SUPPORTING INFORMATION

Tertiary and quaternary carbon formation via gallium-catalyzed nucleophilic addition of organoboronates to cyclopropanes

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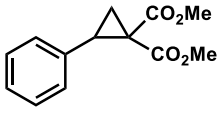
General considerations

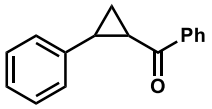
All reactions were carried out in flame-dried glassware under an argon atmosphere. THF, Et_2O, toluene, and CH_2Cl_2 were purged with argon and dried over activated alumina columns. Flash chromatography was performed on 60 Å silica gel (EMD Chemicals Inc.). Preparative plate chromatography was performed on EMD silica gel plates, 60 Å, with UV-254 indicator. Analytical thin layer chromatography was performed on EMD silica gel/TLC plates with fluorescent detector 254 nm. The ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a JEOL ECA-500 or ECX-400P spectrometer using residual solvent peak as an internal standard ($CDCl_3$: 7.26 ppm for ^{1}H NMR and 77.2 ppm for ^{13}C NMR). NMR yields were determined by the addition of 1.0 equivalent of methyl 4-nitrobenzoate as an internal standard to the crude reaction mixture. IR spectra were obtained using a ThermoNicolet Avatar 370 FT-IR instrument. HRMS analyses were performed under contract by UT Austin's mass spectrometric facility via ESI method and a US10252005 instrument. Commercially available compounds were purchased from Aldrich, Acros, Ark Pharm, and Alfa Aesar and were used without further purification. Chemical names were generated using Cambridgesoft ChemBioDraw Ultra 10.0.

1. Preparation of starting materials

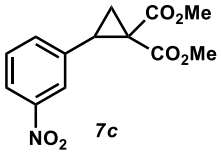
Cyclopropanes ***7a***,[1] ***7b***,[2] ***7c***,[3] ***7d***,[4] ***7e***,[4] ***7f***,[5] ***7g***,[6] ***11a***,[7] ***11c***,[7] ***11e***,[7] and ***11i***[8] were prepared according to literature procedures. Compound ***7h*** is commercially available. The other cyclopropanes were synthesized by procedure A (see below).



7a



7b



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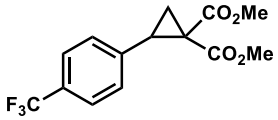

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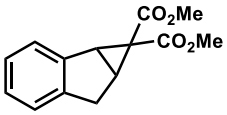

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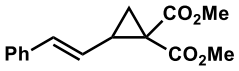

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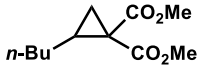

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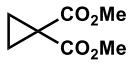

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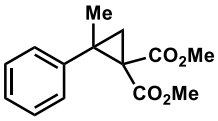

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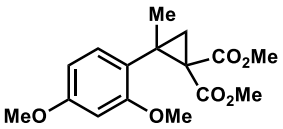

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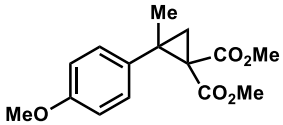

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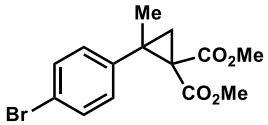

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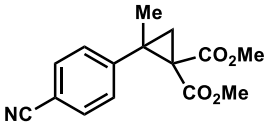
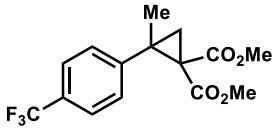


11e



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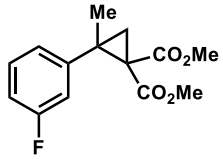

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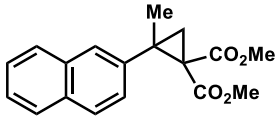
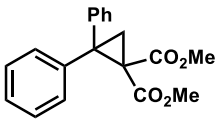


11h



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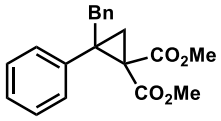
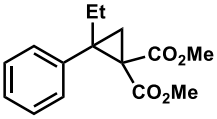


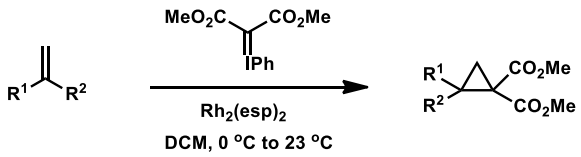
11j



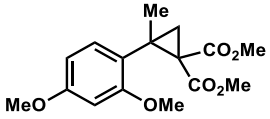
11k

[1] A. F. G. Goldberg, N. R. O'Connor, R. A. Craig, B. M. Stoltz, *Org. Lett.*, **2012**, *14*, 5314.
[2] Miyazawa, Kazuki; Koike, Takashi; Akita, Munetaka, Chem. Eur. J., **2015**, *21*, 11677 .
[3] Mueller, Paul; Fernandez, Daniel, Helv. Chim. Acta, **1995** , *78*, 947.
[4] Chenjie Zhu, Akira Yoshimura, Lei Ji, Yunyang Wei, Victor N. Nemykin, Viktor V. Zhdankin, *Org. Lett.*, **2012**, *14*, 3170.
[5] Marija Skvorcova, Liene Grigorjeva, Aigars Jirgensons, *Org. Lett.*, **2015**, *17*, 2902.
[6] Se´bastien R. Goudreau, David Marcoux, Andre´ B. Charette, *J. Org. Chem.*, **2009**, *74*, 470.
[7] Austin G. Smith, Michael C. Slade, Jeffrey S. Johnson, *Org. Lett.*, **2011**, *13*, 1996.
[8] Ivanov, K. L., Villemson, E. V., Budynina, E. M., Ivanova, O. A., Trushkov, I. V., Melnikov, M. Ya., *Chem. Eur. J.*, **2015**, *21*, 4975.

General procedure A



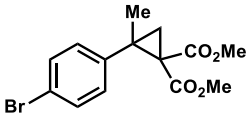
To a flame-dried flask equipped with a stir bar was added olefin (1 equiv) under Argon. Dry DCM (0.2 M) was then added and the reaction mixture was degassed for 10 minutes. After the reaction was cooled to 0 ^{o}C, $Rh_2(esp)_2$ (1 mol%) was added, followed by the addition of iodonium ylide[9] (1.1 equiv) in one portion. The reaction was stirred at this temperature for 3 hours under Argon. After completion monitored by TLC, the solvent was removed via rotary evaporation. The residue was purified via flash column chromatography with a gradient of appropriate eluent on silica gel.



Dimethyl 2-(2,4-dimethoxyphenyl)-2-methylcyclopropane-1,1-dicarboxylate (*11b*)

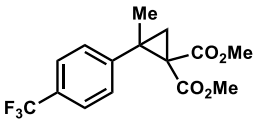
The title compound was synthesized from 2,4-dimethoxy-1-(prop-1-en-2-yl)benzene (534 mg, 3.0 mmol) following general procedure A. After purification via flash column chromatography with a gradient of 10 – 30% ethyl acetate in hexanes as eluent, the product was obtained in 59% yield (545 mg, 1.77 mmol) as a colorless oil. **^{1}H NMR**: (400 MHz, $CDCl_3$): δ 7.07 (d, J = 8.2 Hz, 1H), 6.44 – 6.34 (m, 2H), 3.81 (s, 3H), 3.77 (s, 6H), 3.44 (s, 3H), 1.96 (bs, 1H), 1.67 (d, J = 4.6 Hz, 1H), 1.37 (s, 3H). **^{13}C NMR**: (101 MHz, $CDCl_3$) δ 169.2, 168.9, 160.0, 158.8, 130.1, 122.6, 104.1, 98.6, 55.3, 52.4, 52.0, 39.9, 34.5, 26.4, 23.2. **HRMS**-ESI m/z: [M+Na], calculated for $C_{16}H_{20}O_6$: 331.1158; found 331.1165. **IR (neat):** 2962, 1736, 1720, 1508, 1434, 1208, 1030, 835, 803 cm^{-1}. **R_f**: 0.25 in 20% EtOAc/hexanes.

[9]Honglei Liu, Chunhao Yuan, Yang Wu, Yumei Xiao, Hongchao Guo, *Org. Lett.*, **2015**, *17*, 4220.



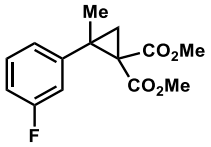
Dimethyl 2-(4-bromophenyl)-2-methylcyclopropane-1,1-dicarboxylate (*11d*)

The title compound was synthesized from 1-bromo-4-(prop-1-en-2-yl)benzene (591 mg, 3.0 mmol) following general procedure A. After purification via flash column chromatography with a gradient of 5 – 10% ethyl acetate in hexanes as eluent, the product was obtained in 90% yield (883 mg, 2.7 mmol) as a colorless oil. **^{1}H NMR**: (400 MHz, $CDCl_3$): δ 7.35 (dd, J = 6.4, 1.8 Hz, 2H), 7.11 (dd, J = 6.4, 1.8, 2H), 3.76 (s, 3H), 3.33 (s, 3H), 2.10 (d, J = 5.3 Hz, 1H), 1.64 (d, J = 5.3 Hz, 1H), 1.43 (s, 3H). **^{13}C NMR**: (101 MHz, $CDCl_3$) δ 168.5, 167.8, 140.3, 131.7, 131.4, 130.1, 129.8, 121.0, 52.7, 52.3, 40.34, 37.3, 24.9, 24.3. **HRMS**-ESI m/z: [M+Na], calculated for $C_{14}H_{15}BrO_4$: 349.0051; found 349.0052. **IR (neat):** 2950, 1750, 1732, 1435, 1260, 1206, 1157, 1031, 700 cm^{-1}. **R_f**: 0.35 in 20% EtOAc/hexanes.



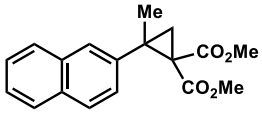
Dimethyl 2-methyl-2-(4-(trifluoromethyl)phenyl)cyclopropane-1,1-dicarboxylate (*11f*)

The title compound was synthesized from 1-(prop-1-en-2-yl)-4-(trifluoromethyl)benzene (558 mg, 3.0 mmol) following general procedure A. After purification via flash column chromatography with a gradient of 5 – 10% ethyl acetate in hexanes as eluent, the product was obtained in 68% yield (645 mg, 2.04 mmol) as a colorless oil. **^{1}H NMR**: (400 MHz, $CDCl_3$): δ 7.50 (d, J = 8.1 Hz, 2H), 7.37 (d, J = 8.1 Hz, 2H), 3.79 (s, 3H), 3.33 (s, 3H), 2.15 (d, J = 5.5 Hz, 1H), 1.71 (d, J = 5.5 Hz, 1H), 1.45 (s, 3H). **^{13}C NMR**: (101 MHz, $CDCl_3$) δ 168.3, 167.9, 145.4, 129.3 (q, J = 32.3 Hz), 128.8, 125.3 (q, J = 3.9 Hz), 124.2 (q, J = 271.9 Hz), 52.7, 52.3, 40.4, 37.3, 24.8, 24.3. **^{19}F NMR**: (376 MHz, CDCl3) δ -62.4 (s). **HRMS**-ESI m/z: [M+Na], calculated for $C_{15}H_{15}F_3O_4$: 339.0820; found 339.0823. **IR (neat):** 2951, 1727, 1435, 1322, 1103, 1064, 842 cm^{-1}. **R_f**: 0.30 in 20% EtOAc/hexanes.



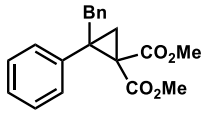
Dimethyl 2-(3-fluorophenyl)-2-methylcyclopropane-1,1-dicarboxylate (*11g*)

The title compound was synthesized from 1-fluoro-3-(prop-1-en-2-yl)benzene (408 mg, 3.0 mmol) following general procedure A. After purification via flash column chromatography with a gradient of 5 – 10% ethyl acetate in hexanes as eluent, the product was obtained in 49% yield (391 mg, 1.47 mmol) as a colorless oil. **^{1}H NMR**: (400 MHz, $CDCl_3$): δ 7.22 (dd, J = 14.2 , 7.8 Hz, 1H), 7.04 (dd, J = 7.8, 0.9 Hz, 1H), 6.96 (d, J =10.1 Hz, 1H), 6.92 – 6.84 (m, 1H), 3.80 (s, 3H), 3.37 (s, 3H), 2.15 (d, J = 5.2 Hz, 1H), 1.68 (d, J = 5.2 Hz, 1H), 1.47 (s, 3H). **^{13}C NMR**: (101 MHz, $CDCl_3$) δ 168.5, 167.9, 162.7 (d, J = 246.5 Hz), 143.8 (d, J = 7.2 Hz), 129.8 (d, J = 8.3 Hz), 124.0 (d, J = 2.6 Hz), 115.5 (d, J = 21.5 Hz), 114.4 (d, J = 20.5 Hz), 52.7, 52.3, 40.5, 37.4, 24.9, 24.3. **^{19}F NMR:** (376 MHz, $CDCl_3$) δ -113.1 (m). **HRMS**-ESI m/z: [M+Na], calculated for $C_{14}H_{15}FO_4$: 289.0852; found 289.0859. **IR (neat):** 2952, 1726, 1435, 1264, 1232, 1199, 1120, 909, 728, 698 cm^{-1}. **R_f**: 0.33 in 20% EtOAc/hexanes.



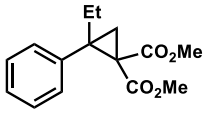
Dimethyl 2-methyl-2-(naphthalen-2-yl)cyclopropane-1,1-dicarboxylate (*11h*)

The title compound was synthesized from 2-(prop-1-en-2-yl)naphthalene (840 mg, 5.0 mmol) following general procedure A. After purification via flash column chromatography with a gradient of 5 – 10% ethyl acetate in hexanes as eluent, the product was obtained in 88% yield (1.311 g, 4.4 mmol) as a colorless oil. **^{1}H NMR**: (400 MHz, $CDCl_3$): 7.80 – 7.72 (m, 4H), 7.45 – 7.41 (m, 3H), 3.86 (s, 3H), 3.27 (s, 3H), 2.33 (d, J = 5.0 Hz, 1H), 1.79 (d, J = 5.0 Hz, 1H), 1.58 (s, 1H). **^{13}C NMR**: (101 MHz, $CDCl_3$) δ 168.9, 168.1, 138.7, 133.3, 132.6, 128.0, 127.9, 127.7, 126.9, 126.6, 126.2, 125.9, 52.8, 52.3, 40.7, 38.3, 25.1, 24.4. **HRMS**-ESI m/z: [M+Na], calculated for $C_{18}H_{18}O_4$: 321.1103; found 321.1109. **IR (neat):** 2950, 1724, 1432, 1223, 1116, 818, 748 cm^{-1}. **R_f**: 0.35 in 20% EtOAc/hexanes.



Dimethyl 2-benzyl-2-phenylcyclopropane-1,1-dicarboxylate (*11j*)

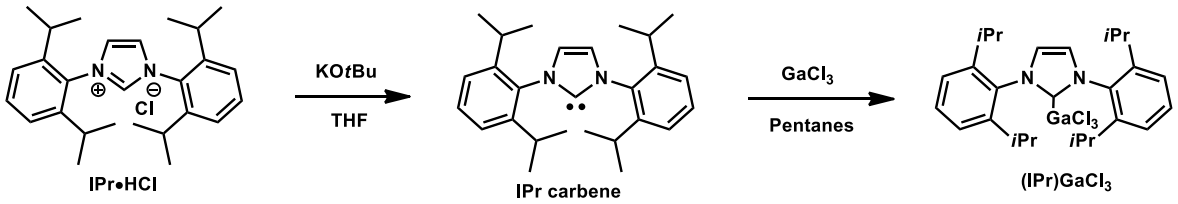
The title compound was synthesized from prop-2-ene-1,2-diyldibenzene (582 mg, 3.0 mmol) following general procedure A. After purification via flash column chromatography with a gradient of 5 – 10% ethyl acetate in hexanes as eluent, the product was obtained in 45% yield (437 mg, 1.35 mmol) as a colorless oil. **^{1}H NMR**: (400 MHz, $CDCl_3$): δ 7.19 – 7.13 (m, 3H), 7.13 – 7.08 (m, 3H), 7.07 – 7.01 (m, 2H), 6.86 – 6.77 (m, 2H), 3.89 (s, 3H), 3.35 (d, J = 14.2 Hz, 1H), 3.32 (s, 3H), 2.73 (d, J = 14.2 Hz, 1H), 2.20 (dd, J = 5.5, 1.2 Hz, 1H), 1.98 (d, J = 5.5 Hz, 1H). **^{13}C NMR**: (101 MHz, $CDCl_3$) δ 169.0, 167.8, 138.6, 138.1, 129.9, 129.4, 128.0, 127.8, 127.2, 126.5, 52.9, 52.3, 43.5, 42.8, 40.7, 23.8. **HRMS**-ESI m/z: [M+Na], calculated for $C_{20}H_{20}O_4$: 347.1259; found 347.1265. **IR (neat):** 1729, 1434, 1260, 1216, 1094, 756, 700 cm^{-1}. **R_f**: 0.35 in 20% EtOAc/hexanes.



Dimethyl 2-ethyl-2-phenylcyclopropane-1,1-dicarboxylate (*11k*)

The title compound was synthesized from but-1-en-2-ylbenzene (396 mg, 3.0 mmol) following general procedure A. After purification via flash column chromatography with a gradient of 5 – 10% ethyl acetate in hexanes as eluent, the product was obtained in 65% yield (511 mg, 1.95 mmol) as a colorless oil. **^{1}H NMR**: (500 MHz, $CDCl_3$): δ 7.31 – 7.19 (m, 5H), 3.82 (s, 3H), 3.32 (s, 3H), 2.14 (dd, J = 5.2, 1.3 Hz, 1H), 2.10 – 1.94 (m, 1H), 1.63 (d, J = 5.2 Hz, 1H), 1.35 (qd, J = 14.5, 7.3 Hz, 1H), 0.79 (t, J = 7.3 Hz, 1H). **^{13}C NMR**: (126 MHz, $CDCl_3$) δ 168.9, 168.0, 138.9, 129.4, 128.1, 127.2, 52.8, 52.2, 43.6, 41.1, 30.4, 23.6, 11.2. **HRMS**-ESI m/z: [M+Na], calculated for $C_{15}H_{18}O_4$: 285.1103; found 285.1107. **IR (neat):** 2949, 1726, 1433, 1278, 1219, 1096, 755, 700 cm^{-1}. **R_f**: 0.35 in 20% EtOAc/hexanes.

2. (IPr)$GaCl_3$ synthesis



A modified procedure of that described previously was used.[10] To a flame-dried 2-neck round bottom flask was added KO*t*Bu (269 mg, 2.4 mmol, 1.2 equiv) under Argon. After that, IPr•HCl (850 mg, 2.0 mmol, 1 equiv) was quickly added. The flask was then evacuated and refilled with Argon (3 times). THF (10 ml) was added via syringe and the mixture was stirred at room temperature under Argon. After 3 hours, the resulting green solution was concentrated under high vacuum for 5 hours. Dry PhMe (10 ml) was then added to the flask via syringe. The resulting mixture was gently heated by a heat gun. After the mixture became nearly homogeneous, it was quickly filtered through a thin pad of oven-dried Celite. The light-yellow filtrate was then concentrated under high vacuum to yield IPr carbene as a flocculent off-white solid (690 mg, 1.78 mmol, 89%). The product was stored in a 250 ml round bottom flask and quickly transferred to a glovebox for the next step.

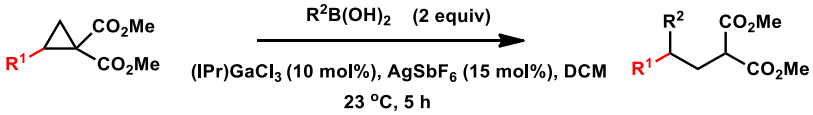
Following a reported procedure,[11] in a glovebox, 100 ml dry pentane was added to the flask containing the carbene product of the previous step. The resulting mixture was stirred for approximately 1 hour. After the IPr carbene was dissolved, $GaCl_3$ (313 mg, 1.78 mmol, 1 equiv) was then added in 1 portion, immediately forming a white precipitate. The solution was stirred for an additional 1 hour before taking it out the glovebox and then filtering it through a Buchner funnel. The white solid was washed with MeOH and dried under high vacuum, obtaining (IPr)$GaCl_3$ in 82% yield (832 mg, 1.46 mmol).**^{1}H NMR**: (400 MHz, Acetone-d_6): δ 8.14 (s, 2H), 7.54 (t, J = 7.8, 2H), 7.38 (d, J = 7.8 Hz, 4H), 2.61 (hept, J = 6.4 Hz, 4H), 1.35 (d, J = 6.8 Hz, 12H), 1.16 (d, J = 6.8 Hz, 12H). **^{13}C NMR:** (101 MHz, Acetone-d_6) δ 145.7, 133.0, 131.3, 127.5, 124.1, 29.0, 25.1, 22.1. **IR (neat):** 3160, 2964, 1466, 1119, 1061, 799, 776, 753 cm^{-1}. Spectral data are consistent with those reported in the literature.[10]

[10] Pompeo, M., Froese, R. D. J., Hadei, N. and Organ, M. G. *Angew. Chem. Int. Ed*., **2012**, *51*, 11354.
[11] (a) N. Marion, E. C. Escudero-Adán, J. Benet-Buchholz, E. D. Stevens, L. Fensterbank, M. Malacria, S. P. Nolan, *Organometallics* **2007**, *26*, 3256. (b) S. Tang, J. Monot, A. El-Hellani, B. Michelet, R. Guillot, C. Bour, V. Gandon, *Chem. Eur. J.* **2012**, *18*, 10239.

3. Procedure for addition reactions

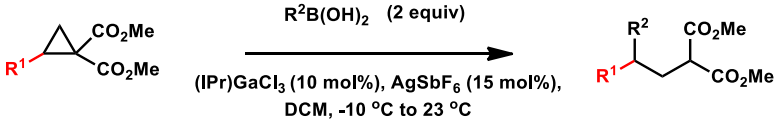
Note: *Reaction yields greatly depend on the quality of the Ga(III) catalyst and the presence of moisture.*

General procedure B



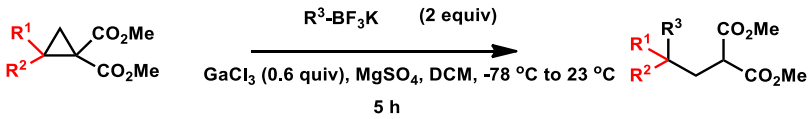
In a glovebox, to a 7 ml vial equipped with a stir bar, was added $AgSbF_6$ (10 mg, 0.03 mmol, 15 mol%). The vial was sealed by a screw cap with silicone septum and removed from the glovebox. The corresponding boronic acid (0.4 mmol, 2 equiv) was added, followed by the addition of the cyclopropane (0.2 mmol, 1 equiv) under Argon. DCM (3 ml) was then added to the vial via syringe. The mixture was allowed to stir under Argon, and $(IPr)GaCl_3$ (11 mg, 0.02 mmol, 10 mol%) was quickly added to the resulting suspension in one portion. The vial was sealed with parafilm and the reaction was stirred at room temperature under Argon for 5 hours. After reaction completion as monitored by TLC, the crude mixture was adsorbed onto silica gel via rotary evaporation. The desired product was purified via flash column chromatography on silica gel with appropriate eluents.

General procedure C

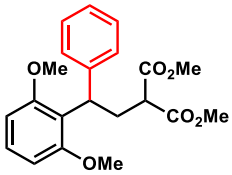


To a 7 ml vial equipped with a stir bar was added $AgSbF_6$ (10 mg, 0.03 mmol, 15 mol%) in a glovebox. The vial was sealed by a screw cap equipped with a silicone septum and taken out the glovebox. Under Argon, the corresponding boronic acid (0.4 mmol, 2 equiv) and $(IPr)GaCl_3$ (11 mg, 0.02 mmol, 10 mol%) were then added. The screw cap of the vial was wrapped completely by parafilm and the vial was cooled to -10 ^{o}C (NaCl/ice cooling bath). DCM (1 ml) was added and the reaction mixture was allowed to stir under Argon. The corresponding cyclopropane (0.2 mmol, 1 equiv) was then dissolved in 2 ml DCM and added dropwise to the reaction solution by syringe pump over 30 minutes at -10 ^{o}C. The reaction was allowed to warm up to room temperature and stirred until completion as monitored by TLC (2 to 5 hours). Silica gel was added to the reaction mixture. The crude product was then concentrated via rotary evaporation and purified via flash column chromatography on silica gel with appropriate solvents.

General procedure D



To a 7 ml vial equipped with a stir bar and a screw cap with silicone septum was added $MgSO_4$ (200 mg). The vial was then flame-dried under high vacuum to completely remove all traces of moisture. The vial was refilled with Argon, and then the corresponding potassium trifluoroborate salt (0.4 mmol, 2 equiv) was added. The reaction mixture was then cooled down to -78 ^oC after the screw cap was wrapped completely by parafilm. Under Argon, DCM (1 ml) was added. In the meantime, $GaCl_3$ (21 mg, 0.12 mmol, 60 mol%) was prepared in a 1 ml vial equipped with a silicone screw cap in a glovebox. The vial containing $GaCl_3$ was removed from the glovebox and DCM (0.2 ml) was added under Argon to dissolve the $GaCl_3$. After $GaCl_3$ was completely dissolved in DCM, the $GaCl_3$ solution was added to the reaction mixture at -78 ^oC by a microsyringe. The corresponding cyclopropanes (0.2 mmol, 1 equiv) was dissolved in DCM (2 ml) and added dropwise to the mixture over 30 minutes at -78 ^oC under Argon. The reaction was warmed up to room temperature over 5 hours. After completion as monitored by TLC, the crude material was adsorbed onto silica gel via rotary evaporation and purified by flash column chromatography on silica gel with appropriate solvents.



Dimethyl 2-(2-(2,6-dimethoxyphenyl)-2-phenylethyl)malonate (*9a*)

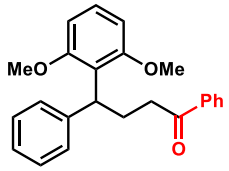
The title compound was synthesized from ***7a*** and (2,6-dimethoxyphenyl)boronic acid following general procedure B. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 99% yield (73.6 mg, 0.198 mmol) as a colorless oil.

*Procedure to synthesize **9a** in large scale:*

Following general procedure B, to a 50 ml round bottom flask equipped with a stir bar was added $AgSbF_6$ (34.3 mg, 0.1 mmol, 2 mol%) in a glove box. The flask was sealed by a rubber septum and took out the glove box. Under Argon atmosphere, (2,6-dimethoxyphenyl)boronic acid (1.81 g, 10.0 mmol, 2 equiv), cyclopropane ***7a*** (1.17 g, 5.0 mmol, 1 equiv), and DCM (25 ml) were added to the flask. (IPr)$GaCl_3$ (28 mg, 0.05 mmol, 1 mol%) was then added in one portion to the resulting suspension. The reaction was

allowed to stir for 48 h at room temperature. After reaction completion, the crude mixture was filtered through a celite bath, concentrated and purified via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent. The product was obtained in 91% yield (1.693 g, 4.55 mmol) as a colorless oil.

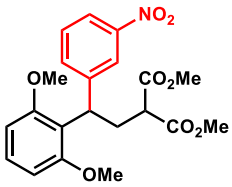
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.27 – 7.22 (m, 4H), 7.19 – 7.12 (m, 1H), 7.09 (d, J = 8.2 Hz, 1H), 6.44 (dd, J = 8.5 Hz, 2.8, 1H), 6.41 (d, J = 2.8 Hz, 1H), 4.32 (dd, J = 8.2, 7.8 Hz, 1H), 3.77 (s, 3H), 3.73 (s, 3H), 3.70 (s, 3H), 3.68 (s, 3H), 3.29 (dd, J = 7.8, 7.3 Hz, 1H), 2.68 – 2.54 (m, 2H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 170.1, 169.9, 159.5, 158.1, 143.9, 128.4, 128.1, 126.2, 124.3, 104.4, 98.7, 55.5, 55.4, 52.6, 52.6, 50.2, 40.6, 34.0. **HRMS**-ESI m/z: [M+Na], calculated for $C_{21}H_{24}O_6$: 395.1471; found 395.1475. **IR (neat):** 2952, 1731, 1609, 1585, 1452, 1435, 1206, 1154, 1031, 734, 699 cm^{-1}. **R_f**: 0.33 in 20% EtOAc/hexanes.



4-(2,6-dimethoxyphenyl)-1,4-diphenylbutan-1-one (*9b*)

The title compound was synthesized from ***7b*** and (2,6-dimethoxyphenyl)boronic acid following general procedure B. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 92% yield (66.2 mg, 0.184 mmol) as a colorless oil.

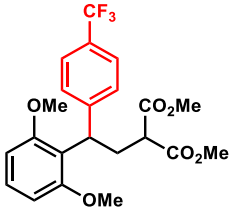
^{1}H NMR: (500 MHz, $CDCl_3$): δ 7.86 (dd, J = 8.3, 1.5 Hz, 2H), 7.53 – 7.50 (m, 1H), 7.43 – 7.38 (m, 2H), 7.29 – 7.24 (m, 4H), 7.17 – 7.11 (m, 2H), 6.44 (dd, J = 8.3, 2.3 Hz, 1H), 6.40 (d, J = 2.3 Hz, 1H), 4.38 (dd, J = 8.0, 8.0 Hz, 1H), 3.77 (s, 3H), 3.70 (s, 3H), 2.94 – 2.91 (m, 2H), 2.49 – 2.33 (m, 2H). **^{13}C NMR:** (126 MHz, $CDCl_3$) δ 200.4, 159.2, 158.0, 144.9, 137.1, 133.0, 128.6, 128.3, 128.2, 128.1, 128.1, 126.0, 125.5, 104.2, 98.7, 55.5, 55.4, 42.2, 37.2, 29.4. **HRMS**-ESI m/z: [M+Na], calculated for $C_{24}H_{24}O_3$: 383.1623; found 383.1624. **IR (neat):** 2936, 2360, 1683, 1610, 1505, 1450, 1290, 1208, 1034, 749, 699 cm^{-1}. **R_f**: 0.50 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2,6-dimethoxyphenyl)-2-(3-nitrophenyl)ethyl)malonate (*9c*)

The title compound was synthesized from ***7c*** and (2,6-dimethoxyphenyl)boronic acid following general procedure B. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 82% yield (68.4 mg, 0.164 mmol) as a colorless oil.

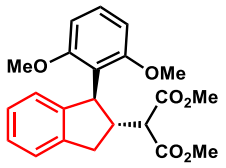
^{1}H NMR: (400 MHz, $CDCl_3$): δ 8.10 – 8.09 (m, 1H), 8.03 – 7.99 (m, 1H), 7.56 (d, J = 7.8 Hz, 1H), 7.40 (dd, J = 8.2, 7.8 Hz, 1H), 7.09 (d, J = 8.2 Hz, 1H), 6.47 (dd, J = 8.5, 2.3 Hz, 1H), 6.41 (d, J = 2.3 Hz, 1H), 4.38 (dd, J = 8.2, 8.2 Hz, 1H), 3.77 (s, 3H), 3.71 (s, 3H), 3.70 (s, 3H), 3.70 (s, 3H), 3.25 (dd, J = 7.3, 7.3 Hz, 1H), 2.65 (dd, J = 8.2, 7.3 Hz, 2H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 169.8, 169.6, 160.0, 158.1, 148.3, 146.4, 134.4, 129.2, 128.3, 122.9, 122.3, 121.4, 104.6, 98.9, 55.4, 52.8, 52.7, 49.9, 40.8, 33.4. **HRMS**-ESI m/z: [M+Na], calculated for $C_{21}H_{23}NO_8$: 440.1321; found 440.1327. **IR (neat):** 2953, 1731, 1609, 1526, 1505, 1348, 1206, 1155, 1032, 732, 686 cm^{-1}. **R_f**: 0.40 in 40% EtOAc/hexanes.



Dimethyl 2-(2-(2,6-dimethoxyphenyl)-2-(4-(trifluoromethyl)phenyl)ethyl)malonate (*9d*)

The title compound was synthesized from ***7d*** and (2,6-dimethoxyphenyl)boronic acid following general procedure B. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 95% yield (83.6 mg, 0.19 mmol) as a colorless oil.

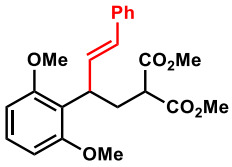
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.50 (d, J = 7.8 Hz, 2H), 7.34 (d, J = 8.2 Hz, 2H), 7.08 (d, J = 8.2 Hz, 1H), 6.46 (dd, J = 8.5, 2.3 Hz, 1H), 6.41 (d, J = 2.3 Hz, 1H), 4.35 (dd, J = 7.8, 8.2 Hz, 1H), 3.78 (s, 3H), 3.72 (s, 3H), 3.70 (s, 3H), 3.69 (s, 3H), 3.26 (dd, J = 6.9, 7.8 Hz, 1H), 2.69 – 2.55 (m, 2H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 169.9, 169.7, 159.8, 158.1, 148.7 (q, J = 32.3 Hz), 128.4, 128.3, 125.3 (q, J = 3.9 Hz), 124.4 (q, J = 271.9 Hz), 104.4, 98.8, 55.4, 52.7, 52.6, 50.1, 40.7, 33.6. **^{19}F NMR:** (376 MHz, $CDCl_3$) δ -62.2 (s). **HRMS**-ESI m/z: [M+Na], calculated for $C_{22}H_{23}F_3O_6$: 463.1344; found 463.1348. **IR (neat):** 2953, 1732, 1610, 1504, 1323, 1155, 1113, 830 cm^{-1}. **R_f**: 0.30 in 20% EtOAc/hexanes.



Dimethyl 2-(1-(2,6-dimethoxyphenyl)-2,3-dihydro-1H-inden-2-yl)malonate (*9e*)

The title compound was synthesized from ***7e*** and (2,6-dimethoxyphenyl)boronic acid following general procedure B. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 90% yield (69.1 mg, 0.18 mmol) as a colorless oil.

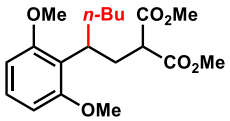
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.23 – 7.21 (m, 1H), 7.17 – 7.08 (m, 2H), 6.87 (d, J = 8.7 Hz, 1H), 6.83 (d, J = 7.8 Hz, 1H), 6.48 (d, J = 2.8 Hz, 1H), 6.41 (dd, J = 8.5, 2.8 Hz, 1H), 4.61 (d, J = 8.7 Hz, 1H), 3.78 (s, 3H), 3.76 (s, 3H), 3.69 (s, 3H), 3.62 (d, J = 7.8, 1H), 3.47 (s, 3H), 3.25 (dd, J = 15.6, 15.6 Hz, 1H), 3.18 – 3.09 (m, 1H), 2.96 (dd, J = 15.6, 15.1 Hz, 1H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 169.2, 169.2, 159.6, 158.7, 145.9, 142.0, 129.7, 126.6, 124.6, 124.3, 123.5, 104.4, 98.5, 55.5, 55.4, 54.7, 52.4, 52.3, 47.7, 47.7, 35.8. **HRMS**-ESI m/z: [M+Na], calculated for $C_{22}H_{24}O_6$: 407.1471; found 407.1478. **IR (neat):** 2950, 2837, 1731, 1610, 1505, 1434, 1206, 1150, 1033, 746 cm^{-1}. **R_f**: 0.40 in 20% EtOAc/hexanes.



(*E*)-methyl 4-(2,6-dimethoxyphenyl)-2-((methylperoxy)methyl)-6-phenylhex-5-enoate (*9f*)

The title compound was synthesized from ***7f*** and (2,6-dimethoxyphenyl)boronic acid following general procedure C. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 76% yield (60.8 mg, 0.152 mmol) as a colorless oil.

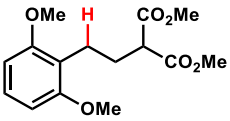
^{1}H NMR: (500 MHz, $CDCl_3$): δ 7.34 – 7.32 (m, 2H), 7.28 – 7.25 (m, 2H), 7.19 – 7.16 (m, 1H), 7.09 (d, J = 8.0 Hz, 1H), 6.47 – 6.40 (m, 3H), 6.32 (dd, J = 15.8, 7.8 Hz, 1H), 3.84 – 3.77 (m, 7H), 3.68 (s, 6H), 3.35 (dd, J = 8.3, 6.5 Hz, 1H), 2.49 – 2.43 (m, 1H), 2.34 – 2.28 (m, 1H). **^{13}C NMR:** (126 MHz, $CDCl_3$) δ 170.1, 170.0, 159.6, 158.1, 137.6, 132.3, 130.1, 128.6, 128.5, 127.2, 126.3, 123.3, 104.5, 98.8, 55.5, 52.6, 52.6, 50.1, 39.8, 34.0. **HRMS**-ESI m/z: [M+Na], calculated for $C_{23}H_{26}O_6$: 421.1627; found 421.1630. **IR (neat):** 2952, 2837, 2360, 1750, 1732, 1609, 1505, 1436, 1207, 1155, 1033, 749 cm^{-1}. **R_f**: 0.27 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2,6-dimethoxyphenyl)hexyl)malonate (*9g*)

The title compound was synthesized from ***7g*** and (2,6-dimethoxyphenyl)boronic acid following general procedure B. After purification via flash column chromatography with a gradient of 0 - 5% ethyl acetate in hexanes as eluent, the product was obtained in 58% yield (44.3 mg, 0.116 mmol) as a colorless oil.

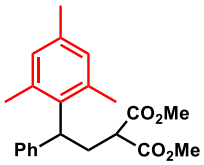
^{1}H NMR: (500 MHz, $CDCl_3$): δ 6.97 (d, J = 8.6 Hz, 1H), 6.44 (dd, J = 8.0, 2.3 Hz, 1H), 6.40 (d, J = 1.7 Hz, 1H), 3.79 (s, 3H), 3.73 (s, 3H), 3.71 (s, 3H), 3.59 (s, 3H), 3.13 (dd, J = 10.0, 4.8 Hz, 1H), 2.97 – 2.95 (m, 1H), 2.33 – 2.24 (m, 1H), 2.10 – 1.99 (m, 1H), 1.59 – 1.56 (m, 3H), 1.27 – 1.01 (m, 4H), 0.81 (t, J = 6.9 Hz, 3H). **^{13}C NMR:** (126 MHz, $CDCl_3$) δ 170.4, 170.1, 159.1, 158.7, 128.3, 124.2, 104.5, 98.4, 55.4, 55.3, 52.5, 52.4, 50.0, 35.7, 35.5, 35.1, 29.7, 22.8, 14.1. **HRMS**-ESI m/z: [M+Na], calculated for $C_{19}H_{28}O_6$: 375.1784; found 375.1787. **IR (neat):** 2954, 2928, 2856, 1751, 1734, 1610, 1505, 1456, 1436, 1207, 1156, 1034, 834 cm^{-1}. **R_f**: 0.30 in 20% EtOAc/hexanes.



Dimethyl 2-(2,6-dimethoxyphenethyl)malonate (*9h*)

The title compound was synthesized from ***7h*** and (2,6-dimethoxyphenyl)boronic acid following general procedure B. After purification via flash column chromatography with a gradient of 0 - 5% ethyl acetate in hexanes as eluent, the product was obtained in 53% yield (31.4 mg, 0.106 mmol) as a colorless oil.

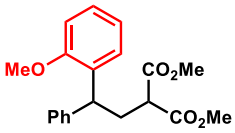
^{1}H NMR: (500 MHz, $CDCl_3$): δ 6.99 (d, J = 8.0 Hz, 1H), 6.42 – 6.39 (m, 2H), 3.78 (s, 3H), 3.77 (s, 3H), 3.72 (s, 6H), 3.35 (t, J = 7.4 Hz, 1H), 2.59 – 2.56 (m, 2H), 2.18 – 2.13 (m, 2H). **^{13}C NMR:** (126 MHz, $CDCl_3$) δ 170.1, 159.5, 158.4, 130.5, 121.3, 103.8, 98.6, 55.5, 55.3, 52.6, 51.1, 29.2, 27.3. **HRMS**-ESI m/z: [M+Na], calculated for $C_{15}H_{20}O_6$: 319.1158; found 319.1160. **IR (neat):** 2952, 2359, 2359, 1733, 1507, 1436, 1208, 1154, 1042, 833 cm^{-1}. **R_f**: 0.55 in 20% EtOAc/hexanes.



Dimethyl 2-(2-mesityl-2-phenylethyl)malonate (*9i*)

The title compound was synthesized from ***7a*** and (2,4,6-trimethylphenyl)boronic acid following general procedure C. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 92% yield (65.1 mg, 0.184 mmol) as a colorless oil.

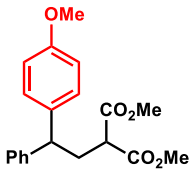
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.27 – 7.23 (m, 2H), 7.18 – 7.14 (m, 3H), 6.82 (s, 2H), 4.55 (dd, J = 10.5, 6.0 Hz, 1H), 3.74 (s, 3H), 3.61 (s, 3H), 3.28 (dd, J = 8.7, 5.5 Hz, 1H), 3.04 – 2.97 (m, 1H), 2.75 – 2.68 (m, 1H), 2.25 (s, 3H), 2.12 (bs, 6H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 170.1, 170.0, 143.1, 137.5, 136.2, 135.9, 130.1(bs), 128.3, 127.1, 125.9, 52.7, 52.7, 50.1, 41.2, 30.6, 21.2, 20.9. **HRMS**-ESI m/z: [M+Na], calculated for $C_{22}H_{26}O_4$: 377.1729; found 377.1735. **IR (neat):** 2952, 1751, 1735, 1609, 1434, 1227, 1151, 699 cm^{-1}. **R_f**: 0.35 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2-methoxyphenyl)-2-phenylethyl)malonate (*9j*)

The title compound was synthesized from ***7a*** and (2-methoxyphenyl)boronic acid following general procedure C. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 91% yield (62.2 mg, 0.182 mmol) as a colorless oil.

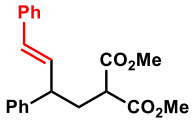
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.30 – 7.26 (m, 2H), 7.22 – 7.18 (m, 3H), 7.16 (m, 2H), 6.84 – 6.83 (d, J = 8.7 Hz, 2H), 3.89 (dd, J = 7.8, 8.2 Hz, 1H), 3.76 (s, 3H), 3.70 (s, 6H), 3.28 (dd, J = 7.3, 7.8 Hz, 1H), 2.67 – 2.59 (m, 2H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 169.9, 158.3, 143.8, 135.5, 128.9, 128.7, 127.9, 126.6, 114.1, 55.3, 52.7, 50.1, 47.9, 34.7. **HRMS**-ESI m/z: [M+Na], calculated for $C_{20}H_{22}O_5$: 365.1365; found 365.1367. **IR (neat):** 2953, 1731, 1609, 1510, 1435, 1246, 1149, 1031, 828, 699 cm^{-1}. **R_f**: 0.35 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(4-methoxyphenyl)-2-phenylethyl)malonate (*9k*)

The title compound was synthesized from ***7a*** and (4-methoxyphenyl)boronic acid following general procedure C. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 89% yield (60.8 mg, 0.178 mmol) as a colorless oil.

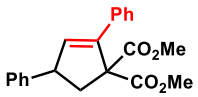
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.31 – 7.25 (m, 2H), 7.23 – 7.13 (m, 5H), 6.83 (d, J = 8.7 Hz, 2H), 3.90 (dd, J = 7.8, 8.2 Hz, 1H), 3.77 (s, 3H), 3.71 (s, 6H), 3.29 (dd, J = 7.3, 7.3 Hz, 1H), 2.65 – 2.62 (m, 2H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 169.9, 169.9, 158.3, 143.8, 135.5, 128.9, 128.7, 127.9, 126.6, 114.1, 55.3, 52.7, 50.1, 47.9, 34.7. **HRMS**-ESI m/z: [M+Na], calculated for $C_{20}H_{22}O_5$: 365.1365; found 365.1372. **IR (neat):** 2951, 1731, 1608, 1509, 1434, 1245, 1149, 1031, 699 cm^{-1}. **R_f**: 0.38 in 20% EtOAc/hexanes.



(*E*)-dimethyl 2-(2,4-diphenylbut-3-en-1-yl)malonate (*9l*)

The title compound was synthesized from ***7a*** and (*E*)-styrylboronic acid following general procedure C. After purification via flash column chromatography with a gradient of 0 - 5% ethyl acetate in hexanes as eluent, the product was obtained in 85% yield (57.5 mg, 0.170 mmol) as a colorless oil.

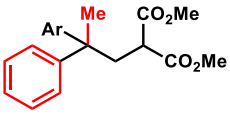
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.39 – 7.20 (m, 10H), 6.44 (d, J = 16.0 Hz, 1H), 6.29 (dd, J = 16.0, 7.8 Hz, 1H), 3.71 (s, 3H), 3.70 (s, 3H), 3.47 (ddd, J =7.8, 7.3, 7.3 Hz, 1H), 3.41 (dd, J = 7.3, 7.3 Hz, 1H), 2.52 – 2.38 (m, 2H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 169.9, 169.8, 142.8, 137.1, 132.3, 130.7, 128.9, 128.6, 127.7, 127.5, 126.9, 126.4, 52.7, 50.0, 47.2, 34.7. **HRMS**-ESI m/z: [M+Na], calculated for $C_{21}H_{22}O_4$: 361.1416; found 361.1418. **IR (neat):** 3026, 2952, 1731, 1493, 1434, 1221, 1149, 965, 745, 694 cm^{-1}. **R_f**: 0.43 in 20% EtOAc/hexanes.



Dimethyl 2,4-diphenylcyclopent-2-ene-1,1-dicarboxylate (*10a*)

The title compound was synthesized from ***7a*** and potassium trifluoro(phenylethynyl)borate following general procedure C at -40 ^{o}C instead of -10 ^{o}C. After purification via flash column chromatography with a gradient of 0 - 5% ethyl acetate in hexanes as eluent, the product was obtained in 66% yield (44.4 mg, 0.132 mmol) as a colorless oil.

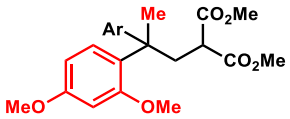
^{1}H NMR: (500 MHz, $CDCl_3$): δ 7.49 – 7.46 (m, 2H), 7.35 – 7.25 (m, 8H), 6.36 (d, J = 2.3 Hz, 1H), 4.17 (ddd, J = 8.0, 8.0, 2.3 Hz, 1H), 3.77 (s, 3H), 3.64 (s, 3H), 3.24 (dd, J = 13.2, 8.0 Hz, 1H), 2.56 (dd, J = 13.2, 8.0 Hz, 1H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 171.8, 171.7, 143.6, 143.0, 136.7, 134.9, 128.8, 128.2, 127.8, 127.6, 127.42, 126.9, 68.0, 53.0, 52.8, 49.3, 46.2. **HRMS**-ESI m/z: [M+Na], calculated for $C_{21}H_{20}O_4$: 359.1259; found 359.1260. **IR (neat):** 2951, 2360, 1730, 1434, 1262, 1197, 1070, 697 cm^{-1}. **R_f**: 0.33 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2,6-dimethoxyphenyl)-2-phenylpropyl)malonate (*12a*)

The title compound was synthesized from ***11a*** and potassium (2,6-dimethoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 92% yield (71 mg, 0.184 mmol) as a colorless oil.

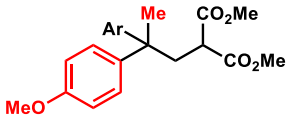
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.29 (d, J = 8.7 Hz, 1H), 7.21 – 7.18 (m, 2H), 7.16 – 7.07 (m, 3H), 6.49 (dd, J = 8.5, 2.5 Hz, 1H), 6.33 (d, J = 2.5 Hz, 1H), 3.80 (s, 3H), 3.64 (s, 3H), 3.47 (s, 3H), 3.32 (s, 3H), 3.28 – 3.19 (m, 2H), 2.75 (dd, J = 12.6, 3.9 Hz, 1H), 1.52 (s, 3H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 170.8, 170.3, 156.0, 158.9, 150.1, 128.6, 127.8, 127.1, 125.9, 125.2, 103.4, 100.2, 55.4, 55.1, 52.7, 52.5, 48.9, 44.4, 37.4, 28.1. **HRMS**-ESI m/z: [M+Na], calculated for $C_{22}H_{26}O_6$: 409.1627; found 409.1632. **IR (neat):** 2950, 2360, 1750, 1731, 1607, 1435, 1258, 1207, 1139, 1029, 699 cm^{-1}. **R_f**: 0.27 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2,4-dimethoxyphenyl)-2-(2,6-dimethoxyphenyl)propyl)malonate (*12b*)

The title compound was synthesized from ***11b*** and potassium (2,6-dimethoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 55% yield (49.1 mg, 0.11 mmol) as a colorless oil.

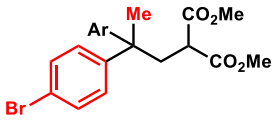
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.19 (d, J = 8.2 Hz, 2H), 6.43 (dd, J = 8.7, 2.3 Hz, 2H), 6.30 (d, J = 2.3 Hz, 2H), 3.78 (s, 6H), 3.54 (s, 6H), 3.38 (s, 6H), 3.20 (dd, J = 6.0, 5.5 Hz, 1H), 3.03 (d, J = 5.5 Hz, 2H), 1.58 (s, 3H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 170.8, 158.9, 158.5, 128.7, 128.3, 103.7, 99.9, 55.5, 55.3, 52.5, 48.8, 42.8, 37.1, 25.1. **HRMS**-ESI m/z: [M+Na], calculated for $C_{24}H_{30}O_8$: 469.1838; found 469.1841. **IR (neat):** 2950, 1732, 1606, 1579, 1501, 1257, 1207, 1142, 1033 cm^{-1}. **R_f**: 0.20 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2,6-dimethoxyphenyl)-2-(4-methoxyphenyl)propyl)malonate (*12c*)

The title compound was synthesized from ***11c*** and potassium (2,6-dimethoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 56% yield (46.6 mg, 0.112 mmol) as a colorless oil.

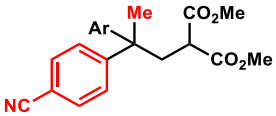
^{1}H NMR: (500 MHz, $CDCl_3$): δ 7.25 (d, J = 2.9 Hz, 1H), 7.06 – 7.00 (m, 2H), 6.76 – 6.72 (m, 2H), 6.47 (dd, J = 8.3, 2.9 Hz, 1H), 6.33 (d, J = 2.9 Hz, 1H), 3.79 (s, 3H), 3.76 (s, 3H), 3.64 (s, 3H), 3.47 (s, 3H), 3.37 (s, 3H), 3.25 – 3.18 (m, 2H), 2.71 (dd, J = 12.0, 3.4 Hz 1H), 1.50 (s, 3H). **^{13}C NMR:** (126 MHz, $CDCl_3$) δ 170.8, 170.4, 159.9, 159.0, 157.1, 142.1, 128.5, 127.3, 126.9, 113.0, 103.3, 100.2, 55.3, 55.2, 52.7, 52.5, 48.9, 43.8, 37.6, 28.1. **HRMS**-ESI m/z: [M+Na], calculated for $C_{23}H_{28}O_7$: 439.1733; found 439.1736. **IR (neat):** 2952, 2836, 1751, 1734, 1608, 1509, 1457, 1248, 1209, 1150, 1034, 831 cm^{-1}. **R_f**: 0.23 in 23% EtOAc/hexanes.



Dimethyl 2-(2-(4-bromophenyl)-2-(2,6-dimethoxyphenyl)propyl)malonate (*12d*)

The title compound was synthesized from ***12d*** and potassium (2,6-dimethoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 – 10% ethyl acetate in hexanes as eluent, the product was obtained in 91% yield (84.5 mg, 0.182 mmol) as a colorless oil.

