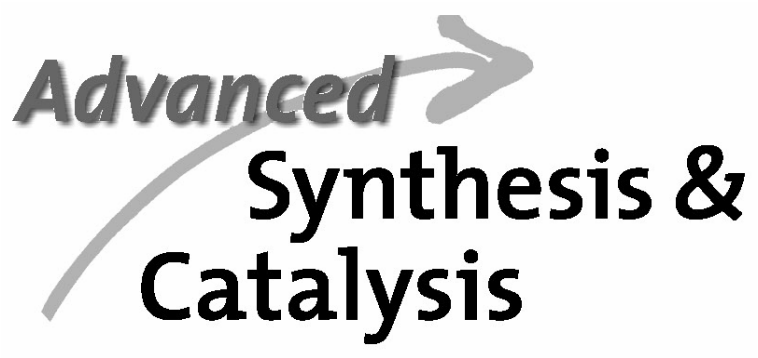

Supporting Information

Supporting Information

for

Cobalt Catalyzed Cross-Coupling Between Functionalized Primary and Secondary Alkyl Halides and Aliphatic Organomagnesium Compounds

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List of contents

I/ General

All reactions were carried out under a nitrogen atmosphere. All starting materials were purchased from commercial sources and used without any further purification. Anhydrous THF was purchased from Carlo Erba. Yields refer to isolated yields of compounds estimated to be = 97 % pure as determined by ^{1}H-NMR (400 MHz), ^{13}C-NMR (100 MHz) and GC analysis (capillary column HP-5MS; 30m x 0.25mm x 0.25µm). All compounds give satisfactory centesimal analysis. The analytical data for the known compounds were found to match with the literature data.

High Resolution Mass Spectra were obtained on a Jeol GCmate II. Ionisation was obtained by electronic impact (EI, 70 eV). Mass spectra are reported as *m/z*.

The Grignard solutions were titrated according to the procedure described by Watson [1].

II) Typical procedure : preparation of 3-methyltridecane

A dry and nitrogen flushed 250 mL four-necked flask, equipped with a mechanical stirrer, a thermometer, a nitrogen inlet and a septum, was charged with THF (25 mL), 2-bromobutane (6.85 g, 50 mmol), $CoCl_2$ (325 mg, 5 mol%), TMEDA (1.16 g, 20 mol%) and LiI (70 mg, 10 mol%). The reaction mixture was cooled to 10°C then a solutio of *n*-decylmagnesium bromide in THF (61 mL, 0.9M, 55 mmol) was added in 80 min. After completion of the addition, the reaction mixture was stirred for 30 min then quenched with aqueous HCl 1M (100 mL). The aqueous phase was extracted with ether (3 x 50 mL), then the combined organic layers were dried with $MgSO_4$ and concentrated *in vacuo*. The crude residue was purified by distillation at a reduced pressure (116°C, 10 Torr) yielding the 3-methyl-tridecane (7.8 g, 79%) as a colorless oil.

III) Analytical data

3-methyltridecane (scheme 1)

Colorless oil. b.p. = 116 °C / 10 Torr

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.84 (d, J = 6.41 Hz, 3H), 0.85 (t, J = 7.33 Hz, 3H), 0.88 (t, J = 7.33 Hz, 3H), 1.1 (m, 2H), 1.26 (m, 19H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 11.42, 14.14, 19.22 (2C), 22.71, 27.12, 29.38, 29.50, 29.68, 29.73, 30.05, 31.94, 34.40, 36.65.

HR-MS (EI, 70 eV) calc : *m/z* = 192.2348

found : *m/z* = 192.2372

2-methyldecane (Table 1, Entry 1)

Colorless oil. b.p. = 78 °C / 10 Torr

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.79 (d, J = 6.87 Hz, 6H), 0.80 (t, J = 7.33 Hz, 3H), 1.15 (m, 2H), 1.26 (m, 12H), 1.44 (sext, J = 6.87 Hz, 1H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 14.12, 22.66, 22.71, 27.44, 27.99, 29.39, 29.71 (2C), 29.98, 31.96, 39.08.

HR-MS (EI, 70 eV) calc : m/z = 156.1878

found : *m/z* = 156.1922

2-methyldodecane[2] (Table 1, Entry 2)

Colorless oil. b.p. = 45 °C / 0,2 Torr

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.86 (d, J = 6.87 Hz, 6H), 0.89 (t, J = 6.87 Hz, 3H), 1.15 (m, 2H), 1.26 (m, 15H), 1.51 (sext., J = 6.87 Hz, 1H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 14.16, 22.43, 22.69, 22.78, 27.54, 28.05, 29.48, 29.78, 29.82, 29.85, 30.06, 32.03, 39.15.

HR-MS (EI, 70 eV) calc : m/z = 184.2191

found : *m/z* = 184.2155

3-methylundecane (Table 1, Entry 3)

Colorless oil. b.p. = 102 °C / 10 Torr

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.82 (d, J = 6.41 Hz, 3H), 0.84 (t, J = 6.87 Hz, 3H), 0.87 (t, J = 6.87 Hz, 3H), 1.08 (m, 2H), 1.27 (m, 15H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 11.41, 14.12, 19.23, 22.72, 27.14, 29.40, 29.53, 29.73, 30.07, 31.96, 34.43, 36.68.

HR-MS (EI, 70 eV) calc : m/z = 170.2035

found : *m/z* = 170.2051

4-methyldodecane (Table 1, Entry 7)

Colorless oil. b.p. = 113 °C / 10 Torr

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.82 (d, J = 6.41Hz, 3H), 0.85 (t, J = 6.87 Hz, 3H), 0.86 (t, J = 6.87 Hz, 3H), 1.06 (m, 2H), 1.28 (m, 17H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 14.14, 14.42, 19.67, 20.16, 22.73, 27.12, 29.41, 29.73, 30.08, 31.97, 32.50, 37.12, 39.44.

HR-MS (EI, 70 eV) calc : m/z = 184.2191

found : *m/z* = 184.2149

4-methyltetradecane (Table 1, Entry 8)

Colorless oil. b.p. = 117 °C / 10 Torr

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.81 (d, J = 6.41Hz, 3H), 0.86 (t, J = 6.87 Hz, 3H), 0.87 (t, J = 6.87 Hz, 3H), 1.05 (m, 2H), 1.24 (m, 21H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 14.14, 14.42, 19.68, 20.15, 22.72, 27.11, 29.40, 29.75 (3C), 30.07, 31.96, 32.49, 37.11. 39.43.

HR-MS (EI, 70 eV) calc : m/z = 212.2504

found : *m/z* = 212.2509

3-Ethyltridecane (Table 1, Entry 9)

Colorless oil. b.p. = 114 °C / 4 Torr

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.81 (t, J = 7.33 Hz, 6H), 0.87 (t, J = 6.87 Hz, 3H), 1.24 (m, 23H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 10.92 (2C), 14.13, 22.72, 25.44 (2C), 26.79, 29.39, 29.70, 29.75, 29.77, 30.19, 31.95, 32.77, 40.39.

HR-MS (EI, 70 eV) calc : m/z = 212.2504

found : *m/z* = 212.2504

6-methylhexadecane (Table 1, Entry 10)

Colorless oil. b.p. = 145 °C / 4 Torr

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.82 (d, J = 6.41 Hz, 3H), 0.86 (t, J = 6.41 Hz, 6H), 1.06 (m, 2H), 1.24 (m, 25H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 14.12 (2C), 19.72, 22.71, 22.74, 26.77, 27.11, 29.38, 29.69, 29.72, 29.76, 30.06, 31.95, 32.28, 32.77, 37.07, 37.12.

HR-MS (EI, 70 eV) calc : m/z = 240.2817

found : *m/z* = 240.2803

5-methyltridecane (Table 1, Entry 11)

Colorless oil. b.p. = 135 °C / 10 Torr

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.77 (d, J = 6.41 Hz, 3H), 0.81 (t, J = 6.41 Hz, 3H), 0.82 (t, J = 6.41 Hz, 3H), 1.2 (m, 21H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 14.13, 14.16, 19.69, 22.72, 23.07, 27.12, 29.36, 29.41, 29.74, 30.07, 31.96, 32.75, 36.81, 37.13.

HR-MS (EI, 70 eV) calc : m/z = 198.2348

found : *m/z* = 198.2339

1-Cyclohexyloctane (Table 1, Entry 12)

Colorless oil. b.p. = 134 °C / 10 Torr

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.81 (m, 2H), 0.86 (t, J = 7.33Hz, 3H), 1.1-1.31 (m, 18H), 1.64 (m, 5H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 14.14, 22.71, 26.48 (2C), 26.79, 29.90, 29.38, 29.71, 30.03, 31.95, 33.47 (2C), 37.59, 37.69.

HR-MS (EI, 70 eV) calc : m/z = 196.2191

found : *m/z* = 196.2163

1-Cyclohexyldecane[3] (Table 1, Entry 13)

Colorless oil. b.p. = 81 °C / 0.3 Torr

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.83 (m, 2H), 0.88 (t, J = 7.33 Hz, 3H), 1.13-1.30 (m, 22H), 1.67 (m, 5H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 14.16, 22.74, 26.48 (2C), 26.79, 26.92, 29.42, 29.72, 29.76, 29.78, 30.06, 31.97, 33.47 (2C), 37.62, 37.70.

HR-MS (EI, 70 eV) calc : m/z = 224.2504

found : *m/z* = 224.2540

***n*-dodecanol[4] (Table 1, Entry 17)**

Colorless oil. b.p. = 262 °C

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.88 (t, J = 6.87 Hz, 3H), 1.29 (m, 18H), 1.41 (s, 1H), 1.56 (quint. ,J = 7.33 Hz, 2H), 3.64 (t, J = 7.33 Hz, 2H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 14.11, 22.67, 25.71, 29.34, 29.42, 29.58, 29.60, 29.62, 29.64, 31.90, 32.78, 63.08.

HR-MS (EI, 70 eV) calc : m/z = 186.1984

found : *m/z* = 186.1969

Methyl 4-methyltetradecanoate (Scheme 2)

Colorless oil.

Purified by flash chromatography (petroleum ether/dichloromethane : 50/50)

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.79 (d, J = 6.41 Hz, 3H), 0.81 (t, J = =7.33 Hz, 3H), 1.18 (m, 18H), 1.35 (m, 2H), 1.59 (m, 1H), 2.23 (m, 2H), 3.59 (s, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 14.09, 19.25, 22.67, 26.89, 29.34, 29.63, 29.66 (3C), 29.91, 31.88 (2C), 32.38, 36.63, 51.43, 174.56.

HR-MS (EI, 70 eV) calc : m/z = 256.2402

found : *m/z* = 256.2384

Ethyl-hexanoate[5] (Table 2, entry 1)

Colorless oil.

Purified by flash chromatography (petroleum ether/dichloromethane : 50/50)

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.80 (t, J = 6.87 Hz, 3H), 1.12 (t, j = 7.33 Hz, 3H), 1.21 (m, 4H), 1.52 (quint. , J = 7.33 Hz, 2H), 2.18 (t, J = 7.33 Hz, 2H), 4.02 (q, J = 7.33 Hz, 2H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 13.69, 14.04, 22.16, 24.50, 31.16, 34.12, 59.91, 173.62.

HR-MS (EI, 70 eV) calc : m/z = 144.1150

found : *m/z* = 144.1136

Ethyl-tetradecanoate[6] (Table 2, entry 2)

Colorless oil.

Purified by flash chromatography (petroleum ether/dichloromethane : 50/50)

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.80 (t, J = 6.87 Hz, 3H), 1.82 (m, 23H), 1.54 (m, 2H), 2.22 (t, J = 7.33 Hz, 2H), 4.04 (q, J = 7.33 Hz, 2H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 14.05, 14.17, 22.64, 24.91, 29.09, 29.22, 29.32, 29.41, 29.55, 29.60 (2C), 29.63, 31.87, 34.29, 60.05, 173.81.

HR-MS (EI, 70 eV) calc : m/z = 256.2402

found : *m/z* = 256.2435

Octanenitrile[7] (Table 2, entry 3)

Colorless oil;

Purified by flash chromatography (petroleum ether/dichloromethane : 50/50)

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.83 (t, J = 6.87 Hz, 3H), 1.24 (m, 6H), 1.39 (m, 2H), 1.60 (quint. , J = 7.33 Hz, 2H), 2.28 (t, J = 7.33 Hz, 2H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 13.86, 16.95, 22.19, 22.37, 25.21, 28.28, 28.46, 31.33, 119.76.

HR-MS (EI, 70 eV) calc : m/z = 125.1204

found : *m/z* = 125.1251

2-Methyldodecan-3-one[8] (Table 2, entry 4)

Colorless oil.

Purified by flash chromatography (petroleum ether/dichloromethane : 50/50)

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.84 (t, J = 6.87 Hz, 3H), 1.05 (d, J = 6.87 Hz, 6H), 1.23 (m, 12H), 1.52 (quint, J = 6.87 Hz, 2H), 2.39 (t, J = 6.87 Hz, 2H), 2.56 (hept. , J = 6.87 Hz, 1H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 14.07, 18.23 (2C), 21.81, 22.63, 23.79, 29.25, 29.30, 29.43, 31.83, 40.34, 40.74, 215.07.

