

# The Role of the *gem*-Difluoro Miety in the Tandem Ring-Closing Metathesis-Olefin Isomerization: Regioselective Preparation of Unsaturated Lactams

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## SUPPORTING INFORMATION

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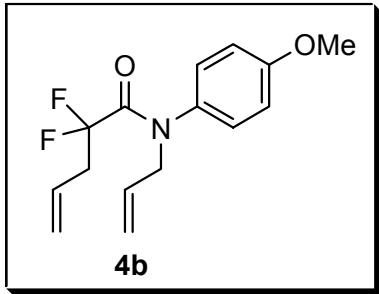
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## General methods.

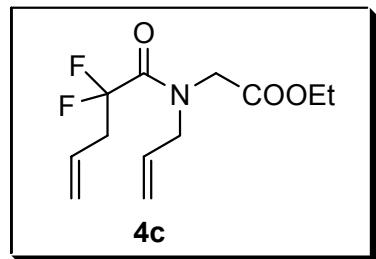
All reactions were carried out under argon or nitrogen atmosphere. The solvents were purified prior to use: THF and Et<sub>2</sub>O were distilled from sodium/benzophenone; CH<sub>2</sub>Cl<sub>2</sub> and CCl<sub>4</sub> were distilled from calcium hydride. All reagents were used as received. The reactions were monitored with the aid of thin-layer chromatography (TLC) using 0.25-mm precoated silica gel plates. Visualization was carried out with UV light and aqueous ceric ammonium molybdate solution or potassium permanganate stain. Flash column chromatography was performed with the indicated solvents on silica gel 60 (particle size 0.040-0.063 mm). Melting points are uncorrected. Chemical shifts are given in ppm ( $\delta$ ), referenced to the residual proton resonances of the solvents or fluorotrichloromethane in <sup>19</sup>F NMR experiments. Coupling constants ( $J$ ) are given in Hertz (Hz). The letters m, s, d, t, and q stand for multiplet, singlet, doublet, triplet, and quartet, respectively. The letters br indicate that the signal is broad.

2,2-Difluoro-4-pentenoic acid,<sup>1</sup> tertiary amides **8**,<sup>2</sup> **13**,<sup>3,4</sup> **22**,<sup>4</sup> and compounds **25**,<sup>4</sup> ( $\pm$ )-**26**,<sup>5</sup> **28**,<sup>6</sup> **30**,<sup>7</sup> ( $\pm$ )-**32**,<sup>8</sup> **34**, (*R*)-**37**,<sup>9</sup> and **39**<sup>10</sup> have been previously described.

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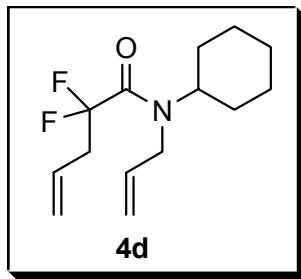


**N-Allyl-2,2-difluoro-N-(4-methoxyphenyl)-4-pentenamide (4b).** Flash chromatography [*n*-hexane-EtOAc (7:1)] ( $R_f = 0.50$ ) afforded **n** as a pale yellow oil (66% overall yield).  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.73 (td,  $J = 17.1, 7.0$  Hz, 2H), 3.74 (s, 3H), 4.16 (d,  $J = 6.4$  Hz, 2H), 5.00-5.14 (m, 4H), 5.62-5.82 (m, 2H), 6.80 (d,  $J = 8.9$  Hz, 2H), 7.03 (d,  $J = 9.0$  Hz, 2H);  $^{13}\text{C-NMR}$  ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  39.7 (t,  $^2J_{\text{CF}} = 23.9$  Hz), 54.9 (t), 55.3 (q), 113.8 (d), 117.8 (t,  $^1J_{\text{CF}} = 256.2$  Hz), 118.9 (t), 120.9 (t), 128.1 (t,  $^3J_{\text{CF}} = 5.5$  Hz), 129.5 (d), 131.6 (d), 133.2 (s), 159.1 (s), 162.8 (t,  $^2J_{\text{CF}} = 28.5$  Hz);  $^{19}\text{F-NMR}$  ( $\text{CDCl}_3$ , 282.4 MHz)  $\delta$  -96.7 (t,  $J_{\text{FH}} = 17.0$  Hz, 2F); HRMS (EI $^+$ ) calcd for  $\text{C}_{15}\text{H}_{17}\text{F}_2\text{NO}_2$  ( $\text{M}^+$ ): 281.1227, found: 281.1218.

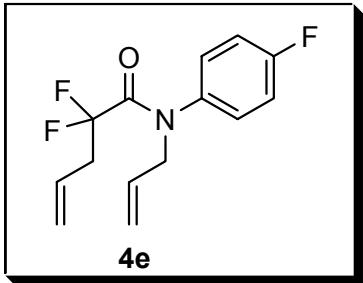


**N-Allyl-2,2-difluoro-N-[ethoxycarbonylmethyl]-4-pentenamide (4c).** Flash chromatography [*n*-hexane-EtOAc (7:1)] ( $R_f = 0.30$ ) afforded **4c** as a pale yellow oil (66% overall yield).  $^1\text{H}$ ,  $^{13}\text{C}$ , and  $^{19}\text{F-NMR}$  showed the presence of two rotamers around the amide bond in a 2:1 ratio.  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  1.20 (t,  $J = 7.2$  Hz, 3H), 2.86 (td,  $J = 18.3, 7.0$  Hz, 2H), 3.94-4.16 (m, 6H), 5.16-5.20 (m, 4H), 5.69-5.80 (m, 2H);  $^{13}\text{C-NMR}$  ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  14.0 (q), 39.0 (t,  $^2J_{\text{CF}} = 23.9$  Hz), 39.2 (t,  $^2J_{\text{CF}} = 23.6$  Hz), 47.5 (t),

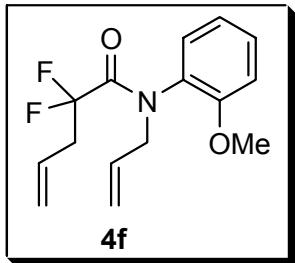
47.6 (t,  $^4J_{\text{CF}} = 6.6$  Hz), 50.4 (t), 51.3 (t,  $^4J_{\text{CF}} = 6.3$  Hz), 61.2 (t), 61.4 (t), 117.9 (t,  $^1J_{\text{CF}} = 254.7$  Hz), 118.3 (t,  $^1J_{\text{CF}} = 255.6$  Hz), 118.6 (t), 118.9 (t), 121.1 (t), 127.8 (t,  $^3J_{\text{CF}} = 5.5$  Hz), 127.9 (t,  $^3J_{\text{CF}} = 5.2$  Hz), 131.3 (d), 132.5 (d), 163.2 (t,  $^2J_{\text{CF}} = 29.6$  Hz), 163.6 (t,  $^2J_{\text{CF}} = 29.9$  Hz), 163.7 (t), 168.7 (s);  $^{19}\text{F}$ -NMR ( $\text{CDCl}_3$ , 282.4 MHz)  $\delta$  -99.9 (t,  $J_{\text{FH}} = 18.6$  Hz, 2F, minor rotamer), -99.7 (t,  $J_{\text{FH}} = 18.6$  Hz, 2F, major rotamer); HRMS (EI $^+$ ) calcd for  $\text{C}_{12}\text{H}_{17}\text{F}_2\text{NO}_3$  ( $\text{M}^+$ ): 261.1177, found: 261.1184.



**N-Allyl-N-cyclohexyl-2,2-difluoro-4-pentenamide (4d).** Prepared directly in one step from 2,2-difluoro-4-pentenoic acid with allylcyclohexylamine as starting material instead of a primary amine. Flash chromatography [*n*-hexane-EtOAc (10:1)] ( $R_f = 0.40$ ) afforded **4d** as a colorless oil (87% yield).  $^1\text{H}$ ,  $^{13}\text{C}$ , and  $^{19}\text{F}$ -NMR showed the presence of two rotamers around the amide bond in a 2:1 ratio.  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  0.98-1.77 (m, 11H), 2.86 (td,  $J = 18.3, 7.0$  Hz, 2H), 3.83 (d,  $J = 5.5$  Hz, 2H, major rotamer), 4.01 (d,  $J = 5.6$  Hz, 2H, minor rotamer), 5.05-5.22 (m, 4H), 5.69-5.86 (m, 2H);  $^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  25.2 (t), 25.6 (t), 25.8 (t), 30.0 (t), 31.7 (t), 39.6 (t,  $^2J_{\text{CF}} = 24.2$  Hz), 45.0 (t), 47.0 (t,  $^4J_{\text{CF}} = 6.3$  Hz), 56.7 (t,  $^4J_{\text{CF}} = 6.6$  Hz), 57.4 (d), 116.2 (t), 116.5 (t), 118.5 (t,  $^1J_{\text{CF}} = 255.9$  Hz), 120.7 (t), 128.6 (t,  $^3J_{\text{CF}} = 5.5$  Hz), 133.9 (d), 136.2 (d), 162.6 (t,  $^2J_{\text{CF}} = 29.0$  Hz), 162.8 (t,  $^2J_{\text{CF}} = 28.8$  Hz);  $^{19}\text{F}$ -NMR ( $\text{CDCl}_3$ , 282.4 MHz)  $\delta$  -99.7 (t,  $J_{\text{FH}} = 18.0$  Hz, 2F, major rotamer), -99.2 (t,  $J_{\text{FH}} = 18.0$  Hz, 2F, minor rotamer); HRMS (EI $^+$ ) calcd for  $\text{C}_{14}\text{H}_{21}\text{F}_2\text{NO}$  ( $\text{M}^+$ ): 257.1591, found: 257.1591.

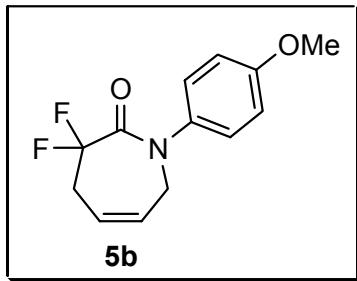


**N-Allyl-2,2-difluoro-N-(4-fluorophenyl)-4-pentenamide (4e).** Flash chromatography [*n*-hexane-EtOAc (15:1)] ( $R_f = 0.50$ ) afforded **4e** as a yellow oil (62% overall yield).  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.74 (td,  $J = 17.1, 7.0$  Hz, 2H), 4.16 (d,  $J = 6.4$  Hz, 2H), 5.03-5.14 (m, 4H), 5.60-5.81 (m, 2H), 6.94-7.11 (m, 4H);  $^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  39.5 (t,  $^2J_{\text{CF}} = 23.9$  Hz), 59.8 (t), 115.7 (d,  $^2J_{\text{CF}} = 23.0$  Hz), 117.9 (t,  $^1J_{\text{CF}} = 256.2$  Hz), 119.2 (t), 121.1 (t), 128.0 (t,  $^3J_{\text{CF}} = 5.5$  Hz), 130.2 (d,  $^3J_{\text{CF}} = 9.2$  Hz), 131.3 (d), 136.5 (s), 162.0 (d,  $^1J_{\text{CF}} = 248.4$  Hz), 162.7 (t,  $^2J_{\text{CF}} = 28.9$  Hz);  $^{19}\text{F}$ -NMR ( $\text{CDCl}_3$ , 282.4 MHz)  $\delta$  -113.5-(-113.4) (m, 1F), -96.5 (t,  $J_{\text{FH}} = 17.0$  Hz, 2F); HRMS (EI $^+$ ) calcd for  $\text{C}_{14}\text{H}_{14}\text{F}_3\text{NO} (\text{M}^+)$ : 269.1027, found: 269.1025.

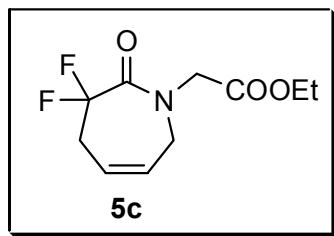


**N-Allyl-2,2-difluoro-N-(2-methoxyphenyl)-4-pentenamide (4f).** Flash chromatography [*n*-hexane-EtOAc (15:1)] ( $R_f = 0.40$ ) afforded **4f** as a pale yellow oil (72% overall yield).  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.70 (td,  $J = 17.3, 7.0$  Hz, 2H), 3.64-3.72 (m, 1H), 3.73 (s, 3H), 4.58 (dd,  $J = 14.5, 5.6$  Hz, 1H), 4.95-5.11 (m, 4H), 5.60-5.77 (m, 2H), 6.83-6.86 (m, 2H), 7.03-7.05 (m, 1H), 7.20-7.26 (m, 1H);  $^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  39.5 (t,  $^2J_{\text{CF}} = 23.9$  Hz), 53.2 (t), 55.3 (q), 111.2 (d), 117.5 (t,  $^1J_{\text{CF}} = 255.9$  Hz), 118.3 (t), 119.8 (d), 120.6 (t), 128.1 (t,  $^3J_{\text{CF}} = 5.2$  Hz), 128.8 (s), 129.6 (d), 130.2 (d), 132.0 (d), 132.0 (d).

155.0 (s), 163.3 (t,  $^2J_{\text{CF}}= 28.2$  Hz);  $^{19}\text{F}$ -NMR ( $\text{CDCl}_3$ , 282.4 MHz)  $\delta$  -101.3 (ddd,  $J_{\text{FF}}= 267.6$  Hz,  $J_{\text{FH}}= 18.6$ , 15.0 Hz, 1F), -97.8 (ddd,  $J_{\text{FF}}= 268.1$  Hz,  $J_{\text{FH}}= 18.3$ , 16.2 Hz, 1F); HRMS (EI $^+$ ) calcd for  $\text{C}_{15}\text{H}_{17}\text{F}_2\text{NO}_2$  ( $\text{M}^+$ ): 281.1227, found: 281.1224.

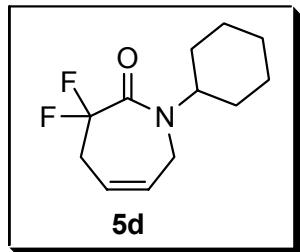


**3,3-Difluoro-1-(4-methoxyphenyl)-1,3,4,7-tetrahydro-2*H*-2-azepinone (5b).** Flash chromatography [*n*-hexane-EtOAc (7:2)] ( $R_f= 0.20$ ) afforded **5b** as a white solid (89% yield). mp: 141-143 °C.  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.87 (tq,  $J= 16.4$ , 2.1 Hz, 2H), 3.74 (s, 3H), 4.24-4.26 (m, 2H), 5.67-5.71 (m, 1H), 5.88-5.92 (m, 1H), 6.83 (d,  $J= 9.1$  Hz, 2H), 7.05 (d,  $J= 9.1$  Hz, 2H);  $^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  34.9 (t,  $^2J_{\text{CF}}= 26.5$  Hz), 49.8 (t,  $^4J_{\text{CF}}= 5.2$  Hz), 55.4 (q), 114.5 (d), 116.6 (t,  $^1J_{\text{CF}}= 248.4$  Hz), 124.7 (t,  $^3J_{\text{CF}}= 6.0$  Hz), 125.4 (d), 127.0 (d), 136.4 (s), 158.5 (s), 163.8 (t,  $^2J_{\text{CF}}= 28.5$  Hz);  $^{19}\text{F}$ -NMR ( $\text{CDCl}_3$ , 282.4 MHz)  $\delta$  -101.3 (t,  $J_{\text{FH}}= 16.5$  Hz, 2F); HRMS (EI $^+$ ) calcd for  $\text{C}_{13}\text{H}_{13}\text{F}_2\text{NO}_2$  ( $\text{M}^+$ ): 253.0914, found: 253.0909. Anal. calcd for  $\text{C}_{13}\text{H}_{13}\text{F}_2\text{NO}_2$ : C, 61.66; H, 5.17; N, 5.53; found: C, 61.56; H, 5.25; N, 5.55.

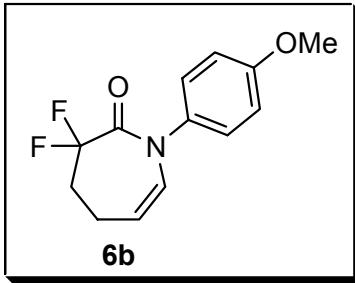


**3,3-Difluoro-1-((ethoxycarbonyl)methyl)-1,3,4,7-tetrahydro-2*H*-2-azepinone (5c).** Flash chromatography [*n*-hexane-EtOAc (3:1)] ( $R_f= 0.20$ ) afforded **5c** as a brown oil (70%

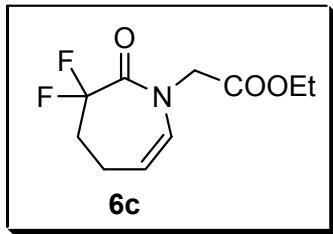
yield).  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  1.21 (t,  $J= 7.1$  Hz, 3H), 2.79 (tq,  $J= 16.0, 2.1$  Hz, 2H), 3.96-3.98 (m, 2H), 4.13 (q,  $J= 7.2$  Hz, 2H), 4.18 (s, 2H), 5.58-5.63 (m, 1H), 5.77-5.82 (m, 1H);  $^{13}\text{C-NMR}$  ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  14.1 (q), 34.6 (t,  $^2J_{\text{CF}}= 26.2$  Hz), 47.8 (t,  $^4J_{\text{CF}}= 4.6$  Hz), 51.2 (t), 61.5 (t), 116.2 (t,  $^1J_{\text{CF}}= 247.8$  Hz), 123.7 (t,  $^3J_{\text{CF}}= 6.0$  Hz), 124.8 (d), 164.5 (t,  $^2J_{\text{CF}}= 29.3$  Hz), 168.1 (s);  $^{19}\text{F-NMR}$  ( $\text{CDCl}_3$ , 282.4 MHz)  $\delta$  -102.0 (t,  $J_{\text{FH}}= 15.9$  Hz, 2F); HRMS (EI $^+$ ) calcd for  $\text{C}_{10}\text{H}_{13}\text{F}_2\text{NO}_3$  ( $\text{M}^+$ ): 233.0864, found: 233.0852.



**1-Cyclohexyl-3,3-difluoro-1,3,4,7-tetrahydro-2H-2-azepinone (5d).** Flash chromatography [*n*-hexane-EtOAc (7:1)] ( $R_f= 0.20$ ) afforded **5d** as a brown solid (82% yield). mp: 73-75 °C.  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  1.03-1.37 (m, 5H), 1.57-1.76 (m, 5H), 2.73 (tq,  $J= 16.6, 2.1$  Hz, 2H), 3.78-3.81 (m, 2H), 4.39-4.46 (m, 1H), 5.53-5.57 (m, 1H), 5.59-5.81 (m, 1H);  $^{13}\text{C-NMR}$  ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  25.3 (t), 25.3 (t), 29.9 (t), 34.8 (t,  $^2J_{\text{CF}}= 26.5$  Hz), 38.9 (t,  $^4J_{\text{CF}}= 5.5$  Hz), 54.0 (d), 116.6 (t,  $^1J_{\text{CF}}= 247.8$  Hz), 124.8 (t,  $^3J_{\text{CF}}= 6.0$  Hz), 125.9 (d), 163.5 (t,  $^2J_{\text{CF}}= 27.6$  Hz);  $^{19}\text{F-NMR}$  ( $\text{CDCl}_3$ , 282.4 MHz)  $\delta$  -100.7 (t,  $J_{\text{FH}}= 16.5$  Hz, 2F); HRMS (EI $^+$ ) calcd for  $\text{C}_{12}\text{H}_{17}\text{F}_2\text{NO}$  ( $\text{M}^+$ ): 229.1278, found: 229.1283. Anal. calcd for  $\text{C}_{12}\text{H}_{17}\text{F}_2\text{NO}$ : C, 62.87; H, 7.47; N, 6.11; found: C, 62.84; H, 7.39; N, 6.18.

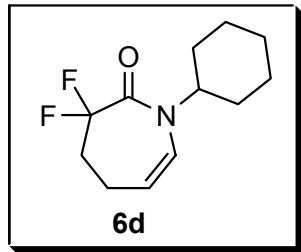


**3,3-Difluoro-1-(4-methoxyphenyl)-1,3,4,5-tetrahydro-2H-2-azepinone (6b).** Flash chromatography [*n*-hexane-EtOAc (7:1)] ( $R_f = 0.10$ ) afforded **6b** as a pale brown solid (93% yield). mp: 94-96 °C.  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.31-2.37 (m, 2H), 2.51-2.66 (m, 2H), 3.74 (s, 3H), 5.58 (dt,  $J = 8.1, 6.7$  Hz, 1H), 5.96 (d,  $J = 8.3$  Hz, 1H), 6.84 (d,  $J = 9.0$  Hz, 2H), 7.09 (d,  $J = 9.0$  Hz, 2H);  $^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  19.8 (t,  $^3J_{\text{CF}} = 5.5$  Hz), 40.2 (t,  $^2J_{\text{CF}} = 23.9$  Hz), 55.4 (q), 114.4 (d), 117.0 (t,  $^1J_{\text{CF}} = 250.7$  Hz), 117.9 (d), 127.1 (d), 130.7 (d), 132.8 (s), 158.7 (s), 164.6 (t,  $^2J_{\text{CF}} = 29.0$  Hz);  $^{19}\text{F}$ -NMR ( $\text{CDCl}_3$ , 282.4 MHz)  $\delta$  -96.0 (t,  $J_{\text{FH}} = 16.0$  Hz, 2F); HRMS (EI $^+$ ) calcd for  $\text{C}_{13}\text{H}_{13}\text{F}_2\text{NO}_2$  ( $\text{M}^+$ ): 253.0914, found: 253.0913. Anal. calcd for  $\text{C}_{13}\text{H}_{13}\text{F}_2\text{NO}_2$ : C, 61.66; H, 5.17; N, 5.53; found: C, 61.55; H, 5.11; N, 5.41.

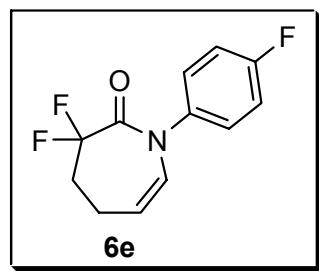


**3,3-Difluoro-1-((ethoxycarbonyl)methyl)-1,3,4,5-tetrahydro-2H-2-azepinone (6c).** Flash chromatography [*n*-hexane-EtOAc (3:1)] ( $R_f = 0.30$ ) afforded **6c** as a pale brown oil (72% yield).  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  1.22 (t,  $J = 7.2$  Hz, 3H), 2.34-2.45 (m, 2H), 2.47-2.58 (m, 2H), 4.13 (s, 2H), 4.14 (q,  $J = 7.1$  Hz, 2H), 5.50 (dt,  $J = 8.5, 6.3$  Hz, 1H), 5.81 (dt,  $J = 8.5, 1.1$  Hz, 1H);  $^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  14.0 (q), 20.0 (t,  $^3J_{\text{CF}} = 5.6$  Hz), 38.8 (t,  $^2J_{\text{CF}} = 23.9$  Hz), 49.5 (t), 61.6 (t), 116.7 (t,  $^1J_{\text{CF}} = 249.8$  Hz), 118.6 (d), 129.2

(d), 164.7 (t,  ${}^2J_{\text{CF}} = 29.9$  Hz), 167.8 (s);  ${}^{19}\text{F}$ -NMR ( $\text{CDCl}_3$ , 282.4 MHz)  $\delta$  -97.2 (t,  $J_{\text{FH}} = 15.5$  Hz, 2F); HRMS (EI $^+$ ) calcd for  $\text{C}_{10}\text{H}_{13}\text{F}_2\text{NO}_3$  ( $\text{M}^+$ ): 233.0864, found: 233.0862.

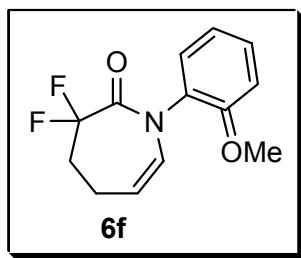


**1-Cyclohexyl-3,3-difluoro-1,3,4,5-tetrahydro-2H-2-azepinone** (6d). Flash chromatography [*n*-hexane-EtOAc (7:1)] ( $R_f = 0.30$ ) afforded **6d** as a pale brown oil (95% yield).  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  0.95-1.10 (m, 1H), 1.25-1.45 (m, 4H), 1.59-1.75 (m, 5H), 2.13-2.21 (m, 2H), 2.43-2.59 (m, 2H), 4.30-4.38 (m, 1H), 5.62 (dt,  $J = 8.3, 7.1$  Hz, 1H), 5.98 (d,  $J = 8.1$  Hz, 1H);  $^{13}\text{C-NMR}$  ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  19.6 (t,  $^3J_{\text{CF}} = 5.2$  Hz), 25.3 (t), 25.5 (t), 30.2 (t), 41.2 (t,  $^2J_{\text{CF}} = 22.0$  Hz), 54.3 (d), 116.9 (t,  $^1J_{\text{CF}} = 250.1$  Hz), 119.8 (d), 126.7 (d), 164.0 (t,  $^2J_{\text{CF}} = 28.5$  Hz);  $^{19}\text{F-NMR}$  ( $\text{CDCl}_3$ , 282.4 MHz)  $\delta$  -94.9 (t,  $J_{\text{FH}} = 16.0$  Hz, 2F); HRMS (EI $^+$ ) calcd for  $\text{C}_{12}\text{H}_{17}\text{F}_2\text{NO} (\text{M}^+)$ : 229.1278, found: 229.1275.



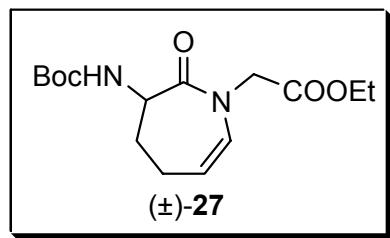
**3,3-Difluoro-1-(4-fluorophenyl)-1,3,4,5-tetrahydro-2*H*-2-azepinone (6e).** Flash chromatography [*n*-hexane-EtOAc (5:1)] ( $R_f = 0.20$ ) afforded **6e** as a pale brown solid (70% yield). mp: 76–78 °C.  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.32–2.39 (m, 2H), 2.53–2.68 (m, 2H), 5.64 (dt,  $J = 8.3, 6.8$  Hz, 1H), 5.98 (d,  $J = 8.3$  Hz, 1H), 7.00–7.14 (m, 2H), 7.15–7.19 (m, 2H);  $^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  19.8 (t,  $^3J_{\text{CF}} = 5.5$  Hz), 40.1 (t,  $^2J_{\text{CF}} = 23.9$  Hz), 116.1 (d,  $^2J_{\text{CF}} = 23.0$  Hz), 117.0 (t,  $^1J_{\text{CF}} = 250.7$  Hz), 118.6 (d), 127.7 (d,  $^3J_{\text{CF}} = 8.6$

Hz), 130.3 (d), 135.9 (d,  $^4J_{\text{CF}} = 2.9$  Hz), 161.4 (d,  $^1J_{\text{CF}} = 247.8$  Hz), 164.5 (t,  $^2J_{\text{CF}} = 29.6$  Hz);  $^{19}\text{F}$ -NMR ( $\text{CDCl}_3$ , 282.4 MHz)  $\delta$  -114.2-(-114.1) (m, 1F), -96.0 (t,  $J_{\text{FH}} = 16.0$  Hz, 2F); HRMS (EI $^+$ ) calcd for  $\text{C}_{12}\text{H}_{10}\text{F}_3\text{NO}$  ( $\text{M}^+$ ): 241.0714, found: 241.0715. Anal. calcd for  $\text{C}_{12}\text{H}_{10}\text{F}_3\text{NO}$ : C, 59.75; H, 4.18; N, 5.81, found: C, 59.76; H, 4.22; N, 5.82.



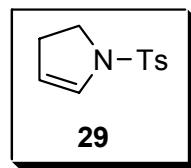
**3,3-Difluoro-1-(2-methoxyphenyl)-1,3,4,5-tetrahydro-2*H*-2-azepinone (6f).** Flash chromatography [*n*-hexane-EtOAc (3:1)] ( $R_f = 0.30$ ) afforded **6f** as a brown solid (91% yield). mp: 58-60 °C.  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.38-2.49 (m, 2H), 2.51-2.62 (m, 2H), 3.74 (s, 3H), 5.43 (dt,  $J = 8.5, 6.4$  Hz, 1H), 5.87 (d,  $J = 8.3$  Hz, 1H), 6.89-6.92 (m, 2H), 6.93-7.06 (m, 1H), 7.08-7.29 (m, 1H);  $^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  20.0 (t,  $^3J_{\text{CF}} = 5.6$  Hz), 39.1 (t,  $^2J_{\text{CF}} = 23.9$  Hz), 55.8 (q), 112.2 (d), 116.5 (d), 116.9 (t,  $^1J_{\text{CF}} = 249.8$  Hz), 121.0 (d), 128.4 (d), 128.9 (s), 129.7 (d), 130.4 (d), 154.7 (s), 164.0 (t,  $^2J_{\text{CF}} = 29.6$  Hz);  $^{19}\text{F}$ -NMR ( $\text{CDCl}_3$ , 282.4 MHz)  $\delta$  -105.4-(-105.2) (m, 2F); HRMS (EI $^+$ ) calcd for  $\text{C}_{13}\text{H}_{13}\text{F}_2\text{NO}_2$  ( $\text{M}^+$ ): 253.0914, found: 253.0918. Anal. calcd for  $\text{C}_{13}\text{H}_{13}\text{F}_2\text{NO}_2$ : C, 61.66; H, 5.17; N, 5.53; found: C, 61.57; H, 5.09; N, 5.42.

**Synthesis of ( $\pm$ )-3-(*tert*-Butoxycarbonylamino)-1-((ethoxycarbonyl)methyl)-1,3,4,5-tetrahydro-2*H*-2-azepinone [( $\pm$ )-27].**



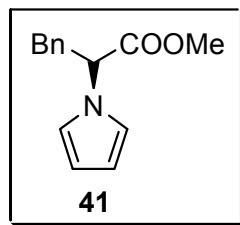
Prepared from ( $\pm$ )-26 with the general procedure described above for compounds 6 (*Method B*). Flash chromatography [*n*-hexane-EtOAc (4:1)] ( $R_f = 0.25$ ) afforded ( $\pm$ )-27 as a colorless oil (51% yield).  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  1.25 (t,  $J = 7.2$  Hz, 3H), 1.41 (s, 9H), 1.86-2.00 (m, 1H), 2.15-2.28 (m, 1H), 2.30-2.40 (m, 1H), 2.40-2.55 (m, 1H), 3.82 (d,  $J = 17.3$  Hz, 1H) 4.17 (q,  $J = 7.2$  Hz, 2H), 4.40-4.50 (m, 1H), 4.47 (d,  $J = 17.3$  Hz, 1H), 5.50-5.58 (m, 2H), 5.83 (dd,  $J = 8.5, 2.1$  Hz, 1H);  $^{13}\text{C-NMR}$  ( $\text{CDCl}_3$ , 75.5 MHz)  $\delta$  14.1 (q), 23.8 (t), 28.3 (q), 35.6 (t), 48.8 (t), 52.6 (d), 61.4 (t), 79.6 (s), 120.5 (d), 128.7 (d), 165.1 (s), 168.5 (s), 172.3 (s); HRMS (EI $^+$ ) calcd for  $\text{C}_{15}\text{H}_{25}\text{N}_2\text{O}_5$  ( $\text{M}+\text{H}^+$ ): 313.1763, found: 313.1821.

**Synthesis of 2,3-dihydro-1-tosyl-1*H*-pyrrole, (29).**



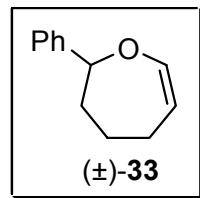
Prepared from 28 with the general procedure described above for compounds 6 (*Method B*). Flash chromatography [*n*-hexane-EtOAc (5:1)] ( $R_f = 0.40$ ) afforded 29 as a white solid (73% yield). Its spectroscopic data matched those previously reported.<sup>6</sup>

**Synthesis of (*R*)-methyl 3-phenyl-2-(1*H*-pyrrol-1-yl)propanoate, (**41**).**



Prepared from **30** with the general procedure described above for compounds **6** (*Method B*). Flash chromatography [*n*-hexane-EtOAc (5:1)] ( $R_f = 0.57$ ) afforded **41** as a brown oil (56% yield). Its spectroscopic data matched those previously reported.<sup>11</sup>

**Synthesis of ( $\pm$ )-2,3,4,5-tetrahydro-2-phenyloxepine, ( $\pm$ )-**33**.**

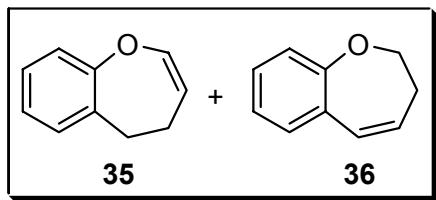


Prepared from ( $\pm$ )-**32** with the general procedure described above for compounds **6** (*Method B*). Flash chromatography [*n*-hexane-*i*-Pr<sub>2</sub>O (8:1)] ( $R_f = 0.40$ ) afforded ( $\pm$ )-**33** as a colorless oil (60% yield). Its spectroscopic data matched those previously reported.<sup>8</sup>

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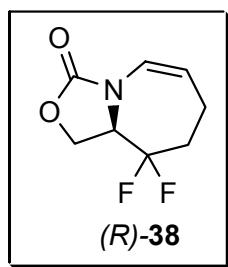
(11) Fang, Y.; Leysen, D; Ottenheijm, H. C. J. *Synt. Commun.* **1995**, 25(12), 1857-1861.

