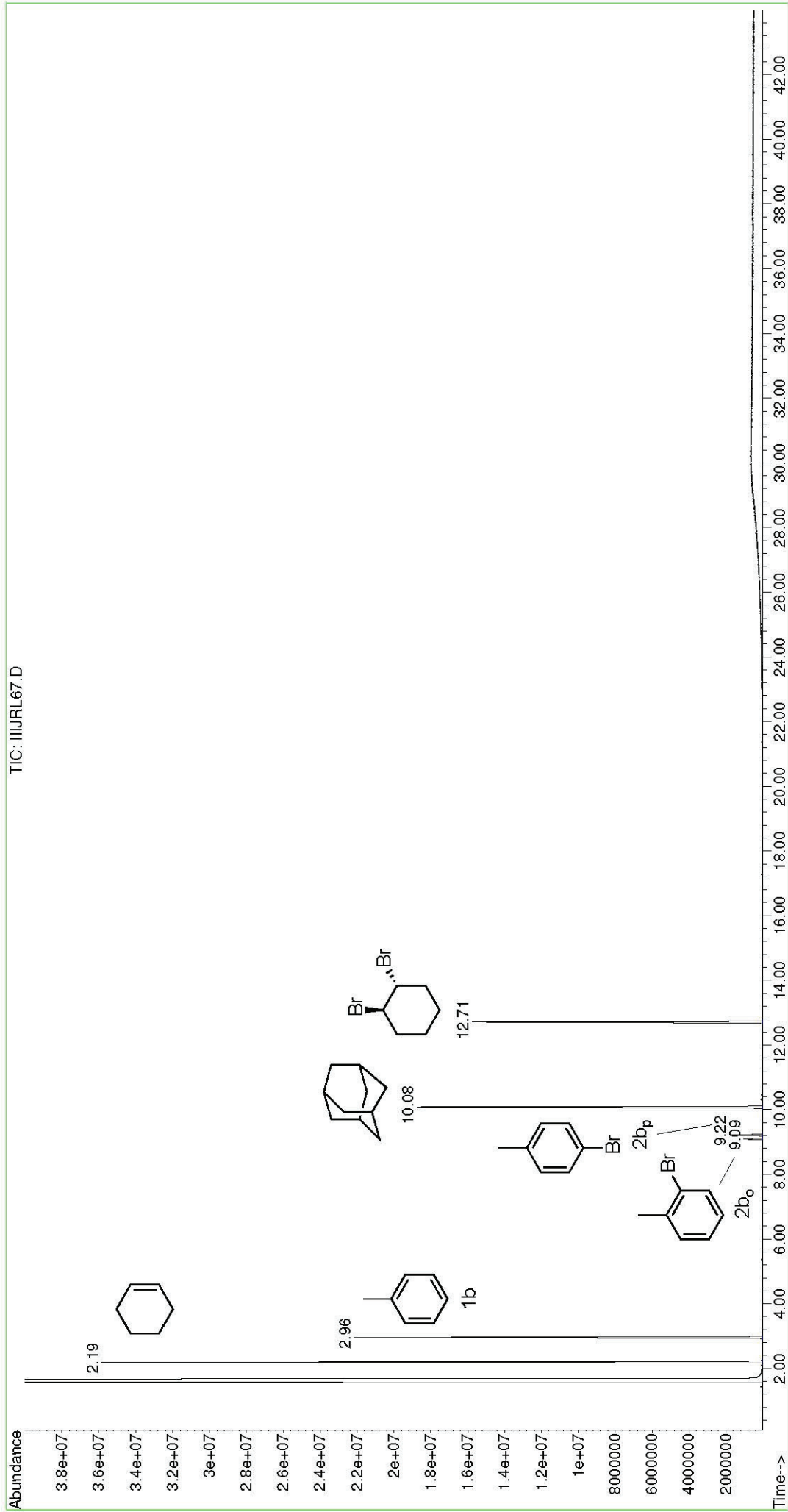
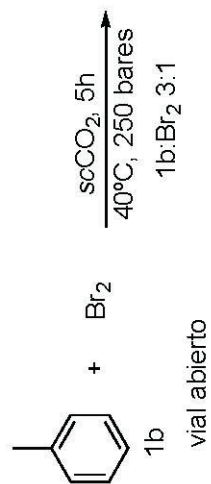
Unknown: Average of 9.199 to 9.231 min.: IIIJRL54.D
Compound in Library Factor = 312



Hit 1 : Benzene, 1-bromo-4-methyl-
C₇H₇Br; MF: 940; RMF: 940; Prob 42.4%; CAS: 106-38-7; Lib: replib; ID: 11700.



File : D:\ASENSIO\MATEO\IIJRL67.D
 Operator :
 Acquired : 16 Jun 2014 21:46 using AcqMethod JMF60
 Instrument : Instrumen
 Sample Name: VIDRIO
 Misc Info :
 Vial Number: 19



File : D:\ASENSIO\MATEO\IIIJRL67.D

Operator :

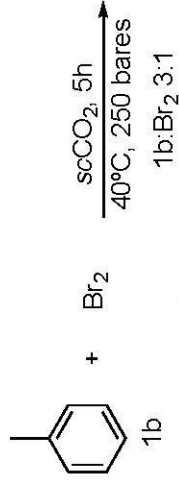
Acquired : 16 Jun 2014 21:46 using AcqMethod JMF60

Instrument : Instrument

Sample Name: VIDRIO

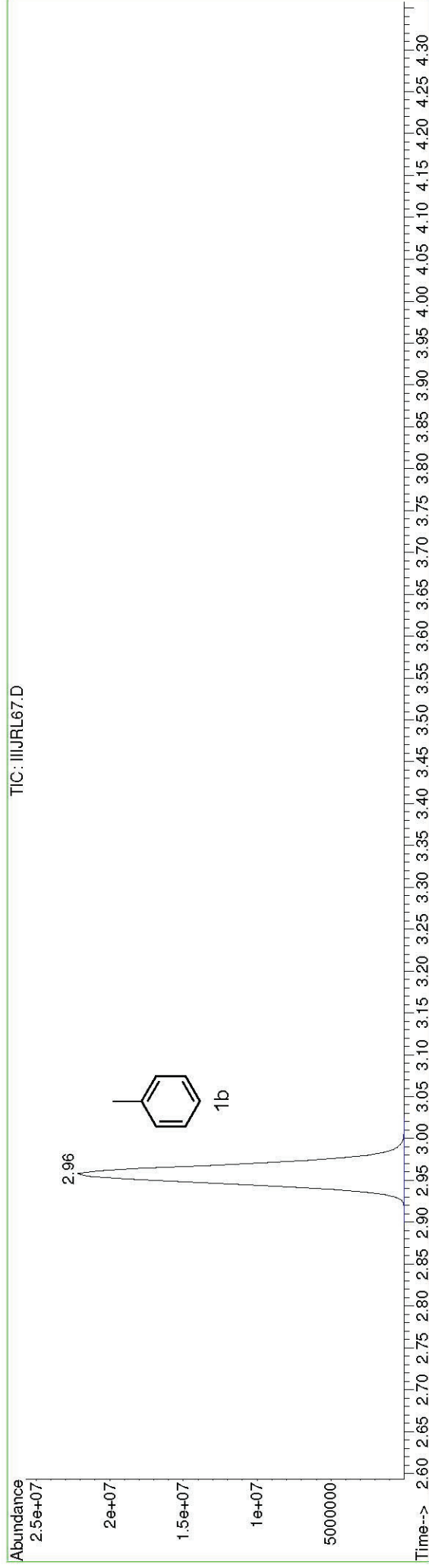
Misc Info :

Vial Number: 19

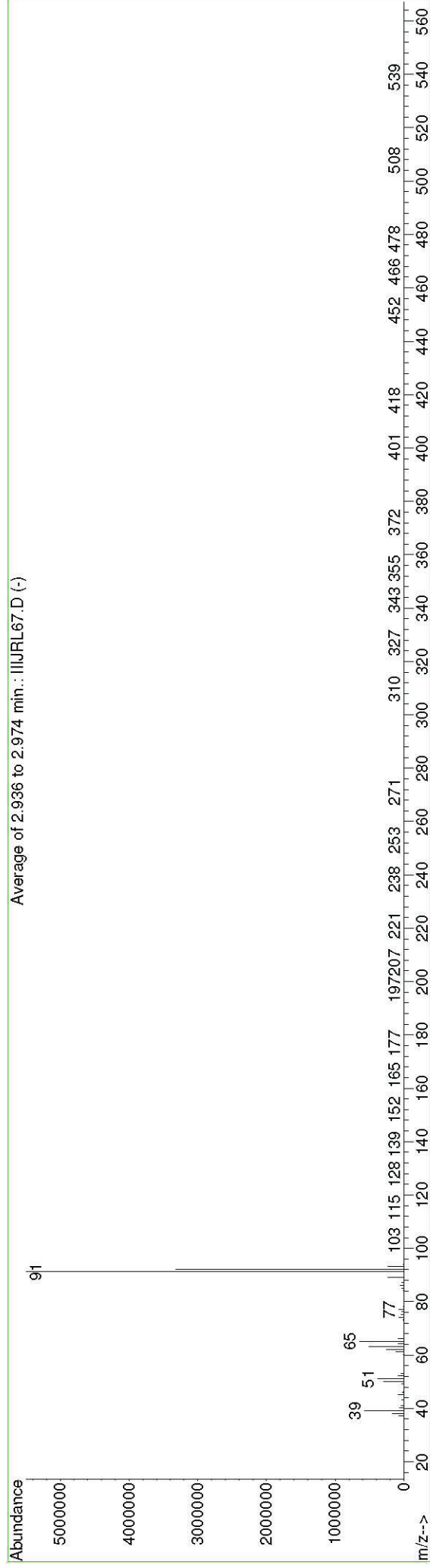


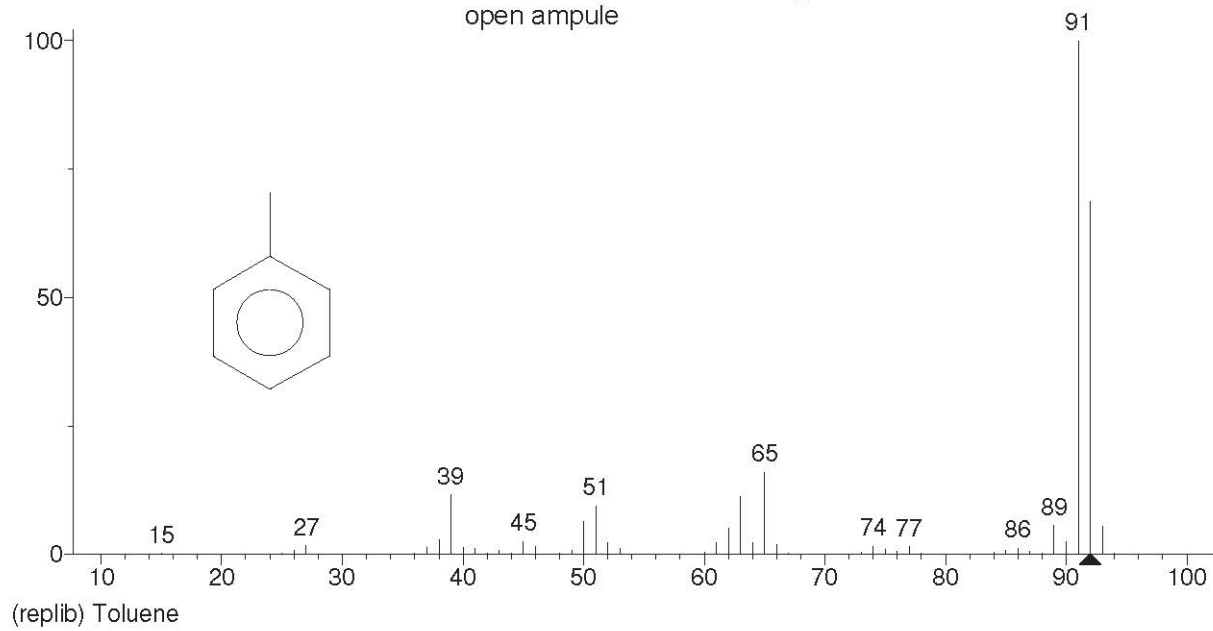
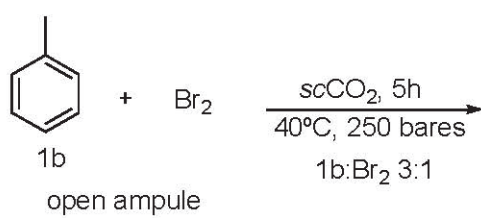
open ampule

TIC: IIJJRL67.D



Average of 2.936 to 2.974 min.: IIJJRL67.D (-)





File : D:\ASENSIO\MATEO\IIIJRL67.D

Operator :

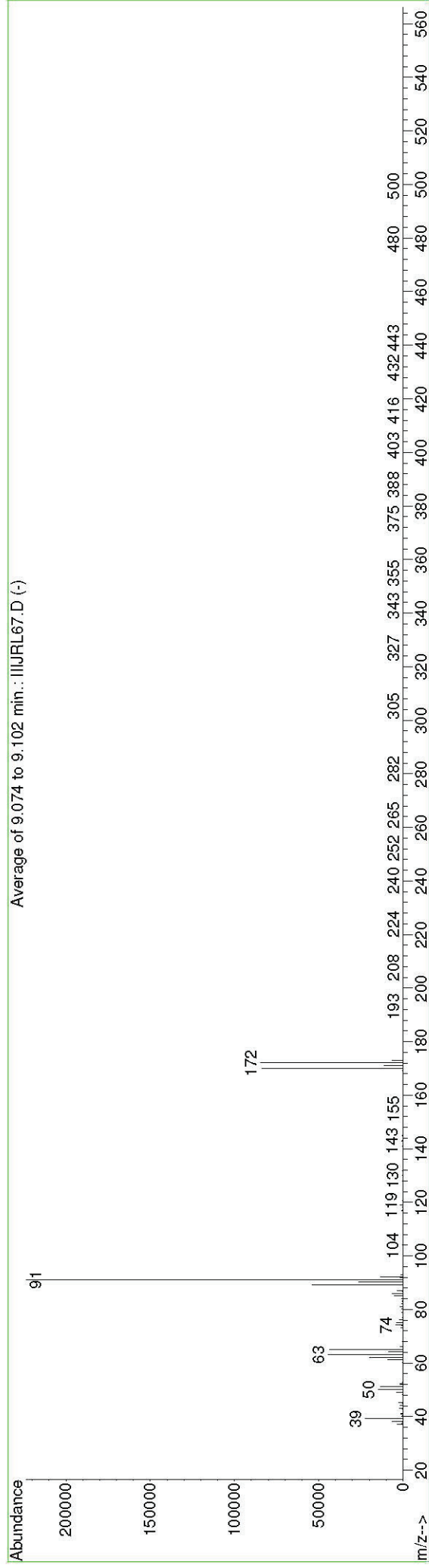
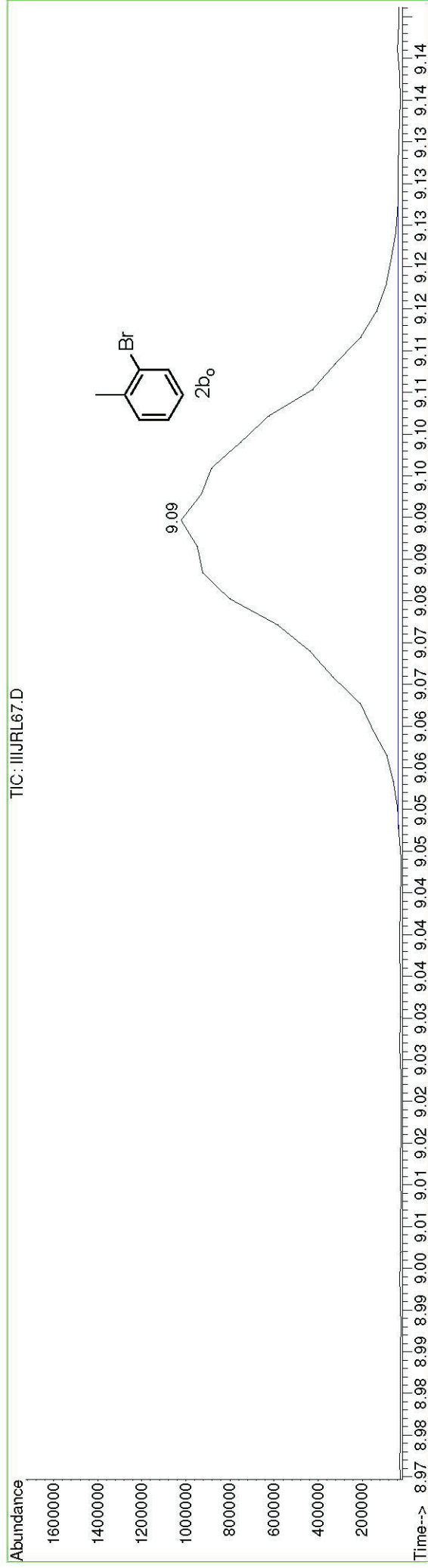
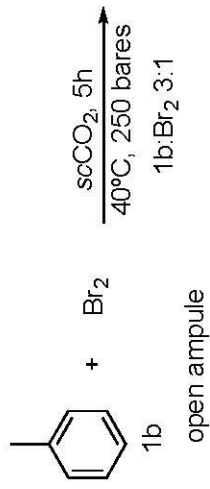
Acquired : 16 Jun 2014 21:46 using AcqMethod JMF60

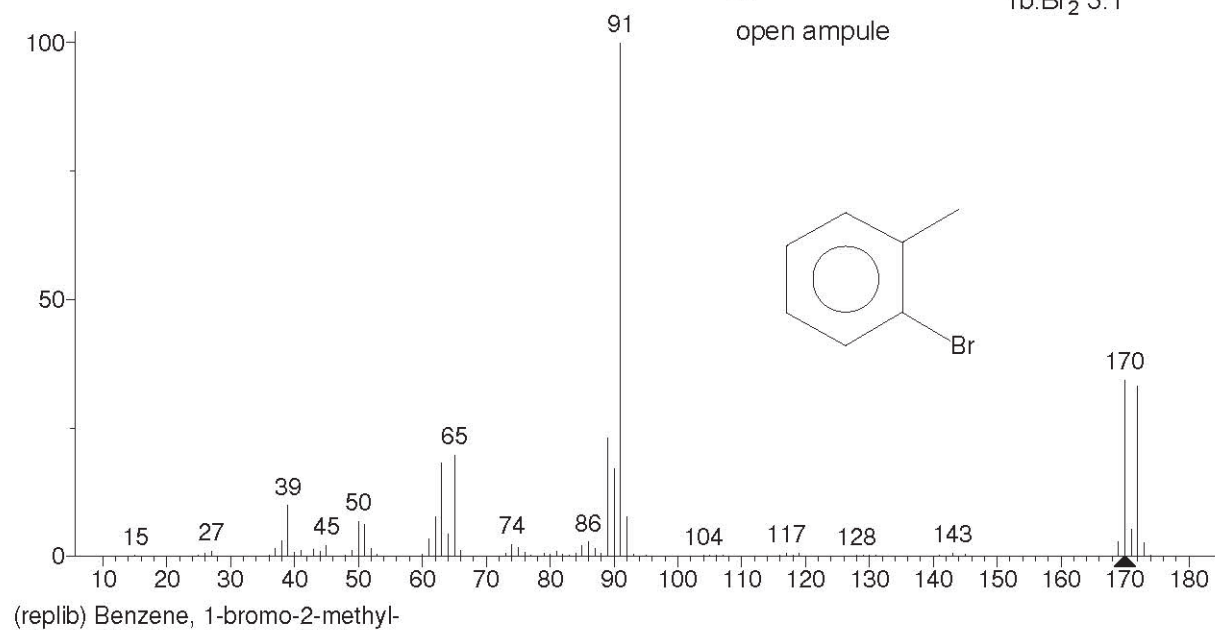
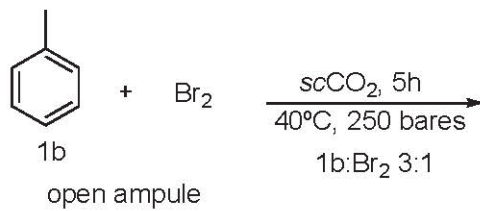
Instrument : Instrumen

Sample Name: VIDRIO

Misc Info :

Vial Number: 19





File : D:\ASENSIO\MATEO\IIIJRL67.D

Operator :

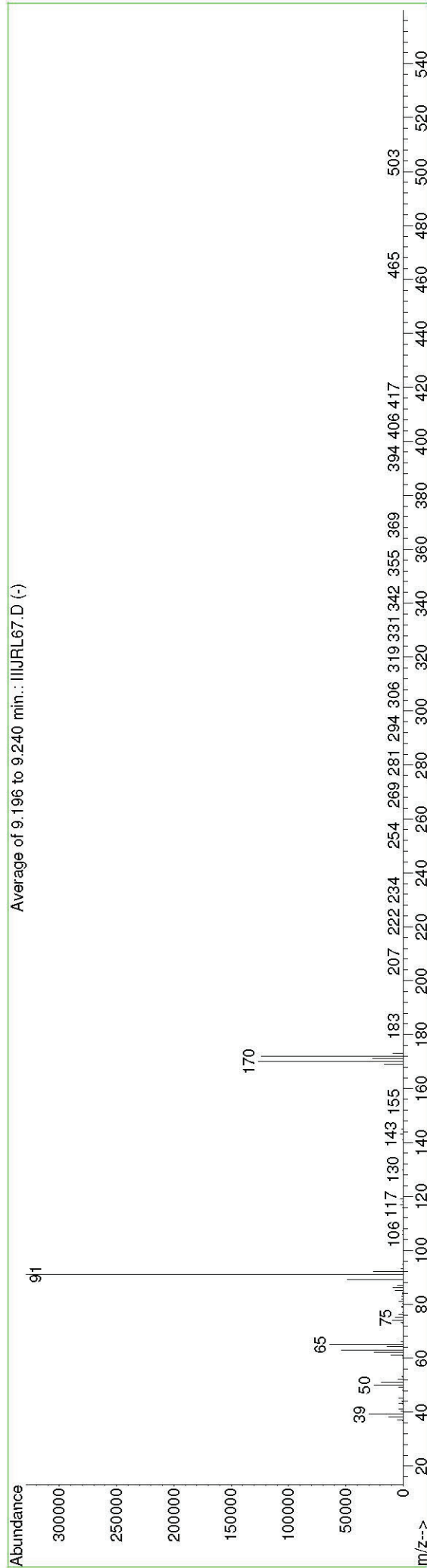
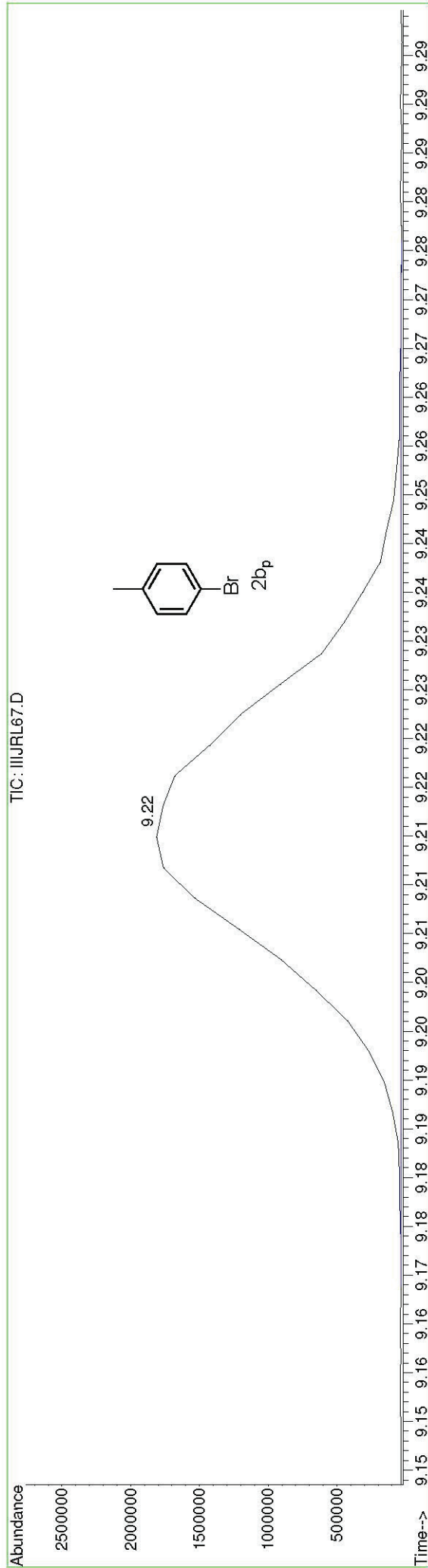
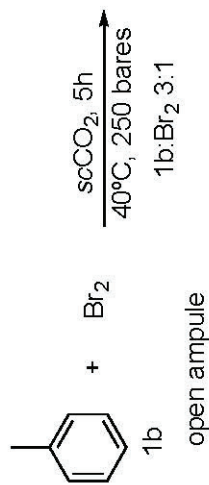
Acquired : 16 Jun 2014 21:46 using AcqMethod JMF60

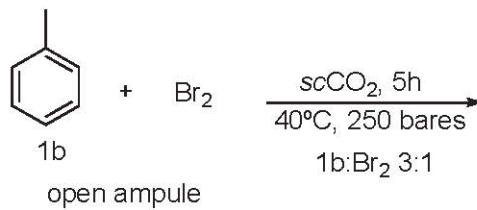
Instrument : Instrumen

Sample Name: VIDRIO

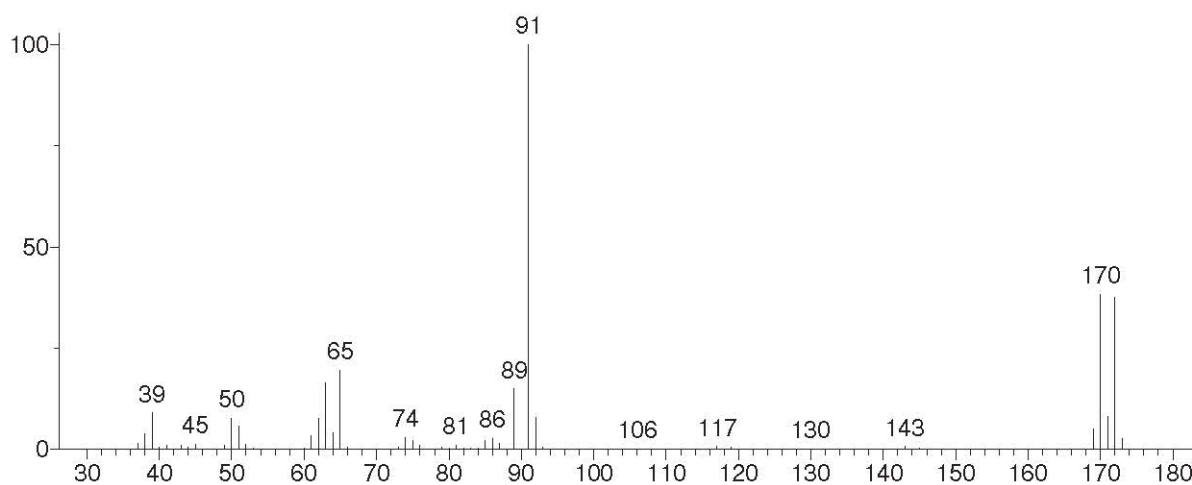
Misc Info :

Vial Number: 19

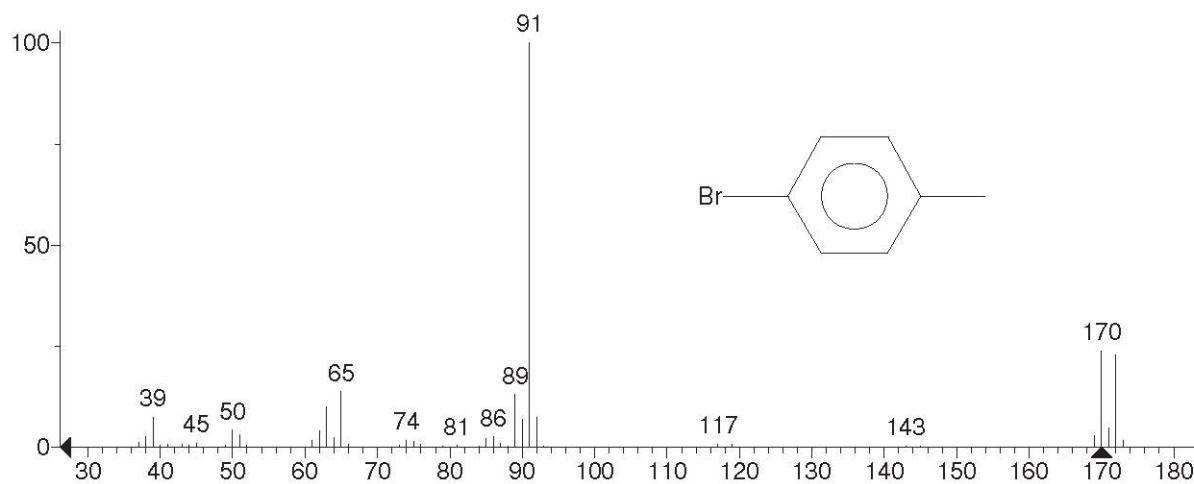




Unknown: Average of 9.196 to 9.240 min.: IIIJRL67.D
Compound in Library Factor = 388



Hit 2 : Benzene, 1-bromo-4-methyl-
C₇H₇Br; MF: 925; RMF: 925; Prob 32.2%; CAS: 106-38-7; Lib: replib; ID: 11700.



File : D:\ASENSIO\MATEO\IIIJRL30.D

Operator :

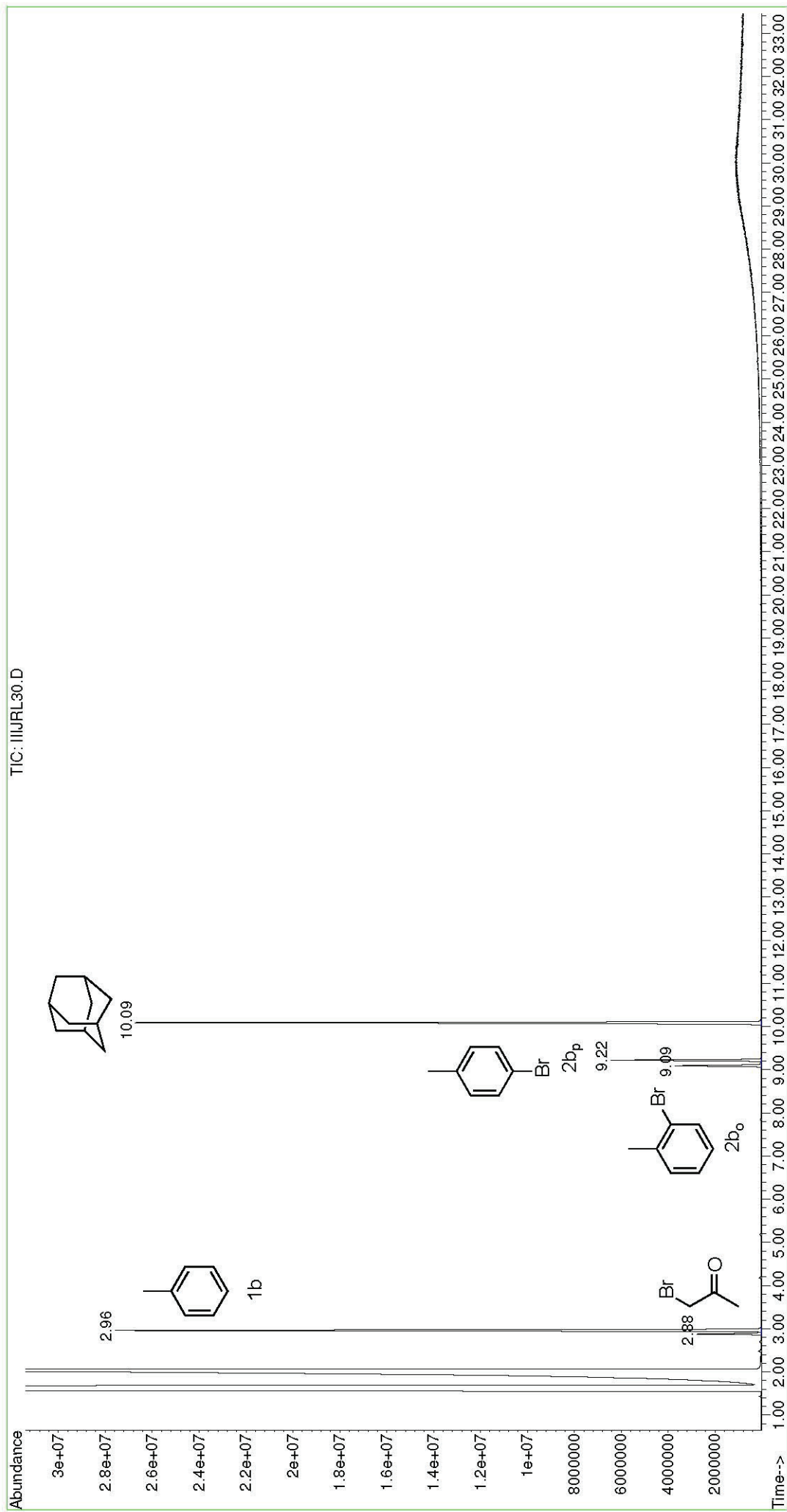
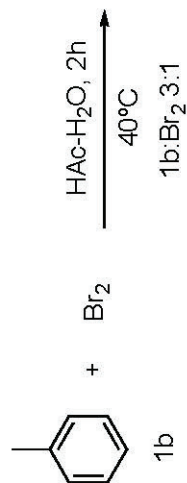
Acquired : 16 Jun 2014 20:56 using AcqMethod JMF60

Instrument : Instrument

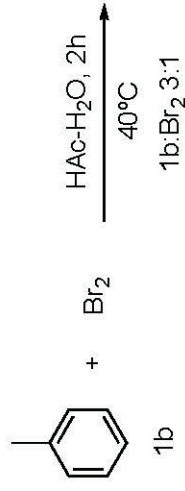
Sample Name: McPh

Misc Info :

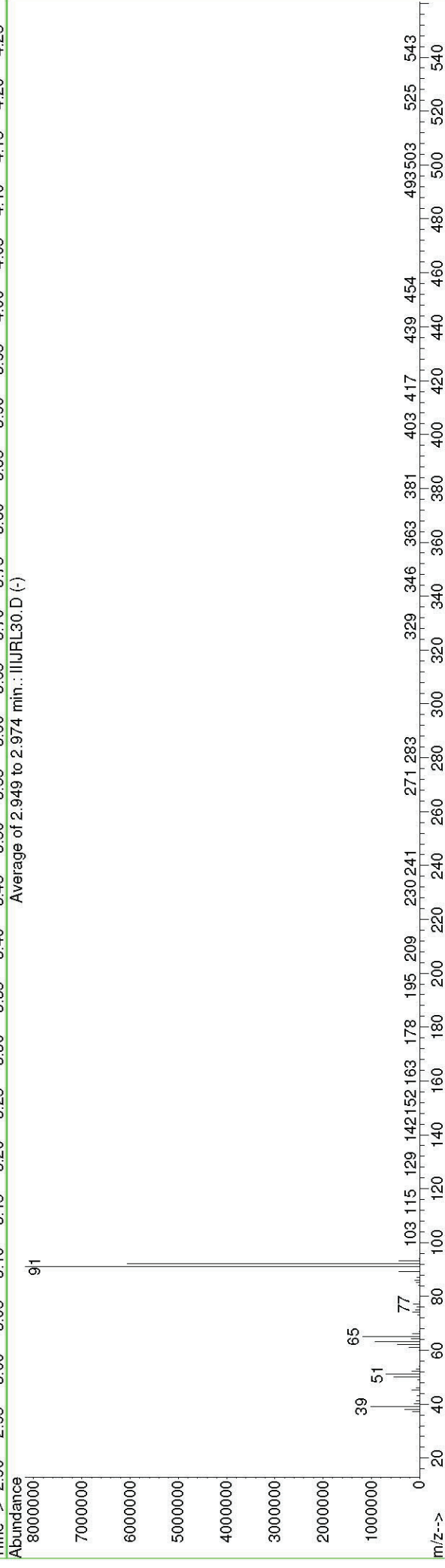
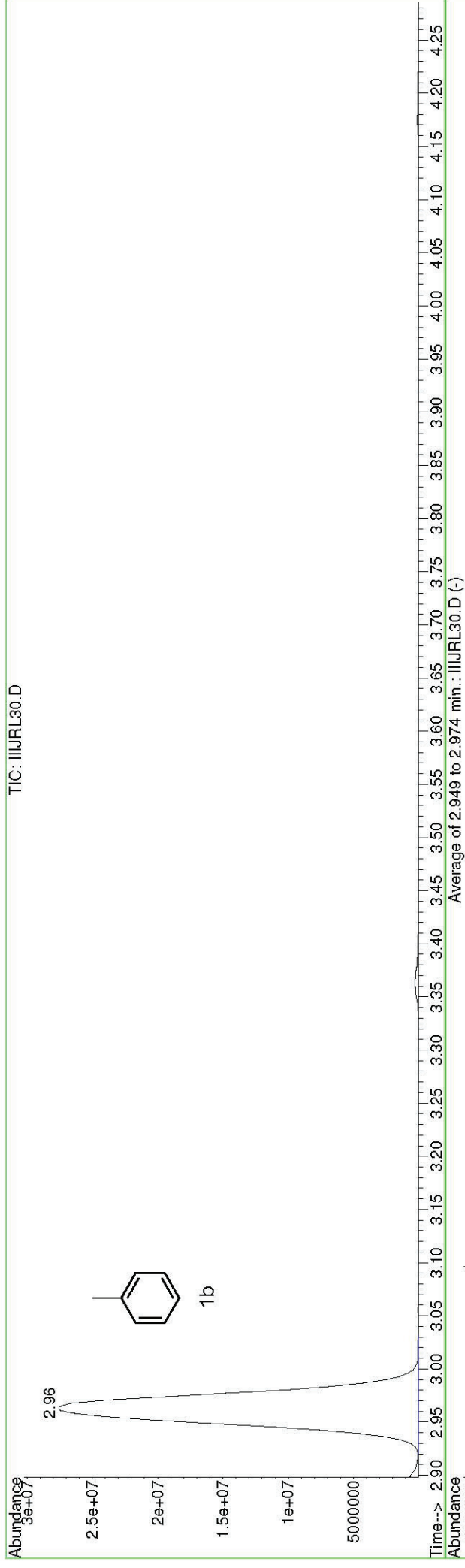
Vial Number: 18

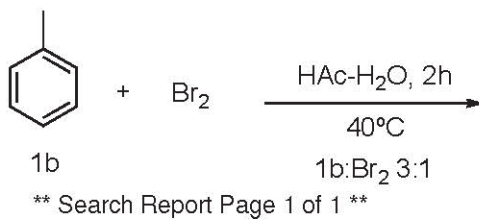


File : D:\ASENSIO\MATEO\IIIJRL30.D
Operator :
Acquired : 16 Jun 2014 20:56 using AcqMethod JMF60
Instrument : Instrument
Sample Name: McPh
Misc Info :
Vial Number: 18

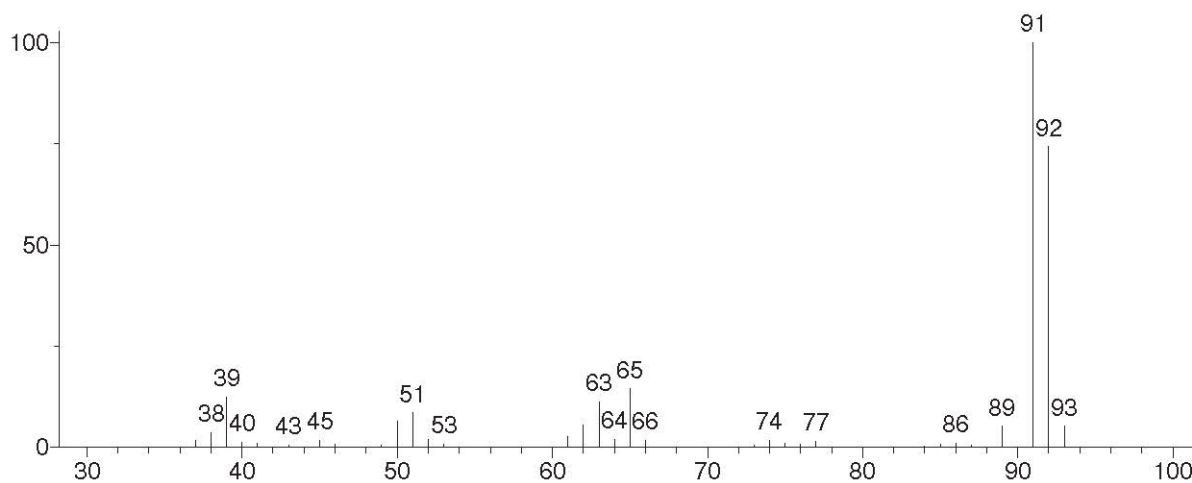


TIC: IIIJRL30.D

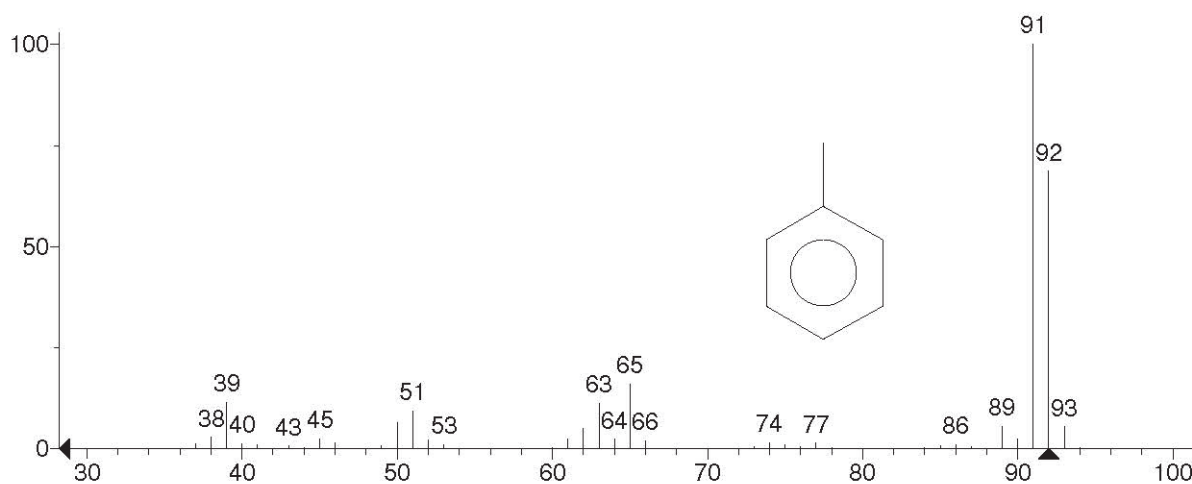




Unknown: Average of 2.949 to 2.974 min.: IIIJRL30.D
Compound in Library Factor = 116



Hit 1 : Toluene
C₇H₈; MF: 946; RMF: 946; Prob 44.4%; CAS: 108-88-3; Lib: replib; ID: 11301.



File : D:\ASENSIO\MATEO\IIIJRL30.D

Operator :

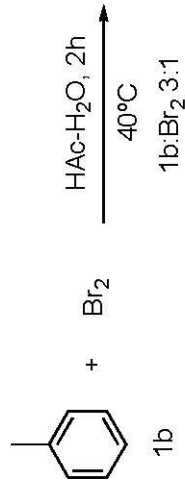
Acquired : 16 Jun 2014 20:56 using AcqMethod JMF60

Instrument : Instrument

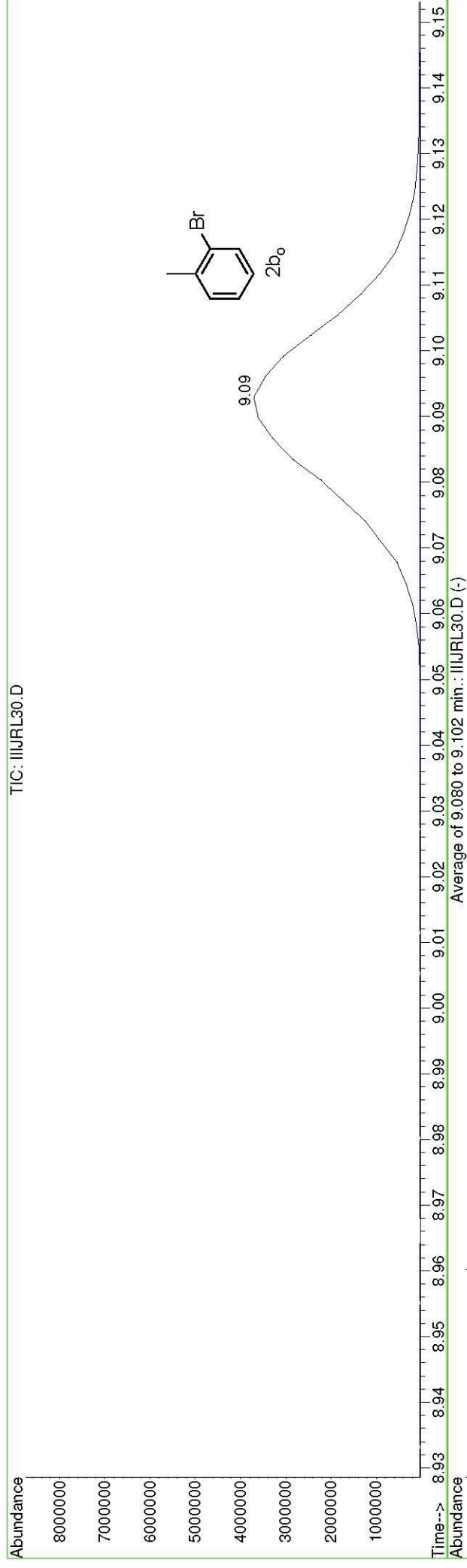
Sample Name: McPh

Misc Info :

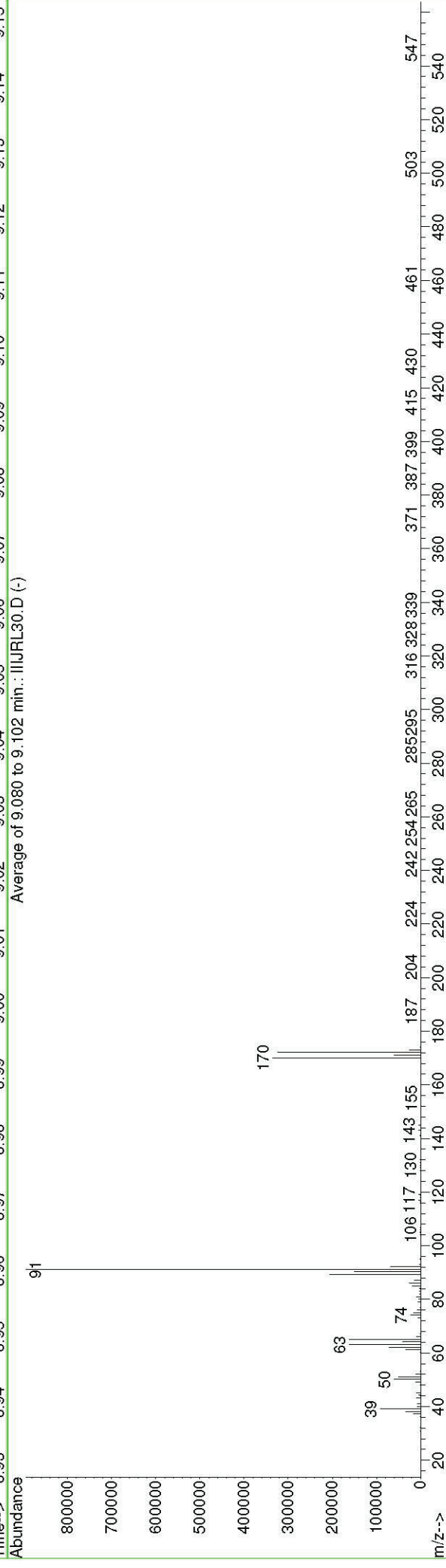
Vial Number: 18

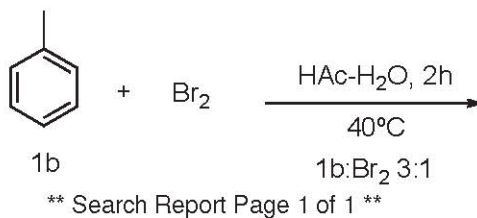


TIC: IIJRL30.D

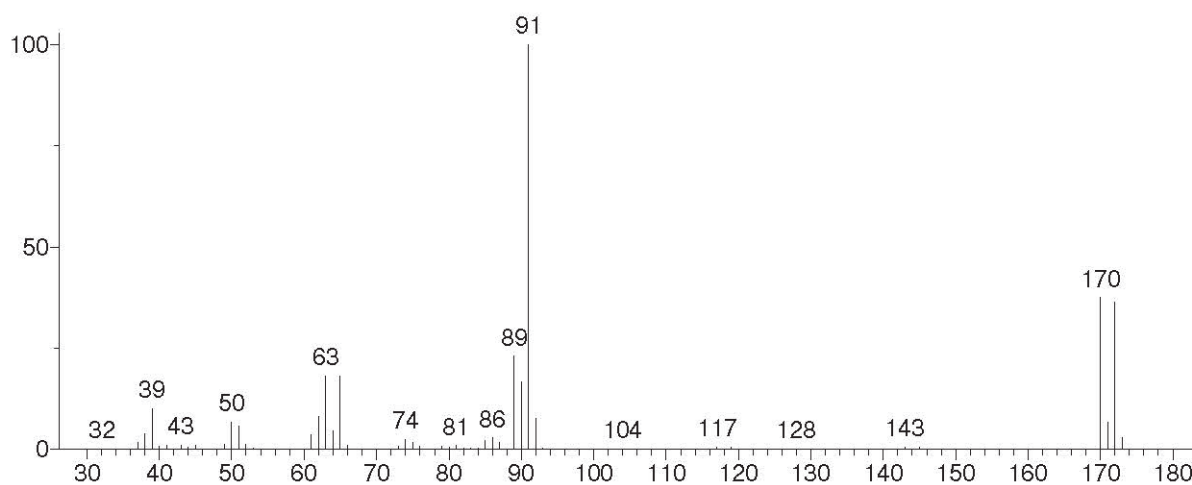


Average of 9.080 to 9.102 min.: IIJRL30.D (-)

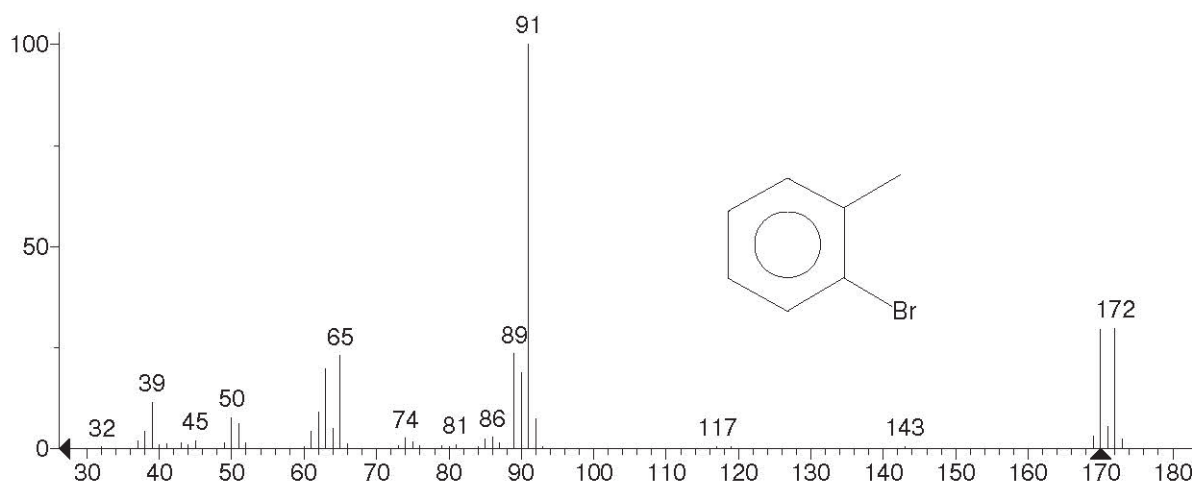




Unknown: Average of 9.080 to 9.102 min.: IIIJRL30.D
Compound in Library Factor = 320



Hit 1 : Benzene, 1-bromo-2-methyl-
C₇H₇Br; MF: 947; RMF: 948; Prob 43.0%; CAS: 95-46-5; Lib: wiley7n; ID: 72508.



File : D:\ASENSIO\MATEO\IIJRL30.D

Operator :

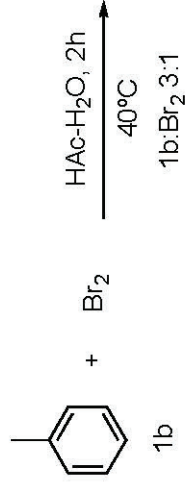
Acquired : 16 Jun 2014 20:56 using AcqMethod JMF60

Instrument : Instrument

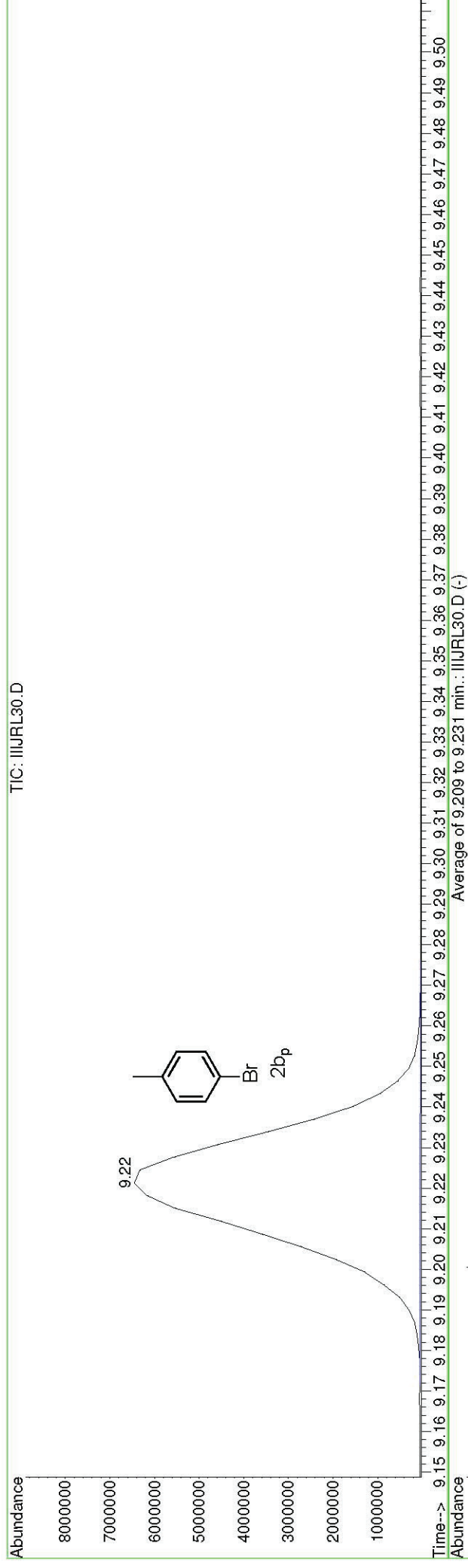
Sample Name: McPh

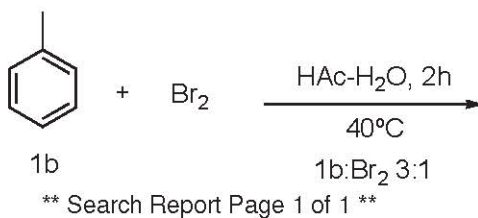
Misc Info :

Vial Number: 18

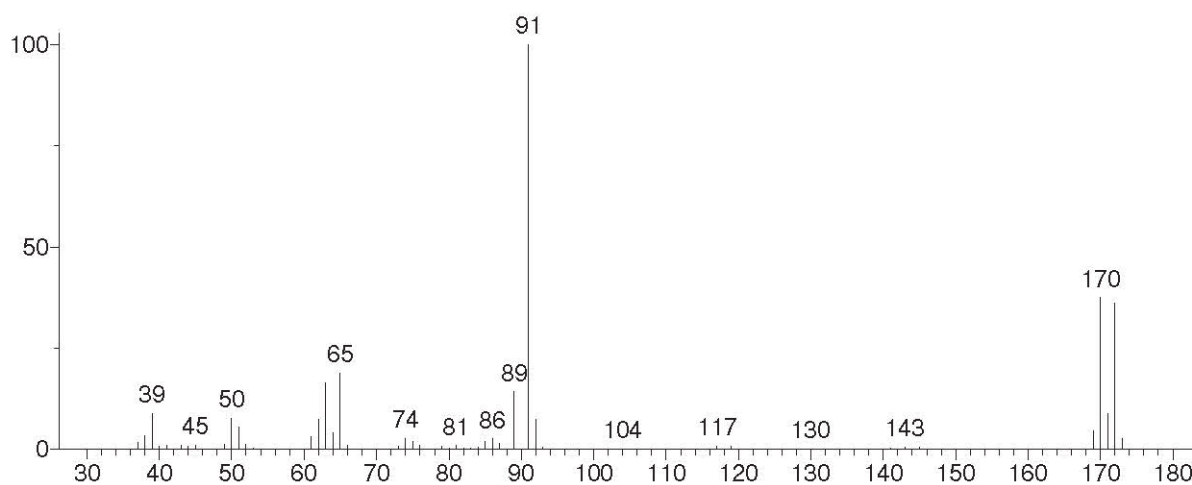


TIC: IIJRL30.D

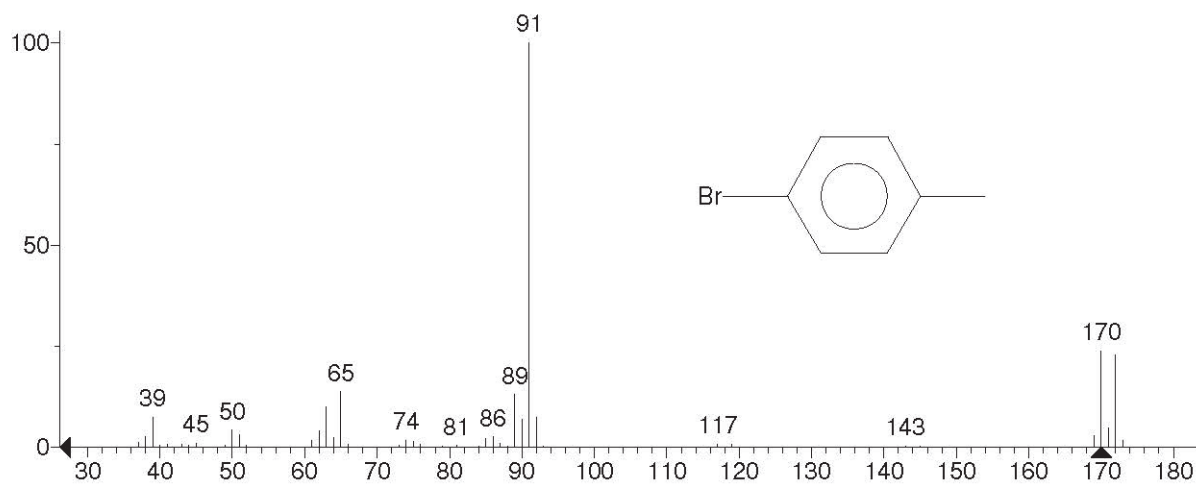




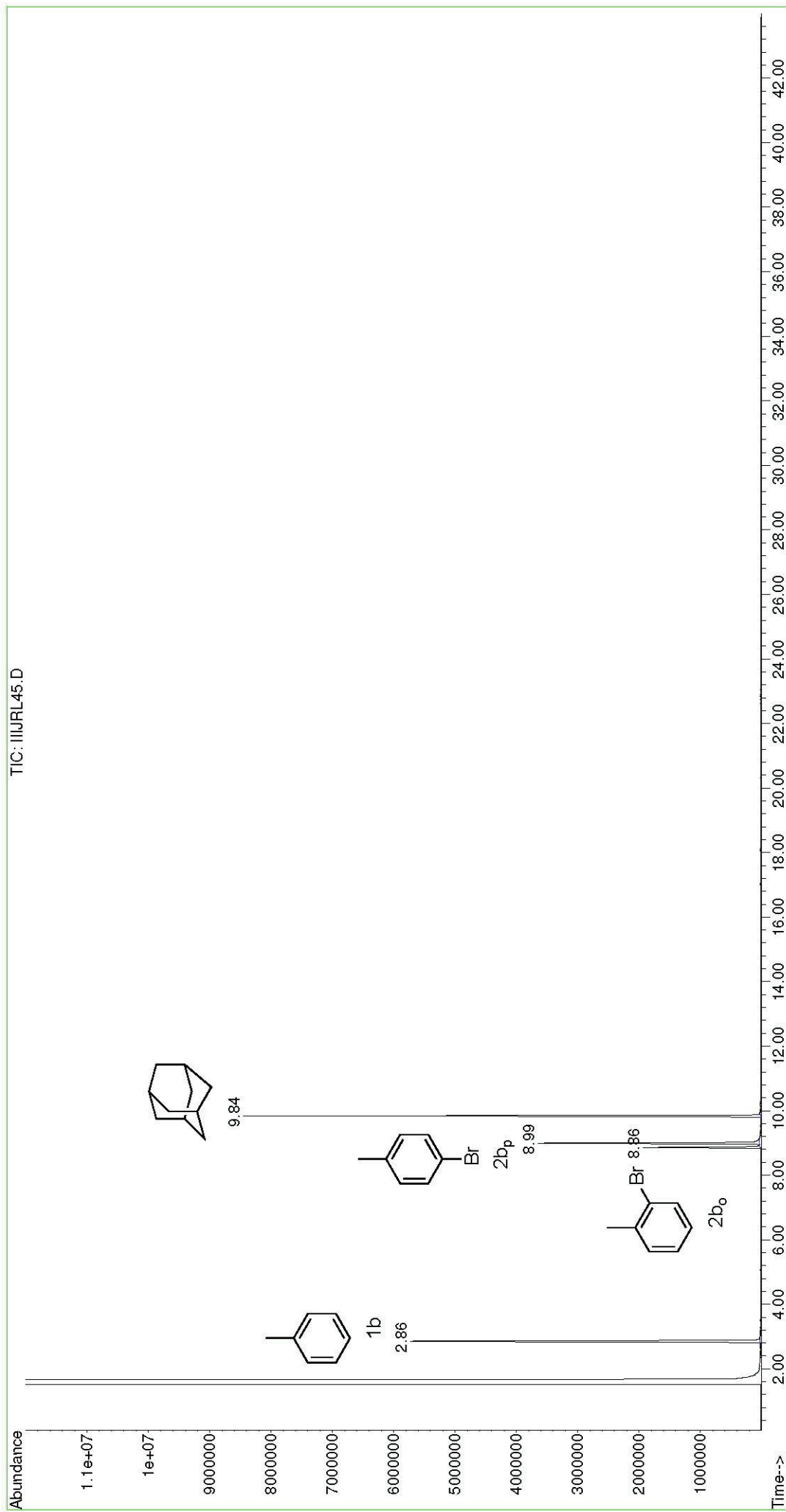
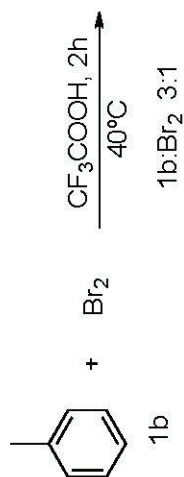
Unknown: Average of 9.209 to 9.231 min.: IIIJRL30.D
Compound in Library Factor = 475



Hit 2 : Benzene, 1-bromo-4-methyl-
C₇H₇Br; MF: 942; RMF: 942; Prob 32.4%; CAS: 106-38-7; Lib: replib; ID: 11700.



File : D:\ASENSIO\JAVI\IIIJRL45.D
Operator :
Acquired : 25 Feb 2014 19:58 using AcqMethod JMF60
Instrument : Instrumenten
Sample Name: IIIJRL45
Misc Info :
Vial Number: 15



File : D:\ASENSIO\JAVI\IIJRL45.D

Operator :

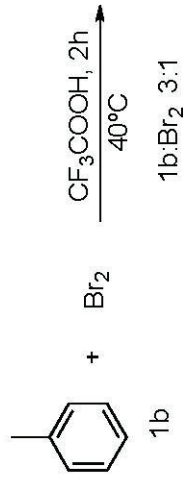
Acquired : 25 Feb 2014 19:58 using AcqMethod JMF60

Instrument : Instrument

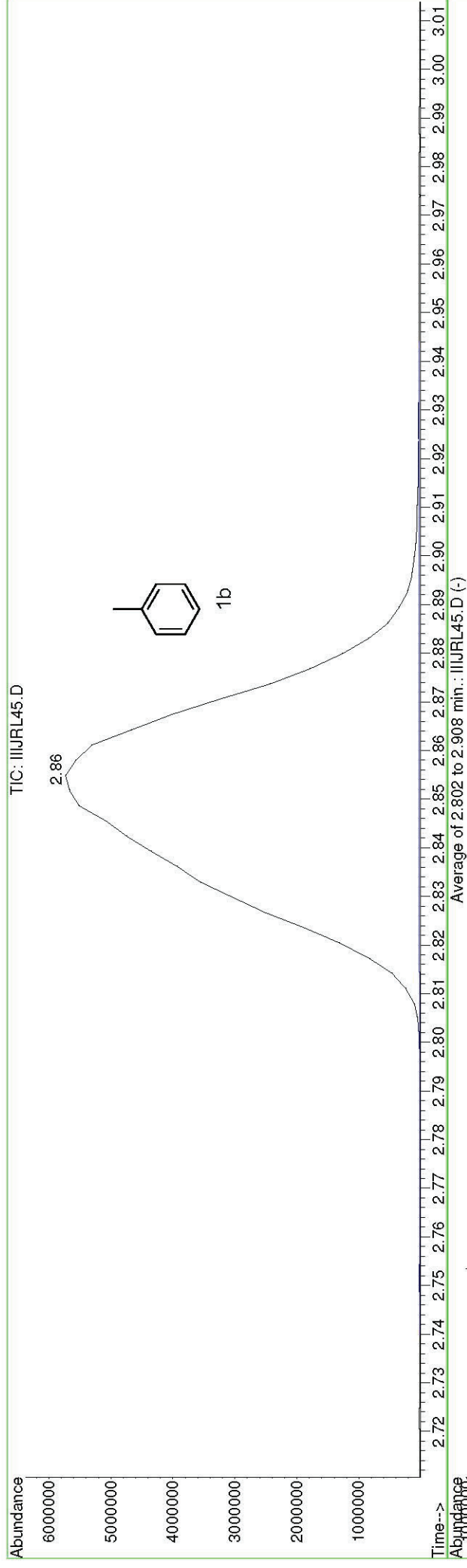
Sample Name: IIJRL45

Misc Info :

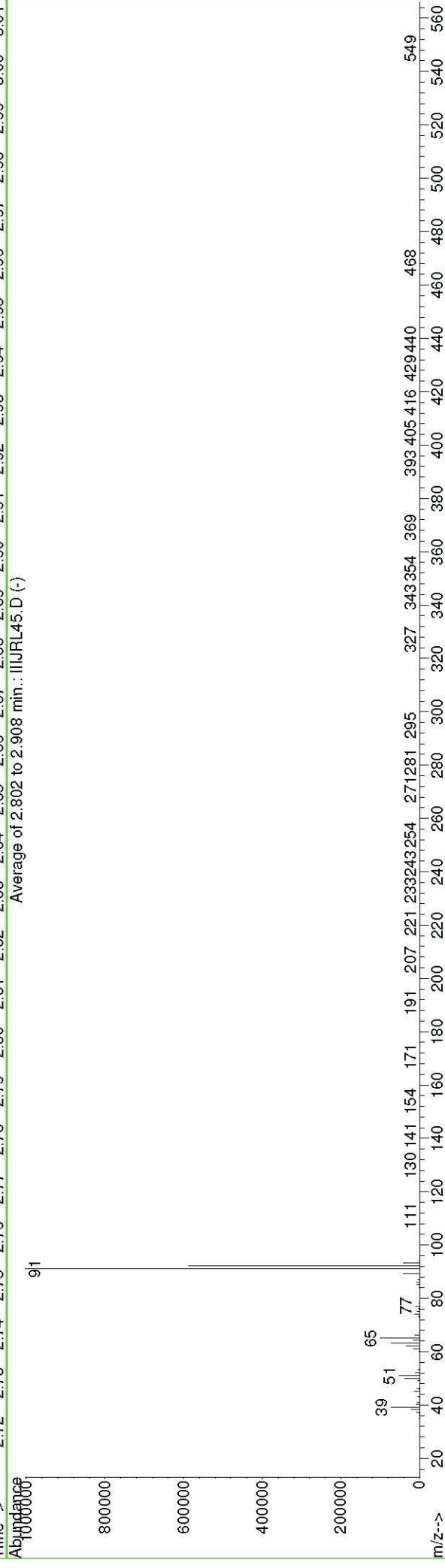
Vial Number: 15

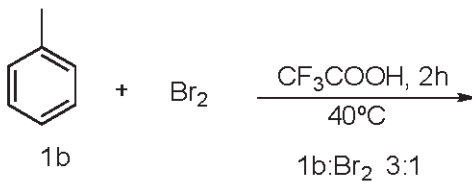


TIC: IIJRL45.D



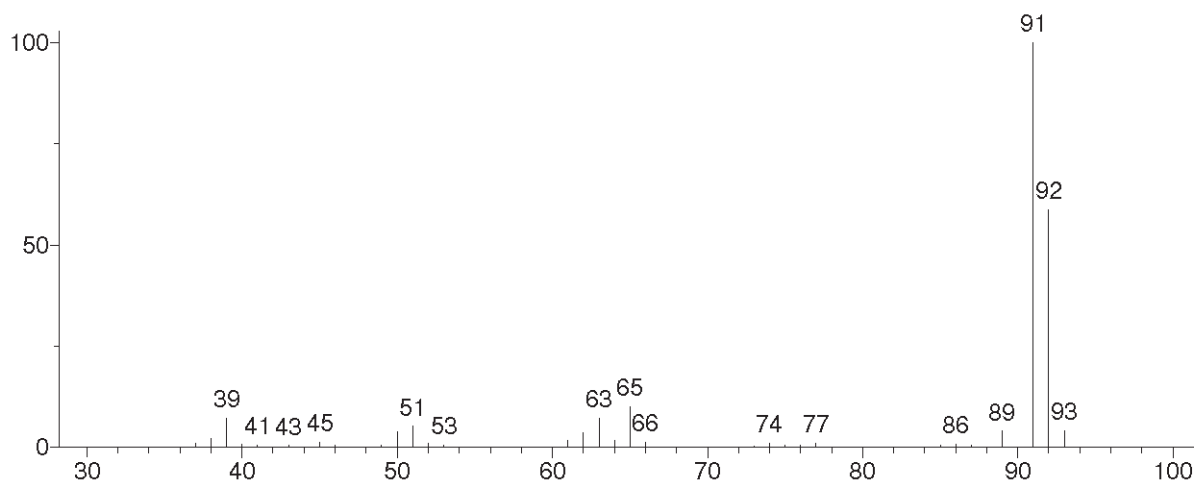
Average of 2.802 to 2.908 min.: IIJRL45.D (-)



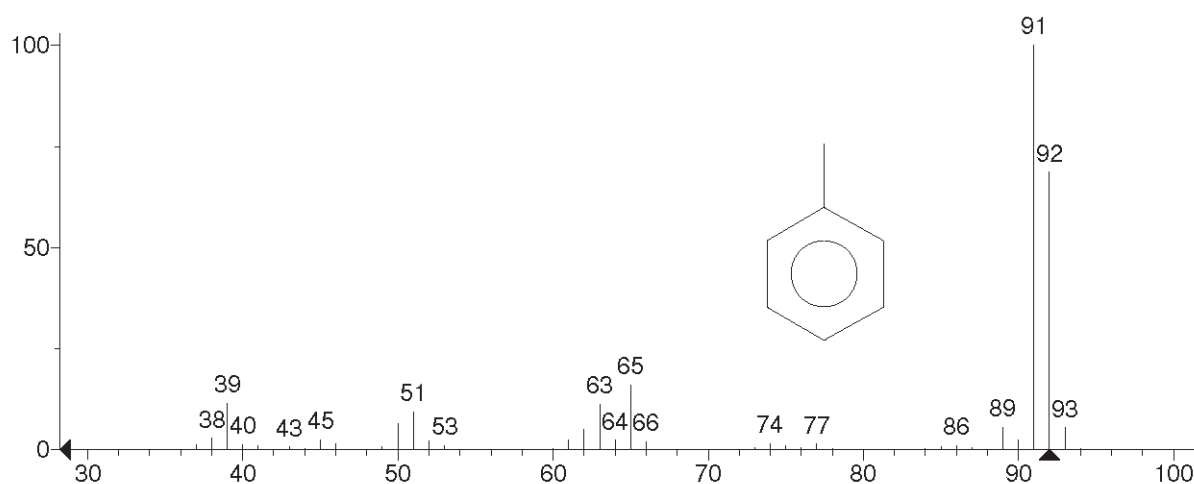


** Search Report Page 1 of 1 **

Unknown: Average of 2.802 to 2.908 min.: IIIJRL45.D
Compound in Library Factor = 102



Hit 2 : Toluene
C₇H₈; MF: 953; RMF: 953; Prob 18.2%; CAS: 108-88-3; Lib: replib; ID: 11301.



File : D:\ASENSIO\JAVI\IIJRL45.D

Operator :

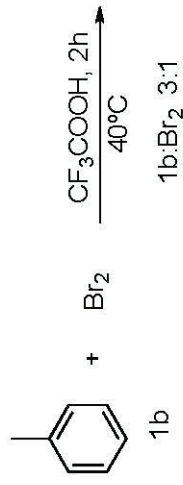
Acquired : 25 Feb 2014 19:58 using AcqMethod JMF60

Instrument : Instrument

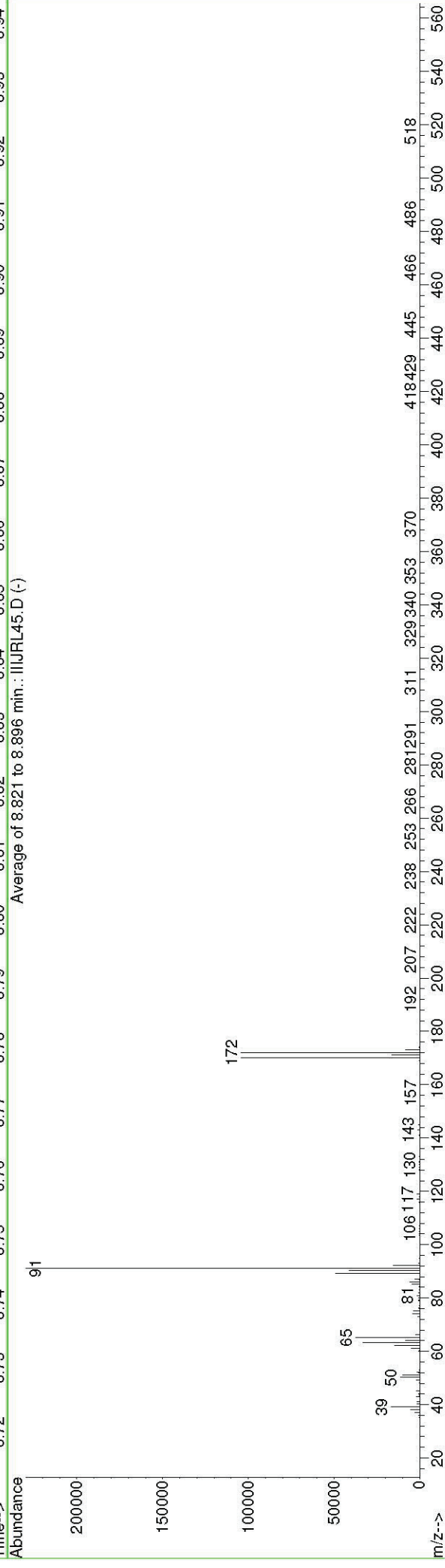
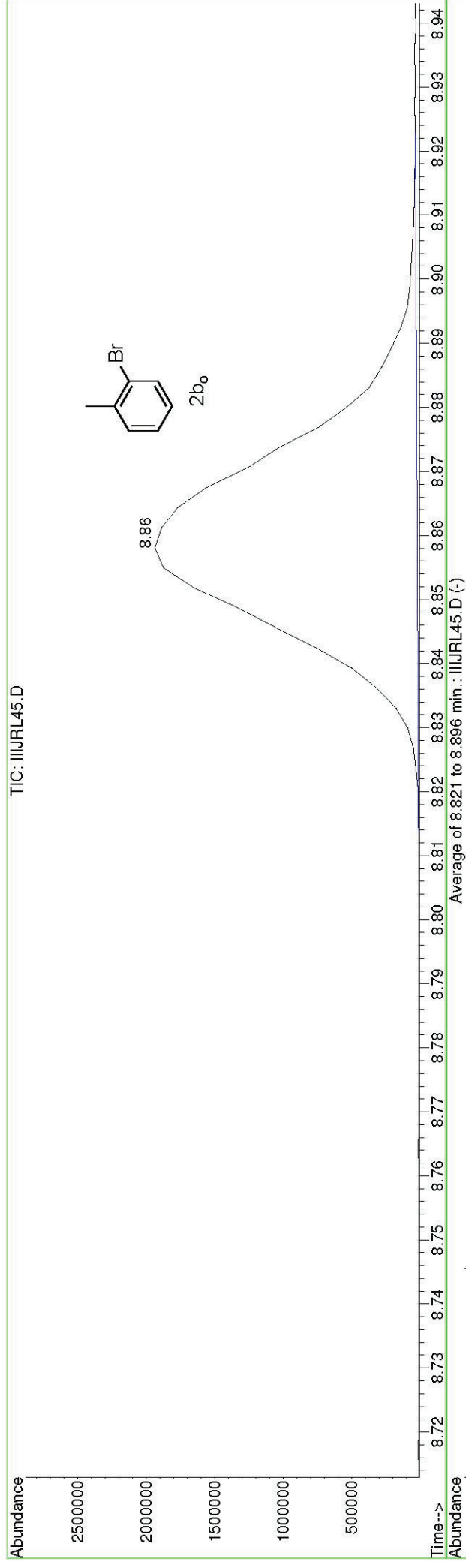
Sample Name: IIJRL45

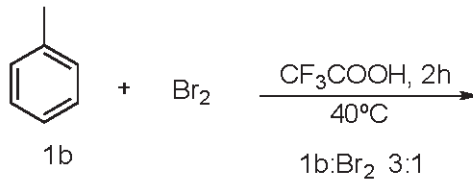
Misc Info :

Vial Number: 15



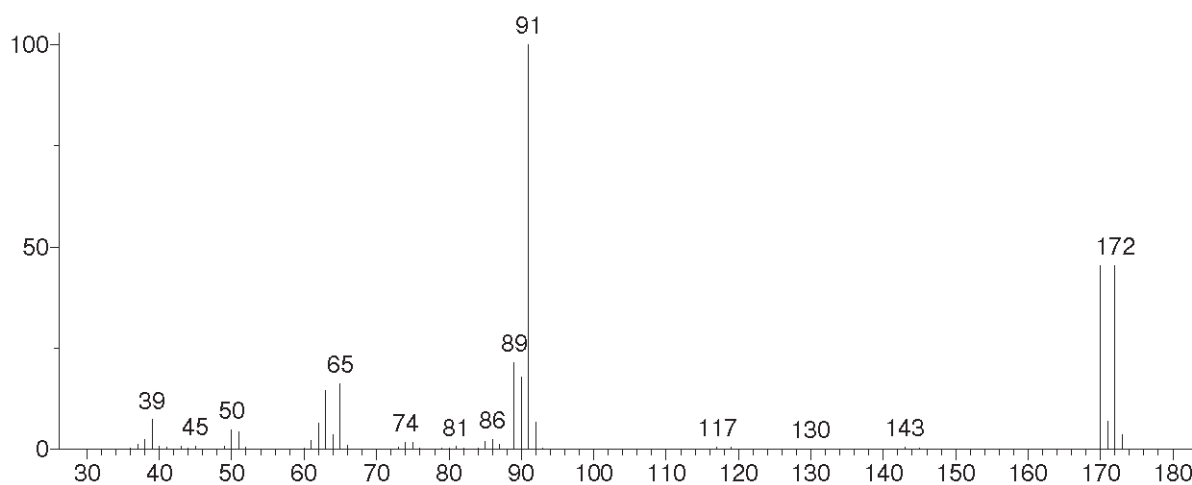
TIC: IIJRL45.D



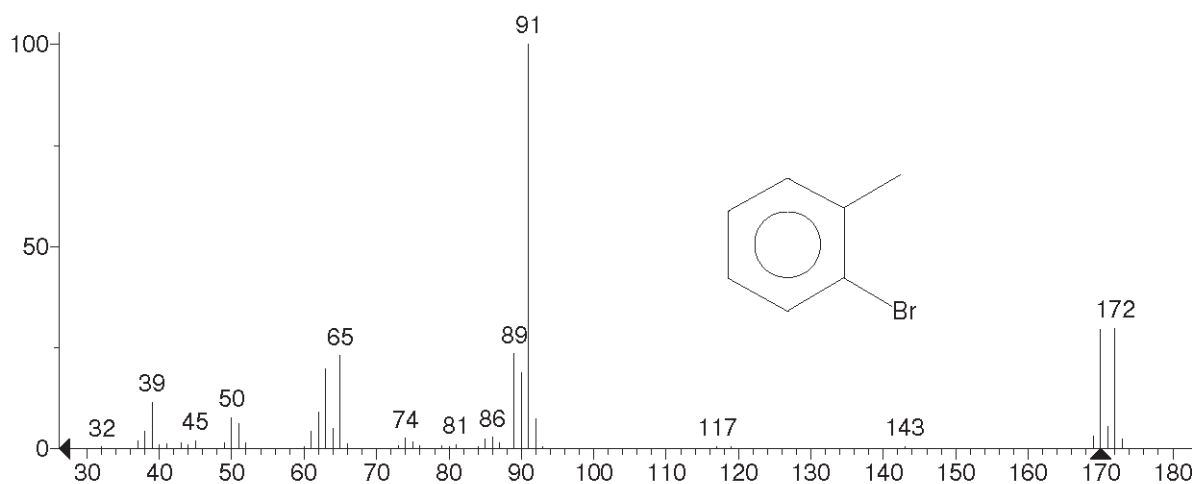


** Search Report Page 1 of 1 **

Unknown: Average of 8.821 to 8.896 min.: IIIJRL45.D
Compound in Library Factor = 184



Hit 1 : Benzene, 1-bromo-2-methyl-
C₇H₇Br; MF: 932; RMF: 933; Prob 39.0%; CAS: 95-46-5; Lib: wiley7n; ID: 72508.