HR-MS (EI, 70 eV) calc : m/z = 198.1984

found : *m/z* = 198.1982

IV) References

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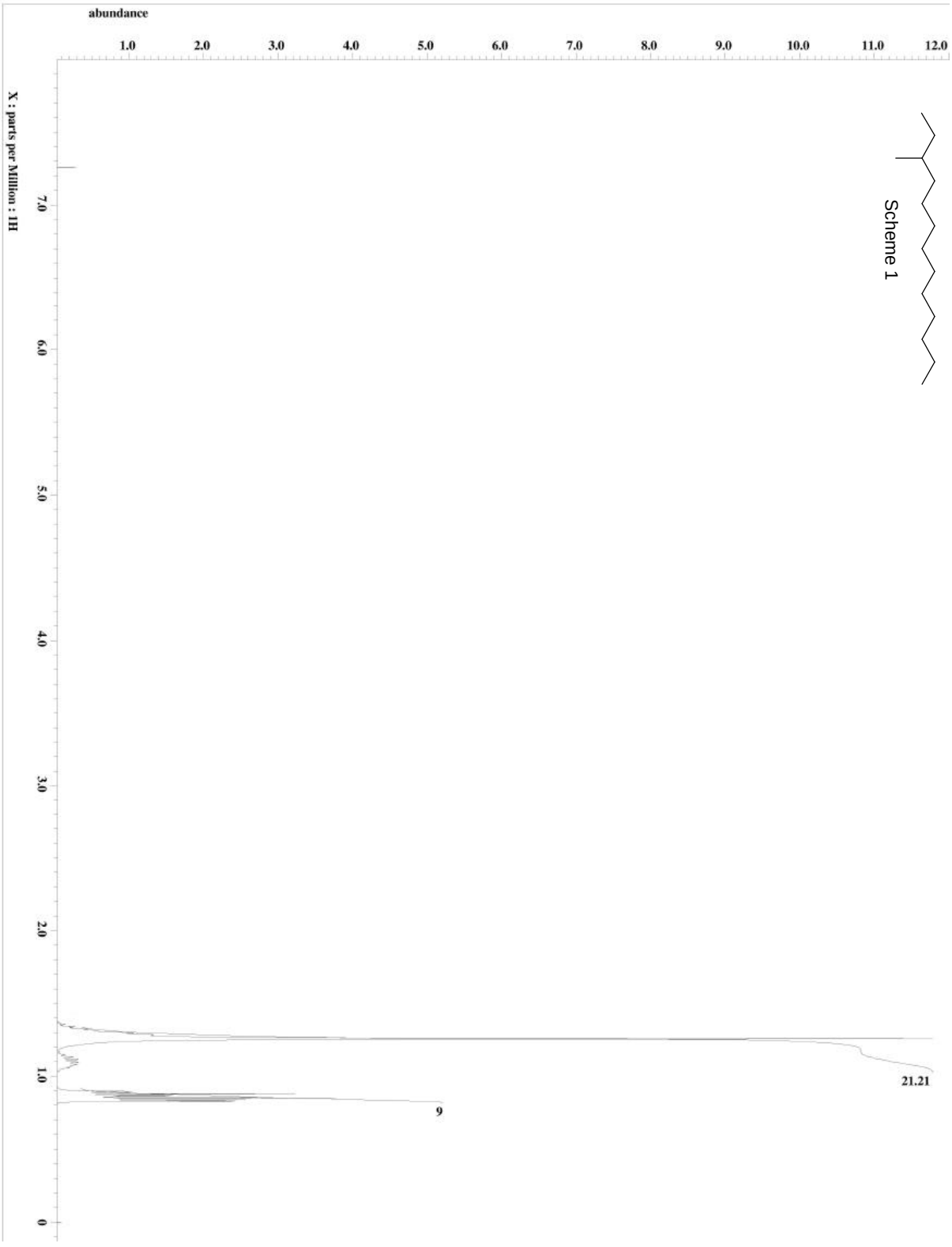
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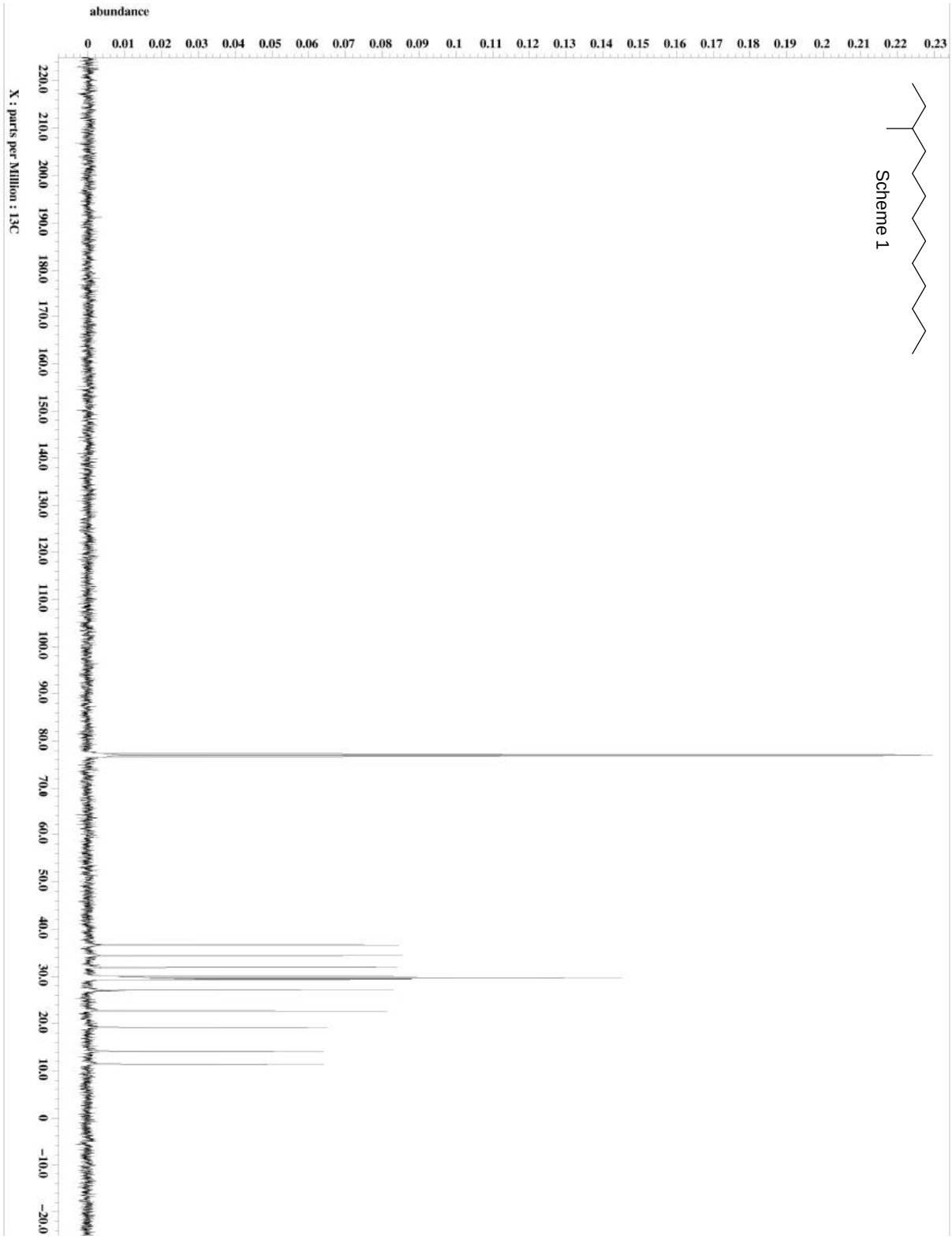
Scheme 1
21.21
9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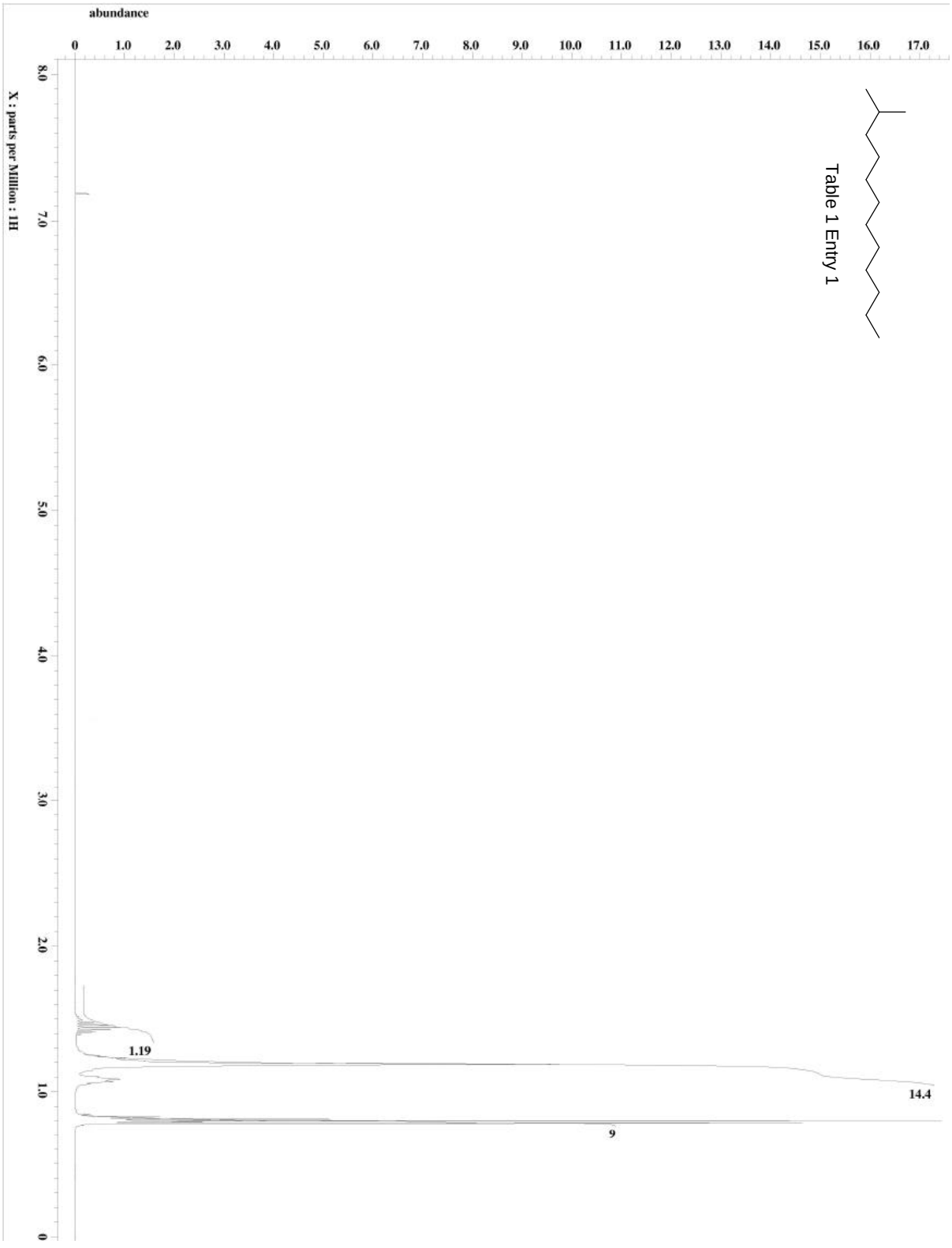
Scheme 1

