Electronic Supplementary Information for

Zn/F Carbenoids:
Preparation, Stability, Structures, and Application to Nucleophilic Monofluoroalkylation

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Abbreviation

THF	tetrahydrofurane
DMF	*N*,*N*-dimethyl formamide
TLC	thin-layer chromatography
NMR	nuclear magnetic resonance
TMS	trimethylsilyl
HRMS	high resolution mass spectroscopy
EtOAc	ethyl acetate
Trt	trityl
Et	ethyl
Me	methyl
Ph	phenyl
TIPS	triisopropyl
TBDPS	*tert*-butyldiphenylsilyl
Bn	benzyl
Ts	*para*-toluenesulfonyl

1. General Experimental Details

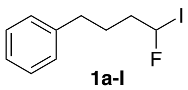
All manipulations employing alkylzinc species were performed under N_2 atmosphere unless stated otherwise using Schlenk technique or nitrogen-filled Glove Box (MBrown, LABSTAR). Solvents were purified under N_2 using The Ultimate Solvent System (Glass Counter) (THF, Et_2O, DMF, toluene). Flash silica gel column chromatography was conducted with Wakogel® FC-40. Preparative TLC was performed on precoated plates (AS ONE, Silica Gel 60 Plate F254, 0.5 mm). Nuclear magnetic resonance (NMR) spectra were acquired on JEOL ECS-400 (400 MHz), JEOL ECX-400P (400 MHz), ECZ-400 (400 MHz), or JEOL ECZ-500R (500 MHz). ^{1}H NMR chemical shifts are reported in ppm and referenced to residual solvent peaks as internal standards ($CDCl_3$: 7.26 ppm and dimethylformamide-d_7: 7.96 ppm). Coupling constants are reported in hertz and J represents $^{3}J_{\mathrm{H–H}}$ unless otherwise noted. The following abbreviations are used: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. ^{13}C{^{1}H} NMR chemical shifts are reported in ppm and referenced to residual solvent peaks as internal standards ($CDCl_3$: 77.16 ppm and dimethylformamide-d_7: 162.62 ppm). ^{19}F NMR chemical shifts are reported in ppm and referenced to hexafluorobenzene as external standards (−164.90 ppm). High-resolution mass spectroscopy (HRMS) was obtained with Thermo Scientific Exactive mass spectrometers for ESI-MS or JMS-T2000 GC for EI-MS. Zinc powder (Kanto Chemical Co. Inc., 1st Grade) was activated by dibromoethane and TMSCl in THF and then dried under vacuum.

__2. Preparation of the Substrates and Reagents__

1-Fluoro-1-haloalkanes **1a-I**[S1], **1a-Br**[S1], **1b-I**[S2], **1c-I**[S1], **1e-I**[S1]and, **1f-I**[S3] are described in the literature but not fully characterized. **1g-Br**[S4] were literature known compounds and prepared according to the literature procedure. These 1-fluoro-1-iodoalkane were thermally stable and resistant to moisture, silica gel, and light. In most cases, the total yield of the four-step preparation was about 30%. **1d-I** was prepared according to the literature procedure.[S2] For literature known 1-Fluoro-1-haloalkanes, ^{1}H, ^{13}C, and ^{19}F NMR were described below. Electrophiles (except for acyl dithiocarbamate derivatives) were literature known compounds or commercially available compounds.

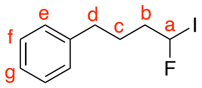
2.1 NMR spectra of 1-Fluoro-1-haloalkanes

(4-fluoro-4-iodobutyl)benzene (**1a-I**)

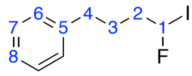


1a-I

for ^{1}H NMR

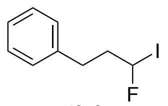


for ^{13}C NMR



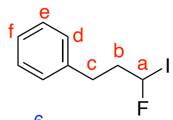
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.32–7.17 (m, 5H, H$_e$–H$_g$), 6.83 (dt, 1H, $^{2}J_{H\text{-}F}$ = 50.8 Hz, $^{2}J_{H\text{-}H}$ = 5.6 Hz, H$_a$), 2.69 (t, 2H, $^{2}J_{H\text{-}H}$ = 7.8 Hz, H$_d$), 2.25–2.15 (m, 2H, H$_b$), 1.88–1.80 (m, 2H, H$_c$); ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 141.27 (C5), 128.62 (C6 or C7), 128.49 (C6 or C7), 126.23 (C8), 75.20 (d, $^{1}J_{C\text{-}F}$ = 254.8 Hz, C1), 42.61 (d, $^{2}J_{C\text{-}F}$ = 19.1 Hz, C2), 34.69 (C4), 28.48 (d, $^{3}J_{C\text{-}F}$ = 3.9 Hz, C3); ^{19}F NMR (367 MHz, CDCl$_3$) δ −134.56 (dt, $^{2}J_{H\text{-}F}$ = 49.5 Hz, $^{3}J_{H\text{-}F}$ = 19.8 Hz). HRMS (EI-TOF) m/z calcd. for $C_{10}H_{12}FI$ [M]$^+$ 277.99622, found 277.99686.

(3-fluoro-3-iodopropyl)benzene (**1b-I**)

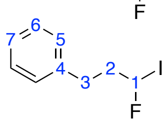


1b-I

for ^{1}H NMR

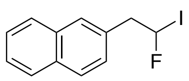


for ^{13}C NMR



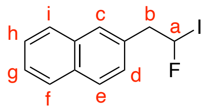
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.32–7.19 (m, 5H, H$_d$–H$_f$), 6.77 (ddd, 2H, $^{2}J_{H\text{-}F}$ = 49.2 Hz, $^{3}J_{H\text{-}H}$ = 6.4 Hz, $^{3}J_{H\text{-}H}$ = 4.8 Hz, H$_a$), 2.86–2.75 (m, 2H, H$_c$), 2.67–2.48 (m, 2H, H$_b$); ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 139.38 (C4), 128.83 (C5 or C6), 128.61 (C5 or C6), 126.64 (C7), 74.38 (d, $^{1}J_{C\text{-}F}$ = 253.0 Hz, C1), 44.85 (d, $^{2}J_{C\text{-}F}$ = 19.2 Hz, C2), 32.91 (d, $^{3}J_{C\text{-}F}$ = 3.8 Hz, C3); ^{19}F NMR (367 MHz, CDCl$_3$) δ −136.57 ($^{2}J_{H\text{-}F}$ = 49.2 Hz, $^{3}J_{H\text{-}F}$ = 20.9 Hz, $^{3}J_{H\text{-}F}$ = 16.9 Hz). HRMS (EI-TOF) m/z calcd. for $C_9H_{10}FI$ [M]$^+$ 263.98057, found 263.98080.

2-(2-fluoro-2-iodoethyl)naphthalene (**1c-I**)

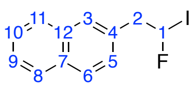


1c-I

for ^{1}H NMR

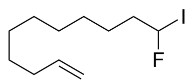


for ^{13}C NMR



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.84–7.82 (m, 2H, H$_h$, H$_g$ and H$_d$), 7.72 (s, 1H, H$_c$), 7.52–7.47 (m, 2H, H$_f$ and H$_i$), 7.36 (d, 1H, $^{3}J_{H\text{-}H}$ = 8.4 Hz, H$_e$), 7.00 (ddd, 1H, $^{2}J_{H\text{-}F}$ = 51.0 Hz, $^{3}J_{H\text{-}H}$ = 6.6 Hz, $^{3}J_{H\text{-}H}$ = 5.6 Hz, H$_a$), 3.87–3.65 {3.81 (ddd, $^{2}J_{H\text{-}H}$ = 15.2 Hz, $^{2}J_{H\text{-}F}$ = 17.0 Hz, $^{3}J_{H\text{-}H}$ = 6.6 Hz), 3.71 (ddd, $^{2}J_{H\text{-}H}$ = 15.2 Hz, $^{2}J_{H\text{-}F}$ = 23.5 Hz, $^{3}J_{H\text{-}H}$ = 5.6 Hz)}; ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 133.55 (C7 or 12), 133.46 (d, $^{3}J_{C\text{-}F}$ = 3.9 Hz, C4), 132,79 (C7 or C12), {128.62, 128.57, 127.88, 127.39, 127.38 126.50, 126.21} (C3, C5, C6, C8, C9, C10 and C11, one carbon overlapped), 75.01 (d, $^{1}J_{C\text{-}F}$ = 254.9 Hz, C1), 50.01 (d, $^{2}J_{C\text{-}F}$ = 19.2 Hz, C2); ^{19}F NMR (367 MHz, CDCl$_3$) δ −135.50 (ddd, $^{2}J_{H\text{-}F}$ = 53.4 Hz, $^{3}J_{H\text{-}F}$ = 23.5 Hz, $^{3}J_{H\text{-}F}$ = 17.0 Hz). HRMS (ESI-TOF) m/z calcd. for $C_{12}H_{10}FI$ [M]$^+$ 299.98057, found 299.98058.

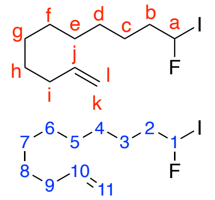
11-fluoro-11-iodoundec-1-ene (**1d-I**)



1d-I

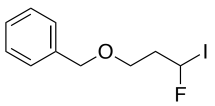
for ^{1}H NMR

for ^{13}C NMR



^{1}H NMR (400 MHz, $CDCl_3$) δ 6.82 (dt, 1H, $^{2}J_{H\text{-}F}$ = 49.6 Hz, $^{3}J_{H\text{-}F}$ = 5.4 Hz, H_a), 5.80 (ddt, $^{3}J_{H\text{-}H}$ = 17.0 Hz, $^{3}J_{H\text{-}H}$ = 10.4 Hz, $^{3}J_{H\text{-}H}$ = 6.4 Hz, 1H, H_j), 4.98 (dd, 1H, $^{3}J_{H\text{-}H}$ = 17.0 Hz, $^{3}J_{H\text{-}H}$ = 2.0 Hz, H_k), 4.92 (dd, 1H, $^{3}J_{H\text{-}H}$ = 10.4 Hz, $^{3}J_{H\text{-}H}$ = 2.0 Hz, H_l), 2.33–2.12 (m, 2H, H_b), 2.04 (dt, 2H, $^{3}J_{H\text{-}H}$ = 7.6 Hz, $^{3}J_{H\text{-}H}$ = 6.4 Hz, H_i), 1.49–1.29 (m, 12H, H_c–H_h); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 139.29 (C10), 114.33 (C11), 75.90 (d, C1, coupling constant cannot be determined due to overlapping with the other peak), 43.42 (d, $^{2}J_{C\text{-}F}$ = 18.2 Hz, C2), 43.24 (C9), {33.92, 29.42, 29.17, 29.02, 28.57} (C4, C5, C6, C7 and C8), 26.86 (d, $^{3}J_{C\text{-}F}$ = 3.8 Hz, C3); ^{19}F NMR (367 MHz, $CDCl_3$) δ −134.01. (dt, $^{2}J_{H\text{-}F}$ = 49.6 Hz, $^{3}J_{H\text{-}F}$ = 25.5 Hz). HRMS (EI-TOF) m/z calcd. for $C_{11}H_{20}FI$ $[M]^+$ 298.05882, found 298.05963.

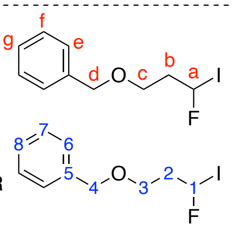
((3-fluoro-3-iodopropoxy)methyl)benzene (**1e-I**)



1e-I

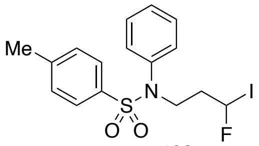
for ^{1}H NMR

for ^{13}C NMR



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38–7.28 (m, 5H, H_e–H_g), 6.99 (dt, 1H, $^{3}J_{H\text{-}H}$ = 48.4 Hz, $^{3}J_{H\text{-}H}$ = 6.0 Hz, H_a), 4.51 (s, 2H, H_d), 3.68–3.47 (m, 2H, H_c), 2.66–2.44 (m, 2H, H_b); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 137.93 (C5), 128.62 (C6 or C7), 127.98 (C8), 127.84 (C6 or C7), 73.67 (d, $^{1}J_{C\text{-}F}$ = 256.5 Hz, C1), 73.38 (C4), 66.85 (d, $^{3}J_{C\text{-}F}$ = 4.8 Hz, C3), 43.74 (d, $^{2}J_{C\text{-}F}$ = 20.0 Hz, C2); ^{19}F NMR (367 MHz, $CDCl_3$) δ −138.64 (ddd, $^{2}J_{H\text{-}F}$ = 48.4 Hz, $^{3}J_{H\text{-}F}$ = 22.4 Hz, $^{3}J_{H\text{-}F}$ = 13.9 Hz). HRMS (EI-TOF) m/z calcd. for $C_{10}H_{12}FIO$ $[M]^+$ 293.99114, found 293.99161.

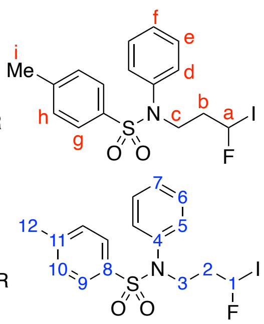
N-(3-fluoro-3-iodopropyl)-4-methyl-*N*-phenylbenzenesulfonamide (**1f-I**)



1f-I

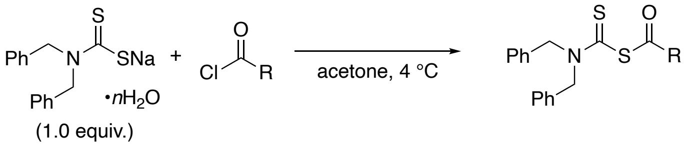
for ^{1}H NMR

for ^{13}C NMR



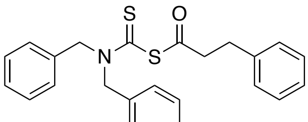
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, 2H $^{3}J_{H\text{-}H}$ = 8.4 Hz, H_g), 7.35–7.31 (m, 3H, H_e and H_f), 7.26 (d, 2H, $^{3}J_{H\text{-}H}$ = 8.4 Hz, H_h), 7.05–7.03 (m, 2H, H_d), 6.89 (ddd, 1H, $^{2}J_{H\text{-}F}$ = 48.1 Hz, $^{3}J_{H\text{-}F}$ = 6.4 Hz, $^{3}J_{H\text{-}F}$ = 5.2 Hz, H_a), 3.77–3.60 (m, 2H, H_c), 2.59–2.35 (m, 2H, H_b), 2.43 (s, 3H, H_i); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 143.89 (C4), 139.06 (C8), 134.64 (C11), {129.65, 129.41, 128.68, 128.41, 127.85} (C5, C6, C7, C9 and C10), 70.59 (d, $^{1}J_{C\text{-}F}$ = 252.1 Hz, C1), 48.19 (d, $^{3}J_{C\text{-}F}$ = 3.9 Hz, C3), 42.43 (d, $^{2}J_{C\text{-}F}$ = 20.1 Hz, C2), 21.70 (C12); ^{19}F NMR (367 MHz, $CDCl_3$) δ −138.80. (ddd, $^{2}J_{H\text{-}F}$ = 48.1 Hz, $^{3}J_{H\text{-}F}$ = 21.3 Hz, $^{3}J_{H\text{-}F}$ = 16.9 Hz). HRMS (ESI-TOF) m/z calcd. for $C_{16}H_{17}O_2NFINaS$ $[M + Na]^+$ 455.99009, found 455.98978.

2.2 General Procedure for Synthesis of Acyl Dithiocarbamate Derivatives



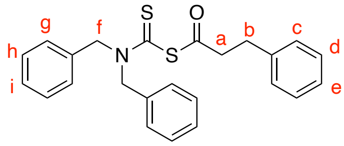
To the 100 mL flask equipped with a magnetic stir bar were added sodium dibenzyldithiocarbamate hydrate (1.0 equiv.) and acetone (dehydrated, 0.075 M). After the solution was cooled to 4 °C, acid chloride was added to the solution. The reaction was then quenched by the addition of sat. $NaHCO_3$ aq. and the resulted solution was extracted by Et_2O by three times. The combined organic phase was washed with brine, dried over Na_2SO_4, concentrated under reduced pressure, and purified by column chromatography.

dibenzylcarbamothioic 3-phenylpropanoic thioanhydride (**7r**)

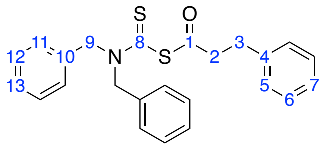


7r

for ^{1}H NMR

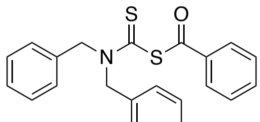


for ^{13}C NMR



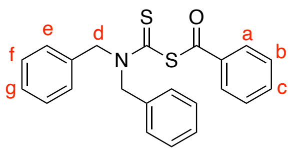
The reaction was performed according to the general procedure using 3-phenylpropionyl chloride (450 μL, 3.00 mmol). The reaction time was 15 min and the obtained crude mixture was purified by silica gel column chromatography using hexane/EtOAc = 10/1 as an eluent to give the titled compound as pale brown sticky oil (654 mg, 54% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.24 (m, 10H, H_e–H_g), 5.08 (s, 4H, H_d), 1.99 (tt, 1H, $^3J_{H–H}$ = 8.0 Hz, $^3J_{H–H}$ = 4.0 Hz, H_a), 1.28–1.24 (m, 2H, H_b or H_c), 1.06–1.01 (m, 2H, H_b or H_c); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.50 (C1), 185.20 (C8), {139.38, 134.57, 129.07, 128.76, 128.47, 128.24, 127.74, 126.72} (C4, C5, C6, C7, C10, C11, C12 and C13), 56.46 (C9), 45.51 (C3), 31.37 (C2). HRMS (ESI-TOF) m/z calcd. for $C_{24}H_{23}ONNaS_2$ $[M + Na]^+$ 428.11133, found 428.11065.

benzoic dibenzylcarbamothioic thioanhydride (**7s**)

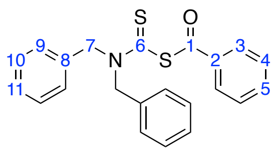


7s

for ^{1}H NMR



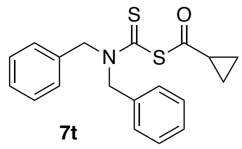
for ^{13}C NMR



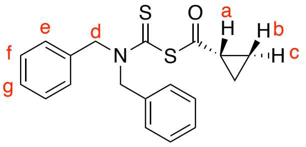
The reaction was performed according to the general procedure using benzoyl bromide (0.36 mL, 3.00 mmol). The reaction time was 15 min and the obtained crude mixture was purified by silica gel column chromatography using hexane/EtOAc = 10/1 as an eluent to give the titled compound as yellow solid (952 mg, 84% yield).

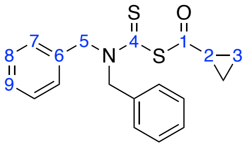
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45–7.33 (m, 15H, H_a–H_c and H_e–H_g), 5.17 (s, 4H, H_d) ; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 186.46 (C1), 185.29 (C6), {135.69, 134.62, 134.44, 129.11, 129.08, 128.25, 127.95 127.79} (C2, C3, C4, C5, C8, C9, C10 and C11), 57.50–56.00 (br, C7). HRMS (ESI-TOF) m/z calcd. for $C_{22}H_{19}ONNaS_2$ $[M + Na]^+$ 400.08003, found 400.07997.

dibenzylcarbamothioic cyclopropanecarboxylic thioanhydride (**7t**)



7t

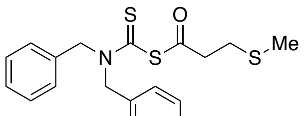
for ^{1}H NMR 

for ^{13}C NMR 

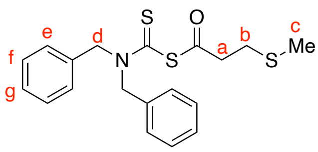
The reaction was performed according to the general procedure using cyclopropanecarbonyl chloride (182 μL, 2.00 mmol). The reaction time was 30 min and the obtained crude mixture was purified by silica gel column chromatography using hexane/EtOAc = 10/1 as an eluent to give **7t** as pale brown sticky oil (579 mg, 85% yield).

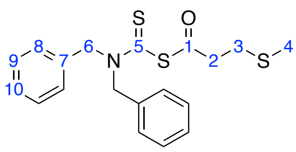
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.24 (m, 10H, H_e–H_g), 5.08 (s, 4H, H_d), 1.99 (tt, 1H, $^{3}J_{H–H}$ = 8.0 Hz, $^{3}J_{H–H}$ = 4.0 Hz, H_a), 1.28–1.24 (m, 2H, H_b or H_c), 1.06–1.01 (m, 2H, H_b or H_c); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 193.27 (C1), 185.50 (C4), 134.67 (C6), {129.06, 128.21, 127.77} (C7, C8, and C9), 56.51 (C5), 22.75 (C2), 11.88 (C3). HRMS (ESI-TOF) m/z calcd. for $C_{19}H_{19}ONNaS_2$ $[M + Na]^+$ 364.08003, found 364.07920.

dibenzylcarbamothioic 3-(methylthio)propanoic thioanhydride (**7u**)



7u

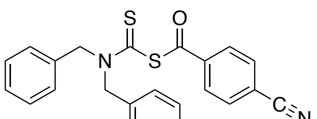
for ^{1}H NMR 

for ^{13}C NMR 

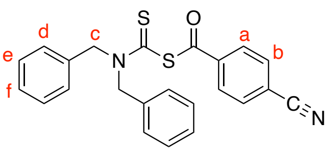
The reaction was performed according to the general procedure using 3-(methylthio)propanoyl chloride (116 μL, 2.00 mmol). The reaction time was 1 h and the obtained crude mixture was purified by silica gel column chromatography using hexane/EtOAc = 20/1 as an eluent to give **7u** as pale brown sticky oil (141 mg, 19% yield).

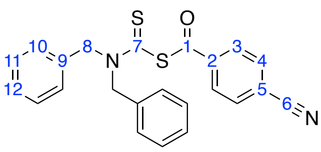
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38–7.25 (m, 10H, H_e–H_g), 5.09 (s, 4H, H_d) 2.95–2.91 (m, 2H, H_a), 2.82–2.78 (m, 2H, H_b), 2.09 (s, 3H, H_c); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 191.74 (C1), 184.80 (C5), 134.59 (C7), 129.08 (C8 or C9), 128.25 (C10), 127.74 (C8 or C9), 56.58 (C6), 43.61 (C2), 29.36 (C3), 15.77 (C4). We could not obtain the corresponding HRMS spectra of **7u** in EI- nor ESI-MS analyses probably due to the lability of **7u** in ionized form.

dibenzylcarbamothioic 3-(methylthio)propanoic thioanhydride (**7v**)



7v

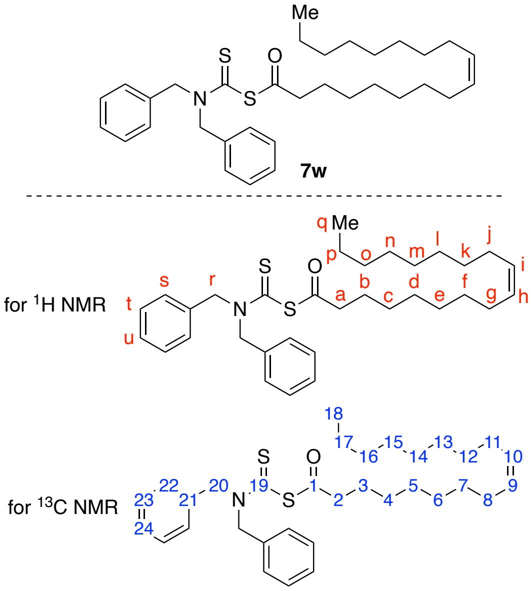
for ^{1}H NMR 

for ^{13}C NMR 

The reaction was performed according to the general procedure using 4-cyanobenzoyl chloride (331 mg, 2.00 mmol). The reaction time was 30 min and the obtained crude mixture was purified by silica gel column chromatography using hexane/EtOAc = 10/1 as an eluent to give **7v** as pale brown sticky oil (201 mg, 25% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, 2H, $^{3}J_{H–H}$ = 8.4 Hz, H_b), 7.77 (d, 2H, $^{3}J_{H–H}$ = 8.4 Hz, H_a), 7.43–7.30 (m, 10H, H_d–H_f), 5.14 (s, 4H, H_c); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 185.28 (C1), 183.31 (C7), {138.95, 134.37, 132.85, 129.15, 128.38, 128.30, 127.73, 117.62, 117.50} (C2, C3, C4, C5, C6, C9, C10, C11, and C12), 56.80 (C8). HRMS (ESI-TOF) m/z calcd. for $C_{23}H_{18}ON_2NaS_2$ $[M + Na]^+$ 425.07528, found 425.07461.

(Z)-dibenzylcarbamothioic oleic thioanhydride (**7w**)

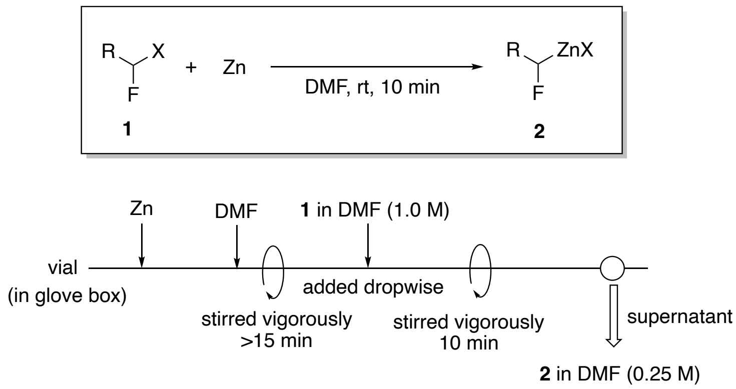


The reaction was performed according to the general procedure using oleic chloride (660 μL, 3.00 mmol). The reaction time was 1 h and the obtained crude mixture was purified by silica gel column chromatography using hexane/EtOAc = 30/1 as an eluent to give **7w** as pale brown sticky oil (484 mg, 84% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39–7.25 (m, 10H, H_s–H_u), 5.38–5.29 (m, 2H, H_h and H_i), 5.09 (s, 4H, H_r), 2.63 (t, 2H, $^3J_{H–H}$ = 7.5 Hz, H_a), 2.03–1.98 (m, 4H, H_j and H_g), 1.71–1.68 (m, 2H, H_b), 1.60–1.40 (m, 20H, H_c–H_f and H_k–H_p), 0.89 (t, 3H, $^3J_{H–H}$ = 7.0 Hz, H_q);^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 193.19 (C1), 185.64 (C19), 134.59 (C21), 130.10 (C9 or C10), 129.72 (C9 or C10), 129.01 (C22 or C23), 128.15 (C24), 127.69 (C22 or C23), 56.38 (C20), 44.07 (C2), {31.97, 31.66, 29.83, 29.69, 29.59, 29.39, 29.13, 20.04, 29.93, 27.29, 27.19, 25.40, 22.76, 14.21} (C3–C8 and C11–C18). HRMS (ESI-TOF) m/z calcd. for $C_{33}H_{47}ONNaS_2$ $[M + Na]^+$ 560.29913, found 560.29860.

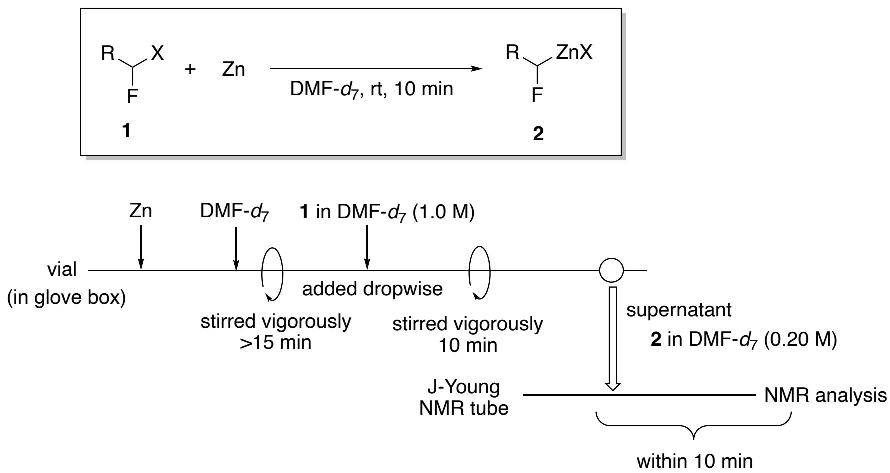
3. Preparation Zinc/Fluorine Carbenoids

3.1 General Procedure for Preparation of Zinc/Fluorine Carbenoids



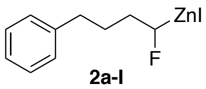
To the vial equipped with a magnetic stir bar were added activated zinc powder (2.0 equiv.) and DMF (dry, 3x mL). After the suspension was stirred vigorously at least 15 min, 1-fluoro-1-haloalkane **1** in DMF (1.00 M, x mL, x mmol) was added in dropwise to the suspension. The solution was further stirred for 10 min at room temperature and then stop stirring. The supernatant of the solution was carefully sucked by a syringe with a needle. The obtained DMF solution of **2** (0.25 M) was used for the next experiments.

3.1 General Procedure for NMR Analysis of Zinc/Fluorine Carbenoids

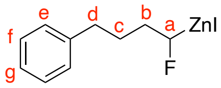


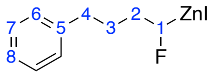
To the vial equipped with a magnetic stir bar were added activated zinc powder (13.1 mg, 0.20 mmol, 2.0 equiv.) and DMF-d_7 (dry, 0.40 mL). After the suspension was stirred vigorously at least 15 min, 1-fluoro-1-haloalkane **1** in DMF-d_7 (1.00 M, 0.10 mL, 0.10 mmol) was added in dropwise to the suspension. The solution was further stirred for 10 min at room temperature and then stop stirring. The supernatant of the solution was carefully transferred to J-Young-type NMR tube and the NMR tube was sealed tightly. The NMR tube was taken out from the glove box and rapidly used for NMR experiments.

(1-fluoro-4-phenylbutyl)zinc(II) iodide (**2a-I**)



2a-I

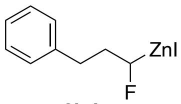
for ^{1}H NMR 

for ^{13}C NMR 

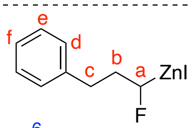
2a-I was prepared according to the general procedure for NMR analysis using **1a-I**. The relative ratio of monoalkylzinc and dialkylzinc (60:1) was determined by ^{19}F NMR using the relative integration values of the peaks at −216.64 ppm (for monoalkylzinc), −217.61 (for dialkylzinc), and −217.63 ppm (for dialkylzinc).

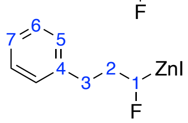
^{1}H NMR (500 MHz, DMF-d_7) δ 7.26–7.12 (m, 5H, H_e–H_g), 4.85 (ddd, 1H, $^{2}J_{H–F}$ = 46.8 Hz, $^{3}J_{H–H}$ = 7.0 Hz, $^{3}J_{H–H}$ = 7.0 Hz, H_a), 2.64–2.56 (m, 2H, H_d), 1.98–1.90 (m, 2H, H_b), 1.79–1.68 (m, 2H, H_c); ^{13}C{^{1}H} NMR (125 MHz, DMF-d_7) δ 143.65 (C5), 128.83 (C6 or C7), 128.63 (C6 or C7), 125.91 (C8), 104.44 (d, $^{1}J_{C–F}$ = 167.8 Hz, C1), 37.94 (d, $^{2}J_{C–F}$ = 17.1 Hz, C2), 36.31 (C4), 30.56 (d, $^{3}J_{C–F}$ = 7.5 Hz, C3); ^{19}F NMR (470 MHz, DMF-d_7) δ −216.64 (major, dt, $^{2}J_{H–F}$ = 46.8 Hz, $^{3}J_{H–F}$ = 29.6 Hz), −217.61 (minor, dt, $^{2}J_{H–F}$ = 47.0 Hz, $^{3}J_{H–F}$ = 30.5 Hz), −217.63 (minor, dt, $^{2}J_{H–F}$ = 47.0 Hz, $^{3}J_{H–F}$ = 30.5 Hz).

(1-fluoro-3-phenylpropyl)zinc(II) iodide (**2b-I**)



2b-I

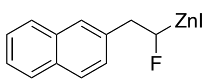
for ^{1}H NMR 

for ^{13}C NMR 

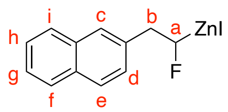
2b-I was prepared according to the general procedure for NMR analysis using **1b-I**. The relative ratio of monoalkylzinc and dialkylzinc (66:1) was determined by ^{19}F NMR using the relative integration values of the peaks at −218.40 ppm (for monoalkylzinc), −219.16 (for dialkylzinc), and −219.03 (for dialkylzinc).

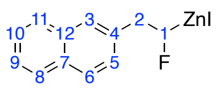
^{1}H NMR (400 MHz, DMF-d_7) δ 7.32–7.07 (m, 5H, H_d-H_f), 4.80 (ddd, 1H, $^{2}J_{H–F}$ = 46.6 Hz, $^{3}J_{H–H}$ = 7.8 Hz, $^{3}J_{H–H}$ = 5.6 Hz, H_a), 2.79–2.62 (m, 2H, H_c), 2.27–2.02 (m, 2H, H_b); ^{13}C{^{1}H} NMR (100 MHz, DMF-d_7) δ 143.86 (C4), 128.89 (C5 or C6), 128.64 (C5 or C6), 125.81 (C7), 103.67 (d, $^{1}J_{C–F}$ = 168.6, C1), 40.69 (d, $^{2}J_{C–F}$ = 17.2 Hz, C2), 34.50 (d, $^{3}J_{C–F}$ = 8.7 Hz, C3); ^{19}F NMR (367 MHz, DMF-d_7) δ −218.40 (major, ddd, $^{2}J_{H–F}$ = 46.0 Hz, $^{3}J_{H–F}$ = 30.8 Hz, $^{3}J_{H–F}$ = 25.3 Hz), −219.03 (minor, ddd, $^{2}J_{H–F}$ = 32.5 Hz, $^{3}J_{H–F}$ = 26.8 Hz, $^{3}J_{H–F}$ = 12.8 Hz), −219.16 (minor, ddd, $^{2}J_{H–F}$ = 32.5 Hz, $^{3}J_{H–F}$ = 26.8 Hz, $^{3}J_{H–F}$ = 12.8 Hz).

(1-fluoro-2-(naphthalen-2-yl)ethyl)zinc(II) iodide (**2c-I**)



2c-I

for ^{1}H NMR 

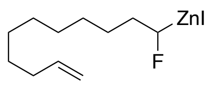
for ^{13}C NMR 

2c-I was prepared according to the general procedure for NMR analysis using **1c-I**. The relative ratio of monoalkylzinc and dialkylzinc (47:1) was determined by ^{19}F NMR using the relative integration values of the peaks at −214.83 ppm (for monoalkylzinc), −215.51 (for dialkylzinc) and, −215.31 ppm (for dialkylzinc).

^{1}H NMR (500 MHz, DMF-d_7) δ 7.83 (d, 1H, $^{3}J_{H–H}$ = 7.5 Hz, H_d or H_e), 7.79 (d, 1H, $^{3}J_{H–H}$ = 7.5 Hz, H_d or H_e), 7.77 (d, 1H, $^{3}J_{H–H}$ = 8.5 Hz, H_i or H_f), 7.75 (s, 1H, H_c), 7.46 (dd, 1H, $^{3}J_{H–H}$ = 8.5 Hz, $^{4}J_{H–H}$ = 1.5 Hz, H_i or H_f), 7.42 (ddd, 1H, $^{3}J_{H–H}$ = 8.5 Hz, $^{3}J_{H–H}$ = 8.5 Hz, $^{4}J_{H–H}$ = 1.5 Hz, H_h or H_g), 7.38 (ddd, 1H, $^{3}J_{H–H}$ = 8.5 Hz, $^{3}J_{H–H}$ = 8.5 Hz, $^{4}J_{H–H}$ = 1.5 Hz, H_h or H_g), 5.07 (ddd, 1H, $^{2}J_{H–F}$ = 46.0 Hz, $^{3}J_{H–H}$ = 7.0 Hz, $^{3}J_{H–H}$ = 7.0 Hz, H_a), 3.31 (dd, 2H, $^{3}J_{H–F}$ = 29.5 Hz, $^{3}J_{H–H}$ = 7.0 Hz, H_b); ^{13}C{^{1}H} NMR (125 MHz, DMF-d_7) δ 140.68 (d, $^{3}J_{C–F}$ = 7.5 Hz, C4), {134.08, 132.48, 129.03, 127.98, 127.86, 127.67, 127.62, 126.17, 125.39} (for C3, C5–C12), 104.01 (d, $^{1}J_{C–F}$ = 173.4 Hz, C1), 44.28 (d, $^{2}J_{C–F}$ = 17.8 Hz, C2); ^{19}F NMR (470 MHz, DMF-d_7) δ −214.83 (major, dt, $^{2}J_{H–F}$ = 46.0 Hz,

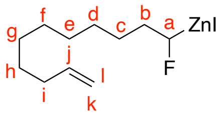
$^3J_{H–F}$ = 29.1 Hz), −215.31 (minor, ddd, $^2J_{H–F}$ = 46.6 Hz, $^3J_{H–F}$ = 32.8 Hz, $^3J_{H–F}$ = 27.8 Hz), −215.51 (minor, ddd, $^2J_{H–F}$ = 46.5 Hz, $^3J_{H–F}$ = 32.9 Hz, $^3J_{H–F}$ = 28.7 Hz).

(1-fluoroundec-10-en-1-yl)zinc(II) iodide (**2d-I**)

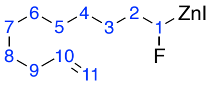


2d-I

for ^{1}H NMR



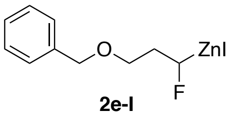
for ^{13}C NMR



2d-I was prepared according to the general procedure for NMR analysis using **1d-I**. The relative ratio of monoalkylzinc and dialkylzinc (90:1) was determined by ^{19}F NMR using the relative integration values of the peaks at −216.31 ppm (for monoalkylzinc), −217.03 (for dialkylzinc) and, −217.03 ppm (for dialkylzinc).

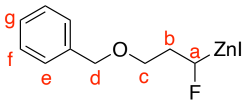
^{1}H NMR (400 MHz, DMF-d_7) δ 5.81–5.70 (m, 1H, H$_j$), 4.93 (d, 1H, $^2J_{H–H}$ = 4.3 Hz, H$_k$), 4,87–4.84 (m, 1H, H$_l$), 4.76 (ddt, 1H, $^2J_{H–F}$ = 47.0 Hz, $^2J_{H–H}$ = 1.2 Hz, $^3J_{H–H}$ = 7 Hz, H$_a$), 1.97 (dt, 2H, $^3J_{H–H}$ = 6.8 Hz, $^3J_{H–H}$ = 5.6 Hz, H$_i$), 1.92-1.77 (m, 2H, H$_b$), 1.38–1.22 (m, 12H, H$_c$-H$_g$); ^{13}C{^{1}H} NMR (100 MHz, DMF-d_7) δ 139.56 (C10), 114.49 (C11), 104.61 (d, $^1J_{C–F}$ = 167.7 Hz, C1), 38.38 (C2), 38.21 (C9), {34.05, 30.11, 29.83, 29.47, 29.26} (C4, C5, C6, C7 and C8), 28.36 (d, $^3J_{C–F}$ = 7.7 Hz, C3); ^{19}F NMR (367 MHz, DMF-d_7) δ −216.31 (major, dt, $^2J_{H–F}$ = 45.1 Hz, $^3J_{F–H}$ = 29.0 Hz), −217.03 (minor, dt, $^2J_{F–H}$ = 45.1 Hz, $^3J_{F–H}$ = 29.5 Hz), −217.03 (minor, dt, $^2J_{F–H}$ = 45.1 Hz, $^3J_{F–H}$ = 29.5 Hz).

(3-(benzyloxy)-1-fluoropropyl)zinc(II) iodide (**2e-I**)

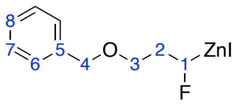


2e-I

for ^{1}H NMR



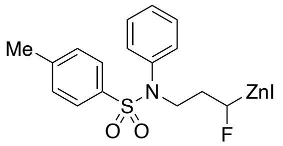
for ^{13}C NMR



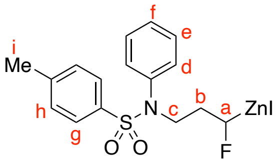
2e-I was prepared according to the general procedure for NMR analysis using **1e-I**. The relative ratio of monoalkylzinc and dialkylzinc (22:1) was determined by ^{19}F NMR using the relative integration values of the peaks at ppm −220.52 (for monoalkylzinc), −221.87ppm (for dialkylzinc), and −222.02 ppm (for dialkylzinc).

^{1}H NMR (400 MHz, DMF-d_7) δ 7.30–7.20 (m, 5H, H$_e$–H$_g$), 4.88 (ddd, 1H, $^2J_{H–F}$ = 46.9 Hz, $^3J_{H–H}$ = 7.3 Hz, $^3J_{H–H}$ = 6.0 Hz, H$_a$), 4.45 (d, 1H, $^2J_{H–H}$ = 12.0 Hz, H$_d$), 4.43 (d, 1H, $^2J_{H–H}$ = 12.0 Hz, H$_d$), 3.68–3.50 (m, 2H, H$_c$), 2.23–2.05 (m, 2H, H$_b$); ^{13}C{^{1}H} NMR (100 MHz, DMF-d_7) δ 139.83 (C5), 128.62 (C6 or C7), 127.89 (C6 or C7), 127.64 (C8), 100.89 (d, $^1J_{C–F}$ =167.0 Hz, C1), 72.71 (C4), 69.70 (d, $^3J_{C–F}$ =6.8 Hz, C3), 38.28 (d, $^2J_{C–F}$ =17.2 Hz, C2); ^{19}F NMR (367 MHz, DMF-d_7) δ −220.52 (major, ddd, $^2J_{H–F}$ = 45.8 Hz, $^3J_{F–H}$ = 33.1 Hz, $^3J_{F–H}$ = 28.9 Hz), −221.87 (minor, ddd, $^2J_{F–H}$ = 44.7 Hz, $^3J_{F–H}$ = 33.5 Hz, $^3J_{F–H}$ = 33.5 Hz), −222.02 (minor, ddd, $^2J_{F–H}$ = 46.1 Hz, $^3J_{F–H}$ = 34.2 Hz, $^3J_{F–H}$ = 32.8 Hz)

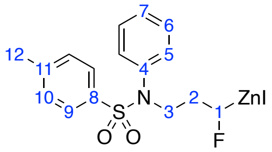
(1-fluoro-3-((4-methyl-*N*-phenylphenyl)sulfonamido)propyl)zinc(II) iodide (**2f-I**)



2f-I



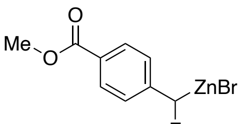
for ^{1}H NMR



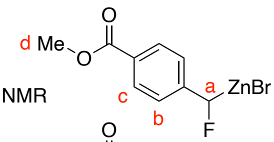
for ^{13}C NMR

2f-I was prepared according to the general procedure for NMR analysis using **1f-I**. The relative ratio of monoalkylzinc and dialkylzinc (26:1) was determined by ^{19}F NMR using the relative integration values of the peaks at −221.0 ppm (for monoalkylzinc) and −221.76–−222.07 ppm (for dialkylzinc). ^{1}H NMR (500 MHz, DMF-d_7) δ 7.44 (d, 2H, $^3J_{H–H}$ = 8.4 Hz, H$_g$), 7.35 (d, 2H, $^3J_{H–H}$ = 8.4 Hz, H$_h$), 7.32–7.25 (m, 3H, H$_e$ and H$_f$), 7.06–7.05 (m, 2H, H$_d$), 4.78 (ddd, 1H, $^2J_{H–F}$ = 46.5 Hz, $^3J_{H–H}$ = 7.5 Hz, $^3J_{H–H}$ = 5.0 Hz, H$_a$), 3.80 (ddd, 1H, $^2J_{H–H}$ = 10.5 Hz, $^3J_{H–H}$ = 7.3 Hz, $^3J_{H–H}$ = 4.8 Hz, H$_c$), 3.72 (ddd, 1H, $^2J_{H–H}$ = 10.5 Hz, $^3J_{H–H}$ = 7.5 Hz, $^3J_{H–H}$ = 5.2 Hz, H$_c$), 2.36 (s, 3H, H$_i$), 2.01–1.87 (m, 2H, H$_b$); ^{13}C{^{1}H} NMR (125 MHz, DMF-d_7) δ 143.97 (C8), 140.15 (C4), 136.12 (C11), {130.08, 129.34, 129.06, 128.03, 127.99}(for C5, C6, C7, C9, C10), 101.06 (d, $^1J_{C–F}$ =168.0 Hz, C1), 49.97 (d, $^3J_{C–F}$ =6.6 Hz, C3), 37.26 (d, $^2J_{C–F}$ =17.4 Hz, C2); ^{19}F NMR (470 MHz, DMF-d_7) δ −221.03 (major, dt, $^2J_{H–F}$ = 46.5 Hz, $^3J_{H–F}$ = 32.0 Hz), −221.76–−222.07 (m)

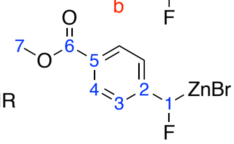
(fluoro(4-(methoxycarbonyl)phenyl)methyl)zinc(II) bromide (**2g-Br**)



2g-Br



for ^{1}H NMR



for ^{13}C NMR

2g-Br was prepared according to the general procedure for NMR analysis using **1g-Br**. The relative ratio of monoalkylzinc and dialkylzinc (5.6:1) was determined by ^{1}H NMR using the relative integration values of the peaks at 7.07 ppm (for monoalkylzinc) and 6.92 ppm (for dialkylzinc).

^{1}H NMR (400 MHz, DMF-d_7) (data for monoalkylzinc) δ 7.76 (d, 2H, $^3J_{H–H}$ = 8.4 Hz, H$_c$), 7.07 (d, 2H, $^3J_{H–H}$ = 8.4 Hz, H$_b$), 5.97 (d, $^2J_{H–F}$ = 47.2 Hz, H$_a$), 3.78 (s, 3H, H$_d$); ^{13}C{^{1}H} NMR (100 MHz, DMF-d_7) δ 167.20 (C6), 157.59 (d, $^2J_{C–F}$ = 10.6 Hz, C2), 129.51 (C4), 123.72 (C5), 120.15 (d, $^2J_{C–F}$ =11.5 Hz, C2), 103.04 (d, $^1J_{C–F}$ =183.0 Hz, C1), 51.64 (C7); ^{19}F NMR (376 MHz, DMF-d_7) δ −224.42 (major, d, $^2J_{H–F}$ = 45.51 Hz), −224.47 (minor, d, $^2J_{H–F}$ = 46.61 Hz), −224.60 (minor, d, $^2J_{H–F}$ = 48.76 Hz).

4. Computational Studies

4.1 General Information of the computational studies

The conformational search in this study was conducted by molecular mechanics simulation using Monte-Carlo Multiple Minimum (MCMM) method (MacroModel in Material Science Suite 2019-4, Force Field: OPLS4). Geometry optimization of obtained conformers was performed by density functional theory (DFT) with M06-2X functionals as implemented in Gaussian 16. Computational time was generously provided by the supercomputer system at the information initiative center of Hokkaido University.

4.2 Detailed computational methods for conformational searches

Firstly, an optimized structure of Zn/F carbenoid **2a-I•2DMF** was generated by DFT calculation (optimization and frequency calculations) using M06-2x functional with the 6-31G(d) basis set for H, C, N, O, F, Zn elements and LANL2DZ pseudopotential for I. Based on the structure, an input structure of **2a-I•2DMF** for conformational search was built in Material Science Suite. Conformational searches were performed using MCMM method torsional sampling. For conformational searches, OPLS4 force field was used under no solvent condition. Given the insufficiency of generic force fields in accurately estimating the geometry around the zinc atom, constrained conformational searches were conducted on the input structure using substructure capability to freeze 5 core atoms (depicted in blue in Figure S1) while allowing all other atoms to freely adopt energetically accessible conformations. Minimization to convergence was performed using Polak-Ribier Conjugate Gradient (PRCG) method with a threshold of 0.1 after 1000 maximum iterations. Intermediate sampling with retaining mirror-image conformations was performed with a maximum of 200 steps and 100 steps per rotatable bond. To eliminate the generation of similar conformational isomers, torsional sampling was performed with root-mean-square deviation (RMSD) cutoff 2 Å. Considering the inability of the force field to accurately estimate relative conformer energies, a large energy window for saving structures of 42.0 kJ/mol (10.04 kcal/mol) was used. Under the conditions for conformational search, 15 conformational isomers of **2a-I•2DMF** were obtained. The conformational search in same procedure were conducted for **2a'•2DMF** to give 23 conformational isomers of **2a'•2DMF**. For ease, calculation of only one diastereomer **2a'•2DMF** with (*S*,*R*) absolute configuration was performed.

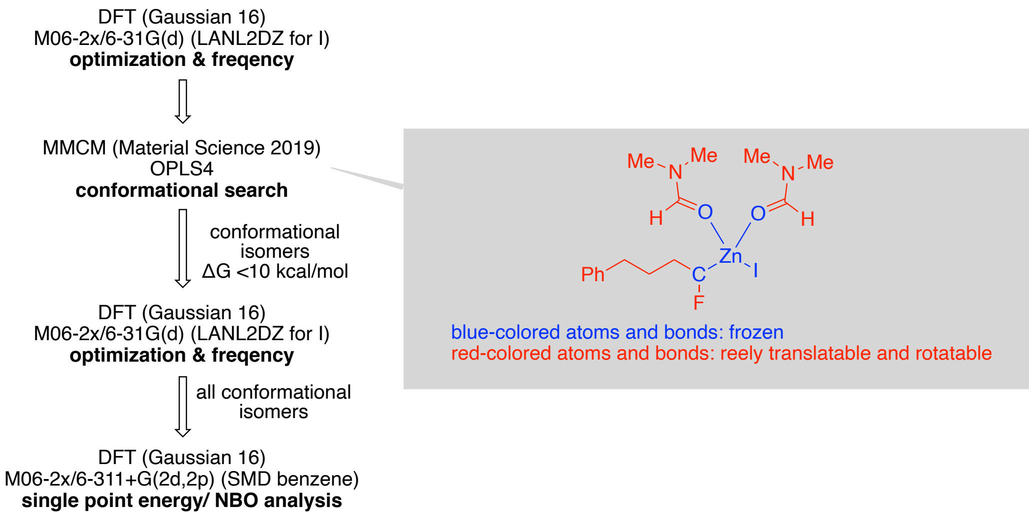


Figure S1. Schematic overview of the conformational searches and evaluation of the relative energies.

4.2 Detailed computational methods for DFT calculations

Geometry optimization calculation of all obtained conformers was performed at the M06-2x/6-31G(d) basis set for H, C, N, O, F, Zn elements and LANL2DZ pseudopotential for I under the condition of tight SCF convergence criteria (scf = tight) and ultrafine integration (int=grid=ultrafine). After optimization of structures, frequency calculations were performed at the same level of the theory to confirm that the obtained structure were stationary point (no imaginary frequencies). Thermal corrections to the Gibbs energy at 278.15 K (25 °C) were calculated by frequency calculation. The single-point energy calculations were performed at the M06-2x/6-311+G(2d,2p) basis set for H, C, N, O, F, Zn elements and SDD pseudopotential for I with solvation in DMF using solvation model based on density (SMD) model. Detailed relative energies and structures of the obtained stable conformers of **2a-I•2DMF** and **2a'•2DMF** are summarized in Table S1 and S2, respectively.

Table S1. Summary of the conformational searches and evaluation of the relative energies of **2a-I•2DMF**.

conformer No.	ΔG [kcal/mol]	Order of relative energy	Eel (Hartree)	E (thermal) (kcal/mol)	S (cal/mol/K)	solvation energy (kcal/mol)	bond length (Å) C1–F	bond length (Å) C1–H	bond length (Å) C1–Zn	bond length (Å) Zn••F	bond angle (°) Zn-C1-F	bond angle (°) C2-C1-Zn	bond angle (°) Zn-C1-H1	bond angle (°) H1-C1-C2	sum of thee bond angles (°)
1	4.25	12	-2775.853215	276.757	194.443	9.92	1.43	1.10	2.01	2.87	111.9	120.6	105.0	106.1	331.8
2	0.00	1	-2775.854374	276.42	205.133	10.41	1.44	1.10	2.02	2.81	107.9	116.4	112.1	108.5	337.0
3	1.00	4	-2775.860552	276.41	188.731	8.8	1.44	1.10	2.03	2.83	108.2	119.6	109.4	107.9	336.9
4	2.46	7	-2775.855436	276.513	194.959	9.22	1.44	1.10	2.02	2.81	107.5	115.2	113.8	108.9	337.9
5	3.68	11	-2775.854469	276.621	193.28	9.86	1.43	1.10	2.02	2.78	105.8	116.9	113.9	108.1	338.9
6	2.98	9	-2775.849738	276.672	205.729	10.6	1.43	1.10	2.00	2.79	107.1	115.6	112.8	109.1	337.5
7	4.59	13	-2775.850194	276.579	199.055	10.49	1.42	1.10	2.01	2.85	111.3	117.3	107.7	107.4	332.5
8	0.58	2	-2775.85749	276.56	197.082	9.86	1.42	1.10	2.02	2.90	114.1	110.0	111.1	108.1	329.3
9	0.80	3	-2775.854121	276.401	202.915	10.42	1.43	1.10	2.02	2.81	108.1	116.1	112.5	103.4	332.0
10	1.74	6	-2775.855773	276.534	196.746	10.02	1.42	1.10	2.01	2.83	110.2	118.2	108.8	107.0	334.0
11	5.27	14	-2775.851675	276.784	194.364	9.47	1.44	1.10	2.01	2.78	106.5	115.2	113.4	108.6	337.1
12	1.57	5	-2775.856821	276.832	196.094	10.23	1.43	1.10	2.02	2.87	111.9	120.6	105.1	106.7	332.3
13	6.58	15	-2775.845618	276.508	201.785	9.94	1.44	1.10	2.00	2.82	109.0	118.6	108.5	109.8	336.9
14	3.51	10	-2775.853192	276.631	196.566	9.53	1.43	1.10	2.01	2.85	110.3	120.7	105.8	108.0	334.5
15	2.53	8	-2775.850516	276.405	204.718	10.22	1.44	1.10	2.01	2.81	108.0	116.6	112.3	108.0	336.9
						Stand. Dev.	0.00699	0.001438	0.007218	0.03537	2.357831	2.783062	3.181449	1.515778	2.883955
						Var.	4.89E-05	2.07E-06	5.21E-05	0.001251	5.559368	7.745437	10.12162	2.297584	8.317194

Table S2. Summary of the conformational searches and evaluation of the relative energies of **2a'•2DMF**.

conformer No.	ΔG [kcal/mol]	Order of relative energy	Eel (Hartree)	E (thermal) (kcal/mol)	S (cal/mol/K)	solvation energy (kcal/mol)	bond length (Å) C1–F	bond length (Å) C1–H	bond length (Å) C1–Zn	bond length (Å) Zn••F	bond angle (°) Zn-C1-F	bond angle (°) C2-C1-Zn	bond angle (°) Zn-C1-H1	bond angle (°) H1-C1-C2	sum of thee bond angles (°)
1	5.69	10	-3252.469306	406.141	229.949	11.36	1.43	1.10	2.04	2.90	112.5	115.1	110.3	107.4	332.7
							1.44	1.10	2.05	2.91	117.7	113.5	112.8	108.5	334.8
2	7.06	15	-3252.46408	406.195	236.548	12.00	1.42	1.10	2.03	2.91	114.1	115.8	107.5	108.5	331.9
							1.44	1.10	2.04	2.92	112.9	114.4	110.7	107.9	333.0
3	4.02	2	-3252.468938	406.245	236.671	12.22	1.43	1.10	2.04	2.90	111.9	113.2	112.6	108.1	333.9
							1.43	1.10	2.03	2.87	110.5	116.2	111.6	107.0	334.8
4	4.60	4	-3252.468391	405.996	235.046	11.85	1.43	1.10	2.03	2.84	108.8	117.5	112.3	107.0	336.9
							1.44	1.10	2.05	2.91	111.8	112.9	113.3	108.4	334.6
5	4.94	8	-3252.466471	405.873	237.531	11.63	1.44	1.10	2.04	2.80	105.8	110.8	120.0	108.9	339.7
							1.44	1.10	2.03	2.83	108.1	114.8	114.4	108.1	337.2
6	4.65	6	-3252.469989	405.822	230.923	11.07	1.44	1.10	2.05	2.91	111.8	111.1	115.2	107.4	333.8
							1.43	1.10	2.03	2.89	111.9	111.8	113.1	107.9	332.8
7	6.39	11	-3252.469485	406.278	227.704	12.35	1.45	1.10	2.05	2.88	109.6	118.7	109.7	107.0	335.4
							1.42	1.10	2.03	2.83	108.5	109.1	118.4	108.5	336.0
8	4.87	7	-3252.466005	405.927	238.945	11.86	1.44	1.10	2.04	2.81	106.3	117.7	113.6	107.9	339.2
							1.45	1.10	2.04	2.72	101.3	117.4	118.1	108.7	344.2
9	6.53	12	-3252.467521	406.172	231.007	11.13	1.44	1.10	2.04	2.75	103.1	116.5	117.7	108.6	342.7
							1.44	1.10	2.03	2.78	105.3	117.8	114.7	108.5	340.9
10	6.80	13	-3252.464248	405.924	236.15	11.52	1.44	1.10	2.03	2.81	107.4	111.9	118.0	108.1	338.1
							1.44	1.10	2.03	2.80	106.6	109.8	120.2	109.1	339.1
11	4.20	3	-3252.462533	405.972	248.652	13.25	1.42	1.10	2.03	2.83	108.6	115.1	113.6	107.3	336.0
							1.44	1.10	2.05	2.92	112.7	114.7	111.0	107.9	333.5
12	7.20	17	-3252.465085	406.164	233.866	12.19	1.45	1.10	2.05	2.95	113.7	115.7	109.2	106.6	331.5
							1.43	1.10	2.03	2.84	108.7	118.2	111.8	106.9	336.9
13	7.12	16	-3252.463611	405.967	236.544	12.04	1.44	1.10	2.04	2.85	109.0	116.9	112.0	107.6	336.5
							1.44	1.10	2.03	2.77	104.2	112.7	119.4	108.5	340.6
14	4.01	1	-3252.465822	405.712	241.494	12.83	1.44	1.10	2.04	2.78	105.1	115.7	116.6	107.6	340.0
							1.42	1.10	2.02	2.82	109.3	114.8	113.1	107.5	335.4
15	6.88	14	-3252.465134	406.166	234.823	11.82	1.44	1.10	2.04	2.88	110.7	111.2	115.7	107.9	334.8
							1.43	1.10	2.03	2.85	109.5	117.1	112.0	107.0	336.1
16	8.10	18	-3252.463425	405.999	233.777	10.87	1.44	1.10	2.03	2.80	105.9	111.5	119.3	108.7	339.5
							1.44	1.10	2.02	2.75	103.9	110.9	120.0	109.0	340.0
17	5.07	9	-3252.468074	406.219	234.88	12.23	1.42	1.10	2.03	2.87	111.3	113.3	112.3	107.4	333.0
							1.44	1.10	2.06	2.89	110.3	126.3	103.8	105.5	335.6
18	4.61	5	-3252.464938	406.076	242.547	13.25	1.43	1.10	2.04	2.87	110.9	118.6	109.5	106.7	334.8
							1.43	1.10	2.03	2.87	111.1	113.7	113.3	107.7	334.7
19	8.39	19	-3252.459847	405.986	240.282	11.50	1.44	1.10	2.03	2.84	108.2	111.7	116.9	109.2	337.7
							1.43	1.10	2.03	2.84	109.1	114.3	113.7	107.9	335.9
20	10.52	23	-3252.461693	406.384	230.591	11.20	1.45	1.10	2.04	2.81	106.0	113.8	116.4	107.5	337.7
							1.44	1.10	2.04	2.78	104.8	118.7	113.4	108.8	340.9
21	8.99	20	-3252.463221	406.295	232.215	11.95	1.44	1.10	2.05	2.79	104.5	122.7	110.9	106.8	340.4
							1.46	1.10	2.06	2.75	101.6	128.4	108.0	106.3	342.7
22	9.47	22	-3252.463166	405.978	229.637	11.12	1.44	1.10	2.03	2.75	103.7	113.0	119.7	108.6	341.3
							1.44	1.98	2.04	2.83	107.9	116.4	113.0	107.5	336.9
23	9.26	21	-3252.460208	406.274	237.582	12.45	1.44	1.10	2.04	2.83	107.7	112.4	116.4	108.8	337.7
							1.45	1.10	2.04	2.76	103.1	123.6	110.7	106.8	341.1
						Stand. Dev.	0.00853	0.13016	0.00890	0.05603	3.59215	4.01771	3.73457	0.82878	3.16148
						Var.	7.28129E-05	0.016942	7.92E-05	0.003139	12.90352	16.14196	13.94699	0.68687	9.994927

ΔG = G(2a')-2G(2a-I•2DMF)+G(ZnI2•2DMF)

4.3 Structures of the most stable conformer of 2a-I•2DMF and 2a'•2DMF

The most stable conformer of **2a-I•2DMF** and **2a'•2DMF** are depicted in Figure S2 and Figure 3, respectively.

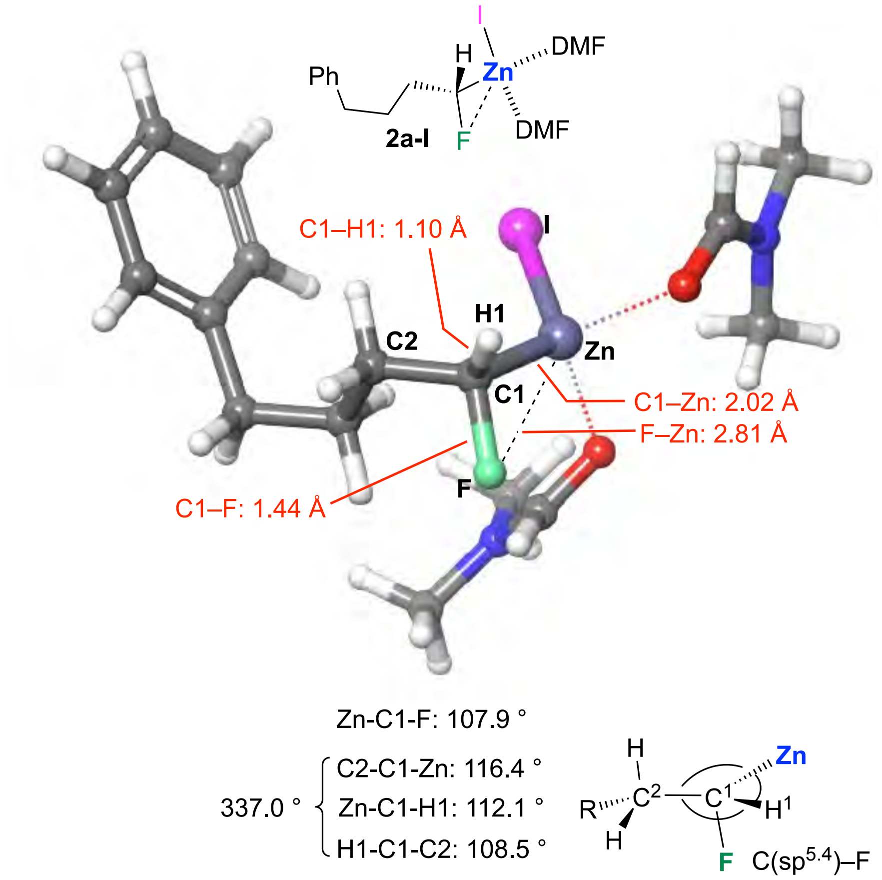


Figure S2. The most stable conformer of **2a-I•2DMF** and the selected bond length and bond angles.

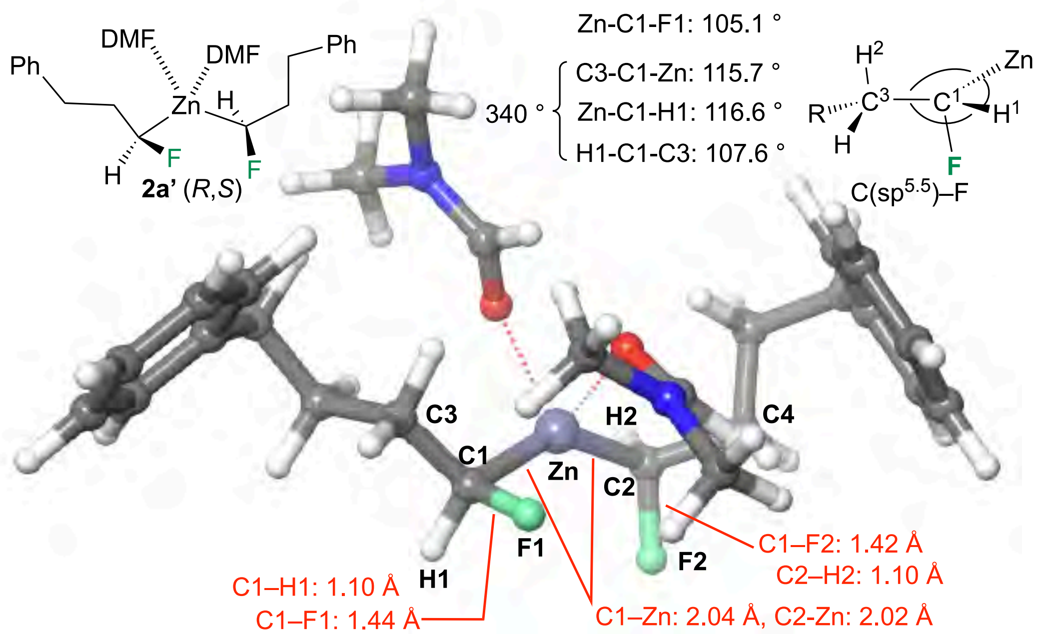
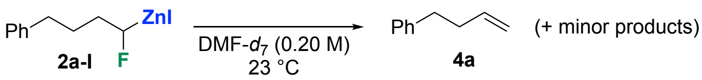


Figure S3. The most stable conformer of **2a'•2DMF** and the selected bond length and bond angles.

5. Kinetic Analysis of Zinc/Fluorine Carbenoids Using NMR spectroscopy

5.1 Decay of 2a-I at 0.20 M in DMF (Figure 7, a)



To the vial equipped with a magnetic stir bar were added activated zinc powder (13.1 mg, 0.20 mmol, 2.0 equiv.) and DMF-d_7 (dry, 0.30 mL). After the suspension was stirred vigorously at least 15 min, **1a-I** in DMF-d_7 (0.50 M, 0.20 mL, 0.10 mmol) was added in dropwise to the suspension. The solution was further stirred for 10 min at room temperature and then stop stirring. The supernatant of the solution was carefully transferred to J-Young-type NMR tube and the NMR tube was sealed tightly. The time of transferring to NMR tube was settled as t = 0. The NMR tube was taken out from the glove box and rapidly used for NMR experiments. The **2a-I** was analyzed by ^{1}H NMR spectroscopy at the specified time. The conversion of **2a-I** was determined by the relative integration values of the peaks at 4.80 ppm (for **2a-I**) and 7.96 ppm (for DMF). The results were summarized in Table S3 and the selected NMR spectra were shown in Figure S4.

Table S3. Decay Profiles of 2a-I in DMF-d_7 (0.20 M at 23 °C)

Time [min]	Relative integration value
31	1.000
46	0.993
74	0.980
104	0.971
134	0.953
164	0.929
194	0.923
224	0.880
254	0.839
284	0.824
314	0.763
344	0.746
374	0.642
404	0.631
434	0.567

Time [min]	Relative integration value
464	0.562
494	0.505
524	0.502
554	0.473
584	0.426
614	0.377
627	0.368
629	0.361
634	0.369
643	0.368
733	0.242
803	0.193
815	0.194
896	0.146
1012	0.077

Time [min]	Relative integration value
1126	0.061
2296	0.002

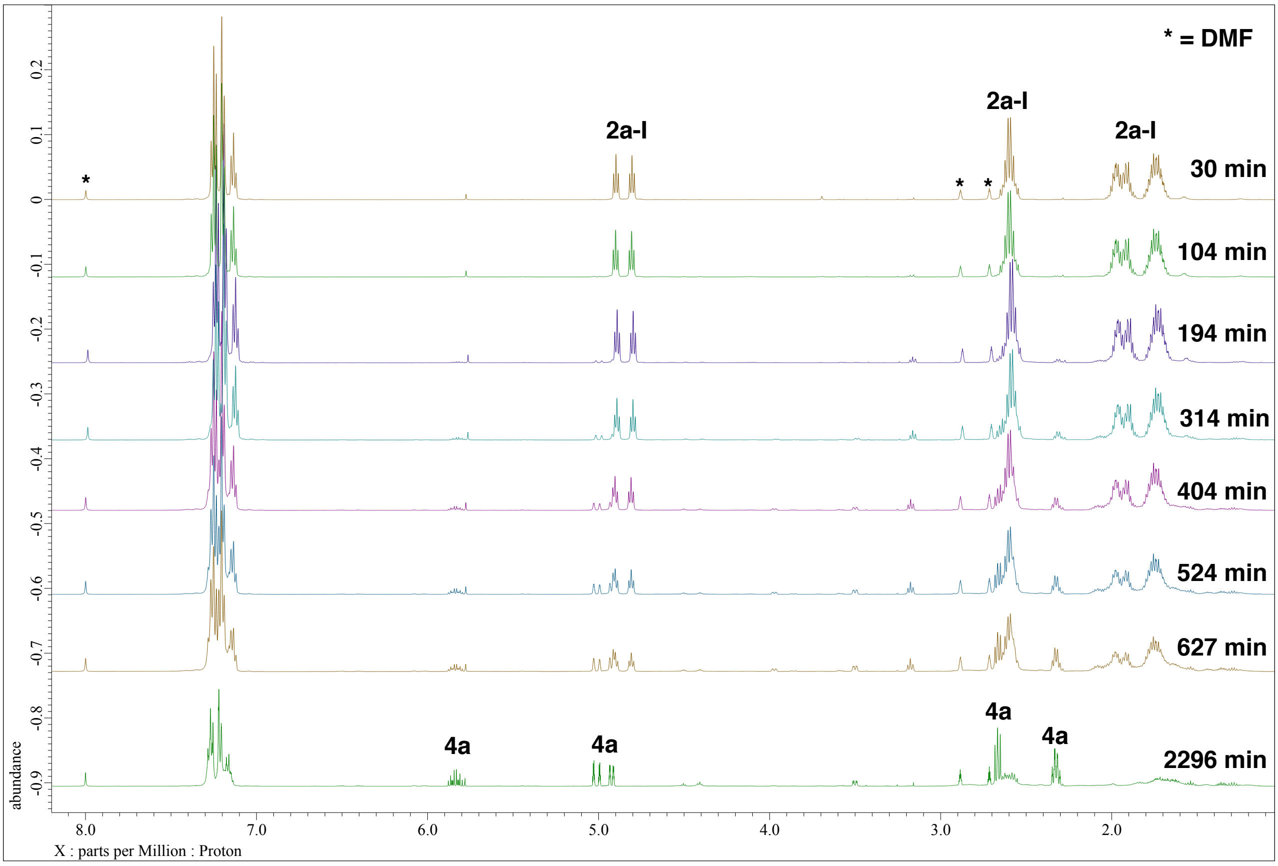
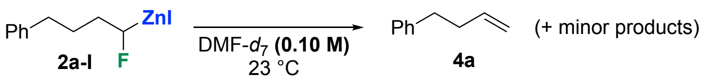


Figure S4. Selected NMR spectra of **2a-I** in DMF-d_7 (0.20 M at 23 °C) for a typical *in situ* ^{1}H NMR experiments.

5.2 Decay of 2a-I at 0.10 M in DMF (Figure 7, a)



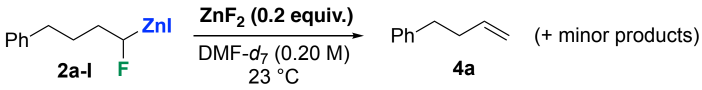
To the vial equipped with a magnetic stir bar were added activated zinc powder (6.6 mg, 0.1 mmol, 2.0 equiv.) and DMF-d_7 (dry, 0.45 mL). After the suspension was stirred vigorously at least 15 min, **1a-I** in DMF-d_7 (1.00 M, 0.05 mL, 0.05 mmol) was added in dropwise to the suspension. The solution was further stirred for 10 min at room temperature and then stop stirring. The supernatant of the solution was carefully transferred to J-Young-type NMR tube and the NMR tube was sealed tightly. The time of transferring to NMR tube was settled as t = 0. The NMR tube was taken out from the glove box and rapidly used for NMR experiments. The **2a-I** was analyzed by ^{1}H NMR spectroscopy at the specified time. The conversion of **2a-I** was determined by the relative integration values of the peaks at 4.80 ppm (for **2a-I**) and 7.96 ppm (for DMF). The results were summarized in Table S4.

Table S4. Decay Profiles of **2a-I** in DMF-d_7 (0.10 M at 23 °C)

Time [min]	Relative integration value
20	1.000
53	0.986
70	0.973
128	1.007
167	1.000
236	1.000
294	0.918
353	0.904
411	0.822
469	0.808
528	0.774
586	0.726
645	0.678
706	0.651
764	0.630

Time [min]	Relative integration value
823	0.603
905	0.555
968	0.555
1068	0.507
1132	0.500
1224	0.425
1279	0.418
1410	0.404
1558	0.336
1716	0.253
1840	0.240
1952	0.226
2000	0.171

5.3 Decay of 2a-I in the presence of ZnF_2 at 0.20 M in DMF (Figure 7, b)



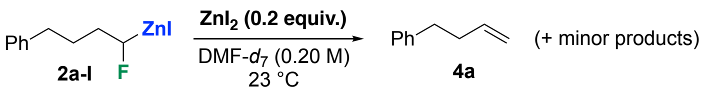
To the vial equipped with a magnetic stir bar were added activated zinc powder (13.1 mg, 0.20 mmol, 2.0 equiv.) and DMF-d_7 (dry, 0.40 mL). After the suspension was stirred vigorously at least 15 min, **1a-I** in DMF (1.00 M, 0.10 mL, 0.10 mmol) was added in dropwise to the suspension. The solution was further stirred for 10 min at room temperature and then stop stirring. The supernatant of the solution was carefully transferred to J-Young-type NMR tube. To the NMR tube was added ZnF_2 (2.07 mg, 0.02 mmol, 0.2 equiv.) before the NMR tube was sealed. The time of transferring to NMR tube was settled as t = 0. The NMR tube was taken out from the glove box and rapidly used for NMR experiments. The **2a-I** was analyzed by ^{1}H NMR spectroscopy at the specified time. The conversion of **2a-I** was determined by the relative integration values of the peaks at 4.80 ppm (for **2a-I**) and 7.96 ppm (for DMF). The results were summarized in Table S5.

Table S5. Decay Profiles of **2a-I** in DMF-d_7 (0.20 M at 23 °C) in the presence of ZnF_2

Time [min]	Relative integration value
17	0.994
40	1.000
69	0.974
98	0.972
127	0.922
157	0.887
186	0.835
215	0.833
244	0.828
274	0.793
303	0.717
332	0.706
361	0.641
391	0.617
420	0.606

Time [min]	Relative integration value
449	0.544
524	0.454

5.4 Decay of 2a-I in the presence of ZnI_2 at 0.20 M in DMF (Figure 7, b)

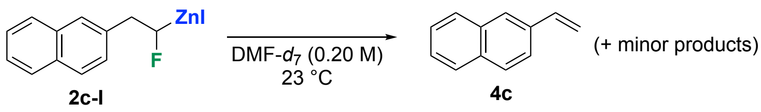


To the vial equipped with a magnetic stir bar were added activated zinc powder (13.1 mg, 0.20 mmol, 2.0 equiv.) and DMF-d_7 (dry, 0.40 mL). After the suspension was stirred vigorously at least 15 min, **1a-I** in DMF (1.00 M, 0.10 mL, 0.10 mmol) was added in dropwise to the suspension. The solution was further stirred for 10 min at room temperature and then stop stirring. The supernatant of the solution was carefully transferred to J-Young-type NMR tube. To the NMR tube was added ZnI_2 (6.38 mg, 0.02 mmol, 0.2 equiv.) before the NMR tube was sealed. The time of transferring to NMR tube was settled as t = 0. The NMR tube was taken out from the glove box and rapidly used for NMR experiments. The **2a-I** was analyzed by ^{1}H NMR spectroscopy at the specified time. The conversion of **2a-I** was determined by the relative integration values of the peaks at 4.80 ppm (for **2a-I**) and 7.96 ppm (for DMF). The results were summarized in Table S6.

Table S6. Decay Profiles of **2a-I** in DMF-d_7 (0.20 M at 23 °C) in the presence of ZnI_2

Time [min]	Relative integration value	Time [min]	Relative integration value
13	1.000	458	0.611
32	1.000	489	0.577
62	1.002	519	0.557
93	0.960	550	0.536
123	0.964	580	0.489
154	0.947	600	0.472
184	0.917	843	0.289
214	0.900		
245	0.855		
275	0.828		
306	0.781		
336	0.757		
367	0.717		
397	0.683		
428	0.658		

5.5 Decay of 2c-I at 0.20 M in DMF (Figure 7, c)

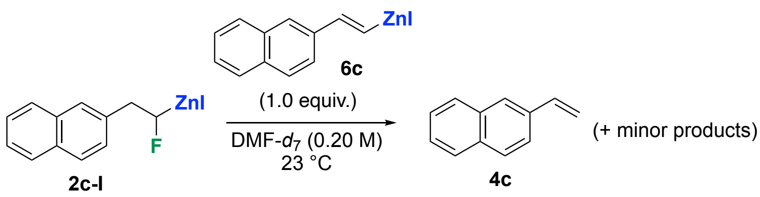


To the vial equipped with a magnetic stir bar were added activated zinc powder (13.1 mg, 0.20 mmol, 2.0 equiv.) and DMF-d_7 (dry, 0.30 mL). After the suspension was stirred vigorously at least 15 min, **1c-I** in DMF-d_7 (0.50 M, 0.20 mL, 0.10 mmol) was added in dropwise to the suspension. The solution was further stirred for 10 min at room temperature and then stop stirring. The supernatant of the solution was carefully transferred to J-Young-type NMR tube. The time of transfering to NMR tube was settled as t = 0. The NMR tube was taken out from the glove box and rapidly used for NMR experiments. The **2c-I** was analyzed by ^{1}H NMR spectroscopy at the specified time. The conversion of **2c-I** was determined by the relative integration values of the peaks at 5.11 ppm (for **2c-I**) and 5.75 ppm (dimethylamine contained in DMF-d_7). The results were summarized in Table S7.

Table S7. Decay Profiles of **2c-I** in DMF-d_7 (0.20 M at 23 °C).

Time [min]	Relative integration value
24	1.000
60	0.999
129	0.966
159	0.954
190	0.938
220	0.929
251	0.922
281	0.887
311	0.882
342	0.867
372	0.859
403	0.828
433	0.817
463	0.785
494	0.769
524	0.743
555	0.737
585	0.733
680	0.640
910	0.518
1009	0.428
1146	0.341
1260	0.314
1322	0.274
1384	0.262
1447	0.236
1509	0.225
1572	0.211
1634	0.185
1697	0.180
1759	0.175
1821	0.155
1884	0.148
1946	0.134
2009	0.124

5.6 Decay of 2c-I in the presence of vinylzinc 6c at 0.20 M in DMF (Figure 7, c)

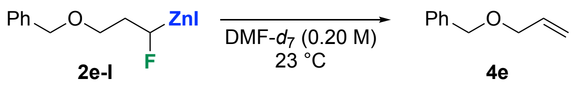


To the vial equipped with a magnetic stir bar were added activated zinc powder (13.1 mg, 0.20 mmol, 2.0 equiv.) and DMF-d_7 (dry, 0.05 mL). After the suspension was stirred vigorously at least 15 min, **1c-I** in DMF-d_7 (0.50 M, 0.20 mL, 0.10 mmol) was added in dropwise to the suspension. The solution was further stirred for 10 min at room temperature and then stop stirring. The supernatant of the solution was carefully transferred to J-Young-type NMR tube. To the NMR tube was added vinylzinc **6c** in DMF-d_7 (0.40 M, 0.25 ml, 0.10 mmol, 1.0 equiv.) before the NMR tube was sealed. The time of transferring to NMR tube was settled as t = 0. The NMR tube was taken out from the glove box and rapidly used for NMR experiments. The **2c-I** was analyzed by ^{1}H NMR spectroscopy at the specified time. The conversion of **2c-I** was determined by the relative integration values of the peaks at 5.11 ppm (for **2c-I**) and 5.75 ppm (dimethylamine contained in DMF-d_7). The results were summarized in Table S8.

Table S8. Decay Profiles of **2c-I** in DMF-d_7 (0.20 M at 23 °C) in the presence of vinylzinc **6c**

Time [min]	Relative integration value
7	1.000
61	0.917
120	0.867
176	0.786
231	0.701
287	0.606
343	0.524
399	0.476
455	0.378
607	0.186
748	0.105
879	0.038
1078	0.008

5.7 Decay of 2e-I at 0.20 M in DMF (Figure 8, b)

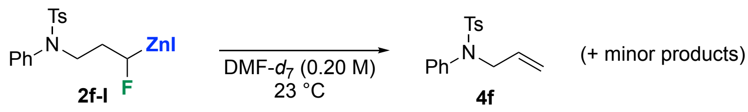


To the vial equipped with a magnetic stir bar were added activated zinc powder (13.1 mg, 0.20 mmol, 2.0 equiv.) and DMF-d_7 (dry, 0.40 mL). After the suspension was stirred vigorously at least 15 min, **1e-I** in DMF-d_7 (1.00 M, 0.10 mL, 0.10 mmol) was added in dropwise to the suspension. The solution was further stirred for 10 min at room temperature and then stop stirring. The supernatant of the solution was carefully transferred to J-Young-type NMR tube. The time of transferring to NMR tube was settled as t = 0. The NMR tube was taken out from the glove box and rapidly used for NMR experiments. The **2e-I** was analyzed by ^{1}H NMR spectroscopy at the specified time. The conversion of **a-I** was determined by the relative integration values of the peaks at 4.94 (for **2e-I**) and 7.96 ppm (for DMF). The results were summarized in Table S9.

Table S9. Decay Profiles of **2e-I** in DMF-d_7 (0.20 M at 23 °C)

Time [min]	Relative integration value	Time [min]	Relative integration value
14	1.000	814	0.317
37	0.997	870	0.273
58	0.994	927	0.239
81	0.994	980	0.202
95	1.000	1033	0.174
127	0.997	1086	0.152
159	0.975	1139	0.134
285	0.848	1193	0.112
345	0.764	1246	0.099
413	0.674	1300	0.078
517	0.584	1365	0.068
592	0.519	1488	0.047
645	0.484	1688	0.024
702	0.416	2199	0.007
758	0.370		

5.8 Decay of 2f-I at 0.20 M in DMF (Figure 8, b)

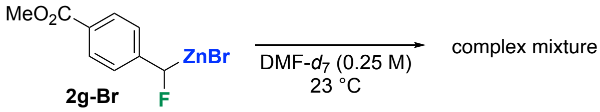


To the vial equipped with a magnetic stir bar were added activated zinc powder (13.1 mg, 0.20 mmol, 2.0 equiv.) and DMF-d_7 (dry, 0.40 mL). After the suspension was stirred vigorously at least 15 min, **1f-I** in DMF-d_7 (1.00 M, 0.10 mL, 0.10 mmol) was added in dropwise to the suspension. The solution was further stirred for 10 min at room temperature and then stop stirring. The supernatant of the solution was carefully transferred to J-Young-type NMR tube. The time of transferring to NMR tube was settled as t = 0. The NMR tube was taken out from the glove box and rapidly used for NMR experiments. The **2f-I** was analyzed by ^{1}H NMR spectroscopy at the specified time. The conversion of **2f-I** was determined by the relative integration values of the peaks at 4.82 ppm (for **2f-I**) and 7.96 ppm (for DMF). The results were summarized in Table S10.

Table S10. Decay Profiles of **2f-I** in DMF-d_7 (0.20 M at 23 °C)

Time [min]	Relative integration value
10	1.000
41	0.997
72	0.997
102	0.993
124	0.987
155	0.980
185	0.977
236	0.977
297	0.974
360	0.958
420	0.915
480	0.859
540	0.846
600	0.758
660	0.722
720	0.650
780	0.572
840	0.510
900	0.477
960	0.425
1020	0.386
1080	0.356
1140	0.314
1217	0.288
1278	0.261
1339	0.225
1400	0.203
1461	0.190
1522	0.183
1583	0.170
1644	0.160
1705	0.141
1766	0.127
1827	0.124
1888	0.111
1949	0.101
2010	0.095
2071	0.095
2123	0.088

5.9 Decay of 2g-Br at 0.20 M in DMF (Figure 8, b)



To the vial equipped with a magnetic stir bar were added activated zinc powder (26.2 mg, 0.40 mmol, 2.0 equiv.) and DMF-d_7 (dry, 0.80 mL). After the suspension was stirred vigorously at least 15 min, **1g-Br** (49.4 mg, 0.20 mmol) was added in dropwise to the suspension. The solution was further stirred for 10 min at room temperature and then stop stirring. The supernatant of the solution was carefully transferred to J-Young-type NMR tube. To the NMR tube was added 3-chloro-4-fluorotoluene (28.9 mg, 0.20 mmol, 1.0 equiv.) as an internal standard before the NMR tube was sealed. The time of transferring to NMR tube was settled as t = 0. The NMR tube was taken out from the glove box and rapidly used for NMR experiments. The **2g-Br** was analyzed by ^{1}H NMR spectroscopy at the specified time. The conversion of **2g-Br** was determined by the relative integration values of the peaks at aound −224 ppm (for **2g-Br** and **2g'**) and −116.51 ppm (for 3-chloro-4-fluorotoluene). The results were summarized in Table S11.

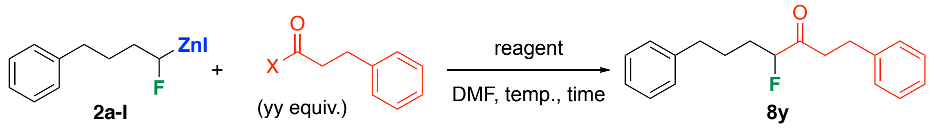
Table S11. Decay Profiles of **2g-Br** in DMF-d_7 (0.25 M at 23 °C)

Time [min]	Relative integration value
23	0.73
43	0.55
65	0.5
219	0.25
312	0.17
441	0.099

6. Optimization of the Conditions for Acylation of Zinc/Fluorine Carbenoids

General procedure: To a test tube equipped with a magnetic stir bar were added acylating reagent (0.20 mmol, 2.0 equiv.) and freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was stirred at the specified temperature, activating reagent was added to the solution. The reaction mixture was stirred for the specified time, and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8y** was determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The results were summarized in the Table S12 below.

Table S12. Optimizatioin of the conditions for acylation of Zn/F carbenoids **2**

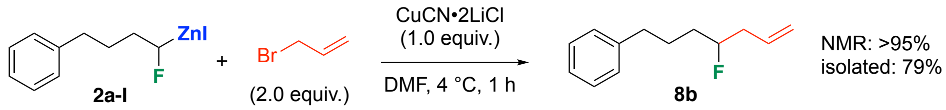


entry	reagent	X	yy	time [h]	temp. [°C]	NMR yield [%]
1	CuCN•2LiCl (1.0 equiv.)	Cl	2	1	4	40
2	CuCN•2LiCl (1.0 equiv.)	Cl	2	1	23	35
3	CuCN•2LiCl (1.0 equiv.)	Cl	5	1	4	21
4	CuCN•2LiCl (1.0 equiv.) + $AlCl_3$ (2.0 equiv.)	Cl	2	1	4	39
5	$Pd(PPh_3)_4$ (10 mol%)	Cl	2	6	4	<5
6	$PdCl_2(PPh_3)_2$ (10 mol%)	Cl	2	6	4	<5
7	$PdCl_2$/SPhos (10 mol%)	Cl	2	6	4	9
8	CuCN•2LiCl (1.0 equiv.)	SC(S)NBn_2	2	1	4	65

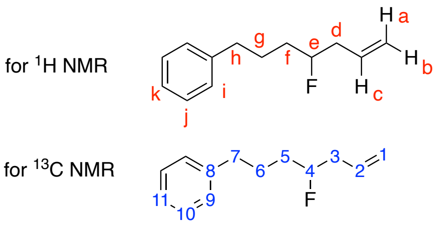
7. Procedures of Copper-Mediated Nucleophilic Monofluoroalkylation and Identification of the Products

7.1 Specific procedure and identification of the products

(4-fluorohept-6-en-1-yl)benzene (**8b**)

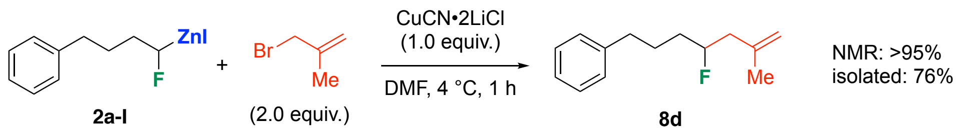


To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, allyl bromide (17.3 μL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8b** was determined to be >95% yield by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane as eluent to give **8b** as yellow oil (15.1 mg, 79% yield).



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.30–7.17 (m, 5H, H$_i$–H$_k$), (ddt, $^3J_{H\text{–}H}$ = 17.2 Hz, $^3J_{H\text{–}H}$ = 10.4 Hz, $^3J_{H\text{–}H}$ = 6.8 Hz, H$_c$), 5.13–5.08 {5.11 (dd, 1H, $^3J_{H\text{–}H}$ = 17.2 Hz, $^2J_{H\text{–}H}$ = 1.2 Hz, H$_a$), 5.10 (dd, 1H, $^3J_{H\text{–}H}$ = 10.4 Hz, $^2J_{H\text{–}H}$ = 1.2 Hz, H$_b$)}, 4.64–4.45 (m, 1H, H$_e$), 2.64 (t, 2H, $^3J_{H\text{–}H}$ = 7.4 Hz, H$_h$), 2.47–2.35 (m, 2H, H$_d$), 1.88–1.50 (m, 4H, H$_f$, H$_g$); ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 142.18 (C8), 133.43 (d, $^3J_{C\text{–}F}$ = 5.8 Hz, C2), 128.53 (C9 or C10), 128.48 (C19 or C10), 125.96 (C11), 117.92 (C1), 93.49 (d, $^1J_{C\text{–}F}$ = 170.6 Hz, C4), 39.69 (d, $^2J_{C\text{–}F}$ = 22.1 Hz, C3), 35.74 (C7), 34.29 (d, $^2J_{C\text{–}F}$ = 22.1 Hz, C5), 26.94 (d, $^3J_{C\text{–}F}$ = 3.8 Hz, C6); ^{19}F NMR (367 MHz, CDCl$_3$) δ −179.83–−180.16 (m). HRMS (EI-TOF) m/z calcd. for $C_{13}H_{17}F$ [M]$^+$ 192.13088 found 192.13130.

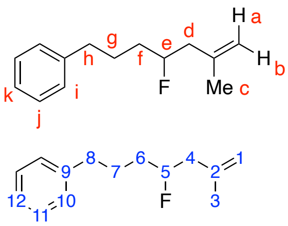
(4-fluoro-6-methylhept-6-en-1-yl)benzene (**8d**)



To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, 3-bromo-2-methylprop-1-ene (20.6 μL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8d** was determined to be >95% yield by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane as eluent to give **8d** as yellow oil (15.7 mg, 76% yield).

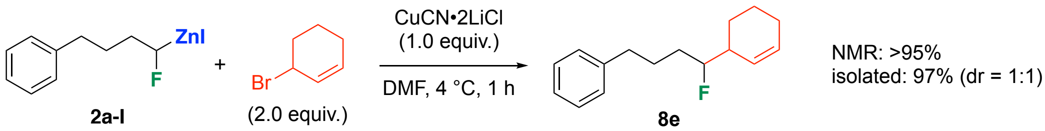
for ^{1}H NMR

for ^{13}C NMR



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.31–7.17 (m, 5H, H$_i$–H$_k$), 4.83 (br, 1H, H$_a$ or H$_b$), 4.76 (br d, 1H, $^2J_{H\text{–}H}$ = 0.8 Hz, H$_a$ or H$_b$), 4.74–4.56 (m, 1H, H$_e$), 2.65 (t, $^3J_{H\text{–}H}$ = 7.2 Hz, H$_h$), 2.37 (ddd, 1H, $^2J_{H\text{–}H}$ = 14.8 Hz, $^3J_{H\text{–}F}$ = 16.6 Hz, $^3J_{H\text{–}H}$ = 7.6 Hz, H$_d$), 2.23 (ddd, 1H, $^2J_{H\text{–}H}$ = 14.8 Hz, $^3J_{H\text{–}F}$ = 29.8 Hz, $^3J_{H\text{–}H}$ = 4.0 Hz, H$_d$), 1.88–1.55 (m, 7H, H$_c$, H$_f$, and H$_g$); ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 142.21 (C9), 141.68 (d, $^3J_{C\text{–}F}$ = 3.9 Hz, C2), 128.54 (C10 or C11), 128.48 (C10 or C11), 125.96 (C12), 113.24 (C1), 92.68 (d, $^1J_{C\text{–}F}$ = 170.6 Hz, C5), 43.61 (d, $^2J_{C\text{–}F}$ = 22.1 Hz, C4), 35.77 (C8), 34.74 (d, $^2J_{C\text{–}F}$ = 21.1 Hz, C6), 27.02 (d, $^3J_{C\text{–}F}$ = 3.9 Hz, C7), 22.90 (C3); ^{19}F NMR (367 MHz, CDCl$_3$) δ −177.69–−178.03 (m). HRMS (EI-TOF) m/z calcd. for. $C_{14}H_{19}F$ [M]$^+$ 206.14653 found 206.14711.

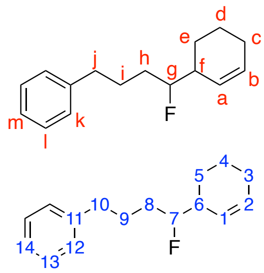
(4-(cyclohex-2-en-1-yl)-4-fluorobutyl)benzene (**8e**)



To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, 3-bromocyclohex-1-ene (23.1 µL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8e** was determined to be >95% yield by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane as eluent to give **8e** as yellow oil (22.5 mg, 97% yield, dr = 1:1).

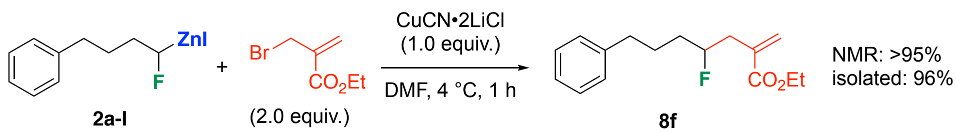
for ^{1}H NMR

for ^{13}C NMR



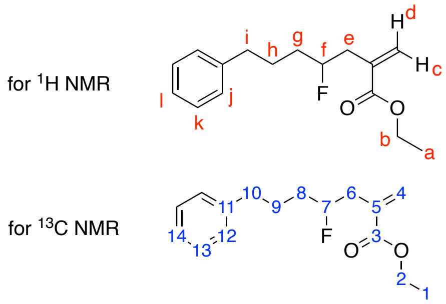
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.30–7.16 (m, 5H, H$_k$–H$_m$), 5.83–5.49 (m, 2H, H$_a$ and H$_b$), 4.43–4.20 (m, 1H, H$_g$), 2.69–2.60 (m, 2h, H$_j$), 2.38–2.30 (m, 1H, H$_f$), 2.00–1.97 (m, 2H, H$_c$), 1.90–1.12 (m, 8H, H$_d$, H$_e$, H$_h$, and H$_i$); ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 142.30 and 142.28 (C11), 130.09 and 129.17 (C2), 128.54 (C12 or C13), 128.47 (C12 or C13), 126.84 and 126.54 (d, $^3J_{C\text{–}F}$ = 6.7 Hz, C1), 125.93 (C14), 97.33 and 96.52 (d, $^1J_{C\text{–}F}$ = 170.6 Hz, C7), 40.06 and 40.03 (d, $^2J_{C\text{–}F}$ = 18.2 Hz and $^2J_{C\text{–}F}$ = 20.1 Hz, C6), 35.84 and 35.81 (C10), 32.02 and 31.88 (d, $^2J_{C\text{–}F}$ = 22.1 Hz and $^2J_{C\text{–}F}$ = 21.1 Hz, C8), 27.29 and 27.14 (d, $^3J_{C\text{–}F}$ = 2.9 Hz and $^2J_{C\text{–}F}$ = 3.8 Hz, C9), 25.26 and 25.21 (C3), 25.12 and 23.82 (d, $^3J_{C\text{–}F}$ = 4.8 Hz, C5), 21.66 and 20.90 (C4); ^{19}F NMR (367 MHz, CDCl$_3$) δ −183.35–−183.66 and −184.27–−184.58 (m). HRMS (EI-TOF) m/z calcd. for. $C_{16}H_{21}F$ [M]$^+$ 232.16218 found 232.16314.

ethyl 4-fluoro-2-methylene-7-phenylheptanoate (**8f**)



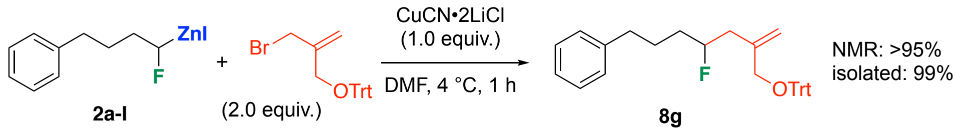
To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, ethyl 2-(bromomethyl)acrylate (27.8 µL, 0.20 mmol, 2.0 equiv.) and

CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8f** was determined to be >95% yield by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane/EtOAc = 16/1 as eluent to give **8f** as yellow oil (25.4 mg, 96% yield).

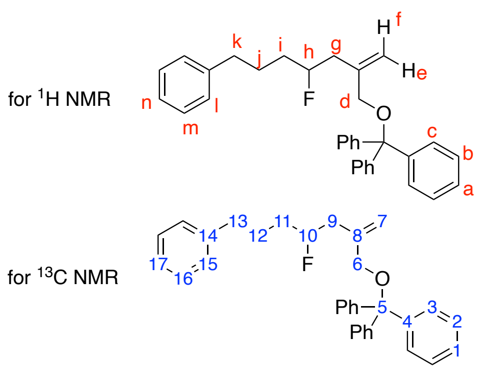


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30–7.16 (m, 5H, H_j–H_l), 6.27 (s, 1H, H_d), 5.67 (s, 1H, H_c), 4.67 (dtt, $^{2}J_{H\text{–}F}$ = 49.6 Hz, $^{3}J_{H\text{–}H}$ = 8.0 Hz, $^{3}J_{H\text{–}H}$ = 8.0 Hz, H_f), 4.11 (q, 2H, $^{3}J_{H\text{–}H}$ = 6.8 Hz, H_b), 2.76–2.54 (m, 4H, H_e and H_i), 1.89–1.55 (m, 4H, H_g and H_h), 1.30 (t, 3H, $^{3}J_{H\text{–}H}$ = 6.8 Hz, H_a); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 166.94 (C3), 142.12 (C11), 136.27 (d, $^{3}J_{C\text{–}F}$ = 3.9 Hz, C5), 128.54 (C12 or C13), 128.47 (C12 or C13), 127.94 (C14), 125.96 (C4), 92.33 (d, $^{1}J_{C\text{–}F}$ = 171.5 Hz, C7), 60.97 (C2), 37.99 (d, $^{2}J_{C\text{–}F}$ = 22.0 Hz, C6), 35.68 (C10), 34.71 (d, $^{2}J_{C\text{–}F}$ = 21.1 Hz, C8), 26.91 (d, $^{3}J_{C\text{–}F}$ = 3.8 Hz, C9), 14.32 (C1); ^{19}F NMR (367 MHz, $CDCl_3$) δ −179.21–−179.59 (m). HRMS (EI-TOF) m/z calcd. for $C_{16}H_{21}F$ $[M]^+$ 232.16218 found 232.16314.

(((4-fluoro-2-methylene-7-phenylheptyl)oxy)methanetriyl)tribenzene (**8g**)



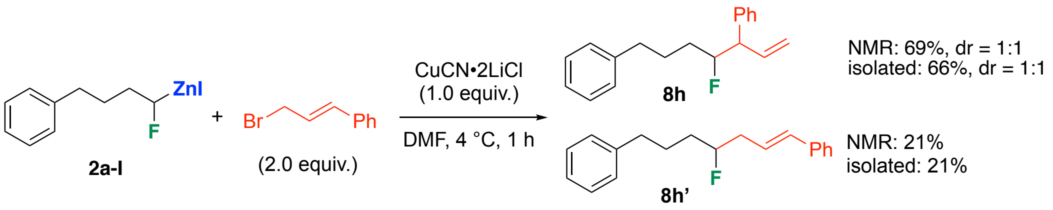
To a test tube equipped with a magnetic stir bar were added *O*-trityl 2-(bromomethyl)prop-2-en-1-ol (78.7 mg, 0.20 mmol, 2.0 equiv.) and DMF (0.20 mL). After the solution was cooled to 4 °C, freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol, 1.0 equiv.) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8g** was determined to be >95% yield by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane as eluent to give **8g** as white amorphous solid (46.6 mg, 99% yield).



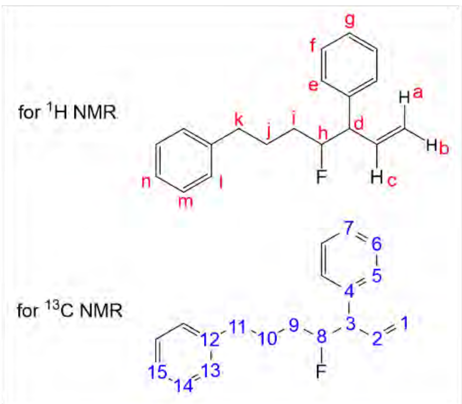
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49–7.46 (m, 6H, H_c), 7.40–7.15 (m, 14H, H_a–H_b and H_l–H_n), 5.36 (s, 1H, H_e or H_f), 5.03 (s, 1H, H_e or H_f), 4.59–4.45 (dtt, 1H, $^{2}J_{H\text{–}F}$ = 49.5 Hz, $^{3}J_{H\text{–}H}$ = 8.0 Hz, $^{3}J_{H\text{–}H}$ = 8.0 Hz, H_h), 3.59 (s, 2H, H_d), 2.65–2.59 (m, 2H, H_k), 2.42–2.24 {2.37 (ddd, 1H, $^{2}J_{H\text{–}H}$ = 15.6 Hz, $^{2}J_{H\text{–}F}$ = 14.5 Hz, $^{3}J_{H\text{–}H}$ = 8.5 Hz, H_g), 2.30 (ddd, 1H, $^{2}J_{H\text{–}H}$ = 15.6 Hz, $^{2}J_{H\text{–}F}$ = 29.3 Hz, $^{3}J_{H\text{–}H}$ = 4.0 Hz, H_g)}, 1.83–1.49 (m, 4H, H_i and H_j); $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) δ 144.24 (C4), 142.28 (d, $^{3}J_{C\text{–}F}$ = 3.9 Hz, C8), 142.18 (C14), {128.75, 128.51, 128.46, 127.95, 127.15, 125.84} (C1, C2, C3, C15, C16, C17), 113.32 (C7), 92.55 (d, $^{1}J_{C\text{–}F}$ = 168.9 Hz, C10), 87.00 (C5), 66.71 (C6), 39.61 (d, $^{2}J_{C\text{–}F}$ = 21.9 Hz, C9), 35.70 (C13), 34.66 (d, $^{2}J_{C\text{–}F}$ = 20.8 Hz, C11), 26.95 (d, $^{3}J_{C\text{–}F}$ = 4.3 Hz, C12);

^{19}F NMR (470 MHz, $CDCl_3$) δ −178.68–−178.99 (m). HRMS (ESI-TOF) m/z calcd. for $C_{33}H_{33}OFNa$ $[M + Na]^+$ 487.24077 found 487.24031.

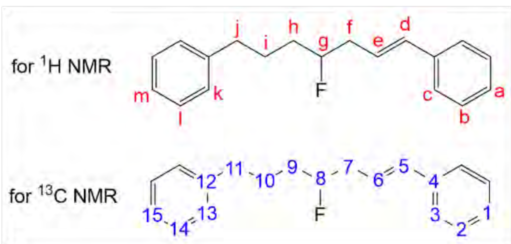
(4-fluorohept-6-ene-1,5-diyl)dibenzene (**8h**) and (*E*)-(4-fluorohept-1-ene-1,7-diyl)dibenzene (**8h'**)



To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, cinnamyl bromide (28.9 µL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8h** and **8h'** was determined to be 69% and 21% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The diastereomeric ratio of **8h** (*syn*-**8h** and *anti*-**8h**) was determined to be 1:1 from ^{1}H NMR spectroscopy. The crude mixture was purified by column chromatography using hexane as eluent to give mixture of *syn*-**8h**, *anti*-**8h**, and **8h'** as colorless oil (23.4 mg, 87% yield). We could not obtain each isomer in pure form even after careful trials.

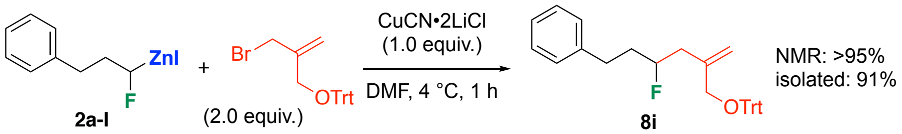


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.14 (m, 10H, H_e, H_f, H_g, H_l, H_m and H_n), 6.27–6.04 (m, 1H, H_c), 5.23–5.11 {5.19 (dd, 1H, $^2J_{H–H}$ = 11.0 Hz, $^3J_{H–H}$ = 20.4 Hz, H_a), 5.14 (dd, 1H, $^2J_{H–H}$ = 11.0 Hz, $^3J_{H–H}$ = 17.2 Hz, H_b)}, 4.87–4.67 (m, 1H, H_h), 3.52–3.41 (m, 1H, H_d), 2.67–2.59 (m, 2H, H_k), 1.93–1.65 (m, 4H, H_i and H_j); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 142.20 and 142.17 (C12), 140.90 and 140.85 (C4), 137.76 and 137.05 (d, $^3J_{C–F}$ = 5.8 Hz and $^3J_{C–F}$ = 4.8 Hz, C2), 128.81-128.35 (C13, C14 and C15), 127.00 and 126.95 (C5), 125.94 and 125.92 (C6), 124.99 and 124.93 (C7), 117.51 and 117.11 (C1), 95.80 and 94.69 (d, $^1J_{C–F}$ =174.4 Hz, C8), 55.02 and 54.83 (d, $^2J_{C–F}$ = 15.4 Hz and $^2J_{C–F}$ = 14.3 Hz, C3), 35.70 and 35.62 (C11), 32.92 and 32.71 (d, $^2J_{C–F}$ = 17.3 Hz, C9), 27.15 and 27.05 (d, $^3J_{C–F}$ = 3.8 Hz, C10); ^{19}F NMR (367 MHz, $CDCl_3$) δ −184.04–−184.48 (m). HRMS (ESI-TOF) m/z calcd. for $C_{19}H_{21}FNa$ $[M + Na]^+$ 291.15195 found 291.15157.

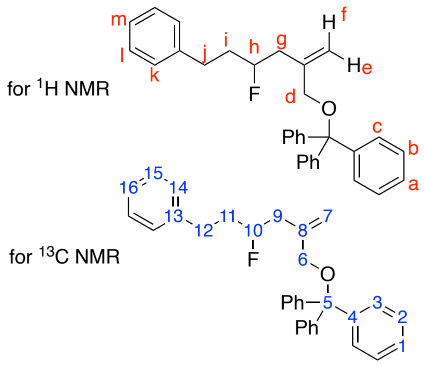


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.14 (m, 10H, H_a, H_b, H_c, H_k, H_l and H_m), 6.48 (d, 1H, $^3J_{H–H}$ = 16.0 Hz, H_d), 6.44–6.14 (m, 1H, H_e), 4.73–4.55 (m, 1H, H_g), 2.70–2.42 (m, 4H, H_f and H_j), 1.69–1.44 (m, 4H, H_h and H_i); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 142.17 (C12, overlapped), 139.92 (C4), 137.41 (C6), 133.03 (C5), 128.81-128.35 (C13, C14 and C15), 127.41 (C3), 126.26 (C2), 125.97 (C1), 93.68 (d, $^1J_{C–F}$ = 168.7 Hz, C8), 38.86 (d, $^2J_{C–F}$ = 22.1 Hz, C7), 35.72 (C11), 34.34 (d, $^2J_{C–F}$ = 21.1 Hz, C9), 26.96 (d, $^3J_{C–F}$ = 4.8 Hz, C10); ^{19}F NMR (367 MHz, $CDCl_3$) δ −177.21–−178.88 (m).

(((4-fluoro-2-methylene-6-phenylhexyl)oxy)methanetriyl)tribenzene (**8i**)

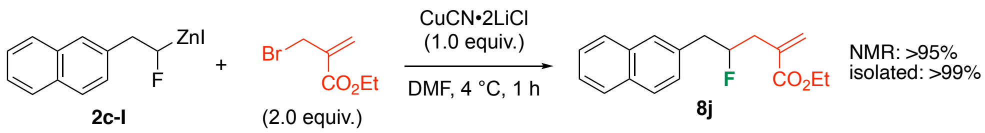


To a test tube equipped with a magnetic stir bar were added *O*-trithyl 2-(bromomethyl)prop-2-en-1-ol (78.7 mg, 0.20 mmol. 2.0 equiv.) and DMF (0.20 mL). After the solution was cooled to 4 °C, freshly prepared **2b-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol, 1.0 equiv.) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8i** was determined to be >95% yield by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane as eluent to give **8i** as yellow oil (40.9 mg, 91% yield).

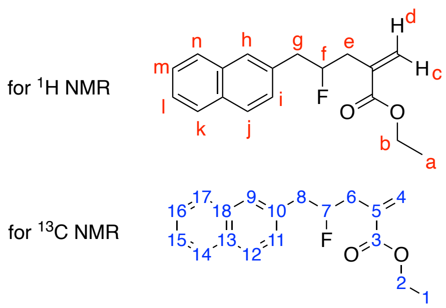


^{1}H NMR (400 MHz, CDCl$_3$) δ 7.46–7.45 (m, 6H, H$_c$), 7.32–7.14 (m, 14H, H$_a$-H$_b$, H$_k$-H$_m$), 5.36 (s, 1H, H$_e$ or H$_f$), 5.03 (s, 1H, H$_e$ or H$_f$), 4.61–4.43 (m, 1H, H$_h$), 3.56 (s, 2H, H$_d$), 2.82–2.59 {2.79 (ddd, 1H, $^2J_{H\text{–}H}$ = 13.6 Hz, $^3J_{H\text{–}F}$ = 6.8 Hz, $^3J_{H\text{–}H}$ = 9.6 Hz, H$_g$), 2.63 (ddd, 1H, $^2J_{H\text{–}H}$ = 13.6 Hz, $^3J_{H\text{–}F}$ = 6.8 Hz, $^3J_{H\text{–}H}$ = 9.6 Hz, H$_g$)}, 2.47–2.26 (m, 2H, H$_j$), 1.96–1.72 (m, 2H, H$_i$); ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 144.22 (C4), 142.21 (d, $^3J_{C\text{–}F}$ = 4.8 Hz, C8), 141.52 (C13), {128.73, 128.56, 128.53, 127.96, 127.14, 126.07} (C1, C2, C3, C14, C15 and C16), 113.40 (C7), 91.85 (d, $^1J_{C\text{–}F}$ = 169.7 Hz, C10), 86.98 (C5), 66.67 (C6), 39.61 (d, $^2J_{C\text{–}F}$ = 21.1 Hz, C9), 36.85 (d, $^2J_{C\text{–}F}$ = 21.1 Hz, C11), 31.45 (d, $^3J_{C\text{–}F}$ = 3.9 Hz, C12); ^{19}F NMR (367 MHz, CDCl$_3$) δ −178.44–−178.84 (m). HRMS (ESI-TOF) m/z calcd. for $C_{32}H_{31}OFNa$ [M + Na]$^+$ 473.22512 found 473.22486.

ethyl 4-fluoro-2-methylene-5-(naphthalen-2-yl)pentanoate (**8j**)

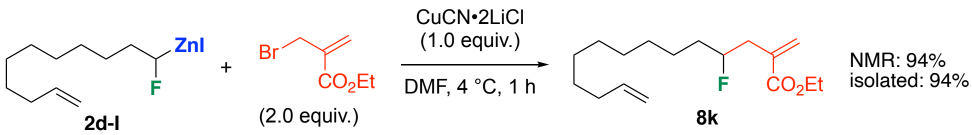


To a test tube equipped with a magnetic stir bar were added freshly prepared **2c-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, ethyl 2-(bromomethyl)acrylate (27.8 µL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8j** was determined to be >95% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane/EtOAc = 20/1 as eluent to give mixture of **8j** as yellow oil (28.6 mg, >99% yield).

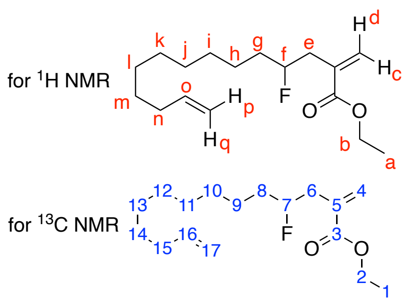


^{1}H NMR (400 MHz, CDCl$_3$) δ 7.84–7.80 (m, 3H, H$_n$, H$_k$ and H$_j$), 7.70 (s, 1H, H$_h$), 7.50–7.43 (m, 2H, H$_m$ and H$_l$), 7.39 (d, 1H, $^3J_{\text{H–H}}$ = 8.0 Hz, H$_i$), 6.31 (s, 1H, H$_d$), 5.72 (s, 1H, H$_c$), 5.11–4.93 (m, 1H, H$_f$), 4.21 (q, 2H, $^3J_{\text{H–H}}$ = 7.2 Hz, H$_b$), 3.20–3.03 {3.15 (ddd, 1H, $^3J_{\text{H–F}}$ = 20.2 Hz, $^2J_{\text{H–H}}$ = 14.1 Hz, $^3J_{\text{H–H}}$ = 6.8 Hz, H$_g$), 3.10 (ddd, 1H, $^3J_{\text{H–F}}$ = 26.3 Hz, $^2J_{\text{H–H}}$ = 14.1 Hz, $^3J_{\text{H–H}}$ = 4.8 Hz, H$_g$)}, 2.79–2.58 {2.72 (ddd, 1H, $^3J_{\text{H–F}}$ = 31.8 Hz, $^2J_{\text{H–H}}$ = 15.0 Hz, $^3J_{\text{H–H}}$ = 2.8 Hz, H$_e$), 2.63 (ddd, 1H, $^3J_{\text{H–F}}$ = 15.0 Hz, $^2J_{\text{H–H}}$ = 15.0 Hz, $^3J_{\text{H–H}}$ = 8.4 Hz, H$_e$)}; ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 166.86 (C3), 136.07 (d, $^3J_{\text{C–F}}$ = 2.9 Hz, C5), 134.55 (d, $^3J_{\text{C–F}}$ = 2.8 Hz, C10), 133.61 (C13 or C18), 132.44 (C13 or C18), {128.19, 128.16, 128.09, 127.83, 127.75, 127.69, 126.16} (C9, C11, C12, C14, C15, C16, and C17), 125.67 (C4), 92.47 (d, $^1J_{\text{C–F}}$ = 172.5 Hz, C7), 60.98 (C2), 41.72 (d, $^2J_{\text{C–F}}$ = 21.0 Hz, C7), 37.65 (d, $^2J_{\text{C–F}}$ = 22.1 Hz, C7), 14.27 (C1); ^{19}F NMR (367 MHz, CDCl$_3$) δ −177.48–−177.86 (m). HRMS (ESI-TOF) m/z calcd. for $C_{18}H_{19}O_2FNa$ [M + Na]$^+$ 309.12613 found 309.12541.

ethyl 4-fluoro-2-methylenetetradec-13-enoate (**8k**)

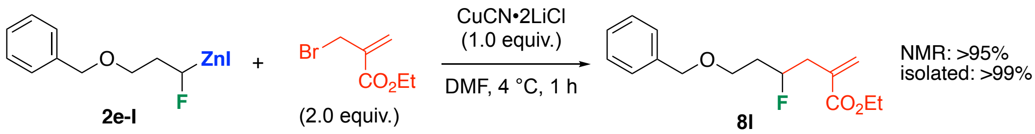


To a test tube equipped with a magnetic stir bar were added freshly prepared **2d-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, ethyl 2-(bromomethyl)acrylate (27.8 μL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8k** was determined to be 94% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by column chromatography using hexane/EtOAc = 10/1 as eluent to give mixture of **8k** as yellow oil (25.0 mg, 94% yield).

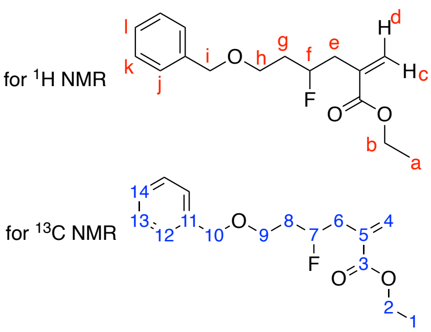


^{1}H NMR (400 MHz, CDCl$_3$) δ 6.27 (s, 1H, H$_d$), 5.86–5.75 (m, 1H, H$_o$), 5.69 (s, 1H, H$_c$), 5.01–4.96 (m, 1H, H$_q$), 4.94–4.90 (m, 1H, H$_p$), 4.73–4.55 (m, 1H, H$_f$), 4.21 (q, 2H, $^2J_{\text{H–H}}$ = 7.1 Hz, H$_b$), 2.68–2.50 (m, 2H, H$_e$), 2.03 (dt, 2H, $^3J_{\text{H–H}}$ = 7.6 Hz, $^3J_{\text{H–H}}$ = 6.8 Hz, H$_n$), 1.70–1.28 (m, 14H, H$_g$-H$_m$), 1.30 (t, 3H, $^2J_{\text{H–H}}$ = 7.2 Hz, H$_a$); ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 166.98 (C3), 139.34 (C16), 136.33 (d, $^3J_{\text{C–F}}$ = 2.8 Hz, C5), 127.86 (C4), 114.26 (C17), 92.54 (d, $^1J_{\text{C–F}}$ = 159.9 Hz, C7), 60.95 (C2), 37.99 (d, $^2J_{\text{C–F}}$ = 22.1 Hz, C6), 35.23 (d, $^2J_{\text{C–F}}$ = 21.0 Hz, C8), 33.93 (C15), {29.57, 29.52, 29.50, 29.23, 29.04, one carbon overlapped} (C10, C11, C12, C13 and C14), 25.13 (d, $^3J_{\text{C–F}}$ = 4.7 Hz, C9), 14.32 (C1); ^{19}F NMR (367 MHz, CDCl$_3$) δ −178.84–−179.22 (m). HRMS (ESI-TOF) m/z calcd. for $C_{17}H_{29}O_2FNa$ [M + Na]$^+$ 307.20438 found 307.20390.

ethyl 6-(benzyloxy)-4-fluoro-2-methylenehexanoate (**8l**)

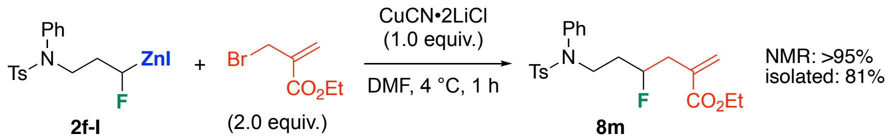


To a test tube equipped with a magnetic stir bar were added freshly prepared **2e-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, ethyl 2-(bromomethyl)acrylate (27.8 µL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8l** was determined to be >95% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane/EtOAc = 99/1 as eluent to give mixture of **8l** as colorless oil (28.1 mg, >99% yield).



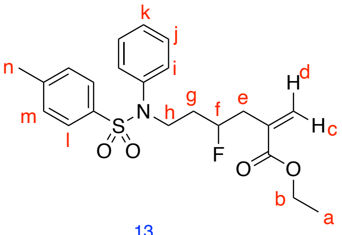
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30–7.19 (m, 5H, H_j–H_l), 6.22 (s, 1H, H_d), 5.63 (s, 1H, H_c), 4.87–7.72 (m, 1H, H_f), 4.45 (s, 2H, H_i), 4.14 (q, 2H, $^{3}J_{H-H}$ = 7.2 Hz, H_b), 3.59–3.51 (m, 2H, H_h), 2.66–2.54 (m, 2H, H_e), 1.90–1.82 (m, 2H, H_g), 1.23 (t, 3H, $^{3}J_{H-H}$ = 7.2 Hz, H_a);$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 166.90 (C3), 138.42 (C11), 136.14 (d, $^{3}J_{C-F}$ = 3.8 Hz, C5), 128.51 (C12 or C13), 128.00 (C14), 127.75 (C12 or C13), 89.85 (d, $^{1}J_{C-F}$ = 170.5 Hz, C7), 73.23 (C10), 66.19 (d, $^{3}J_{C-F}$ = 4.8 Hz, C9), 60.97 (C2), 37.89 (d, $^{2}J_{C-F}$ = 21.1 Hz, C6), 35.46 (d, $^{2}J_{C-F}$ = 21.1 Hz, C8), 14.29 (C1); ^{19}F NMR (367 MHz, $CDCl_3$) δ −181.09–−181.48 (m). HRMS (ESI-TOF) m/z calcd. for $C_{16}H_{21}O_3FNa$ $[M + Na]^+$ 303.13669 found 303.13618.

ethyl 4-fluoro-6-((4-methyl-*N*-phenylphenyl)sulfonamido)-2-methylenehexanoate (**8m**)

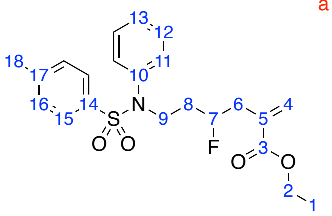


To a test tube equipped with a magnetic stir bar were added freshly prepared **2f-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, ethyl 2-(bromomethyl)acrylate (27.8 µL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8m** was determined to be >95% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane/EtOAc = 10/1 as eluent to give mixture of **8m** as pink oil (33.8 mg, 81% yield).

for ^{1}H NMR

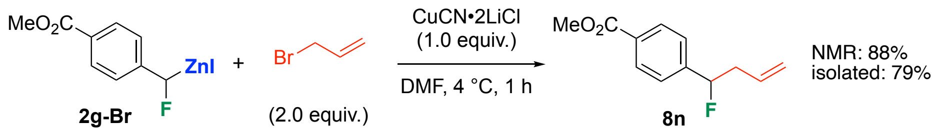


for ^{13}C NMR



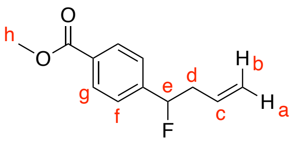
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, 2H, $^3J_{H–H}$ = 8.0 Hz, H_l), 7.32–7.28 (m, 3H, H_j and H_k), 7.23 (d, 2H, $^3J_{H–H}$ = 8.0 Hz, H_l), 7.06–7.01 (m, 2H, H_i), 6.24 (s, 1H, H_d), 5.64 (s, 1H, H_c), 4.82–4.66 (m, 1H, H_f), 4.19 (q, 2H, $^3J_{H–H}$ = 7.2 Hz, H_l), 3.76–3.59 (m, 2H, H_e), 2.59–2.51 (m 2H, H_h), 2.25 (s, 3H, H_n), 1.82–1.70 (m, 4H, H_g), 1.29 (t, 3H, $^3J_{H–H}$ = 7.2 Hz, H_l); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 166.73 (C3), 143.60 (C10), 139.25 (C14), 135.72 (d, $^3J_{C–F}$ = 3.8 Hz, C5), 135.10 (C17), {129.54, 129.21, 128.83, 128.24, 128.13, 127.87} (C4, C11, C12, C13, C15, C16), 89.69 (d, $^1J_{C–F}$ = 172.5 Hz, C7), 61.01 (C2), 47.08 (d, $^3J_{C–F}$ = 3.8 Hz, C9), 37.70 (d, $^2J_{C–F}$ = 21.1 Hz, C6), 34.23 (d, $^2J_{C–F}$ = 22.2 Hz, C6), 21.65 (C18), 14.29 (C1); ^{19}F NMR (367 MHz, $CDCl_3$) δ −181.19–−181.57 (m). HRMS (ESI-TOF) m/z calcd. for $C_{22}H_{26}O_4FNaS$ $[M + Na]^+$ 442.14588 found 442.14536.

methyl 4-(1-fluorobut-3-en-1-yl)benzoate (**8n**)

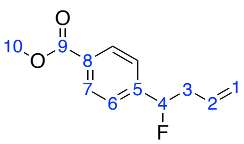


To a test tube equipped with a magnetic stir bar were added freshly prepared **2g-Br** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, allyl bromide (17.3 μL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8n** was determined to be 88% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane/EtOAc = 20/1 as eluent to give mixture of **8n** as colorless oil (16.4 mg, 79% yield).

for ^{1}H NMR

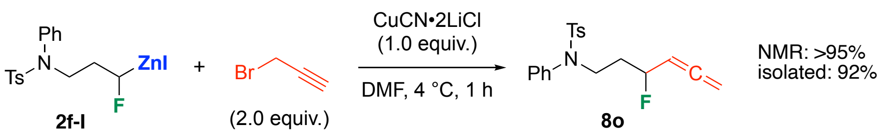


for ^{13}C NMR



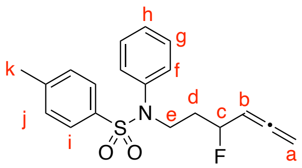
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, 2H, $^3J_{H–H}$ = 8.0 Hz, H_g), 7.39 (d, 2H, $^3J_{H–H}$ = 8.0 Hz, H_f), 5.82–5.72 (m, 2H, H_d), 5.54 (ddd, 1H, $^2J_{H–F}$ = 48.8 Hz, $^3J_{H–H}$ = 8.0 Hz, $^3J_{H–H}$ = 5.2 Hz, H_e), 5.13 (d, 1H, $^3J_{H–H}$ = 17.2 Hz, H_b), 5.12 (d, 1H, $^3J_{H–H}$ = 10.8 Hz, H_a), 3.92 (s, 3H, H_h), 2.74–2.58 (m, 2H, H_d); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 166.85 (C9), 144.87 (d, $^2J_{C–F}$ = 20.1 Hz, C5), 132.27 (d, $^3J_{C–F}$ = 5.7 Hz, C2), 130.16 (C8, 129.88 (C7), 125.125.49 (d, $^3J_{C–F}$ = 7.7 Hz, C6), 118.89 (C1), 93.17 (d, $^1J_{C–F}$ = 174.4 Hz, C4), 52.30 (C10), 41.63 (d, $^2J_{C–F}$ = 24.0 Hz, C3);^{19}F NMR (367 MHz, $CDCl_3$) δ −176.49 (ddd, $^2J_{H–F}$ = 46.6 Hz, $^3J_{H–F}$ = 26.1 Hz, $^3J_{H–F}$ = 18.4 Hz). HRMS (EI-TOF) m/z calcd. for $C_{12}H_{13}O_2F$ $[M]^+$ 208.08941 found 208.08905.

N-(3-fluorohexa-4,5-dien-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (**8o**)

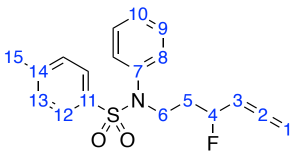


To a test tube equipped with a magnetic stir bar were added freshly prepared **2f-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, propargyl bromide (15.1 µL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8o** was determined to be >95% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by column chromatography using hexane as eluent to give mixture of **8o** as yellow oil (31.6 mg, 92% yield).

for ^{1}H NMR

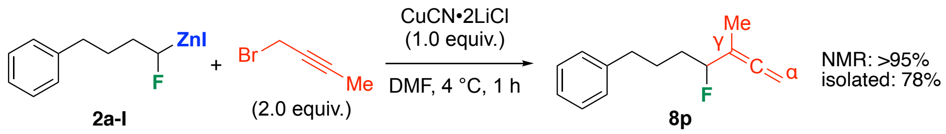


for ^{13}C NMR



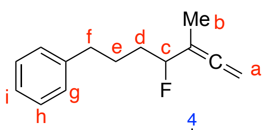
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, 2H, $^{3}J_{H–H}$ = 8.0 Hz, H_i), 7.33–7.29 (m, 3H, H_g and H_h), 7.23 (d, 2H, $^{3}J_{H–H}$ = 8.0 Hz, H_j), 7.06–7.02 (m, 2H, H_f), 5.25 (m, 1H, H_b), 5.12–4.94 (m, 1H, H_c), 4.91–4.79 (m, 2H, H_e), 2.41 (s, 3H, H_k), 1.97–1.80 (m, 2H, H_d); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 208. 81 (d, $^{3}J_{C–F}$ = 11.5 Hz, C2), 143.64 (C7), 139.31 (C11), 135.07 (C14), {129.55, 129.23, 128.83, 128.14, 127.87} (C8, C9, C10, C12, C13), 90.36 (d, $^{2}J_{C–F}$ = 24.0 Hz, C3), 88.67 (d, $^{1}J_{C–F}$ = 168.6 Hz, C4), 77.76 (d, $^{4}J_{C–F}$ = 2.8 Hz, C1), 46.96 (d, $^{3}J_{C–F}$ = 4.8 Hz, C6), 34.49 (d, $^{2}J_{C–F}$ = 23.0 Hz, C5), 21.66 (C15); ^{19}F NMR (367 MHz, $CDCl_3$) δ −170.00–−170.33 (m). HRMS (ESI-TOF) m/z calcd. for $C_{19}H_{20}O_2NFNaS$ $[M + Na]^+$ 368.10910 found 368.10862.

(4-fluoro-5-methylhepta-5,6-dien-1-yl)benzene (**8p**)

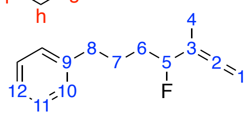


To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, 1-bromobut-2-yne (17.9 µL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8p** was determined to be >95% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by column chromatography using hexane as eluent to give mixture of **8p** as colorless oil (15.9 mg, 78% yield).

for ^{1}H NMR

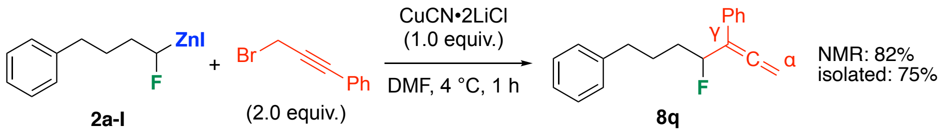


for ^{13}C NMR

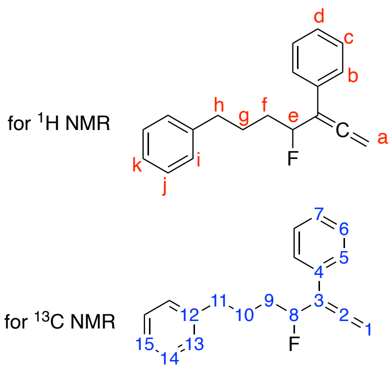


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29–7.16 (m, 5H, H_g–H_i), 4.95–4.71 (m, 3H, H_c and H_a), 2.65 (t, 2H, $^{3}J_{H–H}$ = 7.2 Hz, H_f), 1.88–1.62 (m, 7H, H_b, H_d, and H_e); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.72 (d, $^{3}J_{C–F}$ = 9.9 Hz, C2), 142.17 (C9), 128.54 (C10 or C11), 128.48 (C10 or C11), 125.98 (C12), 98.22 (d, $^{2}J_{C–F}$ = 22.1 Hz, C3), 93.90 (d, $^{1}J_{C–F}$ = 172.4 Hz, C5), 76.08 (C1), 35.67 (C8), 32.88 (d, $^{2}J_{C–F}$ = 33.3 Hz, C6), 27.05 (d, $^{3}J_{C–F}$ = 4.8 Hz, C4), 13.85 (C7); ^{19}F NMR (367 MHz, $CDCl_3$) δ −173.75–−174.03 (m). HRMS (EI-TOF) m/z calcd. for $C_{11}H_{18}F$ $[M]^+$ 204.13088 found 204.13118.

(4-fluorohepta-5,6-diene-1,5-diyl)dibenzene (**8q**)

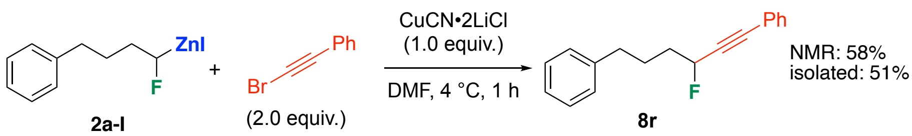


To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, (3-bromoprop-1-yn-1-yl)benzene (28.3 µL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8q** was determined to be 82% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by column chromatography using hexane as eluent to give mixture of **8q** as colorless oil (19.9 mg, 75% yield).



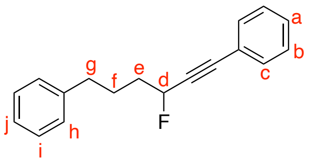
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45–7.16 (m, 10H, H_b–H_d and H_i–H_k), 5.48–5.32 (m, 1H, H_e), 5.24 (br s, 1H, H_a), 5.21 (br s, 1H, H_a), 2.67 (t, 2H, $^{3}J_{H-H}$ = 7.2 Hz, H_h), 2.05–1.70 (m, 4H, H_f and H_g); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 208.99 (d, $^{3}J_{C-F}$ = 8.7 Hz, C2), 142.12 (C12), 134.14 (C4), {128.71, 128.53, 128.49, 127.35, 126.89, 125.98} (C5, C6, C7, C13, C14, and C15), 105.87 (d, $^{2}J_{C-F}$ = 20.2 Hz, C3), 91.60 (d, $^{1}J_{C-F}$ = 171.5 Hz, C8), 80.20 (C1), 35.63 (C11), 33.47 (d, $^{2}J_{C-F}$ = 22.1 Hz, C9), 27.24 (d, $^{3}J_{C-F}$ = 4.7 Hz, C10); ^{19}F NMR (367 MHz, $CDCl_3$) δ −173.75–−174.03 (m). HRMS (EI-TOF) m/z calcd. for. $C_{19}H_{19}F$ $[M]^{+}$ 266.14653 found 266.14626.

(3-fluorohex-1-yne-1,6-diyl)dibenzene (**8r**)

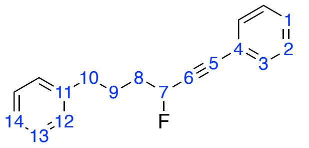


To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, (bromoethynyl)benzene (12.0 µL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8r** was determined to be 58% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane as eluent to give mixture of **8r** as yellow oil (12.9 mg, 51% yield).

for ^{1}H NMR

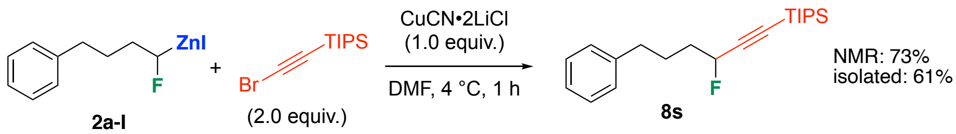


for ^{13}C NMR



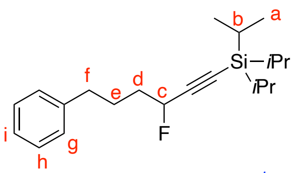
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46–7.20 (m, 10H, H_a–H_c and H_h–H_j), 5.33 (dt, 1H, $^{2}J_{H–F}$ = 49.2 Hz, $^{3}J_{H–H}$ = 6.0 Hz, H_d), 2.72 (t, 2H, $^{3}J_{H–H}$ = 7.2 Hz, H_g), 2.05–1.83 (m, 4H, H_e and H_f); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 141.87 (C11), 131.97 (d, $^{5}J_{C–F}$ = 2.9 Hz, C3), {129.05, 128.58, 128.55, 128.48, 126.09} (C1, C2, C12, C13, C14), 122.04 (d, $^{4}J_{C–F}$ = 3.8 Hz, C3), 88.19 (d, $^{3}J_{C–F}$ = 10.5 Hz, C5), 85.62 (d, $^{2}J_{C–F}$ = 25.9 Hz, C6), 35.63 (d, $^{2}J_{C–F}$ = 23.0 Hz, C8), 35.44 (C10), 25.38 (d, $^{3}J_{C–F}$ = 3.8 Hz, C9); ^{19}F NMR (367 MHz, $CDCl_3$) δ −170.13 (dt, $^{2}J_{H–F}$ = 48.1 Hz, $^{3}J_{H–F}$ = 19.1 Hz). HRMS (EI-TOF) m/z calcd. for $C_{18}H_{17}F$ $[M]^+$ 252.13088 found 252.13139.

(3-fluoro-6-phenylhex-1-yn-1-yl)triisopropylsilane (**8s**)

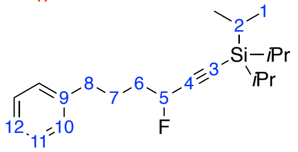


To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, (bromoethynyl)triisopropylsilane (48.7 μL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8s** was determined to be 73% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane as eluent to give mixture of **8s** as yellow oil (20.4 mg, 61% yield).

for ^{1}H NMR

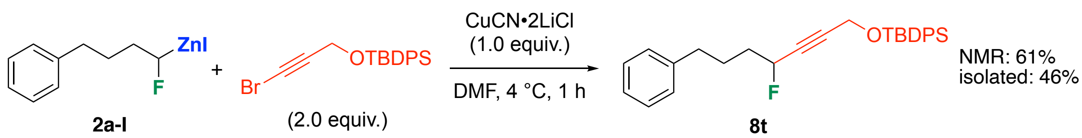


for ^{13}C NMR



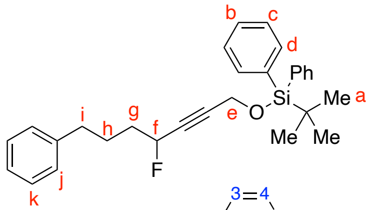
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30–7.16 (m, 5H, H_g–H_i), 5.92–5.04 (m, 1H, H_c), 2.67 (t, 2H, $^{3}J_{H–H}$ = 8.4 Hz, H_f), 1.93–1.80 (m, 4H, H_d and H_e), 1.08–1.06 (m, 21H, H_a and H_b); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 141.90 (C9), 128.52 (C10 and C11, overlapped), 126.03 (C12), 103.76 (d, $^{2}J_{C–F}$ = 25.0 Hz, C4), 93.03 (d, $^{3}J_{C–F}$ = 8.6 Hz, C3), 82.90 (d, $^{1}J_{C–F}$ = 167.7 Hz, C5), 35.69 (d, $^{2}J_{C–F}$ = 23.0 Hz, C6), 35.41 (C8), 26.30 (d, $^{3}J_{C–F}$ = 3.8 Hz, C7), 18.67 (C1), 11.19 (C2); ^{19}F NMR (367 MHz, $CDCl_3$) δ −170.18–−170.41 (m). HRMS (ESI-TOF) m/z calcd. for $C_{21}H_{33}FNaSi$ $[M + Na]^+$ 355.22278 found 355.22221.

tert-butyl((4-fluoro-7-phenylhept-2-yn-1-yl)oxy)diphenylsilane (**8t**)

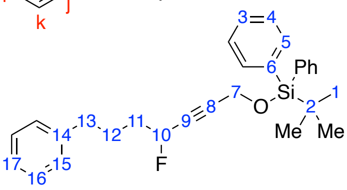


To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, (bromoethynyl)triisopropylsilane (61.2 μL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8t** was determined to be 61% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane as eluent to give mixture of **8t** as colorless oil (20.3 mg, 46% yield).

for ^{1}H NMR

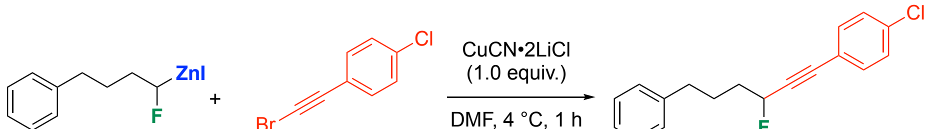


for ^{13}C NMR



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (dd, 4H, $^{3}J_{H–H}$ = 8.8 Hz, $^{4}J_{H–H}$ = 1.2 Hz, H_d), 7.44–7.16 (m, 11H, H_b, H_c, H_j, H_k and H_l), 5.08 (dt, 1H, $^{2}J_{H–F}$ = 50.0 Hz, $^{3}J_{H–H}$ = 6.4 Hz, H_f), 4.37 (dd, 2H, $^{5}J_{H–F}$ = 6.8 Hz, $^{5}J_{H–H}$ = 1.2 Hz, H_e), 2.65 (t, 2H, $^{3}J_{H–H}$ = 7.2 Hz, H_i), 1.85–1.73 (m, 4H, H_g and H_h), 1.07 (s, 9H, H_a); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 141.83 (C14), {135.75, 133.06, 129.99, 128.55, 128.52, 127.86, 126.06} (C3, C4, C5, C6, C15, C16, C17), 86.91 (d, $^{3}J_{C–F}$ = 10.5 Hz, C8), 82.66 (d, $^{1}J_{C–F}$ = 169.8 Hz, C10), 81.81 (d, $^{2}J_{C–F}$ = 26.7 Hz, C9), 52.66 (d, $^{4}J_{C–F}$ = 2.8 Hz, C7), 35.41 (C13), 35.36 (d, $^{2}J_{C–F}$ = 22.9 Hz, C11), 26.80 (C1), 26.24 (d, $^{3}J_{C–F}$ = 3.9 Hz, C12), 19.30 (C2); ^{19}F NMR (367 MHz, $CDCl_3$) δ −171.17–−171.44 (m). HRMS (ESI-TOF) m/z calcd. for $C_{29}H_{33}OFNaSi$ $[M + Na]^+$ 467.21769 found 467.21718.

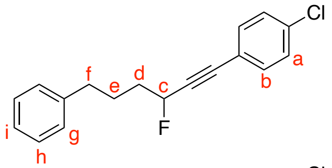
1-chloro-4-(3-fluoro-6-phenylhex-1-yn-1-yl)benzene (**8u**)



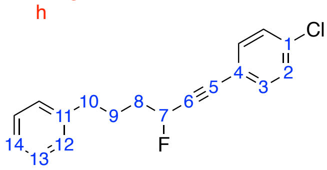
2a-I (2.0 equiv.) **8u**, 57% (48%)

To a test tube equipped with a magnetic stir bar were added 1-(bromoethynyl)-4-chlorobenzene (43.1 mg, 0.20 mmol, 2.0 equiv.) and DMF (0.20 mL). After the solution was cooled to 4 °C, freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol, 1.0 equiv.) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8u** was determined to be 57% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane as eluent to give mixture of **8u** as white amorphous solid (13.8 mg, 48% yield).

for ^{1}H NMR

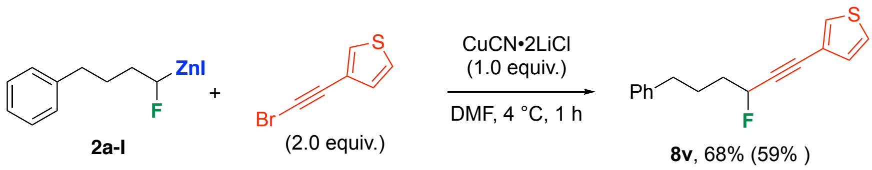


for ^{13}C NMR

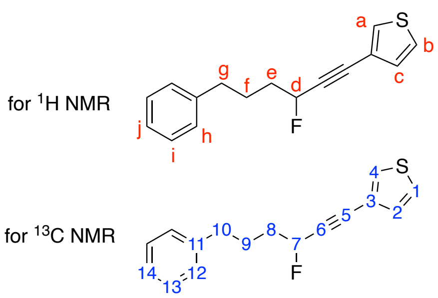


^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27–7.20 (m, 9H, H_a, H_b, and H_g–H_i), 5.33 (dt, 1H, $^{2}J_{H–F}$ = 48.0 Hz, $^{3}J_{H–H}$ = 5.8 Hz, H_c), 2.72 (t, 2H, $^{3}J_{H–H}$ = 7.3 Hz, H_f), 2.15–1.82 (m, 4H, H_d and H_e); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 141.79 (C11), 135.19 (C1), {133.21, 133.19, 128.86, 128.56, 126.12} (C2, C3, C12, C13, and C14), 120.51 (d, $^{4}J_{C–F}$ = 3.6 Hz, C4), 87.40 (d, $^{3}J_{C–F}$ = 10.1 Hz, C5), 86.59 (d, $^{2}J_{C–F}$ = 25.5 Hz, C6), 83.03 (d, $^{1}J_{C–F}$ = 166.5 Hz, C7), 35.53 (d, $^{2}J_{C–F}$ = 22.5 Hz, C8), 35.41 (C10), 26.35 (d, $^{3}J_{C–F}$ = 3.6 Hz, C5); ^{19}F NMR (470 MHz, $CDCl_3$) δ −172.13 (dt, $^{2}J_{H–F}$ = 48.8 Hz, $^{3}J_{H–F}$ = 19.8 Hz). HRMS (EI-TOF) m/z calcd. for $C_{18}H_{16}ClF$ $[M]^+$ 286.09191 found 286.09177.

3-(3-fluoro-6-phenylhex-1-yn-1-yl)thiophene (**8v**)

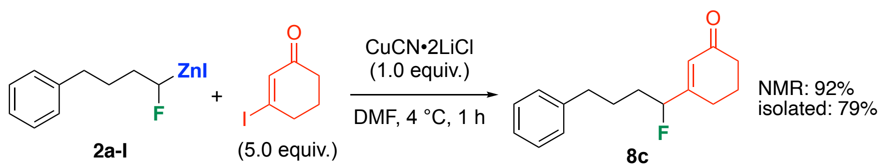


To a test tube equipped with a magnetic stir bar were added 1-(bromoethynyl)-3-ehiophene (37.4 mg, 0.20 mmol, 2.0 equiv.) and DMF (0.20 mL). After the solution was cooled to 4 °C, freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol, 1.0 equiv.) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8v** was determined to be 68% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane as eluent to give mixture of **8v** as clorlessoil (15.2 mg, 59% yield).

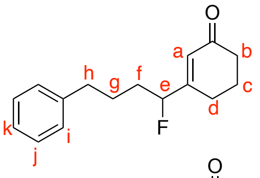


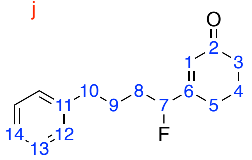
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (d, 1H, $^{3}J_{H–H}$ = 5.0 Hz, H_b), 7.31–7.18 (m, 6H, H_a, and H_h–H_j), 7.12 (dd, 1H, $^{3}J_{H–H}$ = 5.0 Hz, $^{4}J_{H–H}$ = 1.0 Hz, H_b), 5.32 (dt, 1H, $^{2}J_{H–F}$ = 48.0 Hz, $^{3}J_{H–H}$ = 6.0 Hz, H_d), 2.71 (t, 2H, $^{3}J_{H–H}$ = 7.3 Hz, H_g), 2.05–1.85 (m, 4H, H_e and H_f); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 141.85 (C11), {129.97, 129.95, 128.57, 128.54, 126.09, 125.63} (C1, C2, C4, C12, C13, and C14), 120.51 (d, $^{4}J_{C–F}$ = 3.6 Hz, C3), 85.33 (d, $^{2}J_{C–F}$ = 25.5 Hz, C6), 83.41 (d, $^{3}J_{C–F}$ = 10.1 Hz, C5), 83.18 (d, $^{1}J_{C–F}$ = 166.3 Hz, C7), 35.60 (d, $^{2}J_{C–F}$ = 22.8 Hz, C8), 35.42 (C10), 26.37(d, $^{3}J_{C–F}$ = 3.6 Hz, C5); ^{19}F NMR (470 MHz, $CDCl_3$) δ −171.40 (dt, $^{2}J_{H–F}$ = 47.9 Hz, $^{3}J_{H–F}$ = 19.7 Hz). HRMS (EI-TOF) m/z calcd. for $C_{16}H_{15}FS$ $[M]^+$ 258.08730 found 258.08733.

3-(1-fluoro-4-phenylbutyl)cyclohex-2-en-1-one (**8c**)



To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, 3-iodocyclohex-2-en-1-one (60.0 µL, 0.50 mmol, 5.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then quenched with H_2O. The solution was extracted with hexane/EtOAc and dried over Na_2SO_4. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8c** was determined to be 92% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane/EtOAc = 10/1 as eluent to give mixture of **8c** as colorless oil (19.4 mg, 79% yield).

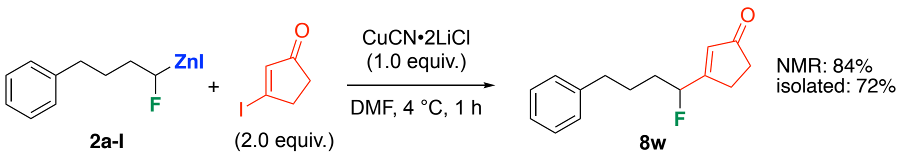
for ^{1}H NMR 

for ^{13}C NMR 

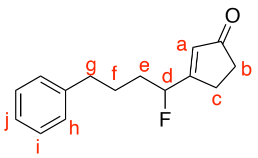
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29–7.15 (m, 5H, H_i–H_k), 6.01 (s, 1H, H_a), 4.95 (dt, 1H, $^{2}J_{H–F}$ = 48.5 Hz, $^{3}J_{H–H}$ = 5.3 Hz, H_e), 2.69–2.63 (m, 2H, H_b), 2.39 (t, 2H, $^{3}J_{H–H}$ = 6.8 Hz, H_h), 2.29–2.15 (m, 2H, H_d), 2.03–1.97 (m, 2H, H_c), 1.82–1.70 (m, 4H, H_f and H_g); ^{13}C{^{1}H} NMR (100 MHz*, $CDCl_3$) δ 199.34 (C2), 161.40 (d, $^{2}J_{C–F}$ = 17.2 Hz, C6), 141.58 (C11), 128.58 (C12 or C13), 128.51 (C12 or C13), 126.16 (C14), 124.70 (d, $^{3}J_{C–F}$ = 9.5 Hz, C1), 93.51 (d, $^{1}J_{C–F}$ = 179.3 Hz, C7), 37.84 (C3), 35.44 (C10), 32.94 (d, $^{2}J_{C–F}$ = 22.9 Hz, C8), 26.39 (d, $^{3}J_{C–F}$ = 2.9 Hz, C5), 24.91 (d, $^{3}J_{C–F}$ = 2.8 Hz, C9), 22.60 (C4); ^{19}F NMR (470 MHz, $CDCl_3$) δ −182.62–−182.88 (m). HRMS (ESI-TOF) m/z calcd. for $C_{16}H_{19}OFNa$ $[M + Na]^+$ 269.13121, found 269.13079.

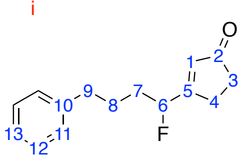
*400 MHz NMR was used for ^{13}C NMR spectroscopy analysis.

3-(1-fluoro-4-phenylbutyl)cyclopent-2-en-1-one (**8w**)



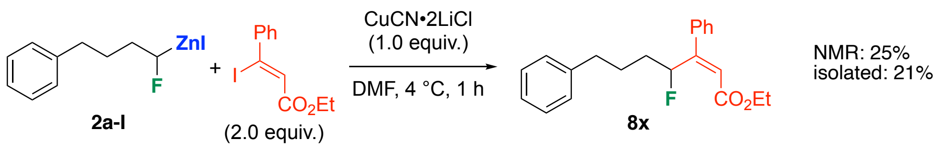
To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, 3-iodocyclopent-2-en-1-one in DMF (0.10 mL, 2.0 M, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then quenched with H_2O. The solution was extracted with hexane/EtOAc and dried over Na_2SO_4. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8w** was determined to be 84% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane/EtOAc = 10/1 as eluent to give mixture of **8w** as colorless oil (16.8 mg, 72% yield).

for ^{1}H NMR 

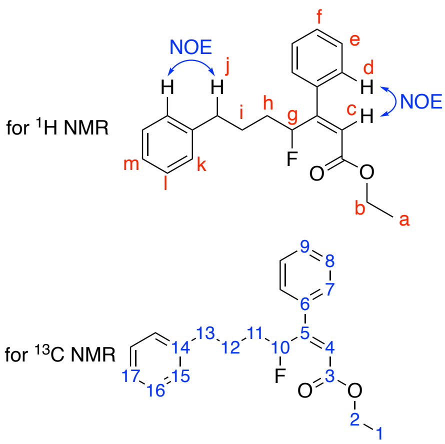
for ^{13}C NMR 

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30–7.15 (m, 5H, H_h–H_j), 6.01 (s, 1H, H_a), 5.27 (dt, 1H, $^{2}J_{H–F}$ = 48.4 Hz, $^{3}J_{H–H}$ = 5.6 Hz, H_d), 2.72–2.65 (m, 2H, H_b), 2.58–2.55 (m, 2H, H_c), 2.43 (m, 2H, H_g), 1.89–1.76 (m, 4H, H_e and H_f); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 208.65 (C2), 177.72 (d, $^{2}J_{C–F}$ = 21.0 Hz, C5), 141.50 (C10), 129.29 (d, $^{3}J_{C–F}$ = 5.7 Hz, C1), 128.60 (C11 or C12), 128.51 (C11 or C12), 126.21 (C13), 91.56 (d, $^{1}J_{C–F}$ = 176.4 Hz, C6), 35.42 (C3), 34.91 (C9), 33.25 (d, $^{2}J_{C–F}$ = 22.9 Hz, C7), 27.51 (d, $^{3}J_{C–F}$ = 4.8 Hz, C4), 26.23 (d, $^{3}J_{C–F}$ = 2.9 Hz, C8); ^{19}F NMR (367 MHz, $CDCl_3$) δ −183.26–−183.52 (m). HRMS (ESI-TOF) m/z calcd. for $C_{15}H_{17}OFNa$ $[M + Na]^+$ 255.11556, found 255.11531.

ethyl (*Z*)-4-fluoro-3,7-diphenylhept-2-enoate (**8x**)

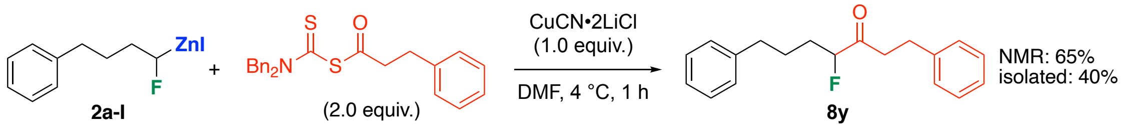


To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, ethyl (*Z*)-3-iodo-3-phenylacrylate (38.0 μL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8x** was determined to be 25% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane/EtOAc = 20/1 as eluent to give mixture of **8x** as colorless oil (7.1 mg, 21% yield).