File : D:\ASENSIO\JAVI\IIIJRL45.D

Operator :

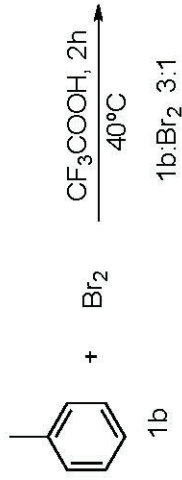
Acquired : 25 Feb 2014 19:58 using AcqMethod JMF60

Instrument : Instrument

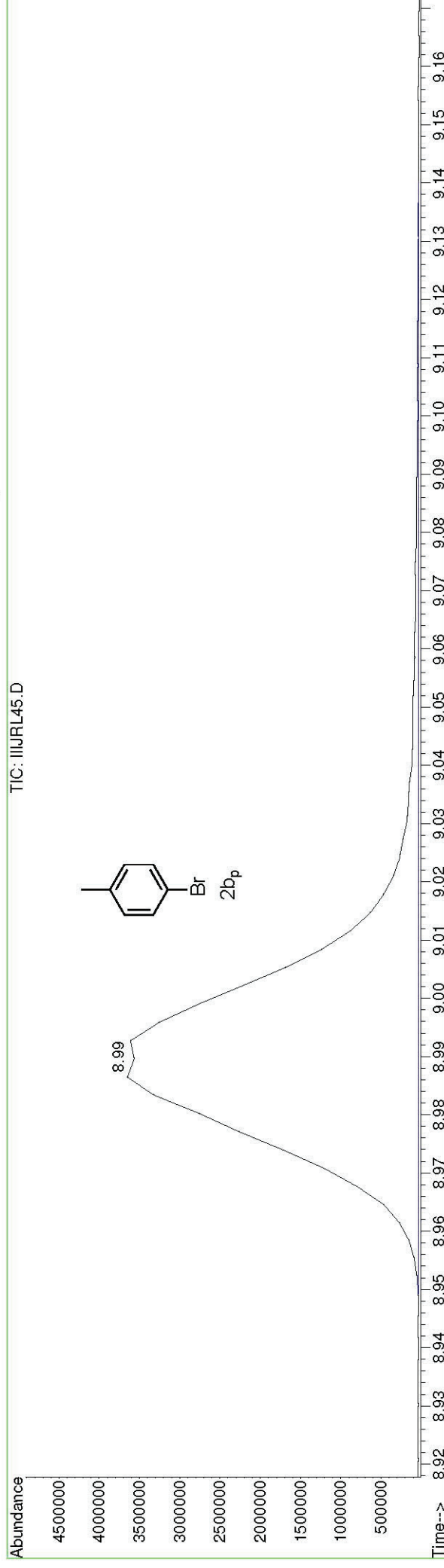
Sample Name: IIIJRL45

Misc Info :

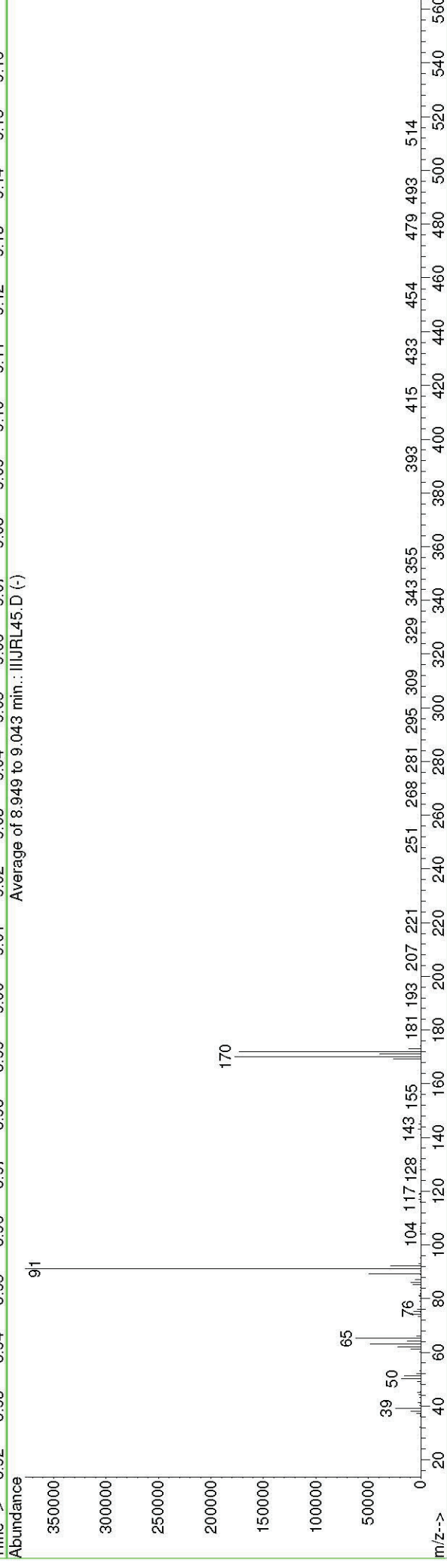
Vial Number: 15

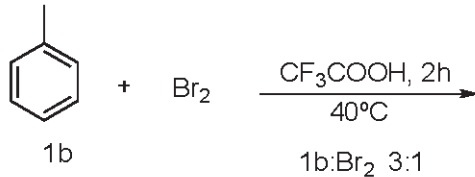


TIC: IIIJRL45.D



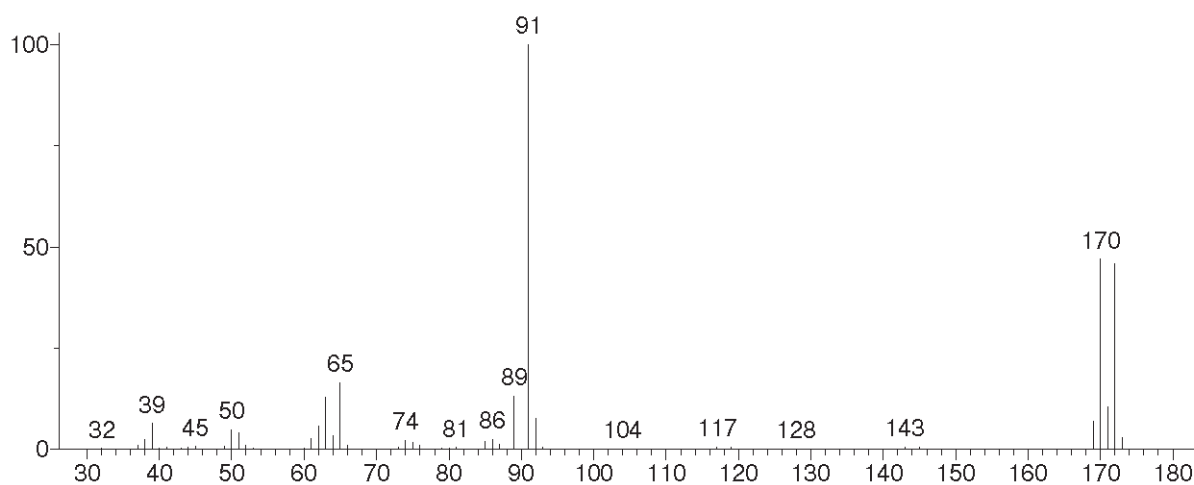
Average of 8.949 to 9.043 min.: IIIJRL45.D (-)



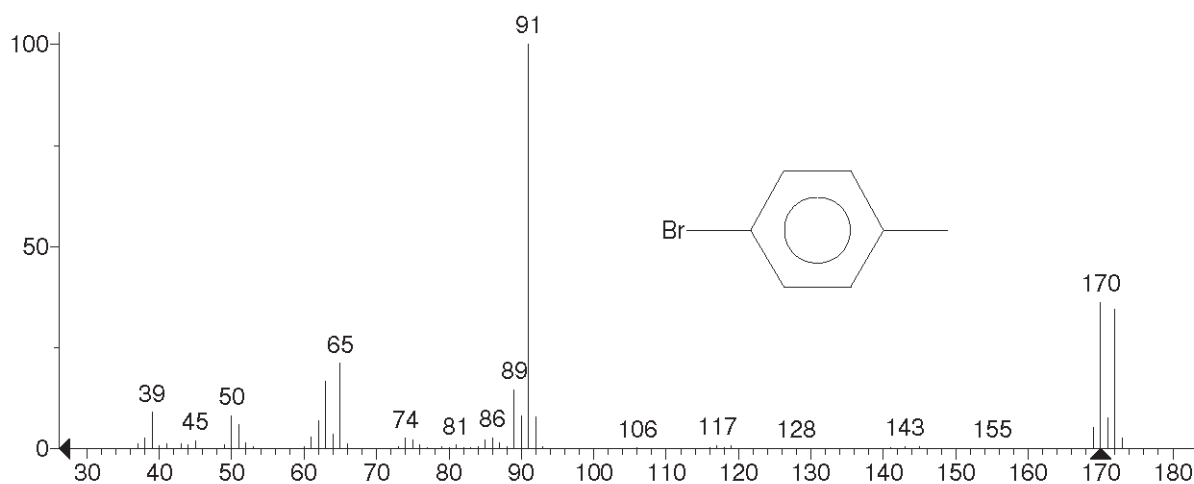


** Search Report Page 1 of 1 **

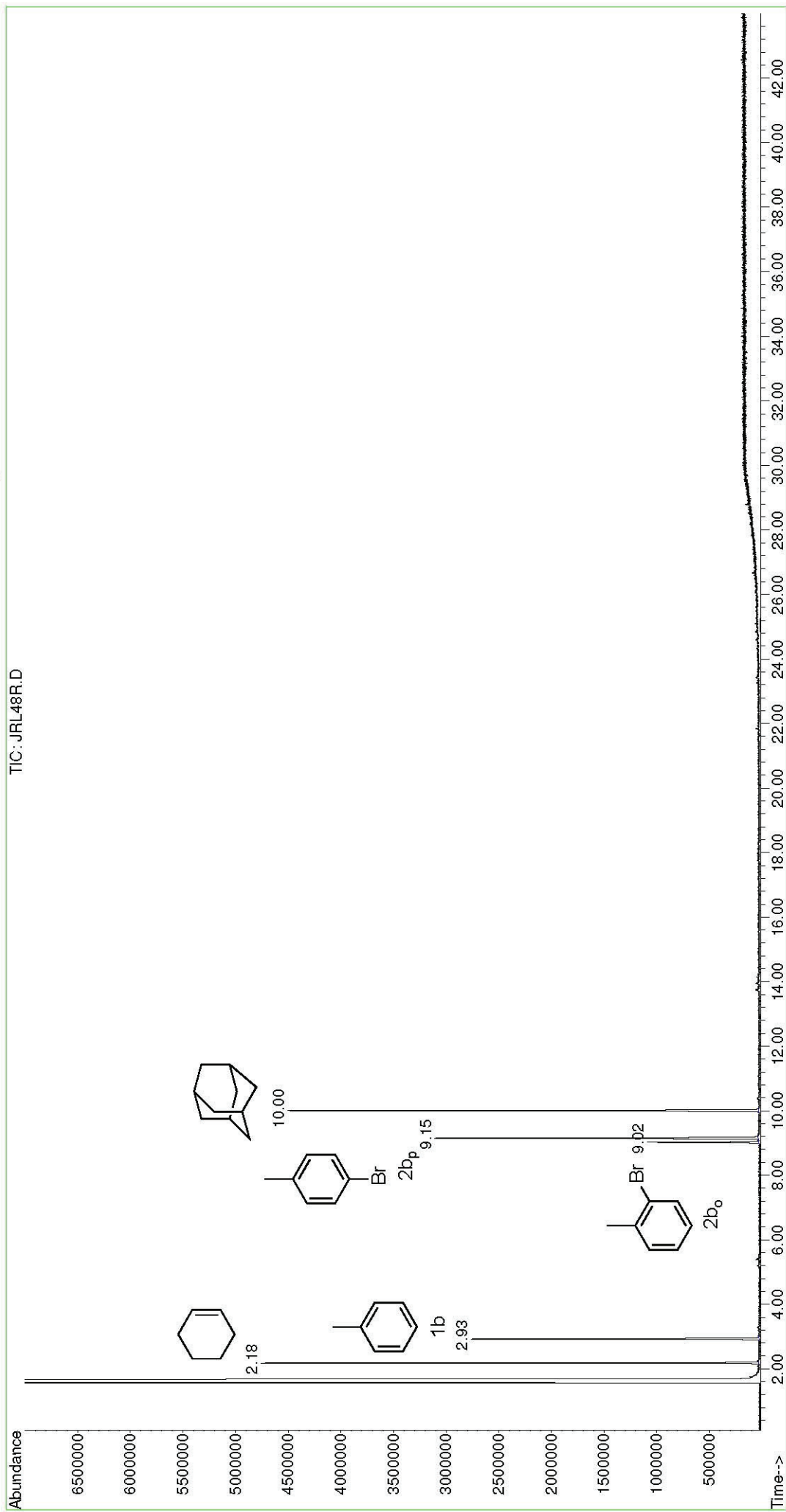
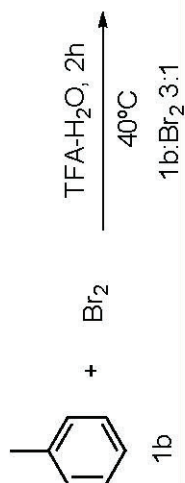
Unknown: Average of 8.949 to 9.043 min.: IIIJRL45.D
Compound in Library Factor = 312



Hit 1 : Benzene, 1-bromo-4-methyl-
C₇H₇Br; MF: 931; RMF: 931; Prob 48.1%; CAS: 106-38-7; Lib: replib; ID: 11701.



File : C:\MSDCHEM\1\DATA\ASENSIO\JAVI\JRL48R.D
 Operator :
 Acquired : 3 Jul 2014 16:12 using AcqMethod JMF60
 Instrument : Instrument
 Sample Name :
 Misc Info :
 Vial Number: 11



File : C:\MSDCHEM\1\DATA\ASENSIO\JAVI\JRL48R.D

Operator :

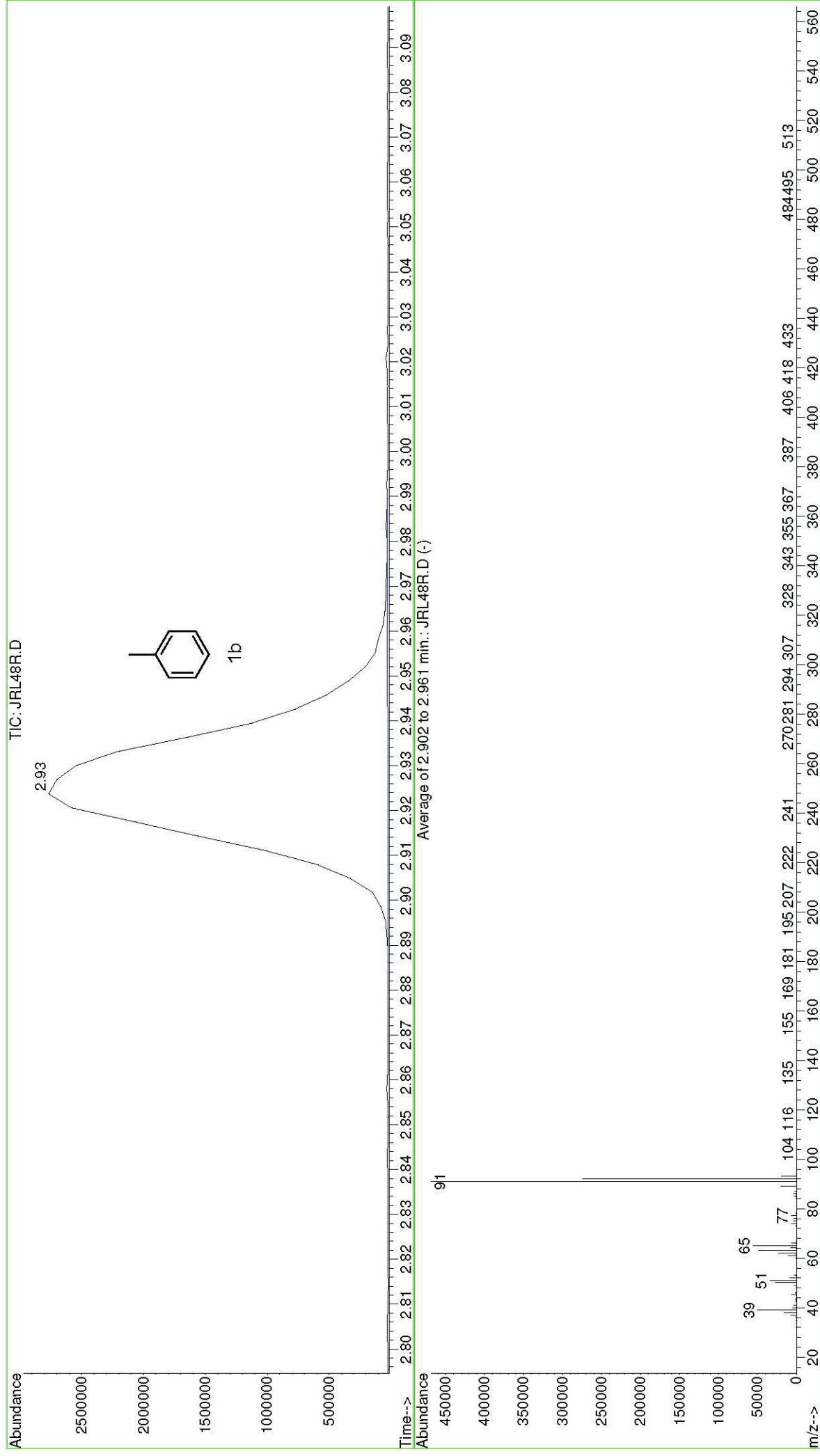
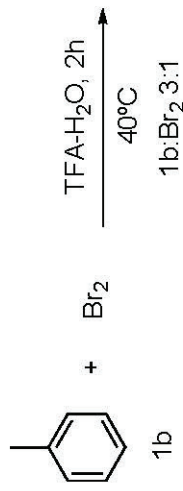
Acquired : 3 Jul 2014 16:12 using AcqMethod JMF60

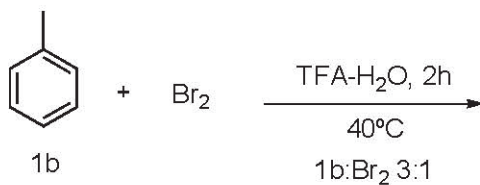
Instrument : Instrument

Sample Name:

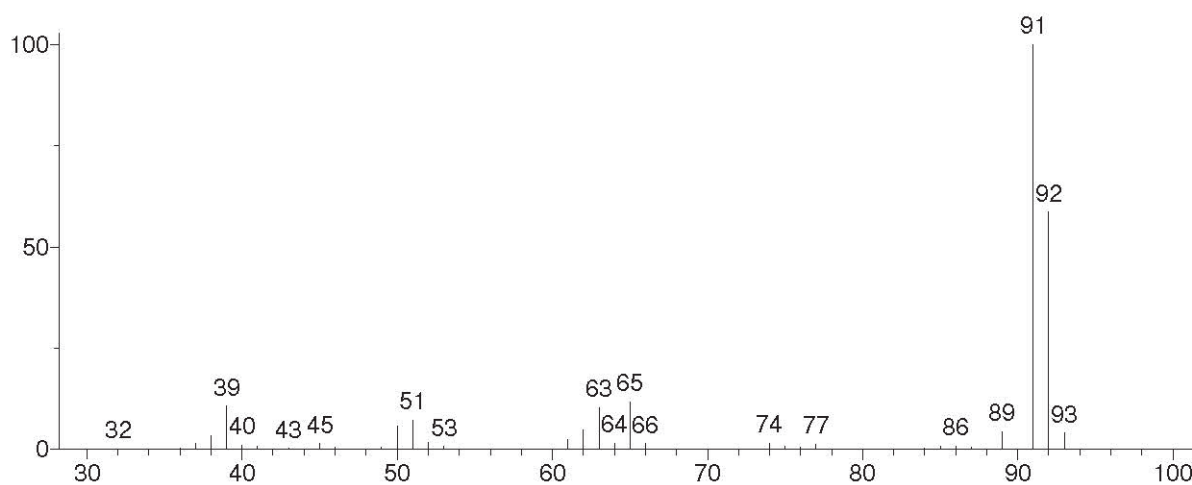
Misc Info :

Vial Number: 11

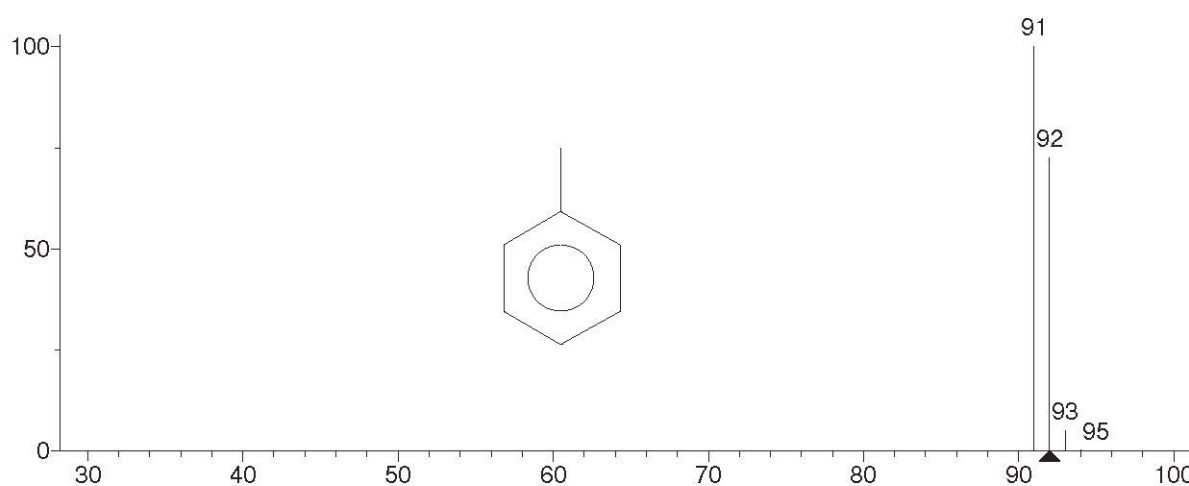




Unknown: Average of 2.902 to 2.961 min.: JRL48R.D
Compound in Library Factor = 101



Hit 2 : Benzene, methyl- (CAS)
C₇H₈; MF: 952; RMF: 952; Prob 21.9%; CAS: 108-88-3; Lib: wiley7n; ID: 5547.



File : C:\MSDCHEM\1\DATA\ASENSIO\JAVI\JRL48R.D

Operator :

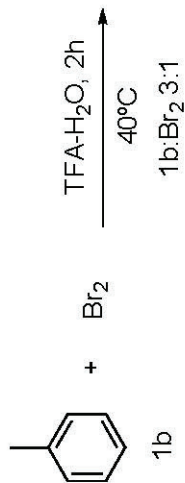
Acquired : 3 Jul 2014 16:12 using AcqMethod JMF60

Instrument : Instrument

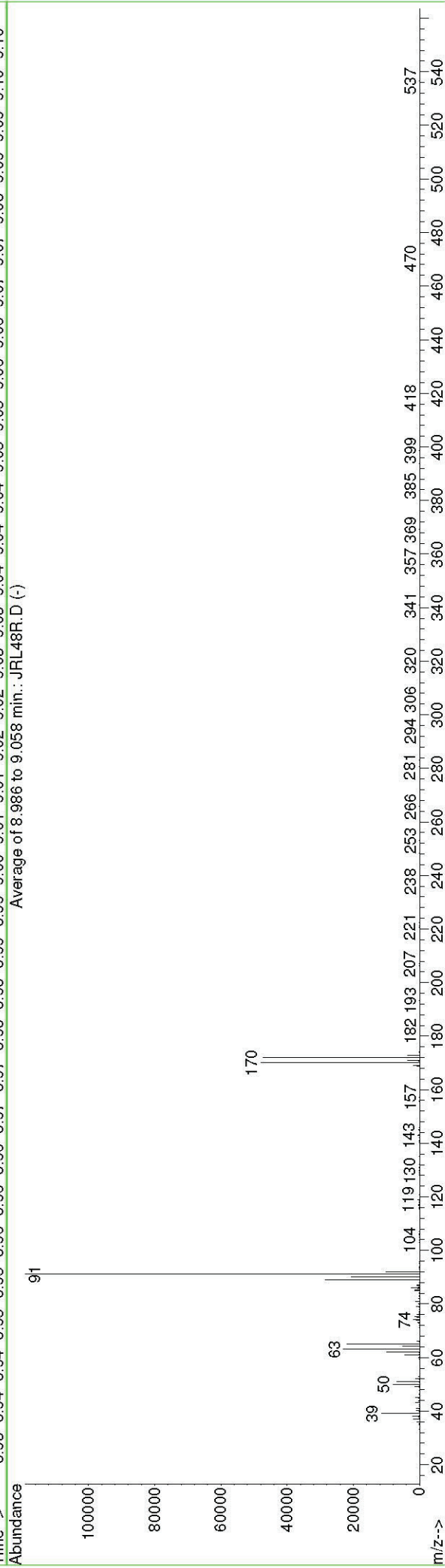
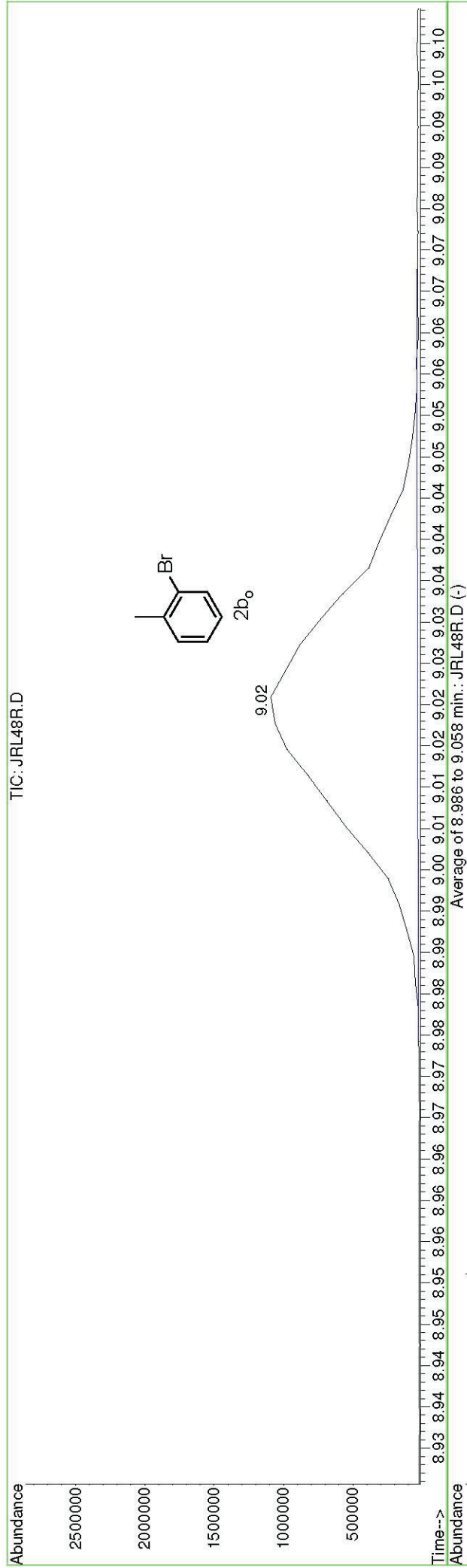
Sample Name:

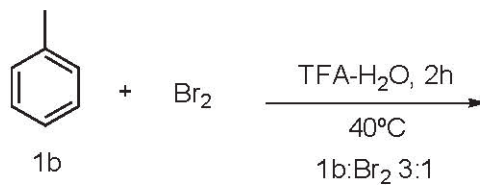
Misc Info :

Vial Number: 11

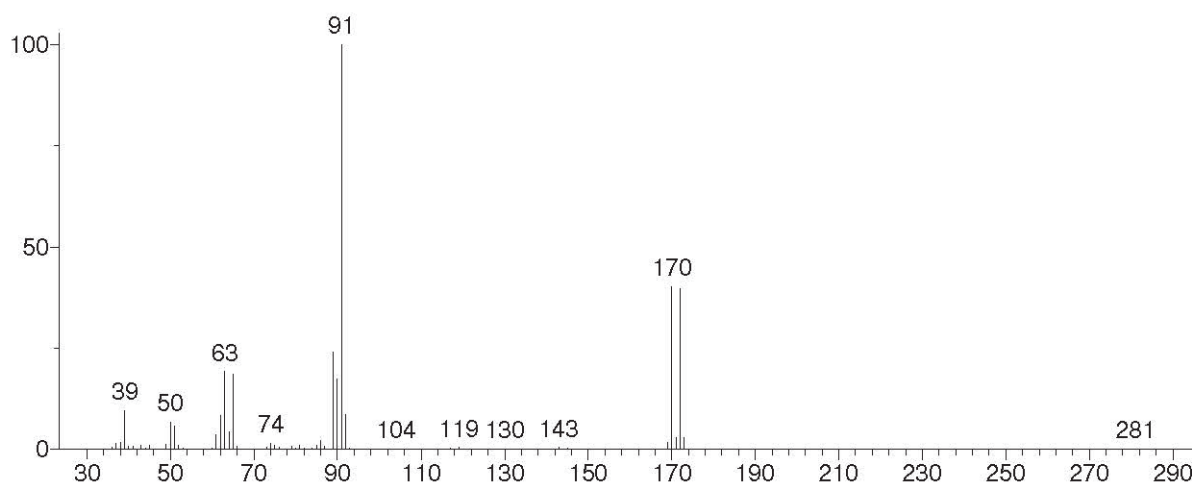


TIC: JRL48R.D

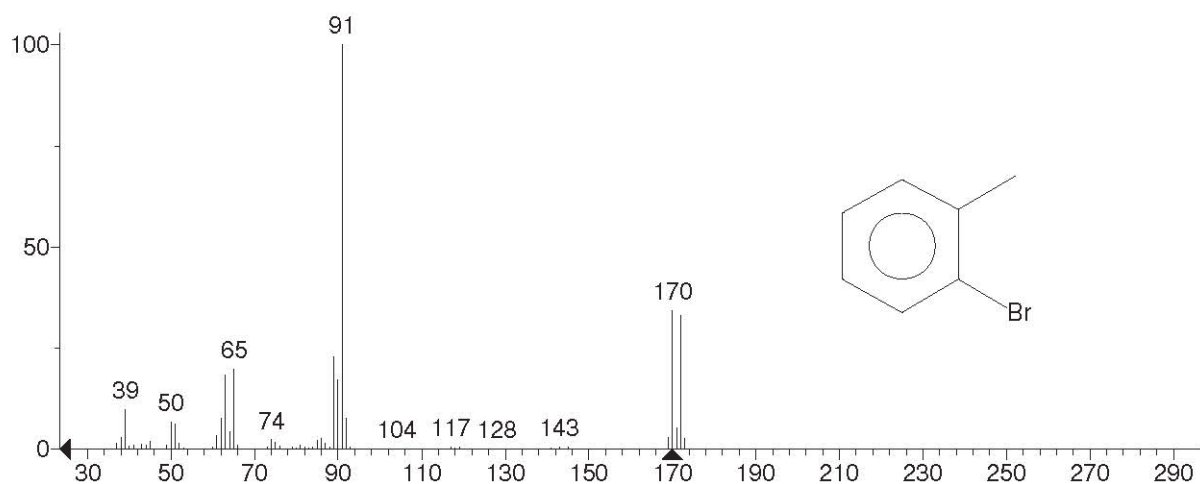




Unknown: Average of 8.986 to 9.058 min.: JRL48R.D
Compound in Library Factor = 205



Hit 2 : Benzene, 1-bromo-2-methyl-
C₇H₇Br; MF: 914; RMF: 914; Prob 15.3%; CAS: 95-46-5; Lib: replib; ID: 11704.



File : C:\MSDCHEM\1\DATA\ASENSIO\JAVI\JRL48R.D

Operator :

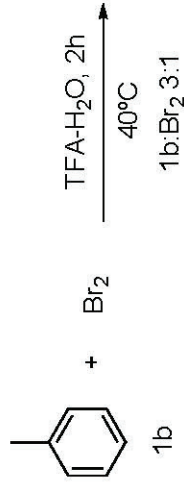
Acquired : 3 Jul 2014 16:12 using AcqMethod JMF60

Instrument : Instrument

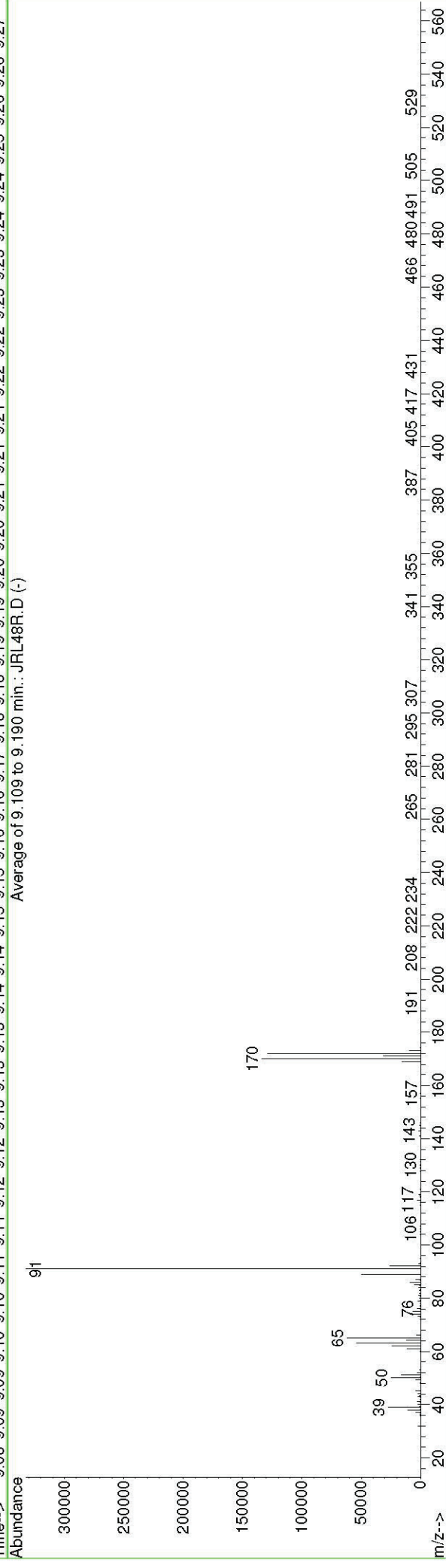
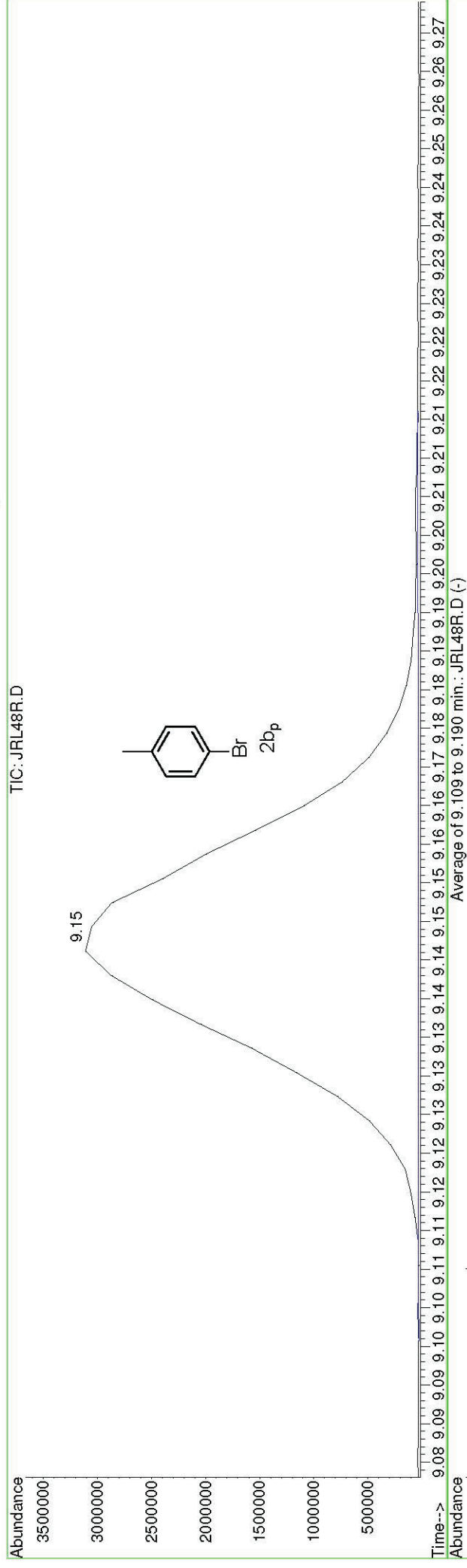
Sample Name:

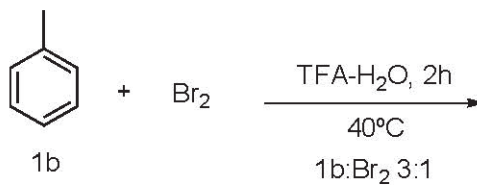
Misc Info :

Vial Number: 11

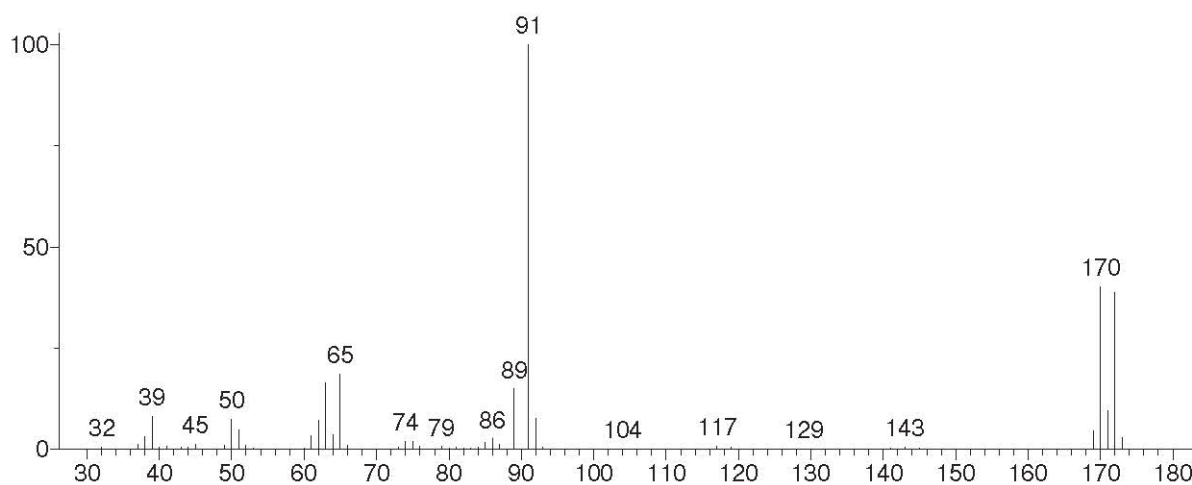


TIC: JRL48R.D

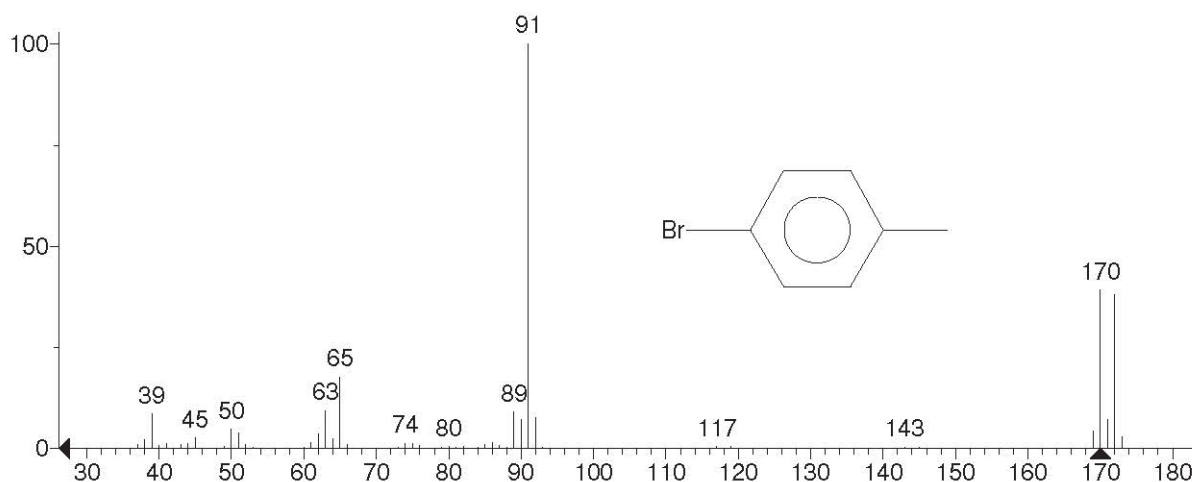




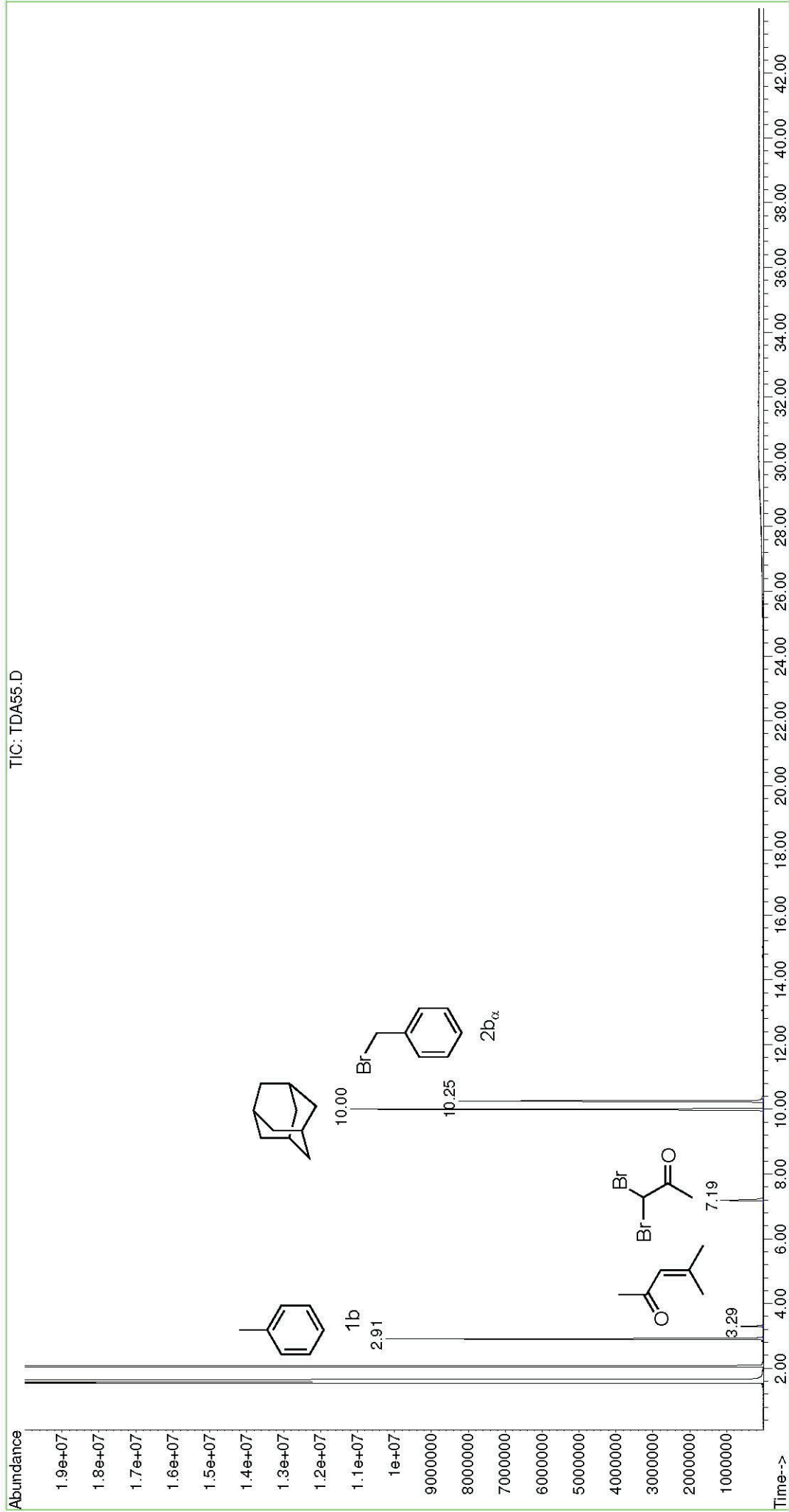
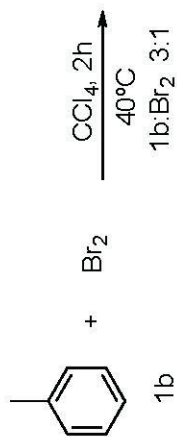
Unknown: Average of 9.109 to 9.190 min.: JRL48R.D
Compound in Library Factor = 327



Hit 2 : Benzene, 1-bromo-4-methyl-
C₇H₇Br; MF: 923; RMF: 924; Prob 27.0%; CAS: 106-38-7; Lib: mainlib; ID: 49322.



File : D:\ASENSIO\THAIS\TDA55.D
Operator :
Acquired : 22 Jan 2014 9:33 using AcqMethod JMF60
Instrument : Instrument
Sample Name :
Misc Info :
Vial Number: 32



File : D:\ASENSIO\THAIS\TDA55.D

Operator :

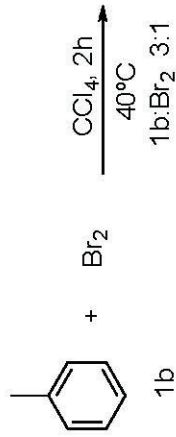
Acquired : 22 Jan 2014 9:33 using AcqMethod JMF60

Instrument : Instrument

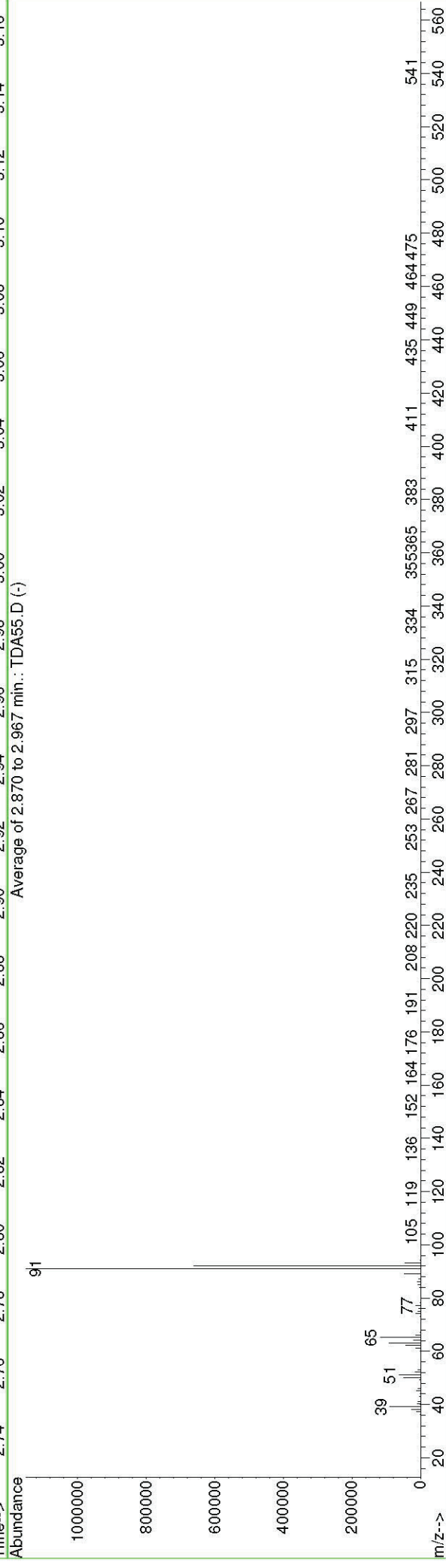
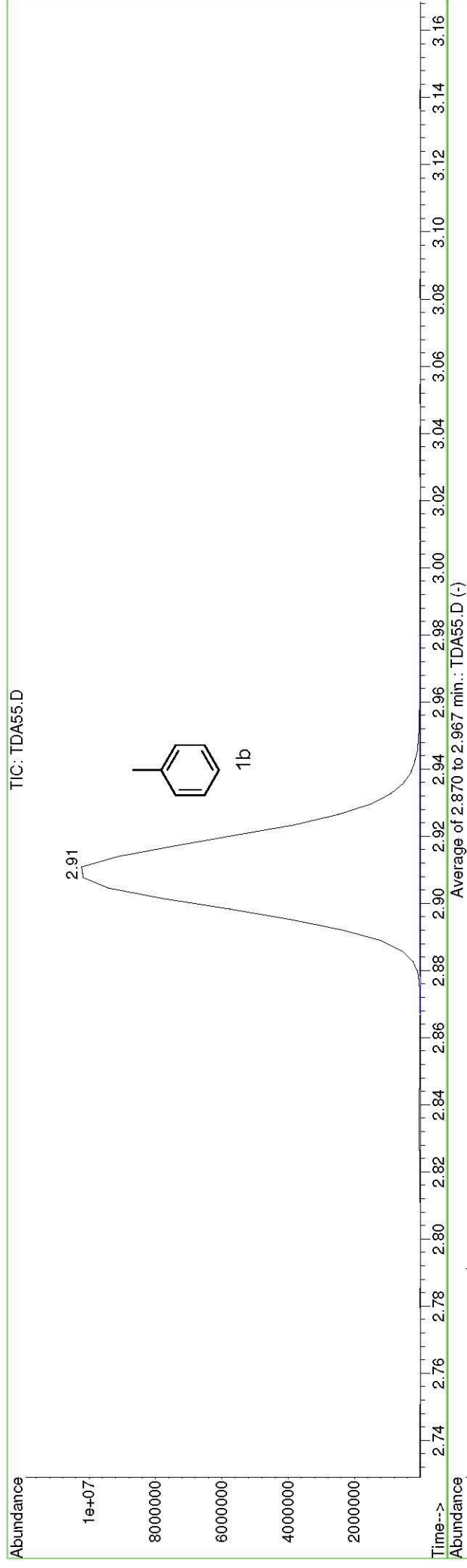
Sample Name:

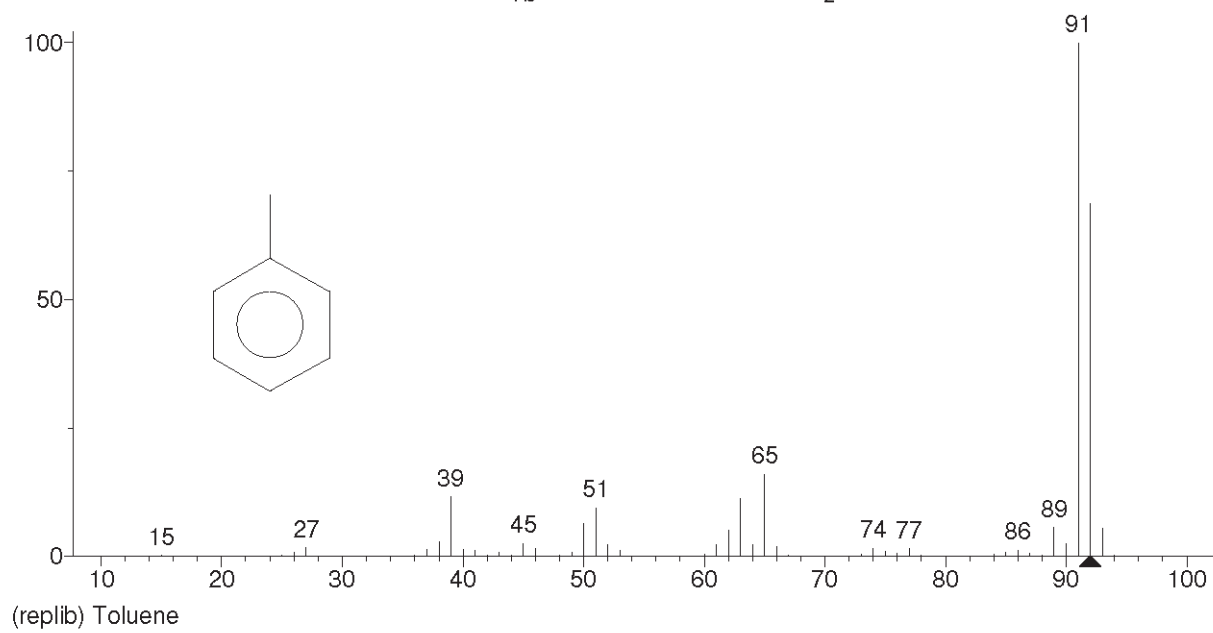
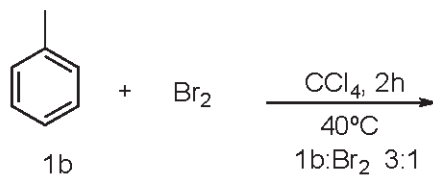
Misc Info :

Vial Number: 32



TIC: TDA55.D





File : D:\ASENSIO\THAIS\TDA55.D

Operator :

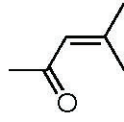
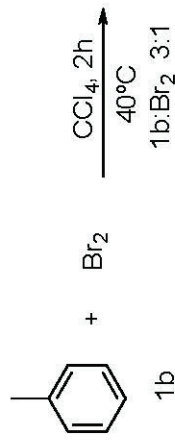
Acquired : 22 Jan 2014 9:33 using AcqMethod JMF60

Instrument : Instrument

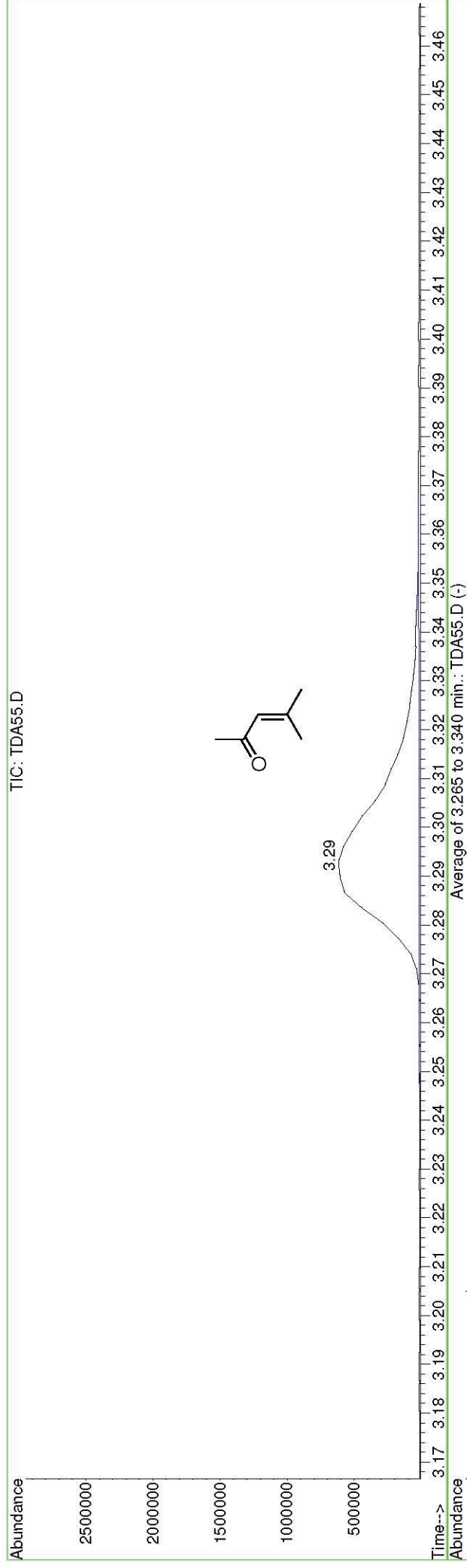
Sample Name:

Misc Info :

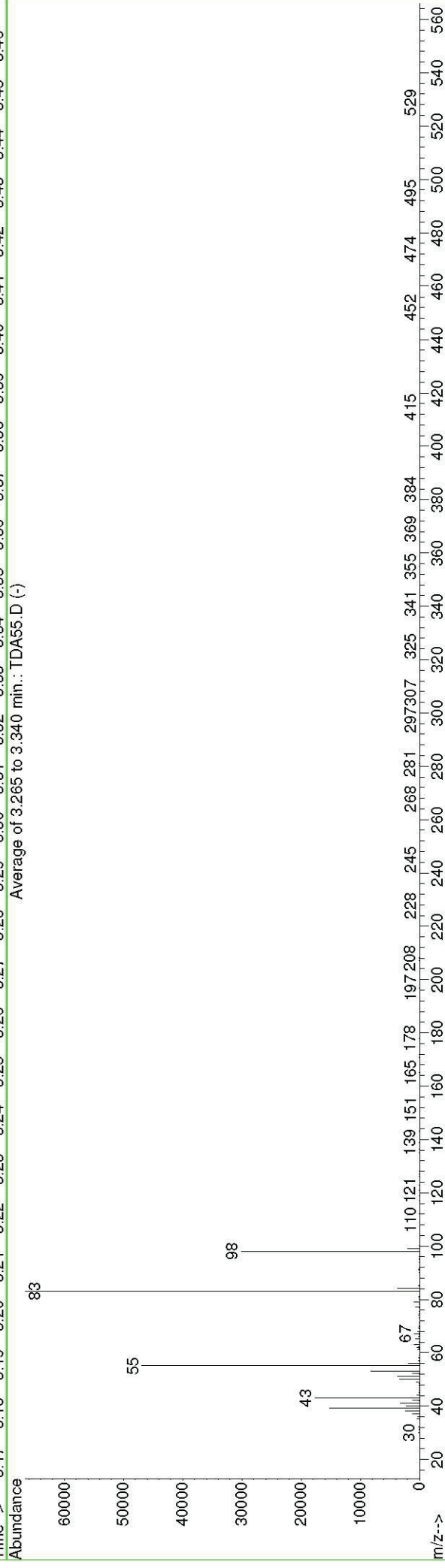
Vial Number: 32



TIC: TDA55.D



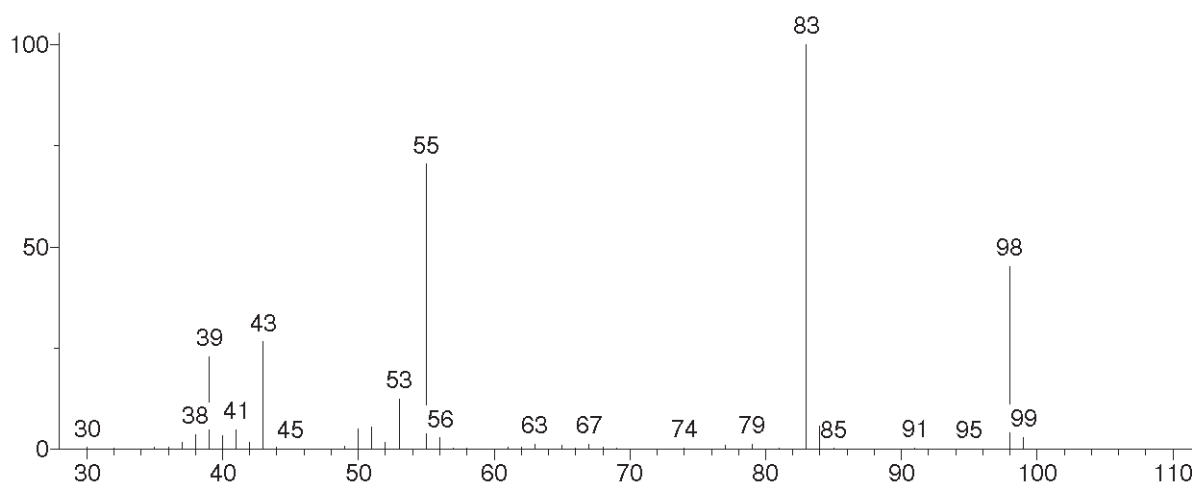
Average of 3.265 to 3.340 min.: TDA55.D (-)



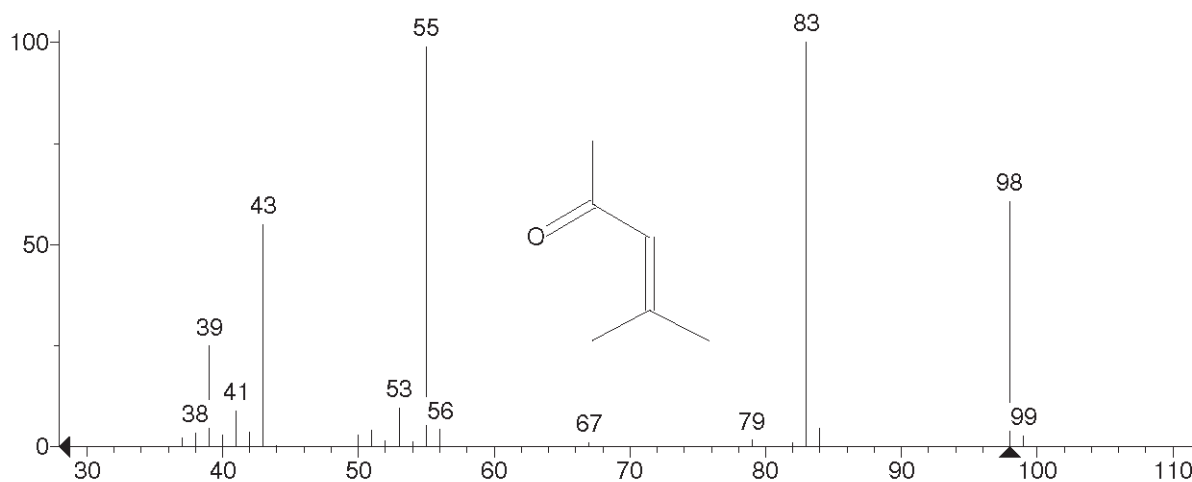


** Search Report Page 1 of 1 **

Unknown: Average of 3.265 to 3.340 min.: TDA55.D
Compound in Library Factor = 109



Hit 1 : 3-Penten-2-one, 4-methyl-
C₆H₁₀O; MF: 921; RMF: 936; Prob 48.2%; CAS: 141-79-7; Lib: wiley7n; ID: 7020.



File : D:\ASENSIO\THAIS\TDA55.D

Operator :

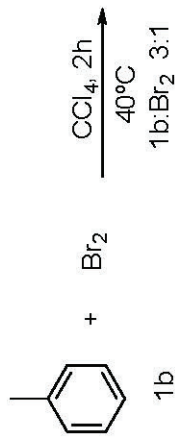
Acquired : 22 Jan 2014 9:33 using AcqMethod JMF60

Instrument : Instrument

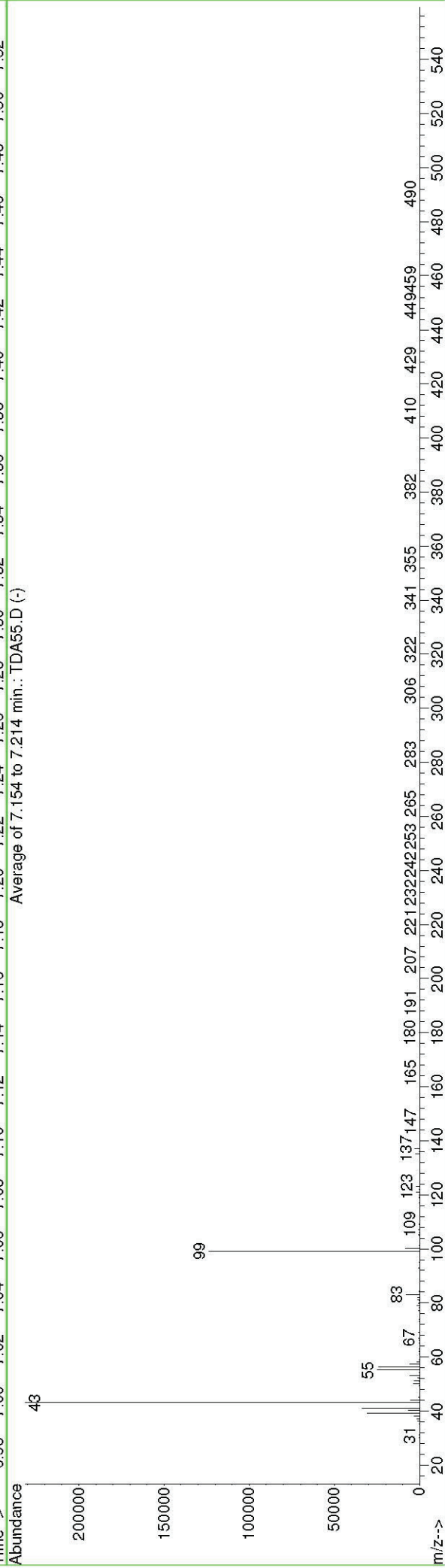
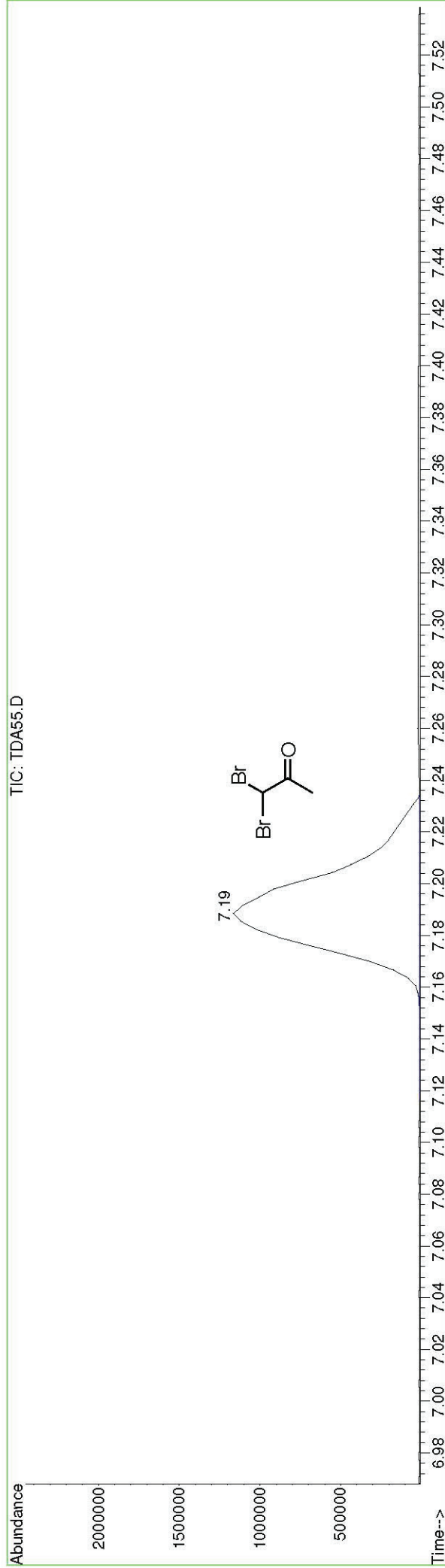
Sample Name:

Misc Info :

Vial Number: 32



TIC: TDA55.D



File : D:\ASENSIO\THAIS\TDA55.D

Operator :

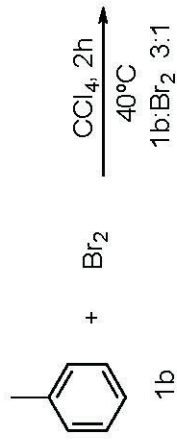
Acquired : 22 Jan 2014 9:33 using AcqMethod JMF60

Instrument : Instrument

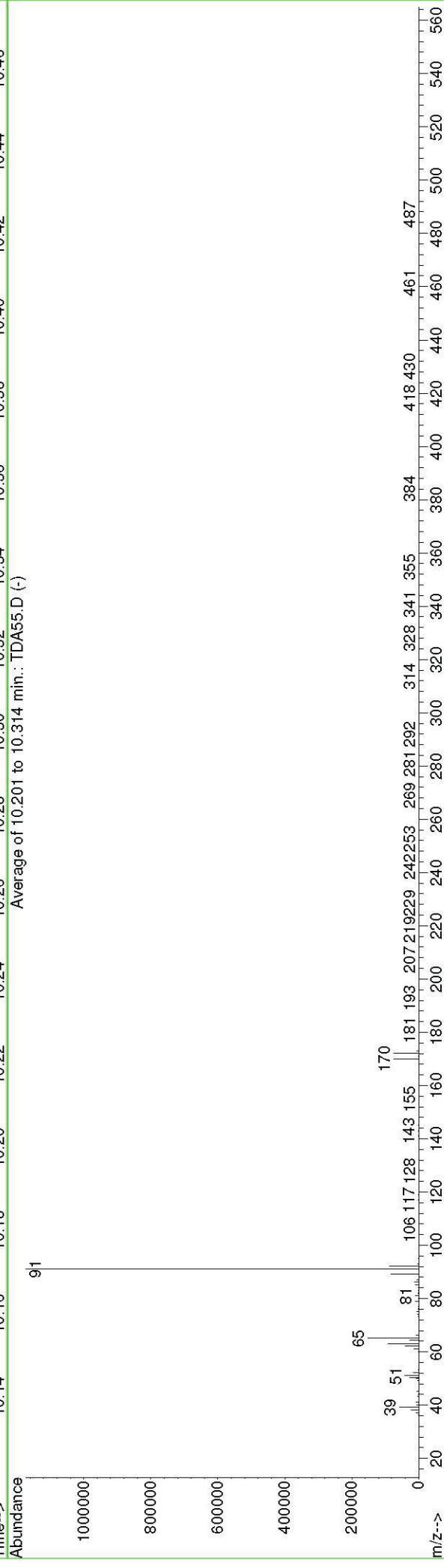
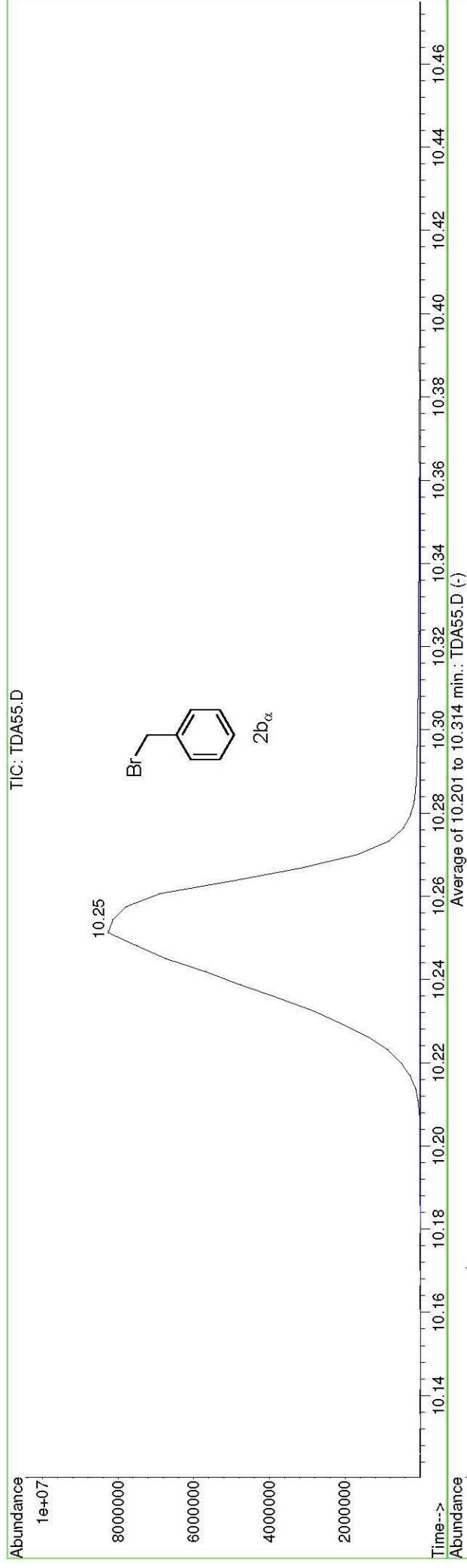
Sample Name:

Misc Info :

Vial Number: 32



TIC: TDA55.D

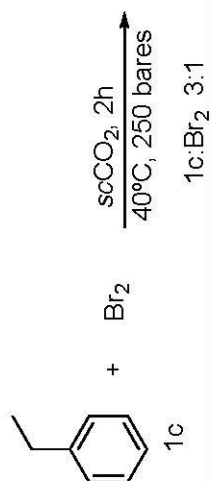


Mass spectrum of 2,4-dichlorobenzonitrile. The x-axis represents the mass-to-charge ratio (m/z) from 30 to 180, and the y-axis represents relative intensity from 0 to 100. The base peak is at m/z 91.

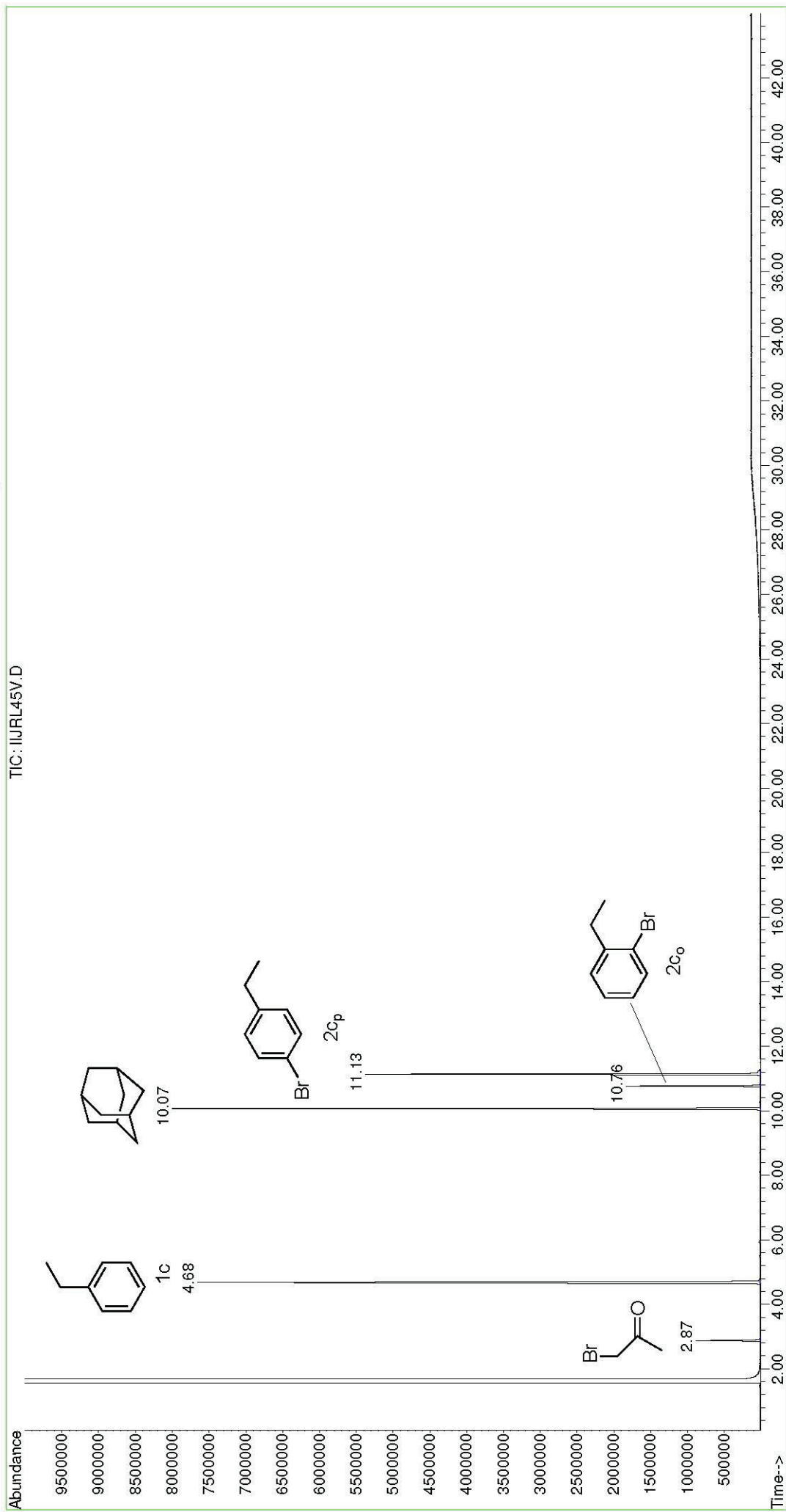
m/z	Relative Intensity (%)
39	~5
45	~2
51	~3
65	~15
75	~5
81	~5
91	100
117	~5
143	~5
170	~10

Mass spectrum of bromobenzene (c1ccccc1Br). The x-axis represents the mass-to-charge ratio (m/z) from 30 to 180, and the y-axis represents relative intensity from 0 to 100. The base peak is at m/z 91. Other labeled peaks include 39, 45, 51, 65, 74, 79, 117, 143, and 170. The chemical structure of bromobenzene is shown above the spectrum.

File : D:\ASENSIO\THAIS\IIJRL45V.D
 Operator :
 Acquired : 5 Dec 2013 1:40 using AcqMethod JMF60
 Instrument : Instrumen
 Sample Name: vidrio
 Misc Info :
 Vial Number: 18



1c:Br₂ 3:1



File : D:\ASENSIO\THAIS\IIJRL45V.D

Operator :

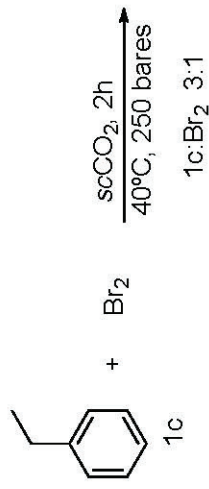
Acquired : 5 Dec 2013 1:40 using AcqMethod JMF60

Instrument : Instrument

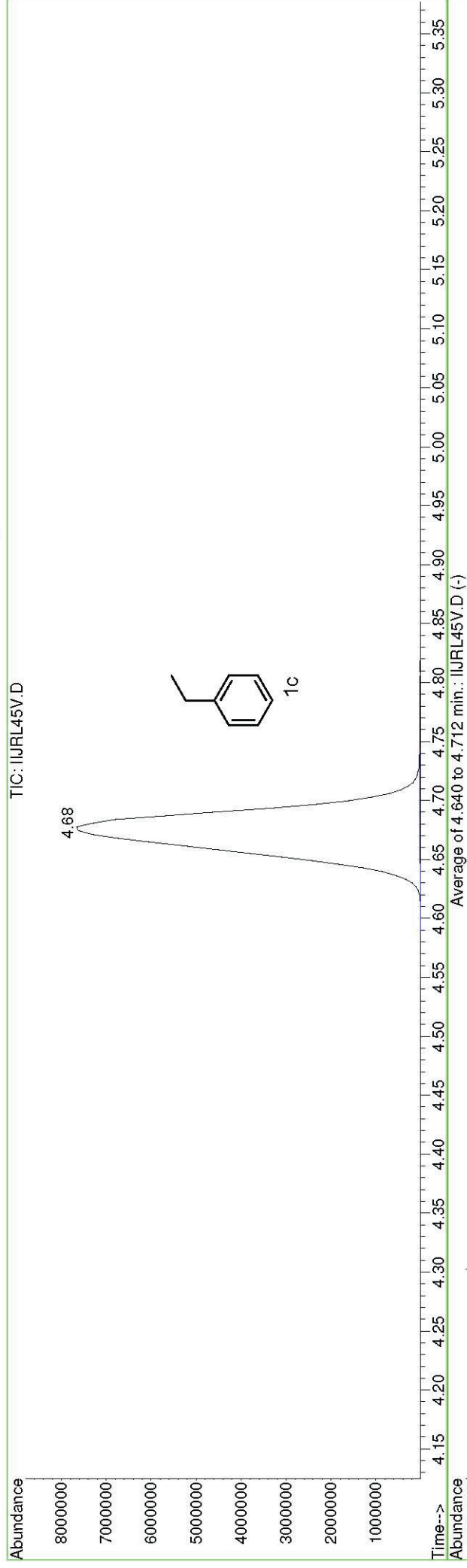
Sample Name: vidrio

Misc Info :

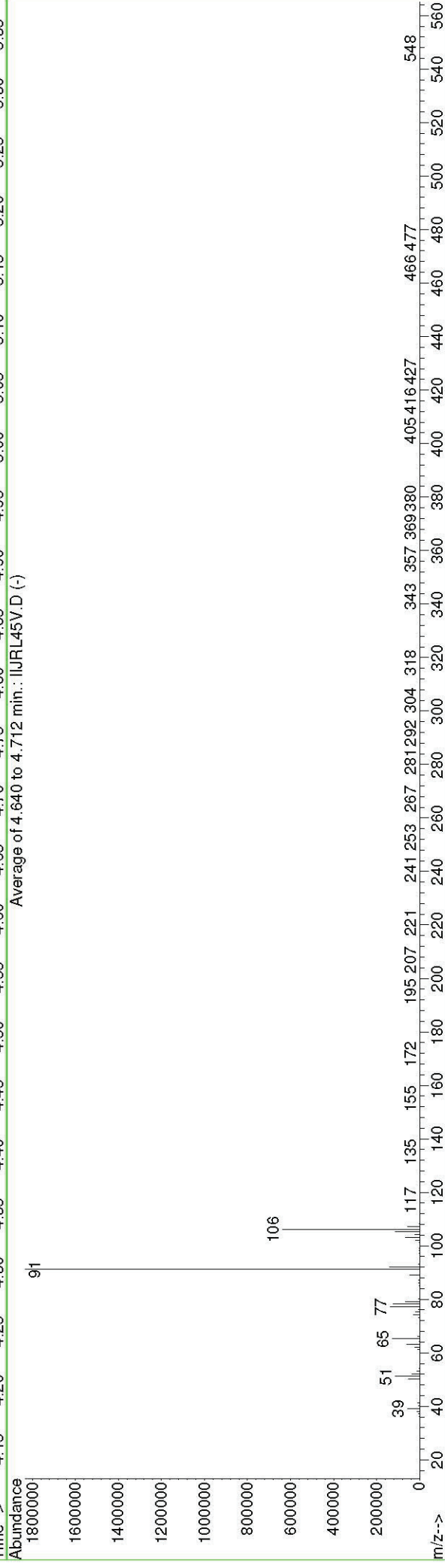
Vial Number: 18

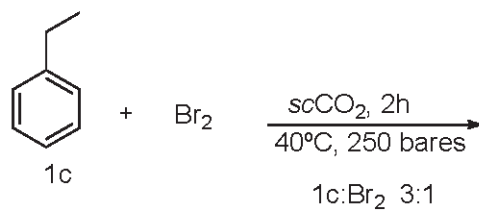


TIC: IIJRL45V.D

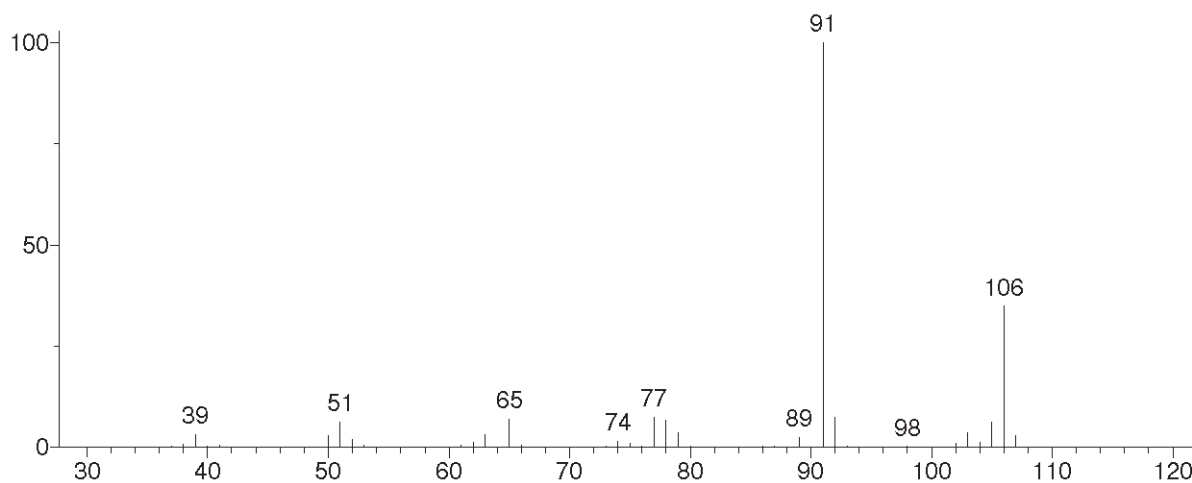


Average of 4.640 to 4.712 min.: IIJRL45V.D (-)

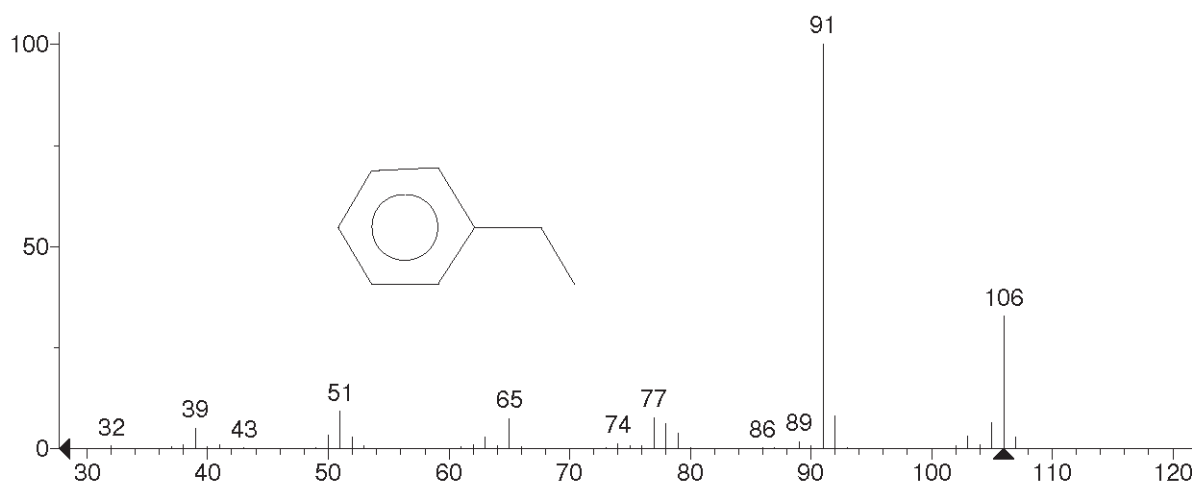




Unknown: Average of 4.640 to 4.712 min.: IJRL45V.D
Compound in Library Factor = -103



Hit 1 : Benzene, ethyl- (CAS)
C₈H₁₀; MF: 933; RMF: 933; Prob 37.6%; CAS: 100-41-4; Lib: wiley7n; ID: 10713.