Équation 1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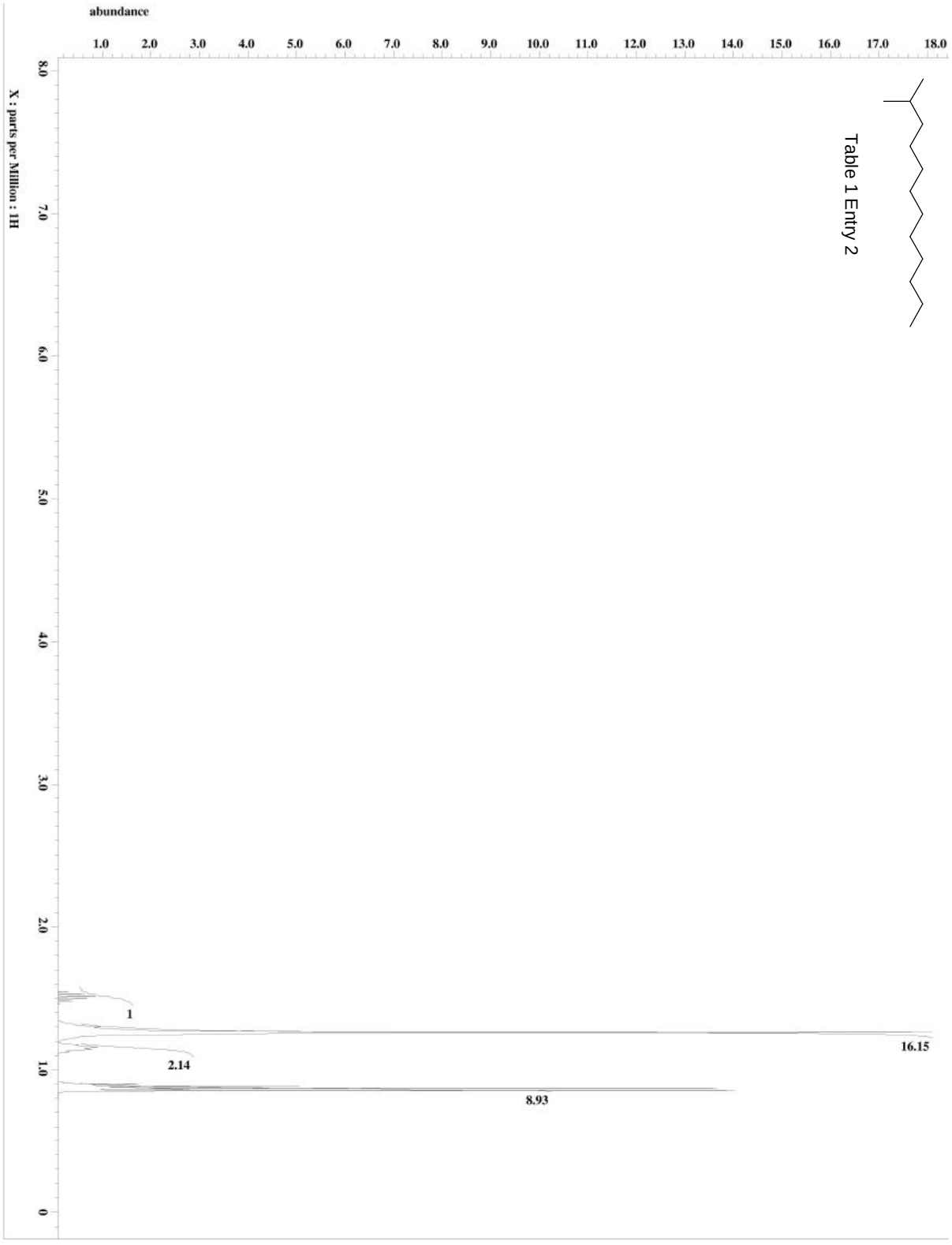
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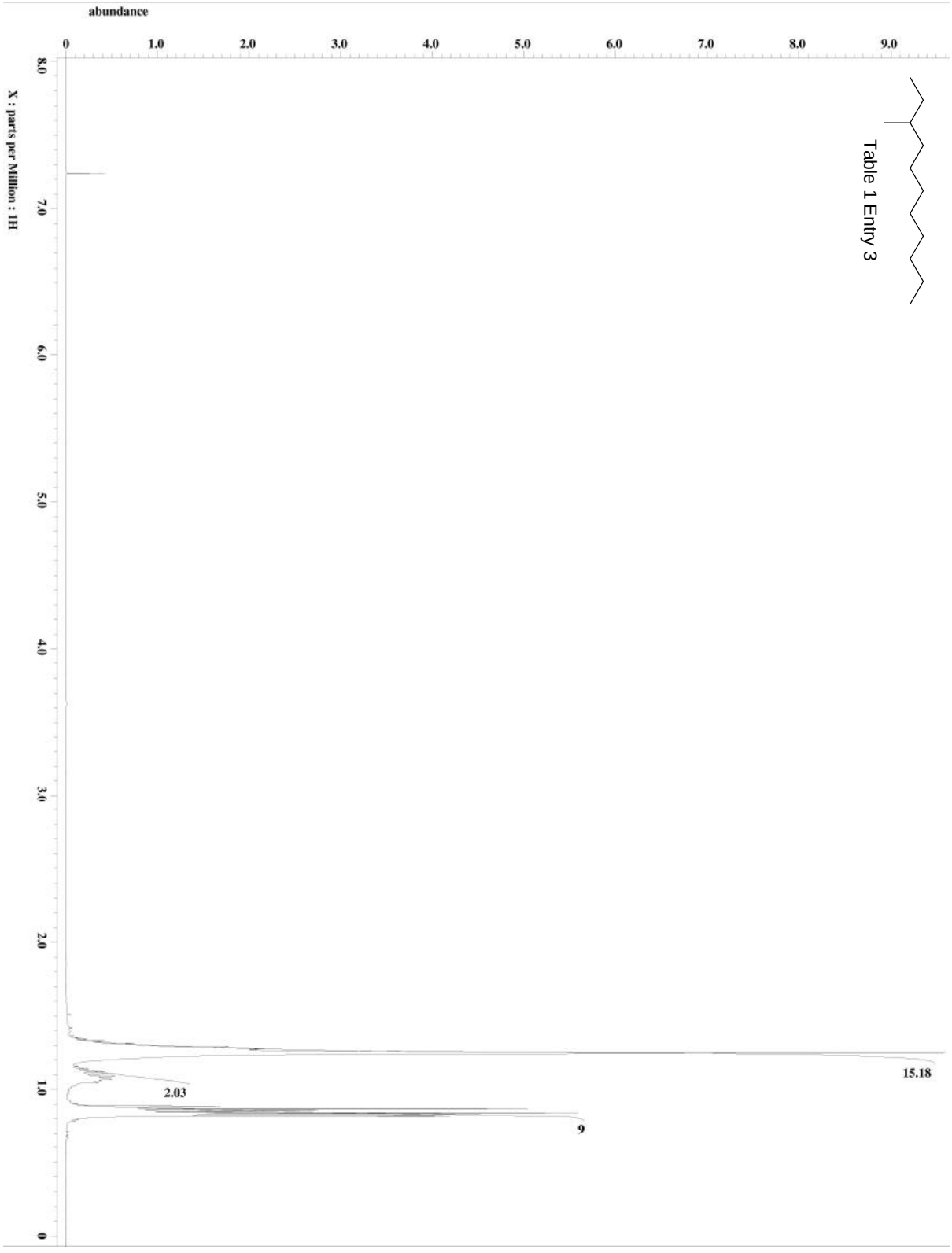
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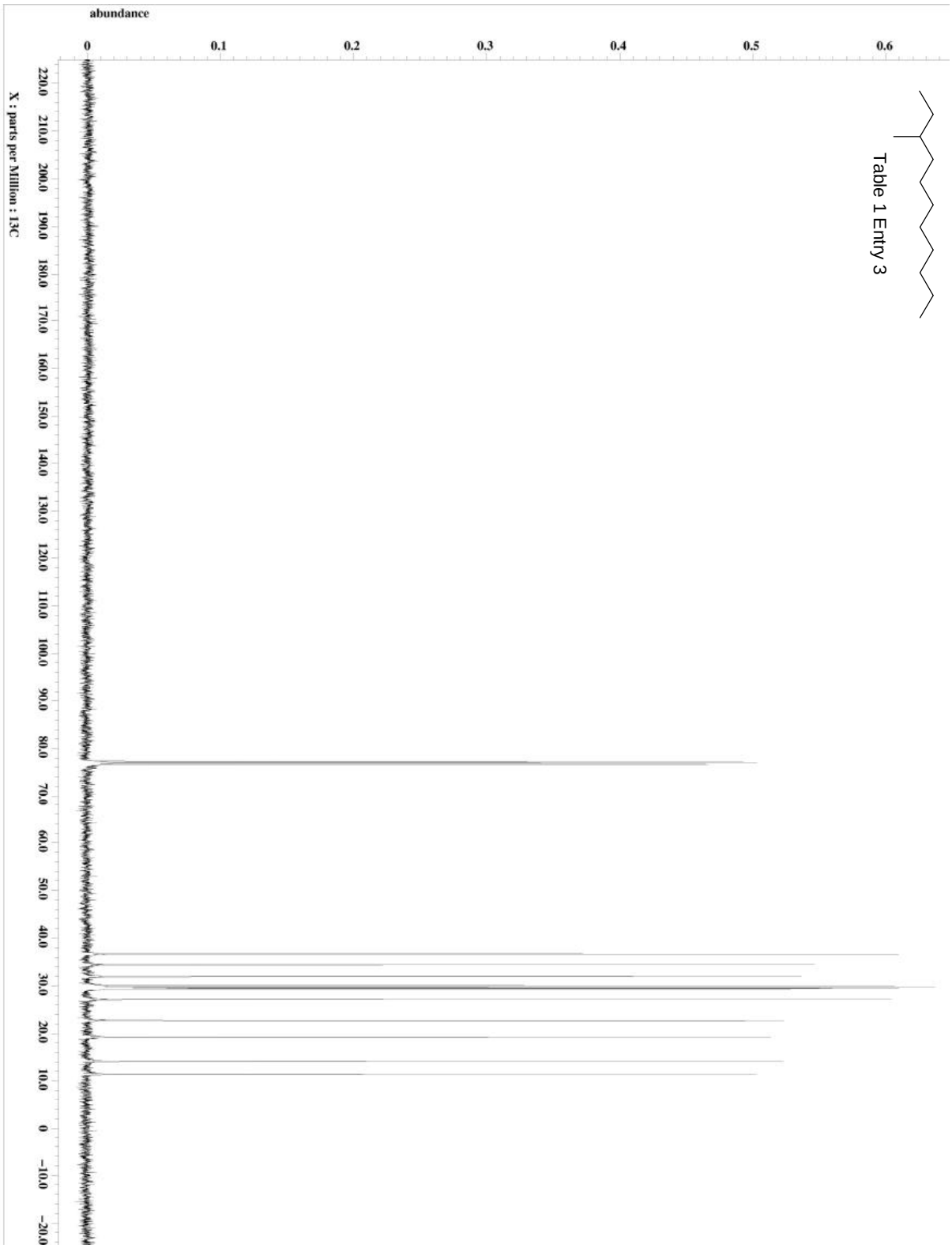
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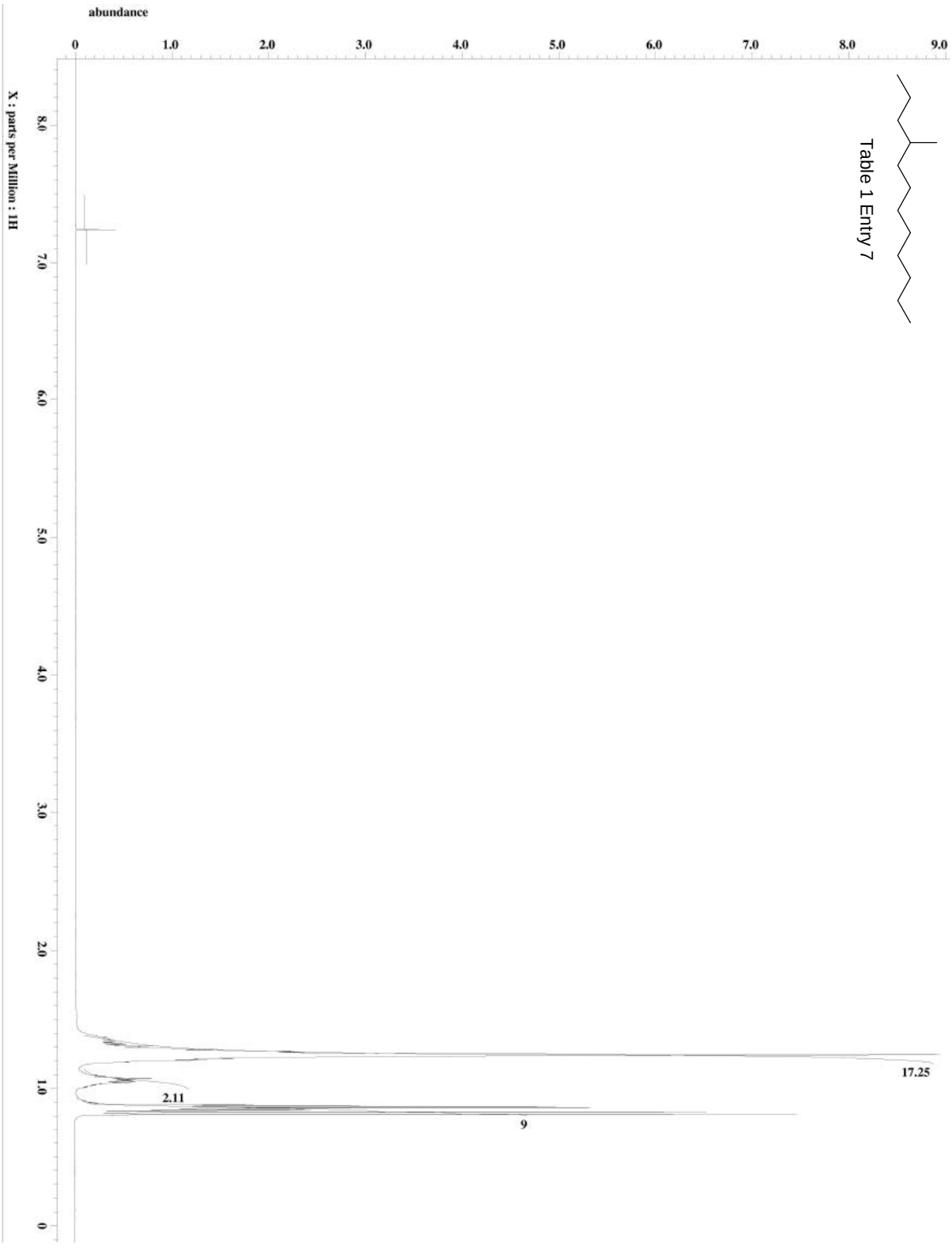
