Supplementary Information

Nucleophilic deoxyfluorination of catechols

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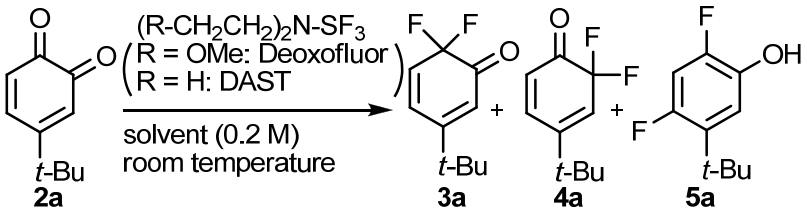
The solvent Effect on the fluorination reaction of 2a

Under a nitrogen atmosphere, Deoxofluoro (6.0 equiv) was added to a solution of **2a** (1.0 equiv) in anhydous solvent (0.2 M) at 0 °C, and the resulting solution was stirred at room temperature for reaction time indicated below. The reaction mixture was quenched with ice-water, the layers were separated, and the aqueous layer was extracted three times with CH_2Cl_2. The combined organic layers were dried (Na_2SO_4), filtered, and concentrated *in vacuo.* The yields of **3a**–**5a** were determined by the ^{19}F NMR (470 MHz, $CDCl_3$) spectra of the crude reaction mixture with 4-fluorotoluene as the internal standard. The solvent, the reaction time, and the yields of **3a**–**5a** are summarized in Table S1.

Table S1 The solvent effect on the fluorination reaction of **2a**

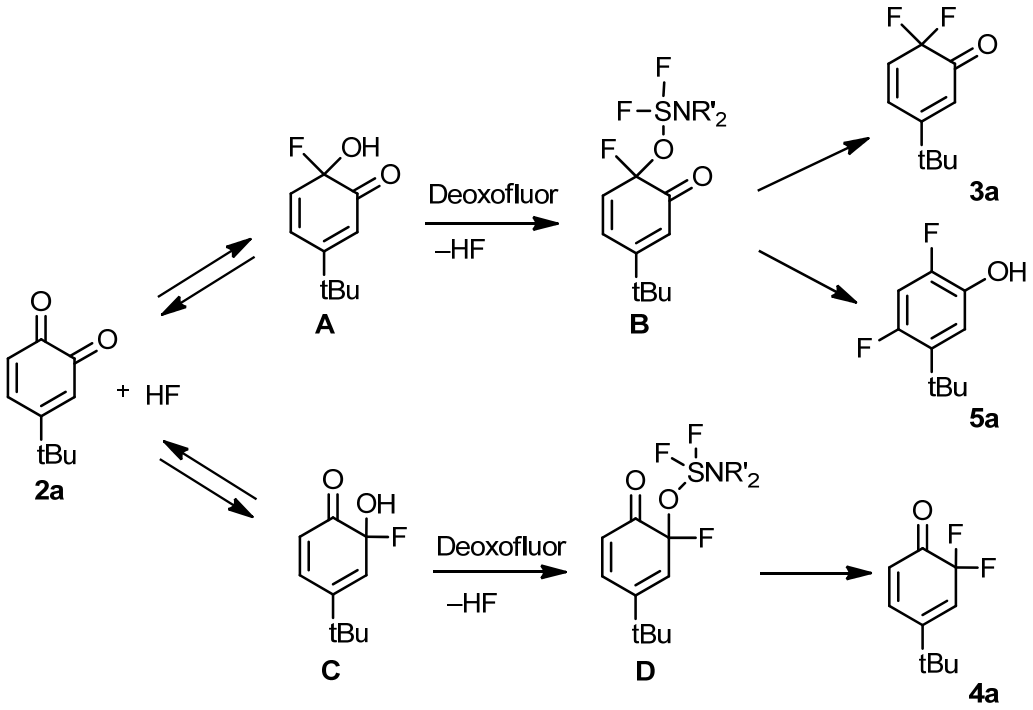


Entry	Reagent	Solvent	Time (h)	Yields[a] 3a	4a	5a
1	Deoxofluor	CH_3CN	4.0	16	2	7
2	Deoxofluor	acetone	6.0	6	0	0
3	Deoxofluor	CH_2Cl_2	2.5	33	18	8
4	Deoxofluor	$CHCl_3$	1.0	43	10	26
5	Deoxofluor	DME	6.0	45	9	13
6	Deoxofluor	THF	6.0	3	4	1
7	Deoxofluor	1.4-Dioxane	6.0	44	3	24
8	Deoxofluor	Et_2O	2.0	22	6	6
9	Deoxofluor	toluene	1.0	36	7	27
10	DAST	$CHCl_3$	1.0	37	9	32

a) ^{19}F-NMR yield using 4-fluorotoluene as an internal standard.

A plausible reaction mechanism for the deoxyfluorination of *ortho*-quinone 2a.

A trace amount of HF in Deoxofluor reacts with **2a** to give a primary intermediate **A**. Then, **A** reacts with Deoxofluor to give **B**, which produces **3a** and **5a** via **B**. As a side path, **2a** and Deoxofluor give **4a** via **C** and **D**.



Experimental Section

General considerations

Reagents: Bu_4NF (TBAF, 1.0 M solution in THF) was obtained from Aldrich Chemical Co. and *n*BuLi (1.6 M solution in *n*-hexane) was purchased from Kanto Chemical Co. Anhydrous THF and chloroform were purchased from Wako Pure Chemical Industries and used without further purification. (–)-Epigallocatechin was a gift from Mitsui Norin Co., Ltd. 3-(Benzyloxy)benzene-1,2-diol (**1g**),[1] 3-methoxy-5-methylbenzene- 1,2-diol (**1h**),[2] and methyl 3-(benzyloxy)-4,5-dihydroxybenzoate (**1i**)[3] were synthesized according to the literature. All other reagents were purchased from Tokyo Chemical Industry Co., Aldrich Chemical Co., Kanto Chemical Co., Kishida Chemical Co., Nacalai Tesque or Wako Pure Chemical Industries and used without further purification. Flash chromatography was performed with silica gel 60 N, spherical neutral (40–50 μm) purchased from Kanto Chemical Co.

Analytical methods. IR spectra were obtained on a JASCO WS/IR-8000. ^{1}H NMR, ^{13}C, and ^{19}F NMR spectra were recorded on a JEOL JMN-A500 or ECA-500 (^{1}H: 500 MHz, ^{13}C: 125 MHz, ^{19}F: 470 MHz) instrument with chemical shifts reported in ppm relative to the residual deuterated solvent or the internal standard tetramethylsilane. Chemical shift of ^{19}F NMR spectra reported in ppm relative to hexafluorobenzene (–164.9 ppm) as an internal standard. The mass spectra were measured on a Bruker micrOTOF, JEOL JMS-700 MStation, and JMS-T100TD spectrometer. Yield refers to isolated yields of compounds greater than 95% purity as determined by ^{1}H NMR analysis. ^{1}H NMR and melting points (where applicable) of all known compounds were taken. All new products were further characterized by elemental analysis or HRMS.

General procedure for the oxidation and deoxyfluorination (Table 1)

Method A. Under a nitrogen atmosphere, an oxidant [$PhI(OAc)_2$ or *o*-chloranil (1.05 equiv)] was added to a solution of a catechol **1** (1.0 equiv) in anhydous $CHCl_3$ (0.2 M) at 0 °C, and the resulting solution was stirred at room temperature for 5 min. Deoxofluor (6.0 equiv) was added at 0 °C, and the reaction mixture was stirred at room temperature for 1 h before being quenched with ice-water. The layers were separated, and the aqueous layer was extracted three times with CH_2Cl_2. The combined organic layers were dried (Na_2SO_4), filtered, and concentrated *in vacuo.* The residue was purified by flash column chromatography to give a mixture of the difluoroketones (**3** and **4**) and the difluorophenol **5**.

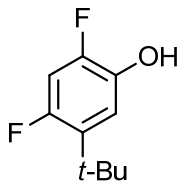
Method B. An oxidant [$PhI(OAc)_2$ or *o*-chloranil (1.05 equiv)] and MgO (2.3 equiv) were added to a solution of a catechol **1** (1.0 equiv) in $CHCl_3$ (0.2 M) at 0 °C, and the resulting solution was stirred at room temperature for 5 min. The reminder of the procedure is the same as described in general procedure A.

General procedure for the reduction of difluoroketone (Table 1)

Method C. $NaBH_4$ (5.0 equiv) and DBU (5.0 equiv) were added to a solution of the above-mentioned mixture of the difluoroketones (**3** and **4**) in MeOH or EtOH (0.1 M) at 0 °C. The reaction mixture was stirred at 50 °C for 30 min before being quenched with saturated aq. NH_4Cl solution. The organic layer was separated, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried (Na_2SO_4), filtered, and concentrated *in vacuo*. The purification of the residue by flash column chromatography afforded the fluorophenol **6** and its regioisomer **7**.

Method D. $NaBH_4$ (5.0 equiv) was added to a solution of the above-mentioned mixture of the difluoroketones (**3** and **4**) in EtOH (0.1 M) at 0 °C. The reaction mixture was stirred at 50 °C for 30 min before being quenched with saturated aq. 1N HCl solution. The organic layer was separated, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried (Na_2SO_4), filtered, and concentrated *in vacuo*. The reminder of the procedure is the same as described in method A.

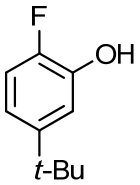
Entry 1 in Table 1: By methods A and C, the use of **1a** (100 mg, 0.60 mmol), *o*-chloranil (155 mg, 0.63 mmol), Deoxofluor (0.66 mL, 3.6 mmol), $NaBH_4$ (114 mg, 3.0 mmol), and DBU (0.45 mL, 3.0 mmol) in EtOH gave **5a** (11 mg, 10%) and a mixture of **6a** and **7a** (53 mg, 53%, **6a**:**7a** = 75:25). Further purification of the mixture of **6a** and **7a** by column chromatography (hexanes–AcOEt 20:1) gave analytically pure **6a** and **7a**.



5-*tert*-Butyl-2,4-difluorophenol (5a)

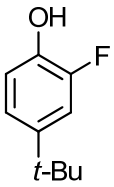
A Colorless oil: ^1H NMR (500 MHz, $CDCl_3$) δ: 1.33 (9H, s), 4.84 (1H, d, J = 4.0 Hz), 6.78 (1H,

dd, J = 10.5, 11.5 Hz), 6.93 (1H, dd, J = 8.0, 10.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 29.8 (d, J = 3.5 Hz), 34.0 (d, J = 3.5 Hz), 104.5 (dd, J = 21.0, 30.0 Hz), 115.3 (dd, J = 2.5, 7.5 Hz), 133.7 (dd, J = 5.0, 13.0 Hz), 138.2 (dd, J =2.4, 13.0 Hz), 148.3 (dd, J = 13.0, 237 Hz), 154.6 (dd, J = 9.5, 242 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –144.3 (1F, dd, J = 11.5, 23.0), –119.6 (1F, dd, J = 10.5, 23.0). IR ($CHCl_3$): 3584 cm^{-1}. HRMS Calcd for $C_{10}H_{12}F_2O$ (M^+) m/z: 186.0856, found: 186.0858.



5-*tert*-Butyl-2-fluorophenol (6a)

A colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ: 1.29 (9H, s), 5.10 (1H, brs), 6.86 (1H, ddd, J = 2.5, 4.5, 8.5 Hz), 6.98 (1H, dd, J = 8.5, 11.5 Hz), 7.03 (1H, dd, J = 2.5, 9.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 31.4, 34.4, 114.5, 114.6 (d, J = 16.5 Hz), 117.5 (d, J = 6.0 Hz), 142.6 (d, J = 14.5 Hz), 148.1 (d, J = 3.5 Hz), 148.9 (d, J = 234 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –149.1 (ddd, J = 4.5, 9.0, 11.5 Hz). IR ($CHCl_3$): 3585, 3568 cm^{-1}. HRMS Calcd for $C_{10}H_{13}FO$ (M^+) m/z: 168.0950, found: 168.0945.

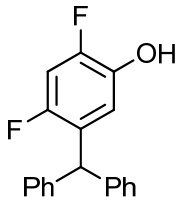


4-*tert*-Butyl-2-fluorophenol (7a)

A colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ: 1.28 (9H, s), 4.99 (1H, brs), 6.92 (1H, t, J = 9.0 Hz), 7.03 (1H, ddd, J = 1.5, 2.5, 9.0 Hz), 7.09 (1H, dd, J = 2.5, 13.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 31.4, 34.2, 112.6 (d, J = 18.0 Hz), 116.5, 121.4 (d, J = 2.5 Hz), 140.8 (d, J = 14.0 Hz), 144.6 (d, J = 5.0 Hz), 150.6 (d, J = 235 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –144.5 (dd, J = 9.0, 13.0 Hz). IR ($CHCl_3$): 3585, 3568 cm^{-1}. HRMS Calcd for $C_{10}H_{13}FO$ (M^+) m/z: 168.0950, found: 168.0957.

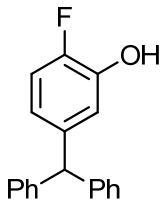
Entry 2 in Table 1: By methods A and C, the use of **1b** (150 mg, 0.54 mmol), *o*-chloranil (183 mg, 0.57 mmol), Deoxofluor (0.60 mL, 3.2 mmol), $NaBH_4$ (102 mg, 2.7 mmol), DBU (0.40 mL,

2.7 mmol) and EtOH gave **5b** (28 mg, 17%) and a mixture of **6b** and 7**b** (83 mg, 51%, **6b**:7**b** = 80:20). Further purification of the mixture of **6b** and **7b** by flash column chromatography (hexanes–AcOEt 5:1) gave analytically pure **6b** and **7b**.



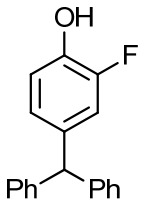
5-Benzhydryl-2,4-difluorophenol (5b)

A colorless solid: mp 100.5–103.0 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 4.85 (1H, d, *J* = 3.5 Hz), 5.73 (1H, s), 6.56 (1H, dd, *J* = 7.5, 10.0 Hz), 6.84 (1H, t, *J* = 10.0 Hz), 7.09 (4H, d, *J* = 7.5 Hz), 7.23 (2H, t, *J* = 7.5 Hz), 7.30 (4H, t, *J* = 7.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 48.9, 103.8 (dd, *J* = 21.5, 27.5 Hz), 118.5 (t, *J* = 2.5 Hz), 126.7, 127.5 (dd, *J* = 3.5, 16.0 Hz), 128.4, 129.1, 139.3 (dd, *J* = 2.5, 13.0 Hz), 142.1, 148.9 (dd, *J* = 12.0, 238 Hz), 153.4 (dd, *J* = 11.0, 241 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –142.3 (1F, m), –126.2 (1F, m). IR ($CHCl_3$): 3582 cm^{-1}. HRMS Calcd for $C_{19}H_{14}F_2O$ (M^+) *m/z*: 296.1013, found: 296.1013.



5-Benzhydryl-2-fluorophenol (6b)

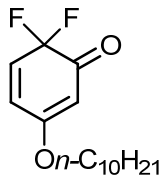
A colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ: 5.07 (1H, d, *J* = 4.5 Hz), 5.49 (1H, s), 6.62 (1H, ddd, *J* = 2.5, 4.5, 8.5 Hz), 6.77 (1H, dd, *J* = 2.5, 8.5 Hz), 6.99 (1H, dd, *J* = 8.5, 10.0 Hz), 7.11 (4H, d, *J* = 7.0 Hz), 7.23 (2H, t, *J* = 7.0 Hz), 7.30 (4H, t, *J* = 7.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 56.1, 115.1 (d, *J* = 18.0 Hz), 118.3, 121.7 (d, *J* = 6.0 Hz), 126.4, 128.4, 129.3, 140.9 (d, *J* = 3.5 Hz), 143.1 (d, *J* = 14.5 Hz), 143.5, 149.6 (d, *J* = 235 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –147.4 (1F, ddd, *J* = 4.5, 8.5, 10.0 Hz). IR ($CHCl_3$): 3580 cm^{-1}. HRMS Calcd for $C_{19}H_{17}O_2$ (M^+) *m/z*: 278.1107, found: 278.1100.



4-Benzhydryl-2-fluorophenol (7b)

A colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ: 4.99 (1H, d, *J* = 4.0 Hz), 5.47 (1H, s), 6.79 (1H, dd, *J* = 2.5, 8.5 Hz), 6.81 (1H, dd, *J* = 2.5, 12.0 Hz), 6.91 (1H, t, *J* = 8.5 Hz), 7.10 (4H, d, *J* = 7.5 Hz), 7.22 (2H, t, *J* = 7.5 Hz), 7.29 (4H, t, *J* = 7.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 55.8, 116.4 (d, *J* = 18.0 Hz), 116.8, 125.6 (d, *J* = 2.5 Hz), 126.5, 128.4, 129.3, 137.0 (d, *J* = 5.0 Hz), 141.7 (d, *J* = 14.5 Hz), 143.5, 150.8 (d, *J* = 236 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –144.1 (1F, m). IR ($CHCl_3$): 3580 cm^{-1}. HRMS Calcd for $C_{19}H_{17}O_2$ (M^+) *m/z*: 278.1107, found: 278.1097.

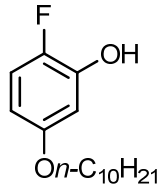
Entry 3 in Table 1: By method B, the use of **1c** (50 mg, 0.19 mmol), MgO (17 mg, 0.43 mmol), $PhI(OAc)_2$ (63 mg, 0.20 mmol), and Deoxofluor (0.21 mL, 1.12 mmol) gave **3c** (33.0 mg, 60%).



3-(*n*-Decyloxy)-6,6-difluorocyclohexa-2,4-dienone (3c)

A colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ: 0.88 (3H, t, *J* = 7.0 Hz), 1.21–1.44 (14H, m), 1.78 (2H, quint, *J* = 7.0 Hz), 3.96 (2H, t, *J* = 7.0 Hz), 5.47 (1H, q, *J* = 2.5 Hz), 6.33 (1H, dd, *J* = 2.5, 10.5 Hz), 6.42 (1H, td, *J* = 5.0, 10.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 14.1, 22.7, 25.7, 28.2, 29.1, 29.3, 29.4, 29.5, 31.8, 70.2, 98.3, 103.1 (t, *J* = 240 Hz), 129.8 (t, *J* = 9.5 Hz), 131.4 (t, *J* = 27.5 Hz), 168.7 (t, *J* = 2.5 Hz), 186.2 (t, *J* = 24.0 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –108.6 (2F, dd, *J* = 2.5, 5.0 Hz). IR ($CHCl_3$): 1678, 1583 cm^{-1}. HRMS Calcd for $C_{16}H_{25}F_2O_2$ [(M+H)$^+$] *m/z*: 287.1817, found: 287.1825.

By method C, the use of **3c** (32.0 mg, 0.11 mmol), $NaBH_4$ (21 mg, 0.55 mmol) and DBU (0.082 mL, 0.55 mmol) in EtOH at 80 °C for 30 min gave **6c** (24.0 mg, 48% for 2 steps from **1c**).

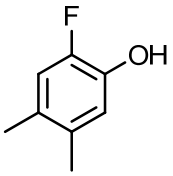


5-(*n*-Decyloxy)-2-fluorophenol (6c)

A colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ: 0.88 (3H, t, *J* = 7.0 Hz), 1.21–1.46 (14H, m), 1.75 (2H, quint, *J* = 6.5 Hz), 3.87 (2H, t, *J* = 6.5 Hz), 5.19 (1H, d, *J* = 4.5 Hz), 6.36 (1H, td, *J* = 3.0, 9.0 Hz), 6.55 (1H, dd, *J* = 3.0, 7.5 Hz), 6.95 (1H, dd, *J* = 9.0, 10.5 Hz). ^{13}C NMR (125 MHz,

$CDCl_3$) δ: 14.1, 22.7, 26.0, 29.1, 29.3, 29.4, 29.6, 31.9, 68.6, 103.5, 106.2 (d, J = 6.0 Hz), 115.3 (d, J = 19.0 Hz), 143.8 (d, J = 15.5 Hz), 145.6 (d, J = 227 Hz), 155.9. ^{19}F NMR (470 MHz, $CDCl_3$) δ: –154.7 (1F, dddd, J = 3.0, 4.5, 7.5, 10.5 Hz). IR ($CHCl_3$): 3580 cm^{-1}. HRMS Calcd for $C_{16}H_{26}FO_2$ [(M+H)$^+$] m/z: 269.1911, found: 269.1910.

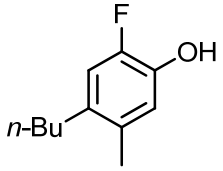
Entry 4 in Table 1: By methods B and D, the use of **1d** (50 mg, 0.36 mmol), MgO (33 mg, 0.82 mmol), $PhI(OAc)_2$ (122 mg, 0.38 mmol), Deoxofluor (1.80 mL, 2.2 mmol), $NaBH_4$ (68 mg, 1.80 mmol) and EtOH gave **6d** (32 mg, 60% from **1d**).



2-Fluoro-4,5-dimethylphenol (6d)

Colorless crystals: mp 48–49.5 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 2.16 (3H, s), 2.17 (3H, s), 4.86 (1H, d, J = 3.5 Hz), 6.77 (1H, d, J = 9.0 Hz), 6.83 (1H, d, J = 11.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 18.9, 19.1, 116.2 (d, J = 18.0 Hz), 118.1, 128.8 (d, J = 6.0 Hz), 132.8 (d, J = 2.5 Hz), 140.7 (d, J = 13.0 Hz) 148.9 (d, J = 234 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –149.3 (1H, ddd, J = 3.5, 9.0, 11.0 Hz). IR ($CHCl_3$): 3584 cm^{-1}. HRMS Calcd for $C_8H_{10}FO$ [(M+H)$^+$] m/z: 141.0710, found: 141.0715. This compound was reported in reference 4 as a mixture of three isomers.

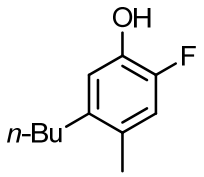
Entry 5 in Table 1: By mthods B and D, the use of **1e** (30 mg, 0.17 mmol), MgO (16 mg, 0.38 mmol), $PhI(OAc)_2$ (56 mg, 0. 17 mmol), Deoxofluor (0.18 mL, 1.0 mmol), $NaBH_4$ (31 mg, 0.83 mmol) and EtOH gave a mixture of **6e** and **7e** (22.6 mg, 70%, **6e**: **7e** = 50: 50). Further purification of the mixture of **6e** and **7e** by flash column chromatography (hexanes–AcOEt 15:1) gave analytically pure **6e** and **7e**.



4-*n*-Butyl-2-fluoro-5-methylphenol (6e)

A colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ: 0.94 (3H, t, J = 7.0 Hz), 1.38 (2H, hex, J = 7.0 Hz), 1.51 (2H, quint, J = 7.0 Hz), 2.21 (3H, s), 2.50 (2H, t, J = 7.0 Hz), 4.91 (1H, d, J = 3.0 Hz),

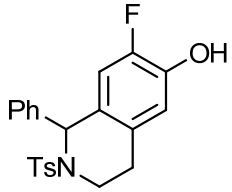
6.77 (1H, d, J = 9.0 Hz), 6.83 (1H, d, J = 12.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 14.0, 18.8, 22.5, 32.2, 32.4, 115.4 (d, J = 17.0 Hz), 118.5, 132.2 (d, J = 2.5 Hz), 133.6 (d, J = 5.0 Hz), 140.6 (d, J = 13.0 Hz), 149.1 (d, J = 232 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –148.9 (1F, ddd, J = 3.0, 9.0, 12.0 Hz). IR ($CHCl_3$): 3584 cm^{-1}. HRMS Calcd for $C_{11}H_{16}FO$ [(M+H)$^+$] *m/z*: 183.1180, found: 183.1182.



5-*n*-Butyl-2-fluoro-4-methylphenol (7e)

A colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ: 0.94 (3H, t, J = 7.0 Hz), 1.38 (2H, hex, J = 7.0 Hz), 1.51 (2H, quint, J = 7.0 Hz), 2.20 (3H, s), 2.49 (2H, t, J = 7.0 Hz), 4.92 (1H, d, J = 3.5 Hz), 6.77 (1H, d, J = 9.0 Hz), 6.83 (1H, d, J = 11.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 14.0, 18.5, 22.6, 32.4, 32.4, 116.6 (d, J = 18.0 Hz), 117.3, 128.3 (d, J = 6.0 Hz), 137.5, 140.8 (d, J = 14.5 Hz), 148.8 (d, J = 234 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –149.1 (1F, ddd, J = 3.5, 9.0, 11.5 Hz). IR ($CHCl_3$): 3584 cm^{-1}. HRMS Calcd for $C_{11}H_{14}FO$ [(M–H)$^-$]) *m/z*: 181.1034, found: 181.1026.

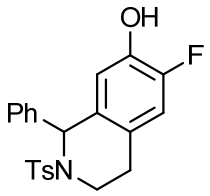
Entry 6 in Table 1: By methods B and D, the use of **1f** (93 mg, 0.24 mmol), $PhI(OAc)_2$ (80 mg, 0. 25 mmol), MgO (22 mg, 0.55 mmol), Deoxofluor (0.26 mL, 1.41 mmol), $NaBH_4$ (44 mg, 1.16 mmol) and EtOH gave a mixture of **6f** and 7**f** (55 mg, 59%, **6f**:7**f** = 58:42) after purification by flash column chromatography (CH_2Cl_2–MeOH 100:1). Further purification of the mixture of **6f** and **7f** by flash column chromatography (hexanes–AcOEt 3:1) gave analytically pure **6f** and **7f**.



7-Fluoro-1-phenyl-2-tosyl-1,2,3,4-tetrahydroisoquinolin-6-ol (6f)

A colorless solid: mp 166.0–167.0 ºC, ^{1}H NMR (500 MHz, $CDCl_3$) δ: 2.34 (3H, s), 2.47 (1H, dd, J = 3.5, 17.5 Hz), 2.58 (1H, ddd, J = 6.0, 11.5, 17.5 Hz), 3.33 (1H, ddd, J = 3.5, 11.5, 14.5 Hz), 3.76 (1H, dd, J = 6.0, 14.5 Hz), 5.29 (1H, brs), 6.13 (1H, s), 6.62 (1H, d, J = 8.5 Hz), 6.70 (1H,

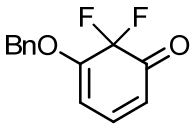
d, J = 10.5 Hz), 7.12 (2H, d, J = 8.0 Hz), 7.15–7.19 (2H, m), 7.23–7.29 (4H, m), 7.55 (2H, d, J = 8.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 21.5, 26.1, 38.6, 58.4, 114.8 (d, J = 18.0 Hz), 116.9 (d, J = 12.0 Hz), 126.3 (d, J = 6.0 Hz), 127.0, 127.8, 128.3, 128.6, 129.4, 130.5 (d, J = 3.5 Hz), 137.6, 141.1, 142.5 (d, J = 15.5 Hz), 143.2, 149.3 (d, J = 236 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –146.1 (1F, m). IR ($CHCl_3$): 3578 cm^{-1}. HRMS Calcd for $C_{22}H_{21}FNO_3S$ [(M+H)$^+$] m/z: 398.1221, found: 398.1220.



6-Fluoro-1-phenyl-2-tosyl-1,2,3,4-tetrahydroisoquinolin-7-ol (7f)

A colorless solid: mp 159.5–160.5 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 2.34 (3H, s), 2.45 (1H, m), 2.57 (1H, ddd, J = 6.5, 11.5, 17.0 Hz), 3.23 (1H, ddd, J = 5.0, 11.5, 14.5 Hz), 3.76 (1H, dd, J = 6.5, 14.5 Hz), 5.10 (1H, d, J = 3.0 Hz), 6.13 (1H, s), 6.63 (1H, d, J = 8.5 Hz), 6.70 (1H, d, J = 11.0 Hz), 7.11 (2H, d, J = 8.0 Hz), 7.15–7.19 (2H, m), 7.23–7.29 (4H, m), 7.55 (2H, d, J = 8.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 21.4, 25.8, 38.6, 58.6, 115.3 (d, J = 18.0 Hz), 116.6 (d, J = 10.5 Hz), 126.5 (d, J = 6.5 Hz), 127.0, 127.7, 128.3, 128.6, 129.3, 130.3 (d, J = 2.5 Hz), 137.6, 140.9, 141.7 (d, J = 15.5 Hz), 143.2, 150.0 (d, J = 238 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –144.9 (1F, m). IR ($CHCl_3$): 3580 cm^{-1}. HRMS Calcd for $C_{22}H_{21}FNO_3S$ [(M+H)$^+$] m/z: 398.1221, found: 398.1223.

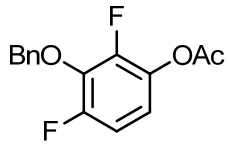
Entry 7 in Table 1: By method A, the use of **1g** (400 mg, 1.85 mmol), $PhI(OAc)_2$ (626 mg, 1.94 mmol), MgO (171 mg, 4.2 mmol) and Deoxofluor (2.05 mL, 11.1 mmol) gave the difluoroketone **3g** (262 mg, 61%) and **5g**. **5g** was isolated as its acetate [**5g-Ac** (**S1**), 37 mg, 7%] due to its unstability.



5-(Benzyloxy)-6,6-difluorocyclohexa-2,4-dienone (3g)

Yellow crystals: mp 102.0–105.0 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 5.05 (2H, s), 5.46 (1H, d, J = 7.0 Hz), 5.93 (1H, td, J = 2.0, 10.0 Hz), 7.05 (1H, dd, J = 7.0, 10.0 Hz), 7.35–7.44 (5H, m). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 71.2, 98.4 (t, J = 5.0 Hz), 102.0 (t, J = 248 Hz), 117.9 (t, J = 3.0

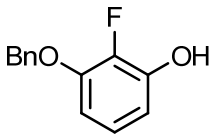
Hz), 127.3, 128.7, 128.8, 134.3, 143.6, 156.7 (t, J = 21.0 Hz), 187.0 (t, J = 23.0 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –117.2 (2F, t, J = 2.0 Hz). IR ($CHCl_3$): 1697, 1647, 1562 cm^{-1}. HRMS Calcd for $C_{19}H_{17}O_2$ [(M+Na)$^+$] m/z: 259.0541, found: 259.0542.



3-(Benzyloxy)-2,4-difluorophenyl acetate (5g-Ac, S1)

A colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ: 2.33 (3H, s), 5.20 (2H, s), 6.79 (1H, ddd, J = 4.5, 7.5, 9.5 Hz), 6.87 (1H, dt, J = 2.0, 9.5 Hz), 7.32–7.47 (5H, m). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 20.4, 76.2 (t, J = 3.0 Hz), 110.7 (dd, J = 14.5, 21.5 Hz), 116.8 (d, J = 8.5 Hz), 128.2, 128.46, 128.49, 135.1 (dd, J = 3.5, 7.0 Hz), 136.0 (dd, J = 12.0, 15.5 Hz), 136.1, 148.3 (dd, J = 6.0, 249 Hz), 153.8 (dd, J = 5.0, 246 Hz), 168.2. ^{19}F NMR (470 MHz, $CDCl_3$) δ: –132.6 (1F, ddd, J = 4.5, 7.5, 9.5 Hz), –143.3 (1F, dt, J = 2.0, 7.5 Hz). IR ($CHCl_3$): 1771 cm^{-1}. HRMS Calcd for $C_{15}H_{13}F_2O_3$ [(M+H)$^+$] m/z: 279.0827, found: 279.0848.

By method D, the reduction of **3g** (262 mg, 1.13 mmol) with $NaBH_4$ (193 mg, 5.64 mmol) in EtOH at 80 °C for 30 min gave **6g** (202 mg, 50% from **1g**).

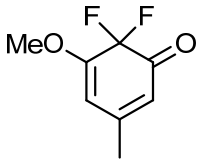


3-(Benzyloxy)-2-fluorophenol (6g)

A colorless solid: mp 50.0–52.0 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 5.13 (2H, s), 5.32 (1H, d, J = 4.5 Hz), 6.57 (1H, dt, J = 1.0, 8.5 Hz), 6.63 (1H, dt, J = 1.0, 8.5 Hz), 6.89 (1H, dt, J = 2.5, 8.5 Hz), 7.34 (1H, t, J = 7.5 Hz), 7.40 (2H, t, J = 7.5 Hz), 7.44 (2H, d, J = 7.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 71.4, 107.0, 109.8, 123.7 (d, J = 5.0 Hz), 127.4, 128.1, 128.6, 136.4, 140.9 (d, J = 235 Hz), 144.6 (d, J = 12.0 Hz), 147.2 (d, J = 9.5 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –165.4 (1F, m). IR ($CHCl_3$): 3578 cm^{-1}. HRMS Calcd for $C_{13}H_{12}F_1O_2$ [(M+H)$^+$] m/z: 219.0816, found: 219.0816.

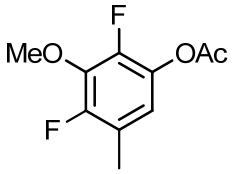
Entry 8 in Table 1: By method B, the use of **1h** (100 mg, 0.65 mmol), $PhI(OAc)_2$ (219 mg, 0.68 mmol), MgO (60 mg, 1.5 mmol) and Deoxofluor (0.72 mL, 3.9 mmol) gave **3h** (66 mg,

58%) and **5h**. **5h** was isolated as its acetate [**5h-Ac** (**S2**), 10.8 mg, 8%] due to its unstability.



6,6-Difluoro-5-methoxy-3-methylcyclohexa-2,4-dienone (3h)

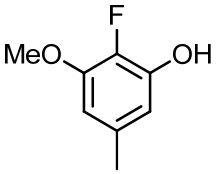
Yellow crystals: mp 84.0–86.0 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 2.13 (3H, s), 3.82 (3H, s), 5.27 (1H, brs), 5.79 (1H, brs). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 24.6, 56.4, 100.9 (t, J = 6.0 Hz), 101.2 (t, J = 246 Hz), 115.9 (t, J = 2.5 Hz), 156.8 (t, J = 20.0 Hz), 156.9, 186.0 (t, J = 23.0 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –117.8 (2F,m). IR ($CHCl_3$): 1690, 1651, 1574 cm^{-1}. HRMS Calcd for $C_8H_8F_2O_2Na$ [(M+Na)$^+$] *m/z*: 197.0385, found: 197.0391.



2,4-Difluoro-3-methoxy-5-methylphenyl acetate (5h-Ac, S2)

A colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ: 2.22 (3H, s), 2.31 (3H, s), 3.99 (3H, s), 6.63 (1H, t, J = 7.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 14.2 (d, J = 3.5 Hz), 20.4, 61.9 (t, J = 2.5 Hz), 117.6 (d, J = 5.0 Hz), 120.7 (dd, J = 13.0, 17.0 Hz), 134.1 (dd, J = 3.5, 12.0 Hz), 137.0 (t, J = 3.5 Hz), 145.9 (dd, J = 5.0, 247 Hz), 151.8 (dd, J = 3.5, 243 Hz), 168.5. ^{19}F NMR (470 MHz, $CDCl_3$) δ: –137.3 (1F, m), –148.9 (1F, t, J = 7.5 Hz). IR ($CHCl_3$): 1775 cm^{-1}. HRMS Calcd for $C_{10}H_{11}F_2O_3$ [(M+H)$^+$] *m/z*: 217.0671, found: 217.0677.

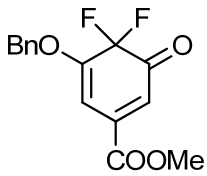
By method C, the reduction of **3h** (50 mg, 0.29 mmol) with $NaBH_4$ (54 mg, 1.44 mmol) and DBU (0.21 mL, 1.44 mL) in EtOH at 80 °C for 30 min gave **6h** (44 mg, 57% from **1h**).



2-Fluoro-3-methoxy-5-methylphenol (6h)[5]

A colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ: 2.26 (3H, s), 3.86 (3H, s), 5.15 (1H, d, *J* = 4.0 Hz), 6.33 (1H, dd, *J* = 1.0, 7.5 Hz), 6.42 (1H, dd, *J* = 1.0, 7.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 21.4, 56.3, 105.7, 109.8, 133.7 (d, *J* = 5.0 Hz), 139.5 (d, *J* = 231 Hz), 143.8 (d, *J* = 12.0 Hz), 147.6 (d, *J* = 8.5 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –171.2 (1F, dt, *J* = 4.0, 7.5 Hz). IR ($CHCl_3$): 3578 cm^{-1}. HRMS Calcd for $C_8H_{10}FO_2$ [(*M*+H)$^+$] *m/z*: 157.0659, found: 157.0655.

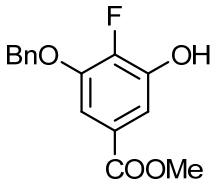
Entry 9 in Table 1: By method A, the use of **1i** (1.00 g, 3.64 mmol), $PhI(OAc)_2$ (1.23 g, 3.82 mmol) and Deoxofluor (4.0 mL, 21.8 mmol) gave difluoroketone **3i** (139 mg, 13%).



Methyl 5-(Benzyloxy)-4,4-difluoro-3-oxocyclohexa-1,5-dienecarboxylate (3i)

Yellow crystals: mp 95.0–100.0 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 3.90 (3H, s), 5.09 (2H, s), 6.02 (1H, d, *J* = 1.5 Hz), 6.60 (1H, q, *J* = 1.5 Hz), 7.35–7.42 (5H, m). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 53.4, 71.5, 97.2 (t, *J* = 5.0 Hz), 101.3 (t, *J* = 248 Hz), 119.7 (t, *J* = 3.5 Hz), 127.6, 128.8, 134.1, 143.0, 156.1 (t, *J* = 21.5 Hz), 164.7, 187.9 (t, *J* = 23.0 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ: –116.4 (2F, d, *J* = 1.5 Hz). IR ($CHCl_3$): 1728, 1701 cm^{-1}. HRMS Calcd for $C_{15}H_{13}F_2O_4$ [(*M*+H)$^+$] *m/z*: 295.0776, found: 295.0775.

By method C with a minor modification, the reduction of **3i** (132 mg, 0.45 mmol) with $NaBH_4$ (20 mg, 0.53 mmol), $CeCl_3 \cdot 7H_2O$ (250 mg, 0.67 mmol) and DBU (0.33 mL, 2.3 mmol) in MeOH gave **9i** (100 mg, 10% from **1i**).



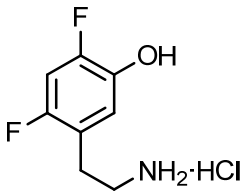
Methyl 3-(Benzyloxy)-4-fluoro-5-hydroxybenzoate (6i)

A colorless solid: 120.0–122.5 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 3.90 (3H, s), 5.16 (2H, s), 5.57 (1H, d, *J* = 4.0 Hz), 7.32–7.47 (7H, m). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 52.4, 71.3, 108.0, 111.7, 125.7 (d, *J* = 3.5 Hz), 127.6, 128.3, 128.7, 135.8, 144.3 (d, *J* = 12.0 Hz), 144.7 (d, *J* =

243 Hz), 147.0 (d, J = 9.5 Hz), 166.2. ^{19}F NMR (470 MHz, $CDCl_3$) δ: –157.2 (1F, dt, J = 4.0, 7.5 Hz). IR ($CHCl_3$): 3574, 1718 cm^{-1}. HRMS Calcd for $C_{15}H_{14}FO_4$ [(M+H)$^+$] m/z: 277.0871, found: 277.0880.

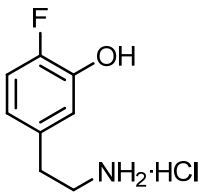
Deoxyfluorination of the protected dopamine (1j)

By methods A and C, the reactions were conducted using **1j** (500 mg, 1.40 mmol), $PhI(OAc)_2$ (478 mg, 1.47 mmol), Deoxofluor (1.57 mL, 8.4 mmol), $NaBH_4$ (265 mg, 7.0 mmol), DBU (1.05 mL, 7.0 mmol) and EtOH. The crude product was roughly purified by flash column chromatography (hexanes–EtOAc 5:1 to 3:1) to afford 250 mg of a mixture of fluorophenols. These products were solved in MeOH (6.6 mL), and $SOCl_2$ (0.96 mL, 13.2 mmol) was slowly added to the solution at 0 °C. The reaction mixture was allowed to warm up to room temperature over 5 min, the solvents were evaporated, and the residue was purified by preparative HPLC (Kanto, Mightysil, RP-18, GP250-10, water, flow 3.0 mL/min) to give **5j** (38.5 mg, 13%, RT = 12.2 min), **6j** (48.6 mg, 18%, RT = 10.0 min) and **7j** (34.6 mg, 13%, RT = 8.9 min).



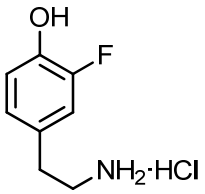
5-(2-Aminoethyl)-2,4-difluorophenol hydrochloride (5j)

A colorless solid: mp 215.0–220.0 ºC. ^{1}H NMR (500 MHz, CD_3OD) δ: 2.95 (2H, t, J = 7.5 Hz), 3.16 (2H, t, J = 7.5 Hz), 6.91 (1H, dd, J = 7.5, 10.0 Hz), 6.98 (1H, t, J = 10.0 Hz). ^{13}C NMR (125 MHz, CD_3OD) δ: 27.7, 40.7, 105.3 (dd, J = 23.0, 27.5 Hz), 119.9 (t, J = 19.0 Hz), 120.3 (dd, J = 3.5, 17.0 Hz), 142.9 (dd, J = 2.5, 12.0 Hz), 151.7 (dd, J = 12.0, 242 Hz), 154.8 (dd, J = 11.0, 237 Hz). ^{19}F NMR (470 MHz, CD_3OD) δ: –135.8 (1F, t, J = 10.0 Hz), –128.6 (1F, t, J = 7.5 Hz). IR (KBr): 3374, 3289, 3071 cm^{-1}. HRMS Calcd for $C_8H_{10}F_2NO$ [(M–Cl)$^+$] m/z: 174.0725, found: 174.0732.



5-(2-Aminoethyl)-2-fluorophenol hydrochloride (6j)

A colorless solid: mp 160.0–162.0 ºC. ^{1}H NMR (500 MHz, CD_3OD) δ: 2.92 (2H, t, *J* = 7.5 Hz), 3.17 (2H, t, *J* = 7.5 Hz), 6.72–6.79 (1H, m), 6.91 (1H, dd, *J* = 2.0, 8.0 Hz), 7.03 (1H, dd, *J* = 8.0, 11.0 Hz). ^{13}C NMR (125 MHz, CD_3OD) δ: 33.8, 42.0, 117.1 (d, *J* = 19.0 Hz), 119.1 (d, *J* = 3.5 Hz), 121.0 (d, *J* = 6.0 Hz), 134.4, 146.3 (d, *J* = 13.0 Hz), 152.2 (d, *J* = 238 Hz). ^{19}F NMR (470 MHz, CD_3OD) δ: –141.4 (1F, m). IR (KBr): 3364, 3036, 2957 cm^{-1}. HRMS Calcd for $C_8H_{11}FNO$ [(*M*–Cl)$^+$] *m/z*: 156.0819, found: 156.0825. This compound was reported in reference 6 as a corresponding HBr salt.

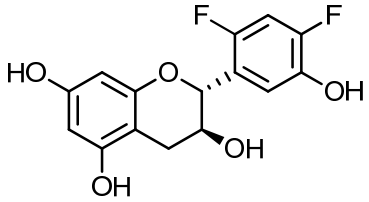


4-(2-Aminoethyl)-2-fluorophenol hydrochloride (7j)[7]

Colorless crystals: mp 230.0–235.0 ºC. ^{1}H NMR (500 MHz, CD_3OD) δ: 2.91 (2H, t, *J* = 7.0 Hz), 3.16 (2H, t, *J* = 7.0 Hz), 6.90–6.96 (2H, m), 7.04 (1H, dd, *J* = 2.0, 11.0 Hz). ^{13}C NMR (125 MHz, CD_3OD) δ: 33.5, 42.0, 117.2 (d, *J* = 18.0 Hz), 119.1 (d, *J* = 3.5 Hz), 125.9 (d, *J* = 3.5 Hz), 129.5 (d, *J* = 6.0 Hz), 145.3 (d, *J* = 13.0 Hz), 152.9 (d, *J* = 240 Hz). ^{19}F NMR (470 MHz, CD_3OD) δ: –138.4 (1F, m). IR (KBr): 3075, 2924 cm^{-1}. HRMS Calcd for $C_8H_{11}FNO$ [(*M*–Cl)$^+$] *m/z*: 156.0819, found: 156.0823.

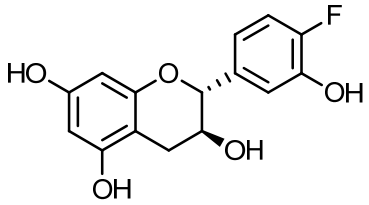
Deoxyfluorination of protected catechins (1k and 1l)

By methods B and C, the reactions were conducted using **1k** (300 mg, 0.51 mmol), $PhI(OAc)_2$ (172 mg, 0.53 mmol), MgO (47 mg, 1.17 mmol), Deoxofluor (0.56 mL, 3.0 mmol), $NaBH_4$ (96 mg, 2.5 mmol), DBU (0.38 mL, 2.5 mmol) and EtOH (2.5 mL). The crude product was dissolved in CH_2Cl_2 (12.6 mL), and CF_3CO_2H (12.6 mL) was added to the solution at 0 °C. The reaction mixture was stirred at 0 °C for 5 min and concentrated *in vacuo*. The residue was purified by flash column chromatography (hexanes–EtOAc 2:3) to afford a mixture of **5k**, **6k** and **7k**. Further purification by preparative HPLC (Kanto, Mightysil, RP-18, GP250-10, water–CH_3CN 2:8, flow 3.0 mL/min) gave **5k** (13.1 mg, 9%, RT = 28.2 min), **6k** (34.0 mg, 23%, RT = 18.8 min) and **7k** (42.1 mg, 28%, RT = 13.3 min).



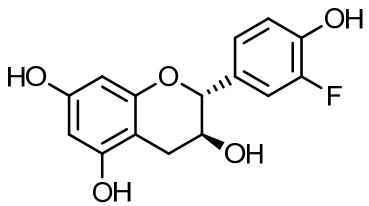
(2*R*,3*S*)-2-(2,4-Difluoro-5-hydroxyphenyl)chroman-3,5,7-triol (5k)

A colorless solid: mp 120.0–127.0 ºC, $[\alpha]_D^{20}$ +16.6 (*c* 0.71, acetone). ^{1}H NMR (500 MHz, acetone-d_6) δ: 2.59 (1H, dd, *J* = 8.0, 16.0 Hz), 2.93 (1H, dd, *J* = 6.0, 16.0 Hz), 4.05–4.13 (1H, m), 4.31 (1H, d, *J* = 5.0 Hz), 4.95 (1H, d, *J* = 8.0 Hz), 5.89 (1H, d, *J* = 2.5 Hz), 6.06 (1H, d, *J* = 2.5 Hz), 7.01 (1H, dd, *J* = 10.0, 11.0 Hz), 7.08 (1H, dd, *J* = 2.0, 9.0 Hz), 8.10 (1H, brs), 8.31 (1H, brs), 8.72 (1H, brs). ^{13}C NMR (125 MHz, acetone-d_6) δ: 29.0, 67.5, 76.3, 95.4, 96.5, 100.4, 104.9 (dd, *J* = 23.0, 27.5 Hz), 117.4 (d, *J* = 3.5 Hz), 123.7 (d, *J* = 14.5 Hz), 142.2 (d, *J* = 12.0 Hz), 151.4 (dd, *J* = 12.0, 242 Hz), 154.2 (dd, *J* = 11.0, 238 Hz), 156.6, 157.3, 157.9. ^{19}F NMR (470 MHz, Acetone-d_6) δ: –135.3 (1F, m), –128.0 (1F, m). IR (KBr): 3510, 3298, 1638, 1620 cm^{-1}. HRMS Calcd for $C_{15}H_{13}FO_5$ [(*M*+H)$^+$] *m/z*: 311.0726, found: 311.0736.



(2*R*,3*S*)-2-(4-Fluoro-3-hydroxyphenyl)chroman-3,5,7-triol (6k)

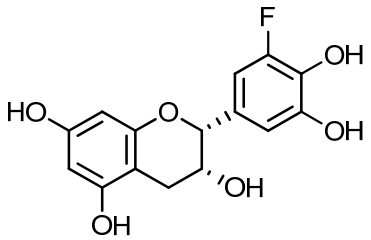
A colorless solid: mp 116.0–119.0 ºC. $[\alpha]_D^{20}$ –6.2 (*c* 0.58, acetone). ^{1}H NMR (500 MHz, acetone-d_6) δ: 2.54 (1H, dd, *J* = 8.5, 16.0 Hz), 2.91 (1H, dd, *J* = 6.0, 16.0 Hz), 3.95–4.02 (1H, m), 4.10 (1H, d, *J* = 4.5 Hz), 4.63 (1H, d, *J* = 8.0 Hz), 5.89 (1H, d, *J* = 2.5 Hz), 6.04 (1H, d, *J* = 2.5 Hz), 6.90 (1H, ddd, *J* = 2.5, 4.5, 8.5 Hz), 7.04–7.10 (2H,m), 8.06 (1H, brs), 8.26 (1H, brs), 8.68 (1H, brs). ^{13}C NMR (125 MHz, acetone-d_6) δ: 29.0, 68.4, 82.2, 95.5, 96.3, 100.6, 116.3 (d, *J* = 18.0 Hz), 117.7, 119.9 (d, *J* = 6.0 Hz), 137.4 (d, *J* = 2.5 Hz), 145.4 (d, *J* = 13.0 Hz), 152.0 (d, *J* = 238 Hz), 156.7, 157.3, 157.8. ^{19}F NMR (470 MHz, acetone-d_6) δ: –140.4 (1F, m). IR (KBr): 3566, 3397, 1634, 1618 cm^{-1}. HRMS Calcd for $C_{15}H_{14}FO_5$ [(*M*+H)$^+$] *m/z*: 293.0820, found: 293.0825.



(2*R*,3*S*)-2-(3-Fluoro-4-hydroxyphenyl)chroman-3,5,7-triol (7k)

A colorless solid: mp 121.0–127.0 ºC, $[\alpha]_D^{20}$ +11.5 (*c* 0.56, acetone). ^{1}H NMR (500 MHz, acetone-d_6) δ: 2.53 (1H, dd, *J* = 8.5, 16.0 Hz), 2.96 (1H, dd, *J* = 6.0, 16.0 Hz), 3.95–4.02 (1H, m), 4.09 (1H, d, *J* = 5.0 Hz), 4.60 (1H, d, *J* = 8.5 Hz), 5.89 (1H, d, *J* = 2.5 Hz), 6.04 (1H, d, *J* = 2.5 Hz), 6.98 (1H, t, *J* = 9.0 Hz), 7.09 (1H, dd, *J* = 2.0, 9.0 Hz), 7.17 (1H, dd, *J* = 2.0, 12.0 Hz), 8.05 (1H, brs), 8.26 (1H, brs), 8.67 (1H, brs). ^{13}C NMR (125 MHz, acetone-d_6) δ: 29.3, 68.4, 82.1, 95.5, 96.3, 100.7, 115.9 (d, *J* = 19.0 Hz), 118.2 (d, *J* = 2.0 Hz), 124.8 (d, *J* = 2.5 Hz), 132.8 (d, *J* = 6.0 Hz), 145.3 (d, *J* = 13.0 Hz), 152.1 (d, *J* = 237 Hz), 156.8, 157.3, 157.9. ^{19}F NMR (470 MHz, acetone-d_6) δ: –139.2 (1F, m). IR (KBr): 3370, 1631, 1605 cm^{-1}. HRMS Calcd for $C_{15}H_{14}FO_5$ [(*M*+H)$^+$] *m/z*: 293.0820, found: 293.0832.

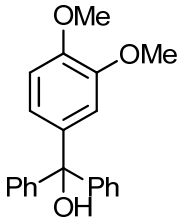
By method B, the oxidation of **1l** (100 mg, 0.14 mmol) was conducted using $PhI(OAc)_2$ (48 mg,0.15 mmol) at 0 °C for 10 min, and the following deoxyfluorination was conducted using Deoxofluor (0.16 mL, 0.84 mmol). The reduction was carried out as per method C using $NaBH_4$ (26 mg, 0.70 mmol) and DBU (0.10 mL, 0.70 mmol) in EtOH (1.4 mL) at 80 °C for 30 min. Work up was basically the same as described for **1k**. Flash Column chromatography (hexanes–EtOAc–AcOH 150:50:1) followed by preparative HPLC (Kanto, Mightysil, RP-18, GP250-10, water–CH_3CN 15:85, flow 3.0 mL/ min) gave **7l** (17.9 mg, 41%, RT = 16.4 min) and a mixture of other regioisomers.



(2*R*,3*R*)-2-(3-Fluoro-4,5-dihydroxyphenyl)chroman-3,5,7-triol (7l)

A colorless solid: mp 193.0–195.0 ºC, $[\alpha]_D^{20}$ –41.2 (*c* 0.53, acetone). ^{1}H NMR (500 MHz, acetone-d_6) δ: 2.73 (1H, dd, *J* = 2.5, 16.0 Hz), 2.85 (1H, dd, *J* = 4.5, 16.0 Hz), 3.73 (1H, d, *J* = 6.0 Hz), 4.22 (1H, brs), 4.89 (1H, brs), 5.93 (1H, d, *J* = 2.5 Hz), 6.02 (1H, d, *J* = 2.5 Hz), 6.82 (1H, dd, *J* = 2.5, 11.5 Hz), 6.85 (1H, s), 7.99 (1H, brs), 8.16 (1H, brs), 8.26 (1H, brs). ^{13}C NMR (125 MHz, acetone-d_6) δ: 28.9, 66.8, 78.9, 95.7, 96.3, 99.8, 106.6 (d, *J* = 20.0 Hz), 110.9, 131.9 (d, *J* = 8.5 Hz), 133.1 (d, *J* = 15.5 Hz), 147.6 (d, *J* = 6.0 Hz), 152.6 (d, *J* = 235 Hz), 156.9, 157.7 (d, *J* = 2.5 Hz). ^{19}F NMR (470 MHz, acetone-d_6) δ: –138.7 (1F, m). IR (KBr): 3476, 3314, 3211, 1636 cm^{-1}. HRMS Calcd for $C_{15}H_{13}FNaO_6$ [(*M*+Na)$^+$] *m/z*: 331.0588, found: 331.0608.

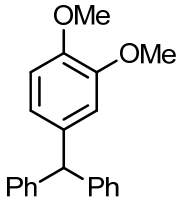
Preparation of catechols (1b–1f)



(3,4-Dimethoxyphenyl)diphenylmethanol (S3)

Under a nitrogen atmosphere, *n*BuLi (1.6 M in hexanes, 5.3 mL, 8.4 mmol) was added to a solution of 4-bromoveratrol (1.52 g, 7.0 mmol) in anhydrous THF (8 mL) at –78 °C. The reaction mixture was stirred at –78 °C for 20 min. Then a solution of benzophenone (1.15 g, 6.3 mmol) in THF (15 mL) was added at −78 °C. The reaction mixture was warm up to room temperatureand stirred for another 30 min at room temperature before being quenched with saturated aq. NH_4Cl solution. The layers were separated, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried (Na_2SO_4), filtered and concentrated *in vacuo*. Recrystallization of the residue from EtOAc gave **S3** (1.33 g, 66%). The mother liquid was concentrated, and the residue was purified by flash column chromatography (hexanes– CH_2Cl_2 1:6) to afford **S3**. Total amount of **S3** was 1.68 g (83%).

A colorless solid: mp 153.5–154.0 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 2.74 (1H, s), 3.68 (3H, s), 3.78 (3H, s), 6.57 (1H, dd, *J* = 2.5, 8.0 Hz), 6.69 (1H, d, *J* = 8.0 Hz), 6.85 (1H, d, *J* = 2.5 Hz), 7.17–7.25 (10H, m). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 55.76, 55.80, 81.9, 110.0, 111.3, 120.6, 127.2, 127.8, 127.9, 139.4, 146.9, 148.1, 148.4. IR ($CHCl_3$): 3597, 1597, 1510 cm^{-1}. HRMS Calcd for $C_{21}H_{20}O_2$ [(*M*–OH)$^+$] *m/z*: 320.1380, found: 320.1406.

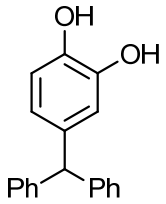


4-Benzhydryl-1,2-dimethoxybenzene (S4)

$NaBH_4$ (1.42 g, 38 mmol) was added to a solution of **S4** (1.20 g, 3.8 mmol) in CF_3CO_2H (8 mL) at 0 °C. The reaction mixture was stirred at 0 °C for 10 min and concetrated in vacuo. EtOAc and saturated aq. $NaHCO_3$ solution were added to the residue, and the layers were separated. The aqueous layer was extracted three times with EtOAc. The combined organic layers were

washed three times with brine, dried ($MgSO_4$), filtered and concentrated in *vacuo*. Recrystallization of the residue from EtOAc gave **S4** (0.90 g, 78%). The mother liquid was concentrated, and the residue was purified by flash column chromatography (hexanes–EtOAc 5:1) to afford **S4**. Total amount of **S4** was 1.16 g (quant.).

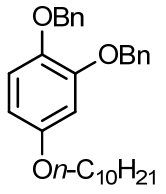
A colorless solid: mp 124–125 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 3.77 (3H, s), 3.86 (3H, s), 5.51 (1H, s), 6.60 (1H, dd, J = 2.0, 8.0 Hz), 6.68 (1H, d, J = 2.0 Hz), 6.79 (1H, d, J = 8.0 Hz), 7.12 (4H, d, J = 7.5 Hz), 7.24 (2H, t, J = 7.5 Hz), 7.29 (4H, t, J = 7.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 55.72, 55.79, 56.3, 110.7, 112.7, 121.4, 126.2, 128.2, 129.3, 136.4, 144.1, 147.4, 148.7. IR (KBr): 1589, 1516 cm^{-1}. HRMS Calcd for $C_{21}H_{20}NaO_2$ [(M+Na)$^+$] *m/z*: 327.1356, found: 327.1355.



4-Benzhydrylbenzene-1,2-diol (1b)

Under a nitrogen atmosphere, BBr_3 (1.0 M in CH_2Cl_2, 0.36 mL, 0.36 mmol) was added to a solution of **S4** (100 mg, 0.33 mmol) in anhydrous CH_2Cl_2 (1.3 mL, 0.3 M) at –78 °C. The reaction mixture was allowed to warm up to room temperature and stirred for another 20 min at room temperature before being quenched with saturated aq. $NaHCO_3$ solution. The aqueous layer was separated and extracted three times with CH_2Cl_2. The combined organic layers were dried ($MgSO_4$), filtered and concentrated *in vacuo*. The residue was purified by flash column chromatography (hexanes–EtOAc 2:1) to afford **1b** (92 mg, quant.).

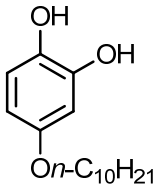
A colorless solid: mp 124–125 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 5.00 (1H, s), 5.05 (1H, s), 5.44 (1H, s), 6.57 (1H, dd, J = 2.0, 8.0 Hz), 6.60 (1H, d, J = 2.0 Hz), 6.78 (1H, d, J = 8.0 Hz), 7.11 (4H, d, J = 7.5 Hz), 7.21 (2H, t, J = 7.5 Hz), 7.28 (4H, t, J = 7.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 56.0, 115.2, 116.6, 122.1, 126.3, 128.3, 129.3, 137.1, 141.8, 143.1, 143.9. IR ($CHCl_3$): 3597, 3557 cm^{-1}. HRMS Calcd for $C_{19}H_{17}O_2$ (M^+) *m/z*: 276.1145, found: 276.1144.



4-Decyloxy-1,2-di(benzyloxy)benzene (S5)

*m*CPBA (80% w/w, 1.63 g, 7.6 mmol) was added to a solution of 3,4-dibenzyloxybezaldehyde[8] (2.0 g, 6.3 mmol) in CH_2Cl_2 (16.5 mL) at 0 °C. The reaction mixture was stirred at room temperature overnight and quenched with a mixture of saturated aq. $Na_2S_2O_3$ solution and saturated aq. $NaHCO_3$ solution. The layers were separated, and the aqueous layer was extracted five times with CH_2Cl_2. The combined organic layers were dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was dissolved in MeOH (16 mL), and K_2CO_3 (1.74 g, 12.6 mmol) was added. The reaction mixture was stirred at room temperature for 1 h and concentrated *in vacuo.* 10% HCl was added to the residue, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried ($MgSO_4$), filtered and concentrated *in vacuo*. The residue was dissolved in acetone (19 mL), and K_2CO_3 (1.74 g, 12.6 mmol), *n*Decyl-Br (1.96 mL, 9.5 mmol) and nBu_4NI (70 mg, 0.19 mmol) were added. The reaction mixture was refluxed for 20 h before being quenched with water and EtOAc. The layers were separated, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried ($MgSO_4$), filtered and concentrated *in vacuo*. The residue was purified by flash column chromatography (hexanes–EtOAc 30:1) to afford **S5** (2.5 g, 88%).

A colorless solid: mp 40.0–42.0 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 0.93 (3H, t, J = 8.0 Hz), 1.25–1.50 (14H, m), 1.76 (2H, quint, J = 8.0 Hz), 3.88 (2H, t, J = 8.0 Hz), 5.11 (2H, s), 5.16 (2H, s), 6.40 (1H, dd, J = 2.5, 8.5 Hz), 6.61 (1H, d, J = 2.5 Hz), 6.88 (1H, d, J = 8.5 Hz), 7.30–7.50 (10H, m). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 14.1, 22.7, 26.0, 29.27, 29.29, 29.4, 29.5, 31.9, 68.3, 71.0, 72.6, 103.2, 105.1, 117.1, 127.3, 127.5, 127.6, 127.7, 128.3, 128.4, 137.1, 137.6, 142.8, 150.2, 154.4. IR ($CHCl_3$): 2928, 2857, 1608, 1593, 1506 cm^{-1}. HRMS Calcd for $C_{30}H_{39}O_3$ [$(M+H)^+$] *m/z*: 447.2894, found: 447.2903.

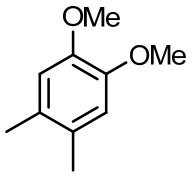


4-(Decyloxy)benzene-1,2-diol (1c)

MeOH (17 mL) was added to a mixture of **S5** (2.5 g, 5.5 mmol) and Pd/C (10% Pd on carbon, 250 mg) at room temperature under nitrogen atomosphere. The flask was evacuated, back-filled with hydrogen. The reaction mixture was stirred for 4 h at room temperature under a hydrogen atomosphere (1 atm) using a balloon and filtered through a Celite pad. The Celite pad was washed with EtOAc, and the combined organic layers were concentrated *in vacuo*. The resulting

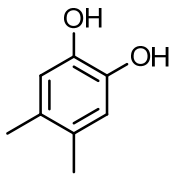
oil was purified by flash column chromatography (hexanes–EtOAc 3:1) to afford **1c** (1.12 g, 77%).

A colorless solid: mp 111.0–113.0 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 0.88 (3H, t, *J* = 7.5 Hz), 1.22–1.37 (12H, m), 1.42 (2H, quint, *J* = 7.5 Hz), 1.74 (2H, quint, *J* = 7.5 Hz), 3.86 (2H, t, *J* = 7.5 Hz), 4.61 (1H, s), 5.23 (1H, brs), 6.34 (1H, dd, *J* = 3.0, 8.5 Hz), 6.50 (1H, d, *J* = 3.0 Hz), 6.76 (1H, d, *J* = 8.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 14.1, 22.7, 26.0, 29.31, 29.32, 29.4, 29.56, 29.58, 31.9, 68.6, 102.9, 106.1, 115.8, 136.8, 144.6, 154.0. IR (KBr): 3412, 3325 cm^{-1}. HRMS Calcd for $C_{16}H_{27}O_3$ [(*M*+H)$^+$] *m/z*: 267.1955, found: 267.1954.



1,2-Dimethoxy-4,5-dimethylbenzene (S6)[9]

Under a nitrogen atmosphere, *n*BuLi (1.6 M in hexanes, 1.6 mL, 2.6 mmol) was added to a solution of 1-bromo-4,5-dimethoxy-2-methylbenzene[10] (500 mg, 2.2 mmol) in anhydrous THF (11 mL) at –78 °C. The reaction mixture was stirred at –78 °C for 30 min. MeI (0.40 mL, 7.8 mmol) was added, and the reaction mixture was allowed to warm up to room temperature and stirred at room temperature for 18 h before being quenched with saturated aq. NH_4Cl solution. The layers were separated, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried (Na_2SO_4), filtered and concentrated in *vacuo* to give **S6** (344 mg, 95%), which was used in the next step without further purification. An analytical sample was obtained by flash column chromatography (hexanes:CH_2Cl_2 1:1). A colorless solid: mp 32.0–36.0 °C. The ^{1}H NMR and ^{13}C NMR were in good agreement with those reported.[9]

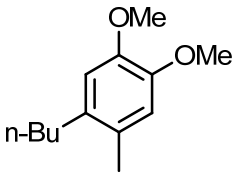


4,5-Dimethylbenzene-1,2-diol (1d)

Under a nitrogen atmosphere, BBr_3 (1.0 M in CH_2Cl_2, 2.2 mL, 2.2 mmol) was added to the solution of **S6** (341 mg, 2.1 mmol) in anhydrous CH_2Cl_2 (3.1 mL, 0.7M) at –78 °C. The reaction mixture was stirred at room temperature for 30 min before being quenched with ice–water. The

layers were separated, and the aqueous layer was extracted three times with CH_2Cl_2. The combined organic layers were washed with brine, dried ($MgSO_4$), filtered and concentrated *in vacuo*. The residue was purified by flash column chromatography (hexanes–EtOAc 4:1) to afford **1d** (223 mg, 79%).

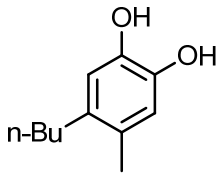
A colorless solid: mp 87–89 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 2.14 (6H, s), 4.90 (2H, brs), 6.65 (2H, s). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 18.7, 116.6, 127.8, 141.7. IR ($CHCl_3$): 3601, 3561 cm^{-1}. HRMS Calcd for $C_8H_{11}O_2$ [(*M*+H)$^+$] *m/z*: 139.0754, found: 139.0754.



1-Butyl-4,5-dimethoxy-2-methylbenzene (S7)

Under a nitrogen atmosphere, *n*BuLi (1.6 M in hexanes, 1.6 mL, 2.56 mmol) was added to a solution of 1-bromo-4,5-dimethoxy-2-methylbenzene[8] (500 mg, 2.2 mmol) in anhydrous THF (11 mL) at –78 °C. The reaction mixture was stirred at –78 °C for 30 min, and then *n*BuI (0.75 mL, 6.6 mmol) was added at −78 °C. The reaction mixture was allowed to warm up to room temperature and stirred at room temperature for 5 h before being quenched with saturated aq. NH_4Cl solution. The layers were separated, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried (Na_2SO_4), filtered and concentrated *in vacuo* to give **S7** (579 mg, quant.), which was used in the next step without further purification. An analytically pure sample was obtained by flash column chromatography (hexanes–EtOAc 5:1).

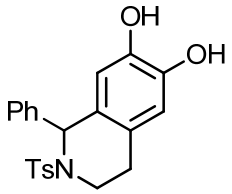
A colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ: 0.96 (3H, t, *J* = 7.5 Hz), 1.41 (2H, hex, *J* = 7.5 Hz), 1.54 (2H, quint, *J* = 7.5 Hz), 2.25 (3H, s), 2.54 (2H, t, *J* = 7.5 Hz), 3.85 (3H, s), 3.87 (3H, s), 6.669 (1H, s), 6.673 (1H, s). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 13.9, 18.6, 22.6, 32.7, 32.8, 55.7, 55.8, 112.3, 113.3, 127.4, 132.9, 146.4, 146.6. IR ($CHCl_3$): 1516, 1206 cm^{-1}. HRMS Calcd for $C_{13}H_{21}O_2$ [(*M*+H)$^+$] *m/z*: 209.1536, found: 209.1536.



4-Butyl-5-methylbenzene-1,2-diol (1e)

Similarly to the preparation of **1d**, **1e** (465 mg, 95%) was obtained from **S7** (579 mg, 2.2 mmol) using BBr_3 (1.0 M in CH_2Cl_2, 3.0 mL, 3.0 mmol).

A colorless solid: mp 52.0–52.5 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 0.93 (3H, t, *J* = 7.5 Hz), 1.37 (2H, hex, *J* = 7.5 Hz), 1.49 (2H, quint, *J* = 7.5 Hz), 2.17 (3H, s), 2.46 (2H, t, *J* = 7.5 Hz), 5.17 (1H, s), 5.18 (1H, s), 6.66 (2H, s). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 14.0, 18.5, 22.6, 32.3, 32.6, 116.0, 117.2, 128.4, 133.9, 140.8, 141.0. IR ($CHCl_3$): 3599, 3559 cm^{-1}. HRMS Calcd for $C_{11}H_{17}O_2$ [(*M*+H)$^+$] *m/z*: 181.1223, found: 181.1224.

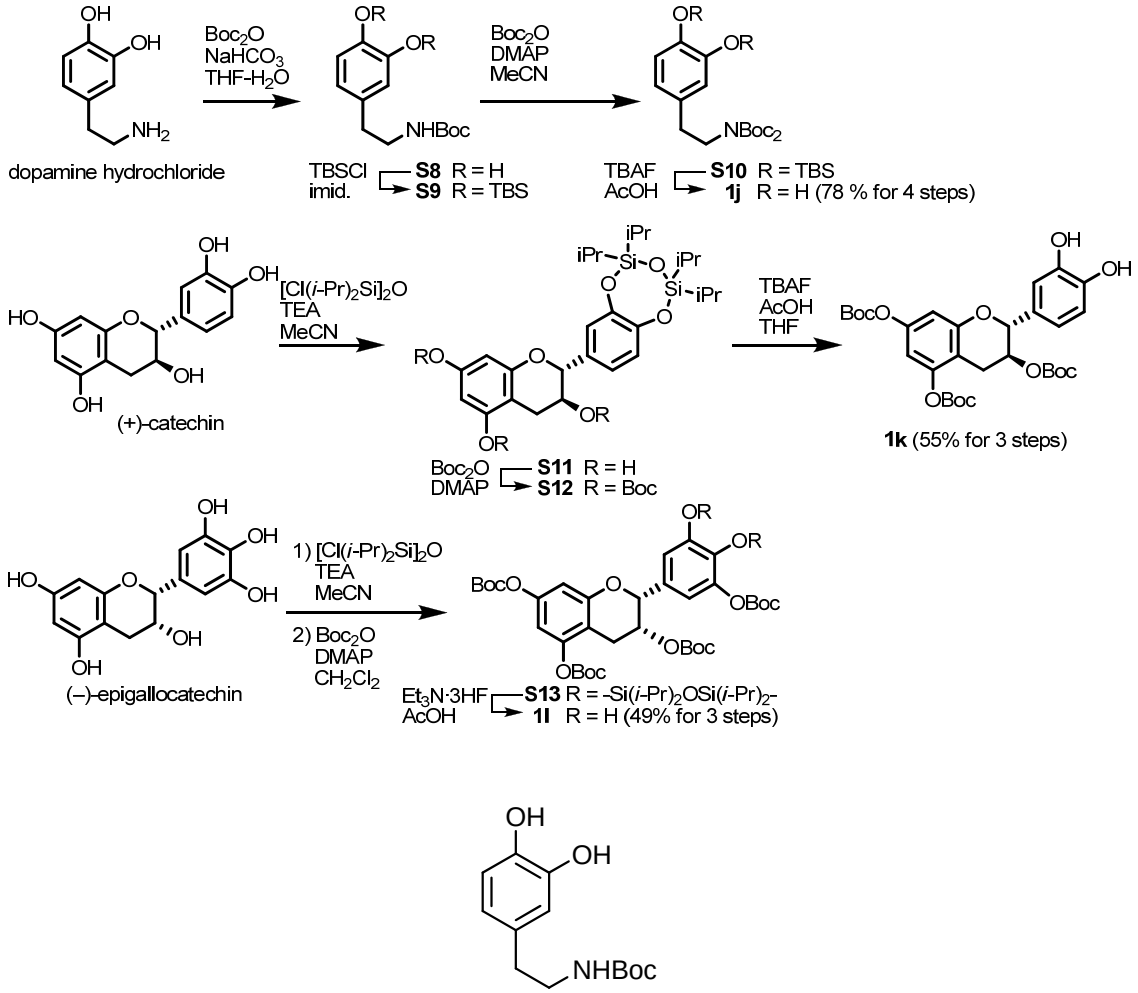


1-Phenyl-2-tosyl-1,2,3,4-tetrahydroisoquinoline-6,7-diol (1i)

Triethylamine (0.16 mL, 1.1 mmol) and TsCl (144 mg, 0.75 mmol) were added to a solution of 1-phenyl-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline (0.20 g, 0.74 mmol)[11] in CH_2Cl_2 (2.5 mL) at room temperature. The reaction mixture was stirred for 1 h before being quenched with 1N HCl solution. The layers were separated, and the aqueous layer was extracted three times with CH_2Cl_2. The combined organic layers were dried (Na_2SO_4), filtered and concentrated *in vacuo*. The reaction mixture was dissolved in anhydrous CH_2Cl_2 (7.4 mL), and BBr_3 (1.0 M in CH_2Cl_2, 1.1 mL, 1.1 mmol) was added at –78 °C. The reaction mixture was stirred for 1 h at the same temperature before being quenched with water. The layers were separated, and the aqueous layer was extracted three times with CH_2Cl_2. The combined organic layers were dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by flash column chromatography (hexanes–EtOAc 1:1) to afford **1i** (293 mg, quant.).

