# Supporting Information

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## Analytical Methods

On-DNA reactions were analyzed by LCMS. Samples (ca. 100 pmol) were injected onto a reverse-phase chromatography column (Targa C18, 5µ, 2.1 x 40 mm) and eluted (15 – 70% solvent B over 7 minutes, 0.36 mL/min flow rate, 10-60% solvent B over 3 minutes, 0.55 mL/min flow rate, or 10-90% solvent B over 1minutes, 1 mL/min flow rate ; Solvent A: 0.75% hexafluoroisopropanol (HFIP) / 0.38% triethylammonium acetate /10 µM EDTA in deionized water; Solvent B: 0.75% HFIP/0.38% TEAA/10 µM EDTA in 90/10 methanol/water) with monitoring at 260 nm. Effluent was analyzed on a ThermoFinnigan Advantage electrospray mass spectrometer in negative ion mode. When necessary, mass deconvolution was achieved using ProMass software (Novatia). Chromatographic purification was likewise achieved using reverse-phase liquid chromatography (Gemini C18 5µ, 30 x 100 mm; Solvent A: pH 7.5 50 mM triethylammonium acetate; Solvent B: 1% water in acetonitrile).

Yields were calculated by examination of the UV and TIC traces of the LCMS chromatograms.

**Materials.** All the reagents were purchased through vendors. They were dissolved in an appropriate solvent before use. DNA headpiece (**HP**) (5′-/5Phos/GAGTCA/iSp9/iUniAmM/iSp9/TGACTCCC-3′) was obtained from Biosearch Technologies, Novato, CA.

**“Headpiece (HP).”** Sequence: 5′-/5Phos/GAGTCA/iSp9/iUniAmM/iSp9/TGACTCCC-3′

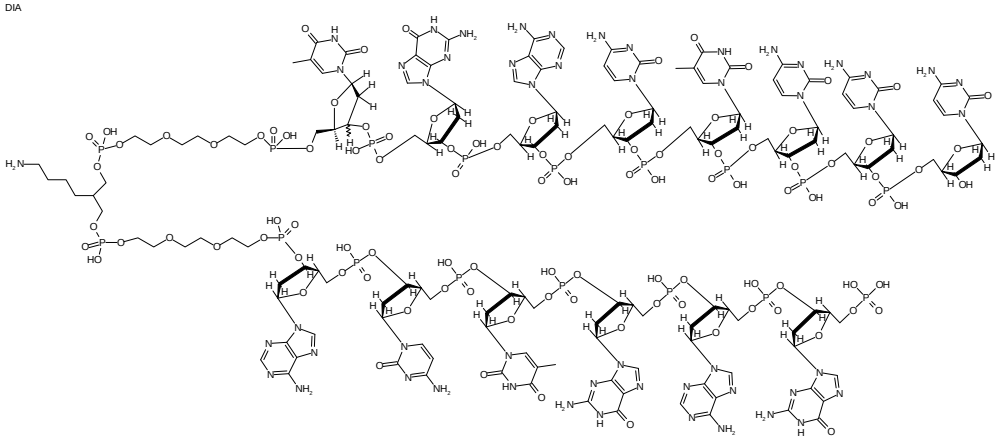


Figure 1. Sequence and structure of the “headpiece.” MW = 4937 D

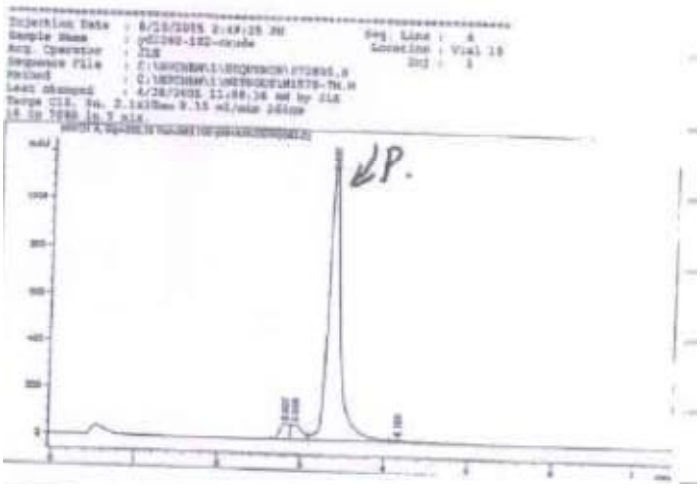
Preparation of **HP-1**

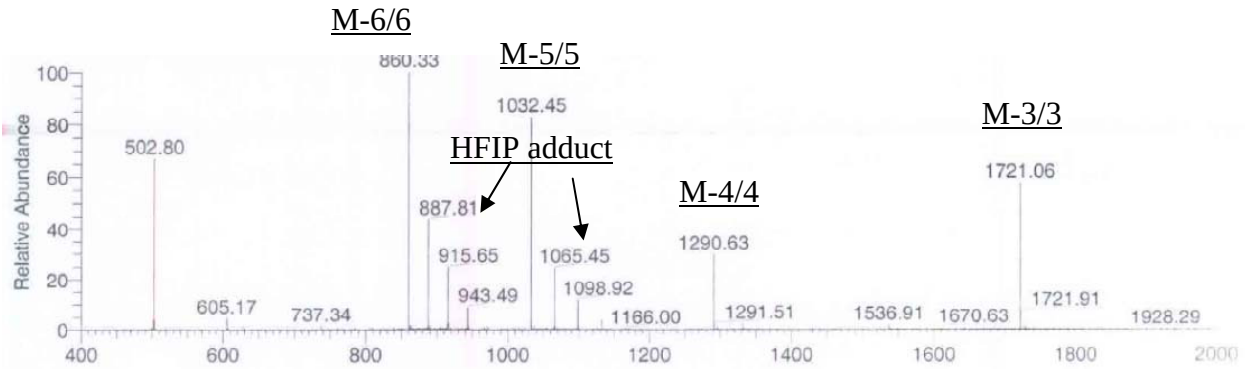
A solution of HP in pH9.4 borate buffer (250 mM) (1 μmol, 350 μL) was added at cold 40 equivalents of 4-iodo benzoic acid (9.92 mg in 70 μL of DMF), followed by 40 equivalents of DMT-MM (10.9 mg in 70 μL of water). After being kept at cold for 10 minutes, the reaction was allowed to proceed at room temperature overnight. The reaction was precipitated by adding 10% 5N NaCl water solution and 2.5 times volume of absolute EtOH. The pellet was redissolved in water (400 μL), followed by adding piperidine (60 μL). The reaction was allowed to proceed at room temperature for a couple hours. The headpiece was precipitated by treating with EtOH, which will be used directly for the next step without further purification.

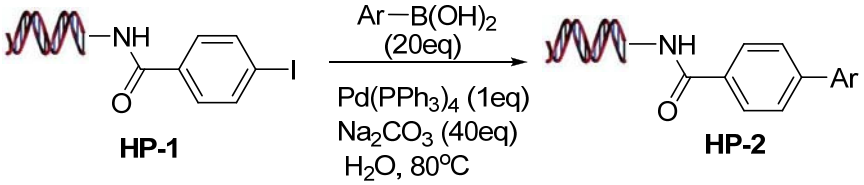
**HP-1**: expected mass 5167.20 (M-3/3=1721.40), observed 5166.18 (M-3/3=1721.06).

In the MS traces, especially in the -5 and -6 charge states, hexafluoroisopropanol (HFIP) adducts (expected mass of HFIP 168, observed +167) were observed. HFIP was a component of the solvents used in the LCMS.

The HFIP adducts were also observed in other samples’ LCMS chromatograms.






General procedure for the coupling of **HP-1** with boronic acids in Table 1.

A 1 mM solution of **HP-1** in water (20 nmol, 20 µL) was added 20 equivalents of boronate (1 µL, 400 mM in $CH_3CN/H_2O$ 1/1) and 40 equivalents of $Na_2CO_3$ (0.5 µL, 1.6 M in water), followed by 1 equivalent of degassed $Pd(PPh_3)_4$ (1 µL, 20 mM in $CH_2Cl_2$/Toluene/$CH_3CN$ 1/2/2). The reaction was allowed to proceed at 80 °C.

Table 1: Suzuki coupling of **HP-1** with boronic acids

| Entry | Boronic acid | Expected | M-3/3 | M-4/4 | M-5/5 | M-6/6 |
|---|---|---|---|---|---|---|

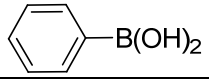
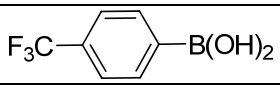
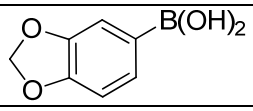
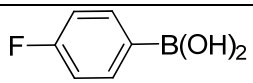
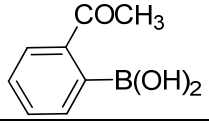
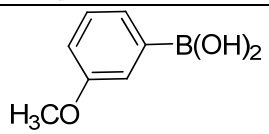
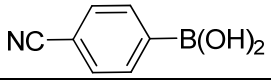
| | | mass | | | | |
|---|---|---|---|---|---|---|
| 1 |  | 5117.4 | 1704.8 | 1278.35 | 1022.48 | 851.9 |
| 2 |  | 5185.4 | 1727.47 | 1295.35 | 1036.08 | 863.23 |
| 3 |  | 5161.41 | 1719.47 | 1289.35 | 1031.28 | 859.24 |
| 4 |  | 5135.39 | 1710.80 | 1282.85 | 1026.08 | 854.90 |
| 5 |  | 5159.44 | 1718.81 | 1288.86 | 1030.89 | 858.91 |
| 6 |  | 5147.42 | 1714.81 | 1285.86 | 1028.48 | 856.90 |
| 7 |  | 5142.41 | 1713.14 | 1284.60 | 1027.48 | 856.07 |

Table 1, entry 1A: LCMS @ 90 min

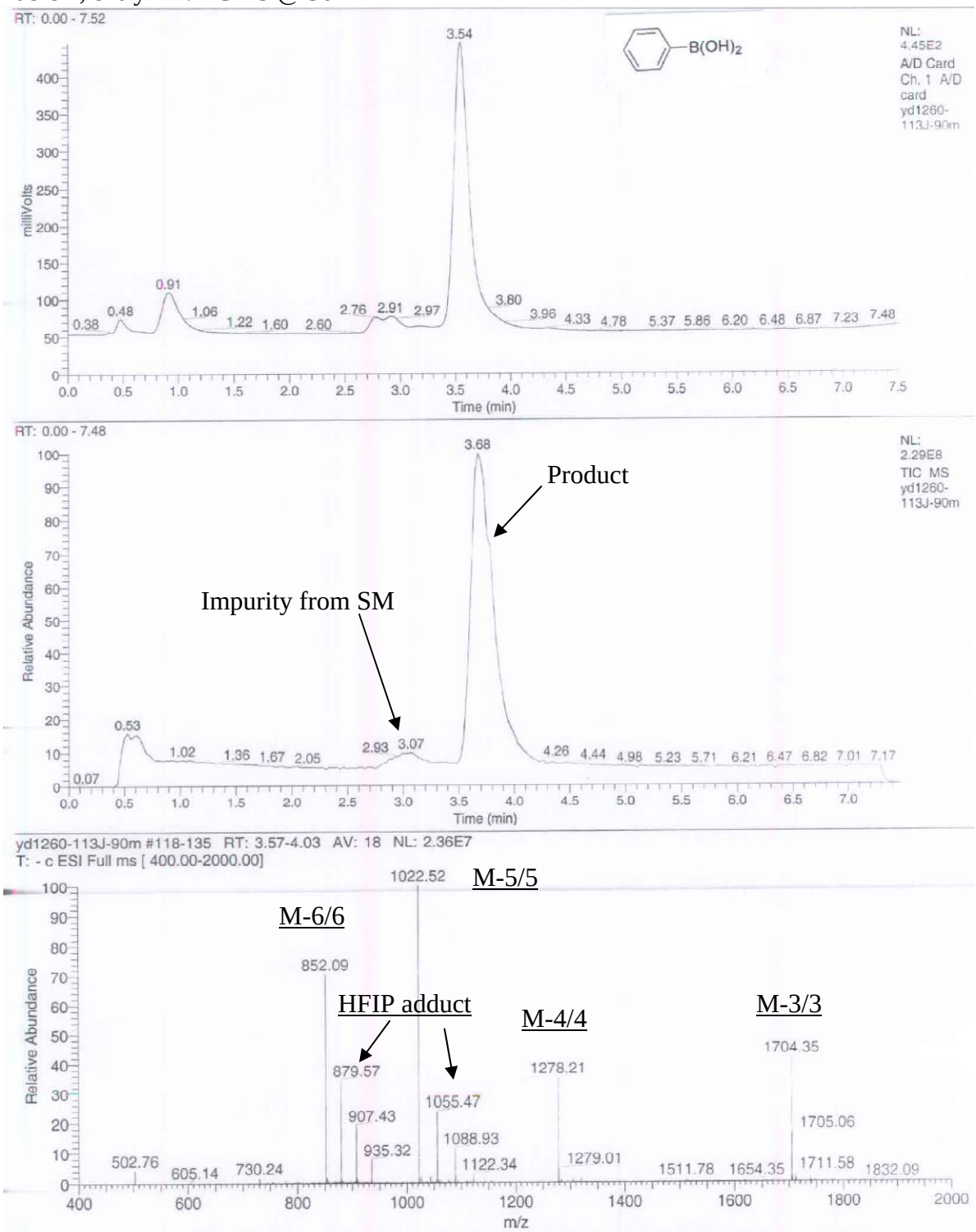
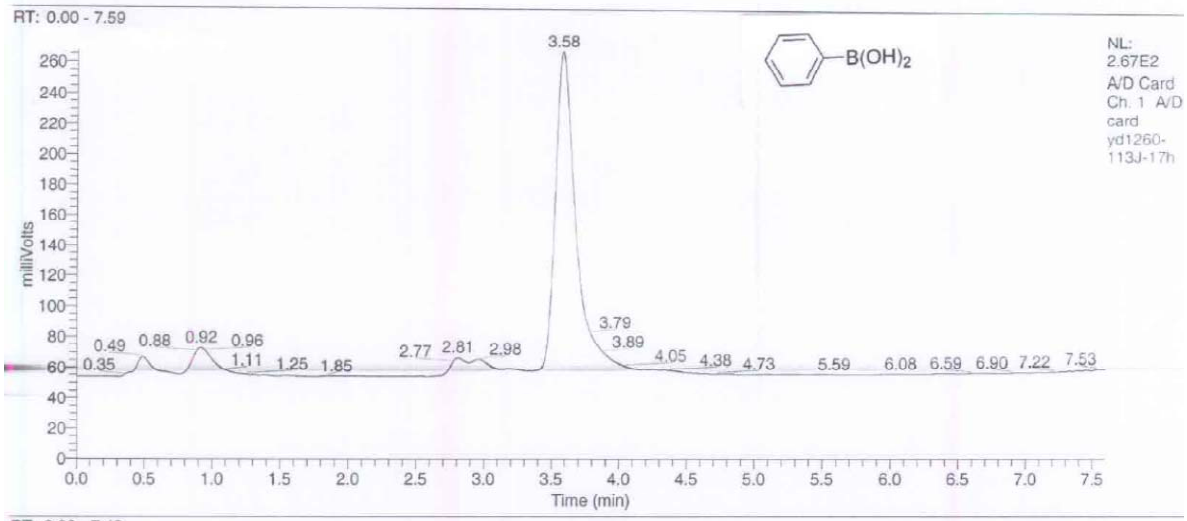
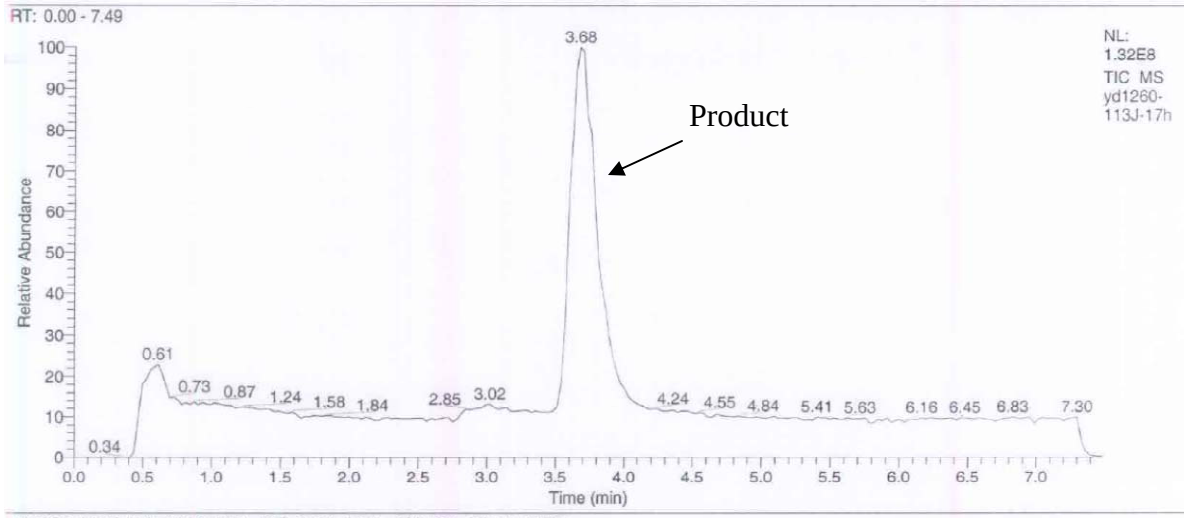


Table 1, entry 1A: LCMS @ 17 h



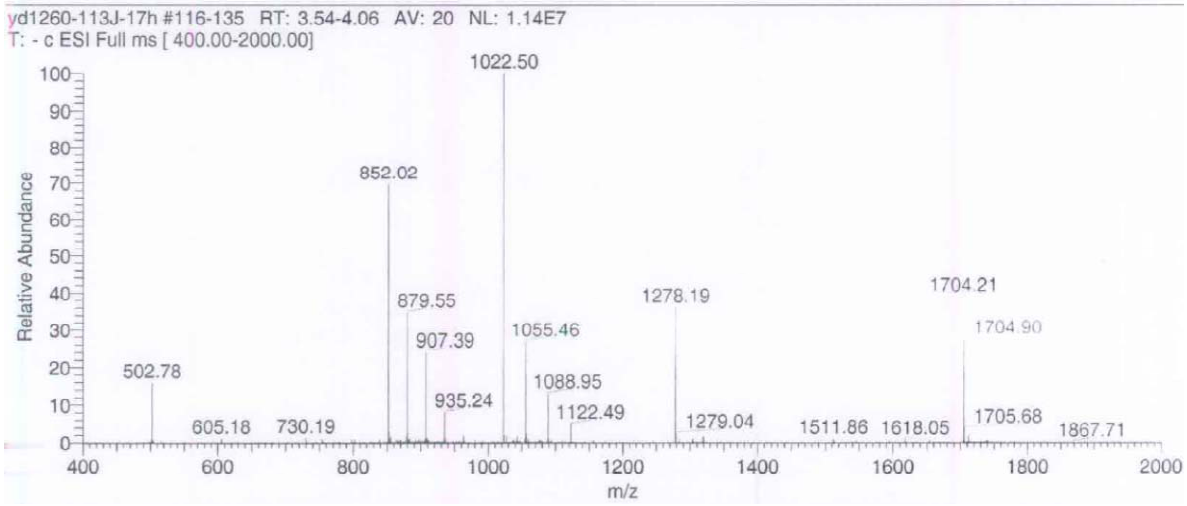



Table 1, entry 2A: LCMS @ 90 min

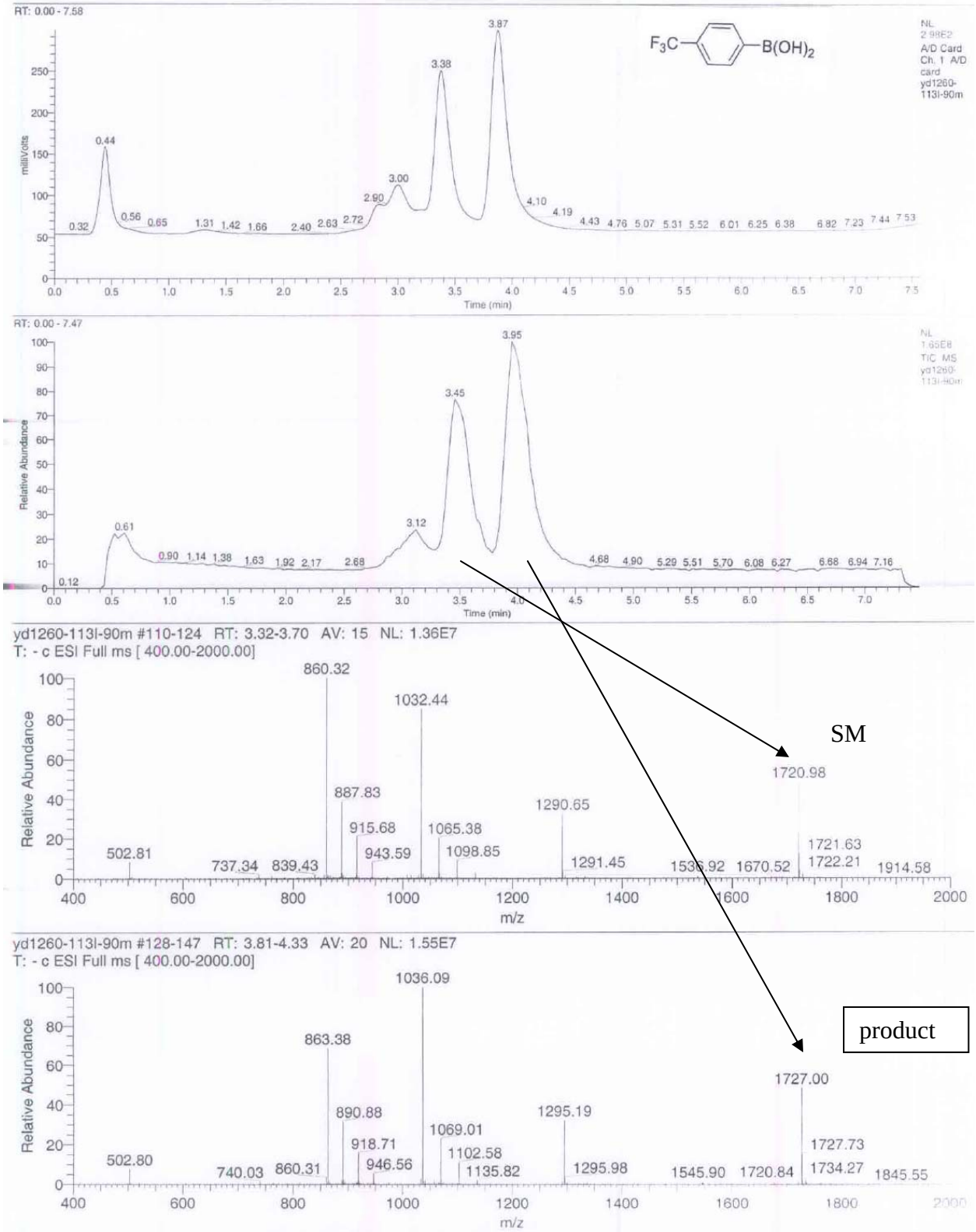


Table 1, entry 2A: LCMS @ 17 h

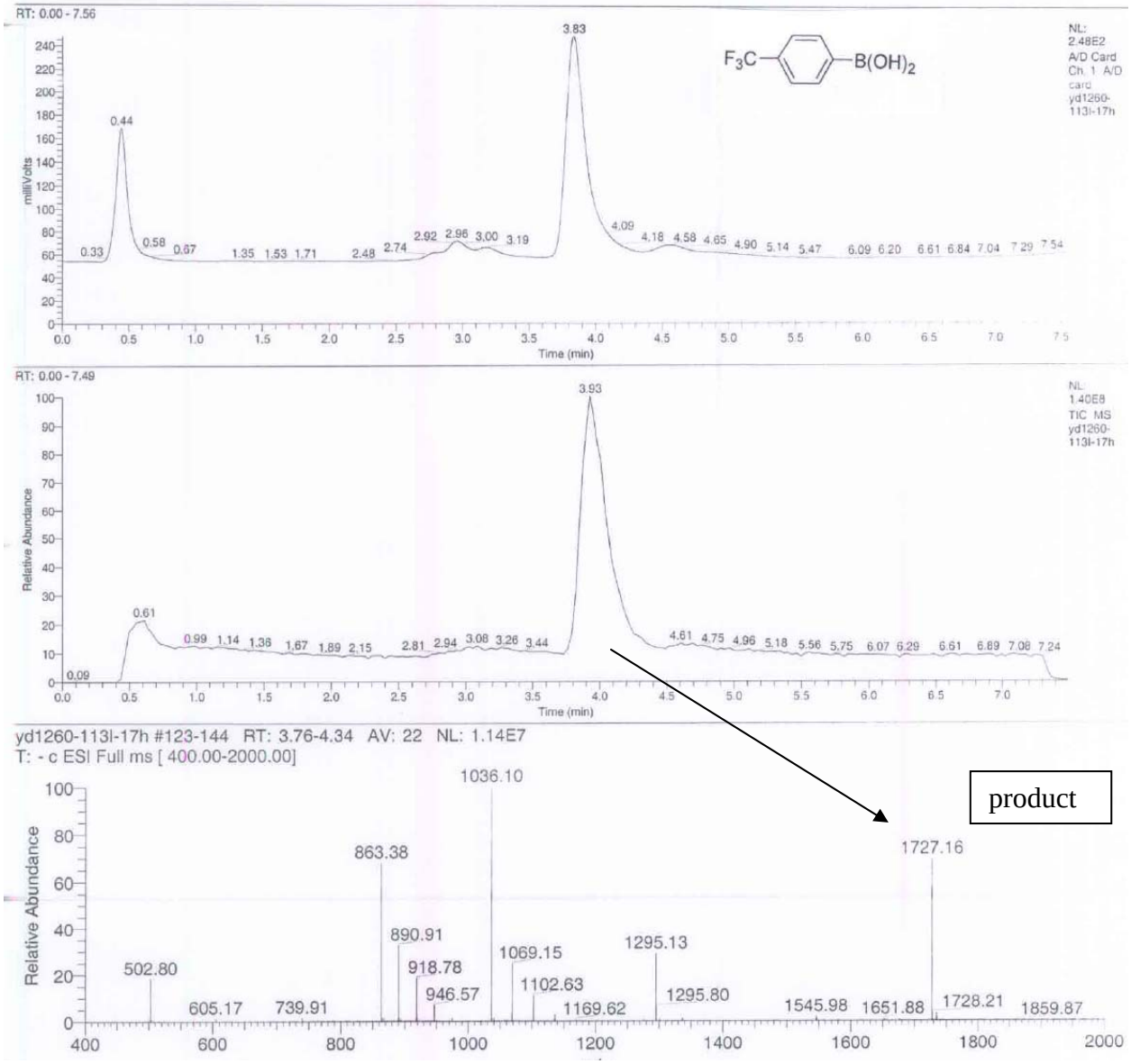


Table 1, entry 3A: LCMS @ 90 min

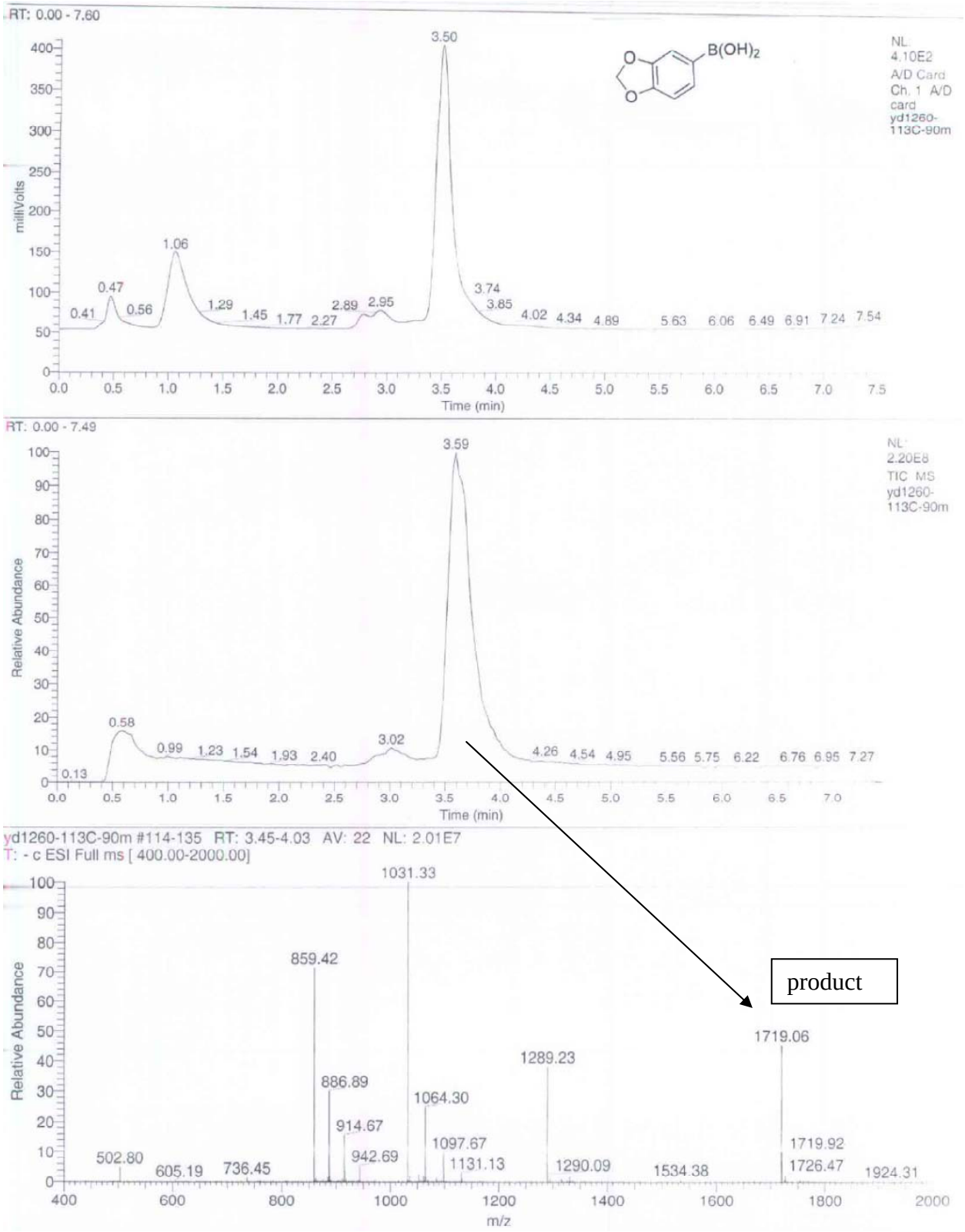


Table 1, entry 3A: LCMS @ 17 h

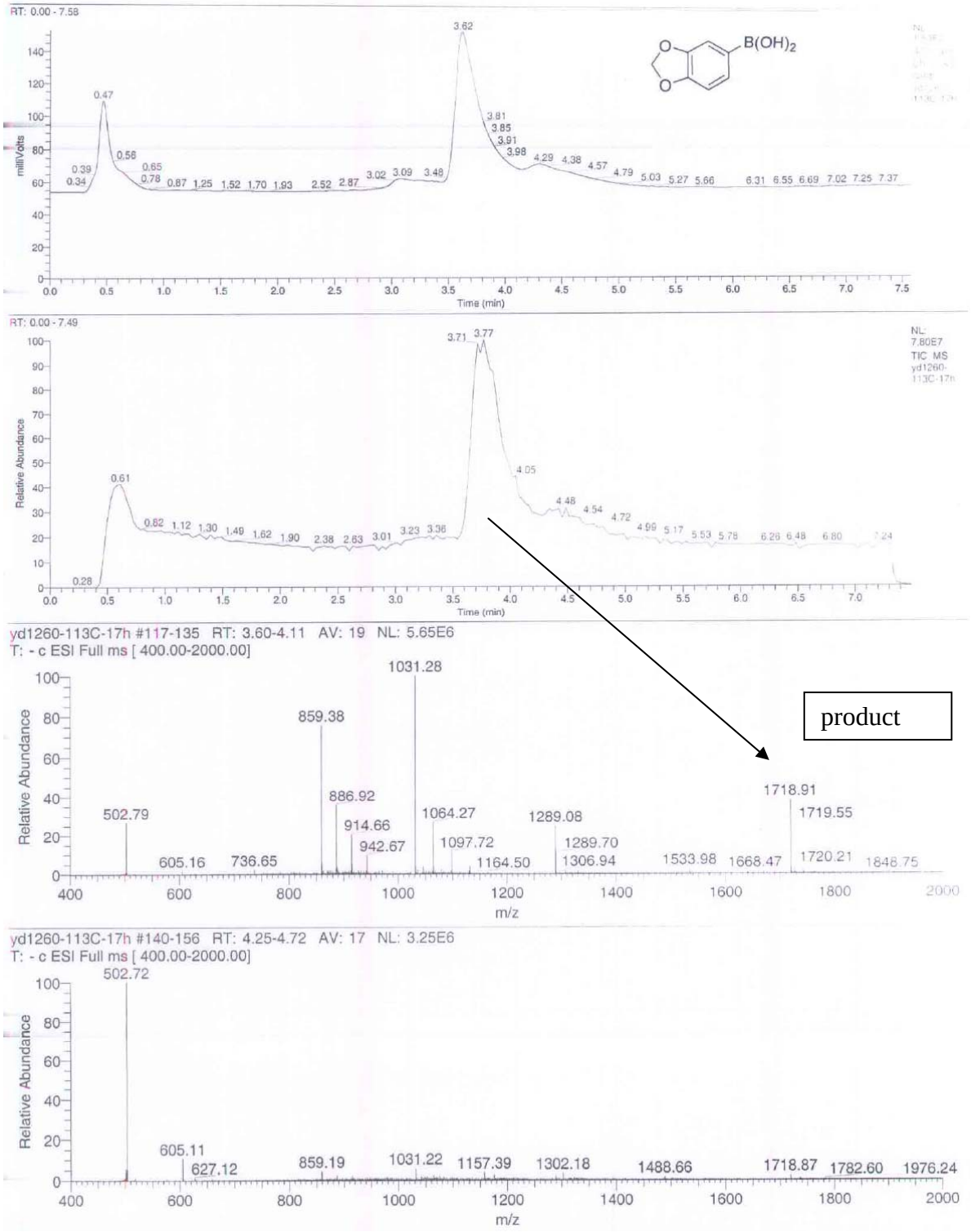


Table 1, entry 4A: LCMS @ 90 min

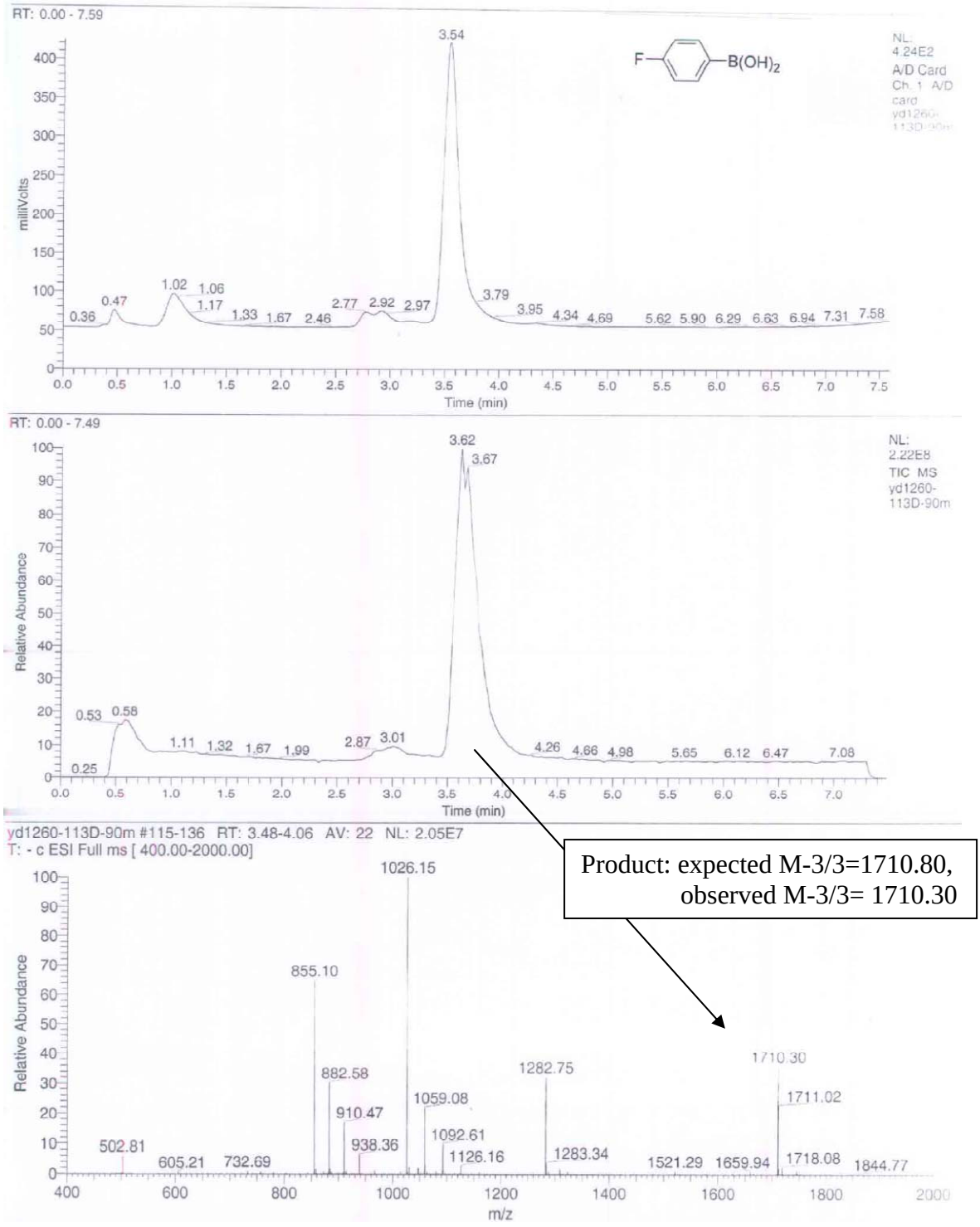
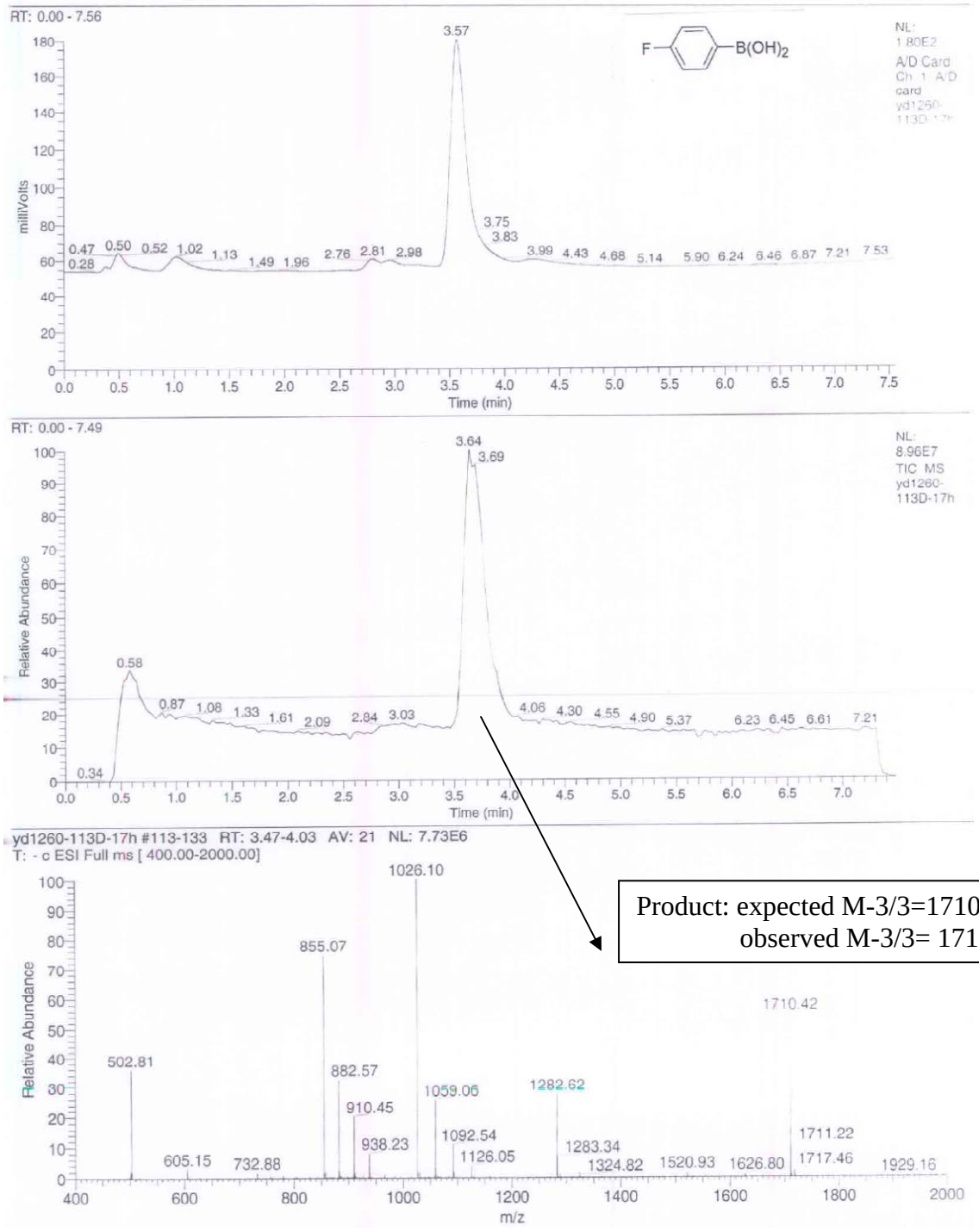