**Synthesis of 4,5-dihydrobenzo[*b*]oxepine (**35**), and 2,3-dihydrobenzo[*b*]oxepine (**36**).**



Prepared from **34** with the general procedure described above for compounds **6** (*Method B*). Flash chromatography [*n*-hexane-EtOAc (30:1)] ( $R_f = 0.40$ ) afforded **35** and **36** as a non separable 2:1 mixture of isomers (70% overall yield). Data for **35**:  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  2.57-2.62 (m, 2H), 4.16 (t,  $J = 4.9$  Hz, 2H), 5.89 (dt,  $J = 11.7, 4.5$  Hz, 1H), 6.25 (d,  $J = 11.7$  Hz, 1H), 6.87-7.11 (m, 4H). Data for **36**:  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  3.40-3.43 (m, 2H), 4.49-4.53 (m, 2H), 5.38-5.45 (m, 1H), 5.75-5.80 (m, 1H), 6.87-7.11 (m, 4H).

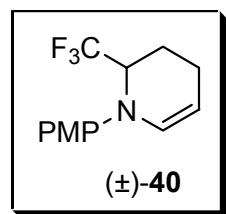
**Synthesis of (*R*)-9,9-difluoro-7,8,9,9a-tetrahydro-1*H*-oxazolo-[3,4-*a*]-3-azepinone [(*R*)-**38**].**



Prepared from (*R*)-**37** with the general procedure described above for compounds **6** (*Method B*). Flash chromatography [*n*-hexane-EtOAc (3:1)] ( $R_f = 0.30$ ) afforded (*R*)-**38** as a pale brown solid (85% yield). mp: 67-70 °C.  $[\alpha]_D^{25} = +40.8$  (*c* 0.5,  $\text{CHCl}_3$ );  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  1.92-2.35 (m, 4H), 4.03-4.16 (m, 1H), 4.40 (td,  $J = 9.2, 1.5$  Hz, 1H), 4.52 (dd,  $J = 9.2, 7.2$  Hz, 1H), 5.15-5.23 (m, 1H), 6.43 (dt,  $J = 9.1, 0.9$  Hz, 1H);  $^{13}\text{C-NMR}$

(CDCl<sub>3</sub>, 75.5 MHz) δ 19.5 (dd, <sup>3</sup>J<sub>CF</sub>= 7.9, 5.5 Hz), 34.3 (dd, <sup>2</sup>J<sub>CF</sub>= 25.0, 23.8 Hz), 60.4 (dd, <sup>2</sup>J<sub>CF</sub>= 40.8, 25.0 Hz), 61.5 (dd, <sup>3</sup>J<sub>CF</sub>= 7.9, 5.5 Hz), 114.0 (d), 121.5 (dd, <sup>1</sup>J<sub>CF</sub>= 250.5, 237.7 Hz), 126.1 (d), 155.8 (s); <sup>19</sup>F-NMR (CDCl<sub>3</sub>, 282.4 MHz) δ -101.5 (ddd, J<sub>FF</sub>= 249.5 Hz, J<sub>FH</sub>= 20.1, 8.8 Hz, 1F), -117.2 (ddd, J<sub>FF</sub>= 250.6 Hz, J<sub>FH</sub>= 21.4, 8.8 Hz, 1F); HRMS (EI<sup>+</sup>) calcd for C<sub>8</sub>H<sub>9</sub>F<sub>2</sub>NO<sub>2</sub> (M<sup>+</sup>): 189.0601, found: 189.0590. Anal. calcd for C<sub>8</sub>H<sub>9</sub>F<sub>2</sub>NO<sub>2</sub>: C, 50.80; H, 4.80; N, 7.40, found: C, 50.78; H, 4.87; N, 7.43.

**Synthesis of 2-(trifluoromethyl)-1,2,3,4-tetrahydro-1-(4-methoxyphenyl) pyridine, (±)-(40).**



Prepared from **39** with the general procedure described above for compounds **6** (*Method B*). Flash chromatography [*n*-hexane-EtOAc (5:1)] (*R*<sub>f</sub>= 0.41) afforded **40** as a yellow oil (75% yield). <sup>1</sup>H-NMR (CDCl<sub>3</sub>, 300 MHz) δ 1.70-2.20 (m, 4H), 3.76 (s, 3H), 4.05-4.17 (m, 1H), 4.80-4.87 (m, 1H), 6.29 (d, *J*= 9.1 Hz, 1H), 6.83 (d, *J*= 9.2 Hz, 2H), 6.98 (d, *J*= 9.2 Hz, 2H); <sup>13</sup>C-NMR (CDCl<sub>3</sub>, 75.5 MHz) δ 17.8 (t), 18.0 (t), 55.6 (q), 58.1 (q, <sup>2</sup>J<sub>CF</sub>= 29.5 Hz), 101.9 (d), 114.5 (d), 120.3 (d), 126.2 (q, <sup>1</sup>J<sub>CF</sub>= 283.7 Hz), 128.9 (d), 141.7 (s), 155.1 (s). <sup>19</sup>F-NMR (CDCl<sub>3</sub>, 282.4 MHz) δ -100.8 (3F).

### Energy calculations for compounds **5a**, **6a**, and **7**.

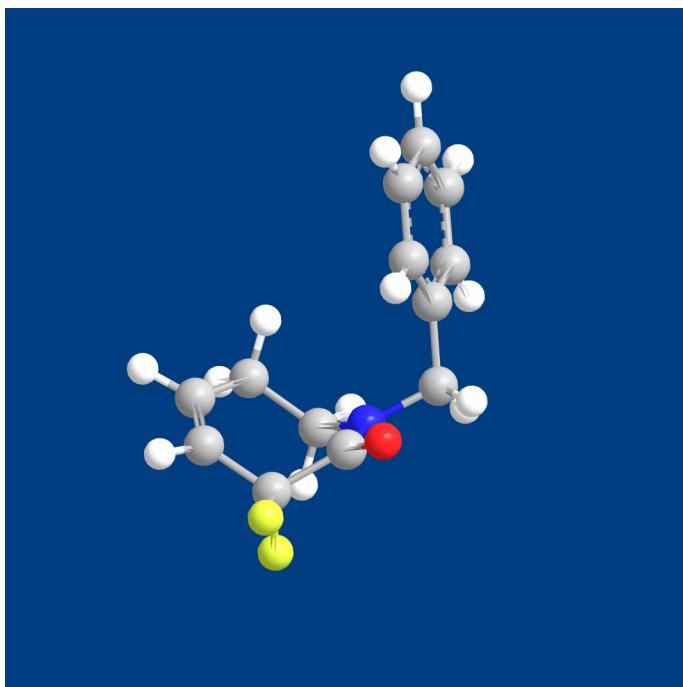
A previous conformational search for each of these compounds allowed for the identification of 4 low-energy conformers for each of **5a**, **6a**, and **7**, which were named as **5a-1**, **5a-2**, **5a-3**, **5a-4**, **6a-1**, **6a-2**, **6a-3**, **6a-4**, **7-1**, **7-2**, **7-3**, and **7-4**. Each one of these conformers was then submitted to an *ab-initio* energy minimization with the Gaussian 03 program.<sup>12</sup> The 6-31G\* basis set was used with default program parameters. The energy results for the energy minimization are as follows:

<b>Compound</b>	<b>Conformer</b>	<b>Absolute Energy HF (Hartrees, En)</b>	<b>Energy above the energy minimum (Hartrees, En)</b>	<b>Energy above the energy minimum (Kcal/mol)</b>
<b>5a</b>	<b>5a-1</b>	-828.0385692	0.0029219	<b>1.8</b>
	<b>5a-2</b>	-828.0386513	0.0028398	<b>1.8</b>
	<b>5a-3</b>	-828.0386515	0.0028396	<b>1.8</b>
	<b>5a-4</b>	-828.0385694	0.0029217	<b>1.8</b>
<b>6a</b>	<b>6a-1</b>	-828.0414911	0.0000000	<b>0.0</b>
	<b>6a-2</b>	-828.0413423	0.0001488	<b>0.1</b>
	<b>6a-3</b>	-828.0413423	0.0001488	<b>0.1</b>
	<b>6a-4</b>	-828.0414911	0.0000000	<b>0.0</b>
<b>7</b>	<b>7-1</b>	-828.0388067	0.0026844	<b>1.7</b>
	<b>7-2</b>	-828.0384929	0.0029982	<b>1.9</b>
	<b>7-3</b>	-828.0384926	0.0029985	<b>1.9</b>
	<b>7-4</b>	-828.0388066	0.0026845	<b>1.7</b>
	<b>Energy Minimum (conf. 6a-1 and 6a-4)</b>	<b>-828.0414911</b>		

The structures for the corresponding conformers and Z-matrixes are described in the next pages.

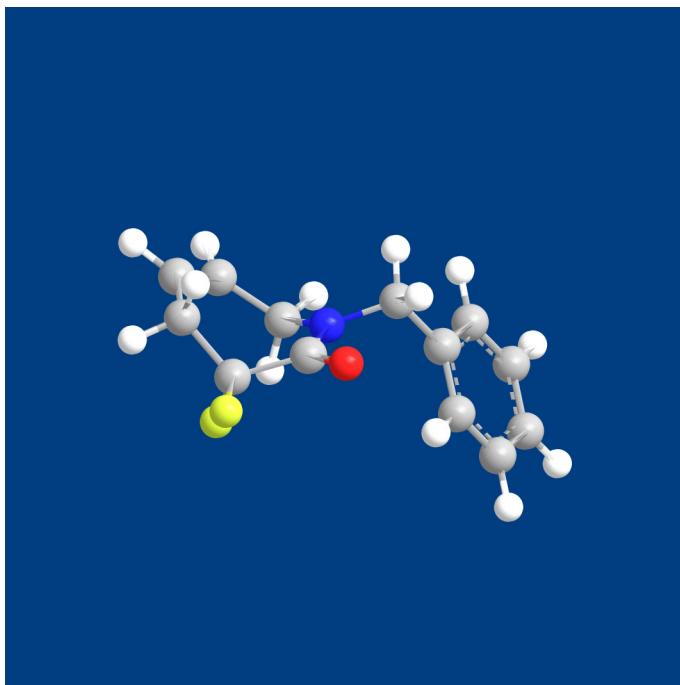
<sup>12</sup> Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

Conformer 5a-1:



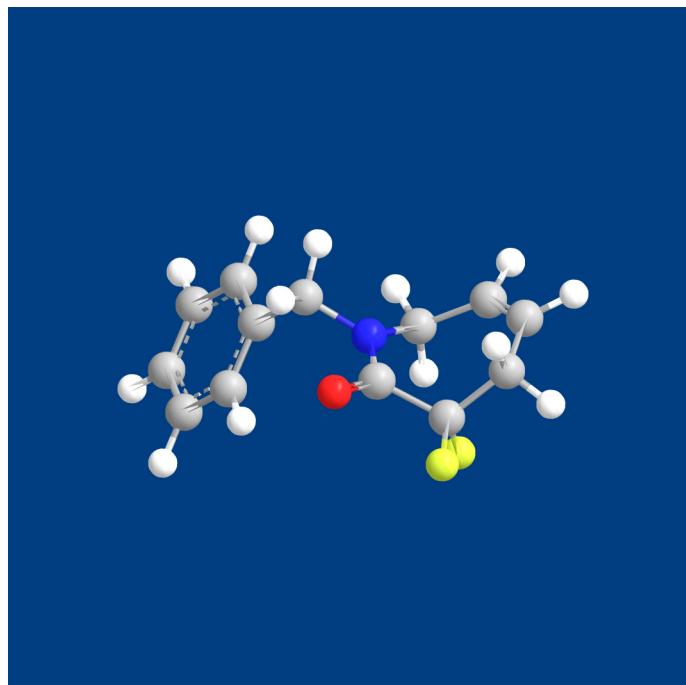
Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.511664( 1)					
3	3	C	2	1.504292( 2)	1	115.914( 30)			
4	4	C	3	1.318883( 3)	2	128.414( 31)	1	350.722( 58)	0
5	5	C	4	1.512871( 4)	3	128.389( 32)	2	359.671( 59)	0
6	6	N	5	1.462601( 5)	4	116.188( 33)	3	318.097( 60)	0
7	7	C	1	1.538195( 6)	2	114.018( 34)	3	62.706( 61)	0
8	8	O	7	1.198400( 7)	1	118.566( 35)	2	105.173( 62)	0
9	9	C	6	1.462931( 8)	5	116.772( 36)	4	236.837( 63)	0
10	10	F	1	1.333626( 9)	2	108.474( 37)	3	183.147( 64)	0
11	11	F	1	1.351353( 10)	2	110.177( 38)	3	299.086( 65)	0
12	12	C	9	1.515986( 11)	6	113.622( 39)	5	72.399( 66)	0
13	13	C	12	1.393586( 12)	9	120.253( 40)	6	65.490( 67)	0
14	14	C	13	1.381700( 13)	12	120.514( 41)	9	179.644( 68)	0
15	15	C	14	1.389250( 14)	13	120.265( 42)	12	359.837( 69)	0
16	16	C	15	1.381741( 15)	14	119.648( 43)	13	-0.144( 70)	0
17	17	C	12	1.386273( 16)	9	120.952( 44)	6	244.737( 71)	0
18	18	H	2	1.086281( 17)	1	107.480( 45)	7	298.578( 72)	0
19	19	H	2	1.086015( 18)	1	106.408( 46)	7	184.654( 73)	0
20	20	H	3	1.076783( 19)	2	113.904( 47)	1	170.377( 74)	0
21	21	H	4	1.076718( 20)	3	117.391( 48)	2	178.269( 75)	0
22	22	H	5	1.079154( 21)	4	107.269( 49)	3	200.256( 76)	0
23	23	H	5	1.083129( 22)	4	110.075( 50)	3	84.485( 77)	0
24	24	H	9	1.077471( 23)	6	107.301( 51)	5	194.593( 78)	0
25	25	H	9	1.084191( 24)	6	107.925( 52)	5	310.419( 79)	0
26	26	H	13	1.075326( 25)	12	119.413( 53)	9	0.282( 80)	0
27	27	H	14	1.075507( 26)	13	119.777( 54)	12	180.209( 81)	0
28	28	H	15	1.075397( 27)	14	120.129( 55)	13	180.124( 82)	0
29	29	H	16	1.075519( 28)	15	120.211( 56)	14	180.262( 83)	0
30	30	H	17	1.076881( 29)	12	119.773( 57)	9	360.033( 84)	0

**Conformer 5a-2:**



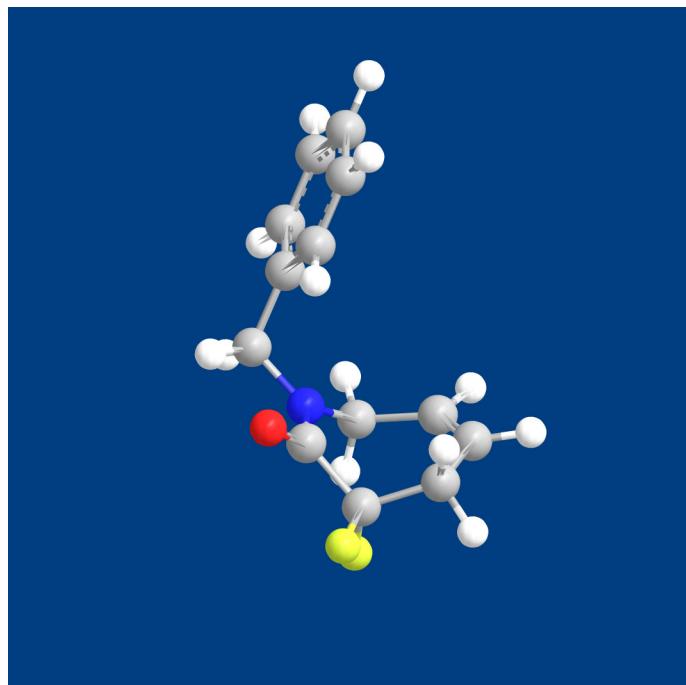
Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.513526( 1)					
3	3	C	2	1.505021( 2)	1	116.291( 30)			
4	4	C	3	1.318671( 3)	2	128.152( 31)	1	347.377( 58)	0
5	5	C	4	1.511995( 4)	3	127.614( 32)	2	359.150( 59)	0
6	6	N	5	1.462569( 5)	4	115.365( 33)	3	318.861( 60)	0
7	7	C	1	1.539479( 6)	2	114.487( 34)	3	65.247( 61)	0
8	8	O	7	1.197881( 7)	1	118.733( 35)	2	111.775( 62)	0
9	9	C	6	1.462584( 8)	5	116.920( 36)	4	238.832( 63)	0
10	10	F	1	1.333227( 9)	2	108.256( 37)	3	185.724( 64)	0
11	11	F	1	1.351530( 10)	2	110.209( 38)	3	301.578( 65)	0
12	12	C	9	1.516327( 11)	6	113.621( 39)	5	288.630( 66)	0
13	13	C	12	1.386311( 12)	9	120.905( 40)	6	116.608( 67)	0
14	14	C	13	1.388998( 13)	12	120.801( 41)	9	179.539( 68)	0
15	15	C	14	1.381872( 14)	13	119.972( 42)	12	360.066( 69)	0
16	16	C	15	1.389102( 15)	14	119.651( 43)	13	359.770( 70)	0
17	17	C	12	1.393525( 16)	9	120.279( 44)	6	295.910( 71)	0
18	18	H	2	1.086602( 17)	1	107.595( 45)	7	300.552( 72)	0
19	19	H	2	1.085795( 18)	1	106.115( 46)	7	186.860( 73)	0
20	20	H	3	1.076808( 19)	2	113.959( 47)	1	166.628( 74)	0
21	21	H	4	1.077028( 20)	3	117.660( 48)	2	177.594( 75)	0
22	22	H	5	1.079364( 21)	4	108.154( 49)	3	200.618( 76)	0
23	23	H	5	1.082294( 22)	4	110.242( 50)	3	85.079( 77)	0
24	24	H	9	1.084038( 23)	6	107.847( 51)	5	50.589( 78)	0
25	25	H	9	1.077537( 24)	6	107.309( 52)	5	166.470( 79)	0
26	26	H	13	1.076869( 25)	12	119.779( 53)	9	359.863( 80)	0
27	27	H	14	1.075518( 26)	13	119.821( 54)	12	180.015( 81)	0
28	28	H	15	1.075377( 27)	14	120.221( 55)	13	179.966( 82)	0
29	29	H	16	1.075429( 28)	15	119.980( 56)	14	180.417( 83)	0
30	30	H	17	1.075365( 29)	12	119.504( 57)	9	-0.235( 84)	0

**Conformer 5a-3:**



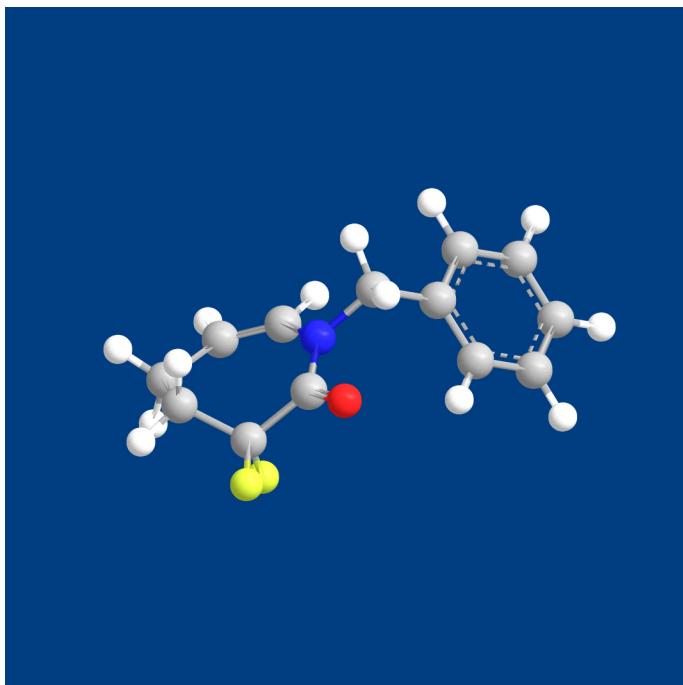
Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.513540( 1)					
3	3	C	2	1.505050( 2)	1	116.304( 30)			
4	4	C	3	1.318711( 3)	2	128.158( 31)	1	12.554( 58)	0
5	5	C	4	1.512046( 4)	3	127.599( 32)	2	0.818( 59)	0
6	6	N	5	1.462552( 5)	4	115.361( 33)	3	41.223( 60)	0
7	7	C	1	1.539567( 6)	2	114.480( 34)	3	294.822( 61)	0
8	8	O	7	1.197845( 7)	1	118.741( 35)	2	248.277( 62)	0
9	9	C	6	1.462579( 8)	5	116.936( 36)	4	120.961( 63)	0
10	10	F	1	1.333226( 9)	2	108.252( 37)	3	174.337( 64)	0
11	11	F	1	1.351489( 10)	2	110.200( 38)	3	58.505( 65)	0
12	12	C	9	1.516297( 11)	6	113.612( 39)	5	71.464( 66)	0
13	13	C	12	1.393539( 12)	9	120.270( 40)	6	64.131( 67)	0
14	14	C	13	1.381868( 13)	12	120.495( 41)	9	179.685( 68)	0
15	15	C	14	1.389123( 14)	13	120.267( 42)	12	359.804( 69)	0
16	16	C	15	1.381862( 15)	14	119.653( 43)	13	-0.101( 70)	0
17	17	C	12	1.386291( 16)	9	120.913( 44)	6	243.446( 71)	0
18	18	H	2	1.085817( 17)	1	106.116( 45)	7	173.203( 72)	0
19	19	H	2	1.086585( 18)	1	107.585( 46)	7	59.516( 73)	0
20	20	H	3	1.076826( 19)	2	113.953( 47)	1	193.290( 74)	0
21	21	H	4	1.077032( 20)	3	117.660( 48)	2	182.400( 75)	0
22	22	H	5	1.079373( 21)	4	108.173( 49)	3	159.492( 76)	0
23	23	H	5	1.082253( 22)	4	110.229( 50)	3	275.029( 77)	0
24	24	H	9	1.077555( 23)	6	107.315( 51)	5	193.618( 78)	0
25	25	H	9	1.084054( 24)	6	107.850( 52)	5	309.507( 79)	0
26	26	H	13	1.075376( 25)	12	119.501( 53)	9	0.242( 80)	0
27	27	H	14	1.075436( 26)	13	119.753( 54)	12	180.121( 81)	0
28	28	H	15	1.075383( 27)	14	120.126( 55)	13	180.095( 82)	0
29	29	H	16	1.075524( 28)	15	120.207( 56)	14	180.181( 83)	0
30	30	H	17	1.076876( 29)	12	119.780( 57)	9	360.120( 84)	0

**Conformer 5a-4:**



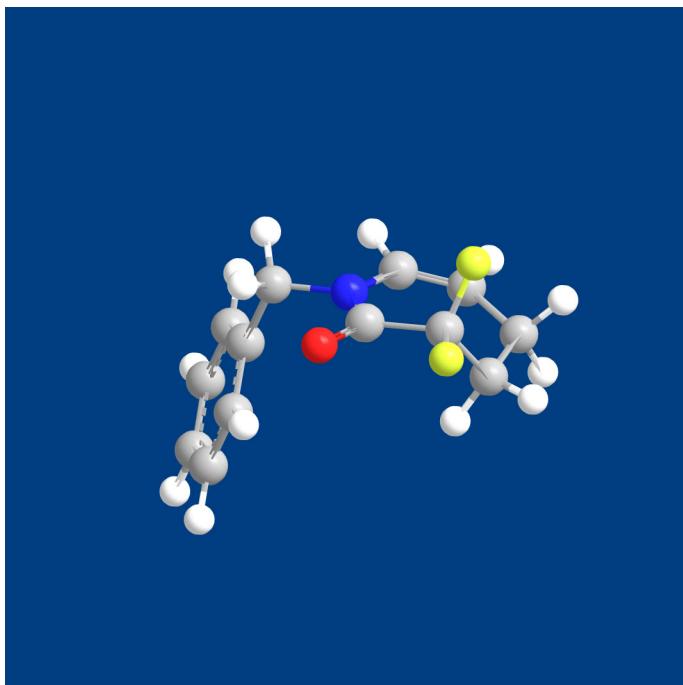
CD	Cent	Atom	Z-MATRIX (ANGSTROMS AND DEGREES)				J
			N1	Length/X	N2	Alpha/Y	
1	1	C					
2	2	C	1	1.511656( 1)			
3	3	C	2	1.504275( 2)	1	115.884( 30)	
4	4	C	3	1.318890( 3)	2	128.408( 31)	1 9.466( 58) 0
5	5	C	4	1.512860( 4)	3	128.419( 32)	2 0.301( 59) 0
6	6	N	5	1.462622( 5)	4	116.231( 33)	3 41.761( 60) 0
7	7	C	1	1.538212( 6)	2	113.983( 34)	3 297.134( 61) 0
8	8	O	7	1.198402( 7)	1	118.574( 35)	2 254.889( 62) 0
9	9	C	6	1.462975( 8)	5	116.768( 36)	4 123.162( 63) 0
10	10	F	1	1.333601( 9)	2	108.479( 37)	3 176.694( 64) 0
11	11	F	1	1.351292( 10)	2	110.182( 38)	3 60.753( 65) 0
12	12	C	9	1.516005( 11)	6	113.631( 39)	5 287.598( 66) 0
13	13	C	12	1.386284( 12)	9	120.946( 40)	6 115.236( 67) 0
14	14	C	13	1.389180( 13)	12	120.813( 41)	9 179.540( 68) 0
15	15	C	14	1.381740( 14)	13	119.969( 42)	12 359.991( 69) 0
16	16	C	15	1.389246( 15)	14	119.648( 43)	13 359.781( 70) 0
17	17	C	12	1.393592( 16)	9	120.261( 44)	6 294.459( 71) 0
18	18	H	2	1.086011( 17)	1	106.420( 45)	7 175.190( 72) 0
19	19	H	2	1.086290( 18)	1	107.484( 46)	7 61.258( 73) 0
20	20	H	3	1.076777( 19)	2	113.912( 47)	1 189.809( 74) 0
21	21	H	4	1.076730( 20)	3	117.387( 48)	2 181.743( 75) 0
22	22	H	5	1.079159( 21)	4	107.262( 49)	3 159.622( 76) 0
23	23	H	5	1.083148( 22)	4	110.053( 50)	3 275.376( 77) 0
24	24	H	9	1.084175( 23)	6	107.915( 51)	5 49.569( 78) 0
25	25	H	9	1.077484( 24)	6	107.306( 52)	5 165.392( 79) 0
26	26	H	13	1.076882( 25)	12	119.773( 53)	9 359.939( 80) 0
27	27	H	14	1.075520( 26)	13	119.820( 54)	12 180.030( 81) 0
28	28	H	15	1.075398( 27)	14	120.223( 55)	13 180.050( 82) 0
29	29	H	16	1.075509( 28)	15	119.956( 56)	14 180.519( 83) 0
30	30	H	17	1.075320( 29)	12	119.414( 57)	9 -0.263( 84) 0

**Conformer 6a-1:**



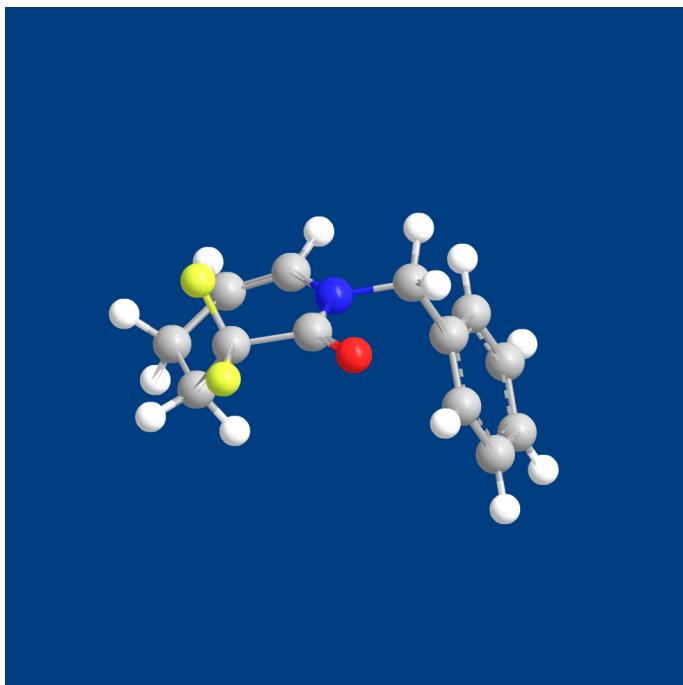
Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.517051( 1)					
3	3	C	2	1.524463( 2)	1	113.027( 30)			
4	4	C	3	1.501049( 3)	2	116.135( 31)	1	310.923( 58)	0
5	5	C	4	1.320233( 4)	3	130.952( 32)	2	4.318( 59)	0
6	6	N	5	1.413347( 5)	4	131.769( 33)	3	-3.713( 60)	0
7	7	C	1	1.537891( 6)	2	114.357( 34)	3	86.135( 61)	0
8	8	O	7	1.195139( 7)	1	118.955( 35)	2	124.476( 62)	0
9	9	C	6	1.470970( 8)	5	114.607( 36)	4	204.878( 63)	0
10	10	F	1	1.333845( 9)	2	109.099( 37)	3	206.173( 64)	0
11	11	F	1	1.348879( 10)	2	110.849( 38)	3	323.244( 65)	0
12	12	C	9	1.515688( 11)	6	113.884( 39)	5	285.419( 66)	0
13	13	C	12	1.386777( 12)	9	120.612( 40)	6	116.411( 67)	0
14	14	C	13	1.388784( 13)	12	120.806( 41)	9	179.293( 68)	0
15	15	C	14	1.381897( 14)	13	119.945( 42)	12	360.058( 69)	0
16	16	C	15	1.388910( 15)	14	119.667( 43)	13	359.770( 70)	0
17	17	C	12	1.393449( 16)	9	120.545( 44)	6	295.429( 71)	0
18	18	H	2	1.083360( 17)	1	107.108( 45)	7	206.976( 72)	0
19	19	H	2	1.085116( 18)	1	108.316( 46)	7	322.198( 73)	0
20	20	H	3	1.086709( 19)	2	108.629( 47)	1	187.705( 74)	0
21	21	H	3	1.085847( 20)	2	108.795( 48)	1	72.774( 75)	0
22	22	H	4	1.076380( 21)	3	114.422( 49)	2	180.744( 76)	0
23	23	H	5	1.073059( 22)	4	117.485( 50)	3	177.647( 77)	0
24	24	H	9	1.082801( 23)	6	107.446( 51)	5	47.344( 78)	0
25	25	H	9	1.076842( 24)	6	107.163( 52)	5	163.030( 79)	0
26	26	H	13	1.076831( 25)	12	119.767( 53)	9	359.595( 80)	0
27	27	H	14	1.075460( 26)	13	119.822( 54)	12	179.996( 81)	0
28	28	H	15	1.075361( 27)	14	120.213( 55)	13	179.953( 82)	0
29	29	H	16	1.075372( 28)	15	119.978( 56)	14	180.396( 83)	0
30	30	H	17	1.074868( 29)	12	119.590( 57)	9	0.022( 84)	0

