Supporting Information

The Journal of Organic Chemistry

Selectivity Guidelines and a Reductive Elimination-Based Model for Predicting the Stereochemical Course of Conjugate Addition Reactions of Organocuprates to γ-Alkoxy-α,β-Enoates

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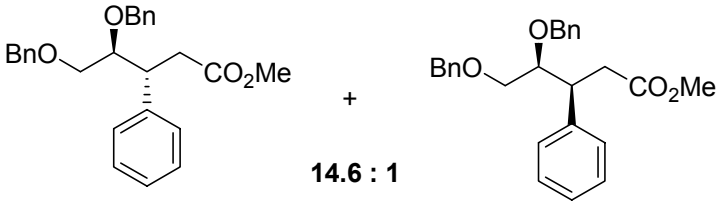
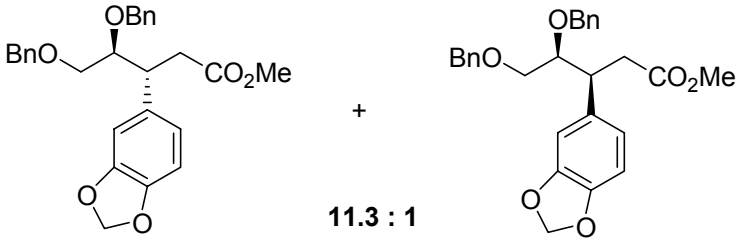
1. General Methods.

Unless otherwise noted all commercially obtained reagents were used without purification. THF was distilled from sodium-benzophenone ketyl prior to use. Dichloromethane and methanol were distilled from calcium hydride. Reactions were carried out under a nitrogen atmosphere in oven-dried glassware using standard syringe, cannula and septa techniques. Reactions were monitored by TLC (Silica Gel 60 F_{254}, 250 μm) and visualized with UV light and ceric ammonium molybdate solution. Flash chromatography was performed on silica gel (32-63 μm, 60 Å pore size).
Aryl bromides **d**[1] and **f**[2,3] were prepared as previously described.

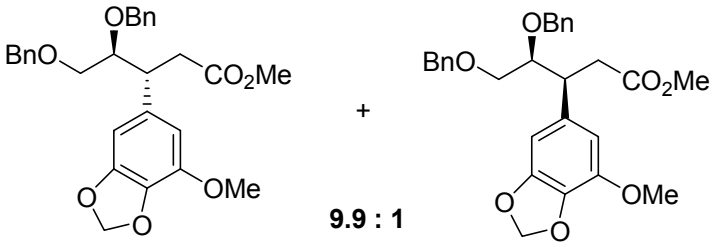
2. Characterization data for cuprate addition product mixtures



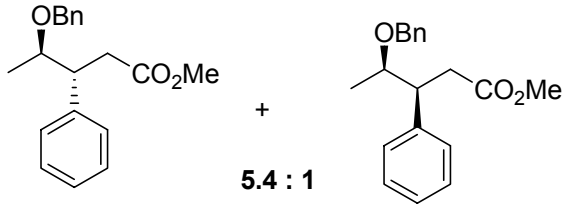
Epimeric mixture 14a: 94%; R_f 0.45 (30% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.55 – 7.15 (m, 15H), 4.80 (d, J = 11.6 Hz, 1H), 4.55 (d, J = 11.6 Hz, 1H), 4.44 (s, 2H), 3.81 – 3.73 (m, 1H), 3.58 – 3.47 (m, 1H), 3.50 (s, 3H), 3.36 (dd, J = 10.5, 5.2 Hz, 1H), 3.04 (dd, J = 16.0, 5.8 Hz, 1H), 2.64 (dd, J=16.0, 9.1 Hz, 1H); HRMS *m/z* (ESI) calcd for $C_{26}H_{28}O_4Na$ $(M+Na)^+$ 427.1879, found 427.1891.



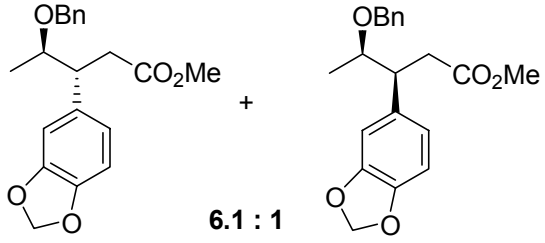
Epimeric mixture 14d: 76%; R_f 0.55 (30% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.63 – 7.15 (m, 10H), 6.68 – 5.59 (m, 3H), 5.92 (s, 2H), 4.75 (d, J = 11.6 Hz, 1H), 4.50 (d, J = 11.6 Hz, 1H), 4.42 (s, 2H), 3.78 – 3.30 (m, 4H), 3.50 (s, 3H), 2.96 (dd, J = 16.0, 5.2 Hz, 1H), 2.53 (dd, J = 16.0, 9.3 Hz, 1H); HRMS *m/z* (ESI) calcd for $C_{27}H_{28}O_6Na$ $(M+Na)^+$ 471.1778, found 471.1756.



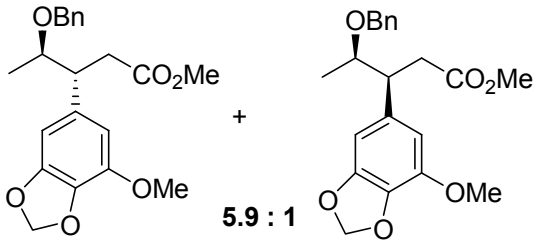
Epimeric mixture 14f: 88%; R_f 0.45 (30% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.51 – 7.25 (m, 10H), 6.66 (d, J = 8.5 Hz, 1H), 6.39 (s, 1H), 5.99 (s, 1H), 5.92 (s, 1H), 4.75 (d, J = 11.6 Hz, 1H), 4.50 (d, J = 11.6 Hz, 1H), 4.43 (s, 2H), 3.94 (s, 3H), 3.81 (s, 3H), 3.68 - 3.32 (m, 4H), 3.51 (s, 3H), 2.93 (dd, J = 16.0, 5.5 Hz, 1H), 2.54 (dd, J = 16.0, 9.4 Hz, 1H); HRMS *m/z* (ESI) calcd for $C_{28}H_{30}O_7Na$ $(M+Na)^+$ 501.1883, found 501.1906.



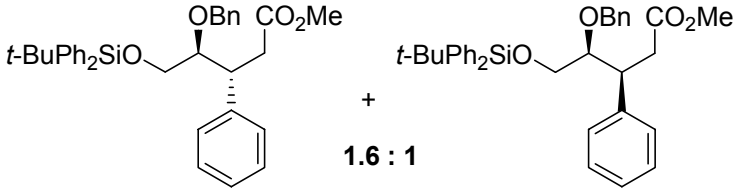
Epimeric mixture 15a: 89%; R_f 0.54 (30% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.50 – 7.19 (m, 10H), 4.65 (d, J = 11.6 Hz, 1H), 4.44 (d, J = 11.6 Hz, 1H), 3.69 – 3.62 (m, 1H), 3.48 (s, 3H), 3.35 – 3.23 (m, 1H), 3.06 (dd, J = 16.0, 6.0 Hz, 1H), 2.62 (dd, J = 16.0, 8.5 Hz, 1H), 1.07 (d, J = 6.0 Hz, 3H); HRMS *m/z* (ESI) calcd for $C_{19}H_{22}O_3Na$ $(M+Na)^+$ 321.1461, found 321.1452.



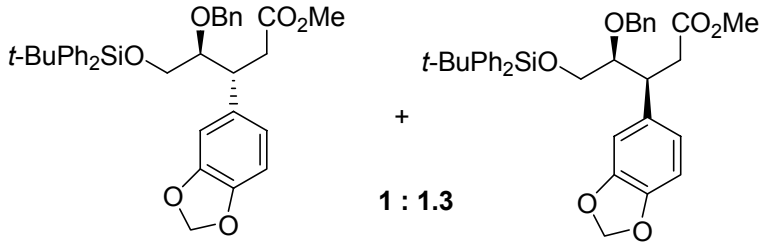
Epimeric mixture 15d: 80%; R_f 0.61 (30% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.60 – 7.20 (m, 5H), 6.90 – 6.55 (m, 3H), 5.92 (s, 2H), 4.62 (d, J = 11.6 Hz, 1H), 4.44 (d, J = 11.6 Hz, 1H), 3.65 - 3.35 (m, 1H), 3.49 (s, 3H), 3.20 – 3.08 (m, 1H), 2.90 (dd, J = 16.0, 5.8 Hz, 1H), 2.51 (dd, J = 16.0, 8.8 Hz, 1H), 1.05 (d, J = 6.0 Hz, 3H); HRMS *m/z* (ESI) calcd for $C_{20}H_{22}O_5Na$ $(M+Na)^+$ 365.1359, found 365.1364.



Epimeric mixture 15f: 82%; R_f 0.46 (30% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.62 – 7.21 (m, 5H), 6.66 (d, J = 8.0 Hz, 1H), 6.37 (s, 1H), 5.92 (s, 2H), 4.62 (d, J = 11.6 Hz, 1H), 4.39 (d, J = 11.6 Hz, 1H), 3.85 (s, 3H), 3.63 – 3.35 (m, 1H), 3.49 (s, 3H), 3.19 – 3.08 (m, 1H), 2.97 (dd, J = 16.0, 6.0 Hz, 1H), 2.52 (dd, J = 16.0, 8.5 Hz, 1H), 1.06 (d, J = 6.0 Hz, 3H); HRMS *m/z* (ESI) calcd for $C_{21}H_{24}O_6Na$ $(M+Na)^+$ 395.1465, found 395.1462.

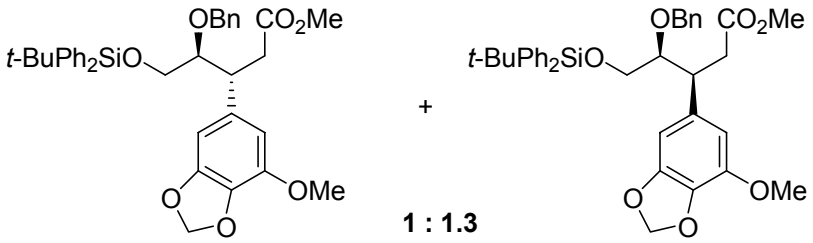


Epimeric mixture 16a: 87%; R_f 0.35 (15% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.69 – 7.57 (m, 5H), 7.47 – 7.22 (m, 15H), 4.67 (d, J = 11.6 Hz, 1H), 4.39 (d, J = 11.6 Hz, 1H), 3.72 - 3.46 (m, 4H), 3.46 (s, 3H), 2.98 (dd, J = 16.0, 5.0 Hz, 1H), 2.62 (dd, J = 16.0, 8.8 Hz, 1H), 1.04 (s, 9H); selected ^{1}H NMR ($CDCl_3$) data for the *syn*-isomer δ 7.69 – 7.57 (m, 5H), 7.47 – 7.22 (m, 15H), 4.57 (d, J = 11.8 Hz, 1H), 4.35 (d, J = 11.8 Hz, 1H), 3.72 - 3.46 (m, 4H), 3.55 (s, 3H), 2.86 (dd, J = 16.0, 7.2 Hz, 1H), 2.72 (dd, J = 16.0, 8.0 Hz, 1H), 1.05 (s, 9H).

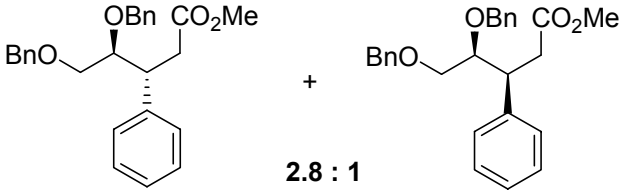


Epimeric mixture 16d: 69%; R_f 0.4 (15% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.67 – 7.50 (m, 5H), 7.47 – 7.17 (m, 10H), 6.69 (d, J = 8.0 Hz, 3H), 5.92 (s, 2H), 4.67 (d, J = 11.6 Hz, 1H), 4.39 (d, J = 11.6 Hz, 1H), 3.72 - 3.39 (m, 4H), 3.46 (s, 3H), 2.93 (dd, J = 16.0, 5.0 Hz, 1H), 2.54 (dd, J = 16.0, 9.4 Hz, 1H), 1.04 (s, 9H); selected ^{1}H NMR ($CDCl_3$) data for the *syn*-isomer δ 7.69 – 7.57 (m, 5H), 7.47 – 7.22 (m, 15H), 6.67 (d, J = 8.0 Hz,

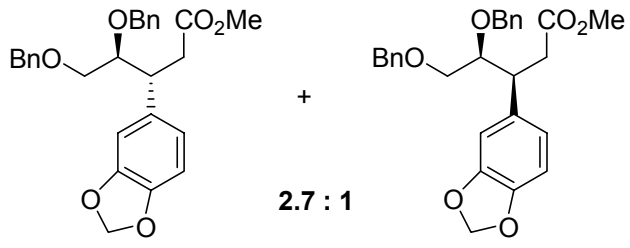
3H), 5.90 (s, 2H), 4.57 (d, J = 11.8 Hz, 1H), 4.34 (d, J = 11.8 Hz, 1H), 3.72 - 3.46 (m, 4H), 3.56 (s, 3H), 2.77 (dd, J = 16.0, 6.9 Hz, 1H), 2.66 (dd, J = 16.0, 8.3 Hz, 1H), 1.05 (s, 9H).



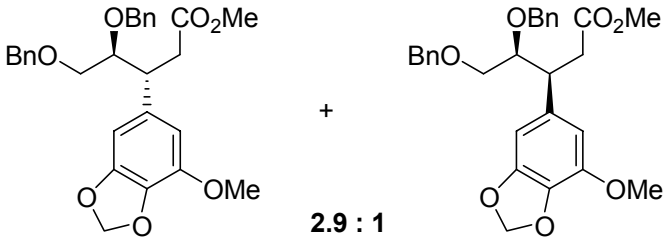
Epimeric mixture 16f: 53%; R_f 0.6 (30% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.65 – 7.50 (m, 5H), 7.45 – 7.20 (m, 10H), 6.45 (m, 2H), 5.95 (s, 2H), 4.67 (d, J = 11.6 Hz, 1H), 4.39 (d, J = 11.6 Hz, 1H), 3.79 (s, 3H), 3.72 - 3.45 (m, 4H), 3.47 (s, 3H), 2.93 (dd, J = 16.0, 5.3 Hz, 1H), 2.52 (dd, J = 16.0, 9.5 Hz, 1H), 1.05 (s, 9H); selected ^{1}H NMR ($CDCl_3$) data for the *syn*-isomer δ 7.65 – 7.5 (m, 5H), 7.45 – 7.20 (m, 10H), 6.39 (s, 2H), 5.92 (s, 2H), 4.60 (d, J = 11.8 Hz, 1H), 4.36 (d, J = 11.8 Hz, 1H), 3.87 (s, 3H), 3.80 - 3.40 (m, 4H), 3.52 (s, 3H), 2.77 (dd, J = 16.0, 6.9 Hz, 1H), 2.66 (dd, J = 16.0, 8.3 Hz, 1H), 1.04 (s, 9H).



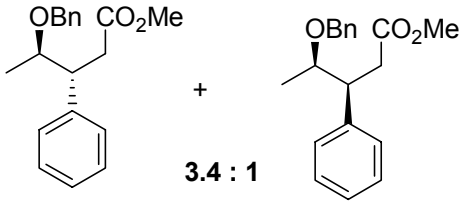
Epimeric mixture 17a: 72%; R_f 0.45 (30% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.55 – 7.15 (m, 15H), 4.80 (d, J = 11.6 Hz, 1H), 4.55 (d, J = 11.6 Hz, 1H), 4.44 (s, 2H), 3.81 – 3.73 (m, 1H), 3.58 – 3.47 (m, 1H), 3.50 (s, 3H), 3.36 (dd, J = 10.5, 5.2 Hz, 1H), 3.04 (dd, J = 16.0, 5.8 Hz, 1H), 2.64 (dd, J=16.0, 9.1 Hz, 1H); selected ^{1}H NMR ($CDCl_3$) data for the *syn*-isomer δ 7.55 – 7.15 (m, 15H), 4.76 (d, J = 11.8 Hz, 1H), 4.57 (d, J = 11.8 Hz, 1H), 4.47 (s, 2H), 3.94 – 3.89 (m, 1H), 3.70 – 3.41 (m, 2H), 3.57 (s, 3H), 2.91 (dd, J = 16.0, 6.9 Hz, 1H), 2.79 (dd, J=16.0, 8.3 Hz, 1H).



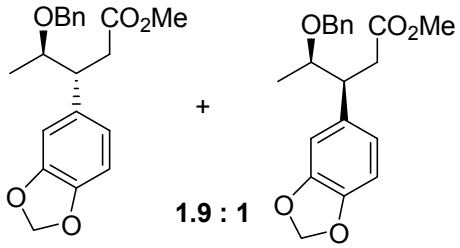
Epimeric mixture 17d: 68%; R_f 0.55 (30% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.63 – 7.15 (m, 10H), 6.67 – 5.59 (m, 3H), 5.89 (s, 2H), 4.75 (d, J = 11.6 Hz, 1H), 4.50 (d, J = 11.6 Hz, 1H), 4.43 (s, 2H), 3.78 – 3.30 (m, 4H), 3.50 (s, 3H), 2.96 (dd, J = 16.0, 5.2 Hz, 1H), 2.53 (dd, J = 16.0, 9.3 Hz, 1H); selected ^{1}H NMR ($CDCl_3$) data for the *syn*-isomer δ 7.63 – 7.15 (m, 10H), 6.67 – 5.59 (m, 3H), 5.91 (s, 2H), 4.72 (d, J = 11.8 Hz, 1H), 4.51 d, J = 11.8 Hz, 1H), 4.44 (s, 2H), 3.87 – 3.79 (m, 1H), 3.78–3.30 (m, 3H), 3.56 (s, 3H), 2.78 (dd, J = 16.0, 6.6 Hz, 1H), 2.69 (dd, J = 16.0, 8.5 Hz, 1H).



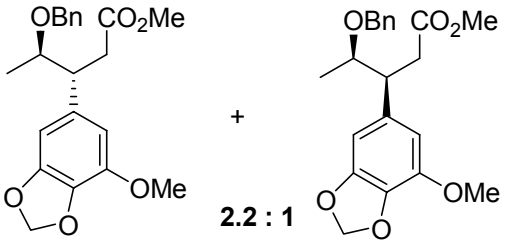
Epimeric mixture 17f: 63%; R_f 0.45 (30% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.45 – 7.20 (m, 10H), 6.45 (d, J = 8.5 Hz, 1H), 6.39 (s, 1H), 5.99 (s, 1H), 5.92 (s, 1H), 4.75 (d, J = 11.6 Hz, 1H), 4.50 (d, J = 11.6 Hz, 1H), 4.43 (s, 2H), 2.94 (dd, J = 16.0, 5.5 Hz, 1H), 2.54 (dd, J = 16.0, 9.4 Hz, 1H); selected ^{1}H NMR ($CDCl_3$) data for the *syn*-isomer δ 7.51 – 7.25 (m, 10H), 6.45 (d, J = 8.5 Hz, 1H), 6.39 (s, 1H), 5.99 (s, 1H), 5.92 (s, 1H), 4.43 (s, 2H), 3.94 (s, 3H), 3.81 (s, 3H), 3.68 – 3.32 (m, 4H), 3.51 (s, 3H), 2.93 (dd, J = 16.0, 6.9 Hz, 1H), 2.54 (dd, J = 16.0, 8.5 Hz, 1H).



Epimeric mixture 18a: 65%; R_f 0.54 (30% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.50 – 7.19 (m, 10H), 4.65 (d, J = 11.6 Hz, 1H), 4.44 (d, J = 11.6 Hz, 1H), 3.69 – 3.62 (m, 1H), 3.48 (s, 3H), 3.35 – 3.23 (m, 1H), 3.06 (dd, J = 16.0, 6.0 Hz, 1H), 2.62 (dd, J = 16.0, 8.5 Hz, 1H), 1.07 (d, J = 6.0 Hz, 3H); selected ^{1}H NMR ($CDCl_3$) data for the *syn*-isomer δ 7.50 – 7.19 (m, 10H), 4.60 (d, J = 11.8 Hz, 1H), 4.46 (d, J = 11.8 Hz, 1H), 3.82 – 3.74 (m, 1H), 3.57 (s, 3H), 3.45 – 3.39 (m, 1H), 2.93 (dd, J = 16.0, 6.6 Hz, 1H), 2.78 (dd, J = 16.0, 8.5 Hz, 1H), 1.06 (d, J = 6.3 Hz, 3H).



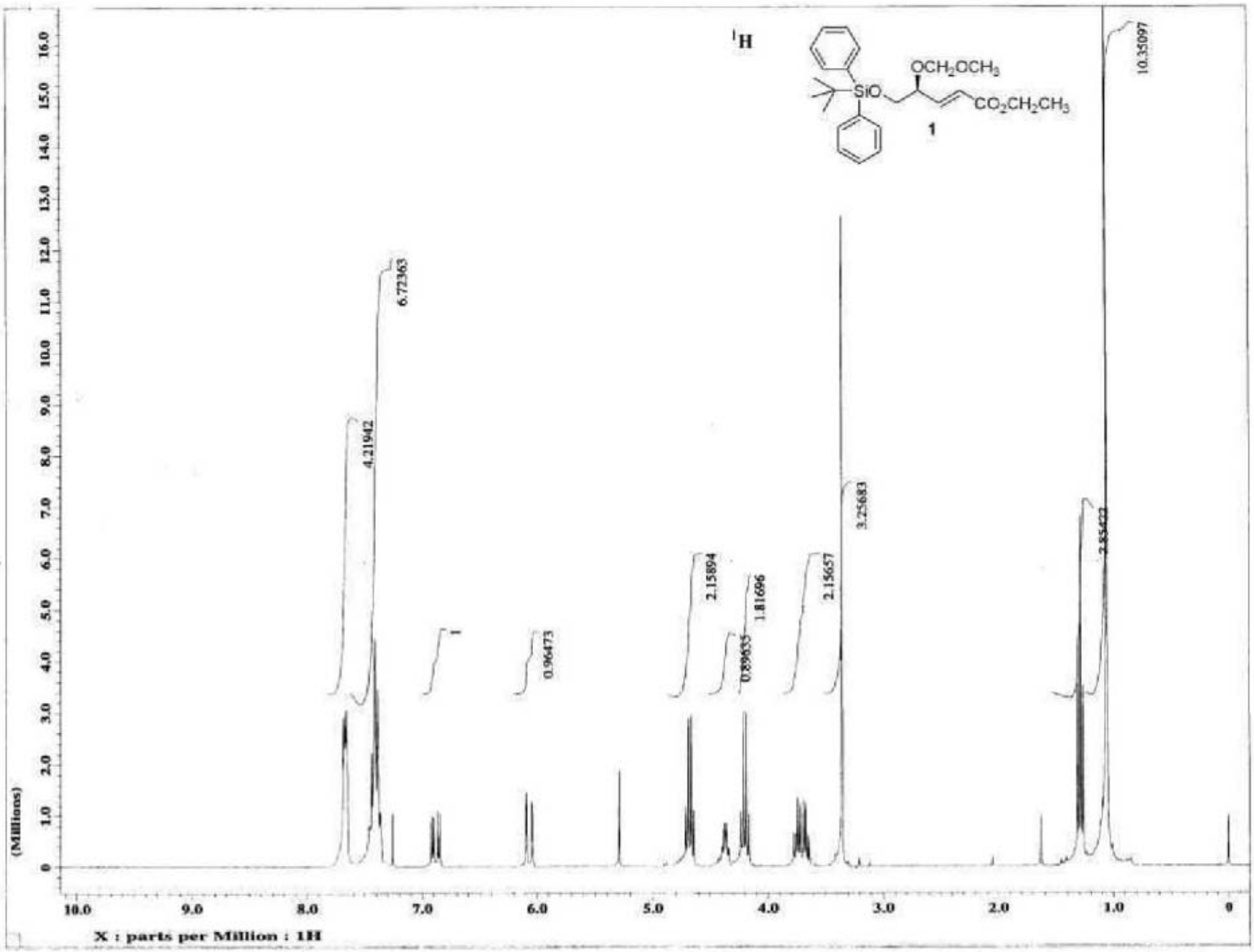
Epimeric mixture 18d: 56%; R_f 0.61 (30% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.50 – 7.20 (m, 5H), 6.90 – 6.60 (m, 3H), 5.91 (s, 2H), 4.62 (d, J = 11.6 Hz, 1H), 4.41 (d, J = 11.6 Hz, 1H), 3.69 – 3.41 (m, 1H), 3.49 (s, 3H), 3.20 – 3.08 (m, 1H), 2.95 (dd, J = 16.0, 5.8 Hz, 1H), 2.52 (dd, J = 16.0, 8.8 Hz, 1H), 1.05 (d, J = 6.0 Hz, 3H); selected ^{1}H NMR ($CDCl_3$) data for the *syn*-isomer δ 7.50 - 7.20 (m, 5H), 6.90 – 6.60 (m, 3H), 5.91 (s, 2H), 4.60 (d, J = 11.8 Hz, 1H), 4.42 (d, J = 11.8 Hz, 1H), 3.84 (s, 3H), 3.80 – 3.67 (m, 1H), 3.59 (s, 3H), 3.32 – 3.21 (m, 1H), 2.84 (dd, J = 16.0, 6.3 Hz, 1H), 2.69 (dd, J = 16.0, 8.8 Hz, 1H), 1.05 (d, J = 6.3 Hz, 3H).



Epimeric mixture 18f: 54%; R_f 0.46 (30% EtOAc/hexanes); selected ^{1}H NMR ($CDCl_3$) data for the *anti*-isomer δ 7.45 – 7.21 (m, 5H), 6.45 (d, J = 8.0 Hz, 1H), 6.37 (s, 1H), 5.92 (s, 2H), 4.59 (d, J = 11.6 Hz, 1H), 4.41 (d, J = 11.6 Hz, 1H), 3.85 (s, 3H), 3.65 – 3.47 (m, 1H), 3.49 (s, 3H), 3.15 – 3.08 (m, 1H), 2.97 (dd, J = 16.0, 5.8 Hz, 1H), 2.52 (dd, J = 16.0, 8.5 Hz, 1H), 1.07 (d, J = 6.0 Hz, 3H); selected ^{1}H NMR ($CDCl_3$) data for the *syn*-isomer δ 7.45 – 7.21 (m, 5H), 6.45 (d, J = 8.0 Hz, 1H), 6.37 (s, 1H), 5.92 (s, 2H), 4.59 (d, J = 11.8 Hz, 1H), 4.40 (d, J = 11.8 Hz, 1H), 3.84 (s, 3H), 3.74 – 3.67 (m, 1H), 3.57 (s, 3H), 3.27 – 3.21 (m, 1H), 2.84 (dd, J = 16.0, 6.3 Hz, 1H), 2.67 (dd, J = 16.0, 8.5 Hz, 1H), 1.06 (d, J = 6.3 Hz, 3H).