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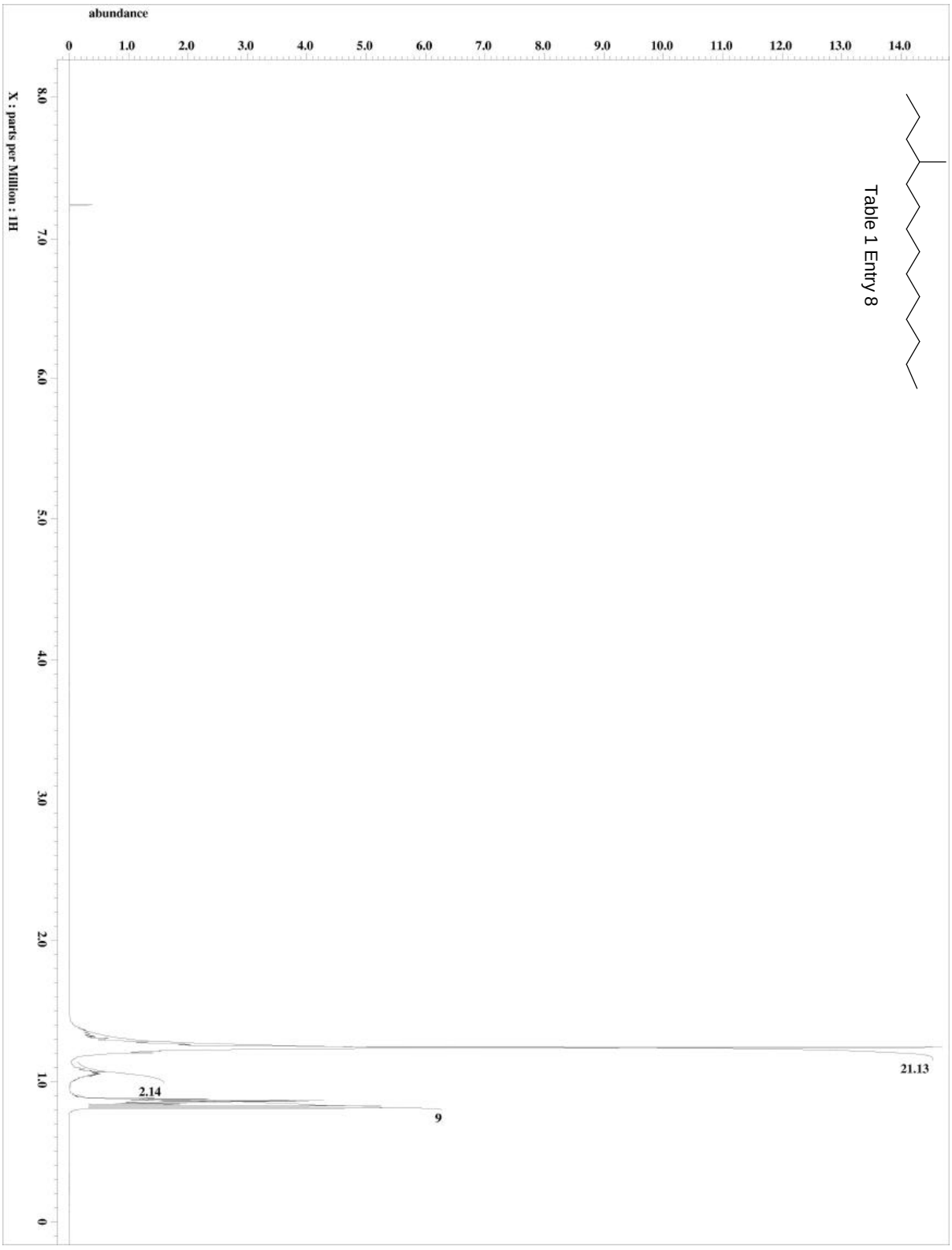
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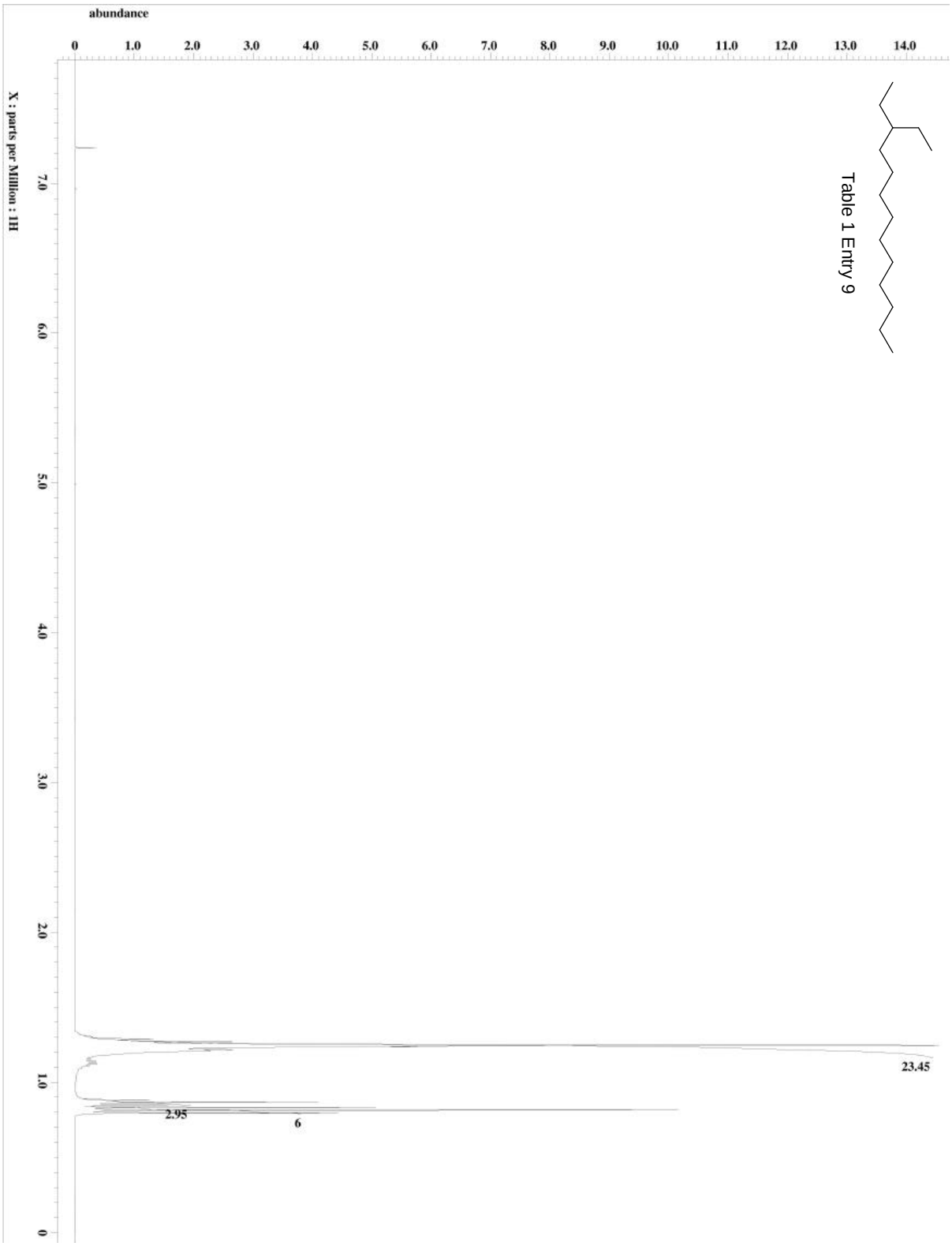
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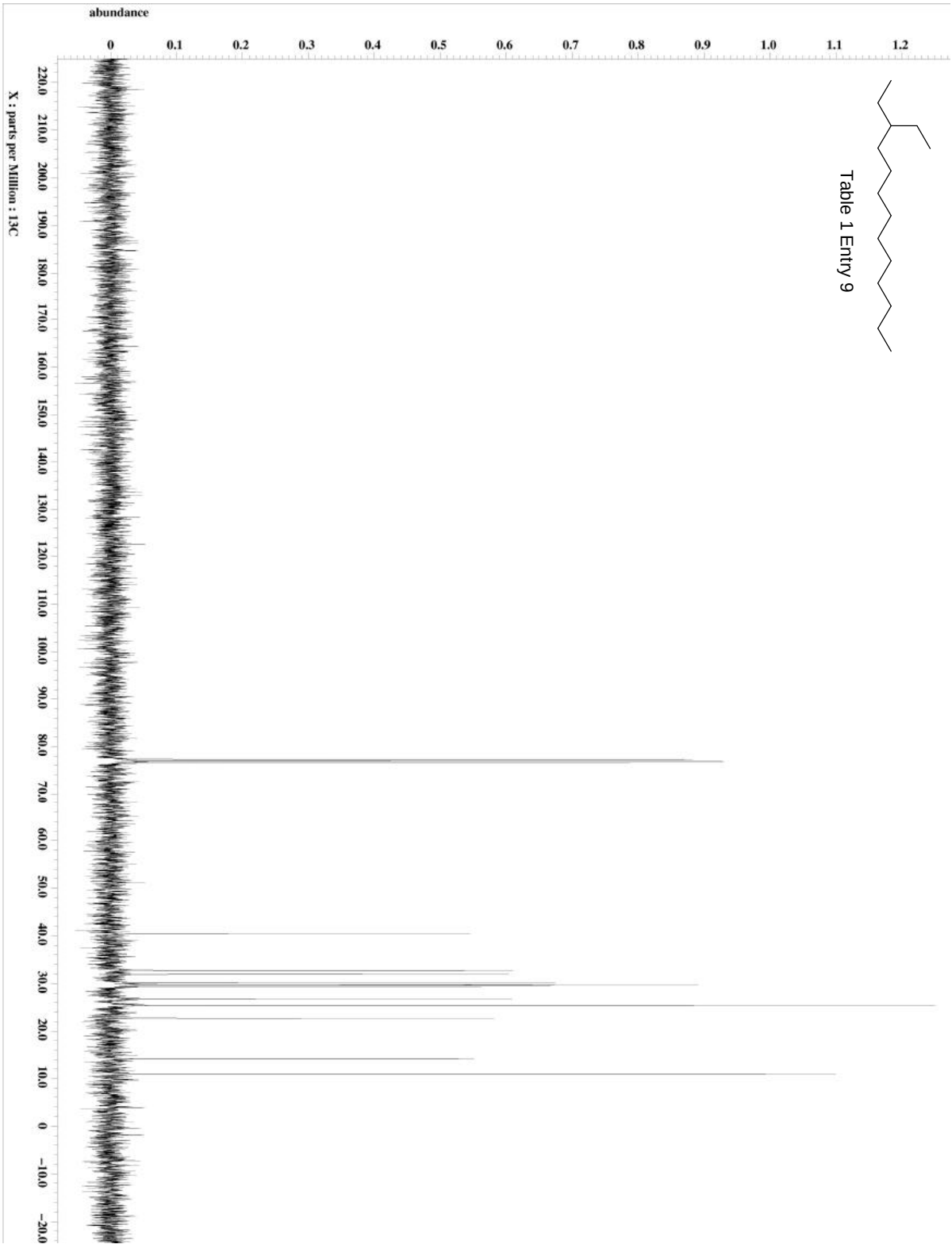
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1.1
1.2
X : parts per Million : 13C