A colorless solid: mp 196.0–196.5 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 2.34 (3H, s), 2.42 (1H, ddd, *J* = 2.0, 5.0, 16.5 Hz), 2.53 (1H, ddd, *J* = 6.5, 11.5, 16.5 Hz), 3.23 (1H, ddd, *J* = 5.0, 11.5, 14.5 Hz), 3.70–3.76 (1H, m), 5.07 (1H, brs), 5.17 (1H, brs), 6.10 (1H, s), 6.47 (1H, s), 6.49 (1H, s), 7.10 (2H, d, *J* = 8.0 Hz), 7.18–7.20 (2H, m), 7.22–7.26 (3H, m), 7.55 (2H, d, *J* = 8.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 21.4, 26.3, 39.1, 58.8, 114.9, 115.3, 126.6, 126.8, 127.1, 127.6, 128.3, 128.7, 129.3, 138.0, 141.7, 141.9, 143.0, 143.1. IR ($CHCl_3$): 3595, 3559, 3448, 3422 cm^{-1}. HRMS Calcd for $C_{22}H_{22}NO_4S$ [(*M*+H)$^+$] *m/z*: 396.1264, found: 396.1260.

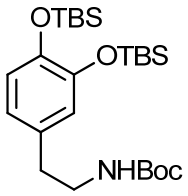
Preparation of the protected dopamine (1j) and catechins (1k and 1l)



***tert*-Butyl 2-(3,4-dihydroxyphenyl)ethylcarbamate (S8)**[12]

Boc_2O (0.67 mL, 2.9 mmol) was added to a solution of dopamine hydrochloride (500 mg, 2.6 mmol) in a mixture of THF (6.7 mL) and saturated aq. $NaHCO_3$ solution (4.0 mL). The reaction mixture was stirred at room temperature for 2 h. The organic layers were separated, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried (Na_2SO_4), filtered and concentrated *in vacuo* to give **S8** (680 mg, quant.), which was pure enough.

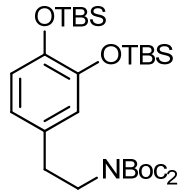
A colorless solid: mp 166.0–167.0 ºC. ^{1}H NMR (500 MHz, DMSO-d_6) δ: 1.37 (9H, s), 2.48 (2H, t, J = 7.5 Hz), 3.03 (2H, dd, J = 6.0, 7.5 Hz), , 6.41 (1H, dd, J = 2.5, 8.0 Hz), 6.55 (1H, d, J = 2.5 Hz), 6.62 (1H, d, J = 8.0 Hz), 6.81 (1H, t, J = 6.0 Hz), 8.70 (2H, brs). ^{13}C NMR (125 MHz, DMSO-d_6) δ: 28.3, 35.1, 42.0, 77.5, 115.5, 116.0, 119.2, 130.2, 143.5, 145.1, 155.5. IR (KBr): 3489, 3377, 3129, 1682 cm^{-1}.



***tert*-Butyl 2-[3,4-bis(*tert*-butyldimethylsilyloxy)phenyl]ethylcarbamate (S9)**

Under a nitrogen atmosphere, imidazole (0.94 g, 14.0 mmol) and TBSCl (1.9 g, 13.0 mmol) were added to a solution of **S9** (1.0 g, 4.0 mmol) in anhydrous CH_3CN (7.9 mL). The reaction mixture was stirred at room temperature for 1 h before being quenched with saturated aq. NH_4Cl solution. The organic layers were separated, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried (Na_2SO_4), filtered and concentrated *in vacuo* to give crude **S9** (3.0 g). An analytically pure compound was obtained by flash column chromatography (hexanes–AcOEt 10: 1).

A colorless solid: mp 68.0–70.0 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 0.185 (6H, s), 0.190 (6H, s), 0.979 (9H, s), 0.982 (9H, s), 1.43 (9H, s), 2.65 (2H, t, J = 6.5 Hz), 3.32 (2H, q, J = 6.5 Hz), 4.49 (1H, brs), 6.62 (1H, dd, J = 2.5, 8.0 Hz), 6.64 (1H, d, J = 2.5 Hz), 6.75 (1H, d, J = 8.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: –4.12, –4.05, 18.4, 25.9, 28.4, 35.4, 41.8, 79.1, 121.0, 121.6, 121.7, 132.0, 145.3, 146.6, 155.8. IR ($CHCl_3$): 3453, 1707 cm^{-1}. HRMS Calcd for $C_{25}H_{47}NO_4SiNa$ [(M+Na)$^+$] *m/z*: 504.2936, found: 504.2933.

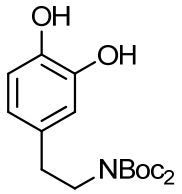


Di(*tert*-butyl) 2-[3,4-bis(*tert*-butyldimethylsilyloxy)phenyl]ethyliminodicarbonate (S10)

Boc_2O (2.7 mL, 12.0 mmol) and DMAP (483 mg, 4.0 mmol) were added to a solution of the above-mentioned crude **S9** (3.0g) in CH_3CN (7.9 mL). The reaction mixture was stirred at 50 °C overnight. Boc_2O (6.4 mL) was added and the reaction mixture was stirred for 1 h. Boc_2O (1.8 mL, 2.0 equiv) and DMAP (145 mg, 0.3 equiv) were added. The reaction mixture was stirred for another 1 h before being quenched with saturated aq. NH_4Cl solution. The organic layers were separated, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried (Na_2SO_4), filtered and concentrated *in vacuo* to give crude **S10** (2.5g). An analytically pure compound was obtained by flash column chromatography (hexanes–AcOEt 20: 1)

A colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ: 0.18 (12H, s), 0.97 (9H, s), 0.98 (9H, s), 1.51

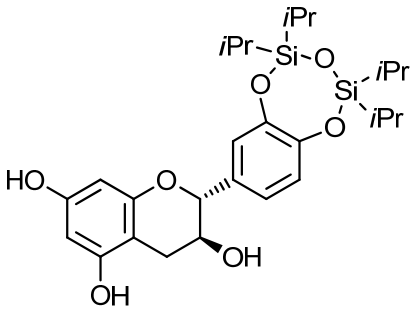
(18H, s), 2.72 (2H, dd, J = 7.5, 8.5 Hz), 3.70 (2H, dd, J = 7.5, 8.5 Hz), 6.64 (1H, dd, J = 2.5, 8.0 Hz), 6.65 (1H, d, J = 2.5 Hz), 6.73 (1H, d, J = 8.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: –4.1, 18.37, 18.41, 25.91, 25.93, 28.1, 34.8, 48.2, 82.1, 120.1, 121.7, 121.8, 131.8, 145.3, 146.5, 152.2. IR ($CHCl_3$): 1778, 1738, 1709, 1688 cm^{-1}. HRMS Calcd for $C_{30}H_{55}NO_6Si_2$ (M^+) *m/z*: 581.3562, found: 581.3573.



Di(*tert*-butyl) 2-(3,4-dihydroxyphenyl)ethyliminodicarbonate (1j)

AcOH (0.68 mL, 12.0 mmol) and TBAF (1.0 M in THF, 12.0 mL, 12.0 mmol) were added to a solution of the above-mentioned crude **S10** (2.5g) in THF (40 mL) at 0 °C. The reaction mixture was stirred 0 °C for 30 min before being quenched with brine. The layers were separated, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by flash column chromatography (hexanes–EtOAc 2:1 to EtOAc only) to afford **1j** (1.10 g, 78% from dopamine hydrochloride).

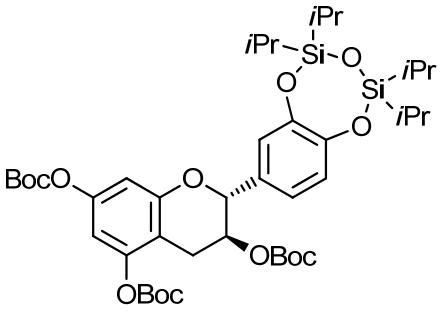
A colorless solid: mp 135.0–136.5 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 1.47 (18H, s), 2.74 (2H, dd, J = 7.0, 7.5 Hz), 3.74 (2H, dd, J = 7.0, 7.5 Hz), 5.76 (1H, brs), 5.96 (1H, s), 6.61 (1H, dd, J = 2.0, 8.0 Hz), 6.70 (1H, d, J = 2.0 Hz), 6.79 (1H, d, J = 8.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 28.0, 34.7, 48.0, 82.6, 115.4, 116.2, 121.3, 131.4, 142.4, 143.6, 152.5. IR ($CHCl_3$): 3597, 3555, 3383, 1775, 1739, 1732, 1686 cm^{-1}. HRMS Calcd for $C_{18}H_{28}NO_6$ [(M+H)$^+$] *m/z*: 354.1911, found: 354.1906.



(2*R*,3*S*)-2-(2,2,4,4-tetraisopropylbenzo[*f*][1,3,5,2,4]trioxadisilepin-7-yl)chroman-3,5,7-triol (S11)

Under a nitrogen atmosphere, 1,3-dichloro-1,1,3,3-tetraisoprpryldisiloxane (2.3 mL,7.2 mmol) and triethylamine (2.1 mL, 15.2 mmol) were added to a solution of (+)-catechin (2.0 g, 6.9 mmol) in CH_3CN (200 mL) at 0 °C. The reaction mixture was stirred at room temperature overnight and quenched with saturated aq. NH_4Cl solution. The layers were separated, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried (Na_2SO_4), filtered and concentrated *in vacuo* to give crude **S11** (4.1g). An analytically pure compound was obtained by flash column chromatography (hexanes–EtOAc 1:1).

A colorless amorphous solid: mp 59.0–61.0 ºC. $[\alpha]_D^{20}$ +0.30 (*c* 0.63, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ: 0.95–1.10 (28H, m), 1.88 (2H, brs), 2.29 (1H, brs), 2.54 (1H, dd, *J* = 8.0, 16.0 Hz), 2.86 (1H, dd, *J* = 5.0, 16.0 Hz), 3.97 (1H, q, *J* = 8.0 Hz), 4.61 (1H, d, *J* = 8.0 Hz), 5.82 (1H, brs), 5.90–6.00 (2H, m), 6.02 (1H, d, *J* = 2.0 Hz), 6.90 (1H, dd, *J* = 2.0, 8.5 Hz), 6.94 (1H, d, *J* = 8.5 Hz), 6.99 (1H, d, *J* = 2.0 Hz) ^{13}C NMR (125 MHz, $CDCl_3$) δ: 12.9, 12.97, 13.01, 16.95, 16.98, 17.00, 17.03, 26.5, 68.1, 80.6, 96.0, 96.3, 100.1, 120.8, 121.2, 122.3, 132.0, 145.5, 145.7, 154.7, 155.1, 155.4. IR ($CHCl_3$): 3593, 3381 cm^{-1}. HRMS Calcd for $C_{27}H_{41}O_7Si_2$ $[(M+H)^+]$ *m/z*: 533.2385, found: 533.2385.

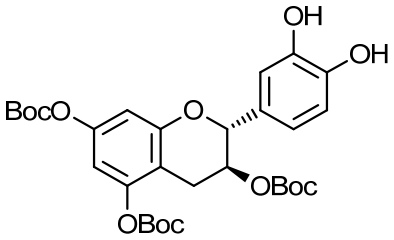


Tri(*tert*-butyl) (2*R*,3*S*)-2-(2,2,4,4-tetraisopropylbenzo[*f*][1,3,5,2,4]trioxadisilepin-7-yl)-chroman- 3,5,7-triyl tricarbonate (S12)

Under a nitrogen atmosphere, Boc_2O (6.3 mL, 28 mmol) and DMAP (421 mg, 3.5mmol) were added to a solution of the above-mentioned crude **S11** (4.1g) in CH_2Cl_2 (70 mL) at 0 °C. The reaction mixture was stirred at room temperature for 3 h before being quenched with saturated aq. NH_4Cl solution. The layers were separated, and the aqueous layer was extracted three times with CH_2Cl_2. The combined organic layers were dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by flash column chromatography (hexanes–EtOAc 20:1) to afford **S12** (3.4 g, 59% from catechin).

A colorless solid: mp 59.0–61.0 ºC. $[\alpha]_D^{20}$ +8.51 (*c* 0.48, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$)

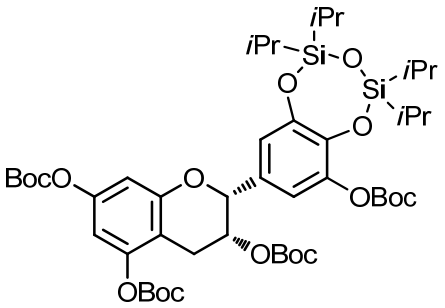
δ: 1.01–1.09 (28H, m), 1.38 (9H, s), 1.51 (9H, s), 1.54 (9H, s), 2.80 (1H, dd, *J* = 6.5, 16.5 Hz), 2.90 (1H, dd, *J* = 6.5, 16.5 Hz), 5.03 (1H, d, *J* = 6.5 Hz), 5.09 (1H, q, *J* = 6.5 Hz), 6.717 (1H, d, *J* = 2.5 Hz), 6.724 (1H, d, *J* = 2.5 Hz), 6.87 (1H, dd, *J* = 2.0, 8.5 Hz), 6.90 (1H, d, *J* = 8.5 Hz), 6.95 (1H, d, *J* = 2.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 12.9, 13.01, 13.04, 13.06, 16.95, 17.00, 17.03, 17.06, 24.1, 27.59, 27.65, 70.8, 78.1, 82.6, 83.7, 83.8, 107.3, 107.9, 110.3, 120.3, 120.5, 122.0, 131.3, 145.4, 145.6, 149.6, 150.1, 150.7, 151.2, 152.3, 154.6. IR ($CHCl_3$): 1759 cm^{-1}. HRMS Calcd for $C_{42}H_{64}O_{13}Si_2$ (M^+) *m/z*: 832.3880, found: 832.3875.



Tri(*tert*-butyl) (2*R*,3*S*)-2-(3,4-dihydroxyphenyl)chroman-3,5,7-triyl tricarbonate (1k)

AcOH (0.66 mL, 11.5 mmol) and Bu_4NF (1.0 M in THF, 11.5 mL, 11.5 mmol) were added to a solution of **S12** (3.2 g, 3.8 mmol) in THF (38 mL) at 0 °C. The reaction mixture was stirred at room temperature for 30 min before being quenched with water and EtOAc. The layers were separated, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by flash column chromatography (hexanes–EtOAc 3:2) to afford **1k** (2.1 g, 93%).

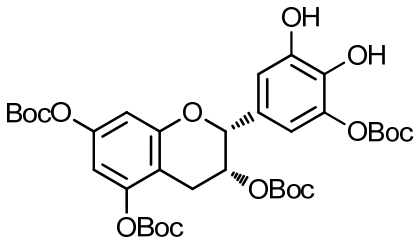
A colorless solid: mp 90.5–93.0 ºC. $[\alpha]_D^{20}$ +0.26 (*c* 0.98, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ: 1.41 (9H, s), 1.51 (9H, s), 1.55 (9H, s), 2.75 (1H, dd, *J* = 5.0, 17.0 Hz), 2.83 (1H, dd, *J* = 5.0, 17.0 Hz), 5.07 (1H, q, *J* = 5.0 Hz), 5.15 (1H, d, *J* = 5.0 Hz), 6.65 (1H, d, *J* = 2.0 Hz), 6.71 (1H, d, *J* = 2.0 Hz), 6.76 (1H, dd, *J* = 2.0, 8.0 Hz), 6.80 (1H, d, *J* = 8.0 Hz), 6.82 (1H, d, *J* = 2.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 27.60, 27.63, 27.7, 70.7, 78.0, 82.9, 84.3, 84.4, 107.9, 108.1, 110.8, 112.9, 115.1, 118.9, 129.4, 143.7, 144.3, 149.6, 150.0, 151.3, 151.9, 152.6, 154.9. IR ($CHCl_3$): 3551, 1751 cm^{-1}. HRMS Calcd for $C_{30}H_{38}NaO_{12}$ [(M+Na)$^+$] *m/z*: 613.2255, found: 613.2265.



Tetra(*tert*-butyl) (2*R*,3*R*)-2-(9-*tert*-butoxycarbonyloxy-2,2,4,4-tetraisopropylbenzo-[*f*][1,3,5,2,4]trioxadisilepin-7-yl)chroman-3,5,7-triyl tricarbonate (S13)

Similarly to the preparation of **S11**, (2*R*,3*R*)-2-(9-*tert*-butoxycarbonyloxy-2,2,4,4-tetra-isopropylbenzo[*f*][1,3,5,2,4]trioxadisilepin-7-yl)chroman-3,5,7-triol was obtained by the reaction of (–)-epigallocatechin (100 mg, 0.33 mmol) with 1,3-dichloro-1,1,3,3-tetraisoprpryl-disiloxane (0.12 mL, 0.36 mmol) and triethylamine (0.12 mL, 0.83 mmol) in CH_3CN (33 mL) at 50 °C overnight followed by work-up and flash column chlomatography (hexanes–EtOAc 1: 1). The Boc protection of the above-mentioned crude product was similarly carried out using Boc_2O (0.29 mL, 2.2 mmol) and DMAP (3.1 mg, 0.025 mmol) at room temperature for 2 h followed by work-up and flash column chromatography (hexanes–EtOAc 7:1) to afford **S13** (159 mg, 50% from epigallocatechin).

A colorless amorphous solid: mp 100.5–103.0 ºC. $[\alpha]_D^{20}$ –4.13 (*c* 0.94, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ: 1.06–1.08 (28H, m), 1.33 (9H, s), 1.52 (9H, s), 1.54–1.55 (18H, m), 2.99 (2H,brs), 4.97 (1H, s), 5.22 (1H, brs), 6.70 (1H, d, *J* = 2.5 Hz), 6.74 (1H, d, *J* = 2.5 Hz), 6.91 (1H, d, *J* = 2.5 Hz), 6.96 (1H, d, *J* = 2.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ:12.99, 13.01, 13.2, 16.78, 16.79, 16.84, 16.92, 16.95, 17.0, 17.1, 26.1, 27.5, 27.60, 27.64, 27.7, 69.1, 82.4, 82.9, 83.6, 83.8, 107.8, 108.0, 109.6, 114.6, 117.6, 130.0, 138.3, 142.6, 146.0, 149.8, 150.0, 151.0. 151.2, 152.8, 155.1. IR ($CHCl_3$): 2984, 2967, 2947, 1759 cm^{-1}. HRMS Calcd for $C_{47}H_{72}NaO_{16}Si_2$ [(*M*+Na)$^+$] *m/z*: 971.4251, found: 971.4223.



Tetra(*tert*-butyl) (2*R*,3*S*)-2-(5-*tert*-butoxycarbonyloxy-3,4-dihydroxyphenyl)chroman-3,5,7-triyl tricarbonate (1l)

AcOH (0.18 mL, 3.1 mmol) and $Et_3N{\cdot}3HF$ (0.20 mL, 1.2 mmol) were added to a solution of **S13** (0.59 g, 0.62 mmol) in THF (6.2 mL, 0.1 M) at 0 °C. The reaction mixture was stirred at room temperature for 1 h before being quenched with water. The layers were separated, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by flash column chromatography (hexanes–EtOAc–AcOH 120:80:1) to afford **1l** (0.43 g, 98%).

A colorless solid: mp 100.0–105.0 ºC. $[\alpha]_D^{20}$ –4.02 (*c* 0.60, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ: 1.34 (9H, s), 1.54 (18H, s), 1.58 (9H, s), 2.96 (1H, dd, *J* = 2.5, 18.0 Hz), 3.01 (1H, dd, *J* = 4.0, 18.0 Hz), 4.95 (1H, brs), 5.24 (1H, brs), 6.08 (2H, brs), 6.70 (1H, d, *J* = 2.0 Hz), 6.71 (1H, d, *J* = 2.0 Hz), 6.81 (1H, d, *J* = 2.0 Hz), 6.88 (1H, d, *J* = 2.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 25.9, 27.56, 27.62, 27.7, 69.3, 82.8, 83.8, 84.0, 84.7, 107.9, 108.1, 109.8, 111.4, 111.9, 129.1, 135.4, 138.9, 146.0, 149.8, 150.0, 150.9, 151.4, 152.3, 152.9, 155.1. IR ($CHCl_3$): 3435, 1763 cm^{-1}. HRMS Calcd for $C_{35}H_{46}NaO_{15}$ [(*M*+Na)$^+$] *m/z*: 729.2729, found: 729.2714.

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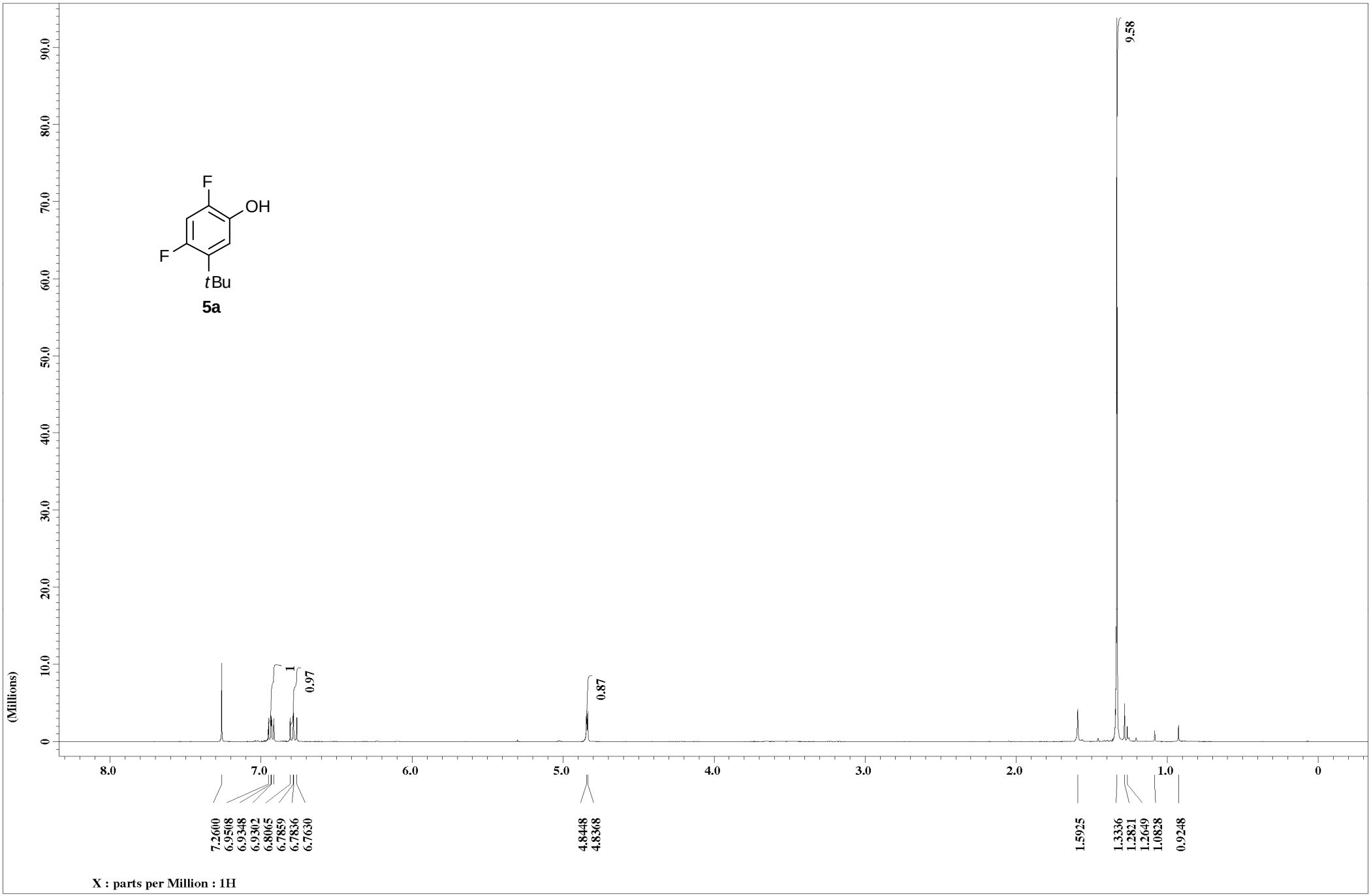
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F
tBu
5a
(Millions)
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80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
9.58
1
0.97
0.87
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2600
6.9508
6.9348
6.9302
6.8065
6.7859
6.7836
6.7630
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4.8368
1.5925
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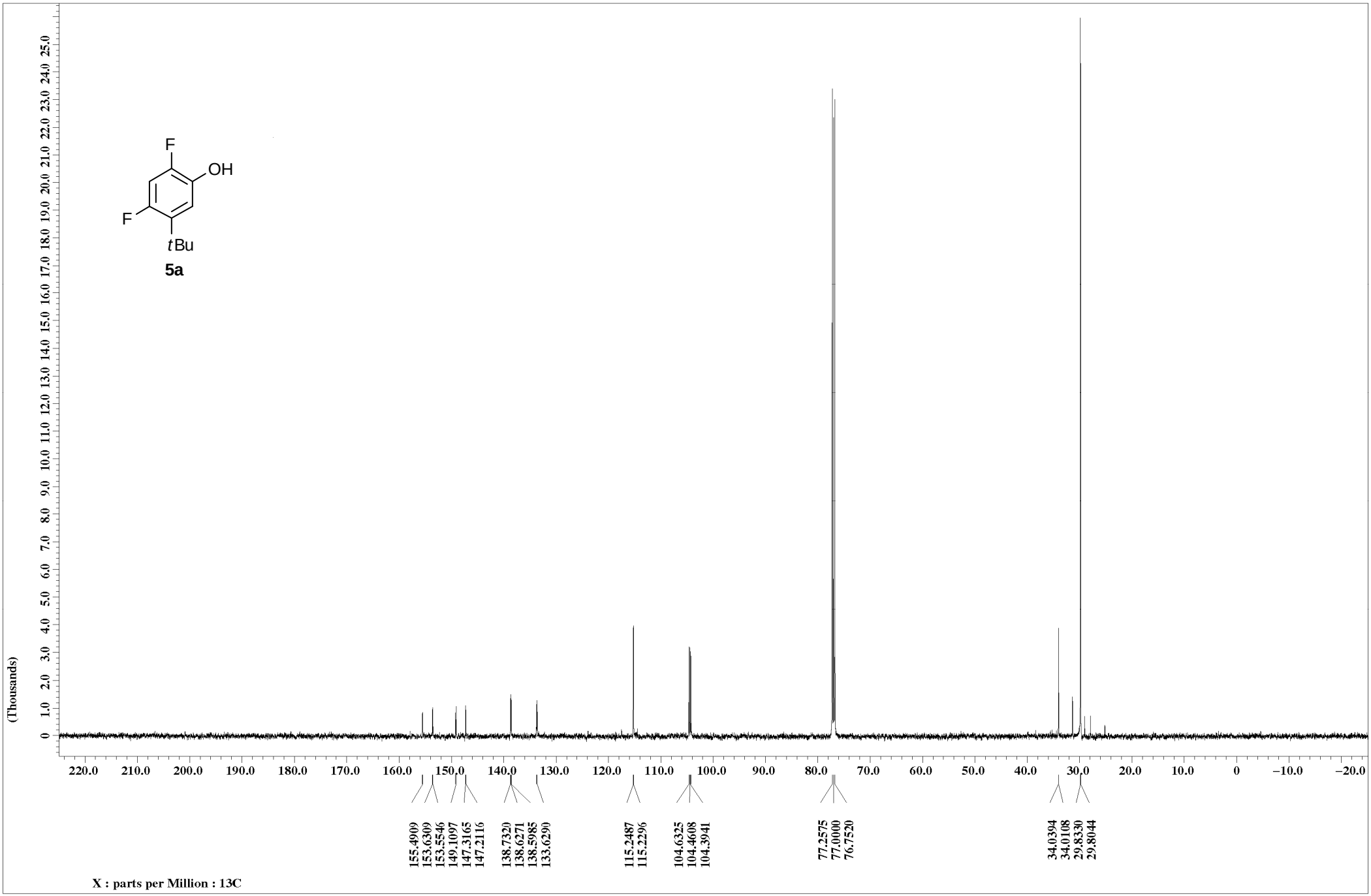
1.2821
1.2649
1.0828
0.9248
X : parts per Million : 1H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OH
F
tBu
5a
(Thousands)
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220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0 −20.0
155.4909
153.6309
153.5546
149.1097
147.3165
147.2116
138.7320
138.6271
138.5985
133.6290
115.2487
115.2296
104.6325
104.4608
104.3941
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77.0000
76.7520
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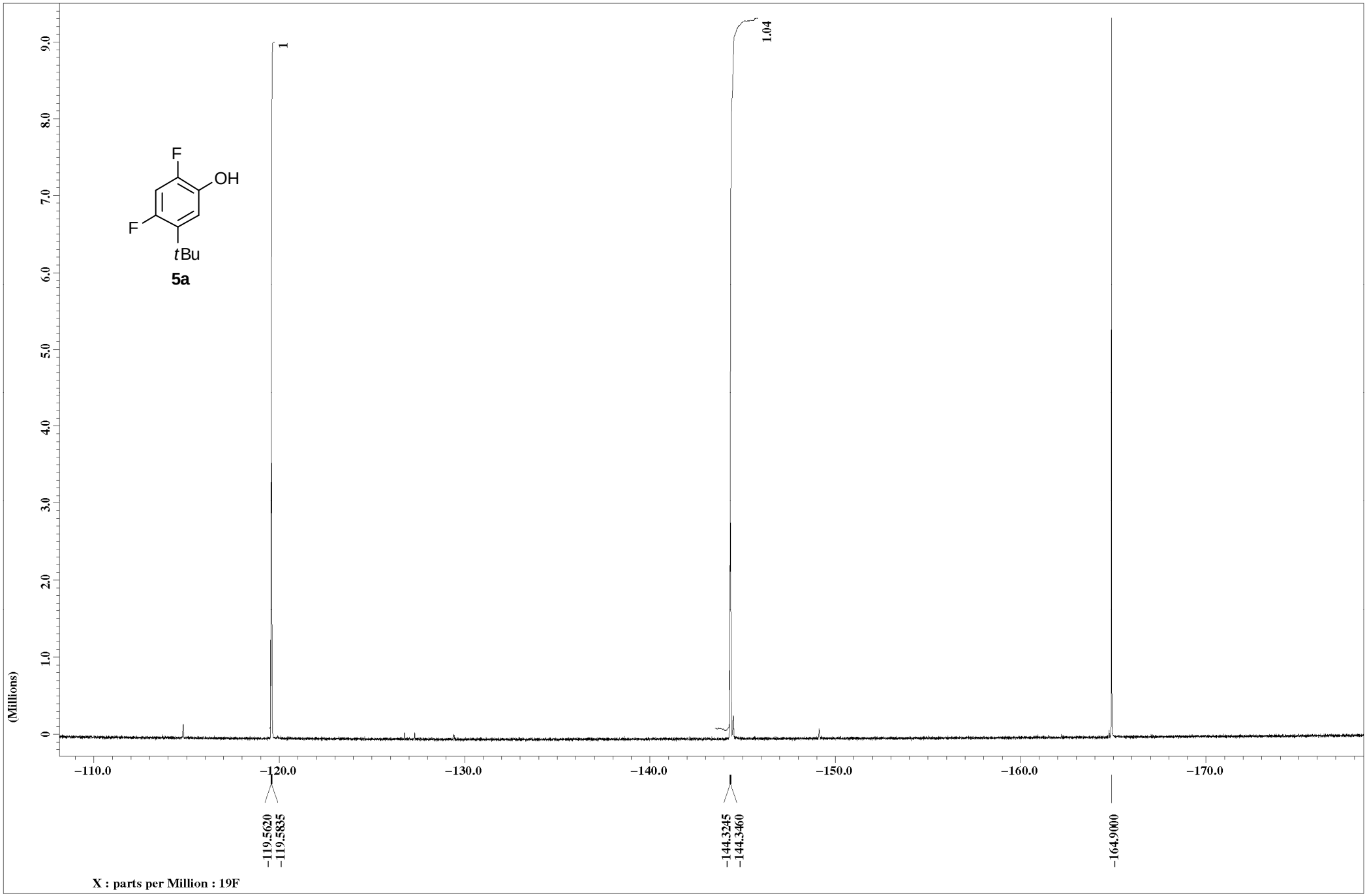
34.0108
29.8330
29.8044
X : parts per Million : 13C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F
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5a
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(Millions)
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6.0
5.0
4.0
3.0
2.0
1.0
0
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−120.0
−130.0
−140.0
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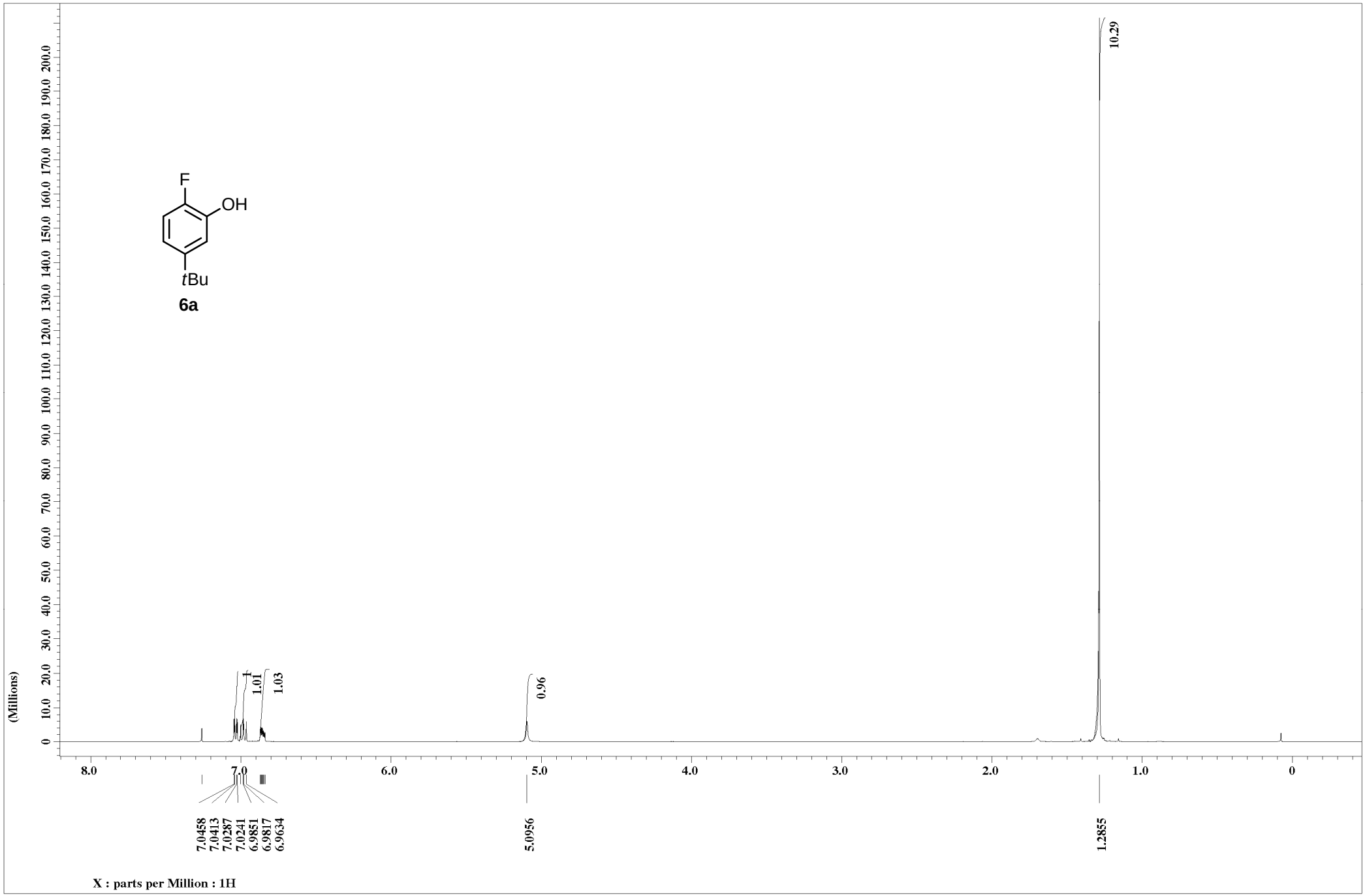
−164.9000
X : parts per Million : 19F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OH
tBu
6a
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50.0
60.0
70.0
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110.0
120.0
130.0
140.0
150.0
160.0
170.0
180.0
190.0
200.0
10.29
1.01
1.03
0.96
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
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7.0241
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1.2855
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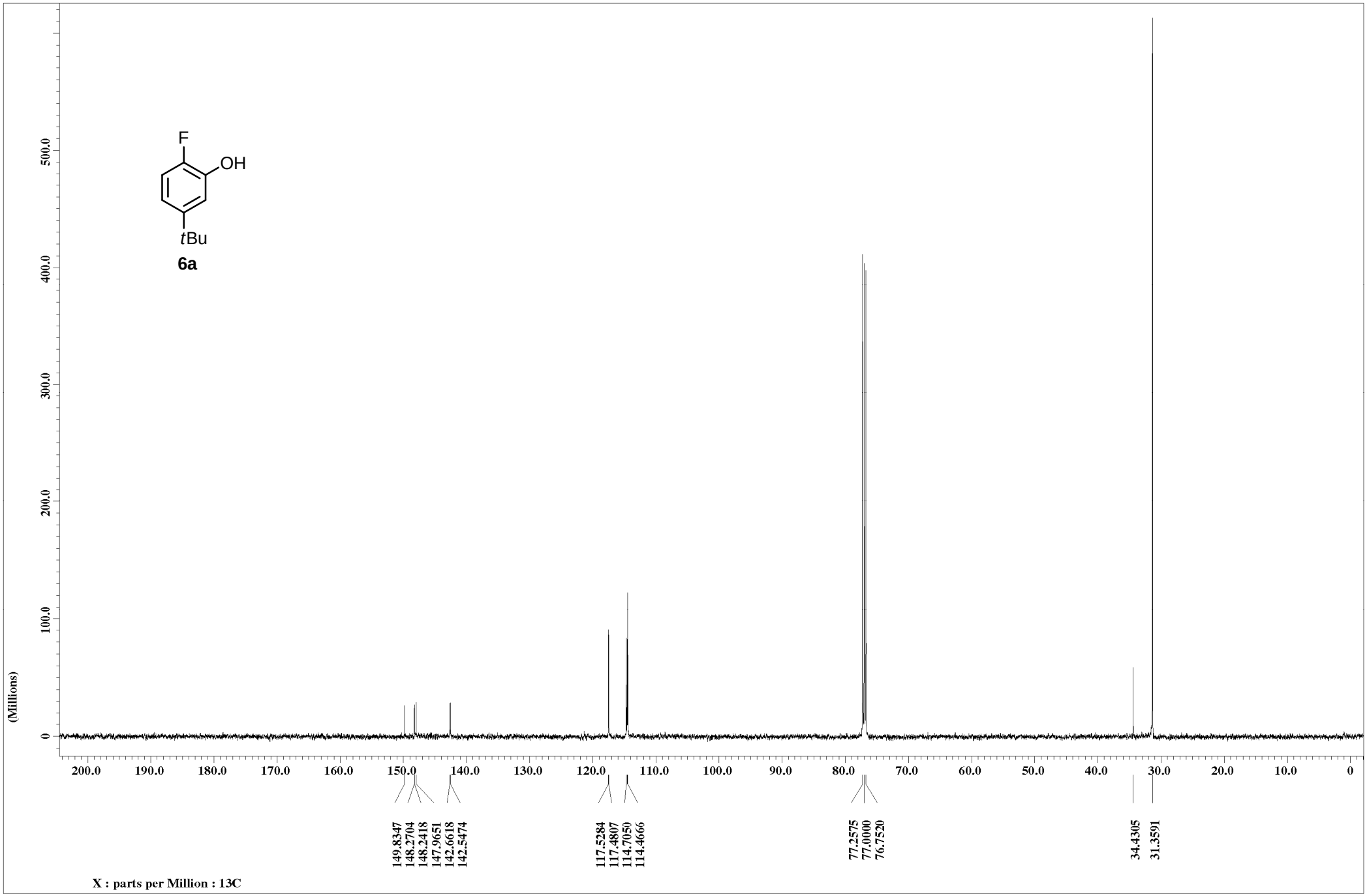
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OH
tBu
6a
(Millions)
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200.0
100.0
0
200.0
190.0
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150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
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148.2704
148.2418
147.9651
142.6618
142.5474
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114.4666
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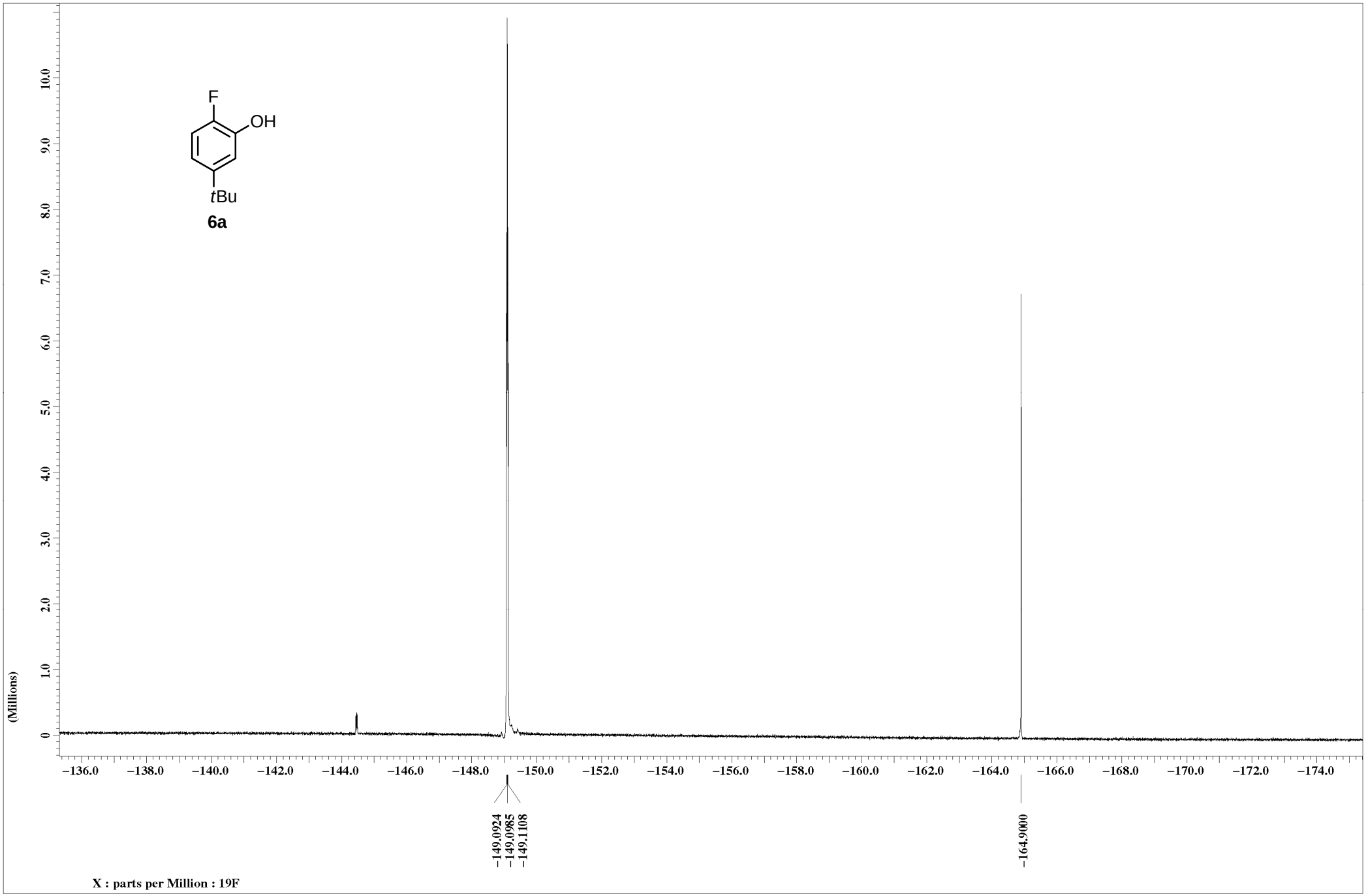
77.0000
76.7520
34.4305
31.3591
X : parts per Million : 13C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tBu
6a
(Millions)
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7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
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−138.0
−140.0
−142.0
−144.0
−146.0
−148.0
−150.0
−152.0
−154.0
−156.0
−158.0
−160.0
−162.0
−164.0
−166.0
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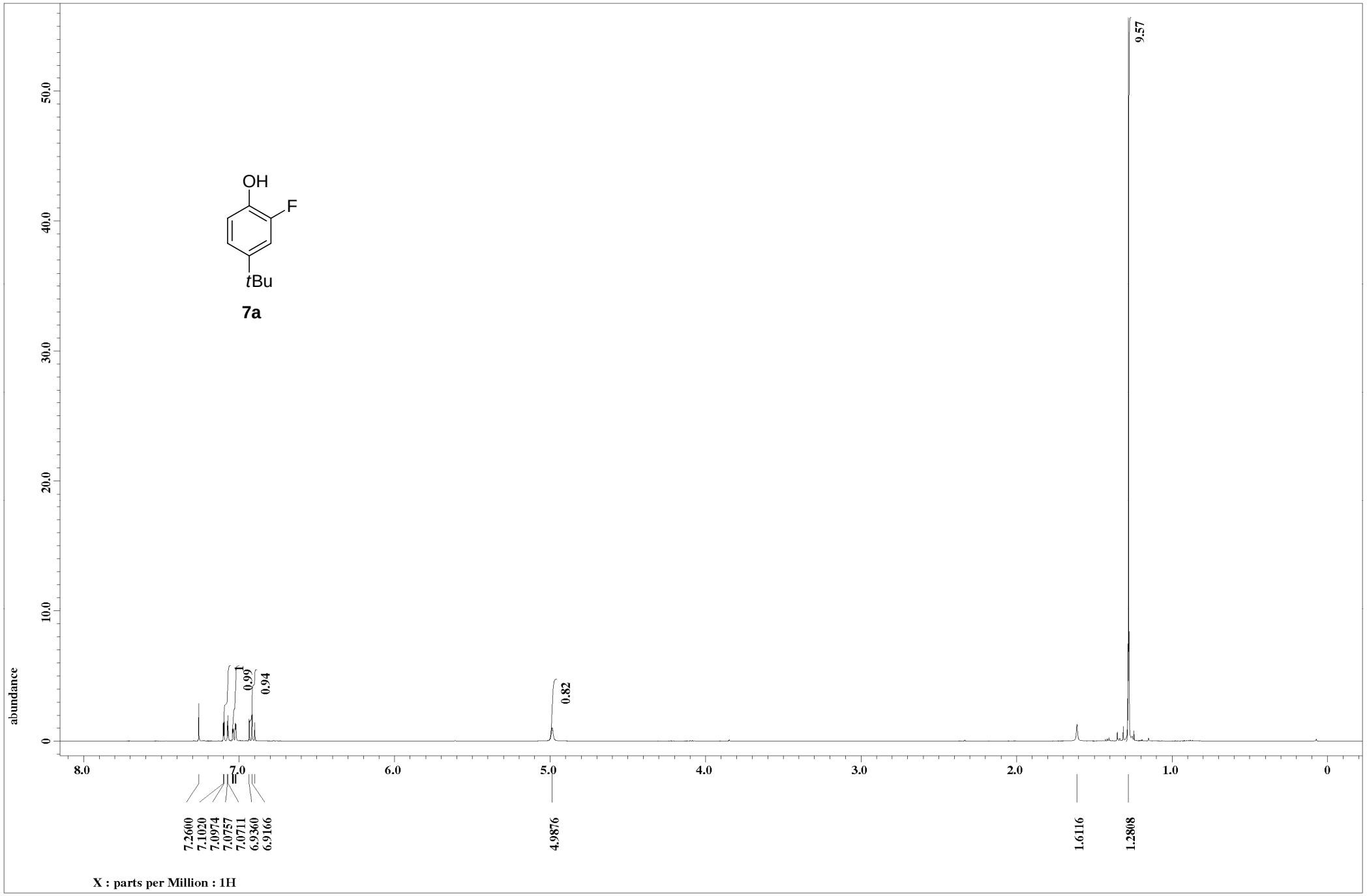
X : parts per Million : 19F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tBu
7a
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10.0
0
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0.99
0.94
0.82
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2600
7.1020
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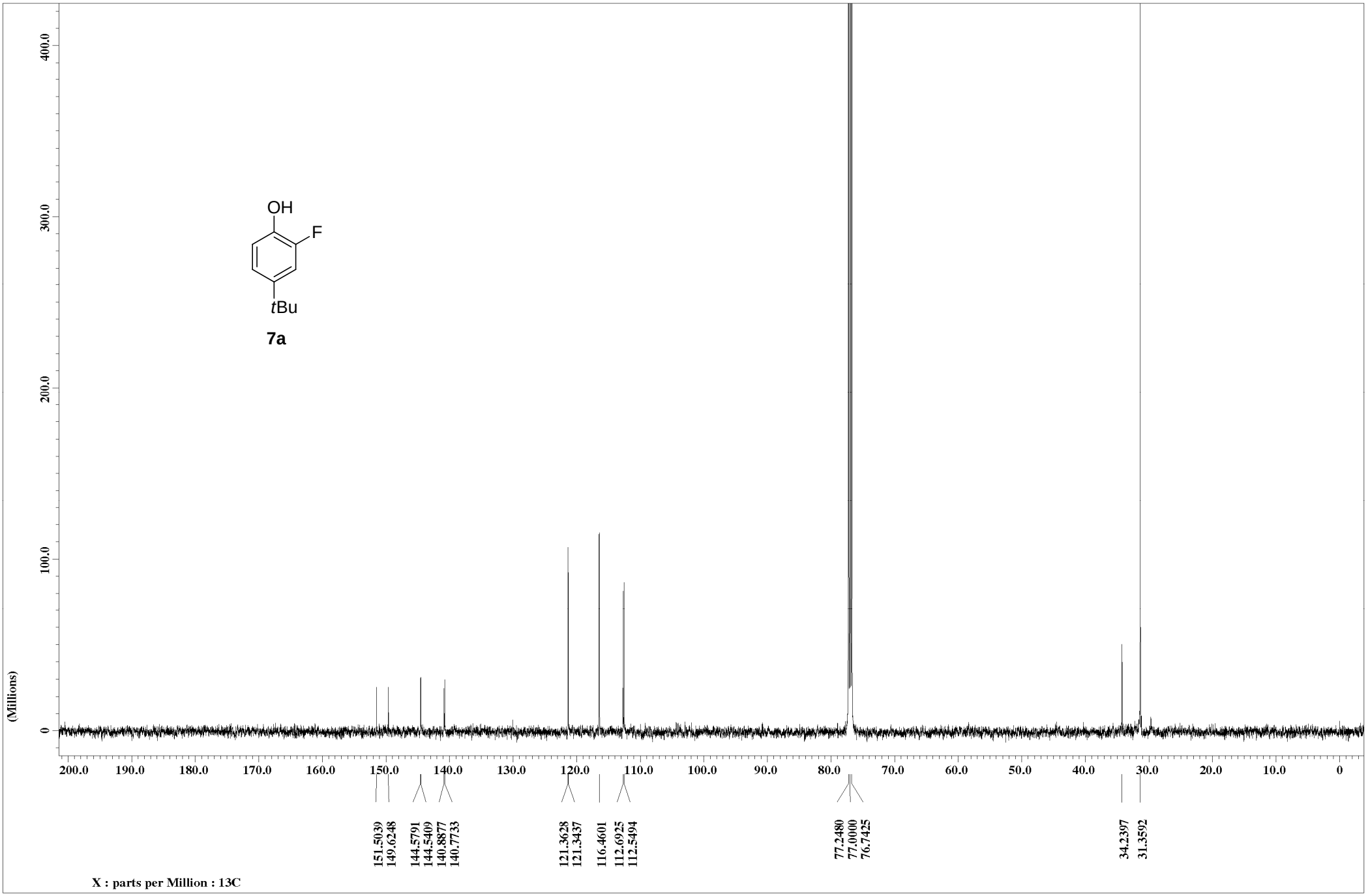
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F
tBu
7a
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200.0
100.0
0
(Millions)
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151.5039
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144.5409
140.8877
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121.3628
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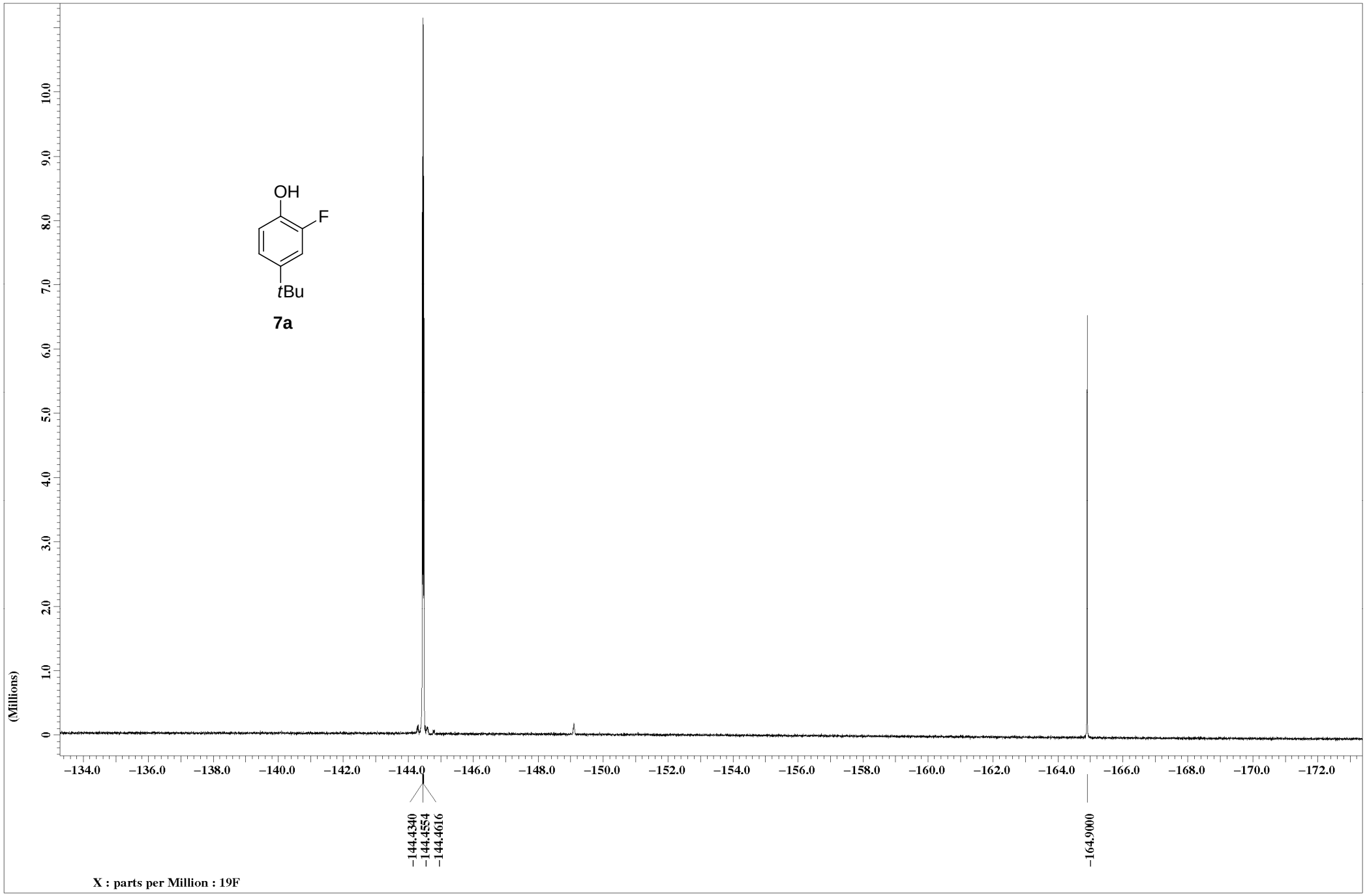
X : parts per Million : 13C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F
tBu
7a
(Millions)
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2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
−134.0
−136.0
−138.0
−140.0
−142.0
−144.0
−146.0
−148.0
−150.0
−152.0
−154.0
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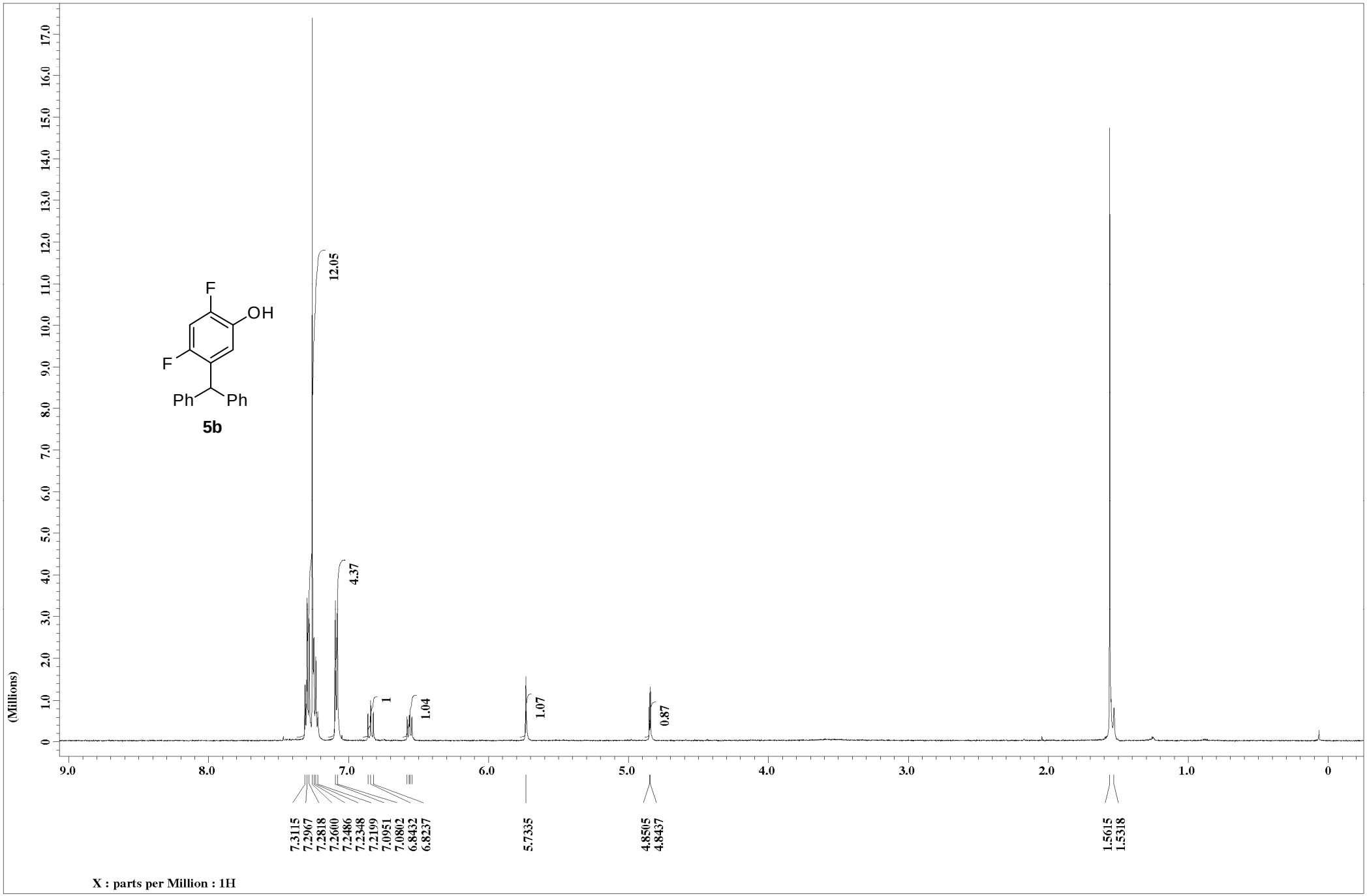
X : parts per Million : 19F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F
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Ph
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(Millions)
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15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
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3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
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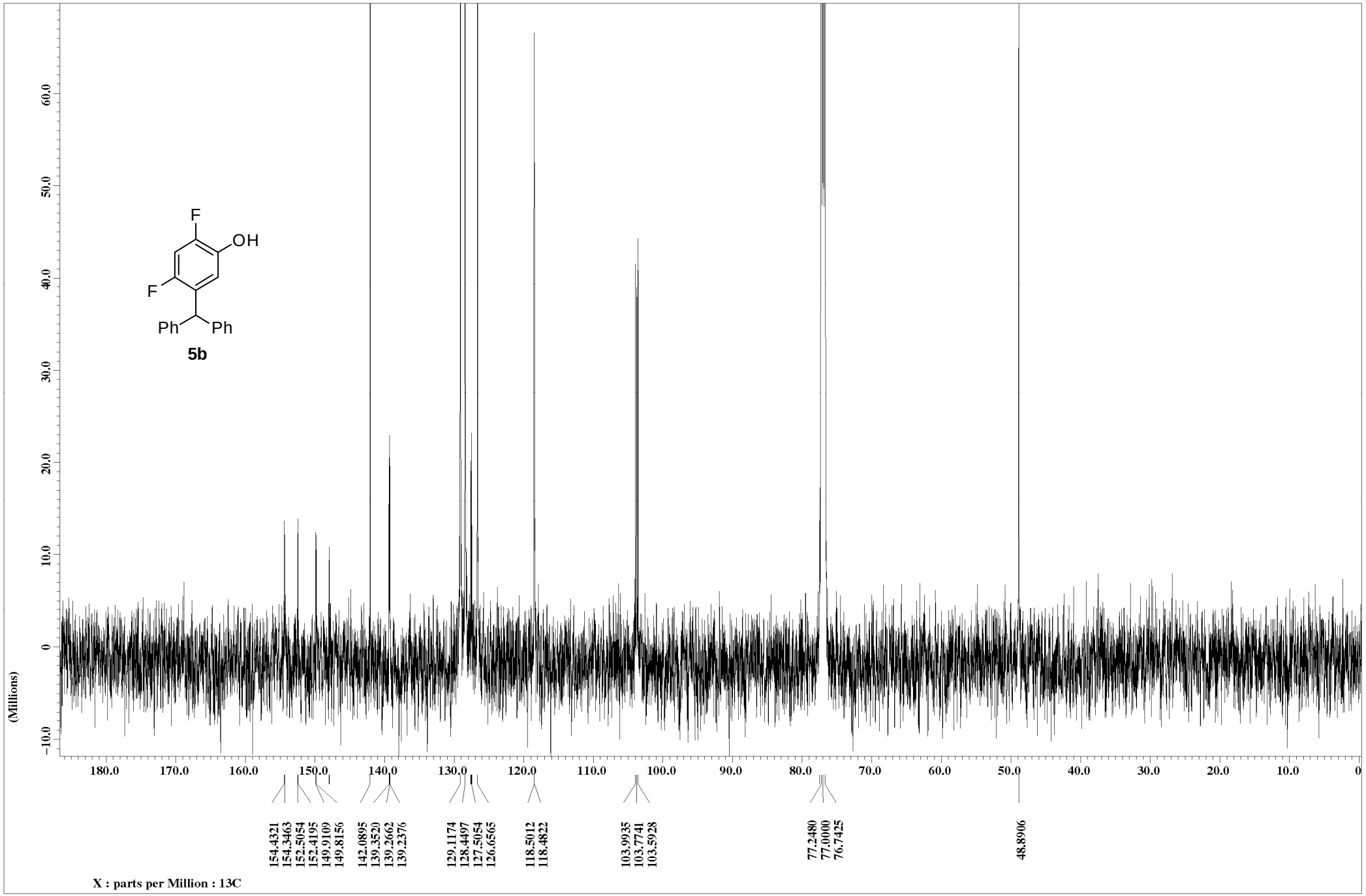
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Ph
Ph
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130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
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139.2376
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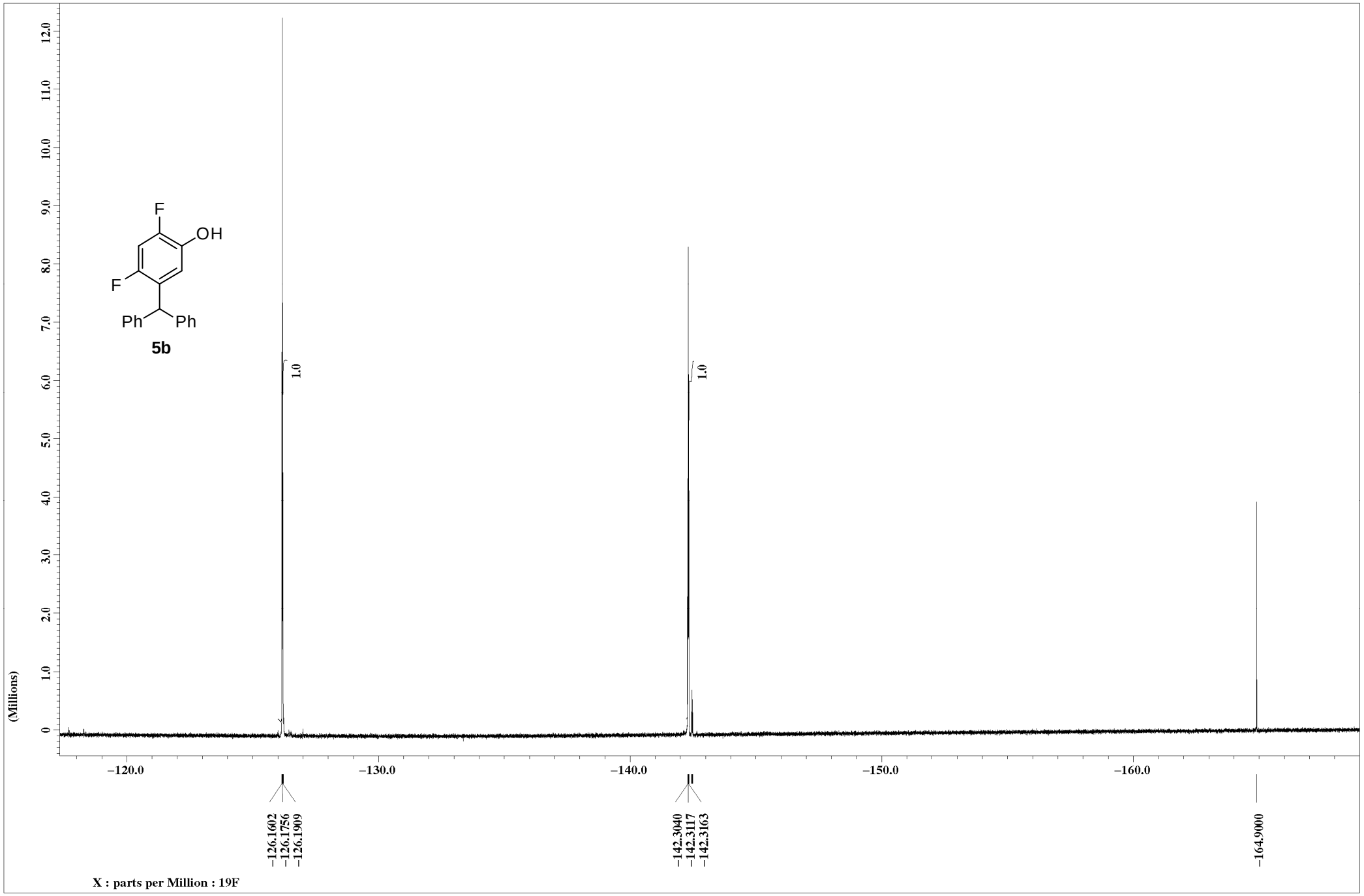
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OH
F
Ph
Ph
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1.0
(Millions)
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10.0
9.0
8.0
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−150.0
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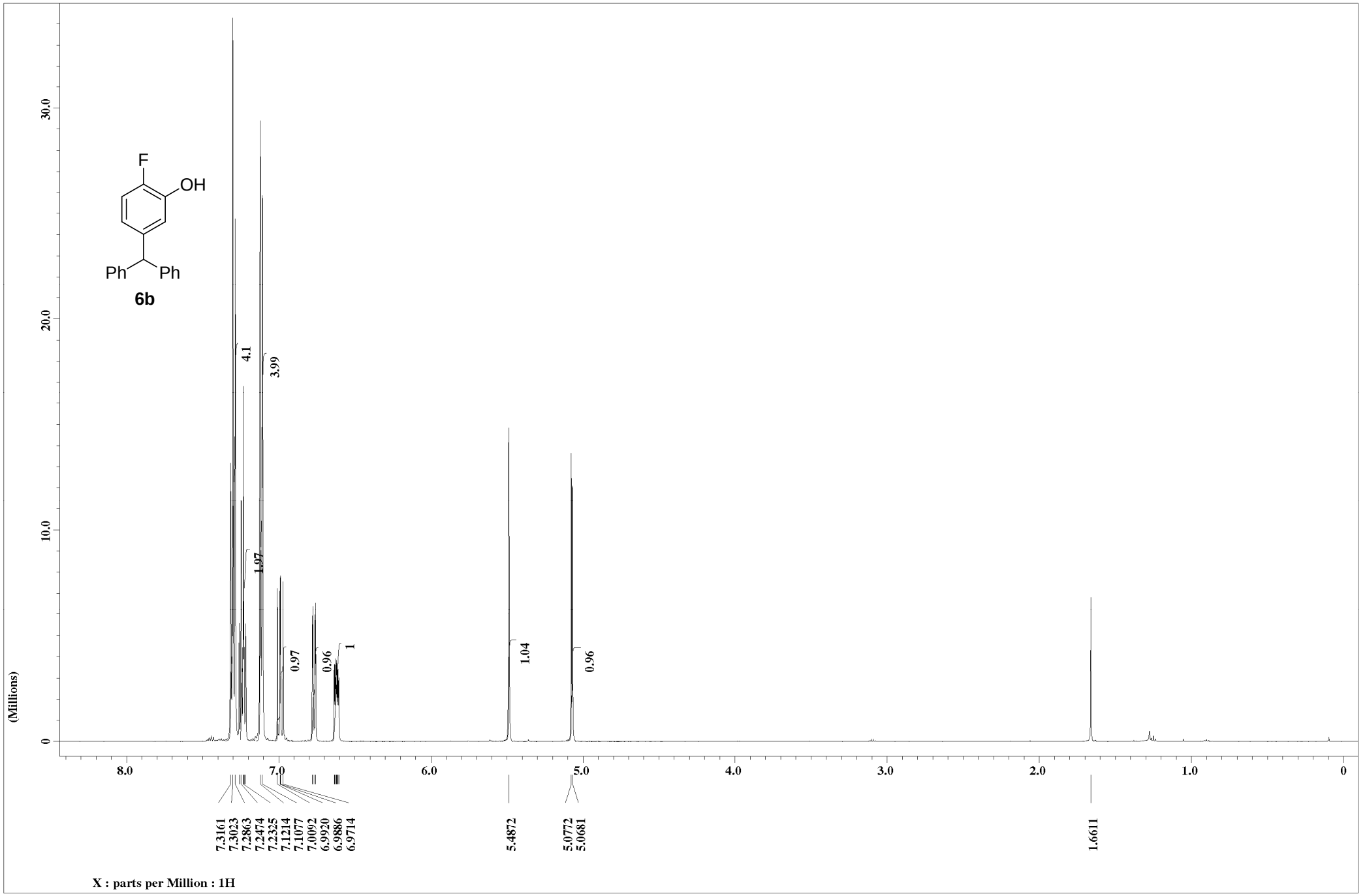
X : parts per Million : 19F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Ph
6b
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0.96
1
1.04
0.96
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
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7.3023
7.2863
7.2474
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7.1214
7.1077
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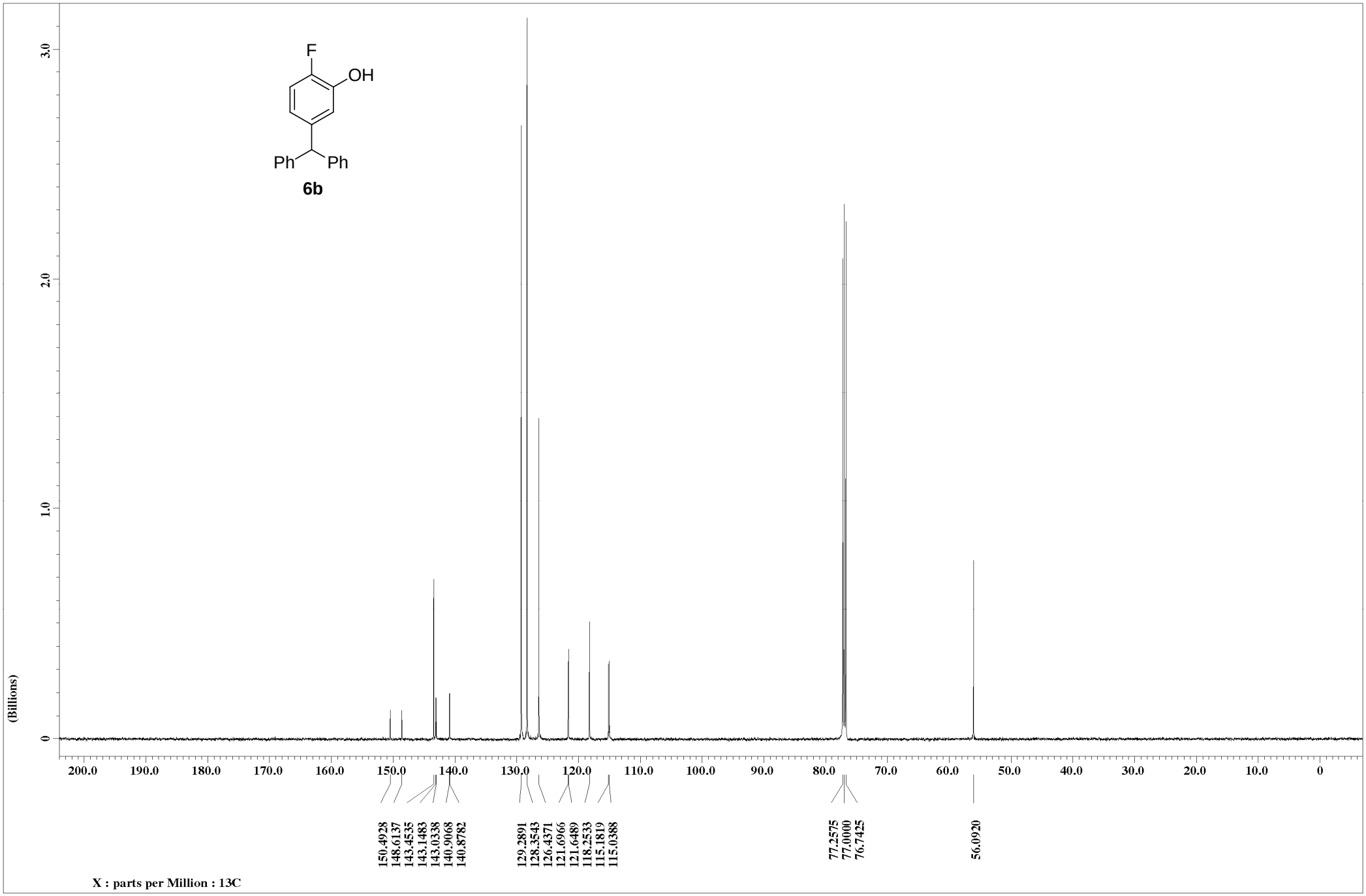
X : parts per Million : 1H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Ph
Ph
6b
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1.0
0
(Billions)
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180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
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148.6137
143.4535
143.1483
143.0338
140.9068
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129.2891
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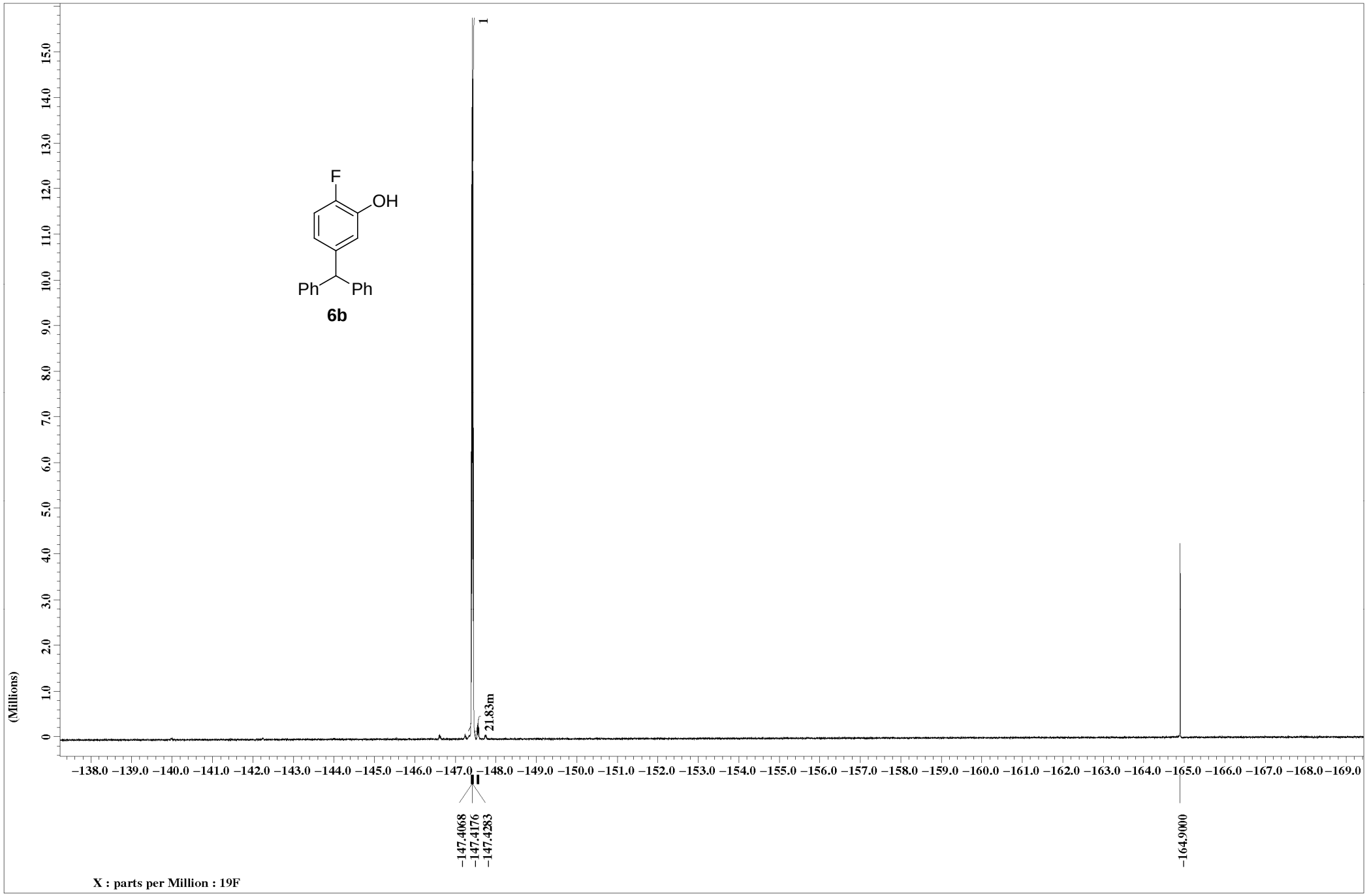
56.0920
X : parts per Million : 13C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Ph
Ph
6b
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21.83m
(Millions)
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4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
−138.0 −139.0 −140.0 −141.0 −142.0 −143.0 −144.0 −145.0 −146.0 −147.0 −148.0 −149.0 −150.0 −151.0 −152.0 −153.0 −154.0 −155.0 −156.0 −157.0 −158.0 −159.0 −160.0 −161.0 −162.0 −163.0 −164.0 −165.0 −166.0 −167.0 −168.0 −169.0
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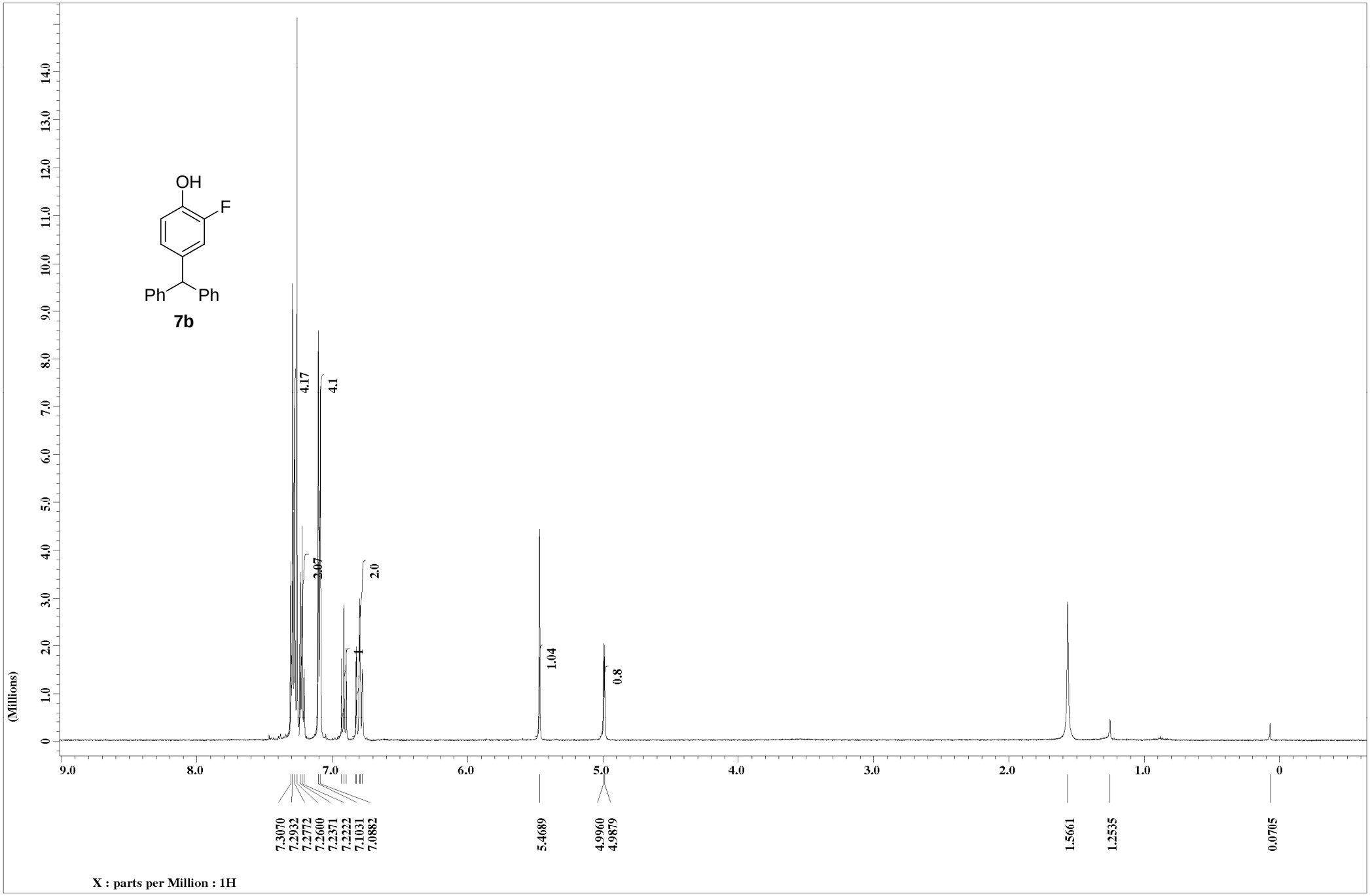
X : parts per Million : 19F