**Conformer 6a-2:**



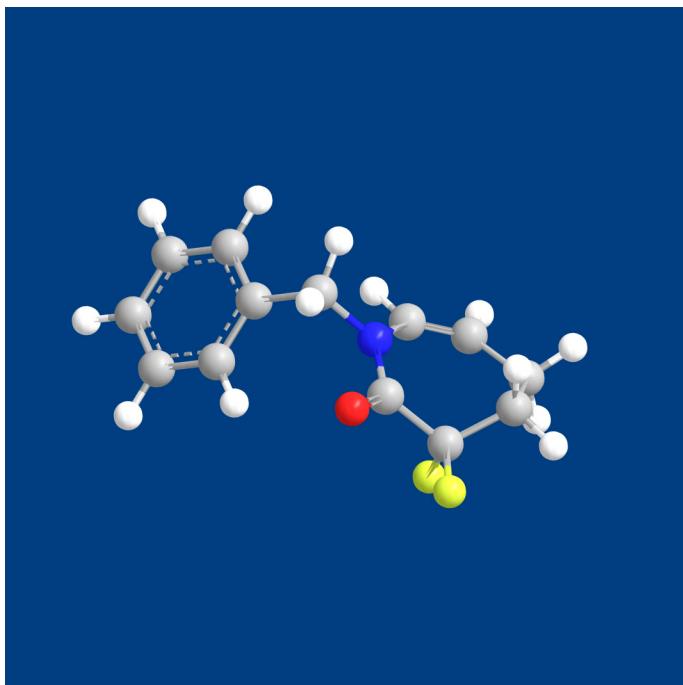
Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.516814( 1)					
3	3	C	2	1.523902( 2)	1	112.910( 30)			
4	4	C	3	1.501209( 3)	2	116.284( 31)	1	311.277( 58)	0
5	5	C	4	1.320777( 4)	3	131.480( 32)	2	6.259( 59)	0
6	6	N	5	1.411764( 5)	4	132.609( 33)	3	-2.708( 60)	0
7	7	C	1	1.536122( 6)	2	113.680( 34)	3	86.262( 61)	0
8	8	O	7	1.195315( 7)	1	118.890( 35)	2	117.825( 62)	0
9	9	C	6	1.471306( 8)	5	115.056( 36)	4	202.812( 63)	0
10	10	F	1	1.333663( 9)	2	109.238( 37)	3	206.116( 64)	0
11	11	F	1	1.348615( 10)	2	110.916( 38)	3	323.305( 65)	0
12	12	C	9	1.515302( 11)	6	113.571( 39)	5	76.685( 66)	0
13	13	C	12	1.393064( 12)	9	120.400( 40)	6	73.687( 67)	0
14	14	C	13	1.382924( 13)	12	120.471( 41)	9	180.152( 68)	0
15	15	C	14	1.388080( 14)	13	120.278( 42)	12	359.762( 69)	0
16	16	C	15	1.382689( 15)	14	119.653( 43)	13	359.886( 70)	0
17	17	C	12	1.387011( 16)	9	120.791( 44)	6	253.358( 71)	0
18	18	H	2	1.083373( 17)	1	107.181( 45)	7	207.201( 72)	0
19	19	H	2	1.085271( 18)	1	108.273( 46)	7	322.492( 73)	0
20	20	H	3	1.086478( 19)	2	108.565( 47)	1	188.226( 74)	0
21	21	H	3	1.085999( 20)	2	108.825( 48)	1	73.278( 75)	0
22	22	H	4	1.076302( 21)	3	114.191( 49)	2	182.988( 76)	0
23	23	H	5	1.072784( 22)	4	116.889( 50)	3	178.444( 77)	0
24	24	H	9	1.076276( 23)	6	107.343( 51)	5	199.188( 78)	0
25	25	H	9	1.082838( 24)	6	107.416( 52)	5	314.906( 79)	0
26	26	H	13	1.074919( 25)	12	119.467( 53)	9	360.560( 80)	0
27	27	H	14	1.075504( 26)	13	119.733( 54)	12	180.182( 81)	0
28	28	H	15	1.075407( 27)	14	120.149( 55)	13	180.199( 82)	0
29	29	H	16	1.075480( 28)	15	120.196( 56)	14	180.315( 83)	0
30	30	H	17	1.076695( 29)	12	119.820( 57)	9	-0.378( 84)	0

**Conformer 6a-3:**



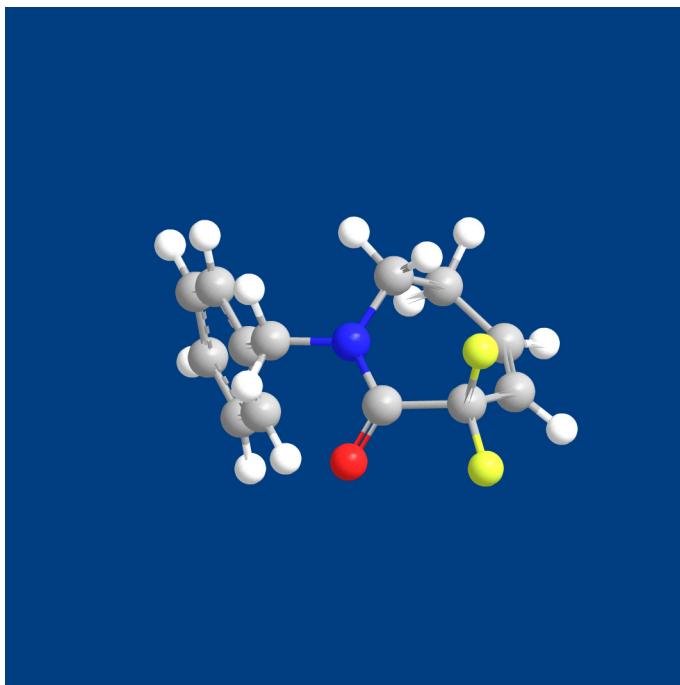
Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.516822( 1)					
3	3	C	2	1.523900( 2)	1	112.913( 30)			
4	4	C	3	1.501212( 3)	2	116.280( 31)	1	48.745( 58)	0
5	5	C	4	1.320785( 4)	3	131.480( 32)	2	353.705( 59)	0
6	6	N	5	1.411786( 5)	4	132.611( 33)	3	362.719( 60)	0
7	7	C	1	1.536121( 6)	2	113.681( 34)	3	273.740( 61)	0
8	8	O	7	1.195306( 7)	1	118.896( 35)	2	242.160( 62)	0
9	9	C	6	1.471274( 8)	5	115.060( 36)	4	157.203( 63)	0
10	10	F	1	1.333667( 9)	2	109.244( 37)	3	153.878( 64)	0
11	11	F	1	1.348611( 10)	2	110.912( 38)	3	36.691( 65)	0
12	12	C	9	1.515274( 11)	6	113.569( 39)	5	283.359( 66)	0
13	13	C	12	1.387002( 12)	9	120.791( 40)	6	106.697( 67)	0
14	14	C	13	1.387899( 13)	12	120.813( 41)	9	180.041( 68)	0
15	15	C	14	1.382689( 14)	13	119.974( 42)	12	359.977( 69)	0
16	16	C	15	1.388090( 15)	14	119.653( 43)	13	359.780( 70)	0
17	17	C	12	1.393059( 16)	9	120.398( 44)	6	286.366( 71)	0
18	18	H	2	1.083374( 17)	1	107.180( 45)	7	152.799( 72)	0
19	19	H	2	1.085266( 18)	1	108.271( 46)	7	37.510( 73)	0
20	20	H	3	1.086001( 19)	2	108.827( 47)	1	286.741( 74)	0
21	21	H	3	1.086480( 20)	2	108.566( 48)	1	171.790( 75)	0
22	22	H	4	1.076303( 21)	3	114.191( 49)	2	176.987( 76)	0
23	23	H	5	1.072780( 22)	4	116.887( 50)	3	181.566( 77)	0
24	24	H	9	1.082840( 23)	6	107.411( 51)	5	45.137( 78)	0
25	25	H	9	1.076289( 24)	6	107.347( 52)	5	160.857( 79)	0
26	26	H	13	1.076697( 25)	12	119.821( 53)	9	360.374( 80)	0
27	27	H	14	1.075481( 26)	13	119.829( 54)	12	180.071( 81)	0
28	28	H	15	1.075407( 27)	14	120.198( 55)	13	180.092( 82)	0
29	29	H	16	1.075506( 28)	15	119.988( 56)	14	180.534( 83)	0
30	30	H	17	1.074935( 29)	12	119.468( 57)	9	-0.559( 84)	0

**Conformer 6a-4:**



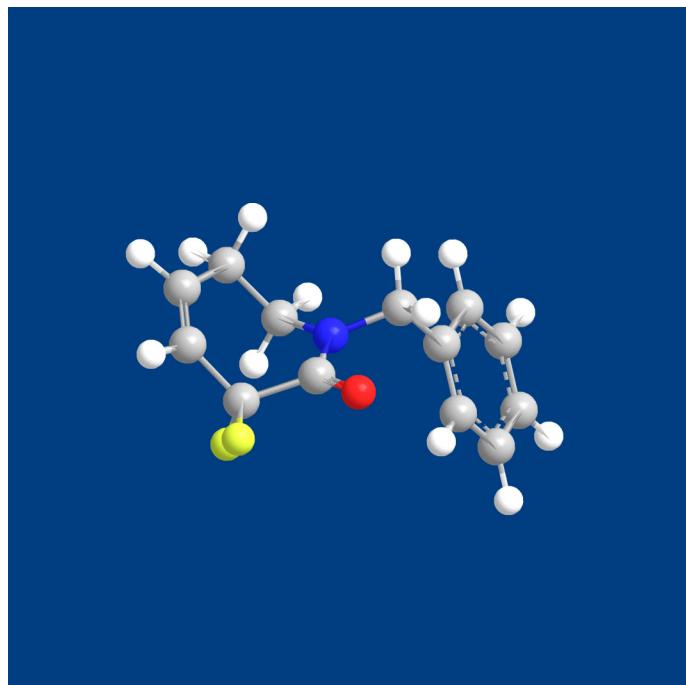
Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.517057( 1)					
3	3	C	2	1.524538( 2)	1	113.042( 30)			
4	4	C	3	1.501077( 3)	2	116.153( 31)	1	48.929( 58)	0
5	5	C	4	1.320227( 4)	3	130.955( 32)	2	355.828( 59)	0
6	6	N	5	1.413371( 5)	4	131.746( 33)	3	363.713( 60)	0
7	7	C	1	1.537877( 6)	2	114.337( 34)	3	273.883( 61)	0
8	8	O	7	1.195126( 7)	1	118.959( 35)	2	235.633( 62)	0
9	9	C	6	1.470938( 8)	5	114.616( 36)	4	154.979( 63)	0
10	10	F	1	1.333845( 9)	2	109.099( 37)	3	153.847( 64)	0
11	11	F	1	1.348830( 10)	2	110.849( 38)	3	36.788( 65)	0
12	12	C	9	1.515696( 11)	6	113.886( 39)	5	74.648( 66)	0
13	13	C	12	1.393458( 12)	9	120.549( 40)	6	64.558( 67)	0
14	14	C	13	1.381990( 13)	12	120.440( 41)	9	179.457( 68)	0
15	15	C	14	1.388910( 14)	13	120.305( 42)	12	359.757( 69)	0
16	16	C	15	1.381899( 15)	14	119.667( 43)	13	359.918( 70)	0
17	17	C	12	1.386778( 16)	9	120.608( 44)	6	243.589( 71)	0
18	18	H	2	1.083362( 17)	1	107.116( 45)	7	153.029( 72)	0
19	19	H	2	1.085105( 18)	1	108.299( 46)	7	37.816( 73)	0
20	20	H	3	1.085850( 19)	2	108.794( 47)	1	287.080( 74)	0
21	21	H	3	1.086716( 20)	2	108.627( 48)	1	172.154( 75)	0
22	22	H	4	1.076384( 21)	3	114.413( 49)	2	179.420( 76)	0
23	23	H	5	1.073076( 22)	4	117.496( 50)	3	182.350( 77)	0
24	24	H	9	1.076850( 23)	6	107.164( 51)	5	197.042( 78)	0
25	25	H	9	1.082800( 24)	6	107.443( 52)	5	312.727( 79)	0
26	26	H	13	1.074857( 25)	12	119.590( 53)	9	359.994( 80)	0
27	27	H	14	1.075374( 26)	13	119.717( 54)	12	180.070( 81)	0
28	28	H	15	1.075363( 27)	14	120.119( 55)	13	180.101( 82)	0
29	29	H	16	1.075461( 28)	15	120.234( 56)	14	180.169( 83)	0
30	30	H	17	1.076832( 29)	12	119.767( 57)	9	0.391( 84)	0

### Conformer 7-1:



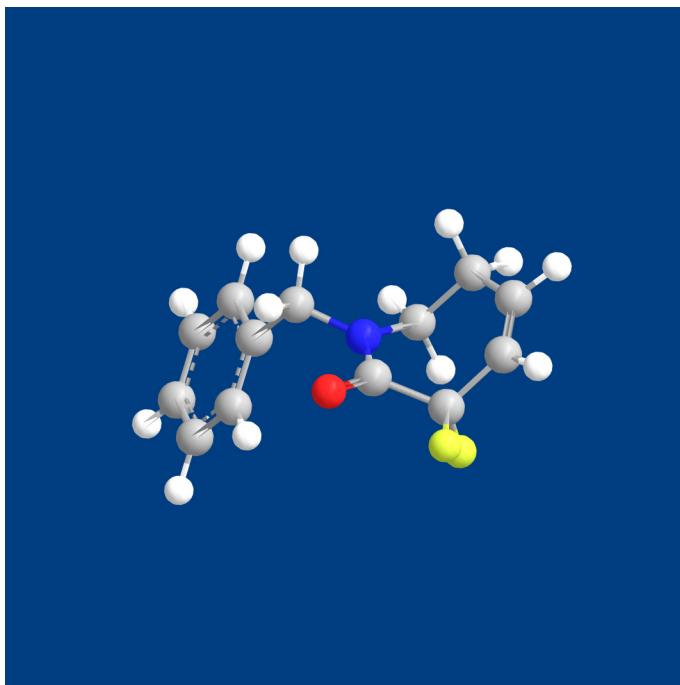
Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.503755( 1)					
3	3	C	2	1.319883( 2)	1	126.988( 30)			
4	4	C	3	1.504473( 3)	2	128.604( 31)	1	1.216( 58)	0
5	5	C	4	1.525728( 4)	3	115.578( 32)	2	9.745( 59)	0
6	6	N	5	1.459205( 5)	4	114.068( 33)	3	296.473( 60)	0
7	7	C	1	1.542800( 6)	2	115.120( 34)	3	44.715( 61)	0
8	8	O	7	1.196557( 7)	1	118.996( 35)	2	114.766( 62)	0
9	9	C	6	1.462111( 8)	5	118.012( 36)	4	251.180( 63)	0
10	10	F	1	1.332955( 9)	2	107.893( 37)	3	164.961( 64)	0
11	11	F	1	1.355559( 10)	2	111.394( 38)	3	280.778( 65)	0
12	12	C	9	1.516496( 11)	6	113.891( 39)	5	72.676( 66)	0
13	13	C	12	1.394075( 12)	9	120.232( 40)	6	68.034( 67)	0
14	14	C	13	1.382172( 13)	12	120.497( 41)	9	179.993( 68)	0
15	15	C	14	1.389203( 14)	13	120.272( 42)	12	359.800( 69)	0
16	16	C	15	1.382022( 15)	14	119.647( 43)	13	-0.135( 70)	0
17	17	C	12	1.386567( 16)	9	120.975( 44)	6	247.587( 71)	0
18	18	H	2	1.074753( 17)	1	113.080( 45)	7	225.383( 72)	0
19	19	H	3	1.077445( 18)	2	116.797( 46)	1	181.178( 73)	0
20	20	H	4	1.087969( 19)	3	107.901( 47)	2	130.863( 74)	0
21	21	H	4	1.086439( 20)	3	108.730( 48)	2	245.747( 75)	0
22	22	H	5	1.080541( 21)	4	108.419( 49)	3	177.843( 76)	0
23	23	H	5	1.080325( 22)	4	110.212( 50)	3	61.061( 77)	0
24	24	H	9	1.077616( 23)	6	107.239( 51)	5	194.872( 78)	0
25	25	H	9	1.083882( 24)	6	107.820( 52)	5	310.657( 79)	0
26	26	H	13	1.075396( 25)	12	119.405( 53)	9	0.497( 80)	0
27	27	H	14	1.075494( 26)	13	119.755( 54)	12	180.223( 81)	0
28	28	H	15	1.075392( 27)	14	120.134( 55)	13	180.180( 82)	0
29	29	H	16	1.075530( 28)	15	120.197( 56)	14	180.315( 83)	0
30	30	H	17	1.076821( 29)	12	119.777( 57)	9	359.700( 84)	0

## Conformer 7-2:



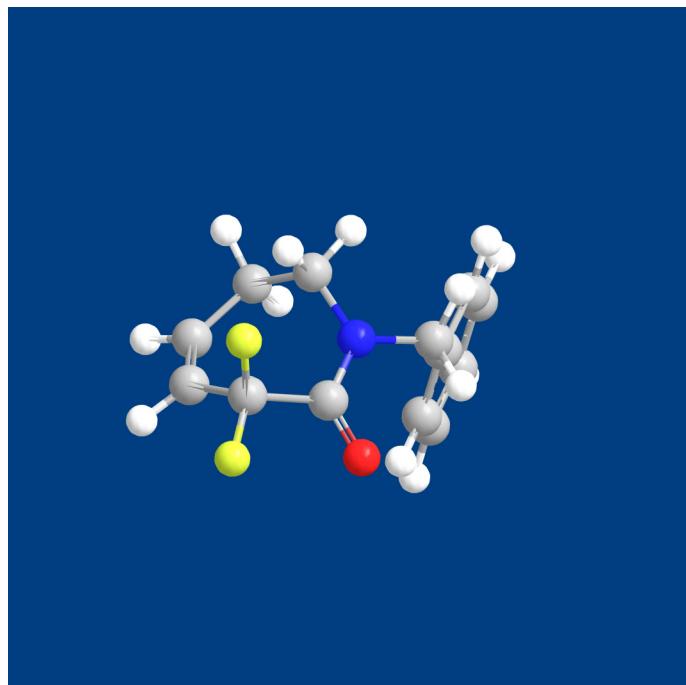
Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.504950( 1)					
3	3	C	2	1.320121( 2)	1	127.499( 30)			
4	4	C	3	1.504552( 3)	2	128.617( 31)	1	1.031( 58)	0
5	5	C	4	1.524326( 4)	3	115.125( 32)	2	7.881( 59)	0
6	6	N	5	1.457810( 5)	4	113.006( 33)	3	297.201( 60)	0
7	7	C	1	1.544298( 6)	2	115.685( 34)	3	45.231( 61)	0
8	8	O	7	1.196187( 7)	1	119.027( 35)	2	120.042( 62)	0
9	9	C	6	1.461185( 8)	5	117.734( 36)	4	253.835( 63)	0
10	10	F	1	1.332776( 9)	2	107.744( 37)	3	165.632( 64)	0
11	11	F	1	1.355822( 10)	2	111.296( 38)	3	281.278( 65)	0
12	12	C	9	1.516053( 11)	6	113.486( 39)	5	285.607( 66)	0
13	13	C	12	1.386213( 12)	9	120.926( 40)	6	117.459( 67)	0
14	14	C	13	1.389155( 13)	12	120.793( 41)	9	179.487( 68)	0
15	15	C	14	1.381760( 14)	13	119.963( 42)	12	360.053( 69)	0
16	16	C	15	1.389256( 15)	14	119.658( 43)	13	359.794( 70)	0
17	17	C	12	1.393496( 16)	9	120.238( 44)	6	296.729( 71)	0
18	18	H	2	1.074778( 17)	1	112.843( 45)	7	225.584( 72)	0
19	19	H	3	1.077494( 18)	2	116.722( 46)	1	180.841( 73)	0
20	20	H	4	1.087847( 19)	3	108.146( 47)	2	129.518( 74)	0
21	21	H	4	1.088393( 20)	3	108.542( 48)	2	244.206( 75)	0
22	22	H	5	1.080505( 21)	4	109.401( 49)	3	178.261( 76)	0
23	23	H	5	1.079333( 22)	4	110.292( 50)	3	61.427( 77)	0
24	24	H	9	1.084590( 23)	6	108.122( 51)	5	47.503( 78)	0
25	25	H	9	1.077908( 24)	6	107.360( 52)	5	163.442( 79)	0
26	26	H	13	1.076921( 25)	12	119.782( 53)	9	359.803( 80)	0
27	27	H	14	1.075533( 26)	13	119.824( 54)	12	179.995( 81)	0
28	28	H	15	1.075386( 27)	14	120.220( 55)	13	179.968( 82)	0
29	29	H	16	1.075424( 28)	15	119.977( 56)	14	180.386( 83)	0
30	30	H	17	1.075348( 29)	12	119.499( 57)	9	359.883( 84)	0

### Conformer 7-3:

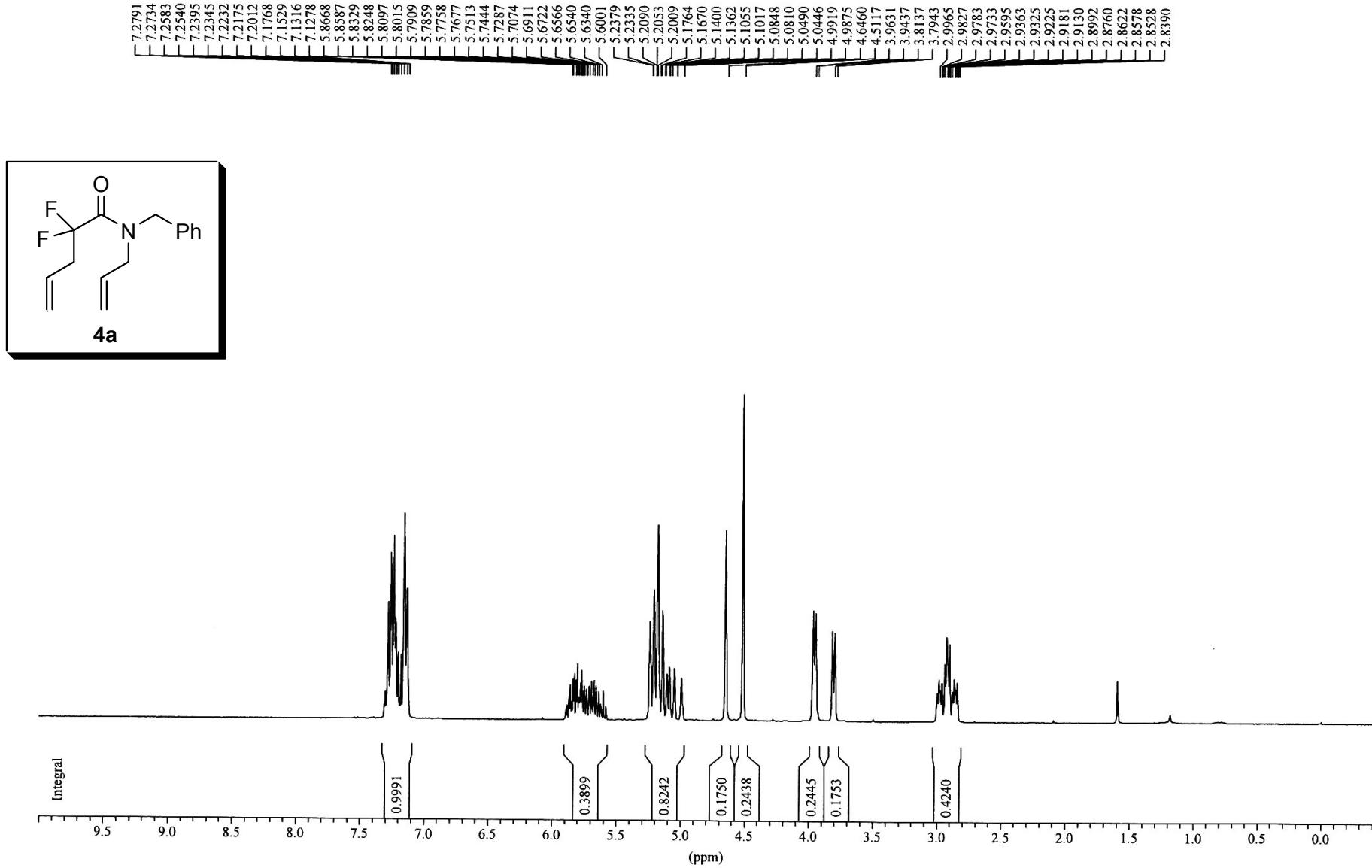


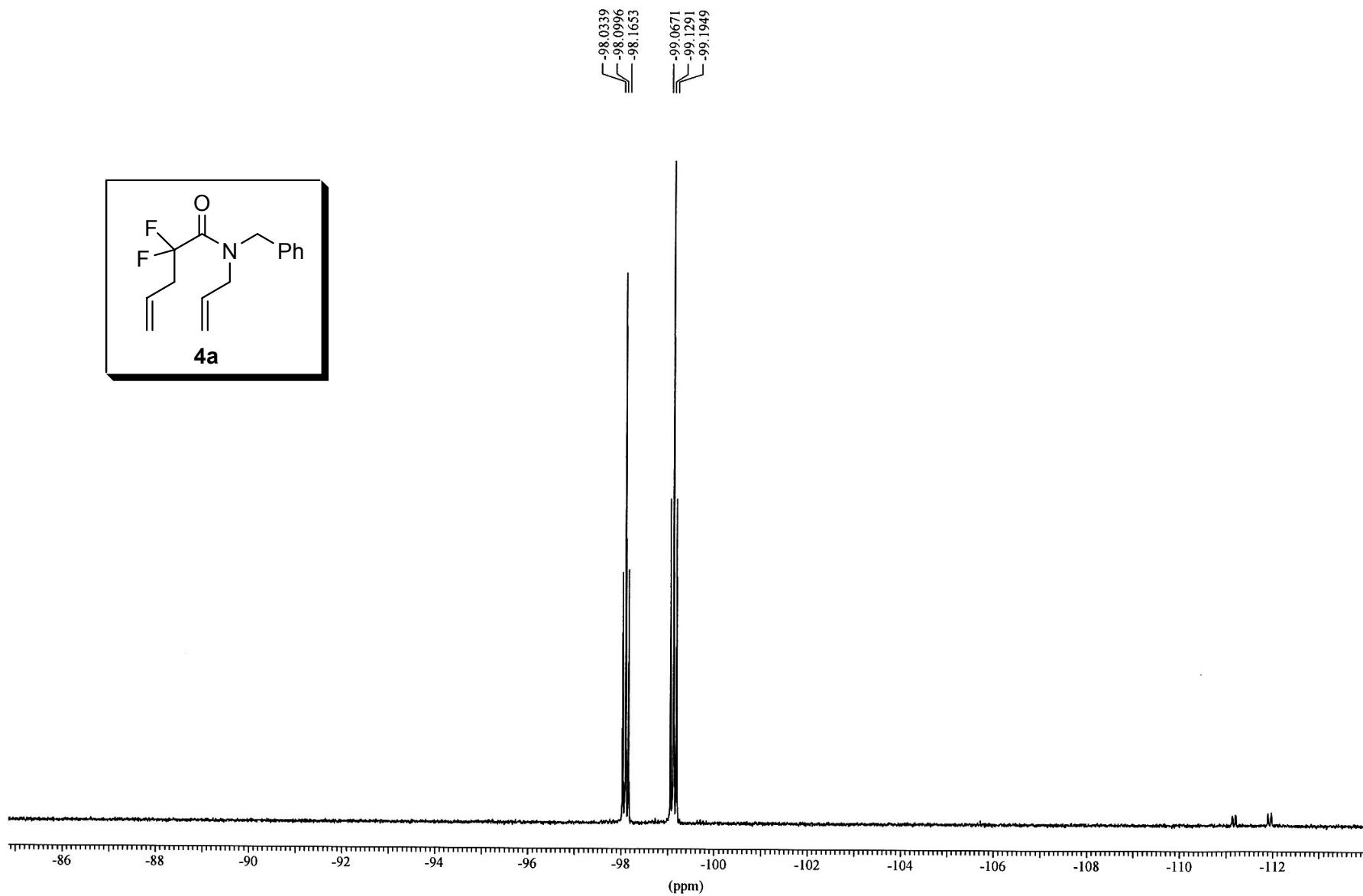
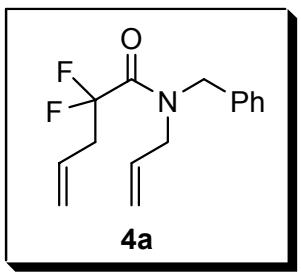
Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.504949( 1)					
3	3	C	2	1.320110( 2)	1	127.509( 30)			
4	4	C	3	1.504540( 3)	2	128.614( 31)	1	359.036( 58)	0
5	5	C	4	1.524306( 4)	3	115.113( 32)	2	351.982( 59)	0
6	6	N	5	1.457804( 5)	4	113.000( 33)	3	62.889( 60)	0
7	7	C	1	1.544271( 6)	2	115.712( 34)	3	314.801( 61)	0
8	8	O	7	1.196230( 7)	1	119.019( 35)	2	239.925( 62)	0
9	9	C	6	1.461220( 8)	5	117.733( 36)	4	106.135( 63)	0
10	10	F	1	1.355849( 9)	2	111.279( 37)	3	78.741( 64)	0
11	11	F	1	1.332764( 10)	2	107.746( 38)	3	194.374( 65)	0
12	12	C	9	1.516045( 11)	6	113.482( 39)	5	74.476( 66)	0
13	13	C	12	1.393507( 12)	9	120.228( 40)	6	63.479( 67)	0
14	14	C	13	1.381728( 13)	12	120.482( 41)	9	179.640( 68)	0
15	15	C	14	1.389264( 14)	13	120.271( 42)	12	359.835( 69)	0
16	16	C	15	1.381748( 15)	14	119.658( 43)	13	-0.102( 70)	0
17	17	C	12	1.386208( 16)	9	120.937( 44)	6	242.788( 71)	0
18	18	H	2	1.074779( 17)	1	112.839( 45)	7	134.494( 72)	0
19	19	H	3	1.077491( 18)	2	116.721( 46)	1	179.183( 73)	0
20	20	H	4	1.088387( 19)	3	108.537( 47)	2	115.638( 74)	0
21	21	H	4	1.087850( 20)	3	108.157( 48)	2	230.330( 75)	0
22	22	H	5	1.080501( 21)	4	109.405( 49)	3	181.827( 76)	0
23	23	H	5	1.079358( 22)	4	110.295( 50)	3	298.665( 77)	0
24	24	H	9	1.077883( 23)	6	107.356( 51)	5	196.639( 78)	0
25	25	H	9	1.084593( 24)	6	108.120( 52)	5	312.575( 79)	0
26	26	H	13	1.075355( 25)	12	119.494( 53)	9	0.147( 80)	0
27	27	H	14	1.075422( 26)	13	119.753( 54)	12	180.121( 81)	0
28	28	H	15	1.075386( 27)	14	120.121( 55)	13	180.076( 82)	0
29	29	H	16	1.075532( 28)	15	120.213( 56)	14	180.160( 83)	0
30	30	H	17	1.076922( 29)	12	119.783( 57)	9	360.142( 84)	0

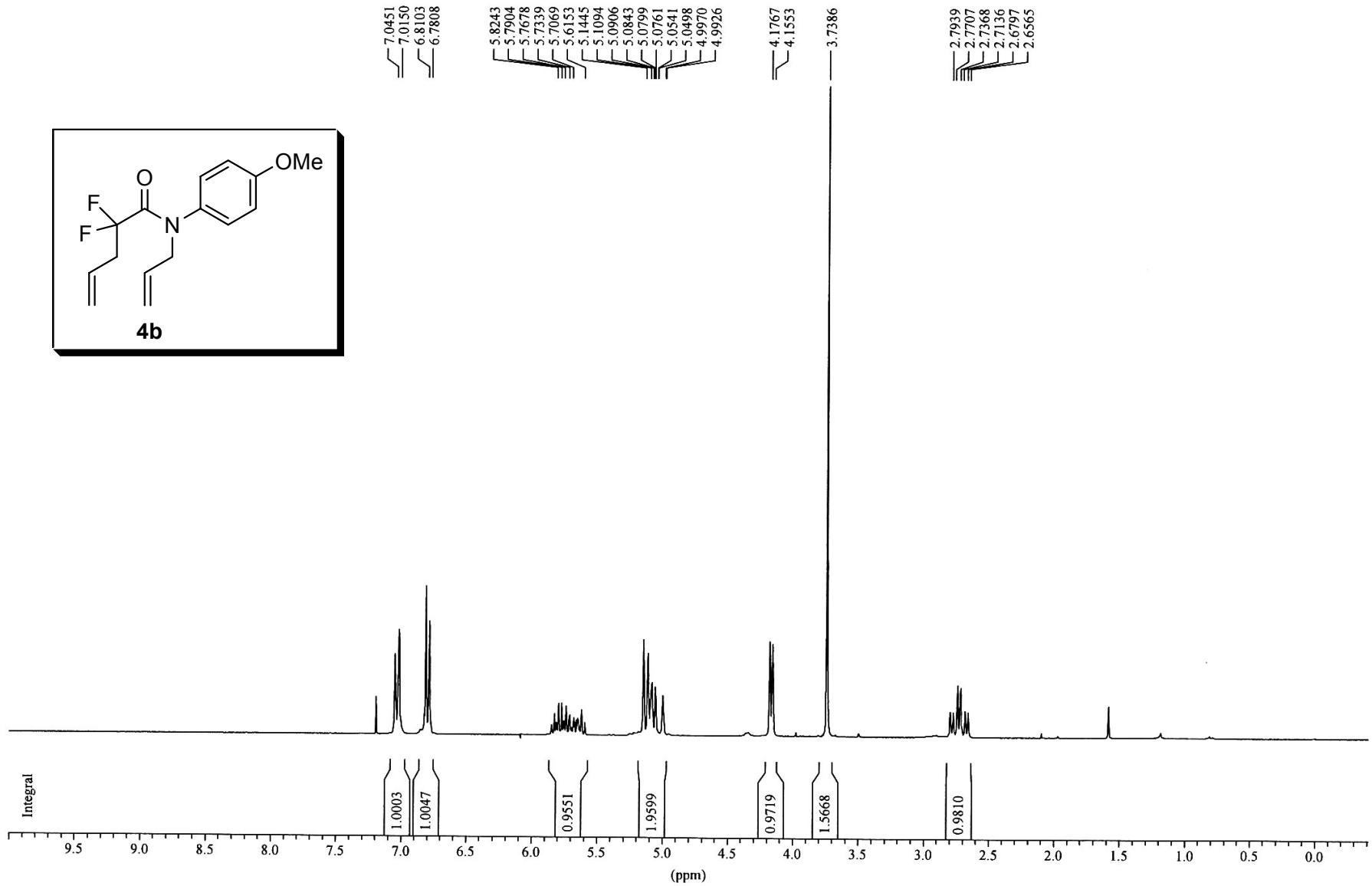
### Conformer 7-4:

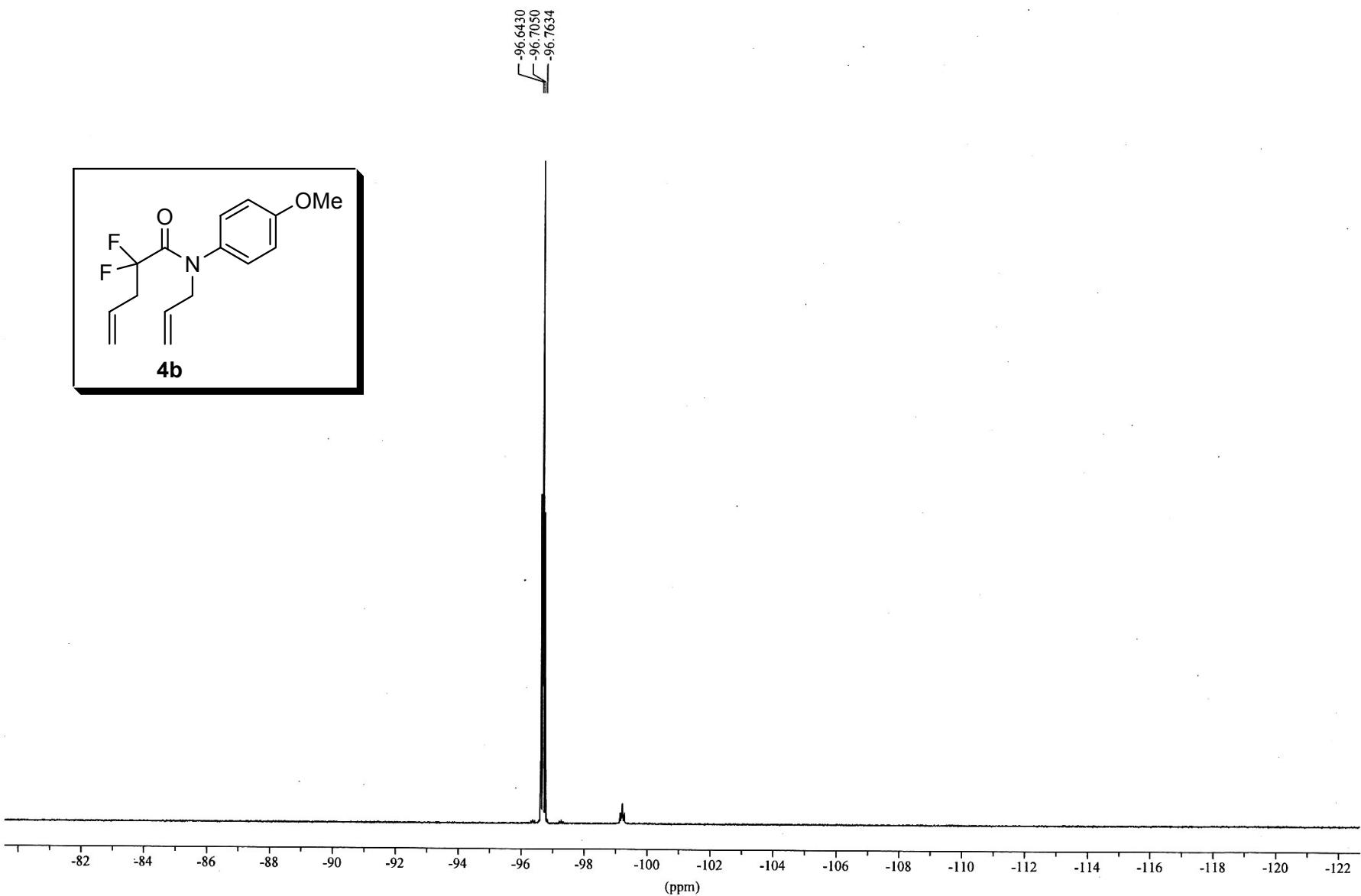
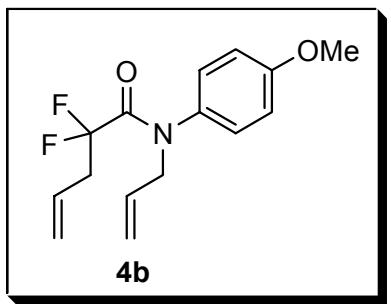


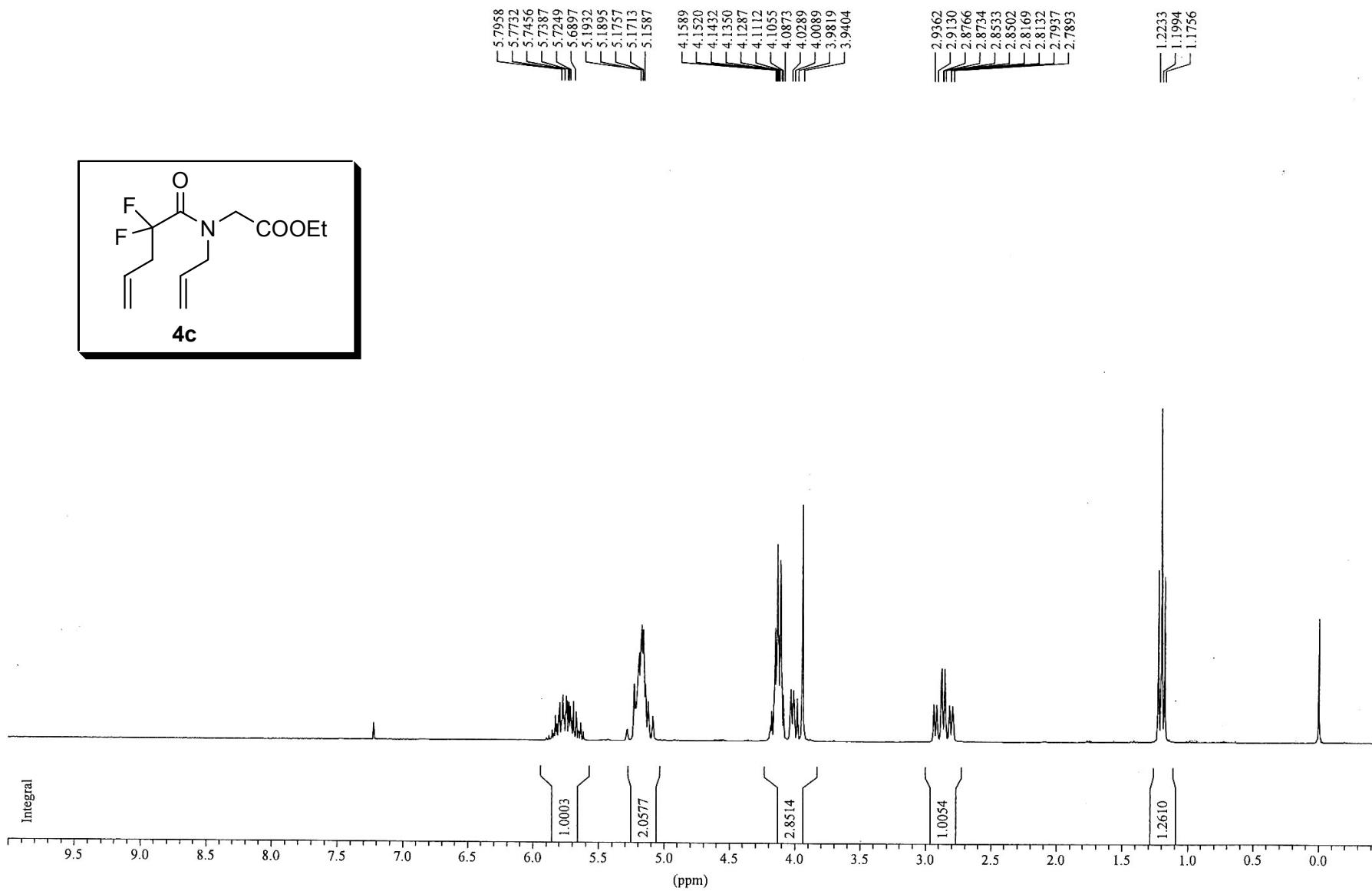
Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.503767( 1)					
3	3	C	2	1.319895( 2)	1	126.984( 30)			
4	4	C	3	1.504480( 3)	2	128.600( 31)	1	358.799( 58)	0
5	5	C	4	1.525715( 4)	3	115.574( 32)	2	350.184( 59)	0
6	6	N	5	1.459188( 5)	4	114.064( 33)	3	63.589( 60)	0
7	7	C	1	1.542830( 6)	2	115.118( 34)	3	315.301( 61)	0
8	8	O	7	1.196534( 7)	1	119.000( 35)	2	245.266( 62)	0
9	9	C	6	1.462057( 8)	5	118.016( 36)	4	108.794( 63)	0
10	10	F	1	1.355472( 9)	2	111.402( 37)	3	79.247( 64)	0
11	11	F	1	1.333001( 10)	2	107.890( 38)	3	195.062( 65)	0
12	12	C	9	1.516516( 11)	6	113.907( 39)	5	287.356( 66)	0
13	13	C	12	1.386598( 12)	9	120.973( 40)	6	112.374( 67)	0
14	14	C	13	1.389112( 13)	12	120.808( 41)	9	179.893( 68)	0
15	15	C	14	1.382049( 14)	13	119.984( 42)	12	359.985( 69)	0
16	16	C	15	1.389173( 15)	14	119.646( 43)	13	359.776( 70)	0
17	17	C	12	1.394053( 16)	9	120.235( 44)	6	291.915( 71)	0
18	18	H	2	1.074748( 17)	1	113.084( 45)	7	134.628( 72)	0
19	19	H	3	1.077441( 18)	2	116.800( 46)	1	178.828( 73)	0
20	20	H	4	1.086445( 19)	3	108.744( 47)	2	114.200( 74)	0
21	21	H	4	1.087956( 20)	3	107.893( 48)	2	229.085( 75)	0
22	22	H	5	1.080540( 21)	4	108.426( 49)	3	182.235( 76)	0
23	23	H	5	1.080318( 22)	4	110.208( 50)	3	299.017( 77)	0
24	24	H	9	1.083883( 23)	6	107.809( 51)	5	49.369( 78)	0
25	25	H	9	1.077617( 24)	6	107.246( 52)	5	165.148( 79)	0
26	26	H	13	1.076820( 25)	12	119.776( 53)	9	360.291( 80)	0
27	27	H	14	1.075527( 26)	13	119.819( 54)	12	180.073( 81)	0
28	28	H	15	1.075389( 27)	14	120.217( 55)	13	180.089( 82)	0
29	29	H	16	1.075490( 28)	15	119.974( 56)	14	180.555( 83)	0
30	30	H	17	1.075386( 29)	12	119.407( 57)	9	359.509( 84)	0

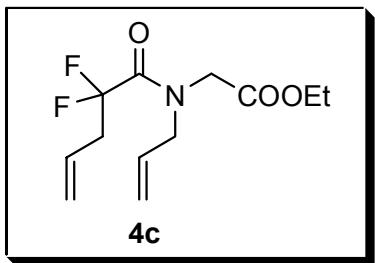




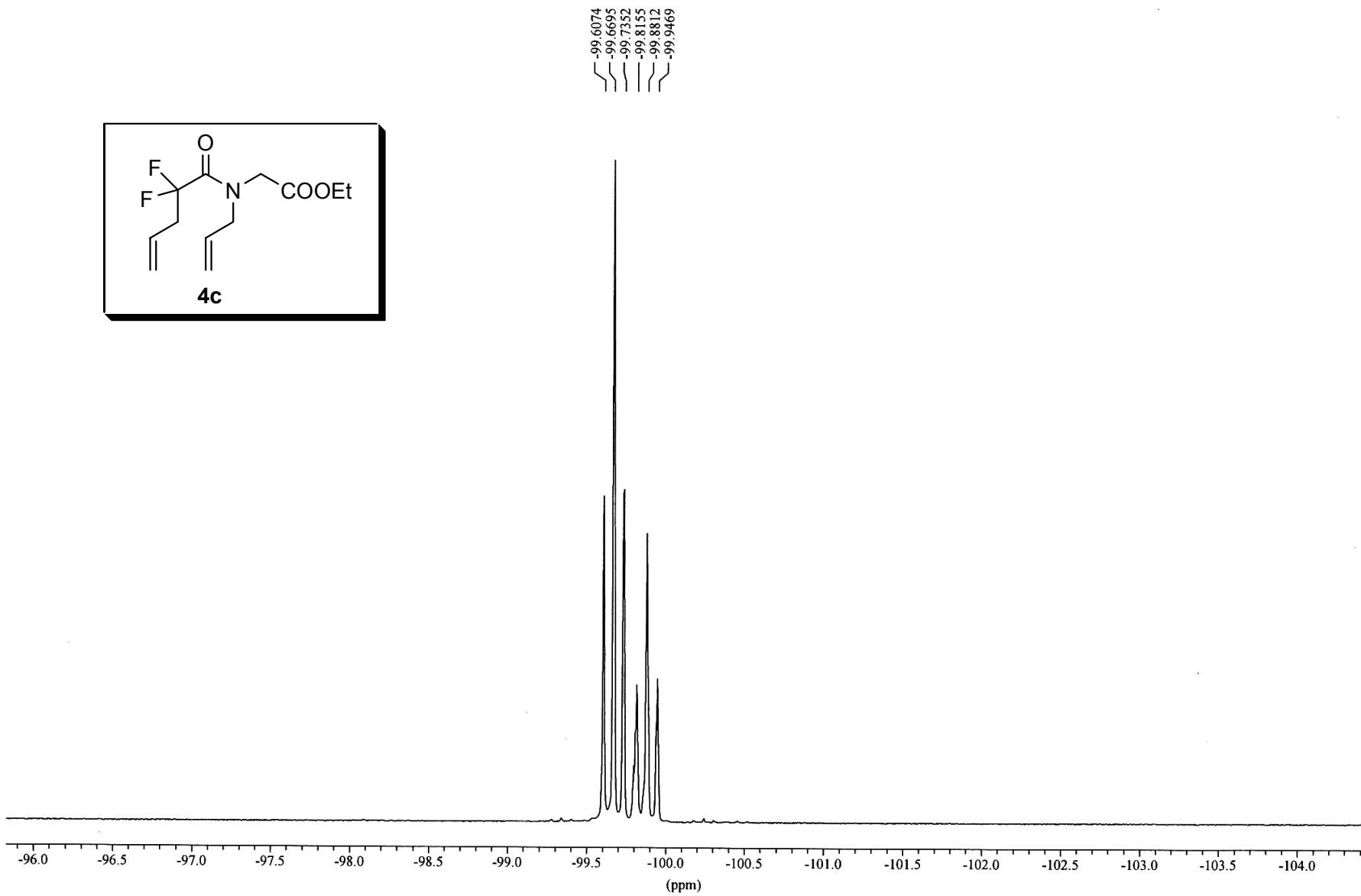


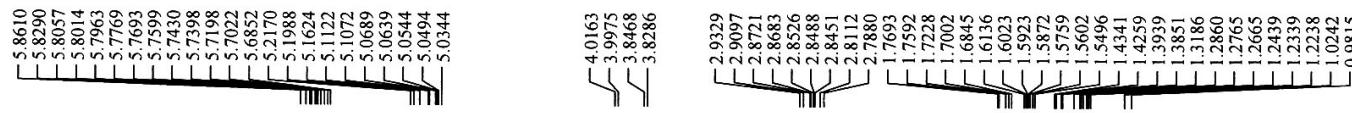
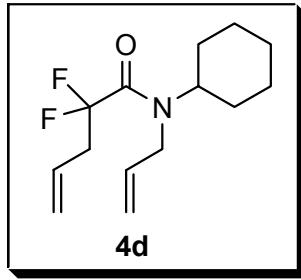
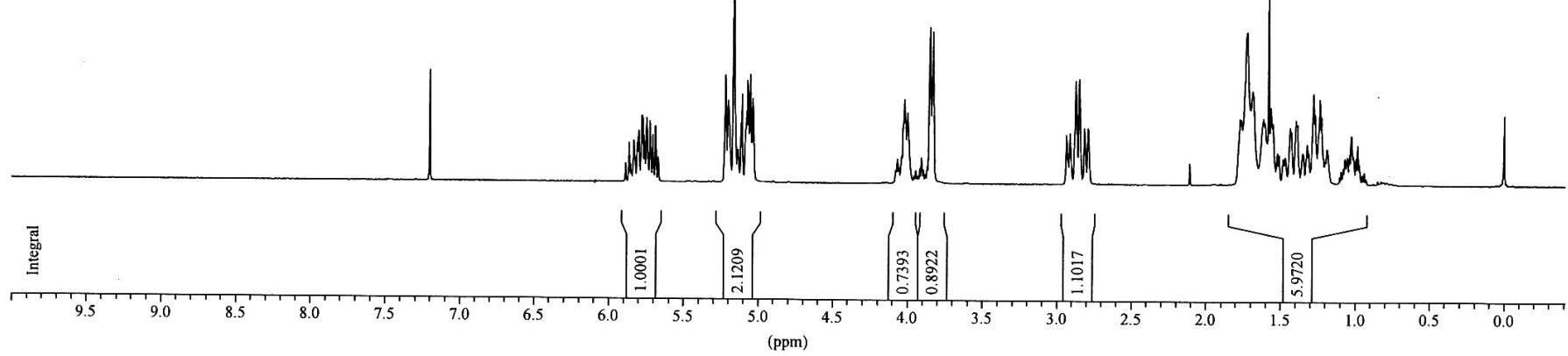


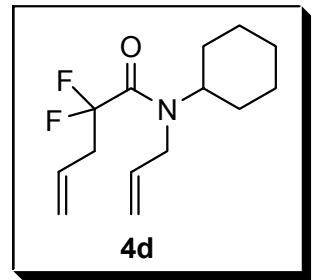




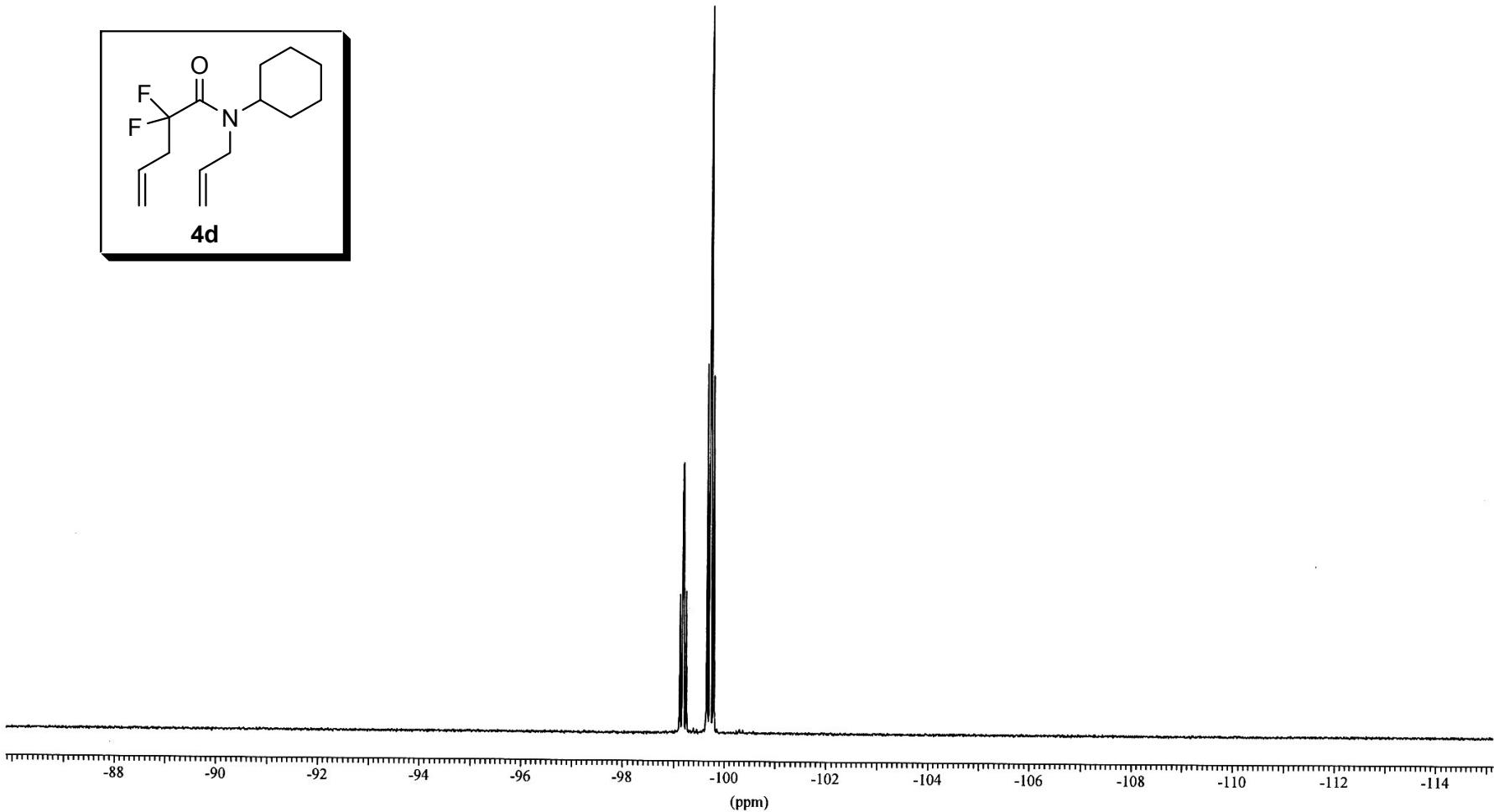
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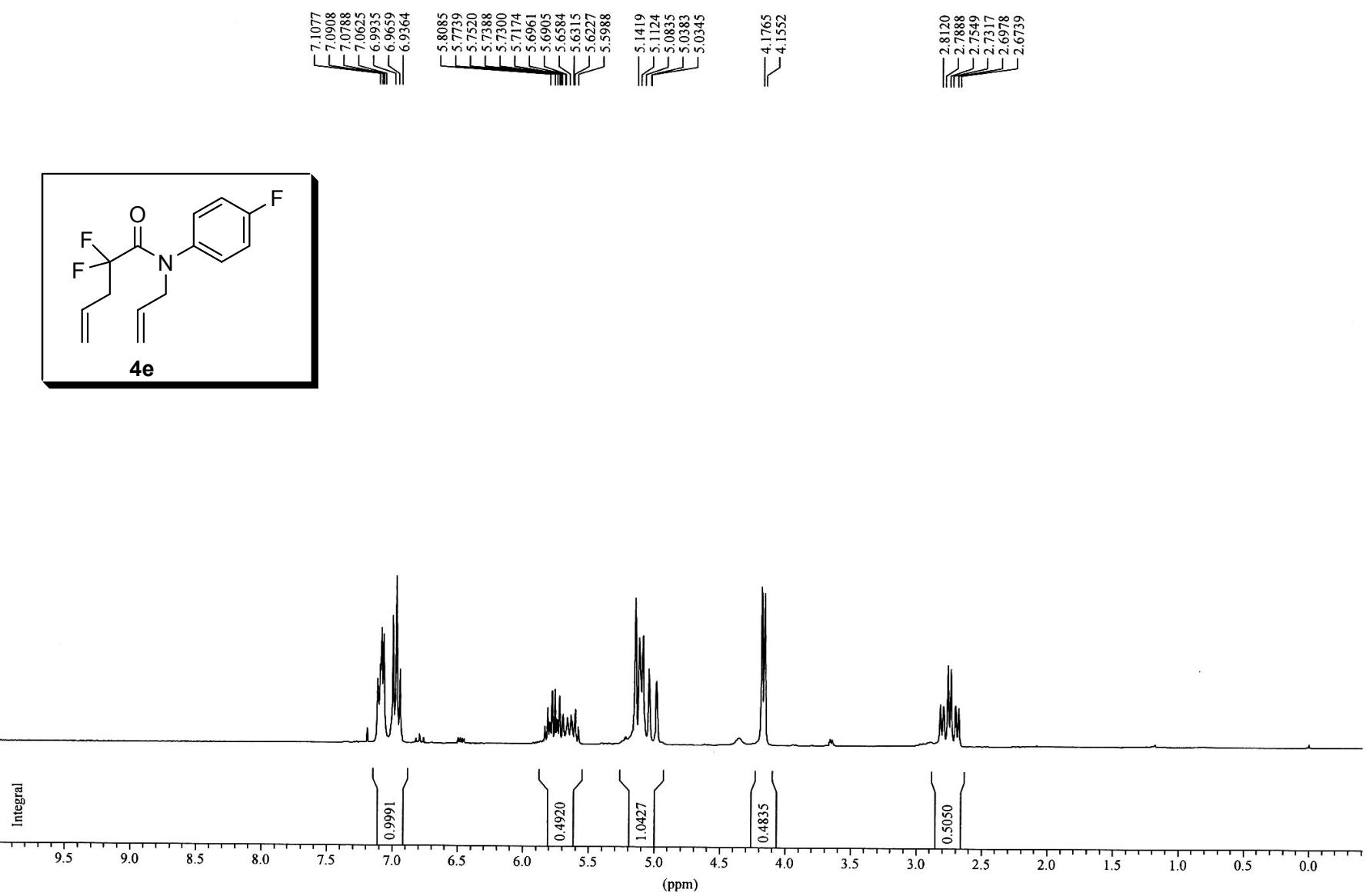