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210.0
200.0
190.0
180.0
170.0
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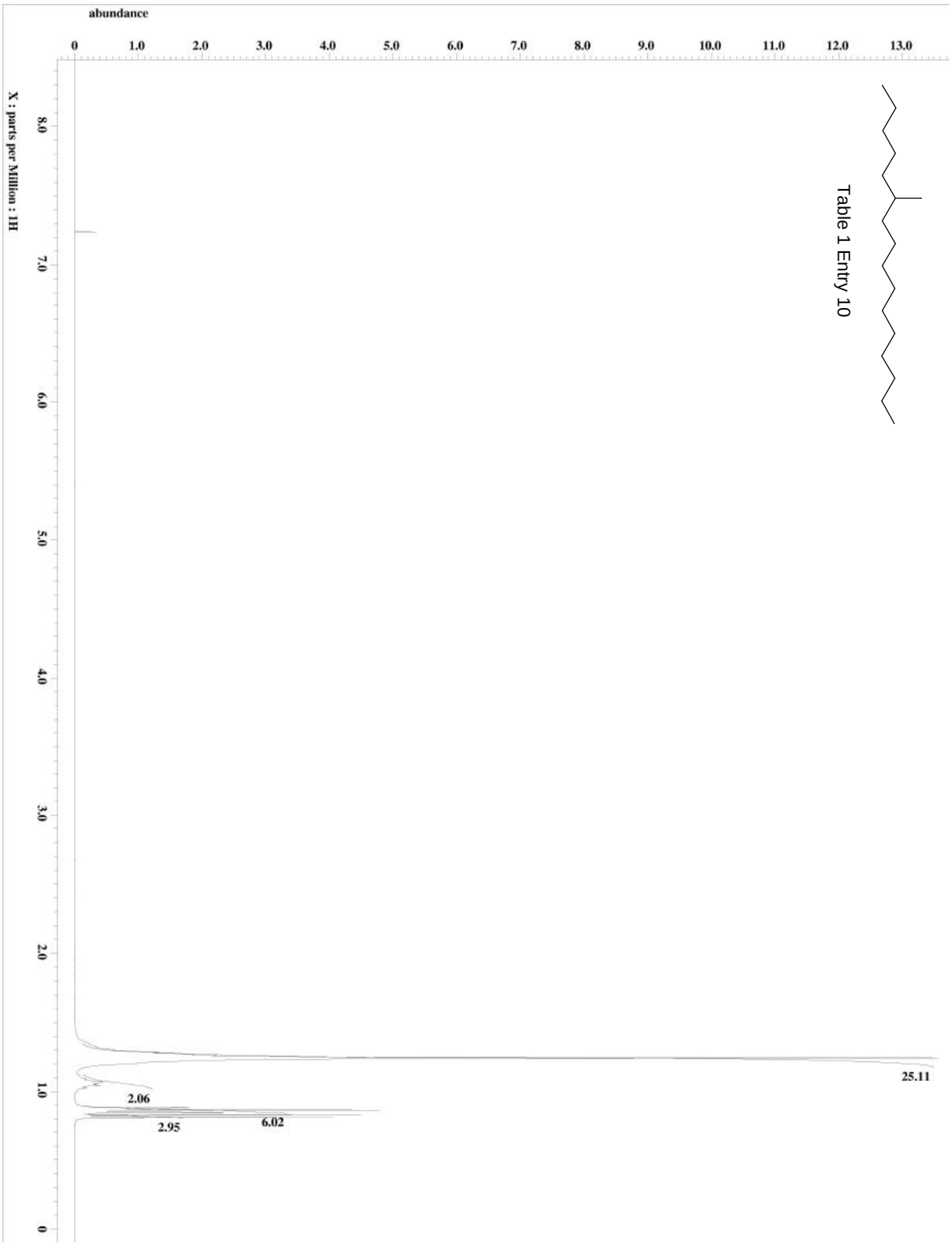
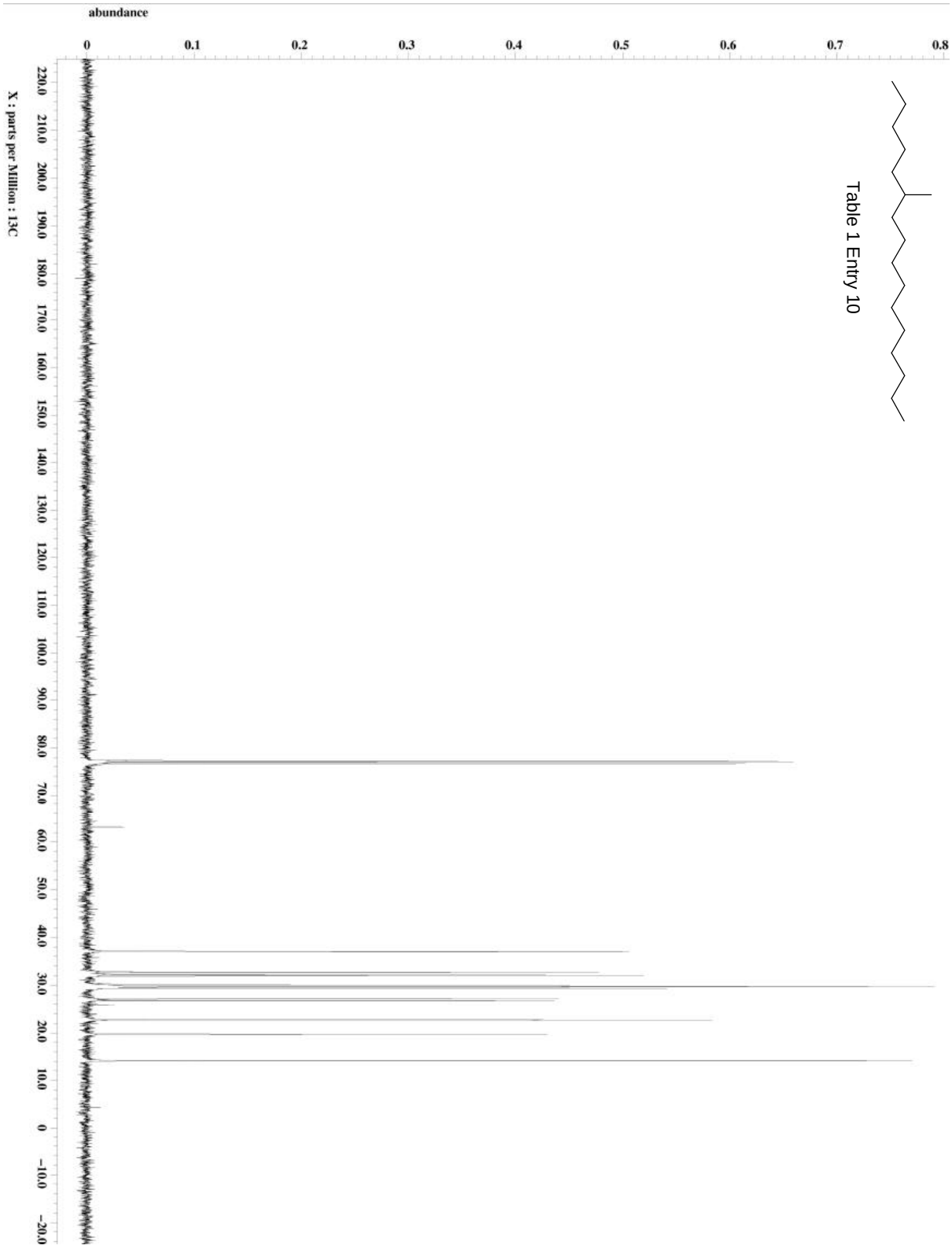
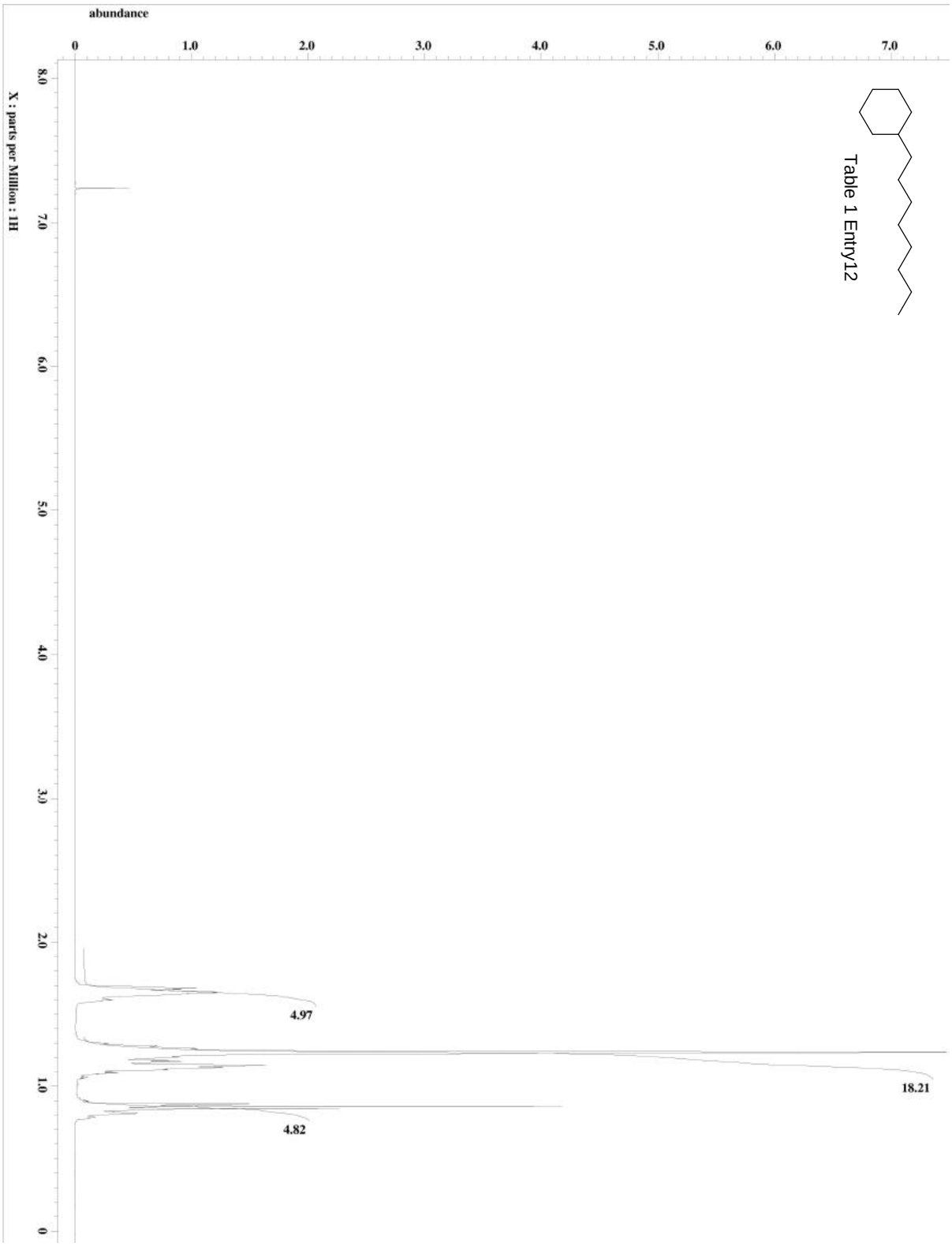
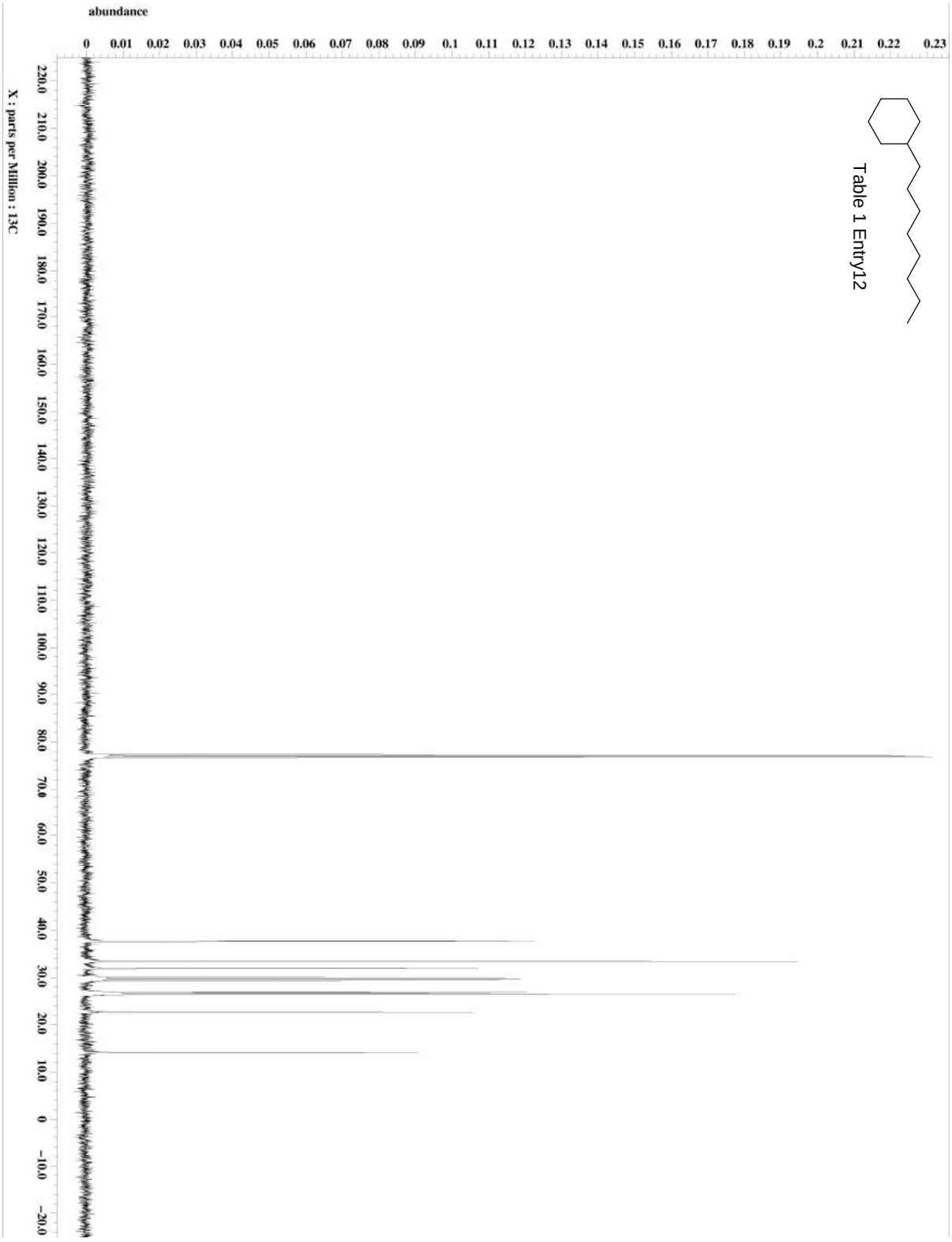
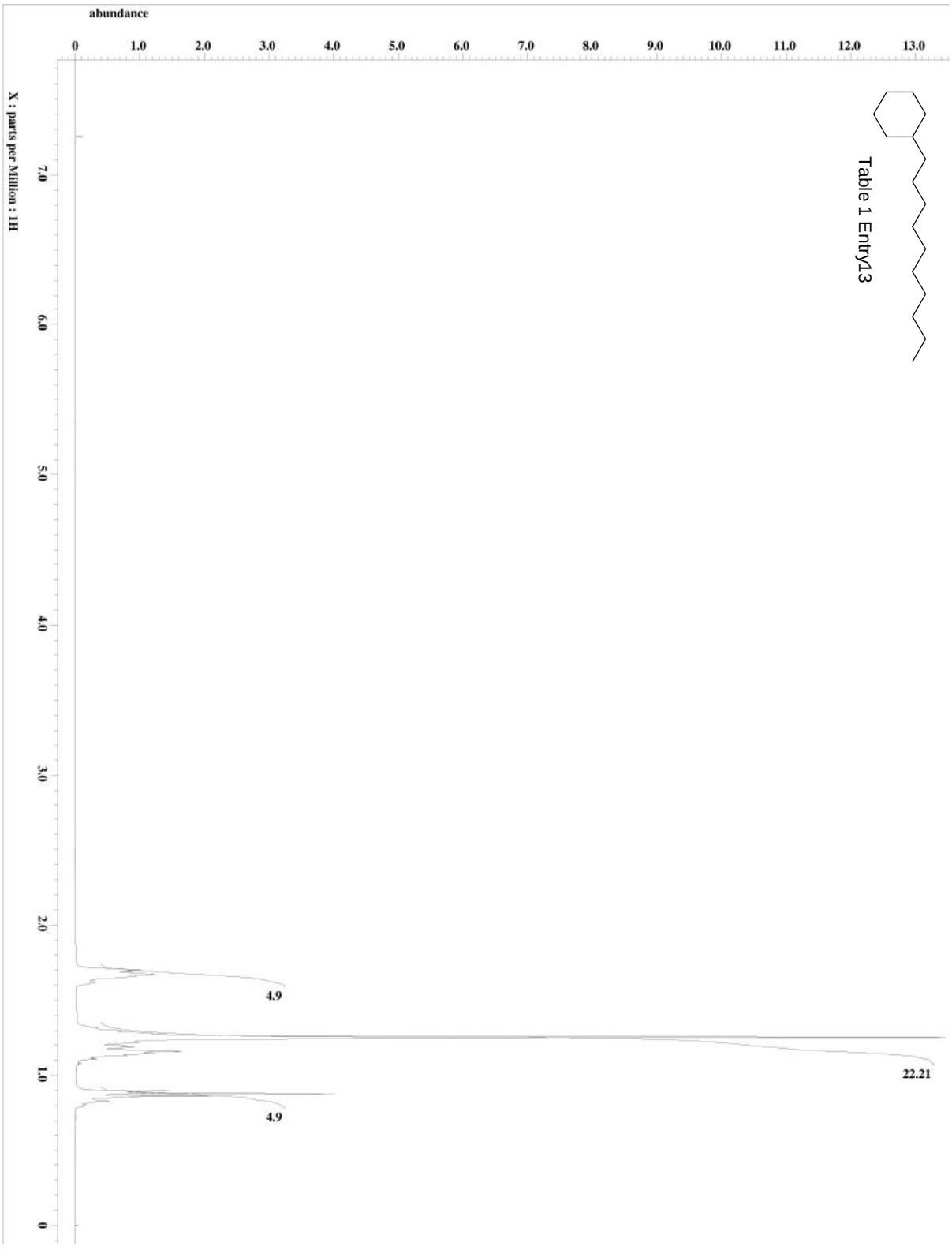
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
Table 1 Entry 9


abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
25.11
2.06
2.95
6.02
Table 1 Entry 10

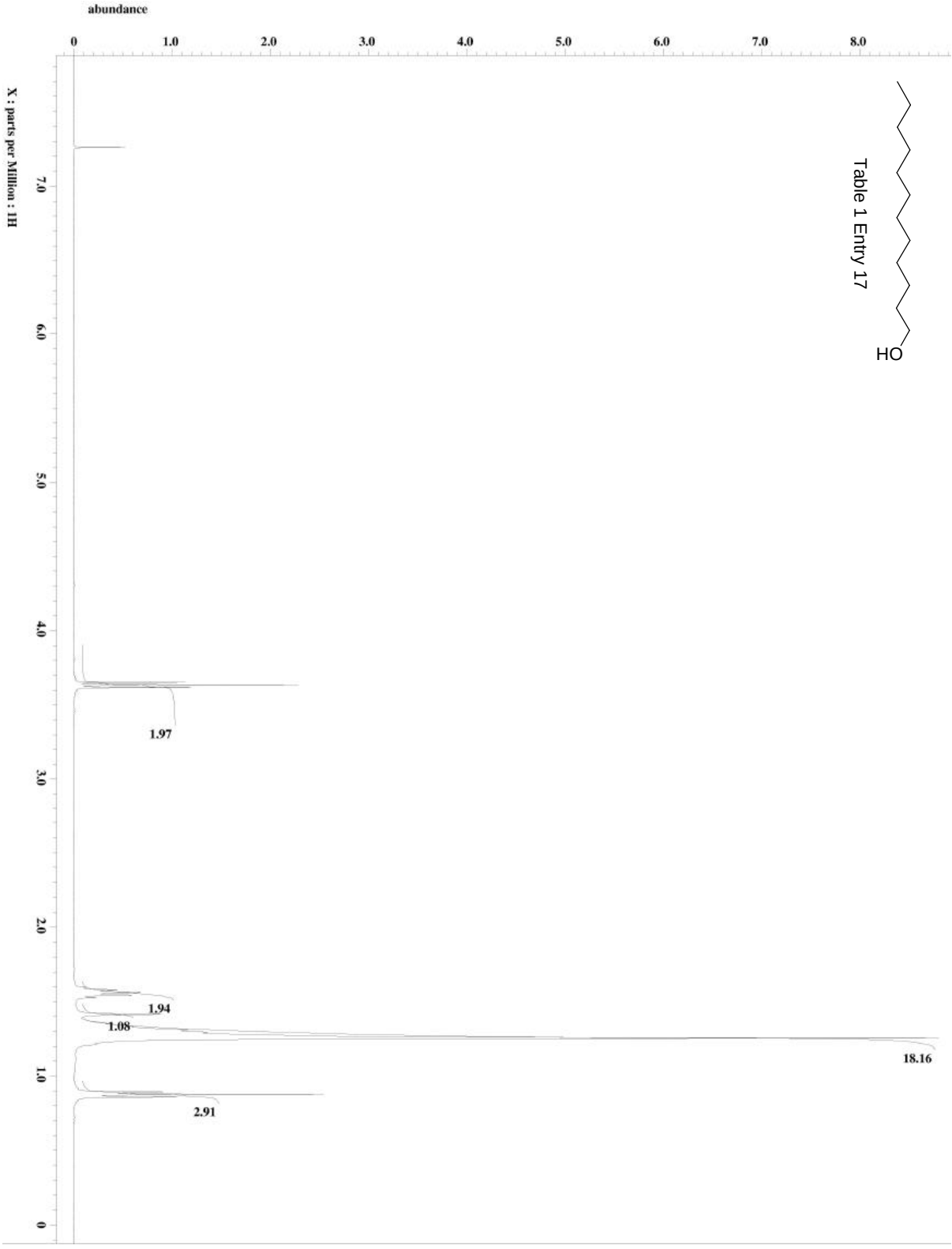

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
X : parts per Million : 13C
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
−20.0
Table 1 Entry 10

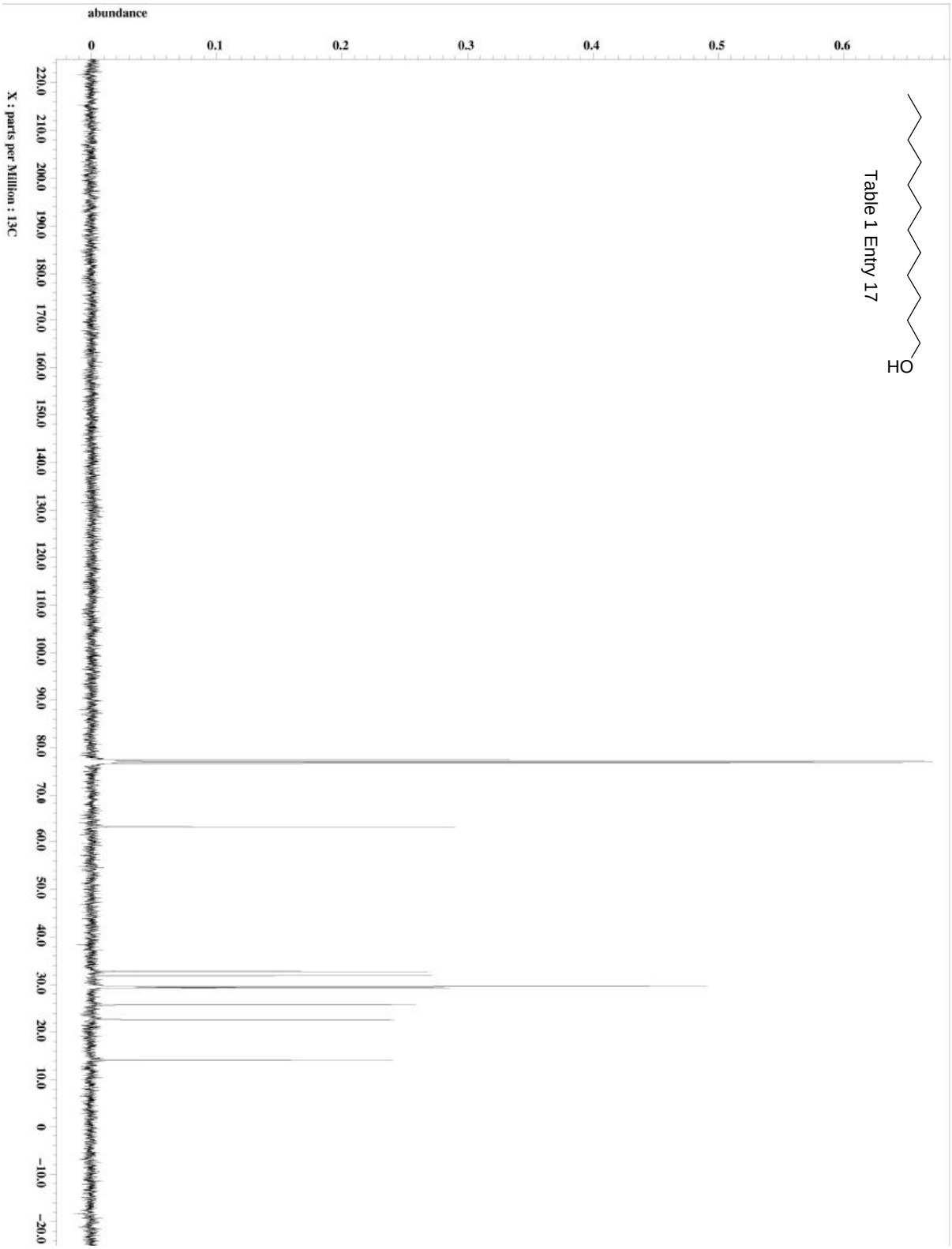

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
X : parts per Million : 1H
Table 1 Entry12
4.97
18.21
4.82

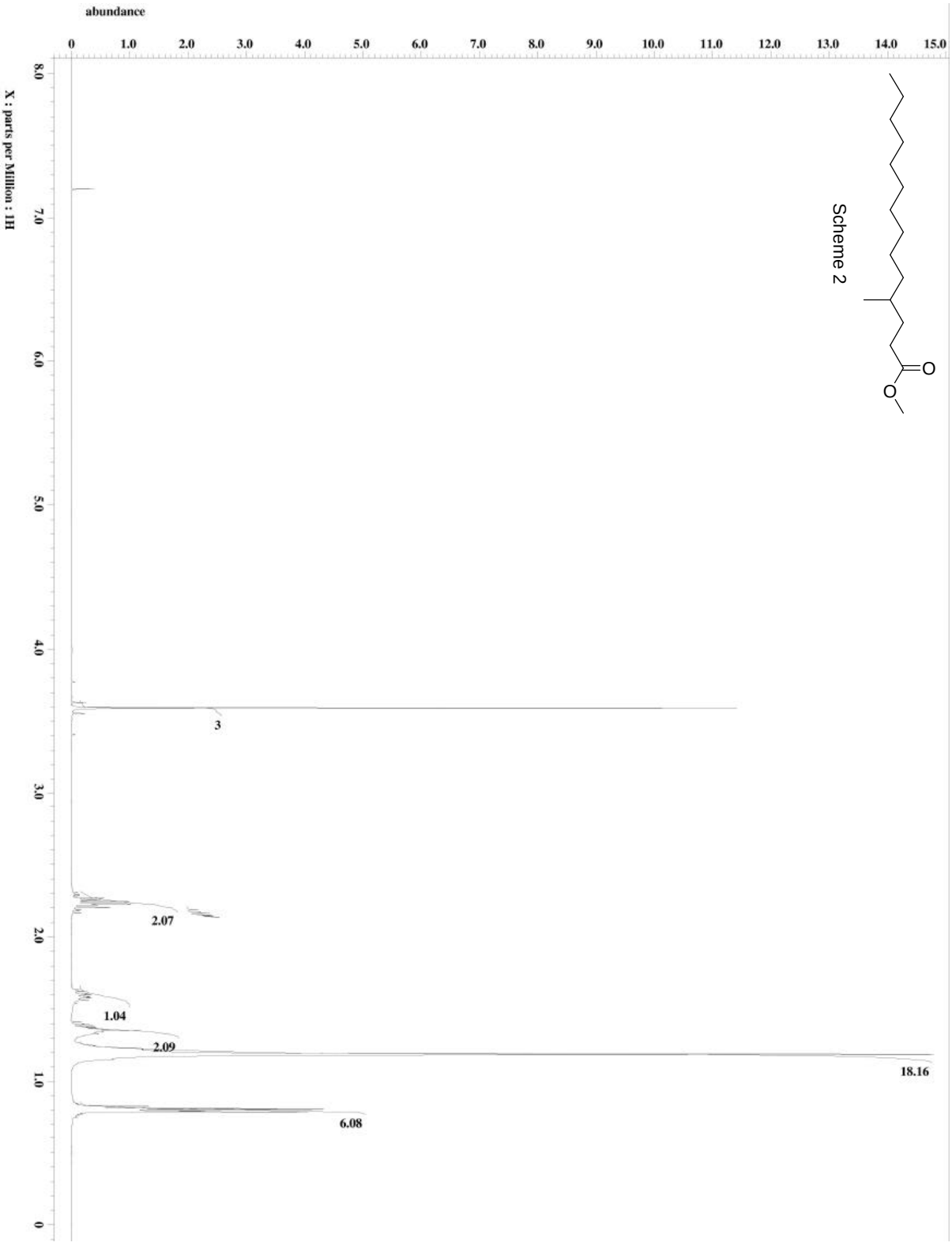

abundance
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17 0.18 0.19 0.2 0.21 0.22 0.23
X : parts per Million : 13C
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
Table 1 Entry12

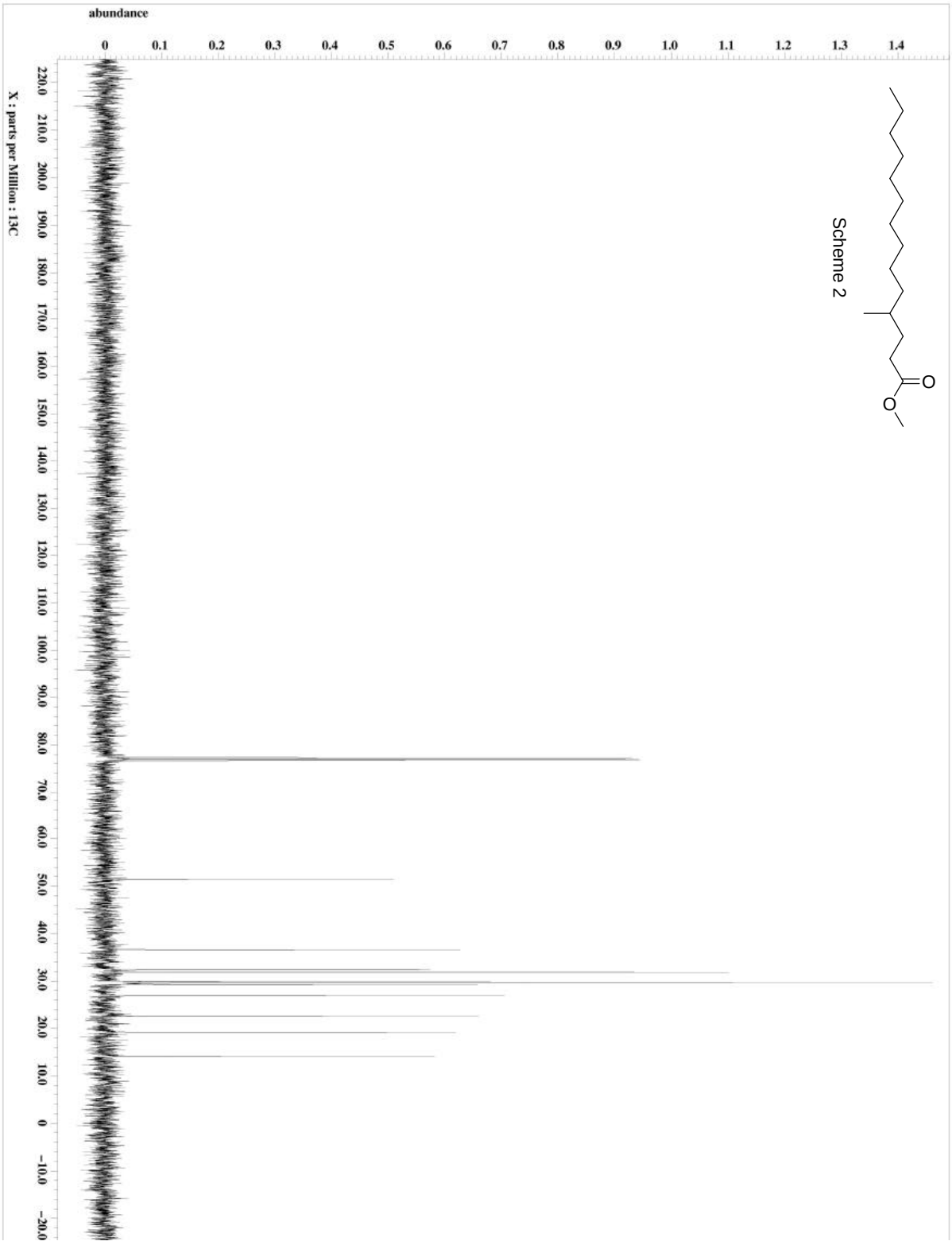

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
X : parts per Million : 1H
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
Table 1 Entry13
4.9
22.21
4.9