File : D:\ASENSIO\THAIS\IIJRL45V.D

Operator :

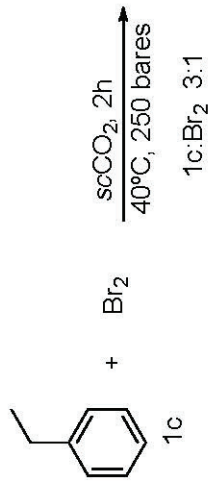
Acquired : 5 Dec 2013 1:40 using AcqMethod JMF60

Instrument : Instrument

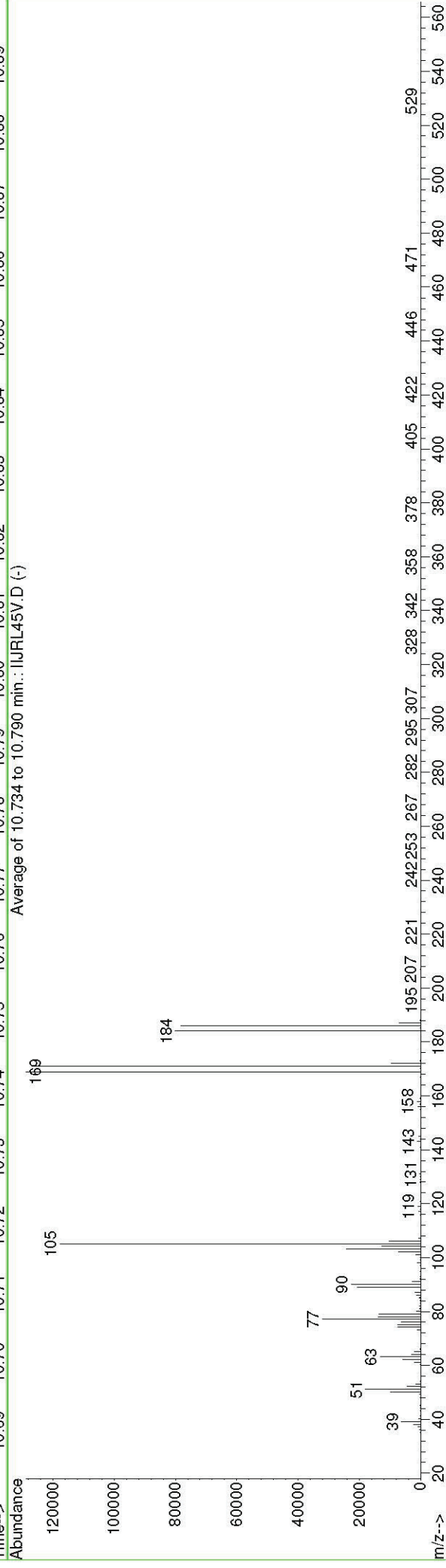
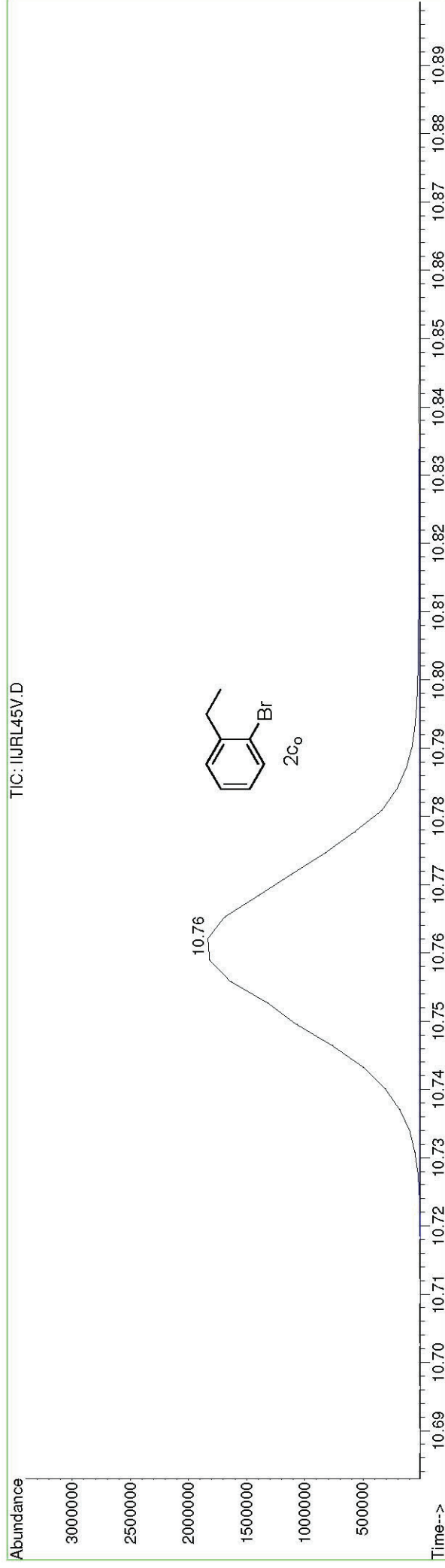
Sample Name: vidrio

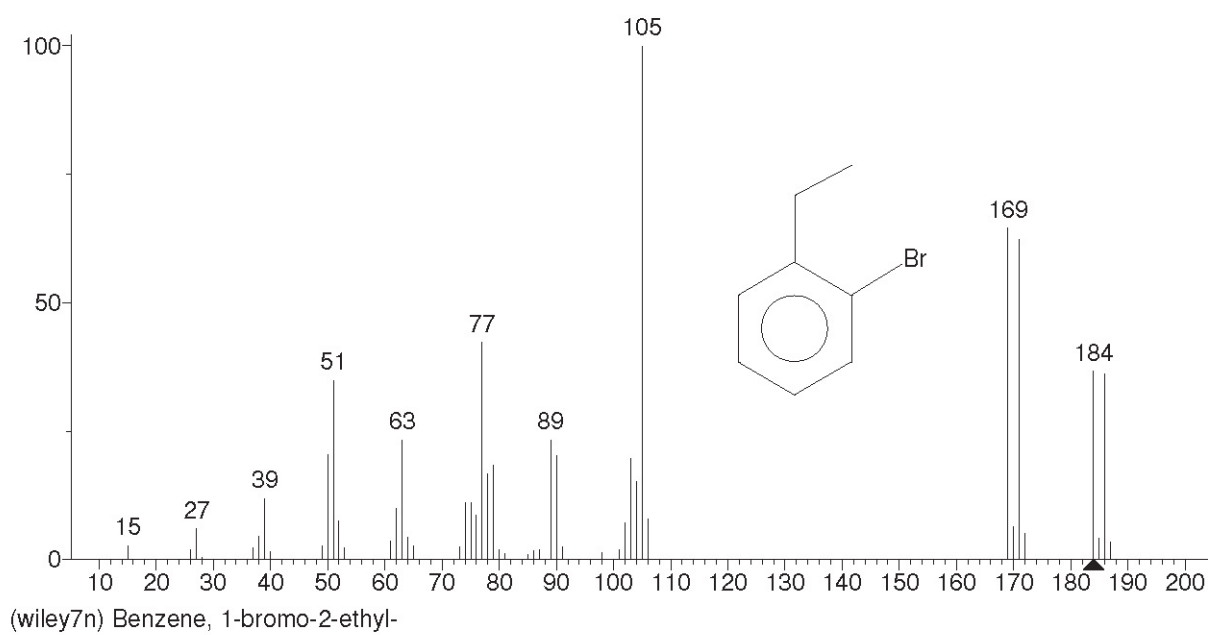
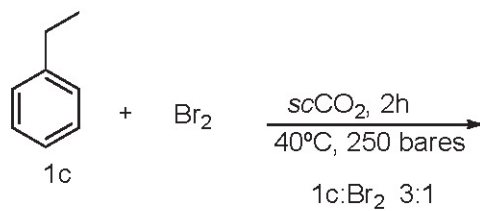
Misc Info :

Vial Number: 18



TIC: IIJRL45V.D





File : D:\ASENSIO\THAIS\IIJRL45V.D

Operator :

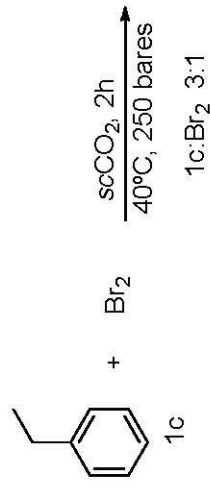
Acquired : 5 Dec 2013 1:40 using AcqMethod JMF60

Instrument : Instrument

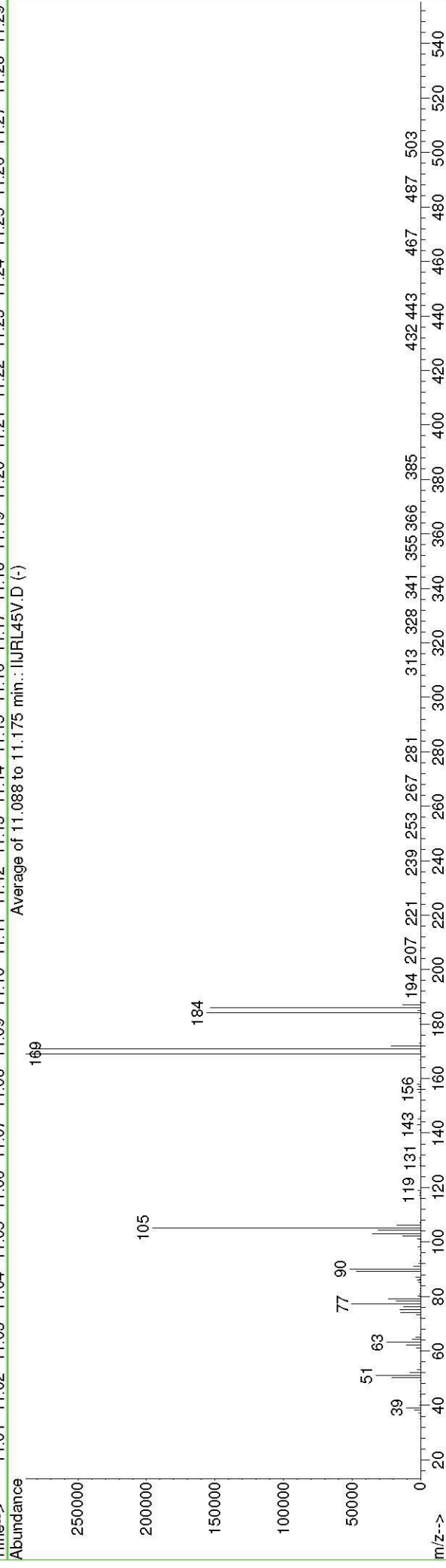
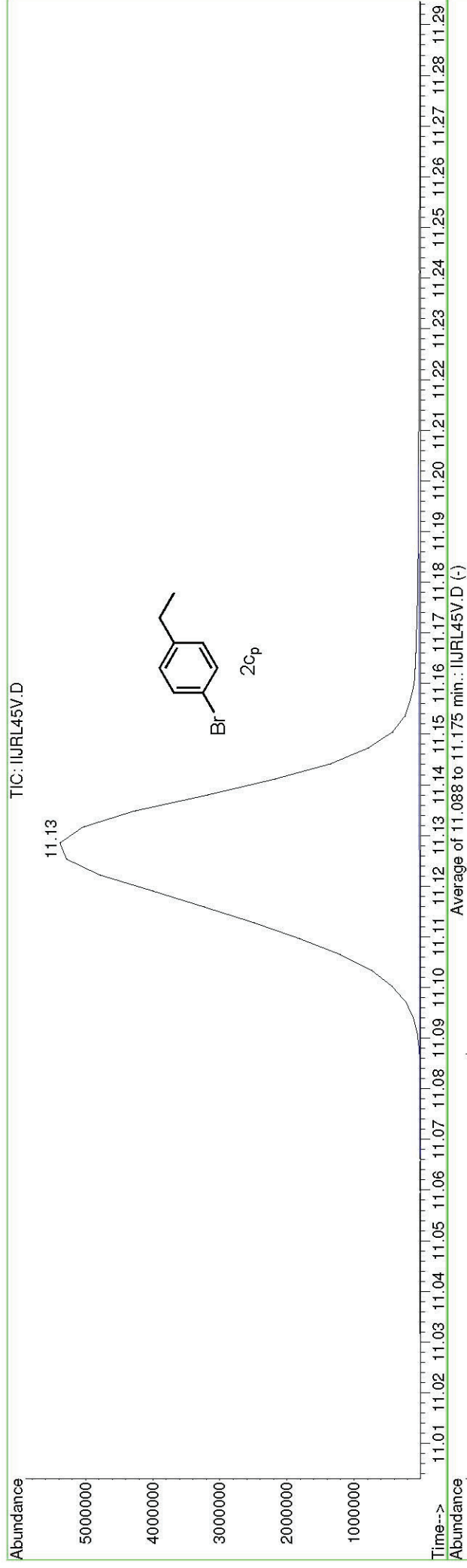
Sample Name: vidrio

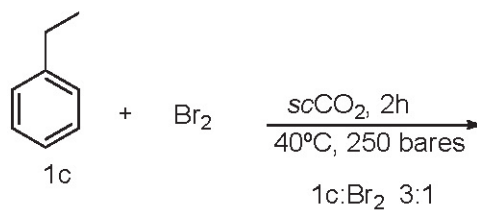
Misc Info :

Vial Number: 18

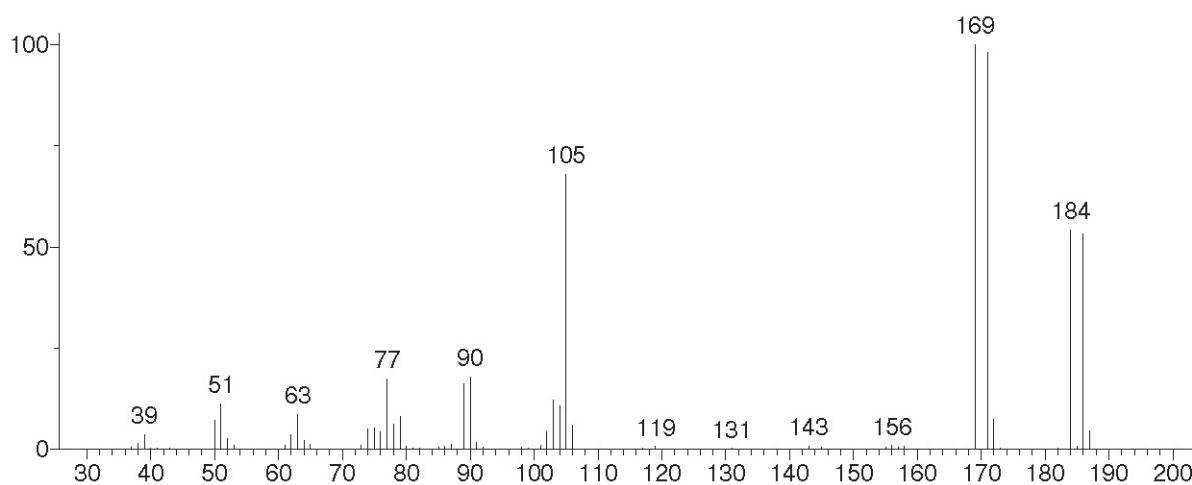


TIC: IIJRL45V.D

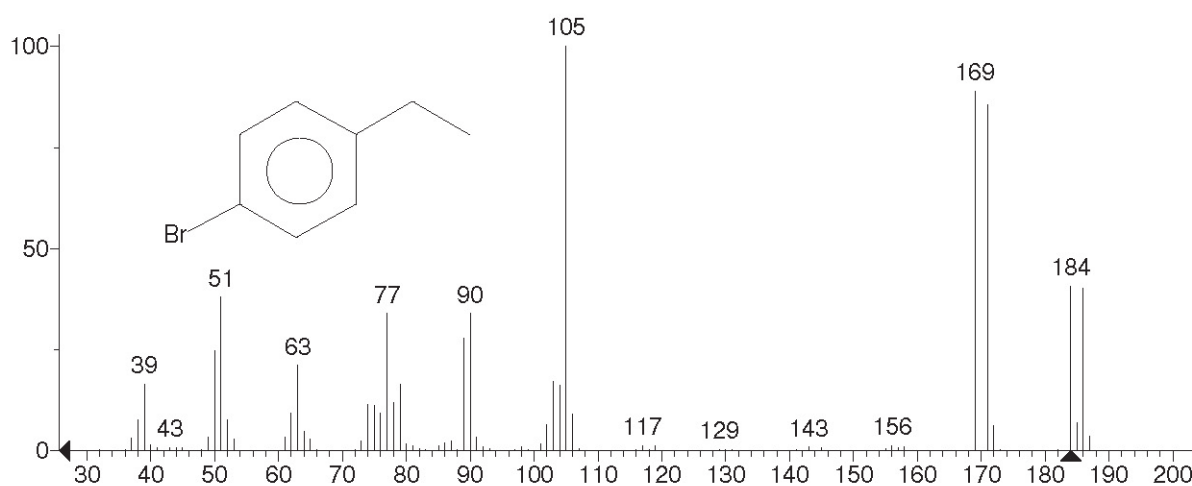




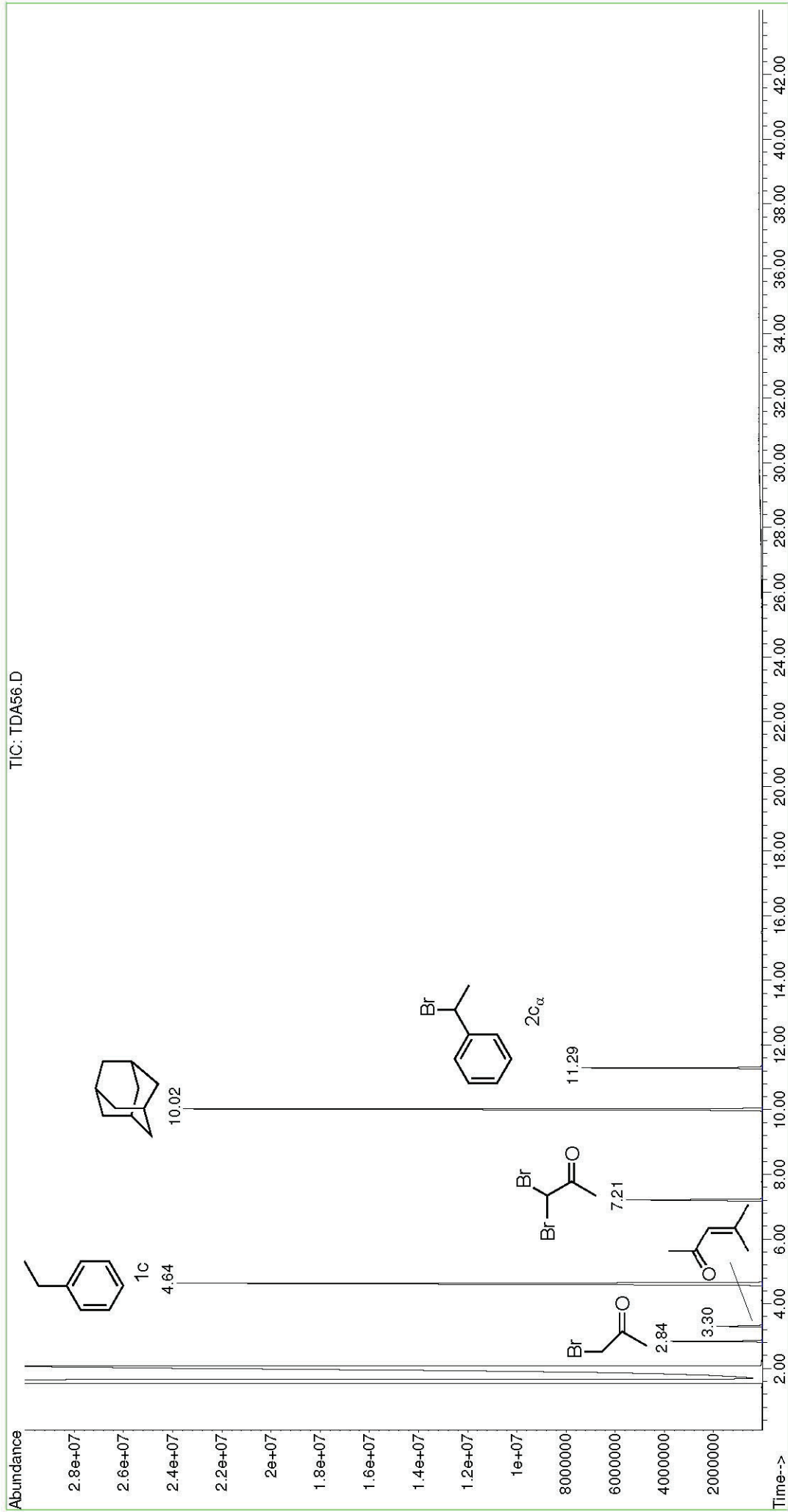
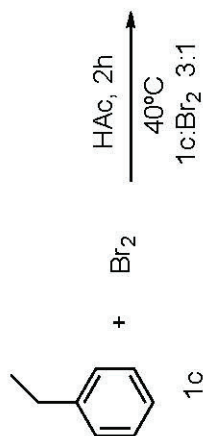
Unknown: Average of 11.088 to 11.175 min.: IJRL45V.D
 Compound in Library Factor = 333



Hit 1 : Benzene, 1-bromo-4-ethyl-
 C₈H₉Br; MF: 897; RMF: 897; Prob 68.6%; CAS: 1585-07-5; Lib: replib; ID: 14019.



File : D:\ASENSIO\THAIS\TDA56.D
 Operator :
 Acquired : 22 Jan 2014 00:18 using AcqMethod JMF60
 Instrument : Instrumen
 Sample Name:
 Misc Info :
 Vial Number: 21



File : D:\ASENSIO\THAIS\TDA56.D

Operator :

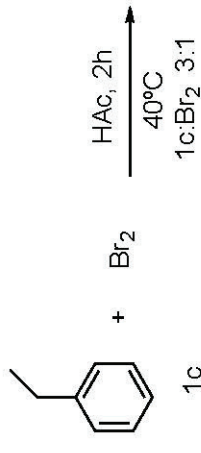
Acquired : 22 Jan 2014 00:18 using AcqMethod JMF60

Instrument : Instrument

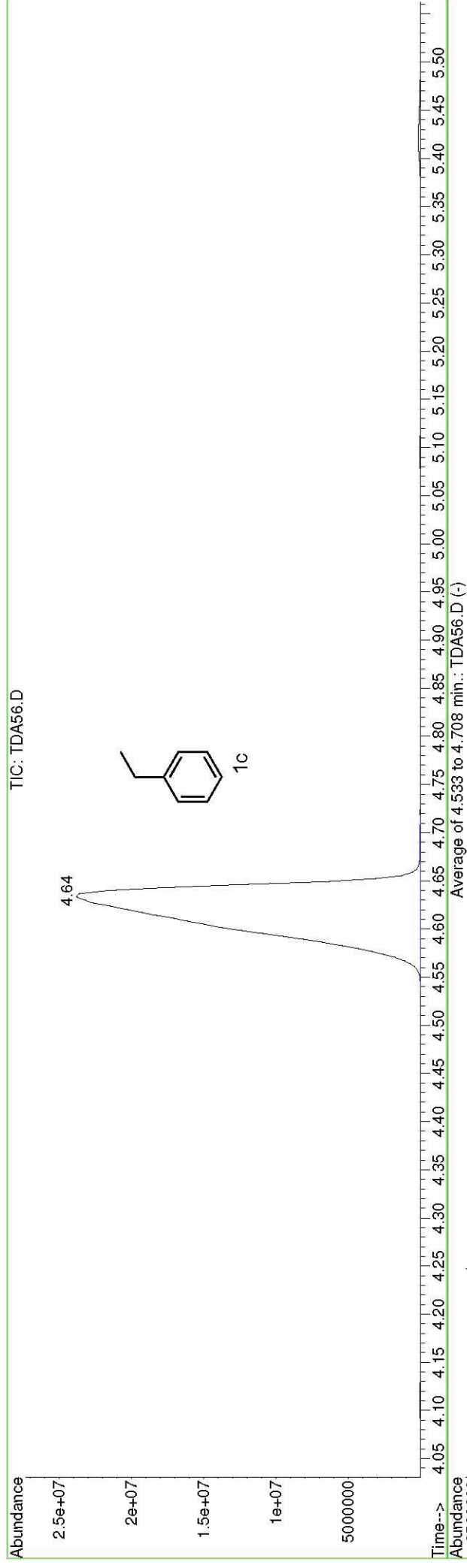
Sample Name:

Misc Info :

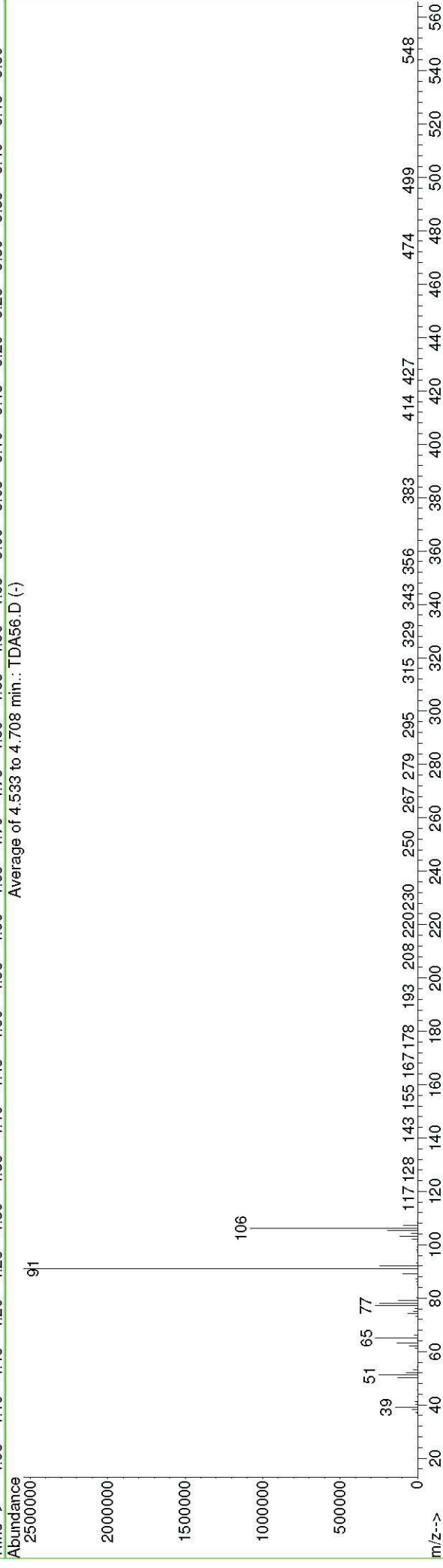
Vial Number: 21

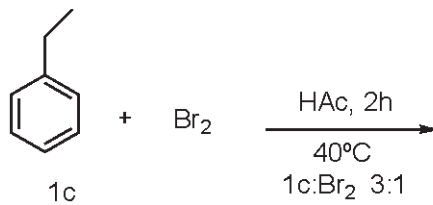


TIC: TDA56.D

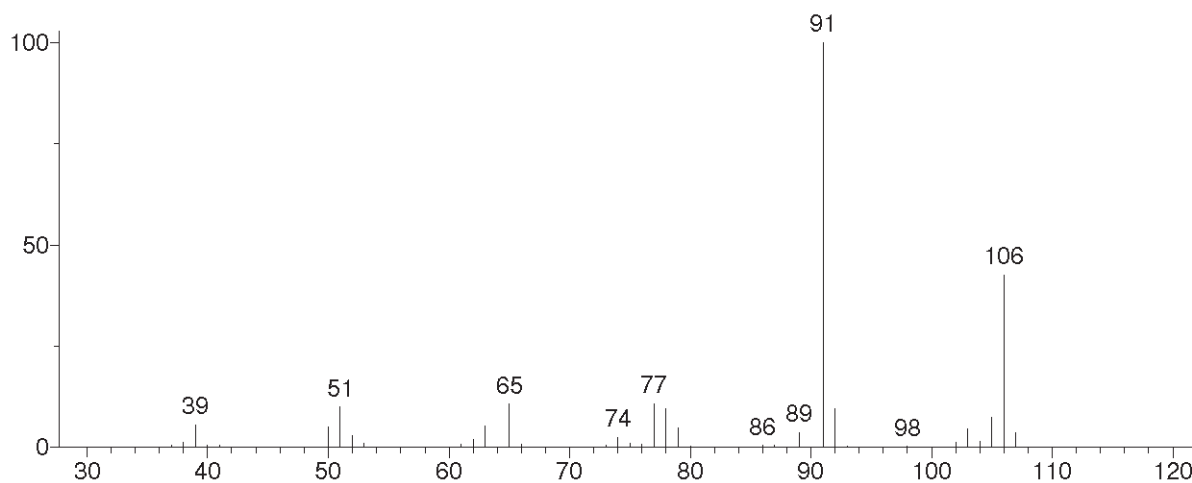


Average of 4.533 to 4.708 min.: TDA56.D (-)

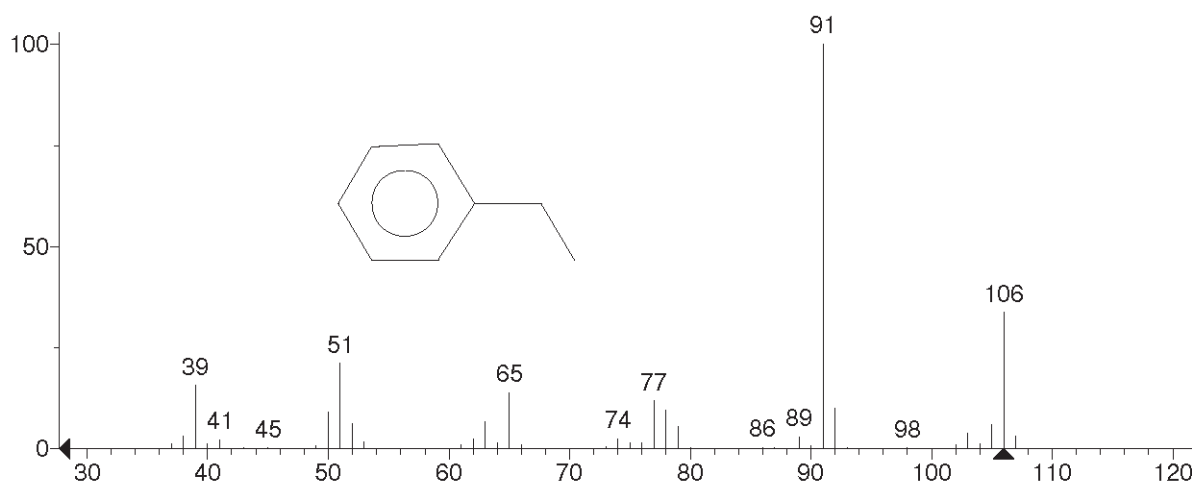




Unknown: Average of 4.533 to 4.708 min.: TDA56.D
Compound in Library Factor = 118



Hit 1 : Ethylbenzene
C₈H₁₀; MF: 953; RMF: 953; Prob 46.8%; CAS: 100-41-4; Lib: replib; ID: 11396.



File : D:\ASENSIO\THAIS\TDA56.D

Operator :

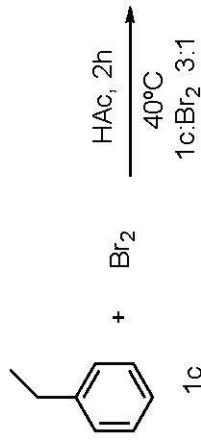
Acquired : 22 Jan 2014 00:18 using AcqMethod JMF60

Instrument : Instrument

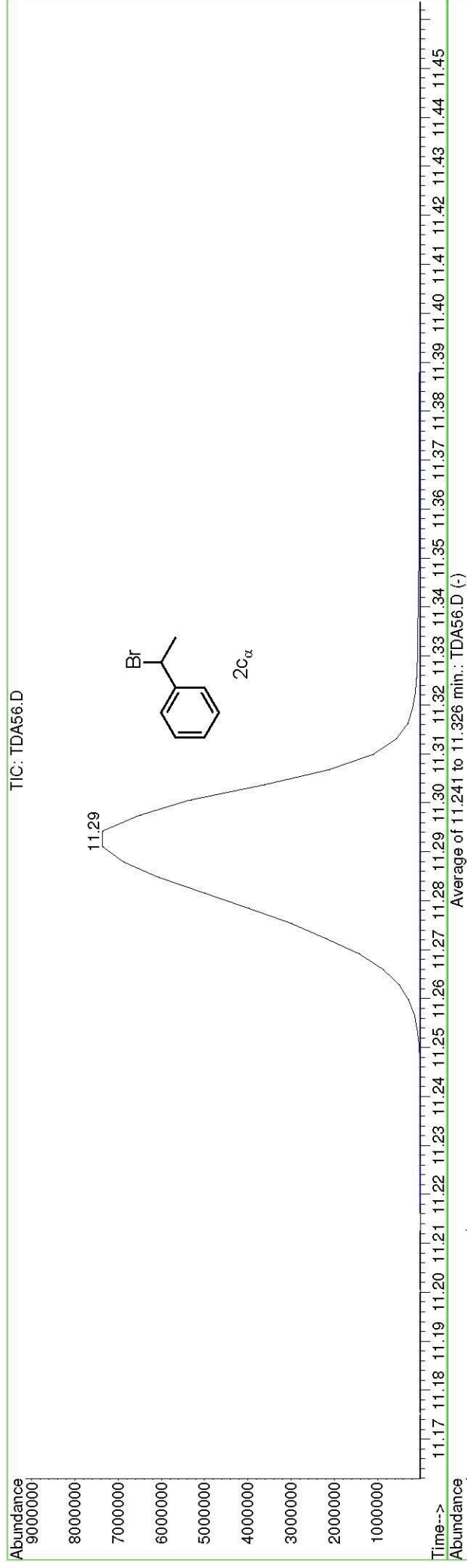
Sample Name:

Misc Info :

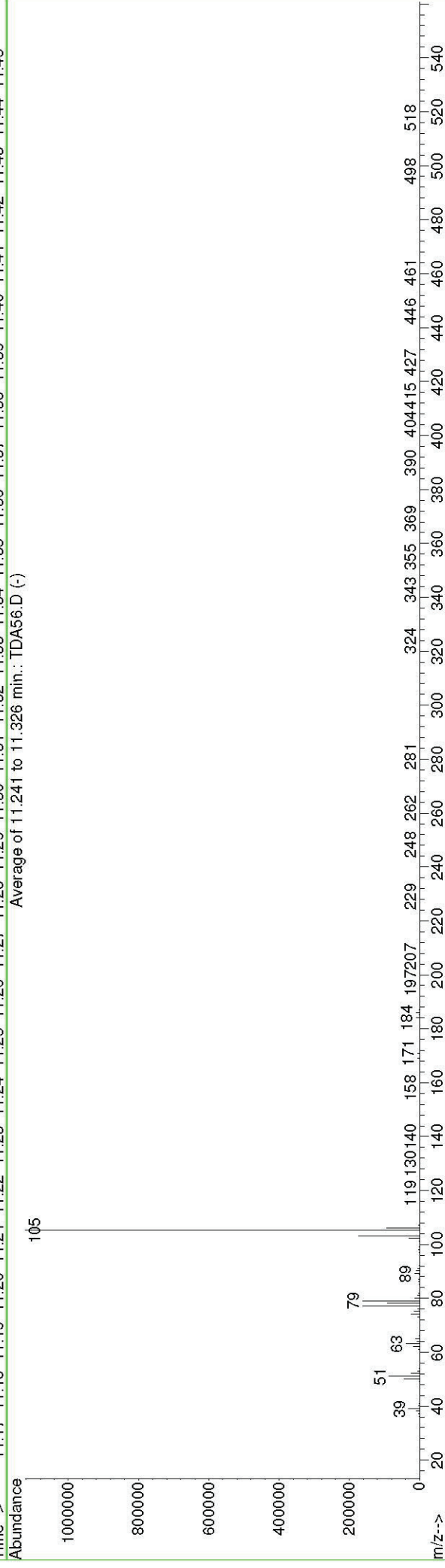
Vial Number: 21

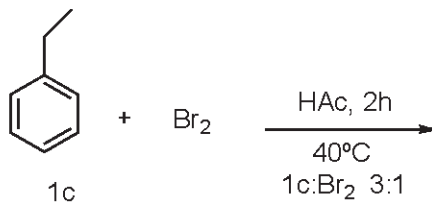


TIC: TDA56.D

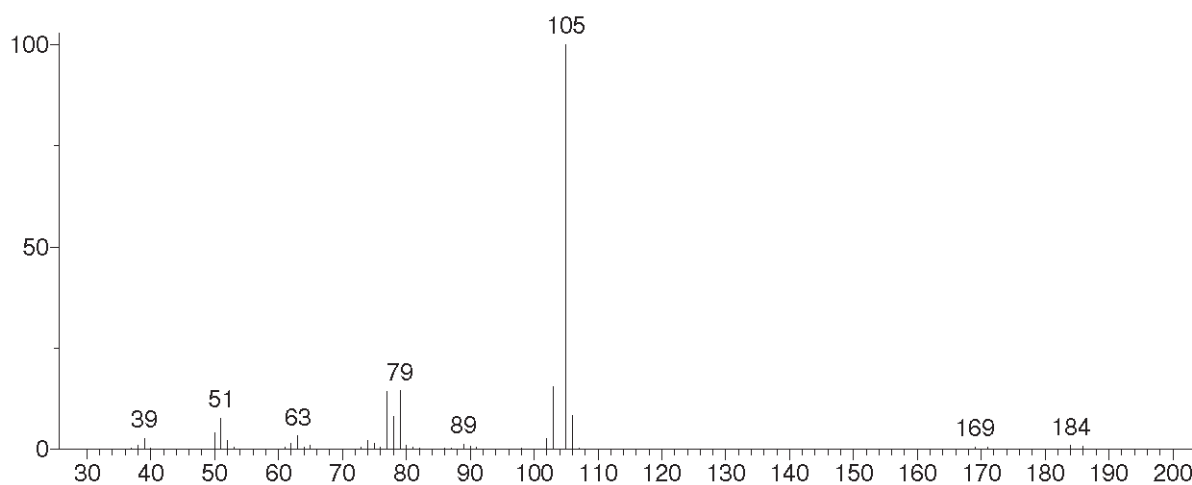


Average of 11.241 to 11.326 min.: TDA56.D (-)

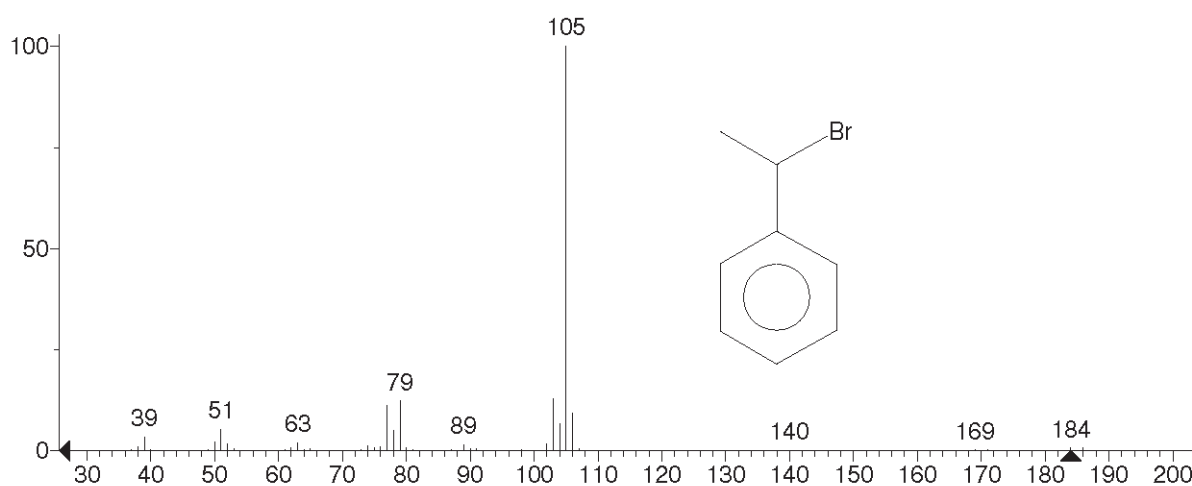




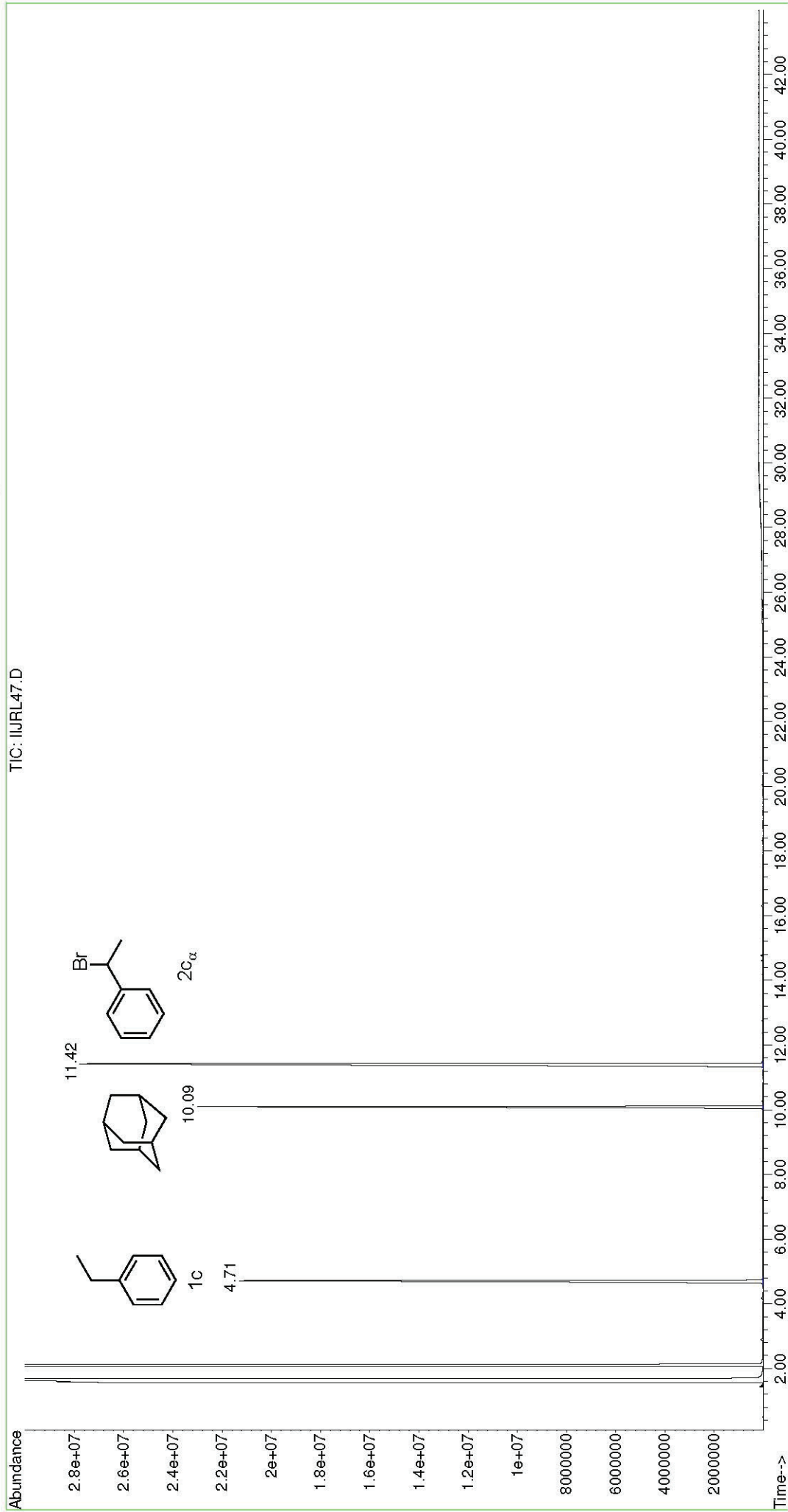
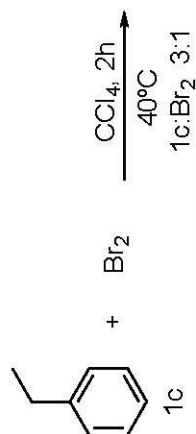
Unknown: Average of 11.241 to 11.326 min.: TDA56.D
Compound in Library Factor = -122



Hit 1 : Benzene, (1-bromoethyl)-
C₈H₉Br; MF: 904; RMF: 904; Prob 26.0%; CAS: 585-71-7; Lib: wiley7n; ID: 91673.



File : D:\ASENSIO\THAIS\IIJRL47.D
 Operator :
 Acquired : 5 Dec 2013 4:17 using AcqMethod JMF60
 Instrument : Instrumen
 Sample Name: CC14
 Misc Info :
 Vial Number: 21



File : D:\ASENSIO\THAIS\IIJRL47.D

Operator :

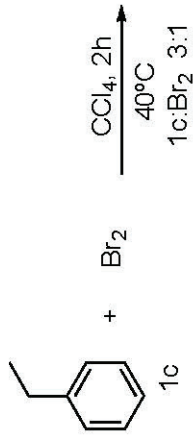
Acquired : 5 Dec 2013 4:17 using AcqMethod JMF60

Instrument : Instrument

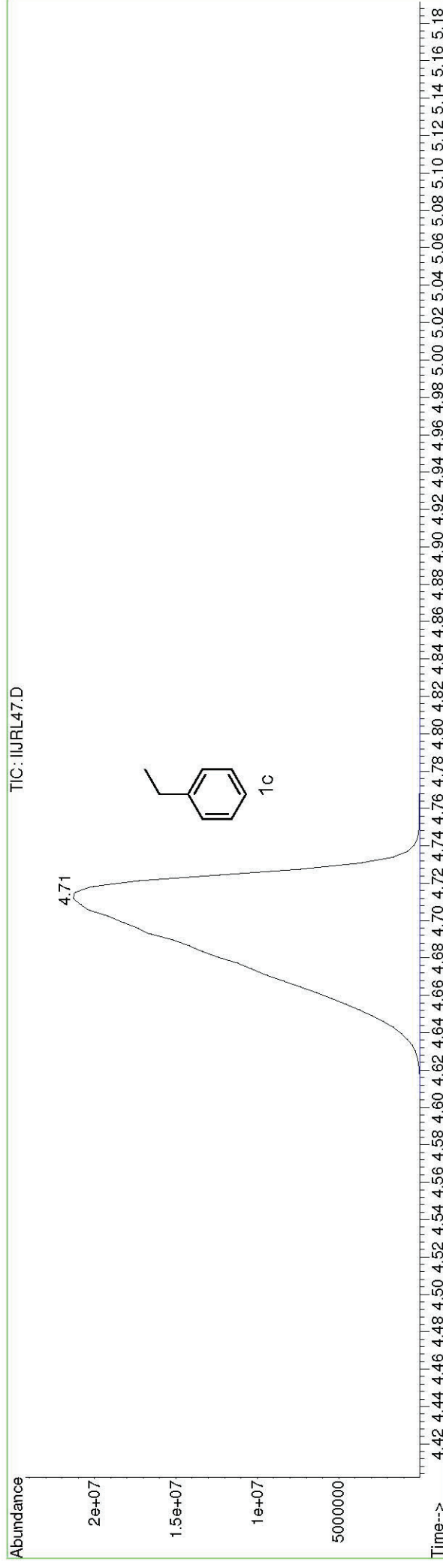
Sample Name: CC14

Misc Info :

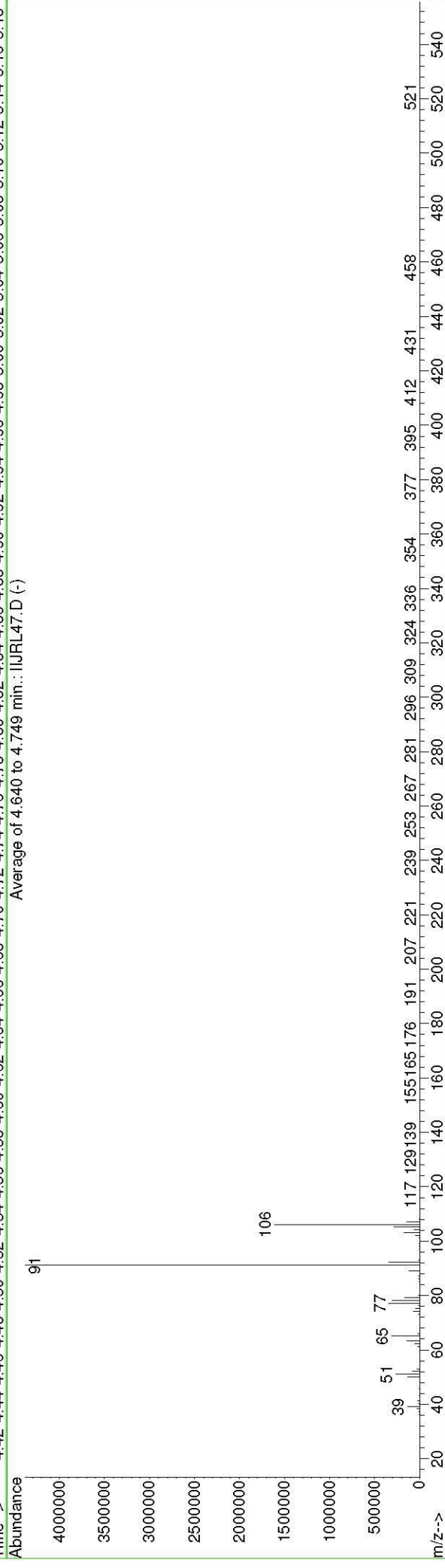
Vial Number: 21

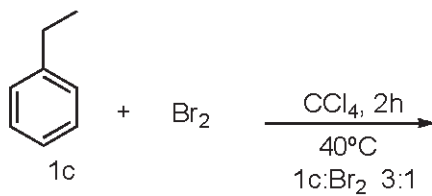


TIC: IIJRL47.D

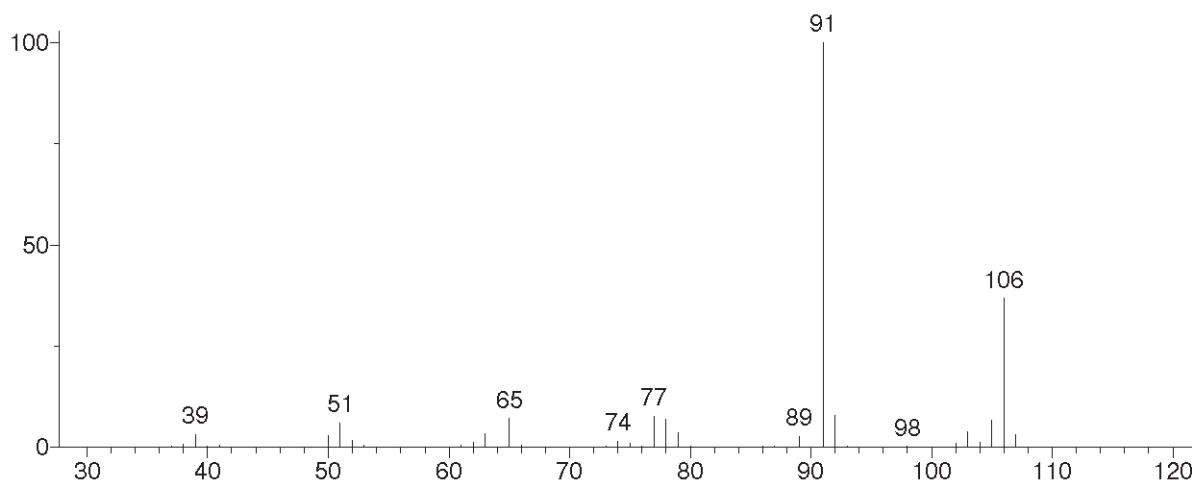


Average of 4.640 to 4.749 min.: IIJRL47.D (-)

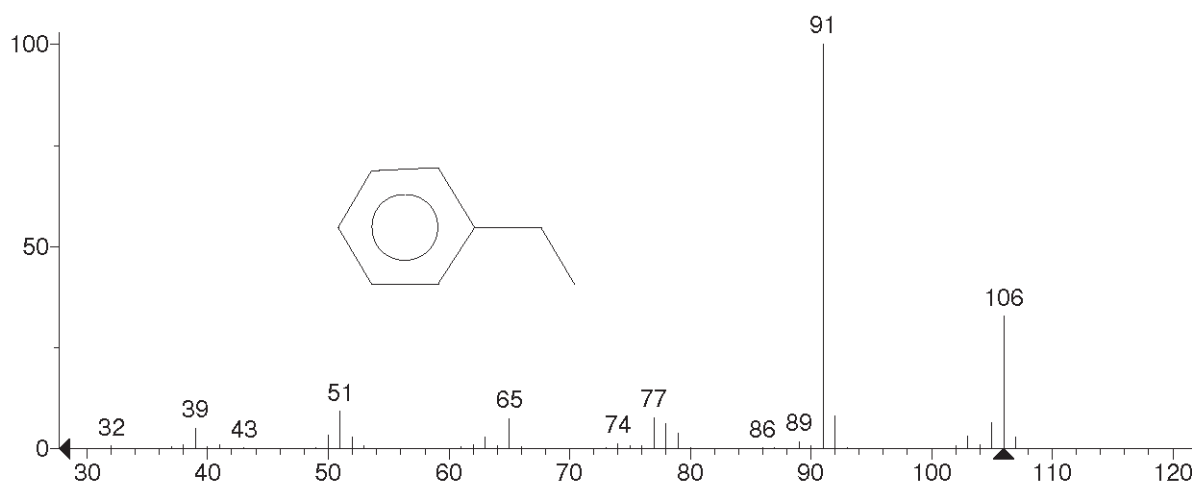




Unknown: Average of 4.640 to 4.749 min.: IJRL47.D
Compound in Library Factor = 118



Hit 1 : Benzene, ethyl- (CAS)
C₈H₁₀; MF: 951; RMF: 951; Prob 48.7%; CAS: 100-41-4; Lib: wiley7n; ID: 10713.



File : D:\ASENSIO\THAIS\IIJRL47.D

Operator :

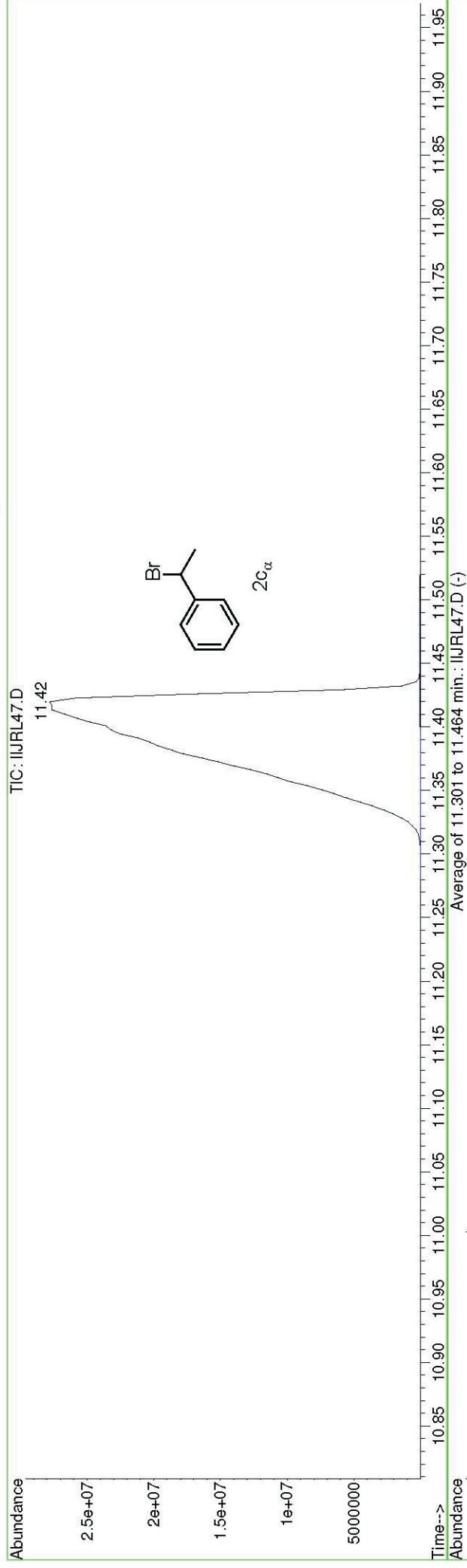
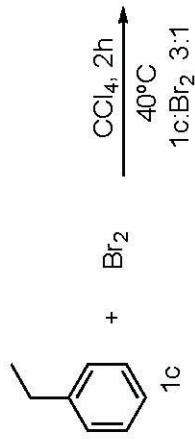
Acquired : 5 Dec 2013 4:17 using AcqMethod JMF60

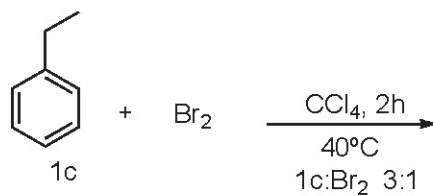
Instrument : Instrument

Sample Name: CC14

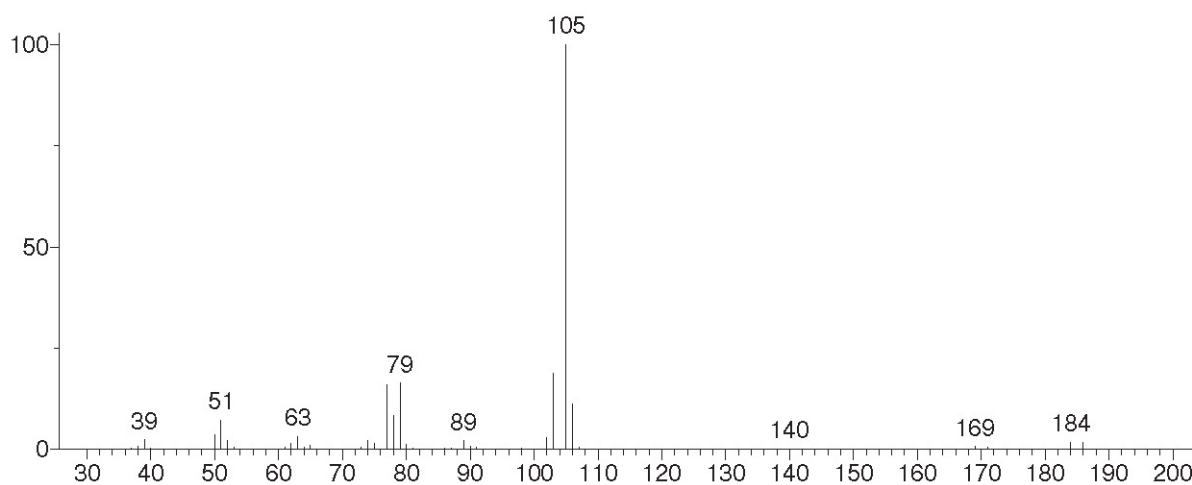
Misc Info :

Vial Number: 21

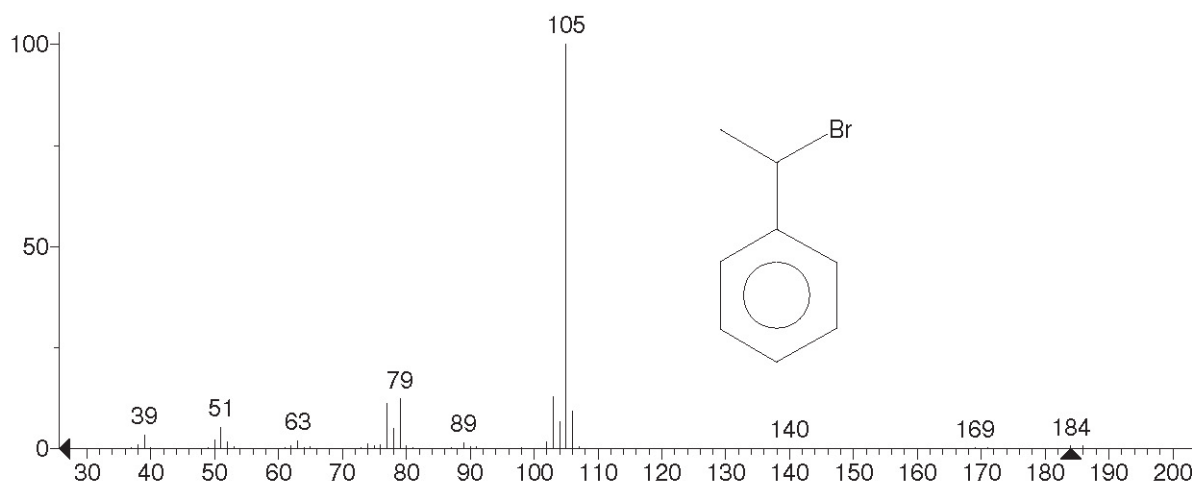




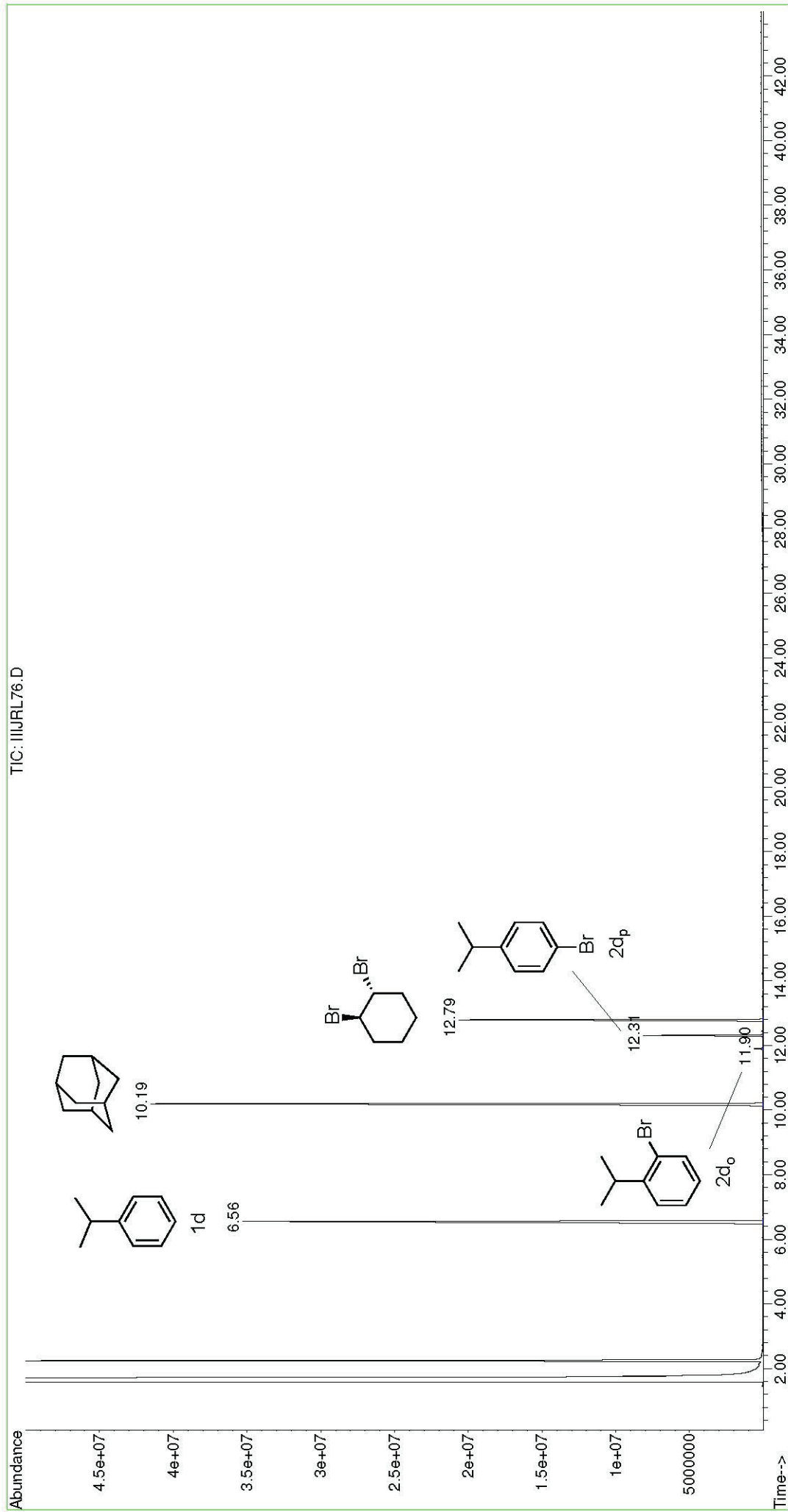
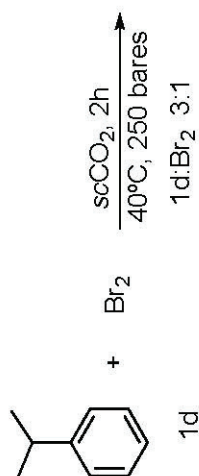
Unknown: Average of 11.301 to 11.464 min.: IJRL47.D
Compound in Library Factor = -113



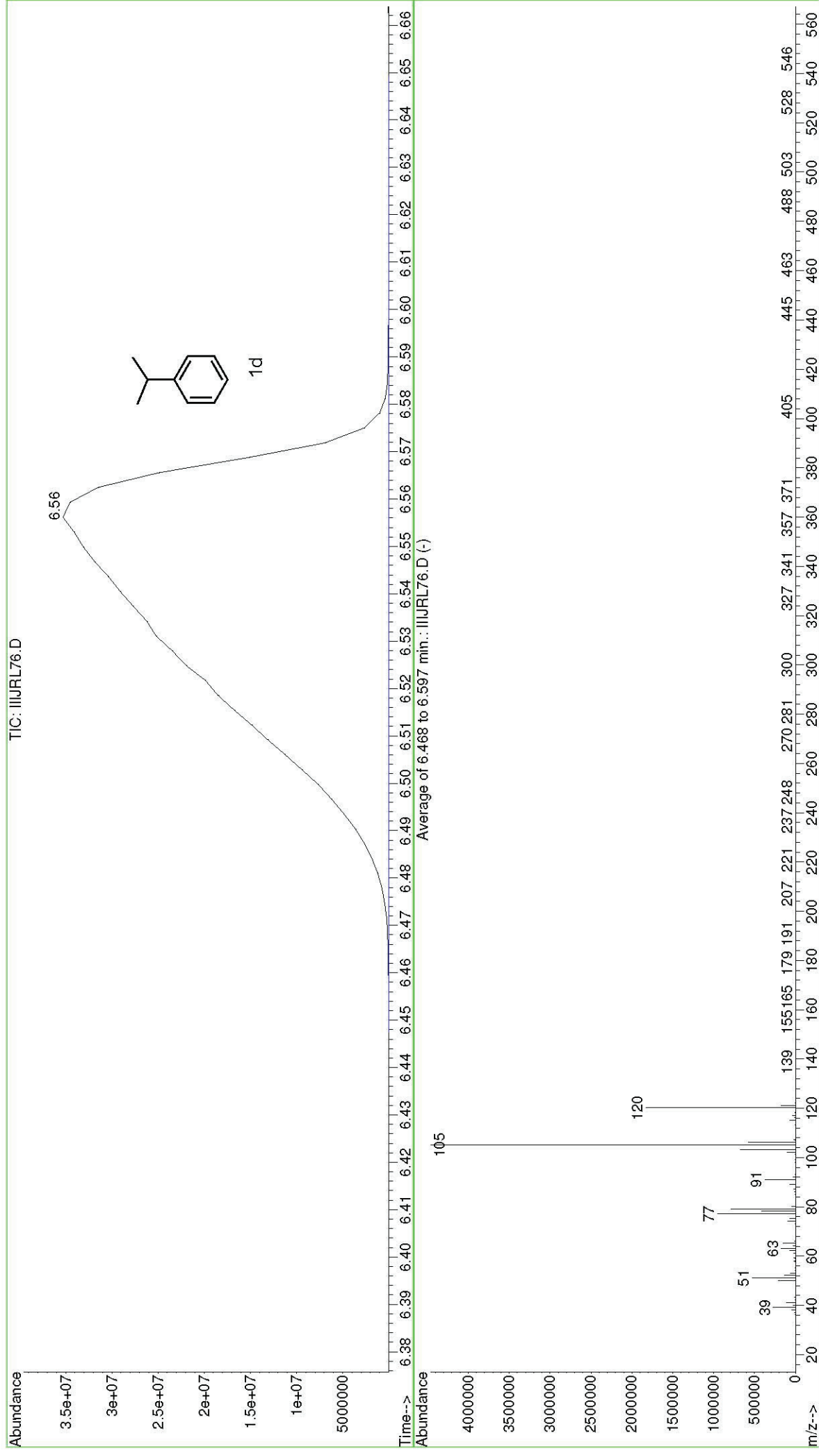
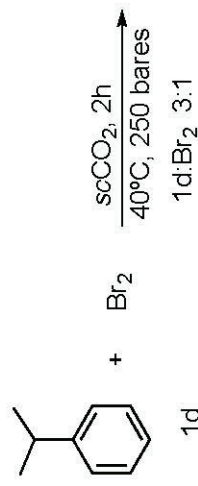
Hit 1 : Benzene, (1-bromoethyl)-
C₈H₉Br; MF: 916; RMF: 916; Prob 31.7%; CAS: 585-71-7; Lib: wiley7n; ID: 91673.

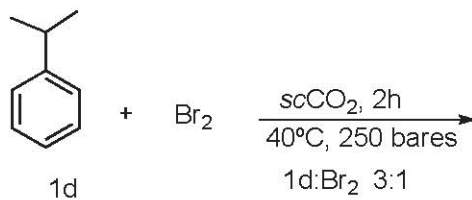


File : C:\MSDCHEM\1\DATA\ASENSIO\IIIJRL76.D
 Operator :
 Acquired : 23 May 2014 18:05 using AcqMethod JMF60
 Instrument : Instrumen
 Sample Name: vidrio
 Misc Info :
 Vial Number: 8

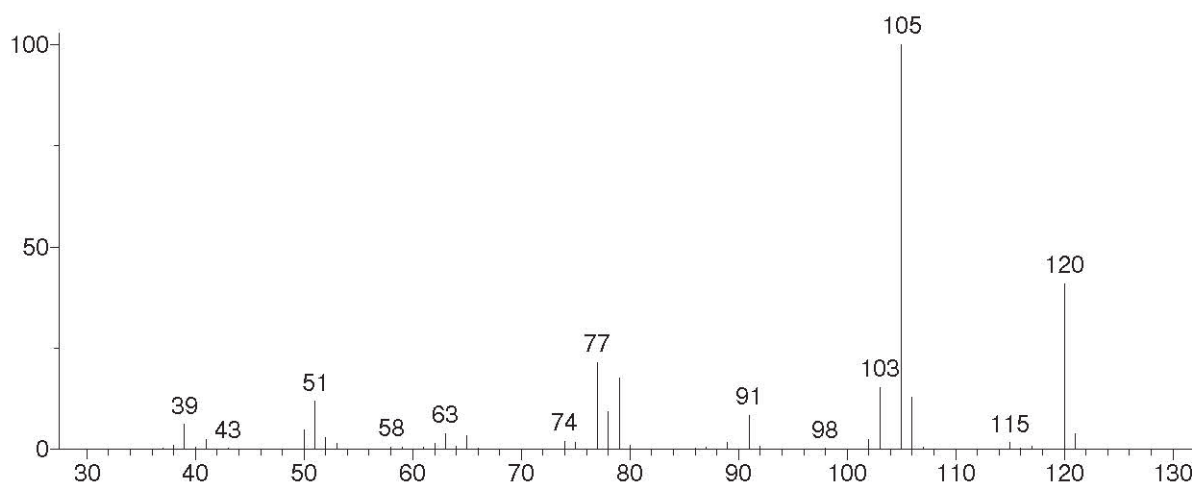


File : C:\MSDCHEM\1\DATA\ASENSIO\IIJRL76.D
Operator :
Acquired : 23 May 2014 18:05 using AcqMethod JMF60
Instrument : Instrument
Sample Name : vidrio
Misc Info :
Vial Number: 8

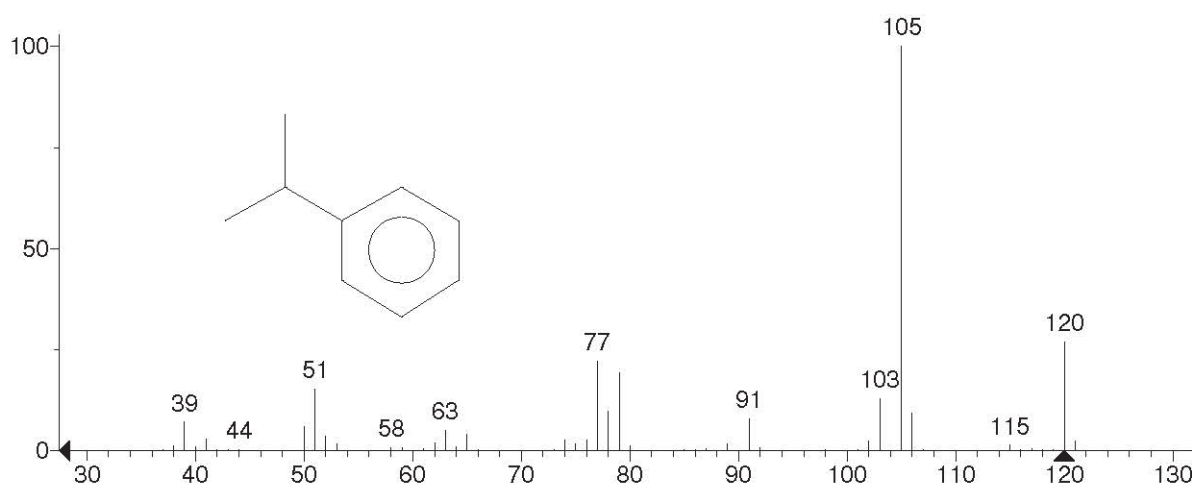




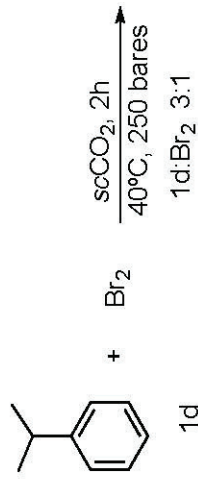
Unknown: Average of 6.468 to 6.597 min.: IIIJRL76.D
Compound in Library Factor = -100



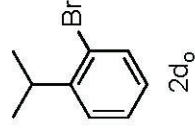
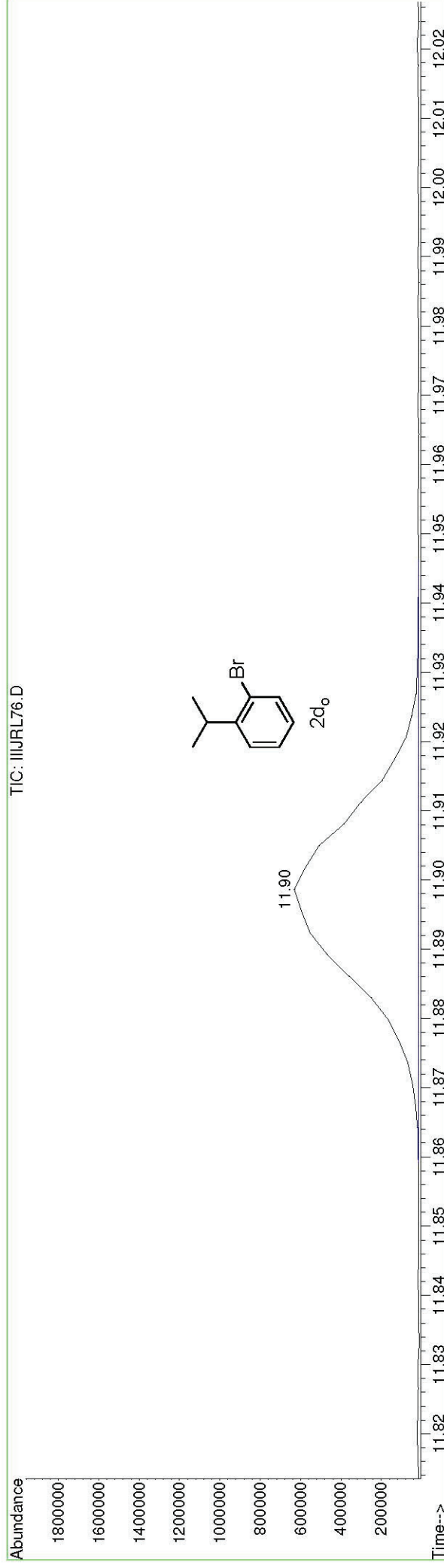
Hit 1 : Benzene, (1-methylethyl)-
C9H12; MF: 941; RMF: 941; Prob 45.2%; CAS: 98-82-8; Lib: mainlib; ID: 61536.