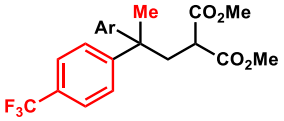
^{1}H NMR: (500 MHz, $CDCl_3$): δ 7.31 – 7.26 (m, 3H), 7.02 – 6.97 (m, 2H), 6.48 (dd, J = 8.6, 2.9 Hz, 1H), 6.32 (d, J = 2.9 Hz, 1H), 3.79 (s, 3H), 3.65 (s, 3H), 3.46 (s, 3H), 3.36 (s, 3H), 3.23 – 3.14 (m, 2 H), 2.72 – 2.66 (m, 1H), 1.49 (s, 3H). **^{13}C NMR:** (126 MHz, $CDCl_3$) δ 170.7, 170.1, 160.2, 158.7, 149.3, 130.7, 128.5, 127.8, 126.3, 118.9, 103.4, 100.1, 55.4, 55.0, 52.8, 52.6, 48.7, 44.1, 37.3, 28.0. **HRMS**-ESI m/z: [M+Na], calculated for $C_{22}H_{25}BrO_6$: 487.0732; found 487.0735. **IR (neat):** 2950, 1731, 1608, 1457, 1435, 1260, 1208, 1140, 1033, 1006, 824, 734 cm^{-1}. **R_f**: 0.30 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2,6-dimethoxyphenyl)-2-(4-isocyanophenyl)propyl)malonate (*12e*)

The title compound was synthesized from ***11e*** and potassium (2,6-dimethoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 84% yield (69.1 mg, 0.168 mmol) as a colorless oil.

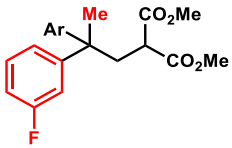
^{1}H NMR: (500 MHz, $CDCl_3$): δ 7.48 (dd, J = 8.6, 1.7 Hz, 2H), 7.30 (d, J = 8.6 Hz, 2H), 7.24 – 7.21 (m, 2H), 6.50 (dd, J = 8.6, 2.9 Hz, 1H), 6.30 (d, J = 2.3 Hz, 1H), 3.80 (s, 3H), 3.66 (s, 3H), 3.44 (s, 3H), 3.32 (s, 3H), 3.22 (dd, J =13.5, 6.3 Hz, 1H), 3.16 (dd, J = 6.3, 5.1 Hz, 1H), 2.70 (dd, J = 13.8, 5.1 Hz, 1H), 1.49 (s, 3H). **^{13}C NMR:** (126 MHz, $CDCl_3$) δ 170.5, 169.9, 160.5, 158.4, 156.3, 131.7, 128.5, 126.6, 125.3, 119.4, 109.0, 103.6, 99.9, 55.4, 54.9, 52.9, 52.6, 48.6, 44.7, 36.8, 28.0. **HRMS**-ESI m/z: [M+Na], calculated for $C_{23}H_{25}NO_6$: 434.1580; found 434.1584. **IR (neat):** 2952, 2225, 1732, 1606, 1503, 1436, 1261, 1208, 1141, 1032, 835, 734 cm^{-1}. **R_f**: 0.27 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2,6-dimethoxyphenyl)-2-(4-(trifluoromethyl)phenyl)propyl)malonate (*12f*)

The title compound was synthesized from ***11f*** and potassium (2,6-dimethoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 95% yield (76.8 mg, 0.19 mmol) as a colorless oil.

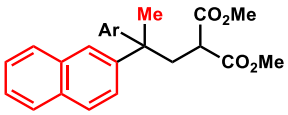
^{1}H NMR: (500 MHz, $CDCl_3$): δ 7.44 (d, J = 8.6 Hz, 2H), 7.31 (d, J = 8.6 Hz, 2H), 7.24 (d, J = 8.2 Hz, 2H), 6.50 (dd, J = 8.6, 2.2 Hz, 1H), 6.32 (d, J = 2.2 Hz, 1H), 3.80 (s, 3H), 3.64 (s, 3H), 3.45 (s, 3H), 3.32 (s, 3H), 3.27 – 3.14 (m, 2H), 2.74 (dd, J = 13.2, 4.6 Hz, 1H), 1.52 (s, 3H).**^{13}C NMR:** (126 MHz, $CDCl_3$) δ 170.6, 170.0, 160.3, 158.6, 154.4, 128.5, 127.4 (q, J = 32.0 Hz), 126.1, 126.0, 125.6 (q, J = 270.7 Hz), 124.7 (q, J = 3.7 Hz), 103.5, 100.0, 55.4, 54.9, 52.7, 52.5, 48.7, 44.4, 37.2, 28.0. **^{19}F NMR:** (470 MHz, $CDCl_3$) δ -62.1 (s). **HRMS**-ESI m/z: [M+Na], calculated for $C_{23}H_{25}F_3O_6$: 477.1501; found 477.1505. **R (neat):** 2953, 1752, 1733, 1611, 1325, 1209, 1159, 1116, 1014, 838, 736 cm^{-1}. **R_f**: 0.33 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2,6-dimethoxyphenyl)-2-(3-fluorophenyl)propyl)malonate (*12g*)

The title compound was synthesized from ***11g*** and potassium (2,6-dimethoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 90% yield (72.7 mg, 0.18 mmol) as a colorless oil.

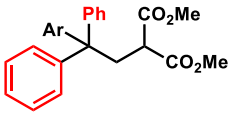
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.28 (d, J = 8.7 Hz, 1H), 7.17 – 7.12 (m, 1H), 6.91 – 6.89 (m, 1H), 6.86 – 6.76 (m, 2H), 6.49 (dd, J = 8.7, 2.3 Hz, 1H), 6.32 (d, J = 2.8 Hz, 1H), 3.80 (s, 3H), 3.66 (s, 3H), 3.46 (s, 3H), 3.35 (s, 3H), 3.25 – 3.17 (m, 2H), 2.69 (dd, J = 12.4, 3.7 Hz, 1H), 1.50 (s, 3H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 170.7, 170.1, 162.7 (d, J = 243.6 Hz), 160.2, 158.8, 153.3 (d, J = 5.9 Hz), 129.0 (d, J = 7.8 Hz), 128.5, 126.3, 121.5, 112.9 (d, J = 21.5 Hz), 112.0 (d, J = 21.5 Hz), 103.4, 100.1, 55.4, 55.0, 52.8, 52.5, 48.8, 44.4, 37.2, 28.1. **^{19}F NMR:** (376 MHz, $CDCl_3$) δ -114.2 (m). **HRMS**-ESI m/z: [M+Na], calculated for $C_{22}H_{25}O_6$: 427.1533; found 427.1537. **IR (neat):** 2952, 1732, 1611, 1582, 1457, 1434, 1259, 1208, 1140, 1033, 782, 699 cm^{-1}. **R_f**: 0.27 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2,6-dimethoxyphenyl)-2-(naphthalen-2-yl)propyl)malonate (*12h*)

The title compound was synthesized from ***11h*** and potassium (2,6-dimethoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 72% yield (62.8 mg, 0.144 mmol) as a colorless oil.

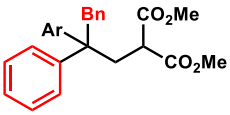
^{1}H NMR: (500 MHz, $CDCl_3$): δ 7.78 – 7.73 (m, 2H), 7.7 – 7.69 (m, 1H), 7.63 (d, J = 8.6 Hz, 1H), 7.44 – 7.38 (m, 2H), 7.35 (d, J = 8.6 Hz, 1H), 7.14 (dd, J = 8.6, 1.8 Hz, 1H), 6.52 (dd, J = 8.6, 2.9 Hz, 1H), 6.32 (d, J = 2.3 Hz, 1H), 3.81 (s, 3H), 3.57 (s, 3H), 3.45 (s, 3H), 3.35 (dd, J = 13.8, 6.3 Hz, 1H), 3.28 – 3.26 (m, 4H), 2.87 (dd, J = 13.5, 5.4 Hz, 1H), 1.61 (s, 3H). **^{13}C NMR:** (126 MHz, $CDCl_3$) δ 170.8, 170.3, 160.1, 159.1, 147.4, 133.4, 131.7, 128.7, 128.1, 127.4, 127.2, 126.8, 125.6, 125.5, 125.1, 123.6, 103.5, 100.1, 55.4, 55.1, 52.7, 52.5, 48.9, 44.5, 37.5, 28.0. **HRMS**-ESI m/z: [M+Na], calculated for $C_{26}H_{28}O_6$: 459.1784, found 459.1787. **IR (neat):** 2951, 1751, 1733, 1608, 1503, 1459, 1435, 1260, 1208, 1143, 1034, 820, 750 cm^{-1}. **R_f**: 0.30 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2,6-dimethoxyphenyl)-2,2-diphenylethyl)malonate (*12i*)

The title compound was synthesized from ***11i*** and potassium (2,6-dimethoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 52% yield (46.6 mg, 0.104 mmol) as a colorless oil.

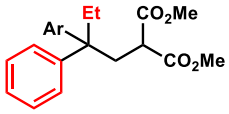
^{1}H NMR: (500 MHz, $CDCl_3$): δ 7.29 – 7.24 (m, 4H), 7.21 – 7.18 (m, 4H), 7.12 – 7.09 (m, 3H), 6.40 (dd, J = 8.6, 2.9 Hz, 1H), 6.35 (d, J = 2.9 Hz, 1H), 3.79 (s, 1H), 3.51 – 3.46 (m, 8H), 3.44 – 3.37 (m, 4H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 170.3, 160.1, 159.3, 146.2, 131.2, 128.6, 127.7, 125.6, 125.5, 103.3, 99.8, 55.4, 54.8, 52.7, 49.9, 36.4. **HRMS**-ESI m/z: [M+Na], calculated for $C_{27}H_{28}O_6$: 471.1784; found 471.1787. **IR (neat):** 2951, 1732, 1608, 1500, 1436, 1262, 1209, 1159, 1030, 700 cm^{-1}. **R_f**: 0.33 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2,6-dimethoxyphenyl)-2,3-diphenylpropyl)malonate (*12j*)

The title compound was synthesized from ***11j*** and potassium (2,6-dimethoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 55% yield (50.8 mg, 0.11 mmol) as a colorless oil.

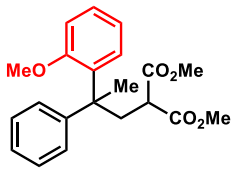
^{1}H NMR: (400 MHz, $CDCl_3$ at 45 ^{o}C): δ 7.19 – 6.99 (m, 9H), 6.57 (d, J = 6.9 Hz, 2H), 6.42 (dd, J = 8.5, 2.8 Hz, 1H), 6.36 (d, J = 2.8 Hz, 1H), 3.80, (s, 3H), 3.68 (d, J = 12.8 Hz, 1H), 3.52 – 3.49 (m, 4H), 3.43 (s, 3H), 3.29 (s, 3H), 3.24 (d, J = 12.8 Hz, 1H), 2.90 (dd, J = 14.0, 6.4 Hz, 1H), 2.66 (dd, J = 14.0, 5.0 Hz, 1H). **^{13}C NMR:** (101 MHz, $CDCl_3$ at 45 ^{o}C): δ 170.0, 169.8, 160.0, 159.2, 147.5, 137.7, 131.0, 128.9, 127.4, 127.3, 126.0, 125.3, 103.6, 100.5, 55.3, 55.0, 52.4, 52.3, 48.8, 48.2, 42.6 (bs), 34.1 (bs). **HRMS**-ESI m/z: [M+Na], calculated for $C_{28}H_{30}O_6$: 485.1940; found 485.1944. **IR (neat):** 2950, 1750, 1732, 1609, 1582, 1501, 1453, 1435, 1261, 1207, 1158, 1032, 836, 701 cm^{-1}. **R_f**: 0.30 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2,6-dimethoxyphenyl)-2-phenylbutyl)malonate (*12k*)

The title compound was synthesized from ***11k*** and potassium (2,6-dimethoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 70% yield (56 mg, 0.14 mmol) as a colorless oil.

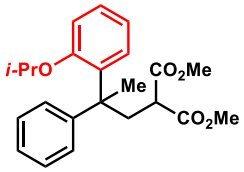
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.33 (d, J = 8.7 Hz, 1H), 7.21 – 7.13 (m, 2H), 7.09 – 7.06 (m, 3H), 6.49 (dd, J = 8.5, 2.8 Hz, 1H), 6.30 (d, J = 2.8 Hz, 1H), 3.79 (s, 3H), 3.60 (s, 3H), 3.43 (s, 3 H), 3.25 (s, 3H), 3.20 – 3.10 (m, 2H), 2.77 (dd , J = 17.4, 8.7 Hz, 1H), 2.25 – 2.13 (m, 1H), 1.94 – 1.85 (m, 1H), 0.58 (dd, J = 7.3, 7.3 Hz, 3H). **^{13}C NMR:** (126 MHz, $CDCl_3$) δ 170.6, 170.2, 159.8, 159.1, 148.2, 128.7, 127.5, 127.4, 126.7, 125.0, 103.5, 100.6, 55.3, 55.1, 52.4, 52.3, 48.5, 47.4, 33.0, 29.4, 8.4. **HRMS**-ESI m/z: [M+Na], calculated for $C_{23}H_{28}O_6$: 423.1784; found 423.1781. **IR (neat):** 2950, 1732, 1607, 1579, 1501, 1435, 1258, 1207, 1147, 1027, 832, 762, 699 cm^{-1}. **R_f**: 0.40 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2-methoxyphenyl)-2-phenylpropyl)malonate (*12m*)

The title compound was synthesized from ***11a*** and potassium (2-methoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 56% yield (39.9 mg, 0.112 mmol) as a colorless oil.

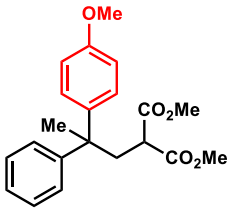
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.29 – 7.23 (m, 2H), 7.22 – 7.14 (m, 3H), 7.14 – 7.08 (m, 2H), 6.82 – 6.77 (m, 2H), 3.78 (s, 3H), 3.58 (s, 3H), 3.58 (s, 3H), 3.25 (dd, J = 5.5, 5.5 Hz, 1H), 2.87 (d, J = 5.5 Hz, 2H), 1.57 (s, 3H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 170.4, 170.4, 157.8, 148.4, 140.0, 128.7, 128.2, 127.5, 126.2, 113.5, 55.3, 52.7, 48.7, 45.5, 40.1, 27.8. **HRMS**-ESI m/z: [M+Na], calculated for $C_{21}H_{24}O_5$: 379.1521; found 379.1525. **IR (neat):** 2952, 1735, 1510, 1436, 1250, 1184, 1032, 701 cm^{-1}. **R_f**: 0.37 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(2-isopropoxyphenyl)-2-phenylpropyl)malonate (*12n*)

The title compound was synthesized from ***11a*** and potassium (2-isopropoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 85% yield (65.3 mg, 0.17 mmol) as a colorless oil.

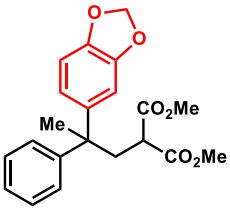
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.26 – 7.24 (m, 2H), 7.21 – 7.17 (m, 3H), 7.09 – 7.07 (m, 2H), 6.77 (d, J = 9.2, 2H), 4.51 (hept, J = 6.1 Hz, 1H), 3.58 (s, 6H), 3.26 (dd, J = 5.9, 5.9 Hz, 1H), 2.87 (d, J = 5.9 Hz, 2H), 1.57 (s, 3H), 1.32 (d, J = 6.0 Hz, 6H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 170.4, 170.4, 156.1, 148.4, 139.7, 128.7, 128.2, 127.5, 126.1, 115.2, 69.7, 52.7, 48.8, 45.5, 40.1, 27.9, 22.2. **HRMS**-ESI m/z: [M+Na], calculated for $C_{23}H_{28}O_5$: 407.1834; found 407.1839. **IR (neat):** 2974, 1751, 1733, 1507, 1434, 1245, 1187, 1147, 701 cm^{-1}. **R_f**: 0.33 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(4-methoxyphenyl)-2-phenylpropyl)malonate (*12o*)

The title compound was synthesized from ***11a*** and potassium (4-methoxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 61% yield (43.4 mg, 0.12 mmol) as a colorless oil.

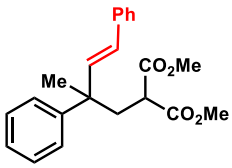
^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.28 – 7.24 (m, 2H), 7.20 – 7.17 (m, 3H), 7.12 – 7.10 (m, 2H), 6.83 – 6.76 (m, 2H), 3.77 (s, 3H), 3.58 (s, 3H), 3.58 (s, 3H), 3.26 (dd, J = 5.9, 5.5 Hz, 1H), 2.87 (d, J = 5.5 Hz, 2H), 1.59 (s, 3H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 170.4, 170.4, 157.8, 148.4, 140.0, 128.7, 128.2, 127.5, 126.2, 113.5, 55.3, 52.7, 48.7, 45.5, 40.1, 27.8. **HRMS**-ESI m/z: [M+Na], calculated for $C_{21}H_{24}O_5$: 379.1521; found 379.1521. **IR (neat):** 2952, 1751, 1733, 1610, 1511, 1435, 1250, 1184, 1150, 1031, 832, 701 cm^{-1}. **R_f**: 0.30 in 20% EtOAc/hexanes.



Dimethyl 2-(2-(benzo[d][1,3]dioxol-5-yl)-2-phenylpropyl)malonate (*12p*)

The title compound was synthesized from ***11a*** and potassium (3,4-methylenedioxyphenyl)trifluoroborate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 42% yield (31.1 mg, 0.084 mmol) as a colorless oil.

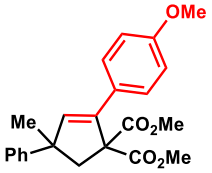
^{1}H NMR: (500 MHz, $CDCl_3$): δ 7.26 – 7.25 (m, 2H), 7.21 – 7.15 (m, 3H), 6.72 (s, 2H), 6.60 (s, 1H), 5.91 (s, 2H), 3.61 (s, 3H), 3.59 (s, 3H), 3.25 (dd, J = 5.7, 5.7 Hz, 1H), 2.89 – 2.79 (m, 2H), 1.55 (s, 3H). **^{13}C NMR:** (126 MHz, $CDCl_3$) δ 170.4, 170.3, 148.1, 147.6, 145.8, 142.1, 128.2, 127.4, 126.3, 120.3, 108.7, 107.6, 101.0, 52.7, 48.7, 45.9, 40.1, 27.9. **HRMS**-ESI m/z: [M+Na], calculated for $C_{21}H_{22}O_6$: 393.1314; found 393.1310. **IR (neat):** 2952, 1734, 1488, 1433, 1233, 1149, 815, 700 cm^{-1}. **R_f**: 0.35 in 20% EtOAc/hexanes.



(*E*)-dimethyl 2-(2-methyl-2,4-diphenylbut-3-en-1-yl)malonate (*12q*)

The title compound was synthesized from ***11a*** and potassium (*E*)-trifluoro(styryl)borate following general procedure D. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 79% yield (55.6 mg, 0.158 mmol) as a colorless oil.

^{1}H NMR: (400 MHz, $CDCl_3$): δ 7.40 – 7.34 (m, 4H), 7.33 – 7.29 (m, 4H), 7.23 – 7.20 (m, 2H), 6.44 (d, J = 16.4 Hz, 1H), 6.34 (d, J = 16.4 Hz, 1H), 3.59 (s, 3H), 3.54 (s, 3H), 3.40 (dd, J = 6.4, 6.0 Hz, 1H), 2.63 (d, J = 6.0, 2H), 1.47 (s, 3H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 170.4, 170.4, 146.3, 137.3, 137.2, 128.7, 128.5, 128.2, 127.5, 126.9, 126.5, 126.4, 52.8, 52.7, 48.6, 43.8, 39.5, 25.5. **HRMS**-ESI m/z: [M+Na], calculated for $C_{22}H_{24}O_4$: 375.1572; found 375.1572. **IR (neat):** 2953, 1752, 1734, 1495, 1435, 1260, 1198, 1152, 700 cm^{-1}. **R_f**: 0.30 in 20% EtOAc/hexanes.

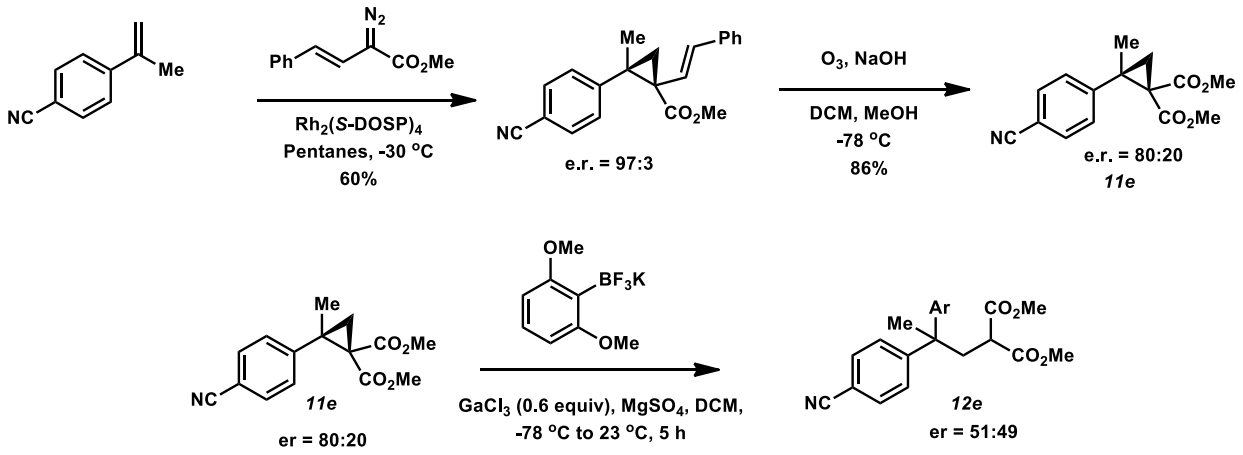


Dimethyl 4-methyl-2,4-diphenylcyclopent-2-ene-1,1-dicarboxylate (*10b*)

The title compound was synthesized from ***11a*** and potassium trifluoro(phenylethynyl)borate following general procedure D with a modification. The reaction was catalyzed by $GaBr_3$ instead of $GaCl_3$. After purification via flash column chromatography with a gradient of 5 - 10% ethyl acetate in hexanes as eluent, the product was obtained in 65% yield (49.4 mg, 0.13 mmol) as a colorless oil.

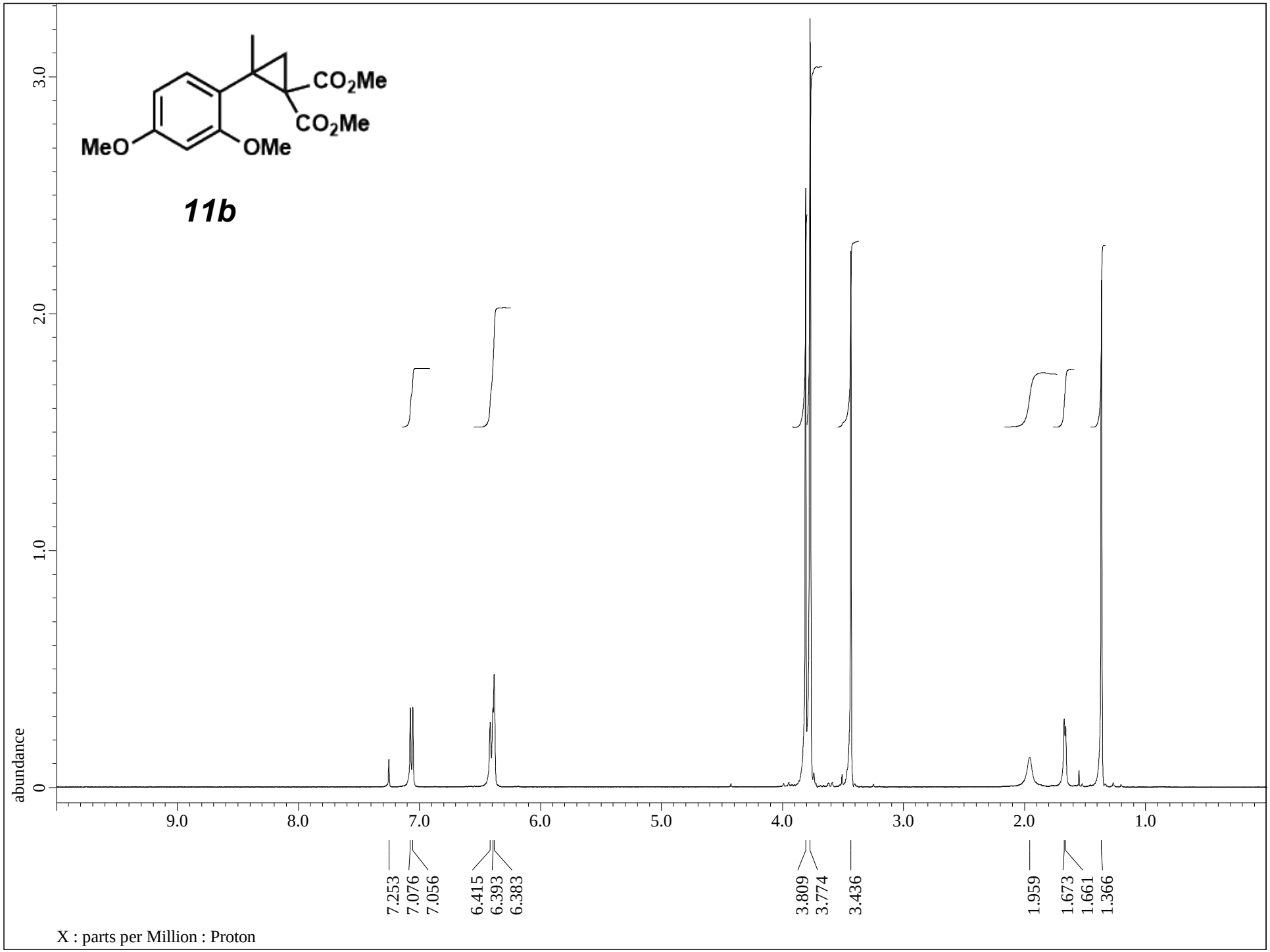
^{1}H NMR: (500 MHz, $CDCl_3$): δ 7.45 – 7.39 (m, 2H), 7.38 – 7.34 (m, 2H), 7.32 – 7.29 (m, 2H), 7.23 – 7.16 (m, 1H), 6.88 – 6.78 (m, 2H), 6.32 (s, 1H), 3.81 (s, 3H), 3.72 (s, 3H), 3.48 (s, 3H), 3.02 (d, J = 13.2 Hz, 1H), 2.89 (d, J = 13.2 Hz, 1H), 1.54 (s, 3H). **^{13}C NMR:** (101 MHz, $CDCl_3$) δ 172.5, 171.8, 159.2, 148.0, 140.6, 139.2, 128.8, 128.4, 127.5 126.3, 126.1, 113.5, 68.1, 55.3, 52.9, 52.6, 52.0, 51.0, 28.0. **HRMS**-ESI m/z: [M+Na], calculated for $C_{23}H_{24}O_5$: 403.1521; found 403.1524. **IR (neat):** 2953, 2359, 1731, 1607, 1512, 1253, 1182, 1089, 1033, 831, 764, 701 cm^{-1}. **R_f**: 0.27 in 20% EtOAc/hexanes.

4. Control experiment



The enantioenriched cyclopropane ***11e*** having an e.r. of 80:20 (HPLC Chiralpak ID, Hexanes/*i*-PrOH = 97:3, 0.75 mL/min, UV-254 detector) was prepared according to the known procedure.[12] Following general procedure D, the reaction between the enantioenriched ***11e*** and potassium (2,6-dimethoxyphenyl)trifluoroborate gave the product ***12e*** with an e.r. of 51:49 (HPLC Chiralpak ID, Hexanes/*i*-PrOH = 80:20, 0.50 mL/min, UV-254 detector).

[12] Austin G. Smith, Michael C. Slade, Jeffrey S. Johnson, *Org. Lett.*, **2011**, *13*, 1996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CO2Me
MeO
OMe
11b
abundance
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1.0
0
9.0
8.0
7.0
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5.0
4.0
3.0
2.0
1.0
7.253
7.076
7.056
6.415
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6.383
3.809
3.774
3.436
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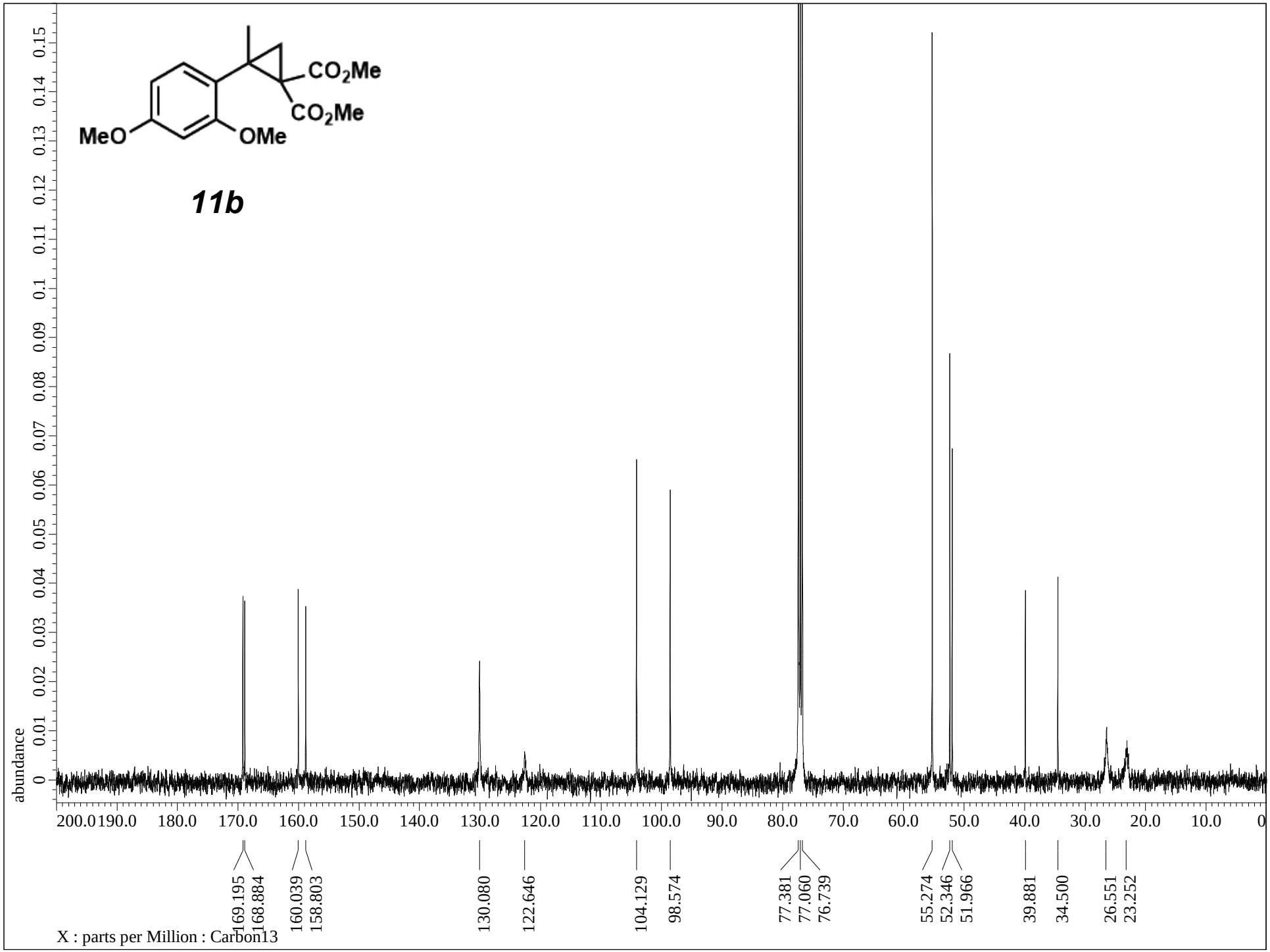
1.673
1.661
1.366
X : parts per Million : Proton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OMe
CO2Me
CO2Me
11b
abundance
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0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
0.15
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190.0
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
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40.0
30.0
20.0
10.0
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130.080
122.646
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98.574
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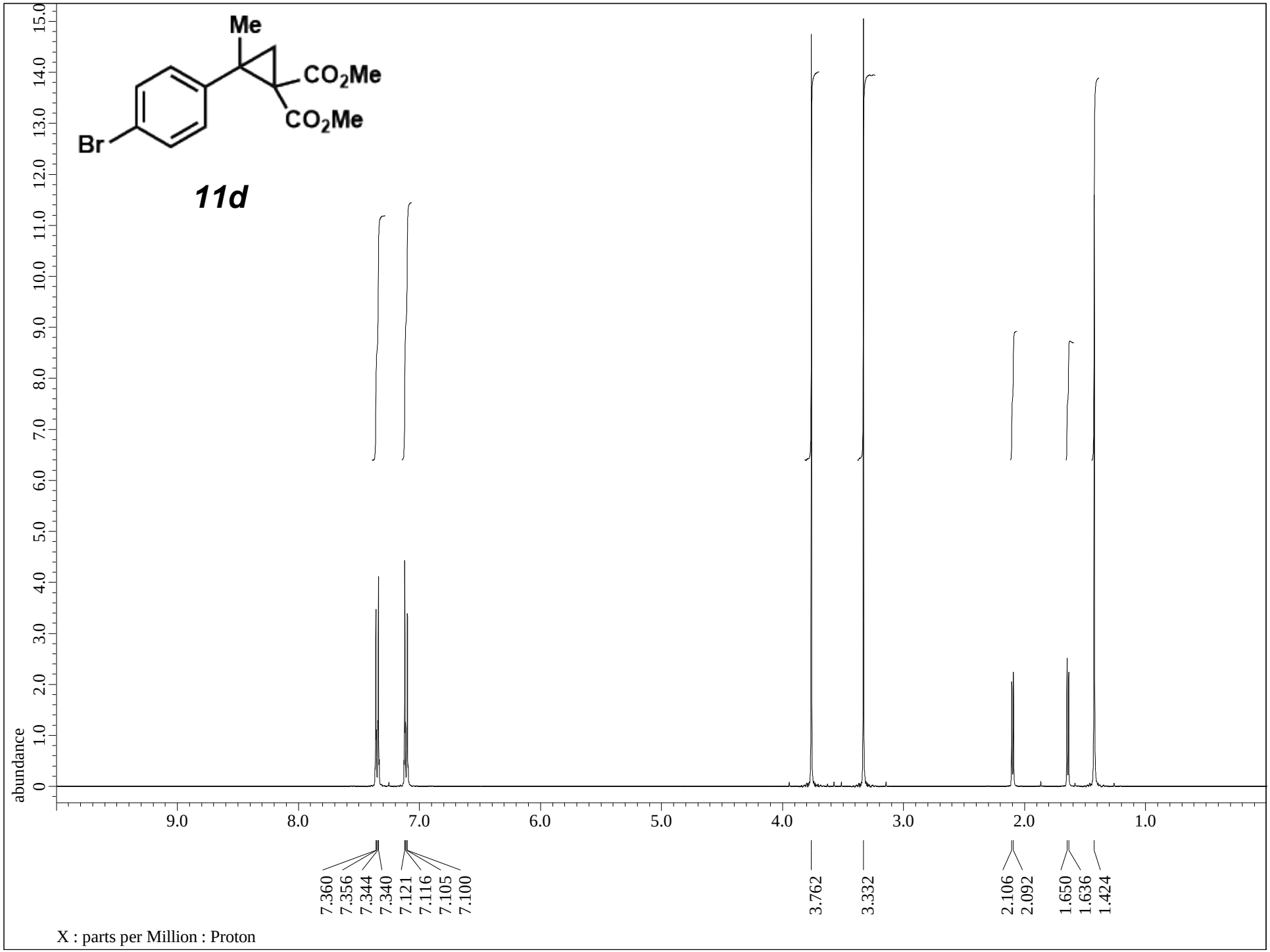
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Br
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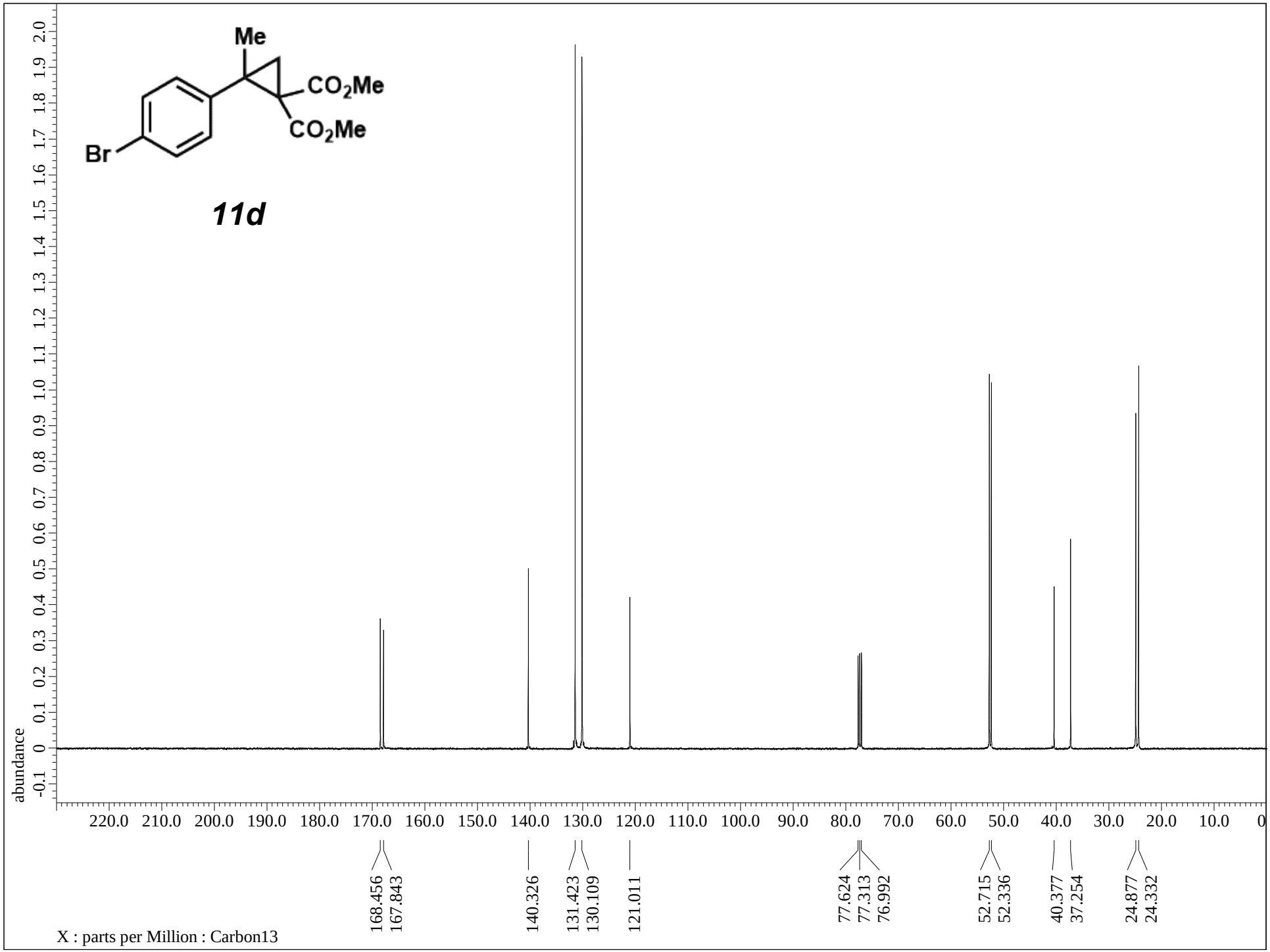
X : parts per Million : Proton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CO2Me
Br
11d
abundance
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220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
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167.843
140.326
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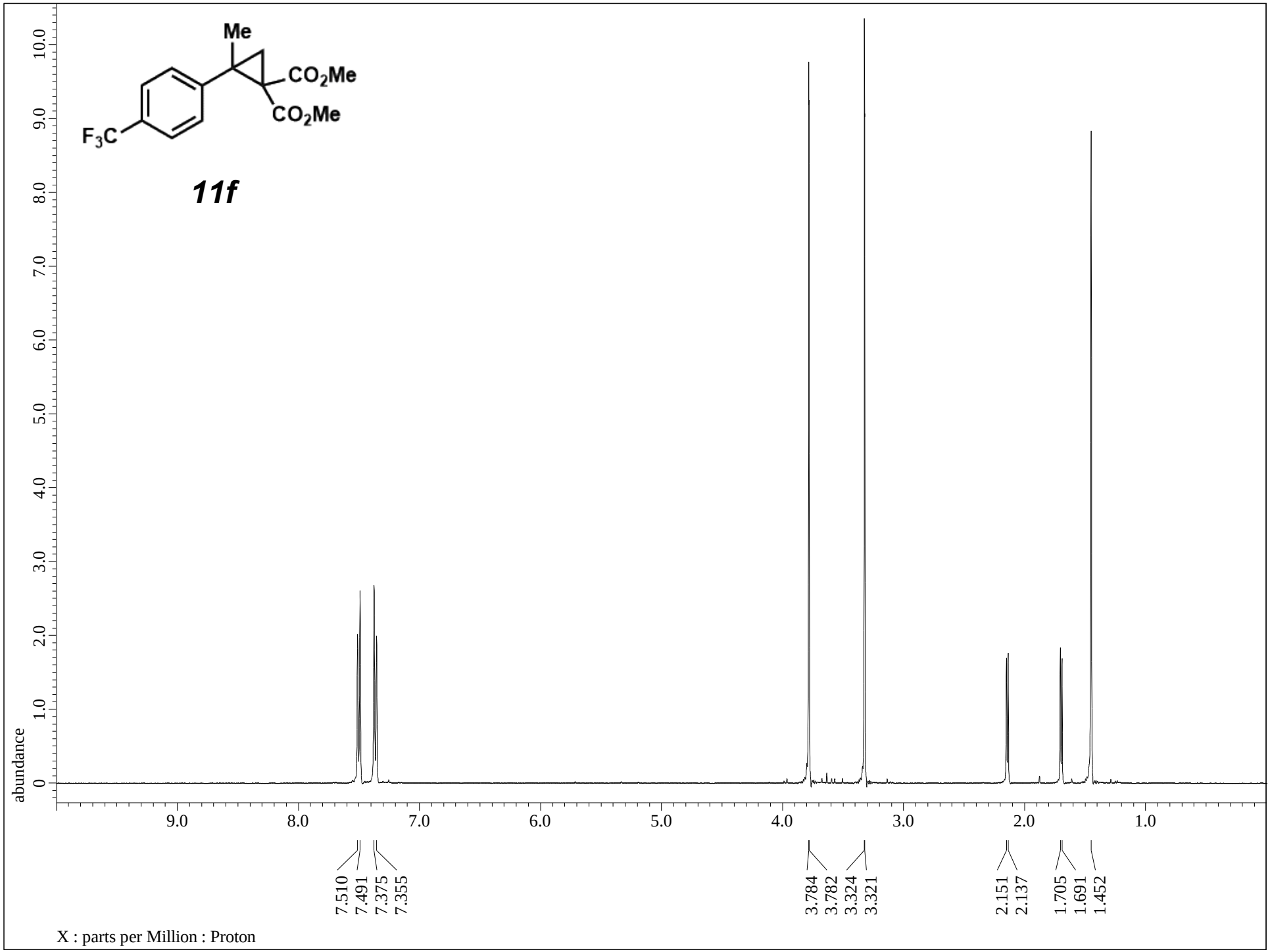
X : parts per Million : Carbon13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CO2Me
F3C
11f
abundance
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2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.510
7.491
7.375
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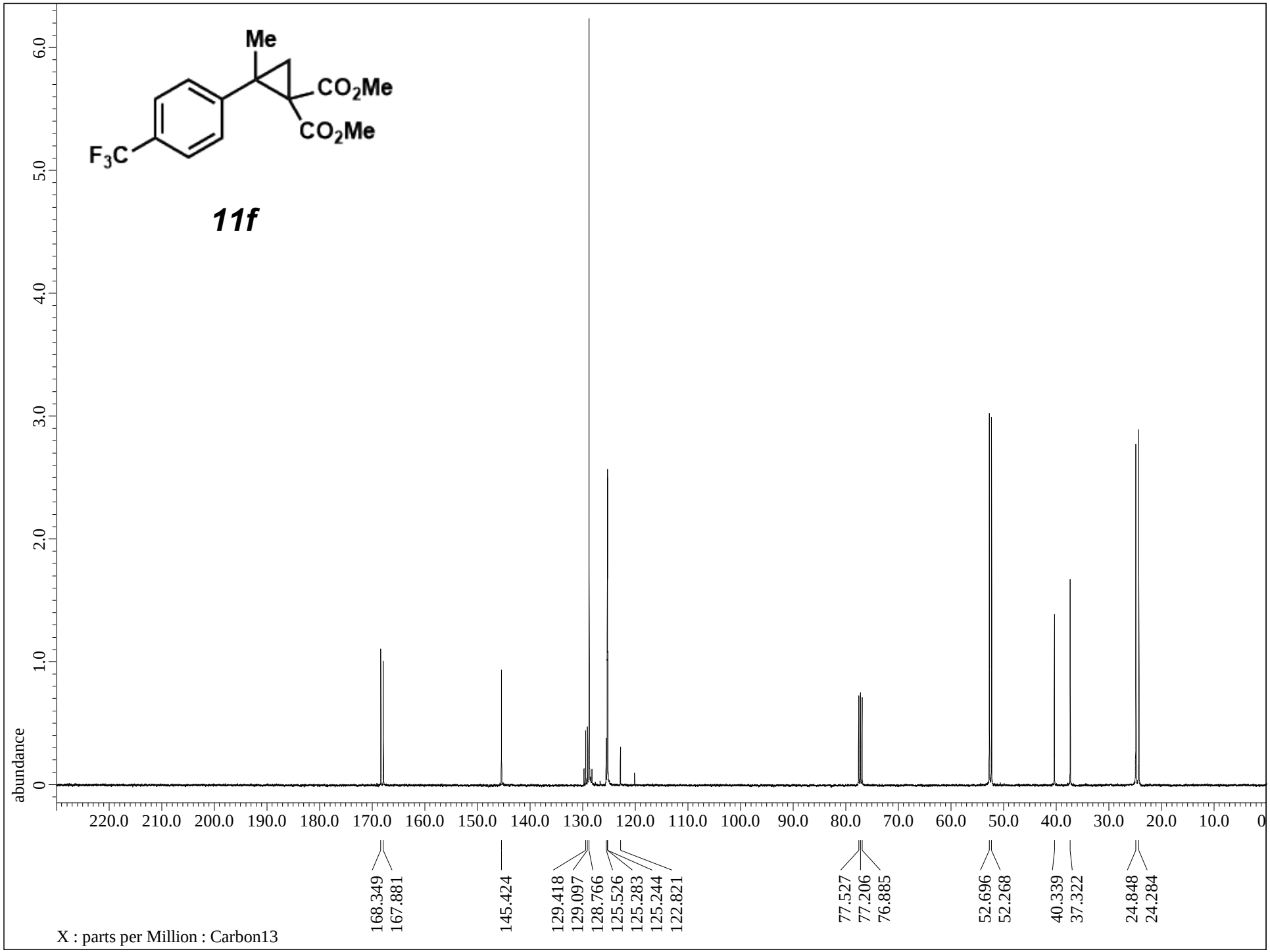
X : parts per Million : Proton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CO2Me
CO2Me
F3C
11f
abundance
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5.0
4.0
3.0
2.0
1.0
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220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
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167.881
145.424
129.418
129.097
128.766
125.526
125.283
125.244
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77.206
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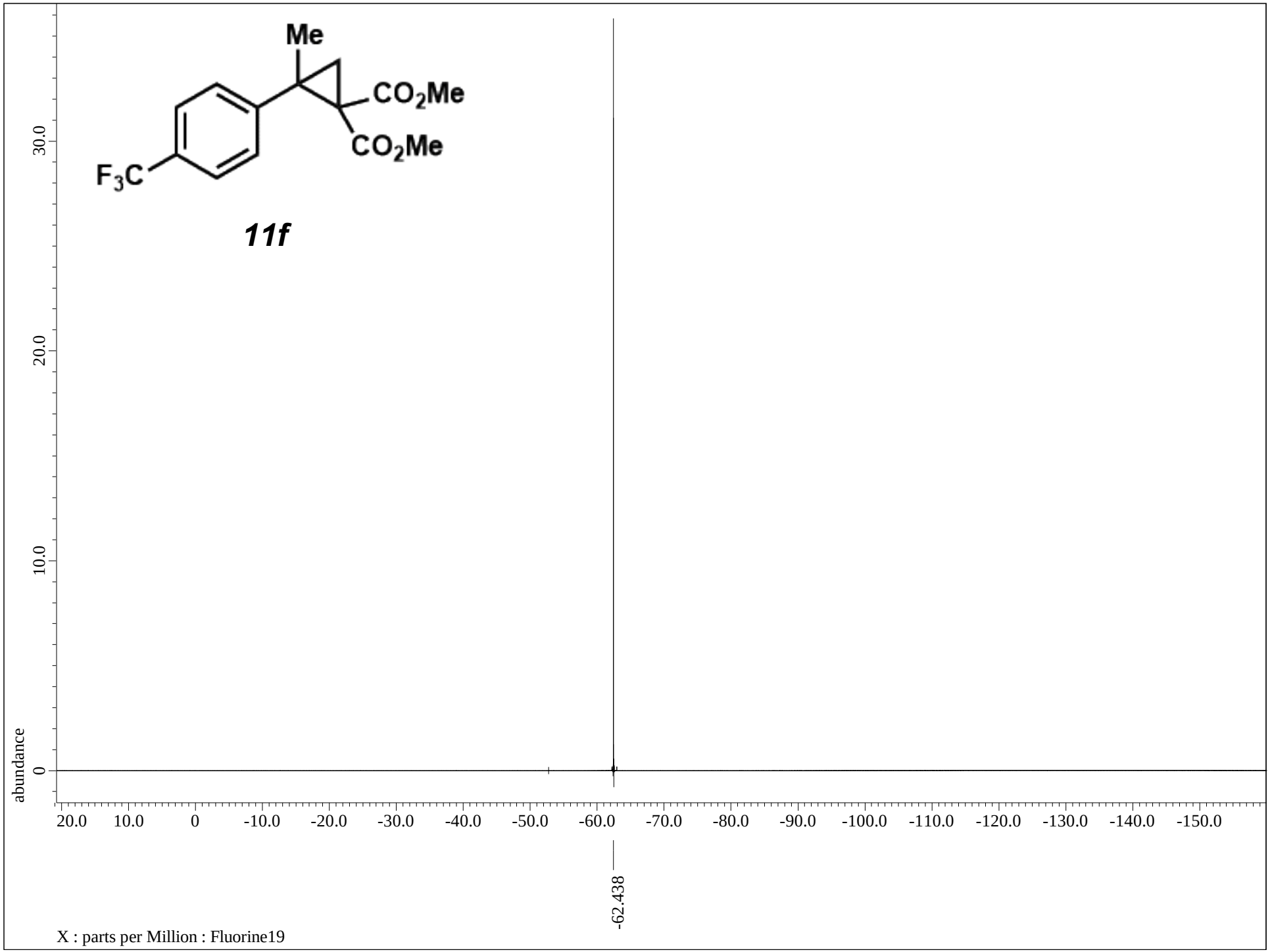
40.339
37.322
24.848
24.284
X : parts per Million : Carbon13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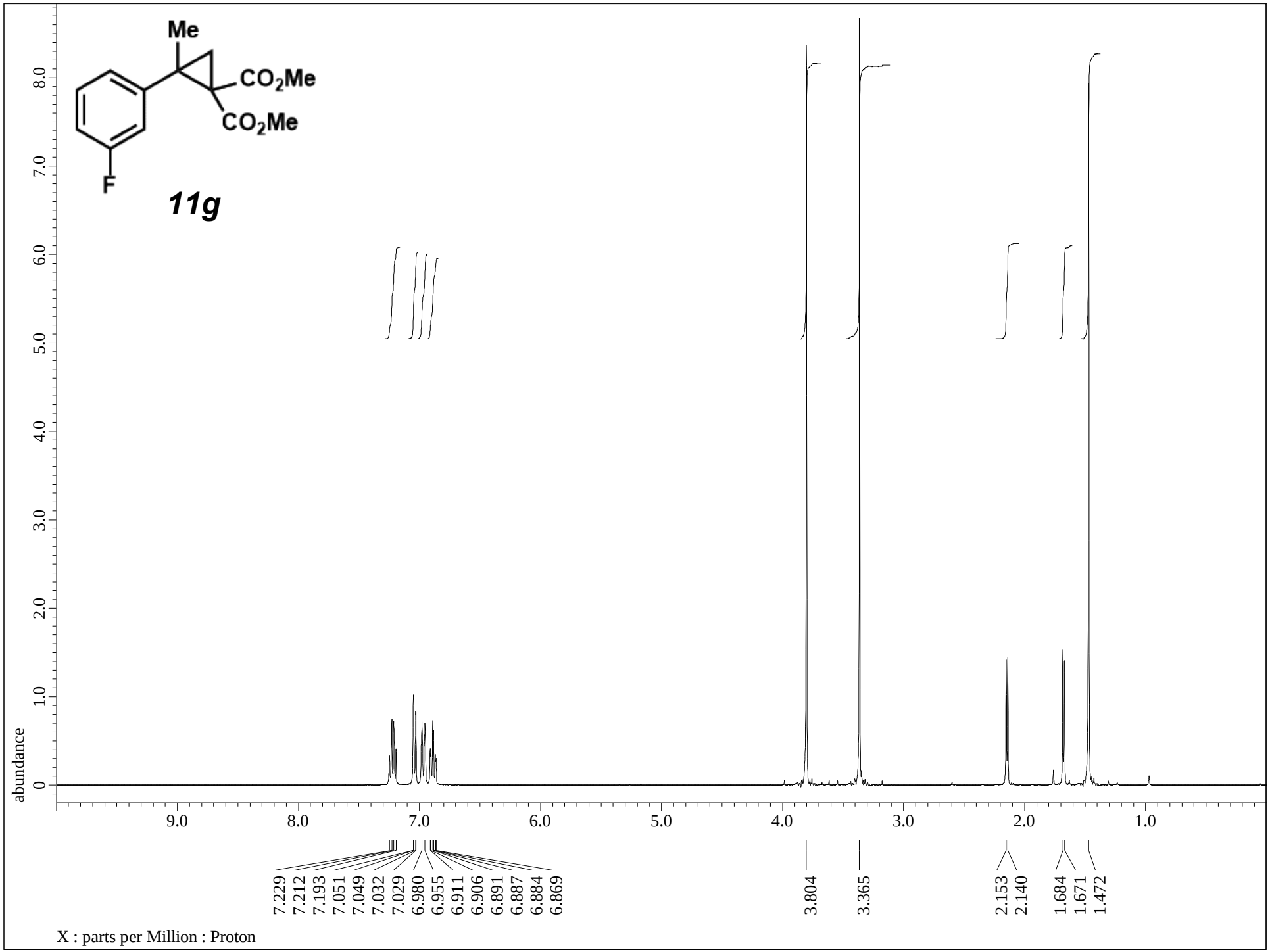
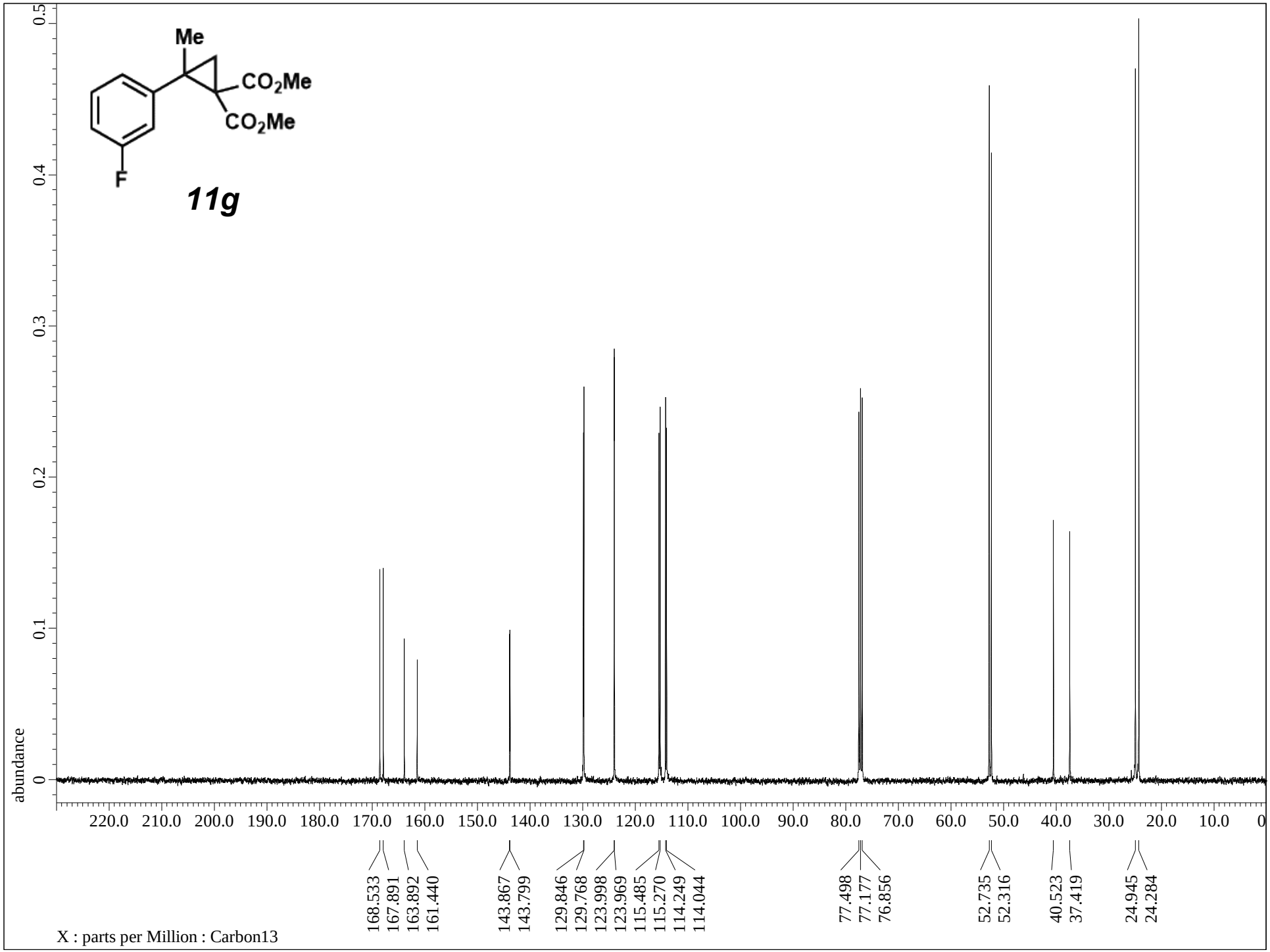
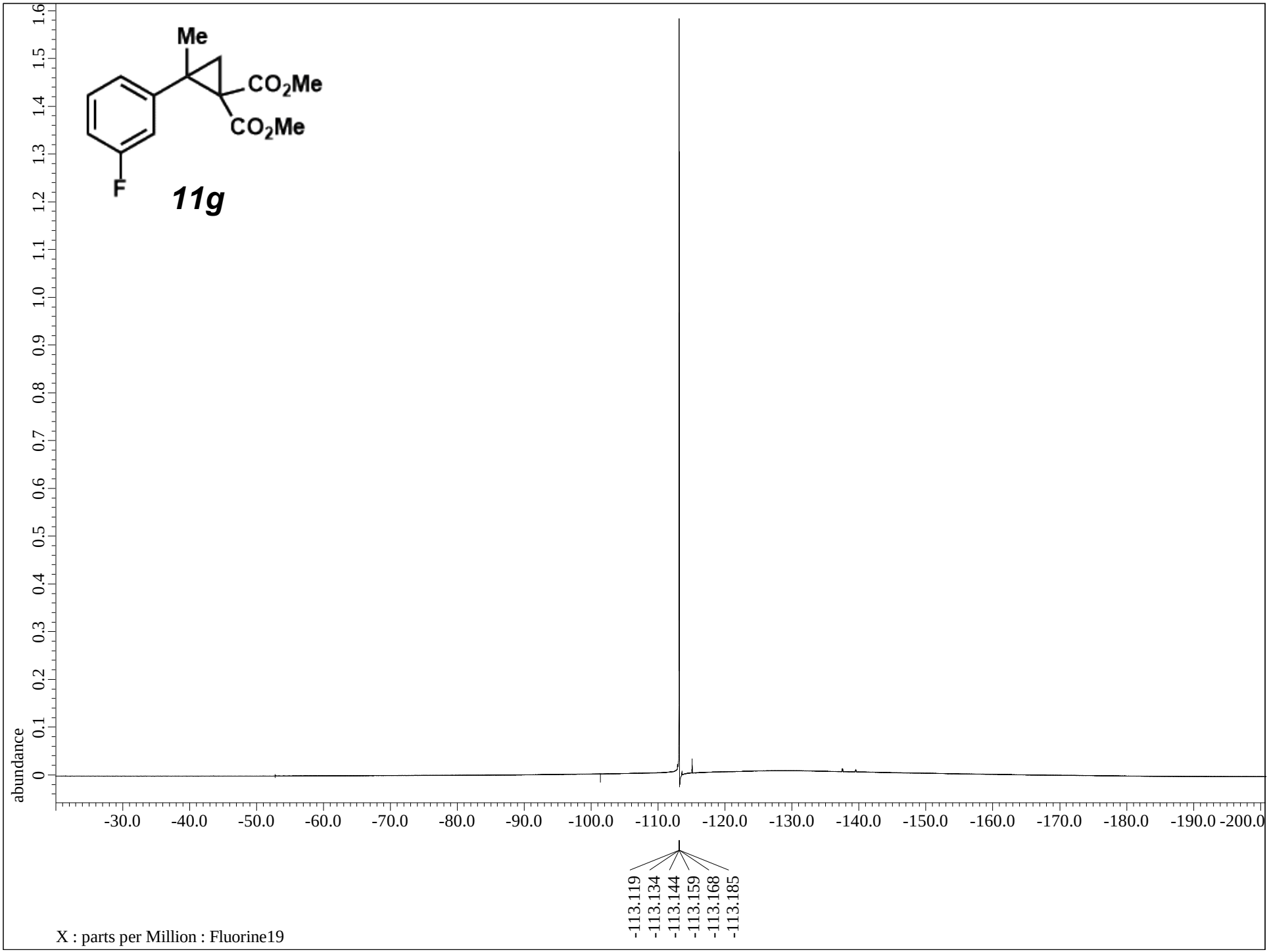
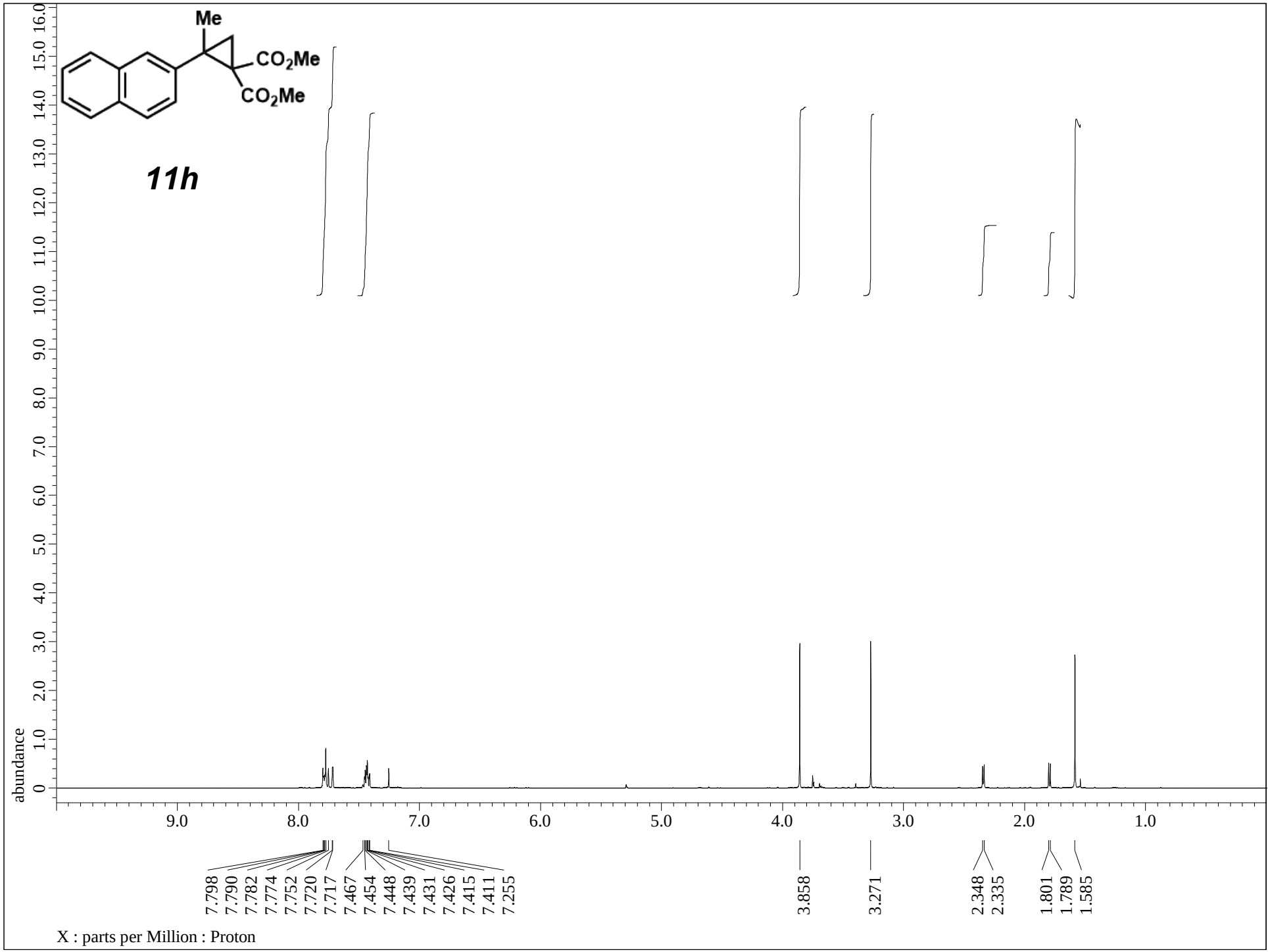
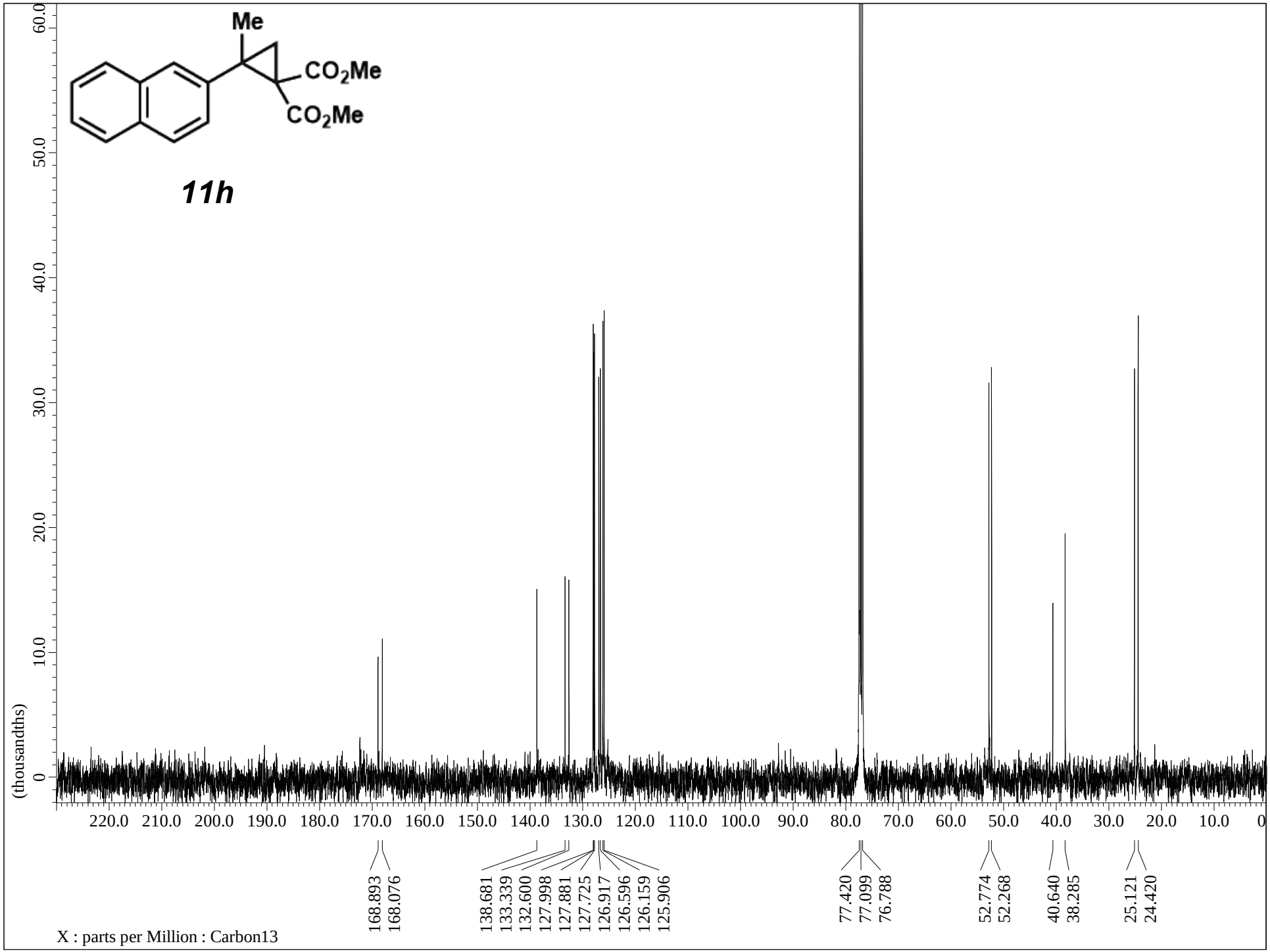
CO2Me
CO2Me
F3C
11f
30.0
20.0
10.0
0
abundance
20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0
-62.438
X : parts per Million : Fluorine19