3. References

1. Gensler, W.J.; Stouffer, J.E. *J. Org. Chem.* **1958**, *23*, 908 –910.
2. Comber, M.F.; Sargent, M.V. *Aust. J. Chem.* **1985**, *38*, 1481–1489.
3. Iinuma M.; Tanaka T.; Matsuura, S. *Yakugaku Zasshi* **1983**, *103*, 997–1000.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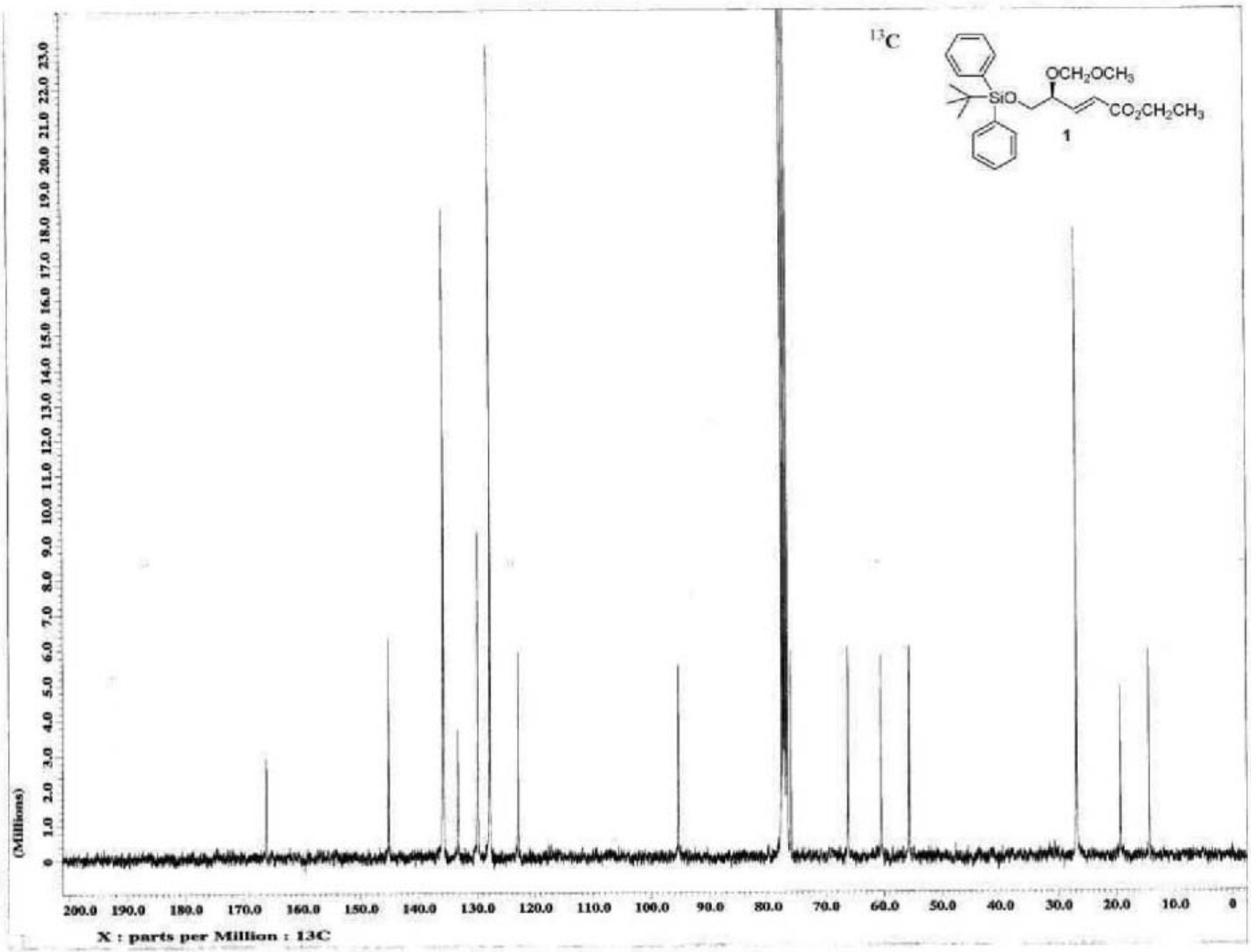
(Millions)
X : parts per Million : 1H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(Millions)
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200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
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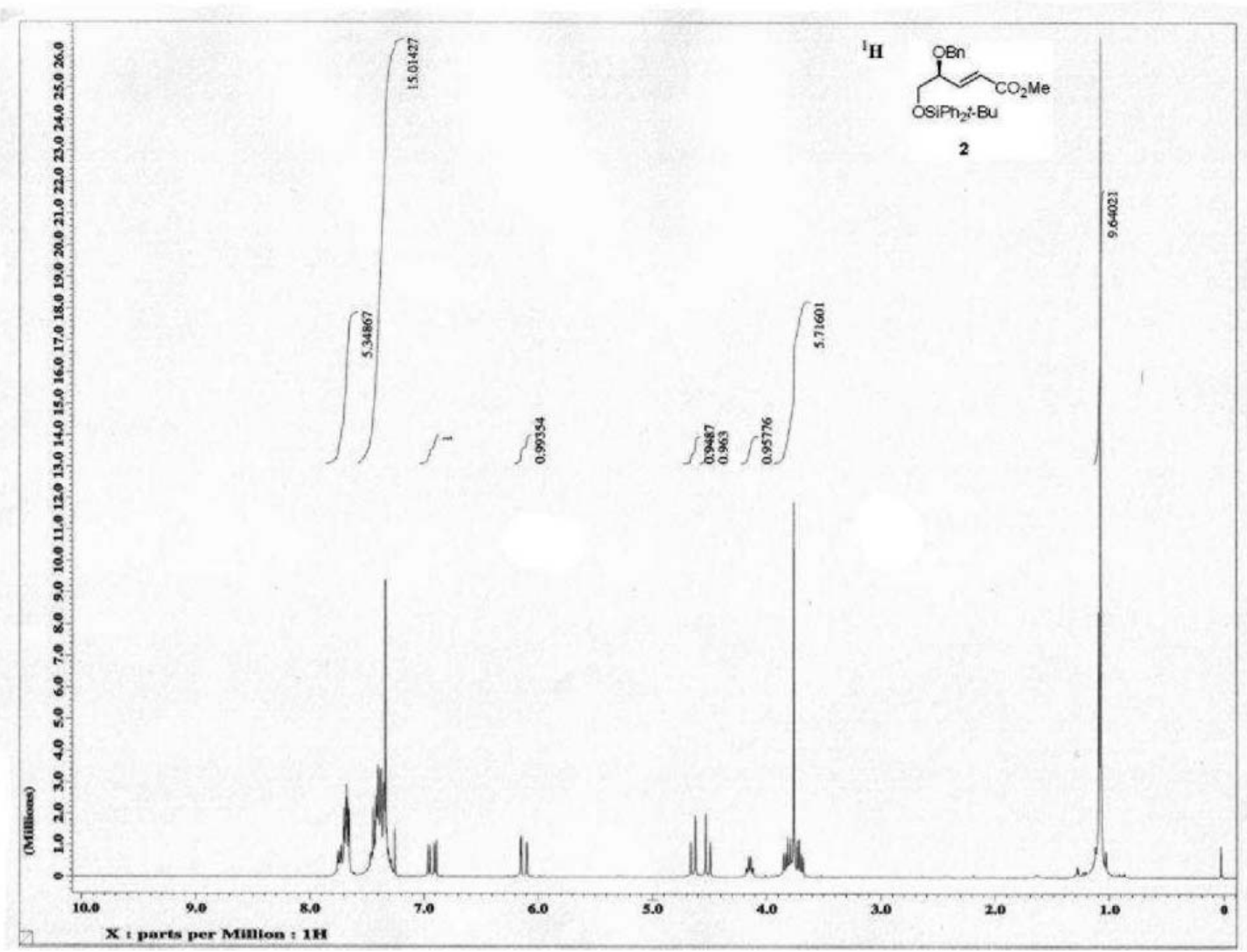
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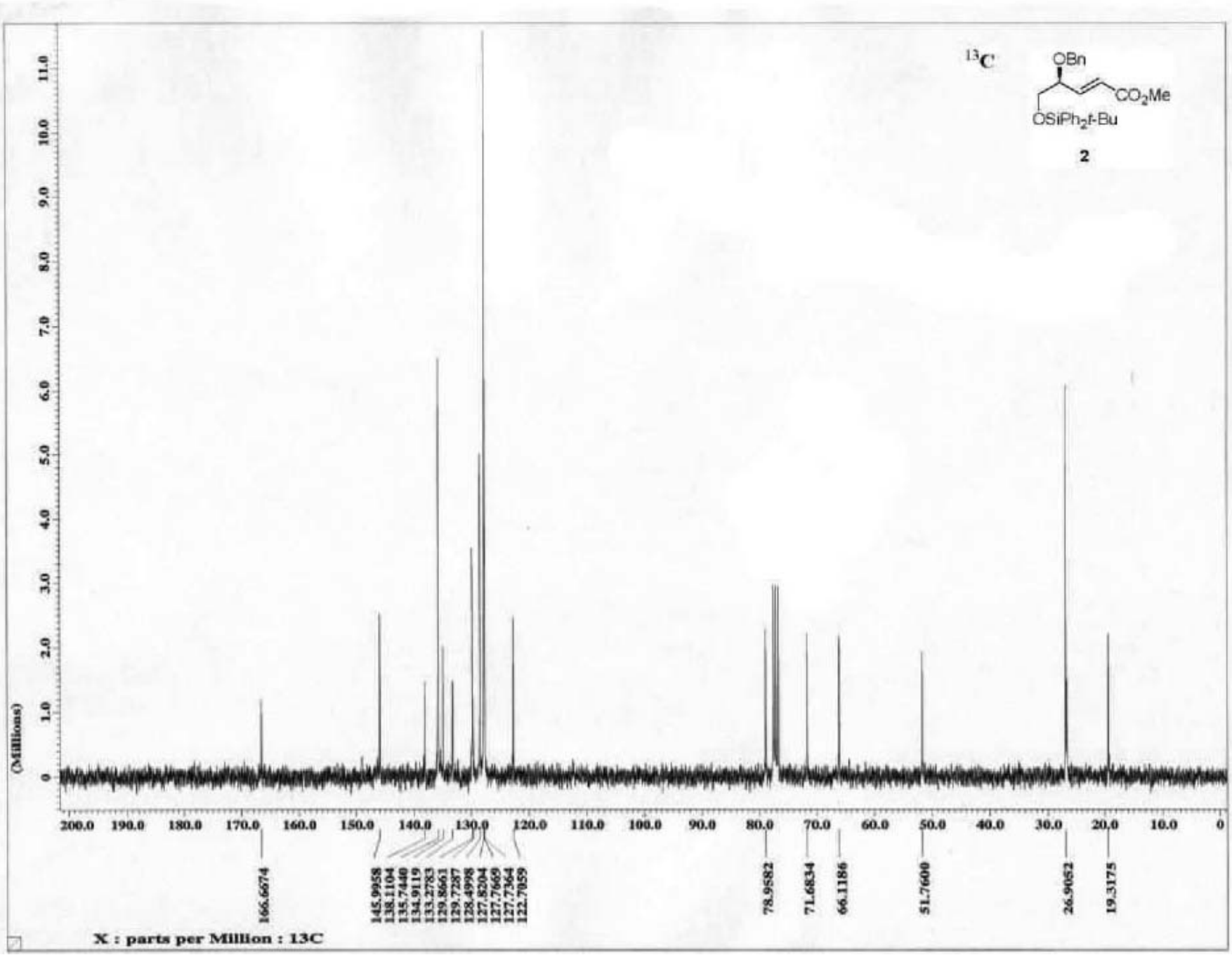
(Millions)
X : parts per Million : 1H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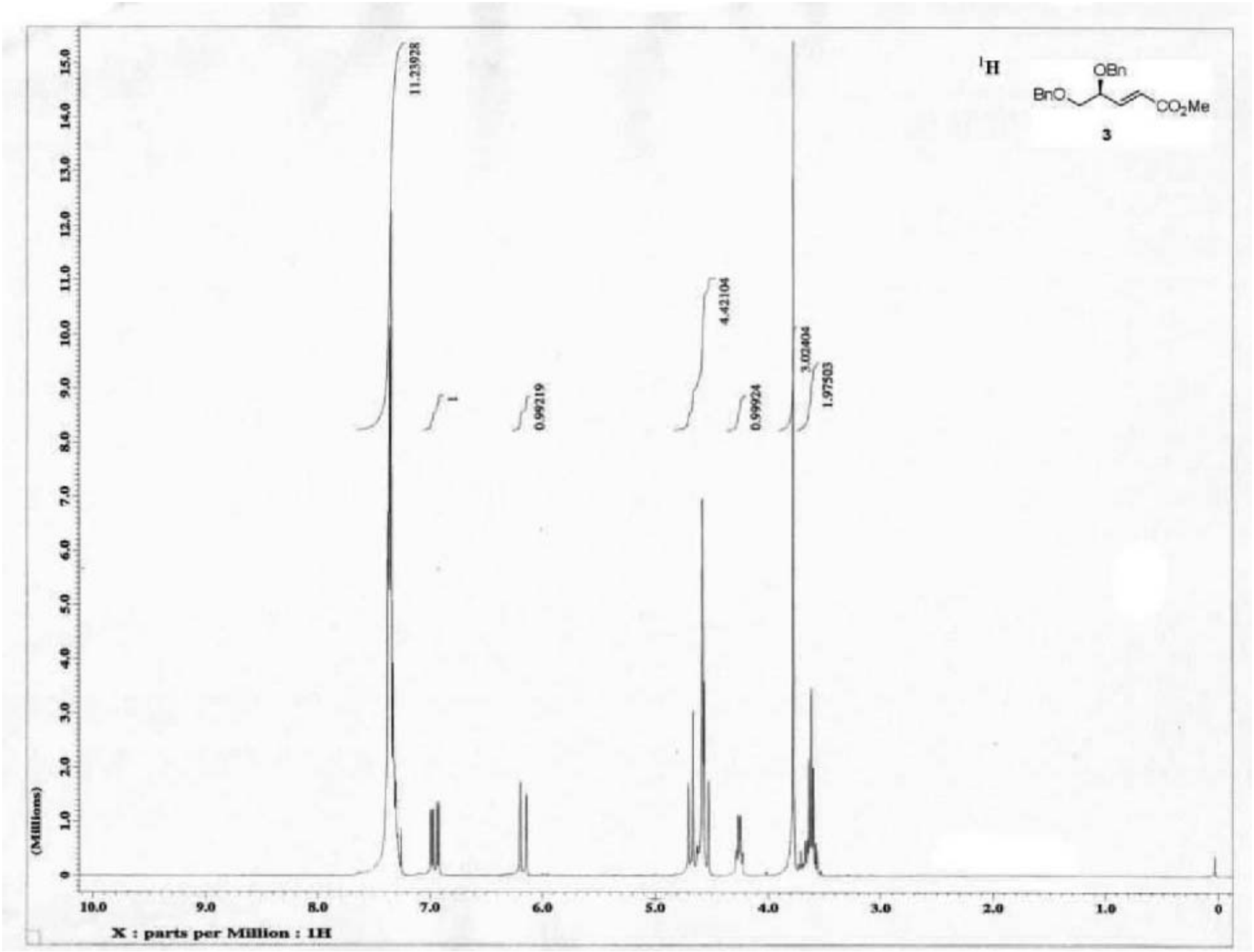
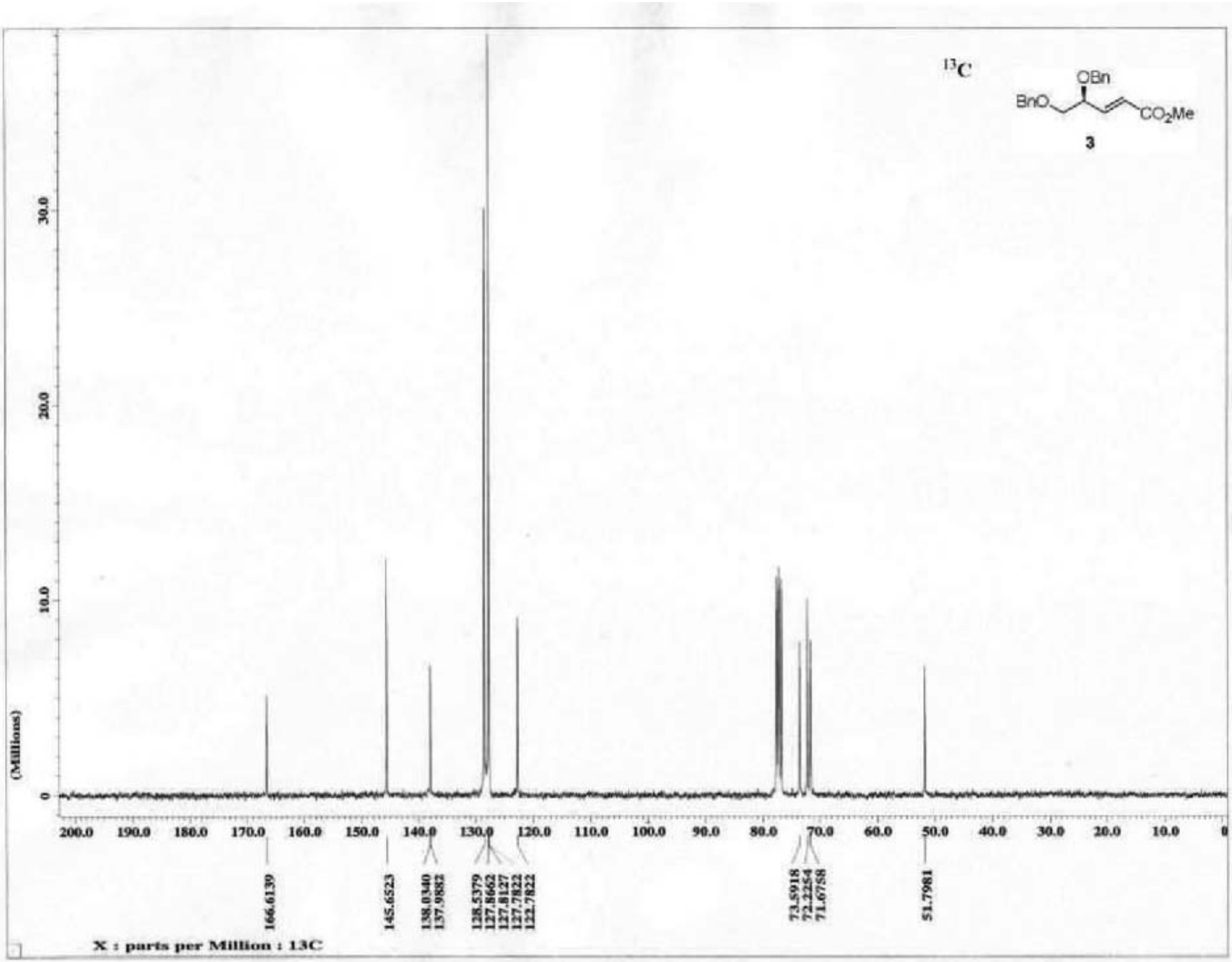
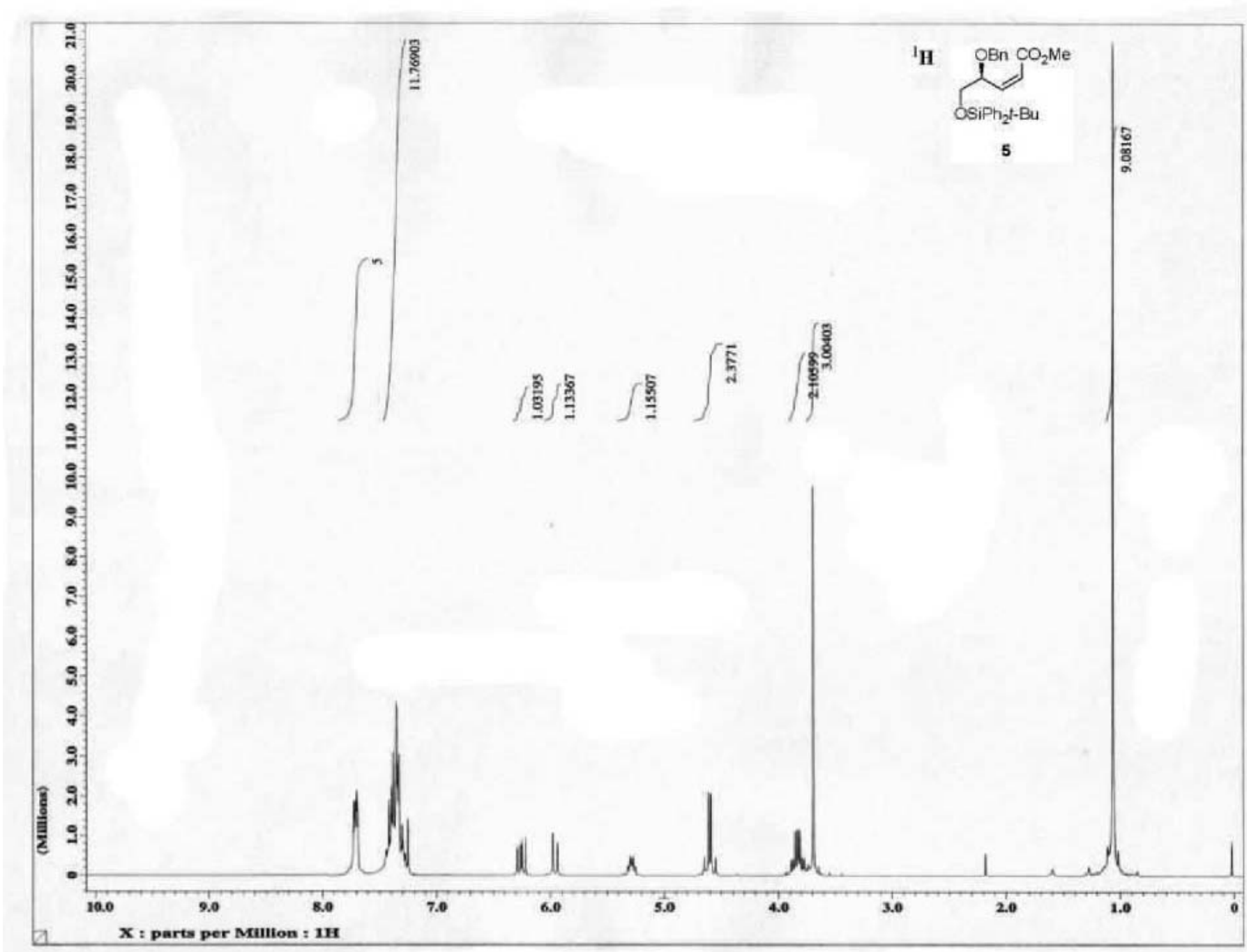
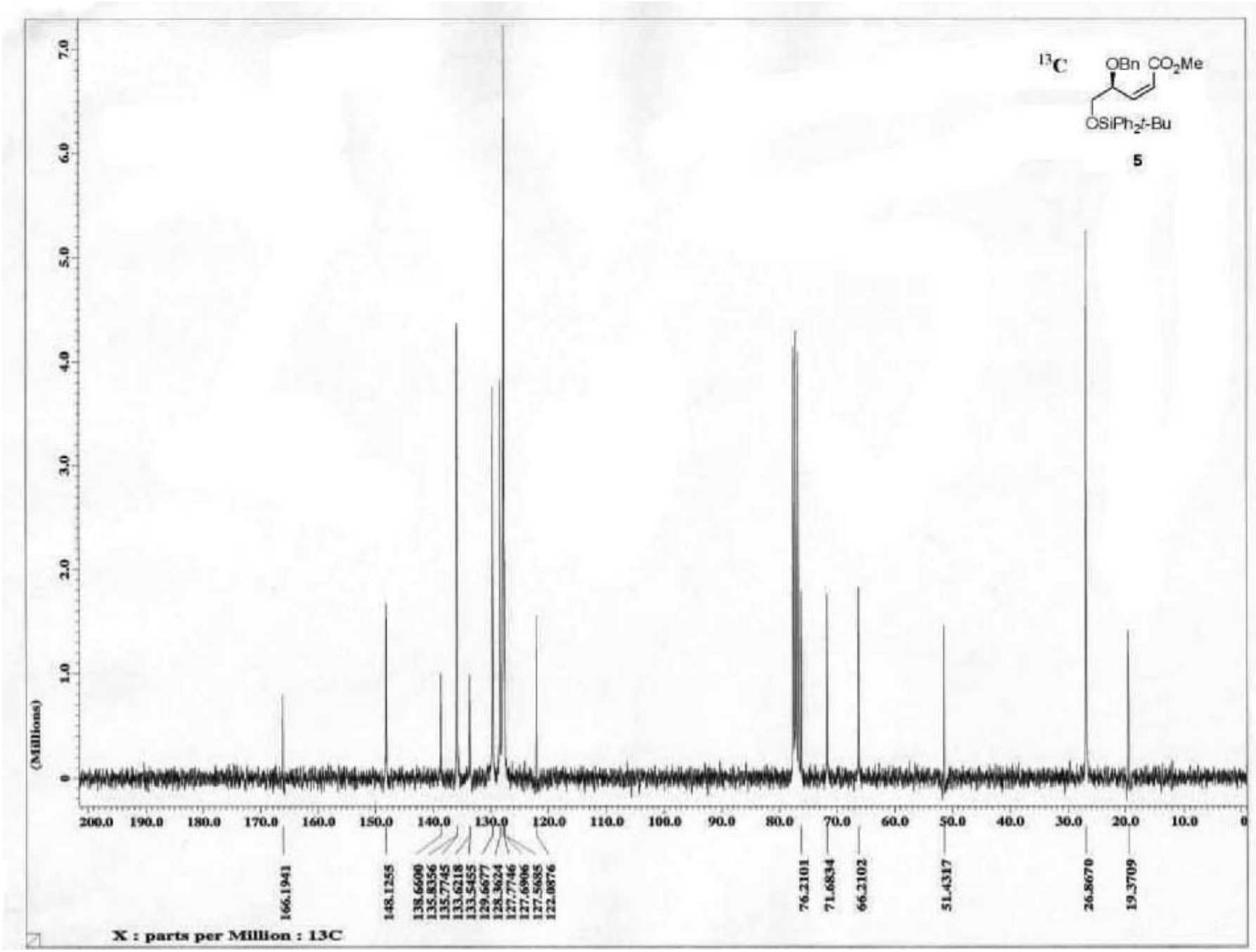
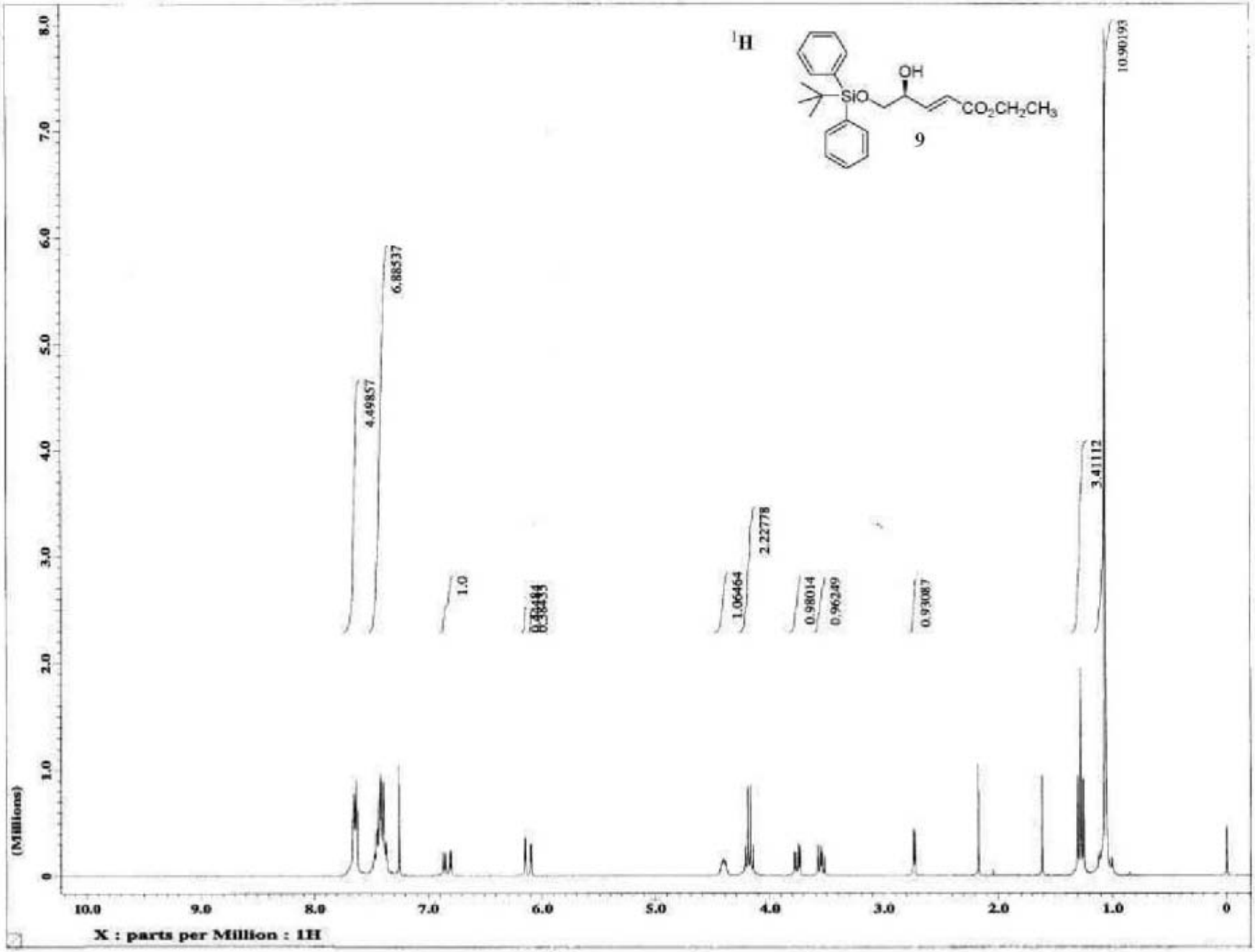
(Millions)
X : parts per Million : 13C
166.6674
145.9958
138.1104
135.7440
134.9119
133.2783
129.8661
129.7287
128.4998
127.8204
127.7669
127.7364
122.7059
78.9582
71.6834
66.1186
51.7600
26.9052
19.3175