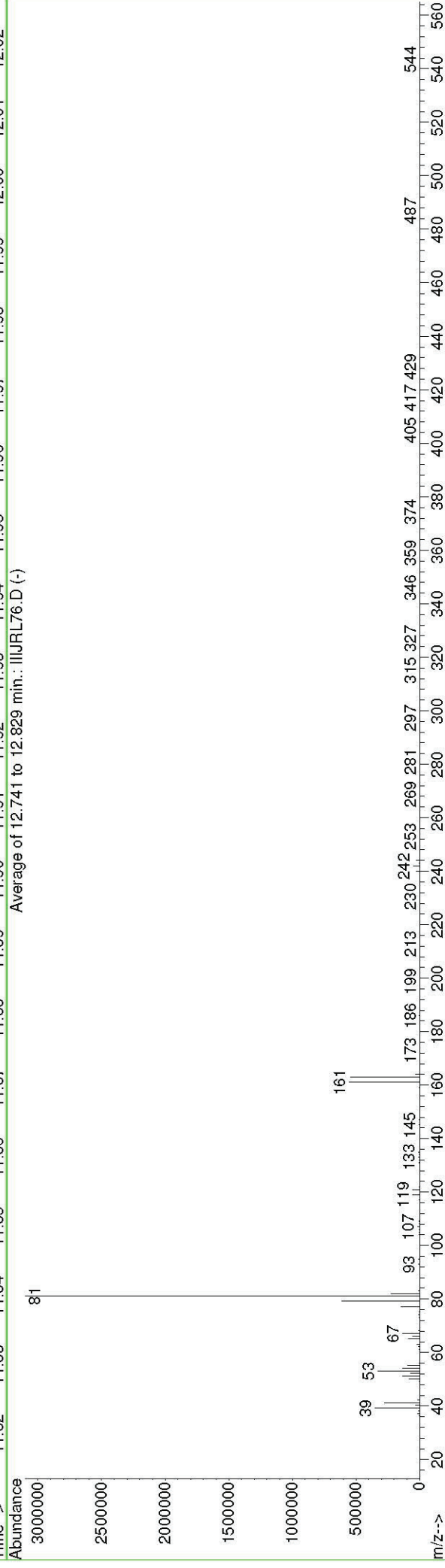
File : C:\MSDCHEM\1\DATA\ASENSIO\IIJURL76.D
 Operator :
 Acquired : 23 May 2014 18:05 using AcqMethod JMF60
 Instrument : Instrument
 Sample Name : vidrio
 Misc Info :
 Vial Number: 8

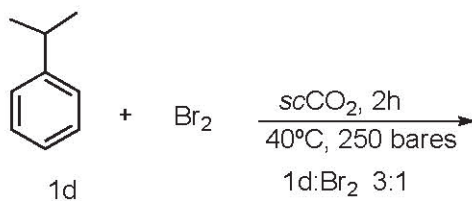


TIC: IIJURL76.D

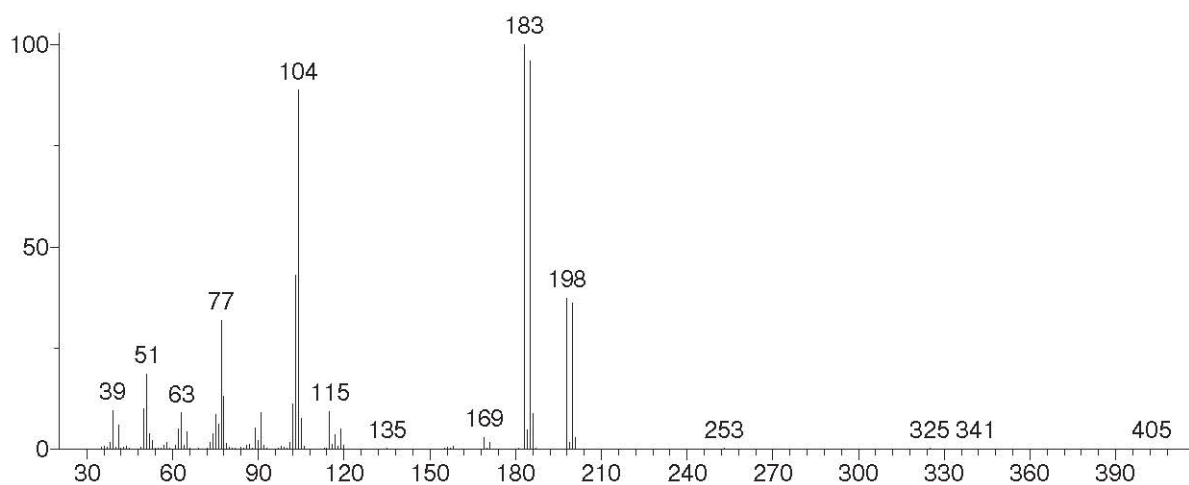


Average of 12.741 to 12.829 min.: IIJURL76.D (-)

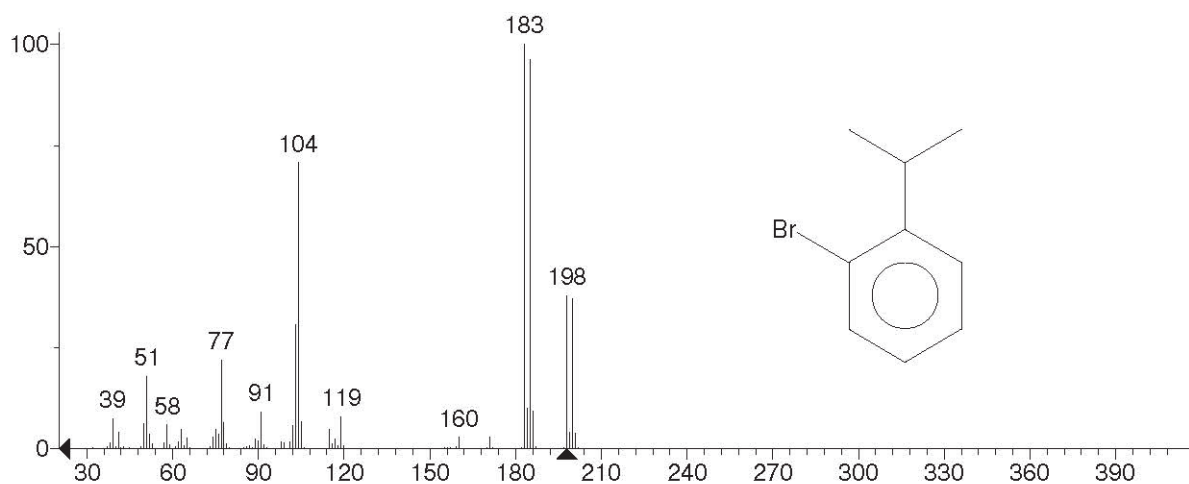




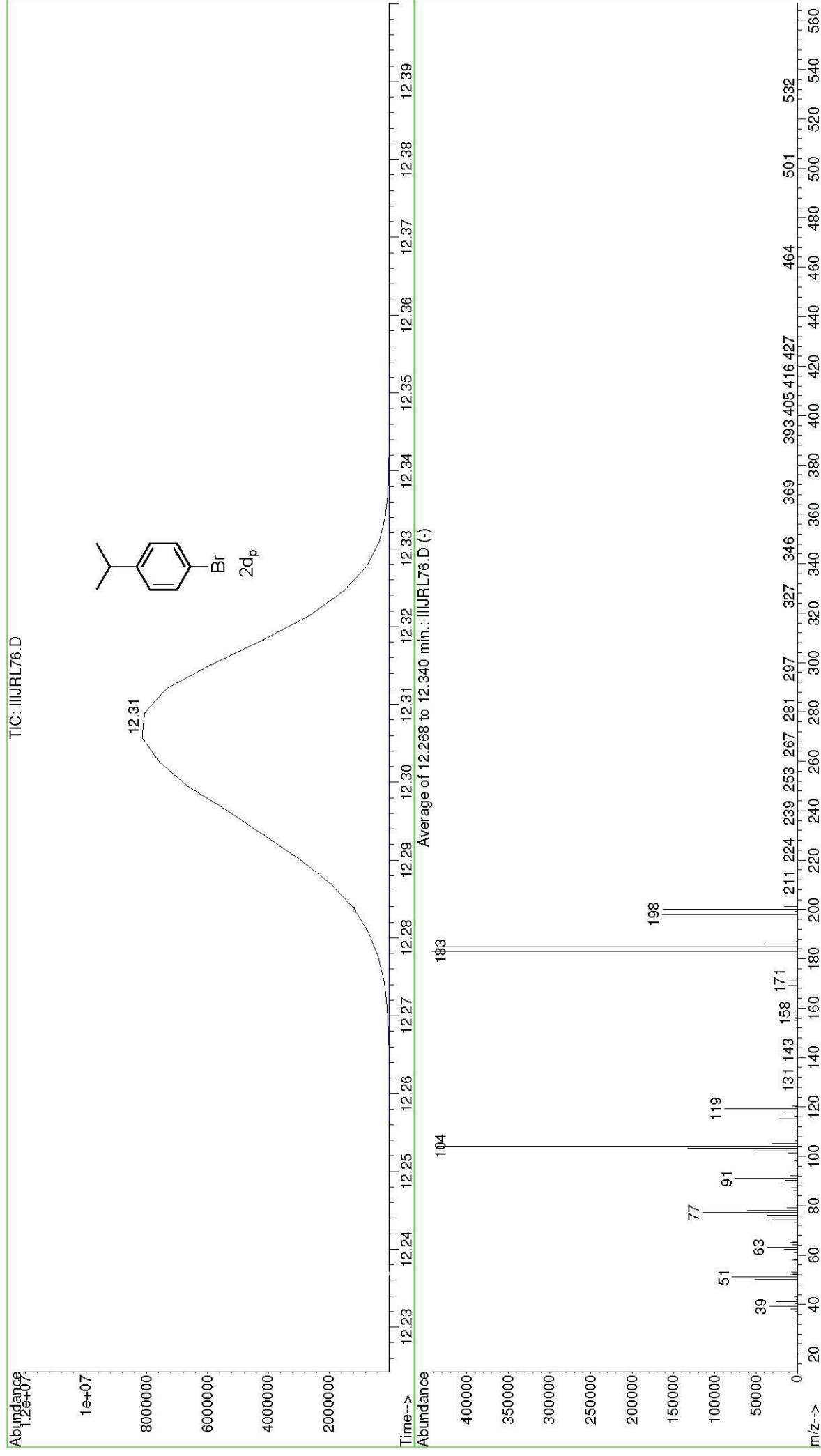
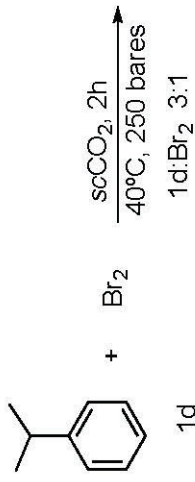
Unknown: Average of 11.874 to 11.927 min.: IIIJRL76.D
 Compound in Library Factor = 191

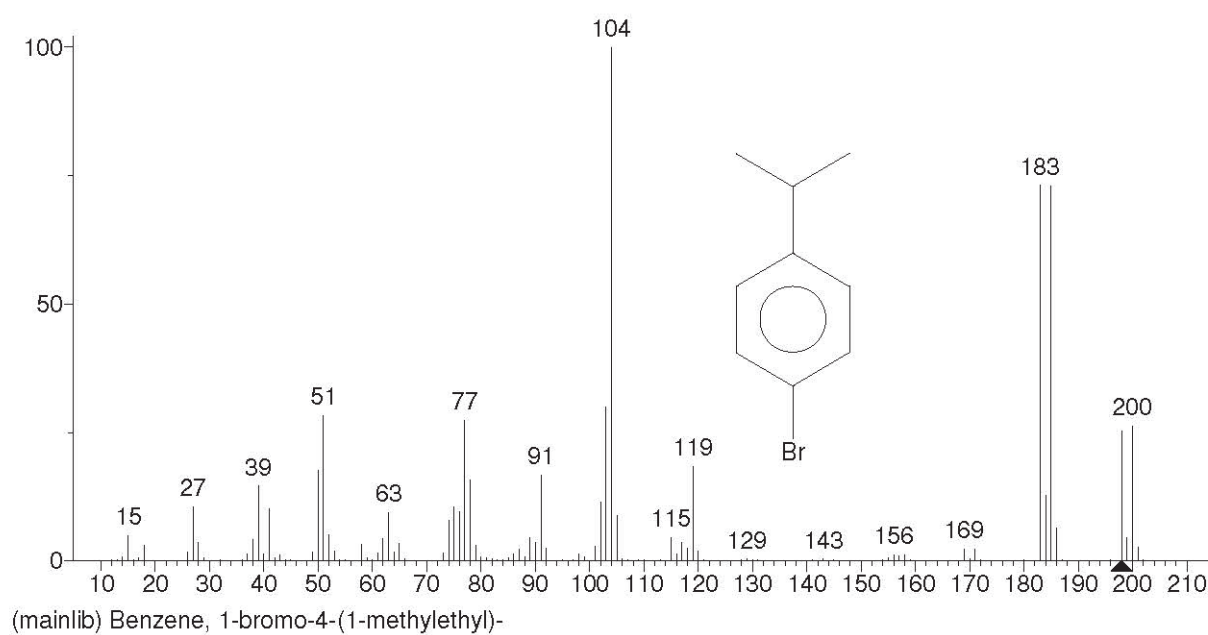
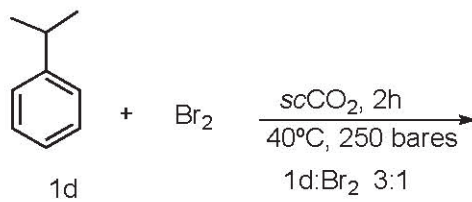


Hit 1 : Benzene, 1-bromo-2-(1-methylethyl)-
 C₉H₁₁Br; MF: 890; RMF: 896; Prob 68.8%; CAS: 7073-94-1; Lib: mainlib; ID: 116050.

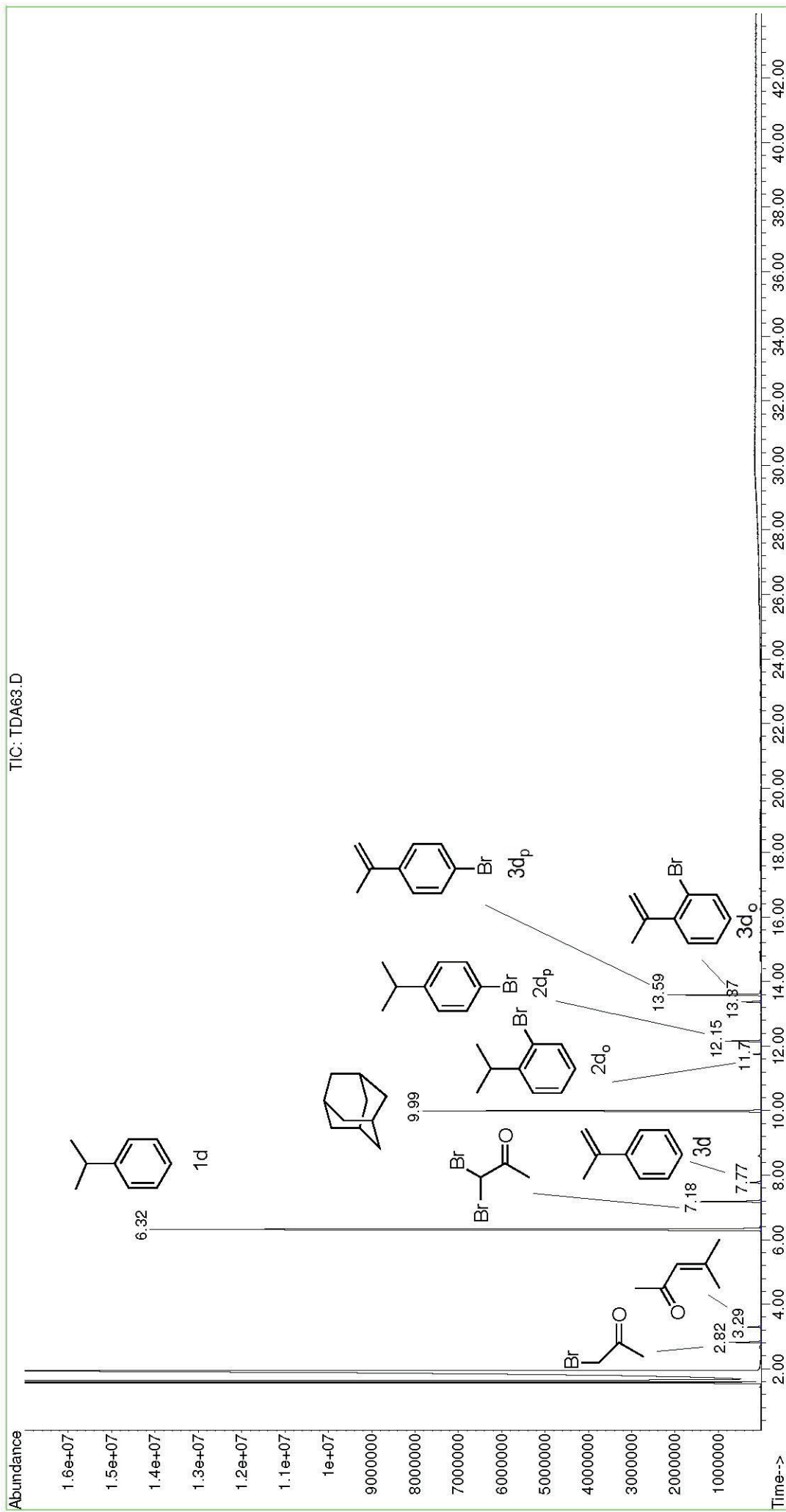
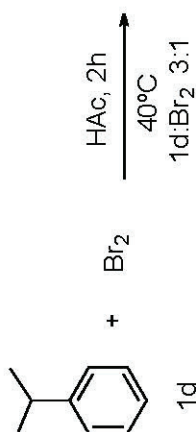


File : C:\MSDCHEM\1\DATA\ASENSIO\IIIJRL76.D
Operator :
Acquired : 23 May 2014 18:05 using AcqMethod JMF60
Instrument : Instrument
Sample Name : vidrio
Misc Info :
Vial Number: 8

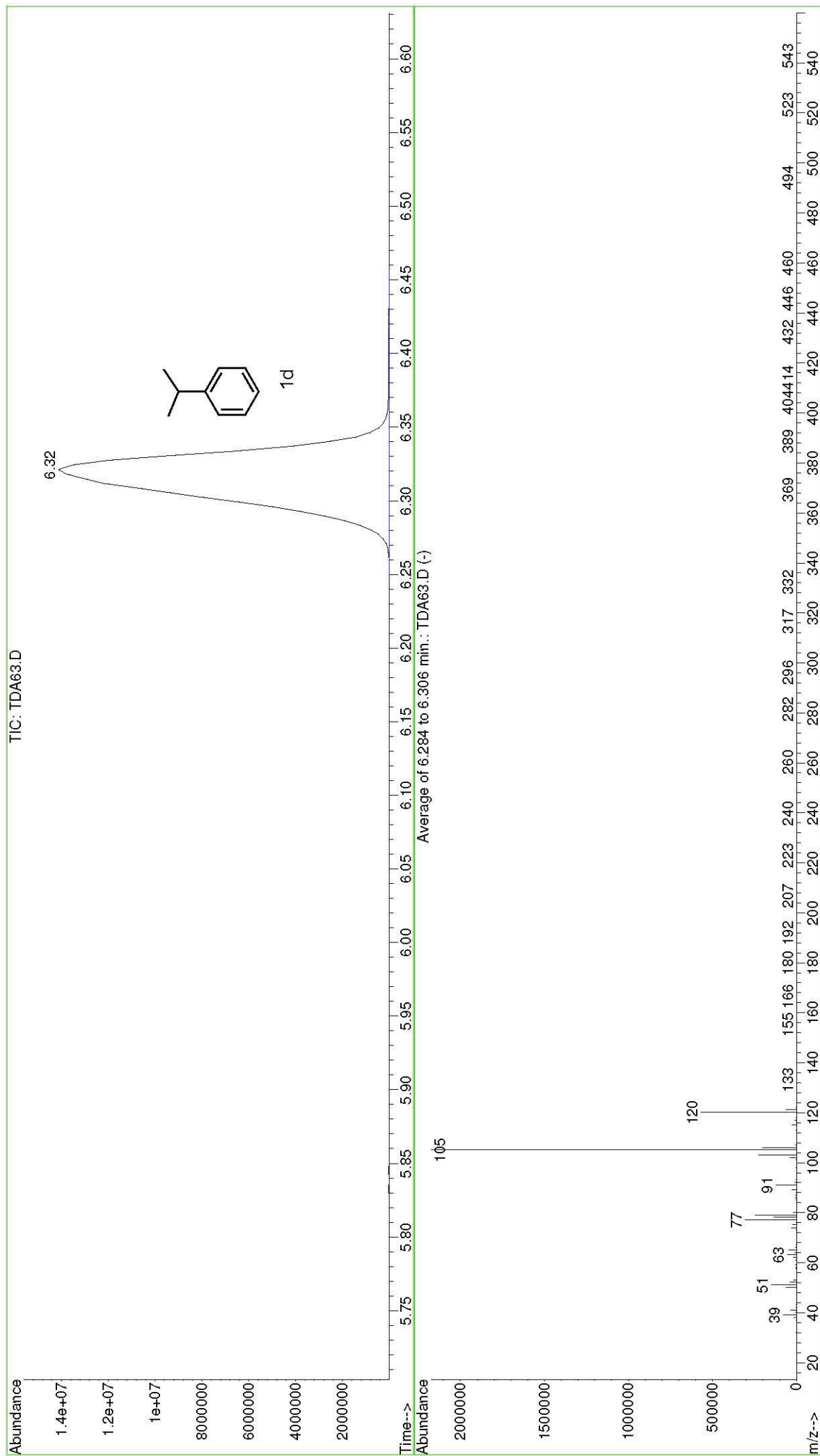
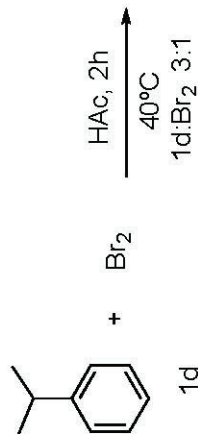


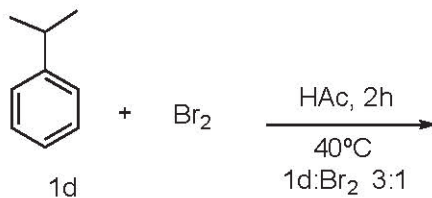


File : D:\ASENSIO\THAIS\TDA63.D
 Operator :
 Acquired : 23 Jan 2014 13:55 using AcqMethod JMF60
 Instrument : Instrumen
 Sample Name: CUMERO 3-1
 Misc Info :
 Vial Number: 6

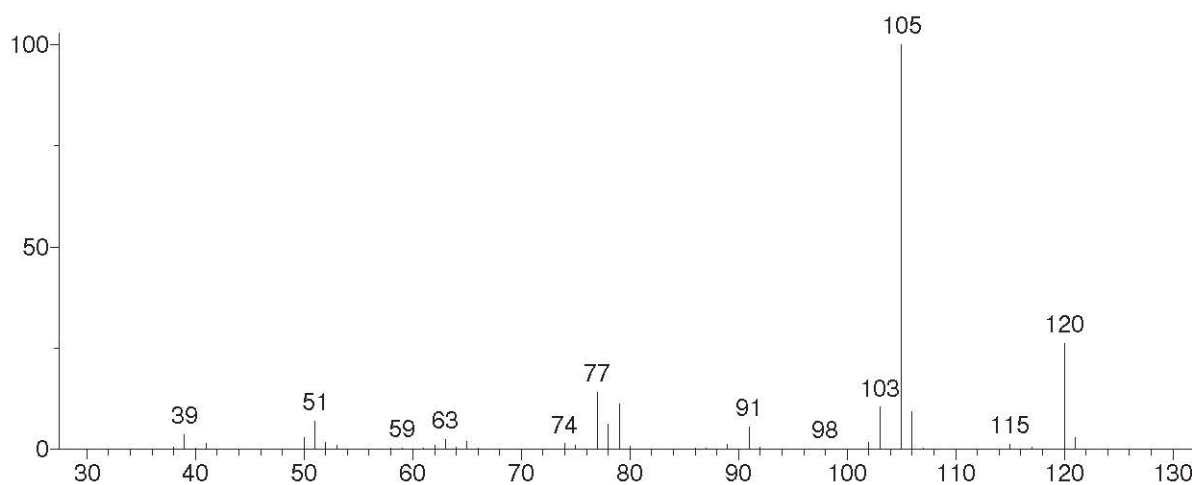


File : D:\ASENSIO\THAIS\TDA63.D
Operator :
Acquired : 23 Jan 2014 13:55 using AcqMethod JMF60
Instrument : Instrumenten
Sample Name : CUMERO 3-1
Misc Info :
Vial Number: 6

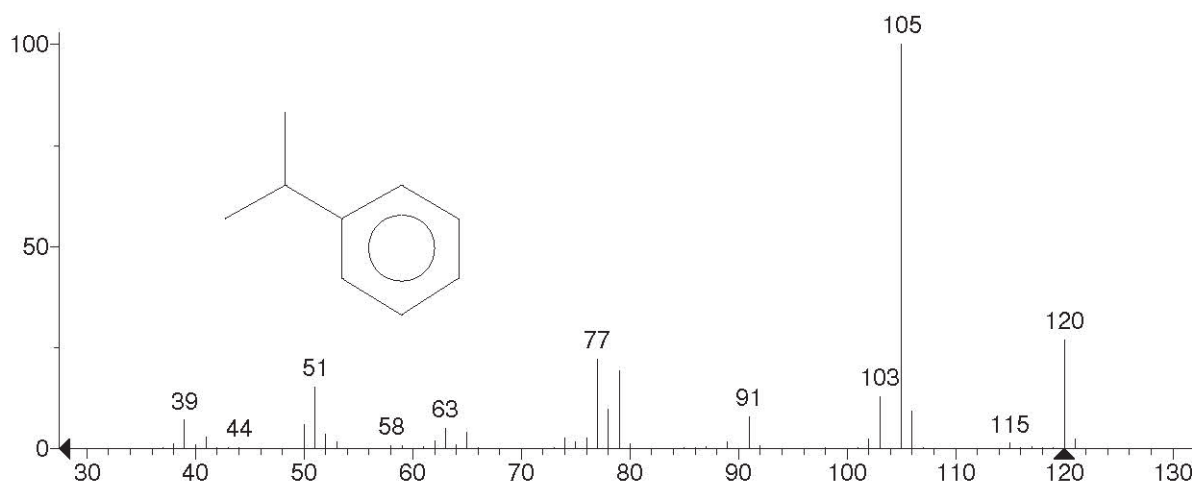




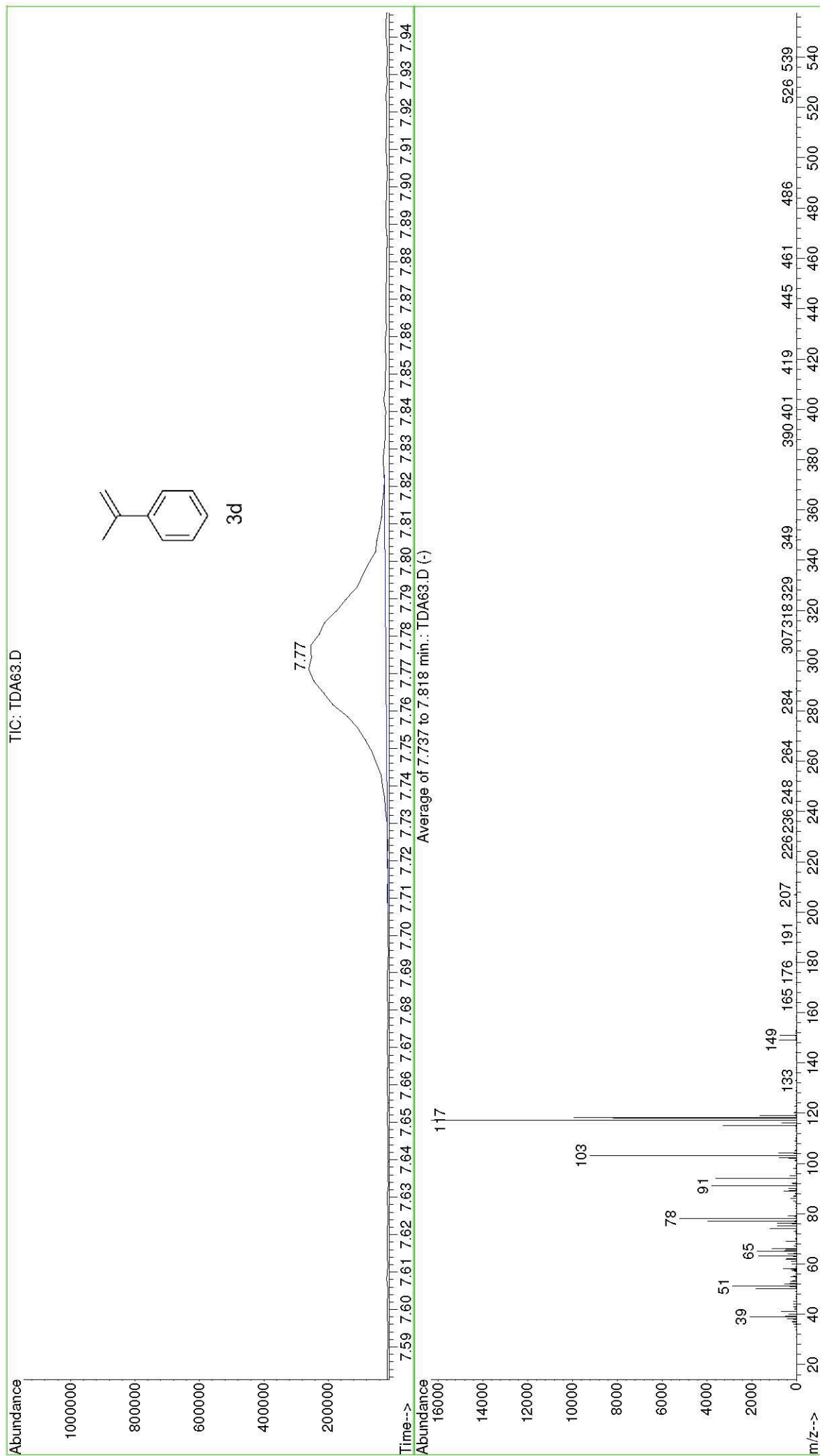
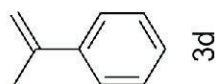
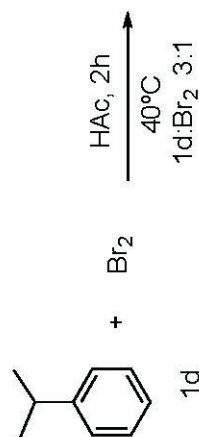
Unknown: Average of 6.284 to 6.306 min.: TDA63.D
Compound in Library Factor = -103

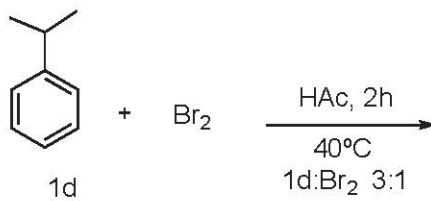


Hit 1 : Benzene, (1-methylethyl)-
C₉H₁₂; MF: 938; RMF: 938; Prob 52.5%; CAS: 98-82-8; Lib: mainlib; ID: 61536.

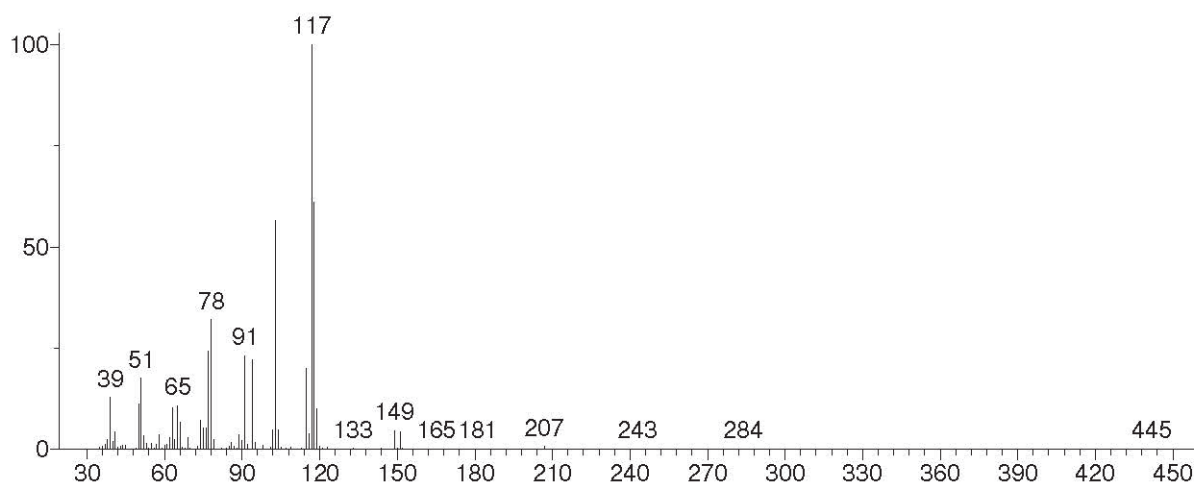


File : D:\ASENSIO\THAIS\TDA63.D
Operator :
Acquired : 23 Jan 2014 13:55 using AcqMethod JMF60
Instrument : Instrumen
Sample Name: CUMERO 3-1
Misc Info :
Vial Number: 6

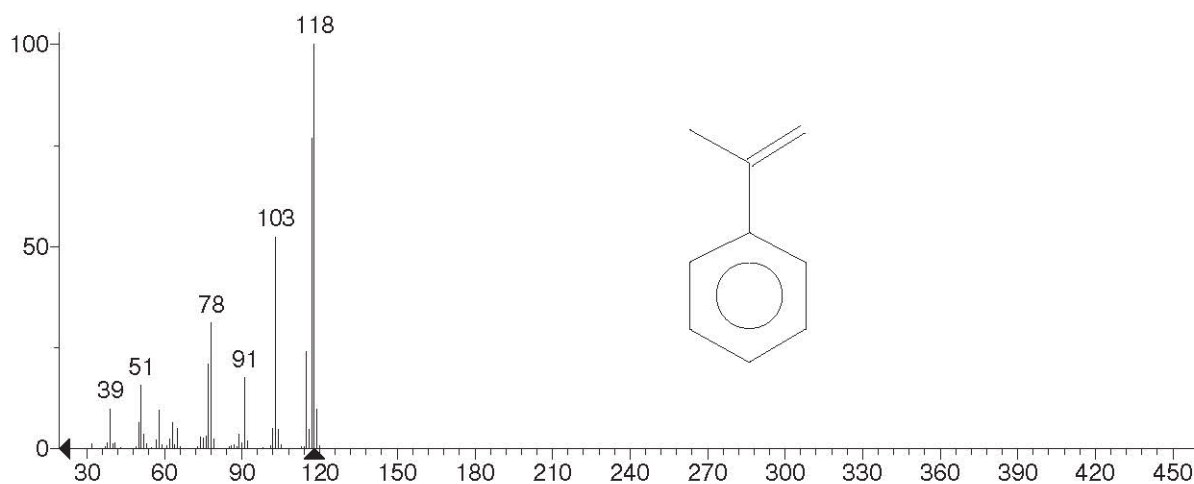




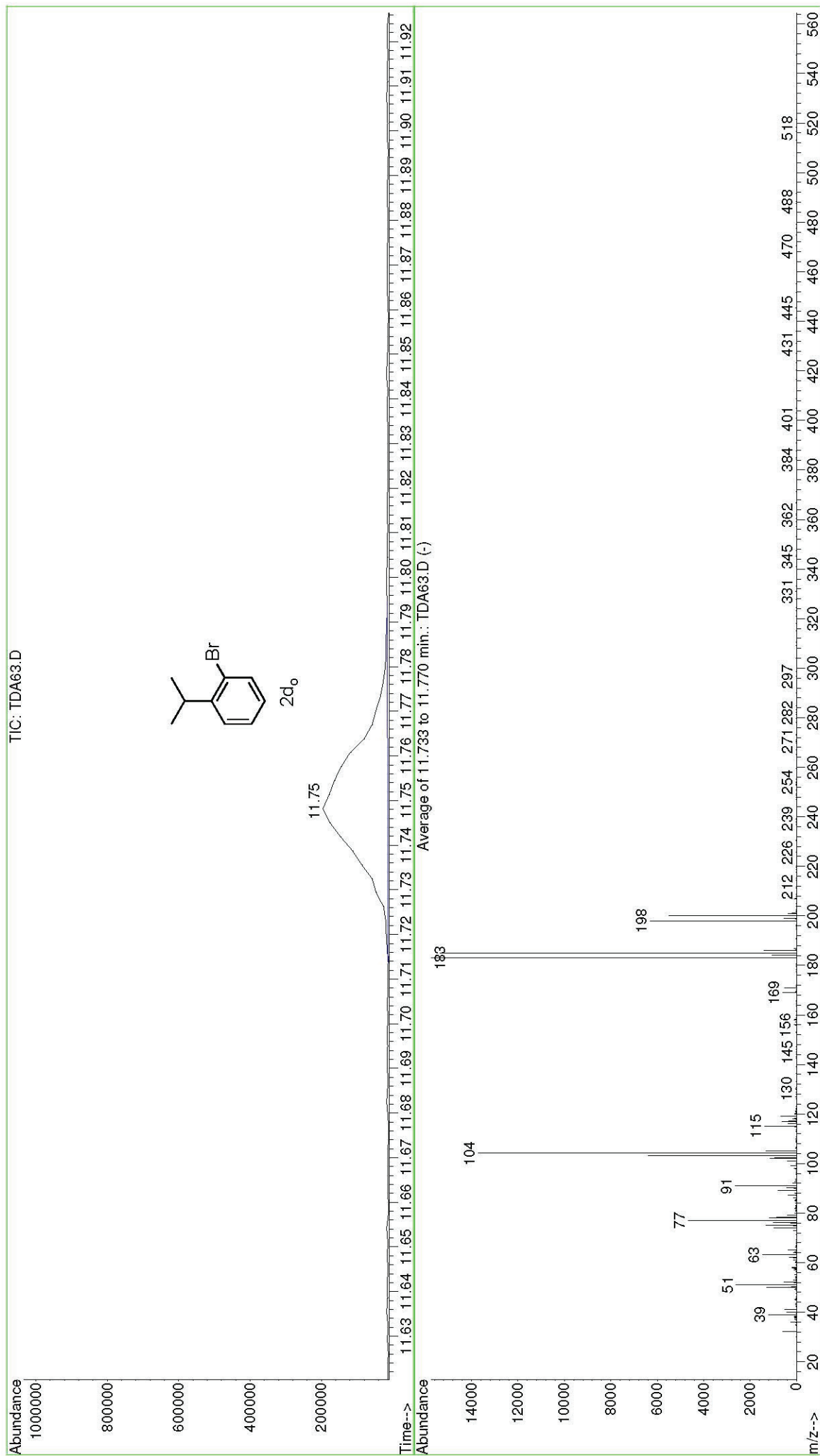
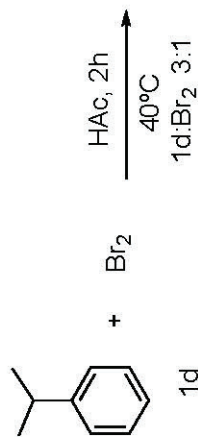
Unknown: Average of 7.737 to 7.818 min.: TDA63.D
Compound in Library Factor = -359

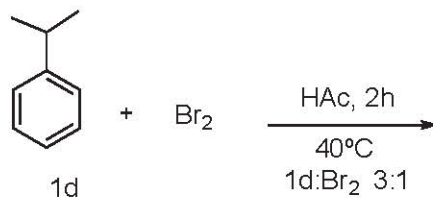


Hit 1 : α -Methylstyrene
C9H10; MF: 840; RMF: 888; Prob 18.1%; CAS: 98-83-9; Lib: wiley7n; ID: 18061.

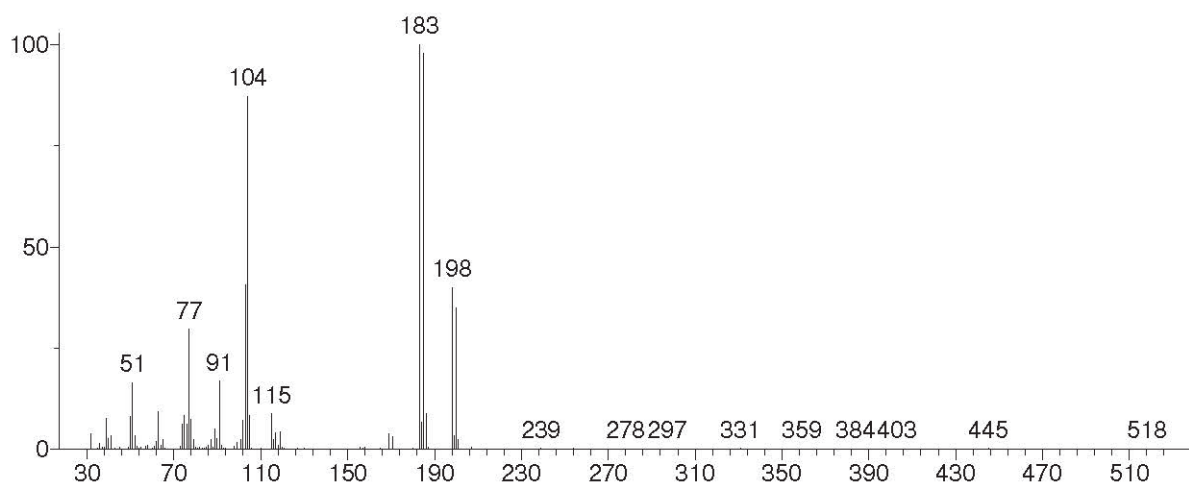


File : D:\ASENSIO\THAIS\TDA63.D
 Operator :
 Acquired : 23 Jan 2014 13:55 using AcqMethod JMF60
 Instrument : Instrument
 Sample Name : CUMERO 3-1
 Misc Info :
 Vial Number: 6

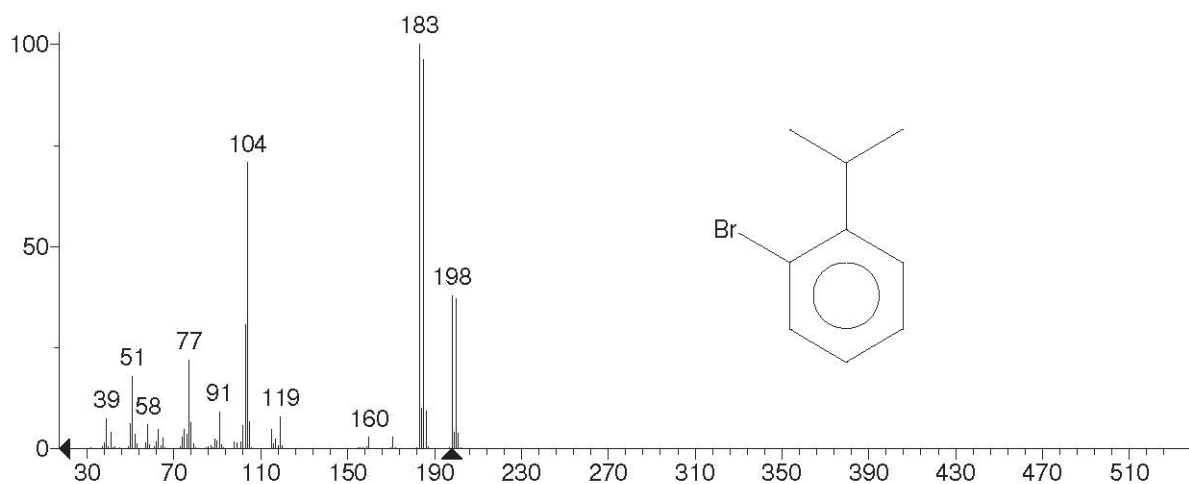




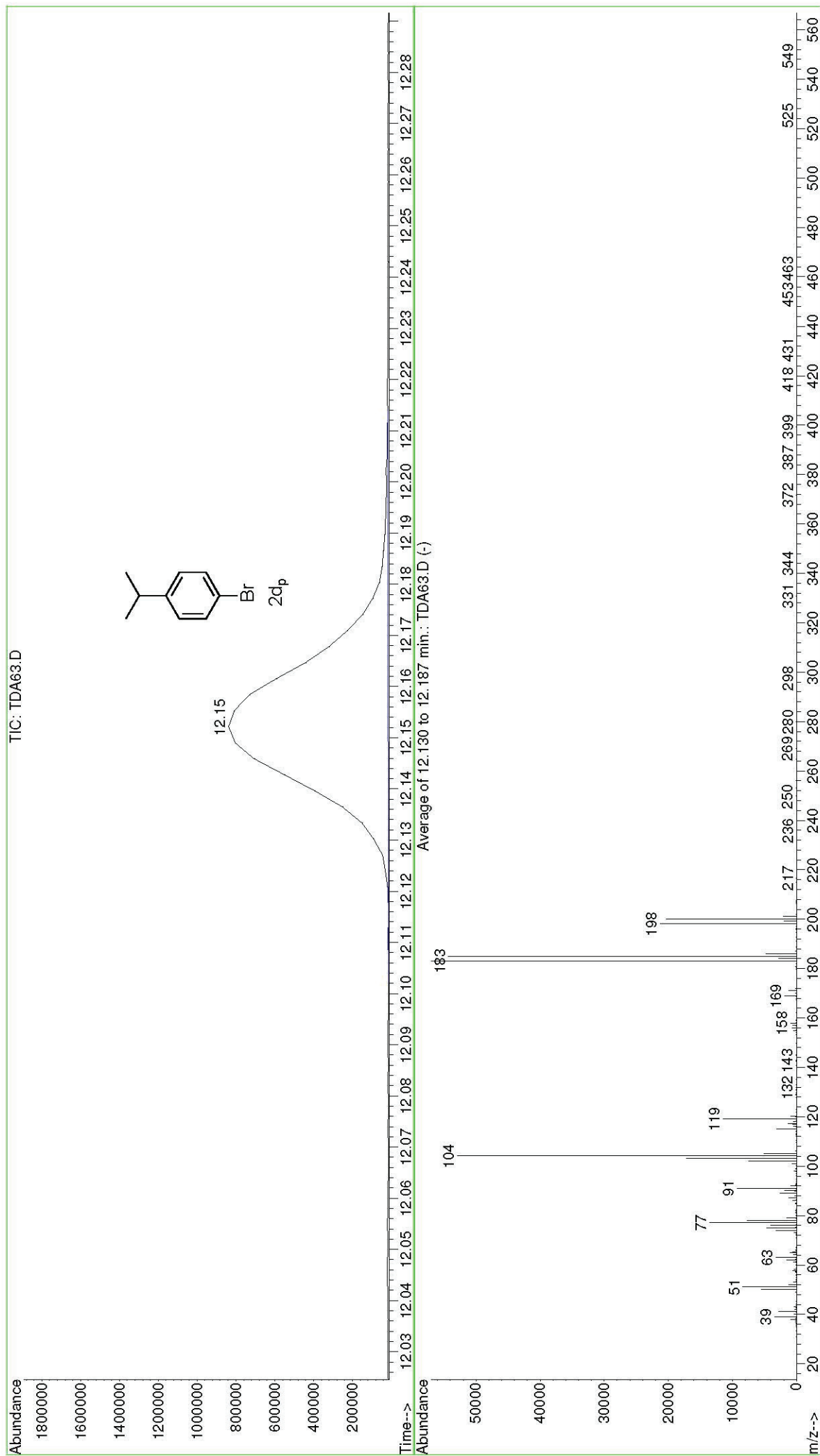
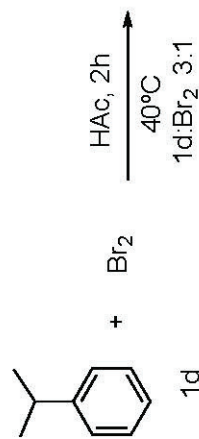
Unknown: Average of 11.733 to 11.770 min.: TDA63.D
Compound in Library Factor = 199

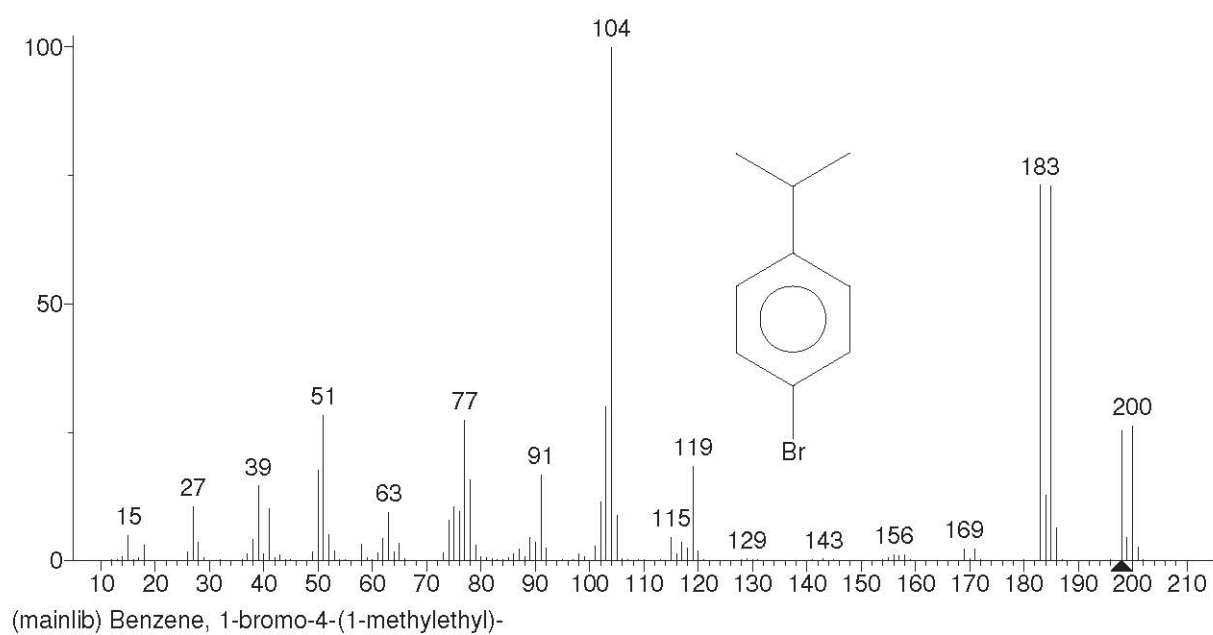
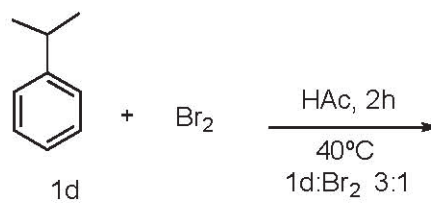


Hit 1 : Benzene, 1-bromo-2-(1-methylethyl)-
C₉H₁₁Br; MF: 900; RMF: 909; Prob 78.1%; CAS: 7073-94-1; Lib: mainlib; ID: 116050.

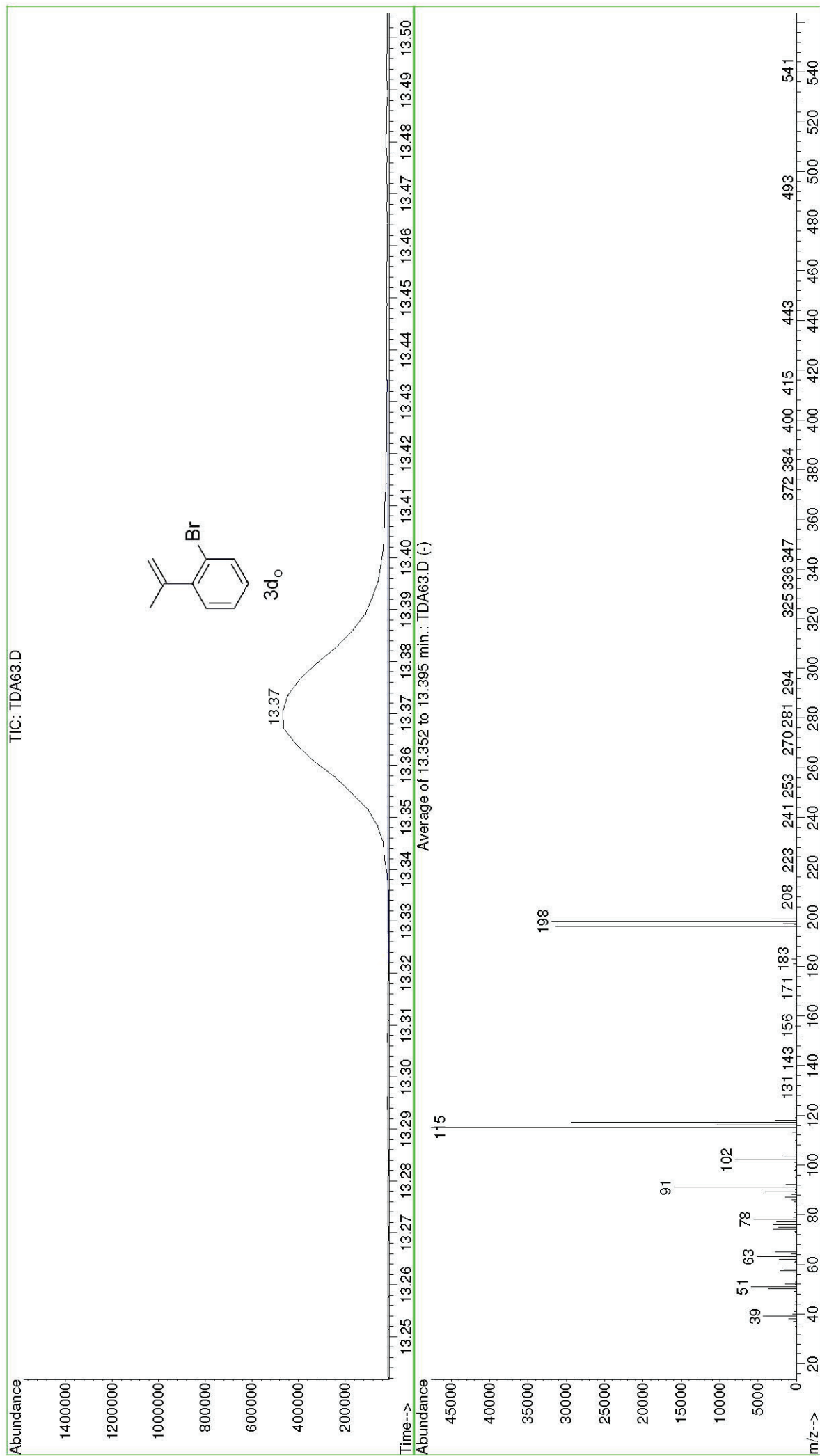
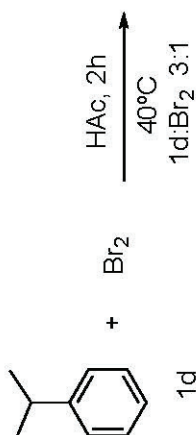


File : D:\ASENSIO\THAIS\TDA63.D
Operator :
Acquired : 23 Jan 2014 13:55 using AcqMethod JMF60
Instrument : Instrument
Sample Name : CUMERO 3-1
Misc Info :
Vial Number: 6





File : D:\ASENSIO\THAIS\TDA63.D
Operator :
Acquired : 23 Jan 2014 13:55 using AcqMethod JMF60
Instrument : Instrument
Sample Name : CUMERO 3-1
Misc Info :
Vial Number: 6



File : D:\ASENSIO\THAIS\TDA63.D

Operator :

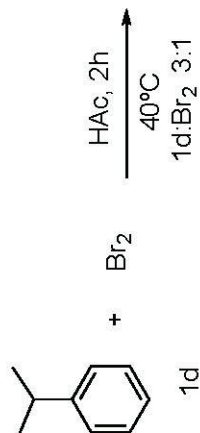
Acquired : 23 Jan 2014 13:55 using AcqMethod JMF60

Instrument : Instrument

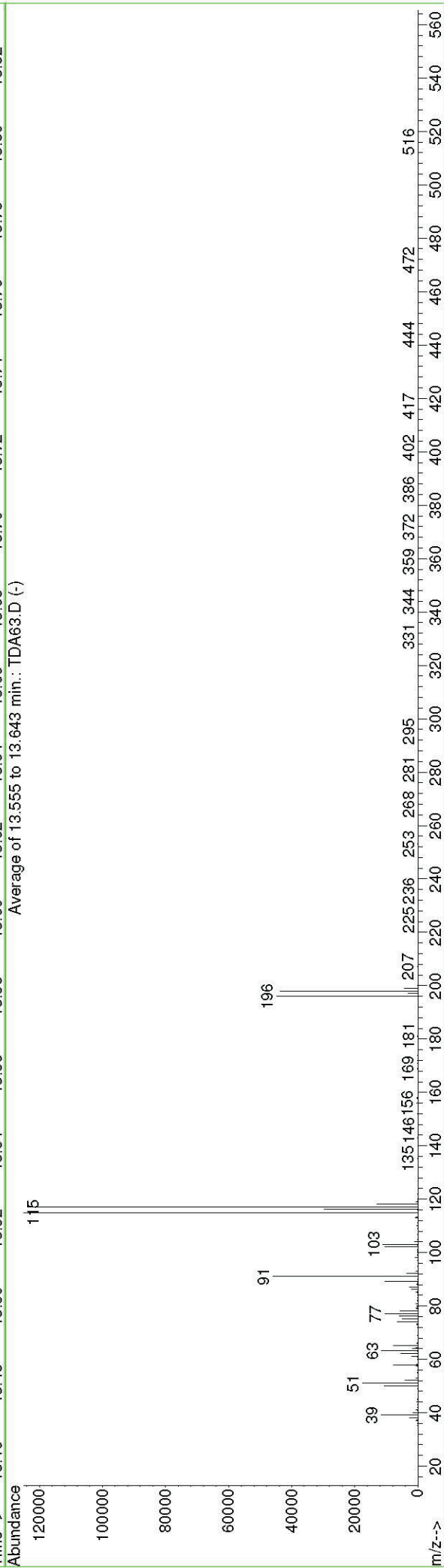
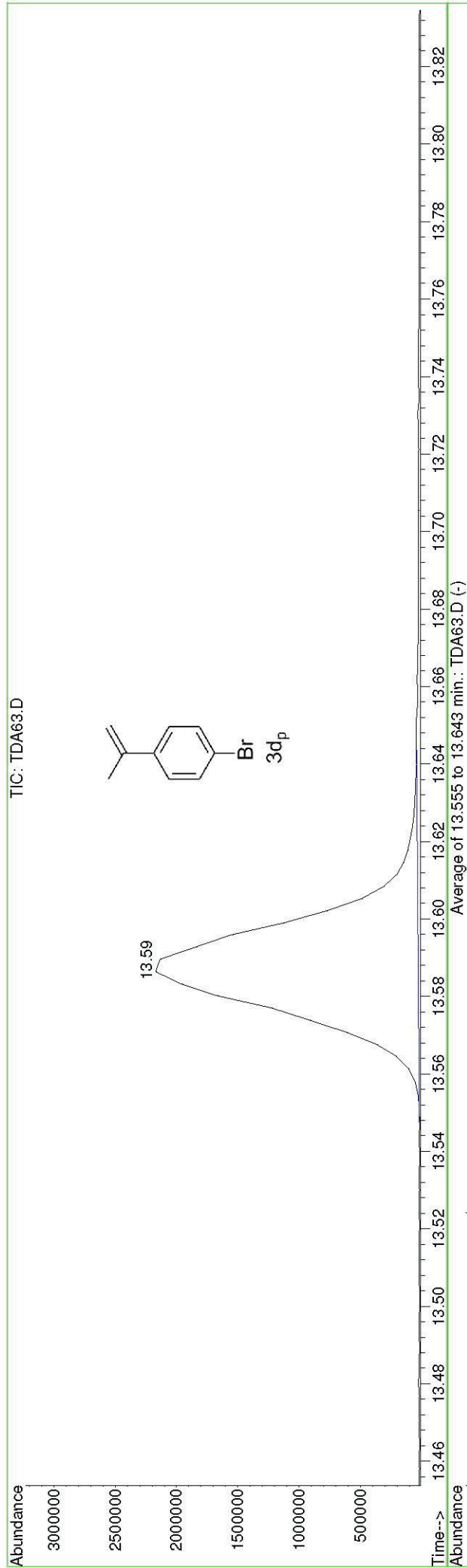
Sample Name: CUMERO 3-1

Misc Info :

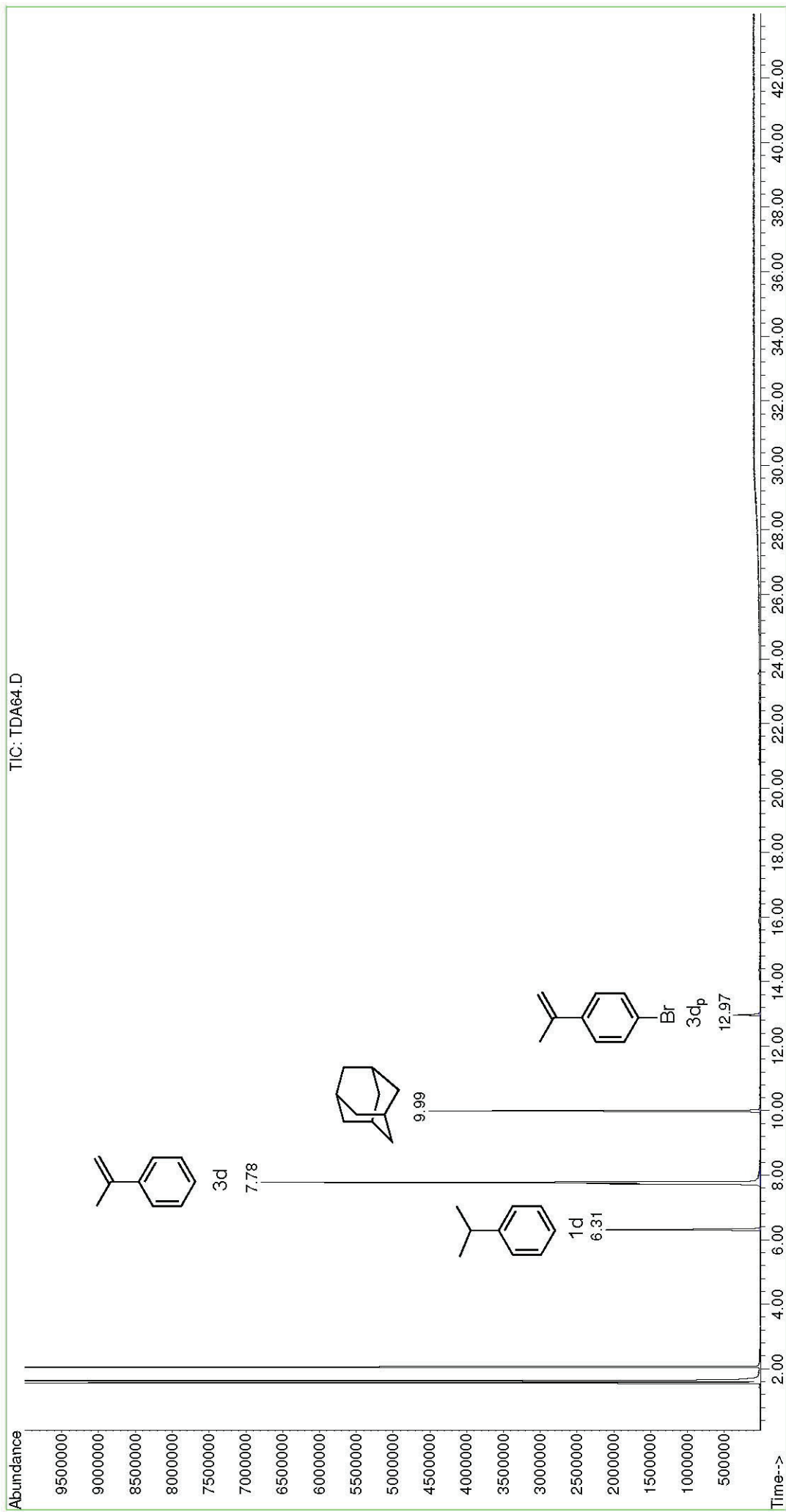
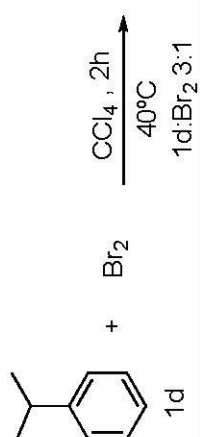
Vial Number: 6



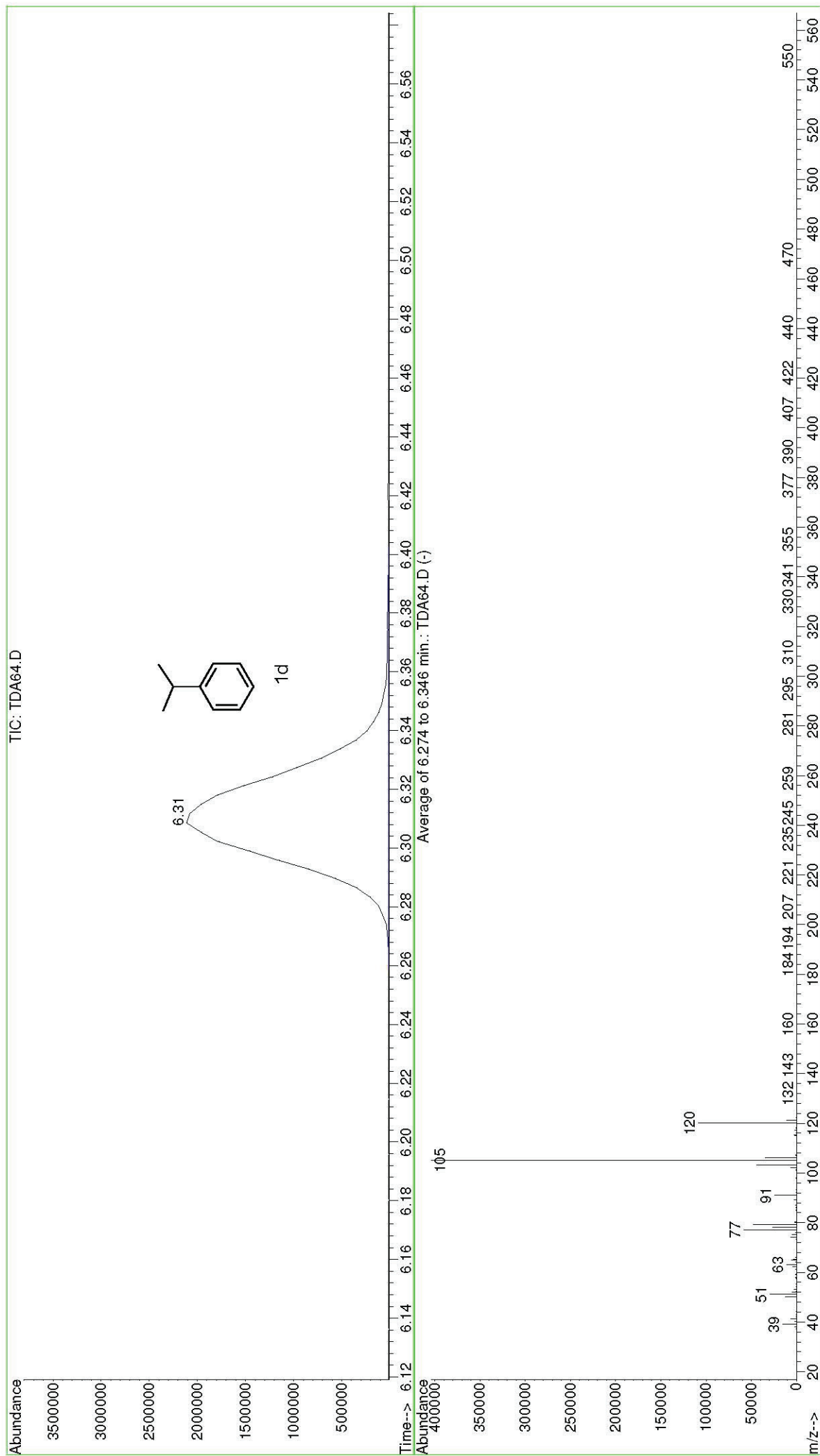
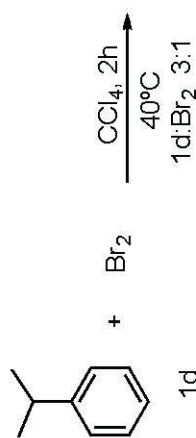
TIC: TDA63.D

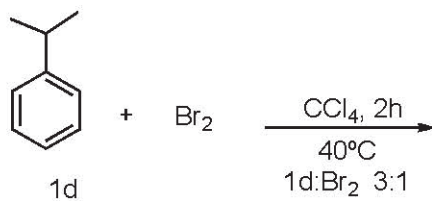


File : D:\ASENSIO\THAIS\TDA64.D
Operator :
Acquired : 23 Jan 2014 16:26 using AcqMethod JMF60
Instrument : Instrumen
Sample Name: CUMENO
Misc Info :
Vial Number: 9

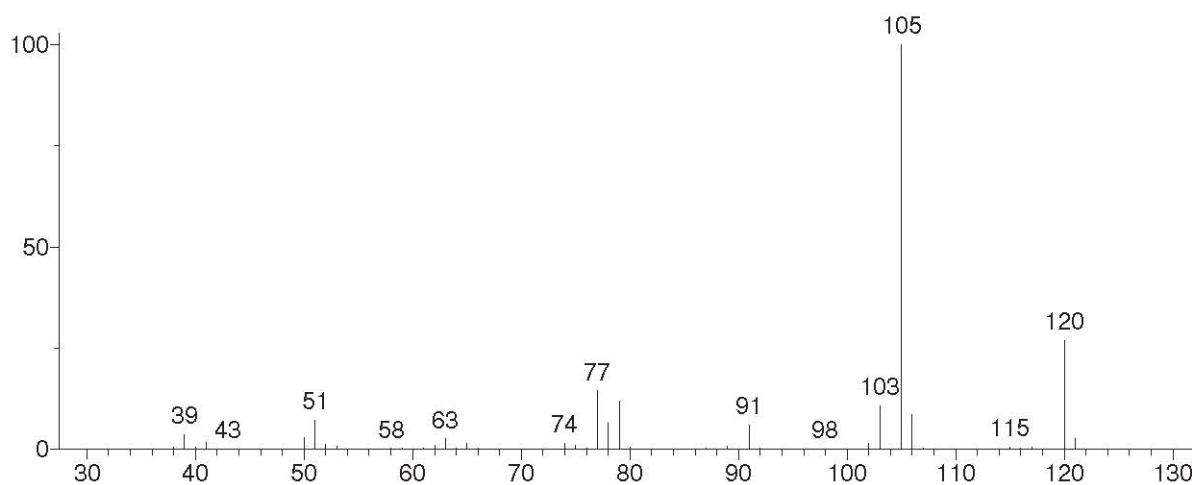


File : D:\ASENSIO\THAIS\TDA64.D
Operator :
Acquired : 23 Jan 2014 16:26 using AcqMethod JMF60
Instrument : Instrument
Sample Name: CUMENO
Misc Info :
Vial Number: 9

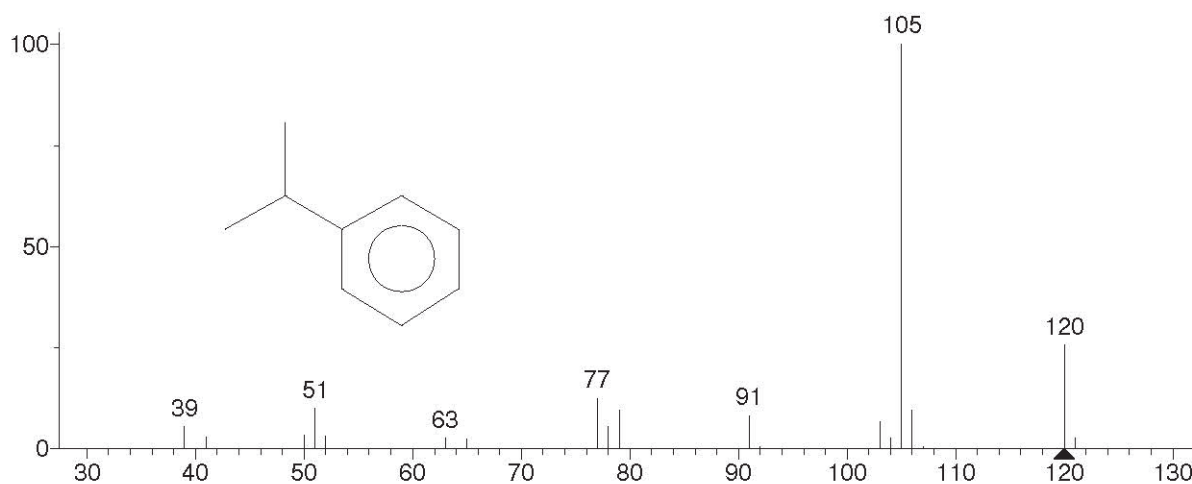




Unknown: Average of 6.274 to 6.346 min.: TDA64.D
Compound in Library Factor = 103



Hit 1 : Benzene, (1-methylethyl)- (CAS)
C₉H₁₂; MF: 916; RMF: 941; Prob 54.6%; CAS: 98-82-8; Lib: wiley7n; ID: 18916.



File : D:\ASENSIO\THAIS\TDA64.D

Operator :

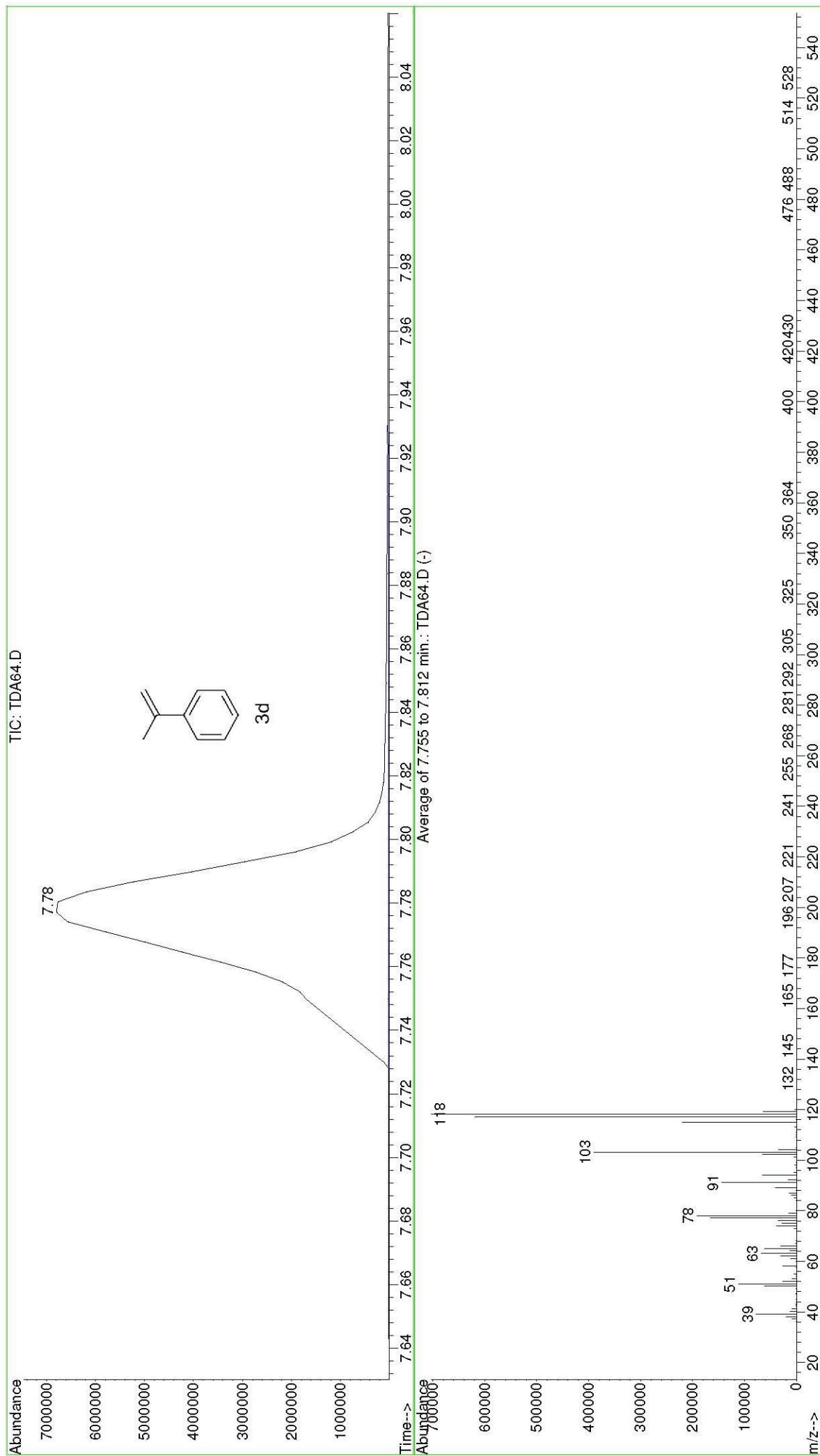
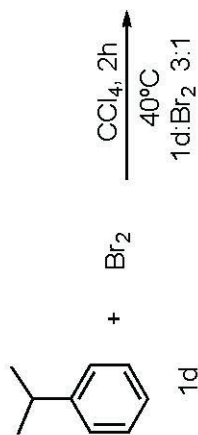
Acquired : 23 Jan 2014 16:26 using AcqMethod JMF60

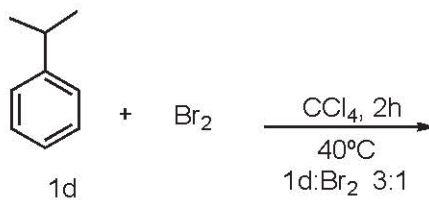
Instrument : Instrument

Sample Name: CUMENO

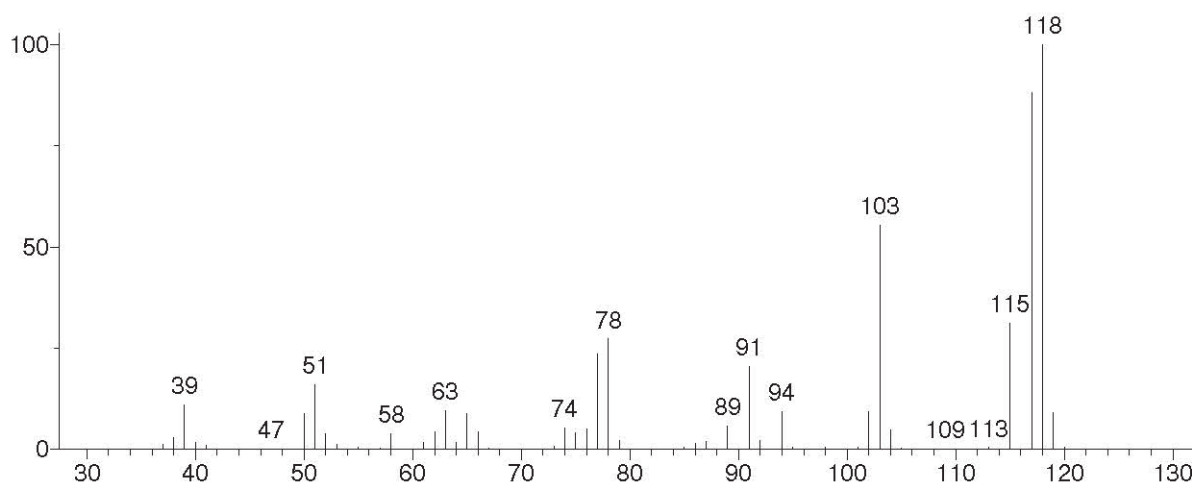
Misc Info :

Vial Number: 9

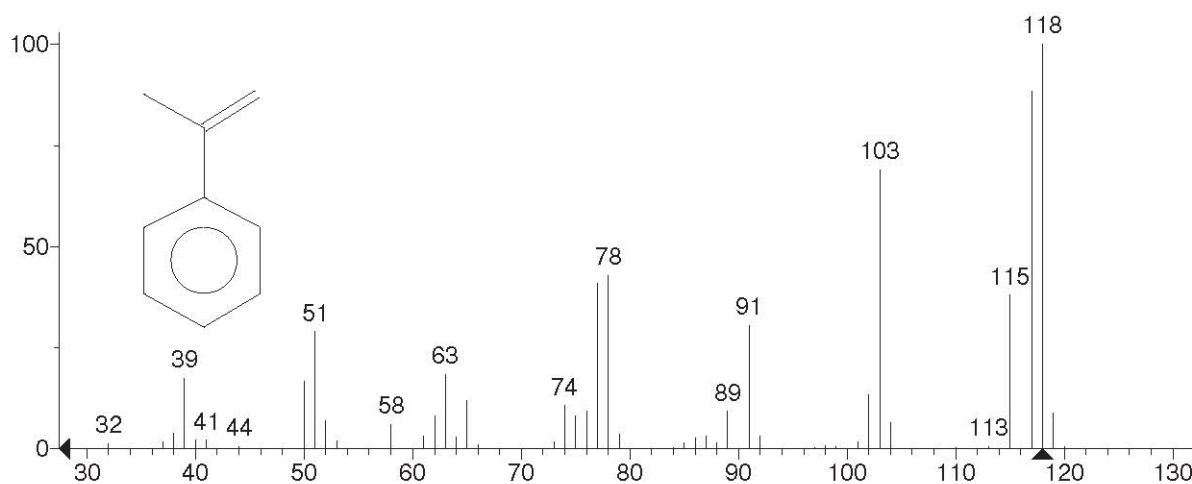




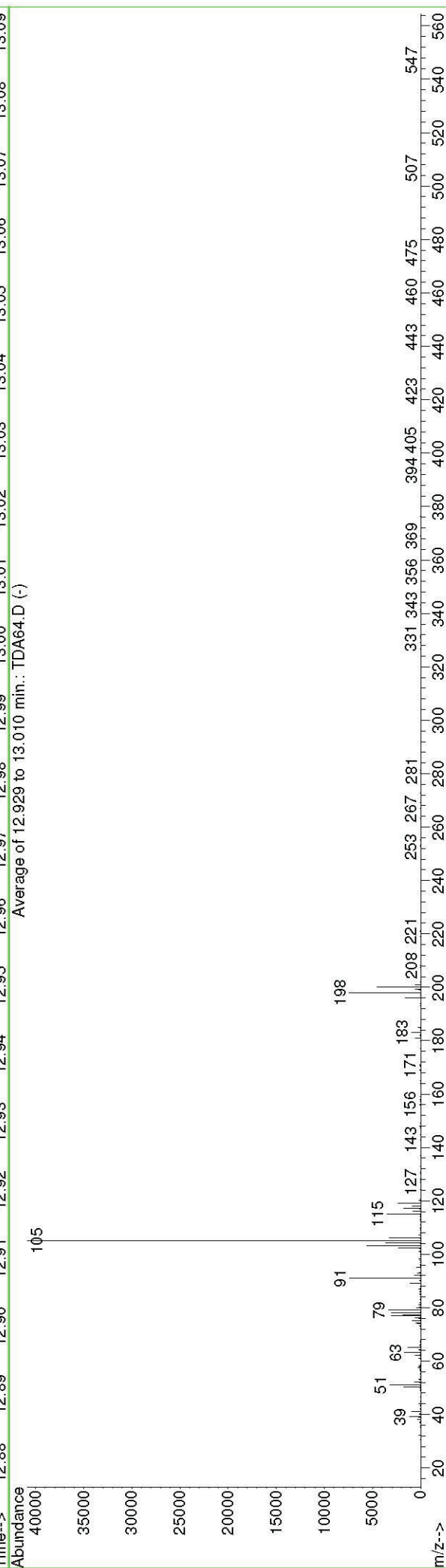
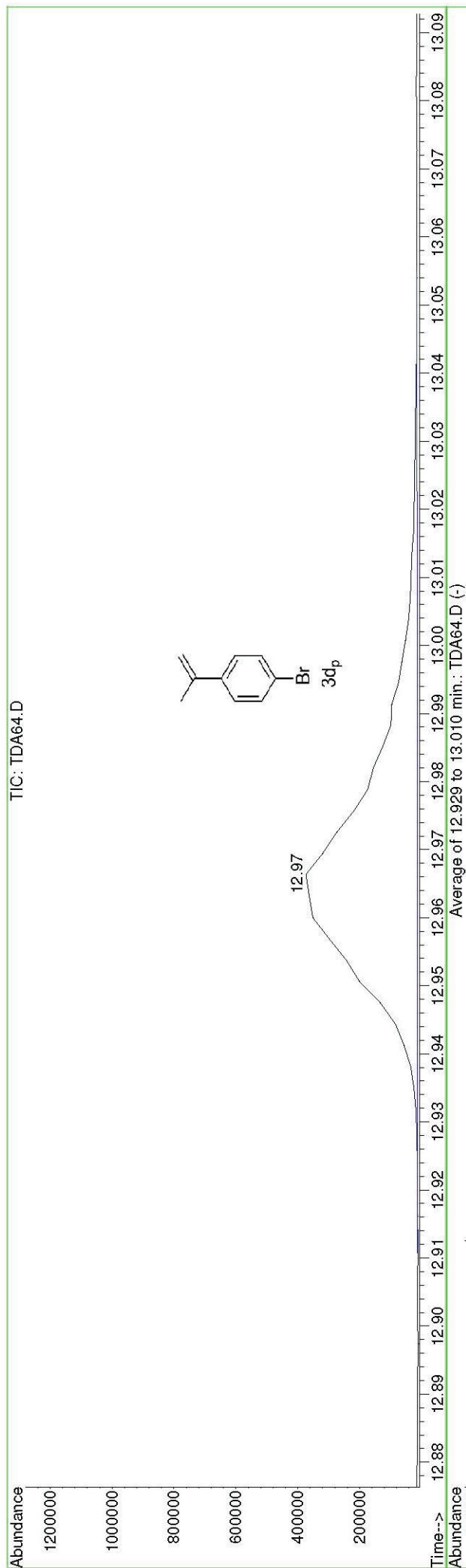
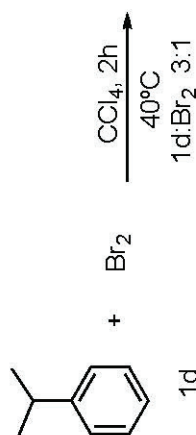
Unknown: Average of 7.755 to 7.812 min.: TDA64.D
Compound in Library Factor = 103



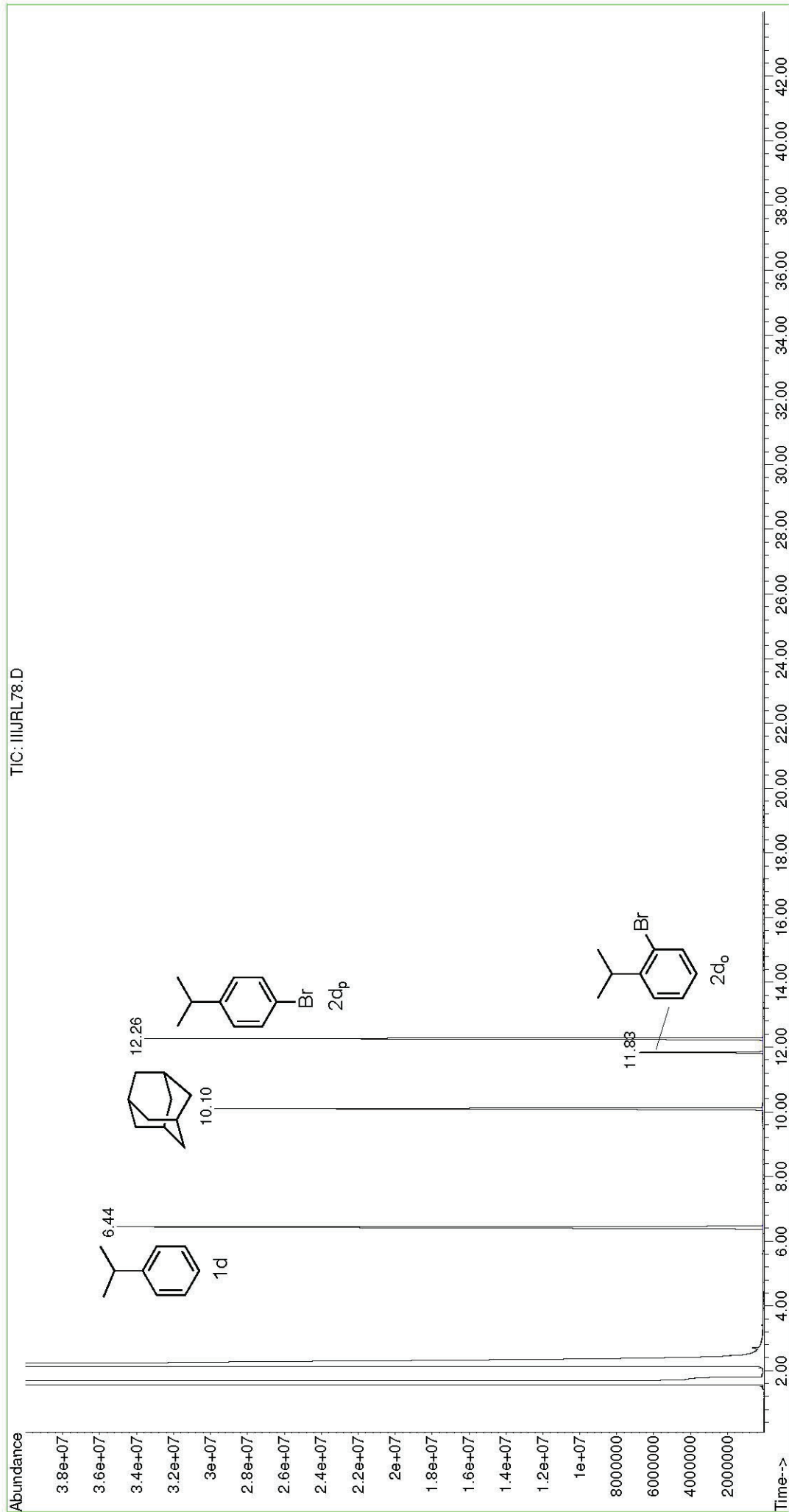
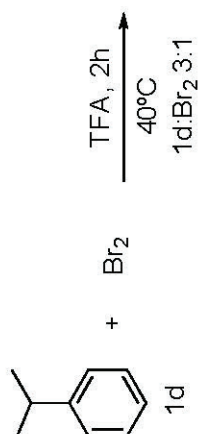
Hit 1 : α -Methylstyrene
C₉H₁₀; MF: 916; RMF: 927; Prob 37.0%; CAS: 98-83-9; Lib: wiley7n; ID: 18064.