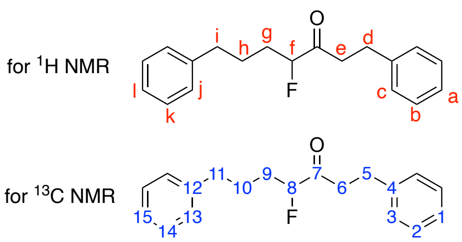


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.15 (m, 10H, H_d–H_f and H_k–H_m), 6.49 (ddd, 1H, $^{2}J_{H\text{–}F}$ = 50.0 Hz, $^{3}J_{H\text{–}H}$ = 9.0 Hz, $^{3}J_{H\text{–}H}$ = 3.6 Hz, H_g), 5.95 (s, 1H, H_c), 4.20 (q, 2H, $^{3}J_{H\text{–}H}$ = 6.8 Hz, H_b), 2.65 (t, 2H, $^{3}J_{H\text{–}H}$ = 7.2 Hz, H_j), 1.98–1.70 (m, 4H, H_h and H_i), 1.29 (t, 3H, $^{3}J_{H\text{–}H}$ = 6.8 Hz, H_a); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 165.57 (C3), 157.64 (d, $^{2}J_{C\text{–}F}$ = 20.1 Hz, C5), 142.90 (C14), 137.51 (C6), {128.93, 128.52, 128.43, 128.27, 125.89} (C7, C8, C9, C15, C16, and C17, overlapped), 120.52 (C4), 90.53 (d, $^{1}J_{C\text{–}F}$ = 167.7 Hz, C10), 60.65 (C2), 35.52 (C13), 34.67 (d, $^{2}J_{C\text{–}F}$ = 20.1 Hz, C11), 27.35 (C12), 14.36 (C1); ^{19}F NMR (367 MHz, $CDCl_3$) δ −172.0 (ddd, $^{2}J_{H\text{–}F}$ = 48.7 Hz, $^{3}J_{H\text{–}F}$ = 32.9 Hz, $^{3}J_{H\text{–}F}$ = 14.9 Hz). HRMS (ESI-TOF) m/z calcd. for $C_{21}H_{23}O_2FNa$ $[M + Na]^+$ 349.15743, found 349.15707.

4-fluoro-1,7-diphenylheptan-3-one (**8y**)



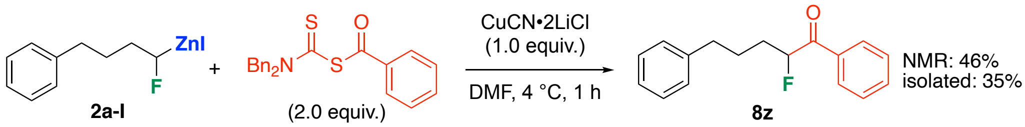
To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, **7r** (81.12 mg, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8y** was determined to be 65% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using toluene to give 8y with impurities. The obtained mixture was further purified by preparative TLC using hexane/EtOAc = 20/1 as eluent to give **8y** as colorless oil (11.37 mg, 40% yield).



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29–7.13 (m, 10H, H_a–H_c and H_j–H_l), 4.81–4.66 (m, 1H, H_f), 2.90–2.89 (m, 4H, H_d and H_i), 2.61 (t, 2H, $^{3}J_{H\text{–}H}$ = 7.2 Hz, H_e), 1.85–1.70 (m, 4H, H_g and H_h); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 209.29 (d, $^{2}J_{C\text{–}F}$ = 24.9 Hz, C7), 141.56 (C4 or C12), 140.87 (C4 or C12), {128.65, 128.55, 128.52} (C2, C3, C13, and C14, overlapped), 126.36 (C1 or C15), 126.14 (C1 or C15), 96.00 (d, $^{1}J_{C\text{–}F}$ =

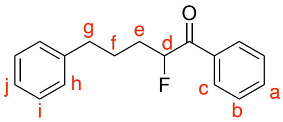
183.1 Hz, C8), 39.87 (C5), 35.46 (C11), 31.58 (d, $^{2}J_{C\text{–}F}$ = 20.0 Hz, C9), 28.83 (C6), 26.33 (C10); ^{19}F NMR (367 MHz, $CDCl_3$) δ −190.39–−190.52. HRMS (ESI-TOF) m/z calcd. for $C_{19}H_{21}OFNa$ [M + Na]$^+$ 307.14686, found 307.14639.

2-fluoro-1,5-diphenylpentan-1-one (**8z**)

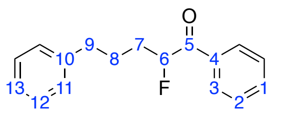


To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, **7s** (75.51 mg, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then quenched with H_2O. The solution was extracted with hexane/EtOAc and dried over Na_2SO_4. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8z** was determined to be 46% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using toluene as eluent to give **8z** with impurities. The obtained mixture was further purified by preparative TLC using hexane/EtOAc = 20/1 as eluent to give **8z** as colorless oil (9.0 mg, 35% yield).

for ^{1}H NMR

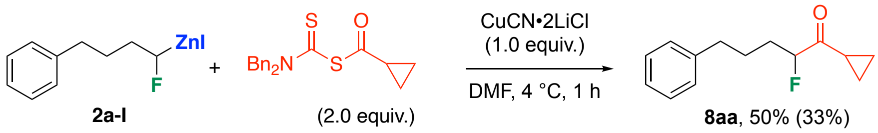


for ^{13}C NMR



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95–7.15 (m, 10H, H_a–H_c and H_h–H_j), 5.64–5.44 (m, 1H, H_d), 2.68 (t, 2H, $^{3}J_{H\text{–}H}$ = 15.1 Hz, H_g), 2.07–1.80 (m, 4H, H_e and H_f); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$); δ 196.86 (d, $^{2}J_{C\text{–}F}$ = 19.3 Hz, C7), 141.52 (C10), 134.33 (C1), 133.88 (C2), 129.00 (d, $^{3}J_{C\text{–}F}$ = 3.9 Hz, C4), {128.87, 128.56, 128.52} (C3, C11, and C12), 126.14 (C13), 93.77 (d, $^{1}J_{C\text{–}F}$ = 183.0 Hz, C6), 35.36 (C9), 32.27 (d, $^{2}J_{C\text{–}F}$ = 21.2 Hz, C6), 26.46 (d, $^{3}J_{C\text{–}F}$ = 2.9 Hz, C8); ^{19}F NMR (367 MHz, $CDCl_3$) δ −188.87–−189.13 (m). HRMS (EI-TOF) m/z calcd. for $C_{17}H_{17}FO$ [M]$^+$ 256.12579, found 256.12576.

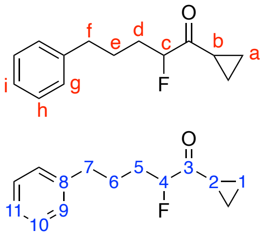
1-cyclopropyl-2-fluoro-5-phenylpentan-1-one (**8aa**)



To a test tube equipped with a magnetic stir bar were added **7t** (68.3 mg, 0.20 mmol, 2.0 equiv.) and freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 ℃, CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol, 1.0 equiv.) was added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8aa** was determined to be 50% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by column chromatography using hexane/EtOAc = 20/1 as eluent to give **8aa** with impurities. The obtained mixture was further purified by preparative TLC using toluene/hexane = 2/1 as eluent to give **8aa** as colorless oil (7.3 mg, 33% yield).

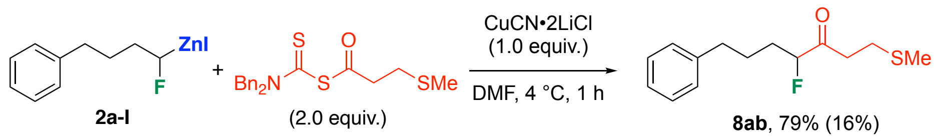
for ^{1}H NMR

for ^{13}C NMR



^{1}H NMR (500 MHz, CDCl$_3$) δ 7.29–7.16 (m, 5H, H$_g$–H$_i$), 4.86 (ddd, 1H, $^2J_{H-F}$ = 50.4 Hz, $^3J_{H-H}$ = 7.1 Hz, $^3J_{H-H}$ = 4.6 Hz, H$_c$), 2.67–2.64 (m, 2H, H$_f$), 2.34–2.27 (m, 1H, H$_b$), 1.93–1.78 (m, 4H, H$_d$ and H$_e$), 1.11–1.08 (m, 2H, H$_a$), 0.99–0.96 (m, 2H, H$_a$); ^{13}C{^{1}H} NMR (125 MHz, CDCl$_3$) δ 209.58 (d, $^2J_{C-F}$ = 23.4 Hz, C3), 141.68 (C8), {128.55, 128.54} (C9 and C10), 126.11 (C11), 96.52 (d, $^1J_{C-F}$ = 58.6 Hz, C4), 35.51 (C7), 31.79 (d, $^2J_{C-F}$ = 21.0 Hz, C5), 26.36 (d, $^3J_{C-F}$ = 3.0 Hz, C6), 16.22 (d, $^3J_{C-F}$ = 2.4 Hz, C2), 12.28 (C1), 12.25 (C1); ^{19}F NMR (470 MHz, CDCl$_3$) δ −191.11–−191.36. HRMS (ESI-TOF) m/z calcd. for $C_{14}H_{17}OFNa$ [M + Na]$^+$ 243.11556, found 243.11521.

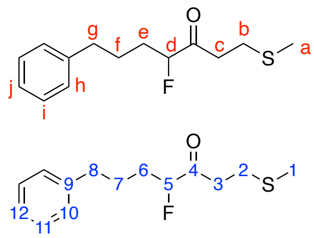
4-fluoro-1-(methylthio)-7-phenylheptan-3-one (**8ab**)



To a test tube equipped with a magnetic stir bar were added **7u** (75.5 mg, 0.20 mmol, 2.0 equiv.) and freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol, 1.0 equiv.) was added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8ab** was determined to be 79% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by column chromatography using toluene/hexane = 20/1 as eluent to give **8ab** with impurities. The obtained mixture was further purified by preparative TLC twice using hexane/EtOAc = 20/1 and hexane/EtOAc/CH_2Cl_2 = 20/20/1 as eluents to give **8ab** as pale brown oil (4.0 mg, 16% yield).

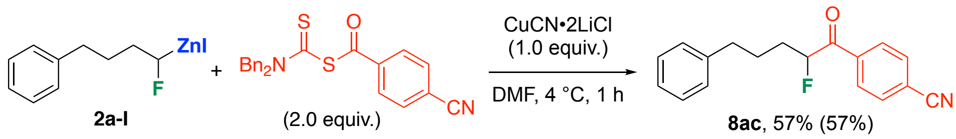
for ^{1}H NMR

for ^{13}C NMR

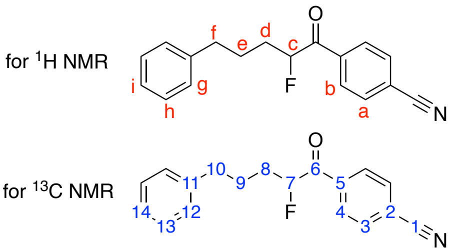


^{1}H NMR (500 MHz, CDCl$_3$) δ 7.23–7.15 (m, 5H, H$_h$–H$_j$), 4.77 (ddd, 1H, $^2J_{H-F}$ = 50.3 Hz, $^3J_{H-H}$ = 7.8 Hz, $^3J_{H-H}$ = 4.0 Hz, H$_d$), 2.96–2.83 (m, 2H, H$_c$), 2.72 (t, 2H, $^3J_{H-H}$ = 7.3 Hz, H$_g$), 2.64 (t, 2H, $^3J_{H-H}$ = 7.0 Hz, H$_g$), 2.10 (s, 3H, H$_a$), 1.90–1.76 (m, 4H); ^{13}C{^{1}H} NMR (125 MHz, CDCl$_3$) δ 208.55 (d, $^2J_{C-F}$ = 25.3 Hz, C4), 141.52 (C9), {128.75, 128.53} (C10 and C11), 126.16 (C12), 98.03 (d, $^1J_{C-F}$ = 183.0 Hz, C5), 38.26 (C2), 35.45 (C8), 31.56 (d, $^2J_{C-F}$ = 20.6 Hz, C6), 27.17 (d, $^3J_{C-F}$ = 2.4 Hz, C3), 26.34 (d, $^3J_{C-F}$ = 2.4 Hz, C7), 15.92 (C1); ^{9}F NMR (470 MHz, CDCl$_3$) δ −192.17–−192.38. HRMS (ESI-TOF) m/z calcd. for $C_{14}H_{19}OFNaS$ [M + Na]$^+$ 277.10329, found 277.10287.

4-(2-fluoro-5-phenylpentanoyl)benzonitrile (**8ac**)

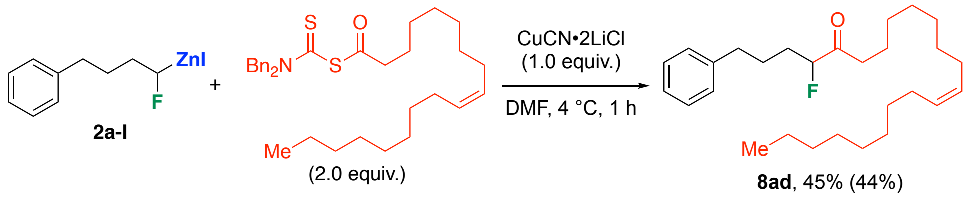


To a test tube equipped with a magnetic stir bar were added **7v** (40.5 mg, 0.20 mmol, 2.0 equiv.) and freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol, 1.0 equiv.) was added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8ac** was determined to be 57% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by column chromatography using hexane/EtOAc = 20/1 as eluent to give **8ac** with impurities. The obtained mixture was further purified by preparative TLC using hexane/toluene = 20/1 a to give **8ac** as colorless oil (16.0 mg, 57% yield).



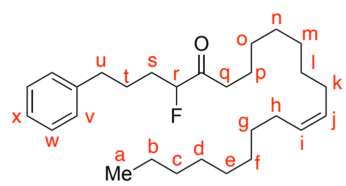
^{1}H NMR (500 MHz, CDCl$_3$) δ 8.00 (d, 2H, $^{3}J_{H–H}$ = 7.5 Hz, H$_a$), 7.75 (d, 2H, $^{3}J_{H–H}$ = 7.5 Hz, H$_b$), 7.30–7.15 (m, 5H, H$_g$–H$_i$), 5.46 (dt, 1H, $^{2}J_{H–F}$ = 49.5 Hz, $^{3}J_{H–H}$ = 5.8 Hz, H$_c$), 2.69 (t, 2H, $^{3}J_{H–H}$ = 7.5 Hz, H$_f$), 2.04–1.82 (m, 4H, H$_d$ and H$_e$); ^{13}C{^{1}H} NMR (125 MHz, CDCl$_3$) δ 196.12 (d, $^{2}J_{C–F}$ = 21.2 Hz, C6), 141.26 (C11), 137.50 (C2), 132.58 (C3), 129.59 (d, $^{3}J_{C–F}$ = 4.8 Hz, C5), {128.61, 128.50} (C12 and C13), 126.24 (C4), 117.86 (C1), 117.03 (C2), 183.25 (d, $^{1}J_{C–F}$ = 183.3 Hz, C7), 35.26 (C10), 31.87 (d, $^{2}J_{C–F}$ = 20.8 Hz, C8), 26.29 (d, $^{3}J_{C–F}$ = 3.0 Hz, C9); ^{19}F NMR (470 MHz, CDCl$_3$) δ −188.42 (dt, $^{2}J_{H–F}$ = 49.8 Hz, $^{3}J_{H–F}$ = 24.7 Hz). HRMS (EI-TOF) m/z calcd. for. $C_{18}H_{16}ONF$ [M]$^{+}$ 281.12104, found 281.12068.

(*Z*)-4-fluoro-1-phenyldocos-13-en-5-one (**8ad**)

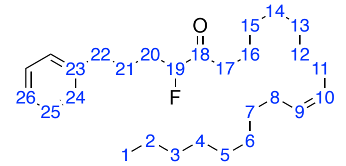


To a test tube equipped with a magnetic stir bar were added **7w** (108 mg, 0.20 mmol, 2.0 equiv.) and freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol, 1.0 equiv.) was added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8ad** was determined to be 45% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by column chromatography using hexane/EtOAc = 40/1 as eluent to give **8ad** with impurities. The obtained mixture was further purified by preparative TLC using hexane/toluene = 20/1 a to give **8ad** as colorless oil (18.3 mg, 44% yield).

for ^{1}H NMR

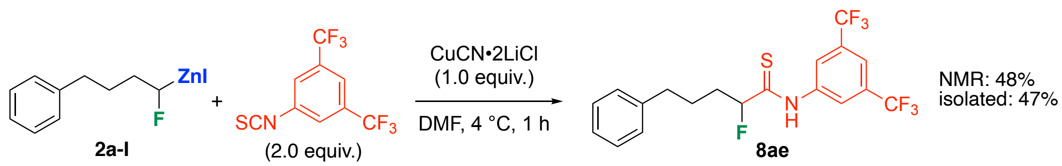


for ^{13}C NMR



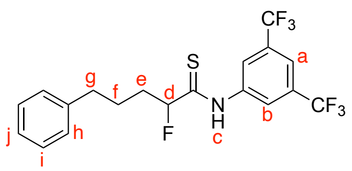
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29–7.15 (m, 5H, H_v–H_x), 5.35–5.29 (m, 2H, H_i and H_j), 4.71–4.65 (m, 1H, H_r), 2.64 (t, 2H, $^{3}J_{H–H}$ = 7.2 Hz, H_u), 2.60–2.48 (m, 2H, H_q), 2.01–1.98 (m, 4H, H_h and H_k), 1.81–1.75 (m, 4H, H_s and H_t), 1.32–1.20 (m, 22H, H_b–H_f and H_l–H_p), 0.87 (t, 3H, $^{3}J_{H–H}$ = 7.2 Hz, H_a); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 210.41 (d, $^{2}J_{C–F}$ = 24.0 Hz, C18), 141.62 (C23), {130.16, 129.89} (C9 and C10), {128.55, 128.52} (C24 and C25), 126.13 (C26), 96.00 (d, $^{1}J_{C–F}$ = 183.1 Hz, C19), {38.21, 35.49, 32.05} (C8, C11, and C22), 31.70 (d, $^{2}J_{C–F}$ = 21.1 Hz, C20), {29.92, 29.84, 29.78, 29.48, 29.43, 29.27, 29.25, 22.84, 22.79} (C2, C3, C4, C5, C6, C7, C12, C13, C14, C15, C16, two carbons overlapped), 27.34 (d, $^{3}J_{C–F}$ = 5.7 Hz, C17), 26.44 (d, $^{3}J_{C–F}$ = 2.9 Hz, C21), 14.27 (C1); ^{19}F NMR (367 MHz, $CDCl_3$) δ −191.52–−191.88 (m). HRMS (ESI-TOF) m/z calcd. for $C_{28}H_{45}OFNa$ $[M + Na]^+$ 439.33467, found 439.33400.

N-(3,5-bis(trifluoromethyl)phenyl)-2-fluoro-5-phenylpentanethioamide (**8ae**)

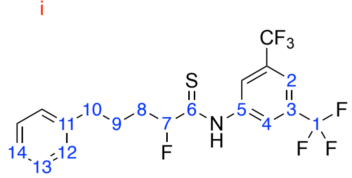


To a test tube equipped with a magnetic stir bar were added freshly prepared **2a-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, 1-isothiocyanato-3,5-bis(trifluoromethyl)benzene (38.0 μL, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then quenched with H_2O. The solution was extracted with hexane/EtOAc and dried over Na_2SO_4. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8ae** was determined to be 48% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane as eluent to give mixture of **8ae** as yellow oil (19.8 mg, 47% yield).

for ^{1}H NMR

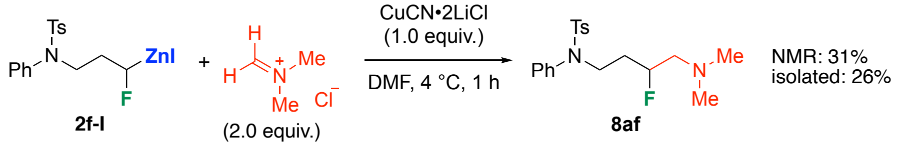


for ^{13}C NMR

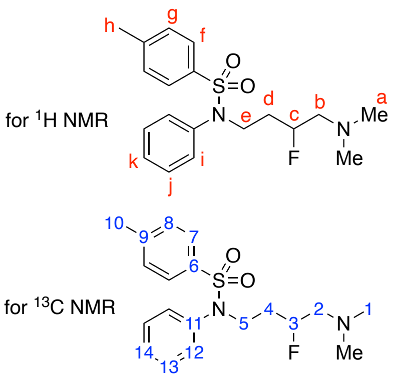


^{1}H NMR (400 MHz, $CDCl_3$) δ 9.49 (d, 1H, $^{4}J_{H–F}$ = 11.6 Hz, H_c), 8.37 (s, 2H, H_b), 7.78 (s, 1H, H_a), 7.31–7.17 (m, 5H, H_h–H_j), 5.34 (ddd, 1H, $^{2}J_{H–F}$ = 51.0 Hz, $^{3}J_{H–H}$ = 7.6 Hz, $^{3}J_{H–H}$ = 3.4 Hz, H_d), 2.76–2.63{2.72 (dt, 1H, $^{2}J_{H–H}$ = 10.0 Hz, $^{3}J_{H–H}$ = 7.0 Hz, H_g), 2.66 (dt, 1H, $^{2}J_{H–H}$ = 10.0 Hz, $^{3}J_{H–H}$ = 7.0 Hz, H_g)}, 2.42–2.23 (m, 1H, H_e), 2.16–2.00 (m, 1H, H_e), 1.91–1.83 (m, 2H, H_f); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 198.85 (d, $^{3}J_{C–F}$ = 11.5 Hz, C6), 141.49 (C11), 138.79 (C5), 132.64 (q, $^{2}J_{C–F}$ = 34.5 Hz, C3), 128.62 (C12 or C13), 128.65 (C12 or C13), 126.23 (C14), 123.15 (m, C4), 122.97 (q, $^{1}J_{C–F}$ = 271.2 Hz, C1), 120.59 (m, C1), 98.66 (d, $^{1}J_{C–F}$ = 192.6 Hz, C7), 35.44 (C10), 35.34 (d, $^{3}J_{C–F}$ = 20.1 Hz, C8), 26.30 (C9); ^{19}F NMR (367 MHz, CDCl3) δ −61.35 (s), −173.74–−174.06 (m). HRMS (ESI-TOF) m/z calcd. for $C_{19}H_{15}NF_7S$ $[M – H]^+$422.08189, found 422.08212.

N-(4-(dimethylamino)-3-fluorobutyl)-4-methyl-*N*-phenylbenzenesulfonamide (**8af**)

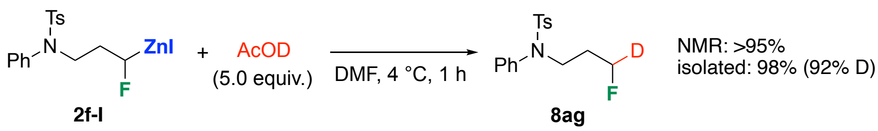


To a test tube equipped with a magnetic stir bar were added freshly prepared **2f-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). After the solution was cooled to 4 °C, Eschenmoser's salt (18.7 mg, 0.20 mmol, 2.0 equiv.) and CuCN•2LiCl in THF (0.10 mL, 1.0 M, 0.10 mmol) were subsequently added to the solution. The reaction mixture was further stirred for 1 hour at 4 °C and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8af** was determined to be 31% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using hexane/EtOAc = 20/1 as eluent to give mixture of **8af** as brown oil (9.6 mg, 26% yield).

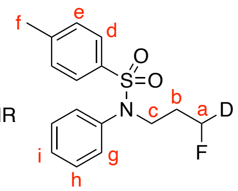


^{1}H NMR (400 MHz, CDCl$_3$) δ 7.44 (d, 2H, $^3J_{H\text{–}H}$ = 8.0 Hz, H$_f$), 7.33–7.28 (m, 3H, H$_j$ and H$_k$), 7.21 (d, 2H, $^3J_{H\text{–}H}$ = 8.0 Hz, H$_g$), 7.04–7.02 (m, 2H, H$_i$), 4.79–4.61 (m, 1H, H$_c$), 3.74–3.59{3.70 (dt, 1H, $^2J_{H\text{–}H}$ = 13.6 Hz, $^3J_{H\text{–}H}$ = 7.2 Hz, H$_e$), 3.64(dt, 1H, $^2J_{H\text{–}H}$ = 13.6 Hz, $^3J_{H\text{–}H}$ = 7.2 Hz, H$_e$)}, 2.54 (ddd, 1H, $^2J_{H\text{–}H}$ = 13.8 Hz, $^3J_{H\text{–}F}$ = 19.2 Hz, $^3J_{H\text{–}H}$ = 8.0 Hz, H$_b$), 2.41 (s, 3H, H$_h$), 2.32 (ddd, 1H, $^2J_{H\text{–}H}$ = 13.8 Hz, $^3J_{H\text{–}F}$ = 30.0 Hz, $^3J_{H\text{–}H}$ = 3.6 Hz, H$_b$), 2.24 (s, 6H, H$_a$), 1.75–1.60 (m, 2H, H$_d$); ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 143.67 (C11), 139.22 (C6), 134.92 (C10), {129.57, 129.25, 128.79, 128.16, 127.89} (C7, C8, C12, C13, and C14), 89.87 (d, $^1J_{C\text{–}F}$ = 172.6 Hz, C3), 63.12 (d, $^2J_{C\text{–}F}$ = 21.0 Hz, C2), 47.08 (d, $^3J_{C\text{–}F}$ = 4.7 Hz, C5), 46.14 (C1), 32.68 (d, $^2J_{C\text{–}F}$ = 21.0 Hz, C4), 21.71 (C10); ^{19}F NMR (367 MHz, CDCl$_3$) δ −182.81–−183.19 (m). HRMS (ESI-TOF) m/z calcd. for $C_{19}H_{26}O_2N_2FS$ [M + H]$^+$ 365.16935, found 365.16898.

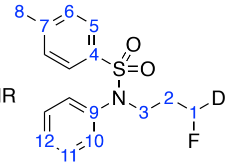
N-(3-fluoropropyl-3-d)-4-methyl-*N*-phenylbenzenesulfonamide (**8ag**)



To a test tube equipped with a magnetic stir bar were added freshly prepared **2f-I** in DMF (0.40 mL, 0.25 M, 0.10 mmol). Acetic acid-*d*$_1$ (28.8 µL, 0.50 mmol, 5.0 equiv.) was subsequently added to the solution. The reaction mixture was further stirred for 1 hour at room temperature and then poured into a slurry of silica gel in hexane. The slurry was then filtered and washed with hexane/EtOAc. The resulted solution was concentrated under reduced pressure to give crude mixture. The NMR yield of **8ag** was determined to be >95% yield respectively by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The crude mixture was purified by preparative TLC using /EtOAc = 8/1 as eluent to give mixture of **8ag** as white solid (30.3 mg, 98% yield, 92% deuteration). The ratio of deuteration was determined by ^{19}F NMR spectroscopy (for D: −220.35–−220.65, for H: −219.68–−220.08) for ^{1}H NMR



for ^{13}C NMR



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, 2H, $^{3}J_{H–H}$ = 8.0 Hz, H_d), 7.32–7.22 (m, 3H, H_h and H_i), 7.23 (d, 2H, $^{3}J_{H–H}$ = 8.0 Hz, H_e), 7.06–7.02 (m, 2H, H_g), 4.46 (dt, 1H, $^{2}J_{H–F}$ = 48.0 Hz, $^{3}J_{H–H}$ = 6.4 Hz, H_e), 3.66 (t, 2H, $^{3}J_{H–H}$ = 6.8 Hz, H_c), 2.40 (s, 3H, H_f), 1.83 (ddt, 2H, $^{3}J_{H–F}$ = 26.0 Hz, $^{3}J_{H–H}$ = 6.4 Hz, $^{3}J_{H–H}$ = 6.4 Hz, H_b); 143.65 (C9), 139.23 (C4), 135.05 (C7), {129.54, 129.34, 128.79, 128.14, 127.86} (C5, C6, C10, C11, and C12), 80.99 (dt, $^{1}J_{C–F}$ = 190.8 Hz, $^{1}J_{C–D}$ = 23.0 Hz, C1), 47.10 (d, $^{3}J_{C–F}$ = 5.8 Hz, C3), 29.58 (d, $^{2}J_{C–F}$ = 21.0 Hz, C2), 21.65 (C8); ^{19}F NMR (367 MHz, $CDCl_3$) δ −220.35–−220.65 (m). HRMS (ESI-TOF) m/z calcd. for $C_{16}H_{17}DO_2NFSNa$ [M + H]$^{+}$ 331.09973, found 331.09919.

8. References in Supporting Information

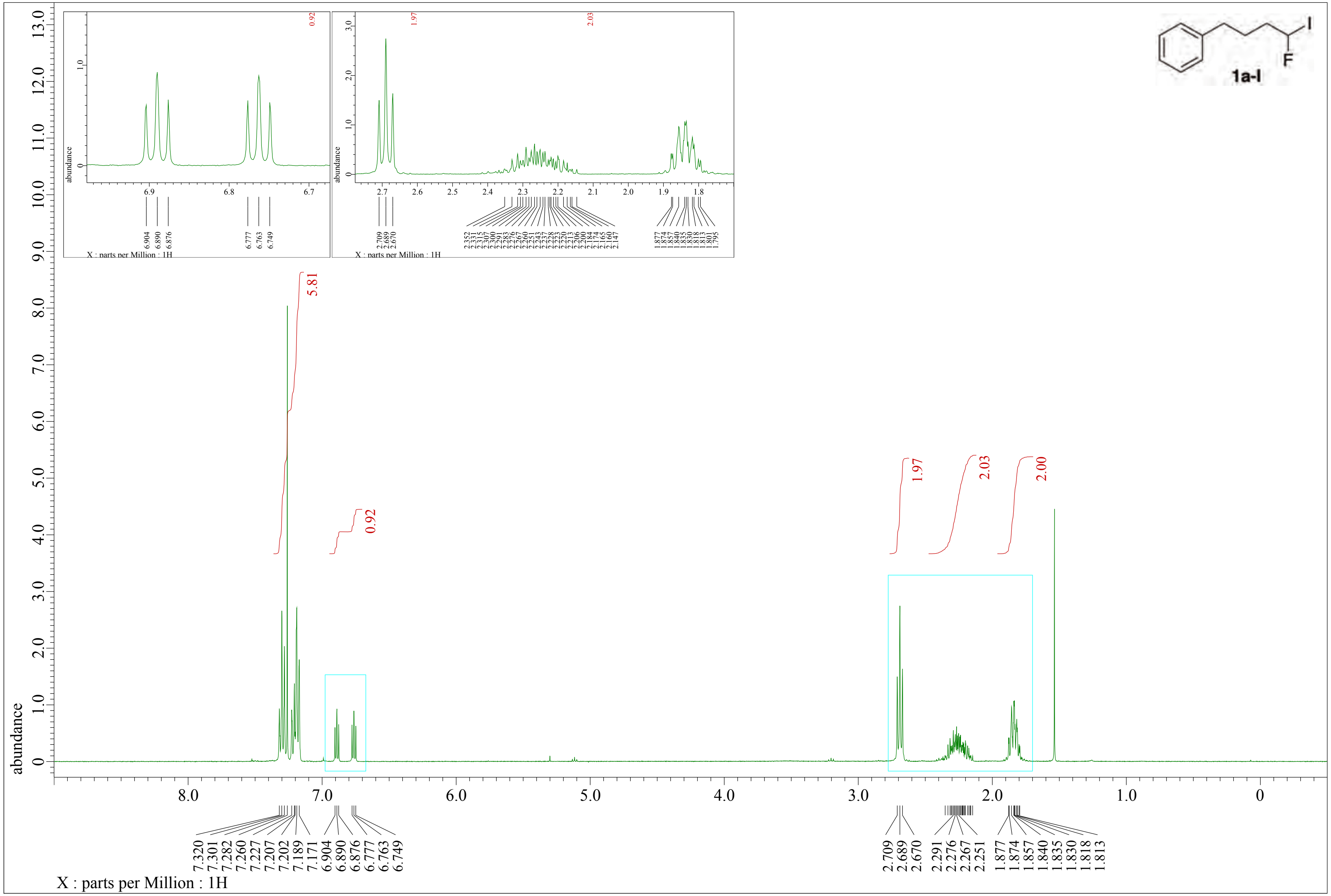
[S1] Jiang, X.; Sakthivel, S.; Kulbitski, K; Nisnevich, G.; Gandelman, M. Efficient synthesis of secondary alkyl fluorides via Suzuki cross-coupling reactioin of 1-halo-1-fluoroalkanes. *J. Am. Chem. Soc.* **2014**, *136*, 9548–9551.

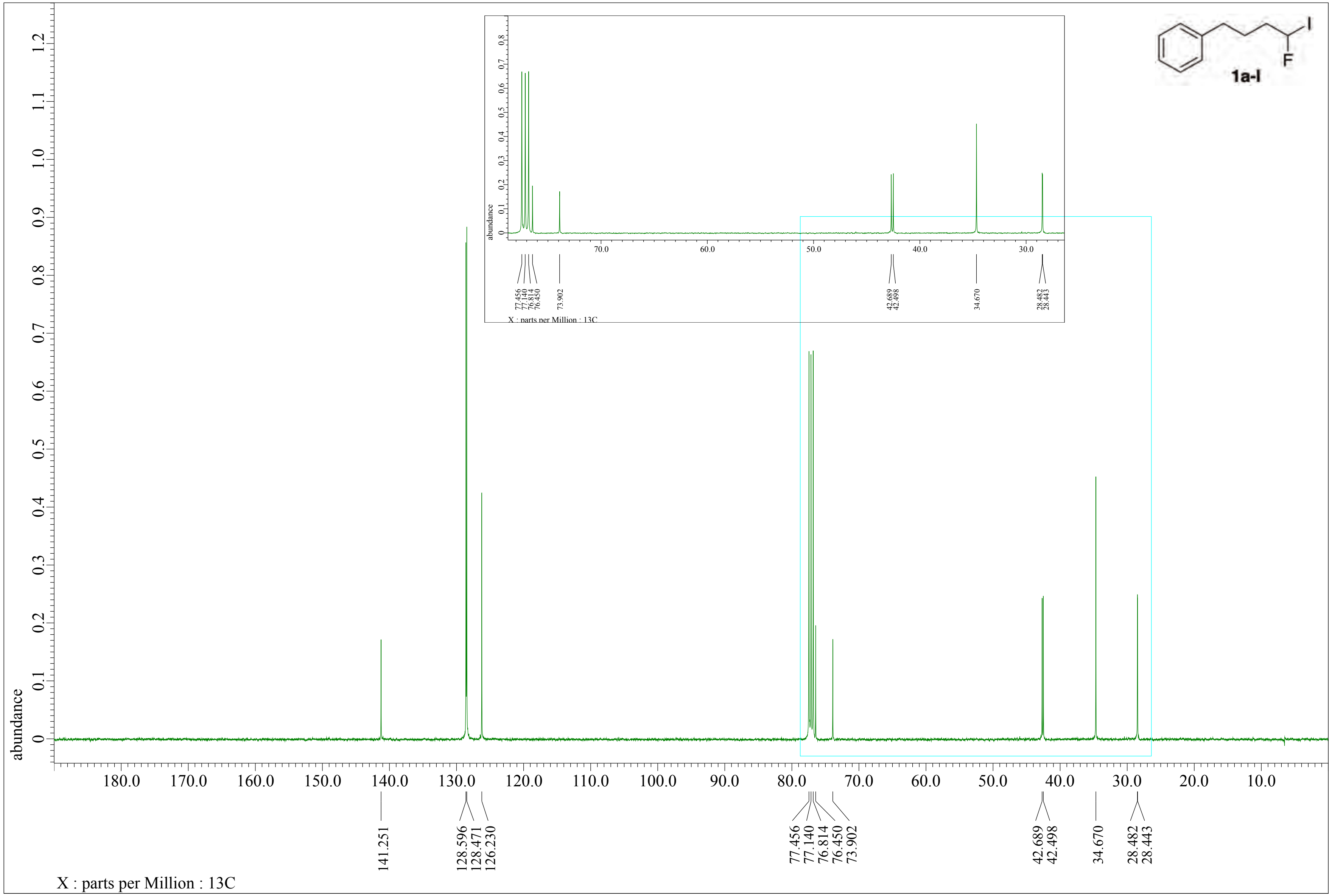
[S2] Wu, B.-B.; Xu, J.; Gao, Q.; Bian, K.-J.; Liu, G.-K.; Wang, X.-S. A general and efficient solution to monofluoroalkylation: Divergent synthesis of aliphatic monofluorides with modular synthetic scaffolds. *Angew. Chem. Int. Ed.* **2022**, *61*, e202208938.

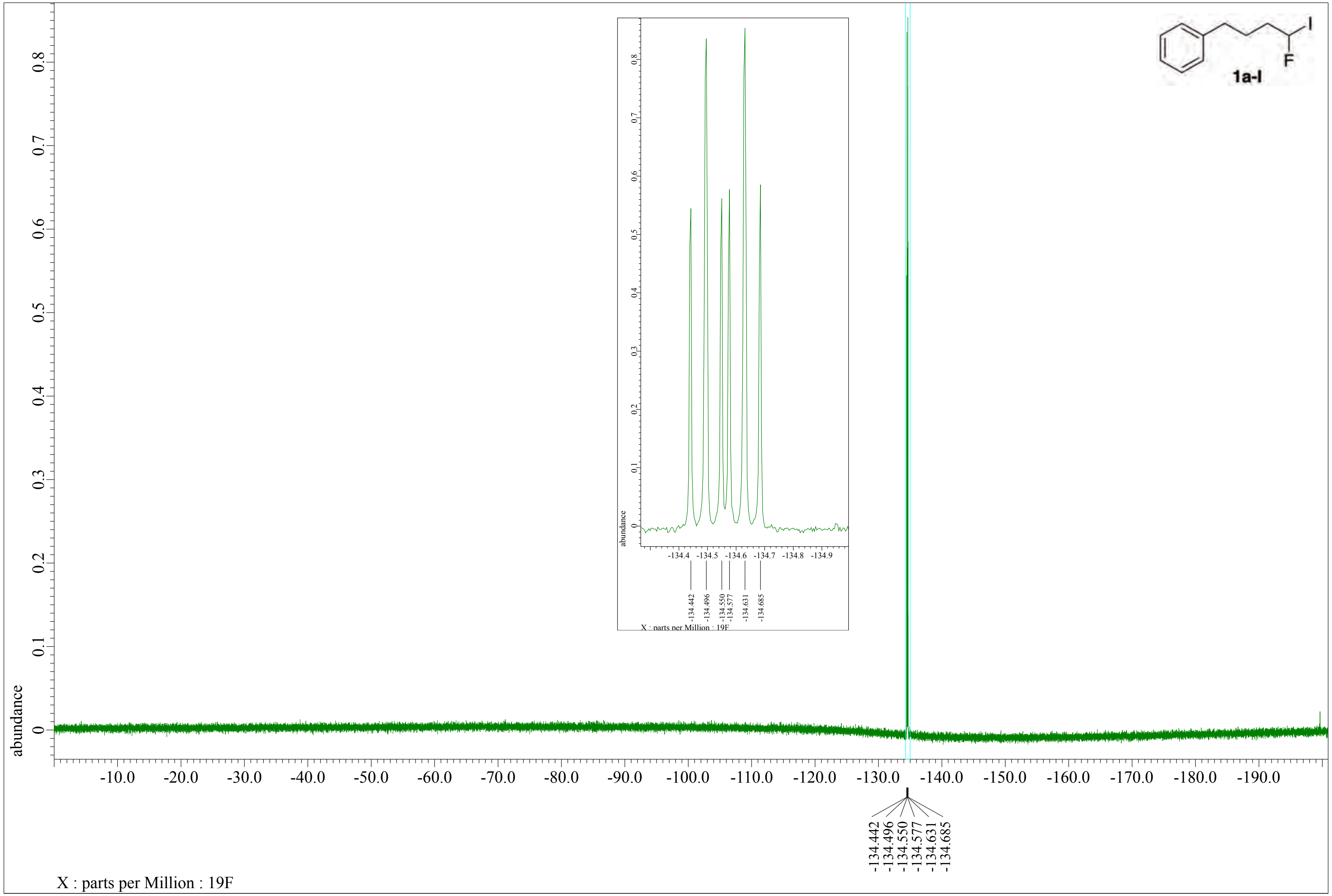
[S3] Jiang, X.; Gandelman, M. Enantioselective Suzuki cross-coupling of unactivated 1-fluoro-1-haloalkanes: Synthesis of chiral β-, γ-, δ-, and ε-fluoroalkanes. *J. Am. Chem. Soc.* **2015**, *137*, 2542–2547.

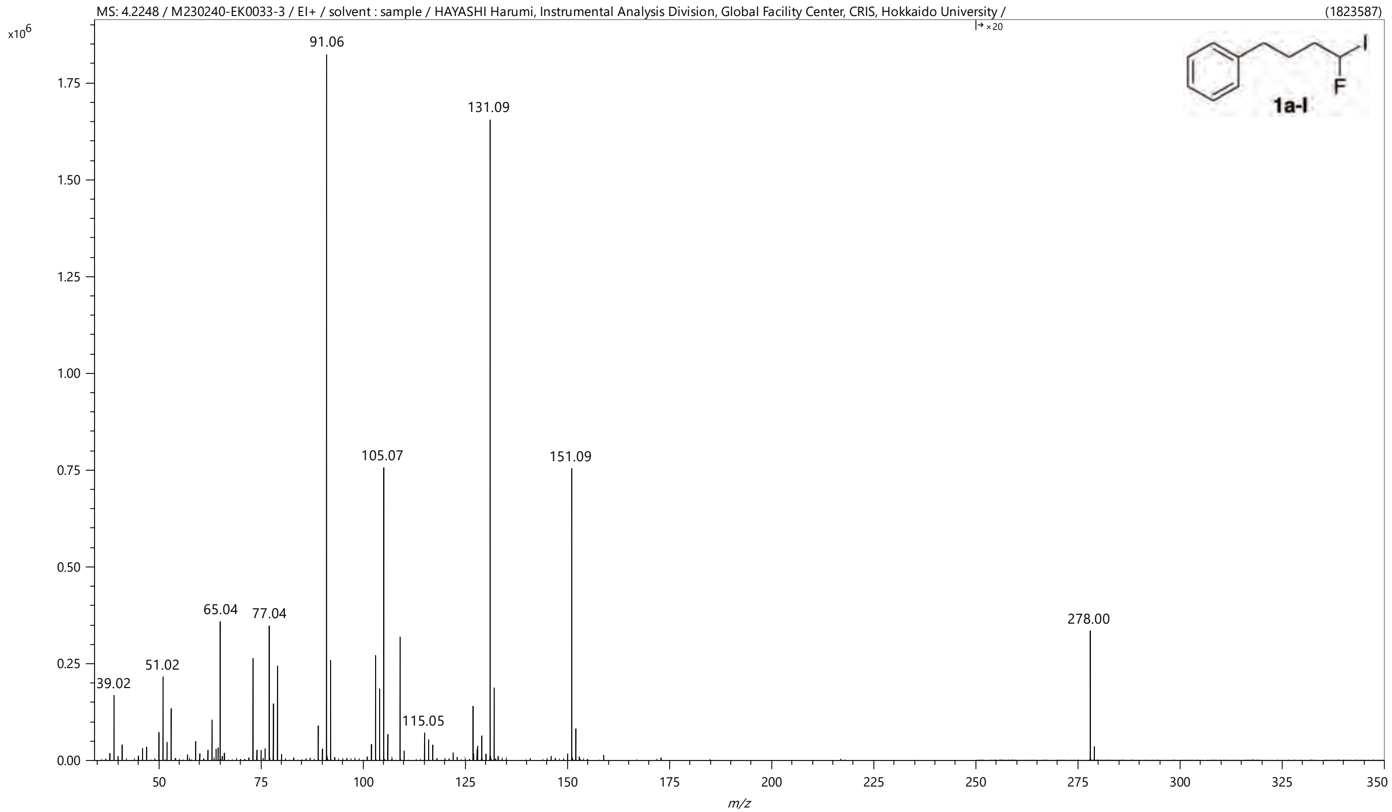
[S4] Huang, W.; Wan, X.; Shen, Q. Cobalt-catalyzed asymmetric cross-coupling reaction of fluorinated secondary benzyl bromides with lithium aryl boronates/$ZnBr_2$. *Org. Lett.* **2020**, *22*, 4327–4332.

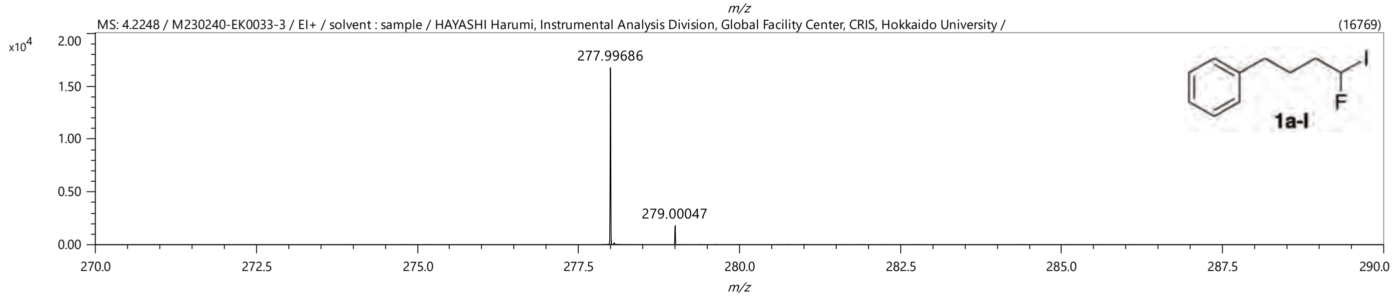
9. NMR and Mass Spectra of the Literature New Compounds

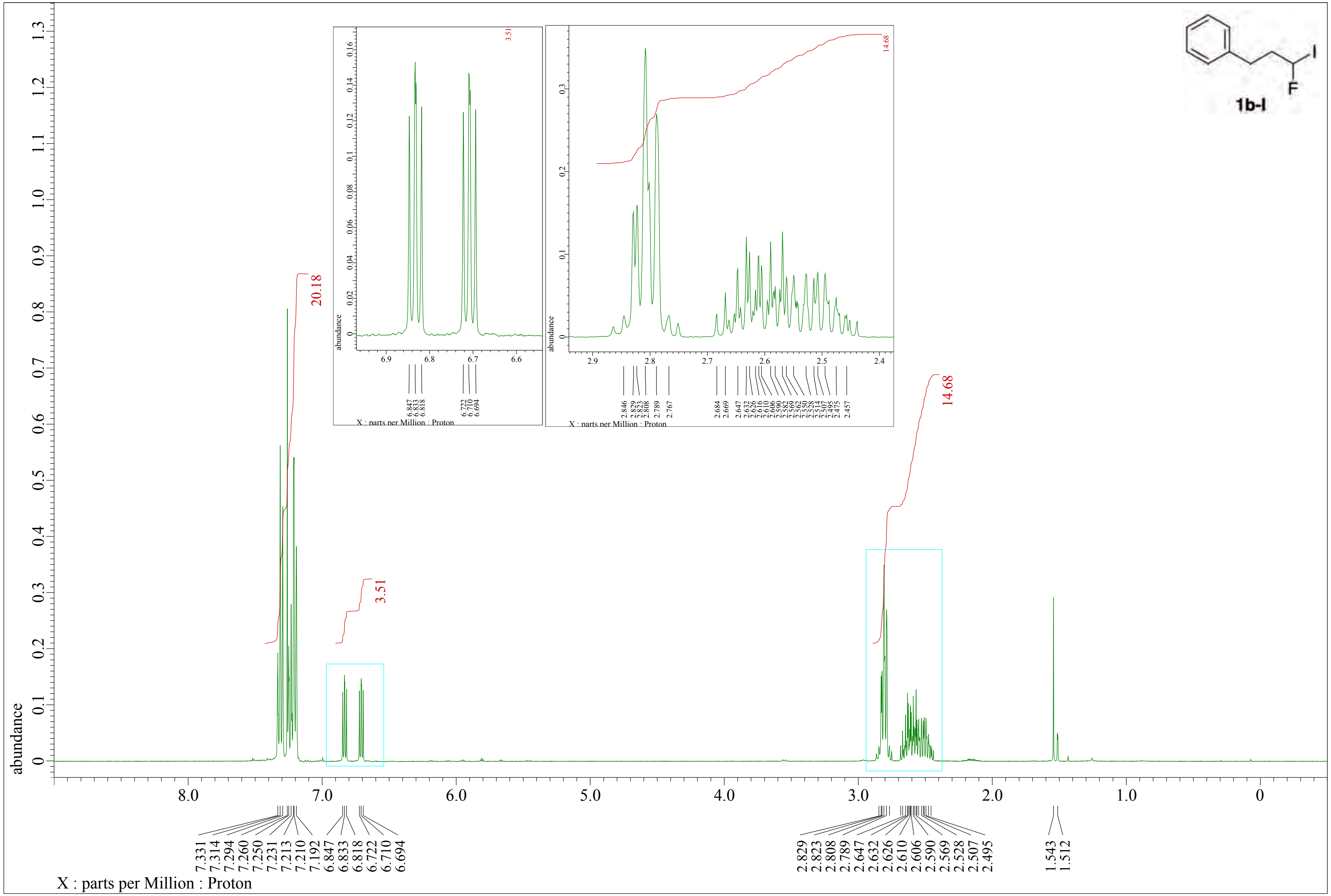



1a-I
abundance
X : parts per Million : 13C
141.251
128.596
128.471
126.230
77.456
77.140
76.814
76.450
73.902
42.689
42.498
34.670
28.482
28.443

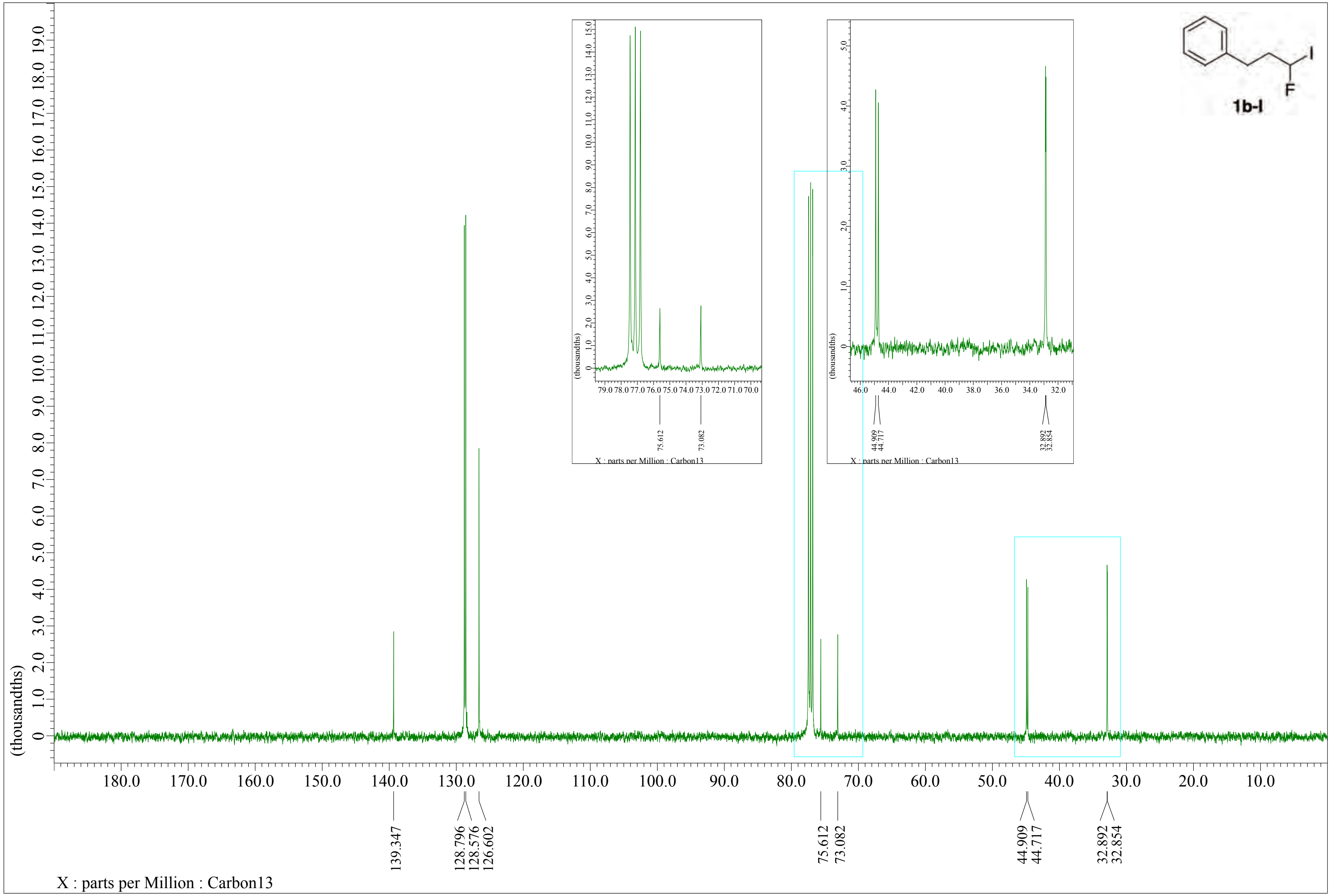

1a-I
abundance
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
-134.442
-134.496
-134.550
-134.577
-134.631
-134.685
X : parts per Million : 19F

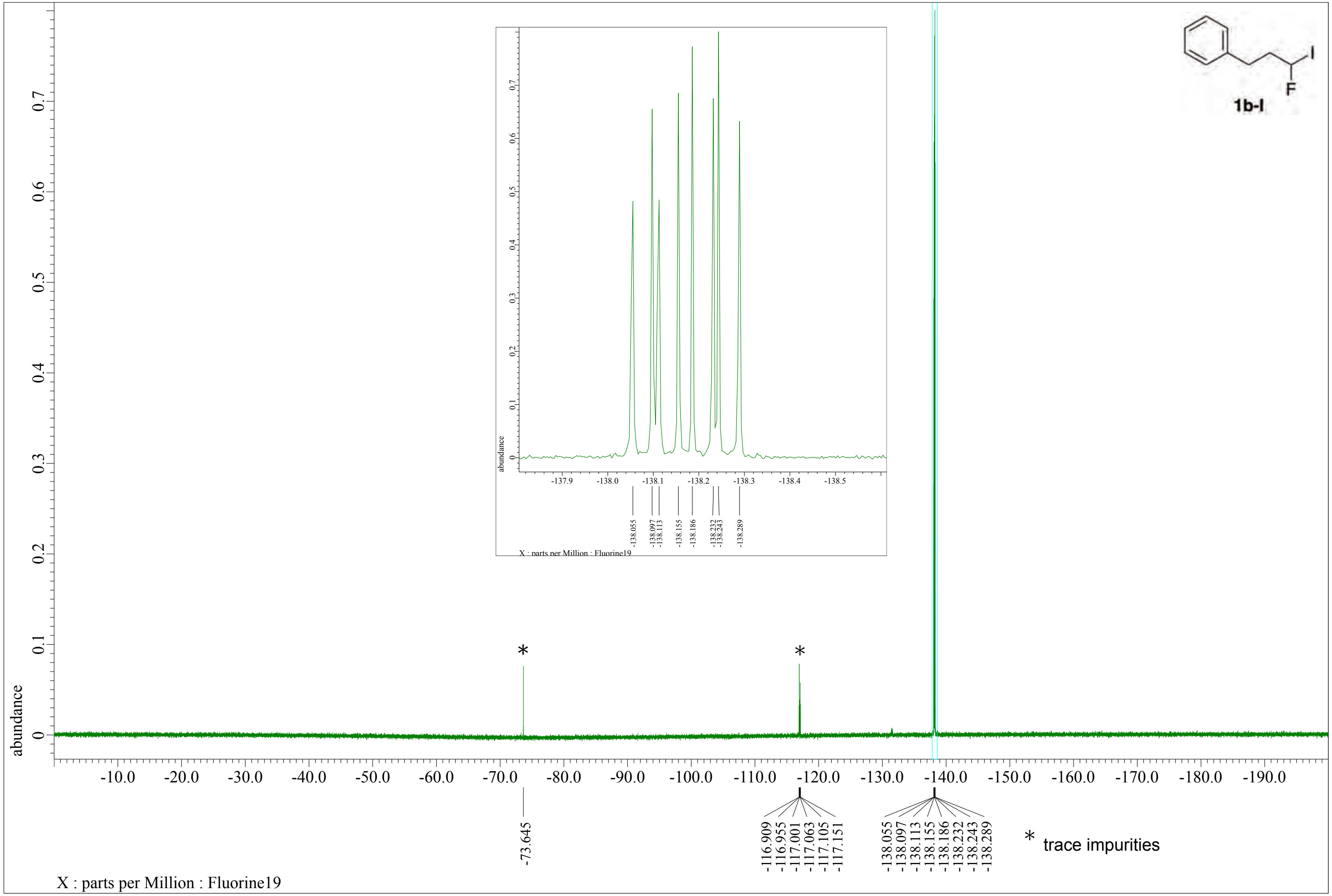

MS: 4.2248 / M230240-EK0033-3 / EI+ / solvent : sample / HAYASHI Harumi, Instrumental Analysis Division, Global Facility Center, CRIS, Hokkaido University /
(1823587)
x10^6
91.06
131.09
105.07
151.09
65.04
77.04
278.00
51.02
39.02
115.05
1a-I
F
I
m/z

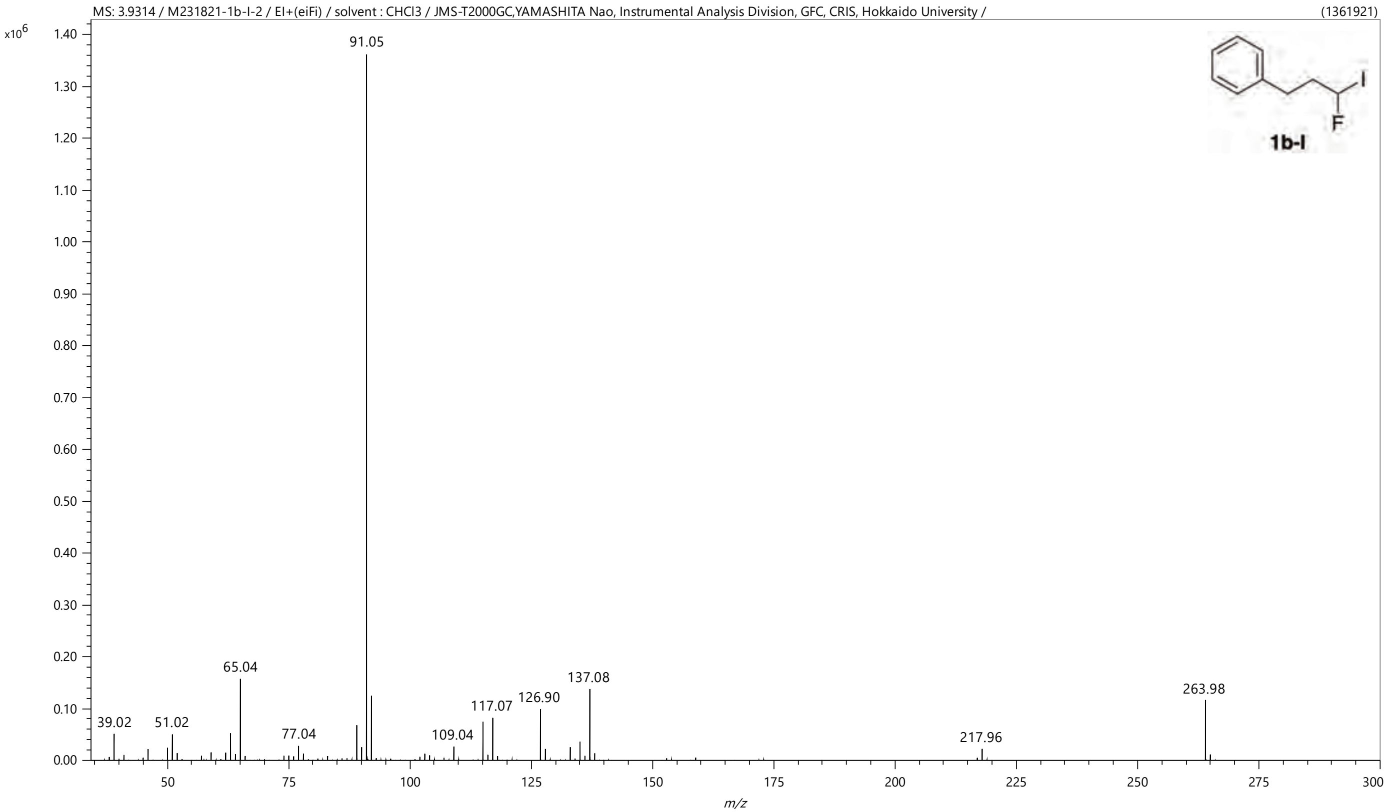

m/z
MS: 4.2248 / M230240-EK0033-3 / EI+ / solvent : sample / HAYASHI Harumi, Instrumental Analysis Division, Global Facility Center, CRIS, Hokkaido University /
(16769)
x10^4
277.99686
279.00047
1a-I
F
I
m/z



1b-I
F
I
abundance
X : parts per Million : Proton
20.18
3.51
14.68
7.331
7.314
7.294
7.260
7.250
7.231
7.213
7.210
7.192
6.847
6.833
6.818
6.722
6.710
6.694
2.829
2.823
2.808
2.789
2.647
2.632
2.626
2.610
2.606
2.590
2.569
2.528
2.507
2.495
1.543
1.512


1b-I
(thousandths)
139.347
128.796
128.576
126.602
75.612
73.082
44.909
44.717
32.892
32.854
X : parts per Million : Carbon13


1b-I
abundance
X : parts per Million : Fluorine19
-73.645
-116.909
-116.955
-117.001
-117.063
-117.105
-117.151
-138.055
-138.097
-138.113
-138.155
-138.186
-138.232
-138.243
-138.289
* trace impurities



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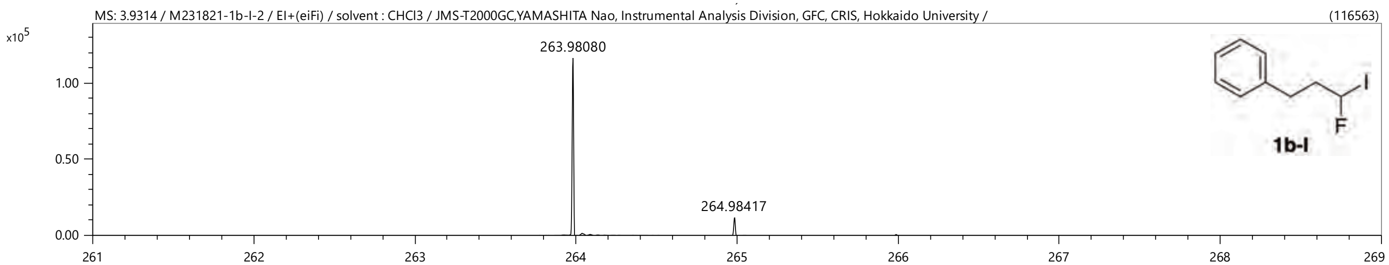
(1361921)
x10^6
91.05
65.04
137.08
117.07
126.90
39.02
51.02
77.04
109.04
217.96
263.98
m/z
1b-I



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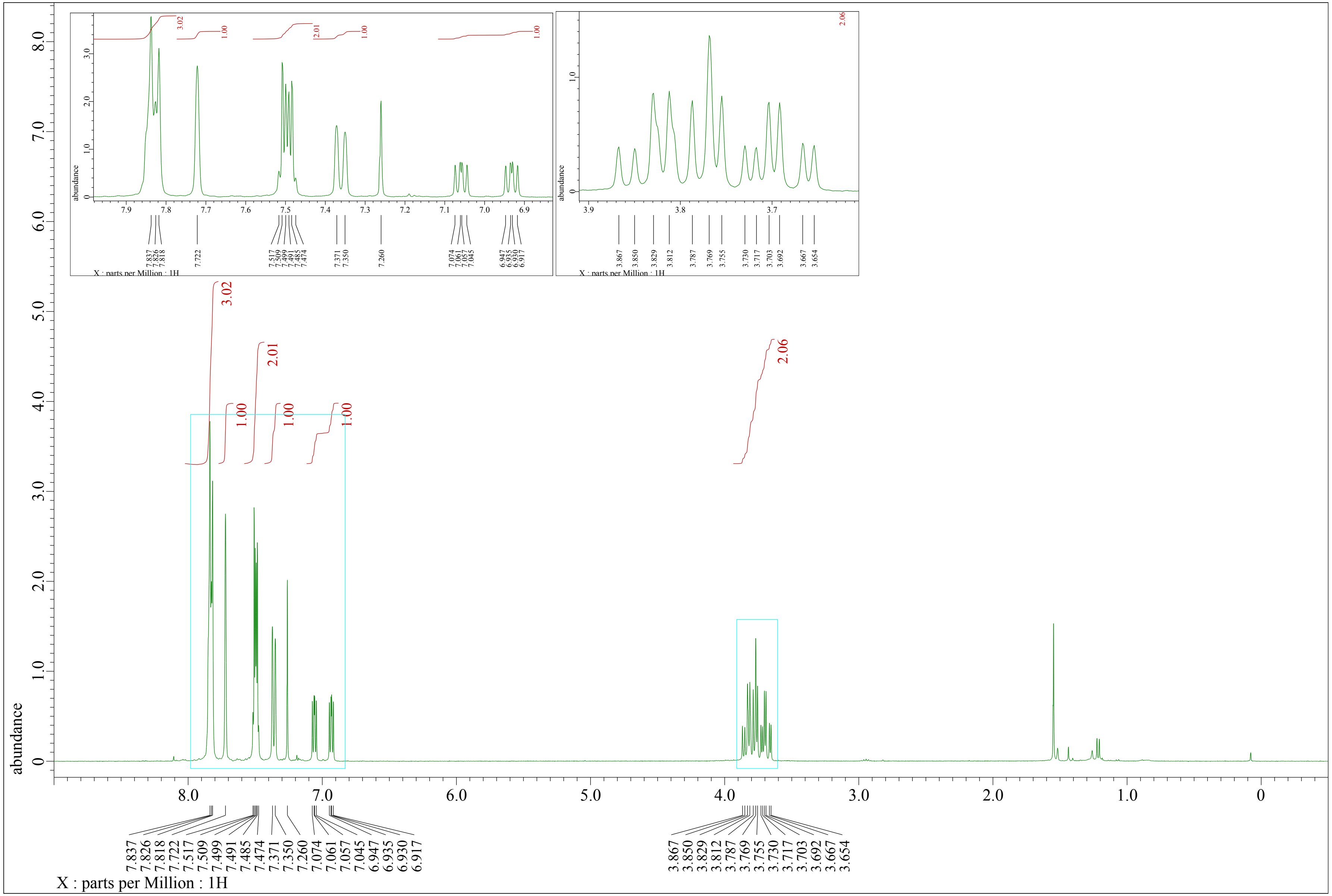
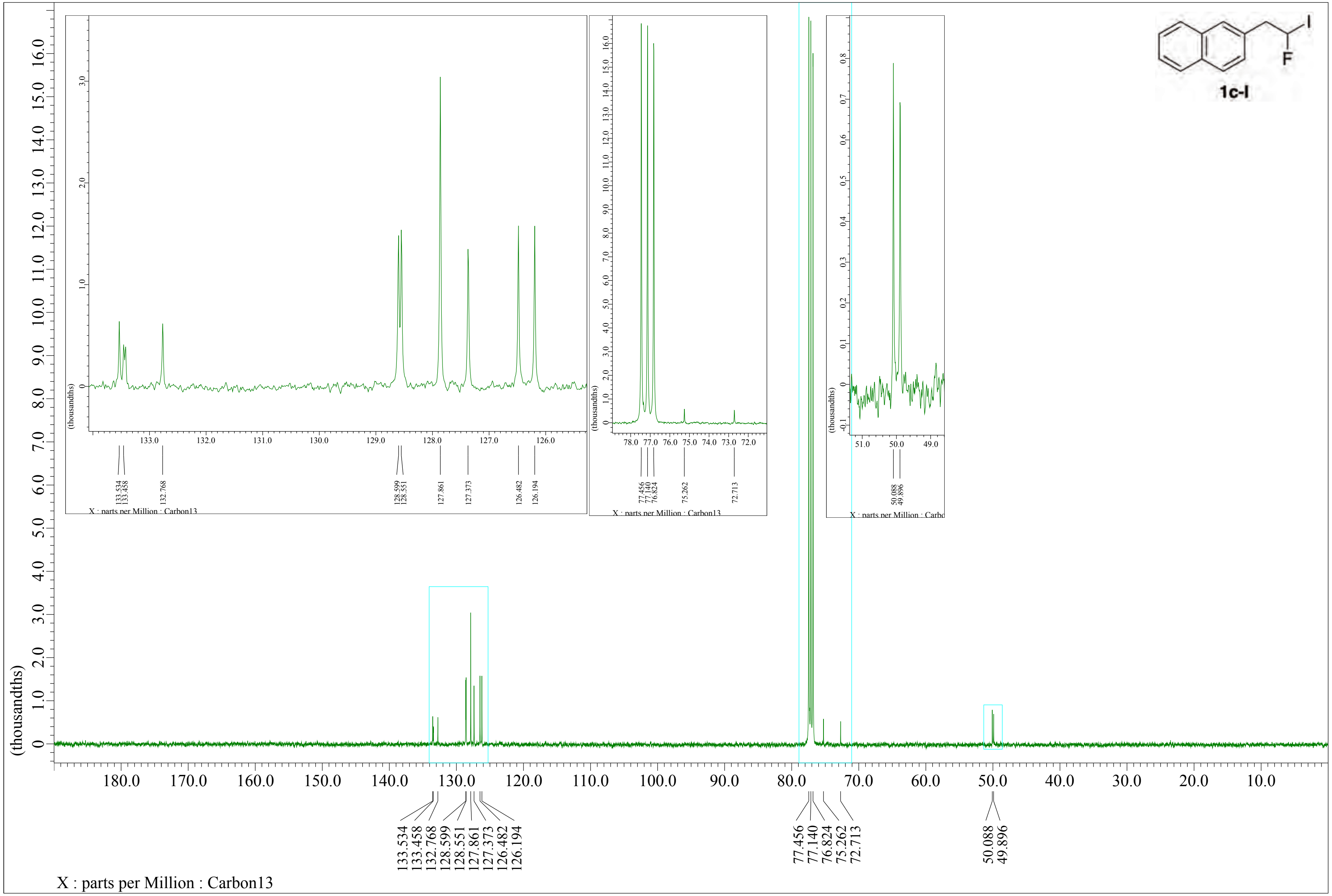
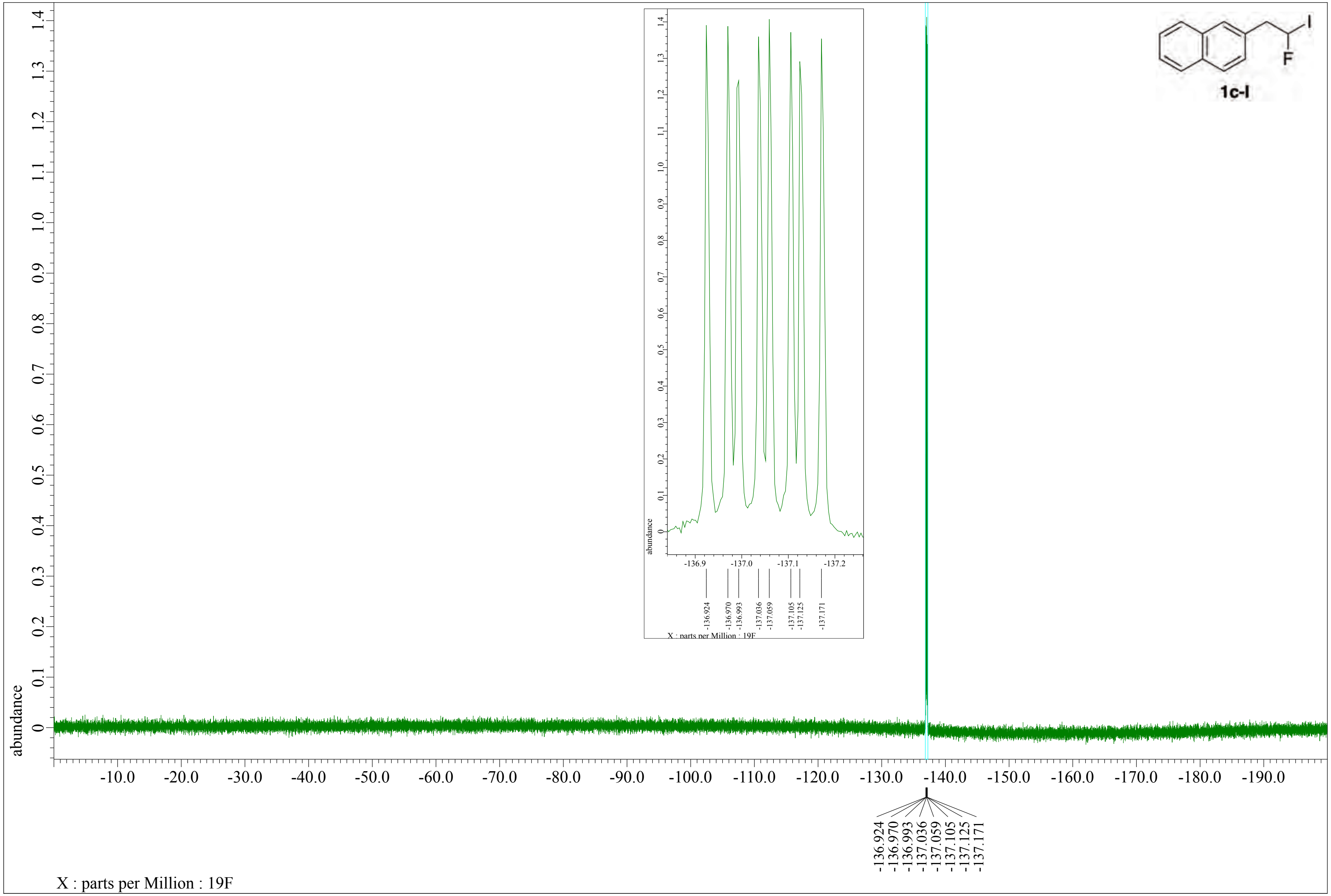
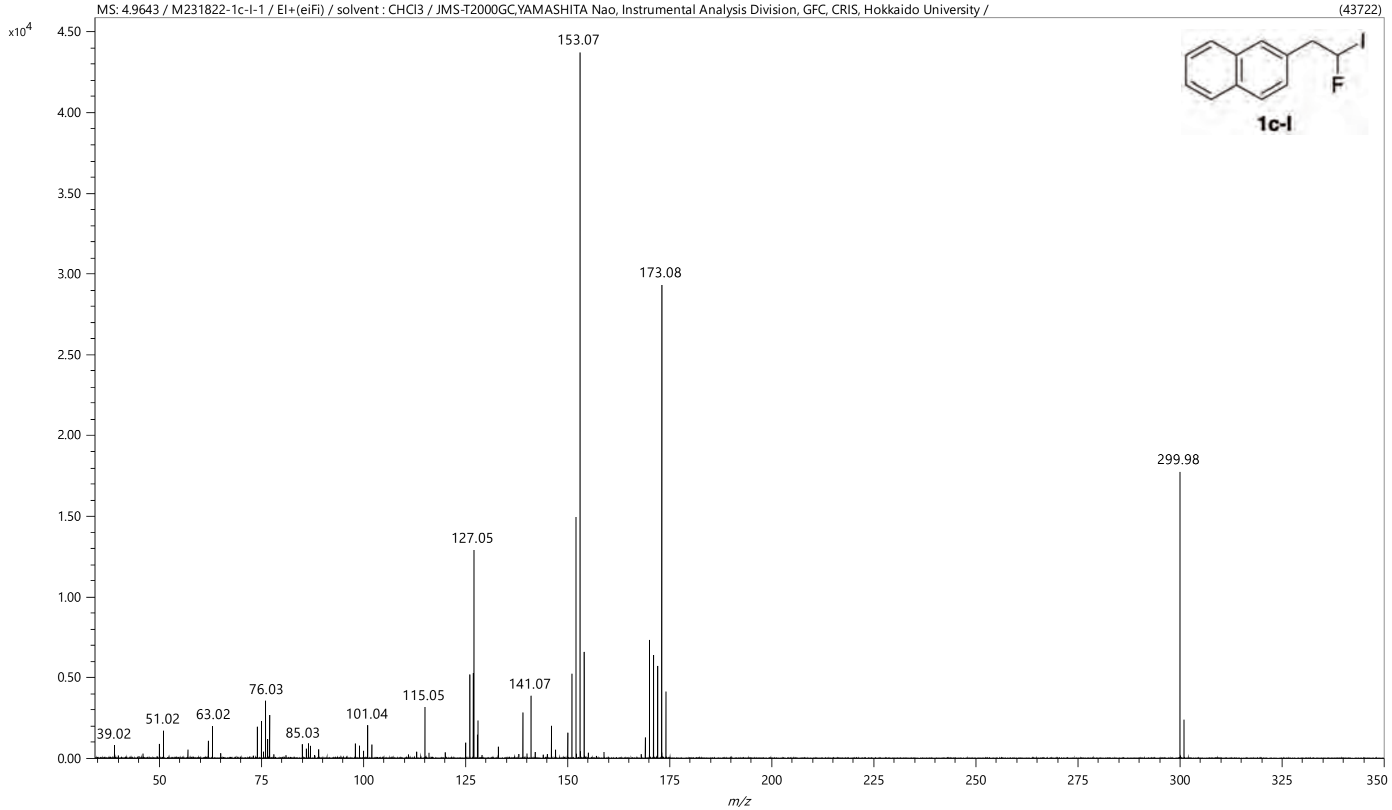
(116563)
x10^5
263.98080
264.98417
1b-I



abundance
X : parts per Million : 1H
3.02
1.00
2.01
1.00
1.00
2.06
7.837
7.826
7.818
7.722
7.517
7.509
7.499
7.491
7.485
7.474
7.371
7.350
7.260
7.074
7.061
7.057
7.045
6.947
6.935
6.930
6.917
3.867
3.850
3.829
3.812
3.787
3.769
3.755
3.730
3.717
3.703
3.692
3.667
3.654


1c-I
X : parts per Million : Carbon13
(thousandths)
133.534
133.458
132.768
128.599
128.551
127.861
127.373
126.482
126.194
77.456
77.140
76.824
75.262
72.713
50.088
49.896


1c-I
abundance
X : parts per Million : 19F
-136.924
-136.970
-136.993
-137.036
-137.059
-137.105
-137.125
-137.171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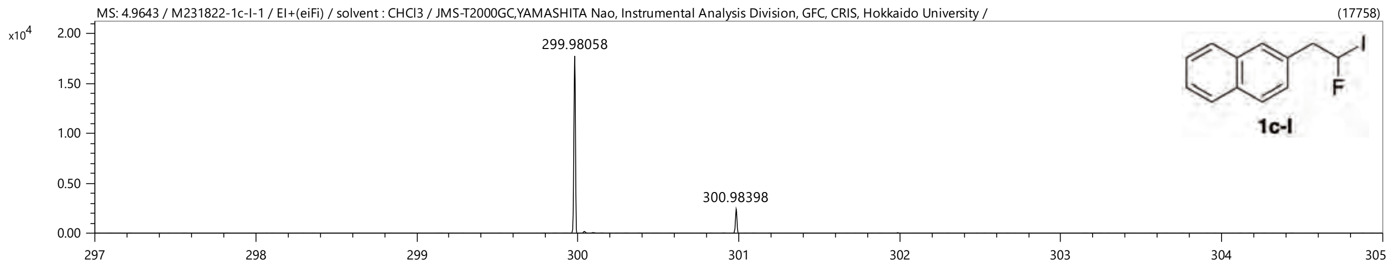
(43722)
x10^4
153.07
173.08
299.98
127.05
141.07
115.05
76.03
101.04
63.02
51.02
85.03
39.02
m/z
F
I
1c-I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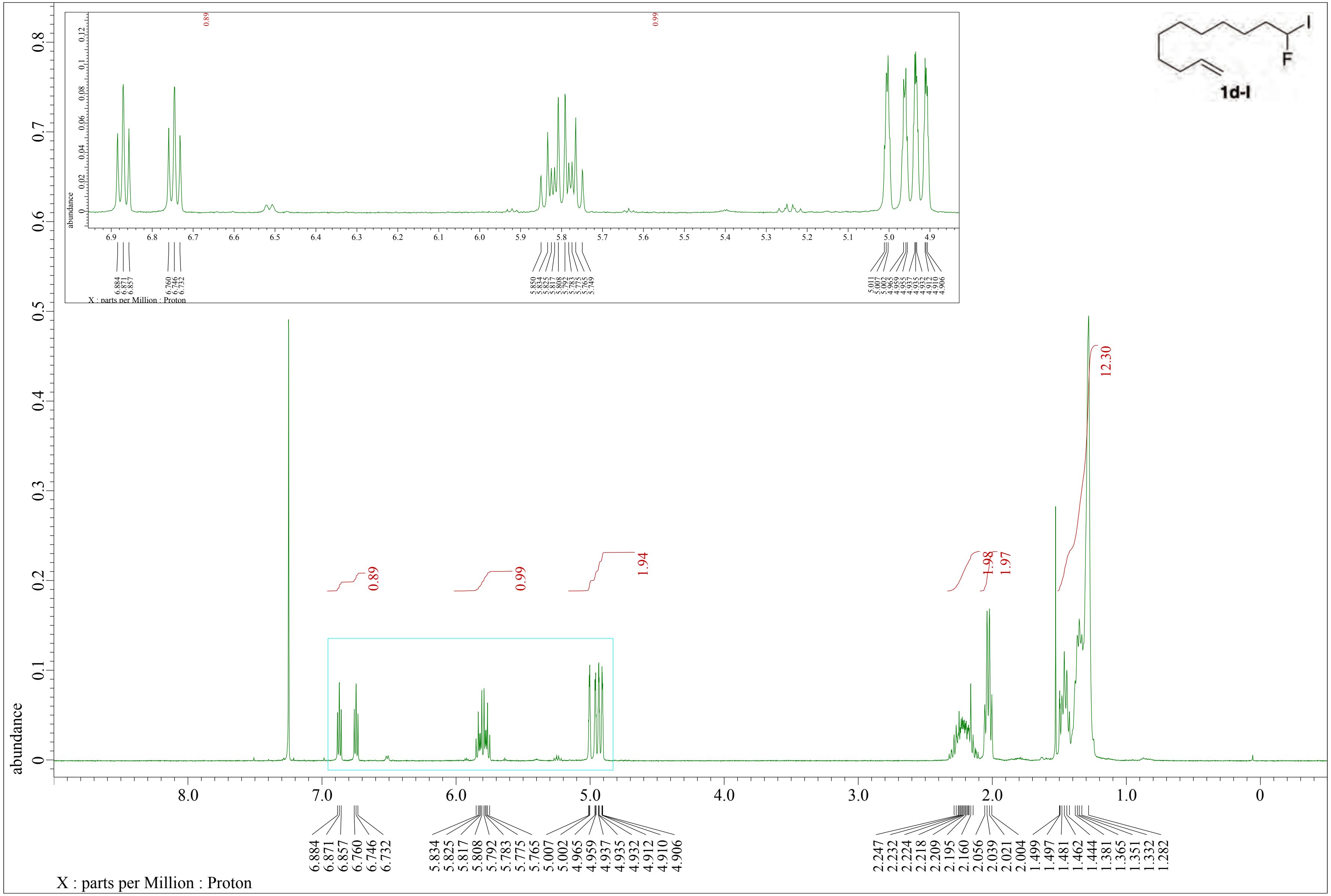
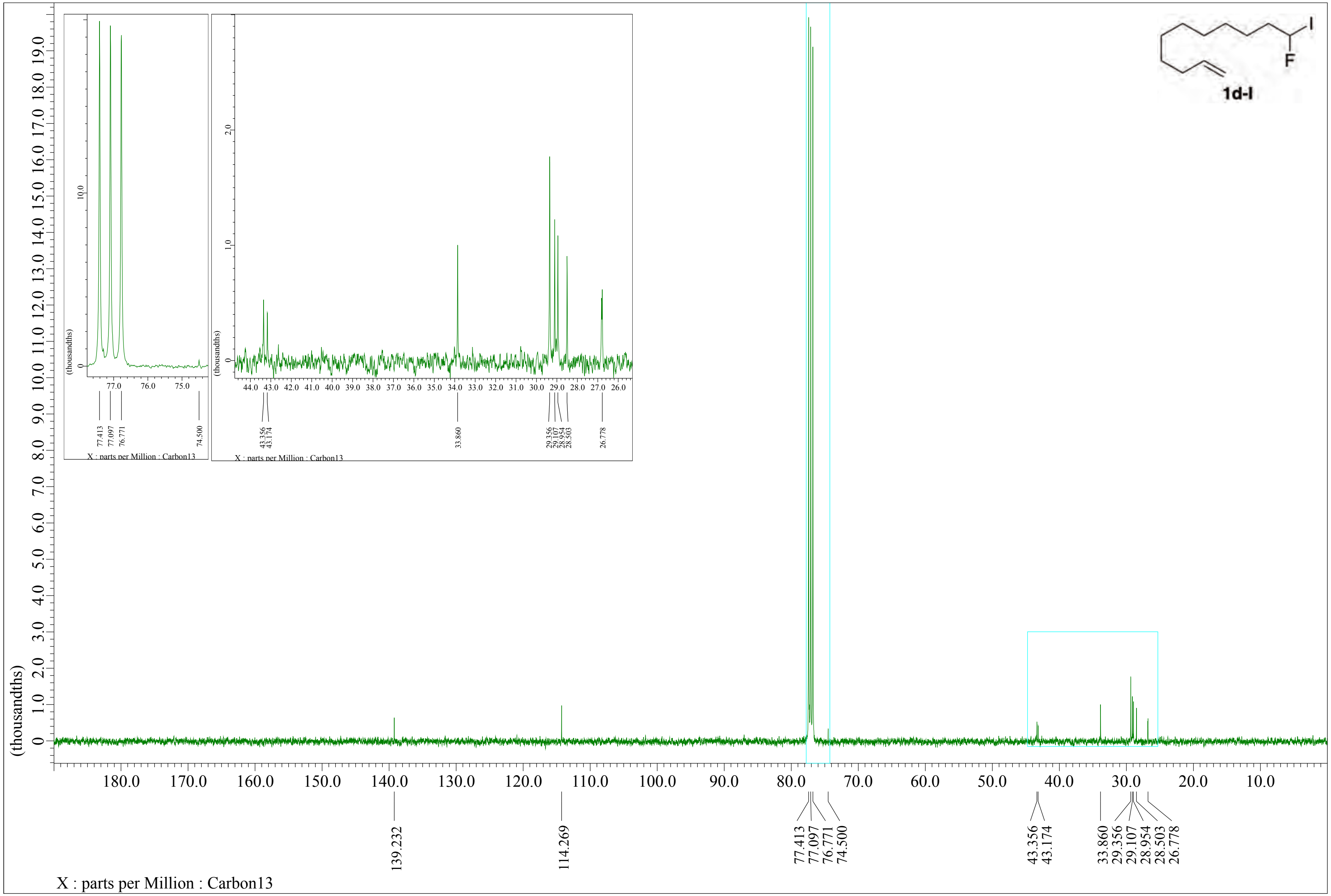
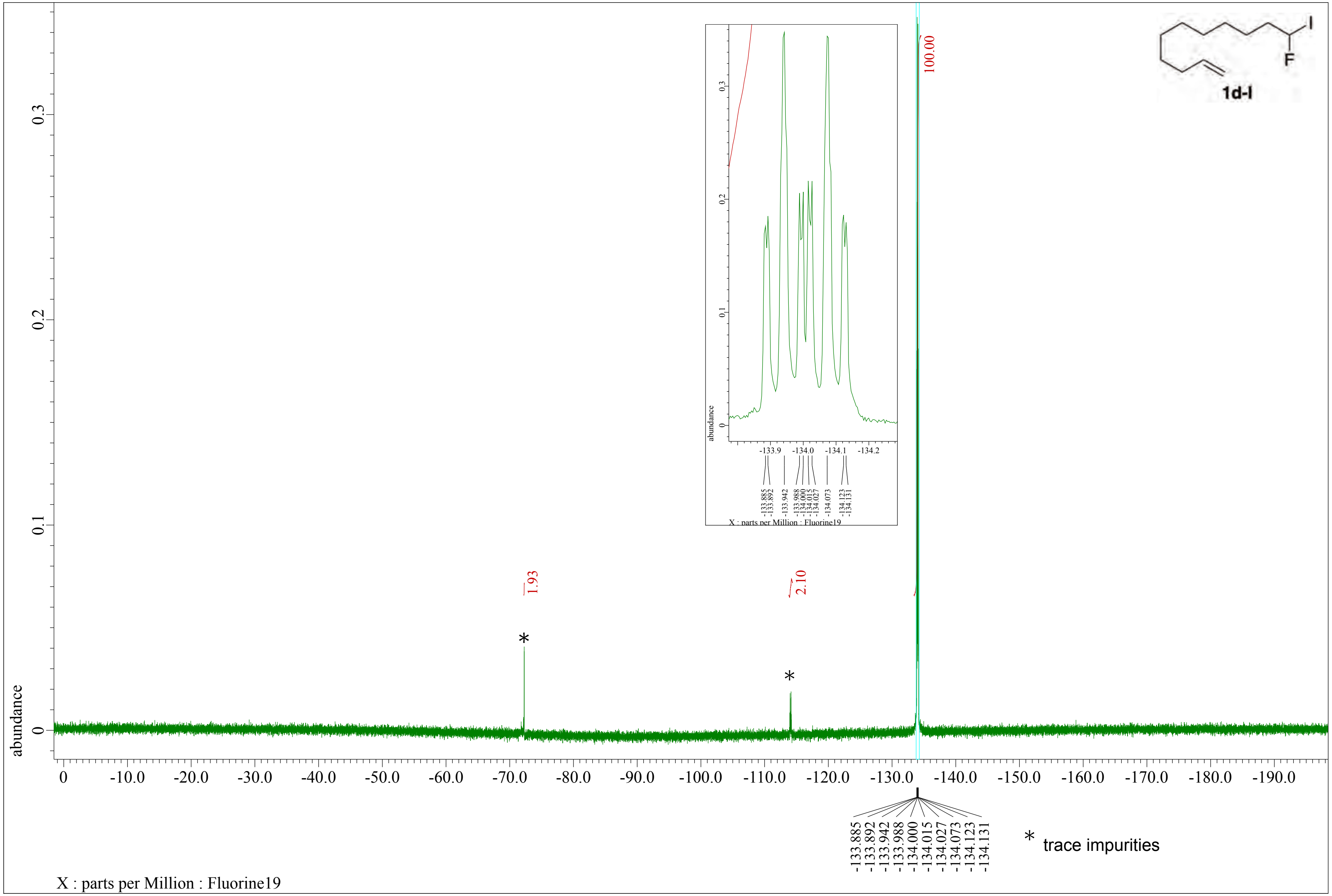
(17758)
x10^4
299.98058
300.98398
F
I
1c-I



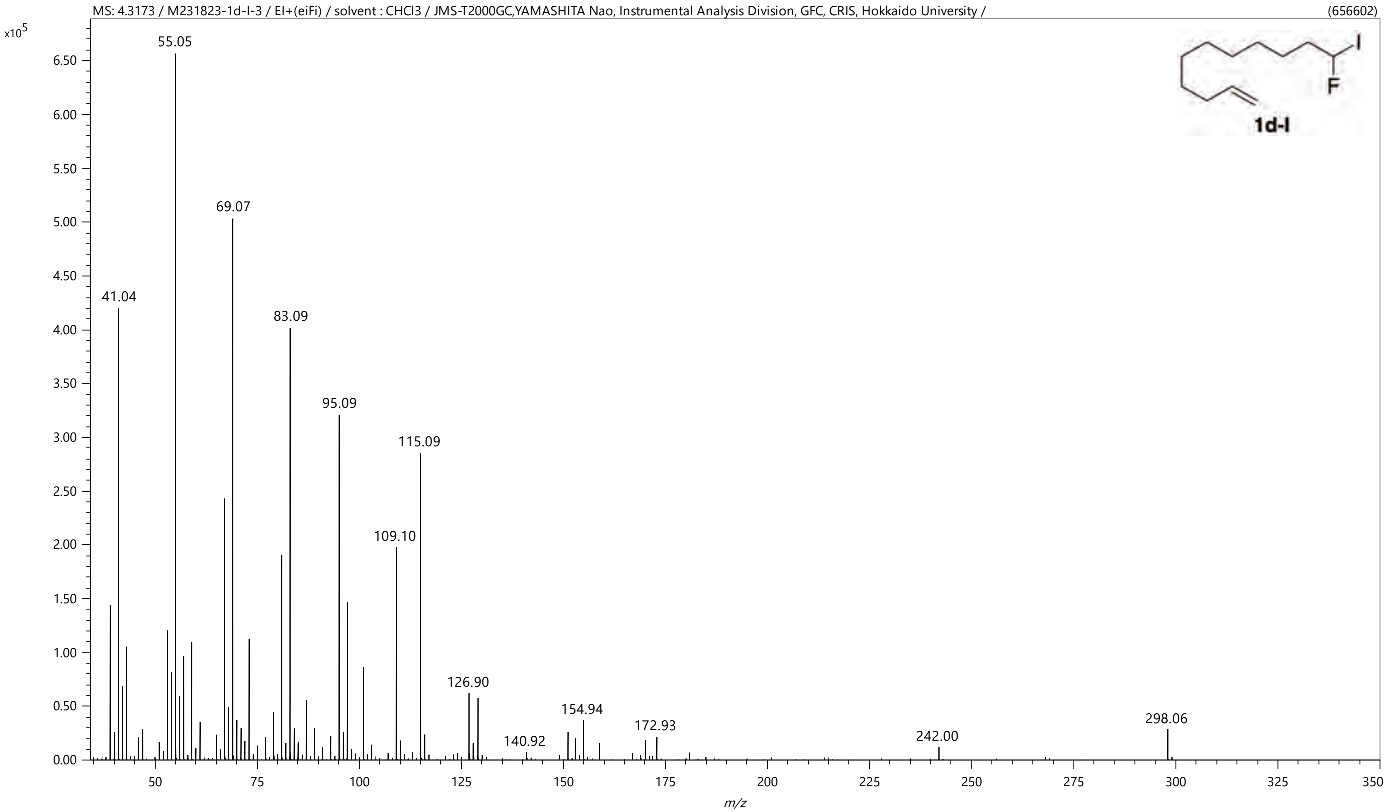
1d-I
abundance
X : parts per Million : Proton
0.89
0.99
1.94
1.98
1.97
12.30
6.884
6.871
6.857
6.760
6.746
6.732
5.834
5.825
5.817
5.808
5.792
5.783
5.775
5.765
5.007
5.002
4.965
4.959
4.937
4.935
4.932
4.912
4.910
4.906
2.247
2.232
2.224
2.218
2.209
2.195
2.160
2.056
2.039
2.021
2.004
1.499
1.497
1.481
1.462
1.444
1.381
1.365
1.351
1.332
1.282



1d-I
(thousandths)
X : parts per Million : Carbon13
139.232
114.269
77.413
77.097
76.771
74.500
43.356
43.174
33.860
29.356
29.107
28.954
28.503
26.778



1d-I
100.00
1.93
2.10
*
*
-133.885
-133.892
-133.942
-133.988
-134.000
-134.015
-134.027
-134.073
-134.123
-134.131
* trace impurities
abundance
X : parts per Million : Fluorine19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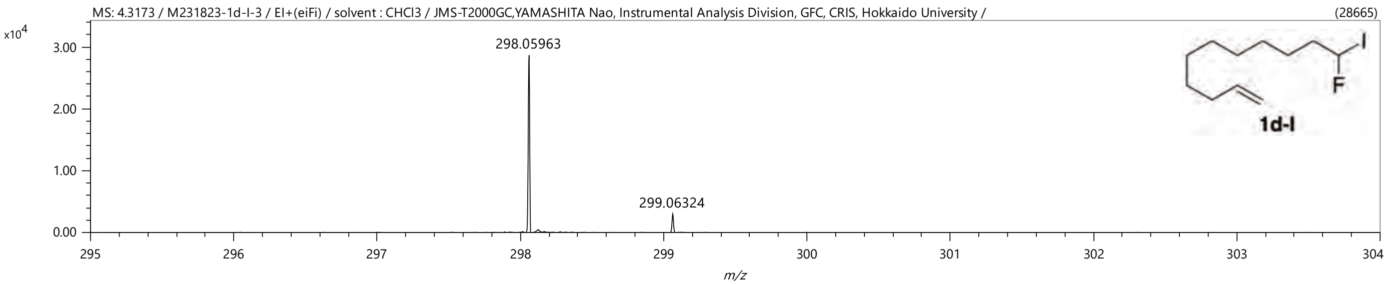
(656602)
x10^5
55.05
69.07
41.04
83.09
95.09
115.09
109.10
126.90
154.94
140.92
172.93
242.00
298.06
m/z
F
I
1d-I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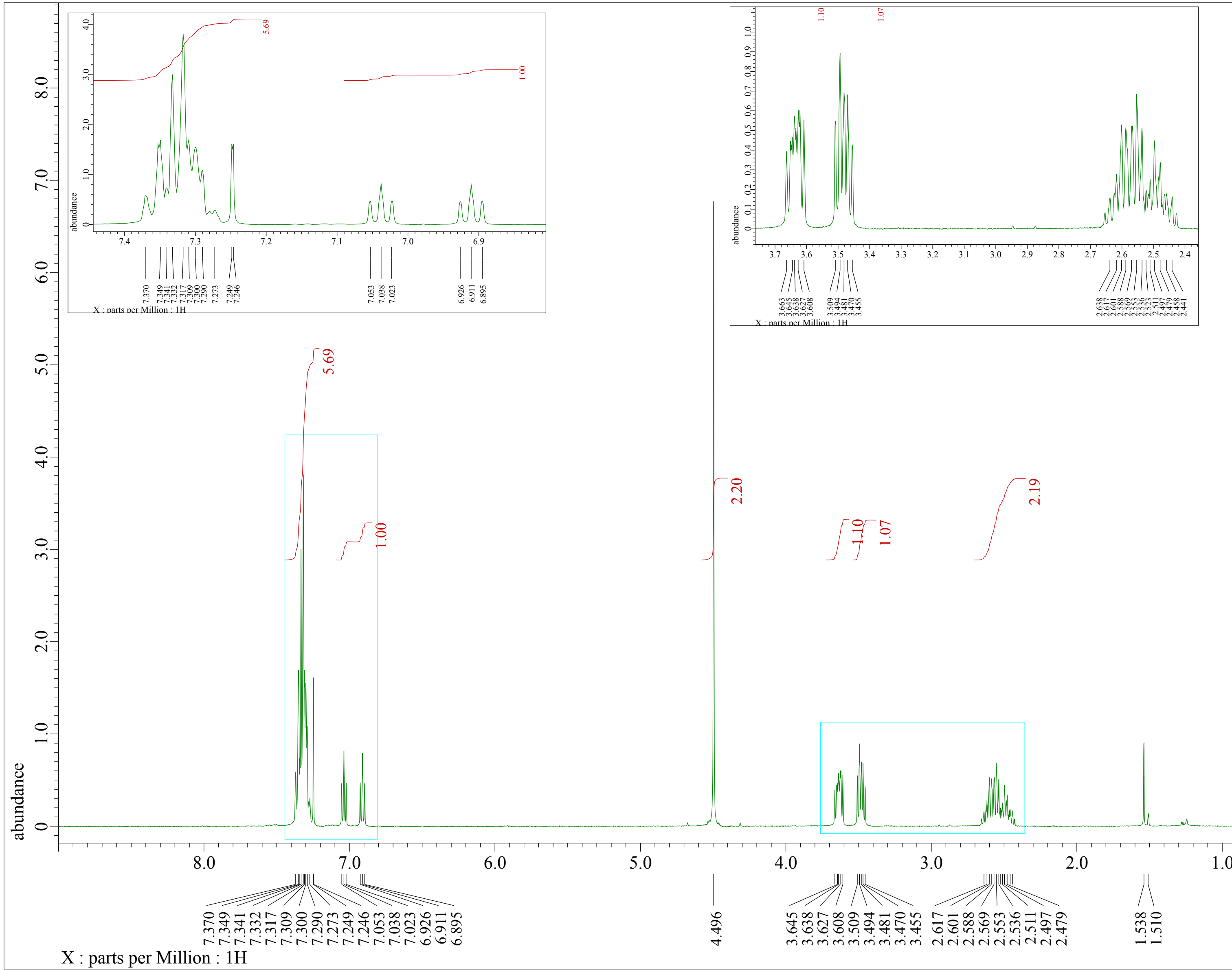
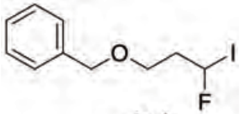
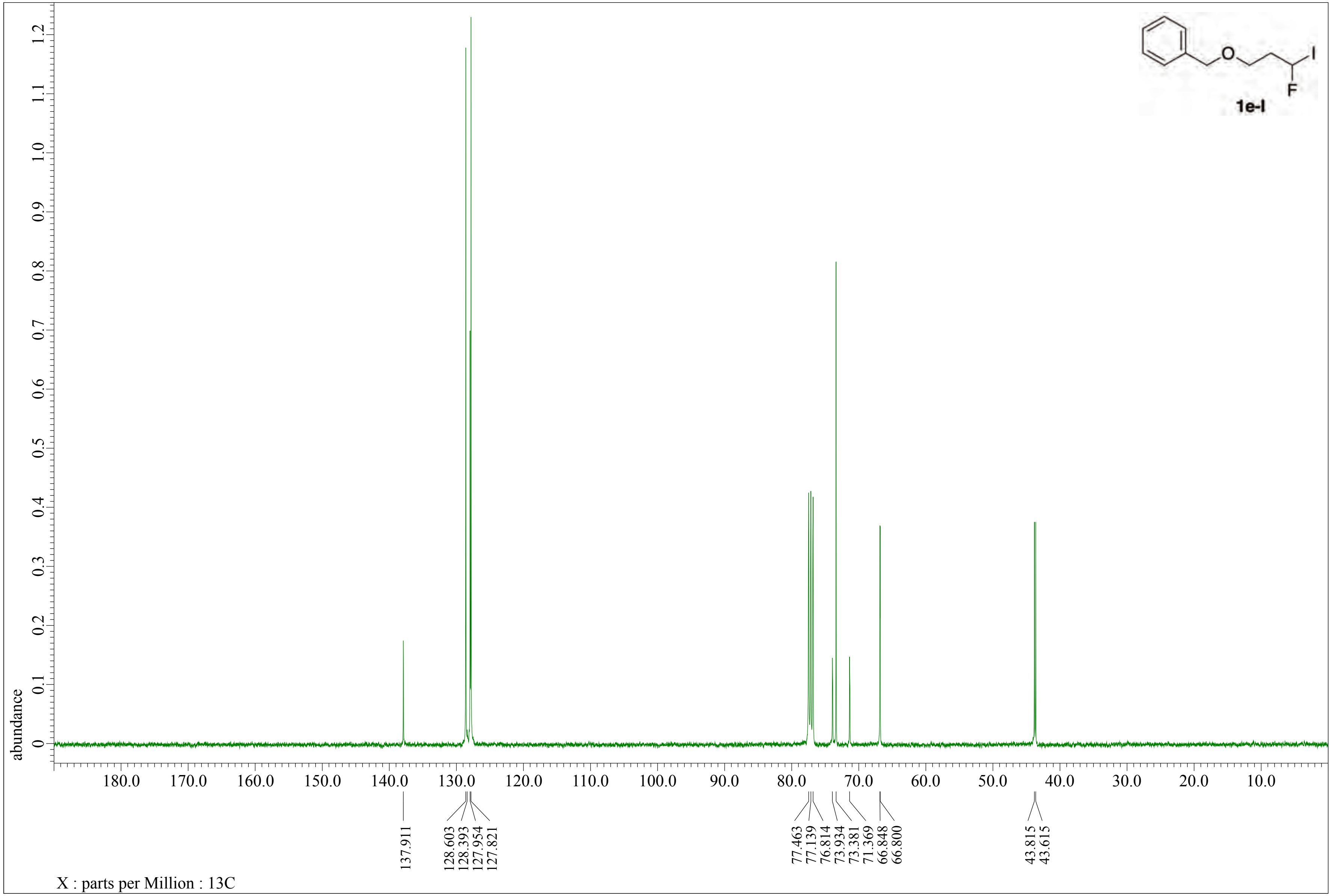
(28665)
x10^4
298.05963
299.06324
m/z
F
I
1d-I

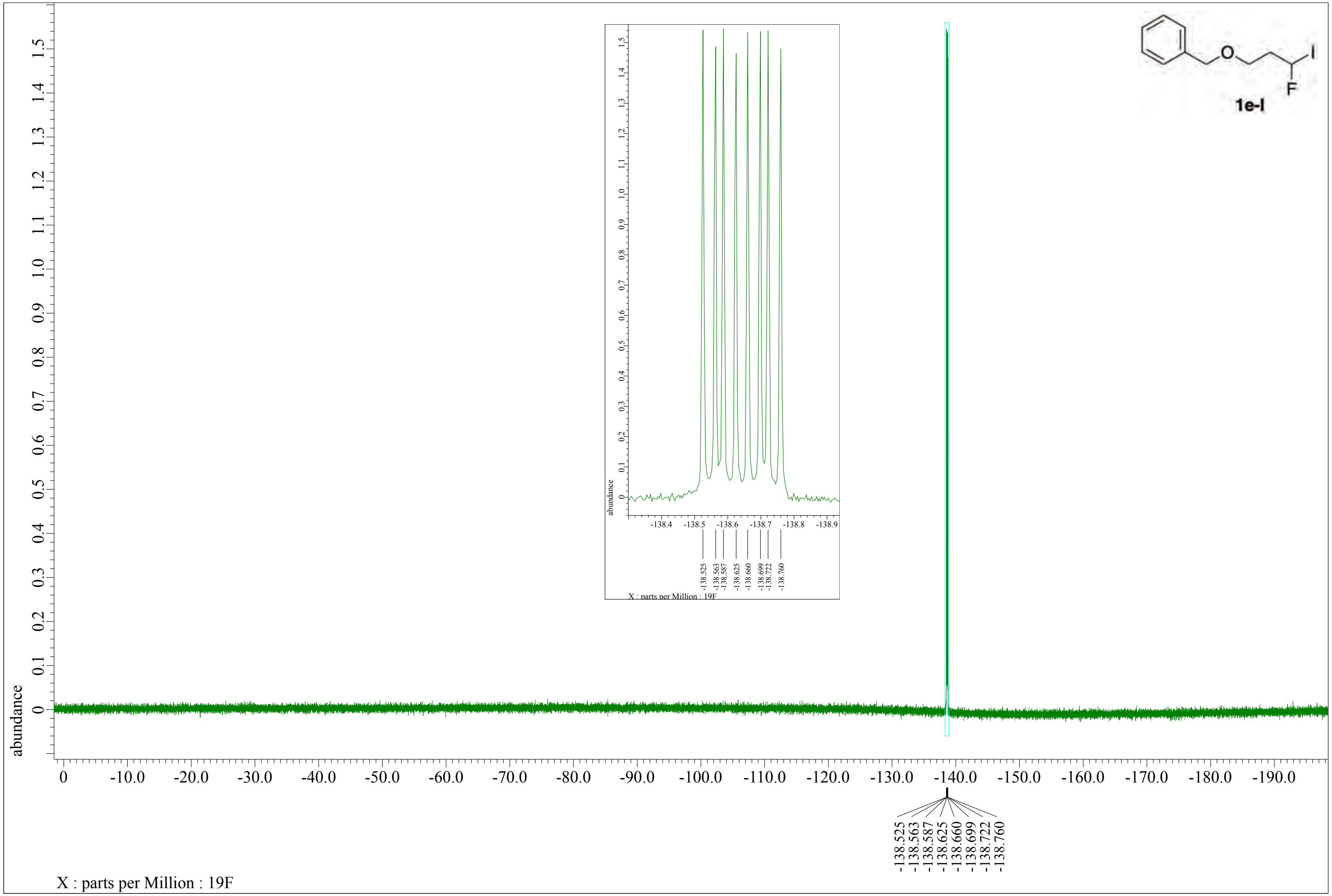


abundance
X : parts per Million : 1H
5.69
1.00
2.20
1.10
1.07
2.19
7.370
7.349
7.341
7.332
7.317
7.309
7.300
7.290
7.273
7.249
7.246
7.053
7.038
7.023
6.926
6.911
6.895
4.496
3.645
3.638
3.627
3.608
3.509
3.494
3.481
3.470
3.455
2.617
2.601
2.588
2.569
2.553
2.536
2.511
2.497
2.479
1.538
1.510

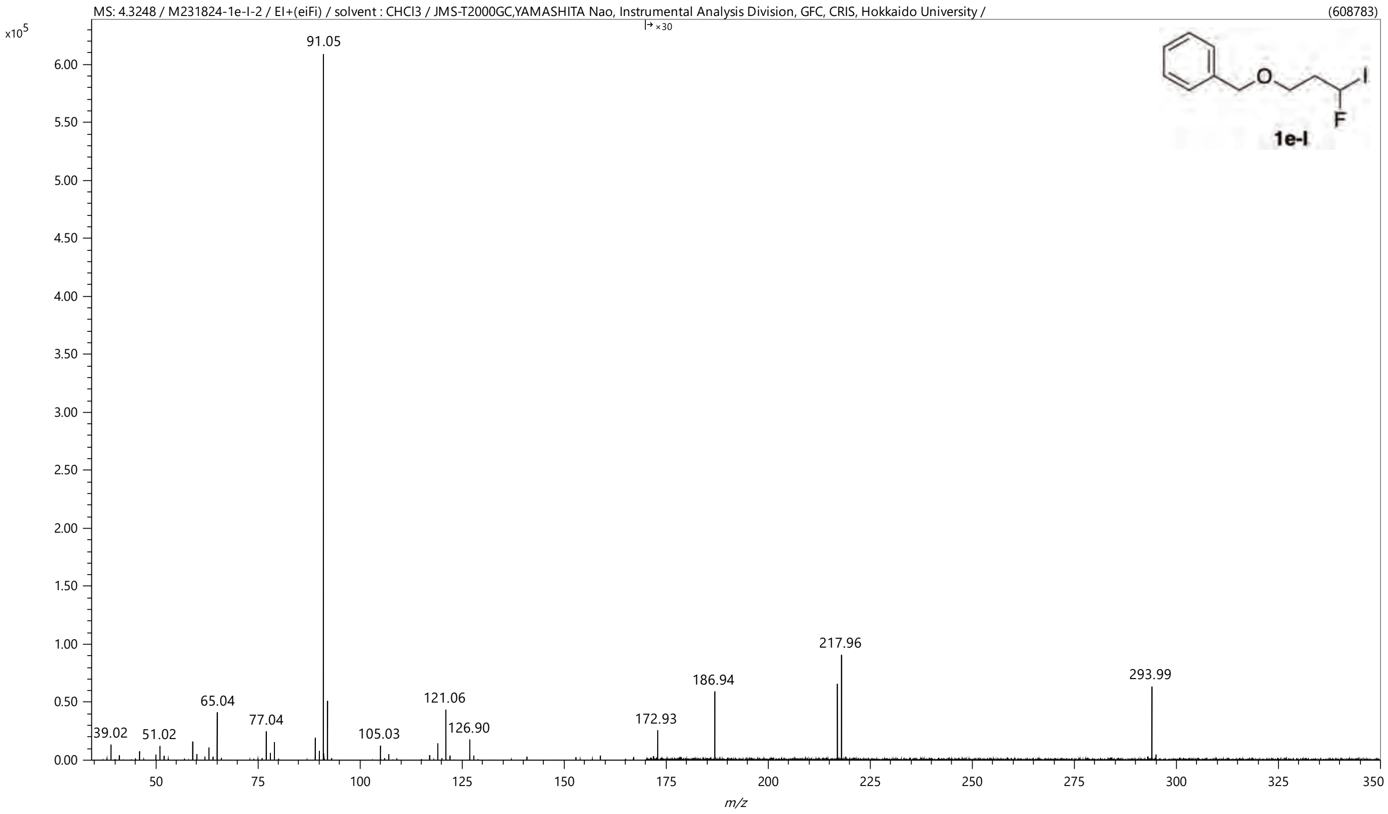


1e-I


1e-I
abundance
X : parts per Million : 13C
137.911
128.603
128.393
127.954
127.821
77.463
77.139
76.814
73.934
73.381
71.369
66.848
66.800
43.815
43.615



1e-I
abundance
X : parts per Million : 19F
-138.525
-138.563
-138.587
-138.625
-138.660
-138.699
-138.722
-138.760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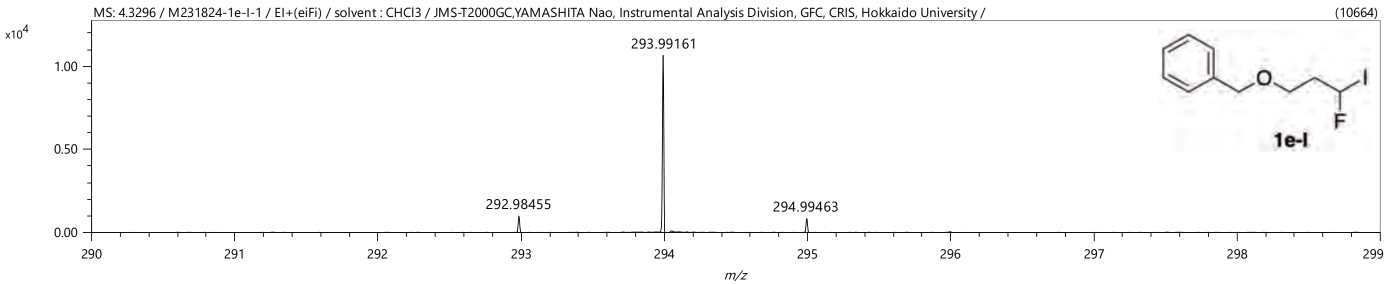
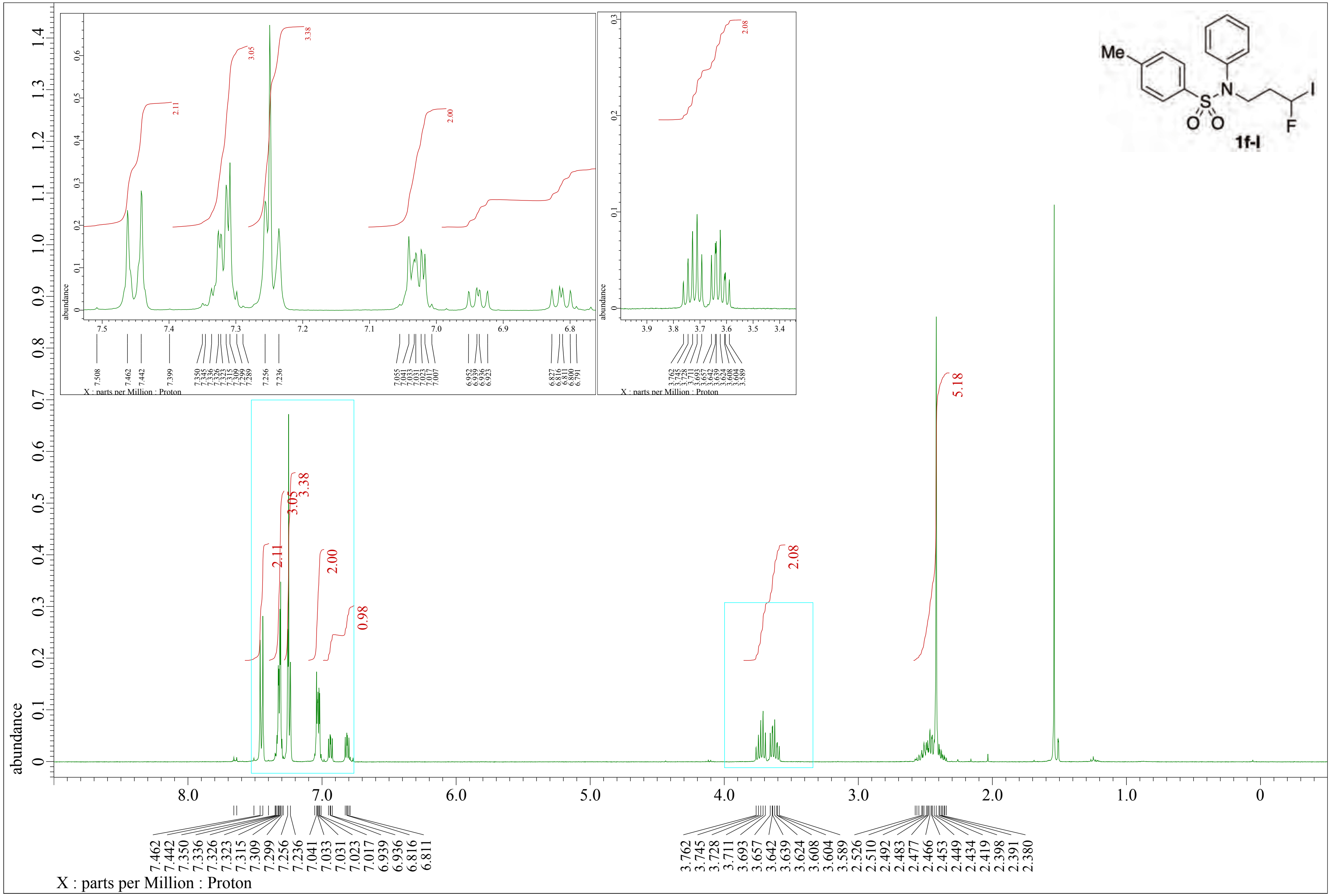
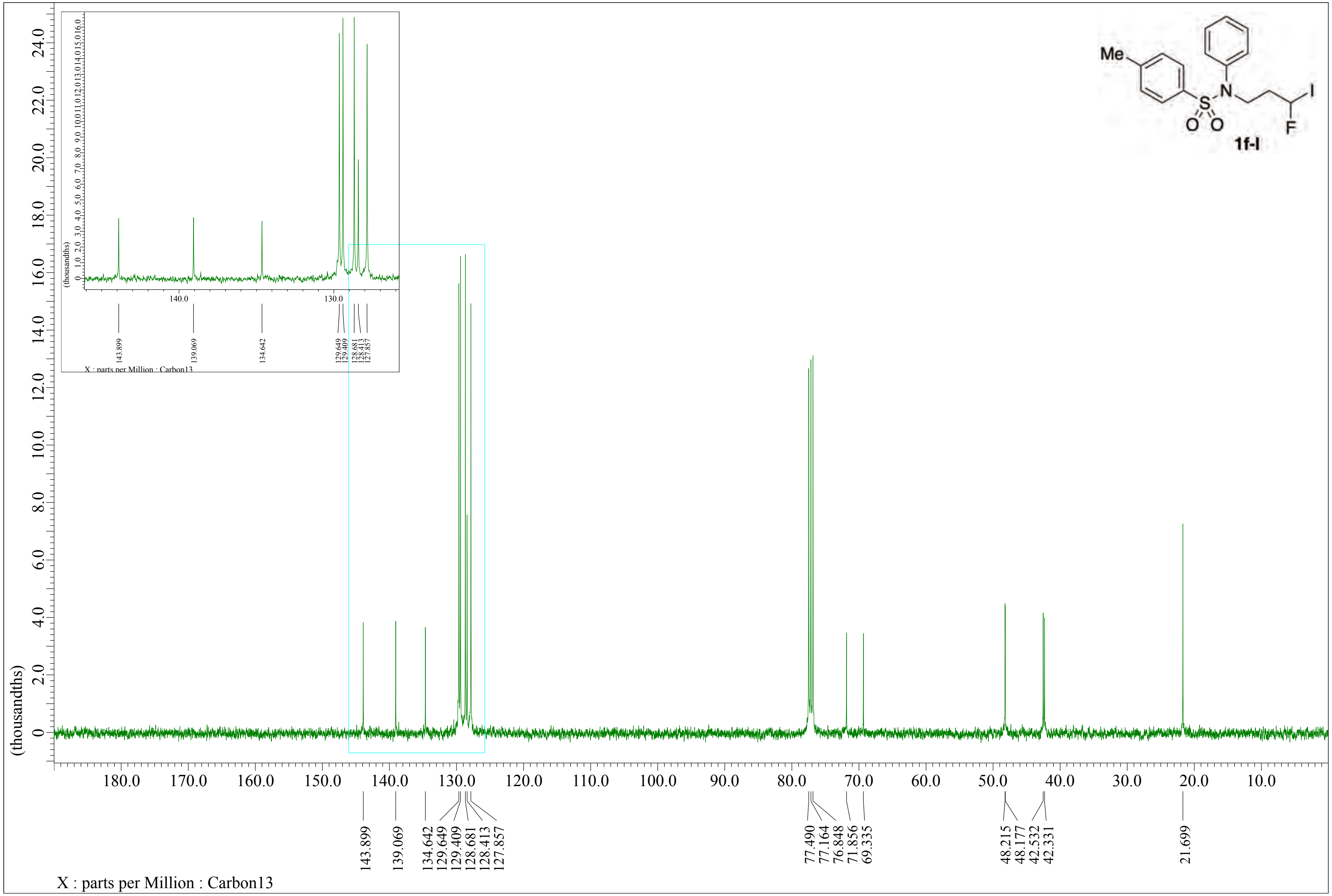
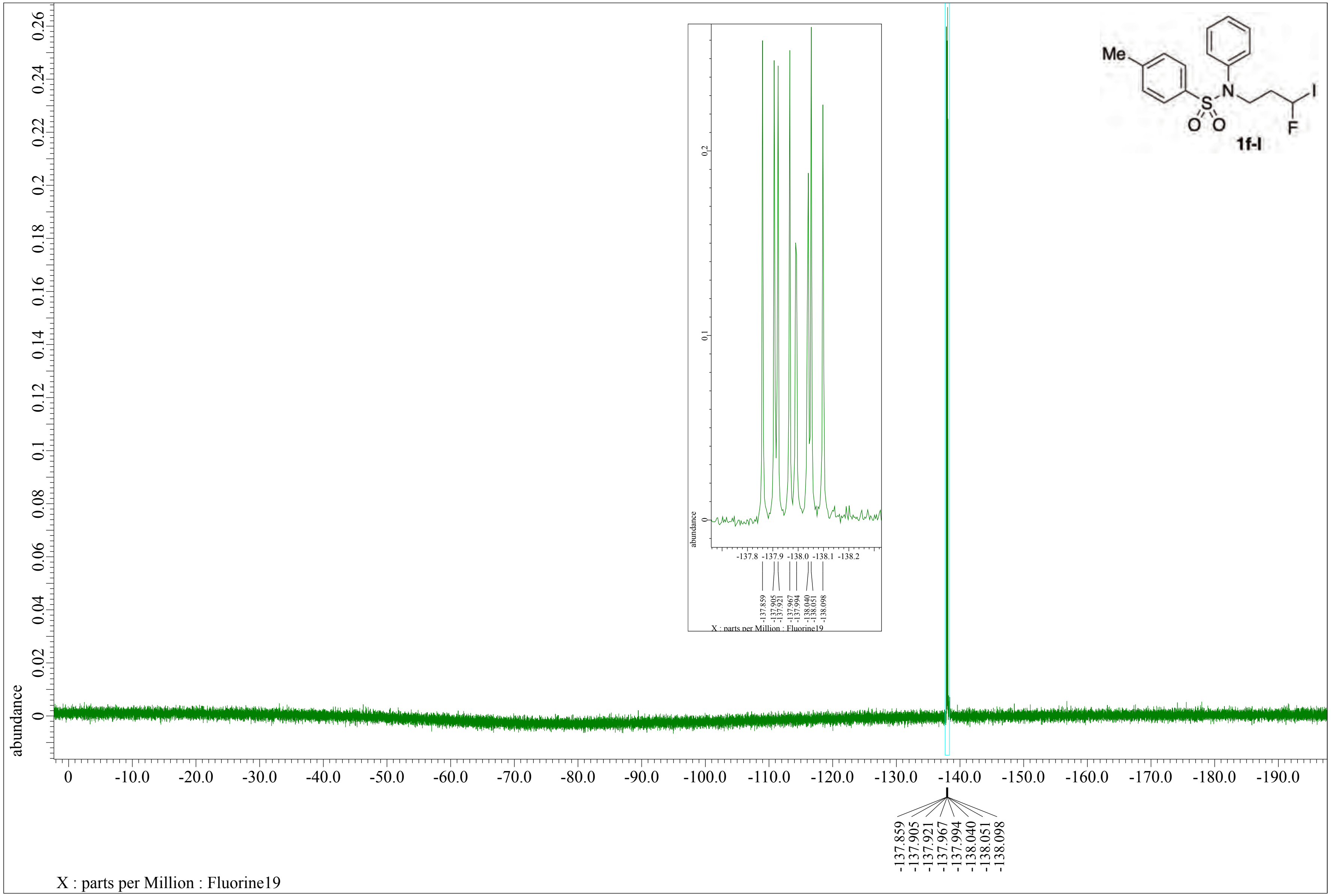
(608783)
x10^5
91.05
217.96
186.94
293.99
172.93
121.06
126.90
105.03
65.04
77.04
39.02
51.02
m/z
1e-I


MS: 4.3296 / M231824-1e-I-1 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,YAMASHITA Nao, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(10664)
x10^4
293.99161
292.98455
294.99463
m/z
1e-I



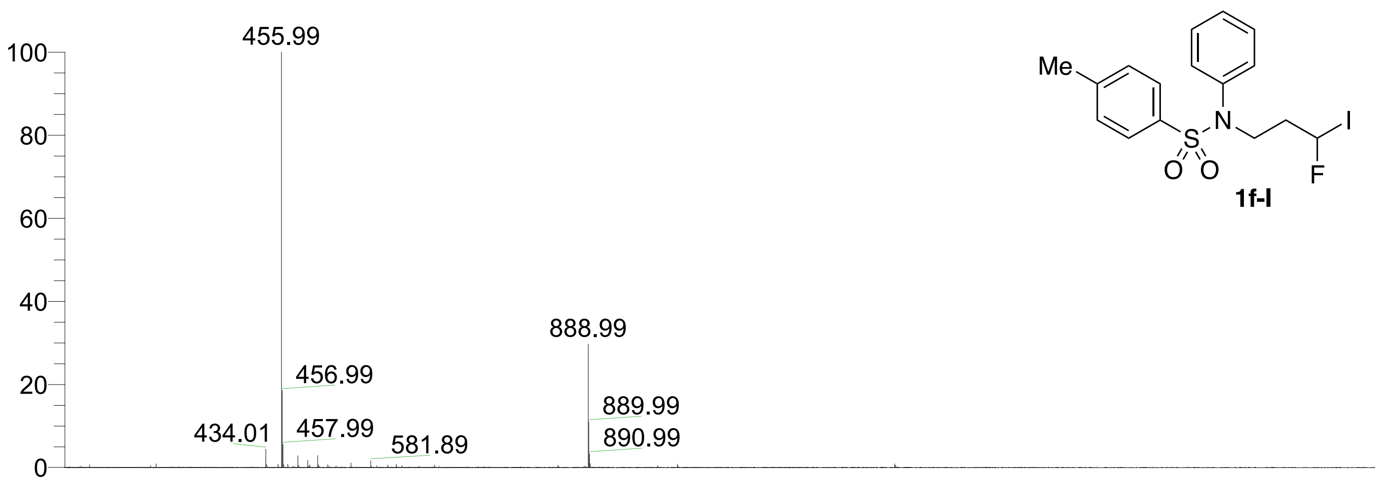
1f-I

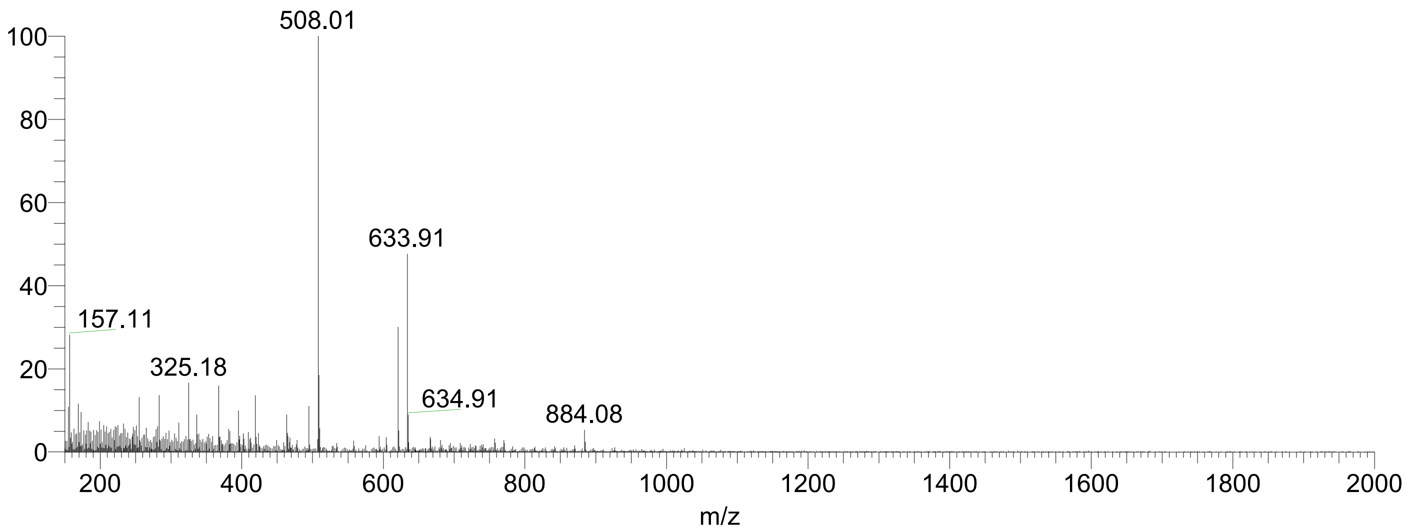

Me
N
S
O O
I
F
1f-I
(thousandths)
X : parts per Million : Carbon13
143.899
139.069
134.642
129.649
129.409
128.681
128.413
127.857
77.490
77.164
76.848
71.856
69.335
48.215
48.177
42.532
42.331
21.699



Me
S
N
O
O
I
F
1f-I
abundance
X : parts per Million : Fluorine19
-137.859
-137.905
-137.921
-137.967
-137.994
-138.040
-138.051
-138.098

Sample No. : C:\Xcalibur\...\1227\BG_231825_1f_ _, Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 11:44:45
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University





Sample No. : C:\Xcalibur\...\1227\231825_1f_I_pn
Instrument : Exactive Plus
Mobile phase solvent : MeOH
Operator name : hayashi harumi
Sample solvent : CHCl3
Date : 12/27/23 15:48:25
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

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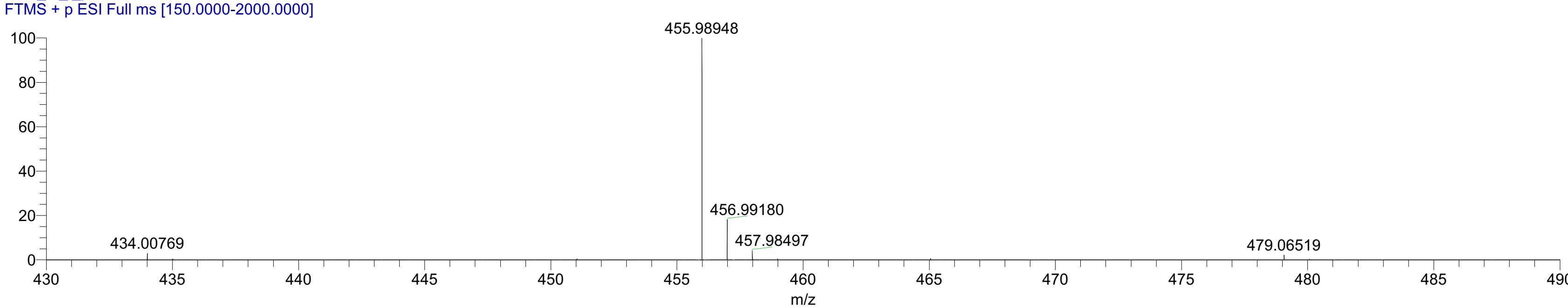
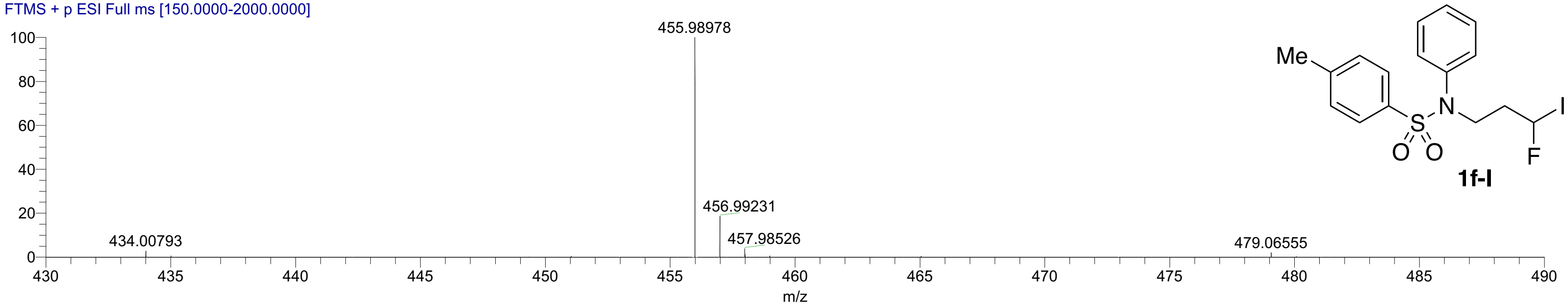
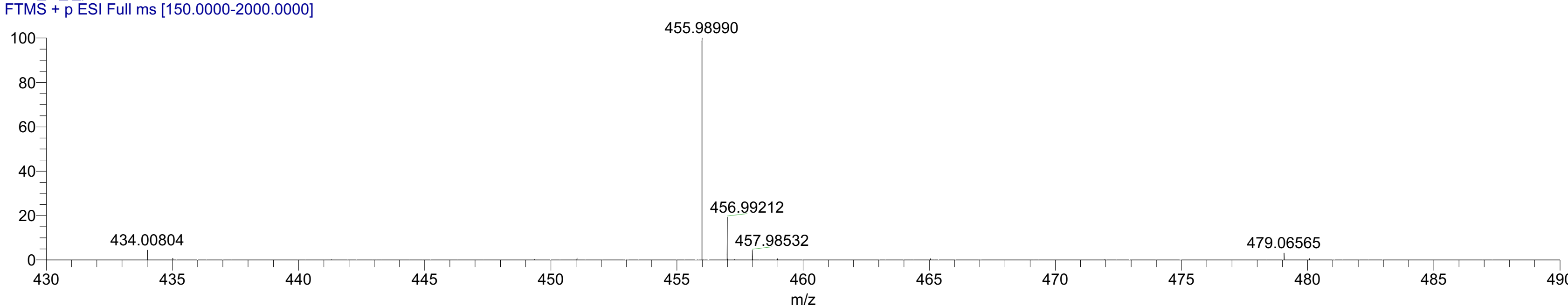
T: FTMS + p ESI Full ms [150.0000-2000.0000]

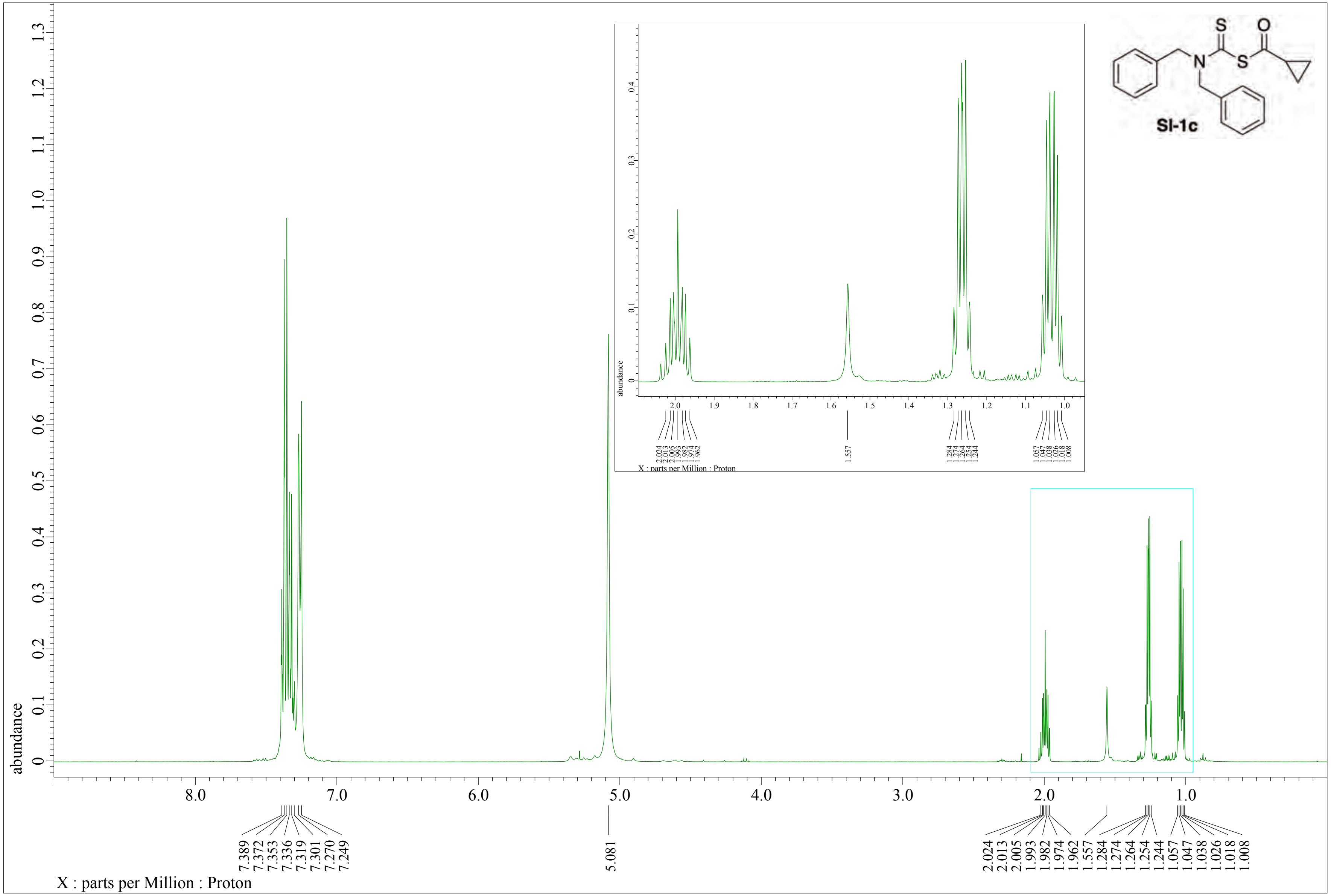


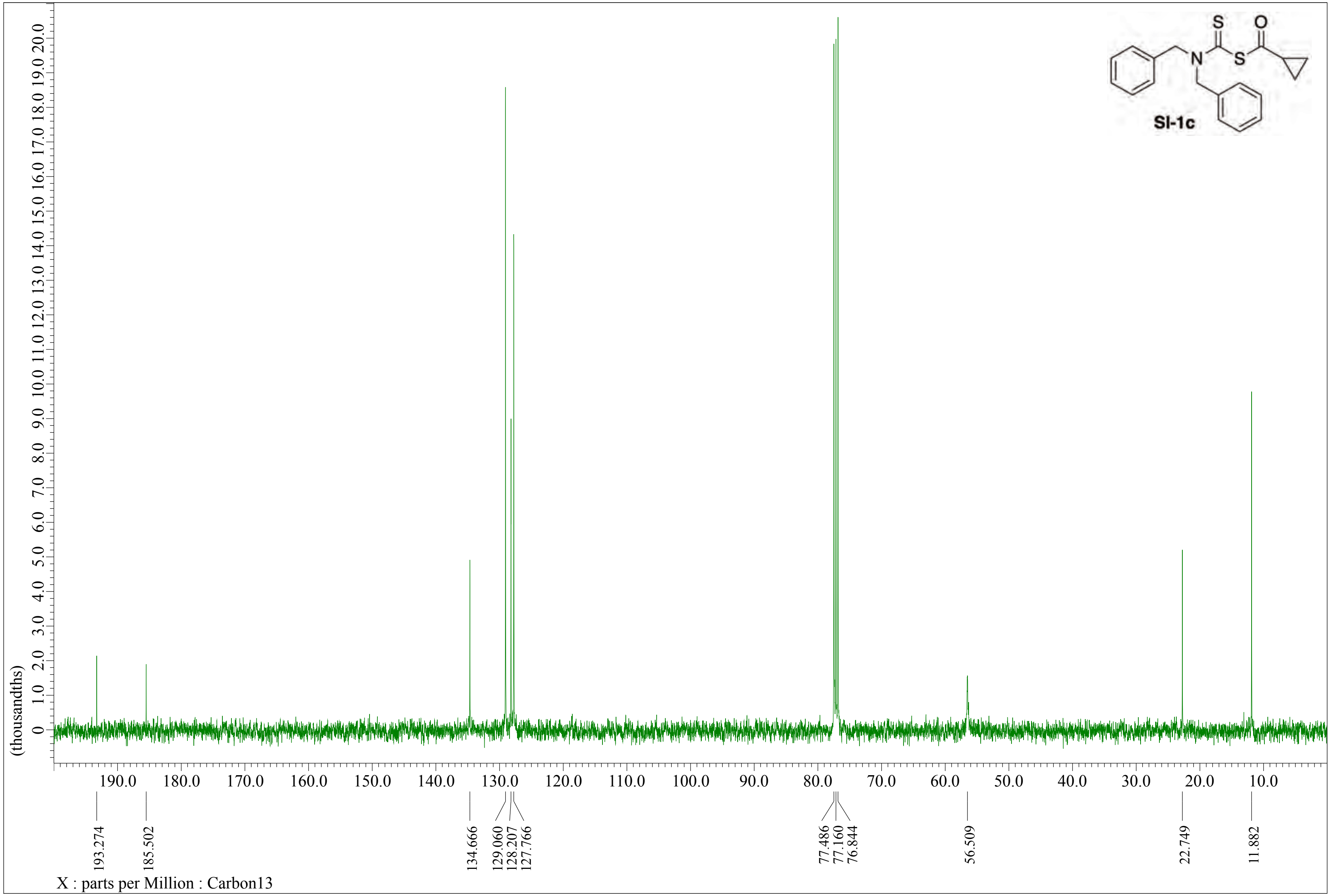
231825_1f_I_pn #26 RT: 0.43 AV: 1 NL: 7.12E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



231825_1f_I_pn #29-32 RT: 0.46-0.49 AV: 2 NL: 4.92E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]




S
O
N
S
SI-1c
abundance
X : parts per Million : Proton
7.389
7.372
7.353
7.336
7.319
7.301
7.270
7.249
5.081
2.024
2.013
2.005
1.993
1.982
1.974
1.962
1.557
1.284
1.274
1.264
1.254
1.244
1.057
1.047
1.038
1.026
1.018
1.008



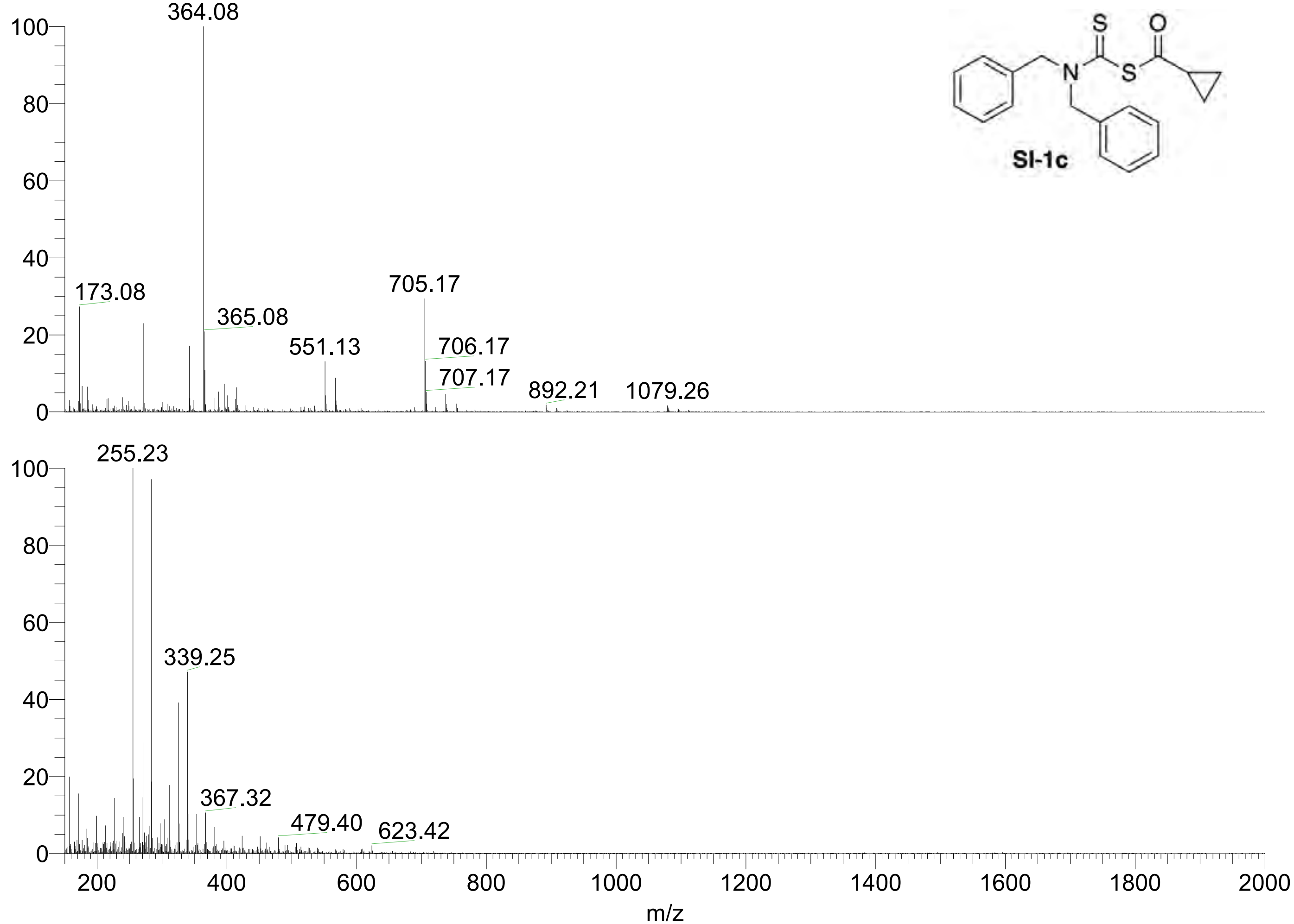
SI-1c
(thousandths)
X : parts per Million : Carbon13
193.274
185.502
134.666
129.060
128.207
127.766
77.486
77.160
76.844
56.509
22.749
11.882

Sample No. : C:\Xcalibur\...\BG_231828_KM_06 _ _ ı
Operator name : hayashi harumi
Date : 01/17/24 13:18:53
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

Instrument : Exactive Plus

Mobile phase solvent : MeOH
Sample solvent : CHCl3

SI-1c

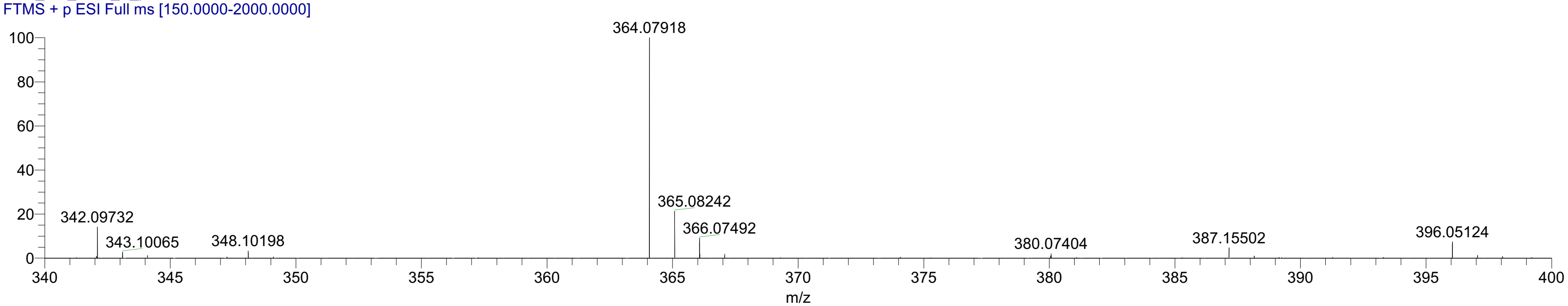


NL: 2.94E7
BG_231828_KM_0629_B_pn#18-31 RT: 0.31-0.50 AV: 7 T: FTMS + c ESI Full ms [150.00-2000.00]

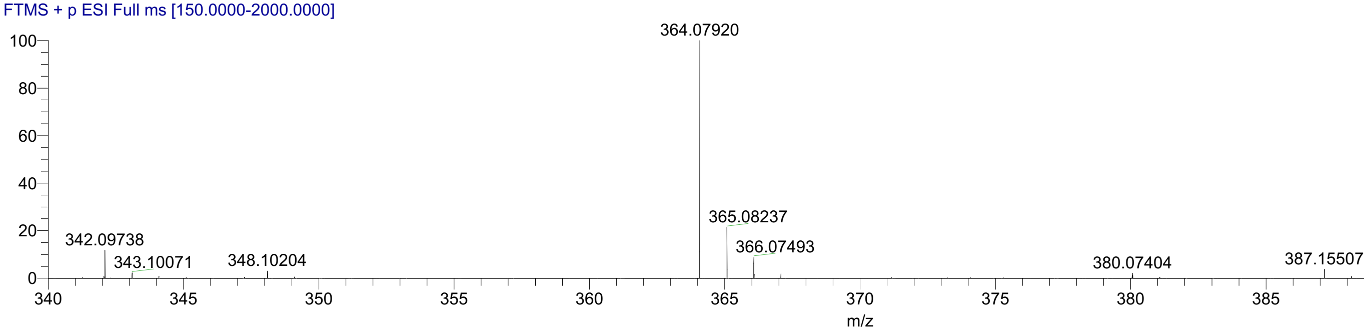
NL: 4.15E6
BG_231828_KM_0629_B_pn#18-31 RT: 0.30-0.49 AV: 7 T: FTMS - c ESI Full ms [150.00-2000.00]

Sample No. : C:\Xcalibur\...\0117\231828_KM_0629_B_pn Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 01/17/24 10:27:35
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

231828_KM_0629_B_pn #21-25 RT: 0.35-0.41 AV: 3 NL: 9.03E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]