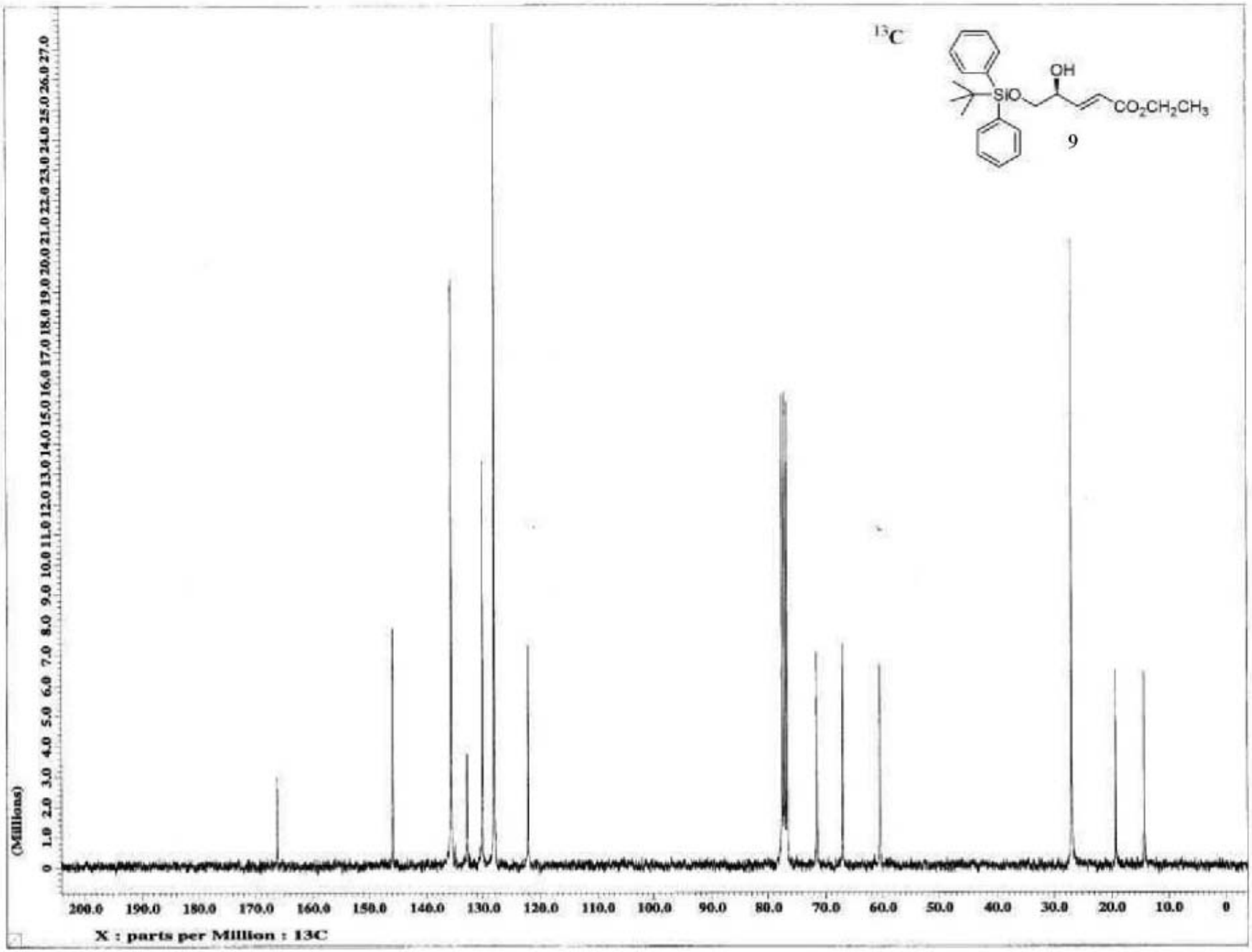

^{1}H
OBn
BnO
CO$_2$Me
3
11.23928
1
0.99219
4.42104
0.99924
3.02404
1.97503
(Millions)
X : parts per Million : 1H

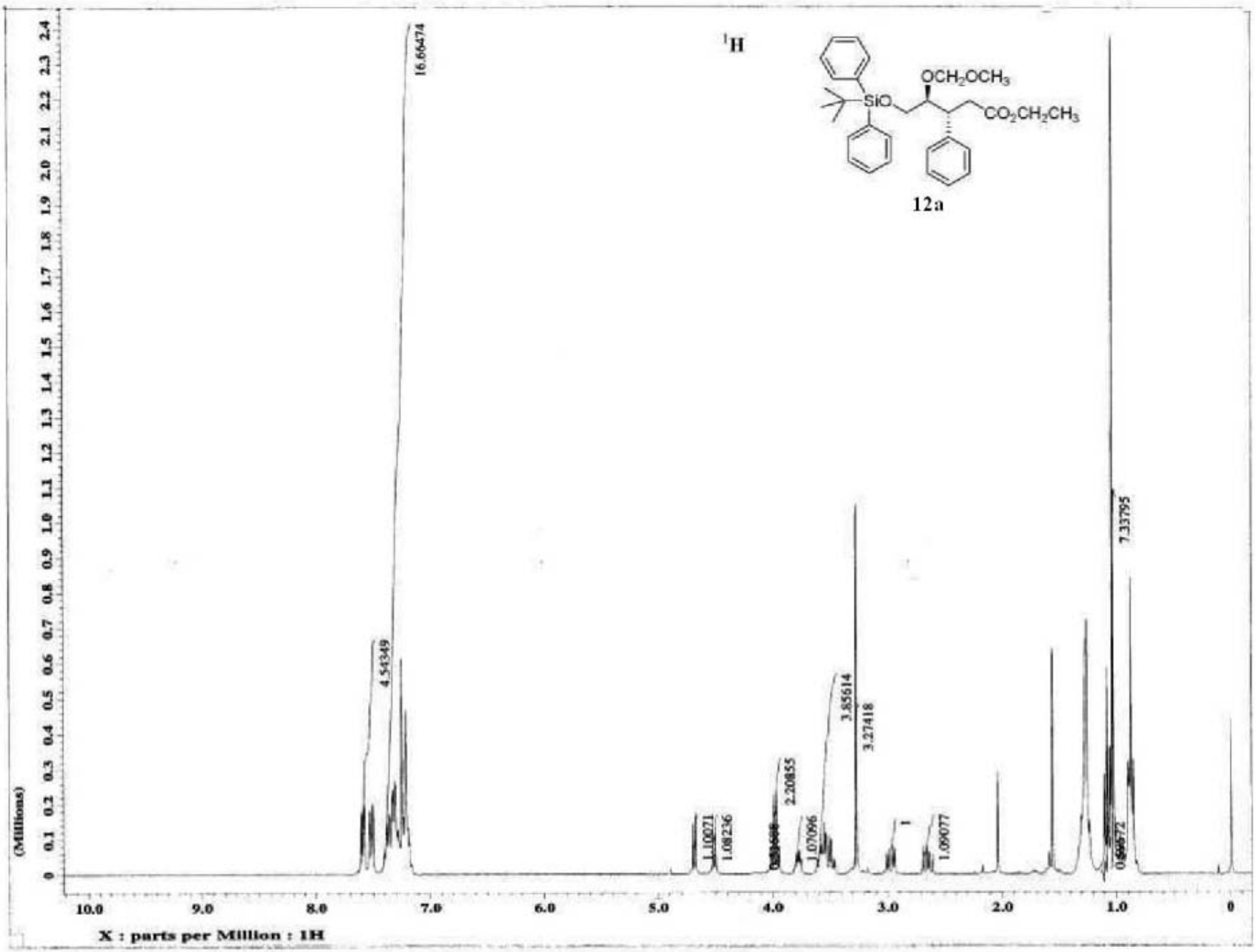

^{13}C
OBn
BnO
CO_2Me
3
(Millions)
30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
166.6139
145.6523
138.0340
137.9882
128.5379
127.8662
127.8127
127.7822
122.7822
73.5918
72.2254
71.6758
51.7981
X : parts per Million : 13C

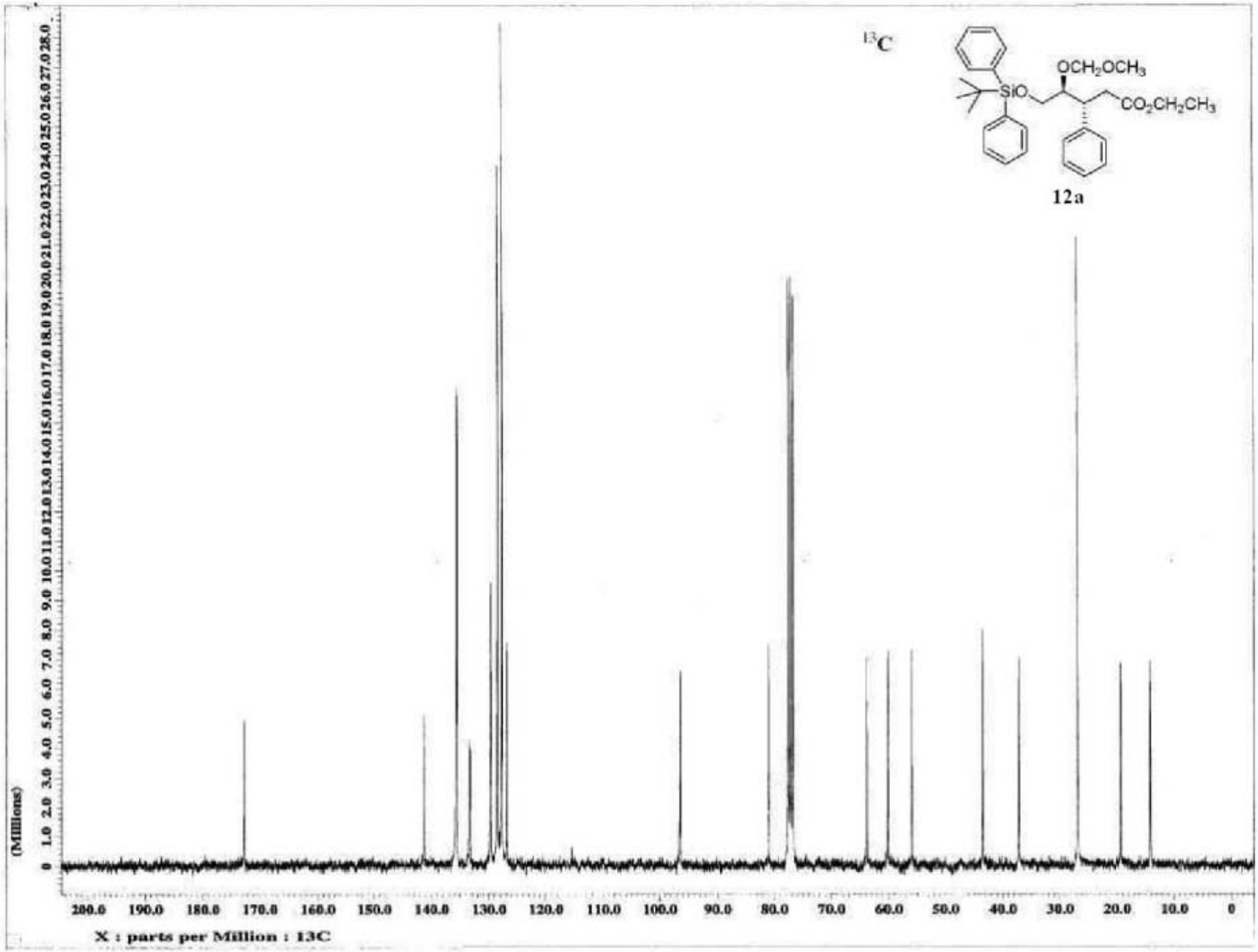

^{1}H
OBn CO$_2$Me
OSiPh$_2$t-Bu
5
11.76903
5
1.03195
1.13367
1.15507
2.3771
2.10599
3.00403
9.08167
(Millions)
X : parts per Million : 1H

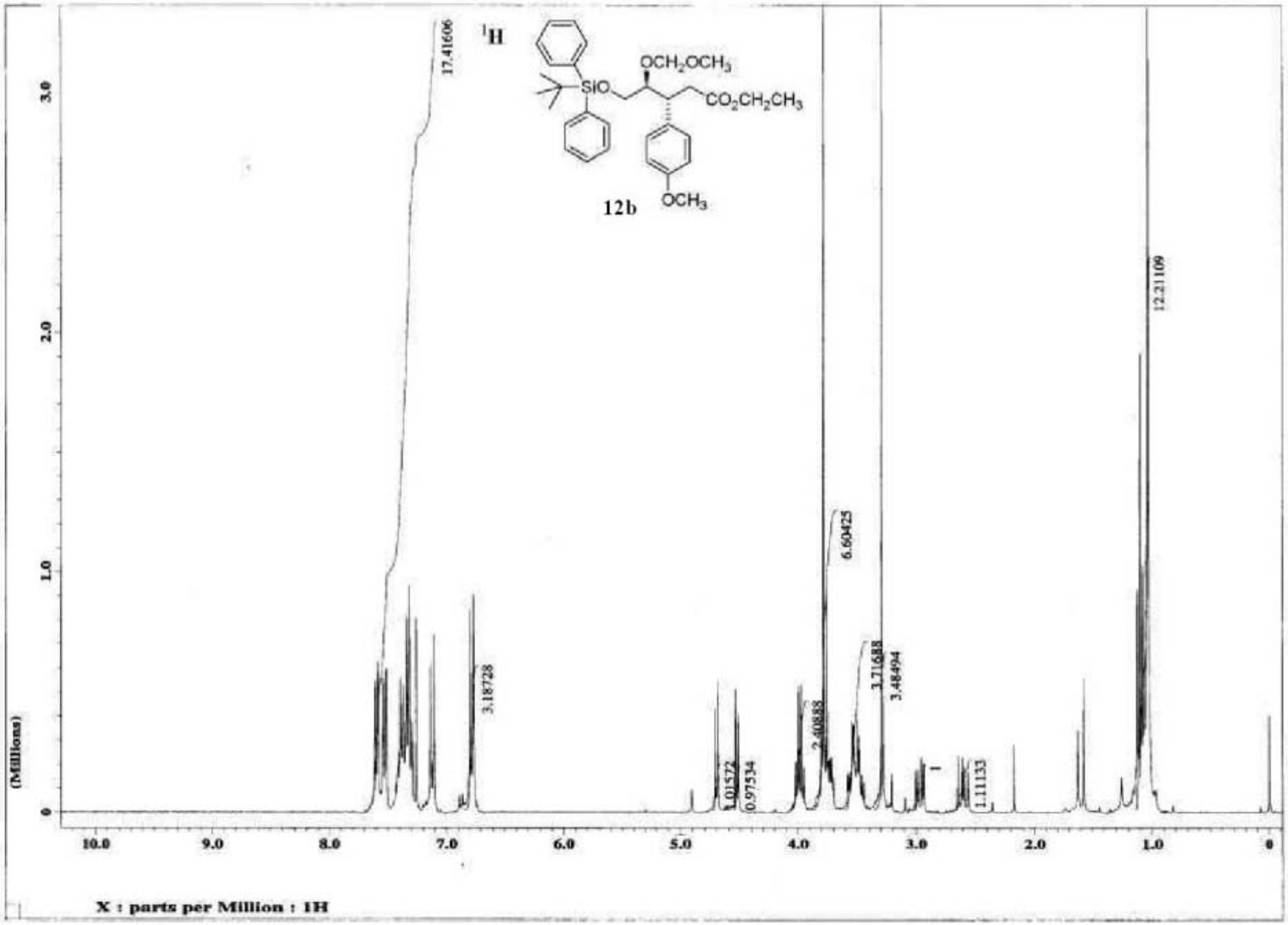

^{13}C
OBn CO$_2$Me
OSiPh$_2$t-Bu
5
(Millions)
X : parts per Million : 13C
166.1941
148.1255
138.6600
135.8356
135.7745
133.6218
133.5455
129.6677
128.3624
127.7746
127.6906
127.5635
122.0876
76.2101
71.6834
66.2102
51.4317
26.8670
19.3709

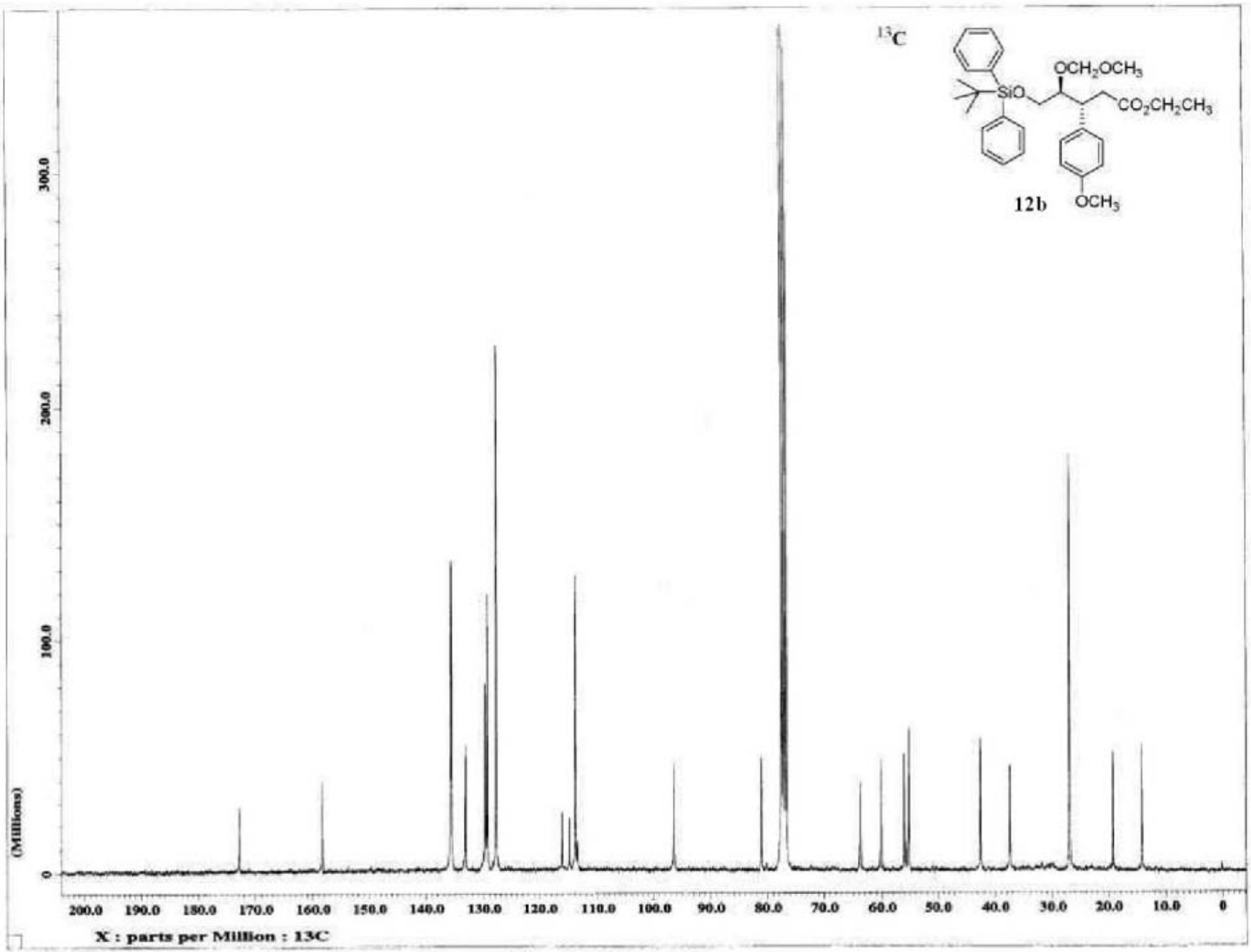

^{1}H
OH
SiO
$CO_2CH_2CH_3$
9
10.90193
6.88537
4.49857
3.41112
2.22778
1.06464
1.0
0.98014
0.96249
0.93087
(Millions)
X : parts per Million : 1H

