

Supporting information

Bridged 1,2,4-Trioxolanes: SnCl₄ - Catalyzed Synthesis and an In Vitro Study against *S. mansoni*

Peter S. Radulov¹, Ivan A. Yaremenko¹, Jennifer Keiser^{2,3} and Alexander O. Terent'ev^{1*}

¹N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, 47 Leninsky Prospekt, 119991 Moscow, Russia

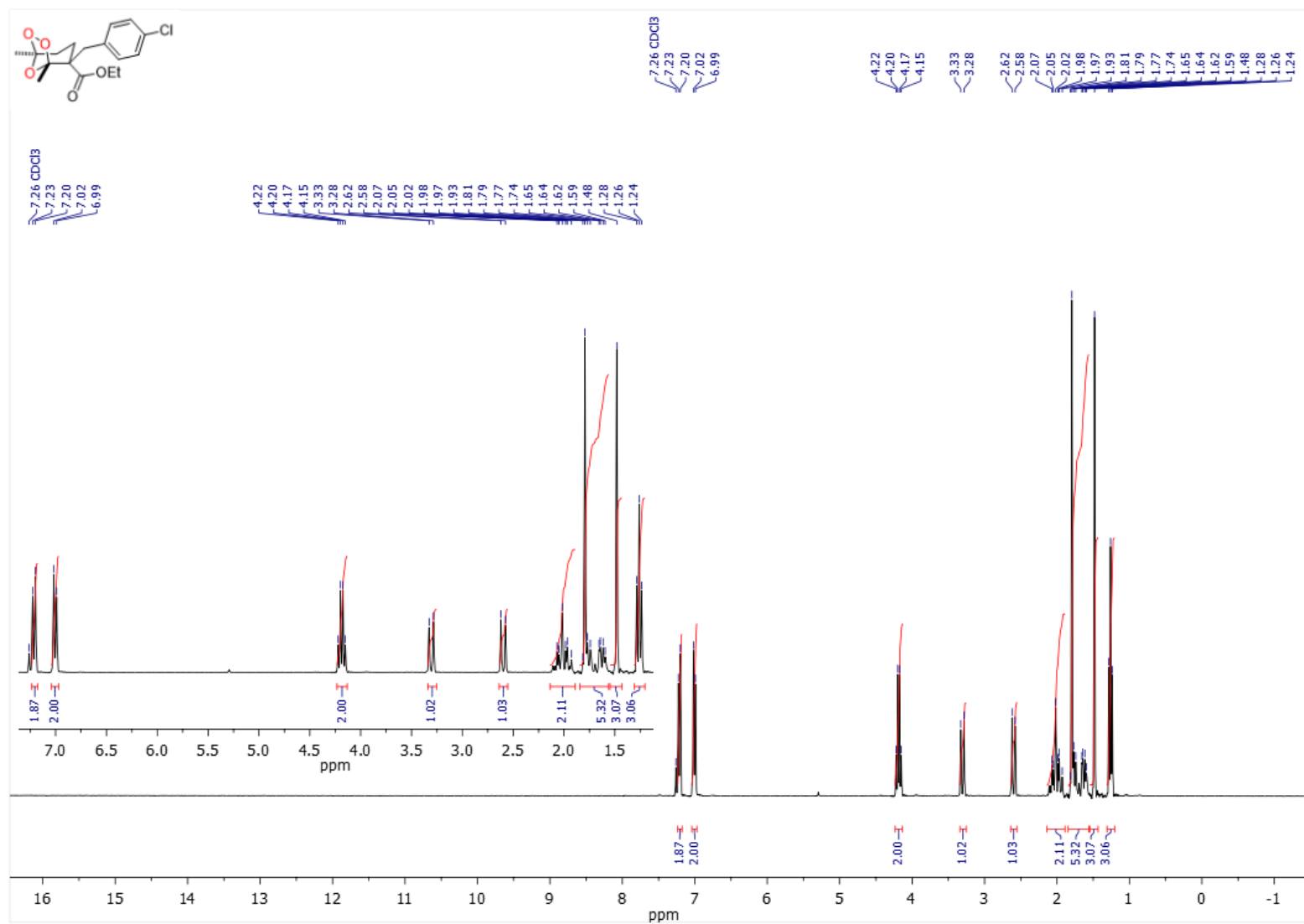
²Department of Medical Parasitology and Infection Biology, Swiss Tropical and Public Health Institute, CH-4123 Allschwil Switzerland