File : D:\ASENSIO\THAIS\TDA64.D
Operator :
Acquired : 23 Jan 2014 16:26 using AcqMethod JMF60
Instrument : Instrument
Sample Name : CUMENO
Misc Info :
Vial Number: 9



File : D:\ASENSIO\MATEO\IIJRL78.D
Operator :
Acquired : 16 Jun 2014 20:05 using AcqMethod JMF60
Instrument : Instrument
Sample Name: SIN TRATAR NaHCO3
Misc Info :
Vial Number: 17



File : D:\ASENSIO\MATEO\IIIJRL78.D

Operator :

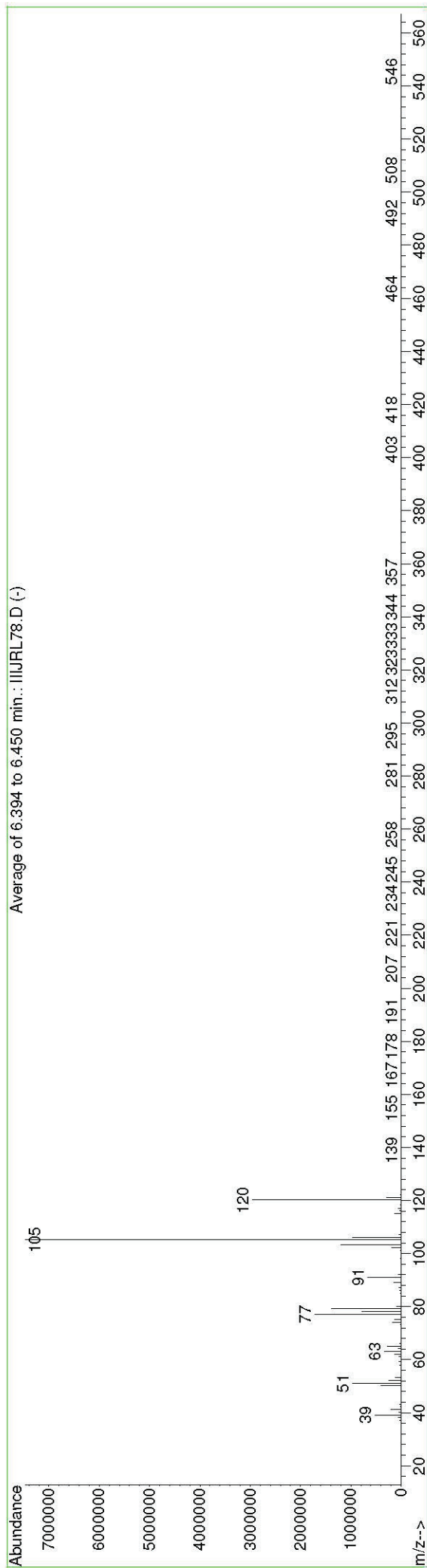
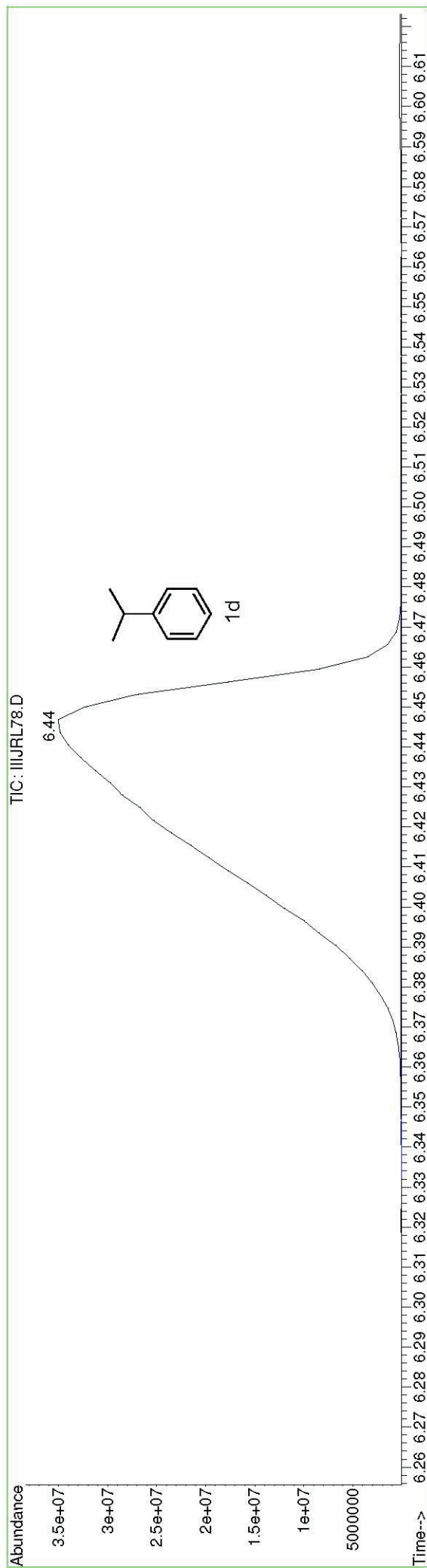
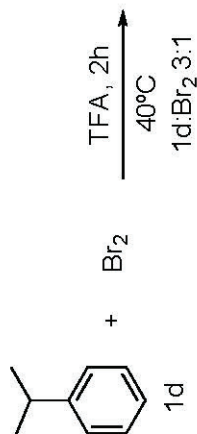
Acquired : 16 Jun 2014 20:05 using AcqMethod JMF60

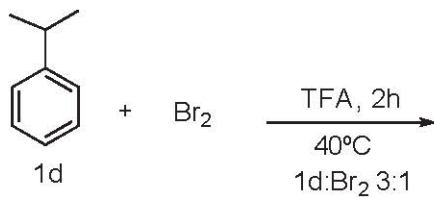
Instrument : Instrument

Sample Name: SIN TRATAR NaHCO3

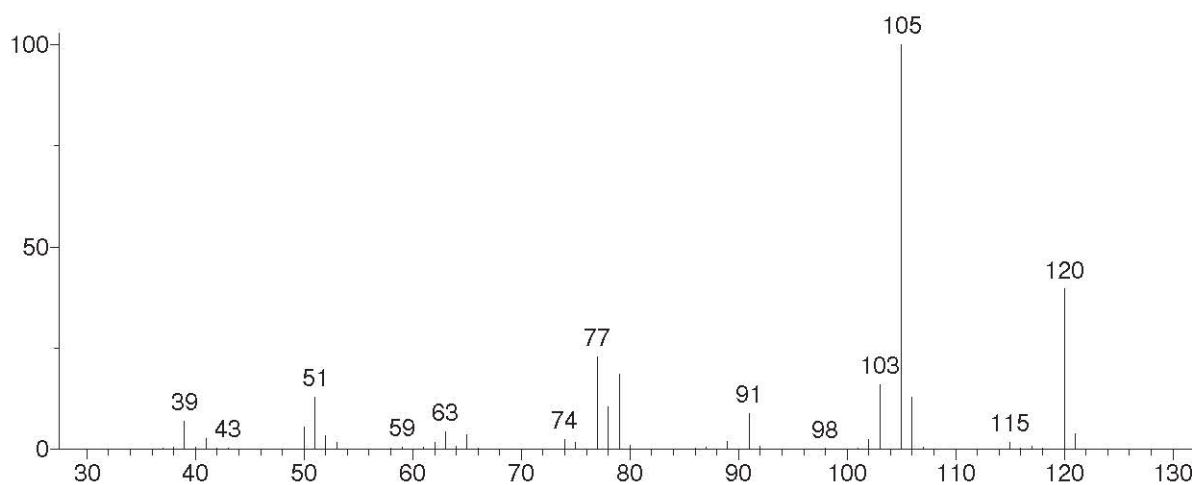
Misc Info :

Vial Number: 17

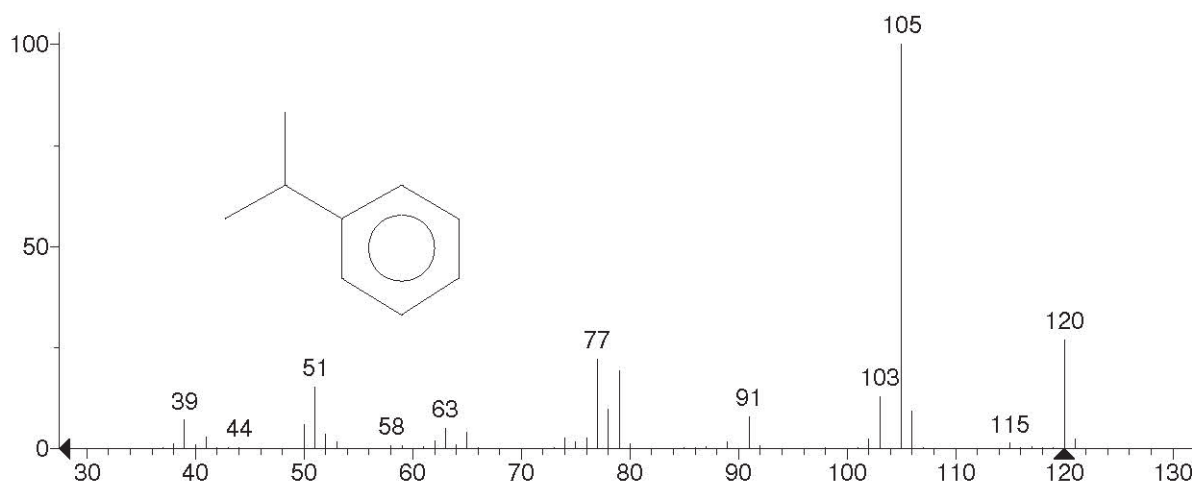




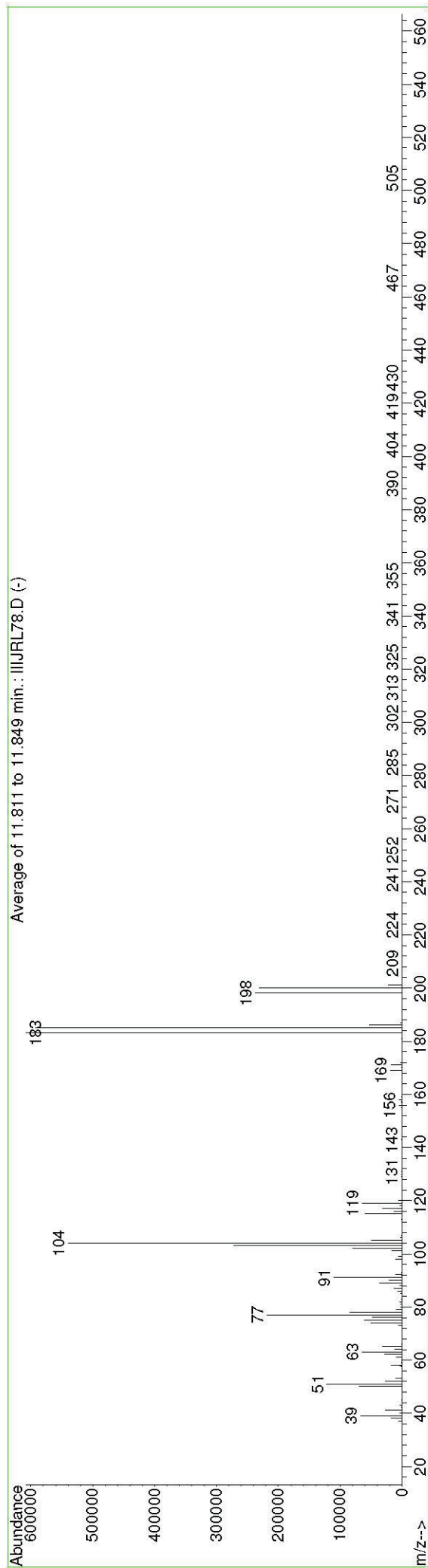
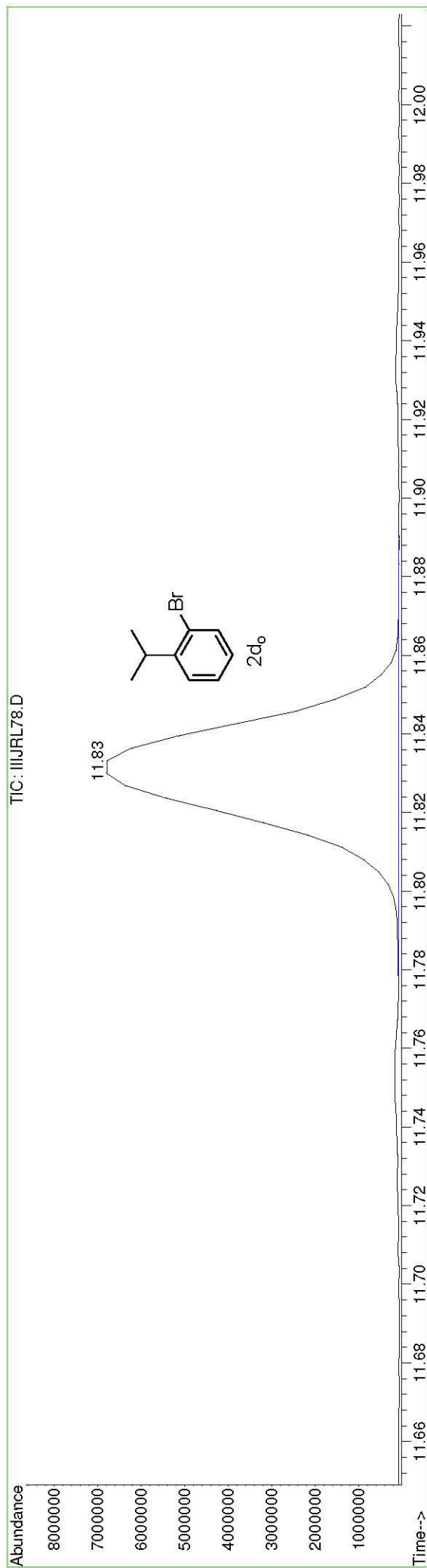
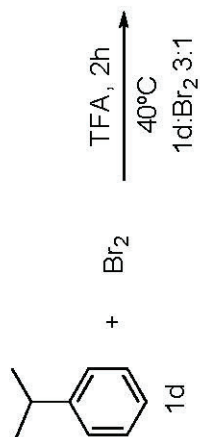
Unknown: Average of 6.394 to 6.450 min.: IIIJRL78.D
 Compound in Library Factor = -103

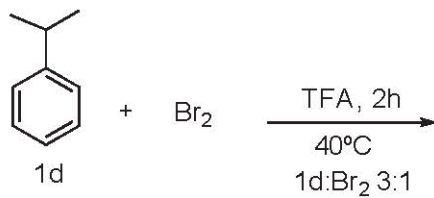


Hit 1 : Benzene, (1-methylethyl)-
 C₉H₁₂; MF: 933; RMF: 933; Prob 43.1%; CAS: 98-82-8; Lib: mainlib; ID: 61536.

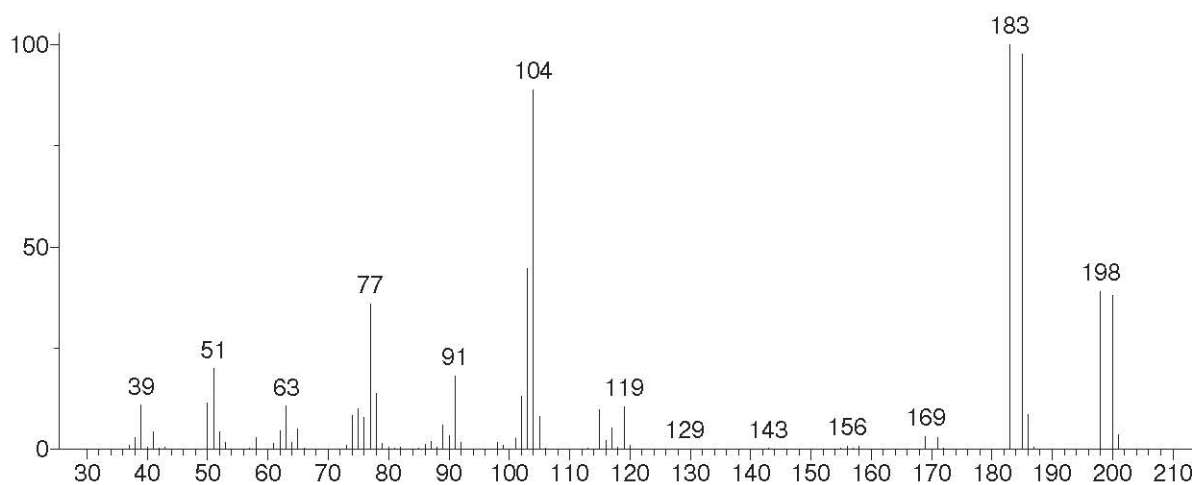


File : D:\ASENSIO\MATEO\IIIJRL78.D
Operator :
Acquired : 16 Jun 2014 20:05 using AcqMethod JMF60
Instrument : Instrument
Sample Name: SIN TRATAR NaHCO3
Misc Info :
Vial Number: 17

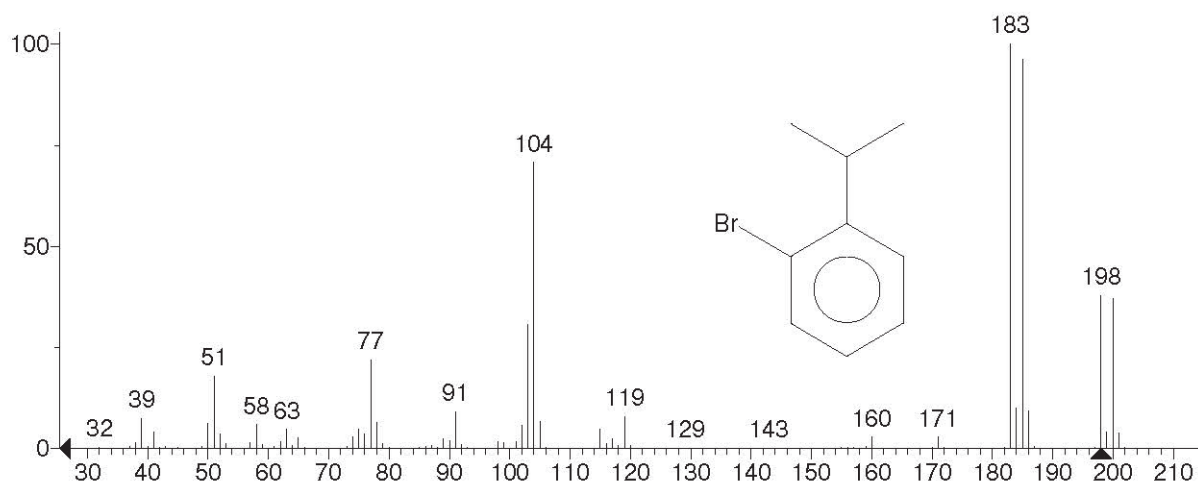




Unknown: Average of 11.811 to 11.849 min.: IIIJRL78.D
Compound in Library Factor = -119



Hit 2 : Benzene, 1-bromo-2-(1-methylethyl)-
C₉H₁₁Br; MF: 871; RMF: 874; Prob 40.6%; CAS: 7073-94-1; Lib: mainlib; ID: 116050.



File : D:\ASENSIO\MATEO\IIIJRL78.D

Operator :

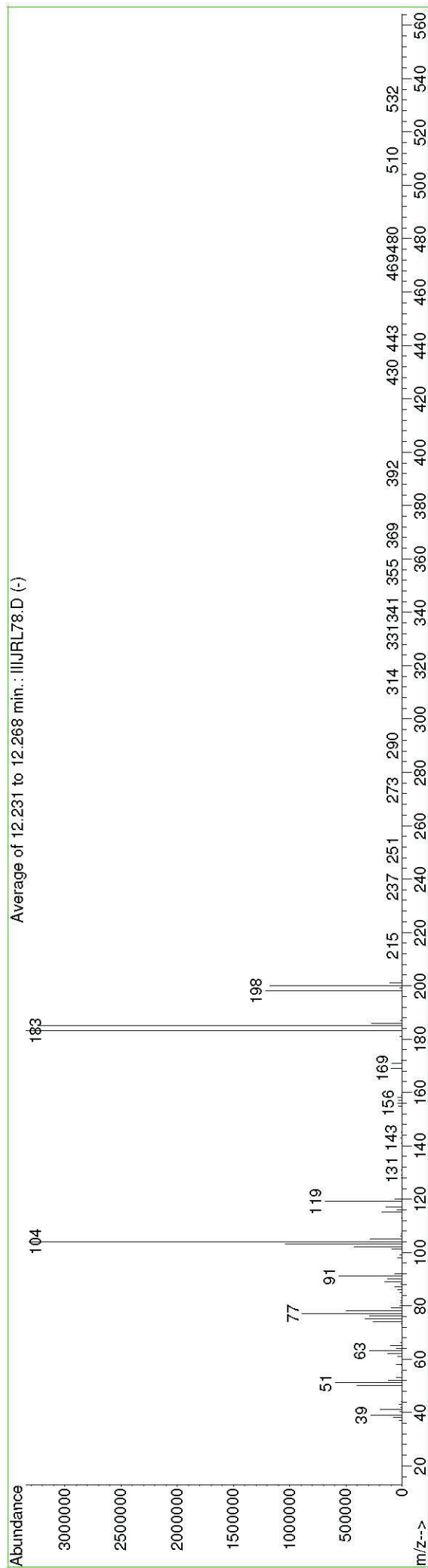
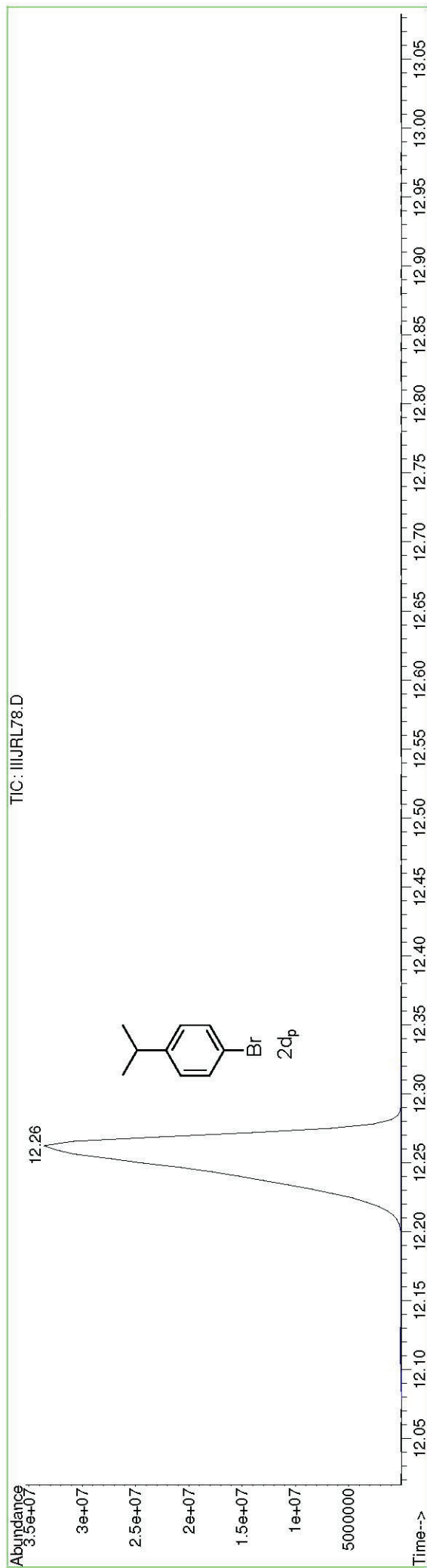
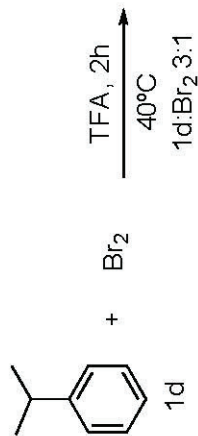
Acquired : 16 Jun 2014 20:05 using AcqMethod JMF60

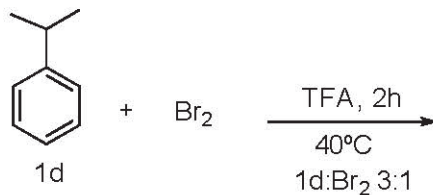
Instrument : Instrument

Sample Name: SIN TRATAR NaHCO3

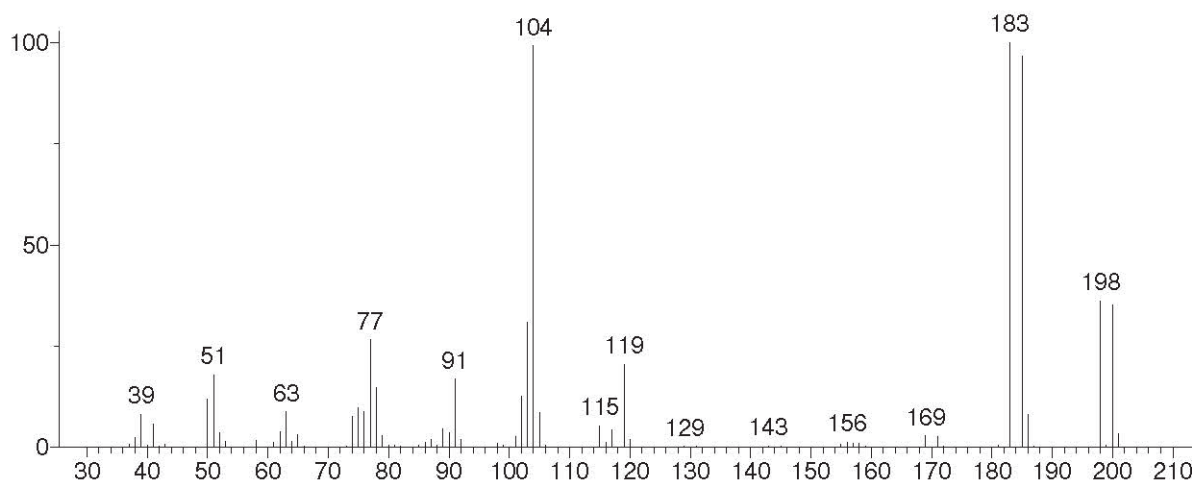
Misc Info :

Vial Number: 17

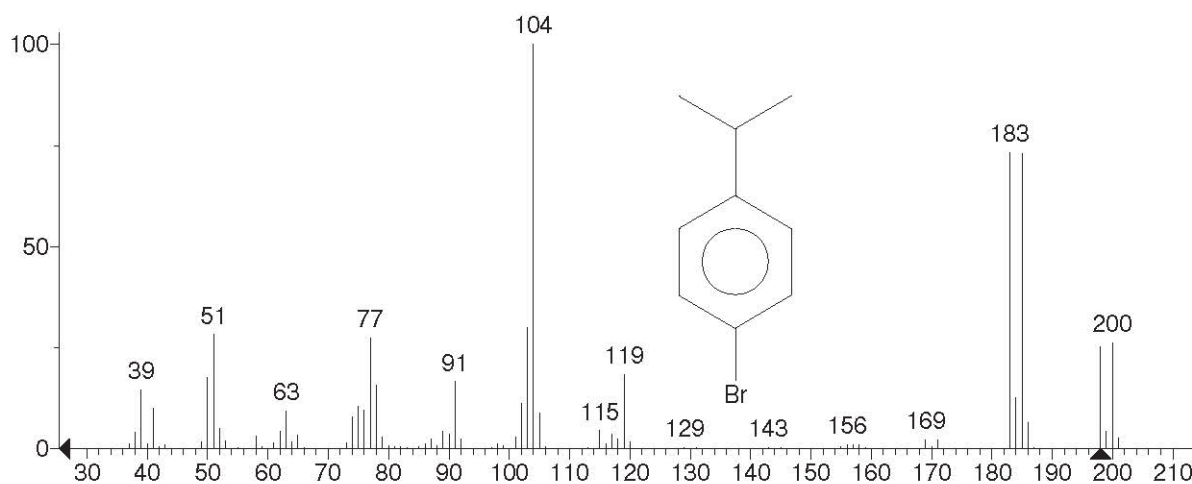




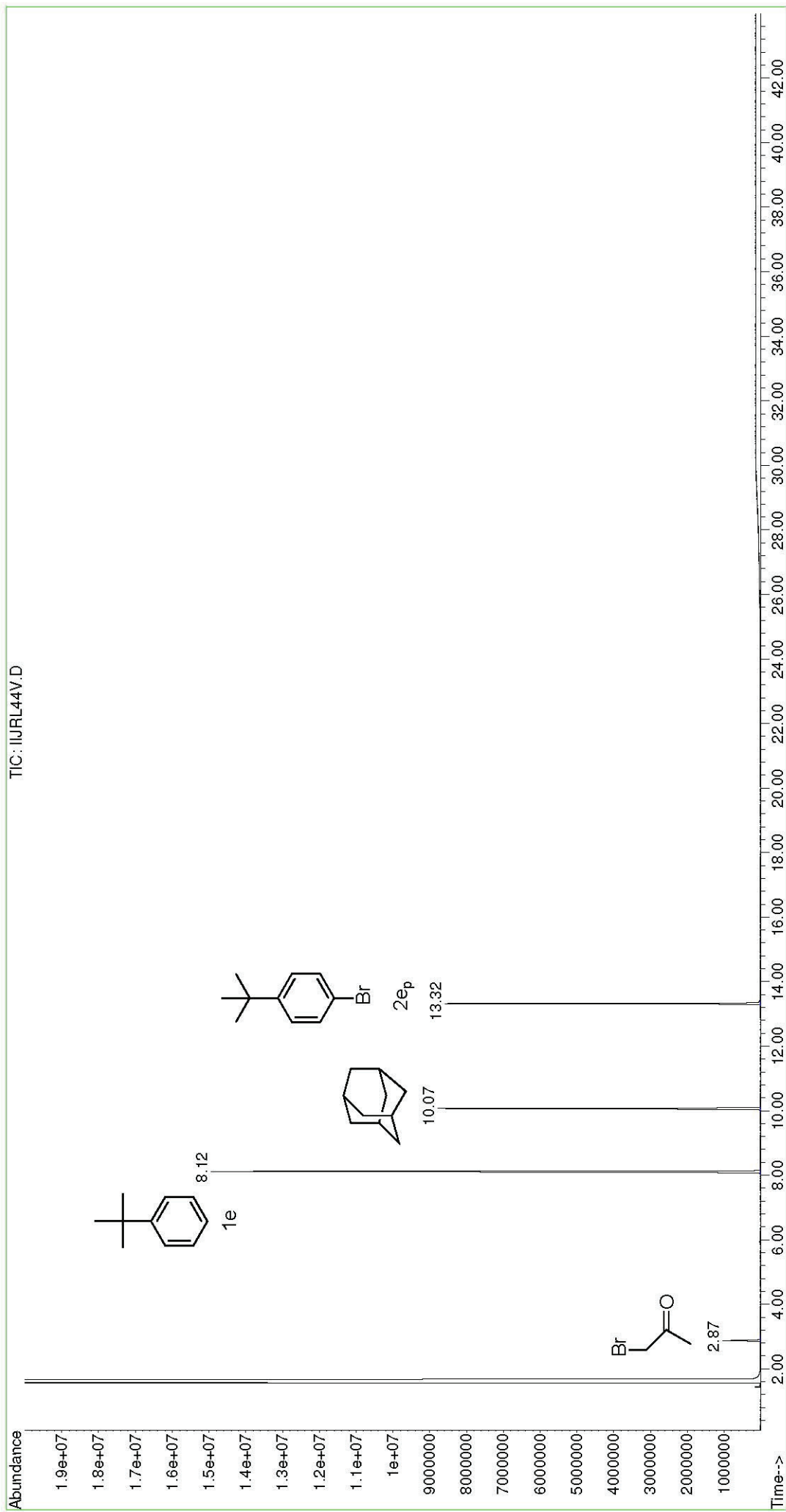
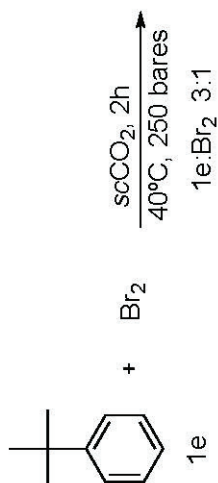
Unknown: Average of 12.231 to 12.268 min.: IIIJRL78.D
 Compound in Library Factor = 224



Hit 1 : Benzene, 1-bromo-4-(1-methylethyl)-
 C₉H₁₁Br; MF: 910; RMF: 911; Prob 62.7%; CAS: 586-61-8; Lib: mainlib; ID: 59111.



File : D:\ASENSIO\THAIS\IIJRL44V.D
Operator :
Acquired : 4 Dec 2013 23:09 using AcqMethod JMF60
Instrument : Instrumen
Sample Name: vidrio
Misc Info :
Vial Number: 15



File : D:\ASENSIO\THAIS\IIJRL44V.D

Operator :

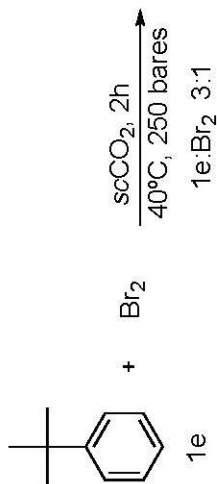
Acquired : 4 Dec 2013 23:09 using AcqMethod JMF60

Instrument : Instrument

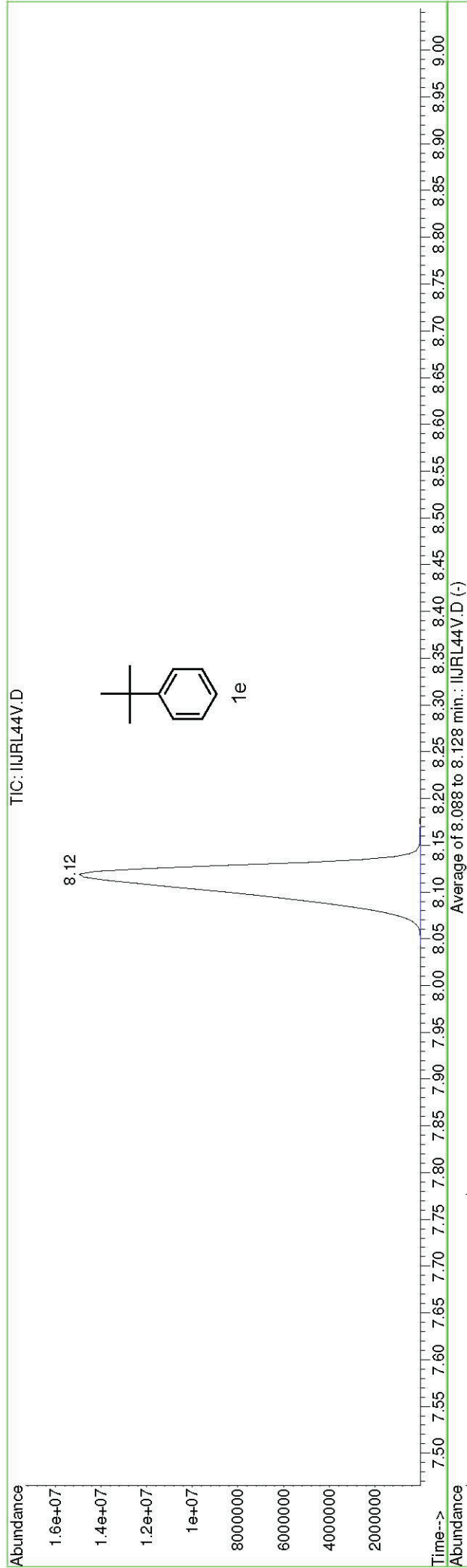
Sample Name: vidrio

Misc Info :

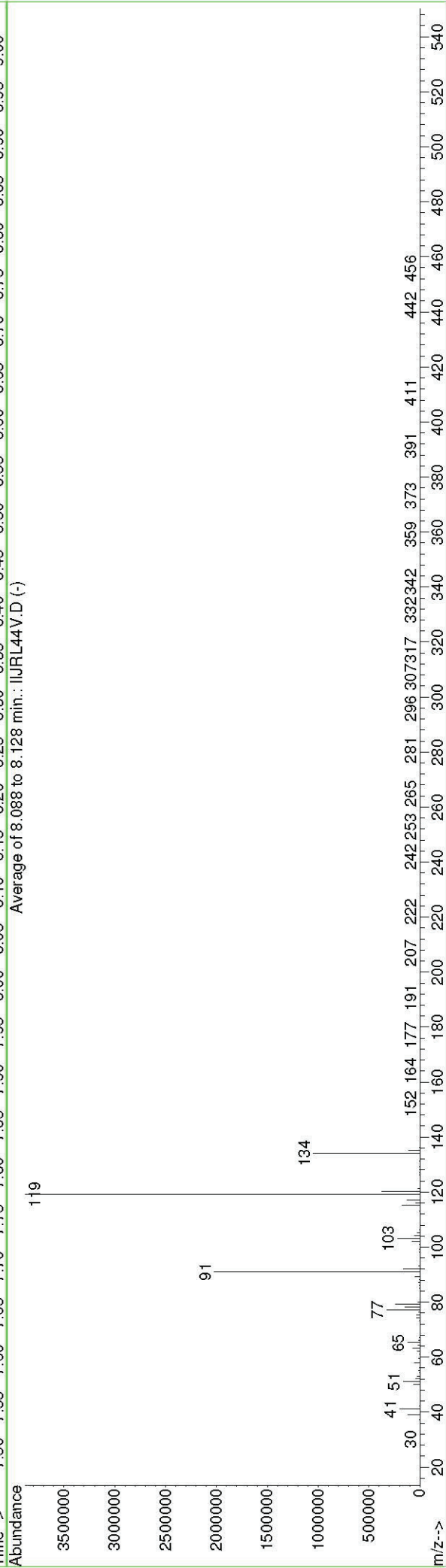
Vial Number: 15

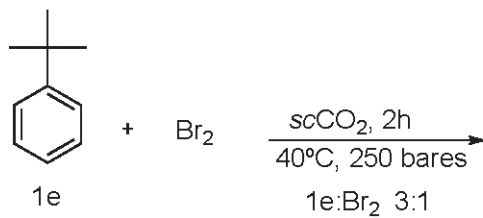


TIC: IIJRL44V.D

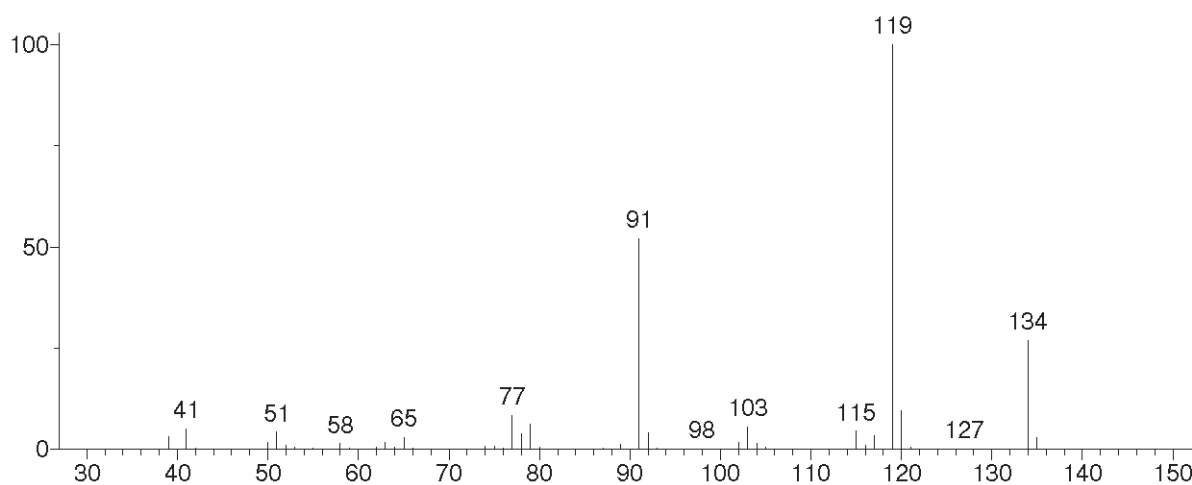


Average of 8.088 to 8.128 min.: IIJRL44V.D (-)

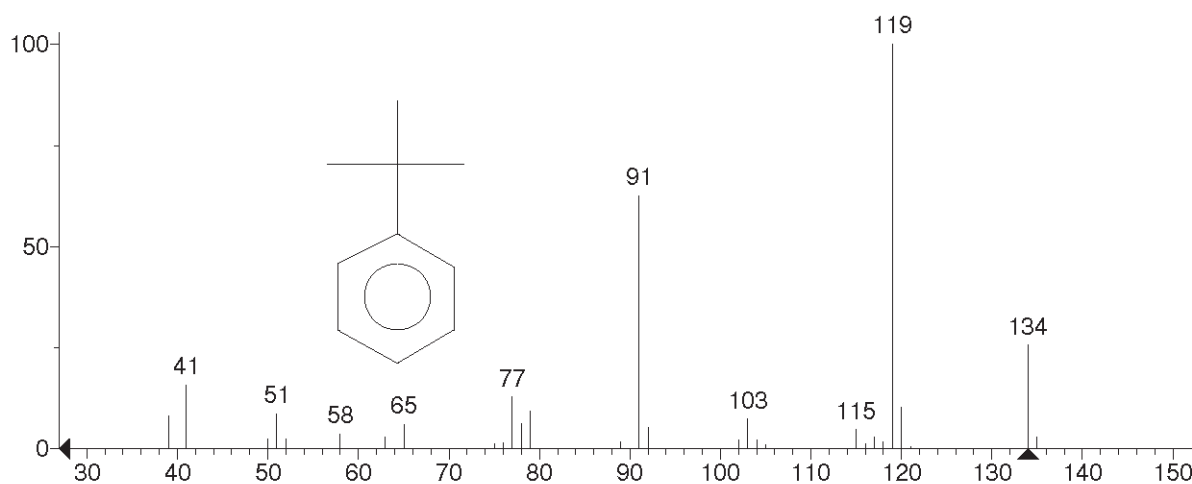




Unknown: Average of 8.088 to 8.128 min.: IJRL44V.D
Compound in Library Factor = 109



Hit 1 : Benzene, (1,1-dimethylethyl)- (CAS)
C₁₀H₁₄; MF: 930; RMF: 936; Prob 37.3%; CAS: 98-06-6; Lib: wiley7n; ID: 29747.



File : D:\ASENSIO\THAIS\IIJRL44V.D

Operator :

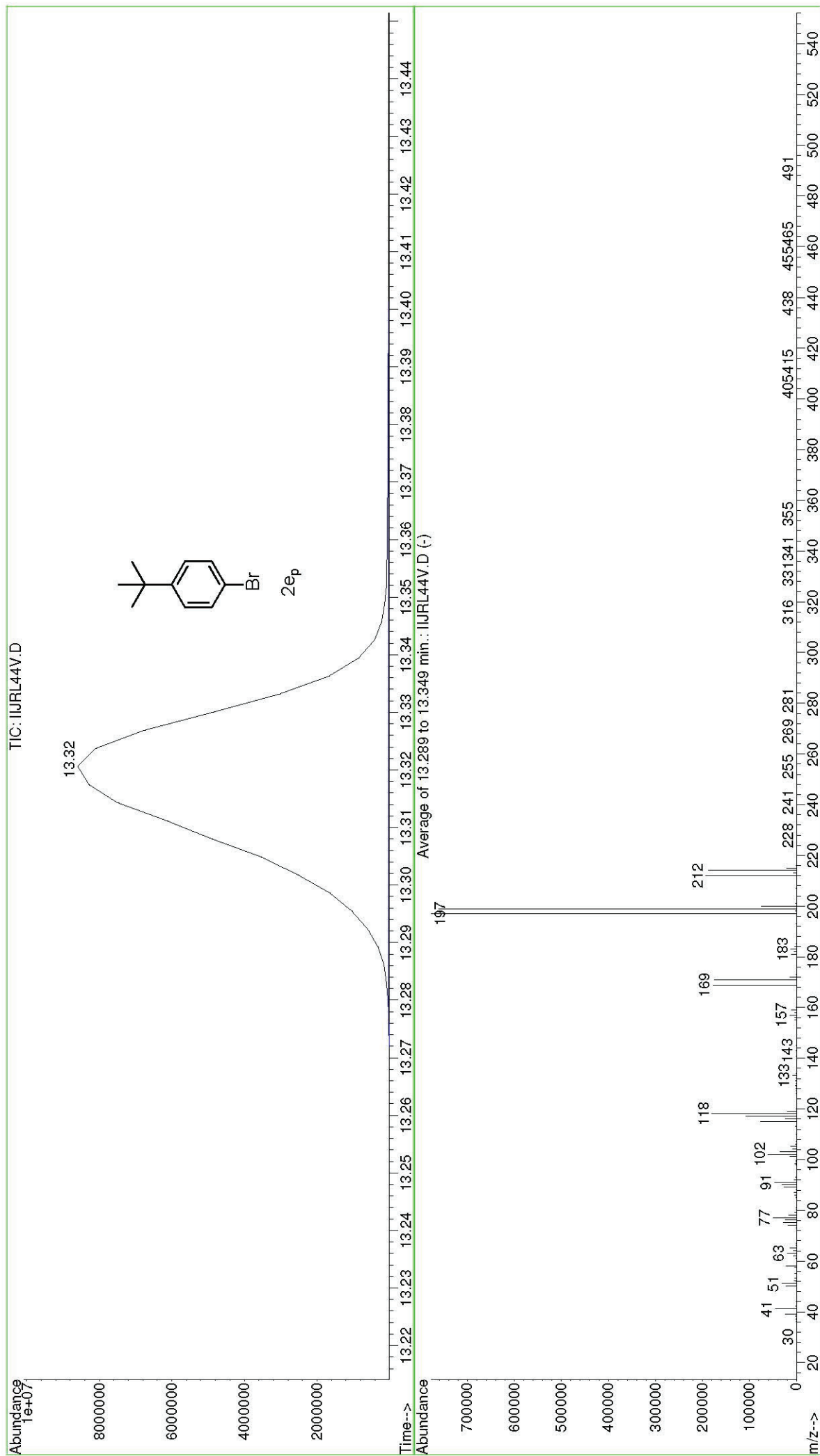
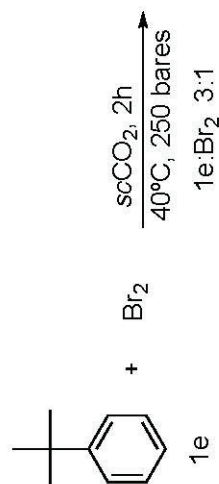
Acquired : 4 Dec 2013 23:09 using AcqMethod JMF60

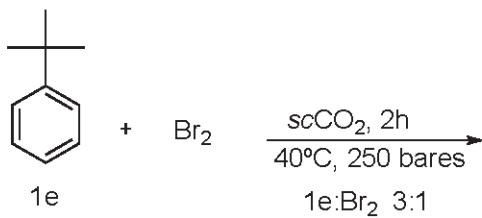
Instrument : Instrument

Sample Name: vidrio

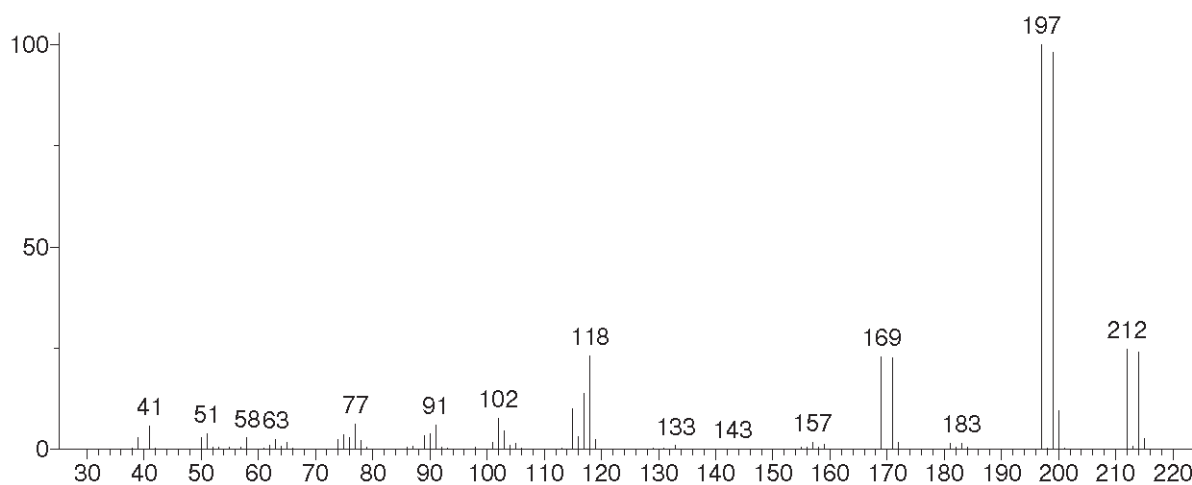
Misc Info :

Vial Number: 15

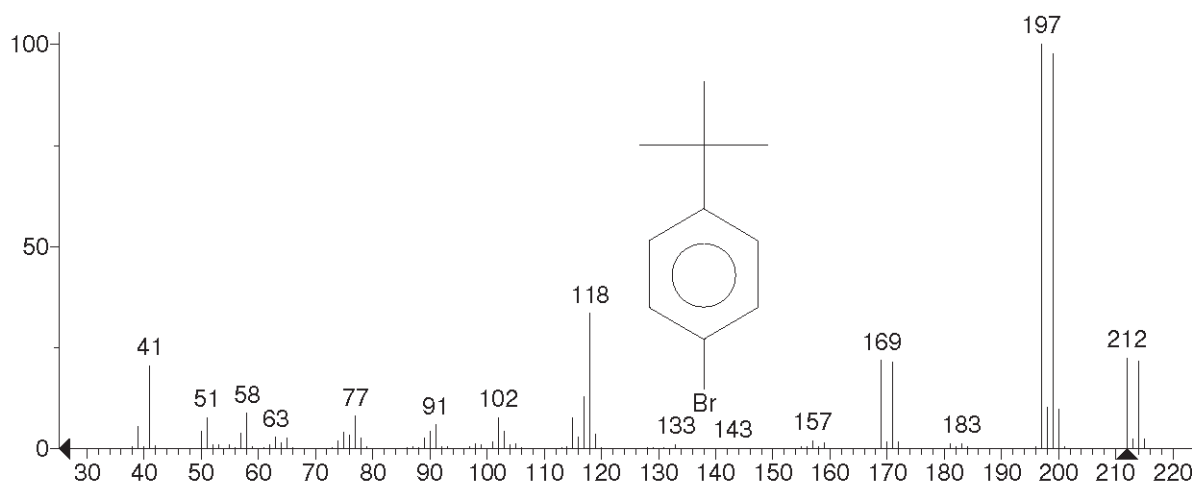




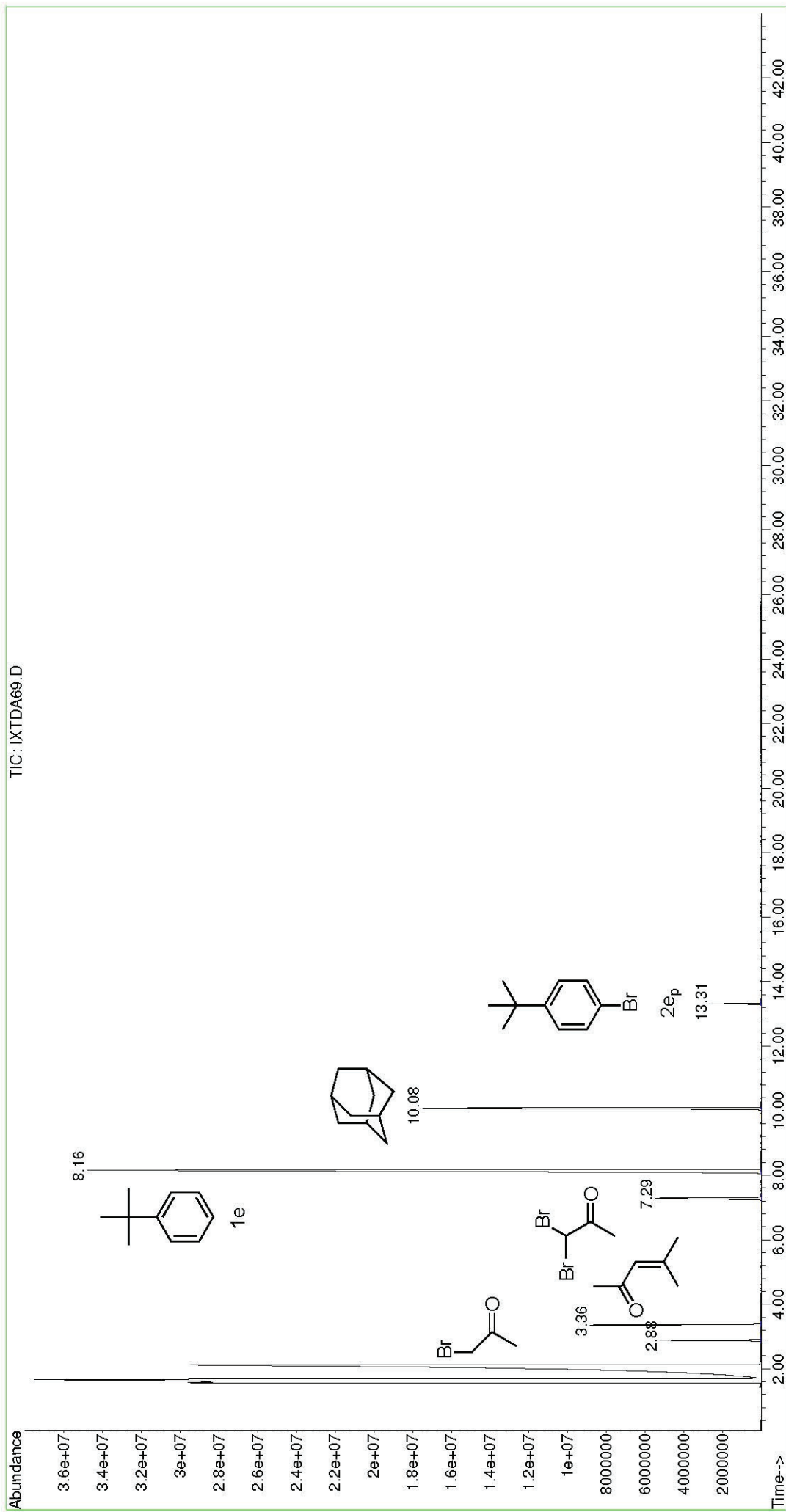
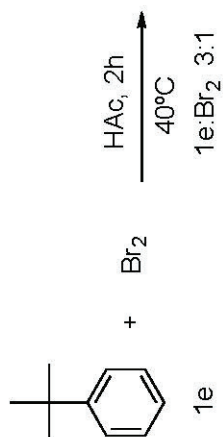
Unknown: Average of 13.289 to 13.349 min.: IJRL44V.D
Compound in Library Factor = 137



Hit 1 : Benzene, 1-bromo-4-(1,1-dimethylethyl)-
C₁₀H₁₃Br; MF: 898; RMF: 898; Prob 51.0%; CAS: 3972-65-4; Lib: mainlib; ID: 122816.



File : D:\ASENSIO\THAIS\IXTDA69.D
Operator :
Acquired : 4 Dec 2013 15:34 using AcqMethod JMF60
Instrument : Instrument
Sample Name: t-but
Misc Info :
Vial Number: 6



File : D:\ASENSIO\THAIS\IXTDA69.D

Operator :

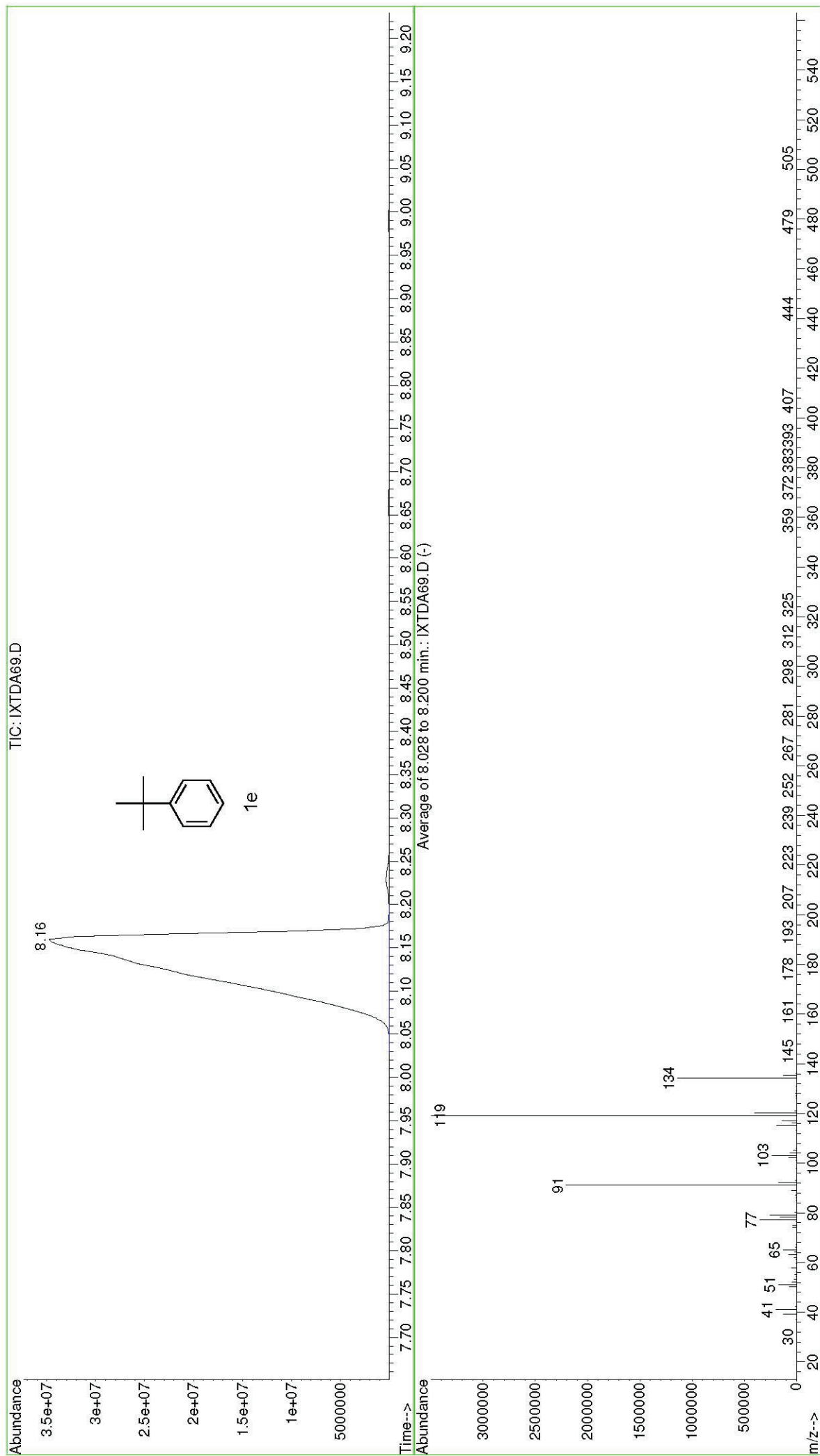
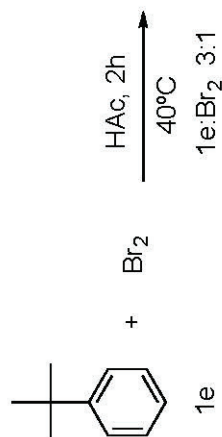
Acquired : 4 Dec 2013 15:34 using AcqMethod JMF60

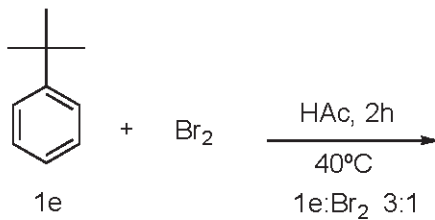
Instrument : Instrument

Sample Name: t-but

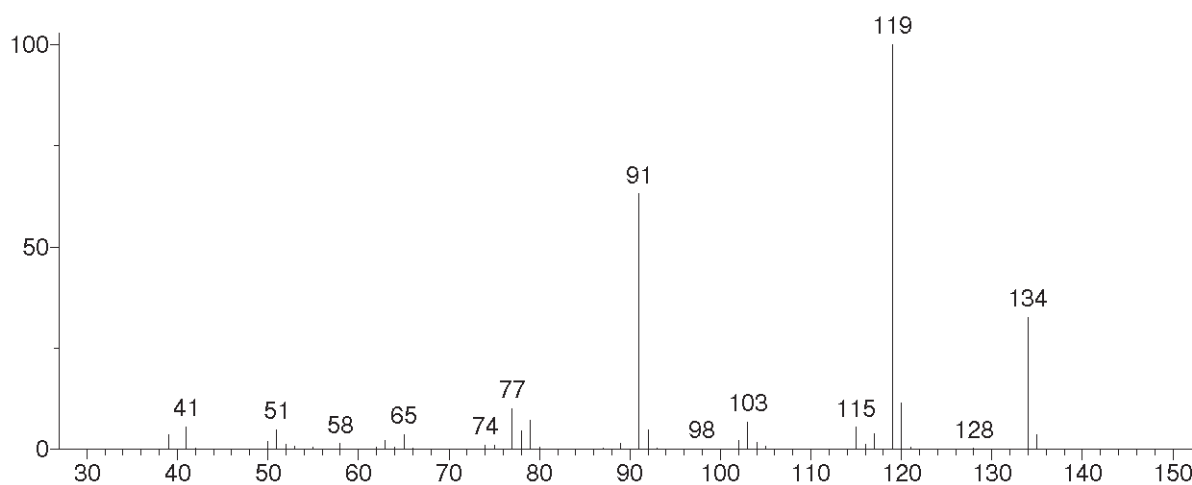
Misc Info :

Vial Number: 6

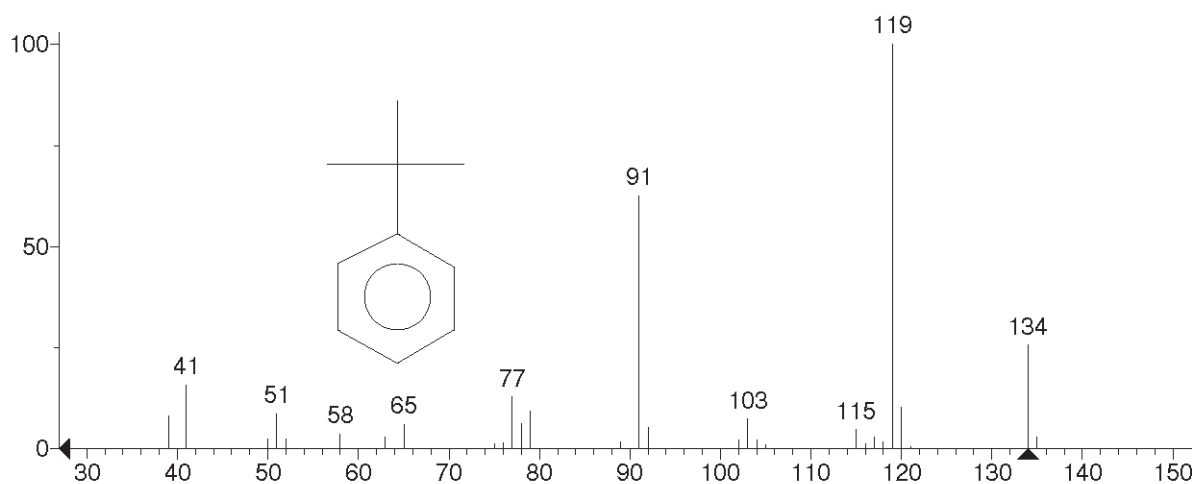




Unknown: Average of 8.028 to 8.200 min.: IXTDA69.D
Compound in Library Factor = 109



Hit 1 : Benzene, (1,1-dimethylethyl)- (CAS)
C₁₀H₁₄; MF: 924; RMF: 930; Prob 40.1%; CAS: 98-06-6; Lib: wiley7n; ID: 29747.



File : D:\ASENSIO\THAIS\IXTDA69.D

Operator :

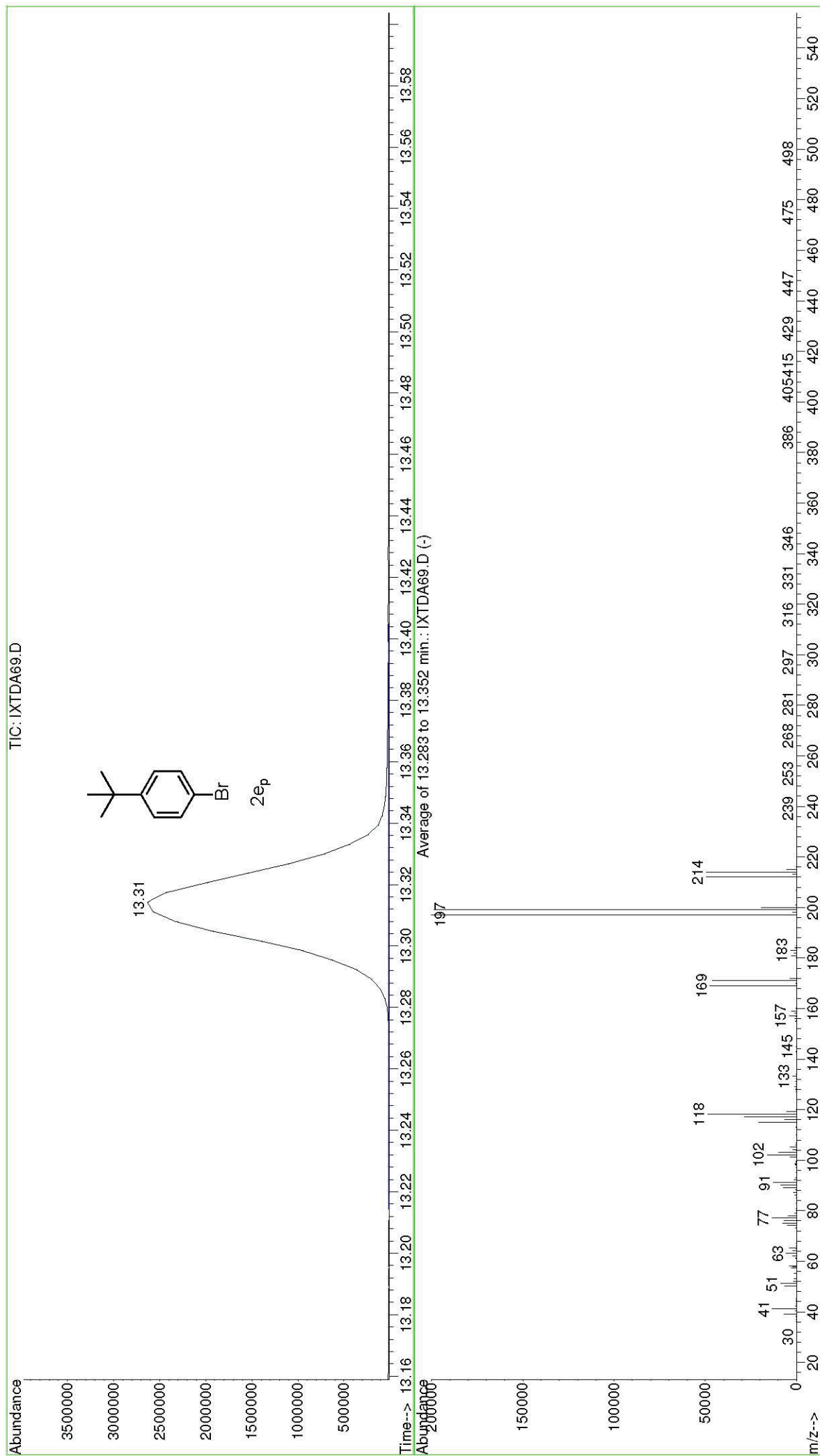
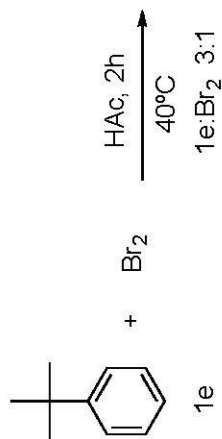
Acquired : 4 Dec 2013 15:34 using AcqMethod JMF60

Instrument : Instrument

Sample Name: t-but

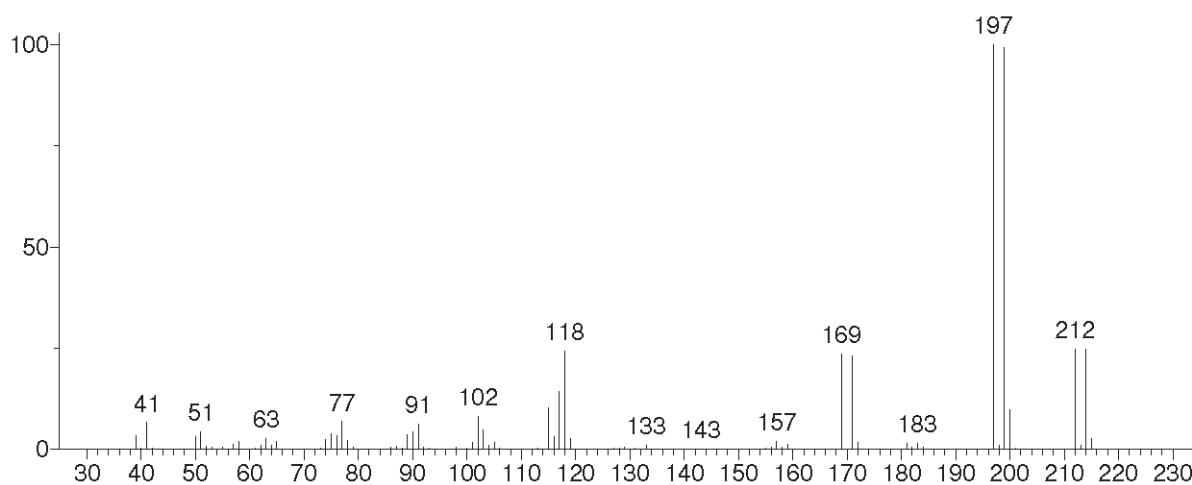
Misc Info :

Vial Number: 6

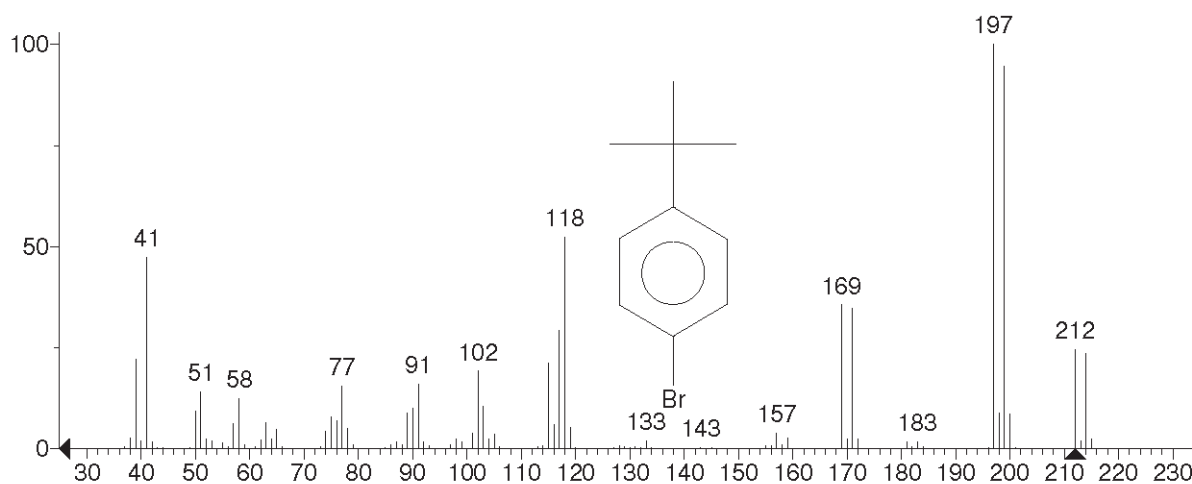




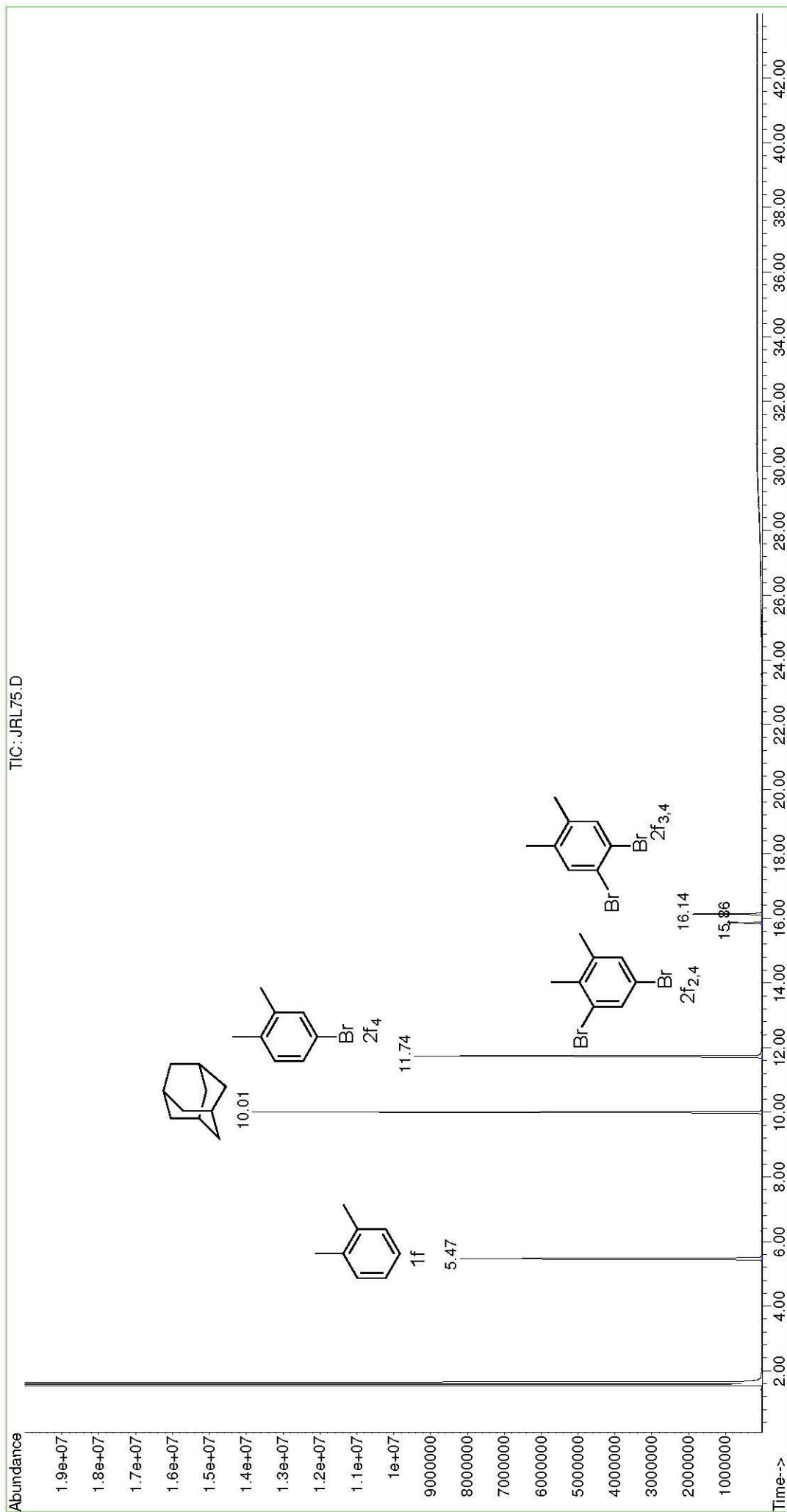
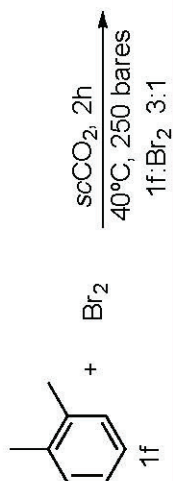
Unknown: Average of 13.283 to 13.352 min.: IXDA69.D
 Compound in Library Factor = 137



Hit 1 : Benzene, 1-bromo-4-(1,1-dimethylethyl)-
 C₁₀H₁₃Br; MF: 899; RMF: 899; Prob 47.9%; CAS: 3972-65-4; Lib: wiley7n; ID: 132463.