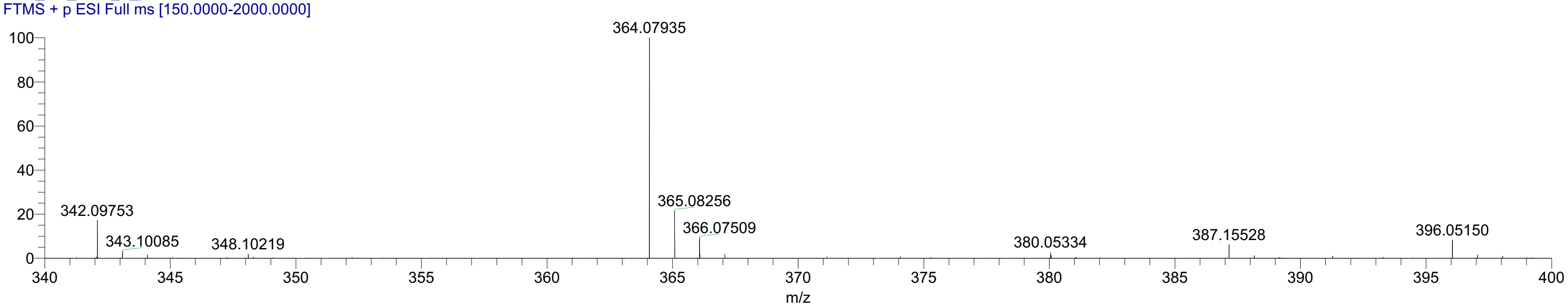


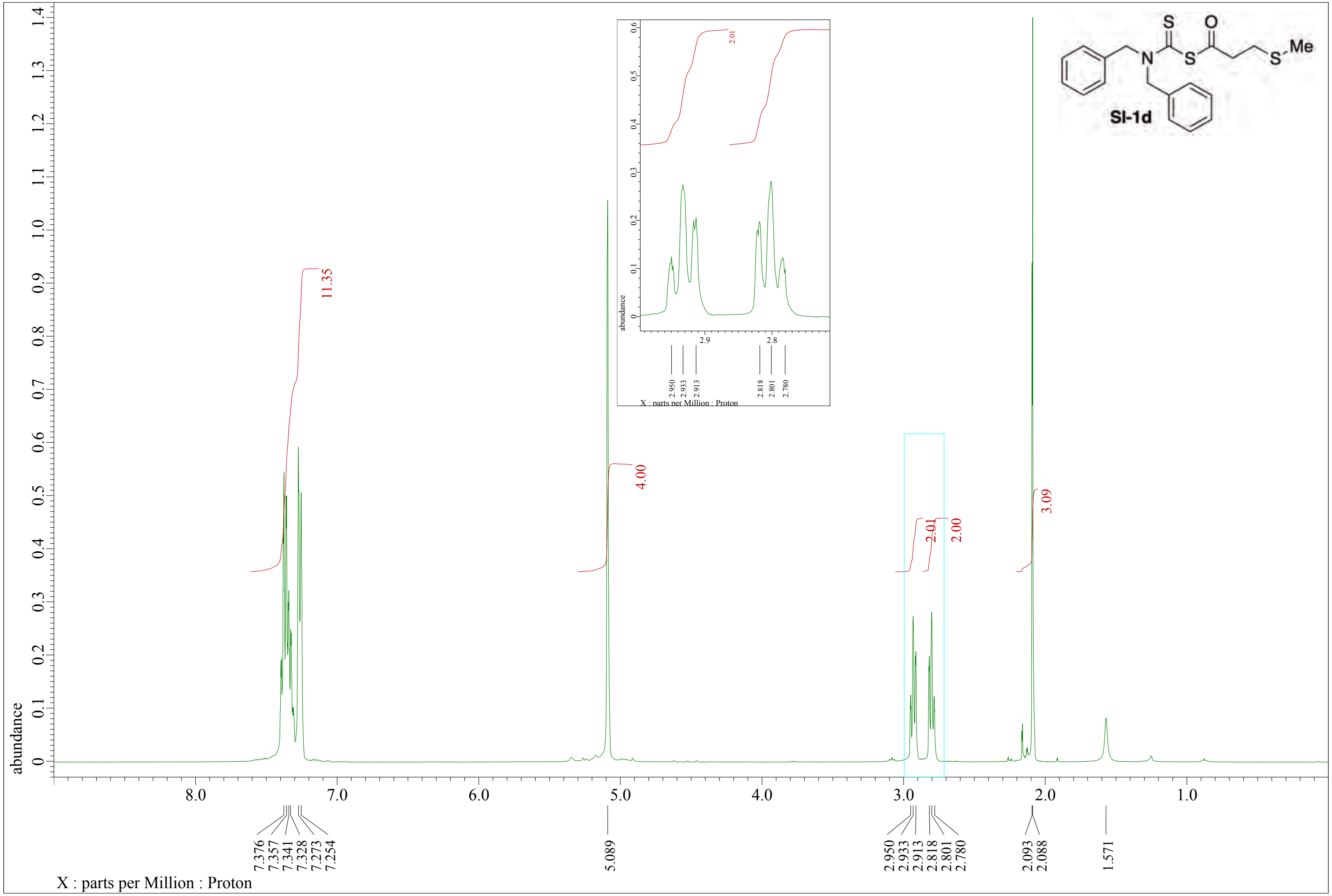
231828_KM_0629_B_pn #25-28 RT: 0.41-0.44 AV: 2 NL: 9.11E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



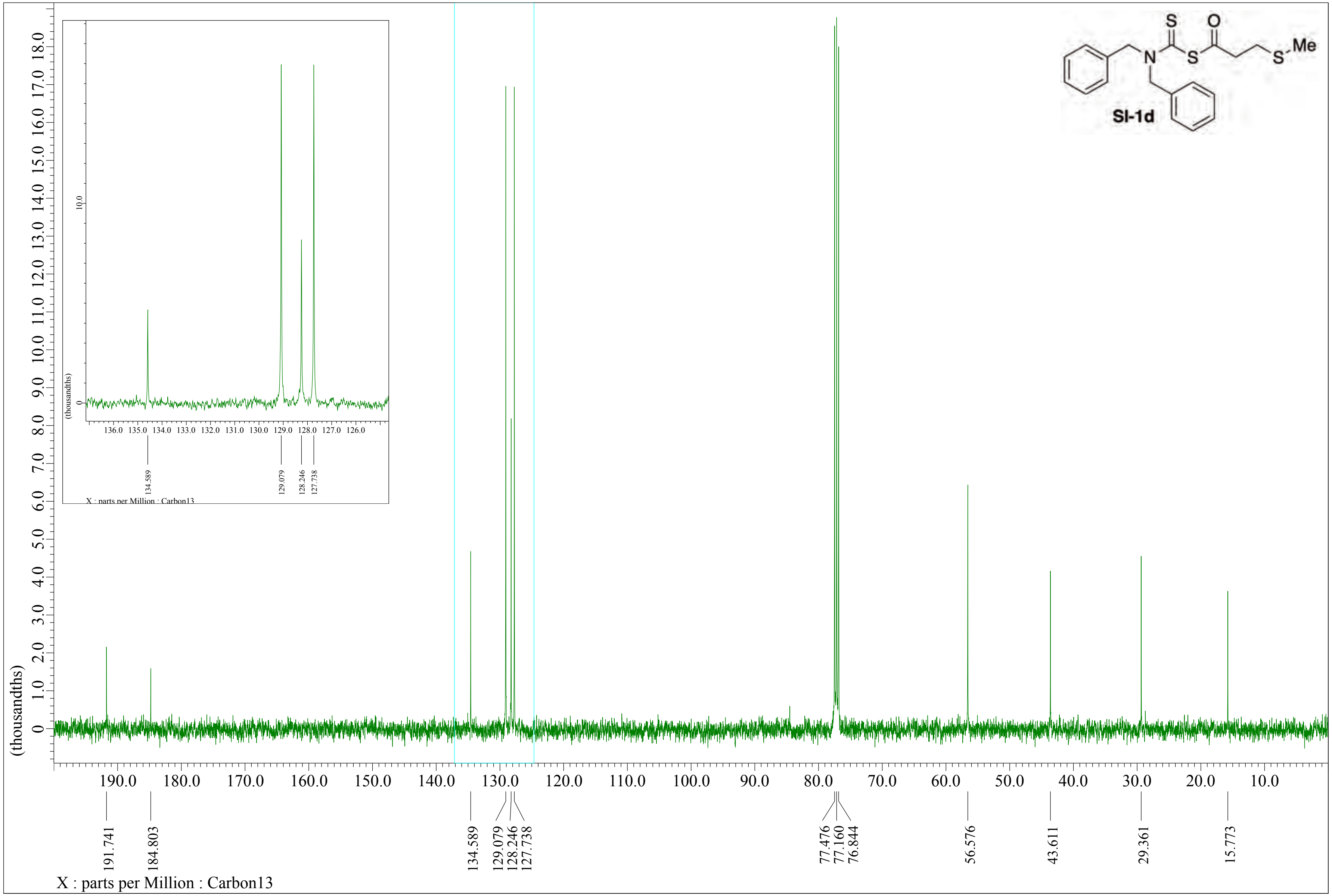
SI-1c

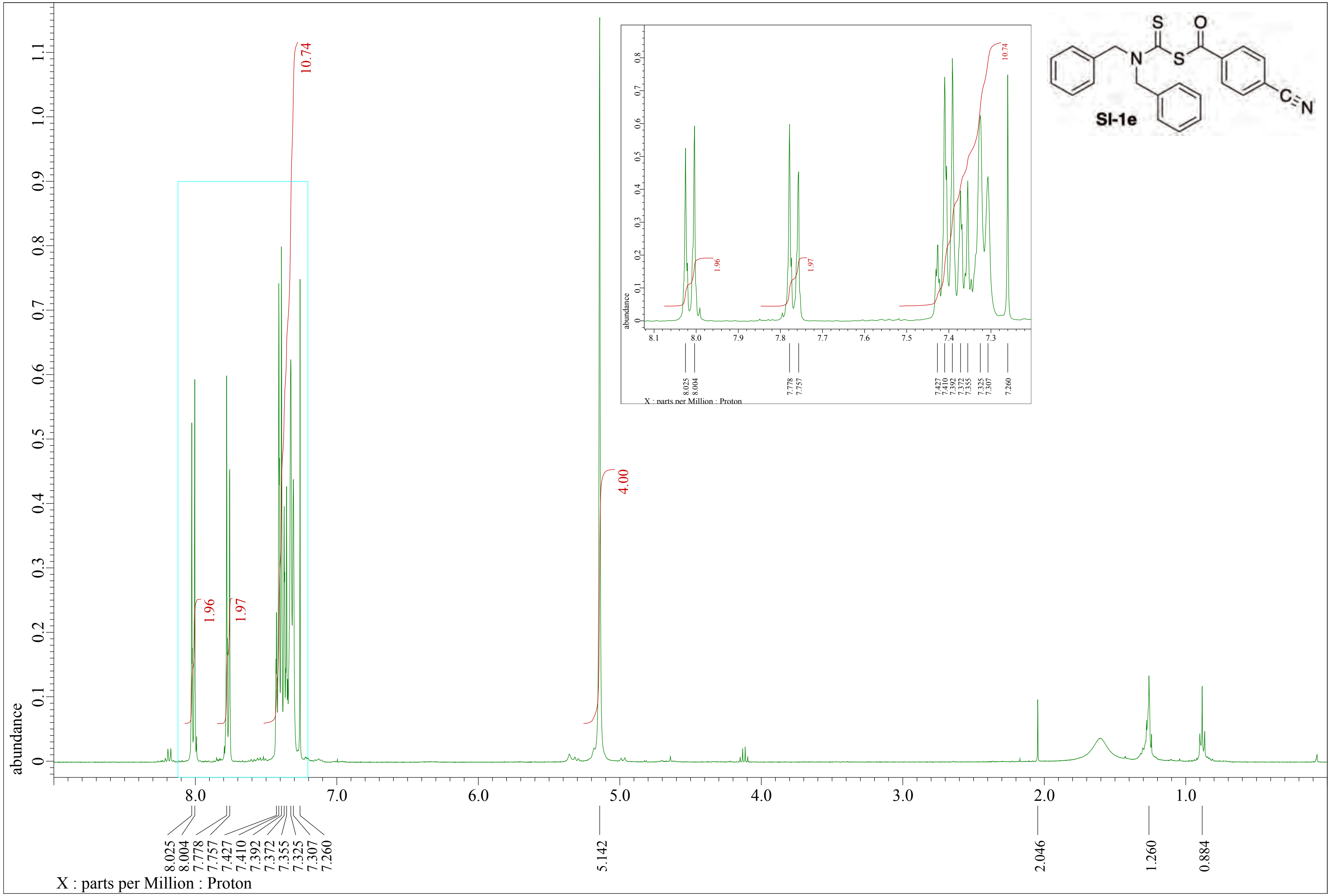
231828_KM_0629_B_pn #29-31 RT: 0.47-0.50 AV: 2 NL: 4.66E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



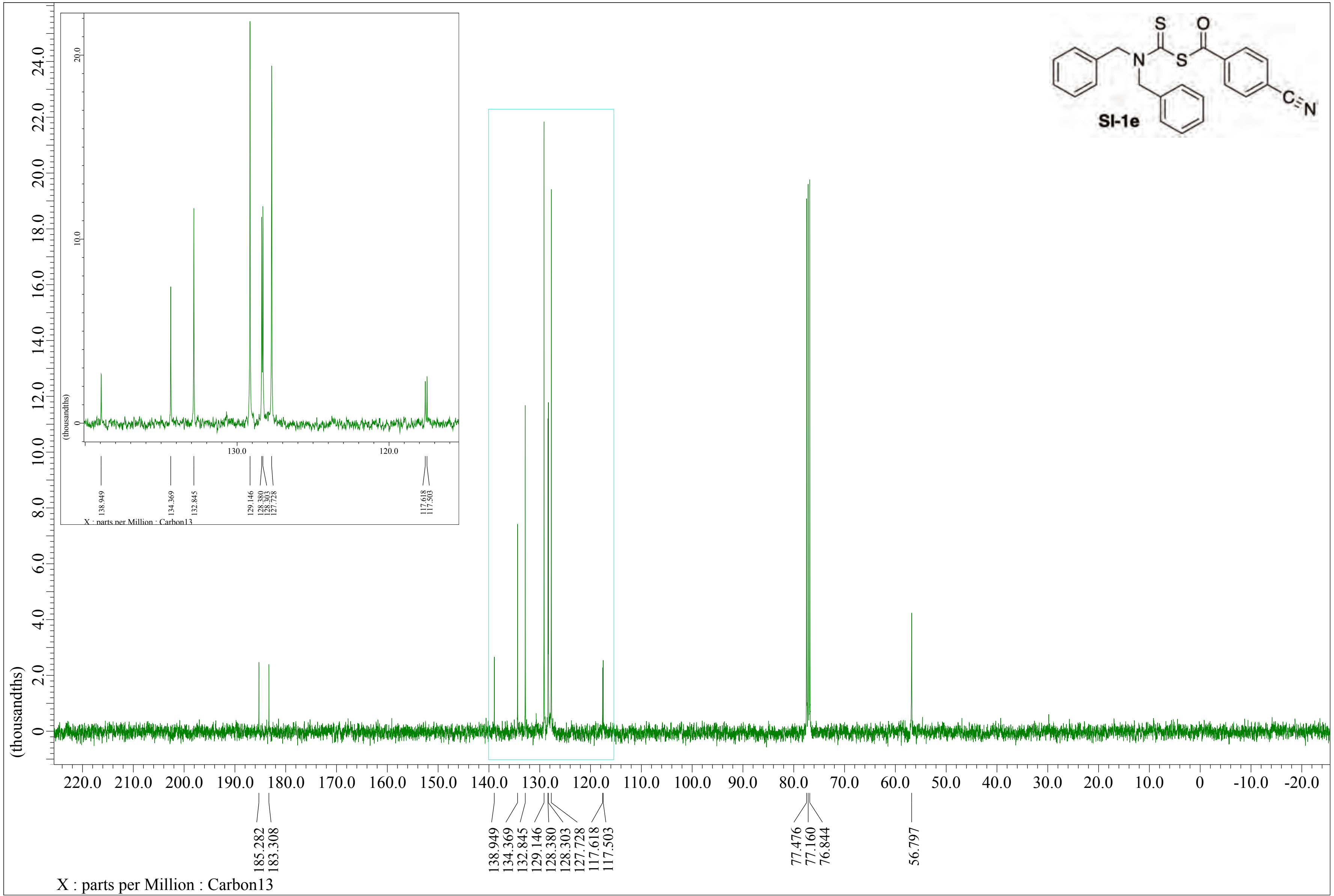


SI-1d
Me
abundance
X : parts per Million : Proton
11.35
4.00
2.01
2.00
3.09
7.376
7.357
7.341
7.328
7.273
7.254
5.089
2.950
2.933
2.913
2.818
2.801
2.780
2.093
2.088
1.571


SI-1d
S
O
N
S
S
Me
(thousandths)
X : parts per Million : Carbon13
191.741
184.803
134.589
129.079
128.246
127.738
77.476
77.160
76.844
56.576
43.611
29.361
15.773

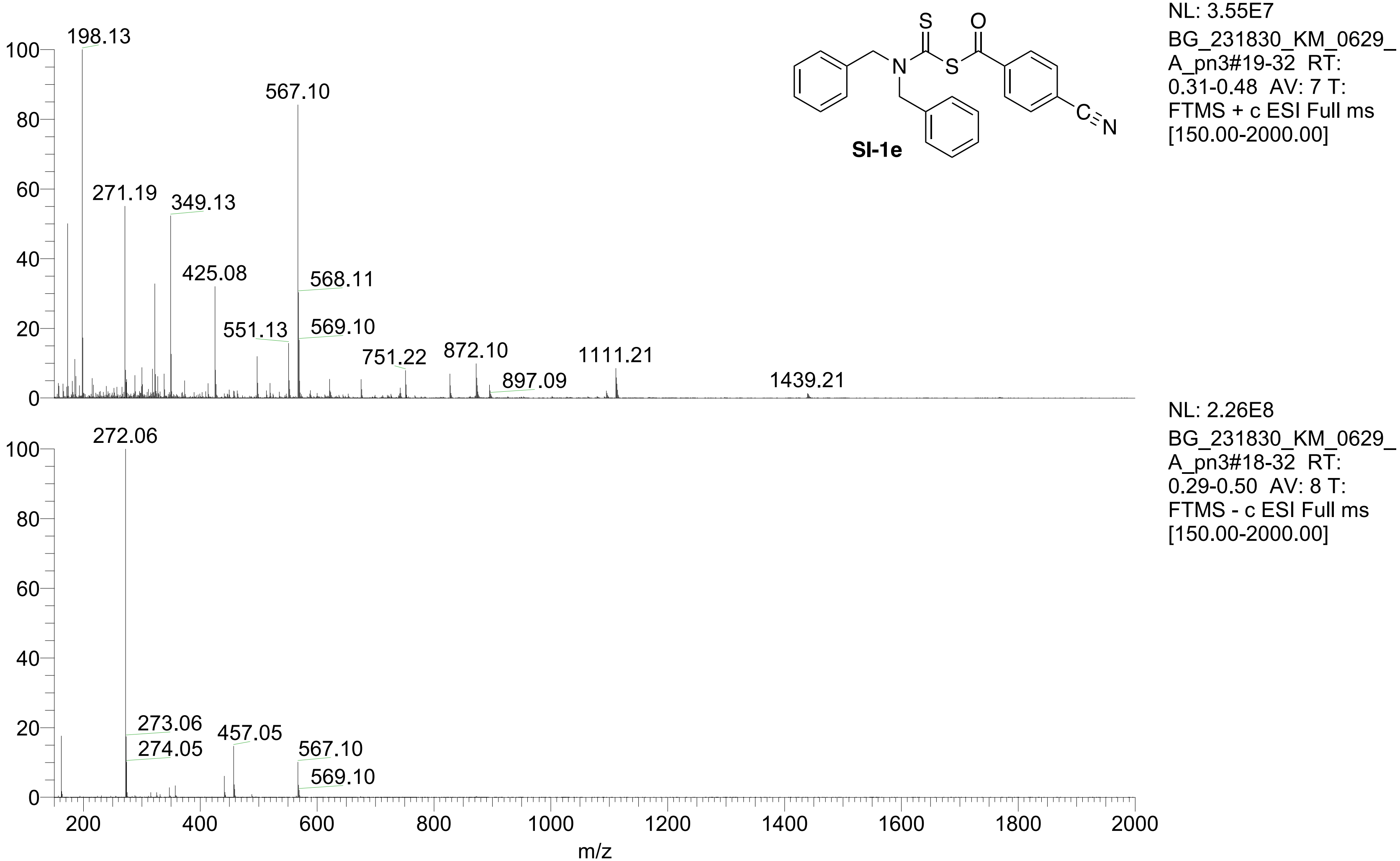


SI-1e
10.74
1.96
1.97
4.00
abundance
X : parts per Million : Proton
8.025
8.004
7.778
7.757
7.427
7.410
7.392
7.372
7.355
7.325
7.307
7.260
5.142
2.046
1.260
0.884


SI-1e
(thousandths)
0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
18.0
20.0
22.0
24.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
185.282
183.308
138.949
134.369
132.845
129.146
128.380
128.303
127.728
117.618
117.503
77.476
77.160
76.844
56.797
X : parts per Million : Carbon13

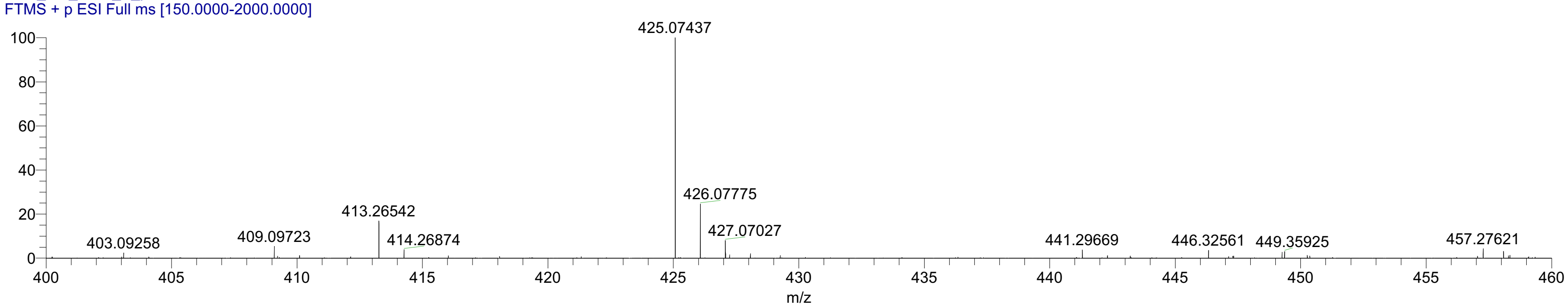
Sample No. : C:\Xcalibur\...\BG_231830_KM_06 _ _ 3
Instrument : Exactive Plus
Mobile phase solvent : MeOH
Operator name : hayashi harumi
Sample solvent : CHCl3
Date : 01/09/24 15:10:22
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

SI-1e

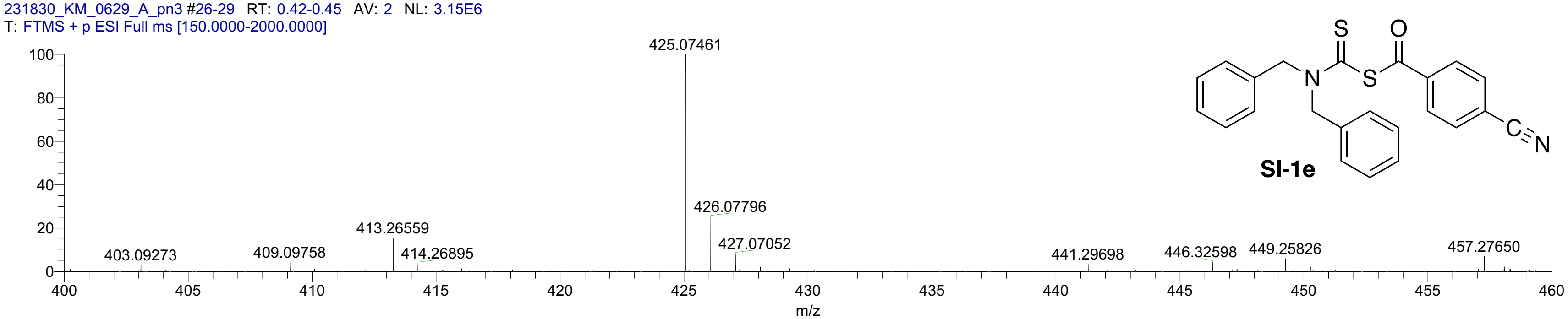


Sample No. : C:\Xcalibur\...\231830_KM_0629_A_pn3 Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 01/09/24 14:59:25
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

231830_KM_0629_A_pn3 #22-25 RT: 0.37-0.39 AV: 2 NL: 3.54E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]

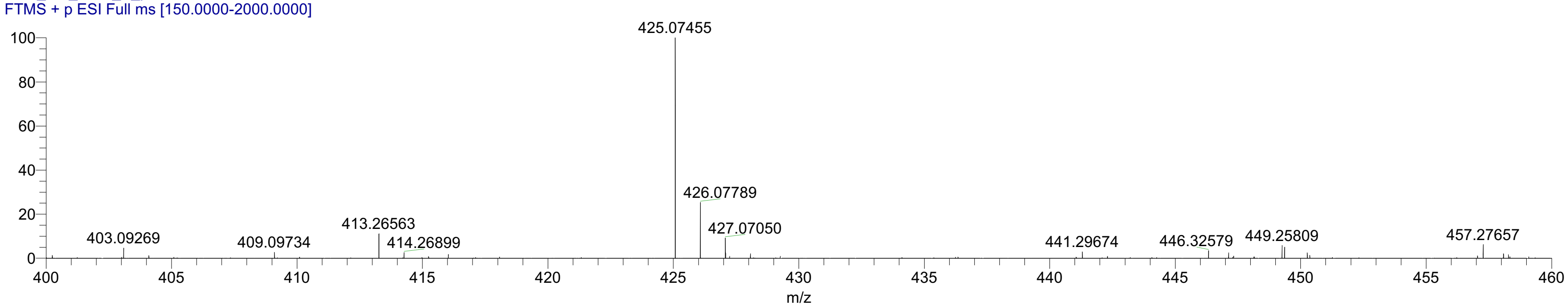


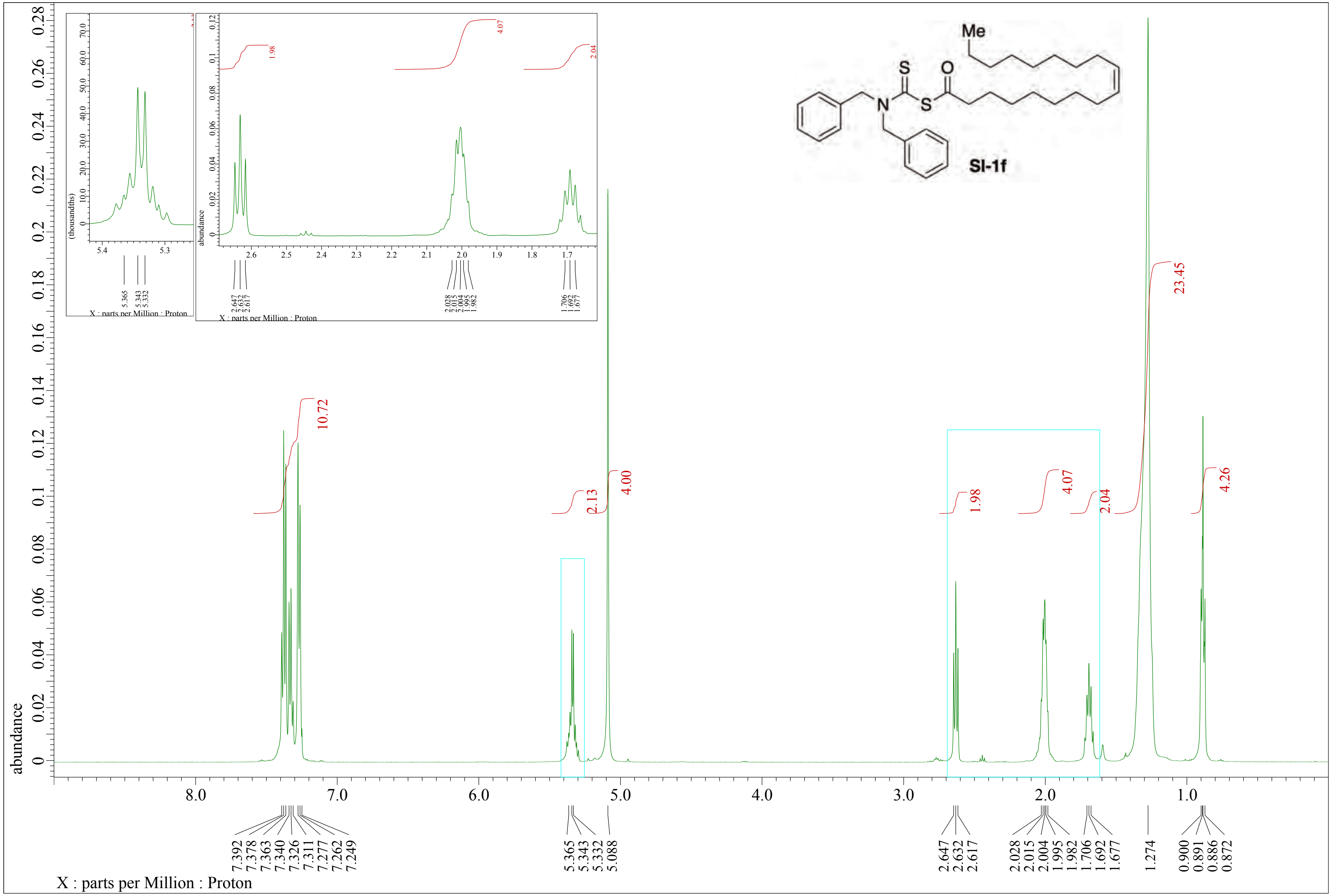
231830_KM_0629_A_pn3 #26-29 RT: 0.42-0.45 AV: 2 NL: 3.15E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



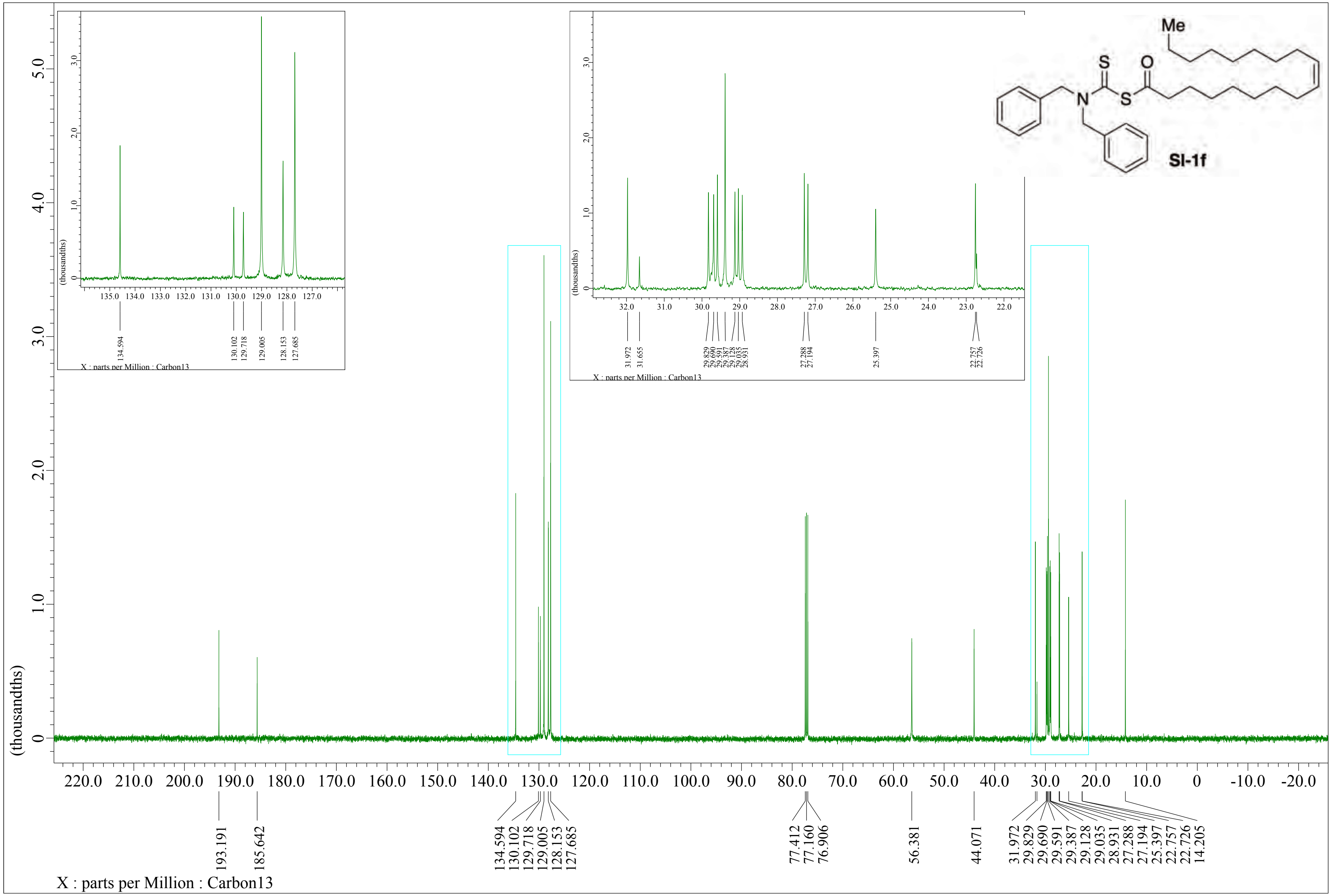
SI-1e

231830_KM_0629_A_pn3 #30-33 RT: 0.48-0.51 AV: 2 NL: 1.66E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]

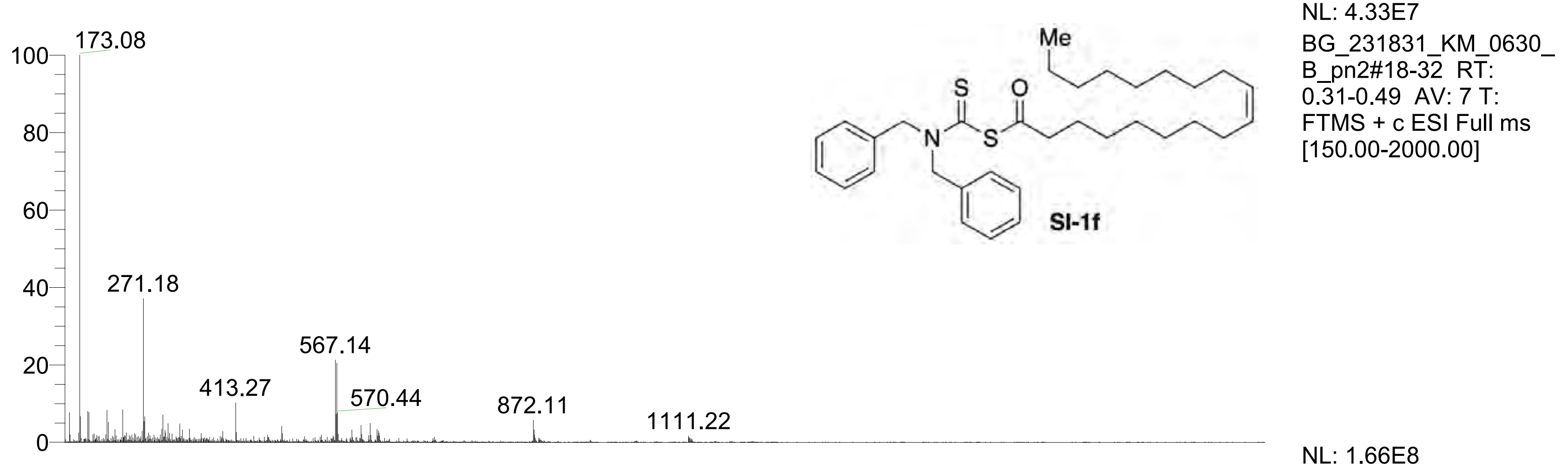




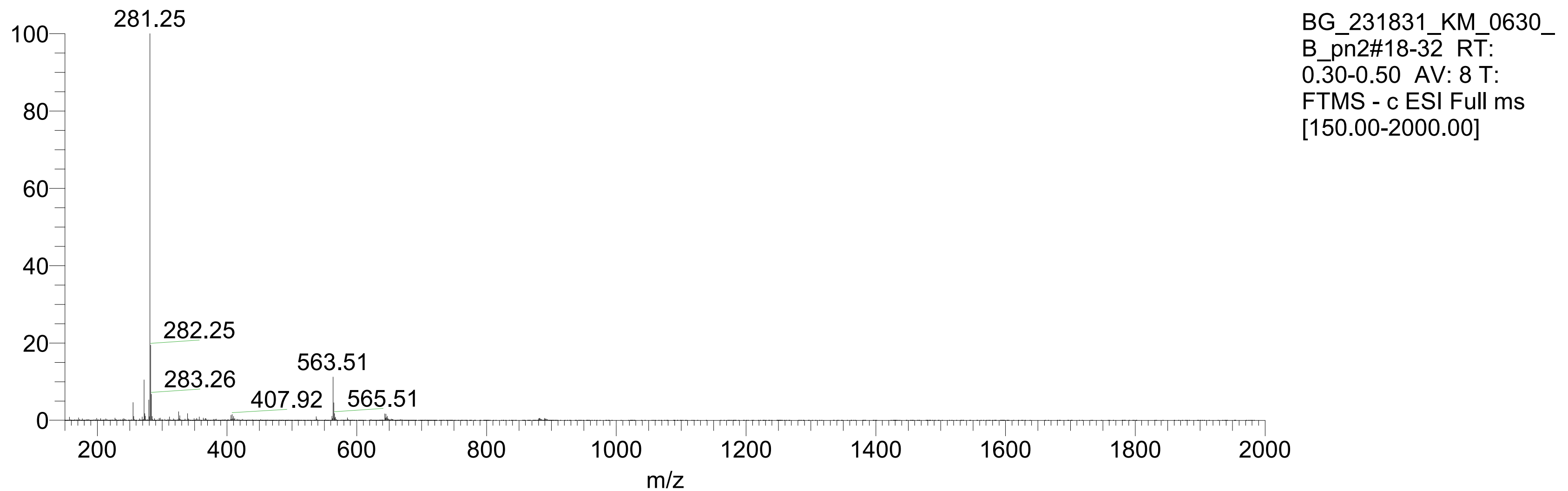
SI-1f
Me
S
O
N
S
abundance
X : parts per Million : Proton
10.72
2.13
4.00
1.98
4.07
2.04
23.45
4.26
7.392
7.378
7.363
7.340
7.326
7.311
7.277
7.262
7.249
5.365
5.343
5.332
5.088
2.647
2.632
2.617
2.028
2.015
2.004
1.995
1.982
1.706
1.692
1.677
1.274
0.900
0.891
0.886
0.872


SI-1f
Me
S
O
N
S
(thousandths)
X : parts per Million : Carbon13
193.191
185.642
134.594
130.102
129.718
129.005
128.153
127.685
77.412
77.160
76.906
56.381
44.071
31.972
29.829
29.690
29.591
29.387
29.128
29.035
28.931
27.288
27.194
25.397
22.757
22.726
14.205

Sample No. : C:\Xcalibur\...\BG_231831_KM_06 _ _, ı2 Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 01/17/24 13:21:51
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

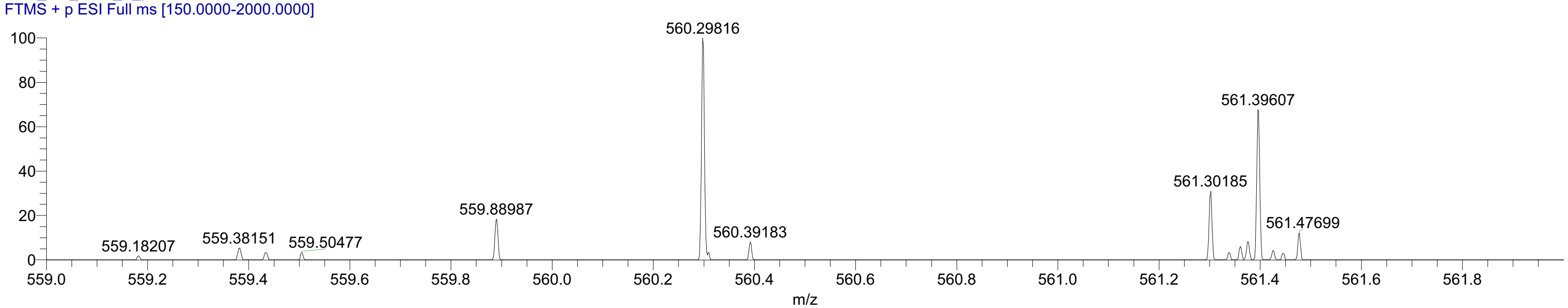


SI-1f

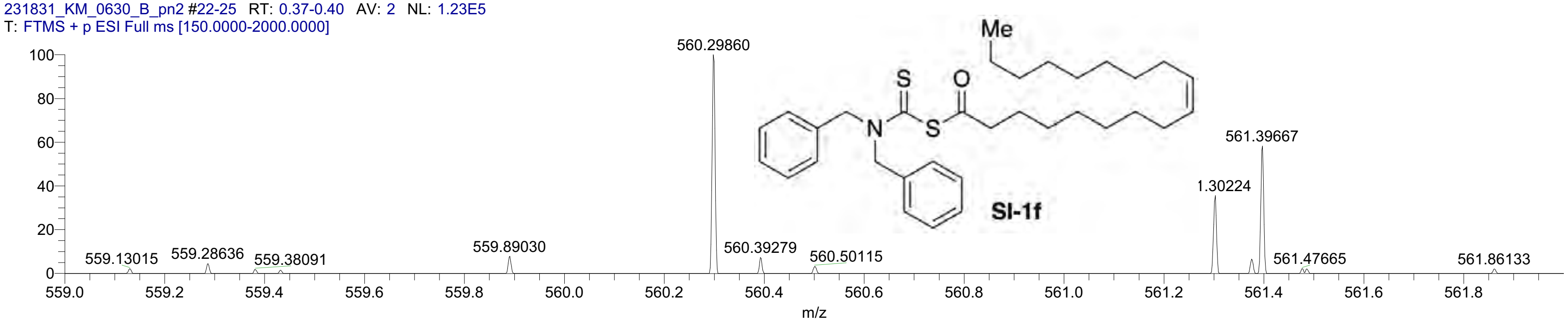


Sample No. : C:\Xcalibur\...\23183 ı_ĸıvı_0630_B_pn2 Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 01/17/24 11:20:00
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

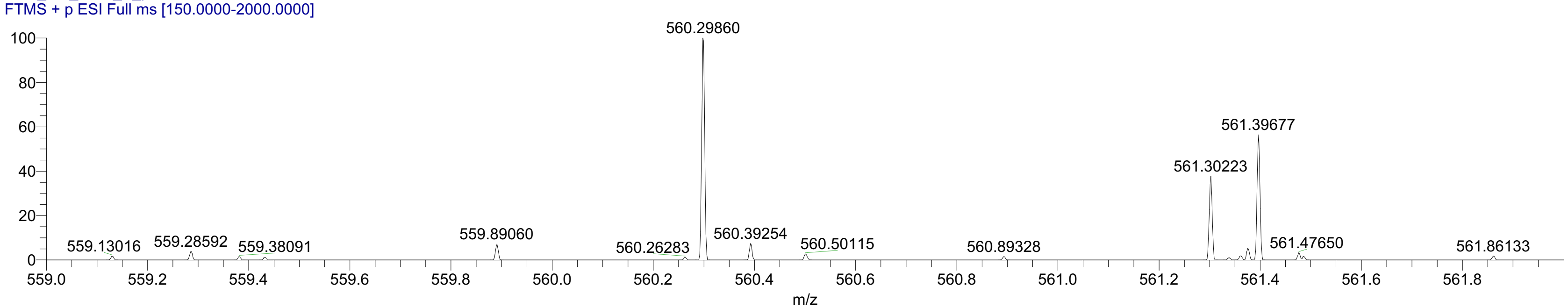
231831_KM_0630_B_pn2 #18-22 RT: 0.31-0.34 AV: 2 NL: 5.00E4
T: FTMS + p ESI Full ms [150.0000-2000.0000]

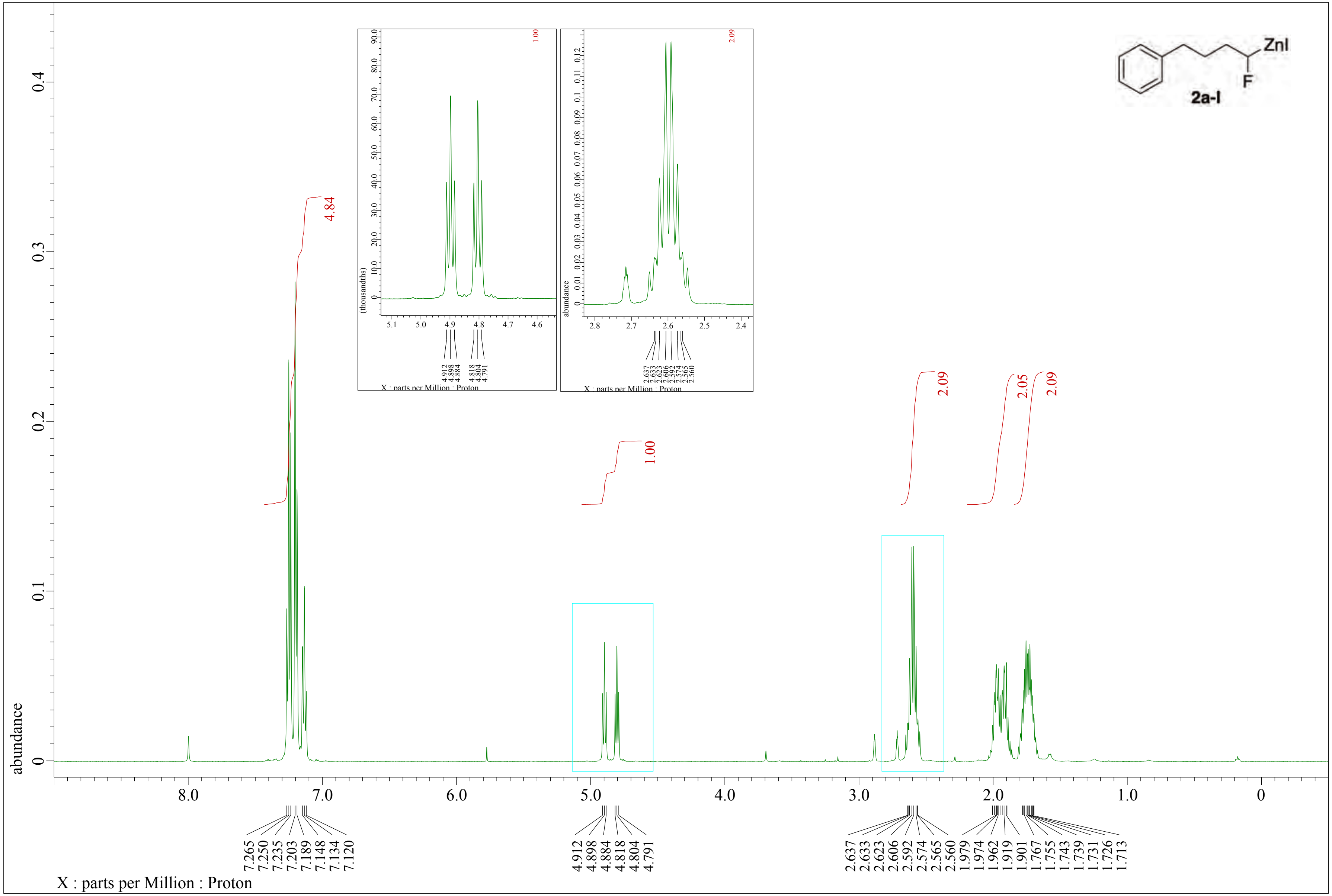


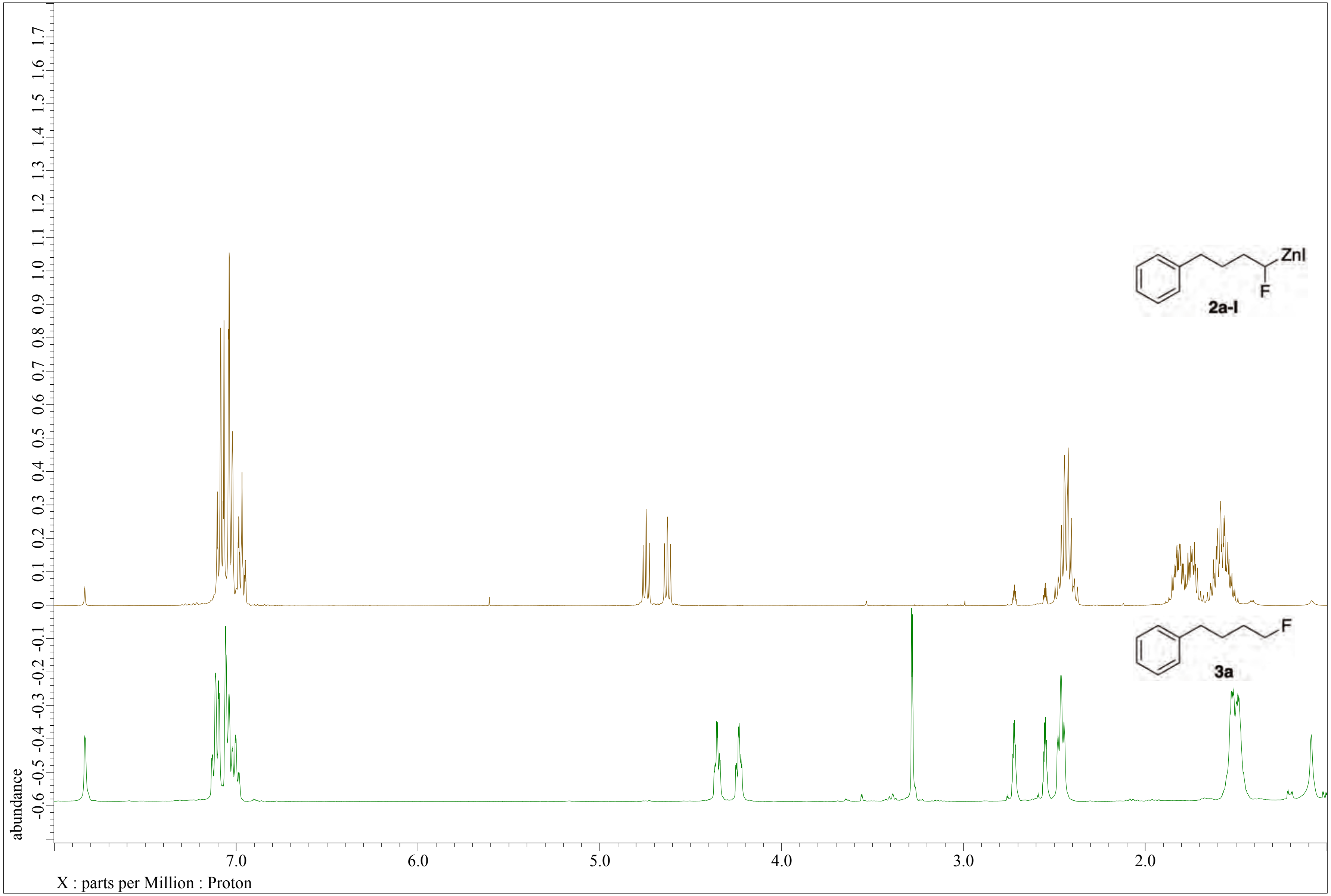
231831_KM_0630_B_pn2 #22-25 RT: 0.37-0.40 AV: 2 NL: 1.23E5
T: FTMS + p ESI Full ms [150.0000-2000.0000]



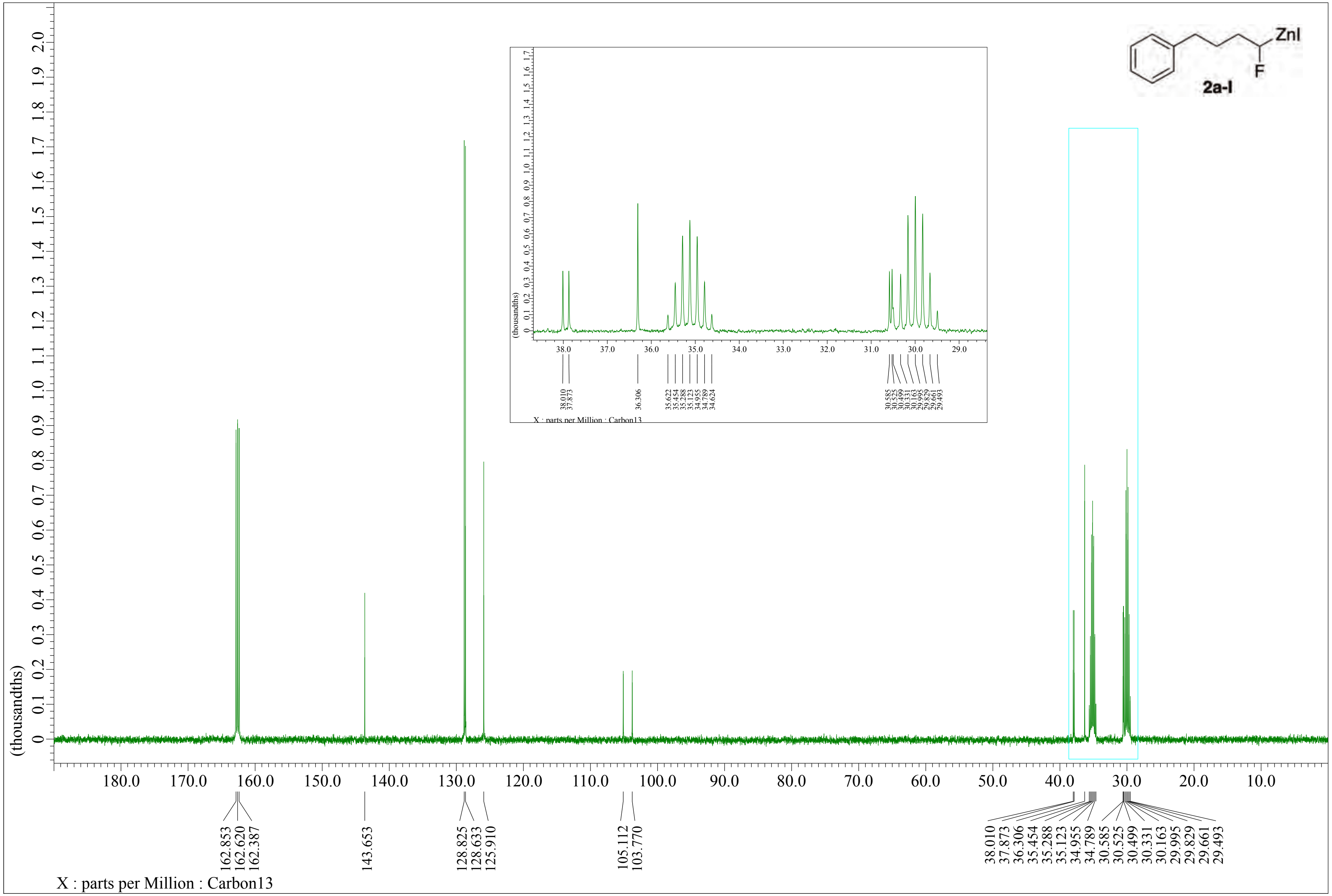
231831_KM_0630_B_pn2 #25-29 RT: 0.40-0.46 AV: 3 NL: 9.96E4
T: FTMS + p ESI Full ms [150.0000-2000.0000]



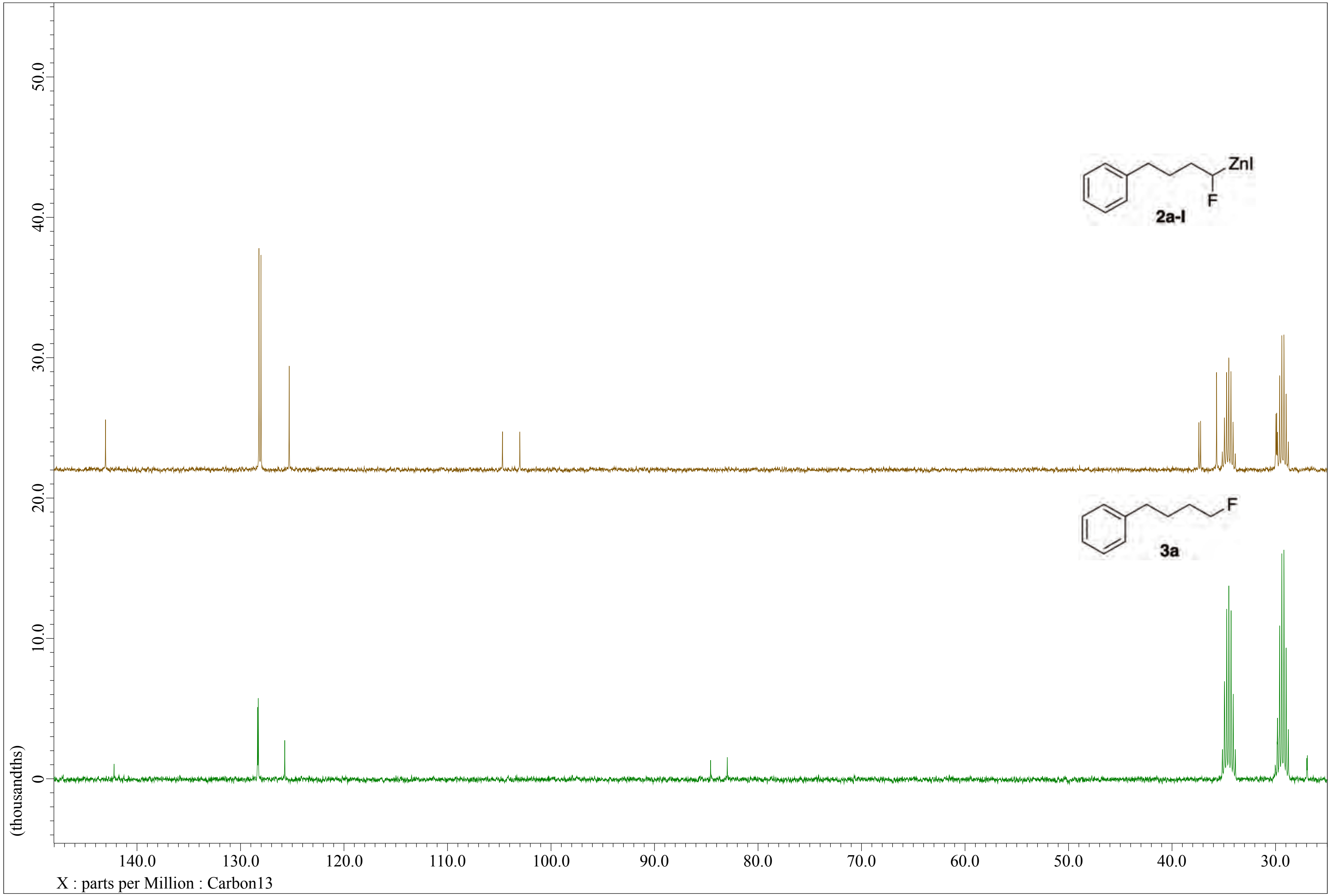

2a-I
X : parts per Million : Proton
abundance
4.84
1.00
2.09
2.05
2.09
7.265
7.250
7.235
7.203
7.189
7.148
7.134
7.120
4.912
4.898
4.884
4.818
4.804
4.791
2.637
2.633
2.623
2.606
2.592
2.574
2.565
2.560
1.979
1.974
1.962
1.919
1.901
1.767
1.755
1.743
1.739
1.731
1.726
1.713



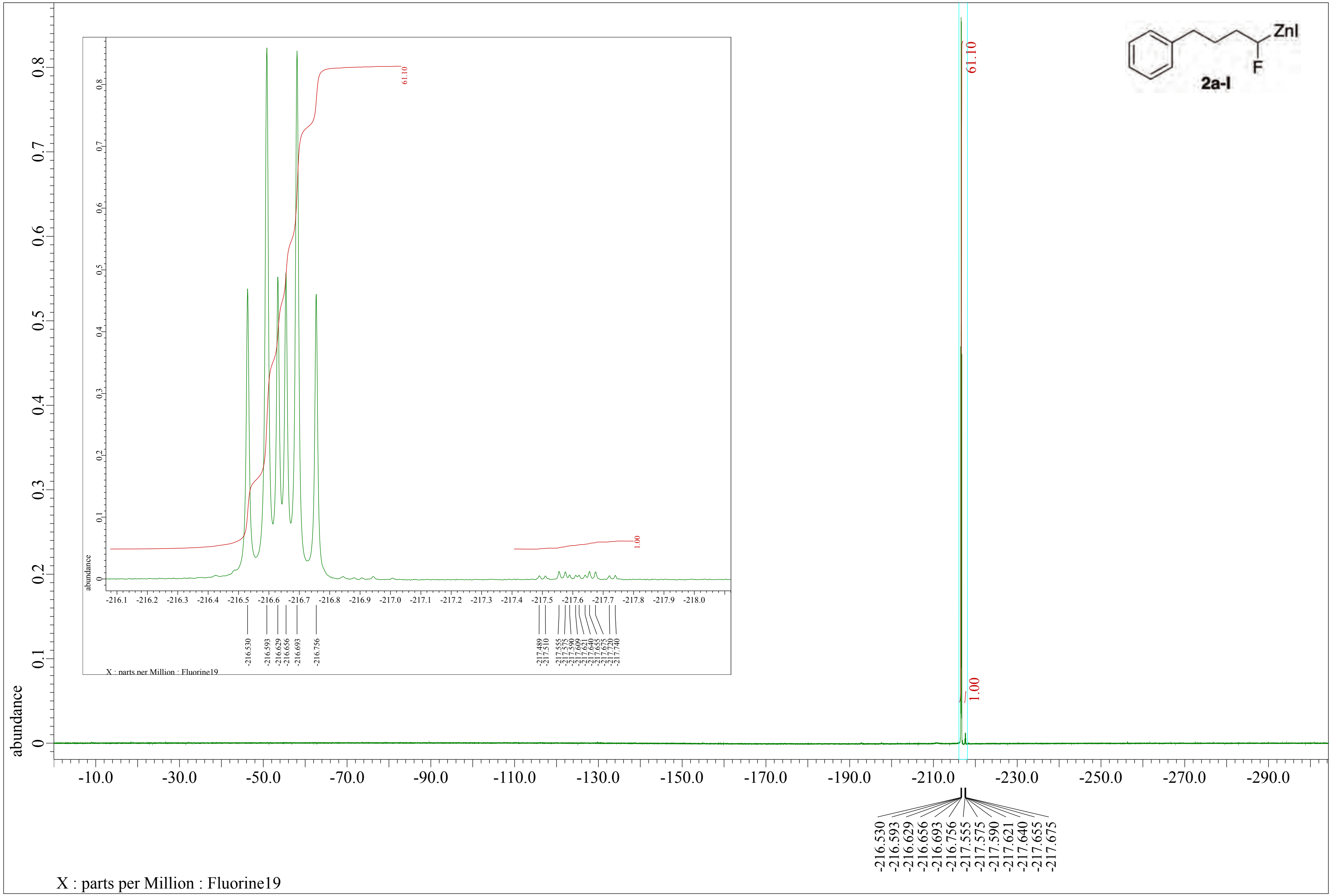
ZnI
F
2a-I
F
3a
abundance
X : parts per Million : Proton

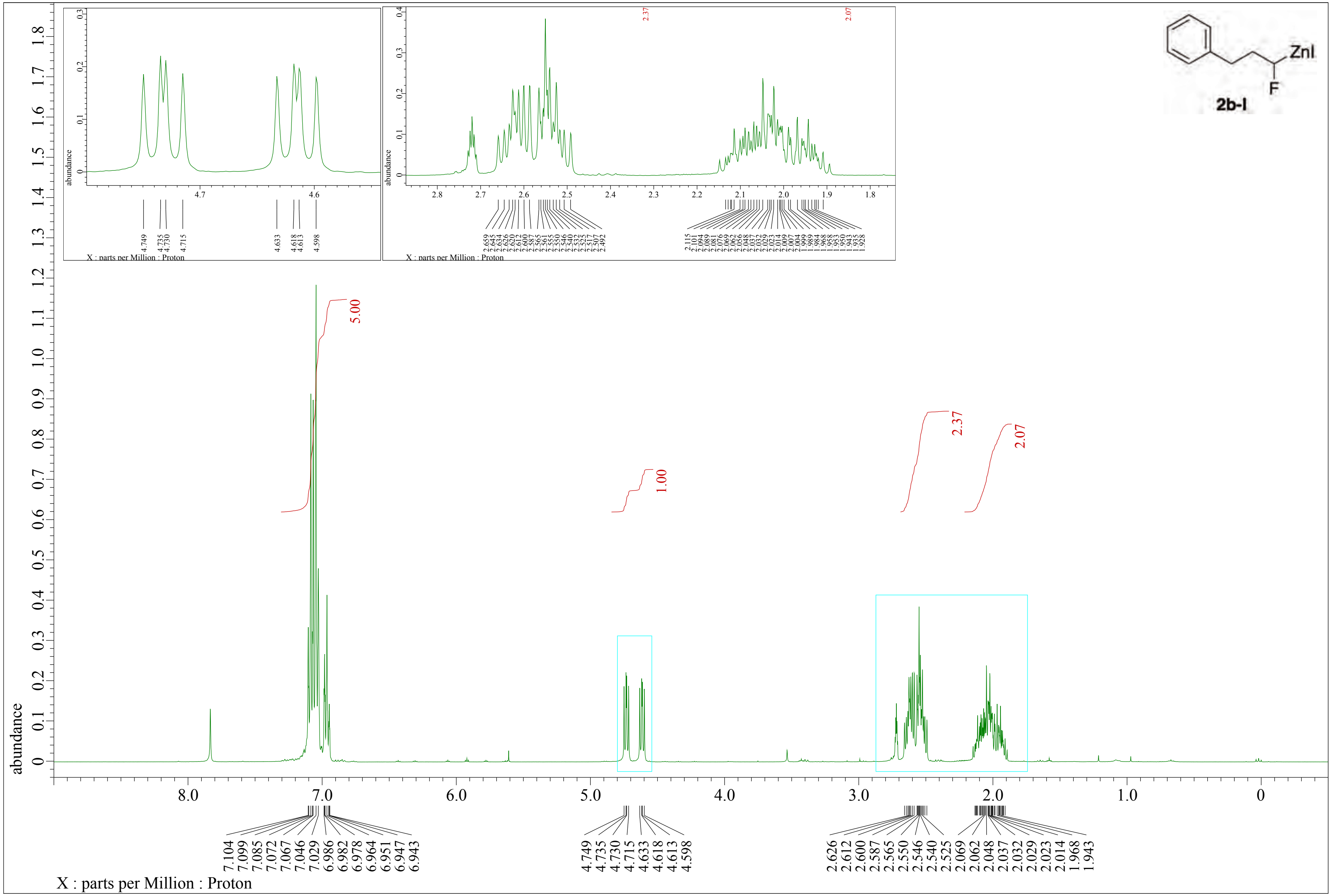


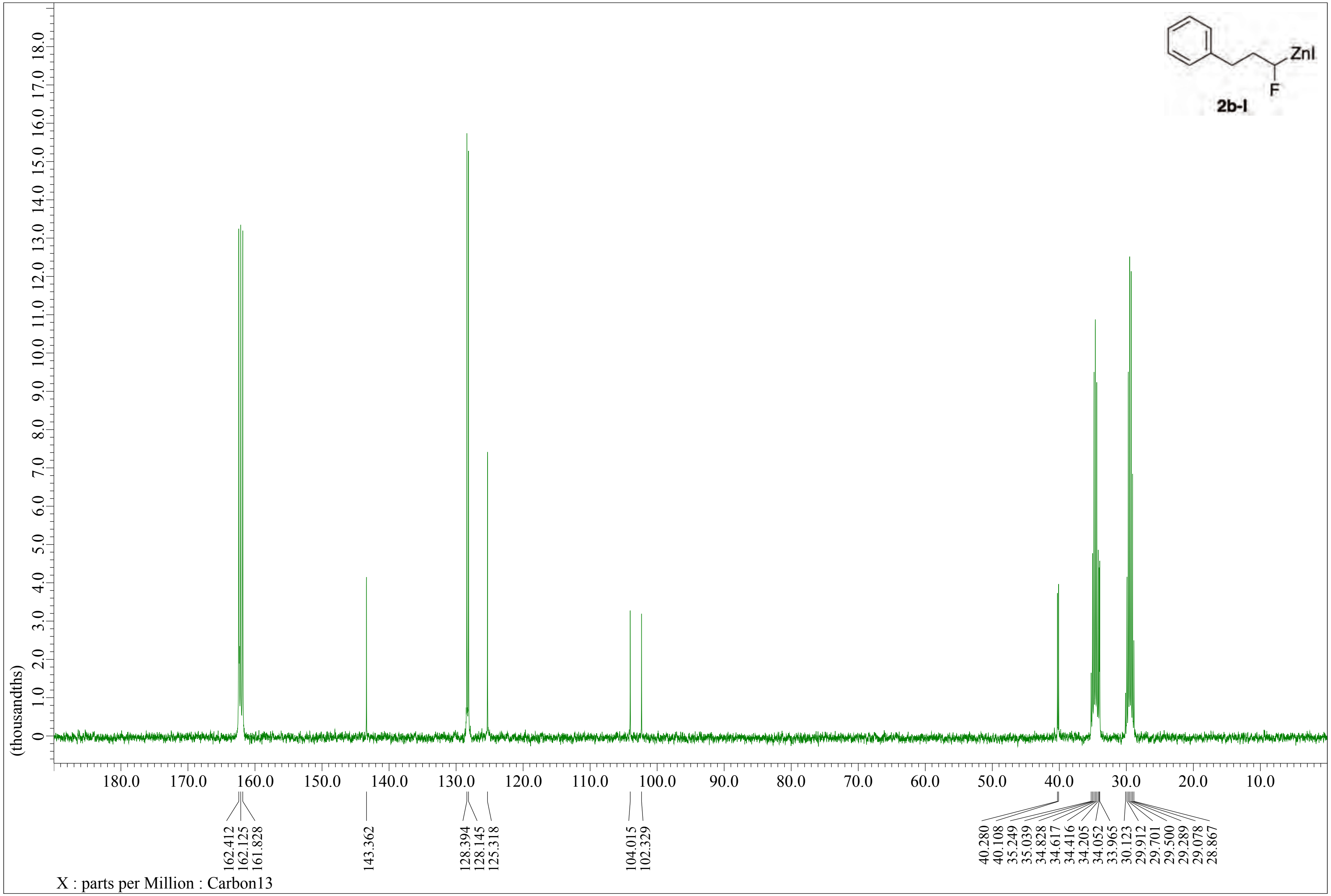
ZnI
F
2a-I
(thousandths)
X : parts per Million : Carbon13
162.853
162.620
162.387
143.653
128.825
128.633
125.910
105.112
103.770
38.010
37.873
36.306
35.454
35.288
35.123
34.955
34.789
30.585
30.525
30.499
30.331
30.163
29.995
29.829
29.661
29.493
35.622
34.624

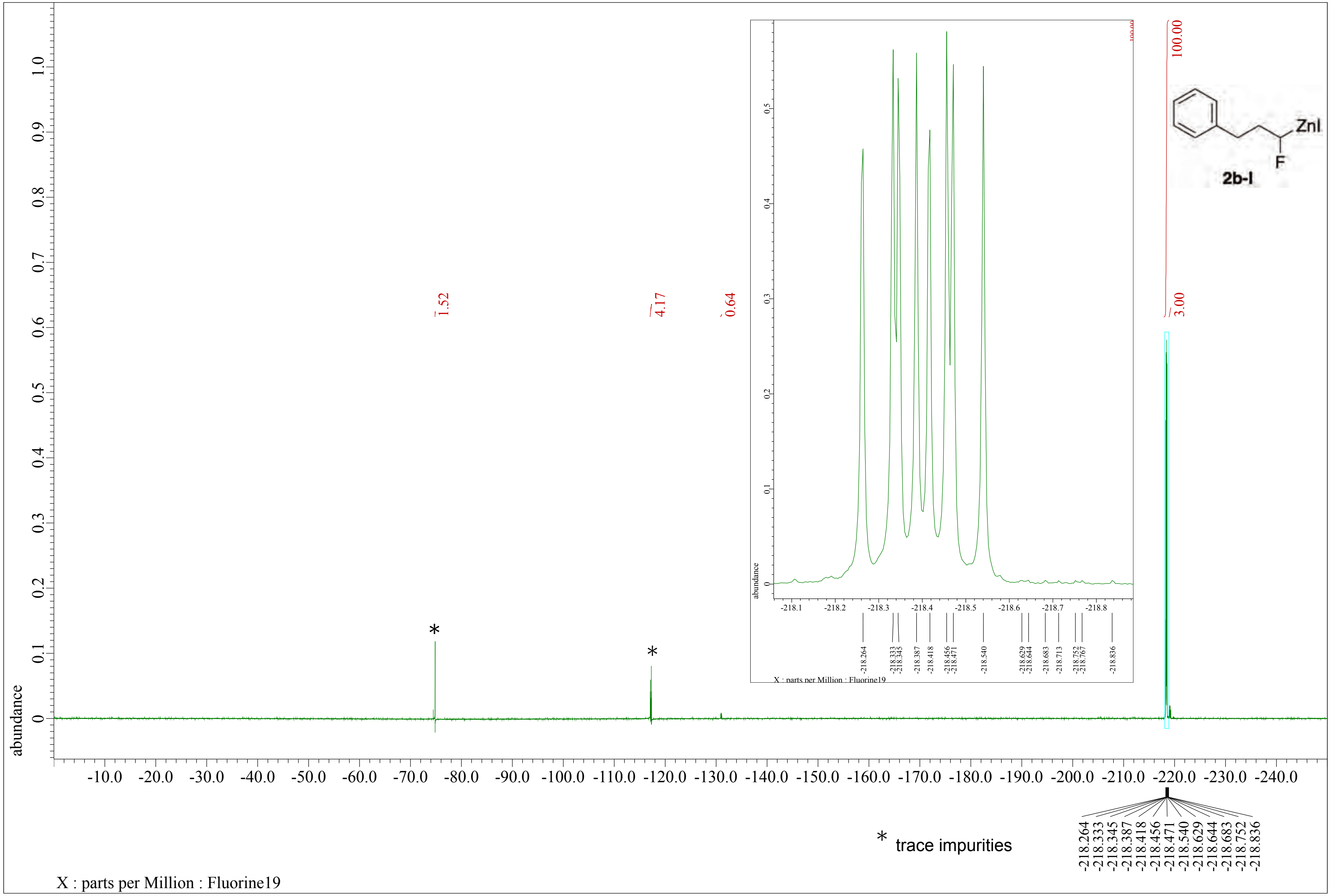


ZnI
F
2a-I
F
3a
50.0
40.0
30.0
20.0
10.0
0
(thousandths)
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
X : parts per Million : Carbon13

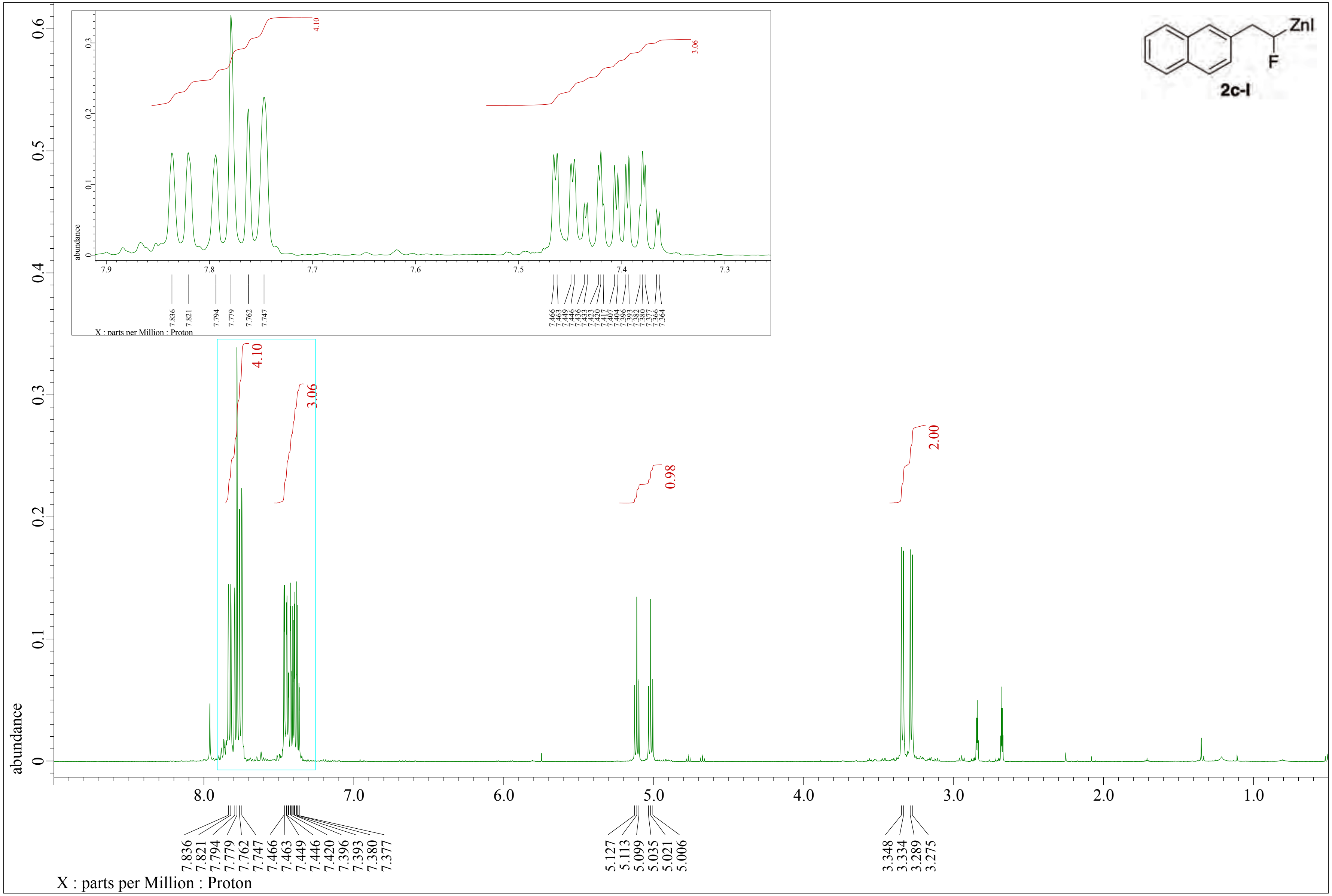

ZnI
F
2a-I
61.10
1.00
abundance
X : parts per Million : Fluorine19
-216.530
-216.593
-216.629
-216.656
-216.693
-216.756
-217.555
-217.575
-217.590
-217.621
-217.640
-217.655
-217.675

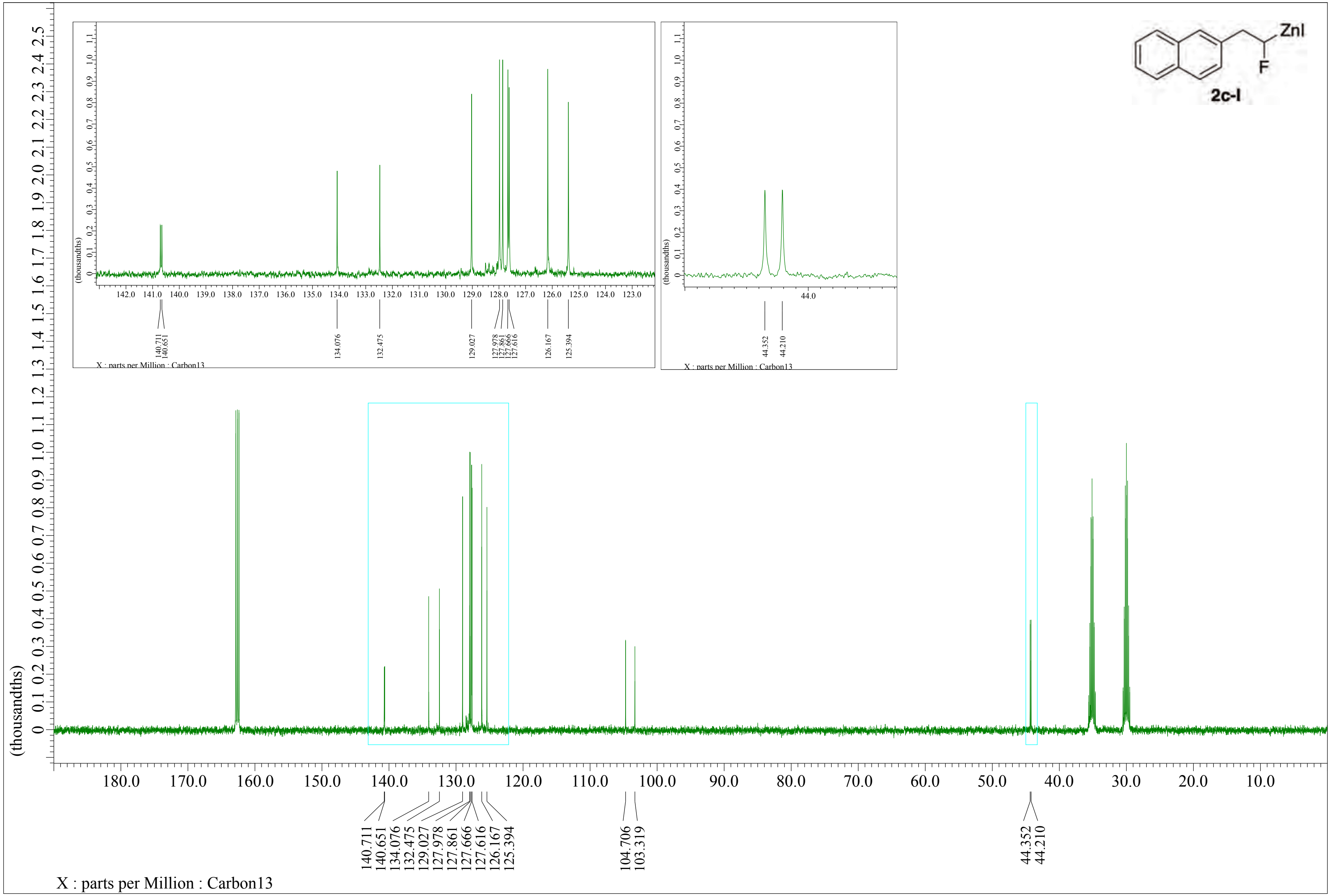

abundance
X : parts per Million : Proton
5.00
1.00
2.37
2.07
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2b-I


ZnI
F
2b-I
(thousandths)
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
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
162.412
162.125
161.828
143.362
128.394
128.145
125.318
104.015
102.329
40.280
40.108
35.249
35.039
34.828
34.617
34.416
34.205
34.052
33.965
30.123
29.912
29.701
29.500
29.289
29.078
28.867
X : parts per Million : Carbon13

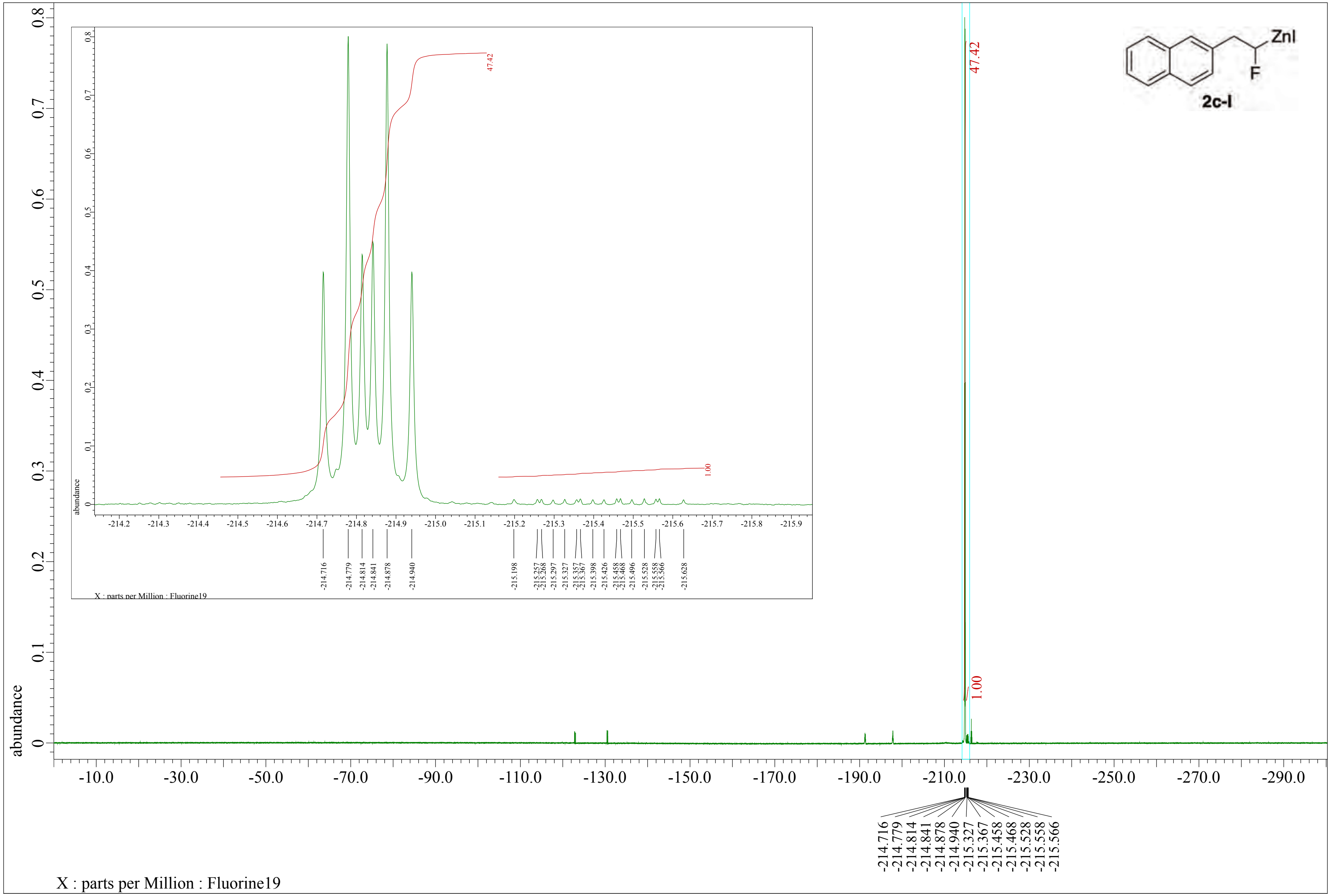


abundance
1.52
4.17
0.64
3.00
100.00
ZnI
F
2b-I
*
* trace impurities
-218.264
-218.333
-218.345
-218.387
-218.418
-218.456
-218.471
-218.540
-218.629
-218.644
-218.683
-218.713
-218.752
-218.767
-218.836
X : parts per Million : Fluorine19

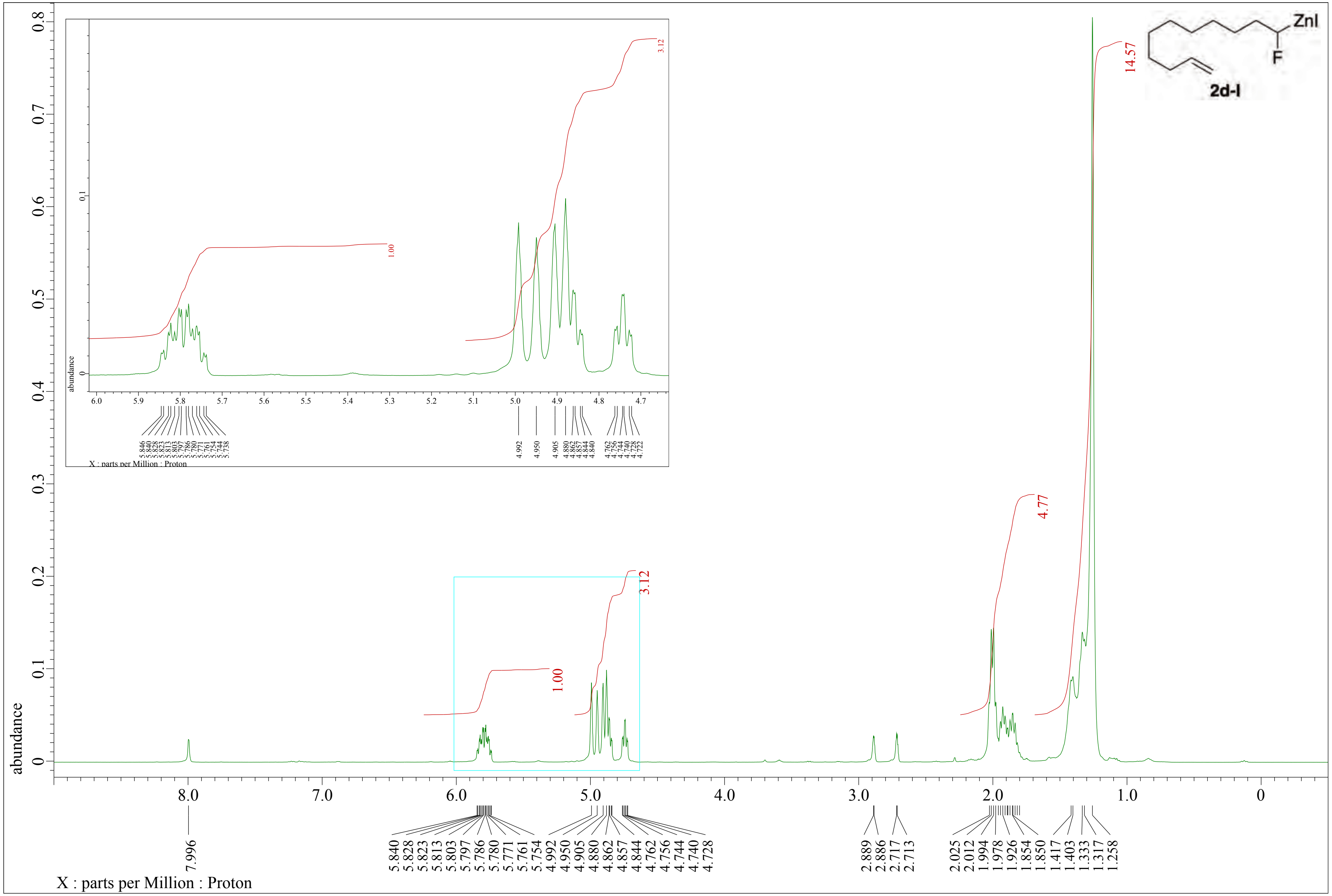

2c-I
ZnI
F
abundance
X : parts per Million : Proton
4.10
3.06
0.98
2.00
7.836 7.821 7.794 7.779 7.762 7.747 7.466 7.463 7.449 7.446 7.420 7.396 7.393 7.380 7.377
5.127 5.113 5.099 5.035 5.021 5.006
3.348 3.334 3.289 3.275
7.836 7.821 7.794 7.779 7.762 7.747
7.466 7.463 7.449 7.446 7.436 7.433 7.423 7.420 7.417 7.407 7.404 7.396 7.393 7.382 7.380 7.377 7.366 7.364

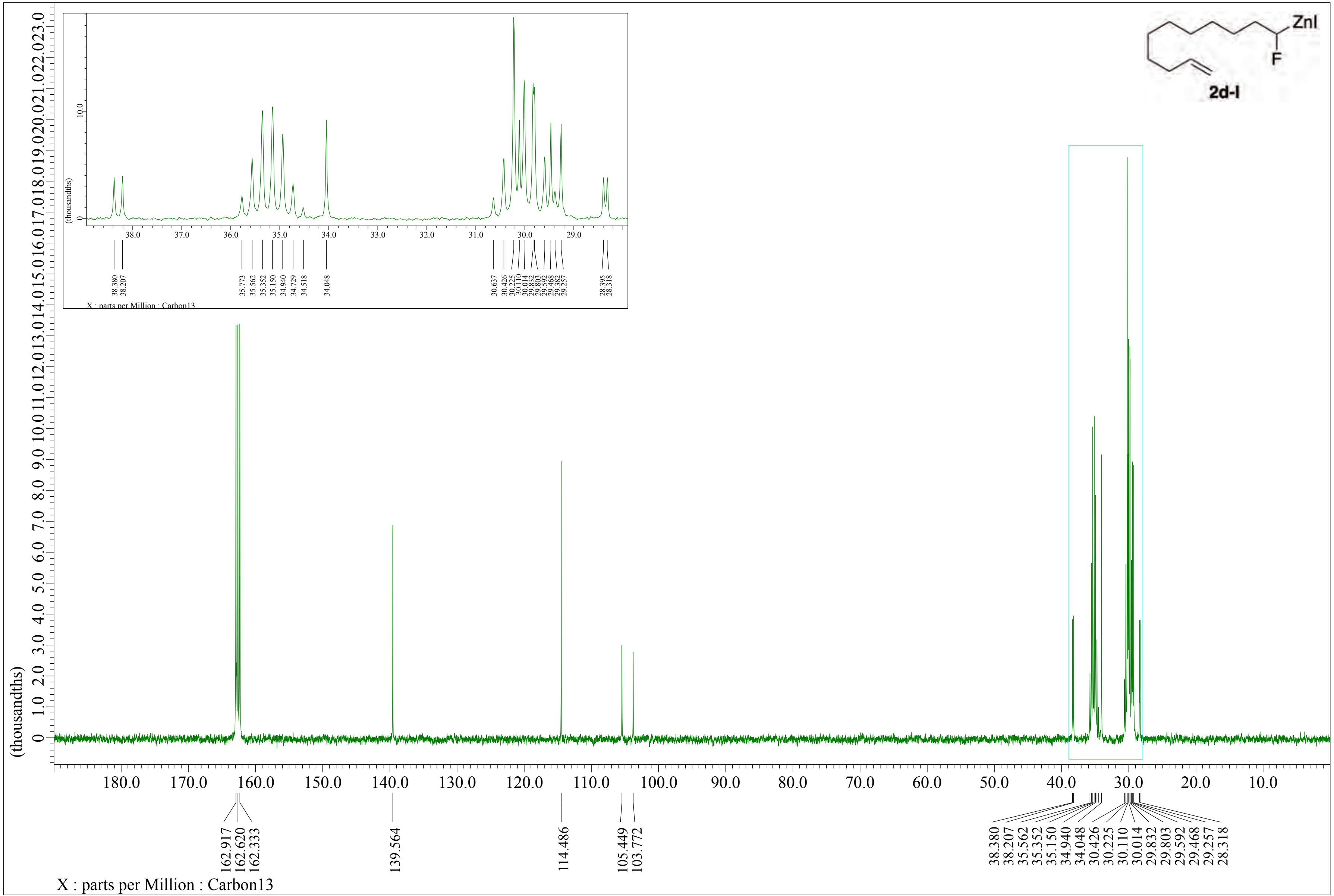


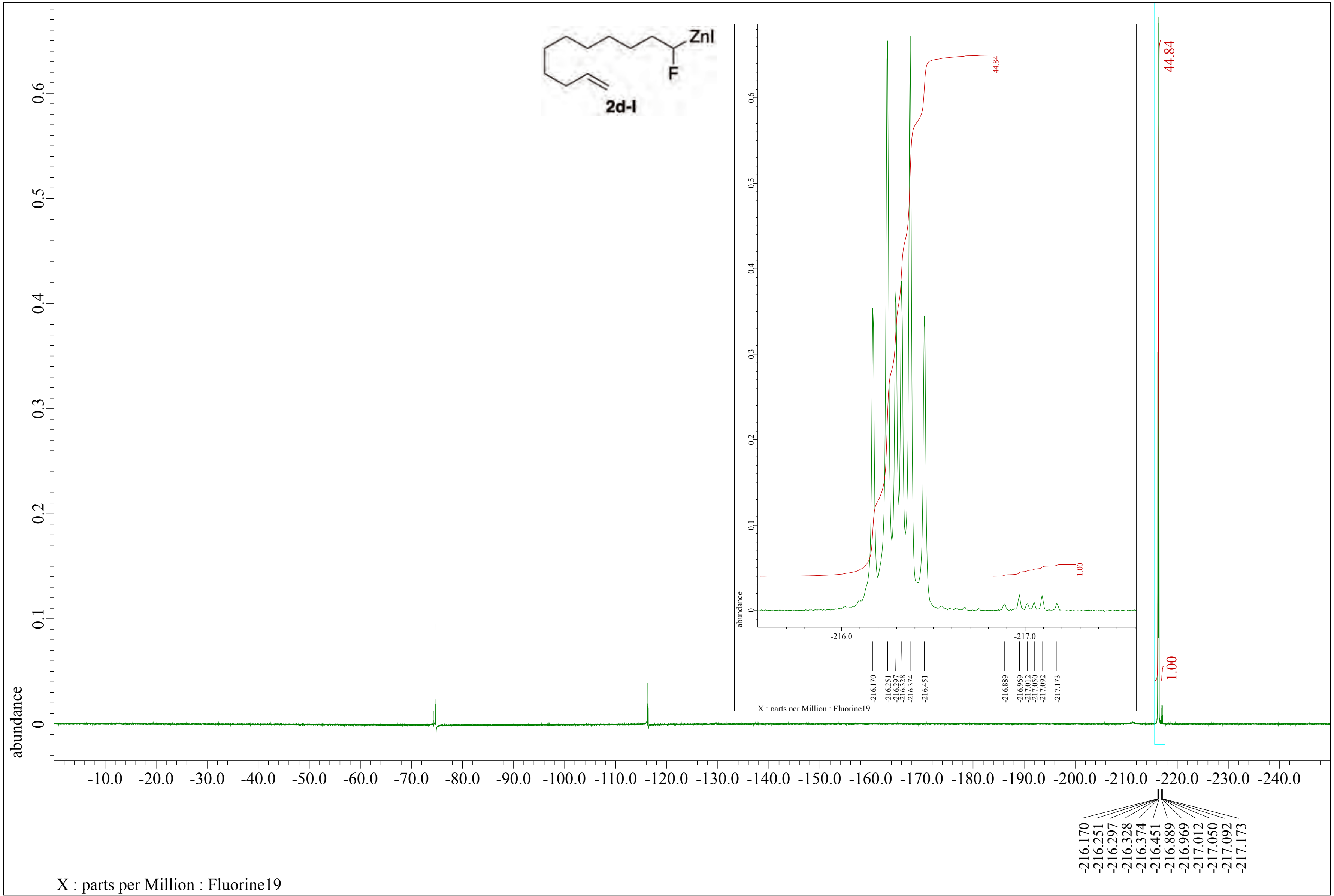
2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 0
(thousandths)
180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
140.711
140.651
134.076
132.475
129.027
127.978
127.861
127.666
127.616
126.167
125.394
104.706
103.319
44.352
44.210
X : parts per Million : Carbon13
ZnI
F
2c-I



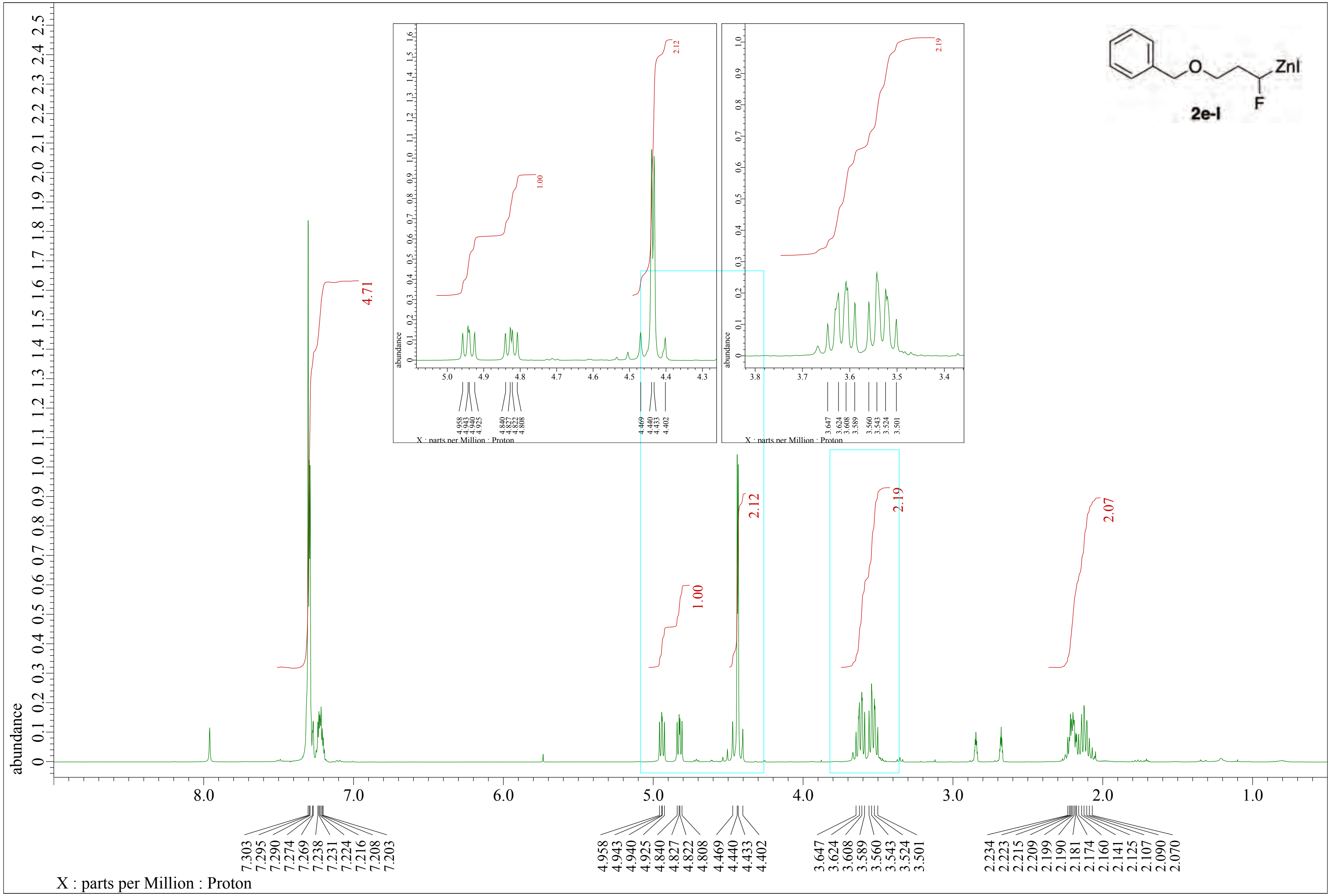
ZnI
F
2c-I
47.42
1.00
abundance
X : parts per Million : Fluorine19
-214.716
-214.779
-214.814
-214.841
-214.878
-214.940
-215.327
-215.367
-215.458
-215.468
-215.528
-215.558
-215.566

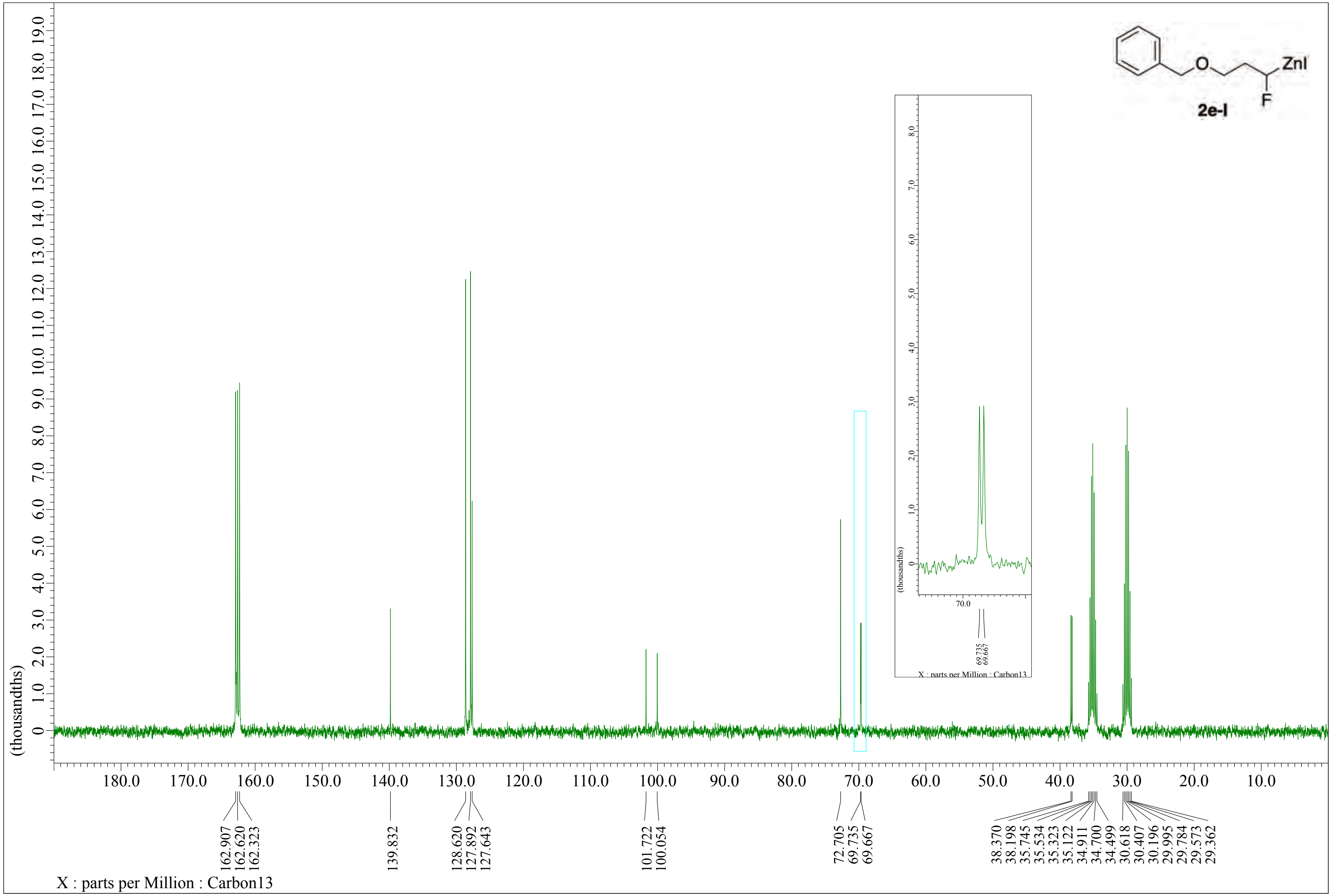

ZnI
F
2d-I
abundance
X : parts per Million : Proton
14.57
4.77
3.12
1.00
7.996
5.840 5.828 5.823 5.813 5.803 5.797 5.786 5.780 5.771 5.761 5.754
4.992 4.950 4.905 4.880 4.862 4.857 4.844 4.762 4.756 4.744 4.740 4.728
2.889 2.886 2.717 2.713
2.025 2.012 1.994 1.978 1.926 1.854 1.850
1.417 1.403 1.333 1.317 1.258


ZnI
F
2d-I
(thousandths)
X : parts per Million : Carbon13
162.917
162.620
162.333
139.564
114.486
105.449
103.772
38.380
38.207
35.562
35.352
35.150
34.940
34.048
30.426
30.225
30.110
30.014
29.832
29.803
29.592
29.468
29.257
28.318

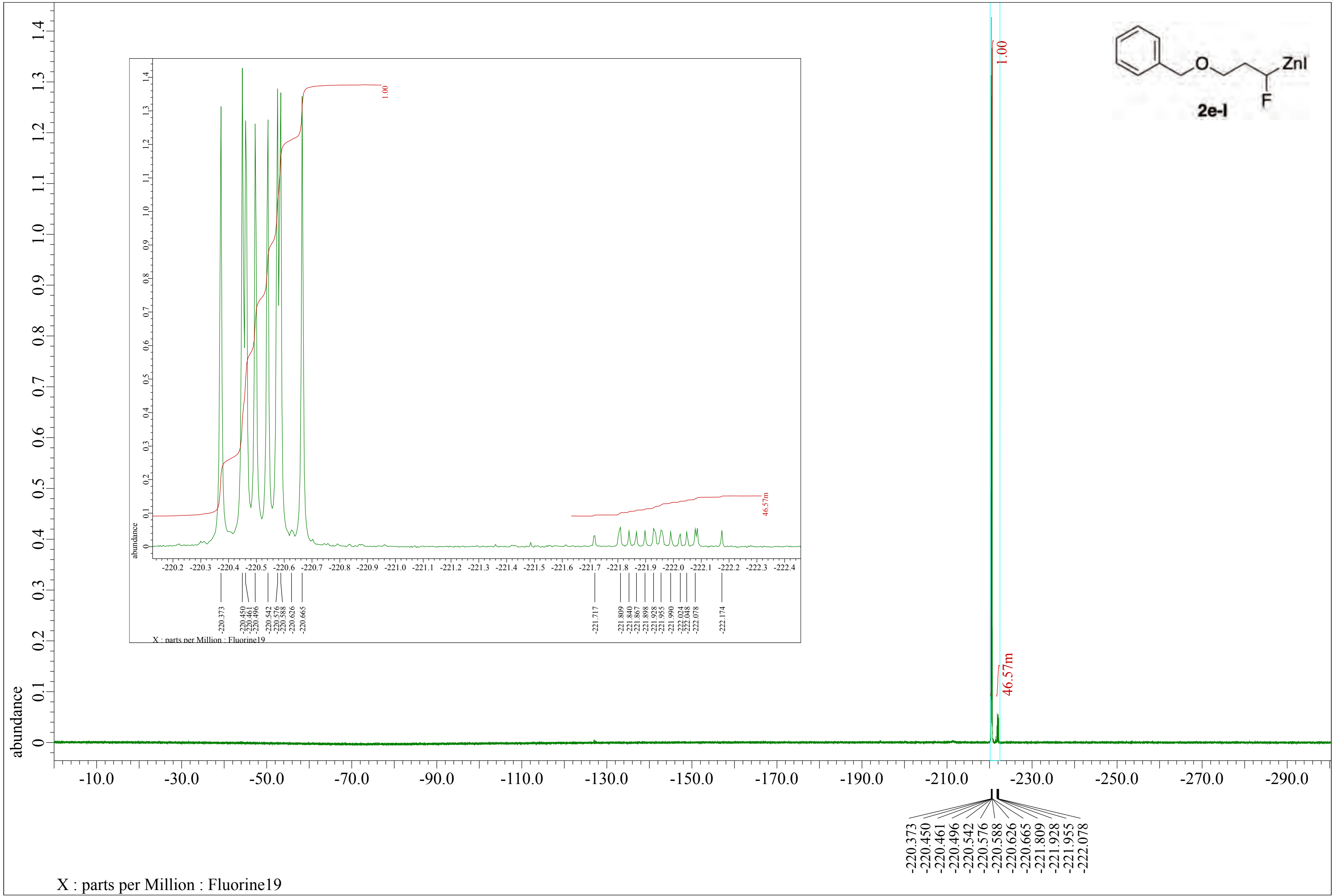


ZnI
F
2d-I
44.84
1.00
abundance
-10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0 -210.0 -220.0 -230.0 -240.0
-216.170
-216.251
-216.297
-216.328
-216.374
-216.451
-216.889
-216.969
-217.012
-217.050
-217.092
-217.173
X : parts per Million : Fluorine19


2e-I
ZnI
O
F
4.71
1.00
2.12
2.19
2.07
abundance
X : parts per Million : Proton
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.303 7.295 7.290 7.274 7.269 7.238 7.231 7.224 7.216 7.208 7.203
4.958 4.943 4.940 4.925 4.840 4.827 4.822 4.808 4.469 4.440 4.433 4.402
3.647 3.624 3.608 3.589 3.560 3.543 3.524 3.501
2.234 2.223 2.215 2.209 2.199 2.190 2.181 2.174 2.160 2.141 2.125 2.107 2.090 2.070

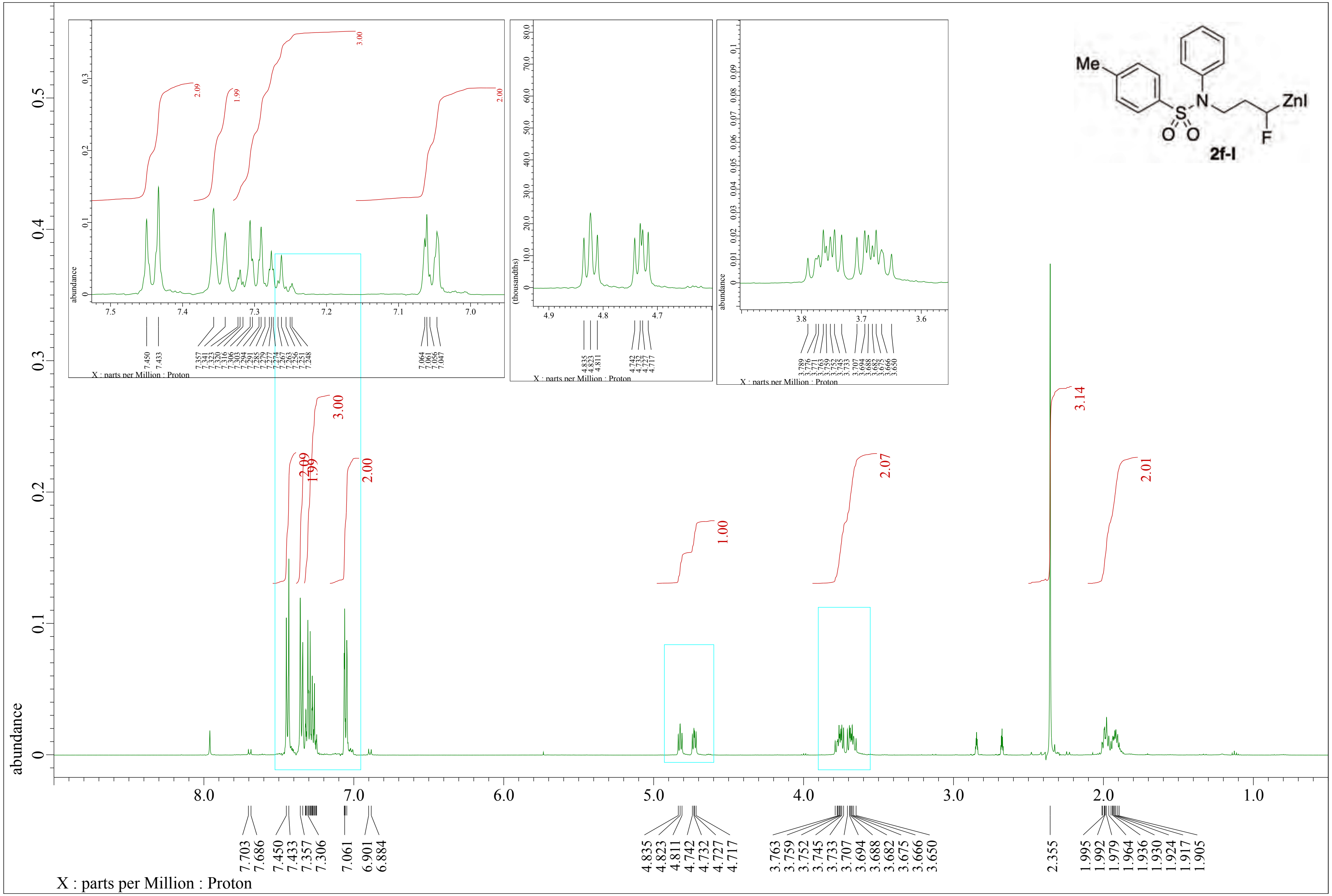


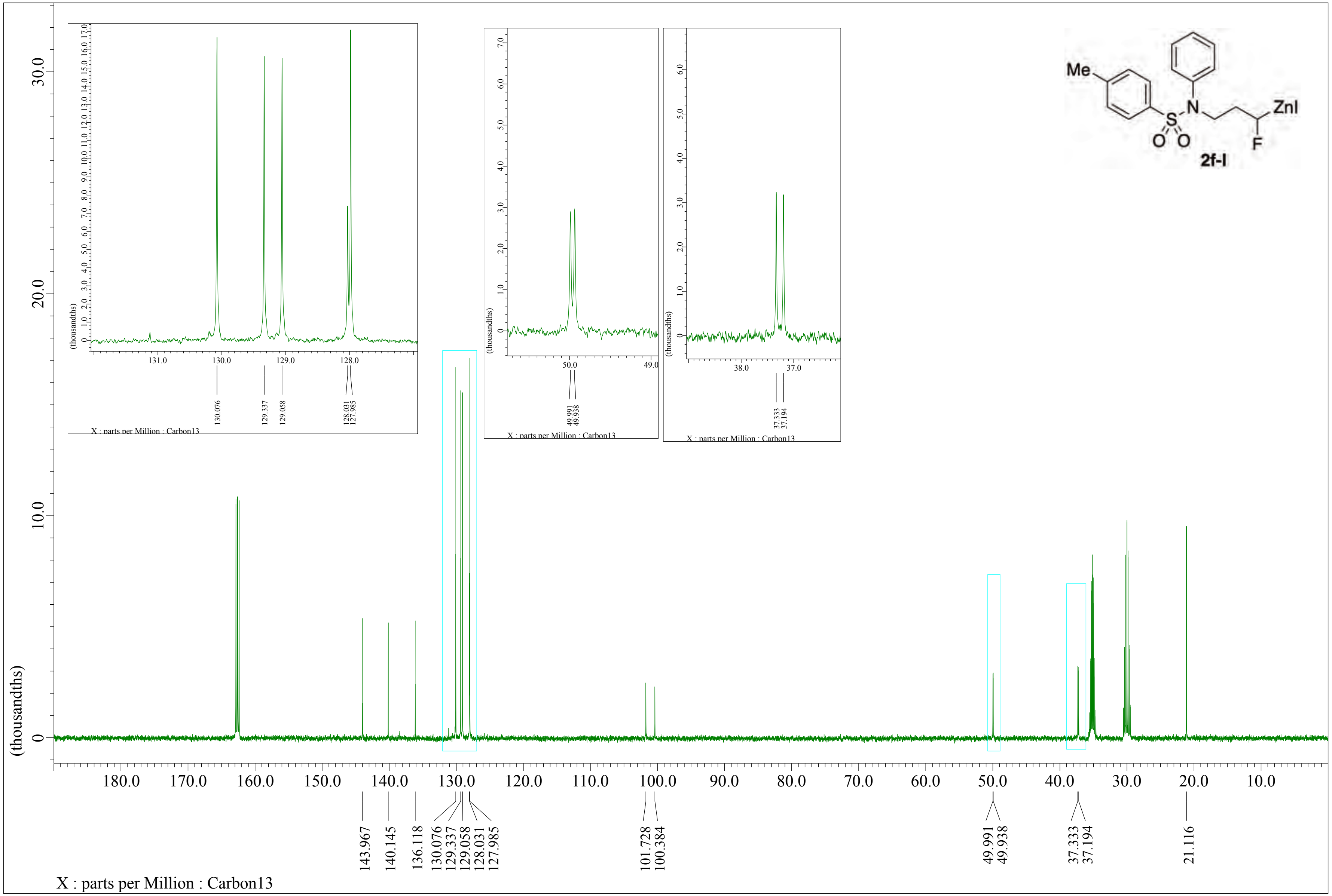
2e-I
(thousandths)
X : parts per Million : Carbon13
162.907
162.620
162.323
139.832
128.620
127.892
127.643
101.722
100.054
72.705
69.735
69.667
38.370
38.198
35.745
35.534
35.323
35.122
34.911
34.700
34.499
30.618
30.407
30.196
29.995
29.784
29.573
29.362



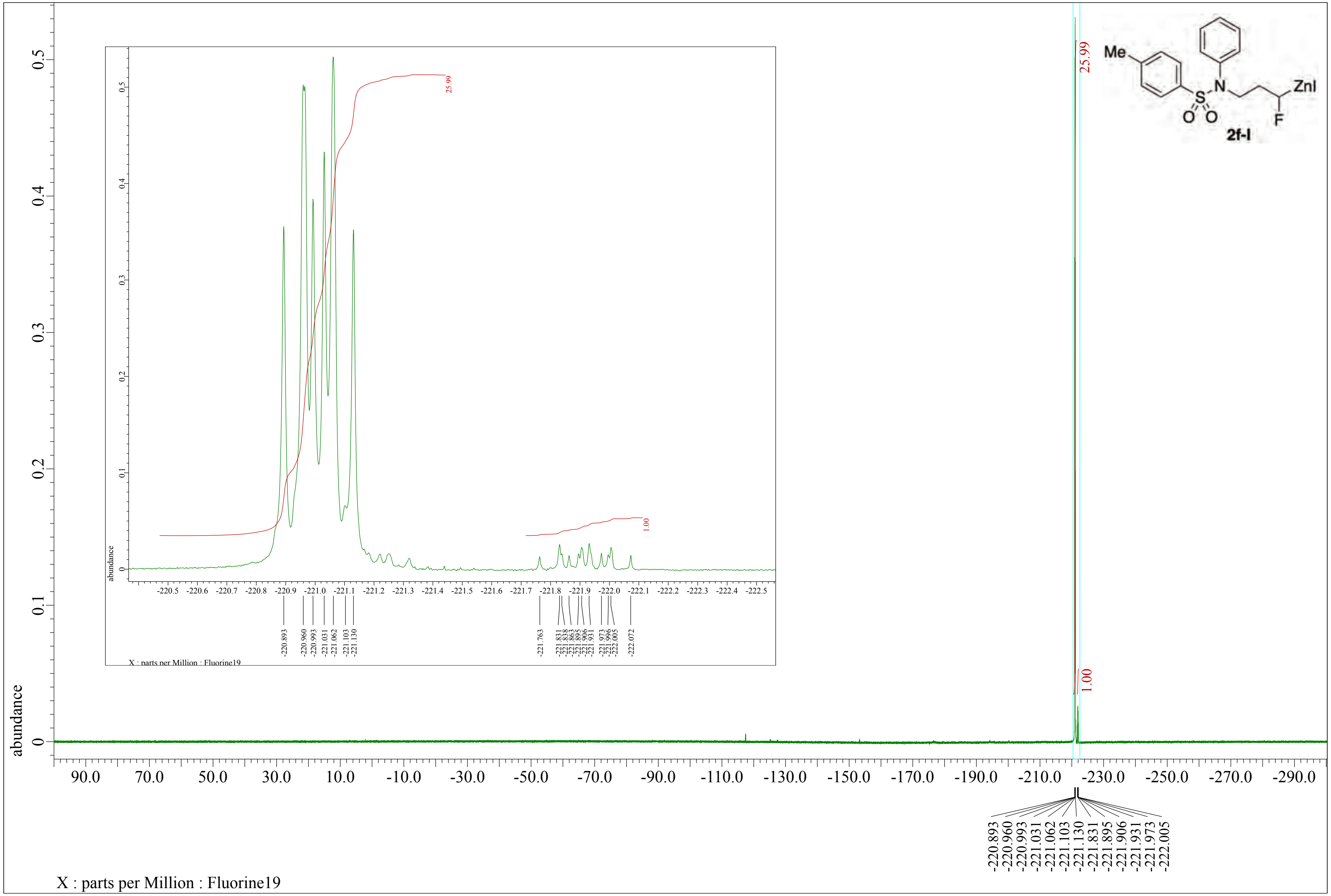
abundance
X : parts per Million : Fluorine19
1.00
46.57m
-220.373
-220.450
-220.461
-220.496
-220.542
-220.576
-220.588
-220.626
-220.665
-221.717
-221.809
-221.840
-221.867
-221.898
-221.928
-221.955
-221.990
-222.024
-222.048
-222.078
-222.174

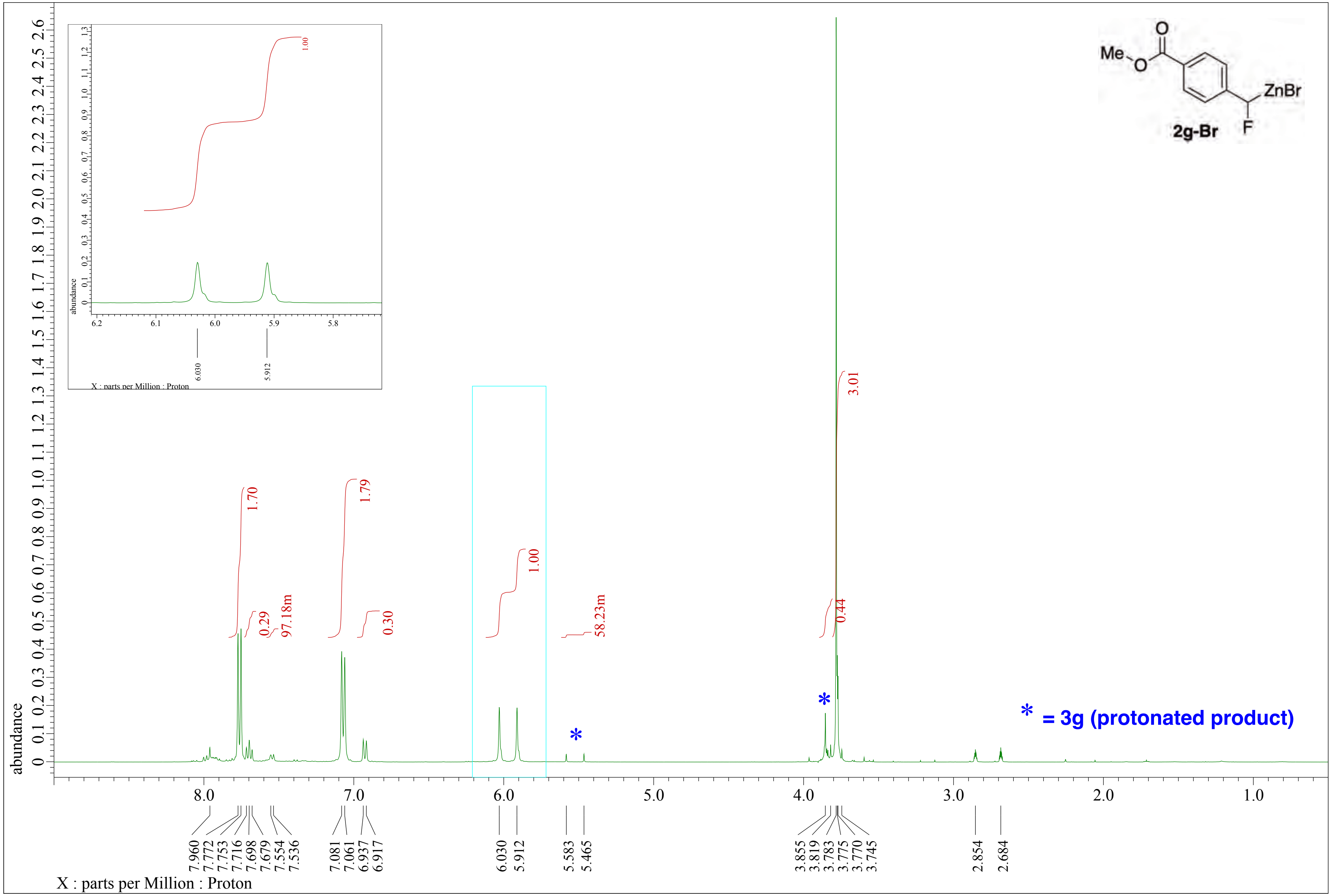
2e-I

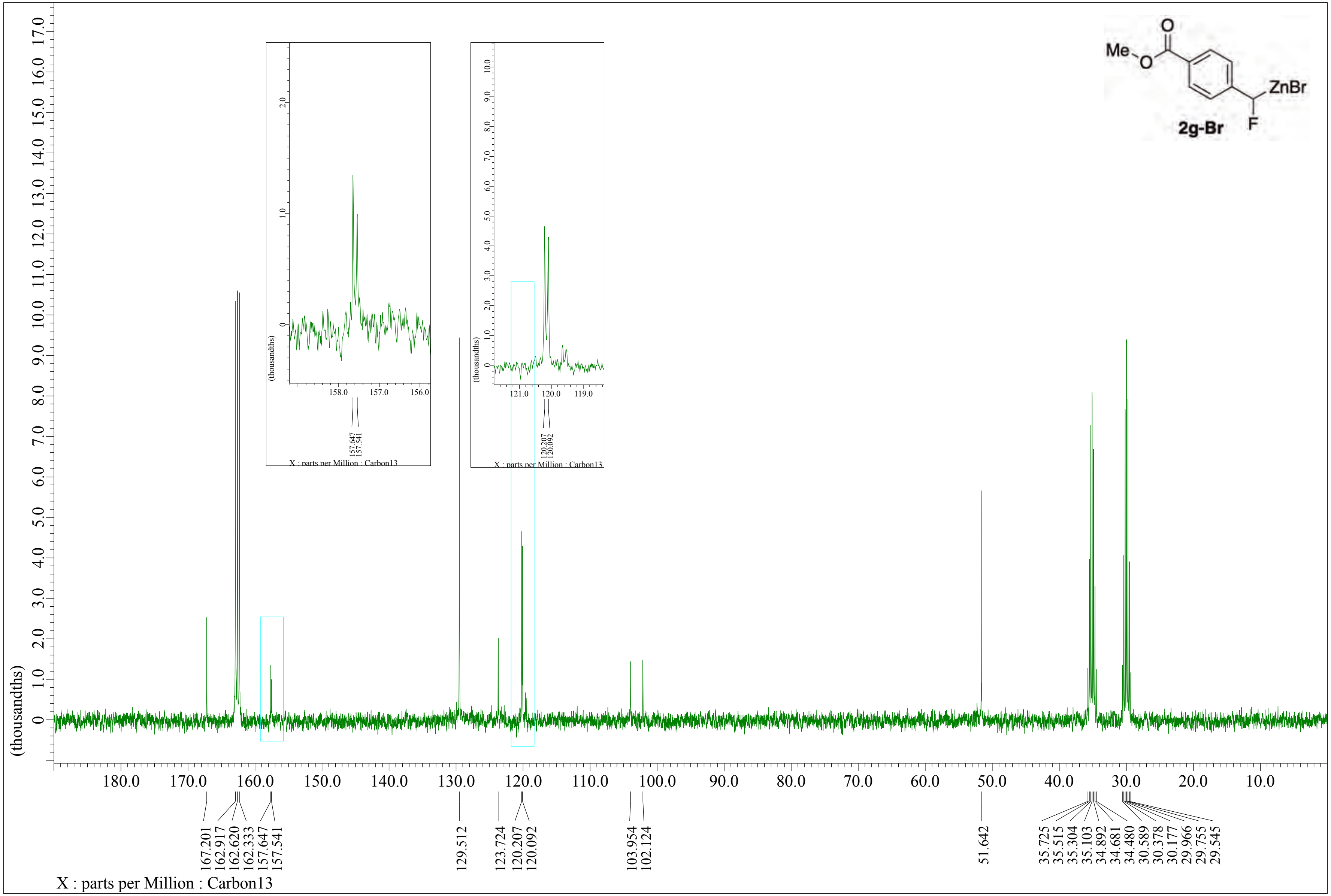

Me
N
S
O O
ZnI
F
2f-I
abundance
X : parts per Million : Proton
8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0
2.09 1.99 3.00 2.00 1.00 2.07 3.14 2.01
7.703 7.686 7.450 7.433 7.357 7.306 7.061 6.901 6.884
4.835 4.823 4.811 4.742 4.732 4.727 4.717
3.763 3.759 3.752 3.745 3.733 3.707 3.694 3.688 3.682 3.675 3.666 3.650
2.355
1.995 1.992 1.979 1.964 1.936 1.930 1.924 1.917 1.905



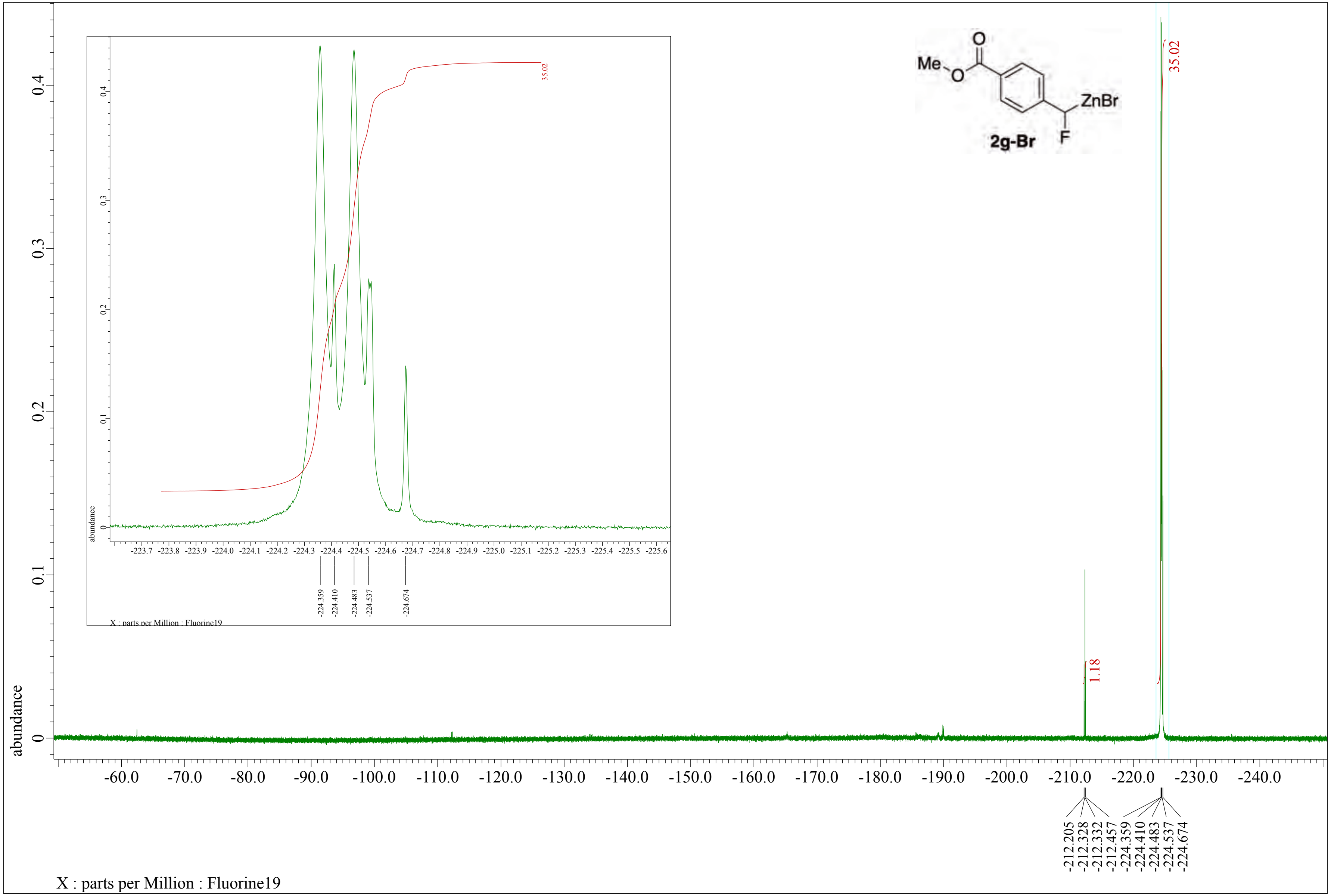
2f-I
Me
ZnI
F
(thousandths)
30.0
20.0
10.0
0
180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
143.967
140.145
136.118
130.076
129.337
129.058
128.031
127.985
101.728
100.384
49.991
49.938
37.333
37.194
21.116
X : parts per Million : Carbon13


25.99
1.00
abundance
X : parts per Million : Fluorine19
-220.893
-220.960
-220.993
-221.031
-221.062
-221.103
-221.130
-221.831
-221.895
-221.906
-221.931
-221.973
-222.005
Me
N
S
O
O
ZnI
F
2f-I

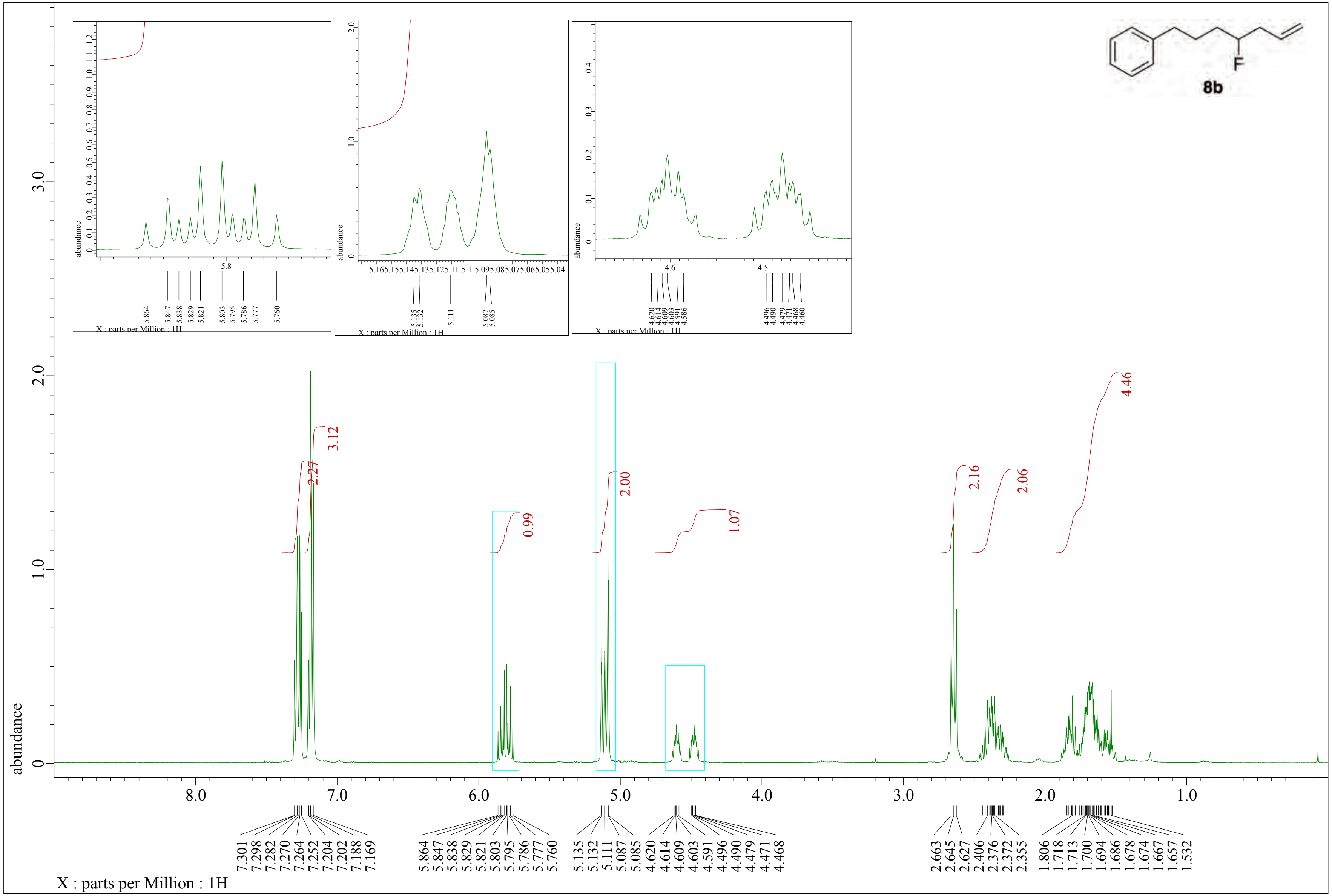

Me
O
O
ZnBr
F
2g-Br
* = 3g (protonated product)
abundance
X : parts per Million : Proton
1.70
0.29
97.18m
1.79
0.30
1.00
58.23m
0.44
3.01
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.960
7.772
7.753
7.716
7.698
7.679
7.554
7.536
7.081
7.061
6.937
6.917
6.030
5.912
5.583
5.465
3.855
3.819
3.783
3.775
3.770
3.745
2.854
2.684



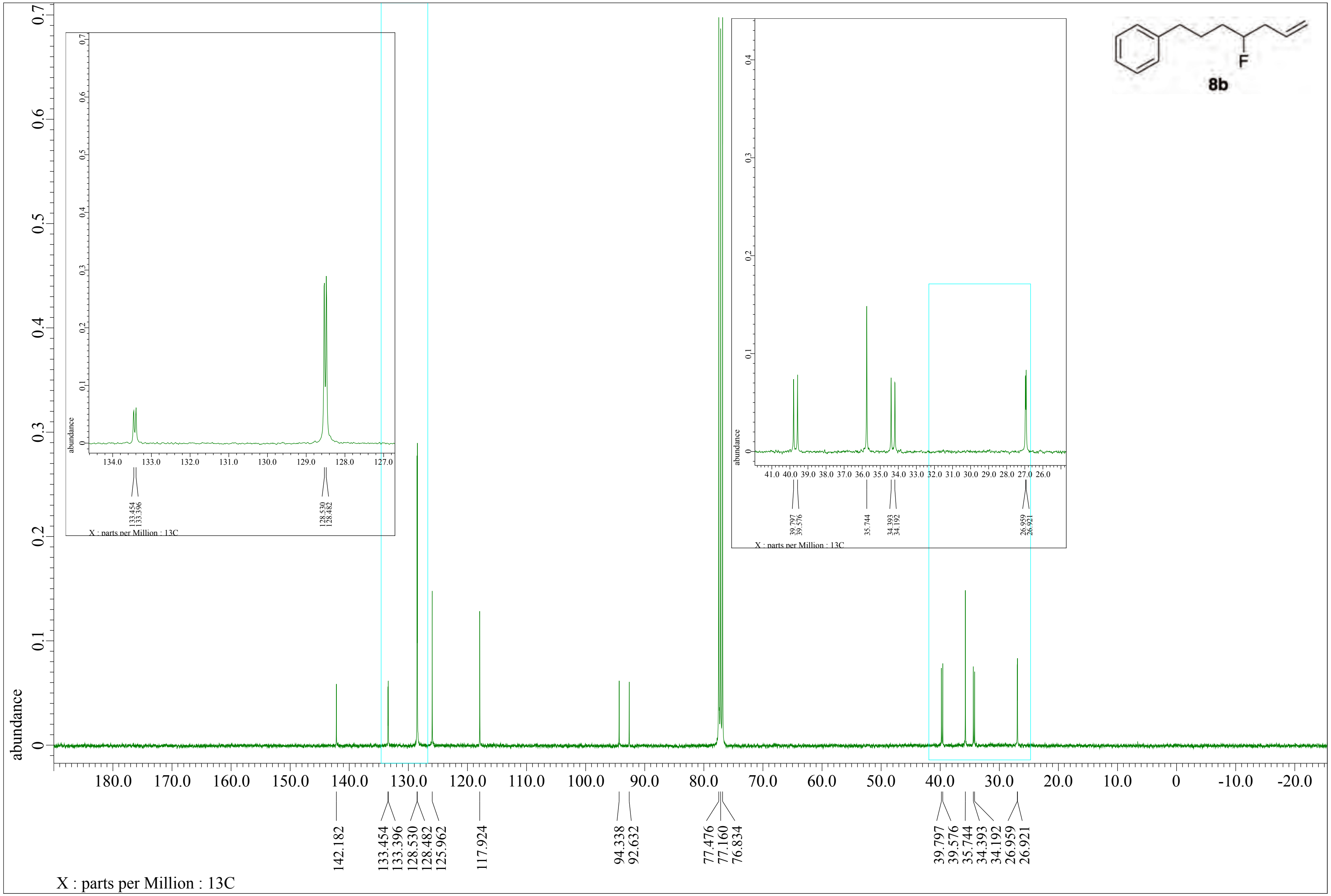
Me
O
O
ZnBr
F
2g-Br
(thousandths)
X : parts per Million : Carbon13
167.201
162.917
162.620
162.333
157.647
157.541
129.512
123.724
120.207
120.092
103.954
102.124
51.642
35.725
35.515
35.304
35.103
34.892
34.681
34.480
30.589
30.378
30.177
29.966
29.755
29.545

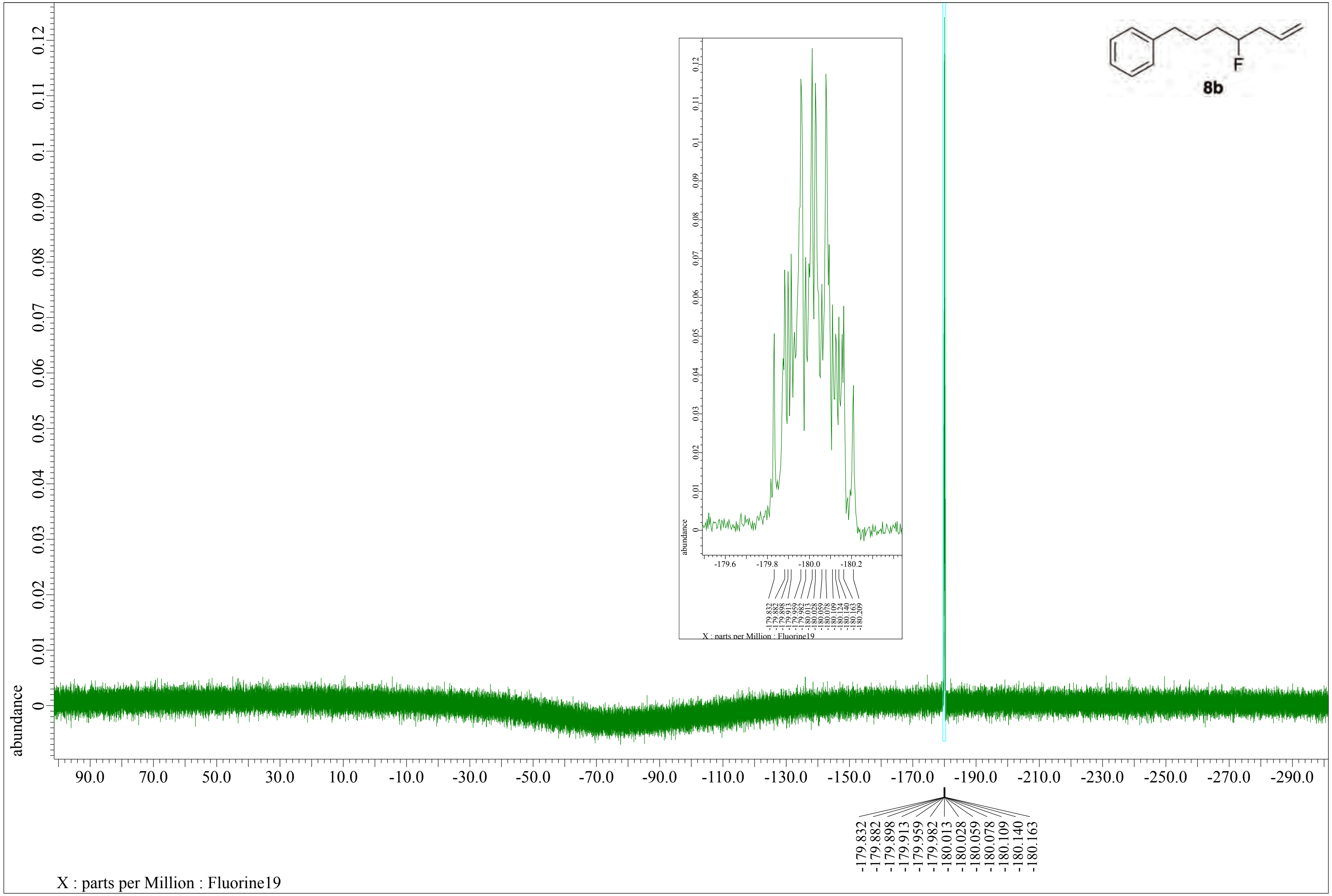


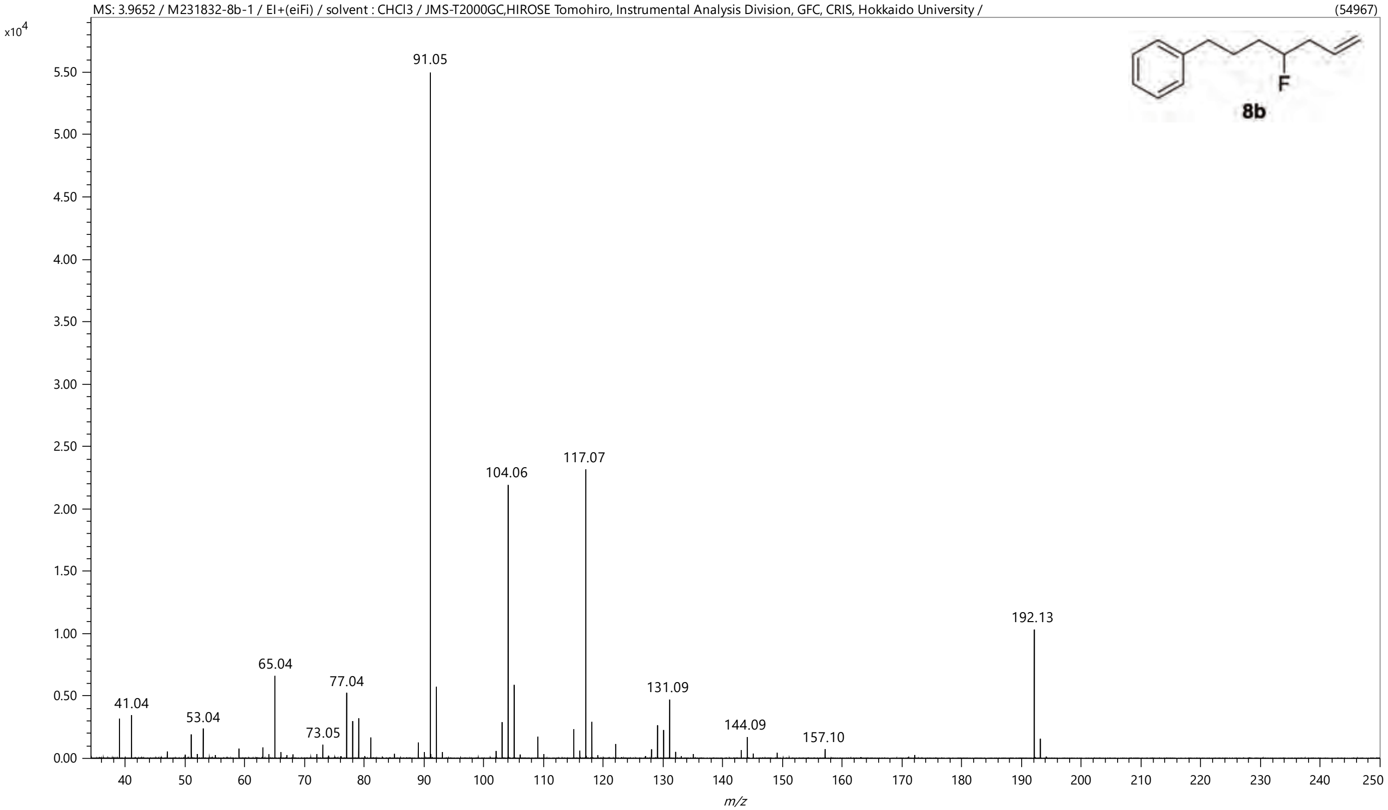
2g-Br
ZnBr
Me
X : parts per Million : Fluorine19
abundance
35.02
1.18
-212.205
-212.328
-212.332
-212.457
-224.359
-224.410
-224.483
-224.537
-224.674