³University of Basel, CH-4003 Basel, Switzerland

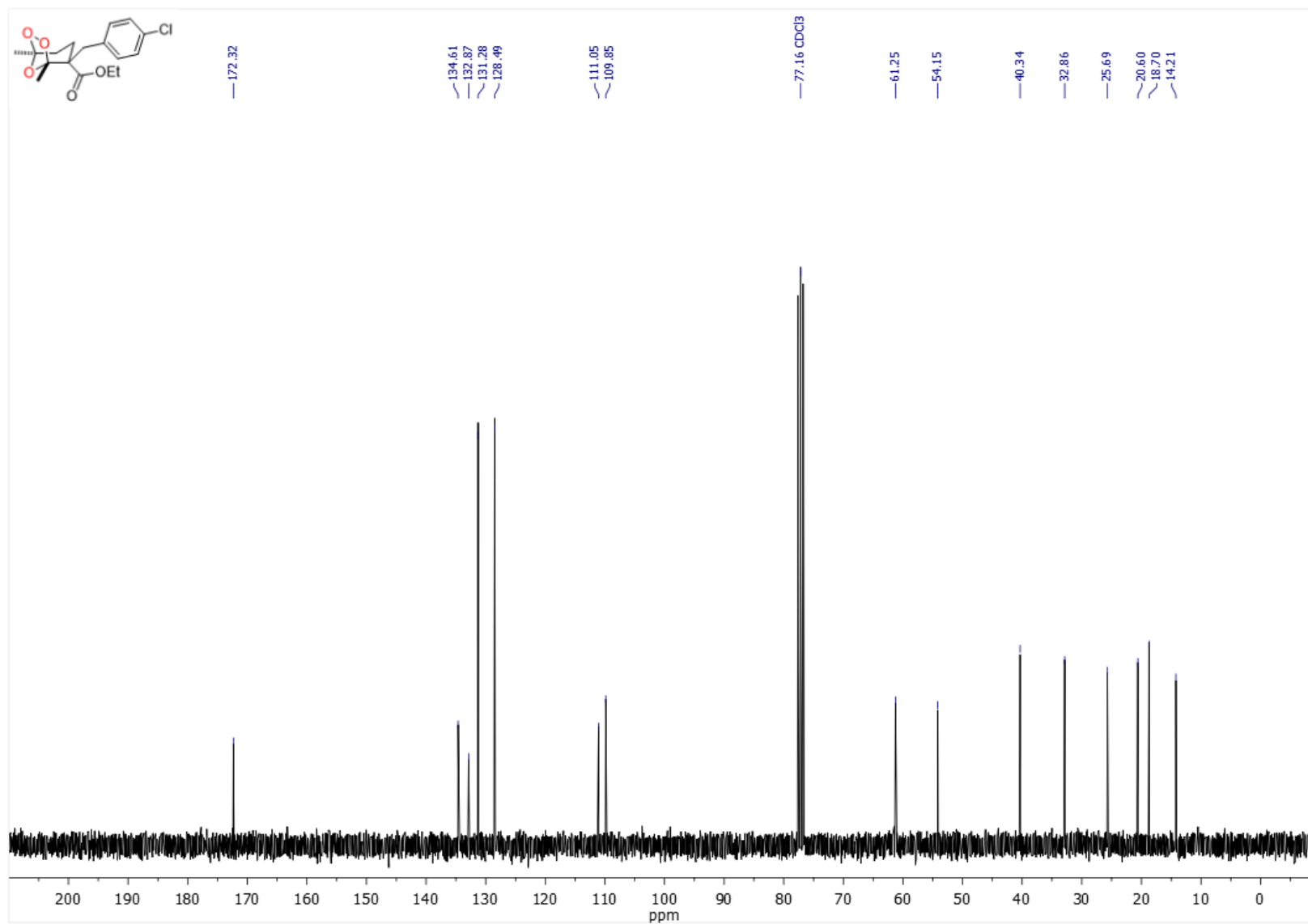
* Correspondence: alterex@yandex.ru; Tel.: +7-916-385-4080

NMR spectra of peroxides 2a-k and 3a-k

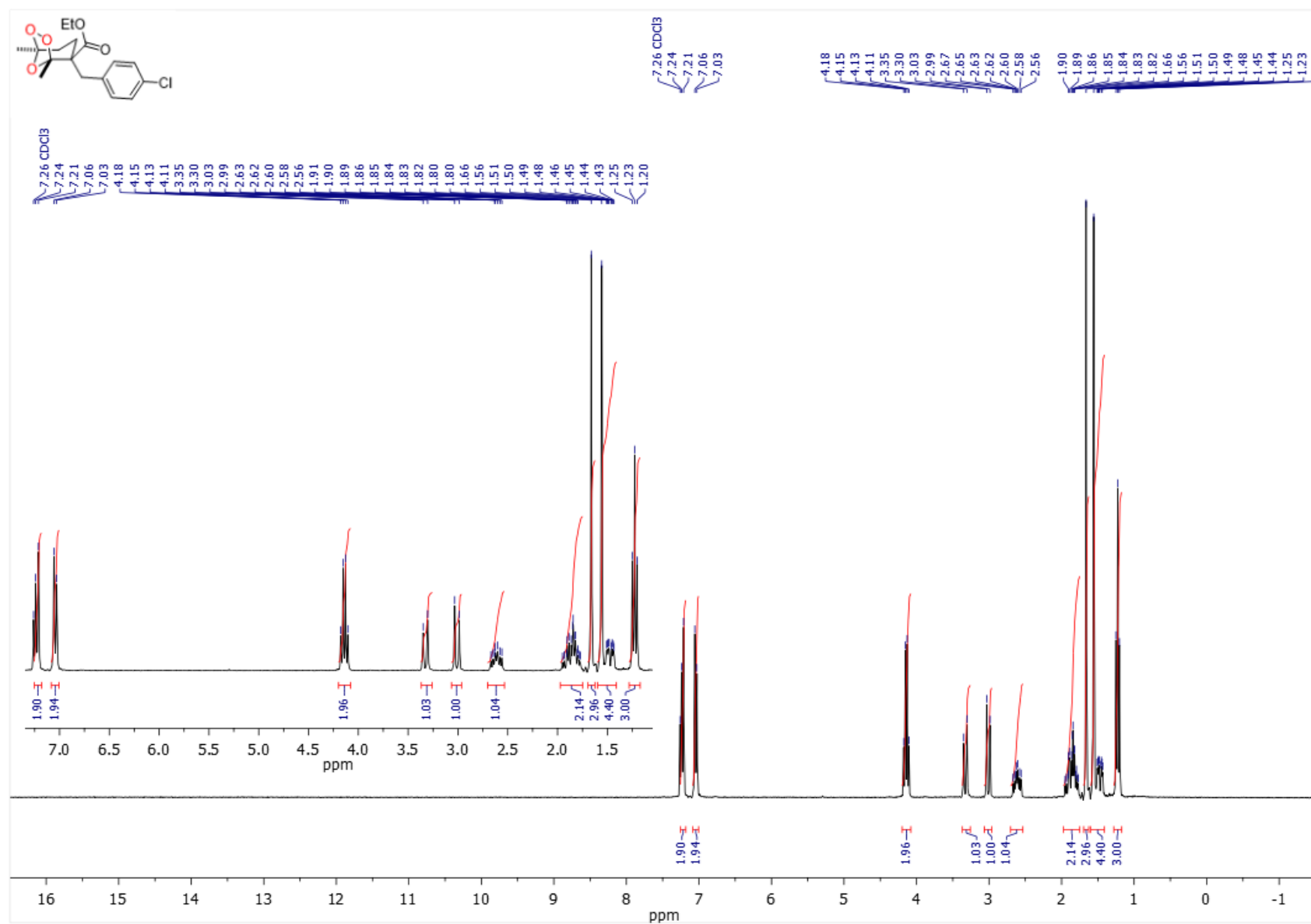
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-(4-chlorobenzyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2a