Table 1, entry 4A: LCMS @ 17 h




Product: expected M-3/3=1710.80, observed M-3/3= 1710.42

Table 1, entry 5A: LCMS @ 90 min

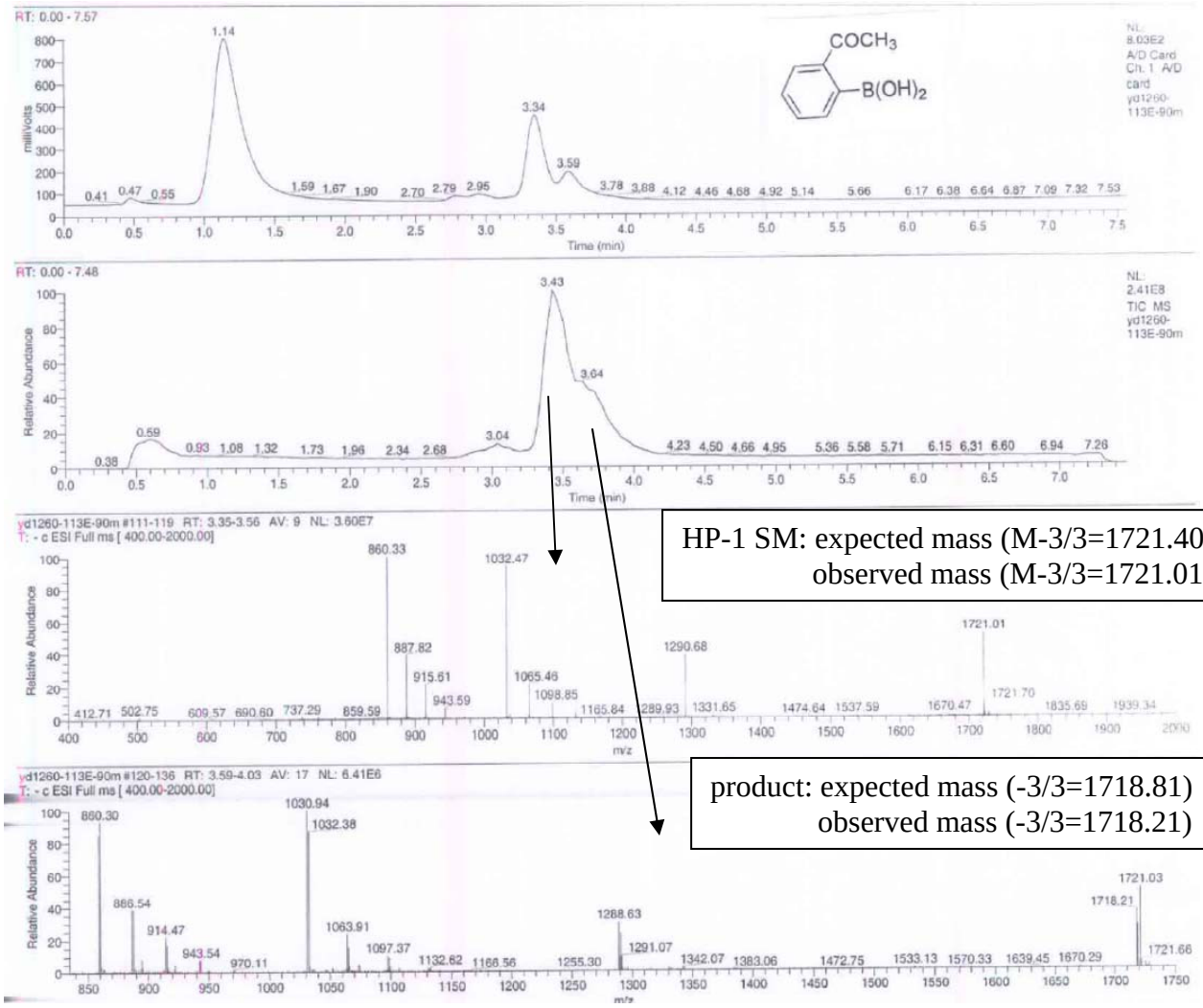


Table 1, entry 5A: LCMS @ 17 h

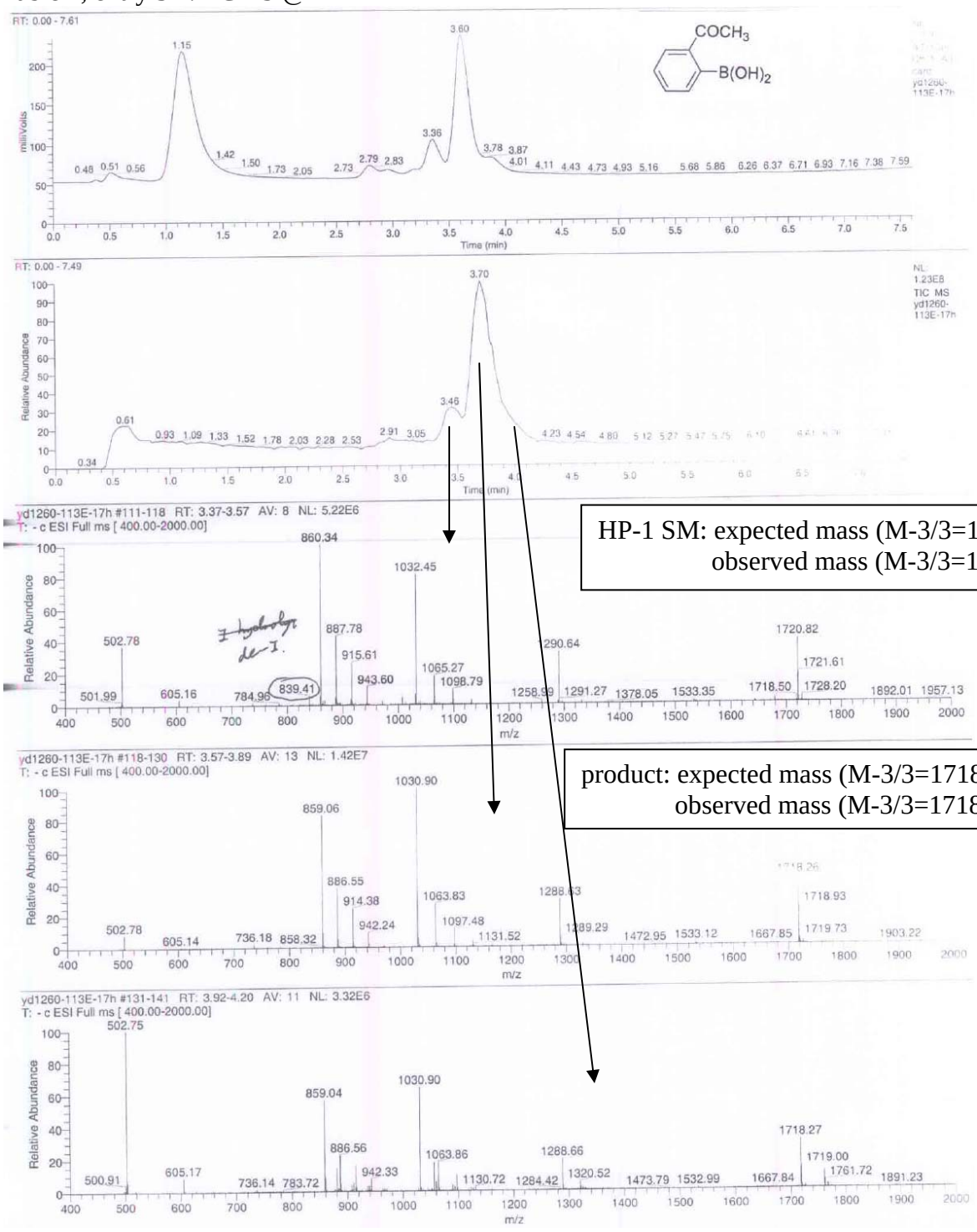
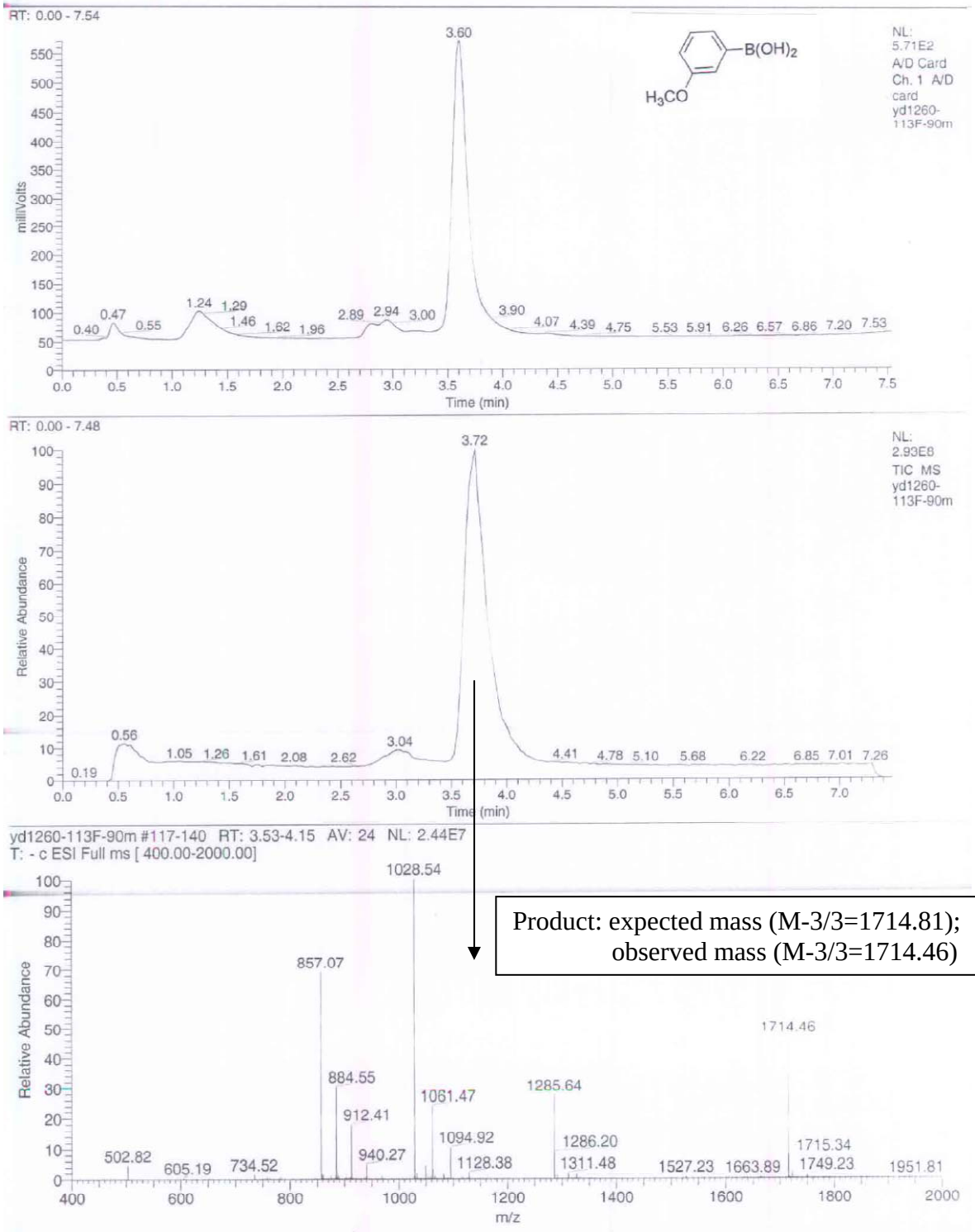
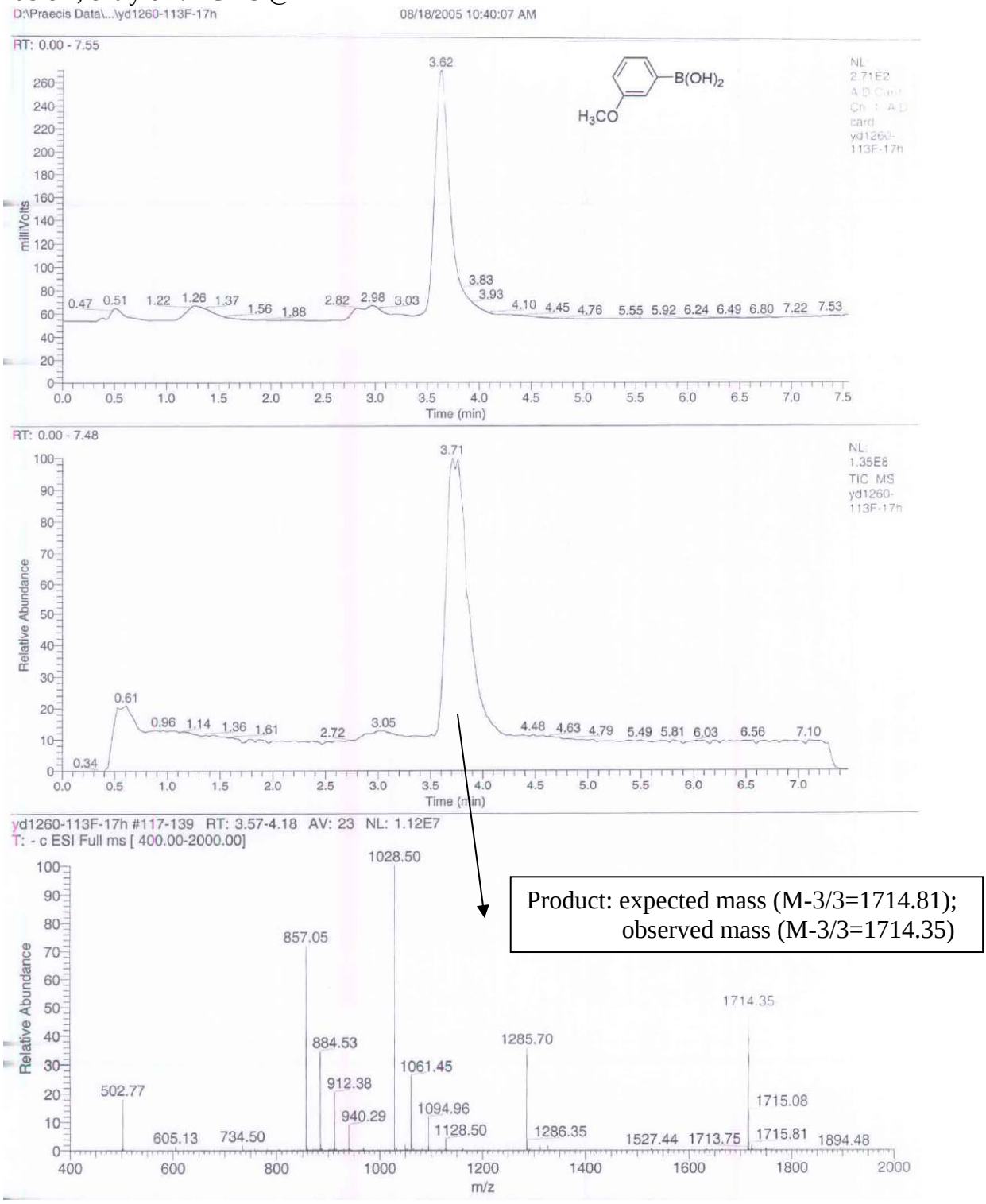


Table 1, entry 6A: LCMS @ 90 min



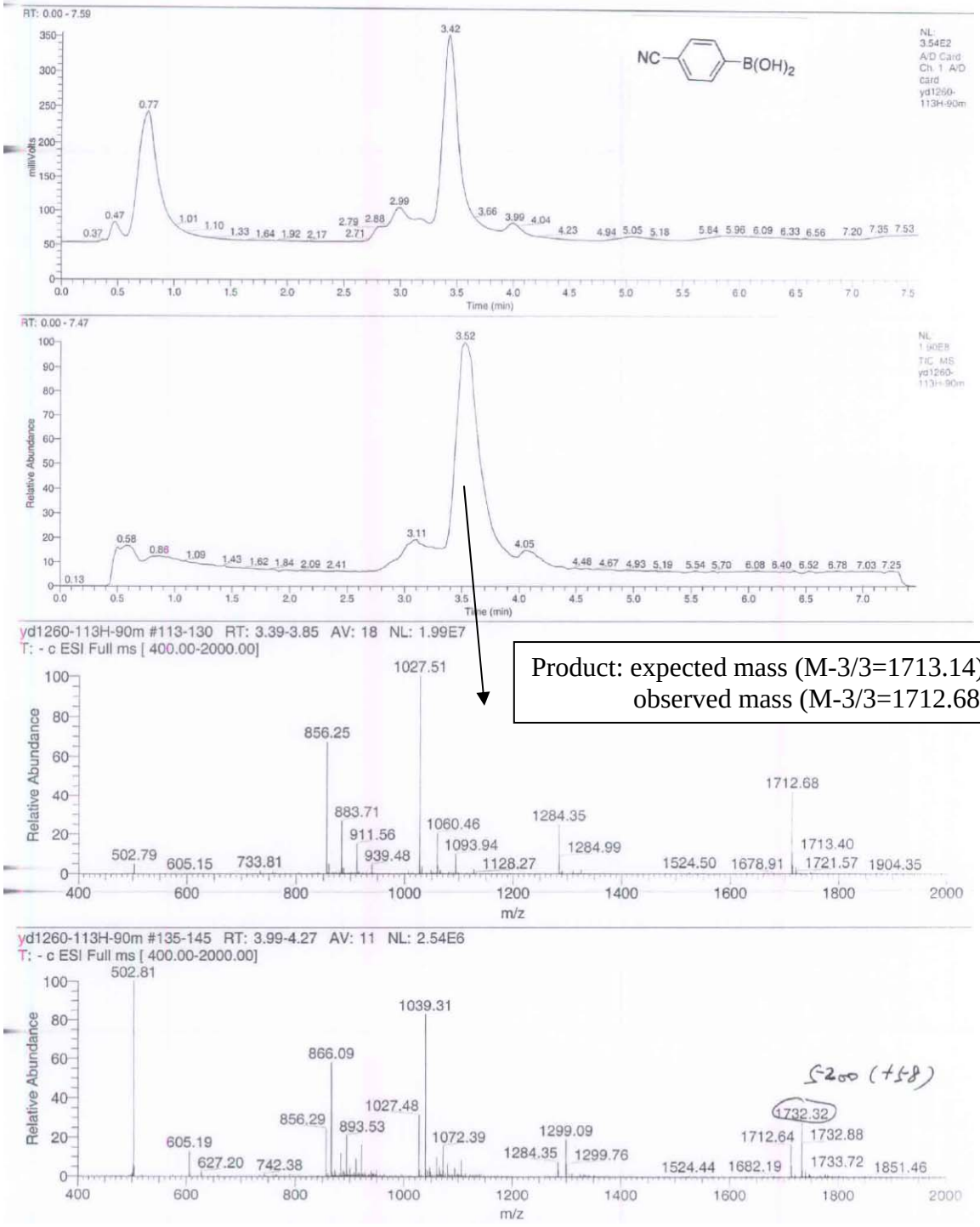

Product: expected mass (M-3/3=1714.81); observed mass (M-3/3=1714.46)

Table 1, entry 6A: LCMS @ 17 h



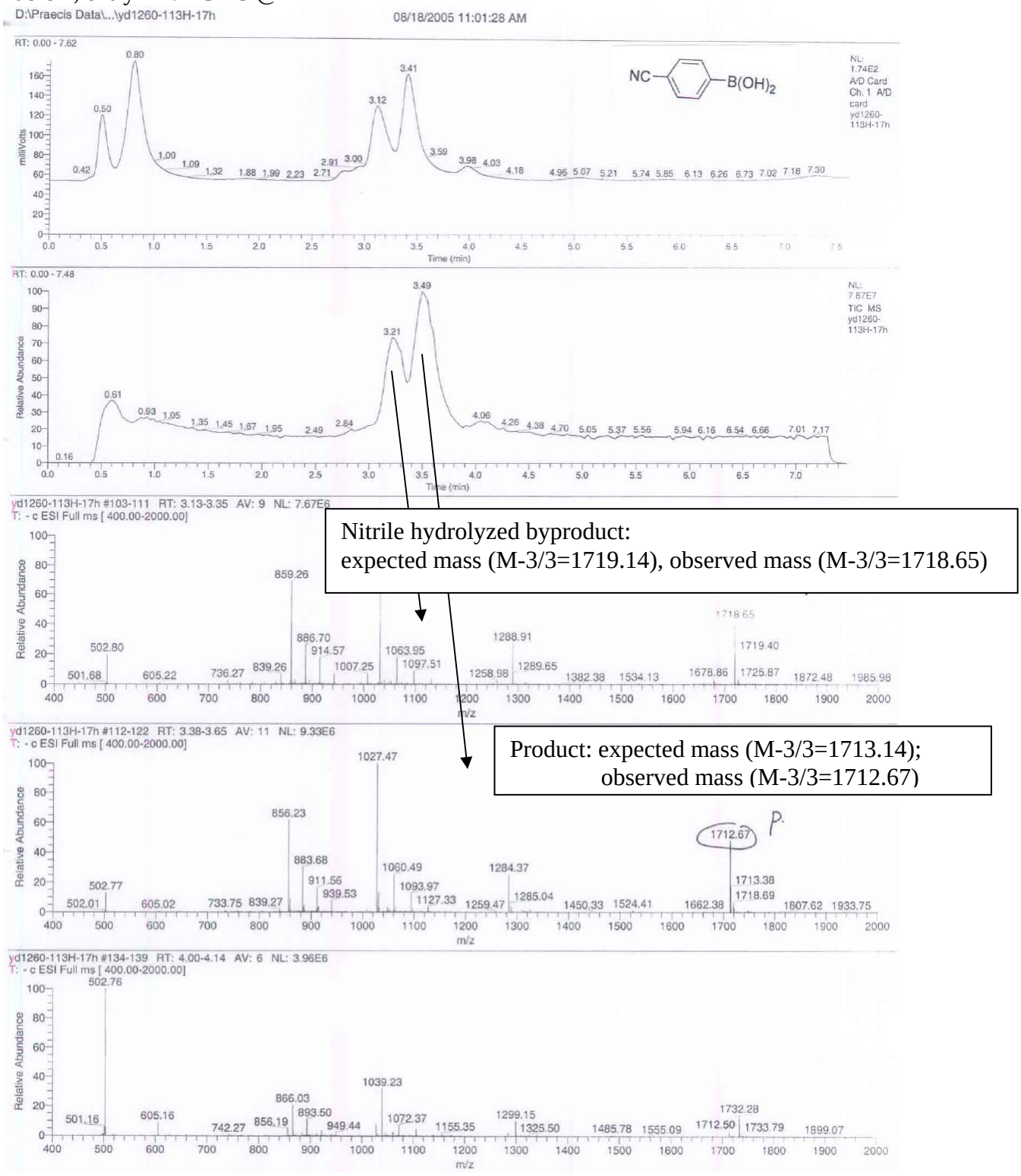

Product: expected mass (M-3/3=1714.81);
observed mass (M-3/3=1714.35)

Table 1, entry 7A: LCMS @ 90 min




Product: expected mass (M-3/3=1713.14);
observed mass (M-3/3=1712.68)

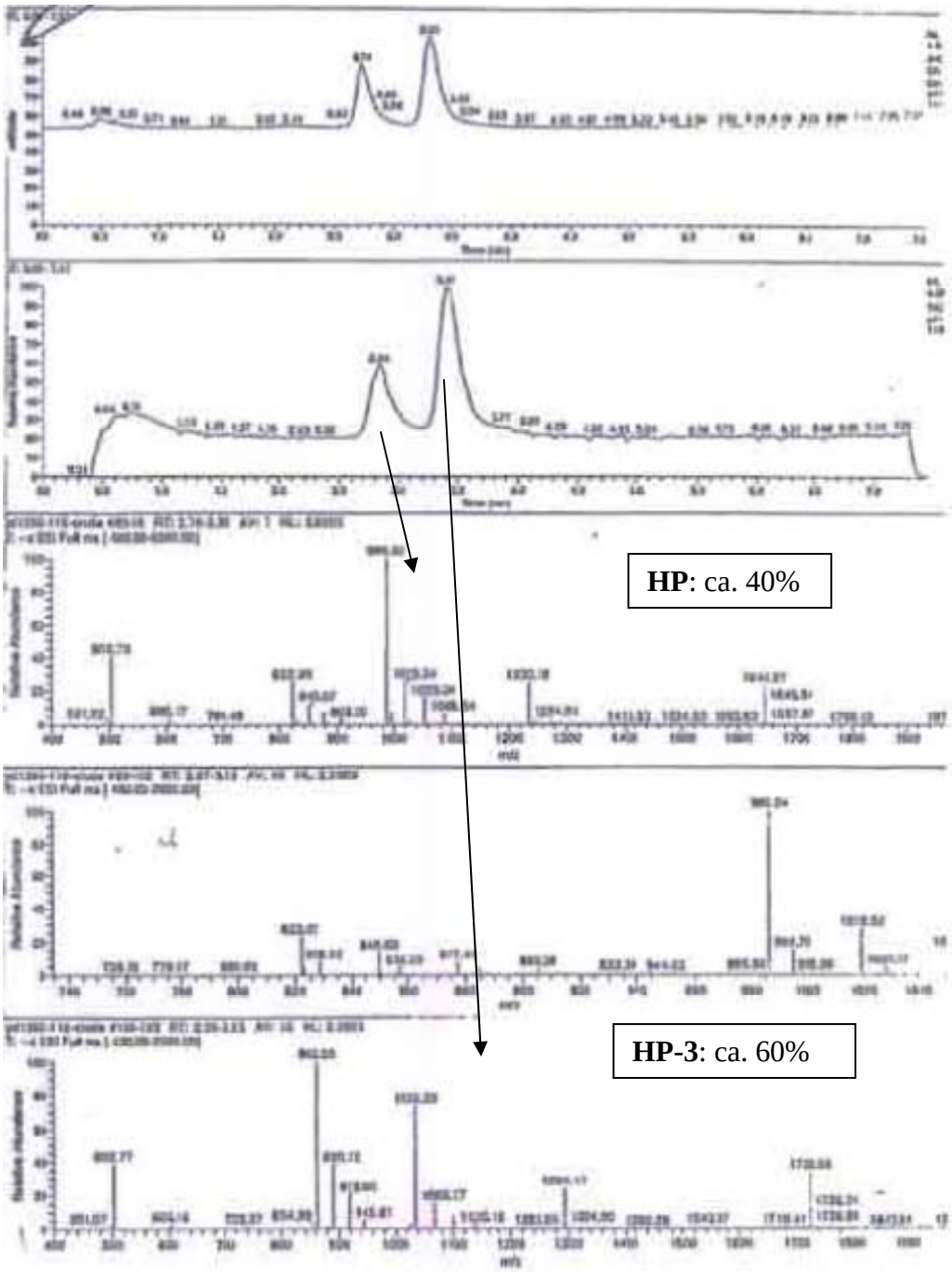
Table 1, entry 7A: LCMS @ 17 h

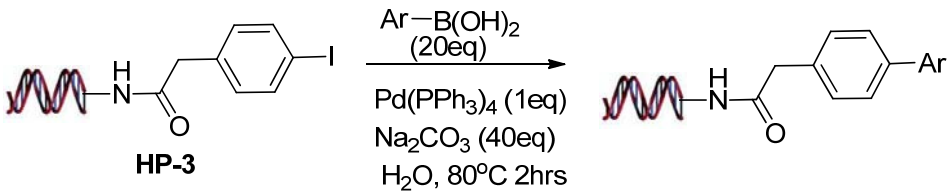


Preparation of **HP-3**

A solution of HP in pH9.4 borate buffer (250 mM) (1 μmol, 300 μL) was added at cold 40 equivalents of 4-iodophenylacetic acid (10.5 mg in 70 μL of DMF), followed by 40 equivalents of DMT-MM (10.9 mg in 70 μL of water). After being kept at cold for 30 minutes, the reaction was allowed to proceed at room temperature for 5 hours. The reaction was further treated with piperidine (44 μL) for 5 minutes, followed with precipitation by 10% 5N NaCl water solution and 2.5 times volume of absolute EtOH. The pellet was redissolved in water and would be used directly for the next step without further purification. It contained about 40% of HP and 60% of **HP-3**.

**HP-3**: expected mass 5181.23 (M-3/3=1726.08), observed 5180 (M-3/3=1725.66)


HP: ca. 40%
HP-3: ca. 60%




General procedure for the coupling of **HP-3** with boronic acids in Table 1.

A solution of **HP-3** in water (20 nmol in 14 µL) was added 20 equivalents of boronate (1 µL, 400 mM in $CH_3CN/H_2O$ 1/1) and 40 equivalents of $Na_2CO_3$ (0.5 µL, 1.6 M in water), followed by 1 equivalent of degassed $Pd(PPh_3)_4$ (1 µL, 20 mM in $CH_2Cl_2$/Toluene/$CH_3CN$ 1/2/2). The reaction was allowed to proceed at 80 °C for 2 h.

Table 1, entry 1B:

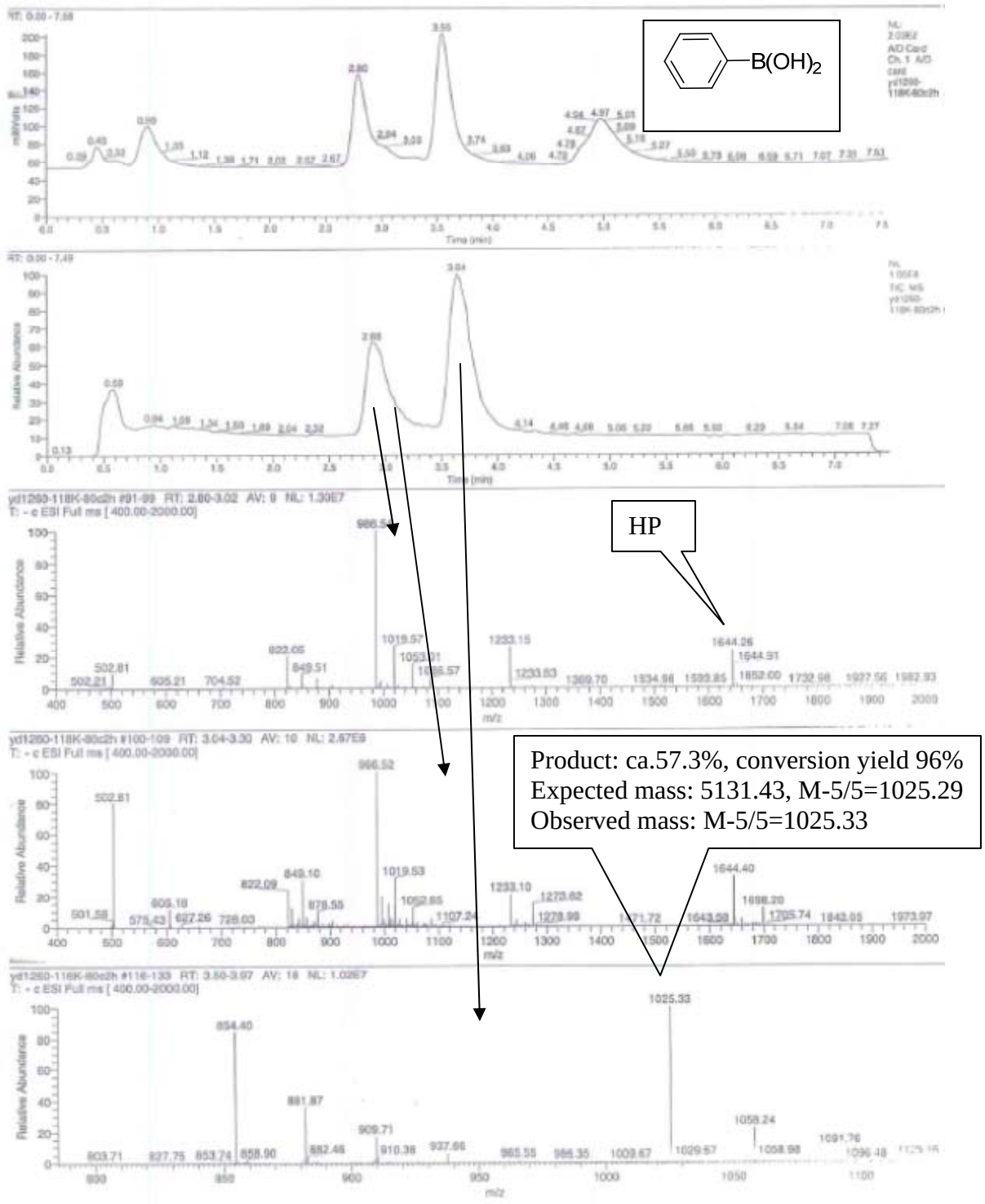


Table 1, entry 2B:

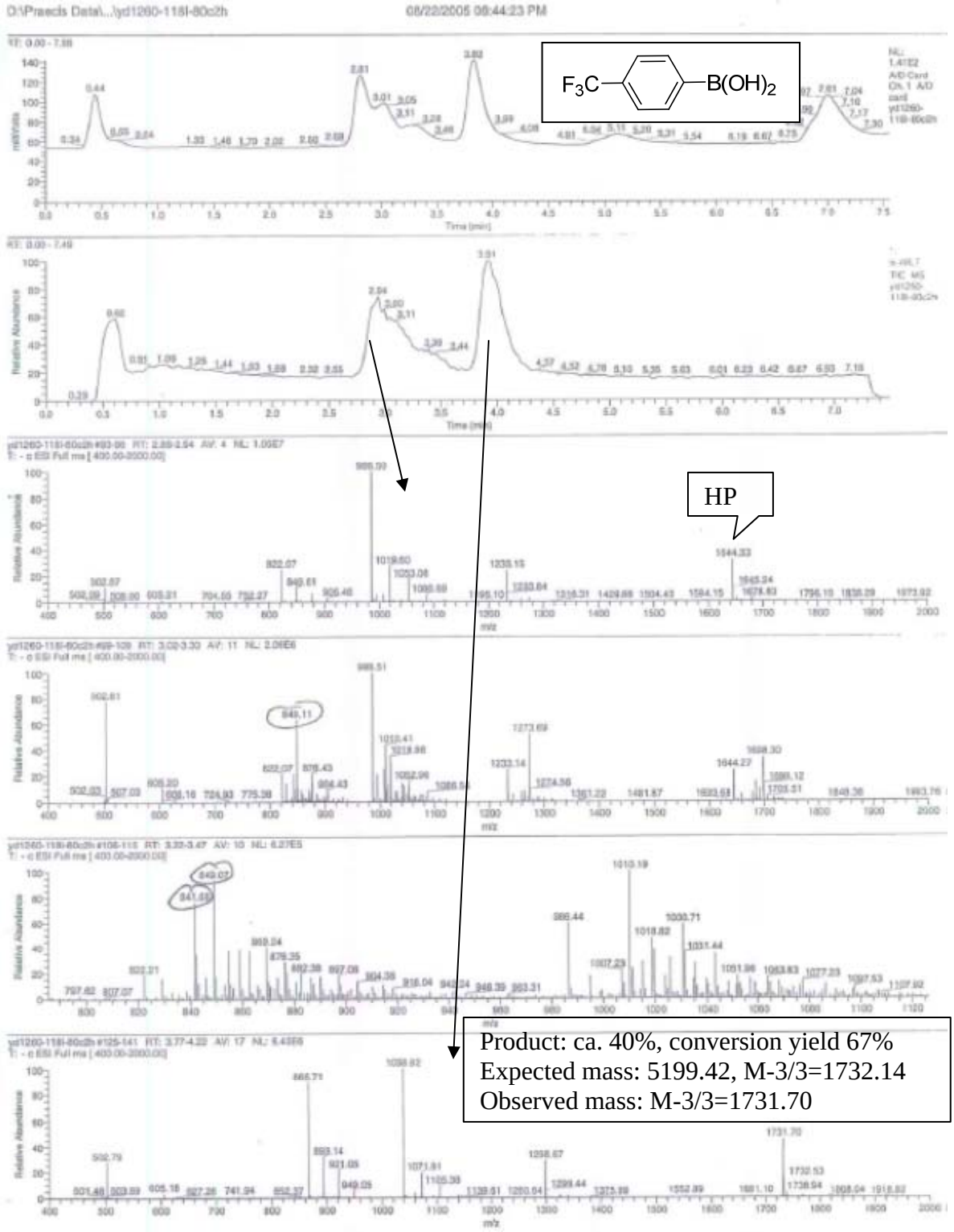
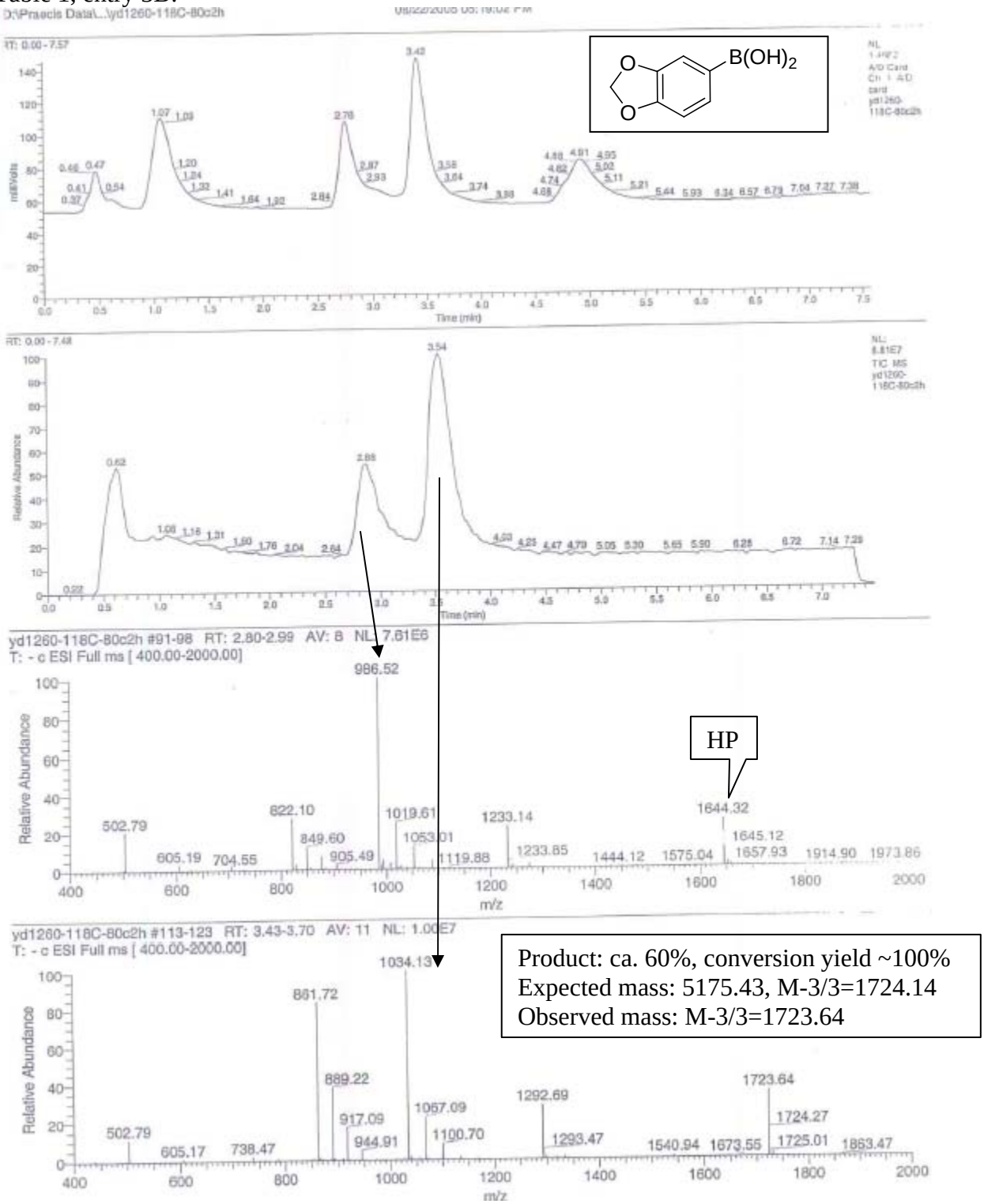


Table 1, entry 3B:




Product: ca. 60%, conversion yield ~100%
Expected mass: 5175.43, M-3/3=1724.14
Observed mass: M-3/3=1723.64

Table 1, entry 4B:

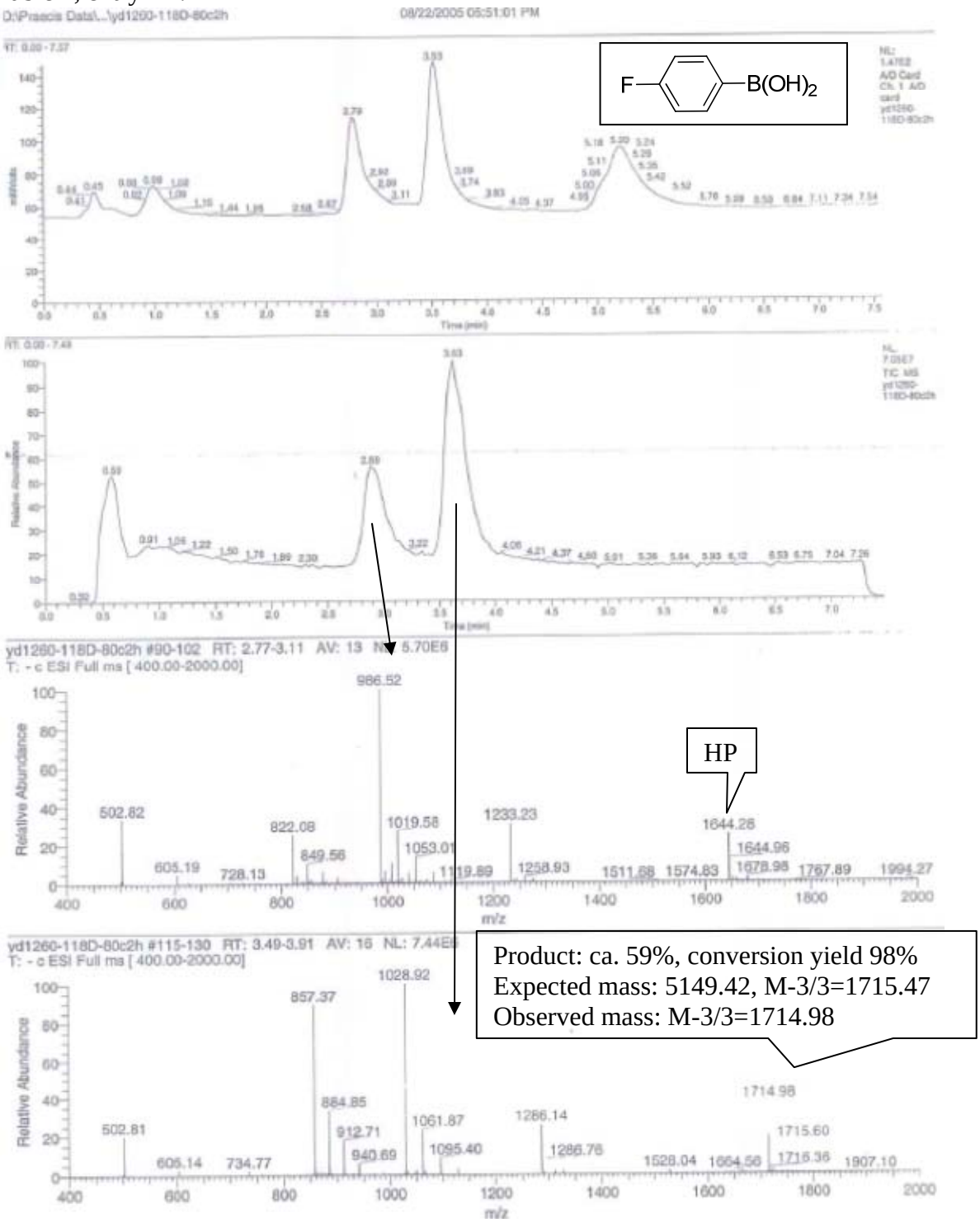


Table 1, entry 5B:

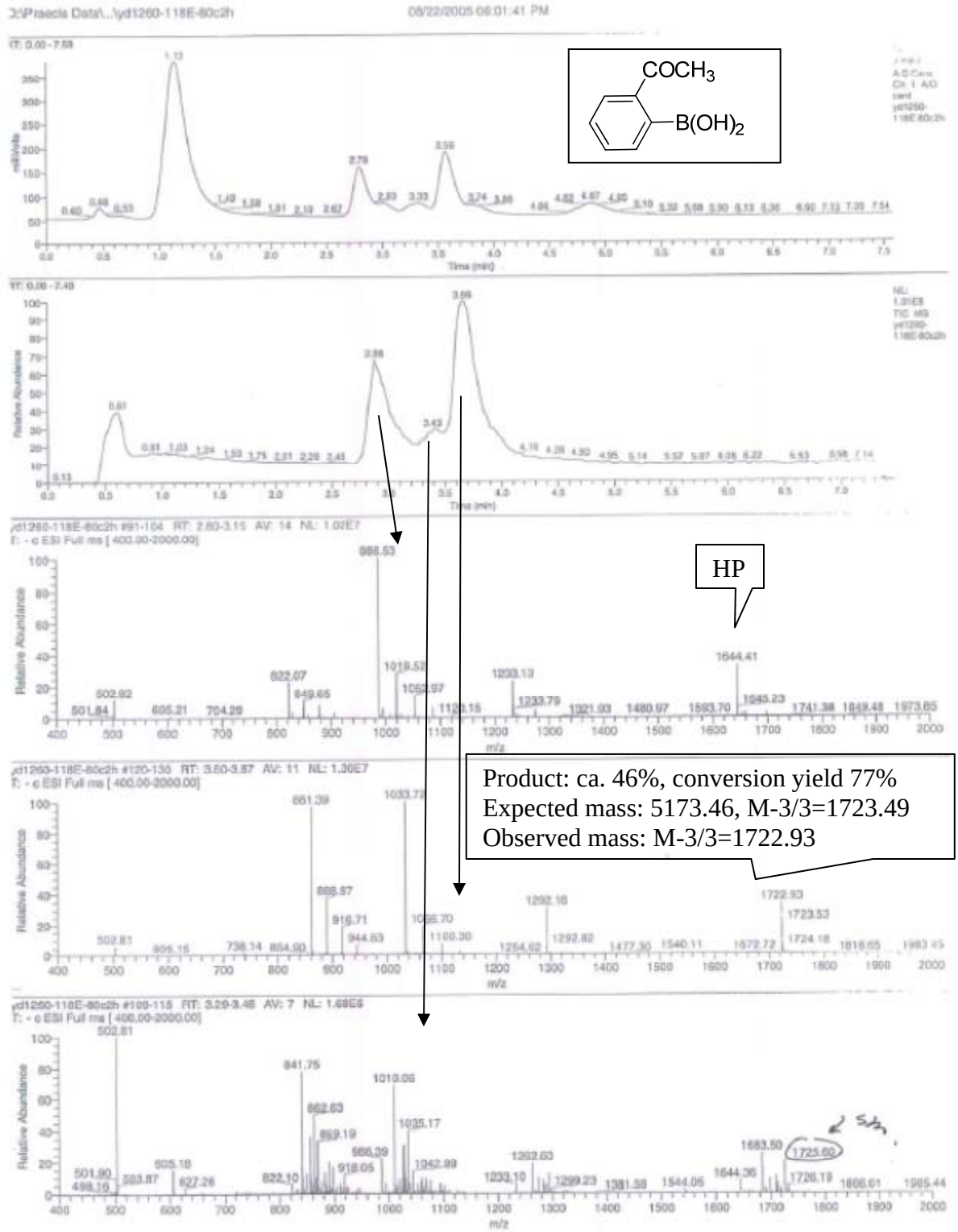


Table 1, entry 6B:

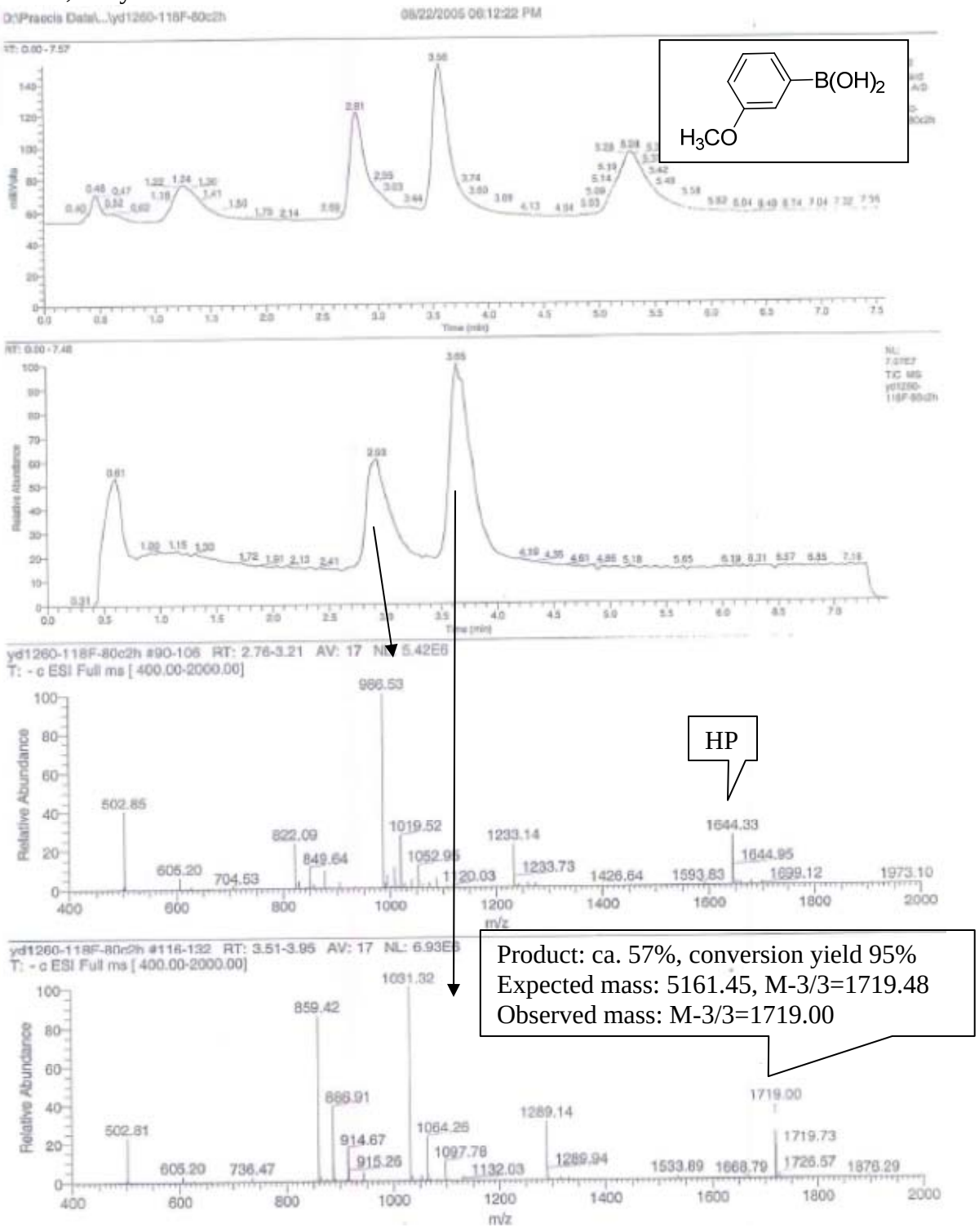
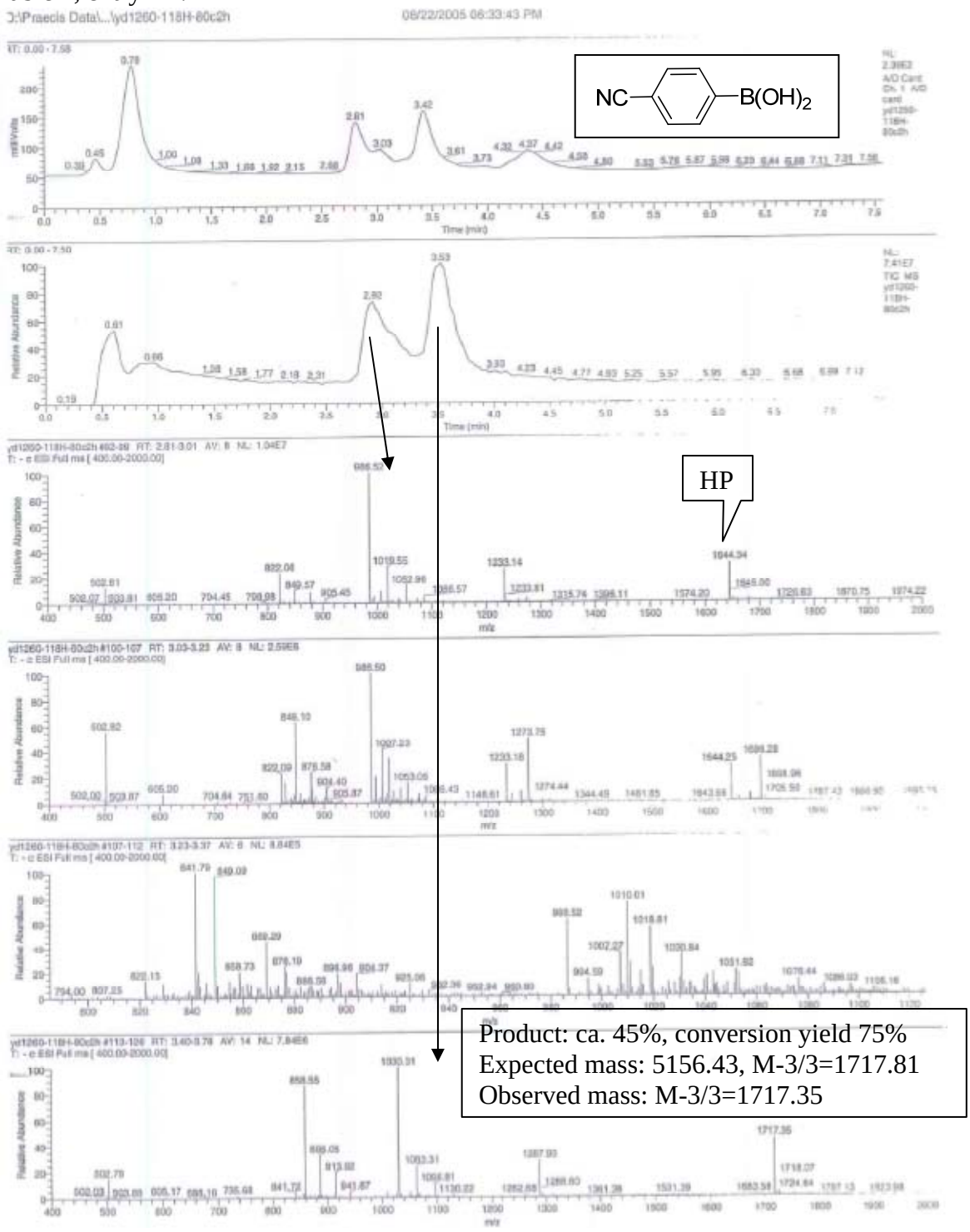


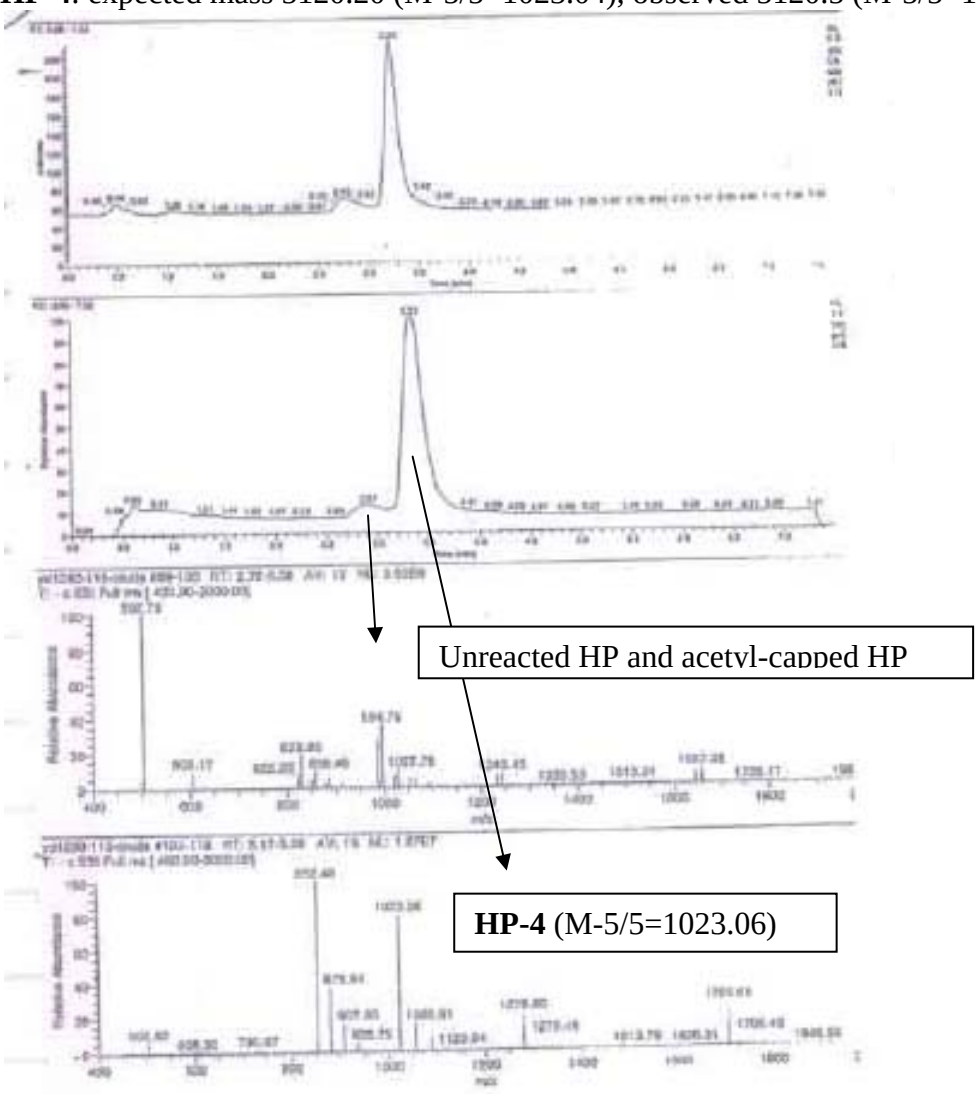
Table 1, entry 7B:

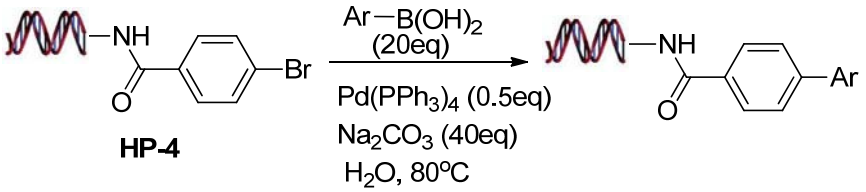


Preparation of **HP-4**

A solution of **HP** in pH9.4 borate buffer (250 mM) (1 μmol, 300 μL) was added 40 equivalents of 4-bromobenzoic acid (8.1 mg in 70 μL of DMF), followed by 40 equivalents of DMT-MM (10.9 mg in 70 μL of water). The reaction was allowed to proceed at room temperature for 5 hours. To the reaction mixture was added piperidine (88 μL, 20% in volume). The reaction was allowed to proceed at room temperature for 5 mins, followed by adding 10% 5 N NaCl water solution and 2.5 times volume of absolute EtOH to precipitate the DNA. The pellet was redissolved in water and it will be used directly for the next step.