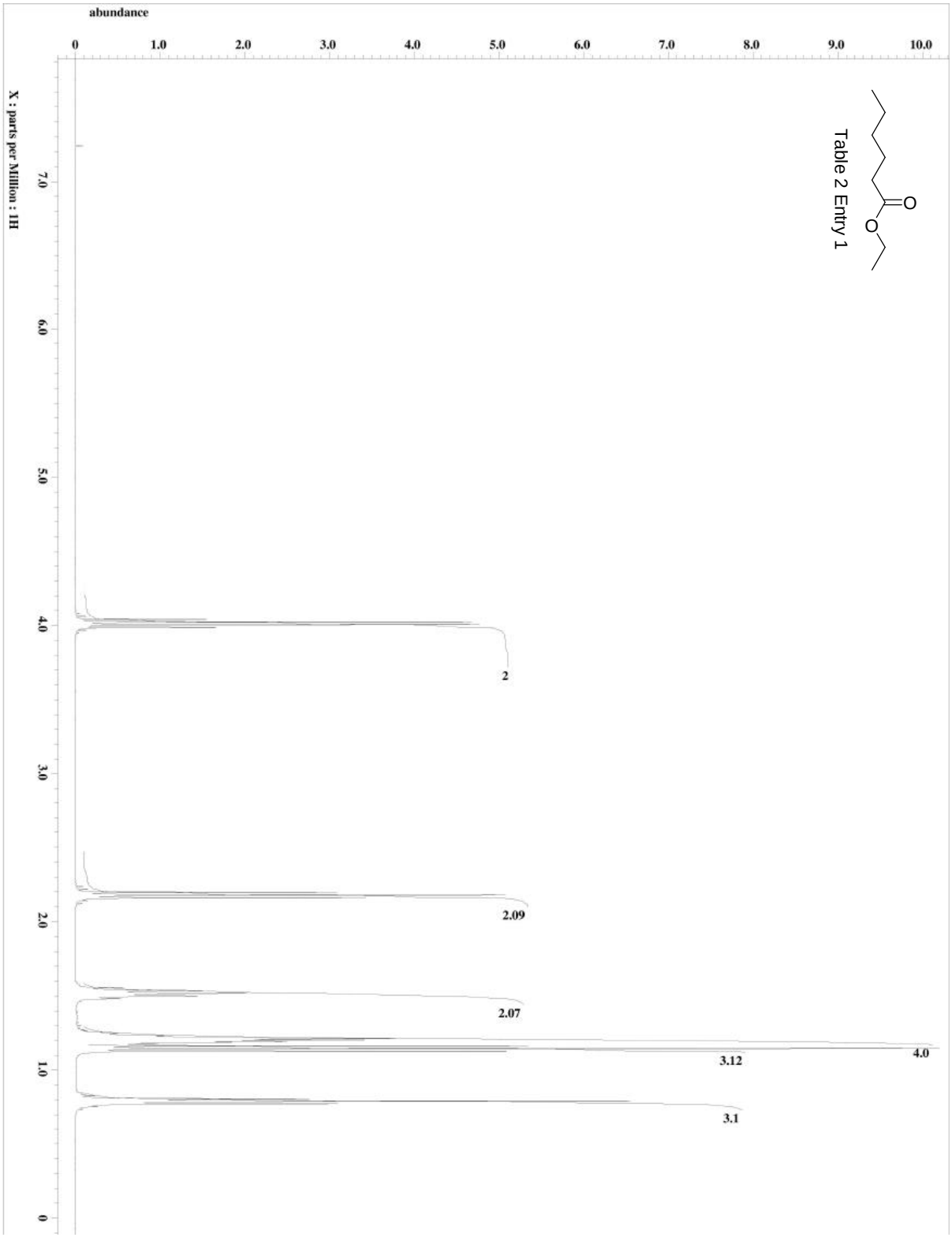

abundance
X : parts per Million : 13C
Table 1 Entry13

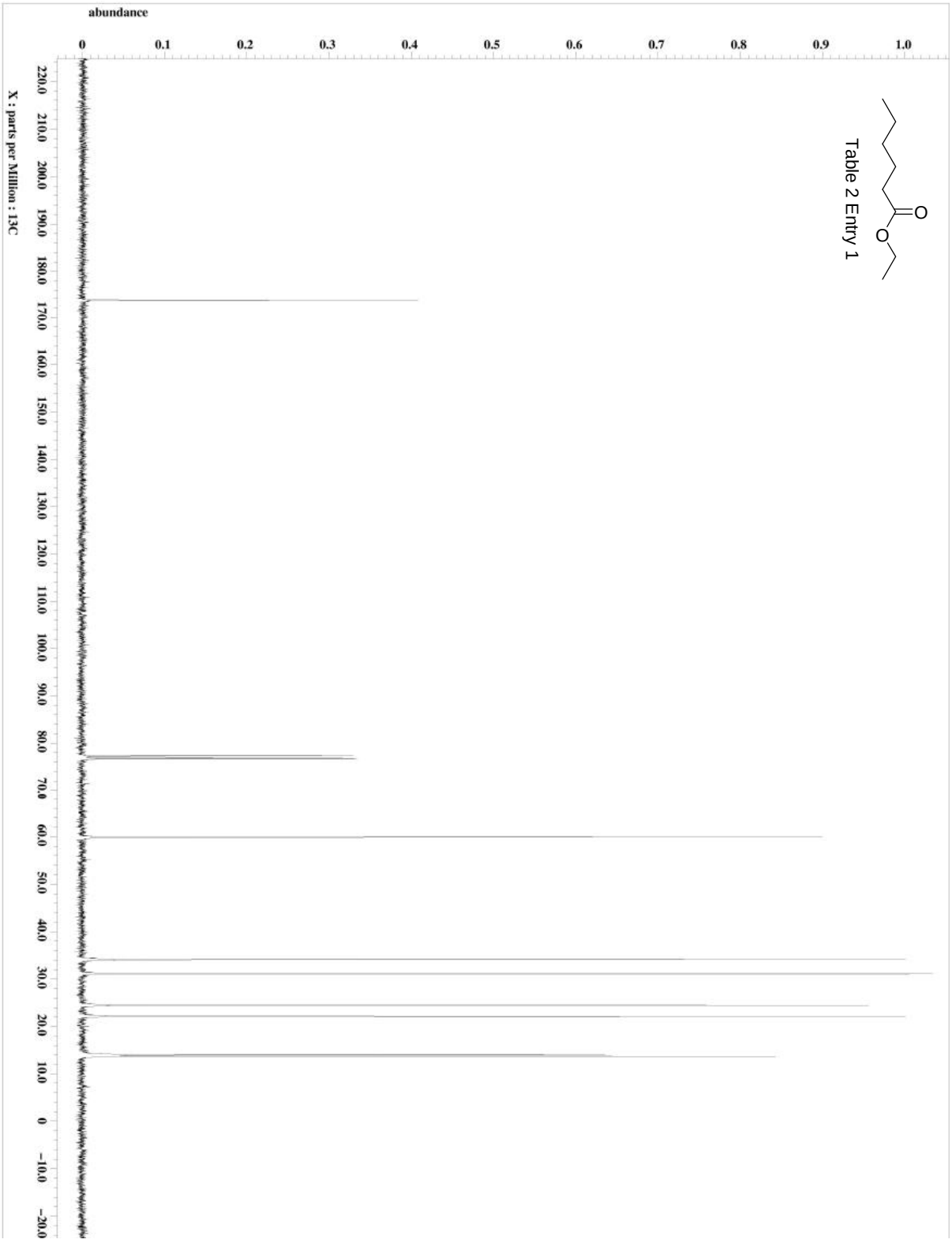

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
X : parts per Million : 1H
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.97
1.94
1.08
18.16
2.91
Table 1 Entry 17
HO

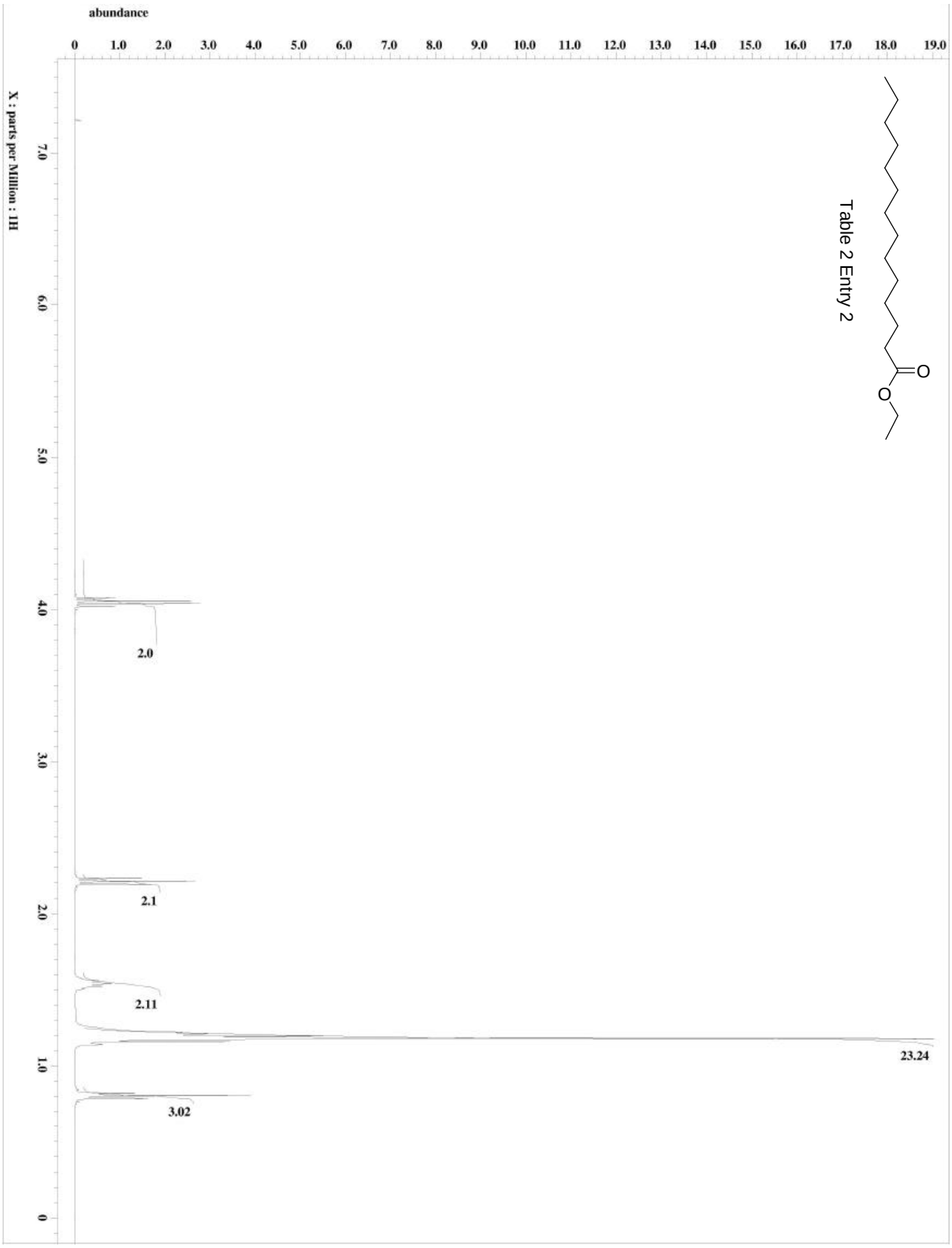

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
X : parts per Million : 13C
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
−20.0
Table 1 Entry 17
HO

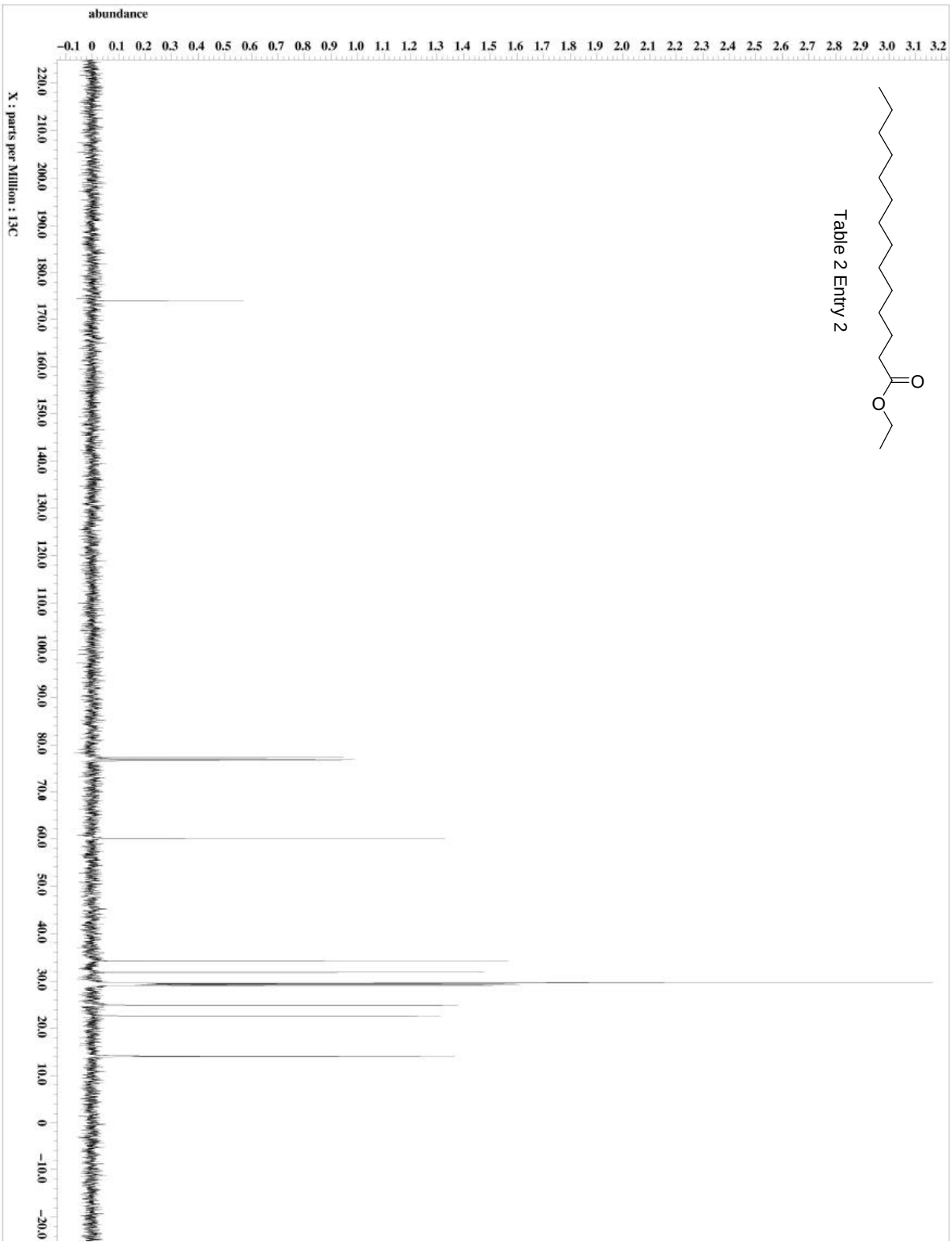

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
3
2.07
1.04
2.09
18.16
6.08
Scheme 2
O
O