OH
F
Ph
Ph
7b
(Millions)
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12.0
11.0
10.0
9.0
8.0
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6.0
5.0
4.0
3.0
2.0
1.0
0
4.17
4.1
2.07
2.0
1.04
0.8
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
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7.2932
7.2772
7.2600
7.2371
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4.9960
4.9879
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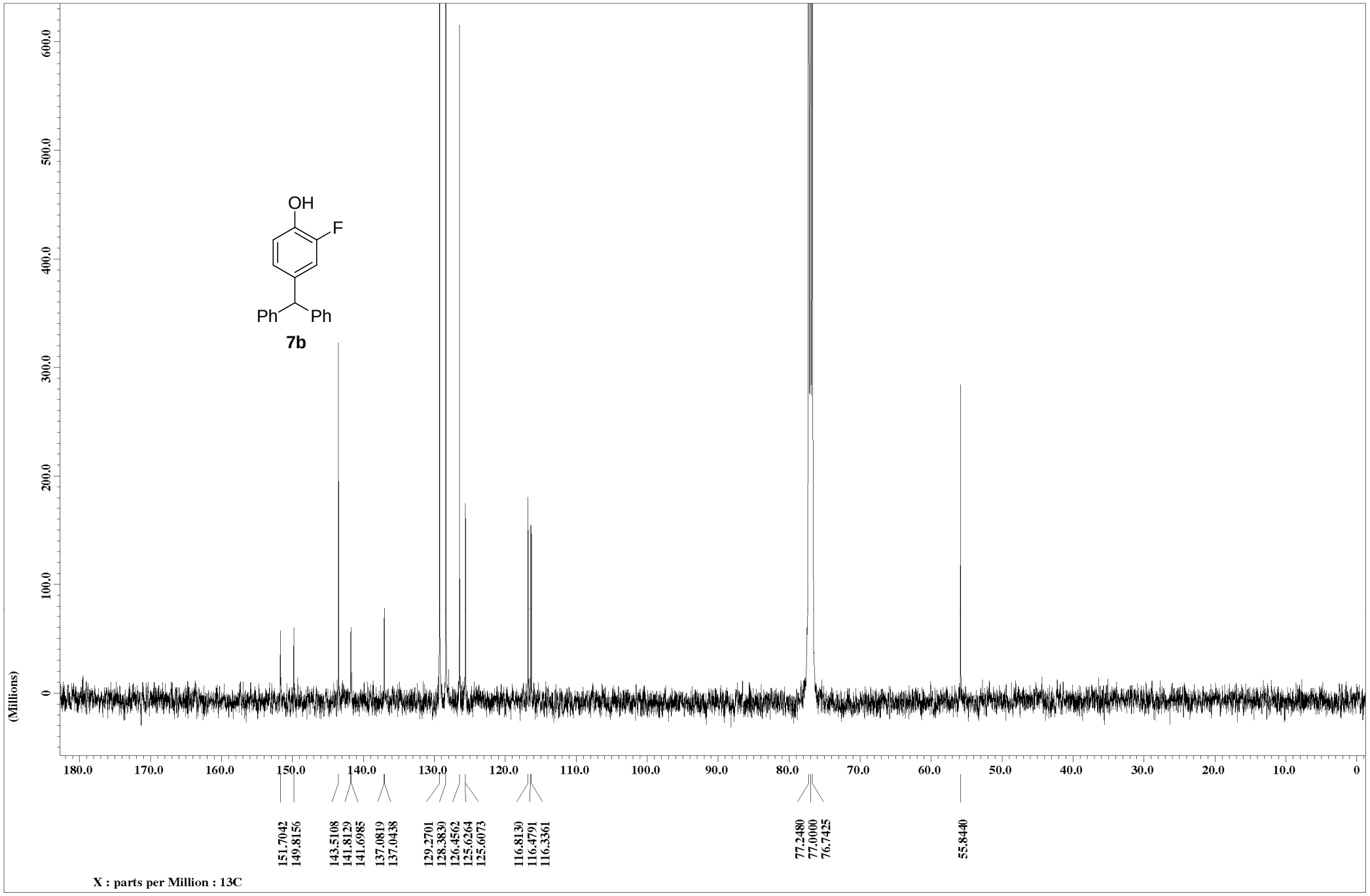
1.2535
0.0705
X : parts per Million : 1H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Ph
Ph
7b
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90.0
80.0
70.0
60.0
50.0
40.0
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20.0
10.0
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141.6985
137.0819
137.0438
129.2701
128.3830
126.4562
125.6264
125.6073
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116.3361
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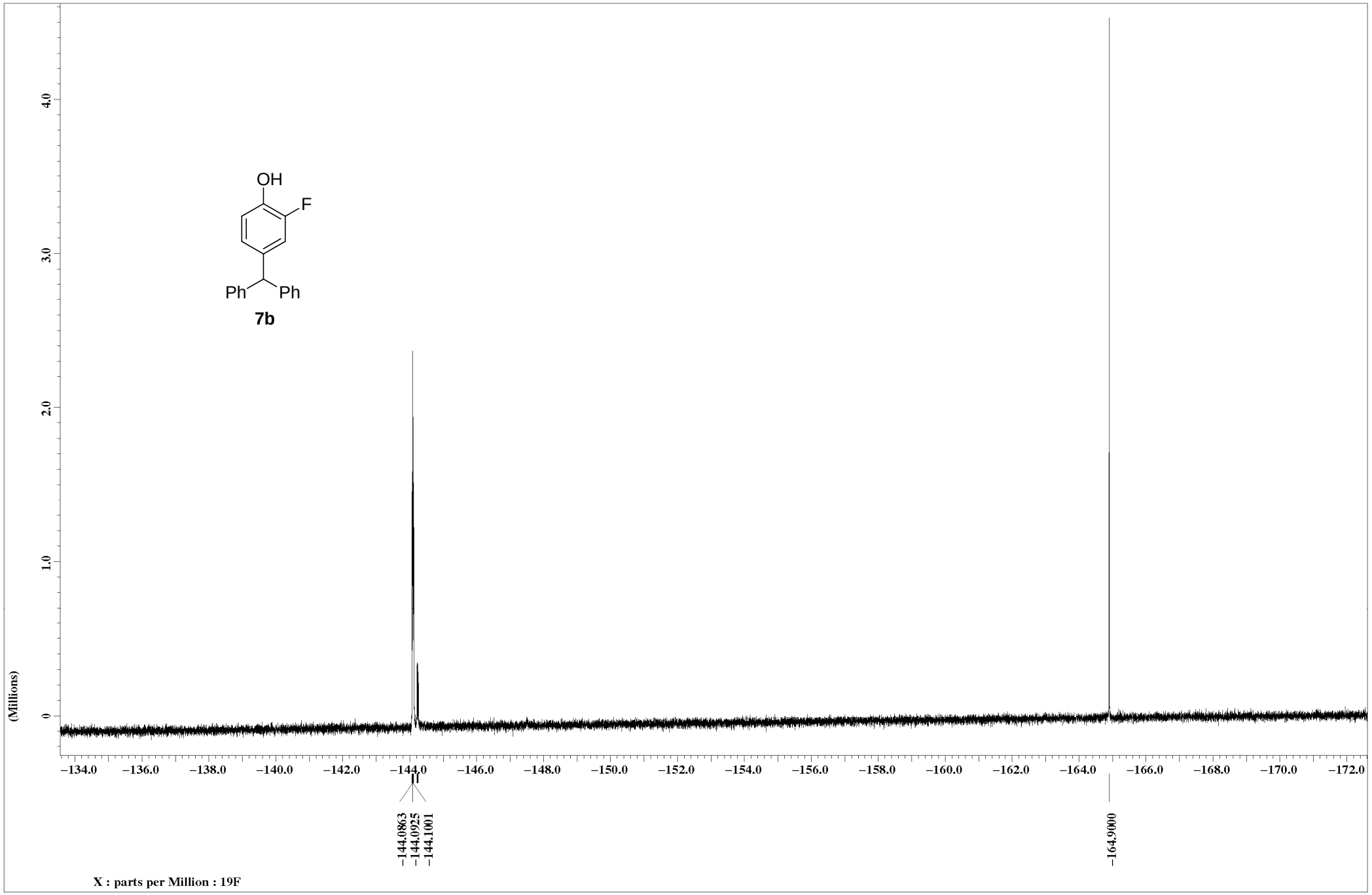
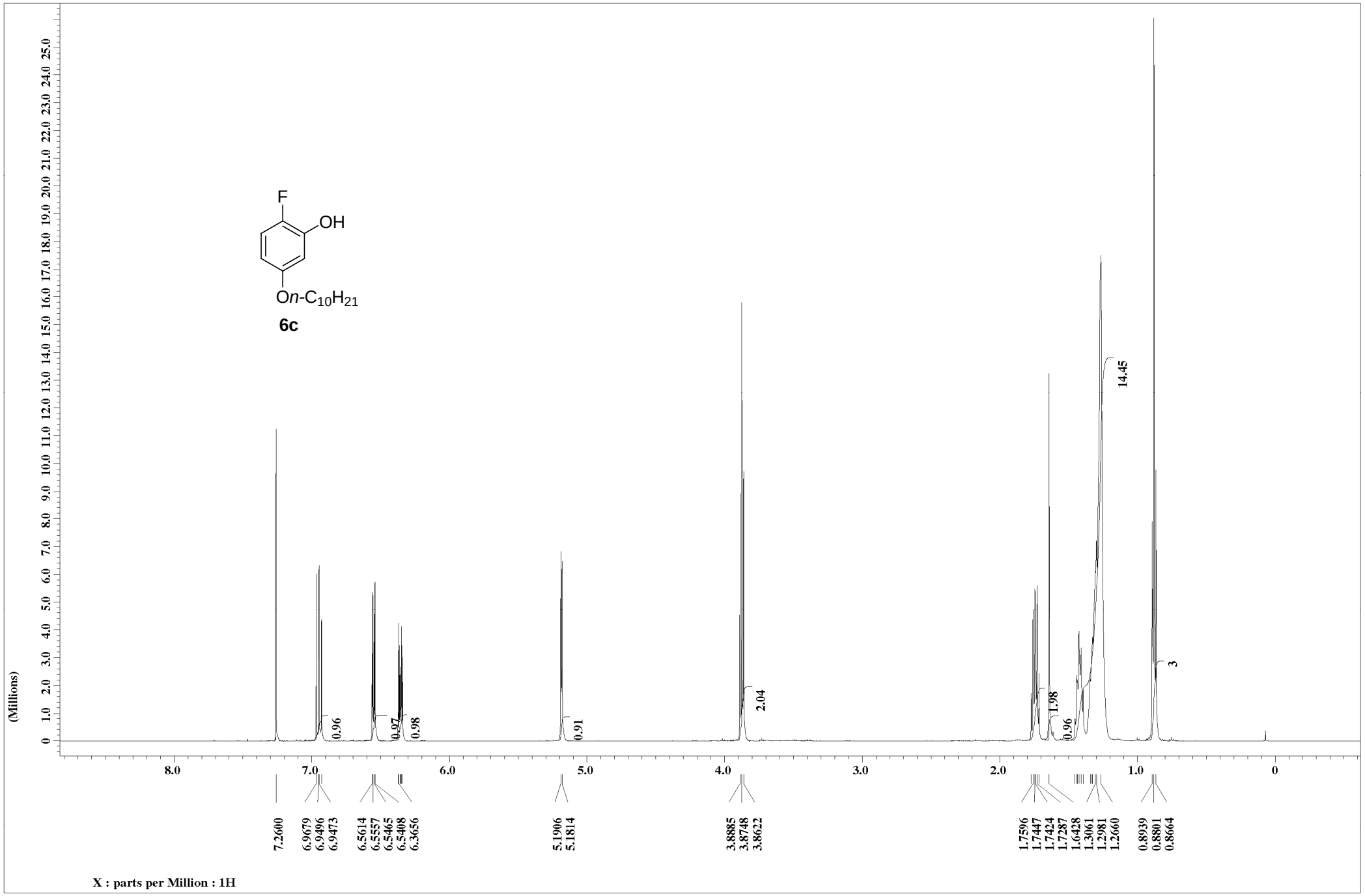
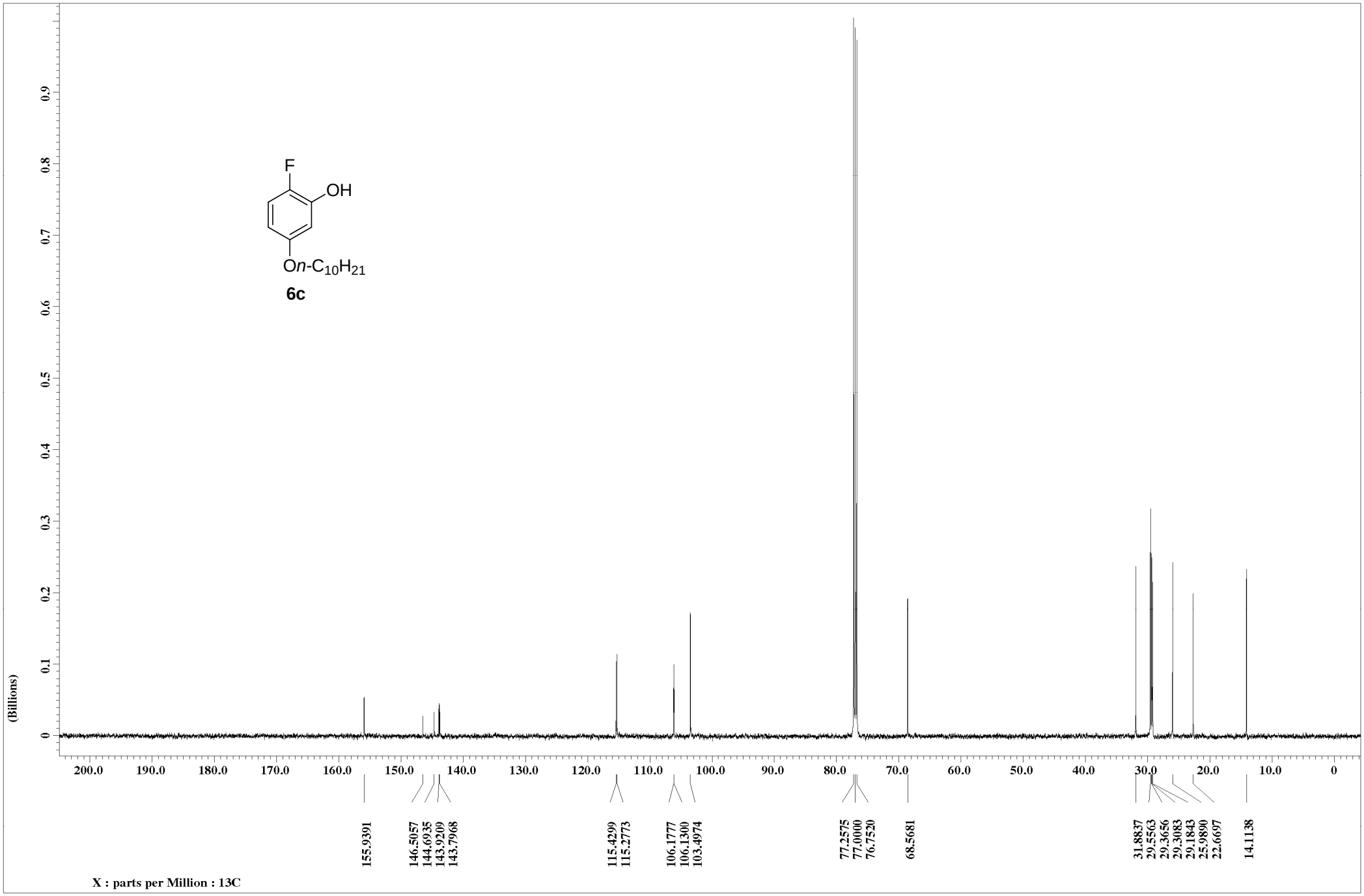
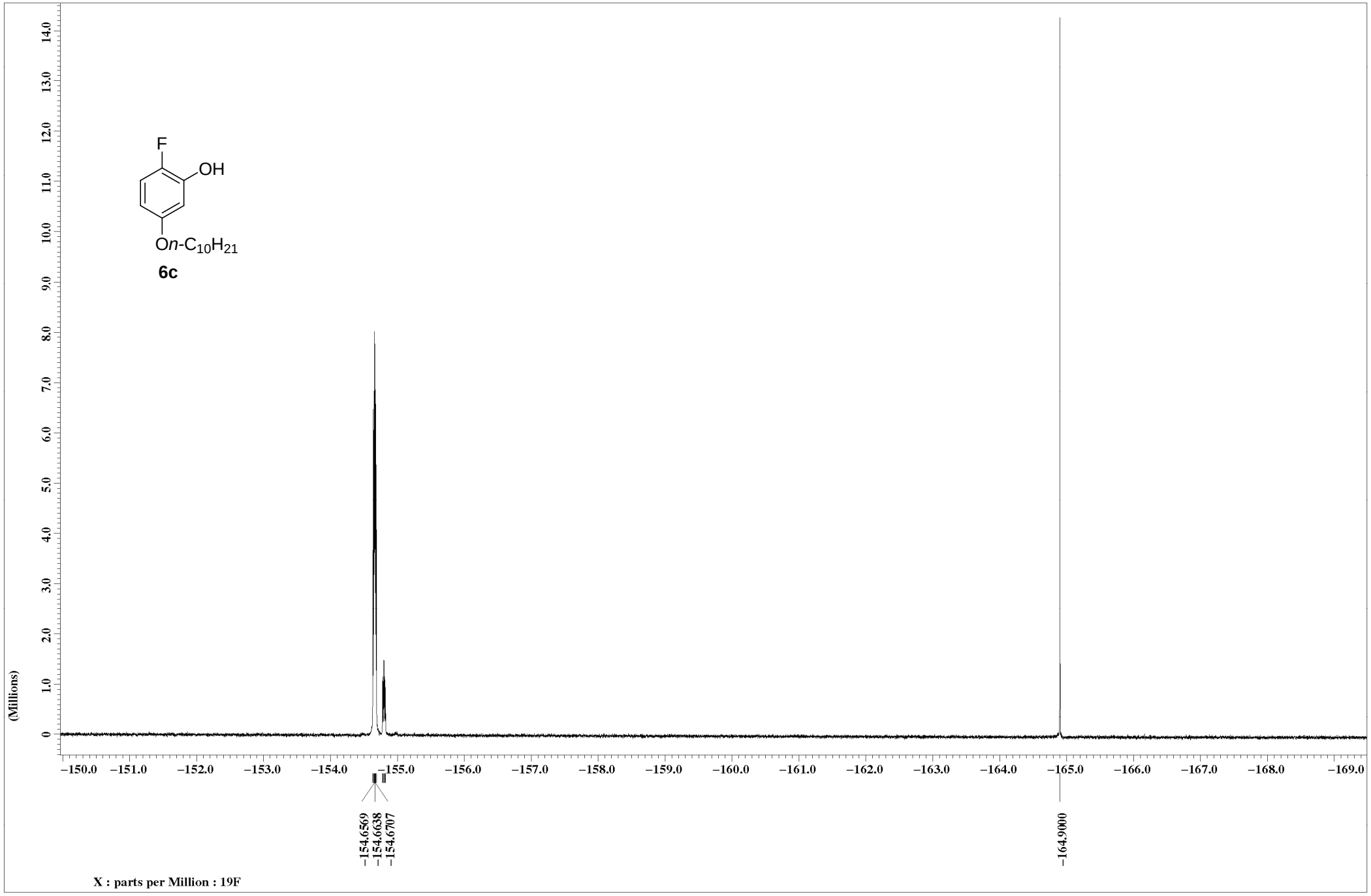
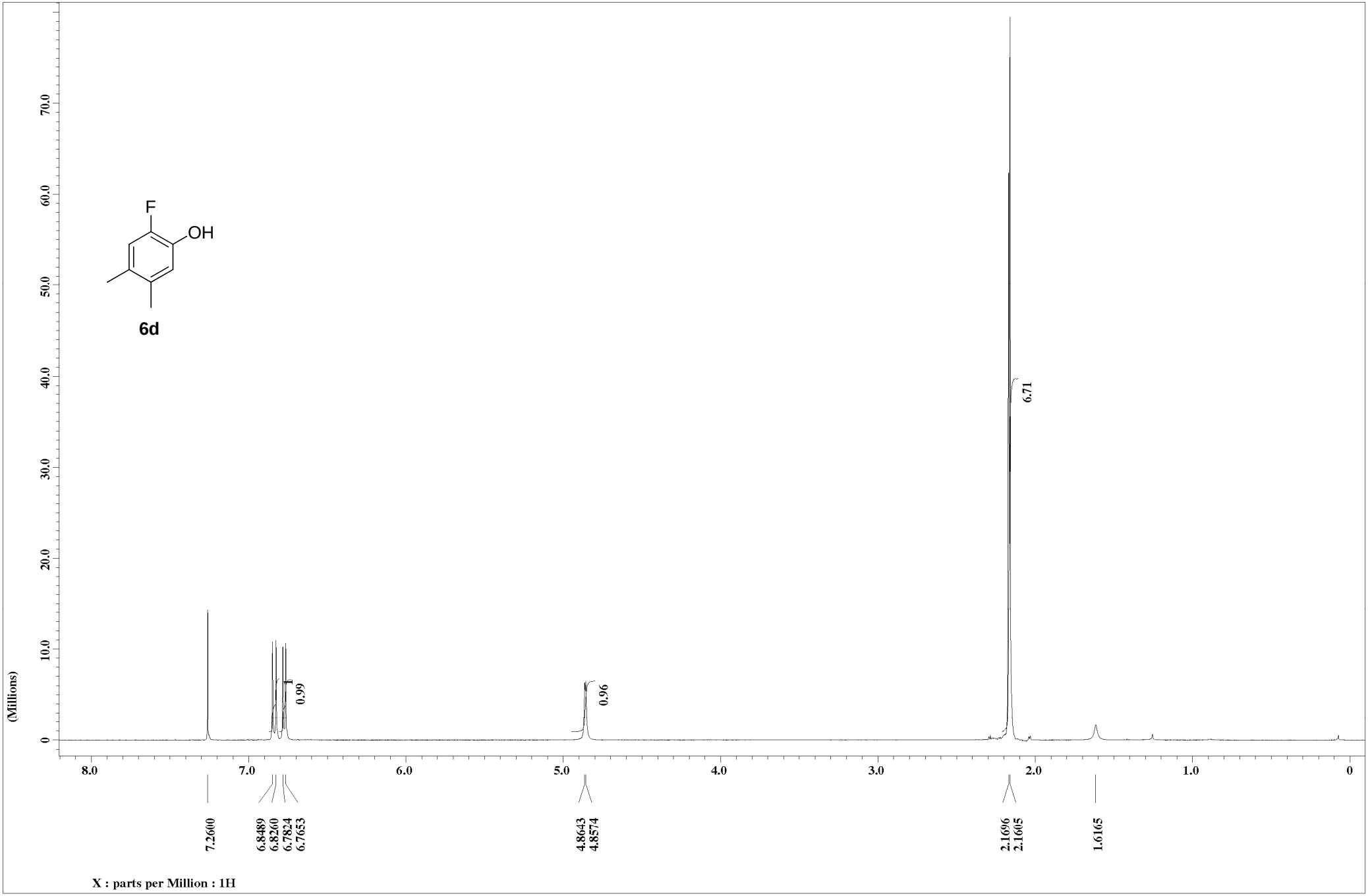
76.7425
55.8440
X : parts per Million : 13C

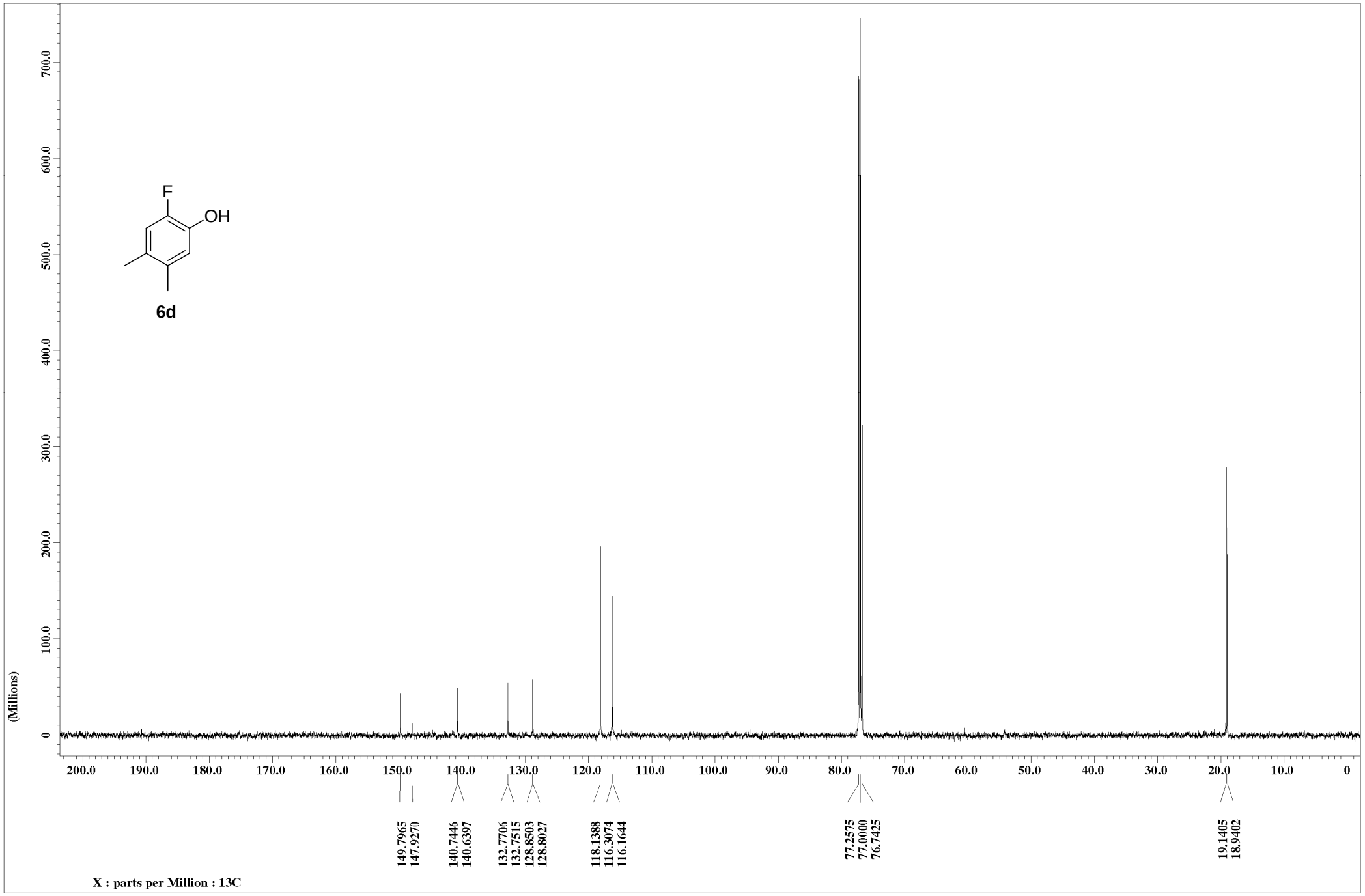

OH
F
Ph
Ph
7b
(Millions)
4.0
3.0
2.0
1.0
0
−134.0
−136.0
−138.0
−140.0
−142.0
−144.0
−146.0
−148.0
−150.0
−152.0
−154.0
−156.0
−158.0
−160.0
−162.0
−164.0
−166.0
−168.0
−170.0
−172.0
−144.0863
−144.0925
−144.1001
−164.9000
X : parts per Million : 19F

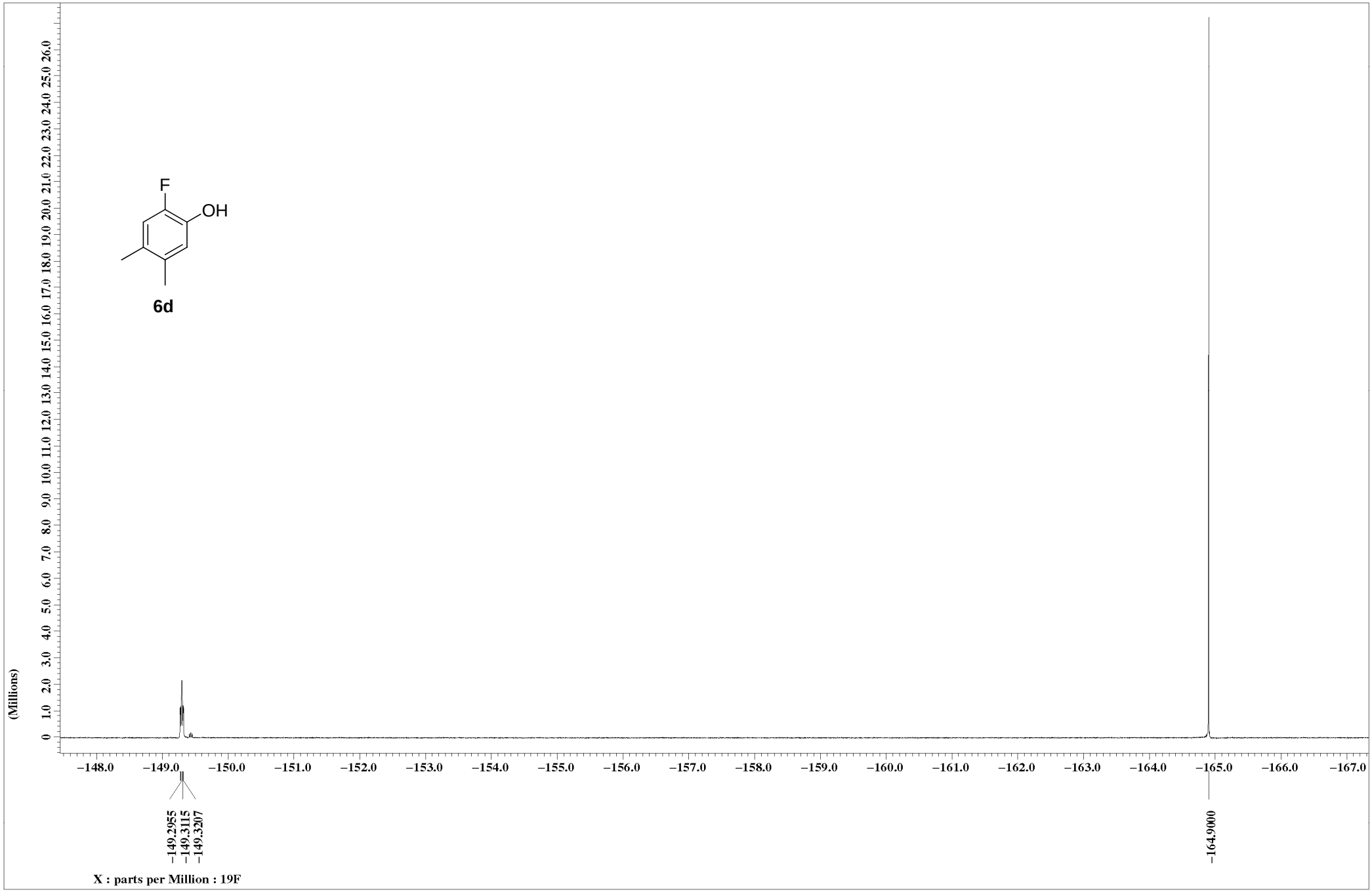

F
OH
On-C10H21
6c
(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0
22.0
23.0
24.0
25.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.96
0.97
0.98
0.91
2.04
1.98
0.96
14.45
3
7.2600
6.9679
6.9496
6.9473
6.5614
6.5557
6.5465
6.5408
6.3656
5.1906
5.1814
3.8885
3.8748
3.8622
1.7596
1.7447
1.7424
1.7287
1.6428
1.3061
1.2981
1.2660
0.8939
0.8801
0.8664
X : parts per Million : 1H

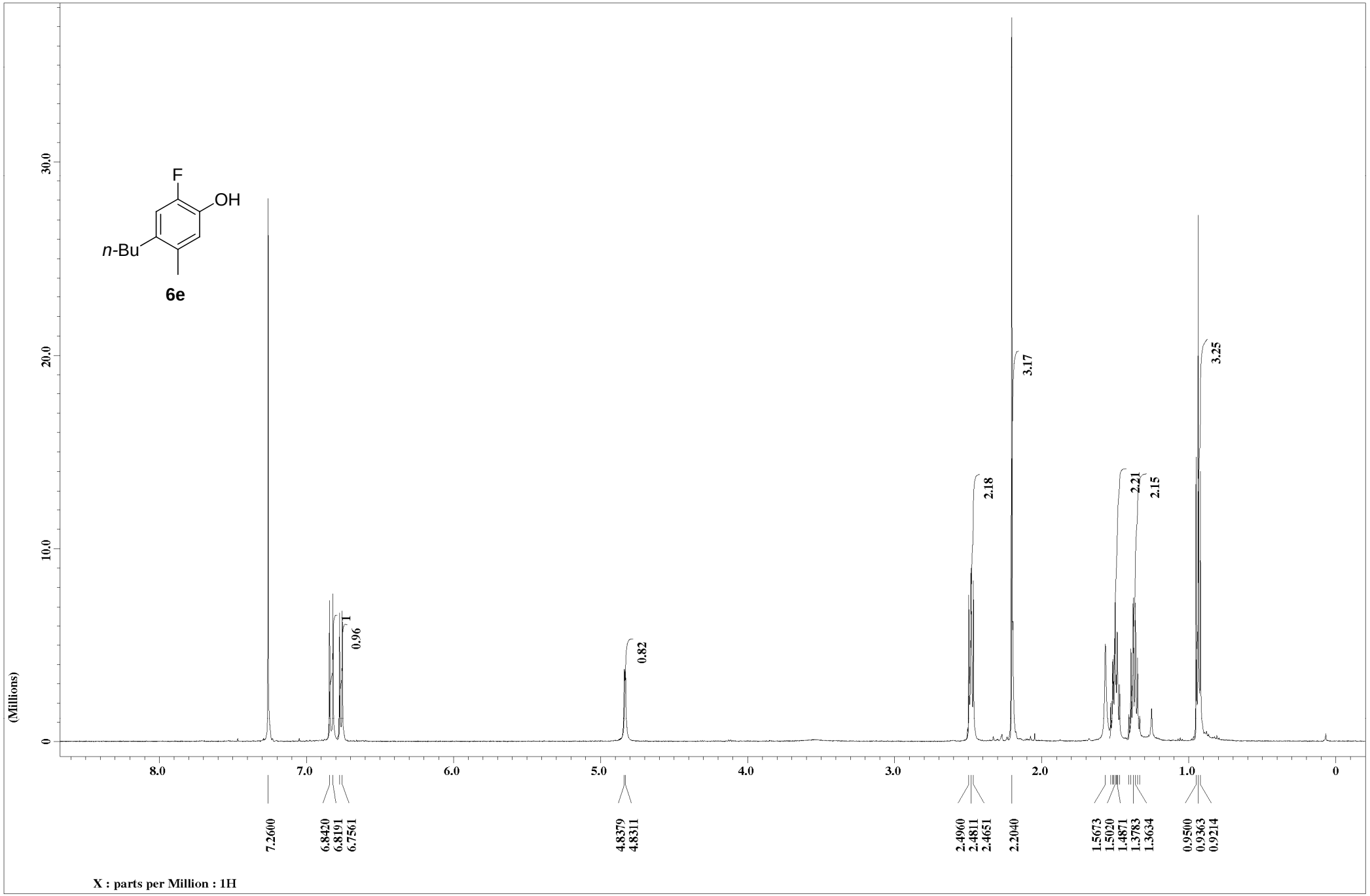

F
OH
On-C10H21
6c
(Billions)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
155.9391
146.5057
144.6935
143.9209
143.7968
115.4299
115.2773
106.1777
106.1300
103.4974
77.2575
77.0000
76.7520
68.5681
31.8837
29.5563
29.3656
29.3083
29.1843
25.9890
22.6697
14.1138
X : parts per Million : 13C

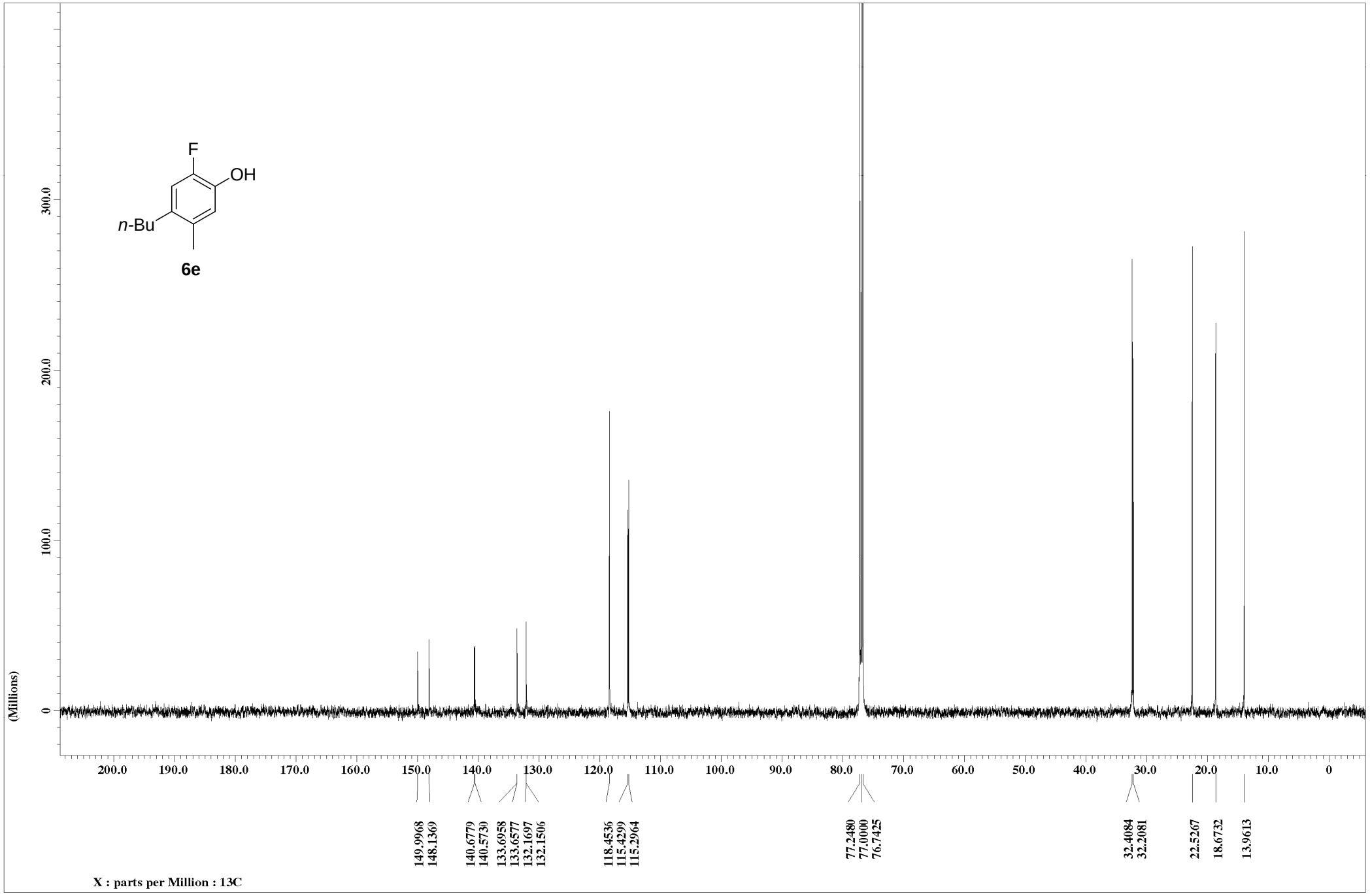

F
OH
On-C10H21
6c
(Millions)
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−150.0 −151.0 −152.0 −153.0 −154.0 −155.0 −156.0 −157.0 −158.0 −159.0 −160.0 −161.0 −162.0 −163.0 −164.0 −165.0 −166.0 −167.0 −168.0 −169.0
−154.6569
−154.6638
−154.6707
−164.9000
X : parts per Million : 19F

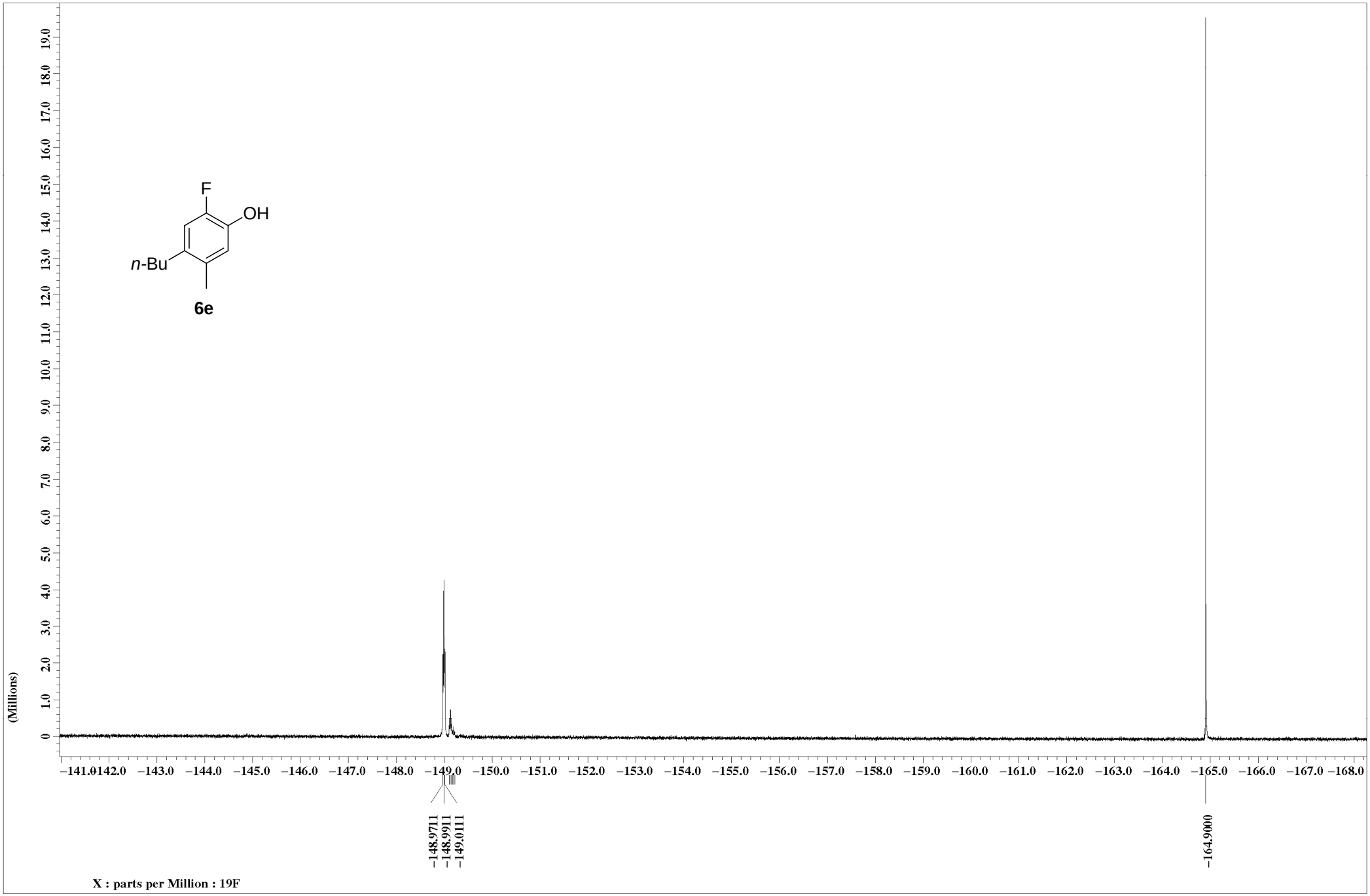

F
OH
6d
(Millions)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
0.99
0.96
6.71
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2600
6.8489
6.8260
6.7824
6.7653
4.8643
4.8574
2.1696
2.1605
1.6165
X : parts per Million : 1H

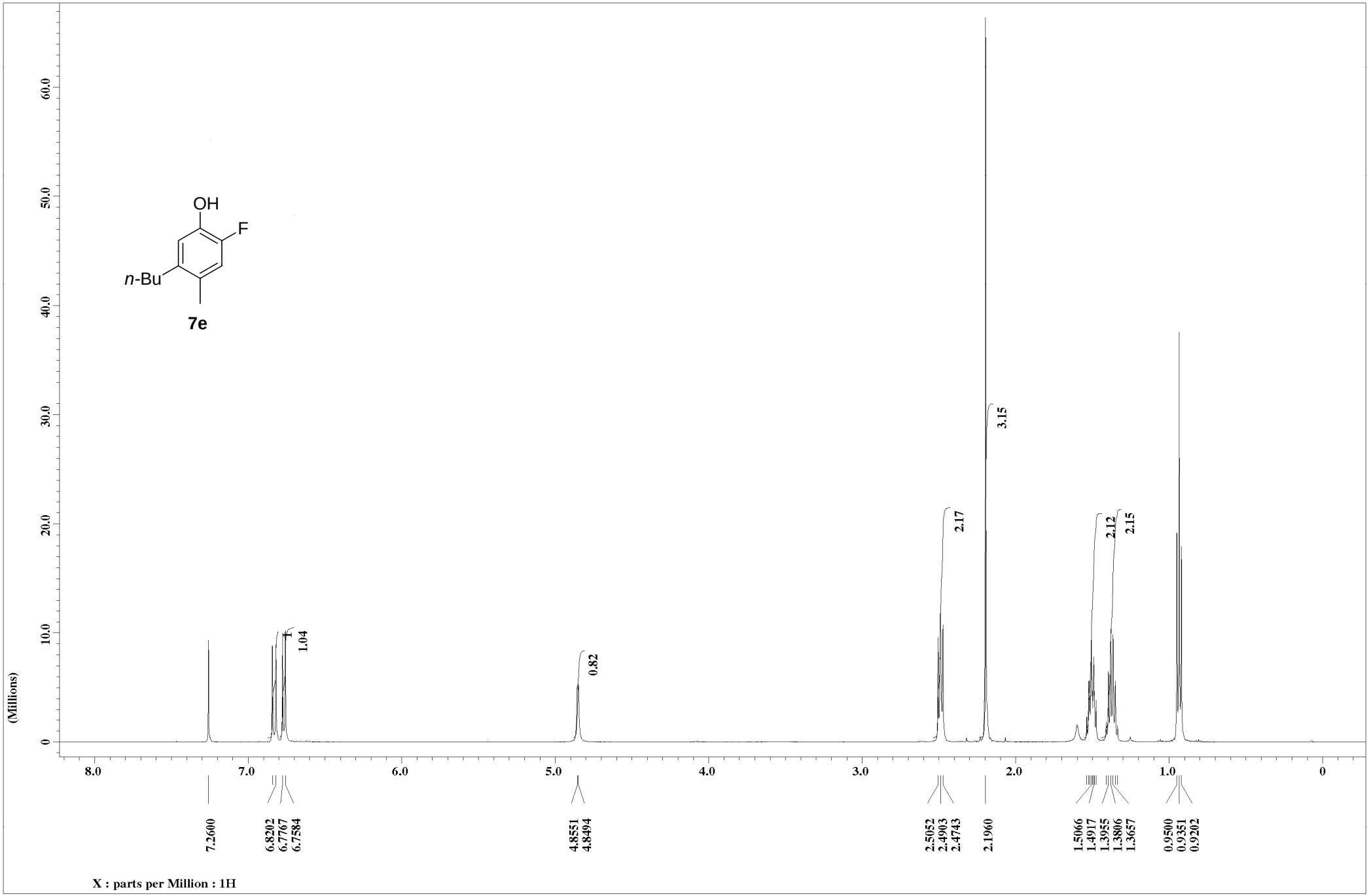

F
OH
6d
(Millions)
700.0
600.0
500.0
400.0
300.0
200.0
100.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
149.7965
147.9270
140.7446
140.6397
132.7706
132.7515
128.8503
128.8027
118.1388
116.3074
116.1644
77.2575
77.0000
76.7425
19.1405
18.9402
X : parts per Million : 13C

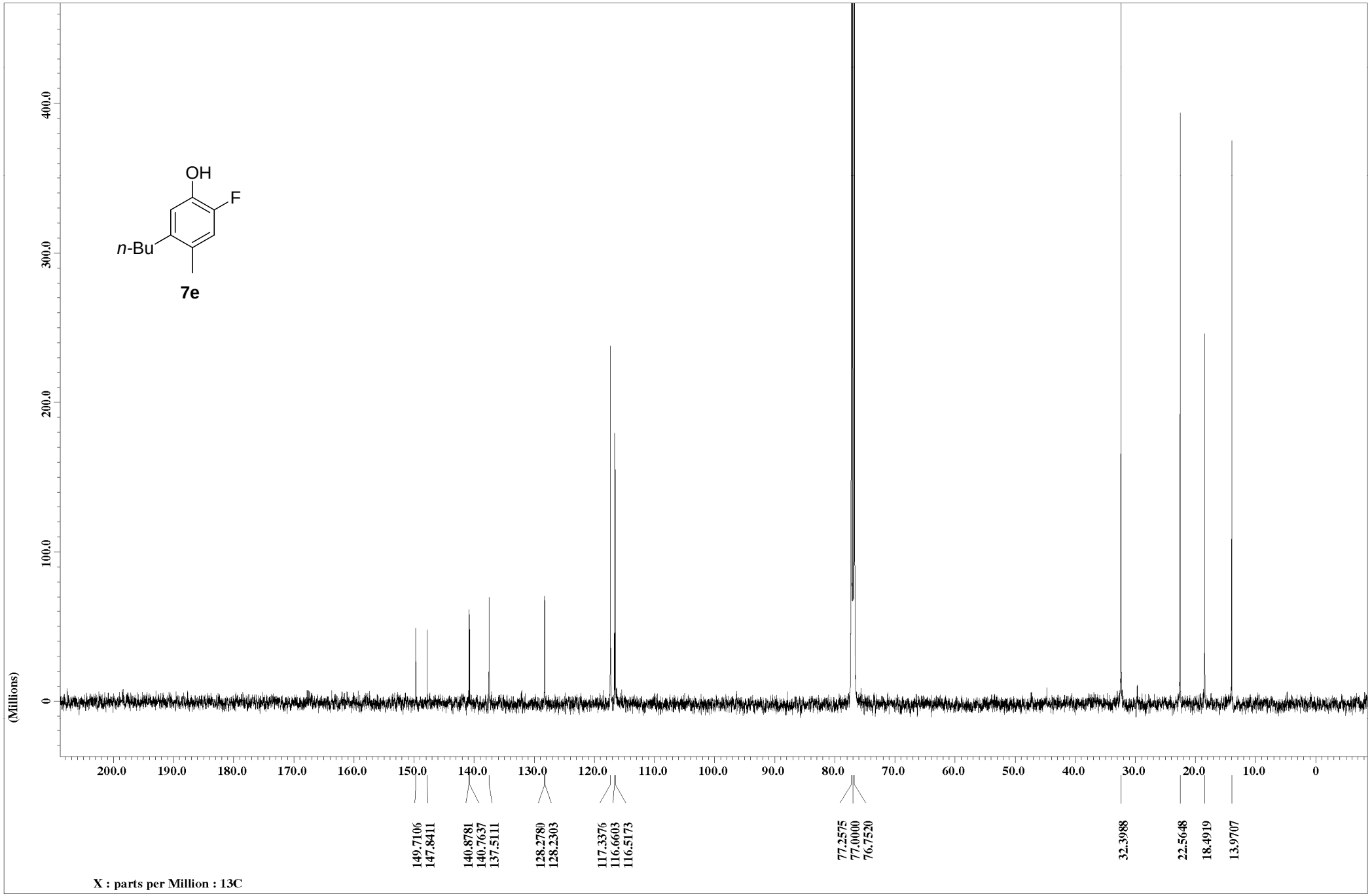

F
OH
6d
(Millions)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0 25.0 26.0
−148.0 −149.0 −150.0 −151.0 −152.0 −153.0 −154.0 −155.0 −156.0 −157.0 −158.0 −159.0 −160.0 −161.0 −162.0 −163.0 −164.0 −165.0 −166.0 −167.0
−149.2955
−149.3115
−149.3207
−164.9000
X : parts per Million : 19F

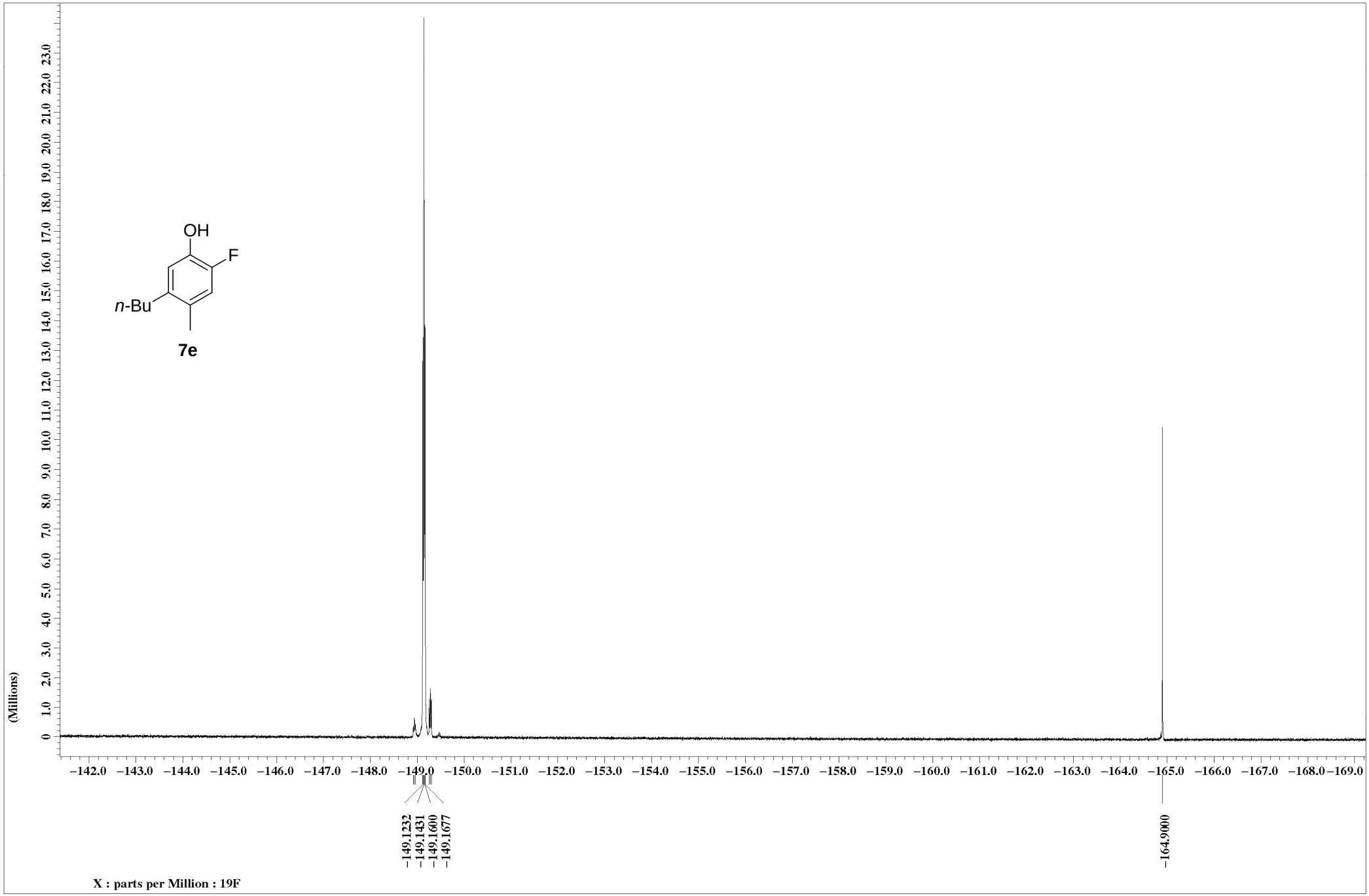

F
OH
n-Bu
6e
(Millions)
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.96
0.82
2.18
3.17
2.21
2.15
3.25
7.2600
6.8420
6.8191
6.7561
4.8379
4.8311
2.4960
2.4811
2.4651
2.2040
1.5673
1.5020
1.4871
1.3783
1.3634
0.9500
0.9363
0.9214
X : parts per Million : 1H

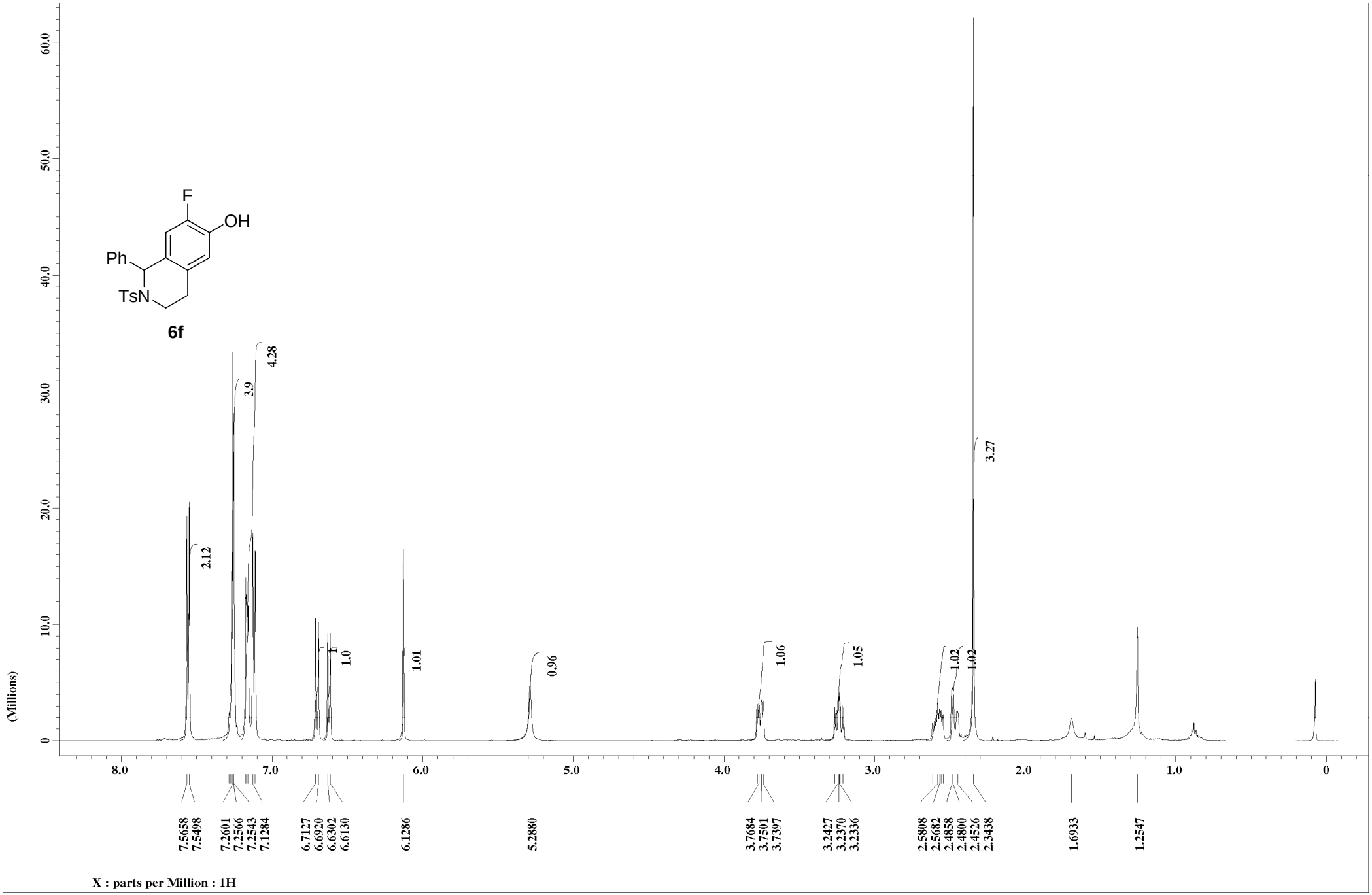

F
OH
n-Bu
6e
(Millions)
300.0
200.0
100.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
149.9968
148.1369
140.6779
140.5730
133.6958
133.6577
132.1697
132.1506
118.4536
115.4299
115.2964
77.2480
77.0000
76.7425
32.4084
32.2081
22.5267
18.6732
13.9613
X : parts per Million : 13C