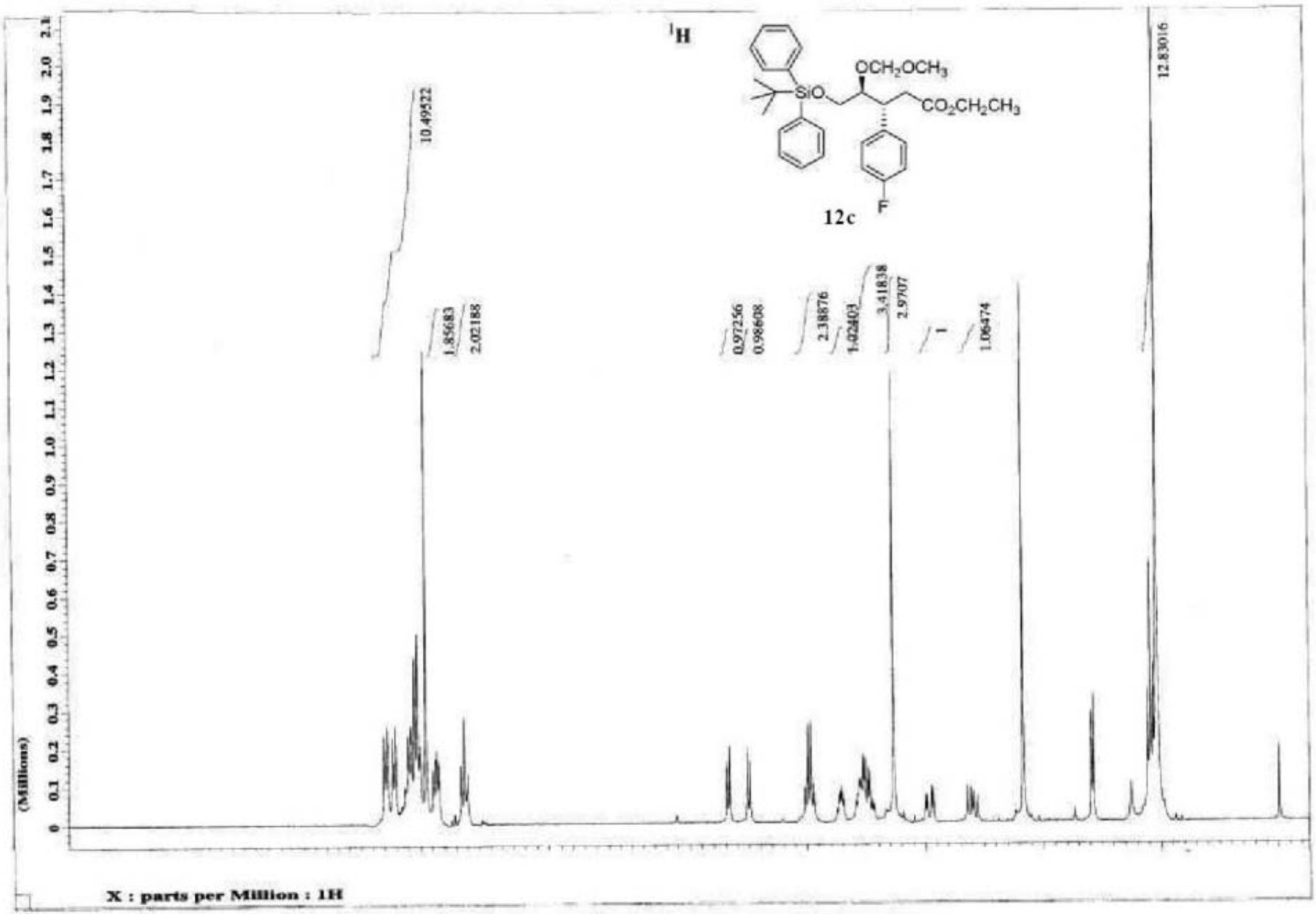

^{13}C
OH
SiO
$CO_2CH_2CH_3$
9
(Millions)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0 25.0 26.0 27.0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : 13C

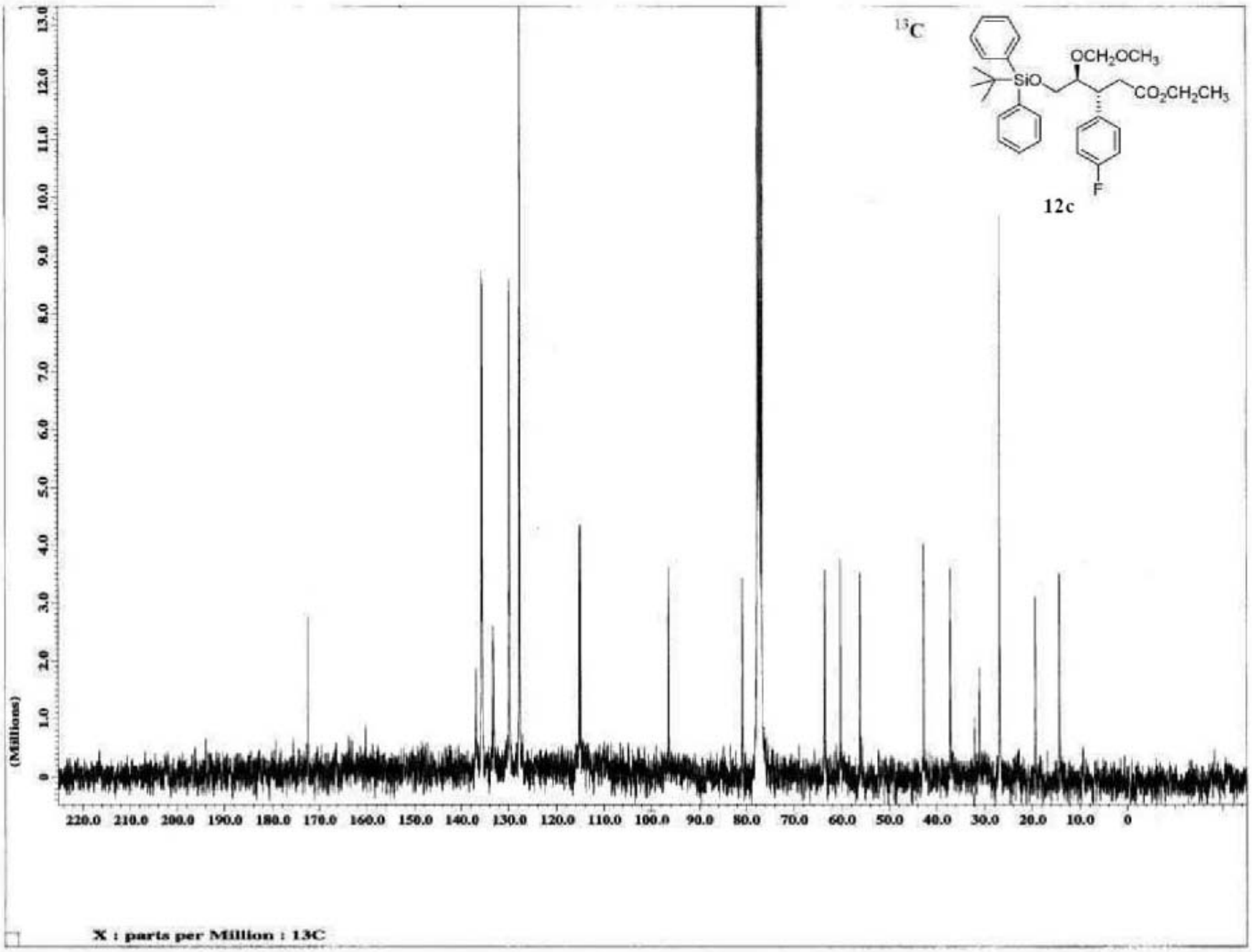

^{1}H
OCH$_2$OCH$_3$
SiO
CO$_2$CH$_2$CH$_3$
12a
16.66474
4.54349
1.10071
1.08236
2.20855
1.07096
3.85614
3.27418
1
1.09077
7.33795
(Millions)
X : parts per Million : 1H

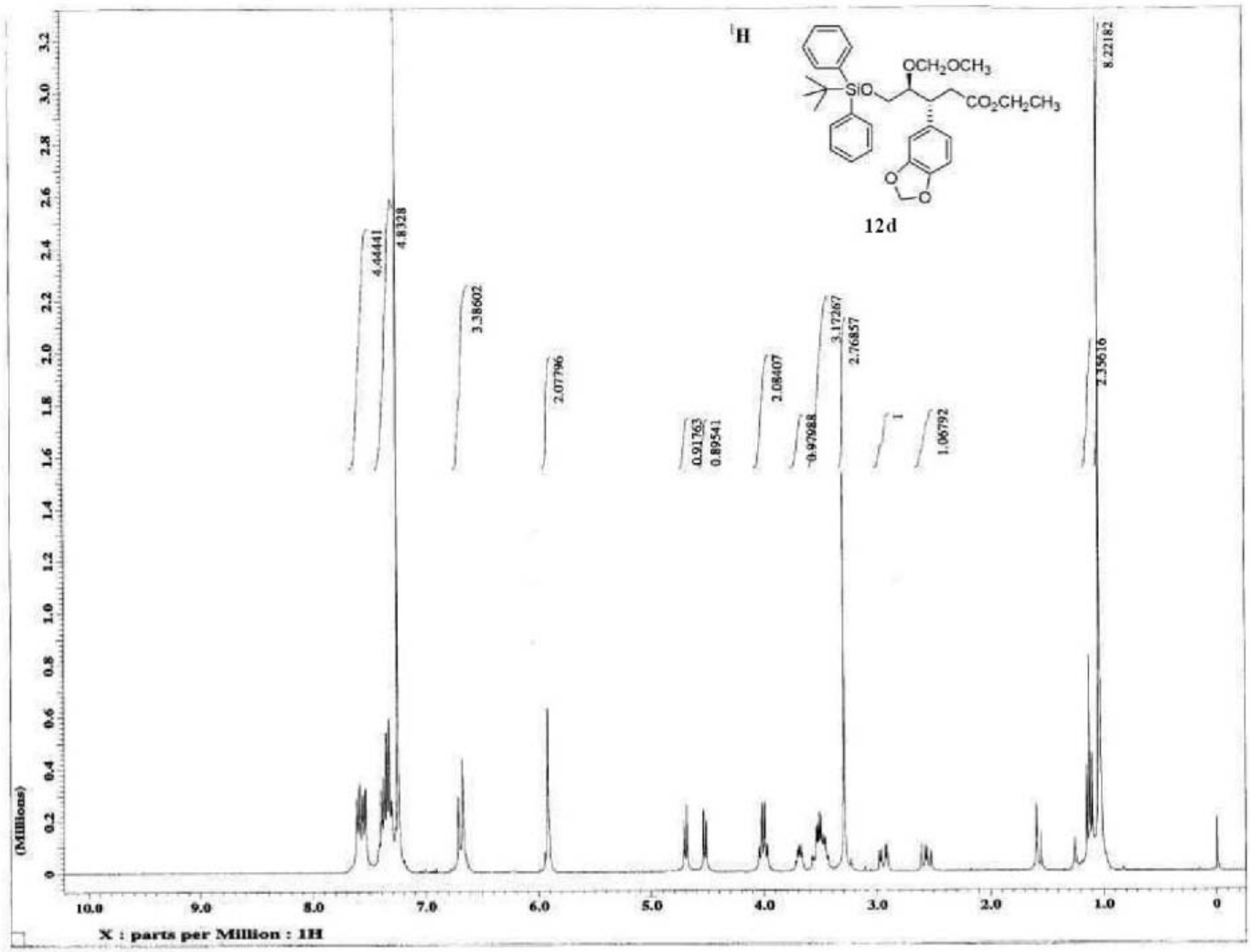

^{13}C
OCH2OCH3
SiO
CO2CH2CH3
12a
(Millions)
X : parts per Million : 13C

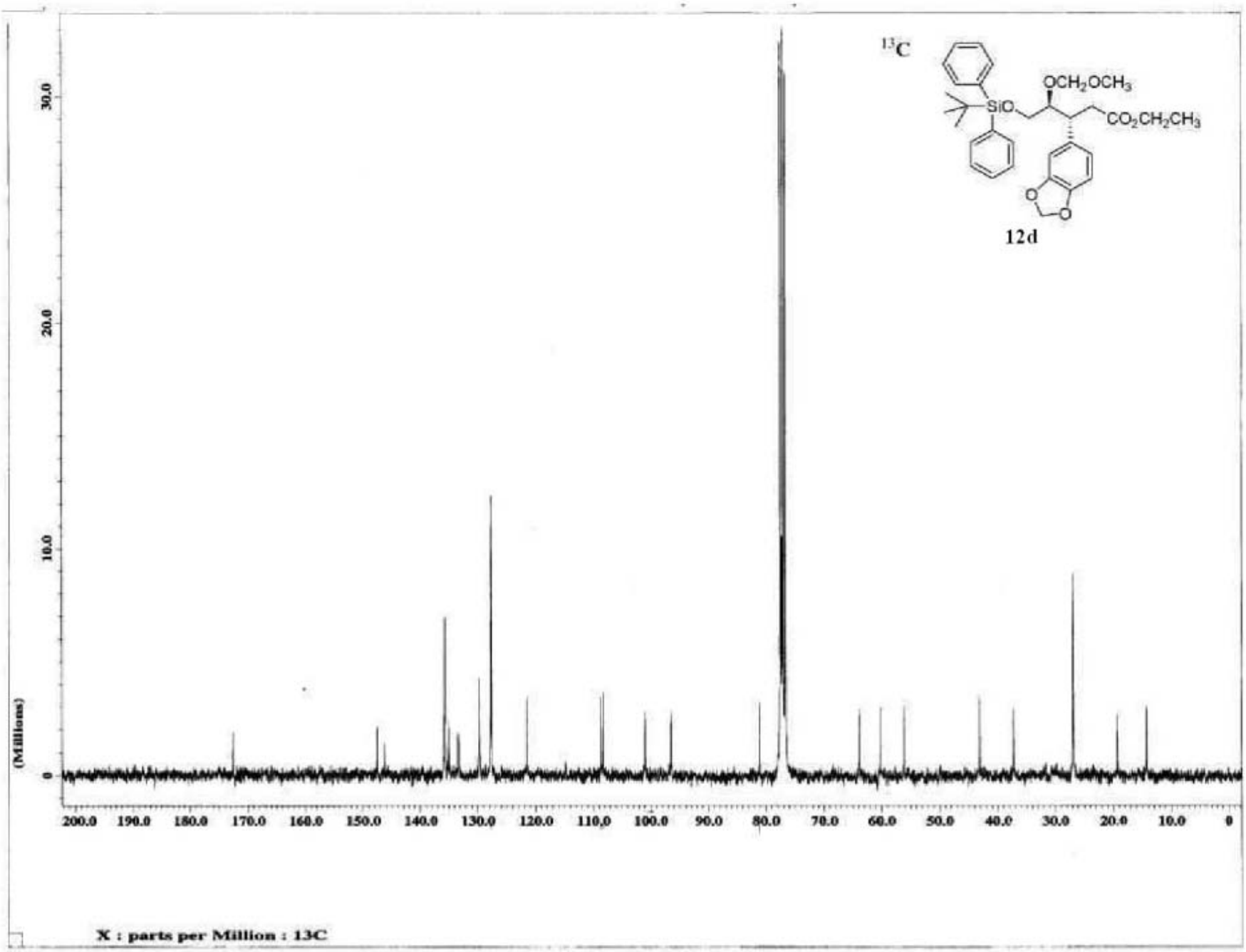

^{1}H
OCH$_2$OCH$_3$
SiO
CO$_2$CH$_2$CH$_3$
OCH$_3$
12b
17.41606
3.18728
1.01572
0.97534
2.40888
6.60425
3.71688
3.48494
1.11133
12.21109
(Millions)
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : 1H

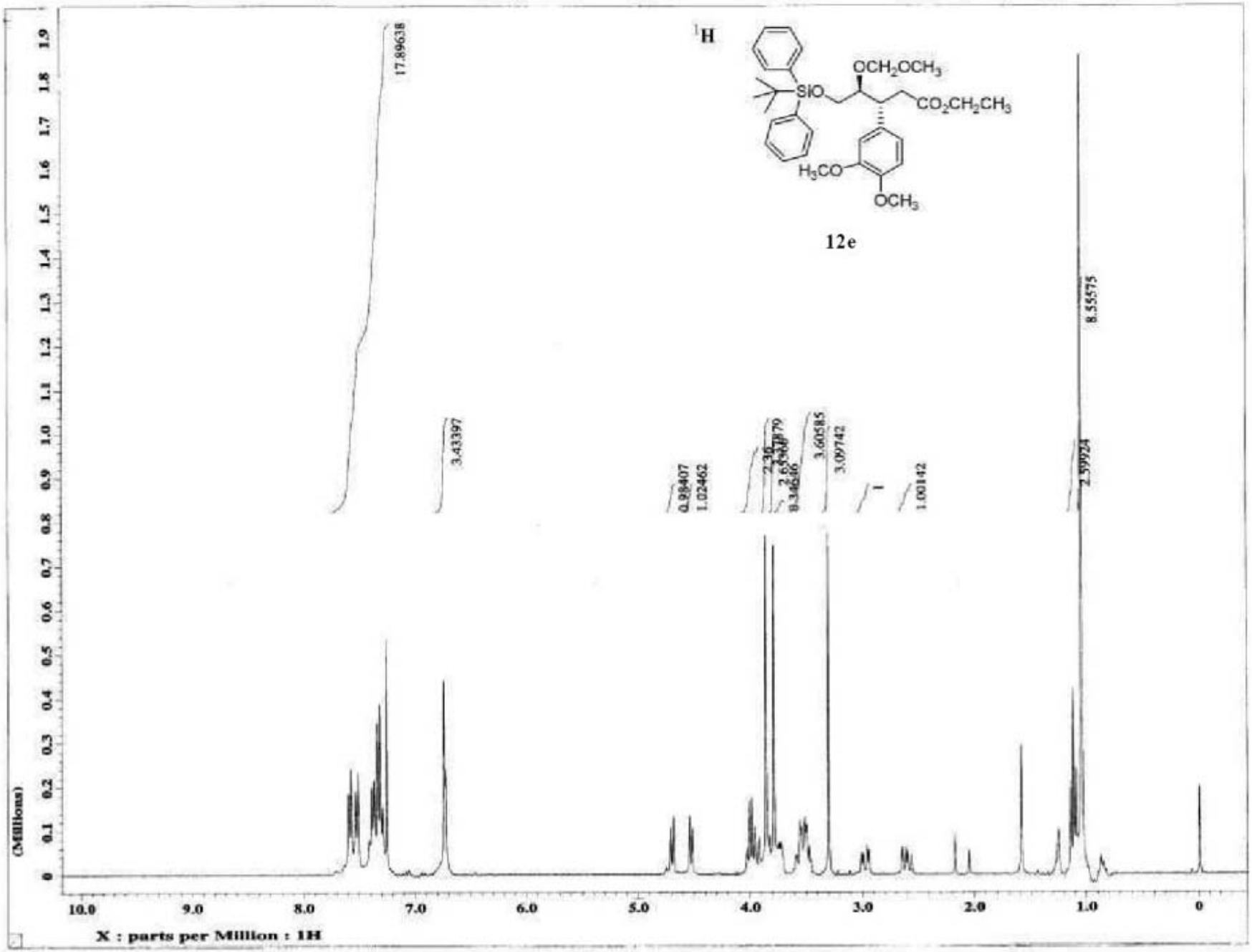

^{13}C
OCH2OCH3
SiO
CO2CH2CH3
OCH3
12b
300.0
200.0
100.0
0
(Millions)
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : 13C

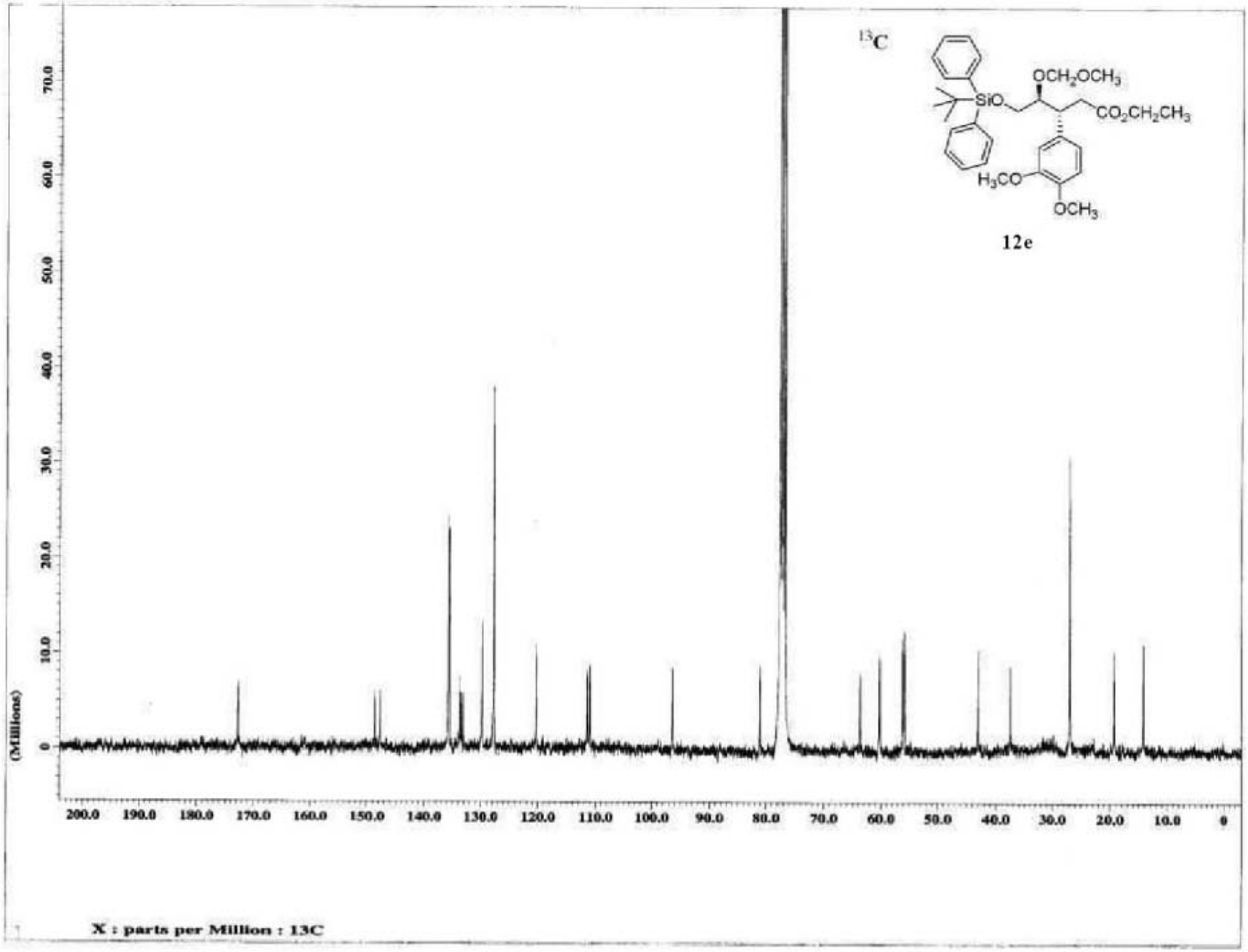

^{1}H
OCH$_2$OCH$_3$
SiO
CO$_2$CH$_2$CH$_3$
F
12c
10.49522
1.85683
2.02188
0.97256
0.98608
2.38876
1.42403
3.41838
2.9707
1
1.06474
12.83016
(Millions)
X : parts per Million : 1H

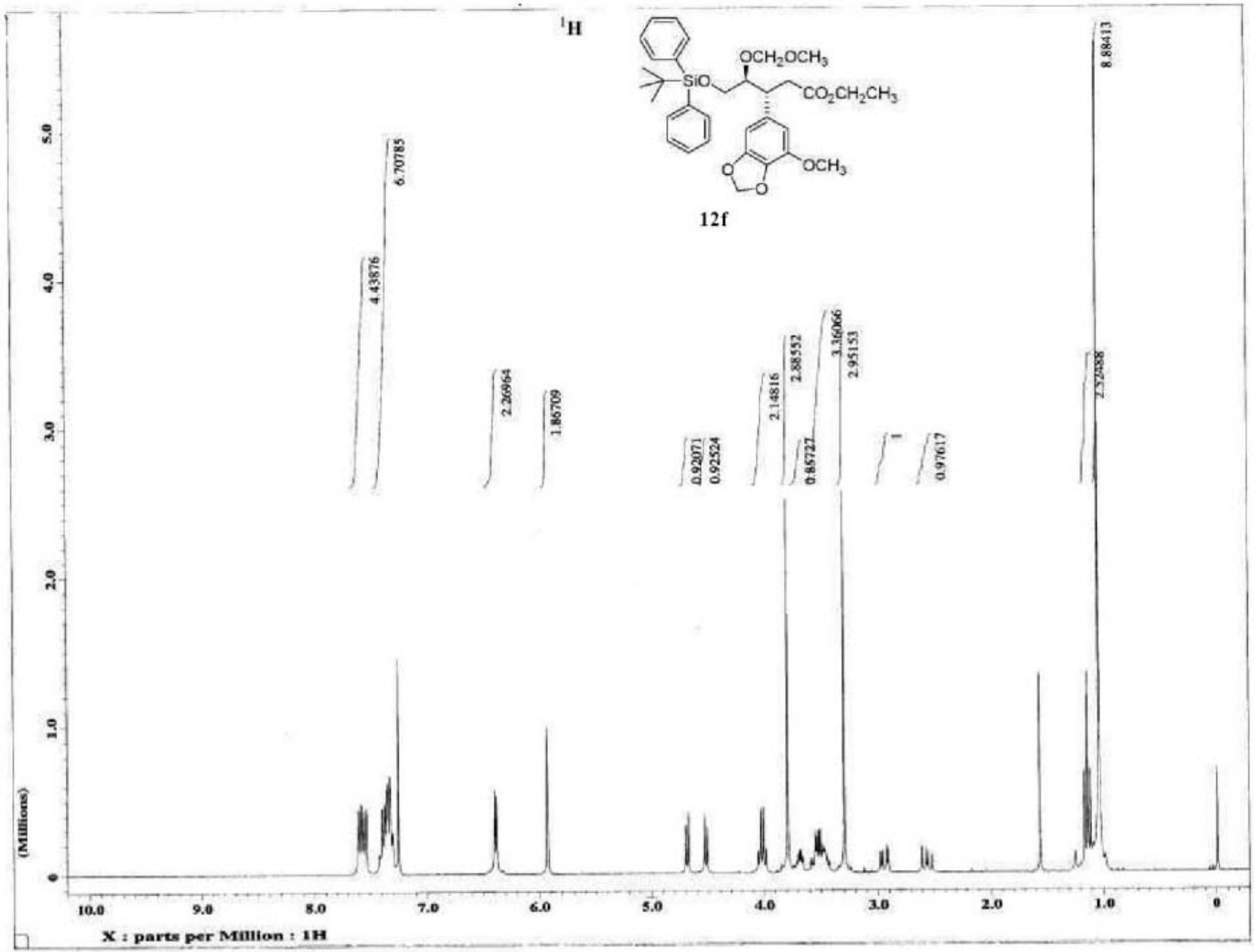

^{13}C
OCH2OCH3
SiO
CO2CH2CH3
F
12c
(Millions)
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : 13C