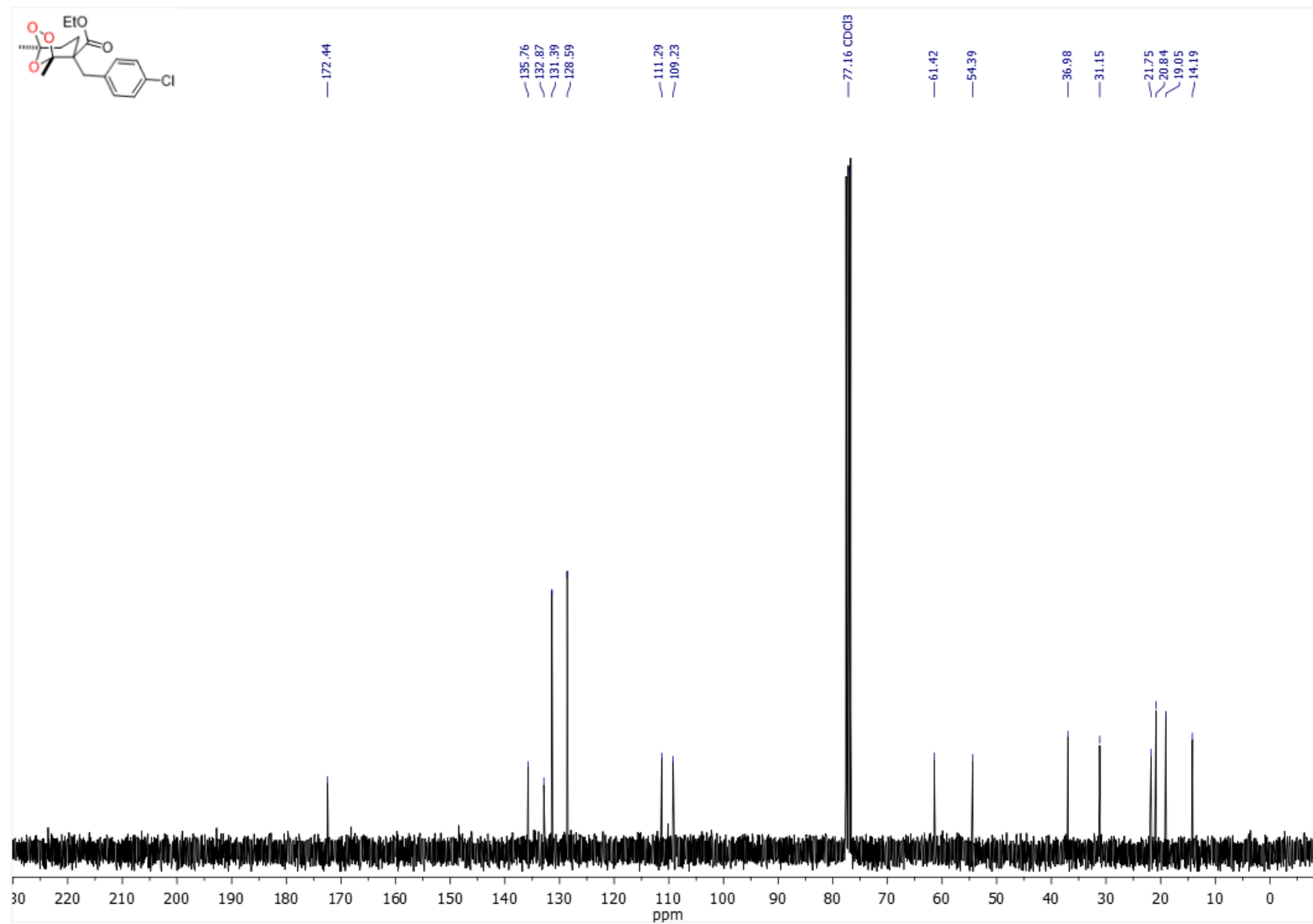
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-(4-chlorobenzyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2a