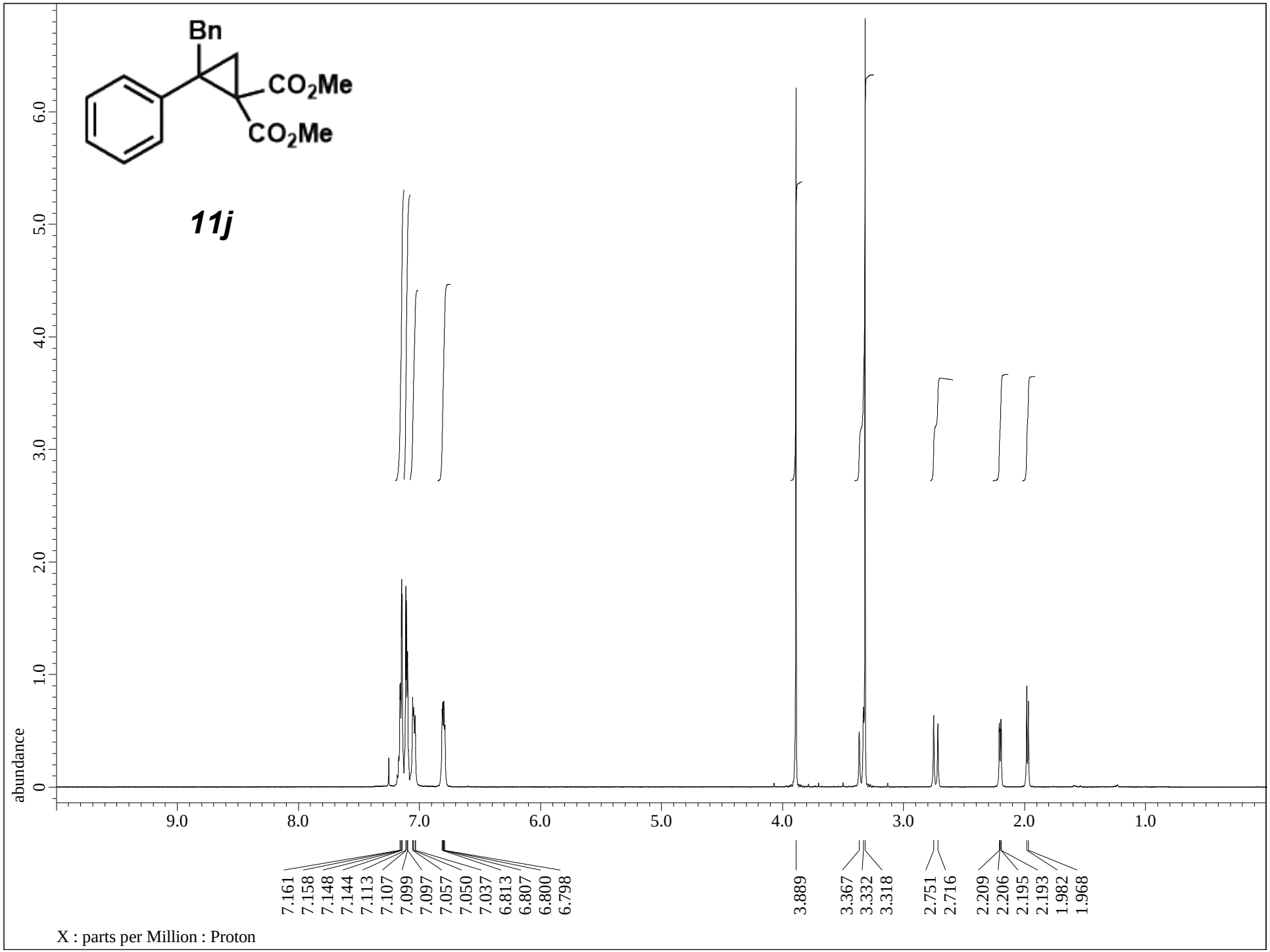

Me
CO2Me
CO2Me
F
11g
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
7.229
7.212
7.193
7.051
7.049
7.032
7.029
6.980
6.955
6.911
6.906
6.891
6.887
6.884
6.869
3.804
3.365
2.153
2.140
1.684
1.671
1.472
X : parts per Million : Proton

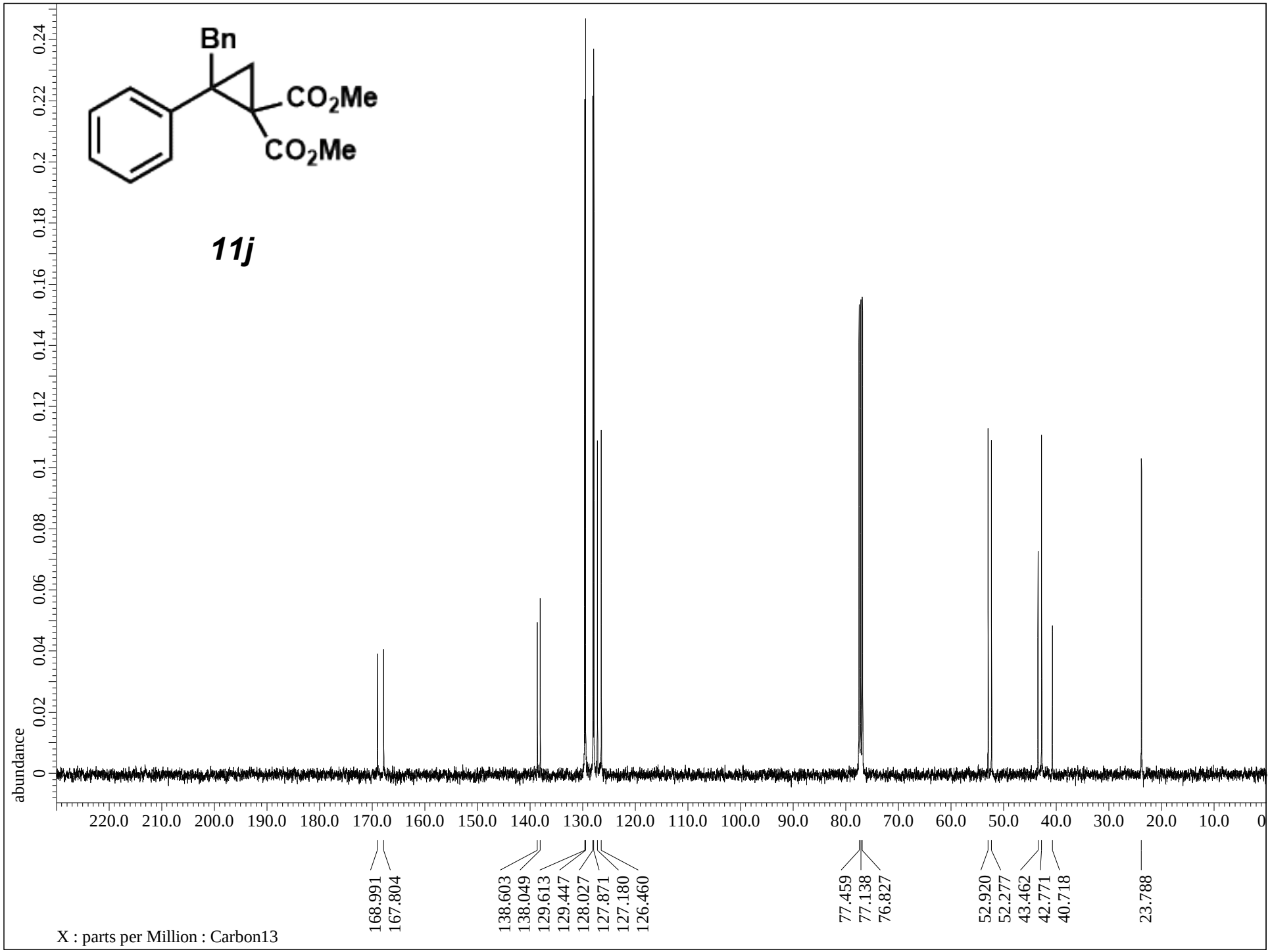

Me
CO2Me
CO2Me
F
11g
abundance
0.5
0.4
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
168.533
167.891
163.892
161.440
143.867
143.799
129.846
129.768
123.998
123.969
115.485
115.270
114.249
114.044
77.498
77.177
76.856
52.735
52.316
40.523
37.419
24.945
24.284
X : parts per Million : Carbon13

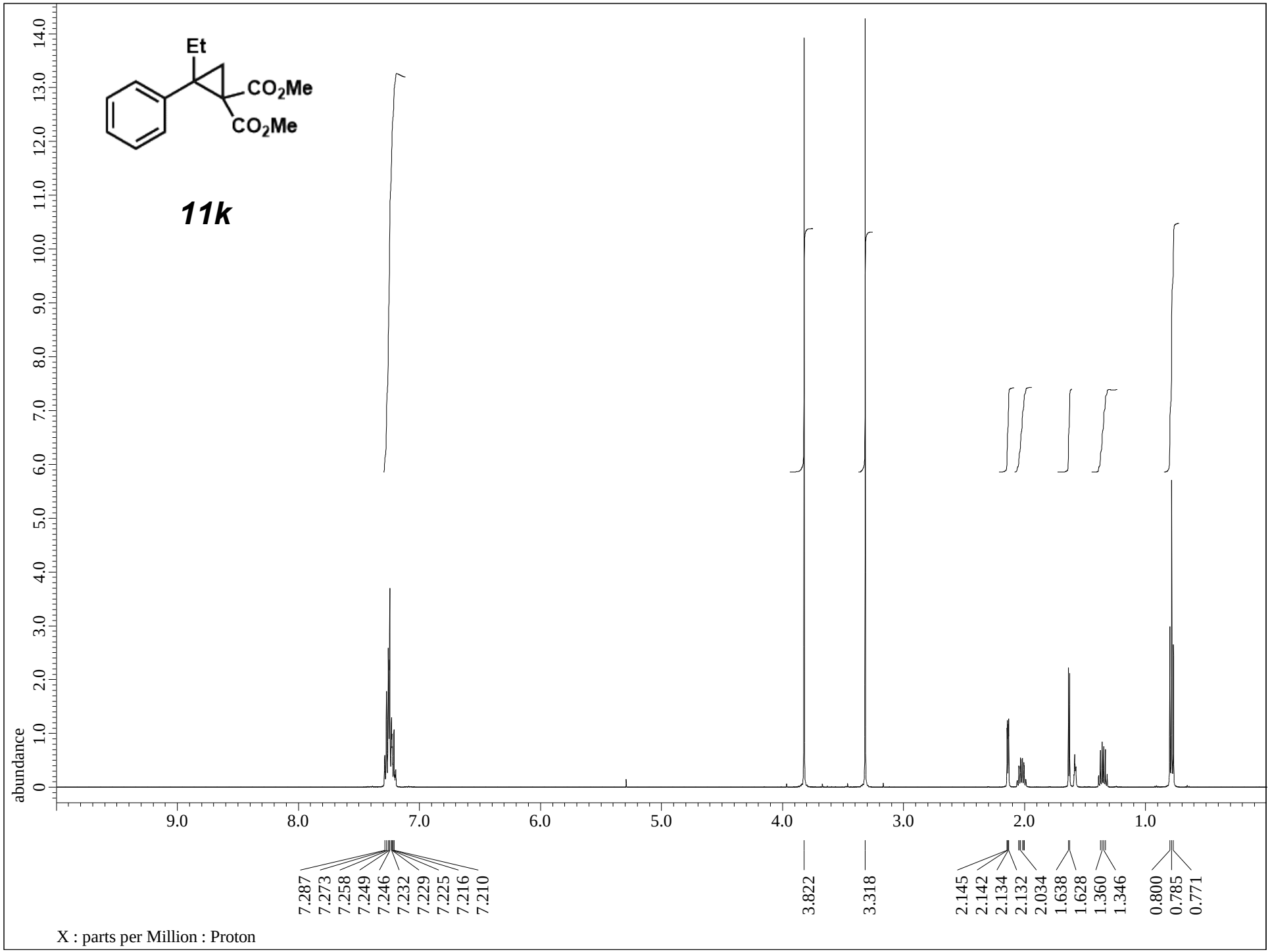

Me
CO2Me
CO2Me
F
11g
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
1.6
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-150.0
-160.0
-170.0
-180.0
-190.0
-200.0
-113.119
-113.134
-113.144
-113.159
-113.168
-113.185
X : parts per Million : Fluorine19

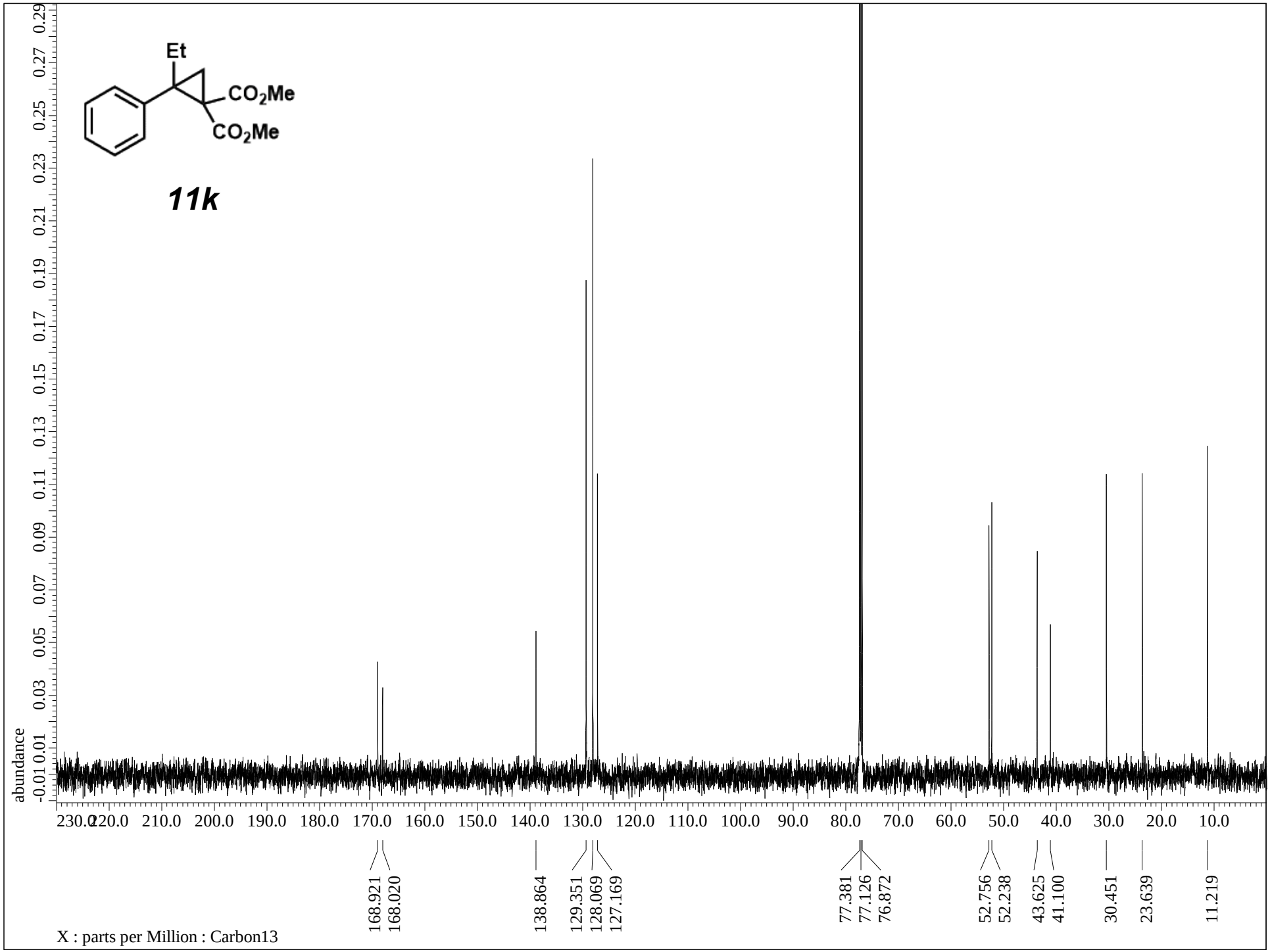

Me
CO2Me
CO2Me
11h
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.798
7.790
7.782
7.774
7.752
7.720
7.717
7.467
7.454
7.448
7.439
7.431
7.426
7.415
7.411
7.255
3.858
3.271
2.348
2.335
1.801
1.789
1.585
X : parts per Million : Proton

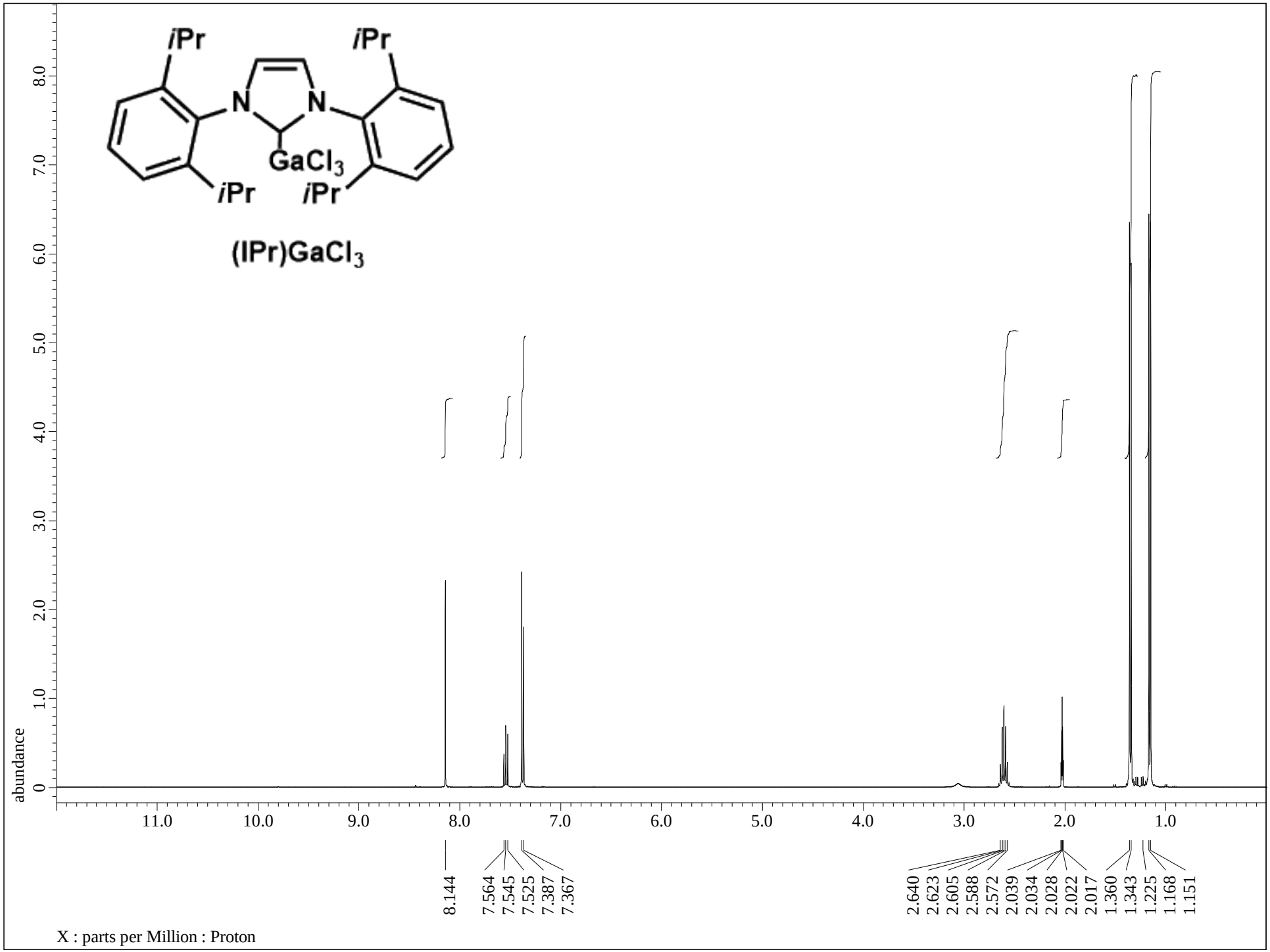

Me
CO2Me
CO2Me
11h
(thousandths)
60.0
50.0
40.0
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
168.893
168.076
138.681
133.339
132.600
127.998
127.881
127.725
126.917
126.596
126.159
125.906
77.420
77.099
76.788
52.774
52.268
40.640
38.285
25.121
24.420
X : parts per Million : Carbon13

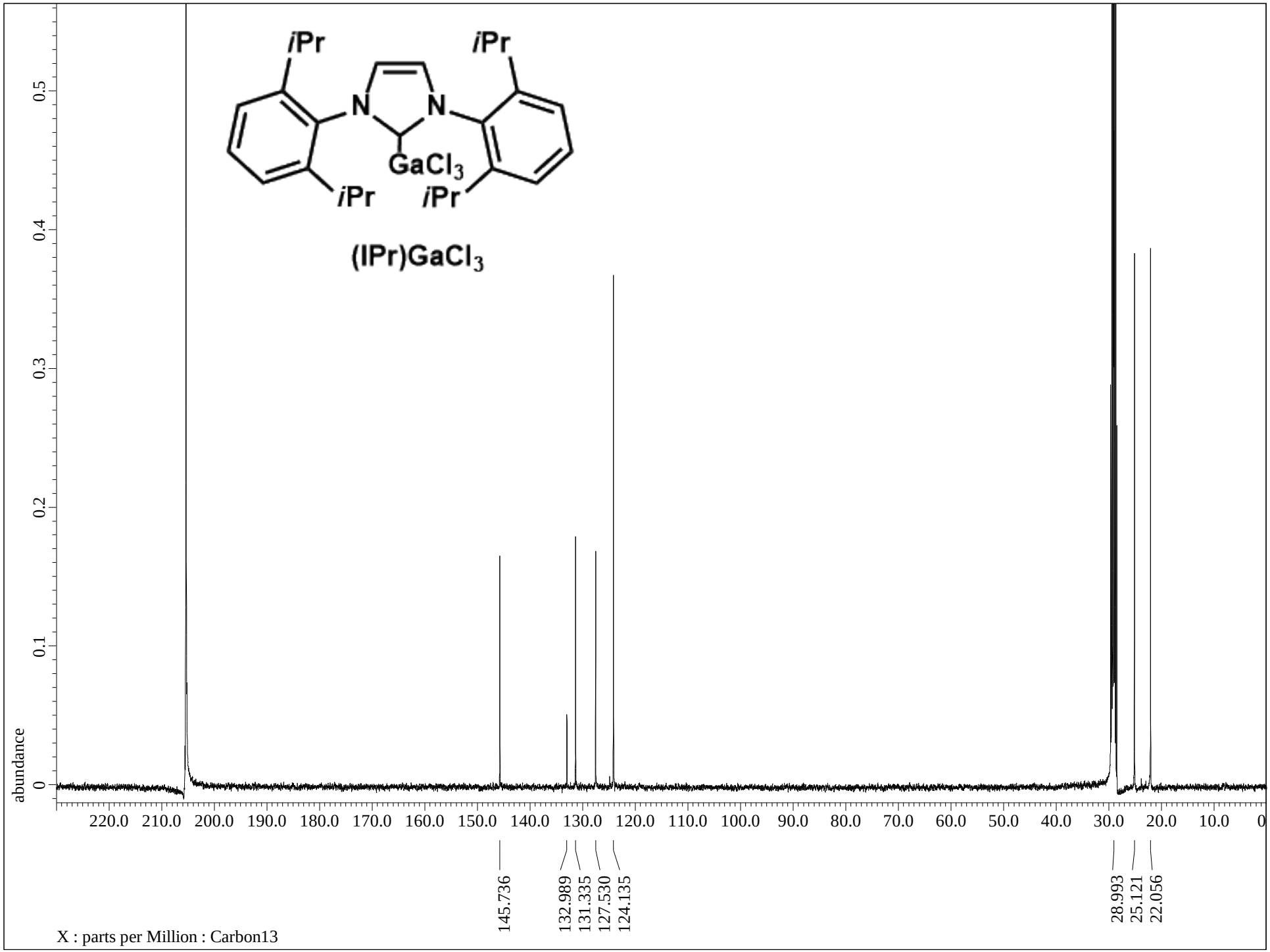

Bn
CO2Me
CO2Me
11j
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.161
7.158
7.148
7.144
7.113
7.107
7.099
7.097
7.057
7.050
7.037
6.813
6.807
6.800
6.798
3.889
3.367
3.332
3.318
2.751
2.716
2.209
2.206
2.195
2.193
1.982
1.968
X : parts per Million : Proton

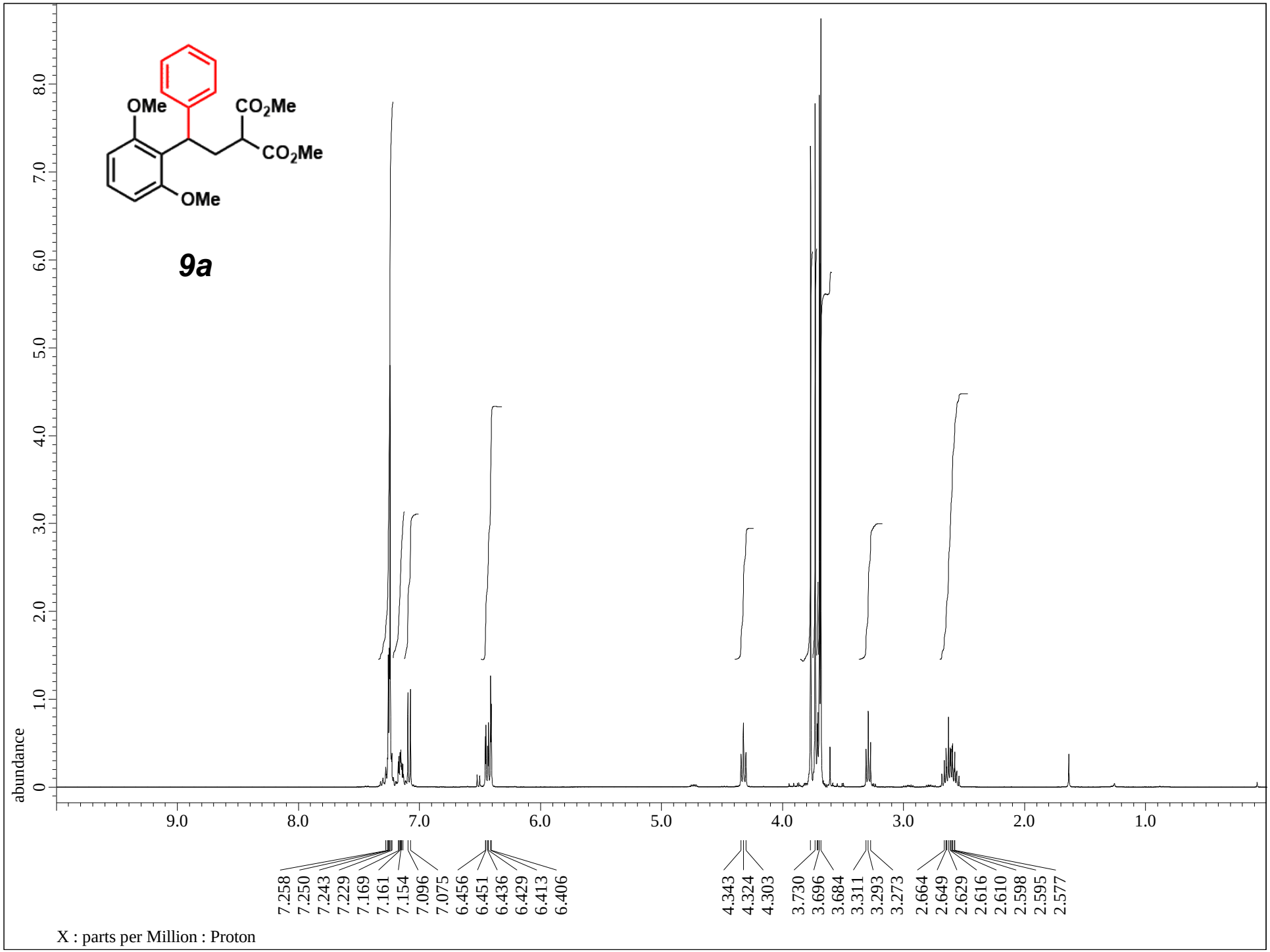

Bn
CO2Me
CO2Me
11j
abundance
0.24
0.22
0.2
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
168.991
167.804
138.603
138.049
129.613
129.447
128.027
127.871
127.180
126.460
77.459
77.138
76.827
52.920
52.277
43.462
42.771
40.718
23.788
X : parts per Million : Carbon13

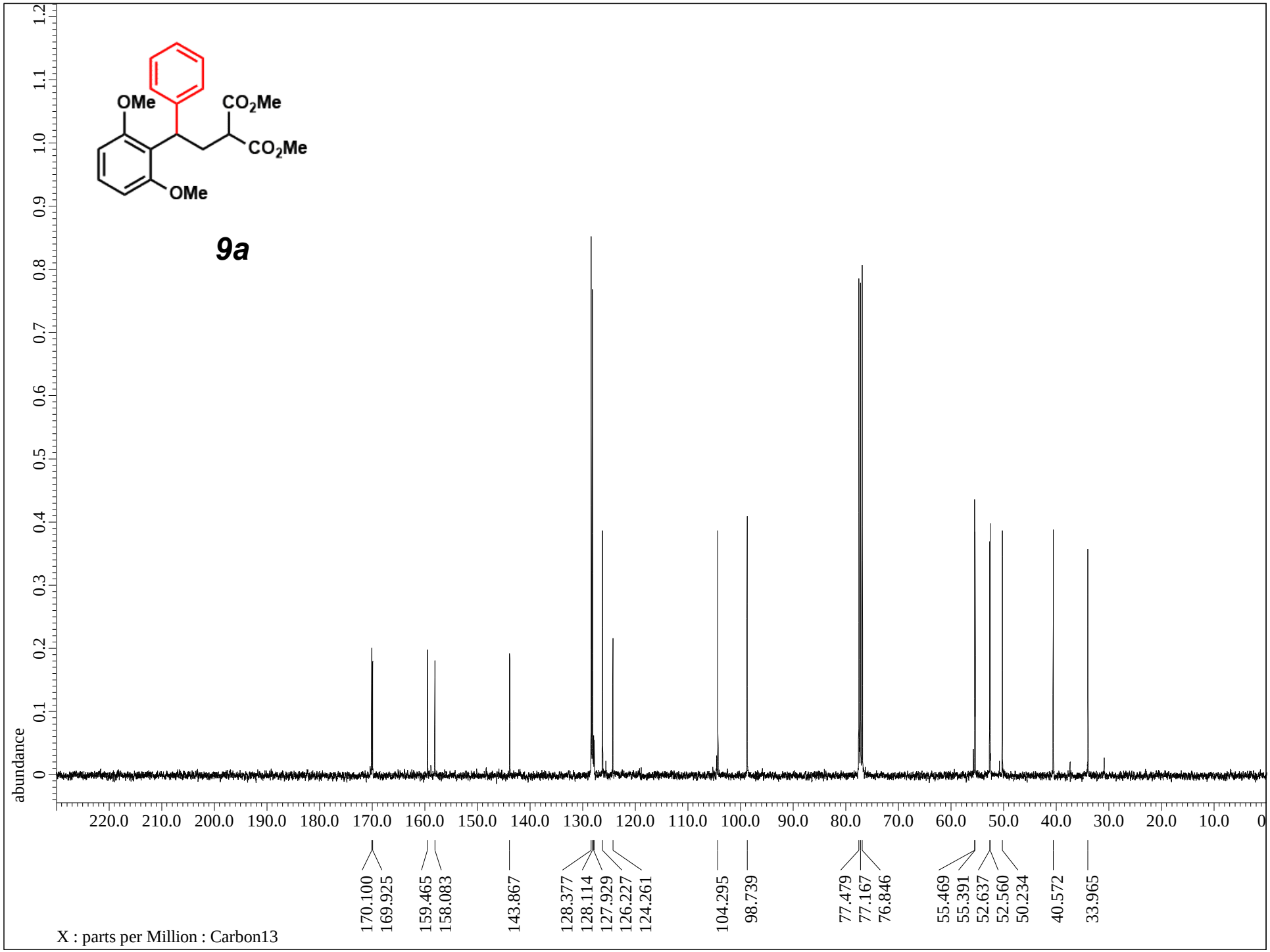

Et
CO2Me
CO2Me
11k
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.287
7.273
7.258
7.249
7.246
7.232
7.229
7.225
7.216
7.210
3.822
3.318
2.145
2.142
2.134
2.132
2.034
1.638
1.628
1.360
1.346
0.800
0.785
0.771
X : parts per Million : Proton