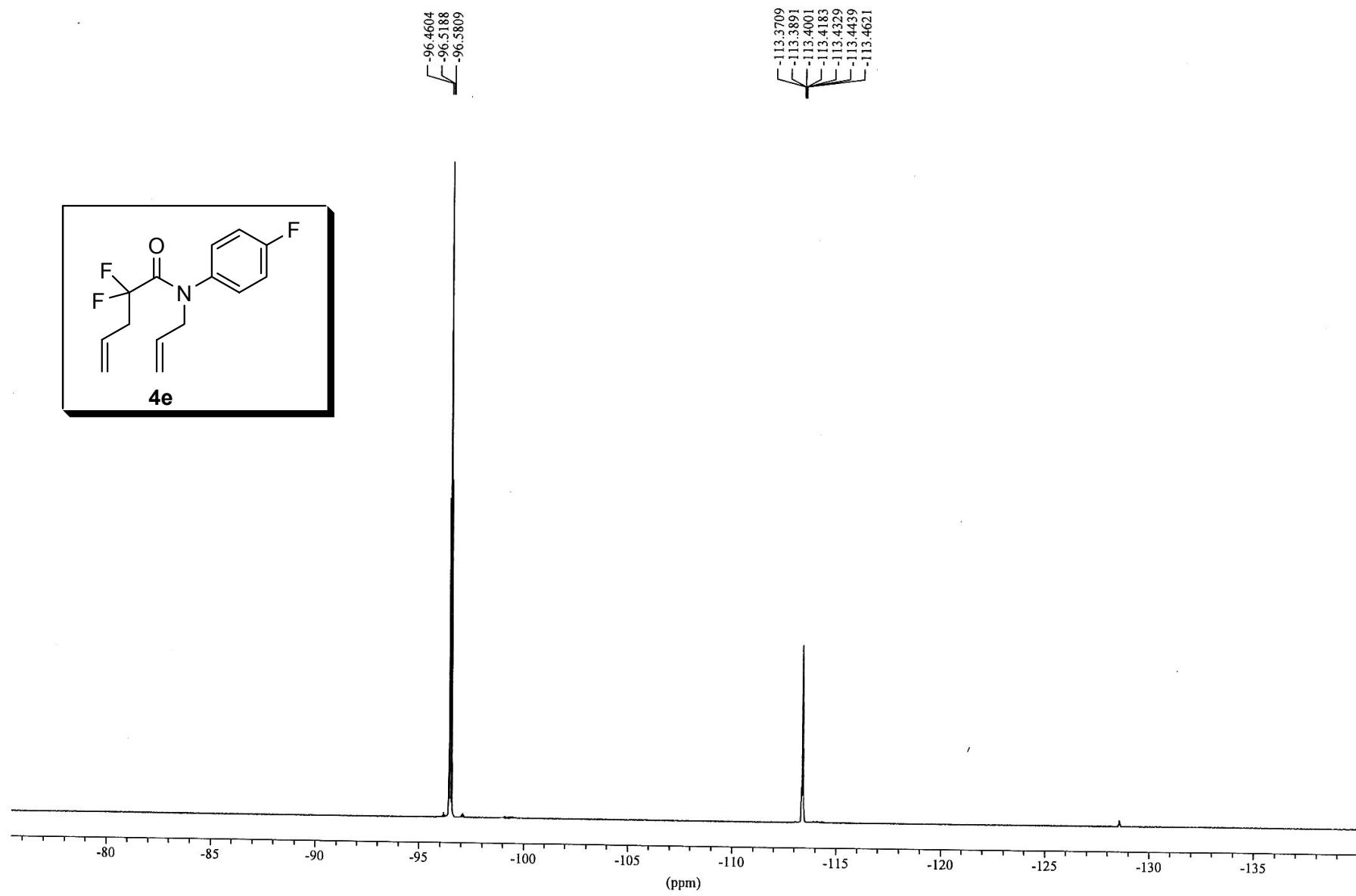


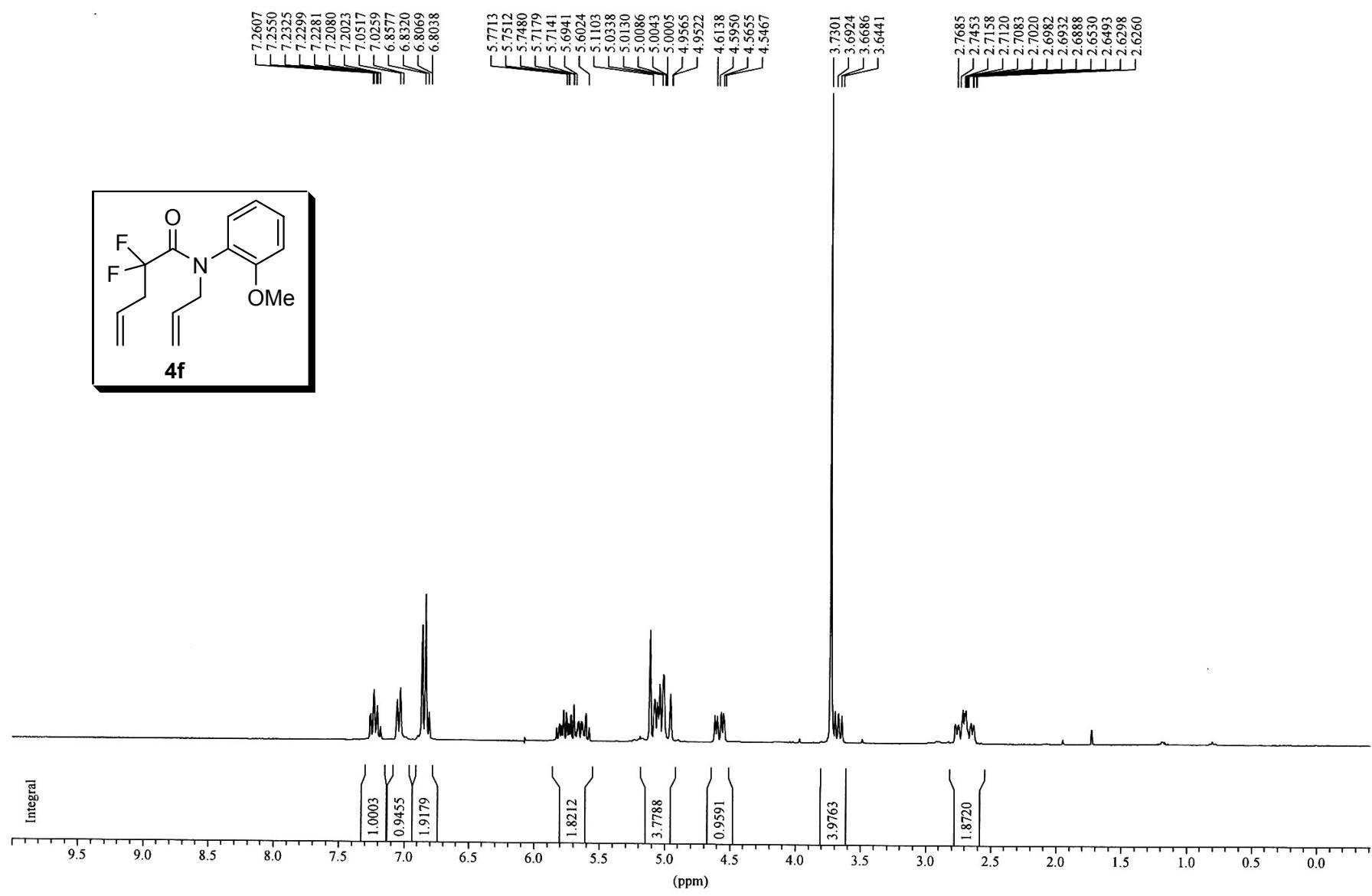


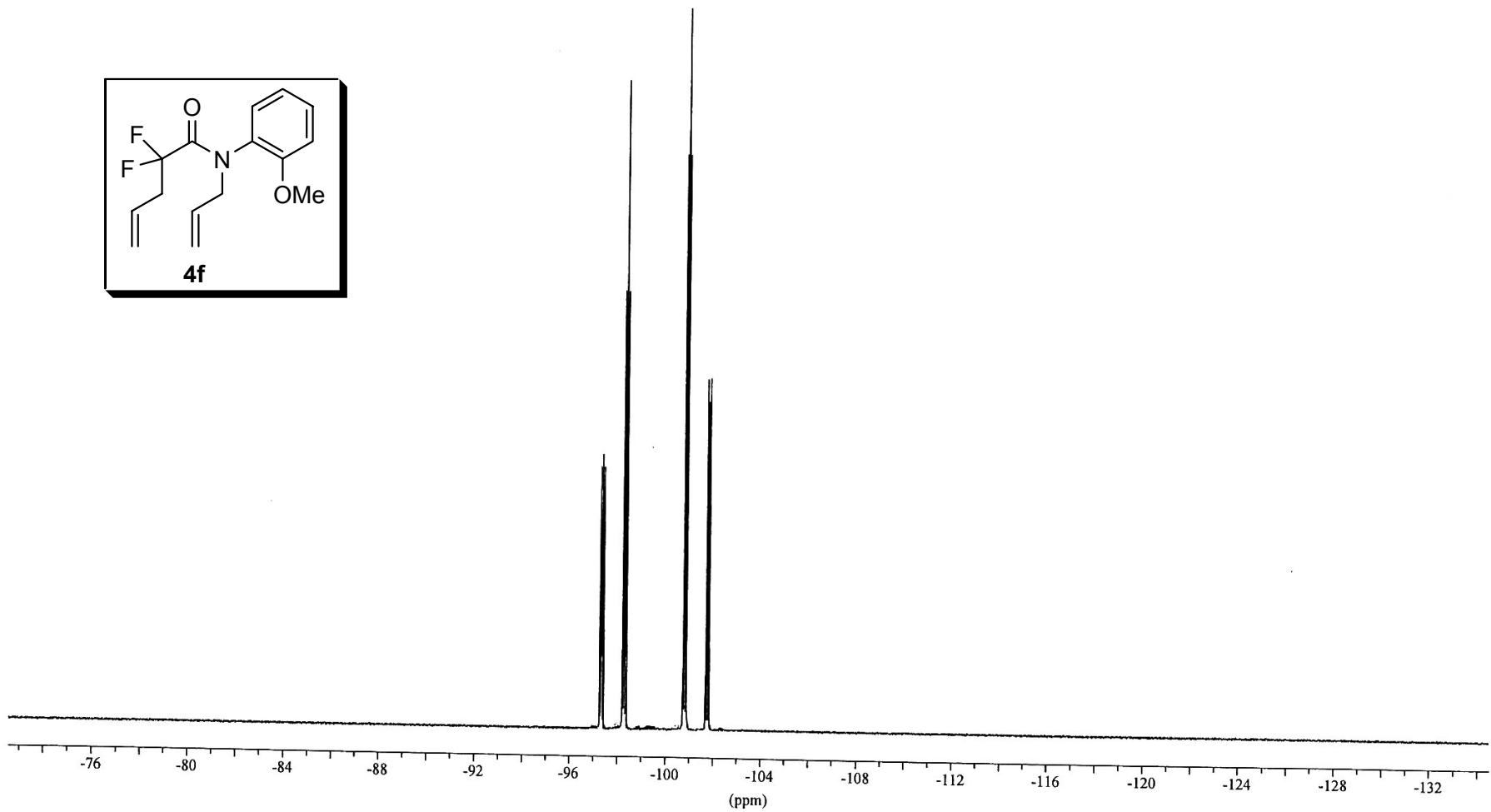
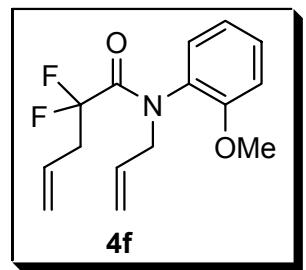
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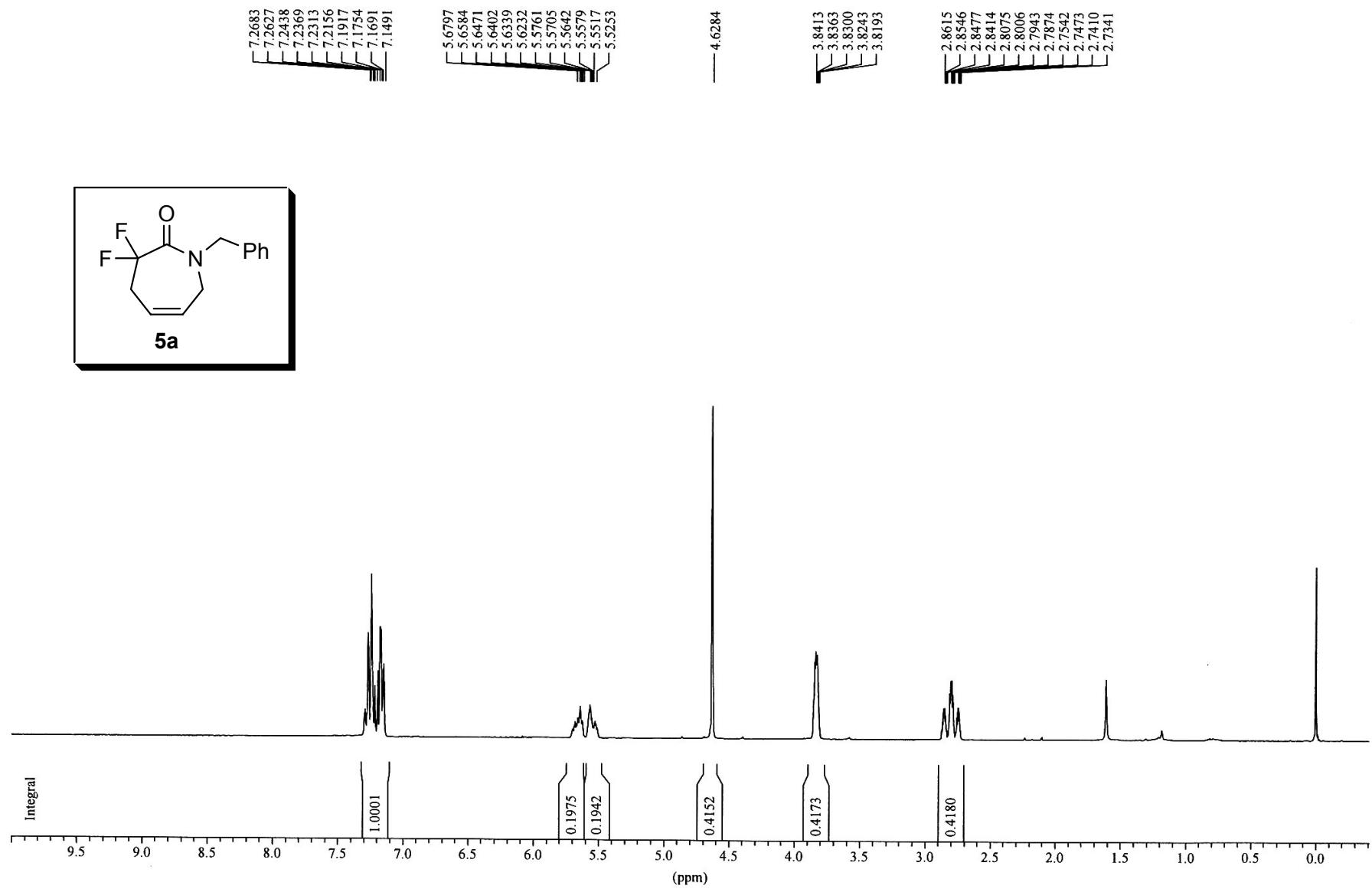


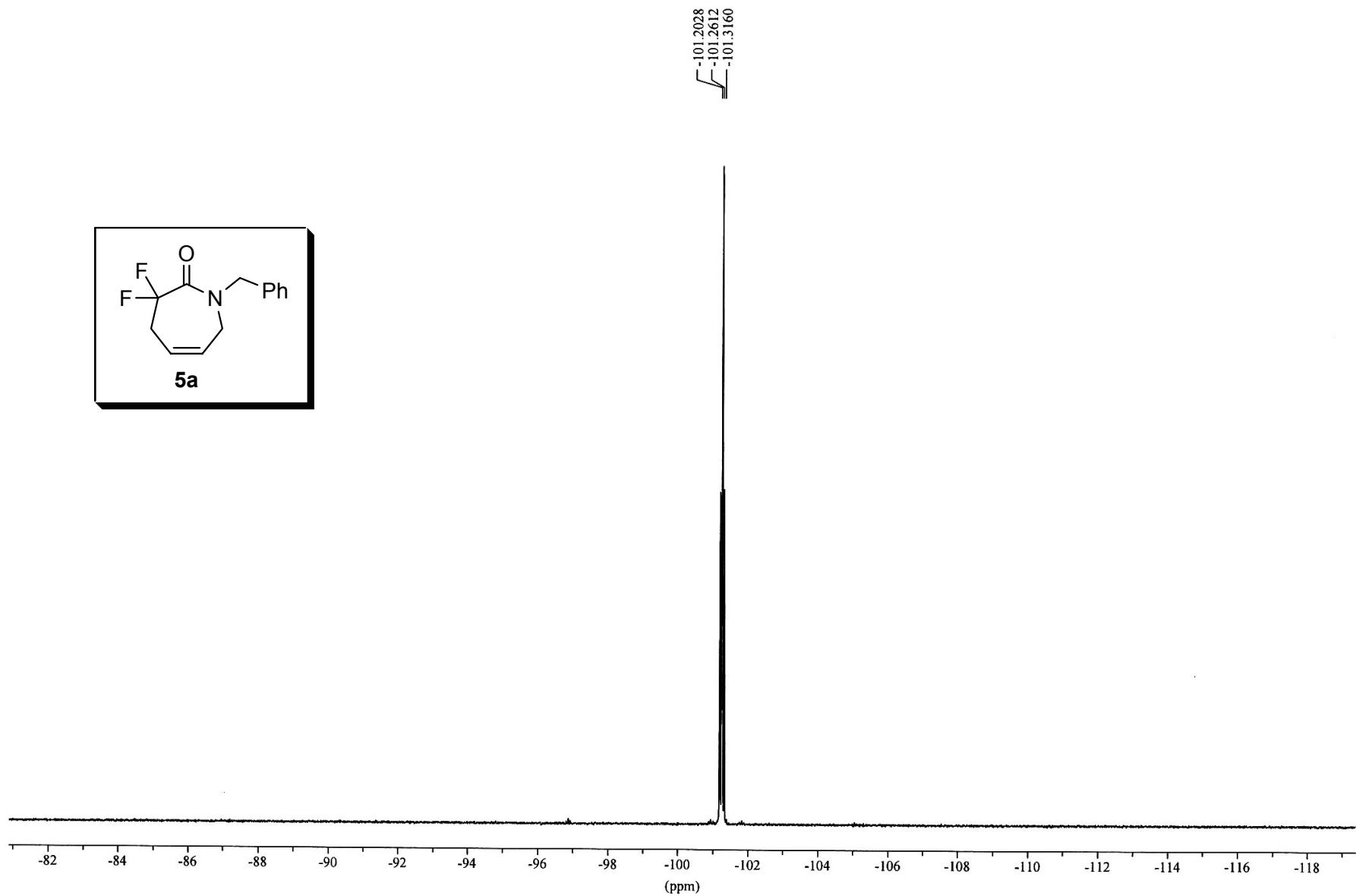
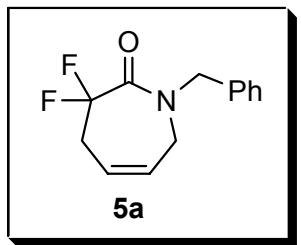


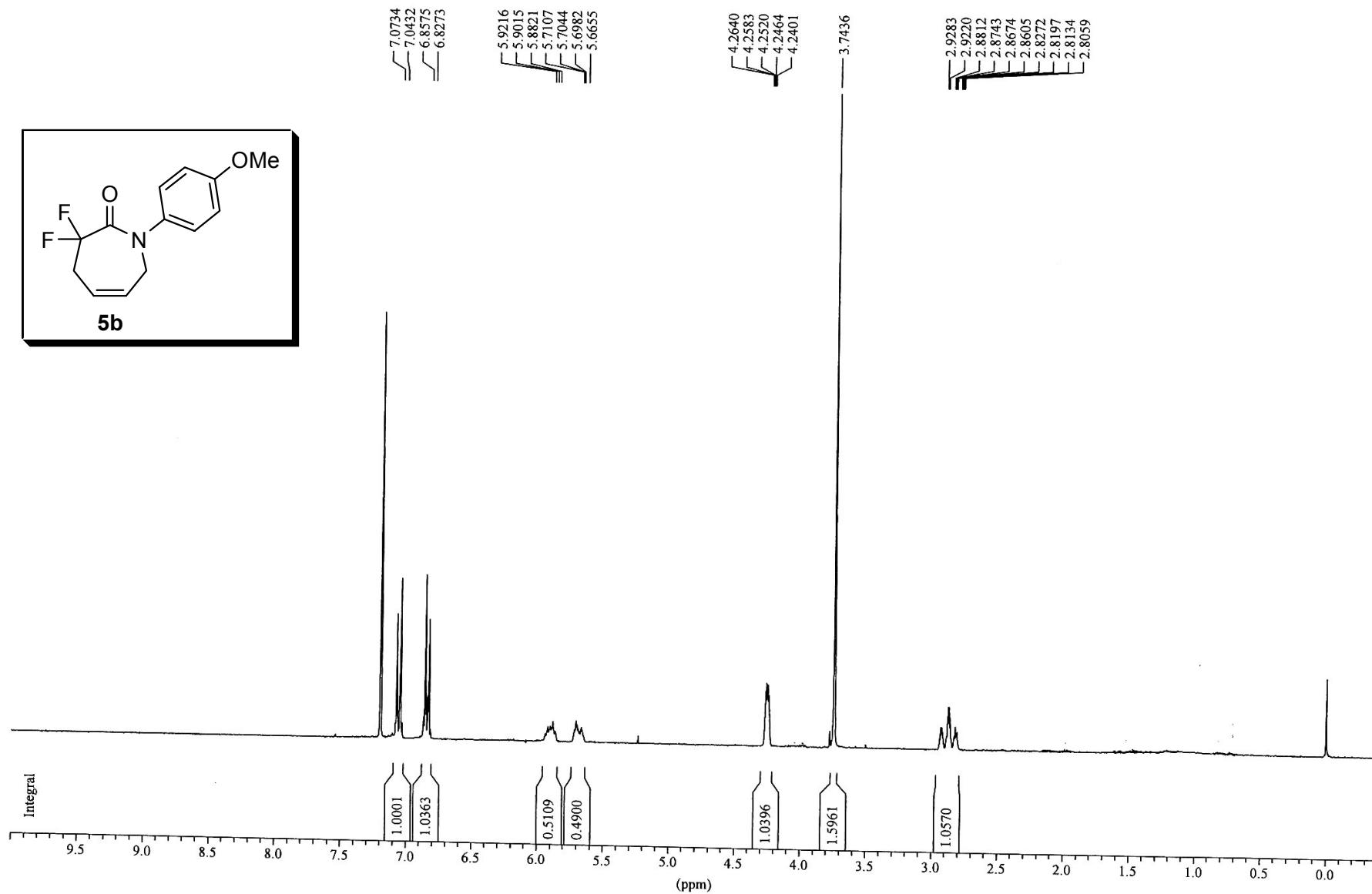


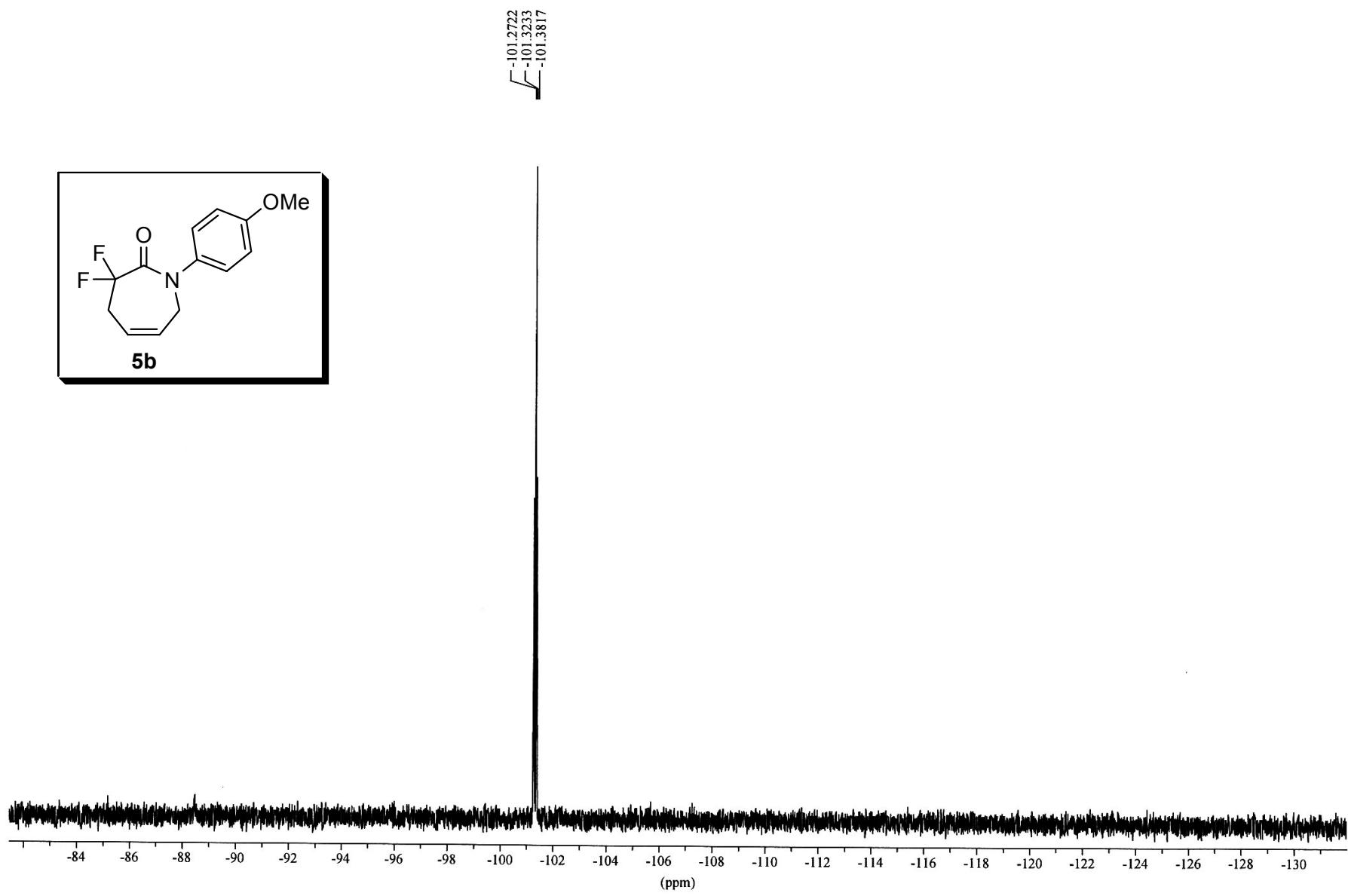


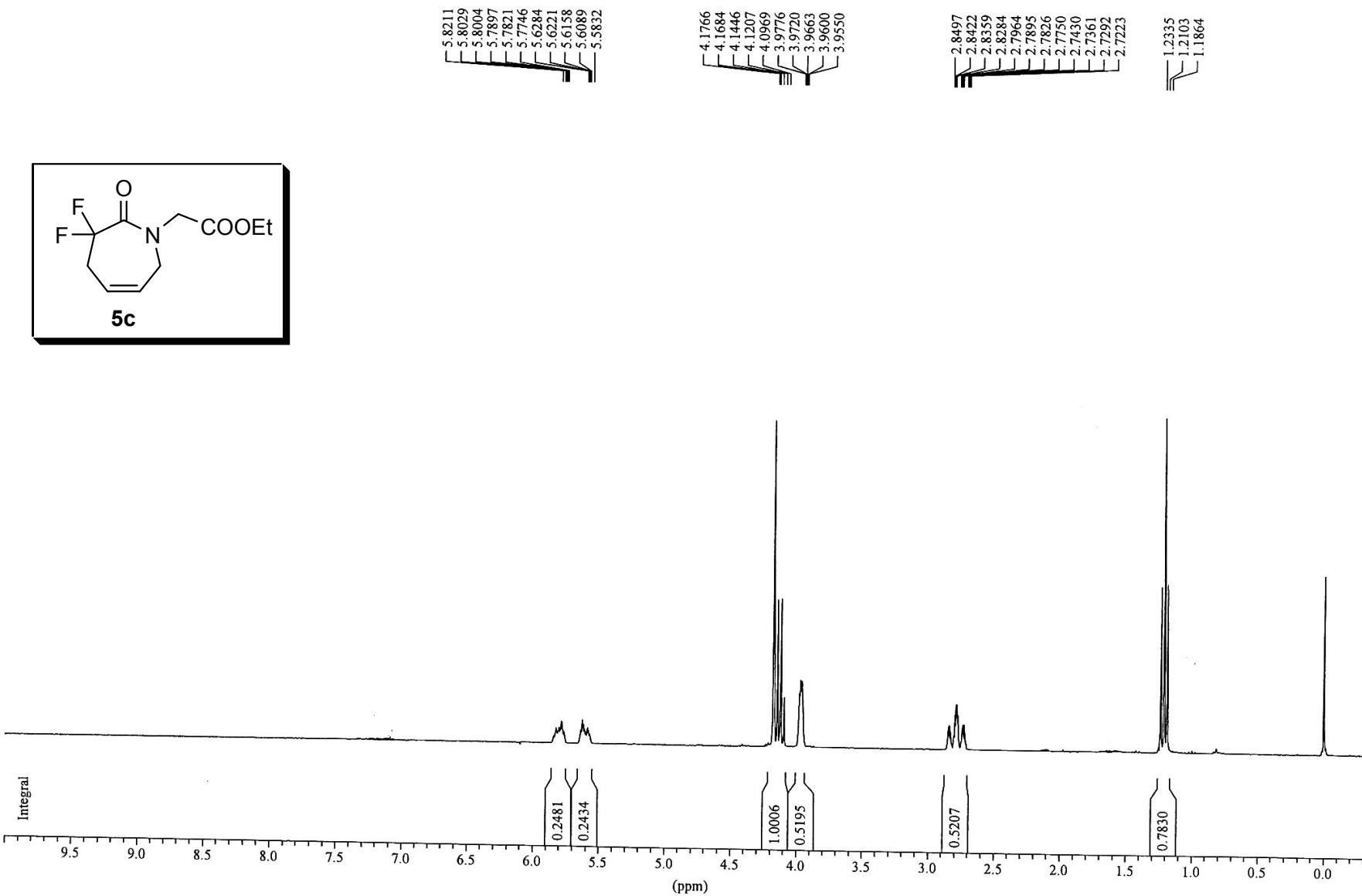


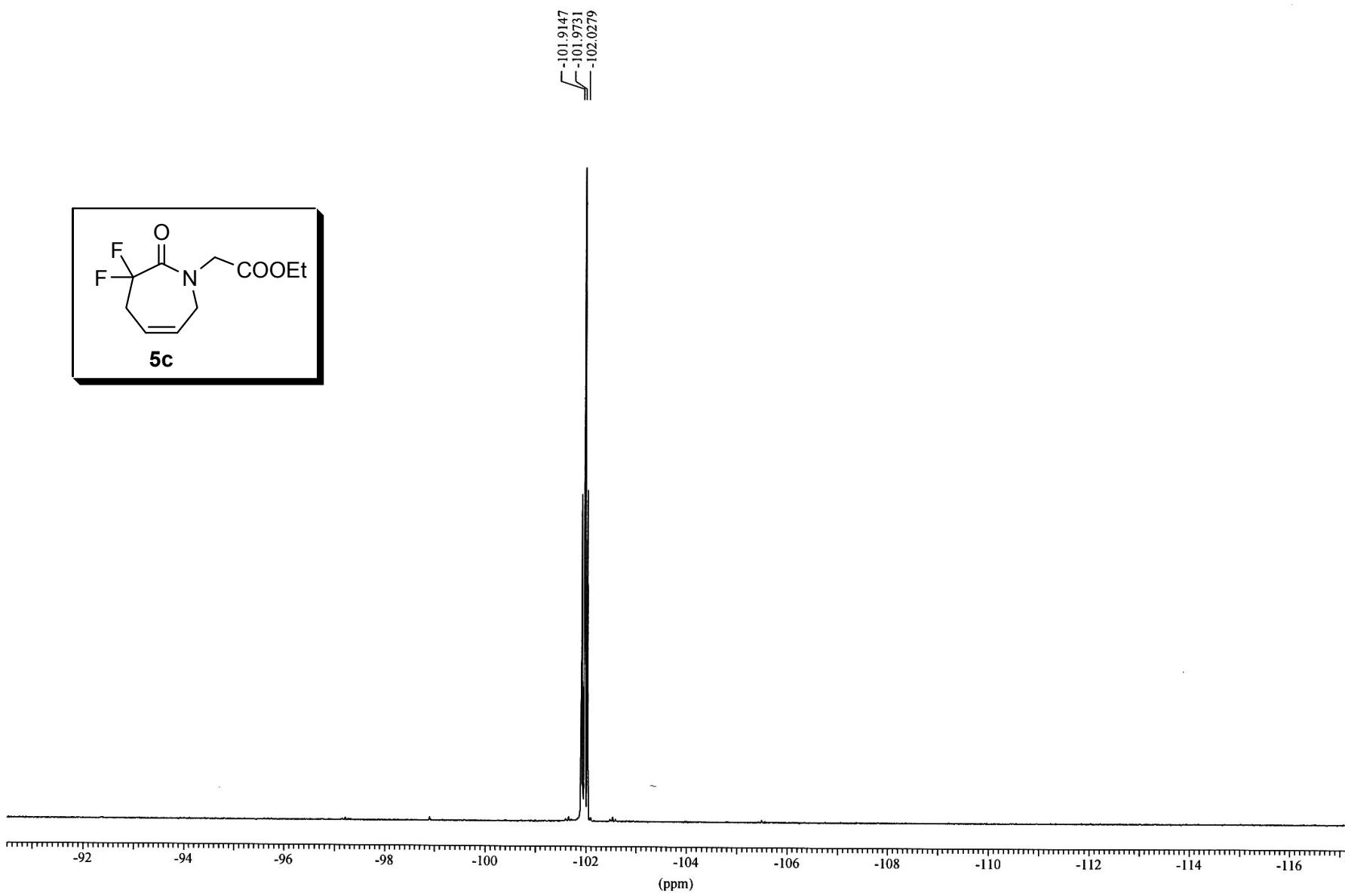


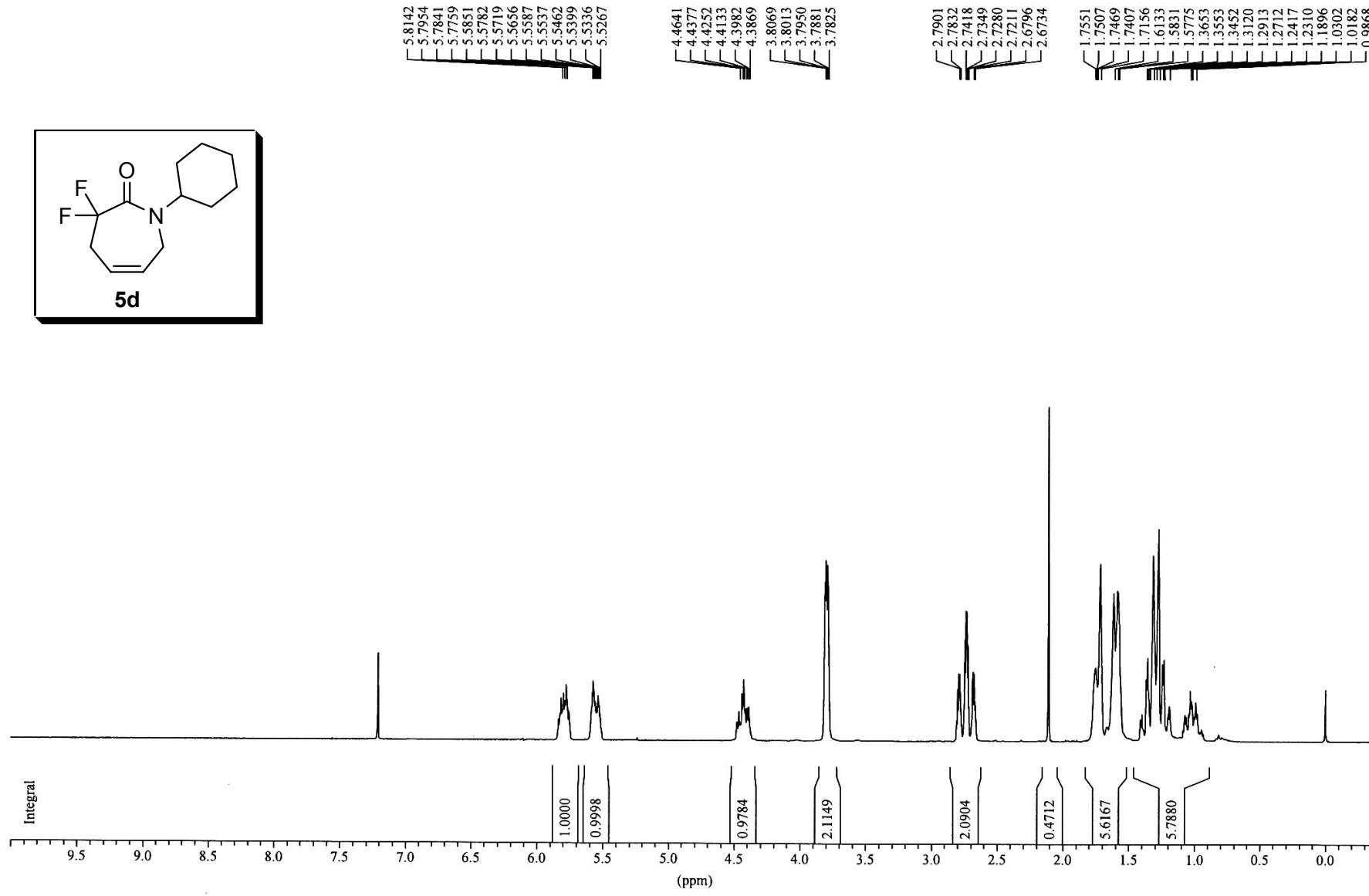


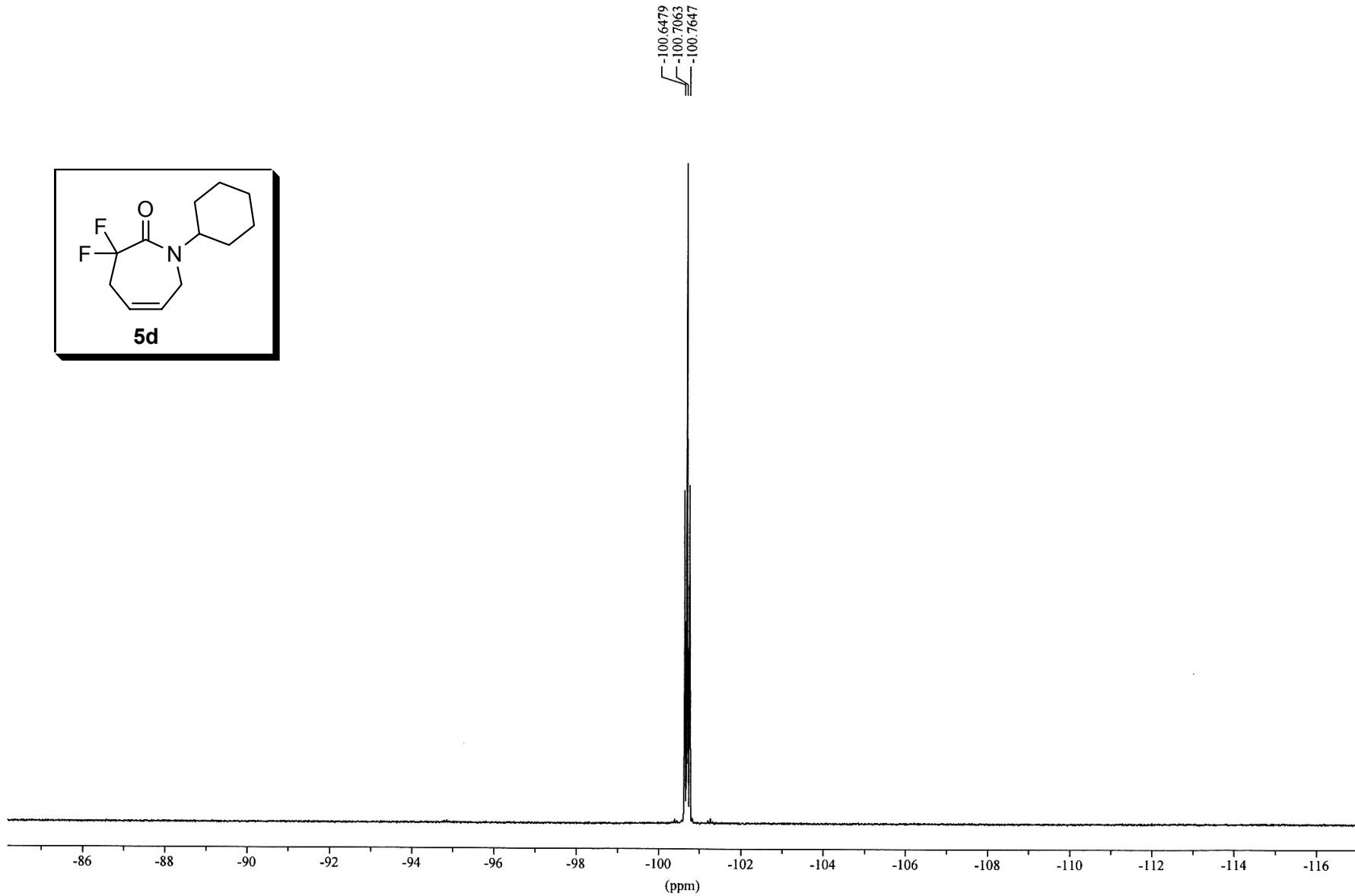
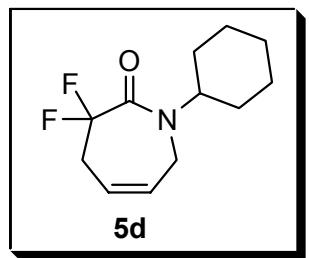