File : C:\MSDCHEM\1\DATA\ISABEL\JRL75.D
Operator :
Acquired : 21 Jan 2014 21:47 using AcqMethod JMF60
Instrument : Instrumen
Sample Name: VIDRIO
Misc Info :
Vial Number: 18



File : C:\MSDCHEM\1\DATA\ISABEL\JRL75.D

Operator :

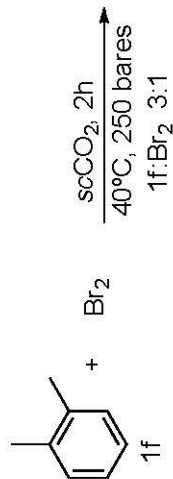
Acquired : 21 Jan 2014 21:47 using AcqMethod JMF60

Instrument : Instrument

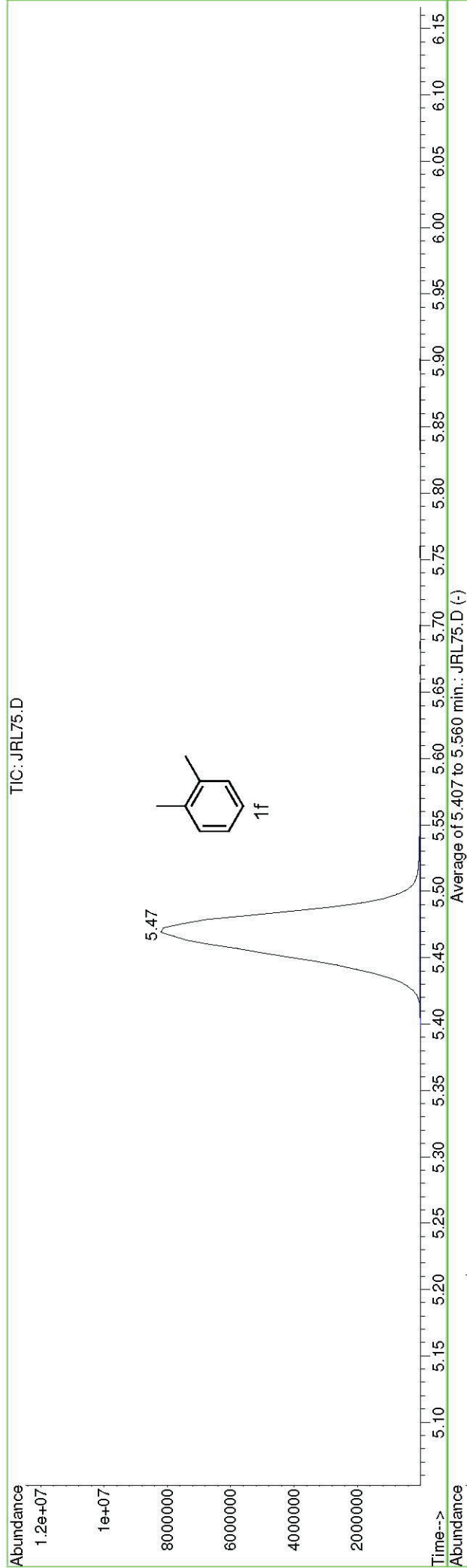
Sample Name: VIDRIO

Misc Info :

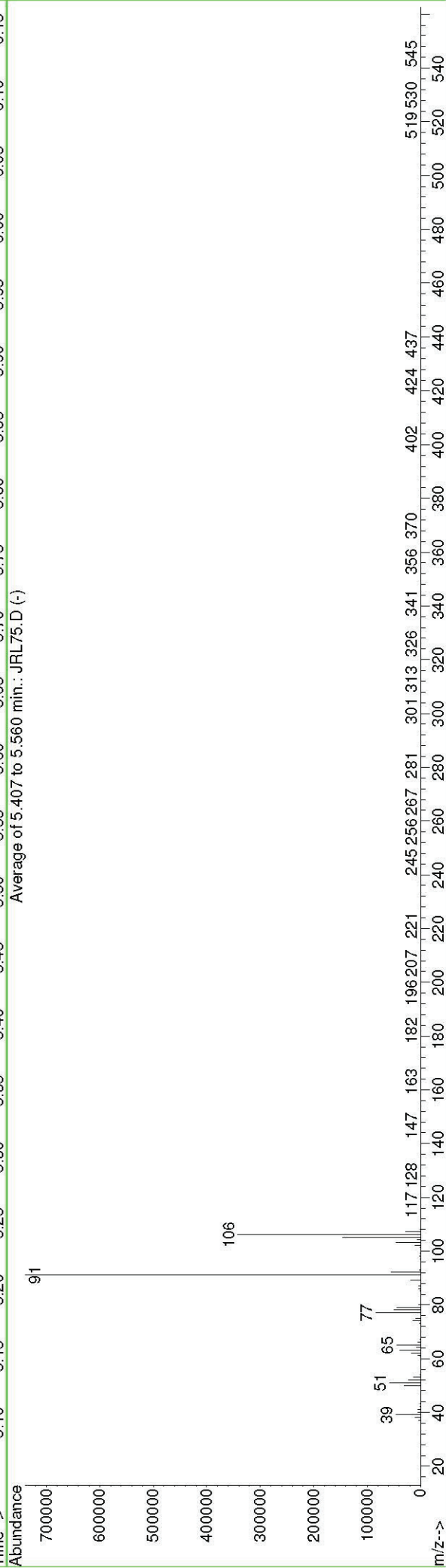
Vial Number: 18

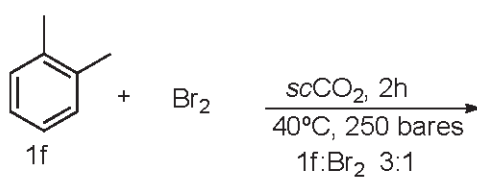


TIC: JRL75.D



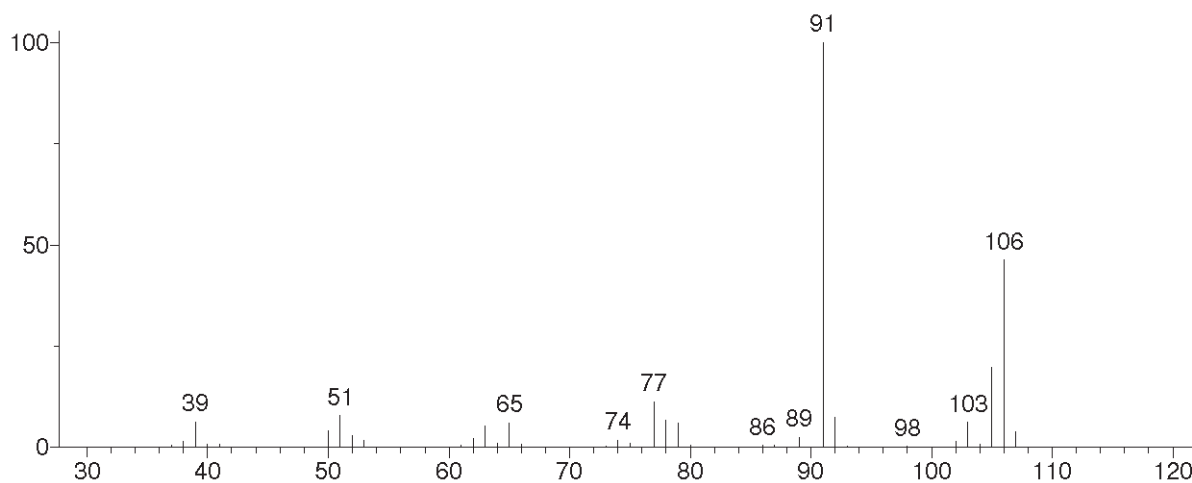
Average of 5.407 to 5.560 min.: JRL75.D (-)





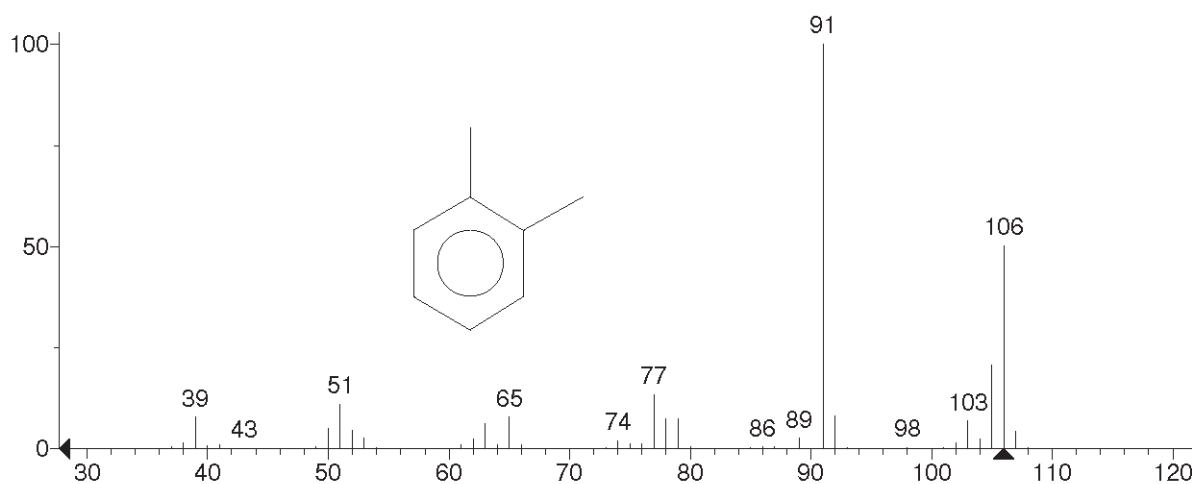
** Search Report Page 1 of 1 **

Unknown: Average of 5.407 to 5.560 min.: JRL75.D
Compound in Library Factor = 165



Hit 1 : o-Xylene

C₈H₁₀; MF: 944; RMF: 944; Prob 24.3%; CAS: 95-47-6; Lib: replib; ID: 11414.



File : C:\MSDCHEM\1\DATA\ISABEL\JRL75.D

Operator :

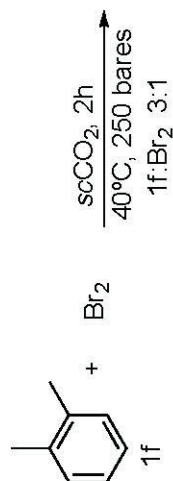
Acquired : 21 Jan 2014 21:47 using AcqMethod JMF60

Instrument : Instrument

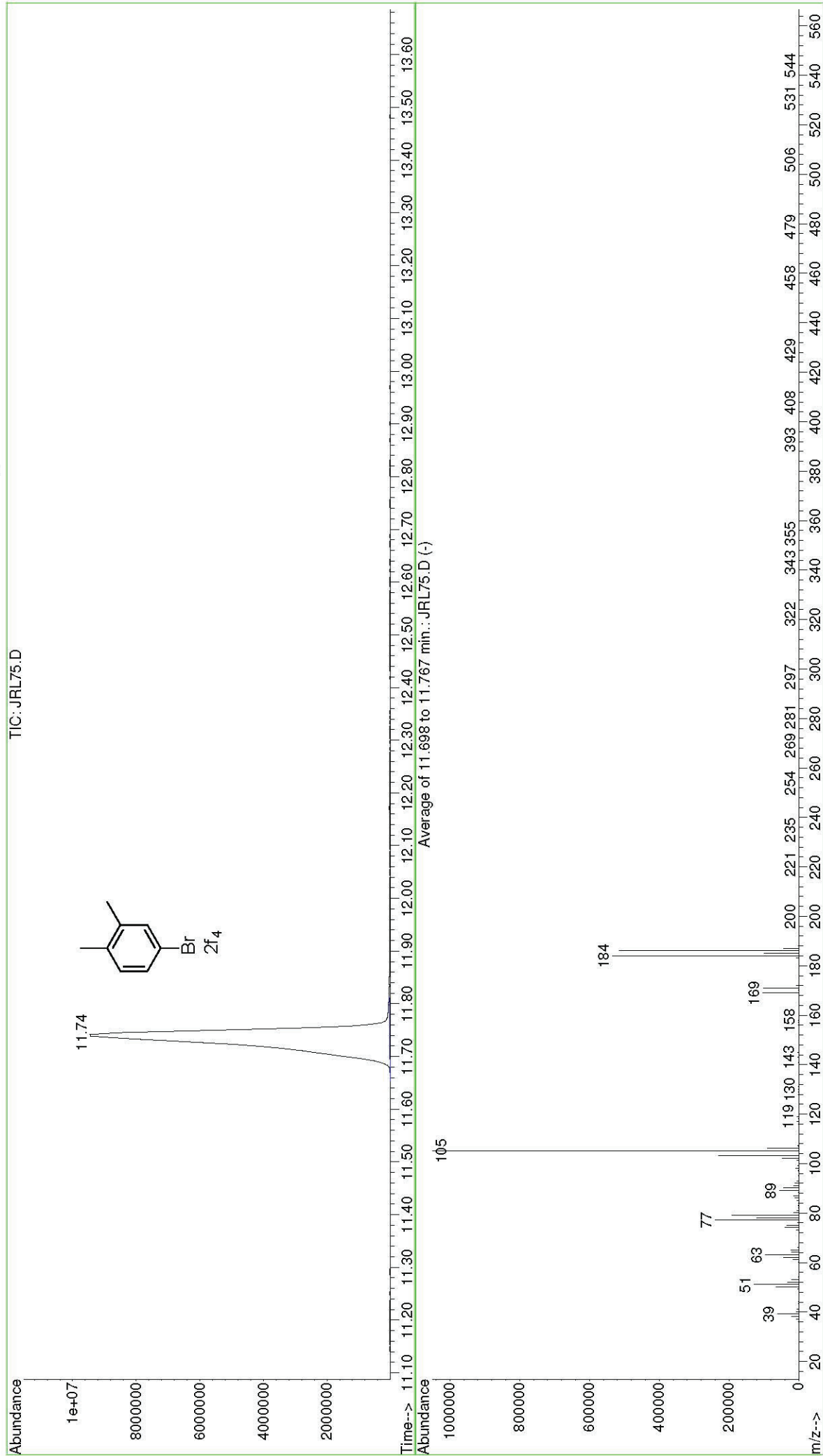
Sample Name : VIDRIO

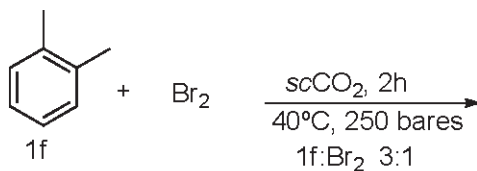
Misc Info :

Vial Number: 18



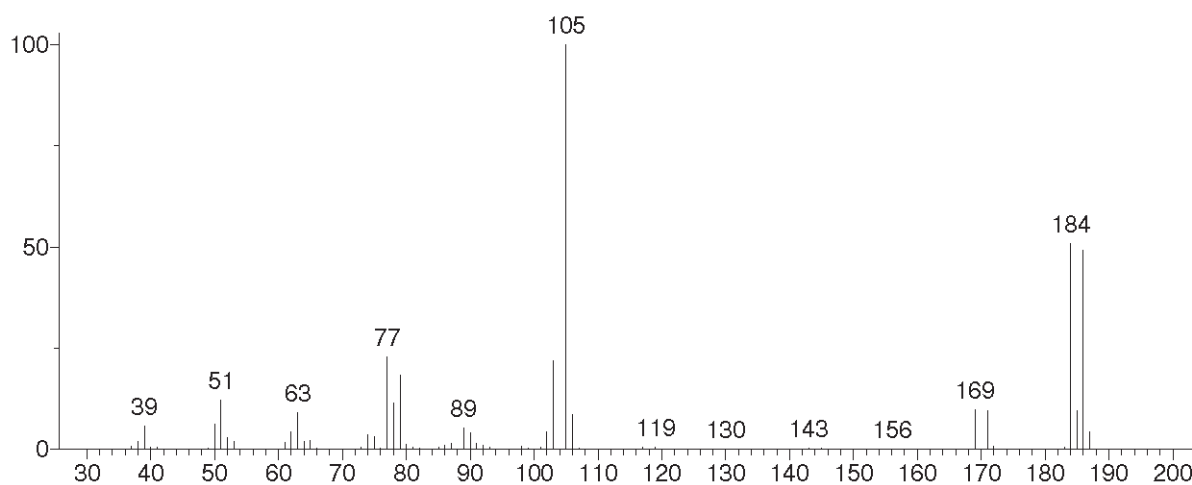
TIC: JRL75.D



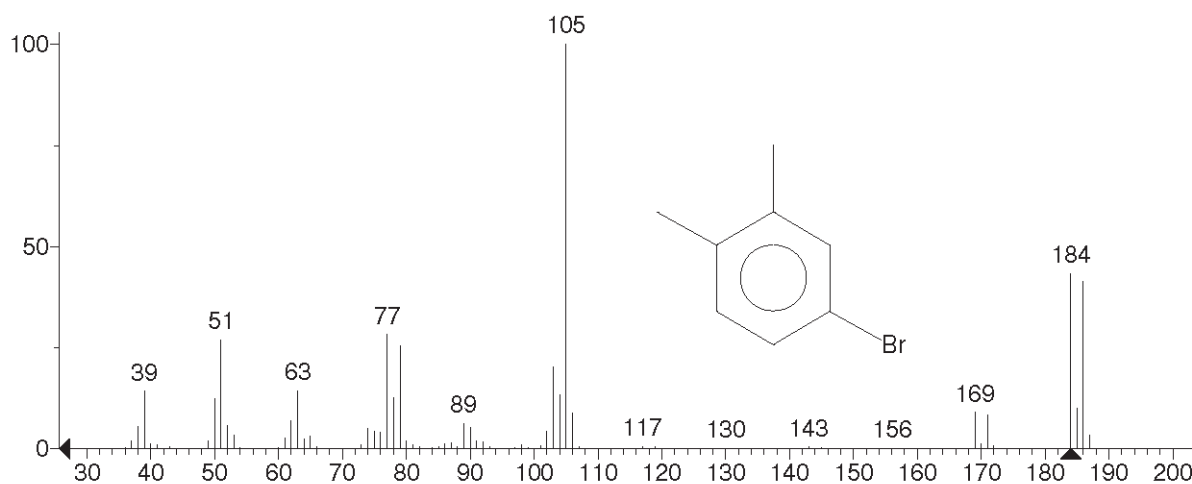


** Search Report Page 1 of 1 **

Unknown: Average of 11.698 to 11.767 min.: JRL75.D
Compound in Library Factor = 167



Hit 1 : Benzene, 4-bromo-1,2-dimethyl-
C₈H₉Br; MF: 913; RMF: 914; Prob 30.9%; CAS: 583-71-1; Lib: mainlib; ID: 62076.



File : C:\MSDCHEM\1\DATA\ISABEL\JRL75.D

Operator :

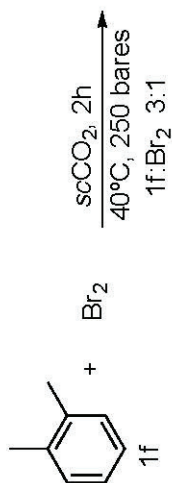
Acquired : 21 Jan 2014 21:47 using AcqMethod JMF60

Instrument : Instrument

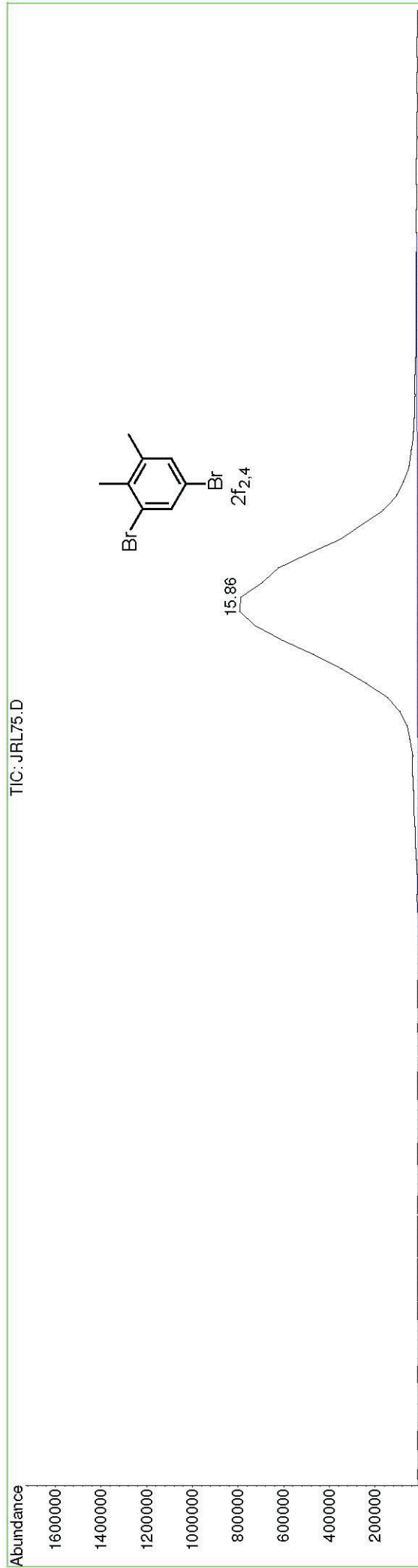
Sample Name: VIDRIO

Misc Info :

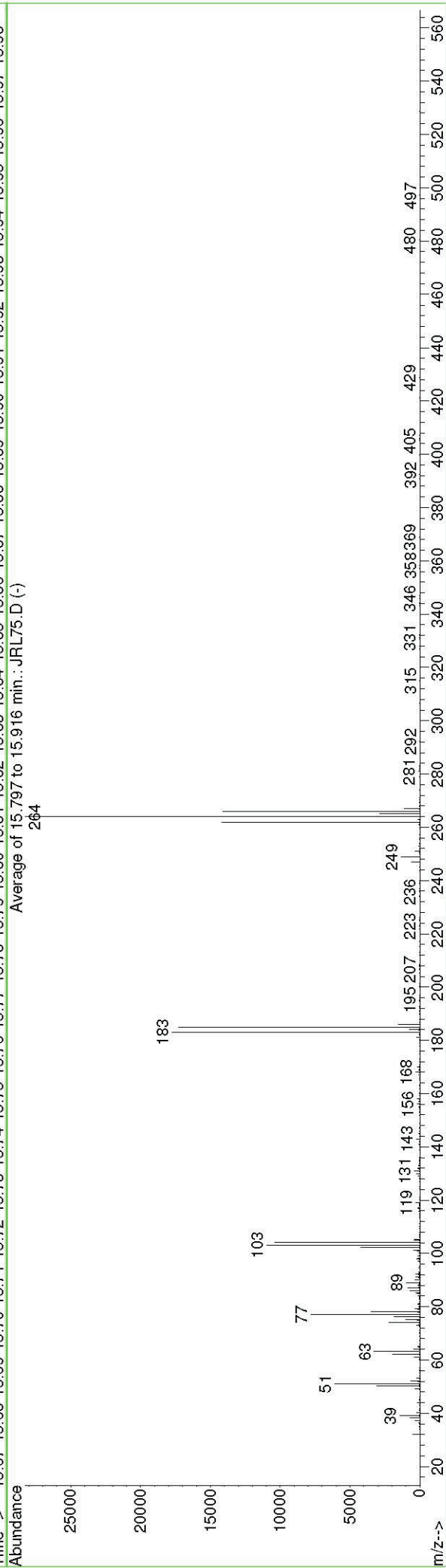
Vial Number: 18

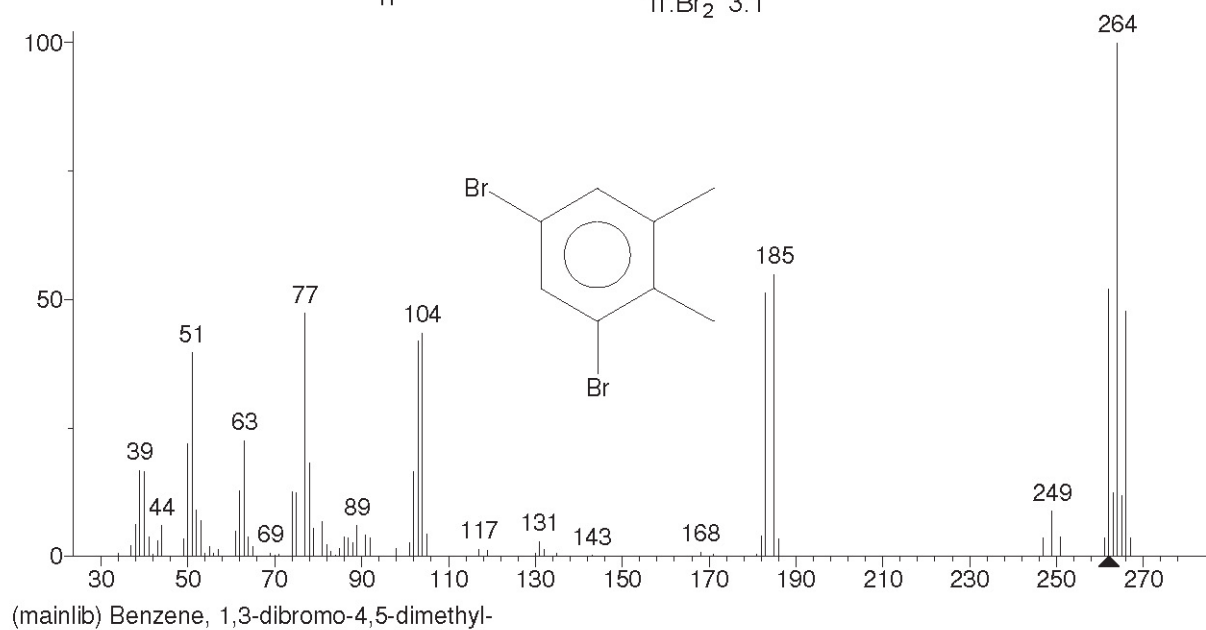
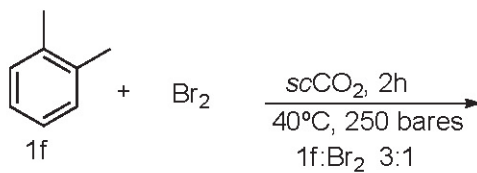


TIC: JRL75.D



Average of 15.797 to 15.916 min.: JRL75.D (-)





(mainlib) Benzene, 1,3-dibromo-4,5-dimethyl-

File : C:\MSDCHEM\1\DATA\ISABEL\JRL75.D

Operator :

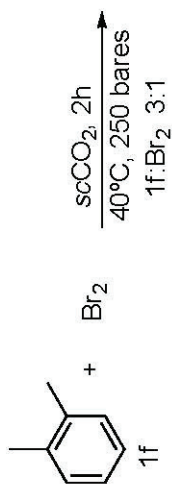
Acquired : 21 Jan 2014 21:47 using AcqMethod JMF60

Instrument : Instrument

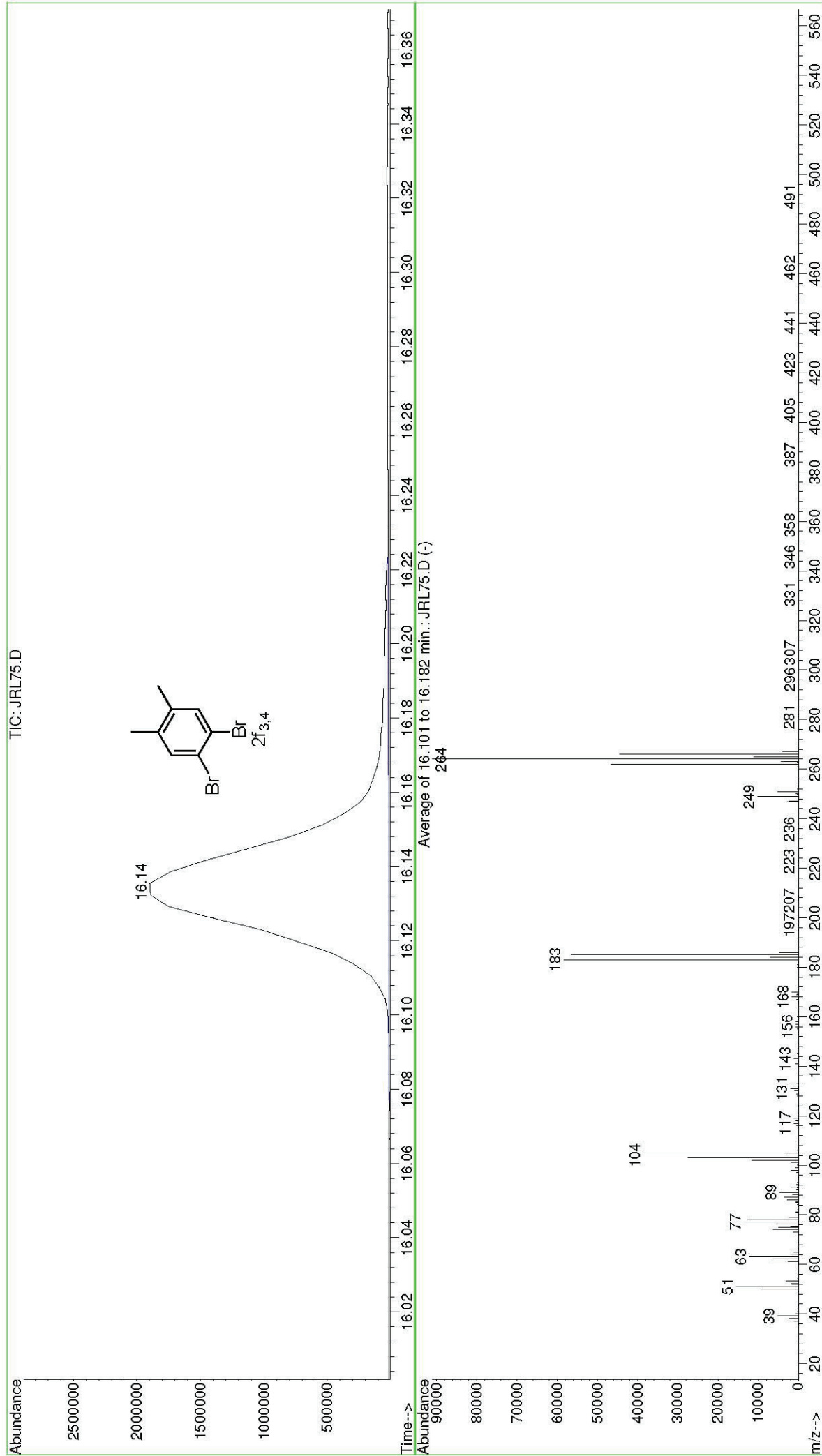
Sample Name: VIDRIO

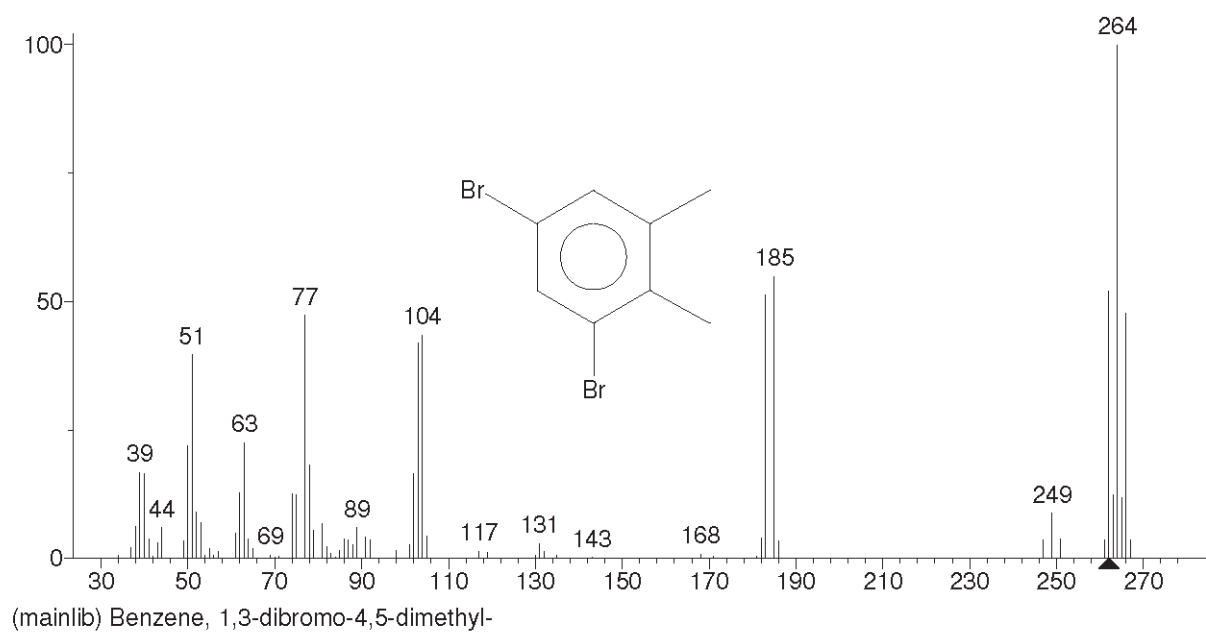
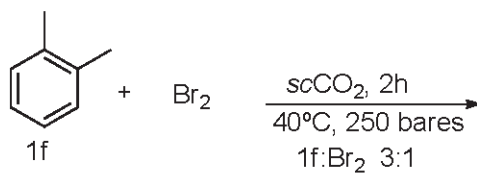
Misc Info :

Vial Number: 18

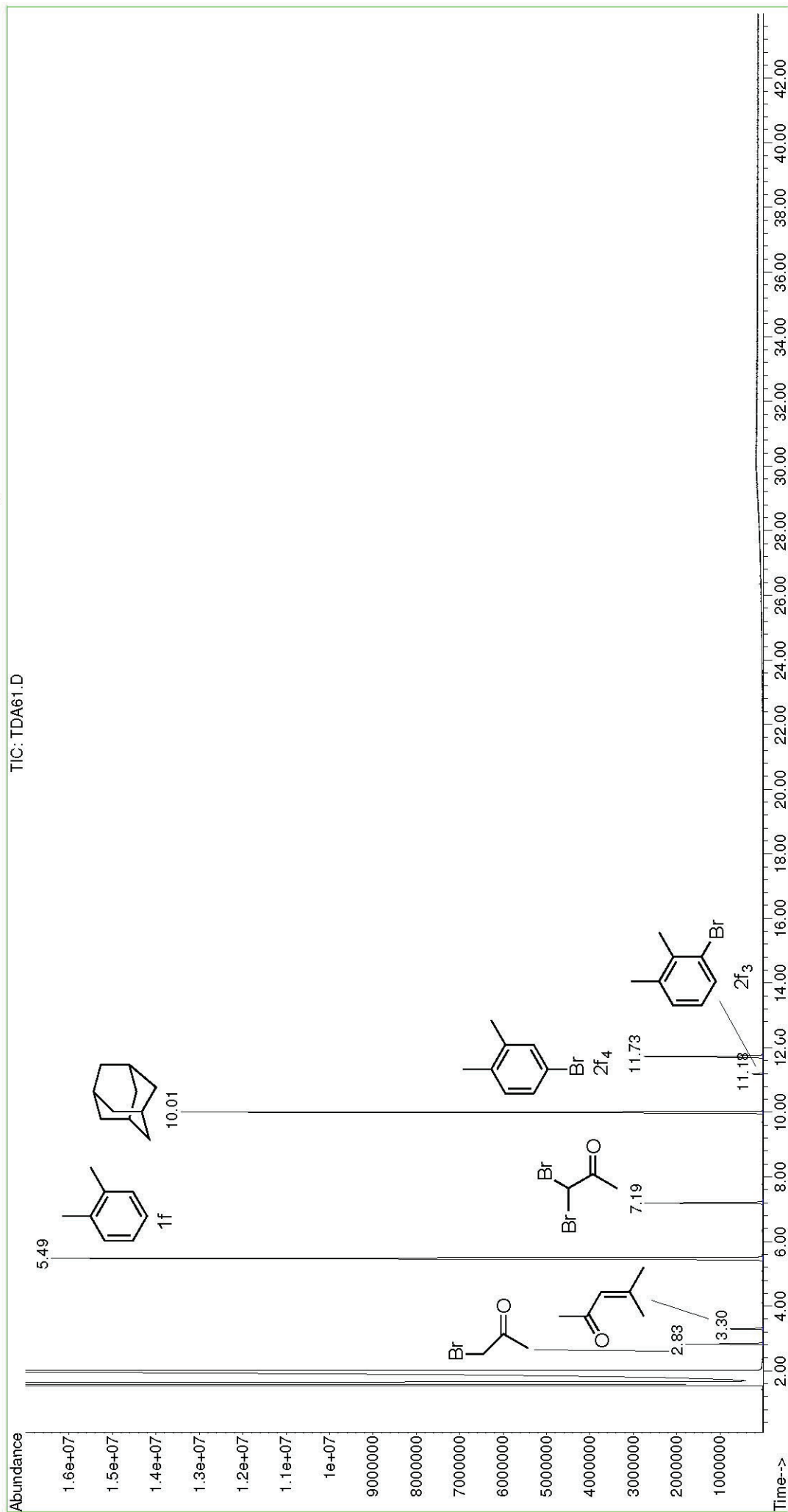
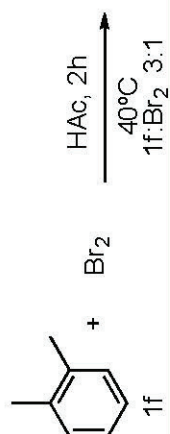


TIC: JRL75.D

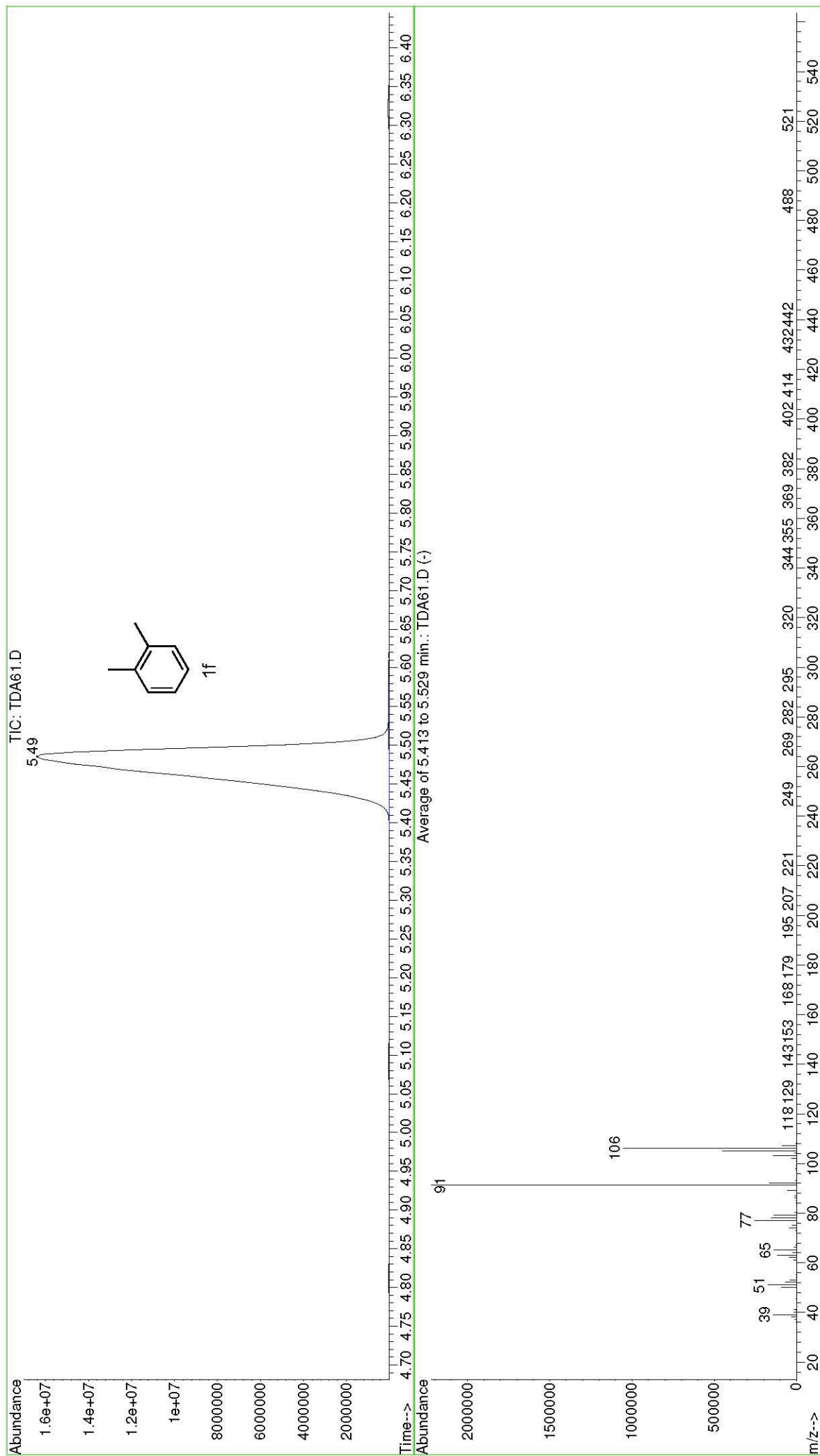
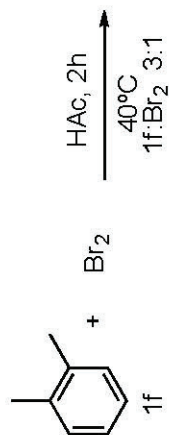


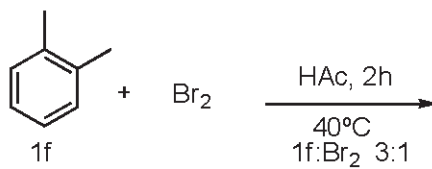


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File      : D:\ASENSIO\THAIS\TDA61.D
Operator  :
Acquired  : 23 Jan 2014 17:17 using AcqMethod JMF60
Instrument : Instrumen
Sample Name : O-XYLENO
Misc Info  :
Vial Number : 10
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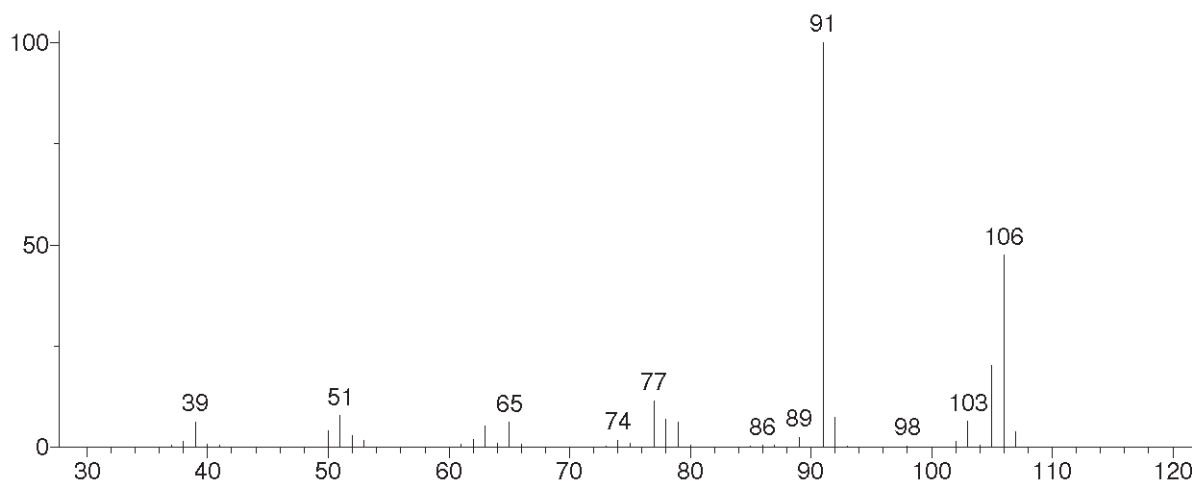
File : D:\ASENSIO\THAIS\TDA61.D
Operator :
Acquired : 23 Jan 2014 17:17 using AcqMethod JMF60
Instrument : Instrument
Sample Name : O-XYLENO
Misc Info :
Vial Number: 10





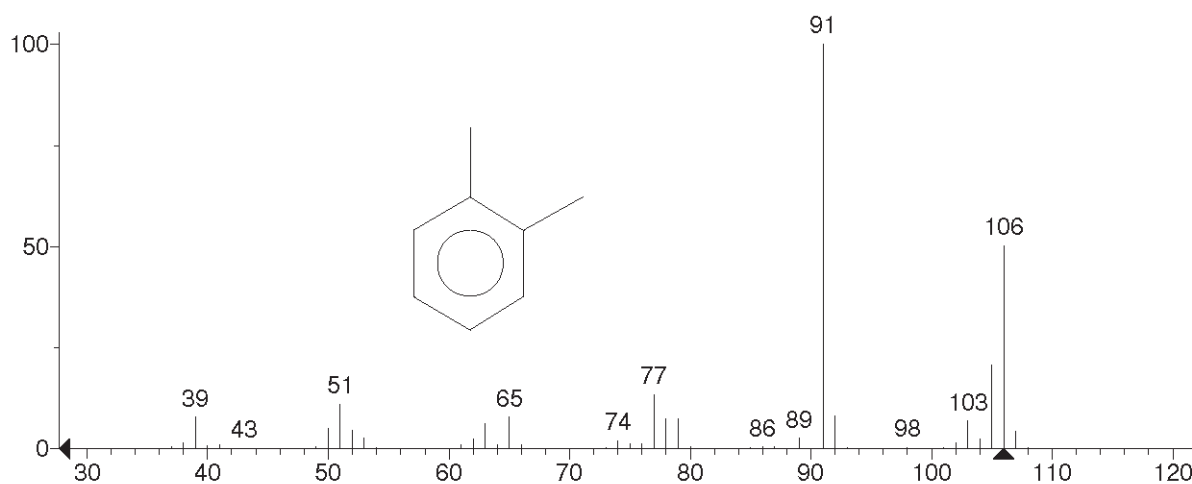
** Search Report Page 1 of 1 **

Unknown: Average of 5.413 to 5.529 min.: TDA61.D
Compound in Library Factor = 141



Hit 1 : o-Xylene

C₈H₁₀; MF: 944; RMF: 944; Prob 24.6%; CAS: 95-47-6; Lib: replib; ID: 11414.



File : D:\ASENSIO\THAIS\TDA61.D

Operator :

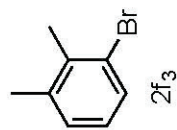
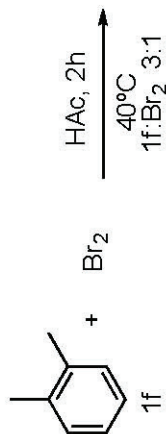
Acquired : 23 Jan 2014 17:17 using AcqMethod JMF60

Instrument : Instrument

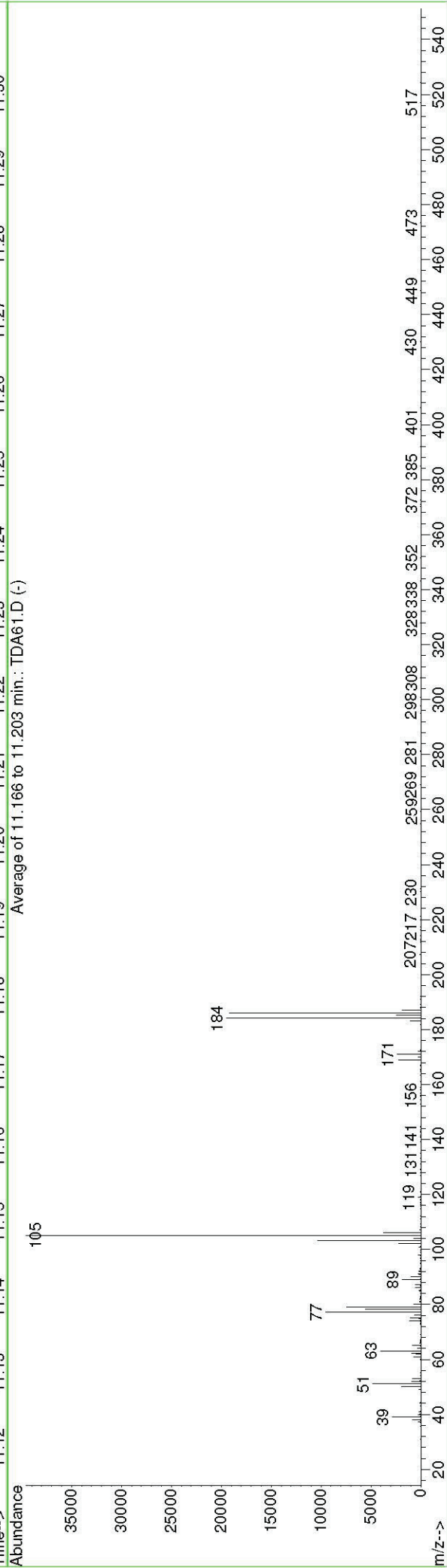
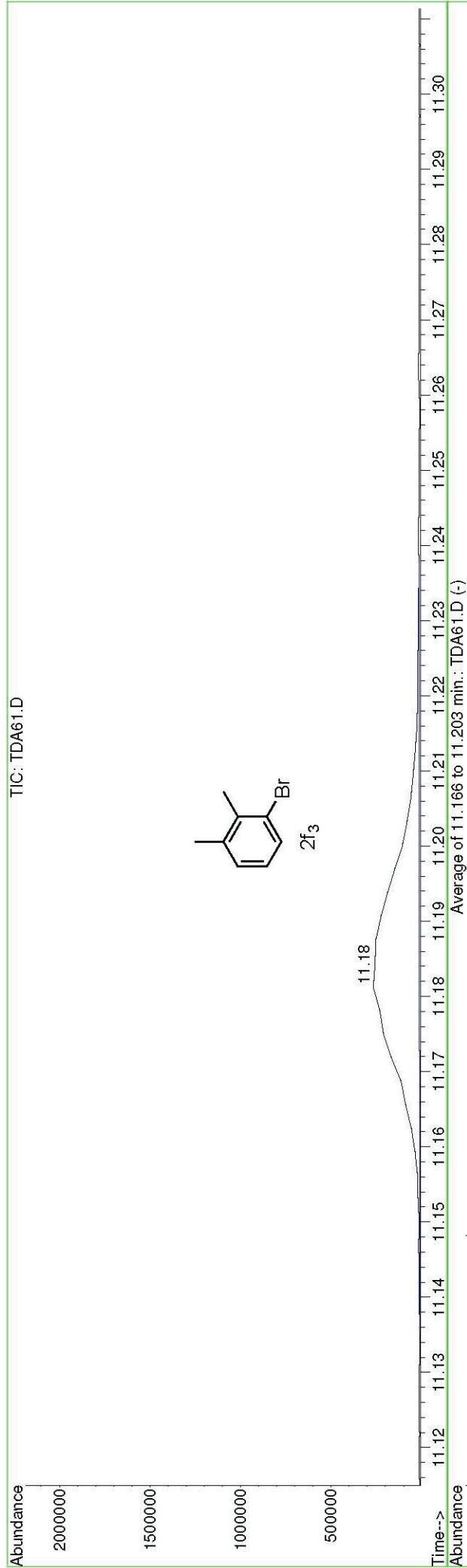
Sample Name : O-XYLENO

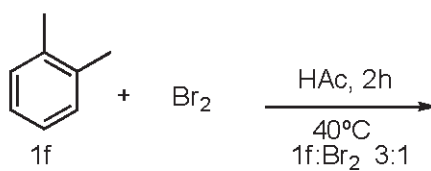
Misc Info :

Vial Number: 10



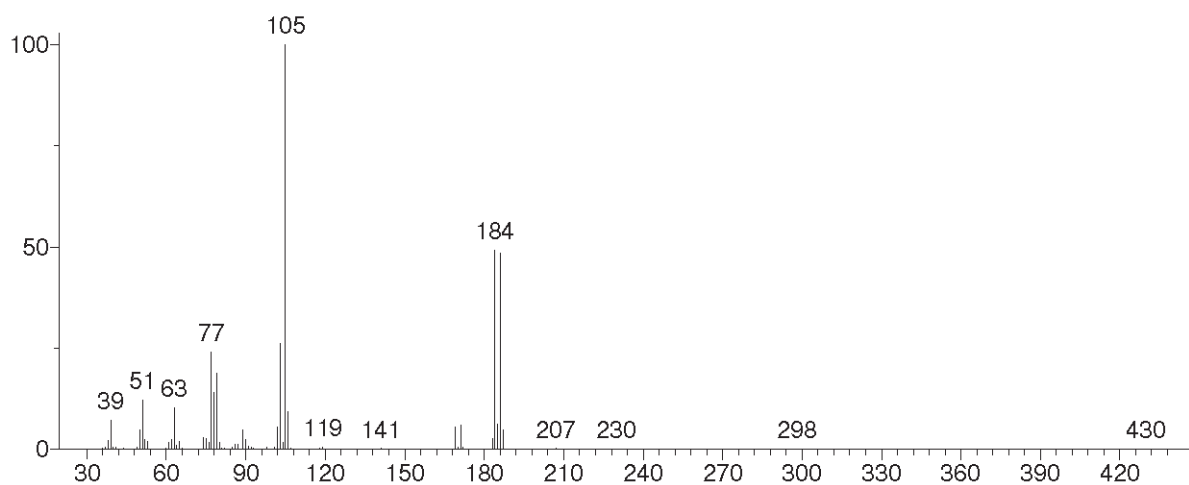
TIC: TDA61.D



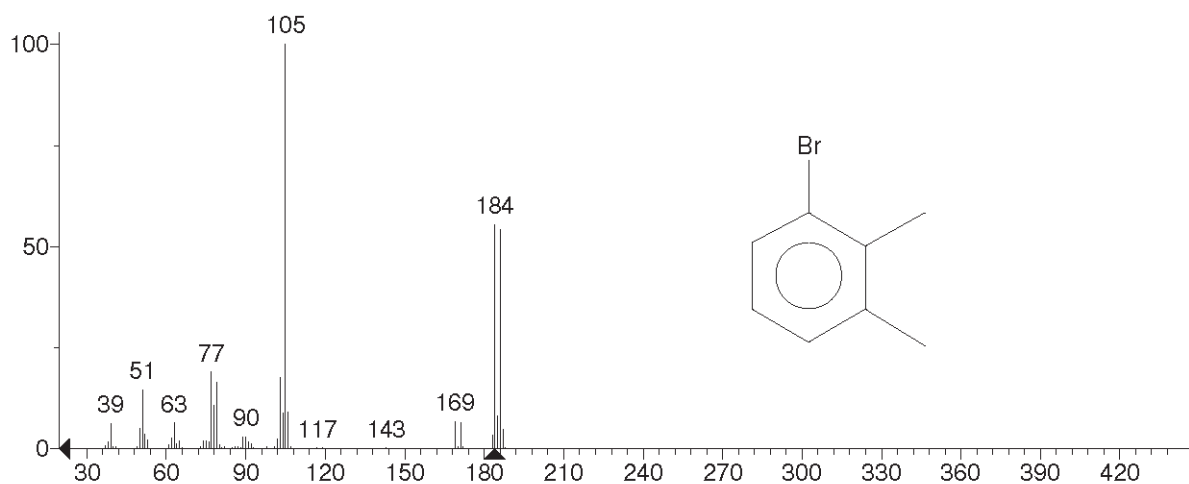


** Search Report Page 1 of 1 **

Unknown: Average of 11.166 to 11.203 min.: TDA61.D
Compound in Library Factor = 137



Hit 1 : Benzene, 1-bromo-2,3-dimethyl-
C₈H₉Br; MF: 892; RMF: 894; Prob 22.2%; CAS: 576-23-8; Lib: mainlib; ID: 62079.



File : D:\ASENSIO\THAIS\TDA61.D

Operator :

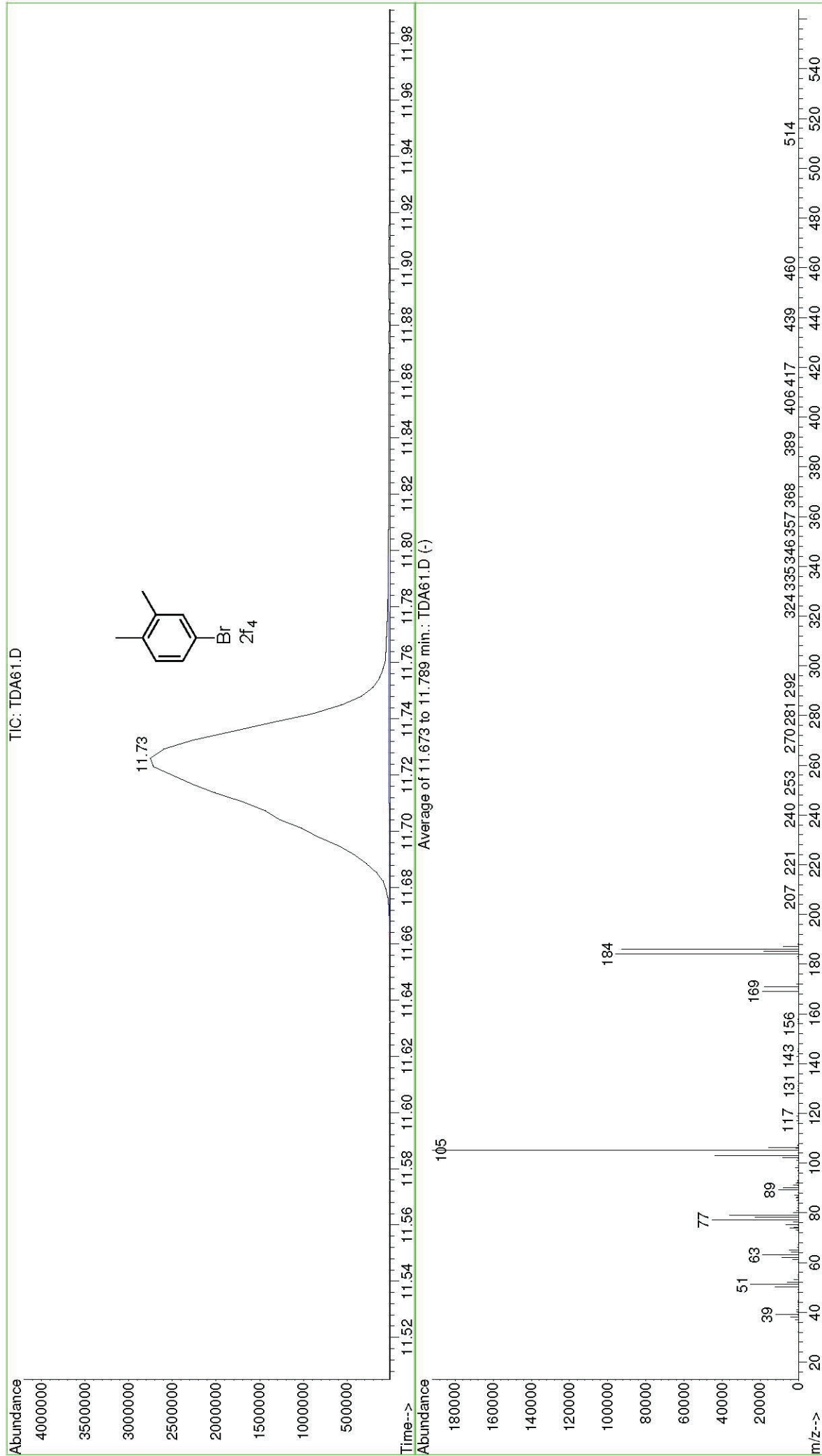
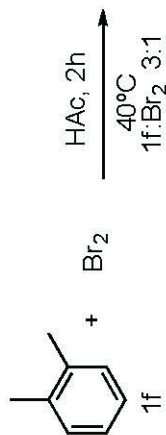
Acquired : 23 Jan 2014 17:17 using AcqMethod JMF60

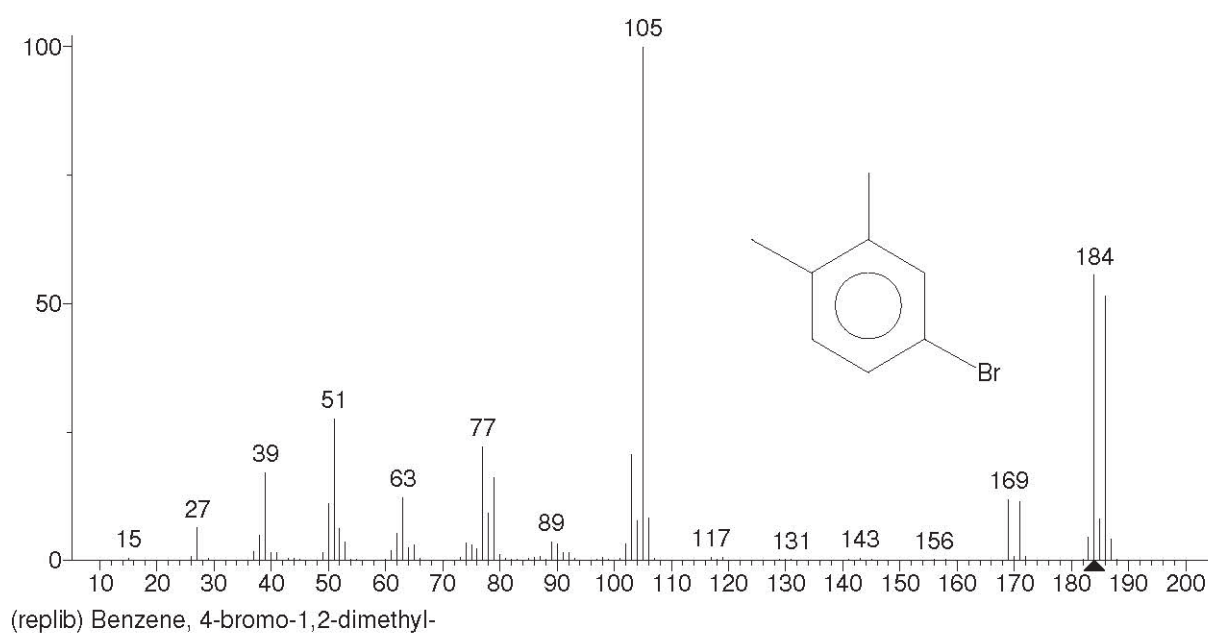
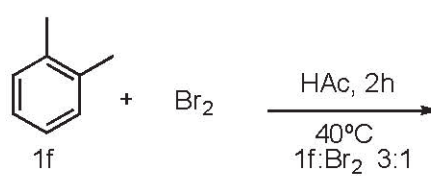
Instrument : Instrument

Sample Name: O-XYLENO

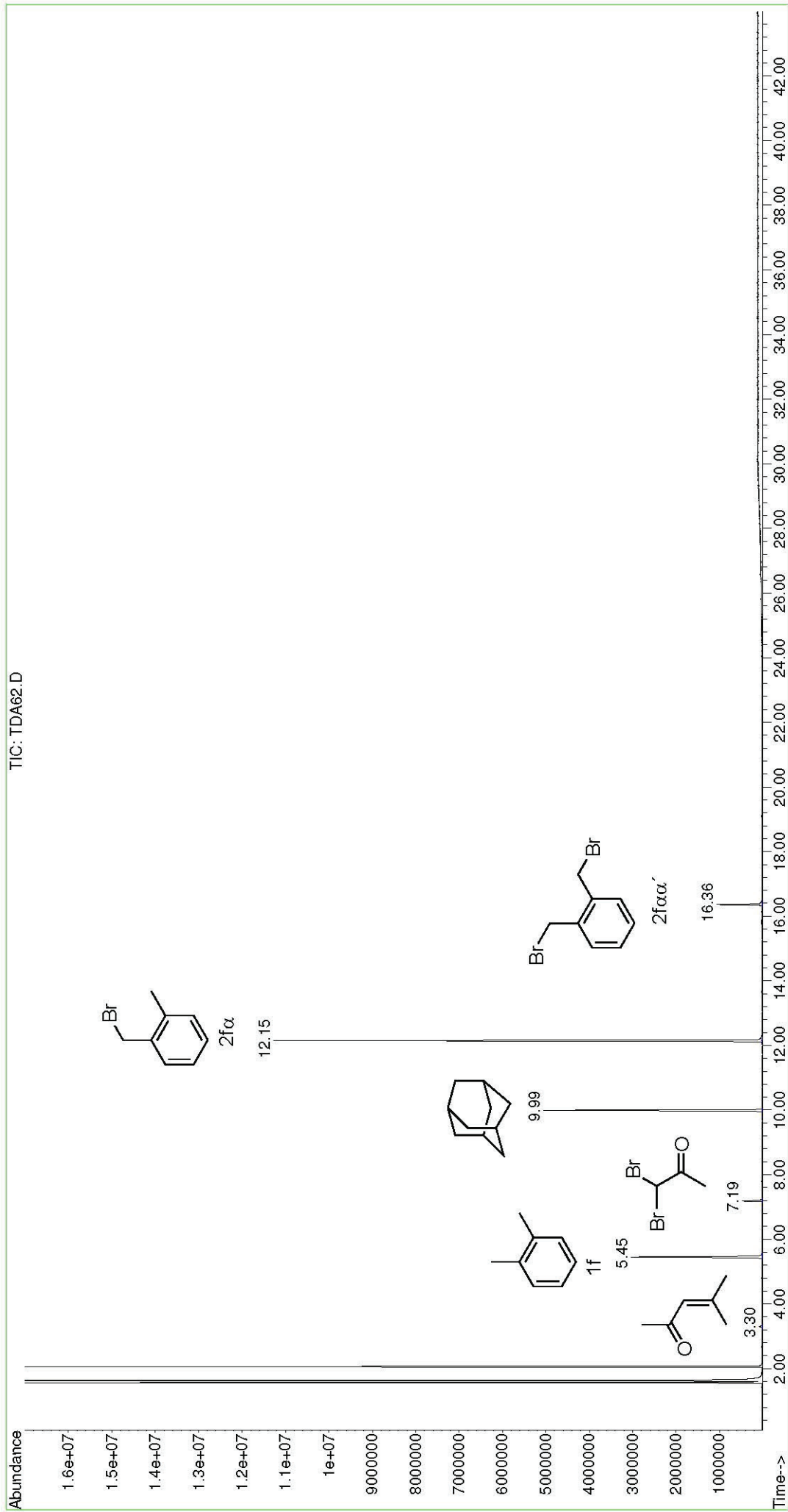
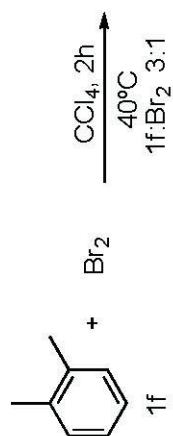
Misc Info :

Vial Number: 10

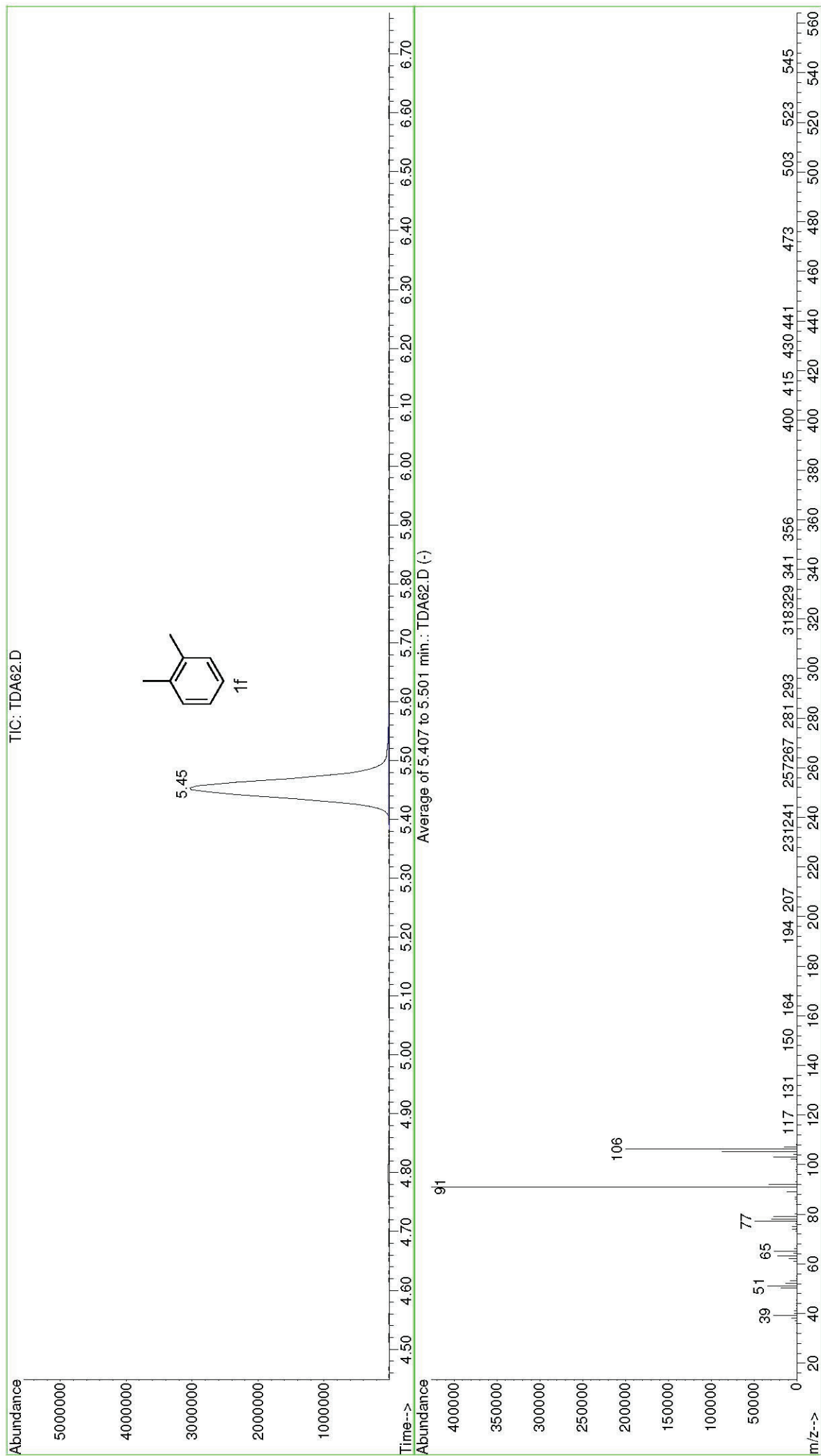
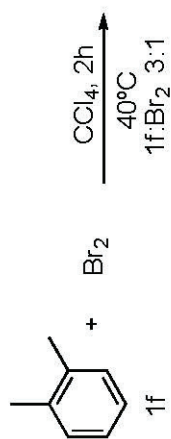


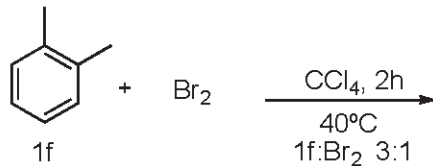


File : D:\ASENSIO\THAIS\TDA62.D
Operator :
Acquired : 23 Jan 2014 14:46 using AcqMethod JMF60
Instrument : Instrumen
Sample Name: O-XYLENO
Misc Info :
Vial Number: 7



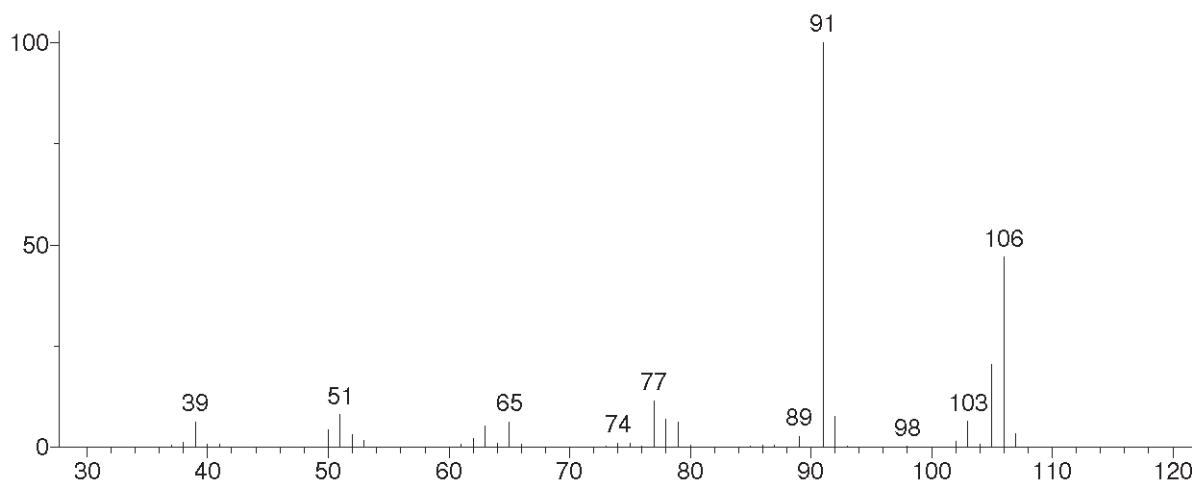
File : D:\ASENSIO\THAIS\TDA62.D
Operator :
Acquired : 23 Jan 2014 14:46 using AcqMethod JMF60
Instrument : Instrument
Sample Name : O-XYLENO
Misc Info :
Vial Number: 7





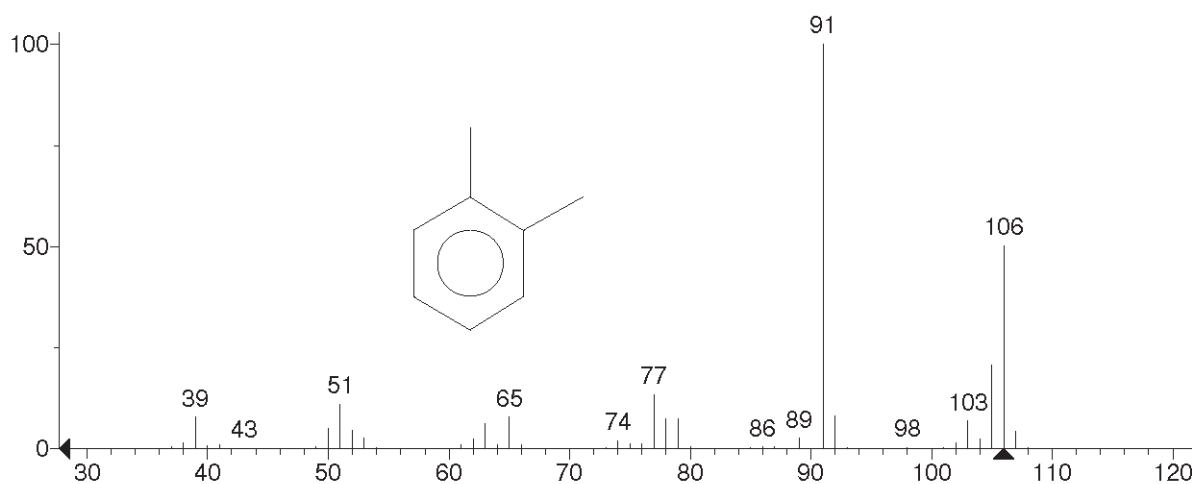
** Search Report Page 1 of 1 **

Unknown: Average of 5.407 to 5.501 min.: TDA62.D
Compound in Library Factor = 113



Hit 1 : o-Xylene

C₈H₁₀; MF: 934; RMF: 934; Prob 20.7%; CAS: 95-47-6; Lib: replib; ID: 11414.



File : D:\ASENSIO\THAIS\TDA62.D

Operator :

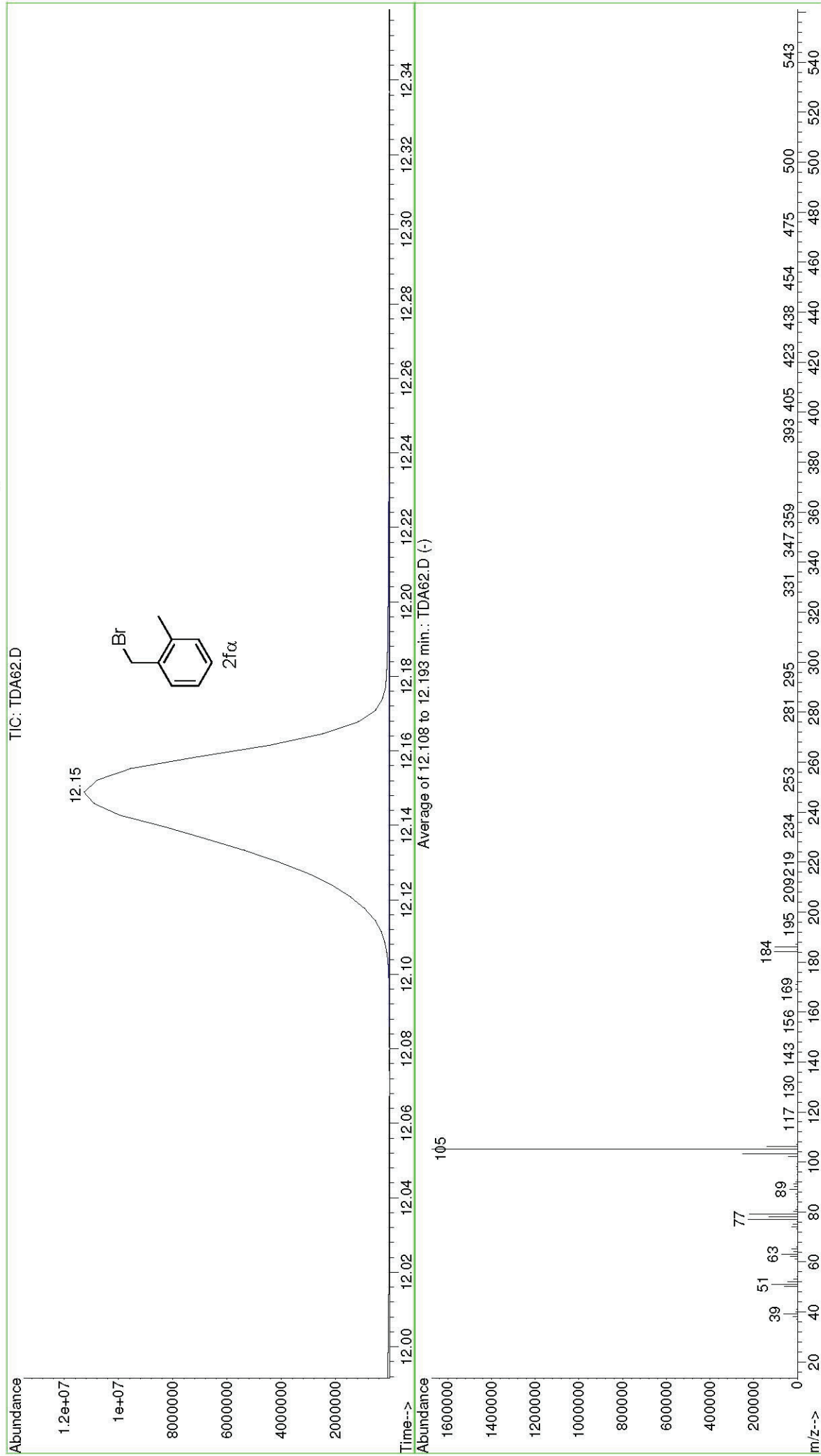
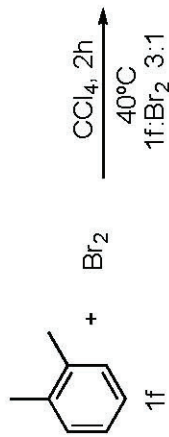
Acquired : 23 Jan 2014 14:46 using AcqMethod JMF60

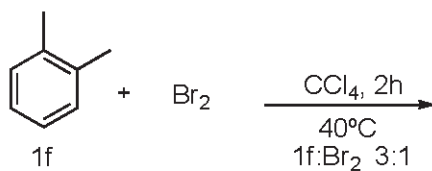
Instrument : Instrument

Sample Name : O-XYLENO

Misc Info :

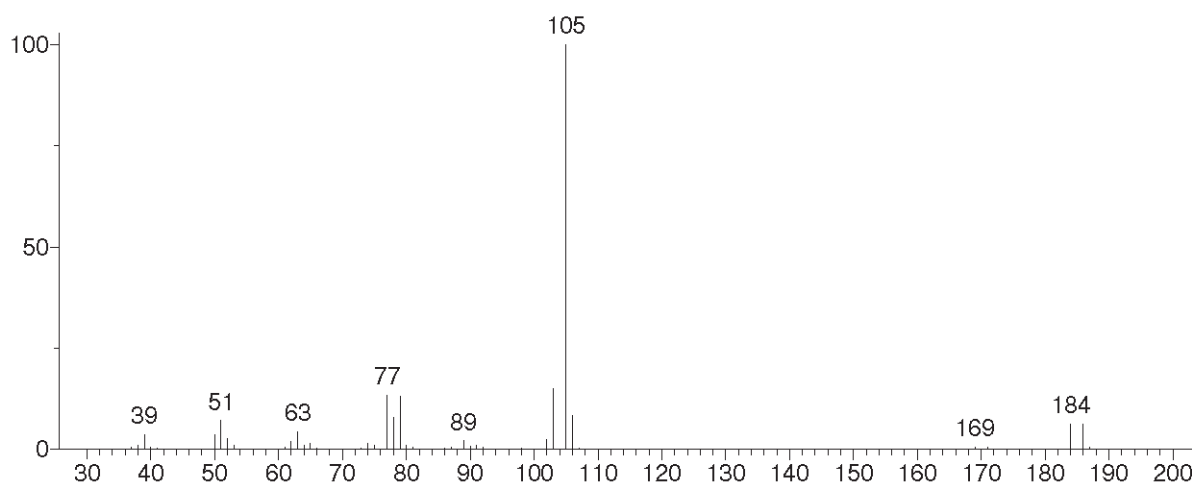
Vial Number: 7



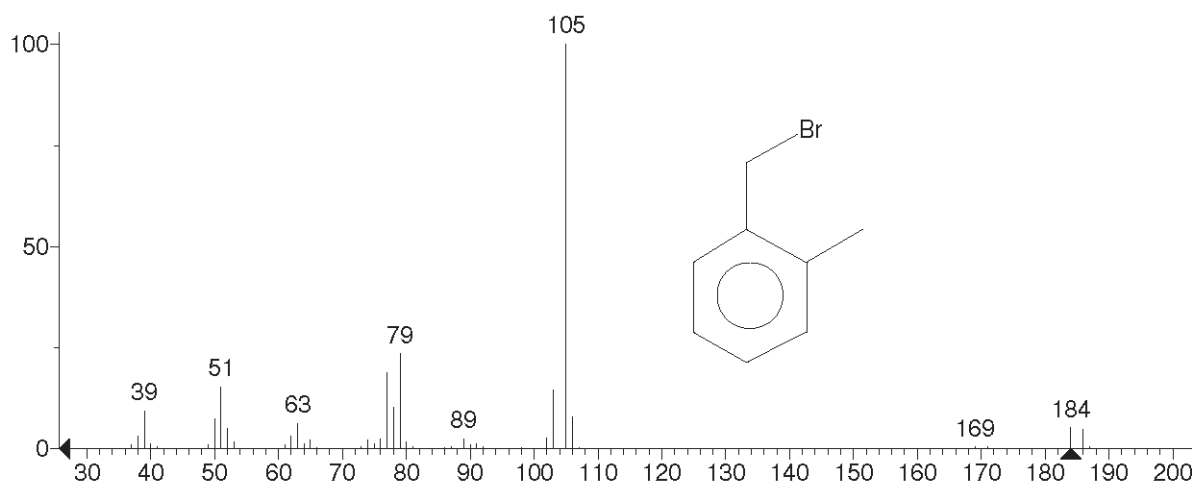


** Search Report Page 1 of 1 **

Unknown: Average of 12.108 to 12.193 min.: TDA62.D
Compound in Library Factor = 160



Hit 1 : Benzene, 1-(bromomethyl)-2-methyl-
C₈H₉Br; MF: 937; RMF: 937; Prob 68.2%; CAS: 89-92-9; Lib: replib; ID: 13832.