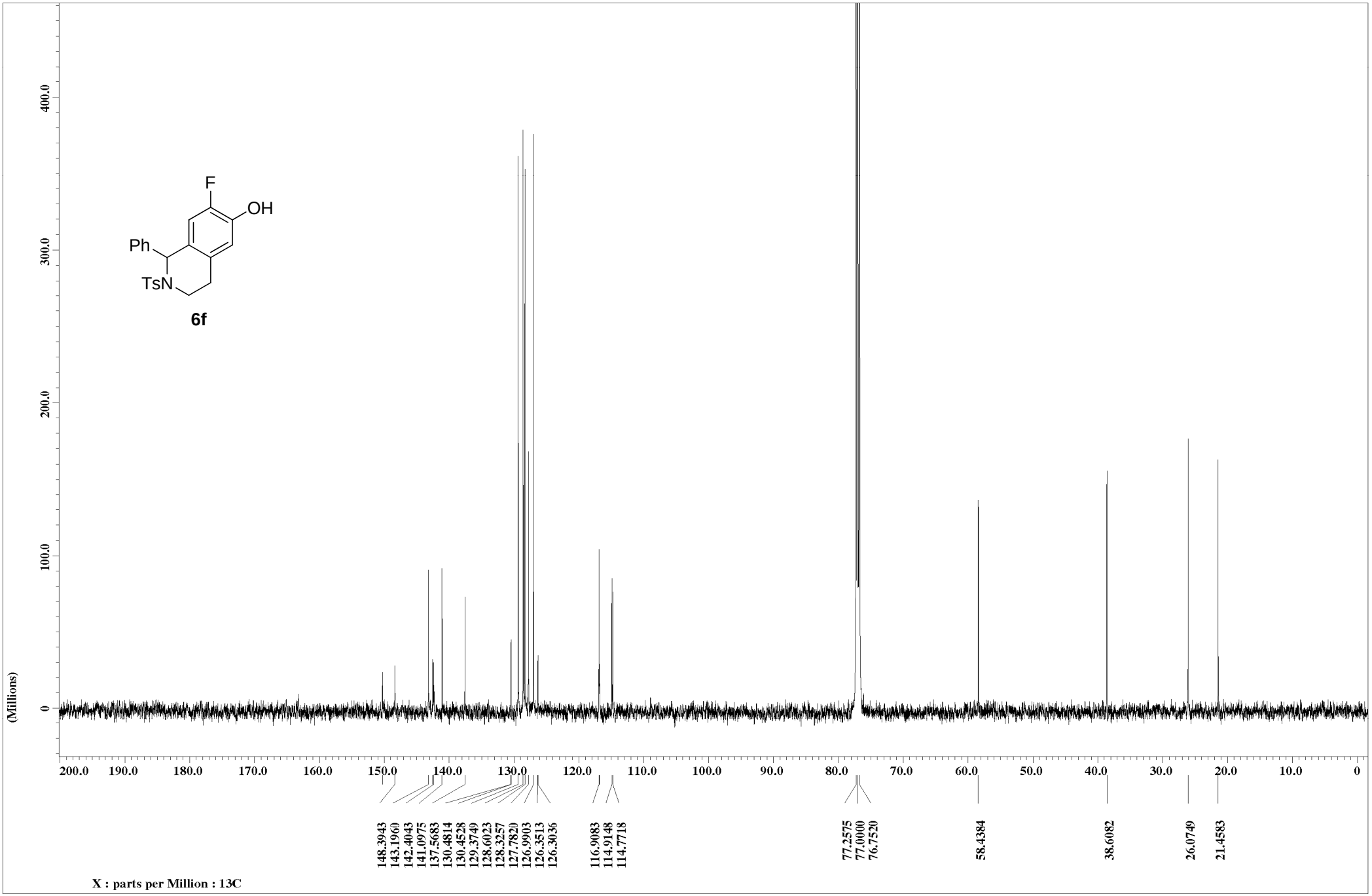

F
OH
n-Bu
6e
(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
−141.0142.0 −143.0 −144.0 −145.0 −146.0 −147.0 −148.0 −149.0 −150.0 −151.0 −152.0 −153.0 −154.0 −155.0 −156.0 −157.0 −158.0 −159.0 −160.0 −161.0 −162.0 −163.0 −164.0 −165.0 −166.0 −167.0 −168.0
−148.9711
−148.9911
−149.0111
−164.9000
X : parts per Million : 19F

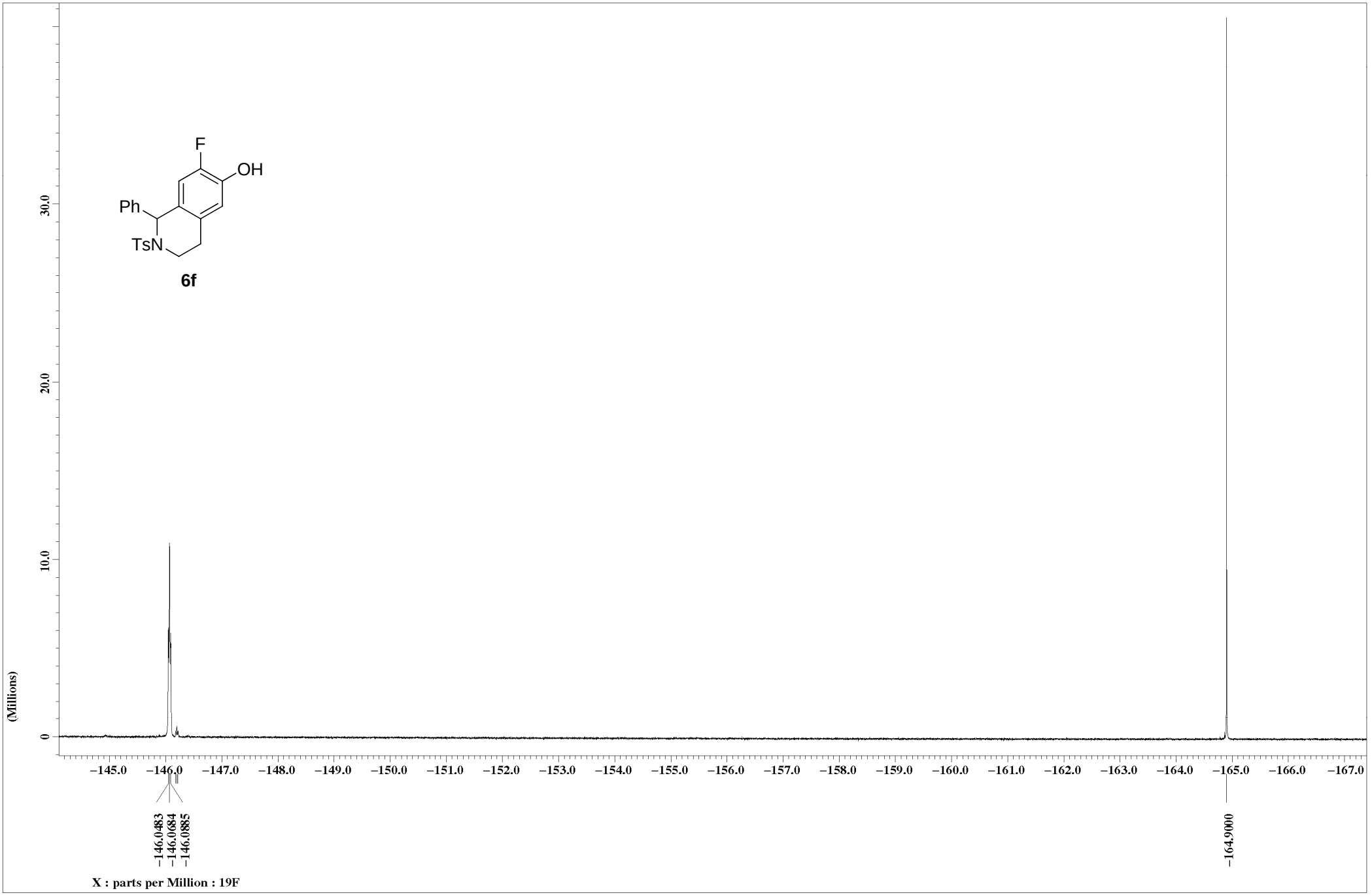

OH
F
n-Bu
7e
(Millions)
60.0
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.04
0.82
2.17
3.15
2.12
2.15
7.2600
6.8202
6.7767
6.7584
4.8551
4.8494
2.5052
2.4903
2.4743
2.1960
1.5066
1.4917
1.3955
1.3806
1.3657
0.9500
0.9351
0.9202
X : parts per Million : 1H

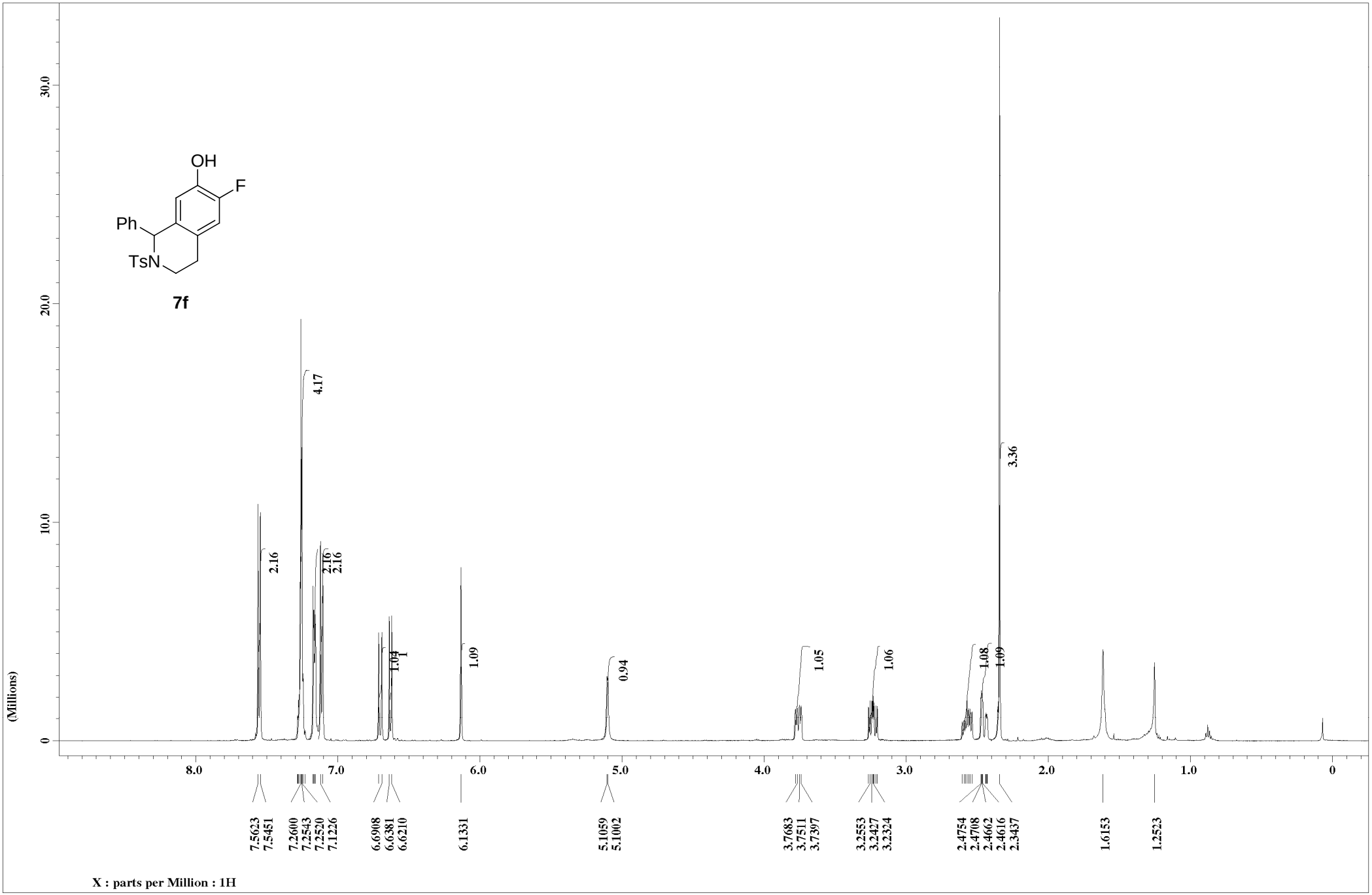

OH
F
n-Bu
7e
(Millions)
400.0
300.0
200.0
100.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
149.7106
147.8411
140.8781
140.7637
137.5111
128.2780
128.2303
117.3376
116.6603
116.5173
77.2575
77.0000
76.7520
32.3988
22.5648
18.4919
13.9707
X : parts per Million : 13C

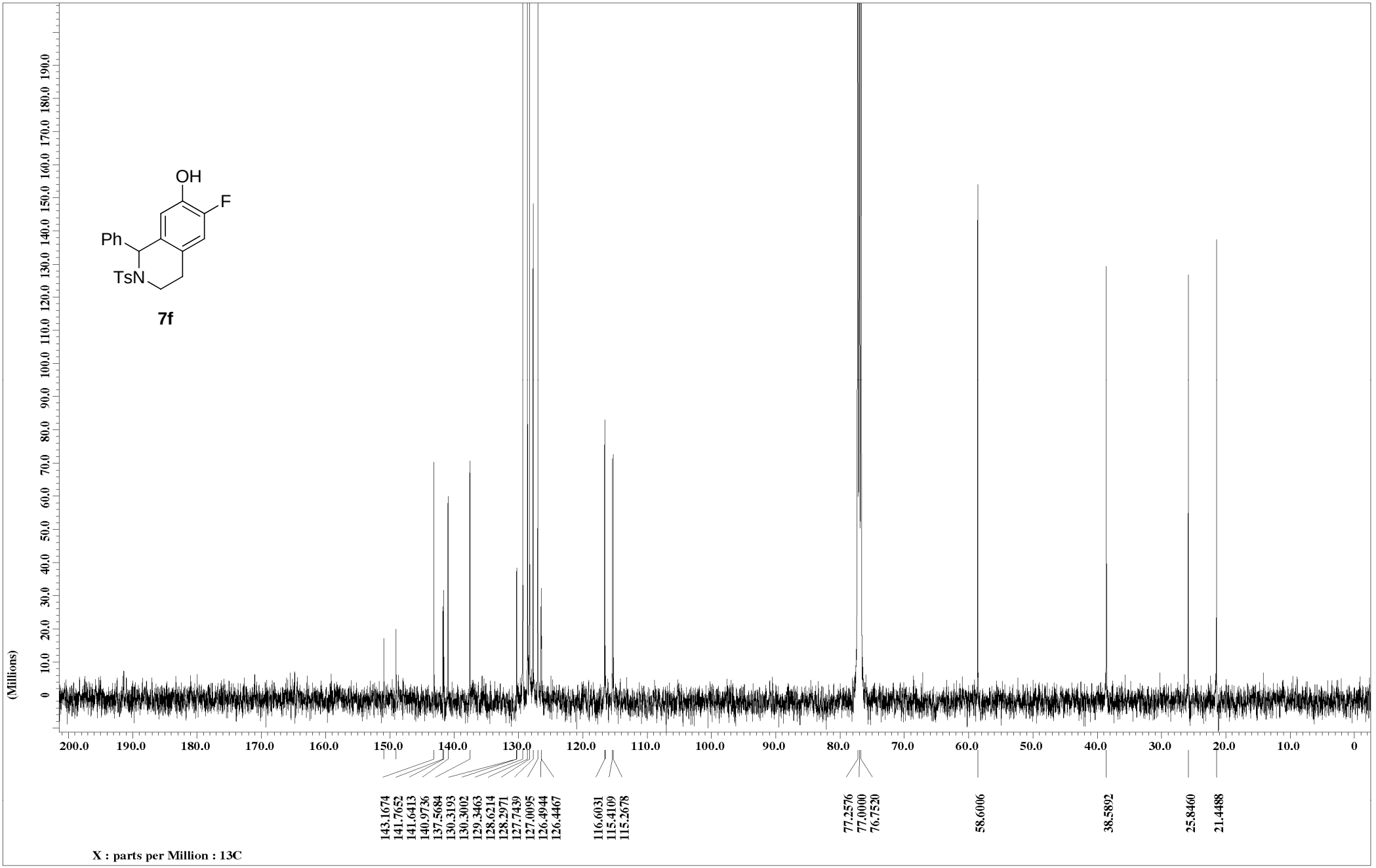

OH
F
n-Bu
7e
(Millions)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0
−142.0 −143.0 −144.0 −145.0 −146.0 −147.0 −148.0 −149.0 −150.0 −151.0 −152.0 −153.0 −154.0 −155.0 −156.0 −157.0 −158.0 −159.0 −160.0 −161.0 −162.0 −163.0 −164.0 −165.0 −166.0 −167.0 −168.0 −169.0
−149.1232
−149.1431
−149.1600
−149.1677
−164.9000
X : parts per Million : 19F

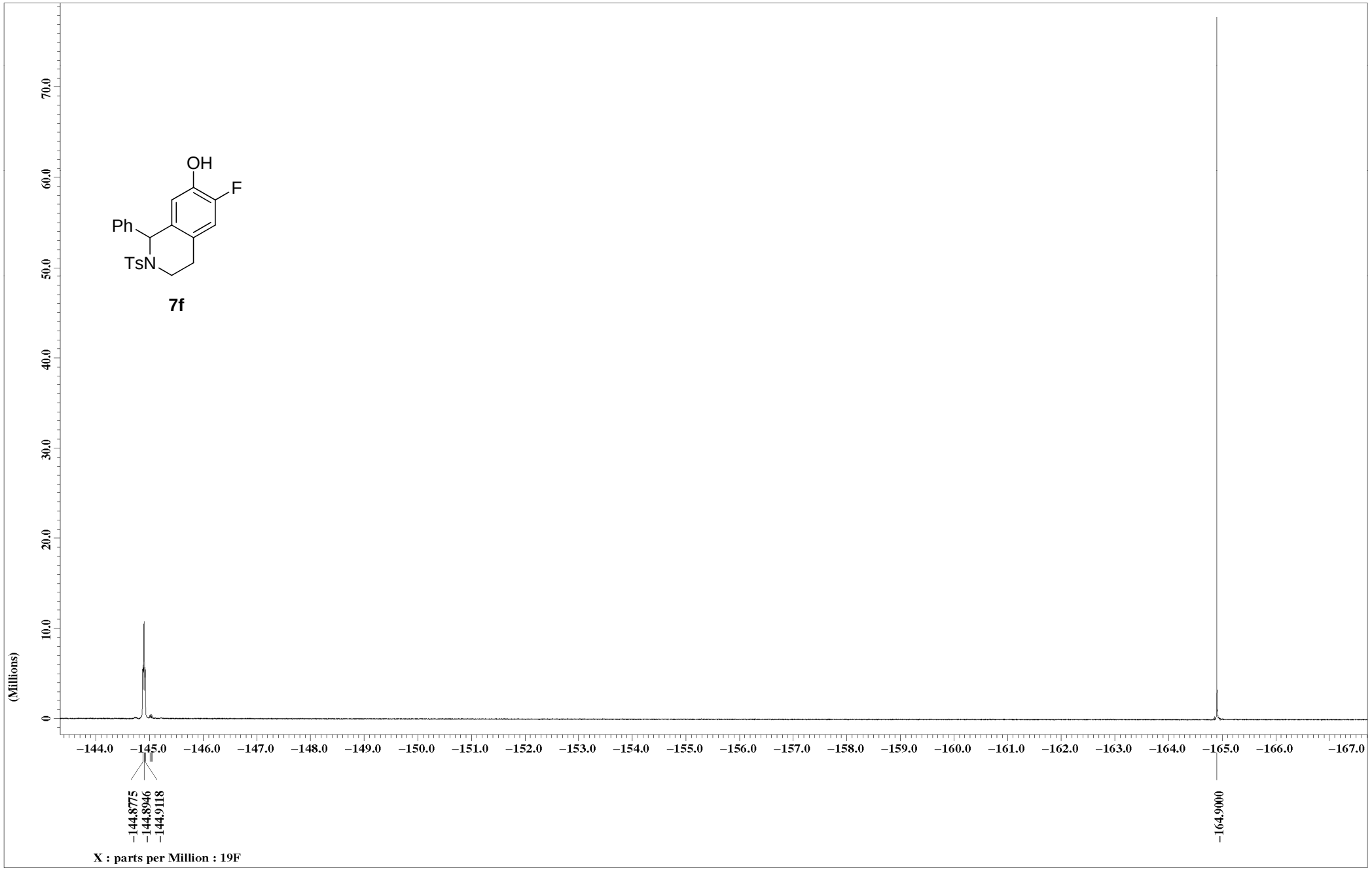

F
OH
Ph
TsN
6f
(Millions)
60.0
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
4.28
3.9
2.12
1.0
1.01
0.96
1.06
1.05
1.02
1.02
3.27
7.5658
7.5498
7.2601
7.2566
7.2543
7.1284
6.7127
6.6920
6.6302
6.6130
6.1286
5.2880
3.7684
3.7501
3.7397
3.2427
3.2370
3.2336
2.5808
2.5682
2.4858
2.4800
2.4526
2.3438
1.6933
1.2547
X : parts per Million : 1H

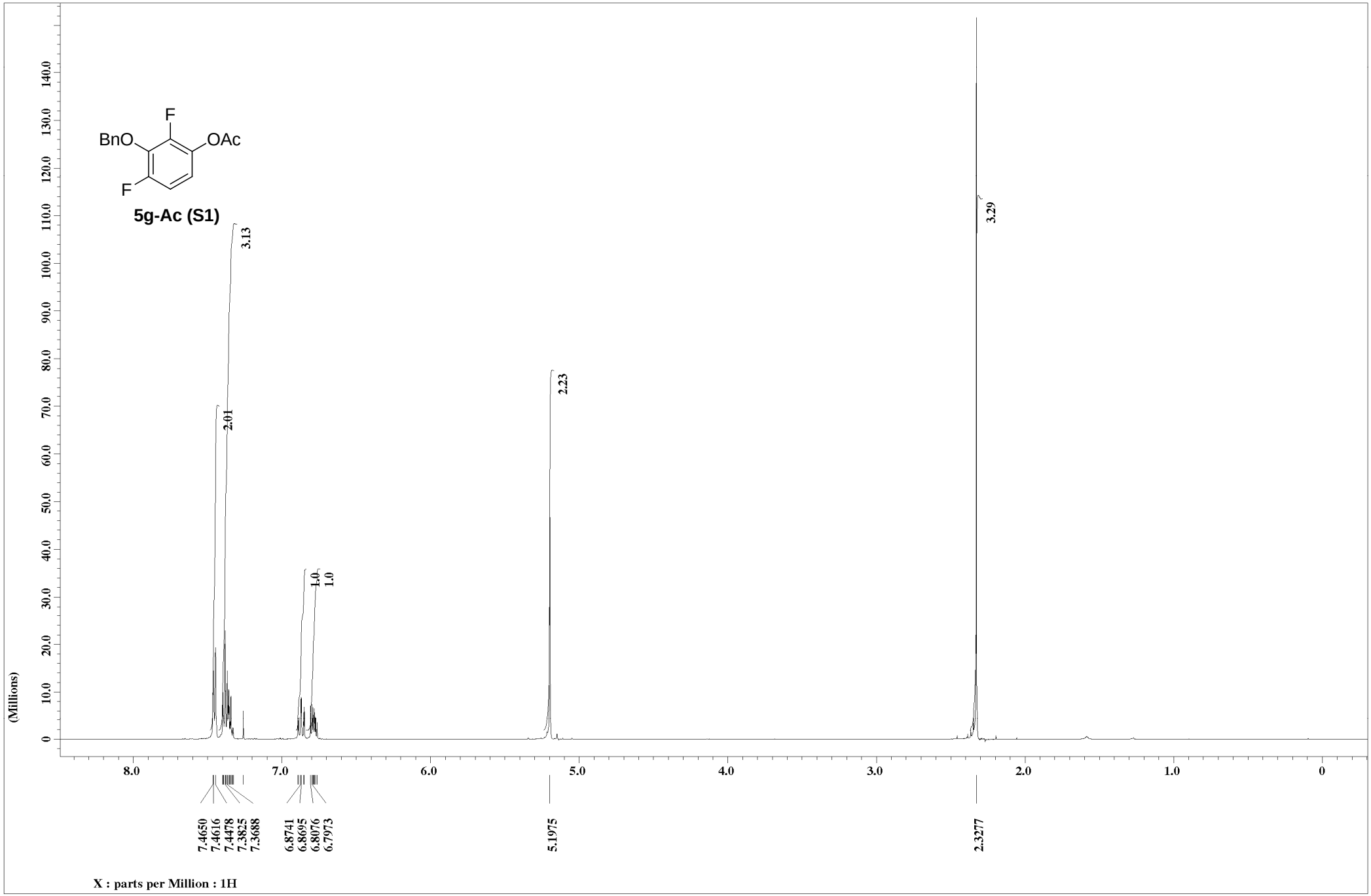

F
OH
Ph
TsN
6f
(Millions)
400.0
300.0
200.0
100.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
148.3943
143.1960
142.4043
141.0975
137.5683
130.4814
130.4528
129.3749
128.6023
128.3257
127.7820
126.9903
126.3513
126.3036
116.9083
114.9148
114.7718
77.2575
77.0000
76.7520
58.4384
38.6082
26.0749
21.4583
X : parts per Million : 13C

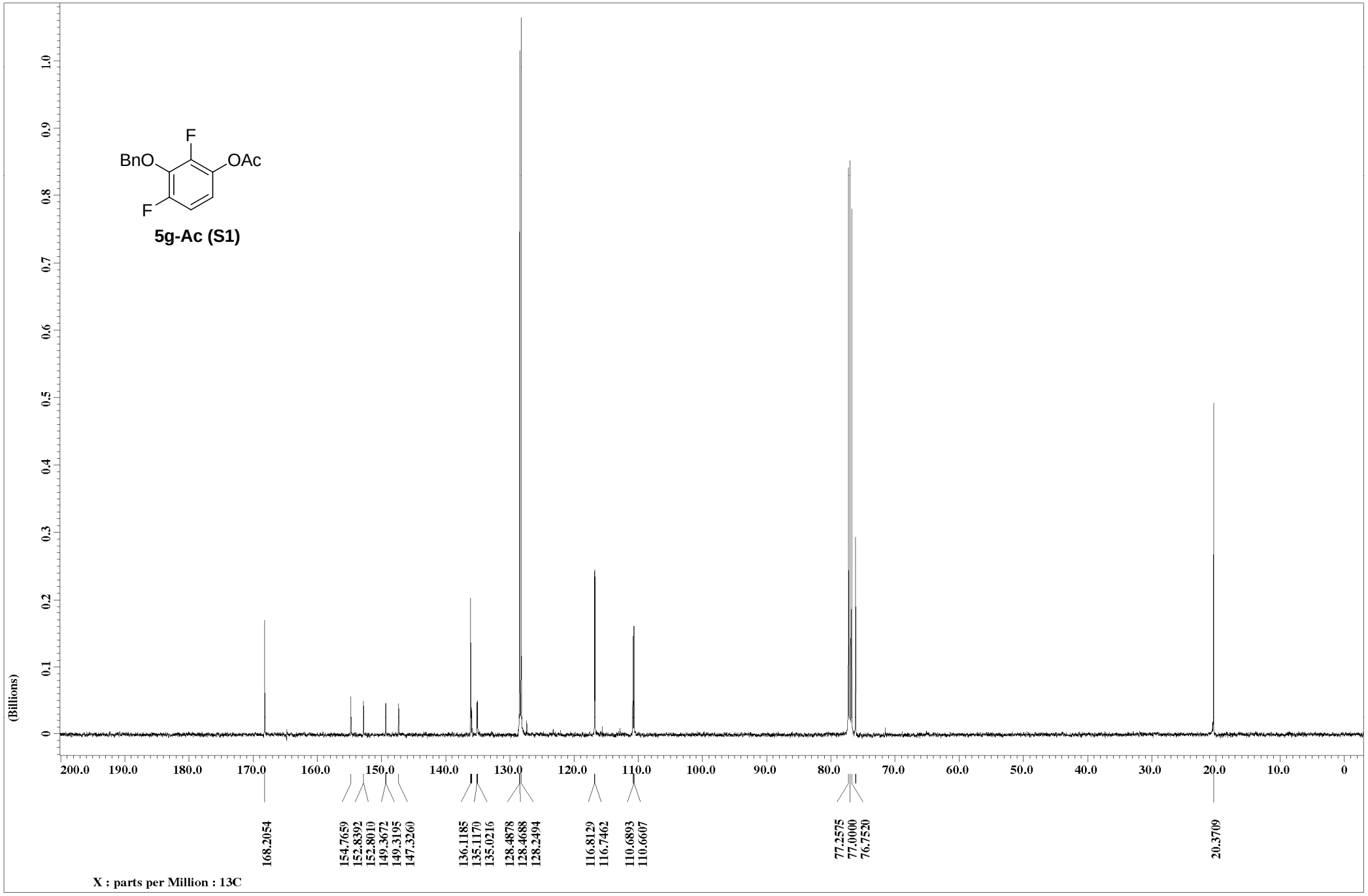

F
OH
Ph
TsN
6f
30.0
20.0
10.0
0
(Millions)
−145.0
−146.0
−147.0
−148.0
−149.0
−150.0
−151.0
−152.0
−153.0
−154.0
−155.0
−156.0
−157.0
−158.0
−159.0
−160.0
−161.0
−162.0
−163.0
−164.0
−165.0
−166.0
−167.0
−146.0483
−146.0684
−146.0885
−164.9000
X : parts per Million : 19F

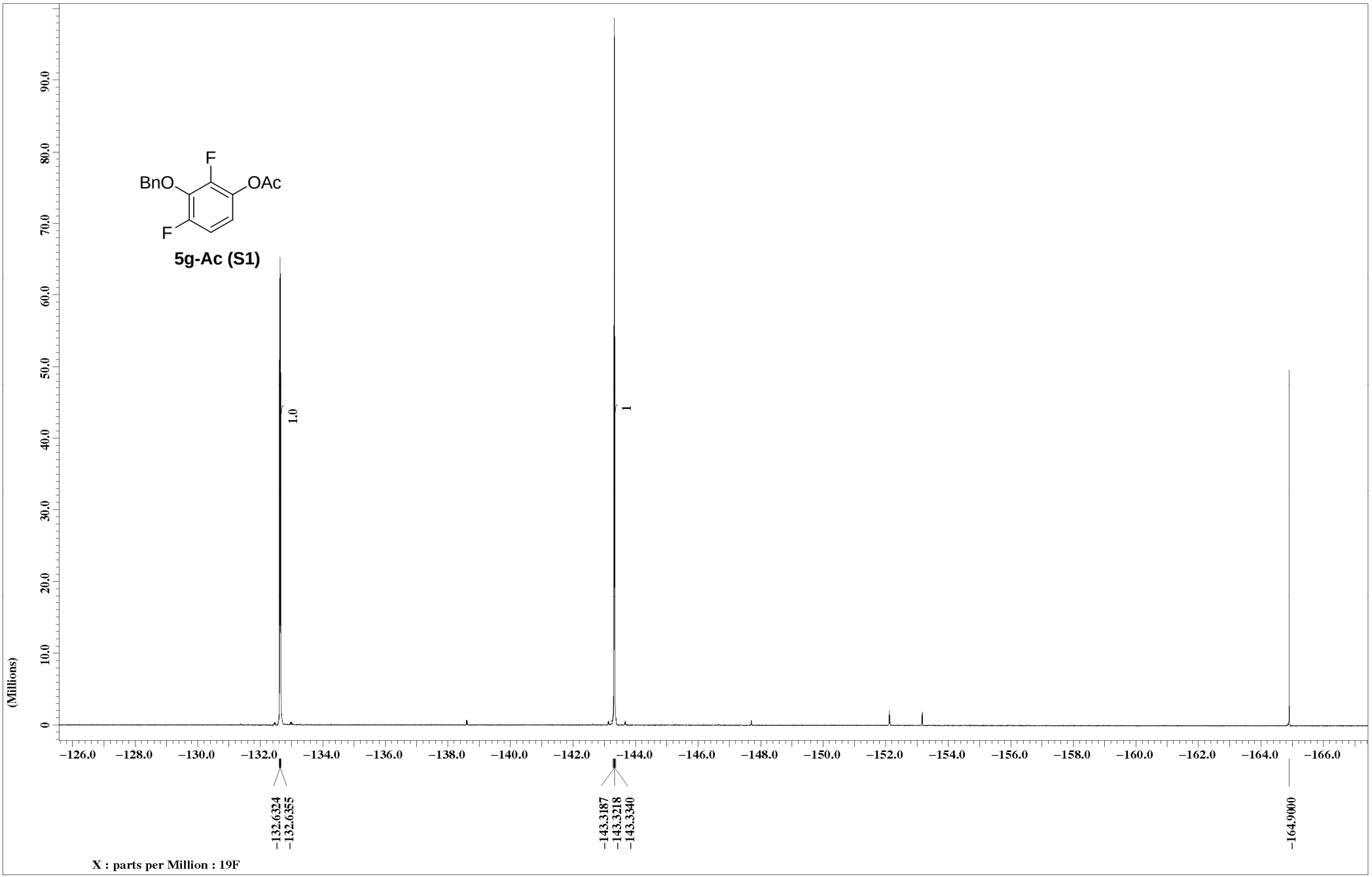

OH
F
Ph
TsN
7f
(Millions)
30.0
20.0
10.0
0
2.16
4.17
2.16
2.16
1.04
1
1.09
0.94
1.05
1.06
1.08
1.09
3.36
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.5623
7.5451
7.2600
7.2543
7.2520
7.1226
6.6908
6.6381
6.6210
6.1331
5.1059
5.1002
3.7683
3.7511
3.7397
3.2553
3.2427
3.2324
2.4754
2.4708
2.4662
2.4616
2.3437
1.6153
1.2523
X : parts per Million : 1H

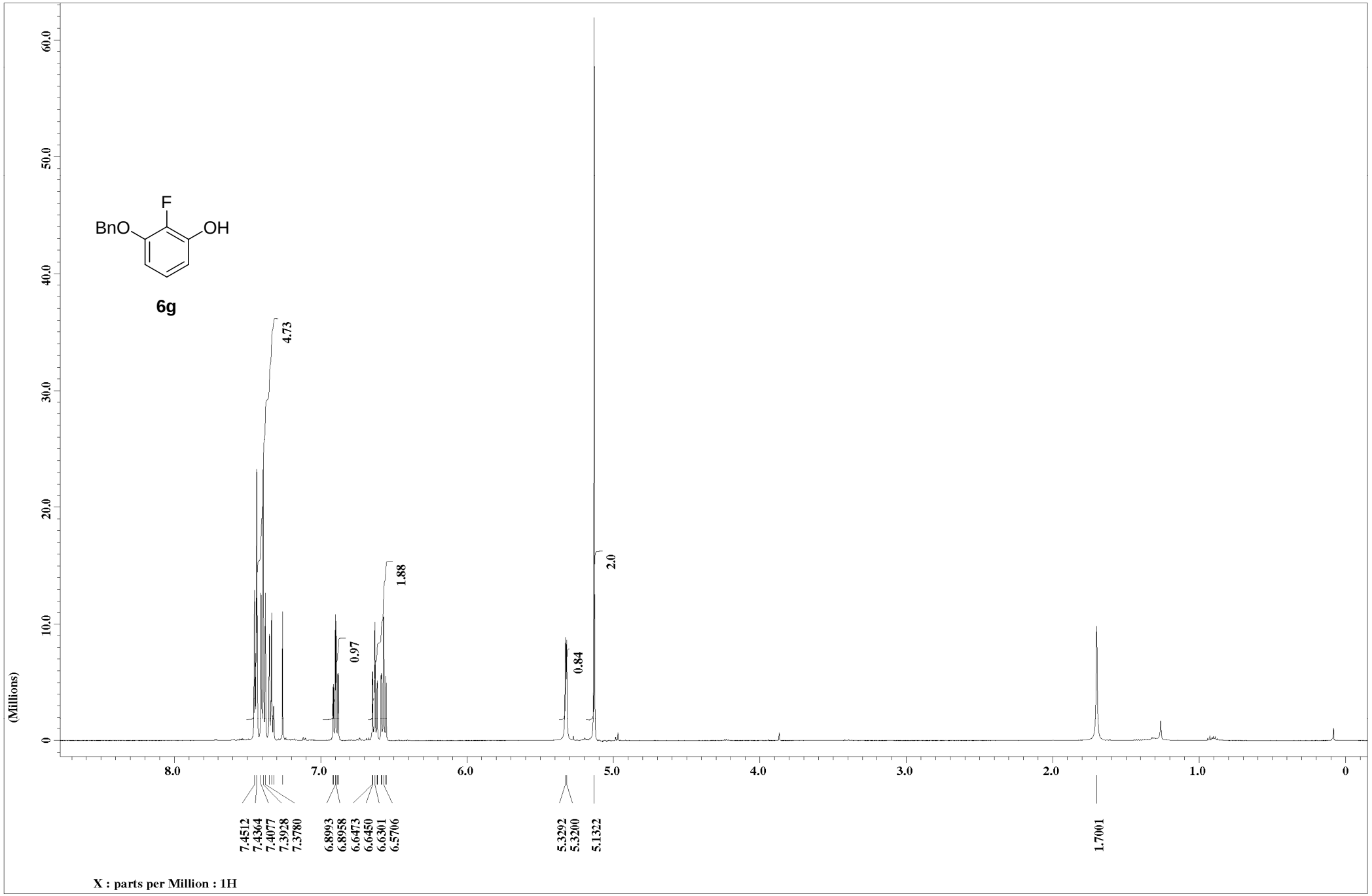

OH
F
Ph
TsN
7f
(Millions)
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
143.1674
141.7652
141.6413
140.9736
137.5684
130.3193
130.3002
129.3463
128.6214
128.2971
127.7439
127.0095
126.4944
126.4467
116.6031
115.4109
115.2678
77.2576
77.0000
76.7520
58.6006
38.5892
25.8460
21.4488
X : parts per Million : 13C

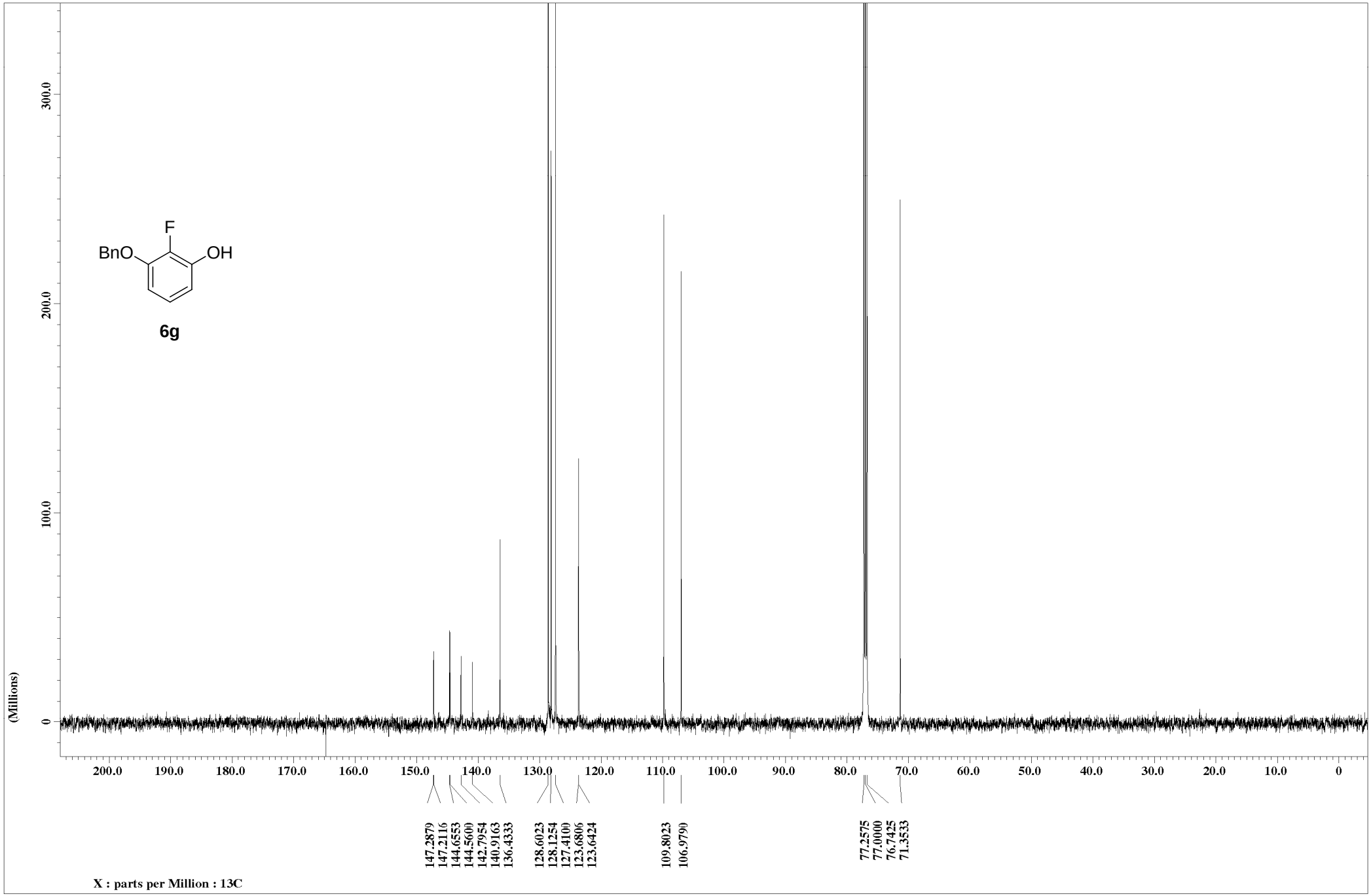

OH
F
Ph
TsN
7f
(Millions)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−144.0
−145.0
−146.0
−147.0
−148.0
−149.0
−150.0
−151.0
−152.0
−153.0
−154.0
−155.0
−156.0
−157.0
−158.0
−159.0
−160.0
−161.0
−162.0
−163.0
−164.0
−165.0
−166.0
−167.0
−144.8775
−144.8946
−144.9118
−164.9000
X : parts per Million : 19F

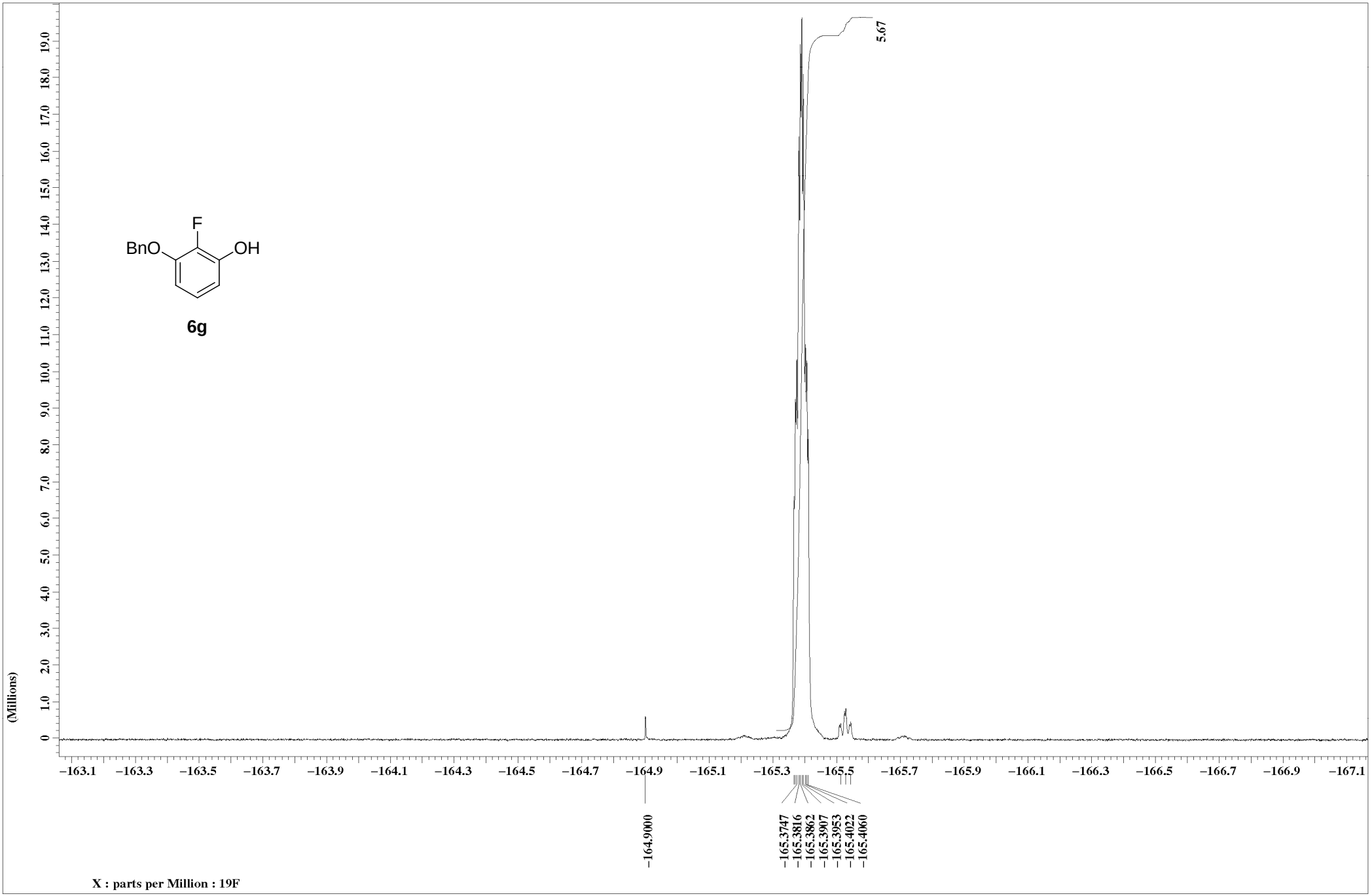

F
BnO
OAc
F
5g-Ac (S1)
3.13
2.01
2.23
3.29
1.0
1.0
(Millions)
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.4650
7.4616
7.4478
7.3825
7.3688
6.8741
6.8695
6.8076
6.7973
5.1975
2.3277
X : parts per Million : 1H

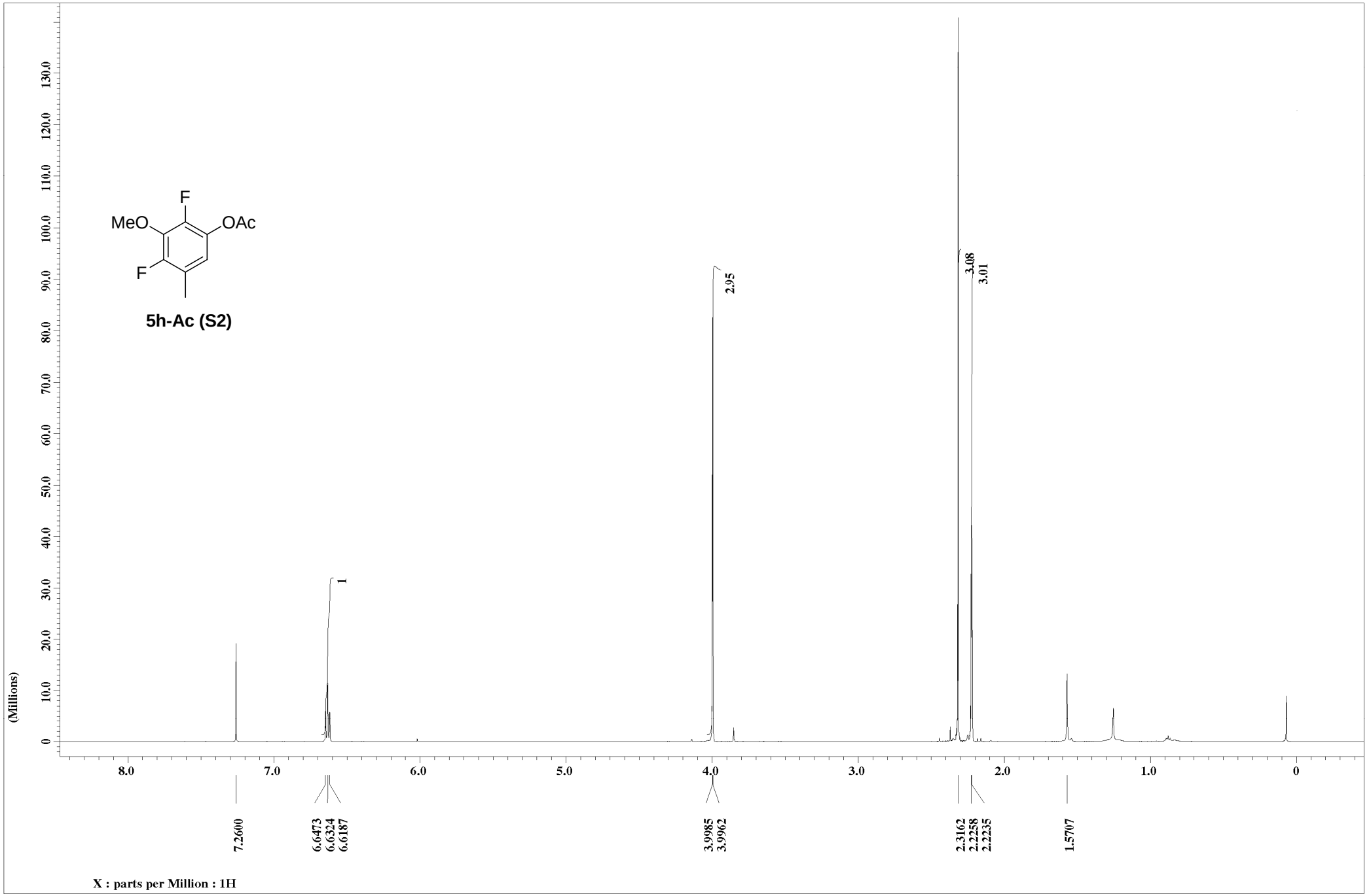

F
BnO
OAc
F
5g-Ac (S1)
(Billions)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
168.2054
154.7659
152.8392
152.8010
149.3672
149.3195
147.3260
136.1185
135.1170
135.0216
128.4878
128.4688
128.2494
116.8129
116.7462
110.6893
110.6607
77.2575
77.0000
76.7520
20.3709
X : parts per Million : 13C

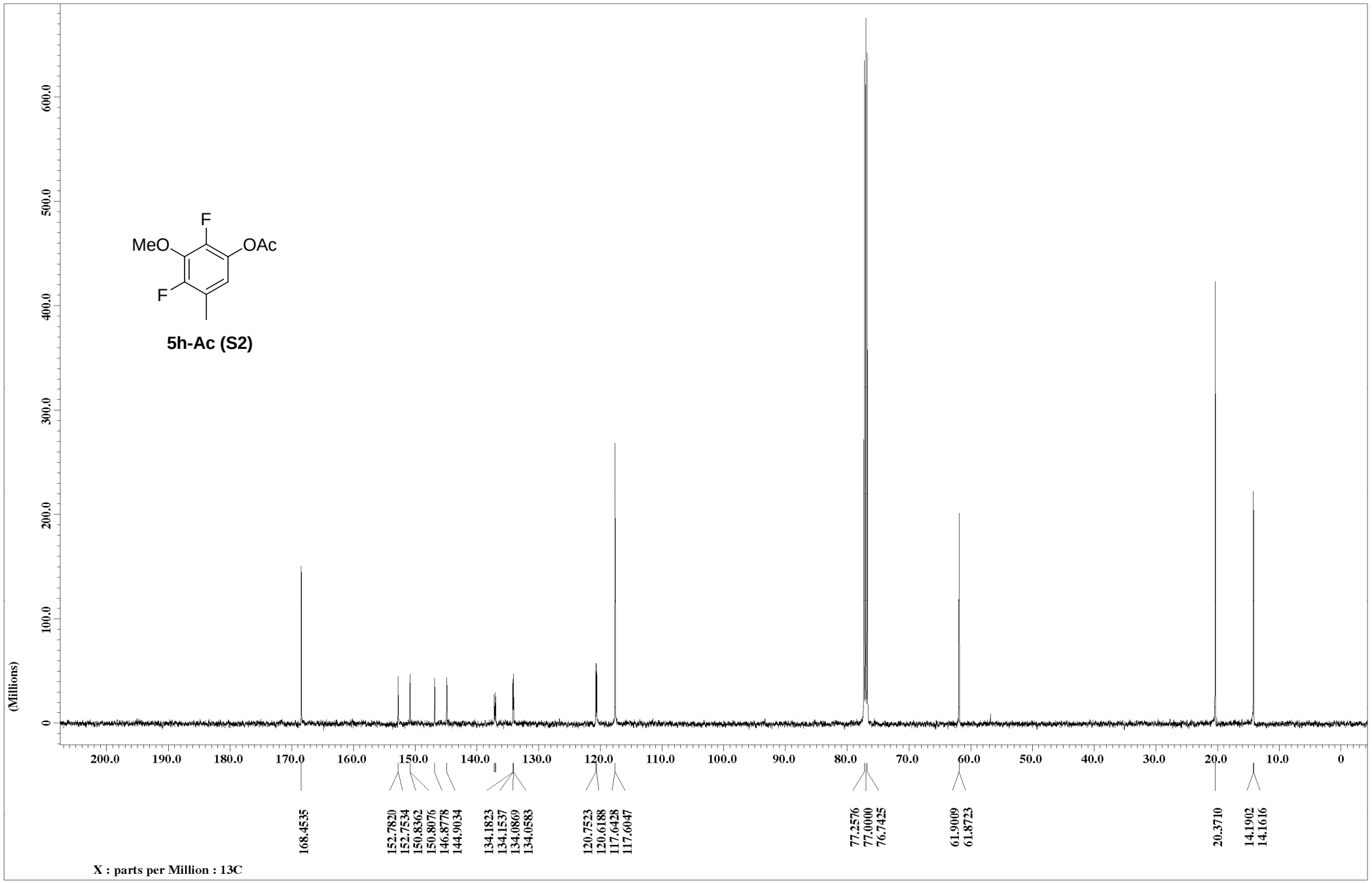

F
BnO
OAc
F
5g-Ac (S1)
(Millions)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
1.0
1
−126.0
−128.0
−130.0
−132.0
−134.0
−136.0
−138.0
−140.0
−142.0
−144.0
−146.0
−148.0
−150.0
−152.0
−154.0
−156.0
−158.0
−160.0
−162.0
−164.0
−166.0
−132.6324
−132.6355
−143.3187
−143.3218
−143.3340
−164.9000
X : parts per Million : 19F

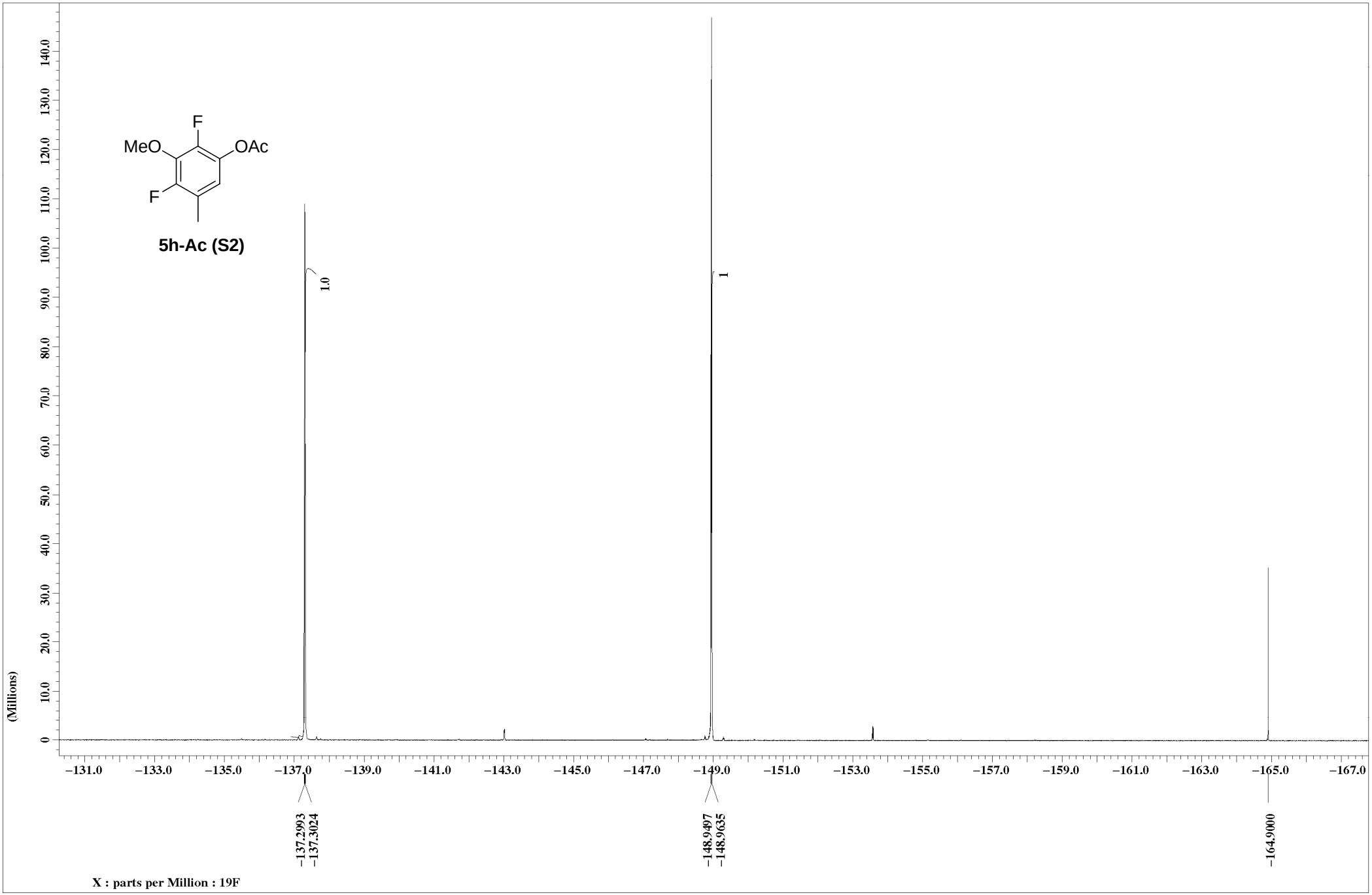

F
BnO
OH
6g
(Millions)
60.0
50.0
40.0
30.0
20.0
10.0
0
4.73
0.97
1.88
0.84
2.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.4512
7.4364
7.4077
7.3928
7.3780
6.8993
6.8958
6.6473
6.6450
6.6301
6.5706
5.3292
5.3200
5.1322
1.7001
X : parts per Million : 1H

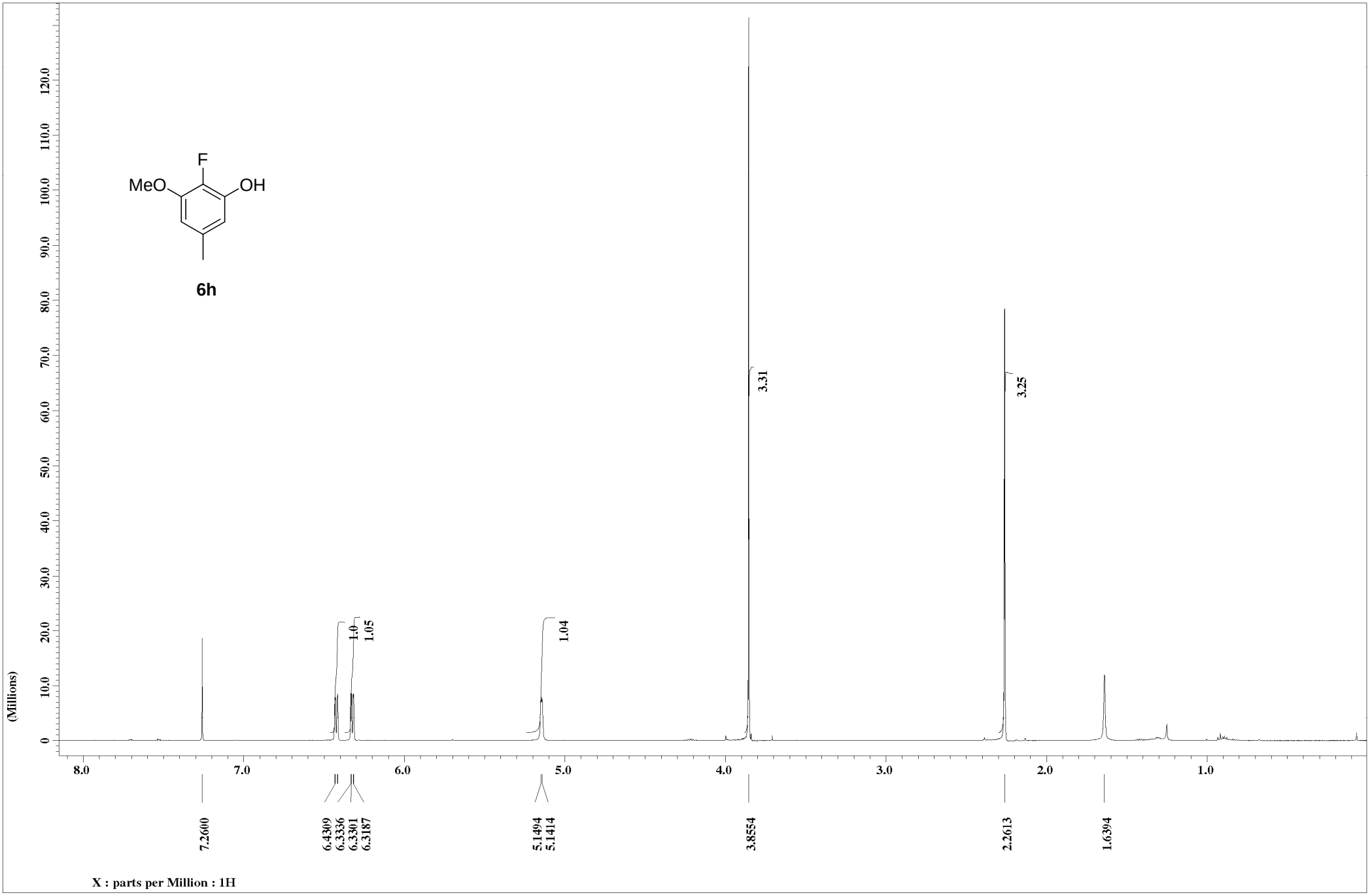

F
BnO
OH
6g
300.0
200.0
100.0
0
(Millions)
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
147.2879
147.2116
144.6553
144.5600
142.7954
140.9163
136.4333
128.6023
128.1254
127.4100
123.6806
123.6424
109.8023
106.9790
77.2575
77.0000
76.7425
71.3533
X : parts per Million : 13C

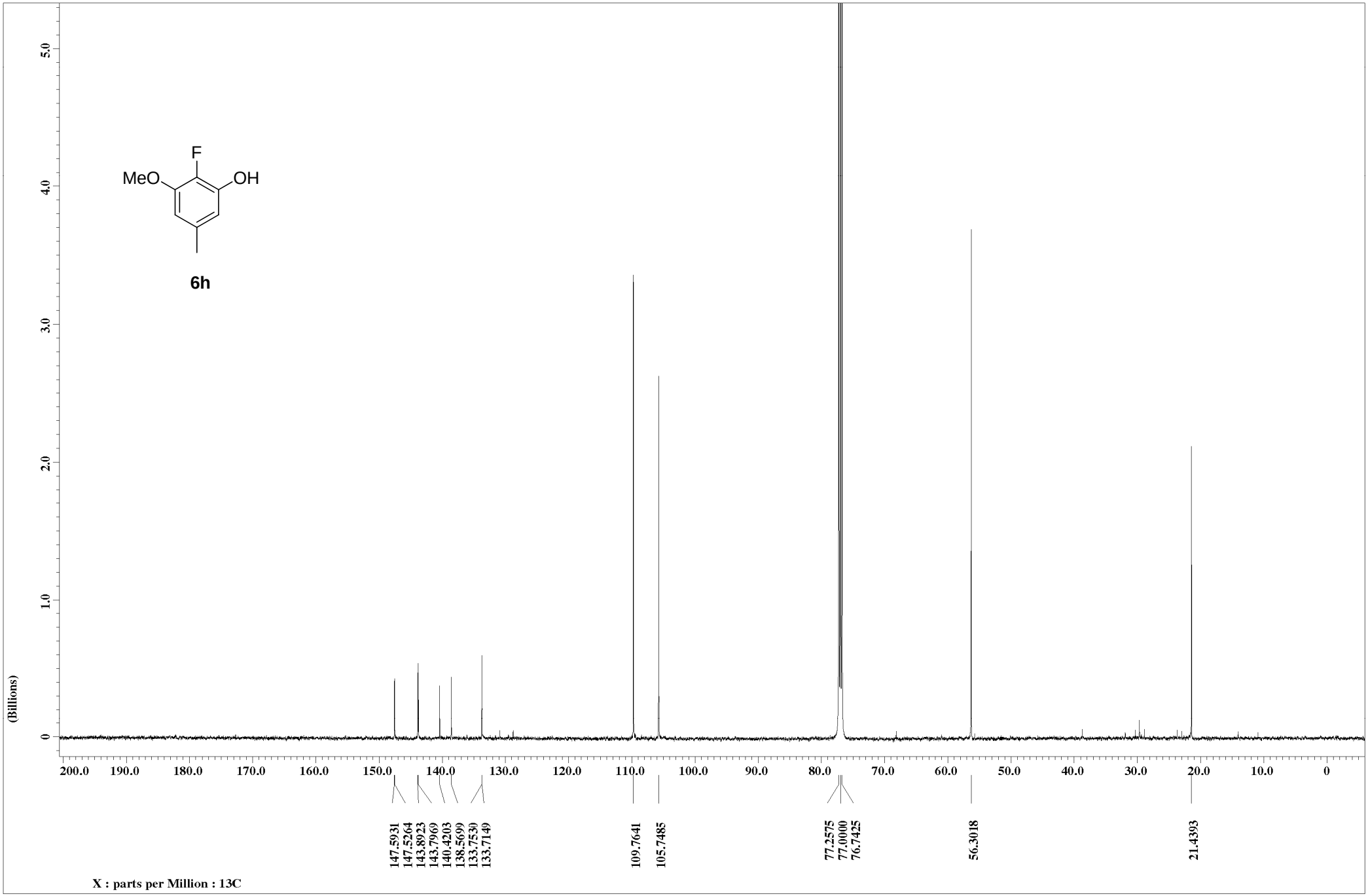

F
BnO
OH
6g
5.67
(Millions)
19.0
18.0
17.0
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−163.1
−163.3
−163.5
−163.7
−163.9
−164.1
−164.3
−164.5
−164.7
−164.9
−165.1
−165.3
−165.5
−165.7
−165.9
−166.1
−166.3
−166.5
−166.7
−166.9
−167.1
−164.9000
−165.3747
−165.3816
−165.3862
−165.3907
−165.3953
−165.4022
−165.4060
X : parts per Million : 19F

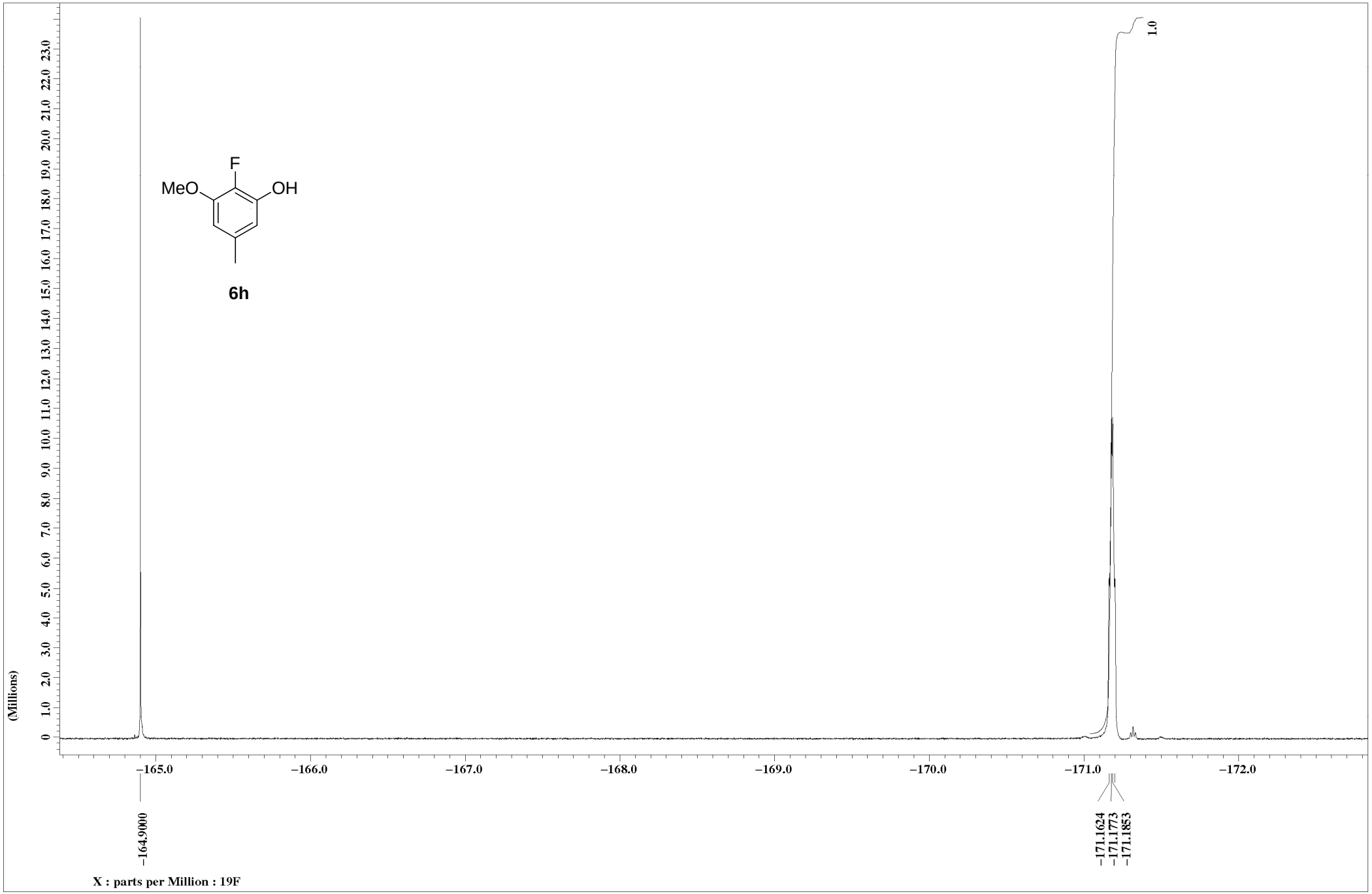

F
MeO
OAc
F
5h-Ac (S2)
(Millions)
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
1
2.95
3.08
3.01
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2600
6.6473
6.6324
6.6187
3.9985
3.9962
2.3162
2.2258
2.2235
1.5707
X : parts per Million : 1H

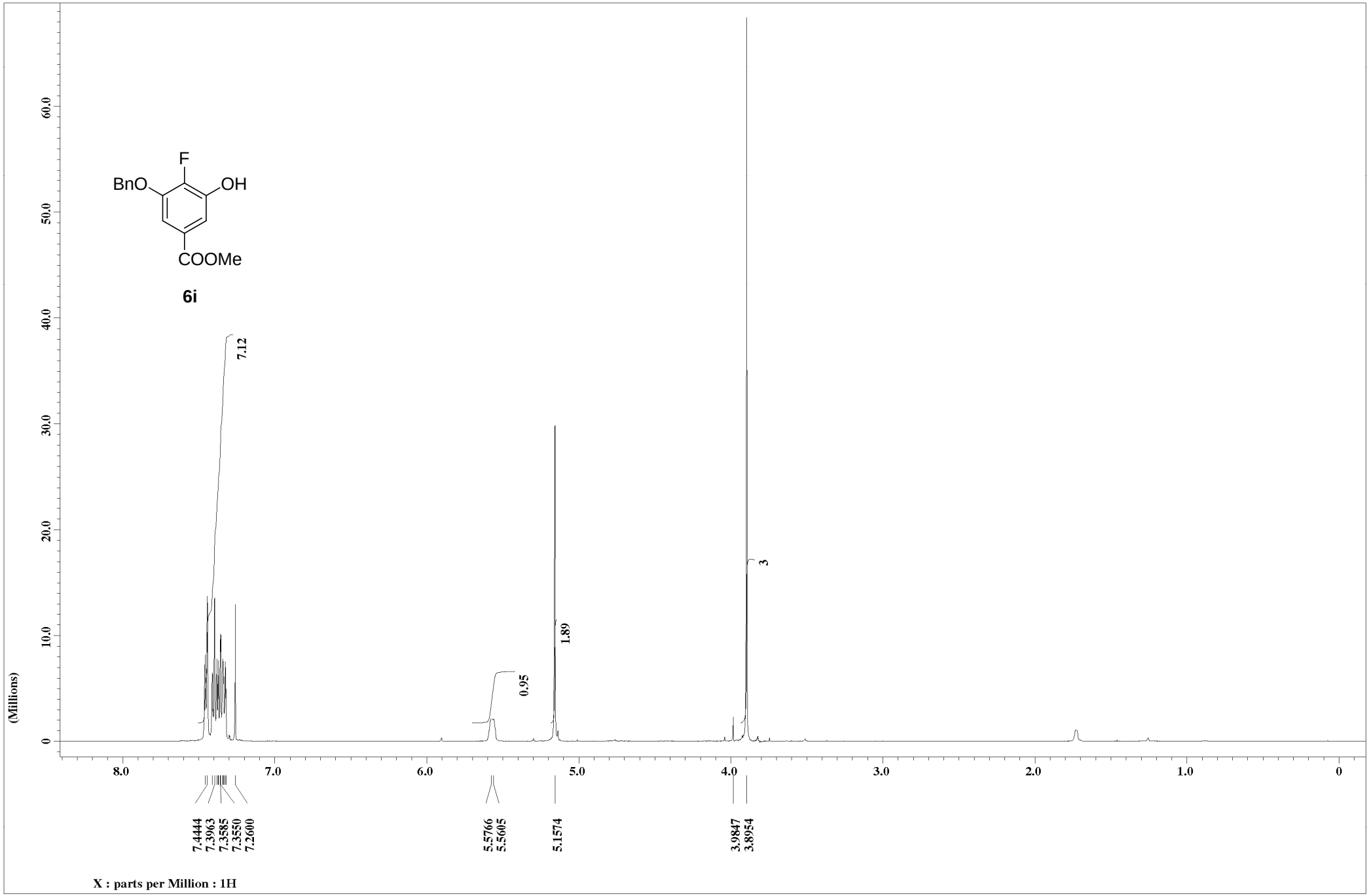

F
MeO
OAc
F
5h-Ac (S2)
(Millions)
600.0
500.0
400.0
300.0
200.0
100.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
168.4535
152.7820
152.7534
150.8362
150.8076
146.8778
144.9034
134.1823
134.1537
134.0869
134.0583
120.7523
120.6188
117.6428
117.6047
77.2576
77.0000
76.7425
61.9009
61.8723
20.3710
14.1902
14.1616
X : parts per Million : 13C