**HP-4**: expected mass 5120.20 (M-5/5=1023.04), observed 5120.5 (M-5/5=1023.06)






General procedure for the coupling of **HP-4** with boronates in Table 1.

A 1 mM solution of **HP-4** in water (20 nmol, 20 μL) was added 20 equivalents of boronate (0.5 μL, 800 mM in DMA) and 40 equivalents of $Na_2CO_3$ (0.5 μL, 1.6 M in water), followed by 0.5 equivalent of degassed $Pd(PPh_3)_4$ (2 μL, 5 mM in $CH_3CN$). The reaction was allowed to proceed at 80 °C for 4 hours.

Table 1, Entry 1C: LCMS @ 4 h

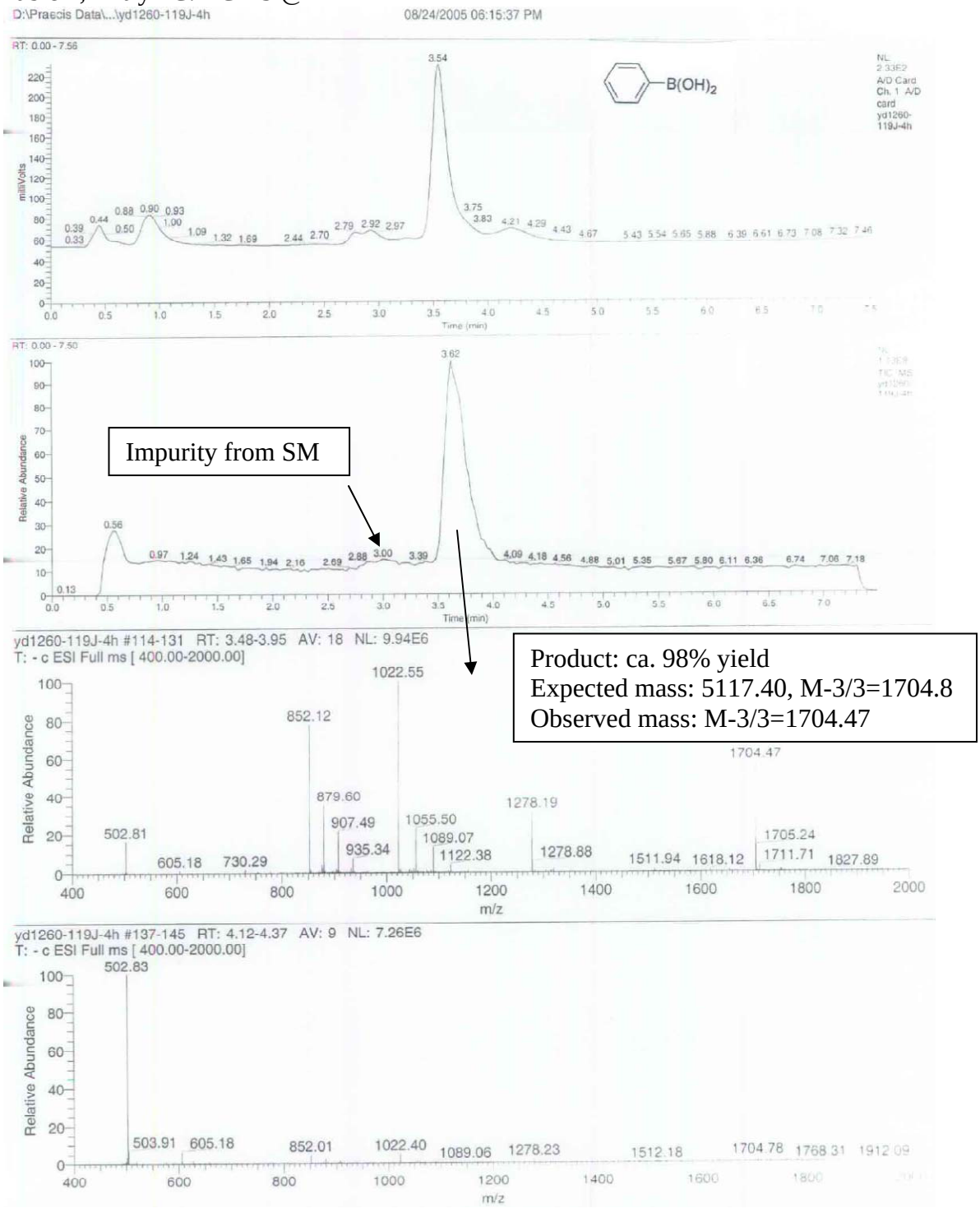
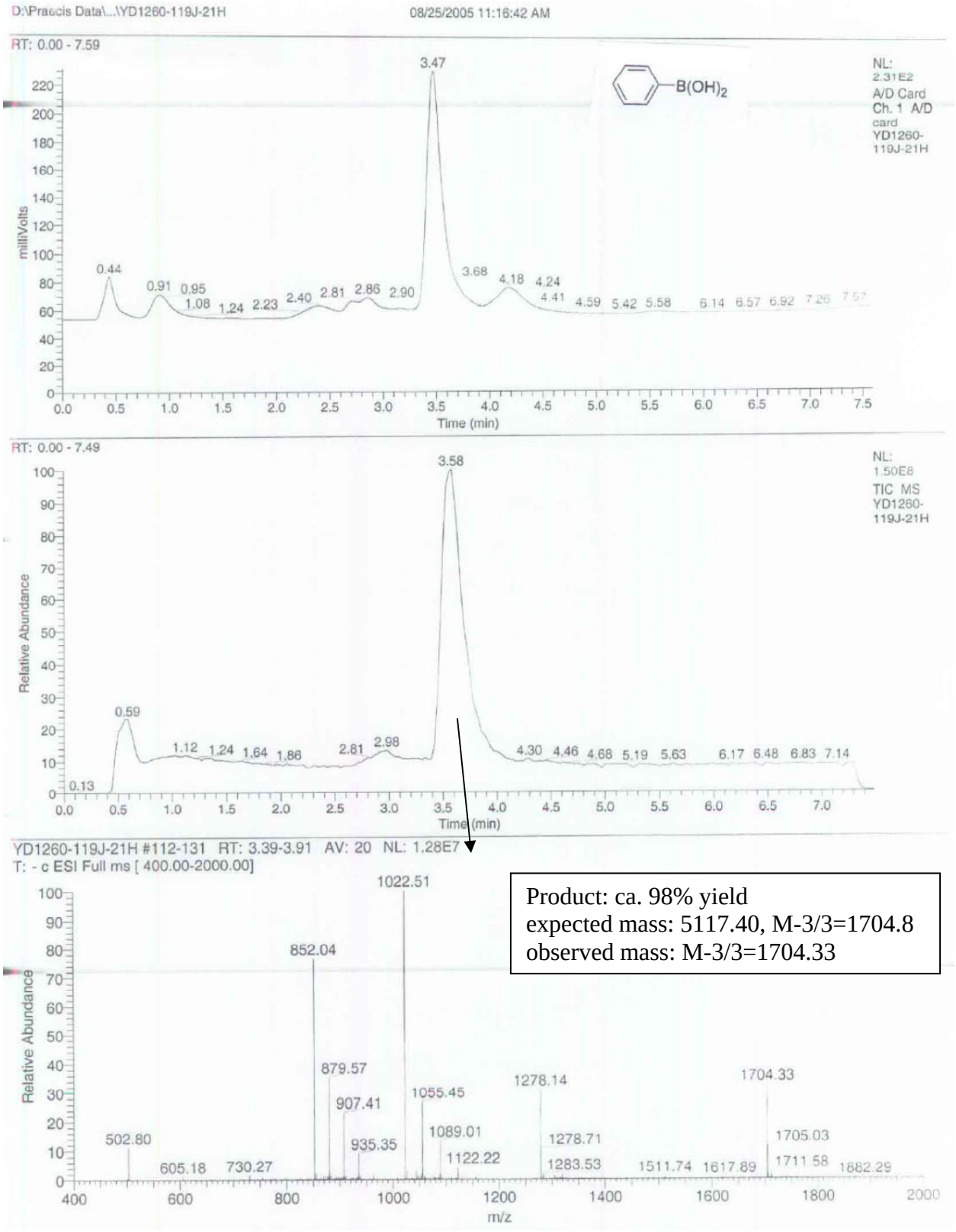


Table 1, entry 1C: LCMS @ 21 h




Product: ca. 98% yield
expected mass: 5117.40, M-3/3=1704.8
observed mass: M-3/3=1704.33

Table 1, entry 2C: LCMS @ 4 h

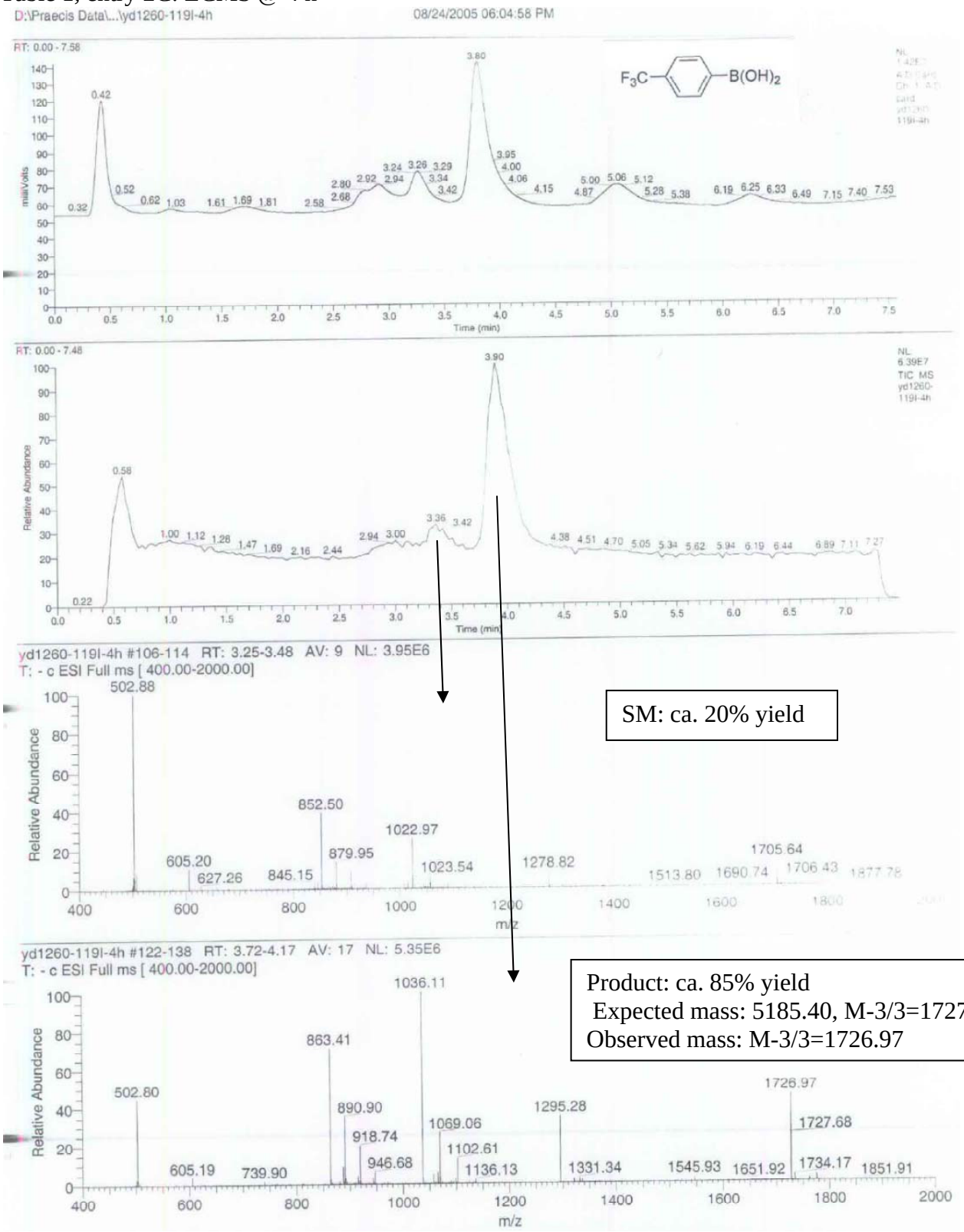
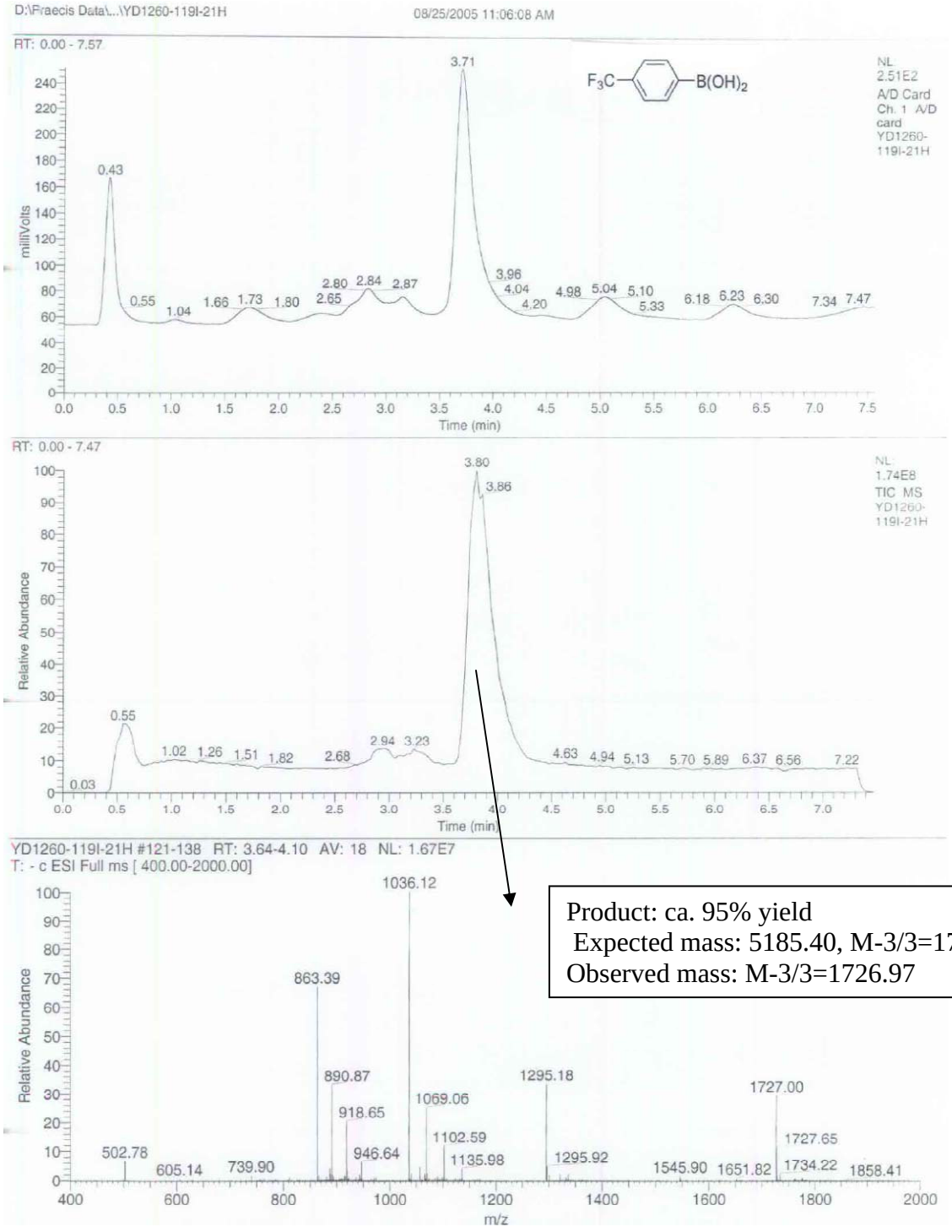
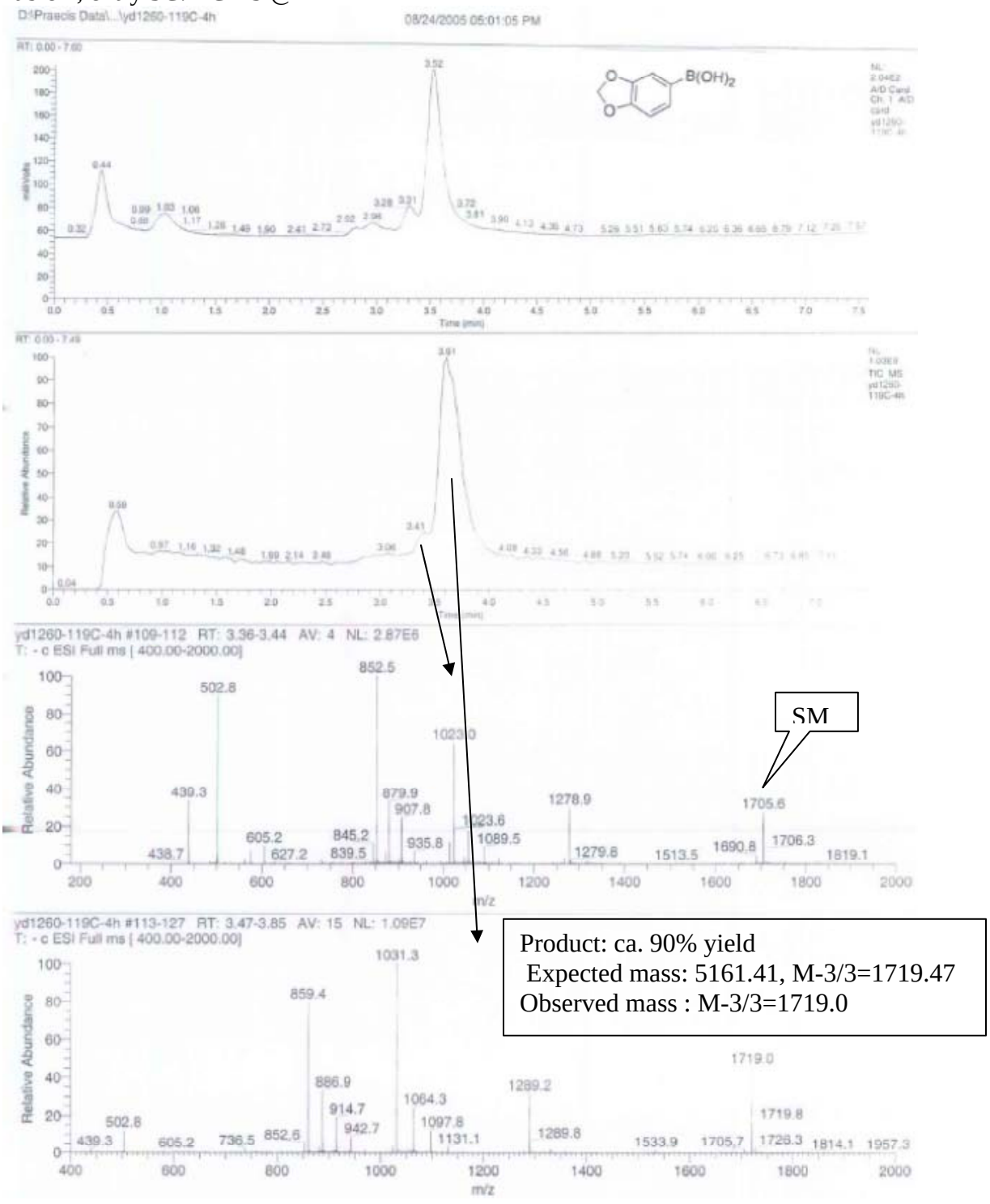


Table 1, entry 2C: LCMS @ 21 h




Product: ca. 95% yield
Expected mass: 5185.40, M-3/3=1727.47
Observed mass: M-3/3=1726.97

Table 1, entry 3C: LCMS @ 4 h




Product: ca. 90% yield
Expected mass: 5161.41, M-3/3=1719.47
Observed mass : M-3/3=1719.0

Table 1, entry 3C: LCMS @ 21 h

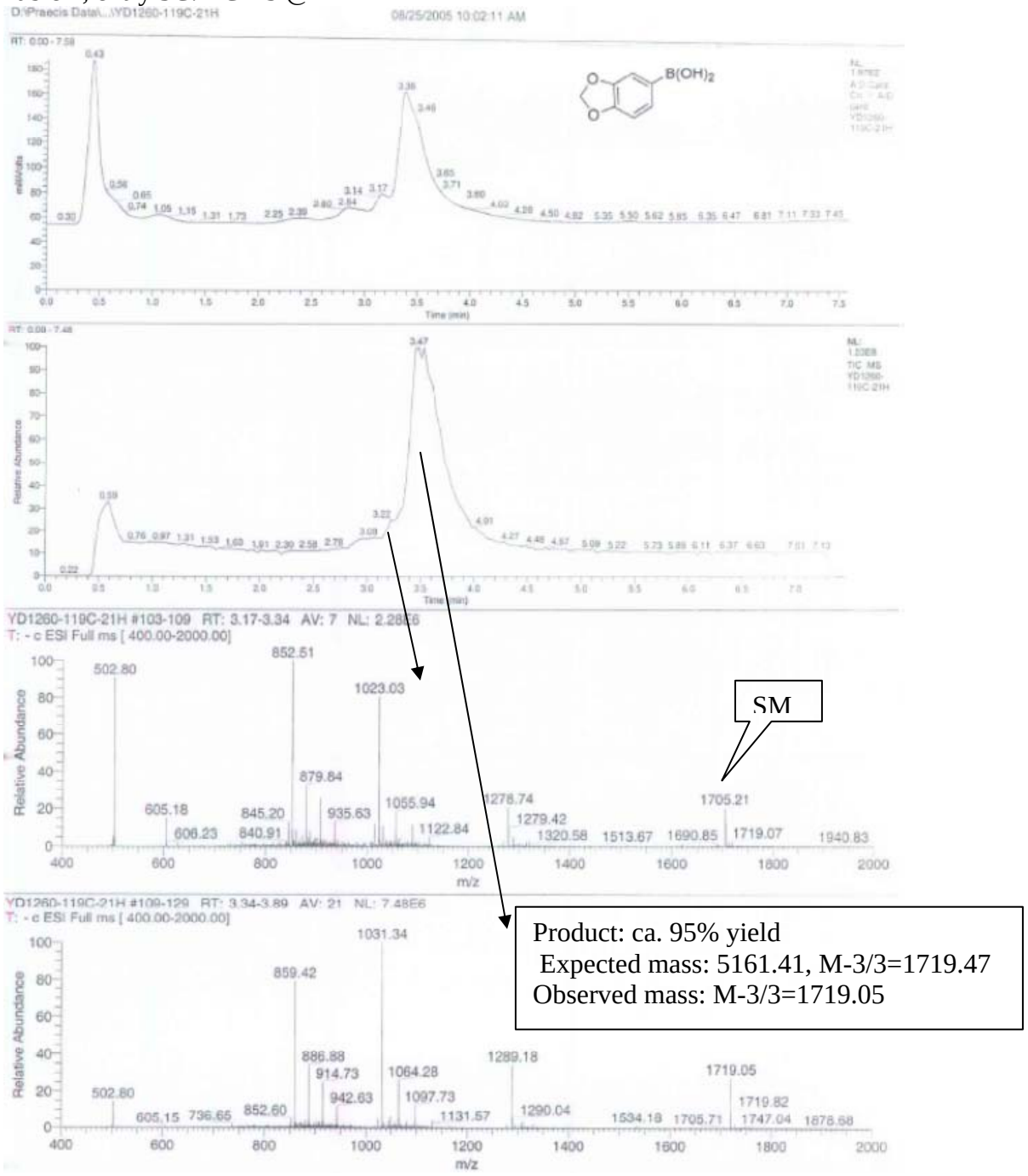


Table 1, entry 4C: LCMS @ 4 h

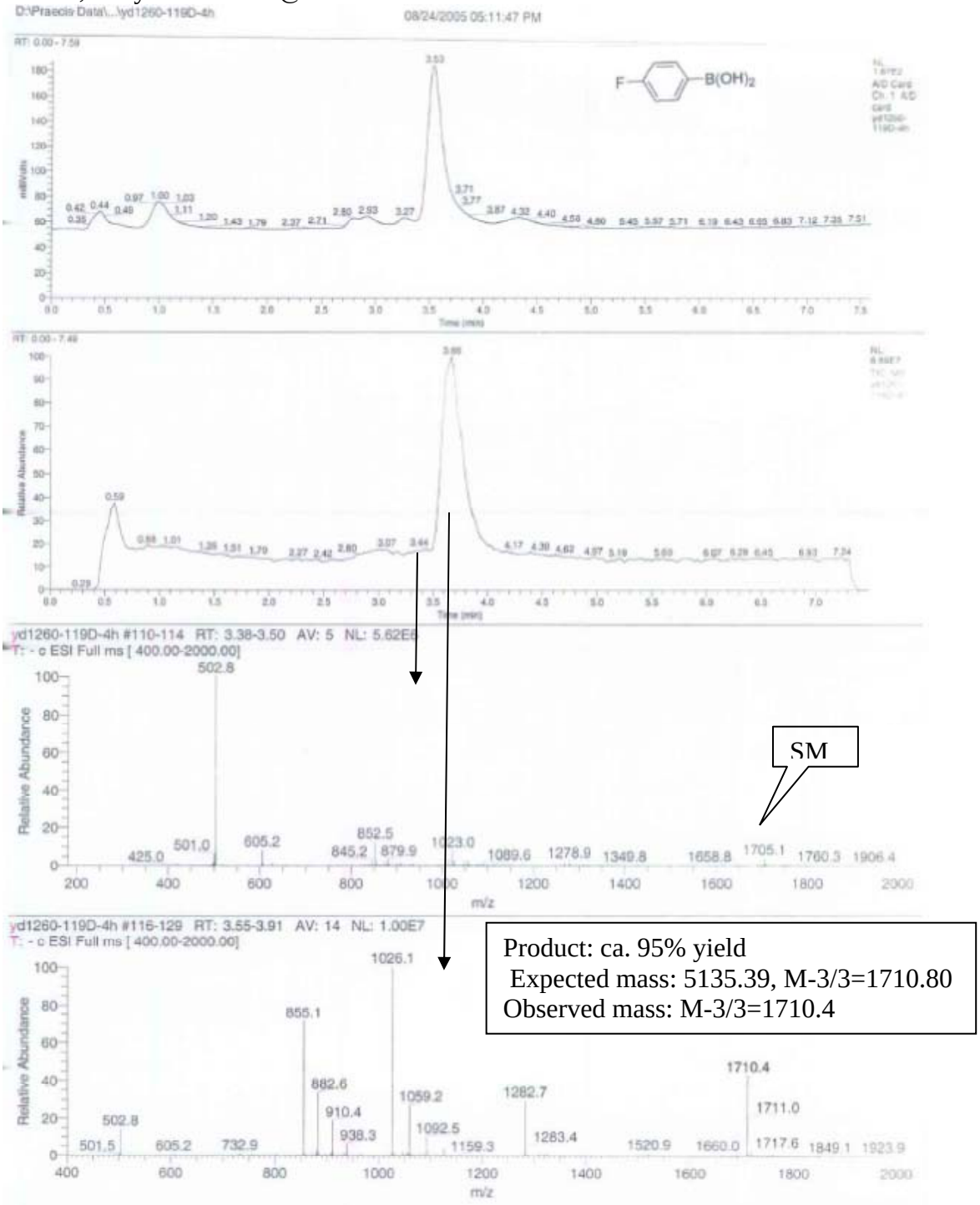
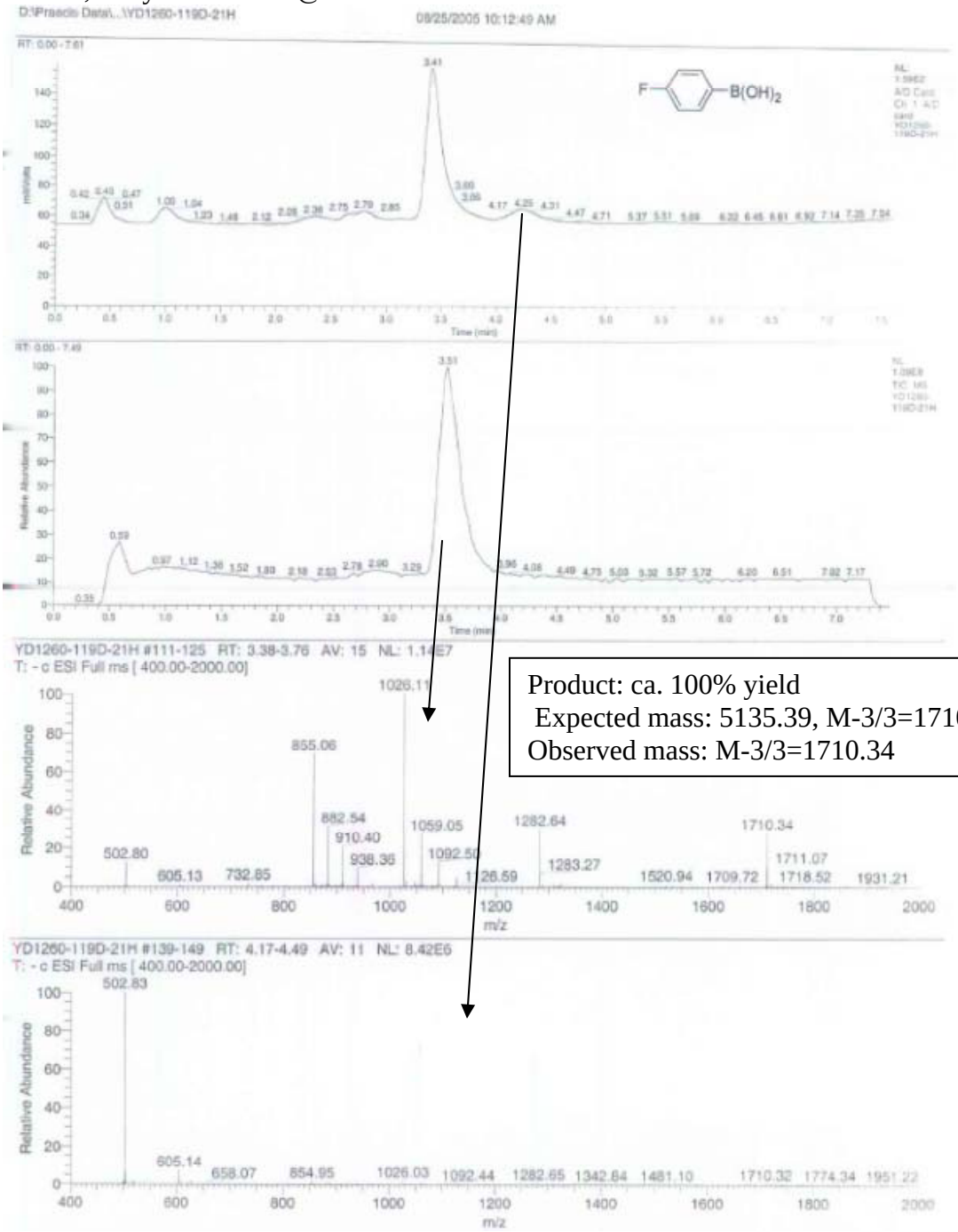


Table 1, entry 4C: LCMS @ 21 h




Product: ca. 100% yield
Expected mass: 5135.39, M-3/3=1710.80
Observed mass: M-3/3=1710.34

Table 1, entry 5C: LCMS @ 4 h

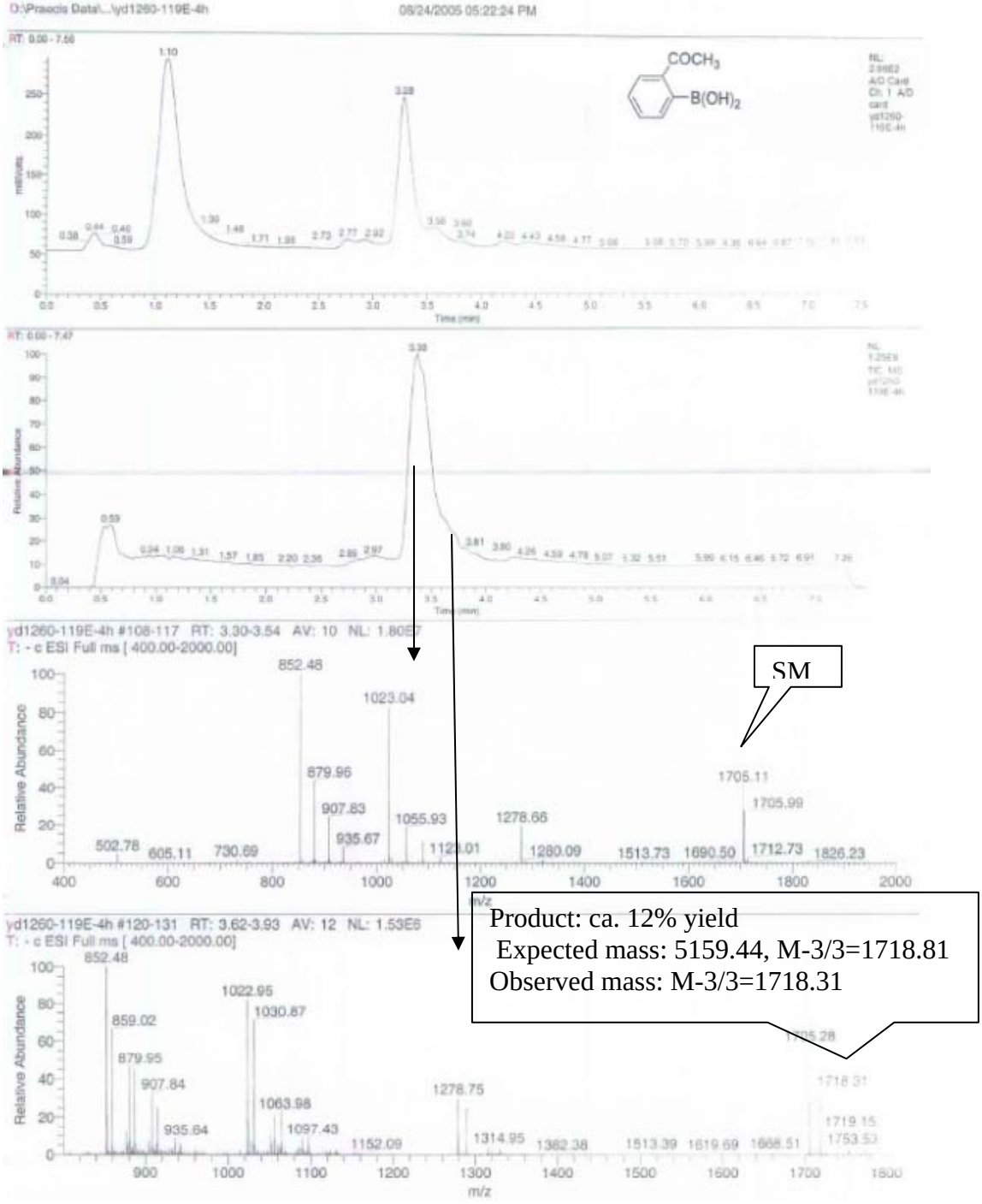


Table 1, entry 5C: LCMS @ 21 h

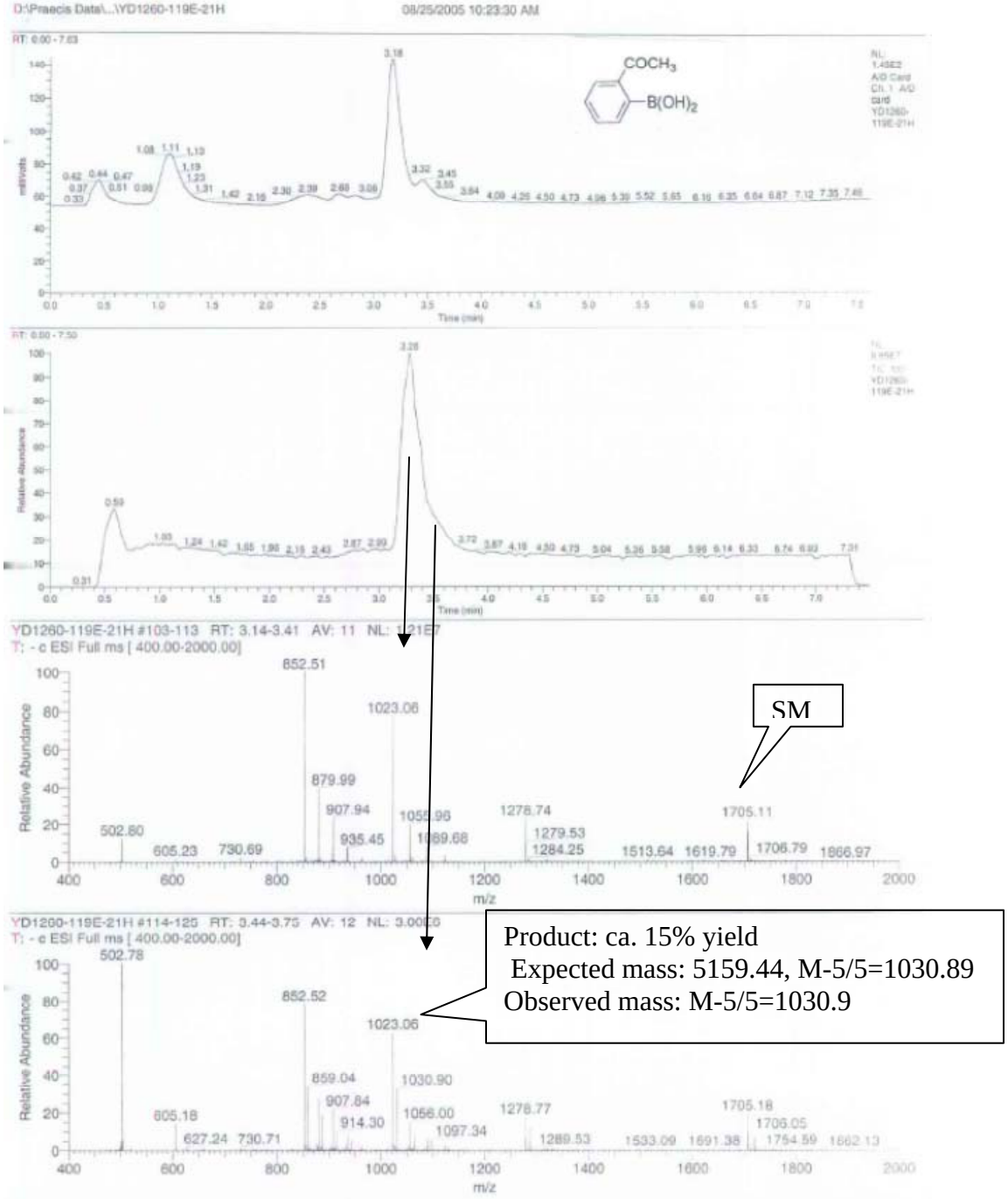
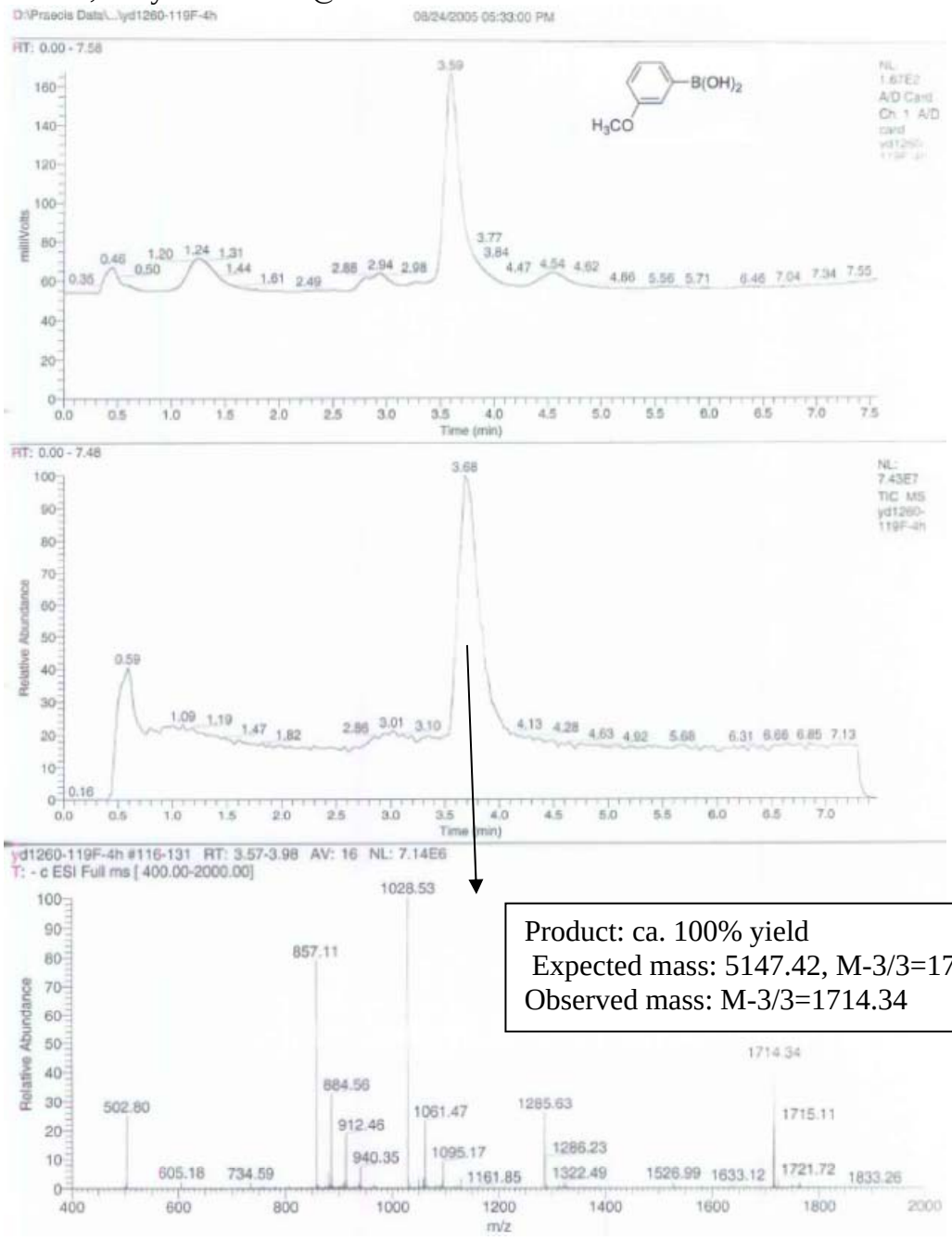


Table 1, entry 6C: LCMS @ 4 h




Product: ca. 100% yield
Expected mass: 5147.42, M-3/3=1714.81
Observed mass: M-3/3=1714.34

Table 3, entry 6: LCMS @ 21 h was very similar to LCMS @ 4 h

Table 1, entry 7C: LCMS @ 4 h

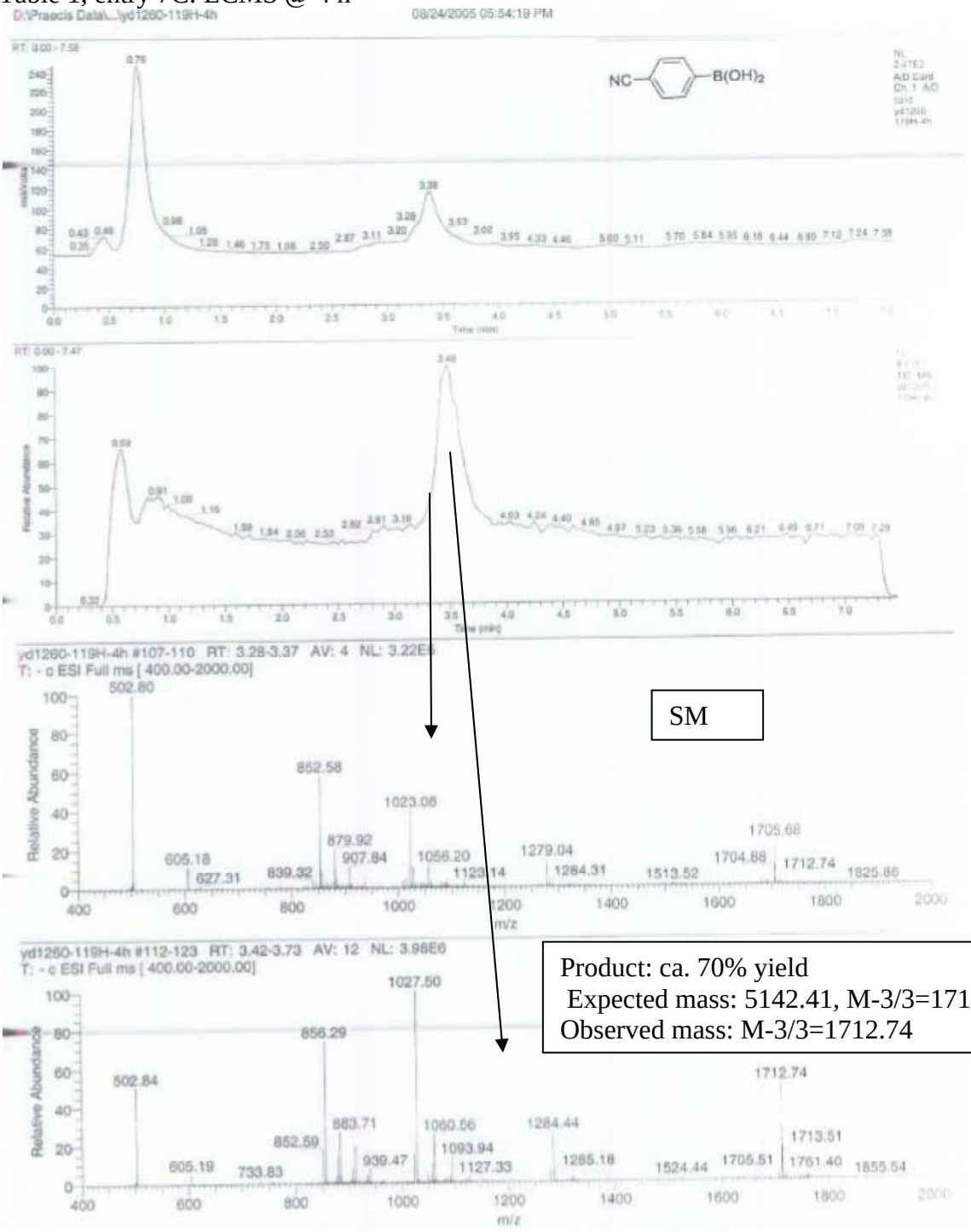
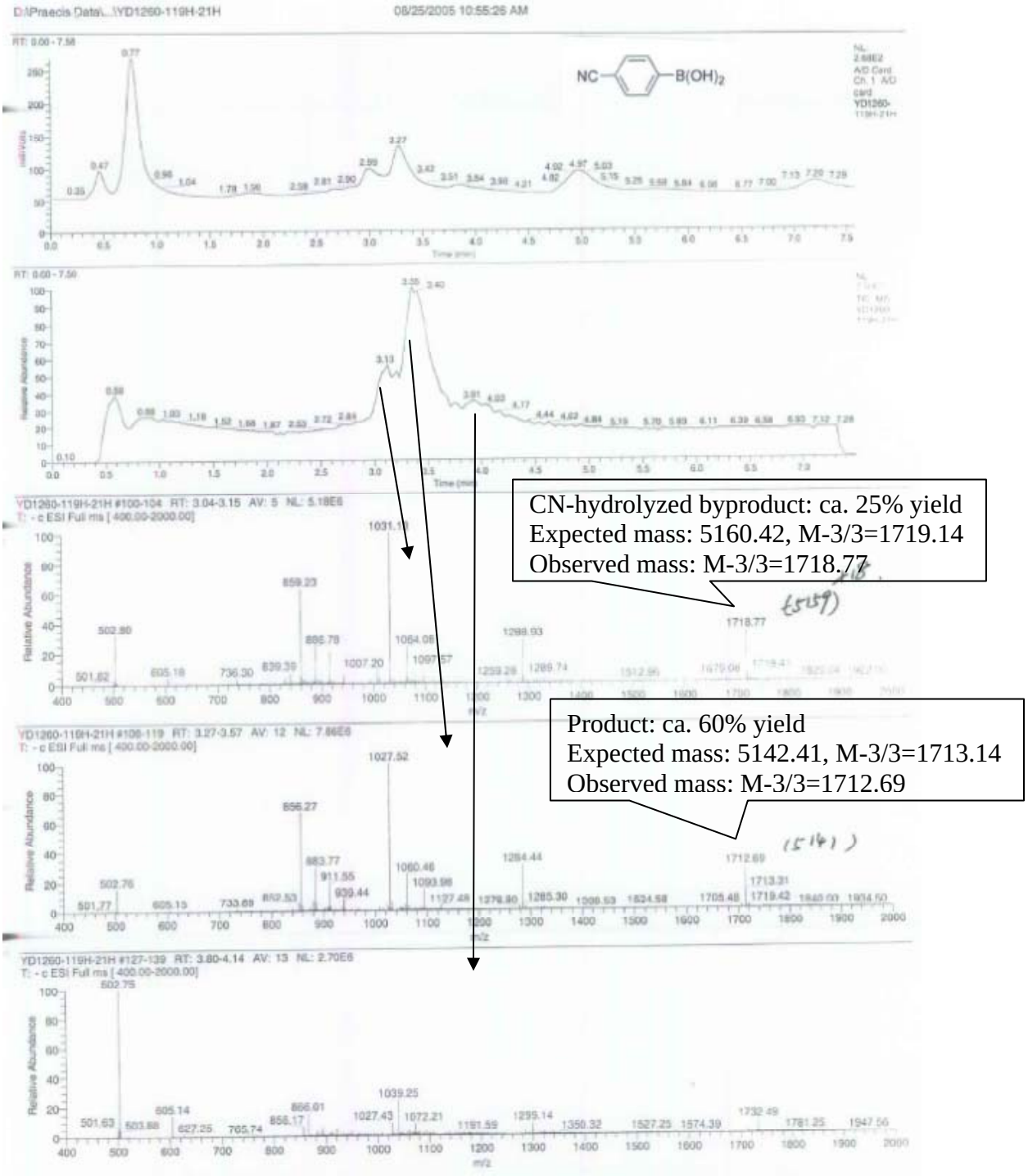


Table 1, entry 7C: LCMS @ 21 h



General procedure for the coupling of **HP-1** with boronic esters in Table 2.