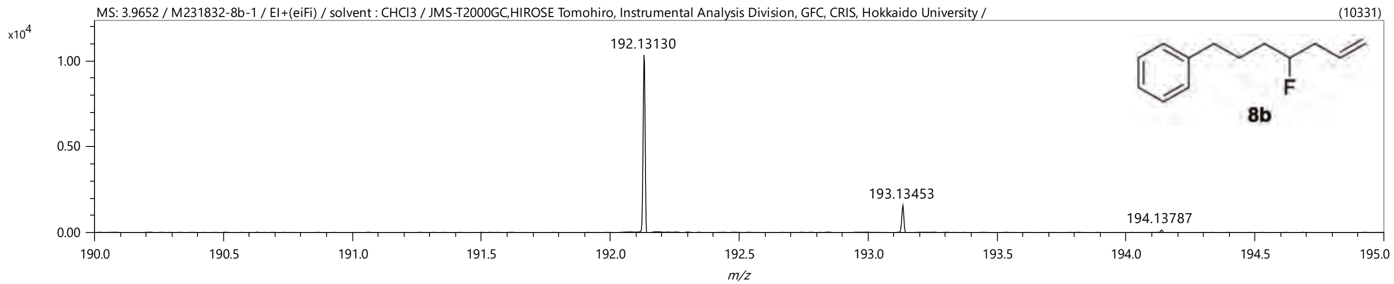


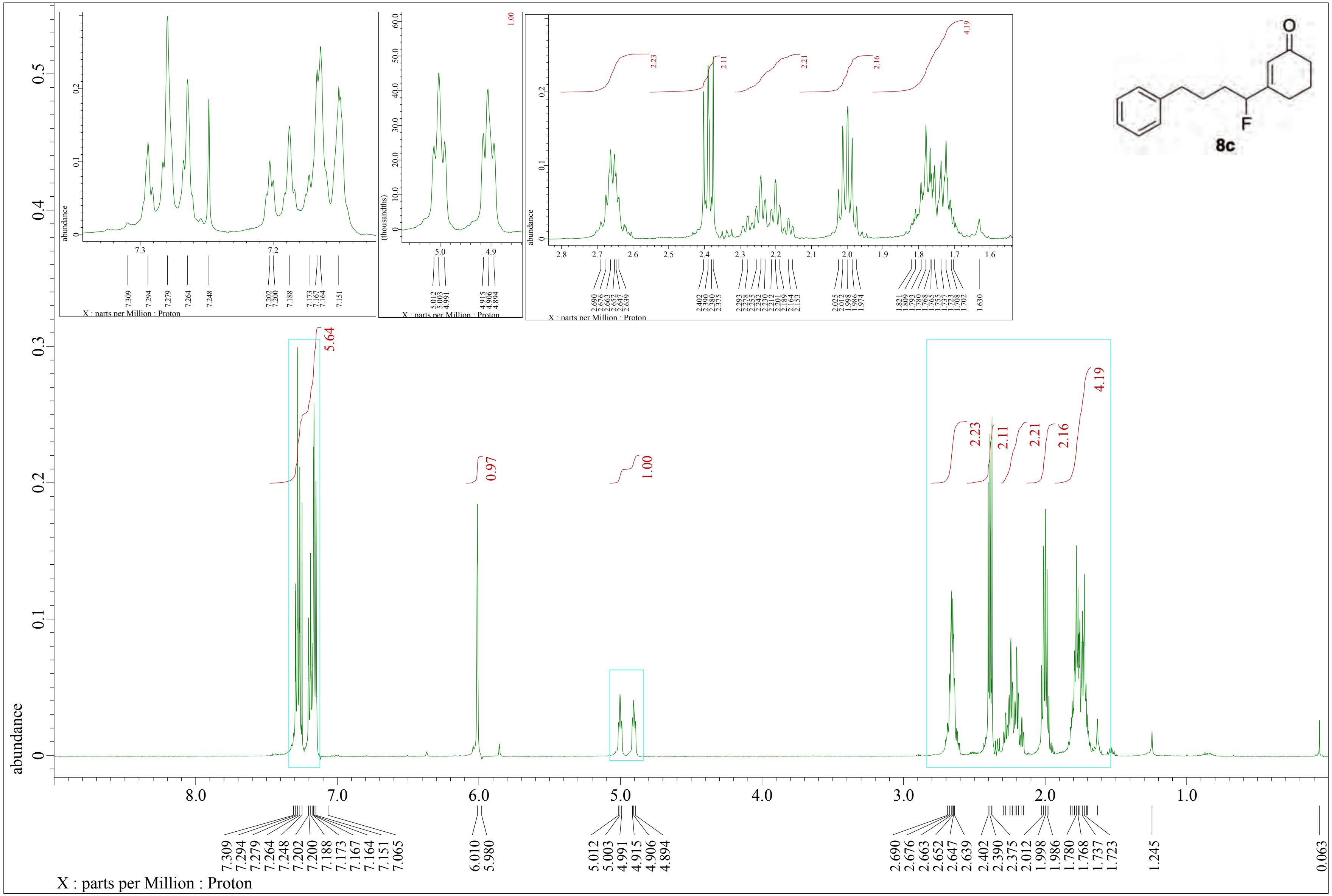
8b
F
abundance
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
3.12
2.27
0.99
2.00
1.07
2.16
2.06
4.46
7.301
7.298
7.282
7.270
7.264
7.252
7.204
7.202
7.188
7.169
5.864
5.847
5.838
5.829
5.821
5.803
5.795
5.786
5.777
5.760
5.135
5.132
5.111
5.087
5.085
4.620
4.614
4.609
4.603
4.591
4.496
4.490
4.479
4.471
4.468
2.663
2.645
2.627
2.406
2.376
2.372
2.355
1.806
1.718
1.713
1.700
1.694
1.686
1.678
1.674
1.667
1.657
1.532

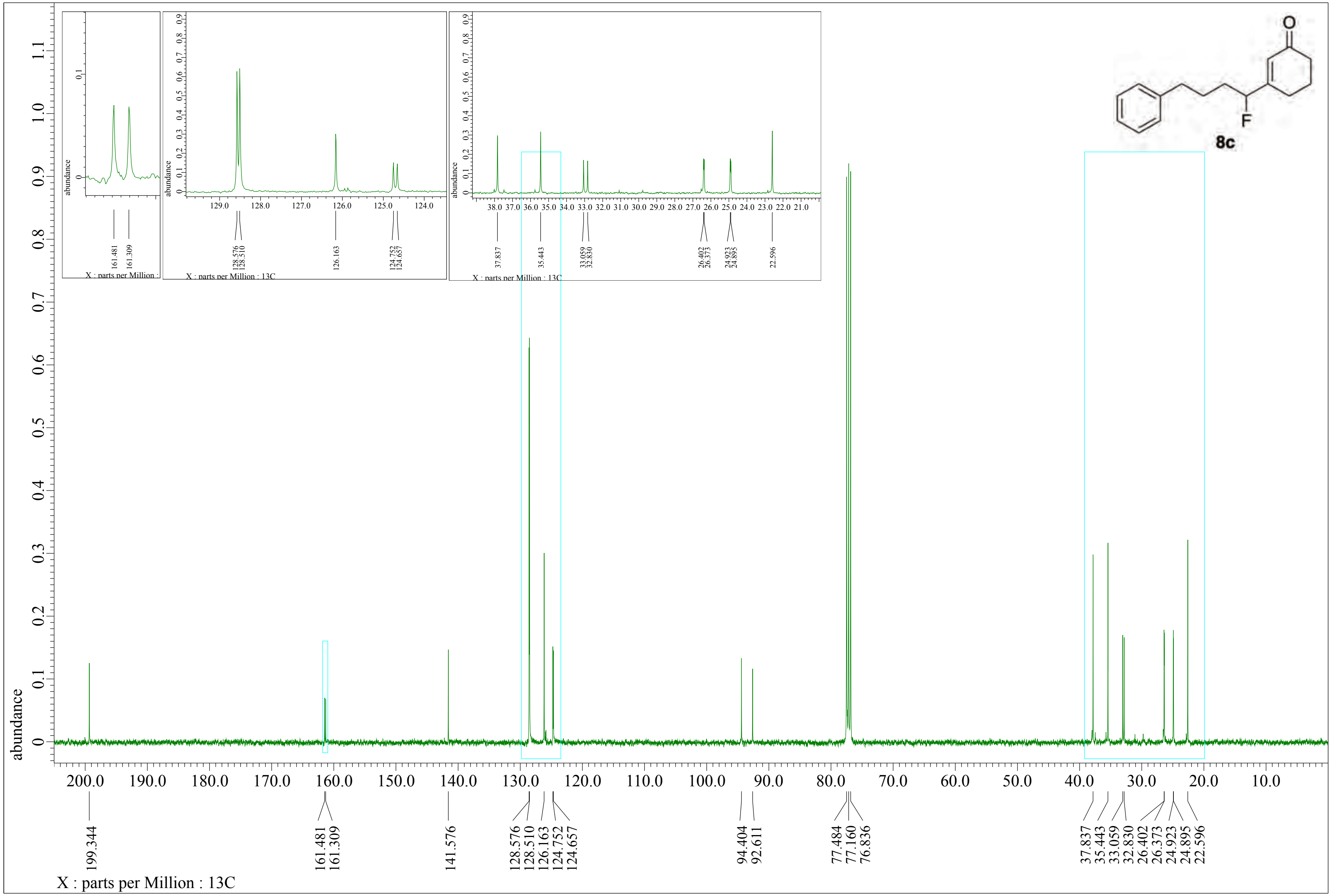

8b
abundance
X : parts per Million : 13C
142.182
133.454
133.396
128.530
128.482
125.962
117.924
94.338
92.632
77.476
77.160
76.834
39.797
39.576
35.744
34.393
34.192
26.959
26.921

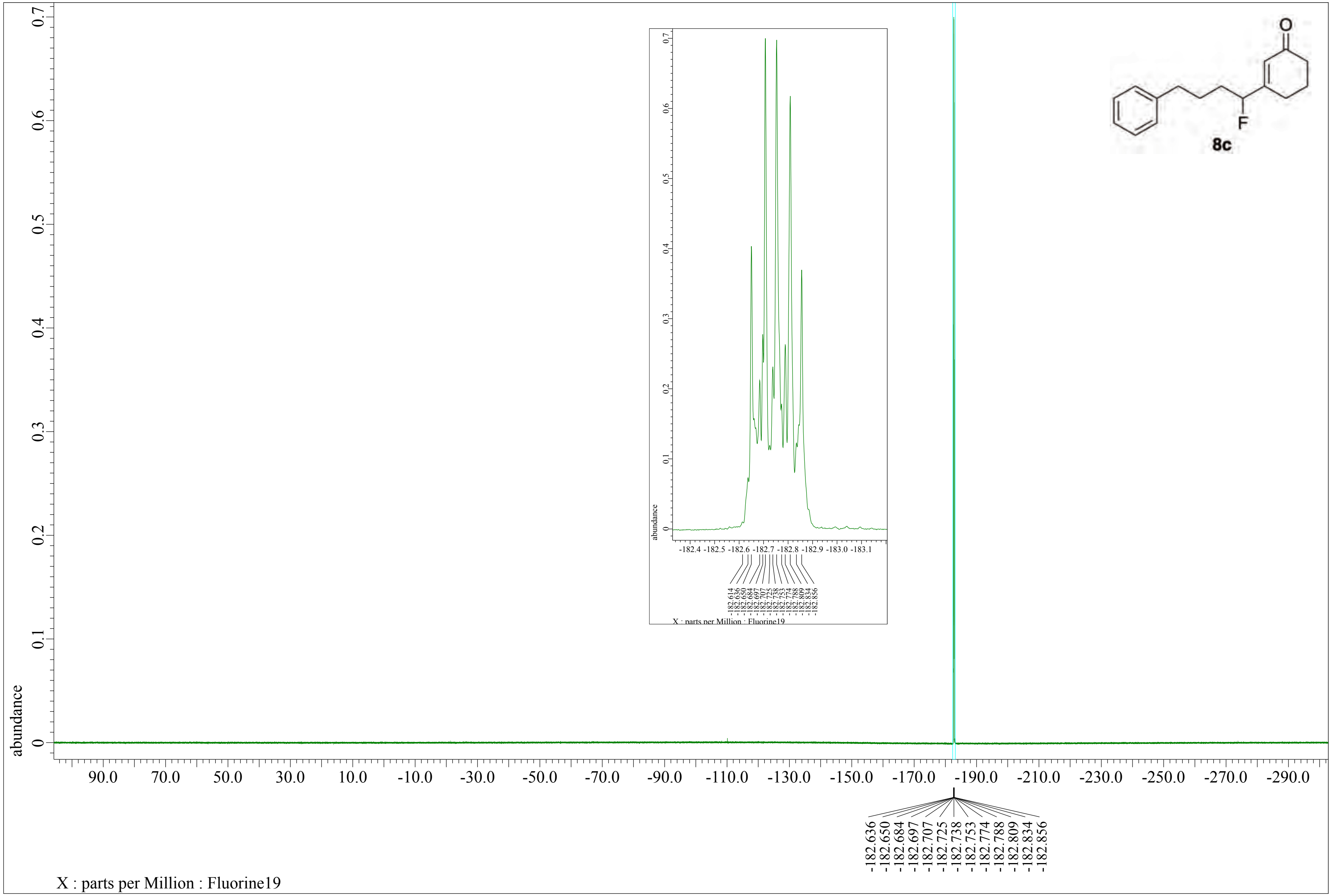

8b
F
abundance
X : parts per Million : Fluorine19
-179.832
-179.882
-179.898
-179.913
-179.959
-179.982
-180.013
-180.028
-180.059
-180.078
-180.109
-180.140
-180.163


MS: 3.9652 / M231832-8b-1 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(54967)
x10^4
91.05
104.06
117.07
192.13
65.04
77.04
41.04
53.04
73.05
131.09
144.09
157.10
m/z
F
8b


MS: 3.9652 / M231832-8b-1 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(10331)
x10^4
192.13130
193.13453
194.13787
m/z
F
8b

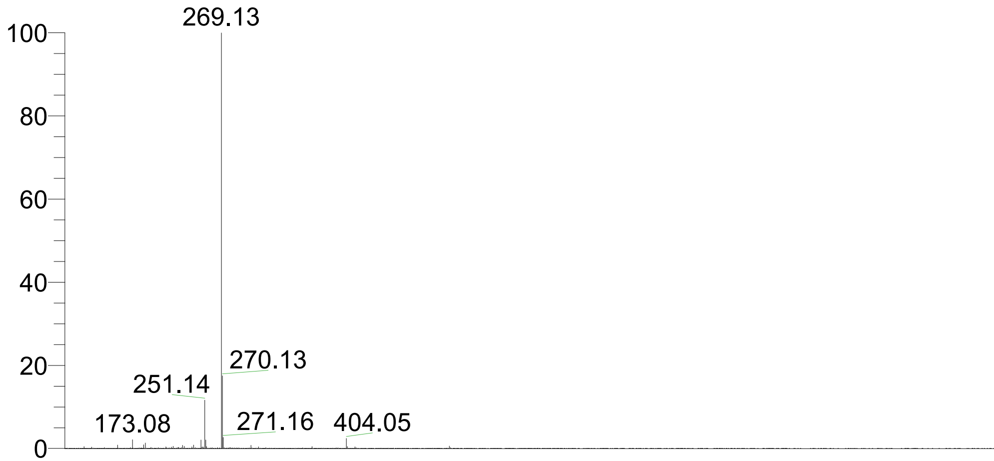

8c
abundance
X : parts per Million : Proton
5.64
0.97
1.00
2.23
2.11
2.21
2.16
4.19
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.309
7.294
7.279
7.264
7.248
7.202
7.200
7.188
7.173
7.167
7.164
7.151
7.065
6.010
5.980
5.012
5.003
4.991
4.915
4.906
4.894
2.690
2.676
2.663
2.652
2.647
2.639
2.402
2.390
2.375
2.012
1.998
1.986
1.780
1.768
1.737
1.723
1.245
0.063

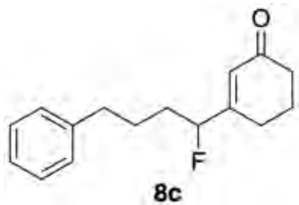

8c
abundance
X : parts per Million : 13C
199.344
161.481
161.309
141.576
128.576
128.510
126.163
124.752
124.657
94.404
92.611
77.484
77.160
76.836
37.837
35.443
33.059
32.830
26.402
26.373
24.923
24.895
22.596


abundance
X : parts per Million : Fluorine19
-182.636
-182.650
-182.684
-182.697
-182.707
-182.725
-182.738
-182.753
-182.774
-182.788
-182.809
-182.834
-182.856

8c

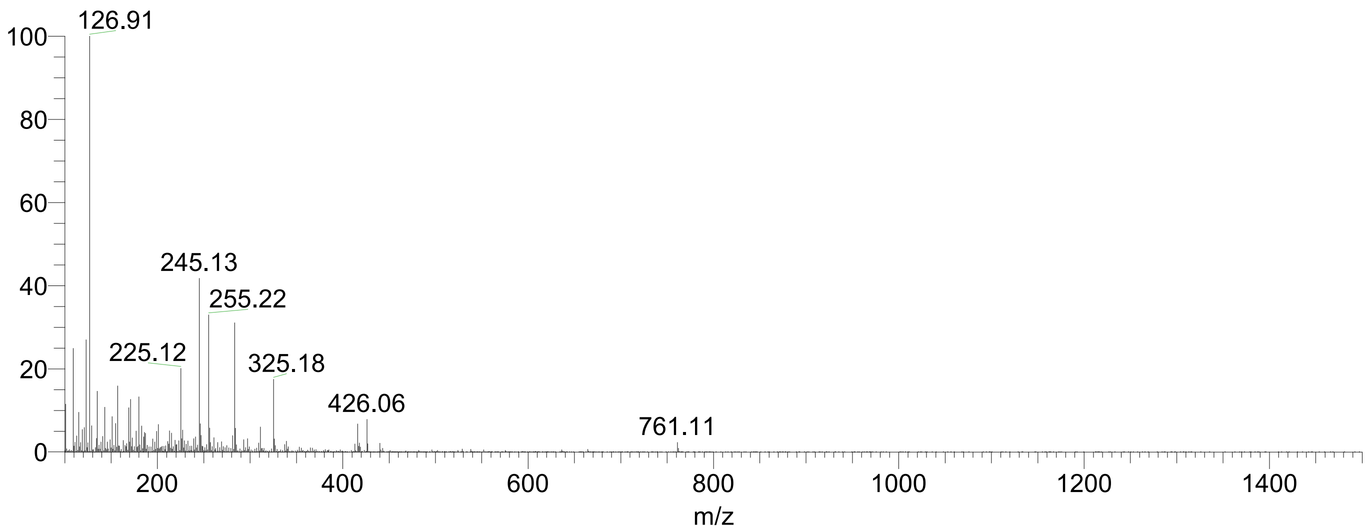
Sample No. : C:\Xcalibur\...\BG_230237_EK002 Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 05/17/23 13:39:43
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University





8c

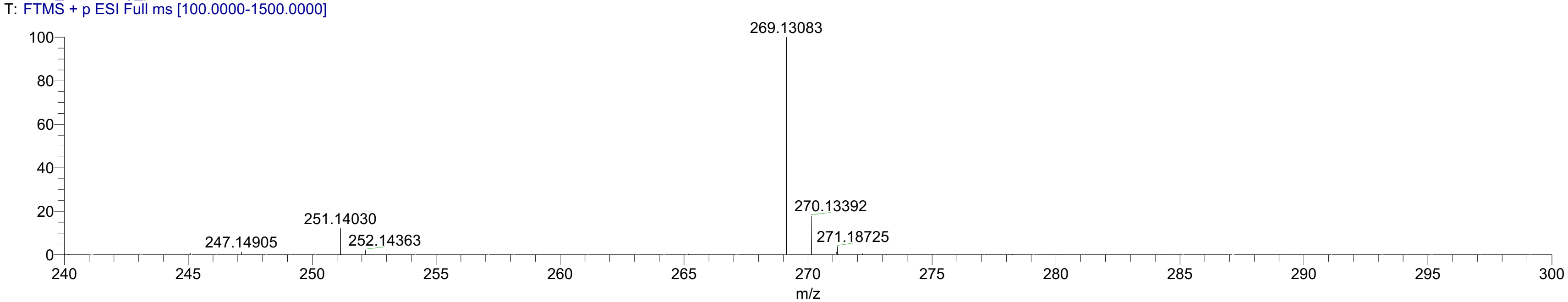
NL: 7.11E8
BG_230237_EK0028by_pn#18-32 RT: 0.31-0.48 AV: 7 T: FTMS + c ESI Full ms [100.00-1500.00]



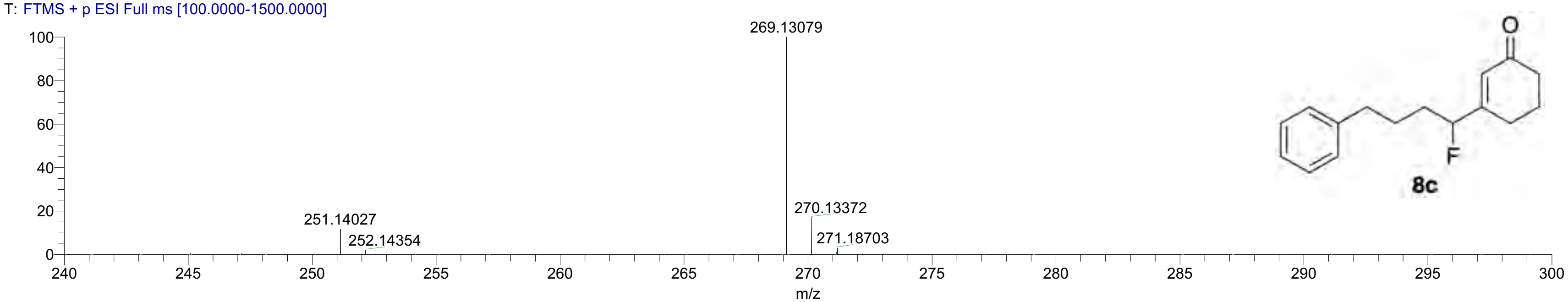
NL: 2.22E7
BG_230237_EK0028by_pn#18-32 RT: 0.30-0.50 AV: 8 T: FTMS - c ESI Full ms [100.00-1500.00]

Sample No. : C:\Xcalibur\...\0517\230237_EK0028by_pn Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 05/17/23 11:32:01
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

230237_EK0028by_pn #22-25 RT: 0.37-0.40 AV: 2 NL: 1.79E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

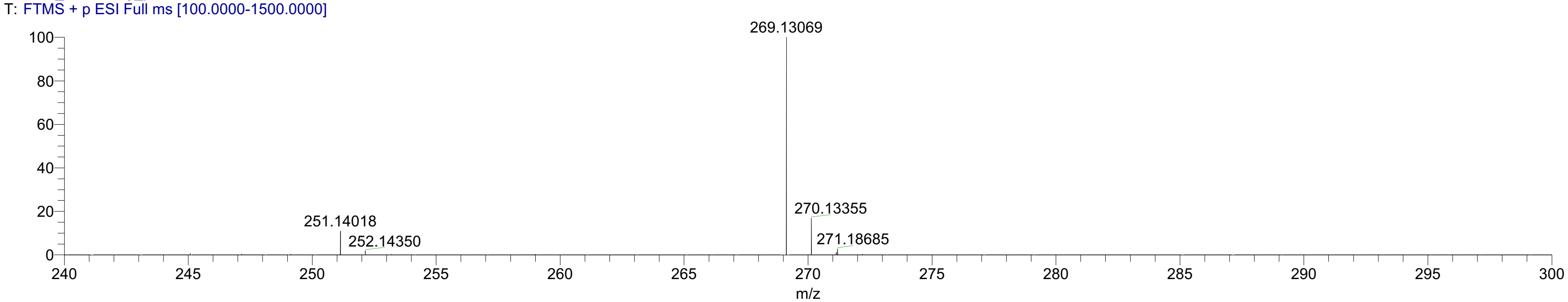


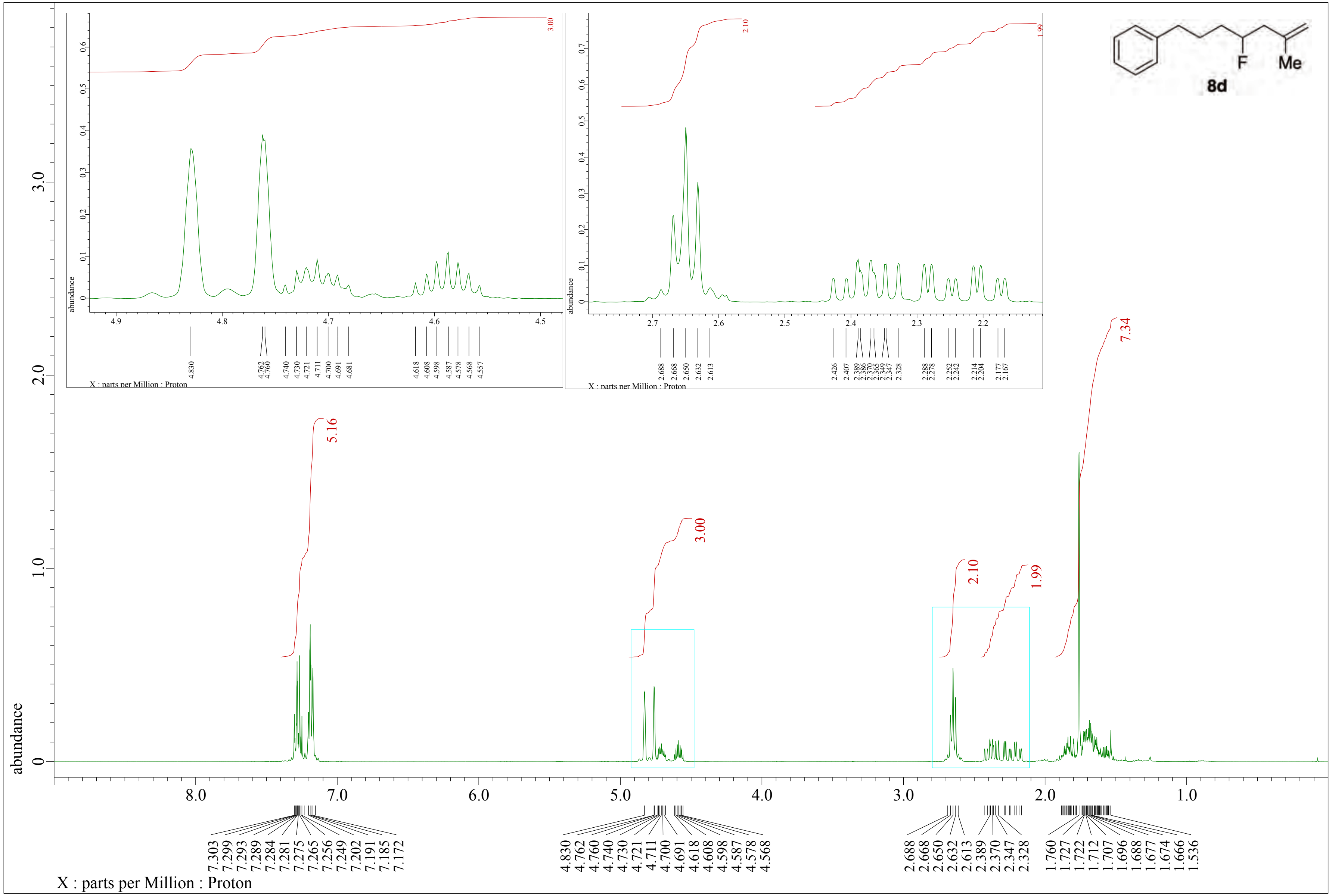
230237_EK0028by_pn #25-29 RT: 0.40-0.45 AV: 3 NL: 2.61E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



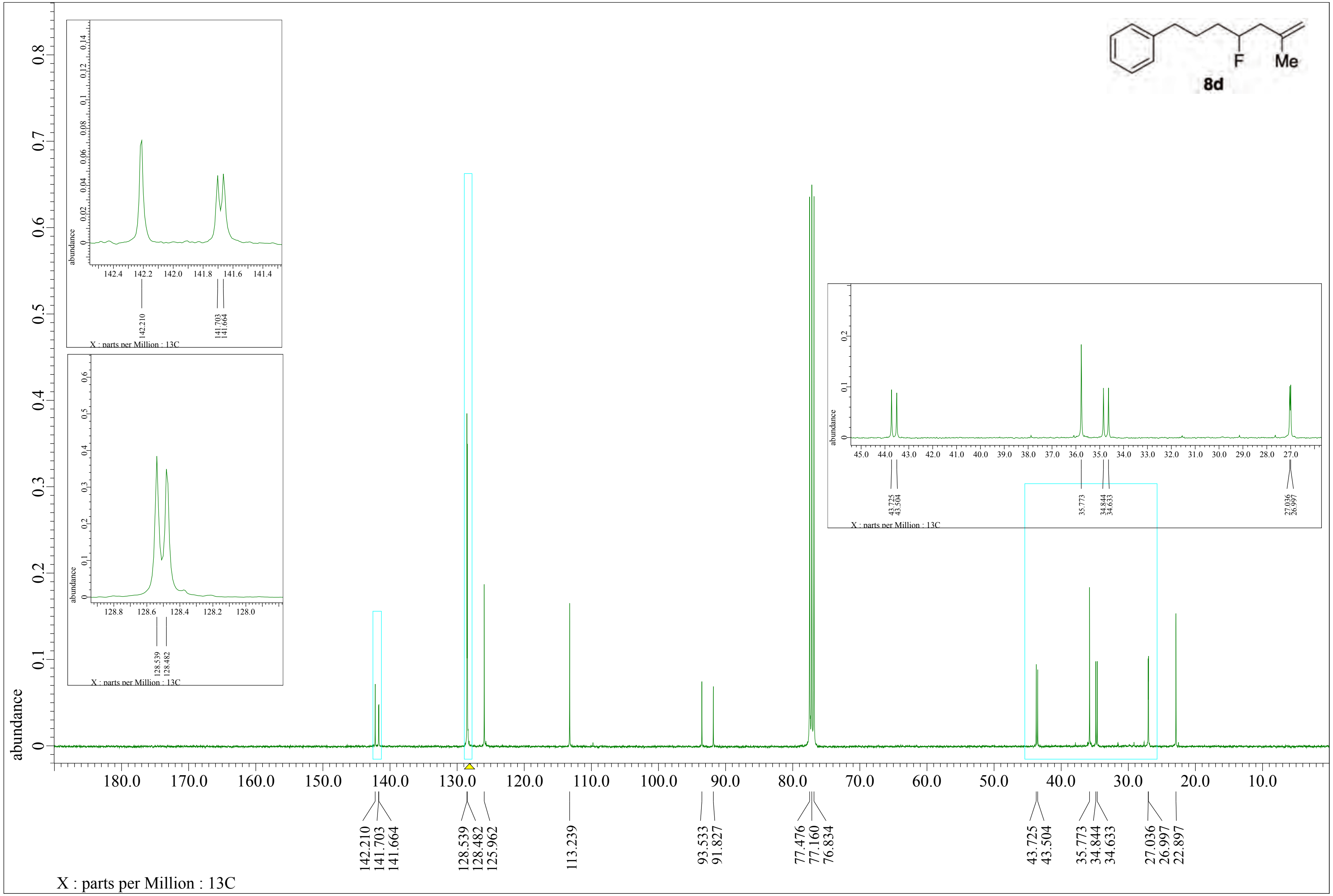
8c

230237_EK0028by_pn #29-32 RT: 0.45-0.48 AV: 2 NL: 2.69E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

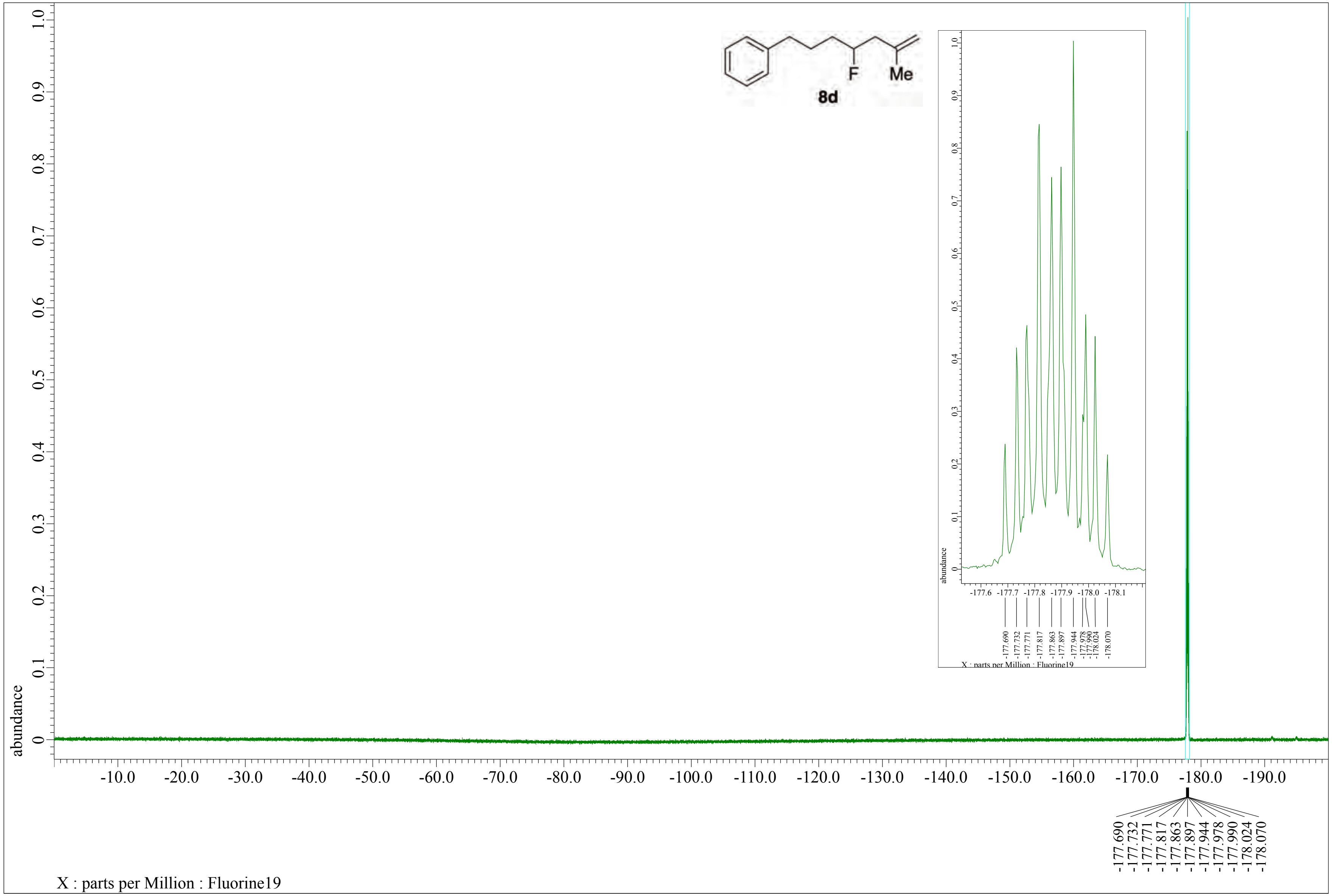


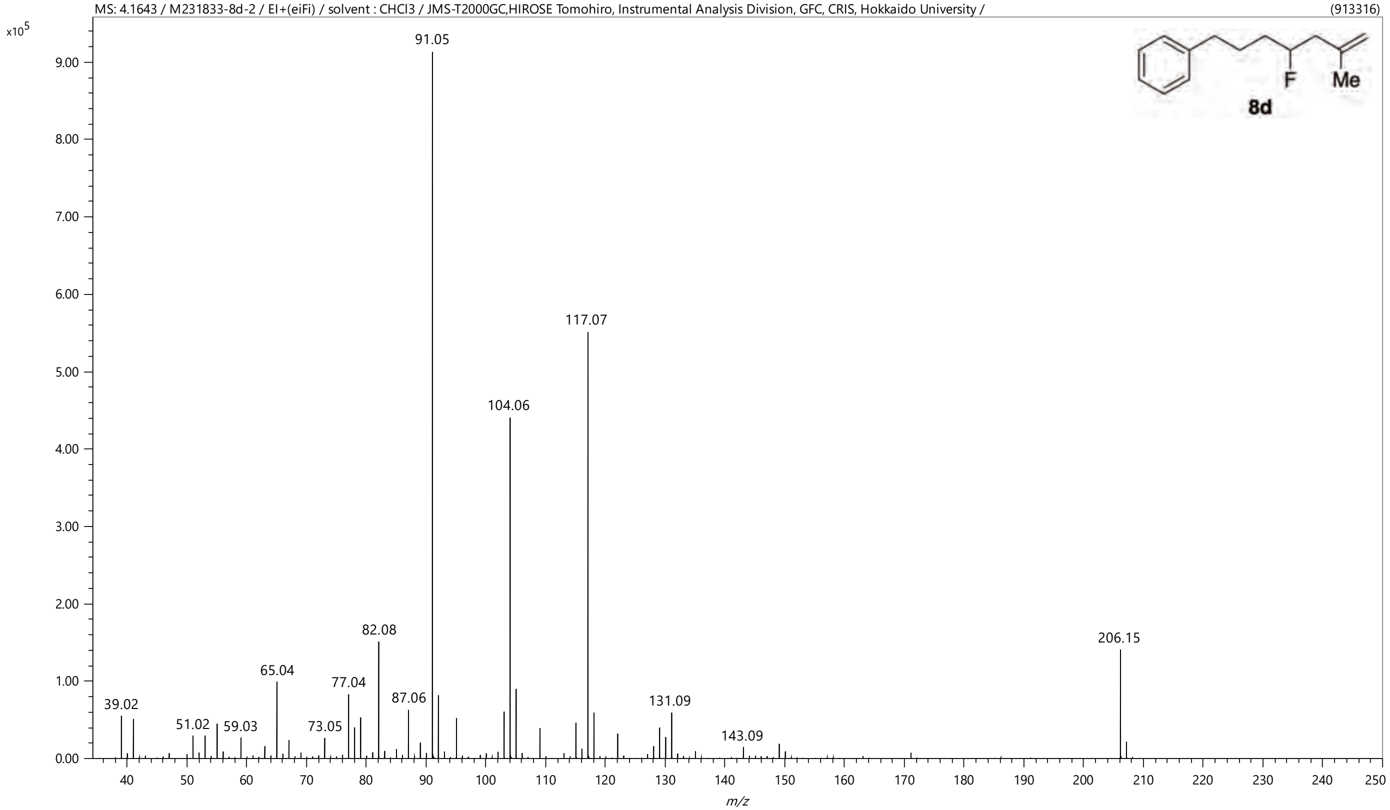


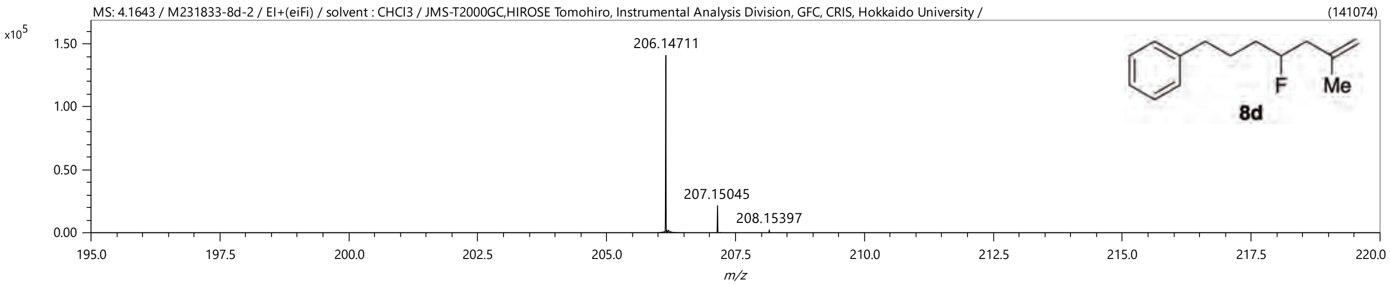
8d
F
Me
abundance
X : parts per Million : Proton
5.16
3.00
2.10
1.99
7.34
7.303 7.299 7.293 7.289 7.284 7.281 7.275 7.265 7.256 7.249 7.202 7.191 7.185 7.172
4.830 4.762 4.760 4.740 4.730 4.721 4.711 4.700 4.691 4.618 4.608 4.598 4.587 4.578 4.568
2.688 2.668 2.650 2.632 2.613 2.389 2.370 2.347 2.328
1.760 1.727 1.722 1.712 1.707 1.696 1.688 1.677 1.674 1.666 1.536

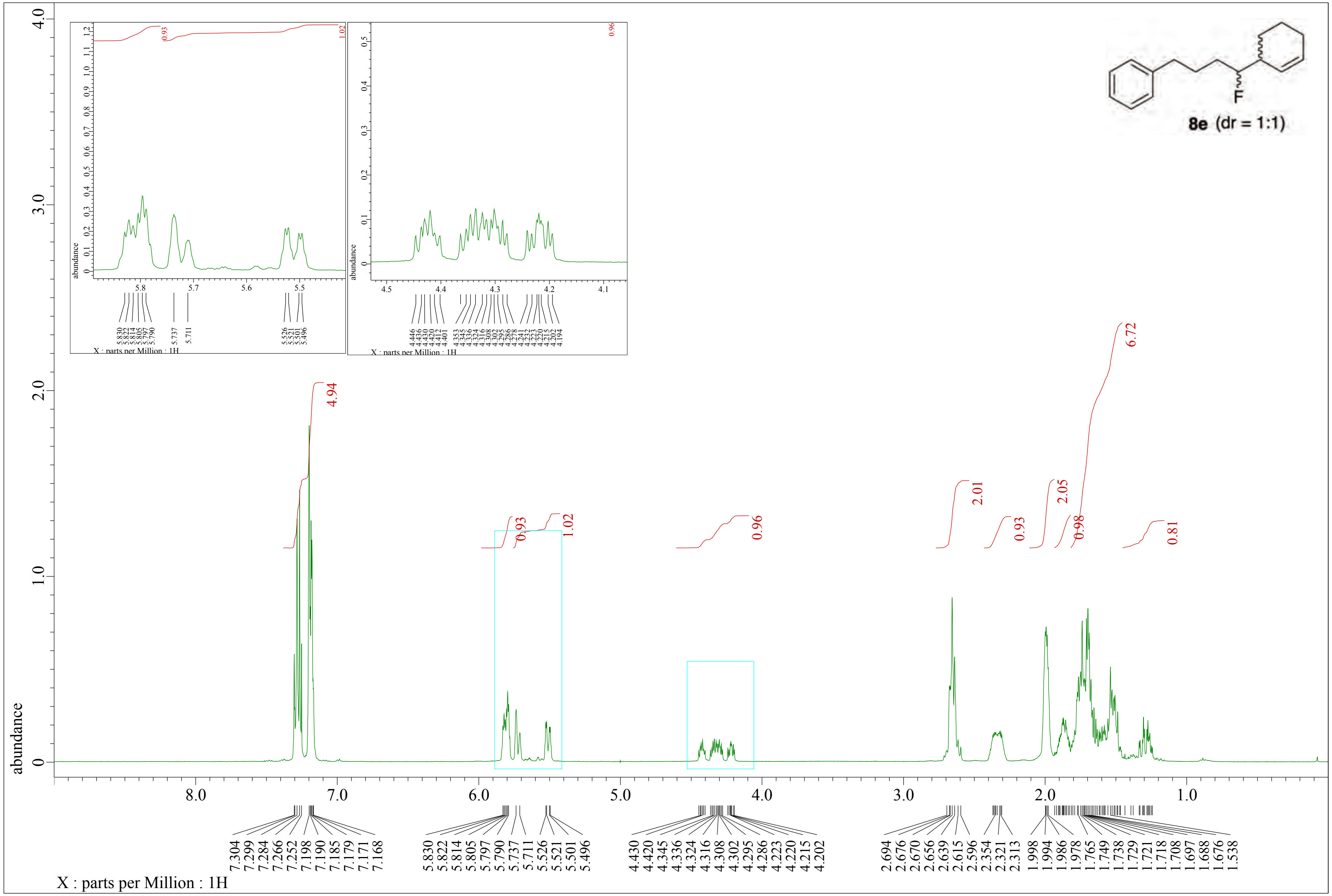


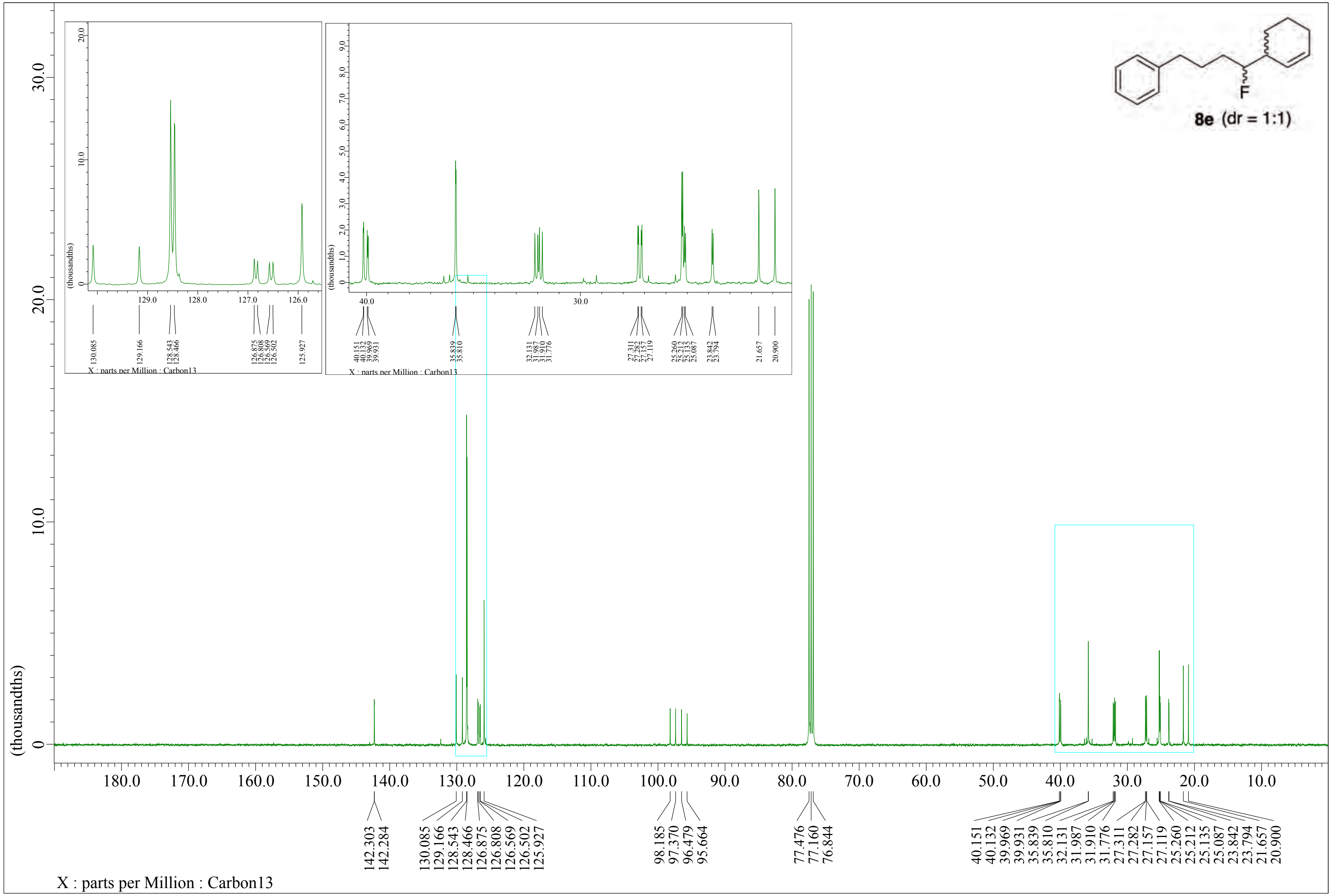
8d
F
Me
abundance
X : parts per Million : 13C
142.210
141.703
141.664
128.539
128.482
125.962
113.239
93.533
91.827
77.476
77.160
76.834
43.725
43.504
35.773
34.844
34.633
27.036
26.997
22.897


F
Me
8d
abundance
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
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
-177.690
-177.732
-177.771
-177.817
-177.863
-177.897
-177.944
-177.978
-177.990
-178.024
-178.070
-177.6 -177.7 -177.8 -177.9 -178.0 -178.1
X : parts per Million : Fluorine19

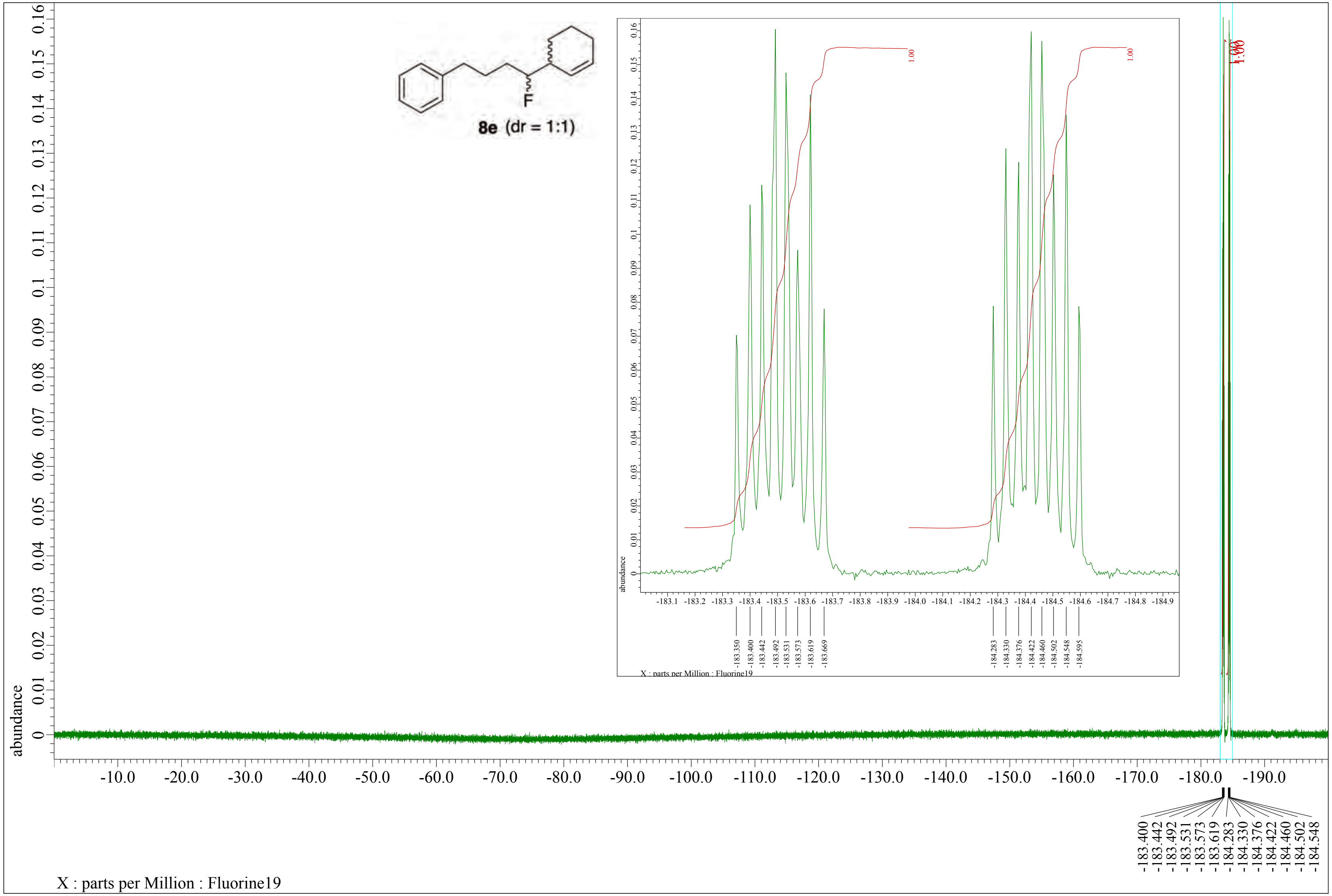

MS: 4.1643 / M231833-8d-2 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(913316)
x10^5
91.05
117.07
104.06
82.08
206.15
65.04
77.04
87.06
131.09
39.02
51.02
59.03
73.05
143.09
m/z
F
Me
8d


MS: 4.1643 / M231833-8d-2 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(141074)
x10^5
206.14711
207.15045
208.15397
m/z
F
Me
8d

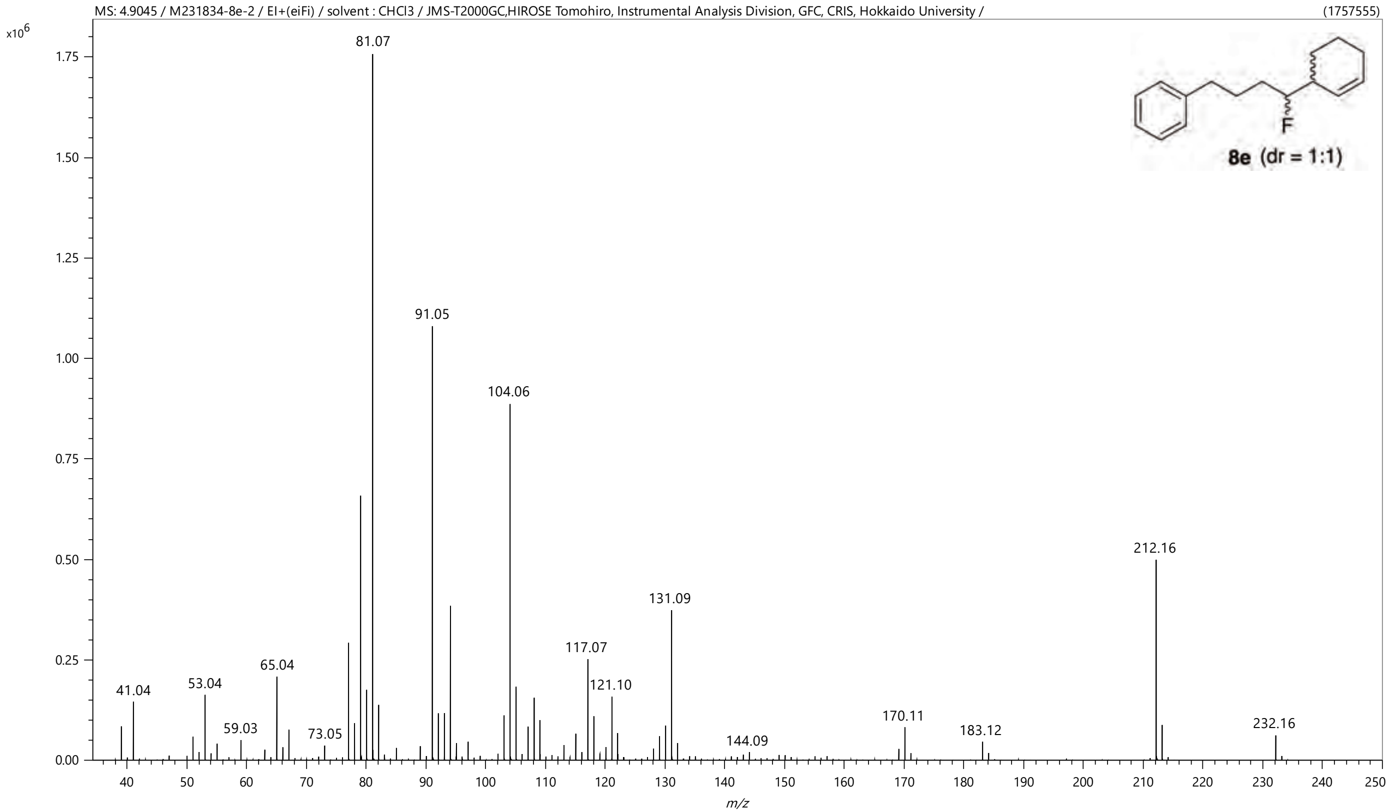

F
8e (dr = 1:1)
abundance
X : parts per Million : 1H
4.94
0.93
1.02
0.96
2.01
0.93
2.05
0.98
6.72
0.81
7.304 7.299 7.284 7.266 7.252 7.198 7.190 7.185 7.179 7.171 7.168
5.830 5.822 5.814 5.805 5.797 5.790 5.737 5.711 5.526 5.521 5.501 5.496
4.430 4.420 4.345 4.336 4.324 4.316 4.308 4.302 4.295 4.286 4.223 4.220 4.215 4.202
2.694 2.676 2.670 2.656 2.639 2.615 2.596 2.354 2.321 2.313
1.998 1.994 1.986 1.978 1.765 1.749 1.738 1.729 1.721 1.718 1.708 1.697 1.688 1.676 1.538

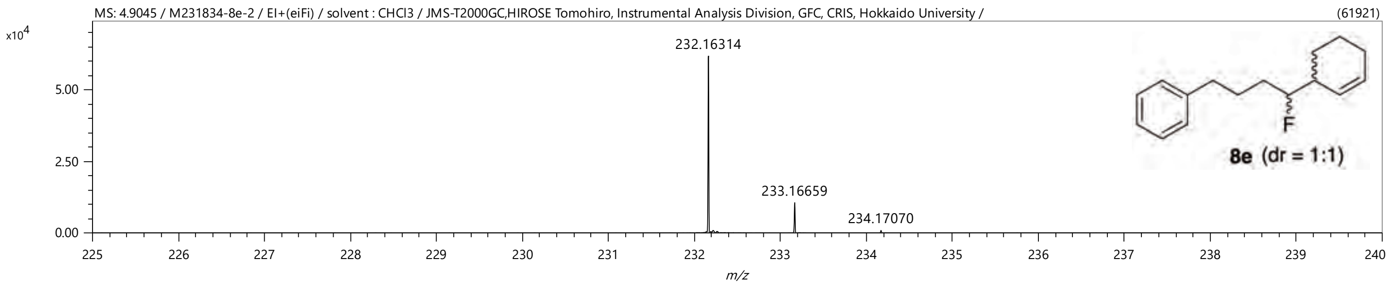


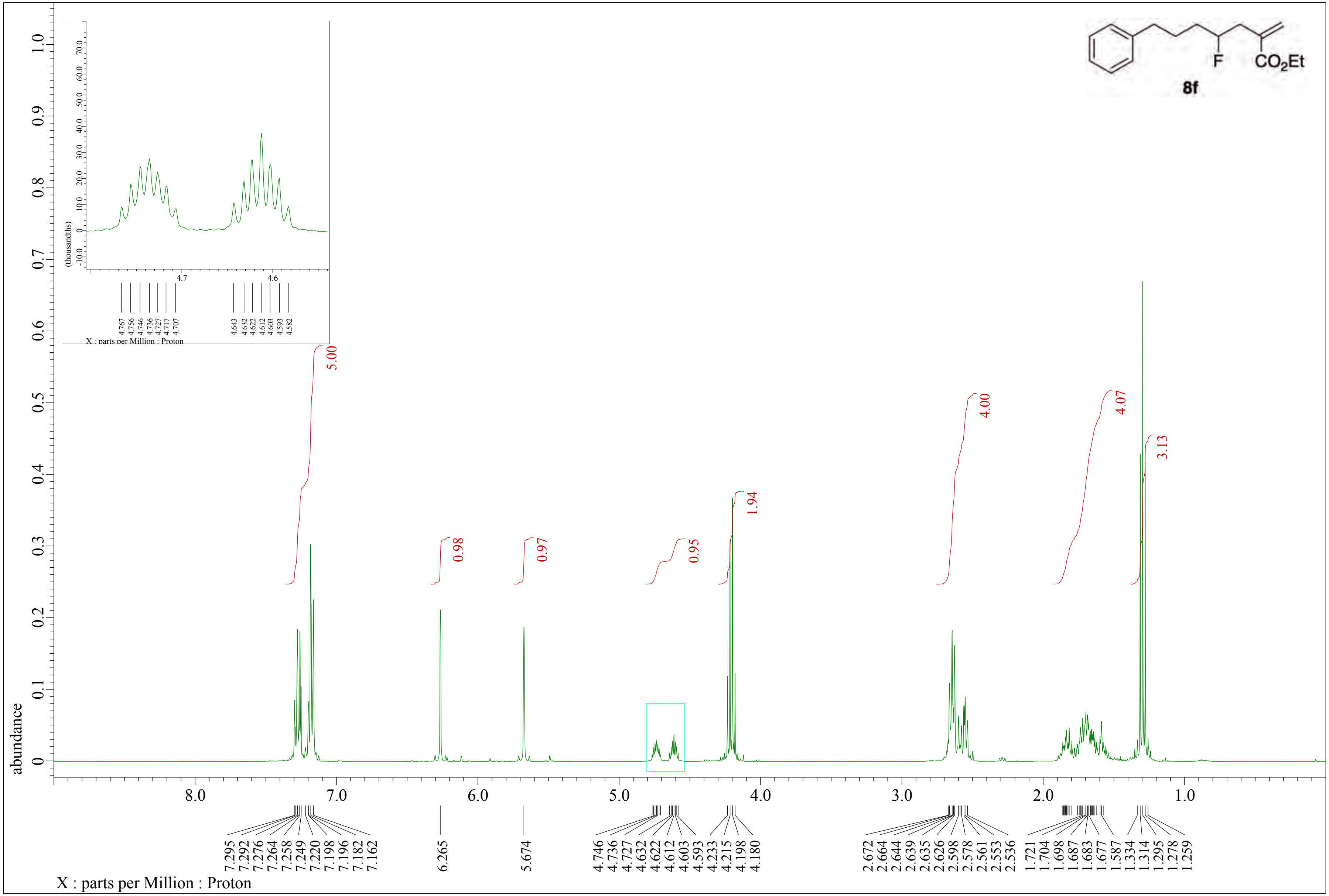
8e (dr = 1:1)
X : parts per Million : Carbon13
(thousandths)
142.303
142.284
130.085
129.166
128.543
128.466
126.875
126.808
126.569
126.502
125.927
98.185
97.370
96.479
95.664
77.476
77.160
76.844
40.151
40.132
39.969
39.931
35.839
35.810
32.131
31.987
31.910
31.776
27.311
27.282
27.157
27.119
25.260
25.212
25.135
25.087
23.842
23.794
21.657
20.900

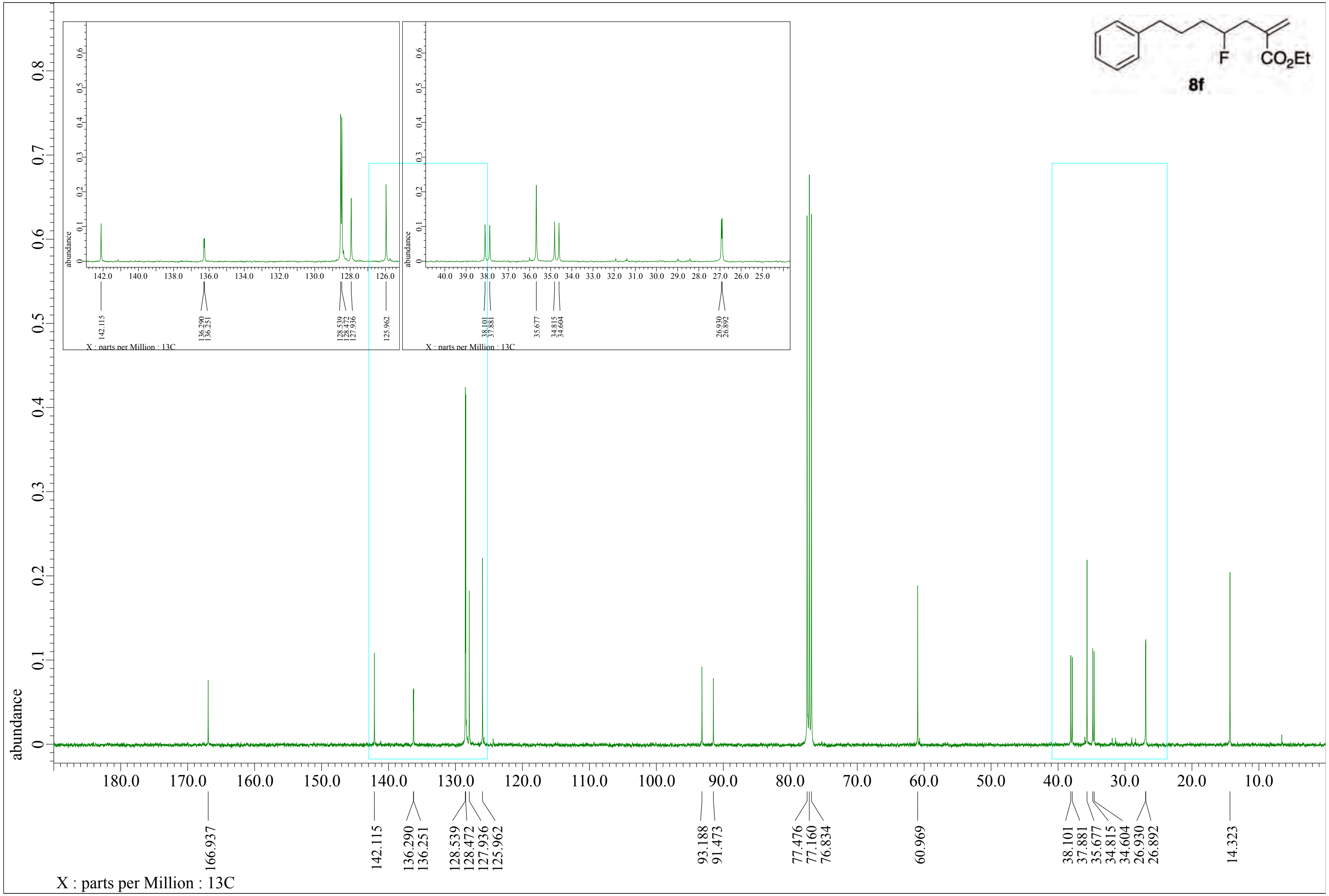


8e (dr = 1:1)
abundance
X : parts per Million : Fluorine19
-183.350
-183.400
-183.442
-183.492
-183.531
-183.573
-183.619
-183.669
-184.283
-184.330
-184.376
-184.422
-184.460
-184.502
-184.548
-184.595
1.00
1.00

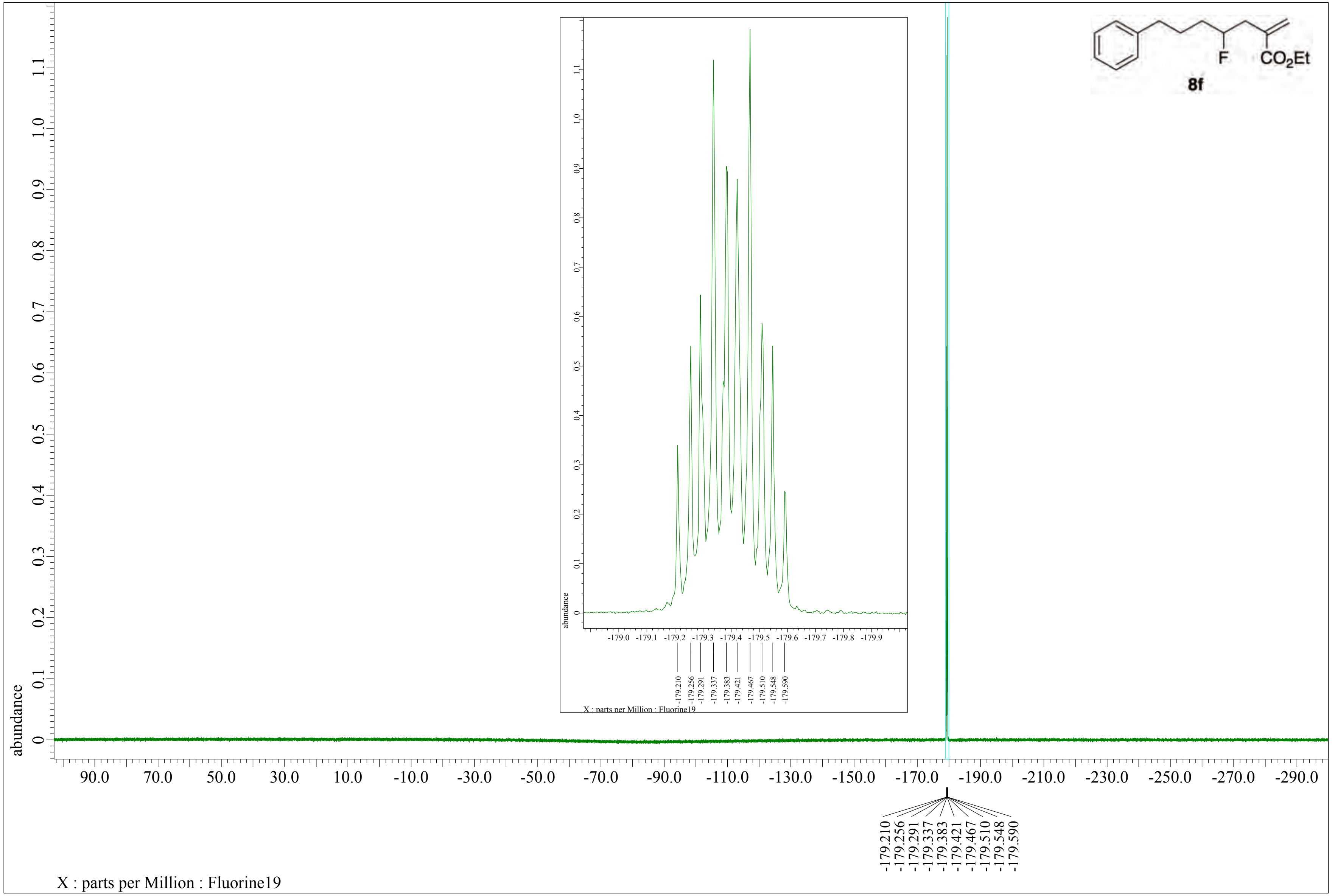

MS: 4.9045 / M231834-8e-2 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(1757555)
x10^6
81.07
91.05
104.06
212.16
131.09
117.07
121.10
65.04
53.04
41.04
59.03
73.05
144.09
170.11
183.12
232.16
m/z
F
8e (dr = 1:1)


MS: 4.9045 / M231834-8e-2 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(61921)
x10^4
232.16314
233.16659
234.17070
m/z
F
8e (dr = 1:1)


8f
F
CO_2Et
X : parts per Million : Proton
abundance
5.00
0.98
0.97
0.95
1.94
4.00
4.07
3.13



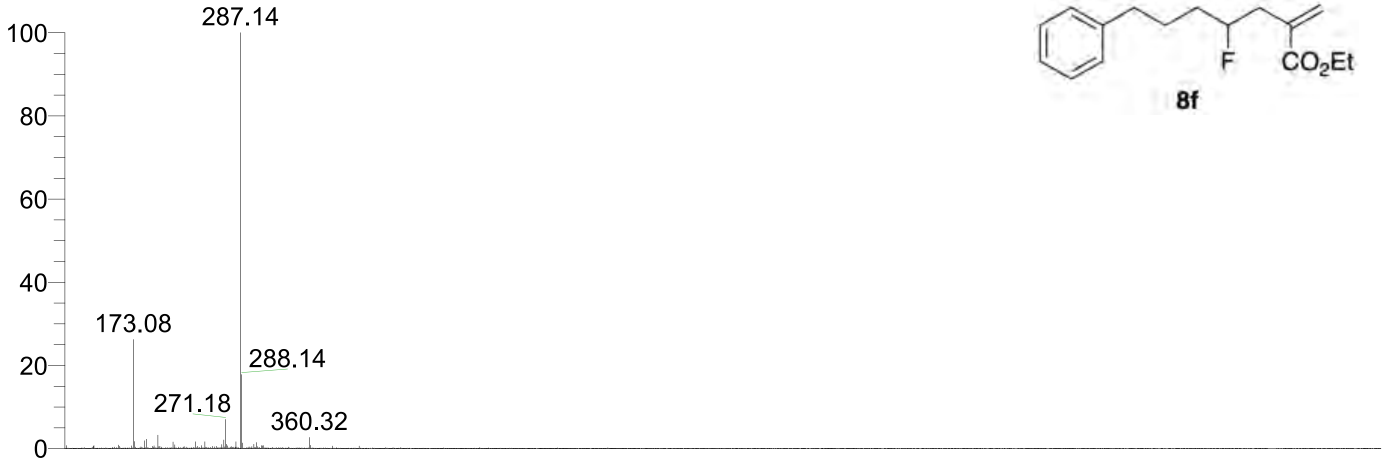
8f
F
CO2Et
abundance
X : parts per Million : 13C
166.937
142.115
136.290
136.251
128.539
128.472
127.936
125.962
93.188
91.473
77.476
77.160
76.834
60.969
38.101
37.881
35.677
34.815
34.604
26.930
26.892
14.323



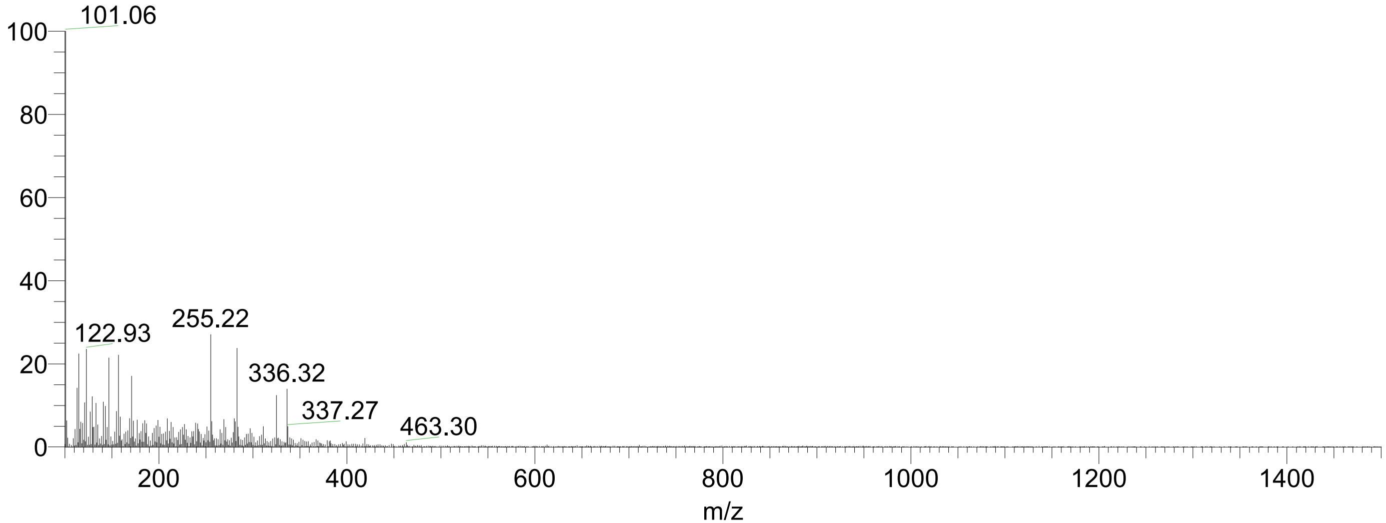
8f
F
CO2Et
abundance
X : parts per Million : Fluorine19
-179.210
-179.256
-179.291
-179.337
-179.383
-179.421
-179.467
-179.510
-179.548
-179.590

Sample No. : C:\Xcalibur\...\1227\BG_231835_8f_, Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 11:47:08
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

NL: 5.67E7
BG_231835_8f_pn#18
-31 RT: 0.31-0.50
AV: 7 T: FTMS + c
ESI Full ms
[100.00-1500.00]

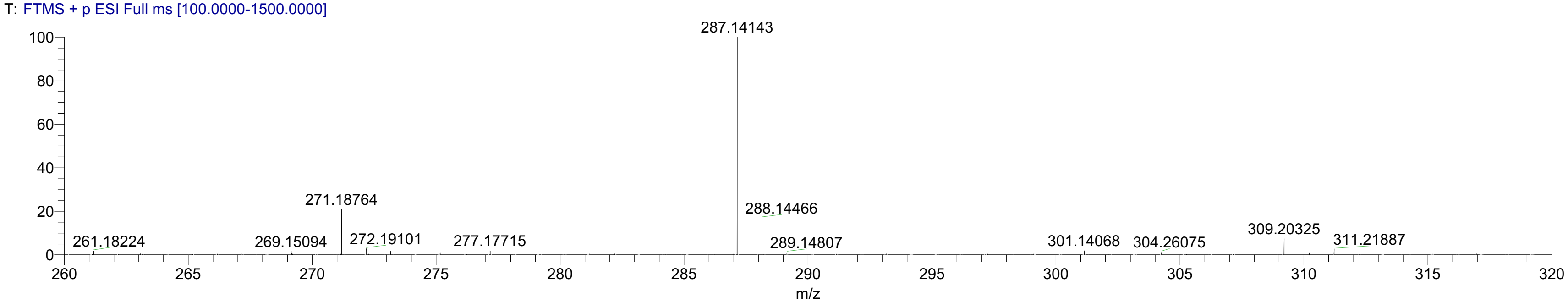


NL: 2.73E6
BG_231835_8f_pn#18
-31 RT: 0.30-0.48
AV: 7 T: FTMS - c ESI
Full ms
[100.00-1500.00]

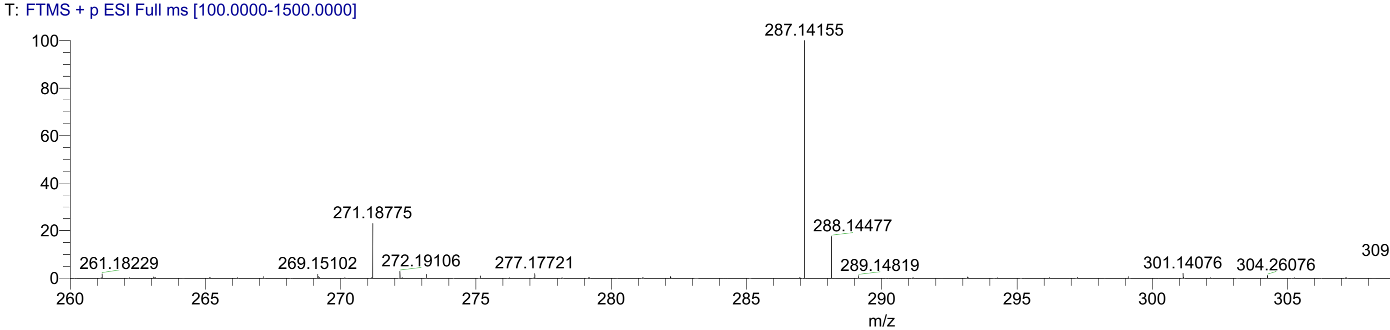


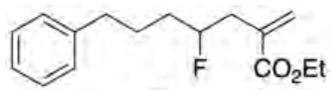
Sample No. : C:\Xcalibur\...\20231227\231835_8f_pn Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/27/23 16:42:26
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

231835_8f_pn #21-25 RT: 0.35-0.41 AV: 3 NL: 2.19E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



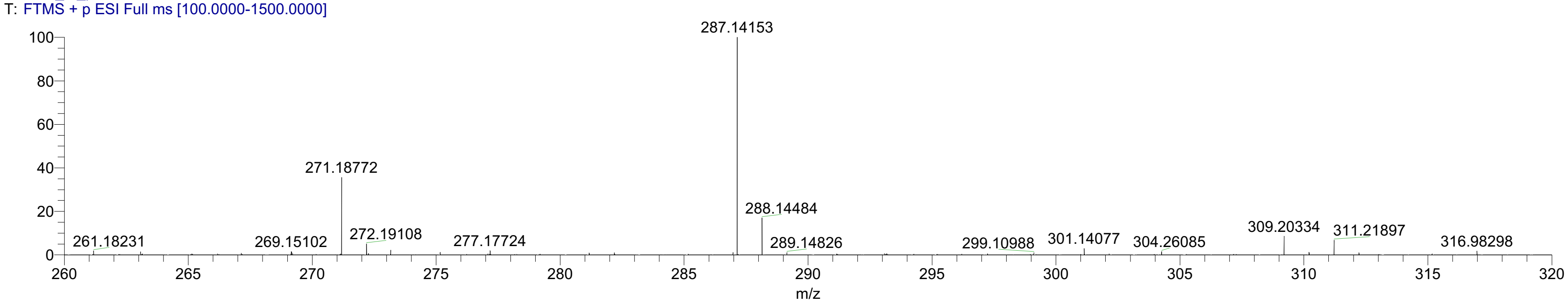
231835_8f_pn #25-28 RT: 0.41-0.44 AV: 2 NL: 1.80E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

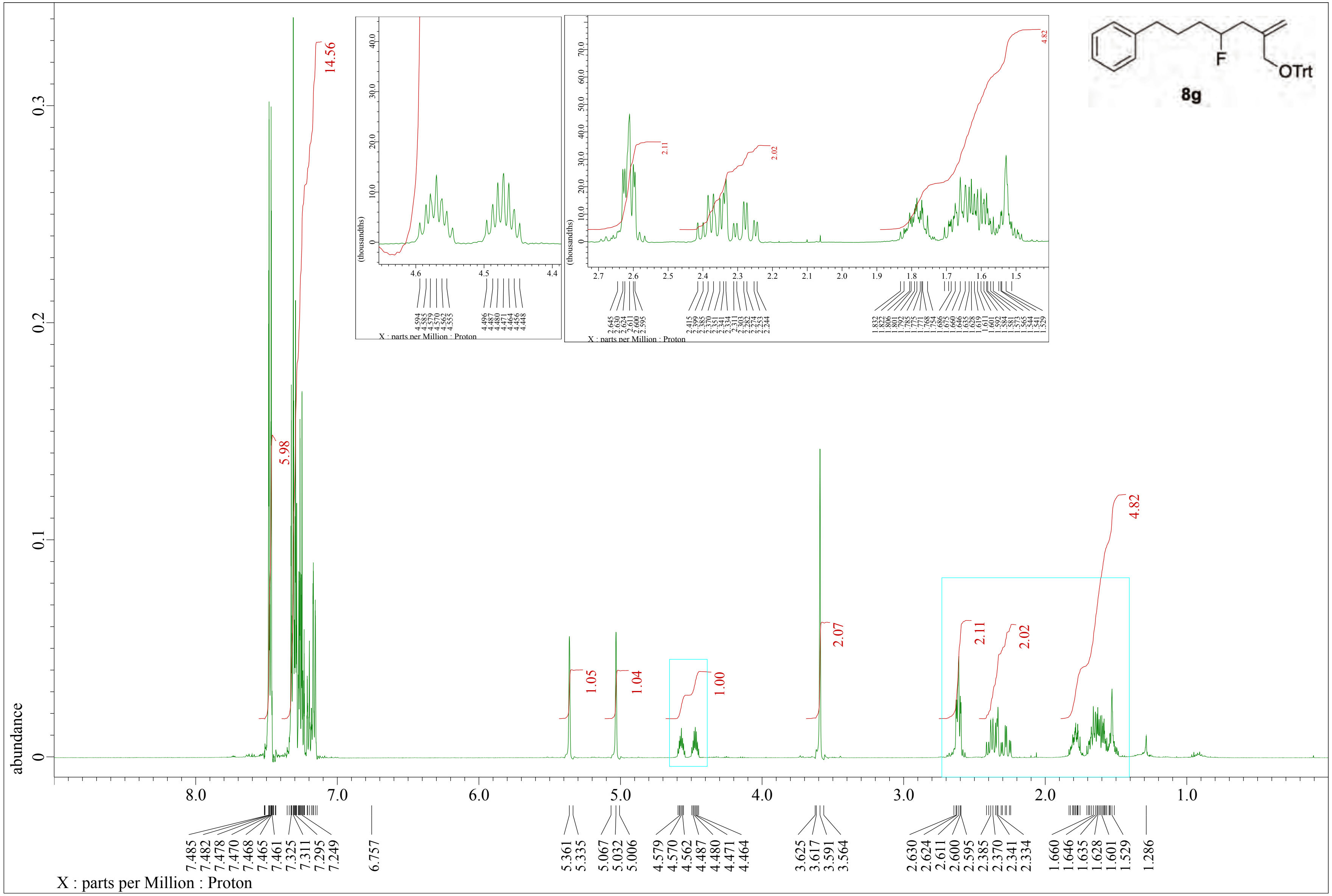


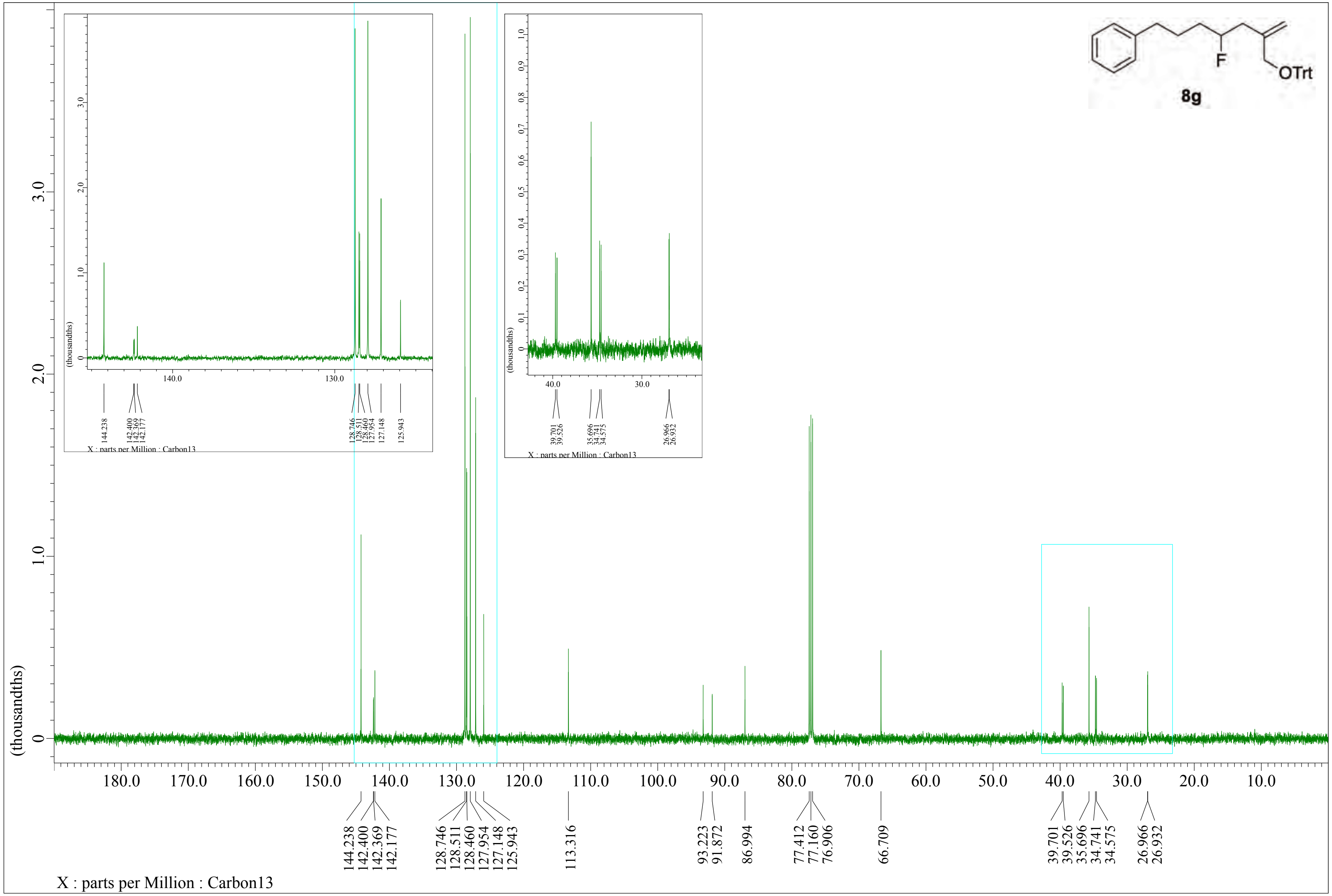


8f

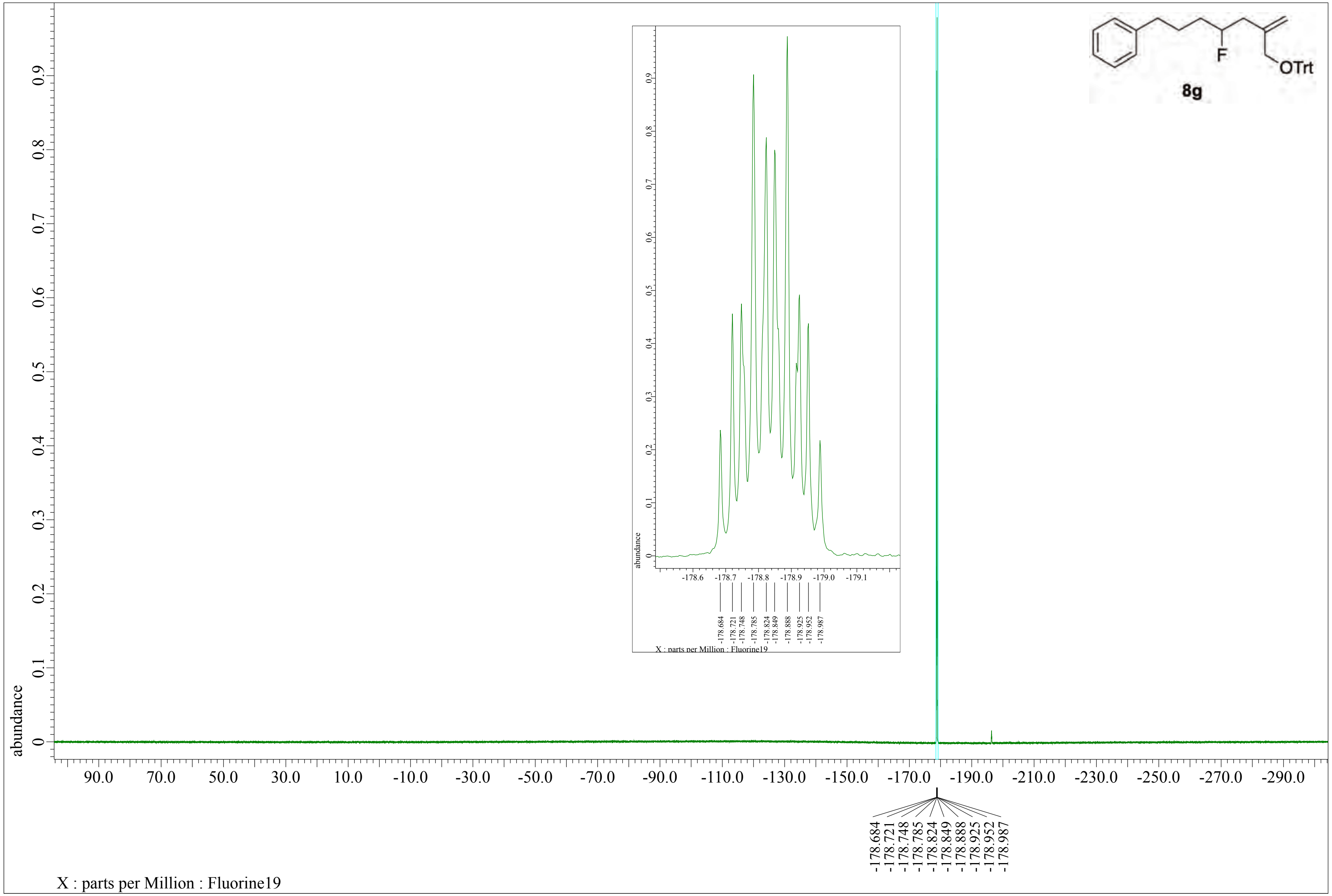
231835_8f_pn #28-31 RT: 0.47-0.50 AV: 2 NL: 6.67E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]



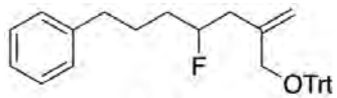

F
OTrt
8g
abundance
0.3
0.2
0.1
0
14.56
5.98
1.05
1.04
1.00
2.07
2.11
2.02
4.82
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.485 7.482 7.478 7.470 7.468 7.465 7.461 7.325 7.311 7.295 7.249
6.757
5.361 5.335
5.067 5.032 5.006
4.579 4.570 4.562 4.487 4.480 4.471 4.464
3.625 3.617 3.591 3.564
2.630 2.624 2.611 2.600 2.595 2.385 2.370 2.341 2.334
1.660 1.646 1.635 1.628 1.601 1.529
1.286
X : parts per Million : Proton


OTrt
F
144.238
142.400
142.369
142.177
128.746
128.511
128.460
127.954
127.148
125.943
113.316
93.223
91.872
86.994
77.412
77.160
76.906
66.709
39.701
39.526
35.696
34.741
34.575
26.966
26.932
X : parts per Million : Carbon13
(thousandths)

8g

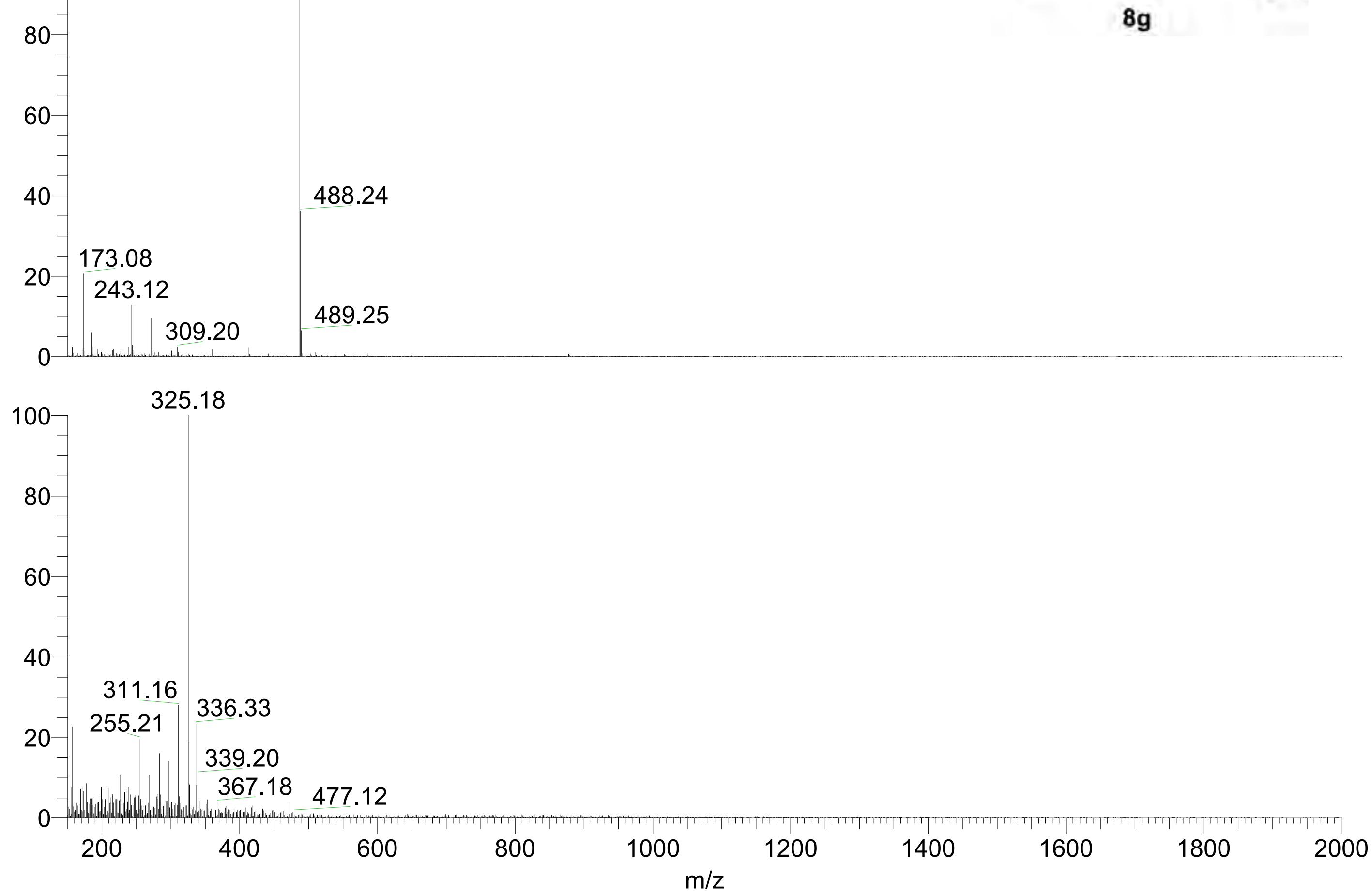

abundance
X : parts per Million : Fluorine19
-178.684
-178.721
-178.748
-178.785
-178.824
-178.849
-178.888
-178.925
-178.952
-178.987
F
OTrt
8g

Sample No. : C:\Xcalibur\...\1227\BG_231836_8g_, Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 11:46:45
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University



8g

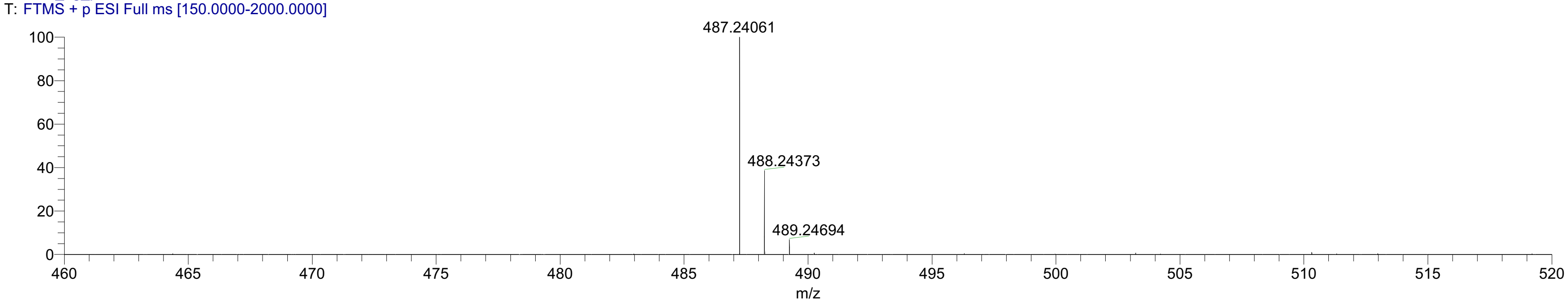
NL: 4.27E7
BG_231836_8g_pn#1
8-30 RT: 0.31-0.47
AV: 6 T: FTMS + c
ESI Full ms
[150.00-2000.00]



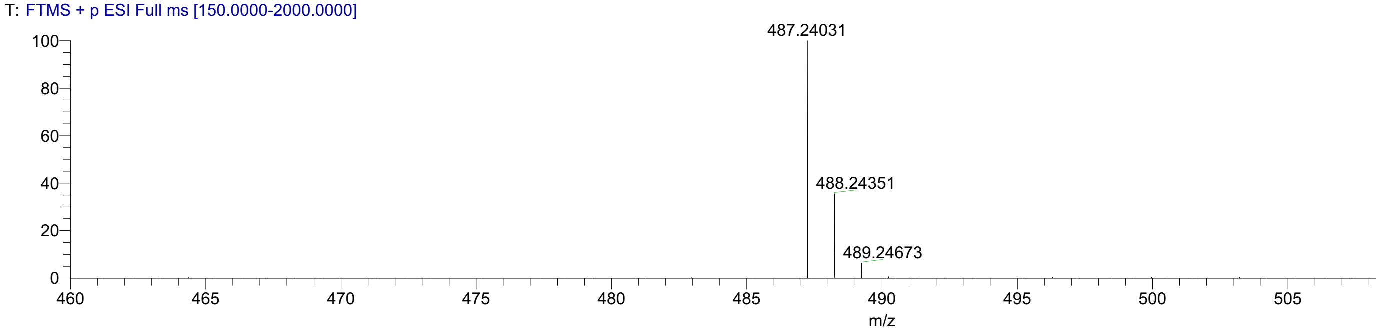
NL: 1.25E6
BG_231836_8g_pn#1
8-31 RT: 0.30-0.49
AV: 7 T: FTMS - c ESI
Full ms
[150.00-2000.00]

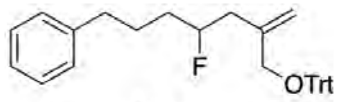
Sample No. : C:\Xcalibur\...\20231227\231836_8g_pn	Instrument : Exactive Plus	Mobile phase solvent : MeOH
Operator name : hayashi harumi	Sample solvent : CHCl3
Date : 12/27/23 16:47:26
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

231836_8g_pn #21-24 RT: 0.35-0.38 AV: 2 NL: 1.11E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



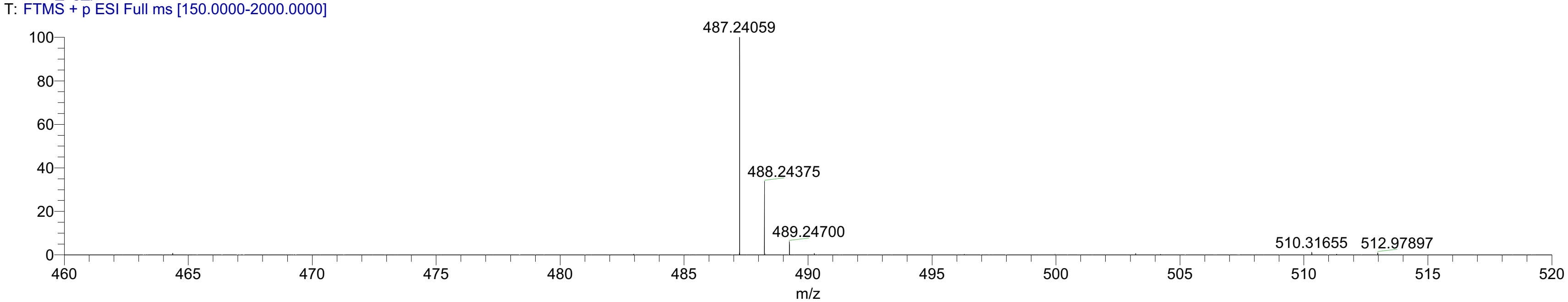
231836_8g_pn #25-28 RT: 0.41-0.44 AV: 2 NL: 1.27E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]

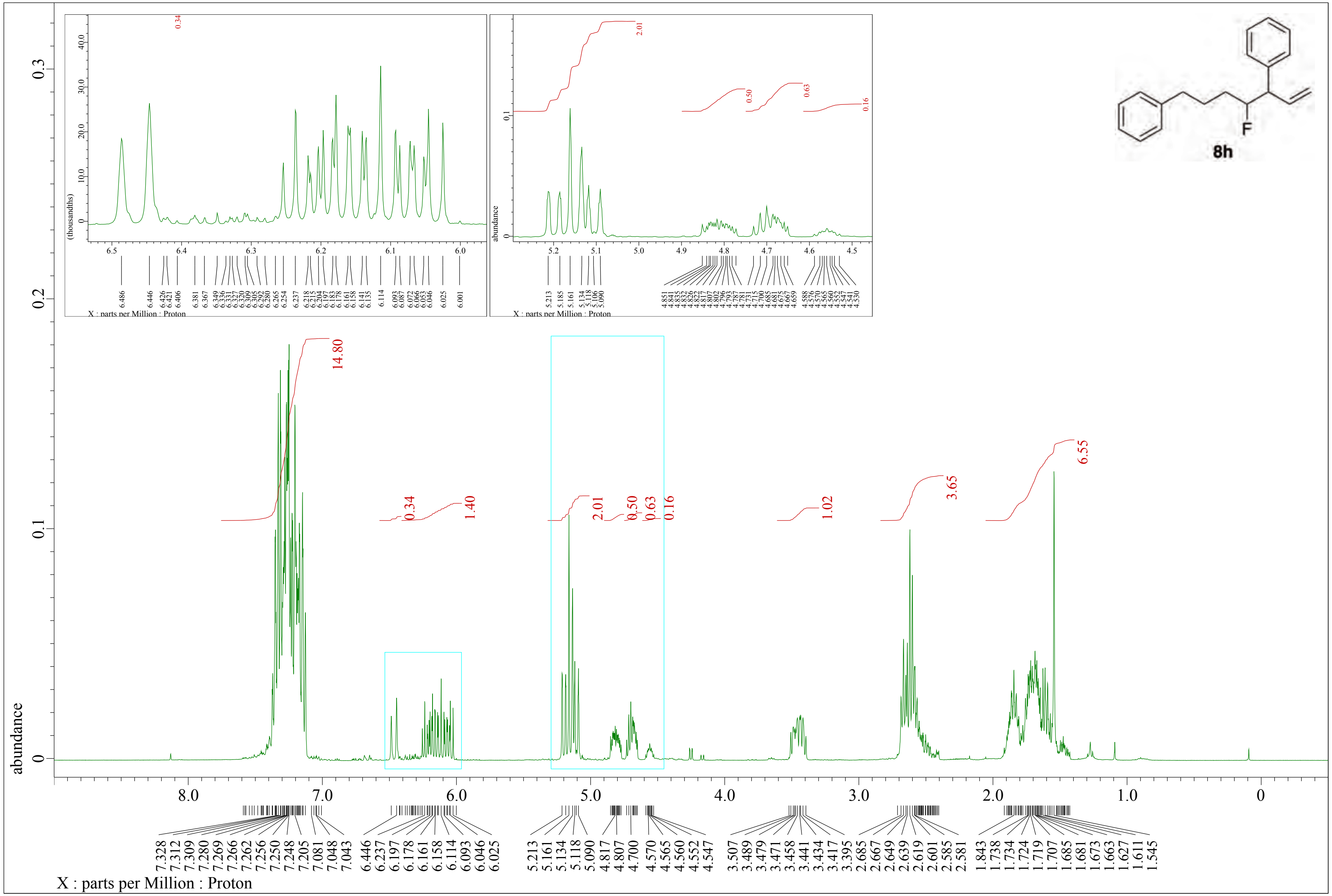




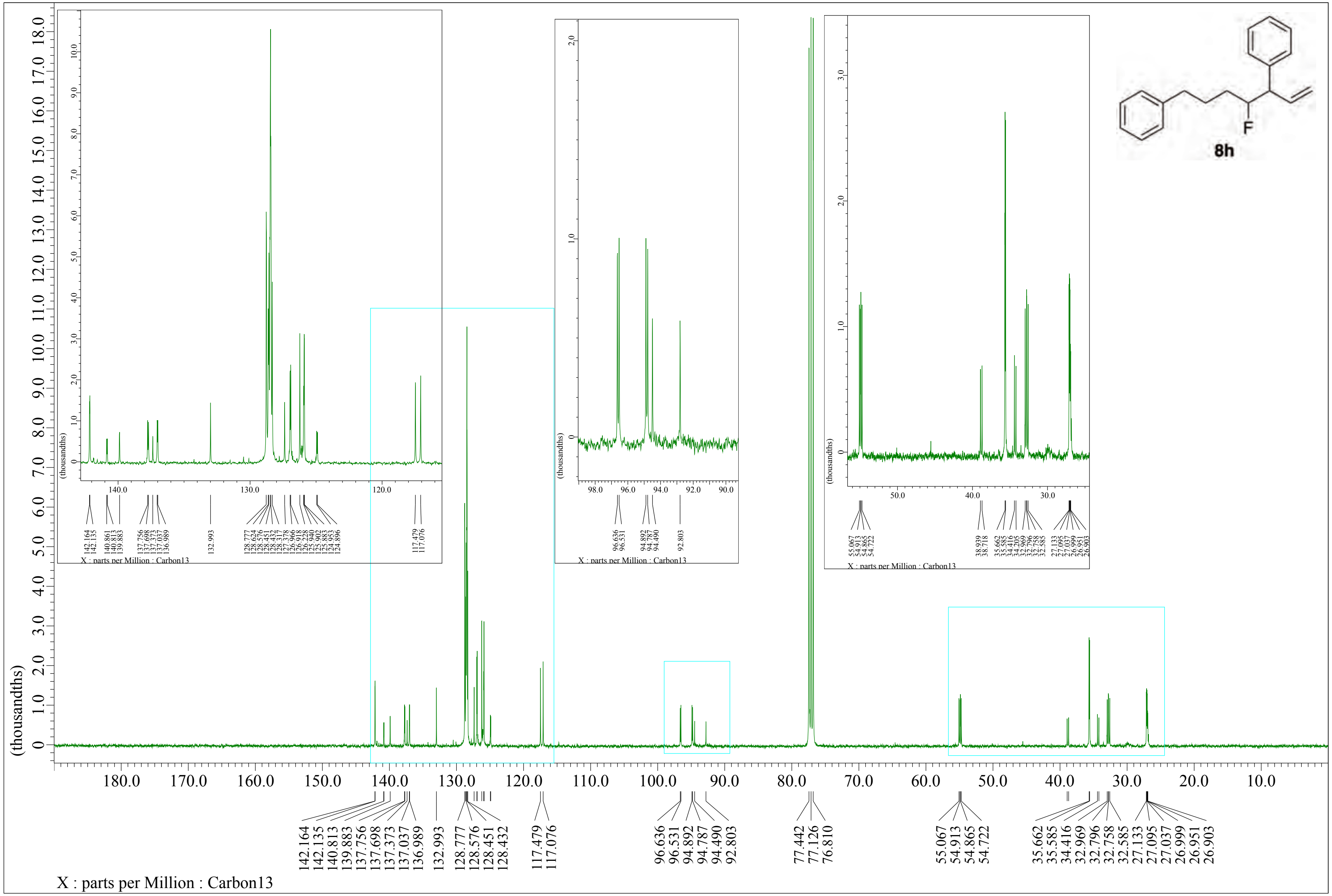
8g

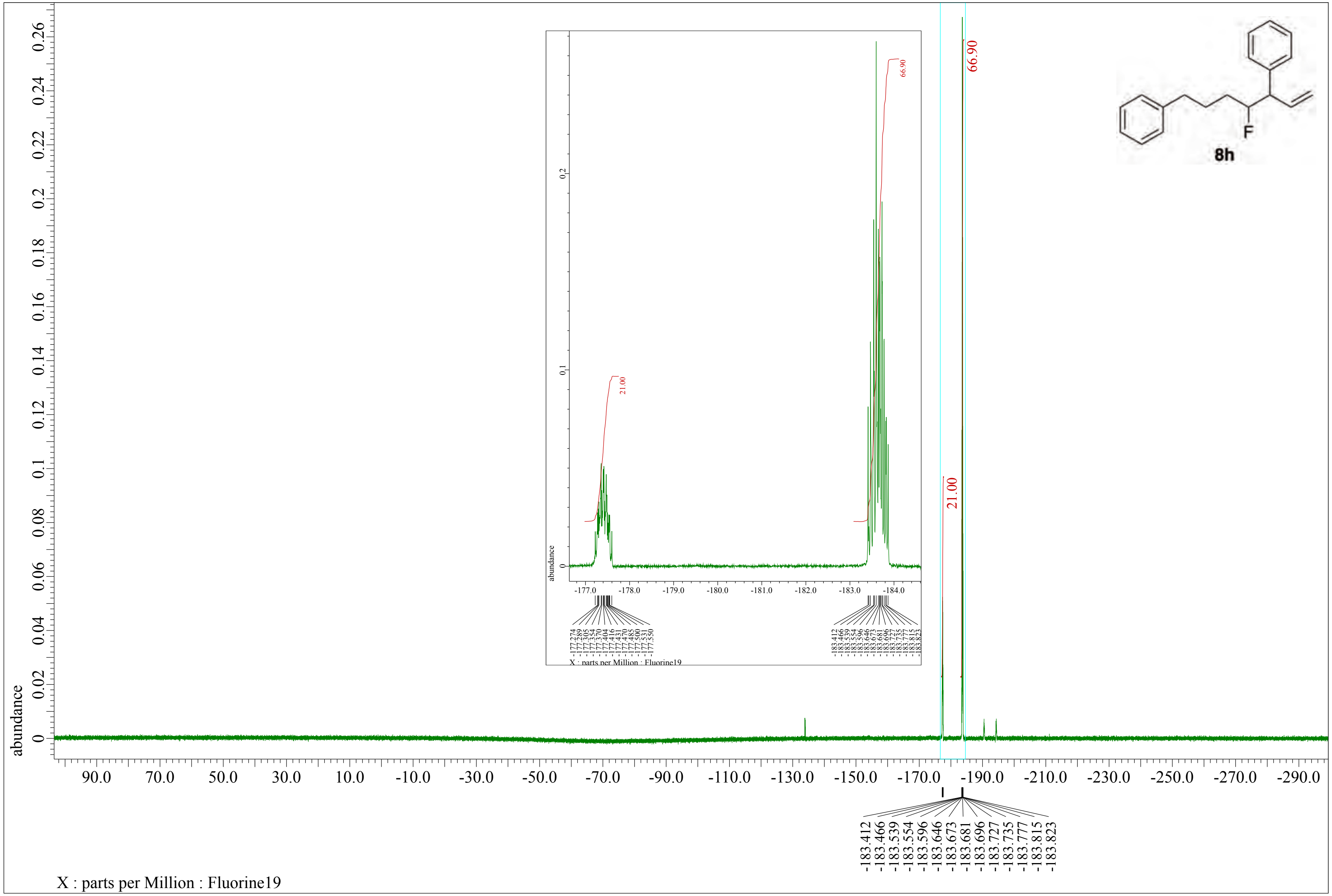
231836_8g_pn #29-31 RT: 0.47-0.51 AV: 2 NL: 7.60E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]





abundance
X : parts per Million : Proton
14.80
0.34
1.40
2.01
0.50
0.63
0.16
1.02
3.65
6.55
8h
F

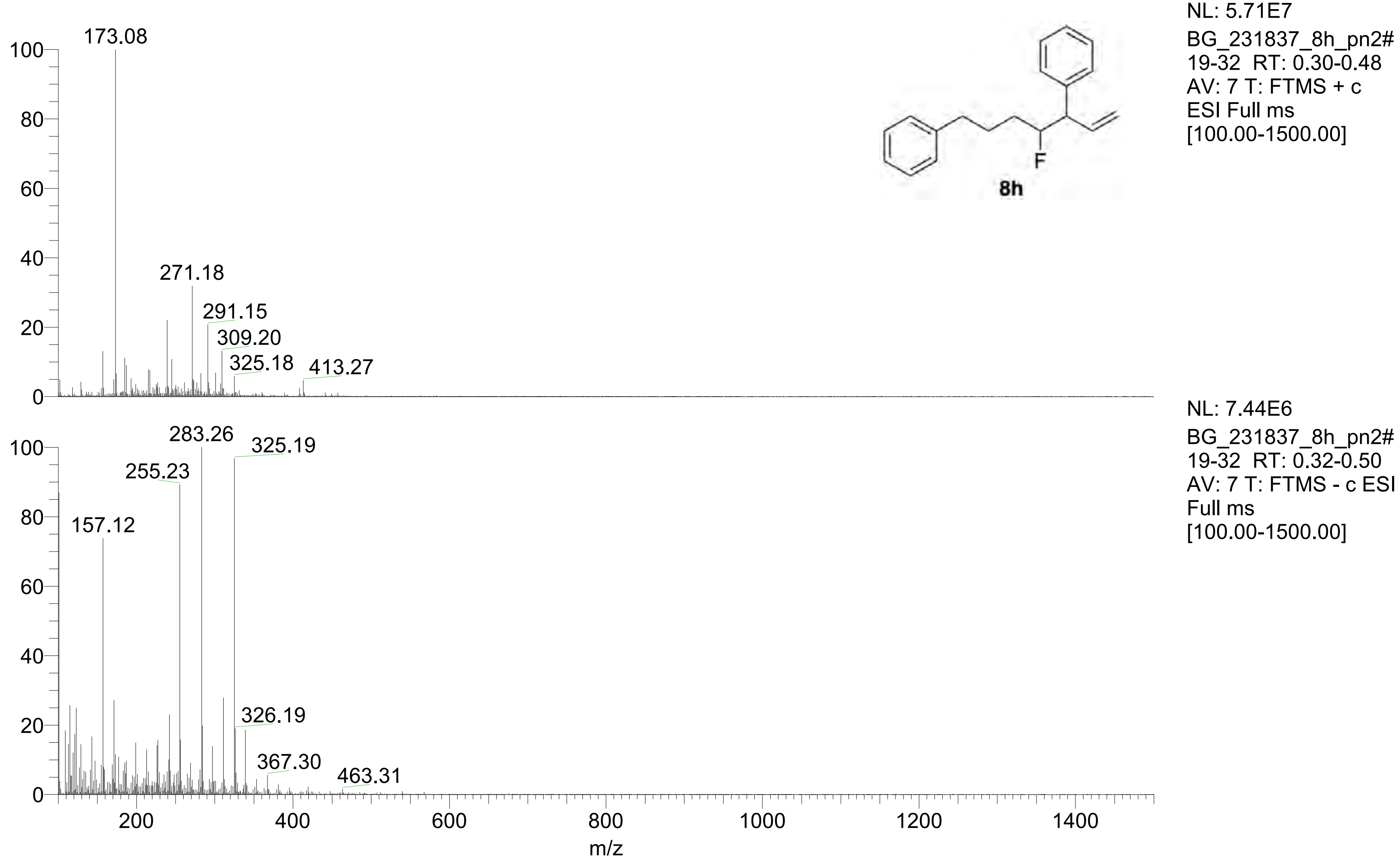

8h
F
(thousandths)
X : parts per Million : Carbon13
142.164
142.135
140.813
139.883
137.756
137.698
137.373
137.037
136.989
132.993
128.777
128.576
128.451
128.432
117.479
117.076
96.636
96.531
94.892
94.787
94.490
92.803
77.442
77.126
76.810
55.067
54.913
54.865
54.722
35.662
35.585
34.416
32.969
32.796
32.758
32.585
27.133
27.095
27.037
26.999
26.951
26.903



abundance
0.26
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
90.0
70.0
50.0
30.0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-170.0
-190.0
-210.0
-230.0
-250.0
-270.0
-290.0
21.00
66.90
-177.0
-178.0
-179.0
-180.0
-181.0
-182.0
-183.0
-184.0
-183.412
-183.466
-183.539
-183.554
-183.596
-183.646
-183.673
-183.681
-183.696
-183.727
-183.735
-183.777
-183.815
-183.823
X : parts per Million : Fluorine19
F

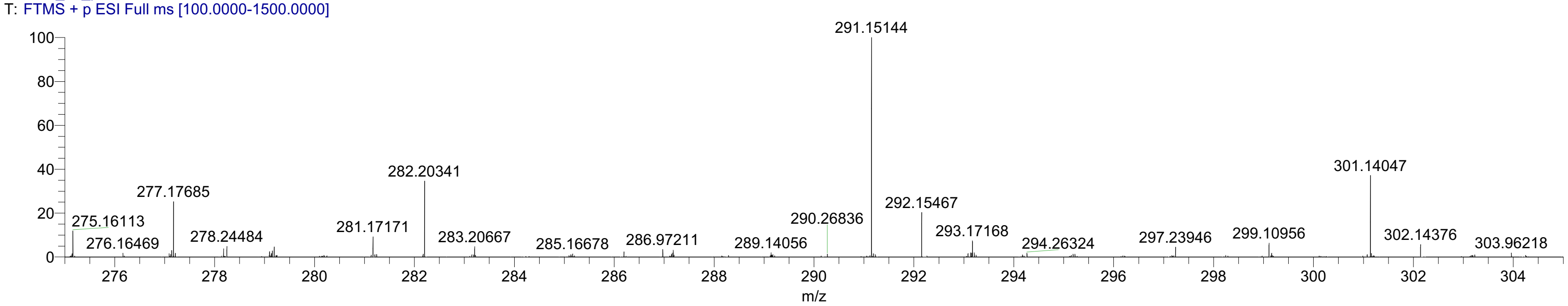
8h

Sample No. : C:\Xcalibur\...\1228\BG_231837_8l _, Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 14:01:15
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

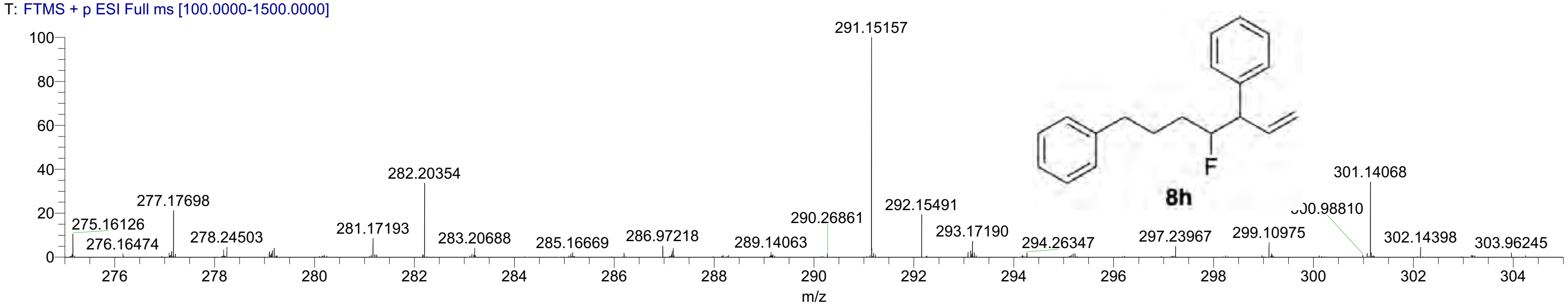


Sample No. : C:\Xcalibur\...\1228\231837_8h_pn2 Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 13:45:21
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

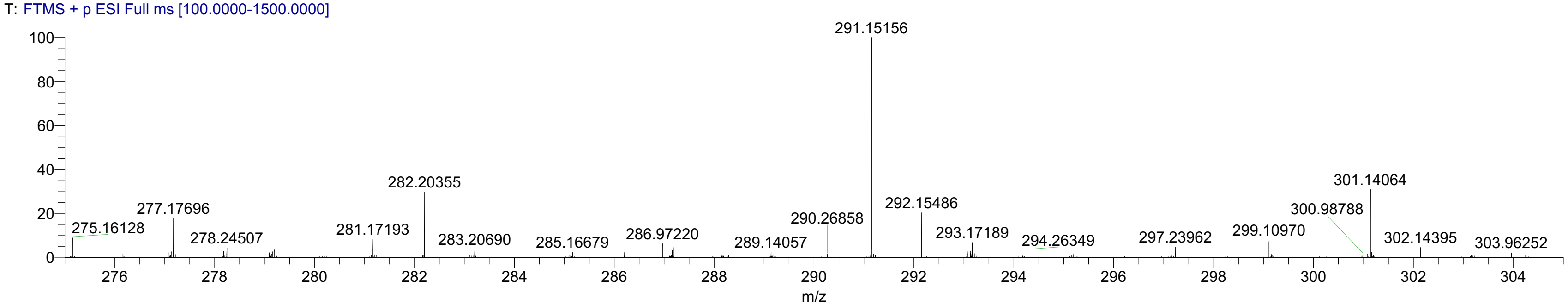
231837_8h_pn2 #22-26 RT: 0.36-0.39 AV: 2 NL: 4.37E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

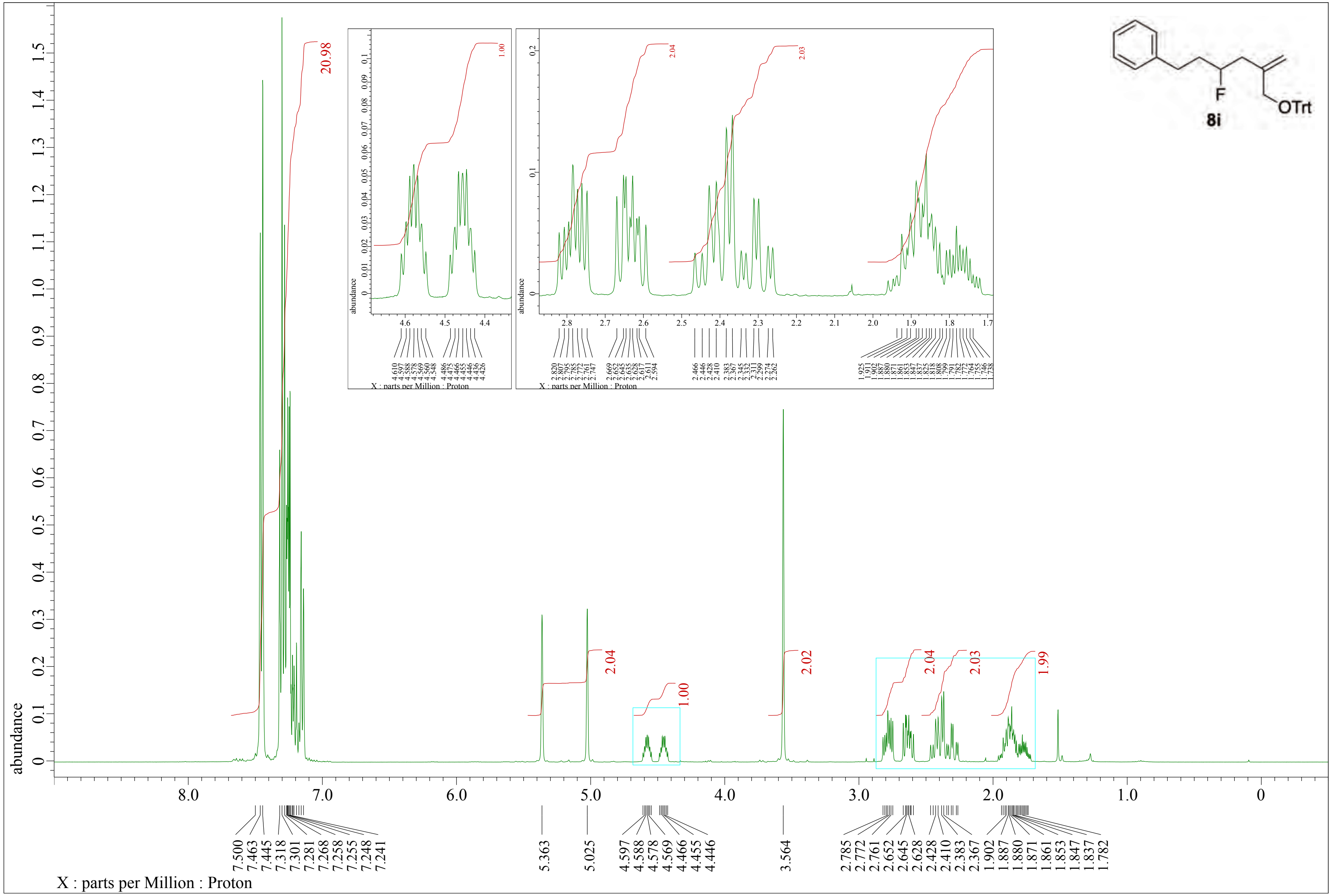


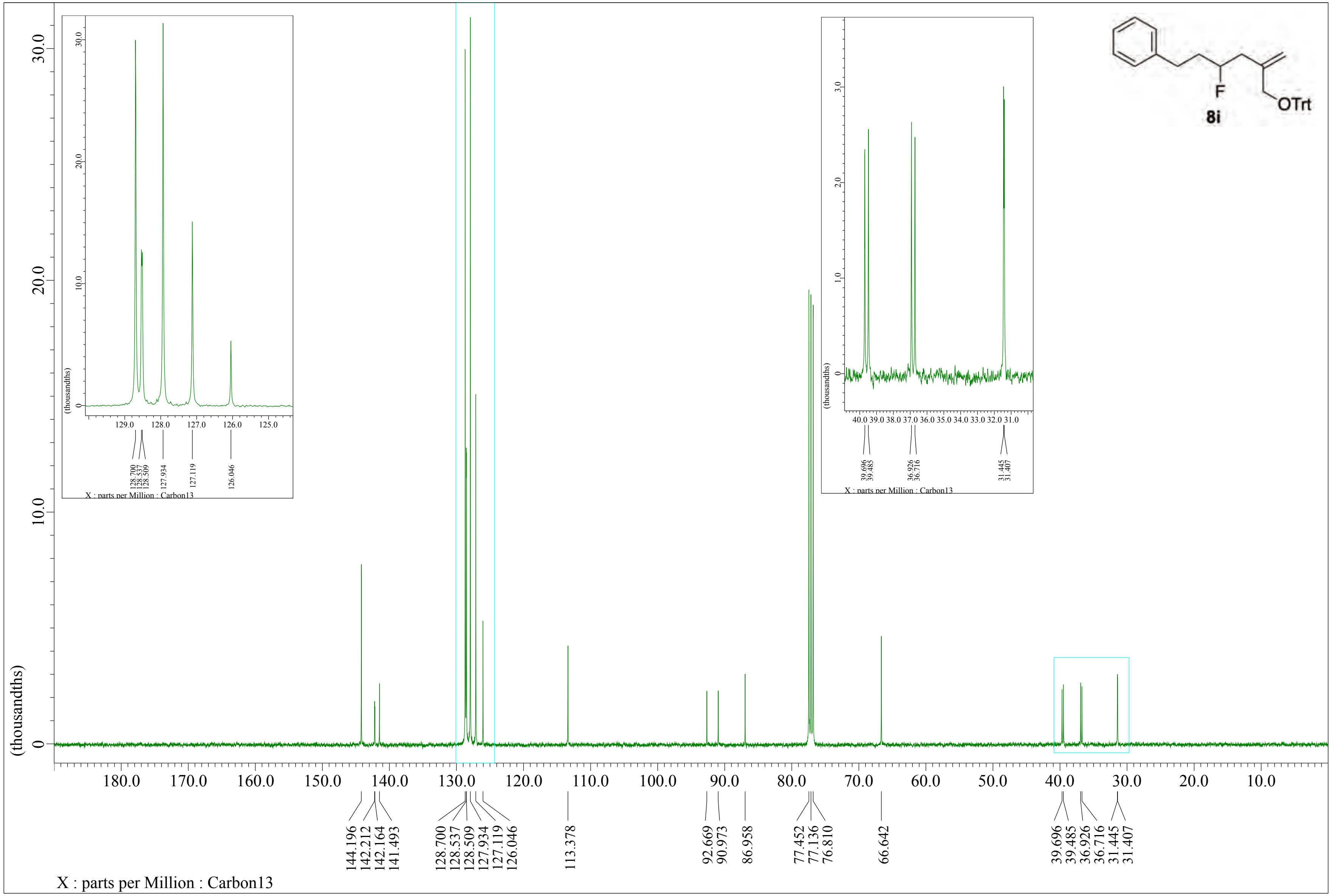
231837_8h_pn2 #26-29 RT: 0.42-0.45 AV: 2 NL: 2.54E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]



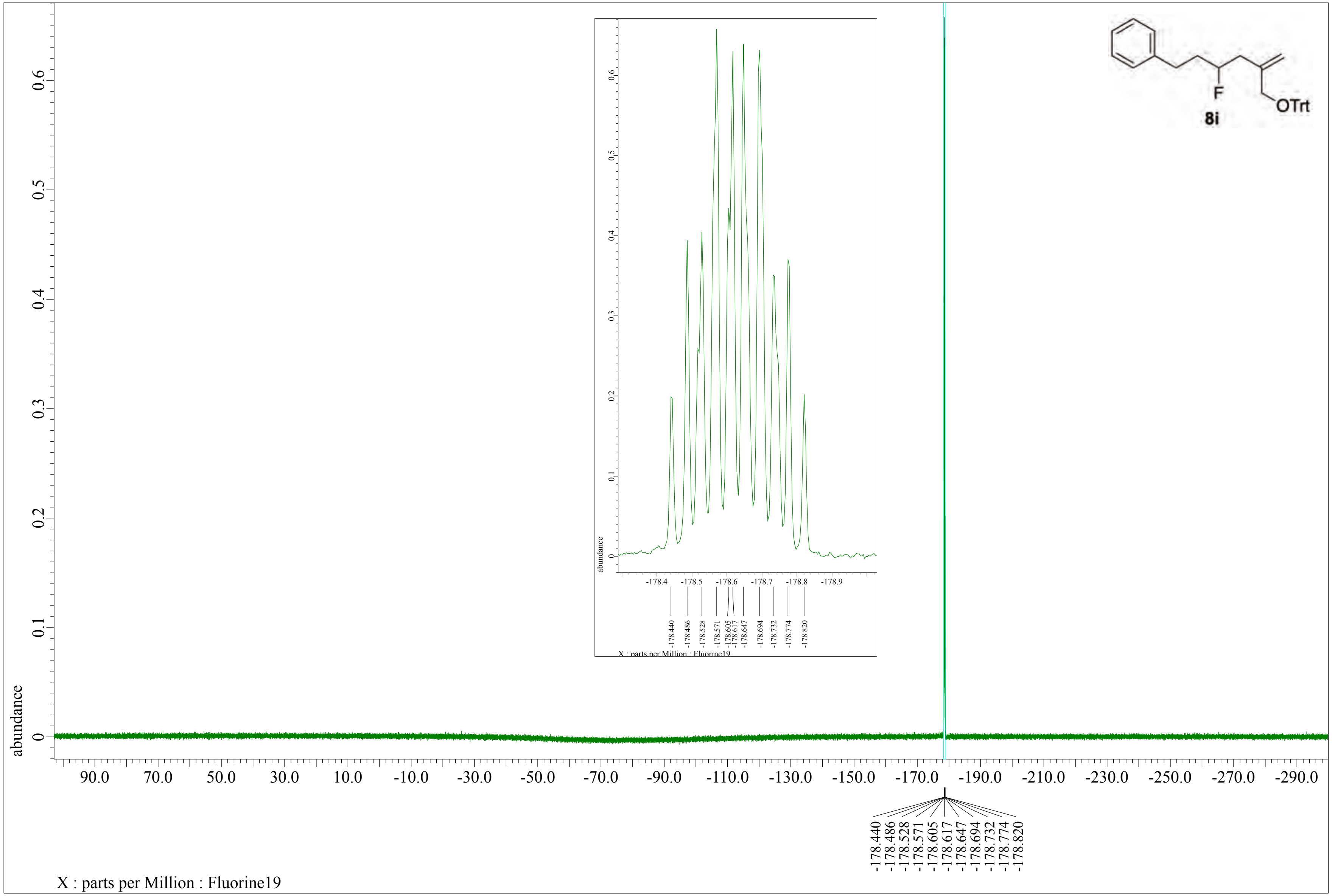
231837_8h_pn2 #29-32 RT: 0.45-0.48 AV: 2 NL: 1.85E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]







8i
F
OTrt
(thousandths)
X : parts per Million : Carbon13
144.196
142.212
142.164
141.493
128.700
128.537
128.509
127.934
127.119
126.046
113.378
92.669
90.973
86.958
77.452
77.136
76.810
66.642
39.696
39.485
36.926
36.716
31.445
31.407

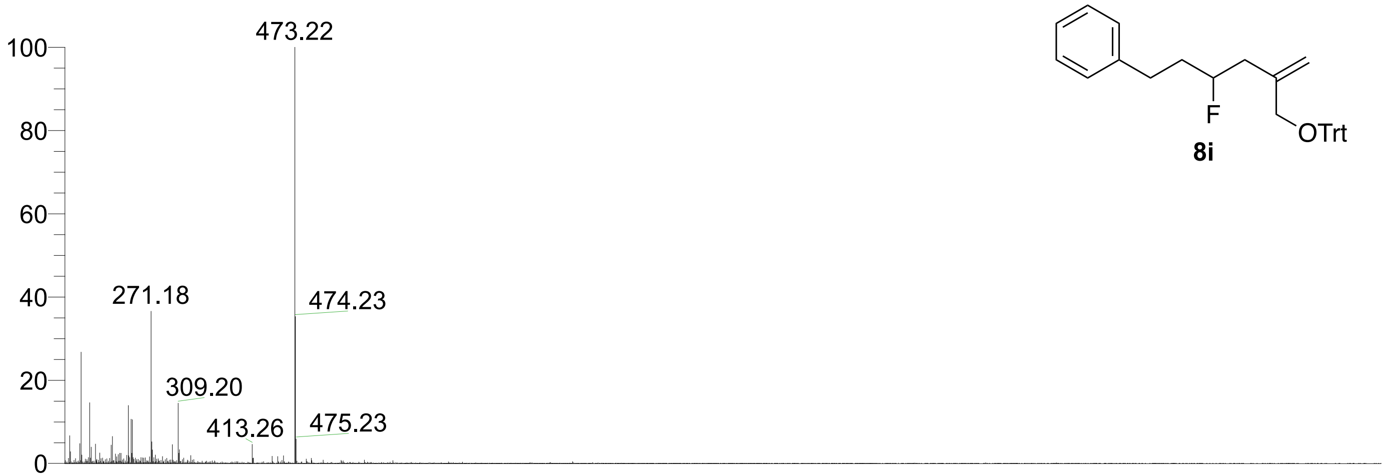


F
OTrt
8i
abundance
X : parts per Million : Fluorine19
-178.440
-178.486
-178.528
-178.571
-178.605
-178.617
-178.647
-178.694
-178.732
-178.774
-178.820

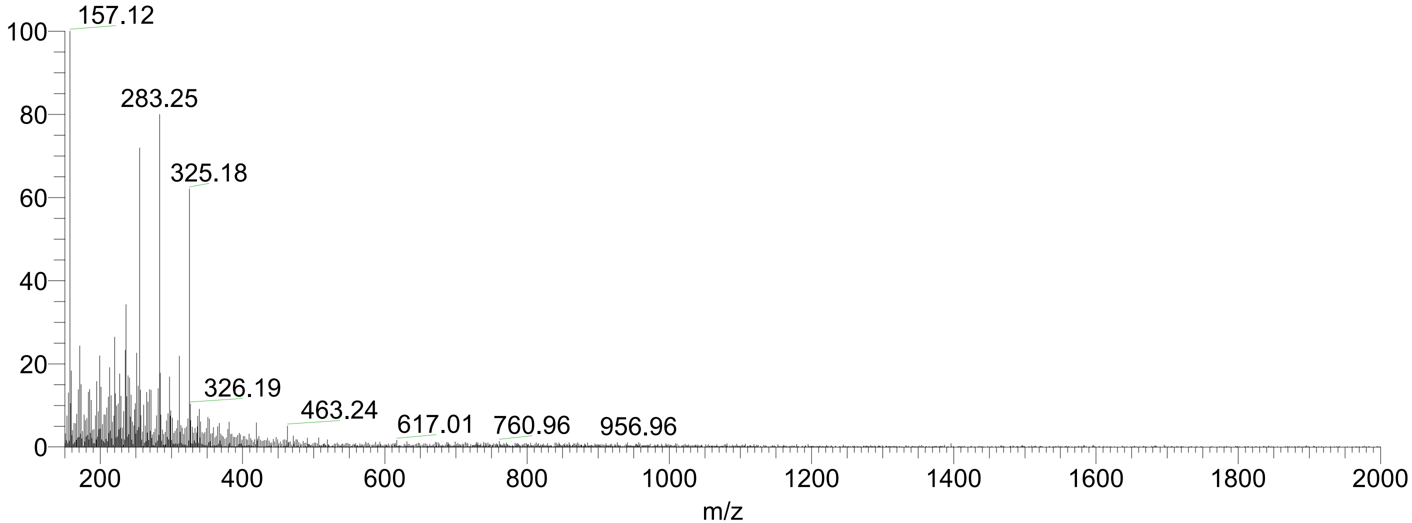
Sample No. : C:\Xcalibur\...\1228\BG_231838_8i_,
Operator name : hayashi harumi
Date : 12/28/23 14:25:49
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

Instrument : Exactive Plus

Mobile phase solvent : MeOH
Sample solvent : CHCl3



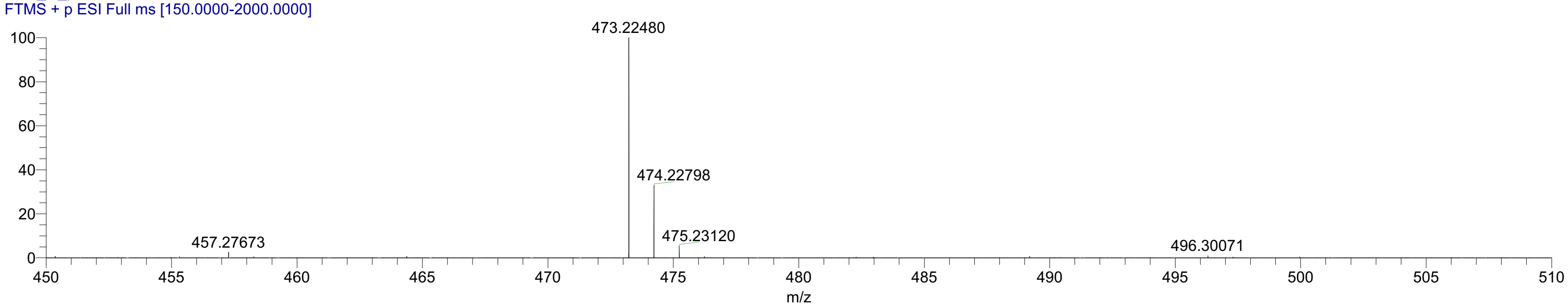
NL: 2.53E7
BG_231838_8i_pn#19
-31 RT: 0.31-0.50
AV: 7 T: FTMS + c
ESI Full ms
[150.00-2000.00]



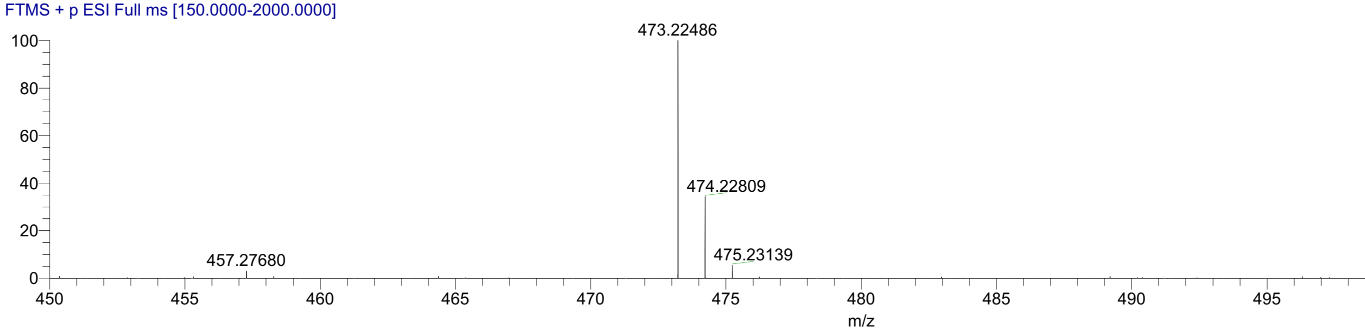
NL: 7.02E5
BG_231838_8i_pn#18
-31 RT: 0.29-0.49
AV: 7 T: FTMS - c ESI
Full ms
[150.00-2000.00]

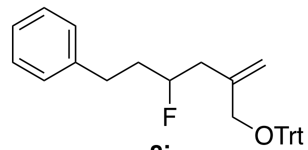
Sample No. : C:\Xcalibur\...\20231228\231838_8i_pn Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 10:27:18
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

231838_8i_pn #21-25 RT: 0.34-0.40 AV: 3 NL: 9.50E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



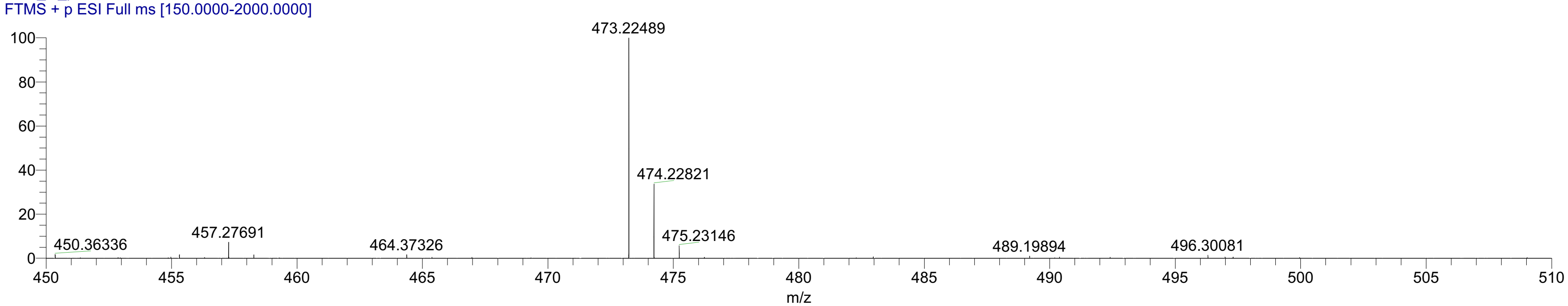
231838_8i_pn #25-28 RT: 0.40-0.44 AV: 2 NL: 7.85E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]

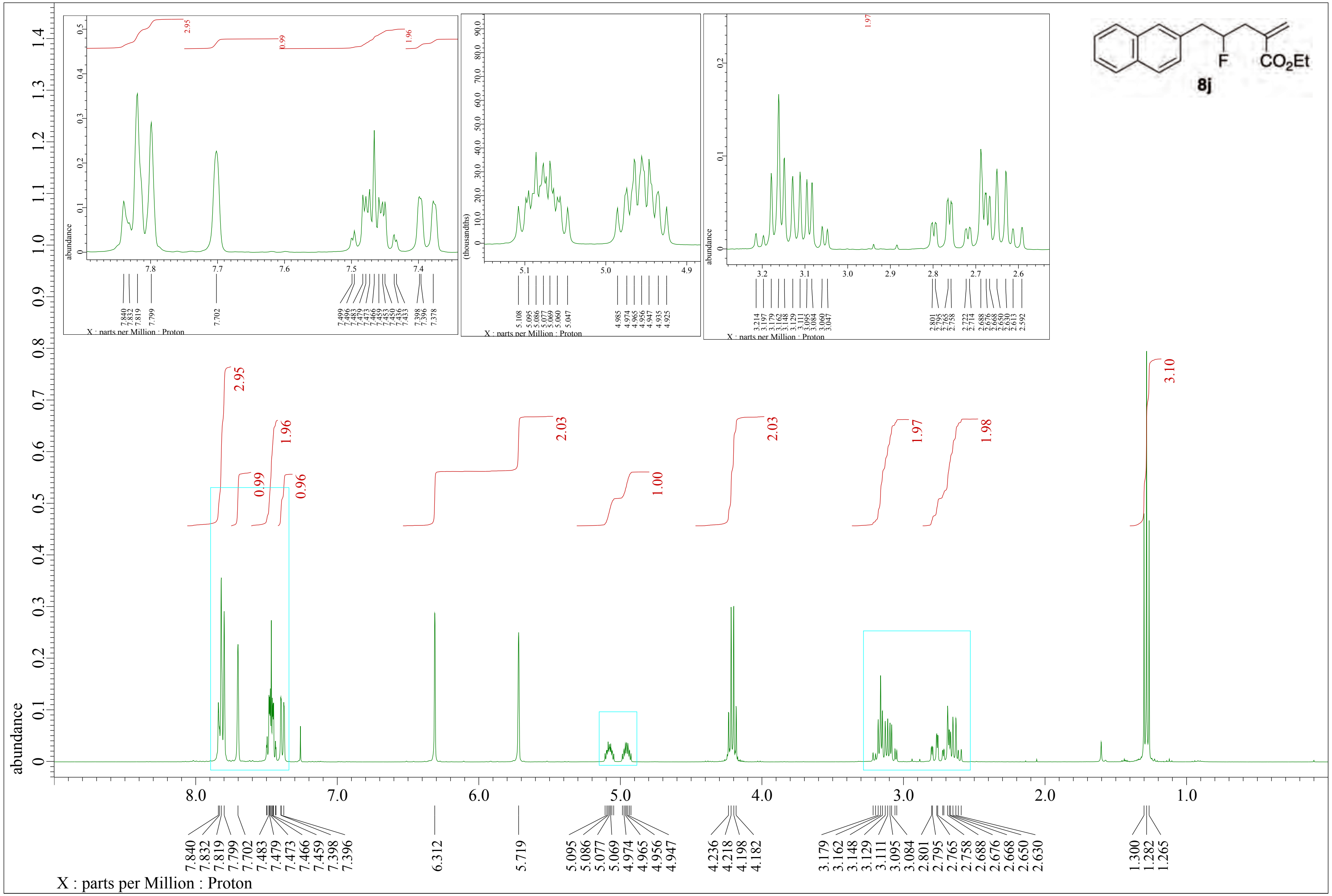


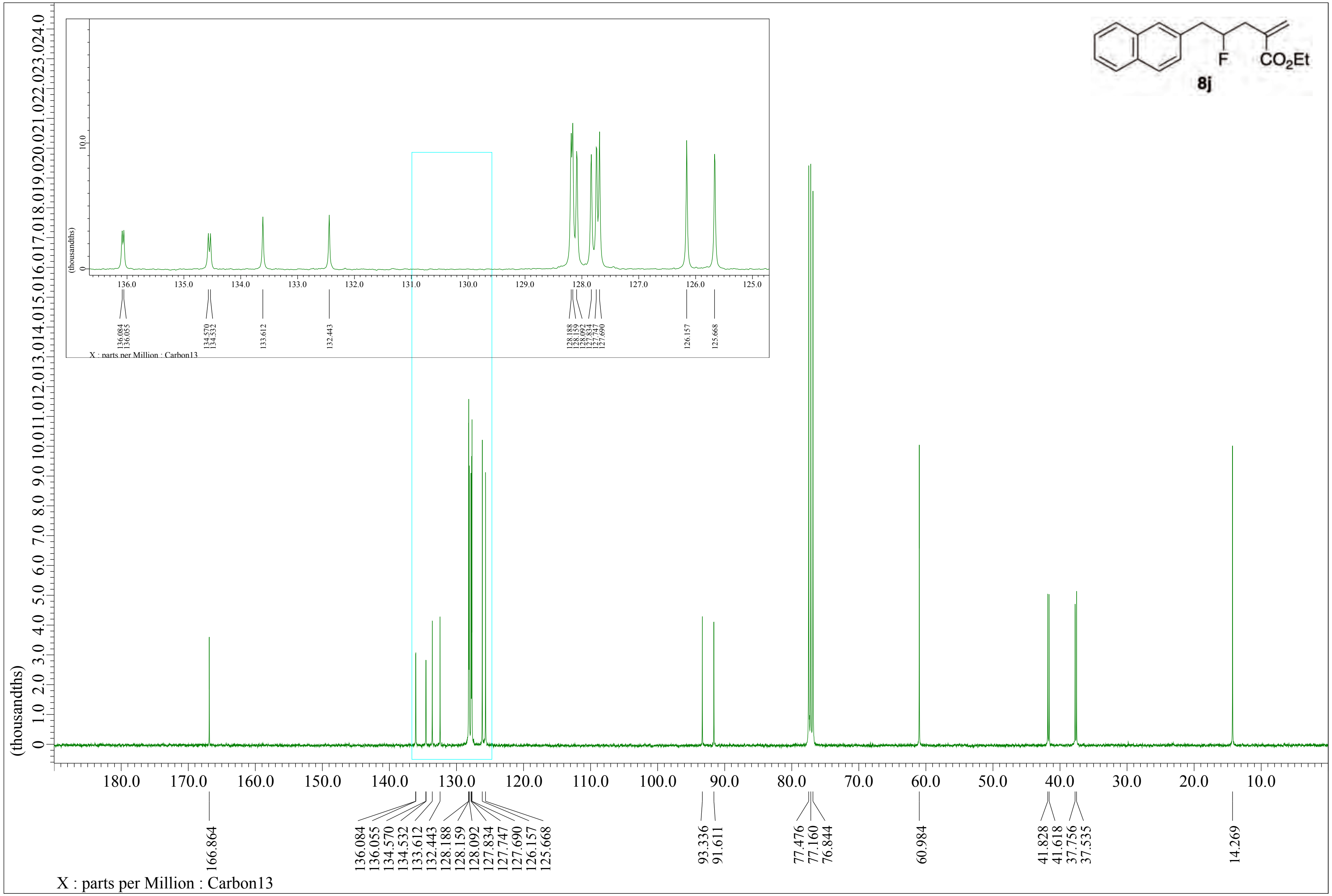


8i

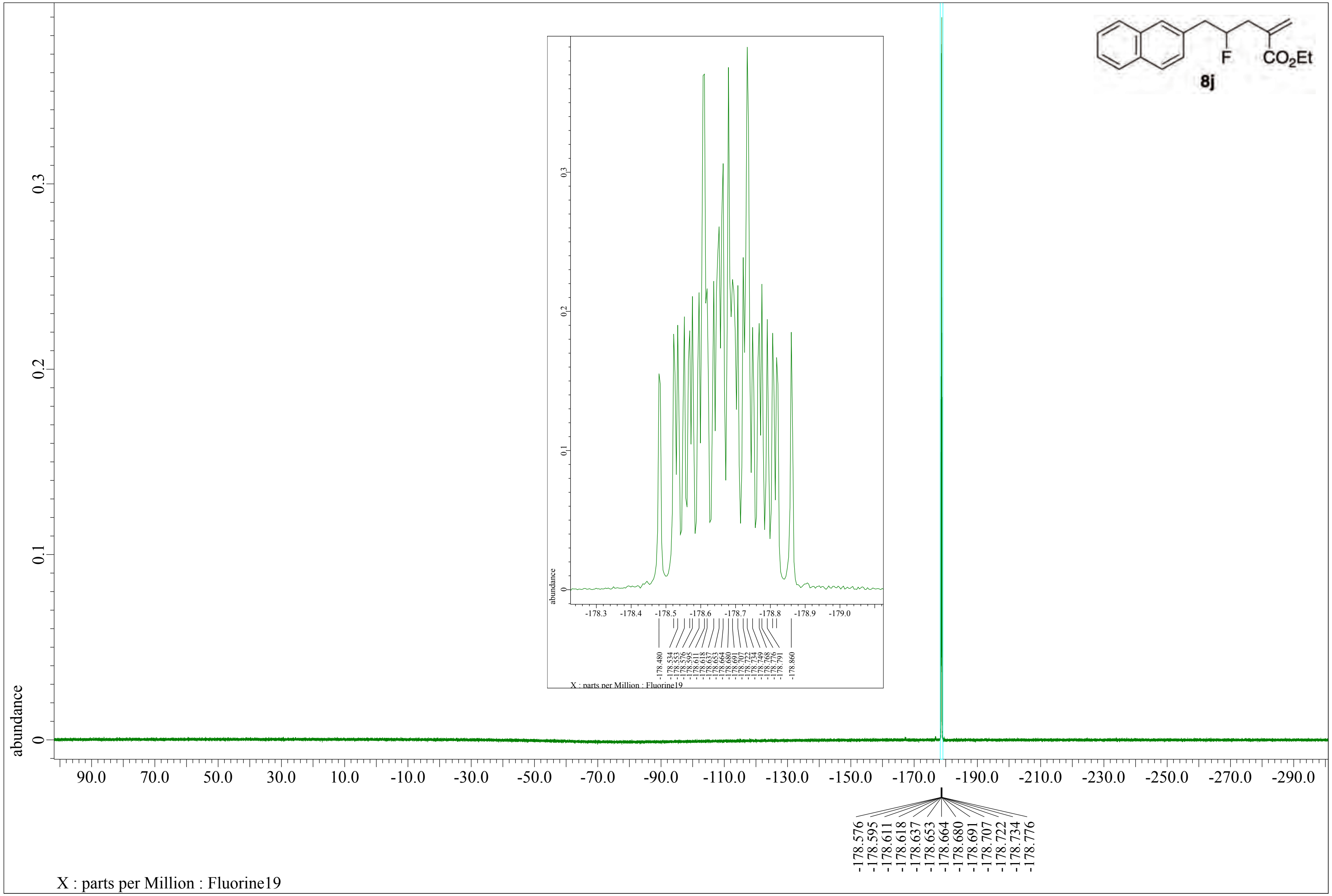
231838_8i_pn #29-32 RT: 0.47-0.50 AV: 2 NL: 3.55E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