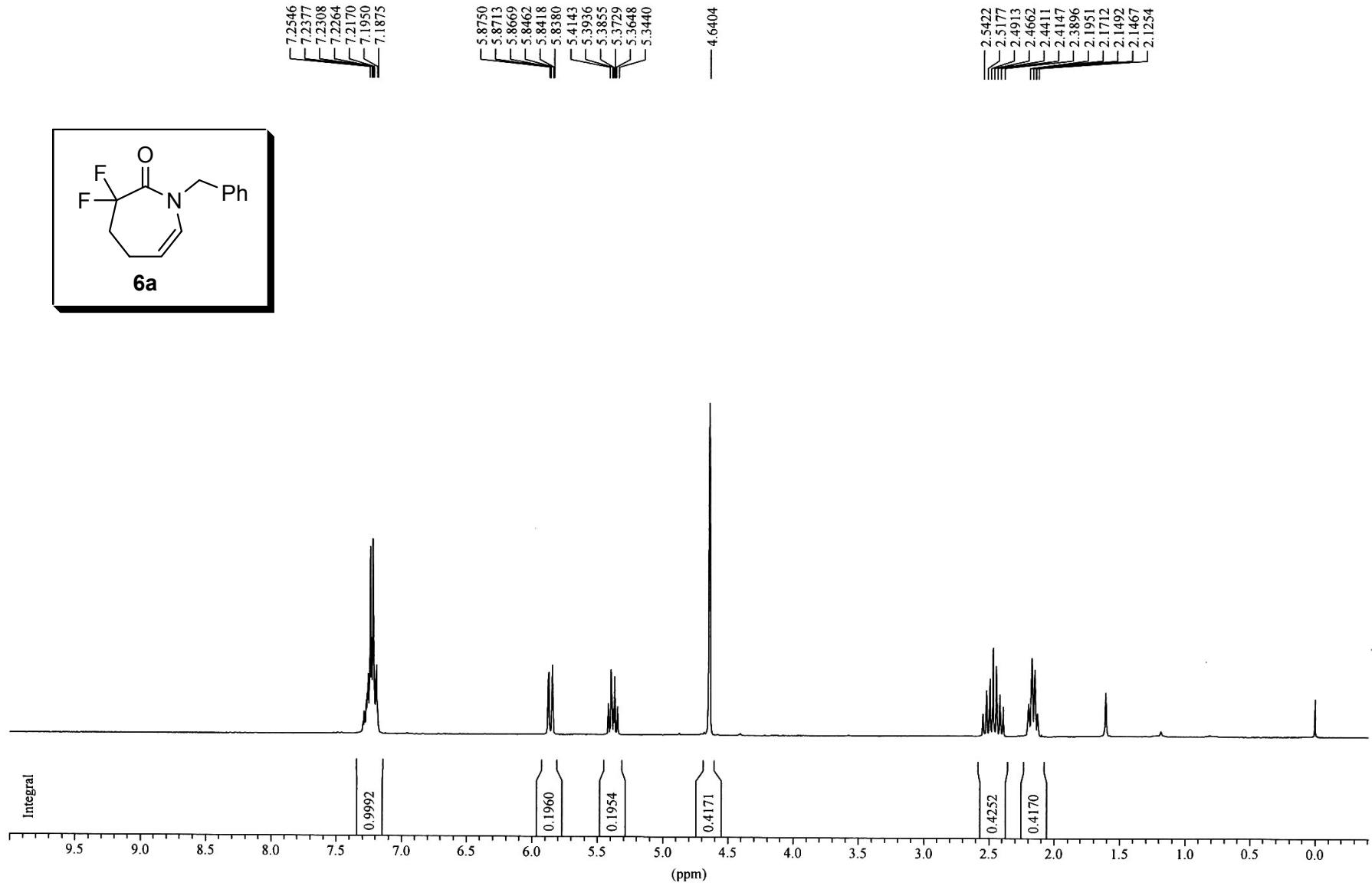


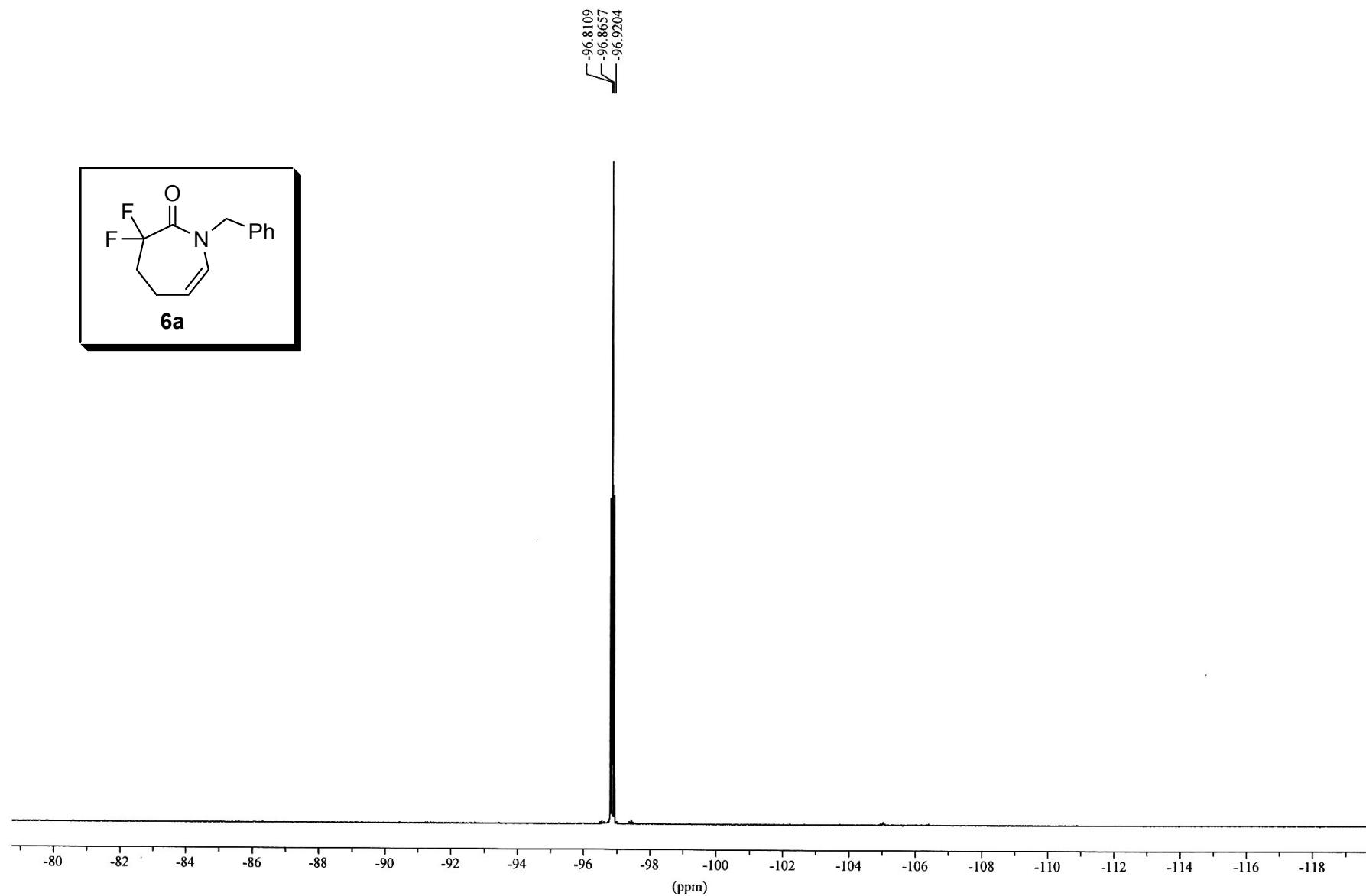
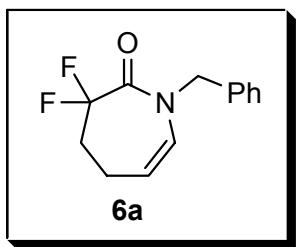


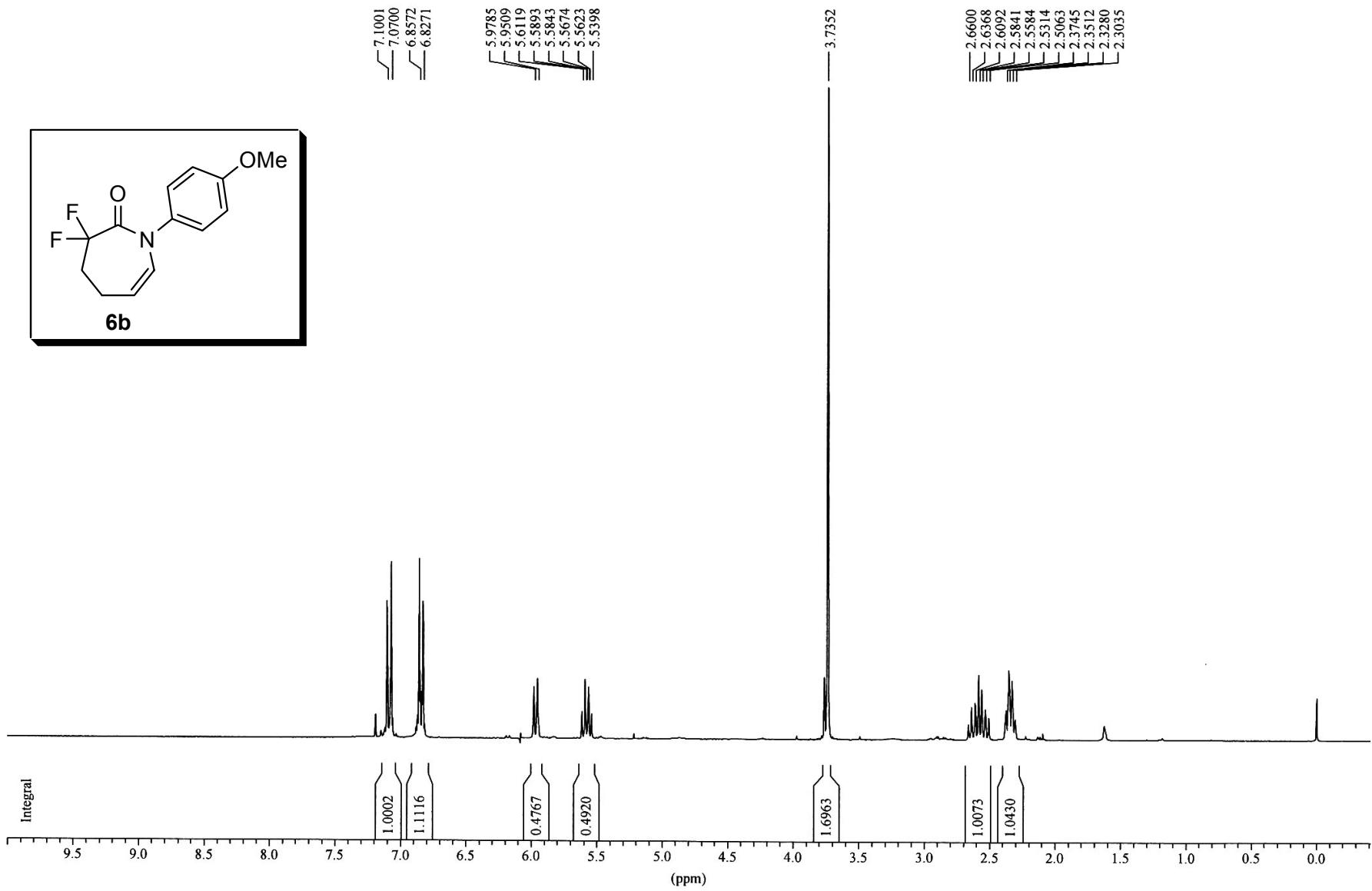


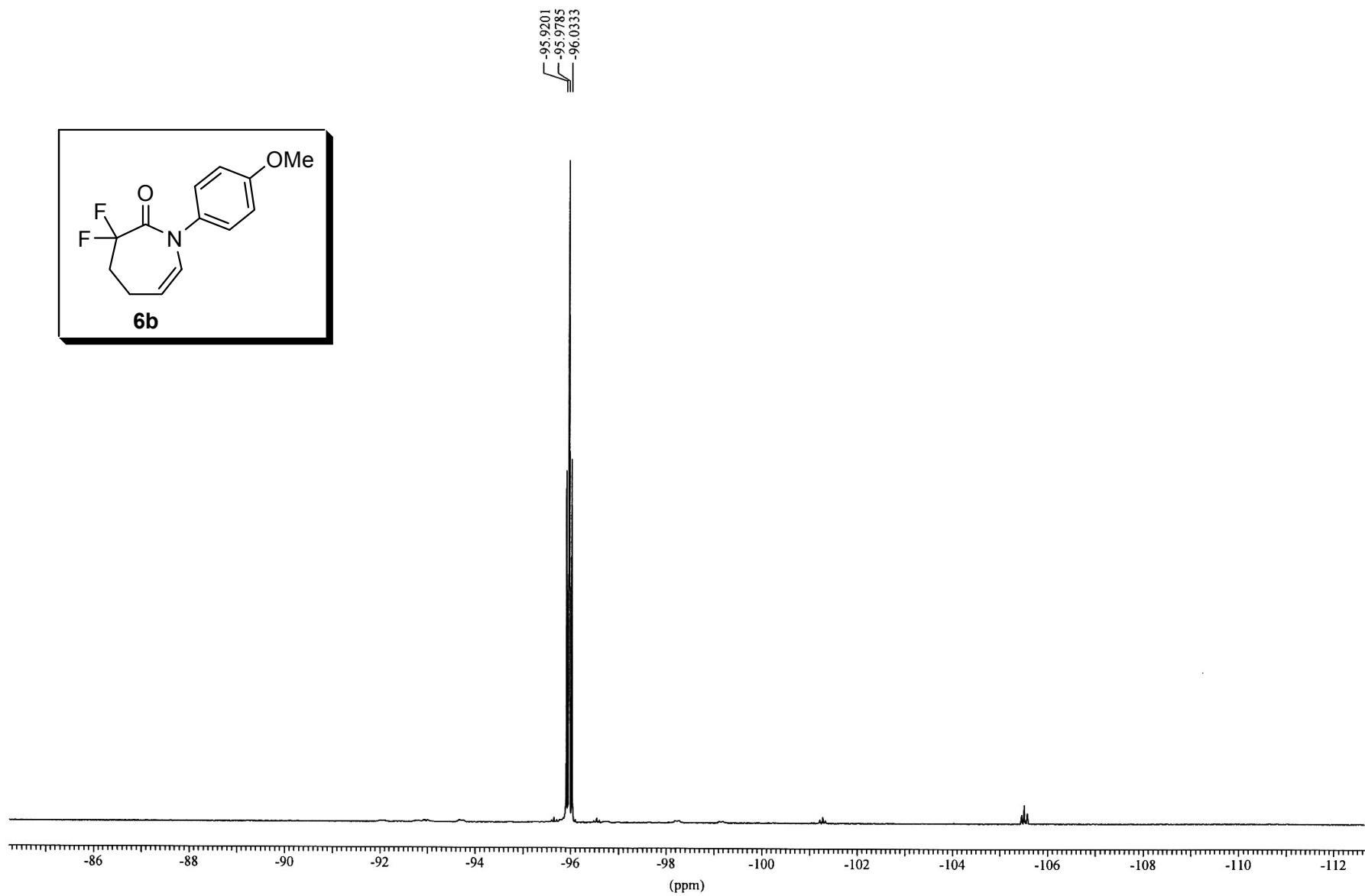
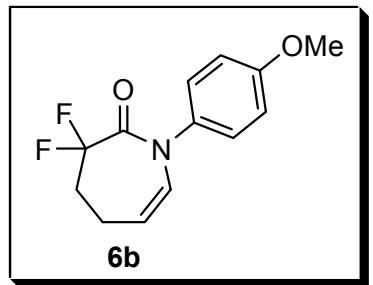


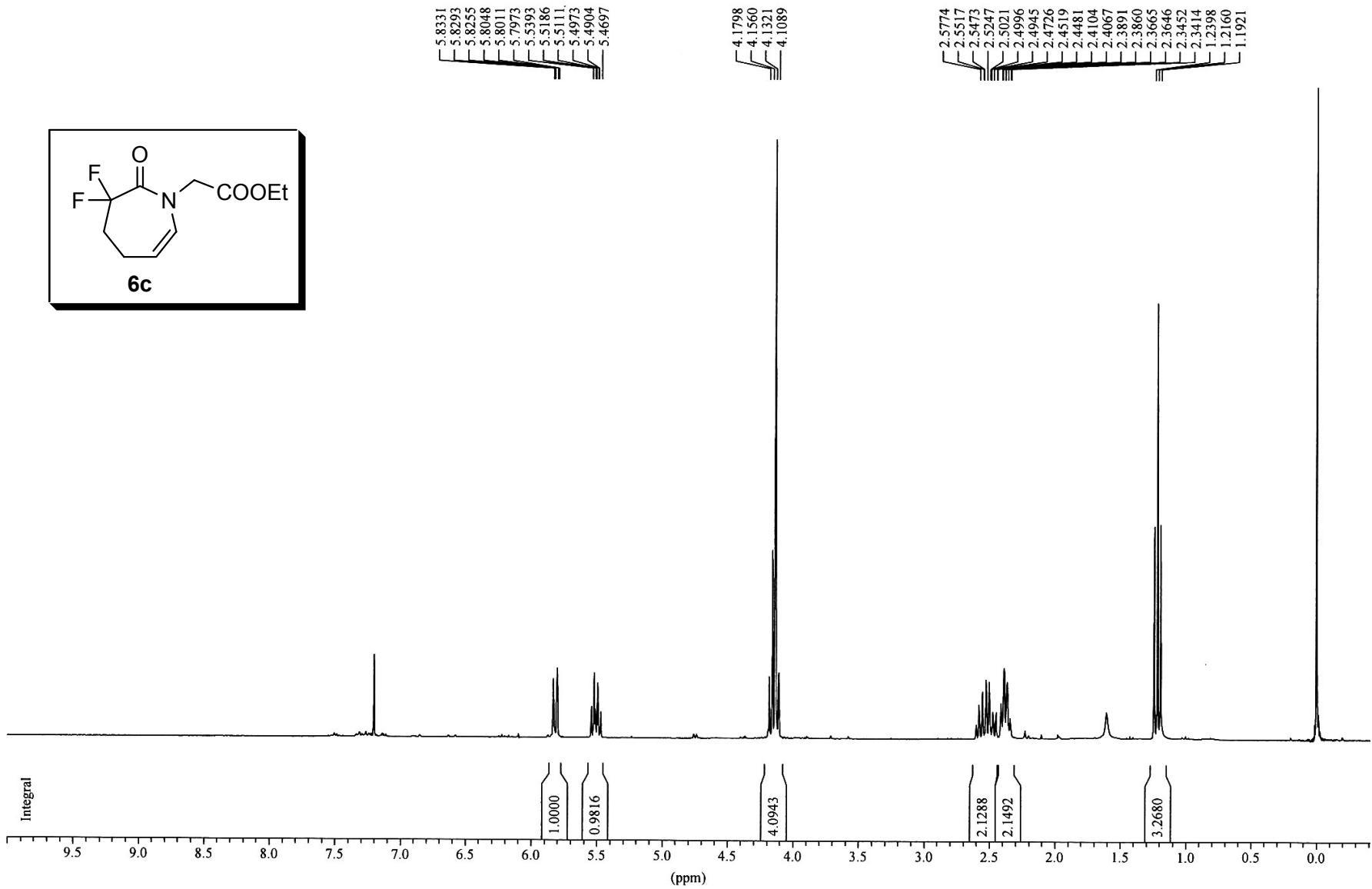


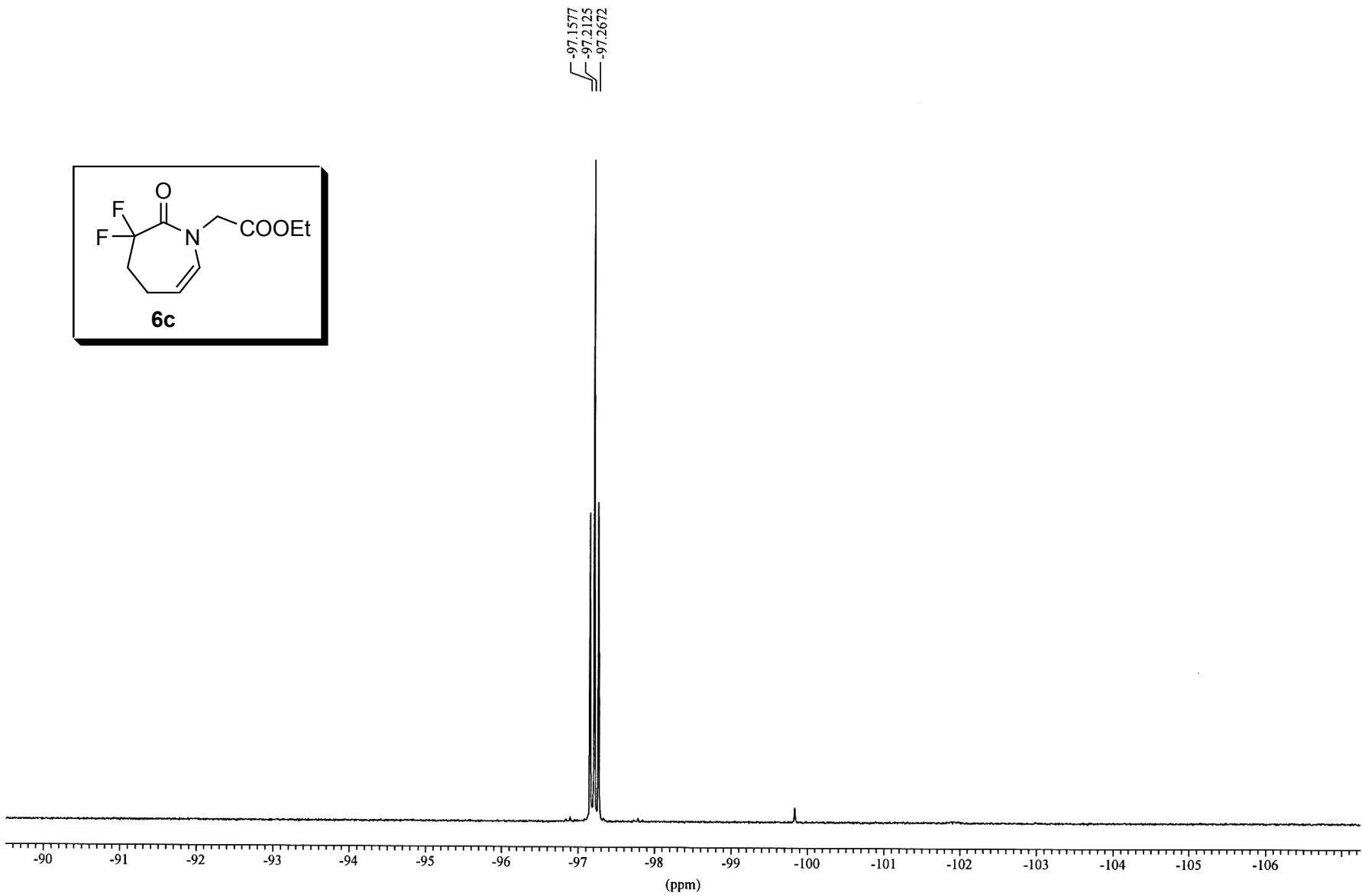
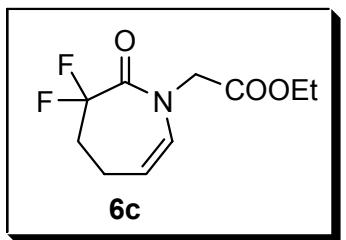


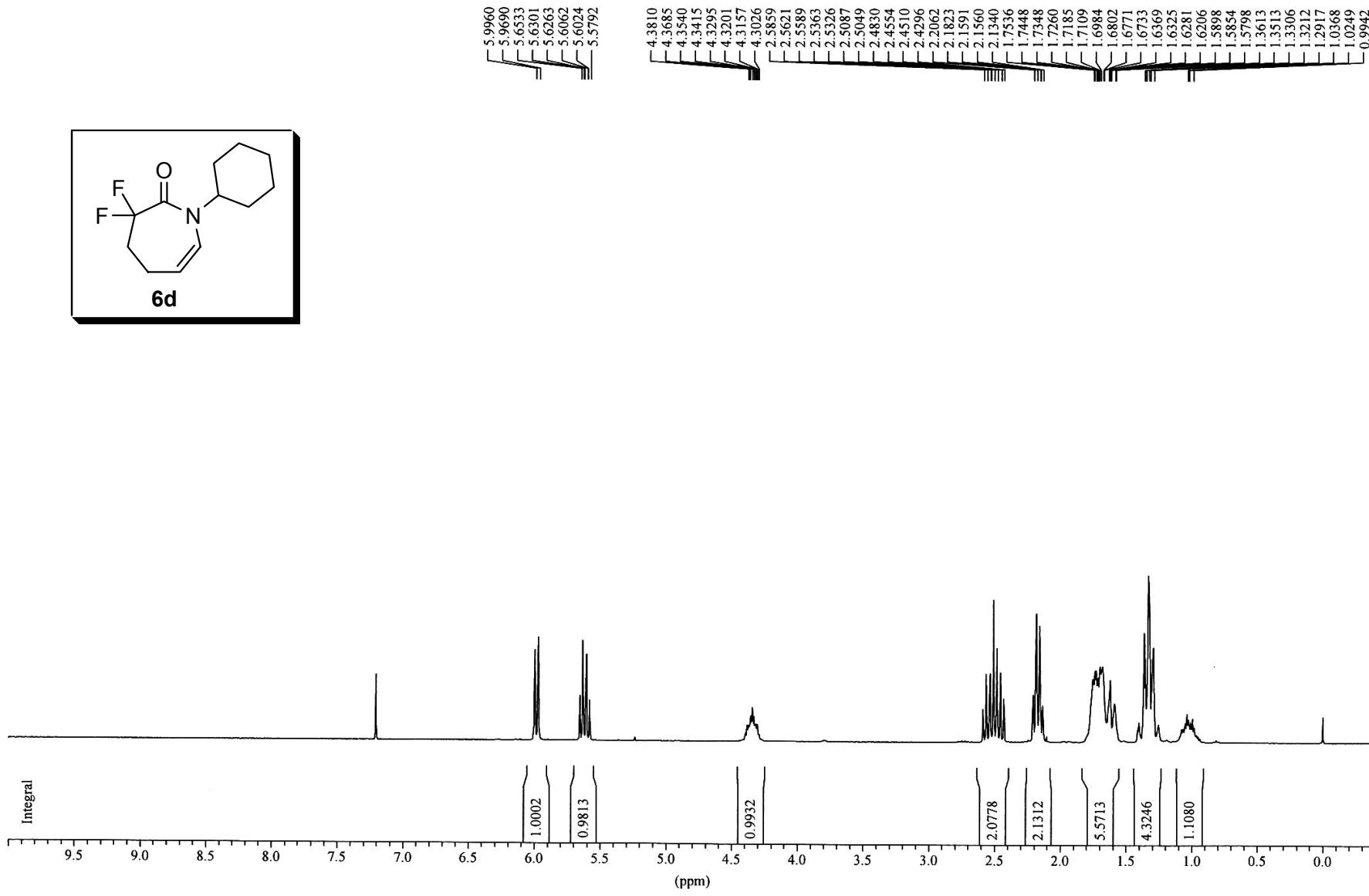


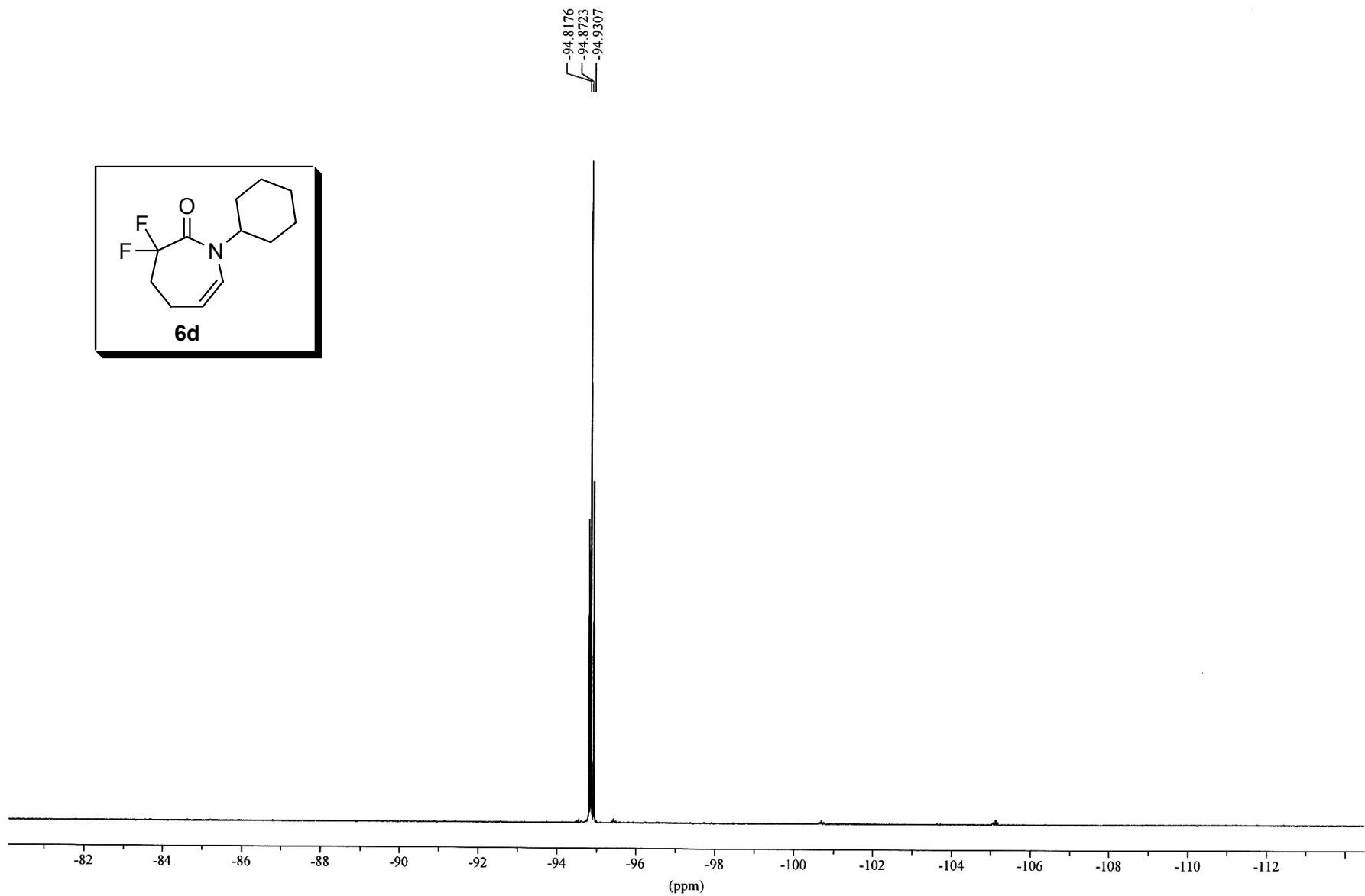
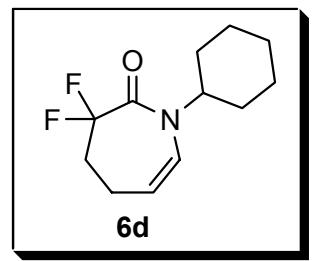