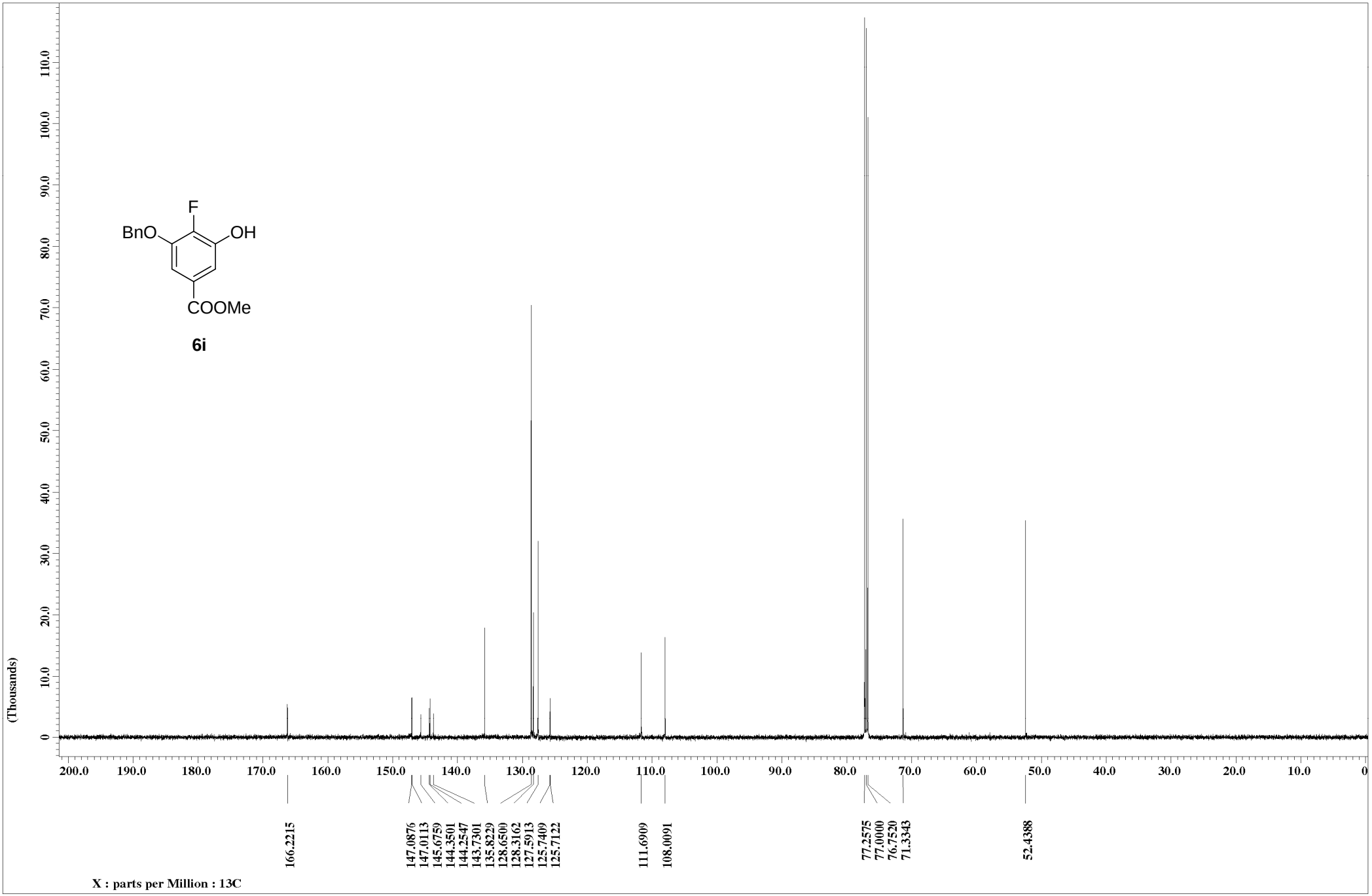

F
MeO
OAc
F
5h-Ac (S2)
1.0
1
(Millions)
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−131.0
−133.0
−135.0
−137.0
−139.0
−141.0
−143.0
−145.0
−147.0
−149.0
−151.0
−153.0
−155.0
−157.0
−159.0
−161.0
−163.0
−165.0
−167.0
−137.2993
−137.3024
−148.9497
−148.9635
−164.9000
X : parts per Million : 19F

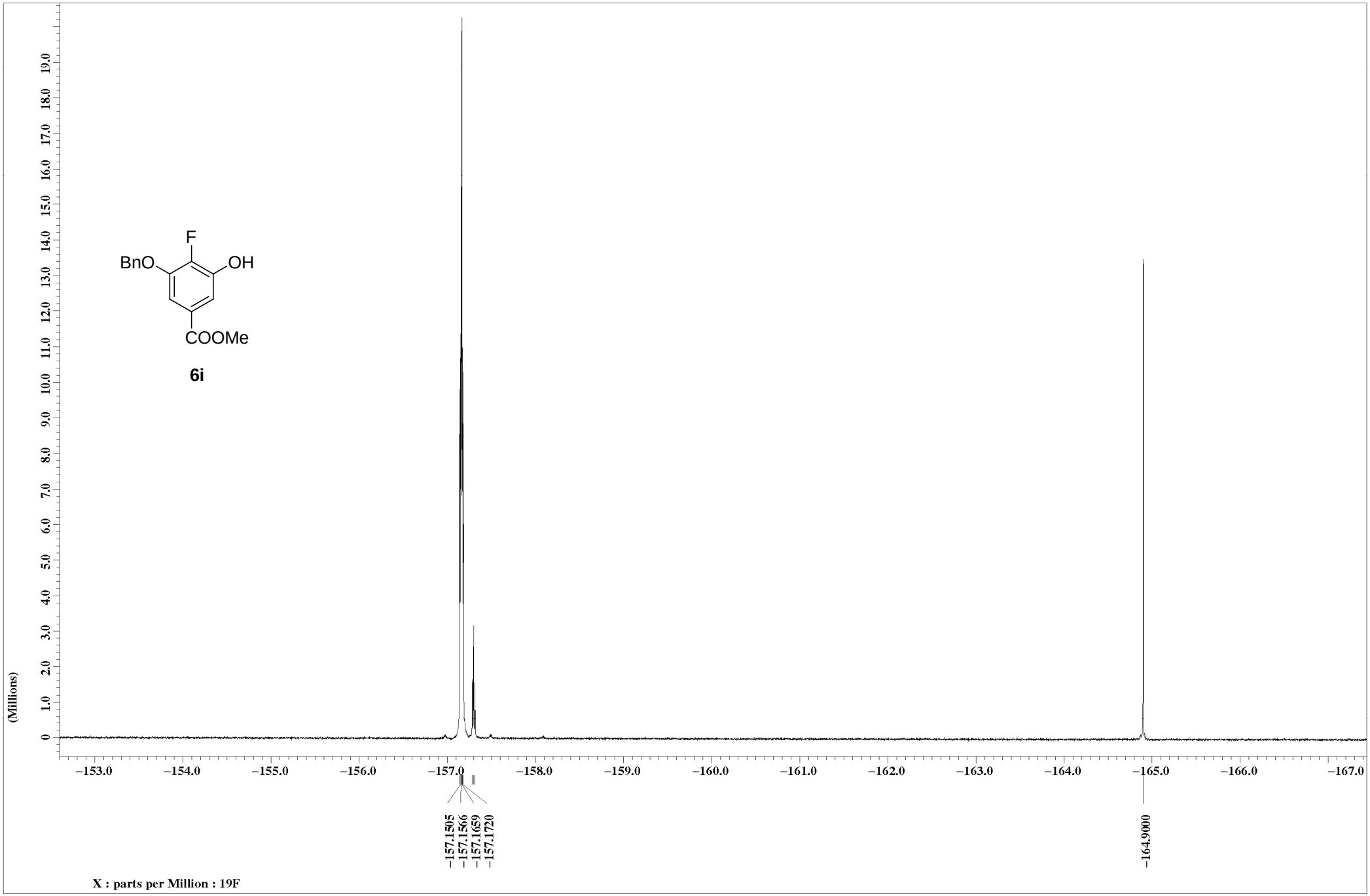

F
MeO
OH
6h
(Millions)
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
3.31
3.25
1.0
1.05
1.04
7.2600
6.4309
6.3336
6.3301
6.3187
5.1494
5.1414
3.8554
2.2613
1.6394
X : parts per Million : 1H

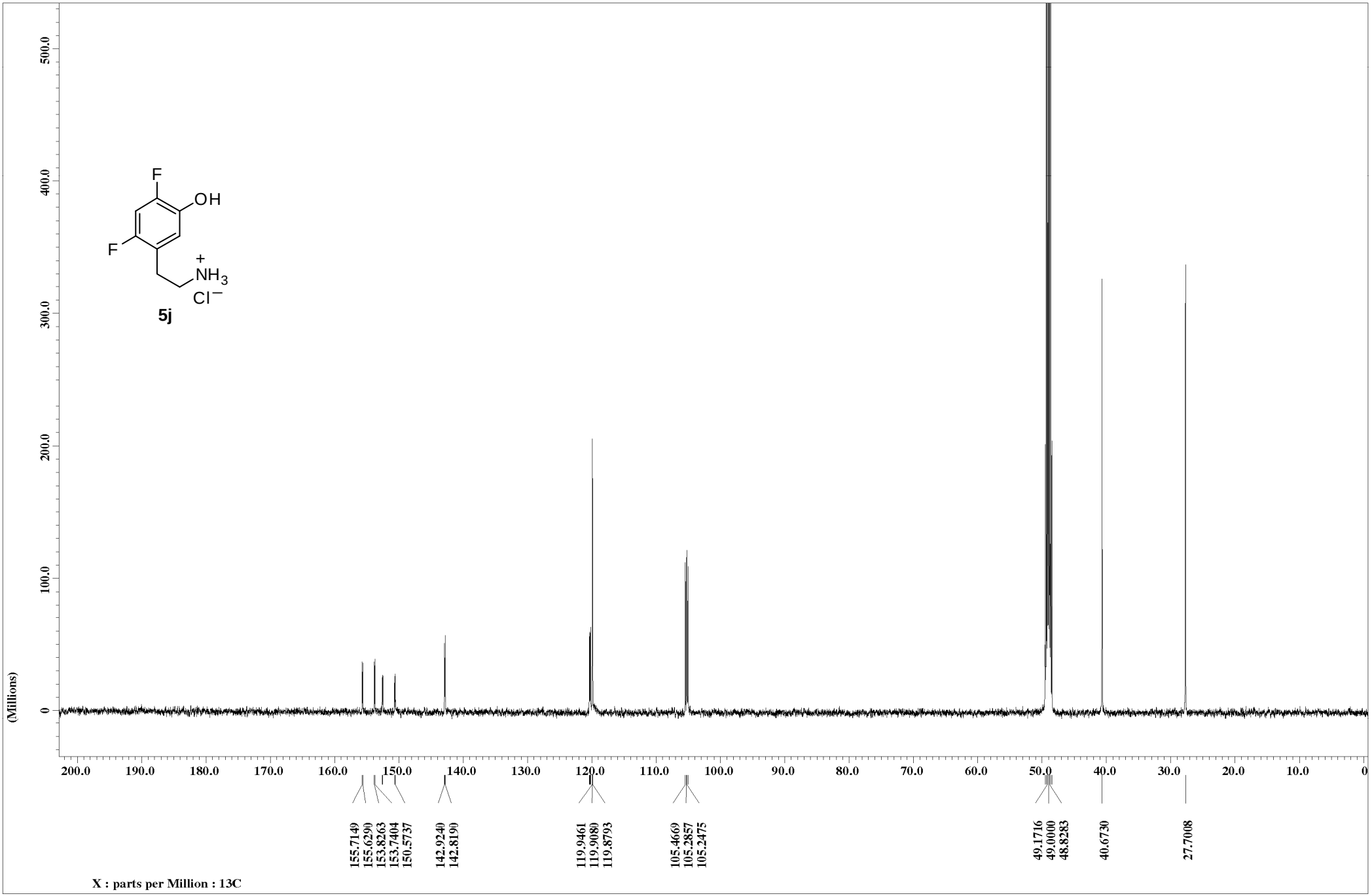

F
MeO
OH
6h
(Billions)
5.0
4.0
3.0
2.0
1.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
147.5931
147.5264
143.8923
143.7969
140.4203
138.5699
133.7530
133.7149
109.7641
105.7485
77.2575
77.0000
76.7425
56.3018
21.4393
X : parts per Million : 13C

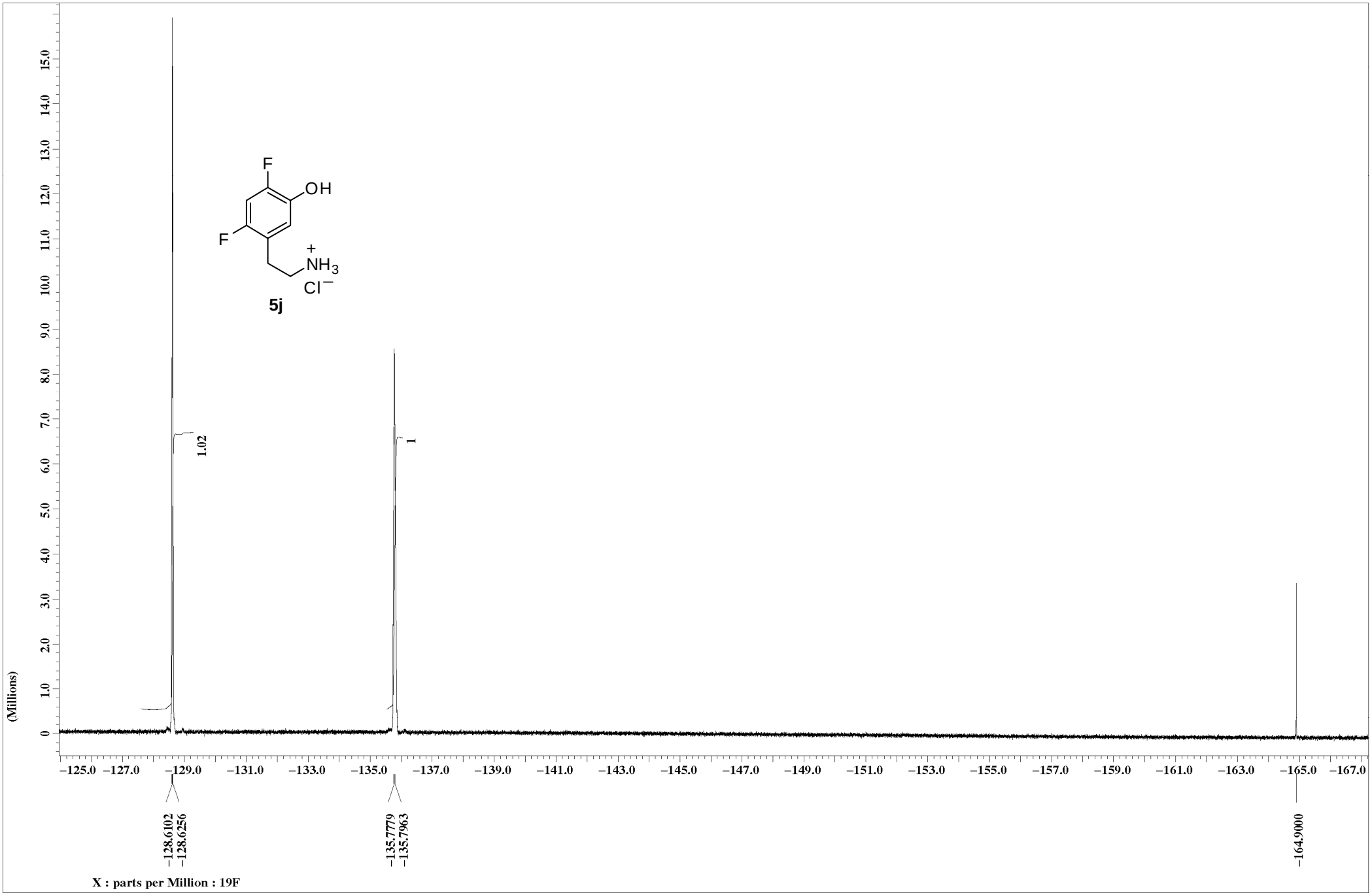

F
MeO
OH
6h
1.0
(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0
22.0
23.0
−165.0
−166.0
−167.0
−168.0
−169.0
−170.0
−171.0
−172.0
−164.9000
−171.1624
−171.1773
−171.1853
X : parts per Million : 19F

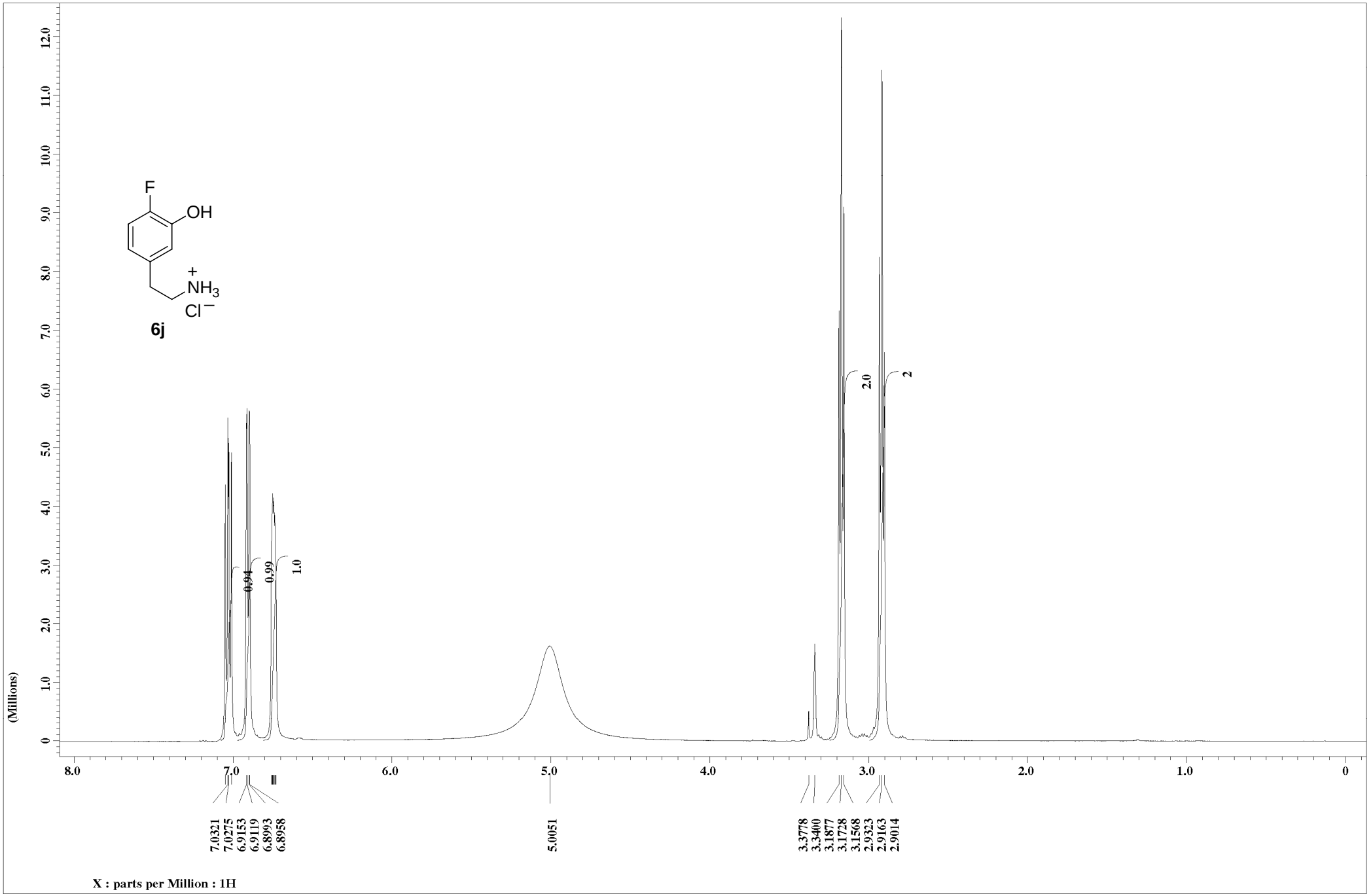

F
BnO
OH
COOMe
6i
7.12
0.95
1.89
3
(Millions)
60.0
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.4444
7.3963
7.3585
7.3550
7.2600
5.5766
5.5605
5.1574
3.9847
3.8954
X : parts per Million : 1H

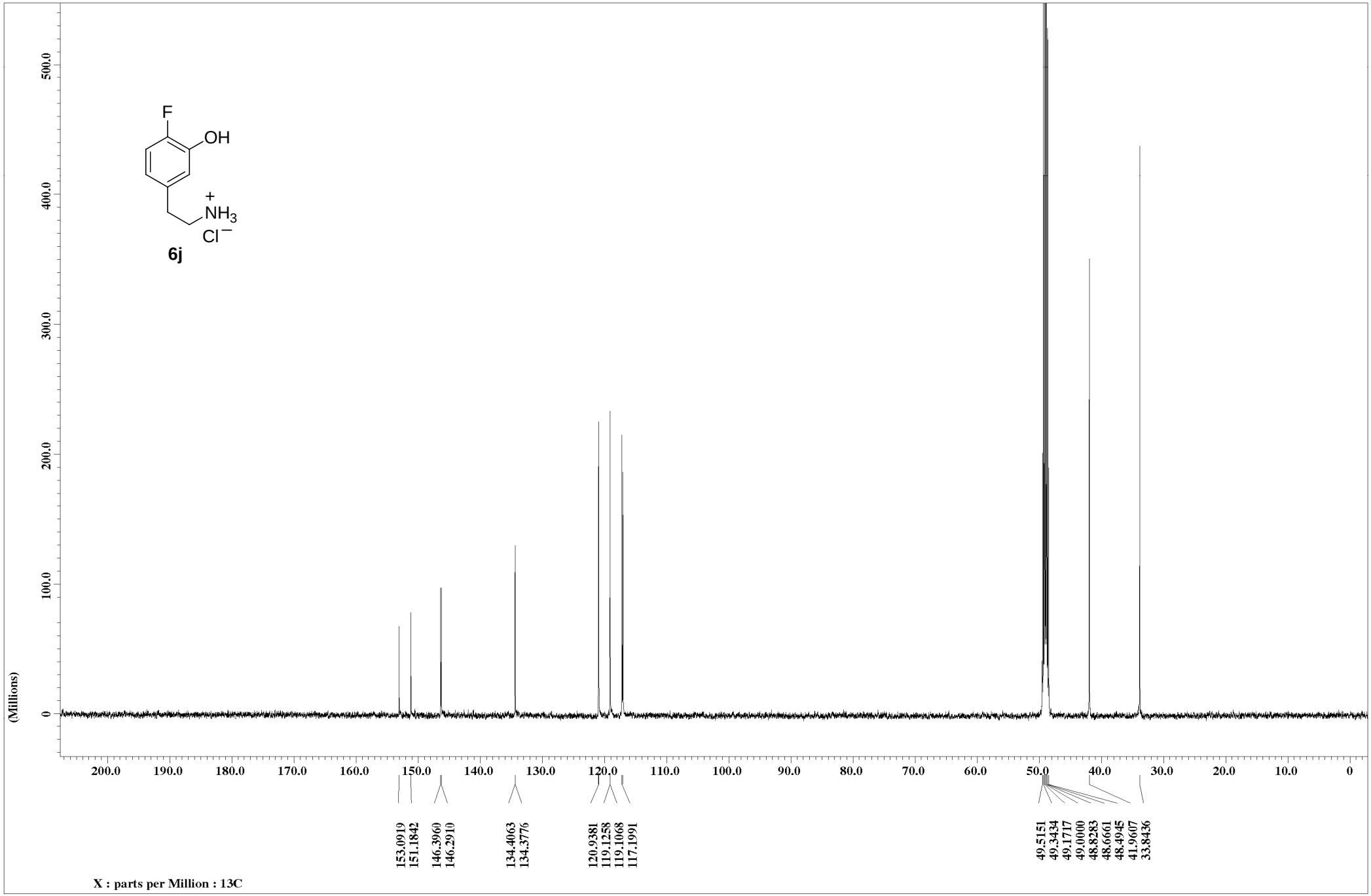

F
BnO
OH
COOMe
6i
(Thousands)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
110.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
166.2215
147.0876
147.0113
145.6759
144.3501
144.2547
143.7301
135.8229
128.6500
128.3162
127.5913
125.7409
125.7122
111.6909
108.0091
77.2575
77.0000
76.7520
71.3343
52.4388
X : parts per Million : 13C

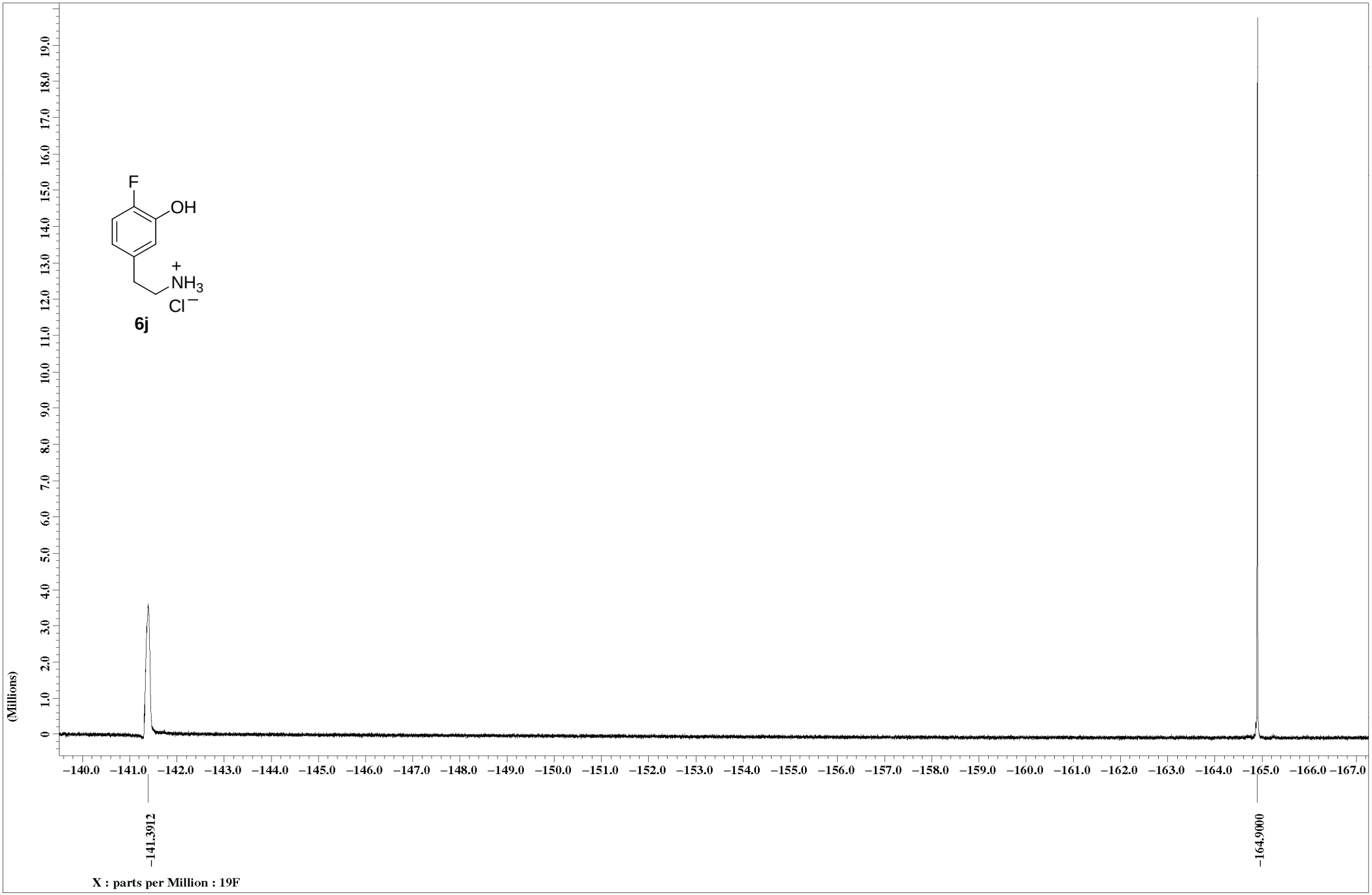

F
BnO
OH
COOMe
6i
(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
−153.0
−154.0
−155.0
−156.0
−157.0
−158.0
−159.0
−160.0
−161.0
−162.0
−163.0
−164.0
−165.0
−166.0
−167.0
−157.1505
−157.1566
−157.1659
−157.1720
−164.9000
X : parts per Million : 19F

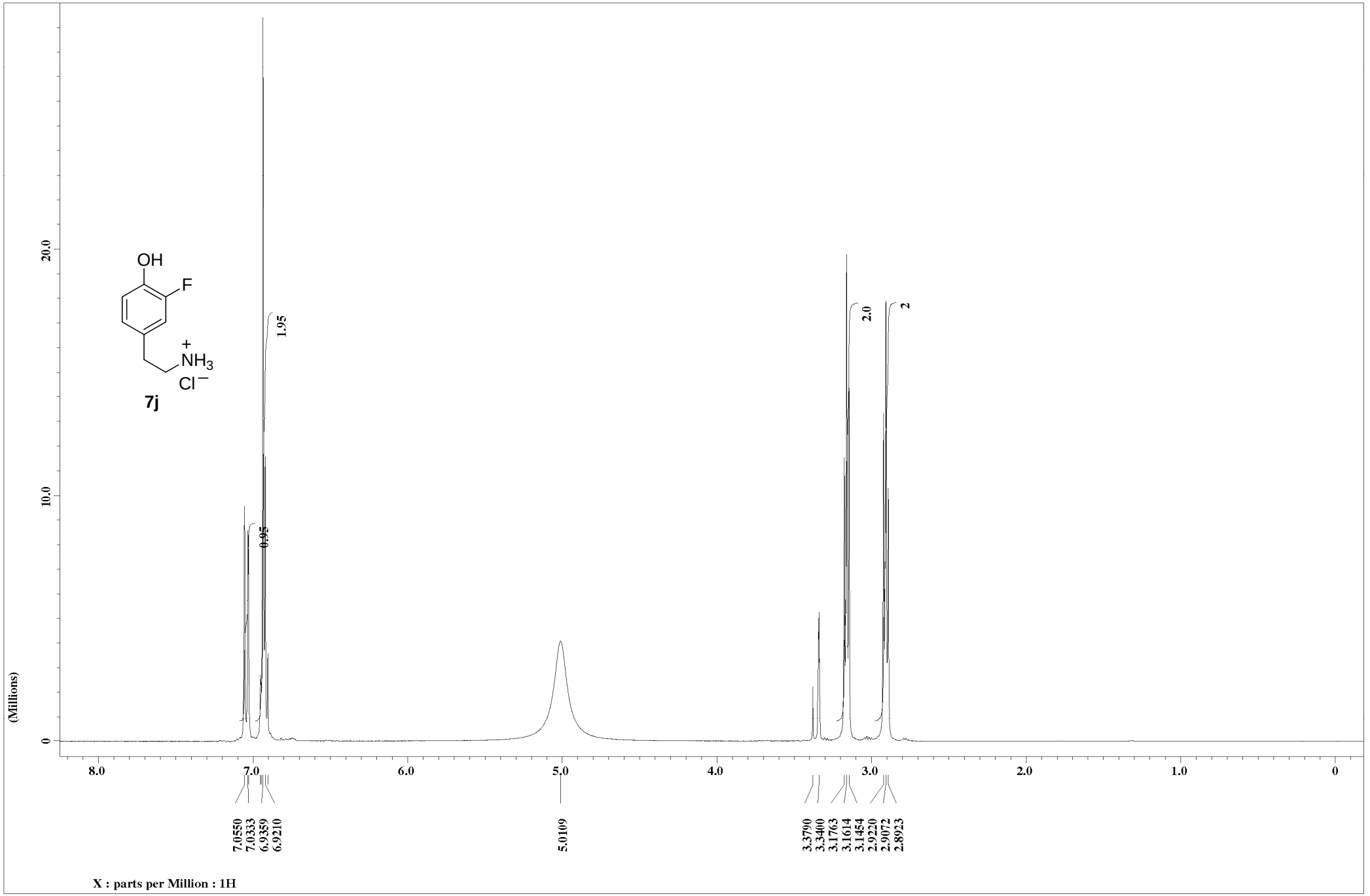

F
OH
F
+
NH3
Cl−
5j
(Millions)
500.0
400.0
300.0
200.0
100.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
155.7149
155.6290
153.8263
153.7404
150.5737
142.9240
142.8190
119.9461
119.9080
119.8793
105.4669
105.2857
105.2475
49.1716
49.0000
48.8283
40.6730
27.7008
X : parts per Million : 13C

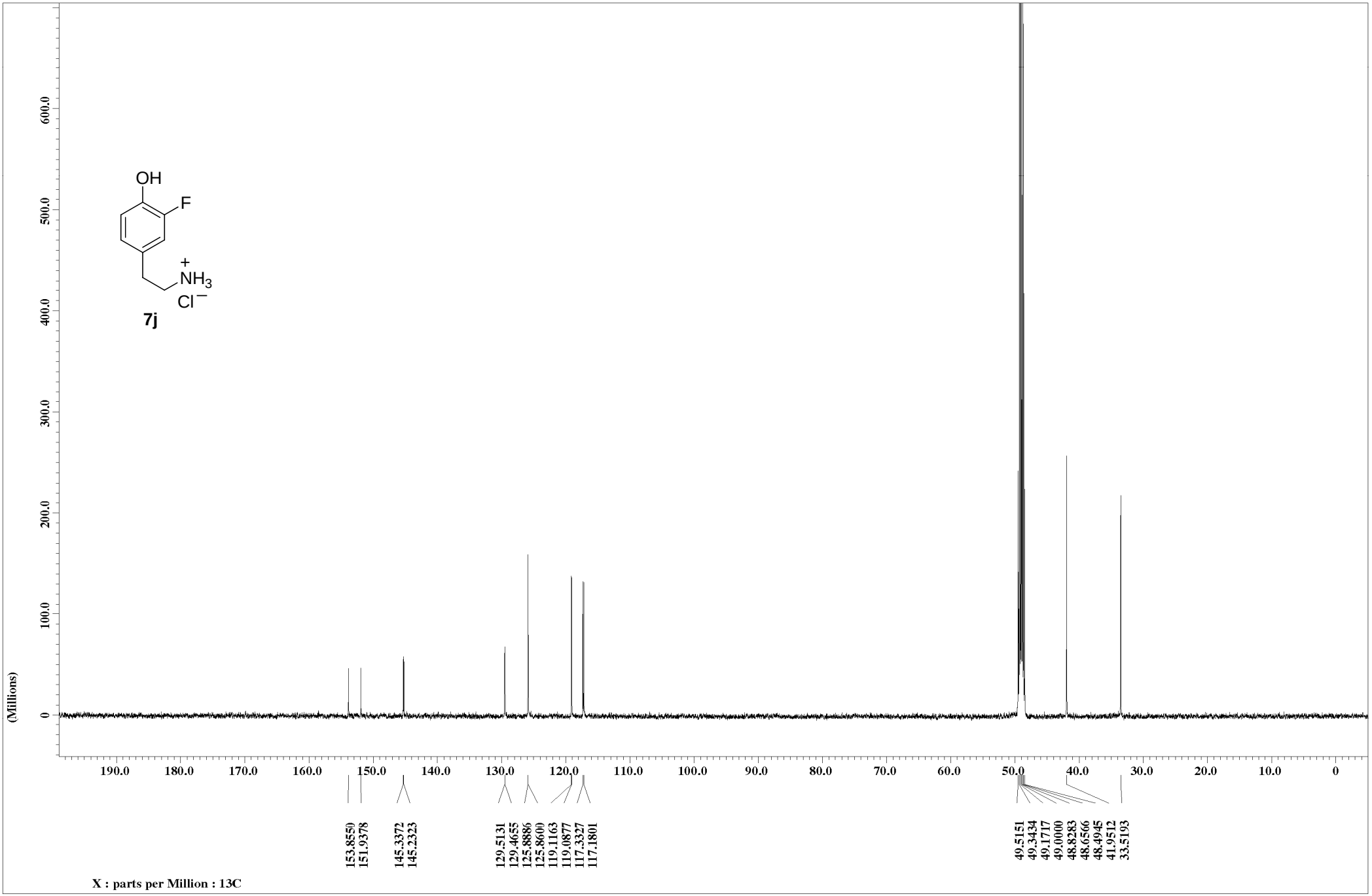

F
OH
F
+
NH3
Cl−
5j
1.02
1
(Millions)
−125.0 −127.0 −129.0 −131.0 −133.0 −135.0 −137.0 −139.0 −141.0 −143.0 −145.0 −147.0 −149.0 −151.0 −153.0 −155.0 −157.0 −159.0 −161.0 −163.0 −165.0 −167.0
−128.6102
−128.6256
−135.7779
−135.7963
−164.9000
X : parts per Million : 19F

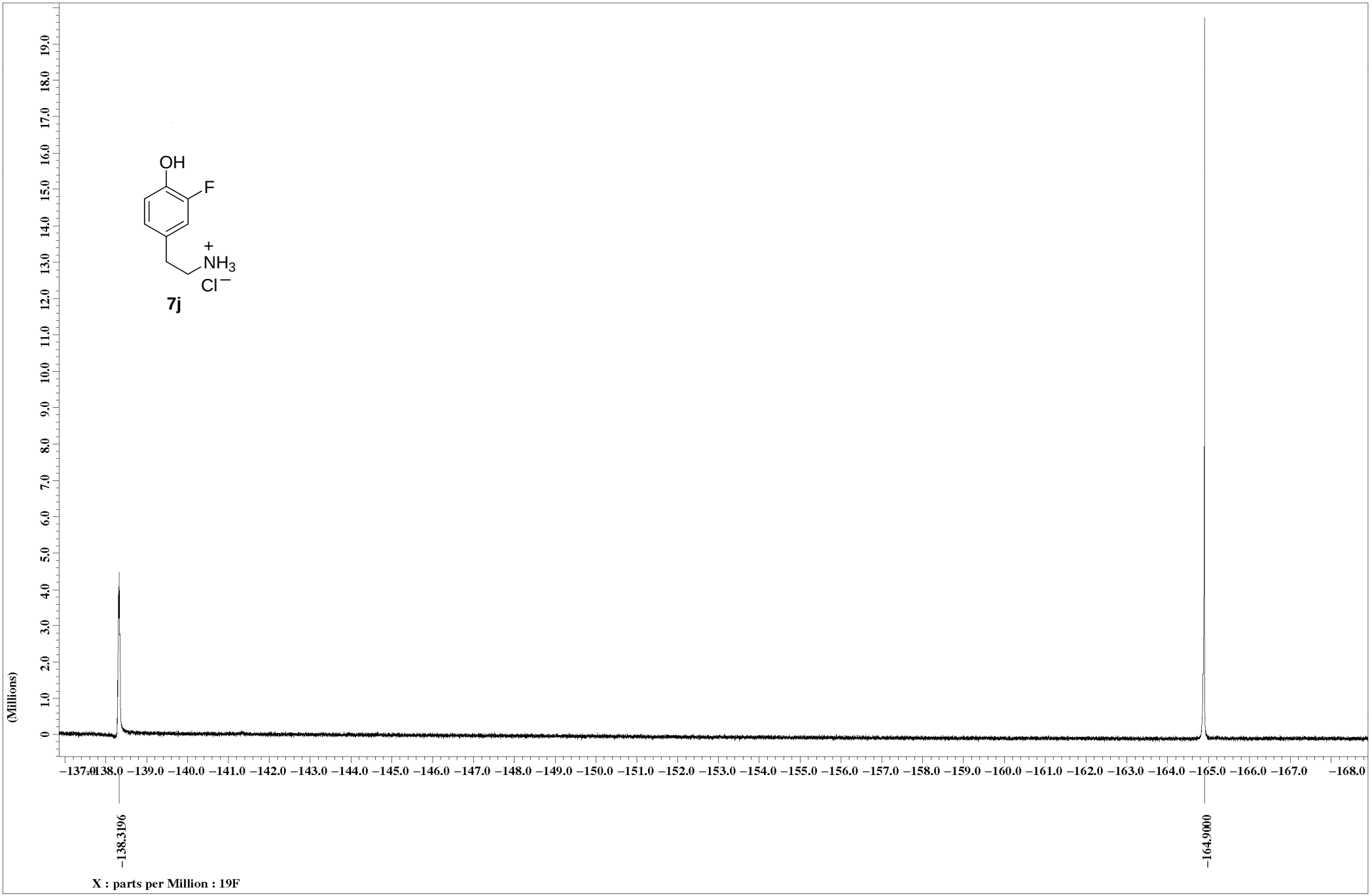

F
OH
+
NH3
Cl−
6j
(Millions)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.94
0.99
1.0
2.0
2
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.0321
7.0275
6.9153
6.9119
6.8993
6.8958
5.0051
3.3778
3.3400
3.1877
3.1728
3.1568
2.9323
2.9163
2.9014
X : parts per Million : 1H

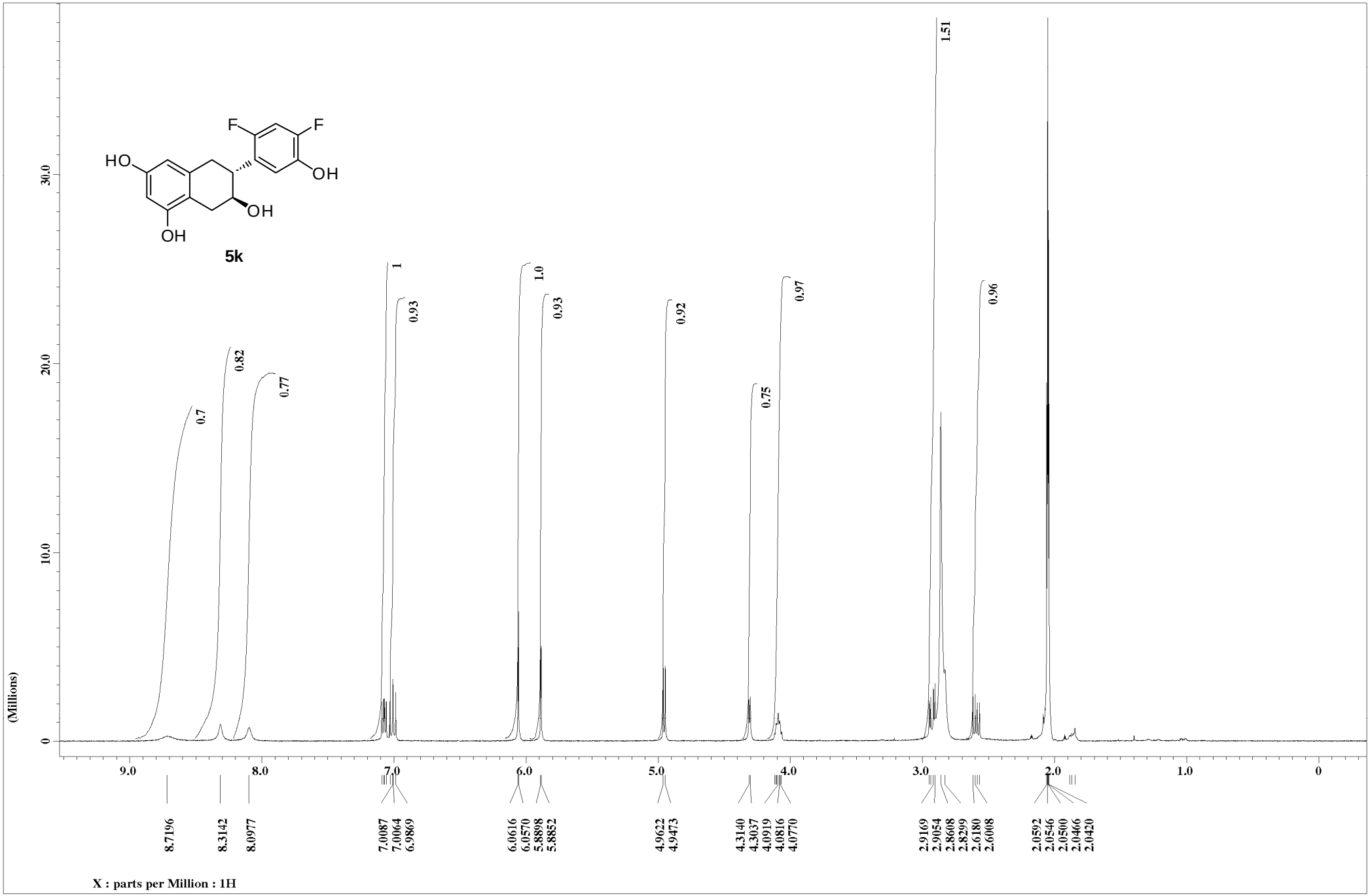

F
OH
+
NH3
Cl−
6j
(Millions)
500.0
400.0
300.0
200.0
100.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
153.0919
151.1842
146.3960
146.2910
134.4063
134.3776
120.9381
119.1258
119.1068
117.1991
49.5151
49.3434
49.1717
49.0000
48.8283
48.6661
48.4945
41.9607
33.8436
X : parts per Million : 13C

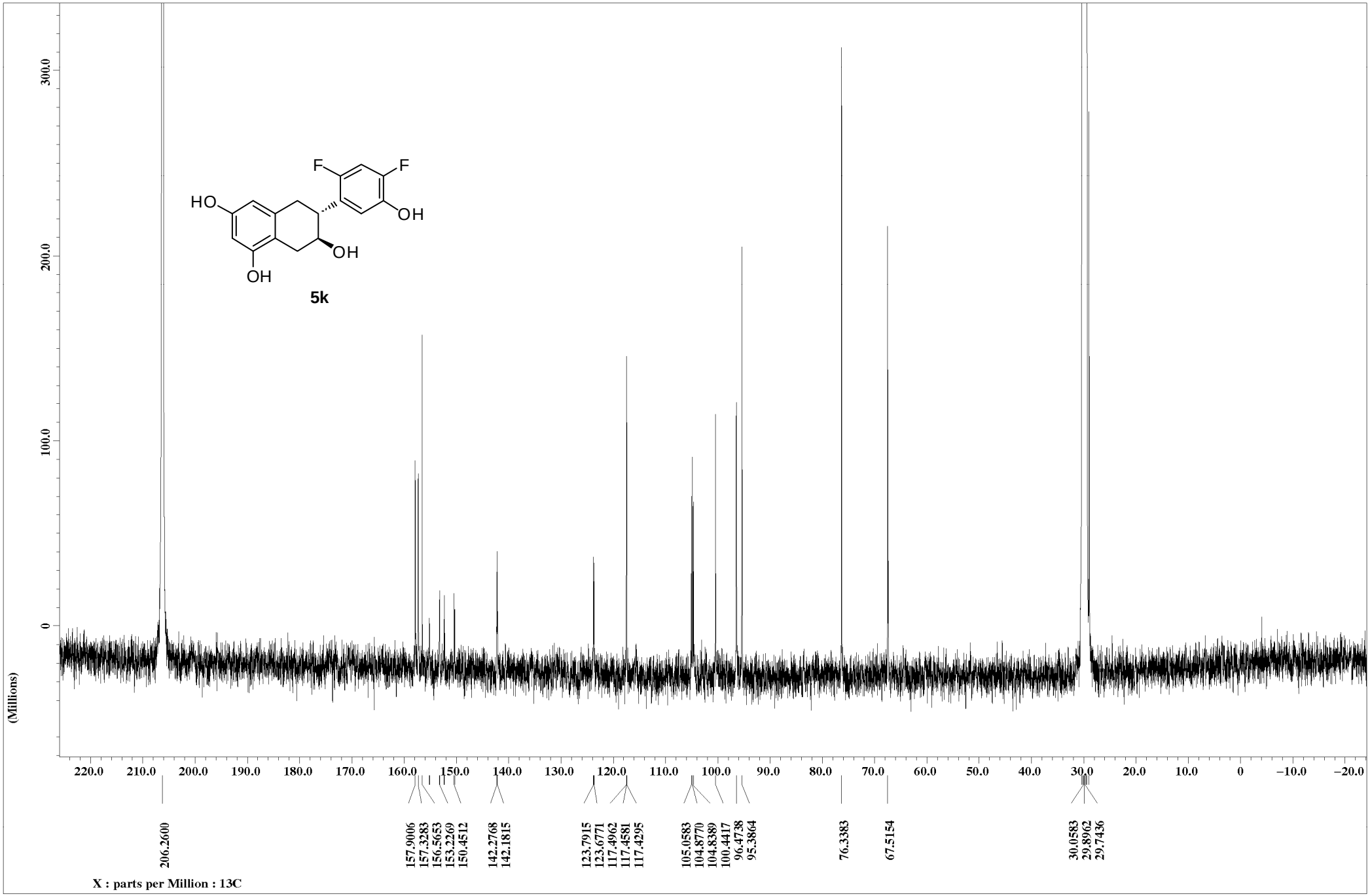

F
OH
+
NH3
Cl−
6j
(Millions)
19.0
18.0
17.0
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−140.0 −141.0 −142.0 −143.0 −144.0 −145.0 −146.0 −147.0 −148.0 −149.0 −150.0 −151.0 −152.0 −153.0 −154.0 −155.0 −156.0 −157.0 −158.0 −159.0 −160.0 −161.0 −162.0 −163.0 −164.0 −165.0 −166.0 −167.0
−141.3912
−164.9000
X : parts per Million : 19F

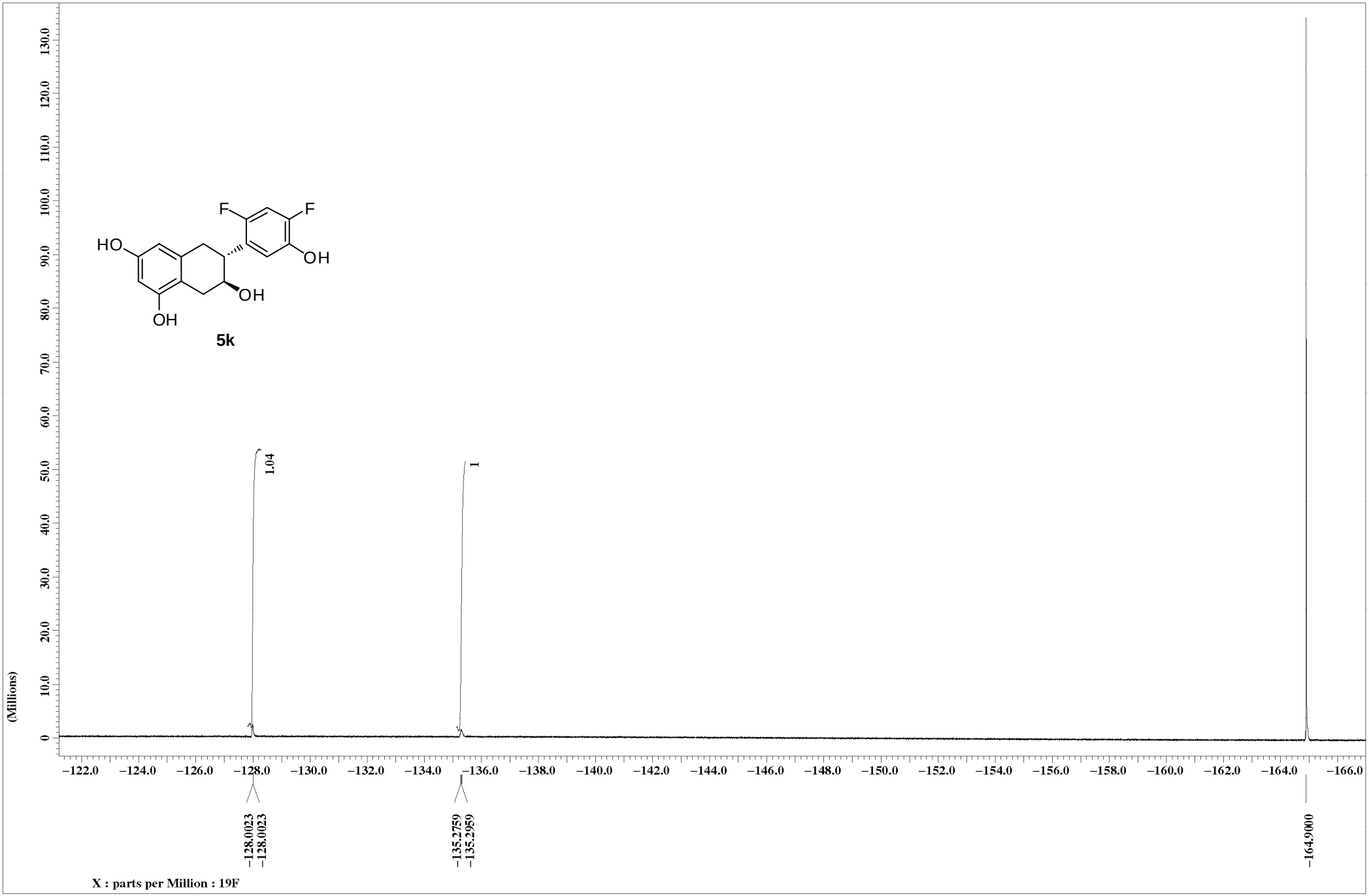

OH
F
+
NH3
Cl−
7j
20.0
10.0
0
(Millions)
1.95
0.95
2.0
2
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.0550
7.0333
6.9359
6.9210
5.0109
3.3790
3.3400
3.1763
3.1614
3.1454
2.9220
2.9072
2.8923
X : parts per Million : 1H

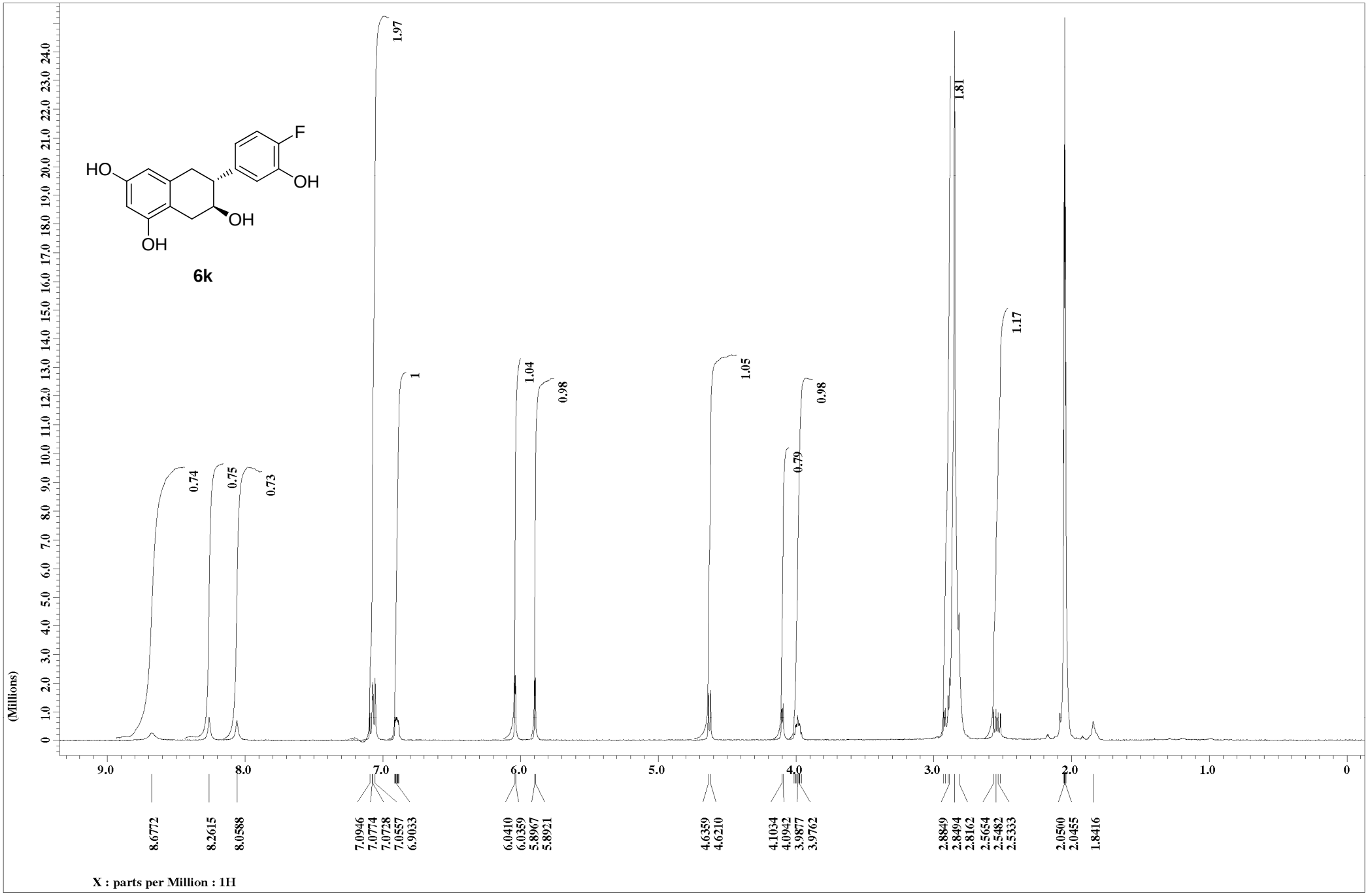

OH
F
+
NH3
Cl−
7j
(Millions)
600.0
500.0
400.0
300.0
200.0
100.0
0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
153.8550
151.9378
145.3372
145.2323
129.5131
129.4655
125.8886
125.8600
119.1163
119.0877
117.3327
117.1801
49.5151
49.3434
49.1717
49.0000
48.8283
48.6566
48.4945
41.9512
33.5193
X : parts per Million : 13C

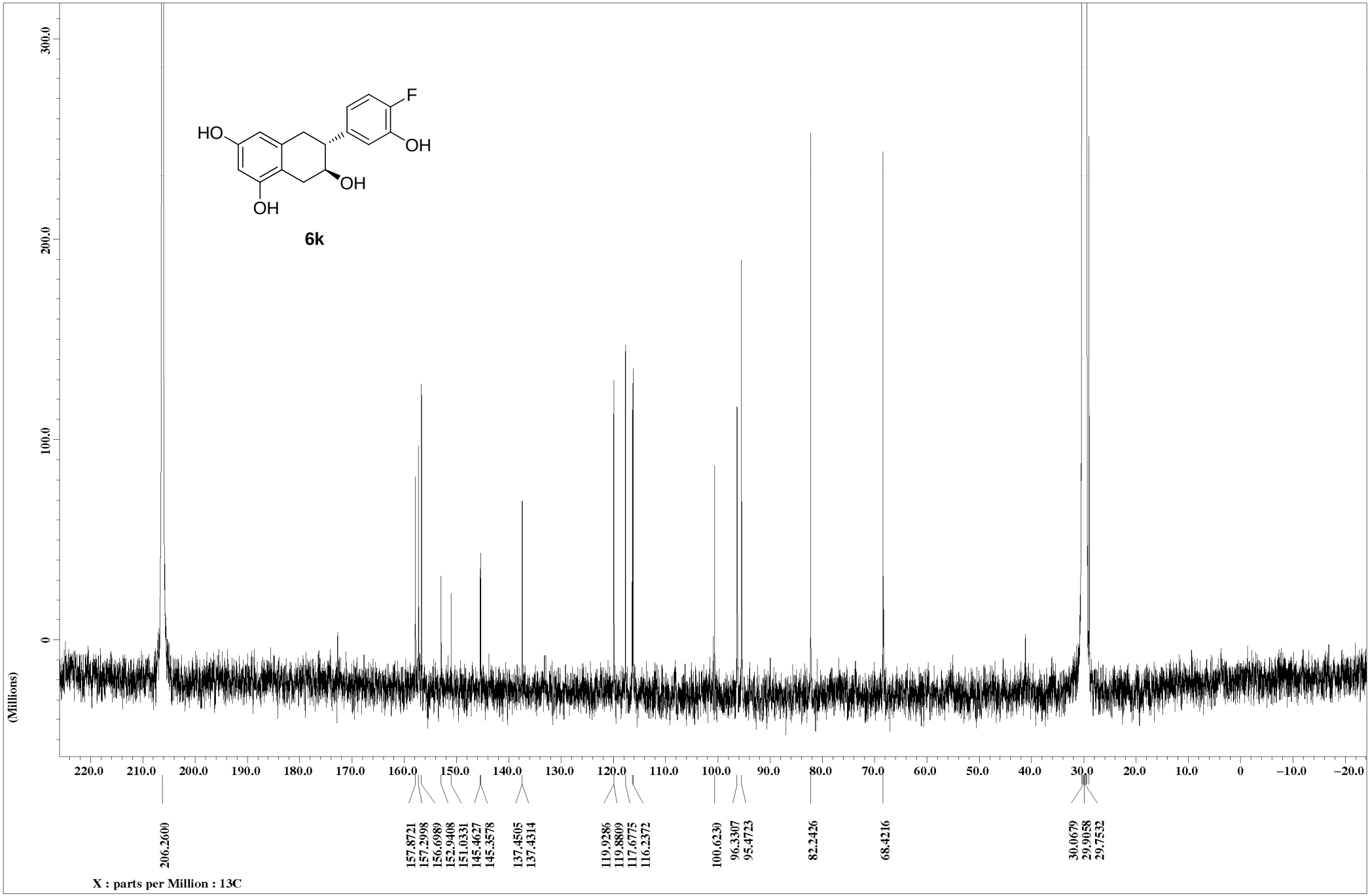

OH
F
+
NH3
Cl−
7j
(Millions)
19.0
18.0
17.0
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−137.0 −138.0 −139.0 −140.0 −141.0 −142.0 −143.0 −144.0 −145.0 −146.0 −147.0 −148.0 −149.0 −150.0 −151.0 −152.0 −153.0 −154.0 −155.0 −156.0 −157.0 −158.0 −159.0 −160.0 −161.0 −162.0 −163.0 −164.0 −165.0 −166.0 −167.0 −168.0
−138.3196
−164.9000
X : parts per Million : 19F

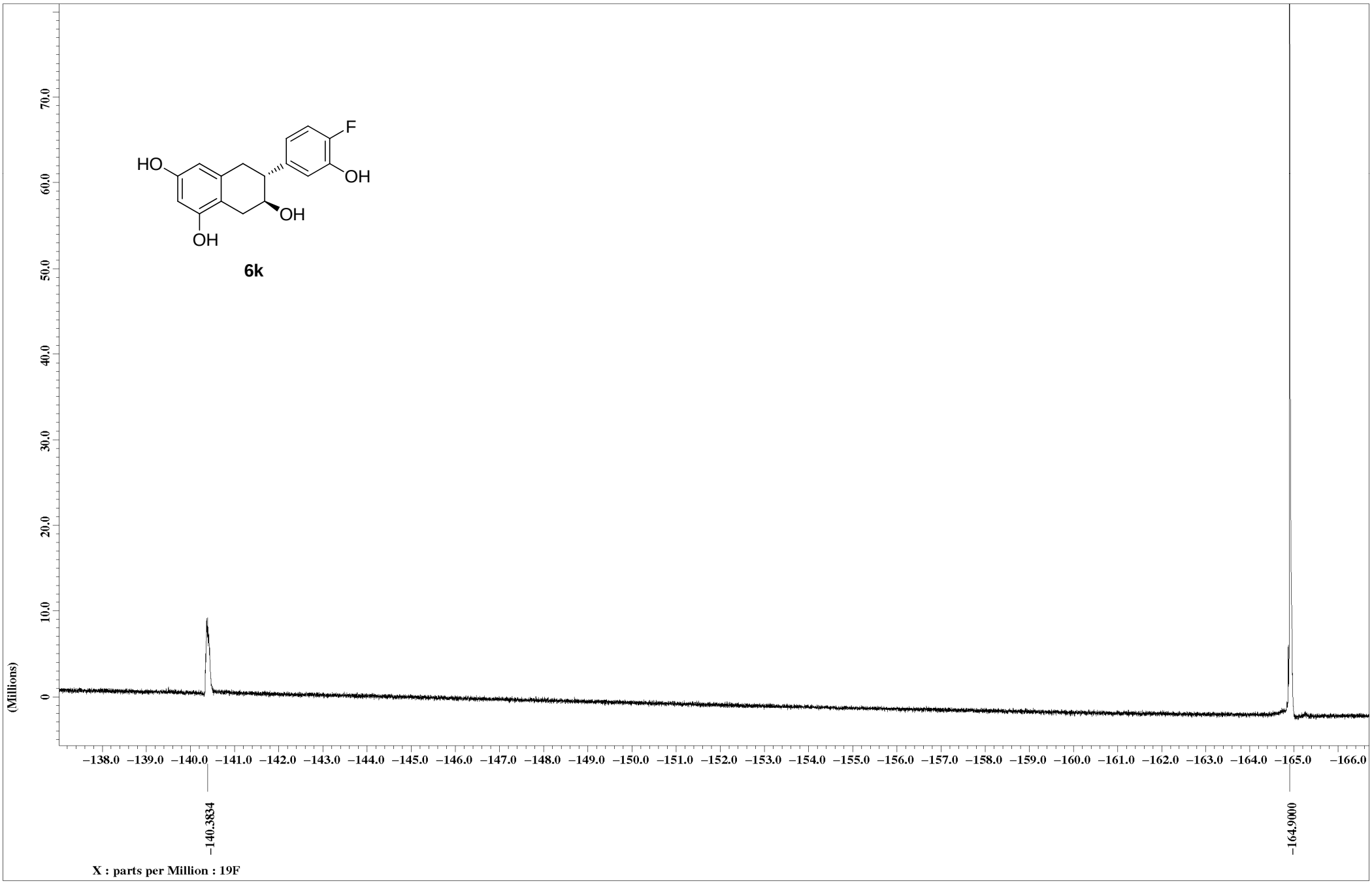

F
F
HO
OH
OH
OH
5k
(Millions)
30.0
20.0
10.0
0
0.7
0.82
0.77
1
0.93
1.0
0.93
0.92
0.75
0.97
1.51
0.96
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.7196
8.3142
8.0977
7.0087
7.0064
6.9869
6.0616
6.0570
5.8898
5.8852
4.9622
4.9473
4.3140
4.3037
4.0919
4.0816
4.0770
2.9169
2.9054
2.8608
2.8299
2.6180
2.6008
2.0592
2.0546
2.0500
2.0466
2.0420
X : parts per Million : 1H

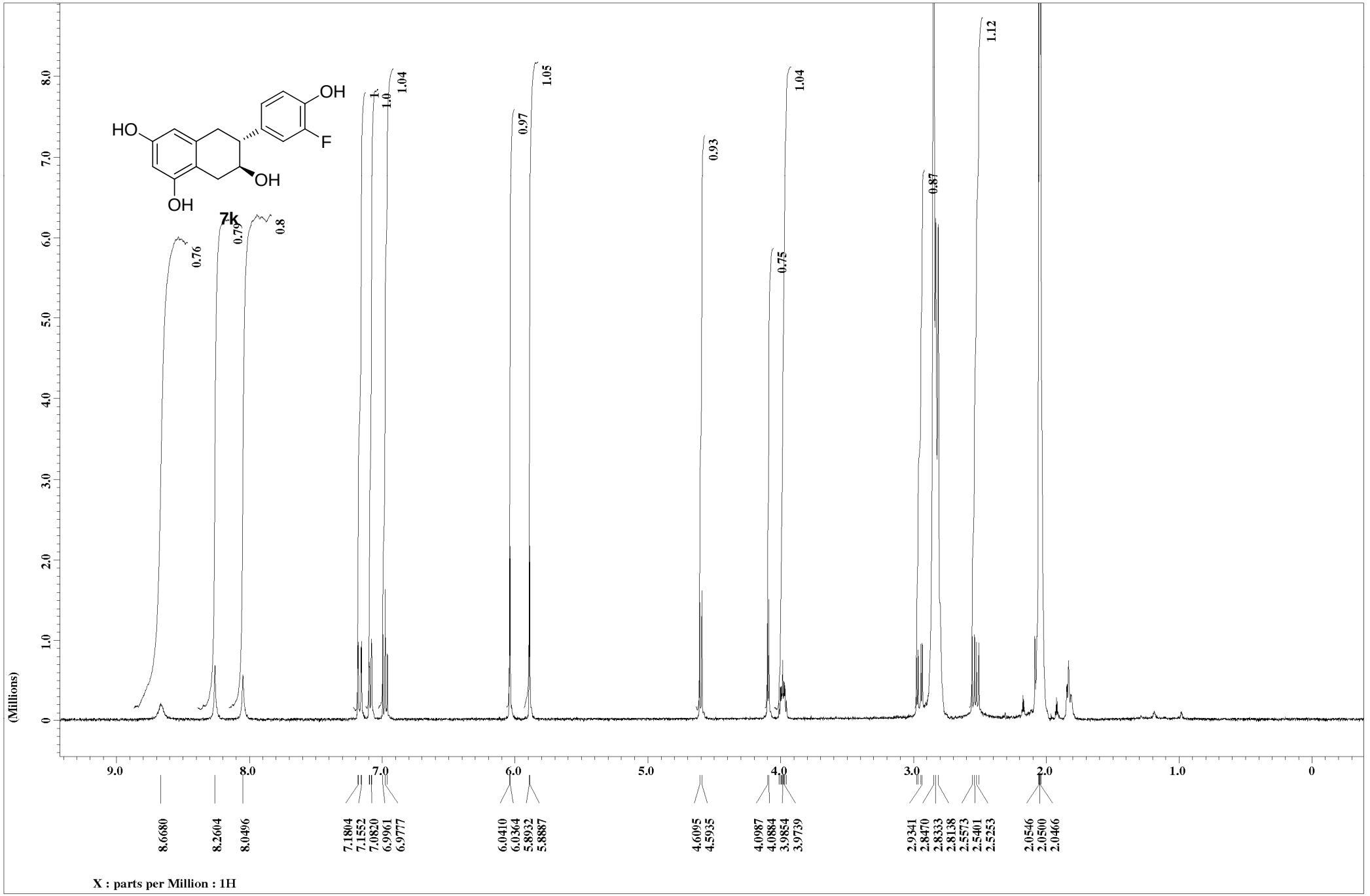

F
F
HO
OH
OH
OH
5k
300.0
200.0
100.0
0
(Millions)
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0 −20.0
206.2600
157.9006
157.3283
156.5653
153.2269
150.4512
142.2768
142.1815
123.7915
123.6771
117.4962
117.4581
117.4295
105.0583
104.8770
104.8389
100.4417
96.4738
95.3864
76.3383
67.5154
30.0583
29.8962
29.7436
X : parts per Million : 13C

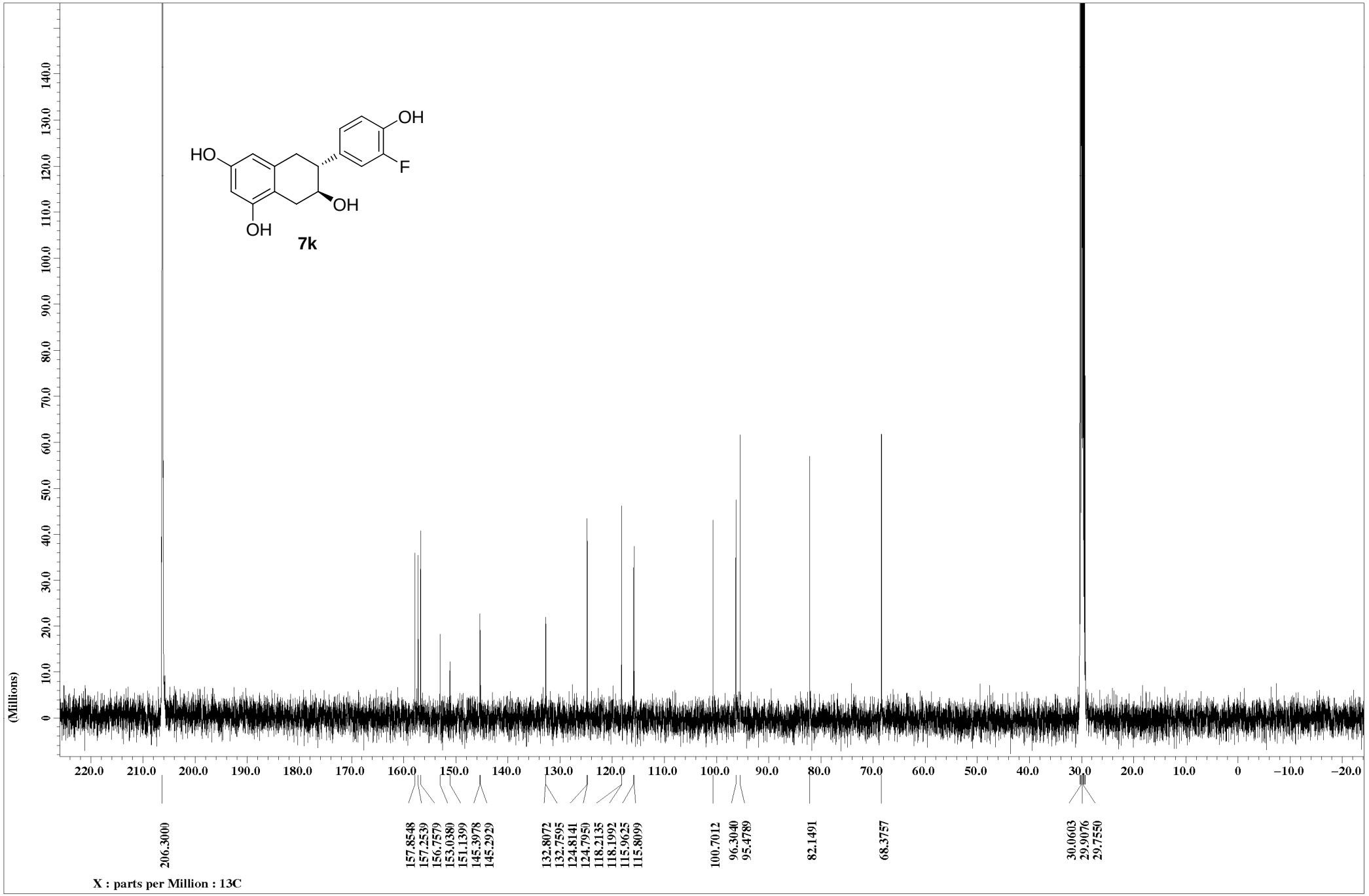

F
F
HO
OH
OH
OH
5k
1.04
1
(Millions)
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−122.0
−124.0
−126.0
−128.0
−130.0
−132.0
−134.0
−136.0
−138.0
−140.0
−142.0
−144.0
−146.0
−148.0
−150.0
−152.0
−154.0
−156.0
−158.0
−160.0
−162.0
−164.0
−166.0
−128.0023
−128.0023
−135.2759
−135.2959
−164.9000
X : parts per Million : 19F