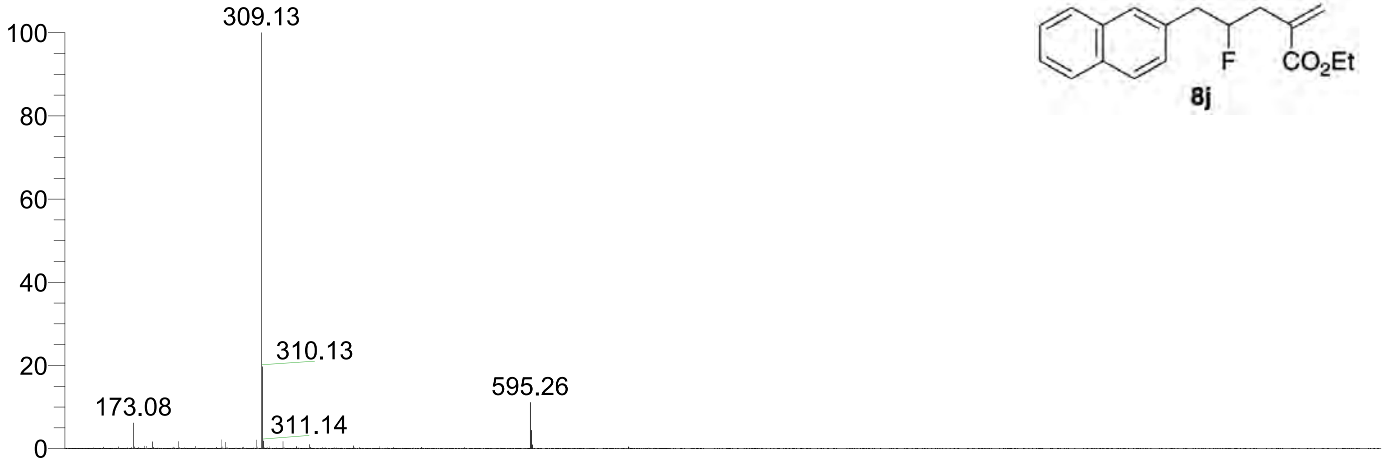

F
CO2Et
8j
abundance
X : parts per Million : Proton
2.95
0.99
1.96
0.96
2.03
1.00
2.03
1.97
1.98
3.10
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.840
7.832
7.819
7.799
7.702
7.483
7.479
7.473
7.466
7.459
7.398
7.396
6.312
5.719
5.095
5.086
5.077
5.069
4.974
4.965
4.956
4.947
4.236
4.218
4.198
4.182
3.179
3.162
3.148
3.129
3.111
3.095
3.084
2.801
2.795
2.765
2.758
2.688
2.676
2.668
2.650
2.630
1.300
1.282
1.265



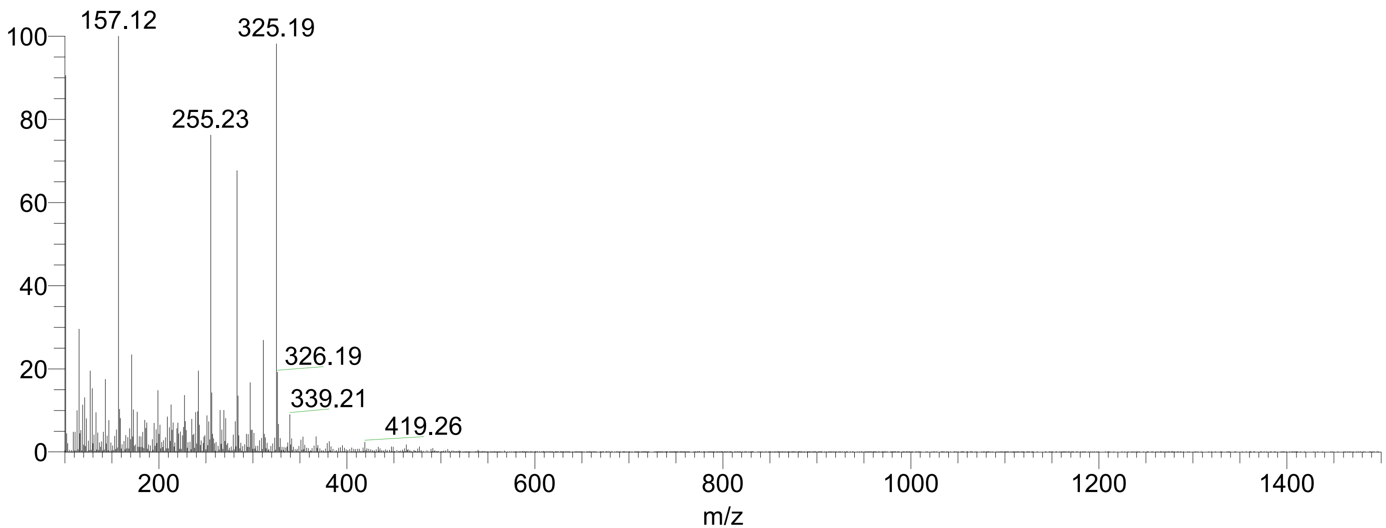
8j
F
CO2Et
(thousandths)
X : parts per Million : Carbon13
166.864
136.084
136.055
134.570
134.532
133.612
132.443
128.188
128.159
128.092
127.834
127.747
127.690
126.157
125.668
93.336
91.611
77.476
77.160
76.844
60.984
41.828
41.618
37.756
37.535
14.269


8j
F
CO2Et
abundance
X : parts per Million : Fluorine19
-178.576
-178.595
-178.611
-178.618
-178.637
-178.653
-178.664
-178.680
-178.691
-178.707
-178.722
-178.734
-178.776

Sample No. : C:\Xcalibur\...\1228\BG_231839_8j_,
Instrument : Exactive Plus
Mobile phase solvent : MeOH
Operator name : hayashi harumi
Sample solvent : CHCl3
Date : 12/28/23 14:01:42
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University



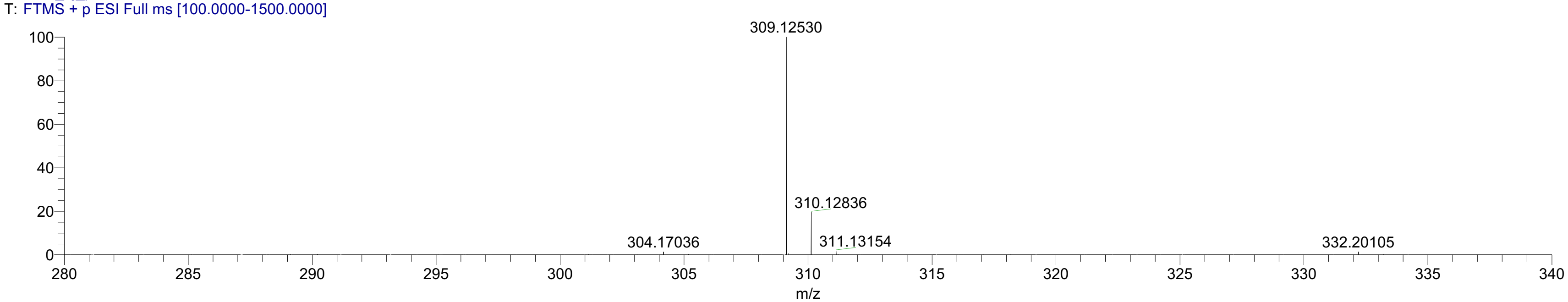
NL: 5.06E8
BG_231839_8j_pn#19
-32 RT: 0.31-0.48
AV: 7 T: FTMS + c
ESI Full ms
[100.00-1500.00]



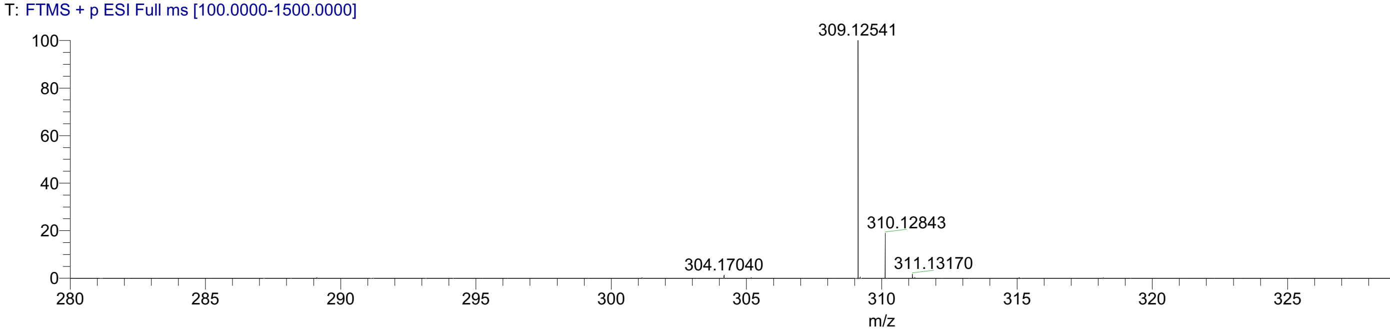
NL: 4.54E6
BG_231839_8j_pn#19
-32 RT: 0.32-0.50
AV: 7 T: FTMS - c ESI
Full ms
[100.00-1500.00]

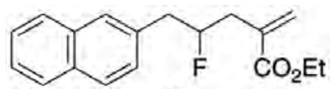
Sample No. : C:\Xcalibur\...\202312\1228\231839_8j_pn Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 10:32:46
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

231839_8j_pn #22-25 RT: 0.37-0.39 AV: 2 NL: 1.91E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



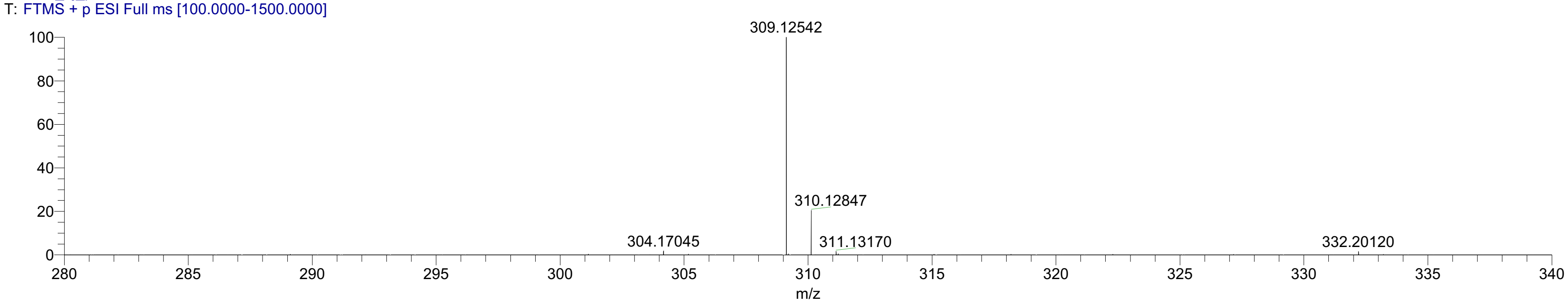
231839_8j_pn #25-29 RT: 0.39-0.45 AV: 3 NL: 1.49E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

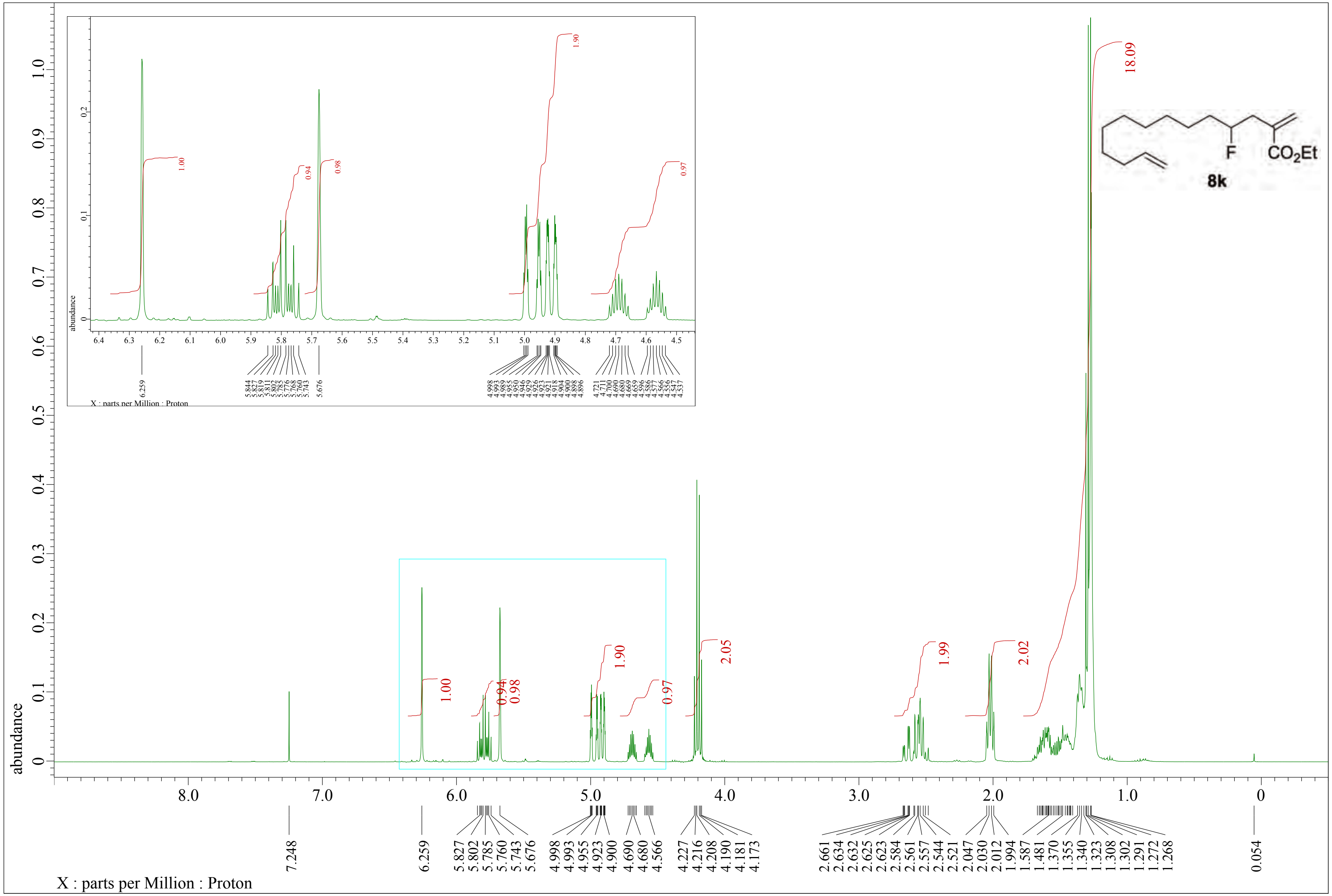


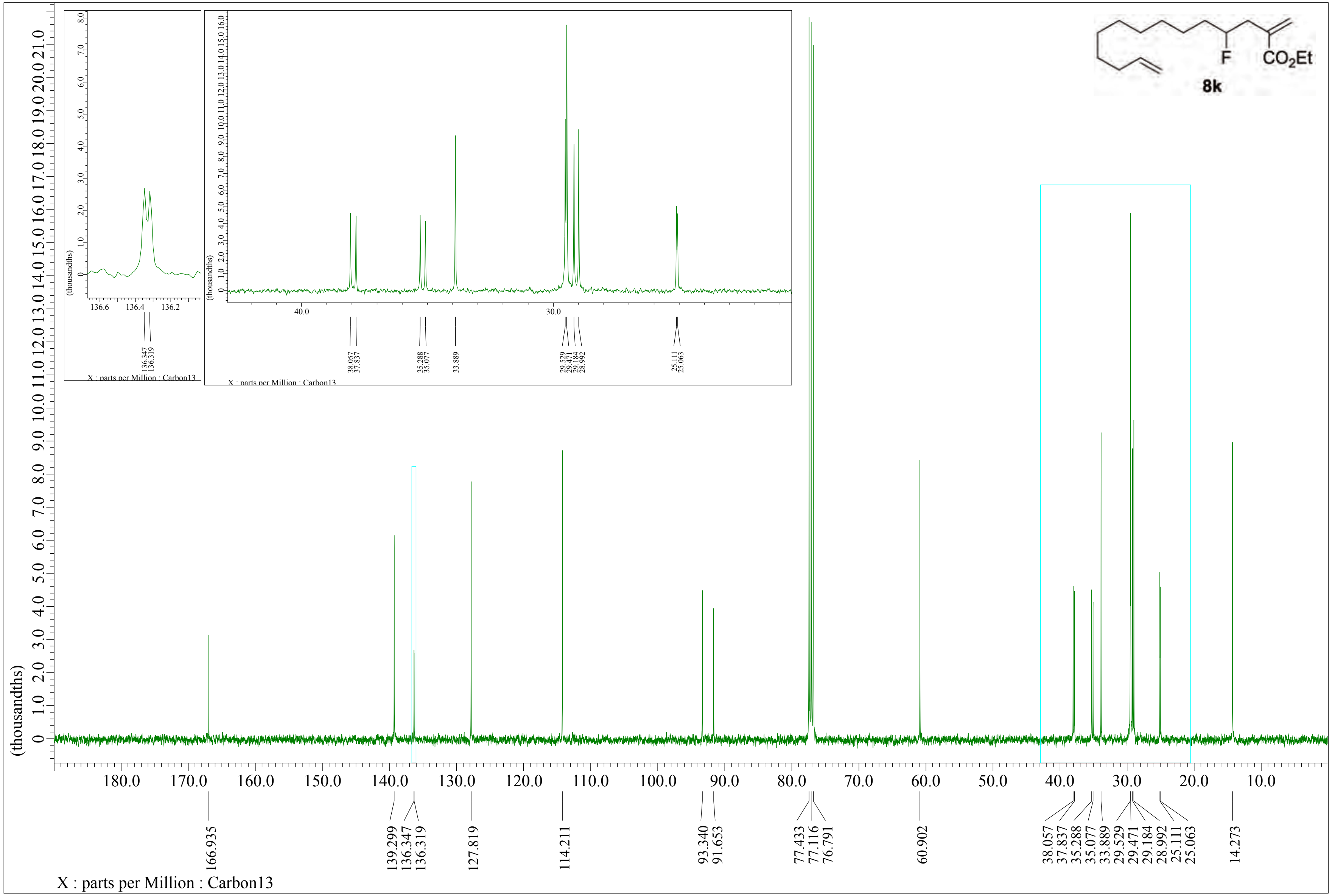


8j

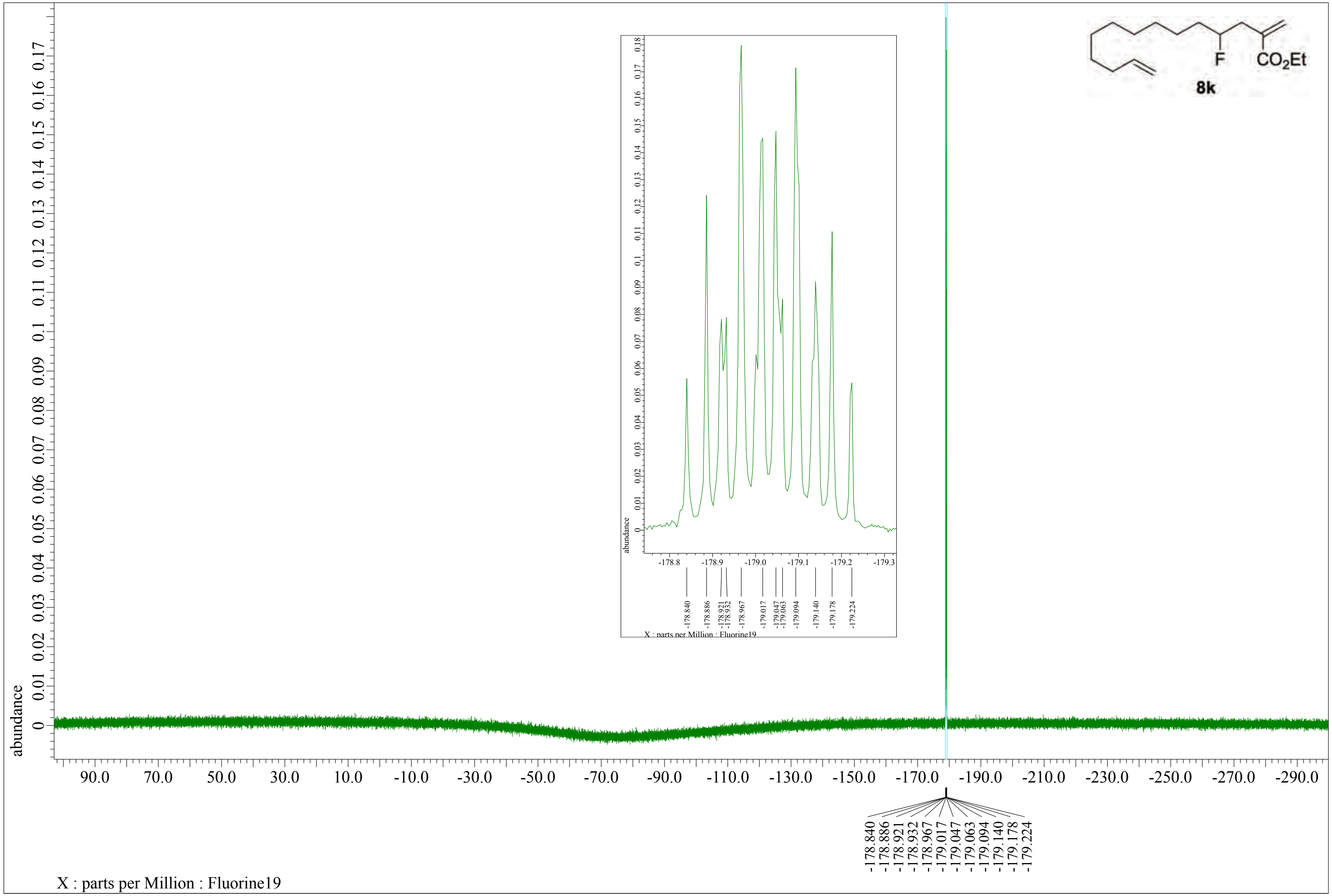
231839_8j_pn #29-32 RT: 0.45-0.48 AV: 2 NL: 7.30E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]




8k
F
CO2Et
abundance
X : parts per Million : Proton
18.09
2.05
1.99
2.02
1.90
1.00
0.94
0.98
0.97



8k
F
CO2Et
(thousandths)
X : parts per Million : Carbon13
166.935
139.299
136.347
136.319
127.819
114.211
93.340
91.653
77.433
77.116
76.791
60.902
38.057
37.837
35.288
35.077
33.889
29.529
29.471
29.184
28.992
25.111
25.063
14.273



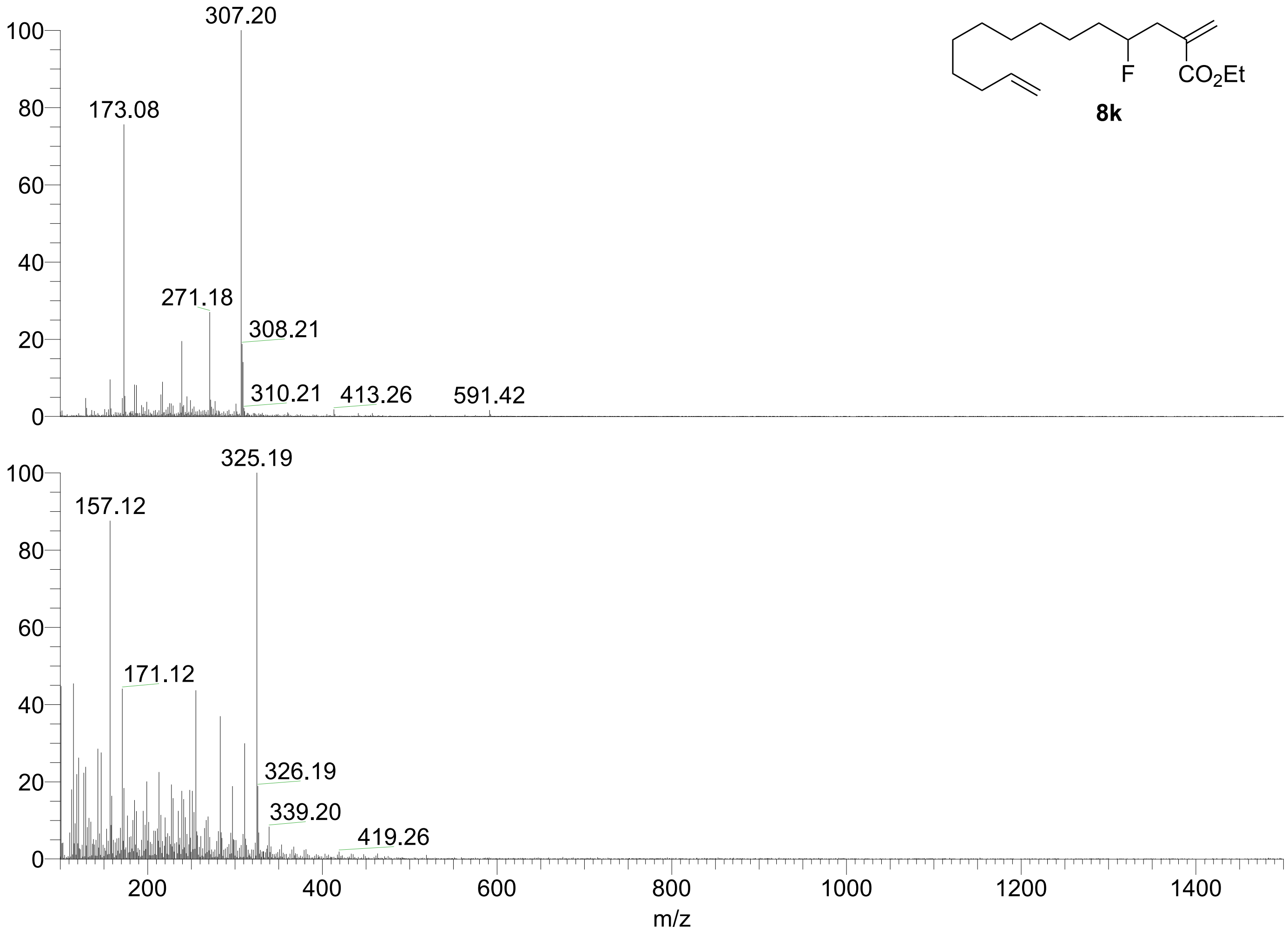
CO2Et
F
8k
abundance
X : parts per Million : Fluorine19
-178.840
-178.886
-178.921
-178.932
-178.967
-179.017
-179.047
-179.063
-179.094
-179.140
-179.178
-179.224

Sample No. : C:\Xcalibur\...\1228\BG_231840_8l _,
Instrument : Exactive Plus
Mobile phase solvent : MeOH
Operator name : hayashi harumi
Sample solvent : CHCl3
Date : 12/28/23 14:02:08
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

8k

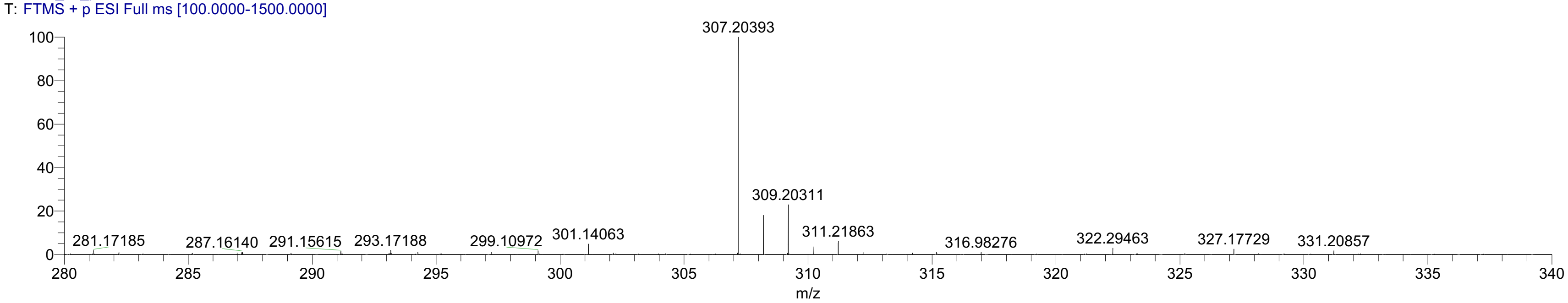
NL: 2.52E7
BG_231840_8k_pn#1
8-31 RT: 0.31-0.50
AV: 7 T: FTMS + c
ESI Full ms
[100.00-1500.00]

NL: 1.63E6
BG_231840_8k_pn#1
8-31 RT: 0.30-0.48
AV: 7 T: FTMS - c ESI
Full ms
[100.00-1500.00]

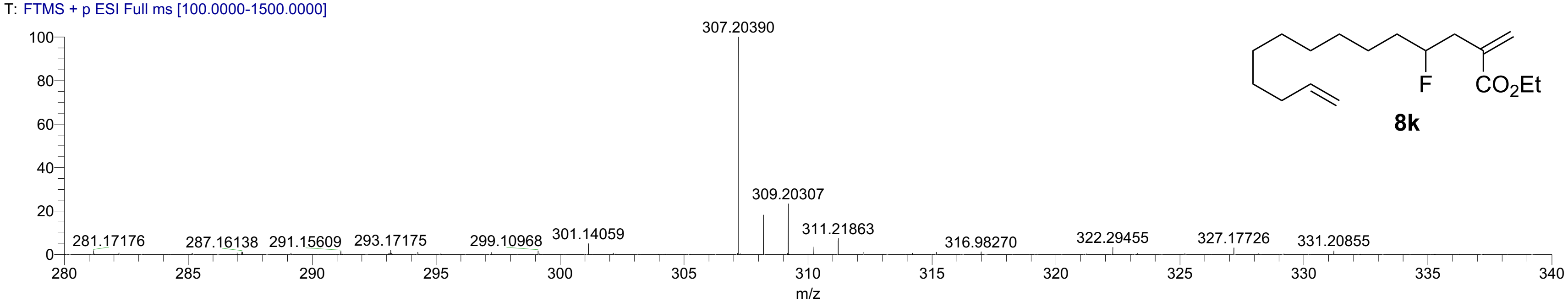


Sample No. : C:\Xcalibur\...\20231228\231840_8k_pn   Instrument : Exactive Plus   Mobile phase solvent : MeOH
Operator name : hayashi harumi   Sample solvent : CHCl3
Date : 12/28/23 10:38:14
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

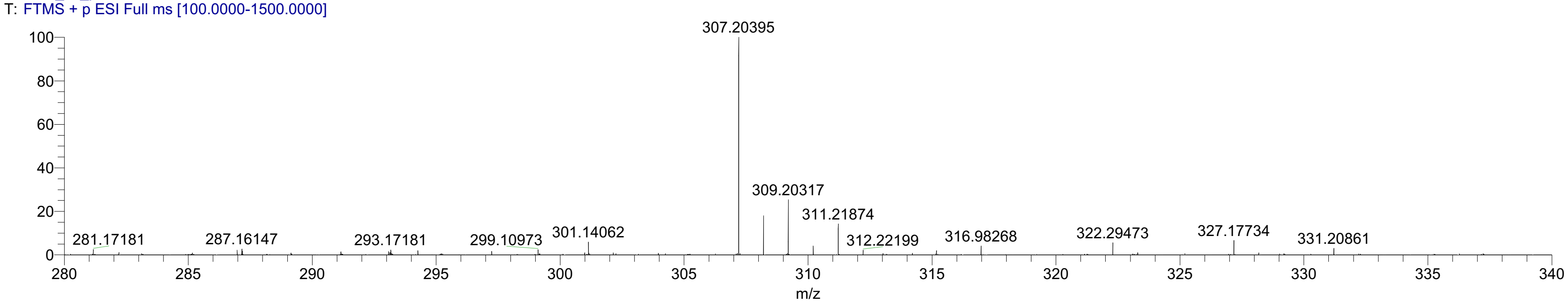
231840_8k_pn #21-25 RT: 0.35-0.41 AV: 3 NL: 9.91E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

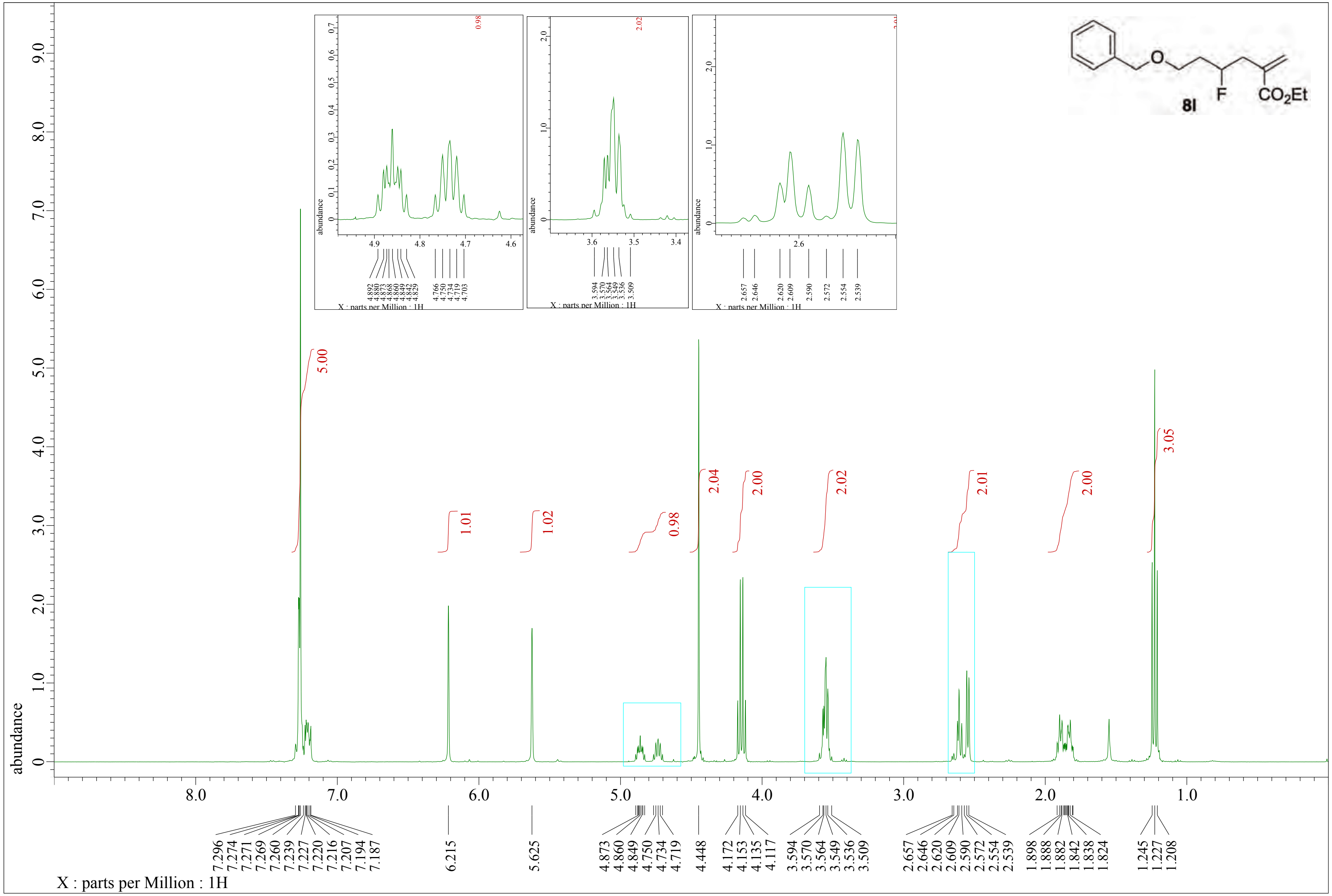


231840_8k_pn #25-28 RT: 0.41-0.44 AV: 2 NL: 8.06E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

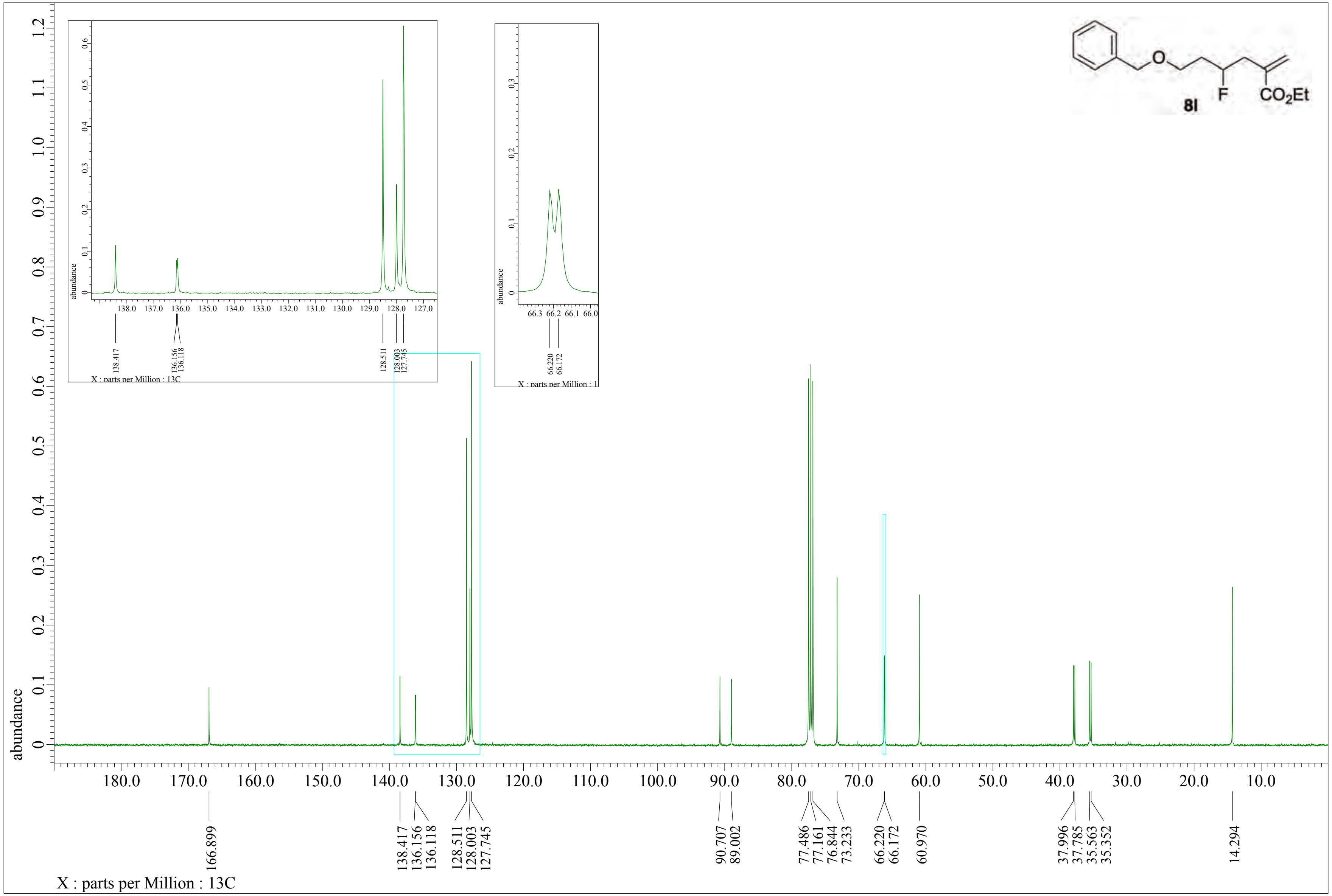


231840_8k_pn #28-31 RT: 0.47-0.50 AV: 2 NL: 2.79E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

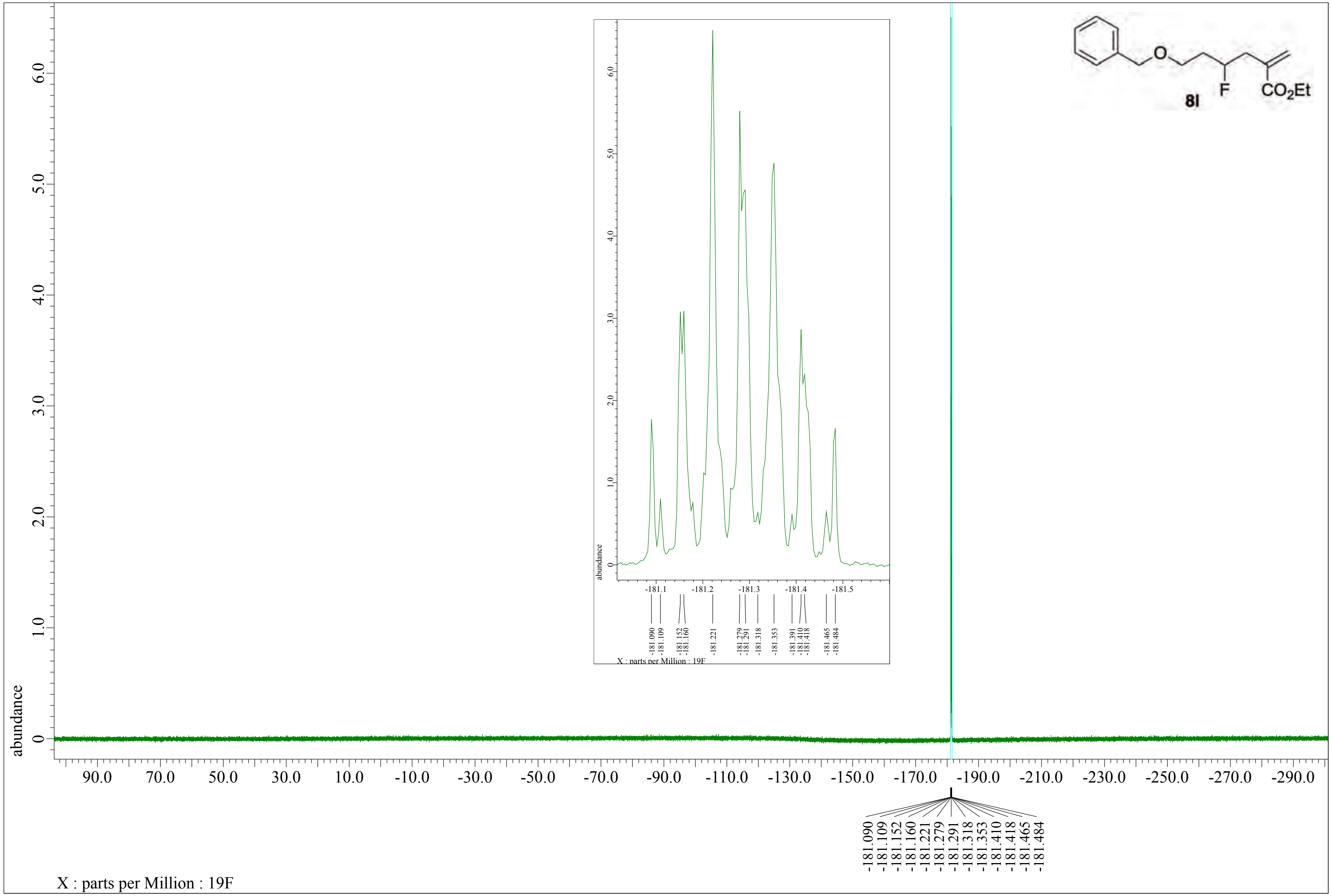




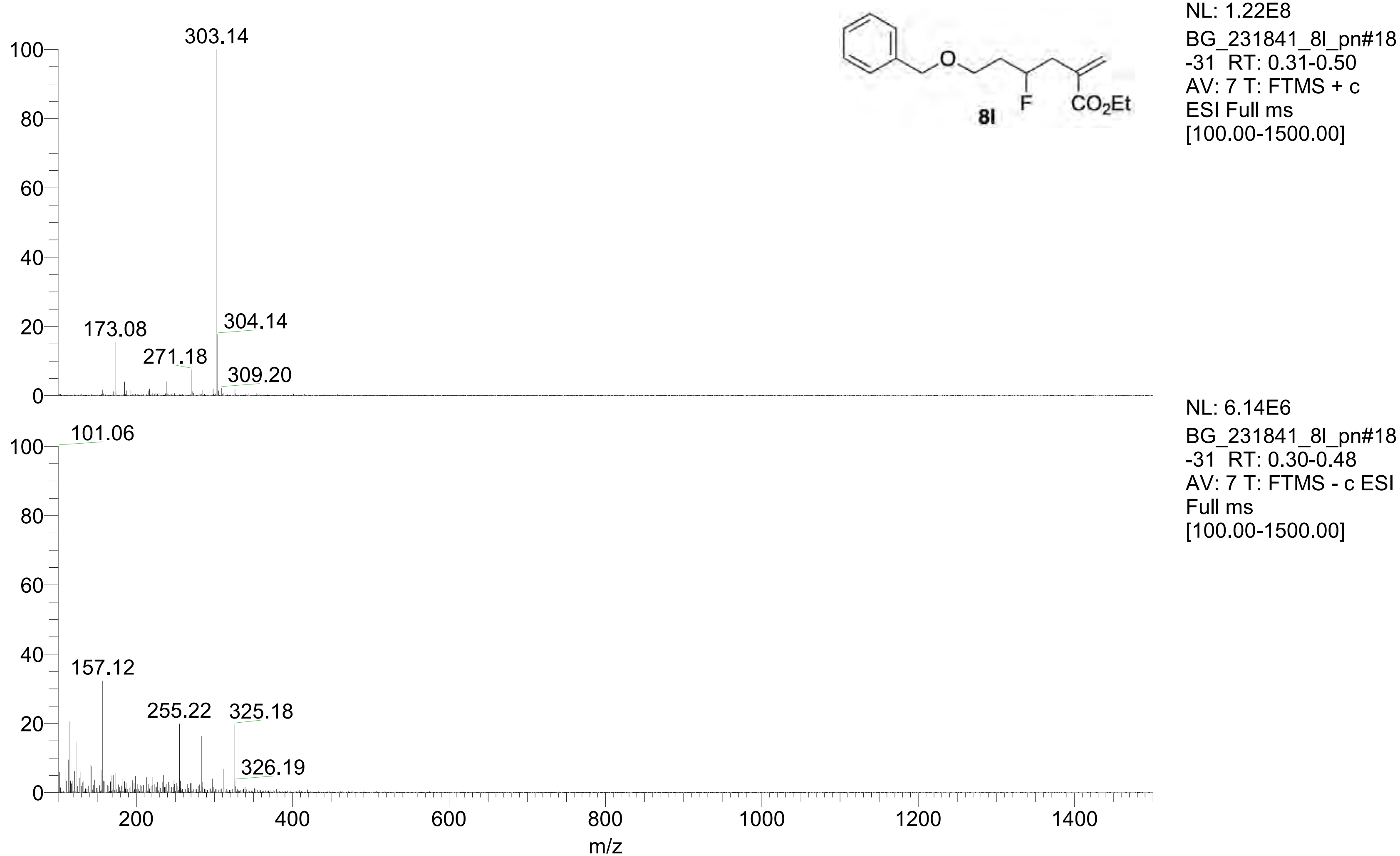
8l
F
CO2Et
O
abundance
X : parts per Million : 1H
5.00
1.01
1.02
0.98
2.04
2.00
2.02
2.01
2.00
3.05
7.296 7.274 7.271 7.269 7.260 7.239 7.227 7.220 7.216 7.207 7.194 7.187
6.215
5.625
4.873 4.860 4.849 4.750 4.734 4.719
4.448
4.172 4.153 4.135 4.117
3.594 3.570 3.564 3.549 3.536 3.509
2.657 2.646 2.620 2.609 2.590 2.572 2.554 2.539
1.898 1.888 1.882 1.842 1.838 1.824
1.245 1.227 1.208



8l
F
CO_2Et
abundance
X : parts per Million : 13C
166.899
138.417
136.156
136.118
128.511
128.003
127.745
90.707
89.002
77.486
77.161
76.844
73.233
66.220
66.172
60.970
37.996
37.785
35.563
35.352
14.294

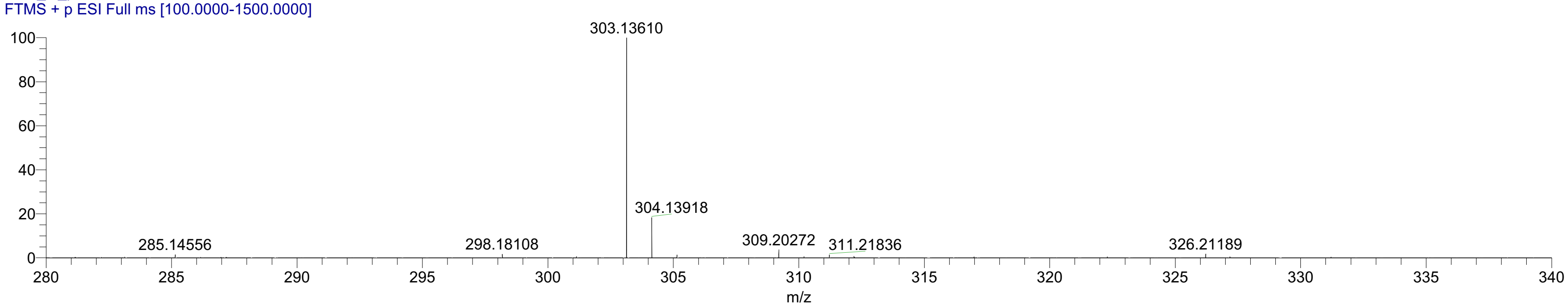

8l
F
CO2Et
abundance
X : parts per Million : 19F
-181.090
-181.109
-181.152
-181.160
-181.221
-181.279
-181.291
-181.318
-181.353
-181.410
-181.418
-181.465
-181.484

Sample No. : C:\Xcalibur\...\1228\BG_231841_8l_,   Instrument : Exactive Plus   Mobile phase solvent : MeOH
Operator name : hayashi harumi   Sample solvent : CHCl3
Date : 12/28/23 14:02:33
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

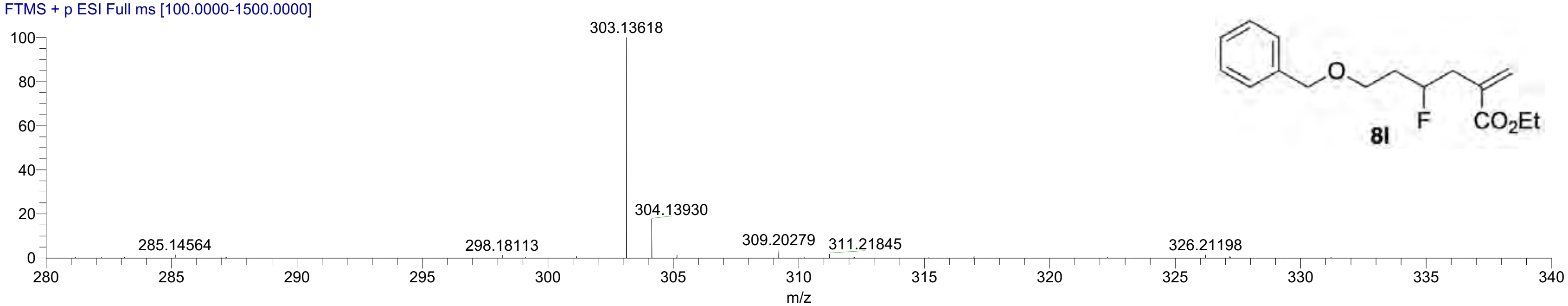


Sample No. : C:\Xcalibur\...\202312\1228\231841_8l_pn Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 10:43:44
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

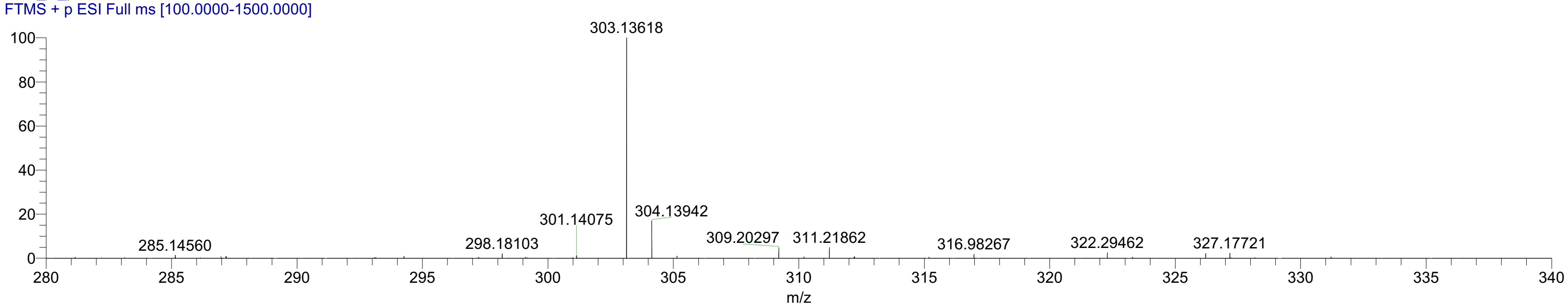
231841_8l_pn #21-25 RT: 0.34-0.40 AV: 3 NL: 4.53E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

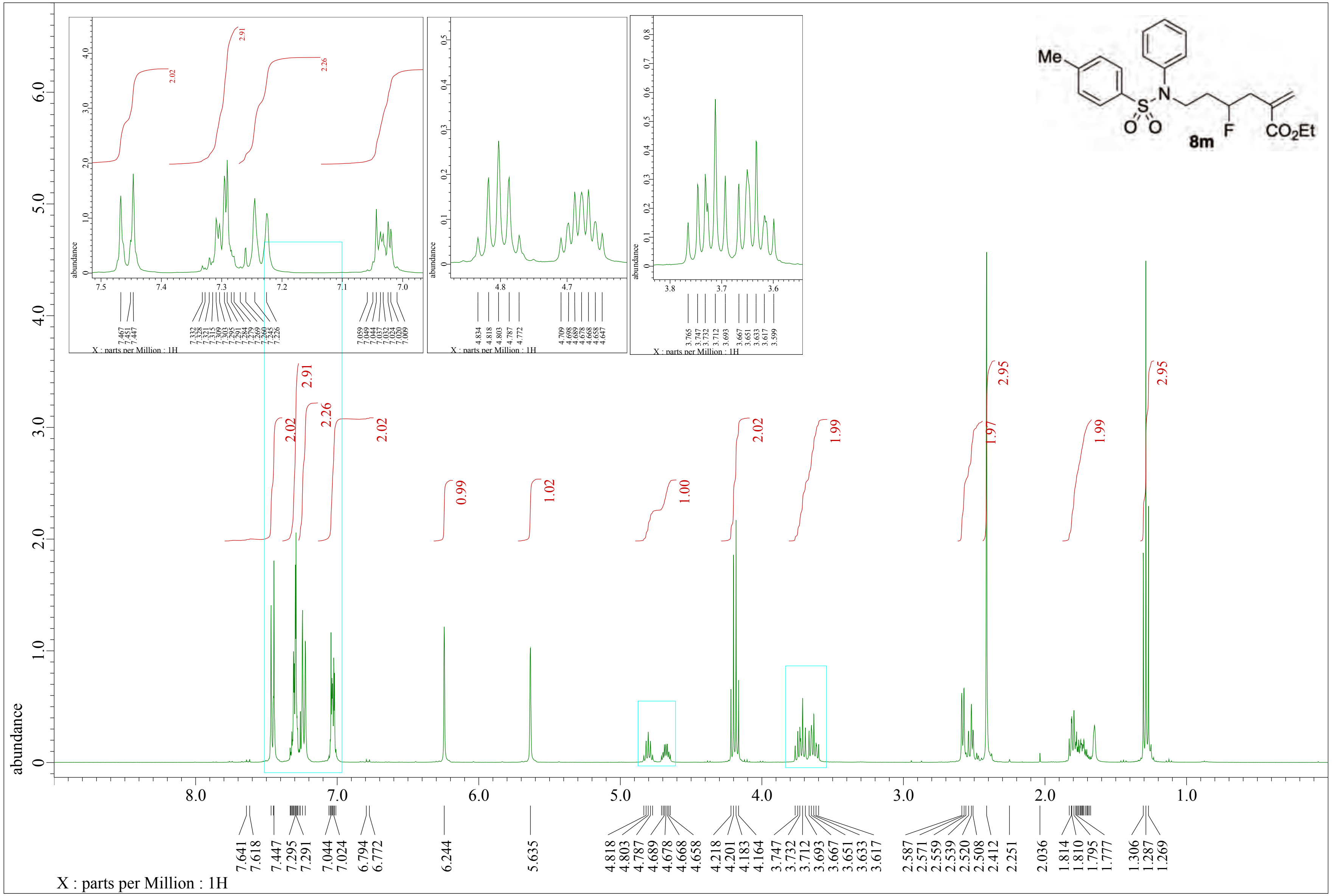


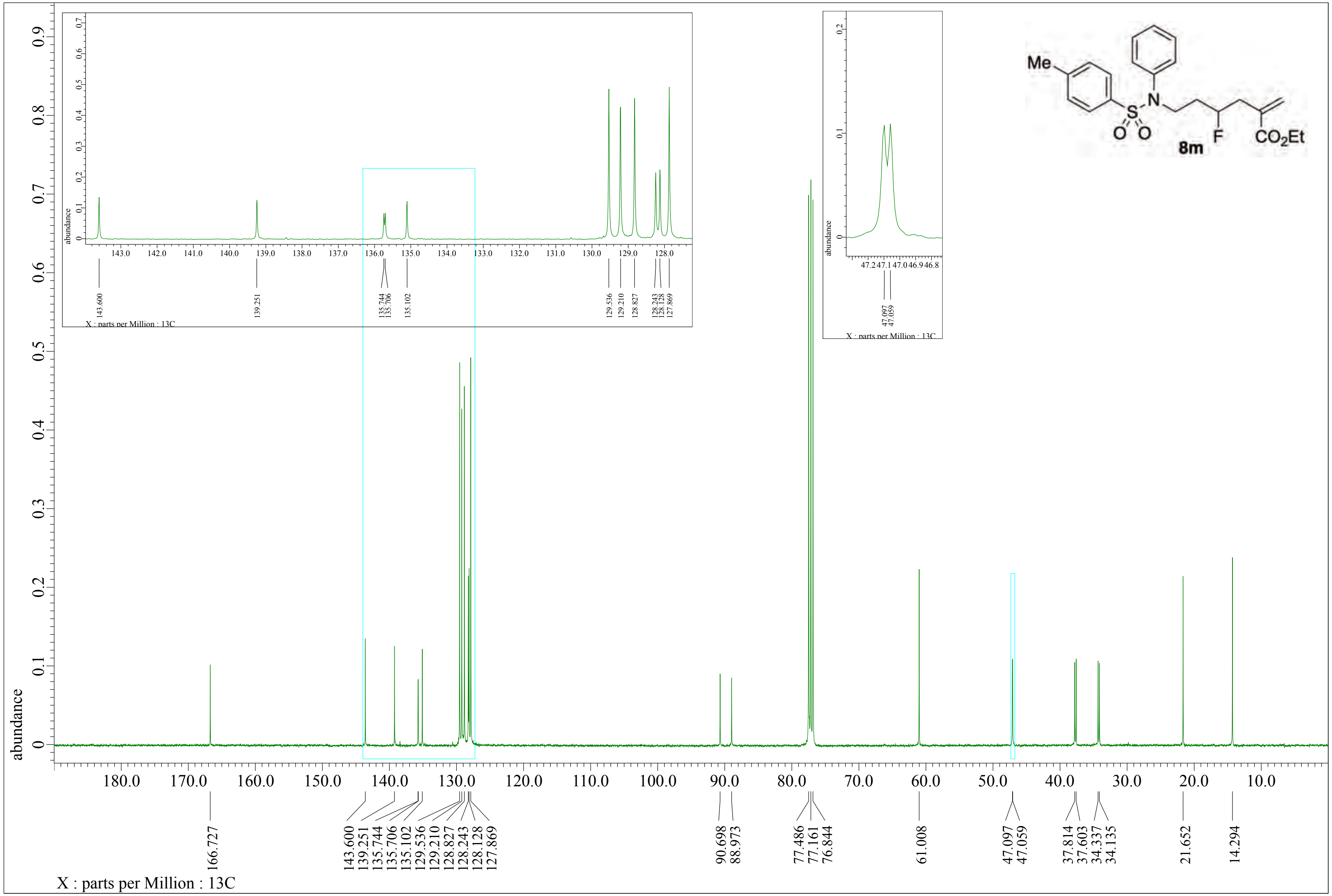
231841_8l_pn #25-28 RT: 0.40-0.43 AV: 2 NL: 3.39E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



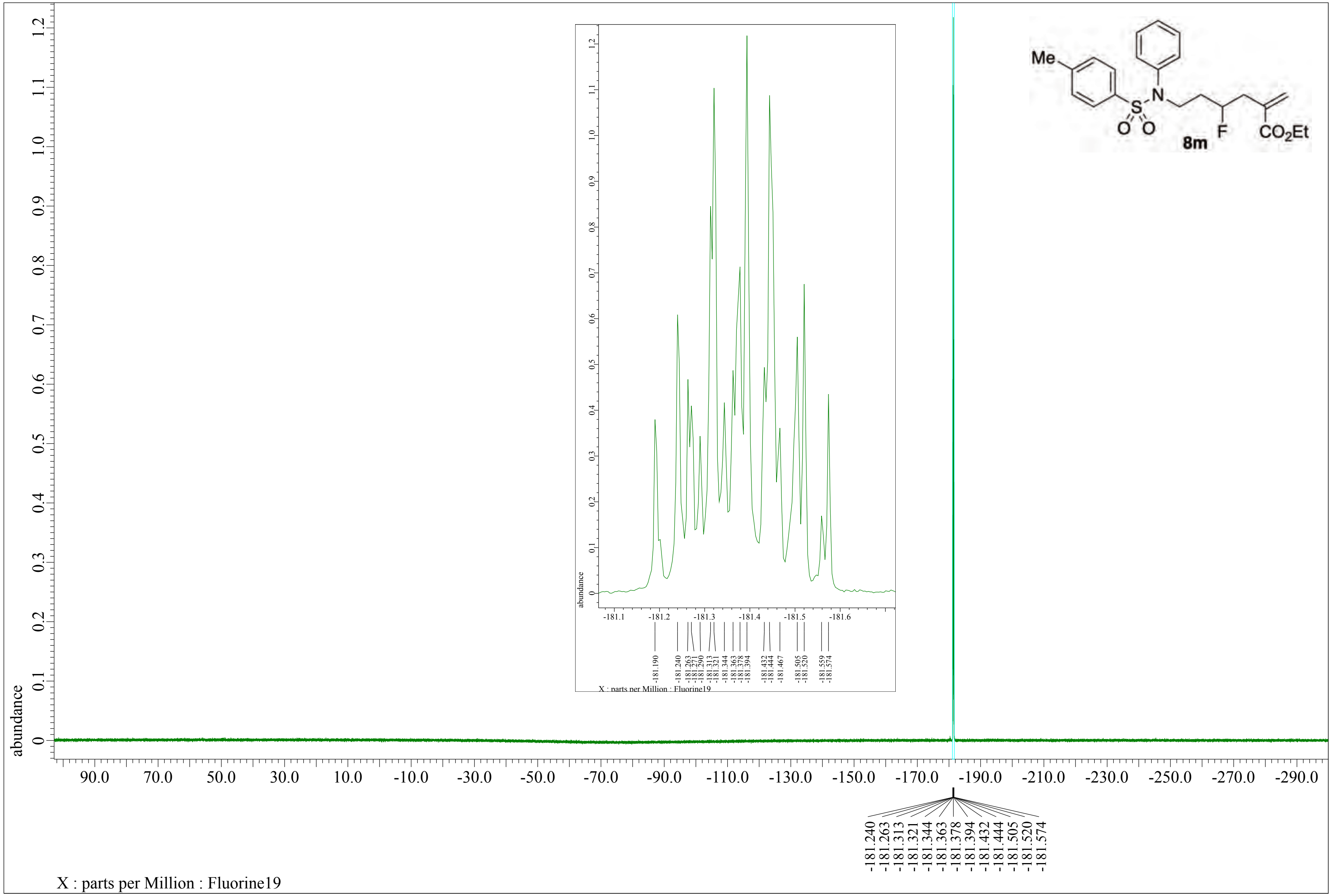
231841_8l_pn #28-31 RT: 0.47-0.50 AV: 2 NL: 1.25E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]




Me
S
N
O O
F
CO2Et
8m
abundance
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
2.02
2.91
2.26
2.02
0.99
1.02
1.00
2.02
1.99
1.97
2.95
1.99
2.95
7.641
7.618
7.447
7.295
7.291
7.044
7.024
6.794
6.772
6.244
5.635
4.818
4.803
4.787
4.689
4.678
4.668
4.658
4.218
4.201
4.183
4.164
3.747
3.732
3.712
3.693
3.667
3.651
3.633
3.617
2.587
2.571
2.559
2.539
2.520
2.508
2.412
2.251
2.036
1.814
1.810
1.795
1.777
1.306
1.287
1.269

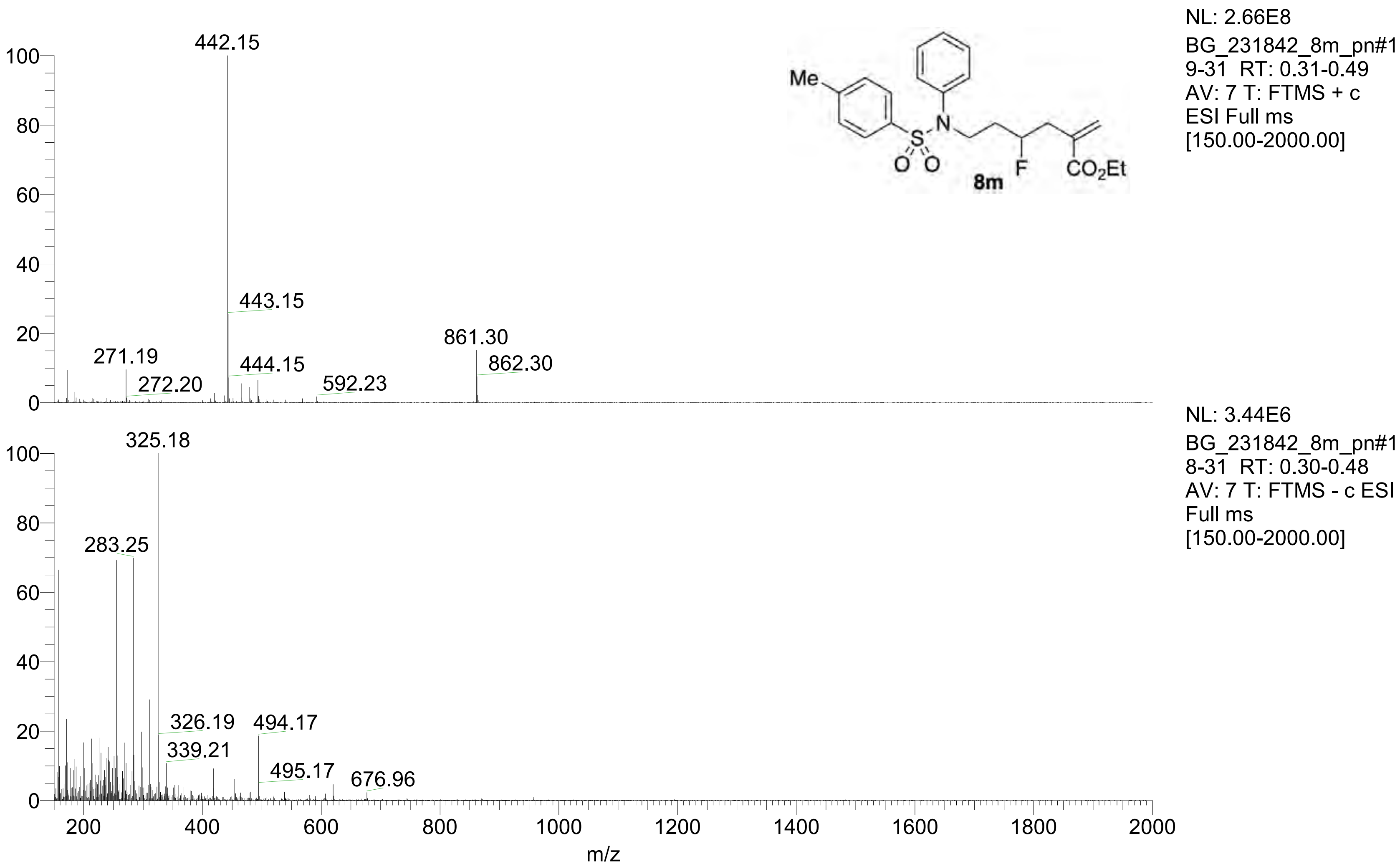


Me
N
S
O O
F
CO_2Et
8m
abundance
X : parts per Million : 13C
166.727
143.600
139.251
135.744
135.706
135.102
129.536
129.210
128.827
128.243
128.128
127.869
90.698
88.973
77.486
77.161
76.844
61.008
47.097
47.059
37.814
37.603
34.337
34.135
21.652
14.294



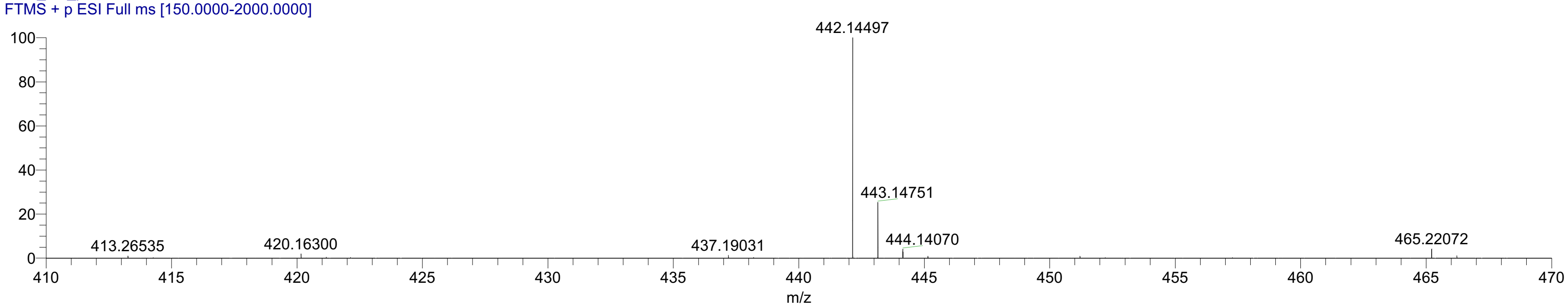
8m
abundance
X : parts per Million : Fluorine19
-181.240
-181.263
-181.313
-181.321
-181.344
-181.363
-181.378
-181.394
-181.432
-181.444
-181.505
-181.520
-181.574

Sample No. : C:\Xcalibur\...\1228\BG_231842_8ı _, Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 14:26:14
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

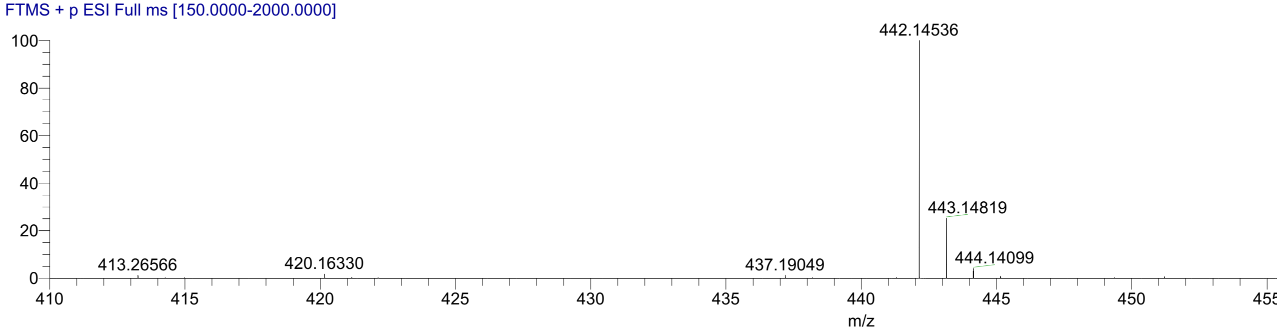


Sample No. : C:\Xcalibur\...\2023121228\231842_8m_pn   Instrument : Exactive Plus   Mobile phase solvent : MeOH
Operator name : hayashi harumi   Sample solvent : CHCl3
Date : 12/28/23 10:48:44
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

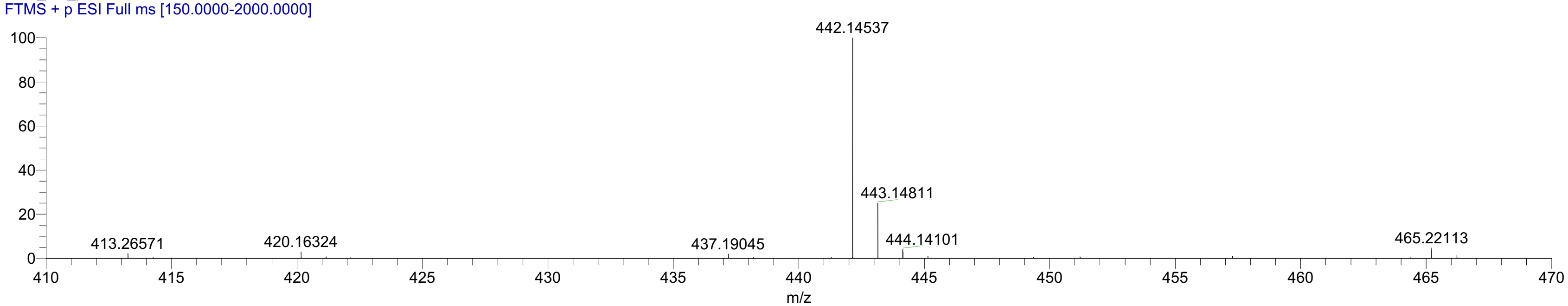
231842_8m_pn #22-25 RT: 0.37-0.40 AV: 2 NL: 1.12E8
T: FTMS + p ESI Full ms [150.0000-2000.0000]

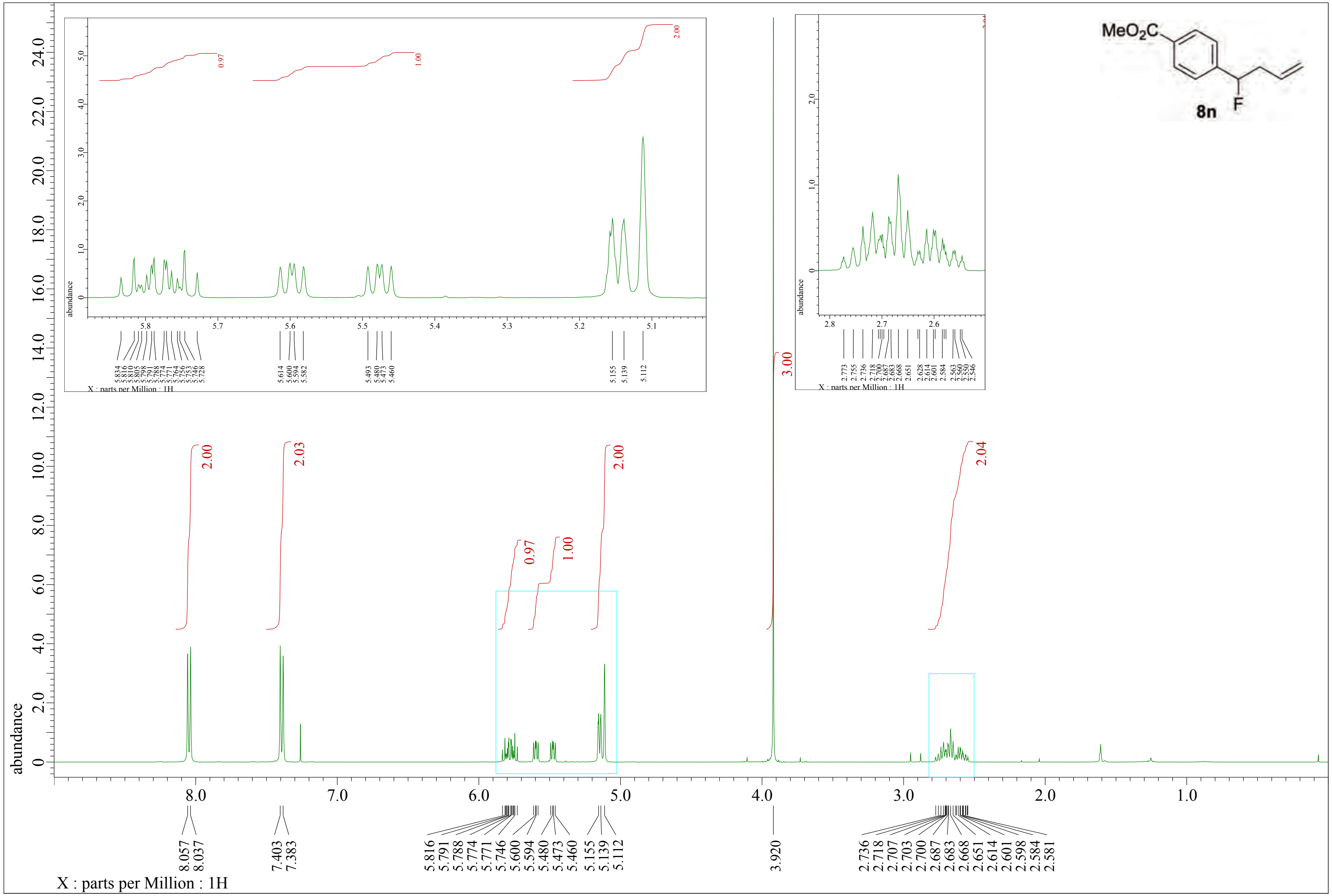


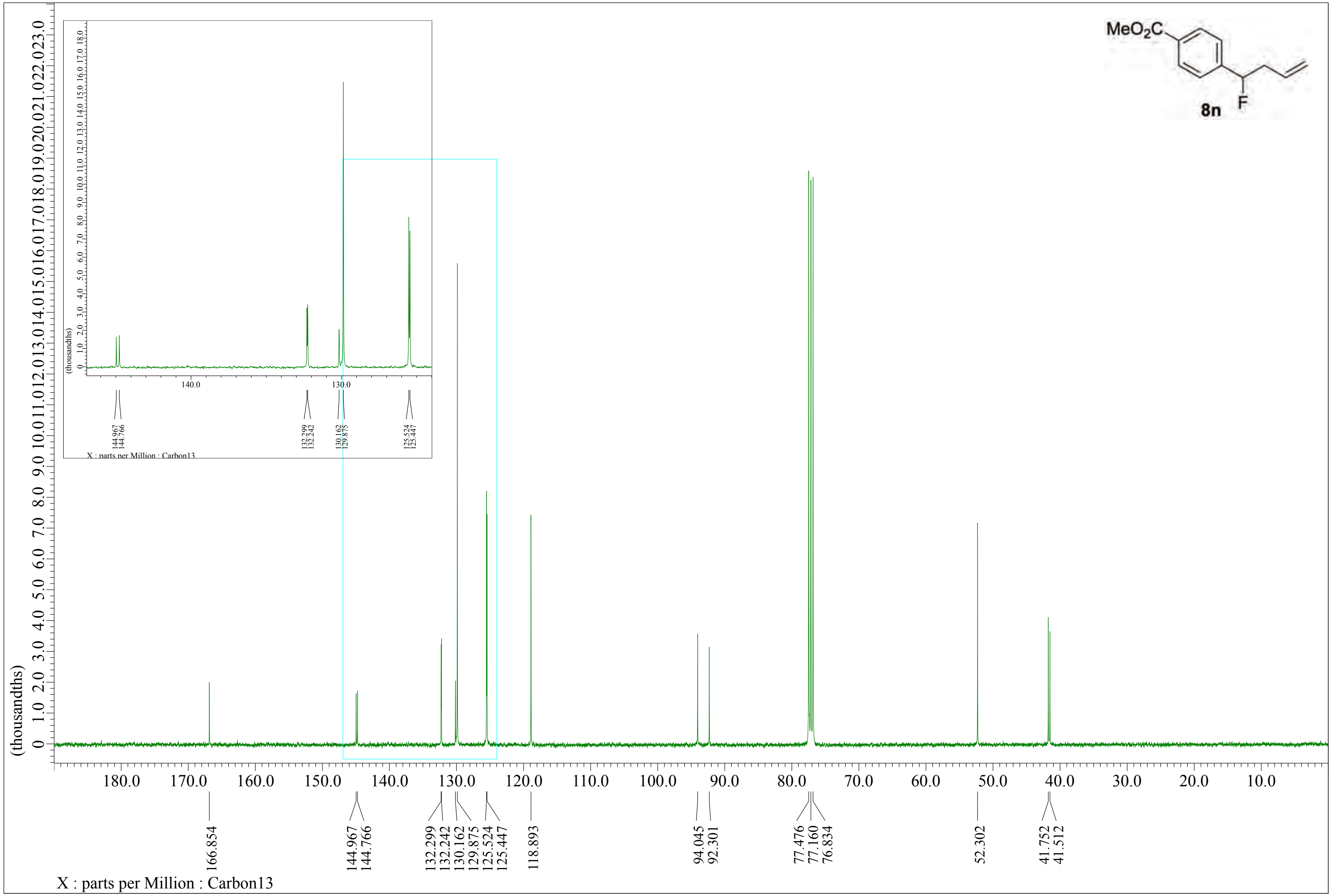
231842_8m_pn #26 RT: 0.43 AV: 1 NL: 7.16E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]

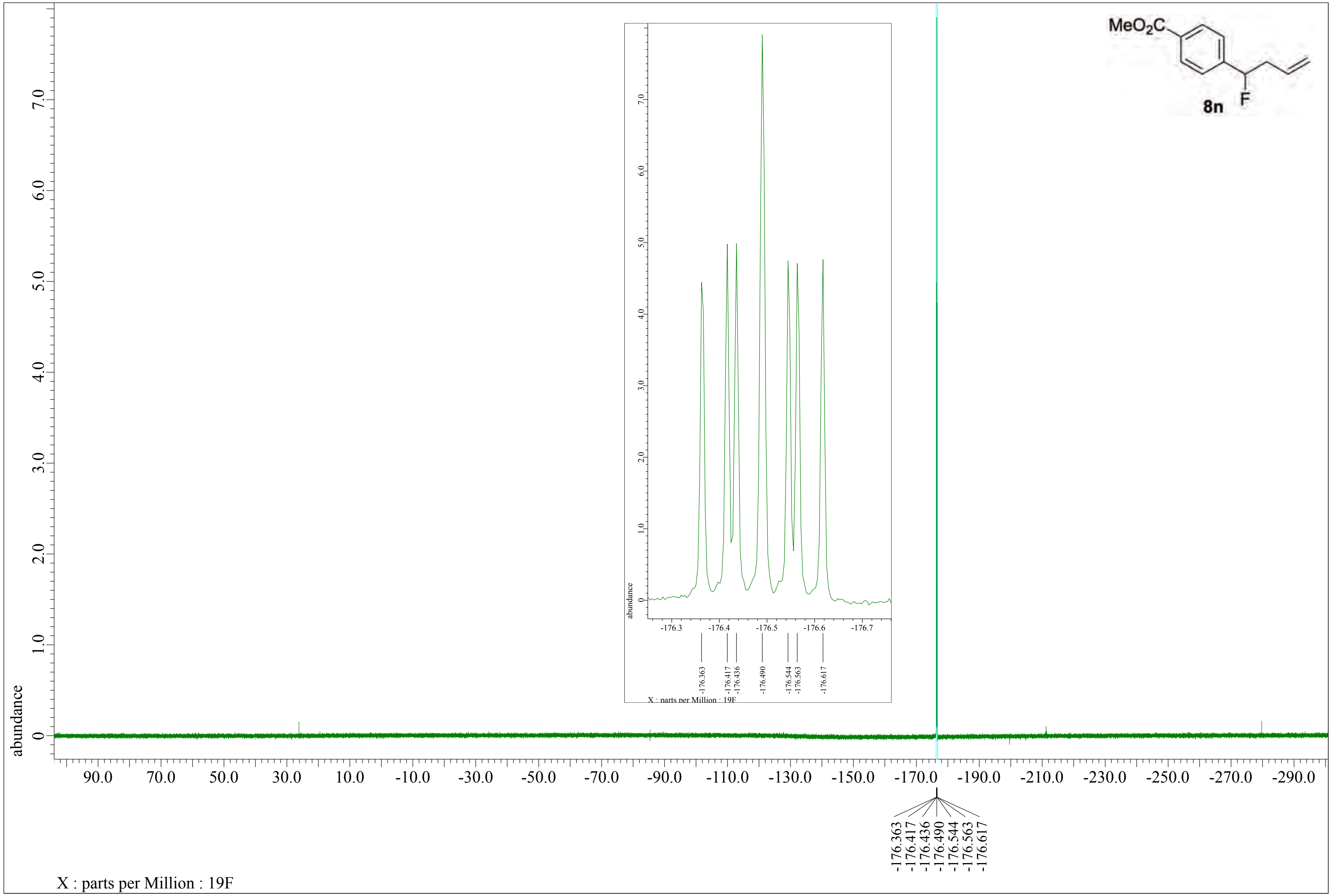


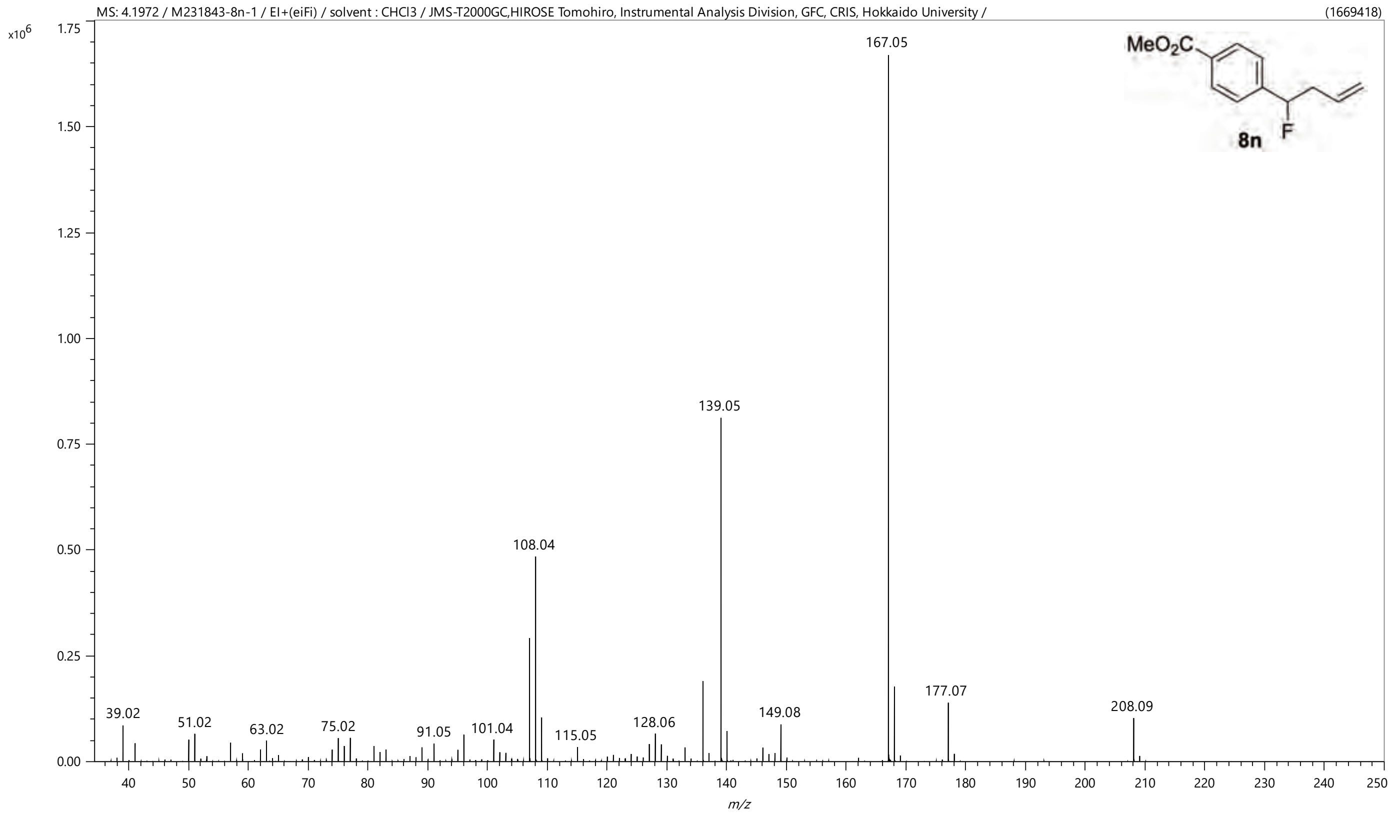
231842_8m_pn #29-32 RT: 0.46-0.49 AV: 2 NL: 4.63E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]

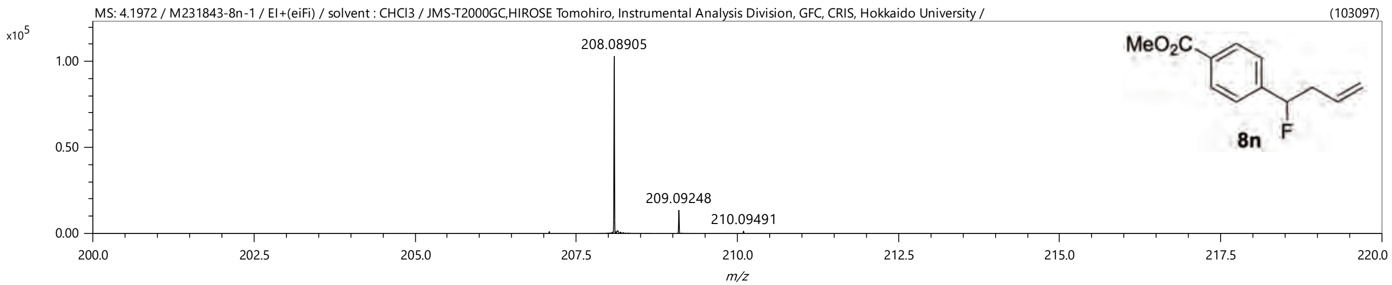


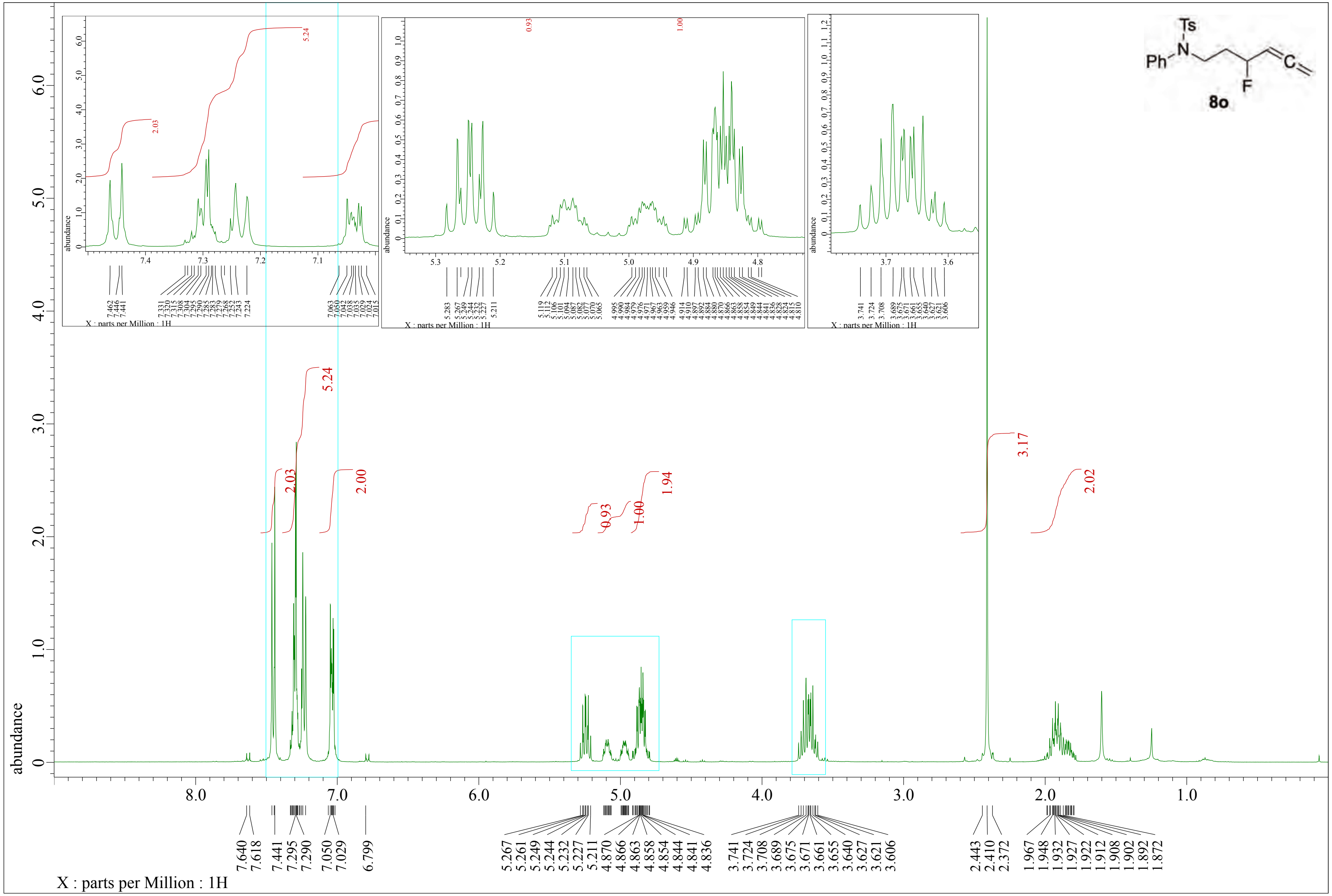

MeO2C
8n
F
X : parts per Million : 1H
abundance
8.057
8.037
7.403
7.383
3.920
2.00
2.03
0.97
1.00
3.00
2.04


MeO2C
F
8n
(thousandths)
X : parts per Million : Carbon13
166.854
144.967
144.766
132.299
132.242
130.162
129.875
125.524
125.447
118.893
94.045
92.301
77.476
77.160
76.834
52.302
41.752
41.512

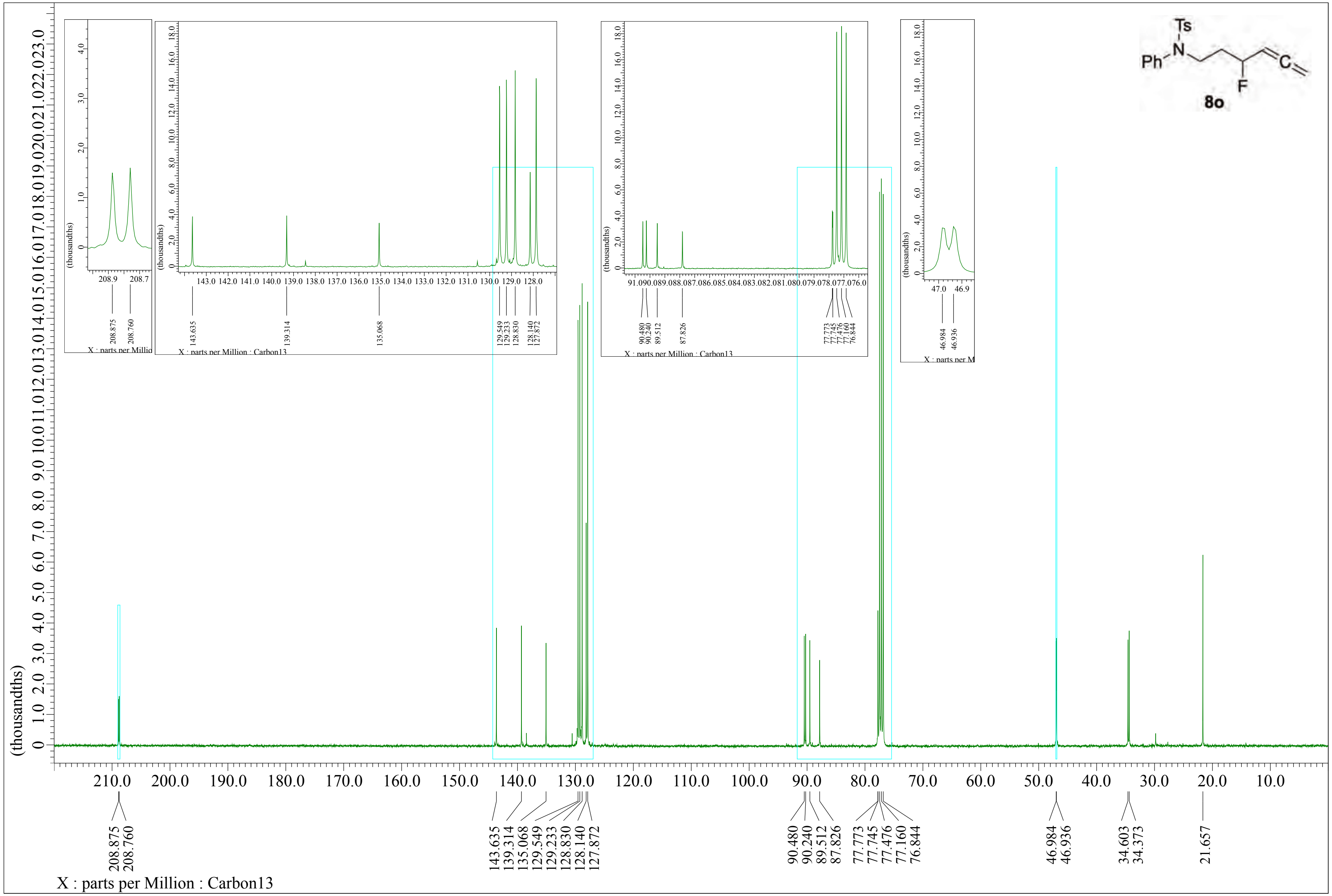

MeO2C
8n
F
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
90.0 70.0 50.0 30.0 10.0 -10.0 -30.0 -50.0 -70.0 -90.0 -110.0 -130.0 -150.0 -170.0 -190.0 -210.0 -230.0 -250.0 -270.0 -290.0
-176.363
-176.417
-176.436
-176.490
-176.544
-176.563
-176.617
X : parts per Million : 19F
-176.3 -176.4 -176.5 -176.6 -176.7


MS: 4.1972 / M231843-8n-1 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(1669418)
x10^6
167.05
139.05
108.04
39.02
51.02
63.02
75.02
91.05
101.04
115.05
128.06
149.08
177.07
208.09
m/z
MeO2C
8n
F

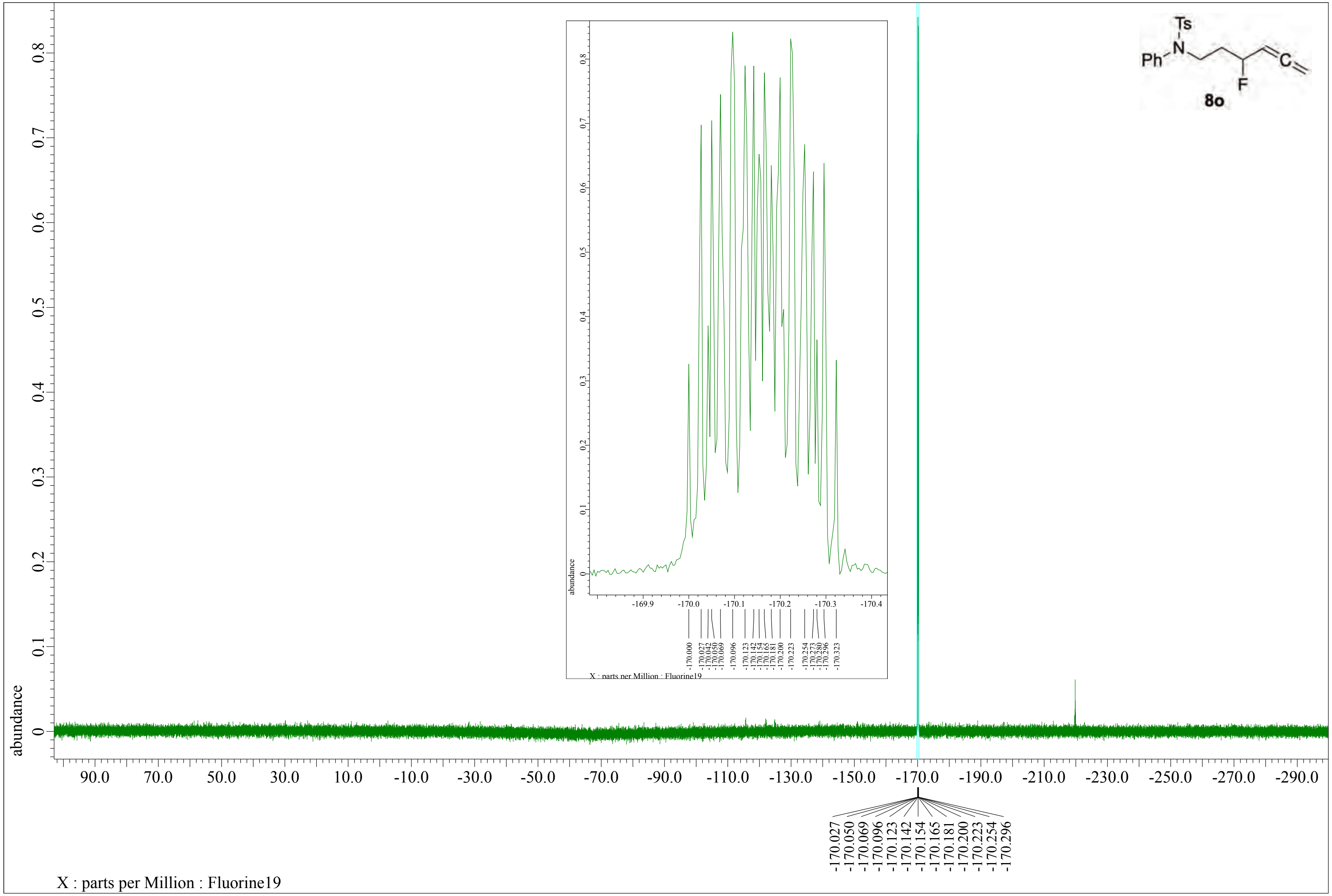

MS: 4.1972 / M231843-8n-1 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(103097)
x10^5
208.08905
209.09248
210.09491
m/z
MeO2C
8n
F



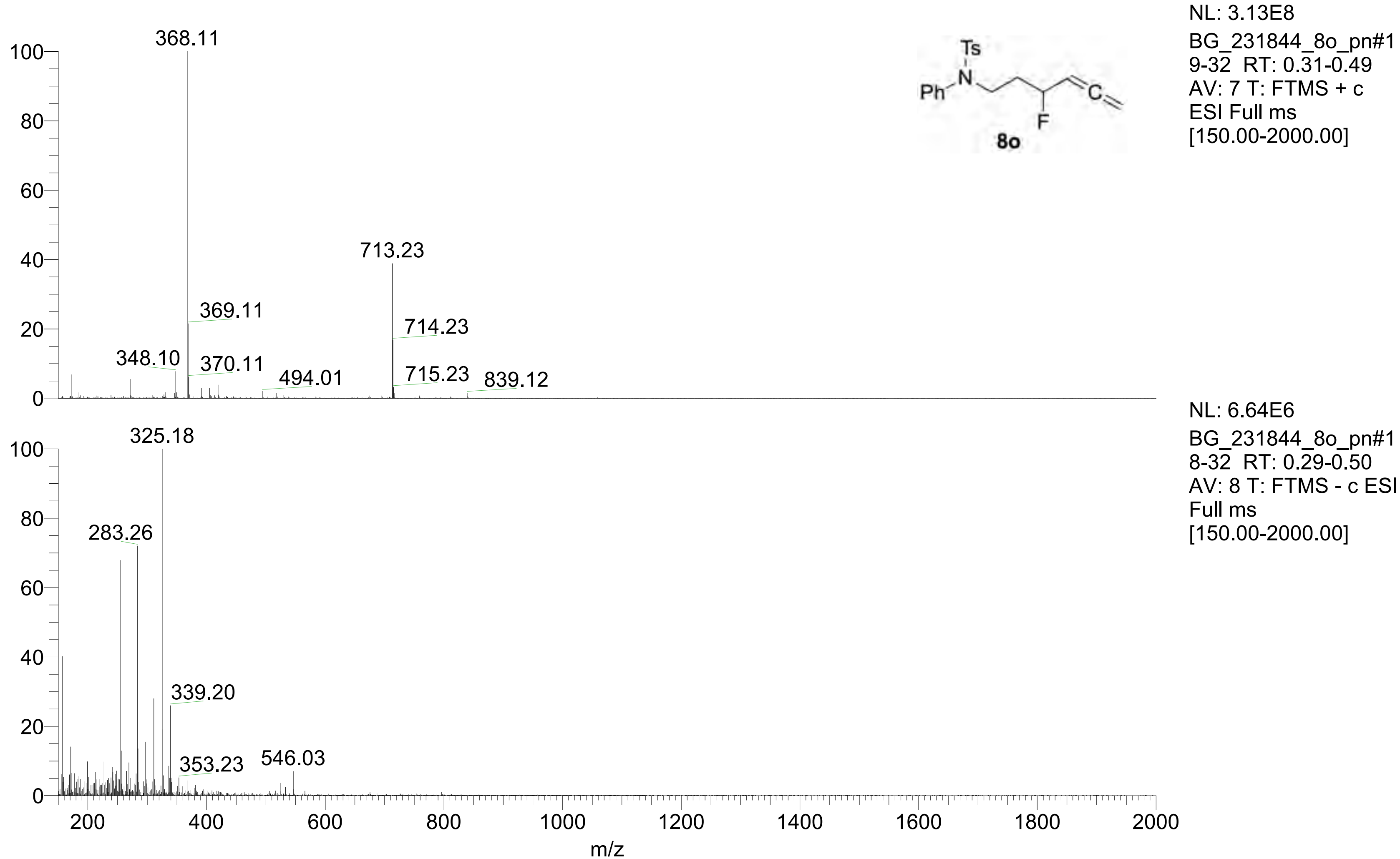
Ts
N
Ph
F
8o
abundance
X : parts per Million : 1H
5.24
2.03
2.00
0.93
1.00
1.94
3.17
2.02
7.640
7.618
7.441
7.295
7.290
7.050
7.029
6.799
5.267
5.261
5.249
5.244
5.232
5.227
5.211
4.870
4.866
4.863
4.858
4.854
4.844
4.841
4.836
3.741
3.724
3.708
3.689
3.675
3.671
3.661
3.655
3.640
3.627
3.621
3.606
2.443
2.410
2.372
1.967
1.948
1.932
1.927
1.922
1.912
1.908
1.902
1.892
1.872



Ts
N
Ph
C
F
8o
(thousandths)
X : parts per Million : Carbon13
208.875
208.760
143.635
139.314
135.068
129.549
129.233
128.830
128.140
127.872
90.480
90.240
89.512
87.826
77.773
77.745
77.476
77.160
76.844
46.984
46.936
34.603
34.373
21.657

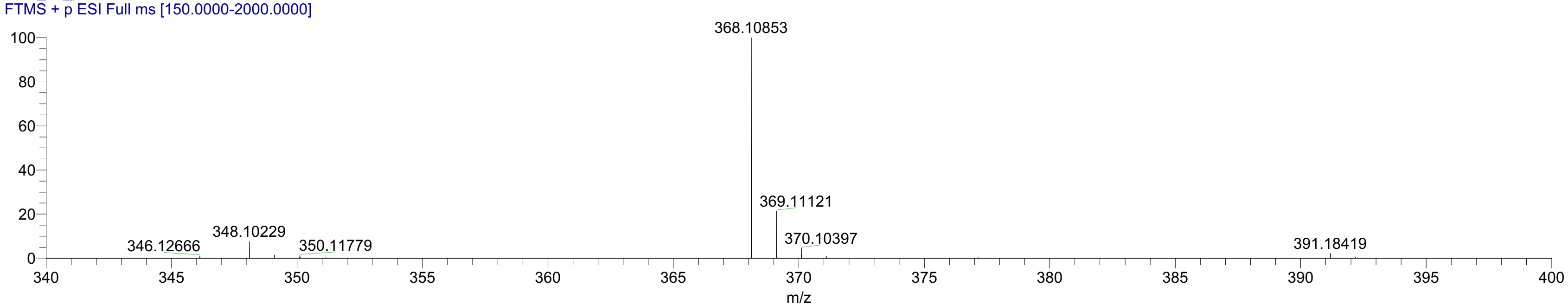

8o
abundance
X : parts per Million : Fluorine19
-170.027
-170.050
-170.069
-170.096
-170.123
-170.142
-170.154
-170.165
-170.181
-170.200
-170.223
-170.254
-170.296

Sample No. : C:\Xcalibur\...\1228\BG_231844_8(_, Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 14:26:38
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

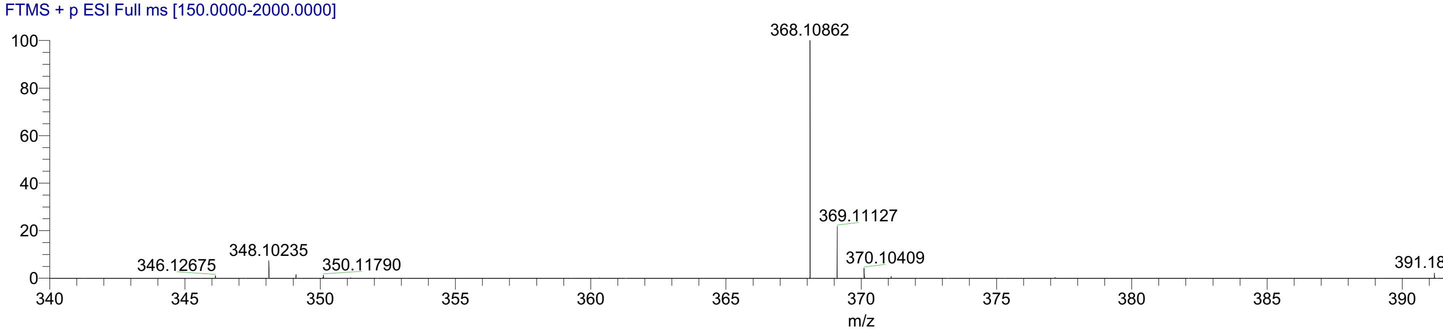


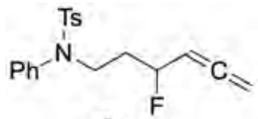
Sample No. : C:\Xcalibur\...\20231228\231844_8o_pn   Instrument : Exactive Plus   Mobile phase solvent : MeOH
Operator name : hayashi harumi   Sample solvent : CHCl3
Date : 12/28/23 11:01:43
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

231844_8o_pn #22-25 RT: 0.37-0.40 AV: 2 NL: 1.03E8
T: FTMS + p ESI Full ms [150.0000-2000.0000]



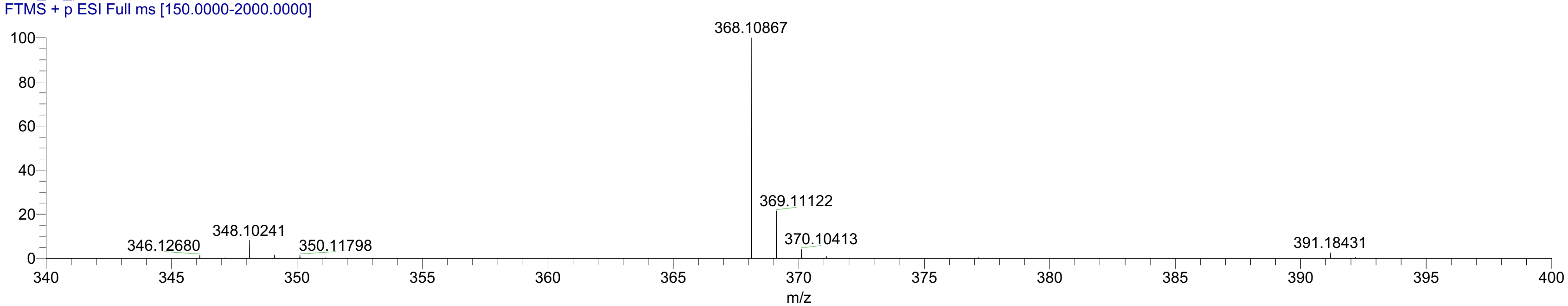
231844_8o_pn #26-29 RT: 0.43-0.46 AV: 2 NL: 7.62E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]

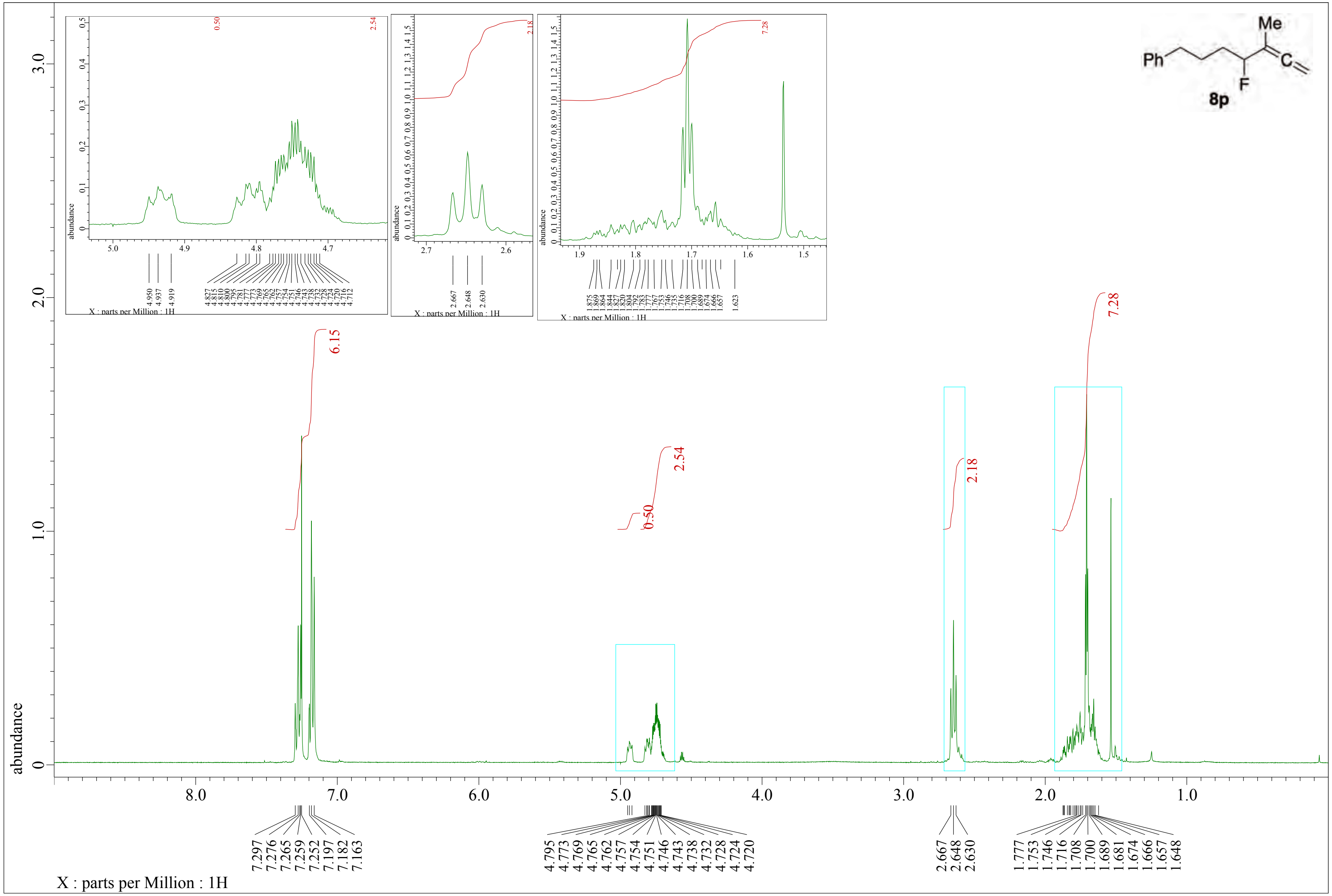


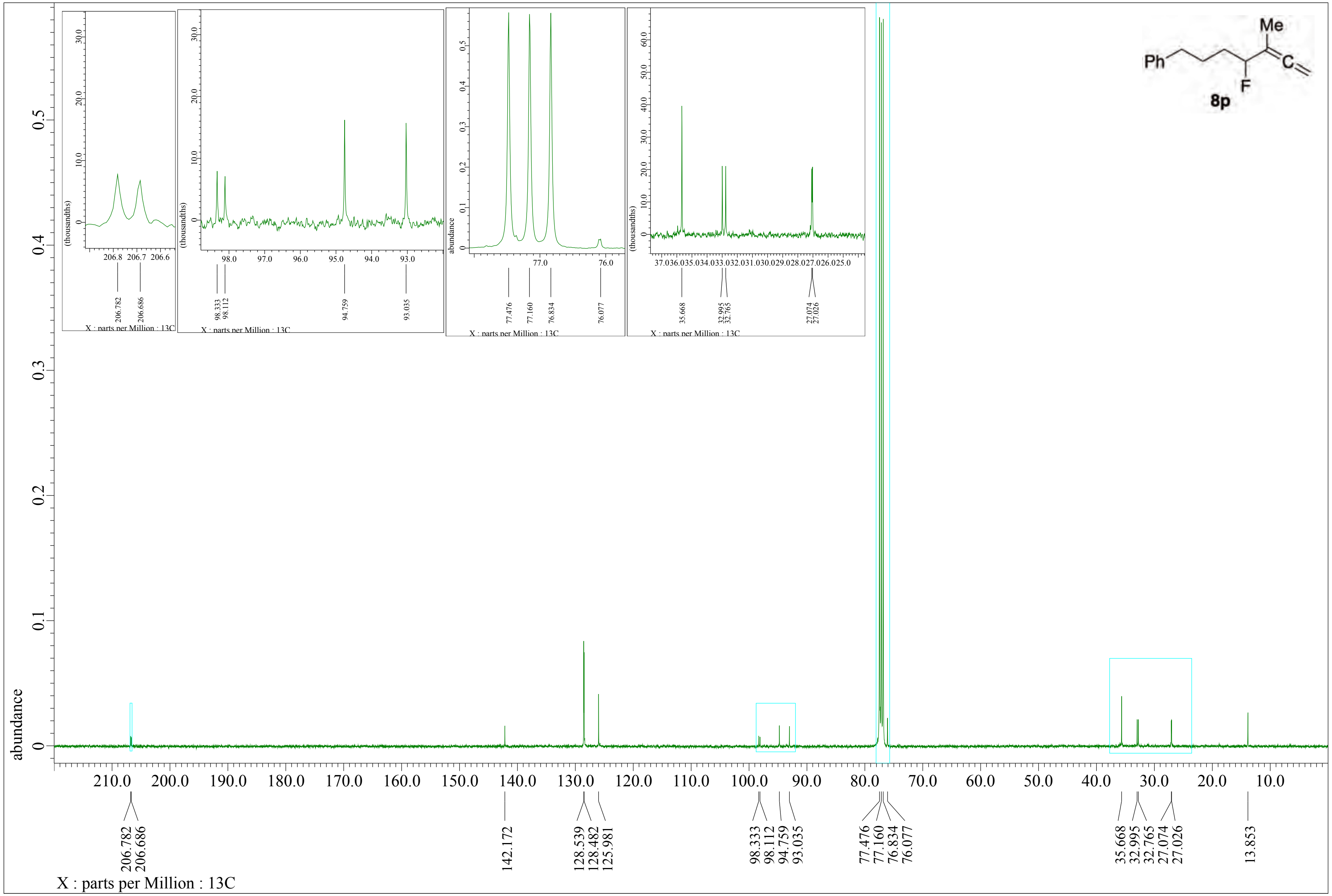


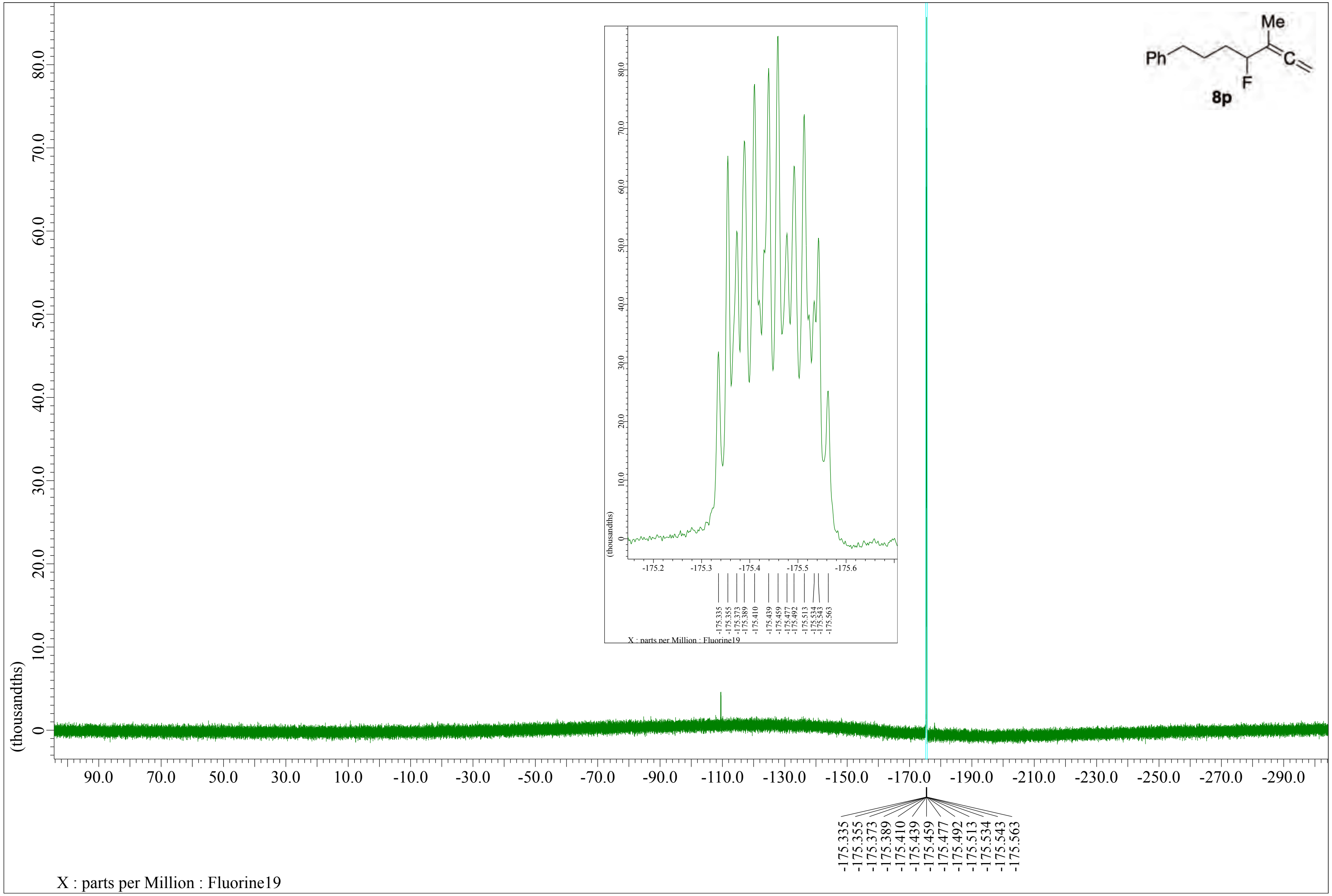
8o

231844_8o_pn #30-33 RT: 0.49-0.52 AV: 2 NL: 3.95E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]

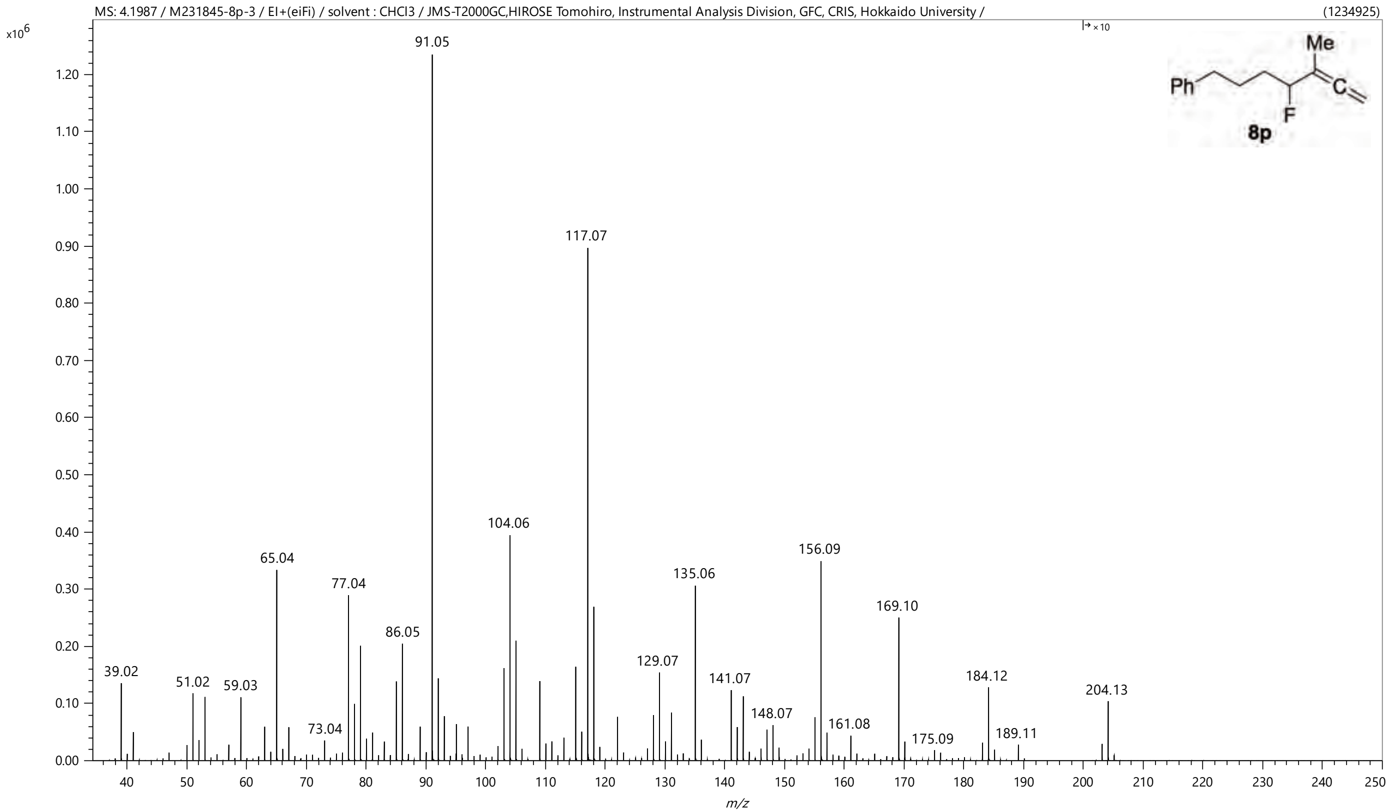


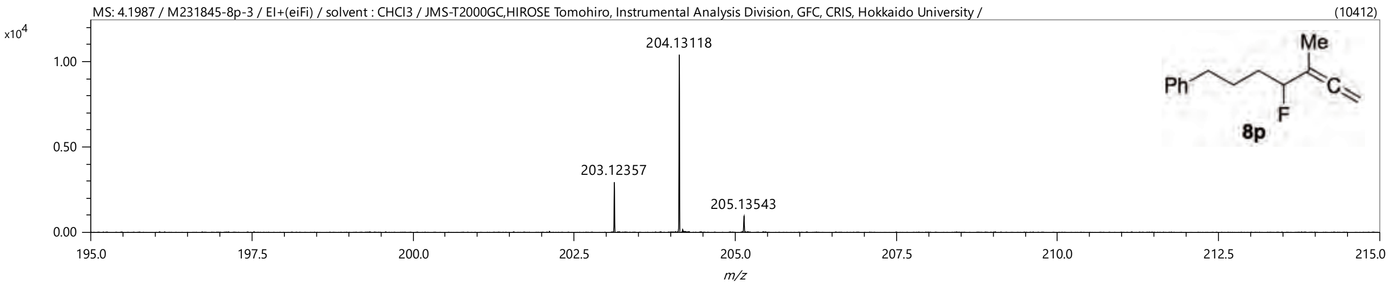

Me
Ph
C
F
8p
abundance
X : parts per Million : 1H
6.15
0.50
2.54
2.18
7.28
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.297
7.276
7.265
7.259
7.252
7.197
7.182
7.163
4.795
4.773
4.769
4.765
4.762
4.757
4.754
4.751
4.746
4.743
4.738
4.732
4.728
4.724
4.720
2.667
2.648
2.630
1.777
1.753
1.746
1.716
1.708
1.700
1.689
1.681
1.674
1.666
1.657
1.648

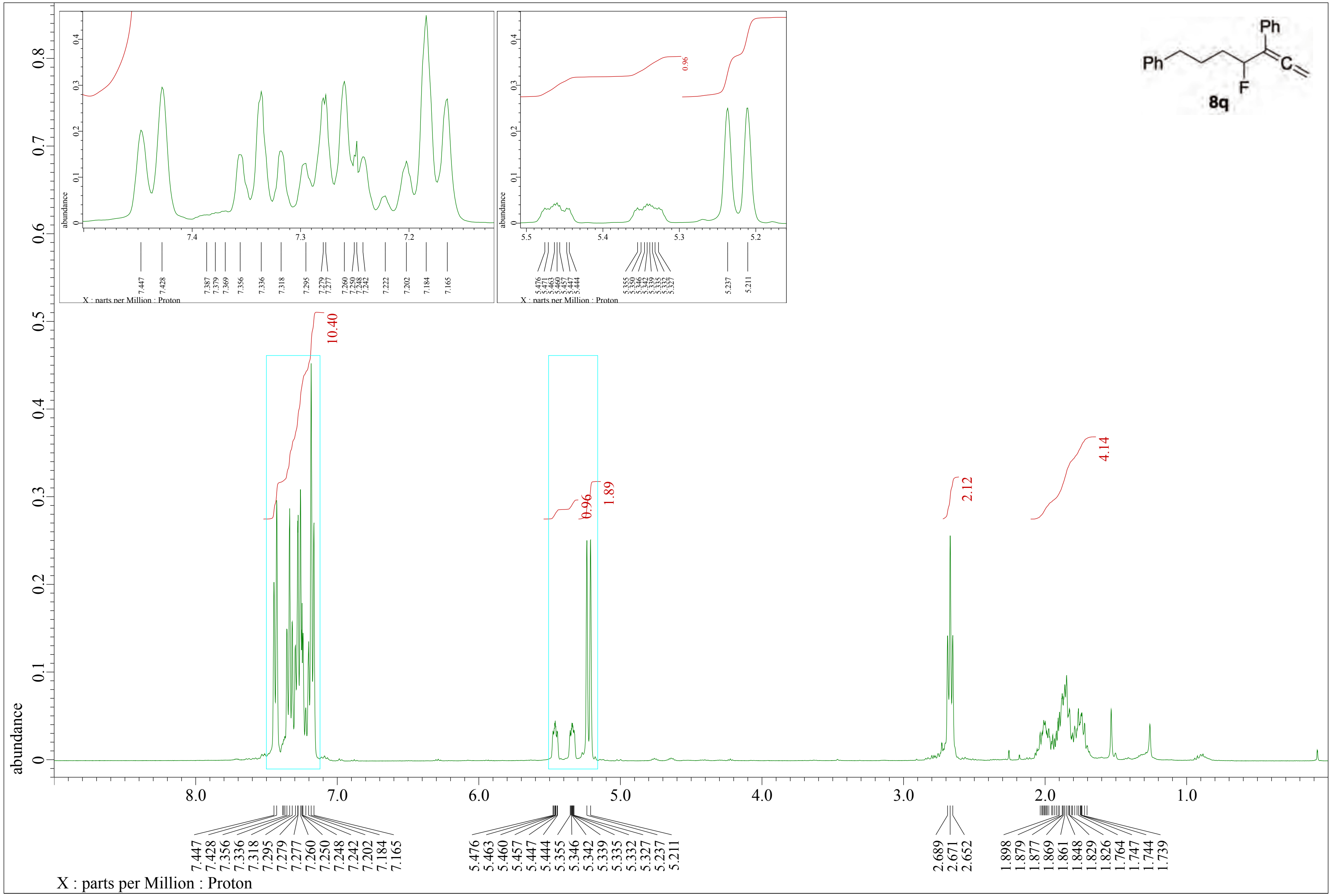

Ph
Me
C
F
8p
abundance
X : parts per Million : 13C
206.782
206.686
142.172
128.539
128.482
125.981
98.333
98.112
94.759
93.035
77.476
77.160
76.834
76.077
35.668
32.995
32.765
27.074
27.026
13.853

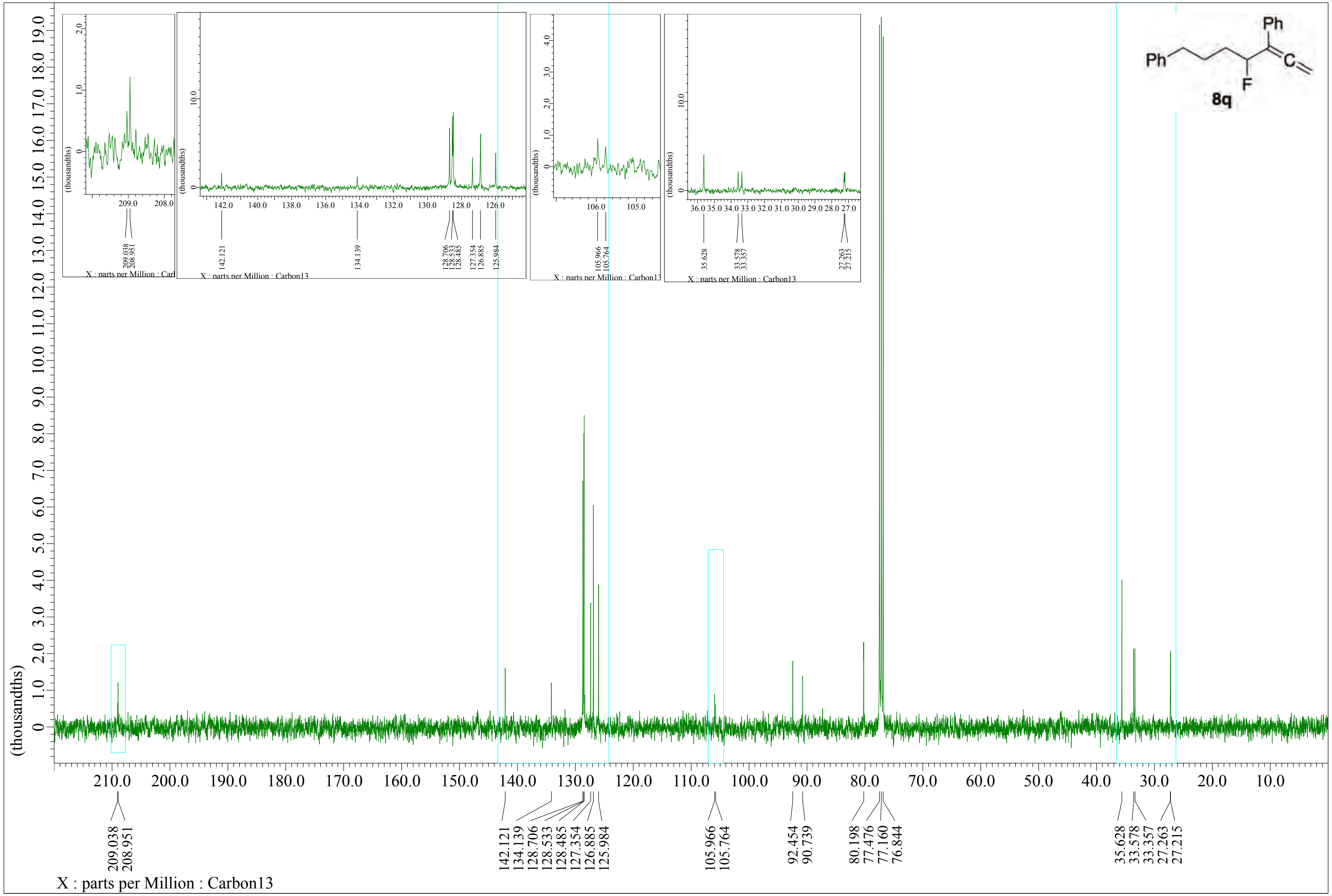


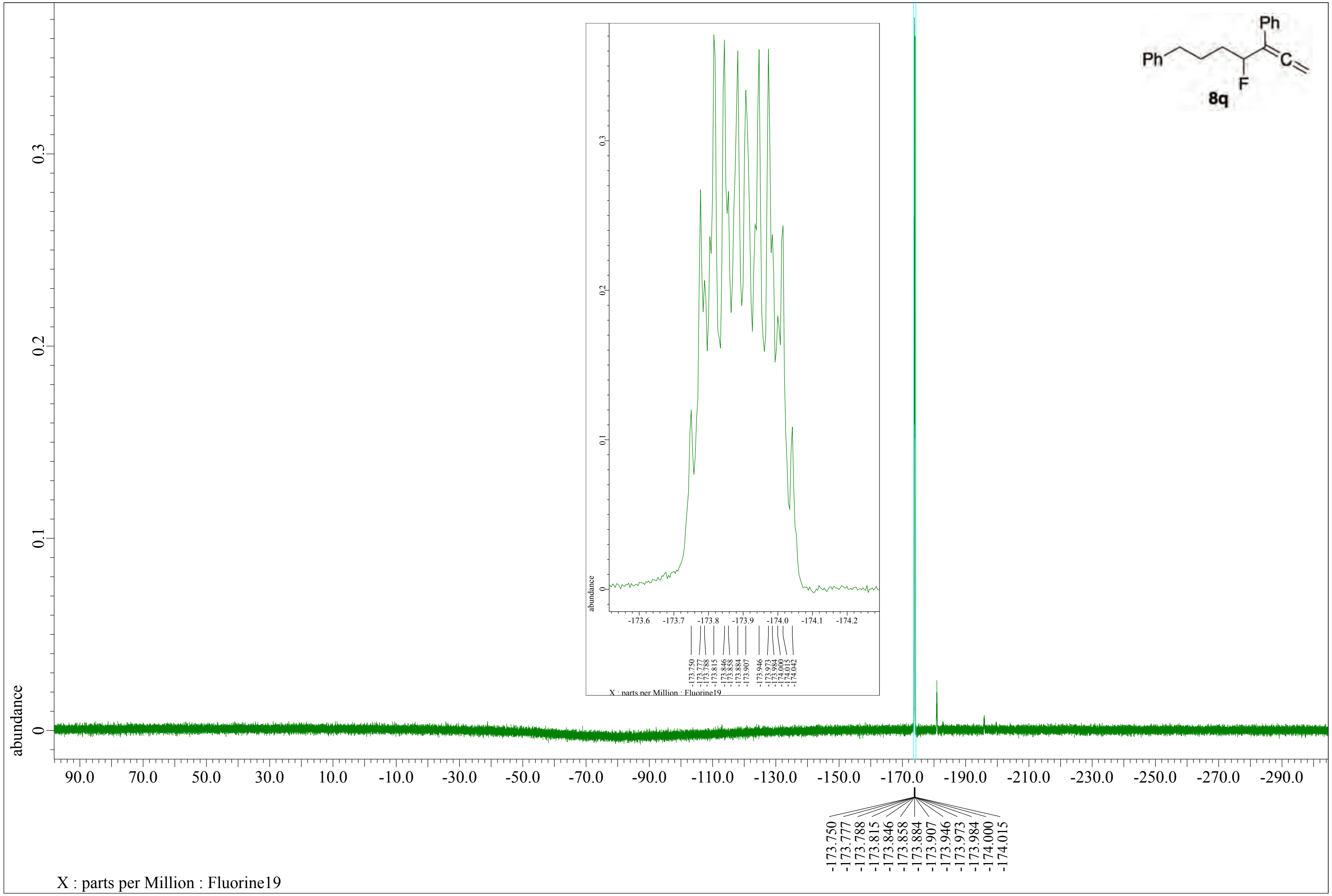
Ph
Me
C
F
8p
(thousandths)
X : parts per Million : Fluorine19
-175.335
-175.355
-175.373
-175.389
-175.410
-175.439
-175.459
-175.477
-175.492
-175.513
-175.534
-175.543
-175.563

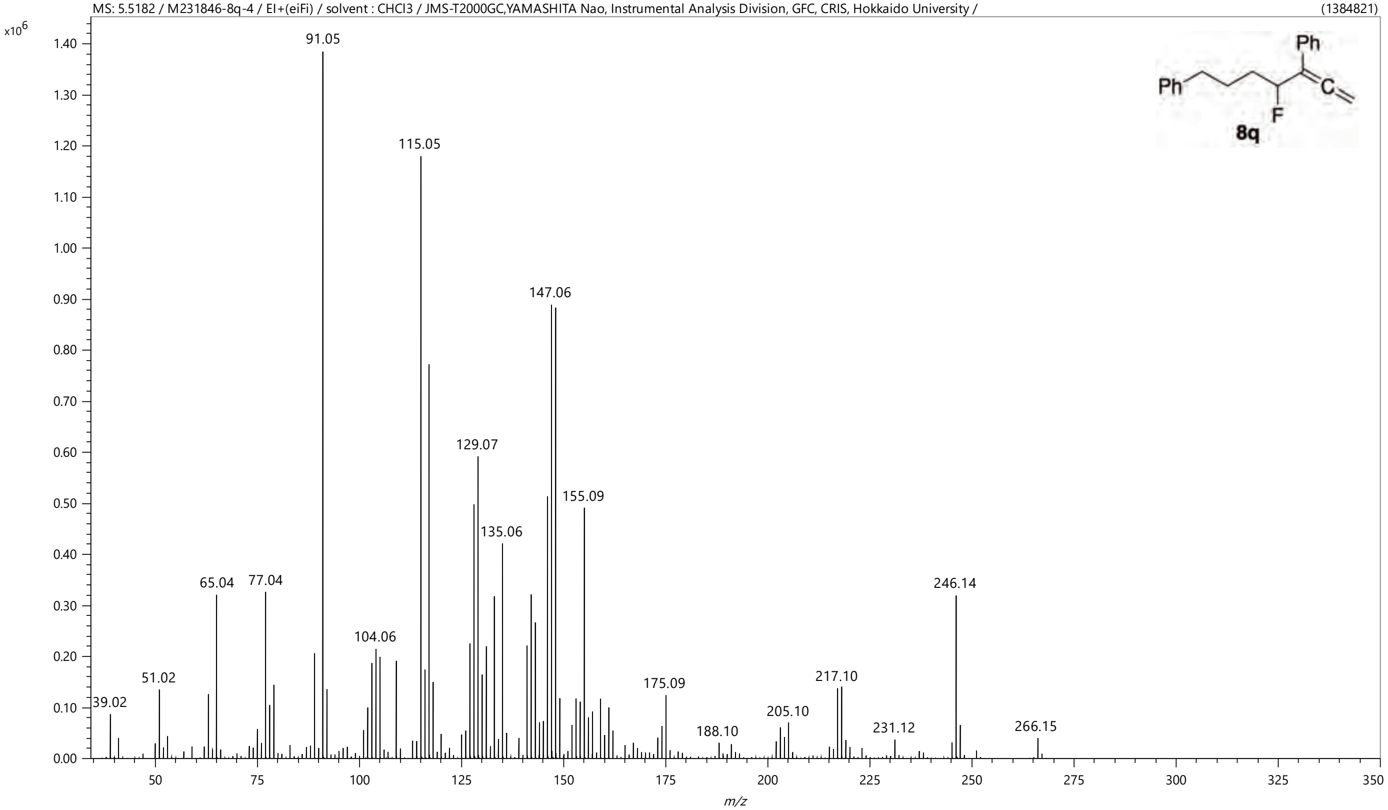

MS: 4.1987 / M231845-8p-3 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(1234925)
x10^6
91.05
117.07
104.06
65.04
77.04
86.05
156.09
135.06
169.10
129.07
141.07
148.07
161.08
175.09
184.12
189.11
204.13
39.02
51.02
59.03
73.04
m/z
Ph
Me
C
F
8p

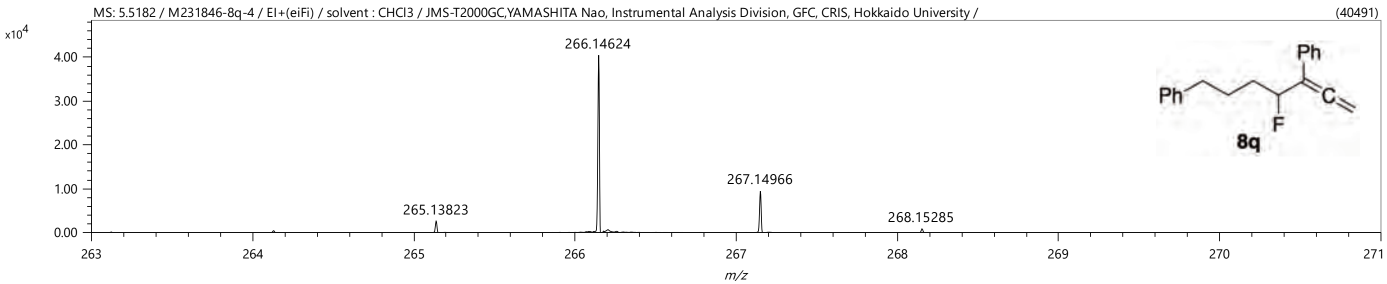

MS: 4.1987 / M231845-8p-3 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(10412)
x10^4
204.13118
203.12357
205.13543
m/z
Ph
Me
C
F
8p

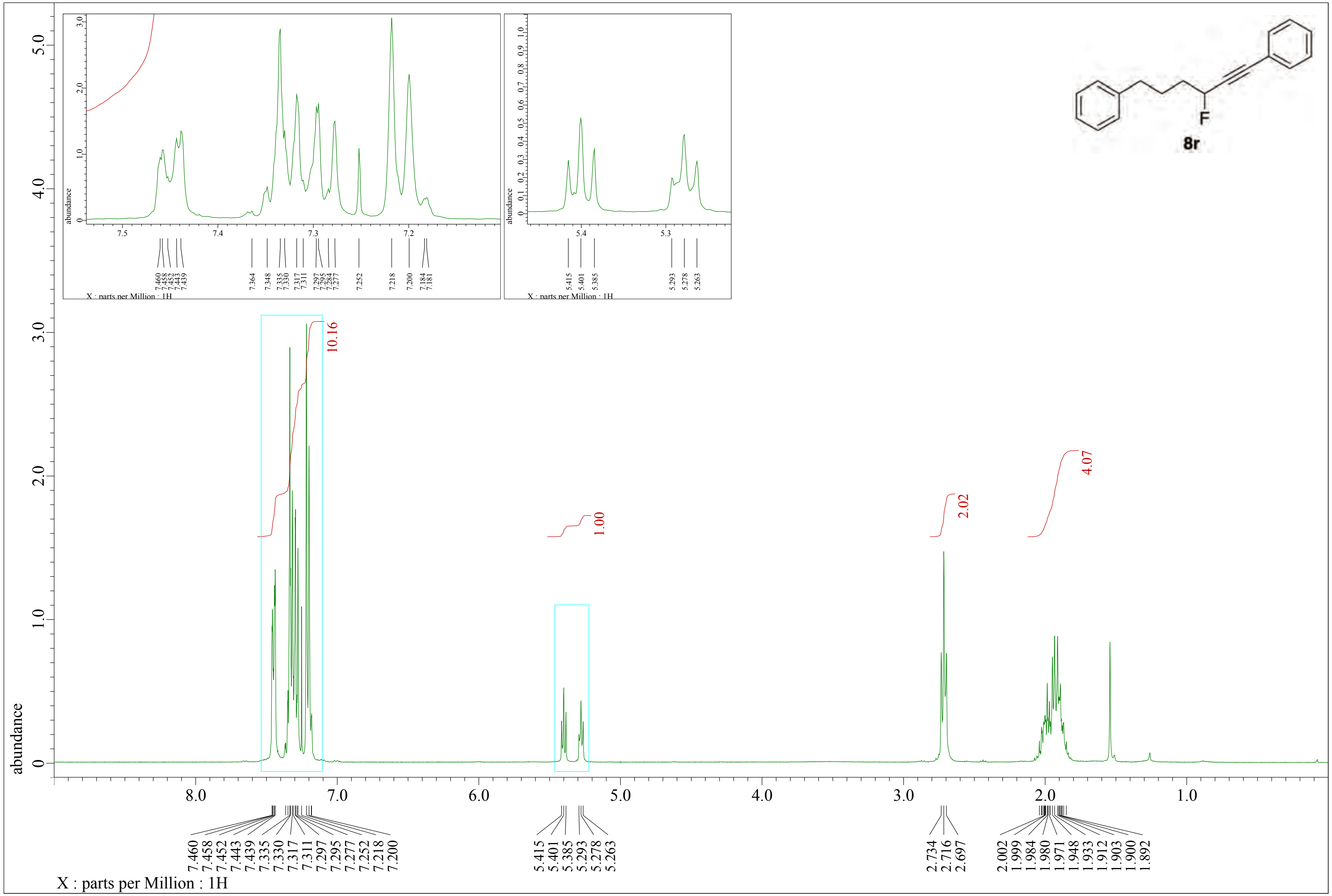

Ph
Ph
F
8q
abundance
X : parts per Million : Proton
10.40
0.96
1.89
2.12
4.14
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.447
7.428
7.356
7.336
7.318
7.295
7.279
7.277
7.260
7.250
7.248
7.242
7.202
7.184
7.165
5.476
5.463
5.460
5.457
5.447
5.444
5.355
5.346
5.342
5.339
5.335
5.332
5.327
5.237
5.211
2.689
2.671
2.652
1.898
1.879
1.877
1.869
1.861
1.848
1.829
1.826
1.764
1.747
1.744
1.739

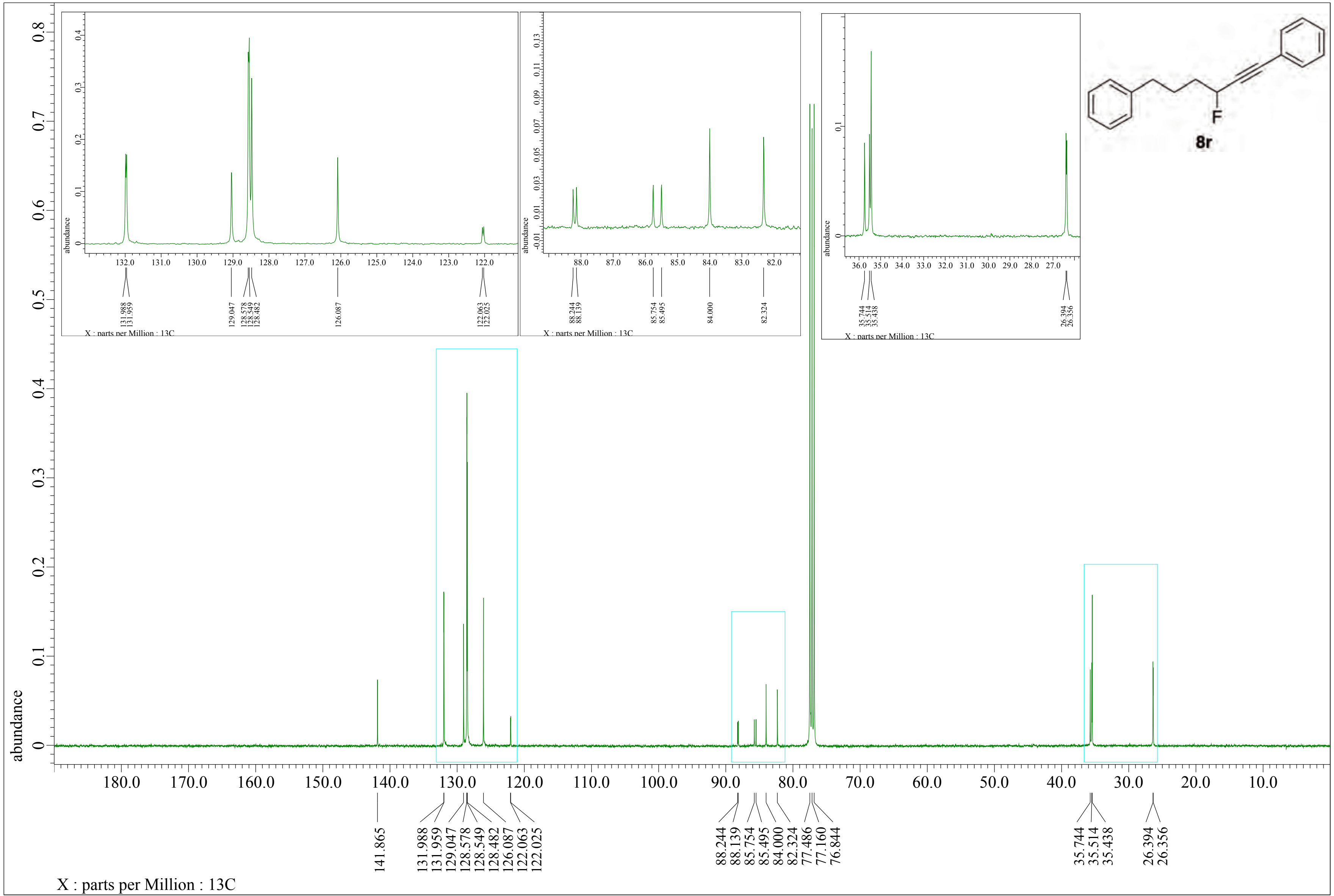

Ph
Ph
C
F
8q
(thousandths)
X : parts per Million : Carbon13
209.038
208.951
142.121
134.139
128.706
128.533
128.485
127.354
126.885
125.984
105.966
105.764
92.454
90.739
80.198
77.476
77.160
76.844
35.628
33.578
33.357
27.263
27.215