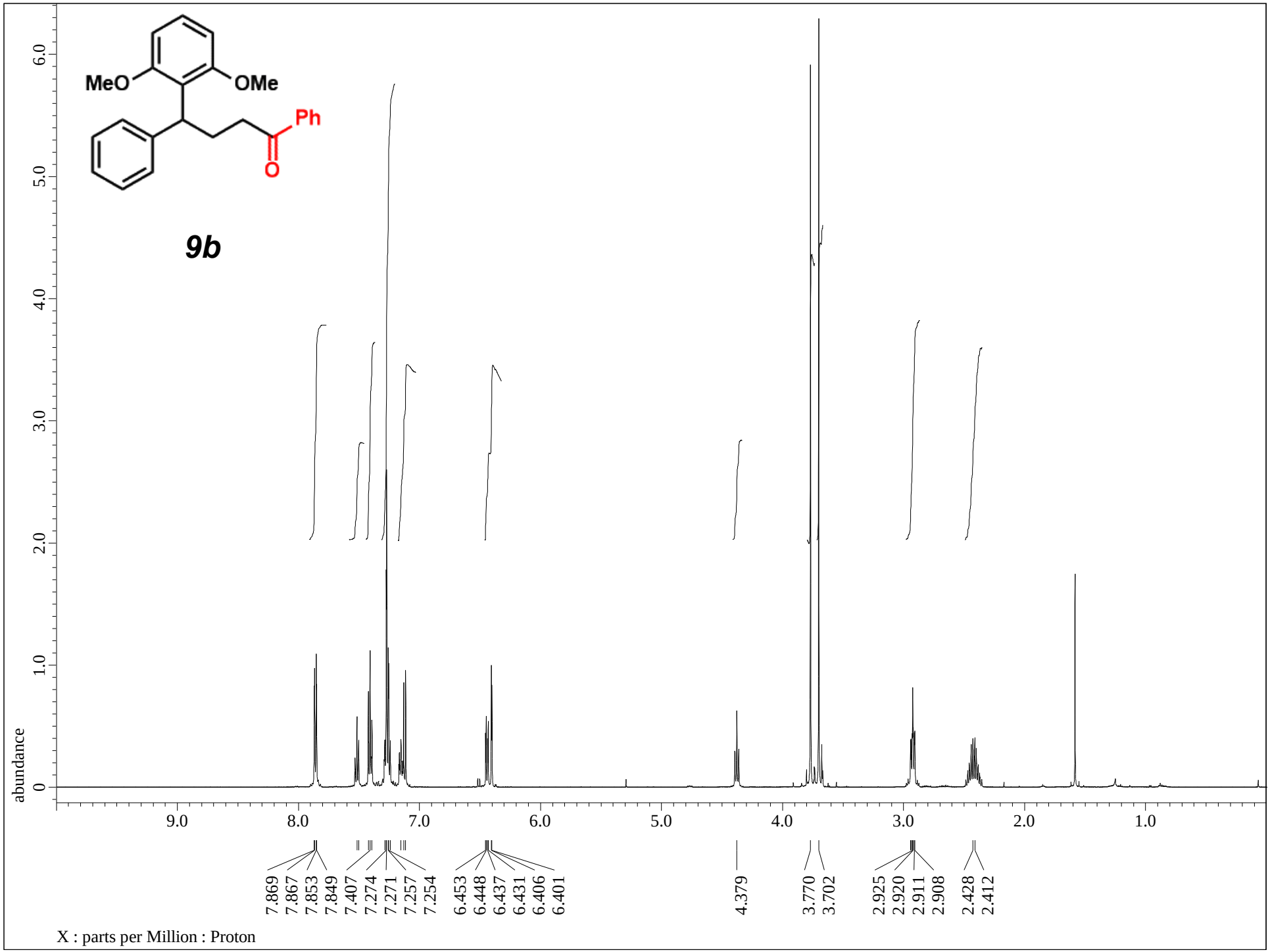


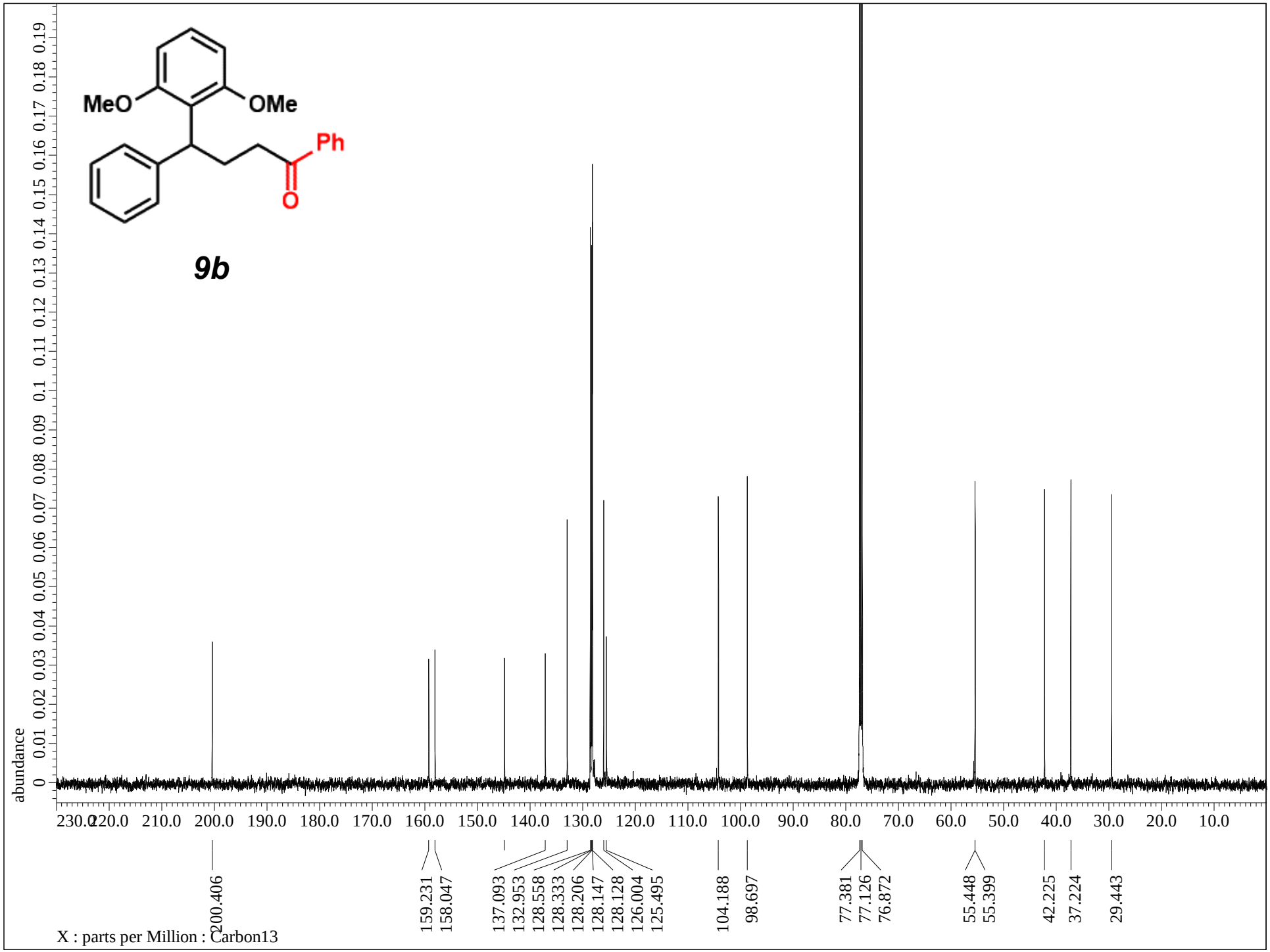

iPr
iPr
N
N
GaCl3
iPr
iPr
(IPr)GaCl3
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.144
7.564
7.545
7.525
7.387
7.367
2.640
2.623
2.605
2.588
2.572
2.039
2.034
2.028
2.022
2.017
1.360
1.343
1.225
1.168
1.151
X : parts per Million : Proton

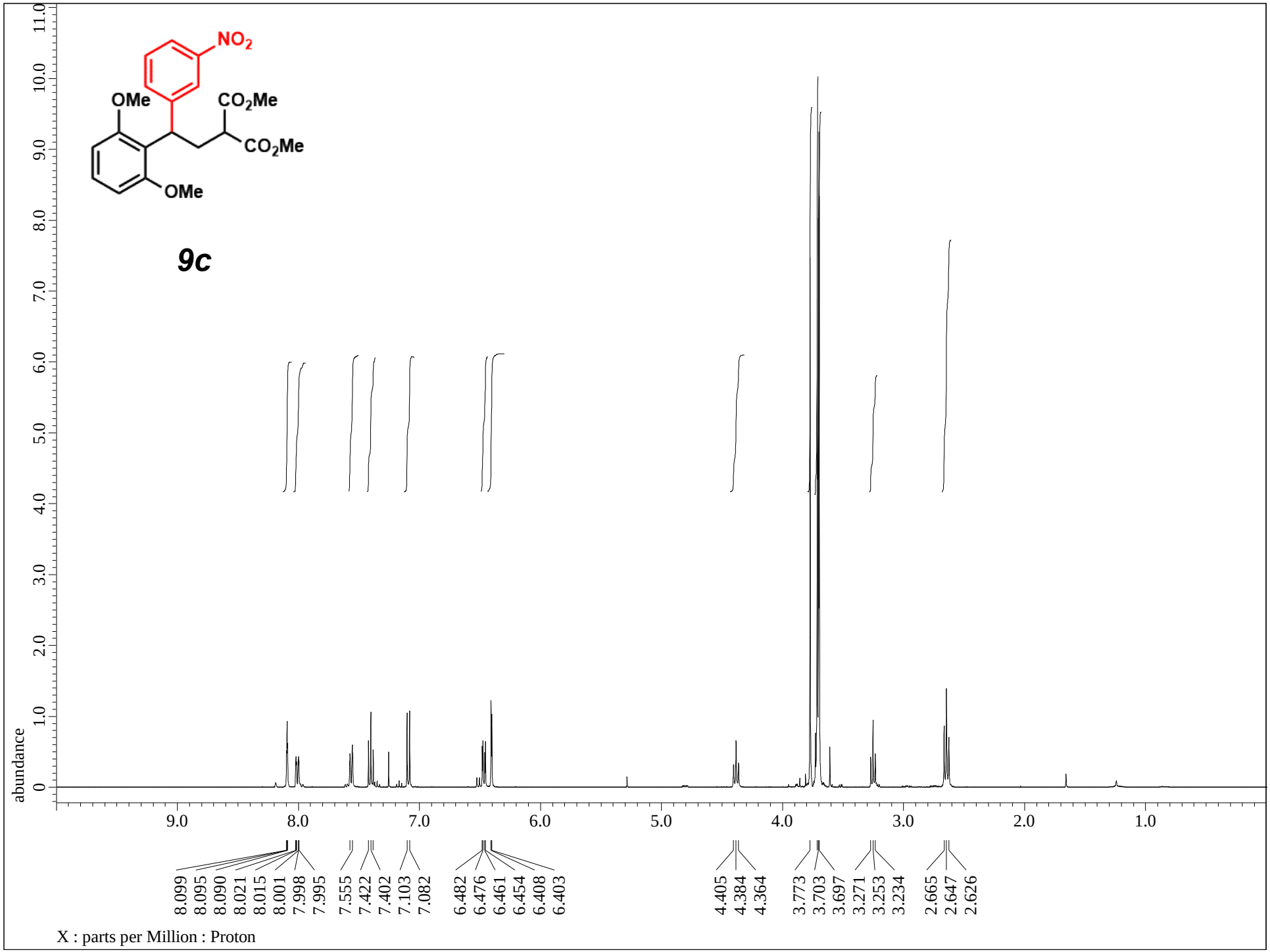

iPr
iPr
N
N
GaCl3
iPr
iPr
(IPr)GaCl3
abundance
0
0.1
0.2
0.3
0.4
0.5
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
145.736
132.989
131.335
127.530
124.135
28.993
25.121
22.056
X : parts per Million : Carbon13

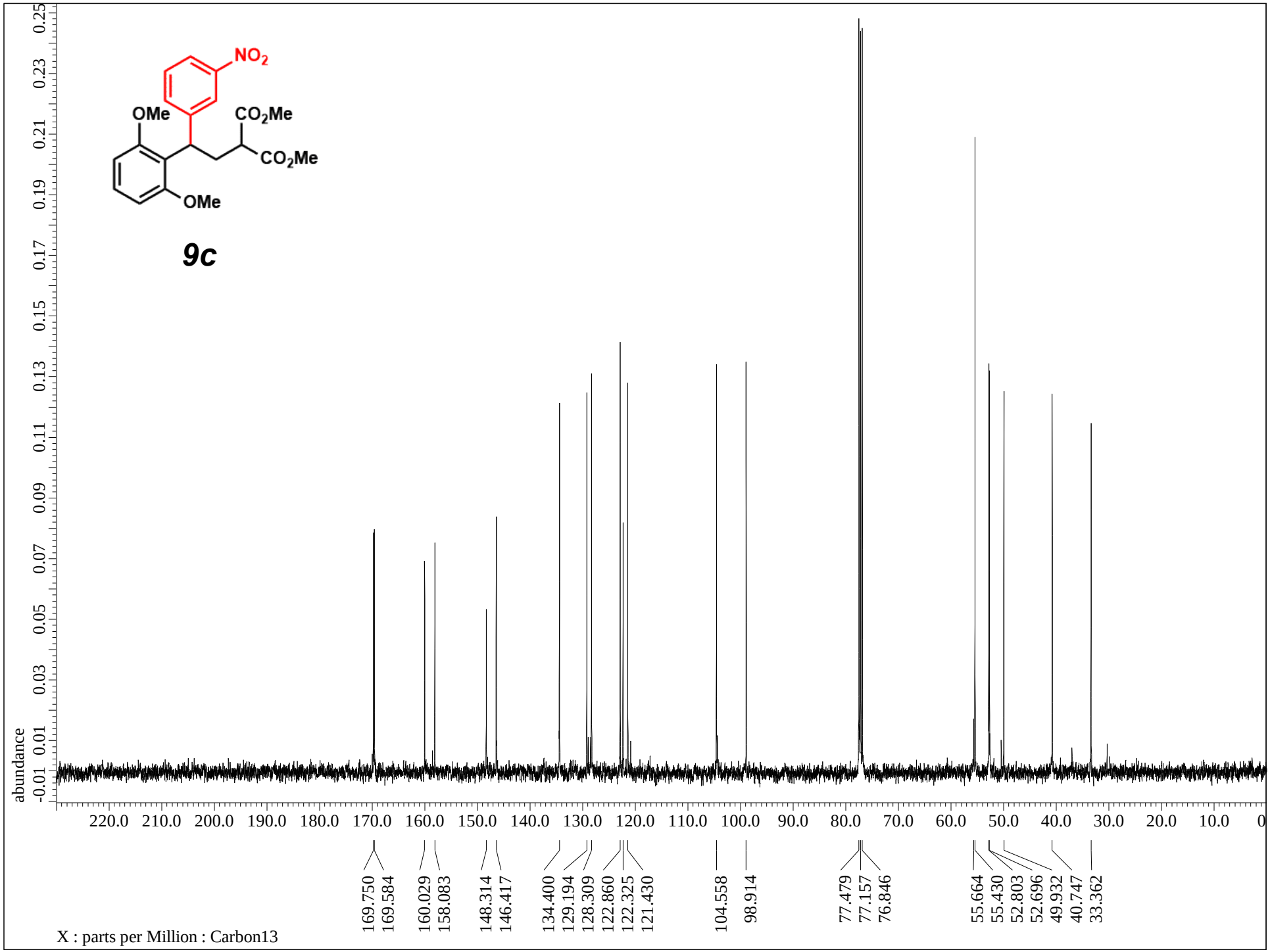

OMe
CO2Me
CO2Me
OMe
9a
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.258
7.250
7.243
7.229
7.169
7.161
7.154
7.096
7.075
6.456
6.451
6.436
6.429
6.413
6.406
4.343
4.324
4.303
3.730
3.696
3.684
3.311
3.293
3.273
2.664
2.649
2.629
2.616
2.610
2.598
2.595
2.577
X : parts per Million : Proton

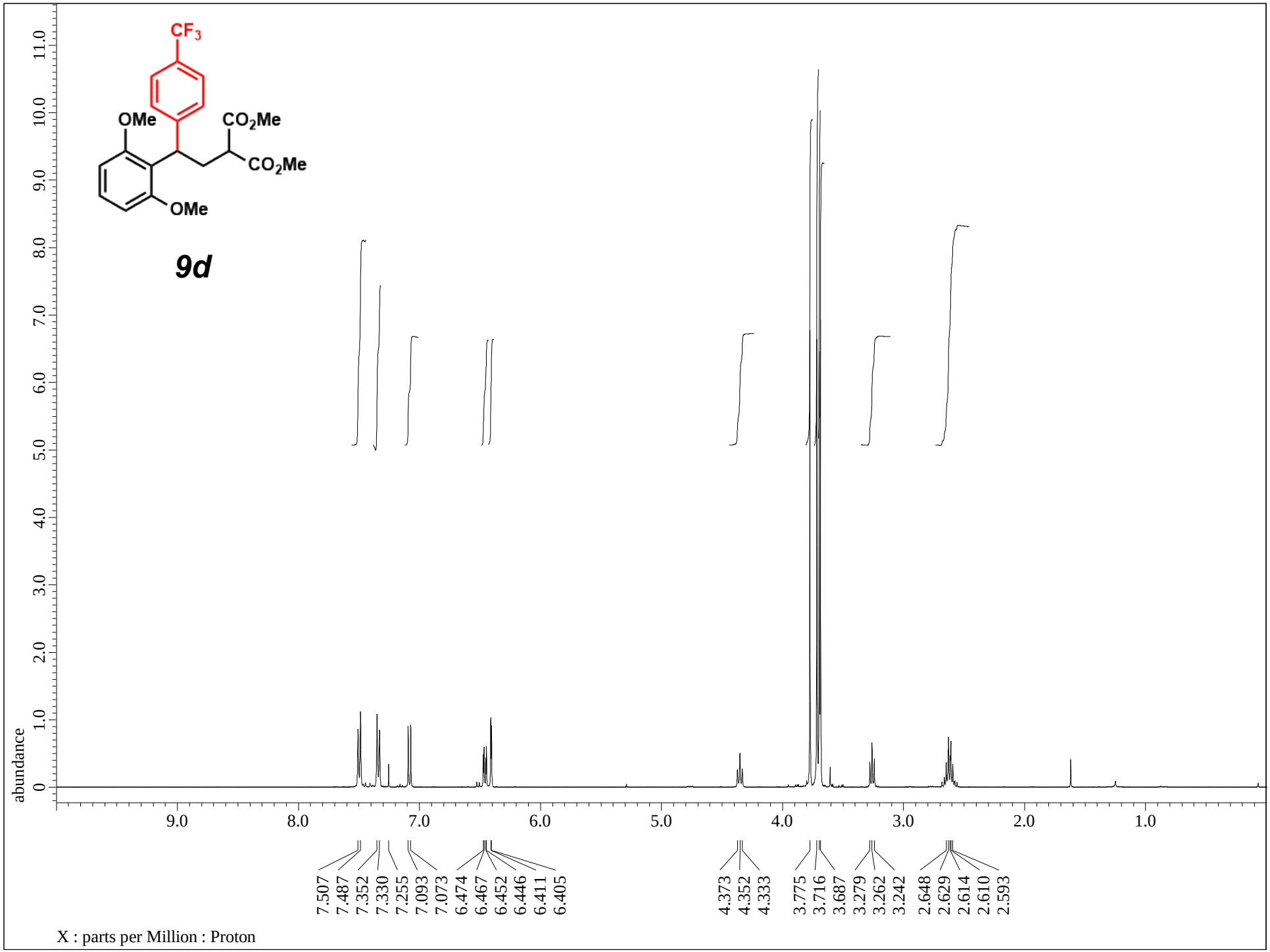

OMe
CO2Me
CO2Me
OMe
9a
abundance
X : parts per Million : Carbon13
170.100
169.925
159.465
158.083
143.867
128.377
128.114
127.929
126.227
124.261
104.295
98.739
77.479
77.167
76.846
55.469
55.391
52.637
52.560
50.234
40.572
33.965

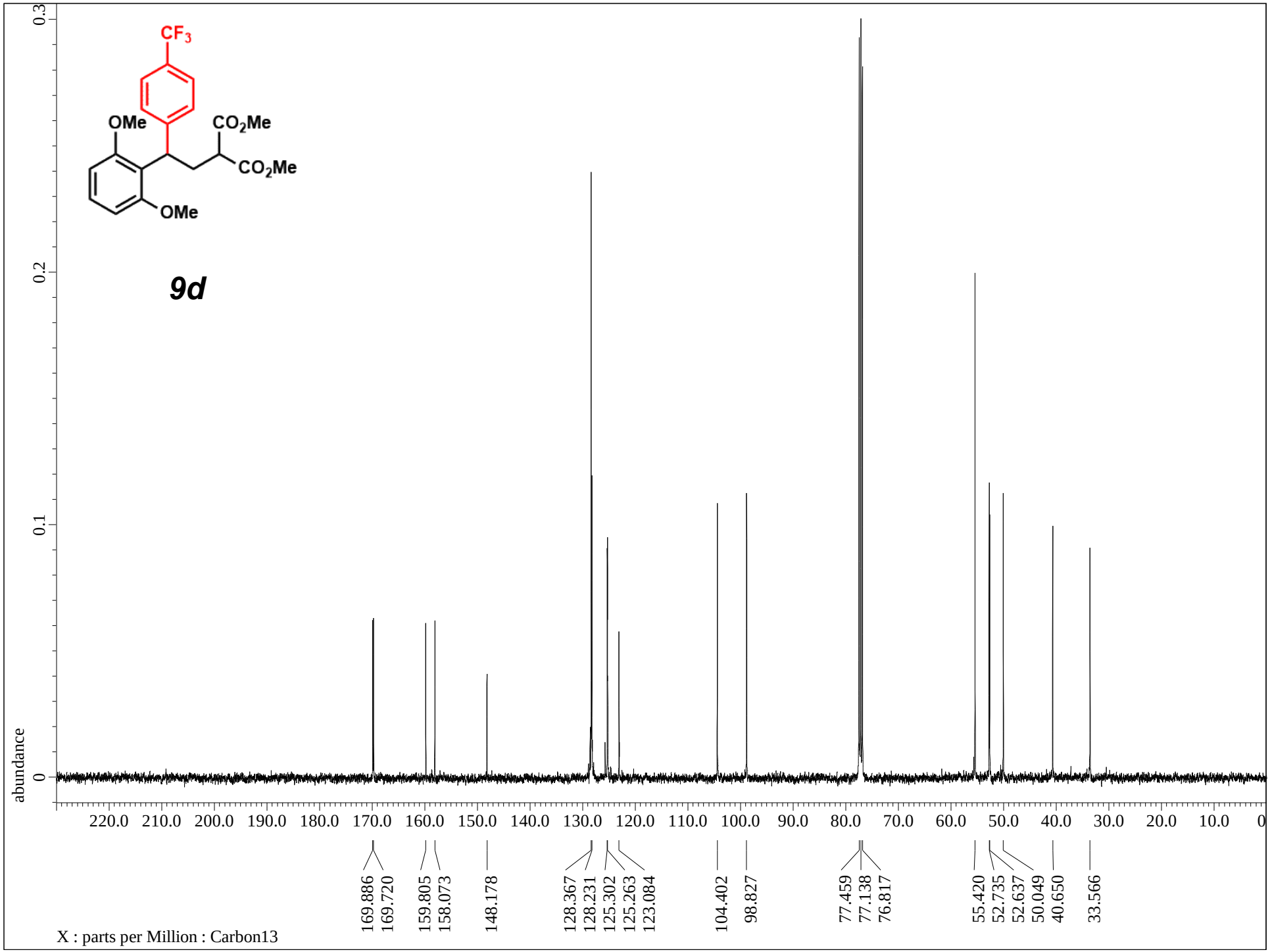

MeO
OMe
Ph
O
9b
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.869
7.867
7.853
7.849
7.407
7.274
7.271
7.257
7.254
6.453
6.448
6.437
6.431
6.406
6.401
4.379
3.770
3.702
2.925
2.920
2.911
2.908
2.428
2.412
X : parts per Million : Proton

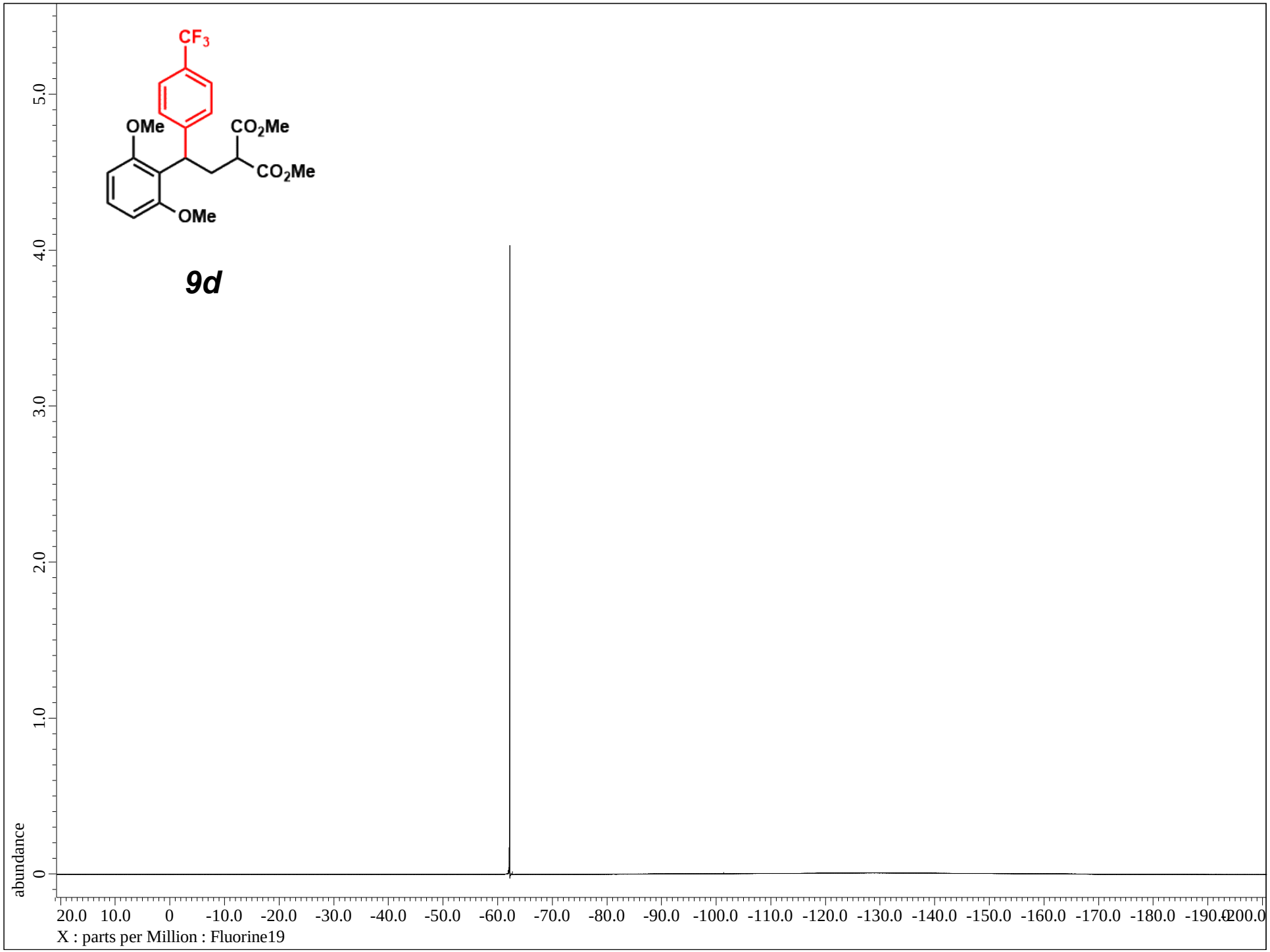

MeO
OMe
Ph
O
9b
abundance
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17 0.18 0.19
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
200.406
159.231
158.047
137.093
132.953
128.558
128.333
128.206
128.147
128.128
126.004
125.495
104.188
98.697
77.381
77.126
76.872
55.448
55.399
42.225
37.224
29.443
X : parts per Million : Carbon13

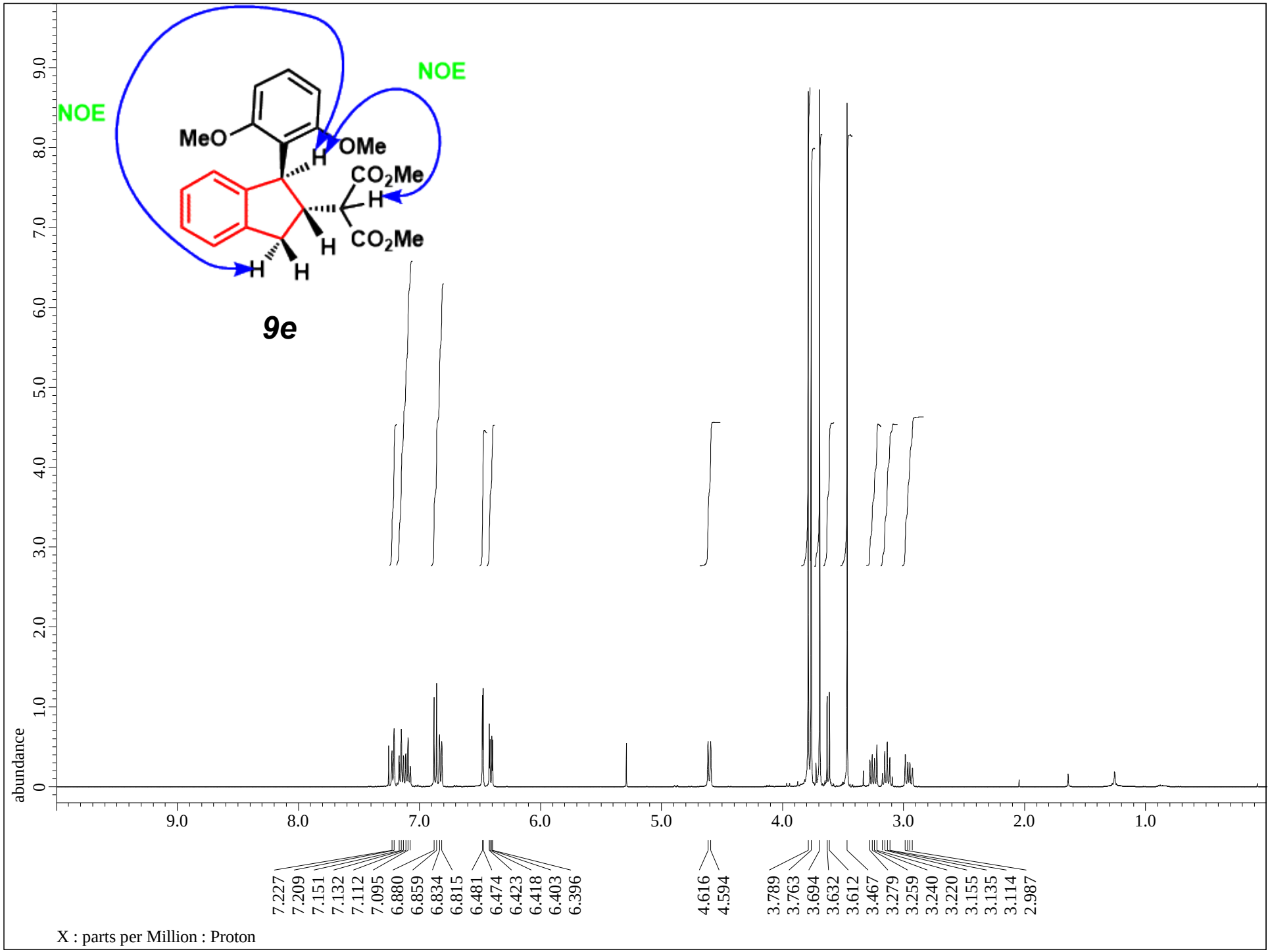

NO2
OMe
CO2Me
CO2Me
OMe
9c
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.099
8.095
8.090
8.021
8.015
8.001
7.998
7.995
7.555
7.422
7.402
7.103
7.082
6.482
6.476
6.461
6.454
6.408
6.403
4.405
4.384
4.364
3.773
3.703
3.697
3.271
3.253
3.234
2.665
2.647
2.626
X : parts per Million : Proton

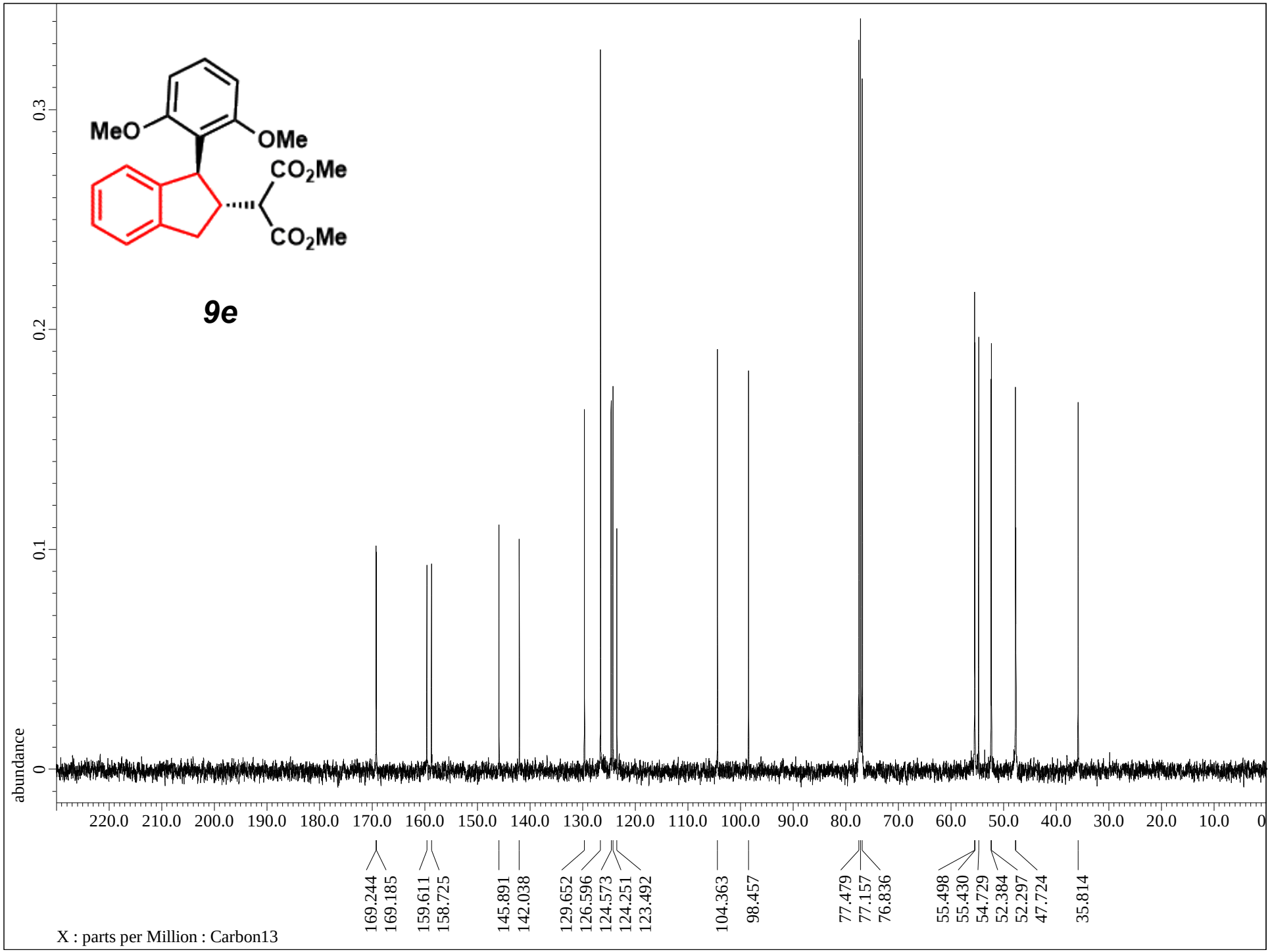

NO2
OMe
CO2Me
CO2Me
OMe
9c
abundance
-0.01 0.01 0.03 0.05 0.07 0.09 0.11 0.13 0.15 0.17 0.19 0.21 0.23 0.25
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
169.750
169.584
160.029
158.083
148.314
146.417
134.400
129.194
128.309
122.860
122.325
121.430
104.558
98.914
77.479
77.157
76.846
55.664
55.430
52.803
52.696
49.932
40.747
33.362
X : parts per Million : Carbon13

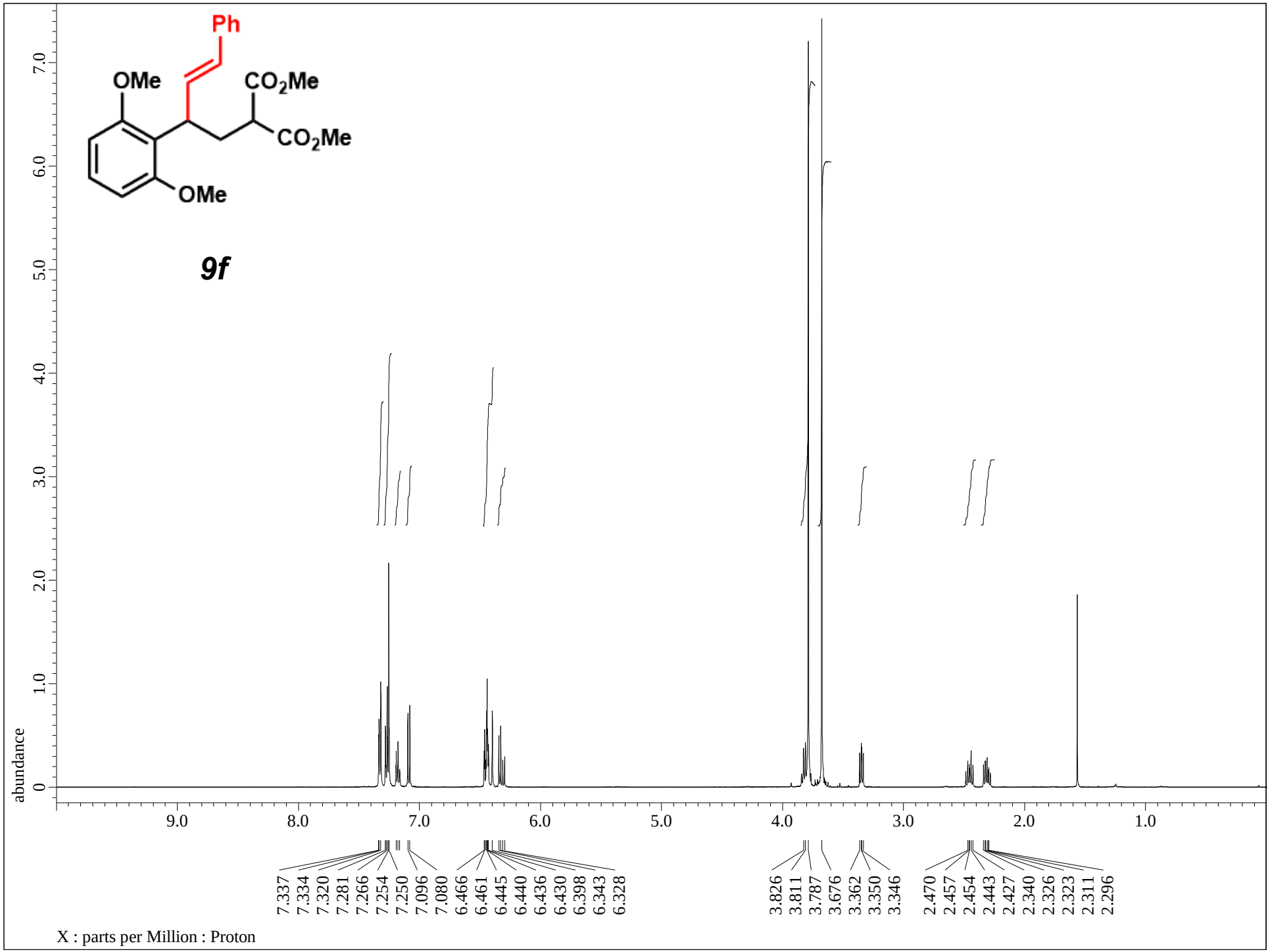

CF3
OMe
CO2Me
CO2Me
OMe
9d
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.507
7.487
7.352
7.330
7.255
7.093
7.073
6.474
6.467
6.452
6.446
6.411
6.405
4.373
4.352
4.333
3.775
3.716
3.687
3.279
3.262
3.242
2.648
2.629
2.614
2.610
2.593
X : parts per Million : Proton

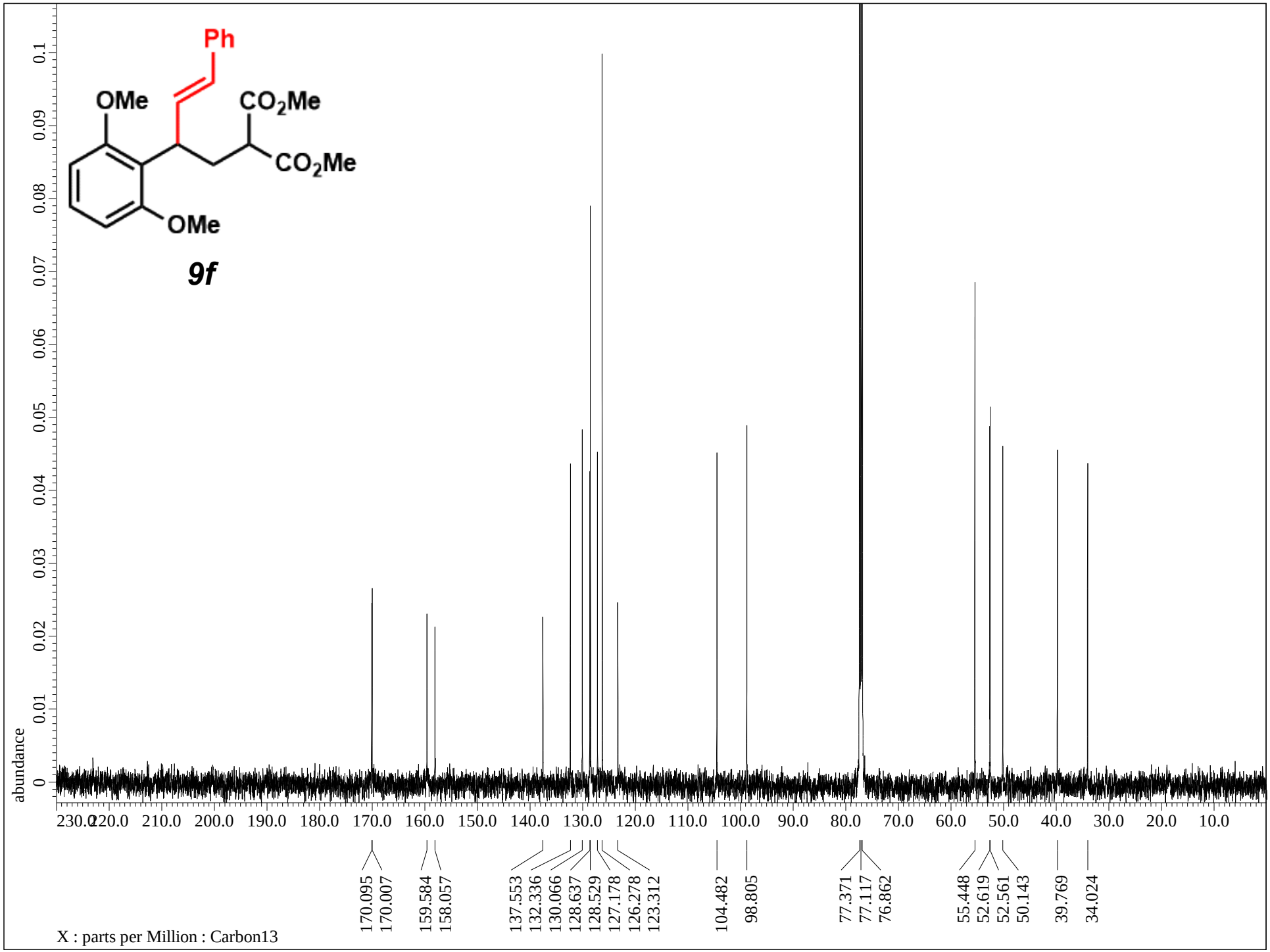

CF3
OMe
CO2Me
CO2Me
OMe
9d
abundance
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
169.886
169.720
159.805
158.073
148.178
128.367
128.231
125.302
125.263
123.084
104.402
98.827
77.459
77.138
76.817
55.420
52.735
52.637
50.049
40.650
33.566
X : parts per Million : Carbon13

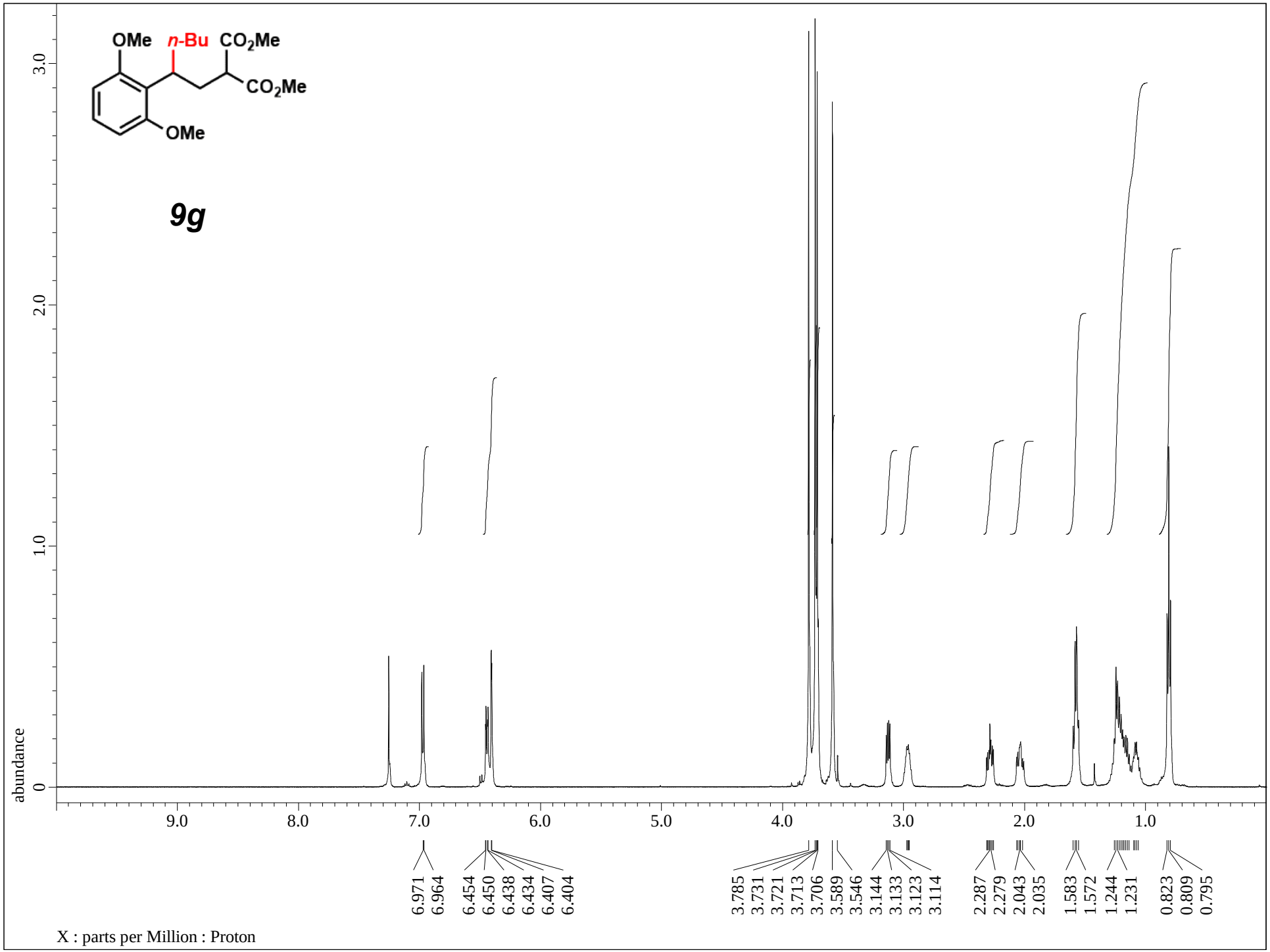

CF3
OMe
CO2Me
CO2Me
OMe
9d
5.0
4.0
3.0
2.0
1.0
0
abundance
20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0
X : parts per Million : Fluorine19

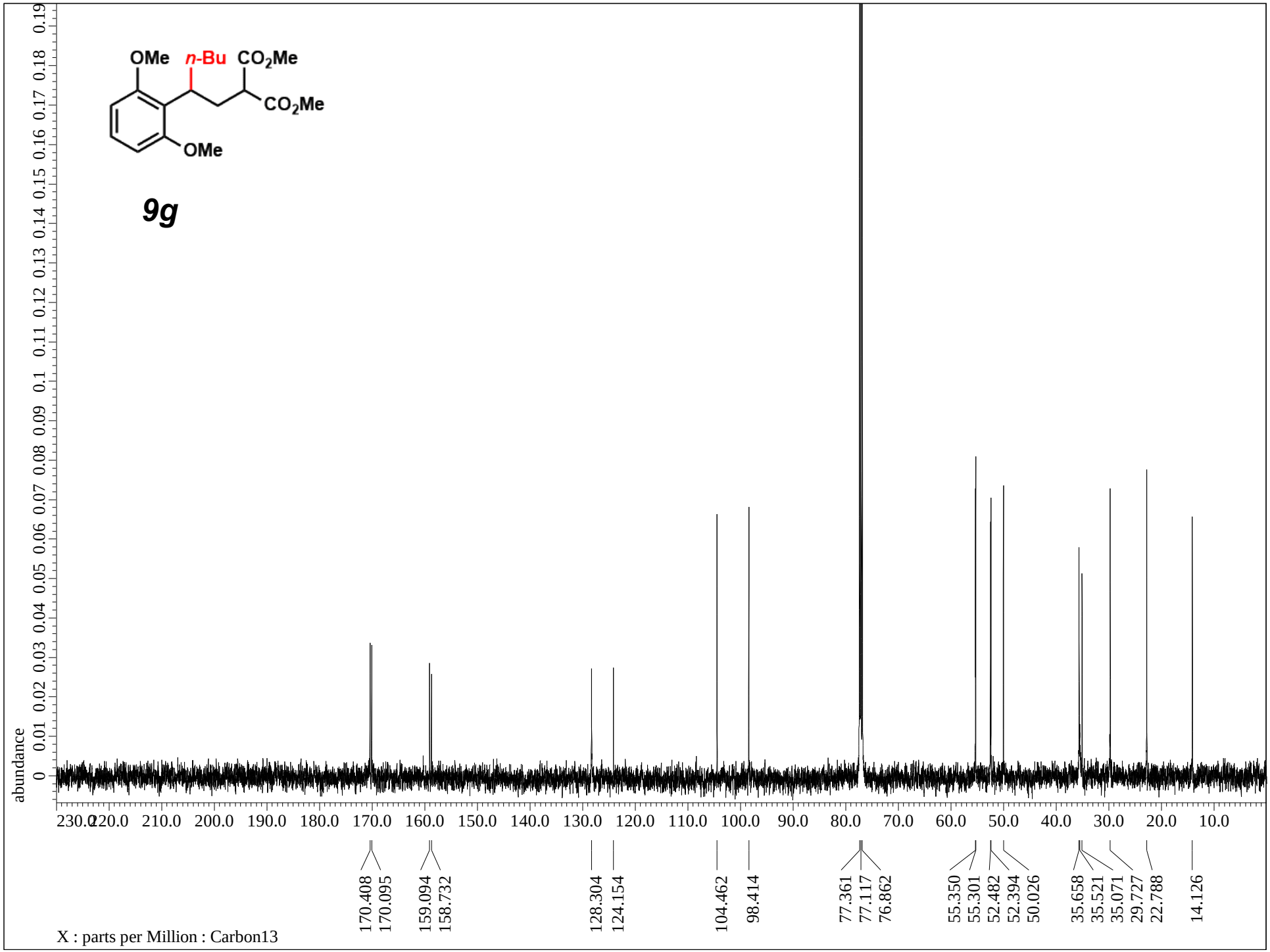

NOE
NOE
MeO
OMe
H
CO2Me
H
CO2Me
H
H
H
9e
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.227
7.209
7.151
7.132
7.112
7.095
6.880
6.859
6.834
6.815
6.481
6.474
6.423
6.418
6.403
6.396
4.616
4.594
3.789
3.763
3.694
3.632
3.612
3.467
3.279
3.259
3.240
3.220
3.155
3.135
3.114
2.987
X : parts per Million : Proton