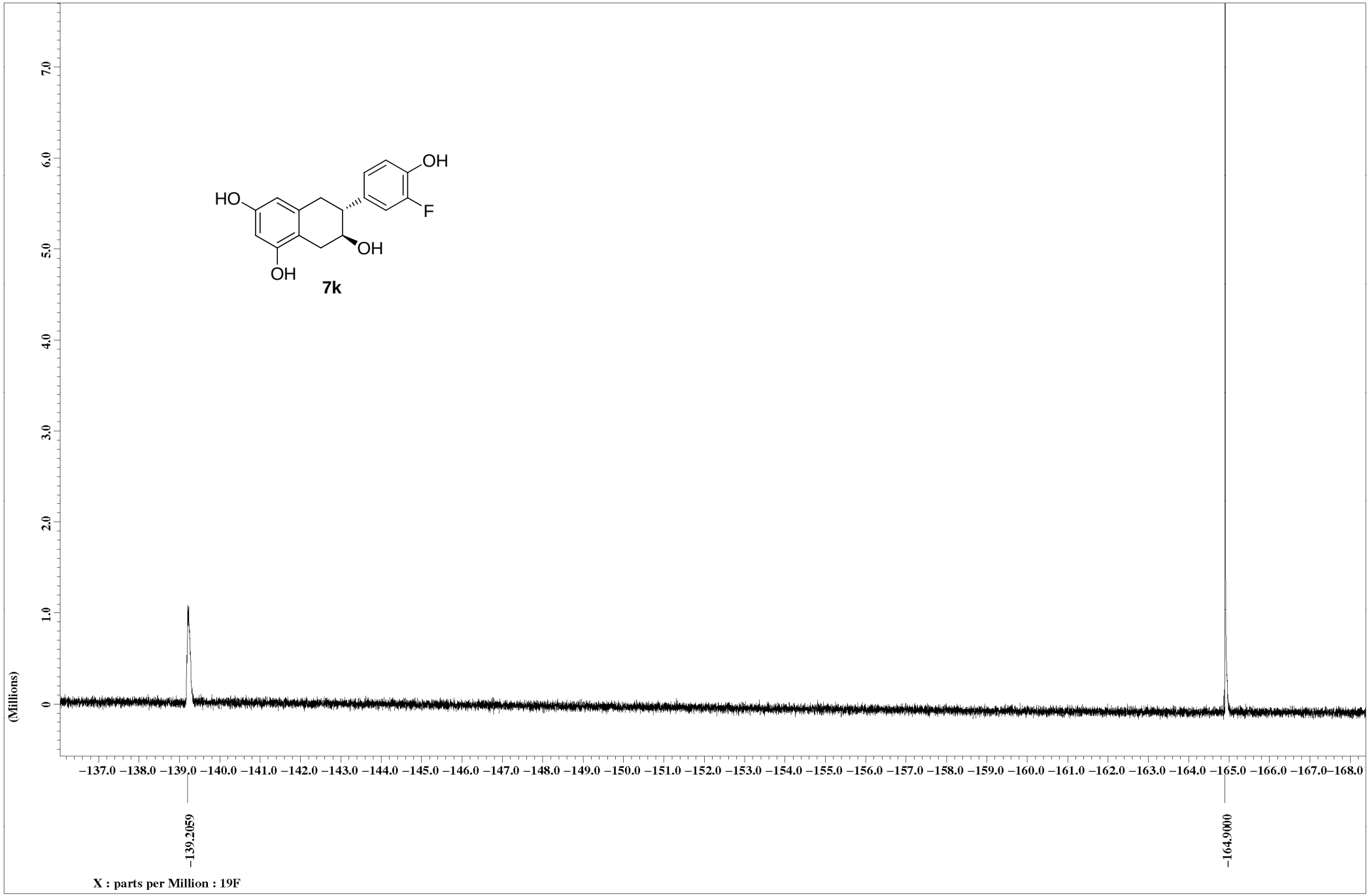

HO
F
OH
OH
OH
6k
(Millions)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0
0.74
0.75
0.73
1.97
1
1.04
0.98
1.05
0.79
0.98
1.81
1.17
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
8.6772
8.2615
8.0588
7.0946
7.0774
7.0728
7.0557
6.9033
6.0410
6.0359
5.8967
5.8921
4.6359
4.6210
4.1034
4.0942
3.9877
3.9762
2.8849
2.8494
2.8162
2.5654
2.5482
2.5333
2.0500
2.0455
1.8416
X : parts per Million : 1H

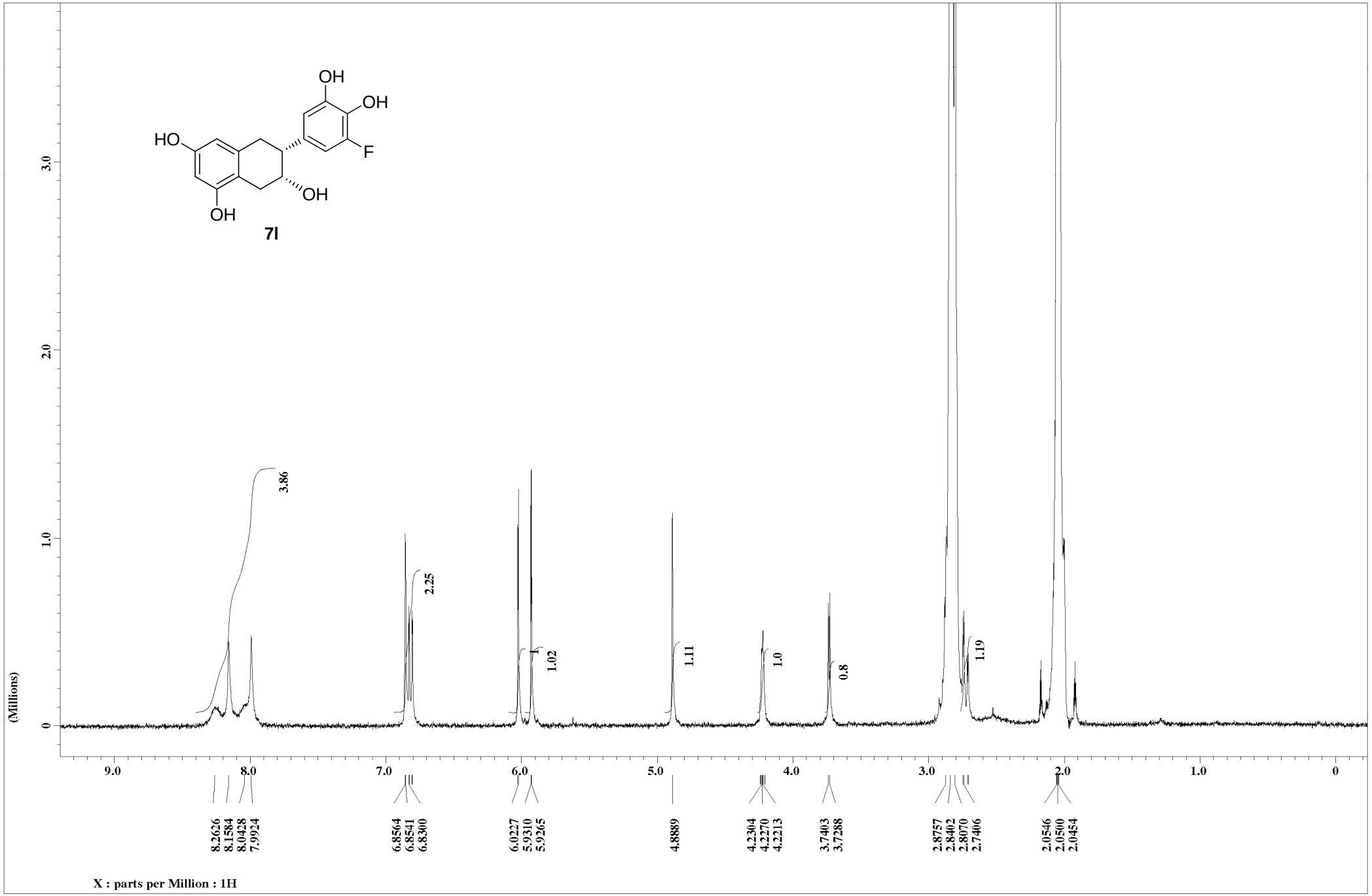

HO
F
OH
OH
OH
6k
300.0
200.0
100.0
0
(Millions)
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0 −20.0
206.2600
157.8721
157.2998
156.6989
152.9408
151.0331
145.4627
145.3578
137.4505
137.4314
119.9286
119.8809
117.6775
116.2372
100.6230
96.3307
95.4723
82.2426
68.4216
30.0679
29.9058
29.7532
X : parts per Million : 13C

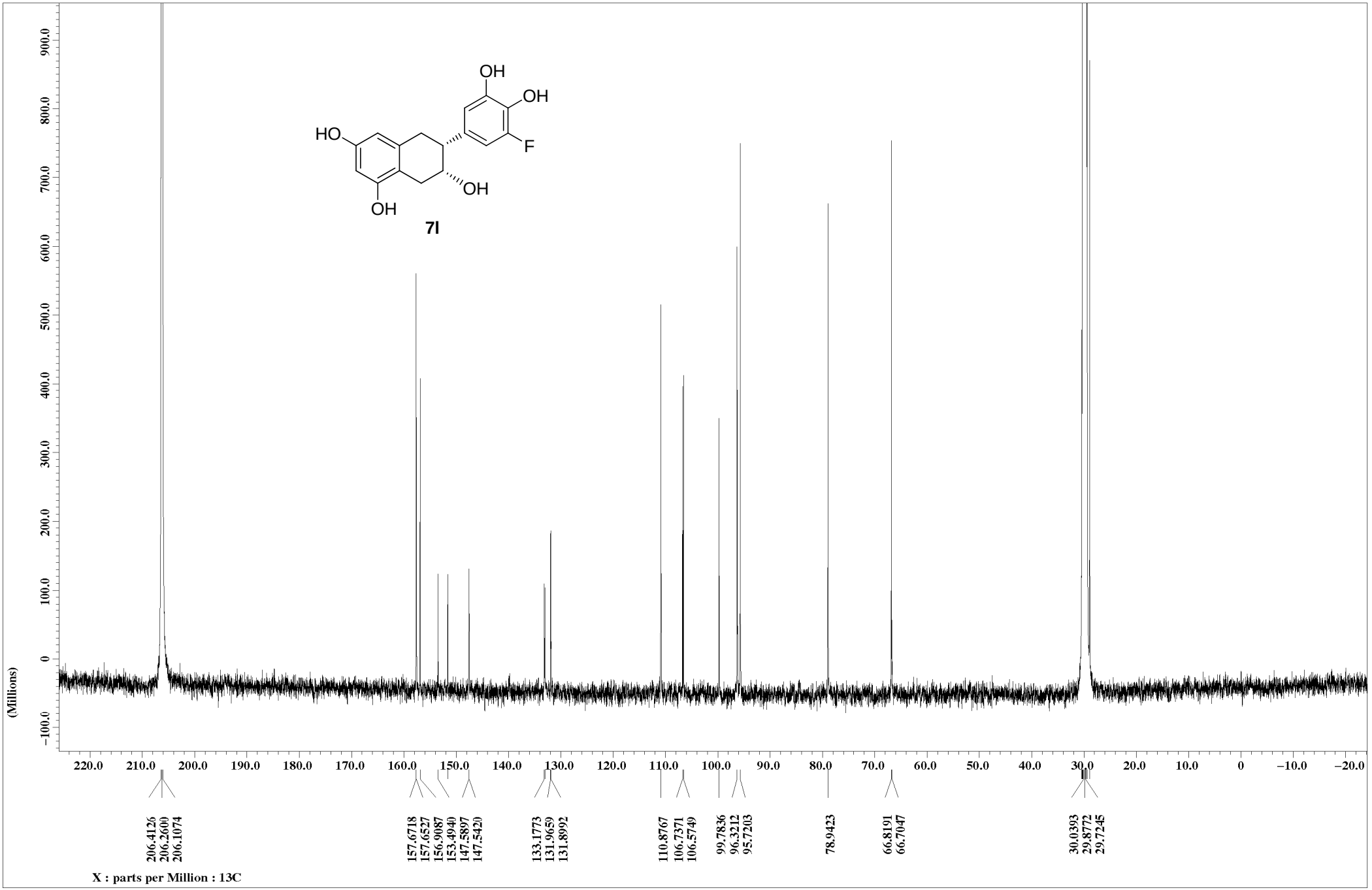

HO
F
OH
OH
OH
6k
(Millions)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−138.0 −139.0 −140.0 −141.0 −142.0 −143.0 −144.0 −145.0 −146.0 −147.0 −148.0 −149.0 −150.0 −151.0 −152.0 −153.0 −154.0 −155.0 −156.0 −157.0 −158.0 −159.0 −160.0 −161.0 −162.0 −163.0 −164.0 −165.0 −166.0
−140.3834
−164.9000
X : parts per Million : 19F

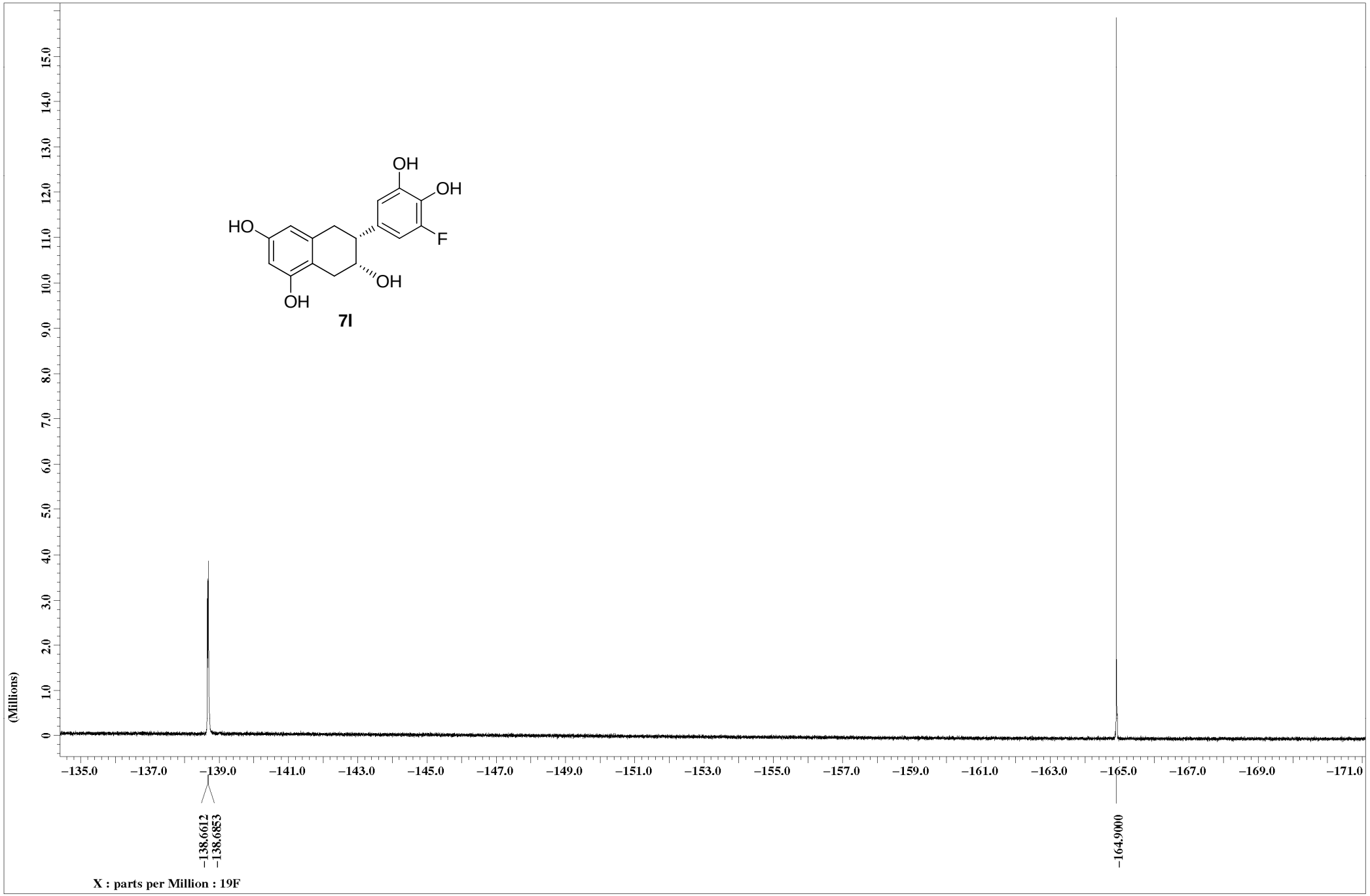

HO
OH
F
OH
OH
7k
0.76
0.79
0.8
1.0
1.04
0.97
1.05
0.93
0.75
1.04
0.87
1.12
(Millions)
8.6680
8.2604
8.0496
7.1804
7.1552
7.0820
6.9961
6.9777
6.0410
6.0364
5.8932
5.8887
4.6095
4.5935
4.0987
4.0884
3.9854
3.9739
2.9341
2.8470
2.8333
2.8138
2.5573
2.5401
2.5253
2.0546
2.0500
2.0466
X : parts per Million : 1H

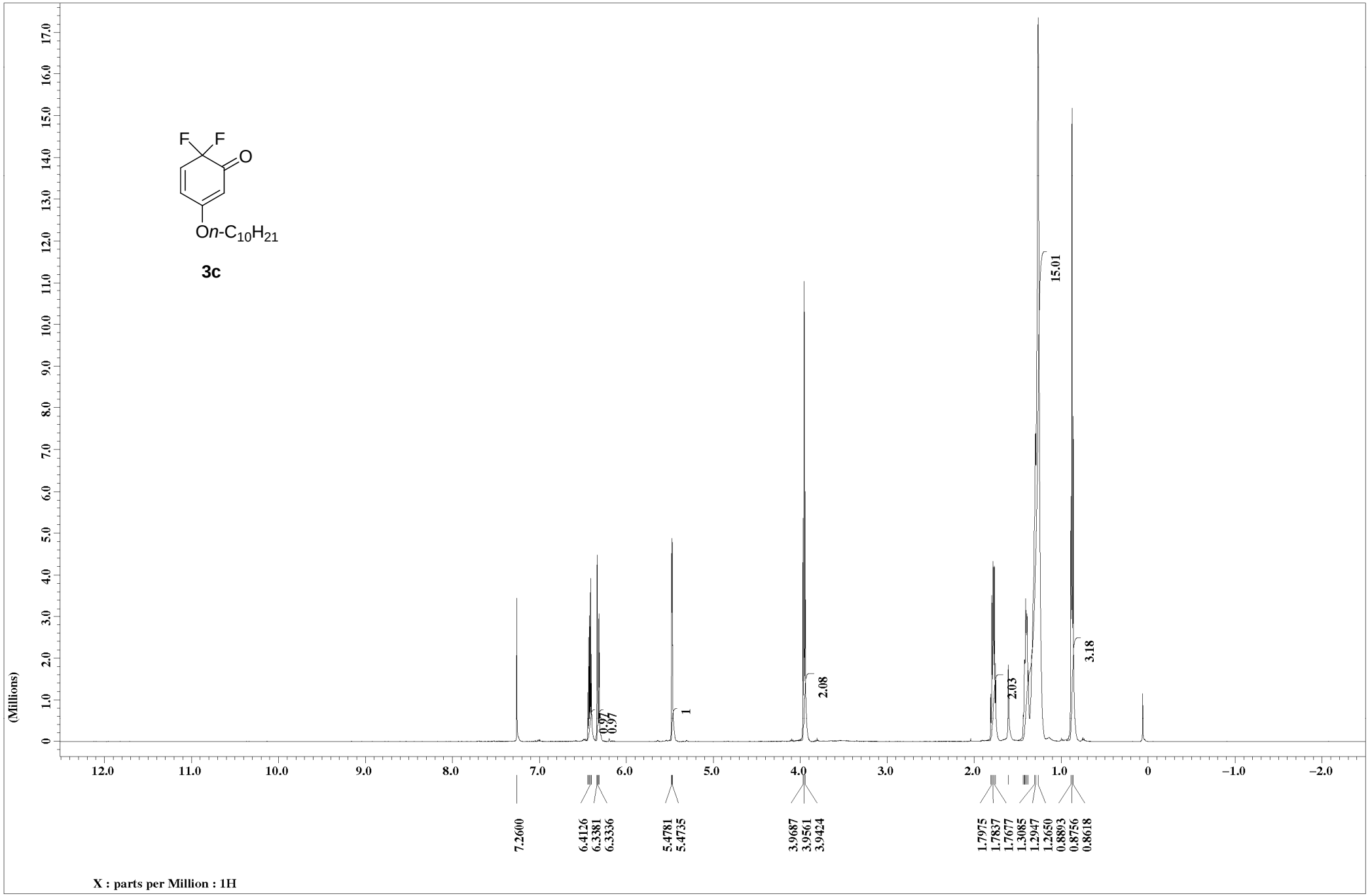

HO
OH
F
OH
OH
7k
(Millions)
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
−20.0
206.3000
157.8548
157.2539
156.7579
153.0380
151.1399
145.3978
145.2929
132.8072
132.7595
124.8141
124.7950
118.2135
118.1992
115.9625
115.8099
100.7012
96.3040
95.4789
82.1491
68.3757
30.0603
29.9076
29.7550
X : parts per Million : 13C

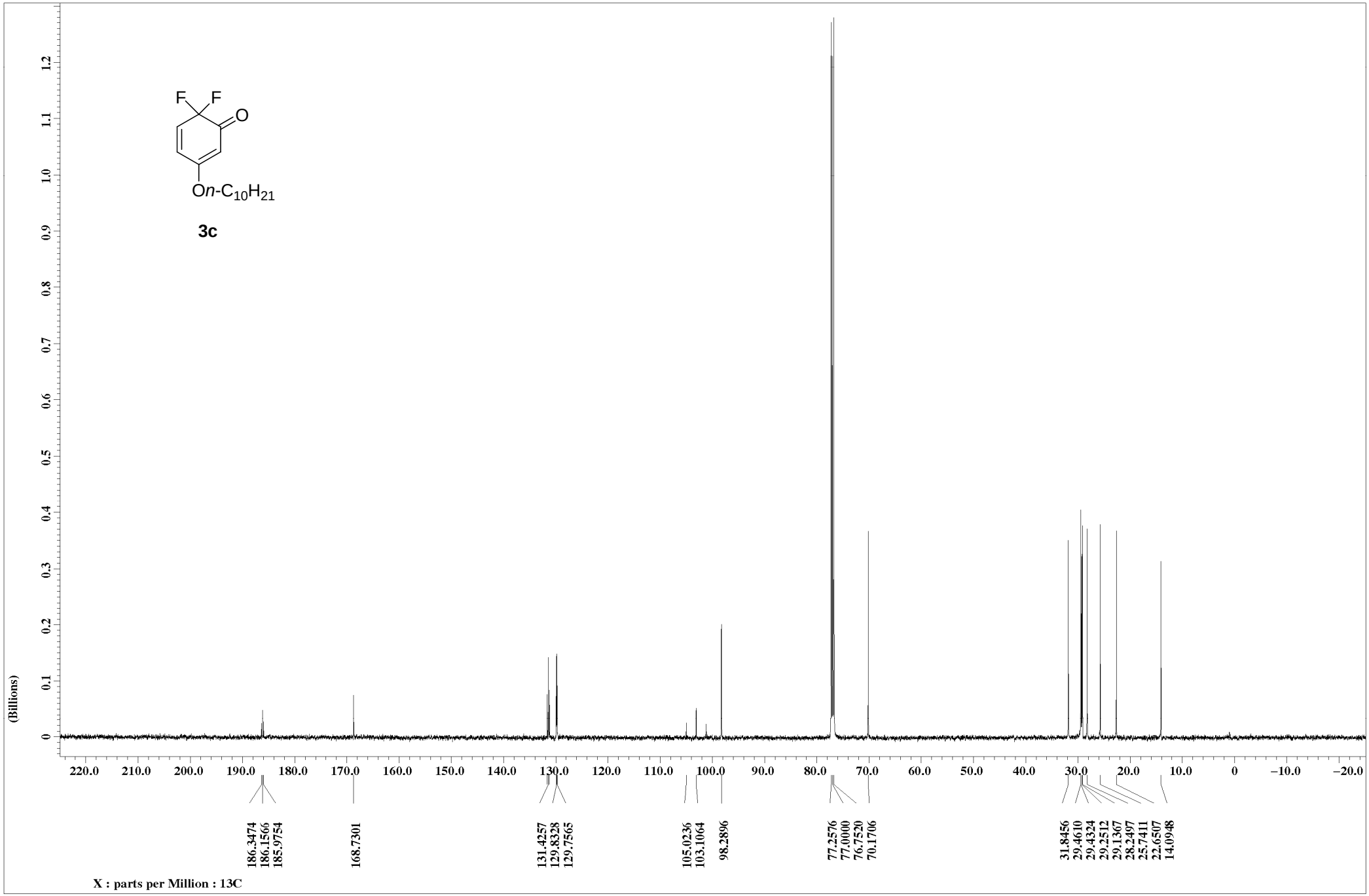

HO
OH
F
OH
OH
7k
(Millions)
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−137.0 −138.0 −139.0 −140.0 −141.0 −142.0 −143.0 −144.0 −145.0 −146.0 −147.0 −148.0 −149.0 −150.0 −151.0 −152.0 −153.0 −154.0 −155.0 −156.0 −157.0 −158.0 −159.0 −160.0 −161.0 −162.0 −163.0 −164.0 −165.0 −166.0 −167.0 −168.0
−139.2059
−164.9000
X : parts per Million : 19F

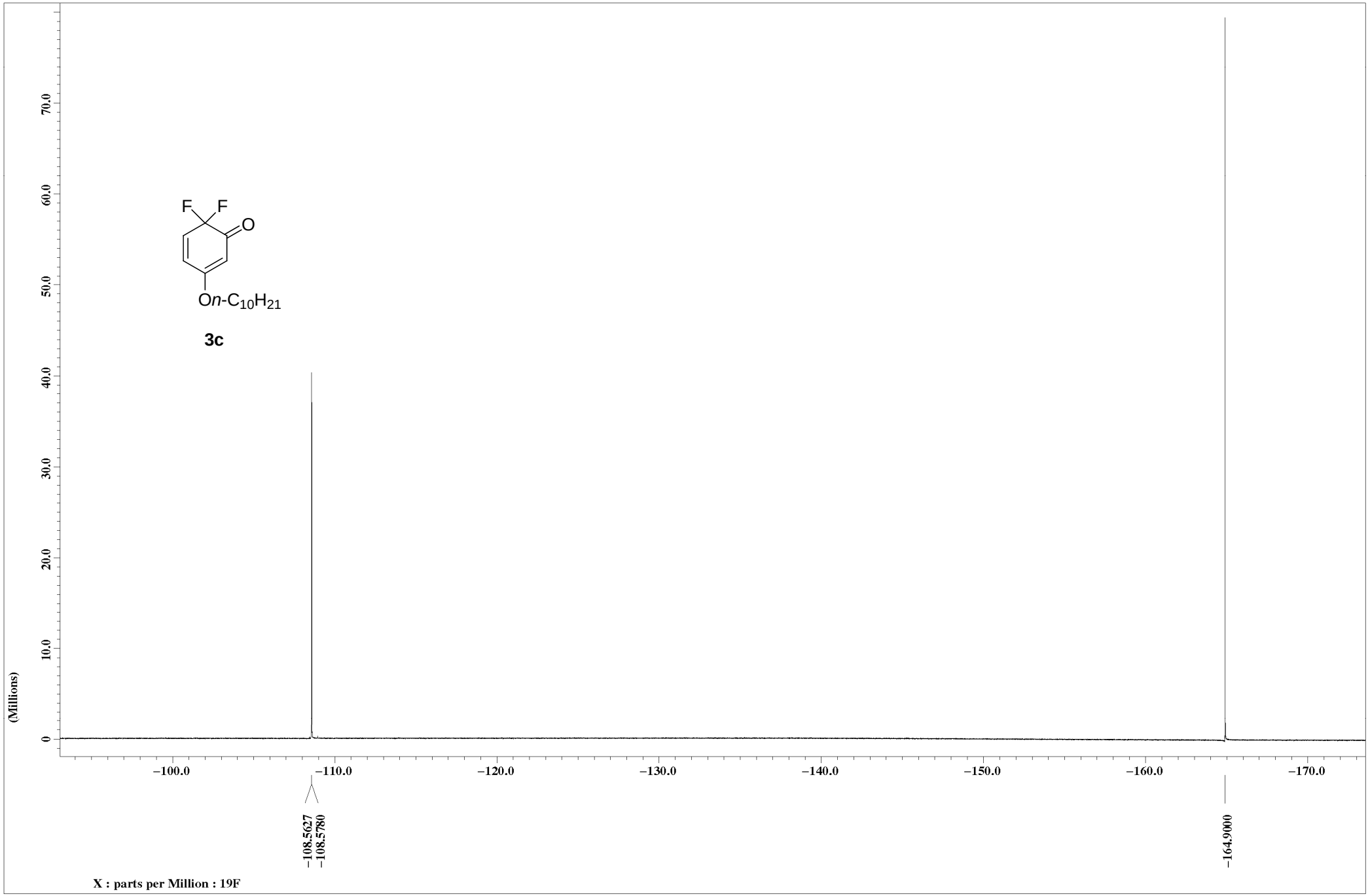

OH
OH
HO
F
OH
OH
7l
3.86
2.25
1.02
1.11
1.0
0.8
1.19
(Millions)
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.2626
8.1584
8.0428
7.9924
6.8564
6.8541
6.8300
6.0227
5.9310
5.9265
4.8889
4.2304
4.2270
4.2213
3.7403
3.7288
2.8757
2.8402
2.8070
2.7406
2.0546
2.0500
2.0454
X : parts per Million : 1H

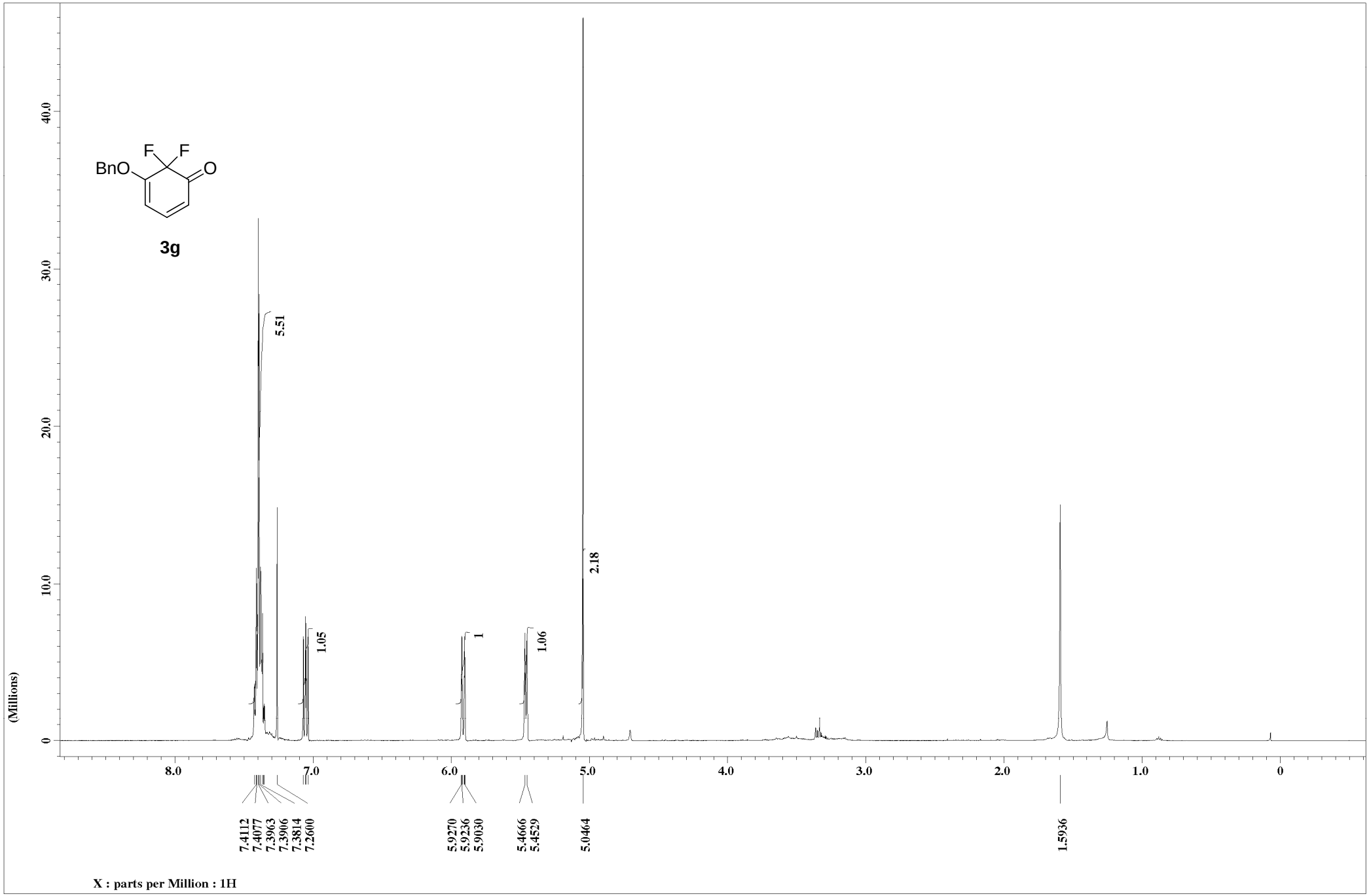

OH
OH
HO
F
OH
OH
7l
(Millions)
900.0
800.0
700.0
600.0
500.0
400.0
300.0
200.0
100.0
0
−100.0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
−20.0
206.4126
206.2600
206.1074
157.6718
157.6527
156.9087
153.4940
147.5897
147.5420
133.1773
131.9659
131.8992
110.8767
106.7371
106.5749
99.7836
96.3212
95.7203
78.9423
66.8191
66.7047
30.0393
29.8772
29.7245
X : parts per Million : 13C

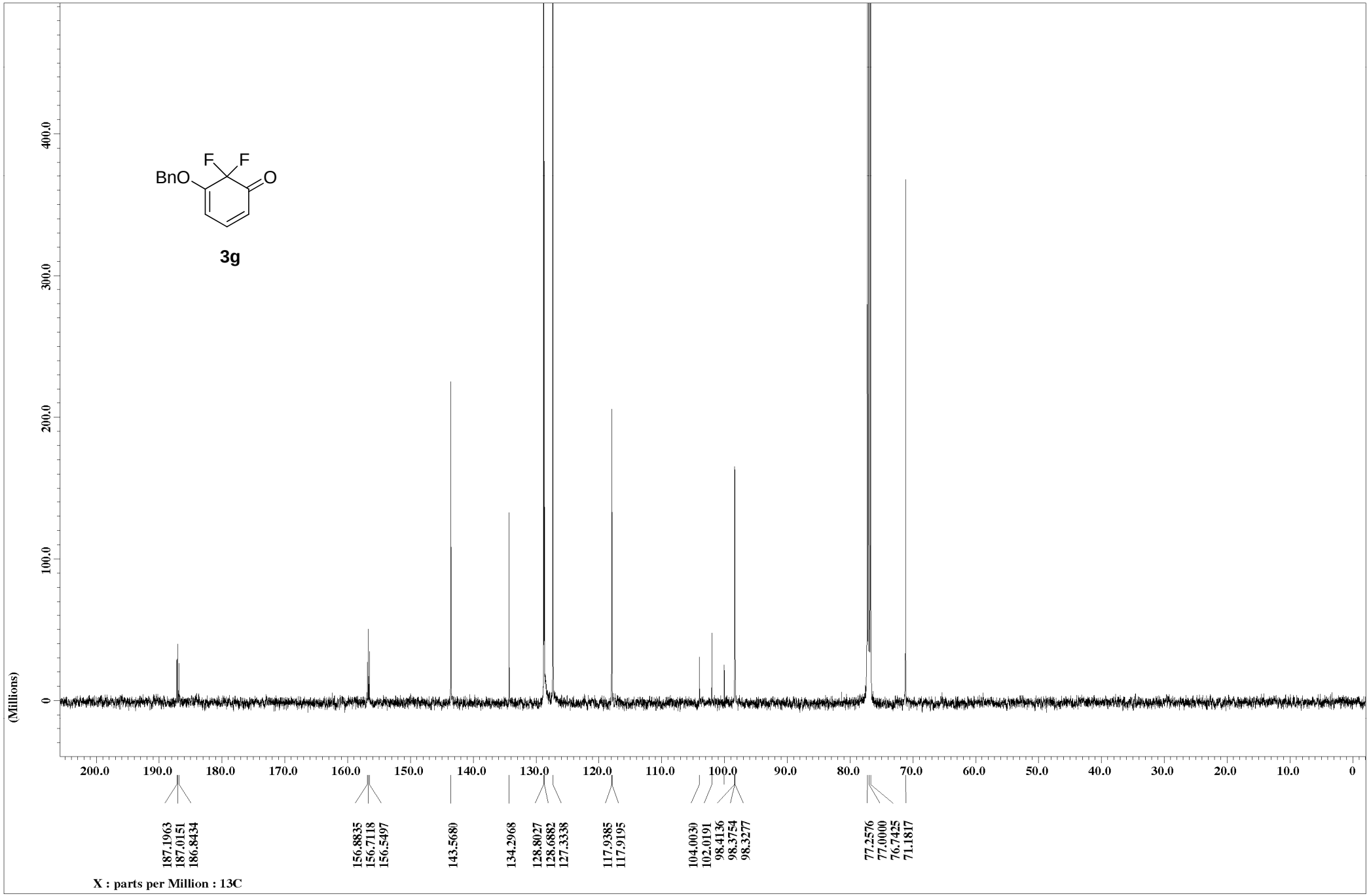

OH
OH
HO
F
OH
OH
7l
(Millions)
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−135.0
−137.0
−139.0
−141.0
−143.0
−145.0
−147.0
−149.0
−151.0
−153.0
−155.0
−157.0
−159.0
−161.0
−163.0
−165.0
−167.0
−169.0
−171.0
−138.6612
−138.6853
−164.9000
X : parts per Million : 19F


F
F
O
On-C10H21
3c
(Millions)
17.0
16.0
15.0
14.0
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
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
−1.0
−2.0
15.01
3.18
2.08
2.03
1
0.97
0.97
7.2600
6.4126
6.3381
6.3336
5.4781
5.4735
3.9687
3.9561
3.9424
1.7975
1.7837
1.7677
1.3085
1.2947
1.2650
0.8893
0.8756
0.8618
X : parts per Million : 1H


F
F
O
On-C10H21
3c
(Billions)
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
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
186.3474
186.1566
185.9754
168.7301
131.4257
129.8328
129.7565
105.0236
103.1064
98.2896
77.2576
77.0000
76.7520
70.1706
31.8456
29.4610
29.4324
29.2512
29.1367
28.2497
25.7411
22.6507
14.0948
X : parts per Million : 13C

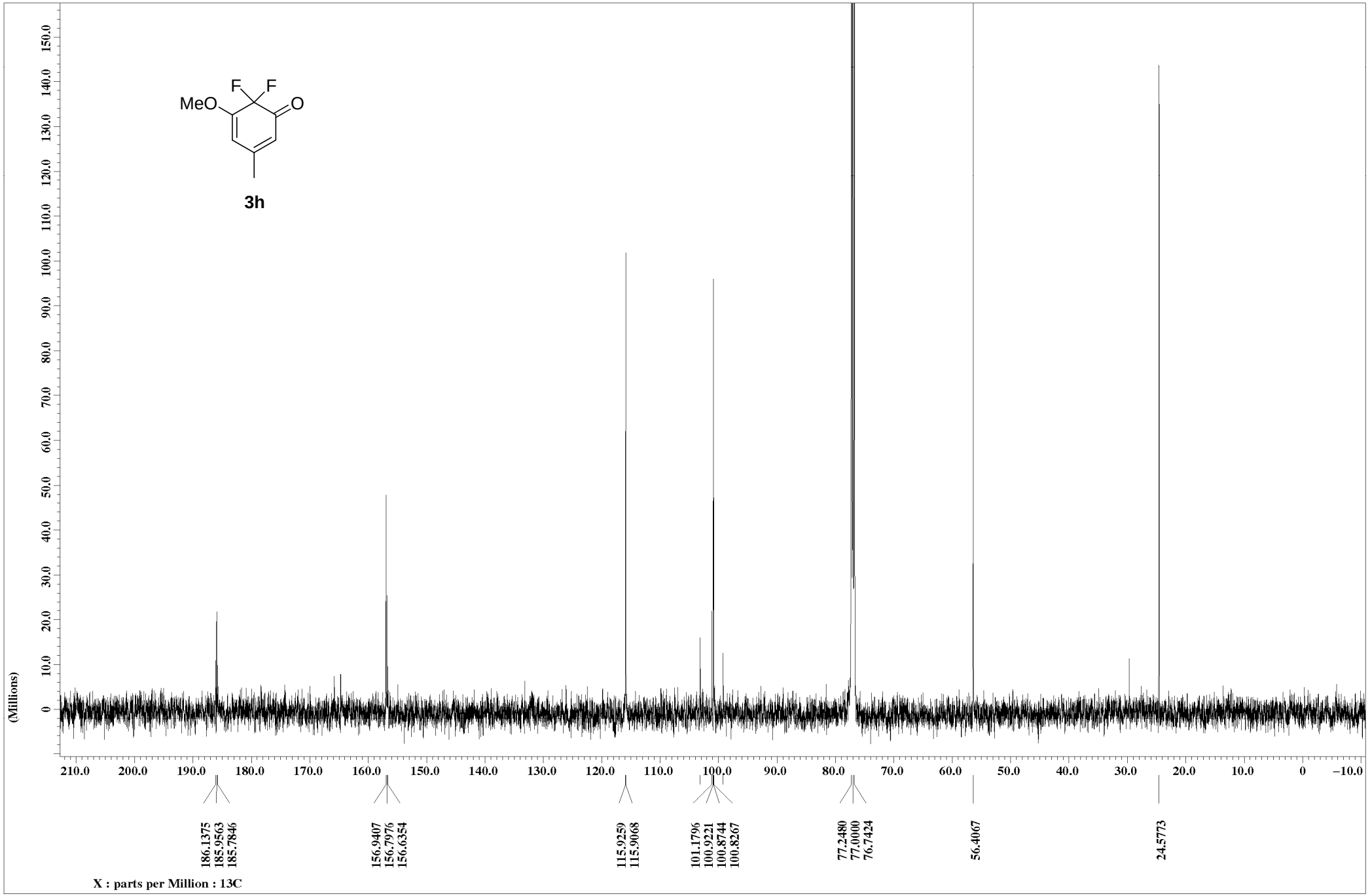

F
F
O
On-C10H21
3c
(Millions)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−100.0
−110.0
−120.0
−130.0
−140.0
−150.0
−160.0
−170.0
−108.5627
−108.5780
−164.9000
X : parts per Million : 19F

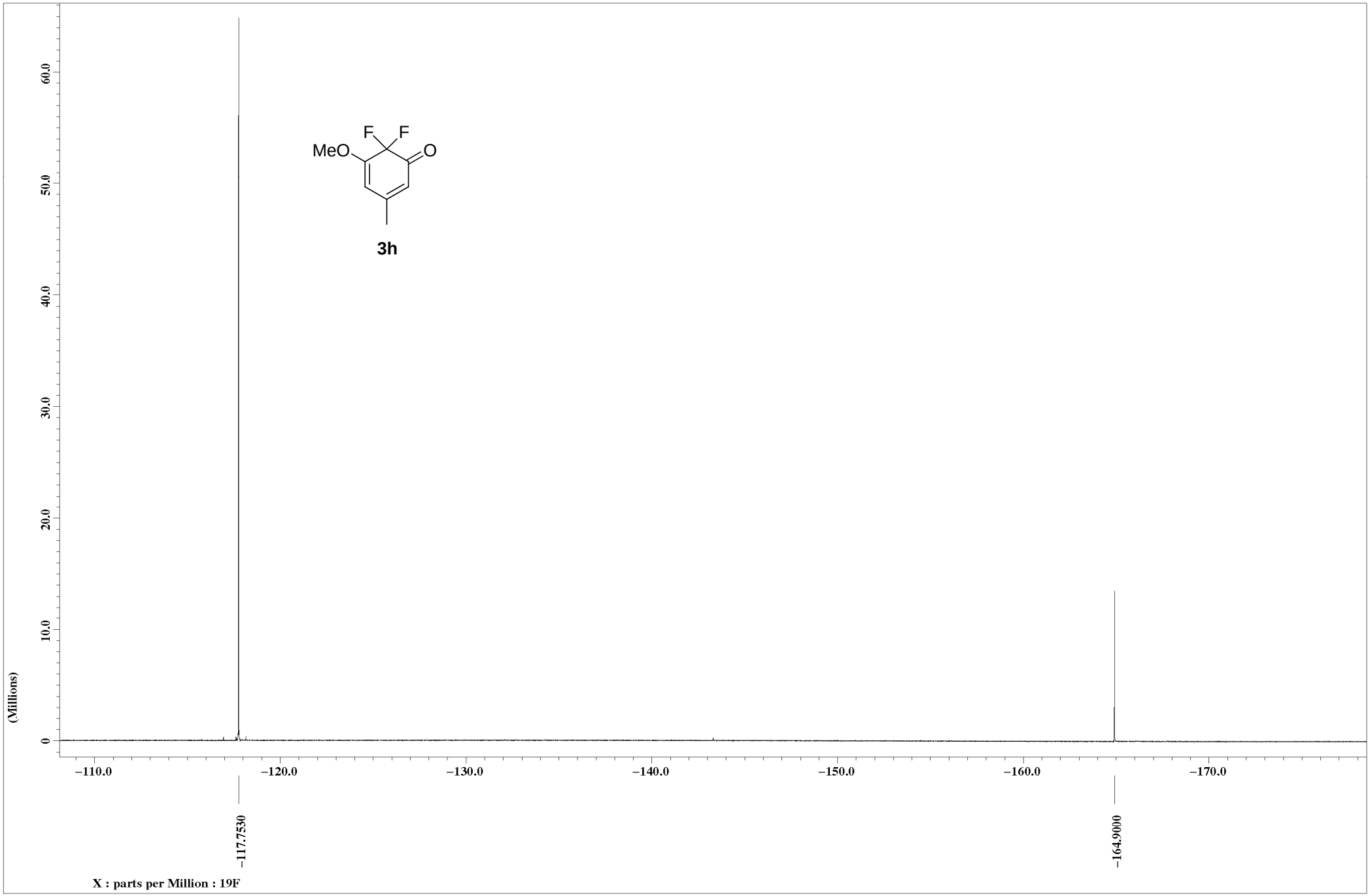

F
F
BnO
O
3g
40.0
30.0
20.0
10.0
0
(Millions)
5.51
1.05
1
1.06
2.18
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.4112
7.4077
7.3963
7.3906
7.3814
7.2600
5.9270
5.9236
5.9030
5.4666
5.4529
5.0464
1.5936
X : parts per Million : 1H

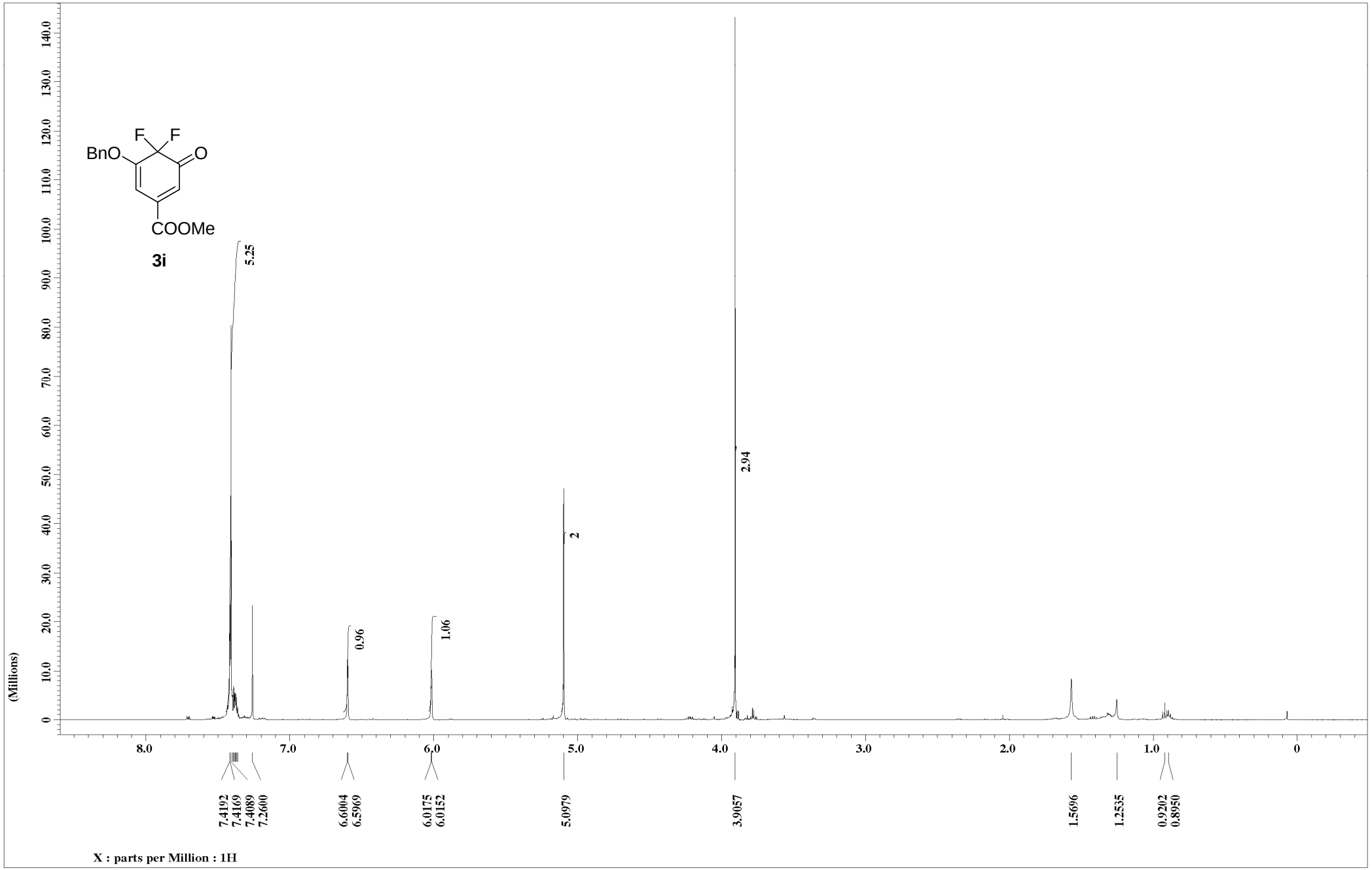

F
F
BnO
O
3g
(Millions)
400.0
300.0
200.0
100.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
187.1963
187.0151
186.8434
156.8835
156.7118
156.5497
143.5680
134.2968
128.8027
128.6882
127.3338
117.9385
117.9195
104.0030
102.0191
98.4136
98.3754
98.3277
77.2576
77.0000
76.7425
71.1817
X : parts per Million : 13C

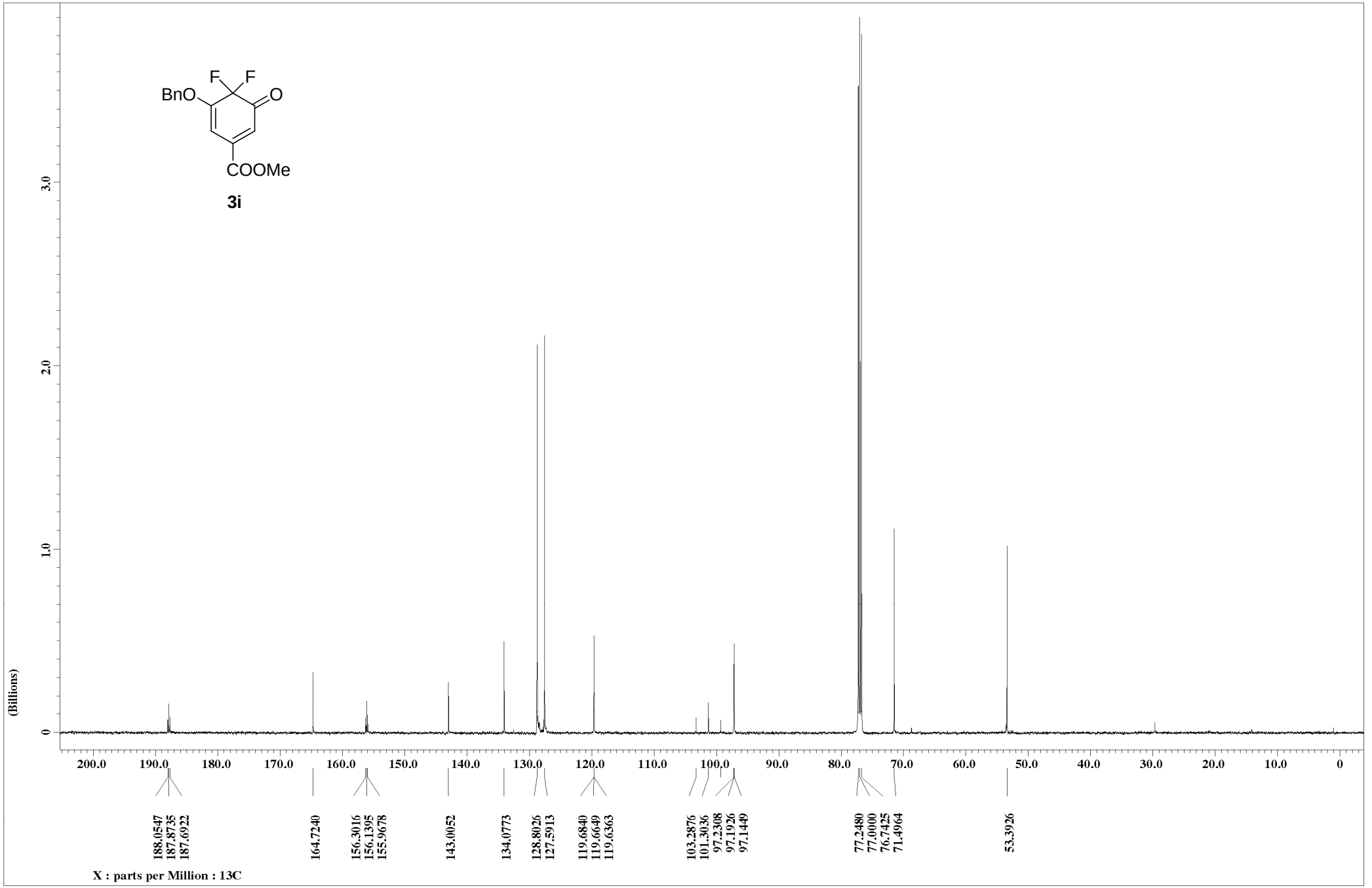

F
F
BnO
O
3g
(Millions)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−110.0
−120.0
−130.0
−140.0
−150.0
−160.0
−170.0
−117.1921
−164.9000
X : parts per Million : 19F

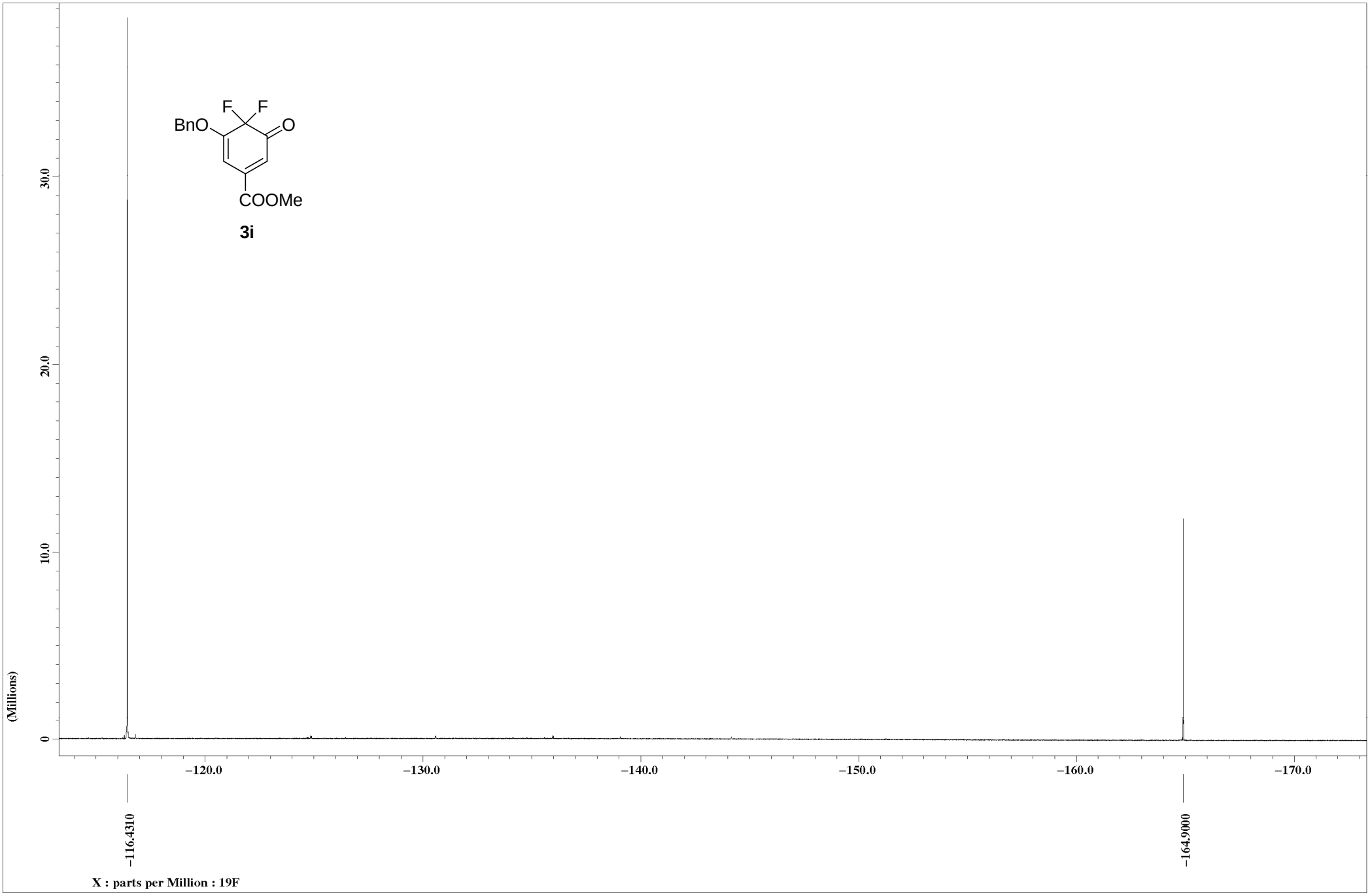

F
F
MeO
O
3h
(Millions)
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
2.86
3
0.92
0.94
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2600
5.7919
5.7873
5.7850
5.2708
5.2674
5.2639
5.2605
3.8233
2.1296
1.2501
X : parts per Million : 1H

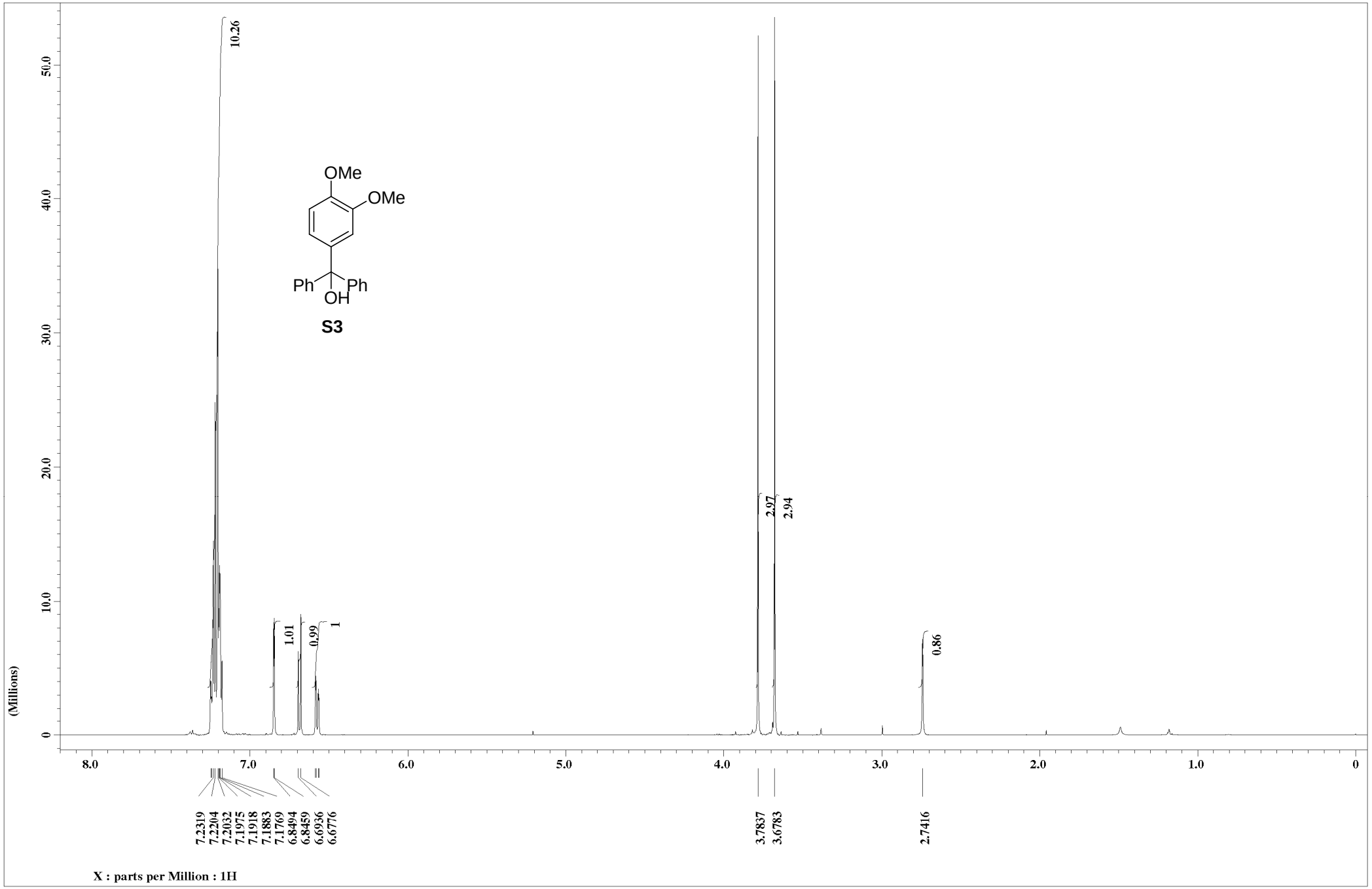

F
F
MeO
O
3h
(Millions)
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
186.1375
185.9563
185.7846
156.9407
156.7976
156.6354
115.9259
115.9068
101.1796
100.9221
100.8744
100.8267
77.2480
77.0000
76.7424
56.4067
24.5773
X : parts per Million : 13C

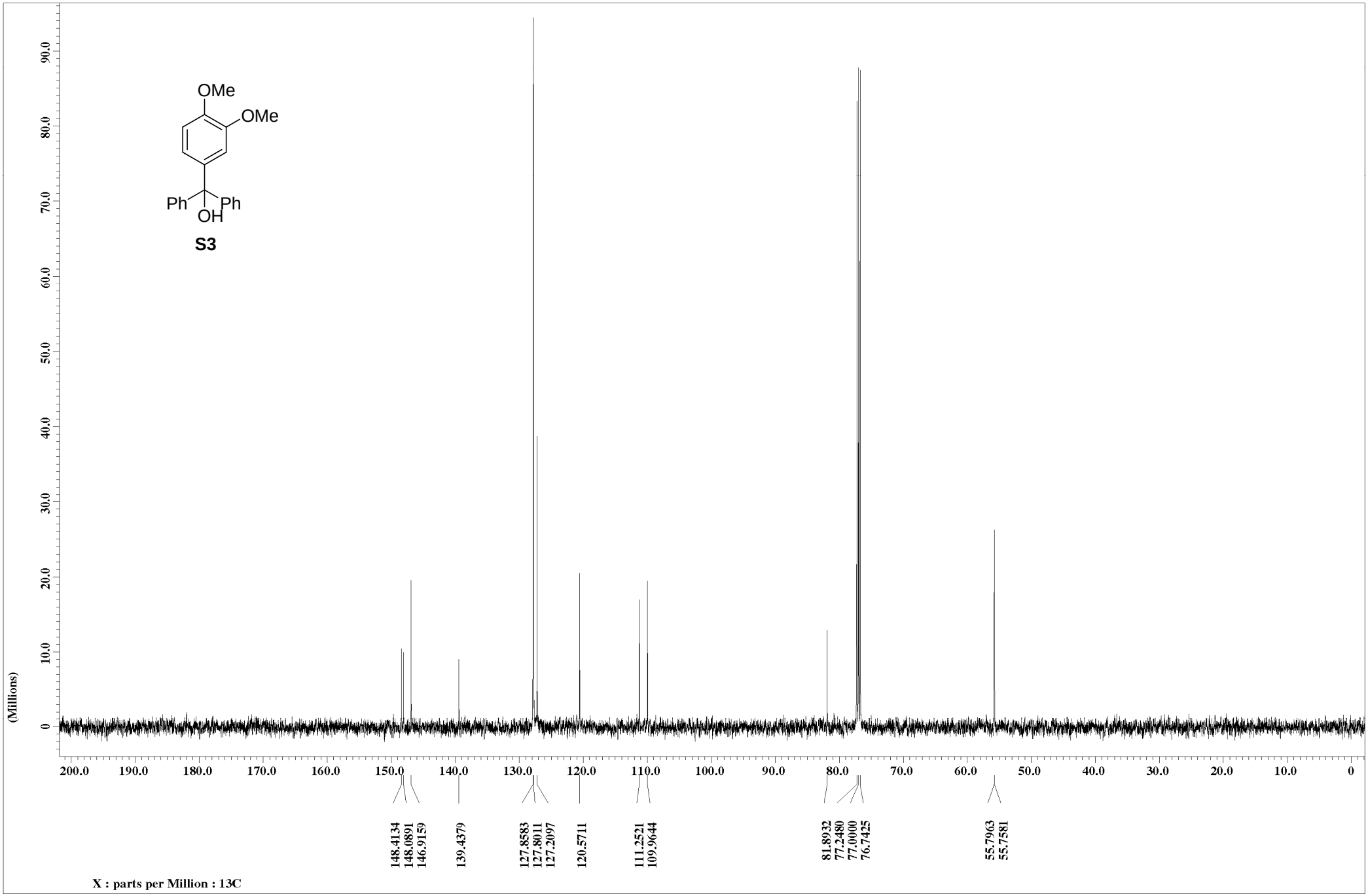

F
F
MeO
O
3h
(Millions)
60.0
50.0
40.0
30.0
20.0
10.0
0
−110.0
−120.0
−130.0
−140.0
−150.0
−160.0
−170.0
−117.7530
−164.9000
X : parts per Million : 19F

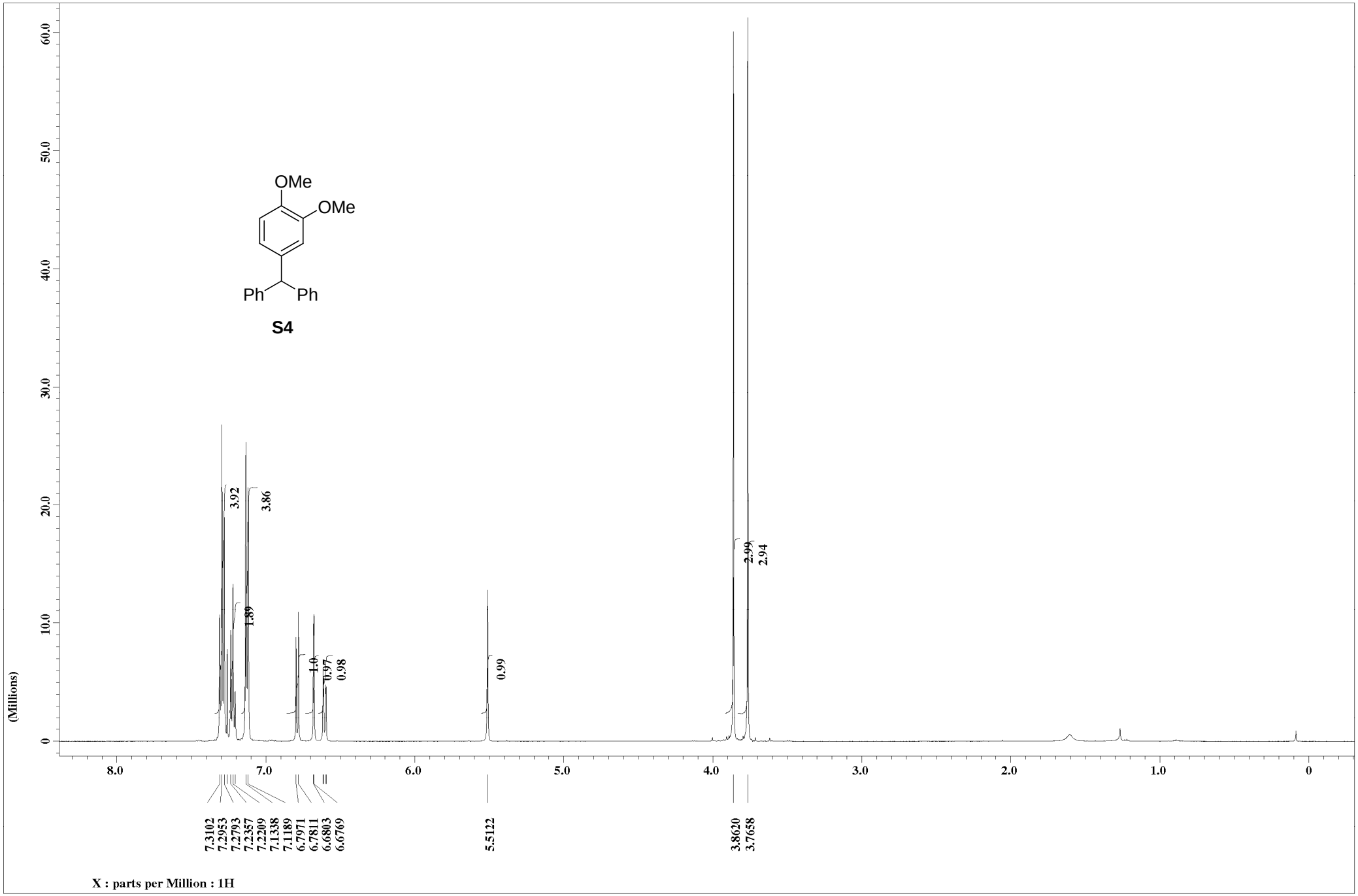

F
F
BnO
O
COOMe
3i
5.25
2.94
2
0.96
1.06
(Millions)
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.4192
7.4169
7.4089
7.2600
6.6004
6.5969
6.0175
6.0152
5.0979
3.9057
1.5696
1.2535
0.9202
0.8950
X : parts per Million : 1H