File : D:\ASENSIO\THAIS\TDA62.D

Operator :

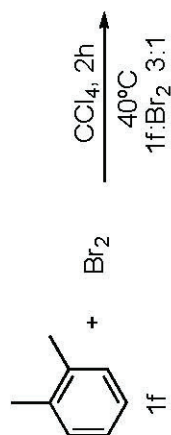
Acquired : 23 Jan 2014 14:46 using AcqMethod JMF60

Instrument : Instrument

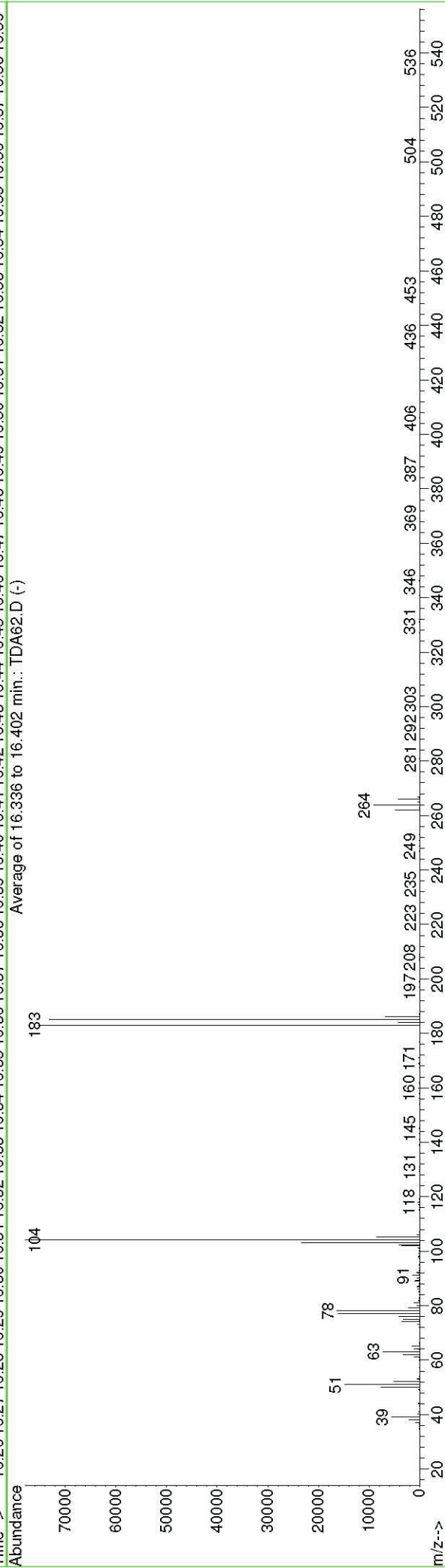
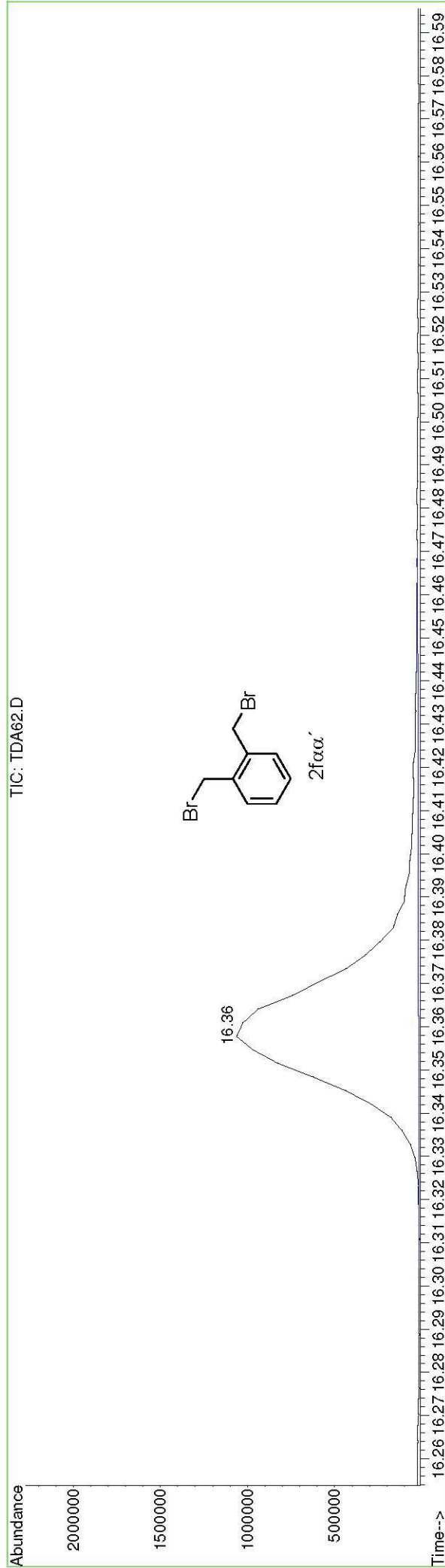
Sample Name: O-XYLENO

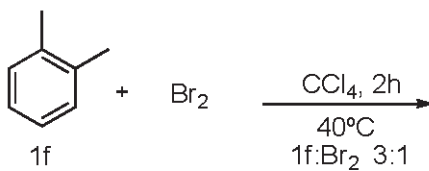
Misc Info :

Vial Number: 7



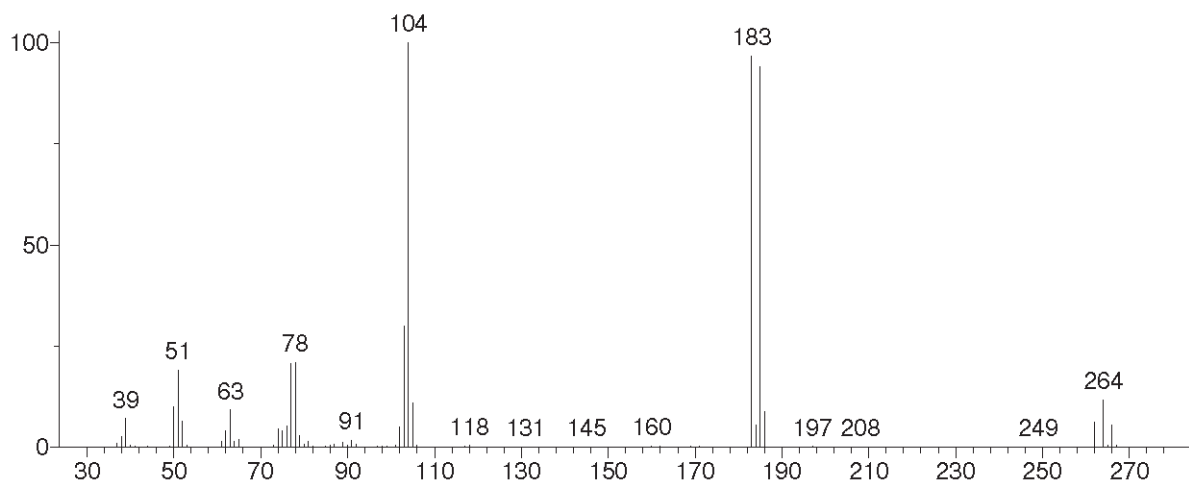
TIC: TDA62.D



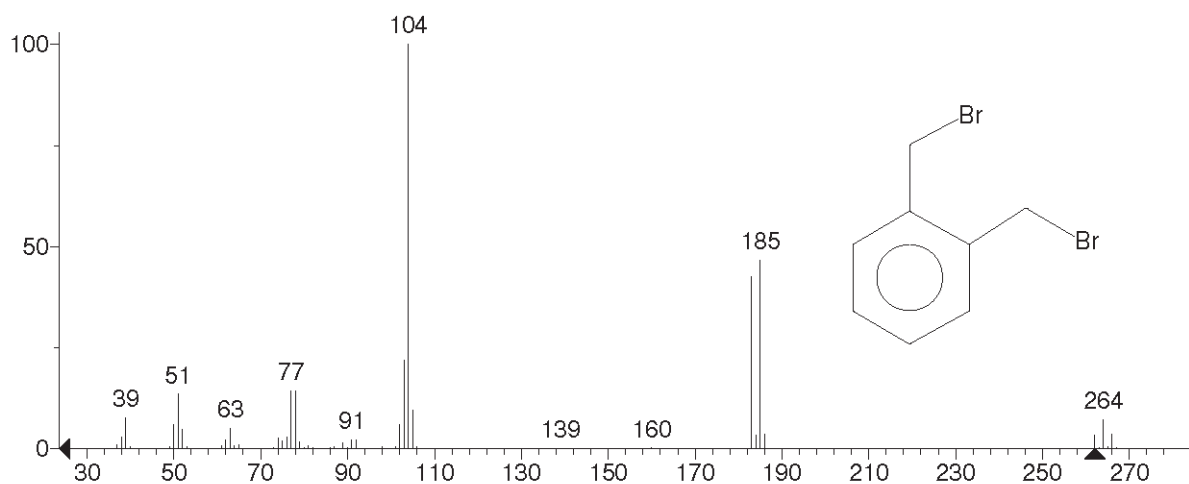


** Search Report Page 1 of 1 **

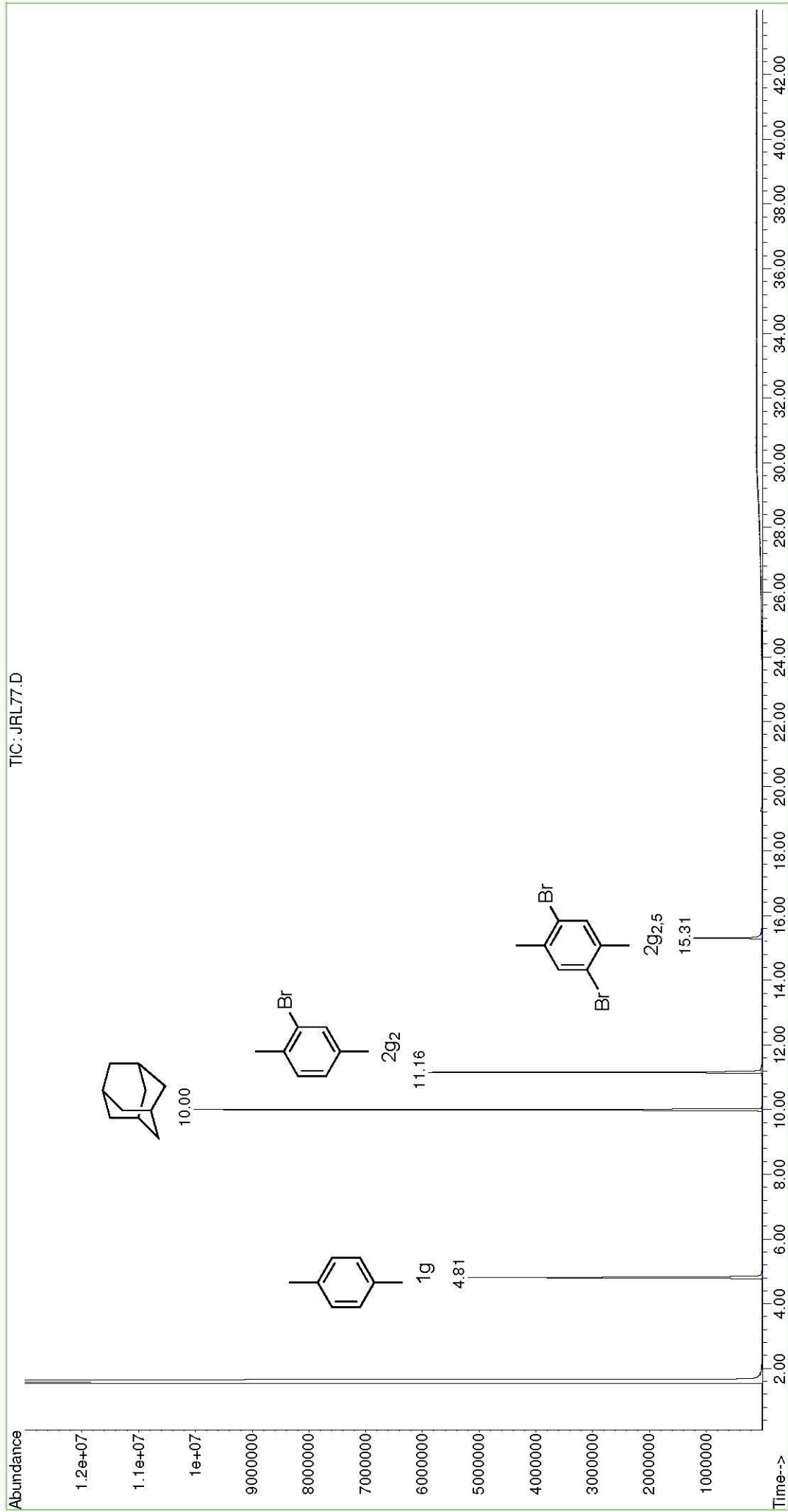
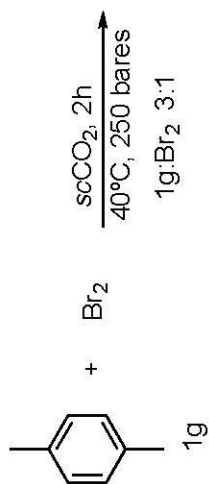
Unknown: Average of 16.336 to 16.402 min.: TDA62.D
Compound in Library Factor = 137



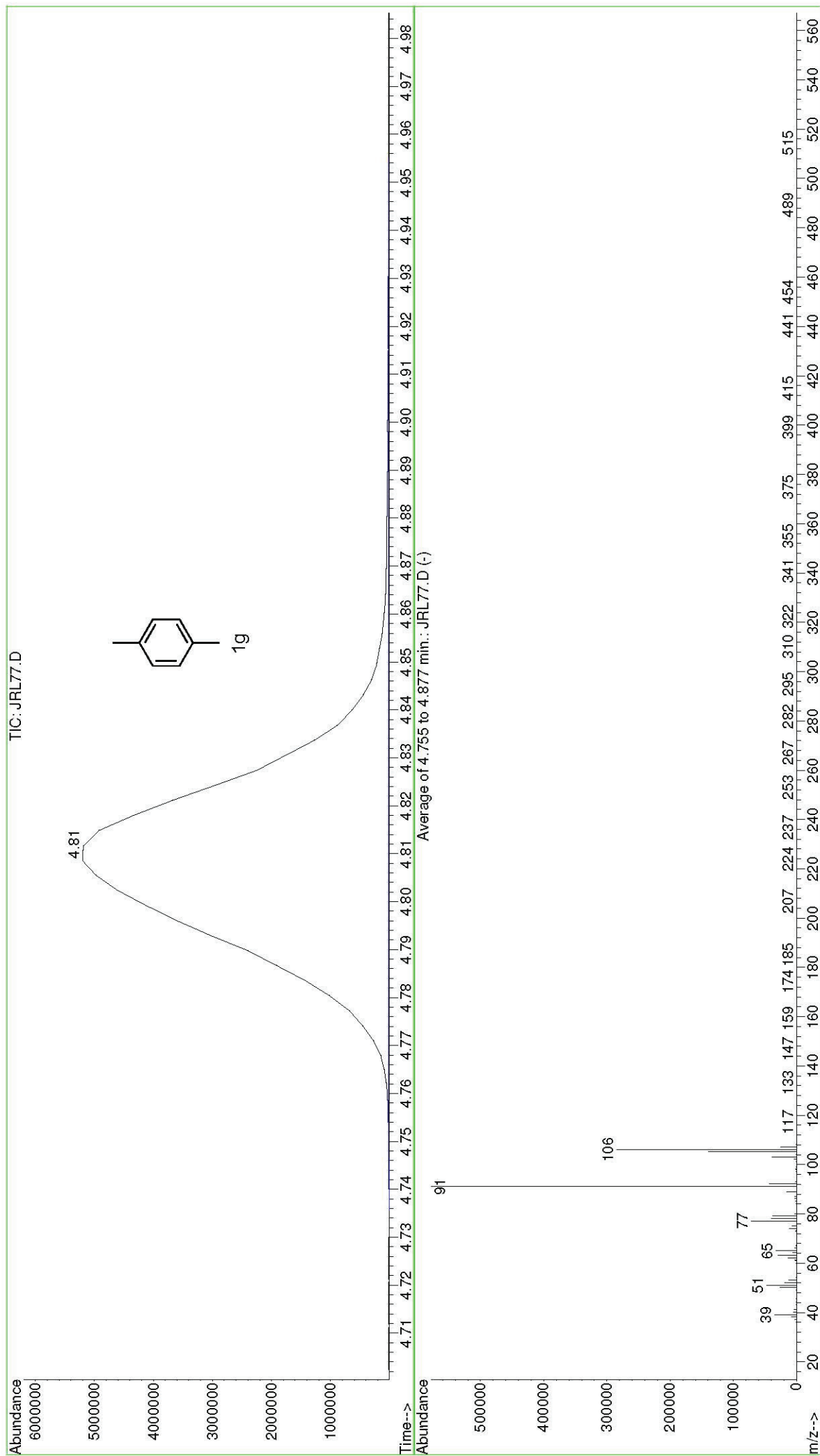
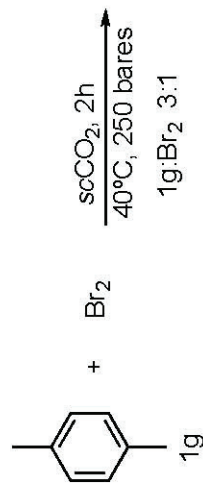
Hit 1 : Benzene, 1,2-bis(bromomethyl)-
C₈H₈Br₂; MF: 896; RMF: 898; Prob 38.4%; CAS: 91-13-4; Lib: replib; ID: 13508.

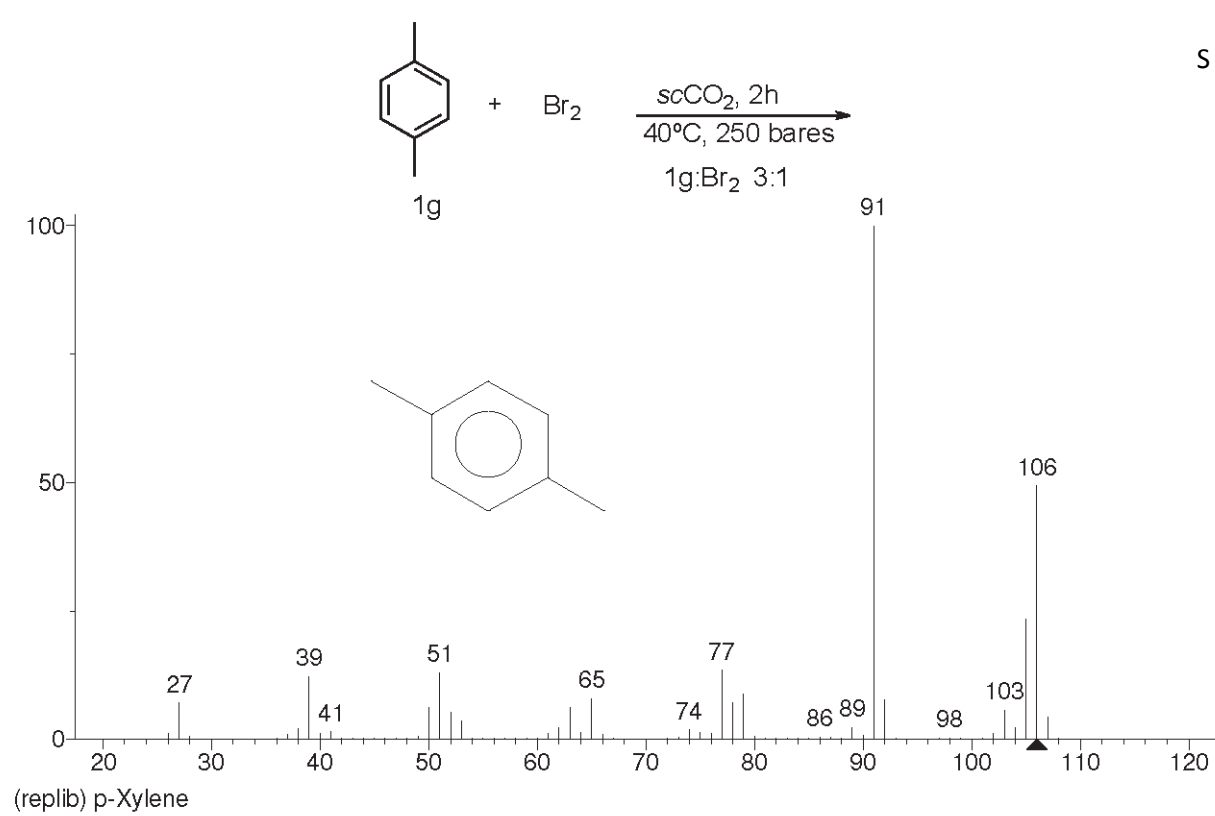


File : D:\ASENSIO\THAIS\JRL77.D
Operator :
Acquired : 22 Jan 2014 5:21 using AcqMethod JMF60
Instrument : Instrumen
Sample Name: VIDRIO-REP
Misc Info :
Vial Number: 27



File : C:\MSDCHEM\1\DATA\ISABEL\JRL77.D
 Operator :
 Acquired : 22 Jan 2014 5:21 using AcqMethod JMF60
 Instrument : Instrument
 Sample Name: VIDRIO-REP
 Misc Info :
 Vial Number: 27





File : C:\MSDCHEM\1\DATA\ISABEL\JRL77.D

Operator :

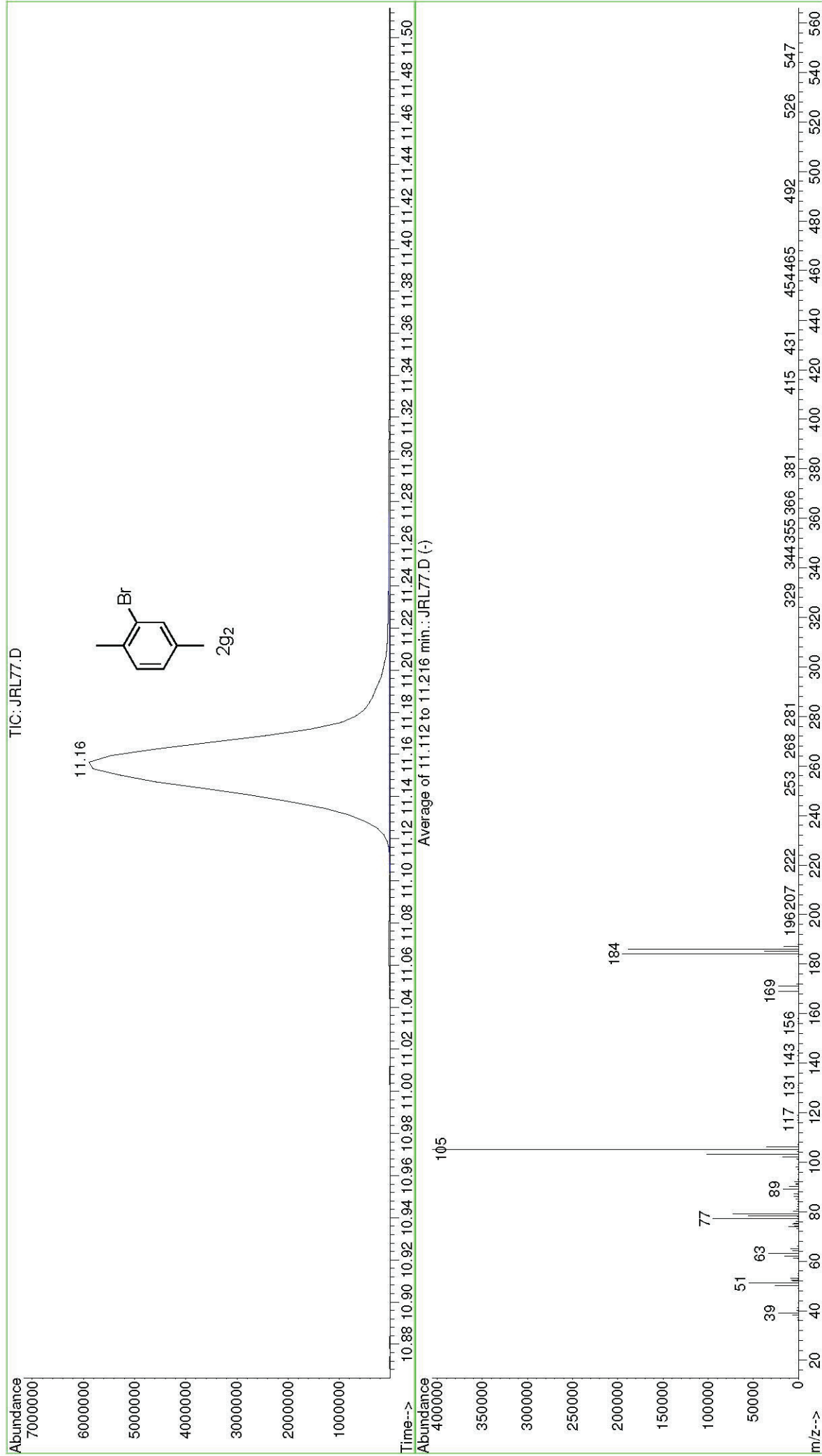
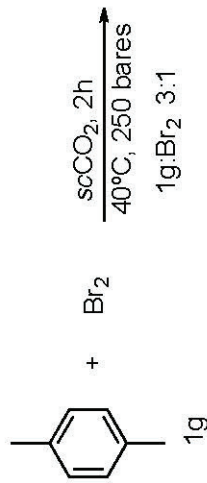
Acquired : 22 Jan 2014 5:21 using AcqMethod JMF60

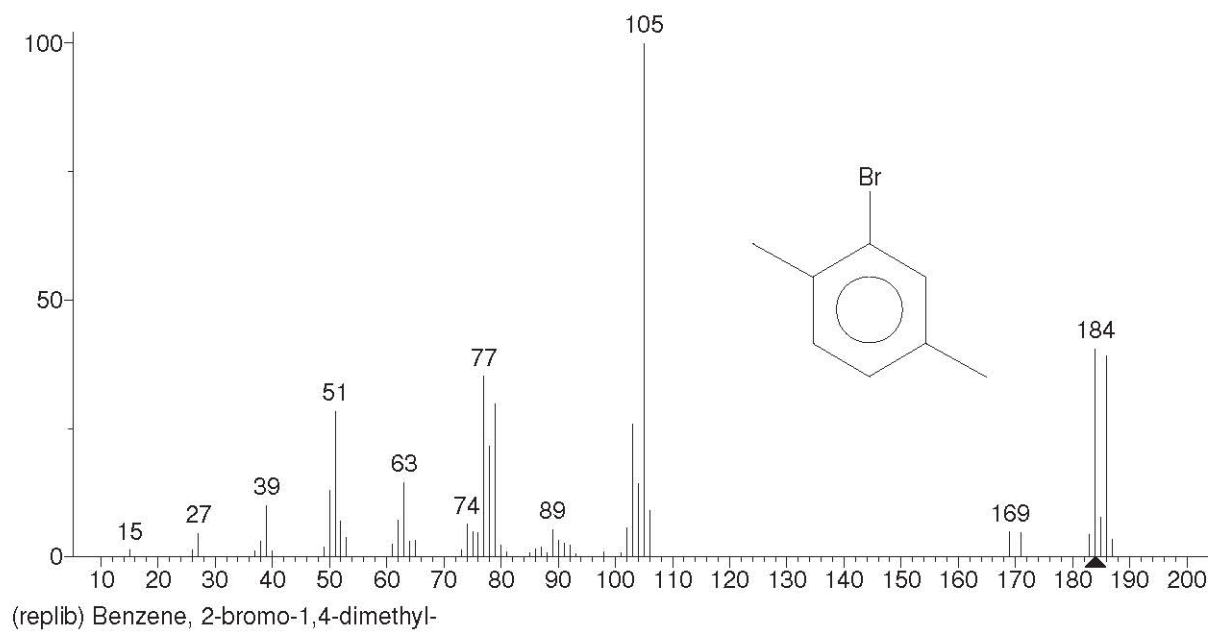
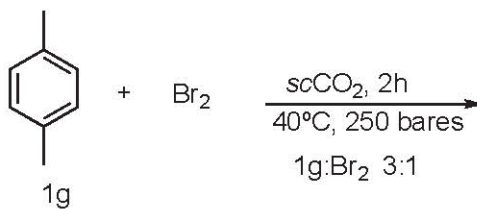
Instrument : Instrument

Sample Name: VIDRIO-REP

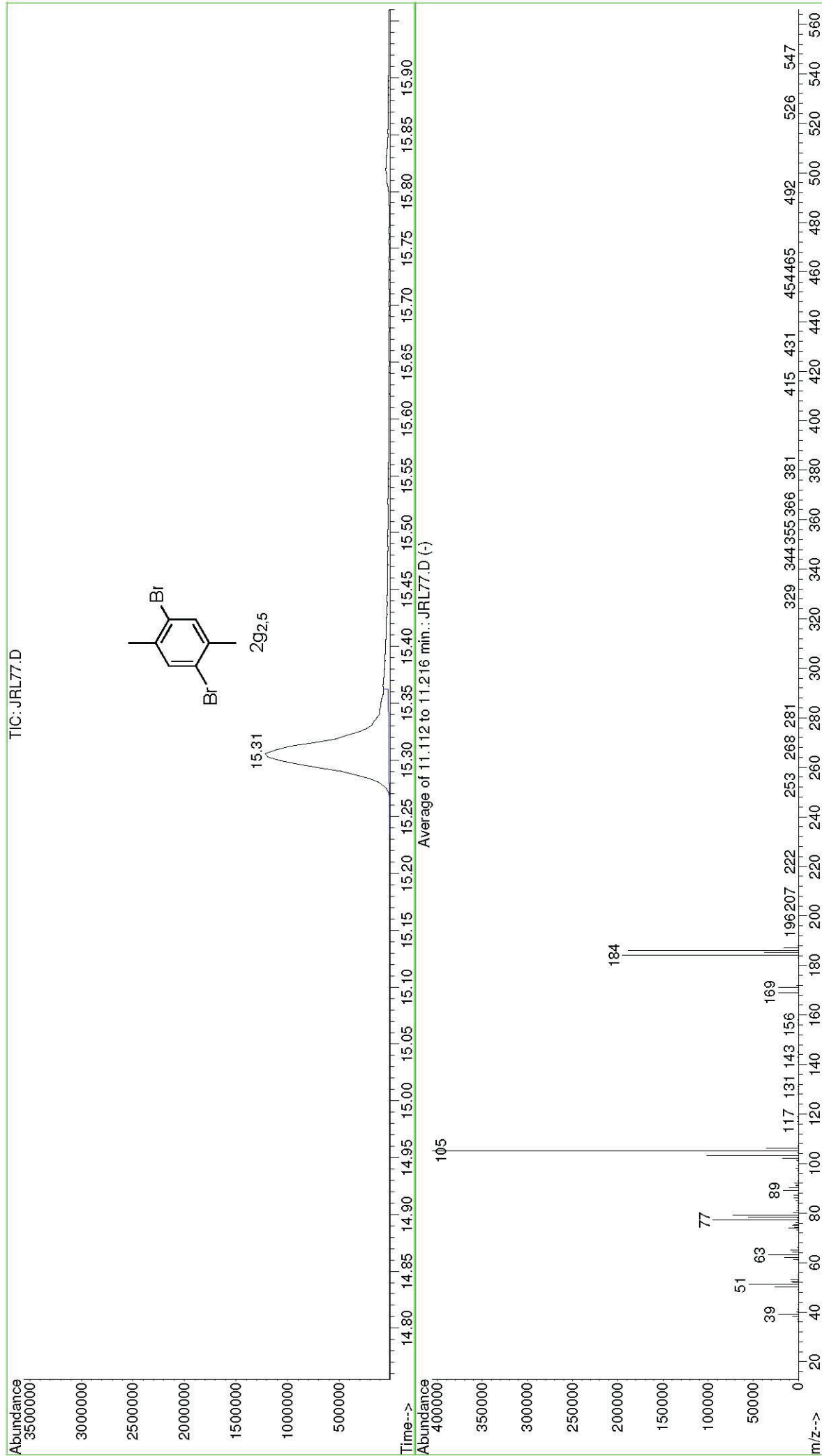
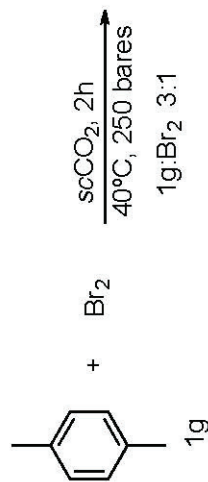
Misc Info :

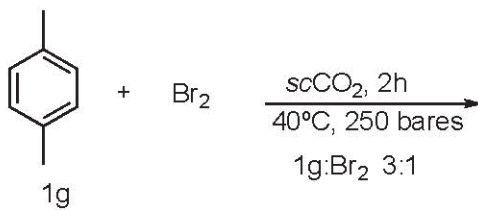
Vial Number: 27



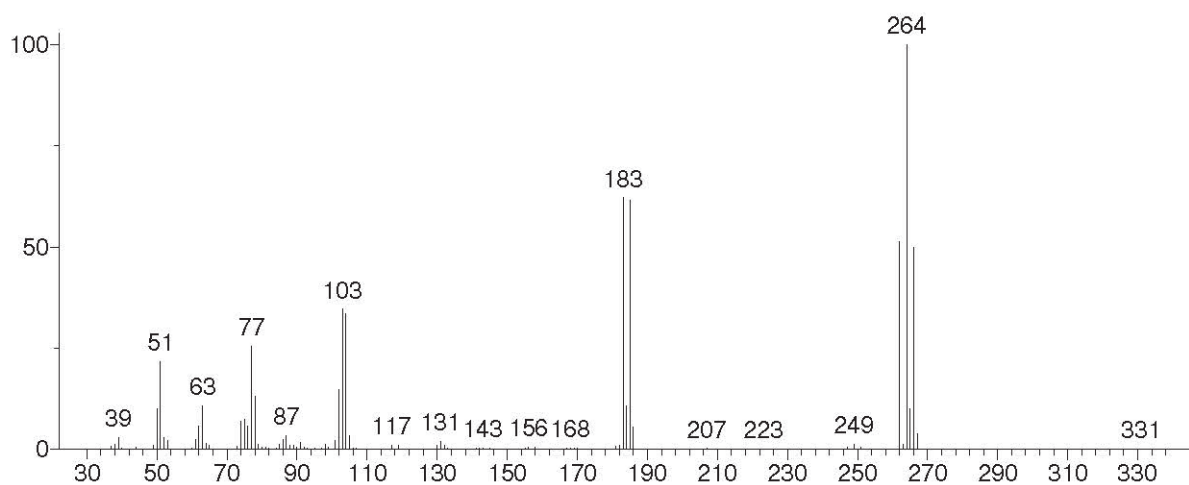


File : C:\MSDCHEM\1\DATA\ISABEL\JRL77.D
 Operator :
 Acquired : 22 Jan 2014 5:21 using AcqMethod JMF60
 Instrument : Instrument
 Sample Name : VIDRIO-REP
 Misc Info :
 Vial Number: 27

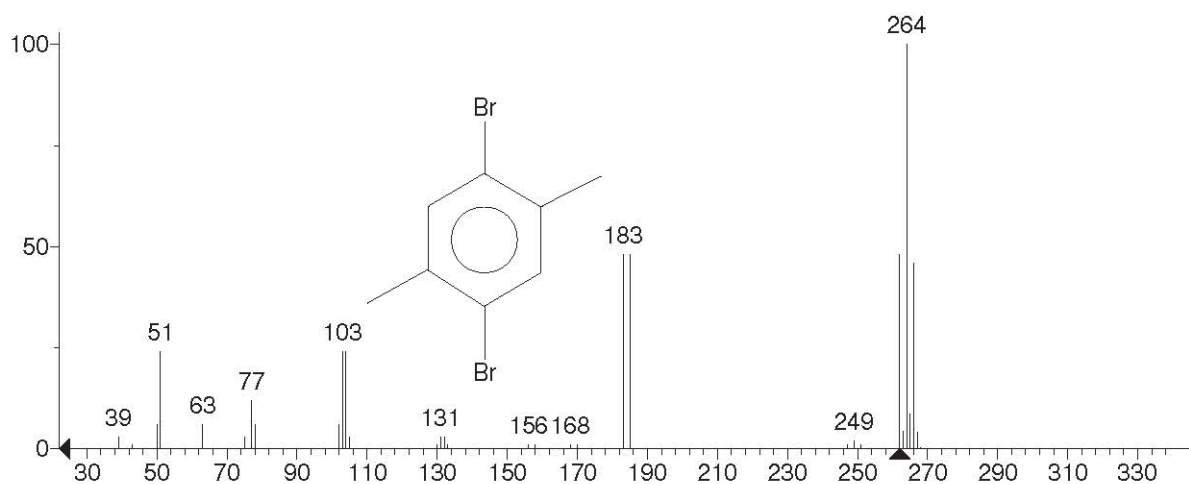




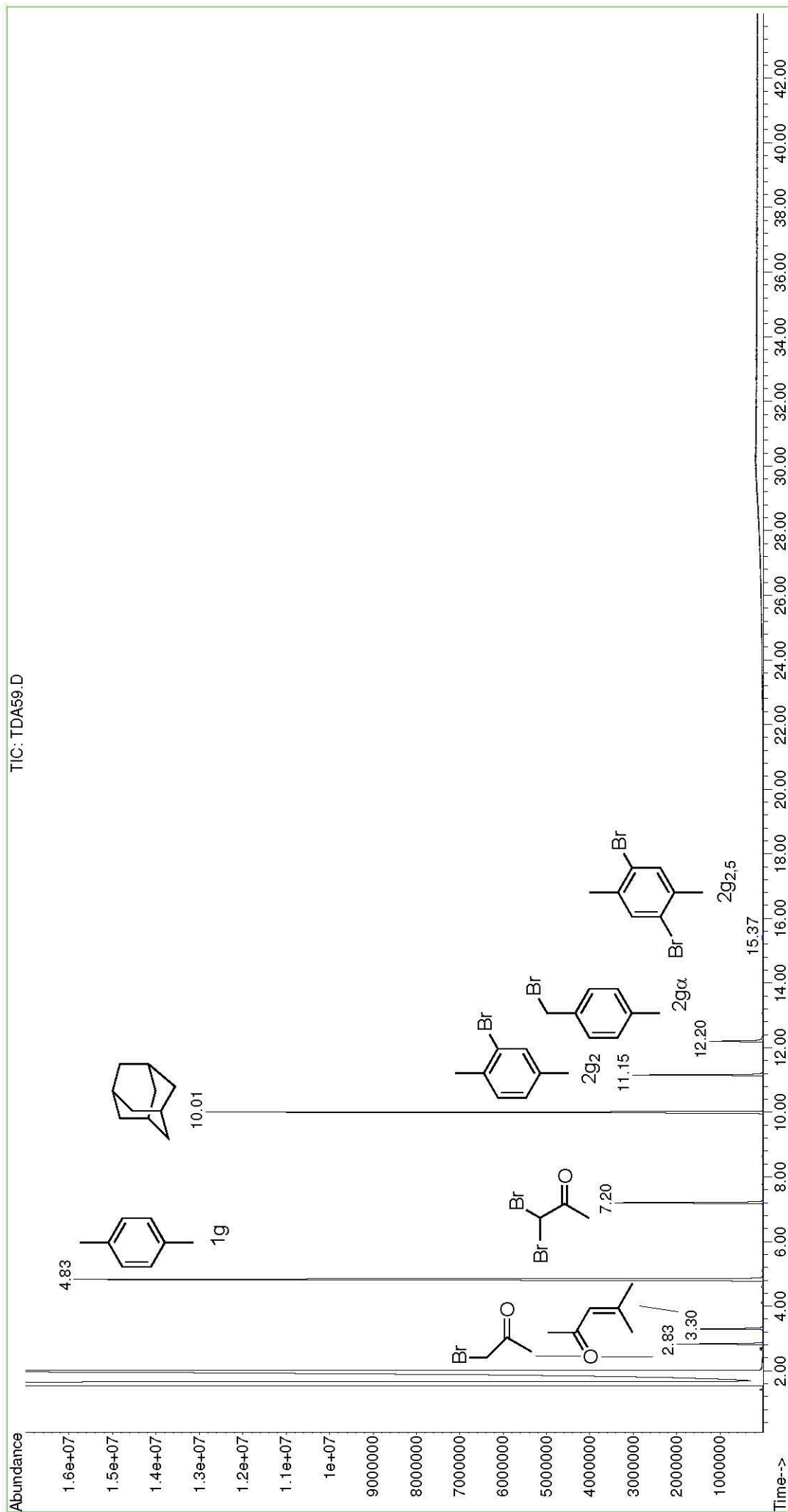
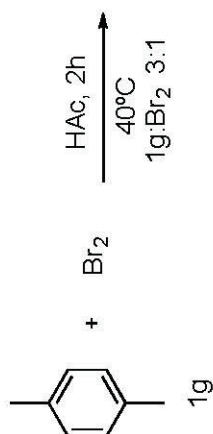
Unknown: Average of 15.268 to 15.362 min.: JRL77.D
Compound in Library Factor = 139



Hit 1 : 2,5-Dibromo-p-xylene
C₈H₈Br₂; MF: 876; RMF: 922; Prob 46.6%; CAS: 1074-24-4; Lib: wiley7n; ID: 201762.



File : D:\ASENSIO\THAIS\TDA59.D
 Operator :
 Acquired : 22 Jan 2014 8:43 using AcqMethod JMF60
 Instrument : Instrument
 Sample Name :
 Misc Info :
 Vial Number: 31



File : D:\ASENSIO\THAIS\TDA59.D

Operator :

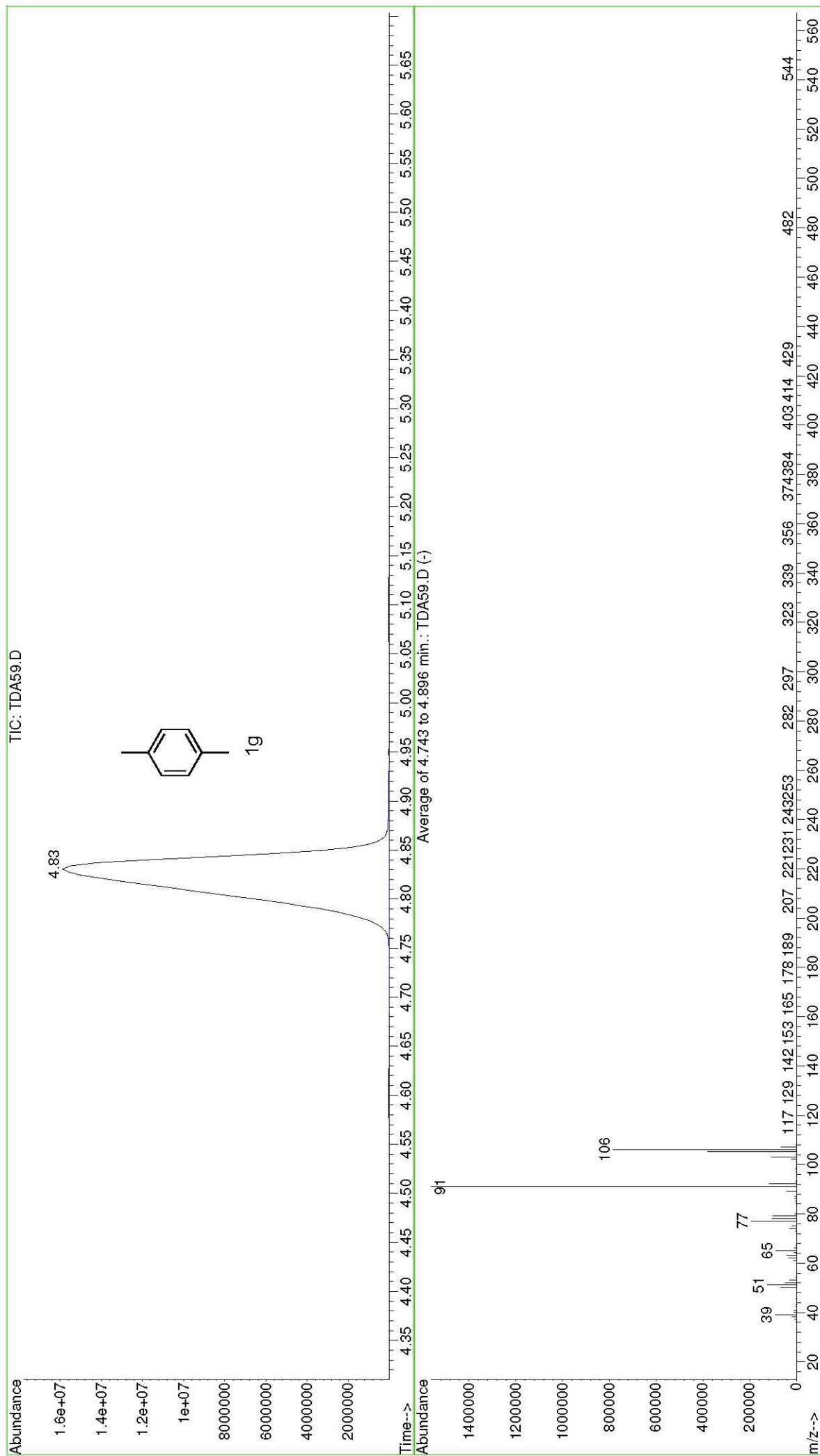
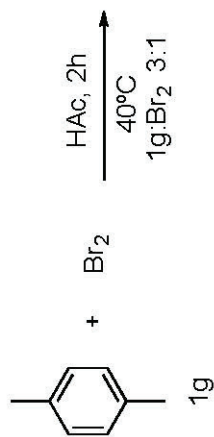
Acquired : 22 Jan 2014 8:43 using AcqMethod JMF60

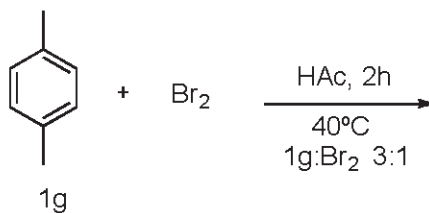
Instrument : Instrument

Sample Name:

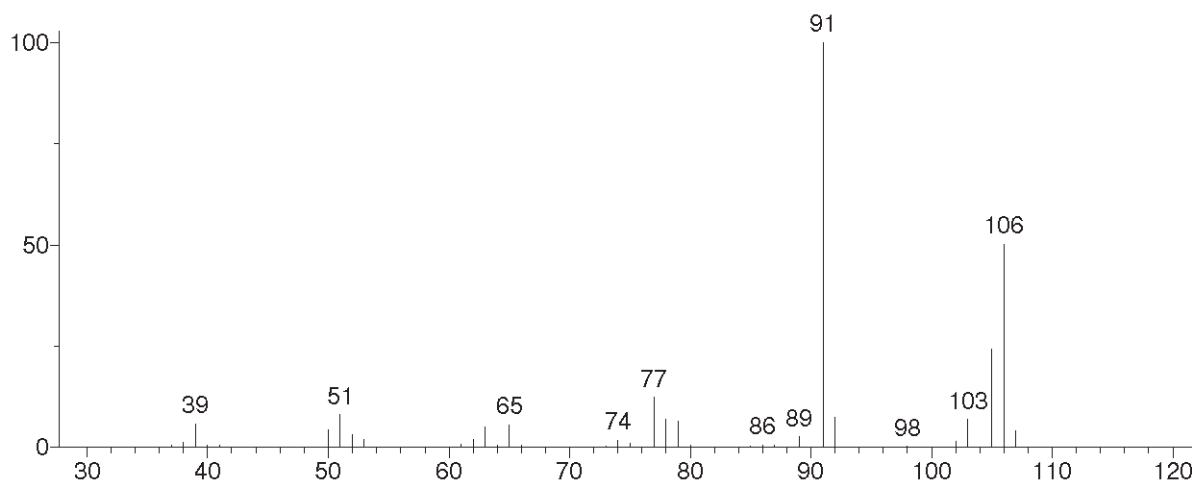
Misc Info :

Vial Number: 31

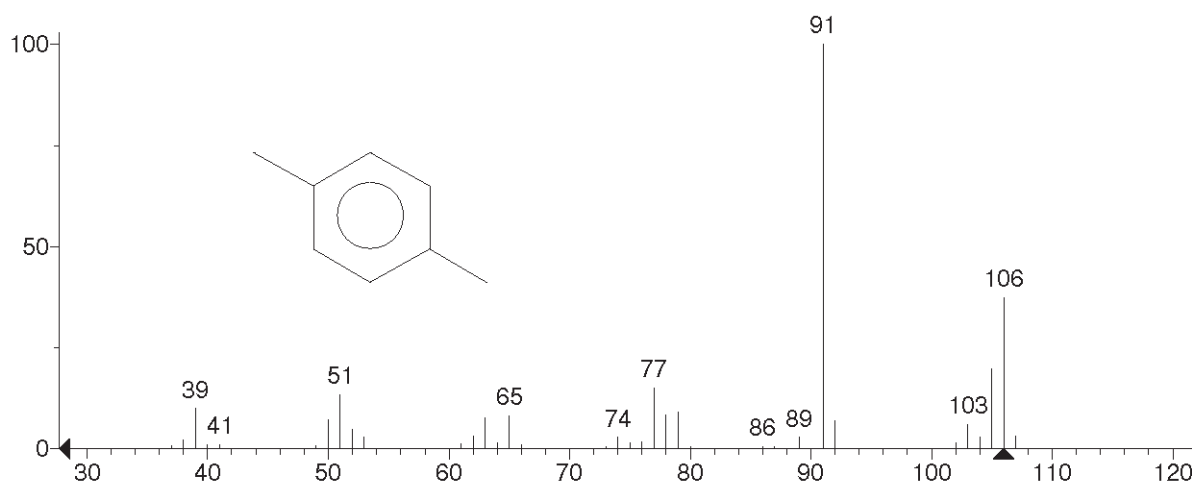




Unknown: Average of 4.759 to 4.871 min.: TDA59.D
Compound in Library Factor = -107



Hit 1 : p-Xylene
C₈H₁₀; MF: 924; RMF: 925; Prob 25.7%; CAS: 106-42-3; Lib: replib; ID: 11407.



File : D:\ASENSIO\THAIS\TDA59.D

Operator :

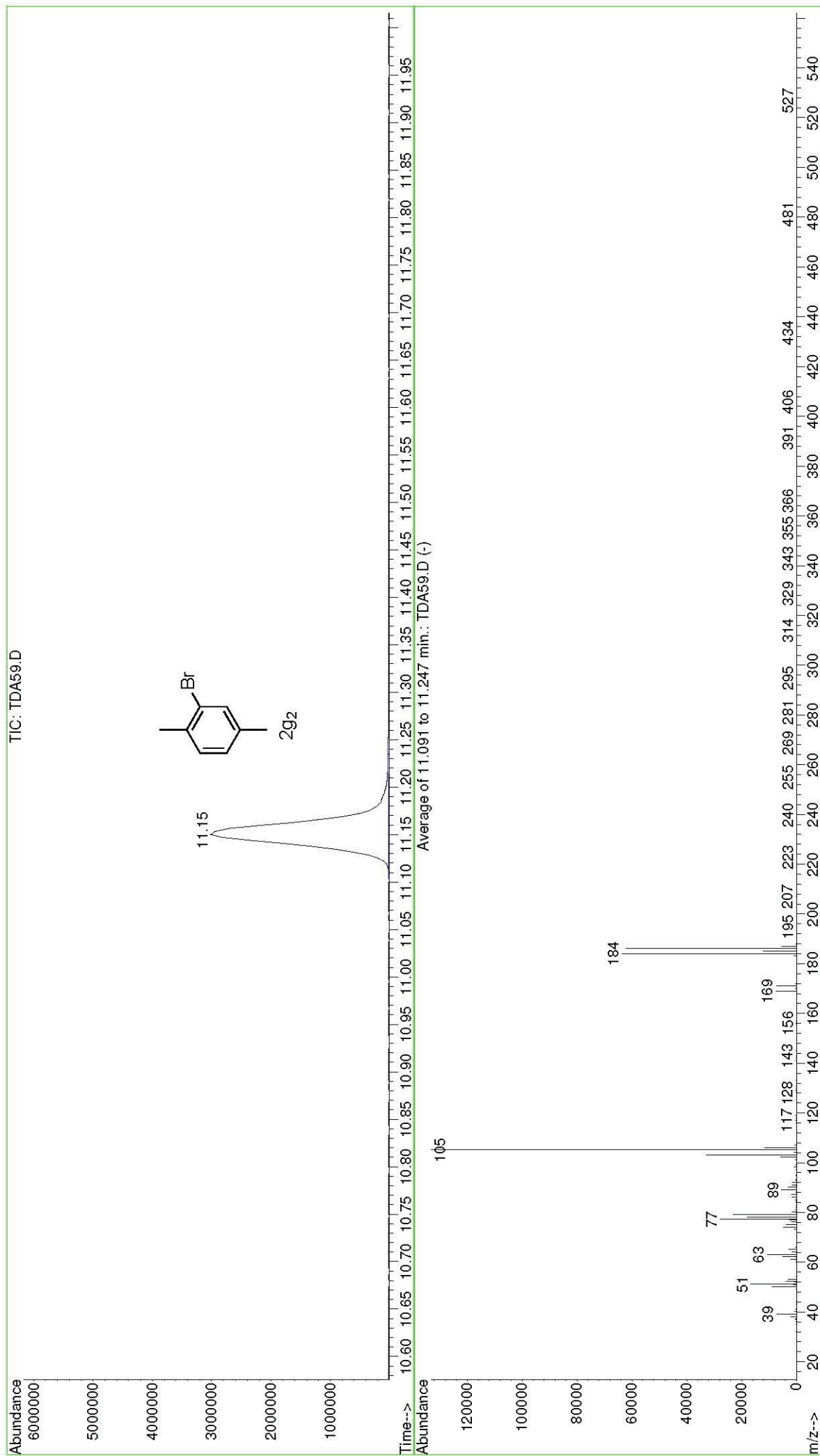
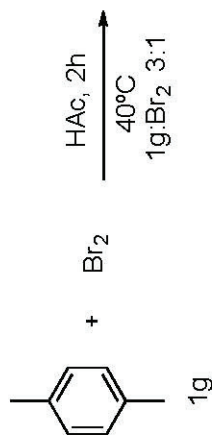
Acquired : 22 Jan 2014 8:43 using AcqMethod JMF60

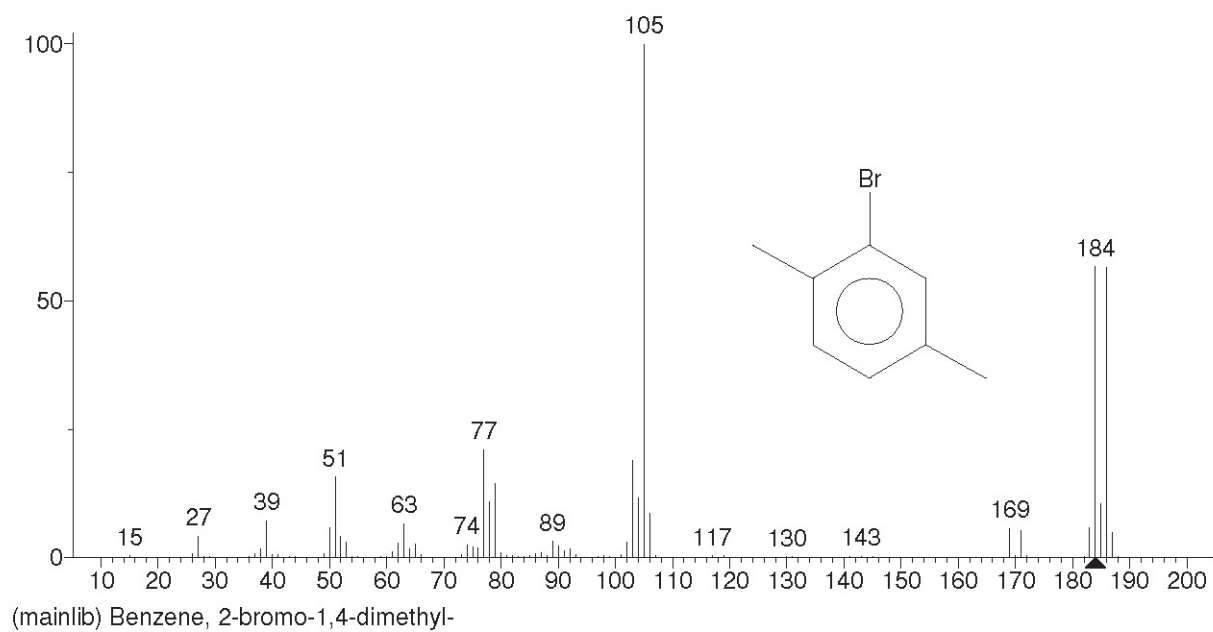
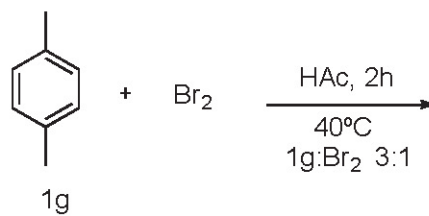
Instrument : Instrument

Sample Name:

Misc Info :

Vial Number: 31





File : D:\ASENSIO\THAIS\TDA59.D

Operator :

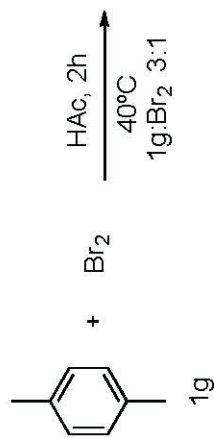
Acquired : 22 Jan 2014 8:43 using AcqMethod JMF60

Instrument : Instrument

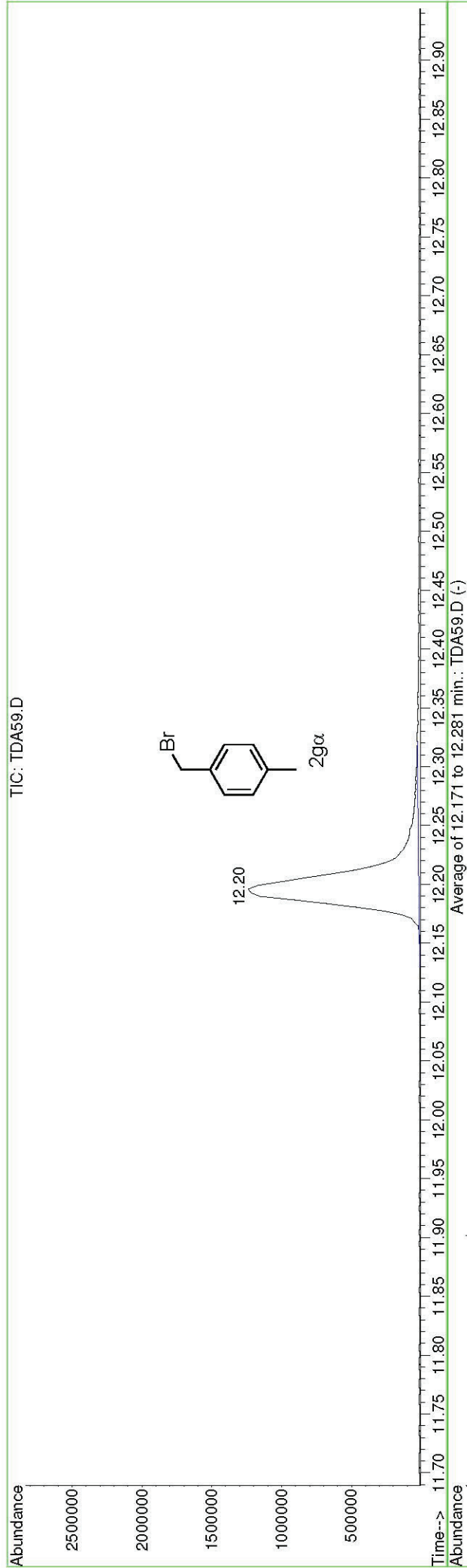
Sample Name:

Misc Info :

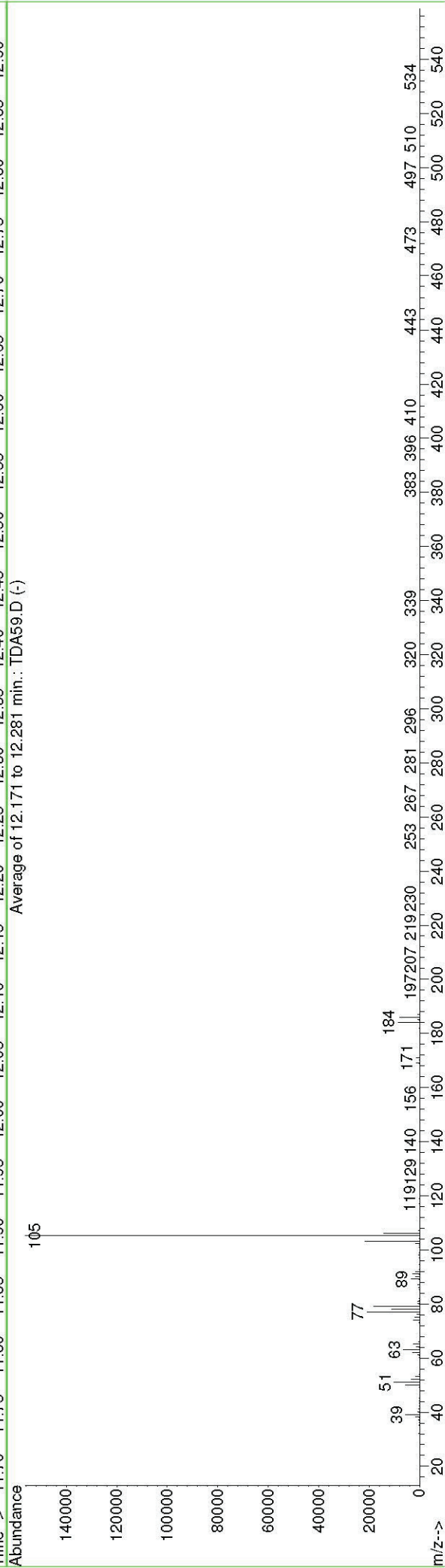
Vial Number: 31

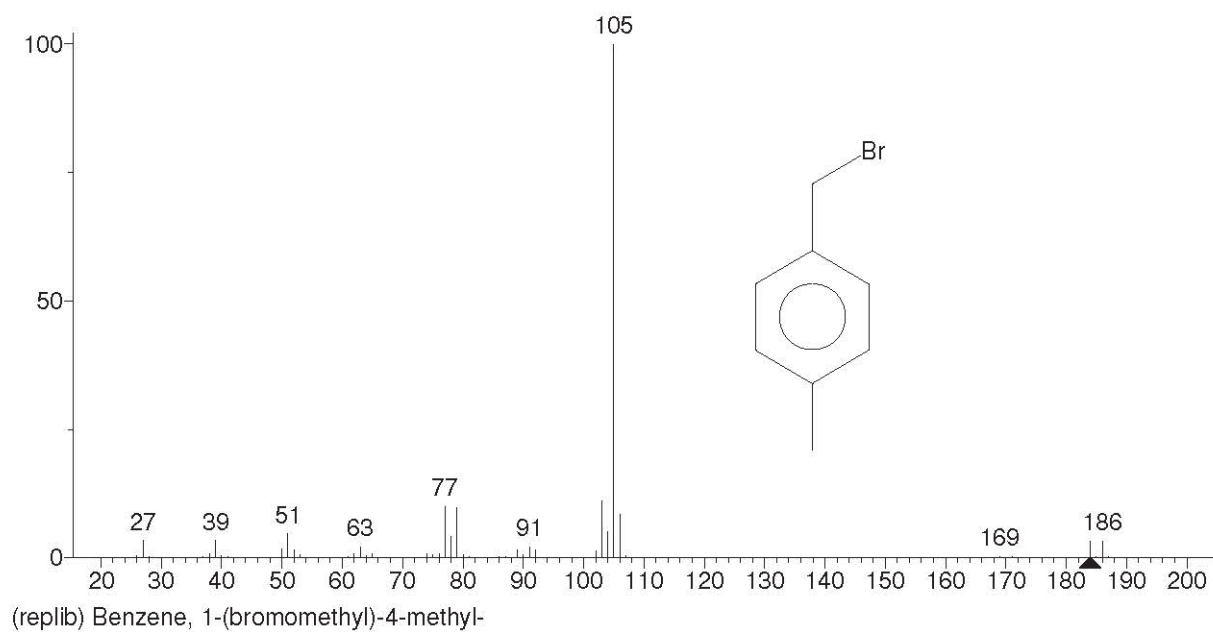
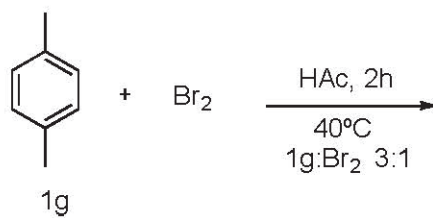


TIC: TDA59.D



Average of 12.171 to 12.281 min.: TDA59.D (-)





File : D:\ASENSIO\THAIS\TDA59.D

Operator :

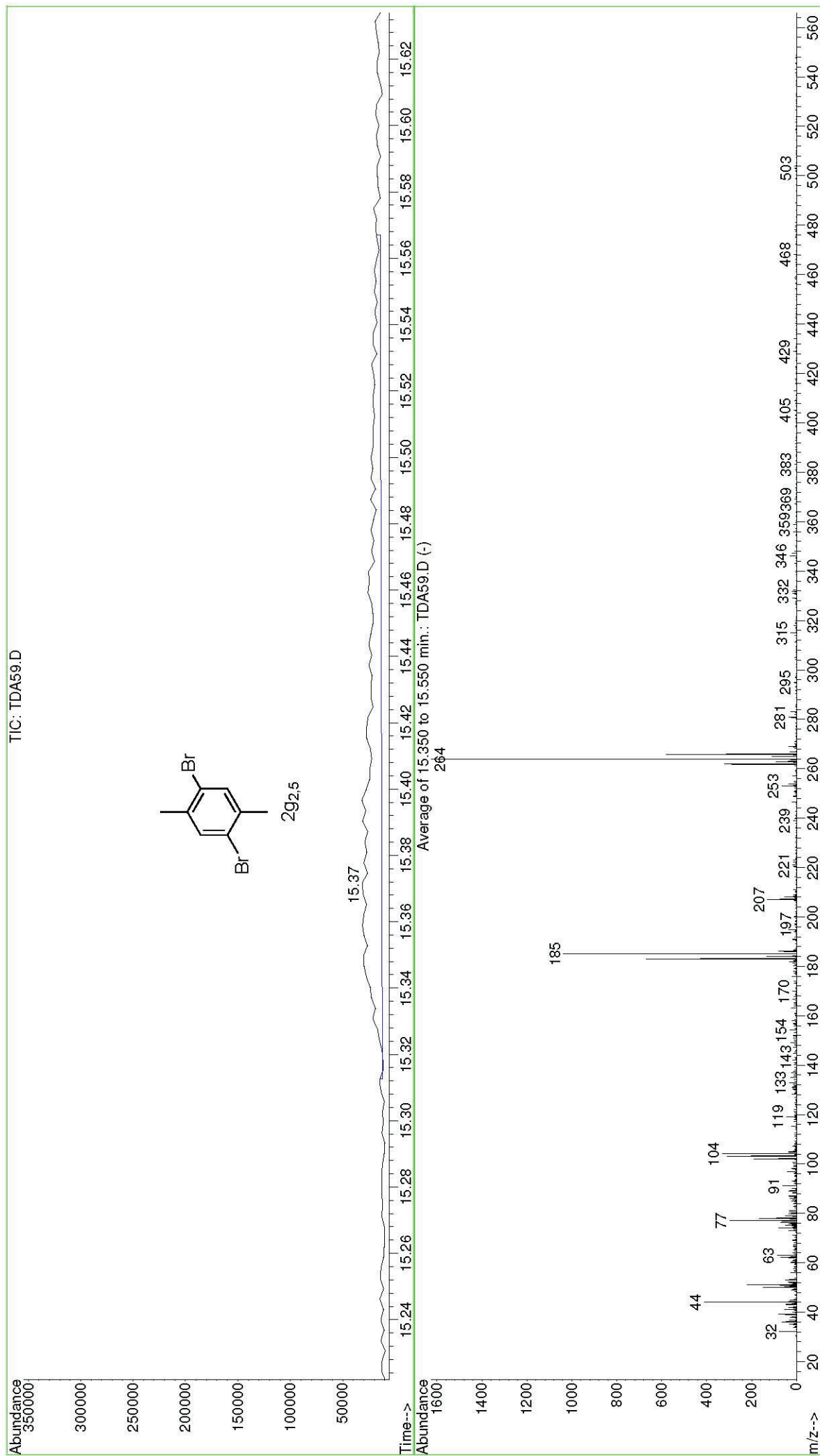
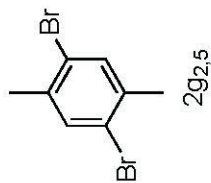
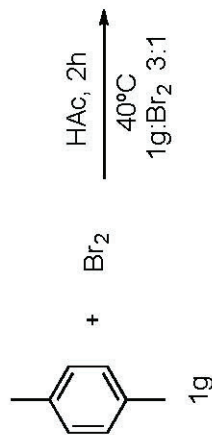
Acquired : 22 Jan 2014 8:43 using AcqMethod JMF60

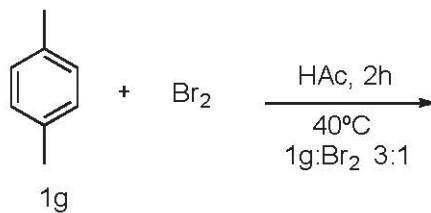
Instrument : Instrument

Sample Name:

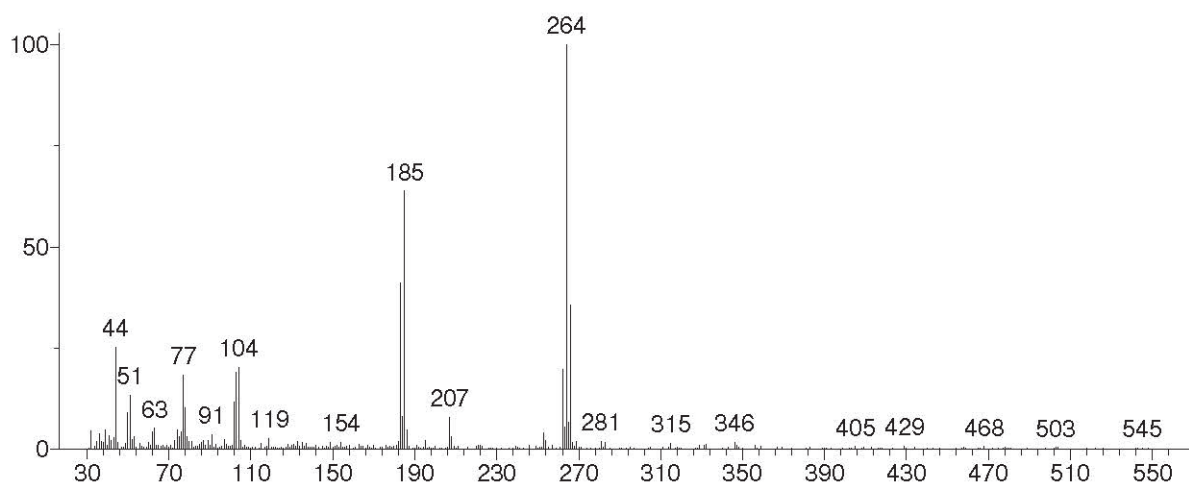
Misc Info :

Vial Number: 31

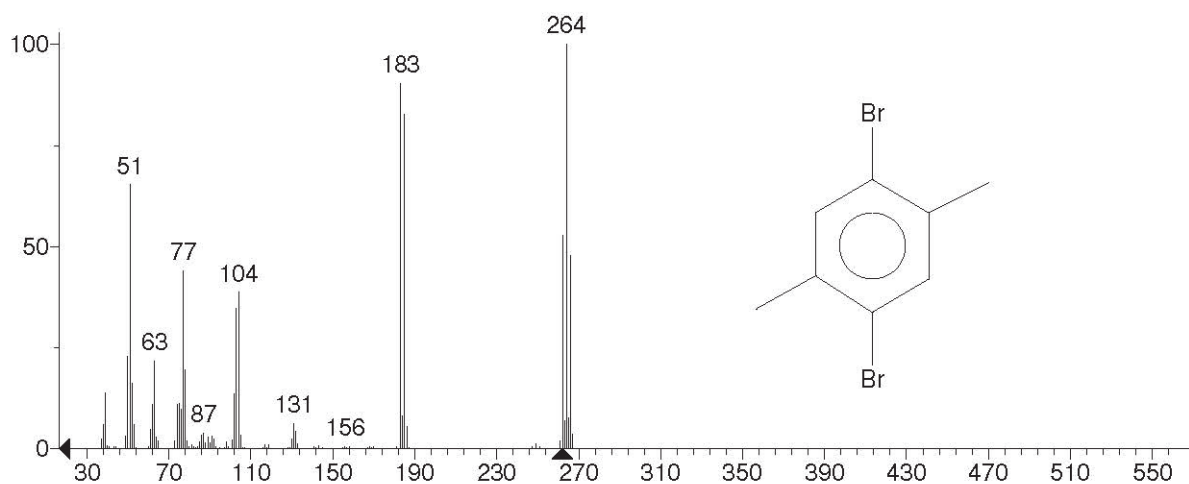




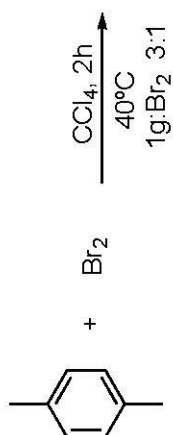
Unknown: Average of 15.350 to 15.550 min.: TDA59.D
Compound in Library Factor = -628



Hit 1 : Benzene, 1,4-dibromo-2,5-dimethyl-
C₈H₈Br₂; MF: 705; RMF: 837; Prob 48.6%; CAS: 1074-24-4; Lib: wiley7n; ID: 201760.

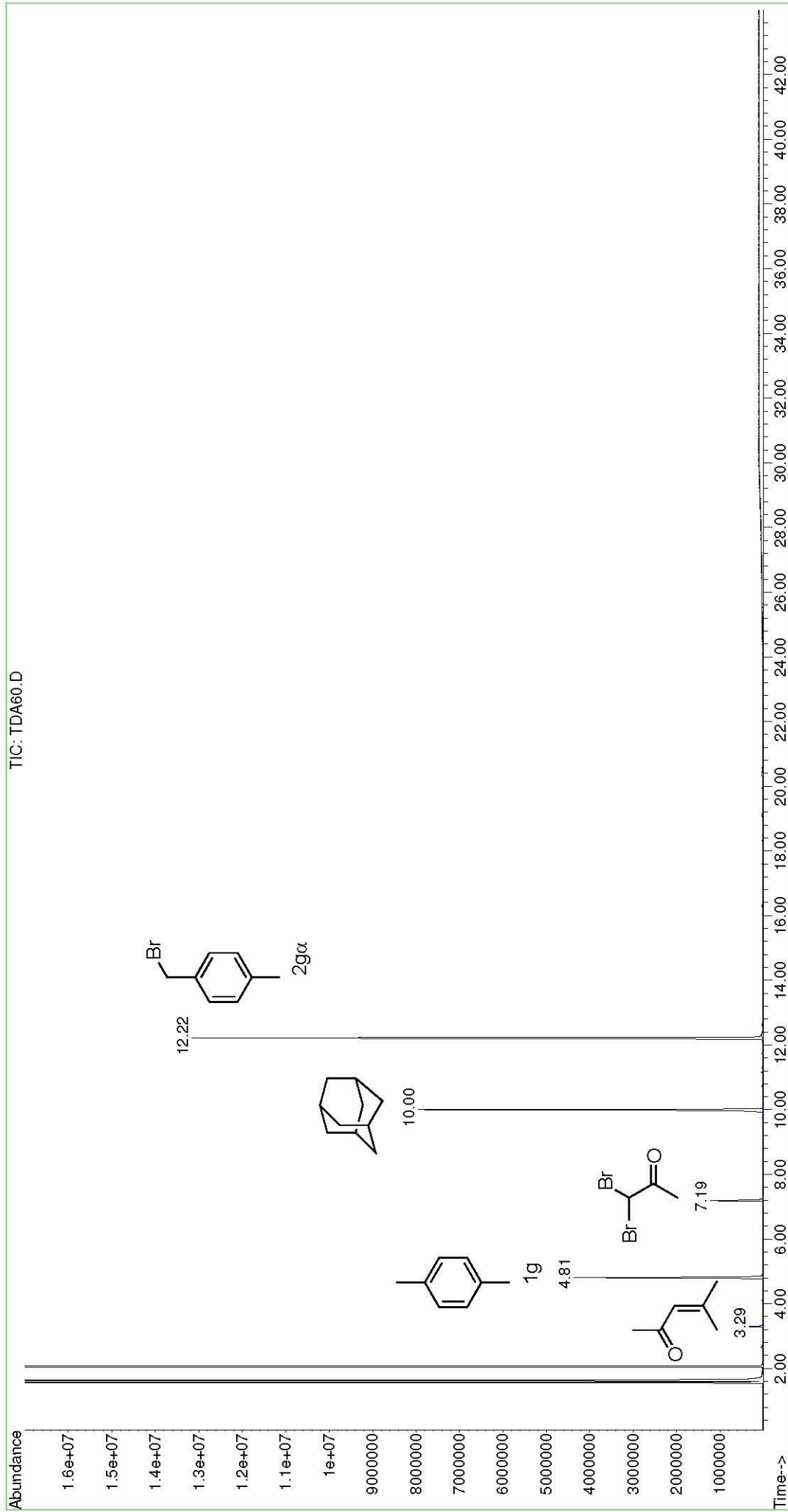


File : D:\ASENSIO\THAIS\TDA60.D
Operator :
Acquired : 22 Jan 2014 7:02 using AcqMethod JMF60
Instrument : Instrument
Sample Name :
Misc Info :
Vial Number: 29



1g

TIC: TDA60.D



File : D:\ASENSIO\THAIS\TDA60.D

Operator :

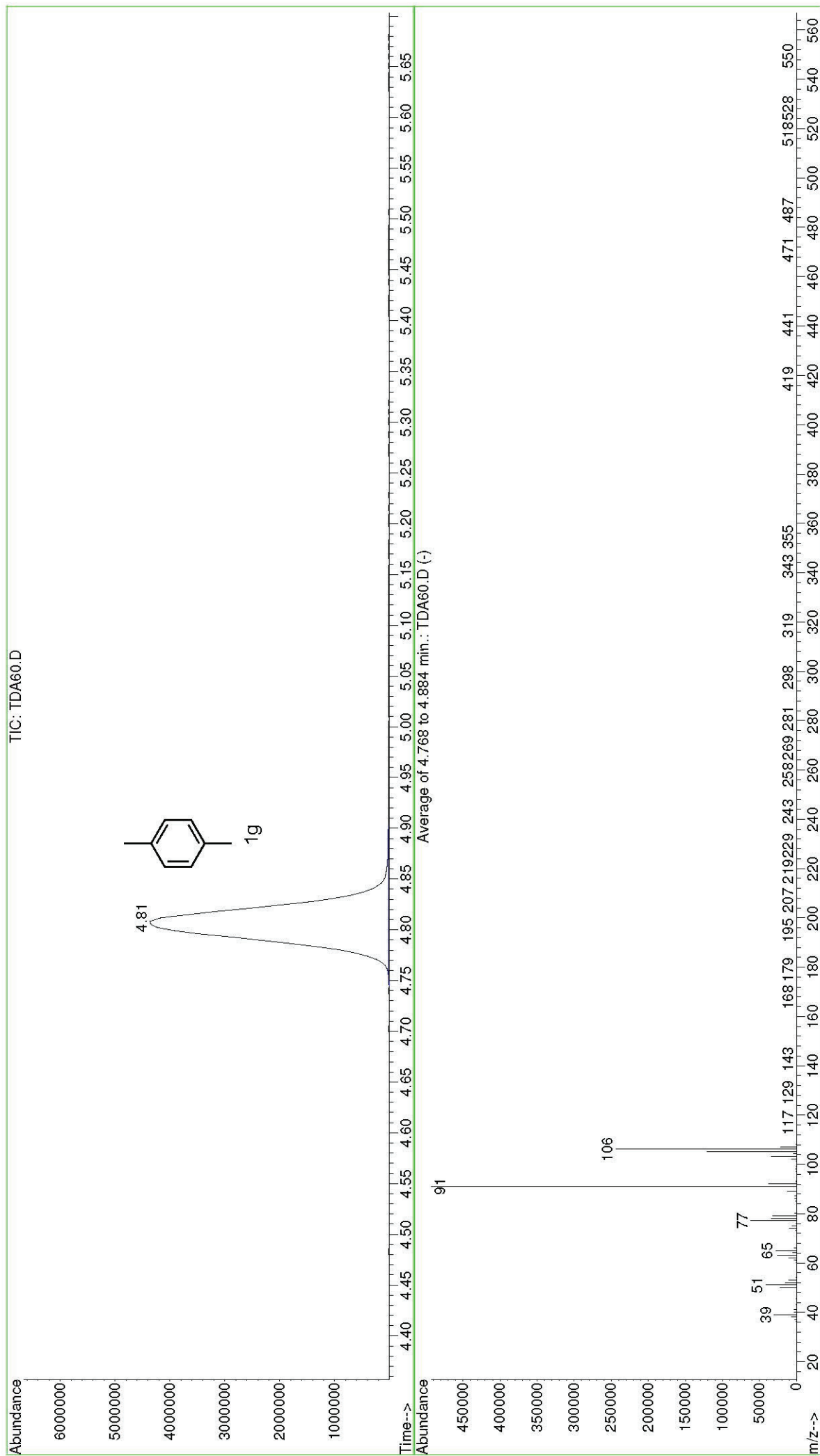
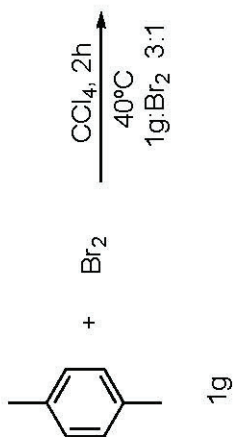
Acquired : 22 Jan 2014 7:02 using AcqMethod JMF60

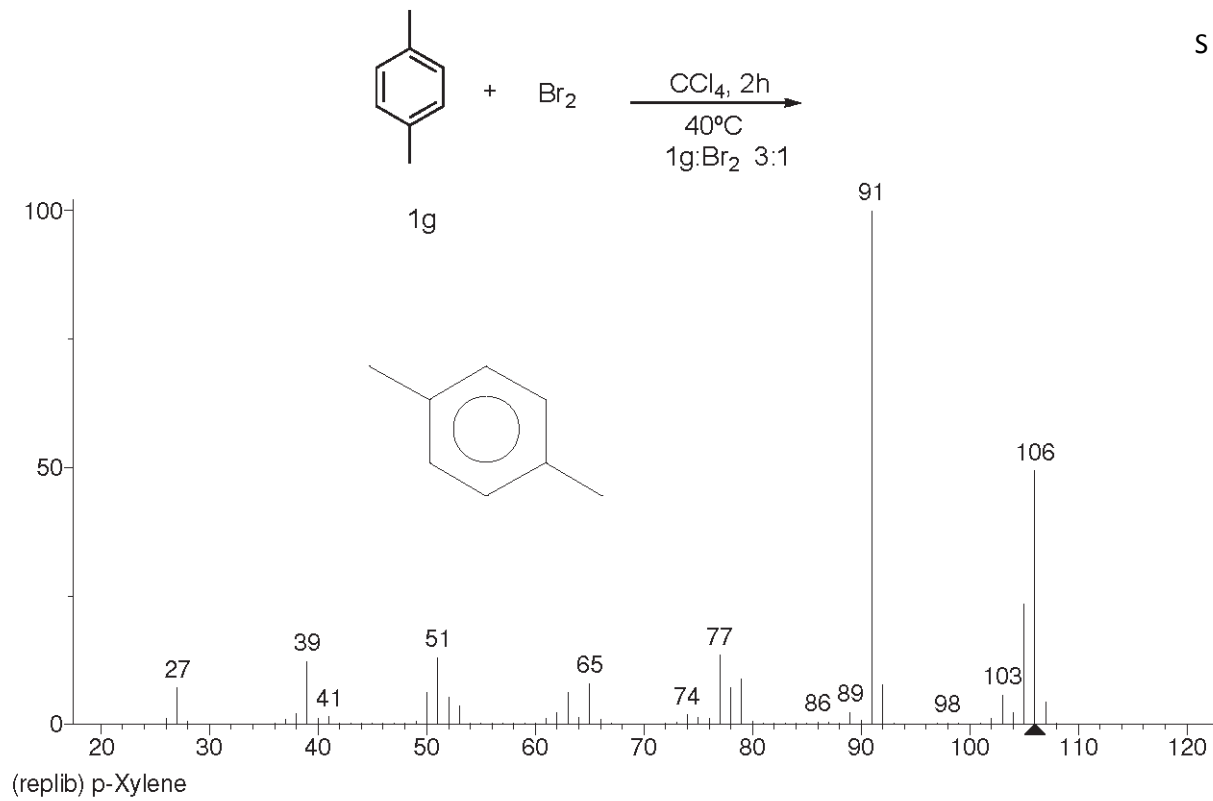
Instrument : Instrument

Sample Name:

Misc Info :

Vial Number: 29





File : D:\ASENSIO\THAIS\TDA60.D

Operator :

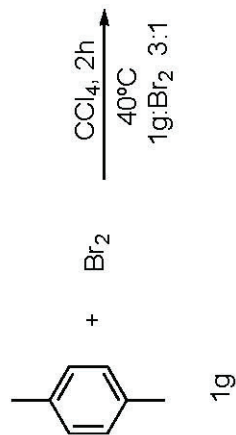
Acquired : 22 Jan 2014 7:02 using AcqMethod JMF60