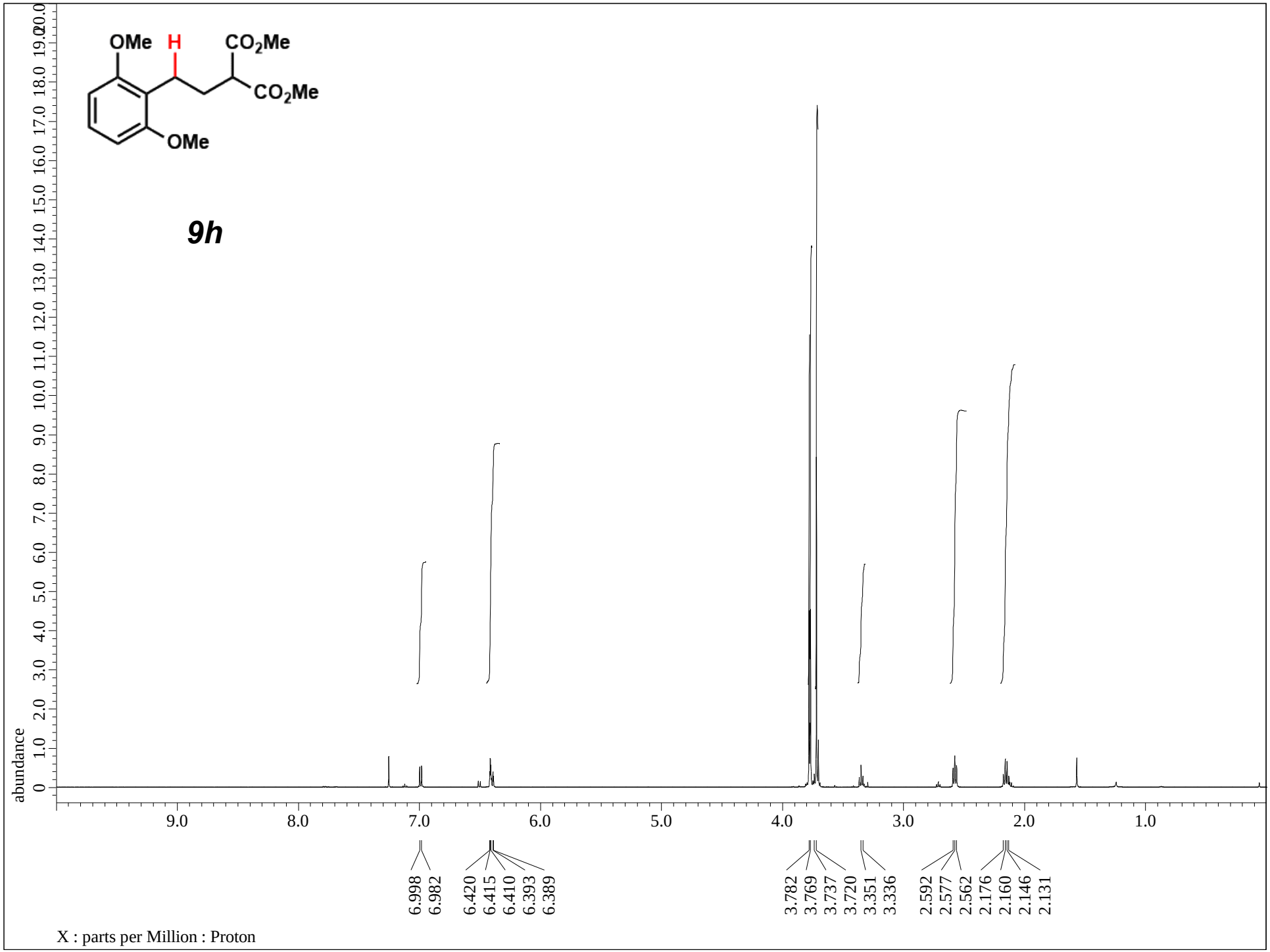

MeO
OMe
CO2Me
CO2Me
9e
abundance
0
0.1
0.2
0.3
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
169.244
169.185
159.611
158.725
145.891
142.038
129.652
126.596
124.573
124.251
123.492
104.363
98.457
77.479
77.157
76.836
55.498
55.430
54.729
52.384
52.297
47.724
35.814
X : parts per Million : Carbon13

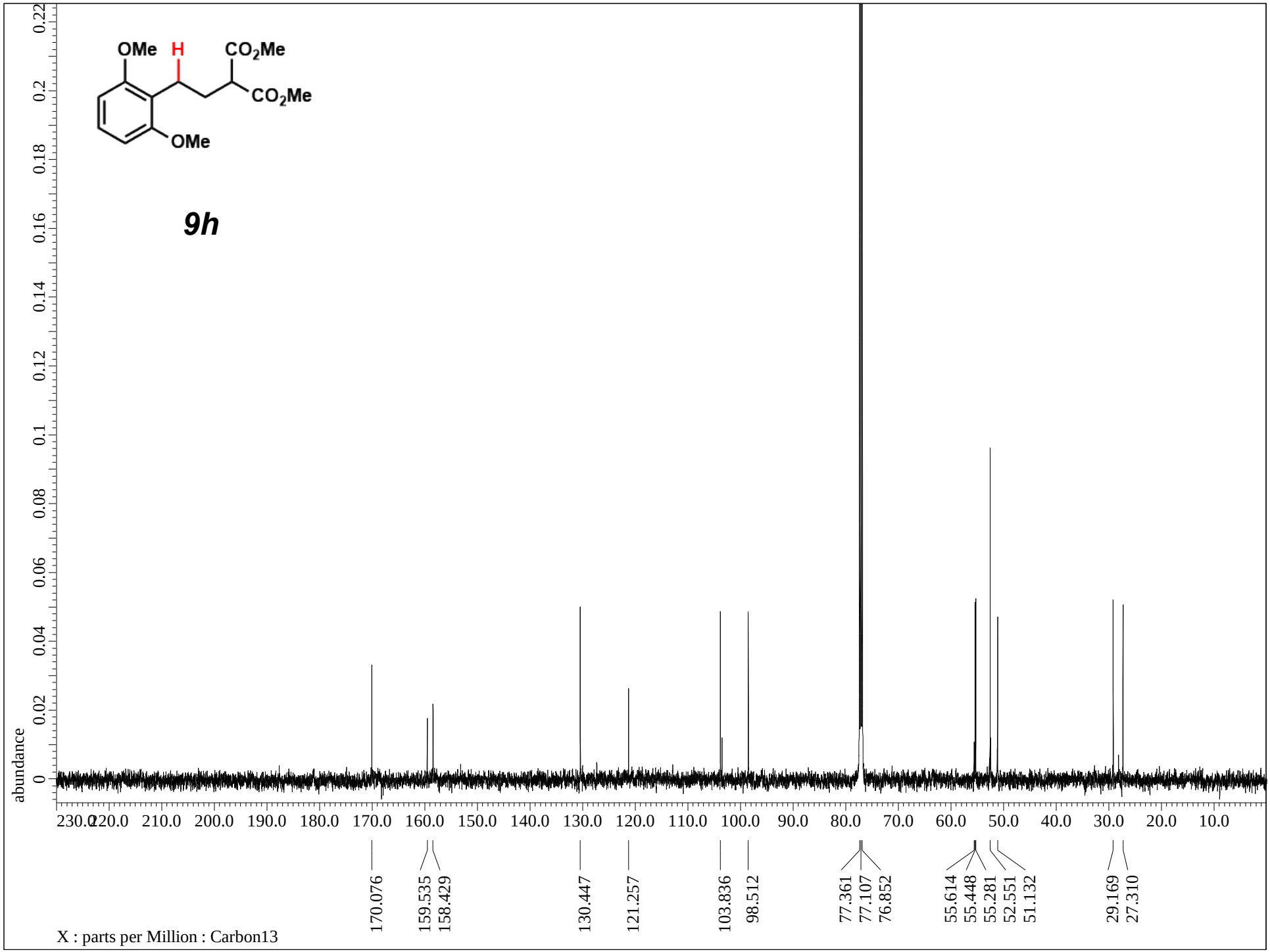

Ph
OMe
CO2Me
CO2Me
OMe
9f
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.337
7.334
7.320
7.281
7.266
7.254
7.250
7.096
7.080
6.466
6.461
6.445
6.440
6.436
6.430
6.398
6.343
6.328
3.826
3.811
3.787
3.676
3.362
3.350
3.346
2.470
2.457
2.454
2.443
2.427
2.340
2.326
2.323
2.311
2.296
X : parts per Million : Proton

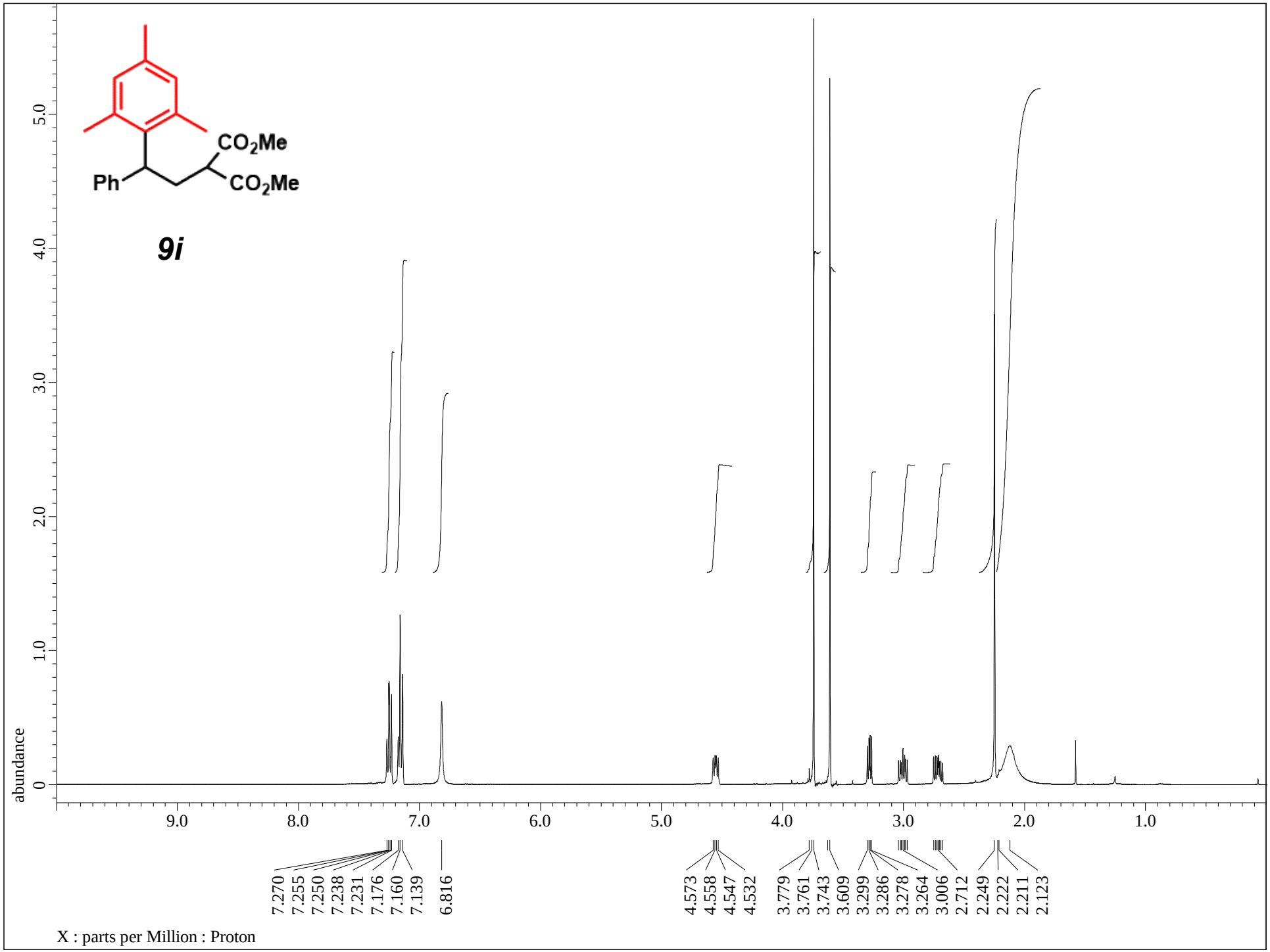

Ph
OMe
CO2Me
CO2Me
OMe
9f
abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
230.0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.095
170.007
159.584
158.057
137.553
132.336
130.066
128.637
128.529
127.178
126.278
123.312
104.482
98.805
77.371
77.117
76.862
55.448
52.619
52.561
50.143
39.769
34.024
X : parts per Million : Carbon13

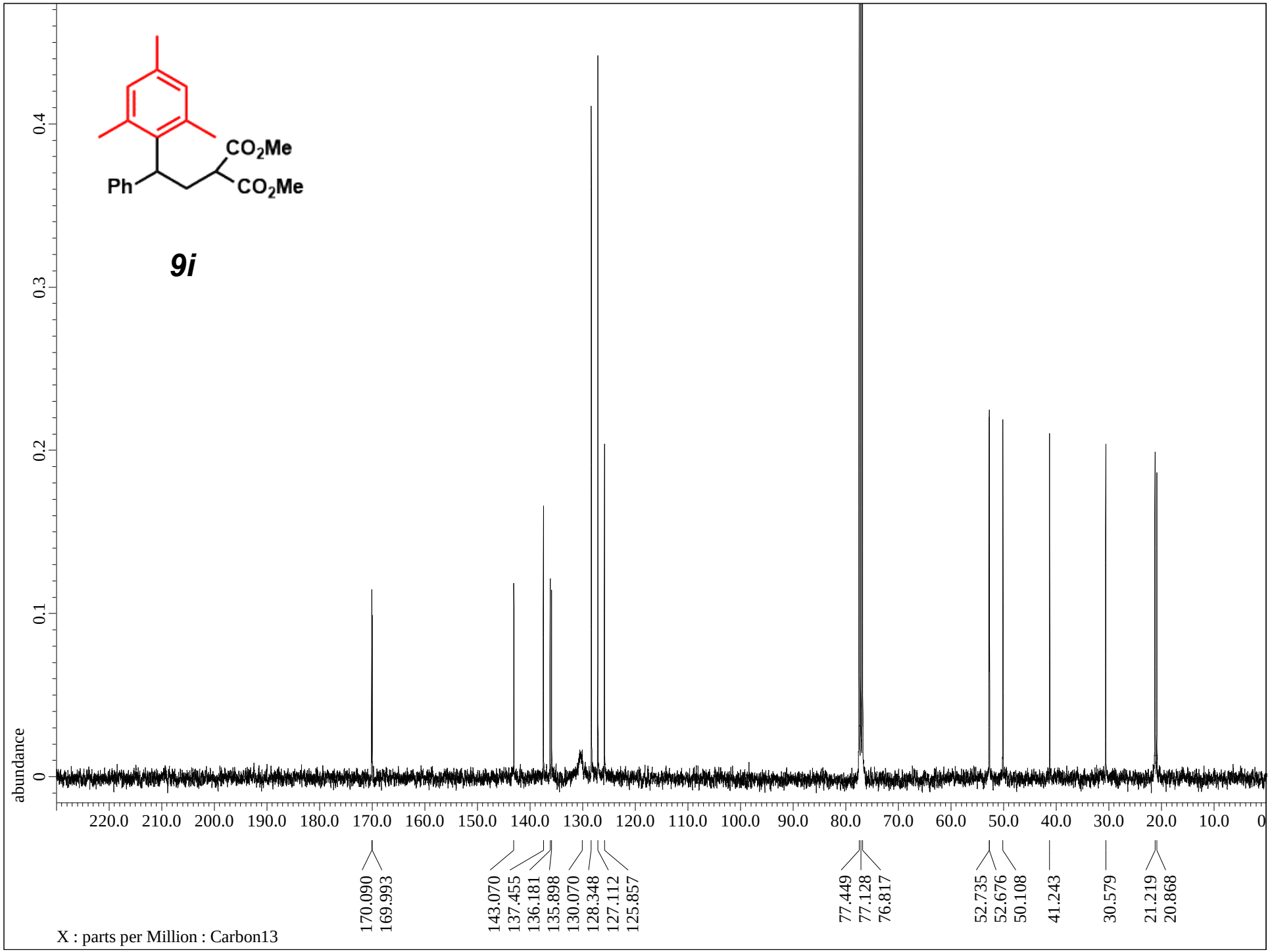

OMe
n-Bu
CO2Me
CO2Me
OMe
9g
abundance
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
6.971
6.964
6.454
6.450
6.438
6.434
6.407
6.404
3.785
3.731
3.721
3.713
3.706
3.589
3.546
3.144
3.133
3.123
3.114
2.287
2.279
2.043
2.035
1.583
1.572
1.244
1.231
0.823
0.809
0.795
X : parts per Million : Proton

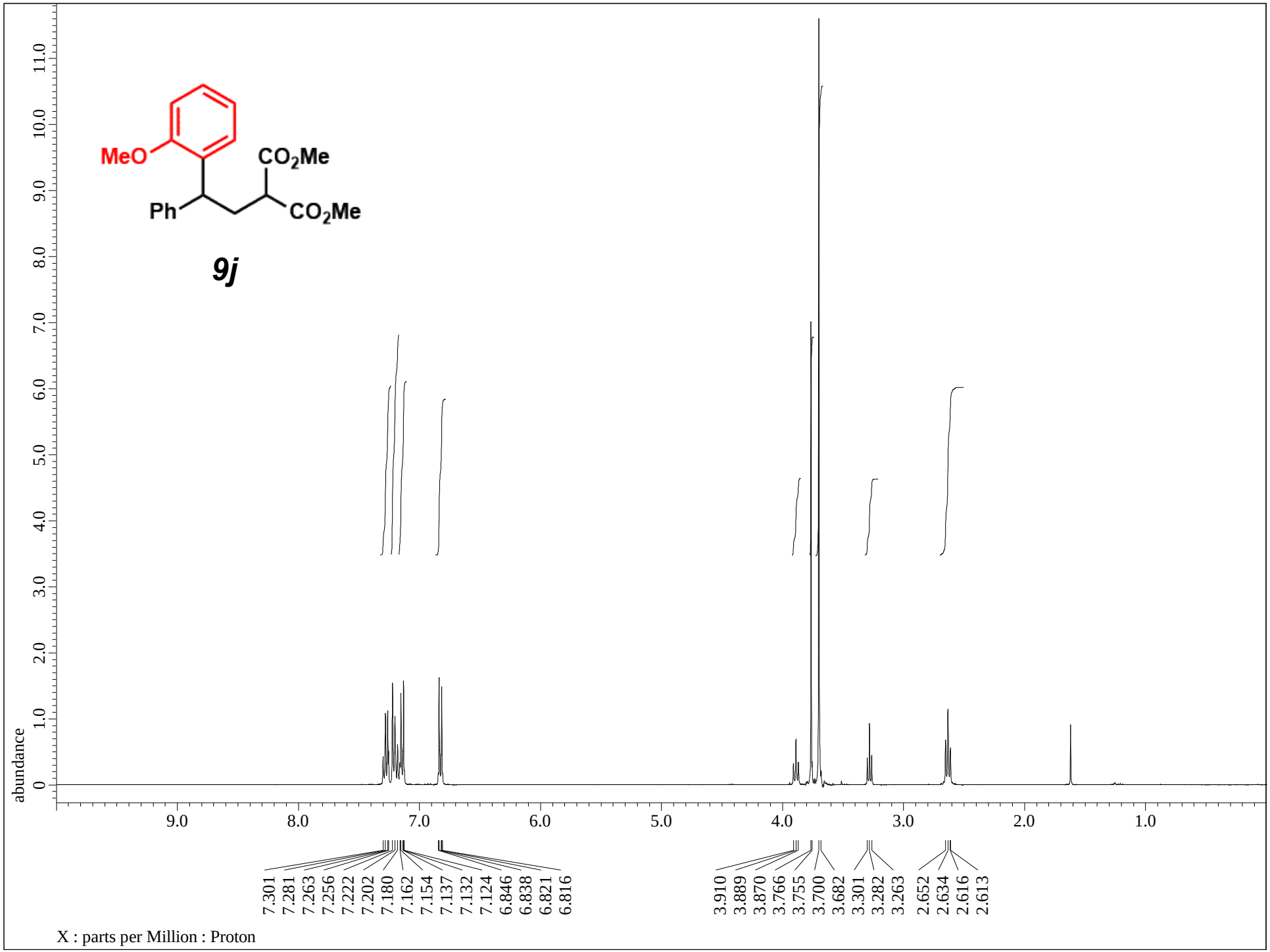

OMe
n-Bu
CO2Me
CO2Me
OMe
9g
abundance
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17 0.18 0.19
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
170.408
170.095
159.094
158.732
128.304
124.154
104.462
98.414
77.361
77.117
76.862
55.350
55.301
52.482
52.394
50.026
35.658
35.521
35.071
29.727
22.788
14.126
X : parts per Million : Carbon13

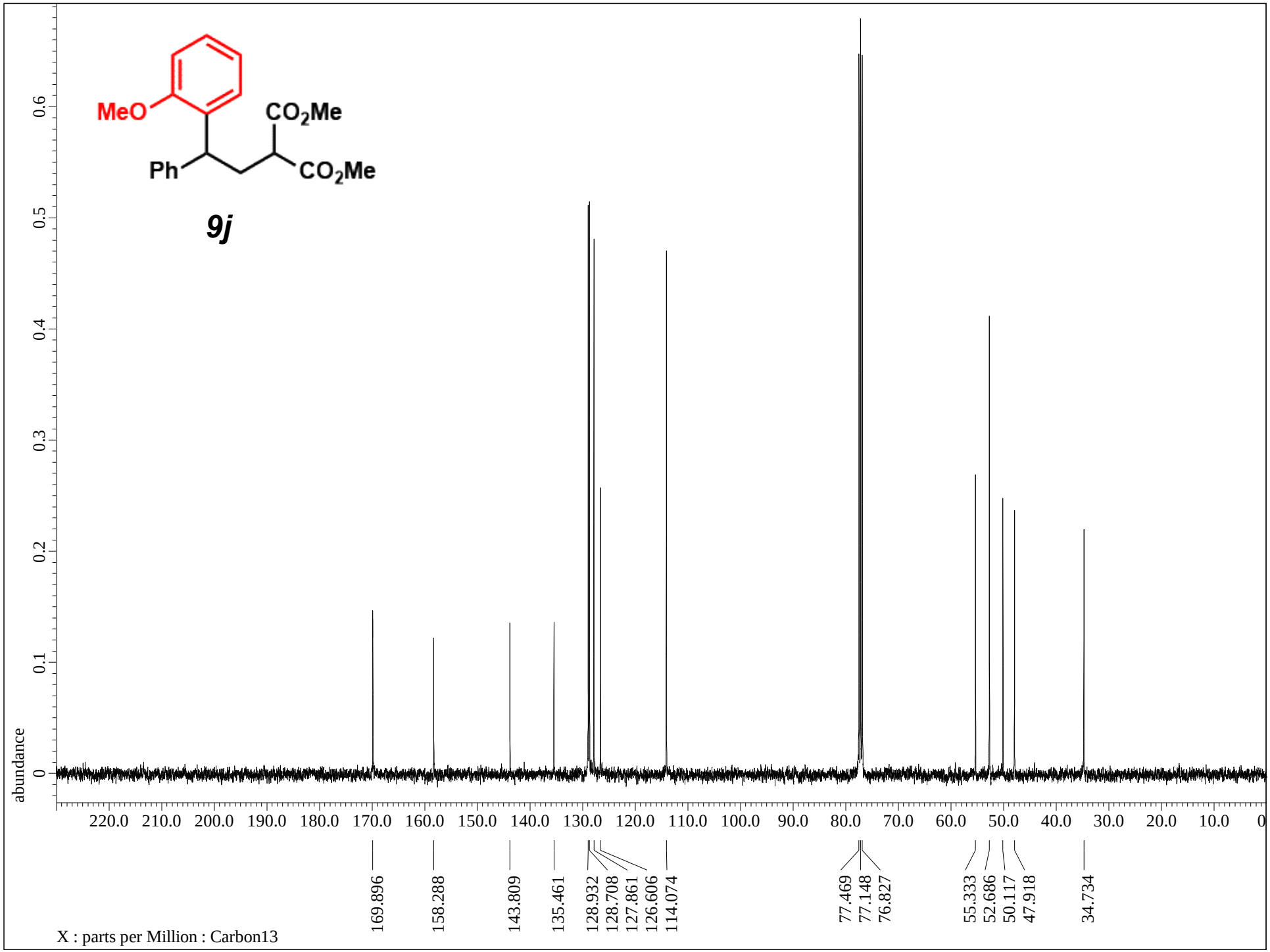

OMe
H
CO2Me
CO2Me
OMe
9h
abundance
X : parts per Million : Proton
6.998
6.982
6.420
6.415
6.410
6.393
6.389
3.782
3.769
3.737
3.720
3.351
3.336
2.592
2.577
2.562
2.176
2.160
2.146
2.131

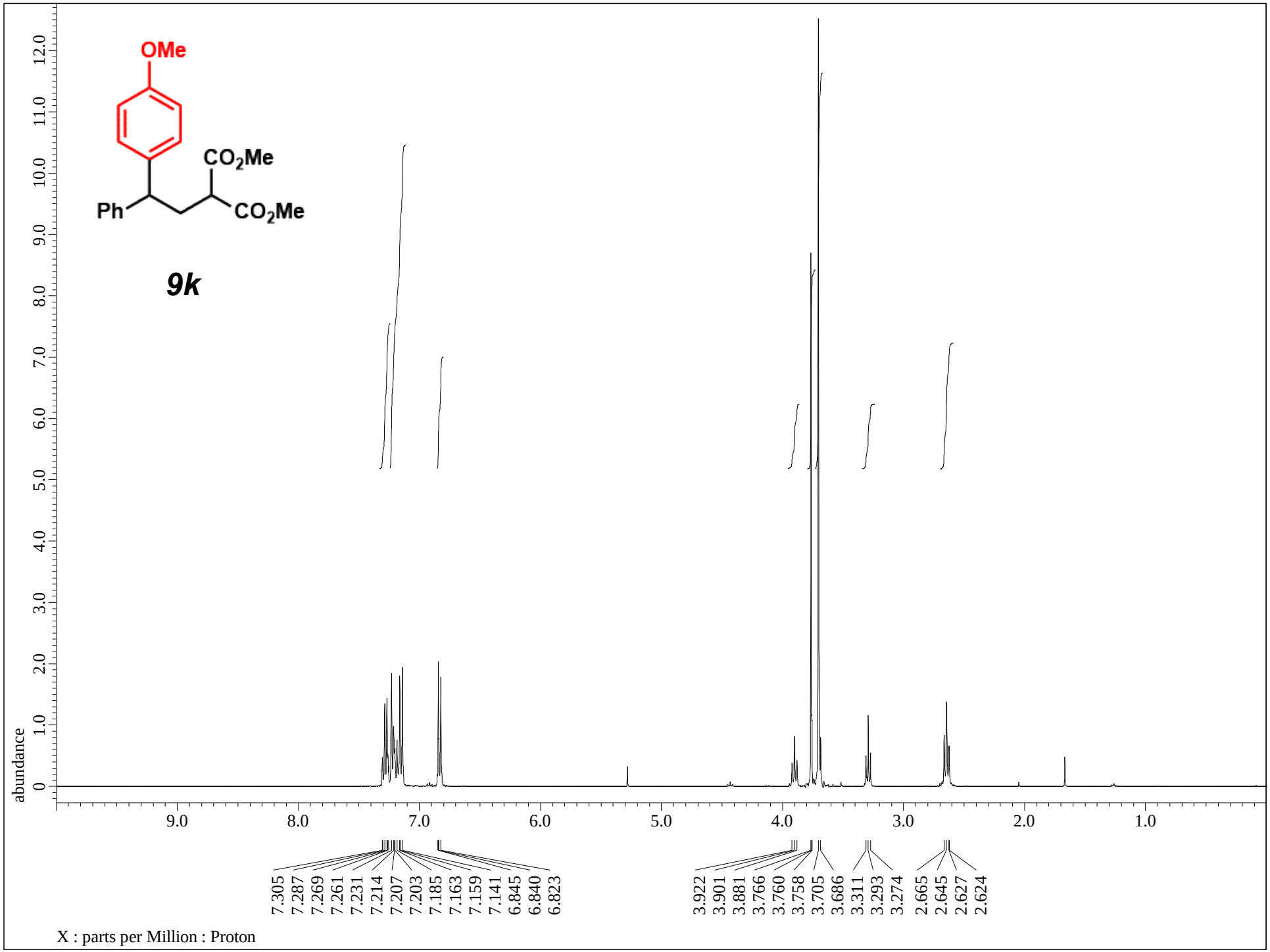

OMe
H
CO2Me
CO2Me
OMe
9h
abundance
0.22
0.2
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
230.0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.076
159.535
158.429
130.447
121.257
103.836
98.512
77.361
77.107
76.852
55.614
55.448
55.281
52.551
51.132
29.169
27.310
X : parts per Million : Carbon13

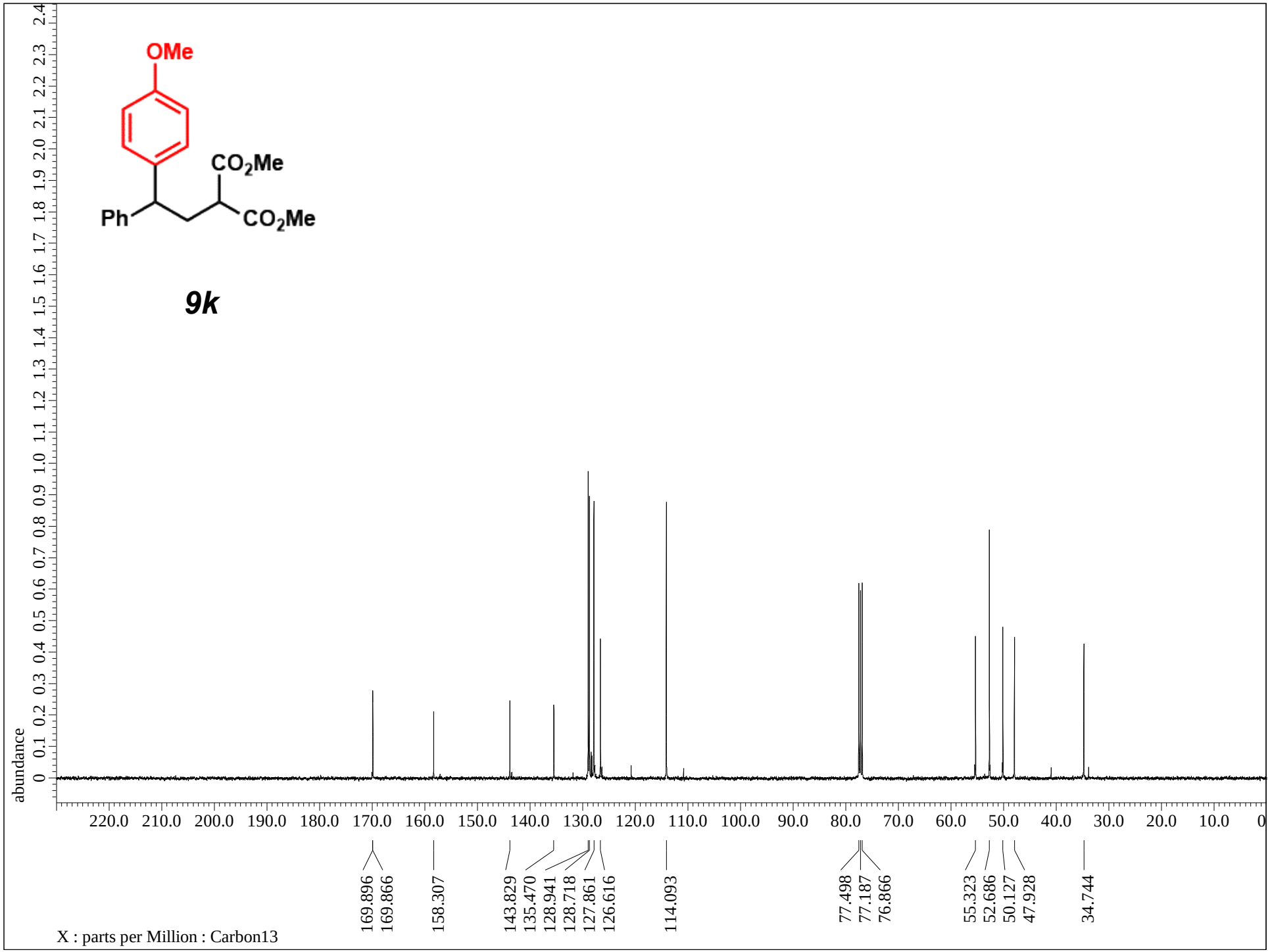

CO2Me
Ph
CO2Me
9i
abundance
0
1.0
2.0
3.0
4.0
5.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.270
7.255
7.250
7.238
7.231
7.176
7.160
7.139
6.816
4.573
4.558
4.547
4.532
3.779
3.761
3.743
3.609
3.299
3.286
3.278
3.264
3.006
2.712
2.249
2.222
2.211
2.123
X : parts per Million : Proton

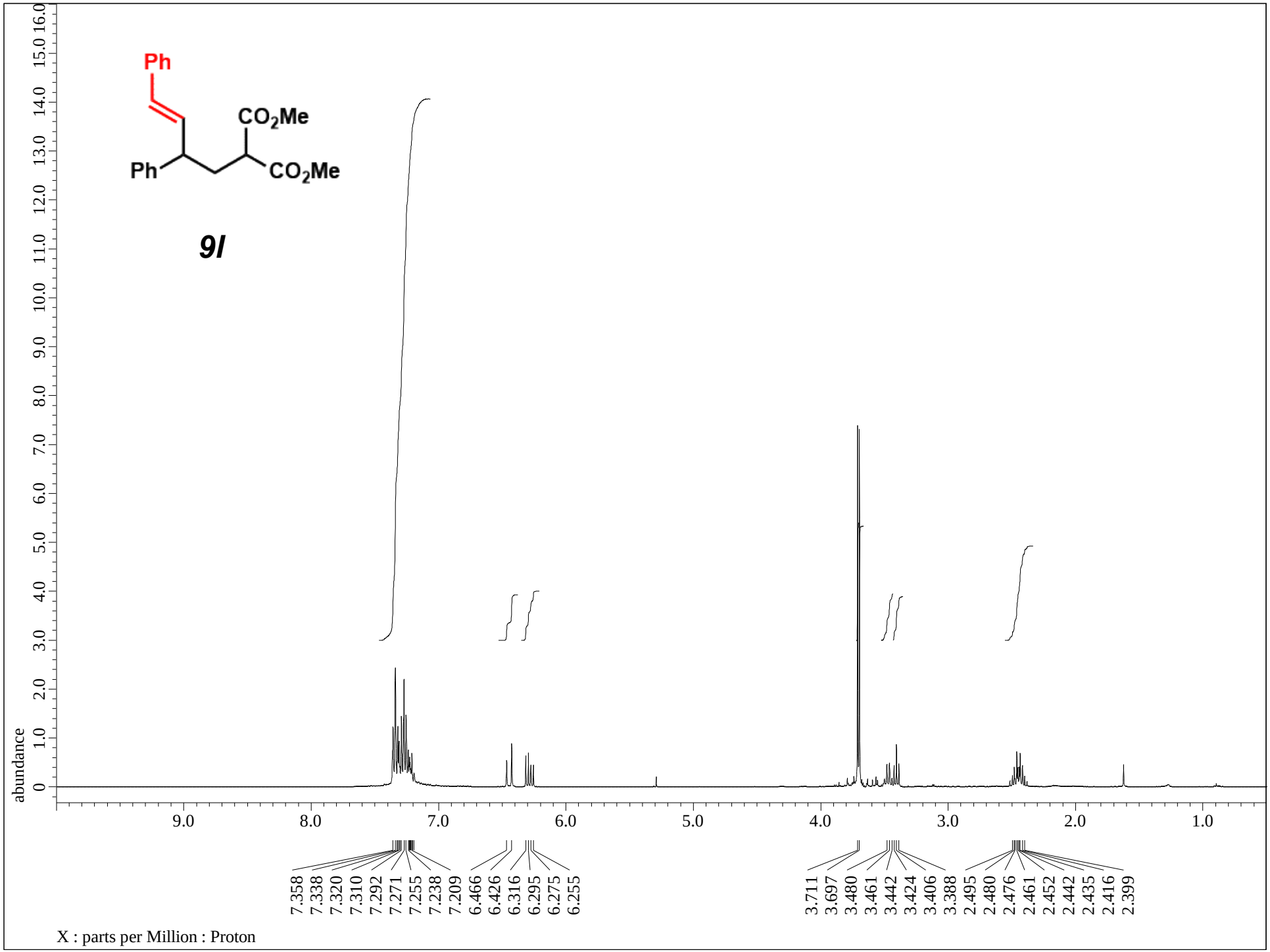

CO2Me
Ph
CO2Me
9i
abundance
0.4
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
170.090
169.993
143.070
137.455
136.181
135.898
130.070
128.348
127.112
125.857
77.449
77.128
76.817
52.735
52.676
50.108
41.243
30.579
21.219
20.868
X : parts per Million : Carbon13

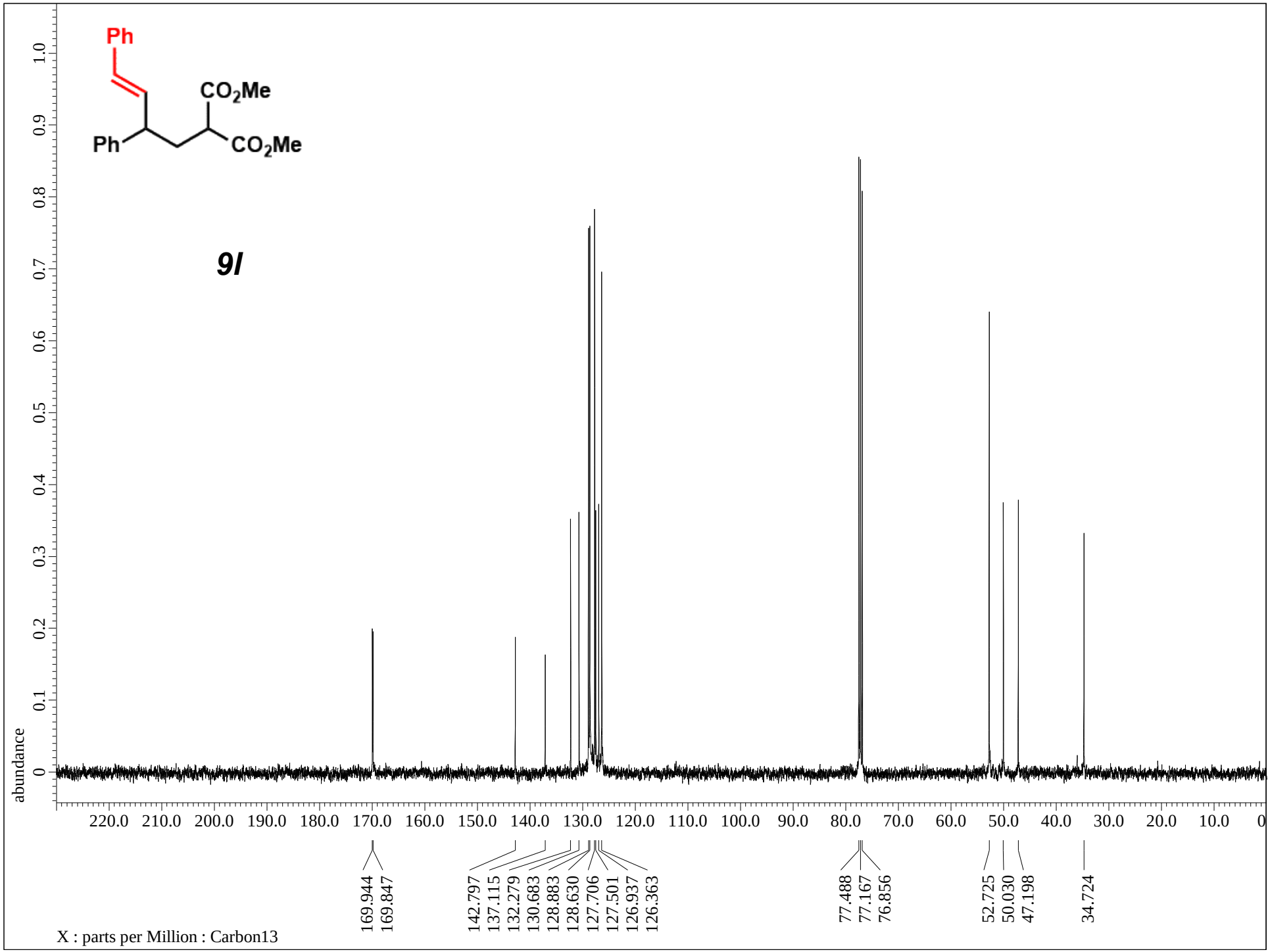


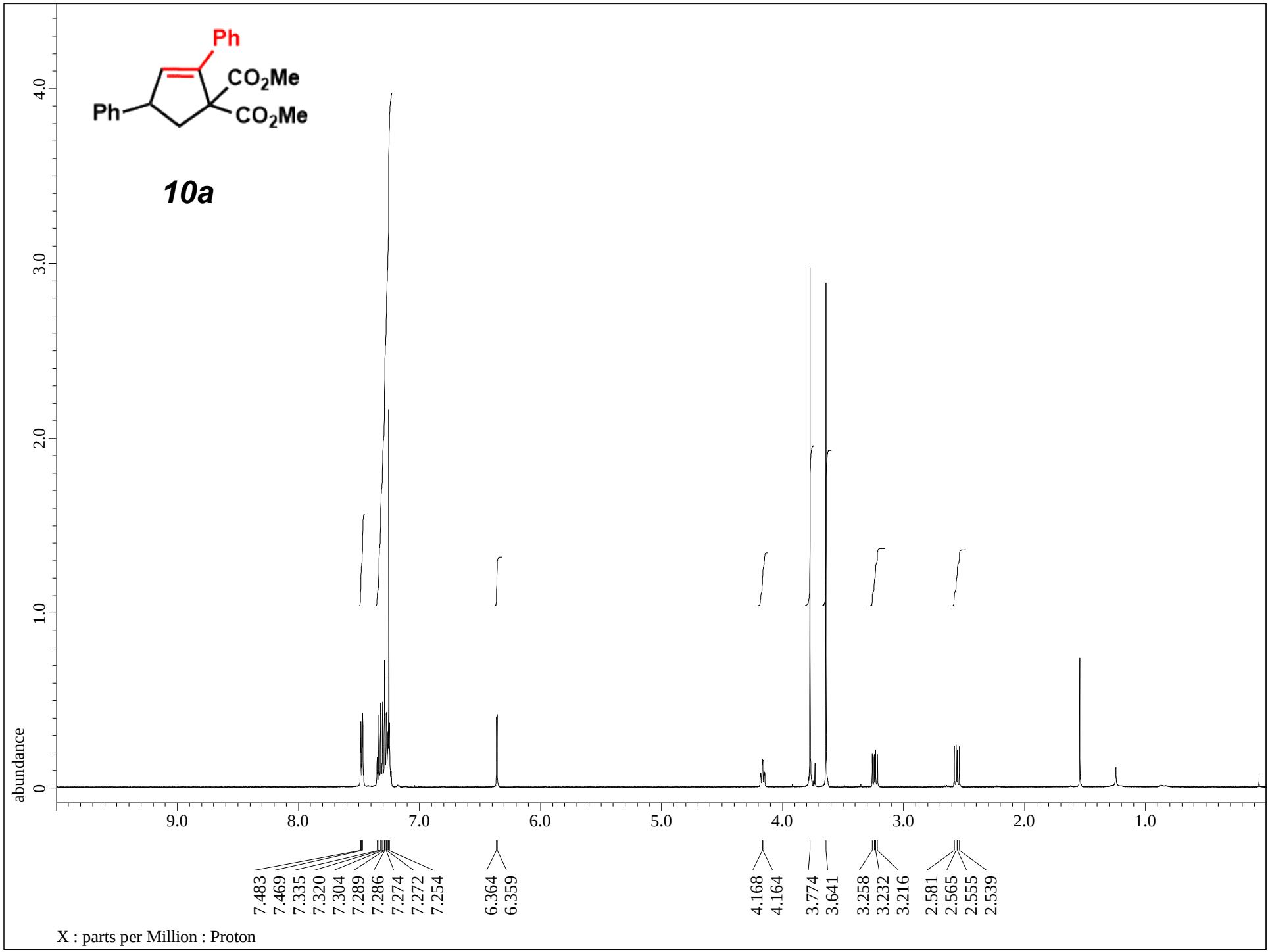

MeO
CO2Me
Ph
CO2Me
9j
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
169.896
158.288
143.809
135.461
128.932
128.708
127.861
126.606
114.074
77.469
77.148
76.827
55.333
52.686
50.117
47.918
34.734
X : parts per Million : Carbon13

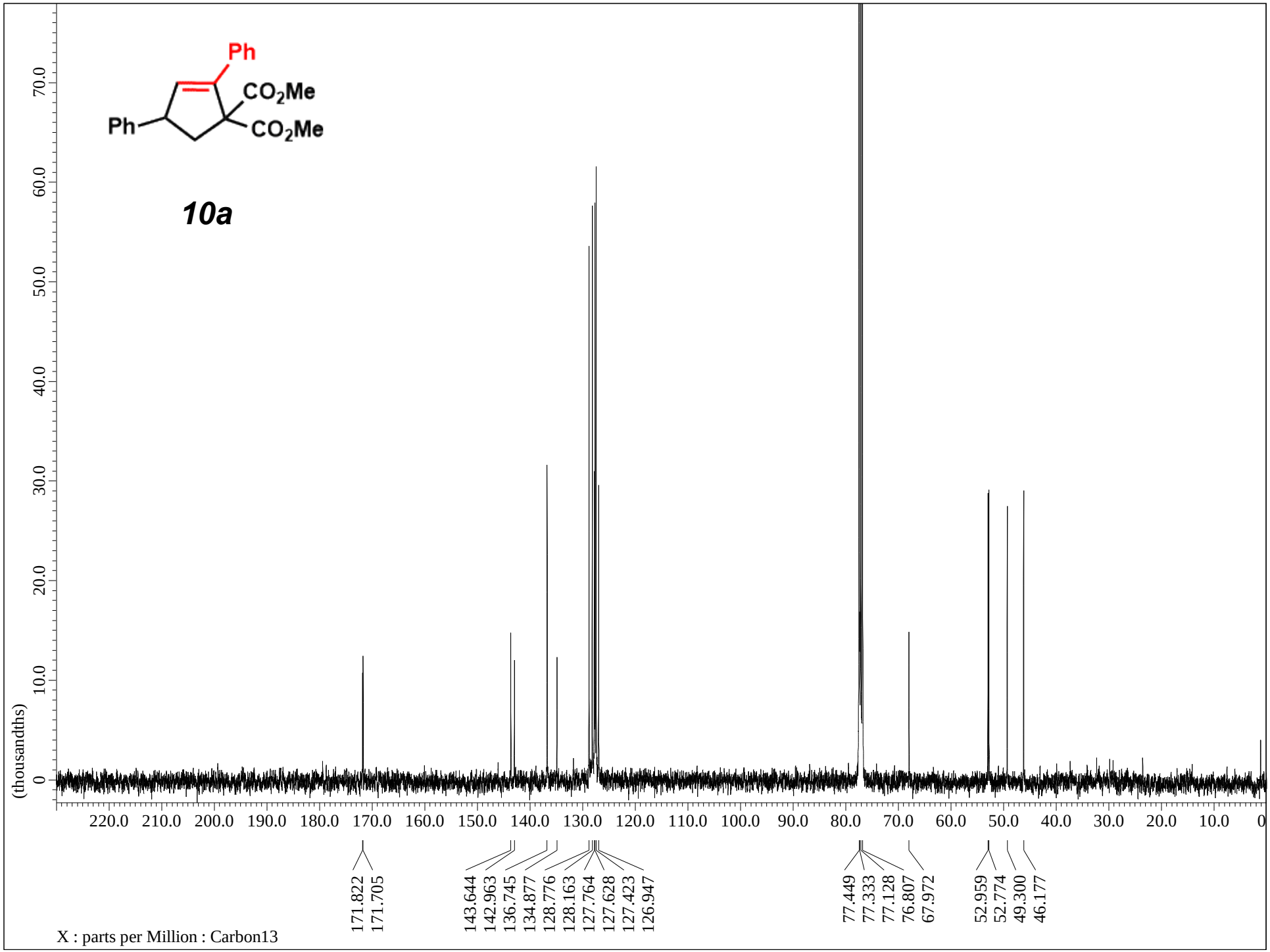

OMe
CO2Me
Ph
CO2Me
9k
abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.305
7.287
7.269
7.261
7.231
7.214
7.207
7.203
7.185
7.163
7.159
7.141
6.845
6.840
6.823
3.922
3.901
3.881
3.766
3.760
3.758
3.705
3.686
3.311
3.293
3.274
2.665
2.645
2.627
2.624
X : parts per Million : Proton

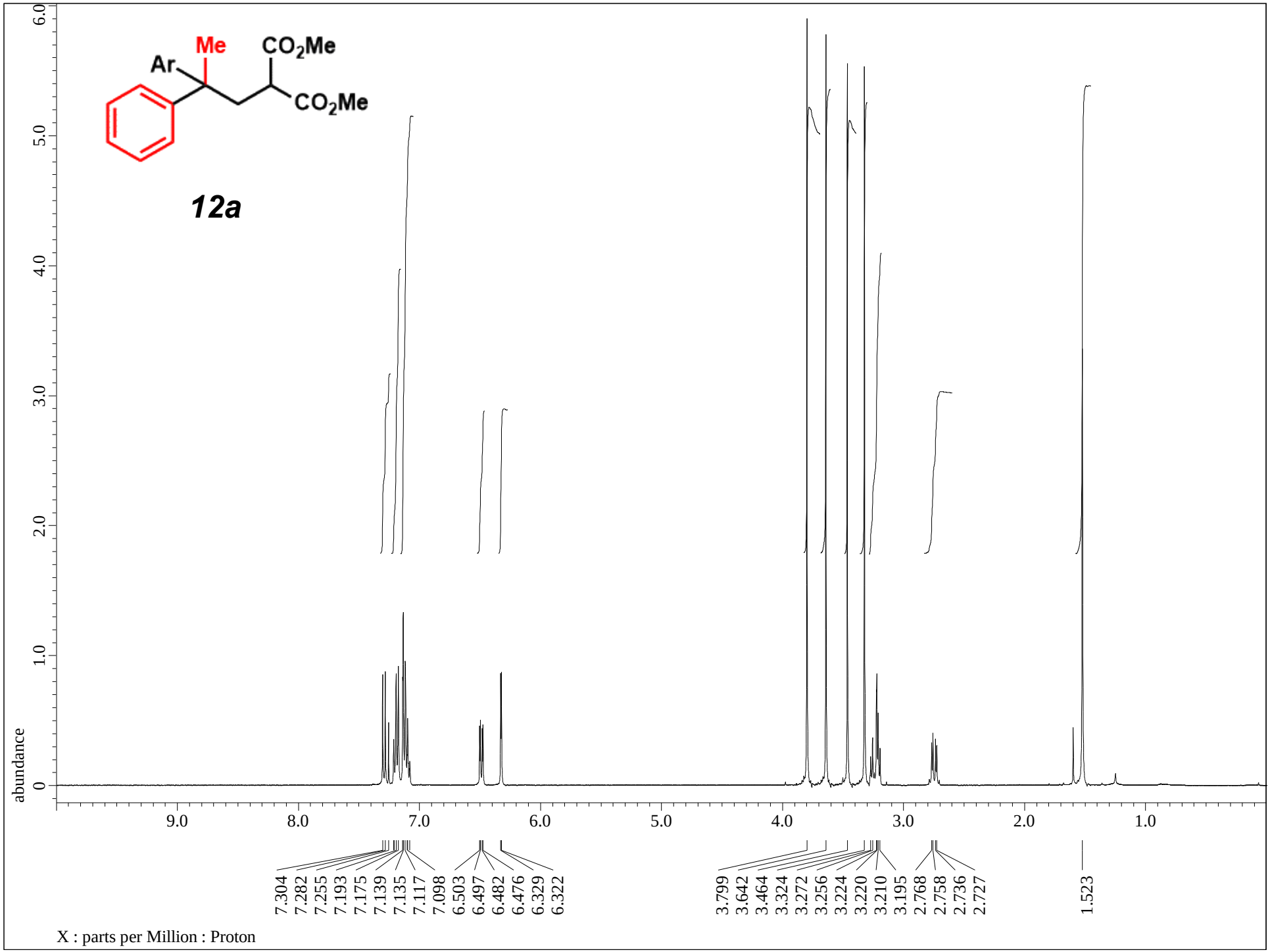

OMe
CO2Me
Ph
CO2Me
9k
abundance
X : parts per Million : Carbon13
169.896
169.866
158.307
143.829
135.470
128.941
128.718
127.861
126.616
114.093
77.498
77.187
76.866
55.323
52.686
50.127
47.928
34.744