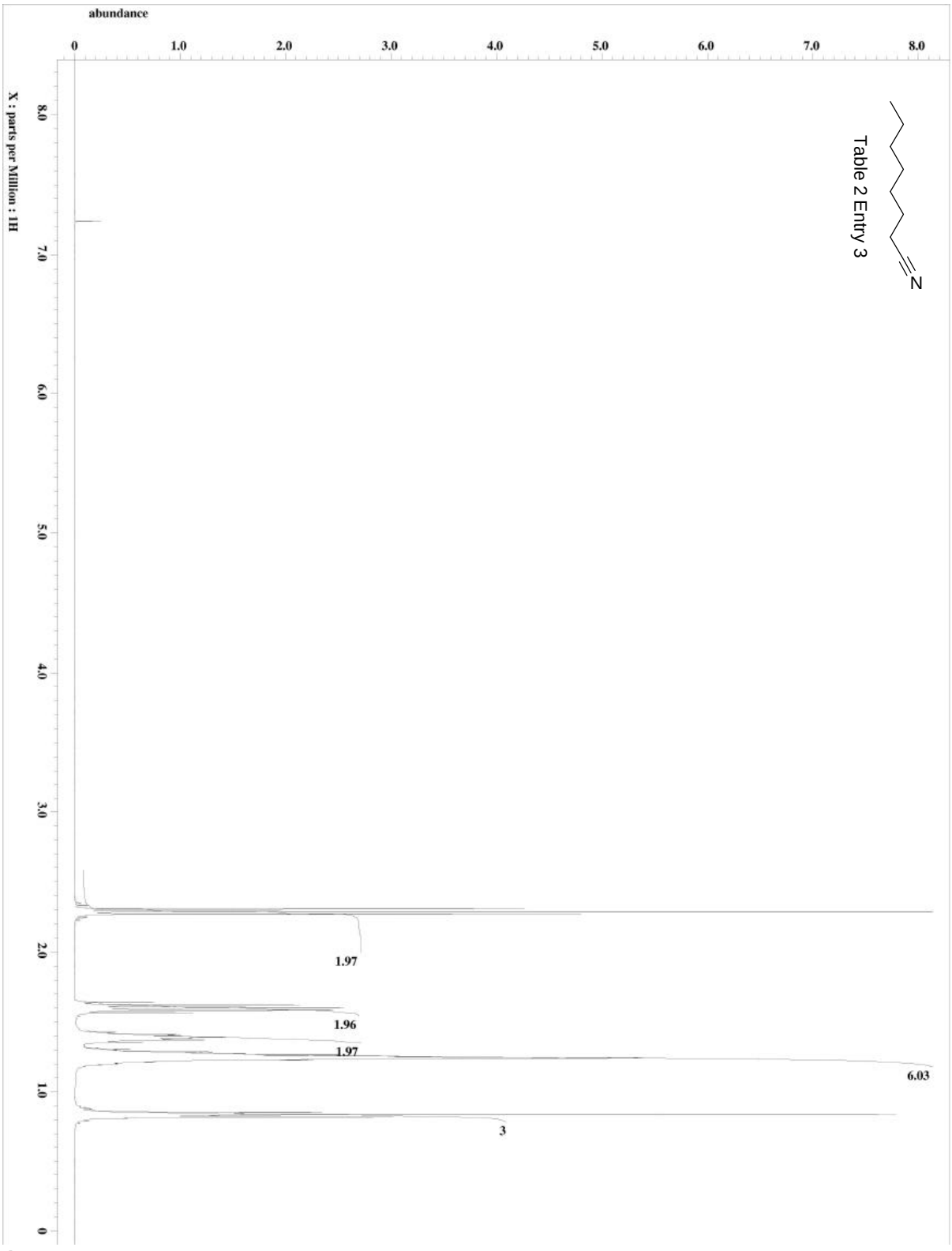

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
X : parts per Million : 13C
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
Scheme 2
O
O


abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
X : parts per Million : 1H
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
Table 2 Entry 1
O
O
2
2.09
2.07
3.12
4.0
3.1

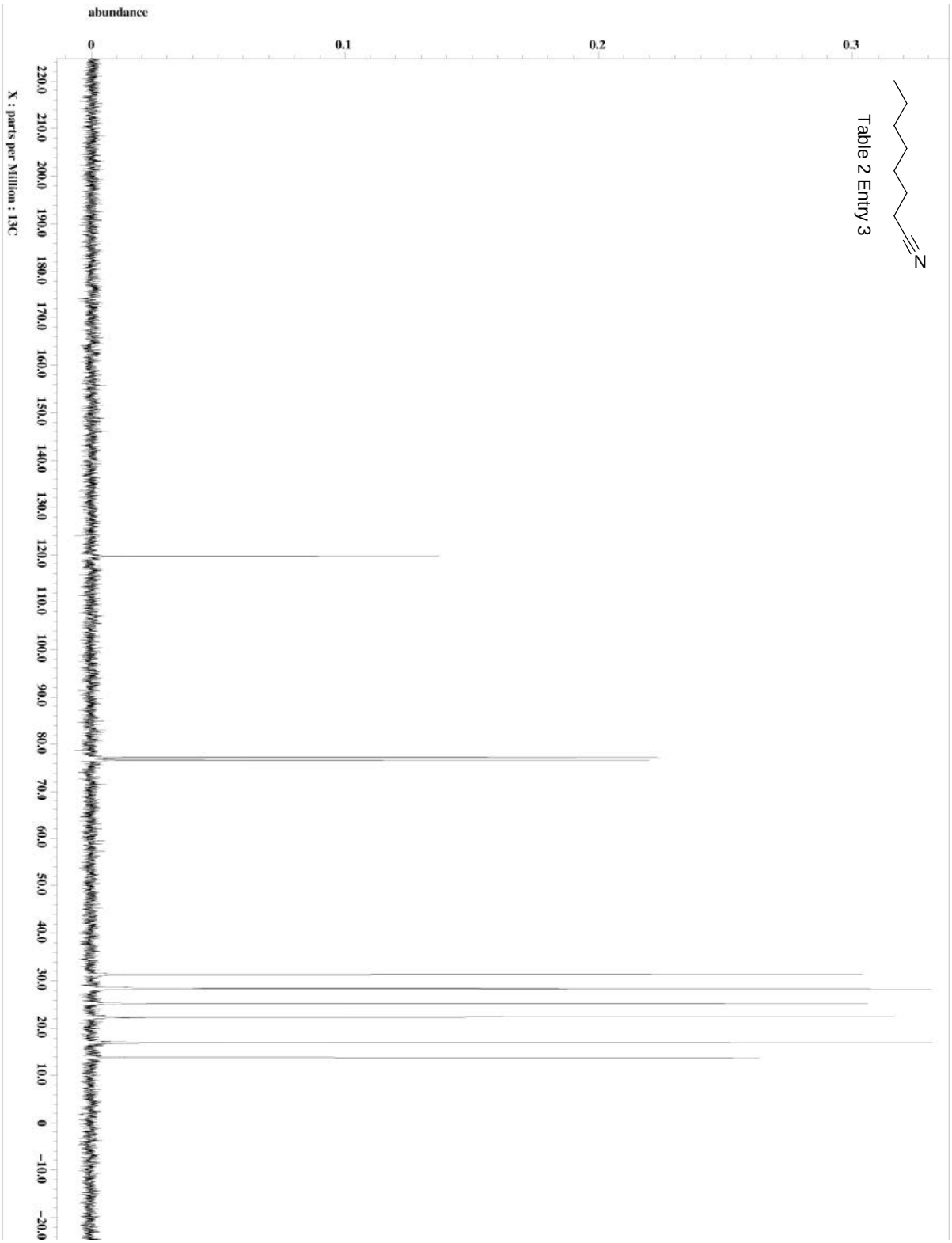

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
X : parts per Million : 13C
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
−20.0
Table 2 Entry 1
O
O

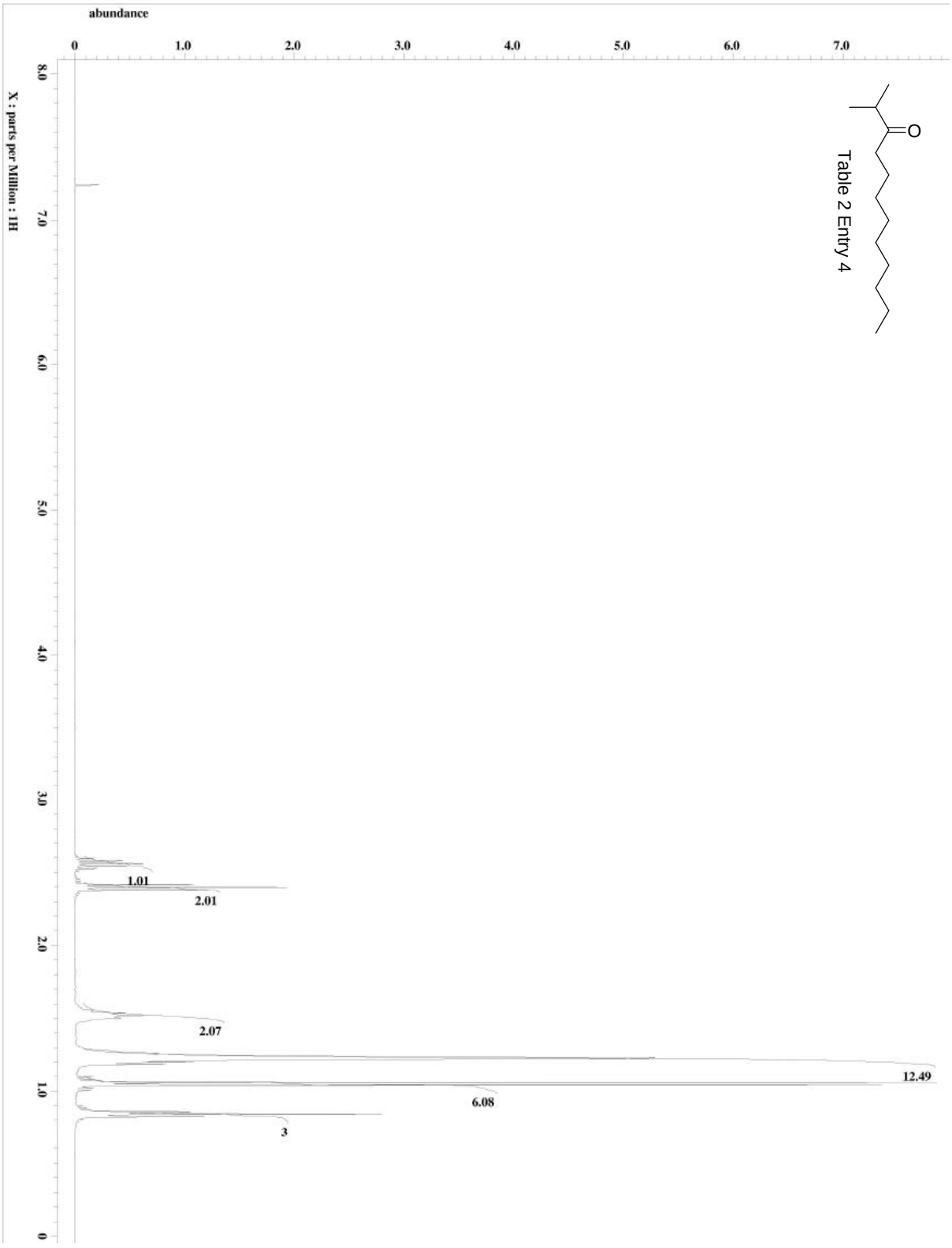

abundance
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0
X : parts per Million : 1H
7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
2.0
2.1
2.11
23.24
3.02
Table 2 Entry 2
O
O


abundance
X : parts per Million : 13C
Table 2 Entry 2
O
O


abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
X : parts per Million : 1H
Table 2 Entry 3
N
1.97
1.96
1.97
6.03
3

Équation 2


abundance
0
0.1
0.2
0.3
X : parts per Million : 13C
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0 −20.0
Table 2 Entry 3
N


abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
X : parts per Million : 1H
1.01
2.01
2.07
12.49
6.08
3
O
Table 2 Entry 4


abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
X : parts per Million : 13C
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
O
Table 2 Entry 4