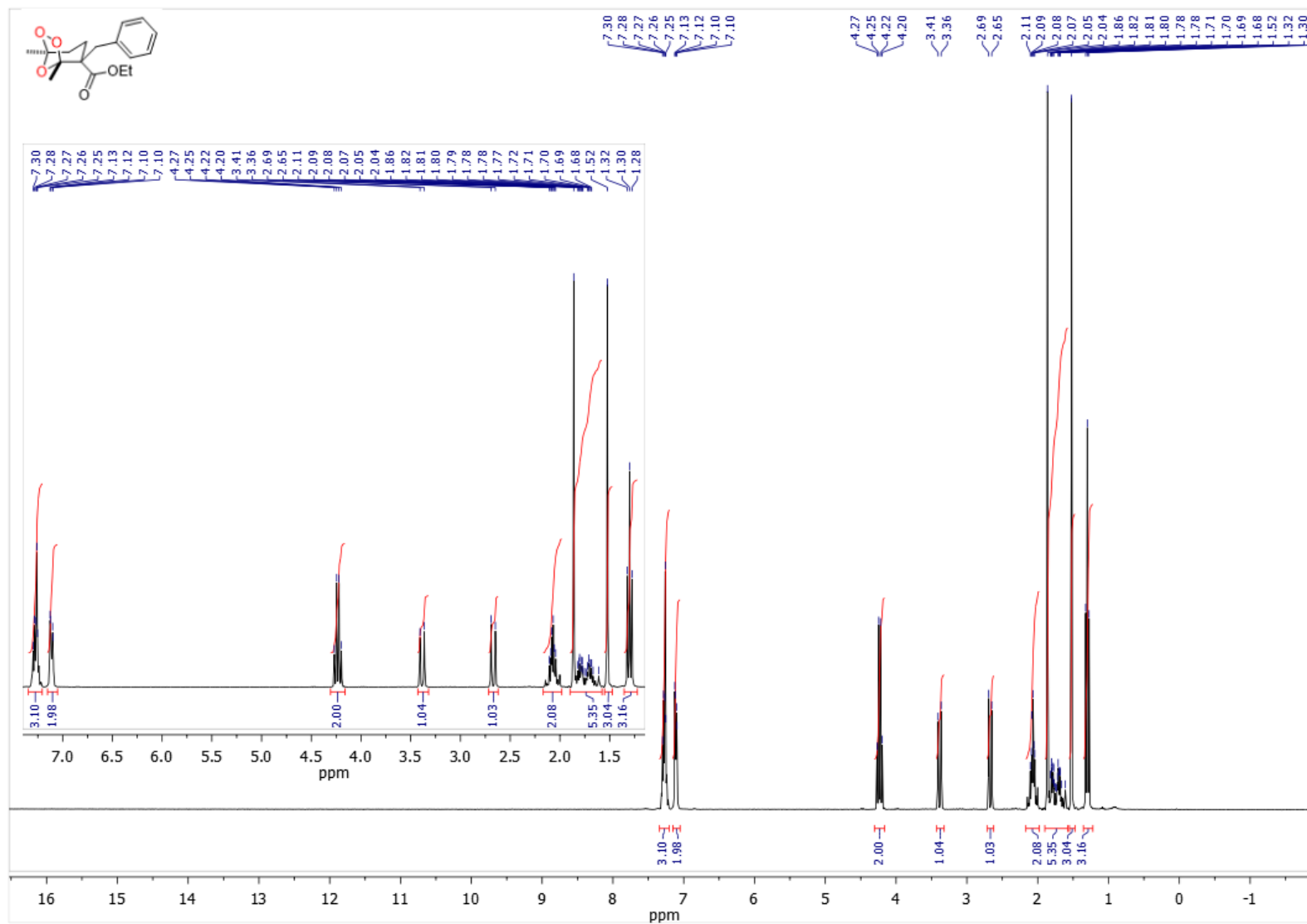
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-(4-chlorobenzyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3a



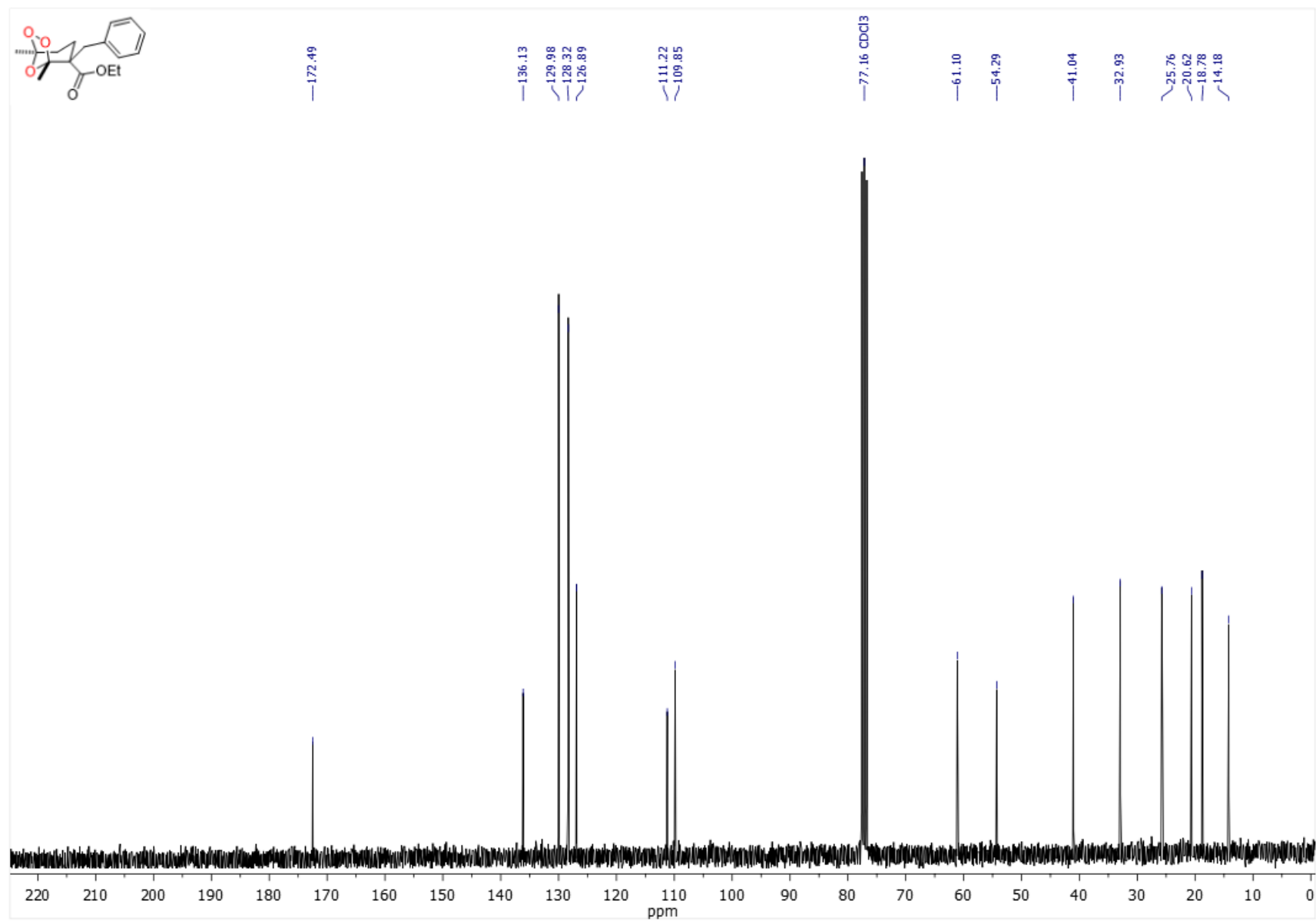
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-(4-chlorobenzyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3a