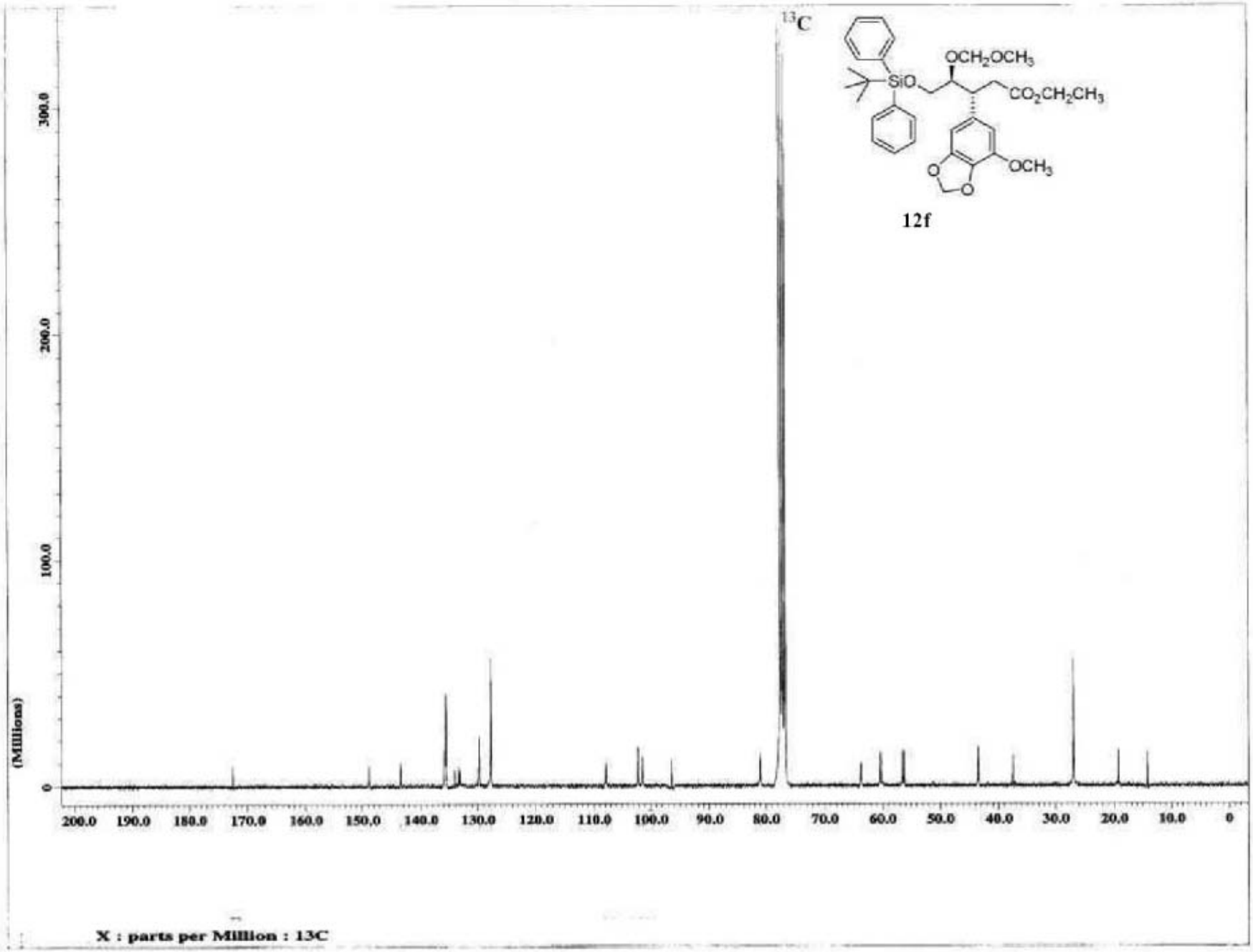

^{1}H
OCH$_2$OCH$_3$
CO$_2$CH$_2$CH$_3$
12d
8.22182
4.44441
4.8328
3.38602
2.07796
0.91763
0.89541
2.08407
0.97988
3.17267
2.76857
1
1.06792
2.35616
(Millions)
X : parts per Million : 1H

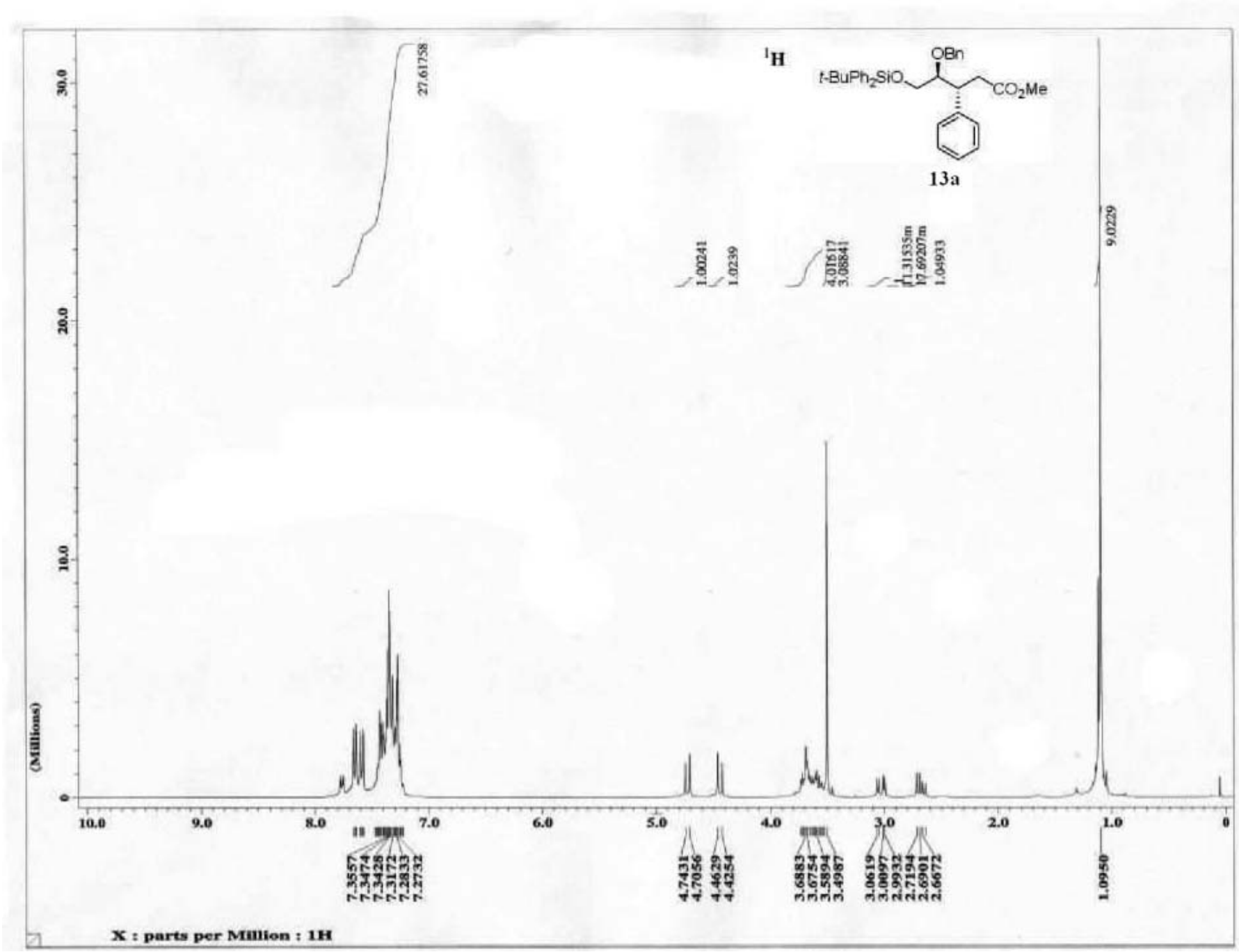

13C
OCH2OCH3
SiO
CO2CH2CH3
12d
30.0
20.0
10.0
0
(Millions)
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : 13C

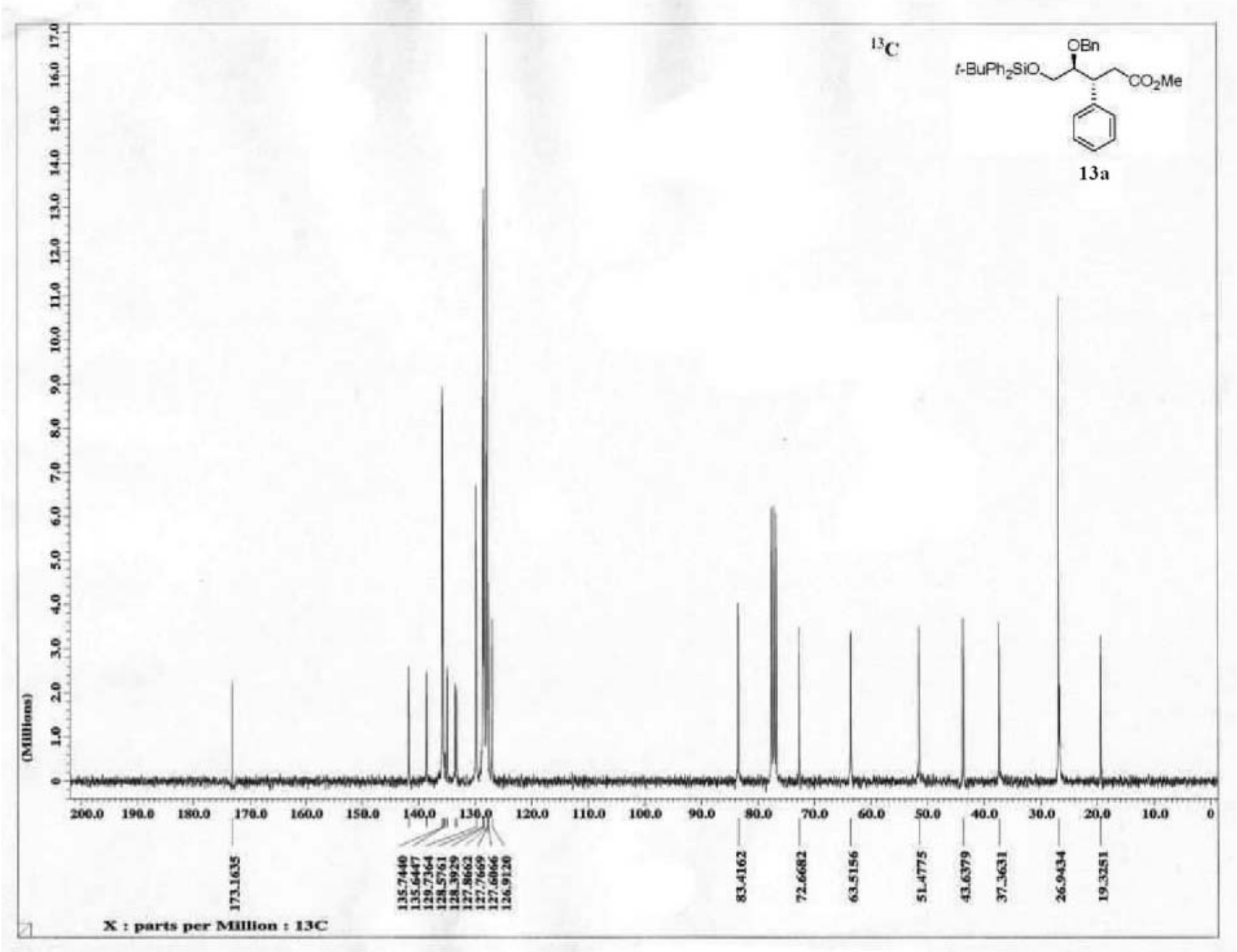

^{1}H
OCH$_2$OCH$_3$
SiO
CO$_2$CH$_2$CH$_3$
H$_3$CO
OCH$_3$
12e
17.89638
3.43397
0.98407
1.02462
3.60585
3.09742
1
1.00142
8.55575
2.59924
(Millions)
X : parts per Million : 1H

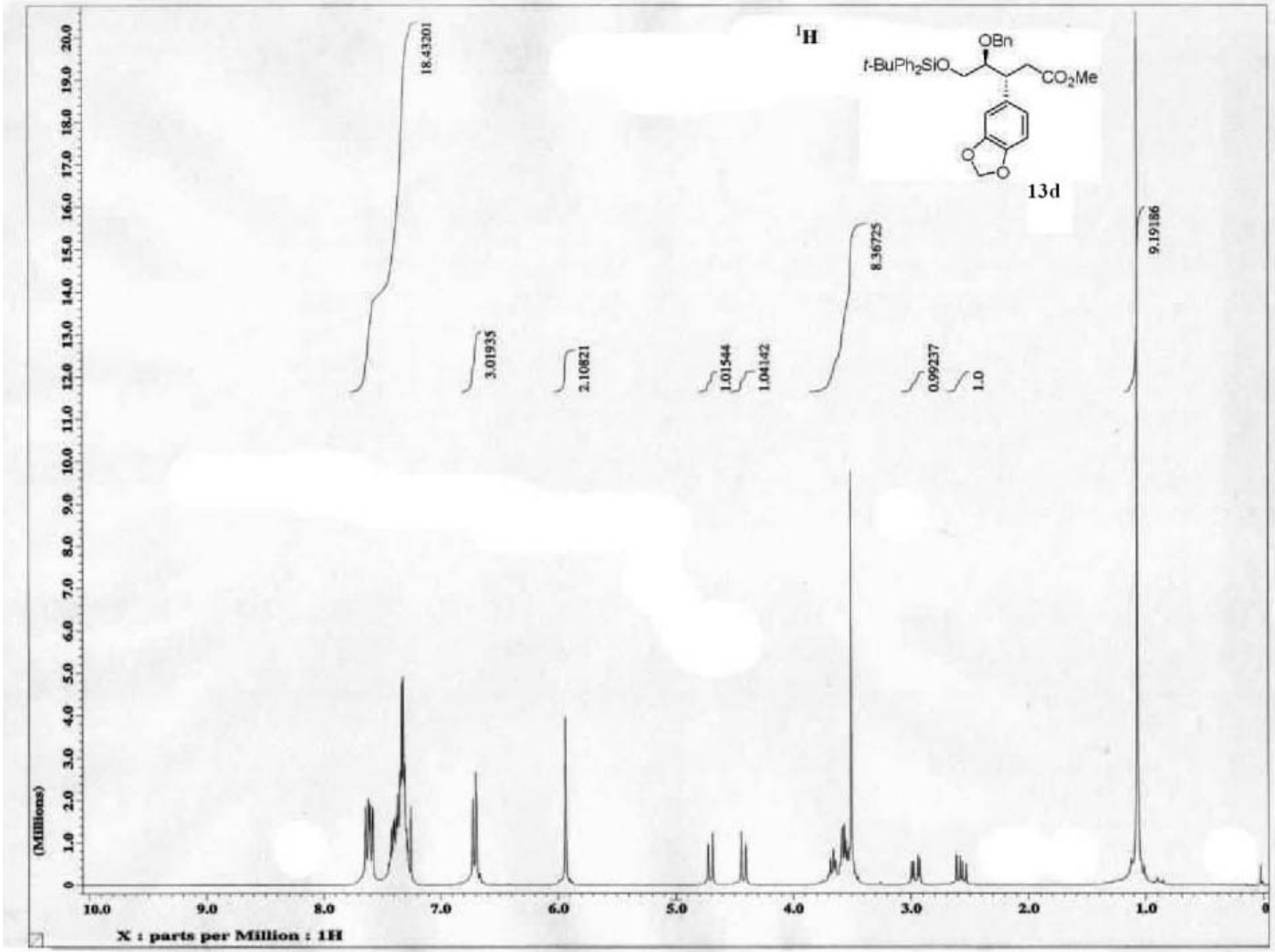

13C
OCH2OCH3
SiO
CO2CH2CH3
H3CO
OCH3
12e
(Millions)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : 13C

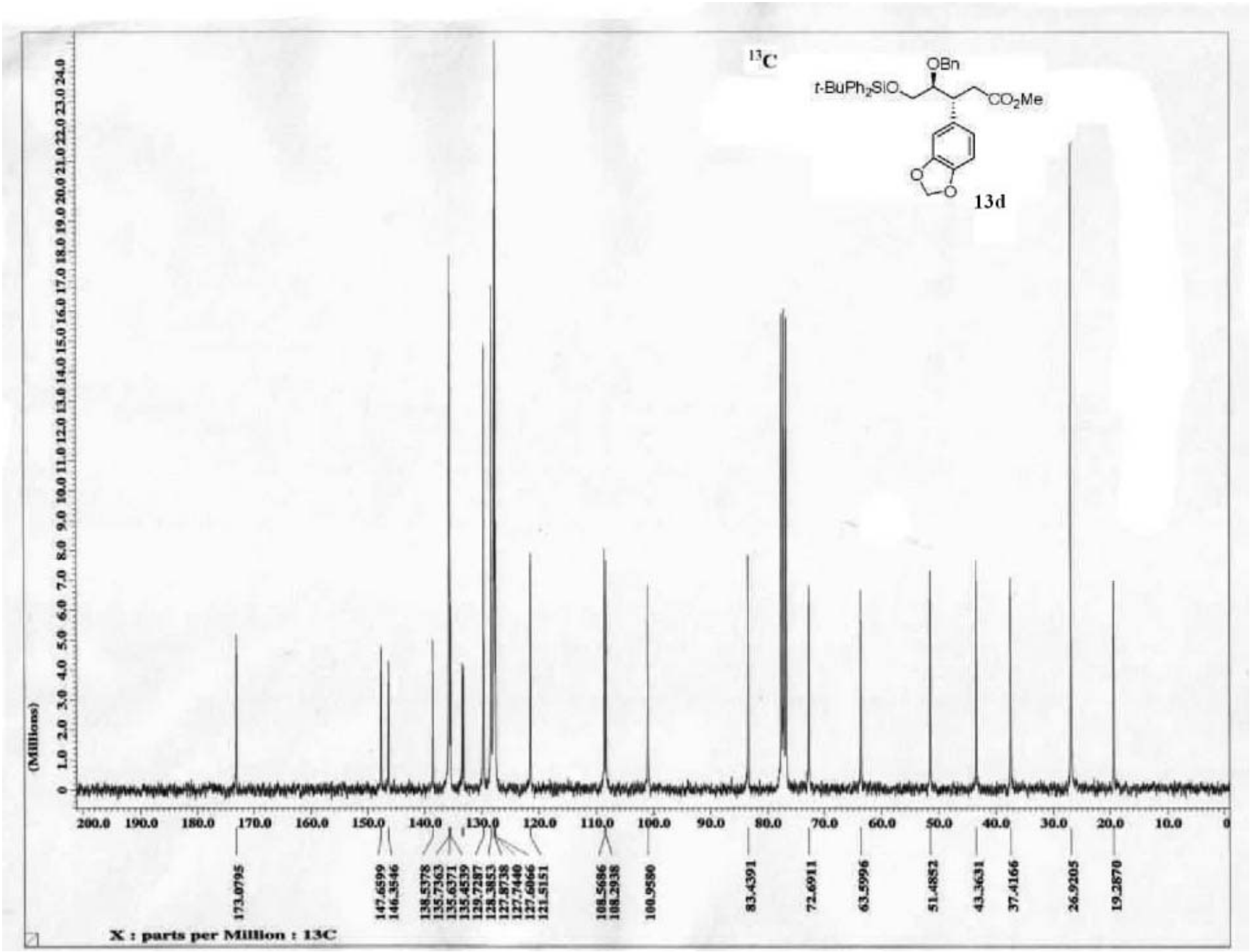

^{1}H
OCH$_2$OCH$_3$
SiO
CO$_2$CH$_2$CH$_3$
OCH$_3$
O
O
12f
8.88413
6.70785
4.43876
2.26964
1.86709
0.92071
0.92524
2.14816
2.88552
0.85727
3.36066
2.95153
1
0.97617
2.52458
(Millions)
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : 1H

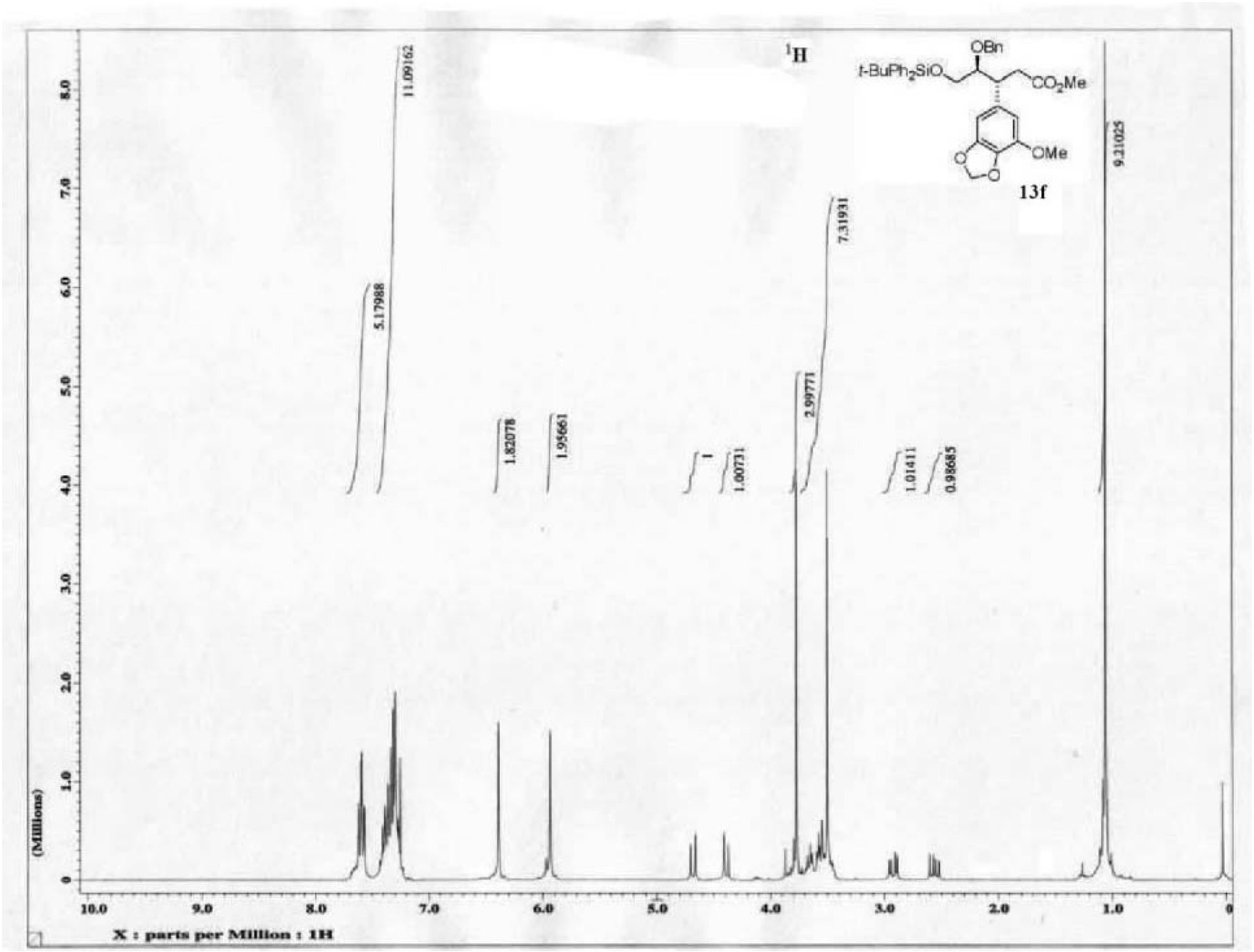

^{13}C
OCH2OCH3
SiO
CO2CH2CH3
OCH3
O
O
12f
300.0
200.0
100.0
0
(Millions)
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : 13C

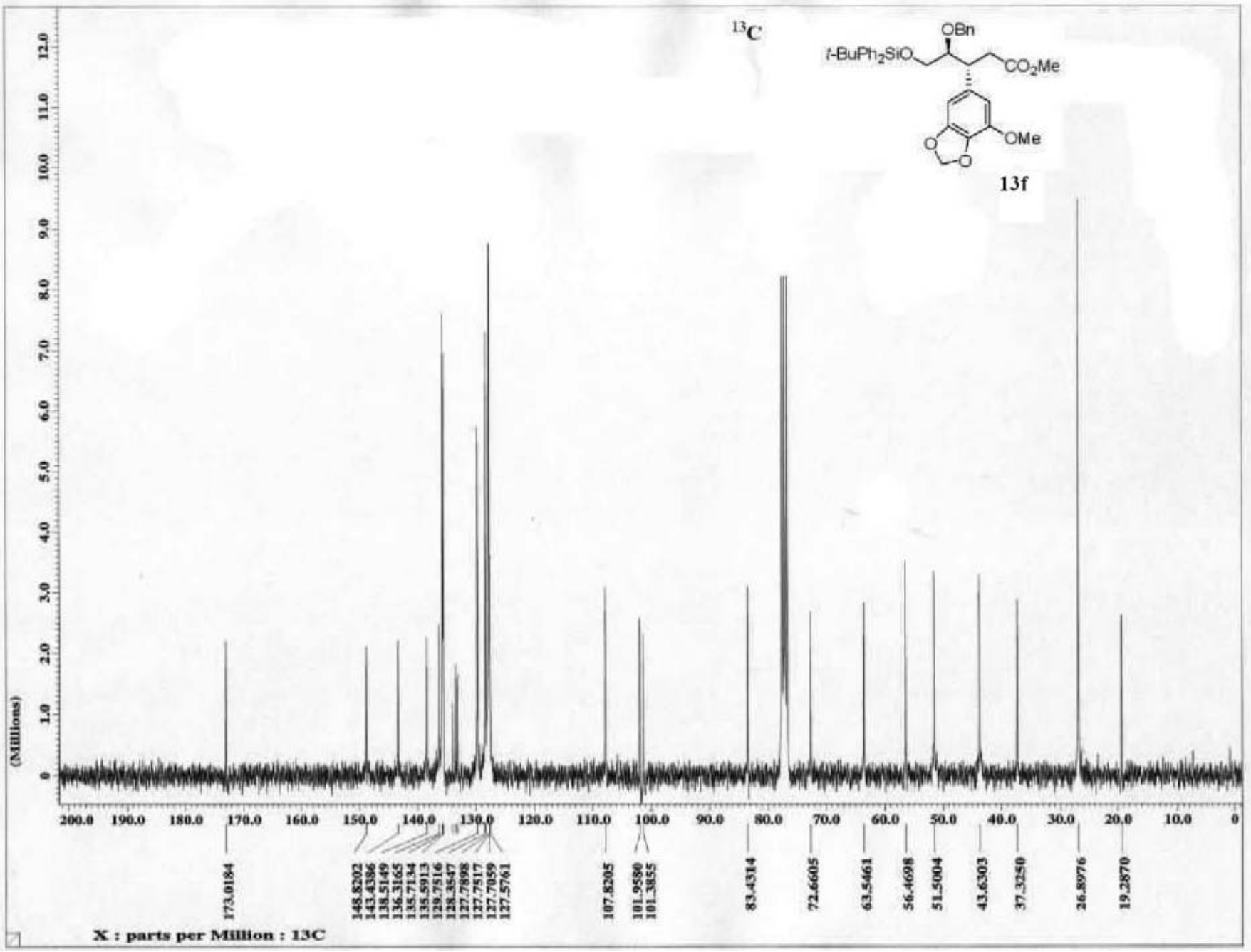

^{1}H
OBn
t-BuPh$_2$SiO
CO$_2$Me
13a
27.61758
1.00241
1.0239
4.01617
3.08841
11.31535m
17.69207m
1.04933
9.0229
(Millions)
30.0
20.0
10.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.3557
7.3474
7.3428
7.3172
7.2833
7.2732
4.7431
4.7056
4.4629
4.4254
3.6883
3.6754
3.5894
3.4987
3.0619
3.0097
2.9932
2.7194
2.6901
2.6672
1.0950
X : parts per Million : 1H