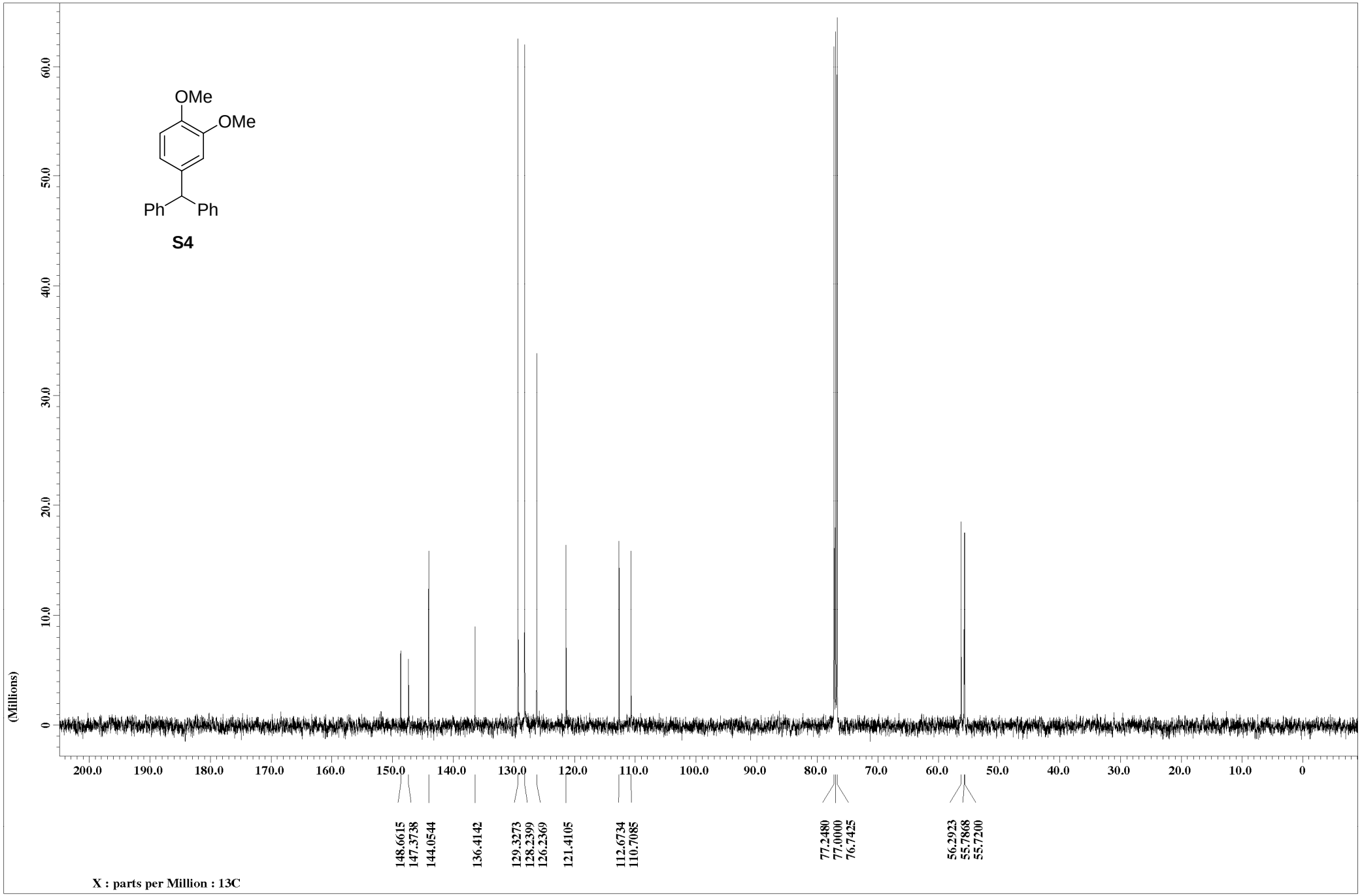

F
F
BnO
O
COOMe
3i
(Billions)
3.0
2.0
1.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
188.0547
187.8735
187.6922
164.7240
156.3016
156.1395
155.9678
143.0052
134.0773
128.8026
127.5913
119.6840
119.6649
119.6363
103.2876
101.3036
97.2308
97.1926
97.1449
77.2480
77.0000
76.7425
71.4964
53.3926
X : parts per Million : 13C

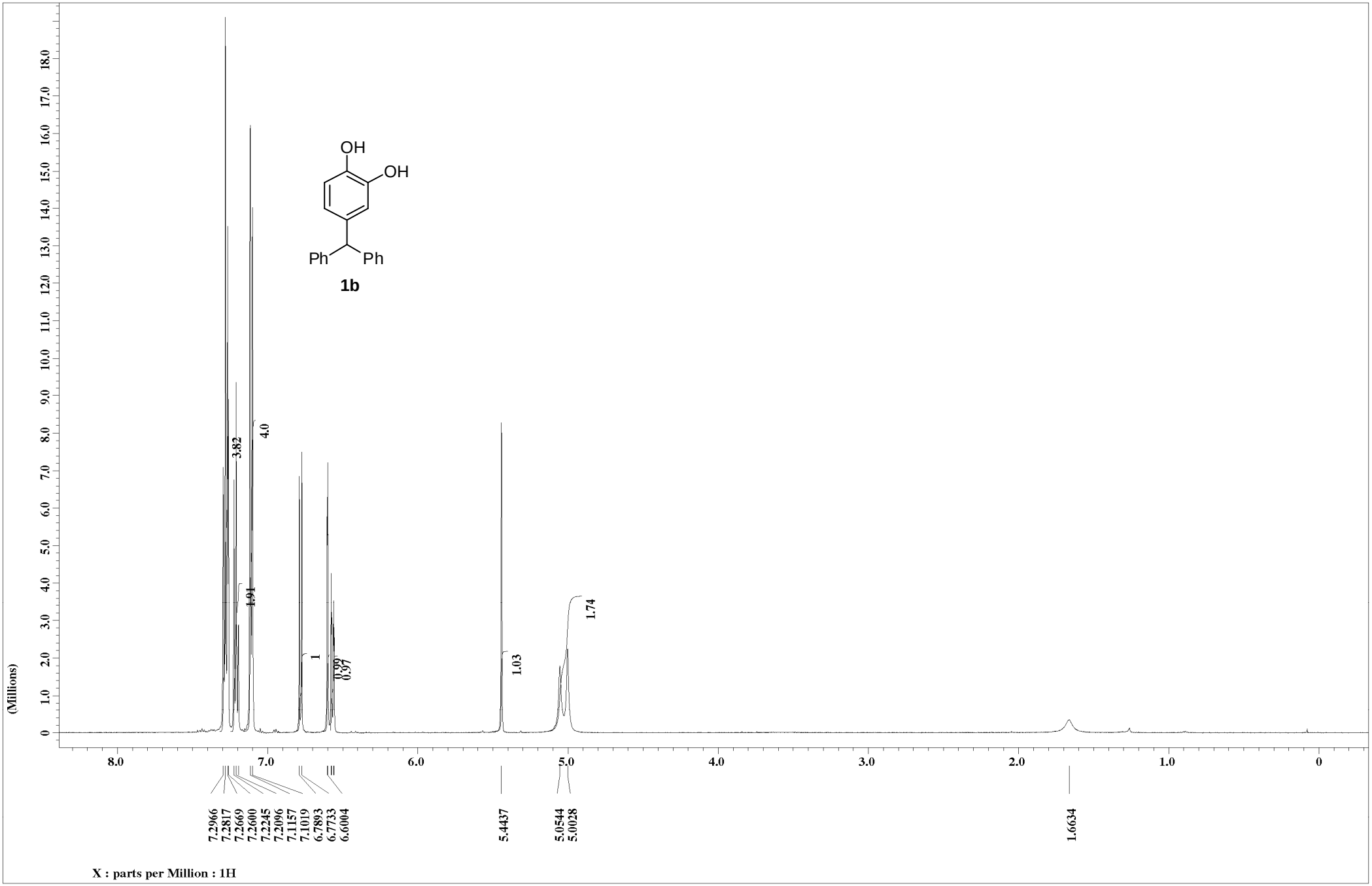

F
F
BnO
O
COOMe
3i
30.0
20.0
10.0
0
(Millions)
−120.0
−130.0
−140.0
−150.0
−160.0
−170.0
−116.4310
−164.9000
X : parts per Million : 19F

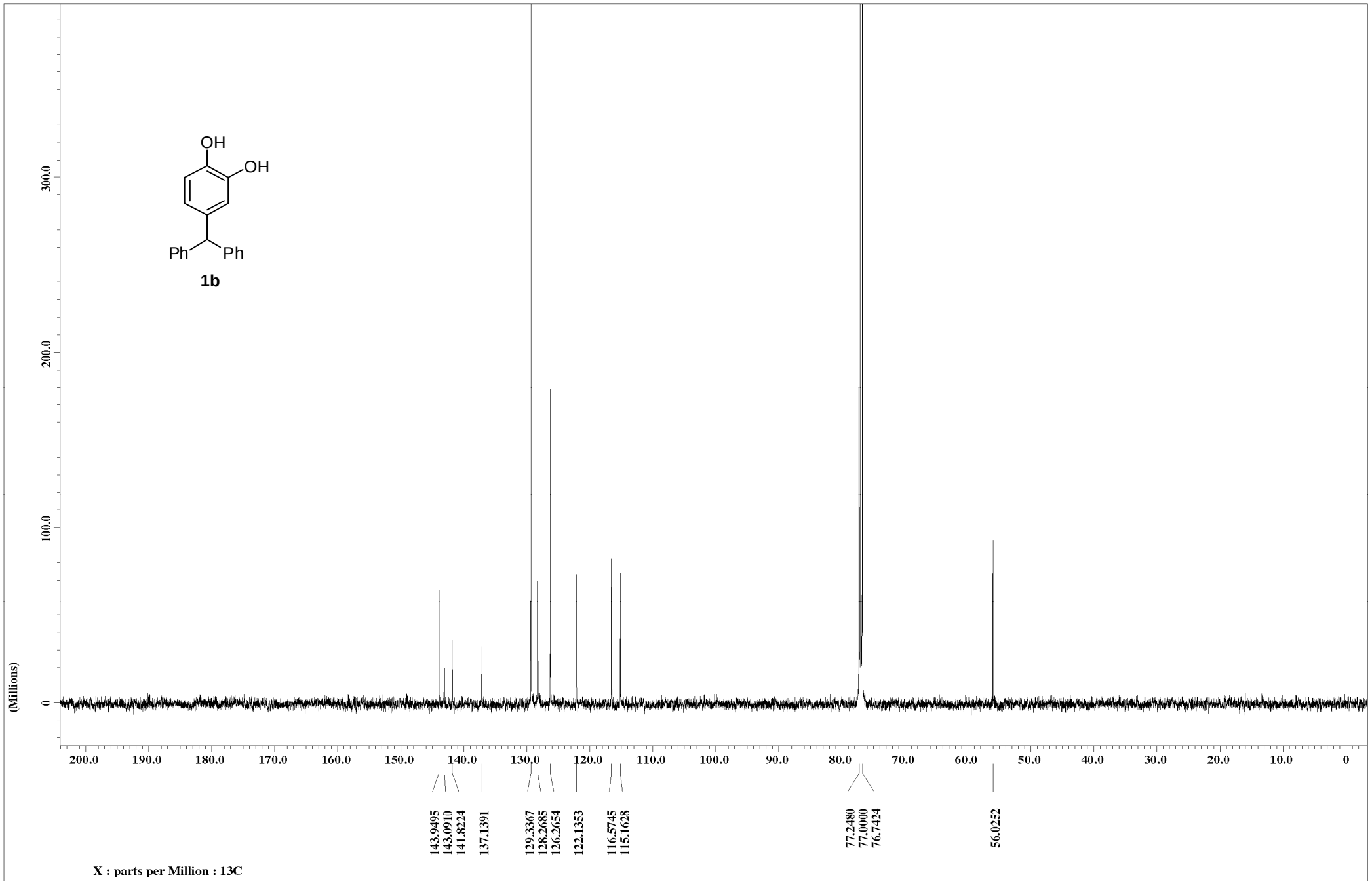

OMe
OMe
Ph
Ph
OH
S3
(Millions)
50.0
40.0
30.0
20.0
10.0
0
10.26
1.01
0.99
1
2.97
2.94
0.86
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2319
7.2204
7.2032
7.1975
7.1918
7.1883
7.1769
6.8494
6.8459
6.6936
6.6776
3.7837
3.6783
2.7416
X : parts per Million : 1H

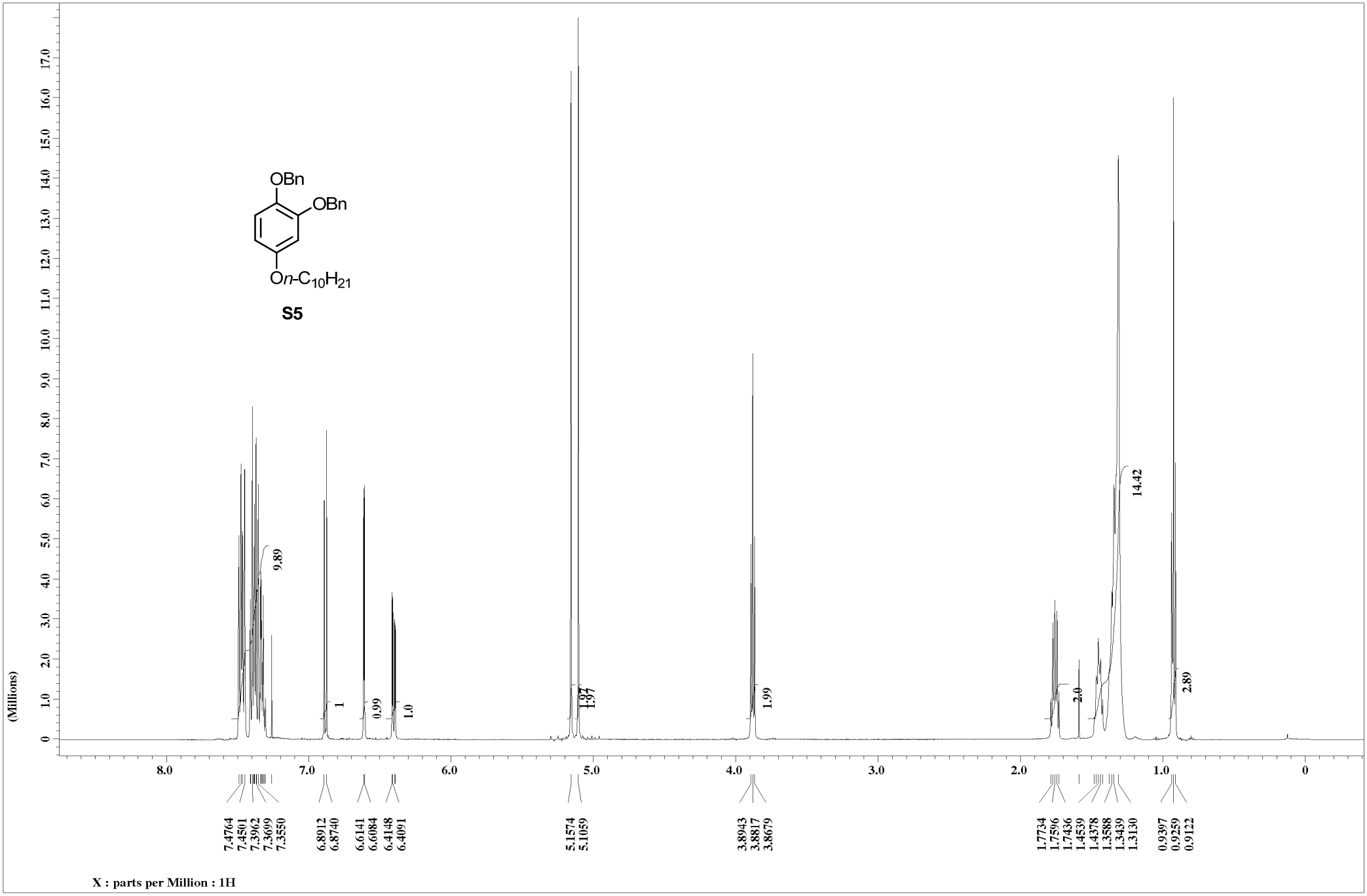

OMe
OMe
Ph
Ph
OH
S3
(Millions)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
148.4134
148.0891
146.9159
139.4379
127.8583
127.8011
127.2097
120.5711
111.2521
109.9644
81.8932
77.2480
77.0000
76.7425
55.7963
55.7581
X : parts per Million : 13C

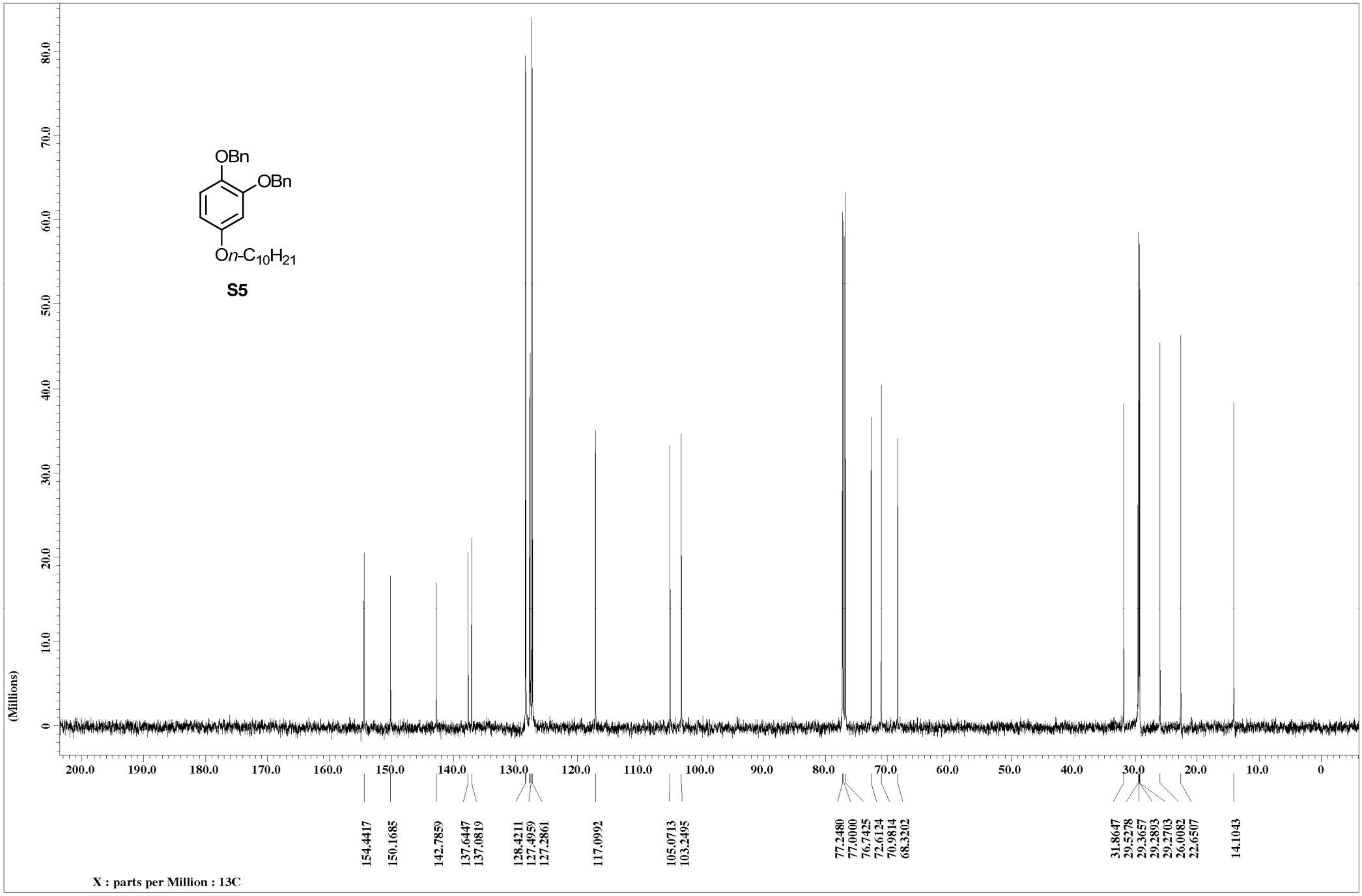

OMe
OMe
Ph
Ph
S4
(Millions)
60.0
50.0
40.0
30.0
20.0
10.0
0
3.92
3.86
1.89
1.0
0.97
0.98
0.99
2.99
2.94
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.3102
7.2953
7.2793
7.2357
7.2209
7.1338
7.1189
6.7971
6.7811
6.6803
6.6769
5.5122
3.8620
3.7658
X : parts per Million : 1H

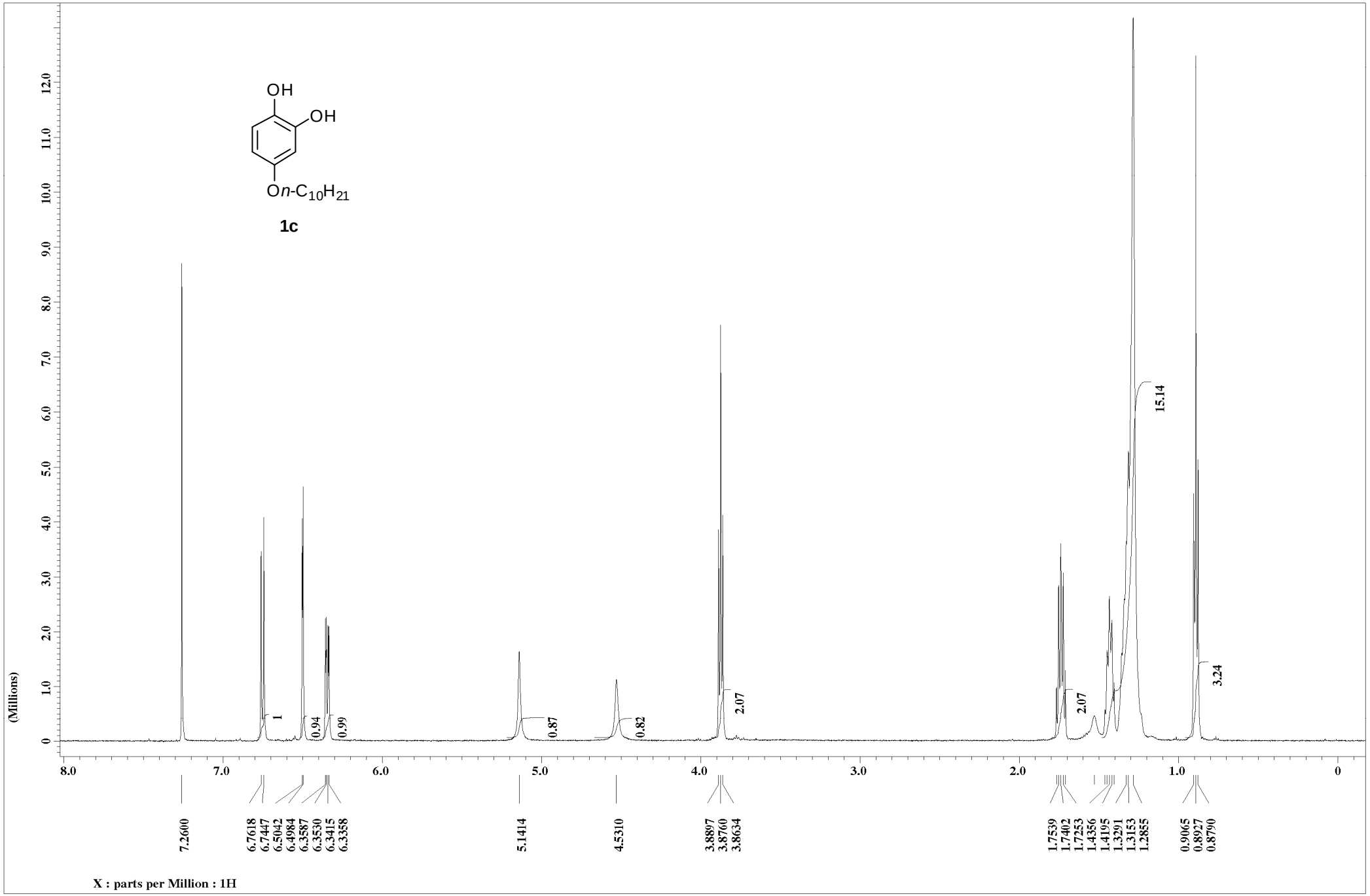

OMe
OMe
Ph
Ph
S4
(Millions)
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
148.6615
147.3738
144.0544
136.4142
129.3273
128.2399
126.2369
121.4105
112.6734
110.7085
77.2480
77.0000
76.7425
56.2923
55.7868
55.7200
X : parts per Million : 13C

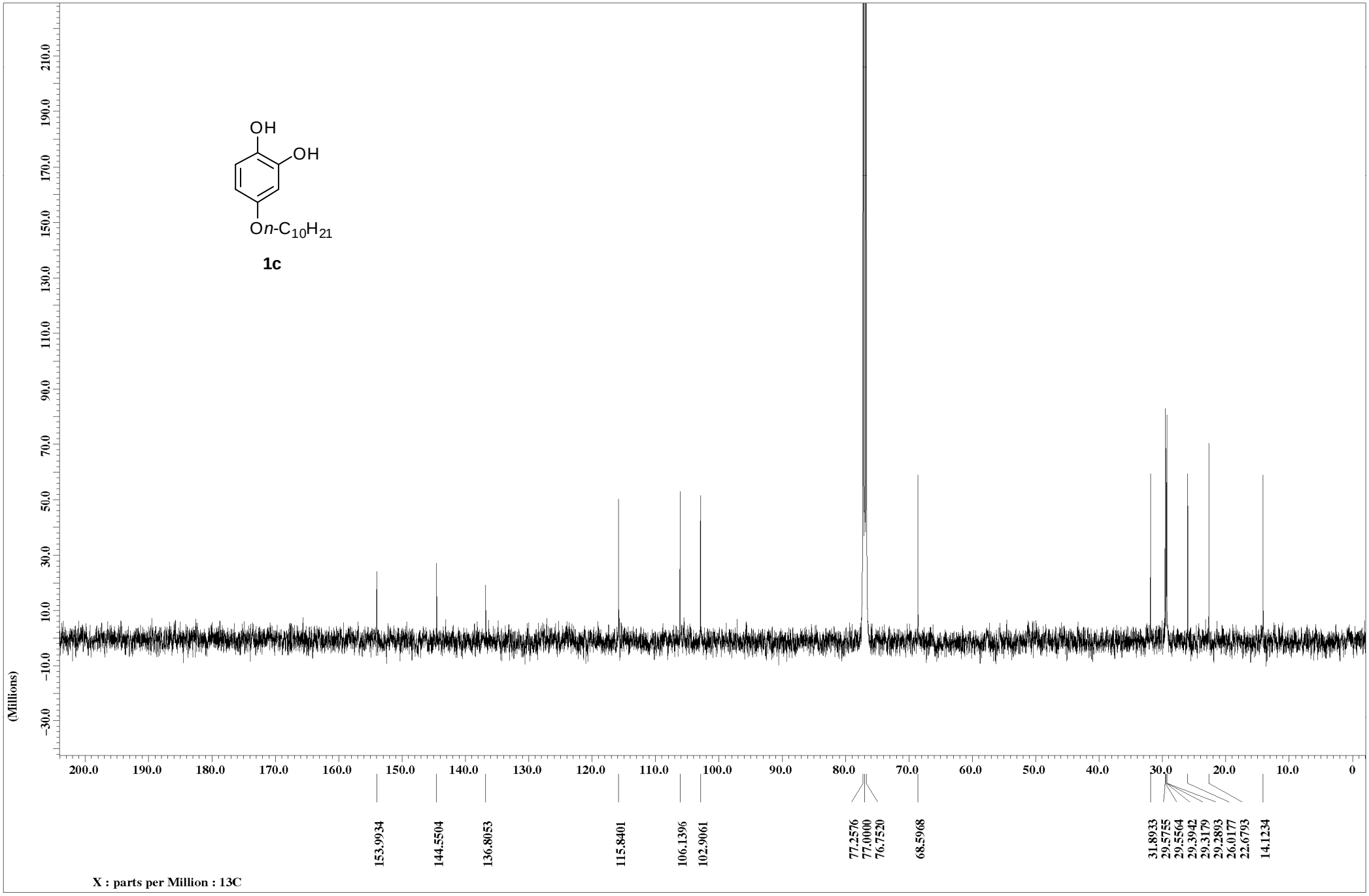

OH
OH
Ph
Ph
1b
(Millions)
18.0
17.0
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
3.82
4.0
1.91
1
0.99
0.97
1.03
1.74
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2966
7.2817
7.2669
7.2600
7.2245
7.2096
7.1157
7.1019
6.7893
6.7733
6.6004
5.4437
5.0544
5.0028
1.6634
X : parts per Million : 1H

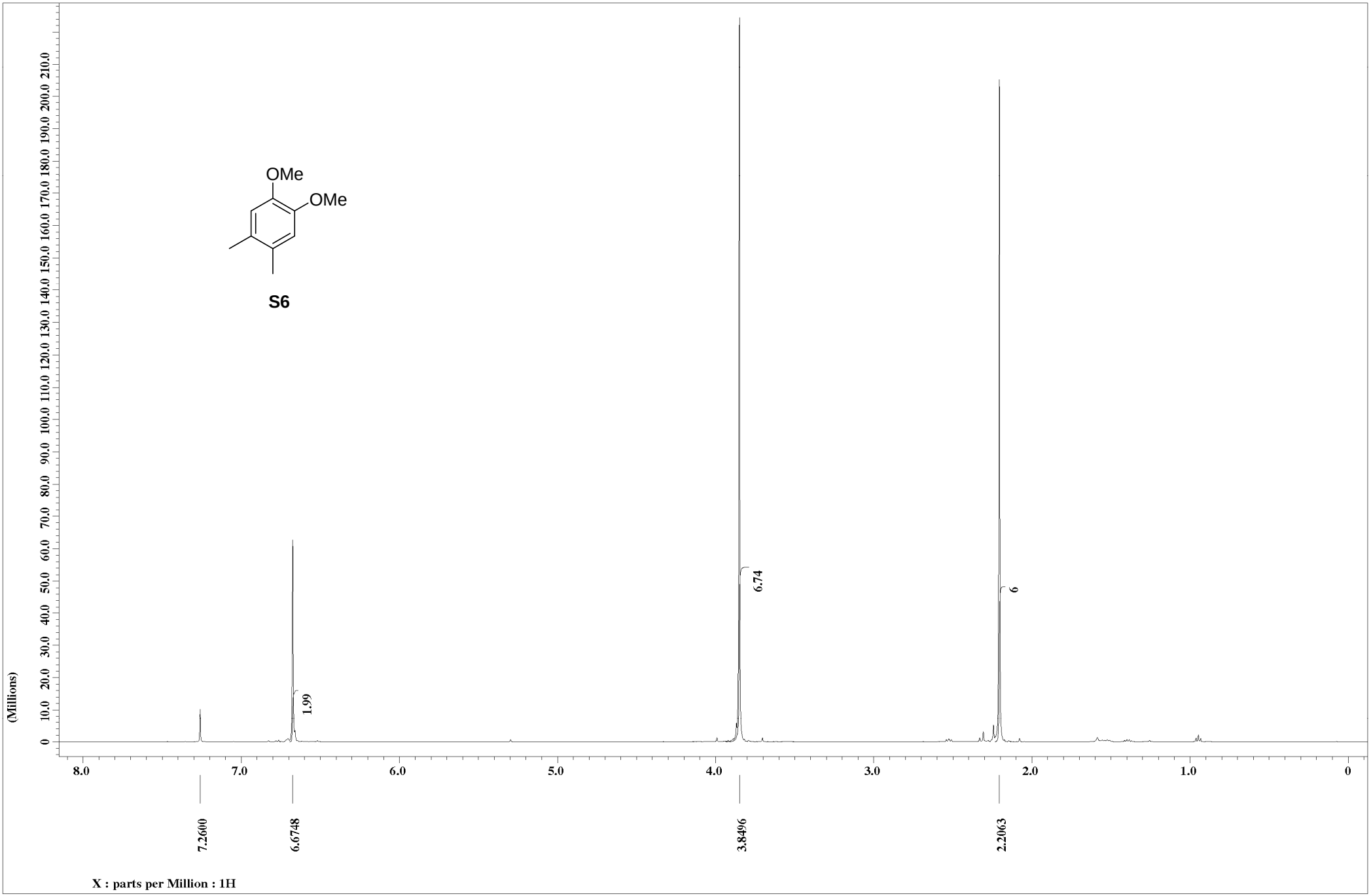

OH
OH
Ph
Ph
1b
300.0
200.0
100.0
0
(Millions)
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
143.9495
143.0910
141.8224
137.1391
129.3367
128.2685
126.2654
122.1353
116.5745
115.1628
77.2480
77.0000
76.7424
56.0252
X : parts per Million : 13C

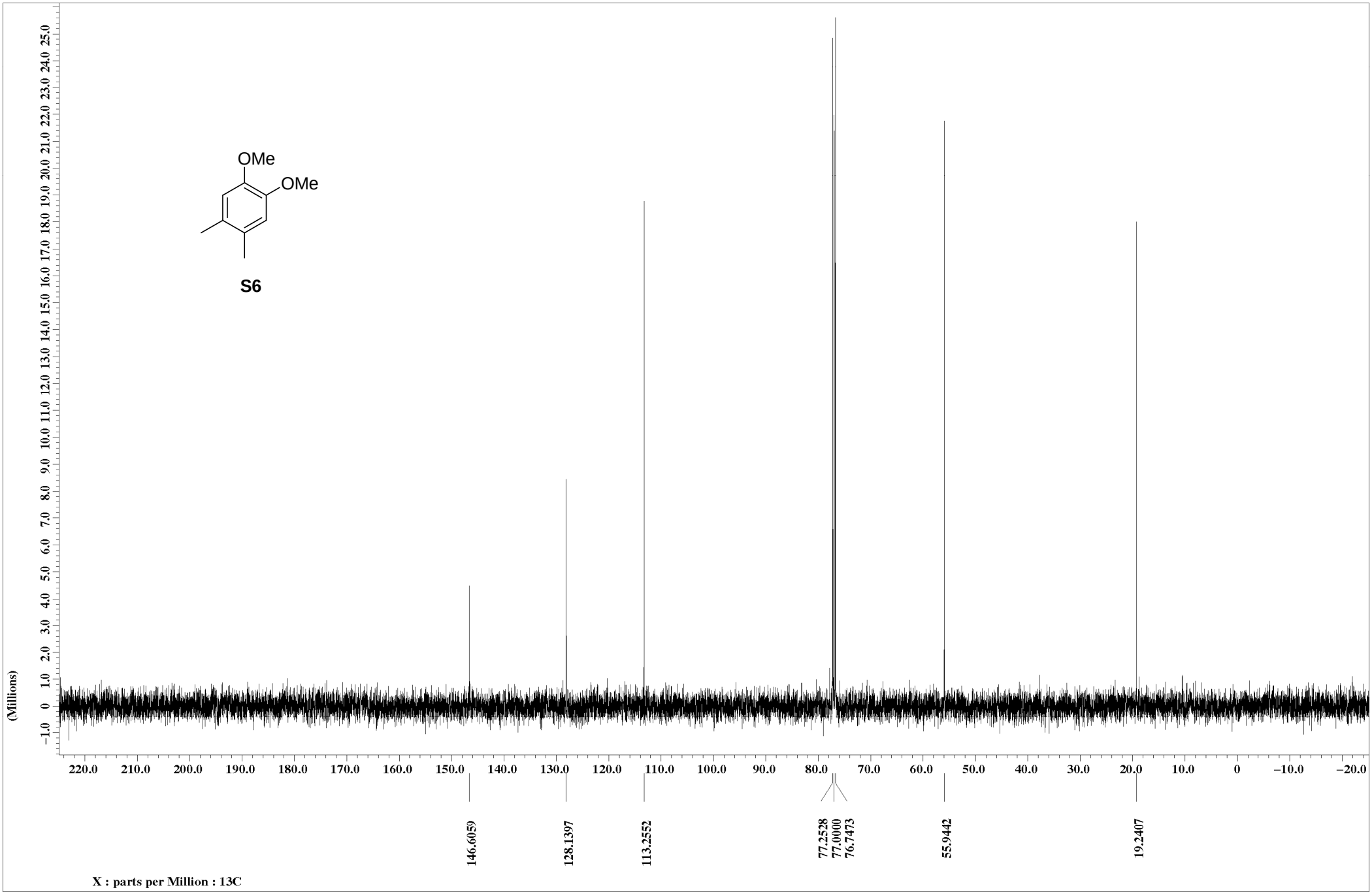

OBn
OBn
On-C10H21
S5
(Millions)
9.89
1
0.99
1.0
1.97
1.99
2.0
14.42
2.89
7.4764
7.4501
7.3962
7.3699
7.3550
6.8912
6.8740
6.6141
6.6084
6.4148
6.4091
5.1574
5.1059
3.8943
3.8817
3.8679
1.7734
1.7596
1.7436
1.4539
1.4378
1.3588
1.3439
1.3130
0.9397
0.9259
0.9122
X : parts per Million : 1H

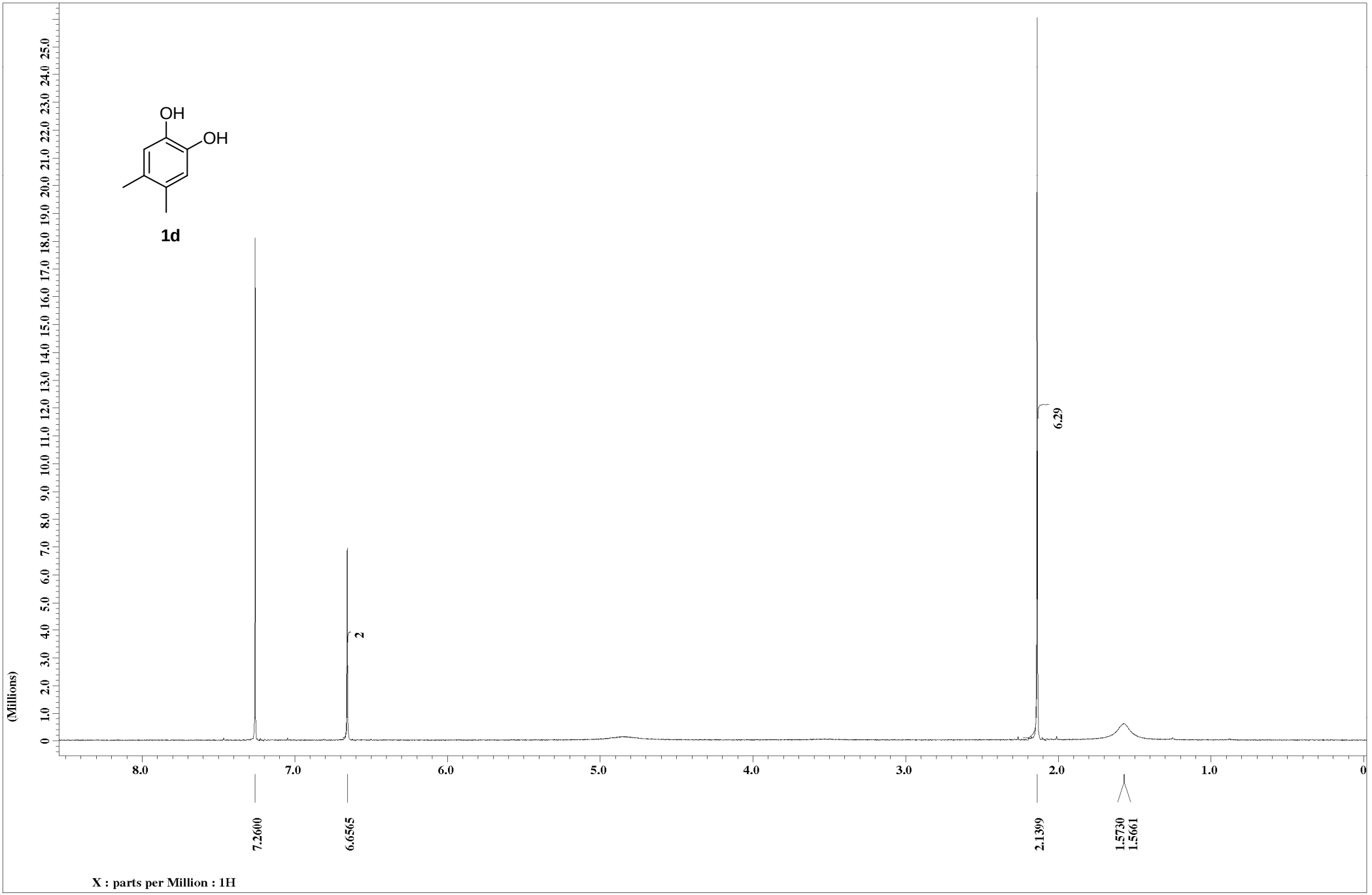

OBn
OBn
On-C10H21
S5
(Millions)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
154.4417
150.1685
142.7859
137.6447
137.0819
128.4211
127.4959
127.2861
117.0992
105.0713
103.2495
77.2480
77.0000
76.7425
72.6124
70.9814
68.3202
31.8647
29.5278
29.3657
29.2893
29.2703
26.0082
22.6507
14.1043
X : parts per Million : 13C

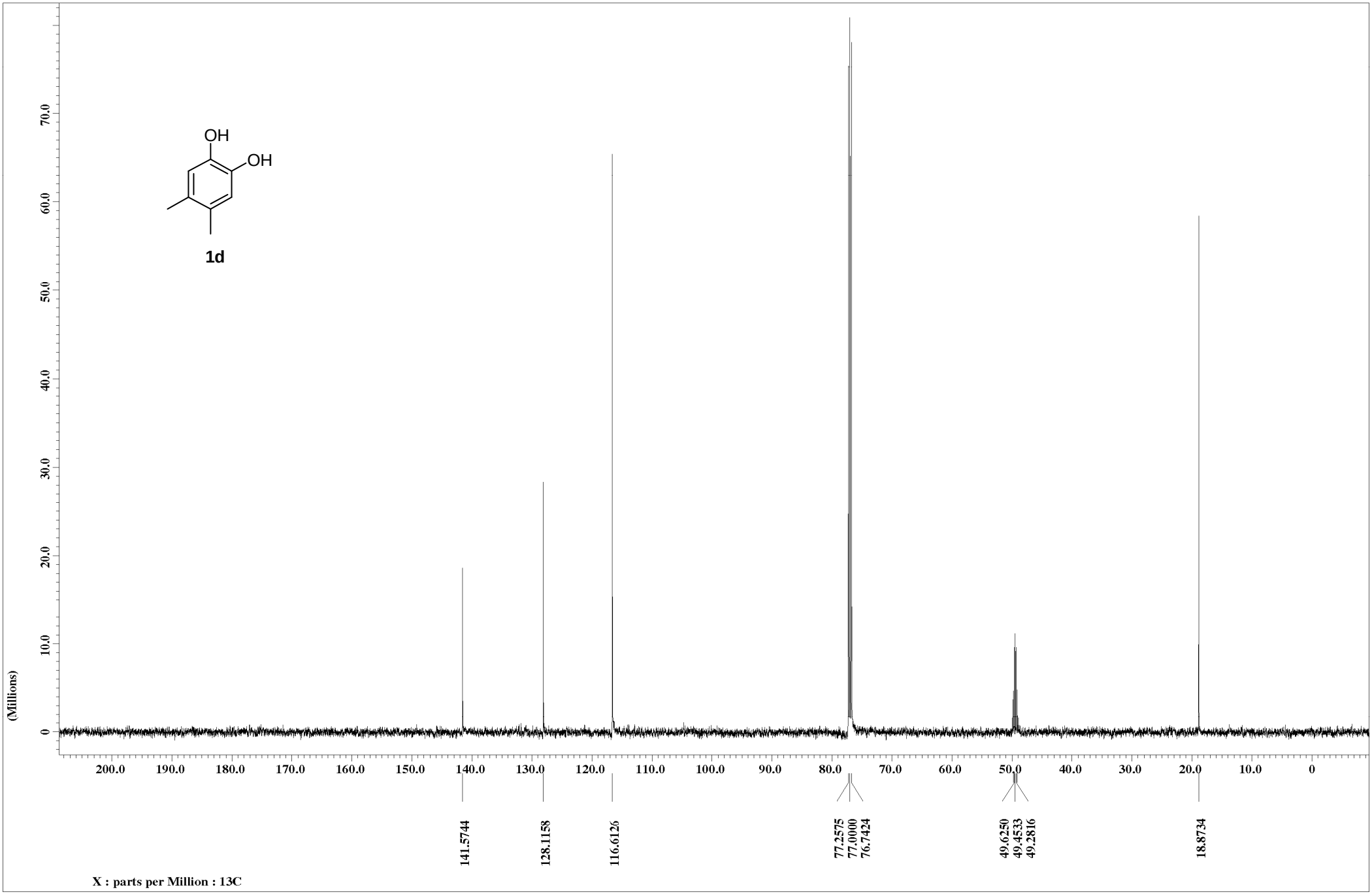

OH
OH
On-$C_{10}H_{21}$
1c
(Millions)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1
0.94
0.99
0.87
0.82
2.07
2.07
15.14
3.24
7.2600
6.7618
6.7447
6.5042
6.4984
6.3587
6.3530
6.3415
6.3358
5.1414
4.5310
3.8897
3.8760
3.8634
1.7539
1.7402
1.7253
1.4356
1.4195
1.3291
1.3153
1.2855
0.9065
0.8927
0.8790
X : parts per Million : 1H

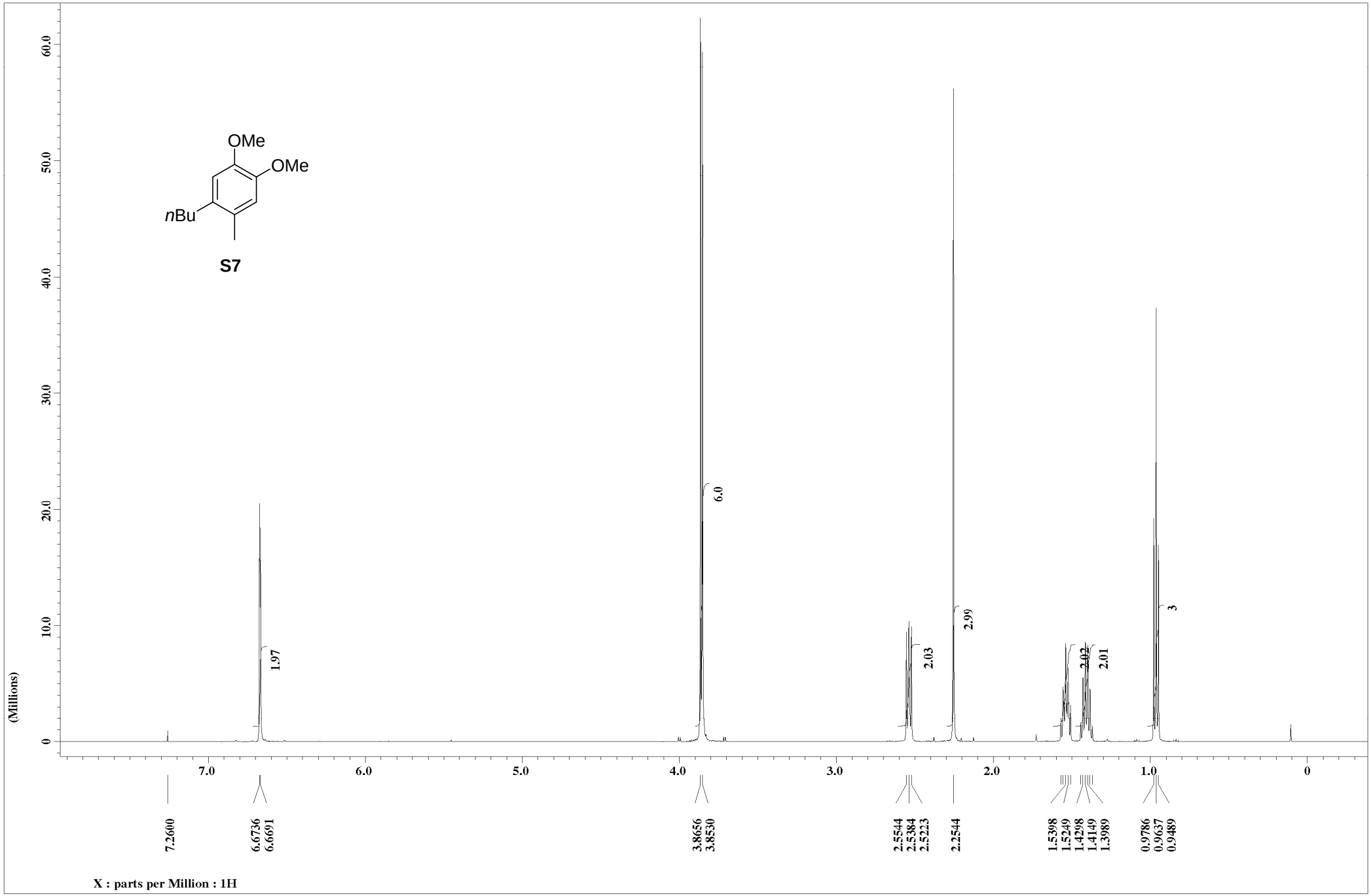

OH
OH
On-C10H21
1c
(Millions)
210.0
190.0
170.0
150.0
130.0
110.0
90.0
70.0
50.0
30.0
10.0
−10.0
−30.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
153.9934
144.5504
136.8053
115.8401
106.1396
102.9061
77.2576
77.0000
76.7520
68.5968
31.8933
29.5755
29.5564
29.3942
29.3179
29.2893
26.0177
22.6793
14.1234
X : parts per Million : 13C

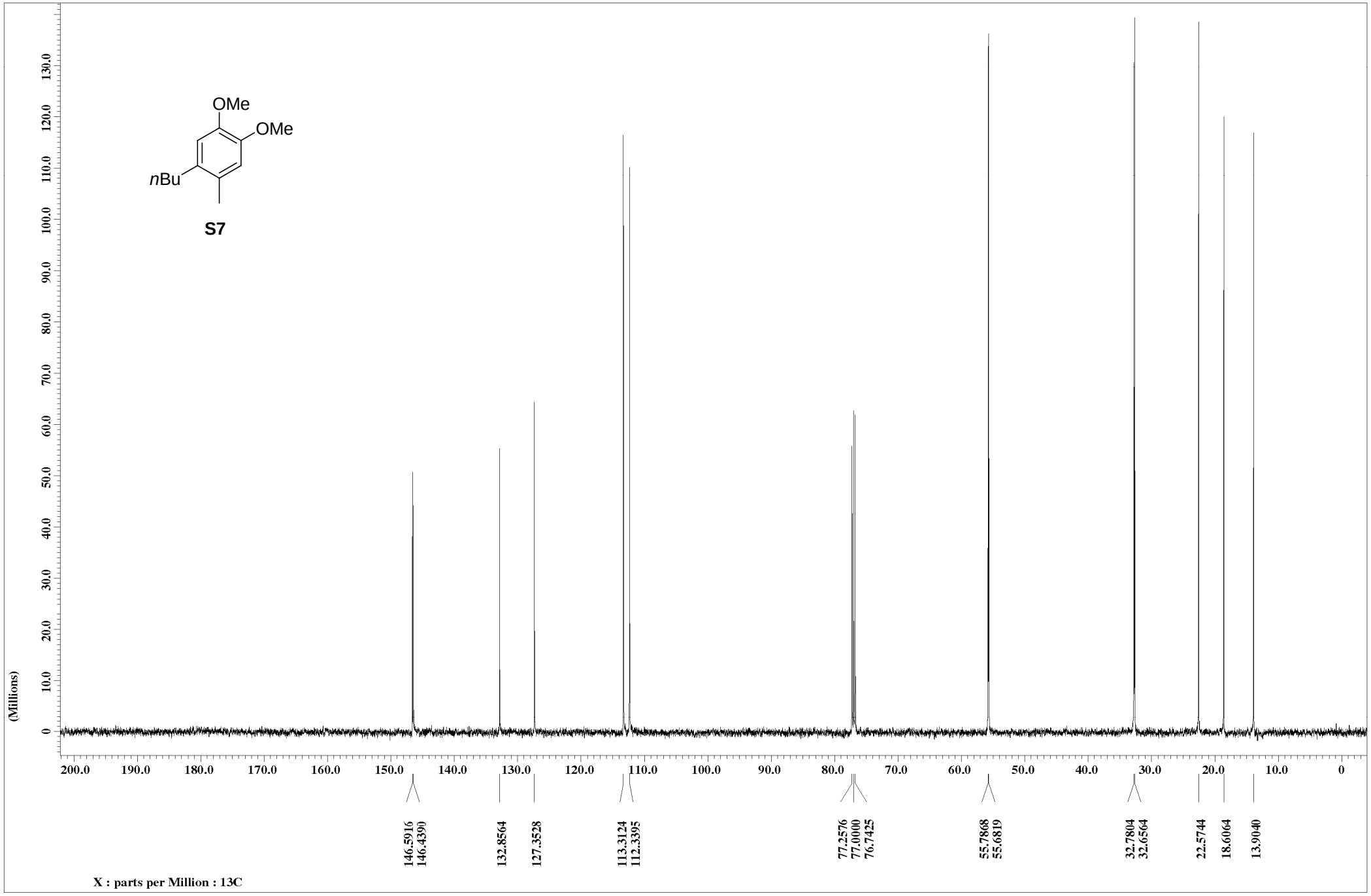

OMe
OMe
S6
(Millions)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
110.0
120.0
130.0
140.0
150.0
160.0
170.0
180.0
190.0
200.0
210.0
1.99
6.74
6
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2600
6.6748
3.8496
2.2063
X : parts per Million : 1H

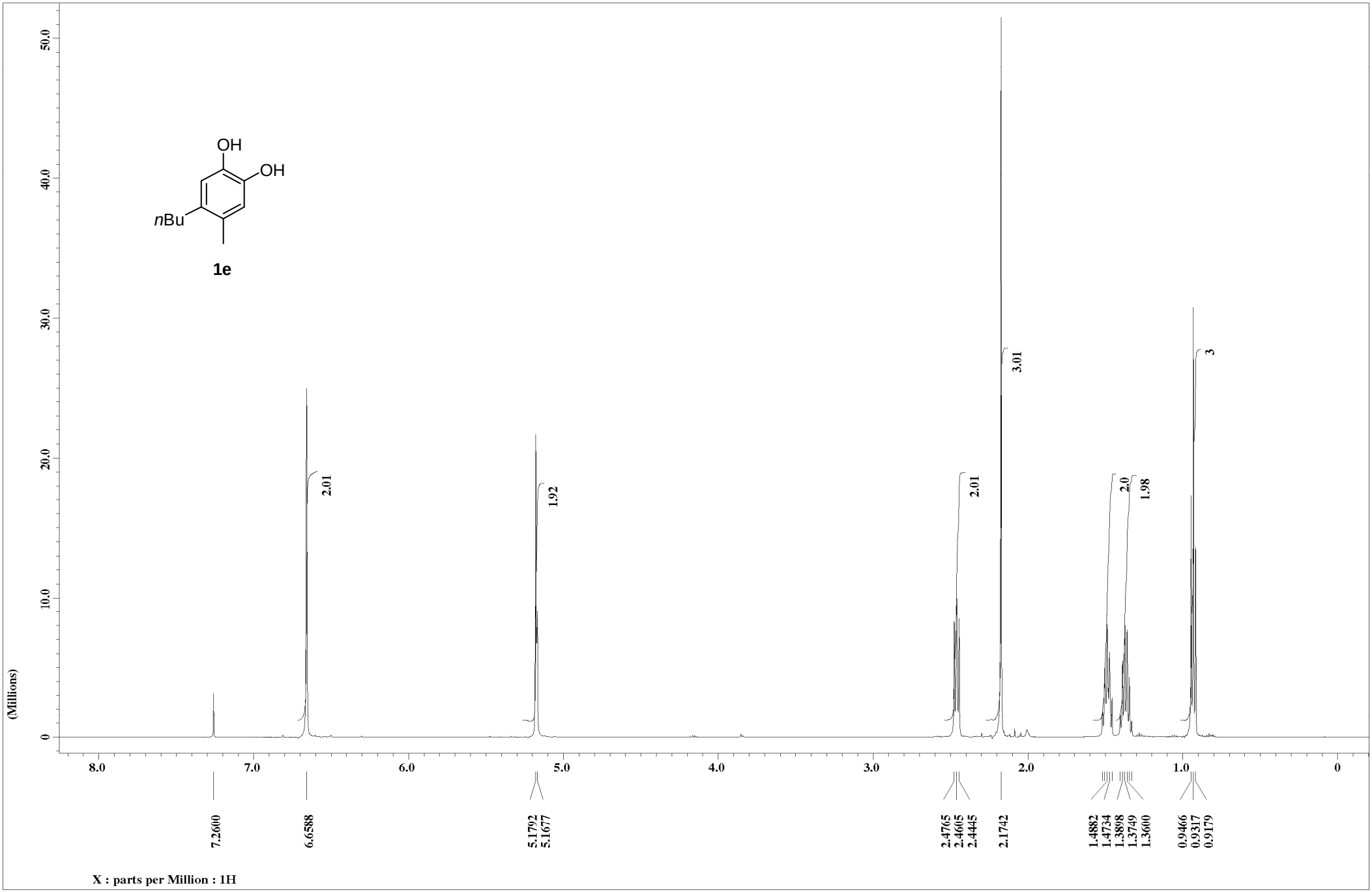

OMe
OMe
S6
(Millions)
25.0
24.0
23.0
22.0
21.0
20.0
19.0
18.0
17.0
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
−20.0
146.6059
128.1397
113.2552
77.2528
77.0000
76.7473
55.9442
19.2407
X : parts per Million : 13C

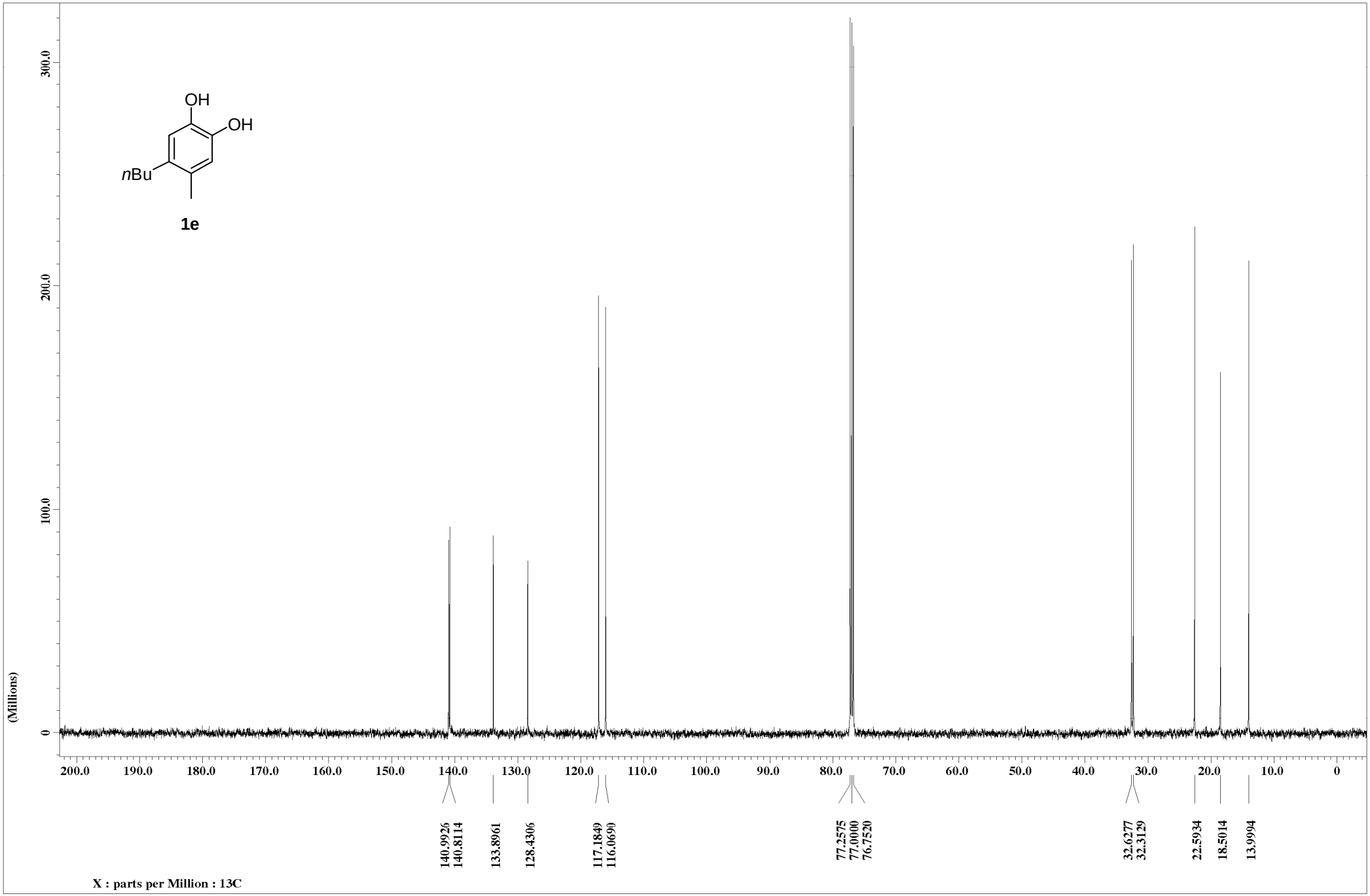

OH
OH
1d
(Millions)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0 25.0
8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
2
6.29
7.2600
6.6565
2.1399
1.5730
1.5661
X : parts per Million : 1H

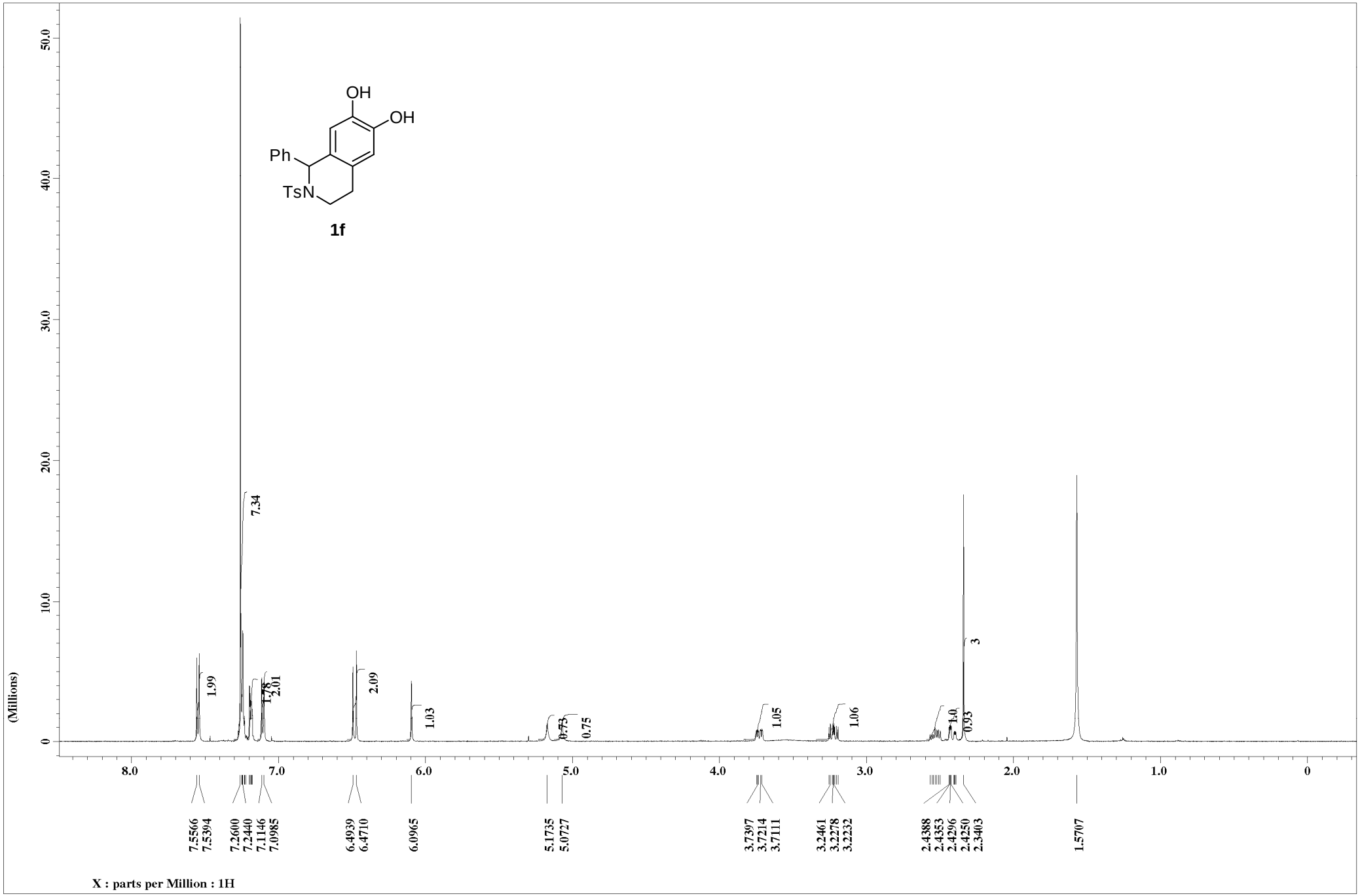

OH
OH
1d
(Millions)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
141.5744
128.1158
116.6126
77.2575
77.0000
76.7424
49.6250
49.4533
49.2816
18.8734
X : parts per Million : 13C

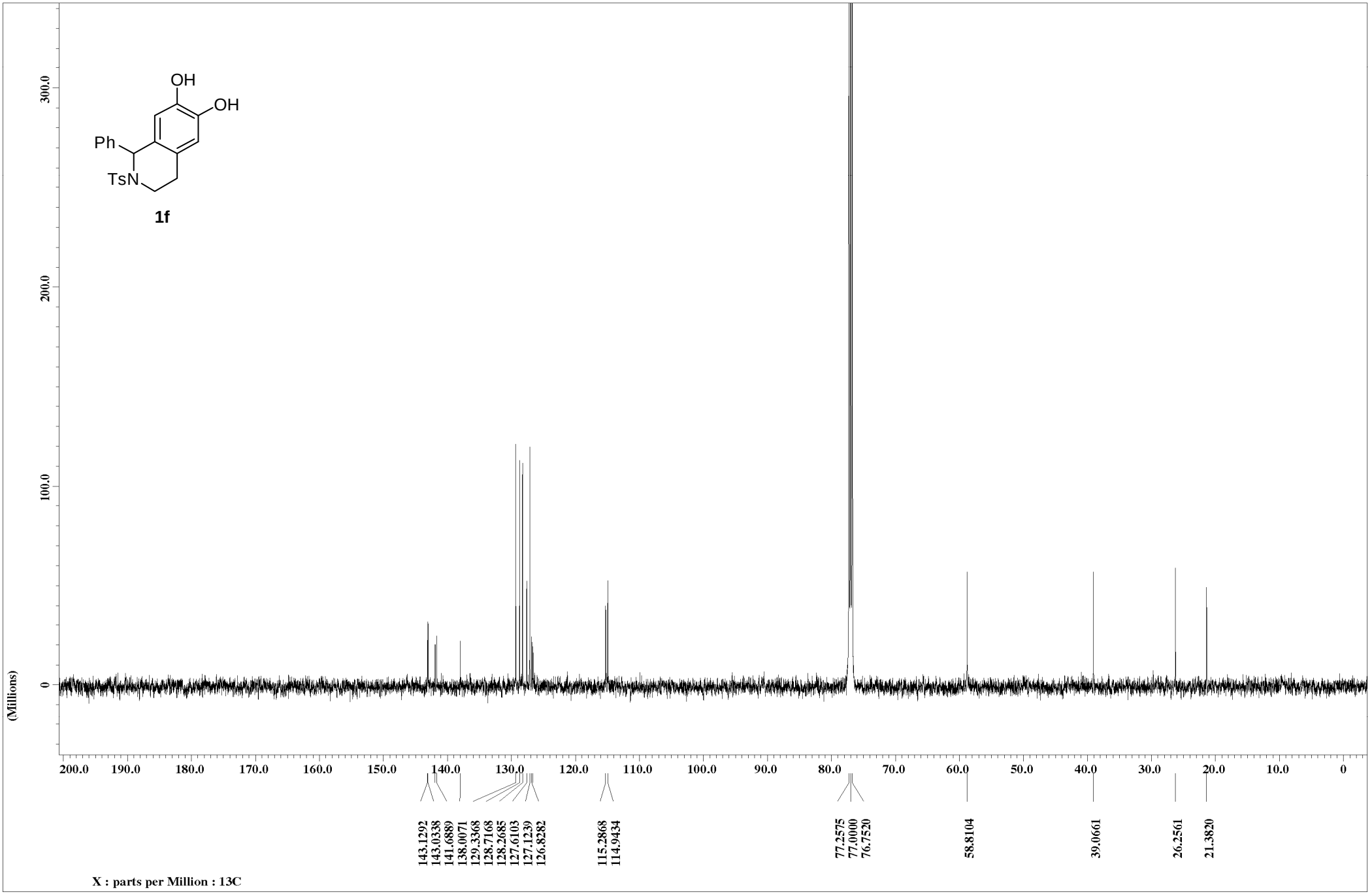

OMe
OMe
nBu
S7
(Millions)
60.0
50.0
40.0
30.0
20.0
10.0
0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.97
6.0
2.03
2.99
2.02
2.01
3
7.2600
6.6736
6.6691
3.8656
3.8530
2.5544
2.5384
2.5223
2.2544
1.5398
1.5249
1.4298
1.4149
1.3989
0.9786
0.9637
0.9489
X : parts per Million : 1H

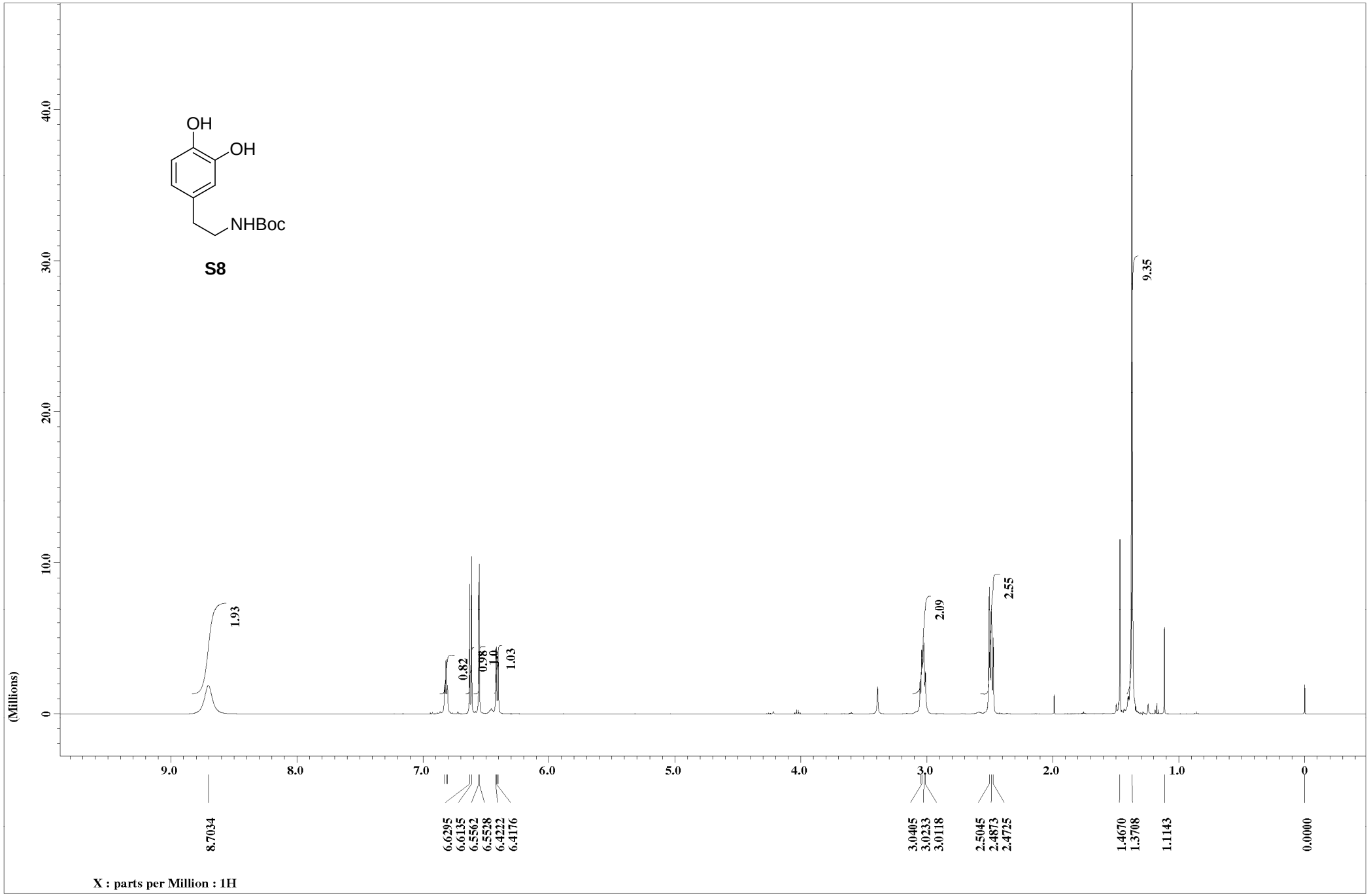

OMe
OMe
nBu
S7
(Millions)
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
146.5916
146.4390
132.8564
127.3528
113.3124
112.3395
77.2576
77.0000
76.7425
55.7868
55.6819
32.7804
32.6564
22.5744
18.6064
13.9040
X : parts per Million : 13C