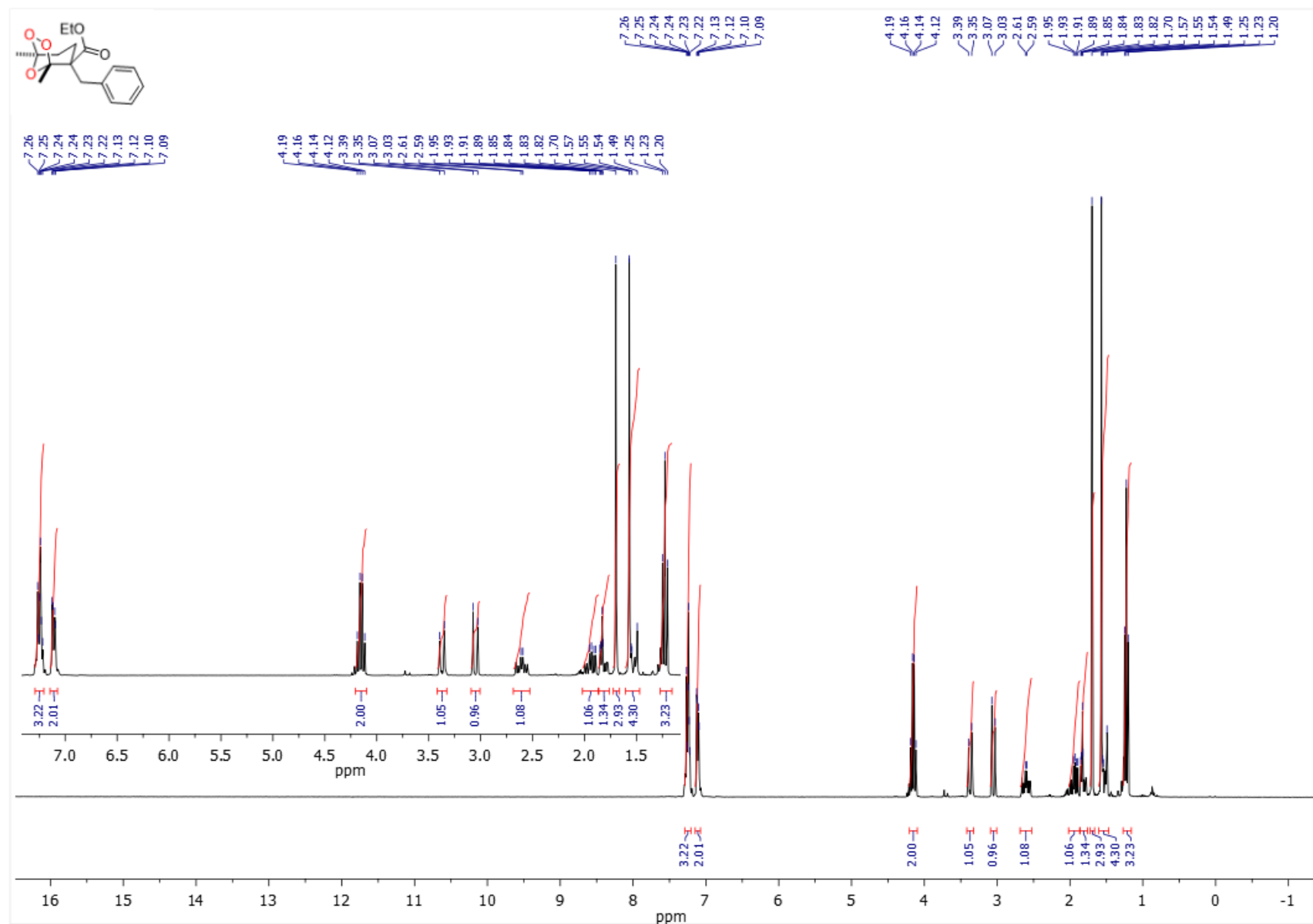
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-benzyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2b