Instrument : Instrument

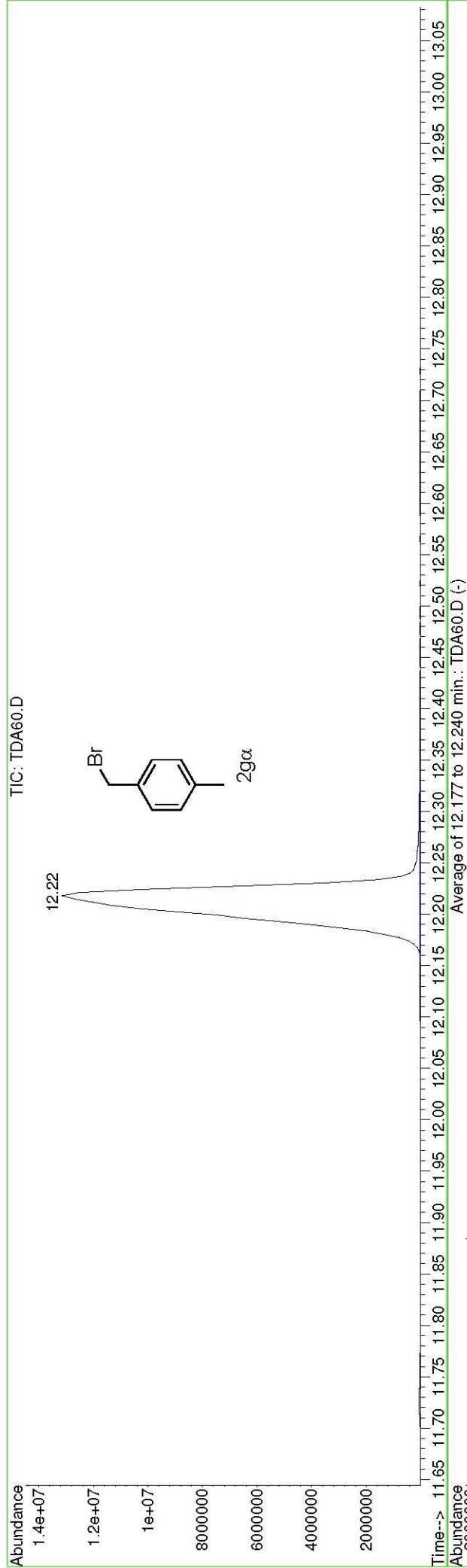
Sample Name:

Misc Info :

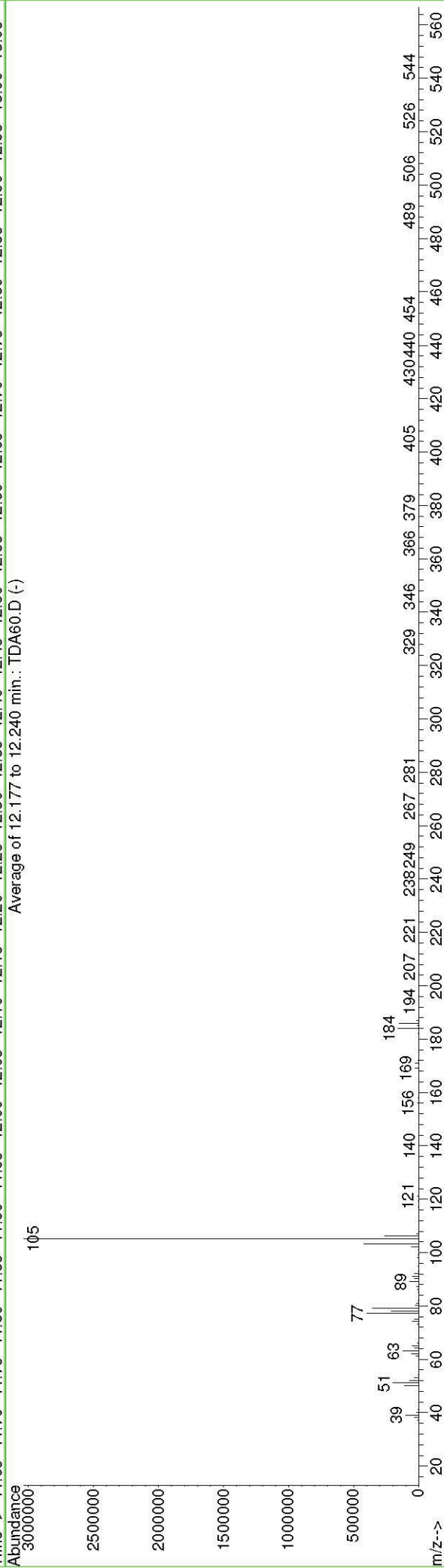
Vial Number: 29

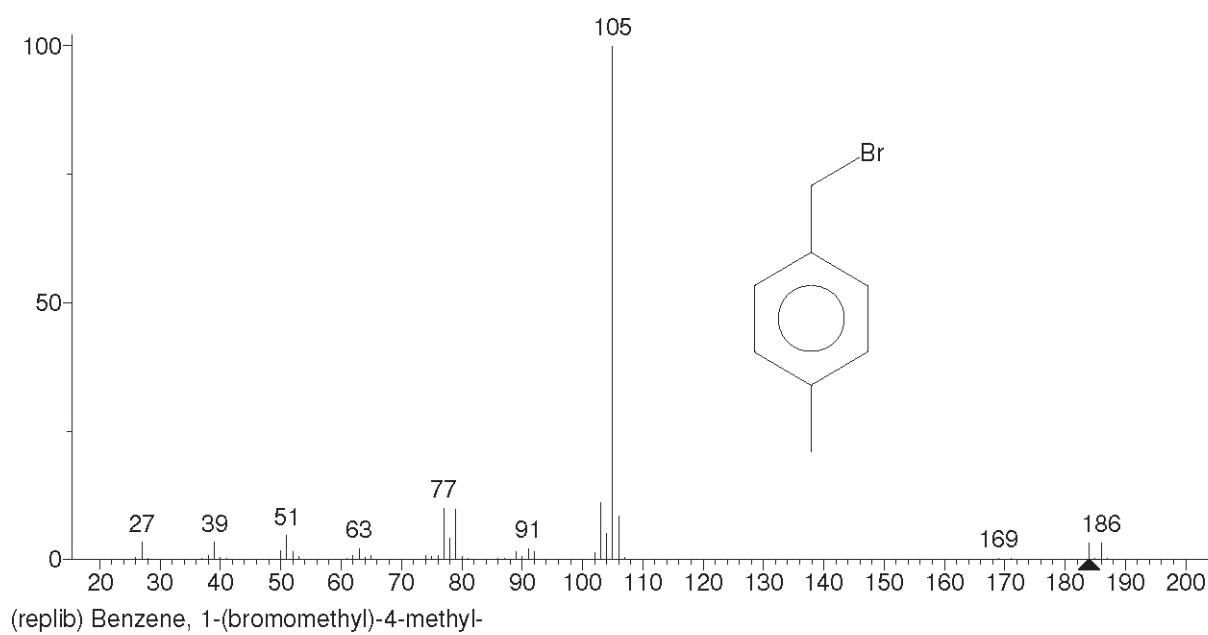
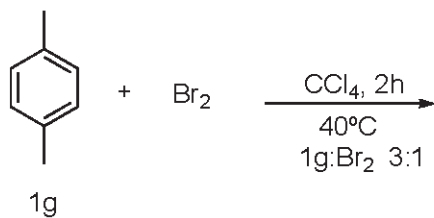


TIC: TDA60.D



Average of 12.177 to 12.240 min.: TDA60.D (-)





File : D:\ASENSIO\THAIS\JRL17.D

Operator :

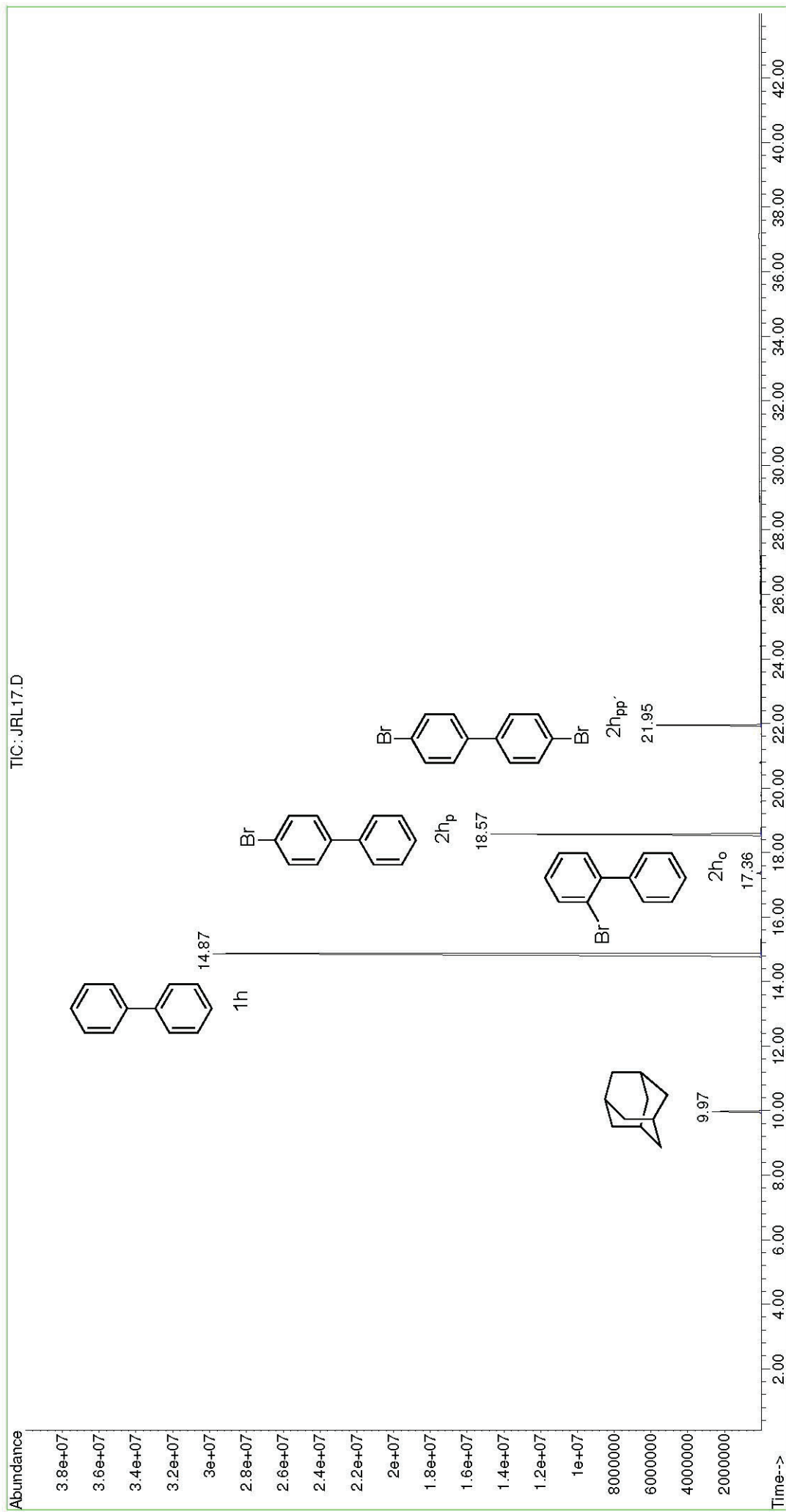
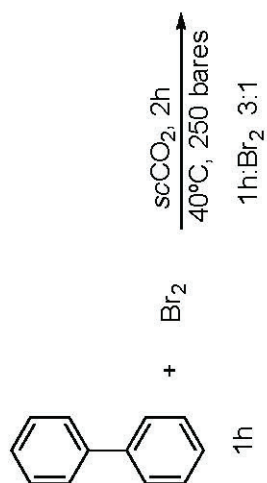
Acquired : 1 Feb 2014 10:20 using AcqMethod JMF60

Instrument : Instrumen

Sample Name: VIDRIO

Misc Info :

Vial Number: 29



File : D:\ASENSIO\THAIS\JRL17.D

Operator :

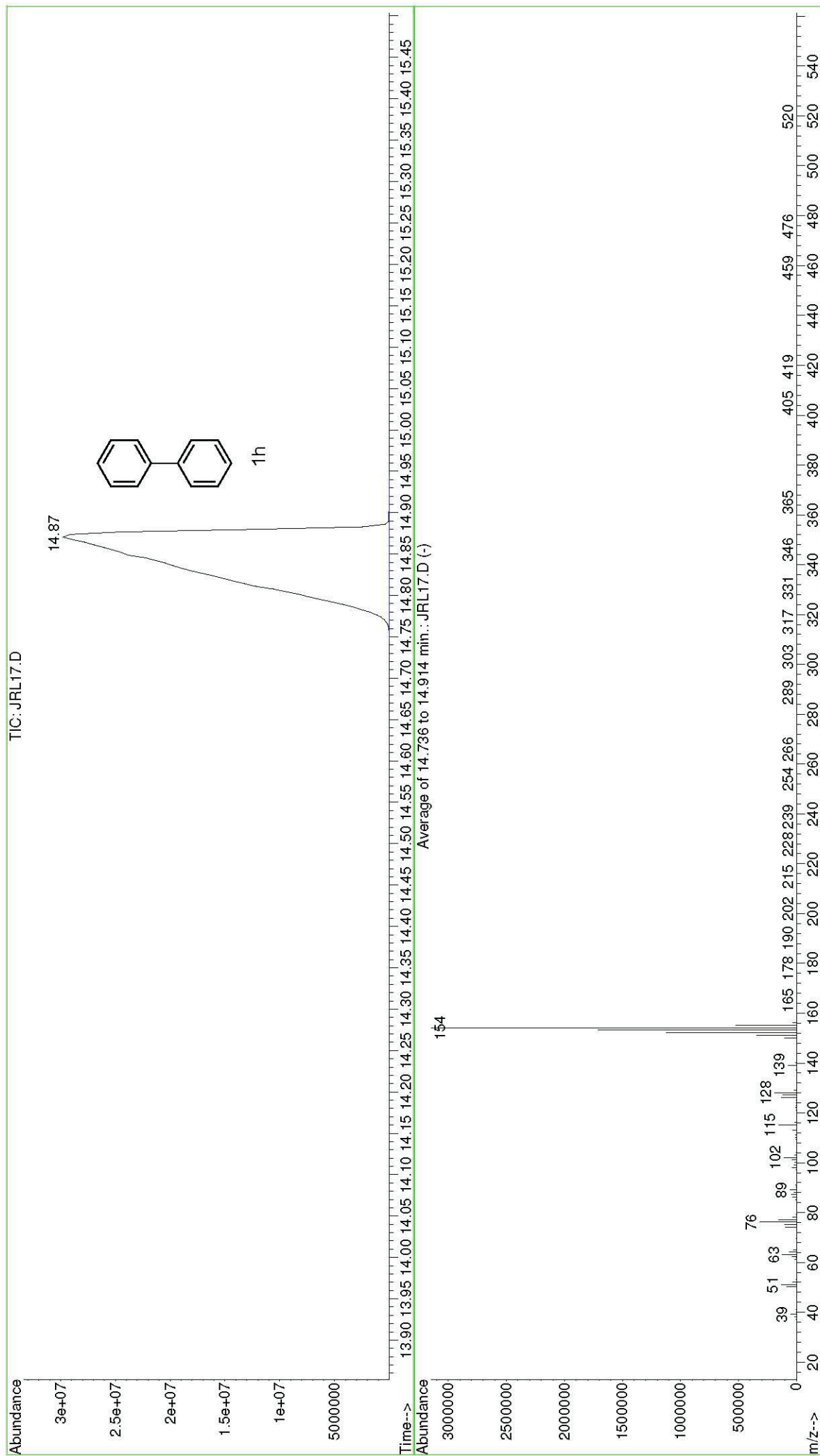
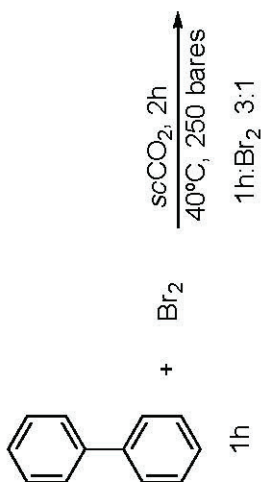
Acquired : 1 Feb 2014 10:20 using AcqMethod JMF60

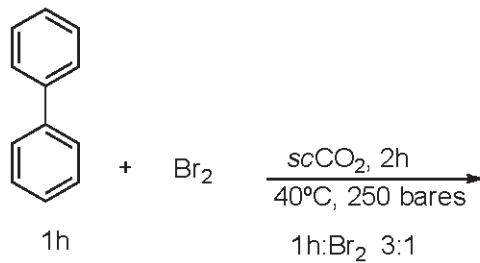
Instrument : Instrument

Sample Name : VIDRIO

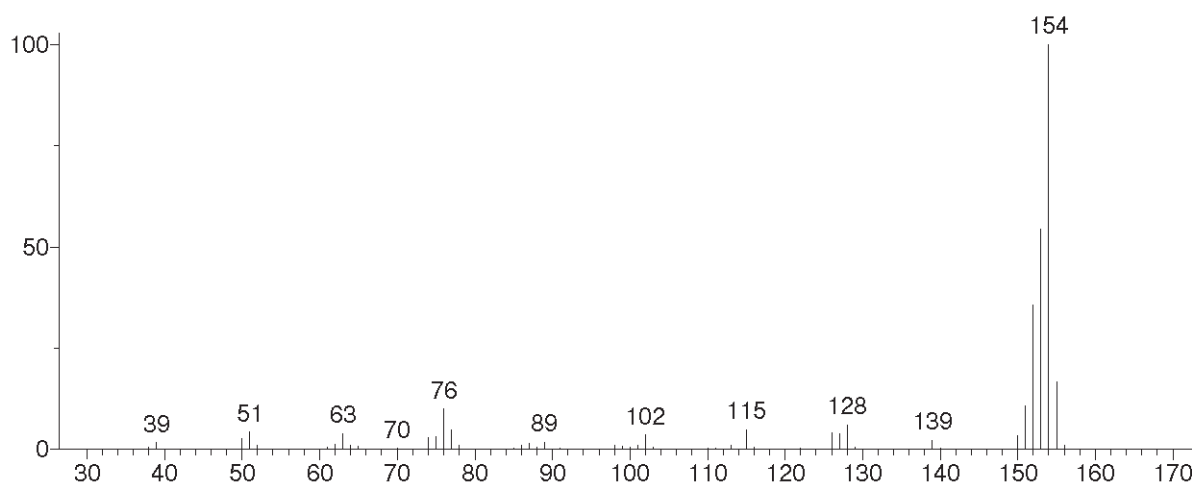
Misc Info :

Vial Number: 29

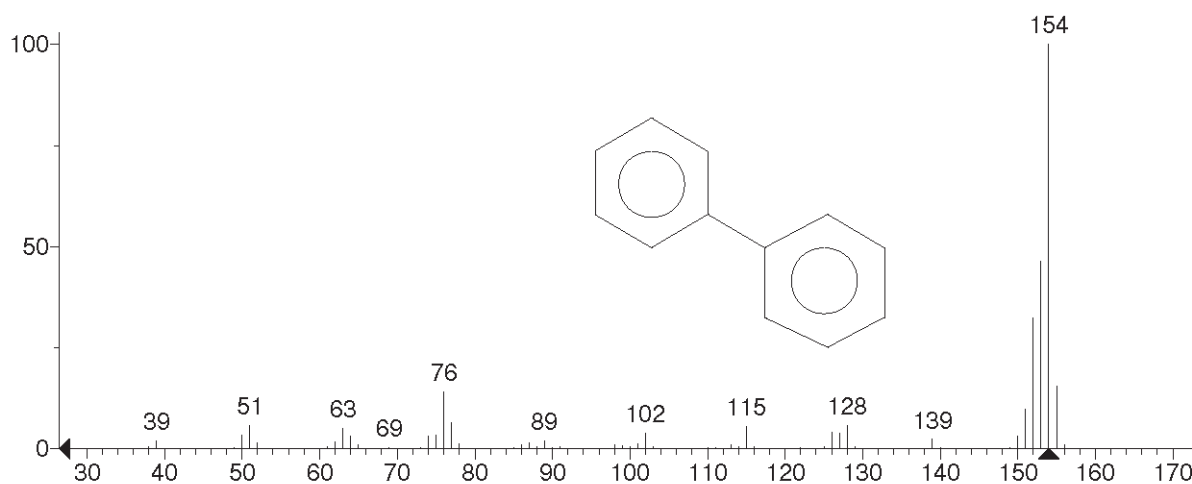




Unknown: Average of 14.758 to 14.917 min.: JRL17.D
Compound in Library Factor = 146



Hit 1 : Biphenyl
C₁₂H₁₀; MF: 963; RMF: 964; Prob 52.0%; CAS: 92-52-4; Lib: replib; ID: 20367.



File : D:\ASENSIO\THAIS\JRL17.D

Operator :

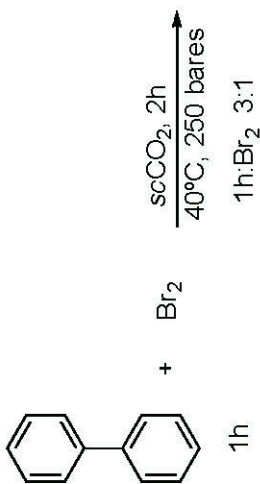
Acquired : 1 Feb 2014 10:20 using AcqMethod JMF60

Instrument : Instrument

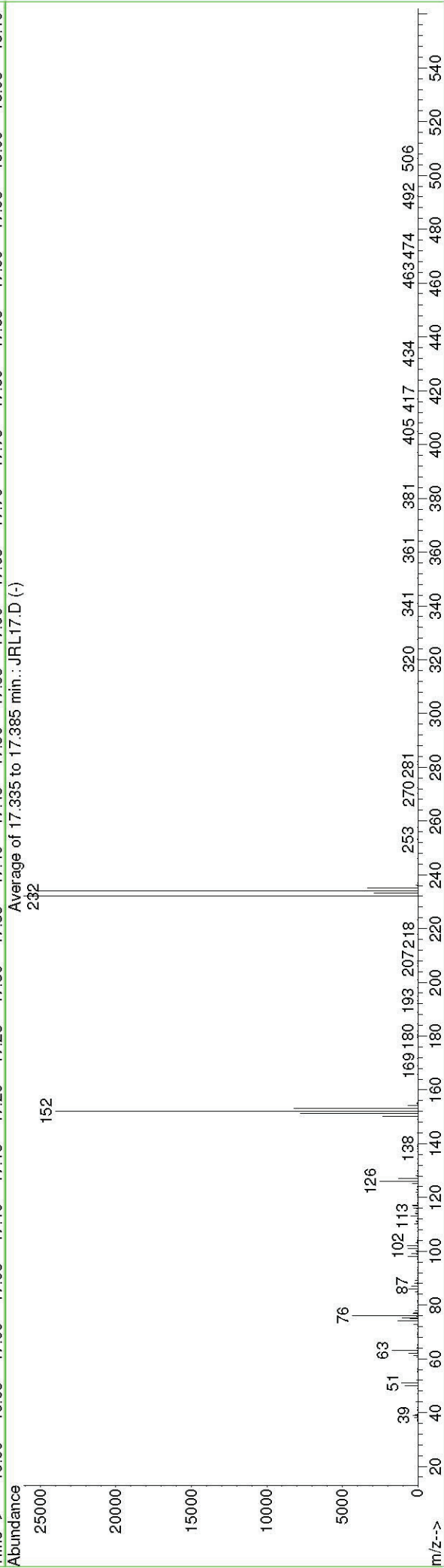
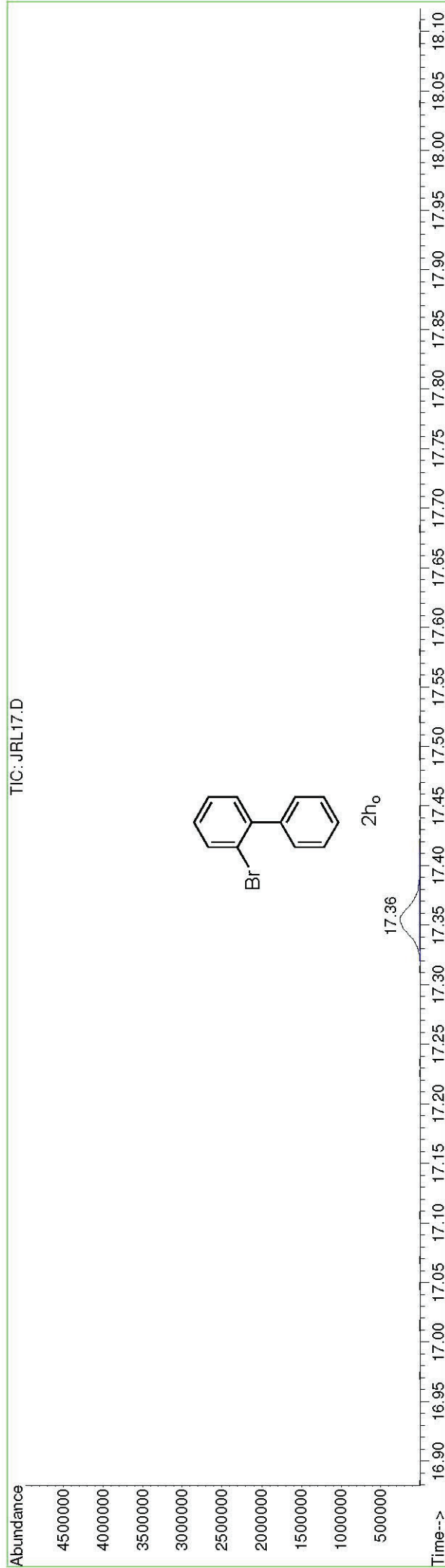
Sample Name: VIDRIO

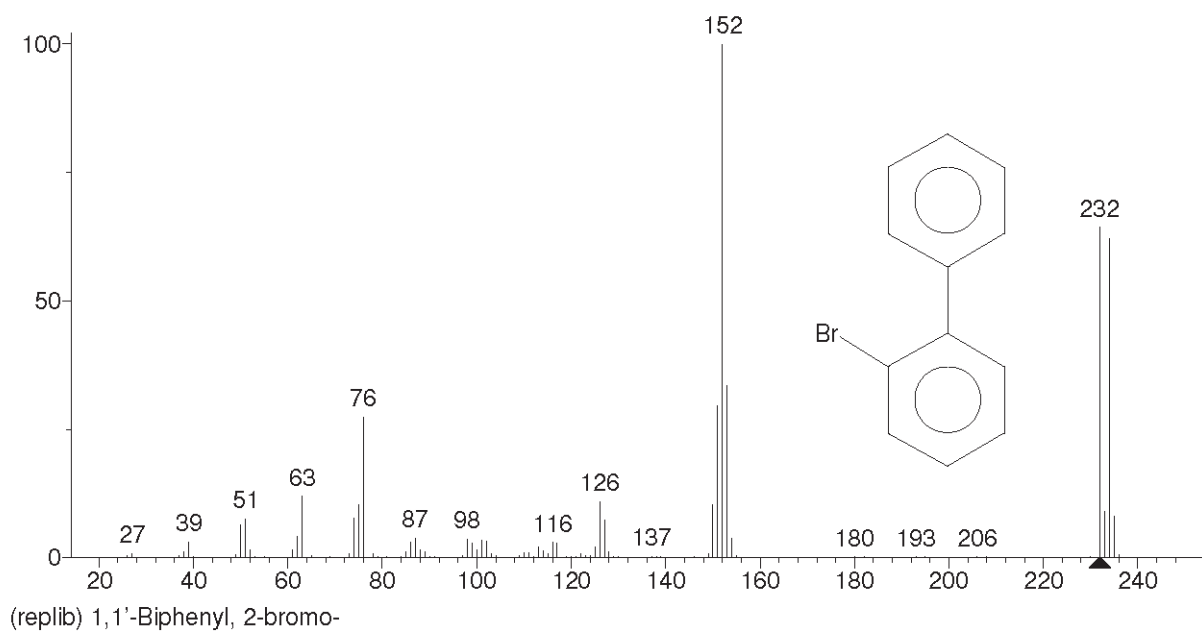
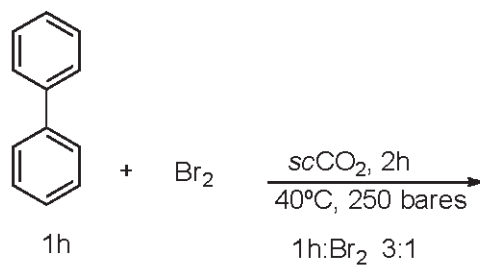
Misc Info :

Vial Number: 29

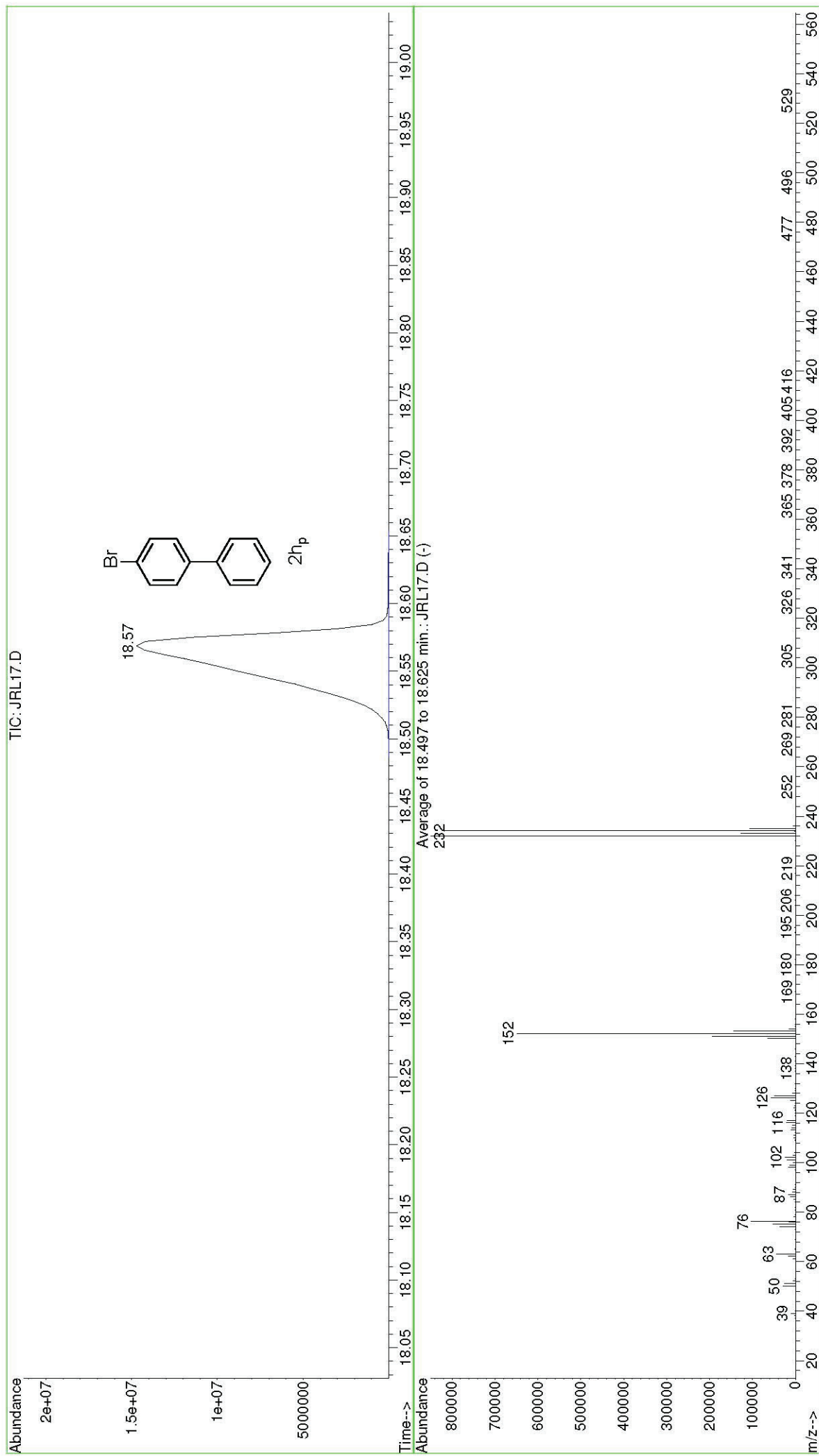
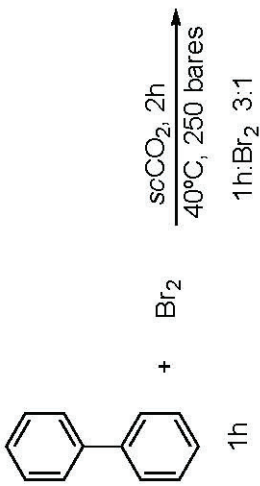


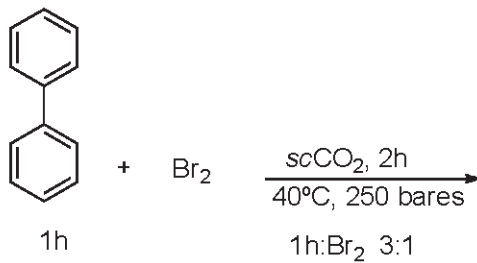
TIC: JRL17.D



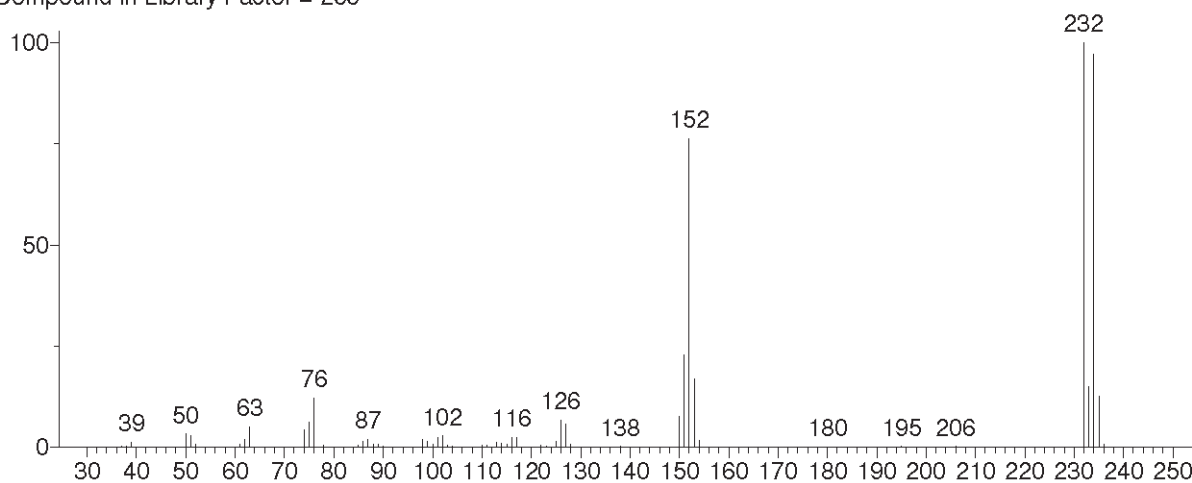


File : D:\ASENSIO\THAIS\JRL17.D
 Operator :
 Acquired : 1 Feb 2014 10:20 using AcqMethod JMF60
 Instrument : Instrument
 Sample Name : VIDRIO
 Misc Info :
 Vial Number: 29





Unknown: Average of 18.497 to 18.625 min.: JRL17.D
Compound in Library Factor = 255



Hit 1 : 1,1'-Biphenyl, 4-bromo- (CAS)
C₁₂H₉Br; MF: 973; RMF: 976; Prob 46.4%; CAS: 92-66-0; Lib: wiley7n; ID: 161792.



File : D:\ASENSIO\THAIS\JRL17.D

Operator :

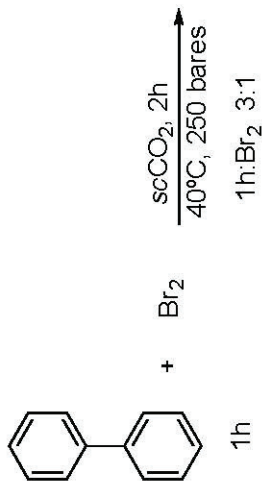
Acquired : 1 Feb 2014 10:20 using AcqMethod JMF60

Instrument : Instrument

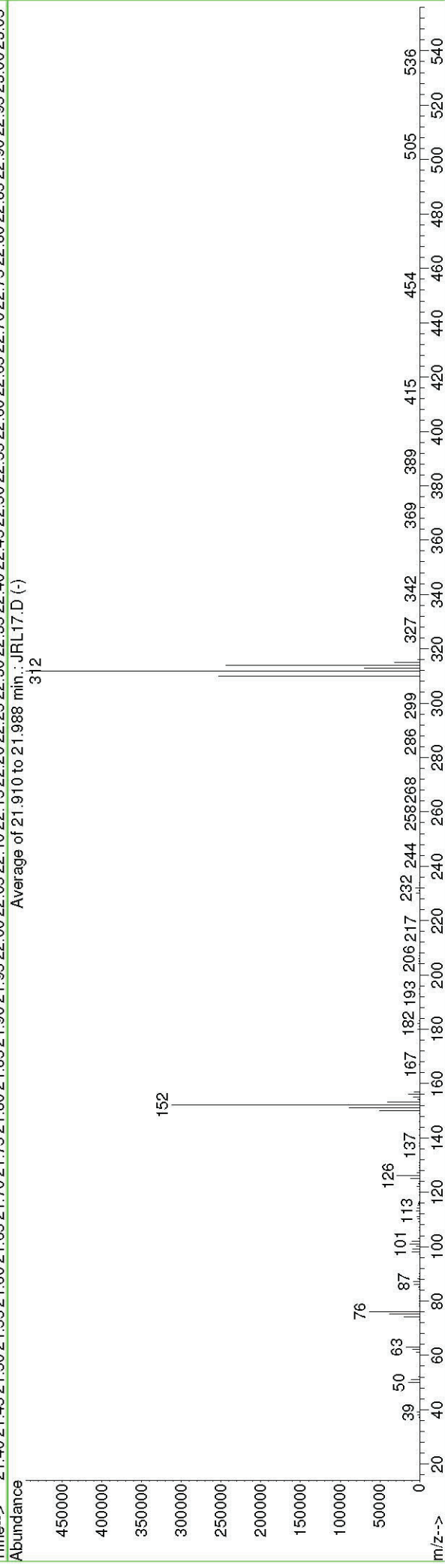
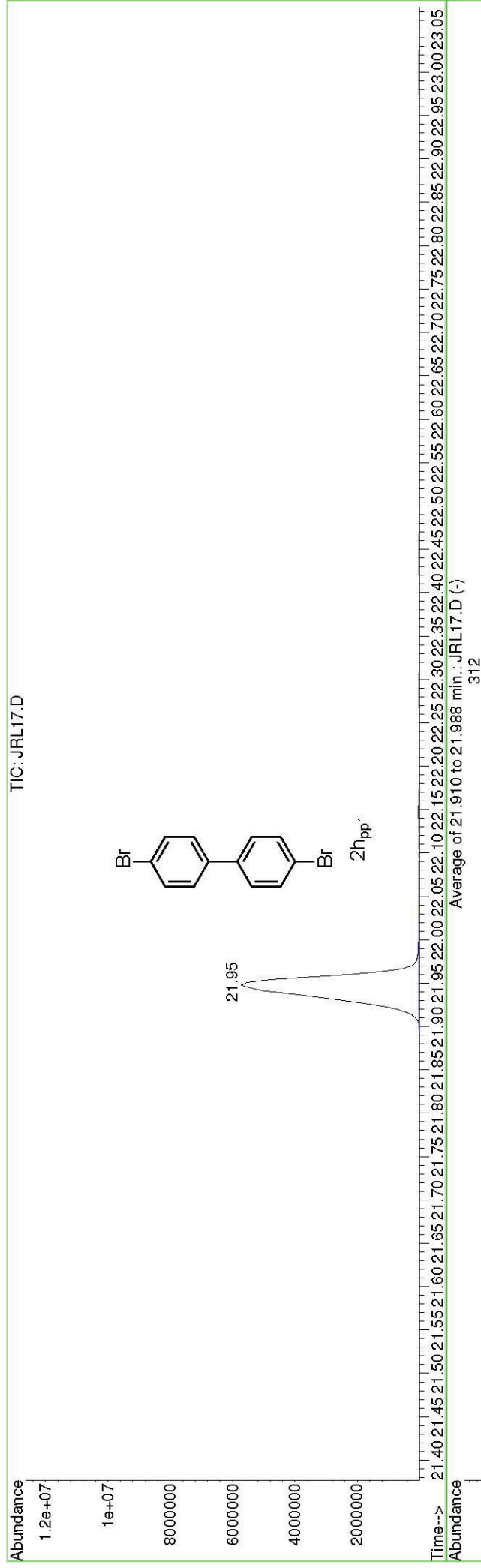
Sample Name: VIDRIO

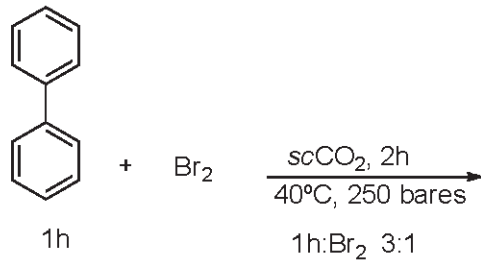
Misc Info :

Vial Number: 29

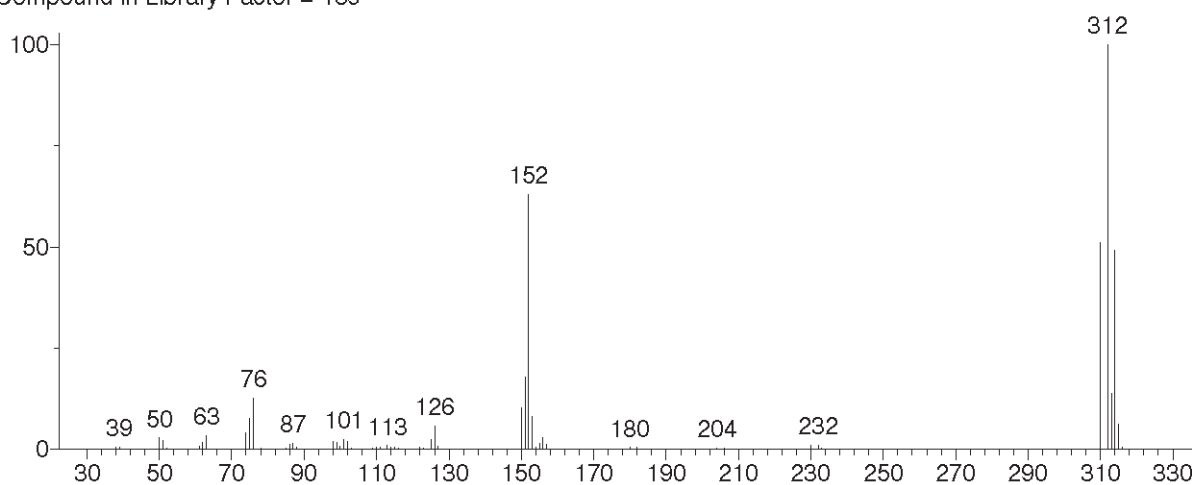


TIC: JRL17.D

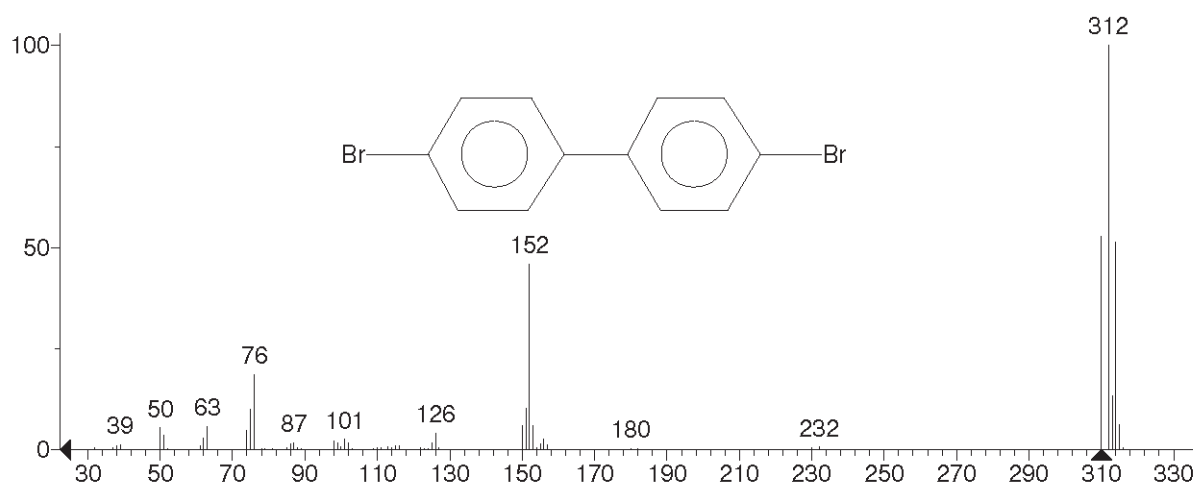




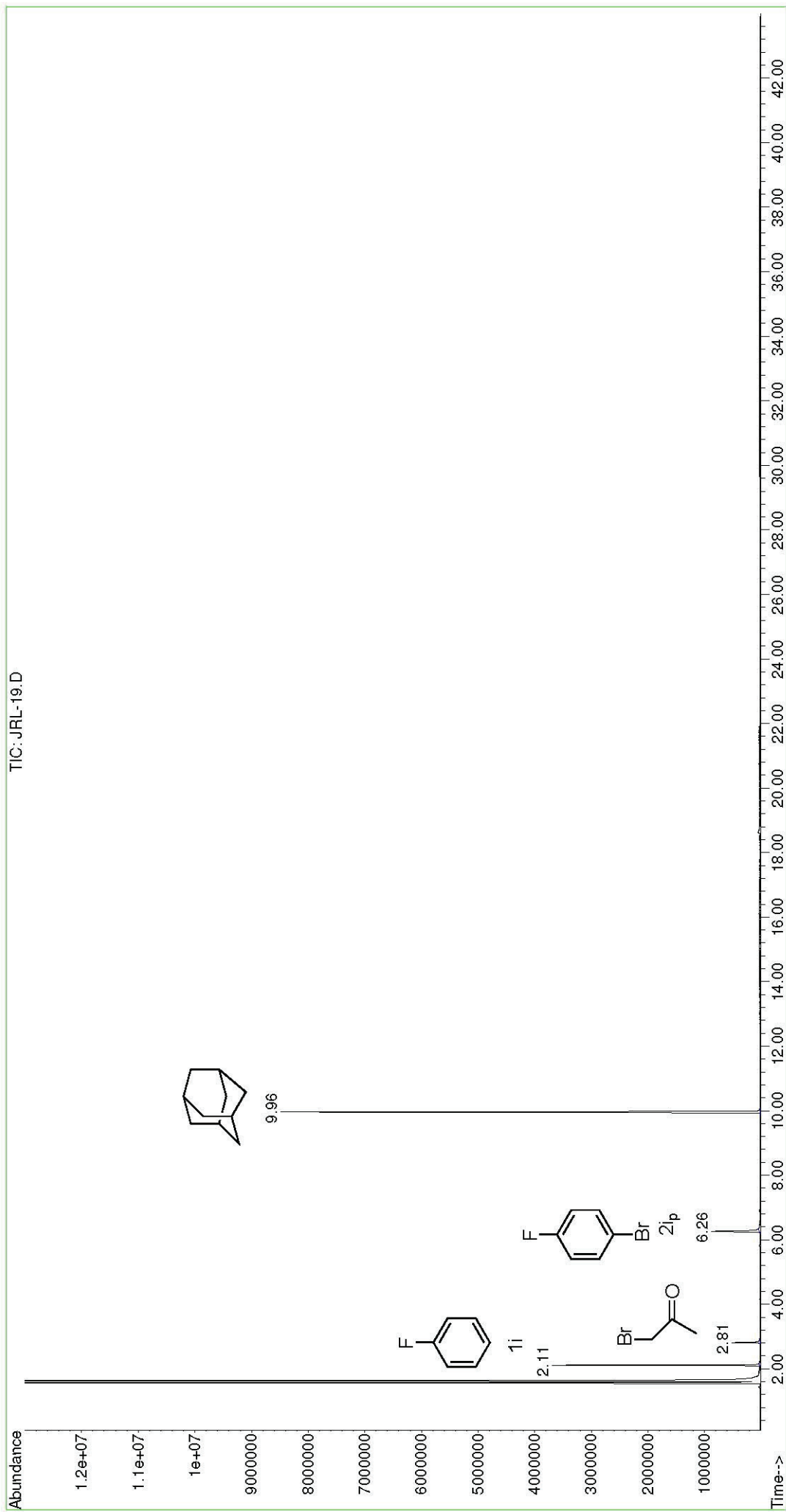
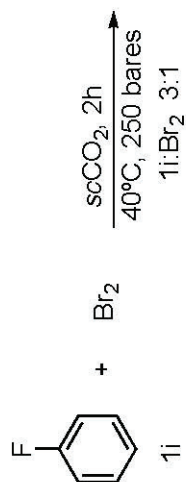
Unknown: Average of 21.910 to 21.988 min.: JRL17.D
Compound in Library Factor = 189



Hit 2 : 1,1'-Biphenyl, 4,4'-dibromo-
C₁₂H₈Br₂; MF: 935; RMF: 935; Prob 29.7%; CAS: 92-86-4; Lib: wiley7n; ID: 259978.



File : D:\ASENSIO\JAVI\JRL-19.D
Operator :
Acquired : 6 Feb 2014 14:14 using AcqMethod JMF60
Instrument : Instrumen
Sample Name: VIDRIO
Misc Info :
Vial Number: 8



File : D:\ASENSIO\JAVI\JRL-19.D

Operator :

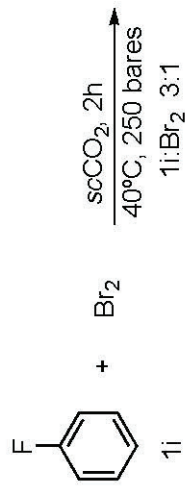
Acquired : 6 Feb 2014 14:14 using AcqMethod JMF60

Instrument : Instrument

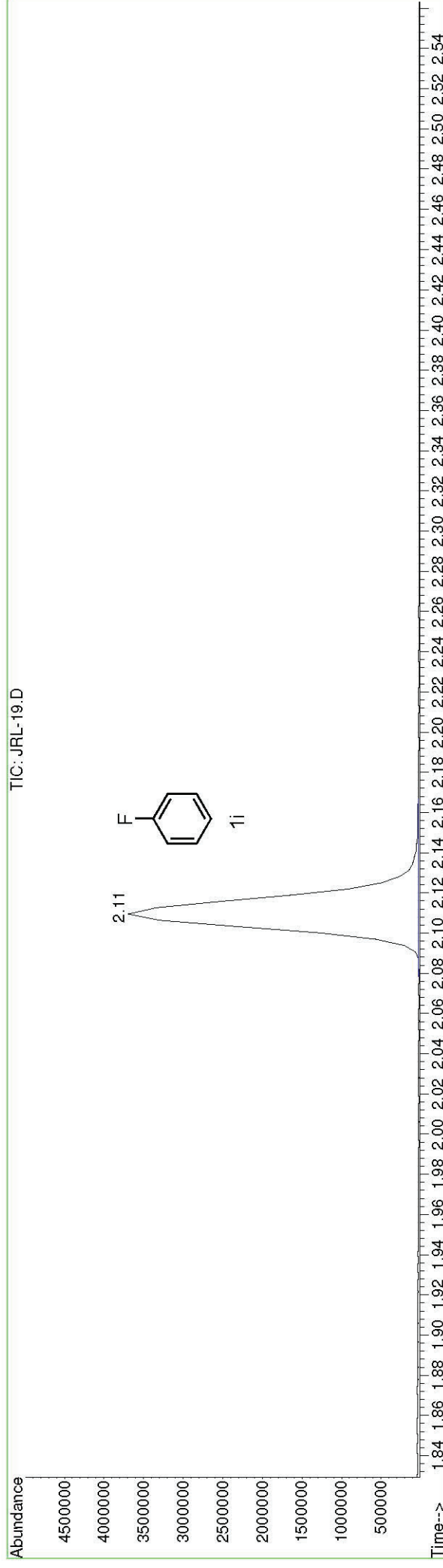
Sample Name: VIDRIO

Misc Info :

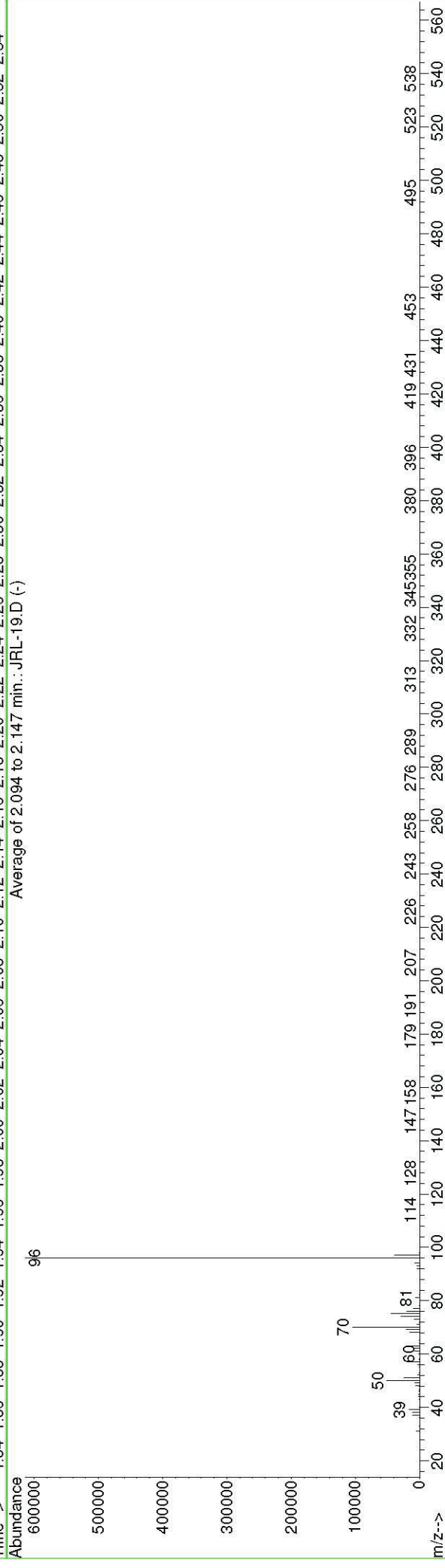
Vial Number: 8

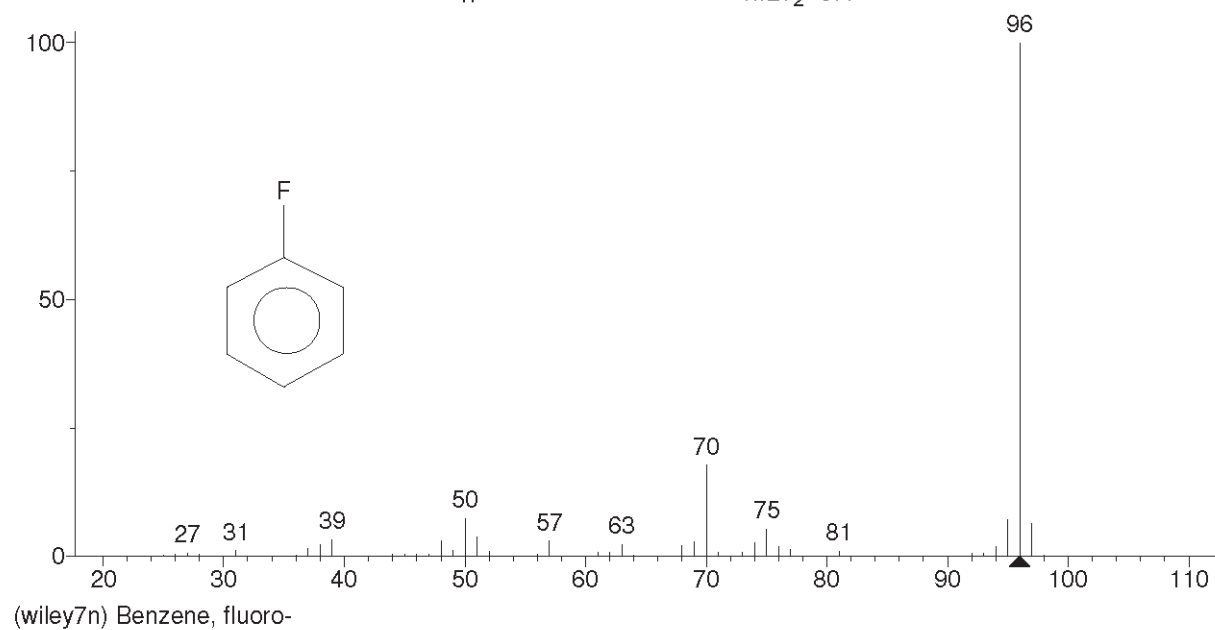
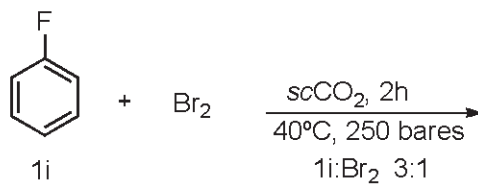


TIC: JRL-19.D



Average of 2.094 to 2.147 min.: JRL-19.D (-)





File : D:\ASENSIO\JAVI\JRL-19.D

Operator :

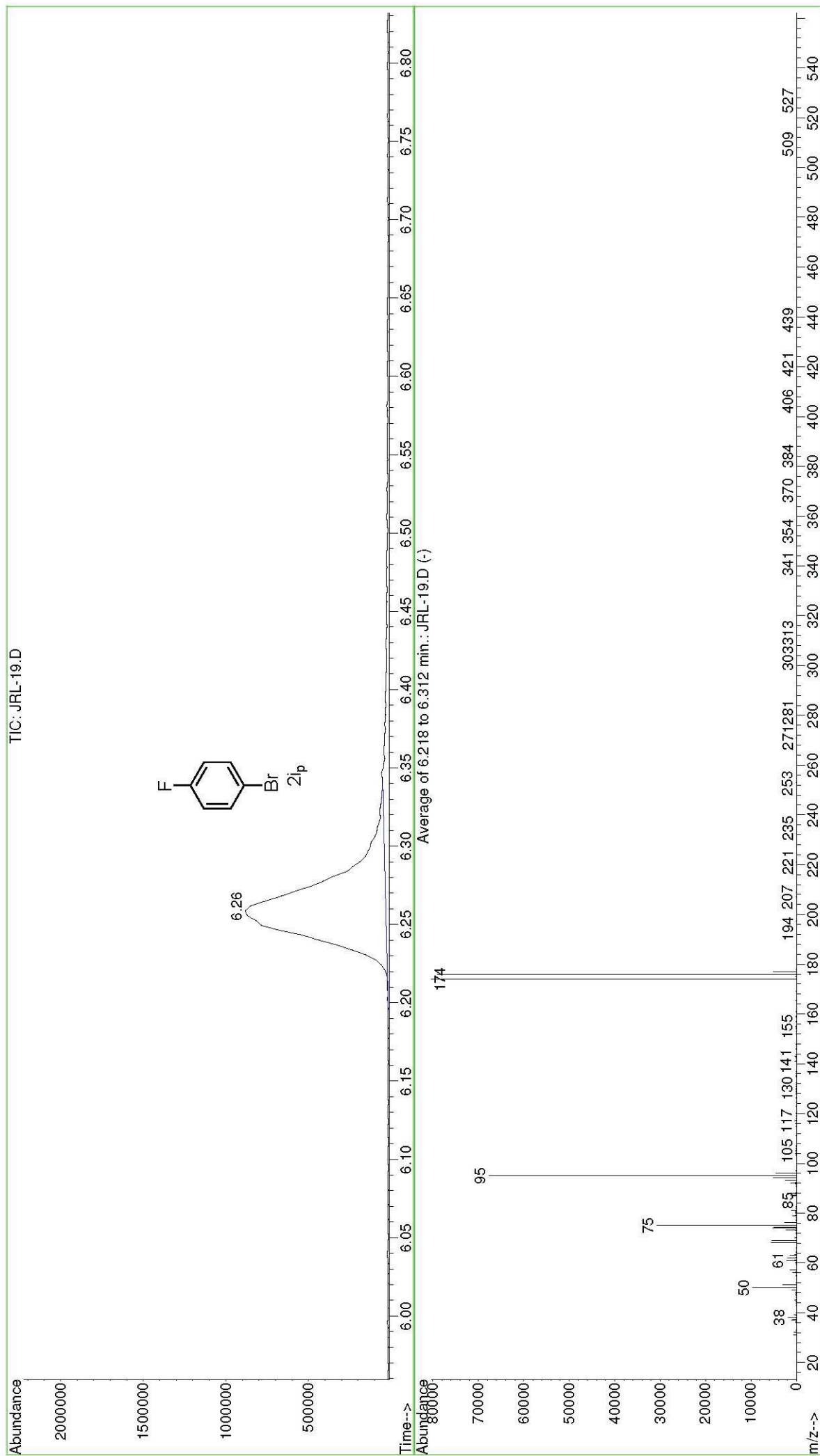
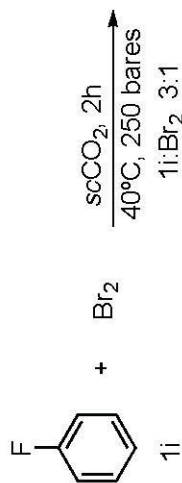
Acquired : 6 Feb 2014 14:14 using AcqMethod JMF60

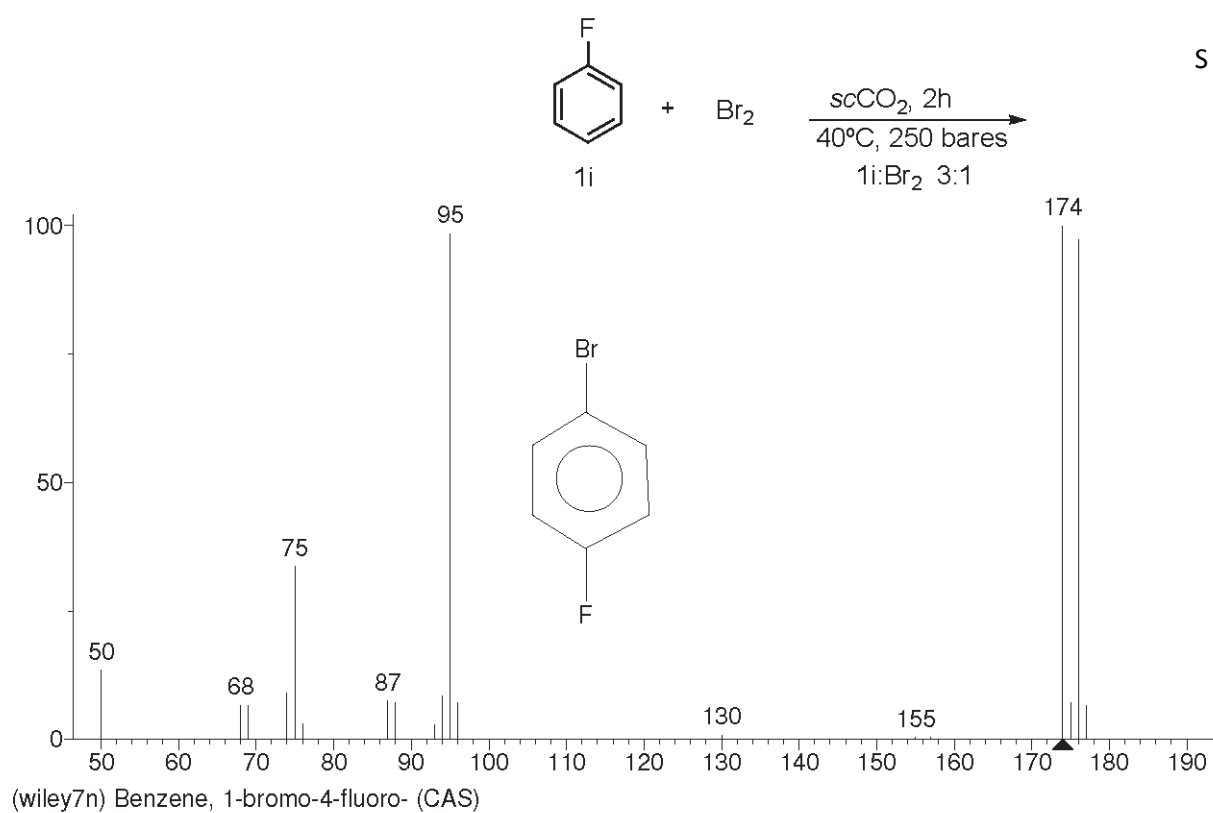
Instrument : Instrument

Sample Name: VIDRIO

Misc Info :

Vial Number: 8





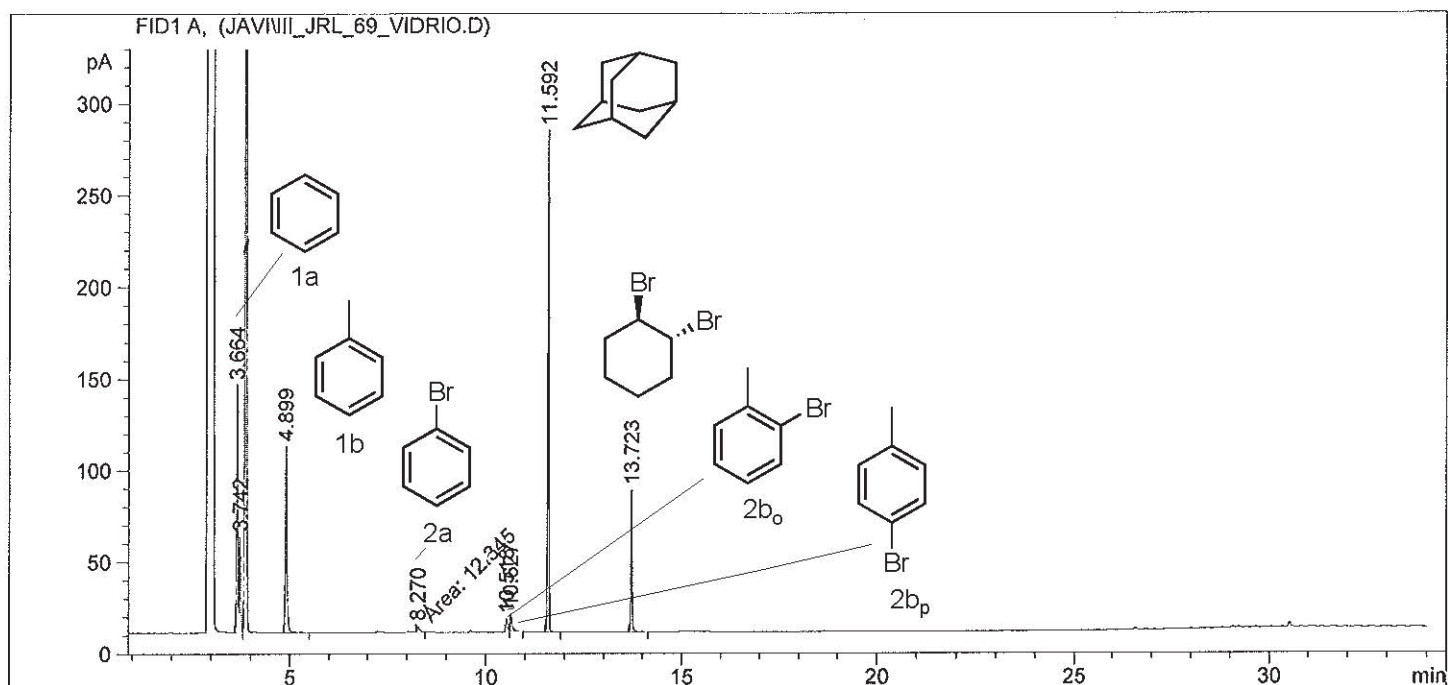
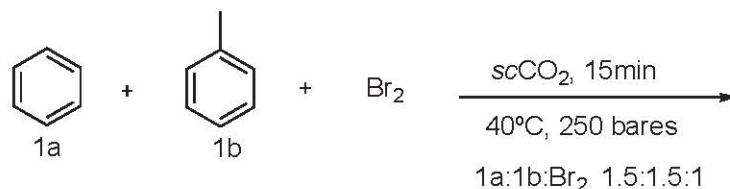
=====

Acq. Operator : javi
Acq. Instrument : Instrument 2 Location : -
Injection Date : 09-May-14, 13:31:55 Inj : 1
Inj Volume : Manually

Acq. Method : C:\CHEM32\2\METHODS\JAIME.M
Last changed : 5/7/2014 11:46:20 AM by javi
Analysis Method : C:\CHEM32\2\METHODS\ROSSELLAM.M
Last changed : 5/9/2014 2:16:45 PM by Rossella
(modified after loading)

Method Info : Columna apolar HP 1 J& W 30 mt, 0,32 mmID, 0,25 microm film thickness
instalada 2-6-2011

Sample Info :



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Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

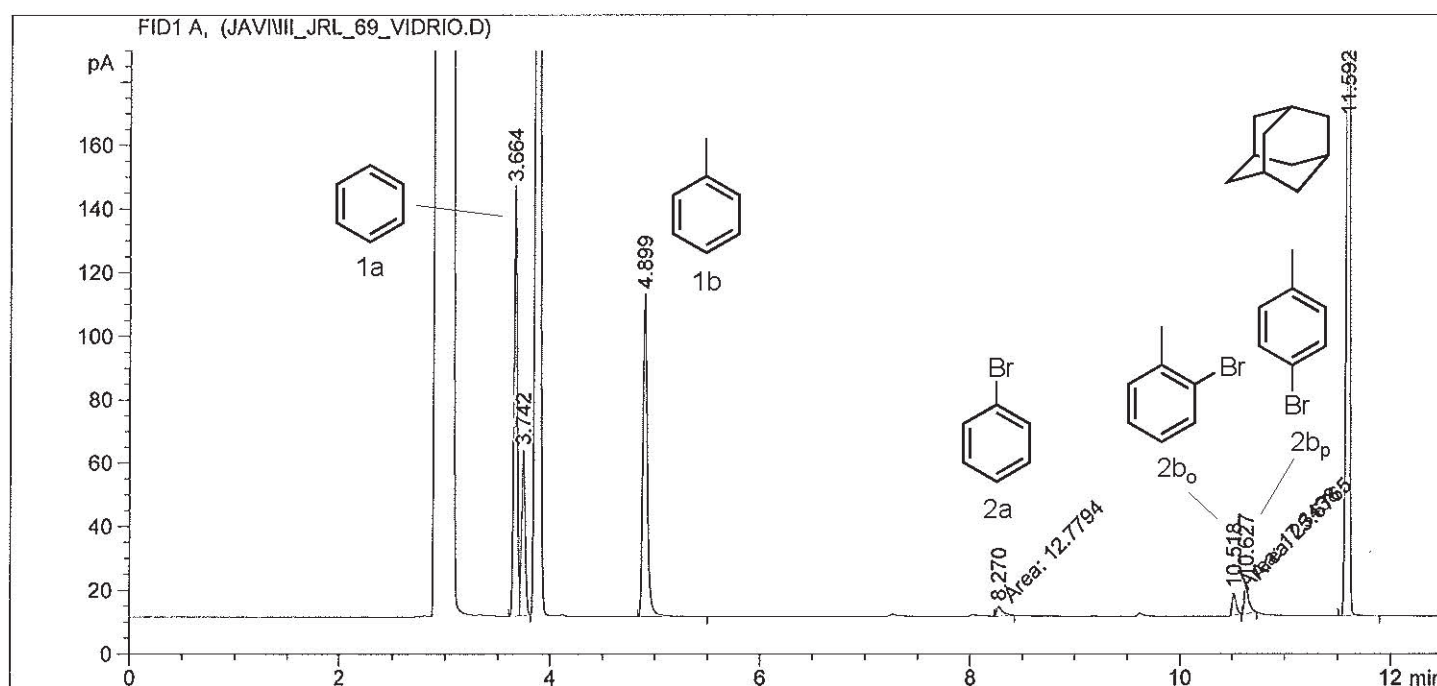
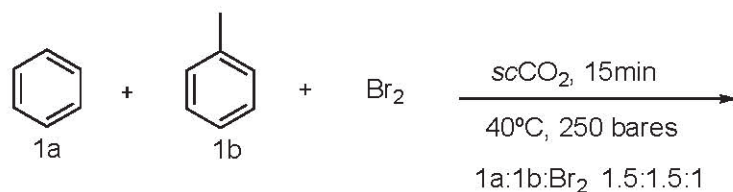
=====

Acq. Operator : javi
Acq. Instrument : Instrument 2
Injection Date : 09-May-14, 13:31:55
Location : -
Inj : 1
Inj Volume : Manually

Acq. Method : C:\CHEM32\2\METHODS\JAIME.M
Last changed : 5/7/2014 11:46:20 AM by javi
Analysis Method : C:\CHEM32\2\METHODS\ROSSELLAM.M
Last changed : 7/29/2014 4:53:58 PM by Rossella
(modified after loading)

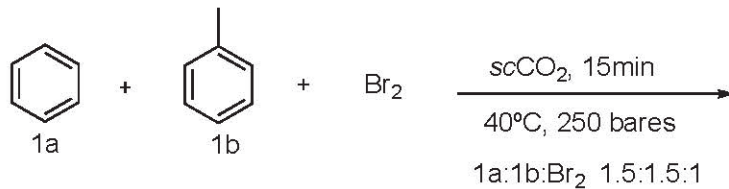
Method Info : Columna apolar HP 1 J& W 30 mt, 0,32 mmID, 0,25 microm film thickness
instalada 2-6-2011

Sample Info :



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs



S 194

Data File C:\CHEM32\2\DATA\JAVI\III_JRL_69_VIDRIO.D

Sample Name: III_JRL_69_vidrio

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	3.664	BV	0.0337	297.69736	134.97183	18.98154
2	3.742	VB	0.0366	122.55346	51.78925	7.81416
3	4.899	BB	0.0454	298.97925	101.45646	19.06328
4	8.270	MM	0.0687	12.34504	2.99344	0.78713
5	10.518	BB	0.0388	17.74319	6.93965	1.13133
6	10.627	BB	0.0483	31.61974	9.37802	2.01611
7	11.592	BB	0.0352	611.90332	272.99268	39.01569
8	13.723	BB	0.0356	175.51039	76.94442	11.19075

Totals : 1568.35174 657.46573

*** End of Report ***

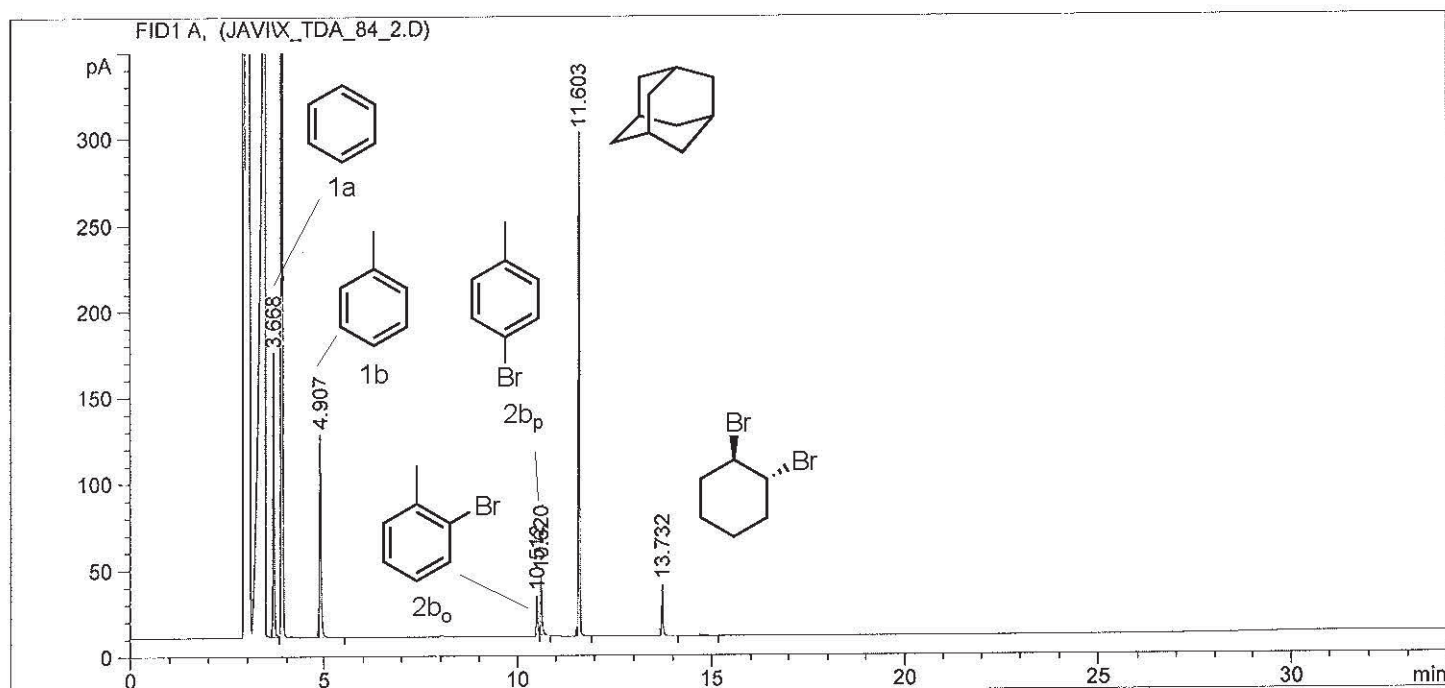
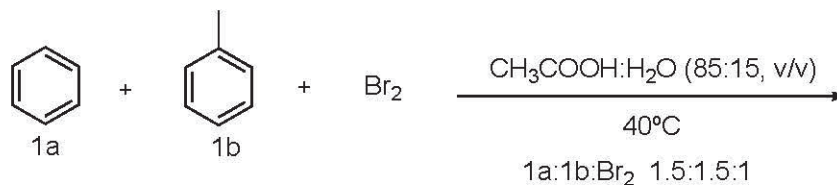
Acq. Operator : javi
Acq. Instrument : Instrument 2
Injection Date : 08-Apr-14, 12:26:57

Location : -
Inj : 1
Inj Volume : Manually

Acq. Method : C:\CHEM32\2\METHODS\JAIME.M
Last changed : 4/8/2014 10:18:54 AM by javi
Analysis Method : C:\CHEM32\2\METHODS\JAIME.M
Last changed : 4/8/2014 1:07:10 PM by Mateo
(modified after loading)

Method Info : Column apolar HP 1 J& W 30 mt, 0,32 mmID, 0,25 microm film thickness
instalada 2-6-2011

Sample Info



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID1 A,

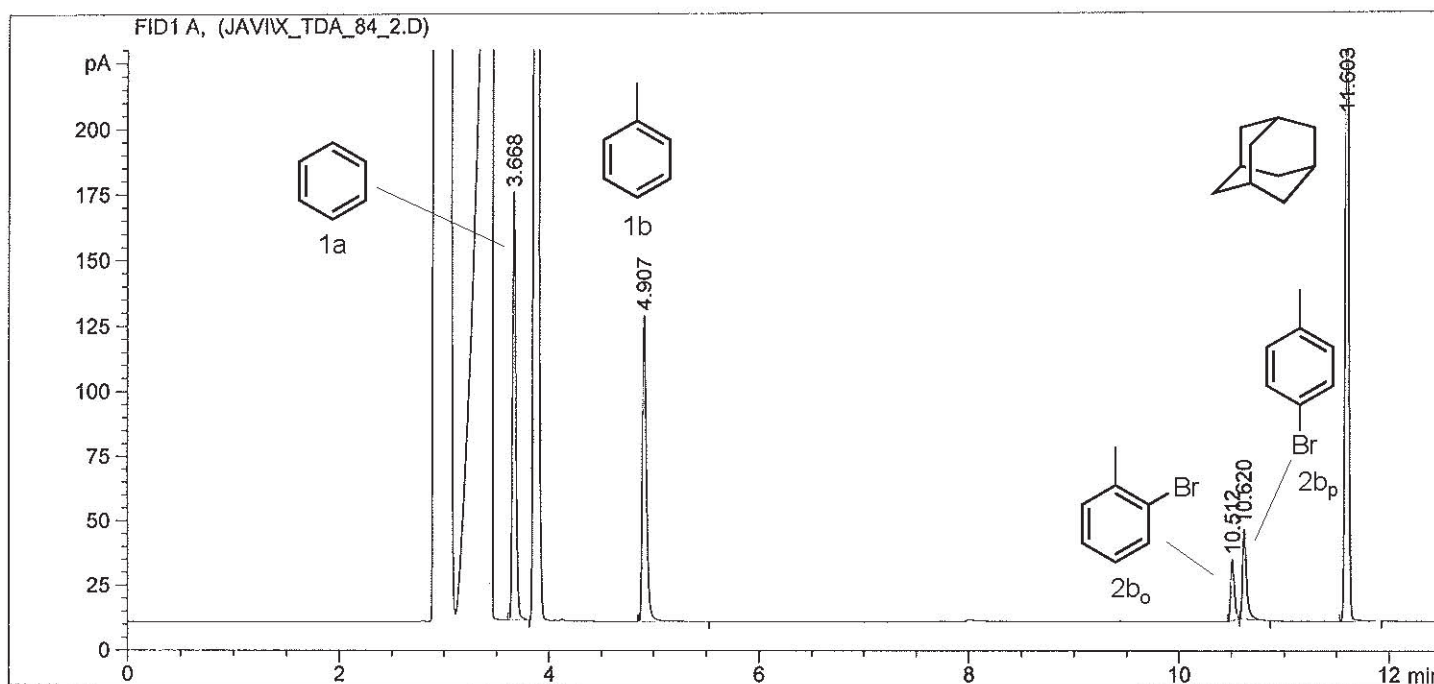
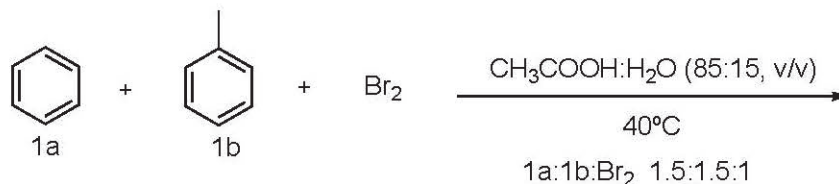
=====

Acq. Operator : javi
Acq. Instrument : Instrument 2 Location : -
Injection Date : 08-Apr-14, 12:26:57 Inj : 1
Inj Volume : Manually

Acq. Method : C:\CHEM32\2\METHODS\JAIME.M
Last changed : 4/8/2014 10:18:54 AM by javi
Analysis Method : C:\CHEM32\2\METHODS\ROSSELLAM.M
Last changed : 7/29/2014 4:53:02 PM by Rossella
(modified after loading)

Method Info : Columna apolar HP 1 J& W 30 mt, 0,32 mmID, 0,25 microm film thickness
instalada 2-6-2011

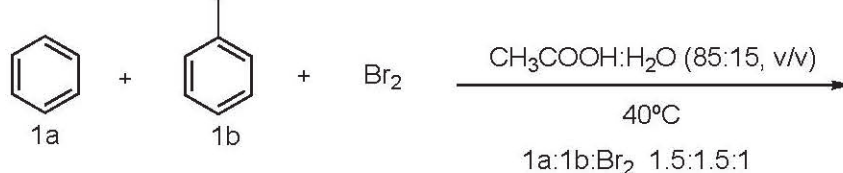
Sample Info :



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Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID1 A,



Data File C:\CHEM32\2\DATA\JAVI\X_TDA_84_2.D

Sample Name: X_TDA_84_2

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	3.668	BB	0.0338	363.10007	163.92003	23.11447
2	4.907	BB	0.0427	329.41364	117.38147	20.97004
3	10.512	BB	0.0359	53.09996	22.98953	3.38027
4	10.620	BB	0.0387	86.42743	33.94022	5.50186
5	11.603	BB	0.0350	649.14209	290.79687	41.32353
6	13.732	BB	0.0369	70.87194	29.61027	4.51161
7	14.599	BB	0.0504	18.82243	5.17991	1.19821

Totals : 1570.87754 663.81830

*** End of Report ***