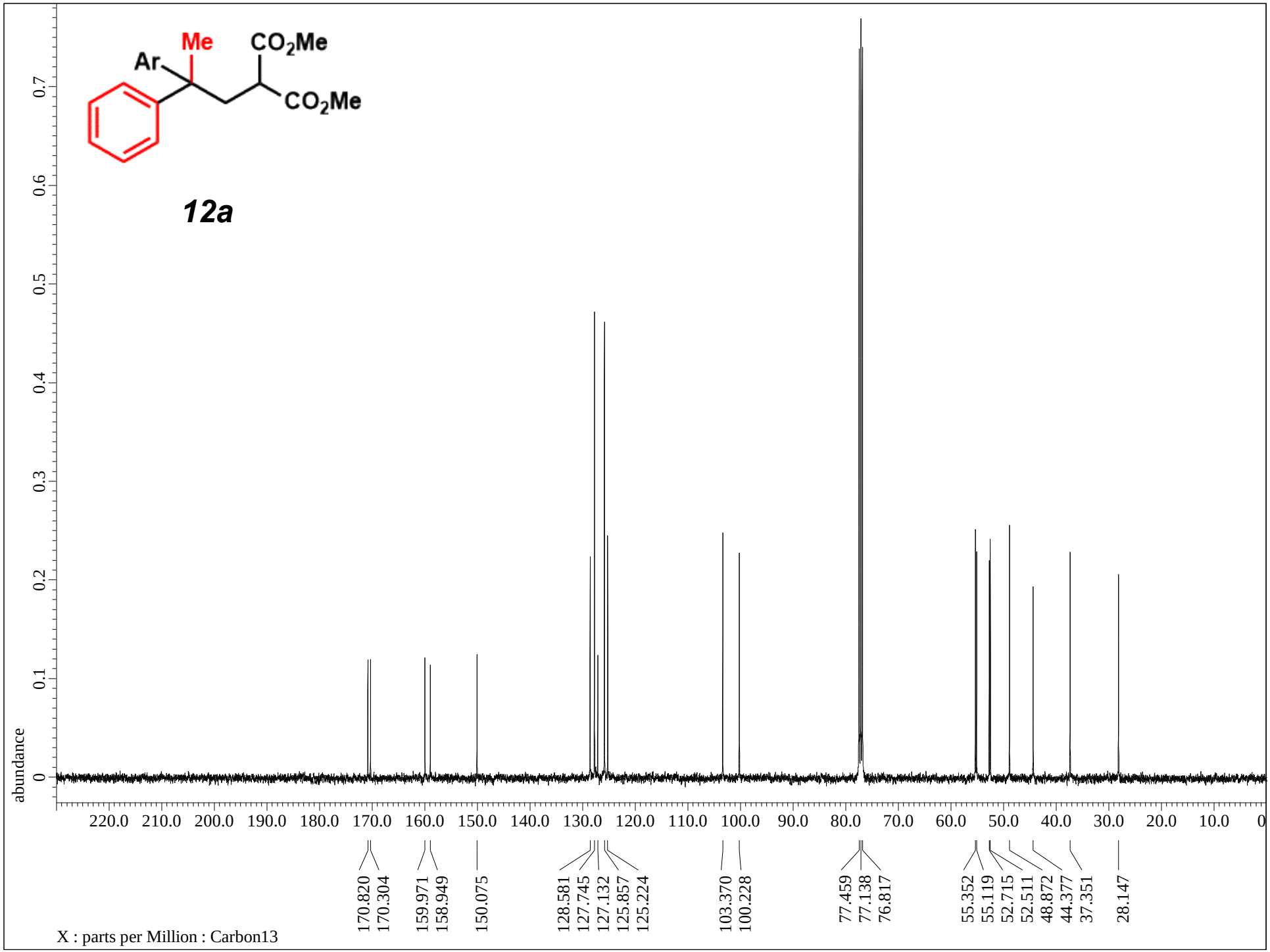

Ph
CO2Me
Ph
CO2Me
9l
abundance
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0
7.358 7.338 7.320 7.310 7.292 7.271 7.255 7.238 7.209
6.466 6.426 6.316 6.295 6.275 6.255
3.711 3.697 3.480 3.461 3.442 3.424 3.406 3.388
2.495 2.480 2.476 2.461 2.452 2.442 2.435 2.416 2.399
X : parts per Million : Proton

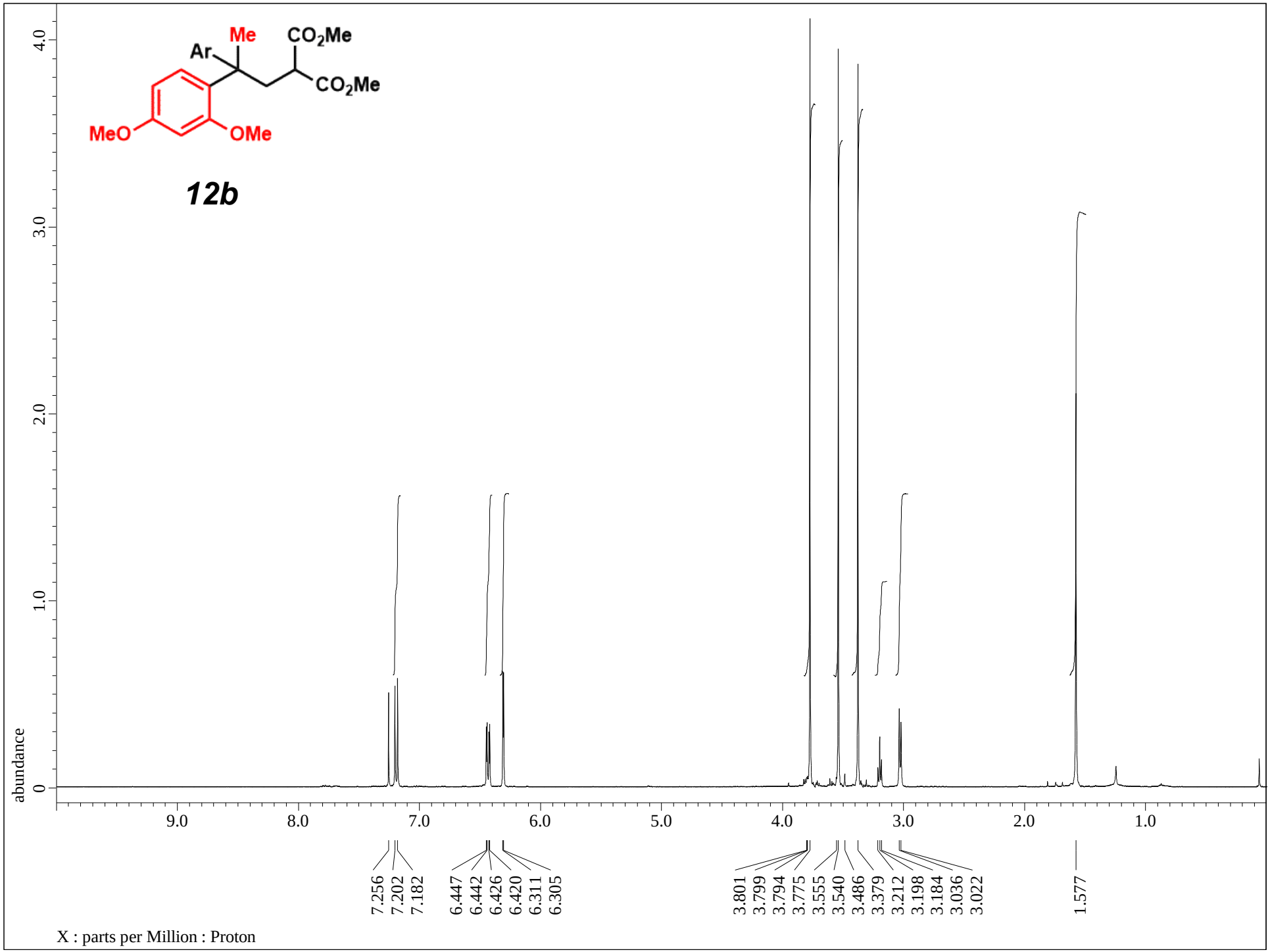

Ph
CO2Me
Ph
CO2Me
9l
abundance
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
169.944
169.847
142.797
137.115
132.279
130.683
128.883
128.630
127.706
127.501
126.937
126.363
77.488
77.167
76.856
52.725
50.030
47.198
34.724
X : parts per Million : Carbon13

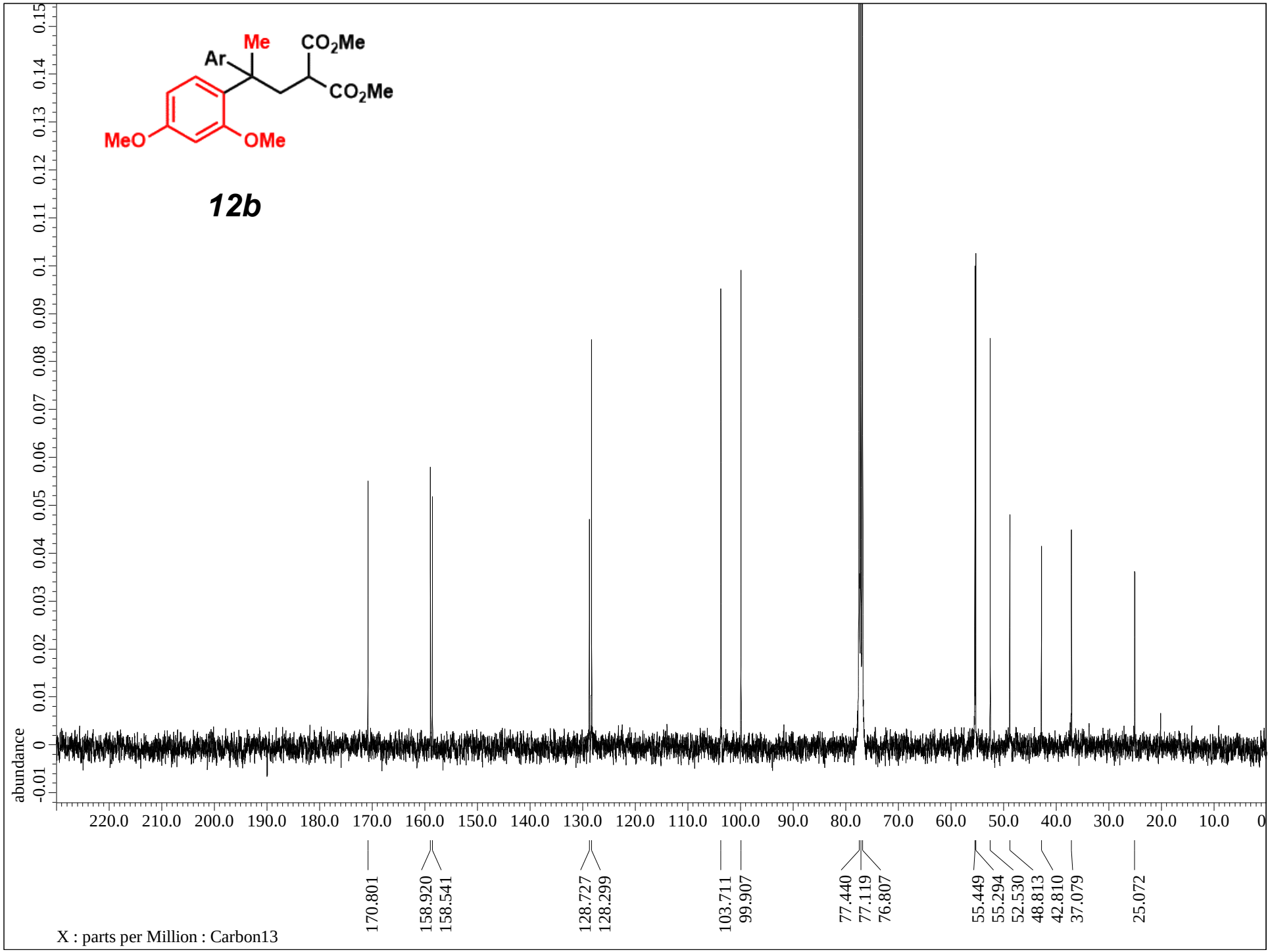

Ph
CO2Me
Ph
CO2Me
10a
abundance
4.0
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.483
7.469
7.335
7.320
7.304
7.289
7.286
7.274
7.272
7.254
6.364
6.359
4.168
4.164
3.774
3.641
3.258
3.232
3.216
2.581
2.565
2.555
2.539
X : parts per Million : Proton

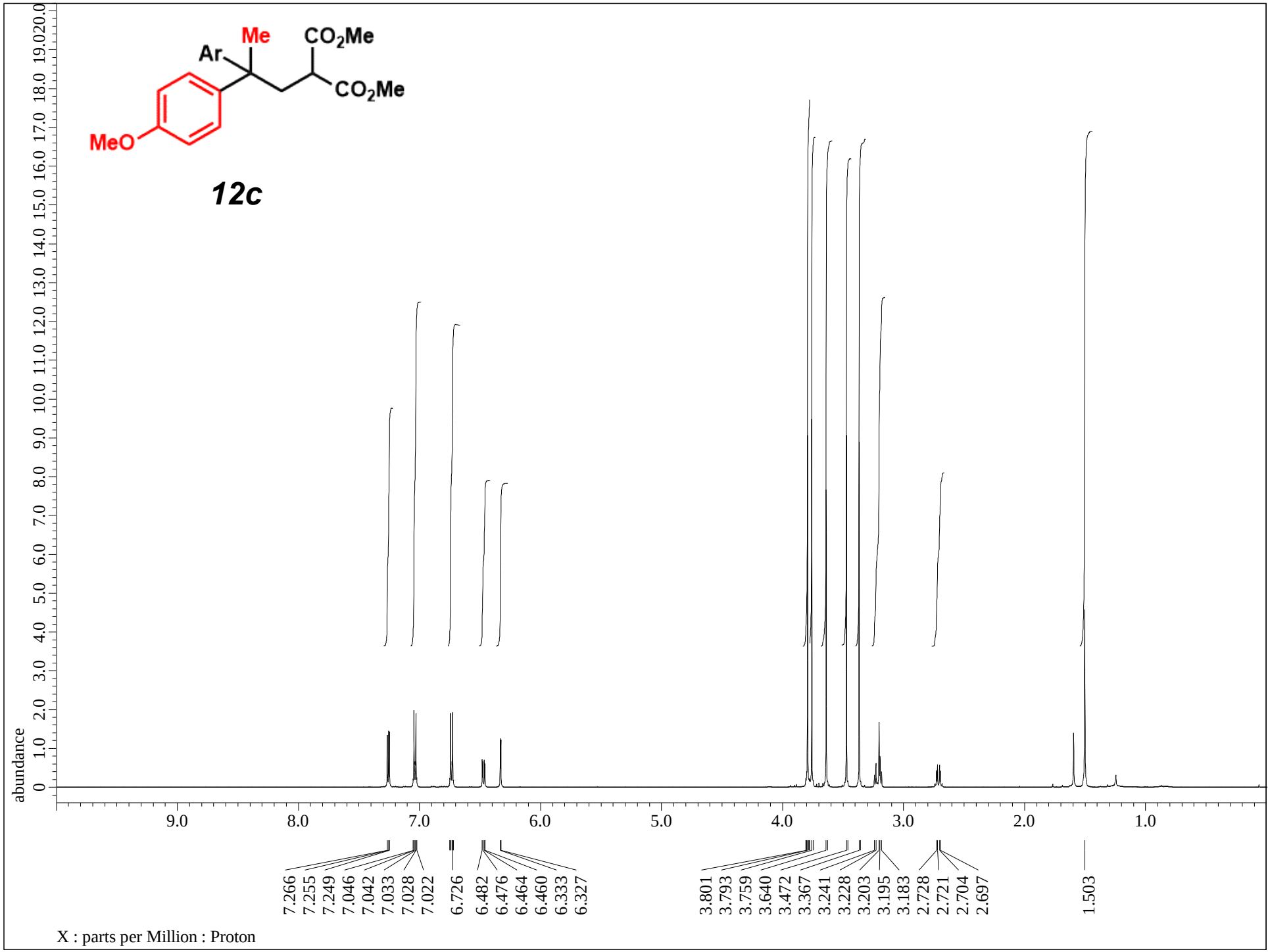

Ph
CO2Me
Ph
CO2Me
10a
(thousandths)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
171.822
171.705
143.644
142.963
136.745
134.877
128.776
128.163
127.764
127.628
127.423
126.947
77.449
77.333
77.128
76.807
67.972
52.959
52.774
49.300
46.177
X : parts per Million : Carbon13

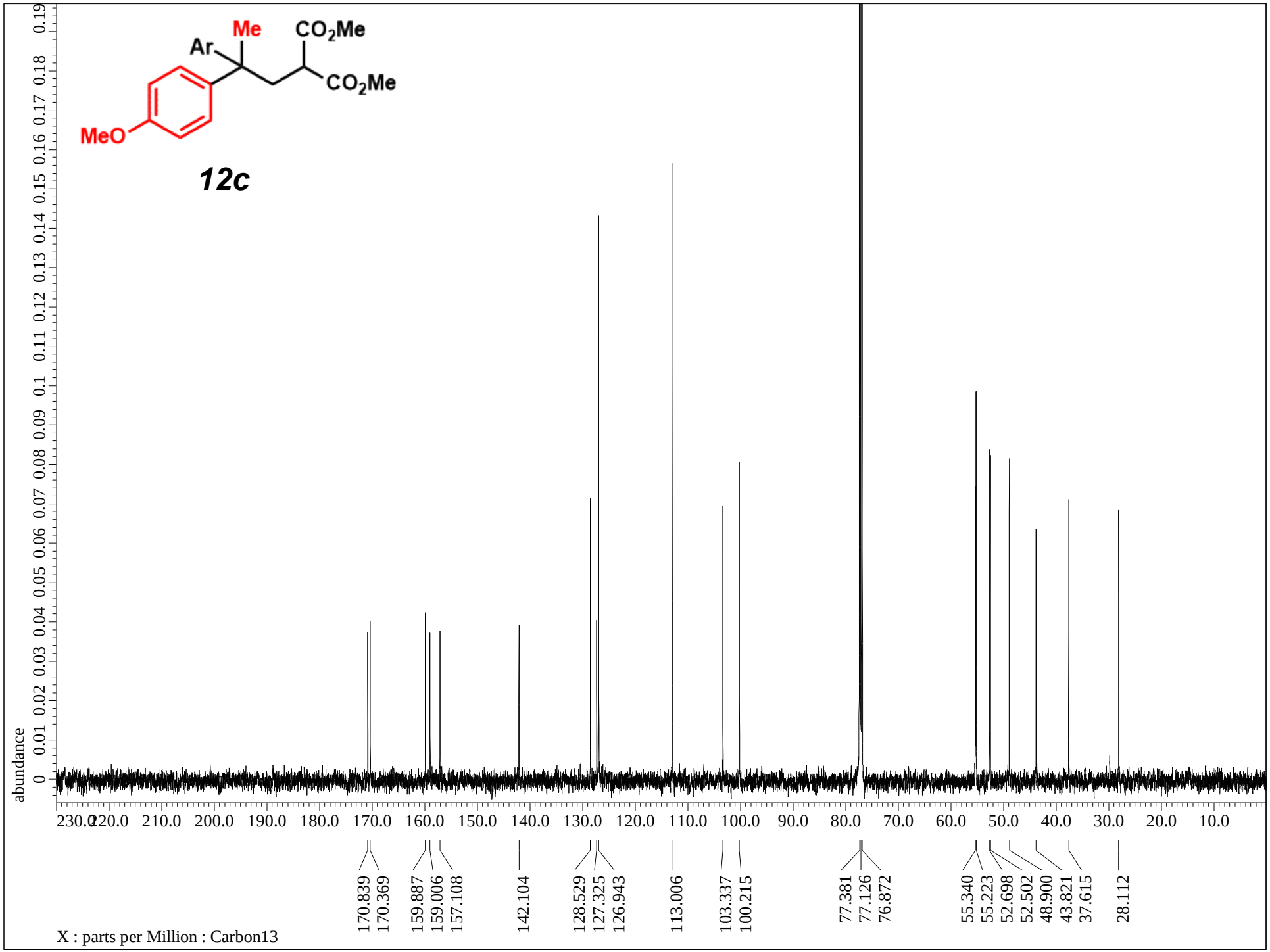

Me
CO2Me
Ar
CO2Me
12a
abundance
6.0
5.0
4.0
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.304
7.282
7.255
7.193
7.175
7.139
7.135
7.117
7.098
6.503
6.497
6.482
6.476
6.329
6.322
3.799
3.642
3.464
3.324
3.272
3.256
3.224
3.220
3.210
3.195
2.768
2.758
2.736
2.727
1.523
X : parts per Million : Proton

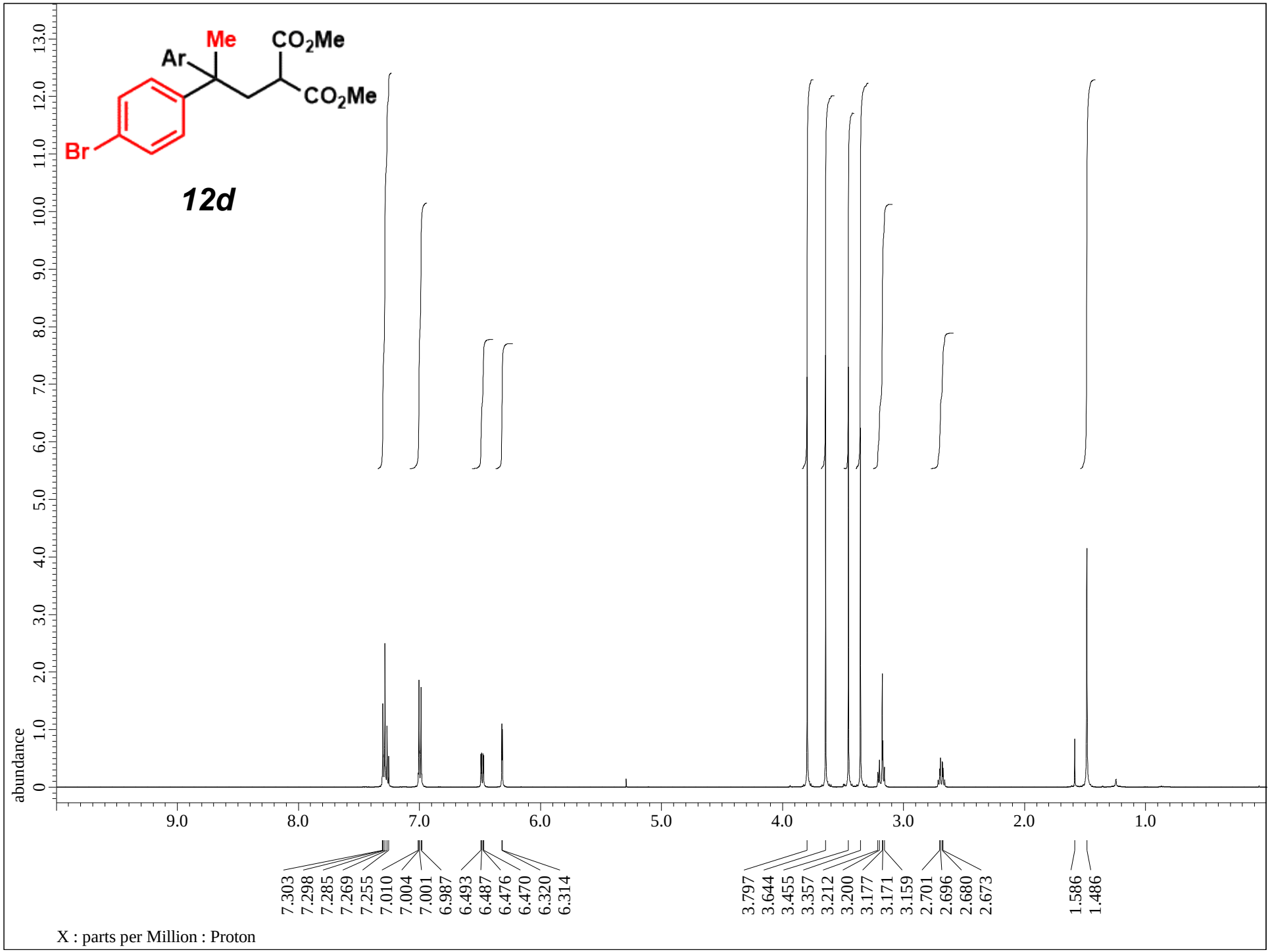

Me
CO2Me
Ar
CO2Me
12a
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
170.820
170.304
159.971
158.949
150.075
128.581
127.745
127.132
125.857
125.224
103.370
100.228
77.459
77.138
76.817
55.352
55.119
52.715
52.511
48.872
44.377
37.351
28.147
X : parts per Million : Carbon13

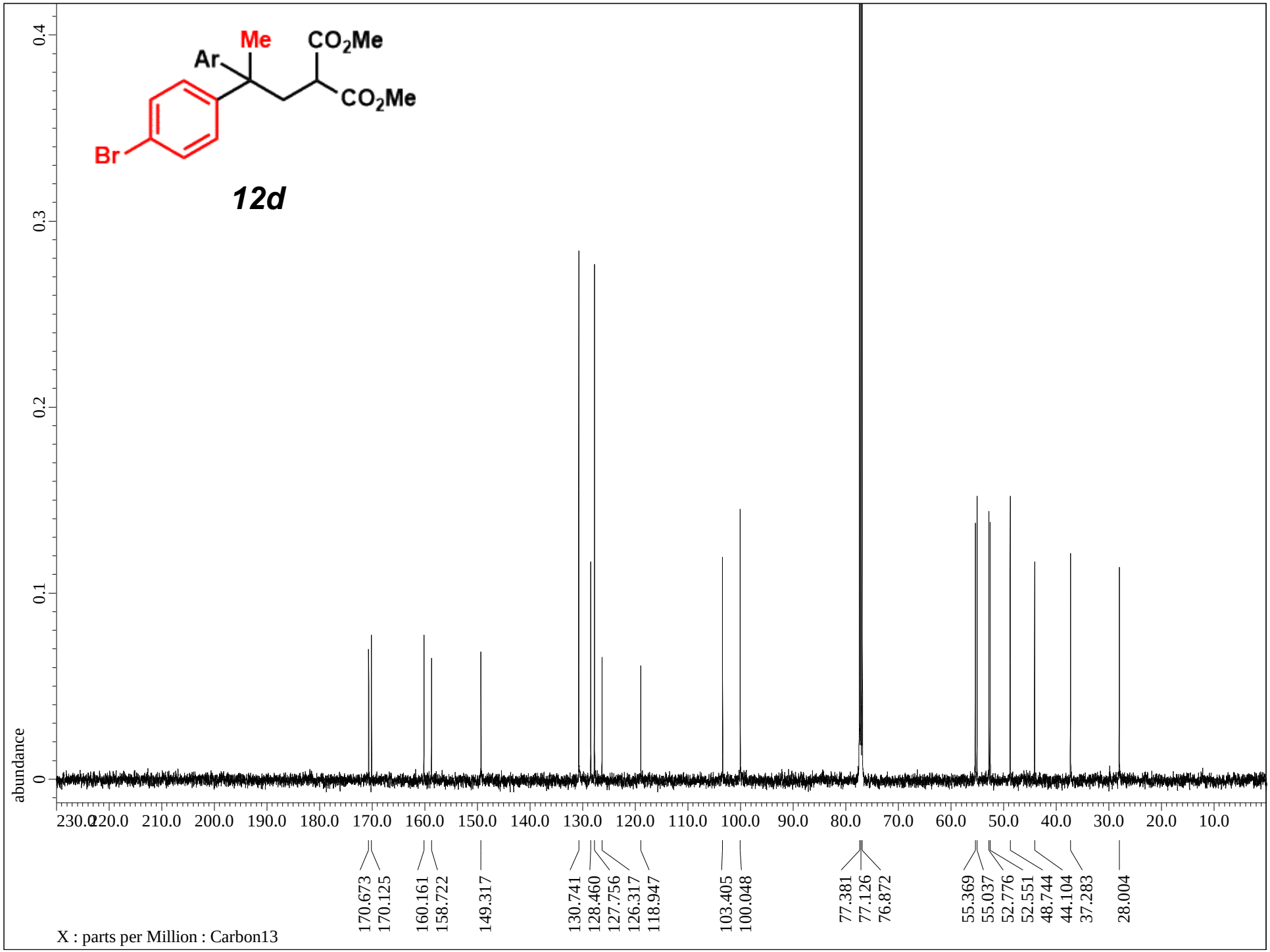

Me
CO2Me
Ar
CO2Me
MeO
OMe
12b
abundance
4.0
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.256
7.202
7.182
6.447
6.442
6.426
6.420
6.311
6.305
3.801
3.799
3.794
3.775
3.555
3.540
3.486
3.379
3.212
3.198
3.184
3.036
3.022
1.577
X : parts per Million : Proton

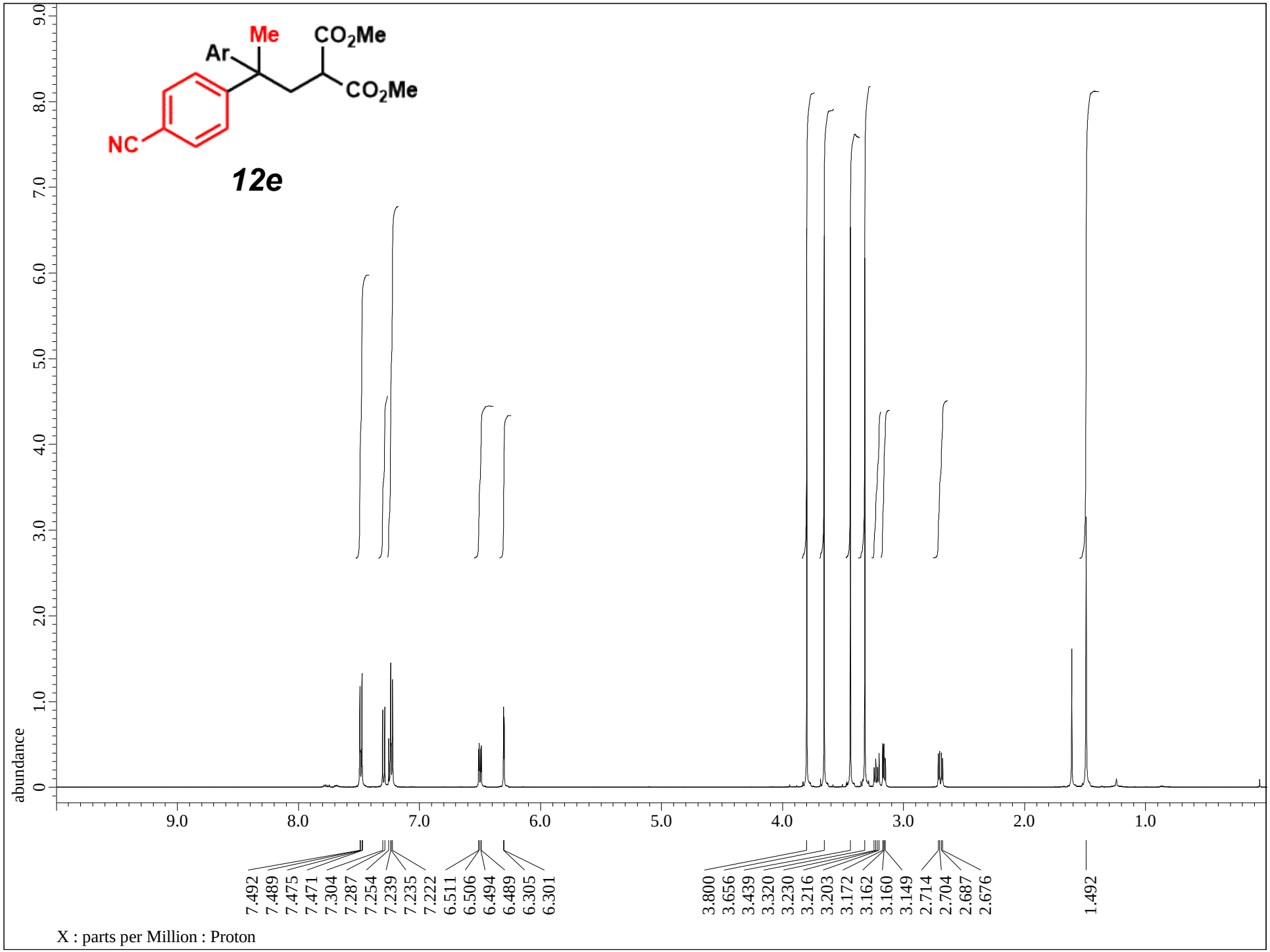

Me
CO2Me
Ar
CO2Me
MeO
OMe
12b
abundance
0.15
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.801
158.920
158.541
128.727
128.299
103.711
99.907
77.440
77.119
76.807
55.449
55.294
52.530
48.813
42.810
37.079
25.072
X : parts per Million : Carbon13

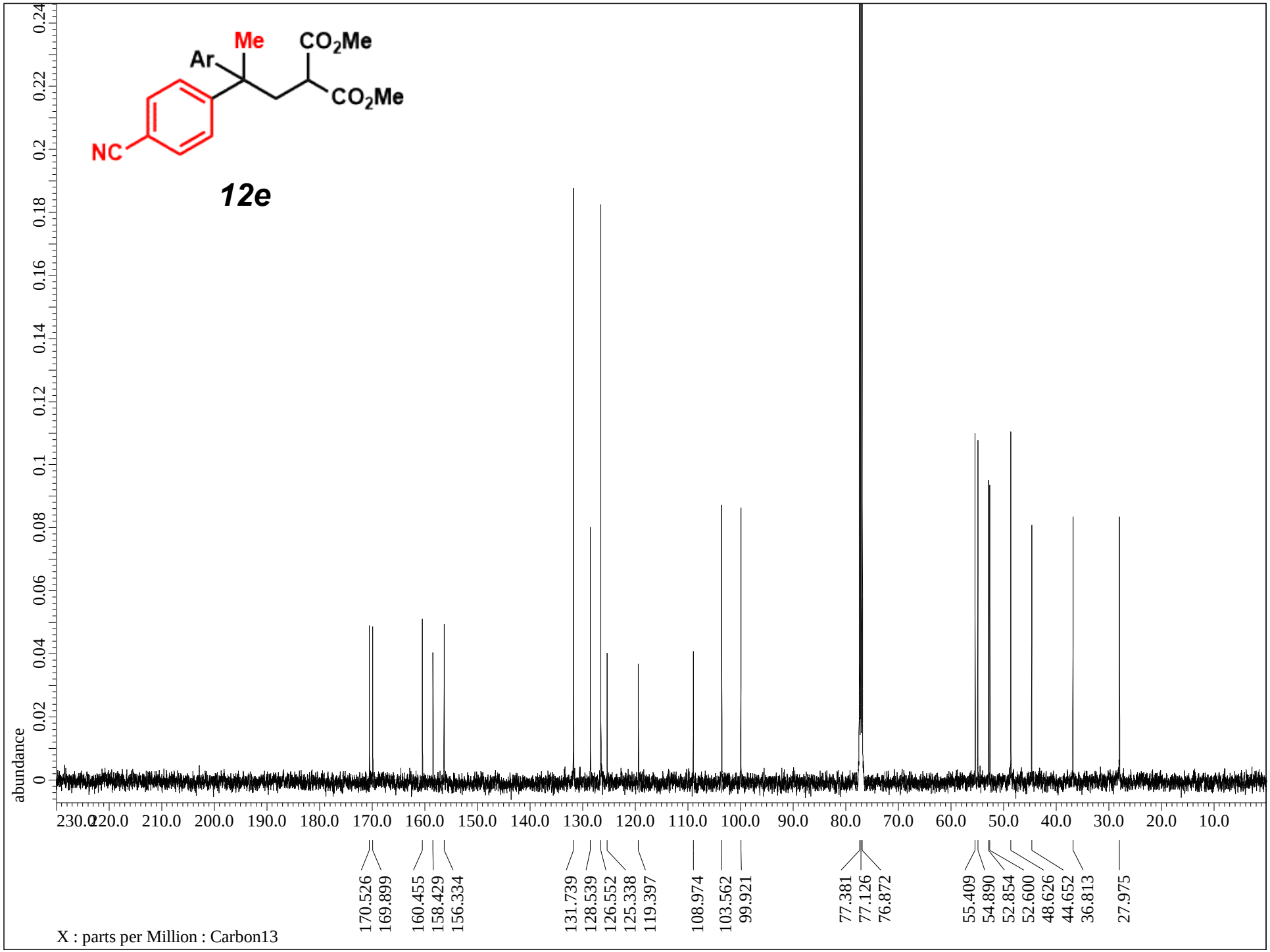

Me
CO2Me
Ar
CO2Me
MeO
12c
abundance
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0
7.266 7.255 7.249 7.046 7.042 7.033 7.028 7.022 6.726 6.482 6.476 6.464 6.460 6.333 6.327
3.801 3.793 3.759 3.640 3.472 3.367 3.241 3.228 3.203 3.195 3.183 2.728 2.721 2.704 2.697 1.503
X : parts per Million : Proton

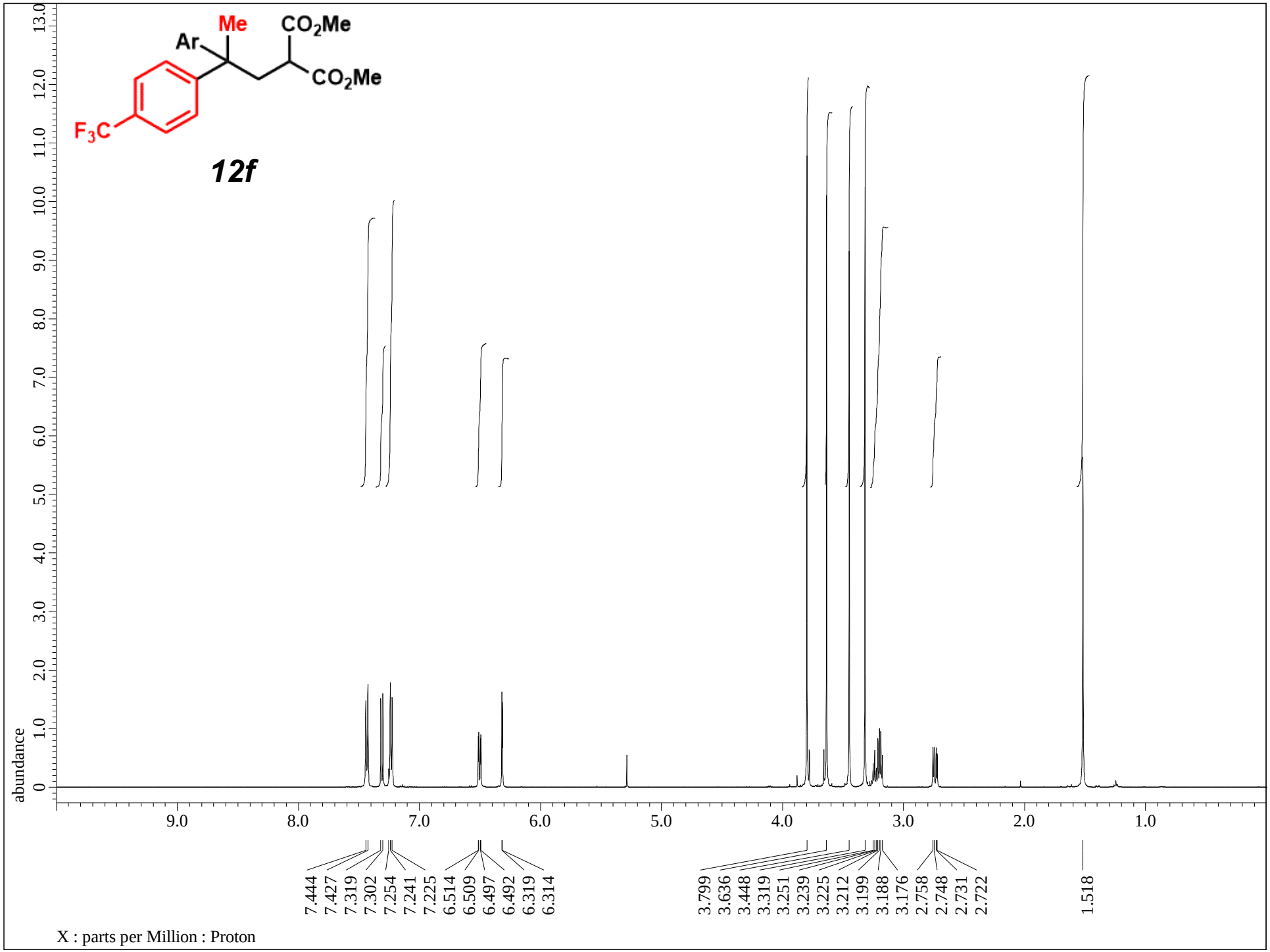

Me
CO2Me
Ar
CO2Me
MeO
12c
abundance
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17 0.18 0.19
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
170.839
170.369
159.887
159.006
157.108
142.104
128.529
127.325
126.943
113.006
103.337
100.215
77.381
77.126
76.872
55.340
55.223
52.698
52.502
48.900
43.821
37.615
28.112
X : parts per Million : Carbon13

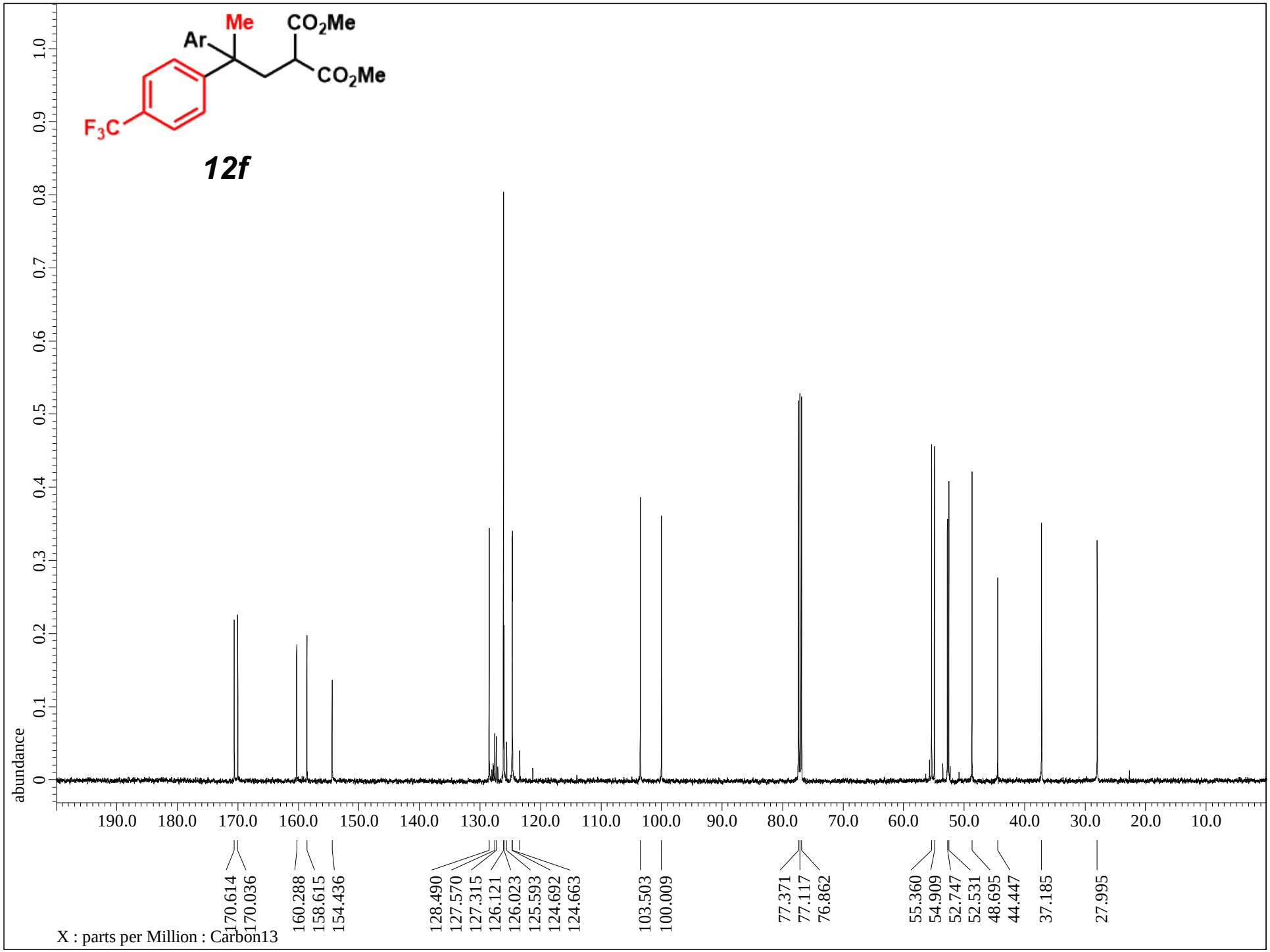

Me
CO2Me
Ar
CO2Me
Br
12d
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.303
7.298
7.285
7.269
7.255
7.010
7.004
7.001
6.987
6.493
6.487
6.476
6.470
6.320
6.314
3.797
3.644
3.455
3.357
3.212
3.200
3.177
3.171
3.159
2.701
2.696
2.680
2.673
1.586
1.486
X : parts per Million : Proton

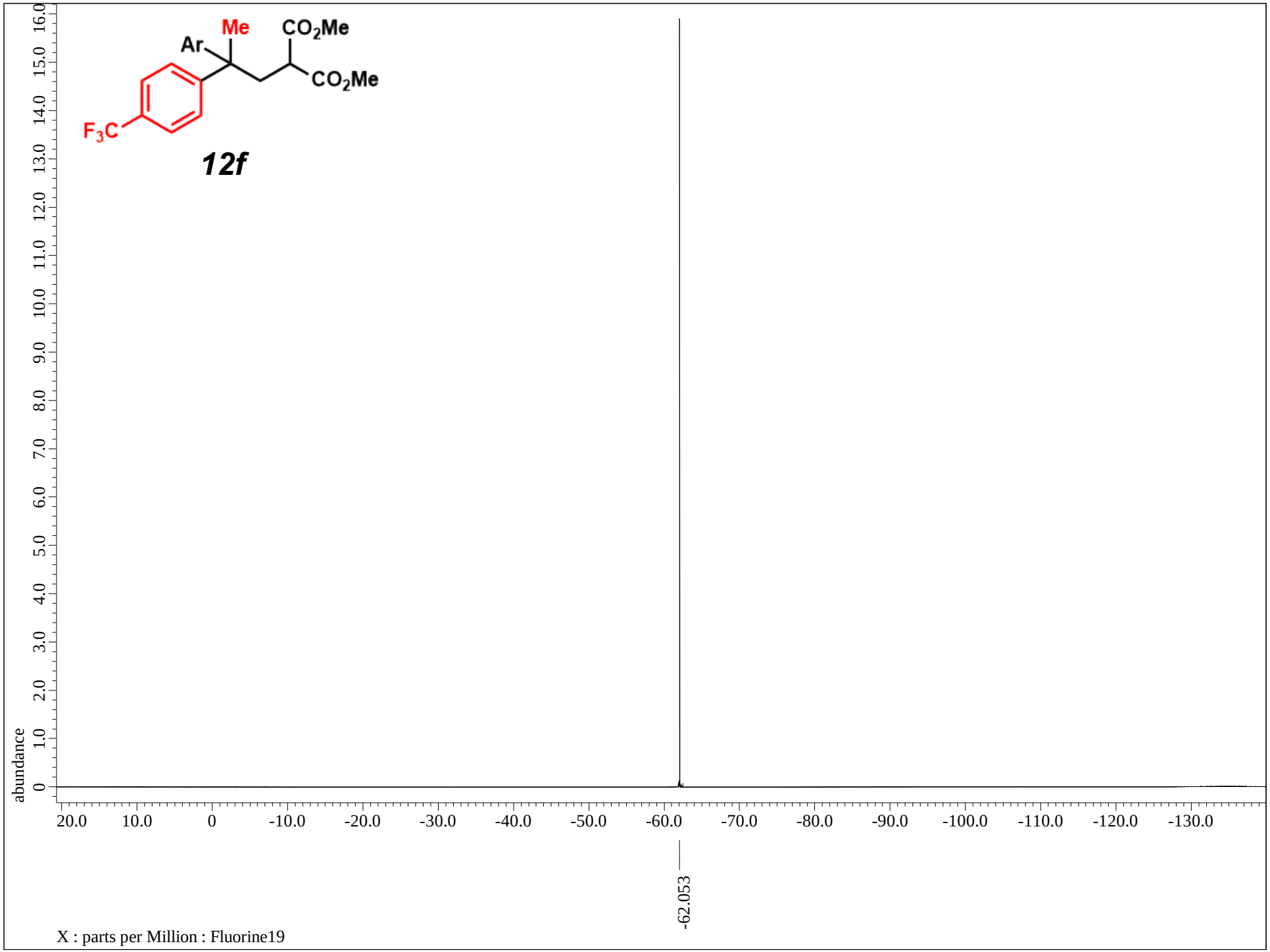

Me
CO2Me
Ar
CO2Me
Br
12d
abundance
0.4
0.3
0.2
0.1
0
230.0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.673
170.125
160.161
158.722
149.317
130.741
128.460
127.756
126.317
118.947
103.405
100.048
77.381
77.126
76.872
55.369
55.037
52.776
52.551
48.744
44.104
37.283
28.004
X : parts per Million : Carbon13