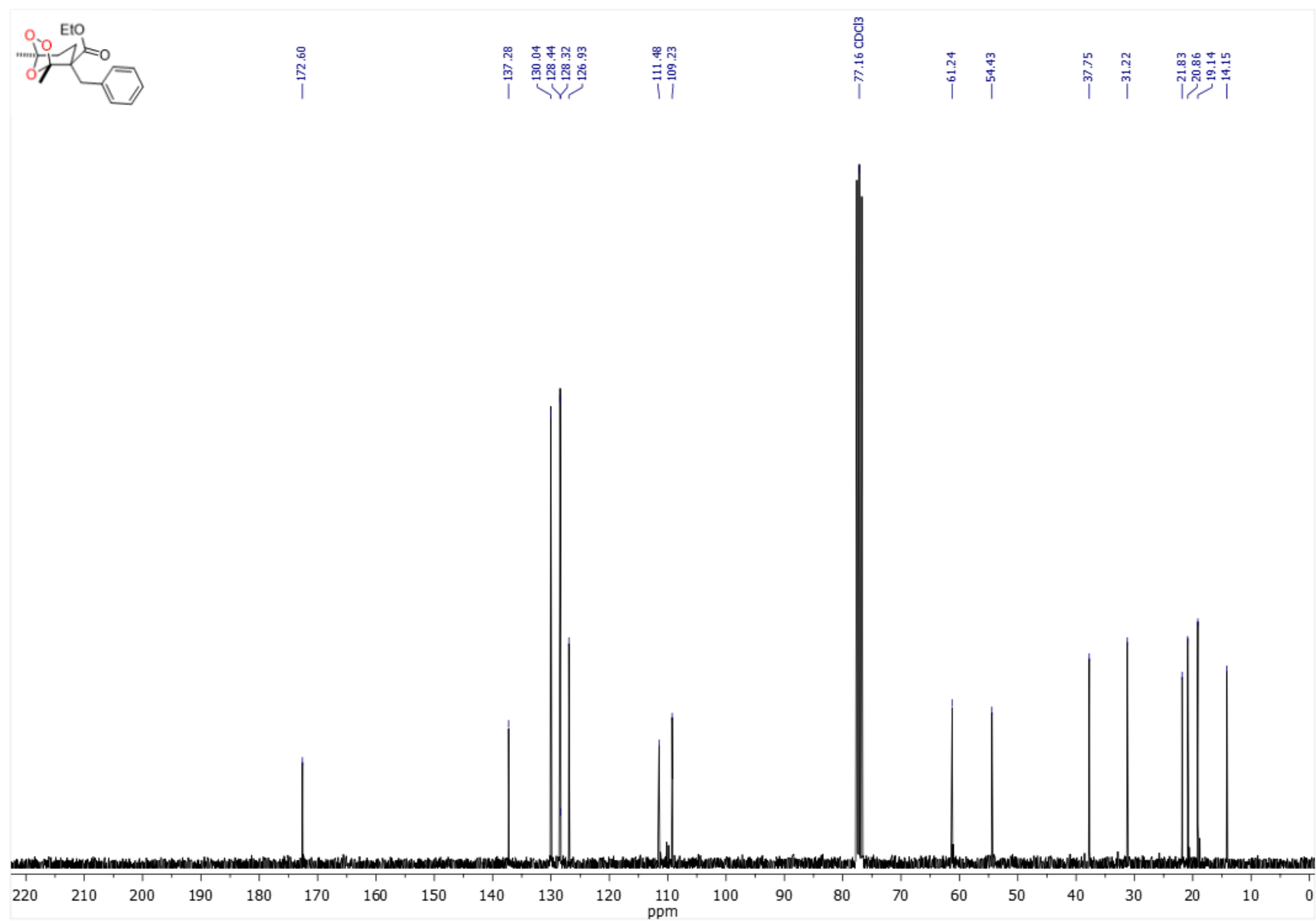
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-benzyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2b



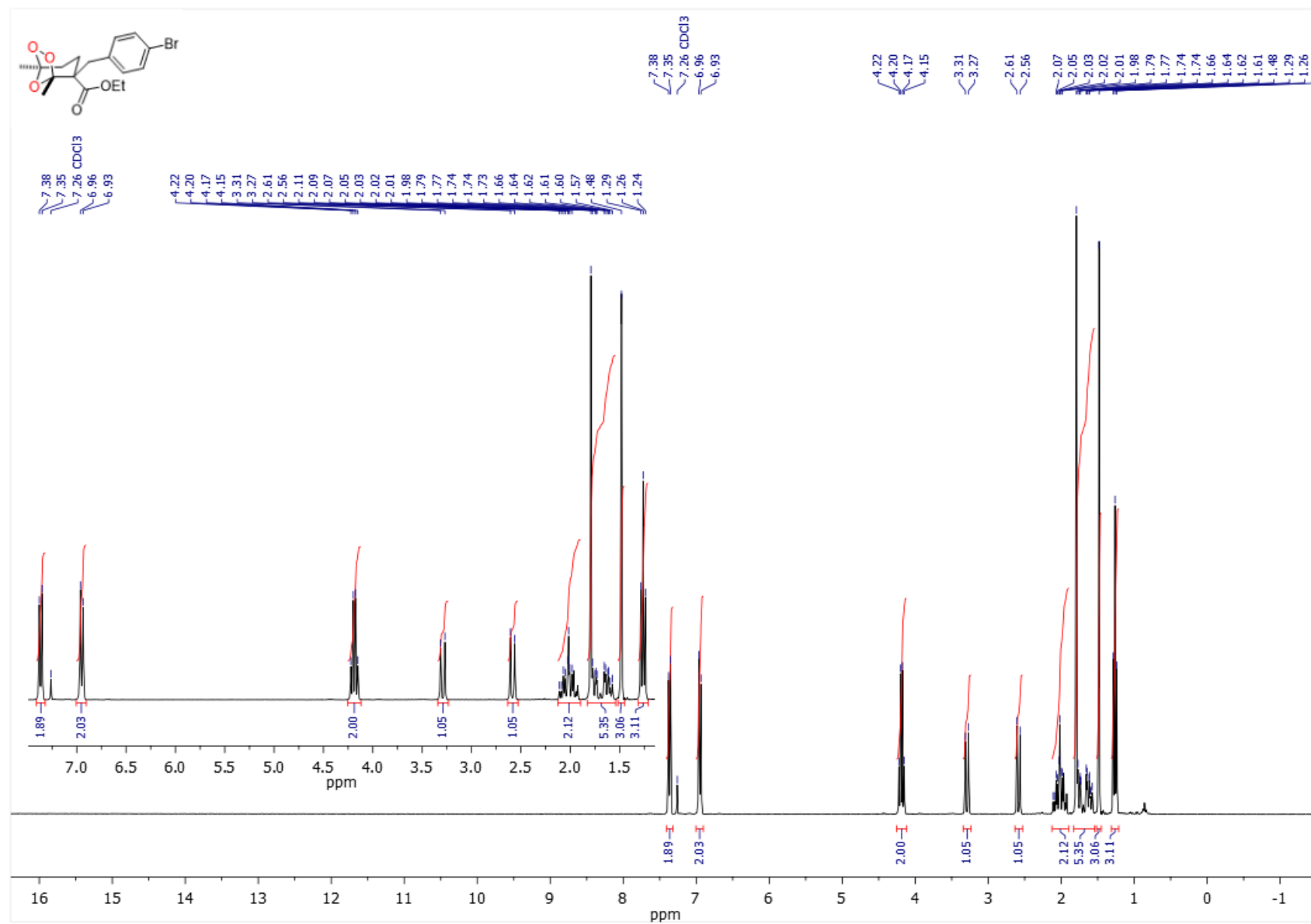
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-benzyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3b