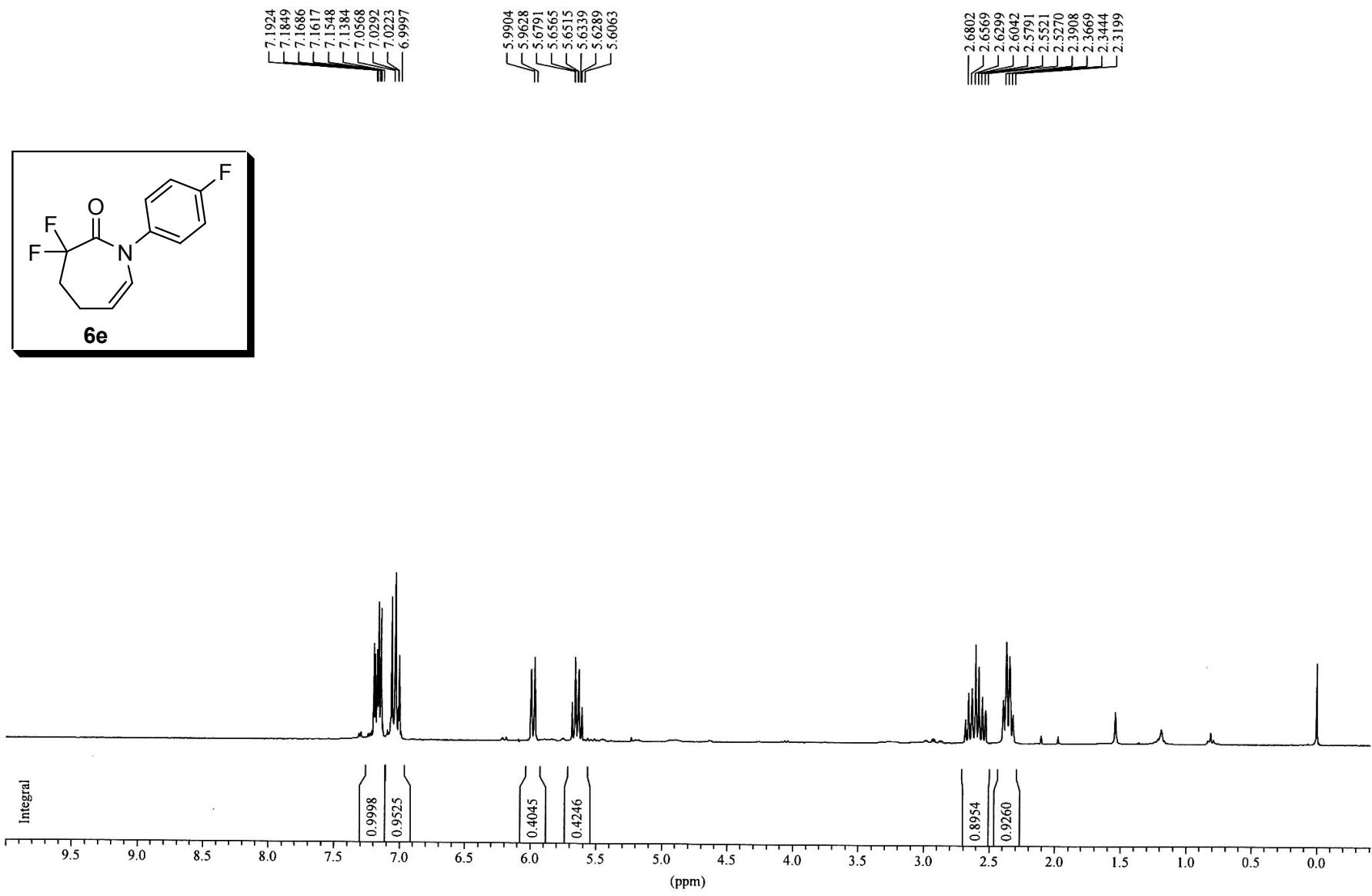


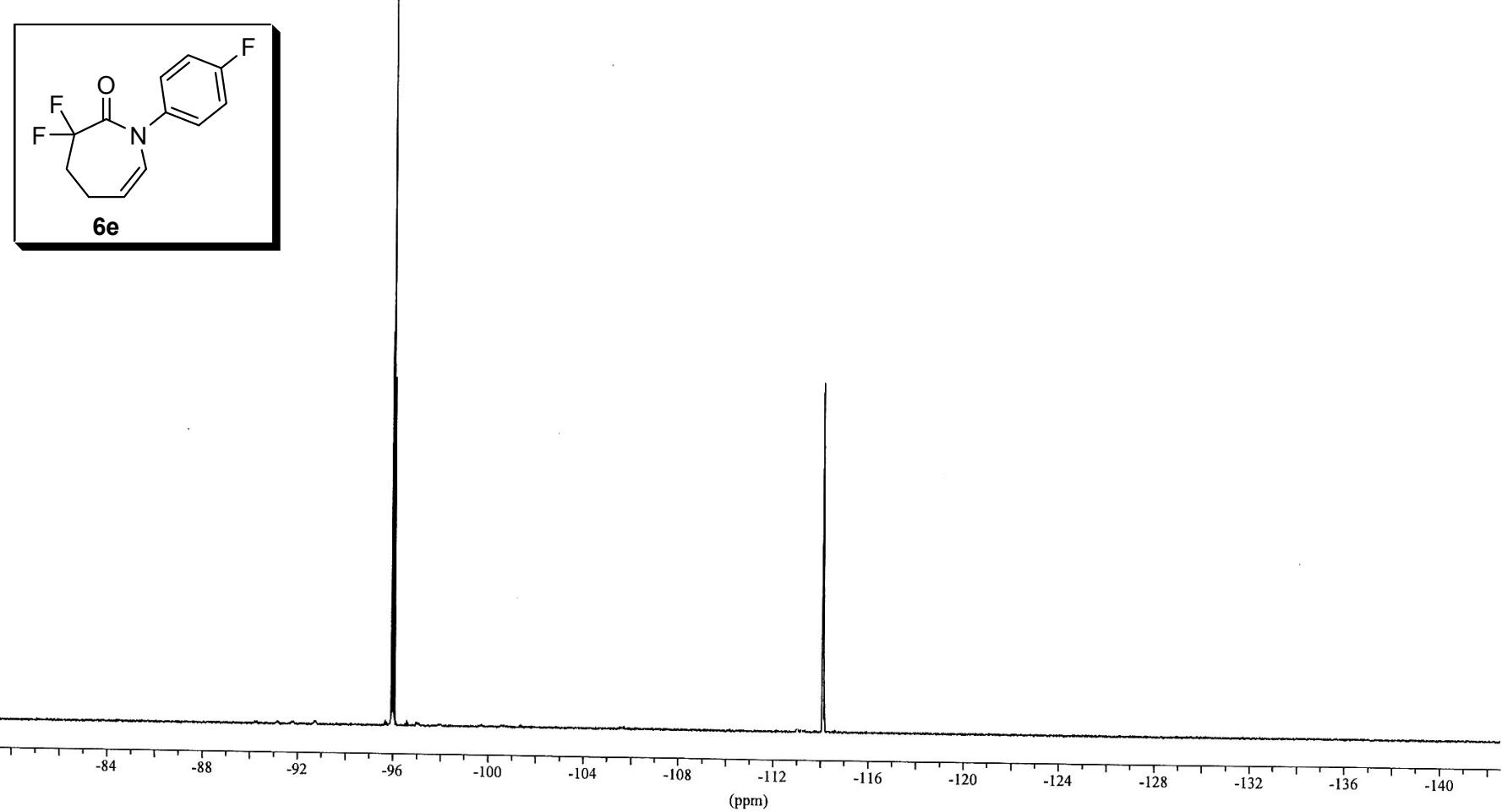


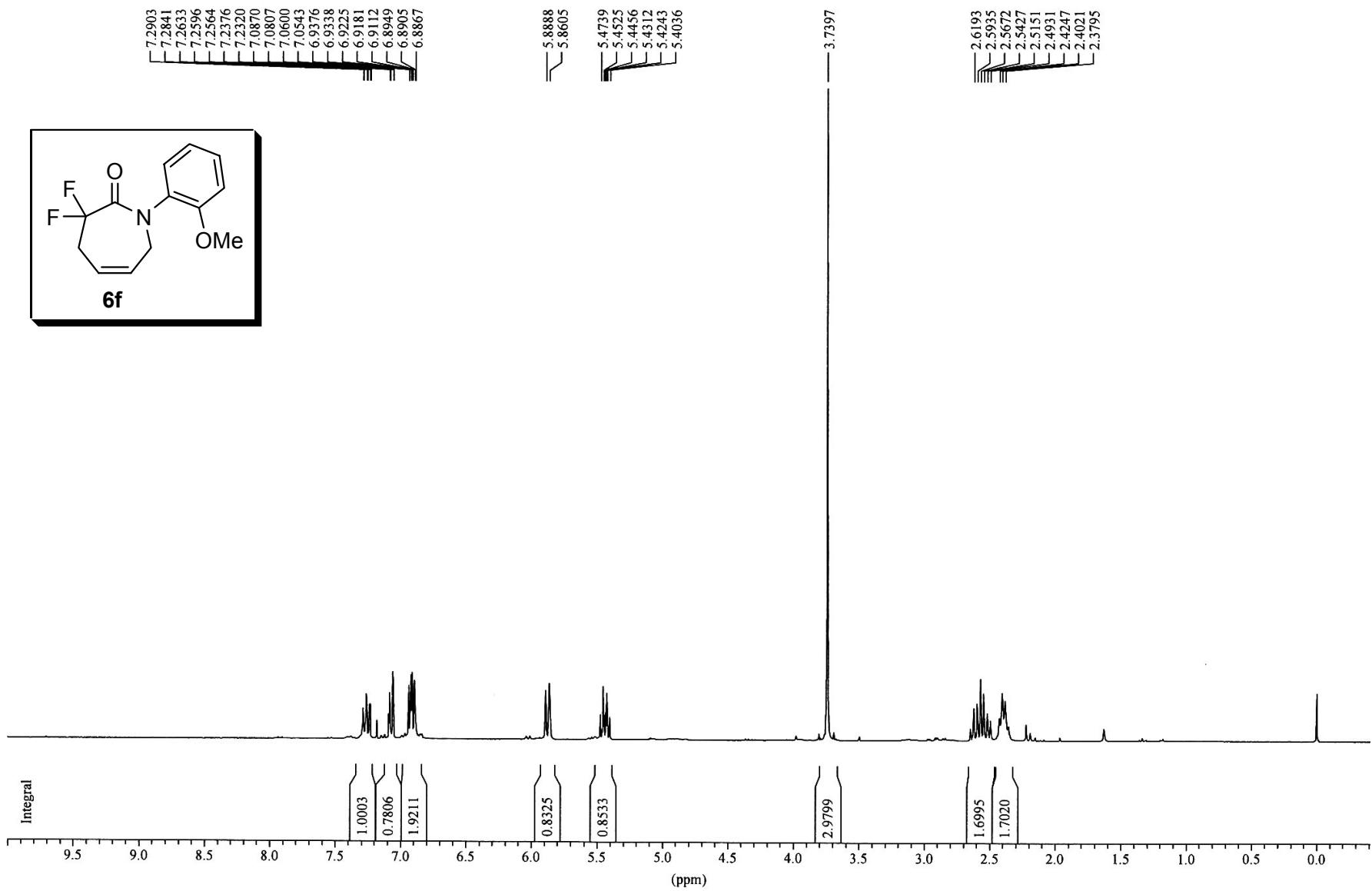


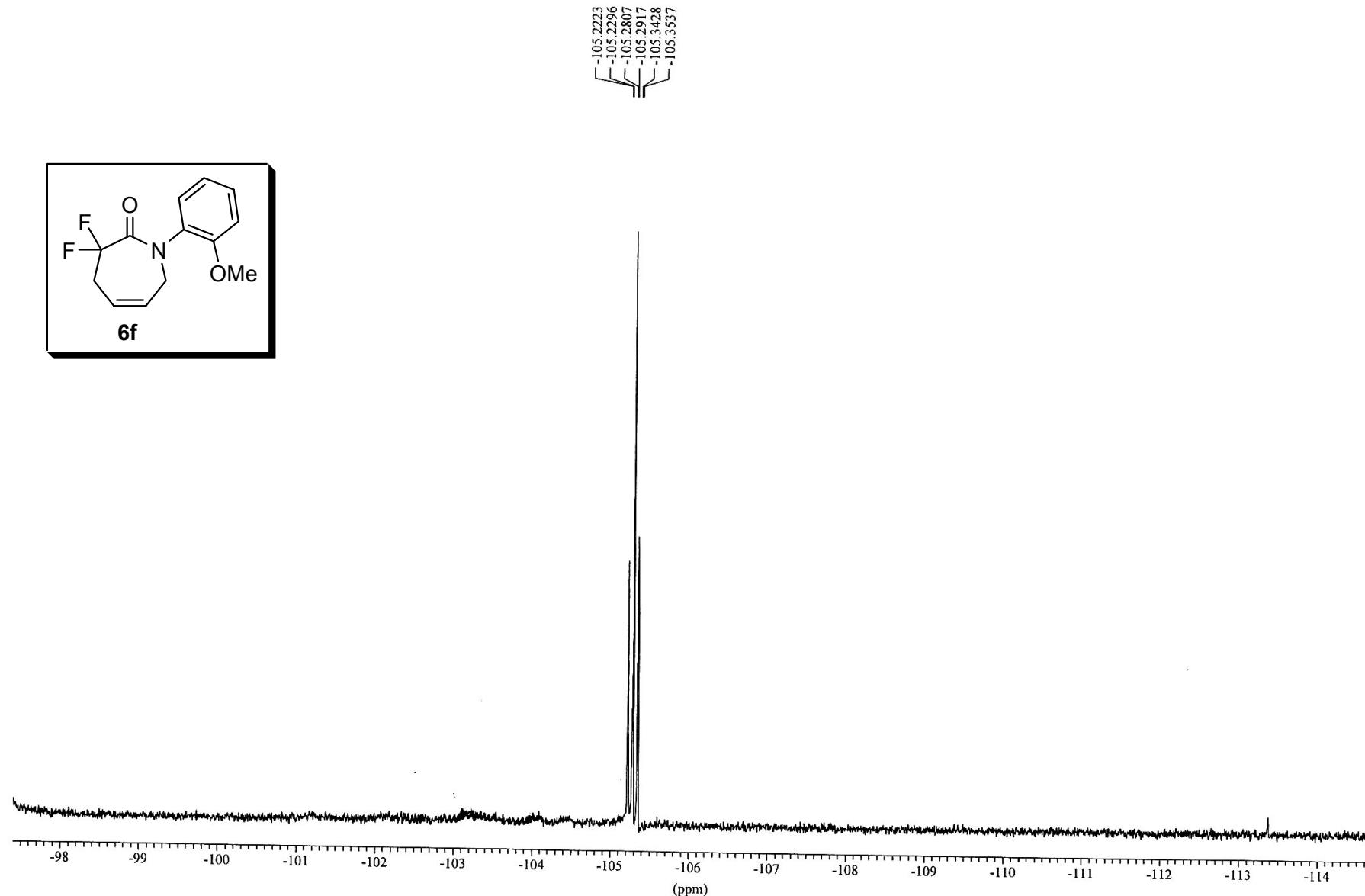
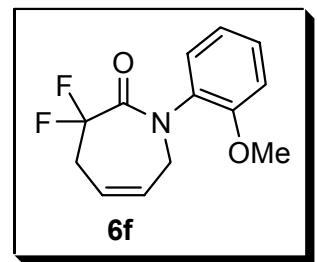


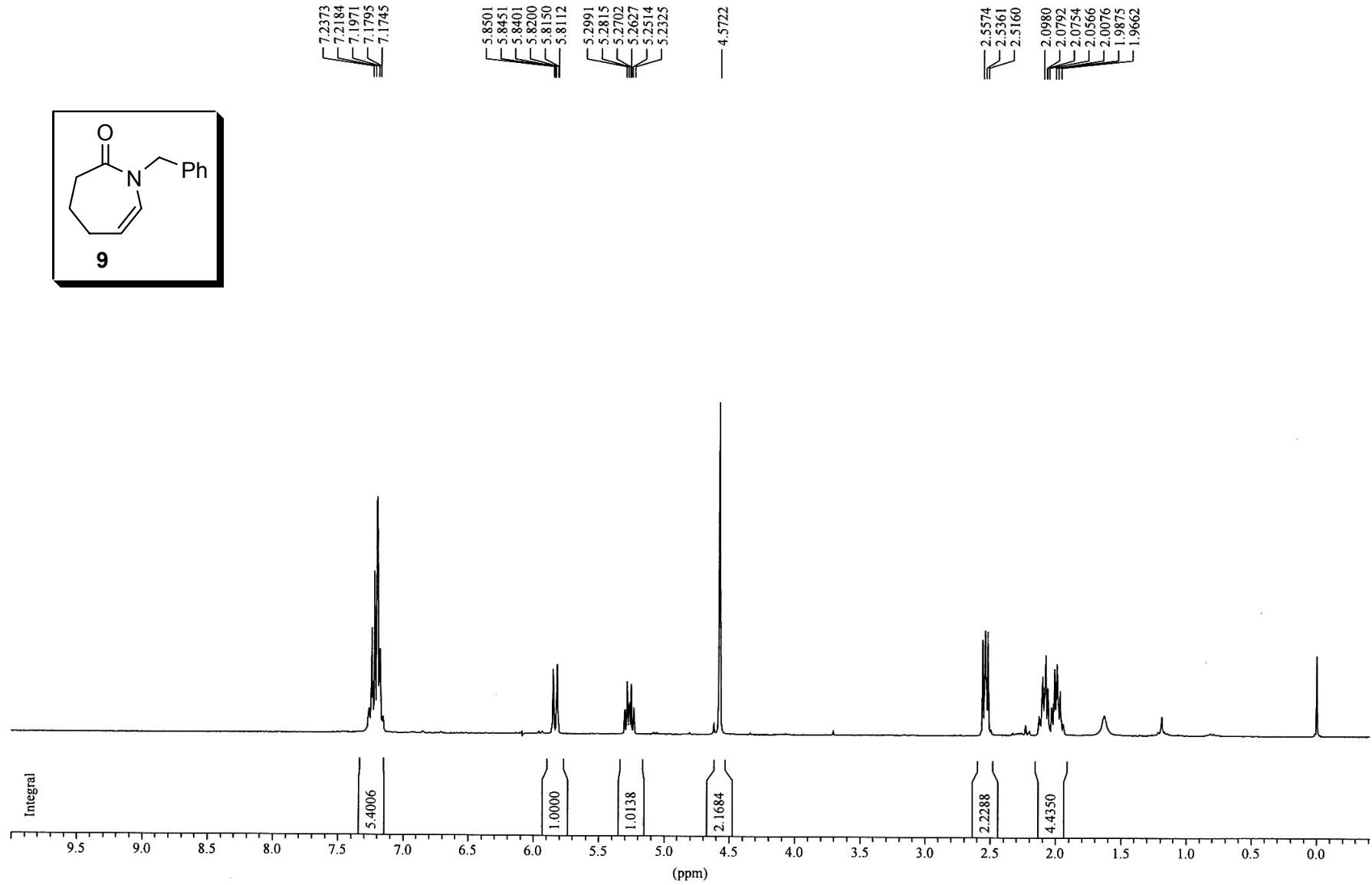


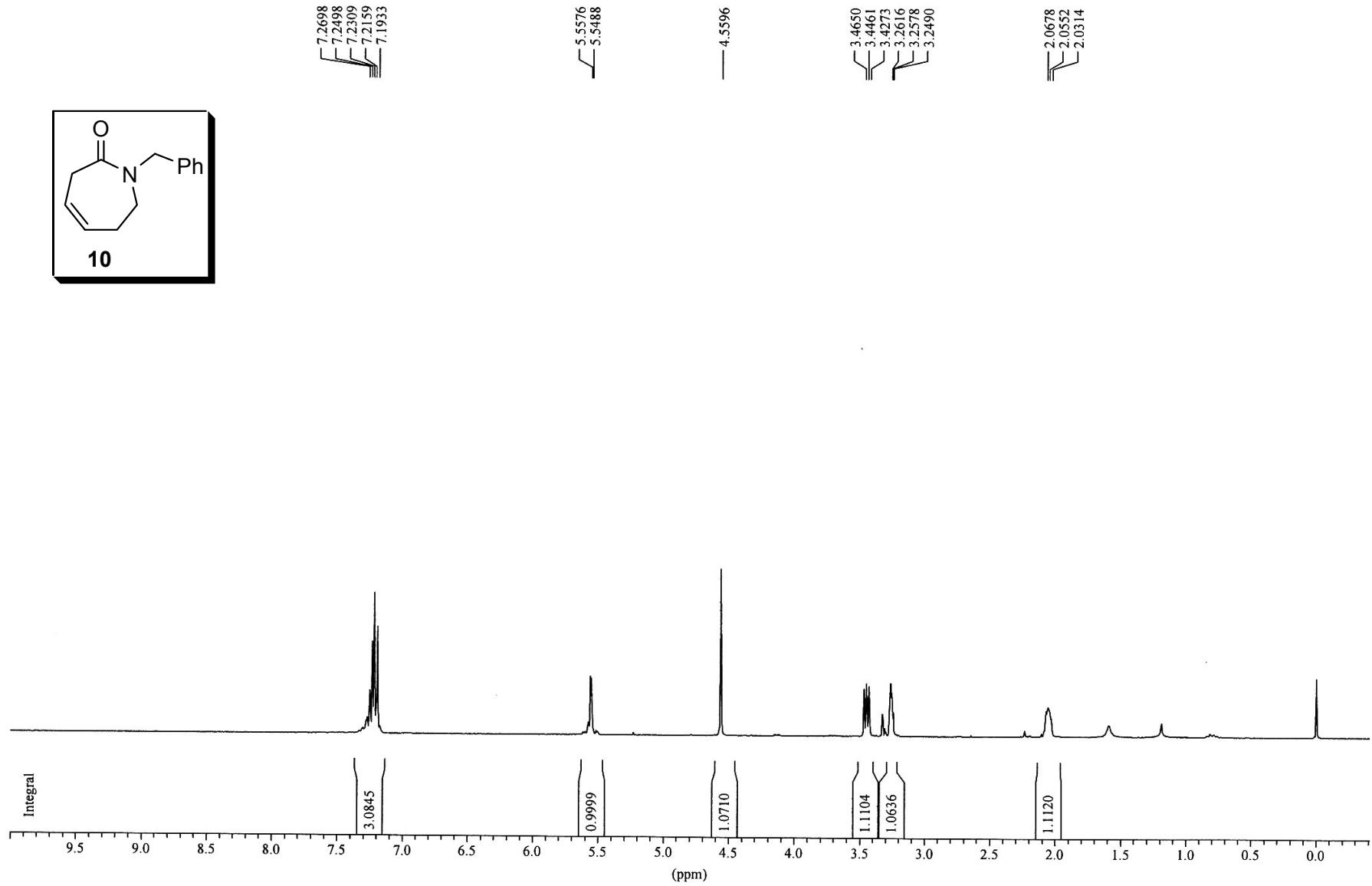


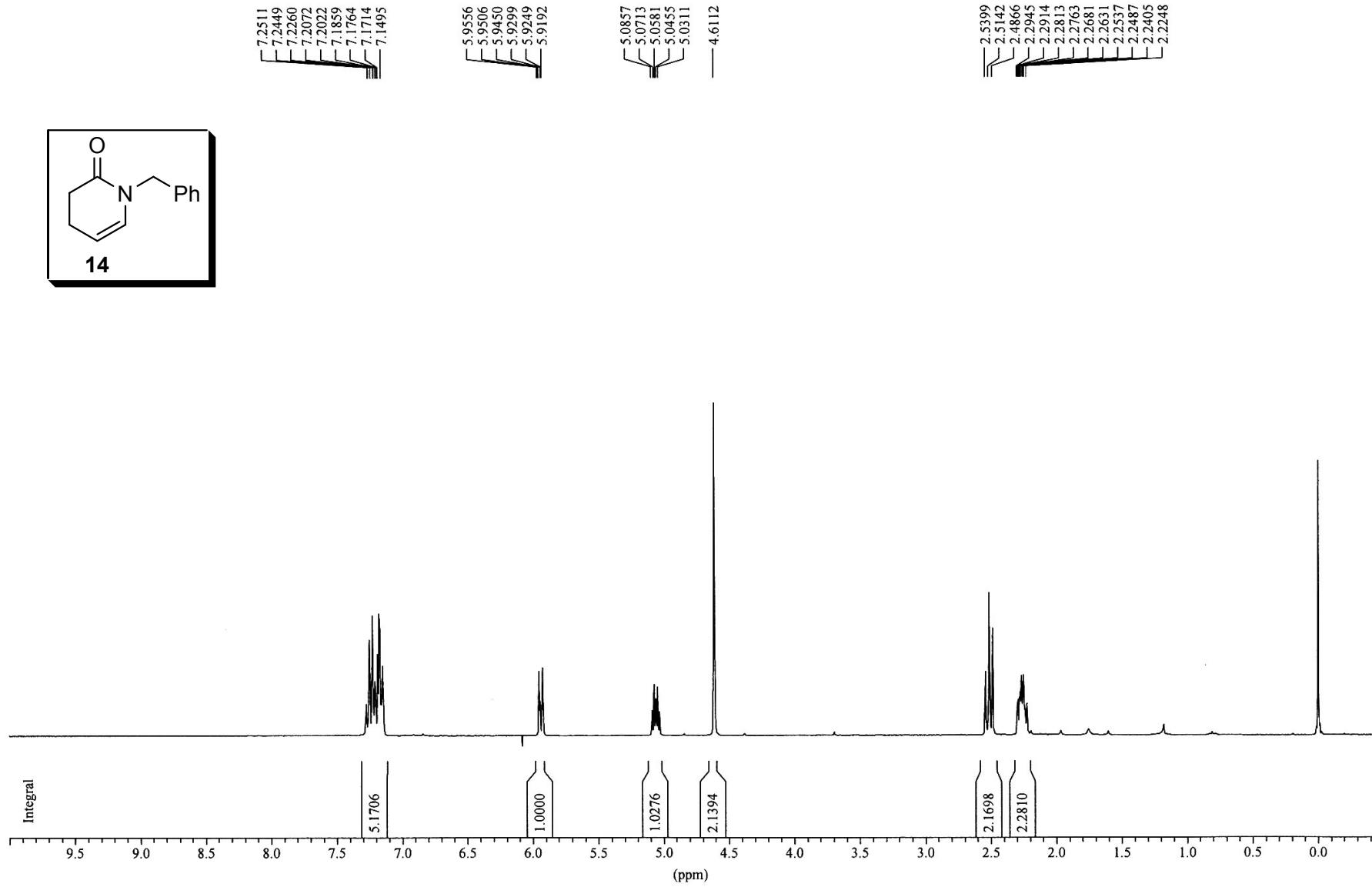


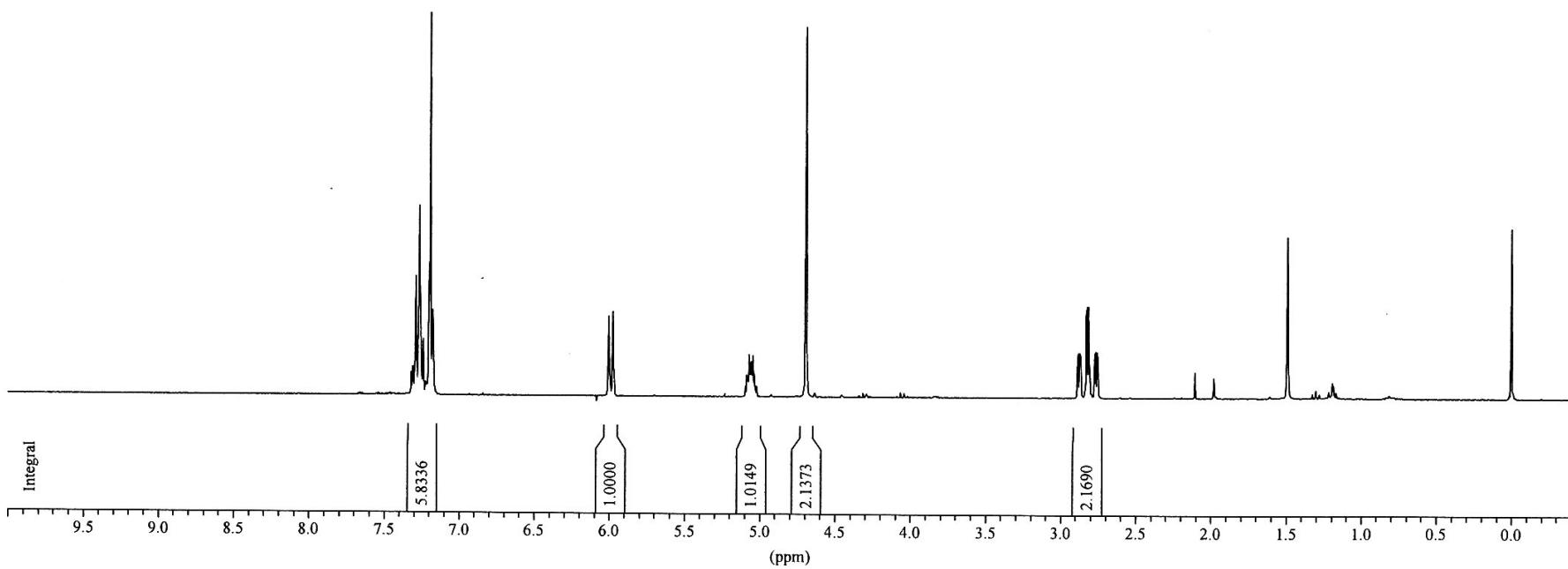
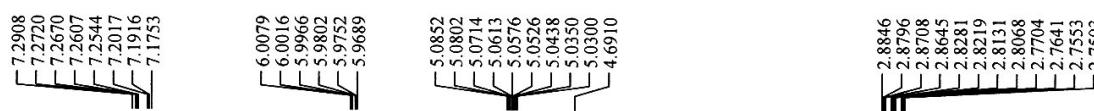
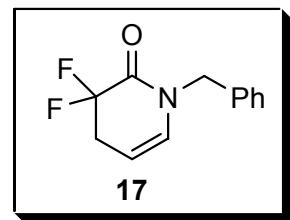