Ph
Ph
F
C
8q
abundance
0.3
0.2
0.1
0
90.0
70.0
50.0
30.0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-170.0
-190.0
-210.0
-230.0
-250.0
-270.0
-290.0
-173.750
-173.777
-173.788
-173.815
-173.846
-173.858
-173.884
-173.907
-173.946
-173.973
-173.984
-174.000
-174.015
-173.6
-173.7
-173.8
-173.9
-174.0
-174.1
-174.2
-174.042
X : parts per Million : Fluorine19

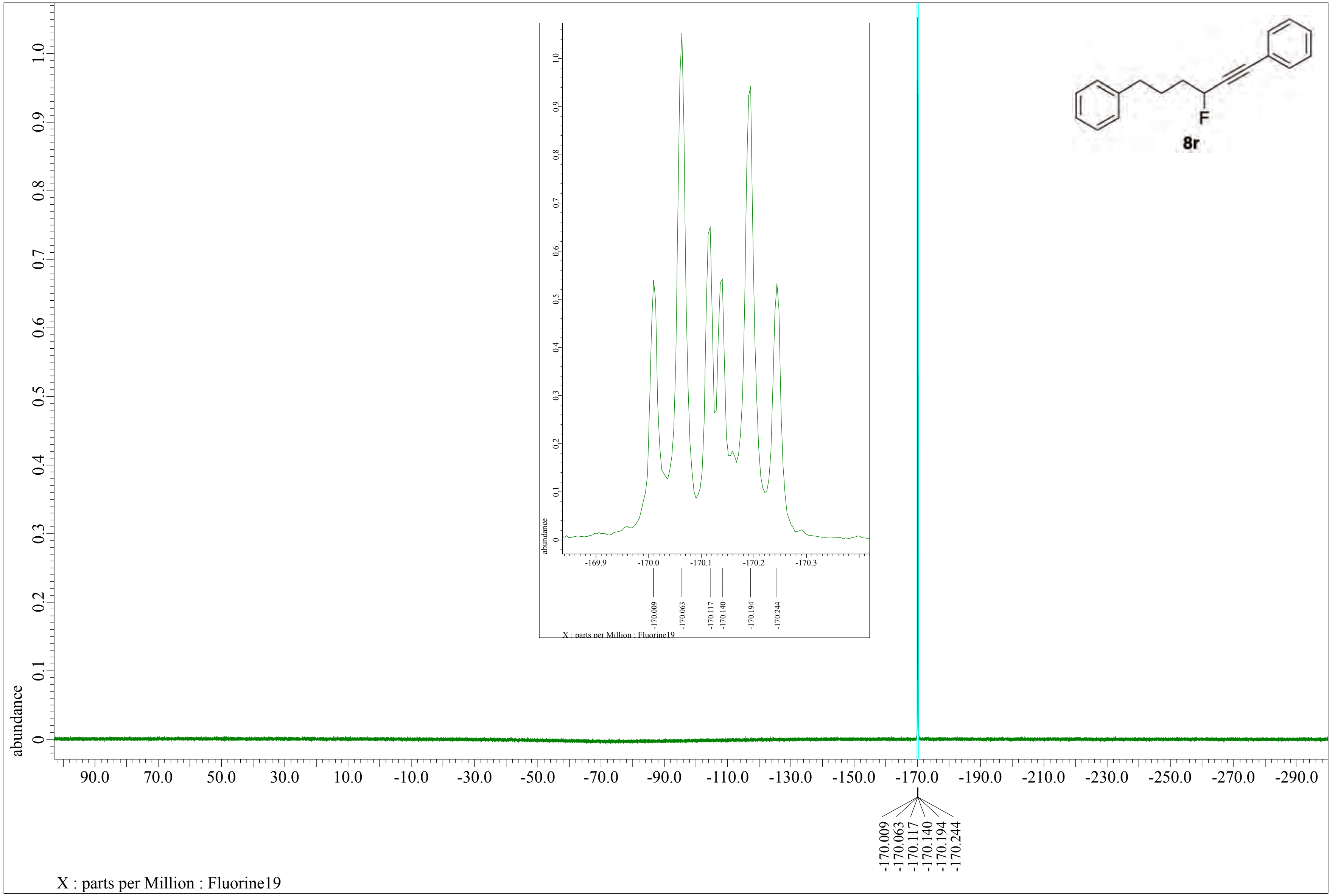

MS: 5.5182 / M231846-8q-4 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,YAMASHITA Nao, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(1384821)
x10^6
91.05
115.05
147.06
129.07
155.09
135.06
65.04
77.04
246.14
104.06
51.02
175.09
217.10
39.02
205.10
188.10
231.12
266.15
m/z
Ph
Ph
F
C
8q

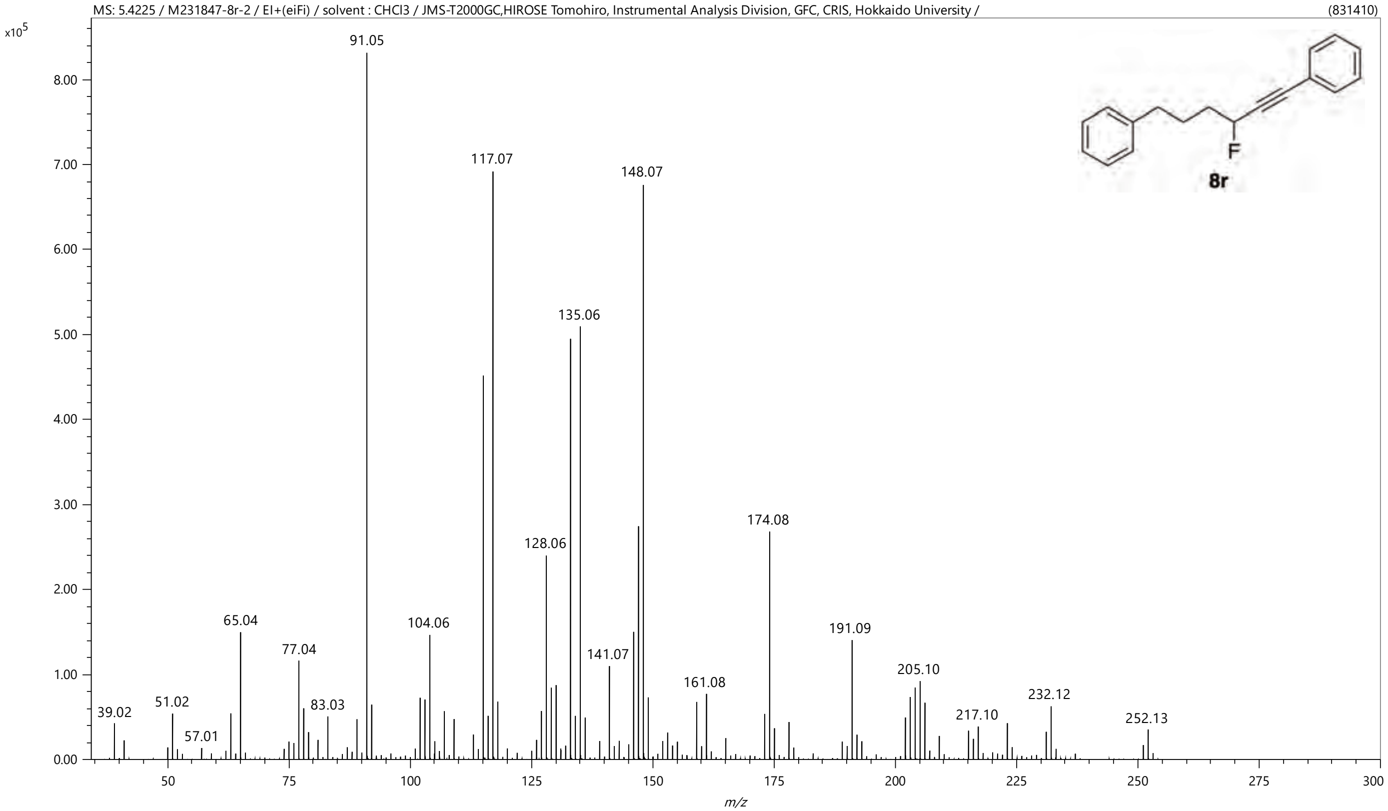

MS: 5.5182 / M231846-8q-4 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,YAMASHITA Nao, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(40491)
x10^4
266.14624
267.14966
265.13823
268.15285
m/z
Ph
Ph
F
C
8q

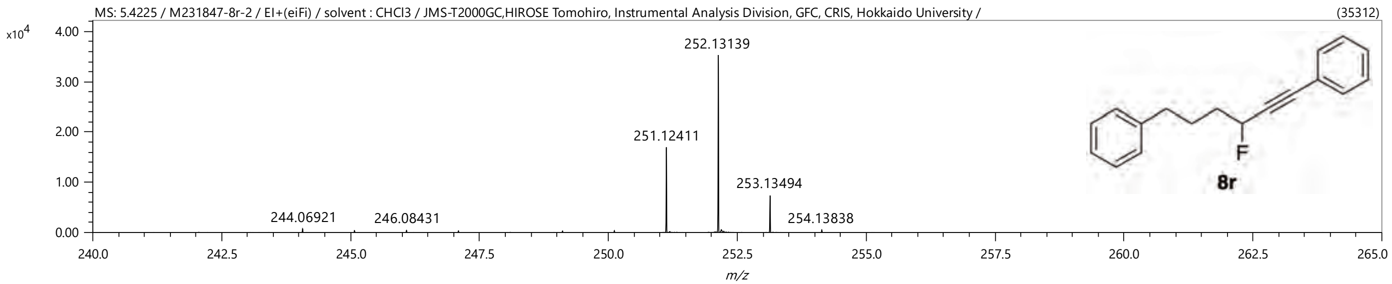

8r
F
abundance
X : parts per Million : 1H
10.16
1.00
2.02
4.07
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.460
7.458
7.452
7.443
7.439
7.335
7.330
7.317
7.311
7.297
7.295
7.277
7.252
7.218
7.200
5.415
5.401
5.385
5.293
5.278
5.263
2.734
2.716
2.697
2.002
1.999
1.984
1.980
1.971
1.948
1.933
1.912
1.903
1.900
1.892
7.364
7.348
7.284
7.184
7.181

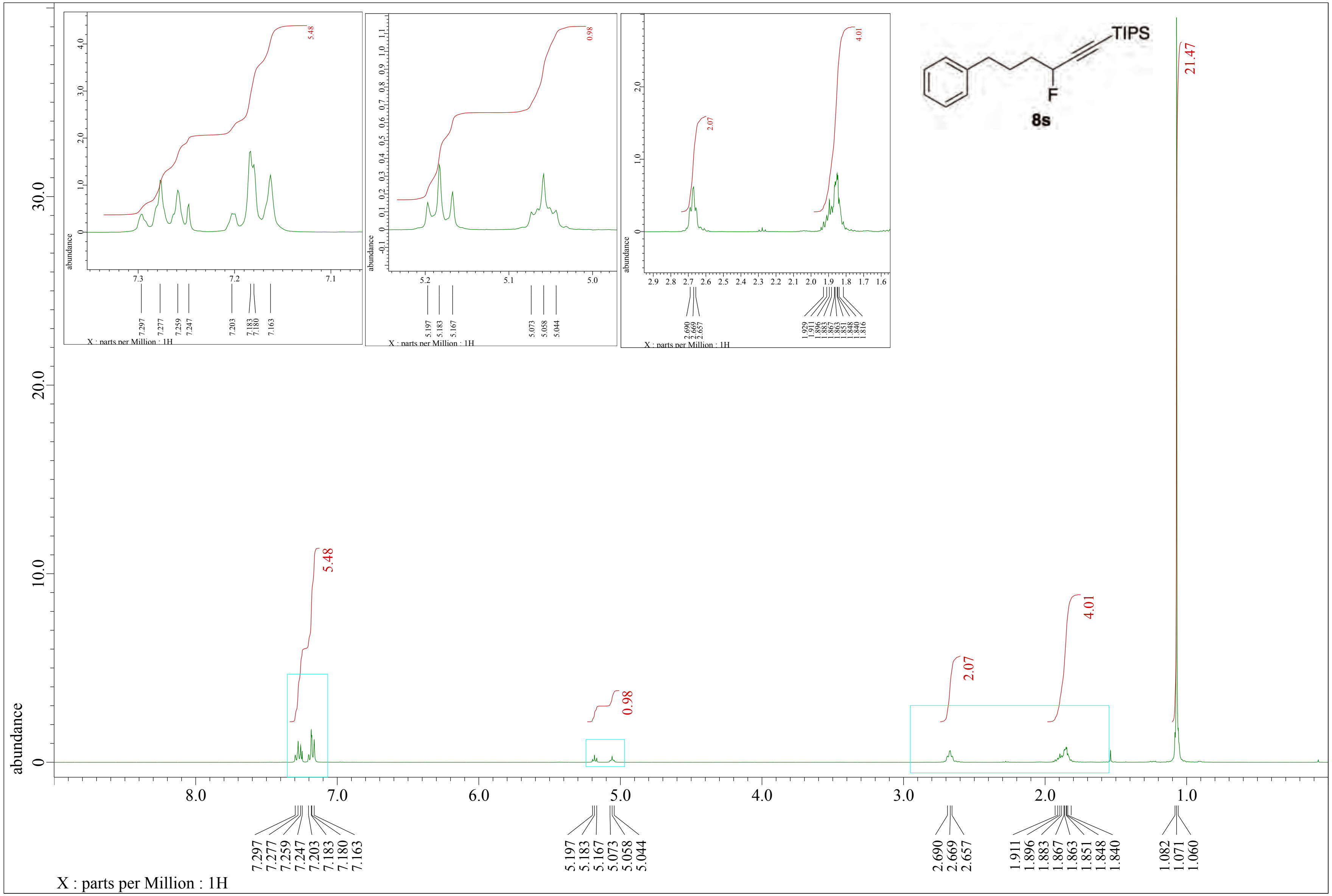


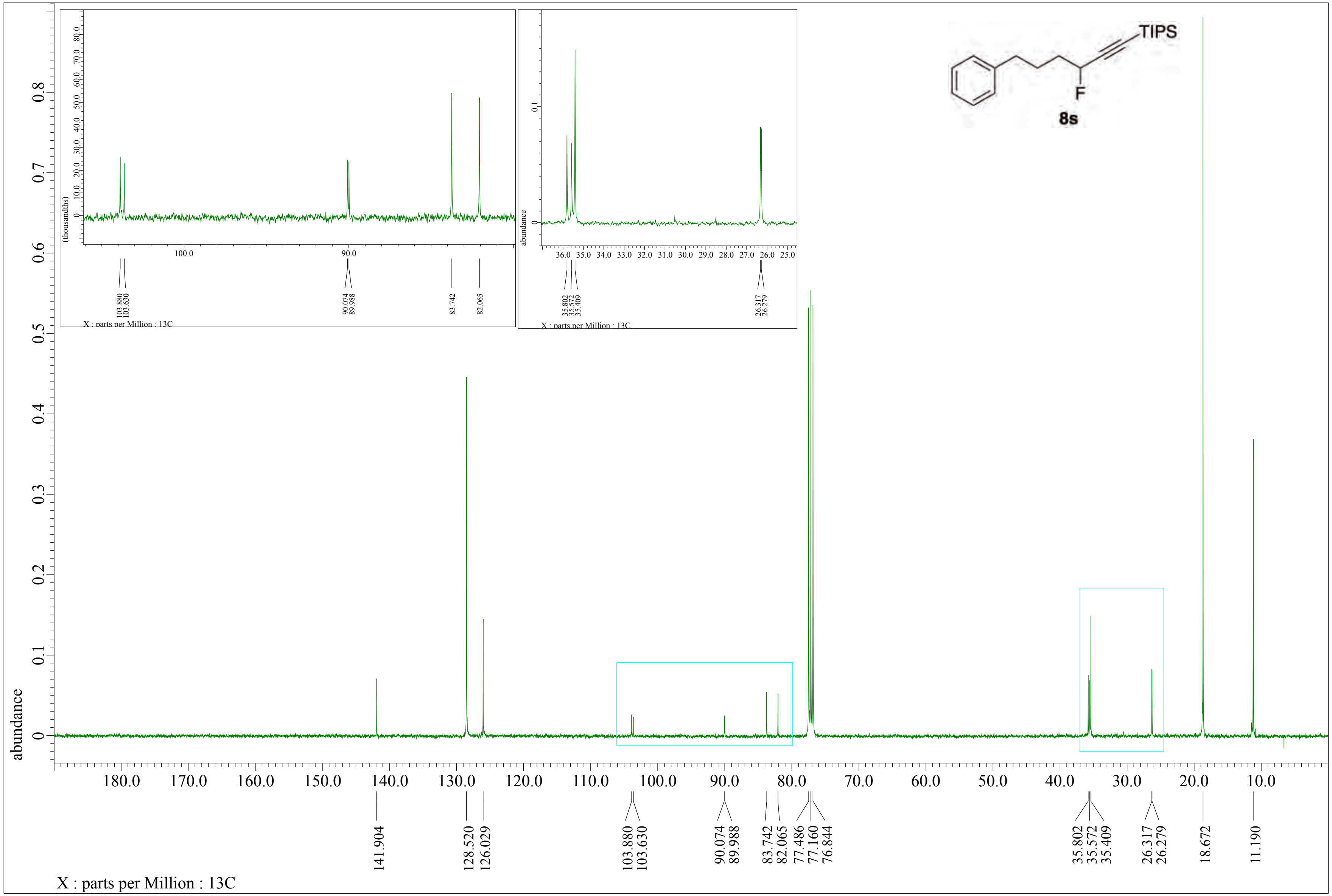
abundance
X : parts per Million : 13C
141.865
131.988
131.959
129.047
128.578
128.549
128.482
126.087
122.063
122.025
88.244
88.139
85.754
85.495
84.000
82.324
77.486
77.160
76.844
35.744
35.514
35.438
26.394
26.356
F
8r

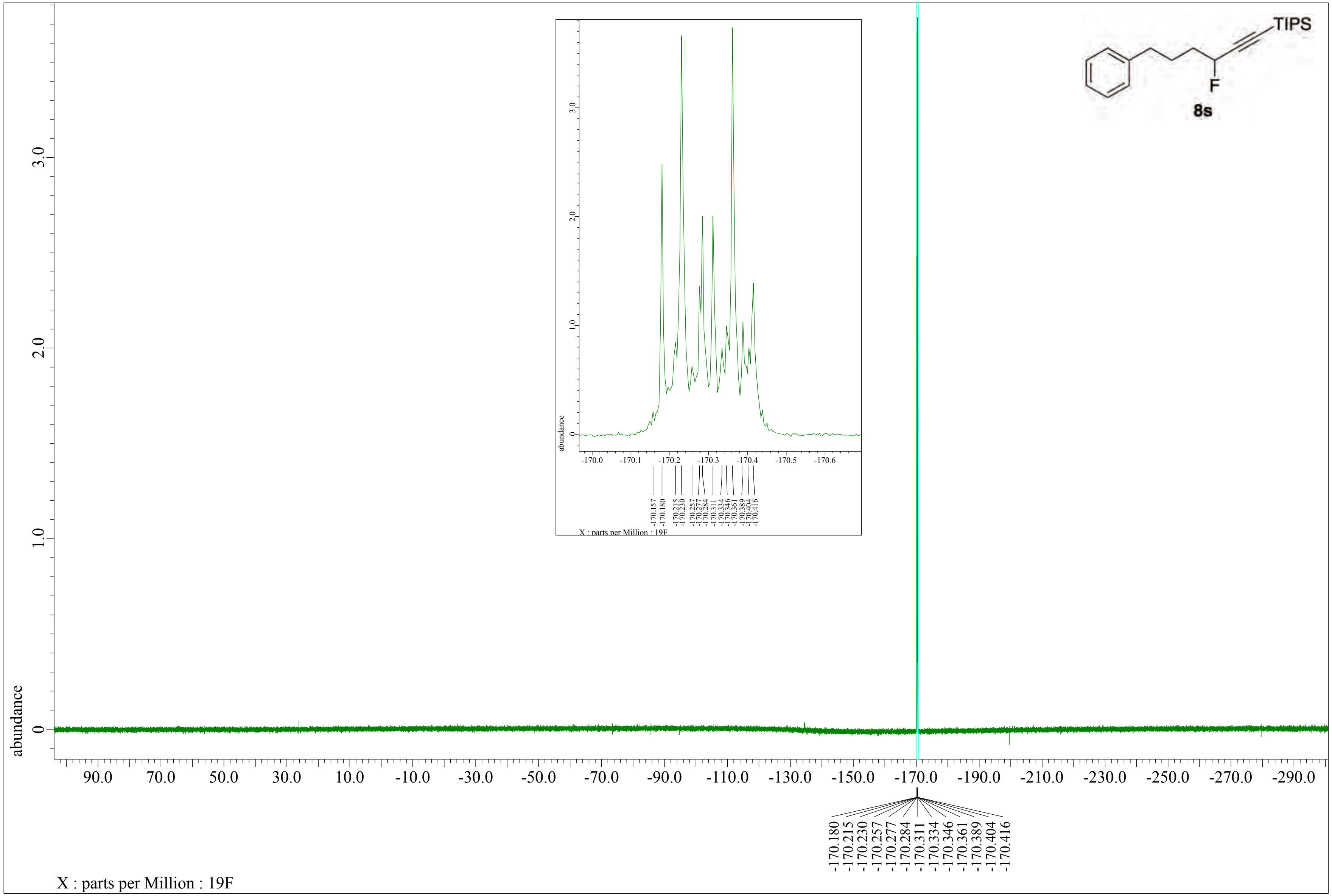

8r
F
abundance
X : parts per Million : Fluorine19
-170.009
-170.063
-170.117
-170.140
-170.194
-170.244


MS: 5.4225 / M231847-8r-2 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(831410)
x10^5
91.05
117.07
148.07
135.06
128.06
174.08
65.04
104.06
191.09
77.04
141.07
205.10
161.08
232.12
39.02
51.02
83.03
217.10
252.13
57.01
m/z
F
8r


MS: 5.4225 / M231847-8r-2 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(35312)
x10^4
252.13139
251.12411
253.13494
244.06921
246.08431
254.13838
m/z
F
8r


TIPS
F
8s
abundance
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
20.0
30.0
5.48
0.98
2.07
4.01
21.47
7.297
7.277
7.259
7.247
7.203
7.183
7.180
7.163
5.197
5.183
5.167
5.073
5.058
5.044
2.690
2.669
2.657
1.911
1.896
1.883
1.867
1.863
1.851
1.848
1.840
1.082
1.071
1.060
1.929
1.816


TIPS
F
8s
abundance
X : parts per Million : 13C
141.904
128.520
126.029
103.880
103.630
90.074
89.988
83.742
82.065
77.486
77.160
76.844
35.802
35.572
35.409
26.317
26.279
18.672
11.190

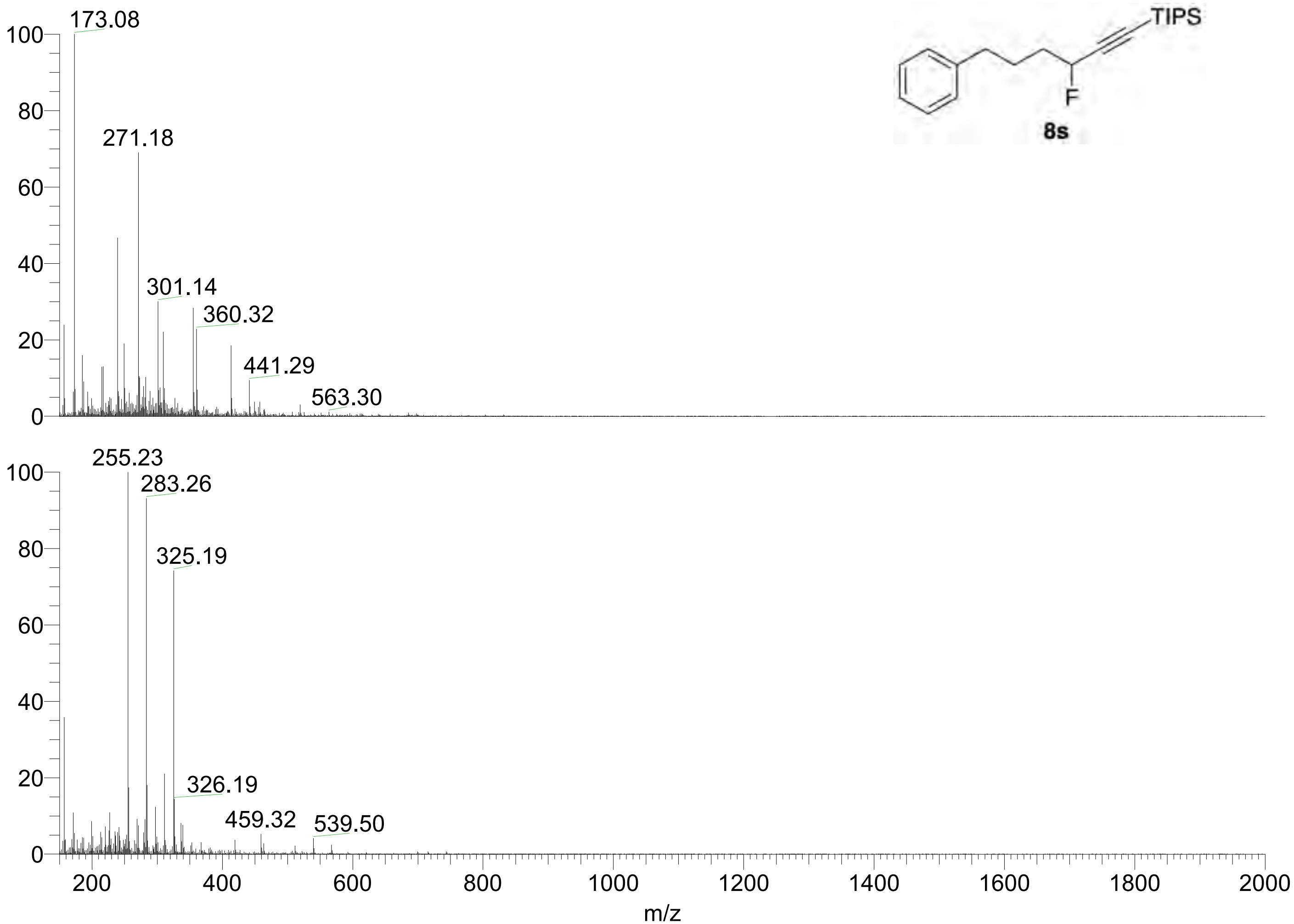


abundance
3.0
2.0
1.0
0
90.0
70.0
50.0
30.0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-170.0
-190.0
-210.0
-230.0
-250.0
-270.0
-290.0
-170.180
-170.215
-170.230
-170.257
-170.277
-170.284
-170.311
-170.334
-170.346
-170.361
-170.389
-170.404
-170.416
X : parts per Million : 19F
-170.0
-170.1
-170.2
-170.3
-170.4
-170.5
-170.6
-170.157
TIPS
F
8s

Sample No. : C:\Xcalibur\...\1228\BG_231848_8s _,
Instrument : Exactive Plus
Mobile phase solvent : MeOH
Operator name : hayashi harumi
Sample solvent : CHCl3
Date : 12/28/23 14:43:34
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

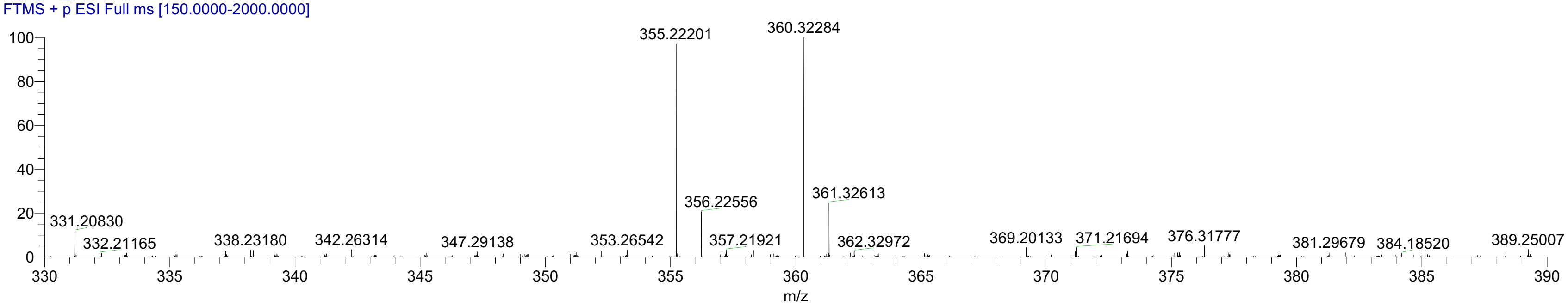
NL: 3.43E7
BG_231848_8s_pn2#1
9-32 RT: 0.31-0.48
AV: 7 T: FTMS + c
ESI Full ms
[150.00-2000.00]

NL: 1.59E7
BG_231848_8s_pn2#1
9-32 RT: 0.32-0.50
AV: 7 T: FTMS - c ESI
Full ms
[150.00-2000.00]

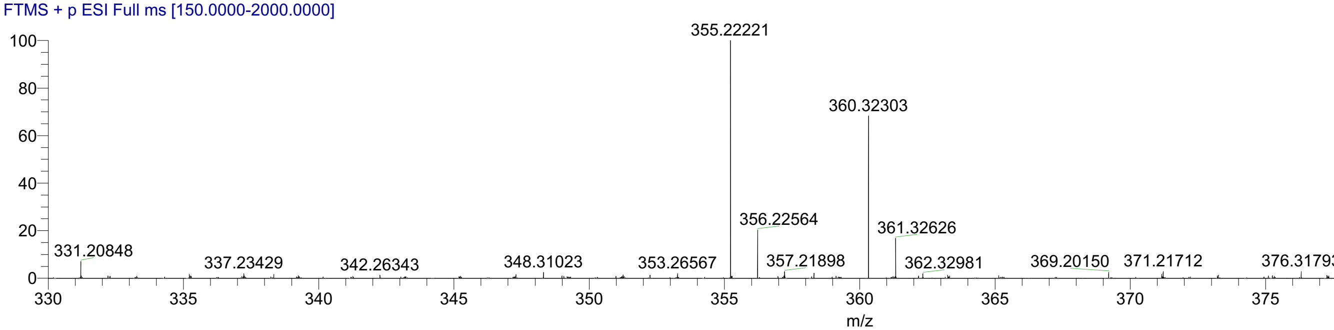


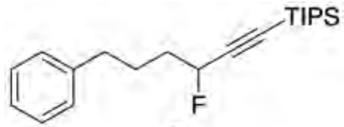
Sample No. : C:\Xcalibur\...\1228\231848_8s_pn2 Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 14:31:28
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

231848_8s_pn2 #22-26 RT: 0.36-0.39 AV: 2 NL: 2.57E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



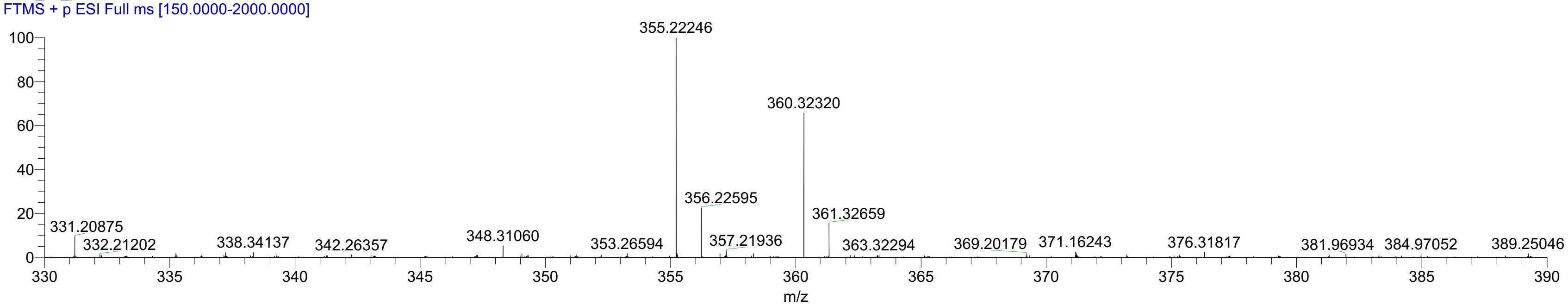
231848_8s_pn2 #26-29 RT: 0.42-0.45 AV: 2 NL: 3.23E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]

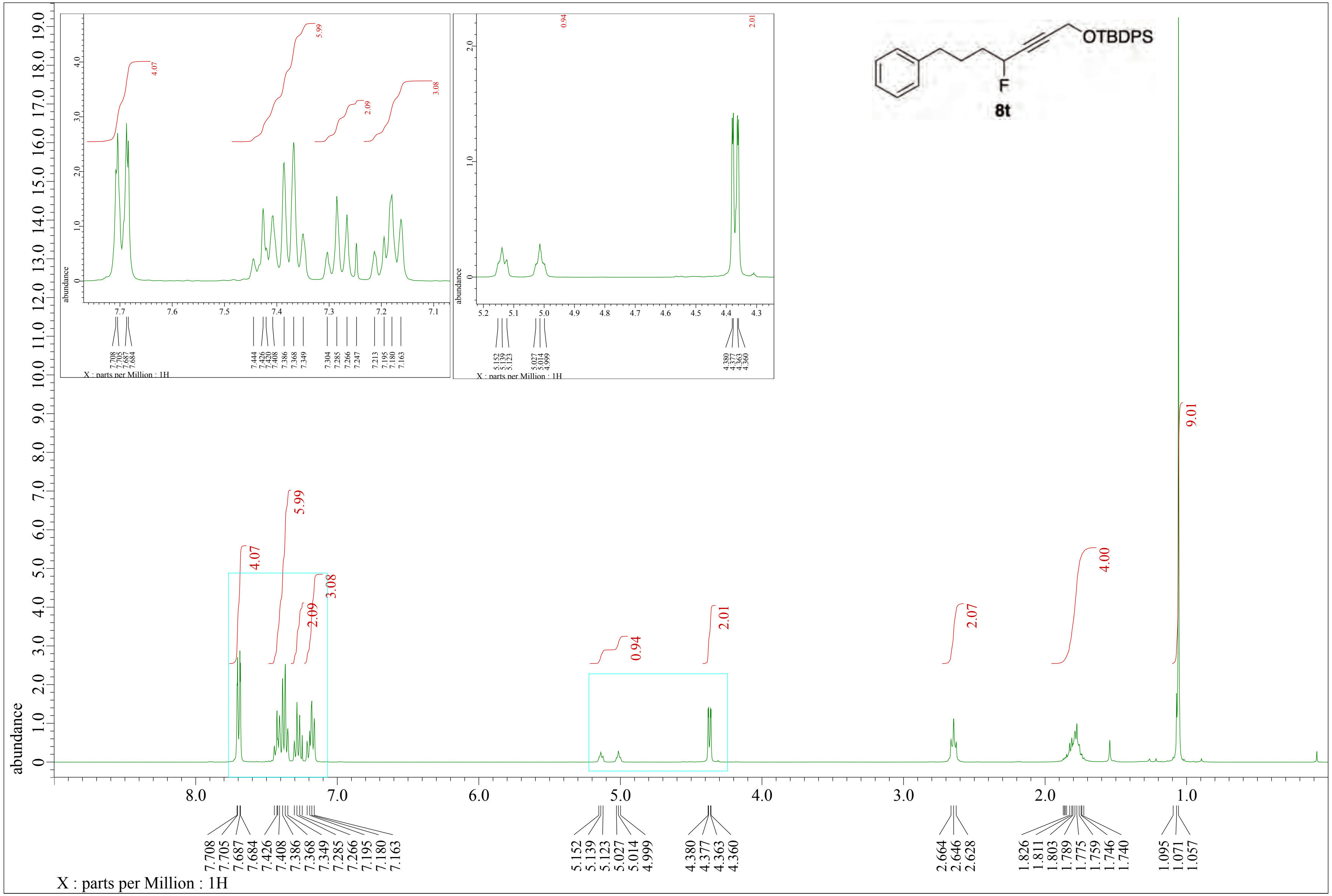


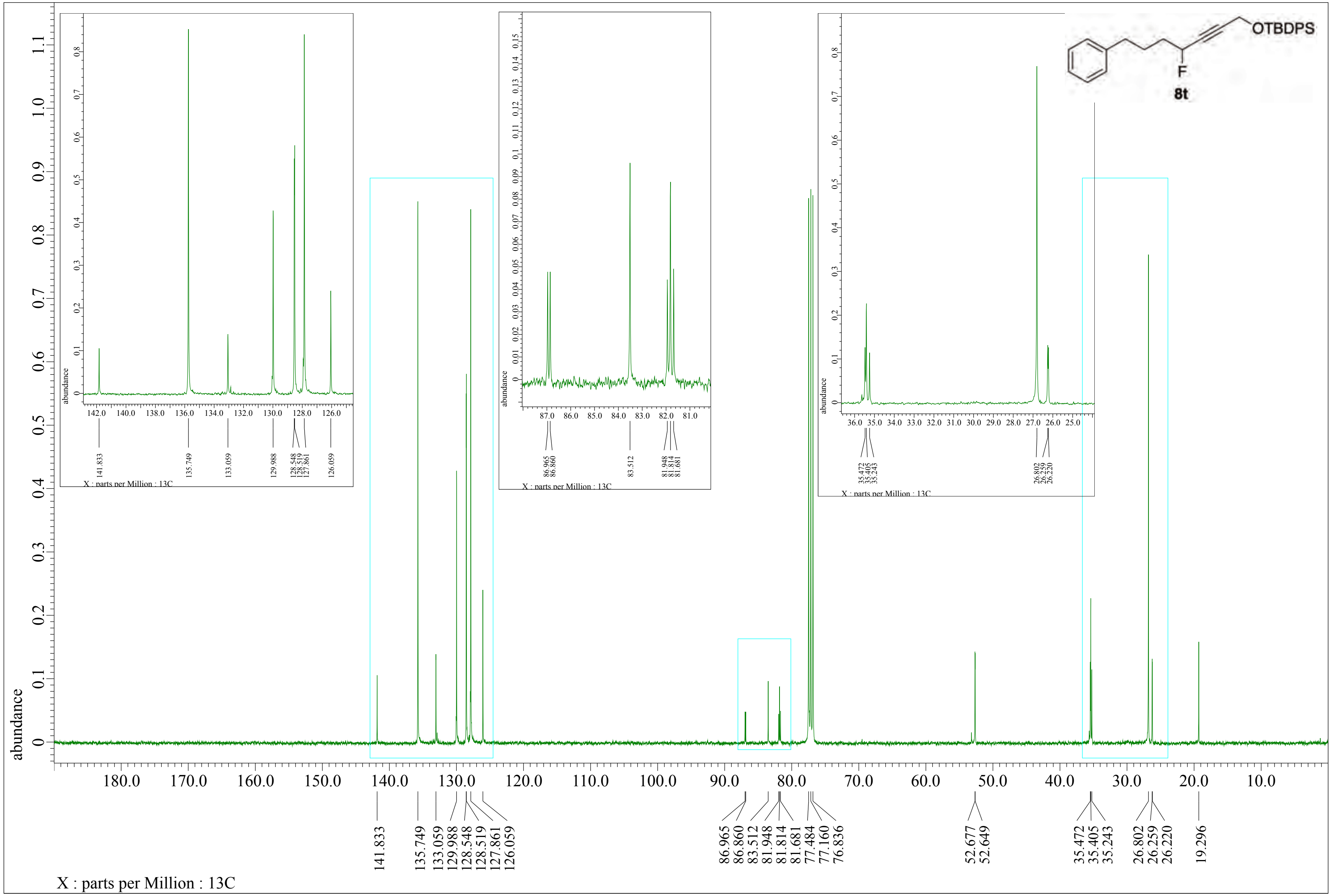


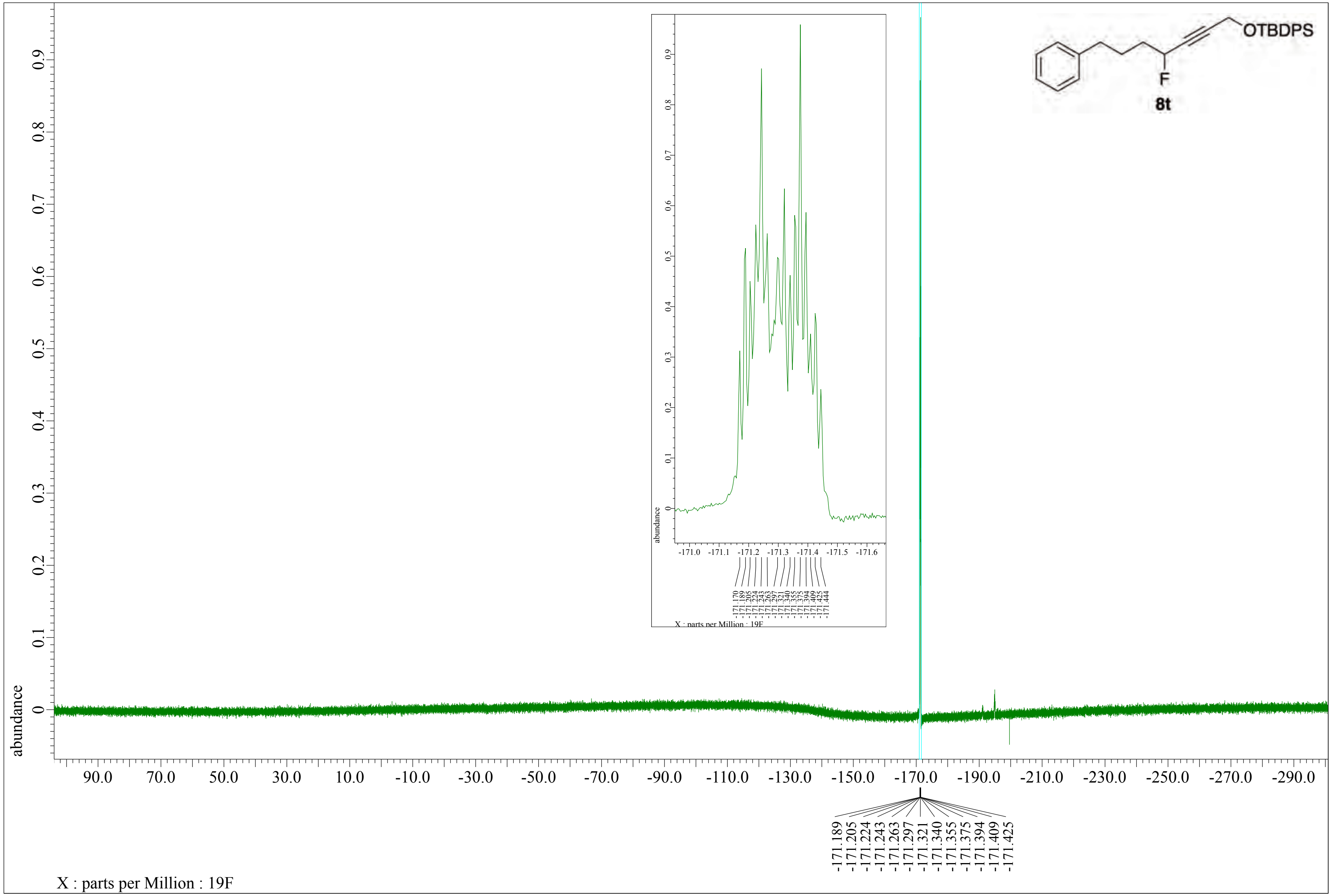
8s

231848_8s_pn2 #30-33 RT: 0.48-0.51 AV: 2 NL: 1.79E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



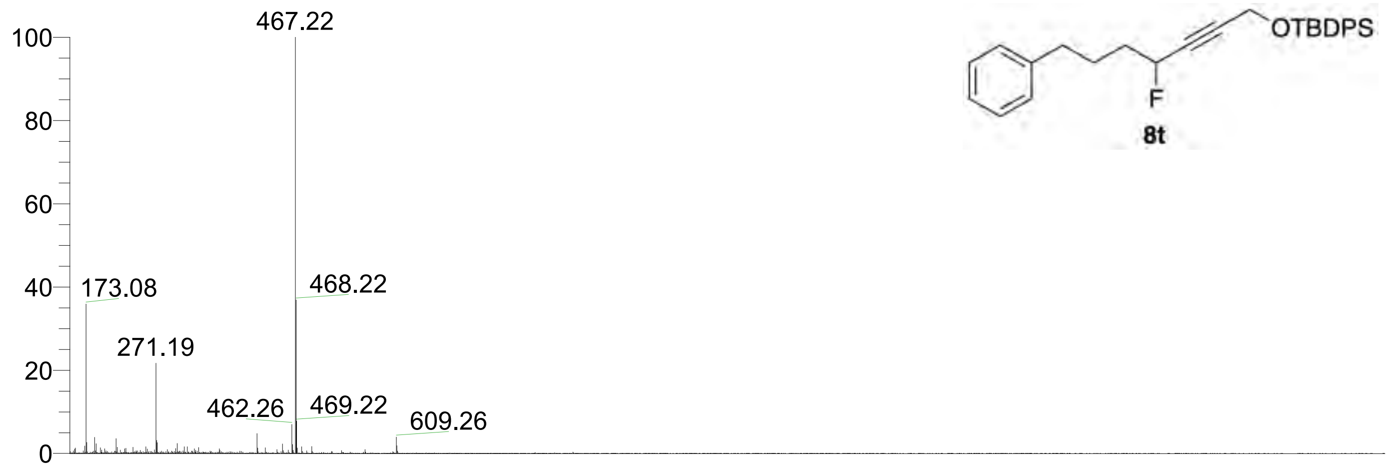

OTBDPS
F
8t
abundance
X : parts per Million : 1H
9.01
4.07
5.99
2.09
3.08
0.94
2.01
2.07
4.00


OTBDPS
F
8t
abundance
X : parts per Million : 13C
141.833
135.749
133.059
129.988
128.548
128.519
127.861
126.059
86.965
86.860
83.512
81.948
81.814
81.681
77.484
77.160
76.836
52.677
52.649
35.472
35.405
35.243
26.802
26.259
26.220
19.296

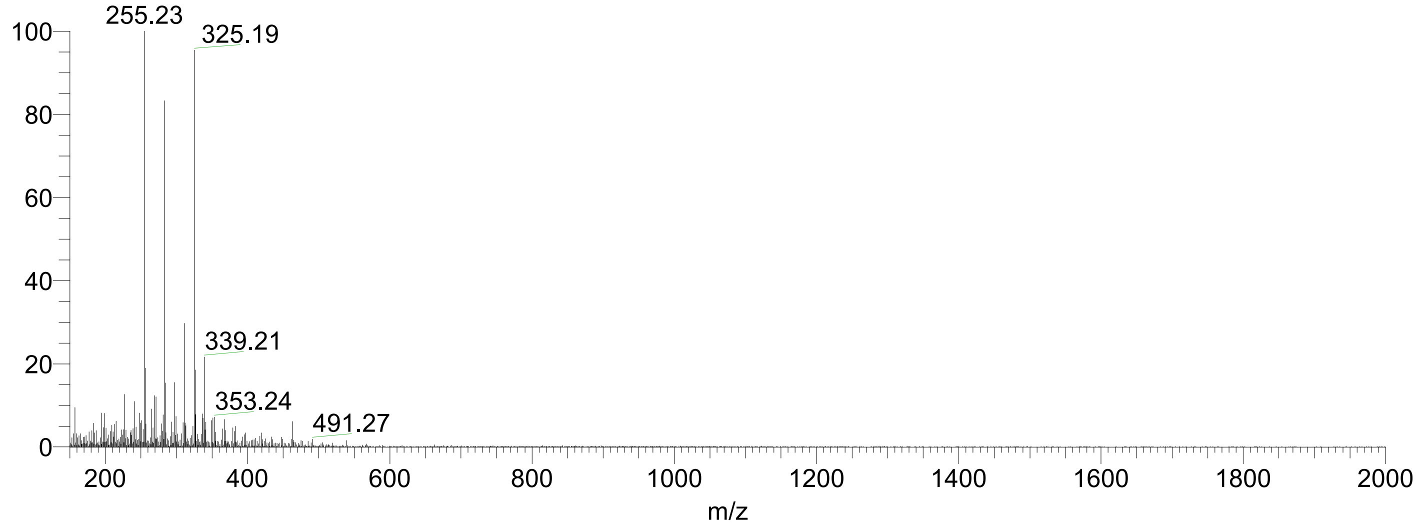


OTBDPS
F
8t
abundance
X : parts per Million : 19F
-171.189
-171.205
-171.224
-171.243
-171.263
-171.297
-171.321
-171.340
-171.355
-171.375
-171.394
-171.409
-171.425

Sample No. : C:\Xcalibur\...\1228\BG_231849_8t_,   Instrument : Exactive Plus   Mobile phase solvent : MeOH
Operator name : hayashi harumi   Sample solvent : CHCl3
Date : 12/28/23 14:27:00
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University



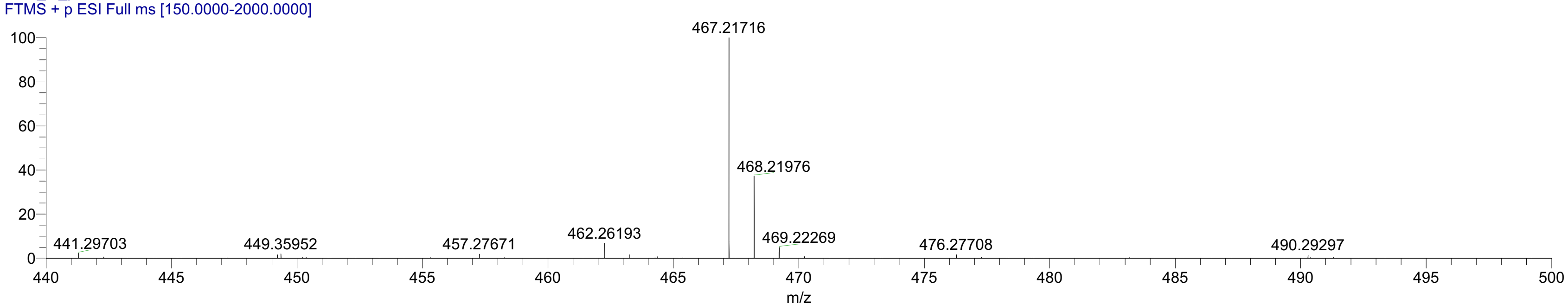
NL: 3.85E7
BG_231849_8t_pn#18-31 RT: 0.31-0.50
AV: 7 T: FTMS + c ESI Full ms [150.00-2000.00]



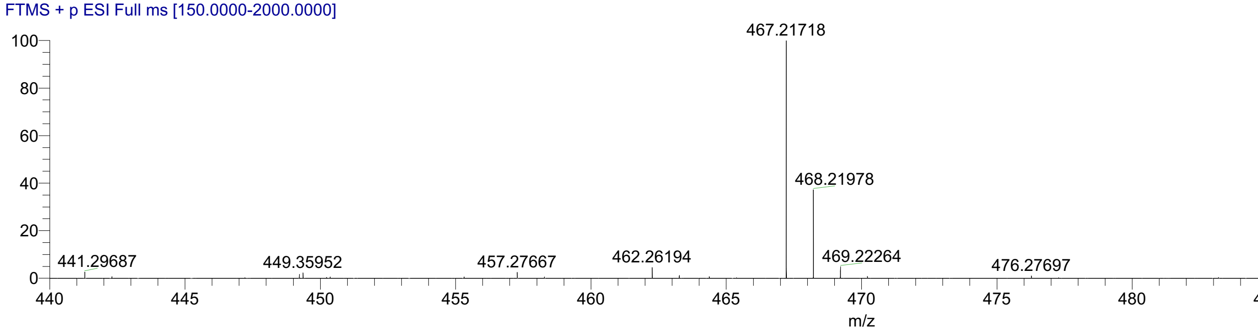
NL: 1.92E6
BG_231849_8t_pn#18-31 RT: 0.30-0.48
AV: 7 T: FTMS - c ESI Full ms [150.00-2000.00]

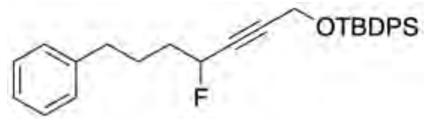
Sample No. : C:\Xcalibur\...\20231228\231849_8t_pn   Instrument : Exactive Plus   Mobile phase solvent : MeOH
Operator name : hayashi harumi   Sample solvent : CHCl3
Date : 12/28/23 11:31:19
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

231849_8t_pn #21-25 RT: 0.34-0.40 AV: 3 NL: 1.25E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



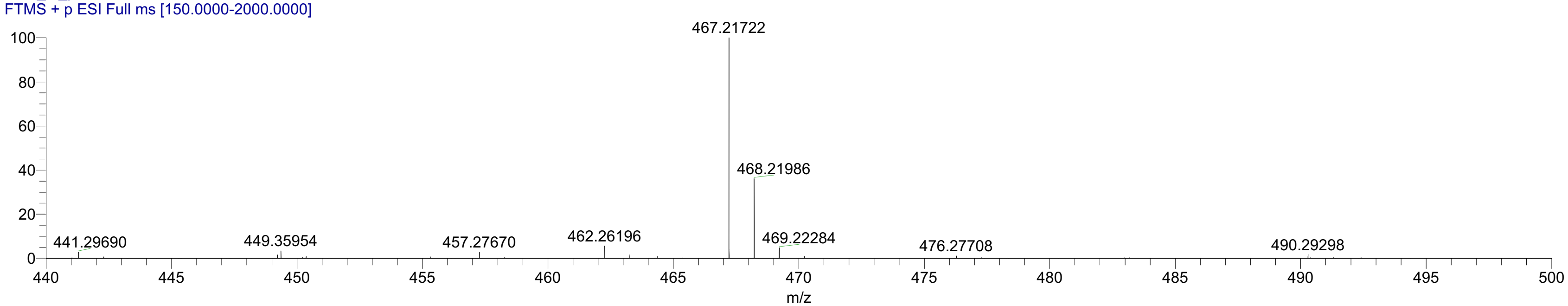
231849_8t_pn #25-28 RT: 0.40-0.44 AV: 2 NL: 1.35E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]

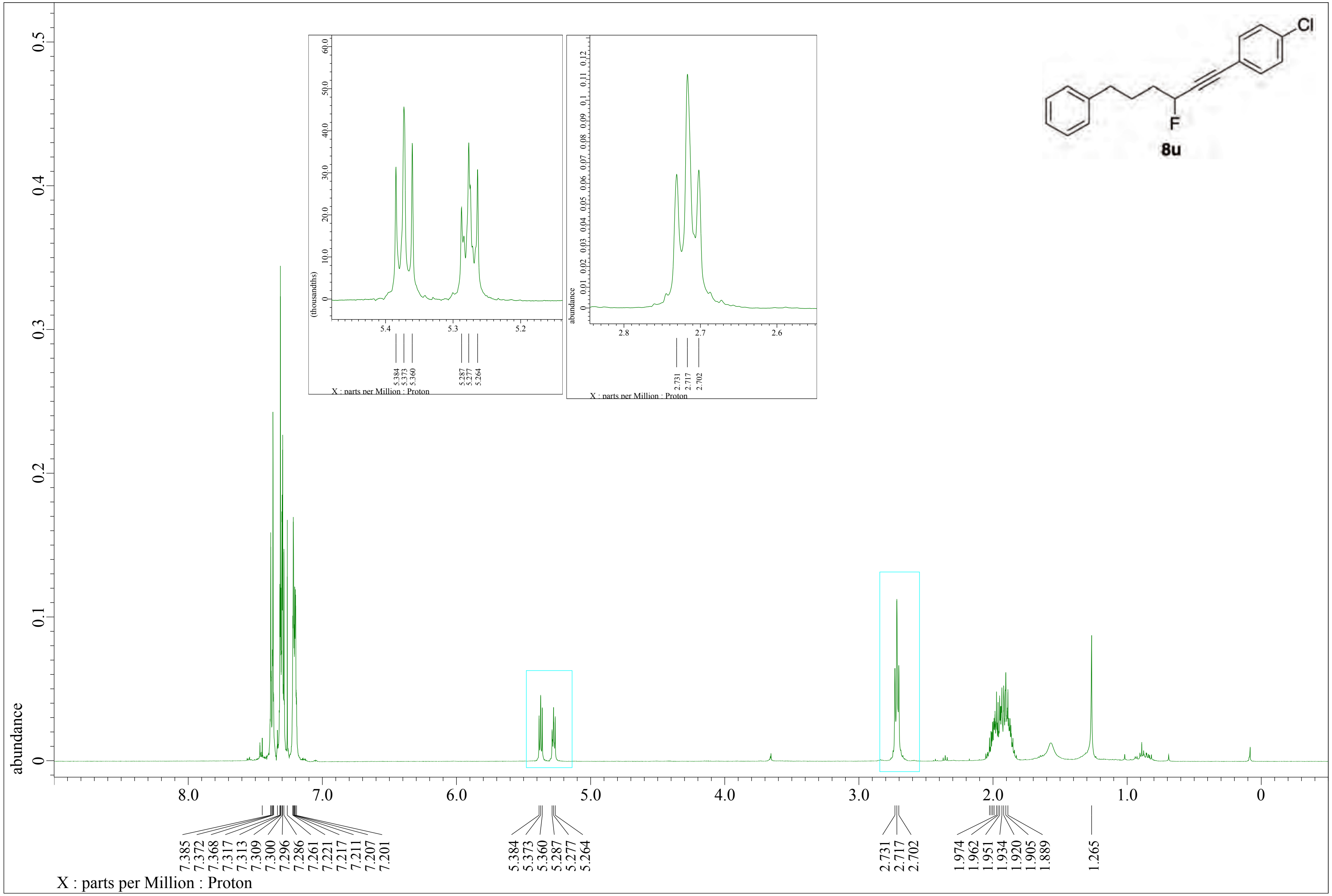




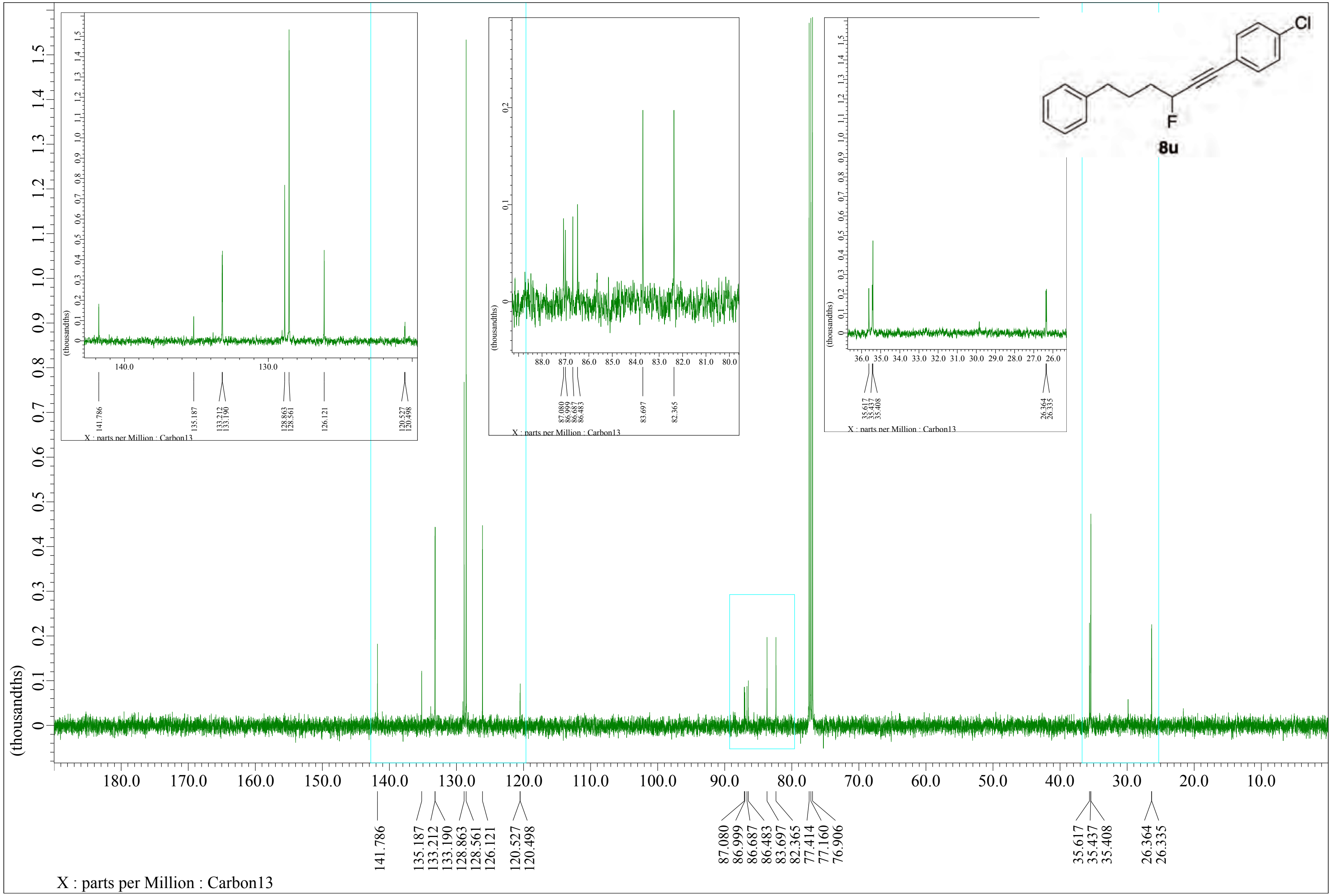
8t

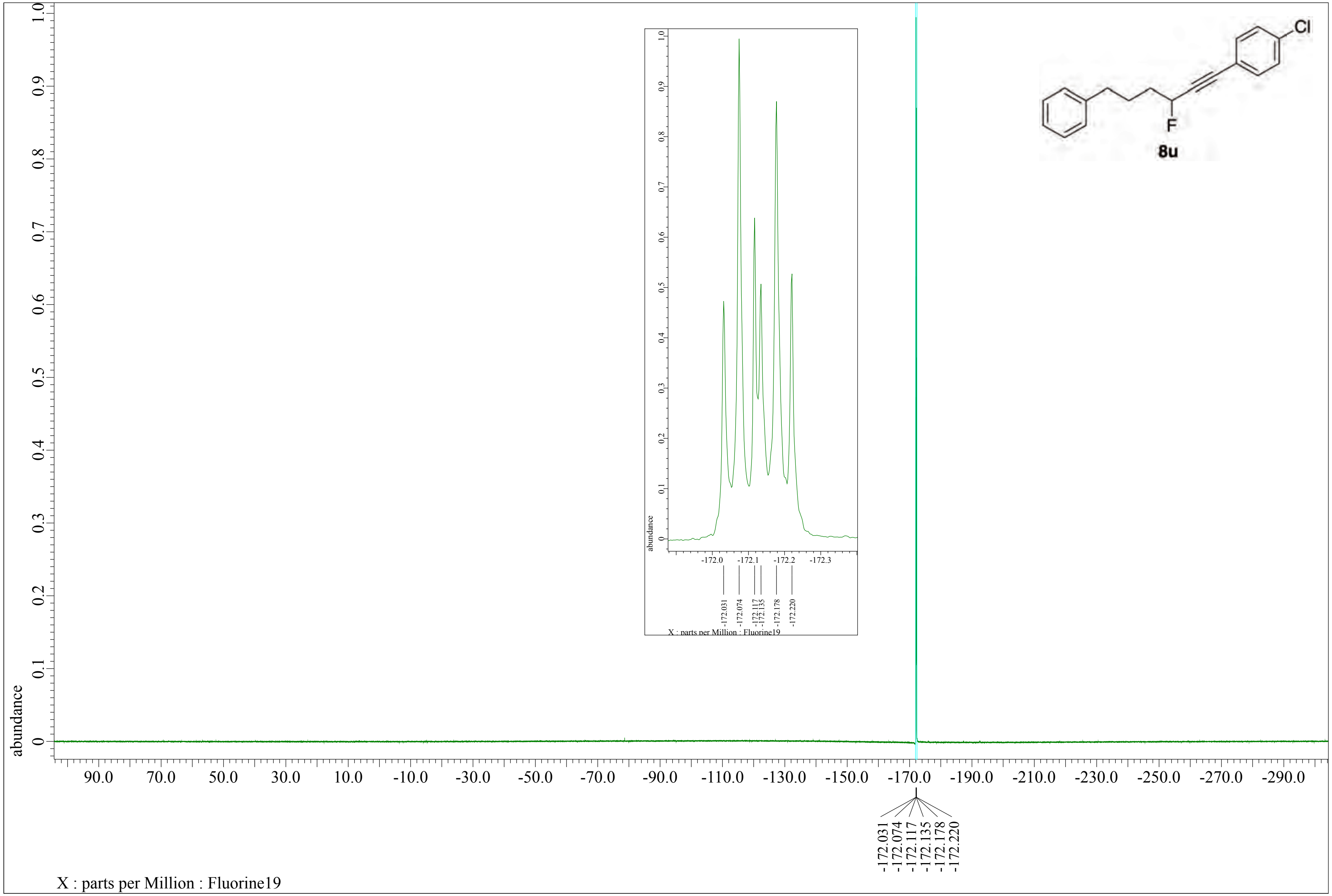
231849_8t_pn #29-32 RT: 0.47-0.50 AV: 2 NL: 7.21E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



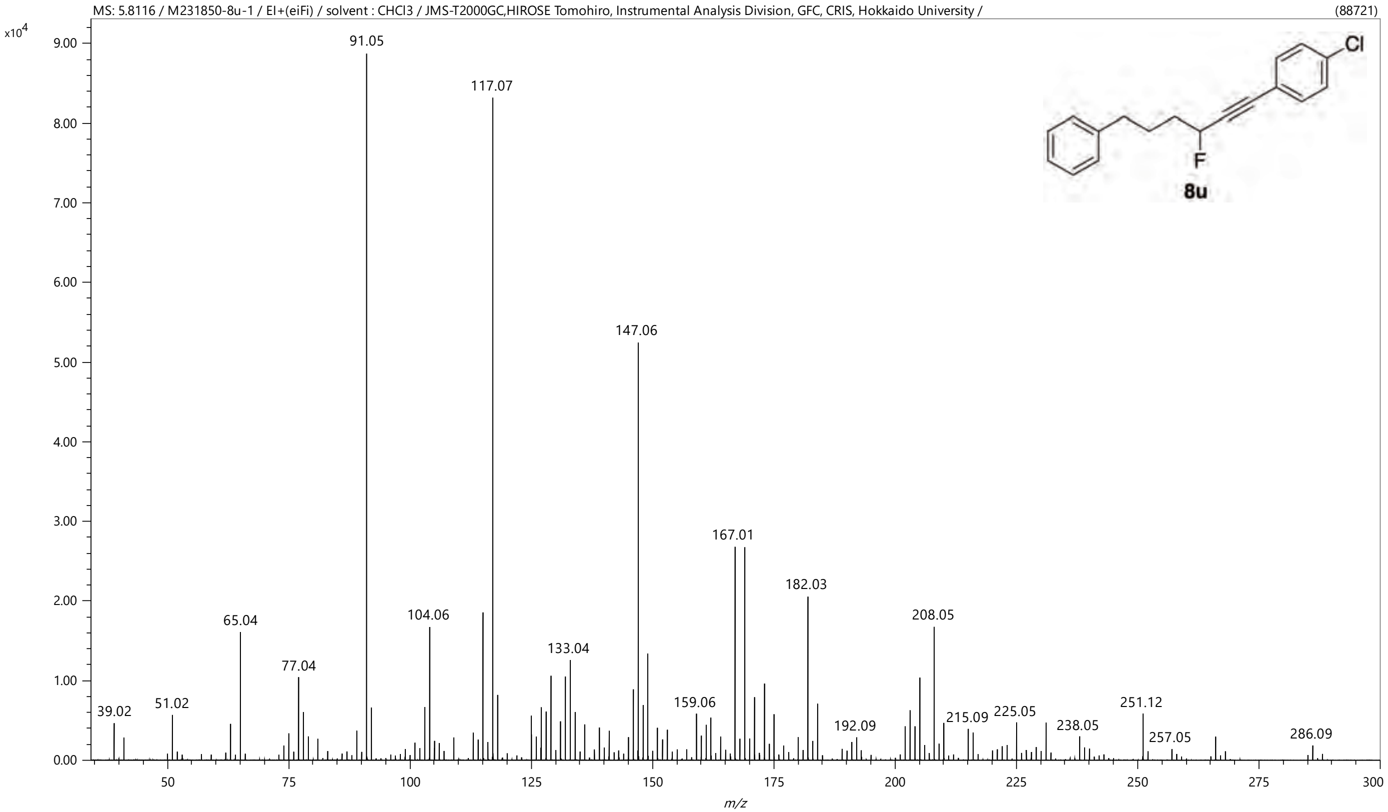


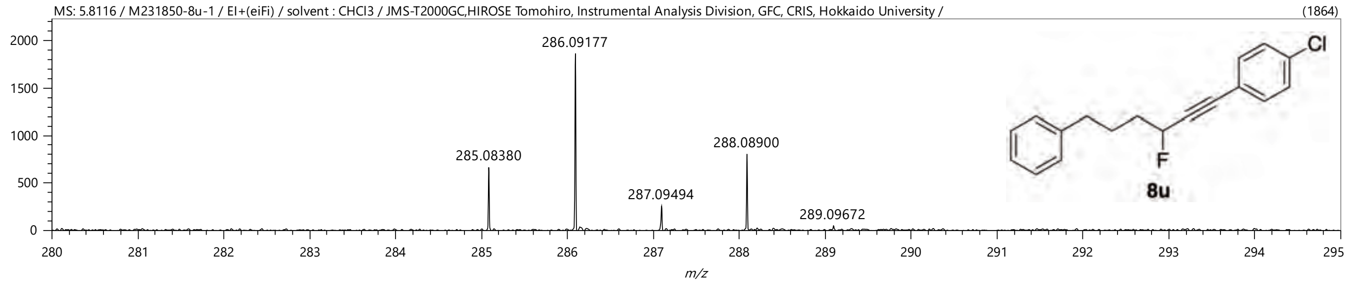
8u
Cl
F
abundance
X : parts per Million : Proton
7.385 7.372 7.368 7.317 7.313 7.309 7.300 7.296 7.286 7.261 7.221 7.217 7.211 7.207 7.201
5.384 5.373 5.360 5.287 5.277 5.264
2.731 2.717 2.702
1.974 1.962 1.951 1.934 1.920 1.905 1.889
1.265

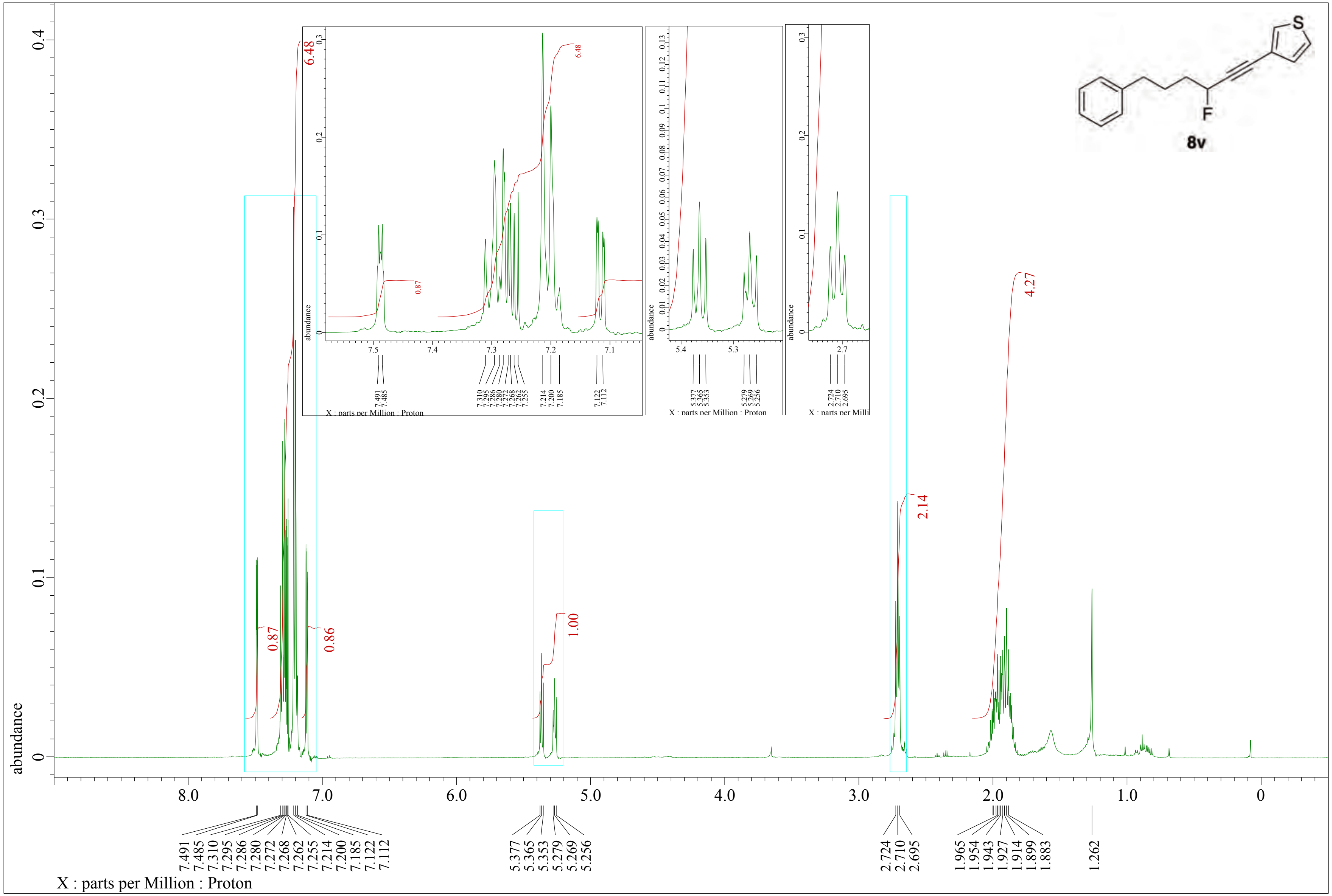

Cl
F
8u
(thousandths)
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5
180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
141.786
135.187
133.212
133.190
128.863
128.561
126.121
120.527
120.498
87.080
86.999
86.687
86.483
83.697
82.365
77.414
77.160
76.906
35.617
35.437
35.408
26.364
26.335
X : parts per Million : Carbon13

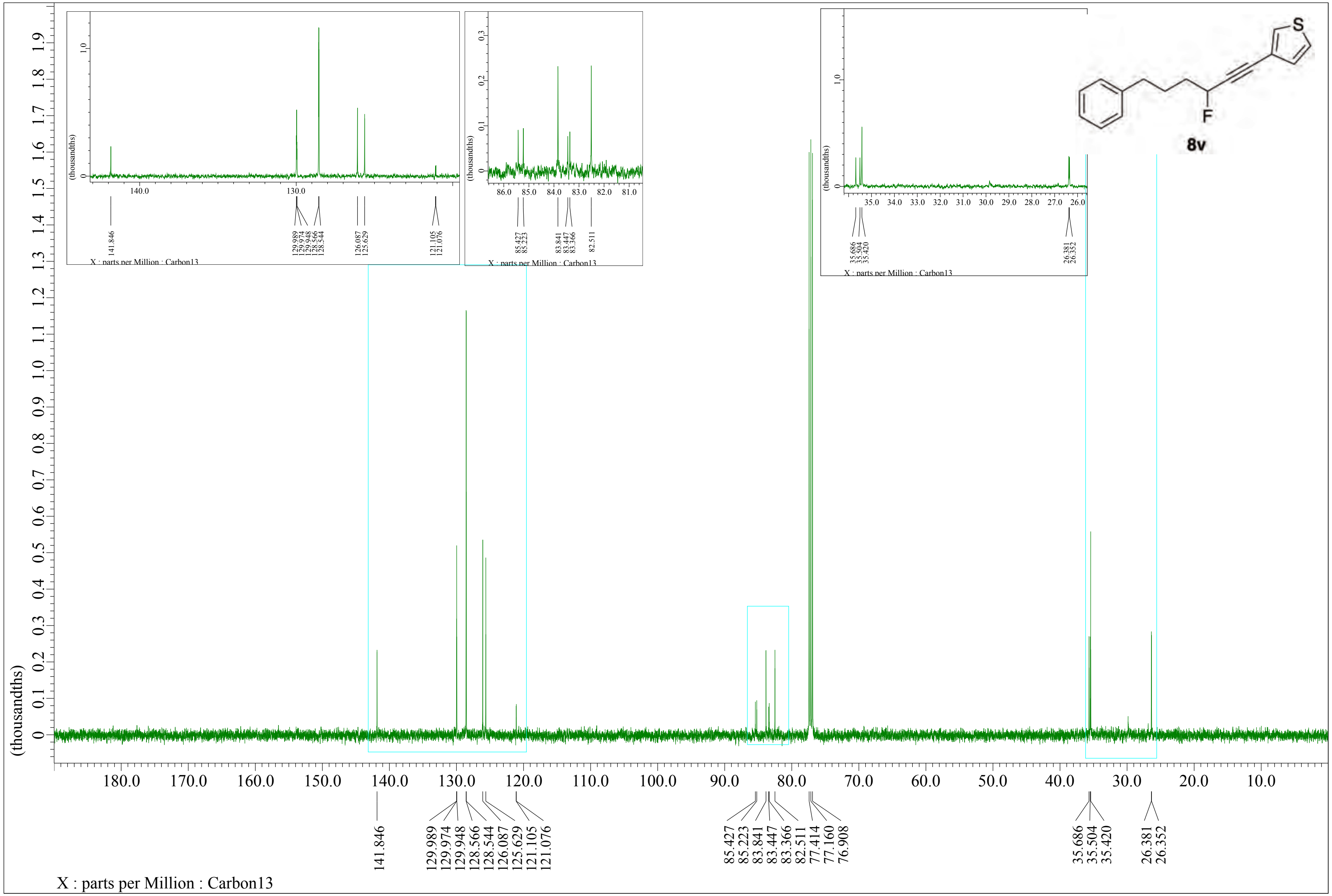


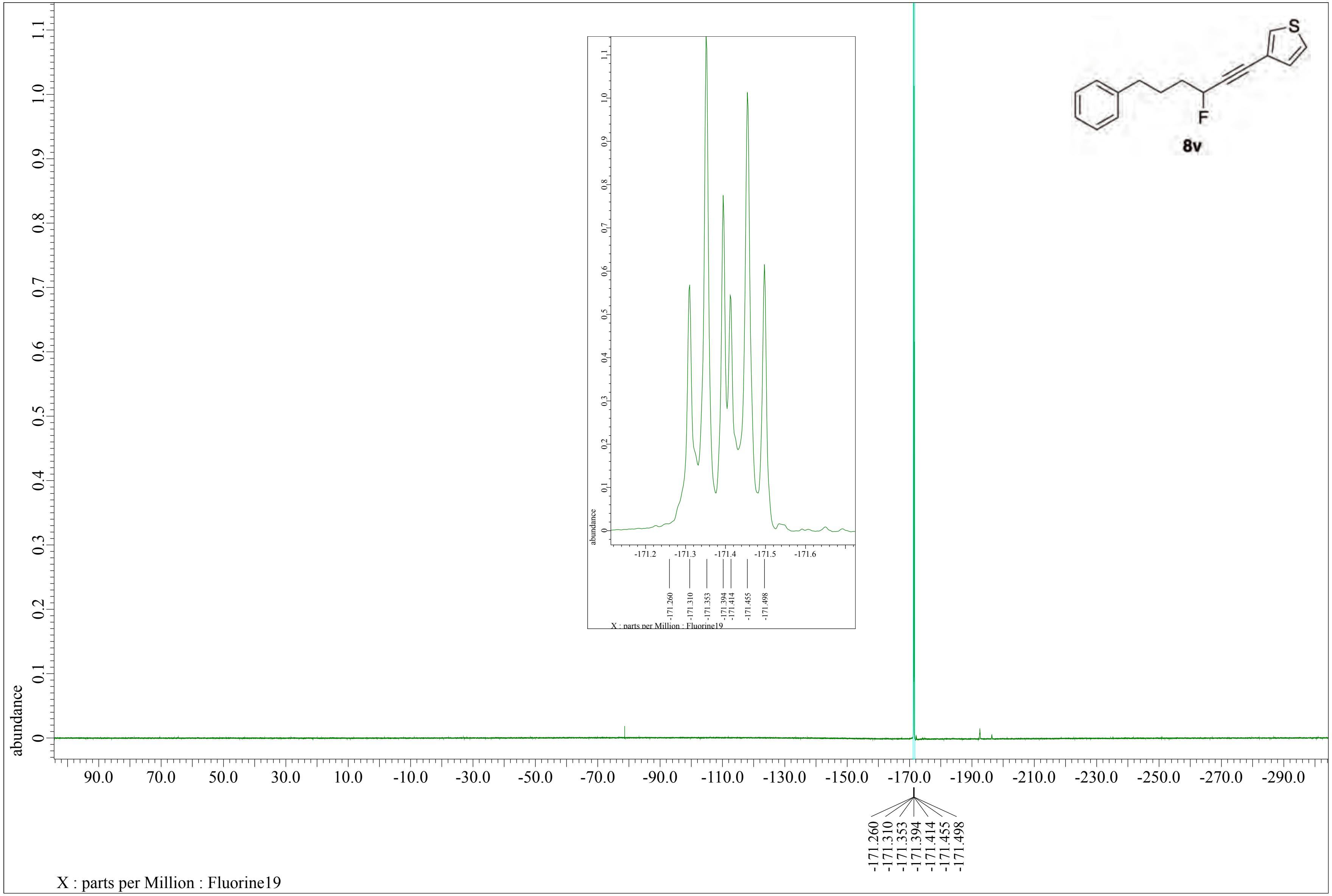
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
90.0
70.0
50.0
30.0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-170.0
-190.0
-210.0
-230.0
-250.0
-270.0
-290.0
-172.031
-172.074
-172.117
-172.135
-172.178
-172.220
X : parts per Million : Fluorine19
-172.0
-172.1
-172.2
-172.3
Cl
F
8u


MS: 5.8116 / M231850-8u-1 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(88721)
x10^4
91.05
117.07
147.06
167.01
182.03
208.05
65.04
104.06
133.04
77.04
39.02
51.02
159.06
192.09
215.09
225.05
238.05
251.12
257.05
286.09
m/z
Cl
F
8u


MS: 5.8116 / M231850-8u-1 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(1864)
286.09177
285.08380
288.08900
287.09494
289.09672
m/z
Cl
F
8u

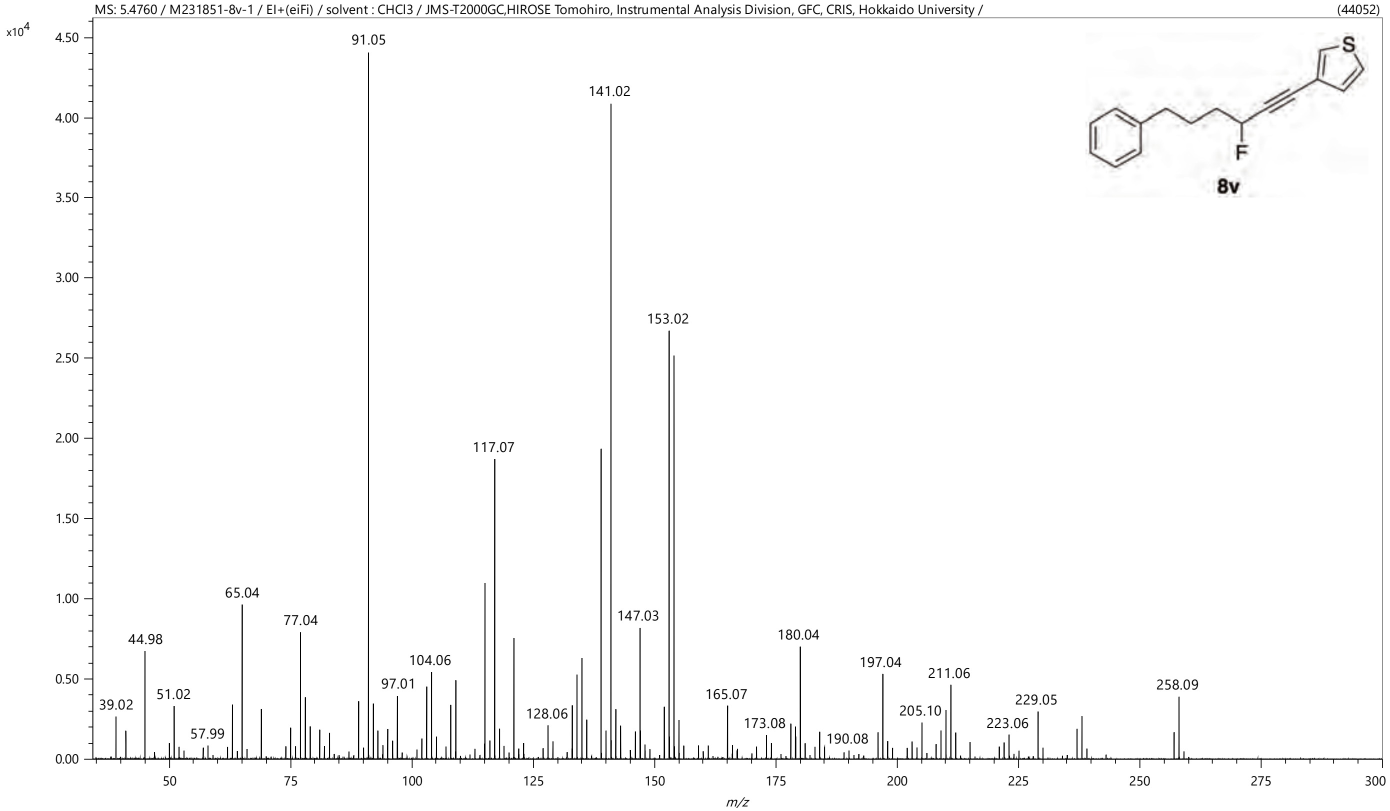

8v
F
S
abundance
X : parts per Million : Proton
6.48
0.87
0.86
1.00
2.14
4.27
7.491
7.485
7.310
7.295
7.286
7.280
7.272
7.268
7.262
7.255
7.214
7.200
7.185
7.122
7.112
5.377
5.365
5.353
5.279
5.269
5.256
2.724
2.710
2.695
1.965
1.954
1.943
1.927
1.914
1.899
1.883
1.262

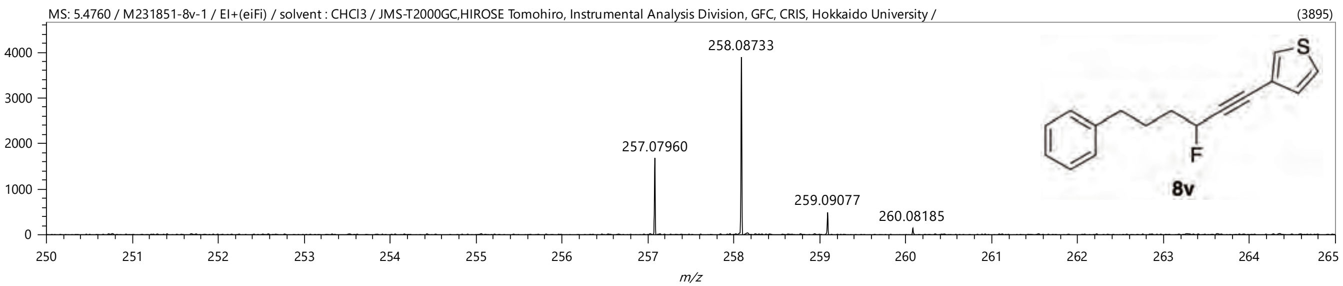

8v
X : parts per Million : Carbon13
(thousandths)
141.846
129.989
129.974
129.948
128.566
128.544
126.087
125.629
121.105
121.076
85.427
85.223
83.841
83.447
83.366
82.511
77.414
77.160
76.908
35.686
35.504
35.420
26.381
26.352

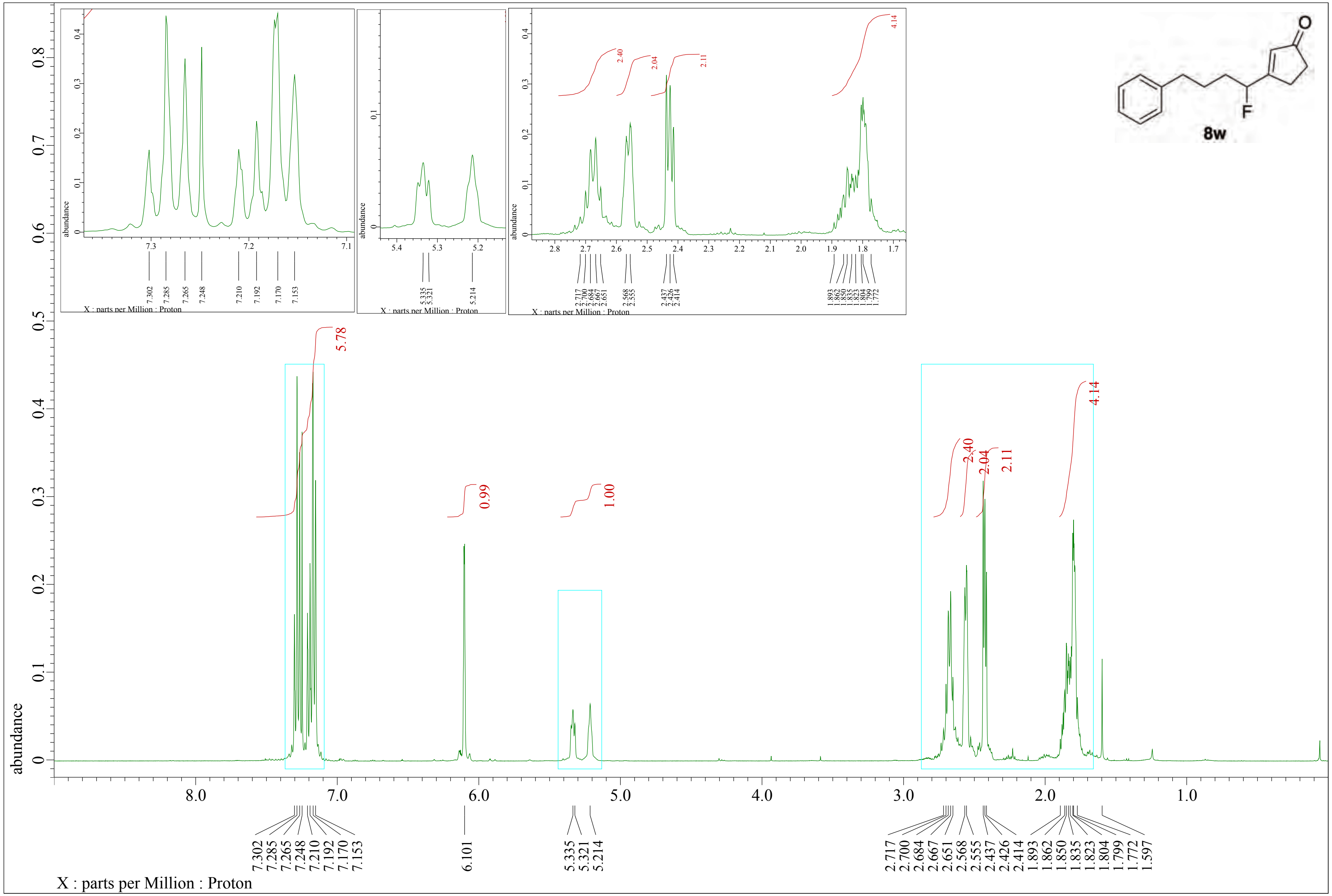


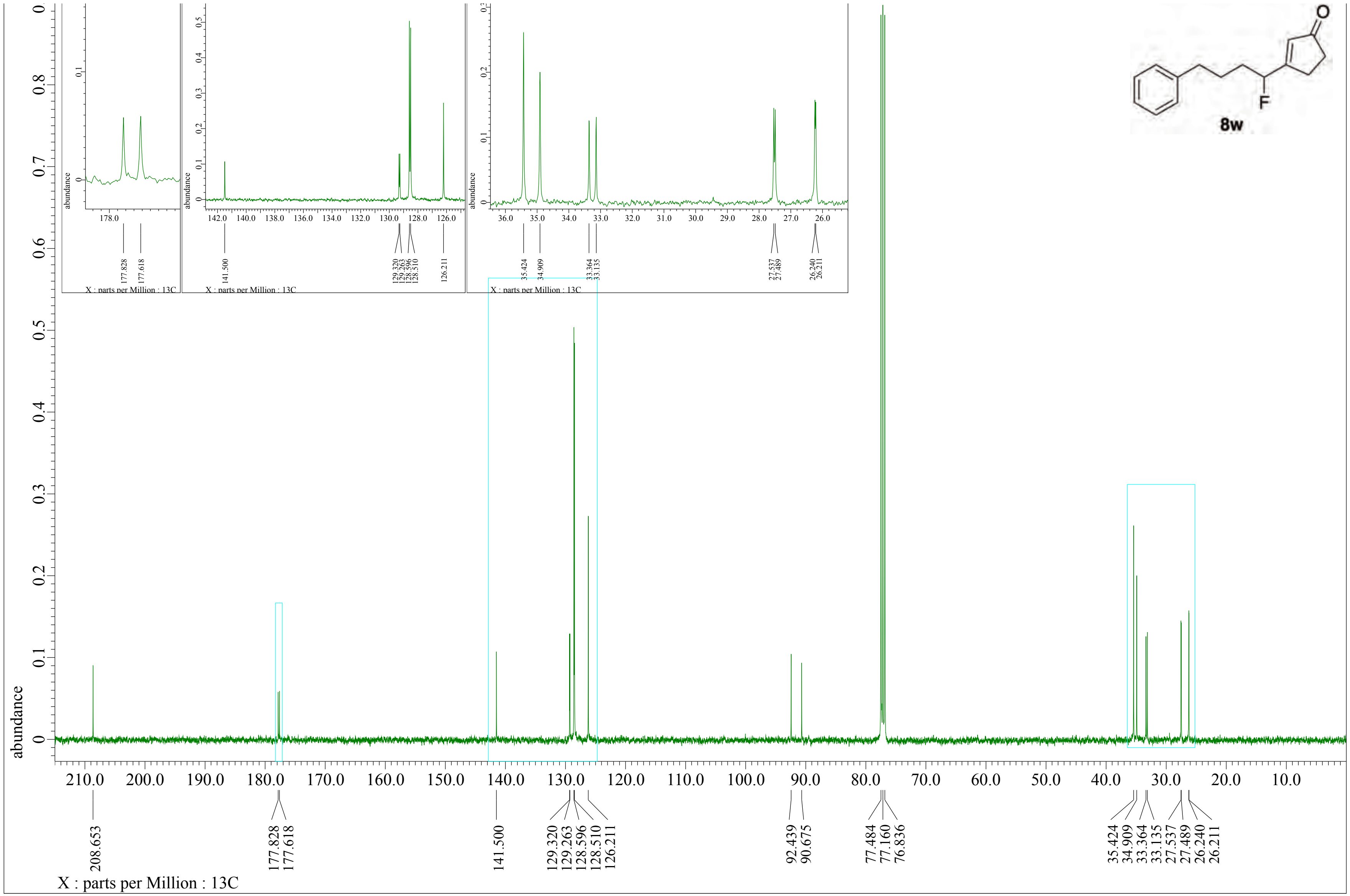
abundance
X : parts per Million : Fluorine19
-171.260
-171.310
-171.353
-171.394
-171.414
-171.455
-171.498

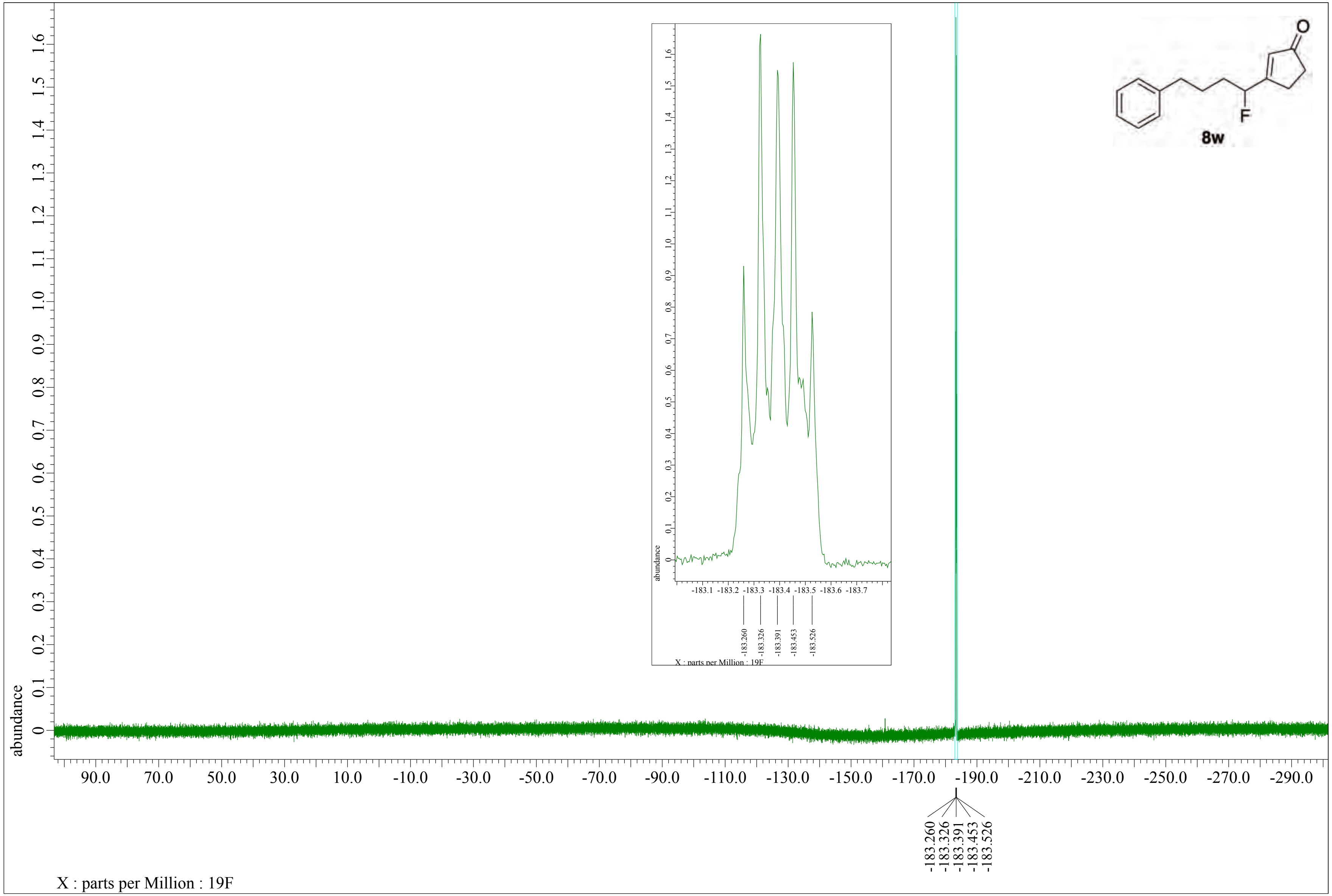
8v


MS: 5.4760 / M231851-8v-1 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(44052)
x10^4
91.05
141.02
153.02
117.07
65.04
77.04
44.98
147.03
180.04
104.06
197.04
211.06
258.09
39.02
51.02
97.01
57.99
128.06
165.07
173.08
190.08
205.10
223.06
229.05
m/z
S
F
8v


MS: 5.4760 / M231851-8v-1 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(3895)
258.08733
257.07960
259.09077
260.08185
m/z
S
F
8v


8w
X : parts per Million : Proton
abundance


8w
F
O
abundance
X : parts per Million : 13C
208.653
177.828
177.618
141.500
129.320
129.263
128.596
128.510
126.211
92.439
90.675
77.484
77.160
76.836
35.424
34.909
33.364
33.135
27.537
27.489
26.240
26.211

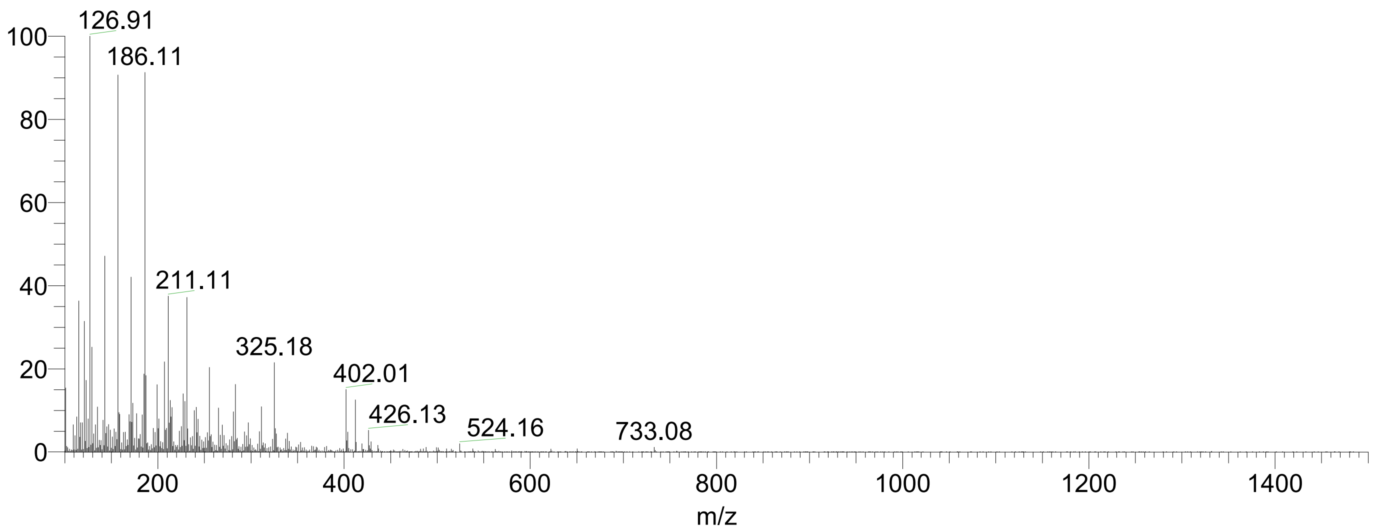


8w
abundance
X : parts per Million : 19F
-183.260
-183.326
-183.391
-183.453
-183.526

Sample No. : C:\Xcalibur\...\0517\BG_230238_E _ɔn Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 05/17/23 13:40:09
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

8w

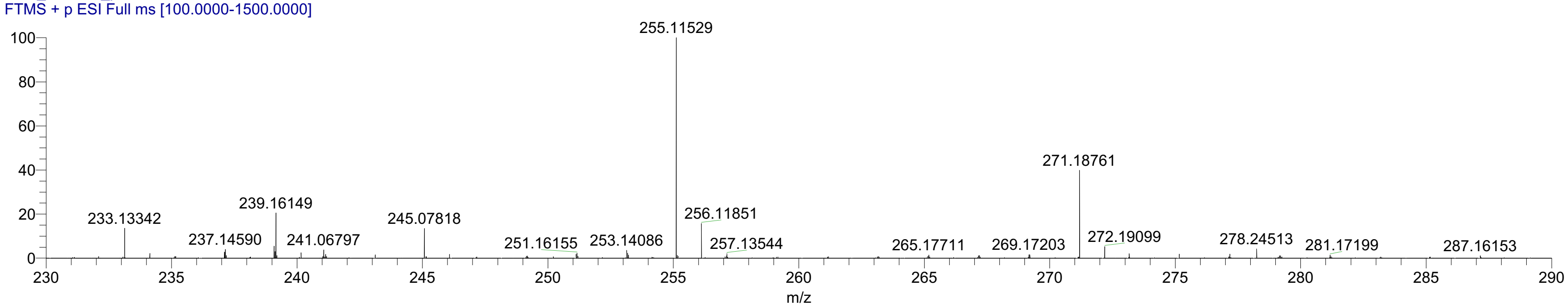
NL: 7.52E7
BG_230238_EK0037_pn#18-32 RT: 0.31-0.49 AV: 7 T: FTMS + c ESI Full ms [100.00-1500.00]



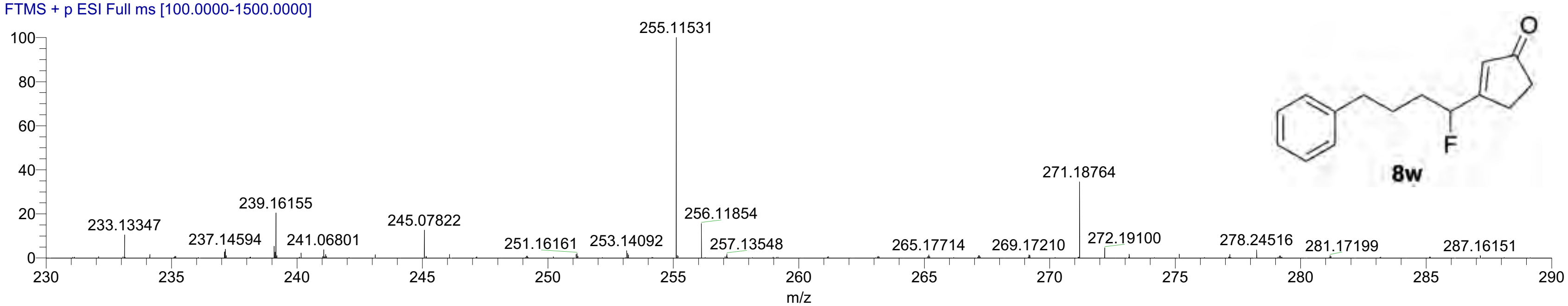
NL: 6.03E6
BG_230238_EK0037_pn#18-32 RT: 0.30-0.50 AV: 8 T: FTMS - c ESI Full ms [100.00-1500.00]

Sample No. : C:\Xcalibur\...\0517\230238_EK0037_pn   Instrument : Exactive Plus   Mobile phase solvent : MeOH
Operator name : hayashi harumi   Sample solvent : CHCl3
Date : 05/17/23 11:39:59
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

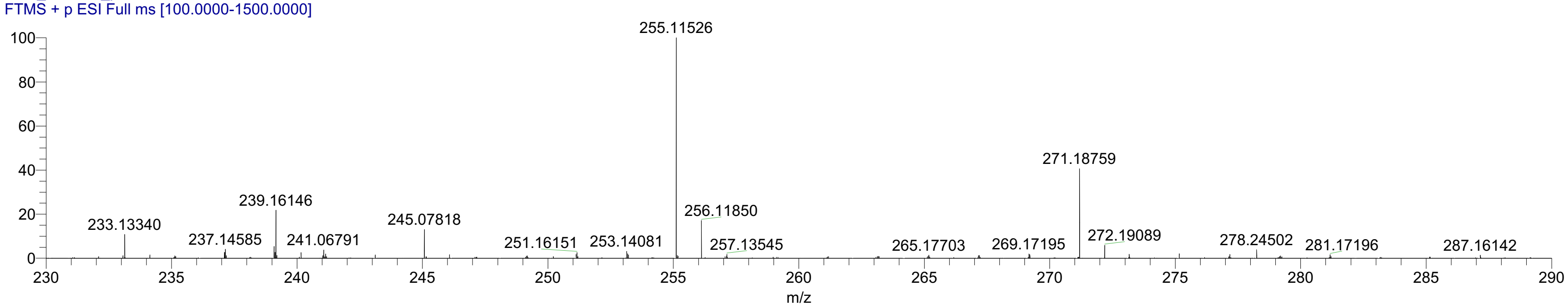
230238_EK0037_pn #22-25 RT: 0.37-0.40 AV: 2 NL: 2.55E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

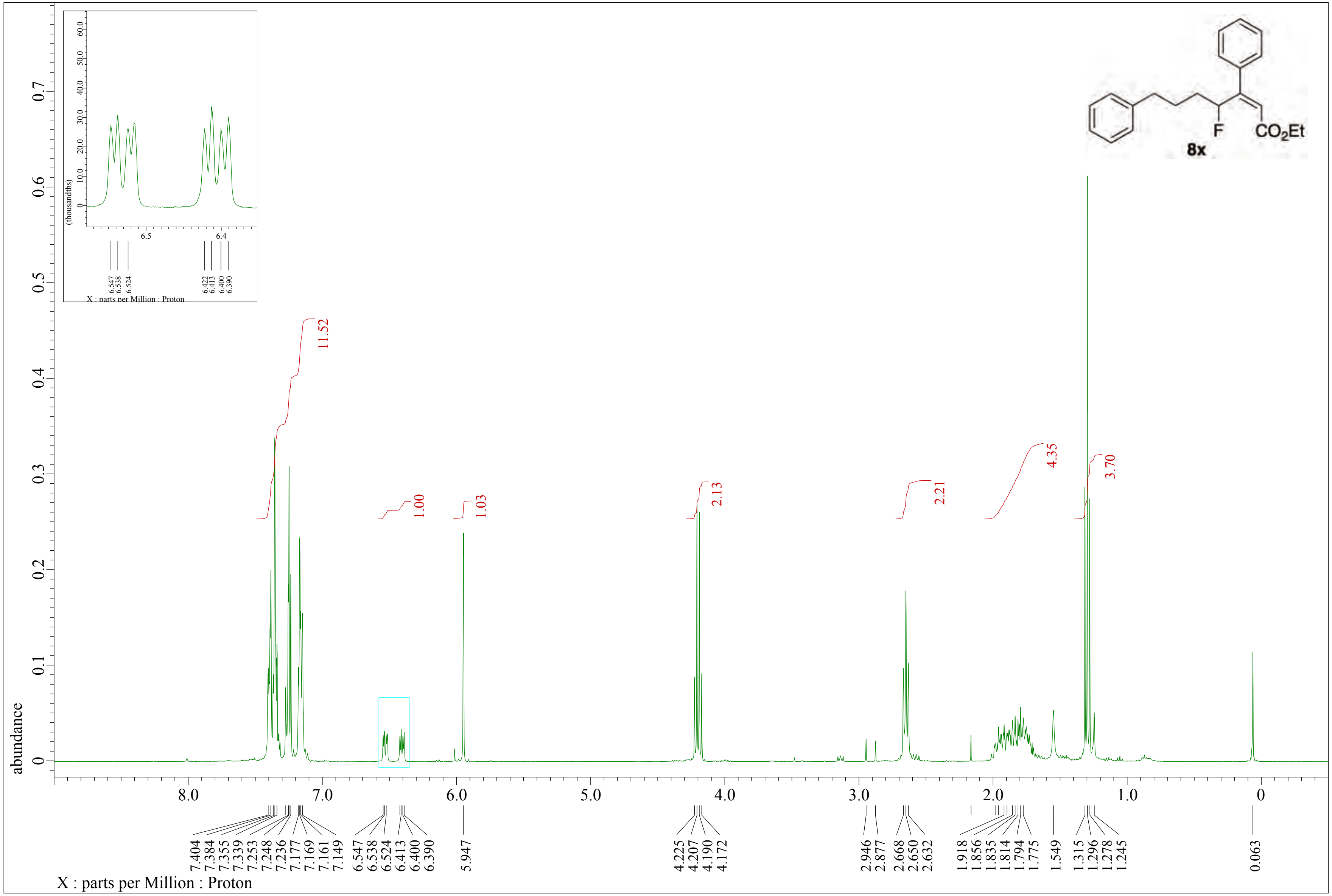


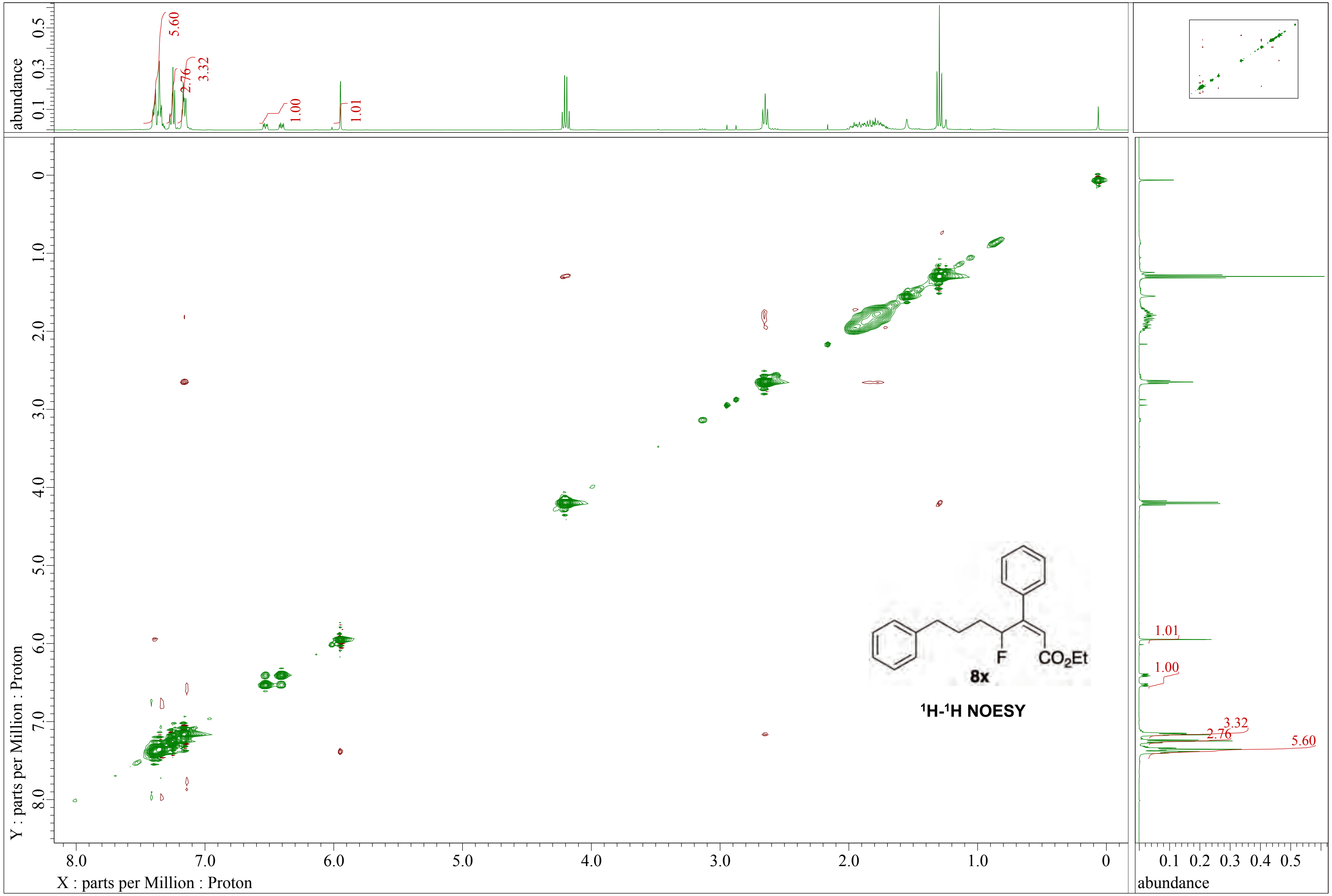
230238_EK0037_pn #25-28 RT: 0.40-0.43 AV: 2 NL: 2.72E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

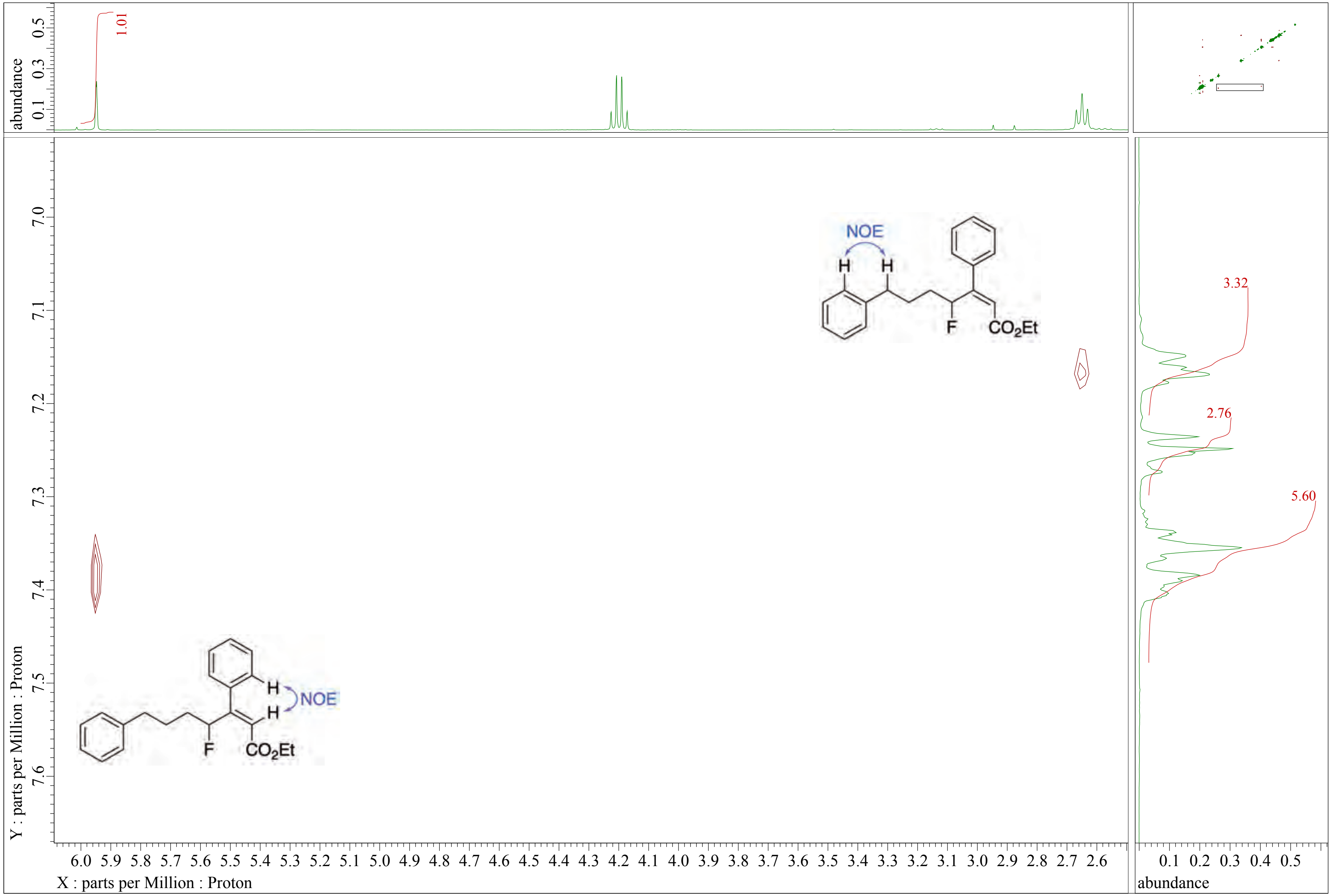


230238_EK0037_pn #28-32 RT: 0.46-0.49 AV: 2 NL: 1.82E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

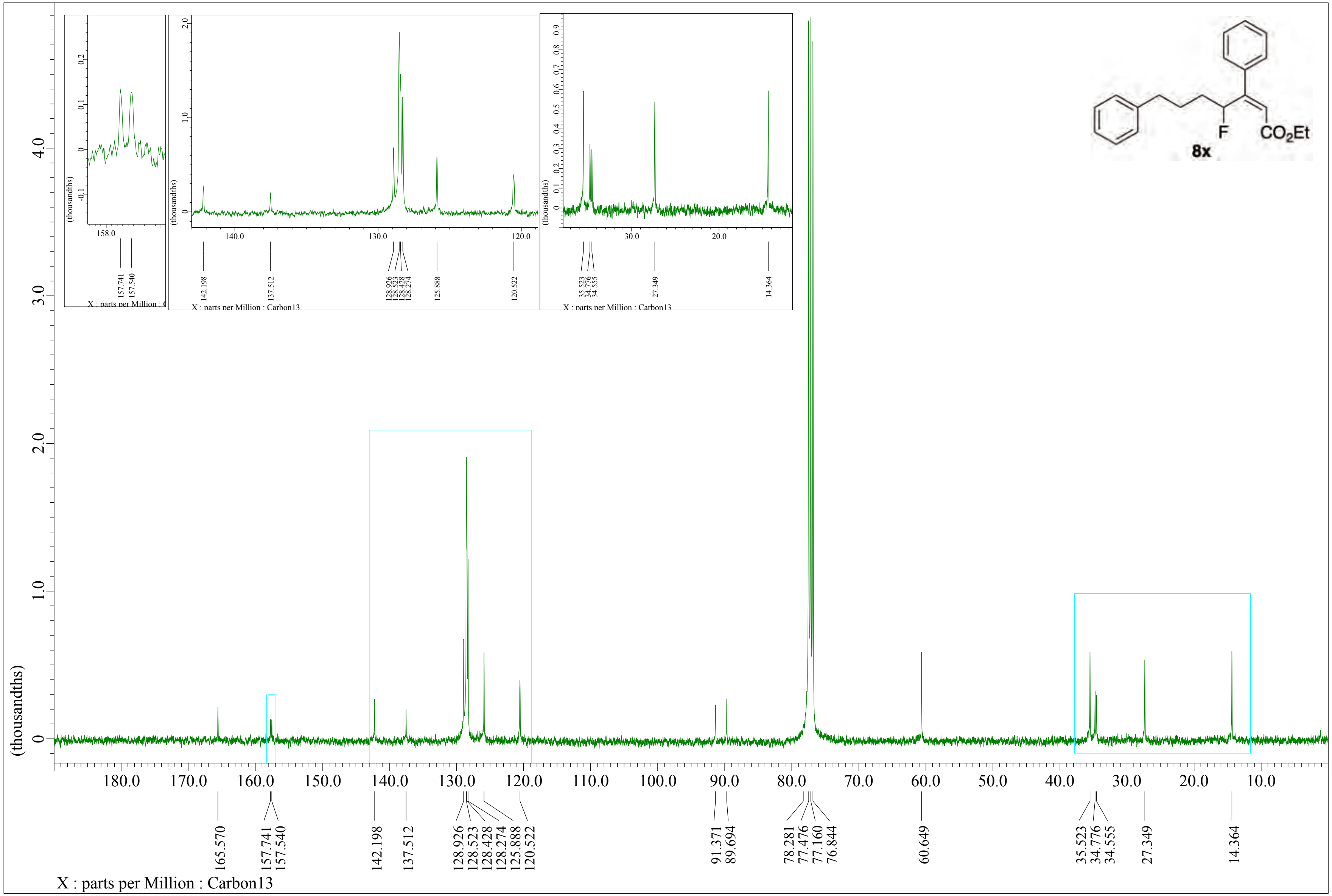



abundance
X : parts per Million : Proton
8x
F
CO2Et
11.52
1.00
1.03
2.13
2.21
4.35
3.70
7.404
7.384
7.355
7.339
7.253
7.248
7.236
7.177
7.169
7.161
7.149
6.547
6.538
6.524
6.413
6.400
6.390
5.947
4.225
4.207
4.190
4.172
2.946
2.877
2.668
2.650
2.632
1.918
1.856
1.835
1.814
1.794
1.775
1.549
1.315
1.296
1.278
1.245
0.063
(thousandths)
6.547
6.538
6.524
6.422
6.413
6.400
6.390
X : parts per Million : Proton

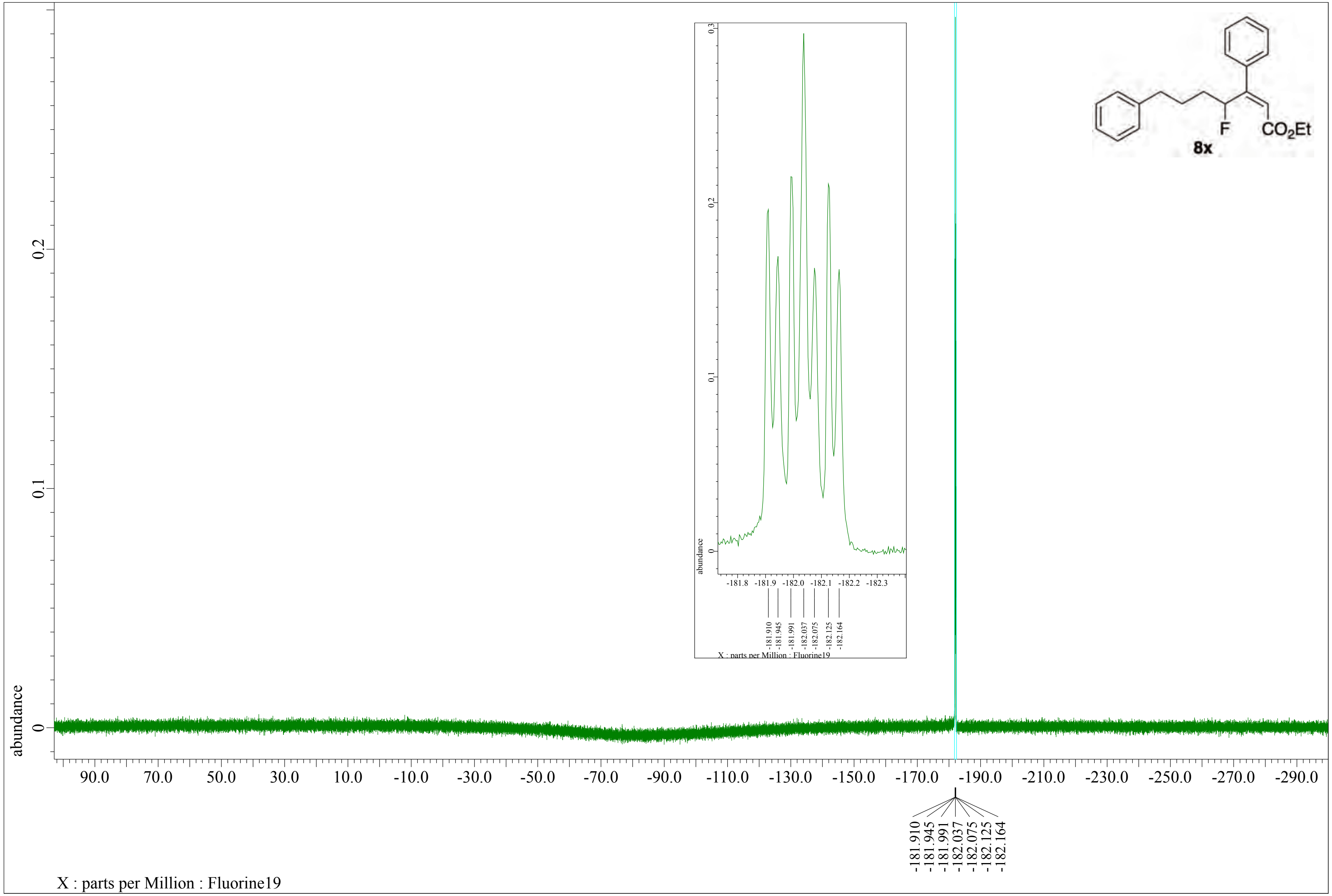

abundance
0.1
0.3
0.5
5.60
2.76
3.32
1.00
1.01
Y : parts per Million : Proton
X : parts per Million : Proton
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
F
CO2Et
8x
1H-1H NOESY
0.1 0.2 0.3 0.4 0.5
abundance



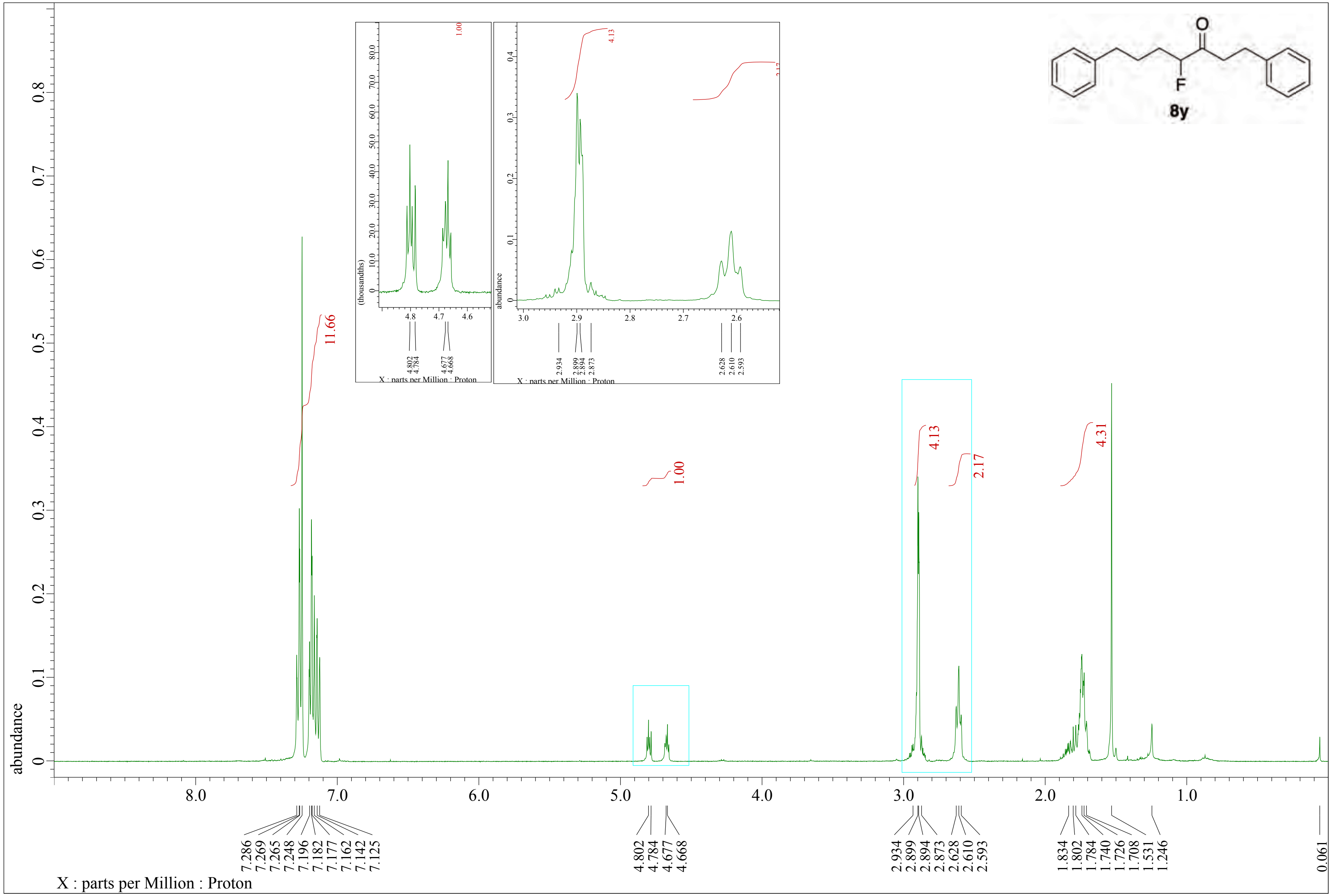
NOE
F
CO_2Et
H
NOE
H
1.01
3.32
2.76
5.60
abundance
Y : parts per Million : Proton
X : parts per Million : Proton

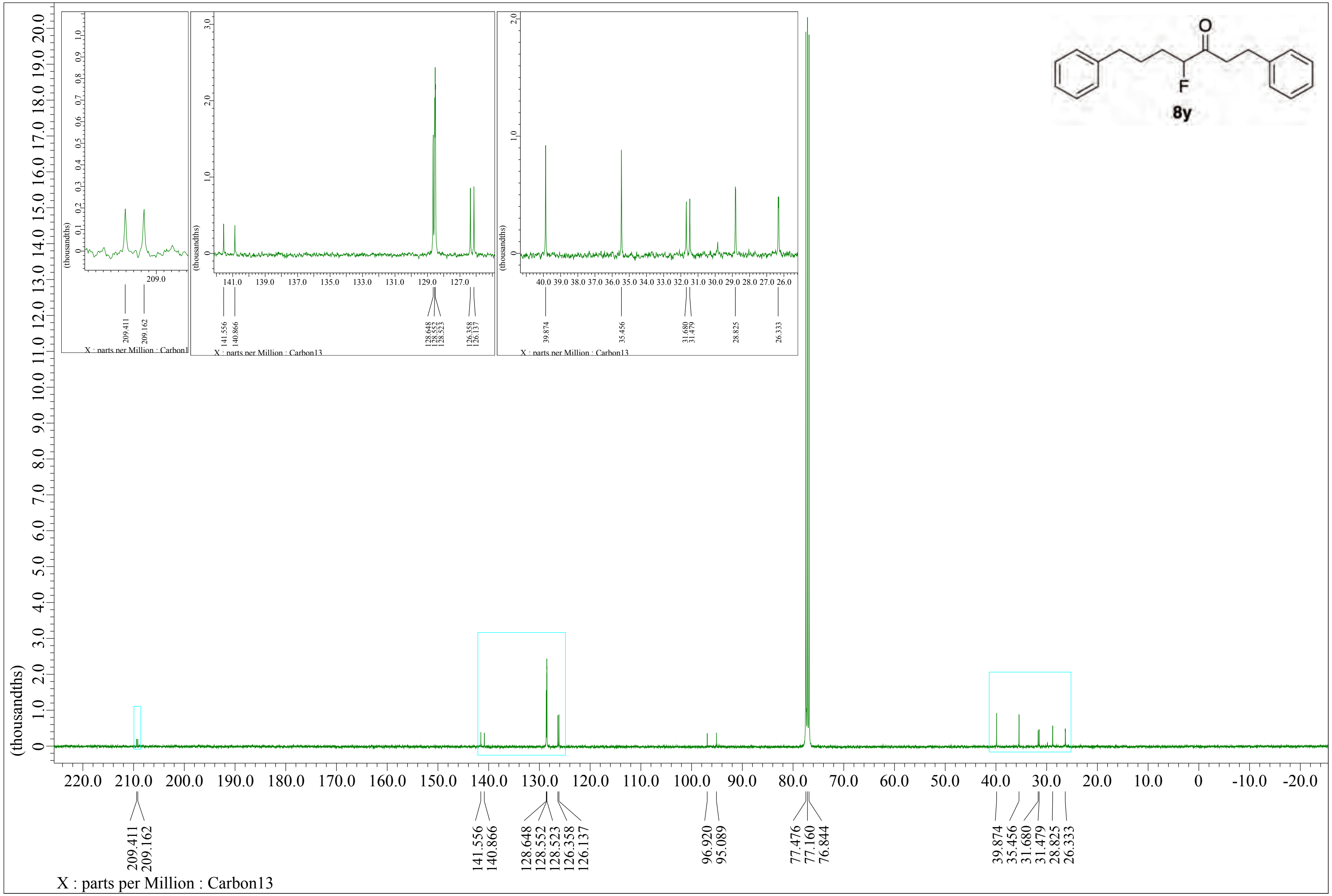


8x
(thousandths)
X : parts per Million : Carbon13
165.570
157.741
157.540
142.198
137.512
128.926
128.523
128.428
128.274
125.888
120.522
91.371
89.694
78.281
77.476
77.160
76.844
60.649
35.523
34.776
34.555
27.349
14.364

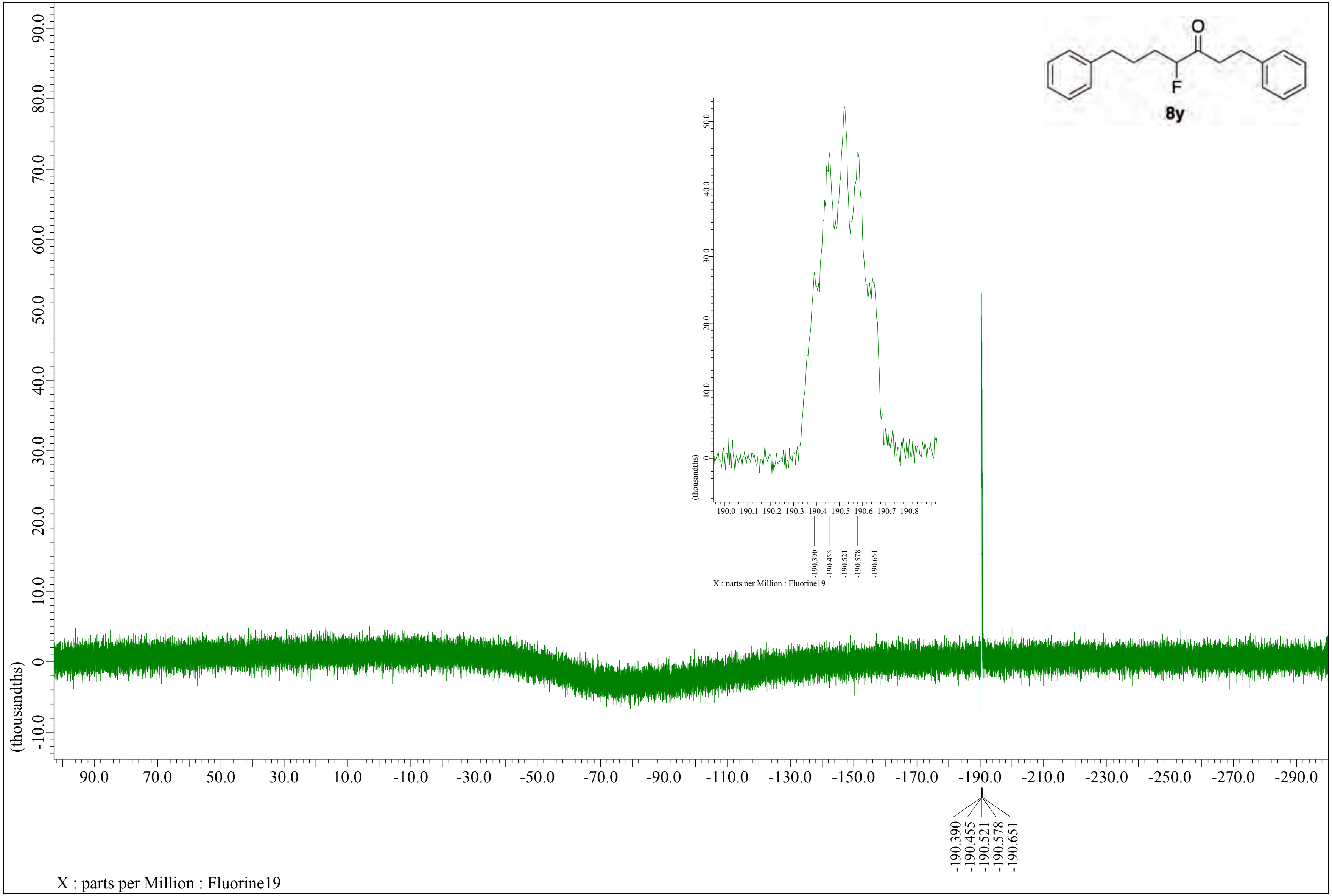


abundance
0
0.1
0.2
90.0
70.0
50.0
30.0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-170.0
-190.0
-210.0
-230.0
-250.0
-270.0
-290.0
-181.910
-181.945
-181.991
-182.037
-182.075
-182.125
-182.164
X : parts per Million : Fluorine19
F
CO2Et
8x


8y
abundance
X : parts per Million : Proton
11.66
1.00
4.13
2.17
4.31
7.286
7.269
7.265
7.248
7.196
7.182
7.177
7.162
7.142
7.125
4.802
4.784
4.677
4.668
2.934
2.899
2.894
2.873
2.628
2.610
2.593
1.834
1.802
1.784
1.740
1.726
1.708
1.531
1.246
0.061

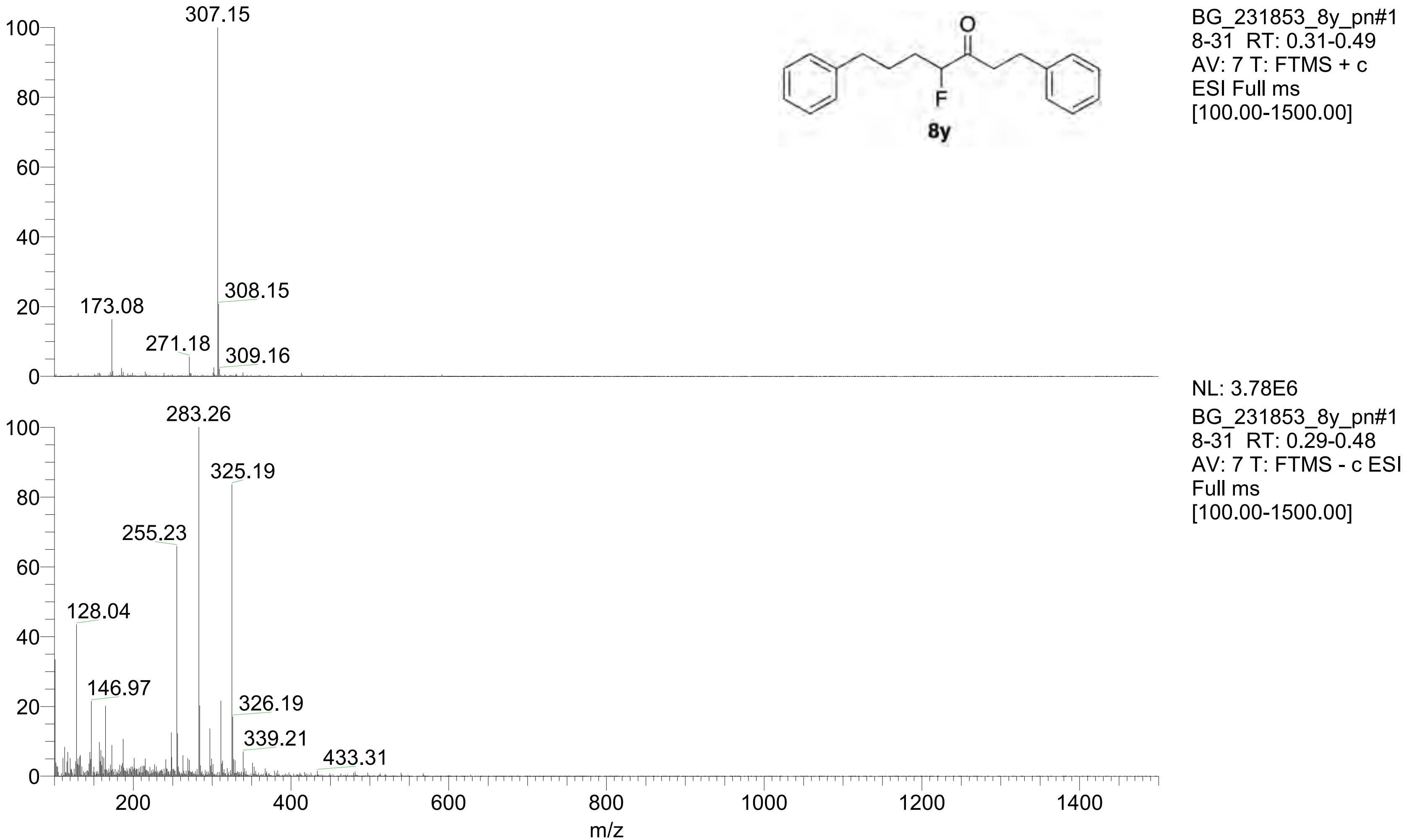


8y
F
O
(thousandths)
X : parts per Million : Carbon13
209.411
209.162
141.556
140.866
128.648
128.552
128.523
126.358
126.137
96.920
95.089
77.476
77.160
76.844
39.874
35.456
31.680
31.479
28.825
26.333



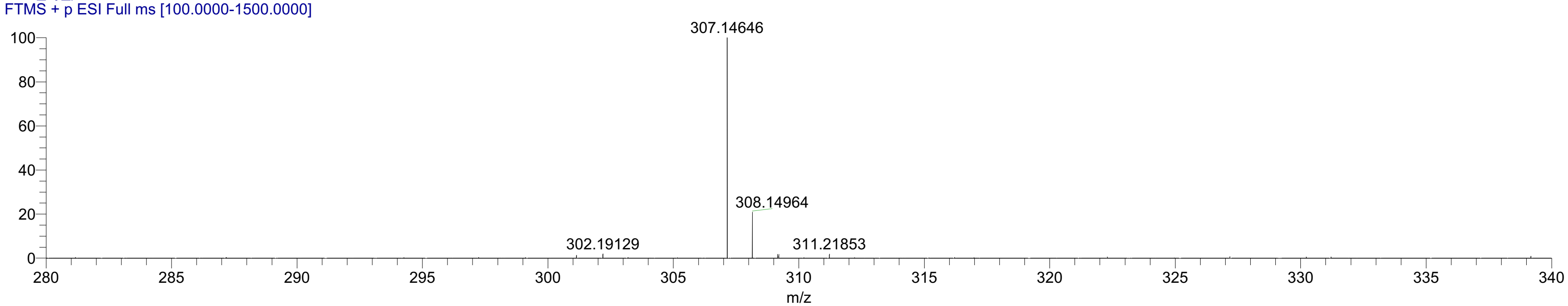
8y
F
O
X : parts per Million : Fluorine19
(thousandths)
-190.390
-190.455
-190.521
-190.578
-190.651

Sample No. : C:\Xcalibur\...\1228\BG_231853_8y_ Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 14:02:57
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

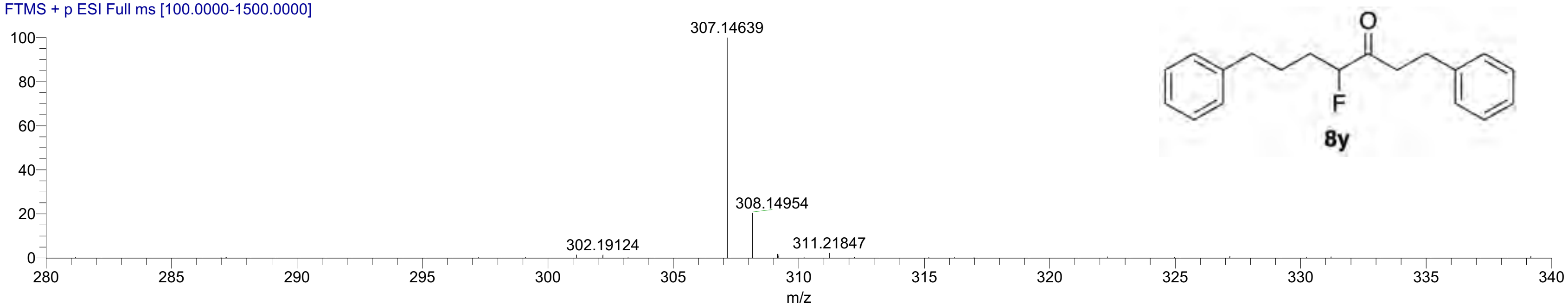


Sample No. : C:\Xcalibur\...\20231228\231853_8y_pn   Instrument : Exactive Plus   Mobile phase solvent : MeOH
Operator name : hayashi harumi   Sample solvent : CHCl3
Date : 12/28/23 11:52:49
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

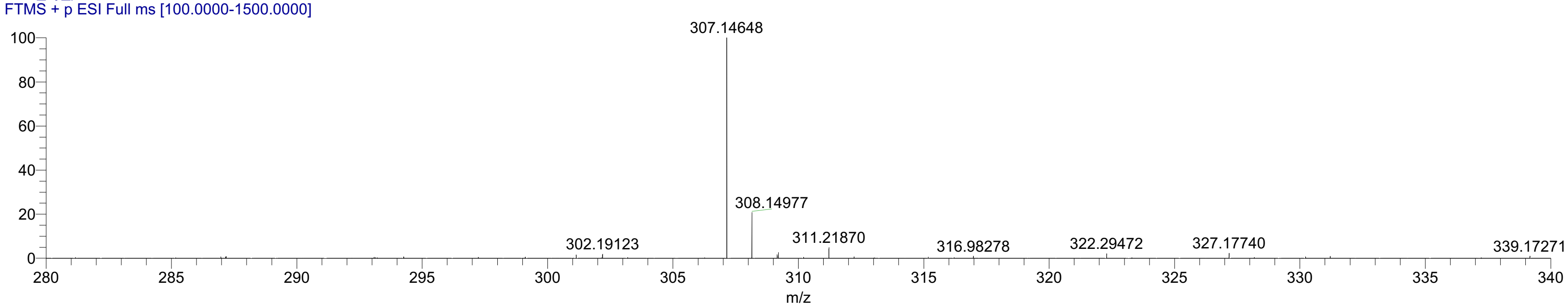
231853_8y_pn #22-25 RT: 0.37-0.40 AV: 2 NL: 2.64E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

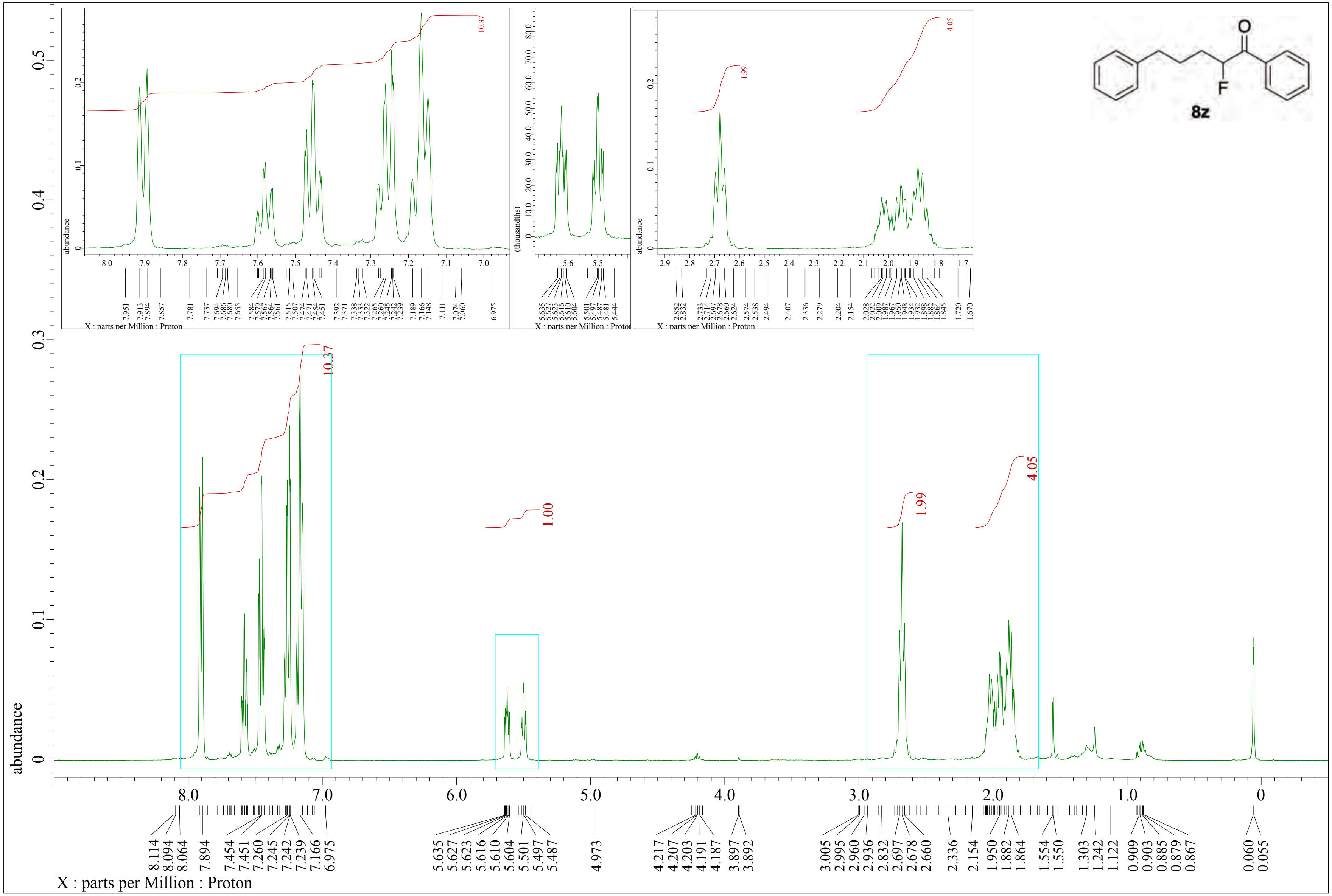


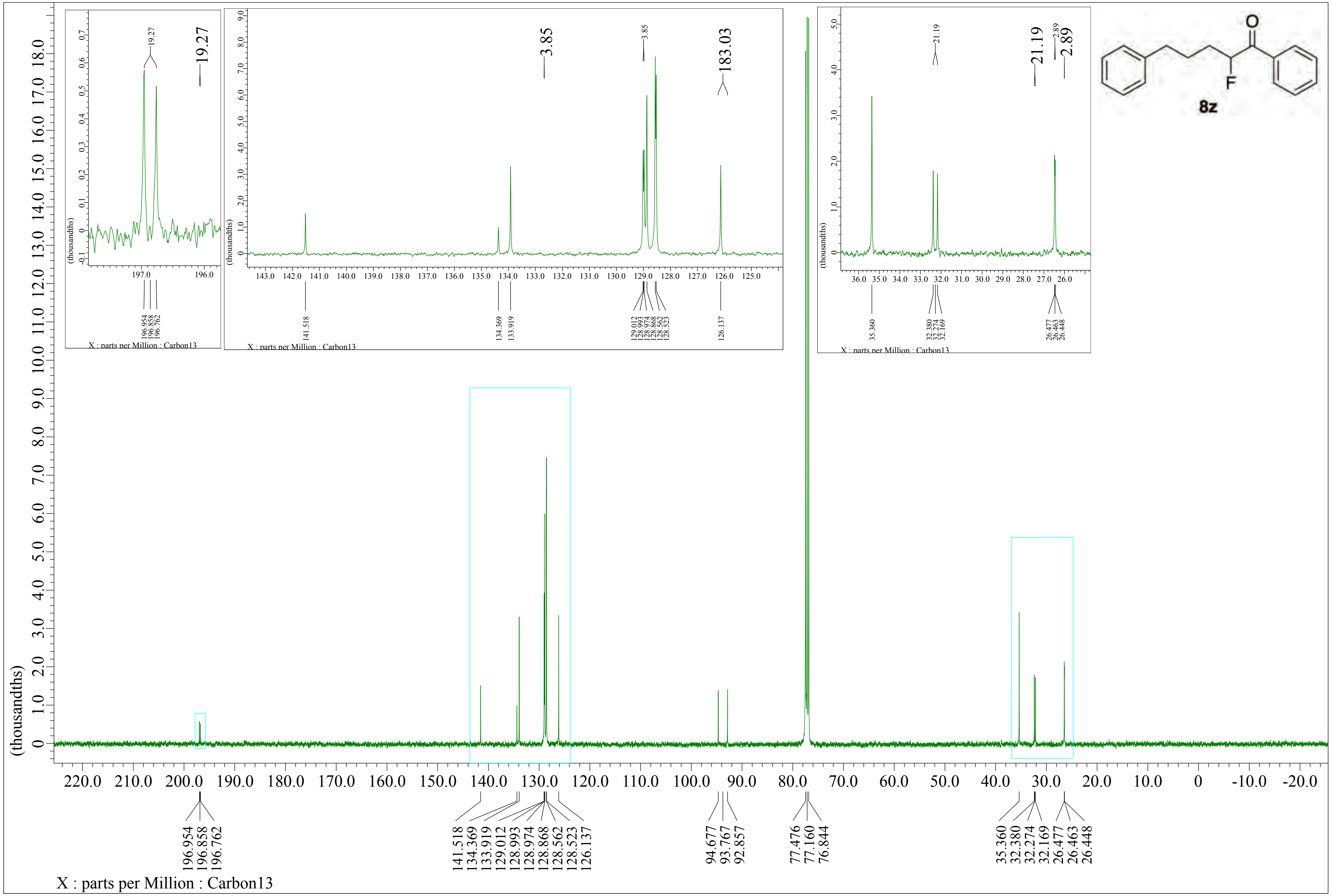
231853_8y_pn #25-28 RT: 0.40-0.43 AV: 2 NL: 2.35E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