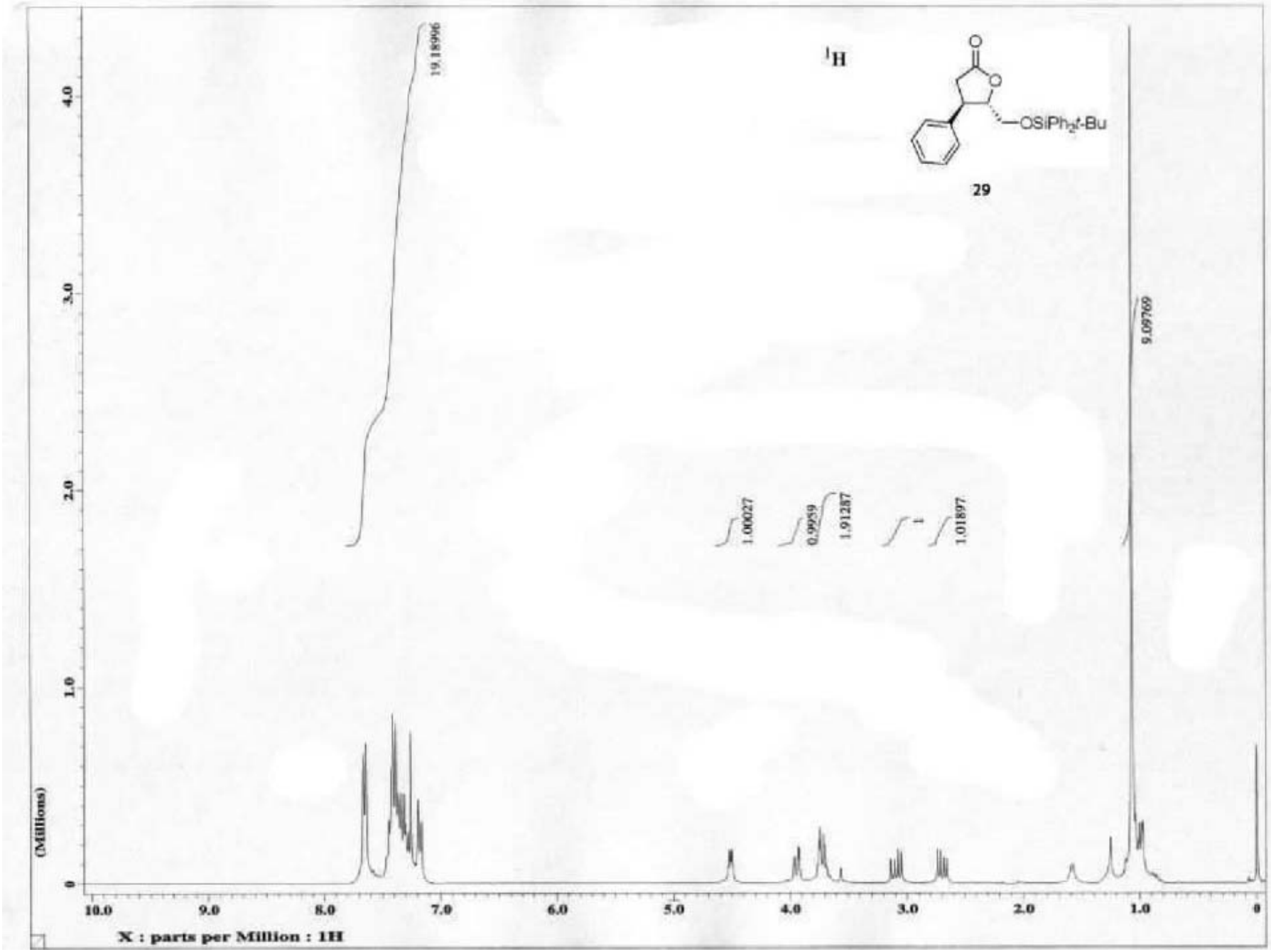

^{13}C
OBn
t-BuPh2SiO
CO2Me
13a
(Millions)
173.1635
135.7440
135.6447
129.7364
128.5761
128.3929
127.8662
127.7669
127.6066
126.9120
83.4162
72.6682
63.5156
51.4775
43.6379
37.3631
26.9434
19.3251
X : parts per Million : 13C

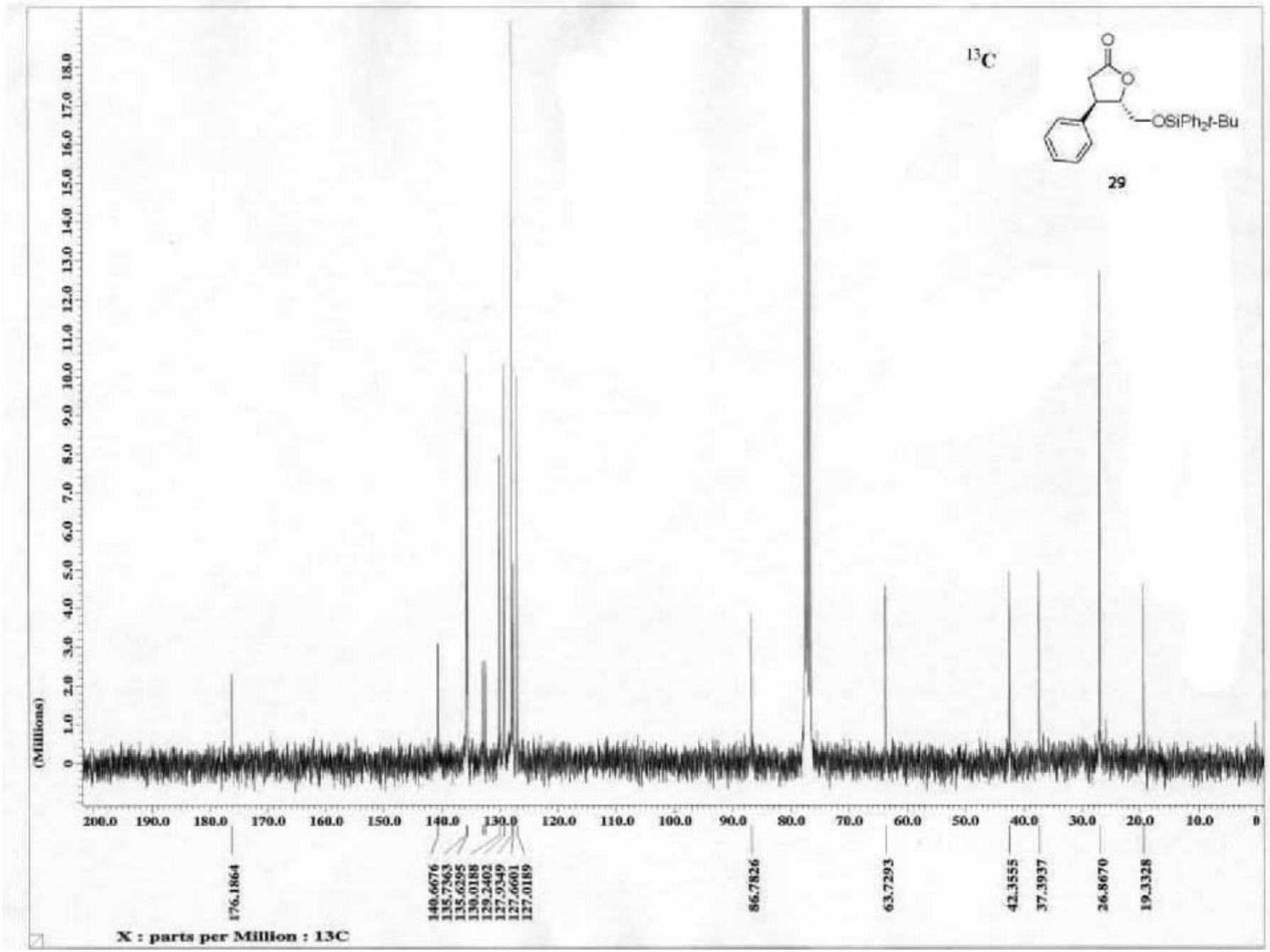

^{1}H
OBn
t-BuPh$_2$SiO
CO$_2$Me
13d
18.43201
3.01935
2.10821
1.01544
1.04142
8.36725
0.99237
1.0
9.19186
(Millions)
X : parts per Million : 1H

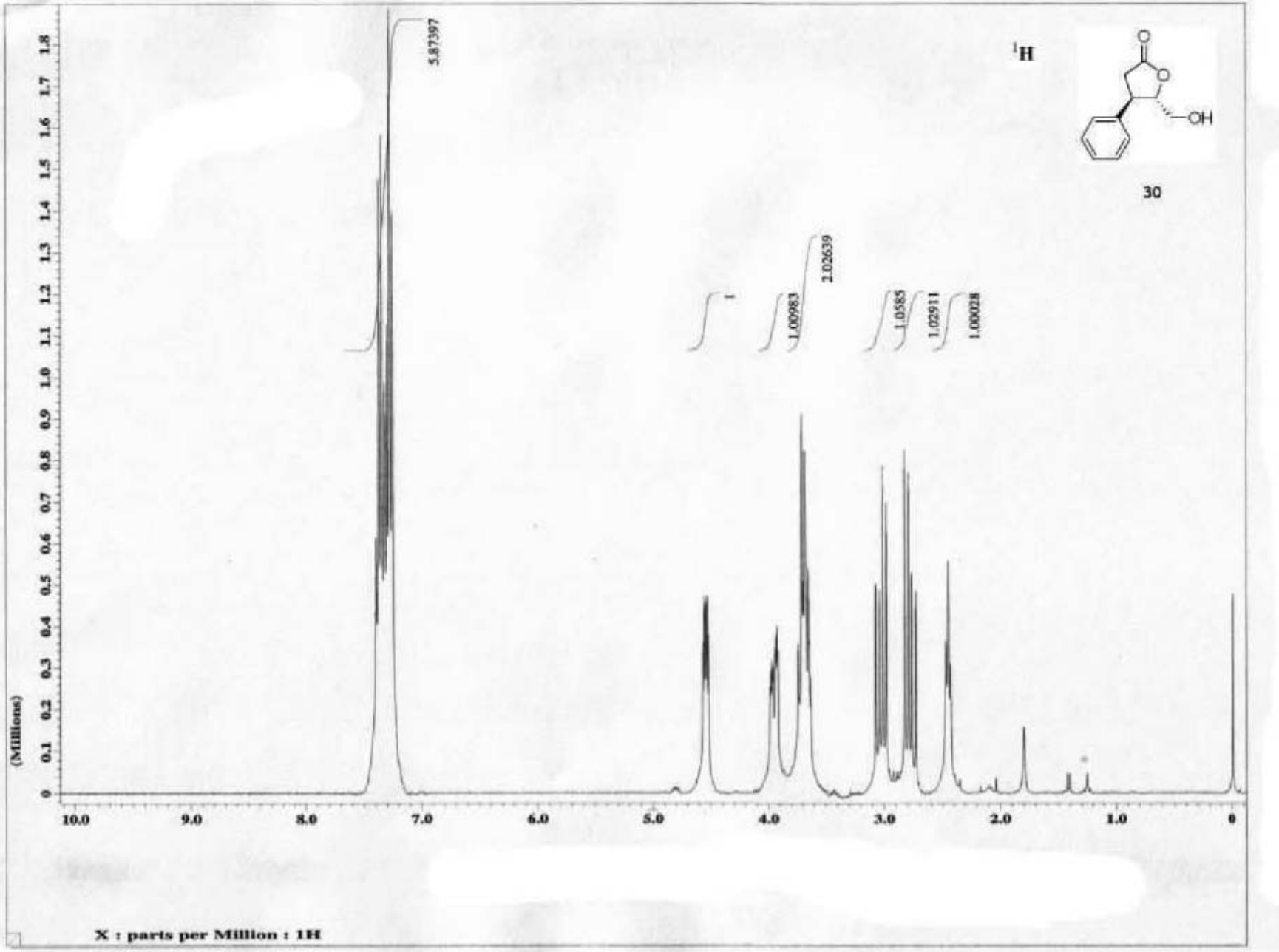

^{13}C
OBn
t-BuPh$_2$SiO
CO$_2$Me
13d
(Millions)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
173.0795
147.6599
146.3546
138.5378
135.7363
135.6371
135.4539
129.7287
128.3853
127.8738
127.7440
127.6066
121.5151
108.5686
108.2938
100.9580
83.4391
72.6911
63.5996
51.4852
43.3631
37.4166
26.9205
19.2870
X : parts per Million : 13C

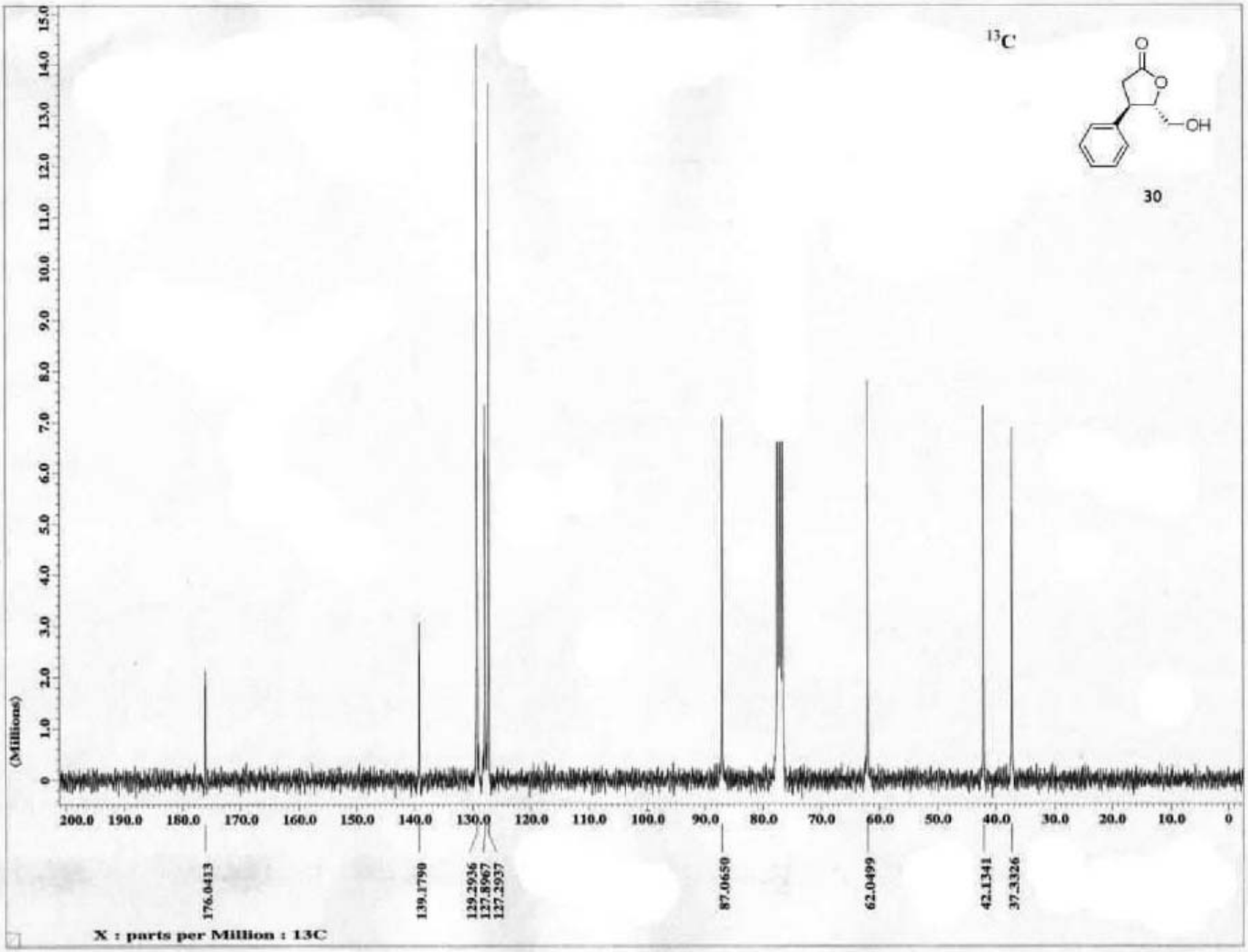

^{1}H
OBn
t-BuPh$_2$SiO
CO$_2$Me
OMe
13f
11.09162
5.17988
1.82078
1.95661
1
1.00731
2.99771
7.31931
1.01411
0.98685
9.21025
(Millions)
X : parts per Million : 1H

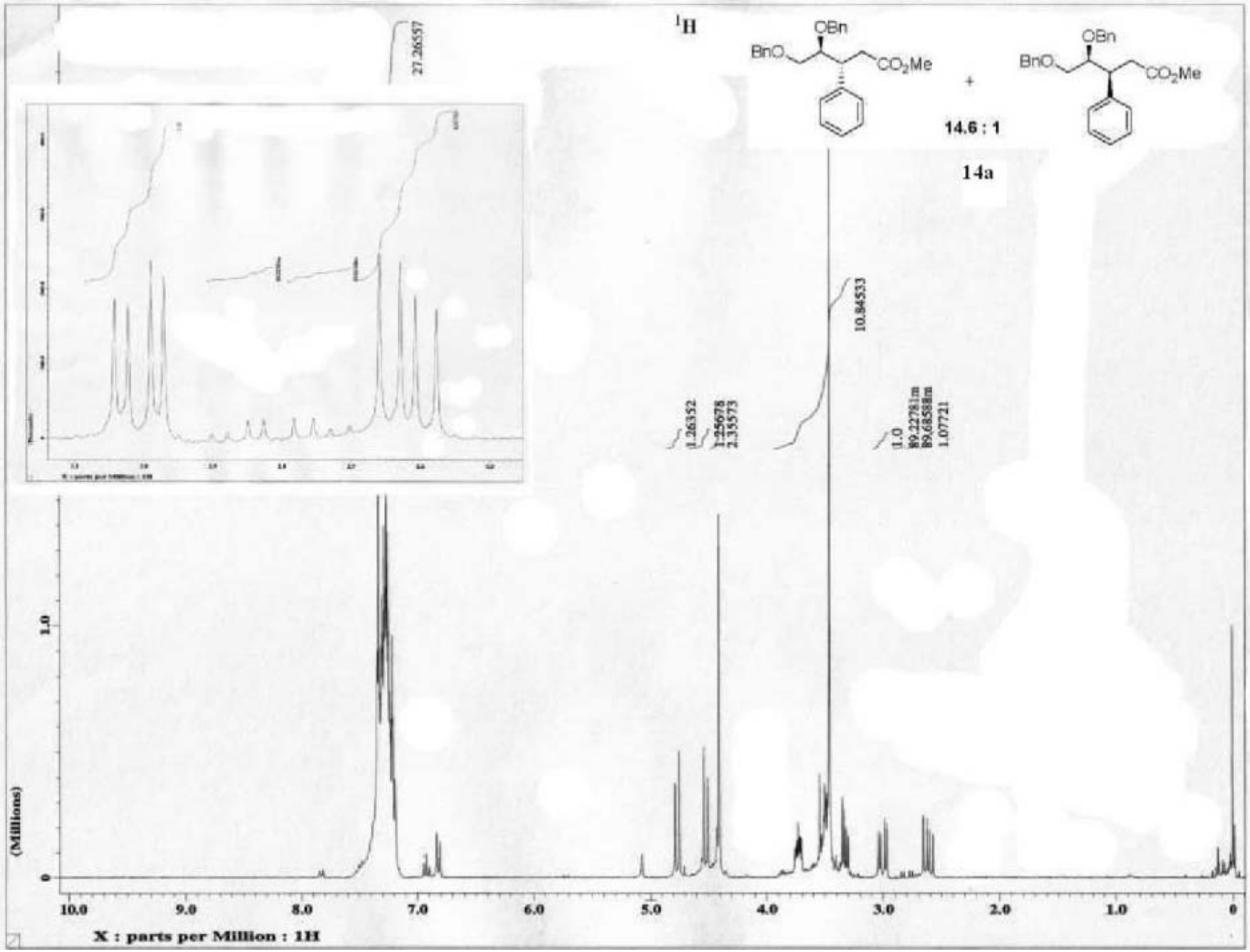

^{13}C
OBn
t-BuPh2SiO
CO2Me
OMe
13f
(Millions)
X : parts per Million : 13C
173.0184
148.8202
143.4386
138.5149
136.3165
135.7134
135.5913
129.7516
128.3847
127.7898
127.7517
127.7059
127.5761
107.8205
101.9580
101.3855
83.4314
72.6605
63.5461
56.4698
51.5004
43.6303
37.3250
26.8976
19.2870

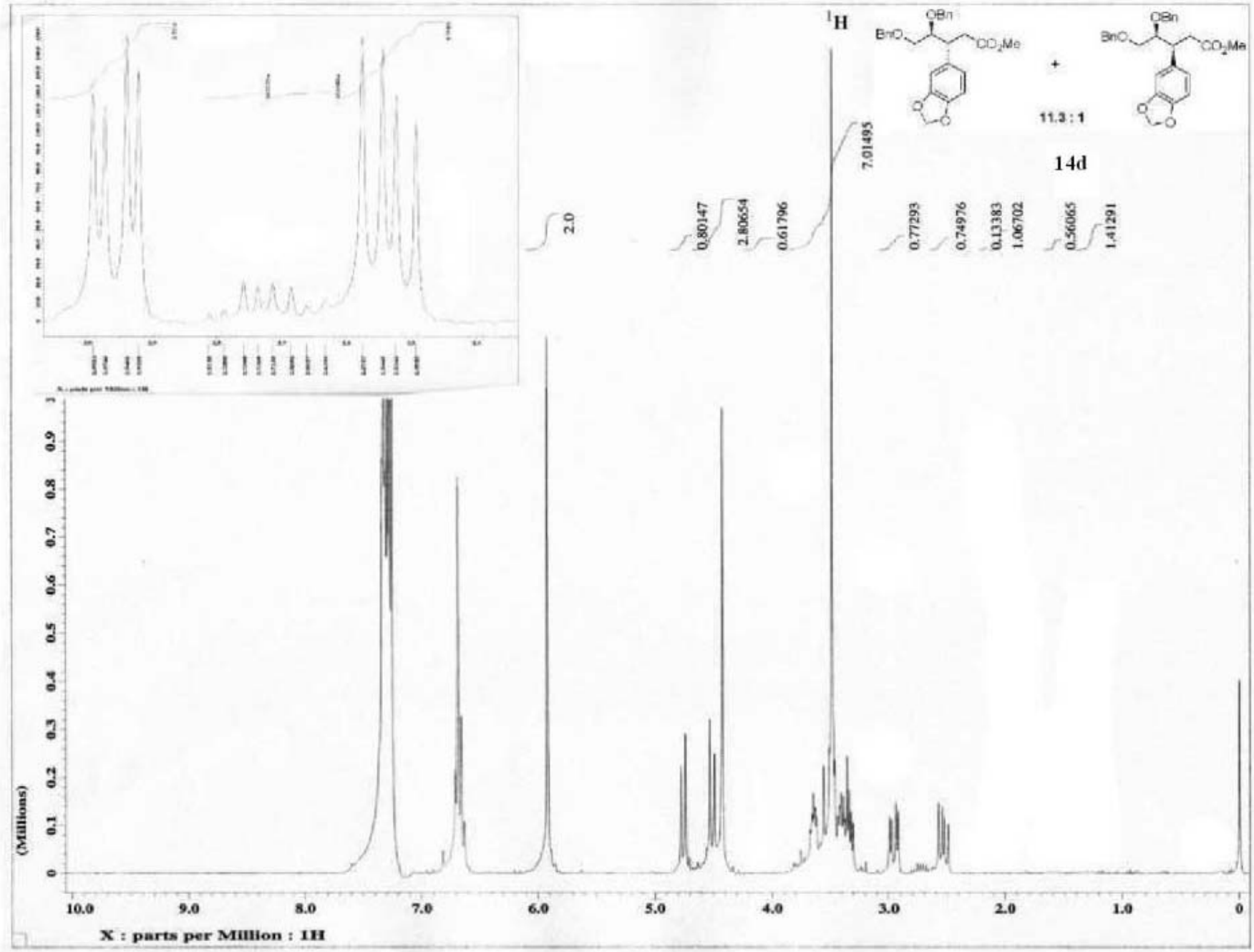

^{1}H
OSiPh$_2$t-Bu
29
19.18906
9.09769
1.00027
0.99959
1.91287
1.01897
(Millions)
X : parts per Million : 1H