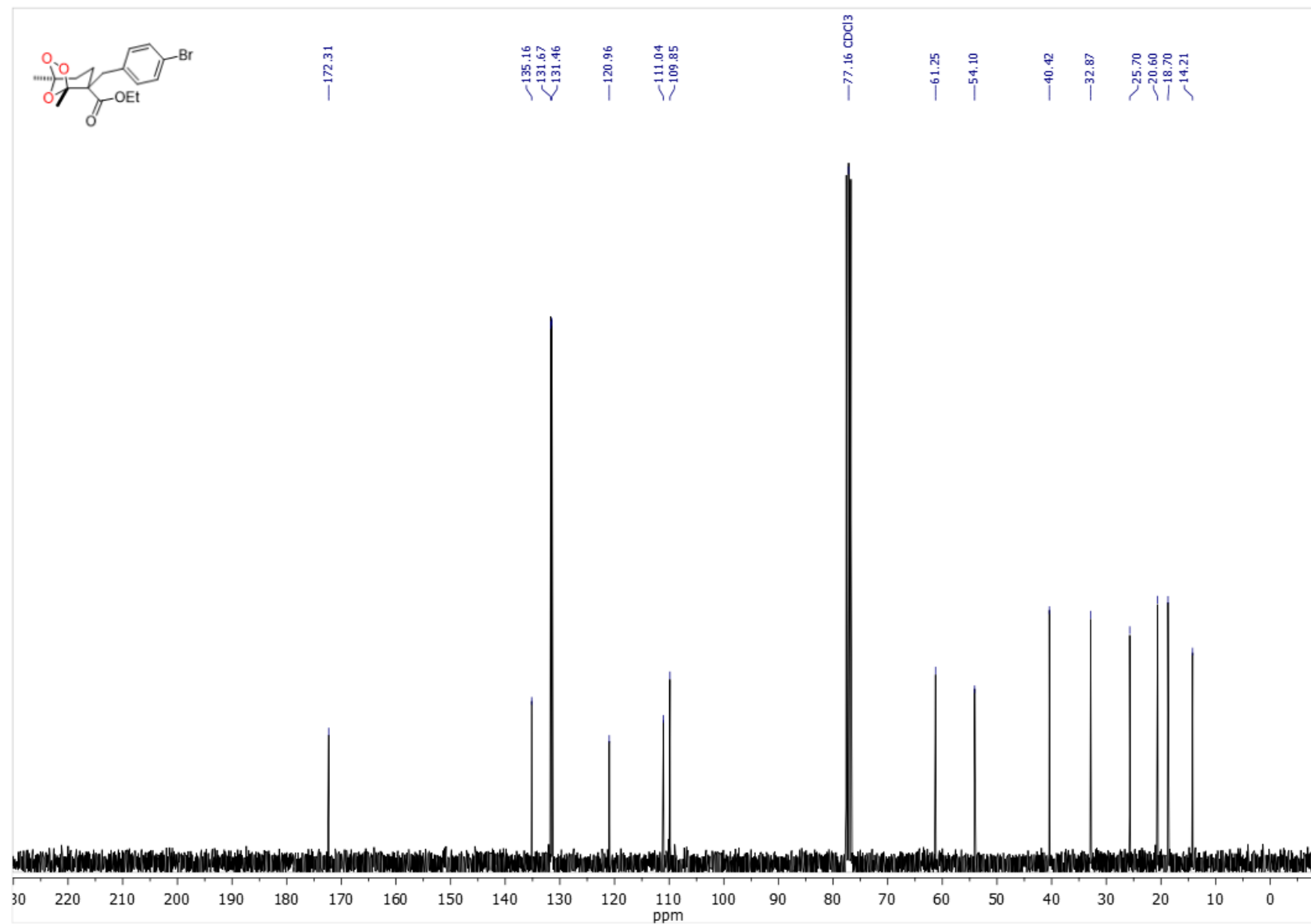
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-benzyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, **3b**