A 1 mM solution of **HP-1** in water (20 nmol, 20 μL) was added 20 equivalents of boronate (0.5 μL, 800 mM in DMA) and 40 equivalents of $Na_2CO_3$ (0.5 μL, 1.6 M in water), followed by 0.5 equivalent of degassed $Pd(PPh_3)_4$ (3 μL, 3.5 mM in $CH_3CN$). The reaction was allowed to proceed at 80 °C for 3 hours 20 mins.

Table 2, entry 1:

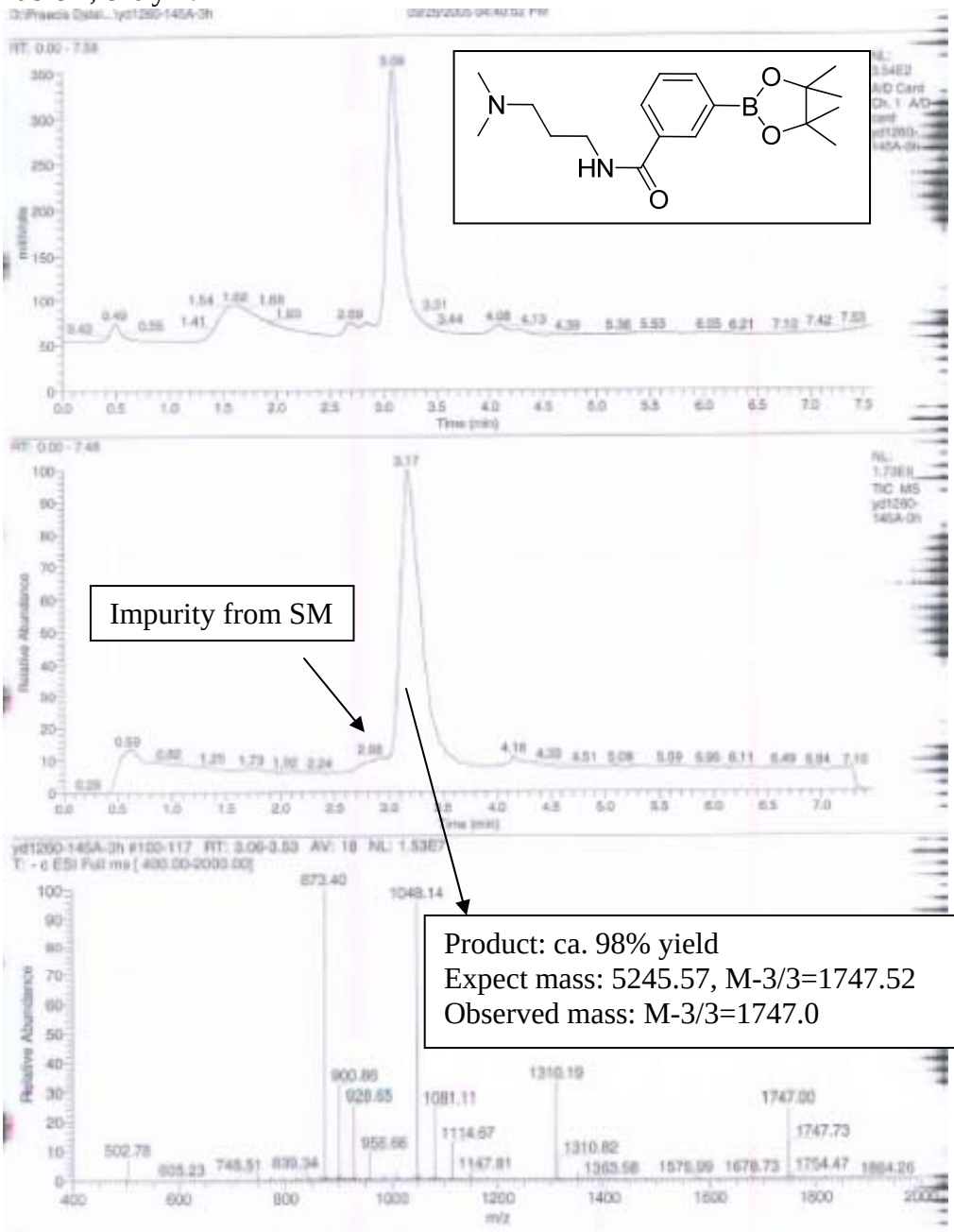


Table 2, entry 2:

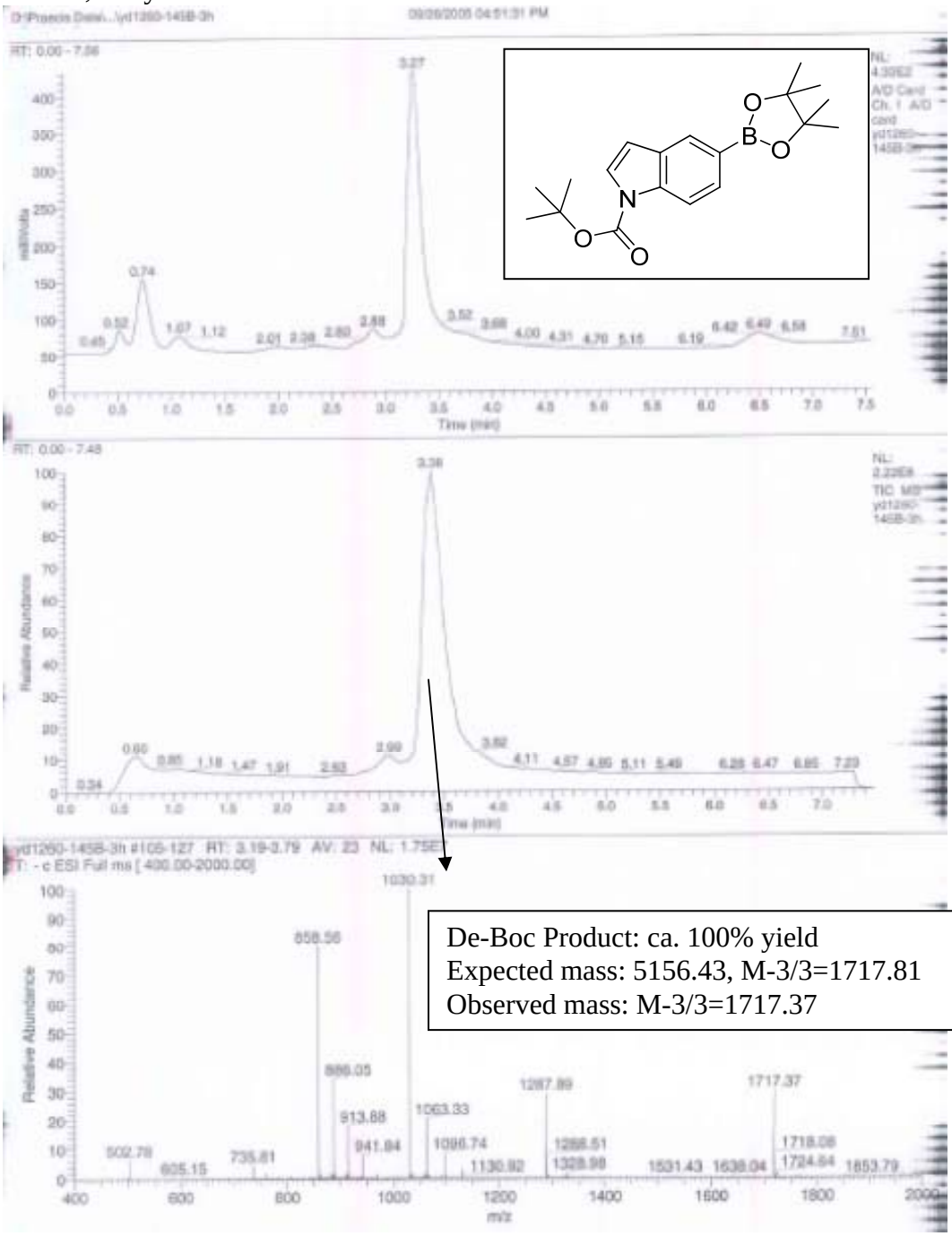
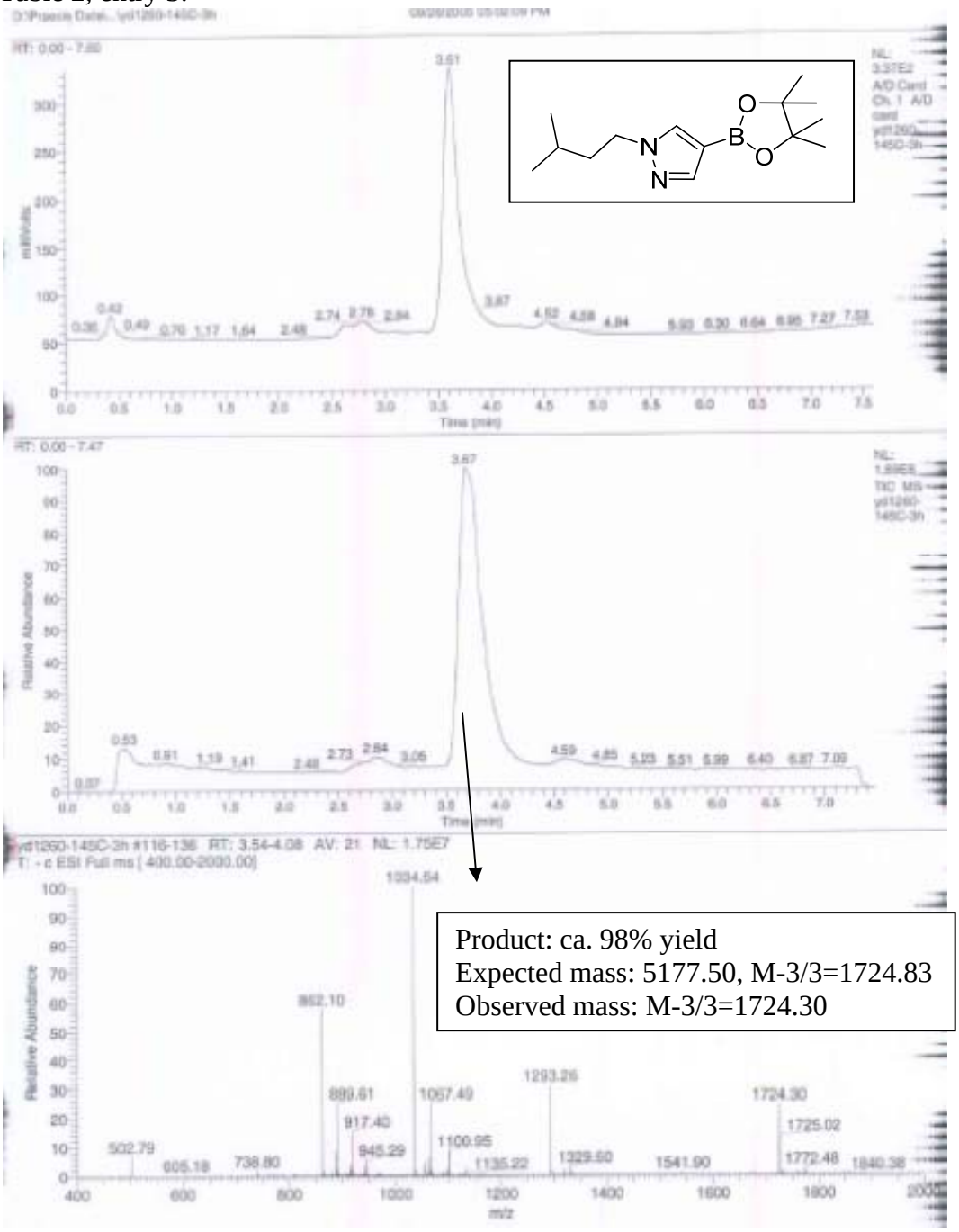


Table 2, entry 3:




Product: ca. 98% yield
Expected mass: 5177.50, M-3/3=1724.83
Observed mass: M-3/3=1724.30

Table 2, entry 4:

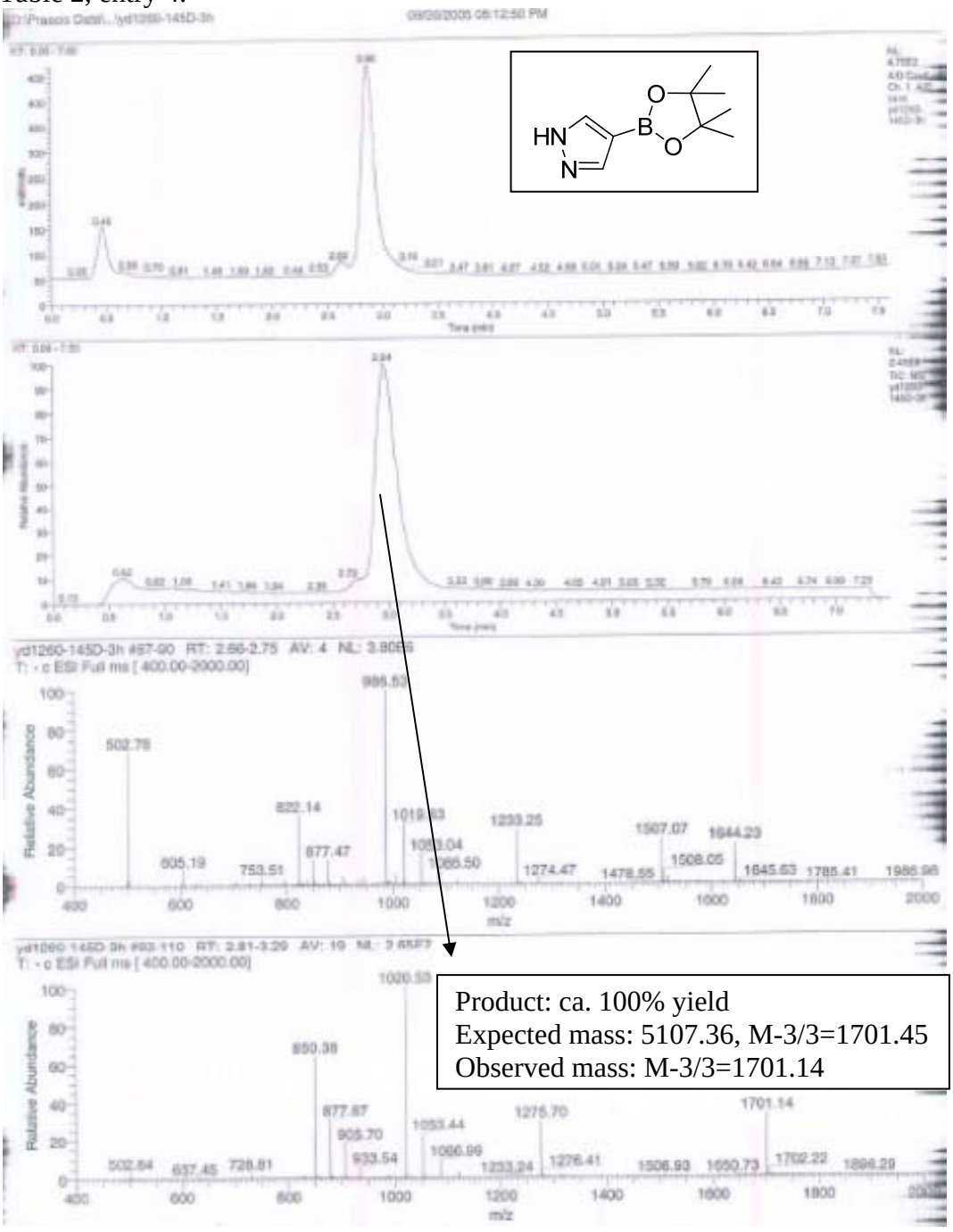


Table 2, entry 5:

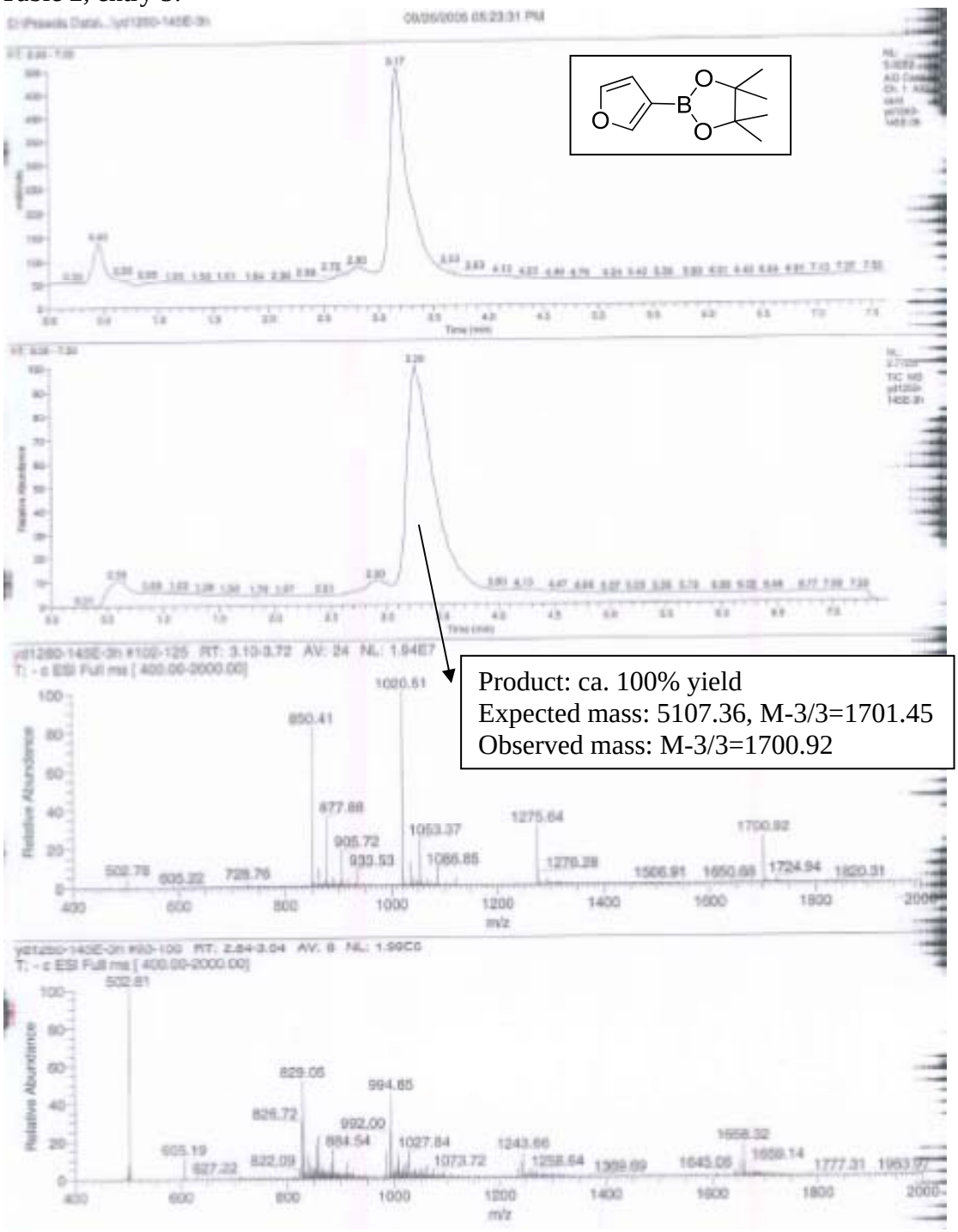
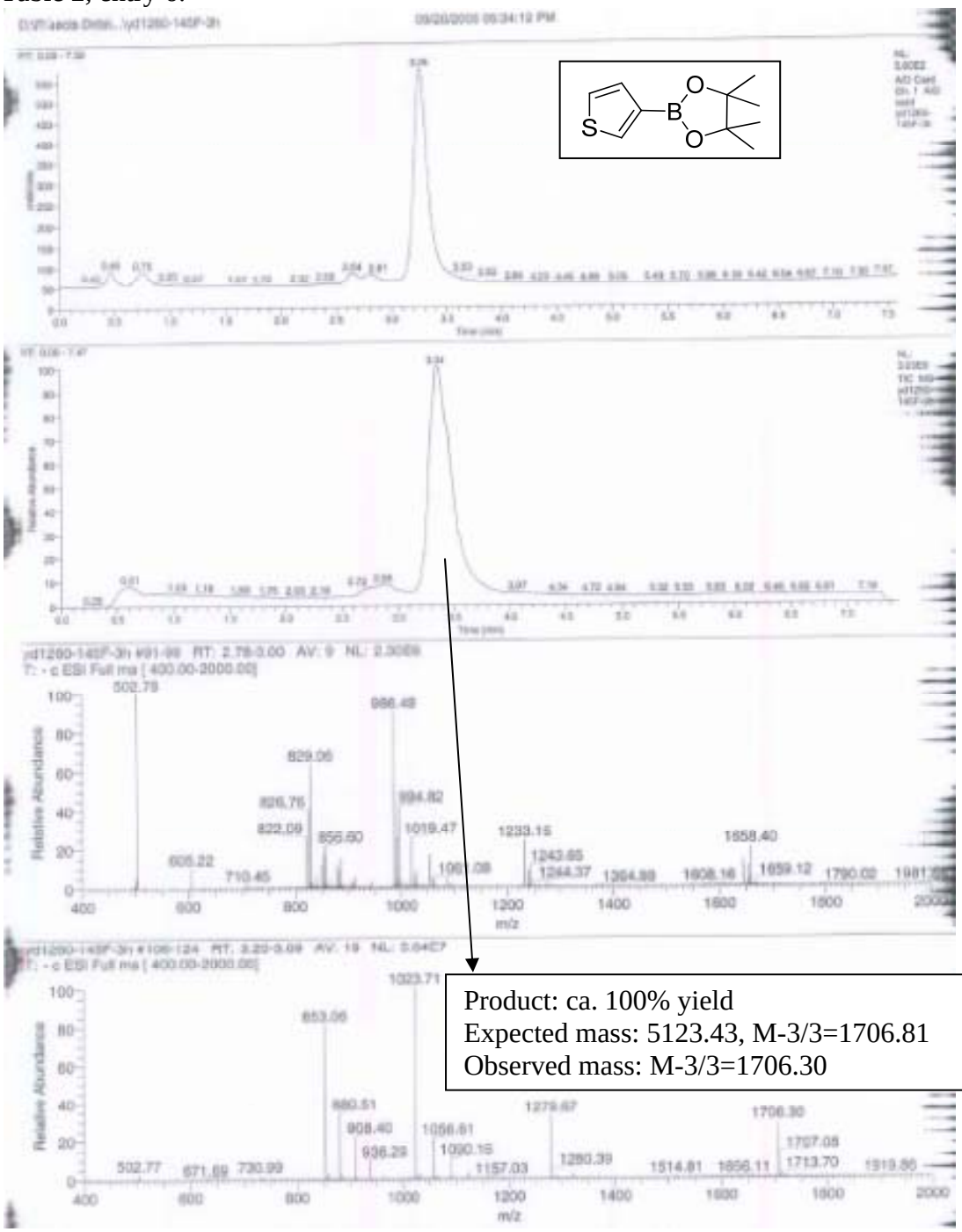
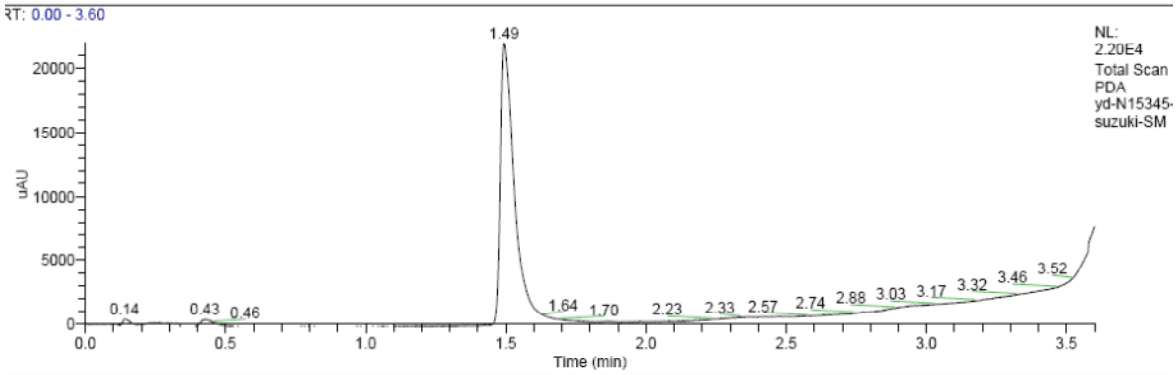


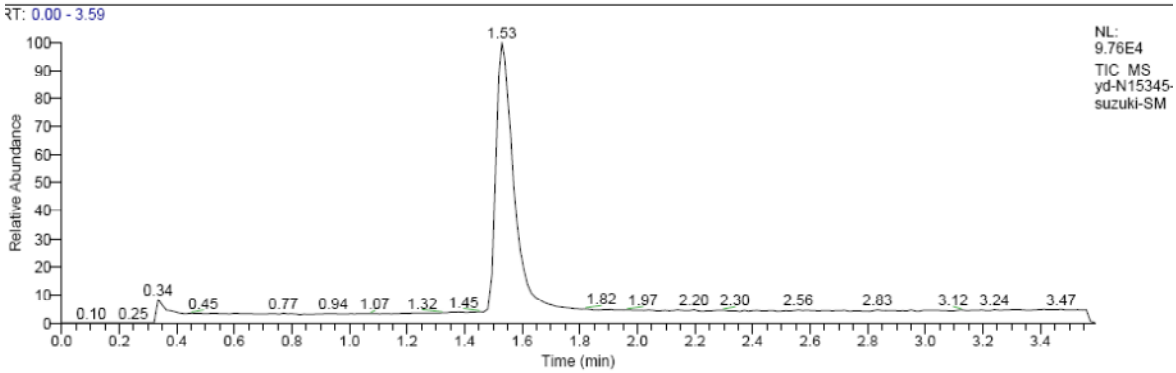
Table 2, entry 6:

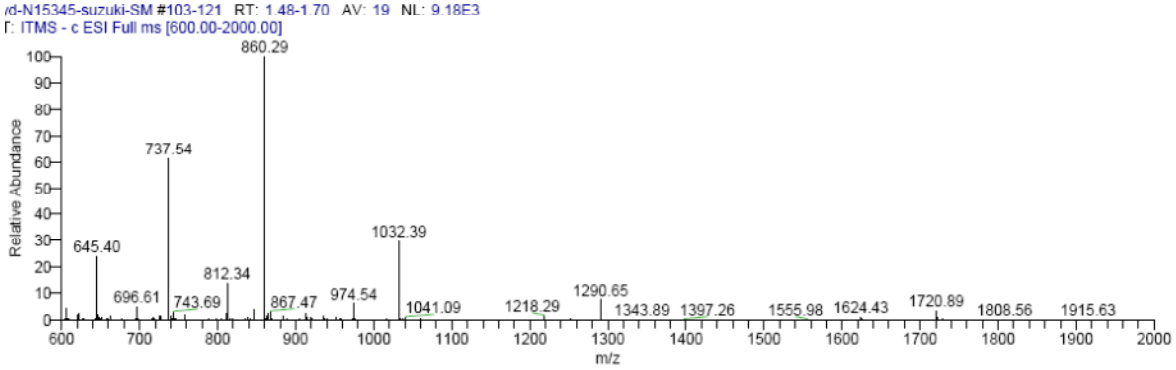



Product: ca. 100% yield
Expected mass: 5123.43, M-3/3=1706.81
Observed mass: M-3/3=1706.30

HP-1 for entry 7-12:



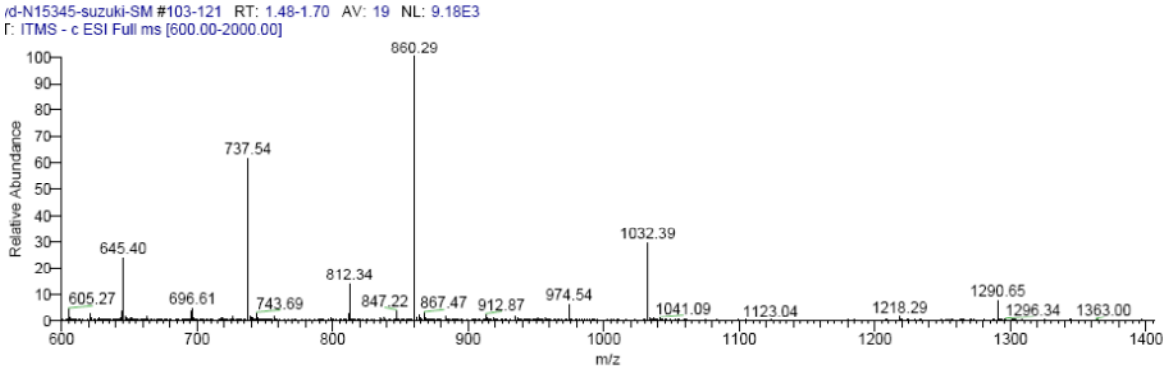



Table 2, entry 7:

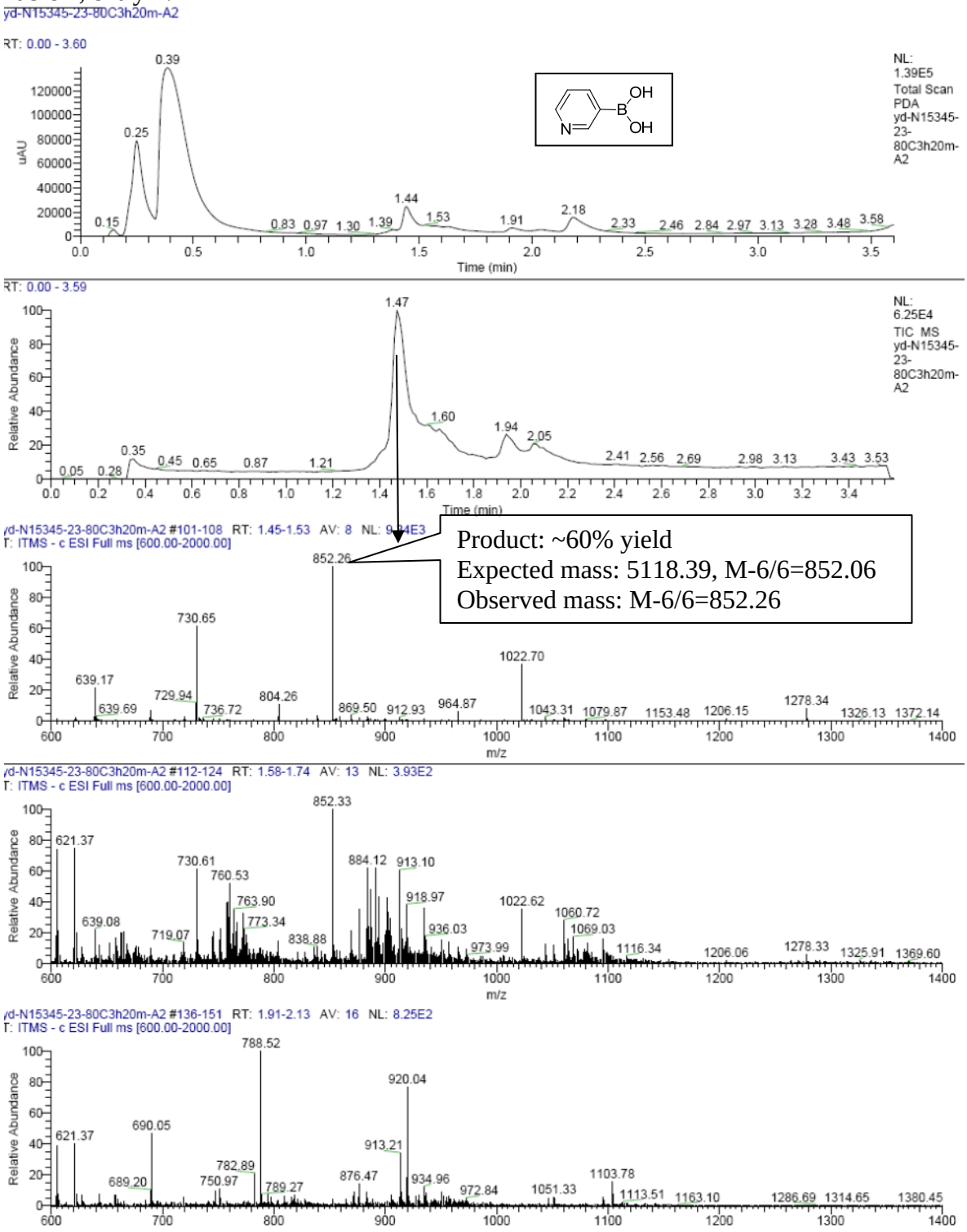


Table 2, entry 7, LCMS @ 16 hrs:

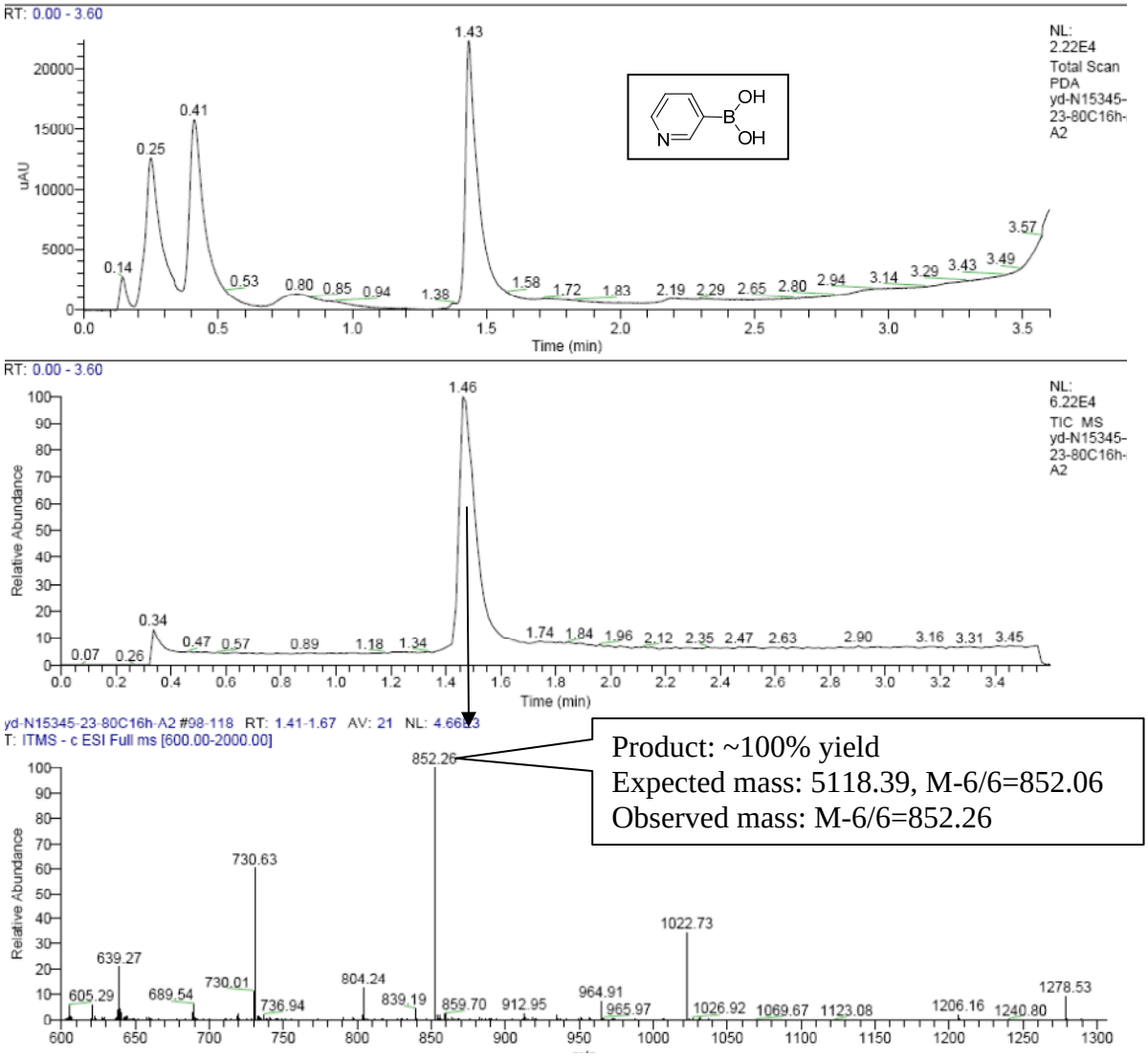
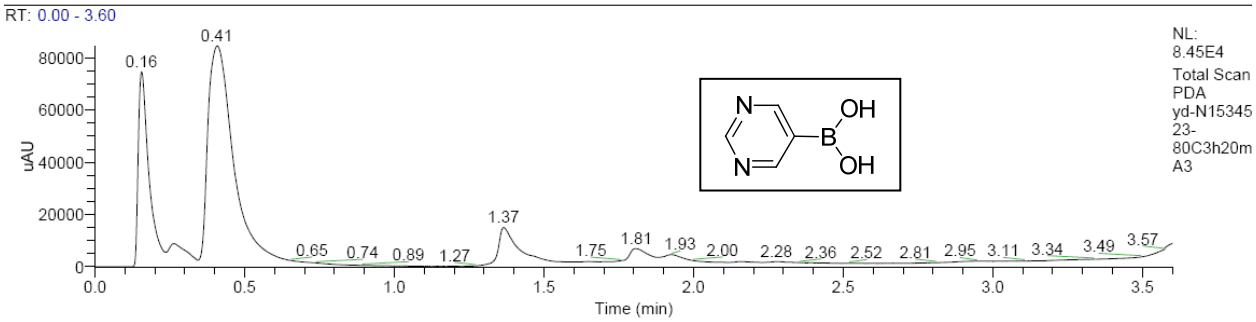
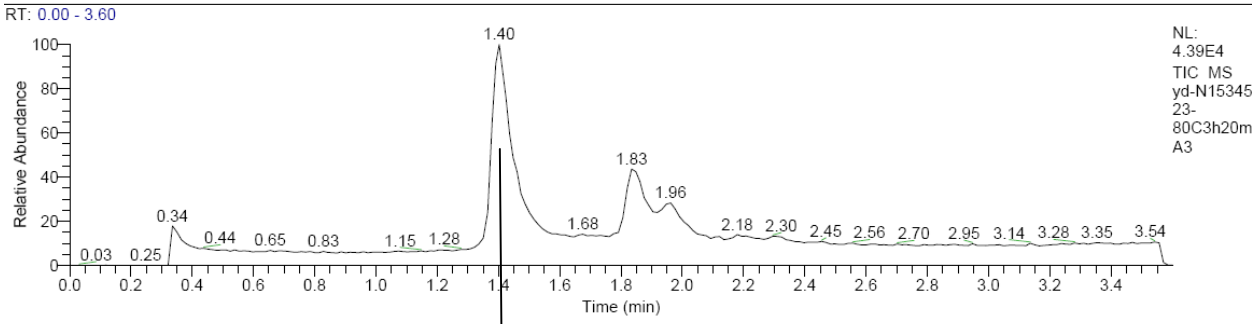
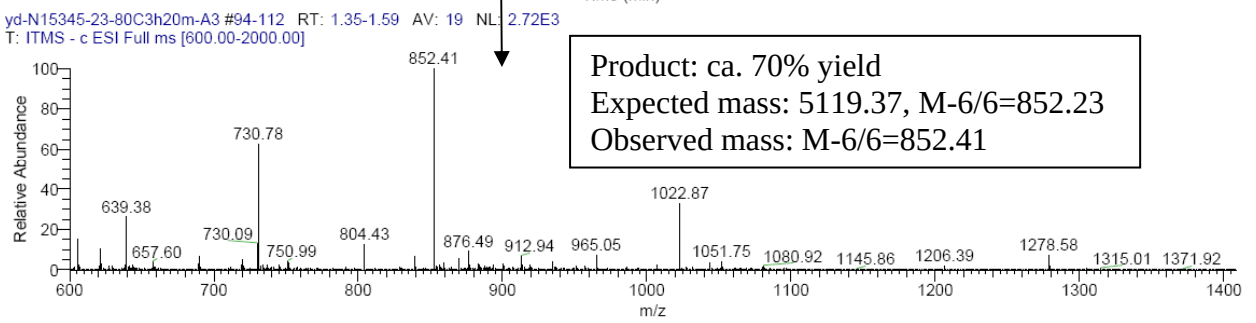


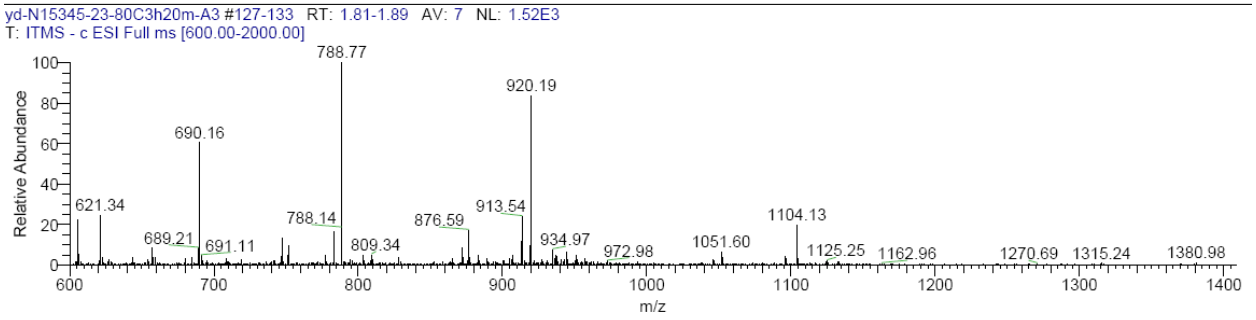
Table 2, entry 8:




Product: ca. 70% yield
Expected mass: 5119.37, M-6/6=852.23
Observed mass: M-6/6=852.41



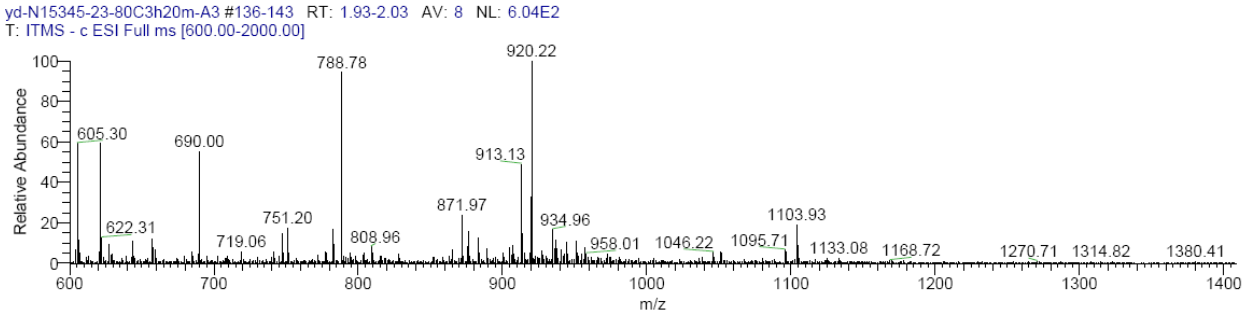



Table 2, entry 8, LCM @ 16 hrs:

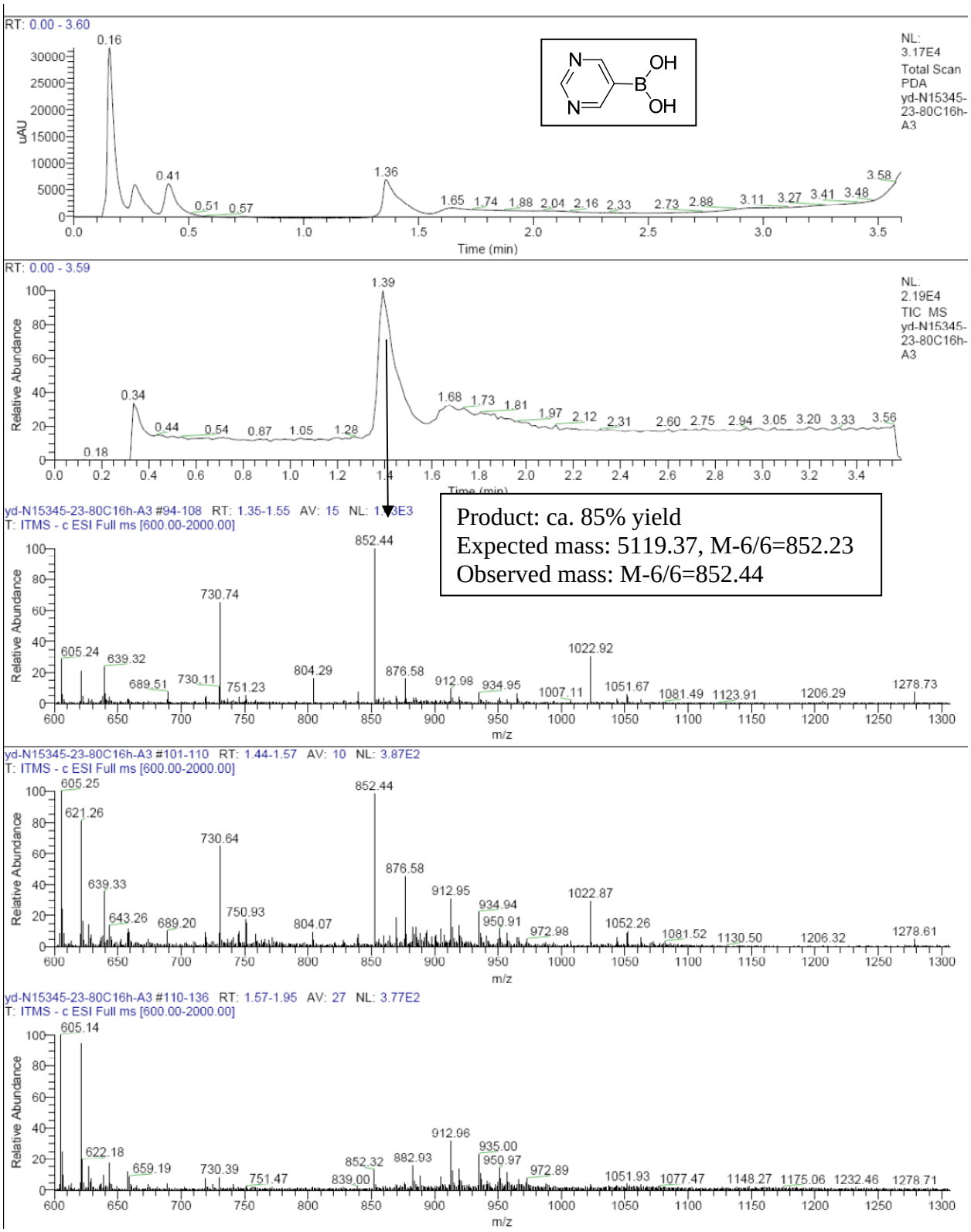


Table 2, entry 9:

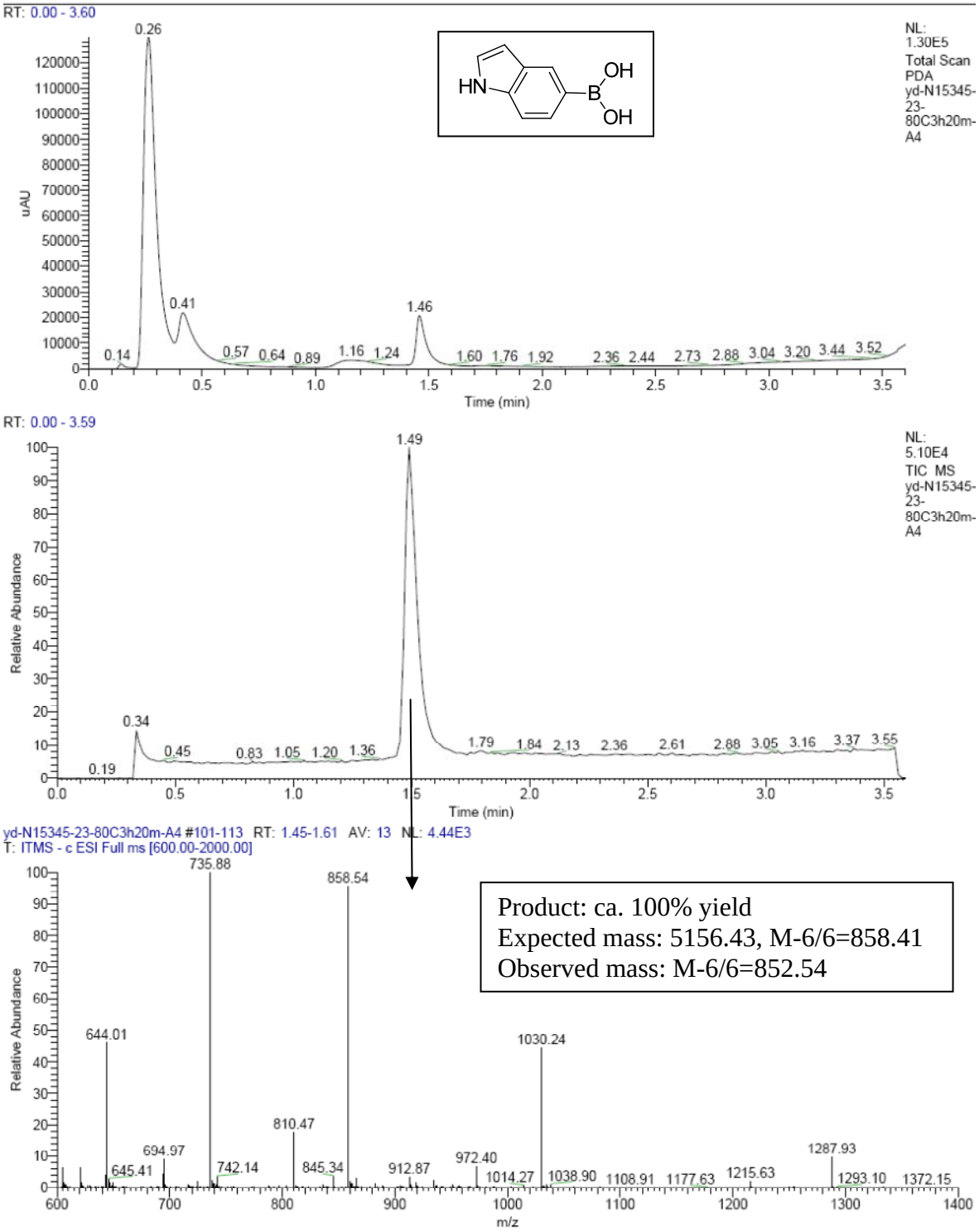


Table 2, entry 10:

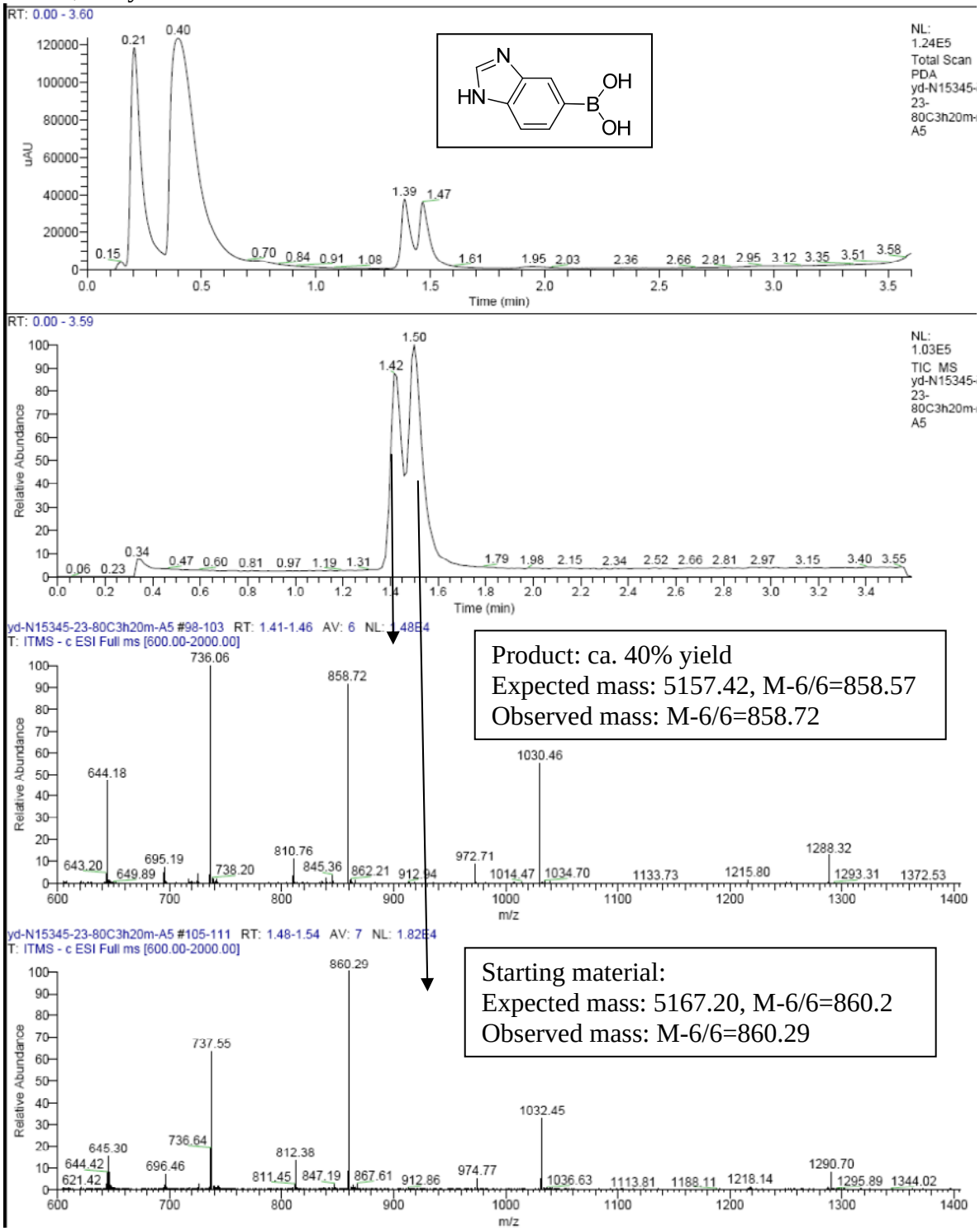


Table 2, entry 10, LCMS @ 16 hrs:

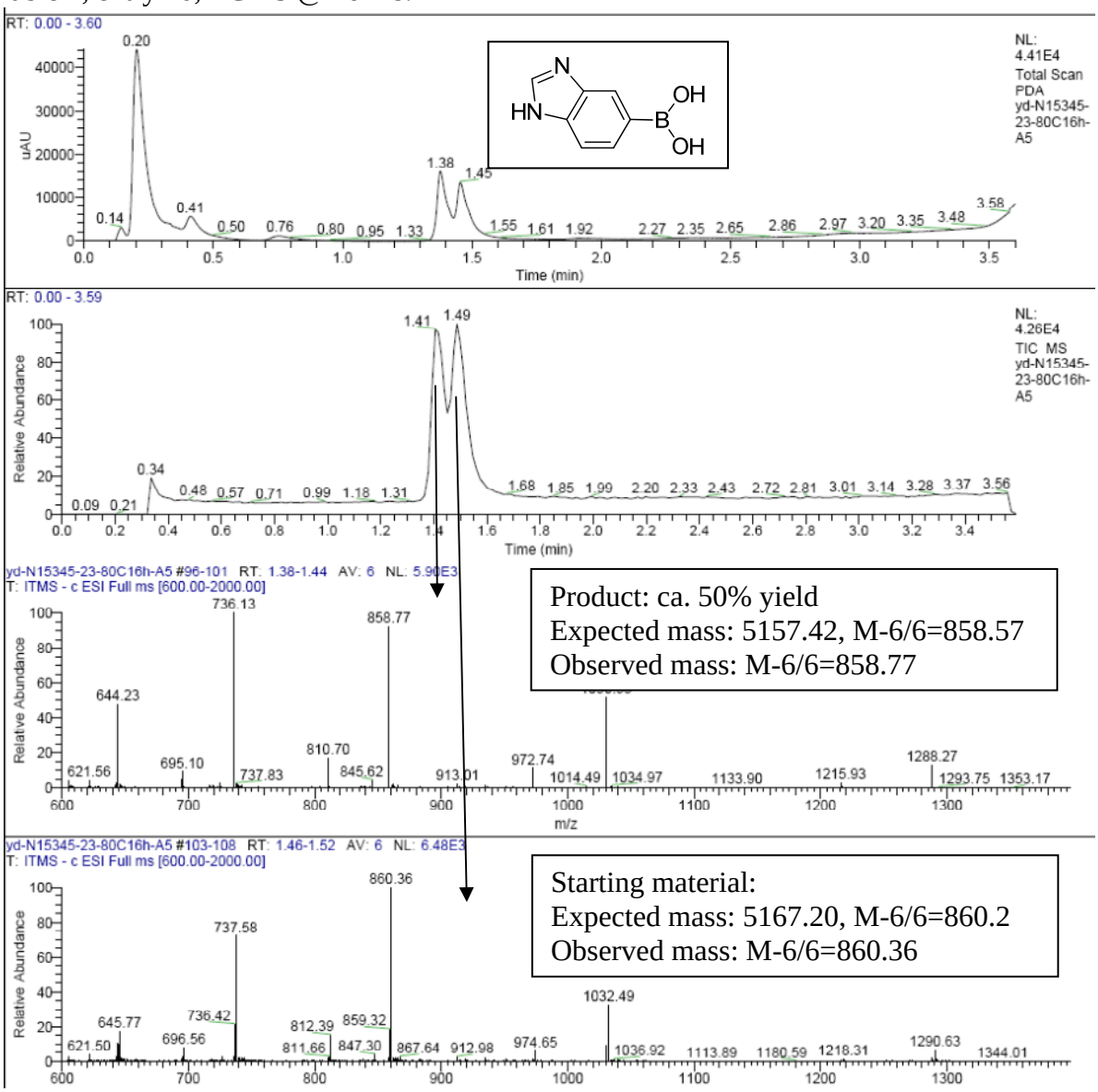


Table 2, entry 11:

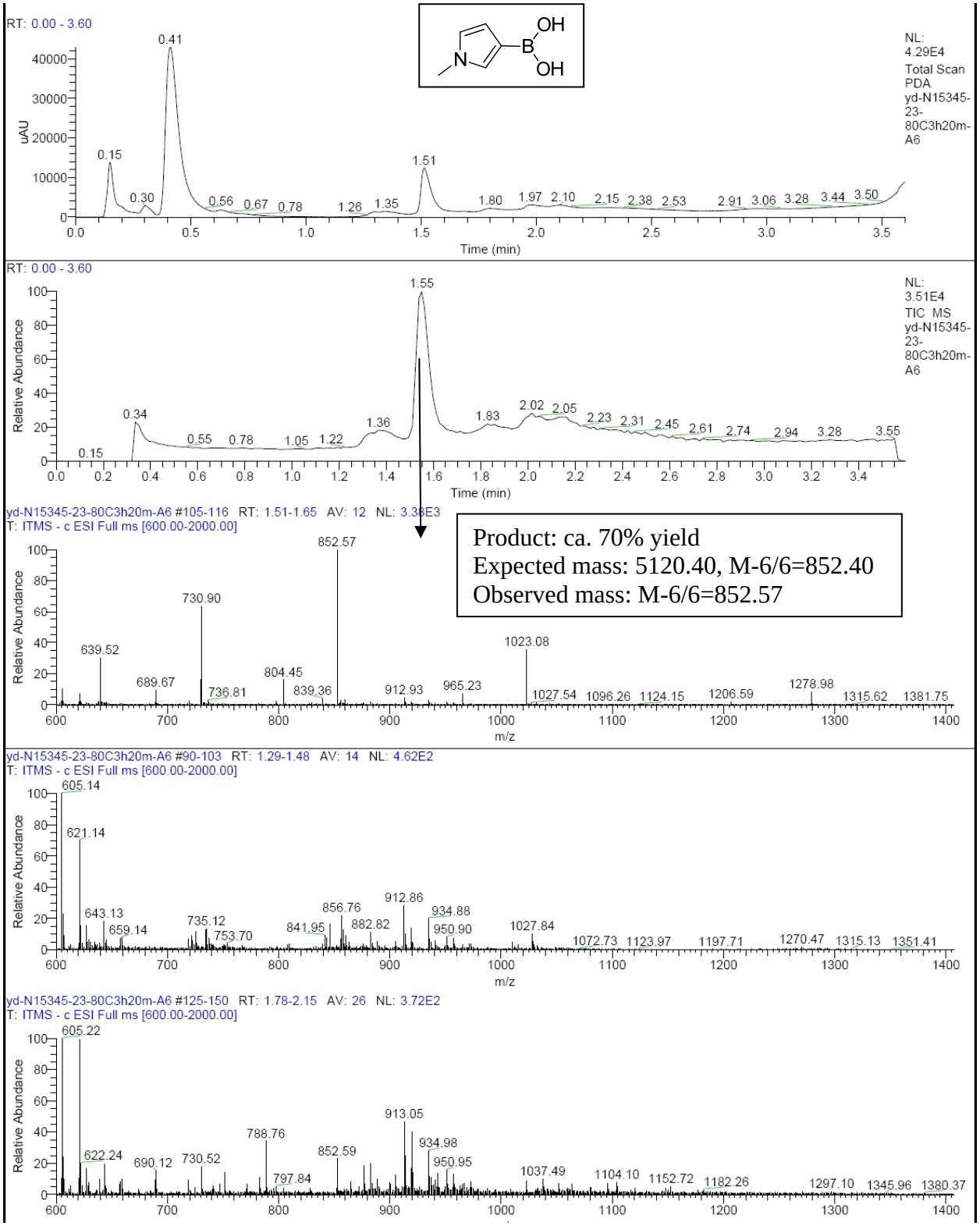
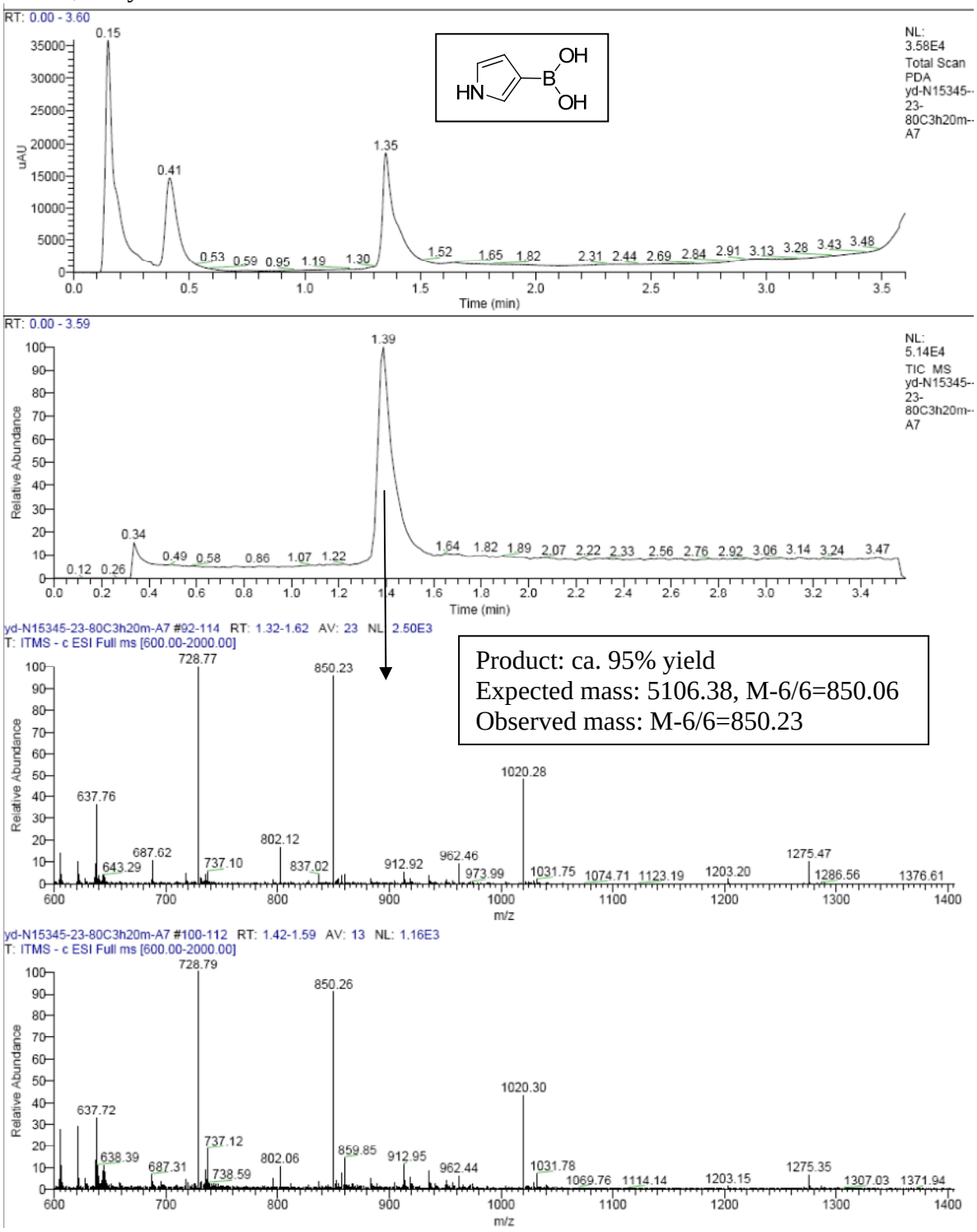
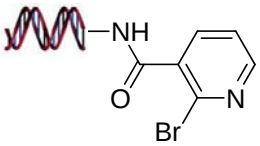


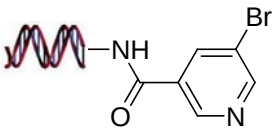
Table 2, entry 12:



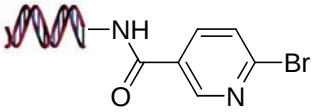
Preparation of **HP-5, 6 & 7**




**HP-5**



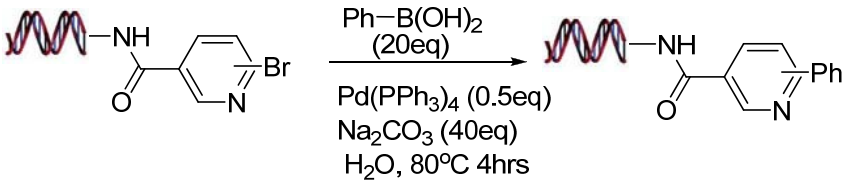

**HP-6**




**HP-7**

A solution of HP in pH9.4 borate buffer (250 mM) (1 μmol, 300 μL) was added at cold 40 equivalents of bromo-nicotinic acid (8.1 mg in 70 μL of DMF), followed by 40 equivalents of DMT-MM (10.9 mg in 70 μL of water). The pH of the reaction solution was adjusted to around 9 with NaOH. The reaction was allowed to proceed at cold overnight. 10% piperidine (44 μL) was added to the reaction. After 15 minutes, the reaction was precipitated by adding 10% 5 N NaCl water solution and 2.5 times volume of absolute EtOH. The pellet was redissolved in water (400 μL), and purified with reverse-phase HPLC (10-40% solvent B).

General procedure for the coupling of **HP-5, 6 & 7** with boronic acids in Table 3.




A 1 mM solution of **HP-5**, **-6**, or **-7** in water (20 nmol, 20 μL) was added 20 equivalents of boronate (0.5 μL, 800 mM in DMA) and 40 equivalents of $Na_2CO_3$ (0.5 μL, 1.6 M in water), followed by 0.33 equivalent of degassed $Pd(PPh_3)_4$ (2 μL, 3.3 mM in $CH_3CN$). The reaction was allowed to proceed at 80 °C for 5 h.

Table 3, entry 1A:

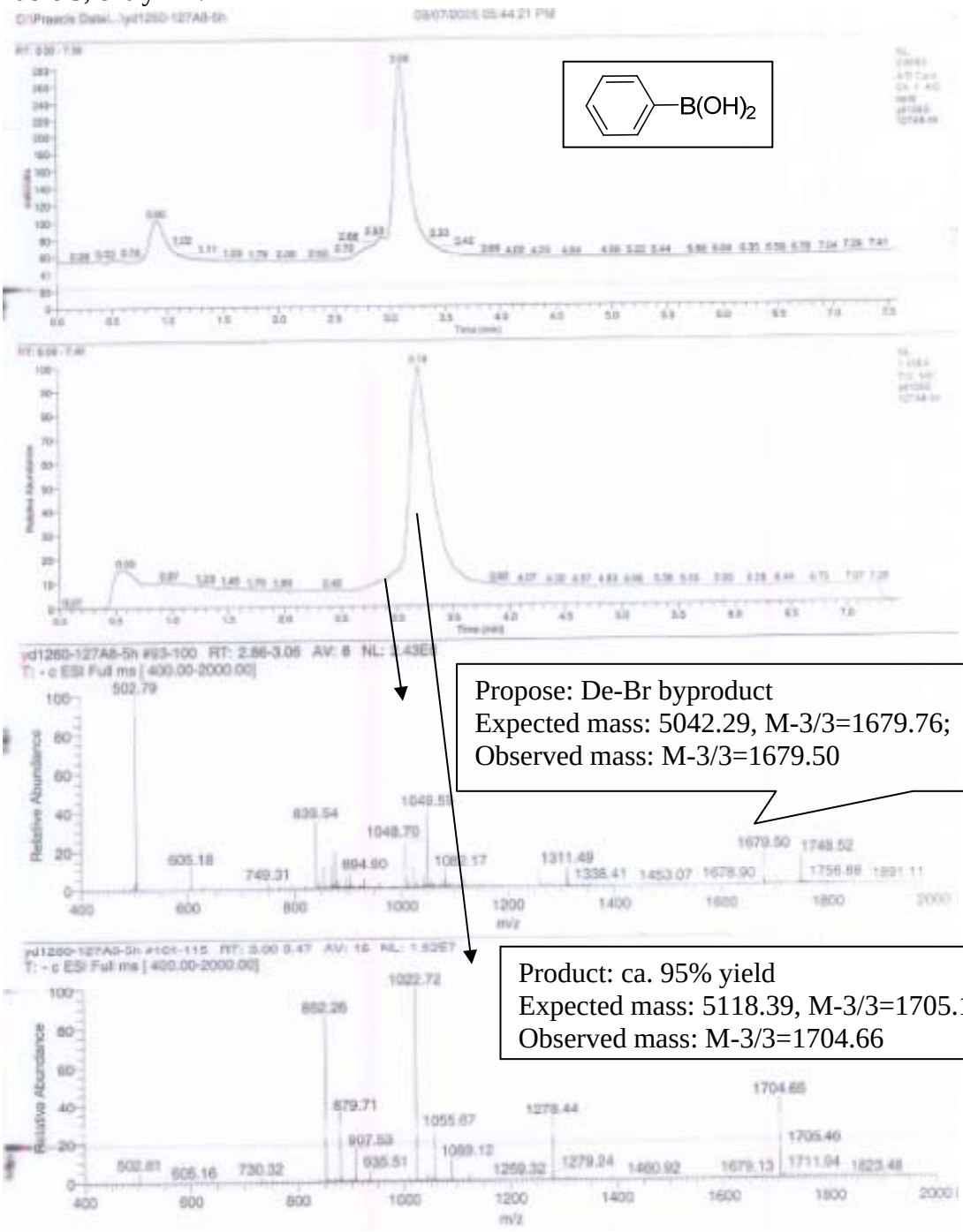


Table 3, entry 2A:

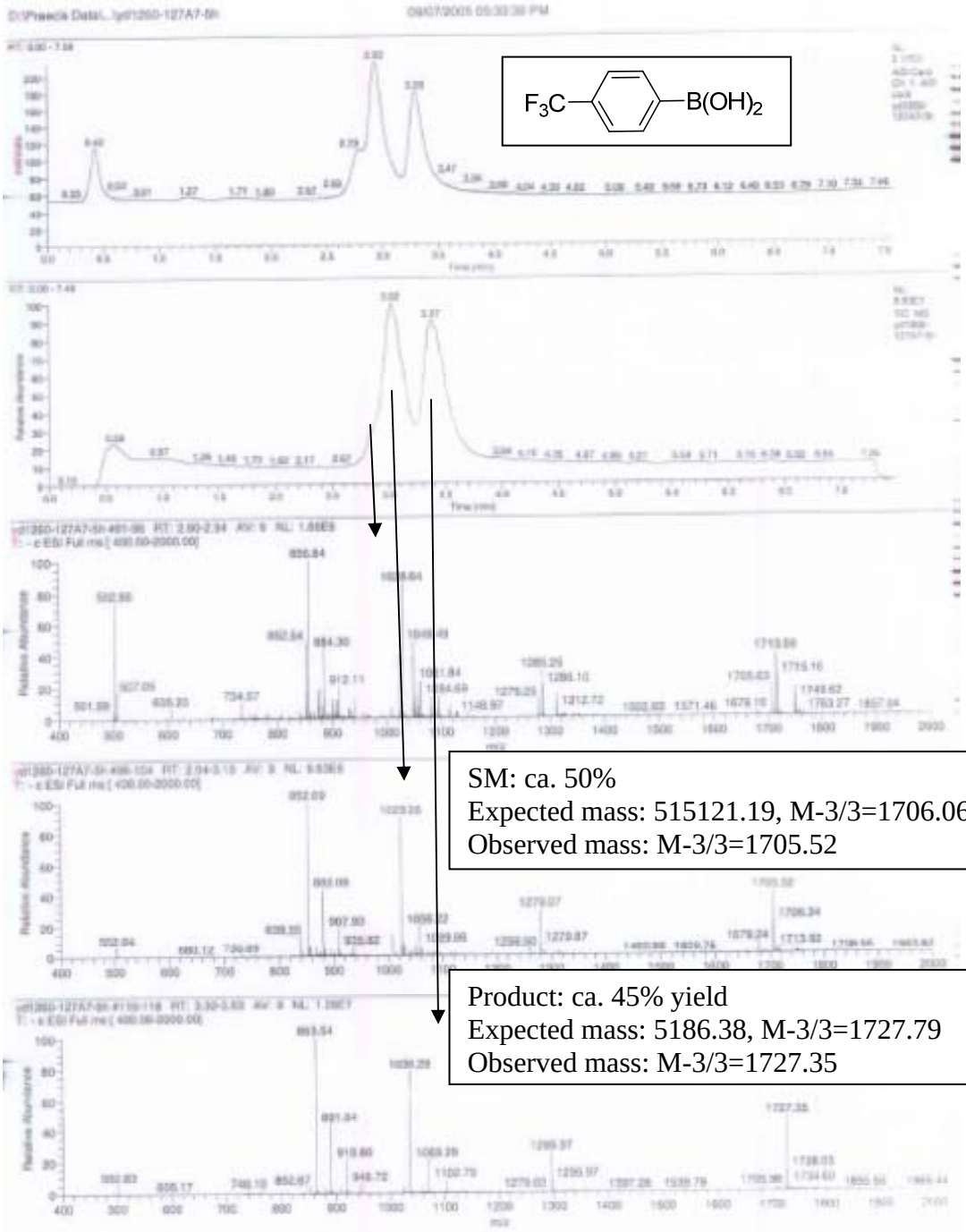


Table 3, entry 3A:

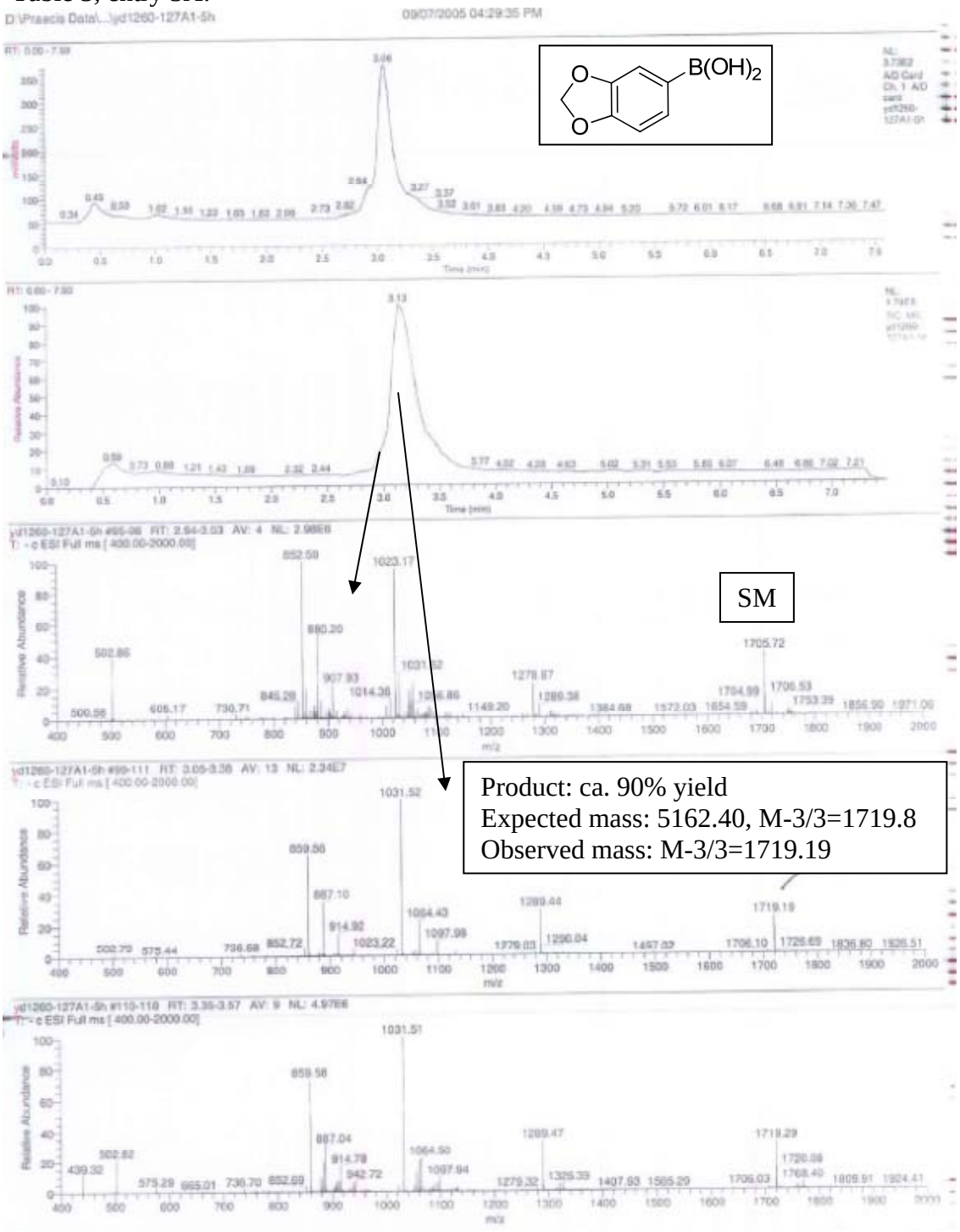


Table 3, entry 4A:

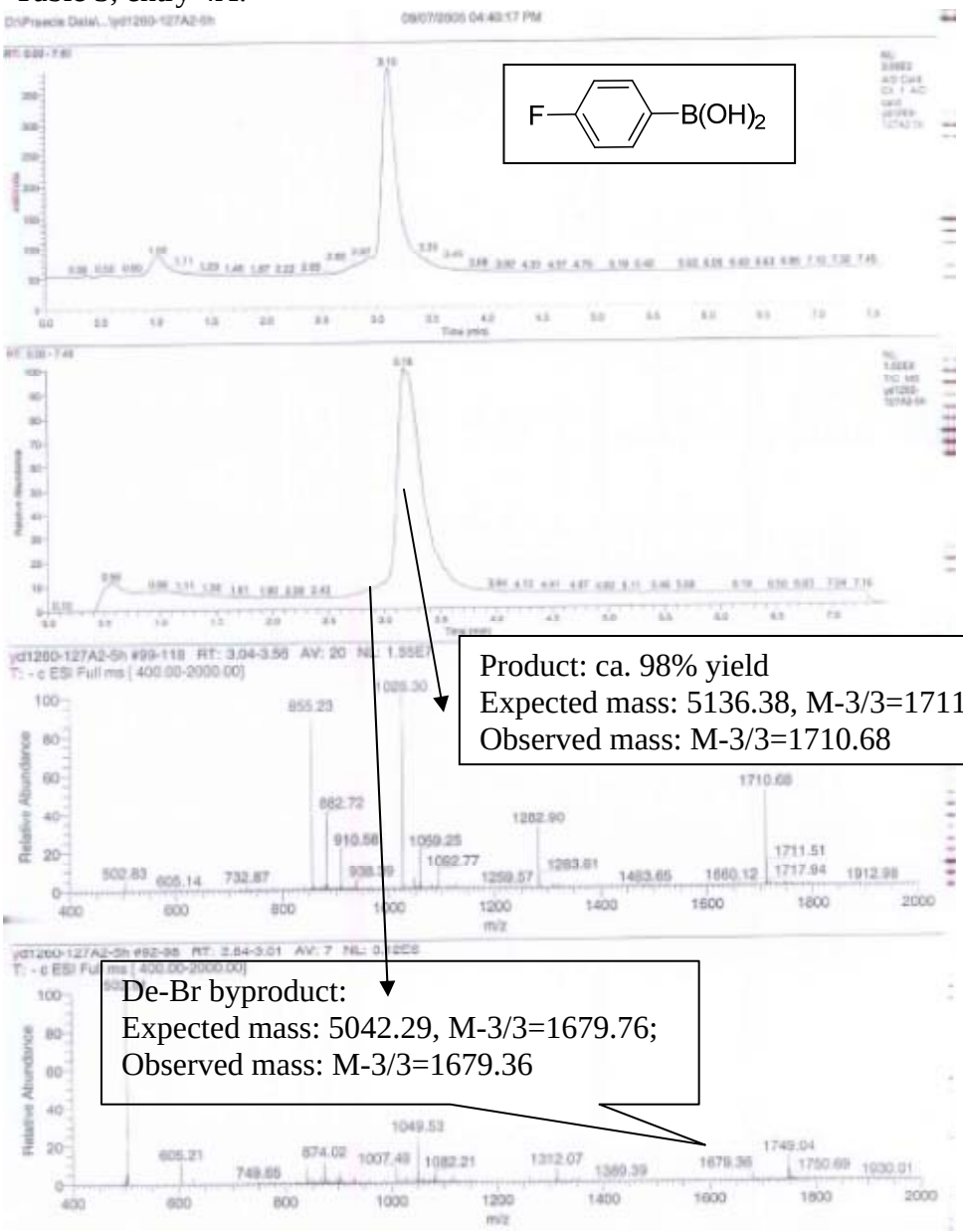


Table 3, entry 5A:

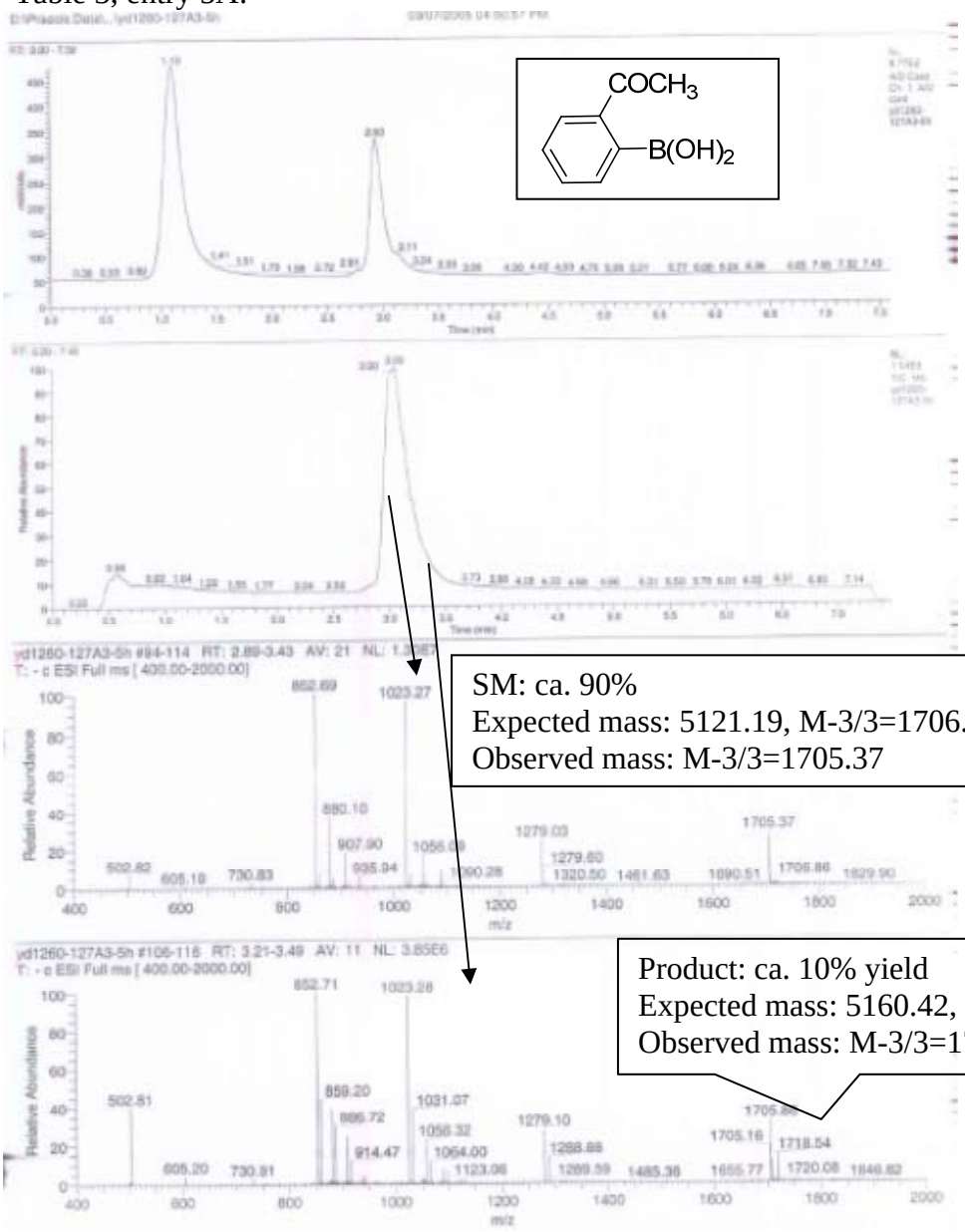


Table 3, entry 6A:

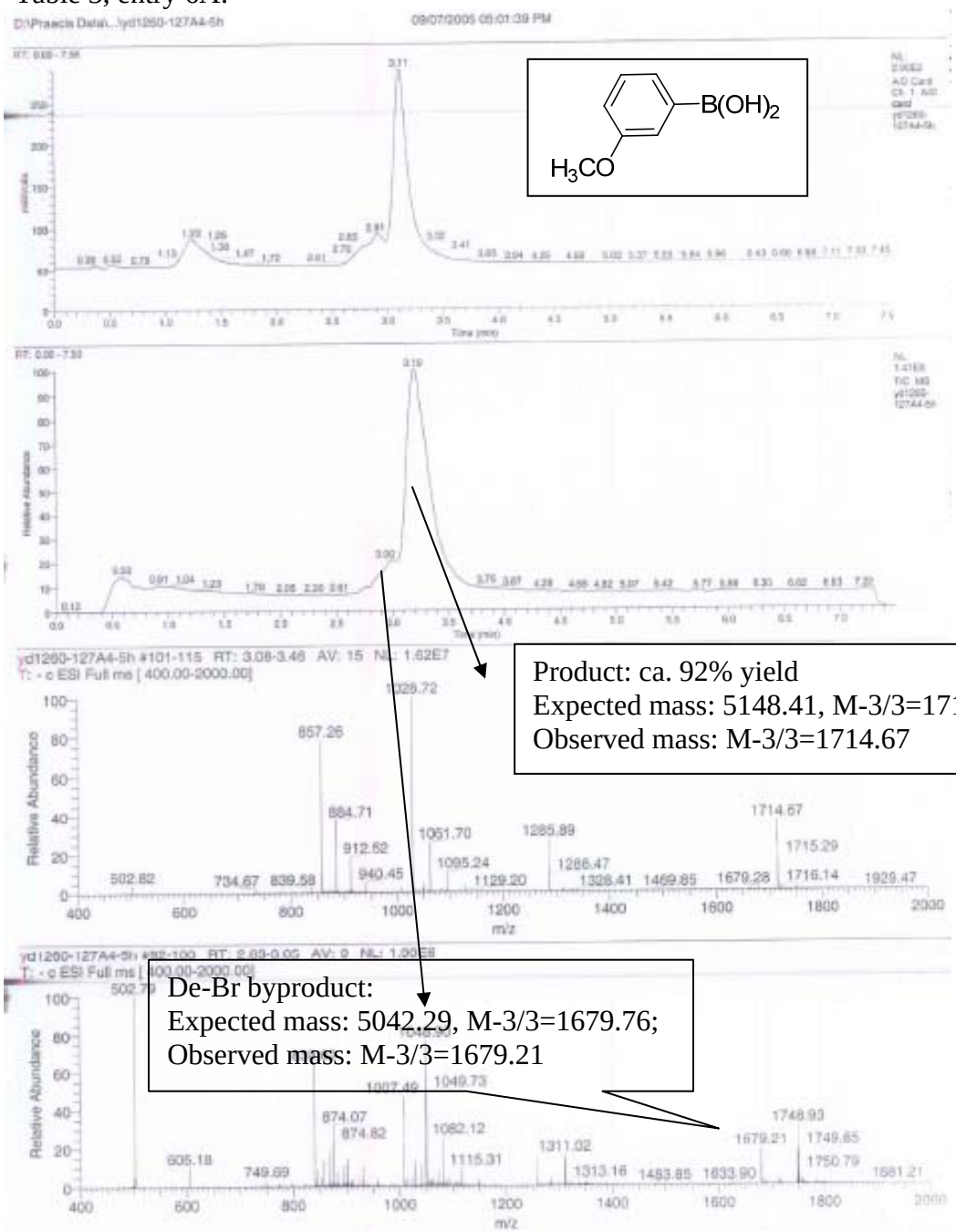


Table 3, entry 7A:

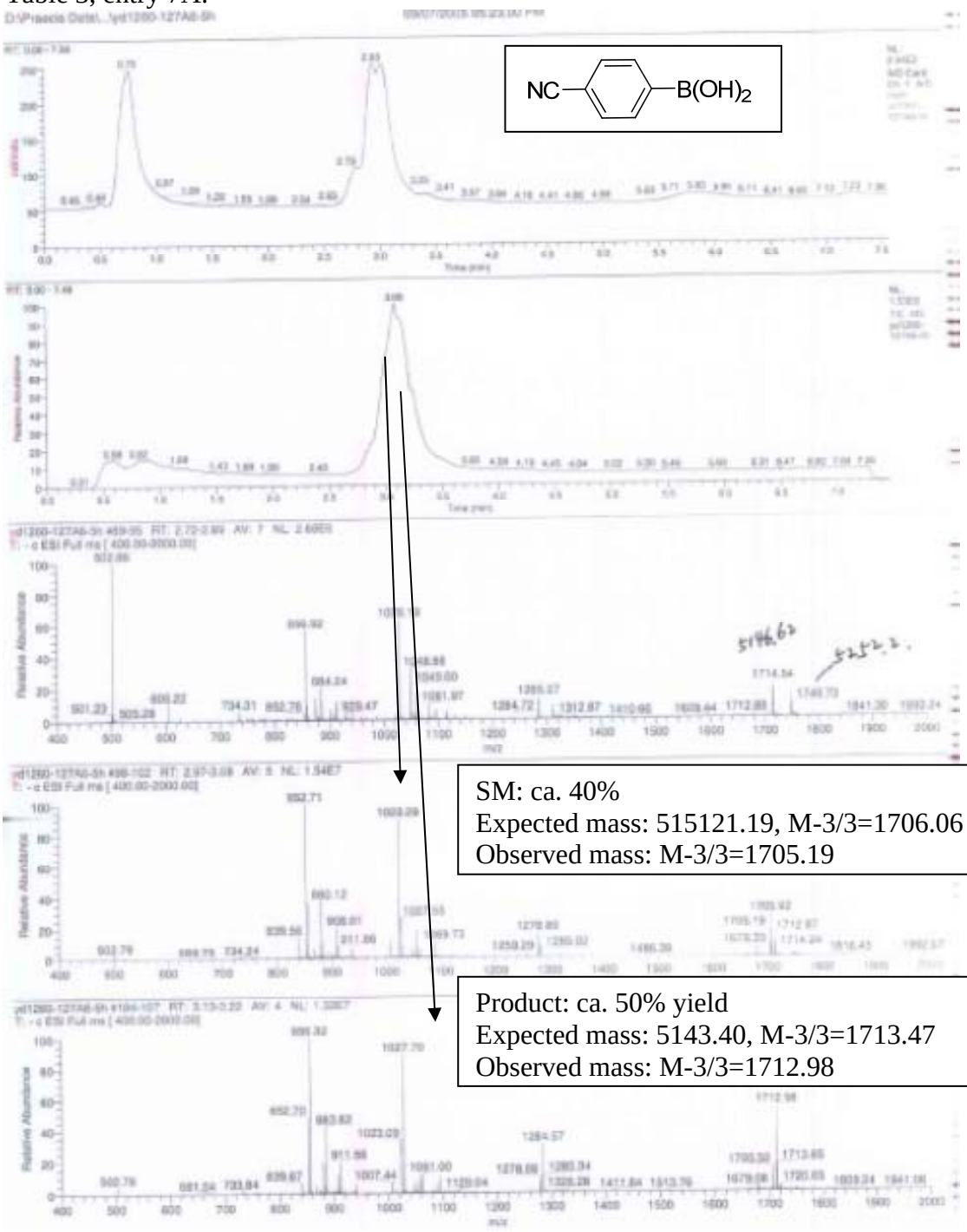


Table 3, entry 8A:

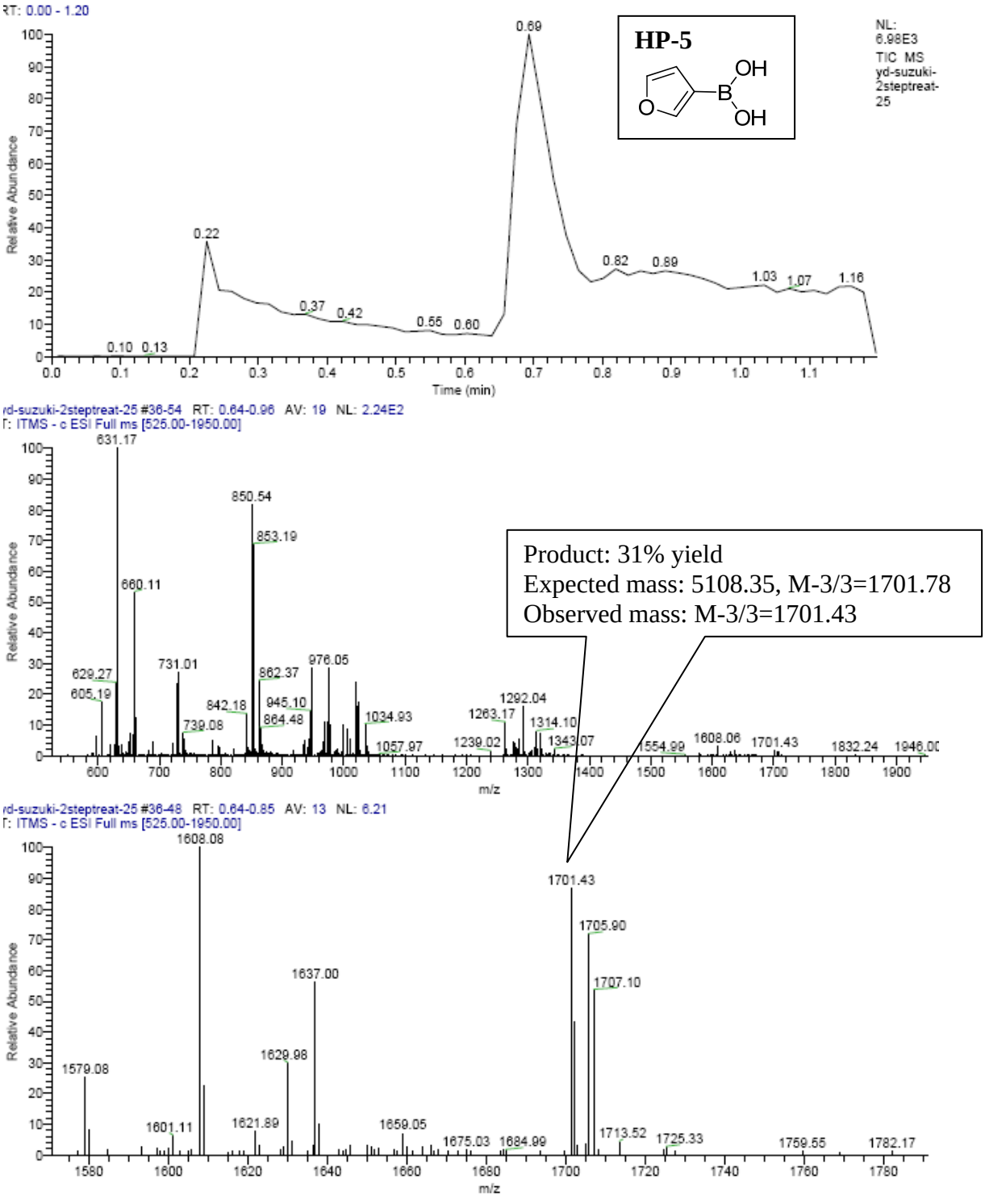
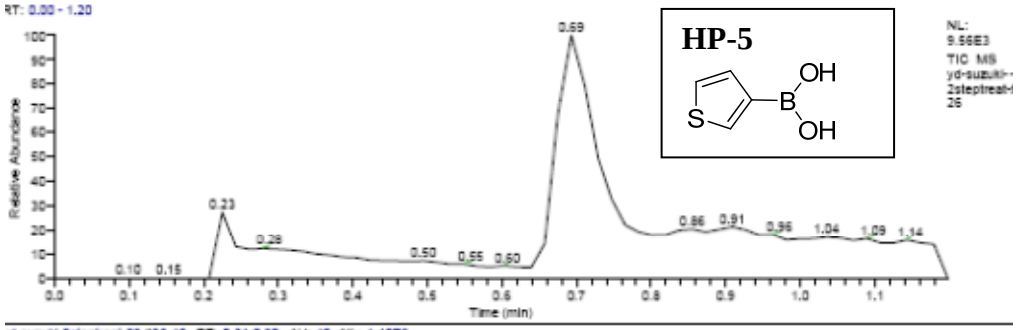
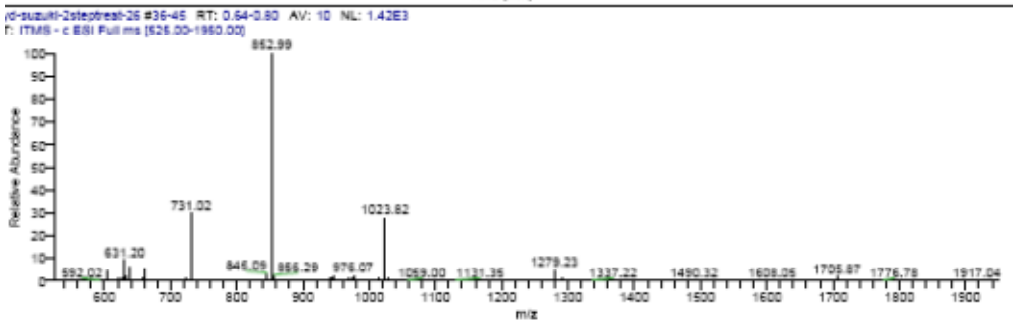
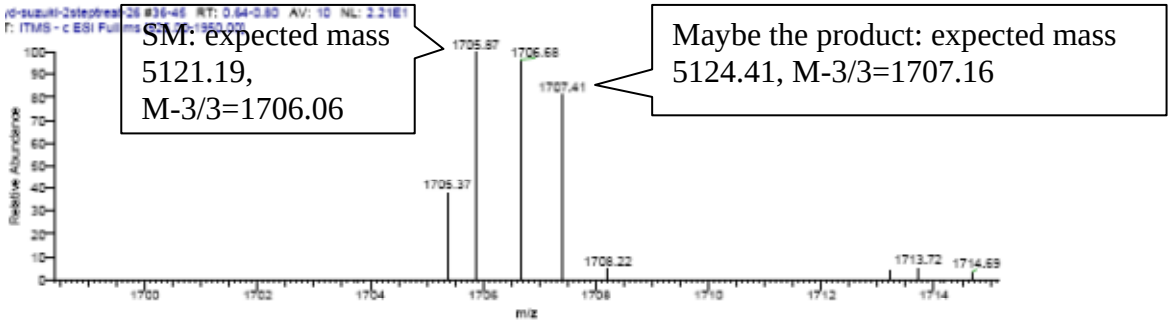


Table 3, entry 9A:



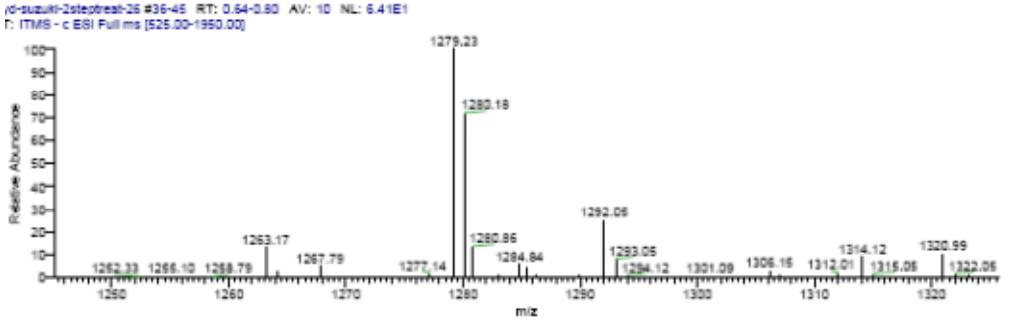
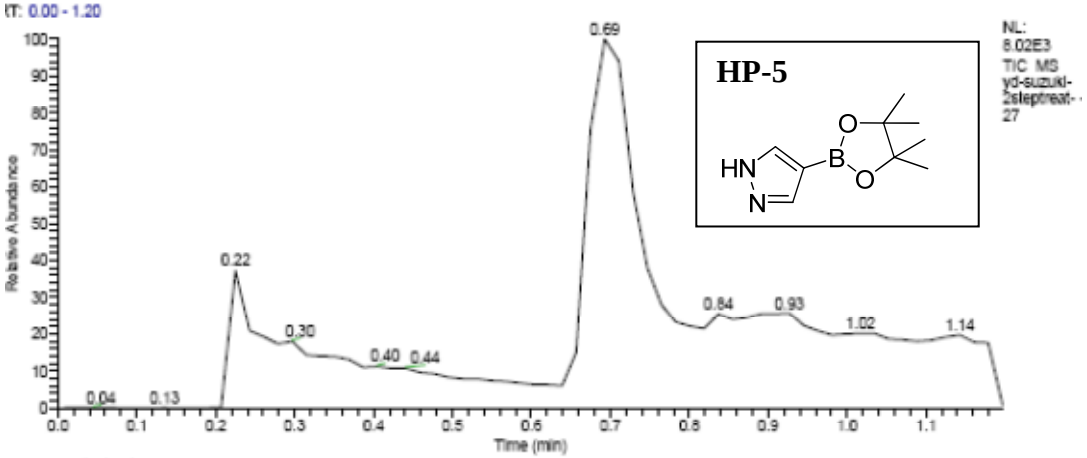
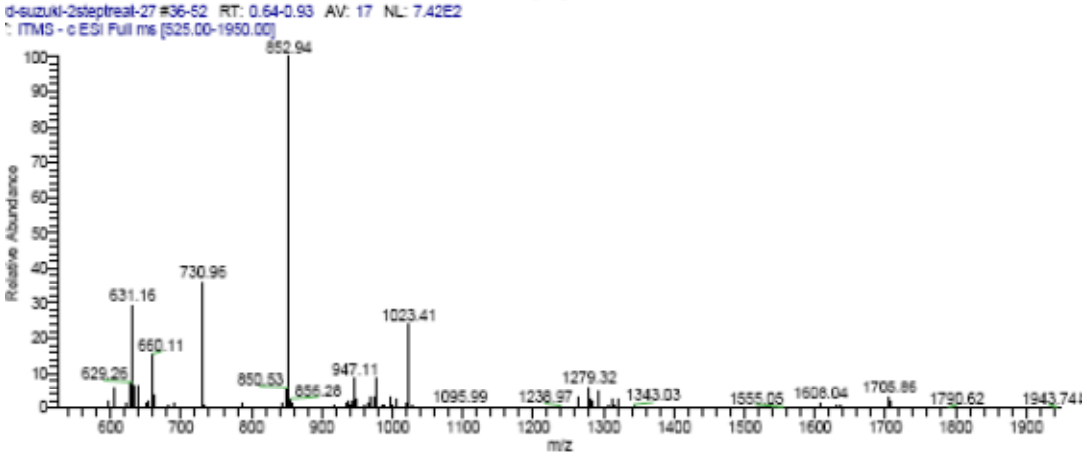



Table 3, entry 10A:



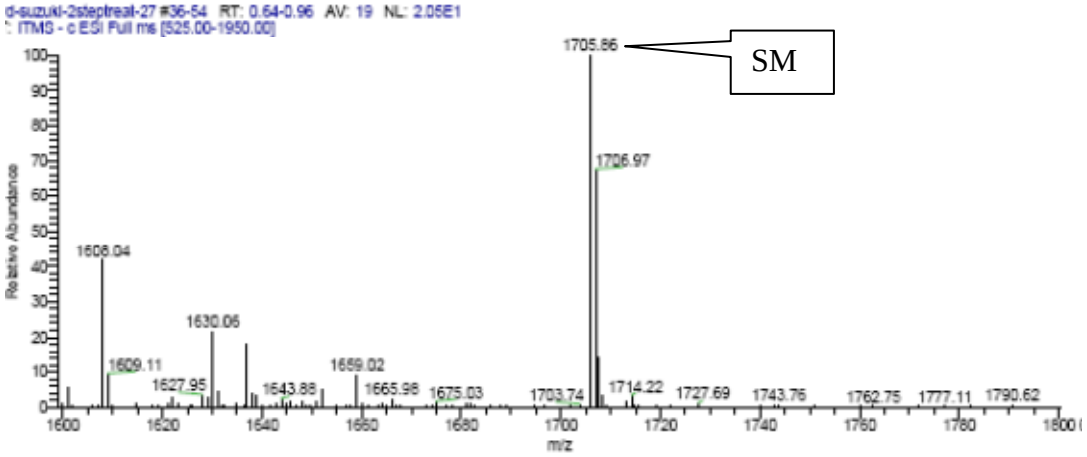



Table 3, entry 11A:

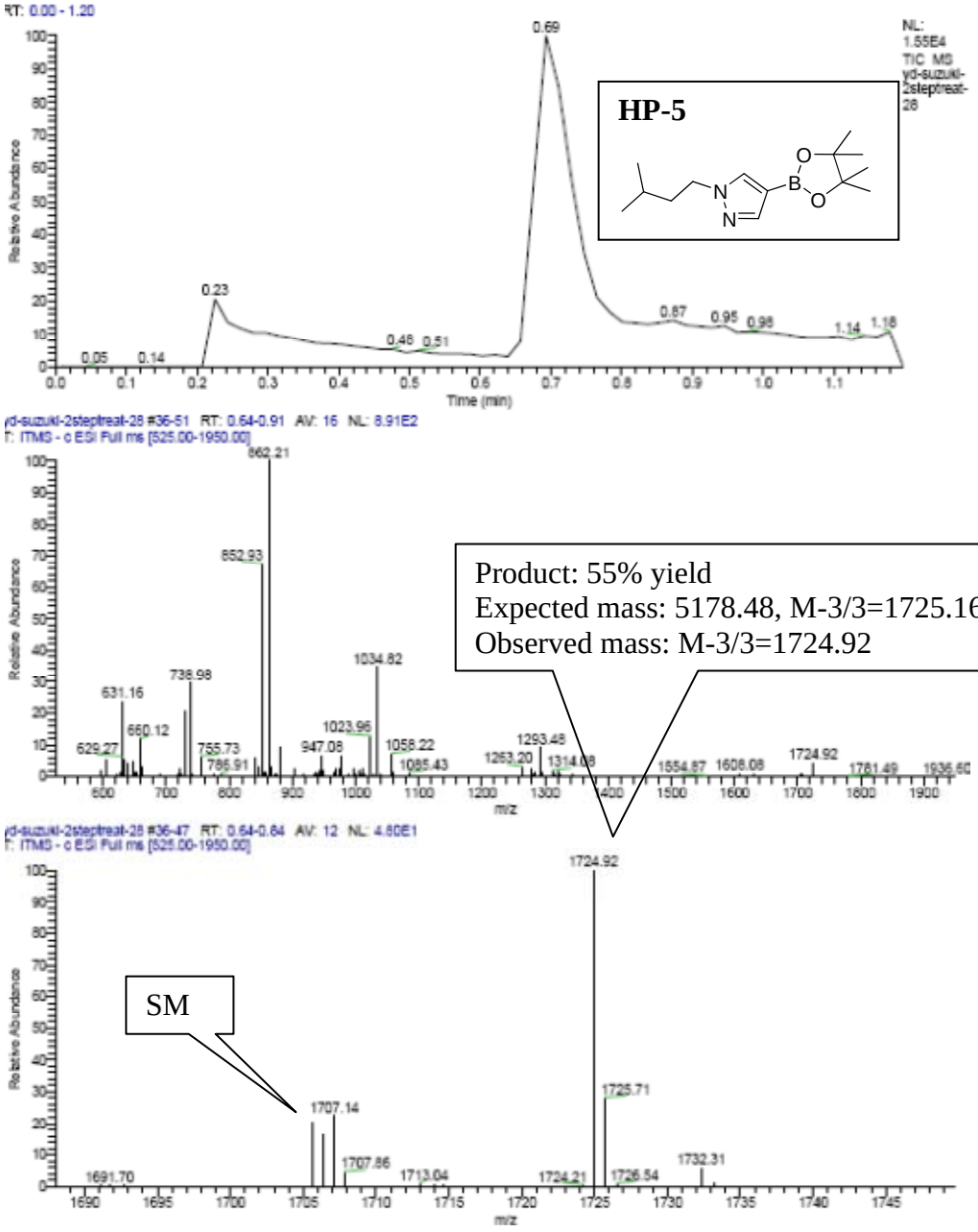


Table 3, entry 1B:

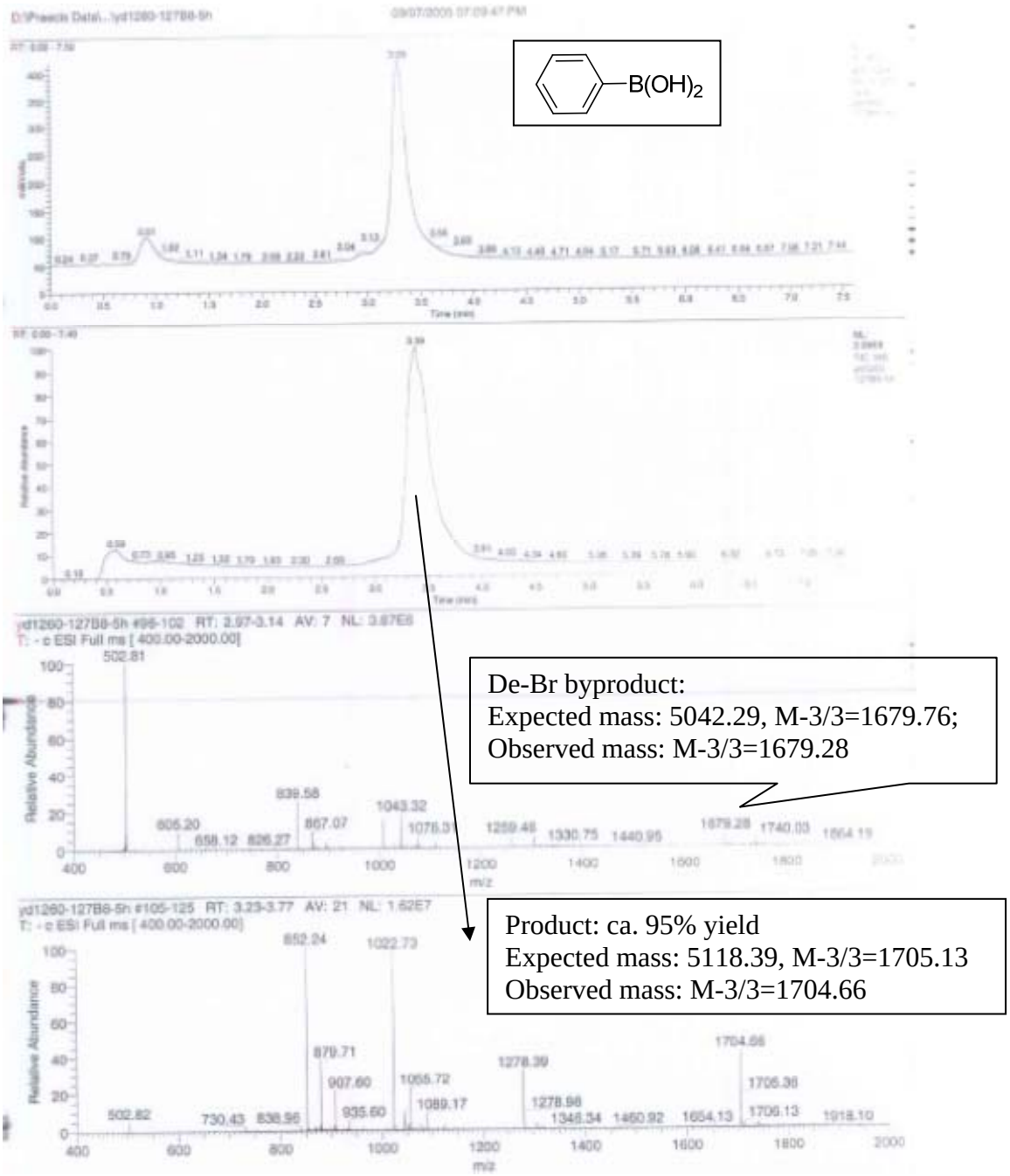


Table 3, entry 2B:

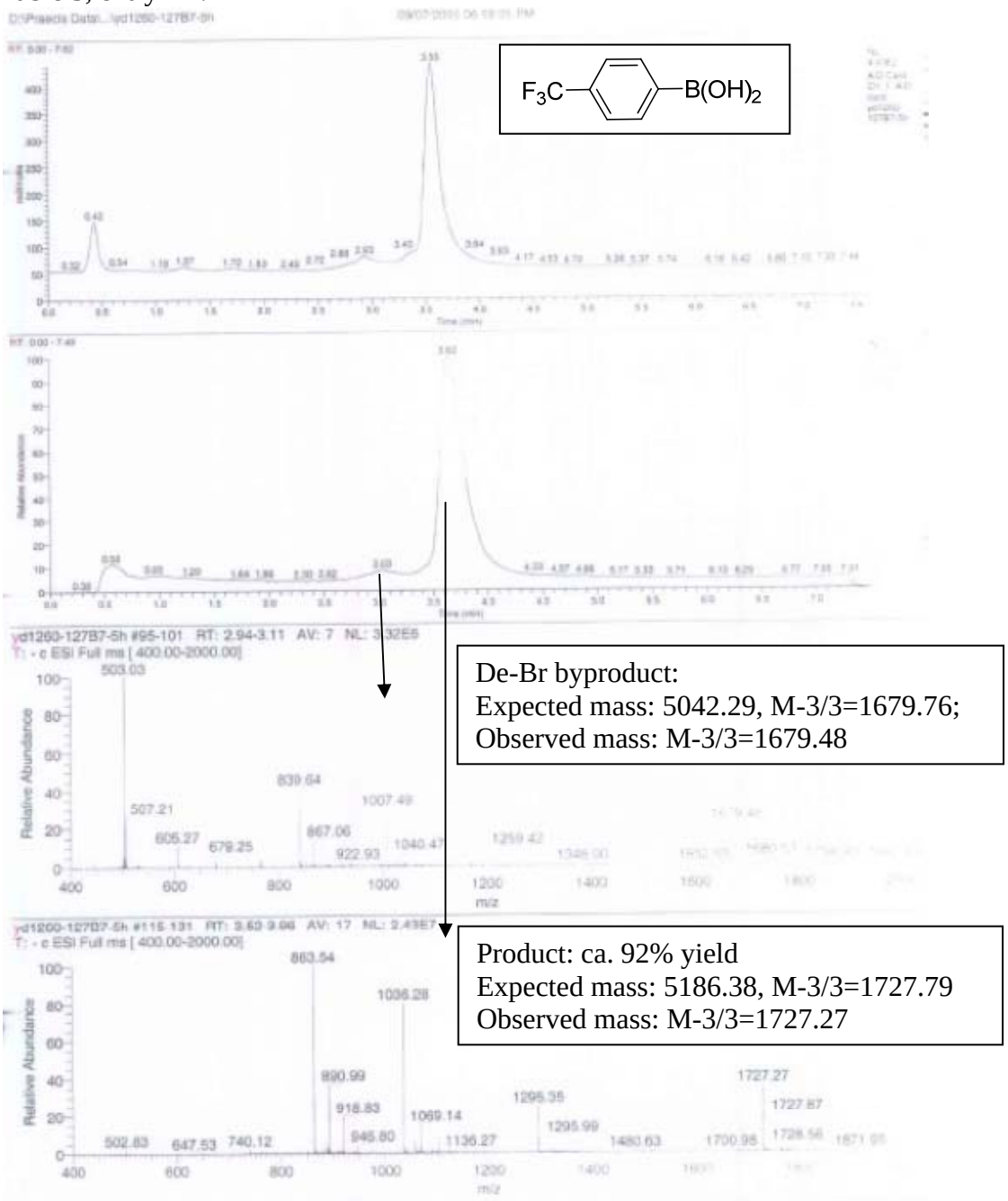


Table 3, entry 3B:

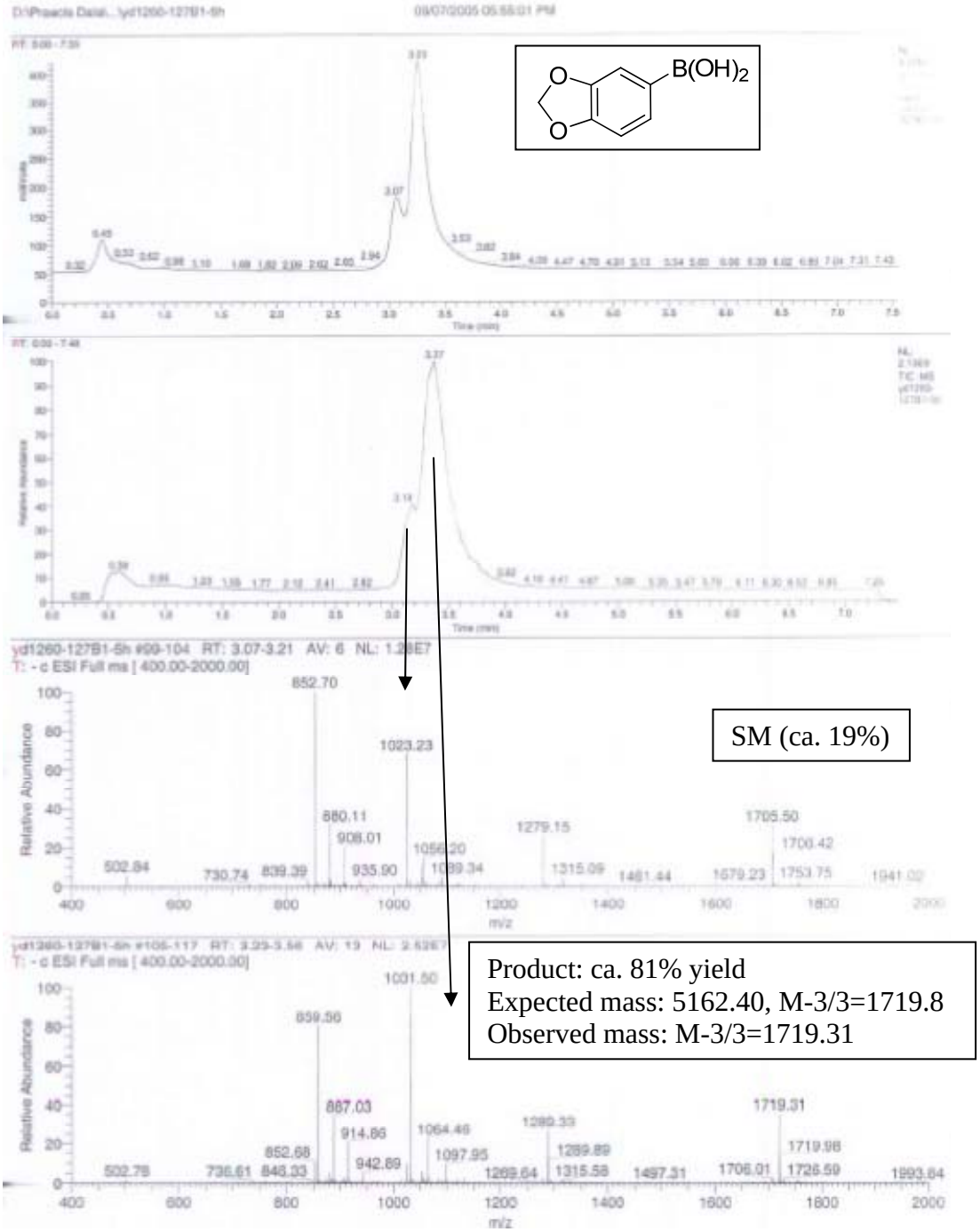
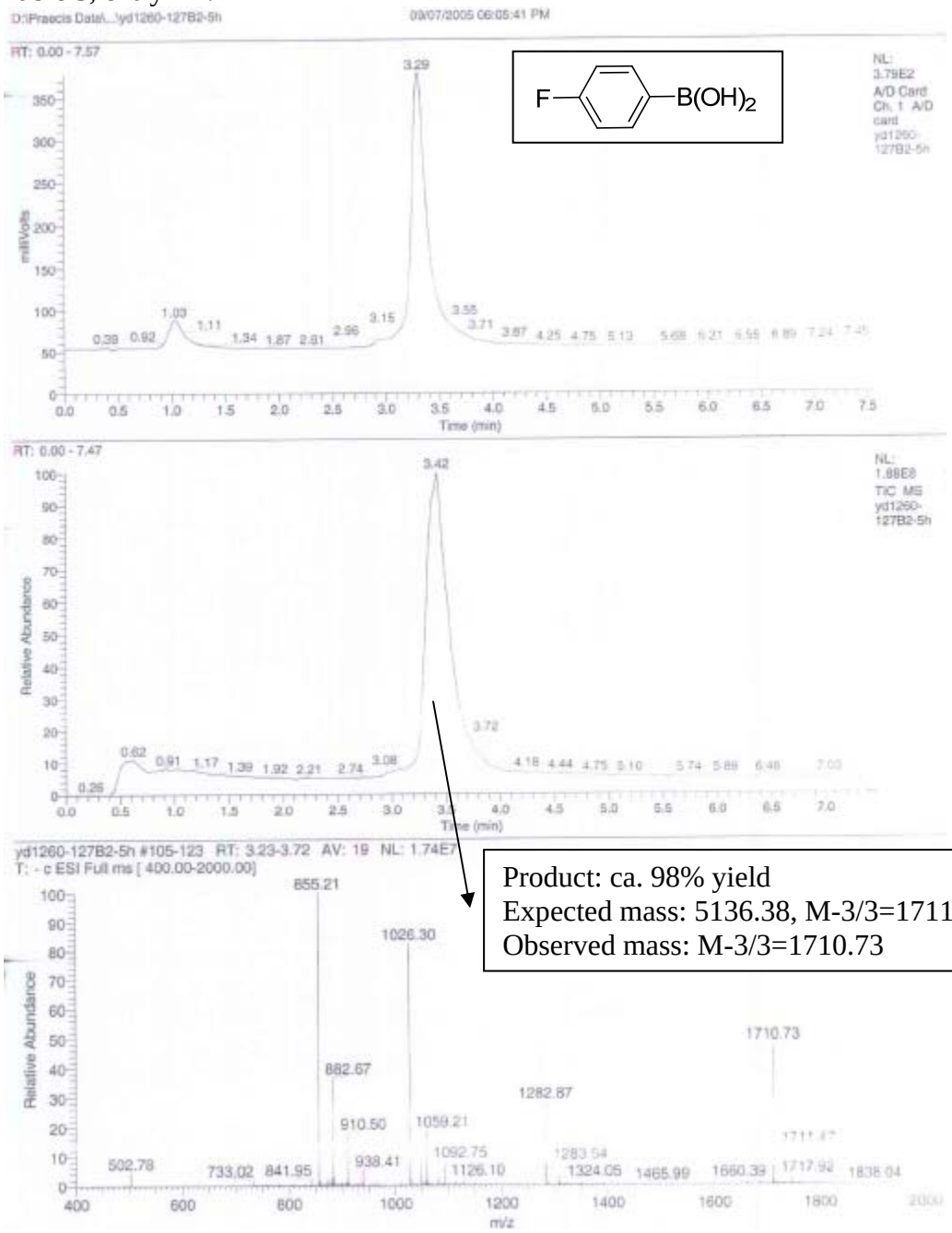


Table 3, entry 4B:




Product: ca. 98% yield
Expected mass: 5136.38, M-3/3=1711.13
Observed mass: M-3/3=1710.73

Table 3, entry 5B:

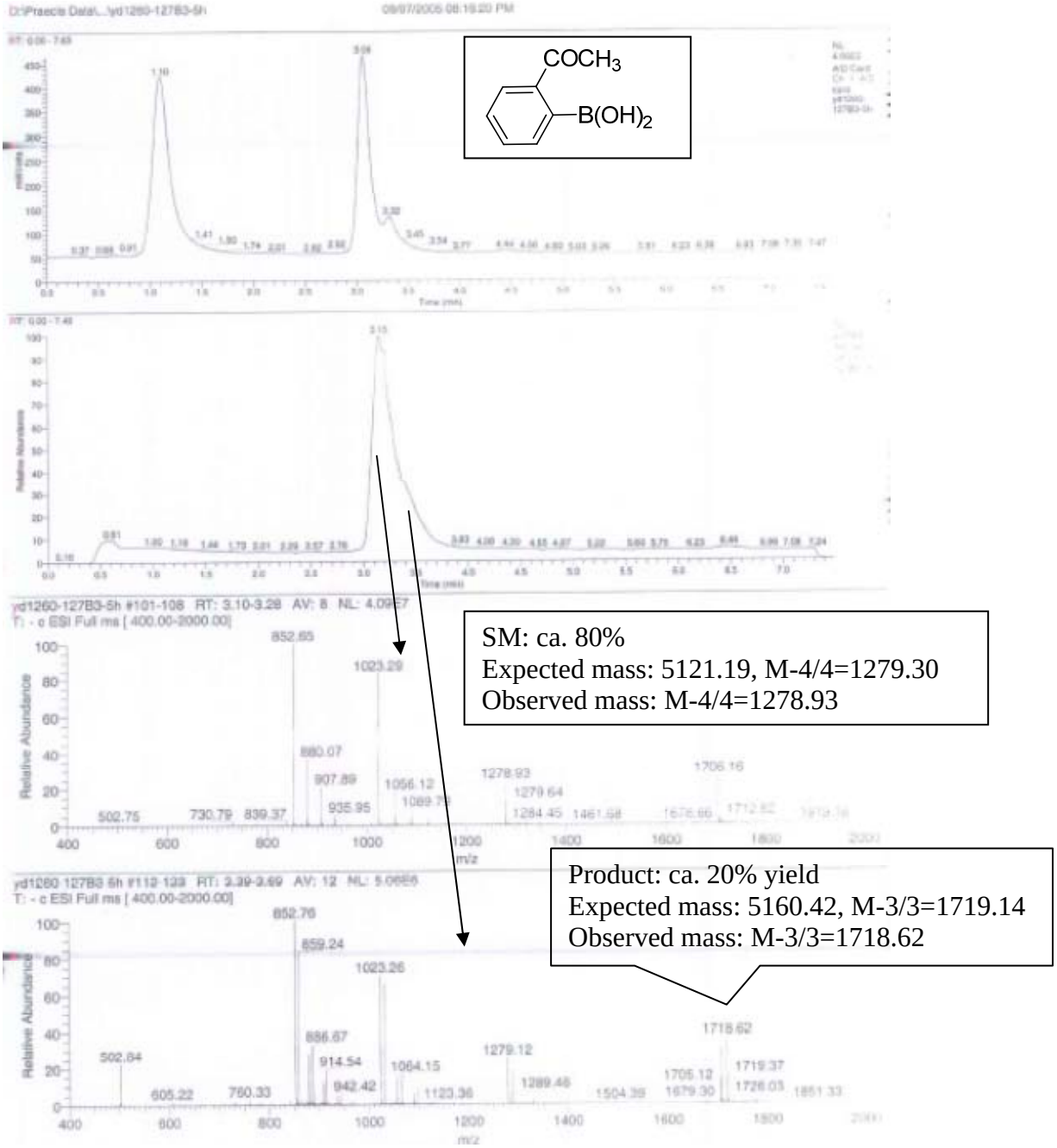


Table 3, entry 6B:

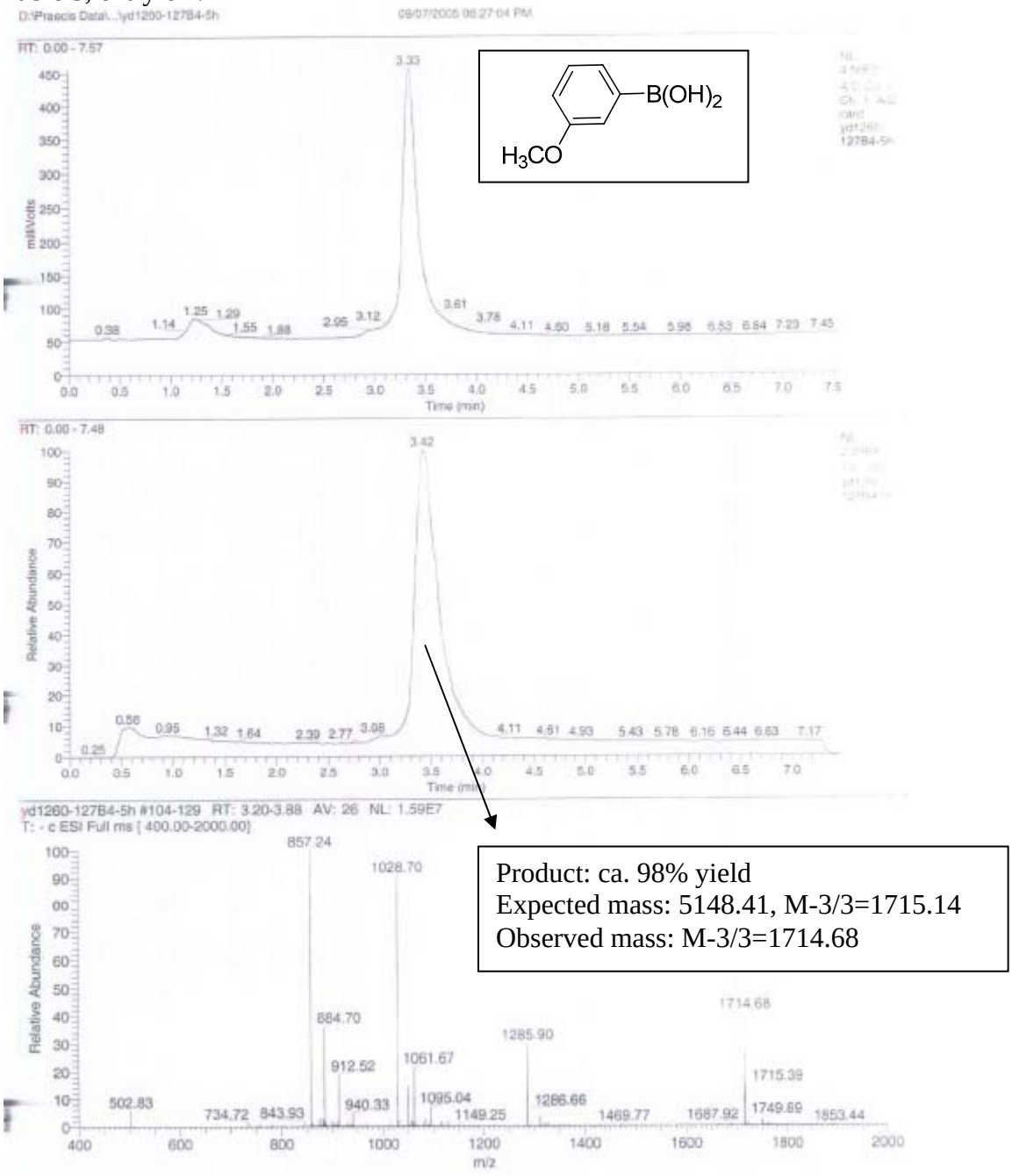


Table 3, entry 7B:

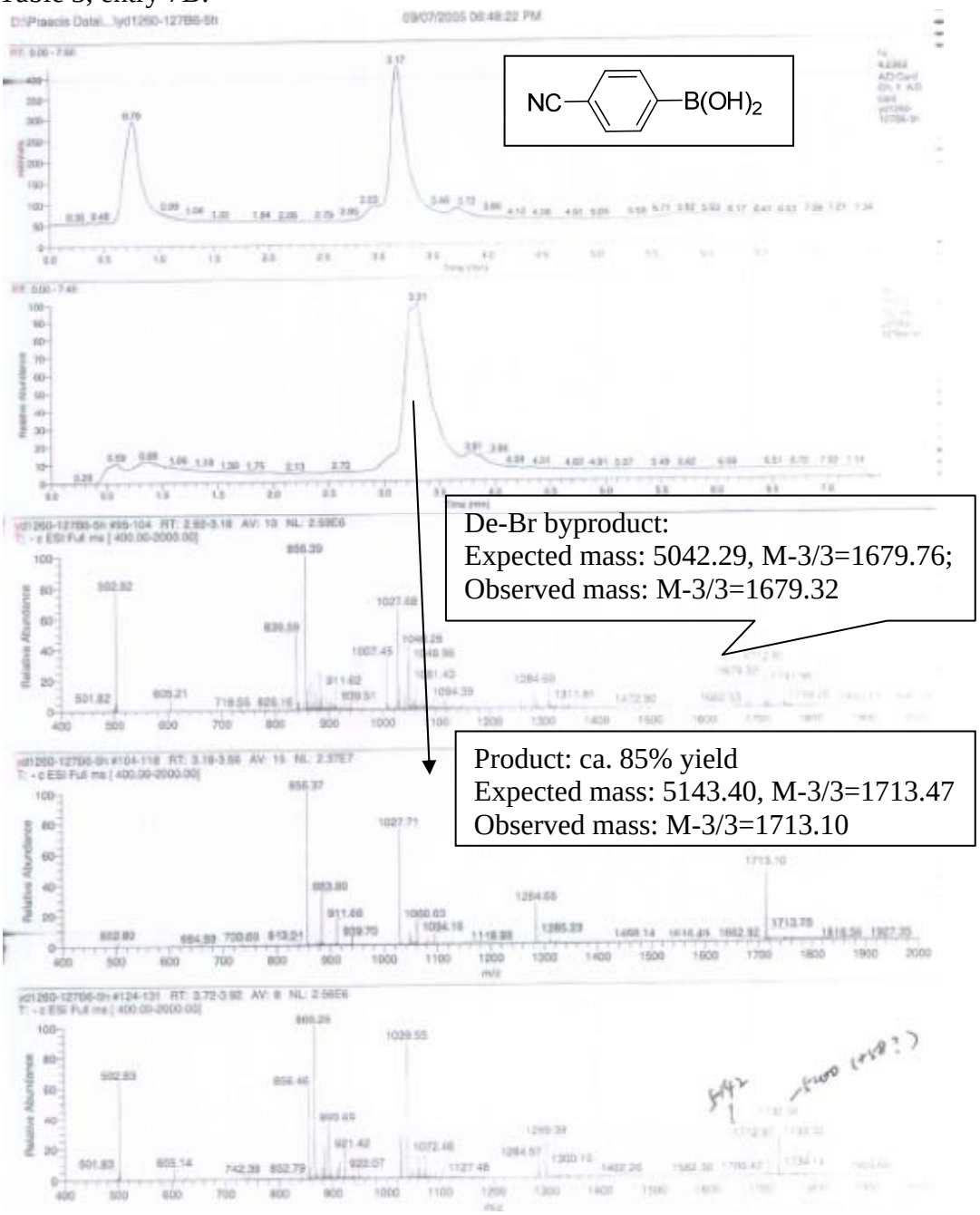


Table 3, entry 8B:

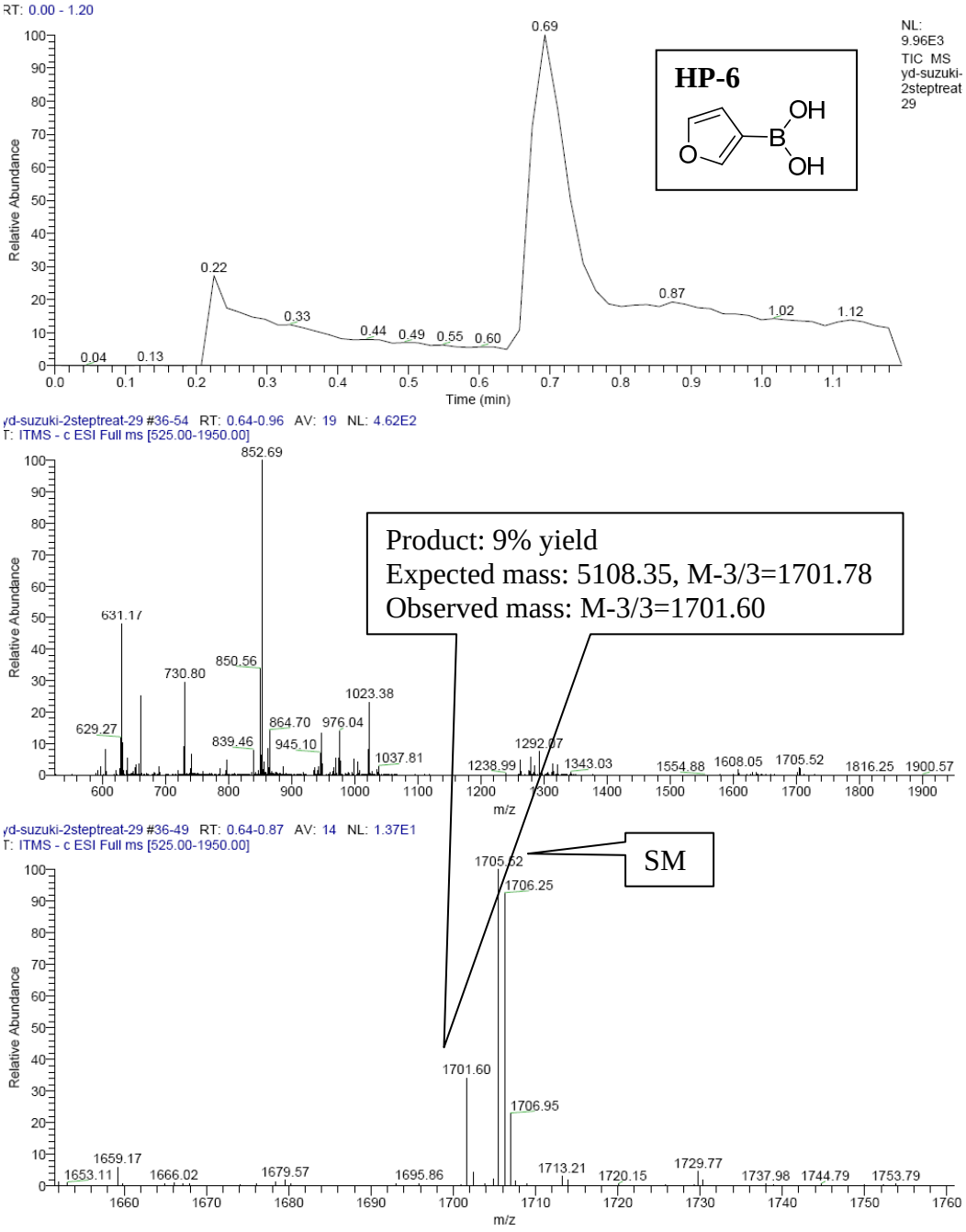
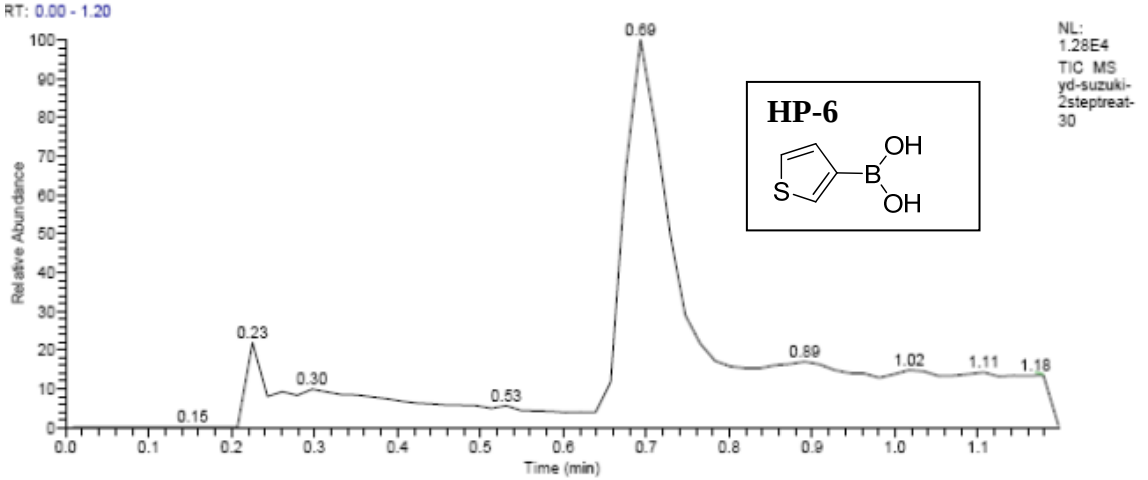
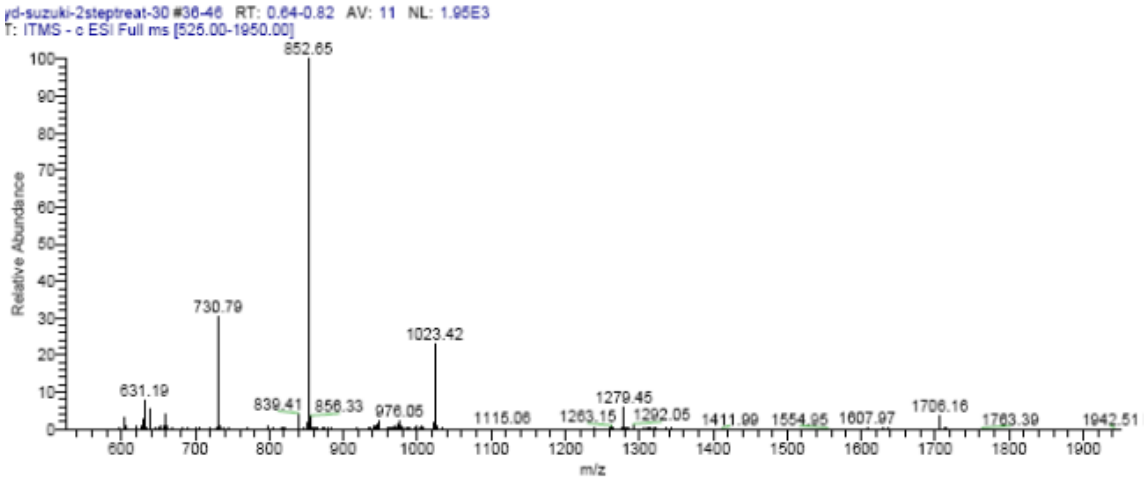


Table 3, entry 9B:



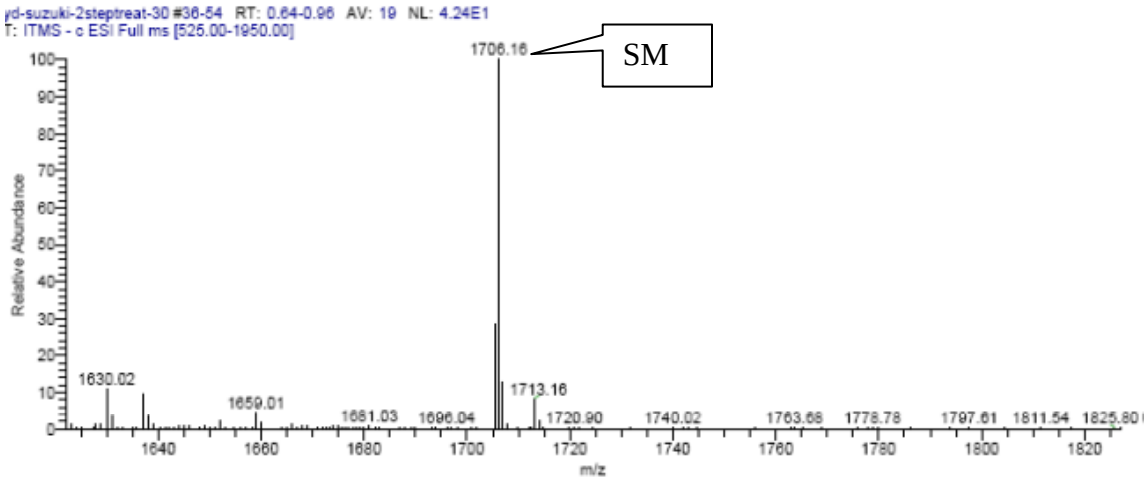



Table 3, entry 10B:

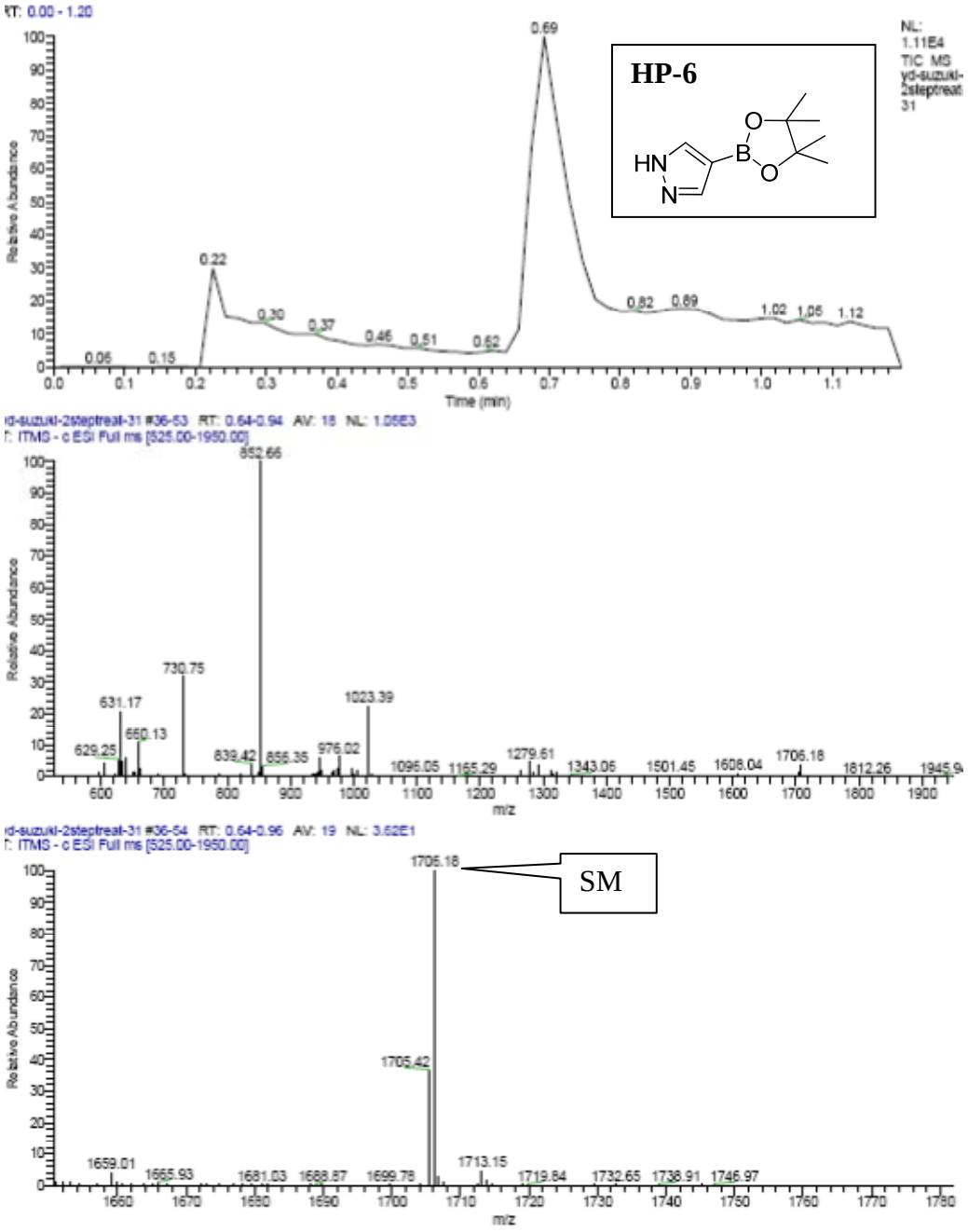


Table 3, entry 11B:

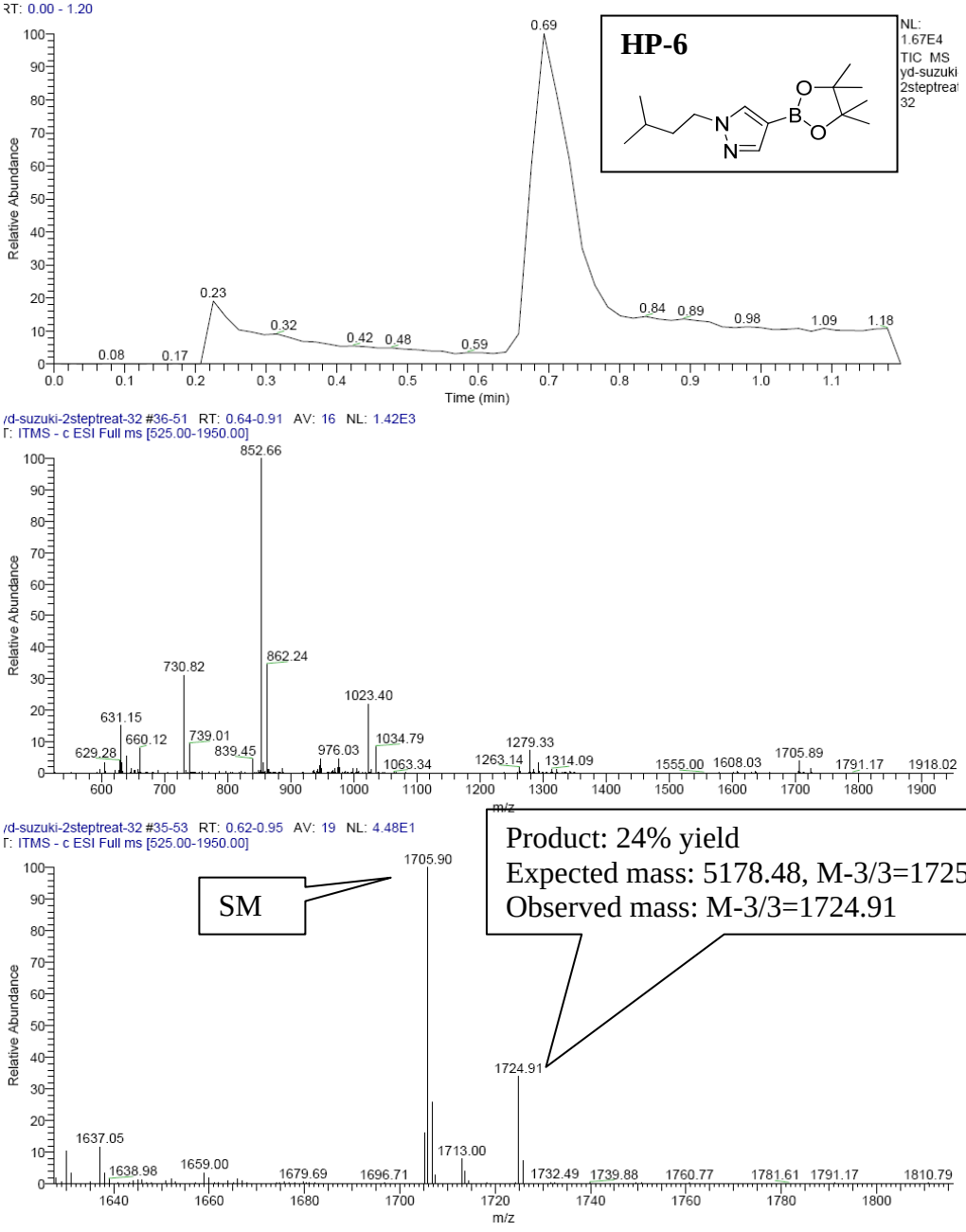


Table 3, entry 1C:

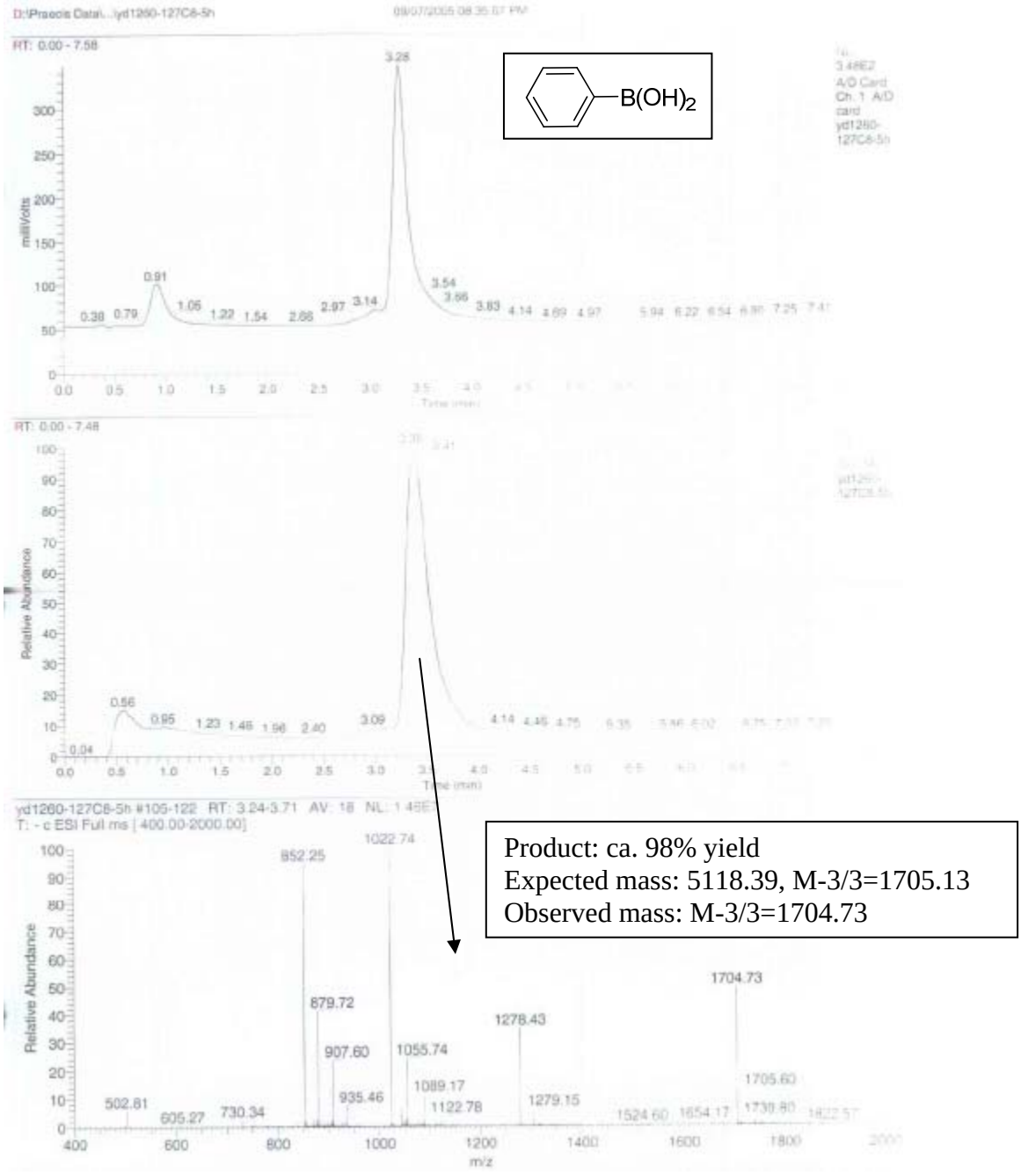


Table 3, entry 2C:

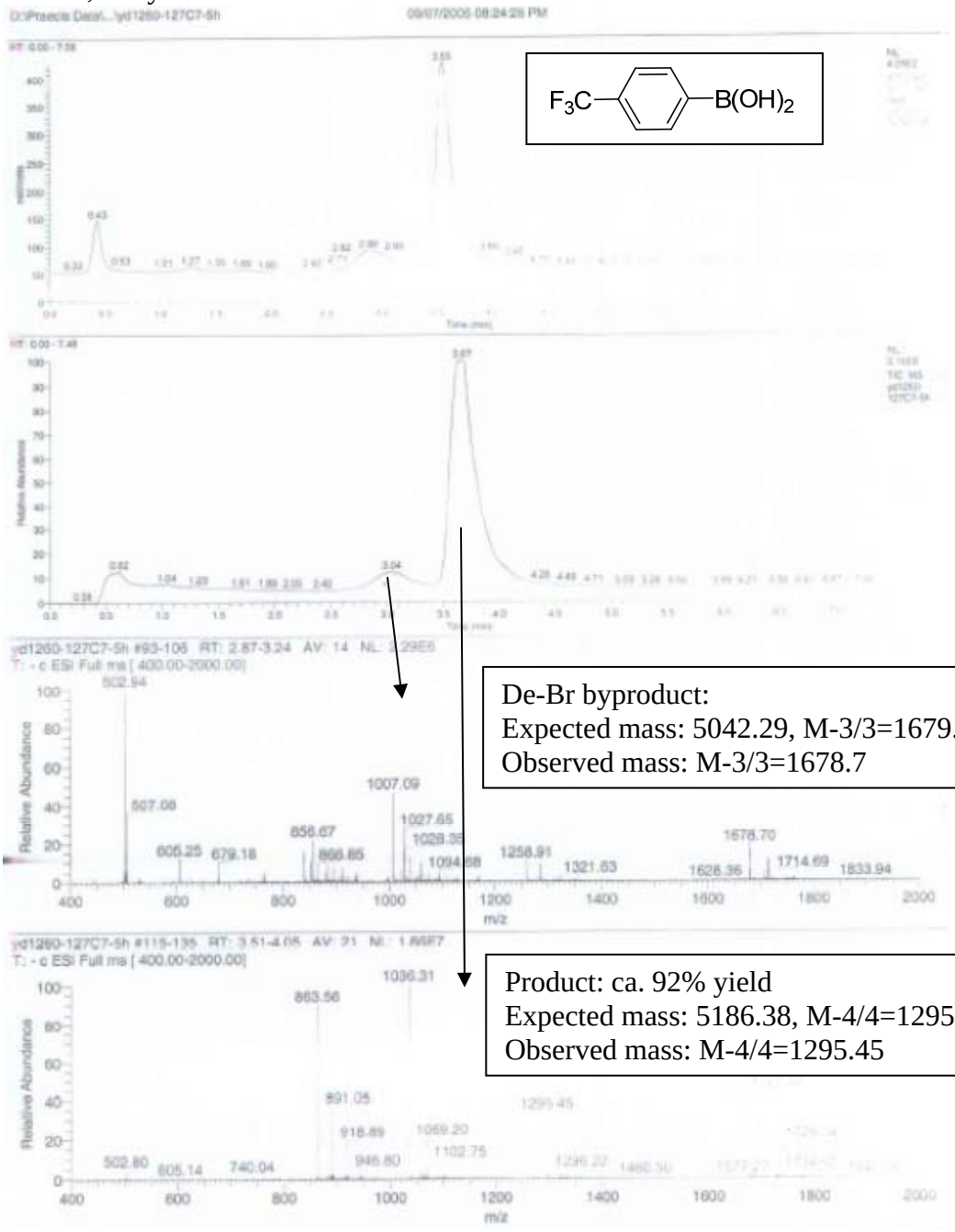
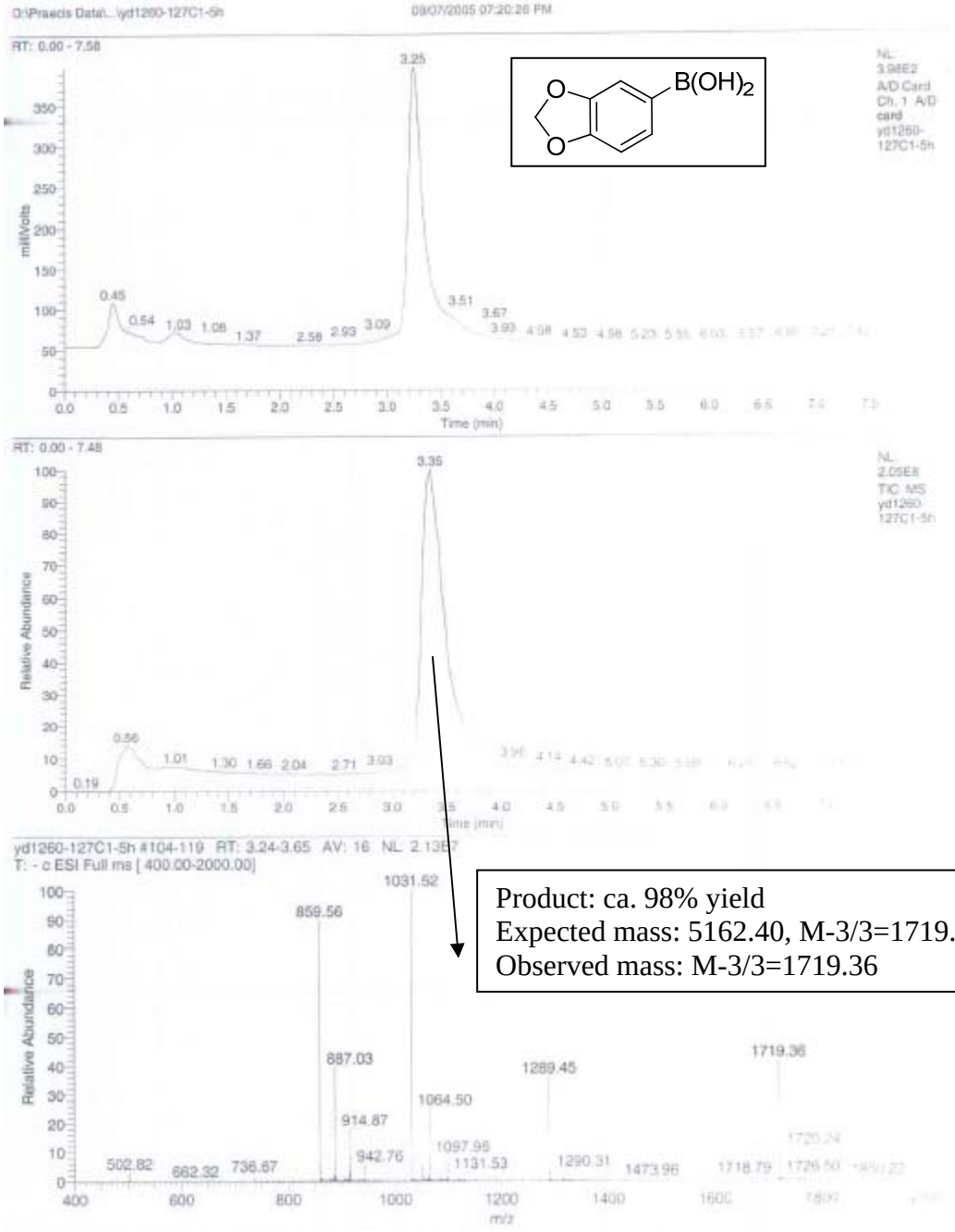


Table 3, entry 3C:




Product: ca. 98% yield
Expected mass: 5162.40, M-3/3=1719.8
Observed mass: M-3/3=1719.36

Table 3, entry 4C:

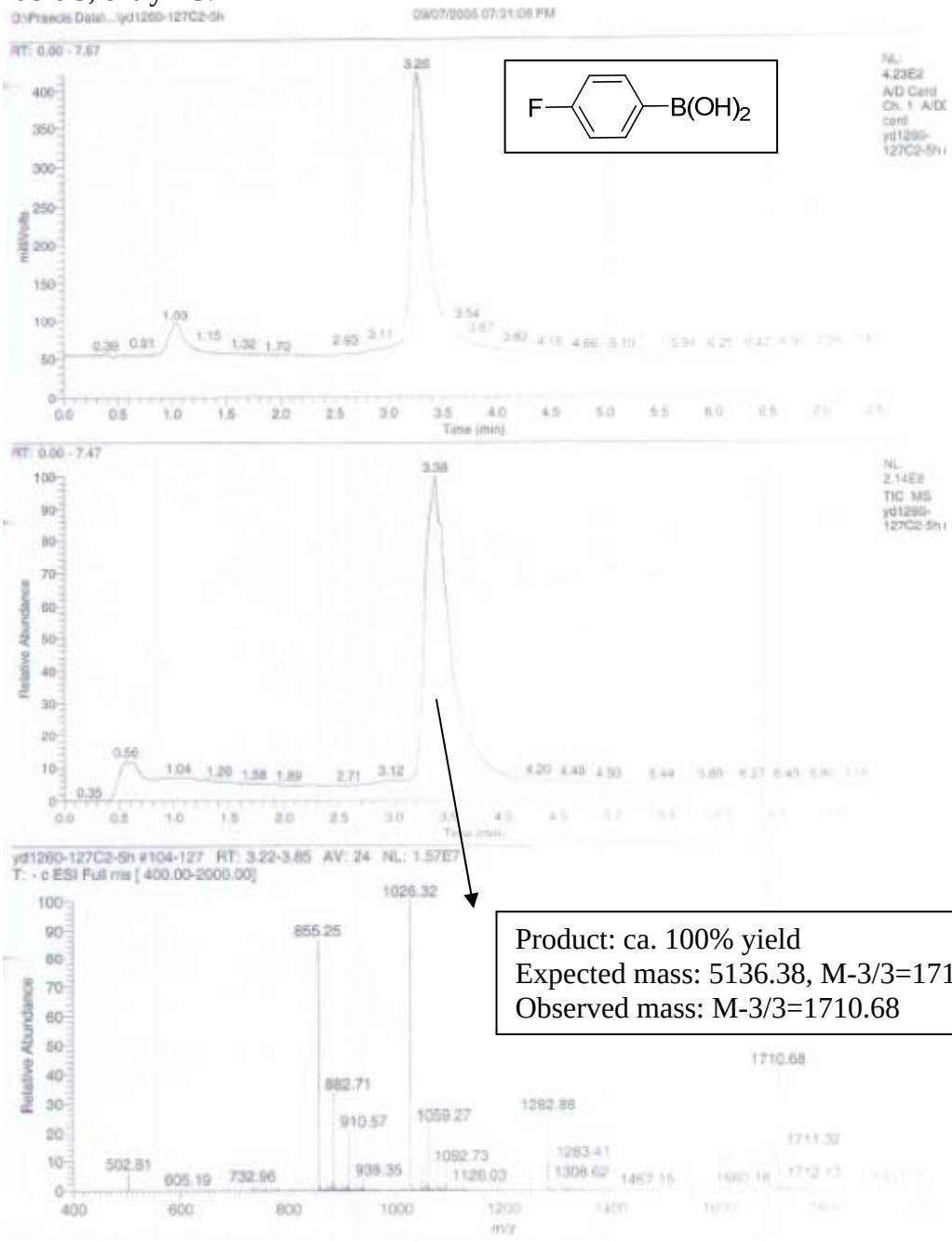


Table 3, entry 5C:

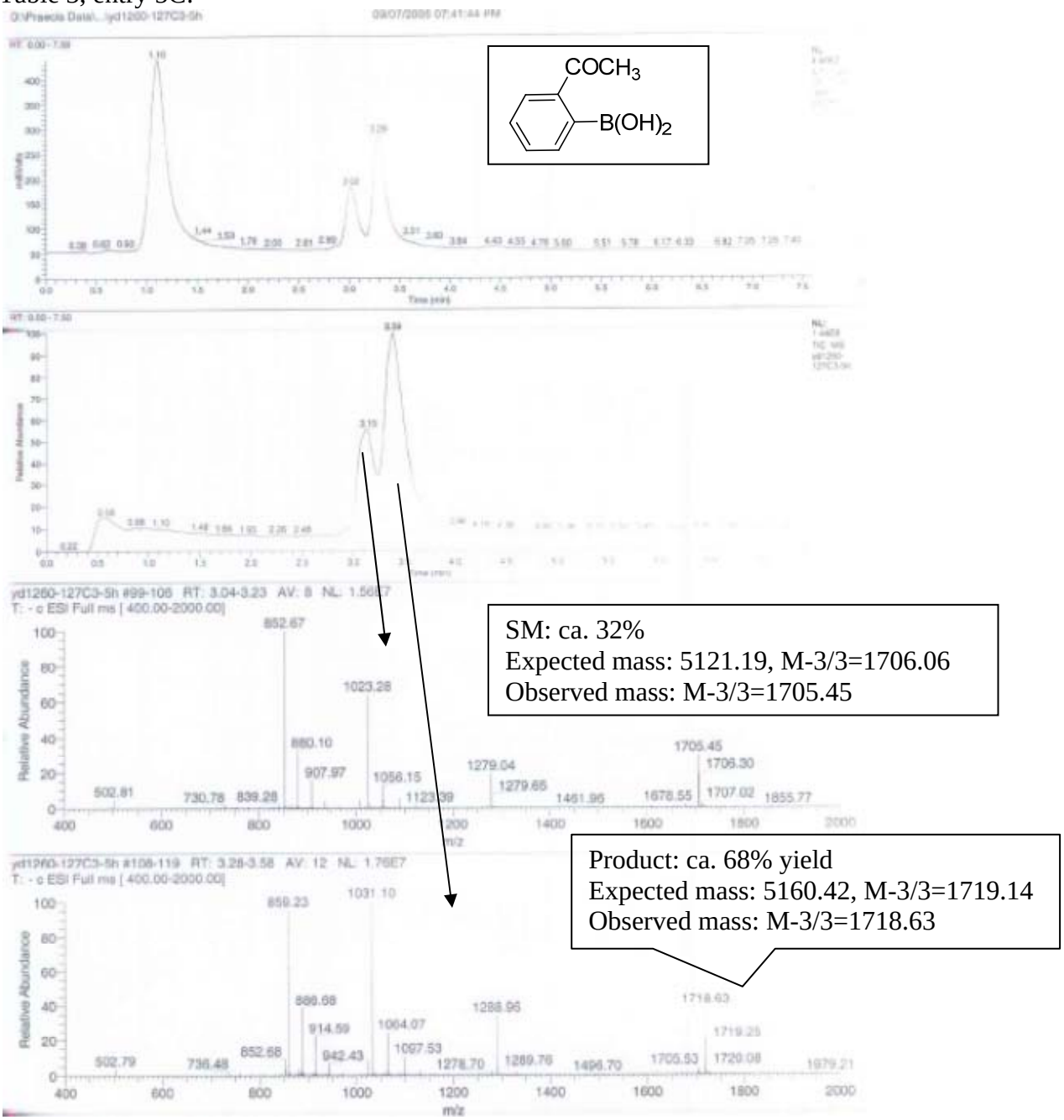


Table 3, entry 6C:

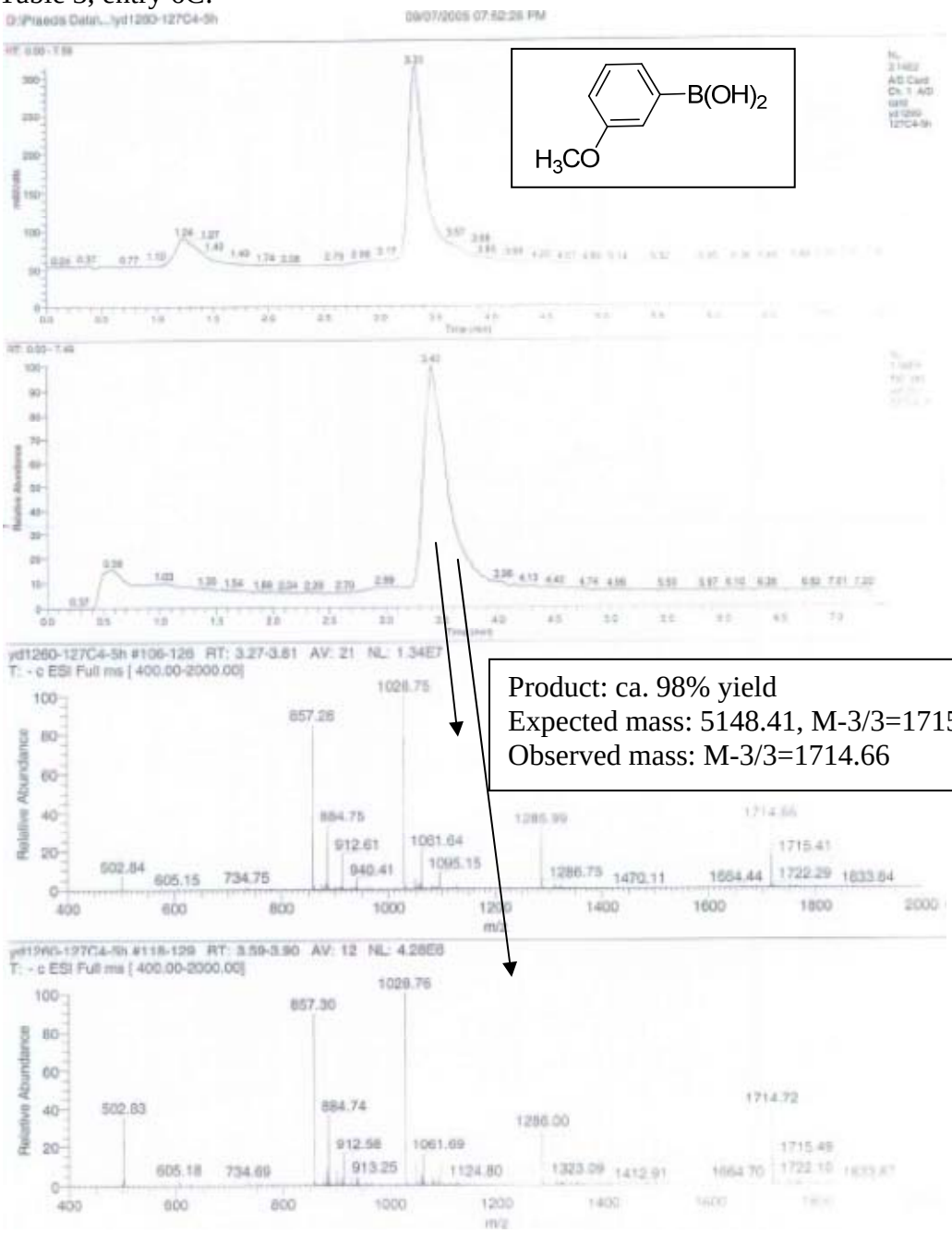


Table 3, entry 7C:

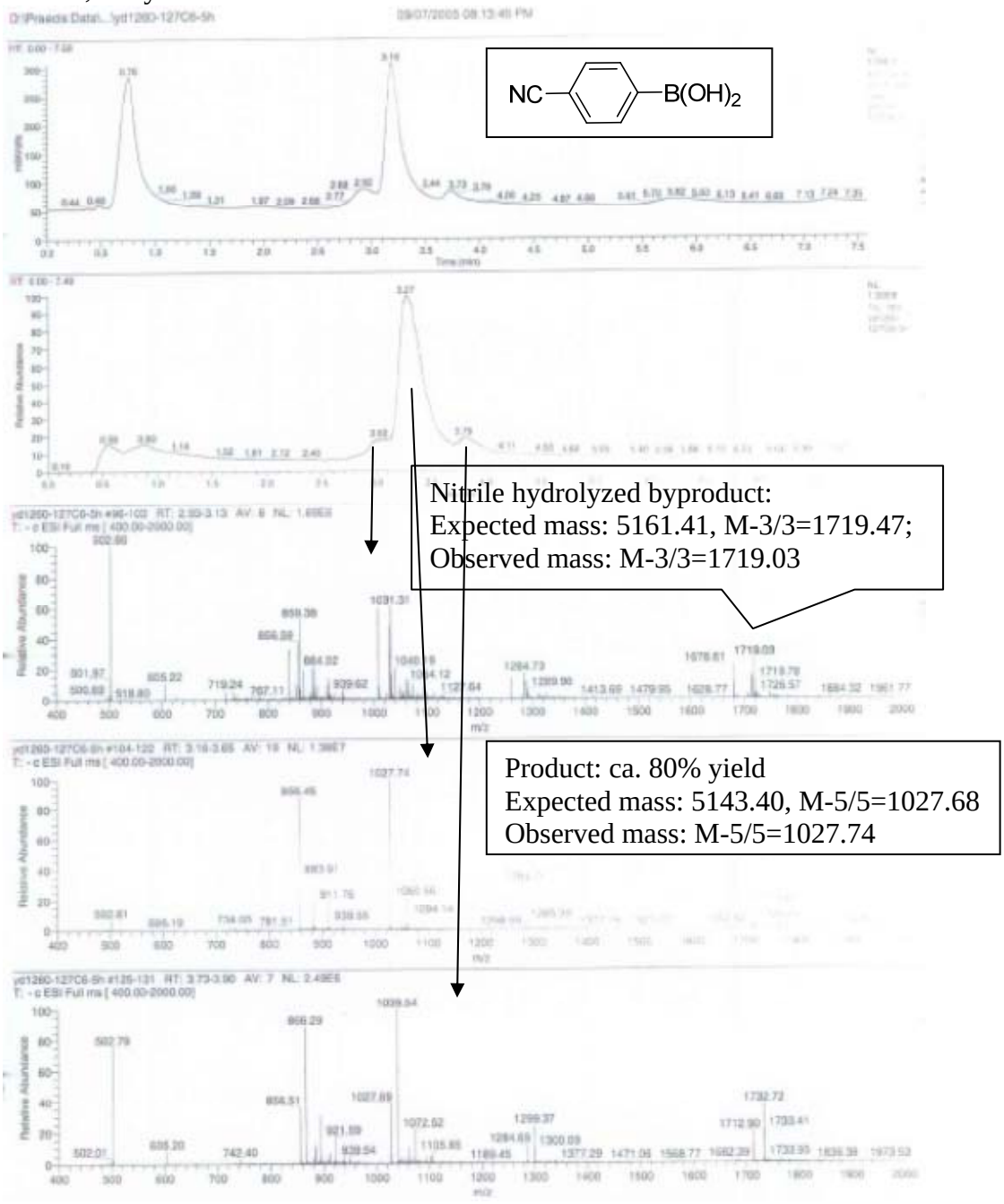


Table 3, entry 8C:

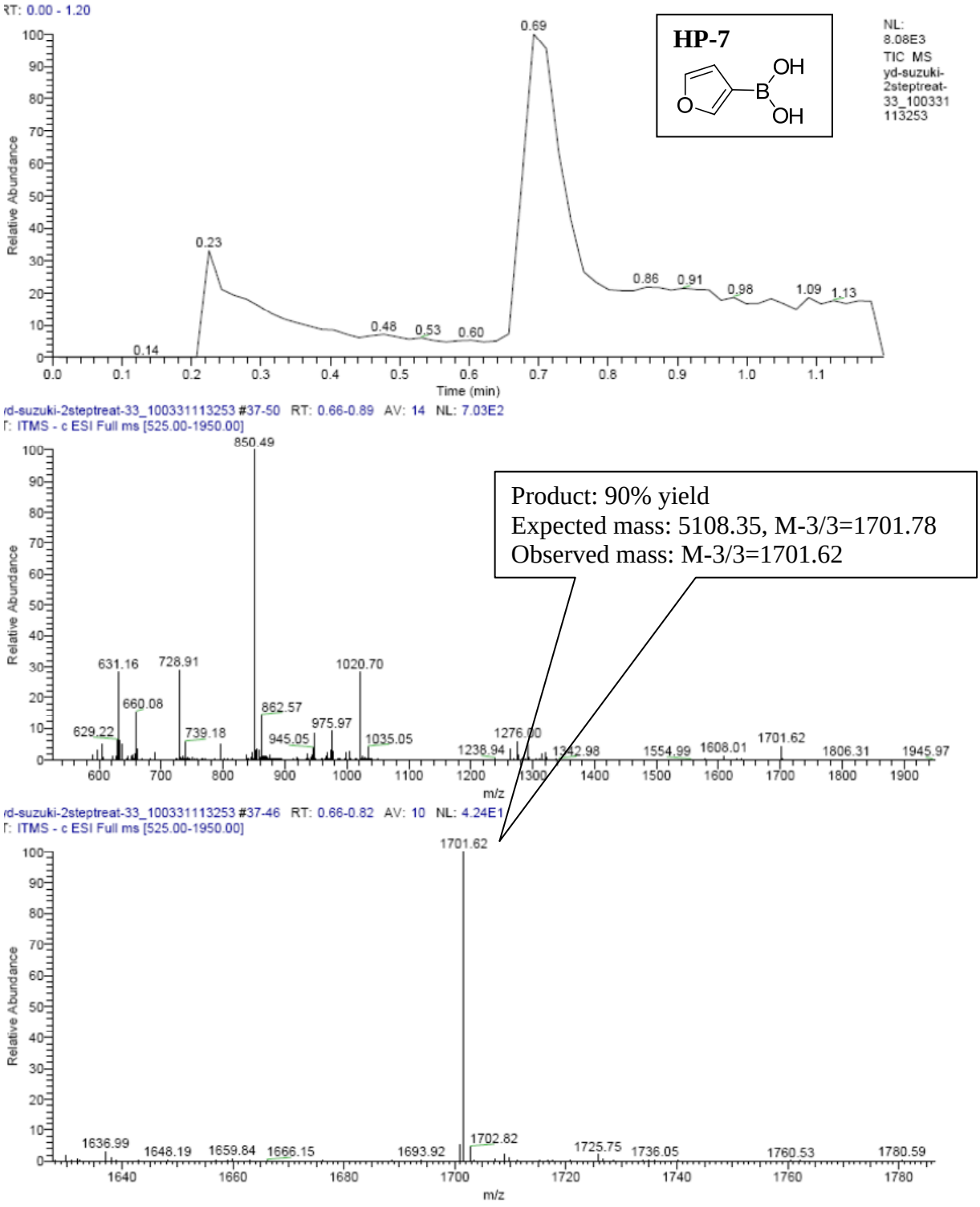


Table 3, entry 9C:

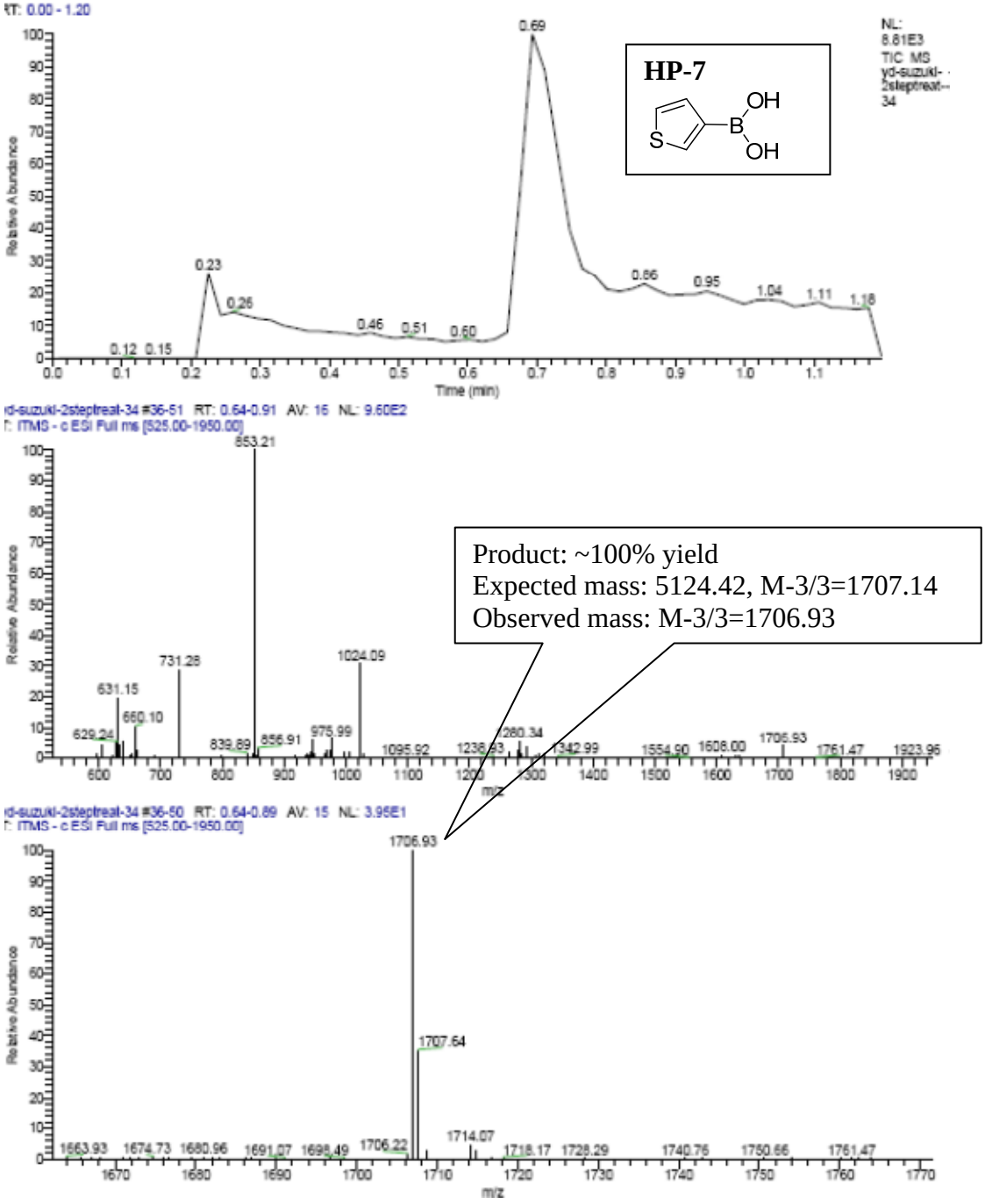


Table 3, entry 10C:

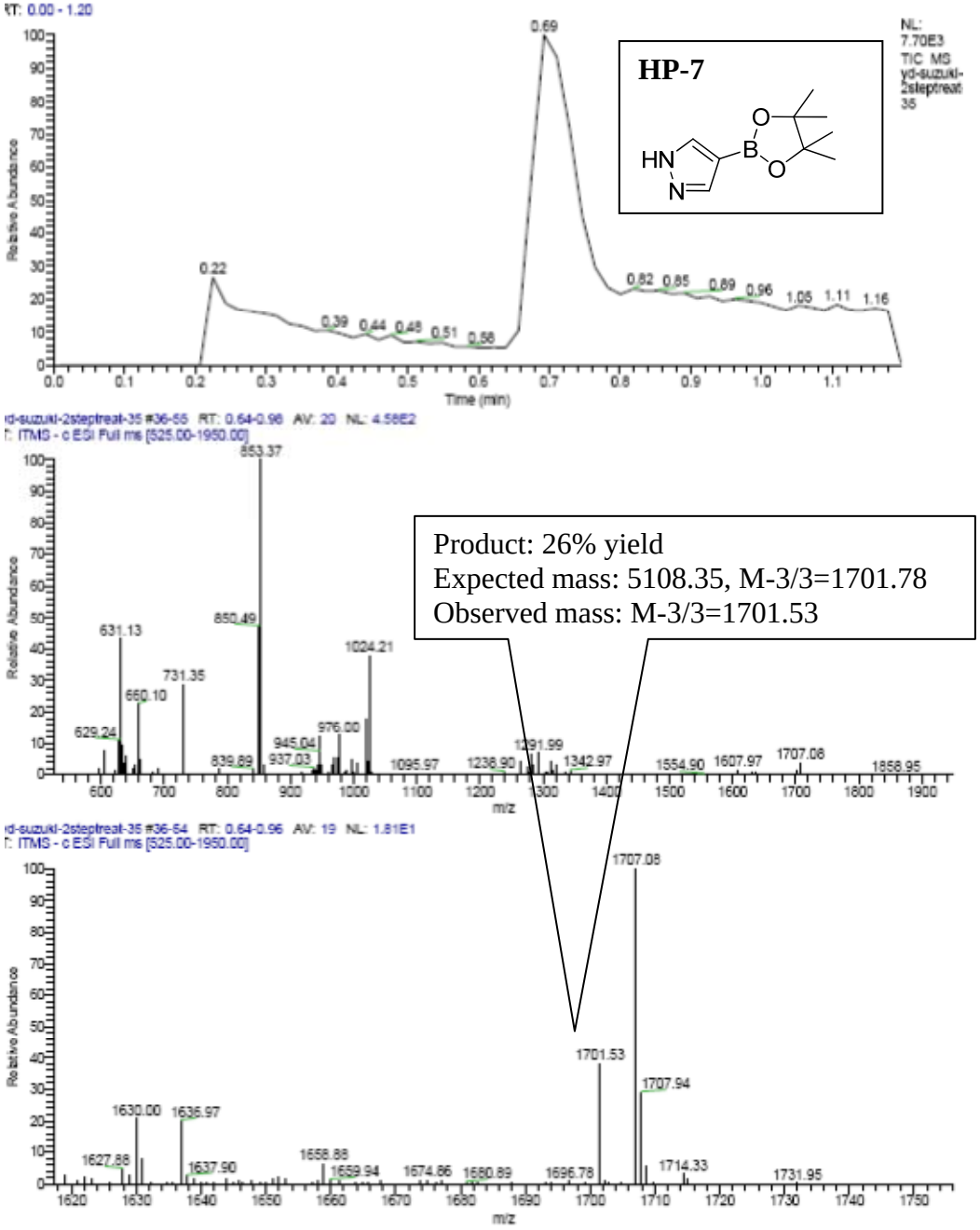
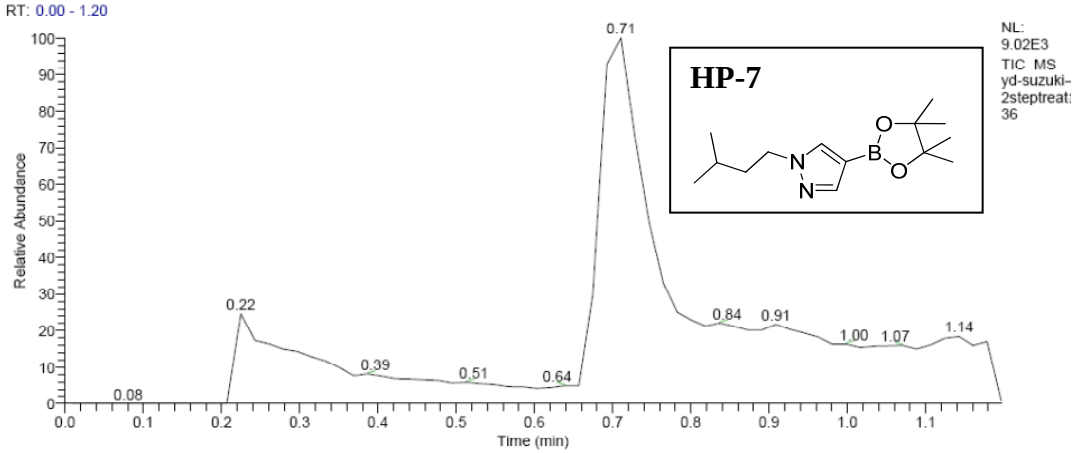
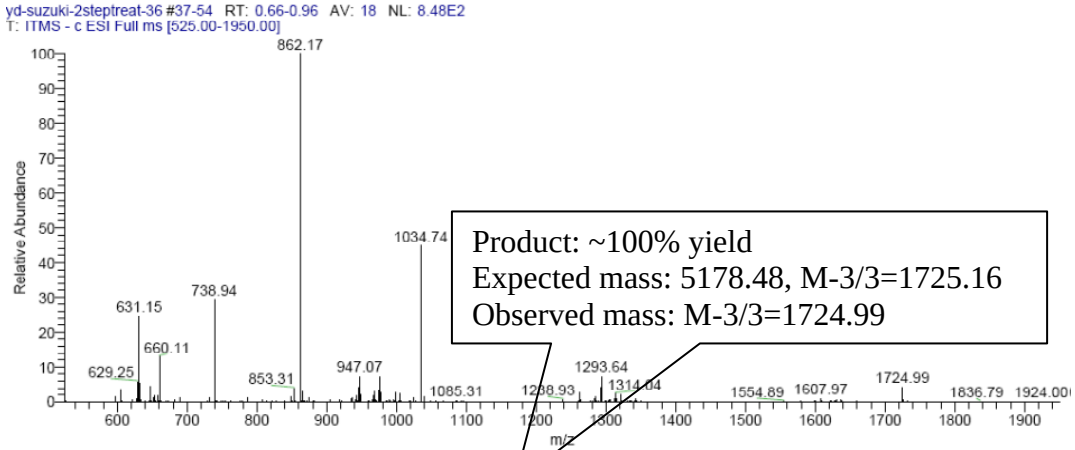
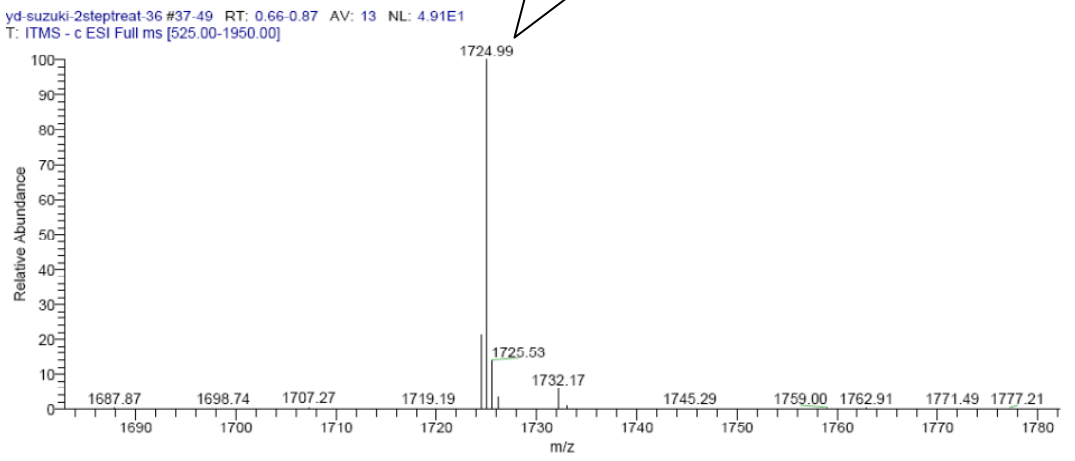


Table 3, entry 11C:



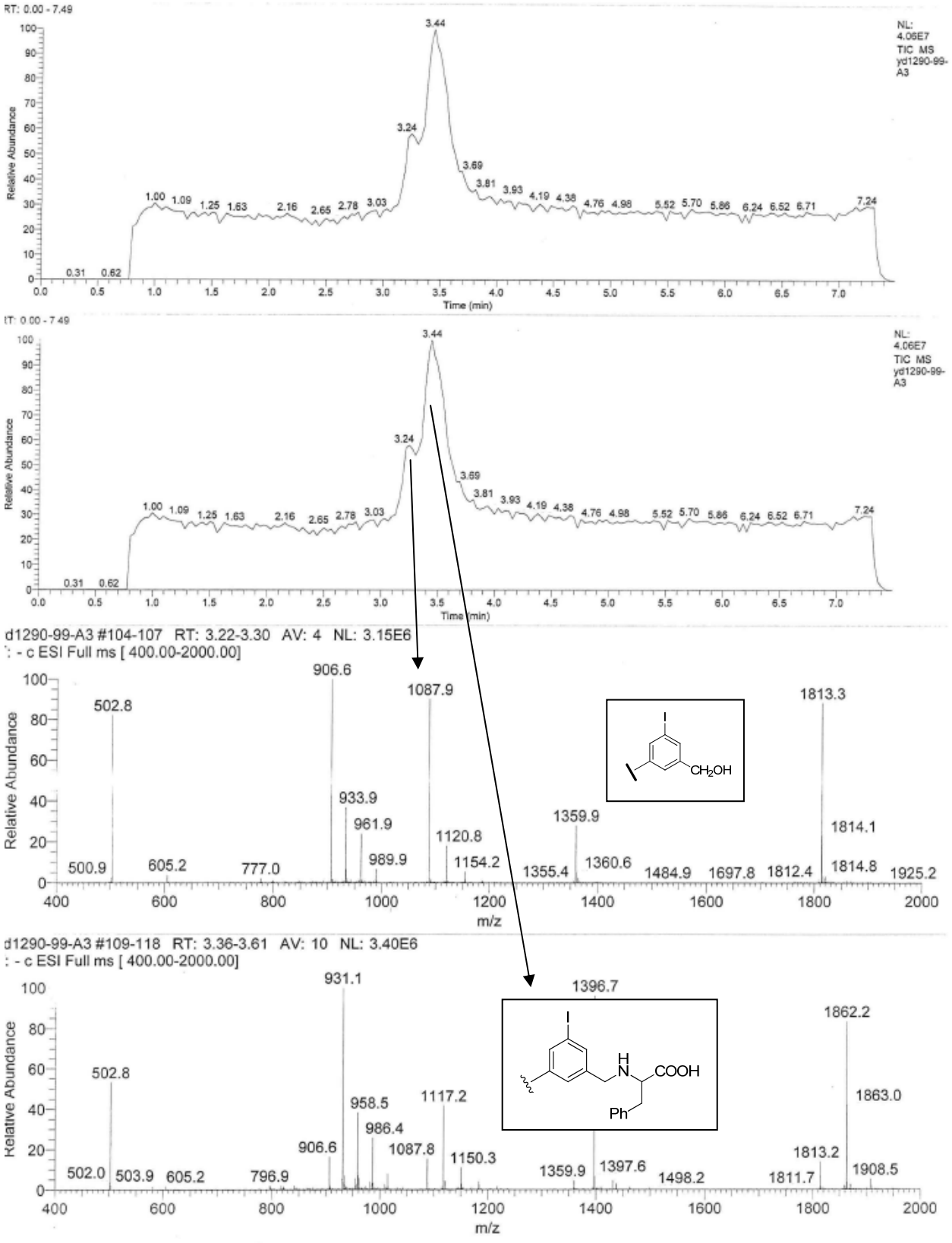

Product: ~100% yield
Expected mass: 5178.48, M-3/3=1725.16
Observed mass: M-3/3=1724.99



Preparation of **HP-8**

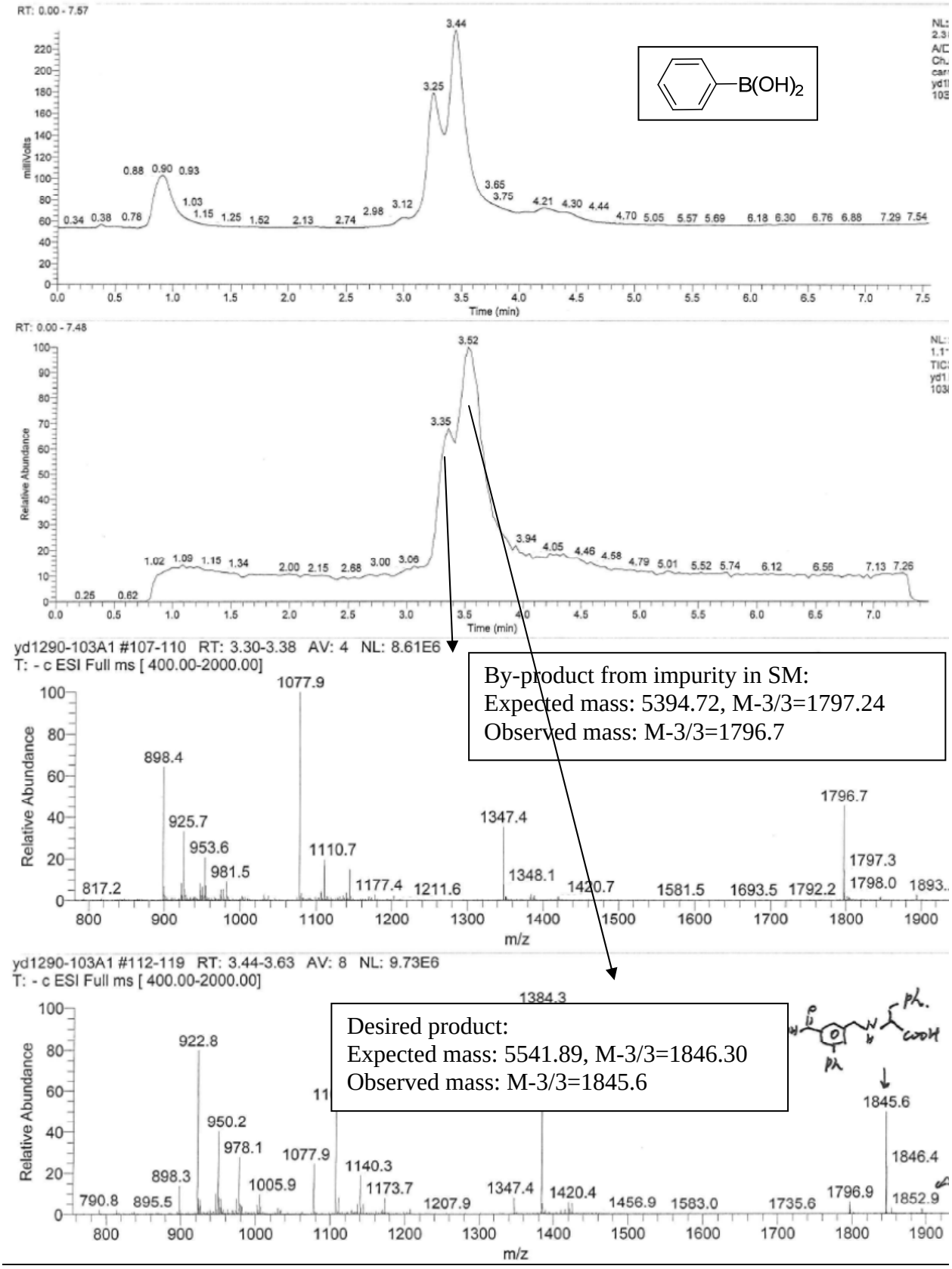
A solution of AOP-HP[1] in pH9.4 borate buffer (250 mM) (0.5 μmol, 500 μL) was added at cold 40 equivalents of 5-formyl 3-iodobenzoic acid (1 M in DMF), followed by 40 equivalents of DMT-MM (400 mM in water). The reaction was kept in cold overnight. The reaction was further treated with piperidine (44 μL) for 5 minutes, followed with precipitation by 10% 5N NaCl water solution and 2.5 times volume of absolute EtOH. The pellet was redissolved in pH5.5 phosphate buffer (250mM) to make 1mM concentration. To the above solution was added 50 equivalents of phenylalanine (400 mM in $H_2O$/DMA 5/1), followed by adding 50 equivalents of $NaCNBH_3$ (400 mM in DMA). The reaction was heated at 50 °C for 3 hours, followed with precipitation by 10% 5N NaCl water solution and 2.5 times volume of absolute EtOH. The pellet of **HP-8** which contained about 25% of reduced starting material was redissolved in water (100 μL), followed by EtOH precipitation once more. The pellet was dissolved in water to make 1 mM concentration of solution, which would be used directly for the next step without further purification.

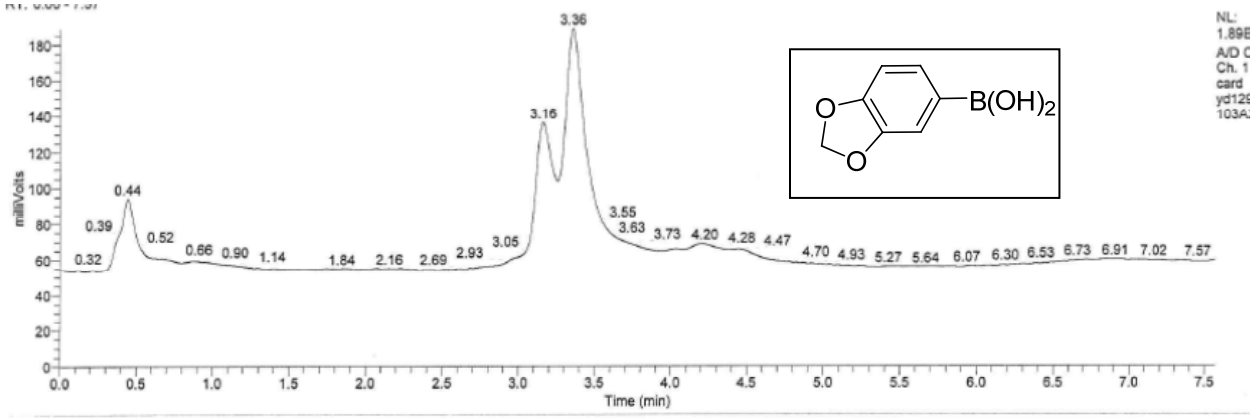
**HP-8**: expected mass 5591.69 (M-3/3=1862.90), observed 5590 (M-3/3=1862.2)

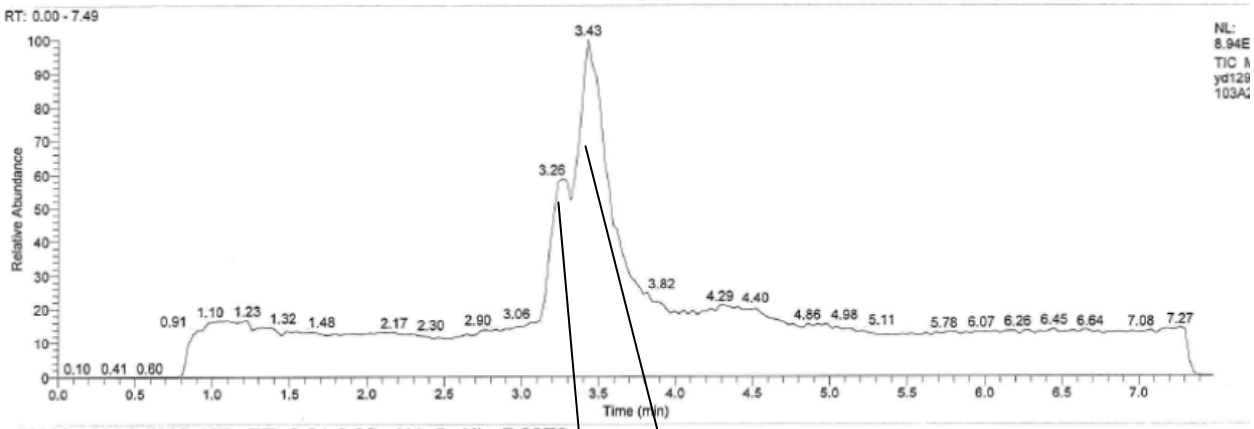

RT: 0.00 - 7.49
Relative Abundance
Time (min)
NL:
4.06E7
TIC MS
yd1290-99-A3
3.44
3.24
3.69
3.81
3.93
4.19
4.38
4.76
4.98
5.52
5.70
5.86
6.24
6.52
6.71
7.24
1.00
1.09
1.25
1.63
2.16
2.65
2.78
3.03
0.31
0.62
d1290-99-A3 #104-107 RT: 3.22-3.30 AV: 4 NL: 3.15E6
: - c ESI Full ms [ 400.00-2000.00]
906.6
1087.9
502.8
1813.3
933.9
961.9
1120.8
1359.9
1814.1
500.9
605.2
777.0
989.9
1154.2
1355.4
1360.6
1484.9
1697.8
1812.4
1814.8
1925.2
CH2OH
m/z
d1290-99-A3 #109-118 RT: 3.36-3.61 AV: 10 NL: 3.40E6
: - c ESI Full ms [ 400.00-2000.00]
931.1
1396.7
1862.2
502.8
958.5
1117.2
986.4
906.6
1087.8
1150.3
1863.0
1813.2
1908.5
502.0
503.9
605.2
796.9
1359.9
1397.6
1498.2
1811.7
COOH
Ph

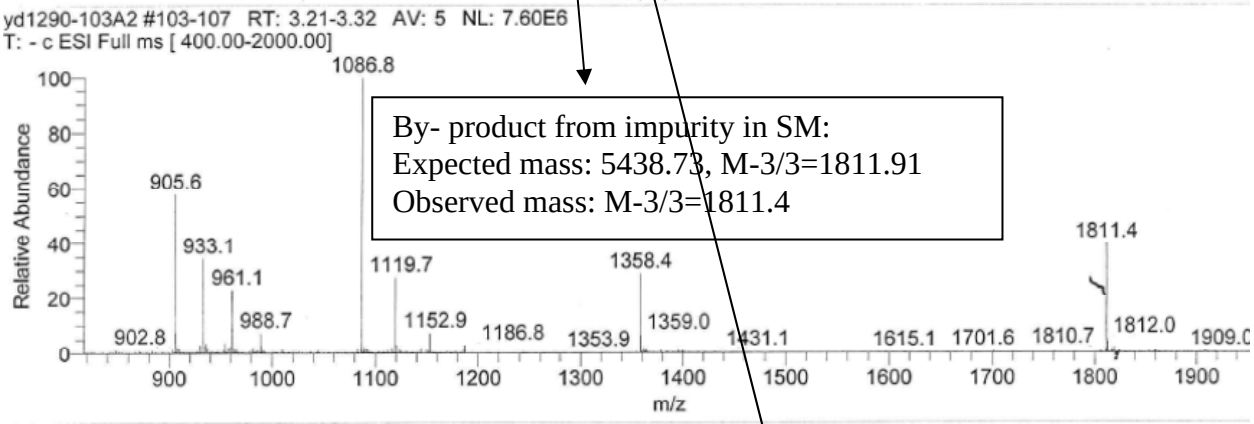
General procedure for the coupling of **HP-8** with boronic acids/esters in Scheme 3.

A 1 mM solution of **HP-8** in water (10 nmol, 10 μL) was added 40 equivalents of boronate (0.67 μL, 600 mM in DMA) and 80 equivalents of $Na_2CO_3$ (0.67 μL, 1.2 M in water), followed by 1 equivalent of degassed $Pd(PPh_3)_4$ (3.3 μL, 3 mM in $CH_3CN$). The reaction was allowed to proceed at 80 °C for 4 hrs.

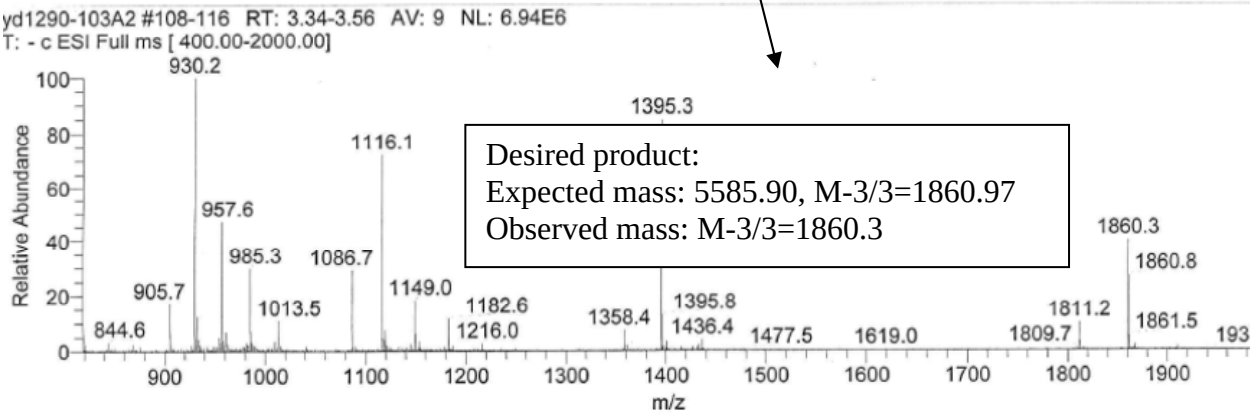

RT: 0.00 - 7.57
B(OH)2
milliVolts
Time (min)
RT: 0.00 - 7.48
Relative Abundance
Time (min)
yd1290-103A1 #107-110 RT: 3.30-3.38 AV: 4 NL: 8.61E6
T: - c ESI Full ms [ 400.00-2000.00]
By-product from impurity in SM:
Expected mass: 5394.72, M-3/3=1797.24
Observed mass: M-3/3=1796.7
Relative Abundance
m/z
yd1290-103A1 #112-119 RT: 3.44-3.63 AV: 8 NL: 9.73E6
T: - c ESI Full ms [ 400.00-2000.00]
Desired product:
Expected mass: 5541.89, M-3/3=1846.30
Observed mass: M-3/3=1845.6
Relative Abundance
m/z



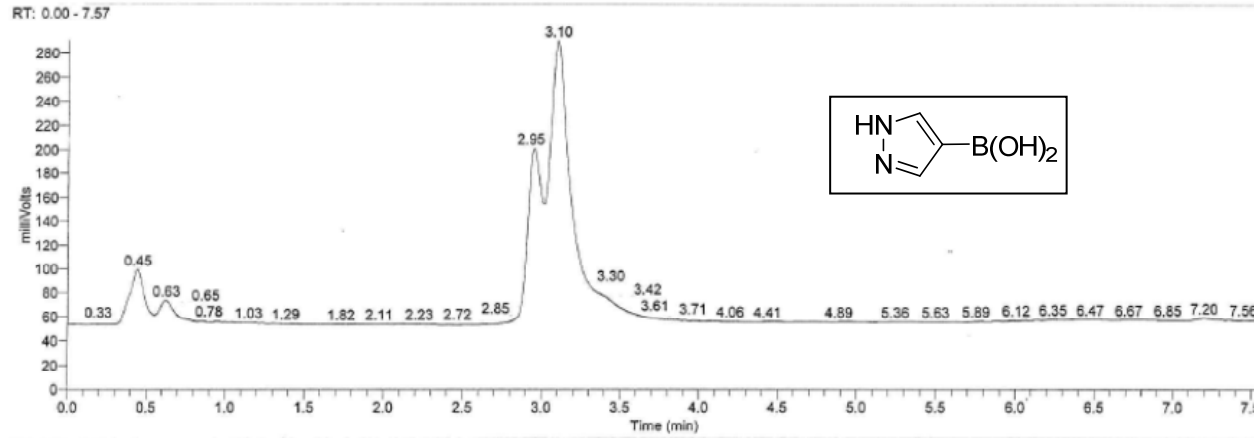



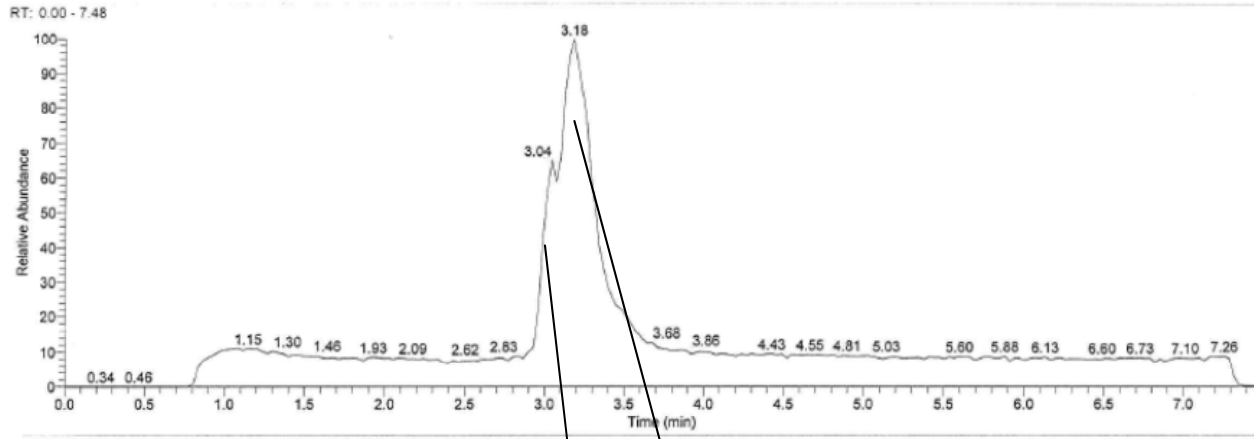



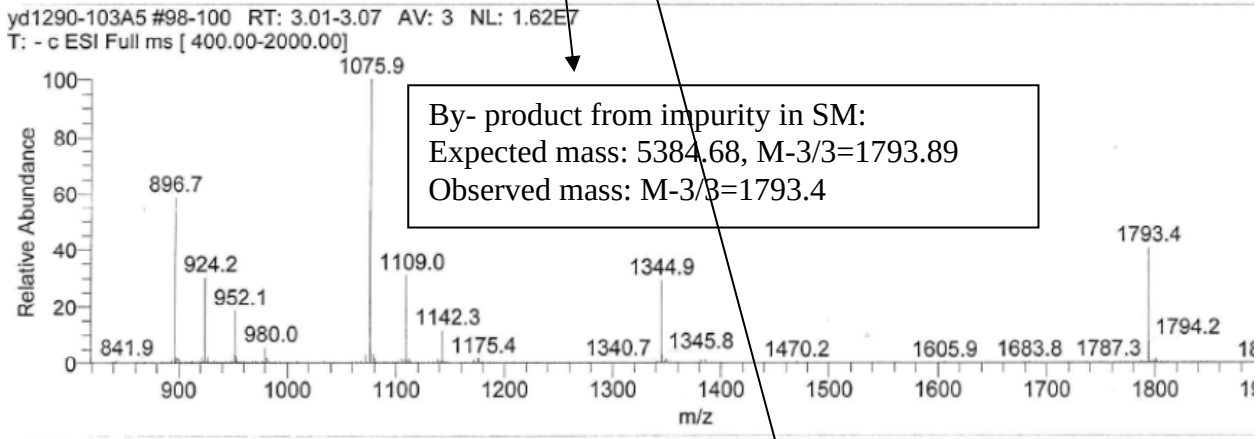

By- product from impurity in SM:
Expected mass: 5438.73, M-3/3=1811.91
Observed mass: M-3/3=1811.4



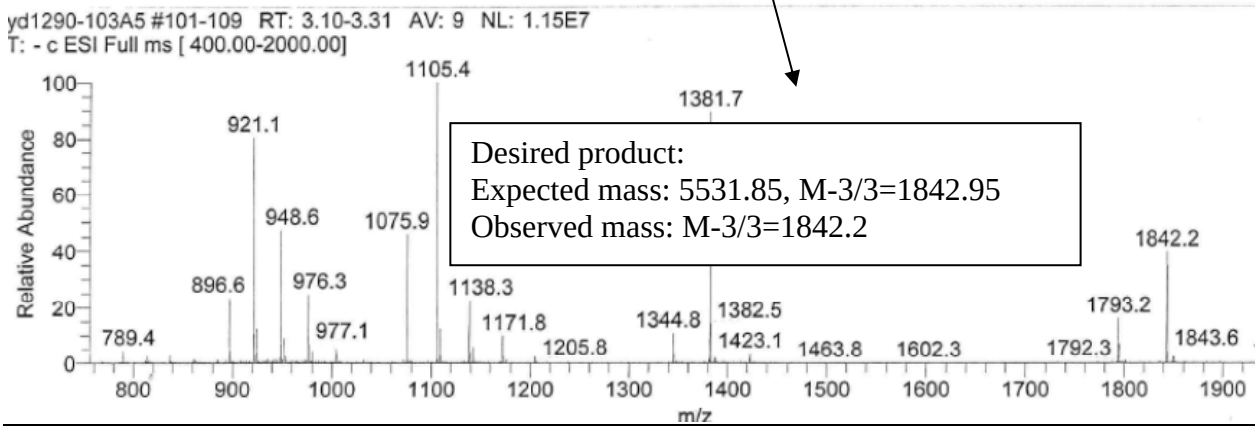

Desired product:
Expected mass: 5585.90, M-3/3=1860.97
Observed mass: M-3/3=1860.3



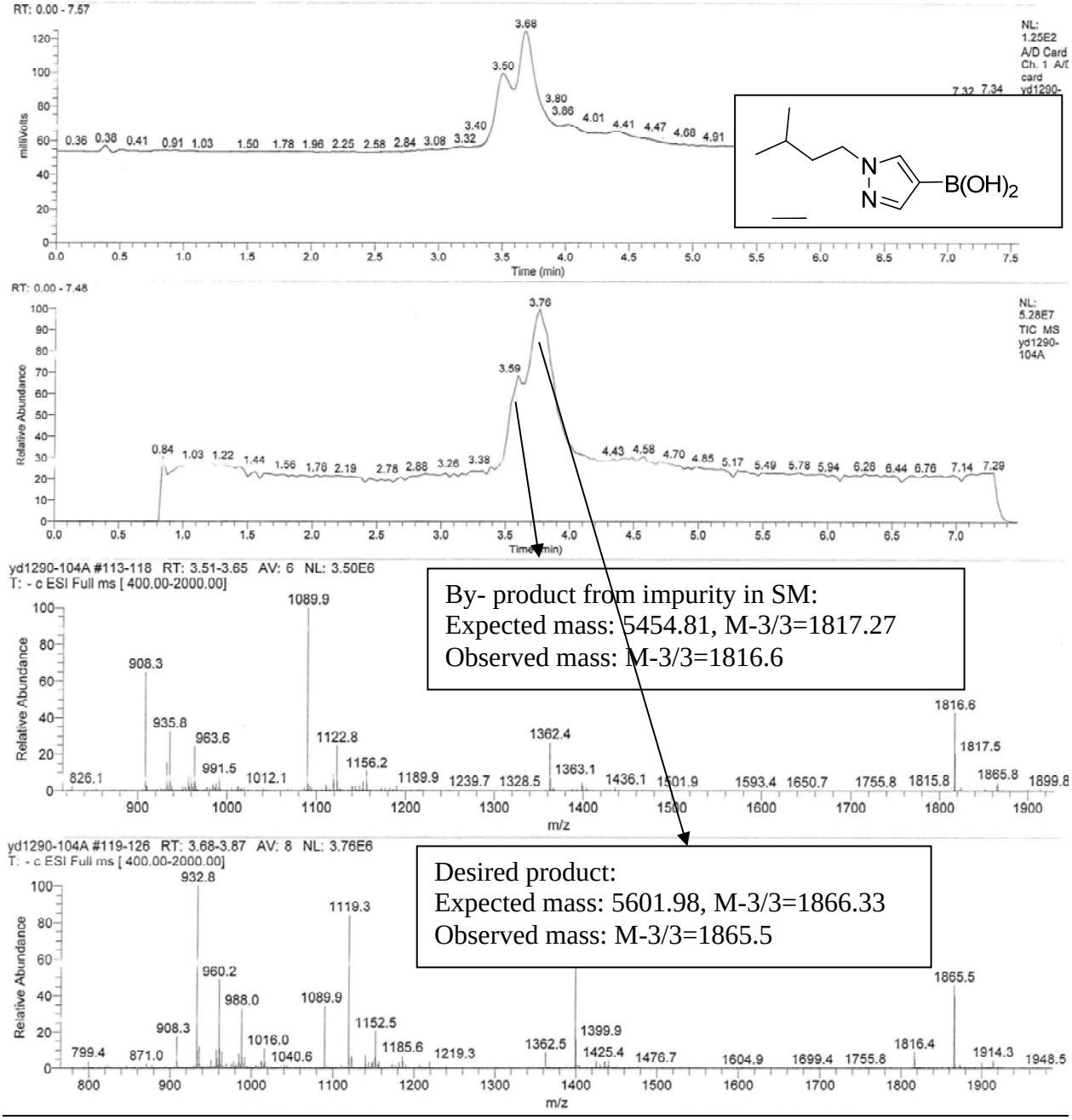



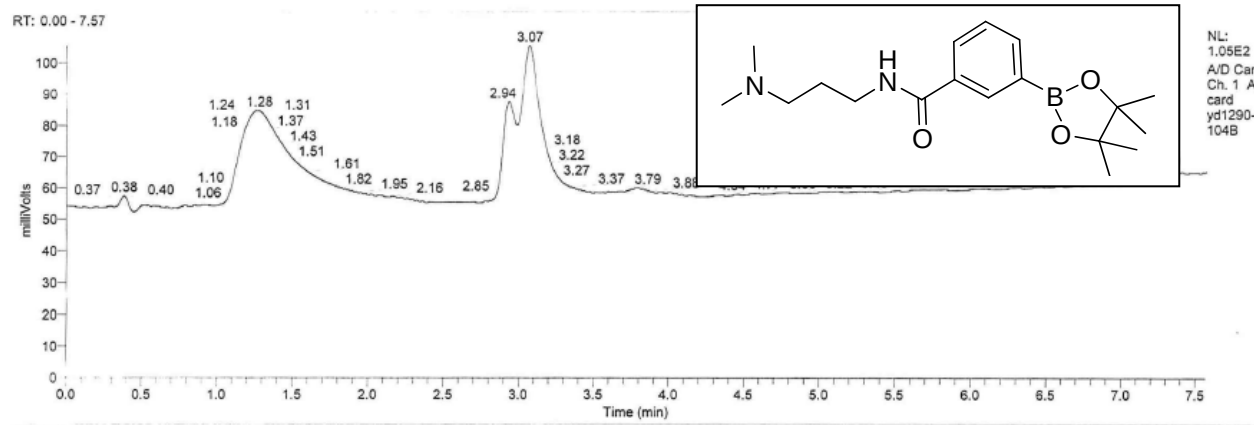



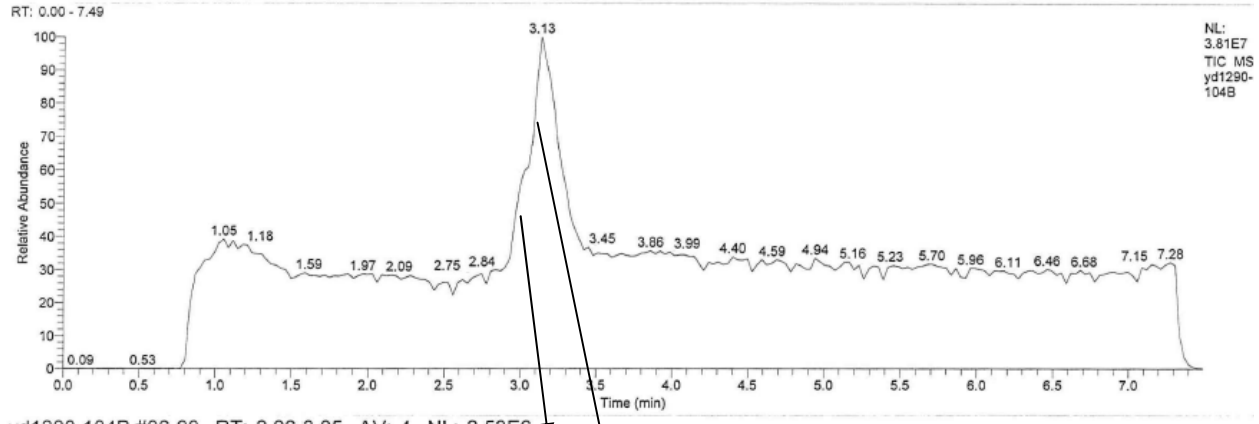

By- product from impurity in SM:
Expected mass: 5384.68, M-3/3=1793.89
Observed mass: M-3/3=1793.4

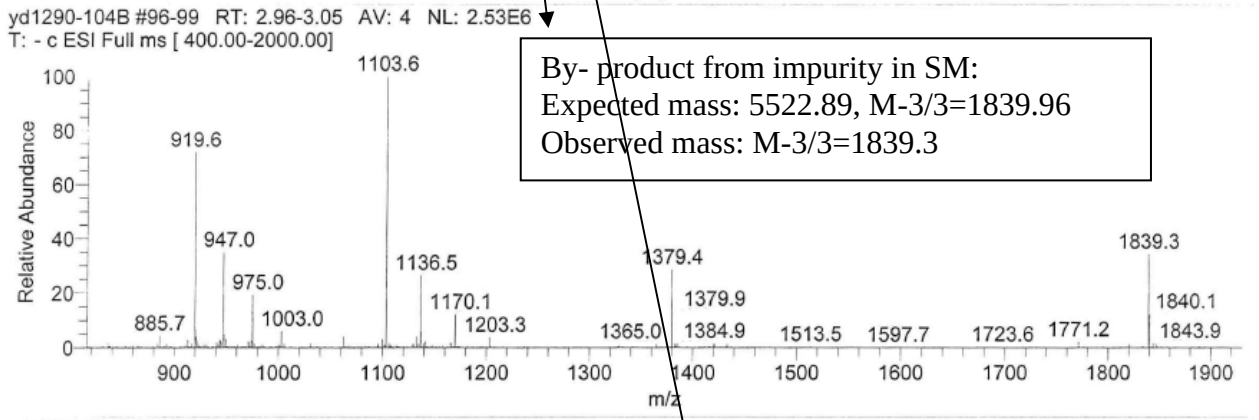



Desired product:
Expected mass: 5531.85, M-3/3=1842.95
Observed mass: M-3/3=1842.2

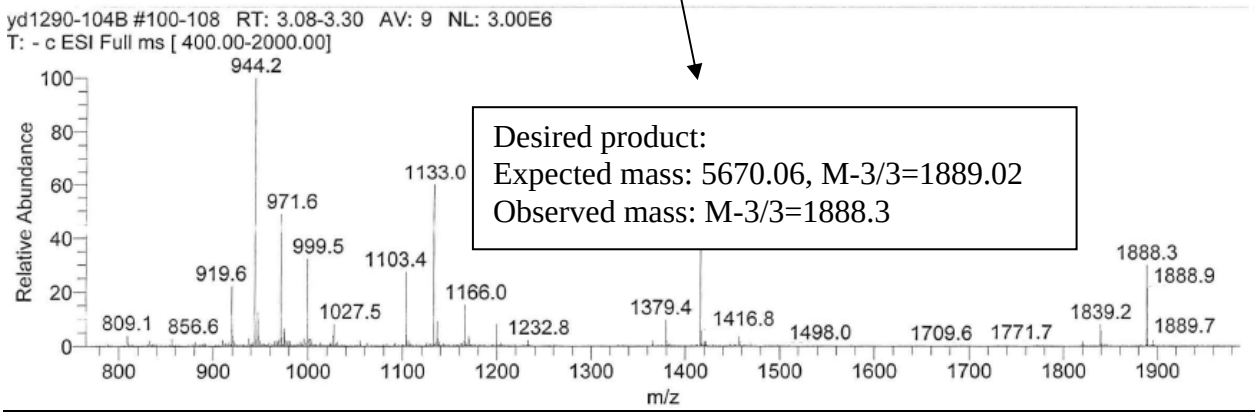

RT: 0.00 - 7.57
NL: 1.25E2
A/D Card
Ch. 1 A/D card
yd1290-
milliVolts
Time (min)
3.68
3.50
3.80
3.86
3.40
3.32
4.01
4.41
4.47
4.68
4.91
7.32
7.34
N
N
B(OH)2
RT: 0.00 - 7.48
NL: 5.28E7
TIC MS
yd1290-104A
Relative Abundance
Time (min)
3.76
3.59
4.43
4.58
4.70
4.85
5.17
5.49
5.78
5.94
6.28
6.44
6.76
7.14
7.29
yd1290-104A #113-118 RT: 3.51-3.65 AV: 6 NL: 3.50E6
T: - c ESI Full ms [ 400.00-2000.00]
Relative Abundance
m/z
1089.9
908.3
935.8
963.6
1122.8
1156.2
991.5
1012.1
826.1
1189.9
1239.7
1328.5
1362.4
1363.1
1436.1
1501.9
1593.4
1650.7
1755.8
1815.8
1816.6
1817.5
1865.8
1899.8
By- product from impurity in SM:
Expected mass: 5454.81, M-3/3=1817.27
Observed mass: M-3/3=1816.6
yd1290-104A #119-126 RT: 3.68-3.87 AV: 8 NL: 3.76E6
T: - c ESI Full ms [ 400.00-2000.00]
Relative Abundance
m/z
932.8
1119.3
960.2
988.0
1089.9
908.3
1016.0
1040.6
1152.5
1185.6
1219.3
799.4
871.0
1362.5
1399.9
1425.4
1476.7
1604.9
1699.4
1755.8
1816.4
1865.5
1914.3
1948.5
Desired product:
Expected mass: 5601.98, M-3/3=1866.33
Observed mass: M-3/3=1865.5




By- product from impurity in SM:
Expected mass: 5522.89, M-3/3=1839.96
Observed mass: M-3/3=1839.3




Desired product:
Expected mass: 5670.06, M-3/3=1889.02
Observed mass: M-3/3=1888.3