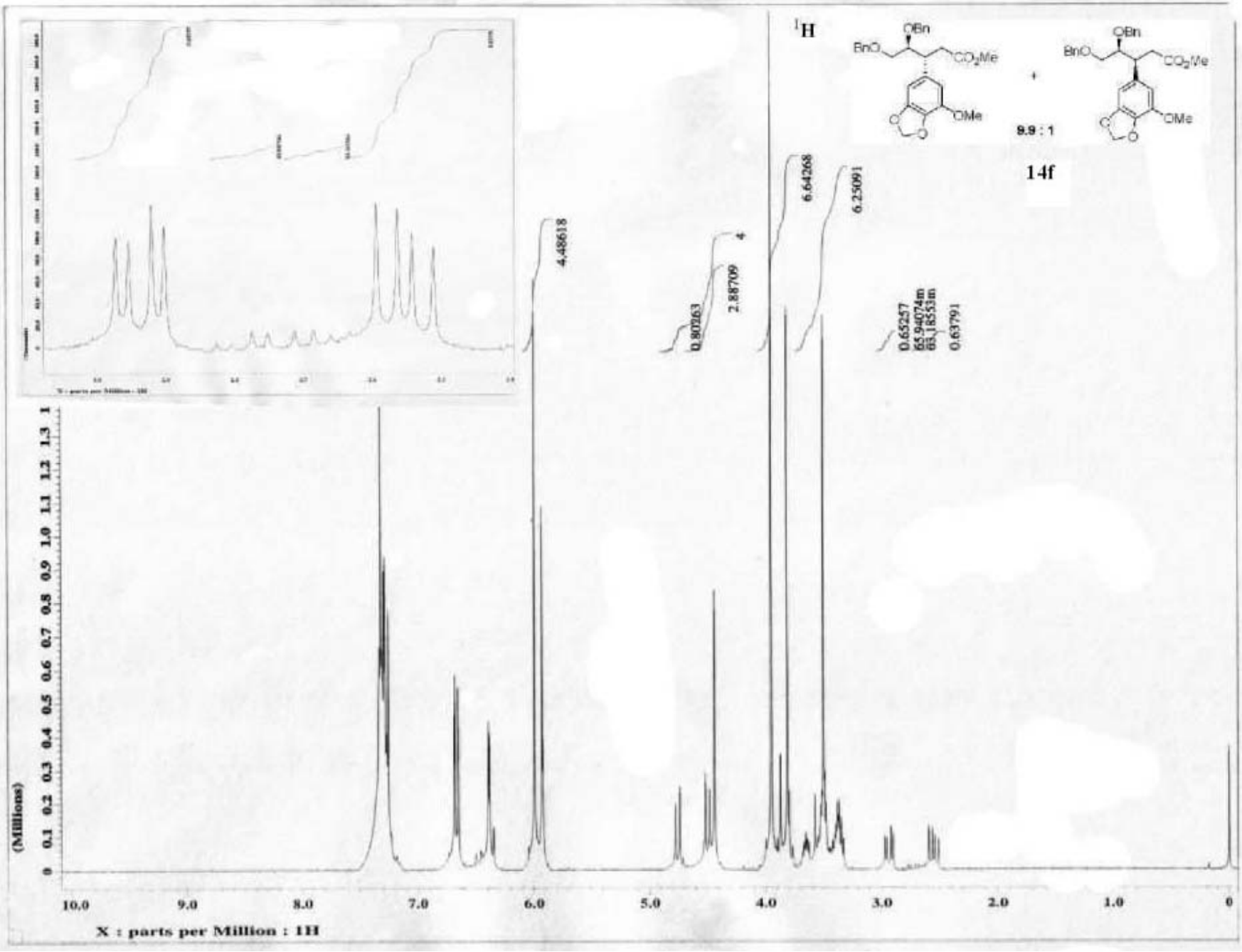

^{13}C
OSiPh$_2$t-Bu
29
(Millions)
X : parts per Million : 13C
176.1864
140.6676
135.7363
135.6295
130.0188
129.2402
127.9349
127.6601
127.0189
86.7826
63.7293
42.3555
37.3937
26.8670
19.3328

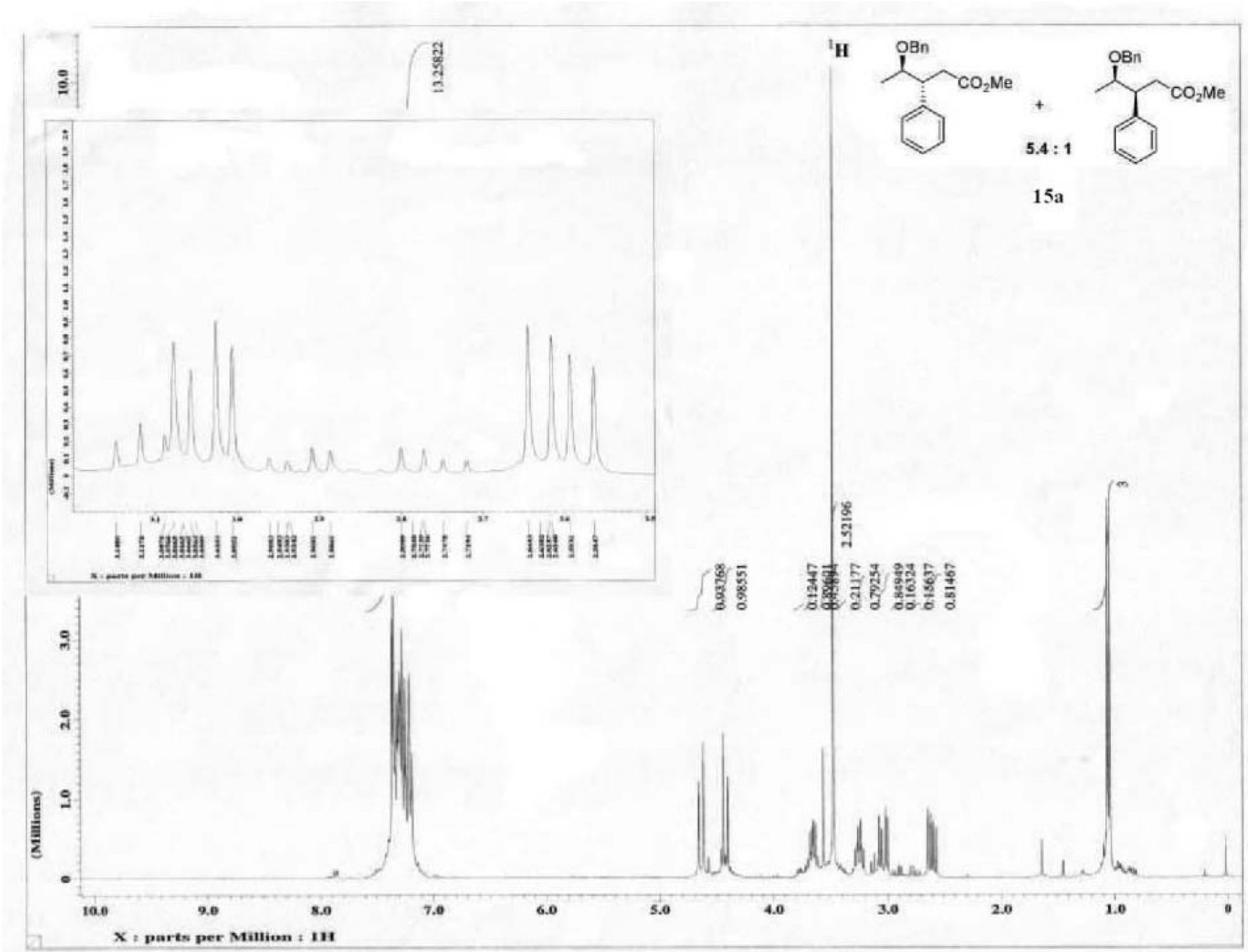

^{1}H
OH
30
5.87397
1
1.00983
2.02639
1.05585
1.02911
1.00028
(Millions)
X : parts per Million : 1H

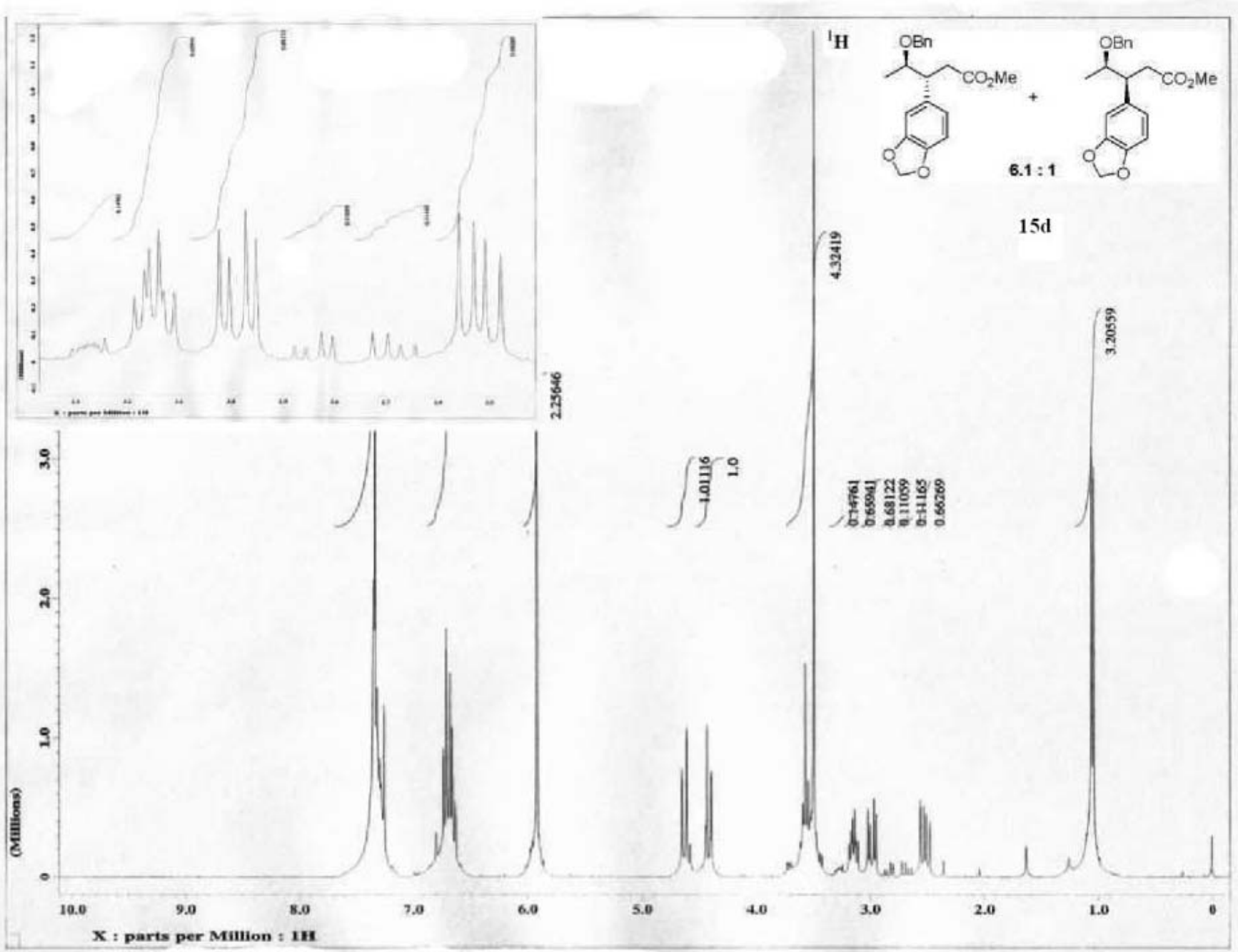

^{13}C
OH
30
(Millions)
X : parts per Million : 13C
176.0413
139.1790
129.2936
127.8967
127.2937
87.0650
62.0499
42.1341
37.3326

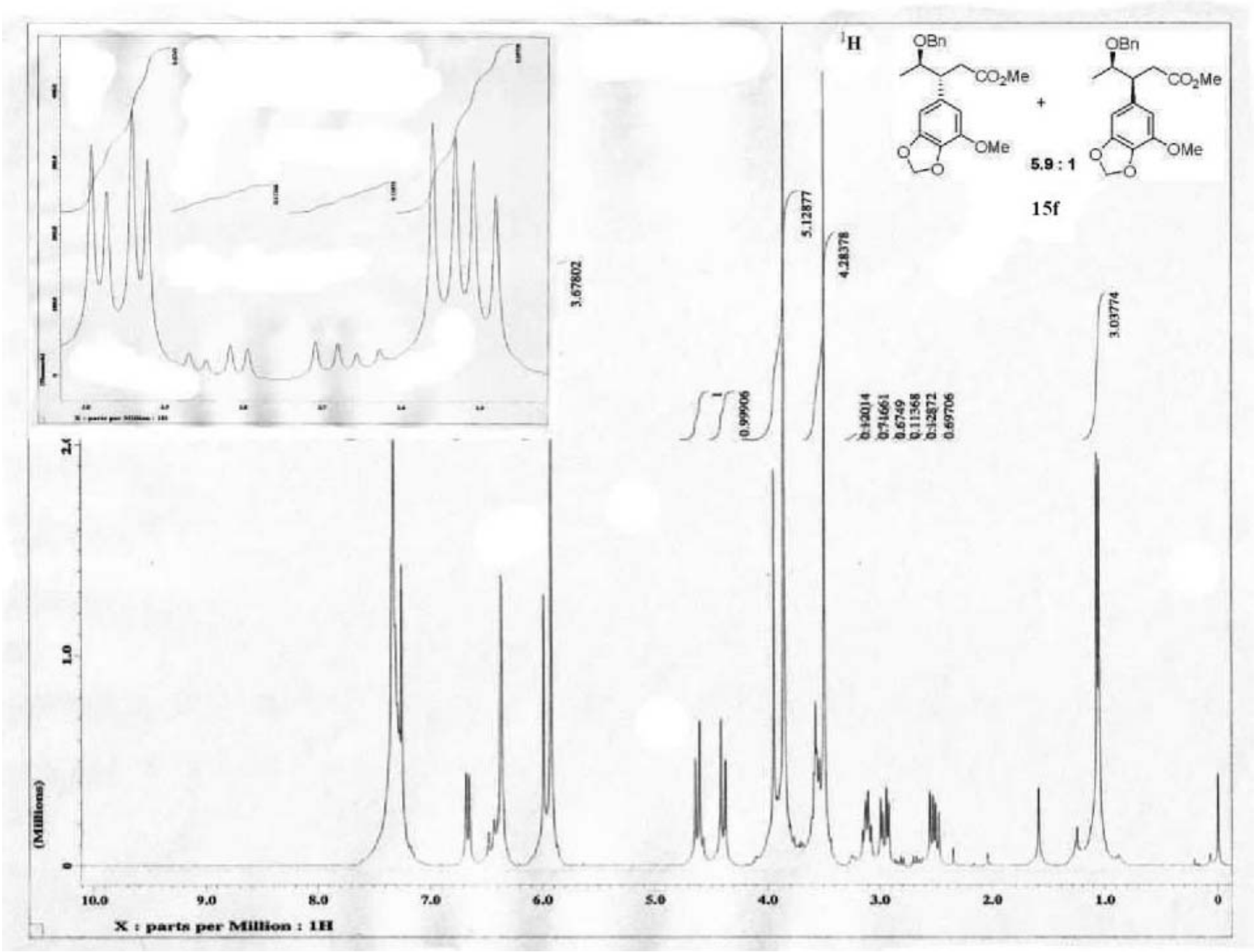

^{1}H
OBn
BnO
CO$_2$Me
+
14.6 : 1
14a
27.26557
10.84533
1.26352
1.25678
2.35573
1.0
89.22781m
89.68588m
1.07721
(Millions)
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : 1H

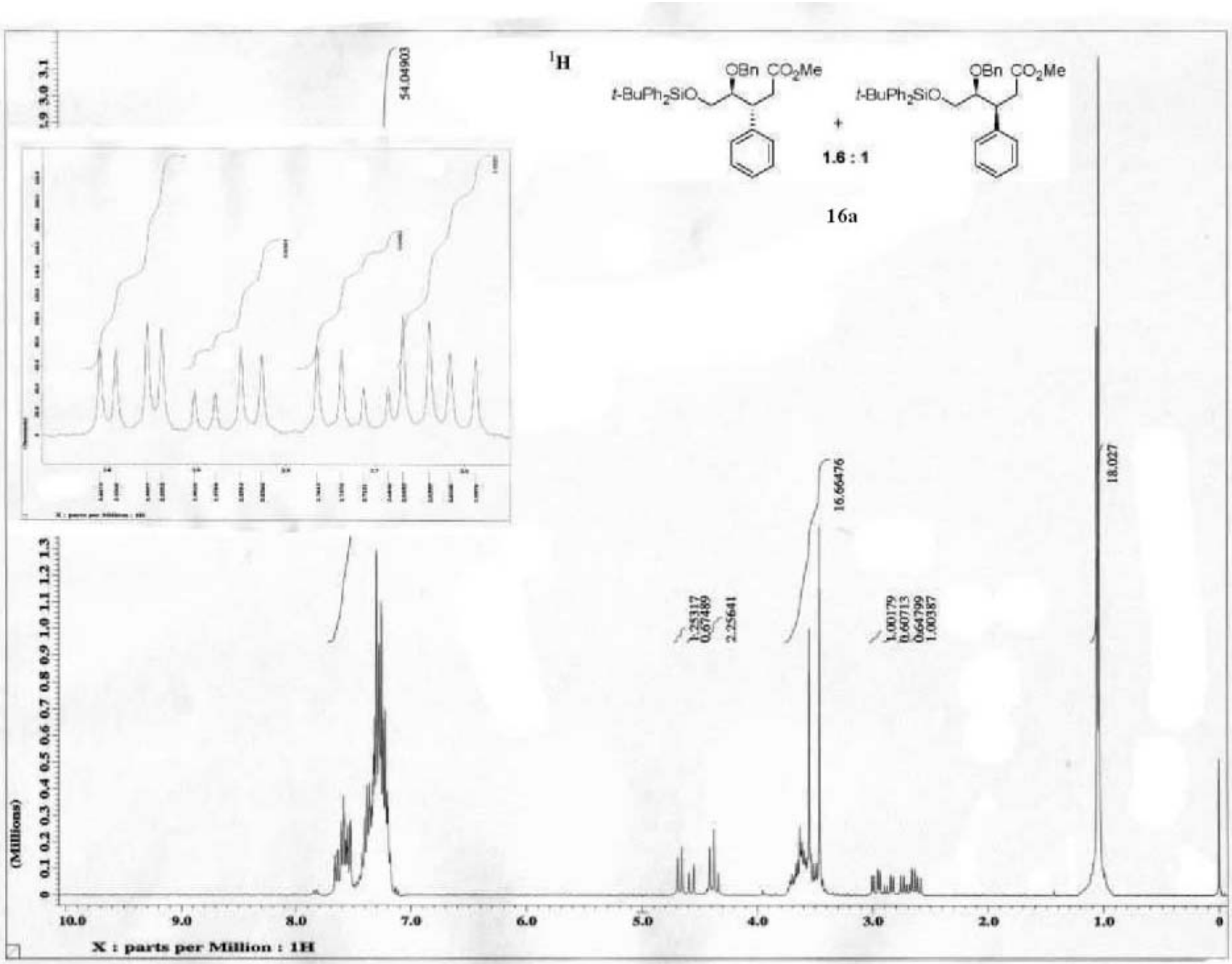

^{1}H
11.3 : 1
14d
2.0
0.80147
2.80654
0.61796
7.01495
0.77293
0.74976
0.13383
1.06702
0.56065
1.41291
(Millions)
X : parts per Million : 1H

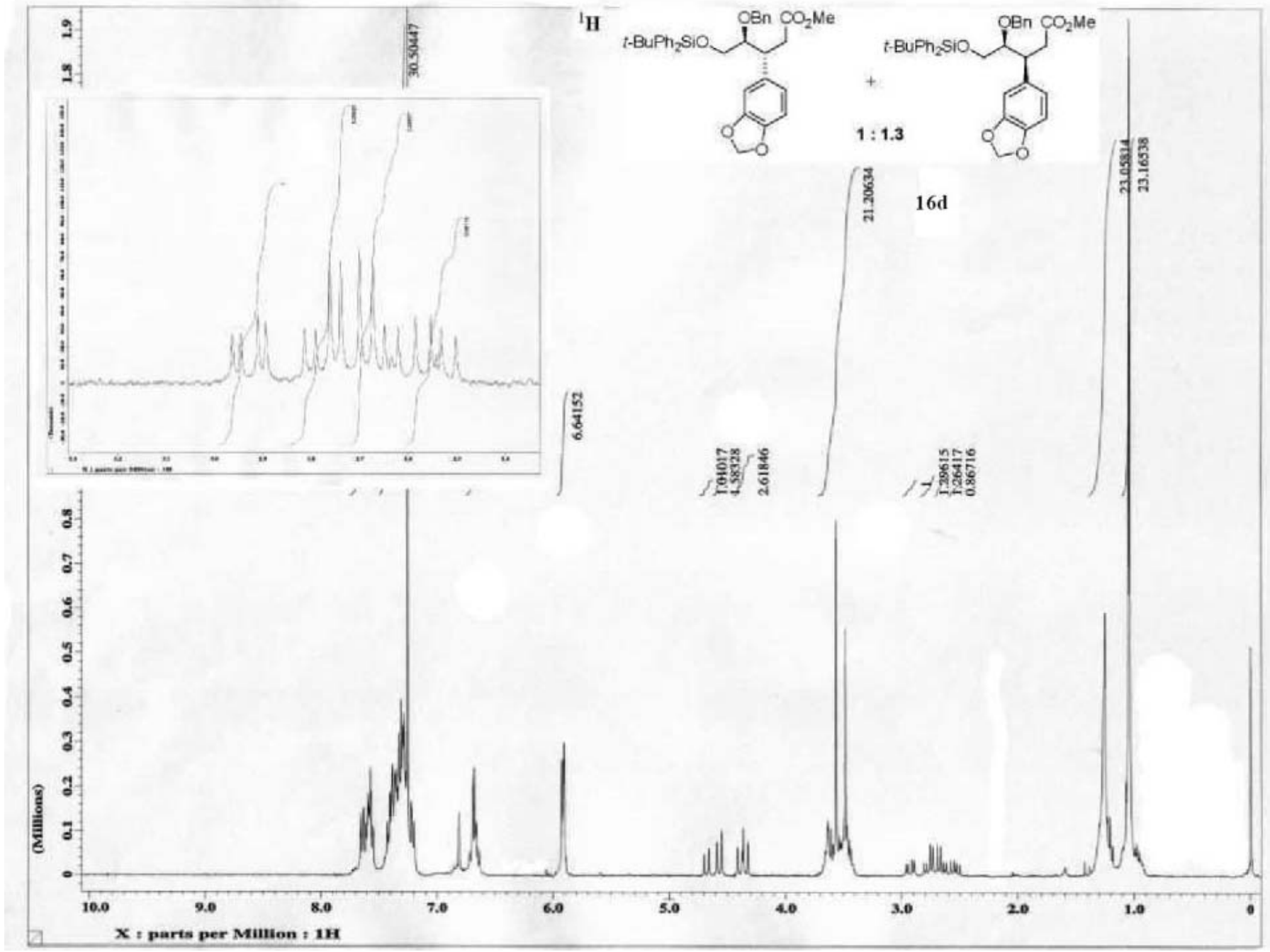

^{1}H
OBn
BnO
CO$_2$Me
OMe
9.9 : 1
14f
4.48618
2.88709
0.80263
6.64268
6.25091
0.65257
65.94074m
63.18553m
0.63791
(Millions)
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
X : parts per Million : 1H

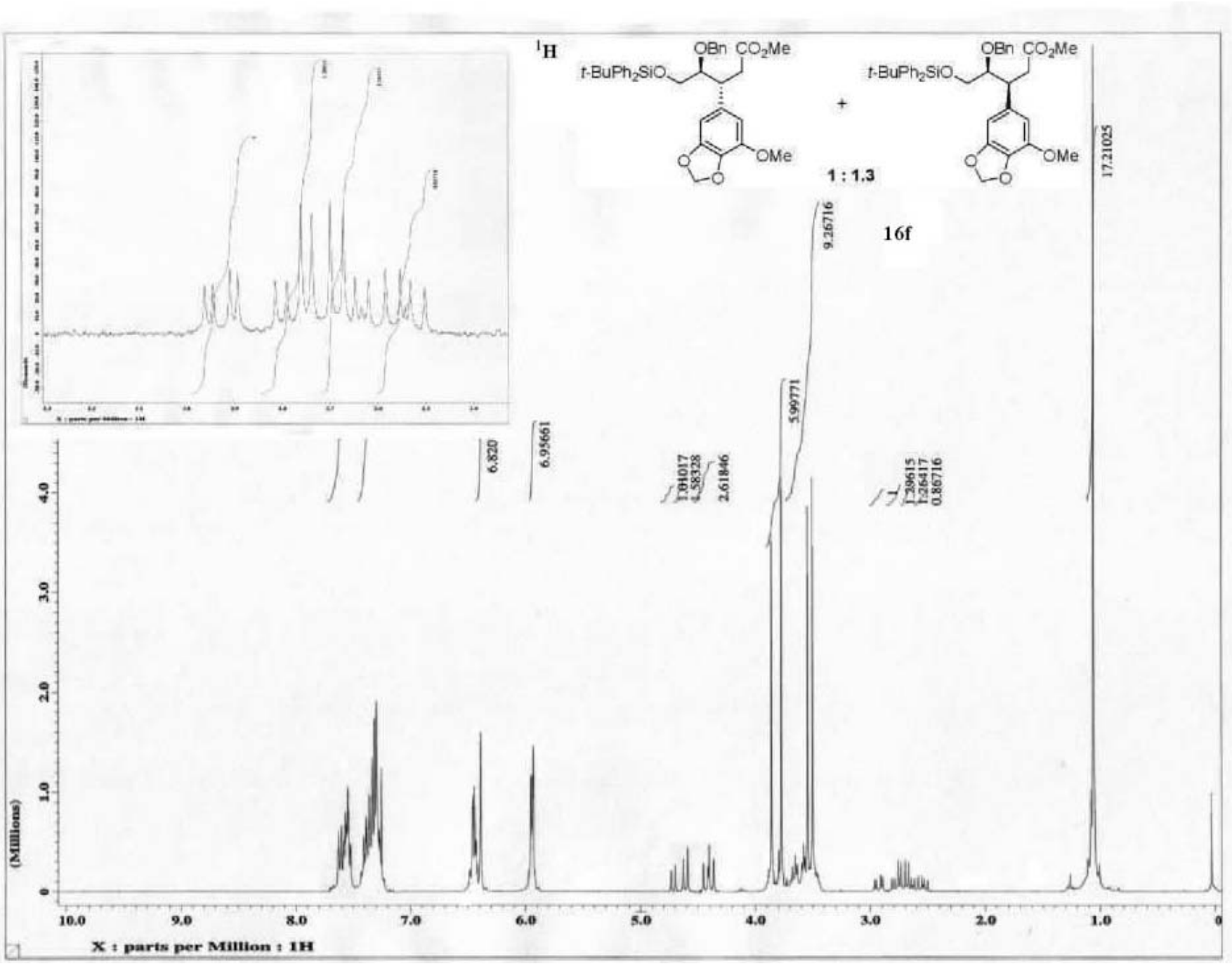

^{1}H
OBn
CO$_2$Me
+
OBn
CO$_2$Me
5.4 : 1
15a
13.25822
10.0
0.93768
0.98551
0.12447
2.52196
0.21177
0.79254
0.84949
0.16324
0.15637
0.81467
(Millions)
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : 1H