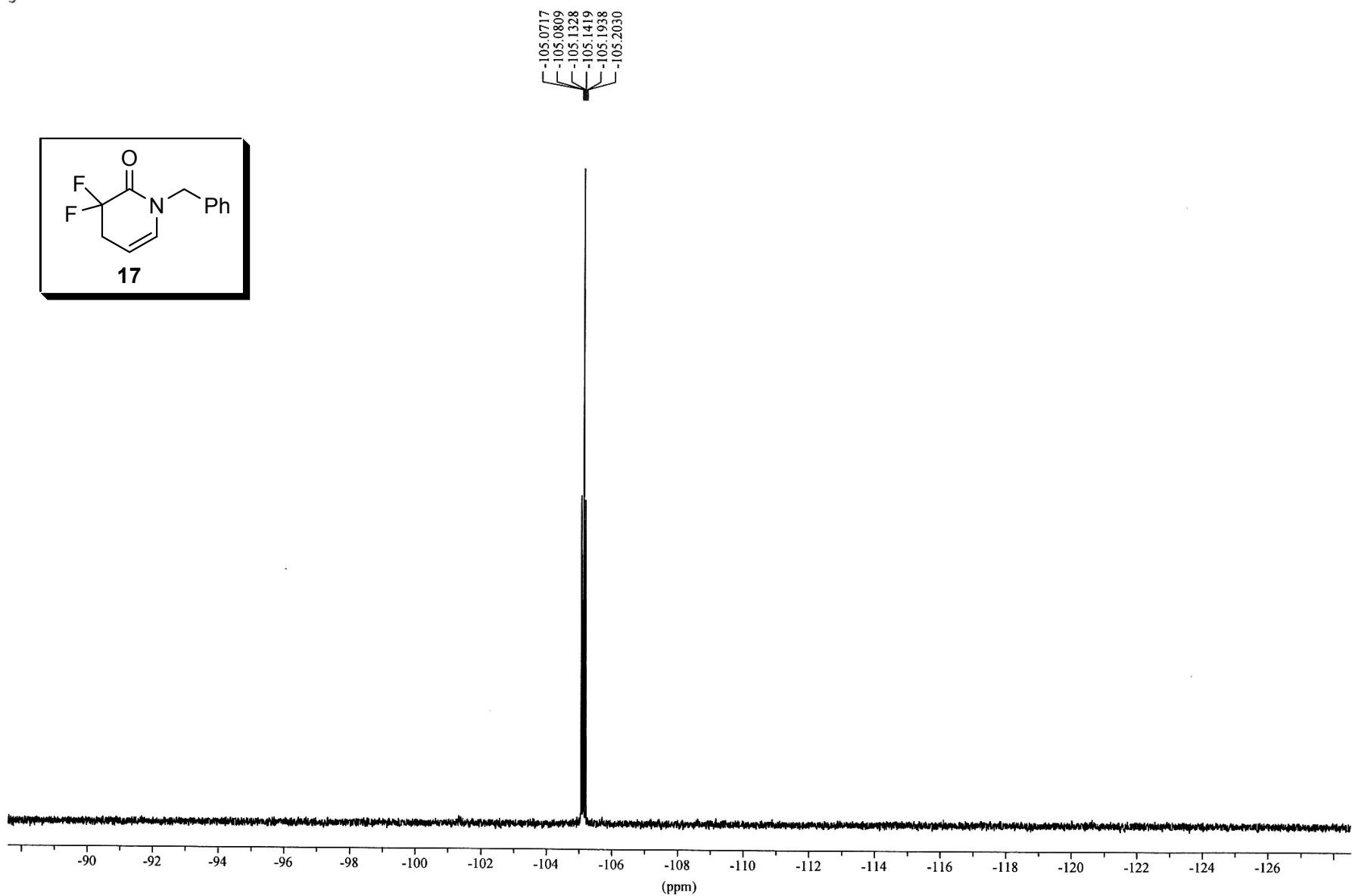


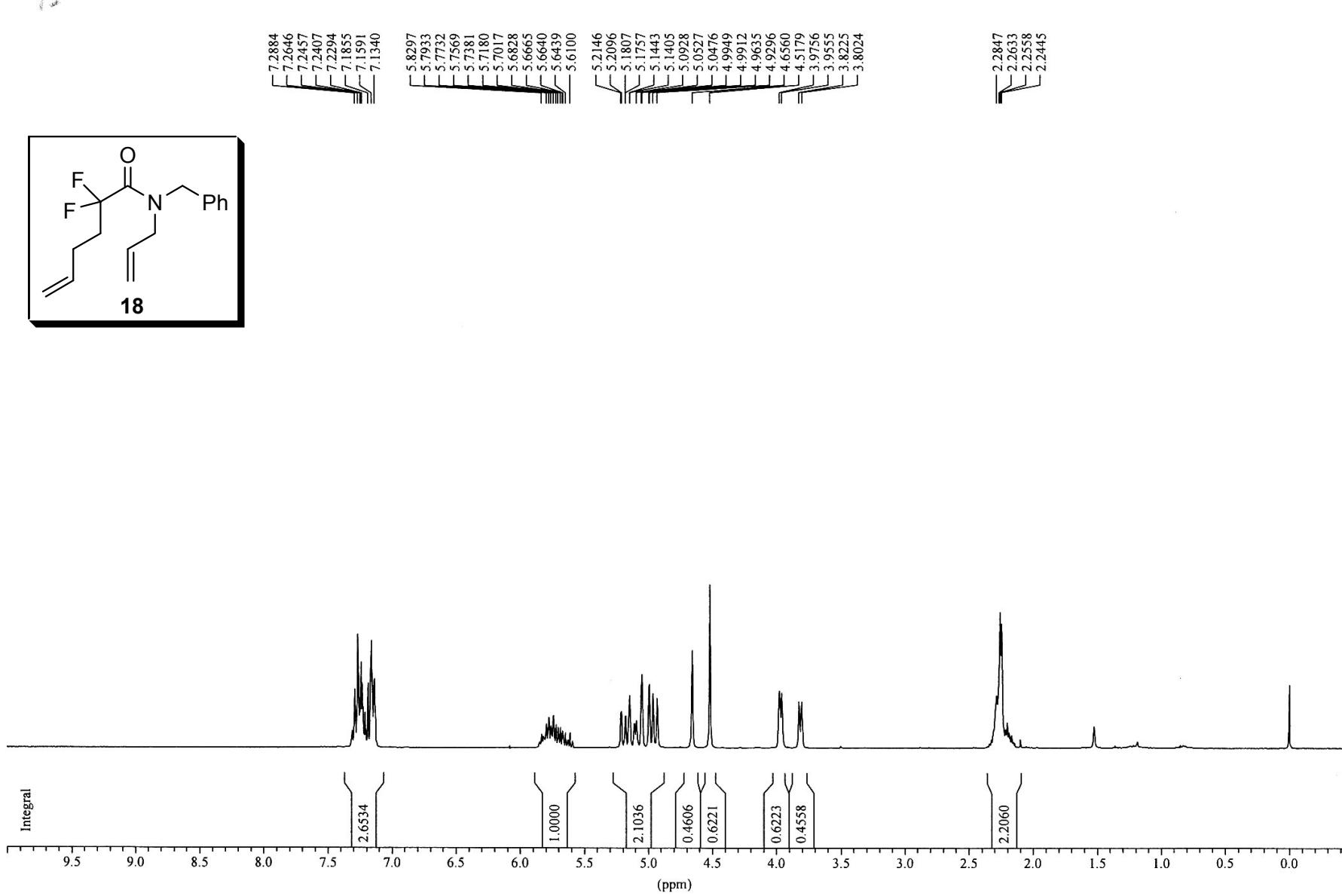




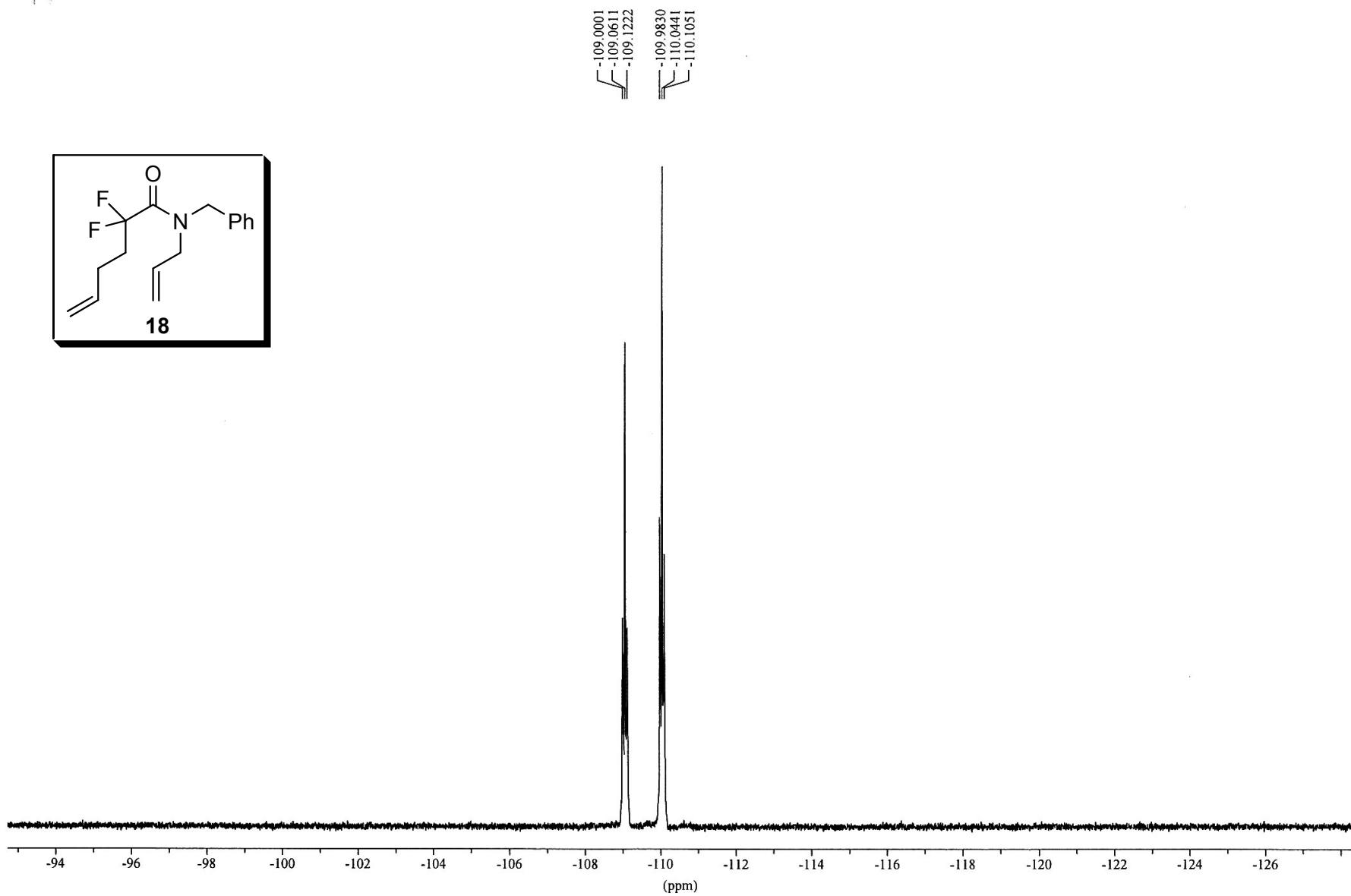
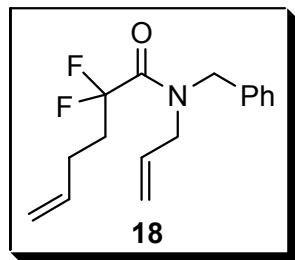


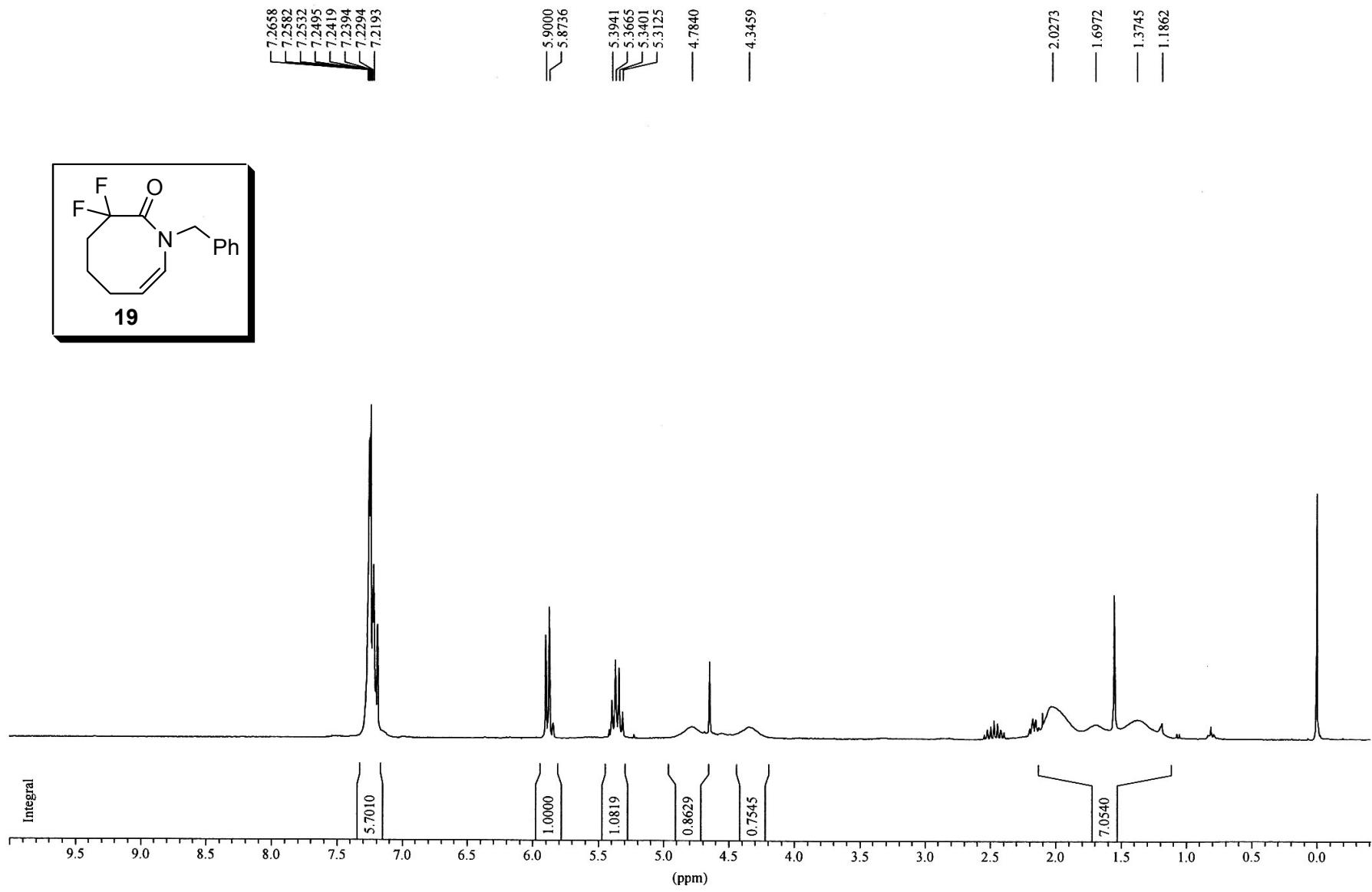


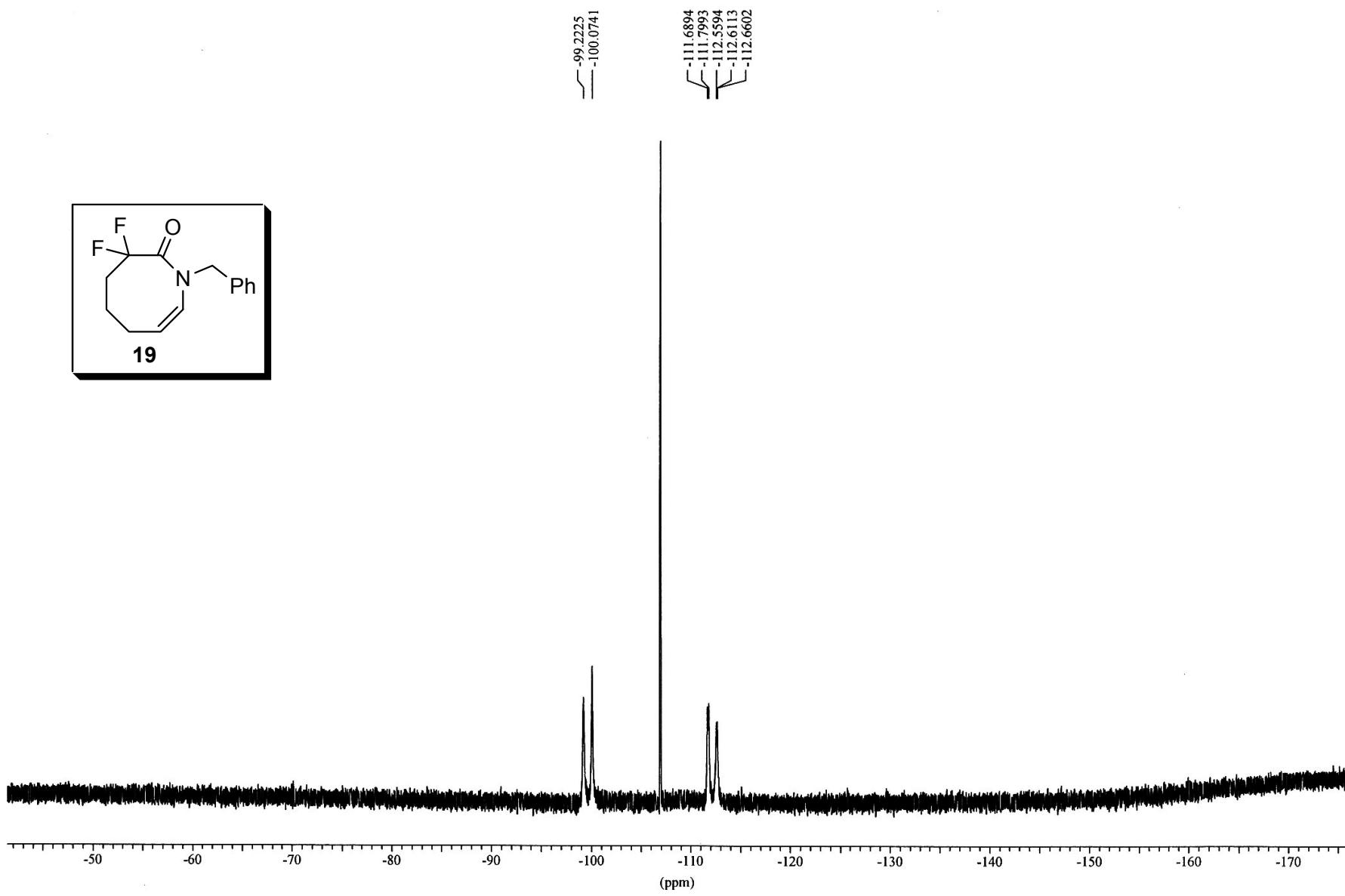
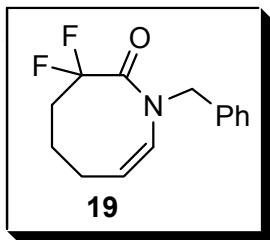


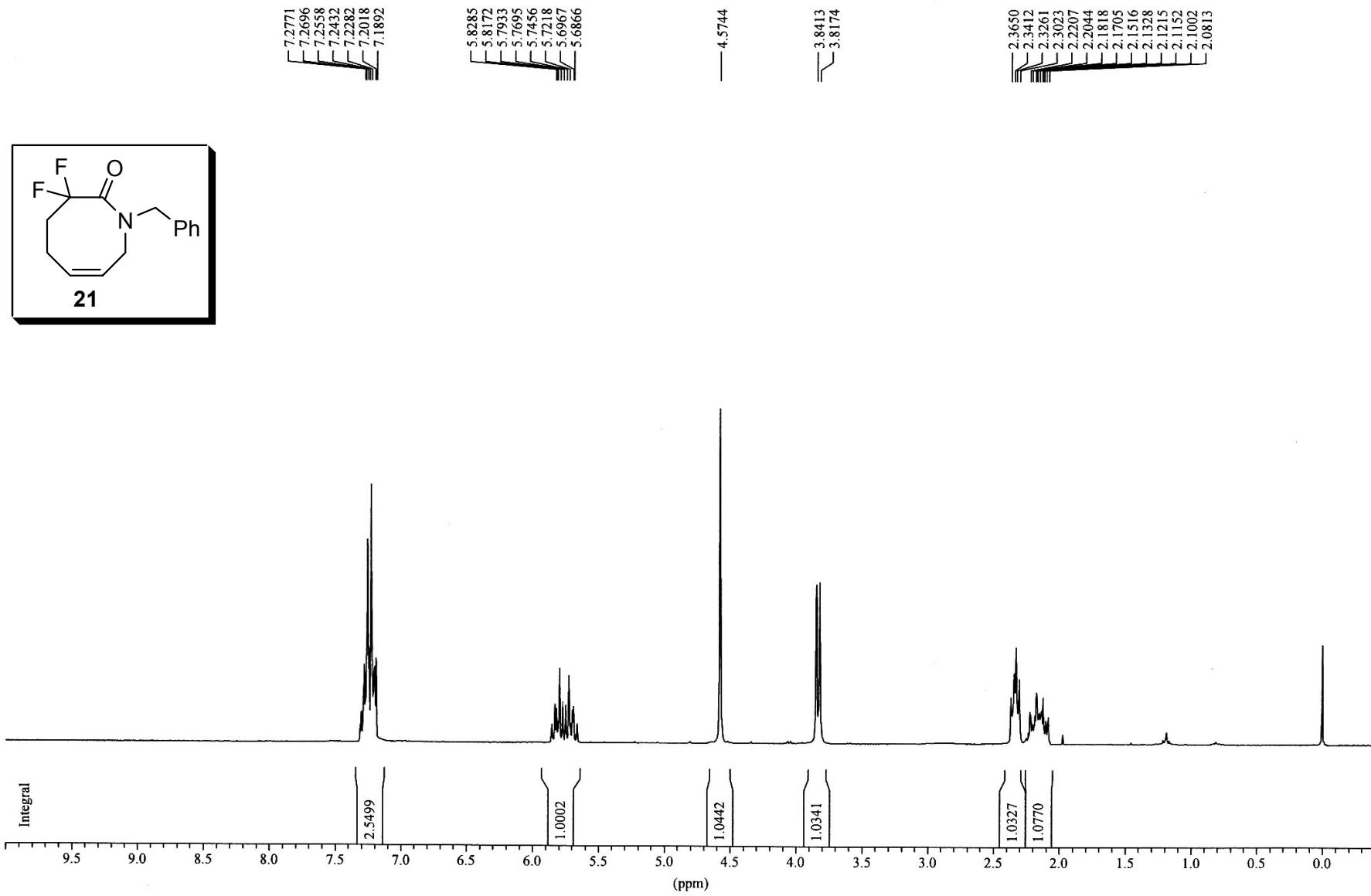
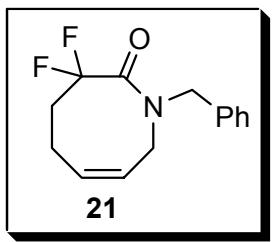


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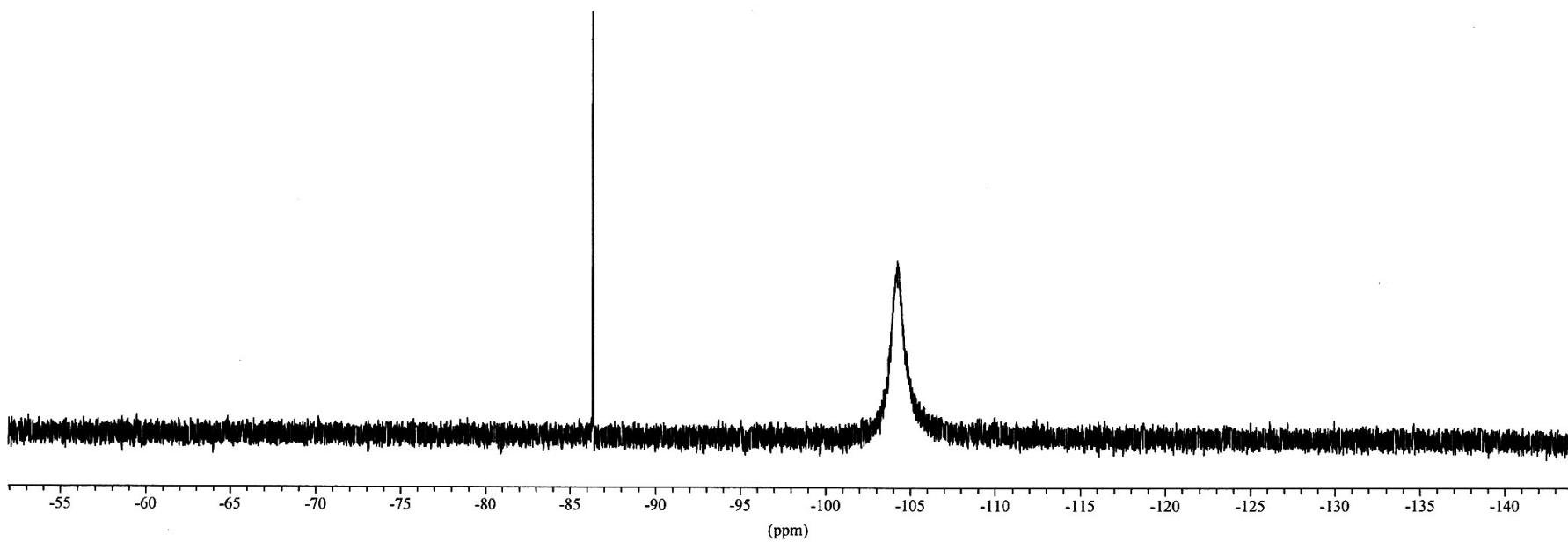
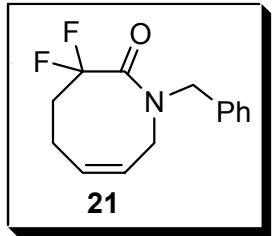


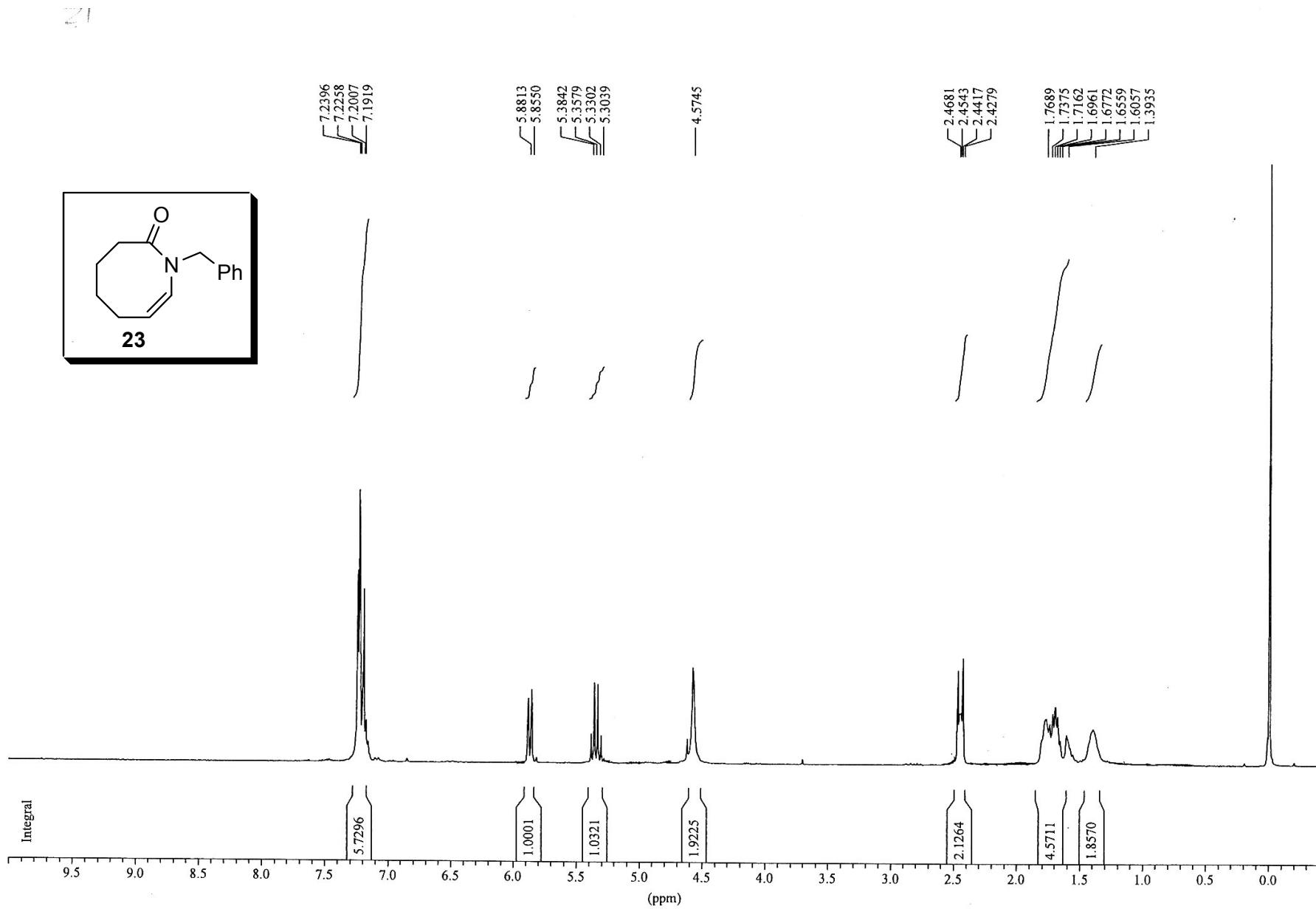


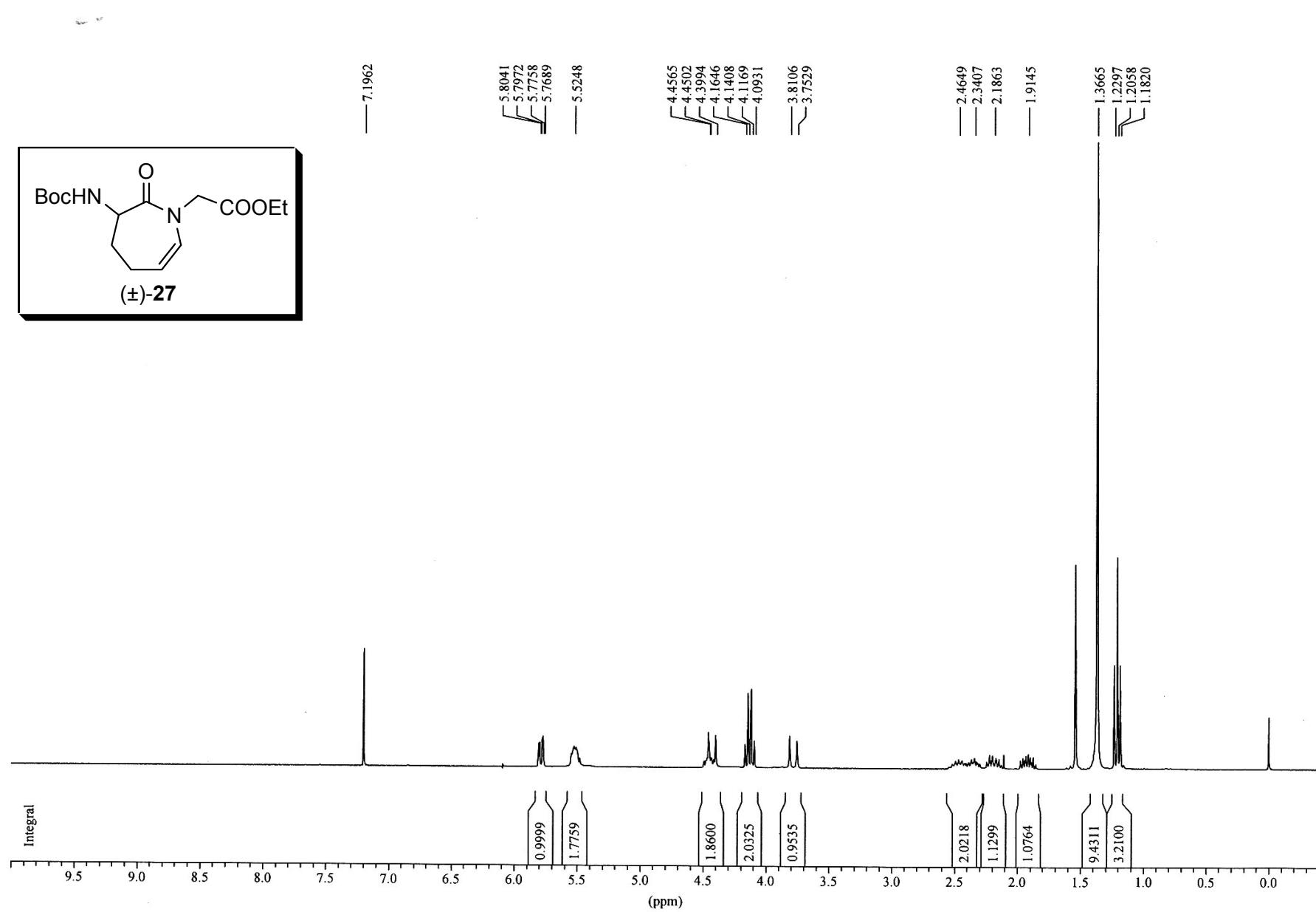




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