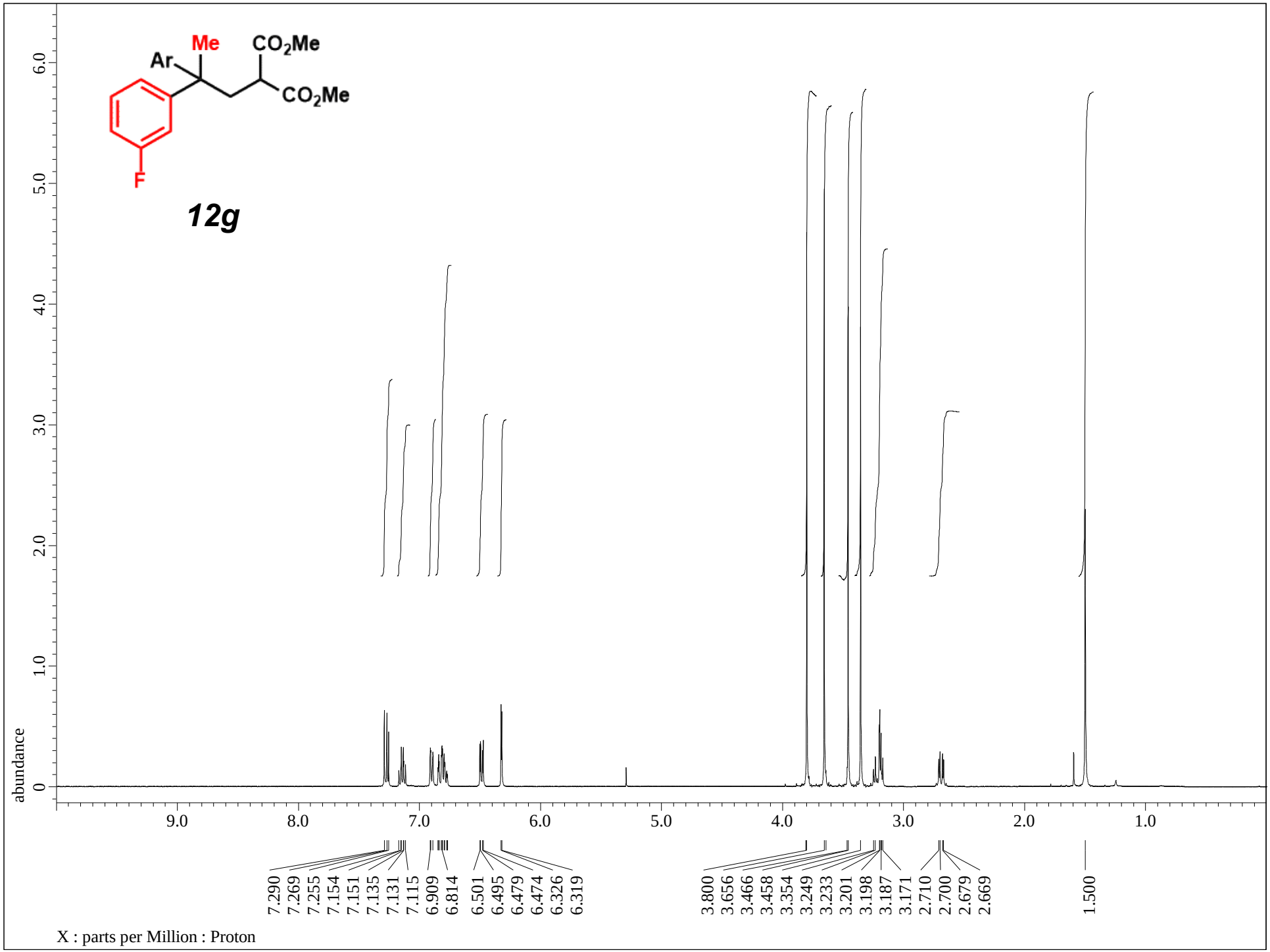

Me
CO2Me
Ar
CO2Me
NC
12e
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.492
7.489
7.475
7.471
7.304
7.287
7.254
7.239
7.235
7.222
6.511
6.506
6.494
6.489
6.305
6.301
3.800
3.656
3.439
3.320
3.230
3.216
3.203
3.172
3.162
3.160
3.149
2.714
2.704
2.687
2.676
1.492
X : parts per Million : Proton

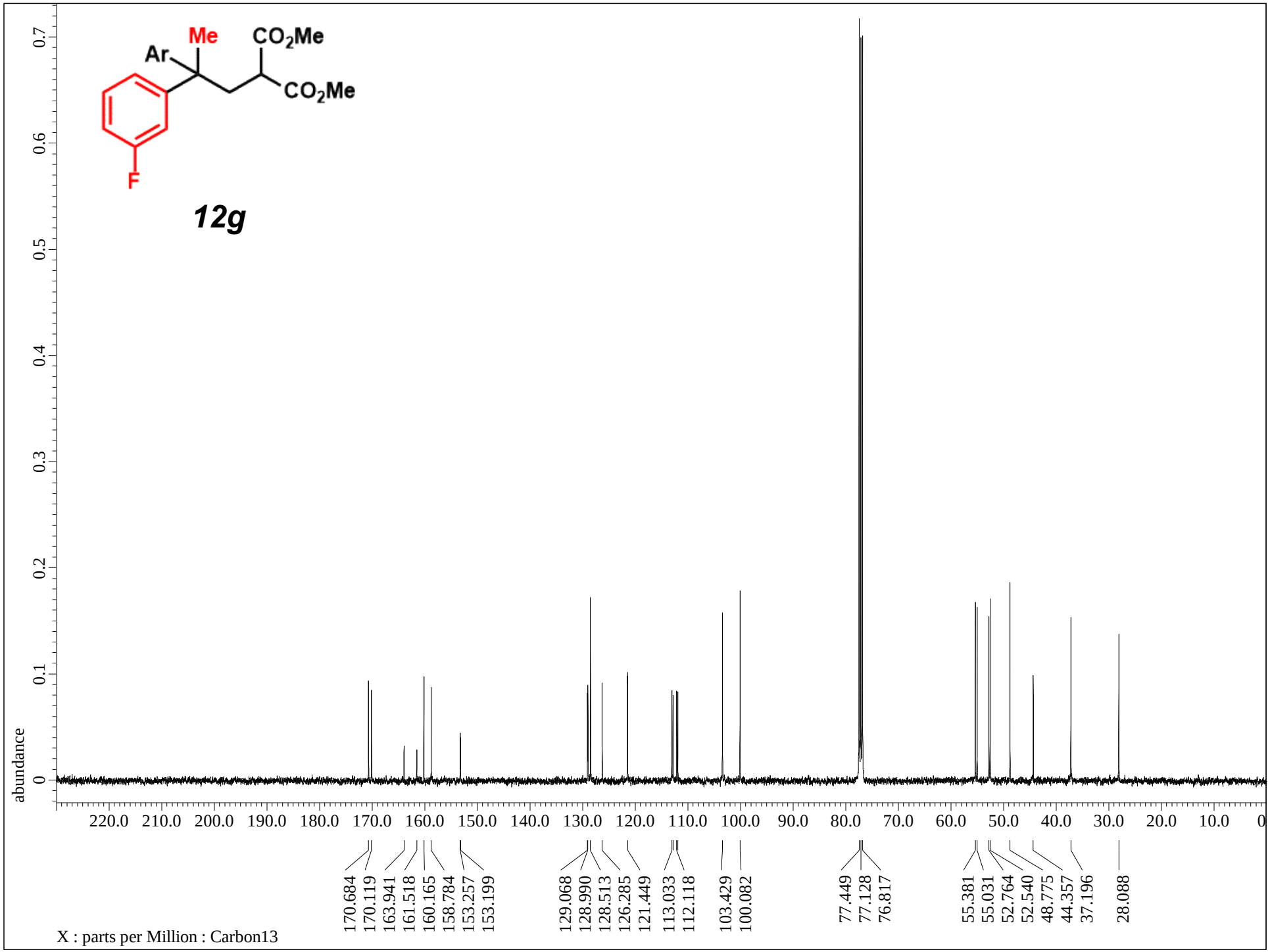

Me
CO2Me
Ar
CO2Me
NC
12e
abundance
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
230.0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.526
169.899
160.455
158.429
156.334
131.739
128.539
126.552
125.338
119.397
108.974
103.562
99.921
77.381
77.126
76.872
55.409
54.890
52.854
52.600
48.626
44.652
36.813
27.975
X : parts per Million : Carbon13

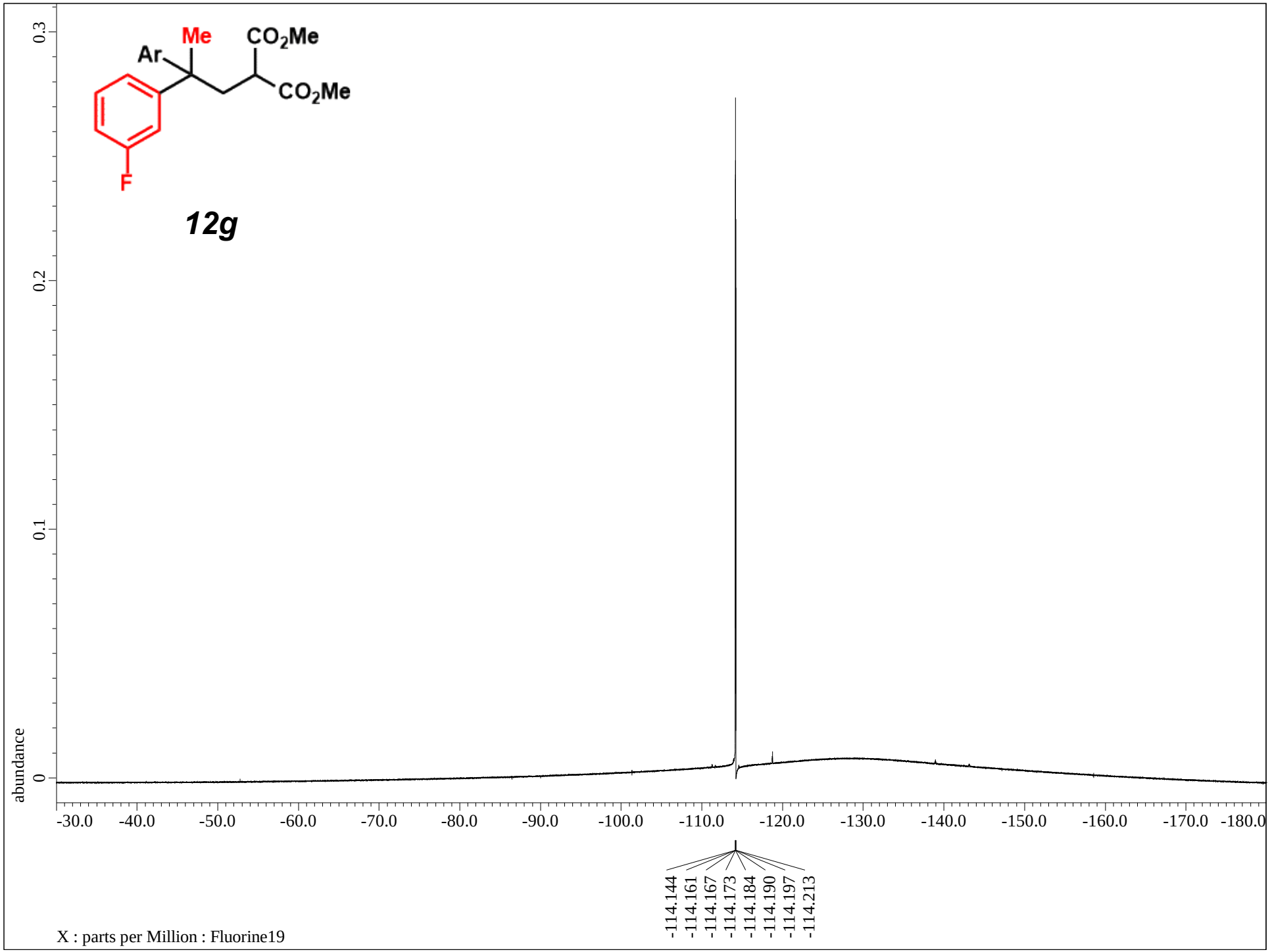

Me
Ar
CO2Me
CO2Me
F3C
12f
abundance
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.444
7.427
7.319
7.302
7.254
7.241
7.225
6.514
6.509
6.497
6.492
6.319
6.314
3.799
3.636
3.448
3.319
3.251
3.239
3.225
3.212
3.199
3.188
3.176
2.758
2.748
2.731
2.722
1.518
X : parts per Million : Proton

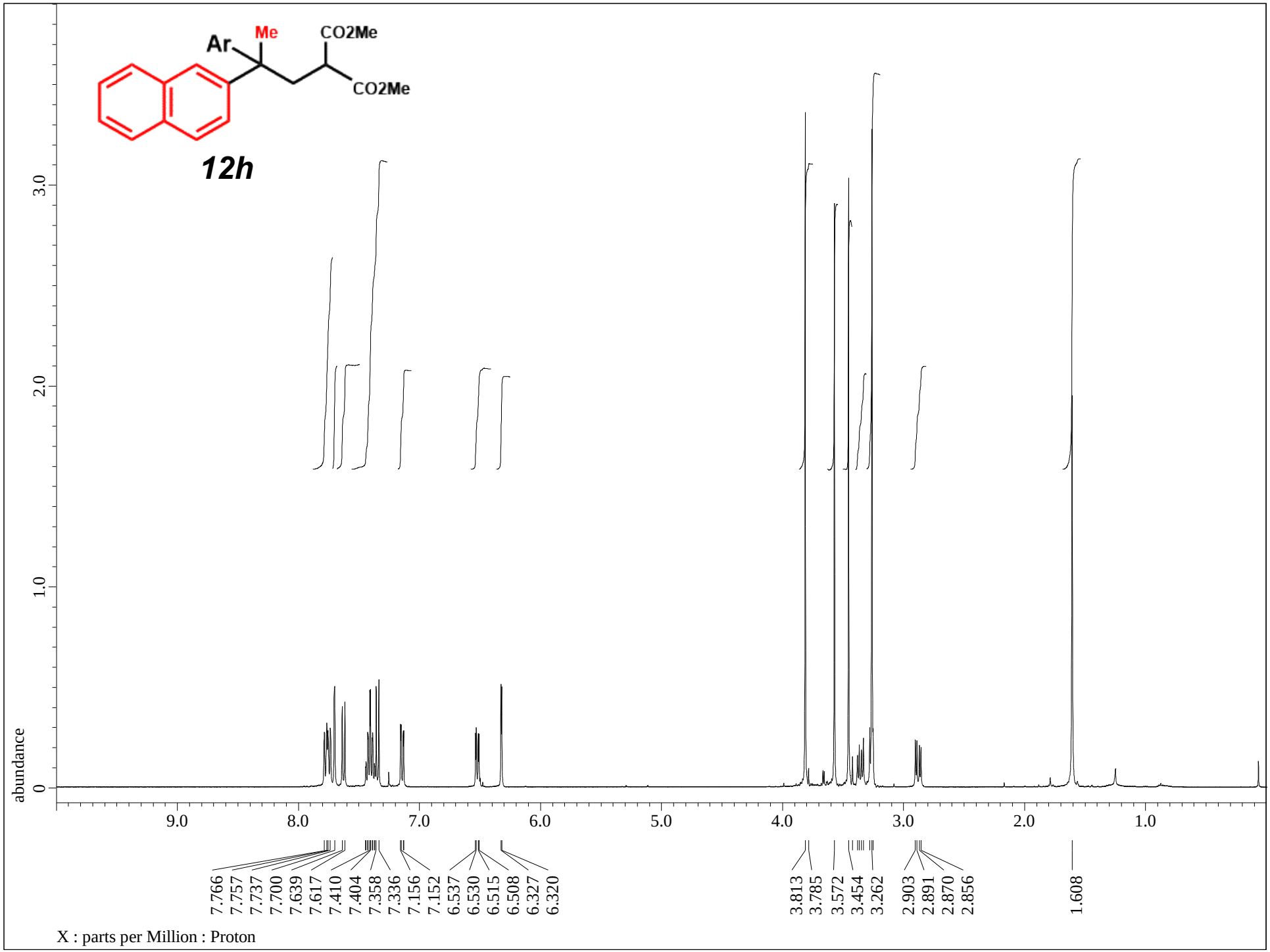

Me
CO2Me
Ar
CO2Me
F3C
12f
abundance
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.614
170.036
160.288
158.615
154.436
128.490
127.570
127.315
126.121
126.023
125.593
124.692
124.663
103.503
100.009
77.371
77.117
76.862
55.360
54.909
52.747
52.531
48.695
44.447
37.185
27.995
X : parts per Million : Carbon13

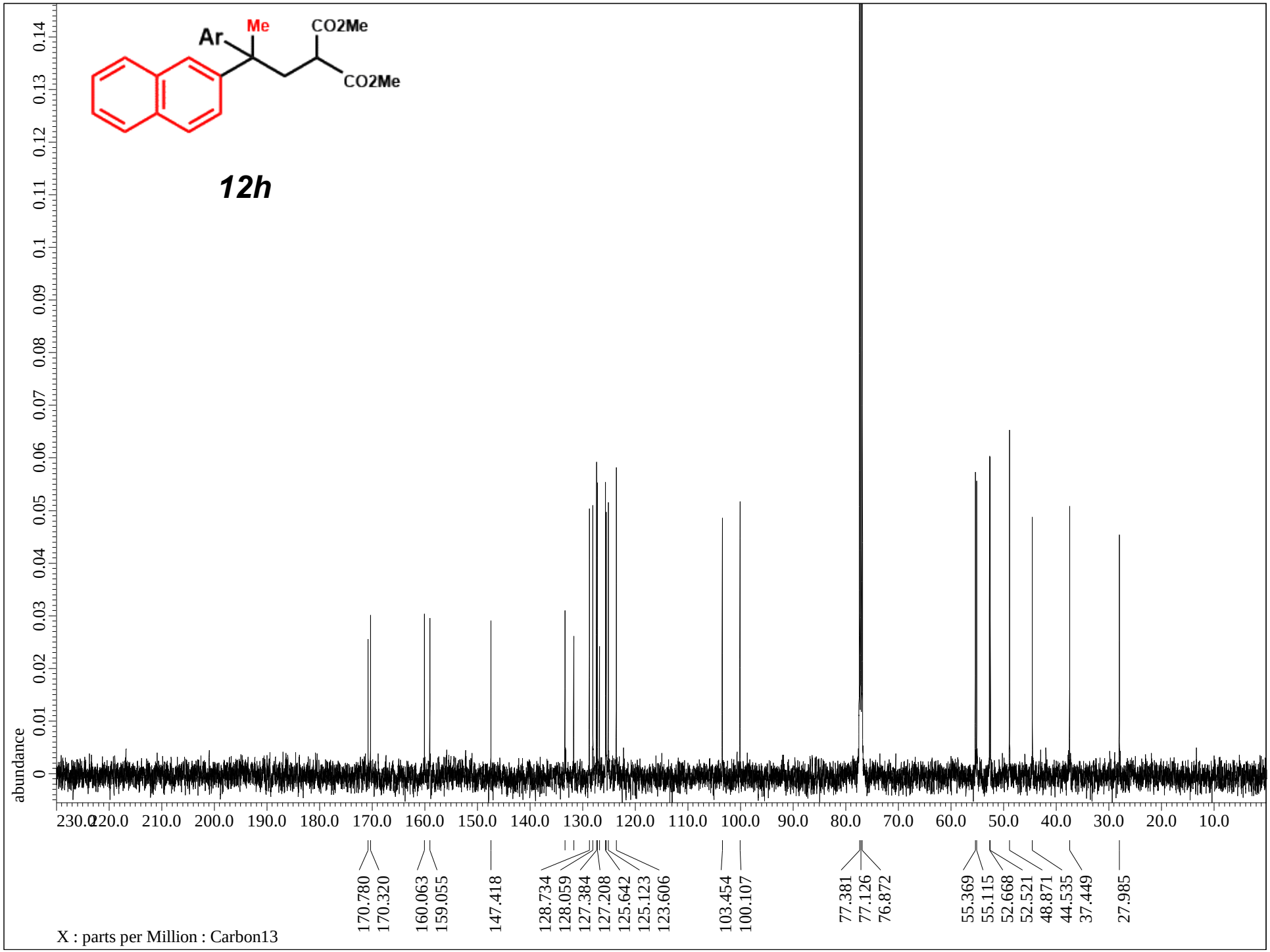

Me
CO2Me
Ar
CO2Me
F3C
12f
abundance
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
20.0
10.0
0
-10.0
-20.0
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-62.053
X : parts per Million : Fluorine19

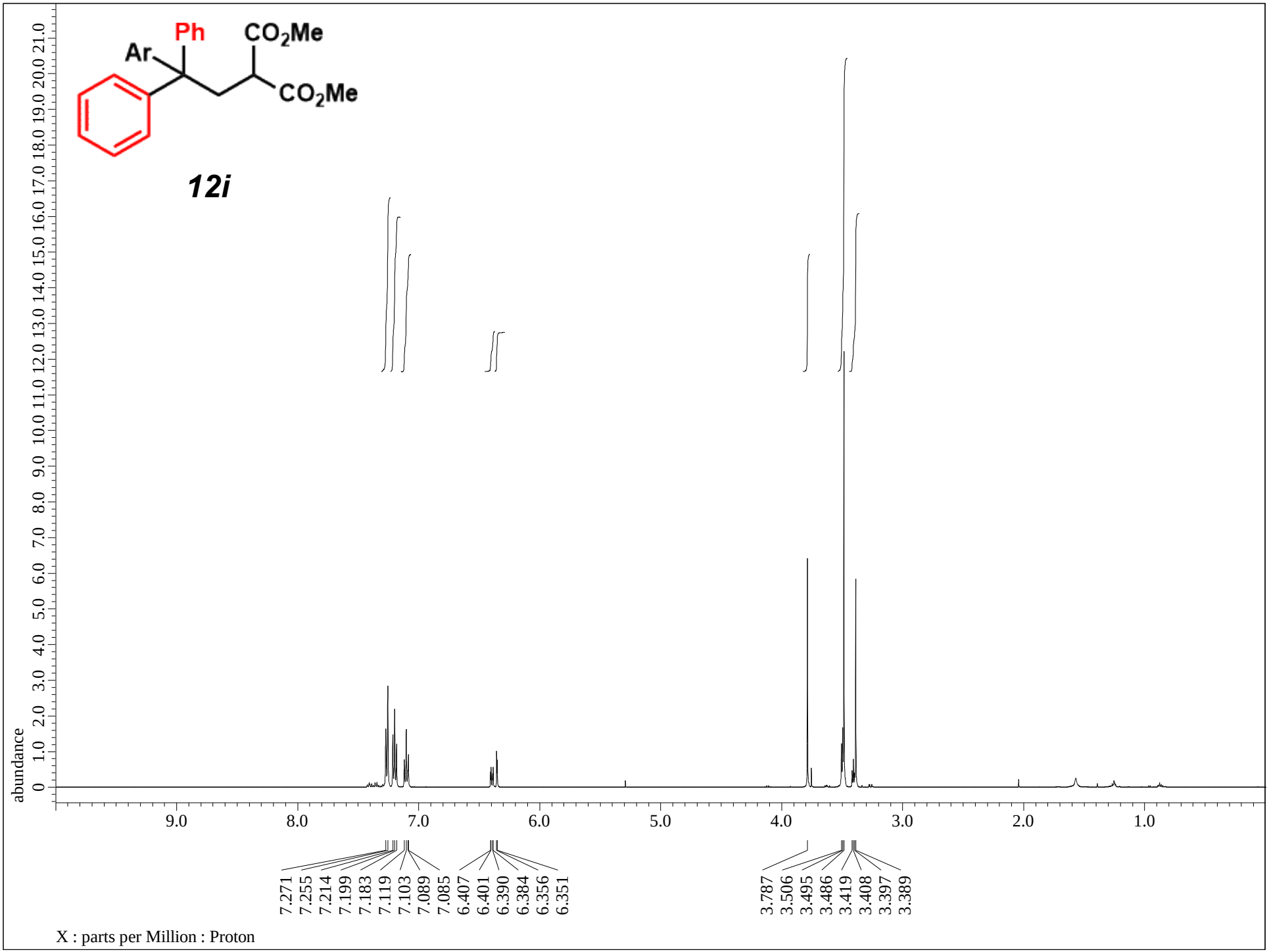

Me
CO2Me
Ar
CO2Me
F
12g
abundance
6.0
5.0
4.0
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.290
7.269
7.255
7.154
7.151
7.135
7.131
7.115
6.909
6.814
6.501
6.495
6.479
6.474
6.326
6.319
3.800
3.656
3.466
3.458
3.354
3.249
3.233
3.201
3.198
3.187
3.171
2.710
2.700
2.679
2.669
1.500
X : parts per Million : Proton

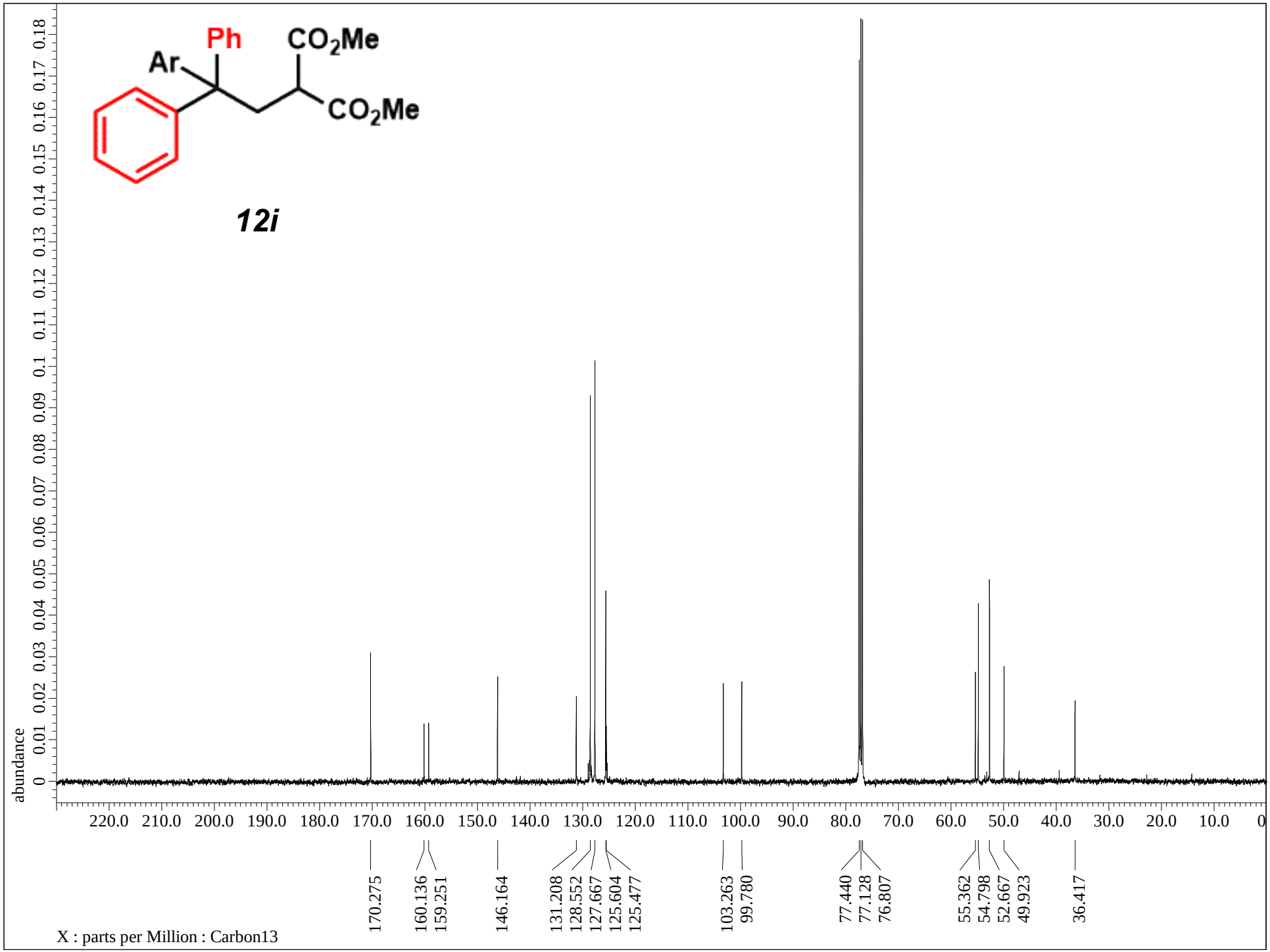

Me
CO2Me
Ar
CO2Me
F
12g
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
170.684
170.119
163.941
161.518
160.165
158.784
153.257
153.199
129.068
128.990
128.513
126.285
121.449
113.033
112.118
103.429
100.082
77.449
77.128
76.817
55.381
55.031
52.764
52.540
48.775
44.357
37.196
28.088
X : parts per Million : Carbon13

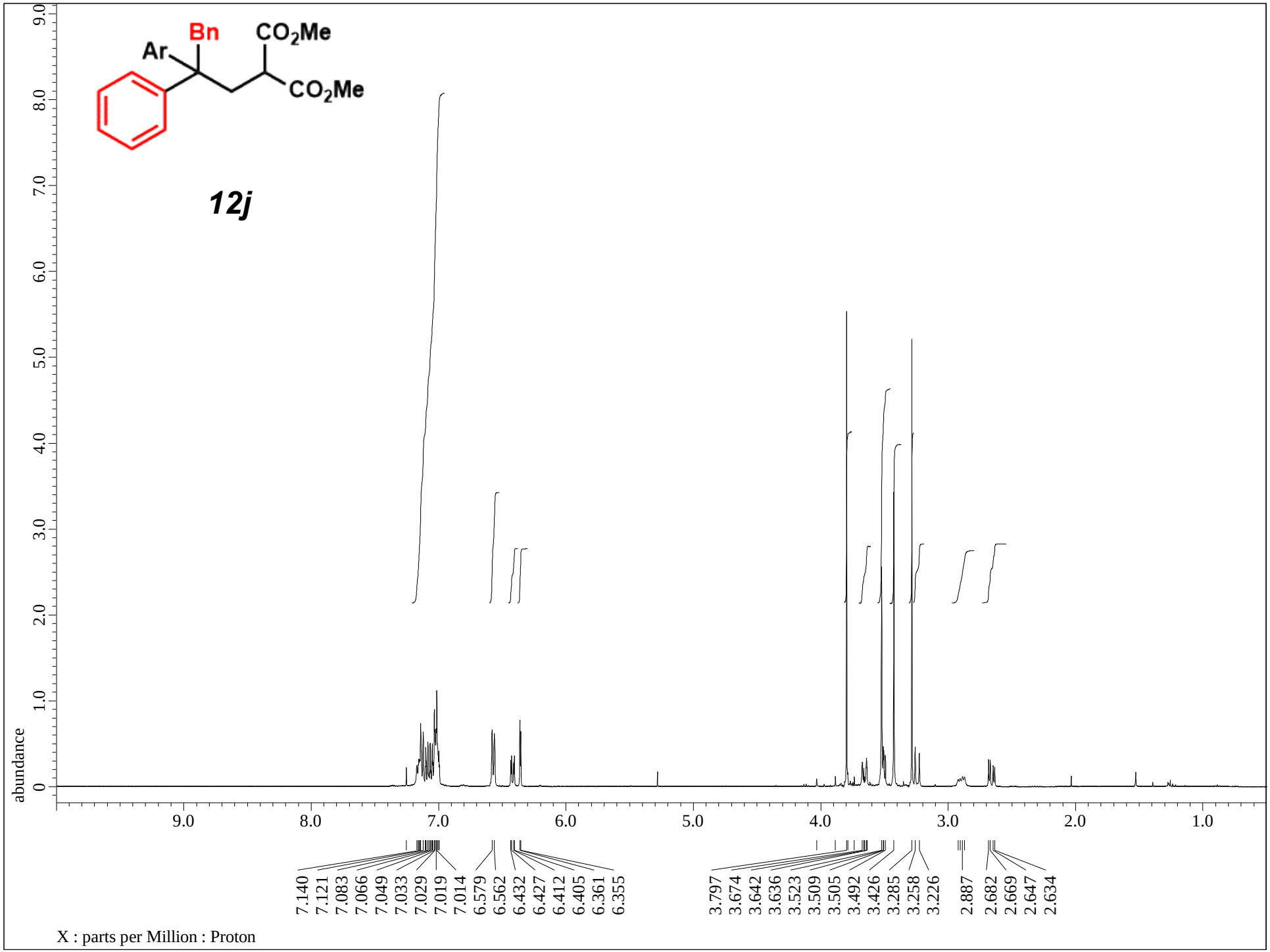

Me
CO2Me
Ar
CO2Me
F
12g
0.3
0.2
0.1
0
abundance
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-150.0
-160.0
-170.0
-180.0
-114.144
-114.161
-114.167
-114.173
-114.184
-114.190
-114.197
-114.213
X : parts per Million : Fluorine19

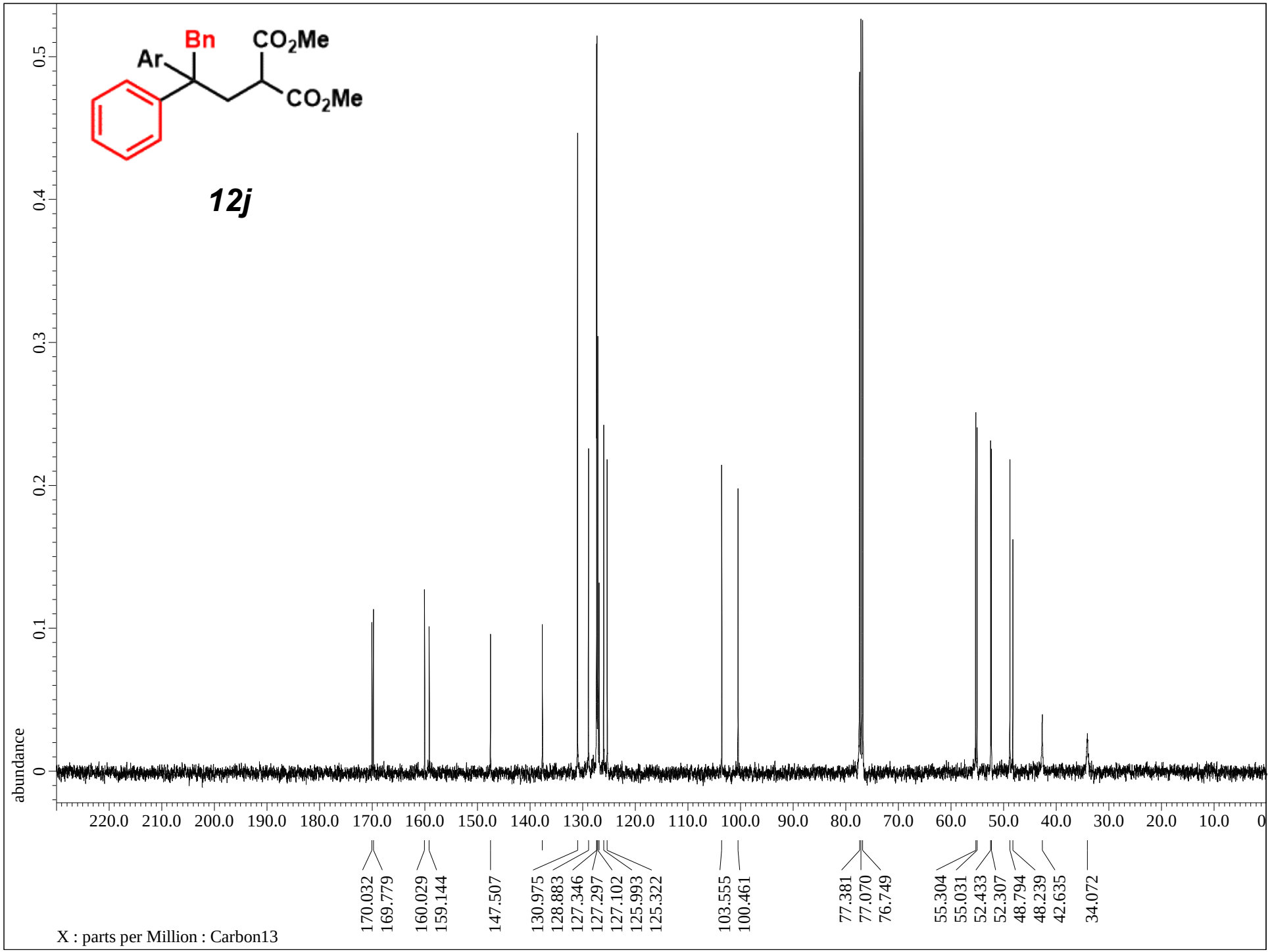

Ar
Me
CO2Me
CO2Me
12h
abundance
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.766
7.757
7.737
7.700
7.639
7.617
7.410
7.404
7.358
7.336
7.156
7.152
6.537
6.530
6.515
6.508
6.327
6.320
3.813
3.785
3.572
3.454
3.262
2.903
2.891
2.870
2.856
1.608
X : parts per Million : Proton

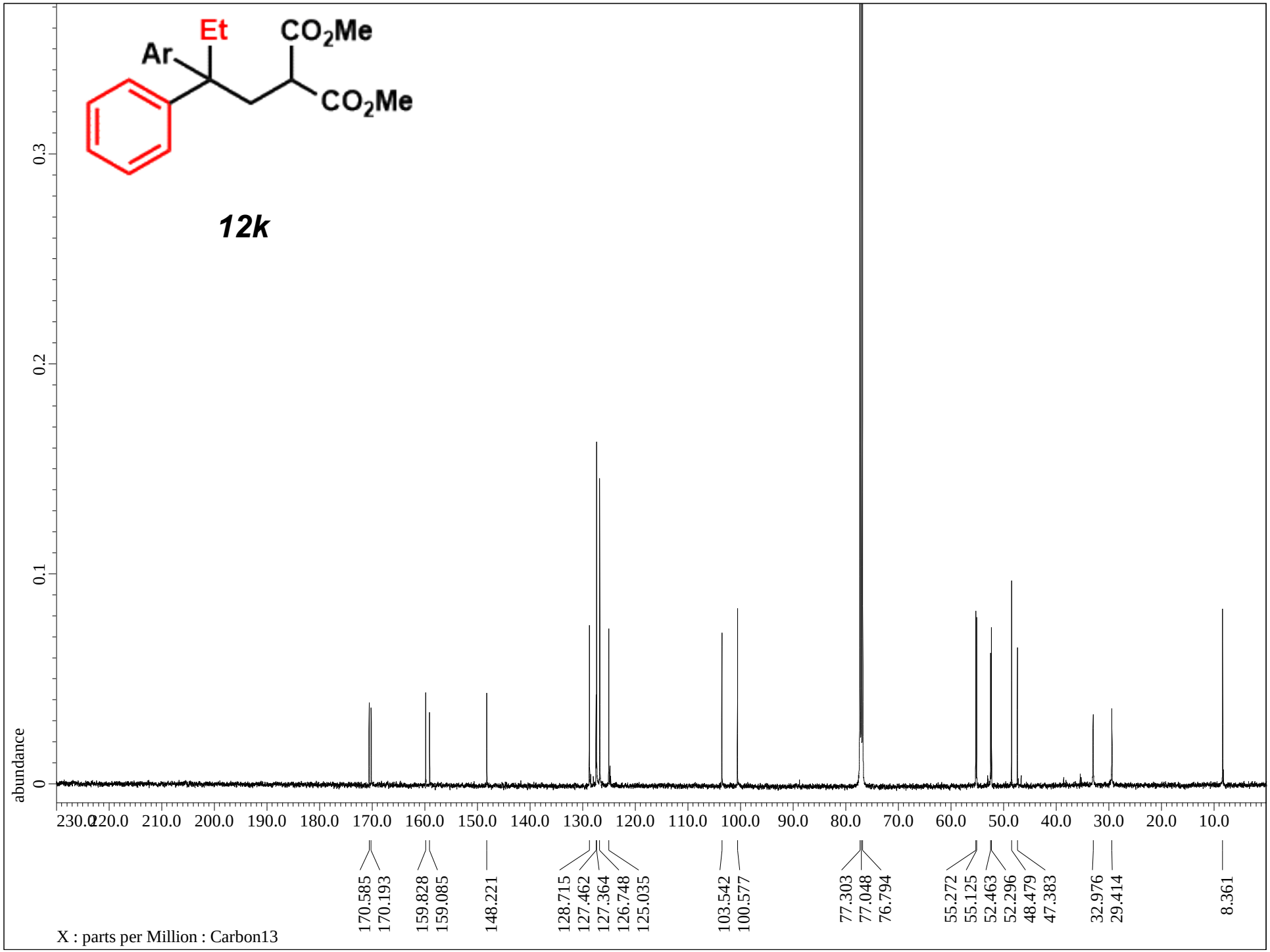

Ar
Me
CO2Me
CO2Me
12h
abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
230.0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.780
170.320
160.063
159.055
147.418
128.734
128.059
127.384
127.208
125.642
125.123
123.606
103.454
100.107
77.381
77.126
76.872
55.369
55.115
52.668
52.521
48.871
44.535
37.449
27.985
X : parts per Million : Carbon13

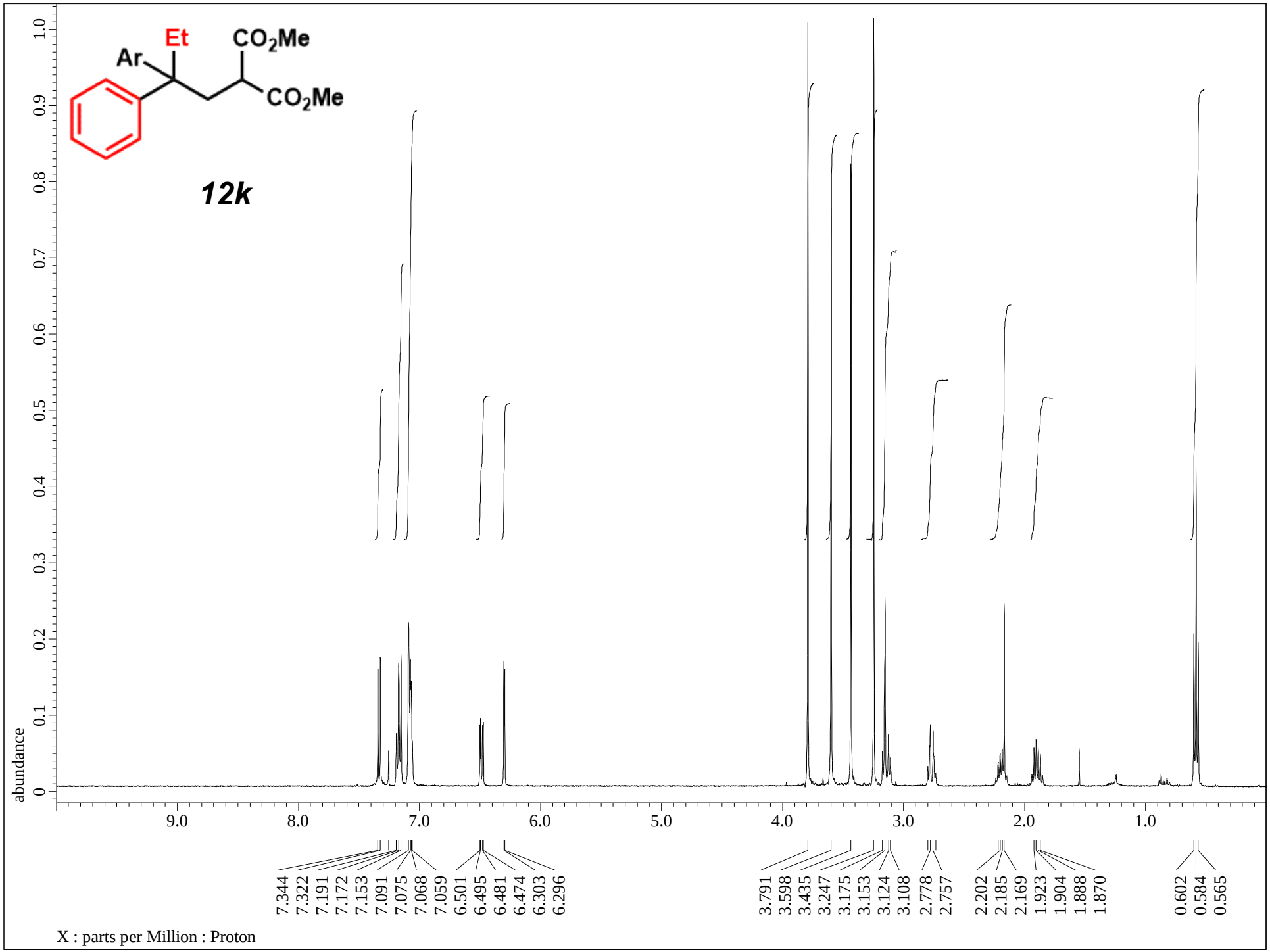

Ar
Ph
CO2Me
CO2Me
12i
abundance
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0
7.271 7.255 7.214 7.199 7.183 7.119 7.103 7.089 7.085
6.407 6.401 6.390 6.384 6.356 6.351
3.787 3.506 3.495 3.486 3.419 3.408 3.397 3.389
X : parts per Million : Proton

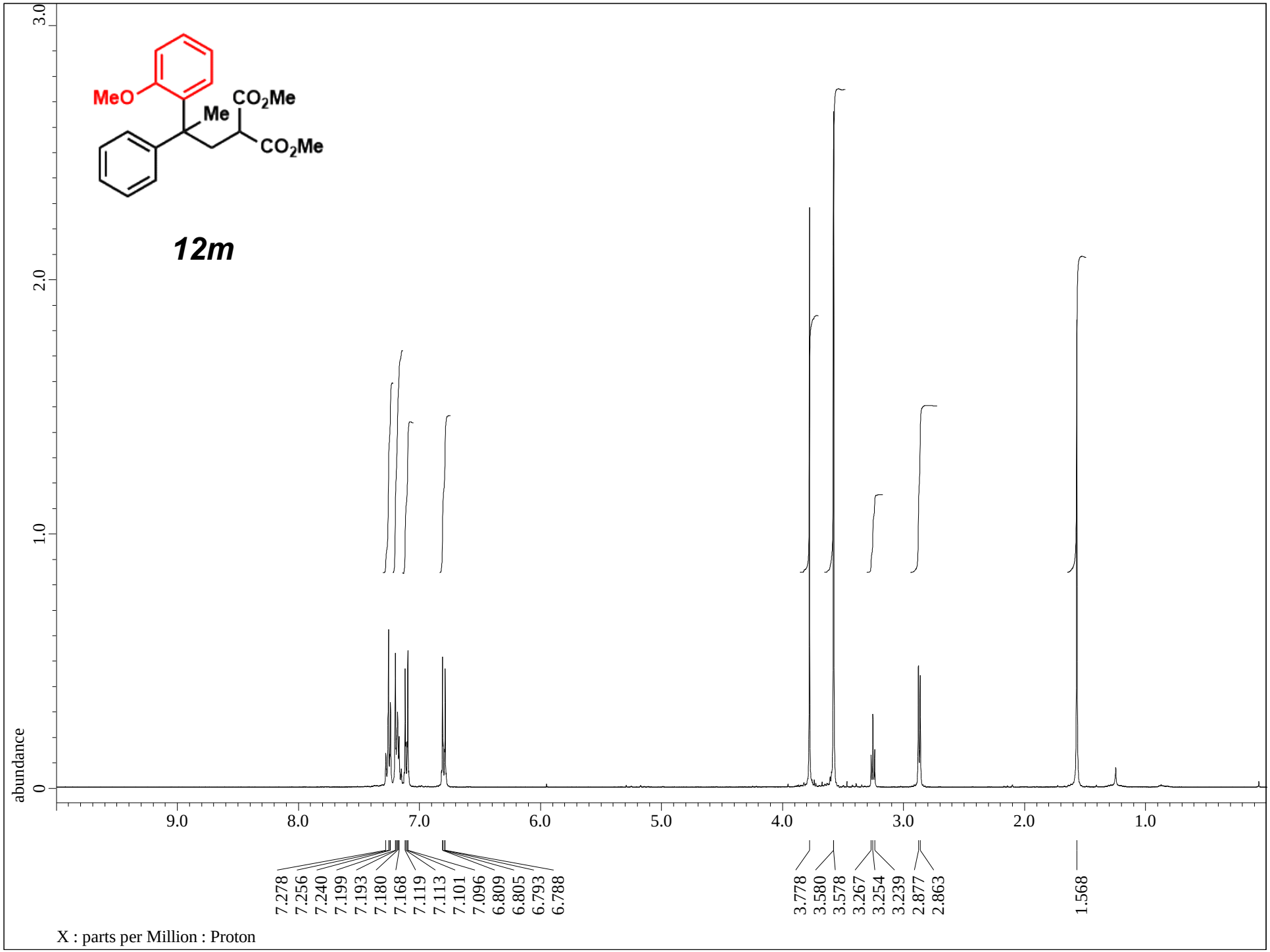

Ph
Ar
CO2Me
CO2Me
12i
abundance
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17 0.18
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
170.275
160.136
159.251
146.164
131.208
128.552
127.667
125.604
125.477
103.263
99.780
77.440
77.128
76.807
55.362
54.798
52.667
49.923
36.417
X : parts per Million : Carbon13

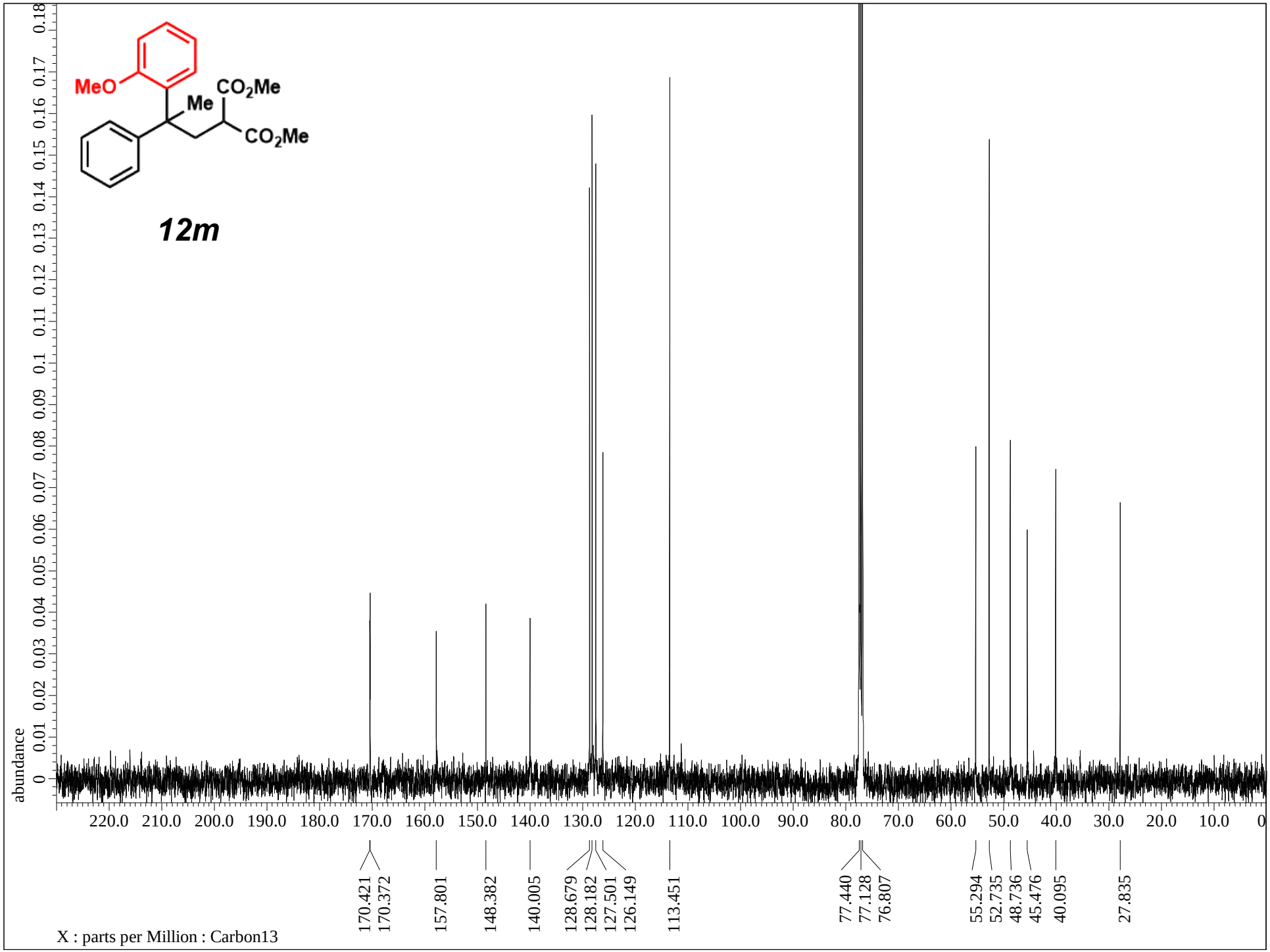

Ar
Bn
CO2Me
CO2Me
12j
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.140
7.121
7.083
7.066
7.049
7.033
7.029
7.019
7.014
6.579
6.562
6.432
6.427
6.412
6.405
6.361
6.355
3.797
3.674
3.642
3.636
3.523
3.509
3.505
3.492
3.426
3.285
3.258
3.226
2.887
2.682
2.669
2.647
2.634
X : parts per Million : Proton