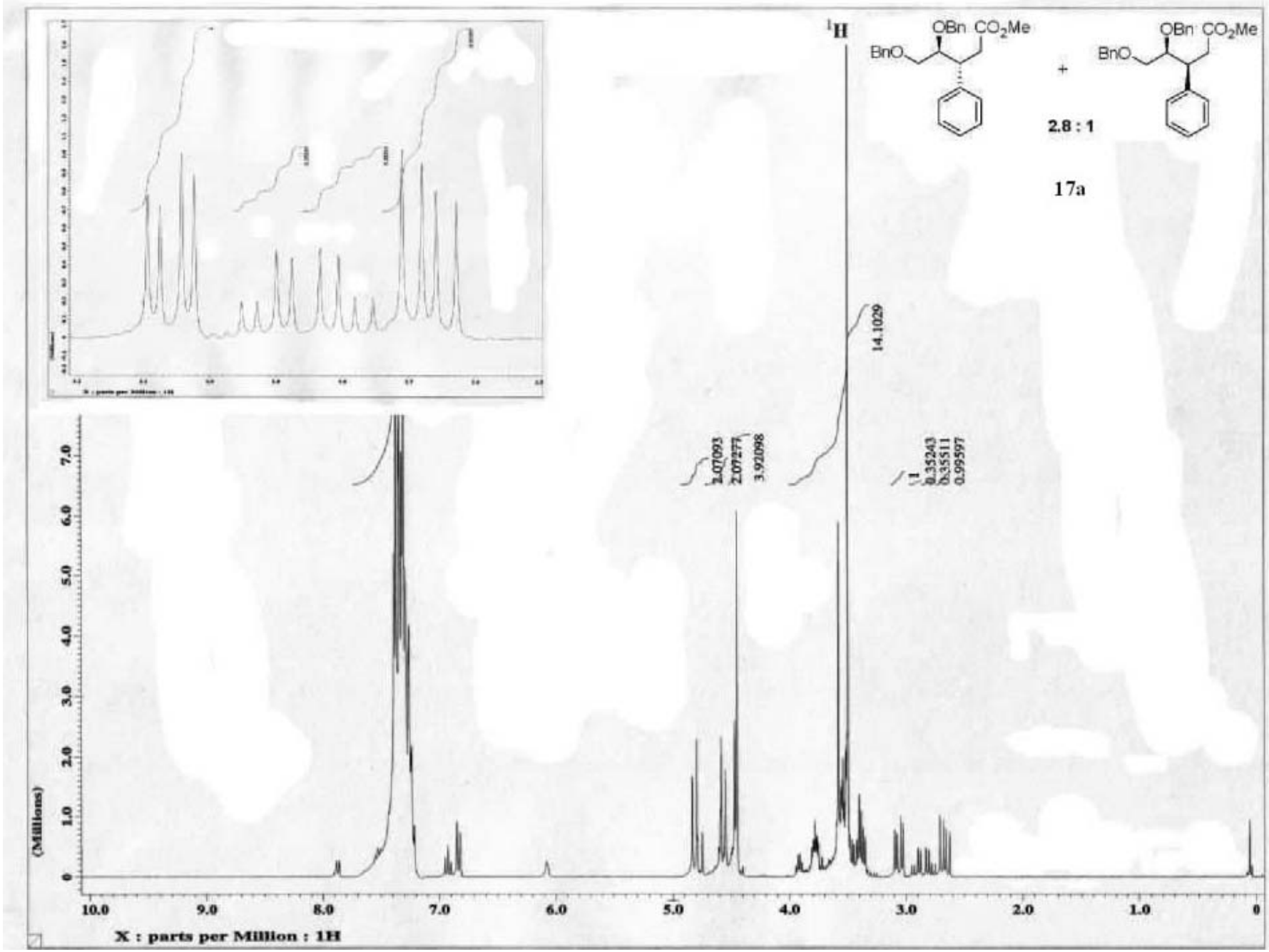

^{1}H
OBn
CO$_2$Me
+
OBn
CO$_2$Me
6.1 : 1
15d
4.32419
3.20559
2.25646
1.01116
1.0
0.74761
0.65941
0.68122
0.11059
0.11165
0.66269
(Millions)
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : 1H

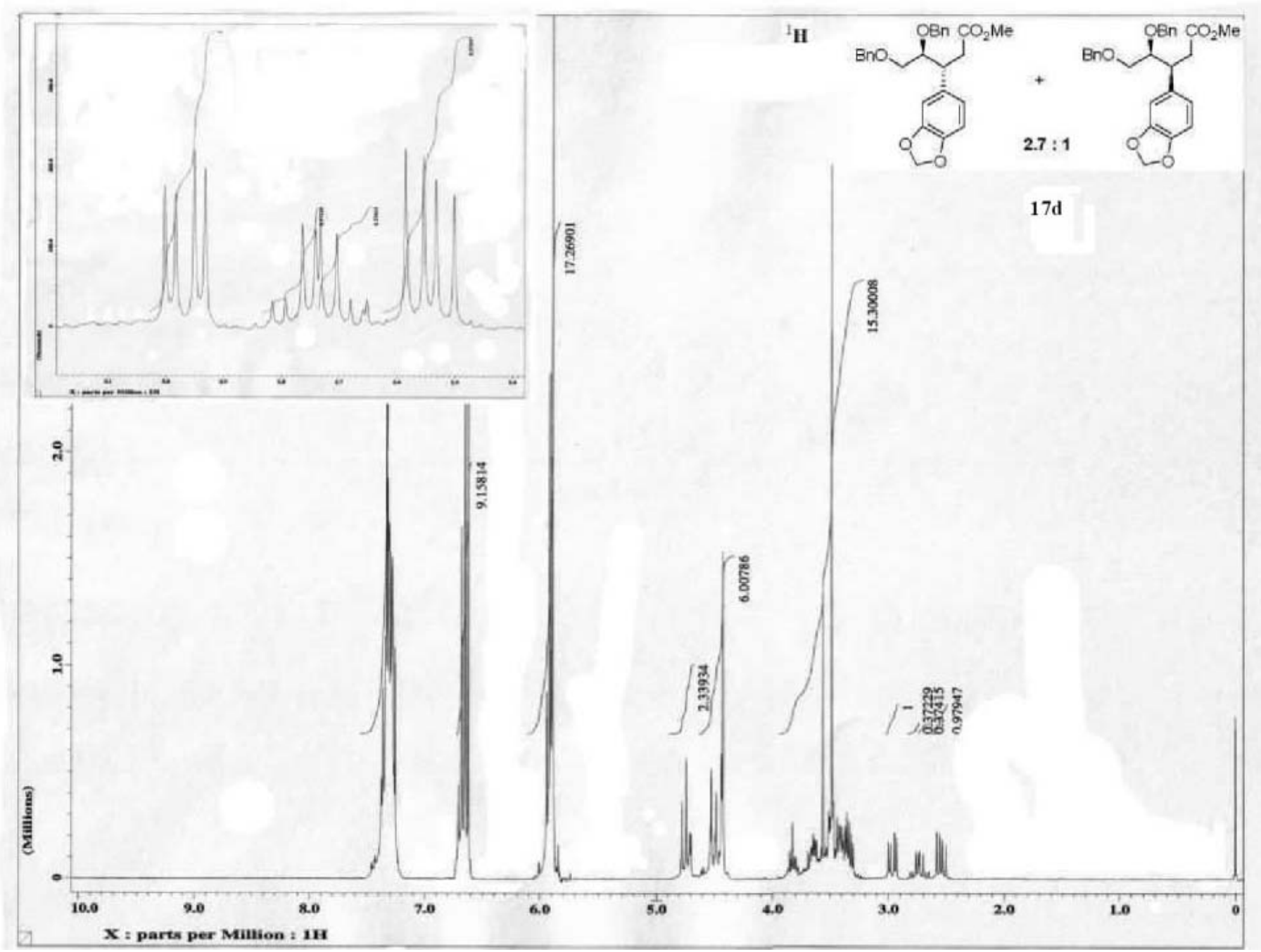

^{1}H
OBn
CO$_2$Me
OMe
+
5.9 : 1
15f
3.67802
5.12877
4.28378
3.03774
0.99906
(Millions)
X : parts per Million : 1H

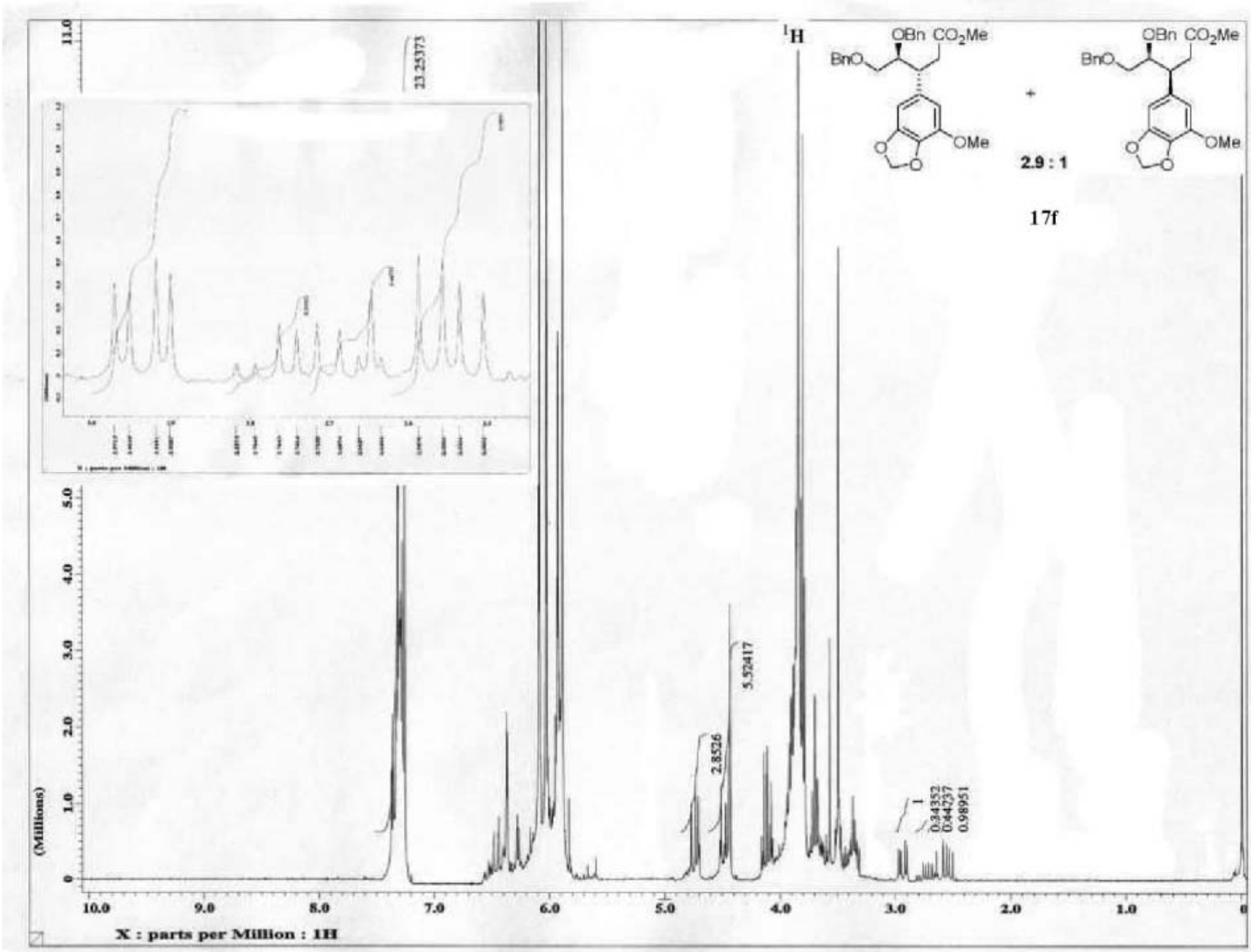

^{1}H
OBn CO$_2$Me
t-BuPh$_2$SiO
+
1.6 : 1
OBn CO$_2$Me
t-BuPh$_2$SiO
16a
54.04903
16.66476
18.027
1.25317
0.67489
2.25641
1.00179
0.60713
0.64799
1.00387
(Millions)
X : parts per Million : 1H

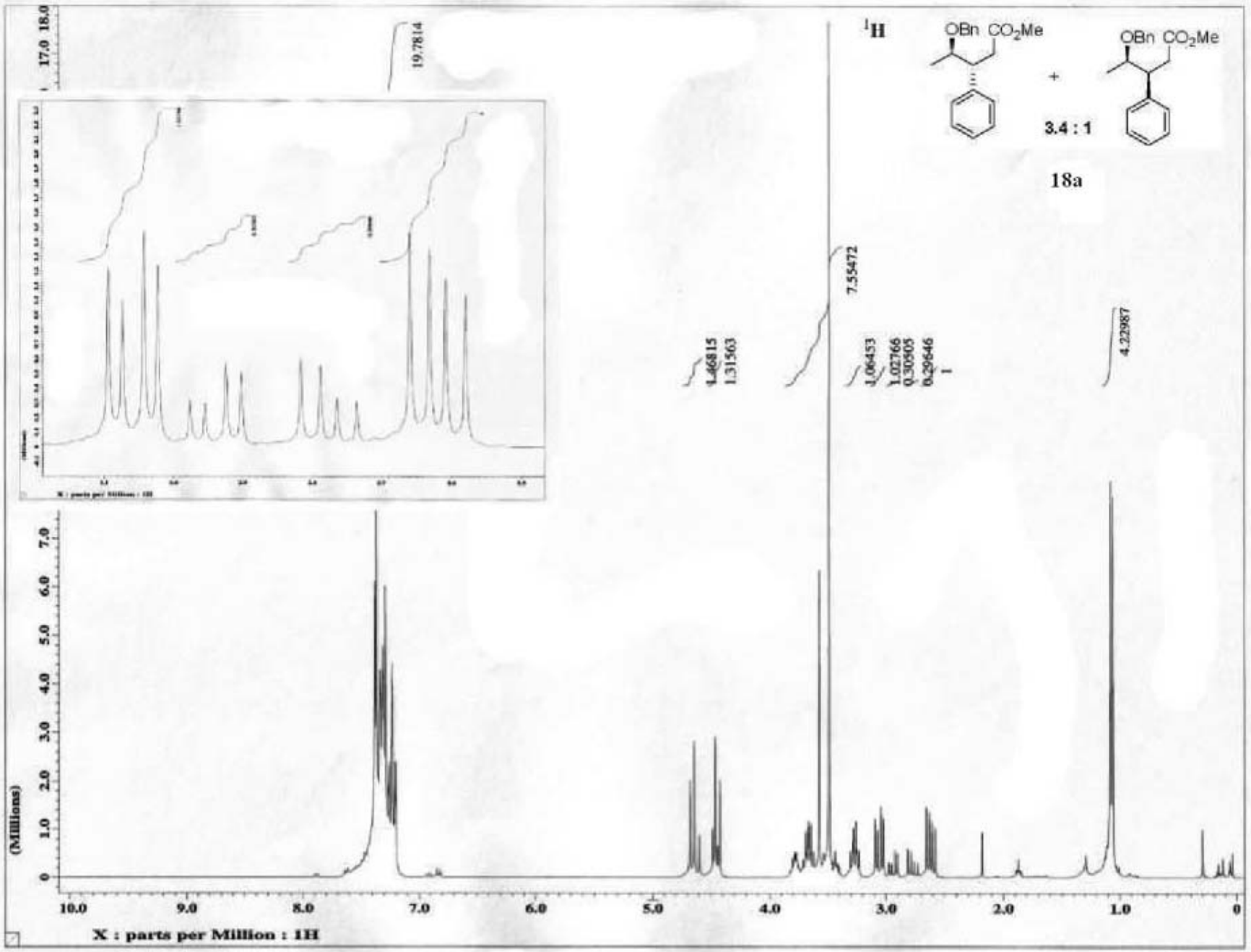

^{1}H
t-BuPh$_2$SiO
OBn
CO$_2$Me
1 : 1.3
16d
21.20634
23.05814
23.16538
6.64152
4.04017
4.58328
2.61846
1.39615
1.26417
0.86716
30.50447
(Millions)
X : parts per Million : 1H

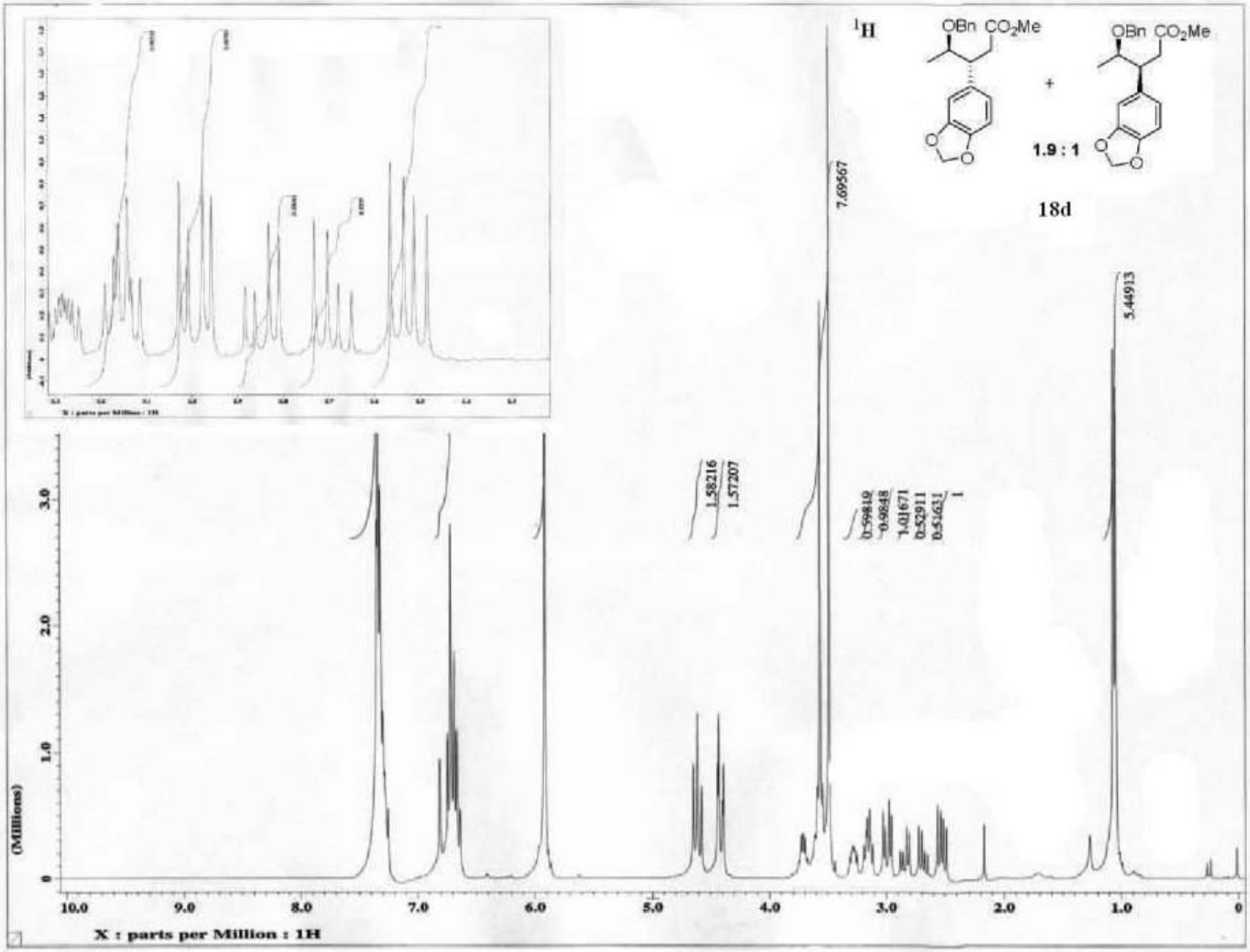

^{1}H
t-BuPh$_2$SiO
OBn CO$_2$Me
OMe
+
1 : 1.3
16f
9.26716
17.21025
5.99771
6.95661
6.820
1.01017
4.58328
2.61846
1.28615
1.26417
0.86716
(Millions)
X : parts per Million : 1H

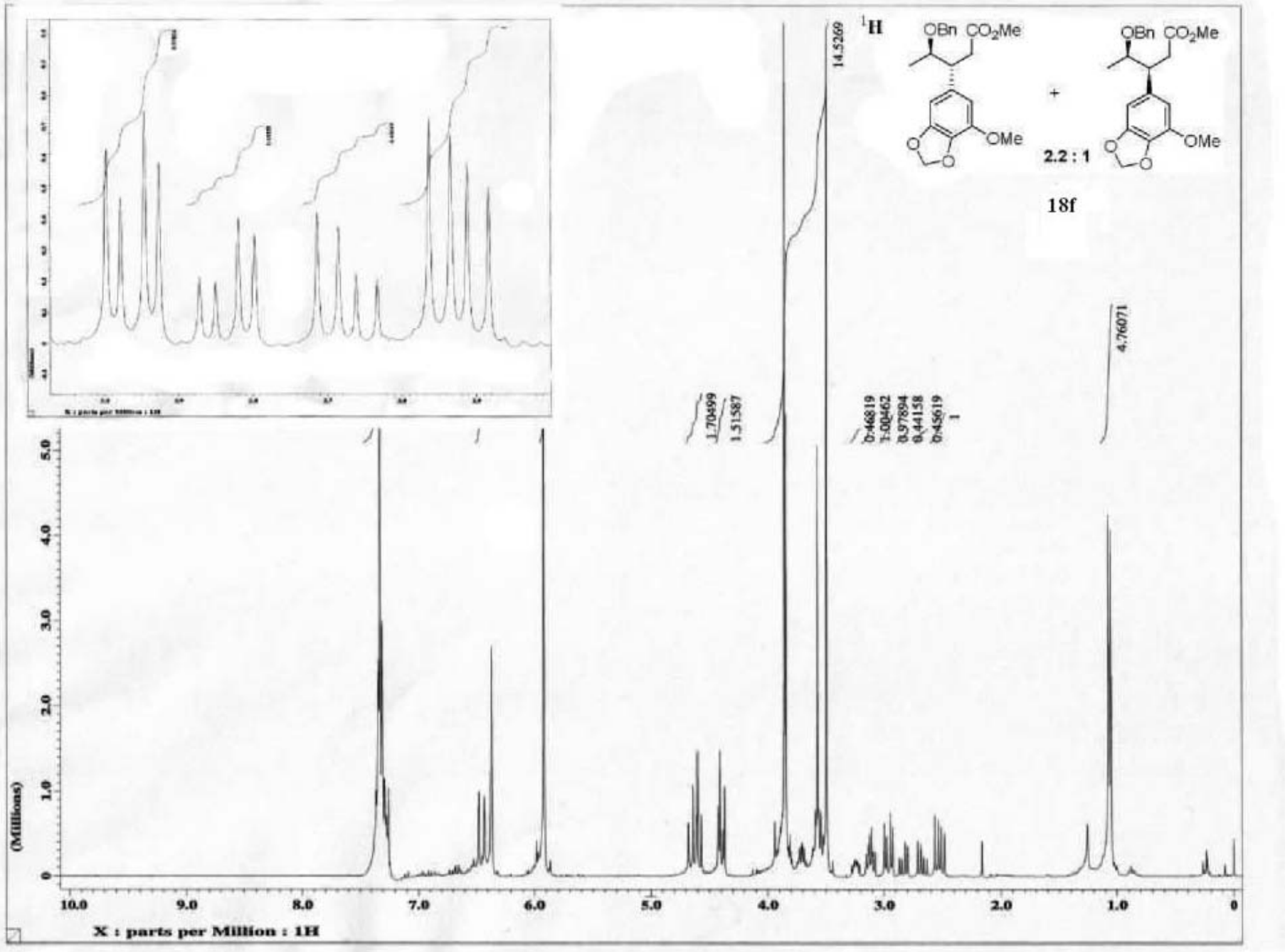

^{1}H
OBn CO$_2$Me
BnO
+
OBn CO$_2$Me
BnO
2.8 : 1
17a
14.1029
2.07093
2.09277
3.92098
1
0.35243
0.35511
0.99597
(Millions)
X : parts per Million : 1H


^{1}H
OBn CO$_2$Me
BnO
+
2.7 : 1
17d
17.26901
15.30008
9.15814
6.00786
2.33934
1
0.37229
0.30415
0.97947
(Millions)
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : 1H


^{1}H
OBn CO$_2$Me
BnO
OMe
+
OBn CO$_2$Me
BnO
OMe
2.9 : 1
17f
23.25373
2.8526
3.52417
1
0.34352
0.84237
0.98951
(Millions)
X : parts per Million : 1H


^{1}H
OBn CO$_2$Me
+
OBn CO$_2$Me
3.4 : 1
18a
19.7814
7.55472
4.22987
1.46815
1.31563
1.06453
1.02766
0.30505
0.29646
(Millions)
X : parts per Million : 1H


^{1}H
OBn CO$_2$Me
+
OBn CO$_2$Me
1.9 : 1
18d
7.69567
5.44913
1.58216
1.57207
0.99819
0.98848
1.01671
0.52911
0.51621
1
(Millions)
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : 1H


^{1}H
OBn CO$_2$Me
OMe
+
2.2 : 1
18f
14.5269
4.76071
1.70499
1.51587
0.46819
1.00462
0.97894
0.44158
0.45619
1
(Millions)
X : parts per Million : 1H