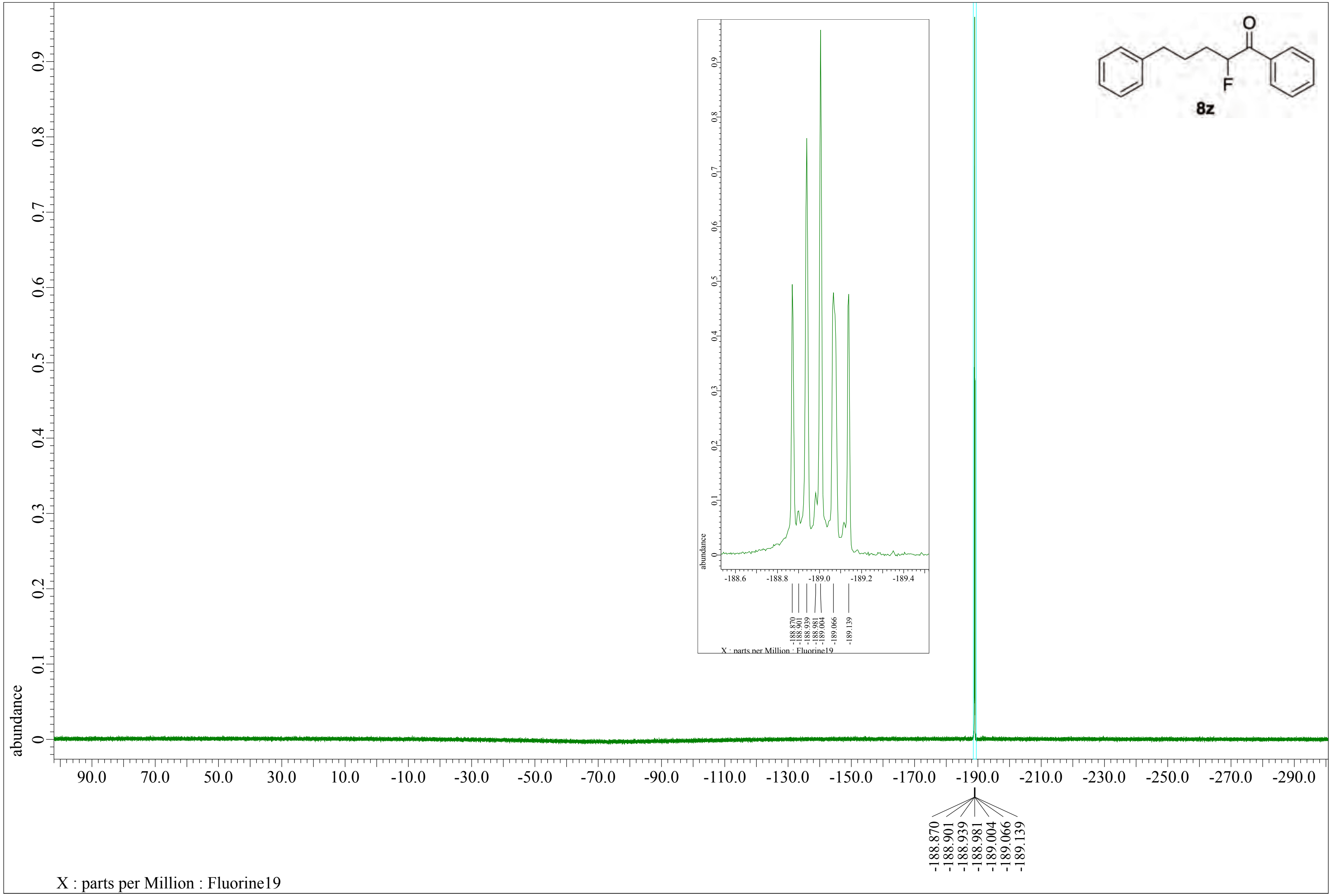


231853_8y_pn #28-31 RT: 0.46-0.49 AV: 2 NL: 7.53E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

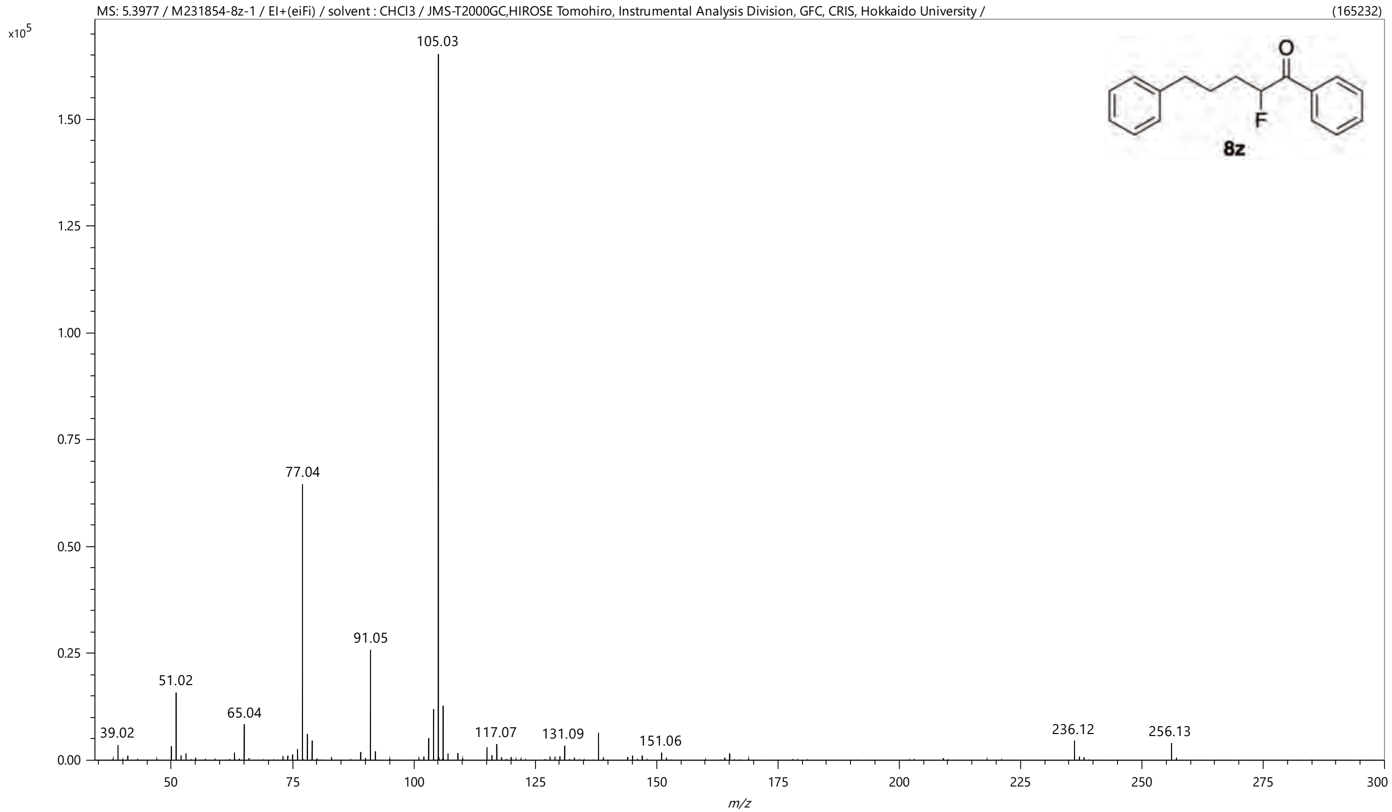


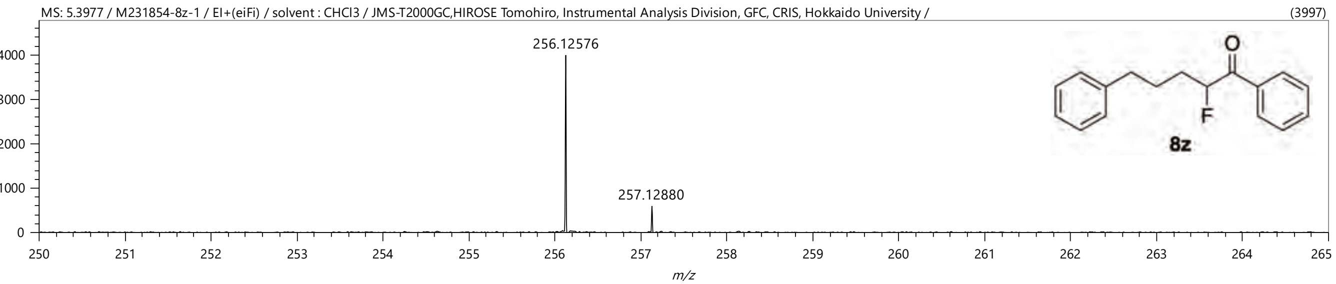

8z
10.37
1.00
1.99
4.05
abundance
X : parts per Million : Proton

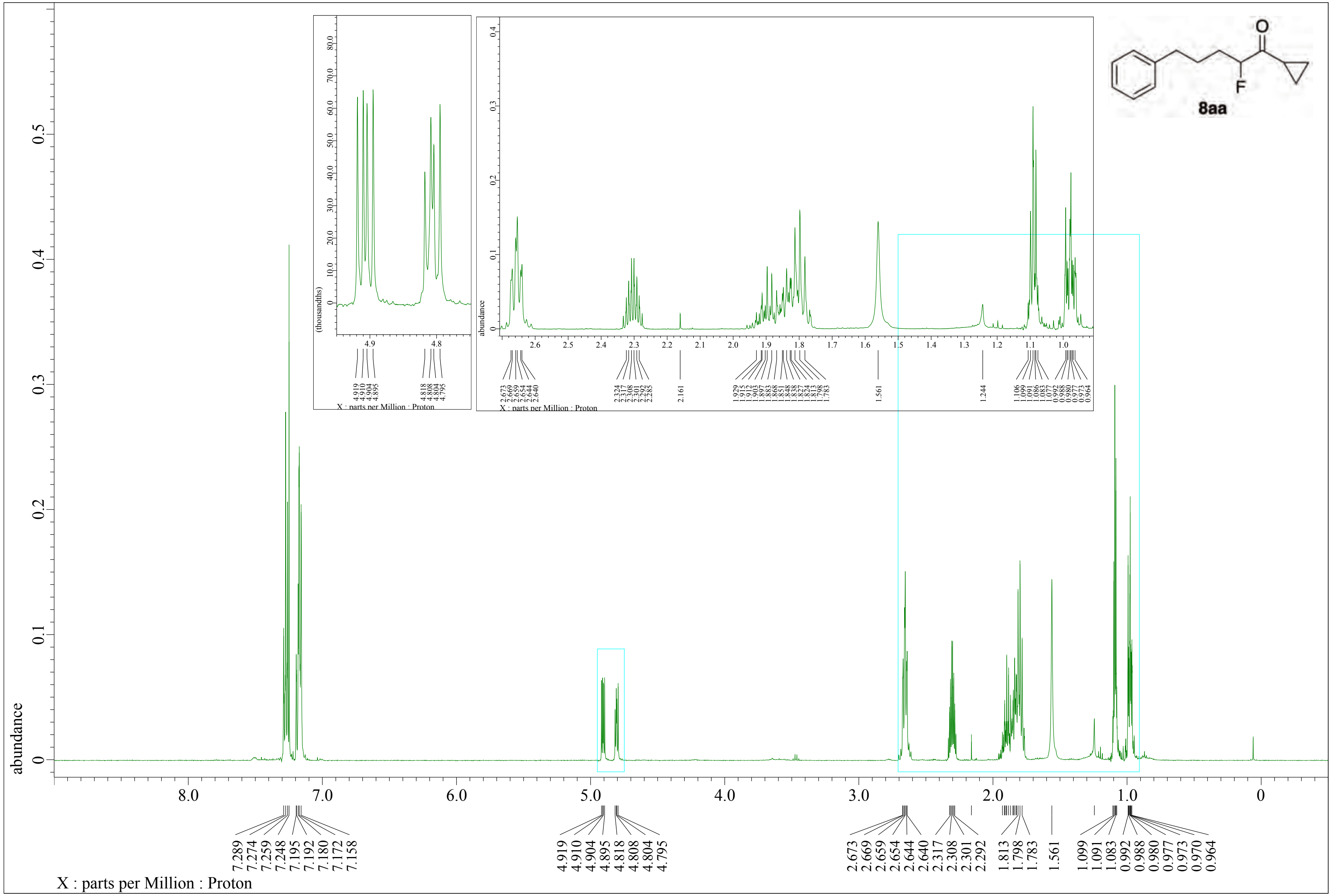

19.27
3.85
183.03
21.19
2.89
8z
X : parts per Million : Carbon13
196.954
196.858
196.762
141.518
134.369
133.919
129.012
128.993
128.974
128.868
128.562
128.523
126.137
94.677
93.767
92.857
77.476
77.160
76.844
35.360
32.380
32.274
32.169
26.477
26.463
26.448
(thousandths)

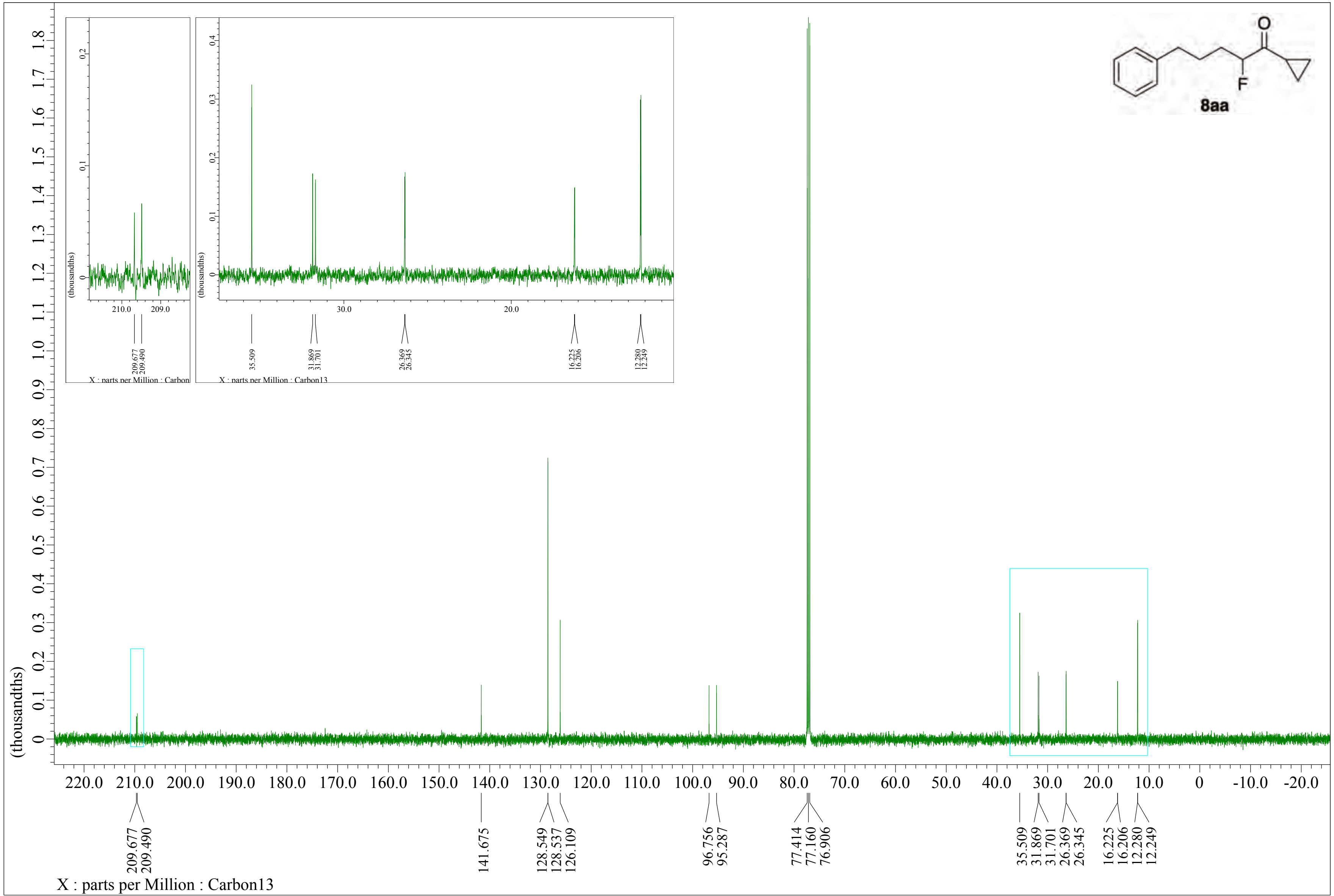


8z
F
O
abundance
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
90.0
70.0
50.0
30.0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-170.0
-190.0
-210.0
-230.0
-250.0
-270.0
-290.0
-188.870
-188.901
-188.939
-188.981
-189.004
-189.066
-189.139
-188.6
-188.8
-189.0
-189.2
-189.4
X : parts per Million : Fluorine19


MS: 5.3977 / M231854-8z-1 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(165232)
x10^5
105.03
77.04
91.05
51.02
65.04
39.02
117.07
131.09
151.06
236.12
256.13
m/z
O
F
8z

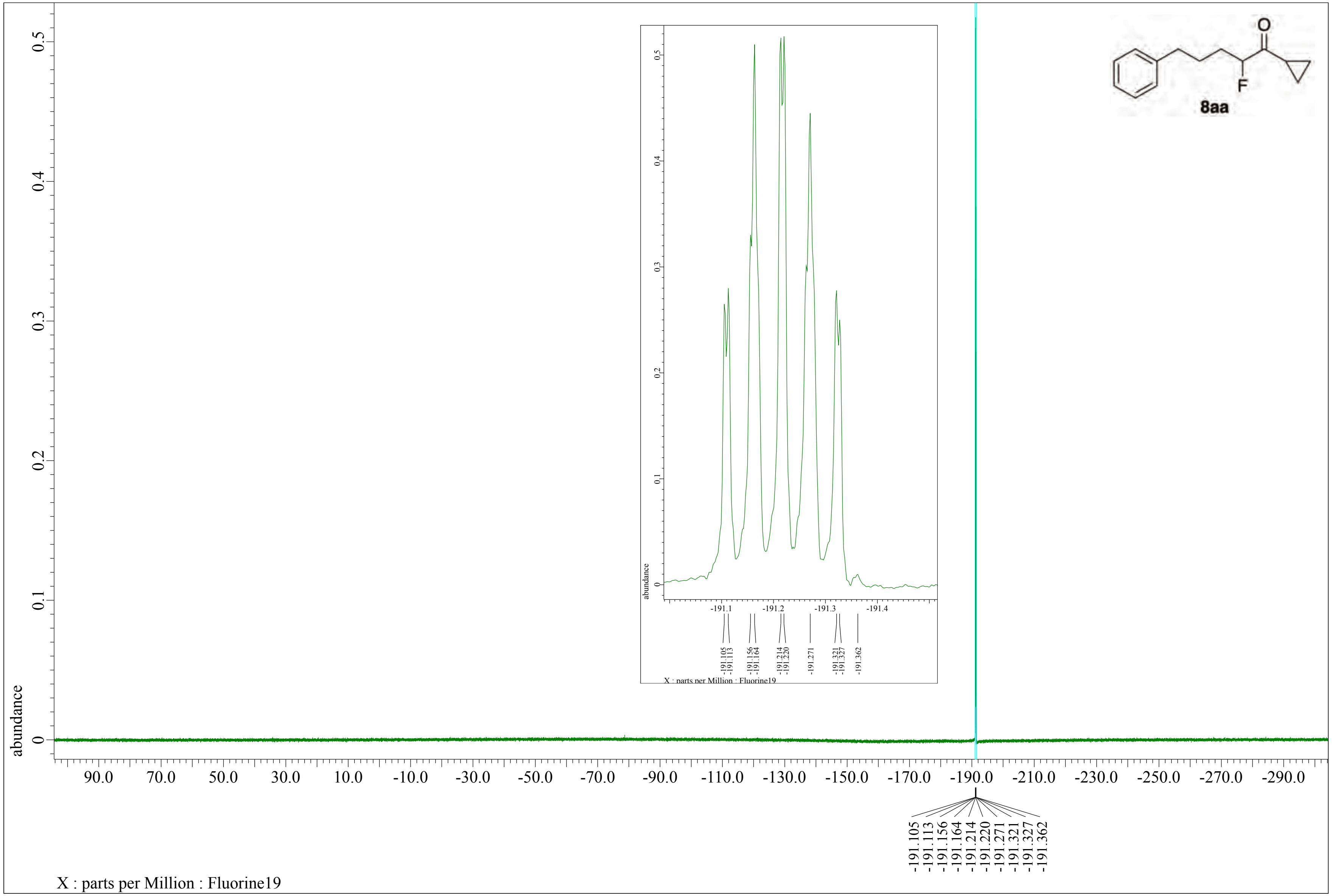

MS: 5.3977 / M231854-8z-1 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(3997)
256.12576
257.12880
m/z
O
F
8z


8aa
O
F
abundance
X : parts per Million : Proton
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.289
7.274
7.259
7.248
7.195
7.192
7.180
7.172
7.158
4.919
4.910
4.904
4.895
4.818
4.808
4.804
4.795
2.673
2.669
2.659
2.654
2.644
2.640
2.317
2.308
2.301
2.292
1.813
1.798
1.783
1.561
1.099
1.091
1.083
0.992
0.988
0.980
0.977
0.973
0.970
0.964

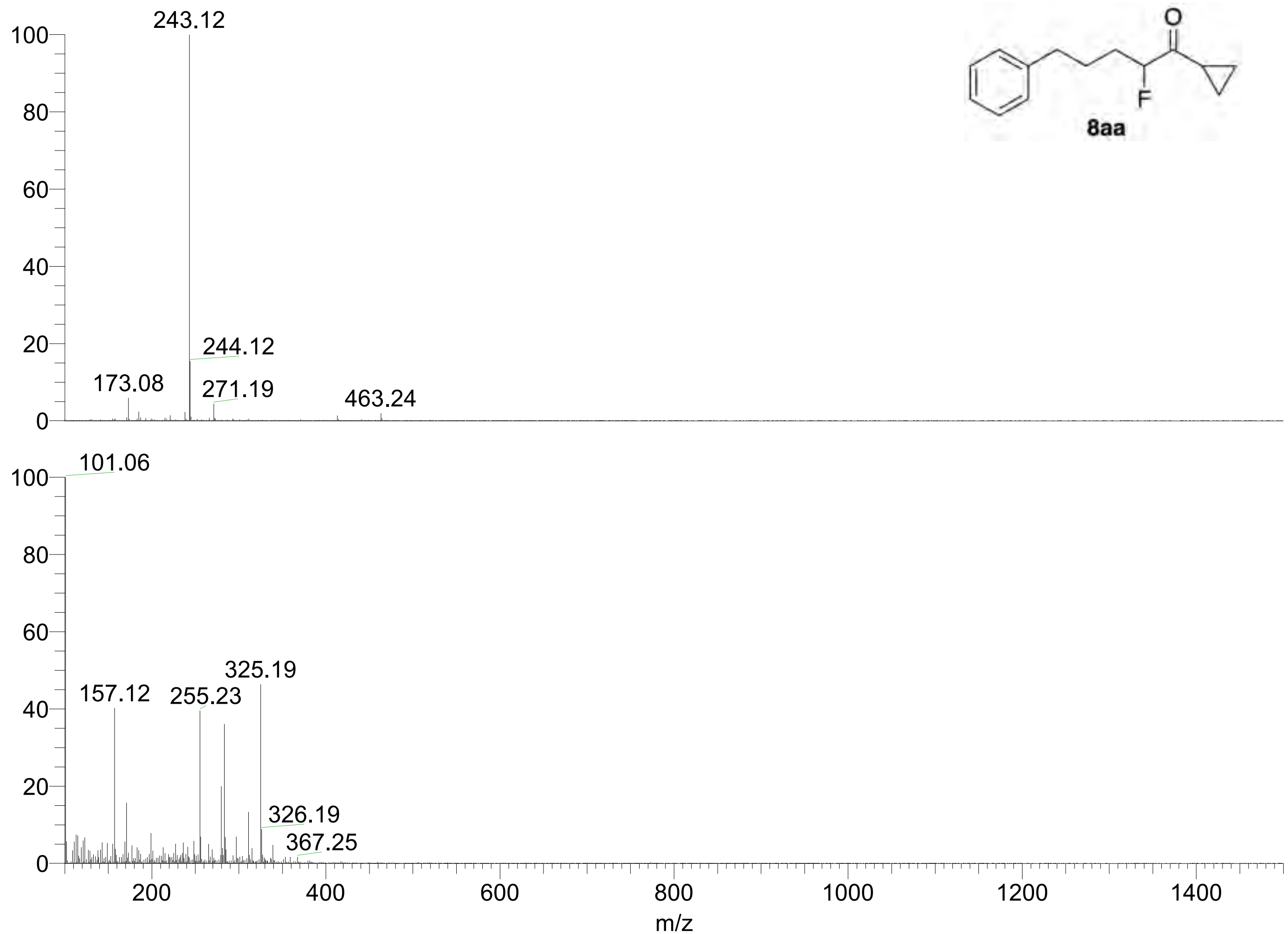


X : parts per Million : Carbon13
(thousandths)
209.677
209.490
141.675
128.549
128.537
126.109
96.756
95.287
77.414
77.160
76.906
35.509
31.869
31.701
26.369
26.345
16.225
16.206
12.280
12.249

8aa


8aa
F
O
abundance
-191.105
-191.113
-191.156
-191.164
-191.214
-191.220
-191.271
-191.321
-191.327
-191.362
X : parts per Million : Fluorine19

Sample No. : C:\Xcalibur\...\1228\BG_231855_8a _,	Instrument : Exactive Plus	Mobile phase solvent : MeOH
Operator name : hayashi harumi	Sample solvent : CHCl3
Date : 12/28/23 14:03:24
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

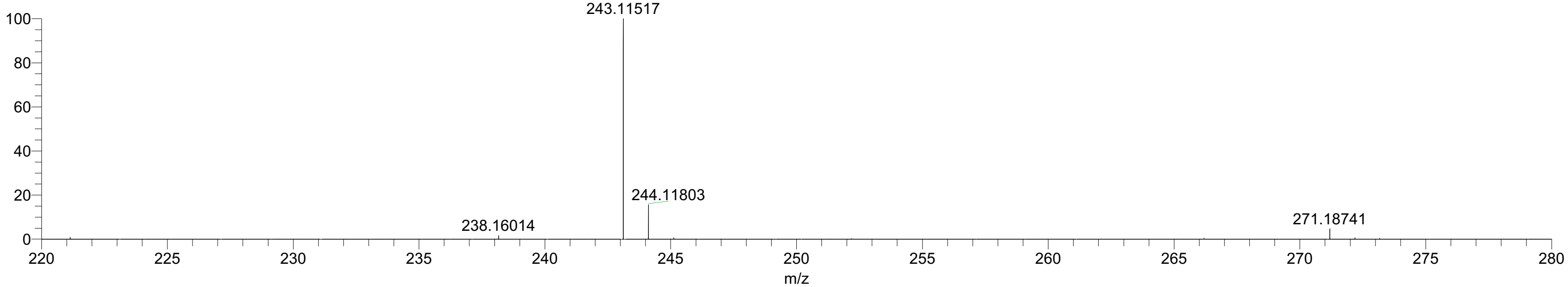


NL: 5.05E8
BG_231855_8aa_pn#
18-32 RT: 0.31-0.49
AV: 7 T: FTMS + c
ESI Full ms
[100.00-1500.00]

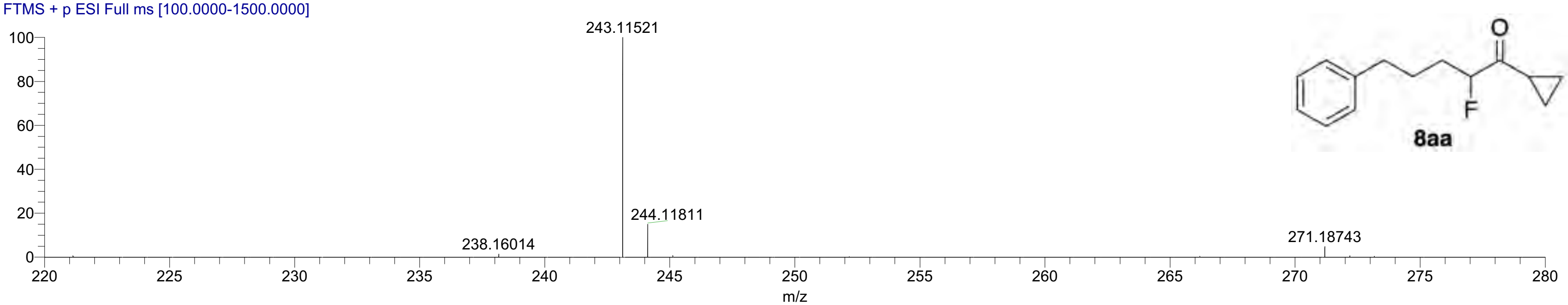
NL: 1.48E7
BG_231855_8aa_pn#
18-32 RT: 0.29-0.51
AV: 8 T: FTMS - c ESI
Full ms
[100.00-1500.00]

Sample No. : C:\Xcalibur\...\1228\231855_8aa_pn
Instrument : Exactive Plus
Mobile phase solvent : MeOH
Operator name : hayashi harumi
Sample solvent : CHCl3
Date : 12/28/23 12:06:15
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

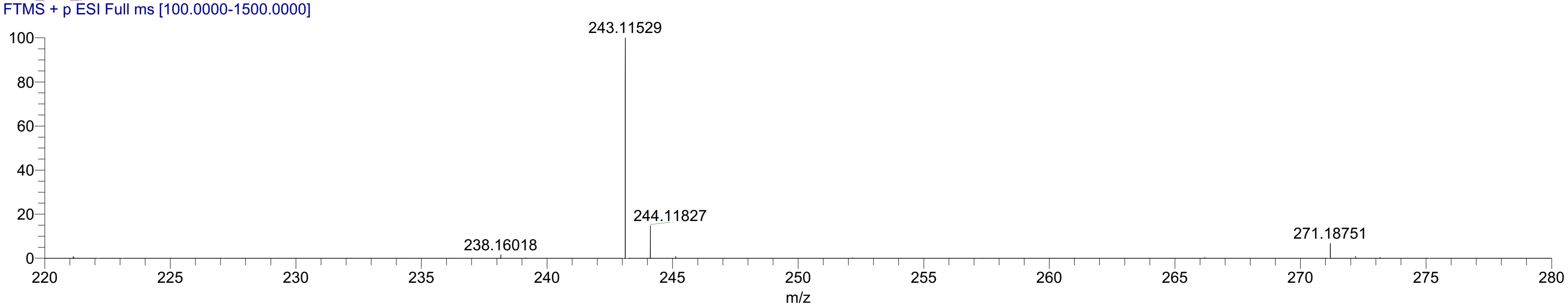
231855_8aa_pn #22-25 RT: 0.37-0.40 AV: 2 NL: 2.16E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

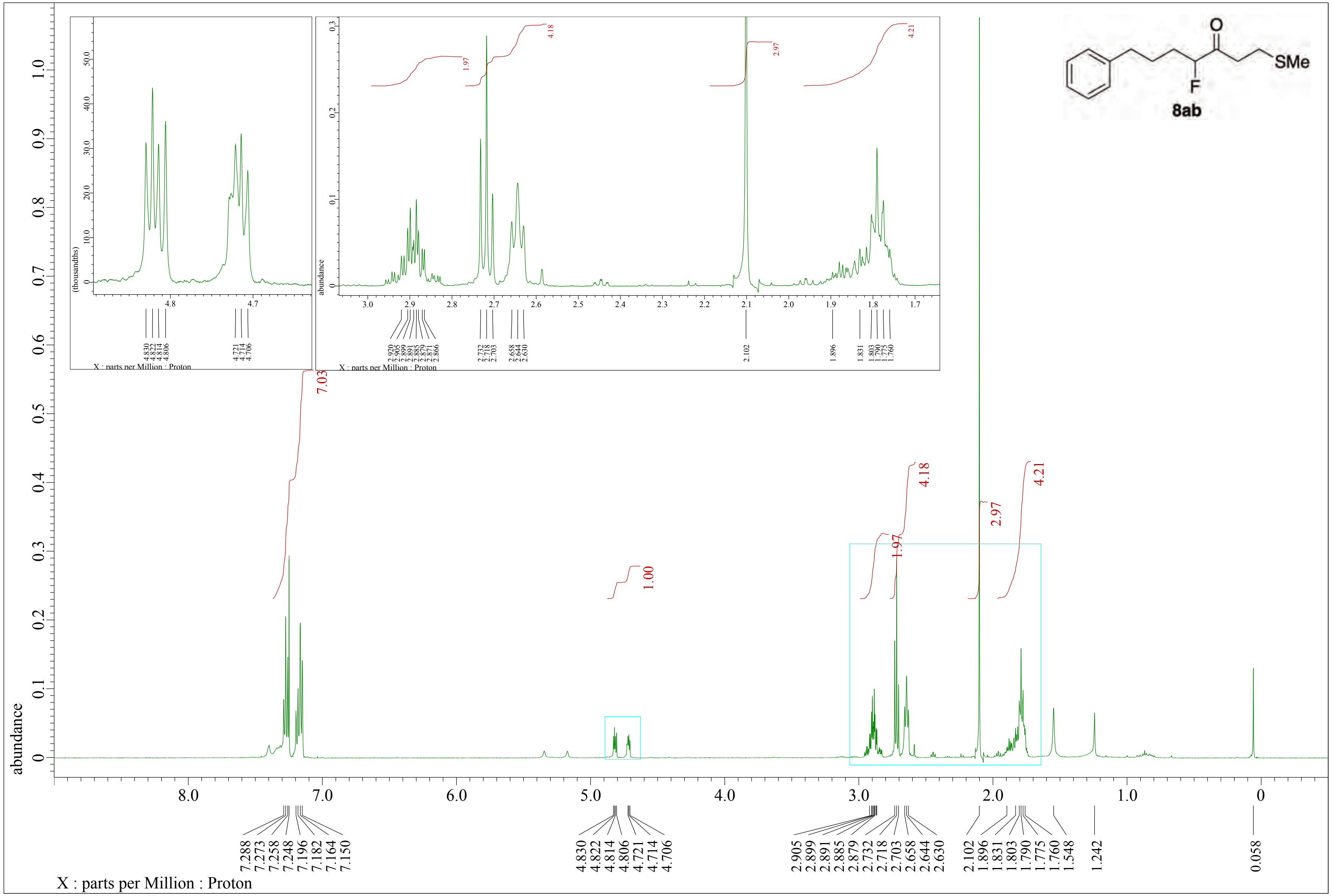


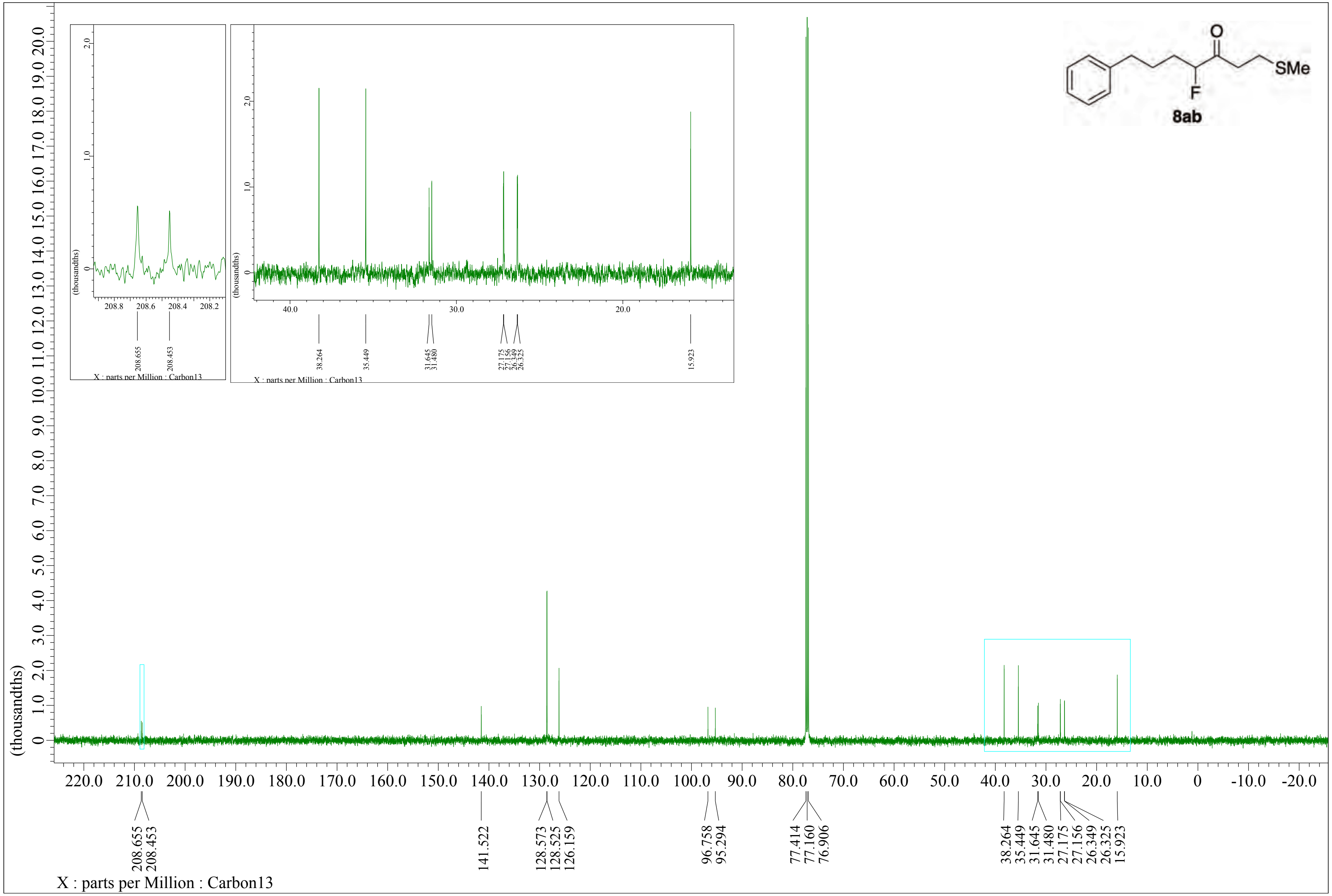
231855_8aa_pn #25-28 RT: 0.40-0.43 AV: 2 NL: 1.64E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



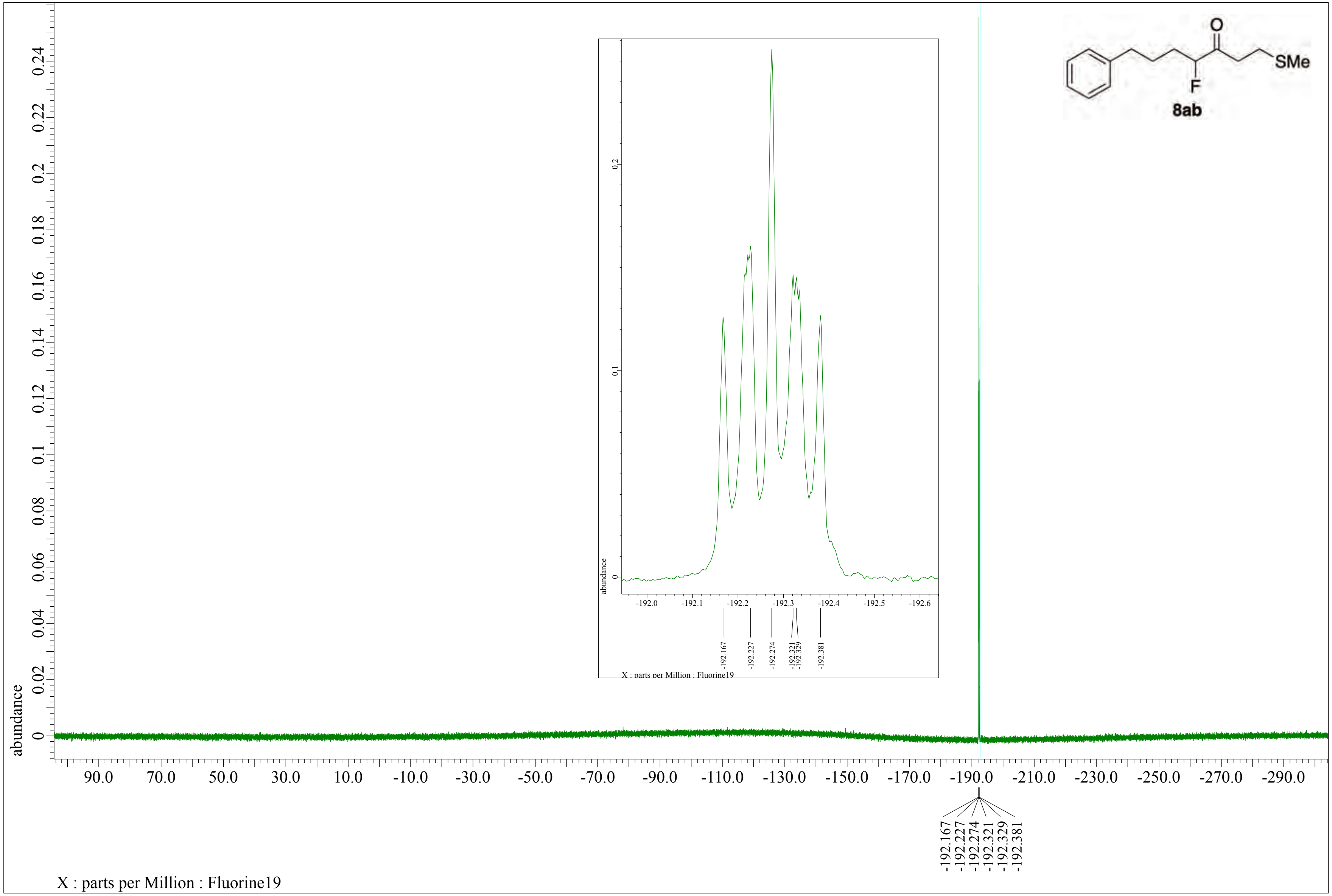
231855_8aa_pn #28-32 RT: 0.46-0.49 AV: 2 NL: 8.06E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]




8ab
SMe
F
O
X : parts per Million : Proton
abundance
7.03
1.00
1.97
4.18
2.97
4.21
7.288
7.273
7.258
7.248
7.196
7.182
7.164
7.150
4.830
4.822
4.814
4.806
4.721
4.714
4.706
2.905
2.899
2.891
2.885
2.879
2.732
2.718
2.703
2.658
2.644
2.630
2.102
1.896
1.831
1.803
1.790
1.775
1.760
1.548
1.242
0.058



8ab
SMe
O
F
(thousandths)
X : parts per Million : Carbon13
208.655
208.453
141.522
128.573
128.525
126.159
96.758
95.294
77.414
77.160
76.906
38.264
35.449
31.645
31.480
27.175
27.156
26.349
26.325
15.923



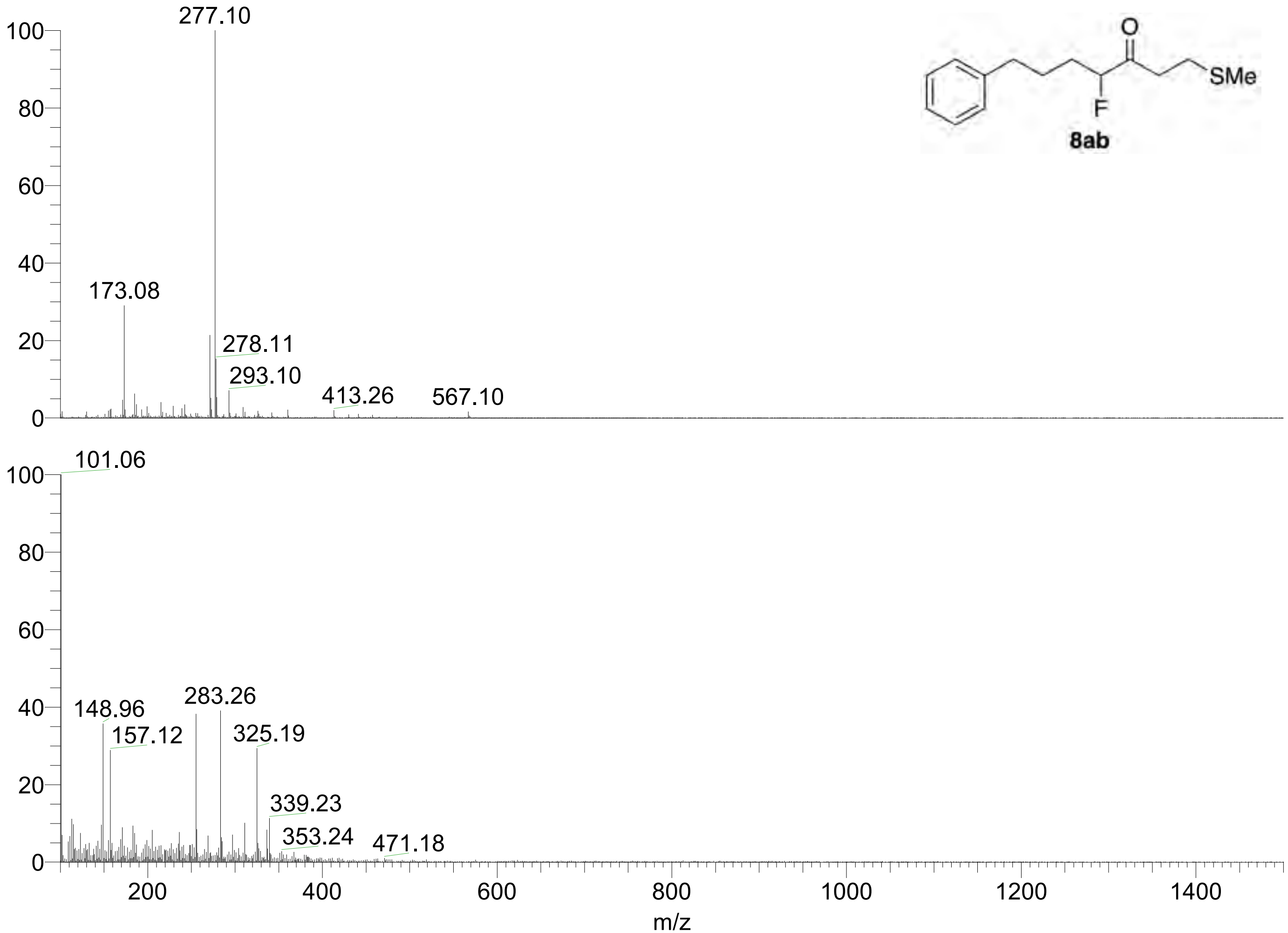
SMe
O
F
8ab
abundance
X : parts per Million : Fluorine19
-192.167
-192.227
-192.274
-192.321
-192.329
-192.381

Sample No. : C:\Xcalibur\...\1228\BG_231856_8a _, Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 14:03:50
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

8ab

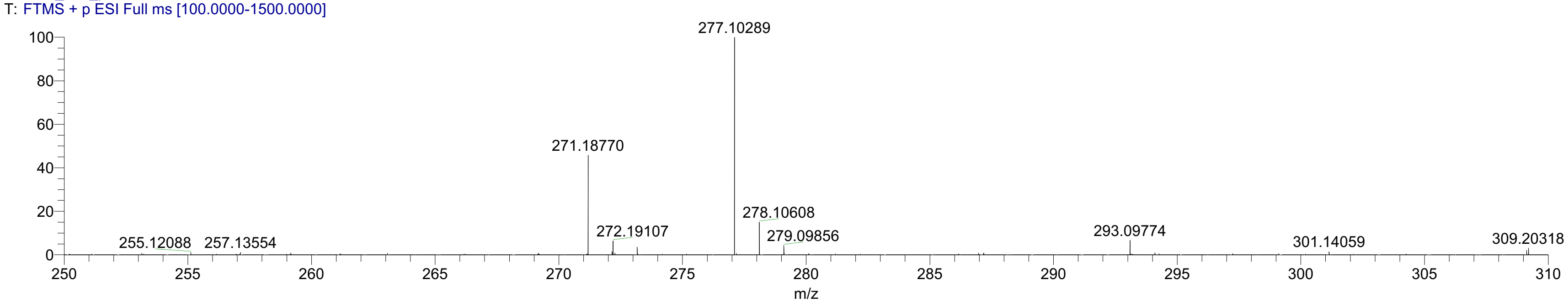
NL: 3.87E7
BG_231856_8ab_pn#
18-31 RT: 0.31-0.50
AV: 7 T: FTMS + c
ESI Full ms
[100.00-1500.00]

NL: 1.88E6
BG_231856_8ab_pn#
18-31 RT: 0.30-0.49
AV: 7 T: FTMS - c ESI
Full ms
[100.00-1500.00]

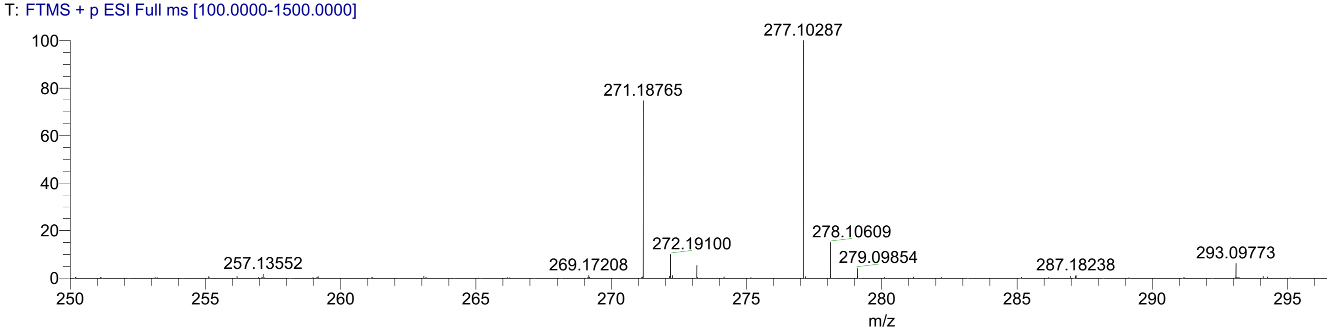


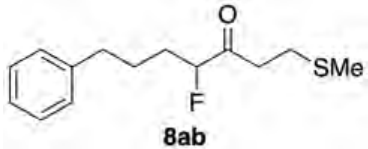
Sample No. : C:\Xcalibur\...\1228\231856_8ab_pn   Instrument : Exactive Plus   Mobile phase solvent : MeOH
Operator name : hayashi harumi   Sample solvent : CHCl3
Date : 12/28/23 12:11:44
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz100_1500pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

231856_8ab_pn #21-25 RT: 0.34-0.41 AV: 3 NL: 1.41E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



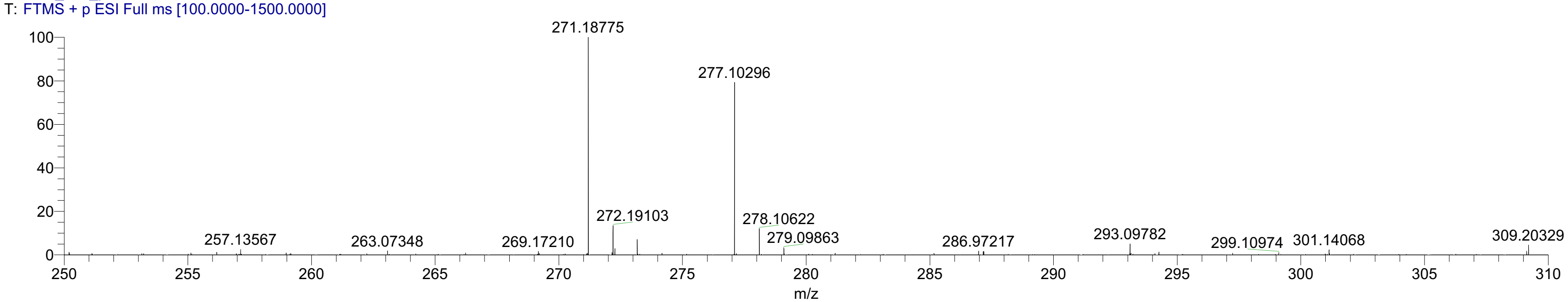
231856_8ab_pn #25-28 RT: 0.41-0.44 AV: 2 NL: 1.35E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

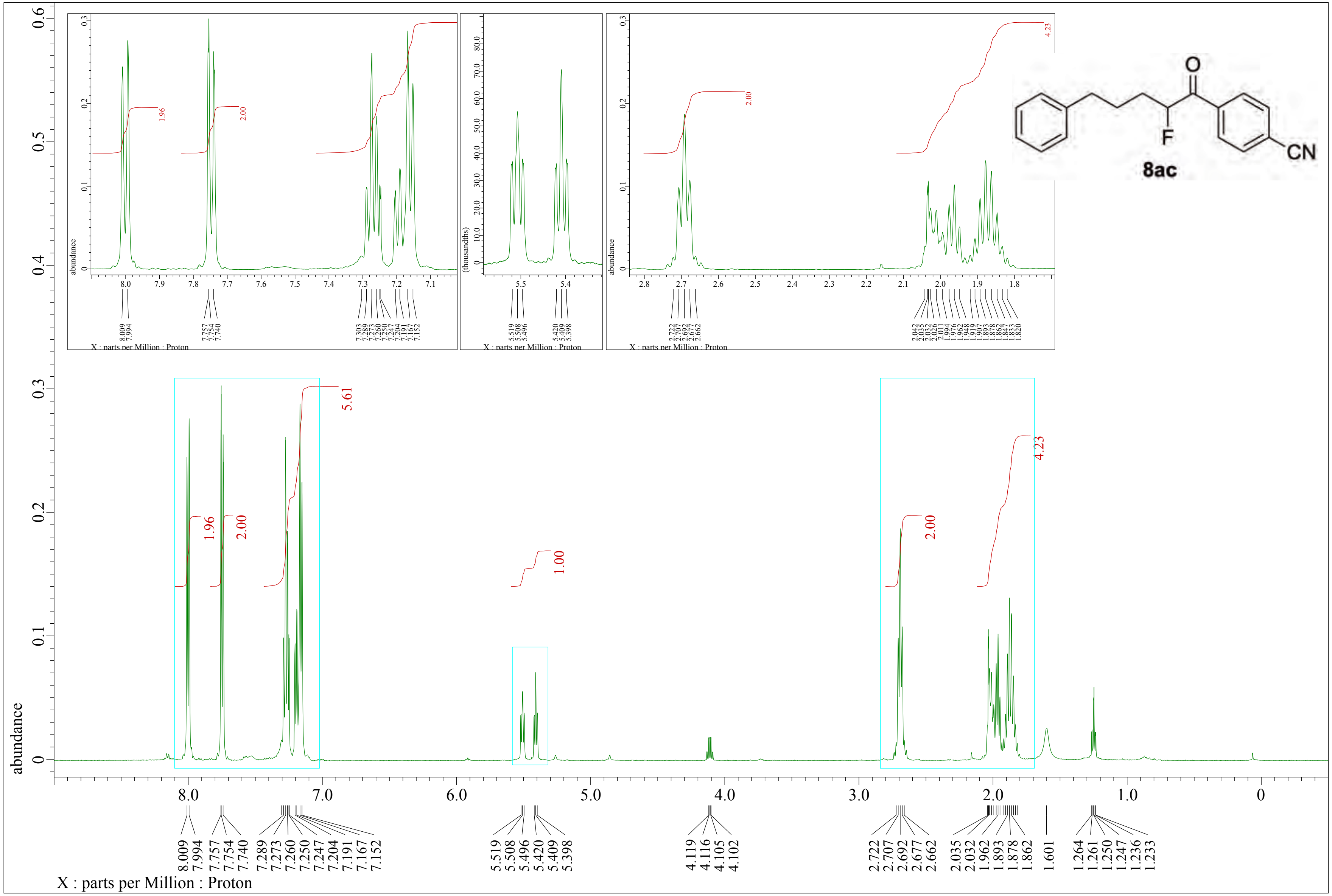


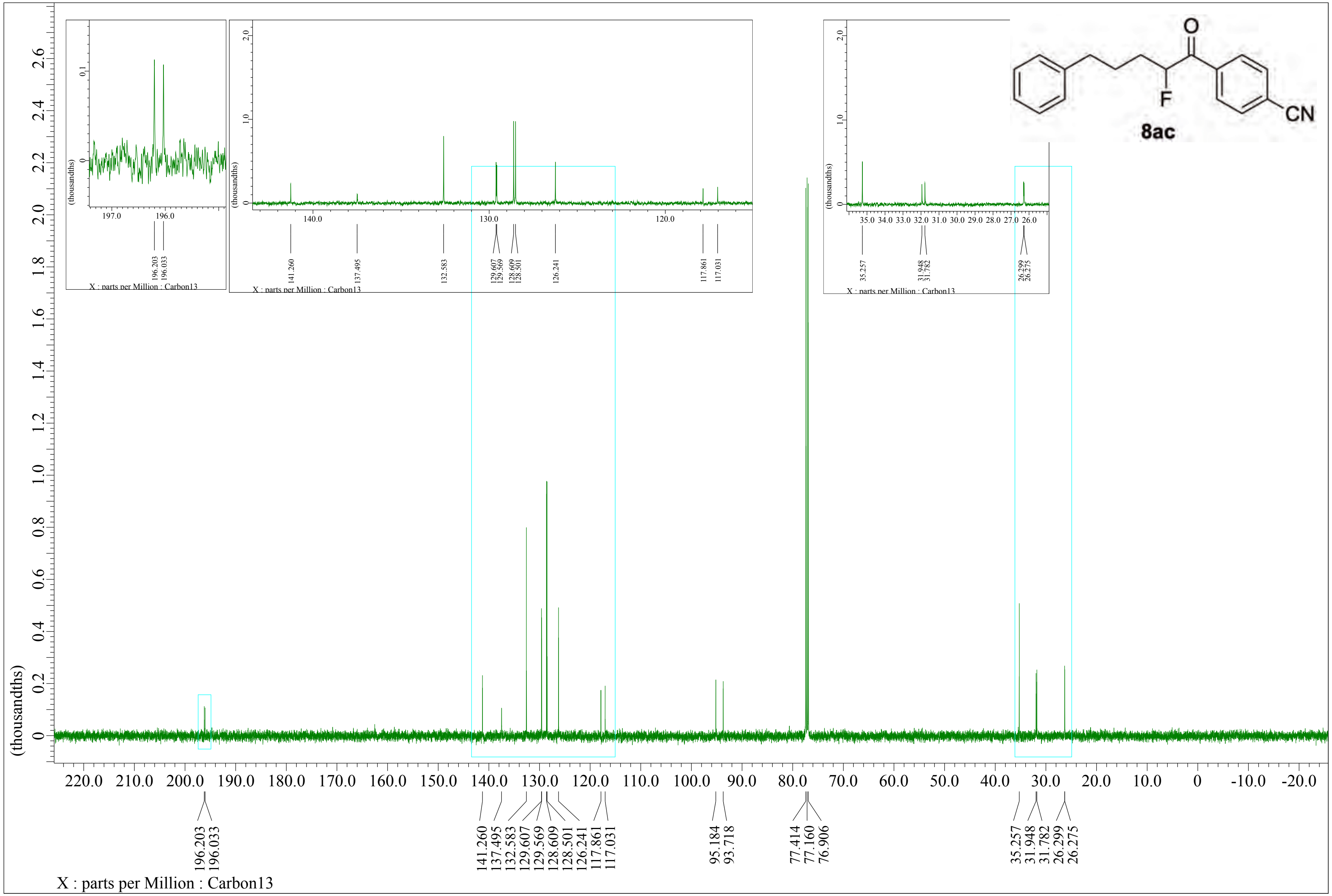


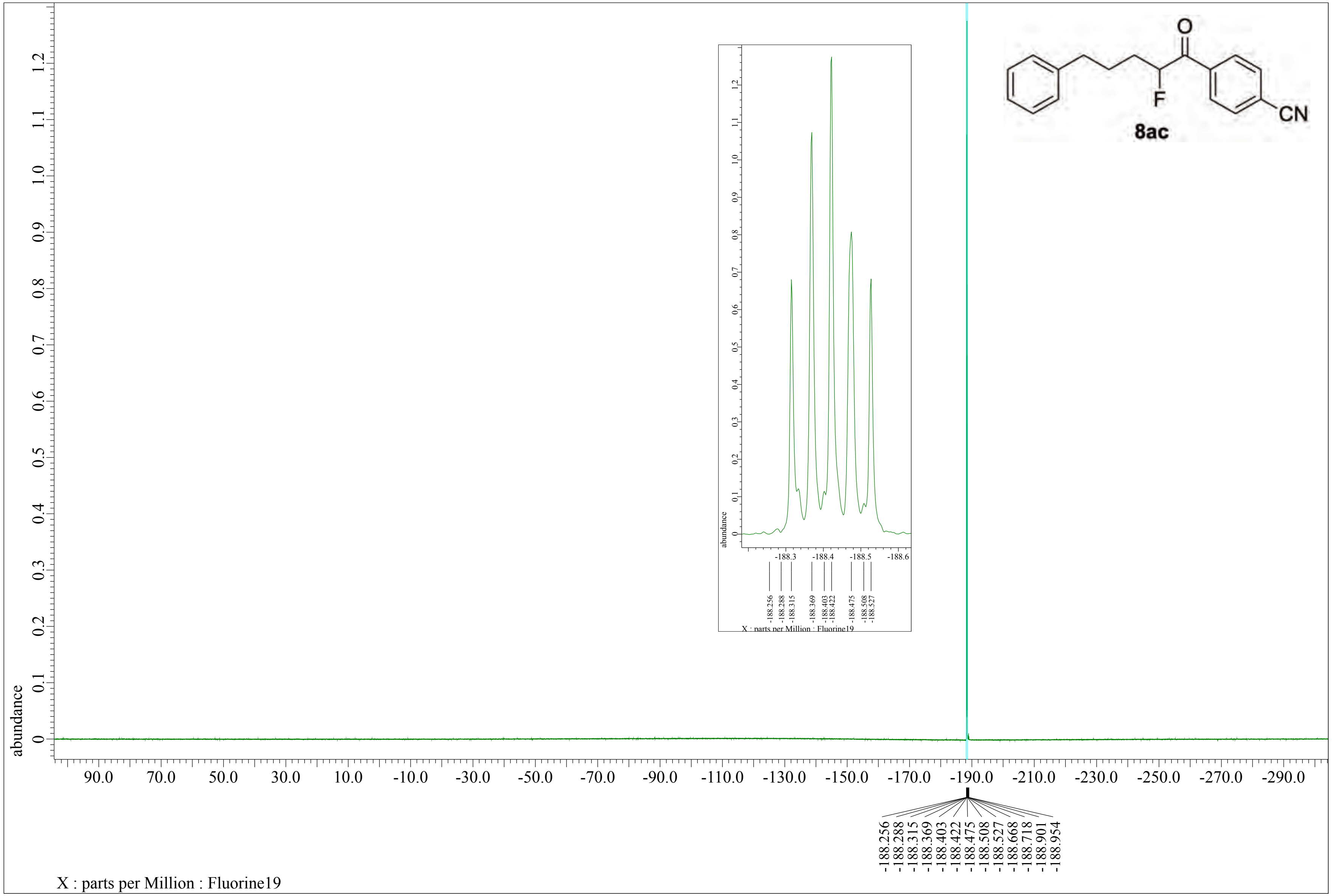
8ab

231856_8ab_pn #28-31 RT: 0.47-0.50 AV: 2 NL: 5.22E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

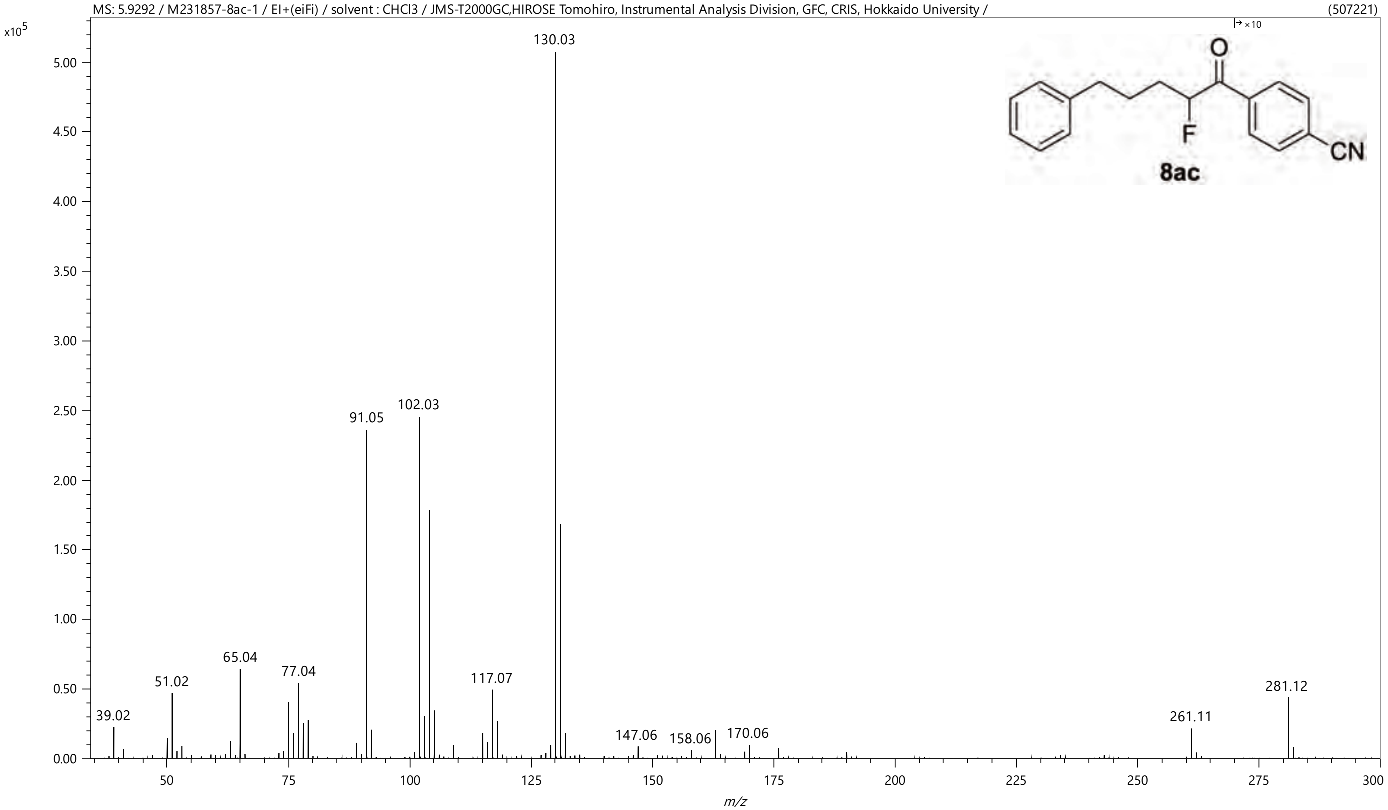


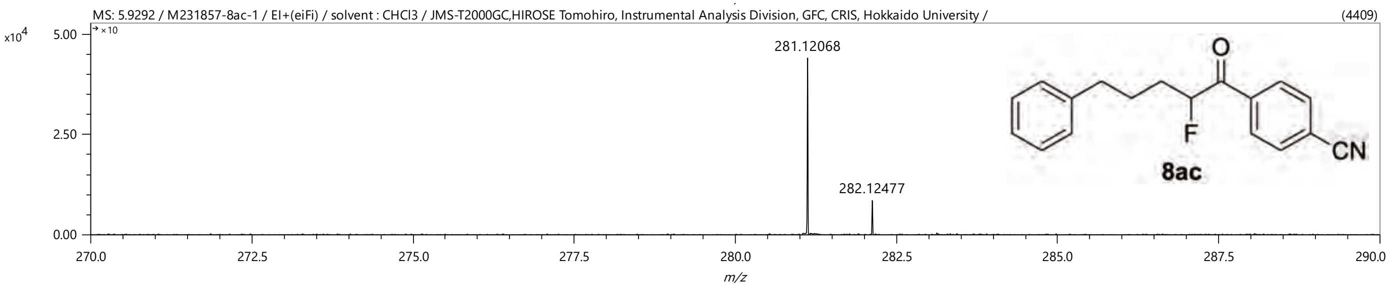

abundance
X : parts per Million : Proton
8.009 7.994 7.757 7.754 7.740 7.289 7.273 7.260 7.250 7.247 7.204 7.191 7.167 7.152
5.519 5.508 5.496 5.420 5.409 5.398
4.119 4.116 4.105 4.102
2.722 2.707 2.692 2.677 2.662
2.035 2.032 1.962 1.893 1.878 1.862
1.601
1.264 1.261 1.250 1.247 1.236 1.233
1.96
2.00
5.61
1.00
2.00
4.23
O
F
CN
8ac

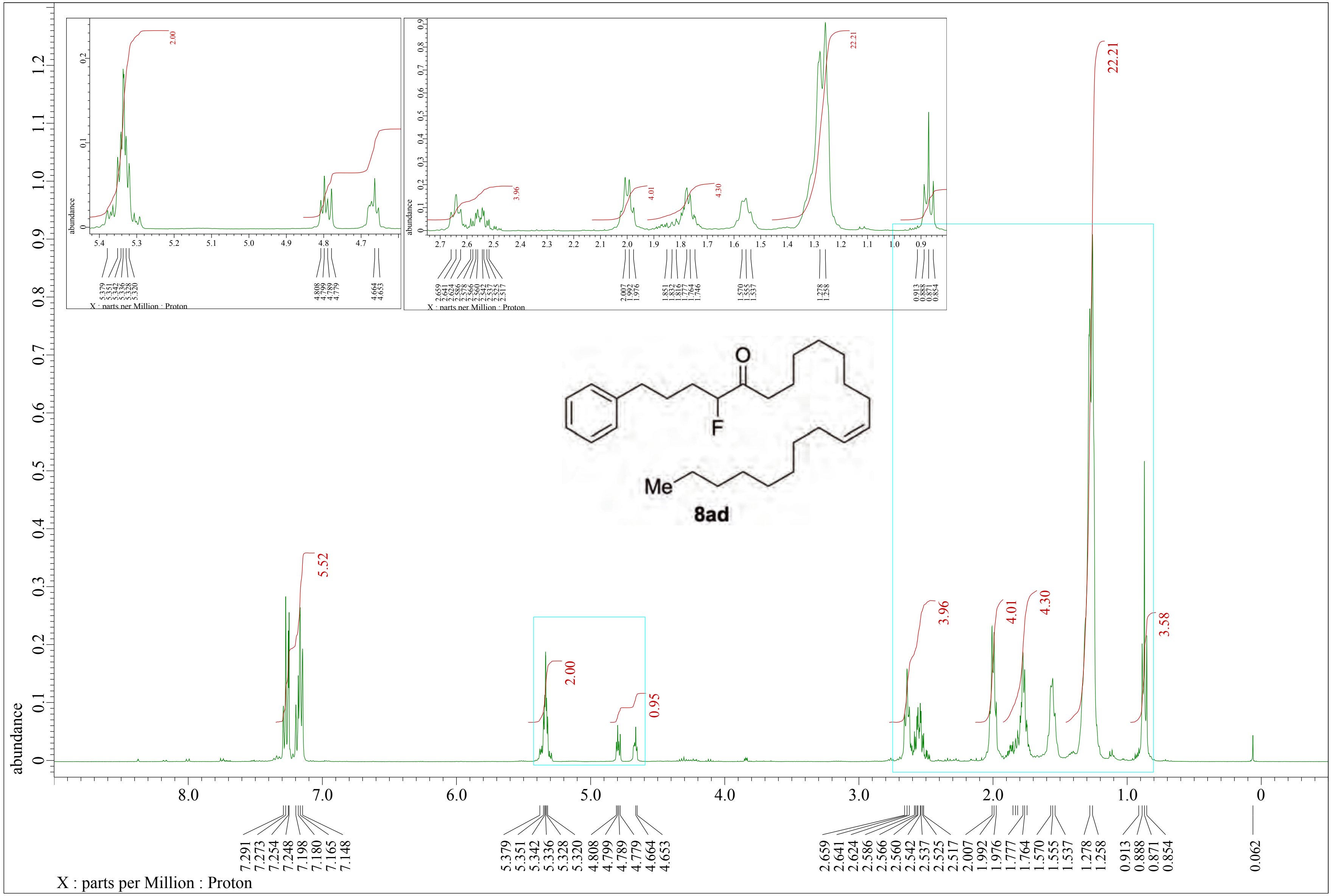

8ac
O
F
CN
(thousandths)
X : parts per Million : Carbon13
196.203
196.033
141.260
137.495
132.583
129.607
129.569
128.609
128.501
126.241
117.861
117.031
95.184
93.718
77.414
77.160
76.906
35.257
31.948
31.782
26.299
26.275



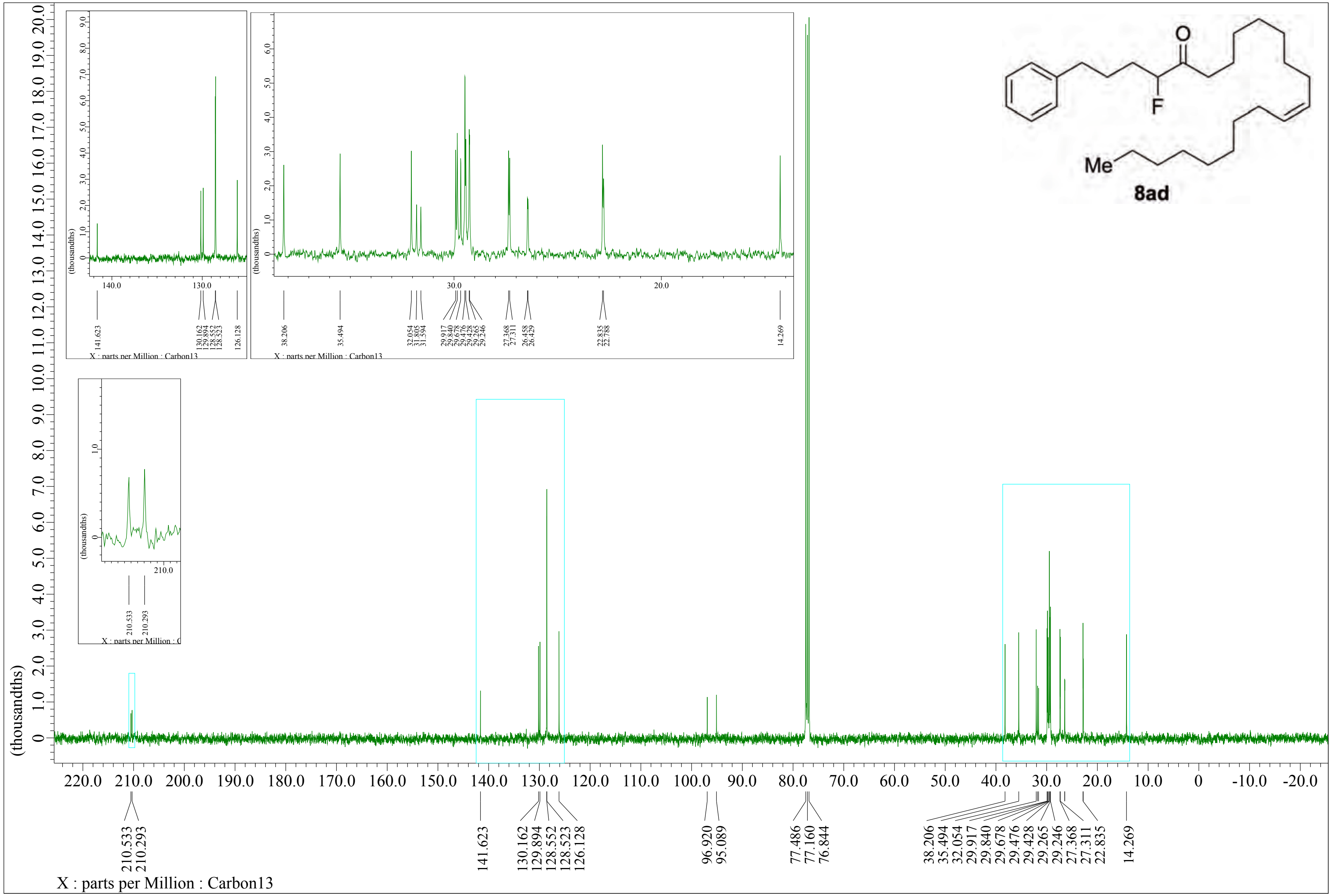
8ac
abundance
X : parts per Million : Fluorine19
-188.256
-188.288
-188.315
-188.369
-188.403
-188.422
-188.475
-188.508
-188.527
-188.668
-188.718
-188.901
-188.954

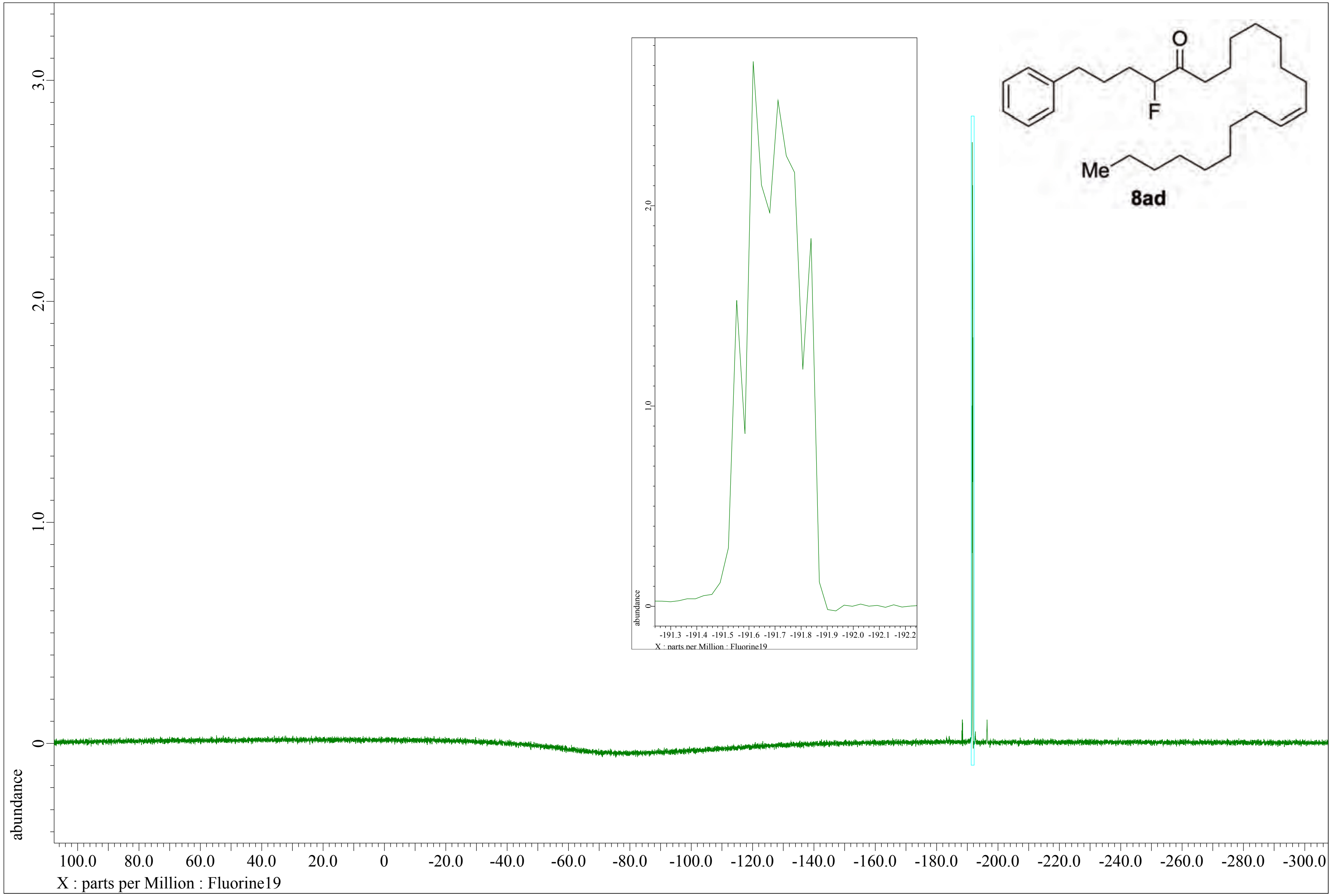

MS: 5.9292 / M231857-8ac-1 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(507221)
x10^5
130.03
91.05
102.03
65.04
77.04
51.02
117.07
39.02
147.06
158.06
170.06
261.11
281.12
8ac
m/z


MS: 5.9292 / M231857-8ac-1 / EI+(eiFi) / solvent : CHCl3 / JMS-T2000GC,HIROSE Tomohiro, Instrumental Analysis Division, GFC, CRIS, Hokkaido University /
(4409)
x10^4
281.12068
282.12477
8ac
m/z



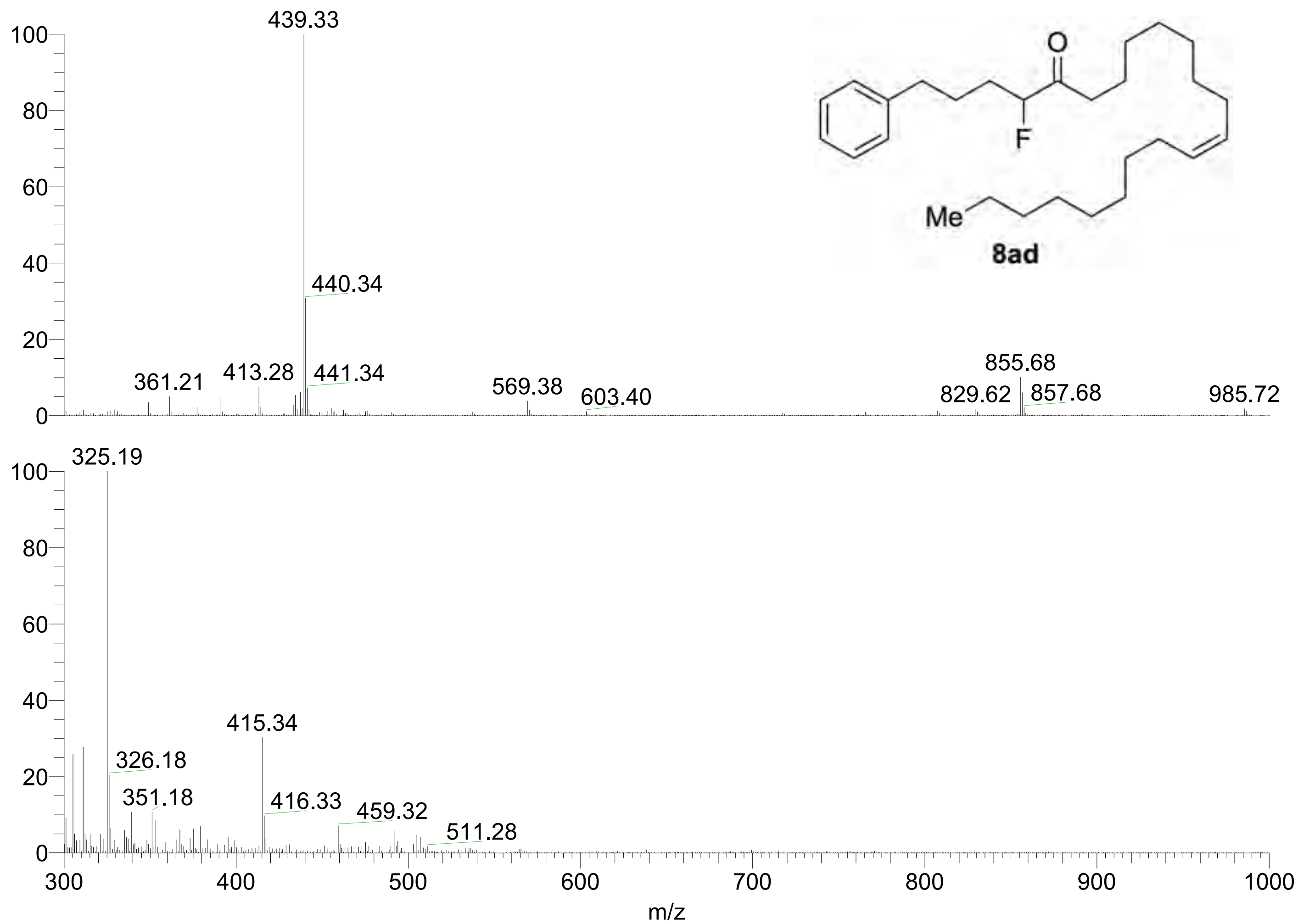
O
F
Me
8ad
abundance
X : parts per Million : Proton
5.52
2.00
0.95
3.96
4.01
4.30
22.21
3.58


O
F
Me
8ad
(thousandths)
X : parts per Million : Carbon13
210.533
210.293
141.623
130.162
129.894
128.552
128.523
126.128
96.920
95.089
77.486
77.160
76.844
38.206
35.494
32.054
31.805
31.594
29.917
29.840
29.678
29.476
29.428
29.265
29.246
27.368
27.311
26.458
26.429
22.835
22.788
14.269



abundance
3.0
2.0
1.0
0
100.0 80.0 60.0 40.0 20.0 0 -20.0 -40.0 -60.0 -80.0 -100.0 -120.0 -140.0 -160.0 -180.0 -200.0 -220.0 -240.0 -260.0 -280.0 -300.0
X : parts per Million : Fluorine19
-191.3 -191.4 -191.5 -191.6 -191.7 -191.8 -191.9 -192.0 -192.1 -192.2
O
F
Me
8ad

Sample No. : C:\Xcalibur\...\1228\BG_231858_8ε _, Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 14:27:48
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

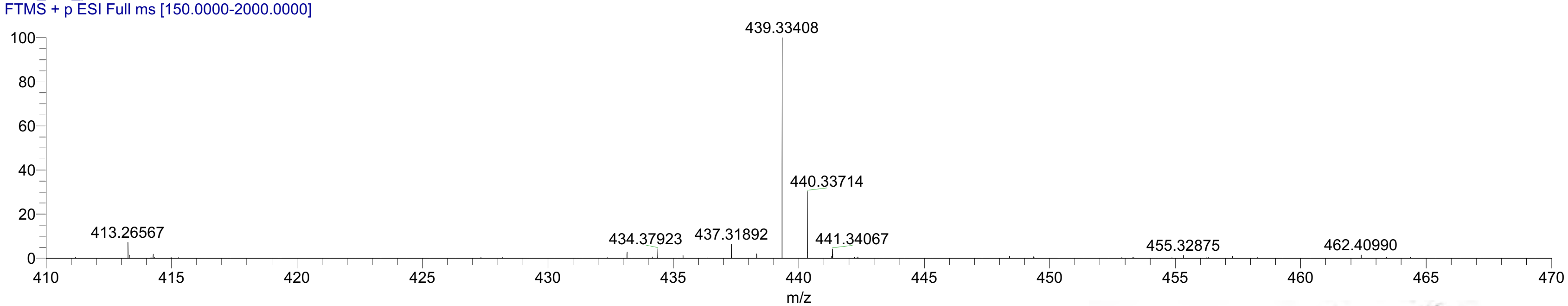


NL: 9.46E7
BG_231858_8ad_pn#
18-31 RT: 0.31-0.49
AV: 7 T: FTMS + c
ESI Full ms
[150.00-2000.00]

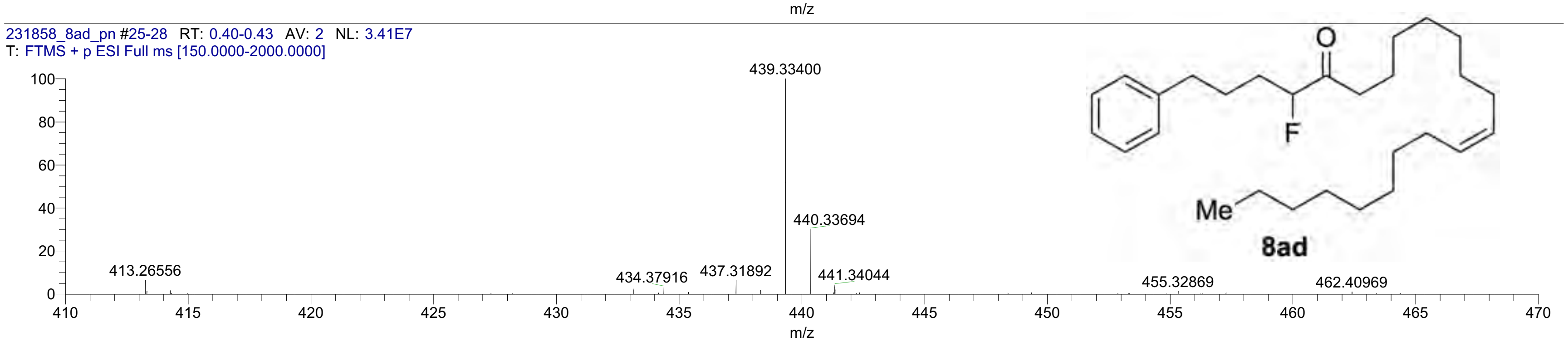
NL: 4.38E6
BG_231858_8ad_pn#
18-31 RT: 0.30-0.48
AV: 7 T: FTMS - c ESI
Full ms
[150.00-2000.00]

Sample No. : C:\Xcalibur\...\1228\231858_8ad_pn　　Instrument : Exactive Plus　　Mobile phase solvent : MeOH
Operator name : hayashi harumi　　Sample solvent : CHCl3
Date : 12/28/23 12:22:12
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

231858_8ad_pn #21-25 RT: 0.34-0.40 AV: 3 NL: 2.77E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]

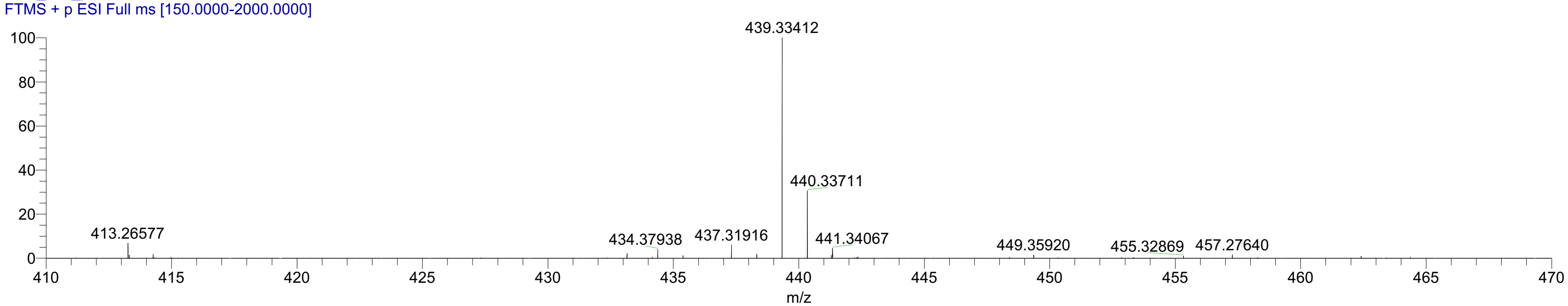


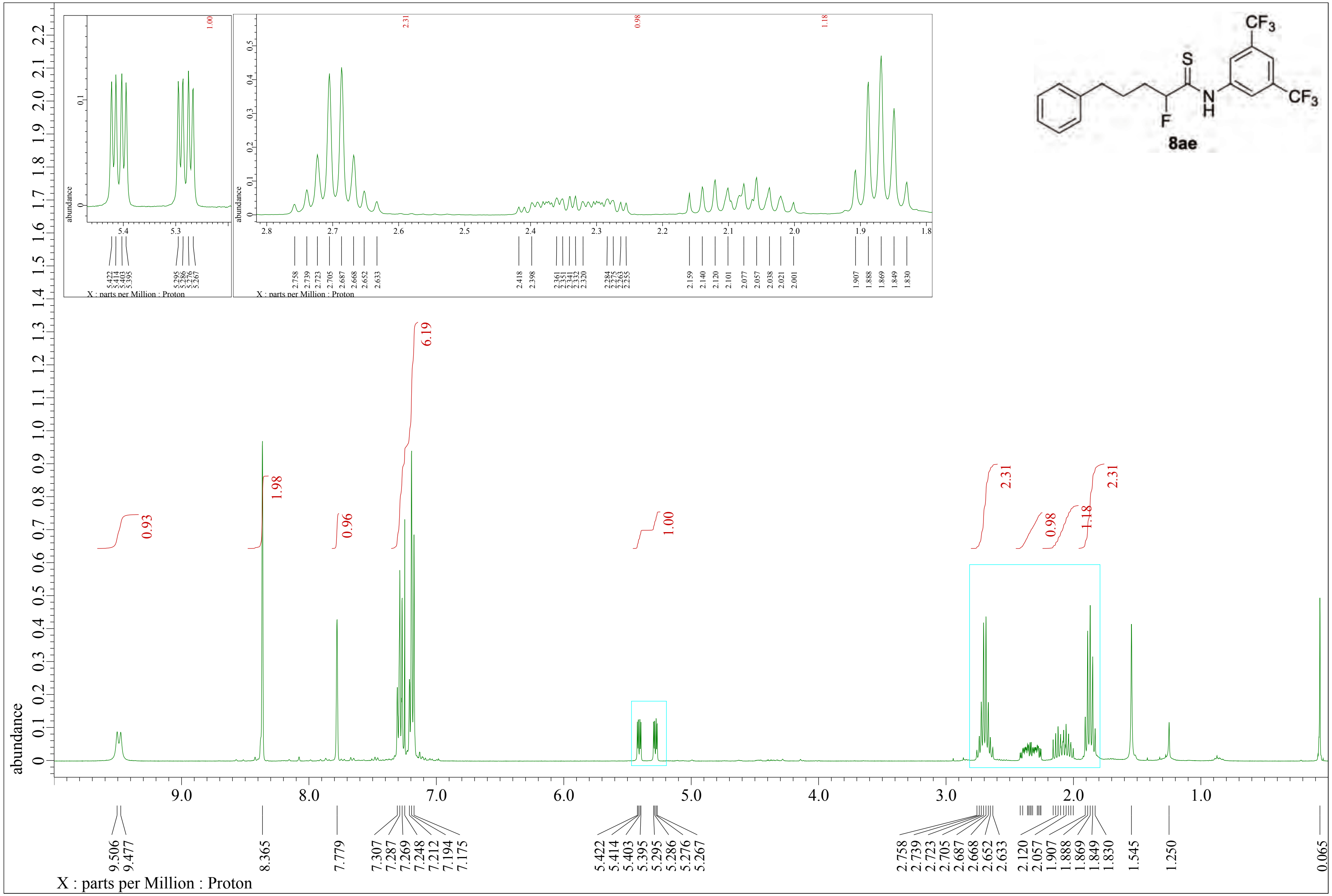
231858_8ad_pn #25-28 RT: 0.40-0.43 AV: 2 NL: 3.41E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]

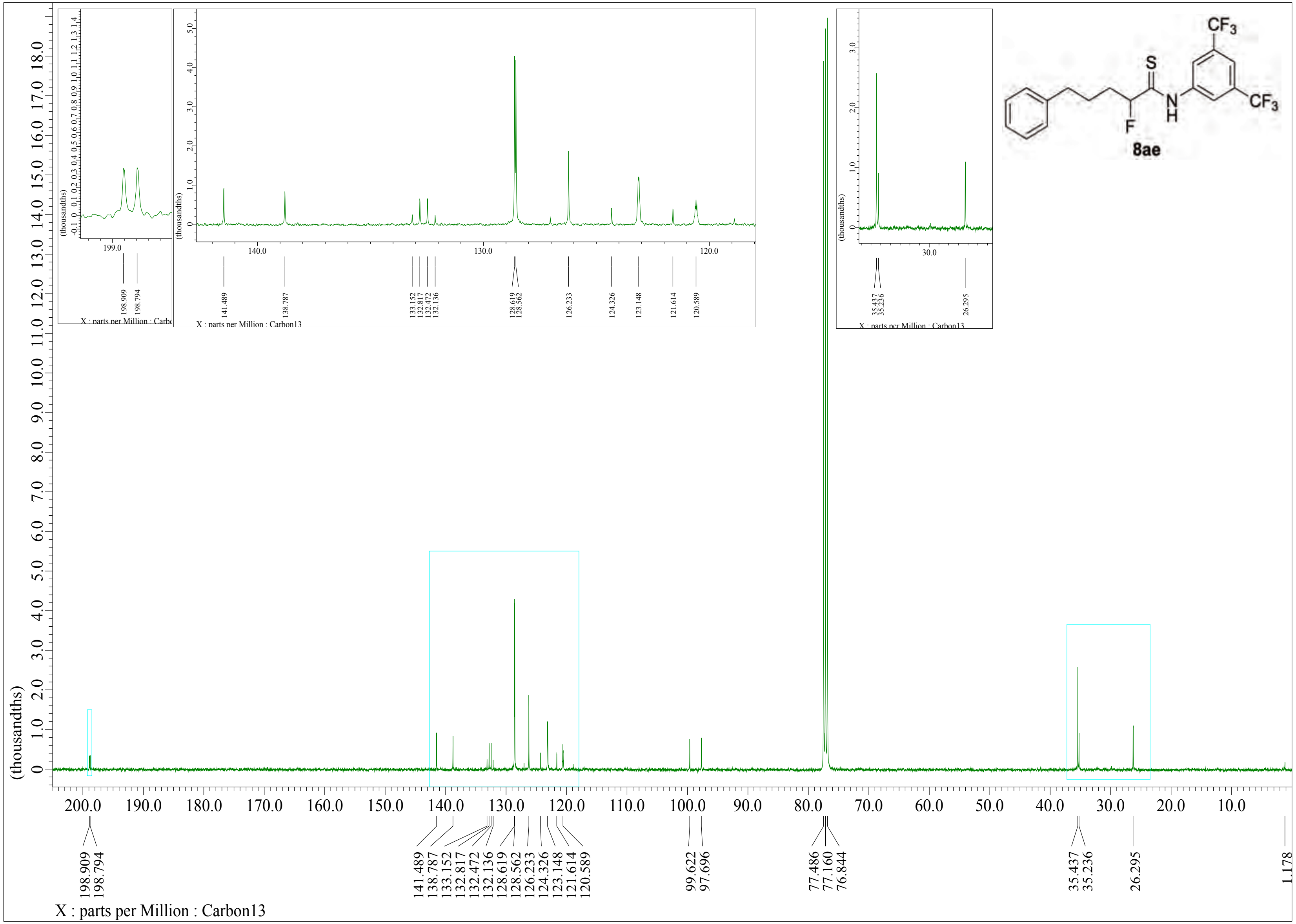


8ad

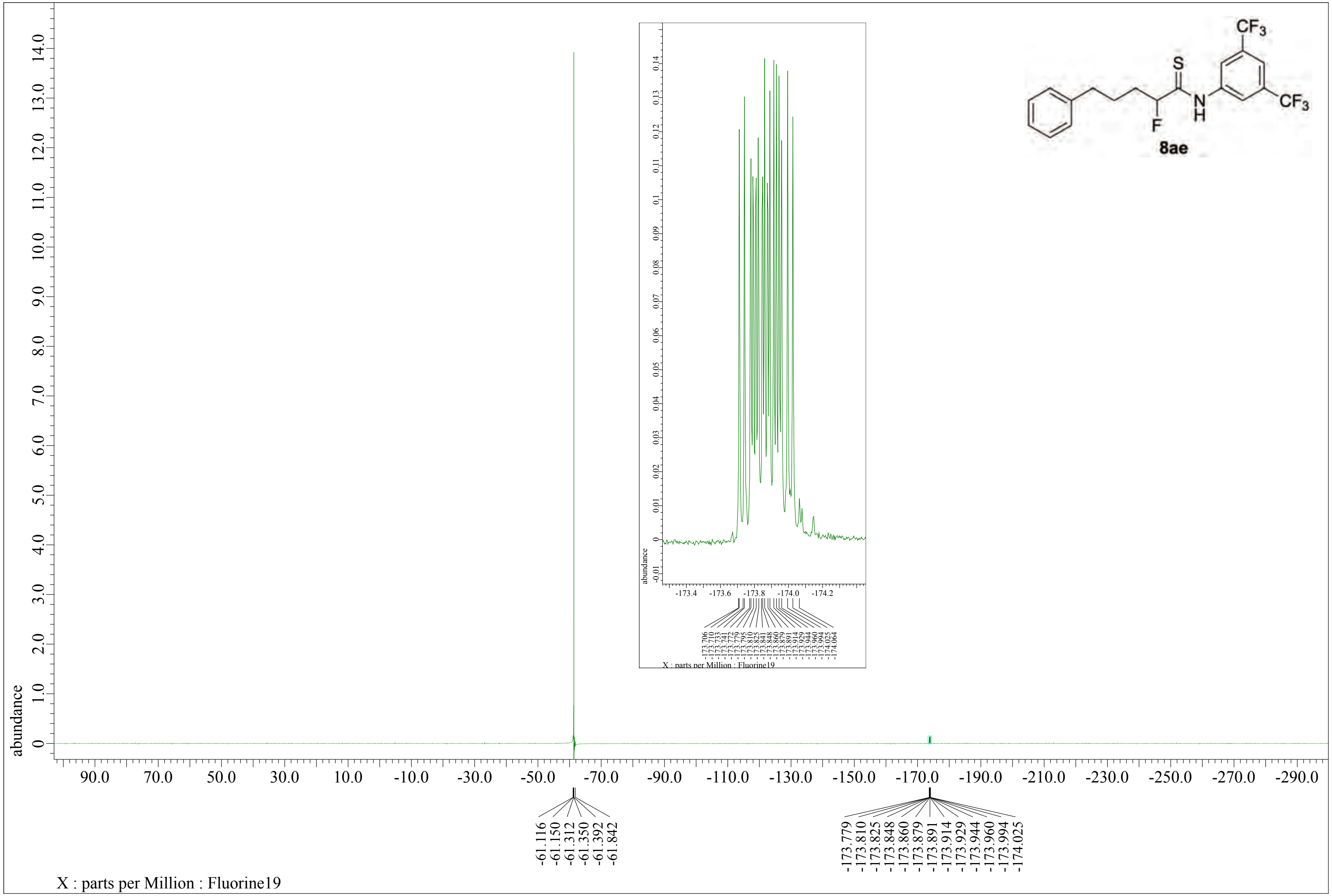
231858_8ad_pn #29-32 RT: 0.46-0.49 AV: 2 NL: 1.73E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



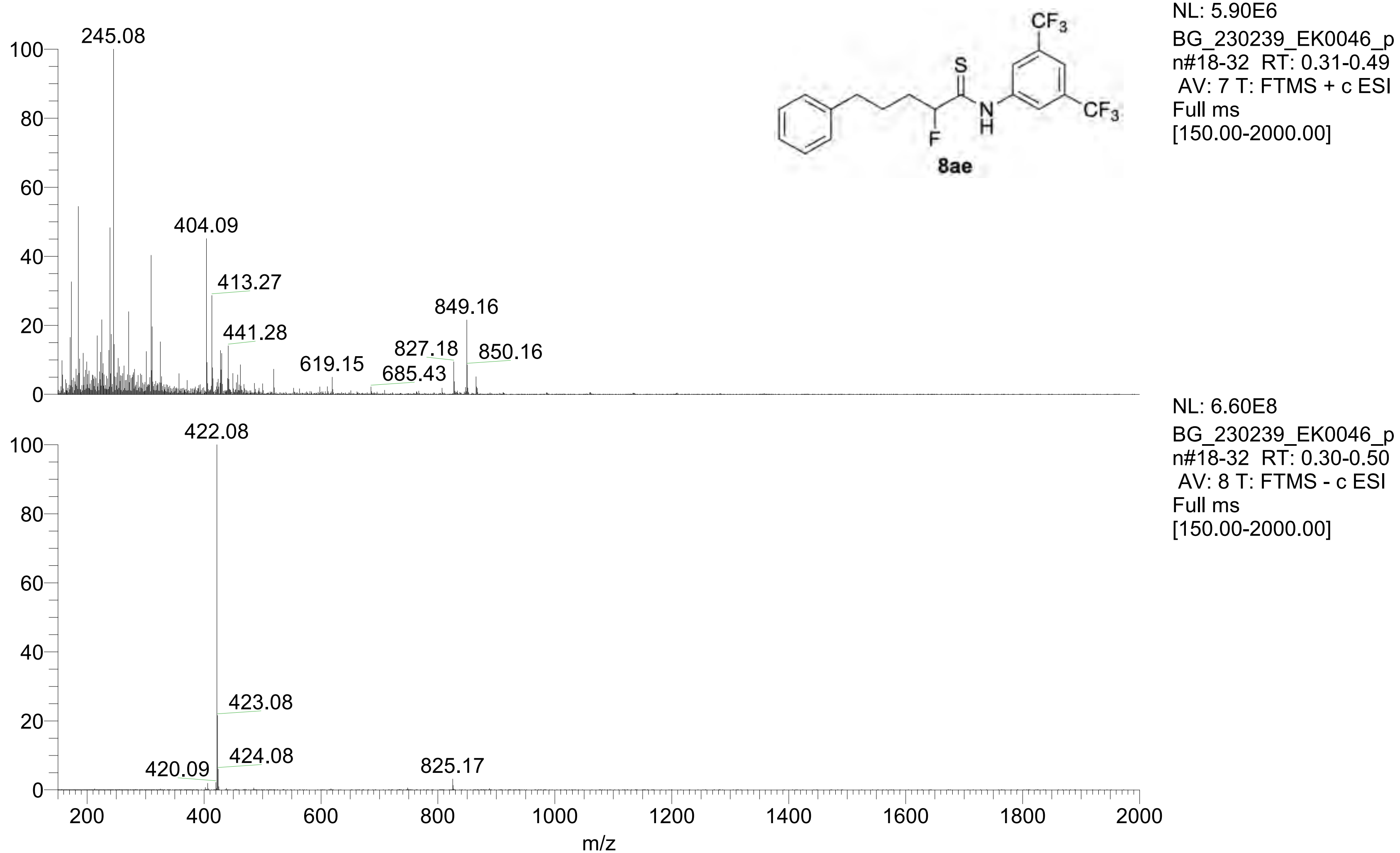

8ae
X : parts per Million : Proton
abundance



8ae
X : parts per Million : Carbon13
(thousandths)
198.909
198.794
141.489
138.787
133.152
132.817
132.472
132.136
128.619
128.562
126.233
124.326
123.148
121.614
120.589
99.622
97.696
77.486
77.160
76.844
35.437
35.236
26.295
1.178

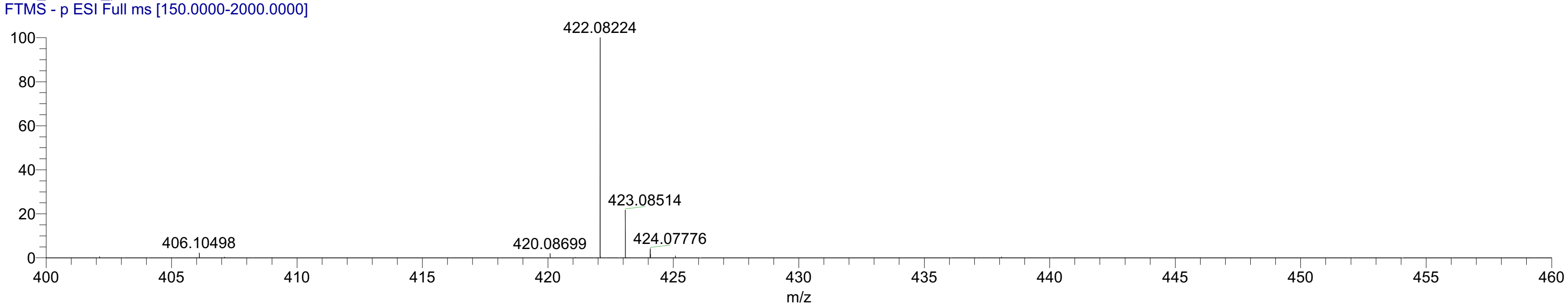


Sample No. : C:\Xcalibur\...\0517\BG_230239_E _ɔn Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 05/17/23 13:40:35
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

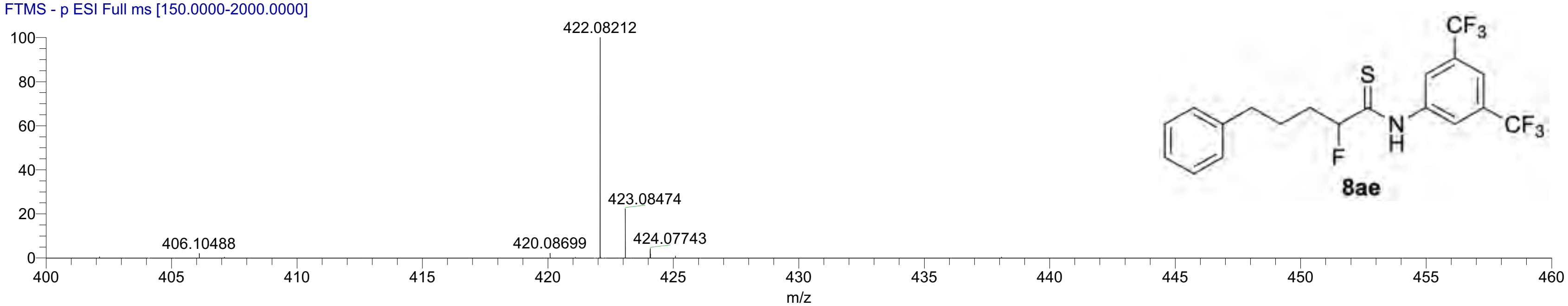


Sample No. : C:\Xcalibur\...\0517\230239_EK0046_pn Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 05/17/23 11:47:31
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

230239_EK0046_pn #18-21 RT: 0.30-0.33 AV: 2 NL: 5.71E7
T: FTMS - p ESI Full ms [150.0000-2000.0000]

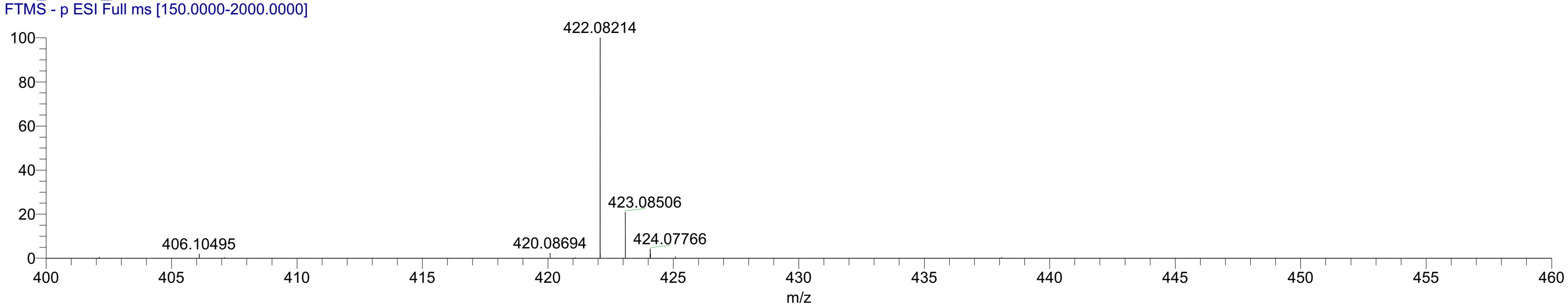


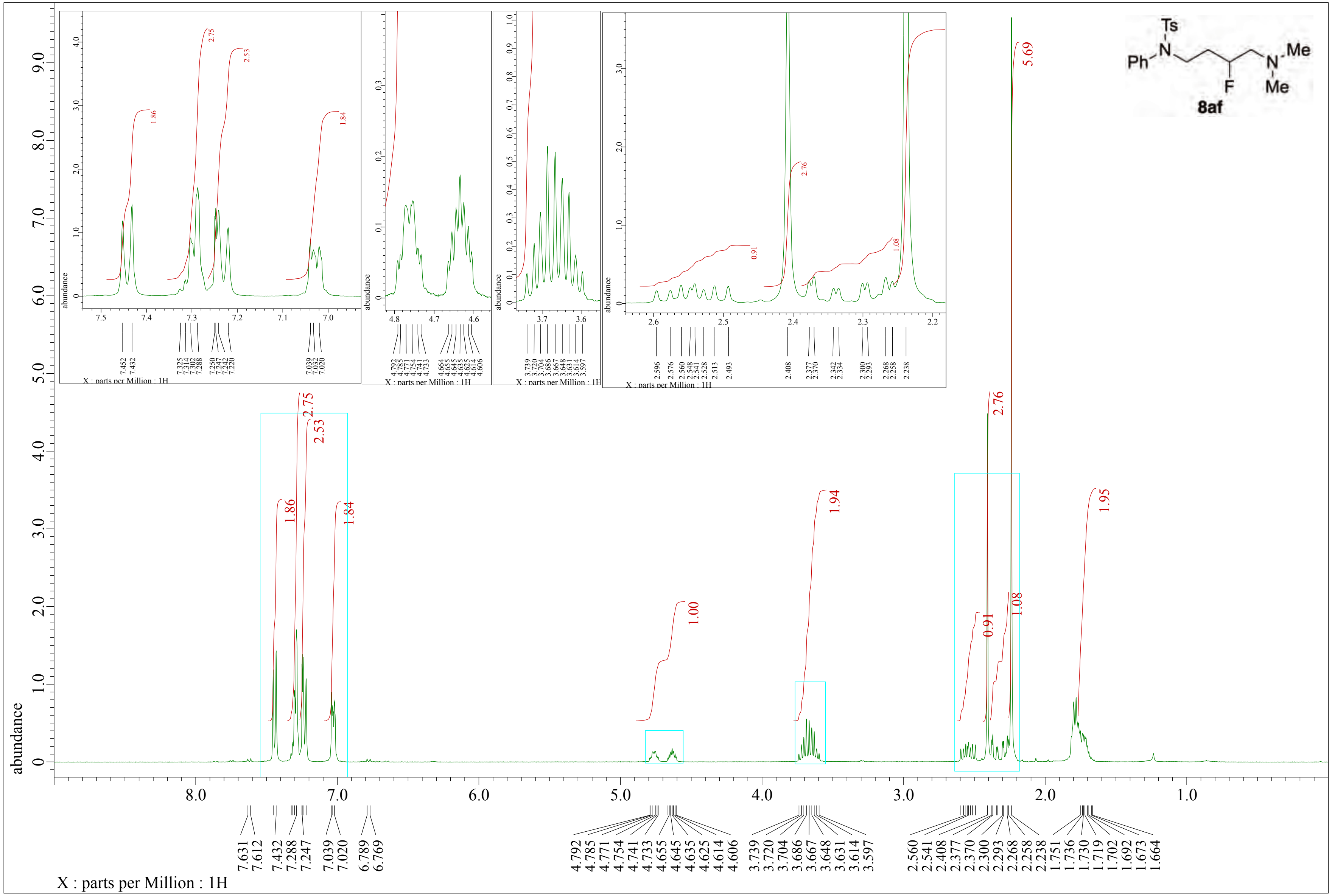
230239_EK0046_pn #22-25 RT: 0.36-0.38 AV: 2 NL: 2.08E8
T: FTMS - p ESI Full ms [150.0000-2000.0000]

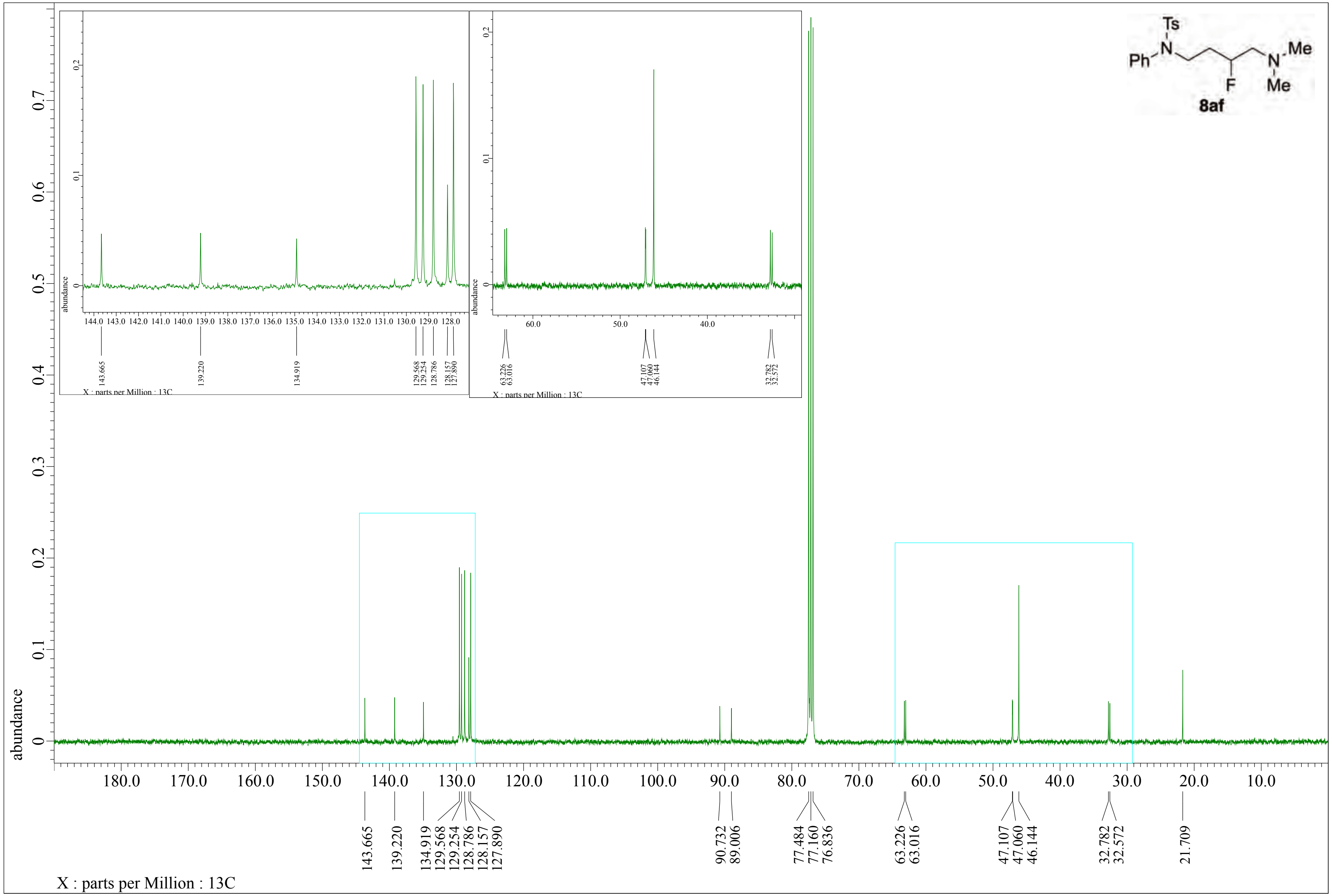


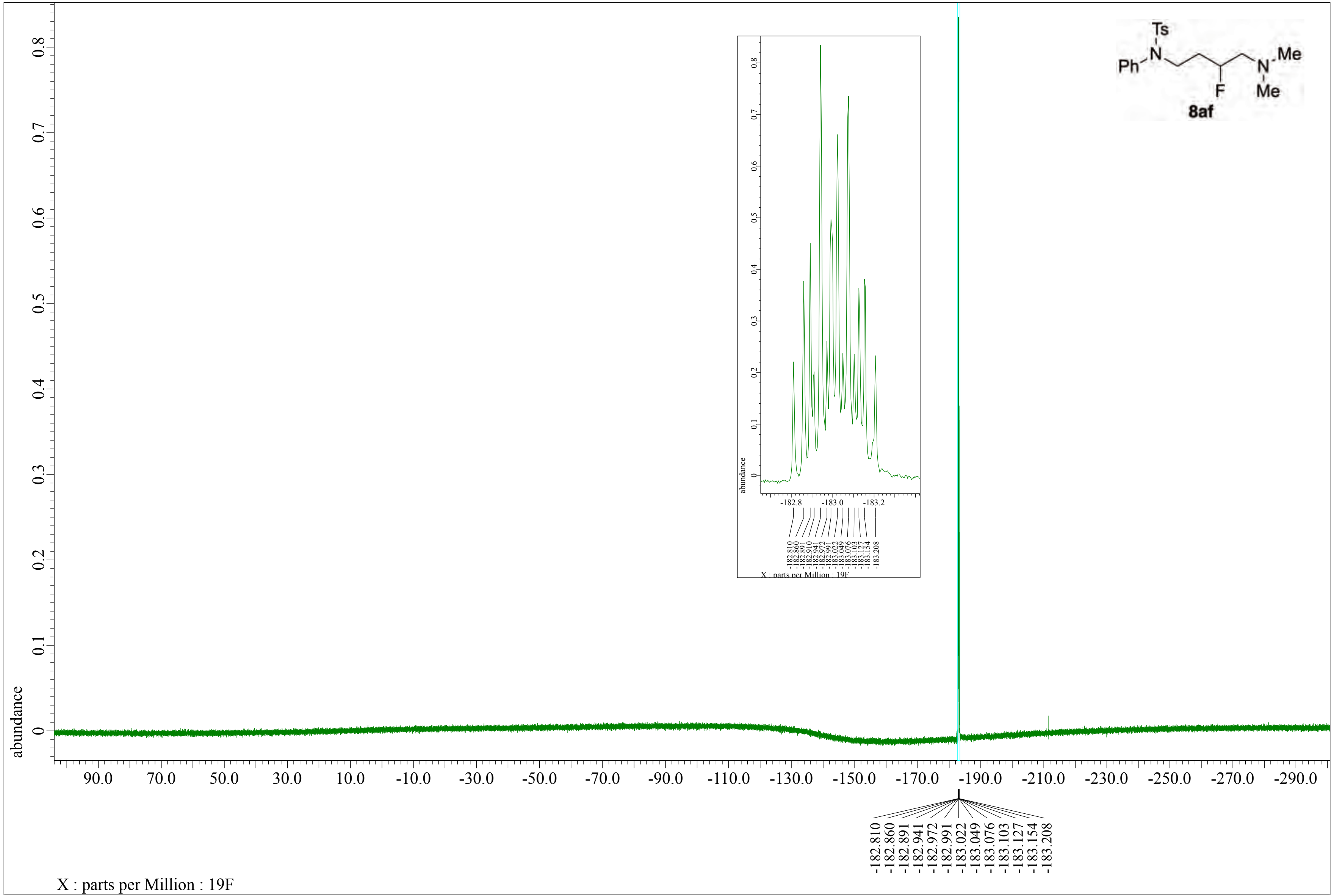
8ae

230239_EK0046_pn #26-29 RT: 0.41-0.44 AV: 2 NL: 1.77E8
T: FTMS - p ESI Full ms [150.0000-2000.0000]

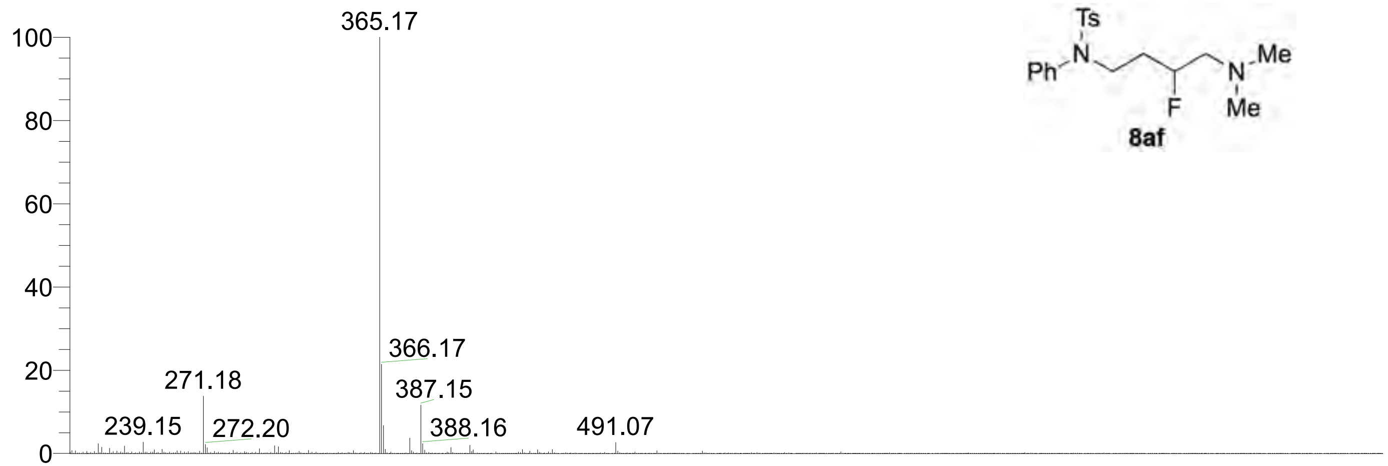



Ts
Ph
N
N
Me
Me
F
8af
abundance
X : parts per Million : 1H
1.86
2.75
2.53
1.84
1.00
1.94
0.91
2.76
1.08
5.69
1.95

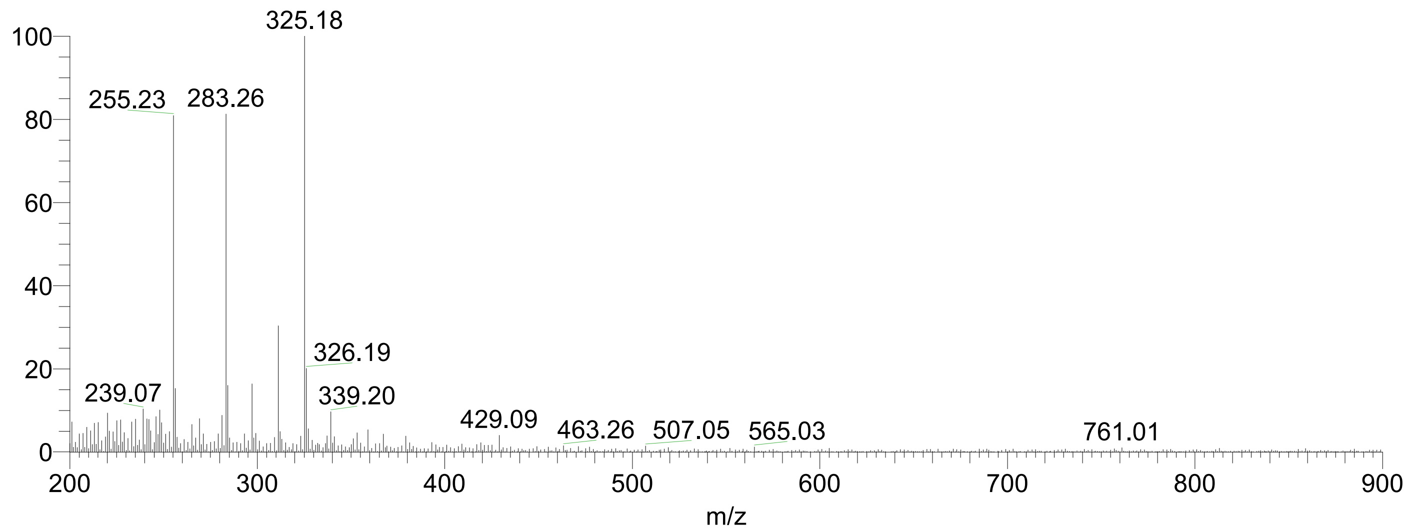

Ts
Ph
N
Me
F
Me
8af
abundance
X : parts per Million : 13C
143.665
139.220
134.919
129.568
129.254
128.786
128.157
127.890
90.732
89.006
77.484
77.160
76.836
63.226
63.016
47.107
47.060
46.144
32.782
32.572
21.709


abundance
X : parts per Million : 19F
-182.810
-182.860
-182.891
-182.941
-182.972
-182.991
-183.022
-183.049
-183.076
-183.103
-183.127
-183.154
-183.208
Ts
Ph
N
Me
N
F
Me
8af

Sample No. : C:\Xcalibur\...\1228\BG_231859_8af_pn Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 12/28/23 14:28:11
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University



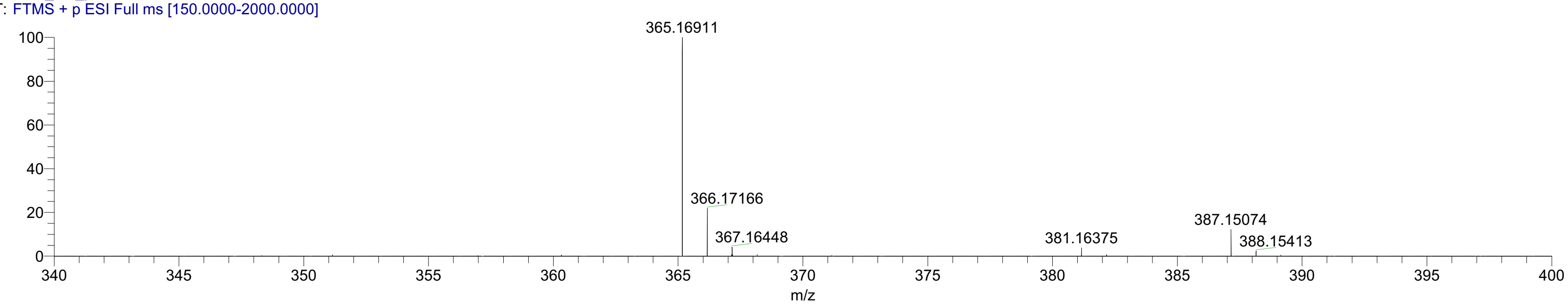
NL: 6.22E7
BG_231859_8af_pn#1
8-31 RT: 0.31-0.50
AV: 7 T: FTMS + c
ESI Full ms
[150.00-2000.00]



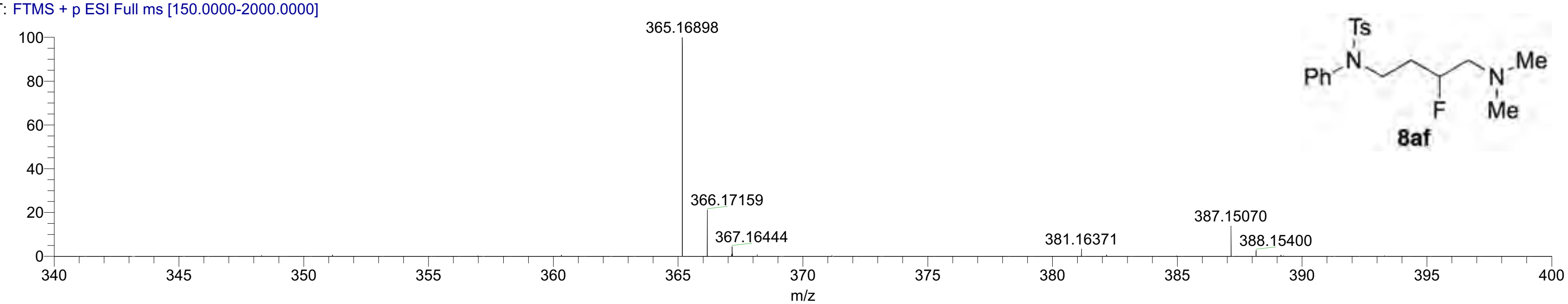
NL: 1.54E6
BG_231859_8af_pn#1
8-31 RT: 0.30-0.49
AV: 7 T: FTMS - c ESI
Full ms
[150.00-2000.00]

Sample No. : C:\Xcalibur\...\1228\231859_8af_pn
Instrument : Exactive Plus
Mobile phase solvent : MeOH
Operator name : hayashi harumi
Sample solvent : CHCl3
Date : 12/28/23 12:27:52
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

231859_8af_pn #21-25 RT: 0.34-0.41 AV: 3 NL: 1.98E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]

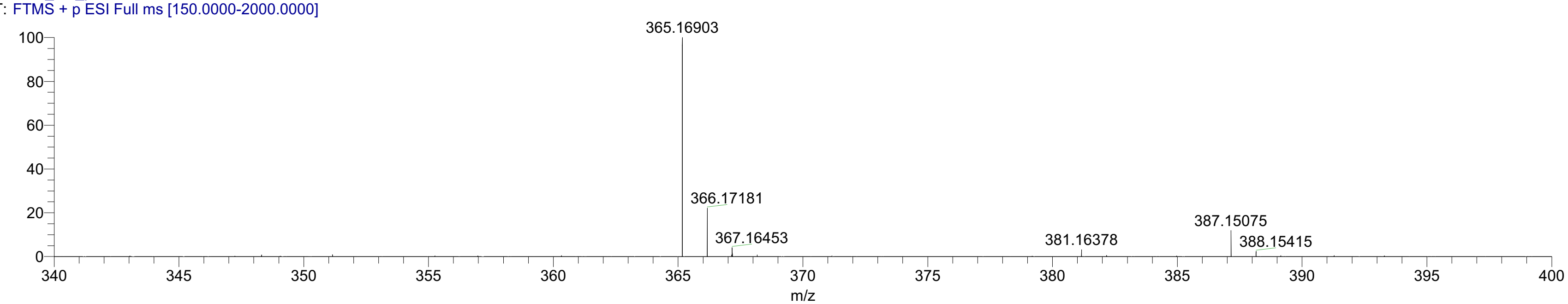


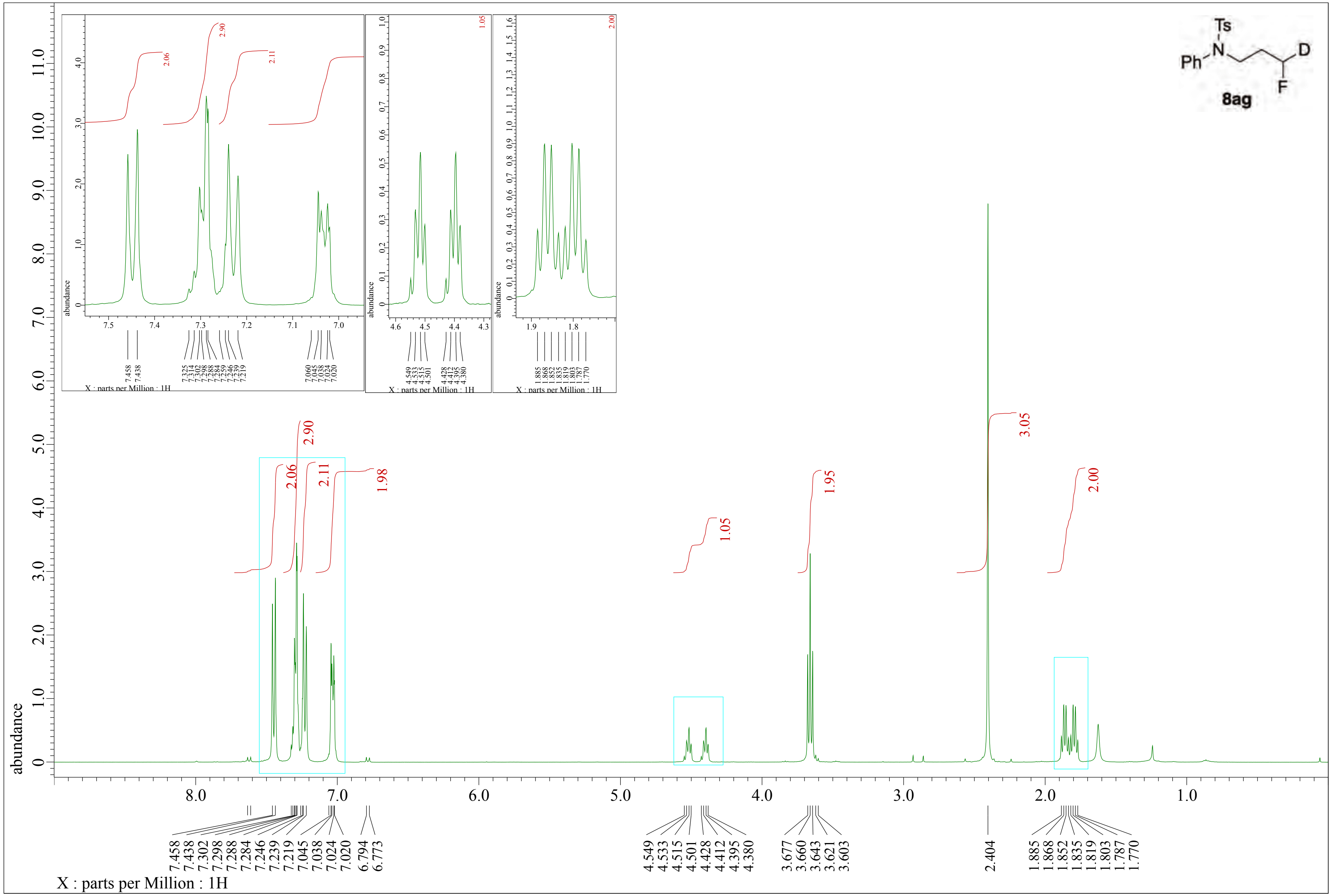
231859_8af_pn #25-28 RT: 0.41-0.44 AV: 2 NL: 1.80E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]

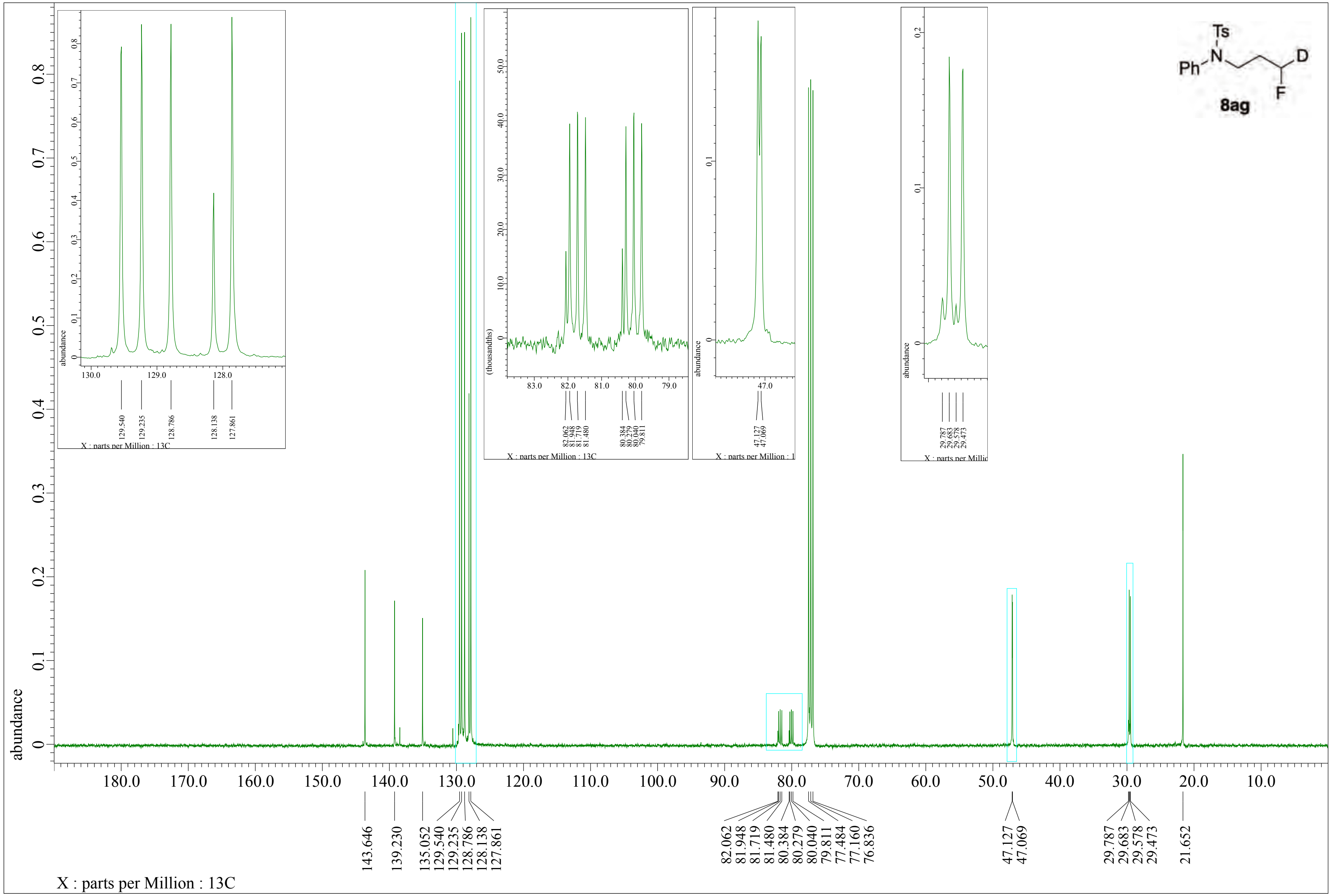


8af

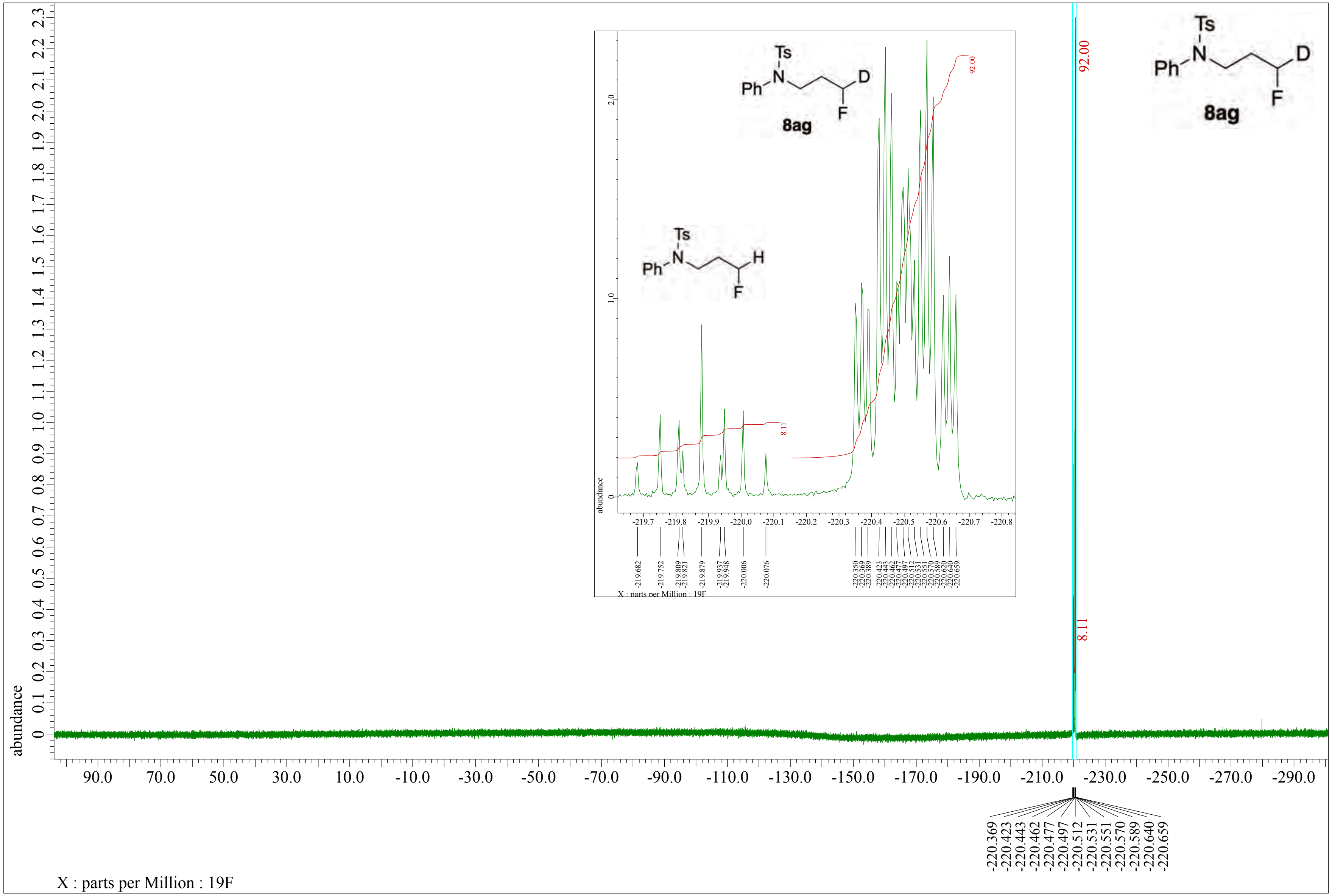
231859_8af_pn #29-31 RT: 0.47-0.50 AV: 2 NL: 1.03E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



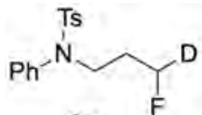

Ts
N
Ph
D
F
8ag
abundance
X : parts per Million : 1H
2.06
2.90
2.11
1.98
1.05
1.95
3.05
2.00
7.458
7.438
7.302
7.298
7.288
7.284
7.246
7.239
7.219
7.045
7.038
7.024
7.020
6.794
6.773
4.549
4.533
4.515
4.501
4.428
4.412
4.395
4.380
3.677
3.660
3.643
3.621
3.603
2.404
1.885
1.868
1.852
1.835
1.819
1.803
1.787
1.770



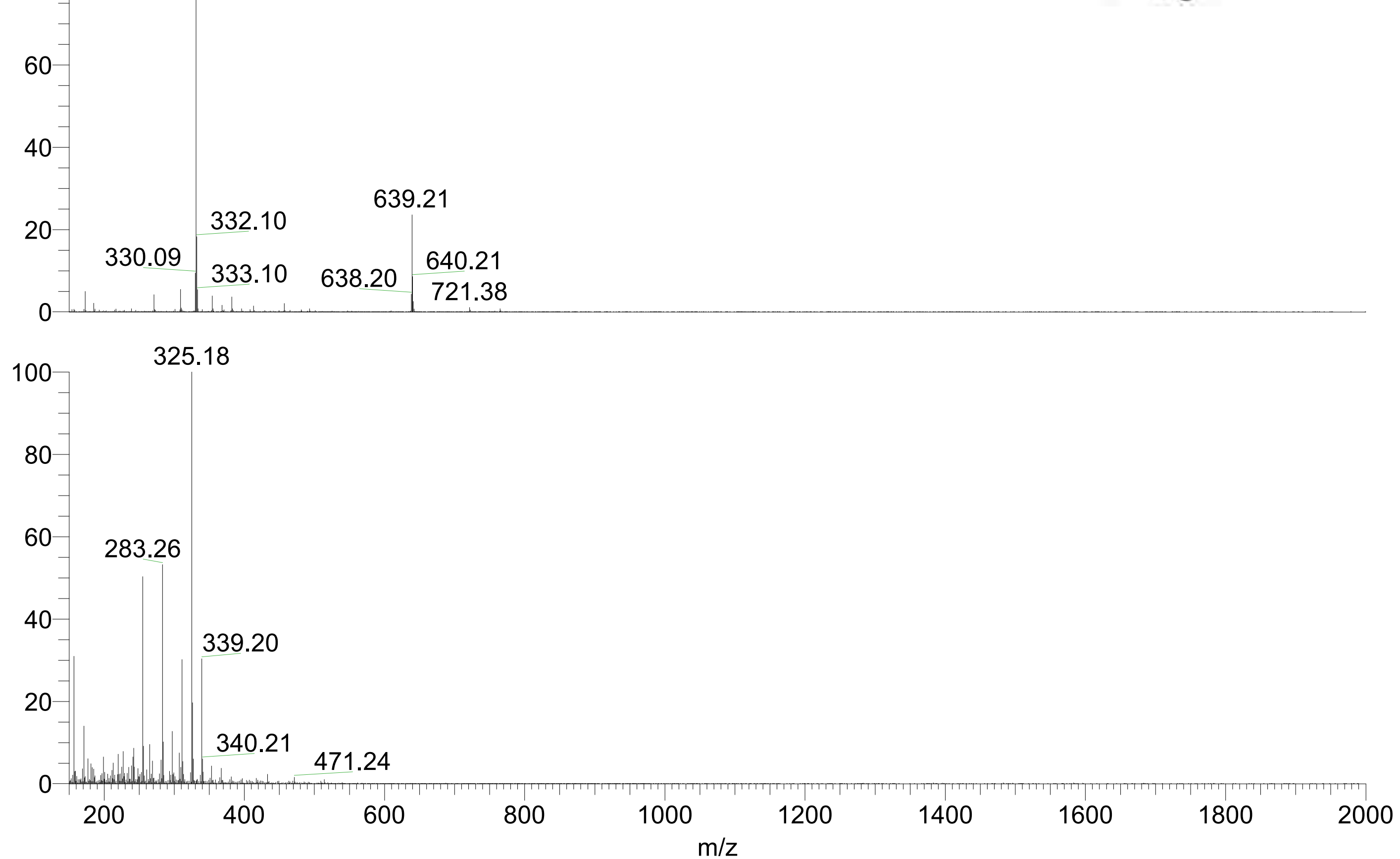
8ag
abundance
X : parts per Million : 13C
143.646
139.230
135.052
129.540
129.235
128.786
128.138
127.861
82.062
81.948
81.719
81.480
80.384
80.279
80.040
79.811
77.484
77.160
76.836
47.127
47.069
29.787
29.683
29.578
29.473
21.652


abundance
X : parts per Million : 19F
92.00
8.11
Ts
N
Ph
D
F
8ag
H
-220.369
-220.423
-220.443
-220.462
-220.477
-220.497
-220.512
-220.531
-220.551
-220.570
-220.589
-220.640
-220.659

Sample No. : C:\Xcalibur\...\0109\BG_231860_8a ... Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 01/09/24 11:30:44
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