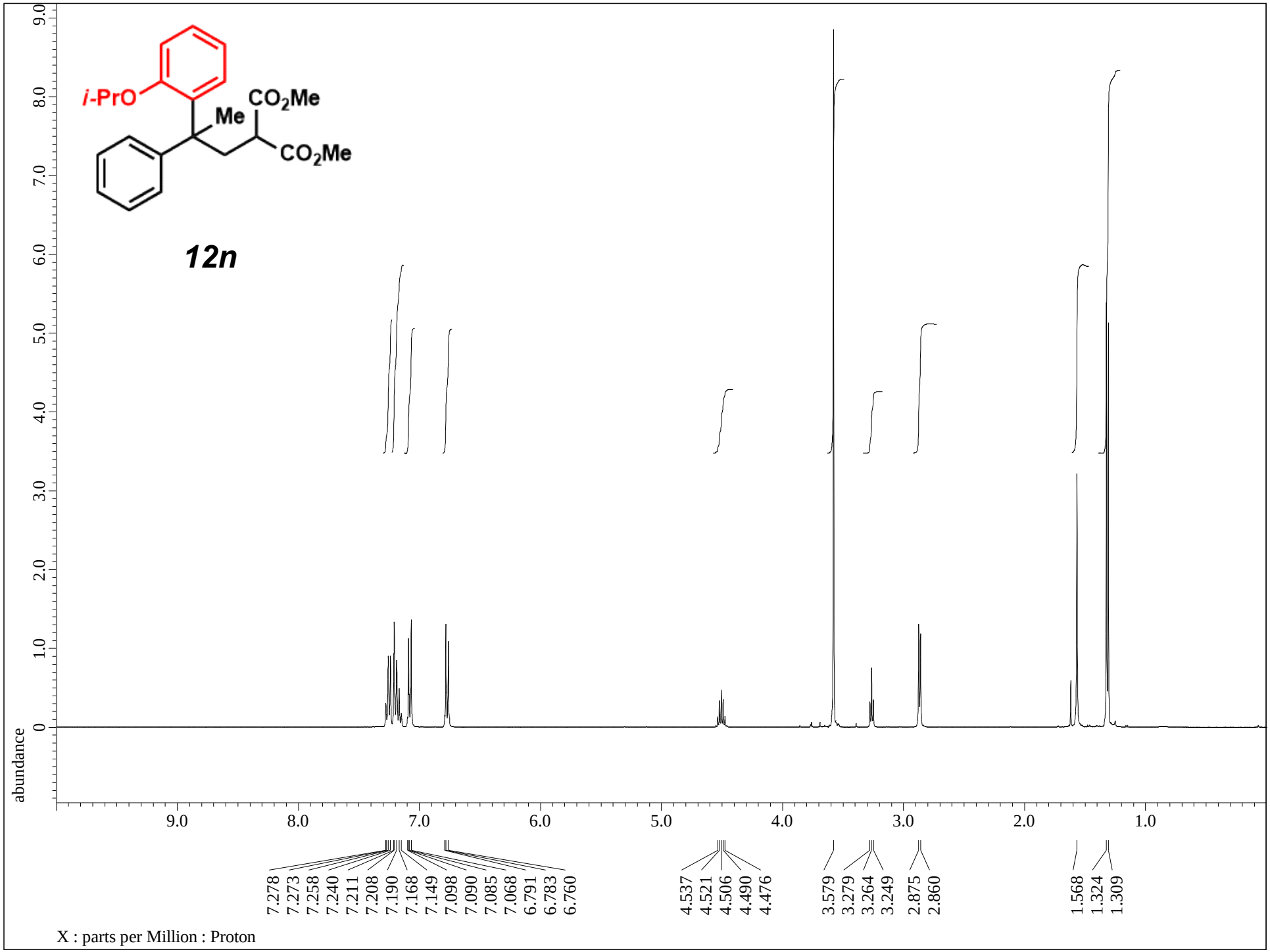

Bn
CO2Me
Ar
CO2Me
12j
abundance
0.5
0.4
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
170.032
169.779
160.029
159.144
147.507
130.975
128.883
127.346
127.297
127.102
125.993
125.322
103.555
100.461
77.381
77.070
76.749
55.304
55.031
52.433
52.307
48.794
48.239
42.635
34.072
X : parts per Million : Carbon13

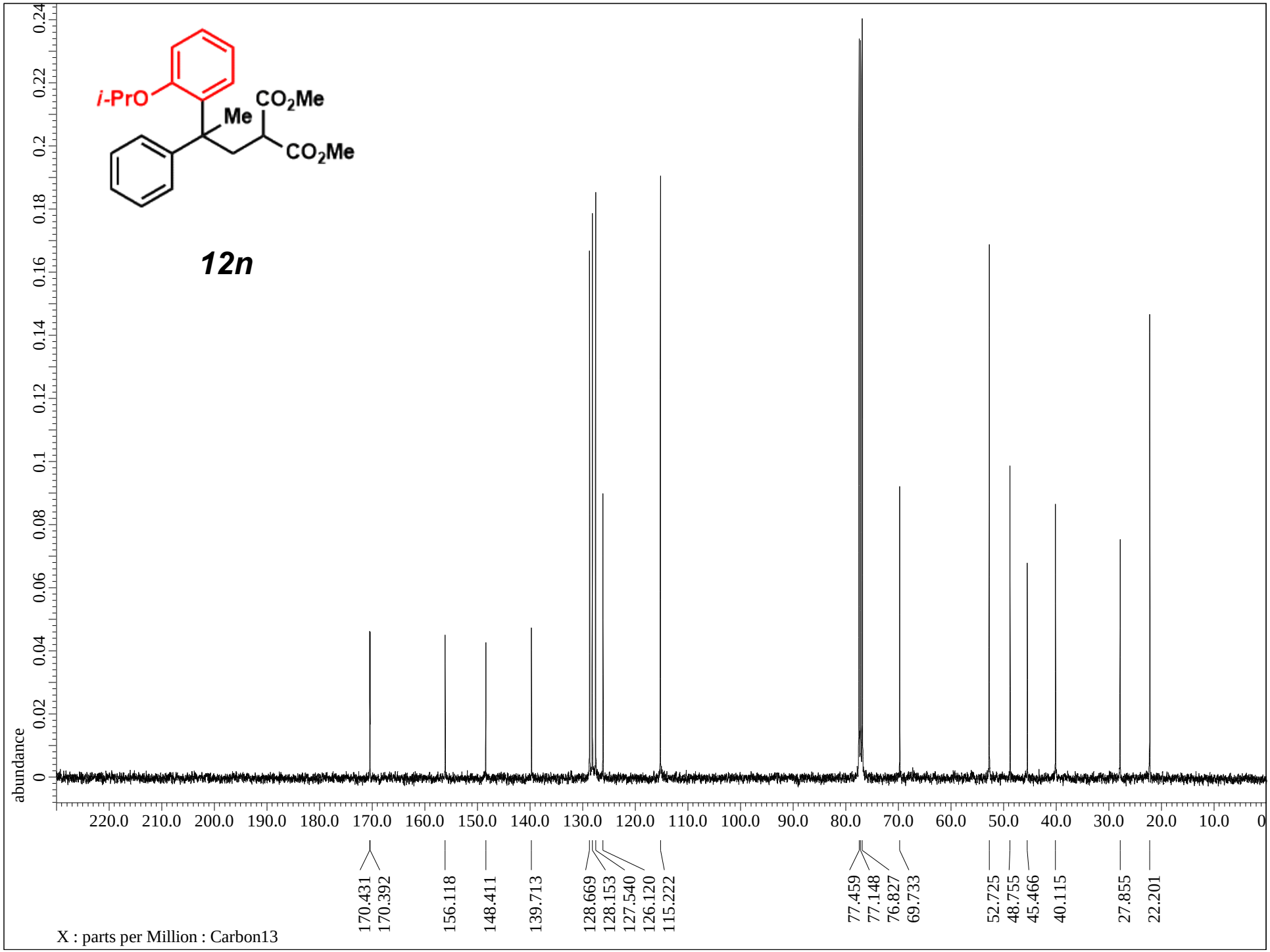

Et
CO2Me
Ar
CO2Me
12k
abundance
0
0.1
0.2
0.3
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
170.585
170.193
159.828
159.085
148.221
128.715
127.462
127.364
126.748
125.035
103.542
100.577
77.303
77.048
76.794
55.272
55.125
52.463
52.296
48.479
47.383
32.976
29.414
8.361
X : parts per Million : Carbon13

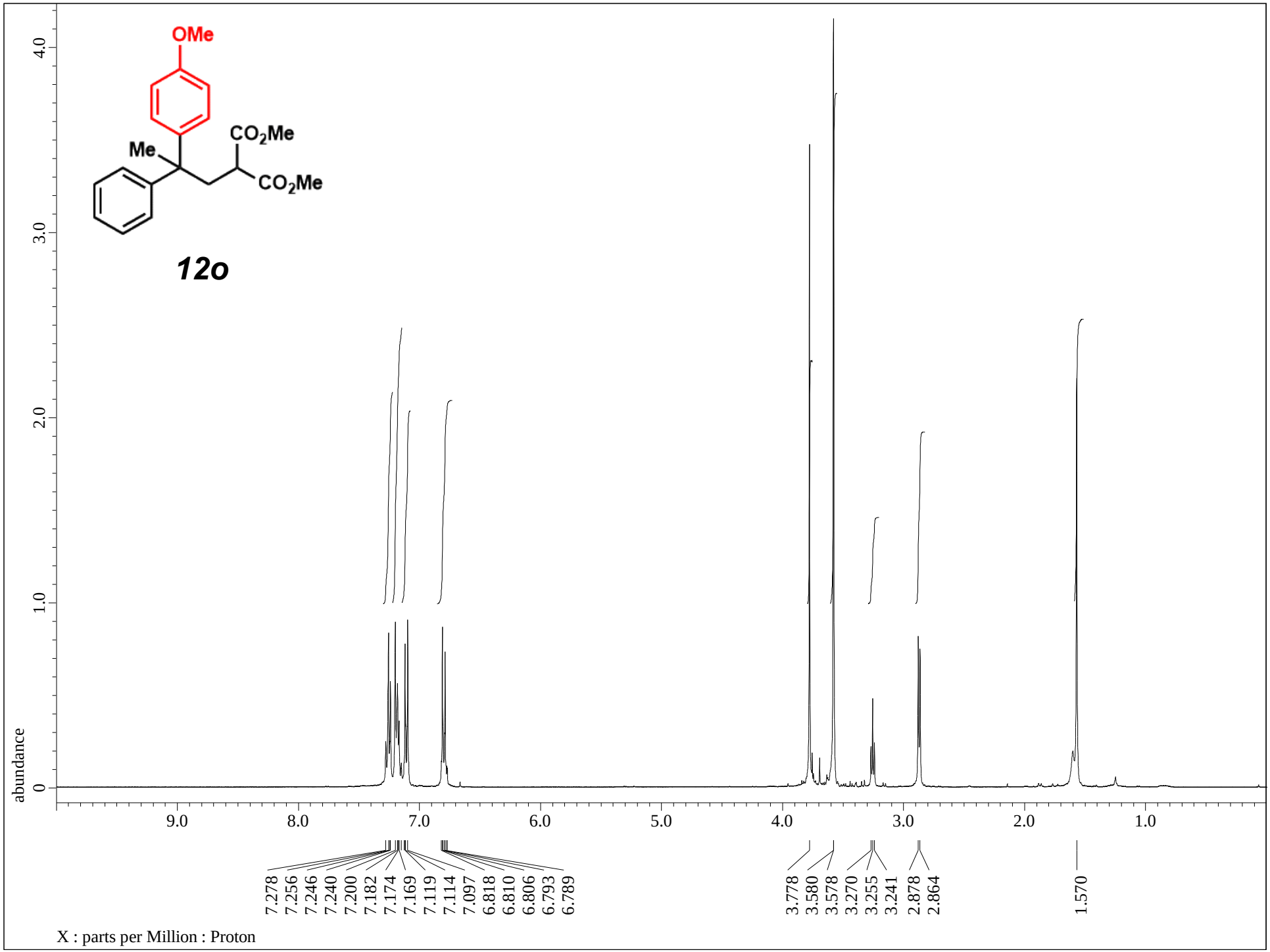

Et
CO2Me
Ar
CO2Me
12k
abundance
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.344
7.322
7.191
7.172
7.153
7.091
7.075
7.068
7.059
6.501
6.495
6.481
6.474
6.303
6.296
3.791
3.598
3.435
3.247
3.175
3.153
3.124
3.108
2.778
2.757
2.202
2.185
2.169
1.923
1.904
1.888
1.870
0.602
0.584
0.565
X : parts per Million : Proton

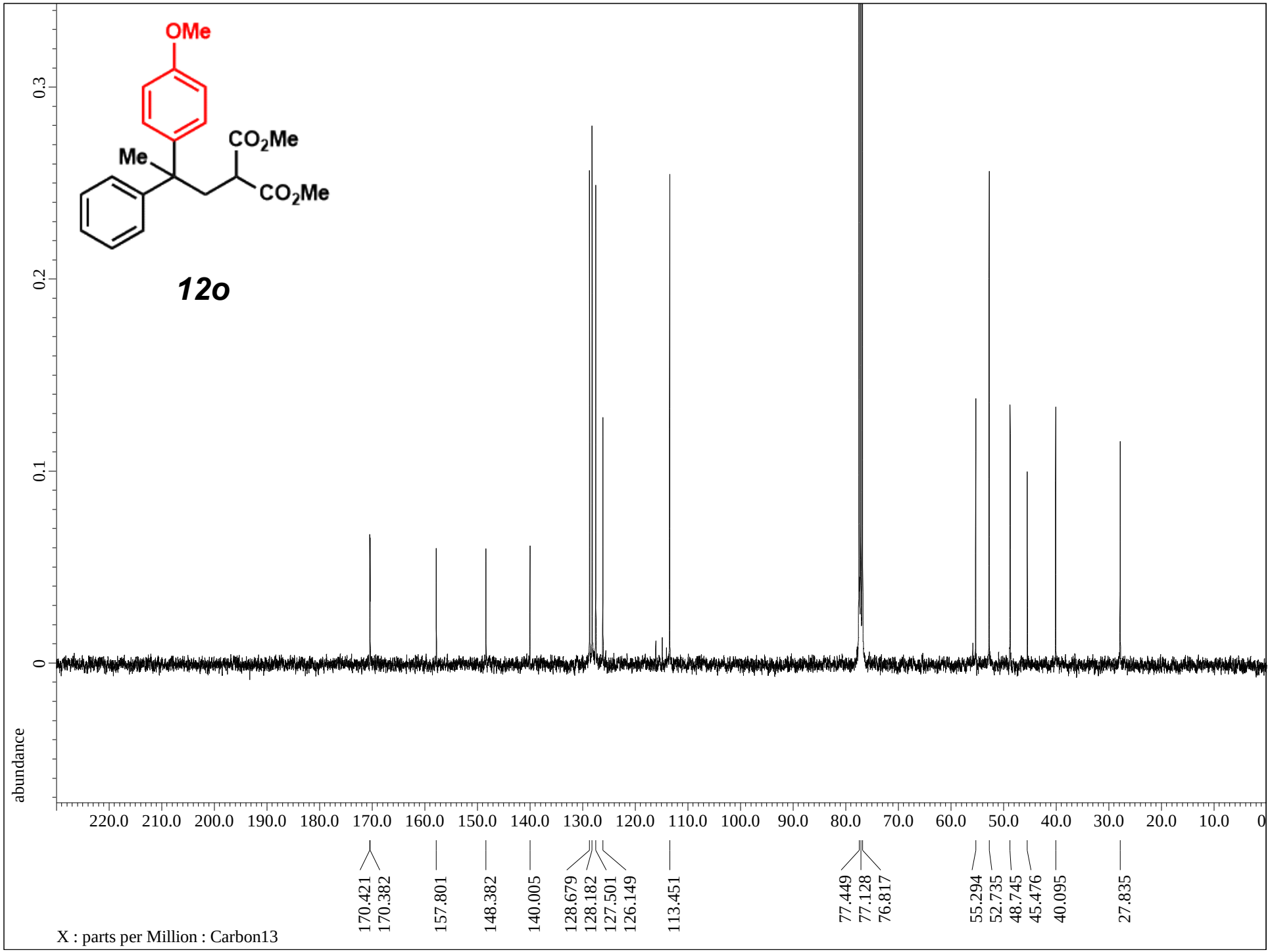

MeO
Me
CO2Me
CO2Me
12m
abundance
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.278
7.256
7.240
7.199
7.193
7.180
7.168
7.119
7.113
7.101
7.096
6.809
6.805
6.793
6.788
3.778
3.580
3.578
3.267
3.254
3.239
2.877
2.863
1.568
X : parts per Million : Proton

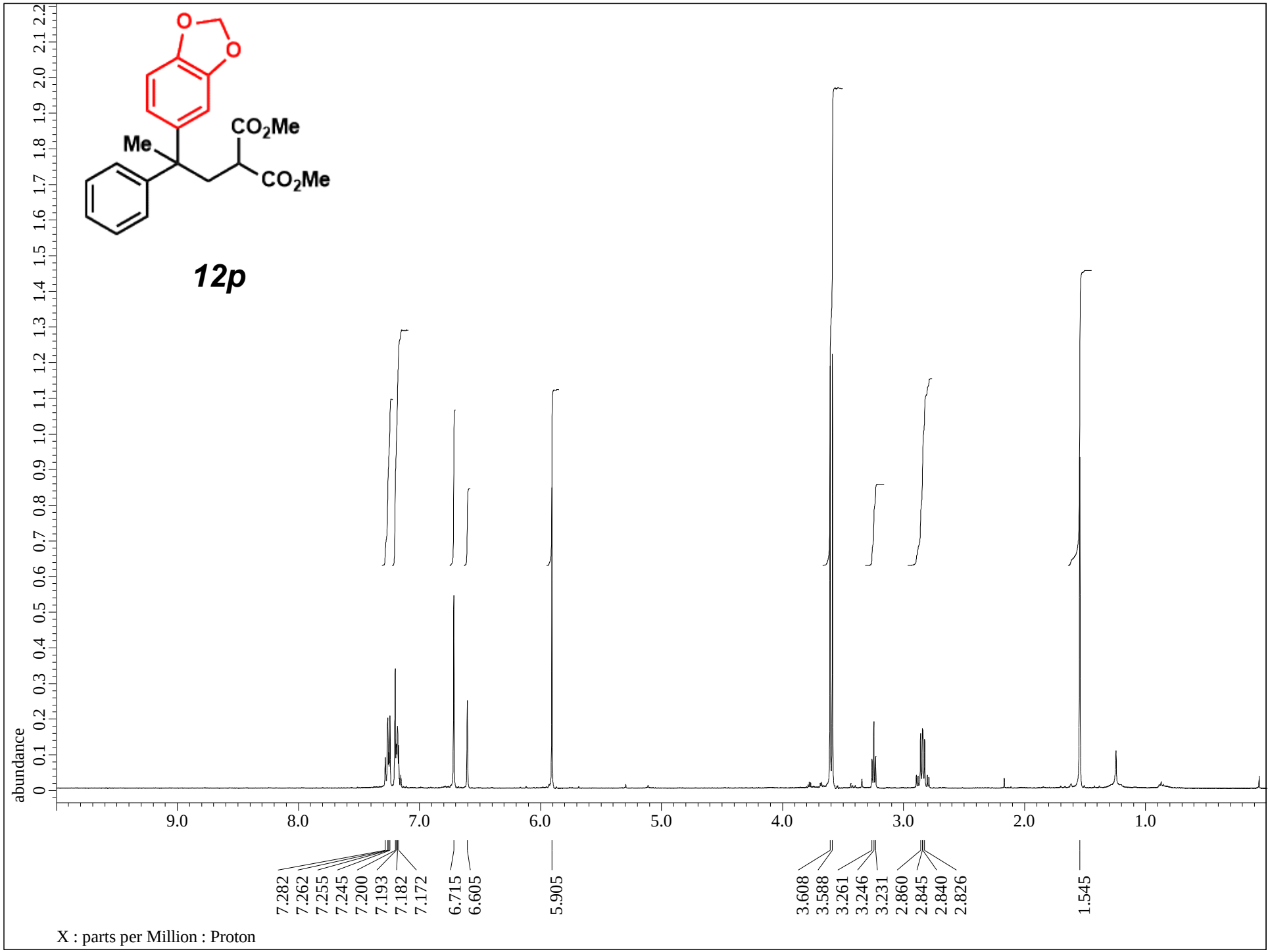

MeO
Me
CO2Me
CO2Me
12m
abundance
0.18
0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.421
170.372
157.801
148.382
140.005
128.679
128.182
127.501
126.149
113.451
77.440
77.128
76.807
55.294
52.735
48.736
45.476
40.095
27.835
X : parts per Million : Carbon13

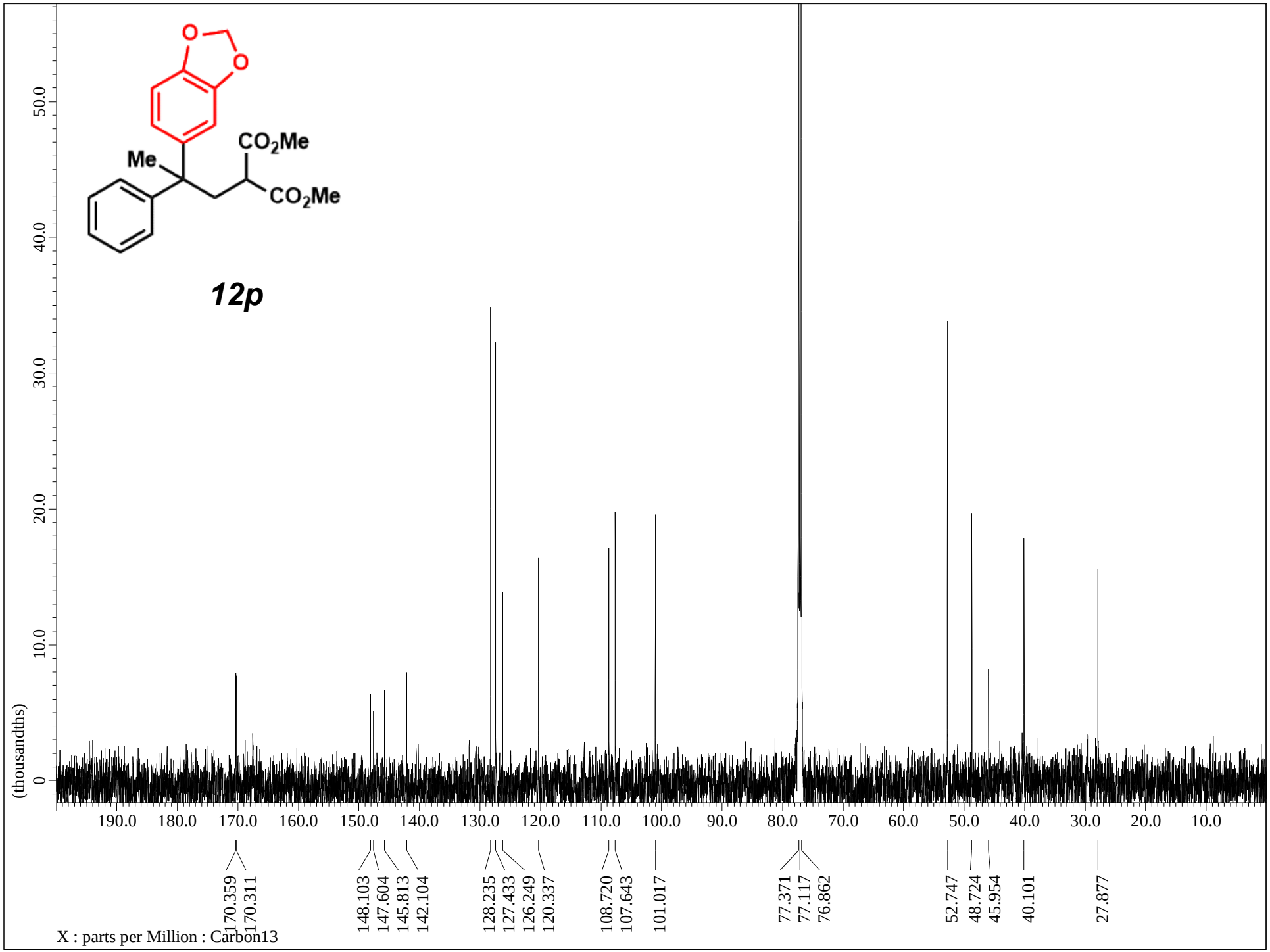

i-PrO
Me
CO2Me
CO2Me
12n
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.278
7.273
7.258
7.240
7.211
7.208
7.190
7.168
7.149
7.098
7.090
7.085
7.068
6.791
6.783
6.760
4.537
4.521
4.506
4.490
4.476
3.579
3.279
3.264
3.249
2.875
2.860
1.568
1.324
1.309
X : parts per Million : Proton

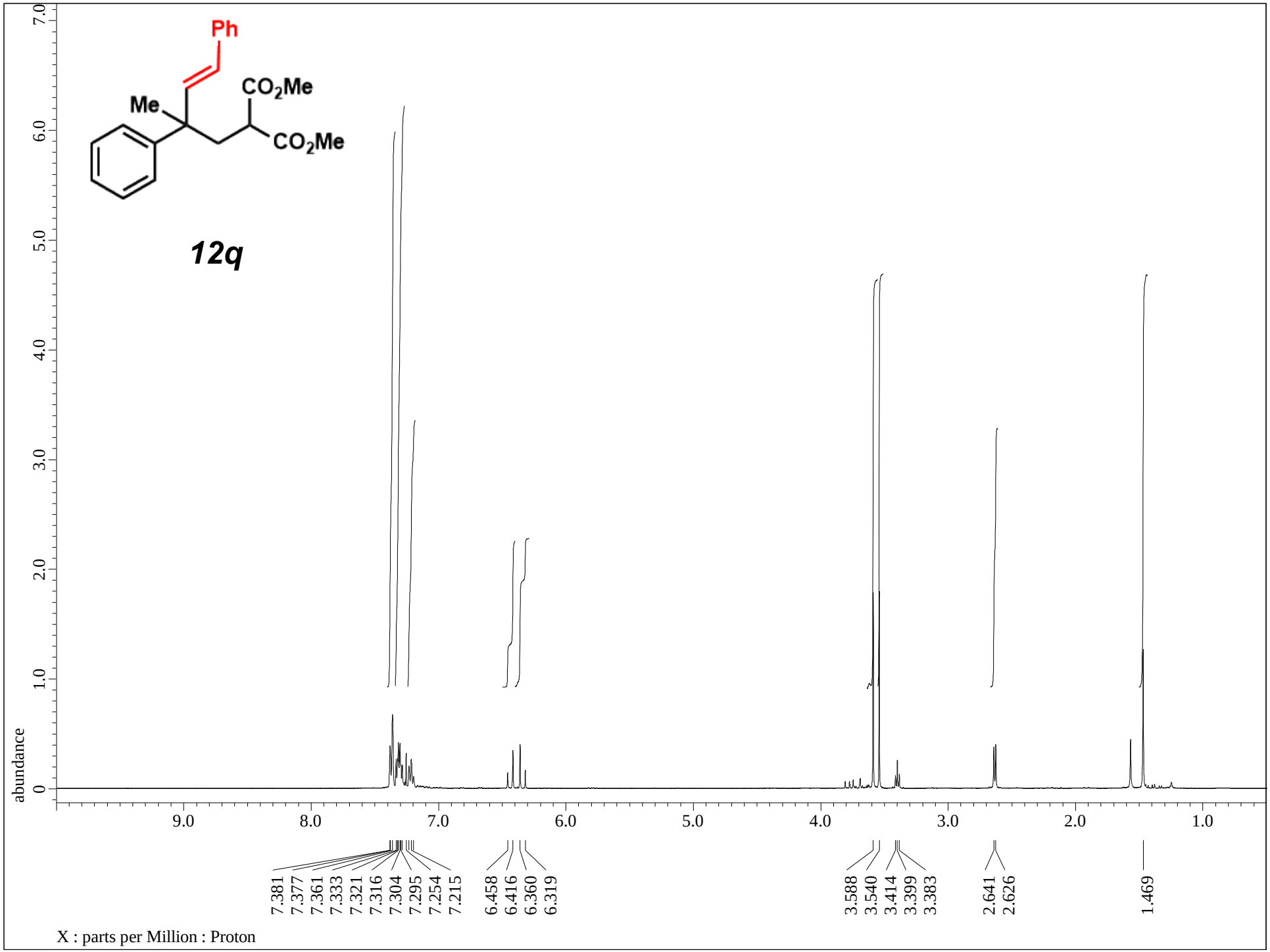

i-PrO
Me
CO2Me
CO2Me
12n
abundance
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
170.431
170.392
156.118
148.411
139.713
128.669
128.153
127.540
126.120
115.222
77.459
77.148
76.827
69.733
52.725
48.755
45.466
40.115
27.855
22.201
X : parts per Million : Carbon13

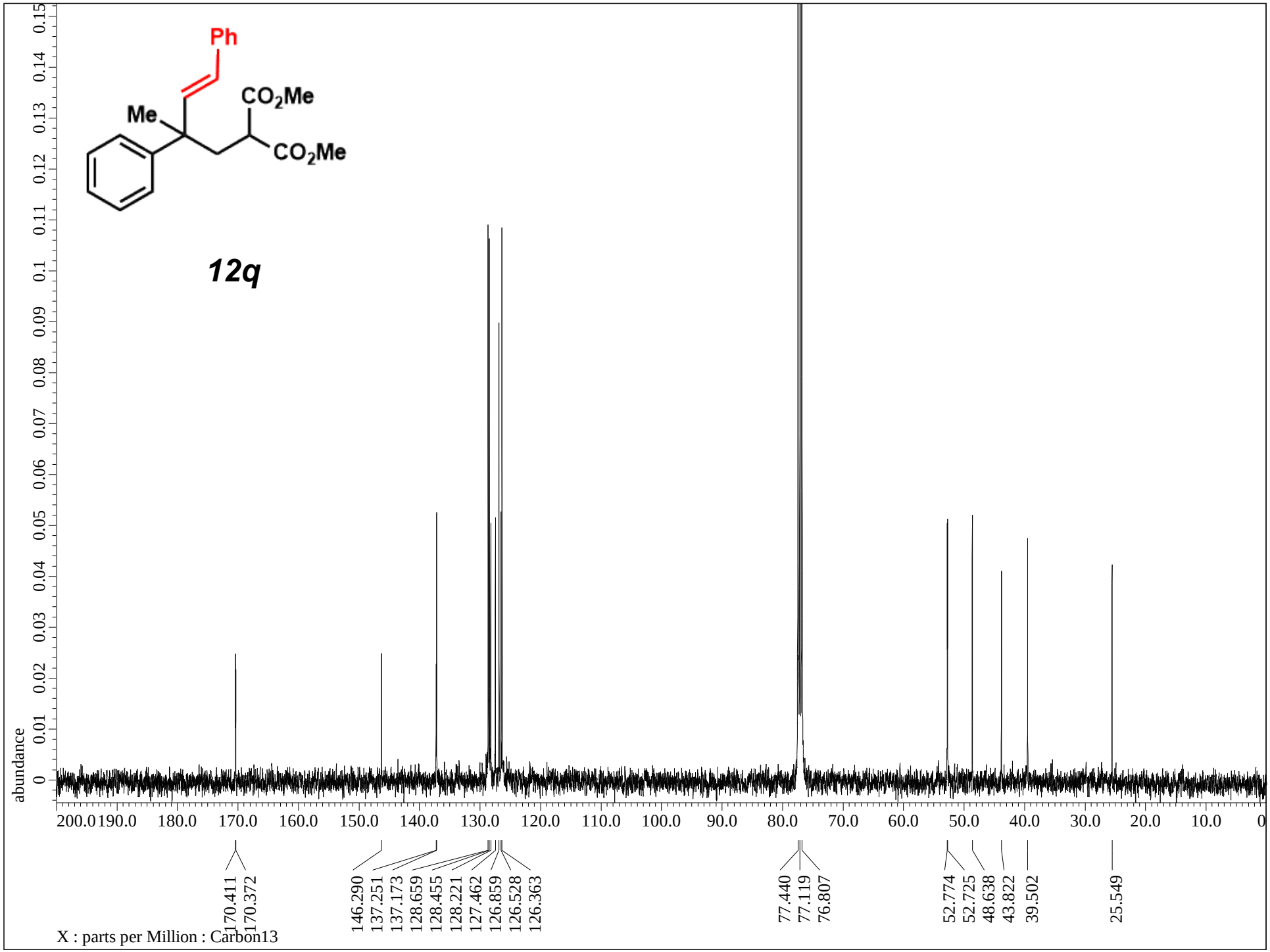

OMe
CO2Me
Me
CO2Me
12o
4.0
3.0
2.0
1.0
0
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.278
7.256
7.246
7.240
7.200
7.182
7.174
7.169
7.119
7.114
7.097
6.818
6.810
6.806
6.793
6.789
3.778
3.580
3.578
3.270
3.255
3.241
2.878
2.864
1.570
X : parts per Million : Proton

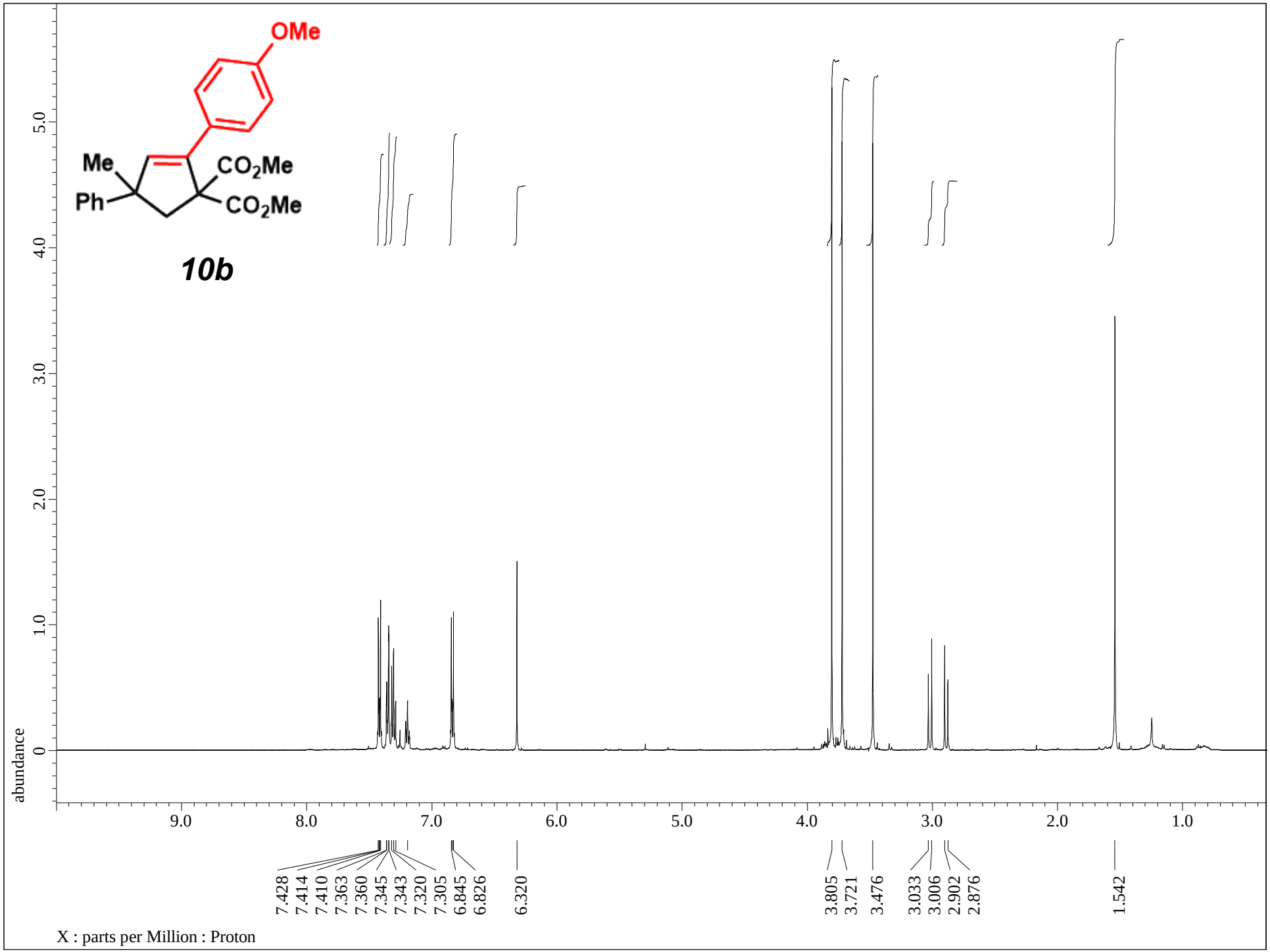

OMe
CO2Me
Me
CO2Me
12o
0.3
0.2
0.1
0
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
170.421
170.382
157.801
148.382
140.005
128.679
128.182
127.501
126.149
113.451
77.449
77.128
76.817
55.294
52.735
48.745
45.476
40.095
27.835
X : parts per Million : Carbon13

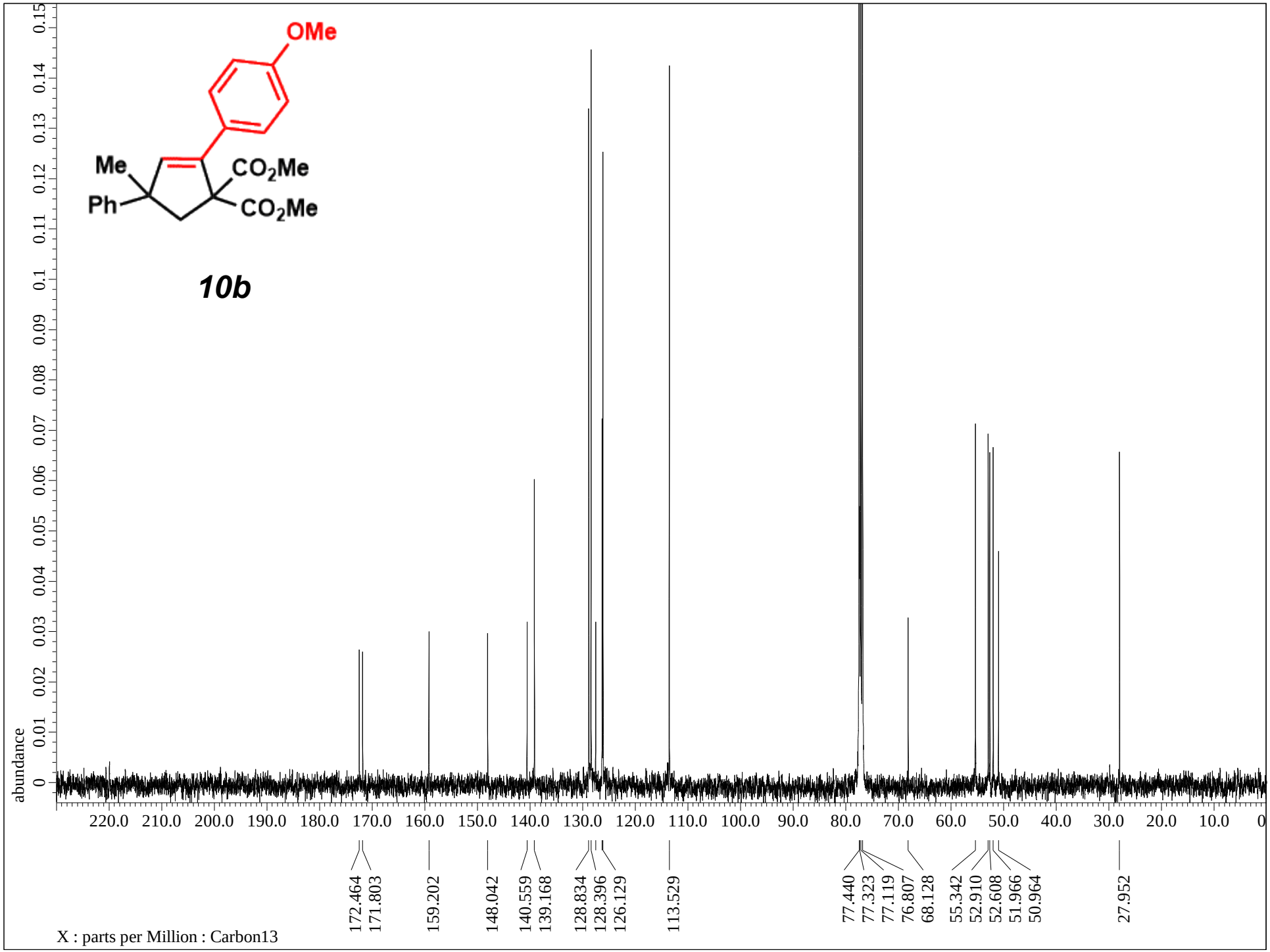

O
O
O
Me
CO2Me
CO2Me
12p
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0
7.282 7.262 7.255 7.245 7.200 7.193 7.182 7.172
6.715 6.605
5.905
3.608 3.588 3.261 3.246 3.231
2.860 2.845 2.840 2.826
1.545
X : parts per Million : Proton


Me
CO2Me
CO2Me
12p
(thousandths)
50.0
40.0
30.0
20.0
10.0
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
170.359
170.311
148.103
147.604
145.813
142.104
128.235
127.433
126.249
120.337
108.720
107.643
101.017
77.371
77.117
76.862
52.747
48.724
45.954
40.101
27.877
X : parts per Million : Carbon13

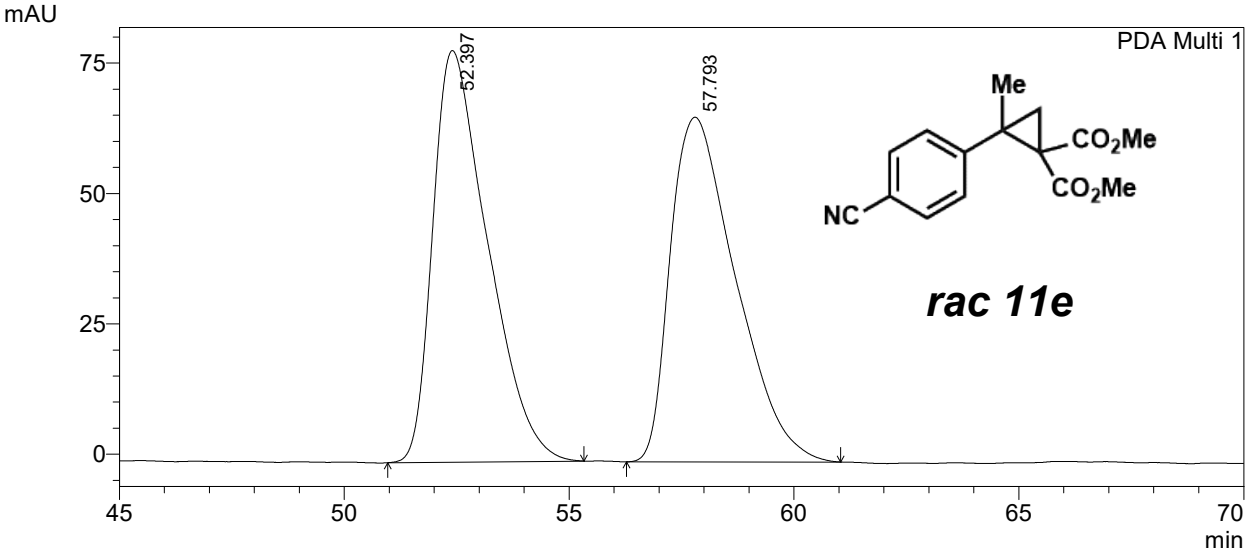

Ph
CO2Me
Me
CO2Me
12q
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.381
7.377
7.361
7.333
7.321
7.316
7.304
7.295
7.254
7.215
6.458
6.416
6.360
6.319
3.588
3.540
3.414
3.399
3.383
2.641
2.626
1.469
X : parts per Million : Proton


Ph
Me
CO2Me
CO2Me
12q
abundance
0.15
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
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
170.411
170.372
146.290
137.251
137.173
128.659
128.455
128.221
127.462
126.859
126.528
126.363
77.440
77.119
76.807
52.774
52.725
48.638
43.822
39.502
25.549
X : parts per Million : Carbon13


OMe
Me
CO2Me
Ph
CO2Me
10b
abundance
0
1.0
2.0
3.0
4.0
5.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.428
7.414
7.410
7.363
7.360
7.345
7.343
7.320
7.305
6.845
6.826
6.320
3.805
3.721
3.476
3.033
3.006
2.902
2.876
1.542
X : parts per Million : Proton


OMe
Me
CO2Me
Ph
CO2Me
10b
abundance
0.15
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
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
172.464
171.803
159.202
148.042
140.559
139.168
128.834
128.396
126.129
113.529
77.440
77.323
77.119
76.807
68.128
55.342
52.910
52.608
51.966
50.964
27.952
X : parts per Million : Carbon13

==== Shimadzu LCsolution Analysis Report ====

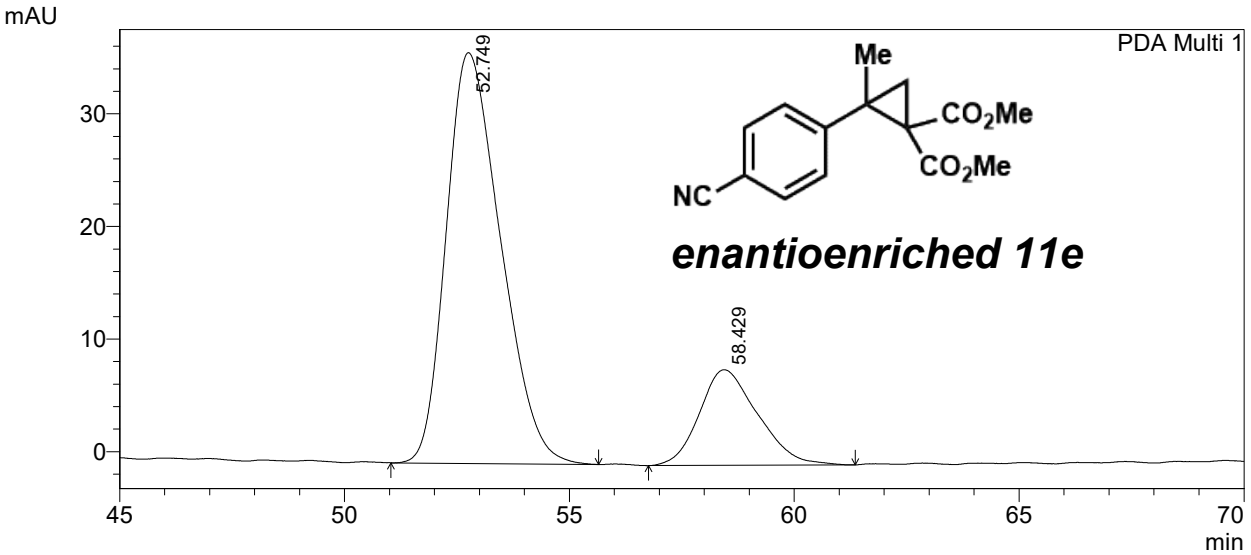


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	52.397	6696416	78920	50.049	54.425
2	57.793	6683391	66087	49.951	45.575
Total		13379807	145008	100.000	100.000



1 PDA Multi 1/254nm 4nm

PeakTable

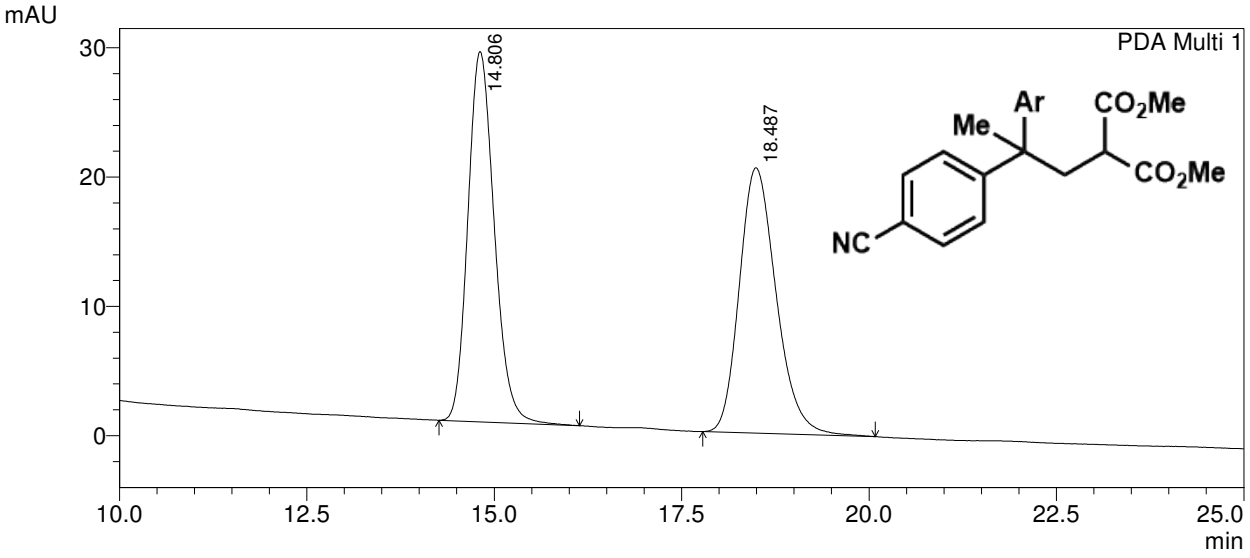
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	52.749	3075346	36489	80.045	81.110
2	58.429	766686	8498	19.955	18.890
Total		3842032	44988	100.000	100.000

==== Shimadzu LCsolution Analysis Report ====

<Chromatogram>

12e from racemic 11e

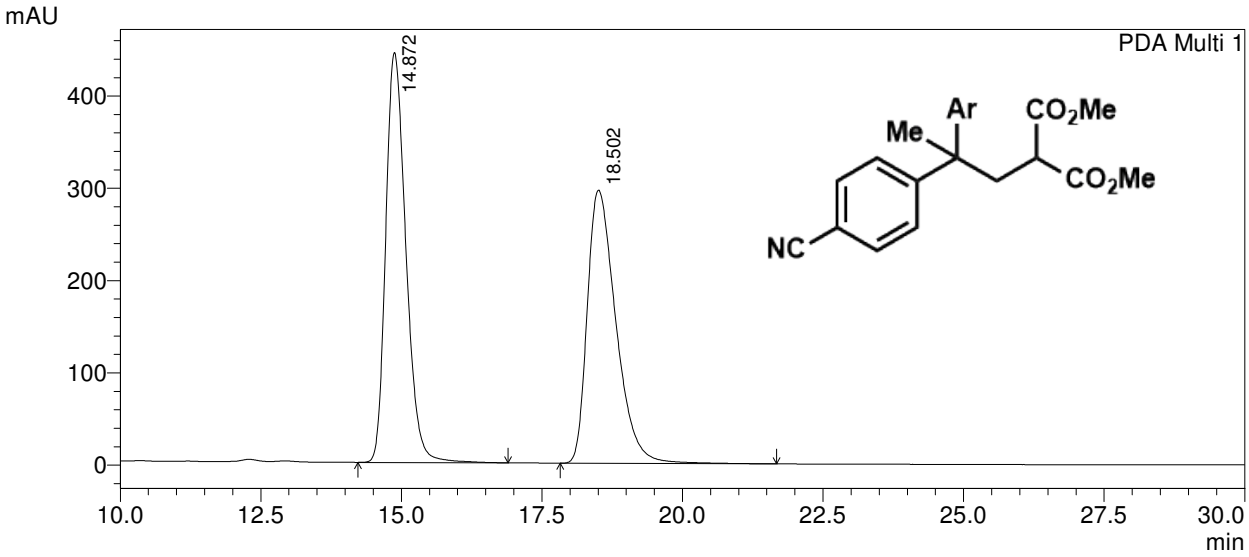


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.806	700718	28630	50.010	58.255
2	18.487	700448	20516	49.990	41.745
Total		1401166	49147	100.000	100.000

12e from enantioenriched 11e



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.872	11054345	444275	51.294	59.992
2	18.502	10496655	296282	48.706	40.008
Total		21551000	740557	100.000	100.000