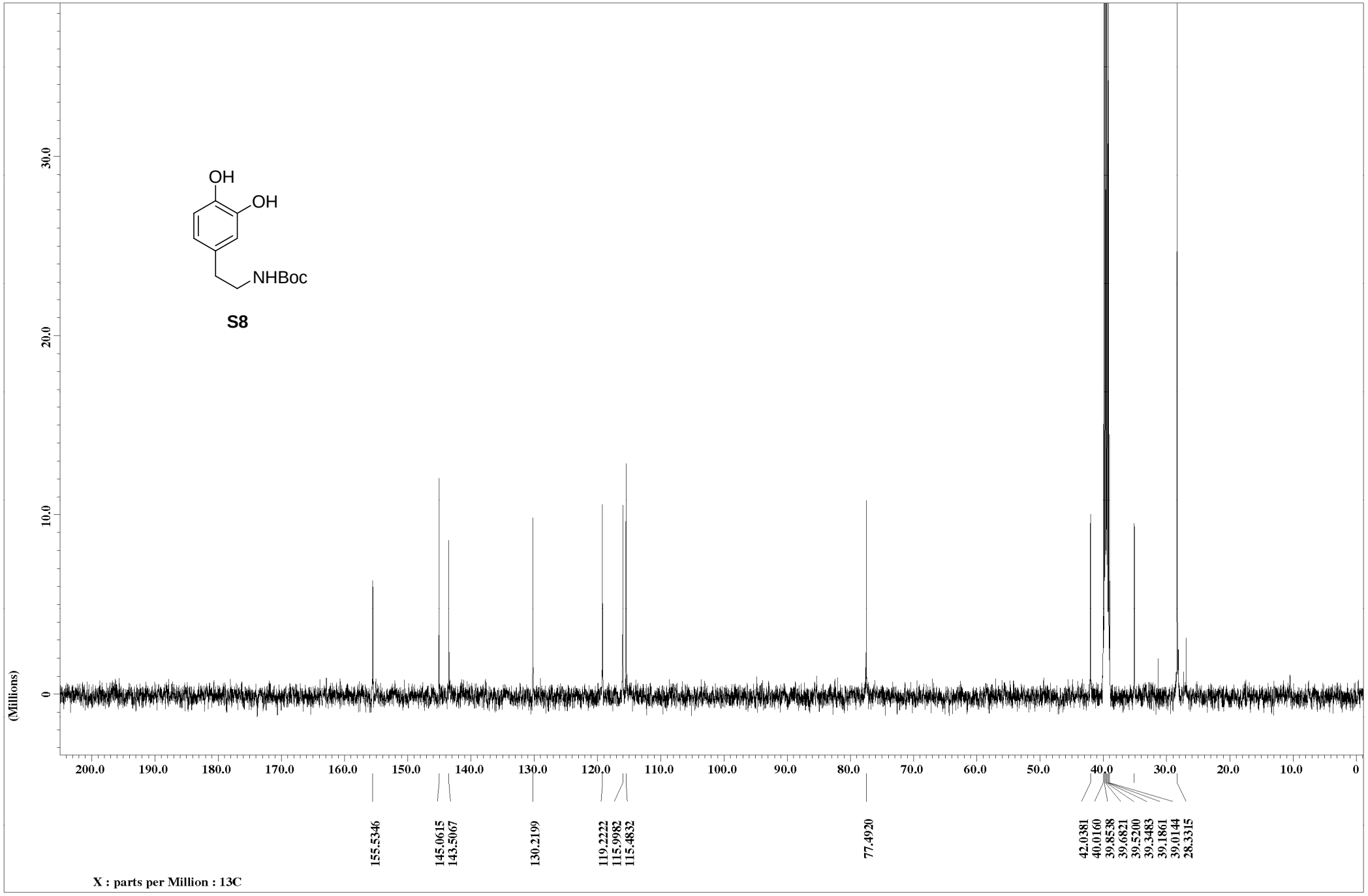

OH
OH
nBu
1e
(Millions)
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2.01
1.92
2.01
3.01
2.0
1.98
3
7.2600
6.6588
5.1792
5.1677
2.4765
2.4605
2.4445
2.1742
1.4882
1.4734
1.3898
1.3749
1.3600
0.9466
0.9317
0.9179
X : parts per Million : 1H

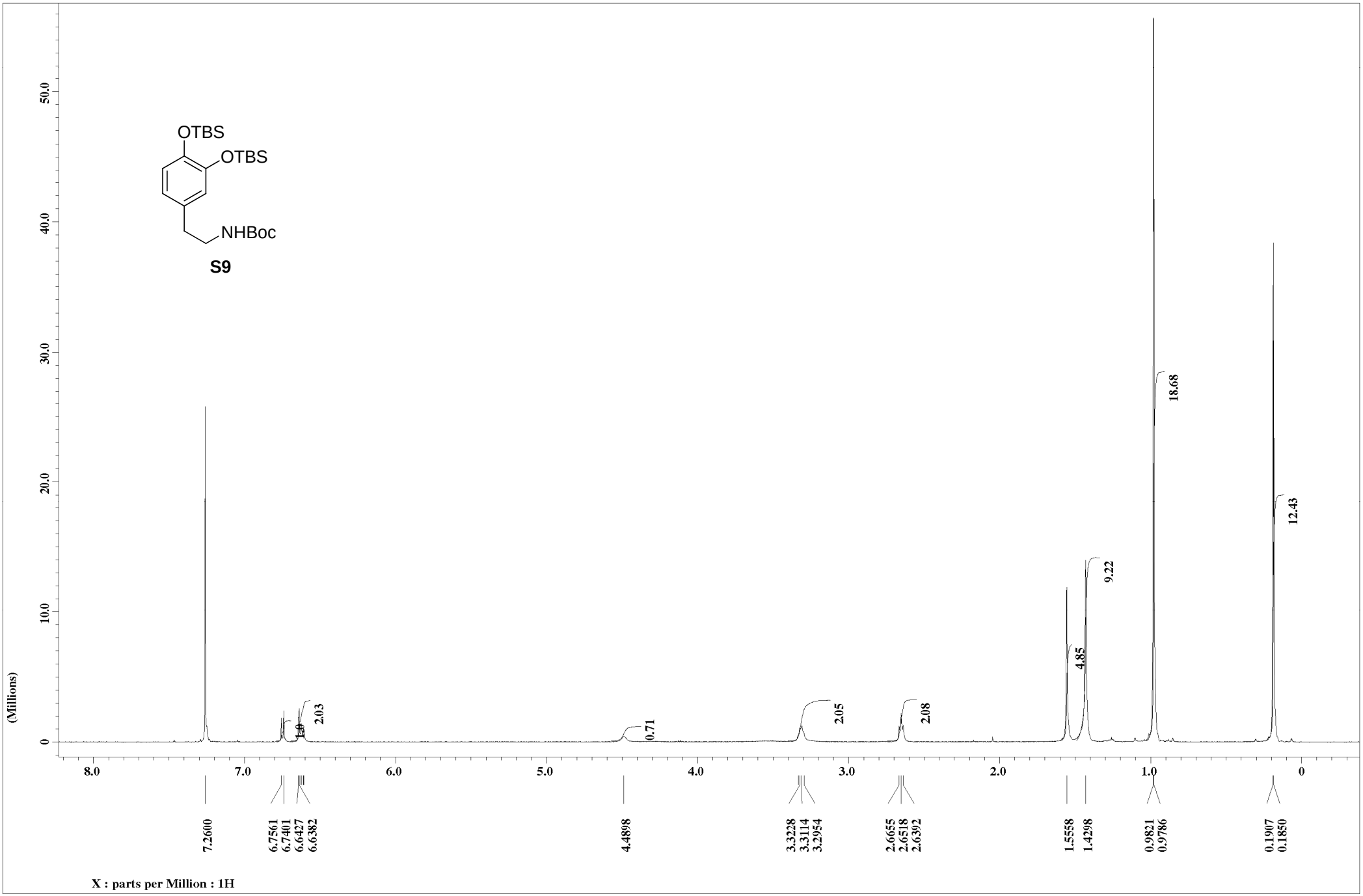

OH
OH
nBu
1e
300.0
200.0
100.0
0
(Millions)
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
140.9926
140.8114
133.8961
128.4306
117.1849
116.0690
77.2575
77.0000
76.7520
32.6277
32.3129
22.5934
18.5014
13.9994
X : parts per Million : 13C

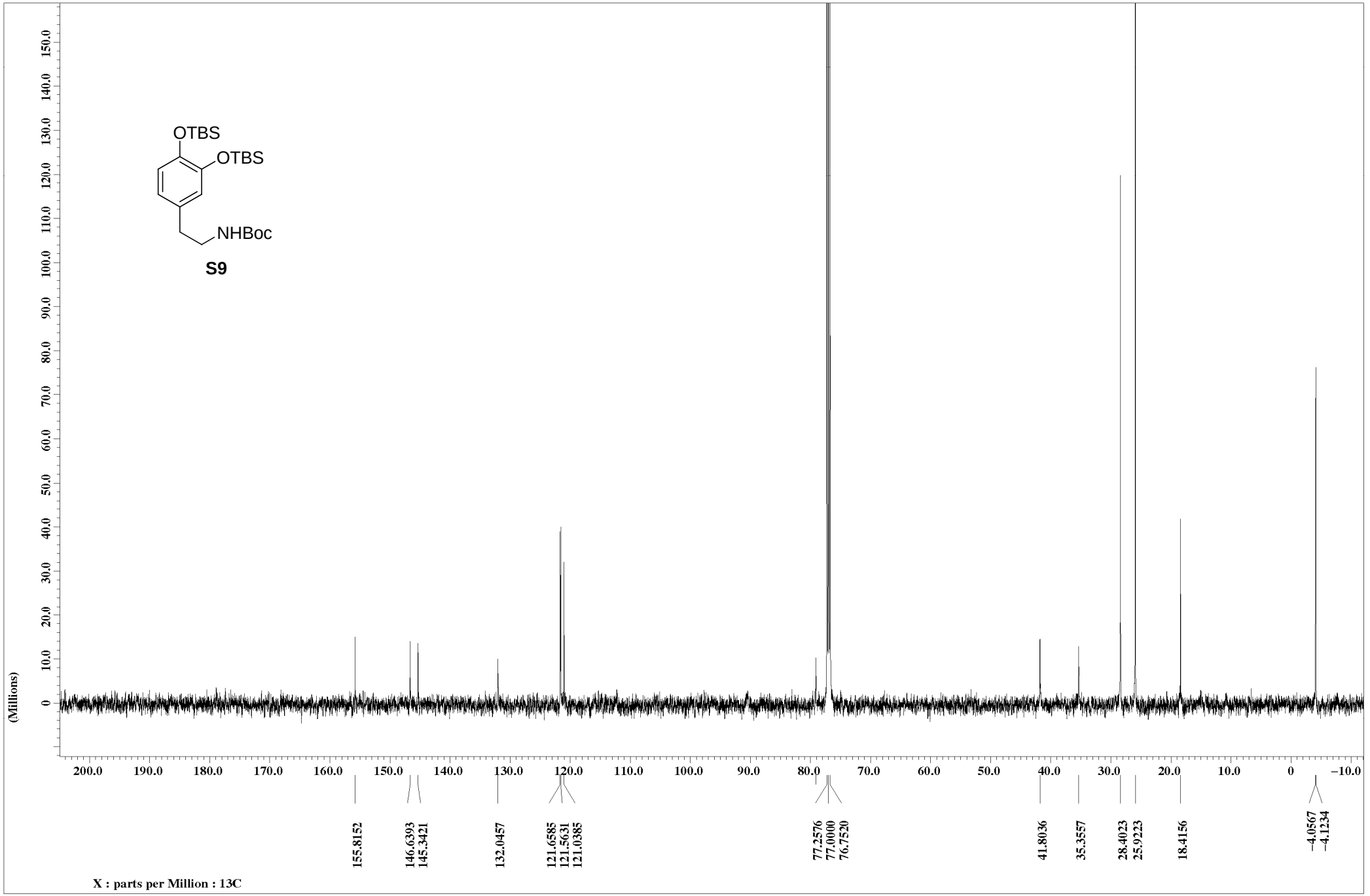

OH
OH
Ph
TsN
1f
(Millions)
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.34
1.99
1.78
2.01
2.09
1.03
0.73
0.75
1.05
1.06
1.0
0.93
3
7.5566
7.5394
7.2600
7.2440
7.1146
7.0985
6.4939
6.4710
6.0965
5.1735
5.0727
3.7397
3.7214
3.7111
3.2461
3.2278
3.2232
2.4388
2.4353
2.4296
2.4250
2.3403
1.5707
X : parts per Million : 1H

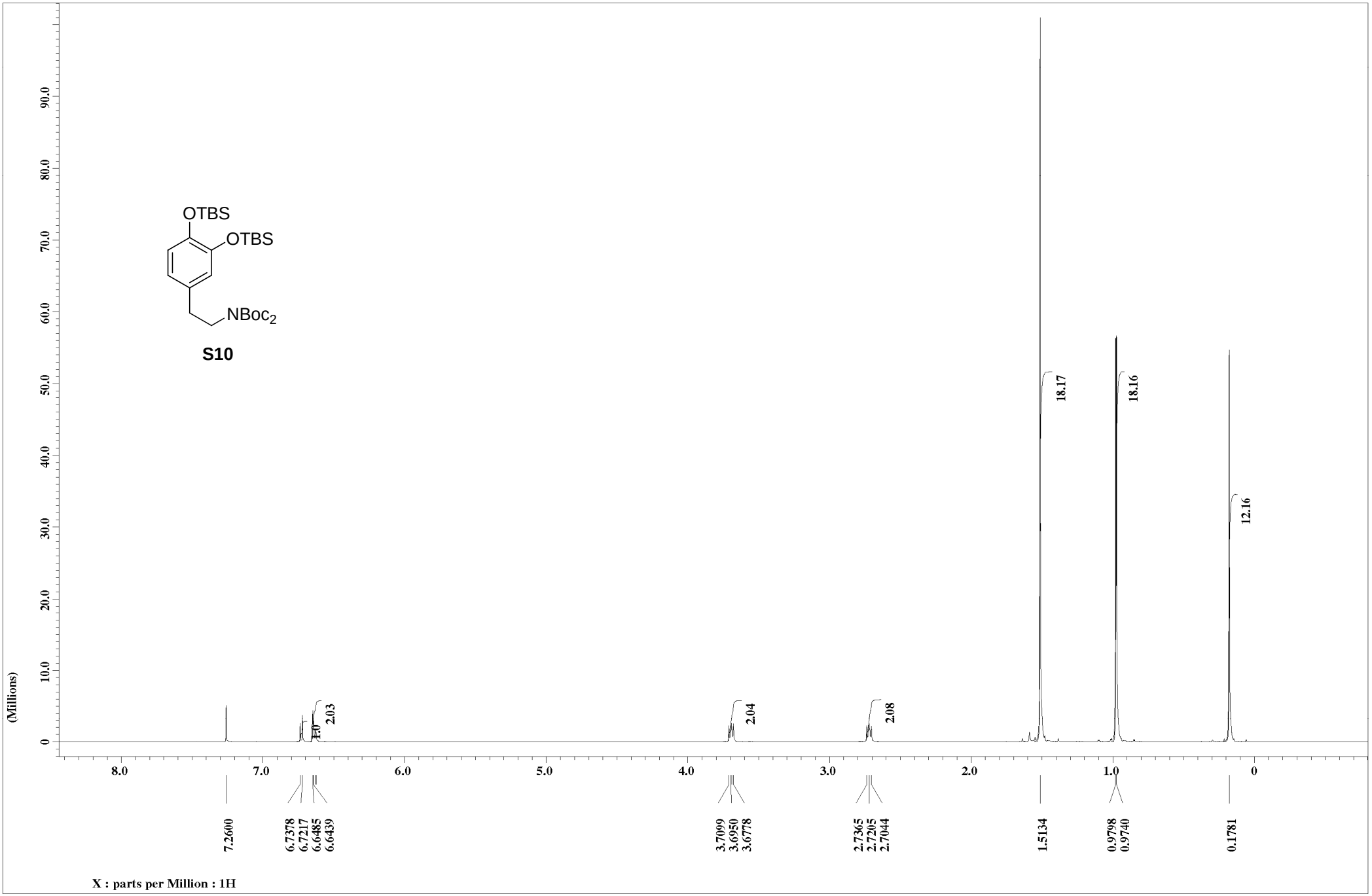

OH
OH
Ph
TsN
1f
300.0
200.0
100.0
0
(Millions)
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
143.1292
143.0338
141.6889
138.0071
129.3368
128.7168
128.2685
127.6103
127.1239
126.8282
115.2868
114.9434
77.2575
77.0000
76.7520
58.8104
39.0661
26.2561
21.3820
X : parts per Million : 13C

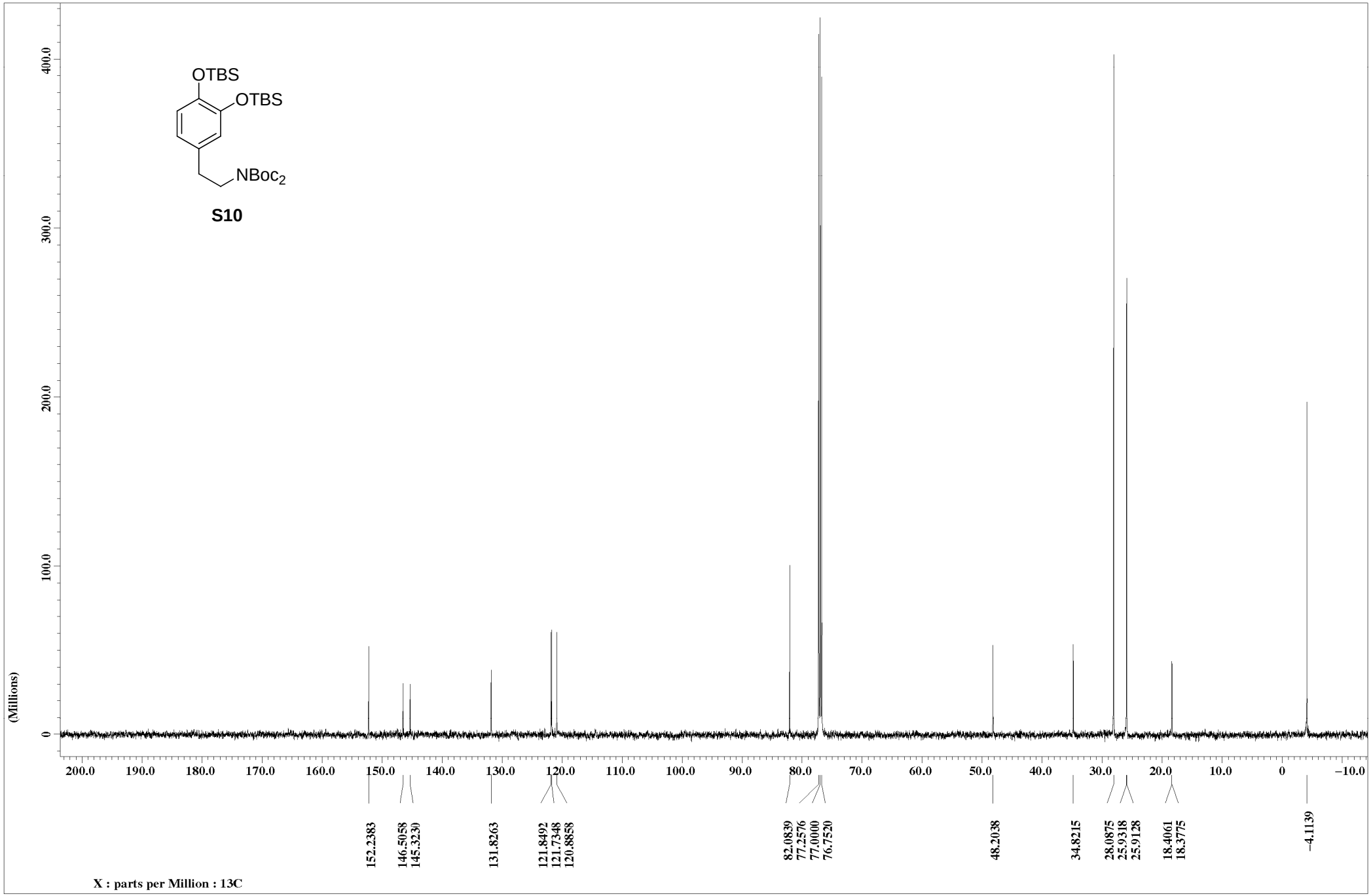

OH
OH
NHBoc
S8
(Millions)
40.0
30.0
20.0
10.0
0
1.93
0.82
0.98
1.0
1.03
2.09
2.55
9.35
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.7034
6.6295
6.6135
6.5562
6.5528
6.4222
6.4176
3.0405
3.0233
3.0118
2.5045
2.4873
2.4725
1.4670
1.3708
1.1143
0.0000
X : parts per Million : 1H

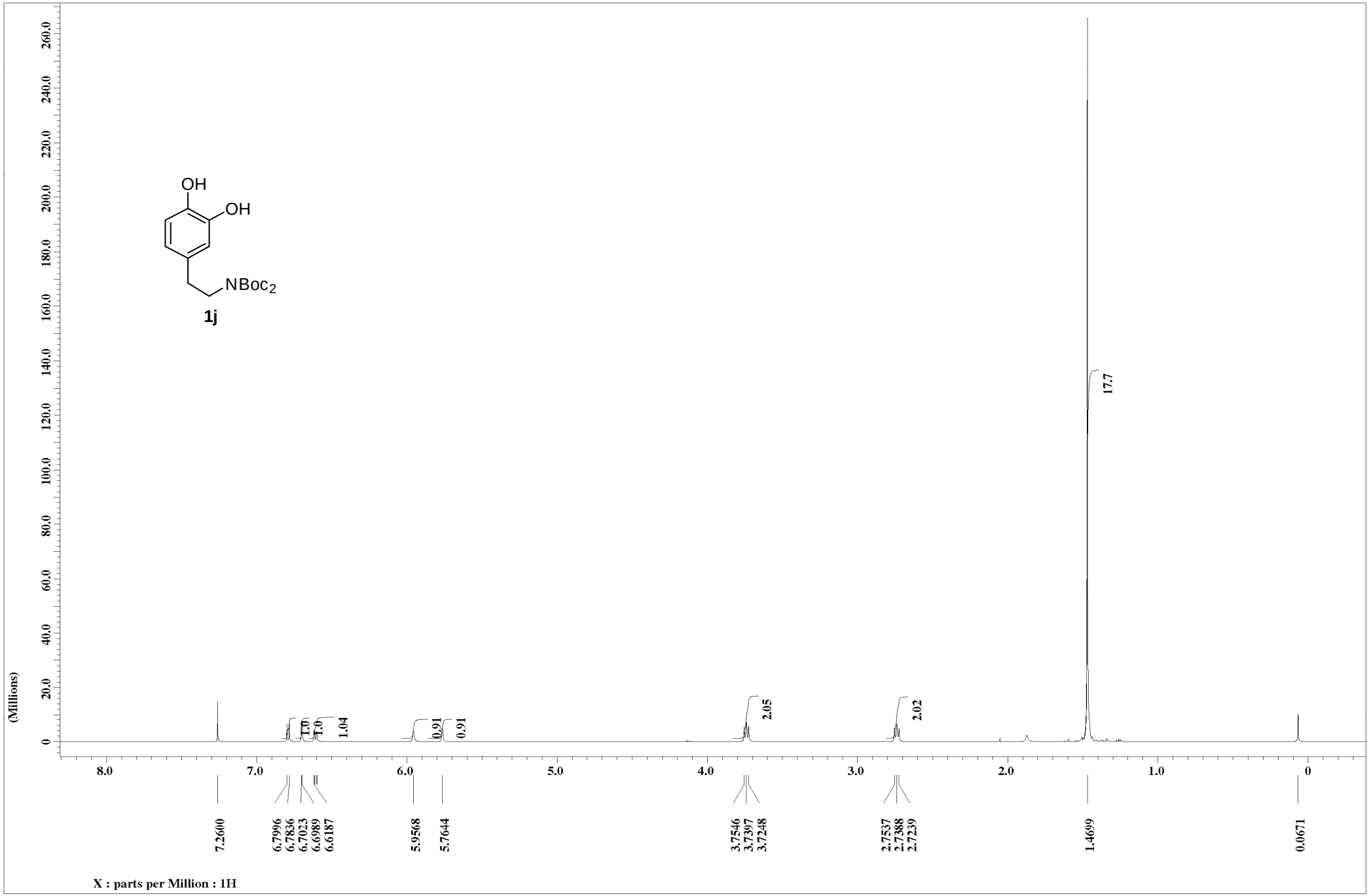

OH
OH
NHBoc
S8
(Millions)
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
155.5346
145.0615
143.5067
130.2199
119.2222
115.9982
115.4832
77.4920
42.0381
40.0160
39.8538
39.6821
39.5200
39.3483
39.1861
39.0144
28.3315
X : parts per Million : 13C

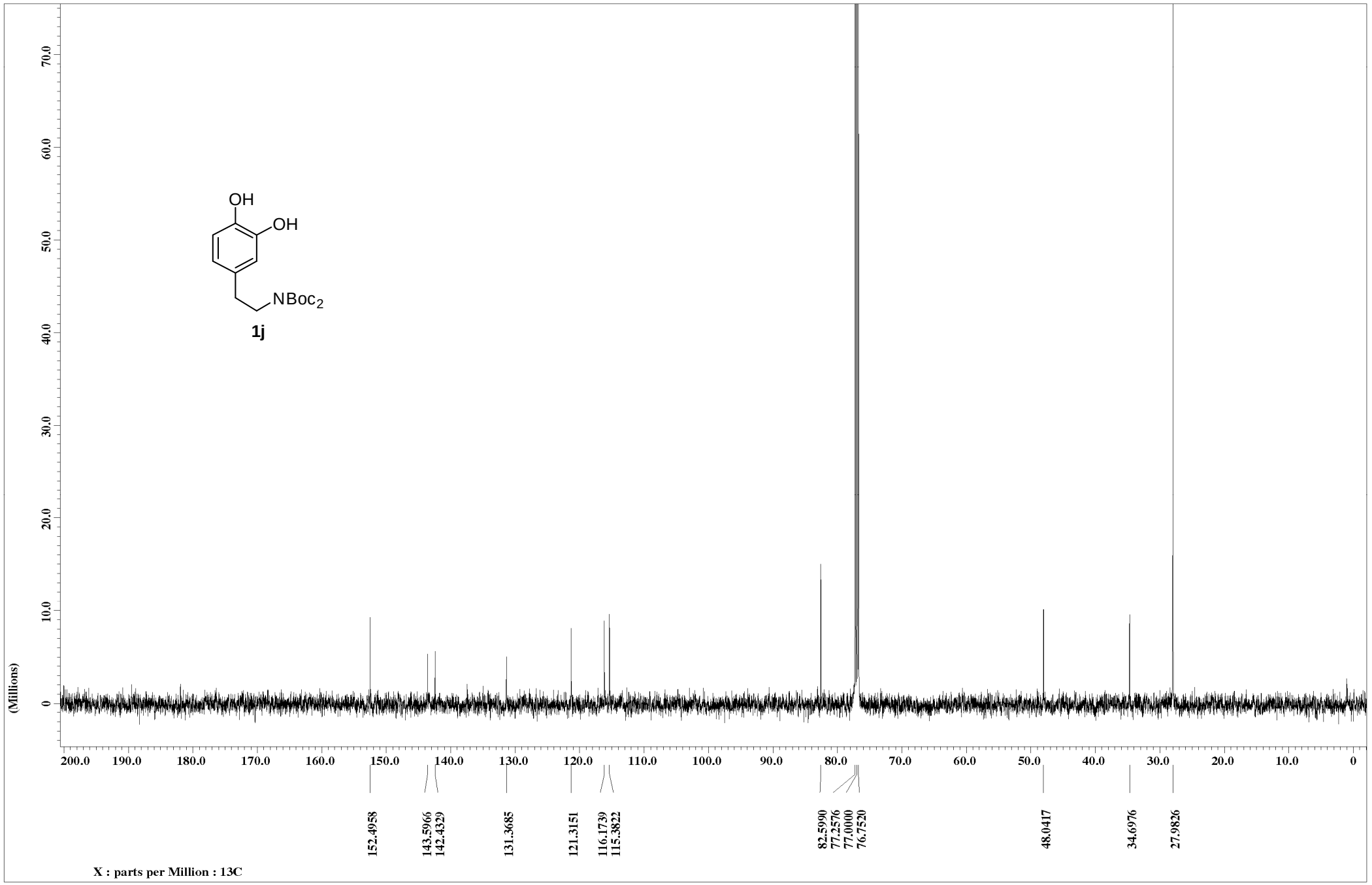

OTBS
OTBS
NHBoc
S9
(Millions)
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.0
2.03
0.71
2.05
2.08
4.85
9.22
18.68
12.43
7.2600
6.7561
6.7401
6.6427
6.6382
4.4898
3.3228
3.3114
3.2954
2.6655
2.6518
2.6392
1.5558
1.4298
0.9821
0.9786
0.1907
0.1850
X : parts per Million : 1H

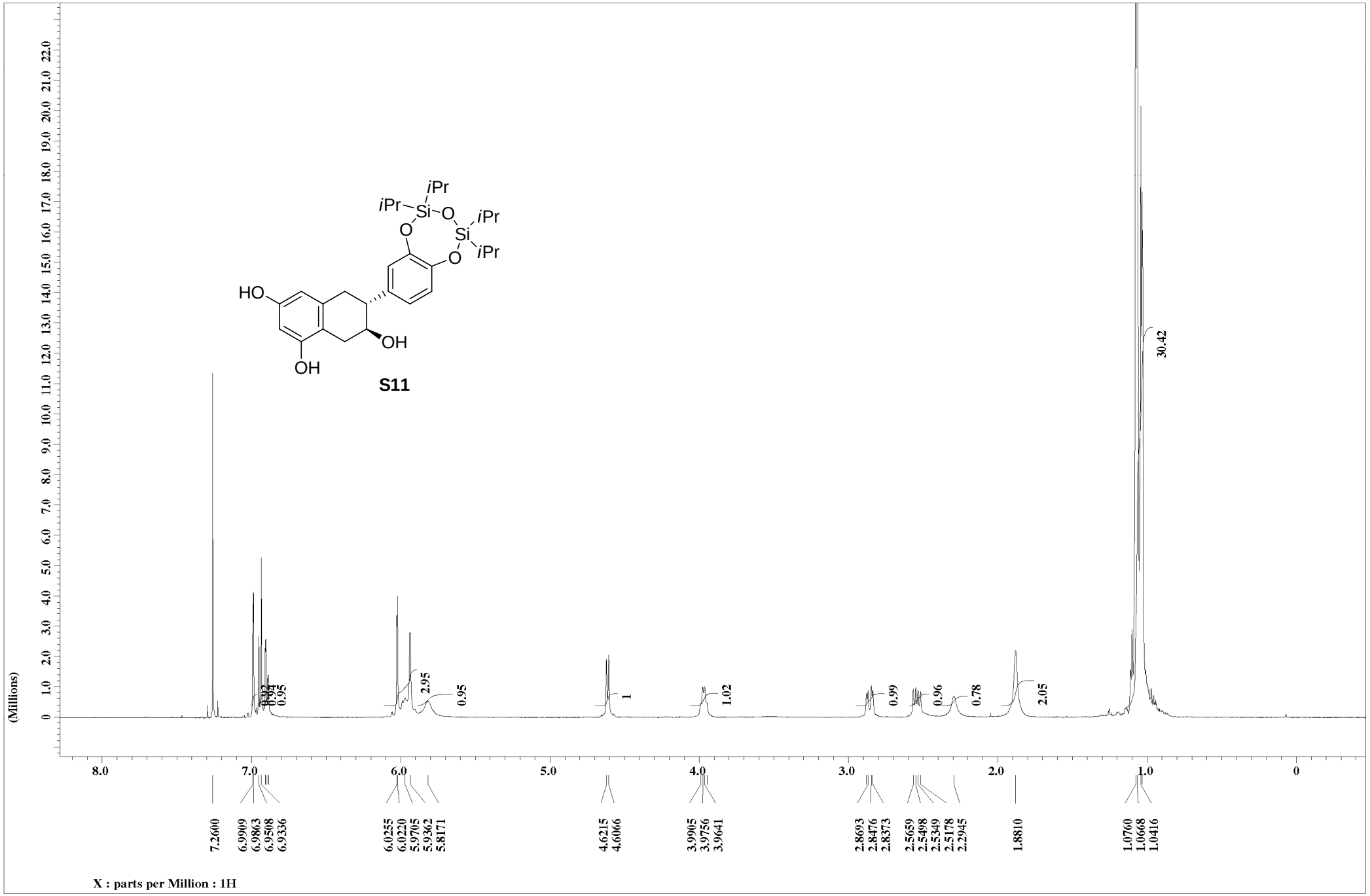

OTBS
OTBS
NHBoc
S9
(Millions)
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
155.8152
146.6393
145.3421
132.0457
121.6585
121.5631
121.0385
77.2576
77.0000
76.7520
41.8036
35.3557
28.4023
25.9223
18.4156
−4.0567
−4.1234
X : parts per Million : 13C

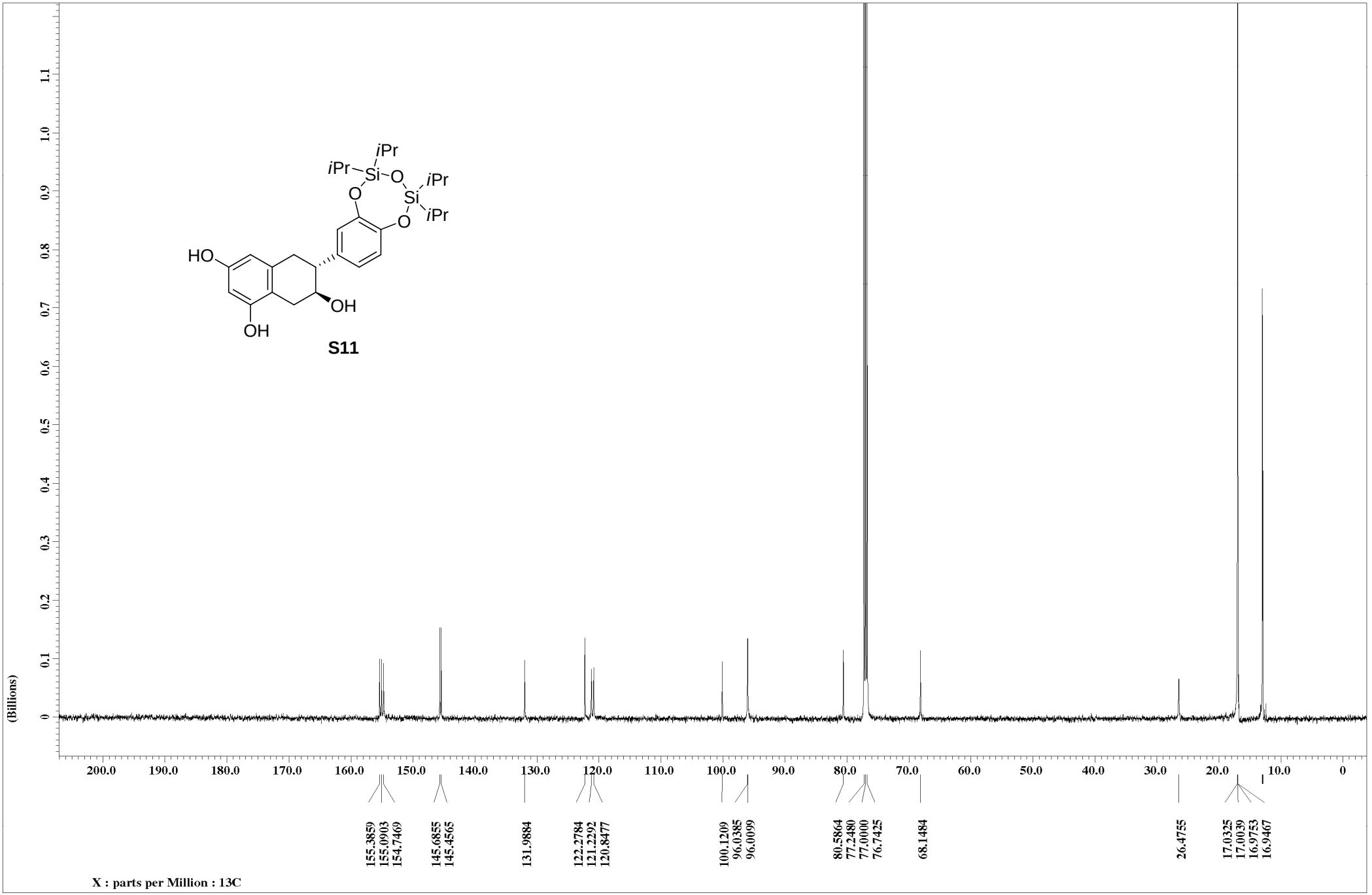

OTBS
OTBS
NBoc2
S10
(Millions)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
18.17
18.16
12.16
2.03
1.0
2.04
2.08
7.2600
6.7378
6.7217
6.6485
6.6439
3.7099
3.6950
3.6778
2.7365
2.7205
2.7044
1.5134
0.9798
0.9740
0.1781
X : parts per Million : 1H

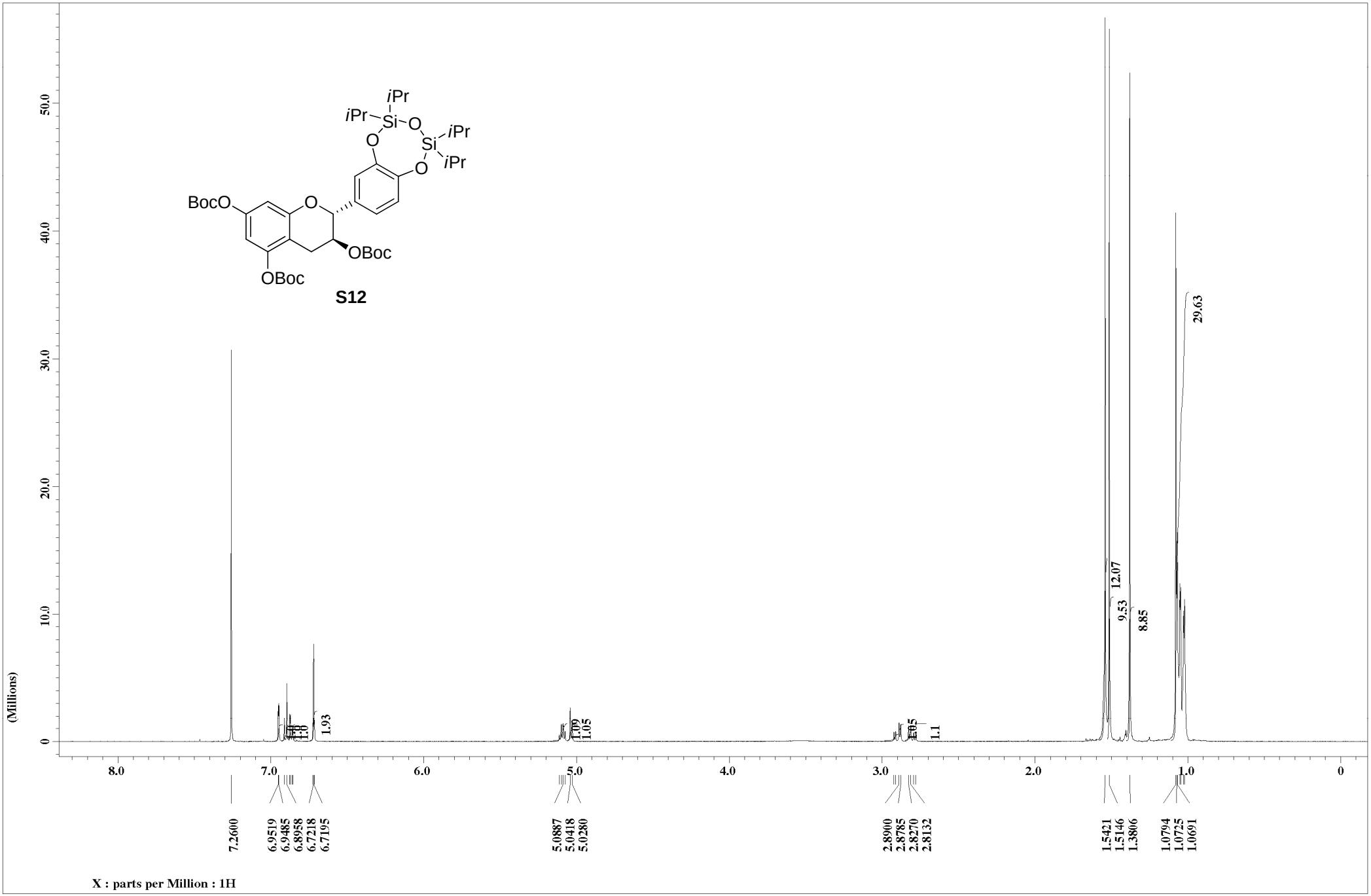

OTBS
OTBS
NBoc2
S10
400.0
300.0
200.0
100.0
0
(Millions)
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0
152.2383
146.5058
145.3230
131.8263
121.8492
121.7348
120.8858
82.0839
77.2576
77.0000
76.7520
48.2038
34.8215
28.0875
25.9318
25.9128
18.4061
18.3775
−4.1139
X : parts per Million : 13C

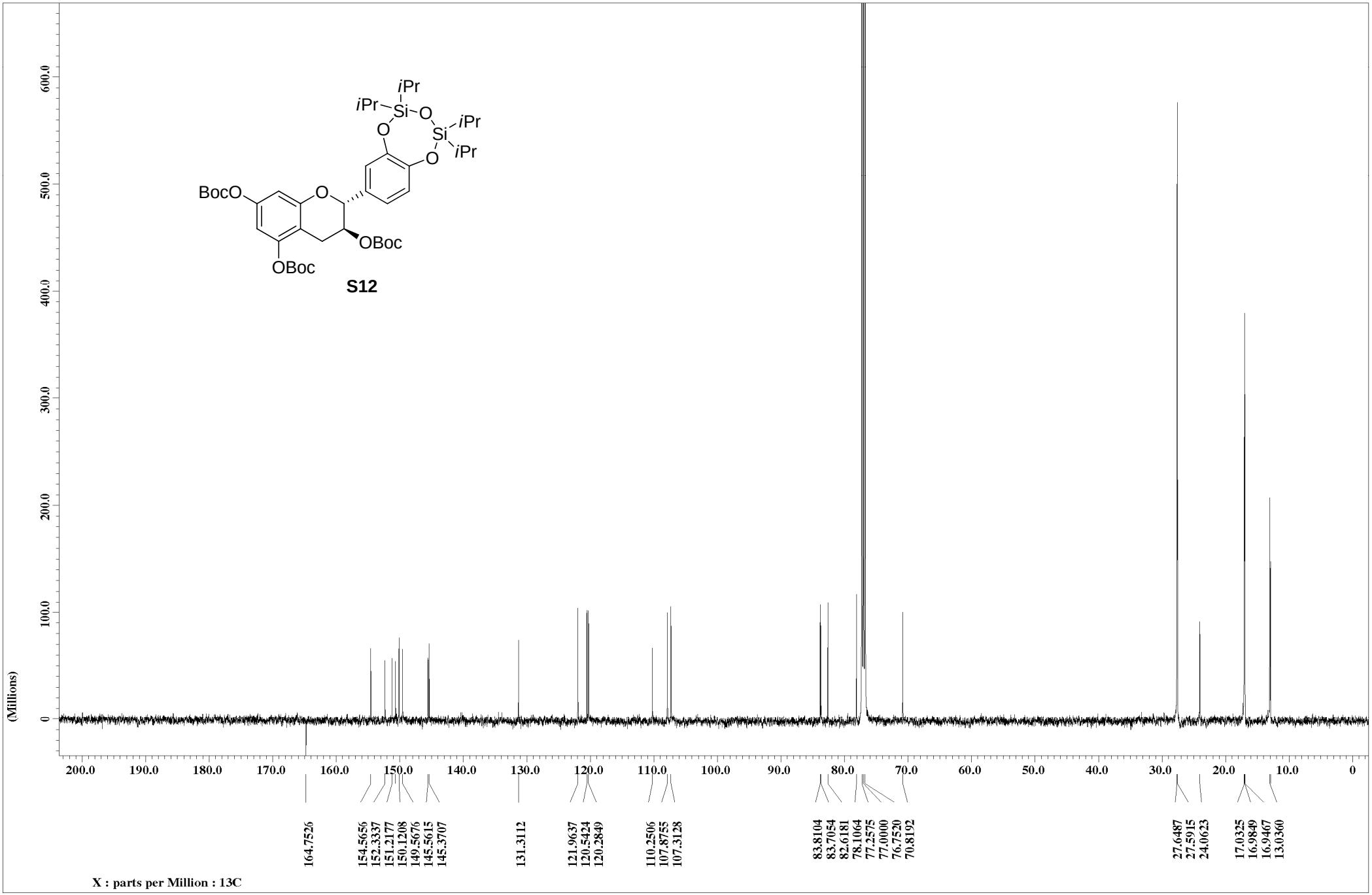

OH
OH
NBoc2
1j
(Millions)
260.0
240.0
220.0
200.0
180.0
160.0
140.0
120.0
100.0
80.0
60.0
40.0
20.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
17.7
1.0
1.0
1.04
0.91
0.91
2.05
2.02
7.2600
6.7996
6.7836
6.7023
6.6989
6.6187
5.9568
5.7644
3.7546
3.7397
3.7248
2.7537
2.7388
2.7239
1.4699
0.0671
X : parts per Million : 1H

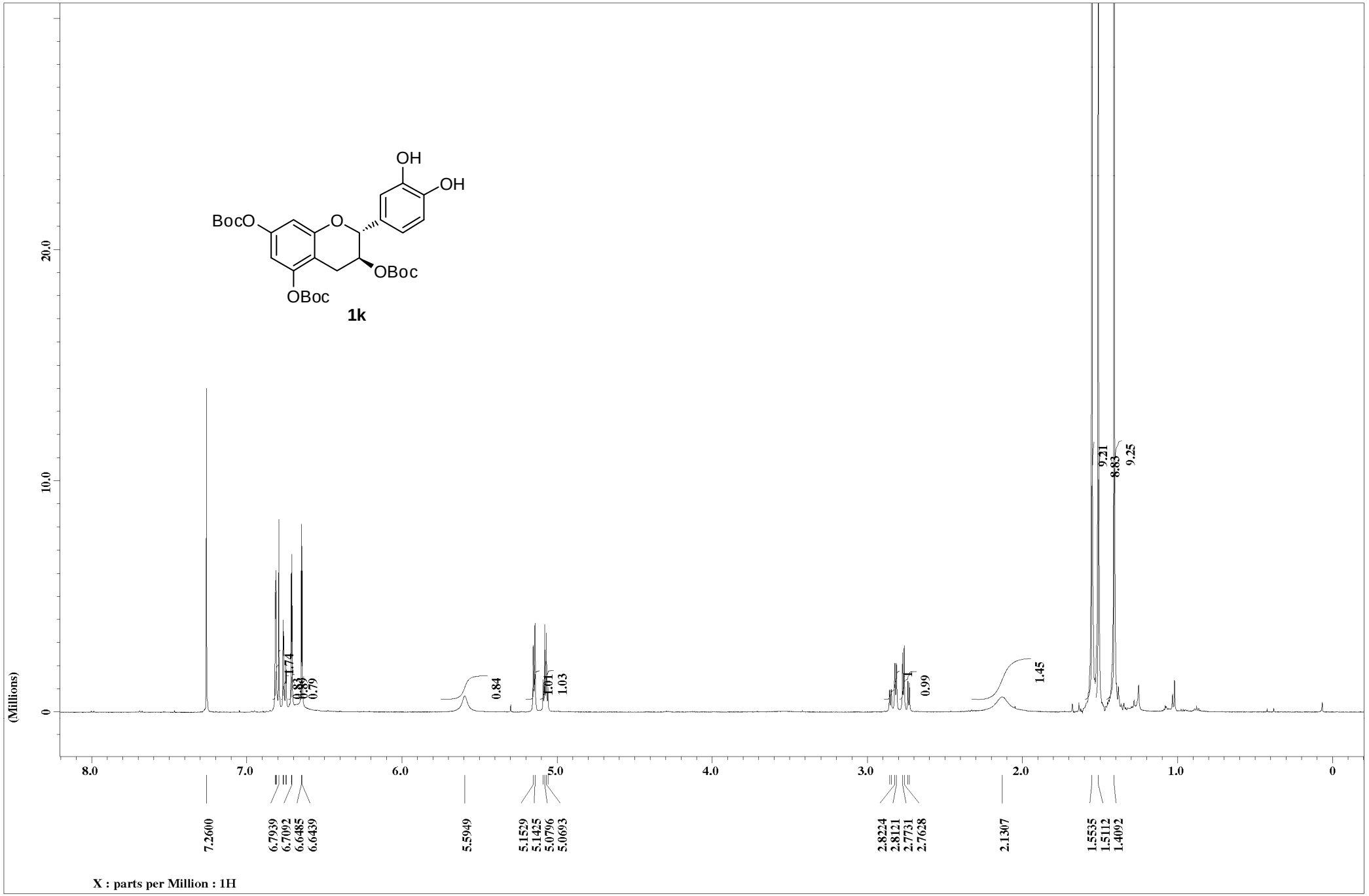

OH
OH
NBoc2
1j
(Millions)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
152.4958
143.5966
142.4329
131.3685
121.3151
116.1739
115.3822
82.5990
77.2576
77.0000
76.7520
48.0417
34.6976
27.9826
X : parts per Million : 13C

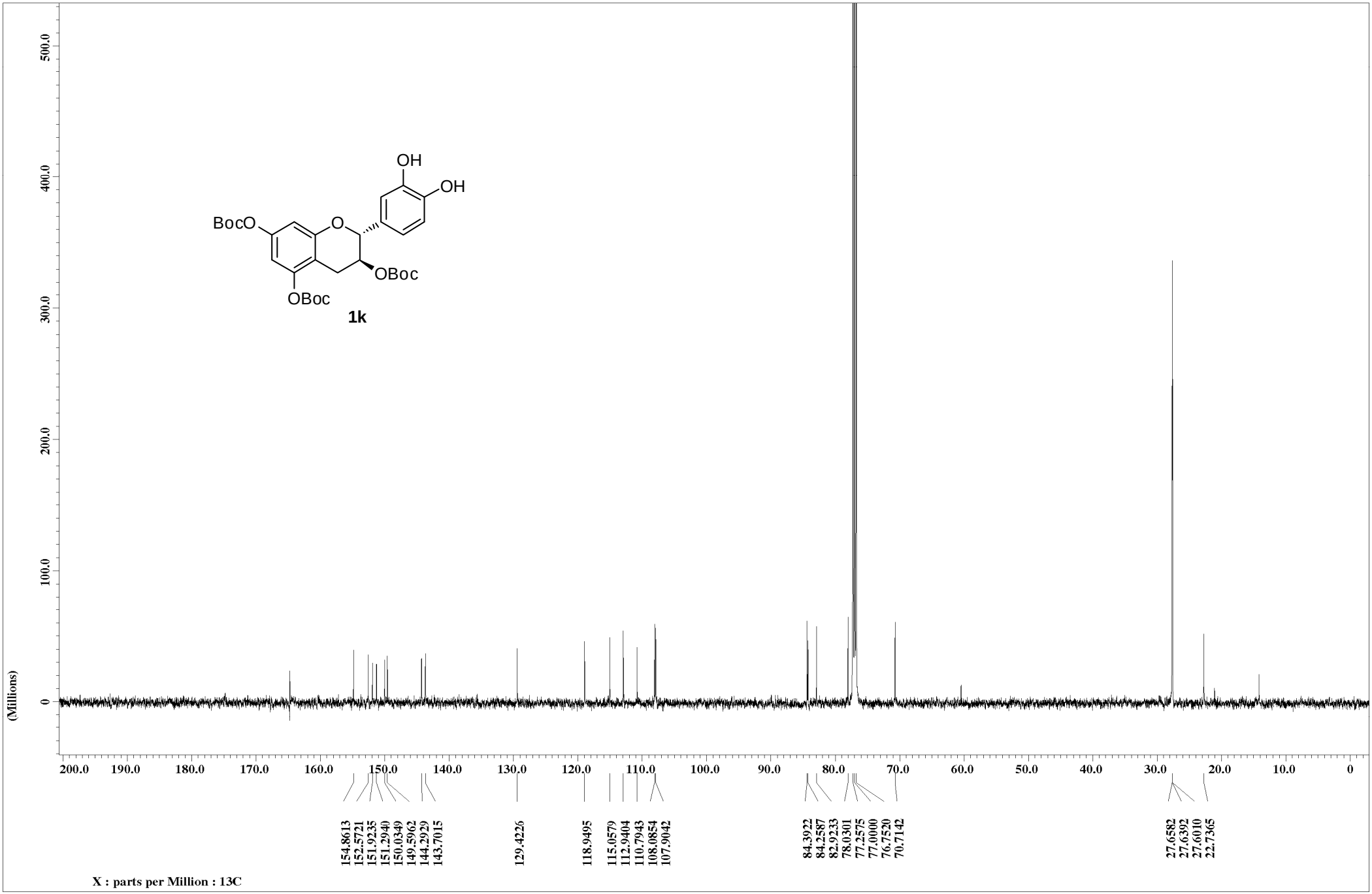

iPr
iPr
Si
O
iPr
O
Si
iPr
O
HO
OH
OH
S11
(Millions)
22.0
21.0
20.0
19.0
18.0
17.0
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
30.42
0.95
0.95
2.95
0.95
1
1.02
0.99
0.96
0.78
2.05
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2600
6.9909
6.9863
6.9508
6.9336
6.0255
6.0220
5.9705
5.9362
5.8171
4.6215
4.6066
3.9905
3.9756
3.9641
2.8693
2.8476
2.8373
2.5659
2.5498
2.5349
2.5178
2.2945
1.8810
1.0760
1.0668
1.0416
X : parts per Million : 1H

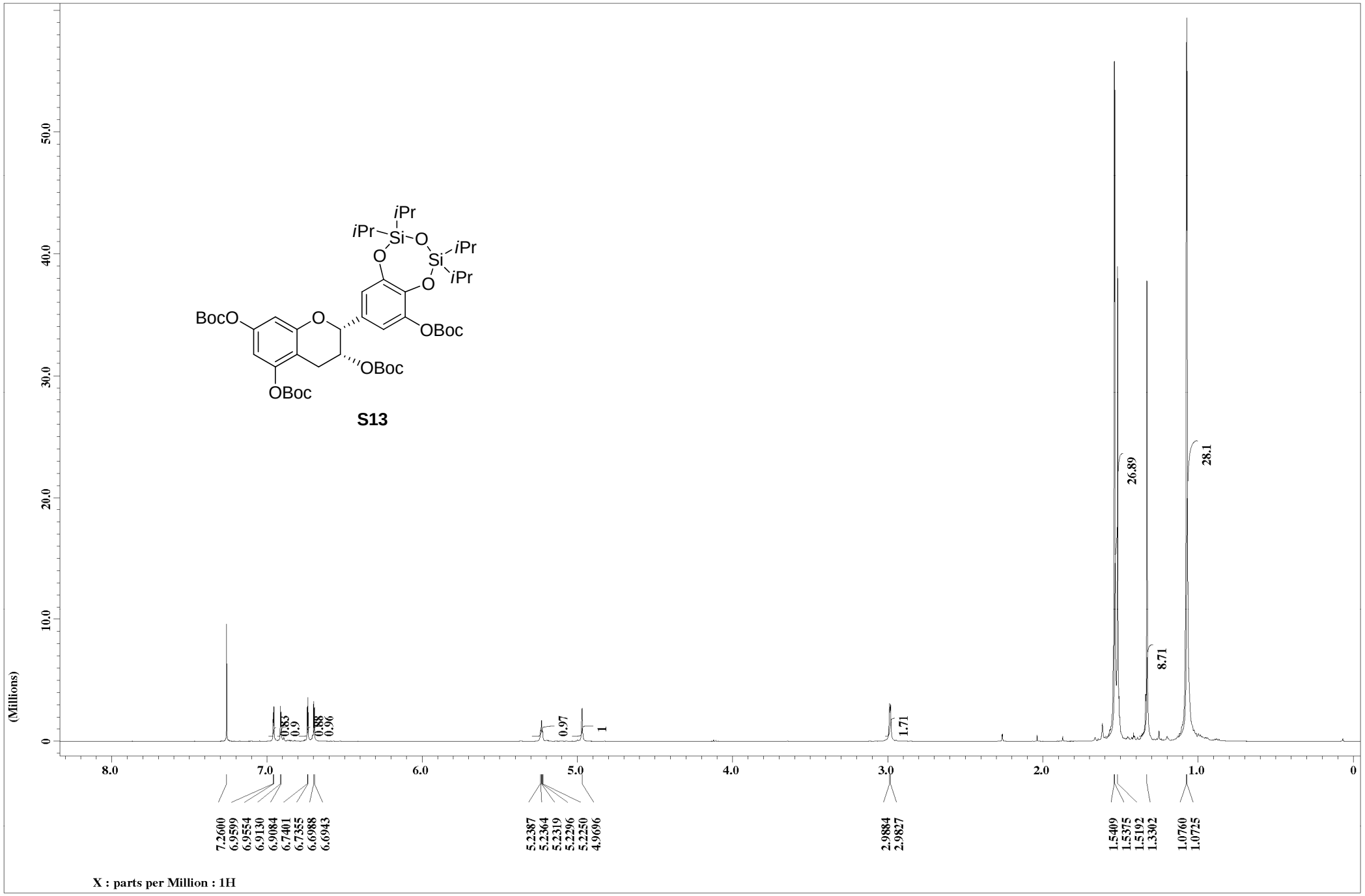

iPr
iPr
Si
O
iPr
O
Si
iPr
O
HO
OH
OH
S11
(Billions)
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
155.3859
155.0903
154.7469
145.6855
145.4565
131.9884
122.2784
121.2292
120.8477
100.1209
96.0385
96.0099
80.5864
77.2480
77.0000
76.7425
68.1484
26.4755
17.0325
17.0039
16.9753
16.9467
X : parts per Million : 13C

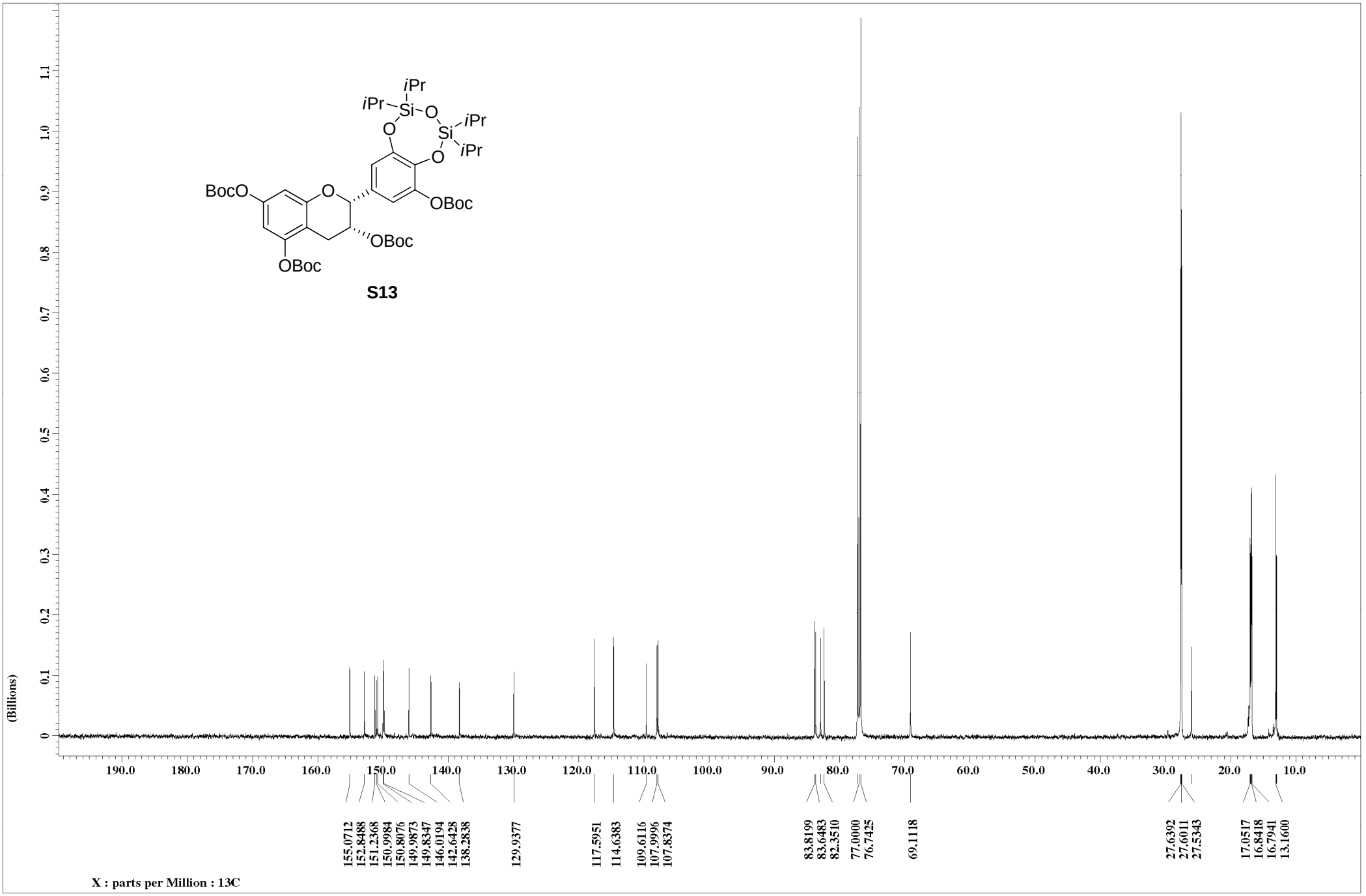

iPr
iPr
Si
O
O
Si
iPr
iPr
O
BocO
O
OBoc
OBoc
S12
(Millions)
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
29.63
12.07
9.53
8.85
1.93
1.1
7.2600
6.9519
6.9485
6.8958
6.7218
6.7195
5.0887
5.0418
5.0280
2.8900
2.8785
2.8270
2.8132
1.5421
1.5146
1.3806
1.0794
1.0725
1.0691
X : parts per Million : 1H

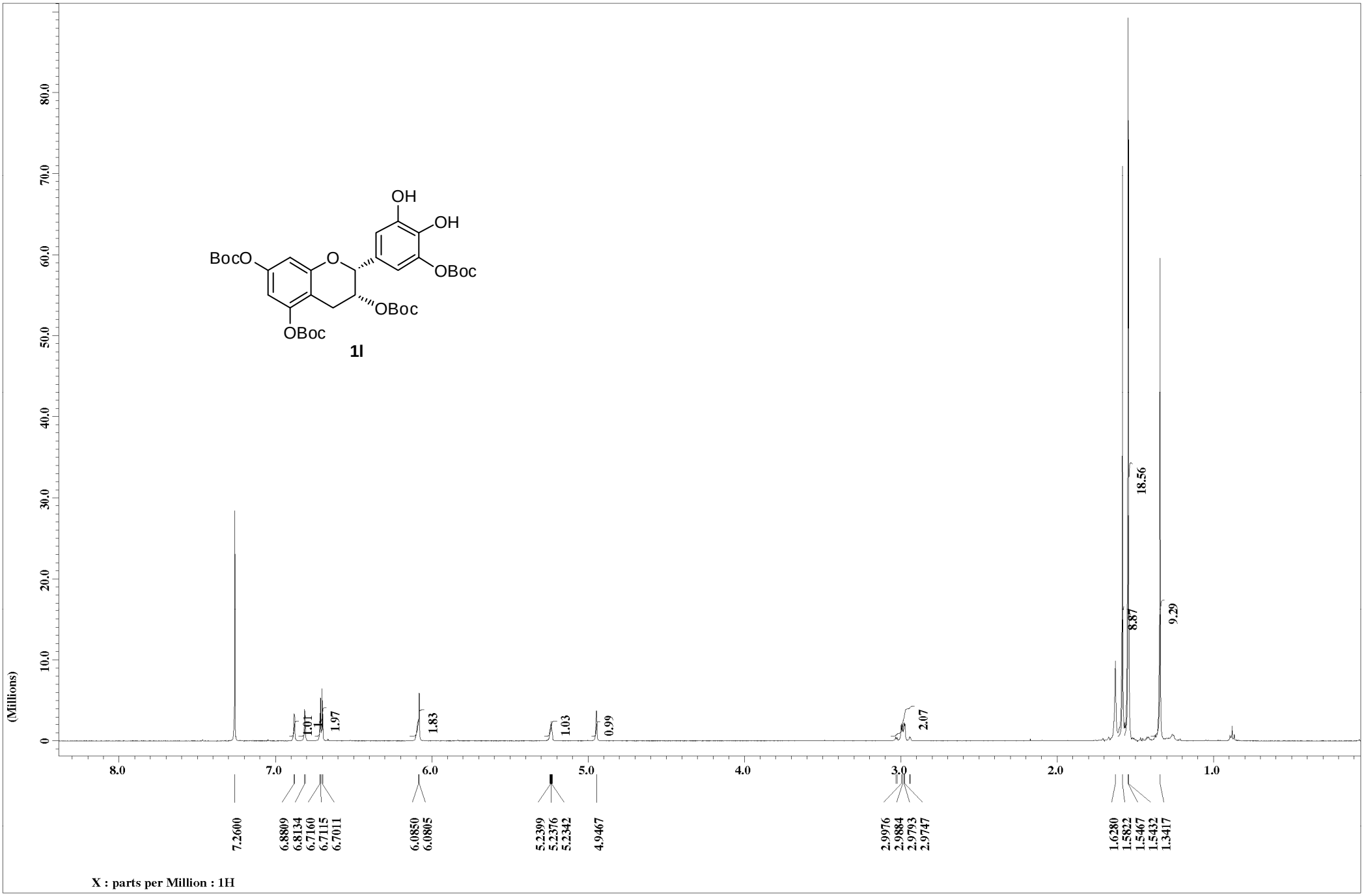

iPr
iPr
Si
O
O
Si
iPr
iPr
O
BocO
O
OBoc
OBoc
S12
(Millions)
600.0
500.0
400.0
300.0
200.0
100.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
164.7526
154.5656
152.3337
151.2177
150.1208
149.5676
145.5615
145.3707
131.3112
121.9637
120.5424
120.2849
110.2506
107.8755
107.3128
83.8104
83.7054
82.6181
78.1064
77.2575
77.0000
76.7520
70.8192
27.6487
27.5915
24.0623
17.0325
16.9849
16.9467
13.0360
X : parts per Million : 13C

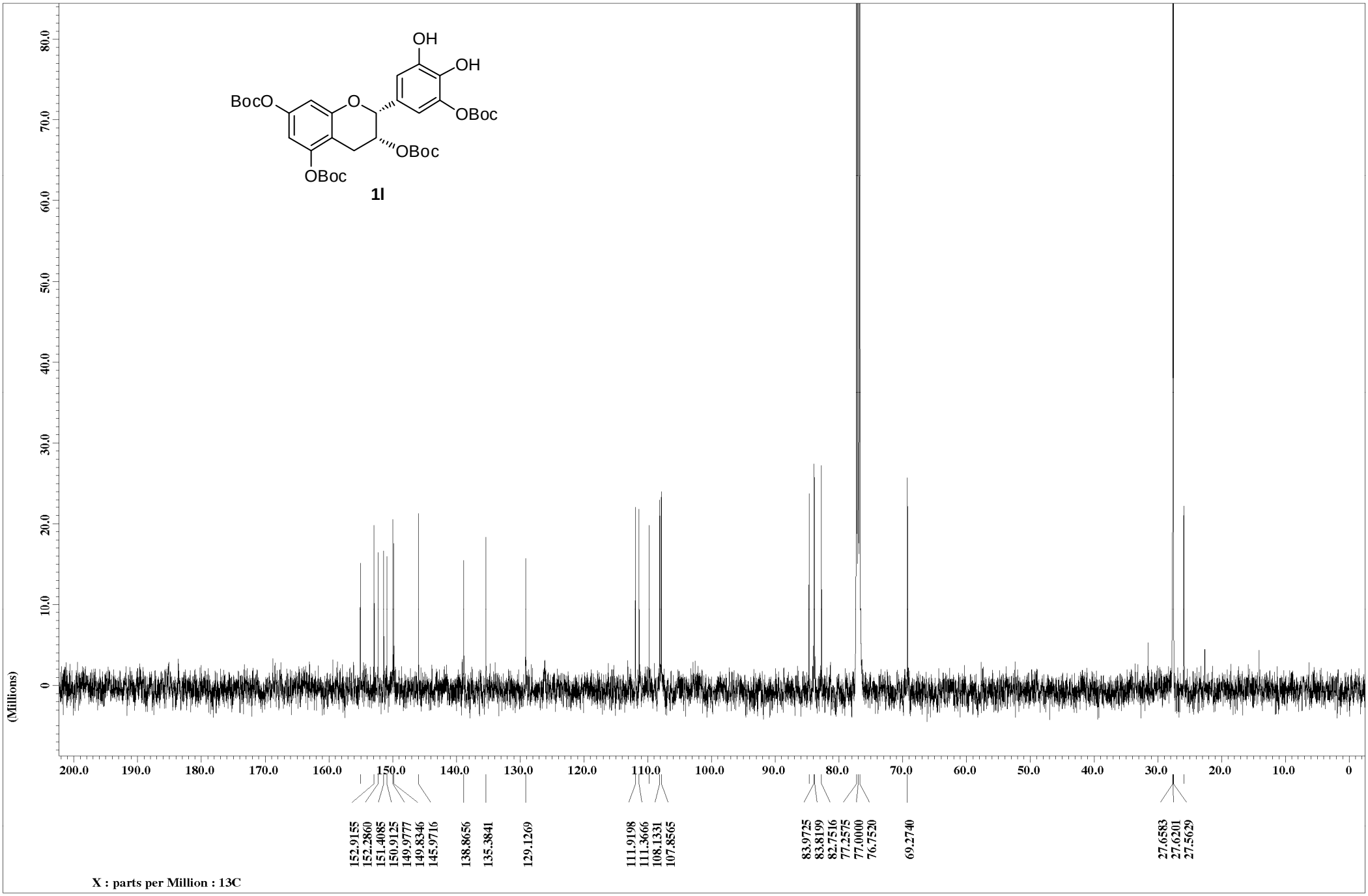

OH
OH
BocO
O
OBoc
OBoc
1k
20.0
10.0
0
(Millions)
9.21
8.83
9.25
1.74
0.83
0.79
0.84
1.01
1.03
0.99
1.45
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2600
6.7939
6.7092
6.6485
6.6439
5.5949
5.1529
5.1425
5.0796
5.0693
2.8224
2.8121
2.7731
2.7628
2.1307
1.5535
1.5112
1.4092
X : parts per Million : 1H


OH
OH
BocO
O
OBoc
OBoc
1k
(Millions)
500.0
400.0
300.0
200.0
100.0
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
154.8613
152.5721
151.9235
151.2940
150.0349
149.5962
144.2929
143.7015
129.4226
118.9495
115.0579
112.9404
110.7943
108.0854
107.9042
84.3922
84.2587
82.9233
78.0301
77.2575
77.0000
76.7520
70.7142
27.6582
27.6392
27.6010
22.7365
X : parts per Million : 13C


iPr
iPr
Si
O
iPr
O
Si
iPr
O
BocO
O
OBoc
OBoc
OBoc
S13
(Millions)
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2600
6.9599
6.9554
6.9130
6.9084
6.7401
6.7355
6.6988
6.6943
5.2387
5.2364
5.2319
5.2296
5.2250
4.9696
2.9884
2.9827
1.5409
1.5375
1.5192
1.3302
1.0760
1.0725
0.83
0.9
0.88
0.96
0.97
1
1.71
26.89
8.71
28.1
X : parts per Million : 1H


iPr
iPr
Si
O
iPr
O
Si
iPr
O
BocO
O
OBoc
OBoc
OBoc
S13
(Billions)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
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
155.0712
152.8488
151.2368
150.9984
150.8076
149.9873
149.8347
146.0194
142.6428
138.2838
129.9377
117.5951
114.6383
109.6116
107.9996
107.8374
83.8199
83.6483
82.3510
77.0000
76.7425
69.1118
27.6392
27.6011
27.5343
17.0517
16.8418
16.7941
13.1600
X : parts per Million : 13C


OH
OH
BocO
O
OBoc
OBoc
OBoc
1l
(Millions)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
1.01
1.97
1.83
1.03
0.99
2.07
18.56
8.87
9.29
7.2600
6.8809
6.8134
6.7160
6.7115
6.7011
6.0850
6.0805
5.2399
5.2376
5.2342
4.9467
2.9976
2.9884
2.9793
2.9747
1.6280
1.5822
1.5467
1.5432
1.3417
X : parts per Million : 1H


OH
OH
BocO
O
OBoc
OBoc
OBoc
1l
(Millions)
80.0
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
152.9155
152.2860
151.4085
150.9125
149.9777
149.8346
145.9716
138.8656
135.3841
129.1269
111.9198
111.3666
108.1331
107.8565
83.9725
83.8199
82.7516
77.2575
77.0000
76.7520
69.2740
27.6583
27.6201
27.5629
X : parts per Million : 13C