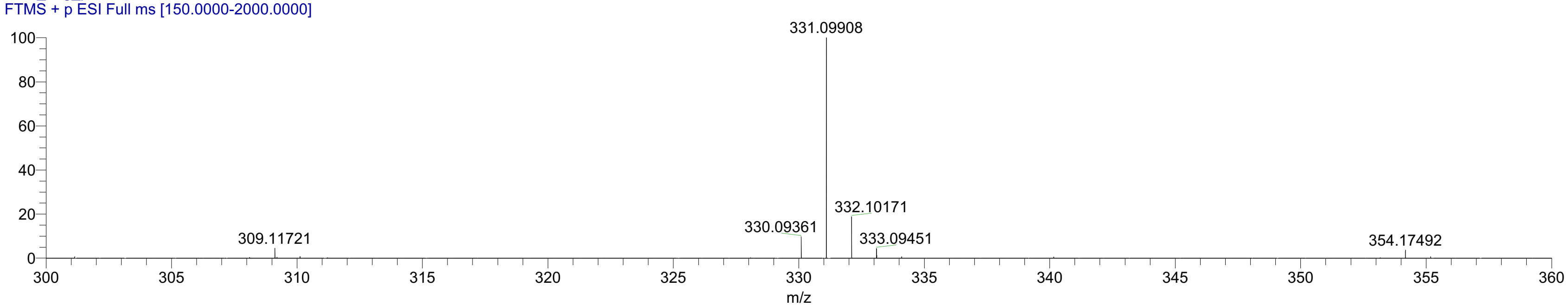


8ag

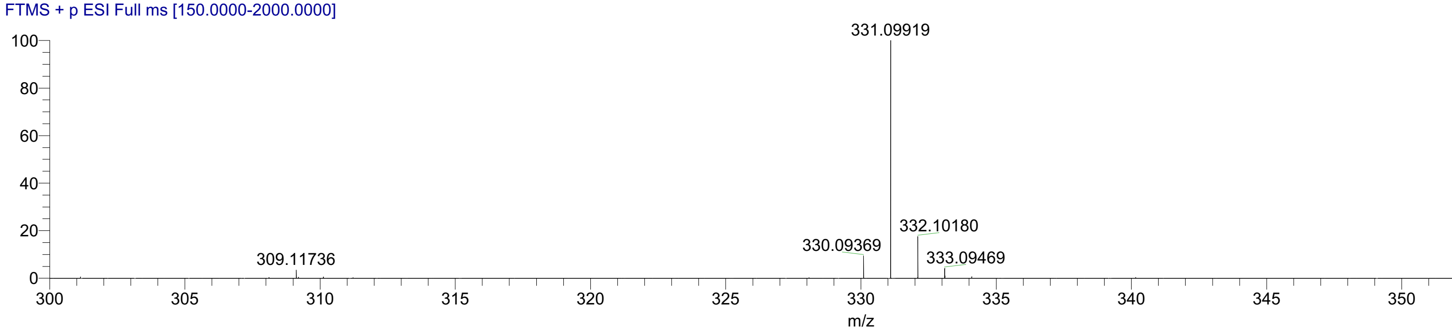


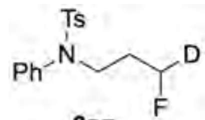
Sample No. : C:\Xcalibur\...\0109\231860_8ag_pn2 Instrument : Exactive Plus Mobile phase solvent : MeOH
Operator name : hayashi harumi Sample solvent : CHCl3
Date : 01/09/24 11:22:19
Instrumental method : C:\Xcalibur\methods\ESI_100ul\S60_100ul_mz150_2000pn.meth
Instrumental Analysis Division, Global Facility Center, Creative Research Institution, Hokkaido University

231860_8ag_pn2 #21-25 RT: 0.34-0.40 AV: 3 NL: 6.32E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



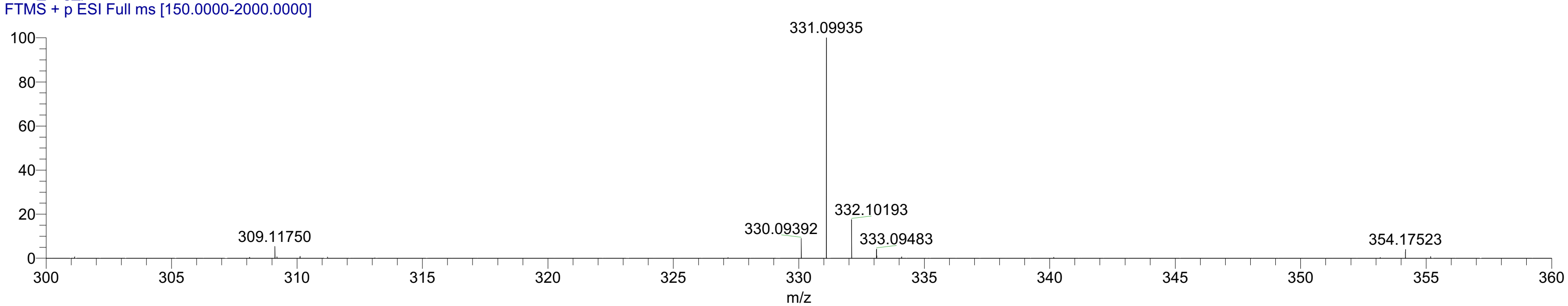
231860_8ag_pn2 #25-28 RT: 0.40-0.43 AV: 2 NL: 5.97E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]





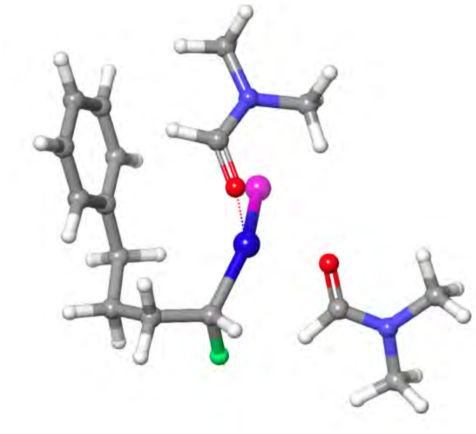
8ag

231860_8ag_pn2 #29-32 RT: 0.47-0.50 AV: 2 NL: 2.62E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



10. Cartesian Coordinates of the Optimized Structures Obtained from DFT Calculations

2a-I•2DMF_conformer-1

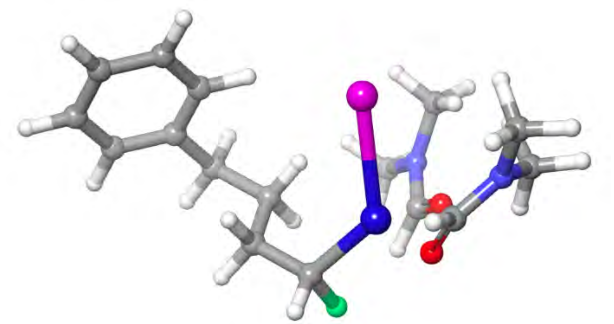


C	0.87677300	2.35197600	-0.67396500
H	1.44258400	2.43459600	-1.61860500
F	1.73788100	2.94441700	0.30298300
Zn	0.64857300	0.37211200	-0.37237300
O	-0.53400600	-0.38765700	-1.82548100
C	-1.52424300	-1.11512900	-1.61209900
N	-1.46357700	-2.43007200	-1.45028800
H	-2.53461400	-0.68831700	-1.56745800
O	2.52359300	-0.34240500	-0.96789500
C	3.42887300	0.37512700	-0.51219700
N	4.72018500	0.04264400	-0.52618400
H	3.20857700	1.35705500	-0.06786400
C	-2.64028800	-3.19672700	-1.08512000

H	-2.53625200	-3.56146900	-0.05766300
H	-3.52468400	-2.56080700	-1.14942700
H	-2.75256100	-4.04920400	-1.76176300
C	-0.19881900	-3.14839700	-1.49450300
H	0.59518700	-2.45494400	-1.76914700
H	0.01895200	-3.56899900	-0.50908400
H	-0.27075600	-3.94938700	-2.23746900
C	5.16080000	-1.23324300	-1.06076900
H	5.66256400	-1.80987300	-0.27739700
H	4.28931700	-1.77966300	-1.41697300
H	5.86064500	-1.06970700	-1.88644300
C	5.73152000	0.92104000	0.02971200
H	5.26142500	1.83335800	0.40084300
H	6.24814400	0.42510600	0.85764400
H	6.46615500	1.18500800	-0.73783300
C	-0.33295100	3.25425200	-0.82660900
H	-0.02584800	4.23686200	-1.21525300
H	-0.97363700	2.79767500	-1.59260100
C	-1.11258800	3.50835100	0.46819000
H	-1.93421300	4.20694200	0.26257000
H	-0.43883000	4.02610800	1.15900200
C	-1.65469500	2.28153000	1.20081700
H	-0.82875000	1.61161300	1.46739700
H	-2.06498900	2.61486100	2.16343900
C	-2.73912100	1.47181600	0.51631500

C	-3.15282400	0.27124200	1.11395600
C	-3.40891300	1.89477800	-0.63502500
C	-4.21484900	-0.46332500	0.59743200
H	-2.63559700	-0.07709100	2.00371700
C	-4.46565200	1.15231100	-1.16703200
H	-3.12049600	2.82367800	-1.11672800
C	-4.87989800	-0.02469900	-0.54931300
H	-4.52744900	-1.37737900	1.09505600
H	-4.97398800	1.50703000	-2.05874600
H	-5.71560000	-0.59026900	-0.95165400
I	0.31613000	-1.29129800	1.72359200

2a-I•2DMF_conformer-2

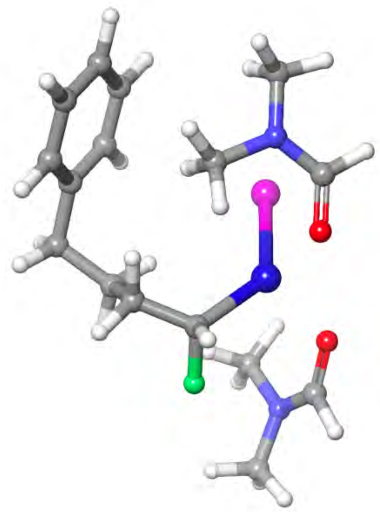


C	0.42506000	-1.18541000	-2.22118700
H	0.33238600	-0.84916200	-3.26098000
F	0.22900100	-2.60668000	-2.28140700
Zn	-1.01592000	-0.40909600	-1.04280000
O	-2.74200400	0.21283100	-1.90444200

C	-3.39688300	1.19531700	-1.50822100
N	-4.15998300	1.21486400	-0.42521000
H	-3.39156100	2.13422800	-2.07684600
O	-1.74107300	-1.89050200	0.19213400
C	-0.87104500	-2.75171700	0.43049300
N	-0.38296400	-2.98703400	1.64404600
H	-0.43760300	-3.35285300	-0.37721000
C	-4.25316500	0.05093900	0.44345900
H	-5.28934800	-0.05512000	0.77609400
H	-3.94142700	-0.83529400	-0.10701100
H	-3.59328000	0.18543800	1.30749600
C	-4.70010200	2.46126200	0.08797300
H	-4.58760300	3.24833800	-0.65974200
H	-5.76027100	2.33708600	0.32455800
H	-4.15144400	2.74951500	0.99099600
C	0.67032200	-3.96241900	1.85430200
H	0.37645400	-4.66745400	2.63762600
H	0.85348000	-4.51165100	0.92904900
H	1.59395700	-3.45667300	2.15638300
C	-0.75994400	-2.15970300	2.78034400
H	-1.52034600	-1.44905200	2.46031500
H	-1.14083100	-2.79236900	3.58773500
H	0.11538400	-1.60559700	3.13417200
C	1.85642300	-0.96488900	-1.76904400
H	2.56255000	-1.42941300	-2.47576400

H	2.05670900	0.11469400	-1.77494600
C	2.12940900	-1.52174900	-0.37355900
H	1.88958200	-2.59346300	-0.37305400
H	1.44968200	-1.03845100	0.34629000
C	3.57937800	-1.33569800	0.09134000
H	3.69396200	-1.76399300	1.09665900
H	4.24527900	-1.90587900	-0.56782800
C	4.01669400	0.11205000	0.10611800
C	3.29531600	1.06361600	0.83434900
C	5.12711800	0.53549800	-0.62543900
C	3.67379600	2.40176100	0.82885600
H	2.41268800	0.76544200	1.39497300
C	5.51694600	1.87346800	-0.62578800
H	5.69090000	-0.19206000	-1.20449100
C	4.78994100	2.81117700	0.10119100
H	3.08626200	3.12439500	1.38679200
H	6.38463800	2.18247900	-1.20108500
H	5.08577500	3.85573700	0.09579900
I	-0.72697600	1.53999400	0.86464500

2a-I•2DMF_conformer-3

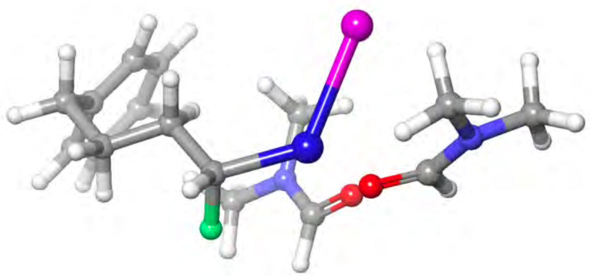


C	-1.14745500	1.41451300	1.45966700
H	-1.21478800	1.37049700	2.55736500
F	-2.37783500	2.03987200	1.05907900
Zn	-1.12281300	-0.47165100	0.71061300
O	-0.42920400	-1.91144500	1.99378700
C	0.60249500	-2.54567900	1.70350900
N	1.81044400	-2.00891100	1.58792300
H	0.56609600	-3.63106000	1.54692000
O	-3.07884000	-1.02977400	0.72545000
C	-4.03951700	-0.24677700	0.65282900
N	-4.28735600	0.57128700	-0.36268900
H	-4.79208600	-0.22088400	1.45197800
C	2.90079500	-2.73793900	0.96529400
H	3.81003900	-2.62782700	1.56255800

H	2.64016000	-3.79527400	0.88902400
H	3.07079400	-2.33930300	-0.04106800
C	1.99590100	-0.57624500	1.76371400
H	1.22961600	-0.20032600	2.44306900
H	2.98694700	-0.39654100	2.18640900
H	1.92952200	-0.06127800	0.79621300
C	-3.33406000	0.67460900	-1.45834700
H	-2.53570000	1.37330600	-1.18495200
H	-2.90827200	-0.30657700	-1.67246100
H	-3.85705900	1.04264700	-2.34359200
C	-5.24831600	1.64951000	-0.22130000
H	-5.90151400	1.45236800	0.63106500
H	-4.71710800	2.59170500	-0.05178900
H	-5.85656700	1.72725400	-1.12593700
C	-0.03479000	2.37783700	1.09925100
H	-0.18173300	3.34829900	1.59926600
H	0.90473600	1.96639700	1.49293000
C	0.10545400	2.61475300	-0.40352800
H	-0.72916300	3.23644600	-0.74859300
H	0.02798800	1.65440000	-0.93269800
C	1.43770200	3.27937200	-0.78522400
H	1.40722100	3.57327500	-1.84077200
H	1.57208500	4.19816600	-0.20087700
C	2.61252400	2.35513200	-0.56150600
C	2.81714200	1.26698900	-1.41698100

C	3.48872800	2.52746900	0.51391100
C	3.86958600	0.37982200	-1.20739300
H	2.13361600	1.10210100	-2.24600400
C	4.54835200	1.64636400	0.72519800
H	3.34038600	3.36726500	1.18885200
C	4.74201000	0.56829200	-0.13574300
H	4.00373600	-0.45873700	-1.88476800
H	5.22327800	1.80480800	1.56142800
H	5.56957800	-0.11711500	0.02342300
I	0.01634900	-1.47468500	-1.56599500

2a-I•2DMF_conformer-4

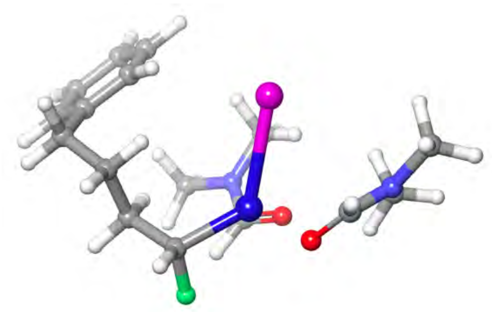


C	-0.48805200	1.39760300	-1.38355100
H	-0.24746200	1.93350000	-2.31130400
F	-1.14883600	2.37421700	-0.56434300
Zn	1.13492800	0.75412400	-0.37136900
O	2.93815000	1.69942600	-0.46682000
C	3.69584200	1.28681900	0.43456500

N	4.85661800	0.68859600	0.21130900
H	3.42361100	1.40062600	1.49269400
O	0.84143500	1.36505500	1.58825500
C	-0.34827500	1.68098900	1.79393200
N	-1.33515100	0.81030700	1.96184600
H	-0.64658700	2.73178100	1.87050100
C	5.58241700	0.04122100	1.28918400
H	6.64137100	0.30840300	1.23850600
H	5.17662800	0.36152500	2.25029300
H	5.47249000	-1.04508800	1.20186200
C	5.26088000	0.35759400	-1.14733700
H	4.71840200	0.99783200	-1.84047800
H	6.33730300	0.51732200	-1.24905100
H	5.01441400	-0.68986500	-1.35271400
C	-1.07590400	-0.62240800	1.98068400
H	-1.28430900	-1.07772300	1.00682700
H	-0.02999700	-0.79665600	2.23268100
H	-1.72858200	-1.08123500	2.72869000
C	-2.72203100	1.23879300	1.89369300
H	-2.76706600	2.32911900	1.91119600
H	-3.17423200	0.88381600	0.96148400
H	-3.28344500	0.83075700	2.73843300
C	-1.52514100	0.33280700	-1.68743600
H	-1.05965600	-0.44127800	-2.31348600
H	-1.80531200	-0.16782100	-0.75173400

C	-2.79200800	0.86489000	-2.35747700
H	-2.55112500	1.20455000	-3.37252600
H	-3.14145100	1.74333600	-1.80158500
C	-3.92228400	-0.17778500	-2.42250900
H	-4.73069800	0.19971900	-3.05903800
H	-3.54440200	-1.09348300	-2.89360100
C	-4.47730700	-0.49970000	-1.05513300
C	-5.44474700	0.32851800	-0.47586100
C	-4.00738800	-1.58690700	-0.31155400
C	-5.92985600	0.08053200	0.80580600
H	-5.82182500	1.17708200	-1.04238900
C	-4.48420100	-1.83704600	0.97433600
H	-3.25885200	-2.24438000	-0.74826700
C	-5.44919600	-1.00457400	1.53682600
H	-6.68756900	0.73127400	1.23201100
H	-4.10708600	-2.68979000	1.53151500
H	-5.82931400	-1.20340300	2.53425100
I	2.05817000	-1.79448800	-0.17674000

2a-I•2DMF_conformer-5

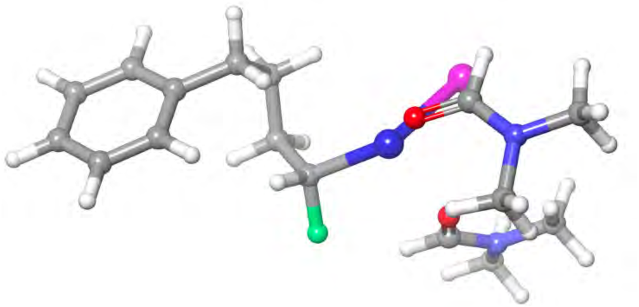


C	0.15774600	-2.49073600	-0.90797300
H	-0.14768800	-2.99423300	-1.83457300
F	0.14739300	-3.51699600	0.09093600
Zn	-1.14725600	-1.08967800	-0.26971100
O	-3.12686400	-1.46779700	-0.43691900
C	-3.99776900	-0.58769200	-0.57122100
N	-4.39290000	0.24382300	0.38125700
H	-4.52263700	-0.46702300	-1.52758400
O	-0.89774100	-1.00694300	1.78461900
C	0.29708700	-1.30375100	2.00581700
N	1.19897000	-0.44980000	2.46898400
H	0.67299500	-2.31002400	1.78552000
C	-5.23768600	1.38499200	0.07714100
H	-4.64137900	2.30209900	0.12924600
H	-5.64425400	1.28535300	-0.93084000
H	-6.06075300	1.43986900	0.79469100
C	-3.78196500	0.20710600	1.70226700
H	-3.33277900	-0.77130300	1.86529800

H	-3.00101500	0.97219400	1.77002500
H	-4.55743400	0.39571900	2.44935100
C	2.59778500	-0.82599900	2.59016000
H	2.95495500	-0.60886900	3.60153200
H	2.70682700	-1.89416900	2.39216100
H	3.19660400	-0.26264300	1.86647000
C	0.86309700	0.94265200	2.72557200
H	-0.19267800	1.09527300	2.50792000
H	1.07901400	1.18352000	3.77138400
H	1.46294100	1.58098600	2.07117500
C	1.60783400	-2.06076800	-1.05966100
H	1.95597700	-1.55251600	-0.14696800
H	2.24924400	-2.94746900	-1.18351900
C	1.80063900	-1.11761400	-2.24239000
H	1.10179200	-0.27508000	-2.15831700
H	1.54116700	-1.63966100	-3.17190500
C	3.23529400	-0.58872500	-2.35587500
H	3.92664400	-1.43265800	-2.47068400
H	3.32164600	0.01139400	-3.27042400
C	3.67949700	0.25700700	-1.18159600
C	2.92506400	1.36348200	-0.77195200
C	4.87025400	-0.01949400	-0.50493100
C	3.36833100	2.18336000	0.26290200
H	1.98665600	1.59642000	-1.26952800
C	5.31720300	0.79802600	0.53313000

H	5.46347200	-0.87924800	-0.80675000
C	4.56873600	1.90722100	0.91853800
H	2.77498600	3.04863200	0.54631300
H	6.25226800	0.56907000	1.03592300
H	4.91763700	2.55277700	1.71889100
I	-1.15935100	1.60925000	-0.76065600

2a-I•2DMF_conformer-6

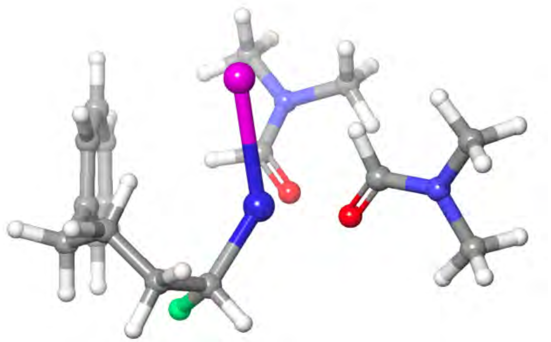


C	1.41139900	-0.40481700	-0.96543100
H	2.07074100	0.40619300	-1.29985300
F	1.05567900	-1.09200400	-2.16725000
Zn	-0.29296400	0.26626200	-0.14428300
O	-0.72901900	2.20932600	0.22332800
C	-1.86200200	2.42784500	0.69469900
N	-2.88172000	2.90103200	-0.01082800
H	-2.08378100	2.23429500	1.75099700
O	-1.79287300	0.23290400	-1.60588800
C	-1.90993200	-0.96726300	-1.92750700

N	-3.05497200	-1.63805500	-1.88750000
H	-1.03386000	-1.54322400	-2.25300500
C	-2.75365300	3.16211700	-1.43644500
H	-3.01768000	4.20400700	-1.64102600
H	-1.72691200	2.96323000	-1.73620100
H	-3.42130900	2.49776500	-1.99230000
C	-4.18651900	3.10277600	0.59148200
H	-4.15304400	2.82276500	1.64567900
H	-4.48605500	4.15158900	0.50363400
H	-4.92915700	2.47854200	0.08486400
C	-4.26017000	-1.03244300	-1.34805800
H	-4.51999300	-1.52096400	-0.40359500
H	-4.06050100	0.02121500	-1.15758800
H	-5.08061000	-1.14237400	-2.06393800
C	-3.09713300	-3.06504800	-2.14981300
H	-2.13342200	-3.39414600	-2.54173200
H	-3.30798700	-3.60472700	-1.22085800
H	-3.87752900	-3.28841400	-2.88310600
C	2.21105500	-1.37603000	-0.11647000
H	1.62466400	-2.29495100	0.00962100
H	3.14373700	-1.65596800	-0.62764800
C	2.52702000	-0.81108400	1.26876500
H	3.12417800	-1.54151000	1.82743400
H	1.59115600	-0.68282300	1.82981000
C	3.27347100	0.53328300	1.24148000

H	2.63583800	1.30315700	0.78834300
H	3.45612900	0.85361300	2.27459500
C	4.58673200	0.46399400	0.49727200
C	4.78851100	1.16538900	-0.69248200
C	5.63091300	-0.33073700	0.98317700
C	5.99583300	1.07573100	-1.38313400
H	3.99065700	1.79468100	-1.07950100
C	6.83806300	-0.42380000	0.29912600
H	5.49369300	-0.87902100	1.91256800
C	7.02430900	0.27935200	-0.89013800
H	6.13066300	1.62976000	-2.30723500
H	7.63673400	-1.04422300	0.69470500
H	7.96575700	0.20724600	-1.42578600
I	-1.83622000	-1.02471300	1.72631100

2a-I•2DMF_conformer-7

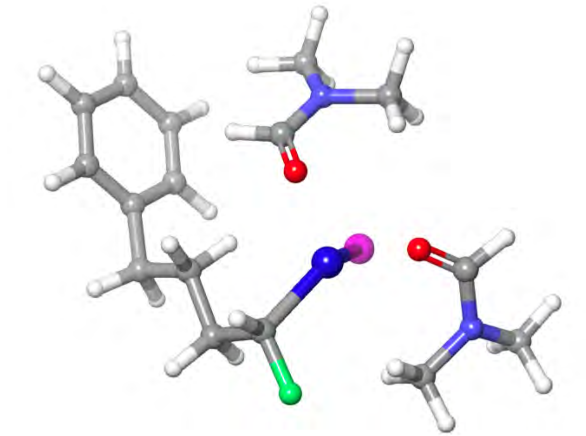


C	-0.21144600	-2.57334900	-0.78680800

H	0.54293800	-3.13440200	-1.35955600
F	-1.35984900	-2.55876400	-1.62244200
Zn	0.50122600	-0.71720500	-0.49093700
O	2.53305000	-0.73898900	-0.87806400
C	3.43212800	-0.36985300	-0.10912500
N	4.73246500	-0.49391900	-0.37891900
H	3.19559000	0.09561000	0.85736400
O	0.11579900	0.73667400	-1.84772500
C	-0.72590400	1.58525400	-1.48727700
N	-0.43301800	2.86246700	-1.27957000
H	-1.77827700	1.31519900	-1.32858300
C	5.74452400	-0.05217100	0.56174000
H	6.38278600	0.70802400	0.10016200
H	5.26514700	0.37470900	1.44443300
H	6.36922500	-0.89687800	0.86924000
C	5.18894800	-1.09078300	-1.62244500
H	4.31939900	-1.36288100	-2.21836500
H	5.80642200	-0.37410100	-2.17298000
H	5.78601400	-1.98307800	-1.40943500
C	-1.40162300	3.76522600	-0.68497900
H	-1.42420100	4.70575500	-1.24287100
H	-2.38922100	3.30326600	-0.70752800
H	-1.12510400	3.96317700	0.35682700
C	0.94366400	3.32387200	-1.33841100
H	1.53938300	2.58093300	-1.86641200

H	0.98092700	4.28131900	-1.86559200
H	1.32867600	3.44407700	-0.31955100
C	-0.54936500	-3.39258100	0.44214900
H	-0.92381200	-4.38286600	0.13592800
H	0.38715500	-3.56413900	0.99212900
C	-1.56780800	-2.75962000	1.39144400
H	-1.17689800	-1.80174400	1.75842300
H	-1.66811700	-3.40901900	2.26844000
C	-2.96279700	-2.55802200	0.76276600
H	-3.10712200	-3.28507600	-0.04197400
H	-3.72345000	-2.77903500	1.52253000
C	-3.28198000	-1.17380900	0.23878100
C	-3.77293100	-0.98709400	-1.05786600
C	-3.22022200	-0.06206100	1.08724800
C	-4.25642200	0.25257600	-1.47173500
H	-3.78707200	-1.83157200	-1.73934800
C	-3.69656200	1.18136000	0.67845100
H	-2.81367000	-0.17415400	2.08914100
C	-4.24144900	1.33774200	-0.59621800
H	-4.65643200	0.36698600	-2.47496900
H	-3.65366000	2.02263600	1.36483100
H	-4.64791300	2.29689600	-0.90709100
I	0.53512600	0.92347100	1.74706300

2a-I•2DMF_conformer-8

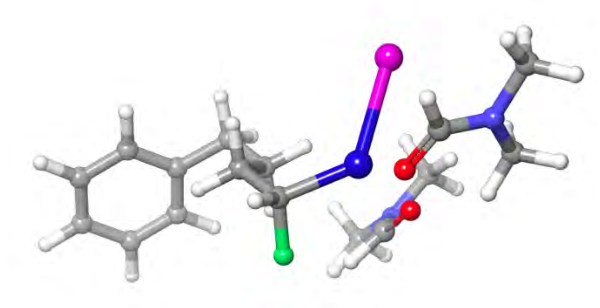


C	-0.88030600	-2.63269900	-0.85582900
H	-0.59889500	-3.02771600	-1.84280900
F	-2.04872400	-3.34355400	-0.48639400
Zn	-1.11638300	-0.63262200	-0.91462700
O	0.27944000	0.29691200	-2.06948900
C	1.17304700	1.03213000	-1.60548500
N	1.04440800	2.33667900	-1.41454800
H	2.15704000	0.62310300	-1.32952900
O	-2.72513600	0.40551800	-1.61537000
C	-3.57501100	0.86245600	-0.82601900
N	-4.19204200	0.17705800	0.12492900
H	-3.88695500	1.91160100	-0.90545100
C	-0.21773400	3.01119200	-1.67457700
H	-0.03234200	3.89196400	-2.29676500
H	-0.88900100	2.32227300	-2.18733200

H	-0.66503400	3.31472500	-0.72237000
C	2.06944000	3.09813900	-0.72352400
H	2.97599800	2.49662400	-0.63216400
H	2.29121600	4.01098200	-1.28373600
H	1.71354200	3.36035400	0.27900500
C	-3.90120000	-1.23435000	0.34249800
H	-4.81923800	-1.73085500	0.66602500
H	-3.55075800	-1.69744000	-0.57792100
H	-3.13299800	-1.35150200	1.11549900
C	-4.95265800	0.85796700	1.15858000
H	-5.12766300	1.89504700	0.86636600
H	-5.91291100	0.35619600	1.30270900
H	-4.38403300	0.84453700	2.09455500
C	0.21984300	-2.99888900	0.13293800
H	-0.13812000	-2.79942900	1.15246100
H	0.46986300	-4.06900500	0.08232700
C	1.45347000	-2.13838200	-0.12317900
H	1.17316100	-1.09062400	0.03622700
H	1.76979700	-2.21868300	-1.17380800
C	2.65242900	-2.40738200	0.79149700
H	2.30520400	-2.44607100	1.83087300
H	3.10474600	-3.37859800	0.56047900
C	3.65975700	-1.29533500	0.63051300
C	4.70649100	-1.38907900	-0.28956700
C	3.49228100	-0.09638900	1.33362000

C	5.57345500	-0.31815700	-0.49917400
H	4.84161100	-2.31278600	-0.84738300
C	4.36426900	0.97130700	1.13661400
H	2.66561600	-0.00223500	2.03487100
C	5.40727900	0.86540000	0.21617300
H	6.38333900	-0.41115300	-1.21646900
H	4.22930700	1.88740700	1.70526600
H	6.09006300	1.69595500	0.06441300
I	-0.81080500	0.88024200	1.44673100

2a-I•2DMF_conformer-9

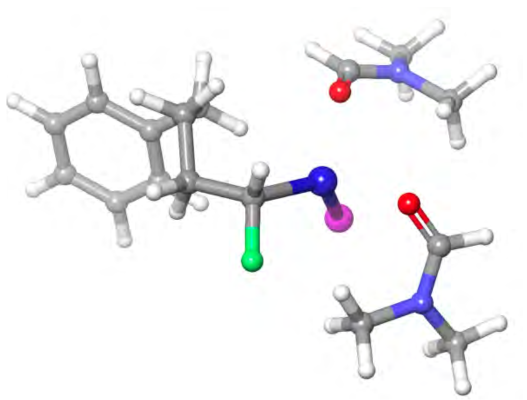


C	-0.70037200	-0.74282600	-1.75229800
H	-0.63679700	-1.54203600	-2.50072100
F	-1.17863600	0.39822300	-2.47892300
Zn	1.09677100	-0.27526900	-0.96748700
O	2.78309900	-0.66417000	-2.02258500
C	3.85116600	-1.03771200	-1.50236400
N	4.68366600	-0.25830100	-0.82781400

H	4.18403900	-2.07911400	-1.60070500
O	1.24154900	1.77337900	-0.81541600
C	0.12348400	2.30998400	-0.68419000
N	-0.24309400	2.98718600	0.39920200
H	-0.63922000	2.22258300	-1.46666500
C	5.78468200	-0.82023400	-0.06581700
H	5.55137300	-0.76529500	1.00282900
H	5.92964200	-1.86605300	-0.34228900
H	6.70191400	-0.26202300	-0.27191400
C	4.37236500	1.14417900	-0.59532600
H	3.62146700	1.47042200	-1.31324200
H	3.97577100	1.26700900	0.41841700
H	5.28809400	1.73010500	-0.71303800
C	0.61374000	3.04449700	1.57425300
H	0.14067100	2.50066800	2.39824000
H	1.56408700	2.56802500	1.33889000
H	0.76914100	4.08714000	1.86703000
C	-1.58123400	3.53281600	0.52675100
H	-2.11628900	3.42125100	-0.41826900
H	-2.12965600	2.99851300	1.31085200
H	-1.52958400	4.59418400	0.78713100
C	-1.79032000	-1.10436100	-0.75696800
H	-2.72871500	-1.33471500	-1.28202800
H	-1.47917700	-2.01569600	-0.22638500
C	-2.05352700	0.00290800	0.26107600

H	-2.35414700	0.90892700	-0.28390600
H	-1.11991500	0.23153700	0.79723800
C	-3.13410800	-0.34513500	1.29483200
H	-2.84411200	-1.26603900	1.81439600
H	-3.17357000	0.44536300	2.05539000
C	-4.50269100	-0.51009700	0.67928800
C	-5.04915500	-1.77337200	0.44488900
C	-5.24024900	0.61363800	0.29538700
C	-6.29822300	-1.91225100	-0.15603400
H	-4.48548600	-2.65636600	0.73610500
C	-6.48845200	0.48236100	-0.30434800
H	-4.82763300	1.60496300	0.47508900
C	-7.02225700	-0.78450500	-0.53212000
H	-6.70598000	-2.90351800	-0.32946400
H	-7.04738100	1.36793400	-0.59165100
H	-7.99656300	-0.89072300	-0.99866400
I	1.94721400	-0.93845700	1.54744300

2a-I•2DMF_conformer-10

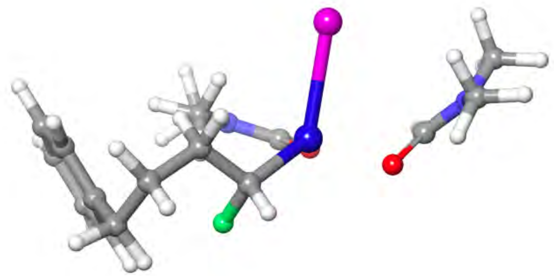


C	-0.34890500	-2.01325400	1.73372300
H	-0.15012000	-2.08567500	2.81453200
F	0.09622600	-3.25282900	1.19789600
Zn	0.73467600	-0.50004900	0.97540300
O	0.51249200	1.26179700	1.99864400
C	0.35358700	2.36680600	1.44938200
N	1.32981000	3.13209100	0.98073800
H	-0.65247400	2.79268100	1.33182200
O	2.77426800	-0.63058500	1.22245000
C	3.58042000	-0.79991400	0.28954600
N	3.53576400	-1.76915000	-0.61228600
H	4.43595200	-0.11984400	0.17503100
C	2.71388100	2.68794200	1.01739700
H	3.33944200	3.49981400	1.39992500
H	2.79076500	1.81258000	1.66227500
H	3.03083800	2.42200700	0.00256000

C	1.04171500	4.30756000	0.17839900
H	-0.01832500	4.55572300	0.25392900
H	1.63595100	5.15394000	0.53358400
H	1.28353500	4.10074300	-0.86961300
C	4.38722700	-1.73308600	-1.78801500
H	3.78196100	-1.48943200	-2.66759800
H	5.15858900	-0.97040900	-1.66538200
H	4.86322300	-2.70685000	-1.93055900
C	2.47898900	-2.77197200	-0.60431200
H	1.99864800	-2.81827100	0.37175100
H	1.72809600	-2.52746500	-1.36339800
H	2.92296200	-3.74536400	-0.83027600
C	-1.85906500	-1.97256500	1.56058700
H	-2.11798800	-2.05064700	0.49669700
H	-2.30045700	-2.85130700	2.04986500
C	-2.45132700	-0.68356000	2.14738700
H	-1.82458400	-0.34062500	2.98225400
H	-3.44532000	-0.87957300	2.56505900
C	-2.57804000	0.45545000	1.12078400
H	-2.78768600	1.39262300	1.65437400
H	-1.62341300	0.59107500	0.59873200
C	-3.66116900	0.20686600	0.09855400
C	-5.00834300	0.30012600	0.46245000
C	-3.34640500	-0.14485200	-1.21558800
C	-6.01705200	0.04704200	-0.46084100

H	-5.26579300	0.57769100	1.48276700
C	-4.35464000	-0.40103100	-2.14337600
H	-2.30187600	-0.20967900	-1.51359600
C	-5.69164700	-0.30634100	-1.76956000
H	-7.05784200	0.12739900	-0.16132000
H	-4.09108000	-0.67251300	-3.16110800
H	-6.47726600	-0.50401200	-2.49235400
I	0.83867000	0.55397600	-1.59566300

2a-I•2DMF_conformer-11

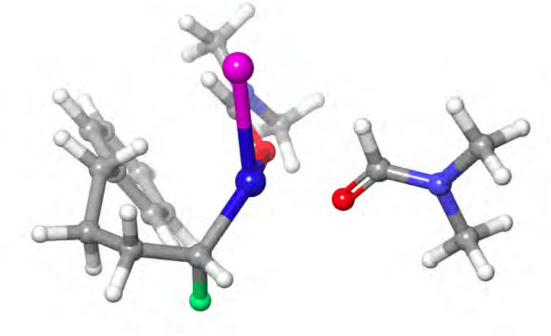


C	-0.66061900	-1.77407400	-0.74077900
H	-0.37170300	-2.71728900	-1.22457300
F	-1.62252800	-1.19209000	-1.63637400
Zn	0.85183600	-0.45642900	-0.59430600
O	2.50557600	-0.77556400	-1.76131100
C	3.40567600	0.05686300	-1.54004800
N	4.59760800	-0.24921900	-1.04544700
H	3.25111400	1.12329900	-1.75247800

O	0.62577700	1.39571800	-1.43422700
C	-0.08665500	2.40255600	-1.28790900
N	-1.14049700	2.49771300	-0.49223200
H	0.14572300	3.31376800	-1.85450300
C	5.50553800	0.78984700	-0.59494400
H	6.51925600	0.57572800	-0.94404600
H	5.18533500	1.75484200	-0.99175900
H	5.49286000	0.83655800	0.49960500
C	4.86833800	-1.60310400	-0.58587600
H	4.19267500	-2.28839000	-1.09458200
H	5.90616800	-1.85790800	-0.81462000
H	4.69828600	-1.65928800	0.49535100
C	-1.91345600	3.72198700	-0.38594800
H	-1.87118300	4.10578600	0.63751200
H	-1.51026900	4.47548200	-1.06557900
H	-2.95659800	3.52025800	-0.64672600
C	-1.56934700	1.33672100	0.28714800
H	-1.77020400	0.50241200	-0.38776700
H	-0.79743700	1.06983900	1.01720400
H	-2.49248500	1.58728100	0.81159700
C	-1.36569300	-2.09683300	0.56580800
H	-0.61528300	-2.55621500	1.22349200
H	-1.67126000	-1.17424000	1.07726800
C	-2.57829400	-3.03057100	0.47775000
H	-2.94498400	-3.22117200	1.49516400

H	-2.25902900	-4.00383500	0.08357500
C	-3.74067900	-2.52688800	-0.39537100
H	-3.44706000	-2.56577600	-1.44596400
H	-4.58511900	-3.21864700	-0.27378000
C	-4.22203400	-1.12608000	-0.08299700
C	-4.40649100	-0.19434300	-1.10870800
C	-4.52669200	-0.73296800	1.22479600
C	-4.90313500	1.08018300	-0.84447100
H	-4.14667800	-0.47599100	-2.12506400
C	-5.01608100	0.54256200	1.49808800
H	-4.38604500	-1.43737100	2.04115100
C	-5.21332300	1.45447600	0.46192000
H	-5.05339900	1.77980400	-1.66244300
H	-5.25145400	0.82156600	2.52094000
H	-5.60923000	2.44412300	0.67138900
I	2.16382600	0.24876100	1.71516000

2a-I•2DMF_conformer-12

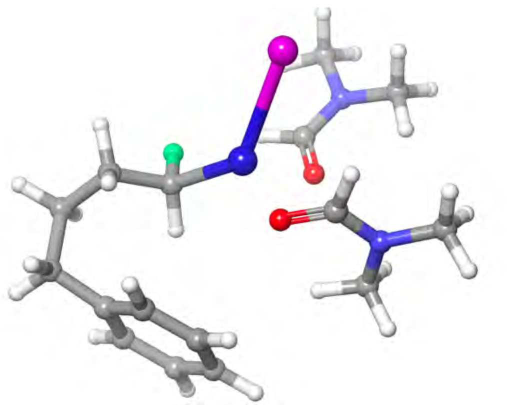


C	0.32243400	-2.01623200	-1.70549300
H	1.30344000	-2.35623300	-2.07185000
F	-0.37964900	-1.62086700	-2.88278700
Zn	0.72461000	-0.44571300	-0.50845500
O	2.37919800	0.56430800	-1.20083200
C	3.43176400	0.72407300	-0.56520300
N	4.51634900	1.31368300	-1.06884200
H	3.52290600	0.38132300	0.47426600
O	-0.37059400	1.24163500	-0.33938900
C	-1.13120500	1.44970000	0.62342600
N	-1.94298100	2.49697800	0.70388200
H	-1.15761600	0.77171600	1.48629000
C	4.53667200	1.81314300	-2.43290200
H	5.32216000	1.30616500	-3.00208700
H	3.56763900	1.61940400	-2.88976200
H	4.73794600	2.88906200	-2.43112400
C	5.72374400	1.47206800	-0.28045500

H	5.56901400	1.05643300	0.71674300
H	6.55838200	0.94967400	-0.75874900
H	5.97789900	2.53287200	-0.18872200
C	-2.75883100	2.73392000	1.87914400
H	-3.80698200	2.82872300	1.58263000
H	-2.66490400	1.89132300	2.56649700
H	-2.43722900	3.65081500	2.38446200
C	-1.99823900	3.48529500	-0.35921700
H	-1.45988500	3.09844900	-1.22309500
H	-3.04295200	3.66477200	-0.62622200
H	-1.54130900	4.42321900	-0.02530800
C	-0.38855000	-3.24403300	-1.15768500
H	-0.29842400	-4.07576800	-1.87139700
H	0.12484900	-3.55353400	-0.23642800
C	-1.88098500	-3.03566900	-0.88237100
H	-2.32980900	-4.00178800	-0.62954500
H	-2.35314300	-2.71730200	-1.81681000
C	-2.19666500	-2.02400400	0.24132100
H	-2.65319500	-2.53536100	1.09526800
H	-1.25269700	-1.61800600	0.63354000
C	-3.08867700	-0.87326400	-0.16783500
C	-2.89029300	-0.20864700	-1.38577000
C	-4.10700400	-0.42352500	0.67730100
C	-3.69381600	0.87061300	-1.74150400
H	-2.09692400	-0.54148900	-2.05225200

C	-4.92139000	0.64958700	0.31698000
H	-4.27639300	-0.93587100	1.62166500
C	-4.71573900	1.30282800	-0.89527600
H	-3.52687400	1.37183800	-2.69091800
H	-5.72317100	0.96545500	0.97913900
H	-5.35545400	2.13147100	-1.18667900
I	1.42319800	-0.80029200	2.13677200

2a-I•2DMF_conformer-13

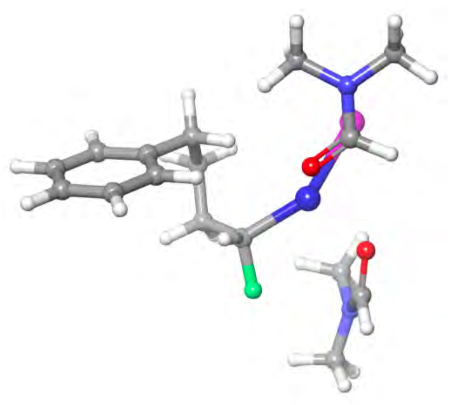


C	-1.41242300	-1.35754100	0.37179300
H	-2.12855900	-0.65116500	0.80726200
F	-0.97653000	-2.13363500	1.49796800
Zn	0.14218800	-0.32347700	-0.35006900
O	-0.14122800	1.45057600	-1.29322000
C	0.84383500	2.21198400	-1.31287000
N	0.99800000	3.24154500	-0.48925200

H	1.65922200	2.06608400	-2.03323800
O	0.97079300	0.68498200	1.31992300
C	1.38856300	-0.25421800	2.02814500
N	2.63365700	-0.34697900	2.48101600
H	0.72424600	-1.08596700	2.30113300
C	2.17782700	4.08344800	-0.53911000
H	2.71670700	4.02569900	0.41187700
H	2.83727100	3.74746600	-1.34122800
H	1.89242000	5.12431600	-0.71979400
C	0.03306700	3.50228400	0.56864500
H	-0.79905000	2.80618600	0.46581800
H	0.51049100	3.34677800	1.54019000
H	-0.32307300	4.53423100	0.49076500
C	3.09510700	-1.54711900	3.15509800
H	3.60833700	-1.28137100	4.08380800
H	2.24269900	-2.18790800	3.38634800
H	3.78422700	-2.09389900	2.50311600
C	3.64717100	0.61030100	2.07253400
H	3.15085800	1.45919600	1.60453000
H	4.21533700	0.93748800	2.94828700
H	4.31761600	0.14260300	1.34390300
C	-2.13925000	-2.32159100	-0.55435100
H	-2.20089700	-1.88995500	-1.56266100
H	-1.50579700	-3.21086700	-0.65267400
C	-3.54746600	-2.71625400	-0.08429100

H	-3.55965300	-2.73214900	1.01305400
H	-3.79834900	-3.73018300	-0.41765000
C	-4.64079700	-1.76351900	-0.60912500
H	-4.67969500	-1.84929800	-1.70208200
H	-5.61707200	-2.08479600	-0.22763400
C	-4.39658600	-0.32298500	-0.23045200
C	-4.78730500	0.15328000	1.02506800
C	-3.69673700	0.53905800	-1.07897100
C	-4.46803700	1.44430300	1.43264700
H	-5.33368400	-0.50694000	1.69483500
C	-3.36704000	1.83113400	-0.67439800
H	-3.39055200	0.19039700	-2.06231600
C	-3.74909800	2.28648200	0.58520700
H	-4.77842400	1.79435700	2.41261500
H	-2.80476500	2.47462300	-1.34429300
H	-3.50030300	3.29553100	0.90177900
I	2.55359400	-1.11989000	-1.31914700

2a-I•2DMF_conformer-14

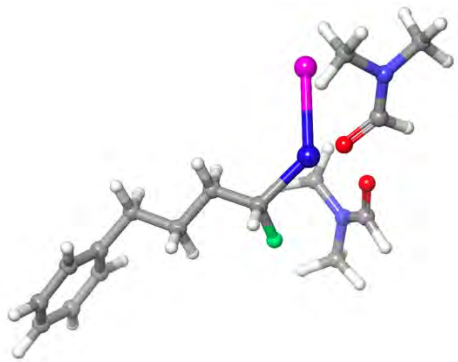


C	0.80788800	-1.66631900	-0.01888100
H	1.56560100	-1.40779000	-0.77305400
F	0.40035200	-2.99394000	-0.37548200
Zn	-0.70806300	-0.37157800	-0.29977900
O	-0.10727200	1.03289000	-1.69058300
C	-0.94078900	1.93946500	-1.88728200
N	-0.75997500	3.19969300	-1.52068300
H	-1.89334100	1.73417300	-2.39382000
O	-2.06431400	-1.27459600	-1.54788800
C	-2.12119700	-2.51284400	-1.63902800
N	-2.33383300	-3.35049700	-0.63190100
H	-2.03204500	-2.99787100	-2.61969300
C	-1.85655800	4.15185400	-1.54977200
H	-1.52015200	5.09417400	-1.98990400
H	-2.67664400	3.74805900	-2.14599900
H	-2.21643600	4.32584300	-0.53000300

C	0.41281600	3.55532300	-0.73346400
H	1.25054000	2.92525200	-1.03169600
H	0.65311000	4.60506000	-0.91439400
H	0.20077700	3.39783700	0.33090800
C	-2.07418500	-4.77026400	-0.79097300
H	-2.86972600	-5.34887300	-0.31482600
H	-2.03592600	-5.02201700	-1.85255300
H	-1.11082100	-5.01300600	-0.33196400
C	-2.41534700	-2.85651700	0.73465500
H	-2.85400400	-1.85726400	0.74392800
H	-3.05168800	-3.53011700	1.31316300
H	-1.41202200	-2.83263500	1.17360000
C	1.50257900	-1.76778100	1.32994900
H	0.90124800	-2.41308500	1.98398100
H	2.48252300	-2.25576500	1.22567700
C	1.66742600	-0.40898900	2.01792300
H	2.30752800	-0.52447700	2.90090900
H	0.69079900	-0.06455100	2.38172300
C	2.23778100	0.69260600	1.11109500
H	1.51788800	0.90748800	0.31132900
H	2.32670600	1.61619700	1.69830800
C	3.57005500	0.36071400	0.48071300
C	3.71209100	0.33213600	-0.90862100
C	4.68920800	0.07820800	1.27043500
C	4.93856500	0.03005300	-1.49721000

H	2.84517500	0.54734200	-1.53129700
C	5.91537200	-0.22524400	0.68764100
H	4.59729500	0.10092500	2.35389600
C	6.04417000	-0.25054000	-0.70015700
H	5.02822600	0.01181000	-2.57924300
H	6.77373900	-0.44106500	1.31685600
H	7.00074400	-0.48770100	-1.15530700
I	-2.19510000	1.24854600	1.28935700

2a-I•2DMF_conformer-15



C	-0.71148900	0.14425000	-0.99406700
H	-0.92047800	-0.23042500	-2.00591800
F	-1.14803700	1.51441700	-1.02949800
Zn	1.25582700	0.12981100	-0.56572700
O	2.59589400	-0.56304100	-1.94807800
C	3.76944100	-0.32924200	-1.59689100
N	4.67738400	-1.26601700	-1.36443600

H	4.11888400	0.70266700	-1.45593900
O	1.96059500	2.05004600	-0.79768800
C	1.21549700	3.04509400	-0.80228900
N	0.43622900	3.42463900	0.20153900
H	1.19541800	3.71602600	-1.67105500
C	5.95083000	-0.93476400	-0.75103400
H	6.76236800	-1.43979400	-1.28172300
H	6.11029500	0.14402000	-0.79359800
H	5.94374500	-1.25072700	0.29774100
C	4.30157900	-2.67189000	-1.38245500
H	3.38038500	-2.78109900	-1.95177700
H	5.10357700	-3.25147300	-1.84676000
H	4.13655700	-3.01529300	-0.35537600
C	-0.60596700	4.41295700	-0.01078400
H	-0.63815600	5.10557800	0.83392000
H	-0.40289400	4.97414500	-0.92492500
H	-1.57077000	3.90567000	-0.11093000
C	0.31128300	2.59060900	1.38765700
H	1.25192400	2.07276500	1.57961500
H	0.06967500	3.22763100	2.24142400
H	-0.49121000	1.86093400	1.23516600
C	-1.62343300	-0.58622700	-0.02694300
H	-1.33943100	-1.64827500	-0.04157700
H	-1.44139400	-0.24894600	1.00469400
C	-3.10961600	-0.43887700	-0.35255400

H	-3.30179100	-0.81840300	-1.36542200
H	-3.37232300	0.62511100	-0.36761300
C	-4.01567600	-1.17560300	0.64162000
H	-3.74761900	-2.23951300	0.65353200
H	-3.82746500	-0.79254600	1.65244600
C	-5.47650900	-1.02025000	0.29963500
C	-6.21969700	0.05063800	0.80219600
C	-6.10393900	-1.91197800	-0.57406300
C	-7.55393700	0.22605000	0.44582800
H	-5.74385600	0.75146800	1.48452400
C	-7.43764200	-1.74206800	-0.93457300
H	-5.53712500	-2.75064400	-0.97208500
C	-8.16781800	-0.67119100	-0.42476700
H	-8.11641800	1.06183600	0.85123300
H	-7.90870400	-2.44855100	-1.61146500
H	-9.20904800	-0.53858800	-0.70159500
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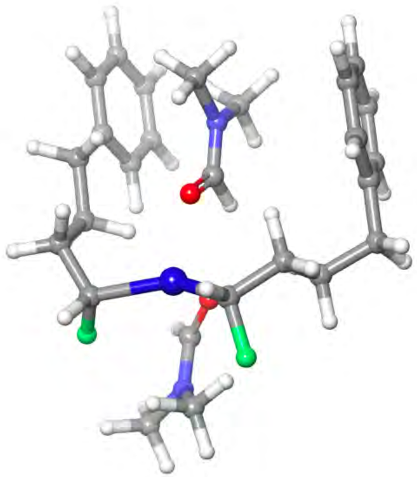

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N	-3.24592200	-2.00467900	1.85273900
H	-1.30608900	-2.35051100	2.38551900
O	0.08618100	0.33469800	-1.10481200
C	0.91548400	0.45852300	-0.19128700
N	2.19077300	0.79979400	-0.37933700
H	0.63804800	0.27007900	0.85493300
C	-4.21170400	-1.28683800	1.03510100
H	-5.17975300	-1.29777300	1.54236100
H	-3.90332300	-0.25291100	0.88562200
H	-4.30969900	-1.78026900	0.06072000
C	-3.64248500	-3.32608600	2.30157500

H	-2.84724000	-3.76509300	2.90765200
H	-4.55137400	-3.25527700	2.90460000
H	-3.82105500	-3.96763300	1.43258800
C	2.70976600	1.05932400	-1.70847400
H	3.47607300	0.31384400	-1.95343800
H	1.88953100	1.00223900	-2.42286300
H	3.15540800	2.05869200	-1.73514600
C	3.15094200	0.82232600	0.70799000
H	2.63397200	0.66449700	1.65692100
H	3.89501400	0.03168900	0.56842100
H	3.64820400	1.79509000	0.73322300
C	-3.00058200	1.24490300	-1.28393300
C	-2.34659600	2.55378100	-0.87727800
H	-1.37898500	2.61571600	-1.39259800
H	-2.94832600	3.41841700	-1.20608600
C	-2.14797600	2.65827800	0.63268500
H	-1.51617700	1.83016900	0.98358500
H	-3.12555700	2.52982800	1.11106100
C	-1.53937600	3.99333700	1.08975400
H	-2.10526600	4.81650300	0.63545200
H	-1.65139800	4.09362700	2.17536900
C	-0.07803800	4.12967900	0.73883600
C	0.90647000	3.82712500	1.68469700
C	0.33309900	4.54497000	-0.53205000
C	2.25870100	3.95643500	1.38153900

H	0.60280500	3.51194200	2.68060100
C	1.68472300	4.65255600	-0.84927300
H	-0.41885300	4.79852000	-1.27483500
C	2.65407100	4.36470500	0.10924000
H	3.00509500	3.74628600	2.14305800
H	1.98118300	4.98132000	-1.84126700
H	3.70893400	4.47362600	-0.12835000
C	-1.87009400	-2.40075800	-1.45348400
H	-2.63098500	-2.64430700	-2.20905700
C	-0.51656900	-2.86558800	-1.96520200
H	-0.55501800	-3.87803300	-2.39605100
H	-0.22056900	-2.18767800	-2.77901100
C	0.54720500	-2.83681200	-0.86062400
H	0.53157000	-3.78414600	-0.30848500
H	0.27920700	-2.05894800	-0.13558300
C	1.94219100	-2.56522100	-1.40981000
H	2.20186600	-3.33659800	-2.14800500
H	1.90590600	-1.61994900	-1.97189100
C	3.05673800	-2.47433800	-0.38961500
C	2.82944300	-2.55726500	0.98622900
C	4.37485000	-2.28983200	-0.82834500
C	3.88442100	-2.46104500	1.89453700
H	1.81916800	-2.70435500	1.35640400
C	5.43024800	-2.19260400	0.07233800
H	4.57004600	-2.23357800	-1.89776900

C	5.18745900	-2.27812800	1.44345500
H	3.68410200	-2.53327600	2.95969700
H	6.44337900	-2.05526200	-0.29405400
H	6.00811500	-2.20713600	2.15050200
F	-2.18274200	-3.26937800	-0.34598900
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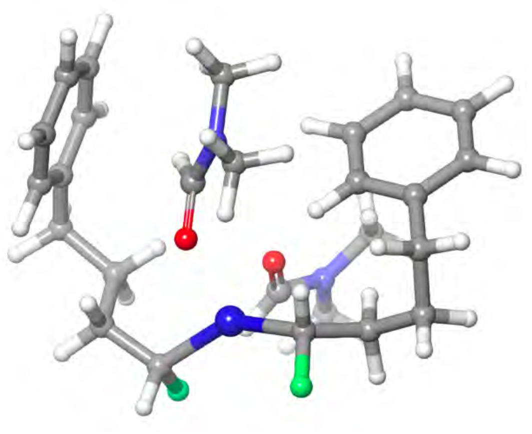
2a'-conformer-2



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N	-1.14330800	-2.32786700	2.62779900
H	0.20654900	-2.97941400	1.21342600
O	1.01558800	0.42034200	-1.31474100

C	1.07350200	1.38488000	-0.54609900
N	0.55905300	2.59034900	-0.81782500
H	1.56794400	1.31666600	0.43504600
C	-2.06187600	-1.31309900	3.11443500
H	-1.68919700	-0.87326300	4.04627500
H	-2.16348900	-0.53361700	2.35908900
H	-3.03777900	-1.76973800	3.30527000
C	-1.04738400	-3.56508300	3.37738000
H	-0.33686600	-4.23475400	2.88931600
H	-0.70537200	-3.36595800	4.39853400
H	-2.02479200	-4.05597300	3.42408000
C	-0.15779100	2.83144800	-2.05722400
H	0.30855500	3.65918500	-2.60137600
H	-0.12509100	1.92571200	-2.66211800
H	-1.19977300	3.08945600	-1.83416700
C	0.63083900	3.68815900	0.12417000
H	1.16451400	3.36606700	1.02039900
H	1.17004000	4.53231400	-0.31960400
H	-0.38037700	4.00748000	0.39915300
C	-1.76858400	-1.00020800	-2.06139700
C	-2.99735800	-1.24611800	-1.19062000
H	-3.21560100	-2.32132900	-1.23014000
H	-2.76242300	-1.02320300	-0.14264800
C	-4.25520000	-0.47038100	-1.60107400
H	-5.10121600	-0.77122600	-0.96899600

H	-4.51139000	-0.73353800	-2.63394000
C	-4.10341100	1.06289600	-1.52066700
H	-3.37104600	1.38801400	-2.26825600
H	-5.05617200	1.52846000	-1.79702800
C	-3.67950200	1.56857300	-0.16112200
C	-4.60785000	2.10861800	0.73258100
C	-2.34320900	1.48479900	0.25084600
C	-4.21980100	2.55765000	1.99356000
H	-5.65063900	2.18084400	0.43218800
C	-1.94984100	1.92628700	1.51113400
H	-1.60524600	1.03840600	-0.41088300
C	-2.88727600	2.46970000	2.38870300
H	-4.96014700	2.97834000	2.66770700
H	-0.90958400	1.81762600	1.81139300
H	-2.58353300	2.81620700	3.37213000
C	1.54775500	-2.82070100	-1.18763500
H	1.64288400	-3.32830700	-2.15651800
C	2.90132600	-2.22106100	-0.84050700
H	3.72132000	-2.93823000	-1.00930100
H	3.06440200	-1.37186800	-1.51637100
C	2.97462500	-1.75594300	0.61350000
H	2.86494400	-2.63986900	1.25209400
H	2.11958900	-1.10082300	0.83009000
C	4.28365300	-1.02658100	0.97536500
H	4.48864500	-1.14179300	2.04549400

H	5.11737200	-1.50125900	0.44264800
C	4.23720200	0.44774500	0.65444300
C	3.98996000	1.38053500	1.66799300
C	4.38617700	0.92081600	-0.65353800
C	3.89179700	2.74187800	1.38811800
H	3.88252100	1.03124500	2.69238100
C	4.27173300	2.27867500	-0.94259700
H	4.59885000	0.21808500	-1.45380900
C	4.02566300	3.19548600	0.07737700
H	3.71689100	3.44887100	2.19476700
H	4.38649200	2.62171900	-1.96648600
H	3.95347200	4.25616600	-0.14532300
F	1.33028200	-3.89108300	-0.24800600
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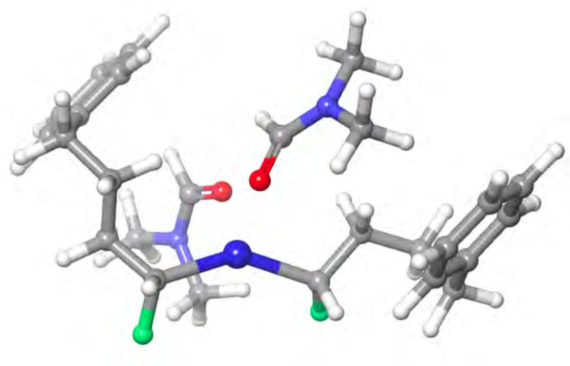
F	-2.02223600	-1.65095800	-3.29810300

2a’-conformer-3



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N	2.79991400	1.84503100	-1.29885600
H	3.13458700	-0.14910400	-1.61779800
O	-0.64724300	-1.01531900	1.02212000
C	-0.69480200	-1.77890700	0.05197700
N	-1.73228600	-2.57484200	-0.22988100
H	0.14074700	-1.84058800	-0.65961700
C	1.94725200	2.92726800	-0.81429100
H	2.24693700	3.84641900	-1.32325700
H	0.90260800	2.72645500	-1.06157200
H	2.05940600	3.06028100	0.26750700
C	4.15974300	2.18032300	-1.67566200
H	4.66650400	1.28934100	-2.04993100
H	4.15072400	2.94749600	-2.45547900

H	4.71095500	2.56218900	-0.80865400
C	-2.96072400	-2.50262000	0.54526900
H	-3.24243400	-3.50249900	0.89064900
H	-2.79682900	-1.84657300	1.39886900
H	-3.77023400	-2.09477200	-0.07195000
C	-1.77023900	-3.35346400	-1.45021400
H	-0.79911000	-3.30779400	-1.94722400
H	-2.00600800	-4.39847800	-1.22595300
H	-2.53534400	-2.95669600	-2.12750600
C	-1.53540400	1.75049500	-0.22195300
C	-2.17829600	0.73883700	-1.15931100
H	-1.40712300	0.29429300	-1.80826900
H	-2.57728600	-0.07663700	-0.54225900
C	-3.30289100	1.28945300	-2.04233100
H	-3.61669500	0.52047800	-2.76190900
H	-2.91787100	2.13536900	-2.62053500
C	-4.53438800	1.75157600	-1.24621900
H	-4.24953900	2.57435800	-0.58246100
H	-5.28004300	2.15170200	-1.94352700
C	-5.15682600	0.63799800	-0.43676200
C	-4.98705100	0.55961900	0.94810000
C	-5.90230700	-0.36453800	-1.06812900
C	-5.55420500	-0.47934300	1.68438500
H	-4.40775200	1.32785000	1.45480300
C	-6.47248900	-1.40453900	-0.33868500

H	-6.04859800	-0.31576100	-2.14532600
C	-6.30097500	-1.46494100	1.04393100
H	-5.41506000	-0.51460200	2.76106500
H	-7.05927000	-2.16386600	-0.84779900
H	-6.75097800	-2.27040000	1.61646600
C	1.42907300	1.35893600	2.25842200
H	1.01758900	1.11843100	3.25082400
C	2.75977900	0.63124200	2.14007300
H	3.24645200	0.88079800	1.18403500
H	3.45298600	0.96678100	2.92848800
C	2.57221000	-0.87964400	2.24070800
H	1.83984400	-1.20784000	1.49247000
H	2.14020800	-1.11991000	3.22048600
C	3.87201900	-1.67732400	2.05961800
H	4.64947200	-1.26353800	2.71298800
H	3.70766400	-2.71330700	2.37895600
C	4.36321600	-1.68846300	0.63190300
C	5.41830900	-0.87603200	0.21009100
C	3.75812400	-2.52887000	-0.31050600
C	5.87606500	-0.92028100	-1.10680700
H	5.89750500	-0.21576700	0.92916200
C	4.20418200	-2.57237900	-1.62784400
H	2.93484400	-3.16655900	0.00489400
C	5.27132500	-1.76865500	-2.03130700
H	6.71247300	-0.29518100	-1.40776100

H	3.72857500	-3.24088000	-2.33956700
H	5.63229700	-1.81123400	-3.05440900
F	1.74475600	2.75132000	2.32588400
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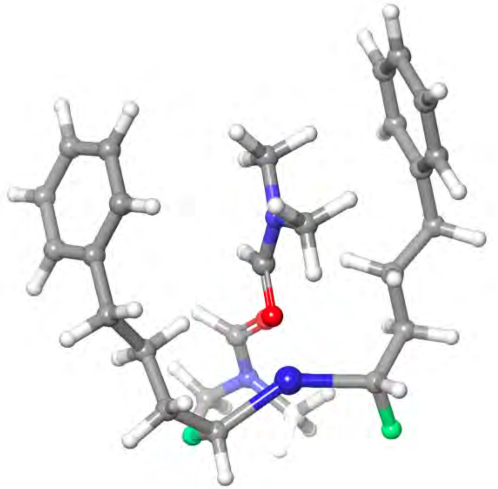
F	-1.18593700	2.87733900	-1.03345200

2a'-conformer-4



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N	2.95051600	-1.70783400	2.15582200
H	2.34145900	0.23302900	2.32888100
O	0.00029200	-0.11849000	-1.64713400
C	-0.66342600	0.60916400	-0.89730400

N	-1.84532900	1.13886900	-1.21888600
H	-0.31105500	0.86209800	0.11286400
C	4.23472400	-1.39746600	2.75610400
H	5.01095400	-1.42582600	1.98498200
H	4.20609700	-0.39840400	3.19582500
H	4.46368000	-2.12483000	3.53950400
C	2.84785900	-3.00836300	1.50925800
H	1.81665500	-3.22677400	1.23698700
H	3.47039800	-3.01479700	0.60848100
H	3.20131200	-3.77456400	2.20398300
C	-2.47185000	0.85274900	-2.49659500
H	-2.60375400	1.77950700	-3.06525000
H	-1.83324100	0.16731100	-3.05207500
H	-3.45232200	0.39748900	-2.32320400
C	-2.59407400	1.95102700	-0.27872500
H	-2.00955800	2.08666700	0.63391200
H	-2.79643700	2.93653700	-0.71452500
H	-3.54329100	1.46417000	-0.03554100
C	0.18372200	-3.29065900	-0.83042700
C	-0.91482000	-3.35707800	0.22252800
H	-1.44732200	-4.31962100	0.15523200
H	-0.46899600	-3.32411200	1.22716400
C	-1.91138200	-2.20451600	0.10338300
H	-2.13849500	-2.00476700	-0.95541900
H	-1.45687900	-1.29019500	0.50400800

C	-3.21731700	-2.47416400	0.86012000
H	-3.68287000	-3.37988000	0.45166300
H	-2.98493600	-2.68823200	1.91034900
C	-4.19780200	-1.32947800	0.78154000
C	-4.91237200	-1.09012100	-0.39827800
C	-4.41932100	-0.48178100	1.86960800
C	-5.83169500	-0.04761100	-0.48339300
H	-4.75784300	-1.74720000	-1.25212600
C	-5.34045100	0.56214500	1.79266900
H	-3.87353500	-0.65399400	2.79413700
C	-6.05301000	0.78114800	0.61648800
H	-6.38672400	0.11003300	-1.40389900
H	-5.50607000	1.20003800	2.65591900
H	-6.77764000	1.58733000	0.55682800
C	3.19504100	-0.91862400	-1.36857100
H	3.73101000	-1.56416200	-2.07785900
C	3.17038000	0.49469400	-1.93094200
H	4.15734800	0.80958200	-2.30492100
H	2.48472000	0.50001500	-2.78997200
C	2.68760300	1.50780500	-0.89272500
H	3.48489400	1.69077500	-0.16160200
H	1.85785400	1.07015300	-0.32708300
C	2.22116000	2.83564500	-1.49937600
H	3.06780500	3.33723600	-1.98566800
H	1.48421500	2.62420100	-2.28476300

C	1.60023900	3.74042500	-0.46376000
C	0.22222700	3.96834000	-0.44081800
C	2.38407600	4.32937200	0.53385200
C	-0.36067700	4.75707900	0.54970100
H	-0.39734700	3.52798400	-1.22025900
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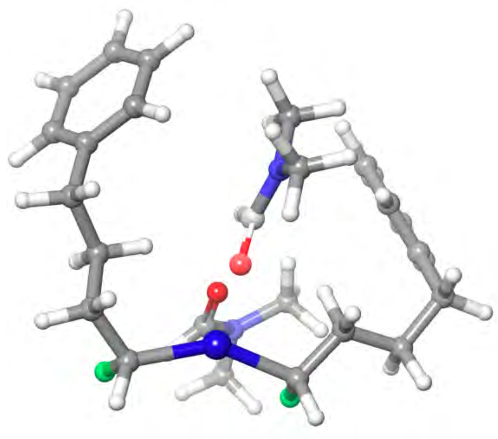
H	3.45968700	4.16740800	0.52692700
C	0.43149500	5.33357400	1.53790400
H	-1.43392700	4.92828600	0.54410200
H	2.43596800	5.57117200	2.28676300
H	-0.01796000	5.95157600	2.30895800
F	4.06040900	-0.86045800	-0.21713000
H	-0.28778800	-3.50576900	-1.80204000
F	1.02466800	-4.41710100	-0.56790000

2a’-conformer-5



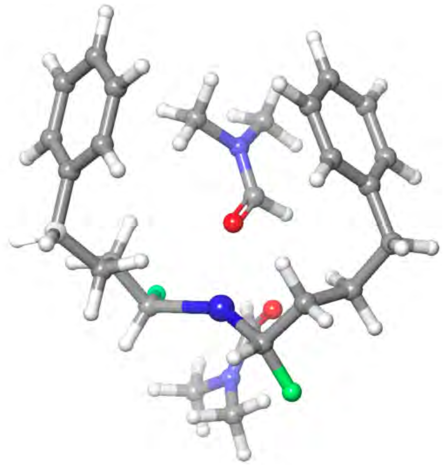
Zn	0.04154200	-2.21928900	-0.90674300
O	-0.10152900	-0.89511000	0.83133200
C	-0.46197500	-1.61189800	1.77809600
N	-1.46019300	-1.30521100	2.60594100
H	0.05713500	-2.55667200	1.98978300
O	0.65303900	-0.50819900	-2.03930300
C	0.63390900	0.62930600	-1.55602900
N	0.73649100	1.74876700	-2.28602500
H	0.52761700	0.79234600	-0.47481500
C	-1.98344200	-2.30824500	3.51262300
H	-2.90216400	-2.74122300	3.10086900
H	-1.24684900	-3.10281900	3.64539300
H	-2.19963500	-1.85758200	4.48535500
C	-2.33686600	-0.18886200	2.29288100
H	-1.78553100	0.56172300	1.72554900

H	-3.17725100	-0.54486500	1.68694900
H	-2.70889400	0.25398300	3.22044200
C	0.85732500	1.69083700	-3.73143800
H	1.83088300	2.08327900	-4.04463500
H	0.76240100	0.65270500	-4.04588700
H	0.06835100	2.29286400	-4.19342800
C	0.77590800	3.05588300	-1.66286100
H	0.77734300	2.94291700	-0.57649300
H	1.68987700	3.58350500	-1.95843400
H	-0.08922900	3.65644900	-1.96738400
C	-1.98474500	-2.17111100	-1.10711200
C	-2.46298600	-0.76312000	-1.41723700
H	-1.97171600	-0.06870500	-0.72014200
H	-2.10658700	-0.49295400	-2.42345000
C	-3.97428800	-0.55481100	-1.33934800
H	-4.33794700	-0.92122400	-0.37151100
H	-4.46683500	-1.16315600	-2.10863100
C	-4.38518200	0.91644700	-1.52106800
H	-3.99646800	1.28081600	-2.48054700
H	-5.47773400	0.99078800	-1.57158400
C	-3.87984900	1.80007100	-0.40545400
C	-4.59427600	1.90322500	0.79150300
C	-2.67444600	2.50064700	-0.51628000
C	-4.12461600	2.68275000	1.84577100
H	-5.53434800	1.36489700	0.89313800

C	-2.19989900	3.28407900	0.53340100
H	-2.10435900	2.42084900	-1.44105400
C	-2.92394700	3.37771900	1.71980600
H	-4.70021700	2.75328200	2.76423200
H	-1.26841800	3.83271900	0.42546300
H	-2.55729000	3.99081900	2.53715500
C	1.67794000	-3.33684600	-0.45504500
H	1.70946700	-4.31531900	-0.95184200
C	3.00916200	-2.64233900	-0.69531200
H	3.85872100	-3.30130600	-0.45401300
H	3.07653900	-2.41551500	-1.76963700
C	3.14212100	-1.34852400	0.10420300
H	3.21686500	-1.58464000	1.17250400
H	2.22325400	-0.76406000	-0.00375100
C	4.33209700	-0.48218900	-0.32384000
H	5.27139700	-1.01106600	-0.11922600
H	4.28574100	-0.32533800	-1.40928500
C	4.32263100	0.85325800	0.37627900
C	4.78916500	0.97682500	1.68789600
C	3.78635200	1.98492800	-0.24419400
C	4.72577500	2.19351600	2.35997500
H	5.20779300	0.10407100	2.18386000
C	3.72290100	3.20693300	0.42252600
H	3.42906400	1.90263500	-1.27026900
C	4.19188300	3.31493500	1.72883300

H	5.09755100	2.26863000	3.37755500
H	3.31875500	4.08147000	-0.08095700
H	4.14780900	4.26672200	2.24908800
F	1.63578000	-3.64087300	0.94832900
H	-2.48632000	-2.87393400	-1.78553500
F	-2.51523800	-2.48327300	0.19837800

2a'-conformer-6



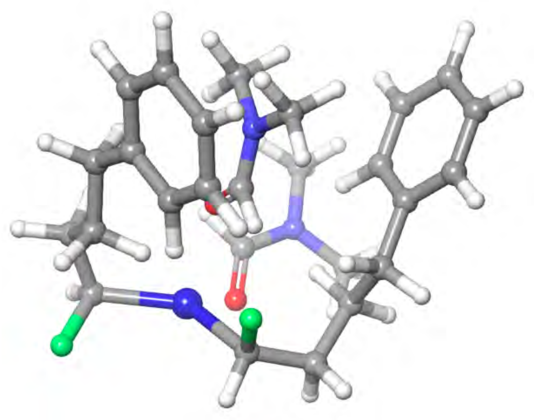
Zn	-1.63117800	-0.46688300	-0.56195500
O	-2.63764500	0.47955400	1.10620700
C	-3.29364900	-0.33813900	1.76563500
N	-4.26818900	-1.11001000	1.28206700
H	-3.12232300	-0.46179600	2.84268400
O	0.22726400	0.33249100	0.06753200
C	0.36773900	0.82808300	1.19341300

N	1.47266800	0.70852600	1.93036800
H	-0.44284900	1.39589100	1.67008700
C	-4.72168900	-2.25882100	2.04040100
H	-4.25561600	-3.16916300	1.64824000
H	-4.43113600	-2.14733400	3.08676000
H	-5.80990500	-2.34323500	1.97599600
C	-4.65497600	-1.05518200	-0.11993400
H	-4.29144900	-0.13705100	-0.58410800
H	-4.24978800	-1.91804700	-0.66090800
H	-5.74716500	-1.08134200	-0.18345500
C	2.61884000	-0.04423100	1.45394700
H	2.82339200	-0.88090400	2.12987800
H	2.40724200	-0.42819000	0.45554700
H	3.49788900	0.60777700	1.41423200
C	1.56615100	1.28563100	3.25323900
H	0.67184800	1.87653700	3.46183500
H	1.66322500	0.49600500	4.00654700
H	2.43915700	1.94358900	3.31102800
C	-2.09197200	0.54964100	-2.25434600
C	-1.29990000	1.84197100	-2.36973300
H	-0.23575400	1.57843200	-2.29833500
H	-1.44895400	2.33001700	-3.34718600
C	-1.66539800	2.84869500	-1.27994100
H	-1.63978900	2.35869100	-0.29761400
H	-2.70324300	3.15798000	-1.44025700

C	-0.75705500	4.09159800	-1.25414000
H	-0.54575800	4.40326600	-2.28516400
H	-1.28690200	4.92387600	-0.77747400
C	0.53984200	3.86710100	-0.51301800
C	1.63185700	3.22825100	-1.10947300
C	0.66847300	4.28442200	0.81644100
C	2.81198200	3.01271700	-0.40196700
H	1.55996000	2.90758600	-2.14493200
C	1.85446300	4.09547500	1.52137000
H	-0.16956800	4.78717600	1.29420800
C	2.93272600	3.45668400	0.91303300
H	3.64508300	2.50952600	-0.88493500
H	1.93935200	4.45679400	2.54301000
H	3.86380600	3.31447500	1.45580100
C	-1.43774700	-2.34681800	0.23012000
H	-2.12328200	-3.10451700	-0.18634500
C	-0.01941300	-2.87144500	0.05837400
H	0.67139700	-2.24898500	0.64325600
H	0.08203700	-3.90064400	0.44067300
C	0.38476100	-2.82554200	-1.41493800
H	0.47633300	-1.77668100	-1.73297300
H	-0.41504500	-3.26884900	-2.02449800
C	1.69754000	-3.55756800	-1.72951100
H	1.61827000	-4.59736100	-1.38999100
H	1.83909700	-3.58750900	-2.81613000

C	2.90554500	-2.91119800	-1.09567700
C	3.42310500	-3.37038000	0.11795600
C	3.52837800	-1.82105300	-1.71300100
C	4.53994900	-2.76844700	0.69403400
H	2.94785600	-4.21591700	0.60973400
C	4.64400100	-1.21488800	-1.14225900
H	3.13544800	-1.45232100	-2.65795700
C	5.15648300	-1.68979100	0.06400700
H	4.93328200	-3.14748600	1.63305900
H	5.11947400	-0.37666900	-1.64362100
H	6.03326400	-1.22599400	0.50622000
F	-1.71456800	-2.36358200	1.64113400
H	-1.91926900	-0.03513400	-3.16950200
F	-3.47685600	0.90552100	-2.30401300

2a’-conformer-7



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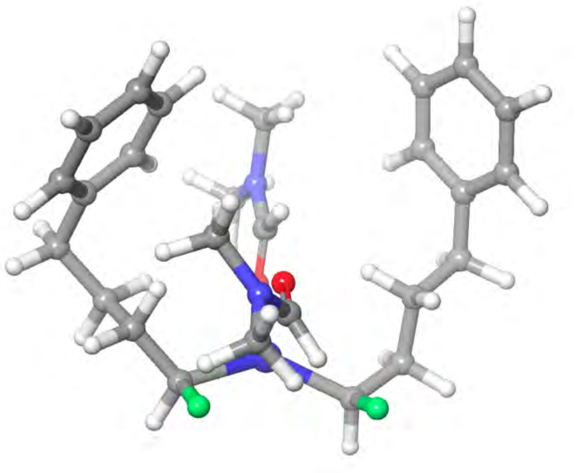
O	-0.24597200	-0.68382000	0.91015700
C	0.32862900	0.30939600	0.42504100
N	0.67860500	1.38889600	1.11956900
H	0.59774800	0.33891900	-0.63725000
O	-2.46049400	-2.44169800	0.09866200
C	-2.70838500	-1.85317200	1.15514600
N	-3.75845300	-1.04237100	1.33719700
H	-2.06118400	-1.95136600	2.03660600
C	1.22247600	2.56464400	0.46263400
H	2.21553800	2.79351200	0.86355000
H	1.31645000	2.37134900	-0.60745400
H	0.54405500	3.41262600	0.61607500
C	0.43869500	1.47953600	2.54371100
H	0.07837000	0.51487900	2.90082400

H	1.37327100	1.73783600	3.05331300
H	-0.30615300	2.25793400	2.74715400
C	-4.70947000	-0.79253300	0.26739400
H	-4.69085300	0.26869600	-0.00507100
H	-4.42758200	-1.39623600	-0.59445600
H	-5.71757400	-1.06169800	0.59857400
C	-3.96791100	-0.33982100	2.58656900
H	-3.15248800	-0.56568200	3.27675000
H	-3.99103200	0.74070400	2.40496000
H	-4.91736900	-0.63859300	3.04307200
C	0.75391200	-3.78220000	0.56650000
C	1.80541500	-3.03887200	1.37761500
H	1.28030100	-2.48538000	2.17024200
H	2.50049500	-3.73199400	1.87596000
C	2.60367700	-2.04949300	0.52135200
H	1.92333800	-1.60977500	-0.21884500
H	3.35928000	-2.58284700	-0.06612900
C	3.24566000	-0.93759900	1.34502000
H	2.49020900	-0.55238700	2.04784200
H	4.04146200	-1.35591600	1.97555400
C	3.79938600	0.24311600	0.57160400
C	4.53856100	1.21487700	1.25933800
C	3.57129200	0.43329900	-0.79432500
C	5.03112700	2.34274600	0.61198000
H	4.73121300	1.07502500	2.32150700

C	4.06454000	1.56475600	-1.44692800
H	2.99796900	-0.29198800	-1.36461400
C	4.79174200	2.52384800	-0.75031800
H	5.60552000	3.07852000	1.16762300
H	3.87608200	1.68964300	-2.50937100
H	5.17633100	3.40070700	-1.26215800
C	-0.34950600	-1.60344700	-2.32821300
H	-0.05218400	-2.36272100	-3.06341600
C	-1.61645200	-0.94659200	-2.85497100
H	-1.46660900	-0.54668900	-3.87115300
H	-2.36028100	-1.75036400	-2.93921900
C	-2.18650700	0.15828500	-1.95737300
H	-2.09104400	-0.18381600	-0.92085900
H	-3.25999500	0.29430200	-2.14506200
C	-1.49490300	1.51055500	-2.14312600
H	-0.41020200	1.35235800	-2.18664000
H	-1.76040500	1.91115900	-3.12984900
C	-1.80885800	2.56286400	-1.09772800
C	-1.64206100	3.91542400	-1.41943100
C	-2.21271900	2.24907900	0.20560400
C	-1.85650100	4.91982100	-0.48141200
H	-1.33401300	4.17965600	-2.42852100
C	-2.43134700	3.25296500	1.14990400
H	-2.33712300	1.20920400	0.50181400
C	-2.25229200	4.59186600	0.81398900

H	-1.71849900	5.95966800	-0.76218400
H	-2.74491300	2.98603600	2.15640300
H	-2.42587300	5.37104700	1.54962600
F	0.71520100	-0.62123200	-2.41148100
H	0.24504700	-4.49832900	1.22742200
F	1.46527900	-4.57765800	-0.37530700

2a'-conformer-8



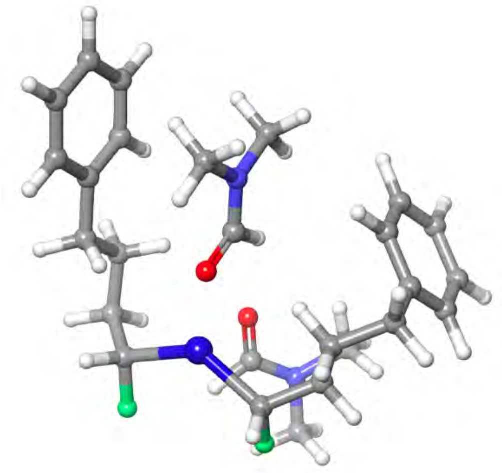
Zn	0.35480300	-2.00581600	1.03231600
O	0.21095900	-0.83768100	-0.80813800
C	0.58662800	-1.62652100	-1.69117200
N	1.41560900	-1.29866500	-2.68366000
H	0.22533200	-2.66200600	-1.70556800
O	-0.23087600	-0.25262100	2.08012200

C	-0.51898700	0.80808200	1.51340500
N	-0.79786000	1.94290900	2.16892100
H	-0.56047500	0.88127400	0.41840800
C	1.99661900	-2.33547400	-3.51330100
H	3.03223500	-2.51976200	-3.20805300
H	1.42934400	-3.25981100	-3.39270100
H	1.97323900	-2.03389300	-4.56463800
C	2.02072400	0.01929600	-2.75095700
H	1.53804100	0.67324500	-2.02408500
H	3.08927700	-0.04348500	-2.51657100
H	1.89961500	0.43203400	-3.75784400
C	-0.72911800	2.00633000	3.61798100
H	-1.69842900	2.31109800	4.02523000
H	-0.46342700	1.02072000	3.99664400
H	0.02813100	2.73682800	3.92305800
C	-1.12585000	3.16406100	1.46200300
H	-1.22075300	2.95532700	0.39414200
H	-2.08050300	3.56062500	1.82500700
H	-0.34824100	3.92121900	1.62034500
C	2.38297800	-2.17662000	0.86858300
C	3.17265700	-0.90503000	0.61950500
H	4.19692600	-1.14220000	0.28234100
H	2.69748300	-0.35002900	-0.19856400
C	3.23850900	0.00460900	1.84145900
H	3.67959400	-0.53315700	2.69070000

H	2.21969400	0.27766300	2.14611200
C	4.05664300	1.28063400	1.58336000
H	4.03887200	1.91454200	2.47862800
H	5.10423600	1.00960000	1.40756900
C	3.54569400	2.06580700	0.39782700
C	2.29612900	2.69483300	0.44521400
C	4.28200300	2.15220600	-0.78480800
C	1.80189900	3.39106600	-0.65405500
H	1.71224200	2.63770500	1.36330000
C	3.79373600	2.84945600	-1.88910000
H	5.25207200	1.66393700	-0.83928200
C	2.55016000	3.47073700	-1.82830700
H	0.83648000	3.88599300	-0.59787300
H	4.38760900	2.90695700	-2.79683300
H	2.16688600	4.01742000	-2.68431300
C	-1.22031400	-3.28824600	0.85925500
H	-1.12072200	-4.19264600	1.47404300
C	-2.61473100	-2.72636400	1.07729900
H	-3.38448100	-3.49775200	0.91143400
H	-2.69450400	-2.41635600	2.12985100
C	-2.90870800	-1.53303300	0.17434100
H	-2.84798300	-1.84696400	-0.87465500
H	-2.11965700	-0.78471800	0.30352300
C	-4.26600200	-0.87377900	0.44386800
H	-5.07450800	-1.57223400	0.19632800

H	-4.35185900	-0.65678400	1.51649000
C	-4.42277700	0.40378400	-0.34124600
C	-3.99989600	1.62372800	0.19515900
C	-4.92793900	0.39370900	-1.64348400
C	-4.08929300	2.80153600	-0.54276400
H	-3.60818800	1.64282200	1.21198100
C	-5.01544300	1.56686500	-2.38789700
H	-5.25722900	-0.54863300	-2.07504200
C	-4.59772600	2.77672100	-1.83926300
H	-3.77448800	3.74471800	-0.10324500
H	-5.41536700	1.53744300	-3.39711300
H	-4.67333400	3.69403000	-2.41489300
F	-1.20190700	-3.76837400	-0.49708500
H	2.91311100	-2.77990400	1.61761600
F	2.50626000	-2.92585100	-0.36081600

2a’-conformer-9



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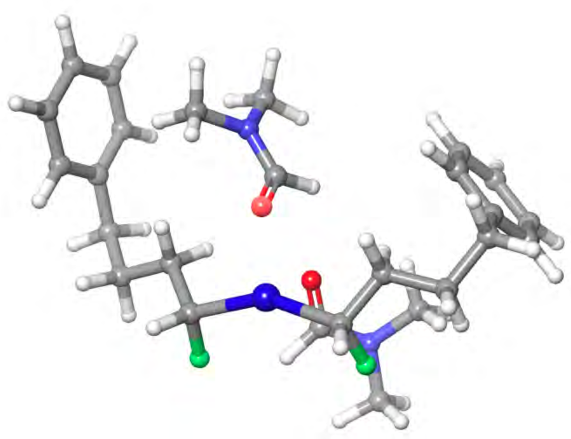
O	-0.99451000	-0.96593400	1.04846100
C	-1.81915100	-1.87356800	1.24937200
N	-3.04607100	-1.68190500	1.73542500
H	-1.56550700	-2.92270100	1.03596700
O	0.94462500	0.08305500	-1.10733000
C	0.92067300	0.96911800	-0.24026100
N	1.70831800	2.04518600	-0.26321800
H	0.22636300	0.91476000	0.60975400
C	-3.55035800	-0.34093900	1.97056100
H	-4.01694400	-0.28931800	2.95942800
H	-2.72386500	0.36752200	1.91203300
H	-4.29413600	-0.08037900	1.20883400
C	-4.02162500	-2.75367800	1.67404400

H	-3.50999900	-3.70246900	1.50538100
H	-4.58154900	-2.80559700	2.61221900
H	-4.70971700	-2.57953300	0.84050100
C	1.67952300	3.02392700	0.80305200
H	1.39706300	4.00877900	0.41299300
H	0.95278700	2.71829100	1.55854300
H	2.67089500	3.09349700	1.26296300
C	2.69171200	2.23558300	-1.31667100
H	2.66744200	1.36873300	-1.97506800
H	2.45454100	3.14132100	-1.88505200
H	3.68702200	2.33214300	-0.87193200
C	-2.03849300	-1.44540800	-1.83406400
C	-2.74654400	-0.11633400	-1.63550900
H	-3.81486100	-0.20964000	-1.89844300
H	-2.71068600	0.15583800	-0.57222200
C	-2.12281400	1.01447400	-2.44681900
H	-2.11991100	0.75300800	-3.51286200
H	-1.07134400	1.13626300	-2.15779600
C	-2.86041800	2.35161400	-2.26773800
H	-2.35508900	3.12884900	-2.85365000
H	-3.87622600	2.25939100	-2.66976500
C	-2.93928800	2.77970200	-0.82154000
C	-4.13027200	2.66669400	-0.10096500
C	-1.80744300	3.26333700	-0.15580500
C	-4.19701600	3.02723400	1.24349600

H	-5.01705900	2.28895600	-0.60472000
C	-1.86955500	3.63132100	1.18586400
H	-0.87169400	3.36181800	-0.70568200
C	-3.06528400	3.51173600	1.89274400
H	-5.13602700	2.93388100	1.78180200
H	-0.99050200	4.03457100	1.68074900
H	-3.11452200	3.80404000	2.93707000
C	0.87909700	-3.22434200	-0.24758700
H	1.61920800	-3.60608400	-0.96477800
C	1.55149500	-3.08672600	1.11514000
H	0.76514400	-3.06762800	1.88061100
H	2.17361100	-3.96810200	1.33721000
C	2.38366000	-1.81410800	1.27069800
H	2.90112700	-1.83391300	2.23857400
H	1.69899900	-0.95617000	1.29991700
C	3.40195100	-1.61753700	0.15206200
H	4.04296100	-2.50832200	0.08932500
H	2.87347000	-1.55686500	-0.80825300
C	4.29166100	-0.39694600	0.27910700
C	5.26996300	-0.16285600	-0.69634400
C	4.19434600	0.51113200	1.33658000
C	6.13010700	0.92605700	-0.61526500
H	5.35750900	-0.85864000	-1.52806800
C	5.05837500	1.60489900	1.42635000
H	3.44633100	0.36068900	2.10984000

C	6.03043400	1.81723700	0.45352200
H	6.88390700	1.07782100	-1.38220700
H	4.97731500	2.28492200	2.27056300
H	6.70695300	2.66305100	0.52821600
F	-0.05541900	-4.30085100	-0.08261600
H	-2.11261200	-1.72591000	-2.89313100
F	-2.86613000	-2.40411300	-1.14223600

2a'-conformer-10



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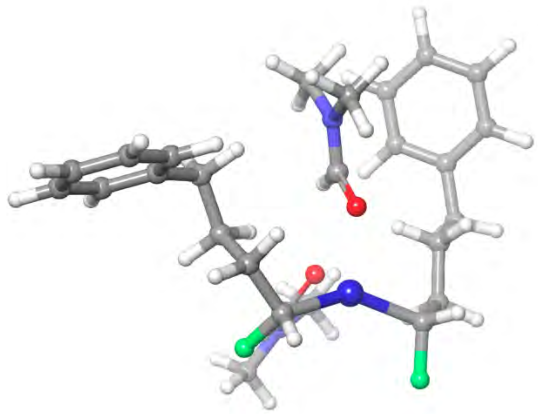
O	-0.74661800	-0.79509100	0.78504500
C	-1.23413100	-1.77153300	1.37464400
N	-2.41097900	-1.75671400	2.00174900
H	-0.68577900	-2.72271100	1.42421600
O	0.55161300	0.39588300	-1.65094900

C	0.62435000	1.22311900	-0.73257400
N	1.63353800	2.08458600	-0.58650200
H	-0.15883600	1.29543500	0.03416200
C	-3.02280100	-3.00522700	2.41336200
H	-3.76908400	-3.31616600	1.67355100
H	-2.25833400	-3.78060000	2.49132800
H	-3.50513000	-2.88216200	3.38710700
C	-3.30659700	-0.62699400	1.81912700
H	-2.72535900	0.27333400	1.61724400
H	-3.96628100	-0.82103400	0.96627700
H	-3.90370600	-0.48282400	2.72348700
C	2.78325900	2.04012800	-1.47594700
H	3.63731900	1.58561900	-0.96357700
H	2.52048500	1.44761400	-2.35118100
H	3.04817300	3.05794500	-1.77821300
C	1.70786700	2.97755400	0.55185400
H	0.81180900	2.86424500	1.16576900
H	2.59006200	2.73799700	1.15448900
H	1.78232400	4.01675700	0.21468900
C	-2.09851600	-1.61379100	-1.80072100
C	-2.65781500	-0.20114300	-1.82495500
H	-2.37943300	0.29874400	-0.88666100
H	-2.14895900	0.35301600	-2.62770800
C	-4.17102700	-0.10276800	-2.01291400
H	-4.66905600	-0.73059900	-1.26365300

H	-4.44409400	-0.51333600	-2.99354200
C	-4.69741600	1.33957500	-1.90876900
H	-4.19240100	1.95937500	-2.66019800
H	-5.76746500	1.35842800	-2.14654300
C	-4.48119800	1.93652600	-0.53839400
C	-5.39011000	1.68920500	0.49433500
C	-3.35103100	2.70830000	-0.25157400
C	-5.17854700	2.19371900	1.77529800
H	-6.27651000	1.09315500	0.28678900
C	-3.13111000	3.21302800	1.02809900
H	-2.63684500	2.91257900	-1.04654800
C	-4.04512800	2.95678400	2.04774500
H	-5.90210800	1.99505000	2.56080400
H	-2.24974700	3.81665600	1.22718100
H	-3.87943500	3.35385200	3.04452500
C	1.53719700	-2.46506400	-0.57387000
H	2.11037100	-3.05965700	-1.29883800
C	2.48905000	-1.48066400	0.08891500
H	2.82961100	-0.76556200	-0.67381700
H	1.93703600	-0.89165700	0.83957300
C	3.69225100	-2.14385500	0.76038300
H	4.33205900	-2.59823600	-0.00799300
H	3.32762800	-2.96935100	1.37987300
C	4.51066400	-1.19584400	1.64360200
H	3.88020700	-0.85066100	2.47242300

H	5.33946100	-1.75276000	2.10106400
C	5.08067500	0.01603400	0.93750400
C	4.99526200	1.28494300	1.51795200
C	5.74761200	-0.10039300	-0.28754700
C	5.56738000	2.40127400	0.90853400
H	4.48418600	1.39422200	2.47234700
C	6.31902400	1.01048500	-0.90305000
H	5.82502600	-1.07454300	-0.76327500
C	6.23445100	2.26734100	-0.30595100
H	5.49423600	3.37436600	1.38649500
H	6.83493200	0.89361400	-1.85154800
H	6.68397600	3.13236900	-0.78373200
F	1.16418100	-3.40267400	0.45111300
H	-2.38109900	-2.12728800	-2.72883200
F	-2.82418800	-2.30752800	-0.76459000

2a’-conformer-11



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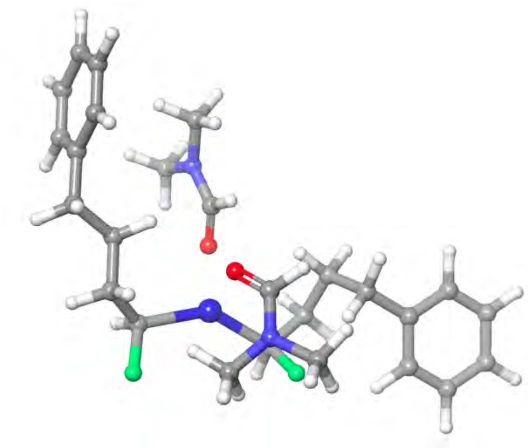
O	-0.81703700	-1.40475600	0.78792300
C	-0.43093200	-2.44682100	1.34218500
N	-1.09962800	-3.05459000	2.32645300
H	0.50880400	-2.93050000	1.04071200
O	-0.08988300	0.62194000	-1.40325200
C	-0.24002000	1.33732000	-0.40804400
N	0.03888400	2.64426600	-0.37448800
H	-0.62151200	0.92908900	0.53896400
C	-0.60767200	-4.27949600	2.92715900
H	-1.31996100	-5.09418500	2.76162200
H	0.34891200	-4.54822400	2.47573600
H	-0.46933200	-4.14458700	4.00486000
C	-2.38222400	-2.55132100	2.78166000
H	-2.63633900	-1.67146100	2.19095800

H	-3.15162500	-3.31796000	2.64419400
H	-2.32982900	-2.28654000	3.84286100
C	-0.13329000	3.42526800	0.83317300
H	-0.85786100	4.22929000	0.66757700
H	-0.50773500	2.78189000	1.63177800
H	0.82588300	3.85694500	1.13996800
C	0.57606600	3.32153200	-1.54024600
H	0.65099900	2.60288400	-2.35510400
H	-0.08446800	4.14442100	-1.83085900
H	1.56844000	3.72607600	-1.31078100
C	-1.95470500	-2.15053200	-2.11402500
C	-3.18573600	-1.85170600	-1.26718300
H	-4.10317700	-2.22322200	-1.75069600
H	-3.10141100	-2.38621800	-0.30893700
C	-3.29894200	-0.36006200	-0.97930800
H	-3.28007700	0.21495100	-1.91591900
H	-2.41210400	-0.05655800	-0.41583700
C	-4.53338900	0.04169800	-0.16434400
H	-5.44524500	-0.11845400	-0.75112600
H	-4.60528400	-0.60888800	0.71768400
C	-4.43839500	1.48180800	0.27553900
C	-3.66003200	1.82799100	1.38573600
C	-5.05601300	2.50630700	-0.44398000
C	-3.51738000	3.15644400	1.77589700
H	-3.17162700	1.03802400	1.95510600

C	-4.90851300	3.83889600	-0.06503400
H	-5.66102200	2.25366700	-1.31142600
C	-4.14052500	4.16921500	1.04813400
H	-2.92896000	3.40329400	2.65589200
H	-5.40119800	4.61986800	-0.63655800
H	-4.03655900	5.20603100	1.35359100
C	1.79576500	-1.98477200	-1.22041600
H	2.14575500	-2.42852200	-2.16205400
C	2.71001600	-0.81326700	-0.88819500
H	3.77155100	-1.07078500	-1.01733000
H	2.49058700	-0.00425000	-1.60134400
C	2.50051200	-0.30422900	0.53892400
H	2.96006000	-1.01109300	1.24065600
H	1.42738200	-0.30320400	0.77056100
C	3.06523400	1.10295300	0.78126100
H	2.55438100	1.80771000	0.11040200
H	2.83773600	1.41743600	1.80856100
C	4.55411400	1.19009800	0.54755100
C	5.44899100	0.69477800	1.50019600
C	5.07103700	1.72563200	-0.63349800
C	6.82201400	0.73532200	1.28077100
H	5.06004000	0.27344600	2.42483000
C	6.44463100	1.76792300	-0.85994500
H	4.38517400	2.10907100	-1.38605600
C	7.32490900	1.27339500	0.09791500

H	7.50158900	0.34805300	2.03413400
H	6.82679000	2.18735700	-1.78586500
H	8.39613900	1.30665000	-0.07495200
F	2.07814400	-2.99201200	-0.22949500
H	-2.15126700	-1.76235900	-3.12565100
F	-1.90476400	-3.56541100	-2.25769000

2a’-conformer-12



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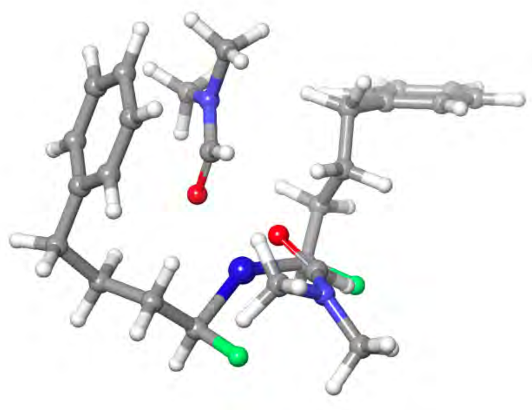
O	-0.02249600	0.74988100	1.16840300
C	-1.01037100	1.01720000	1.87154500
N	-1.67933200	2.16524400	1.86419600
H	-1.39278600	0.28361500	2.59634600
O	0.75756900	-0.76194100	-1.36646500
C	1.34319500	-1.38628100	-0.47260200

N	2.36998400	-2.21104700	-0.67999600
H	1.04638700	-1.28009100	0.58003100
C	-2.96677600	2.28005700	2.52434700
H	-3.75736200	2.30609100	1.76696300
H	-3.12854800	1.41944800	3.17715200
H	-2.99890900	3.19555100	3.12155200
C	-1.30812000	3.25700800	0.97294800
H	-0.25714700	3.18741600	0.69780800
H	-1.92722300	3.22192300	0.07254300
H	-1.47472100	4.20195500	1.49718000
C	2.91360300	-2.41014600	-2.01117000
H	2.83412400	-3.46474400	-2.29465200
H	2.35029000	-1.79644700	-2.71263900
H	3.96861300	-2.11700500	-2.01687900
C	3.03759300	-2.88554300	0.41705800
H	2.59284200	-2.57240300	1.36393900
H	2.93477600	-3.97133200	0.31451600
H	4.09945300	-2.62347400	0.42280200
C	1.25962200	2.48498300	-1.31343300
C	2.41412900	2.57338800	-0.32424300
H	3.11204200	3.37146000	-0.62511300
H	2.03456500	2.85784900	0.66786500
C	3.16661100	1.24977200	-0.19087000
H	3.26654500	0.76832200	-1.17617100
H	2.58292300	0.56308900	0.43449100

C	4.55665400	1.41731400	0.43351400
H	5.14926700	2.09147400	-0.19740400
H	4.45515800	1.90963000	1.40826400
C	5.29421700	0.11095800	0.59967700
C	5.85995900	-0.52840600	-0.51000000
C	5.43198800	-0.49509700	1.85069800
C	6.55824700	-1.72539000	-0.37144600
H	5.76887100	-0.06470500	-1.49043200
C	6.13105700	-1.69257700	1.99726800
H	5.00003700	-0.01104500	2.72339500
C	6.70079700	-2.31032300	0.88681300
H	7.00386500	-2.19544400	-1.24362300
H	6.23774900	-2.13811000	2.98196500
H	7.25470900	-3.23718000	0.99945900
C	-2.16423700	0.76626600	-1.42405900
H	-2.39331400	1.21433300	-2.40148200
C	-2.58157000	-0.69510100	-1.50819600
H	-3.61865900	-0.79413600	-1.86237900
H	-1.94386000	-1.15214200	-2.27721700
C	-2.42015600	-1.49940900	-0.21566600
H	-1.39887400	-1.35719000	0.16327700
H	-2.53570600	-2.56968800	-0.43272200
C	-3.41251900	-1.12854400	0.90301600
H	-3.14900000	-1.69001100	1.80949100
H	-3.30964800	-0.06358000	1.12504500

C	-4.85170300	-1.41567600	0.54778100
C	-5.64159200	-0.44415000	-0.07525200
C	-5.41525800	-2.66614900	0.81248000
C	-6.96259000	-0.71782400	-0.41902000
H	-5.19632500	0.52066000	-0.30334400
C	-6.73587400	-2.94328100	0.46947700
H	-4.81055500	-3.42928600	1.29852200
C	-7.51499500	-1.96721900	-0.14639000
H	-7.56259900	0.04752900	-0.90268200
H	-7.15812700	-3.92001100	0.68728100
H	-8.54615300	-2.17927800	-0.41235000
F	-3.08881000	1.42872300	-0.52811000
H	1.70448600	2.37214900	-2.31474600
F	0.66514000	3.78548200	-1.31624700

2a’-conformer-13



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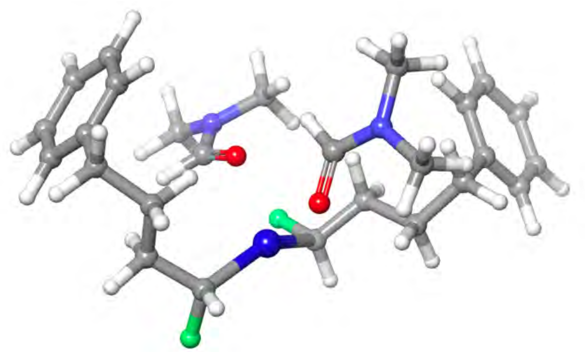
O	0.83500800	-1.28085600	-0.91421600
C	0.69779000	-2.48968700	-1.16166800
N	1.53428400	-3.18968100	-1.92968500
H	-0.15705200	-3.05036900	-0.75647200
O	0.54321200	0.92906800	1.11372000
C	0.35309300	1.46538300	0.01430700
N	-0.35119000	2.59043100	-0.15052800
H	0.74838800	1.02817000	-0.91218000
C	1.47826600	-4.63937100	-1.91949500
H	2.23945200	-5.03712000	-1.23907000
H	0.49434800	-4.96431900	-1.57634500
H	1.65008800	-5.02746300	-2.92722700
C	2.79812500	-2.58880100	-2.32047500
H	2.65898600	-1.51351900	-2.42993500
H	3.54407400	-2.77651400	-1.54019100
H	3.12619500	-3.02196400	-3.26865200
C	-0.56876000	3.16562800	-1.46111600
H	-0.14926500	4.17666400	-1.50744500
H	-0.07720500	2.54914300	-2.21609000
H	-1.64170100	3.21284900	-1.67640300
C	-0.89466500	3.30225200	0.99002700
H	-0.72781900	2.70470000	1.88513900
H	-0.39719000	4.27341600	1.09585500
H	-1.96810100	3.46828000	0.84928000

C	2.45067900	-1.88745800	1.54763600
C	3.50846500	-0.94509500	1.00119600
H	4.46008000	-1.47978200	0.83898200
H	3.18315600	-0.57032700	0.02067800
C	3.75057300	0.22928700	1.94511100
H	4.20423600	-0.13944700	2.87360500
H	2.79087800	0.68727200	2.21838100
C	4.66122300	1.31111000	1.34143600
H	4.95142200	2.02088100	2.12452500
H	5.58410200	0.84361300	0.97650600
C	3.99823900	2.06861100	0.21653500
C	4.13874900	1.66893400	-1.11566300
C	3.20234300	3.18533800	0.49131300
C	3.51231500	2.36717100	-2.14594500
H	4.75668000	0.80385700	-1.34493500
C	2.58519600	3.89566800	-0.53421500
H	3.07806100	3.50502600	1.52366800
C	2.74010500	3.49027400	-1.85906000
H	3.64321300	2.04465300	-3.17478000
H	1.99066100	4.77563600	-0.29936200
H	2.27174600	4.05174000	-2.66264100
C	-1.39716800	-1.68063500	1.52622300
H	-1.62267900	-1.95312600	2.56621800
C	-2.42777000	-0.64916800	1.08577500
H	-3.44450000	-0.93511000	1.39391900

H	-2.19729800	0.29994200	1.59641400
C	-2.42491000	-0.42809500	-0.42563800
H	-2.78871000	-1.34026500	-0.91382100
H	-1.39451400	-0.28933900	-0.77674800
C	-3.27633200	0.76924600	-0.86975700
H	-2.88763400	1.67524700	-0.38499300
H	-3.16646800	0.91343900	-1.95280600
C	-4.73998400	0.61904000	-0.53141800
C	-5.55770400	-0.21997600	-1.29376400
C	-5.30252600	1.27774400	0.56335500
C	-6.90011000	-0.39405300	-0.97345600
H	-5.13228400	-0.74113800	-2.14875500
C	-6.64556300	1.10698800	0.89021900
H	-4.67544100	1.92827500	1.16968100
C	-7.44933200	0.27064600	0.12108100
H	-7.51998500	-1.04809900	-1.57953000
H	-7.06371800	1.62772200	1.74656500
H	-8.49698200	0.13679600	0.37217800
F	-1.68395500	-2.87126300	0.77217000
H	2.76280700	-2.22113300	2.54606500
F	2.51409400	-3.07316400	0.72831600

2a’-conformer-14



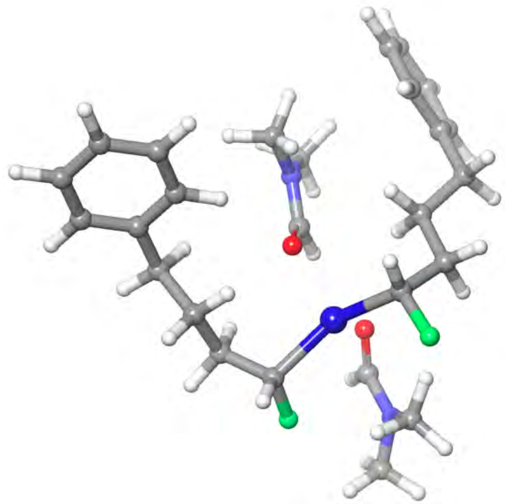
Zn	0.56643400	-1.24810300	1.20012300
O	1.08246700	0.30515200	-0.28183700
C	1.61730100	1.30917200	0.21000800
N	1.15302000	2.55165800	0.08121900
H	2.55822300	1.23689900	0.77662200
O	-0.28191000	-2.29659500	-0.45978500
C	-0.67081300	-1.70858300	-1.47254700
N	-1.57438900	-2.20849600	-2.32706600
H	-0.28091800	-0.71664500	-1.73692100
C	1.70180600	3.62568500	0.88433200
H	1.02523200	3.85385800	1.71558700
H	2.67277600	3.32379800	1.28109200
H	1.83778300	4.52029500	0.26882500
C	-0.14948200	2.77905300	-0.51605300
H	-0.35174400	1.98250400	-1.23175600
H	-0.91958100	2.76519400	0.26177400
H	-0.14583200	3.74430600	-1.02949900

C	-2.19820700	-3.49679300	-2.08442100
H	-2.03437000	-4.15798400	-2.94127100
H	-1.75390500	-3.93355600	-1.19109200
H	-3.27596600	-3.36641500	-1.93542000
C	-2.02031700	-1.45804200	-3.48263100
H	-1.49385400	-0.50204100	-3.52401300
H	-1.81774900	-2.01546600	-4.40304000
H	-3.09765000	-1.26576400	-3.41808700
C	-0.94800400	-0.07601200	1.89878900
C	-2.12961300	0.10271500	0.96068500
H	-2.70547000	0.99958900	1.23613300
H	-1.77518000	0.27750700	-0.07065000
C	-3.05184100	-1.11348200	0.97447500
H	-3.54818000	-1.18063400	1.95143100
H	-2.45545400	-2.02932300	0.86209200
C	-4.11515400	-1.08035500	-0.13445300
H	-3.60537800	-1.10183000	-1.10692100
H	-4.73213500	-1.98590200	-0.07437300
C	-4.99998500	0.14055600	-0.07351200
C	-4.78310400	1.23010200	-0.91945900
C	-6.03260400	0.22268800	0.86458600
C	-5.57523300	2.37232900	-0.83524400
H	-3.97808500	1.18026800	-1.65055900
C	-6.82798800	1.36067000	0.95355200
H	-6.21329300	-0.61846200	1.53040800

C	-6.60177900	2.44031200	0.10225600
H	-5.39155600	3.20890100	-1.50300700
H	-7.62776900	1.40482200	1.68671800
H	-7.22292600	3.32806500	0.16927800
C	2.24280900	-2.23133500	1.75155800
H	2.18759700	-3.31712300	1.56997200
C	3.52182700	-1.72418300	1.10198700
H	3.63198900	-0.64944900	1.30351400
H	4.40116600	-2.20678400	1.55932100
C	3.53908300	-1.96757600	-0.40416600
H	2.61514200	-1.57364400	-0.84676200
H	3.55006500	-3.04809300	-0.59627000
C	4.74508500	-1.32300000	-1.10849000
H	5.67008900	-1.66718900	-0.63017200
H	4.78034200	-1.65837000	-2.15170900
C	4.68950200	0.18544900	-1.07674100
C	3.91261300	0.88296400	-2.00742100
C	5.36672000	0.91949700	-0.09892600
C	3.82050800	2.27130600	-1.97037100
H	3.36995300	0.32380800	-2.76647800
C	5.27657000	2.30998500	-0.05337900
H	5.97158100	0.39138400	0.63427100
C	4.50637200	2.99116200	-0.99328600
H	3.21287200	2.79351900	-2.70399200
H	5.81702900	2.86076700	0.71117700

H	4.44362700	4.07531900	-0.96720300
F	2.42886900	-2.09425900	3.15300500
H	-1.34632600	-0.32581000	2.89173900
F	-0.36625300	1.23164500	2.05729400

2a'-conformer-15



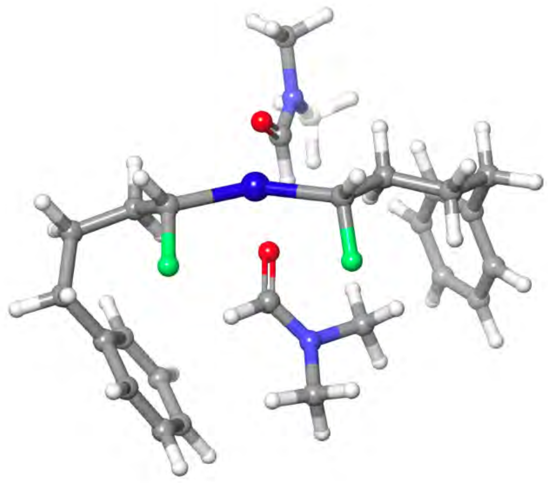
Zn	-0.07232000	1.74854700	0.64229800
O	-1.60960900	1.86924600	-0.89449800
C	-1.88251300	2.93490600	-1.46379100
N	-2.16967500	4.08918400	-0.86543200
H	-1.94601700	2.97787100	-2.56056700
O	0.55037600	-0.17312200	-0.10145200
C	-0.07989900	-0.72637200	-1.01406200
N	-0.06037900	-2.03907900	-1.23385600

H	-0.72270100	-0.14852400	-1.69133500
C	-2.14965200	5.31939500	-1.63548000
H	-1.18659400	5.82157600	-1.49571900
H	-2.28304600	5.09588900	-2.69594300
H	-2.95954700	5.97552000	-1.30651400
C	-1.99837400	4.23957400	0.57214500
H	-2.21627900	3.30820300	1.09230100
H	-0.96834100	4.54479800	0.78681500
H	-2.68751200	5.00931700	0.92810200
C	0.72821300	-2.90741800	-0.37326900
H	1.75933500	-2.98998600	-0.73415800
H	0.74162900	-2.49016100	0.63518000
H	0.26095900	-3.89413000	-0.35555500
C	-0.80903300	-2.64143100	-2.32170800
H	-1.36917000	-1.86567400	-2.84770000
H	-0.12960900	-3.12955500	-3.02831000
H	-1.51246200	-3.37940600	-1.92571700
C	-1.14556900	1.25321800	2.29397400
C	-2.48484700	0.55982200	2.06989500
H	-2.96078000	0.32732300	3.03614200
H	-3.17104100	1.24135600	1.54681300
C	-2.34291600	-0.71391300	1.23736700
H	-1.43484100	-1.25970000	1.53553100
H	-2.21000700	-0.43907500	0.18456700
C	-3.55153700	-1.64890500	1.34759800

H	-3.68365000	-1.93773200	2.39802800
H	-4.45811900	-1.10451300	1.05685000
C	-3.41348700	-2.89263400	0.50173200
C	-2.49895300	-3.89125300	0.85758700
C	-4.18652100	-3.08672800	-0.64546600
C	-2.38144400	-5.05858100	0.10786300
H	-1.89008200	-3.75831900	1.74975000
C	-4.07373800	-4.25294000	-1.40168300
H	-4.90103800	-2.32092500	-0.93752700
C	-3.17476400	-5.24695200	-1.02417600
H	-1.68060400	-5.83001200	0.41530600
H	-4.69655200	-4.38791000	-2.28111900
H	-3.09362400	-6.16166500	-1.60331600
C	1.25101800	3.03964000	-0.22977200
H	1.85683800	3.64197100	0.46353900
C	2.20014300	2.30632600	-1.16571700
H	1.61757700	1.68134800	-1.85951500
H	2.76680700	3.01522000	-1.78735500
C	3.15794900	1.41744200	-0.36992800
H	2.63474600	1.03026600	0.51370600
H	4.00178800	2.00695200	0.00859200
C	3.68174400	0.22508800	-1.17687600
H	2.81515400	-0.30287800	-1.59793700
H	4.27869500	0.58040700	-2.02578800
C	4.48881000	-0.74276300	-0.34578100

C	3.87795200	-1.41520100	0.71951800
C	5.83794300	-0.98826700	-0.60049500
C	4.59571000	-2.31322000	1.50191000
H	2.82747900	-1.21968200	0.92754600
C	6.56237100	-1.88604800	0.18213600
H	6.32632100	-0.47053000	-1.42261500
C	5.94317700	-2.55261500	1.23457900
H	4.10587700	-2.82547200	2.32516900
H	7.61227500	-2.06346200	-0.03185800
H	6.50577300	-3.25198500	1.84544300
F	0.55893300	4.00817500	-1.03596800
H	-0.56885500	0.62147300	2.98738400
F	-1.45200400	2.43567400	3.03561800

2a’-conformer-16



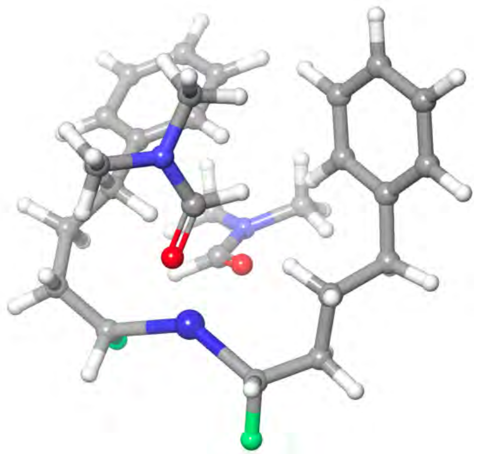
Zn	0.53831200	-1.47950300	1.33797600
O	0.36286300	0.06828900	-0.22685900
C	0.93919600	1.08604100	0.19466500
N	0.37896700	2.29497900	0.22059800
H	1.97256600	1.03548200	0.56774000
O	-0.57157900	-2.76210100	0.04096800
C	-1.16825300	-2.29800000	-0.93638700
N	-2.03647200	-2.99880900	-1.67930100
H	-1.01884500	-1.25831100	-1.25567700
C	0.98788700	3.36038800	0.99202200
H	0.42326900	3.51138100	1.91917400
H	2.01466400	3.08845000	1.23903700
H	0.99508800	4.28994800	0.41405500
C	-1.03374300	2.44327700	-0.08177000

H	-1.34302600	1.67266800	-0.78878800
H	-1.61789900	2.33464200	0.83864300
H	-1.21085600	3.43045500	-0.51710800
C	-2.33544200	-4.38558300	-1.37299600
H	-2.00692700	-5.03256600	-2.19327400
H	-1.81091300	-4.65858500	-0.45868100
H	-3.41399400	-4.51114100	-1.23406900
C	-2.65621800	-2.42301600	-2.85459700
H	-2.33525200	-1.38480500	-2.96058700
H	-2.36571600	-2.98002700	-3.75205800
H	-3.74815300	-2.44879900	-2.76439500
C	-0.90408400	-0.57068100	2.44502800
C	-2.24666300	-0.58970900	1.73469900
H	-2.09870600	-0.24692100	0.69971400
H	-2.58934000	-1.63396100	1.66895900
C	-3.33473100	0.26225700	2.38567800
H	-2.95096000	1.27859300	2.53775200
H	-3.56164300	-0.13777000	3.38213100
C	-4.62941600	0.31674000	1.55789300
H	-4.98960500	-0.70562900	1.38691600
H	-5.40872900	0.83726600	2.12687300
C	-4.44053100	1.01211500	0.23069200
C	-4.45120800	2.40834700	0.16140800
C	-4.21769100	0.29500500	-0.94874000
C	-4.24978000	3.07138400	-1.04621300

H	-4.62344000	2.98042300	1.07076300
C	-4.02377200	0.95235700	-2.16216800
H	-4.20099000	-0.79332600	-0.90671900
C	-4.03703600	2.34410500	-2.21515000
H	-4.26776700	4.15700500	-1.07655400
H	-3.87873000	0.37989900	-3.07430300
H	-3.89035400	2.85704300	-3.16055000
C	2.51607600	-1.83102400	1.10776400
H	3.00721400	-2.61642000	1.69784600
C	2.86590700	-2.02063200	-0.35891100
H	2.40038400	-2.96615400	-0.67304200
H	2.37141500	-1.23630800	-0.94553800
C	4.35458700	-2.06985400	-0.72688900
H	4.44590800	-2.24062200	-1.80873500
H	4.81854900	-2.94051700	-0.24584500
C	5.17512200	-0.82997200	-0.33603000
H	5.30801500	-0.81403600	0.74794100
H	6.17717800	-0.92376100	-0.77728500
C	4.58625800	0.50009300	-0.75392600
C	3.90885000	0.66633700	-1.96515600
C	4.72700800	1.61660200	0.07615900
C	3.37561500	1.90109300	-2.32972400
H	3.78258300	-0.18529400	-2.62869000
C	4.21919200	2.85903200	-0.29309600
H	5.23550700	1.50093000	1.02985000

C	3.52904100	3.00487300	-1.49537000
H	2.84095200	2.00023500	-3.26993800
H	4.35354000	3.71401200	0.36460100
H	3.11787500	3.96925000	-1.77945000
F	3.13871600	-0.60388800	1.54339100
H	-1.05319200	-0.87775800	3.48889400
F	-0.52691400	0.81810900	2.52281600

2a’-conformer-17



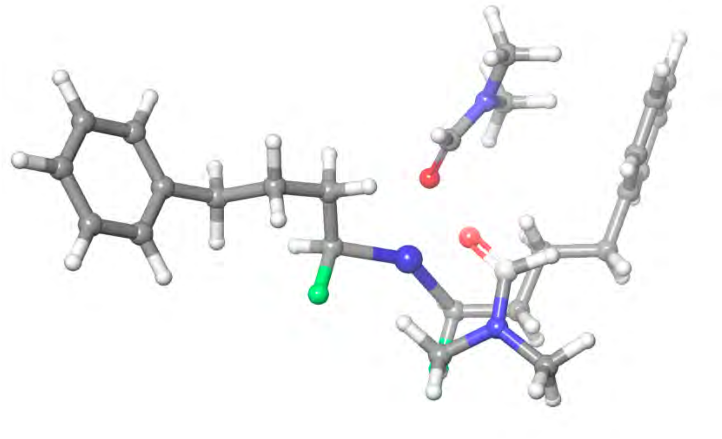
Zn	0.54714400	-2.38237900	-0.16918300
O	0.19390000	-0.70343100	1.18757000
C	1.22836600	-0.26467900	1.72188600
N	1.23400800	0.66070000	2.68063800
H	2.21731300	-0.64528500	1.43650200
O	-0.18580600	-1.37786600	-1.94930300

C	-0.77270000	-0.30348300	-2.10016900
N	-0.66291100	0.47038200	-3.18606000
H	-1.44307700	0.10847200	-1.33042800
C	-0.00702300	1.20738200	3.19410200
H	-0.25440700	2.14874300	2.68893400
H	-0.80639500	0.48454700	3.02979900
H	0.10368600	1.39597100	4.26528300
C	2.46992400	1.31372000	3.07199200
H	3.31466200	0.79853500	2.61020700
H	2.46338100	2.35549400	2.73038400
H	2.58259900	1.28578200	4.15992400
C	0.19455700	0.08561300	-4.29207600
H	0.92425600	0.87852400	-4.48769500
H	0.71209500	-0.83565400	-4.02683600
H	-0.40431900	-0.07401500	-5.19470000
C	-1.36534600	1.73541300	-3.28785100
H	-2.02109700	1.86380100	-2.42327300
H	-0.64923800	2.56426900	-3.32054800
H	-1.97281600	1.75560100	-4.19829200
C	-0.94036300	-3.66609300	0.35137200
C	-1.99707500	-3.03174900	1.24860200
H	-2.75526600	-3.76825600	1.55625000
H	-1.51721200	-2.67000600	2.16886700
C	-2.65137200	-1.84615000	0.54789100
H	-3.24671600	-2.18069800	-0.31250700

H	-1.84661000	-1.22430200	0.14583000
C	-3.50998400	-0.96038500	1.45943600
H	-4.44854800	-1.46388000	1.71729600
H	-2.96542300	-0.80640700	2.40050000
C	-3.79004300	0.38292900	0.82895400
C	-2.73397300	1.28559500	0.64236000
C	-5.06056200	0.75331600	0.38900300
C	-2.94497400	2.52353900	0.04233800
H	-1.73620500	0.99246400	0.96855900
C	-5.27697800	1.98972800	-0.21922900
H	-5.89078400	0.06463900	0.52428000
C	-4.22197200	2.87997200	-0.39416200
H	-2.11319300	3.21255800	-0.09100500
H	-6.27453600	2.25803300	-0.55409800
H	-4.39171100	3.84555900	-0.86066800
C	2.57953600	-2.41260700	-0.47964900
H	2.78395700	-3.45264400	-0.77475500
C	3.35536600	-1.54624800	-1.47079100
H	4.36788900	-1.95356900	-1.60576400
H	2.85508900	-1.60479900	-2.44833100
C	3.50518800	-0.07929500	-1.05041400
H	4.28562900	0.39667800	-1.65670700
H	3.86704100	-0.05531700	-0.01418200
C	2.20379500	0.71236300	-1.17102600
H	1.99415000	0.88604200	-2.23752100

H	1.38201800	0.09097700	-0.81019400
C	2.15538200	2.03479700	-0.43937600
C	0.92435800	2.52954200	0.01054400
C	3.29882000	2.80151700	-0.20048200
C	0.83397200	3.75591600	0.66283200
H	0.02832700	1.92834300	-0.14843500
C	3.21456000	4.03173000	0.45129600
H	4.26718800	2.43489800	-0.52907100
C	1.98295300	4.51570100	0.88342900
H	-0.13201400	4.11910800	1.00548000
H	4.11608100	4.61286300	0.62140700
H	1.91687600	5.47351200	1.39008400
F	3.27813300	-2.26819700	0.77207500
H	-1.46067800	-4.08313100	-0.52710700
F	-0.43093300	-4.78755700	1.05403100

2a'-conformer-18



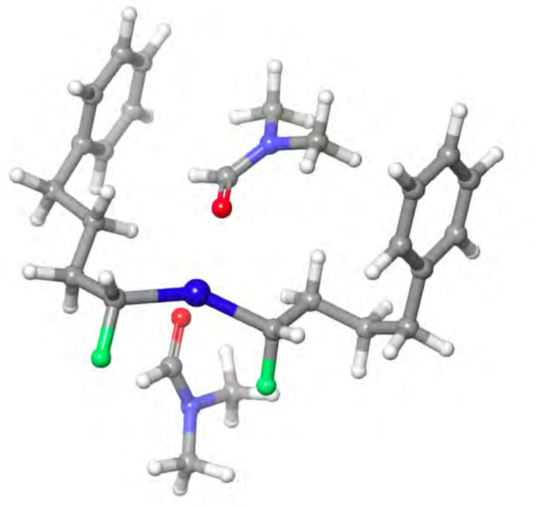
Zn	0.17797400	1.28447400	1.09085600
O	1.00818700	1.93199000	-0.88291700
C	0.85977600	3.15568800	-0.75725500
N	0.39157600	3.95728100	-1.71882200
H	1.12977900	3.66660800	0.18130600
O	0.21743800	-0.83114700	0.93657200
C	0.58618600	-1.62185700	0.06053200
N	-0.10685800	-2.69962300	-0.31292800
H	1.54094100	-1.49340100	-0.47336800
C	-0.05450600	5.29553400	-1.37888400
H	-1.13948100	5.29964600	-1.22604300
H	0.43115200	5.61815100	-0.45605400
H	0.20684300	5.99149000	-2.18072100
C	-0.20209500	3.35292600	-2.89781200

H	0.33314500	2.43352800	-3.13152600
H	-1.25369100	3.11701200	-2.69515700
H	-0.13072600	4.04957300	-3.73660000
C	-1.40257600	-2.99771300	0.27723900
H	-1.41301500	-4.03066100	0.63973100
H	-1.57696700	-2.31420700	1.10660000
H	-2.20157900	-2.87170600	-0.46246900
C	0.38279700	-3.59016200	-1.34631500
H	1.34696900	-3.23302400	-1.71474400
H	0.51554700	-4.60005400	-0.94365200
H	-0.33179700	-3.63193500	-2.17499600
C	-1.71238400	1.61146400	0.41258000
C	-2.07381900	0.66442900	-0.72052300
H	-1.28214400	0.71009700	-1.48259200
H	-2.06002100	-0.35896000	-0.32203000
C	-3.42535500	0.92840600	-1.39301100
H	-3.52203900	0.30035600	-2.28911700
H	-3.46107500	1.97197200	-1.72653400
C	-4.63092700	0.66624100	-0.47511500
H	-4.59650300	1.35204200	0.37781400
H	-5.55332900	0.89197800	-1.02357800
C	-4.68449600	-0.75766400	0.02648100
C	-5.04575300	-1.79996100	-0.83467400
C	-4.35312400	-1.07652100	1.34569000
C	-5.08689300	-3.11839400	-0.38959400

H	-5.31111900	-1.56832600	-1.86415600
C	-4.39346500	-2.39448700	1.79852100
H	-4.06514900	-0.27886400	2.02666600
C	-4.76117100	-3.42086800	0.93225400
H	-5.38287500	-3.91032700	-1.07169600
H	-4.13994000	-2.61743800	2.83103600
H	-4.80145700	-4.44725000	1.28463700
C	1.71263600	1.97561400	2.22813800
H	1.71033600	1.58609900	3.25599200
C	3.09750000	1.72594900	1.63442300
H	3.25475100	2.42568600	0.80224600
H	3.90169300	1.91844100	2.36133000
C	3.18453300	0.30608800	1.08724800
H	2.51861400	0.25372800	0.21853800
H	2.79081000	-0.40952600	1.82344700
C	4.57604700	-0.15609800	0.64176500
H	5.01416500	0.59118100	-0.03055500
H	5.24106200	-0.24040300	1.50958000
C	4.46044600	-1.48268200	-0.06834900
C	4.39440000	-1.54703900	-1.46303200
C	4.30282700	-2.66786700	0.65800000
C	4.19222700	-2.76144100	-2.11687000
H	4.50536600	-0.63248300	-2.04077900
C	4.09501200	-3.88312300	0.01157600
H	4.34417600	-2.63218200	1.74436000

C	4.04370900	-3.93513400	-1.38064600
H	4.15788300	-2.79101400	-3.20222400
H	3.98235700	-4.79264800	0.59441000
H	3.89269600	-4.88380700	-1.88746500
F	1.58740600	3.39463600	2.37015100
H	-2.51711900	1.60275700	1.16066500
F	-1.76348300	2.93706600	-0.15561500

2a'-conformer-19



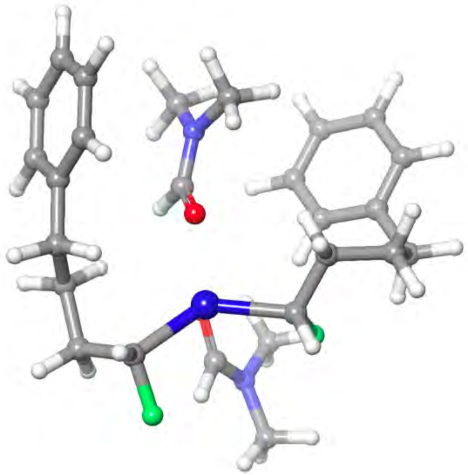
Zn	0.07929600	0.88464600	-0.96917600
O	-0.54318600	0.73594300	1.13267100
C	-1.03785400	1.64594500	1.80824300
N	-0.64400700	2.91752900	1.80846700

H	-1.87299300	1.43853200	2.49610600
O	-0.80992100	-1.04948100	-1.18910500
C	-0.96848400	-1.78231500	-0.20628300
N	-1.96980700	-2.65754900	-0.07954200
H	-0.28313000	-1.74994500	0.65130500
C	0.43807000	3.36742800	0.93564100
H	0.91852100	4.22828400	1.40712700
H	1.18228700	2.57820100	0.81567700
H	0.04295200	3.65981400	-0.04419700
C	-1.41269400	3.93975100	2.49214800
H	-2.20478900	3.47599800	3.08415000
H	-0.76292700	4.51729700	3.15586800
H	-1.86731100	4.61813400	1.76195200
C	-2.07085000	-3.53685100	1.06739700
H	-1.95753800	-4.58204100	0.75924300
H	-1.28822300	-3.29294500	1.78866400
H	-3.04963300	-3.41252300	1.54031800
C	-2.97384600	-2.80609000	-1.12068100
H	-2.82355400	-2.02057500	-1.85987500
H	-2.87263900	-3.78593800	-1.60048200
H	-3.97219000	-2.72018400	-0.68082700
C	2.06615300	0.52259600	-0.79113800
C	2.39672200	-0.63448900	0.14269800
H	1.80777600	-0.55621800	1.06886700
H	2.07626400	-1.56026500	-0.36033600

C	3.87765100	-0.73912300	0.53069400
H	4.04510600	-1.64386200	1.12944100
H	4.13901800	0.11297400	1.16780400
C	4.82814600	-0.74817300	-0.67308300
H	4.52754800	-1.53778400	-1.37440000
H	4.73293400	0.20721600	-1.19964300
C	6.26018800	-0.95559100	-0.24888800
C	7.03539300	0.12539600	0.18050200
C	6.82836500	-2.23127300	-0.22137000
C	8.34166800	-0.06164800	0.62239700
H	6.60391800	1.12383200	0.16263200
C	8.13520900	-2.42484000	0.21861700
H	6.23680700	-3.08154700	-0.55384600
C	8.89694700	-1.33919600	0.64246100
H	8.92938400	0.79180000	0.94788500
H	8.56032700	-3.42437300	0.22705600
H	9.91727200	-1.48668500	0.98316500
C	-1.35070900	2.08949500	-1.77595500
H	-1.59768100	1.73621500	-2.78961400
C	-2.67083900	2.25085700	-1.03403400
H	-2.49521300	2.74801200	-0.06656800
H	-3.34721400	2.91823500	-1.59164700
C	-3.35920900	0.91236200	-0.78364000
H	-2.71652900	0.27921300	-0.15999800
H	-3.48431000	0.37564600	-1.73468800

C	-4.72446100	1.04873800	-0.09995200
H	-4.60281700	1.61728400	0.83192800
H	-5.40153400	1.62943100	-0.73744000
C	-5.33091500	-0.29826500	0.20463600
C	-6.19403600	-0.92098300	-0.70090100
C	-4.99787500	-0.98096300	1.37866800
C	-6.72013200	-2.18431200	-0.43914500
H	-6.45988300	-0.40358600	-1.61977500
C	-5.52904500	-2.23944600	1.65193100
H	-4.32418600	-0.51058900	2.09251500
C	-6.39157300	-2.84771800	0.74097700
H	-7.39392400	-2.64735600	-1.15380600
H	-5.27974000	-2.74155100	2.58302600
H	-6.81055500	-3.82628300	0.95379500
F	-0.85293700	3.41525700	-1.96408800
H	2.56016500	0.32772800	-1.75296900
F	2.75282200	1.66493400	-0.26211000

2a’-conformer-20



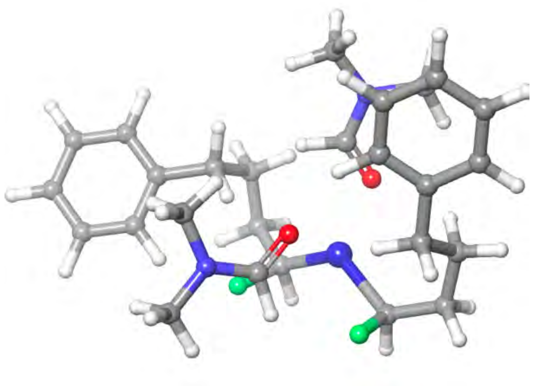
Zn	-0.10968100	-1.57344900	-0.92645500
O	-0.71927300	-1.38152300	1.18006000
C	-1.53270400	-2.31678800	1.24370100
N	-2.63202900	-2.31303700	1.99905000
H	-1.36866300	-3.24811400	0.67798900
O	0.93379100	0.23004400	-0.76117700
C	1.17306300	0.86650200	0.27463300
N	1.44819300	2.16856300	0.30195700
H	1.17689900	0.37919800	1.25906500
C	-3.03731500	-1.10310900	2.69030500
H	-3.47393800	-1.36640900	3.65756400
H	-2.16176800	-0.47216700	2.83763000
H	-3.77565600	-0.55600900	2.09253200
C	-3.63948400	-3.34209000	1.82760700

H	-3.20903700	-4.18979900	1.29160900
H	-3.99788900	-3.68190300	2.80349500
H	-4.48314000	-2.94968700	1.24886200
C	1.74713500	2.86008300	1.53807700
H	0.98238000	3.61799500	1.73644300
H	1.77213200	2.14350300	2.36235800
H	2.72833000	3.33814000	1.46414900
C	1.32727500	2.97869900	-0.89684800
H	1.25135700	2.31735600	-1.75902800
H	0.42639100	3.60066500	-0.82474700
H	2.21057500	3.61618100	-0.99455800
C	-1.87898300	-0.97187100	-1.75548700
C	-1.84911600	0.44824700	-2.30414300
H	-1.24878400	1.10752900	-1.66589900
H	-1.28948300	0.37879200	-3.24898600
C	-3.19450100	1.12841800	-2.57935000
H	-3.82347800	0.47168200	-3.19416500
H	-3.01417100	2.03835300	-3.16804800
C	-3.99115400	1.52517800	-1.31883600
H	-4.87622900	2.09356300	-1.62862000
H	-4.33868500	0.61739700	-0.82292000
C	-3.19579800	2.35449000	-0.33745700
C	-2.33603800	1.74216300	0.58520800
C	-3.28809300	3.74797600	-0.33254200
C	-1.61988900	2.50428300	1.50303200

H	-2.22977600	0.66033100	0.56824400
C	-2.56507800	4.51572600	0.57891500
H	-3.94824100	4.23731900	-1.04535800
C	-1.73543000	3.89500300	1.50913200
H	-0.97502600	2.00539800	2.22440900
H	-2.66388700	5.59738800	0.57371300
H	-1.19628900	4.48992100	2.24172800
C	0.94909800	-3.30907200	-0.83572900
H	1.51258200	-3.52541100	-1.75349200
C	1.85643900	-3.55175400	0.36743800
H	1.21407400	-3.80687000	1.22021300
H	2.52063400	-4.41605000	0.21303600
C	2.67348100	-2.31848400	0.75210600
H	3.33112400	-2.55915200	1.59639400
H	1.97355800	-1.55324700	1.10866900
C	3.49666800	-1.74144500	-0.40401600
H	4.32717100	-2.42424900	-0.63289900
H	2.87558800	-1.70195700	-1.30601500
C	4.03490400	-0.34824100	-0.15708000
C	4.13338300	0.55871800	-1.21752100
C	4.41799700	0.08568500	1.11576200
C	4.61124500	1.85038300	-1.02081600
H	3.81345900	0.24564700	-2.20832000
C	4.89890500	1.37845000	1.31943200
H	4.34436200	-0.59384500	1.96025400

C	4.99957400	2.26659300	0.25173800
H	4.68030500	2.53404300	-1.86255600
H	5.19790400	1.69044300	2.31643400
H	5.37936900	3.27230100	0.40856300
F	-0.04706100	-4.34511700	-0.77845100
H	-2.29758000	-1.62000500	-2.53722800
F	-2.86614500	-1.05311900	-0.69472100

2a'-conformer-21



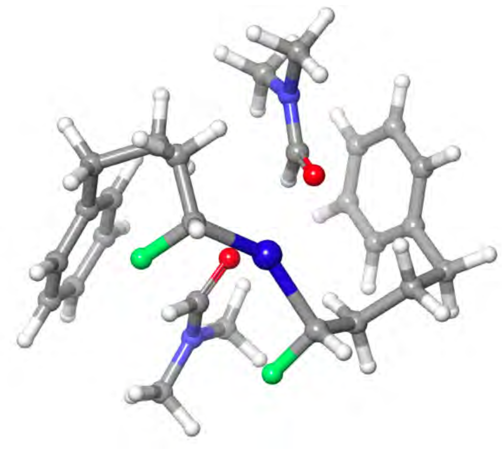
Zn	-0.26484100	-1.54796100	1.03901900
O	0.00230100	-0.53659400	-0.86087500
C	0.67741100	-1.26373900	-1.60998200
N	1.54114100	-0.80088200	-2.51471200
H	0.57027000	-2.35296700	-1.58236000
O	-1.29080500	0.16751200	1.64649100
C	-1.04897800	1.27021300	1.13469600

N	-1.82398500	2.34337800	1.27664100
H	-0.15426600	1.42779600	0.51855700
C	2.41284200	-1.70100600	-3.24337700
H	3.45548300	-1.51306700	-2.96448400
H	2.16183700	-2.73338700	-2.99479800
H	2.29999800	-1.55169900	-4.32196400
C	1.77038500	0.62200900	-2.69106100
H	1.00959800	1.16923100	-2.13493000
H	2.76442300	0.89613900	-2.31905200
H	1.70149200	0.87182900	-3.75454800
C	-3.11367800	2.25829900	1.94116300
H	-3.90602400	2.47747600	1.21685900
H	-3.24131000	1.24899900	2.32915700
H	-3.15560400	2.98027300	2.76297300
C	-1.46809200	3.61815300	0.68882900
H	-0.53996100	3.51594800	0.12136300
H	-2.26553300	3.94831700	0.01656300
H	-1.32511600	4.37038600	1.47177800
C	1.72206400	-1.74012500	1.55495100
C	2.58484600	-0.78359800	2.36267800
H	2.39251100	-0.99377800	3.42355900
H	3.64813900	-1.01116100	2.18956800
C	2.33339000	0.70655300	2.12706200
H	2.97745400	1.30672300	2.78333600
H	1.29604200	0.92388800	2.41507400

C	2.54503000	1.15538800	0.67157500
H	1.98958900	0.47337700	0.02046800
H	2.11371800	2.15862600	0.54018900
C	3.99507900	1.20736700	0.24867100
C	4.62892300	0.09574700	-0.31880900
C	4.73910900	2.37709400	0.42853200
C	5.96763700	0.15983100	-0.69939800
H	4.06325800	-0.82448600	-0.43131300
C	6.07759200	2.44261400	0.05191500
H	4.25821300	3.24885200	0.86789800
C	6.69643400	1.33244900	-0.51751500
H	6.44473200	-0.71343500	-1.13539900
H	6.63650500	3.36223900	0.19860200
H	7.73944300	1.38112500	-0.81519000
C	-1.49164700	-3.11283500	0.54318100
H	-1.08728600	-4.06253300	0.92142100
C	-2.98136600	-3.11636300	0.84666900
H	-3.47304100	-3.87392700	0.21564700
H	-3.11295700	-3.44037500	1.88808000
C	-3.68371000	-1.76762700	0.66481800
H	-3.31311600	-1.06664600	1.42190100
H	-4.76095100	-1.88862500	0.84004000
C	-3.43976000	-1.16567400	-0.72247000
H	-2.36529500	-1.15621500	-0.92410600
H	-3.87945300	-1.83070400	-1.47952200

C	-3.98385700	0.23079700	-0.90829300
C	-5.30013800	0.56441300	-0.56707900
C	-3.18056400	1.22709800	-1.47330500
C	-5.80141100	1.84381500	-0.79270300
H	-5.94566200	-0.19329800	-0.13073000
C	-3.68112100	2.50551800	-1.71590000
H	-2.15287800	0.98024400	-1.73607100
C	-4.99422300	2.82157800	-1.37265500
H	-6.82834700	2.07602800	-0.52557900
H	-3.04788800	3.25339700	-2.18685300
H	-5.38836300	3.81506300	-1.56476800
F	-1.36223700	-3.23379000	-0.88941800
H	1.86174400	-2.73404100	2.00252300
F	2.35097000	-1.88614400	0.25096800

2a'-conformer-22



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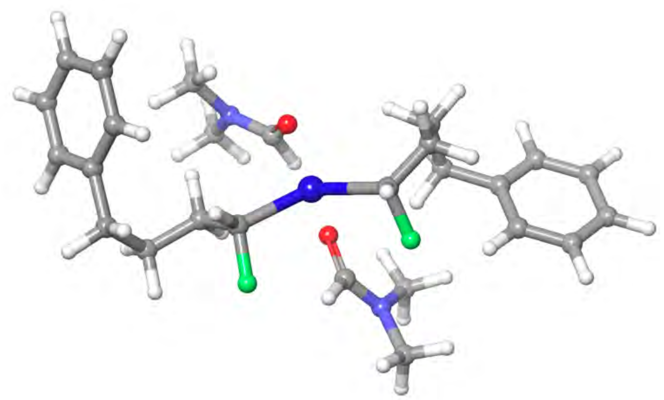
O	-0.52680700	0.51145000	0.06435200
C	-1.48815600	1.29304700	-0.03706200
N	-1.69634400	2.31890300	0.78470700
H	-2.24649800	1.15930600	-0.81787700
O	1.56446900	-1.20054500	-1.27604600
C	1.51054800	-1.51435200	-0.07911000
N	1.67977000	-2.76377500	0.36783100
H	1.30270000	-0.77102300	0.70278500
C	-2.71504400	3.30320200	0.49445500
H	-2.25056500	4.23919600	0.16509100
H	-3.36183700	2.92967600	-0.30137900
H	-3.32340100	3.48717500	1.38599500
C	-0.76195500	2.61446300	1.84995300
H	-0.09922300	1.75831400	1.97829100

H	-0.16745700	3.50120600	1.59888400
H	-1.31461600	2.79941400	2.77708600
C	1.44410400	-3.10138400	1.75513700
H	2.33277400	-3.56817500	2.19456800
H	1.21011500	-2.19442600	2.31530500
H	0.60107500	-3.79841600	1.83021700
C	1.92862700	-3.85739400	-0.55187600
H	2.12139000	-3.44327700	-1.54045600
H	2.79584800	-4.43325700	-0.21305300
H	1.05643000	-4.52003700	-0.59647000
C	0.71060600	2.00311400	-2.24301600
C	1.78213800	2.38132500	-1.23439800
H	1.86251900	3.47800100	-1.14906000
H	1.48676800	2.00762100	-0.24374600
C	3.14406500	1.80684400	-1.61387400
H	3.50643400	2.30257000	-2.52309200
H	3.04170100	0.73985700	-1.85106600
C	4.19667100	1.96998300	-0.50430500
H	5.18976600	1.73996100	-0.90681800
H	4.21895600	3.01741500	-0.17892200
C	3.93442300	1.07579400	0.68360100
C	3.18032800	1.51244400	1.77729900
C	4.42919000	-0.23237100	0.70351500
C	2.93843100	0.67470600	2.86473200
H	2.79014100	2.52766400	1.77858600

C	4.19923200	-1.07207900	1.79007600
H	5.01065900	-0.58980700	-0.14336100
C	3.45691400	-0.61858100	2.87924200
H	2.36138400	1.03990200	3.70965100
H	4.60756000	-2.07950500	1.78964900
H	3.29005500	-1.26553900	3.73596800
C	-1.46663000	-1.16515100	-2.55238000
H	-1.56456600	-1.26749500	-3.64147800
C	-1.41567500	-2.56906200	-1.96356500
H	-2.16919300	-3.23334700	-2.41771600
H	-0.43312300	-2.98908500	-2.22177500
C	-1.60842200	-2.60590500	-0.44128900
H	-1.01485900	-1.80587500	0.01391800
H	-1.22281700	-3.55734200	-0.04996300
C	-3.08787800	-2.43824400	-0.01077200
H	-3.71586200	-2.35639100	-0.90077300
H	-3.41719100	-3.33921400	0.52247300
C	-3.35971400	-1.24945100	0.88160800
C	-2.65073700	-1.07142600	2.07465800
C	-4.35056900	-0.31864500	0.56000700
C	-2.93778600	-0.01425200	2.93259300
H	-1.86457900	-1.77820000	2.33391900
C	-4.65349200	0.73481400	1.42169800
H	-4.88702600	-0.42700300	-0.37877800
C	-3.95211400	0.88790600	2.61464600

H	-2.37861200	0.09950600	3.85740500
H	-5.43932300	1.43778000	1.15816400
H	-4.19079000	1.70429000	3.29118200
F	-2.71583600	-0.58523000	-2.12967600
H	1.02755200	2.34706000	-3.23650900
F	-0.43164400	2.81594500	-1.91512700

2a’-conformer-23



Zn	-0.07544200	0.27389100	-0.95066300
O	0.75299800	0.76205400	1.01894500
C	1.33019500	1.84951400	0.85274500
N	2.43795800	2.21801200	1.49856800
H	0.92451900	2.60216700	0.16542300
O	-0.85967600	-1.52473200	-0.15674700
C	-1.07993600	-1.56479700	1.06175200
N	-2.20128800	-2.04216400	1.60576900

H	-0.34220400	-1.18921400	1.78359600
C	3.15593600	3.41619200	1.11182700
H	4.11741900	3.14476600	0.66238100
H	2.57018900	3.97307700	0.37872700
H	3.33670400	4.04982700	1.98584800
C	3.09465100	1.33444000	2.44580900
H	2.42791200	0.50144900	2.66462800
H	4.02991900	0.94981800	2.02218900
H	3.31525500	1.88678300	3.36469500
C	-3.32506900	-2.44561400	0.77463200
H	-4.16874500	-1.76317700	0.93269600
H	-3.02069100	-2.40399800	-0.27005000
H	-3.63309200	-3.46334900	1.03413800
C	-2.43892200	-1.95430600	3.03243300
H	-1.53026300	-1.62273100	3.53848900
H	-3.24233400	-1.23693200	3.23508800
H	-2.72978400	-2.93228800	3.42776100
C	1.66129800	0.18762700	-2.02060000
C	2.47694100	-1.08345900	-2.19984100
H	2.00058700	-1.65245200	-3.01026800
H	3.48812000	-0.82836400	-2.55314600
C	2.57056300	-1.99365300	-0.97361200
H	3.11306400	-2.91295100	-1.23215700
H	1.55355000	-2.28784500	-0.68452200
C	3.24581100	-1.33843800	0.24243000

H	2.75815900	-0.37824500	0.42210700
H	3.06593900	-1.96283100	1.12750400
C	4.73491600	-1.14001400	0.08517900
C	5.25846100	0.03912100	-0.45810200
C	5.62643500	-2.14543800	0.47137300
C	6.63411600	0.20559300	-0.60371800
H	4.56812400	0.81019200	-0.78833300
C	7.00104600	-1.98305800	0.32496800
H	5.23285100	-3.06663100	0.89636200
C	7.51047800	-0.80292900	-0.21166300
H	7.02244200	1.12647800	-1.02970900
H	7.67567800	-2.77621300	0.63418500
H	8.58245800	-0.67179300	-0.32439100
C	-1.68460900	1.51213900	-0.78954200
H	-2.33204900	1.59076200	-1.67478600
C	-2.54592400	1.18983200	0.42026200
H	-2.95315200	0.17907200	0.28220900
H	-1.90099100	1.14959700	1.31144800
C	-3.70141400	2.15981400	0.68596400
H	-3.30582400	3.18052800	0.71710800
H	-4.14150500	1.95268000	1.67131500
C	-4.81415600	2.08381000	-0.37329500
H	-5.59412500	2.81382300	-0.12649200
H	-4.41015200	2.37218700	-1.34932700
C	-5.42945300	0.70732900	-0.47014800

C	-5.12323200	-0.15371000	-1.52741100
C	-6.30071300	0.24824200	0.52419400
C	-5.68015300	-1.42946700	-1.60040500
H	-4.44184500	0.18490300	-2.30464300
C	-6.86074300	-1.02496600	0.45762000
H	-6.55267600	0.90735600	1.35252200
C	-6.55313600	-1.86949000	-0.60852900
H	-5.43379700	-2.07794500	-2.43623600
H	-7.54579500	-1.35556100	1.23310900
H	-6.99500000	-2.85959500	-0.66722100
F	-1.19090600	2.84565900	-0.57834200
H	1.52373200	0.62006900	-3.02036200
F	2.50724900	1.16261300	-1.35564500