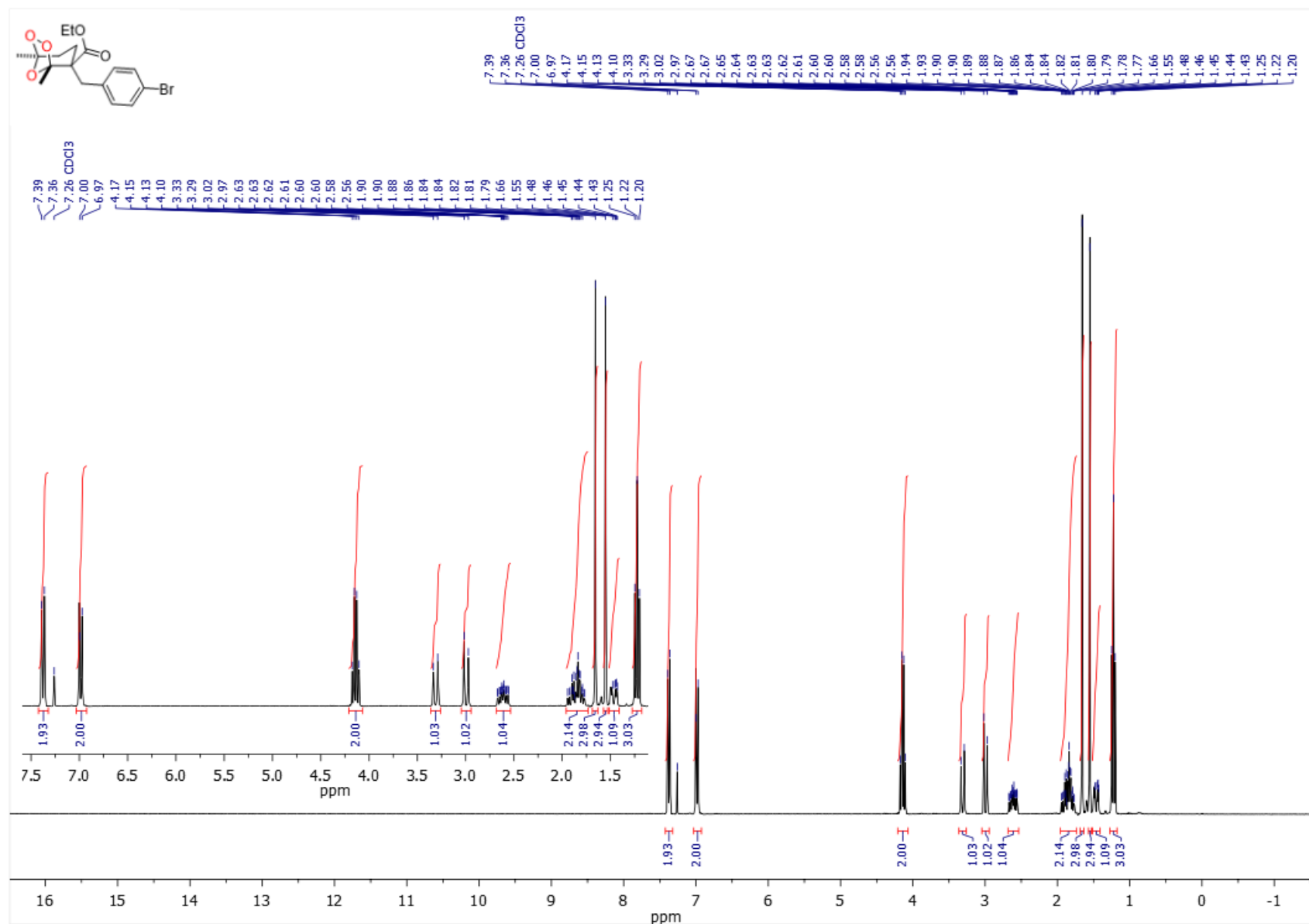
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-(4-bromobenzyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2c



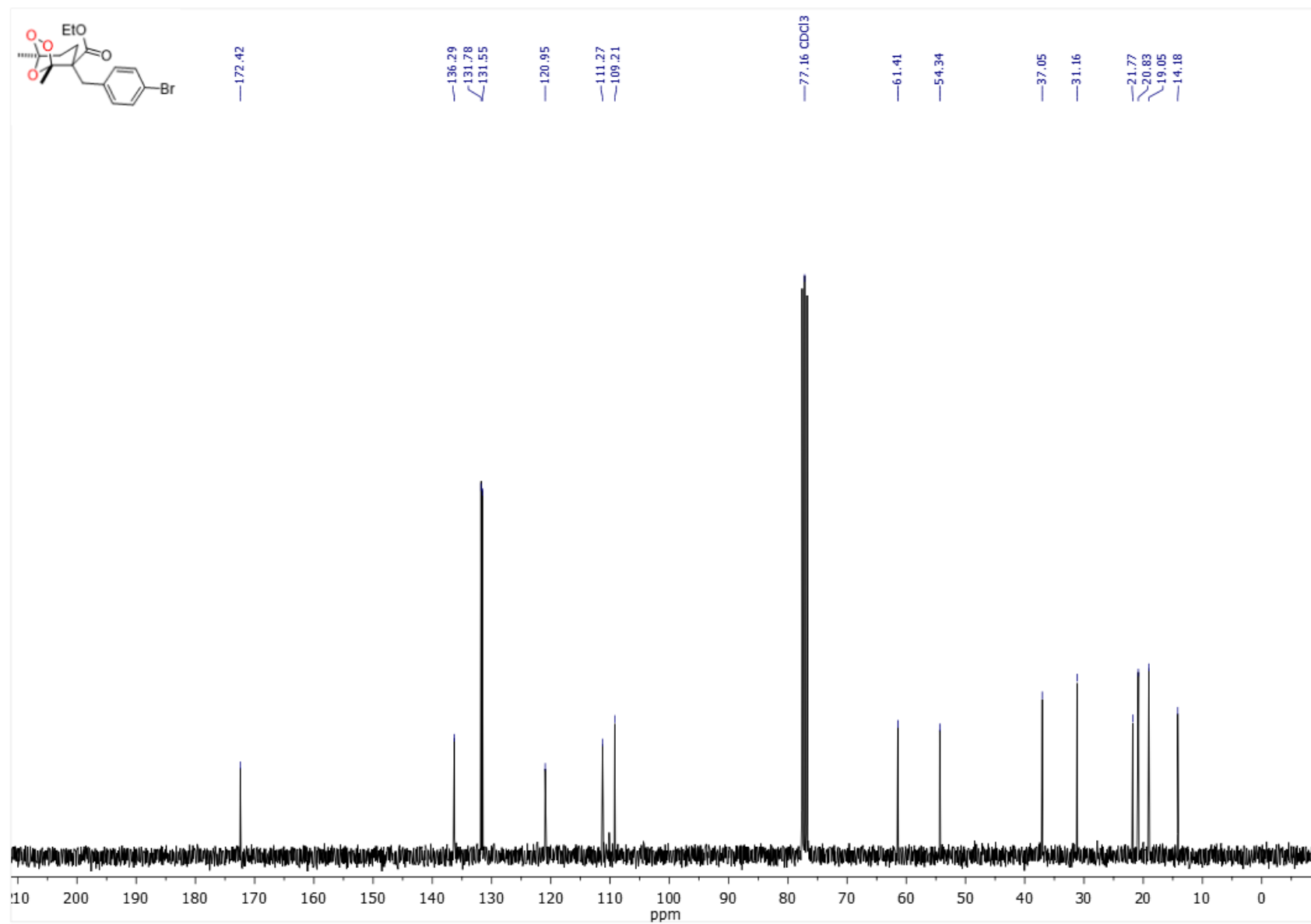
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-(4-bromobenzyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2c



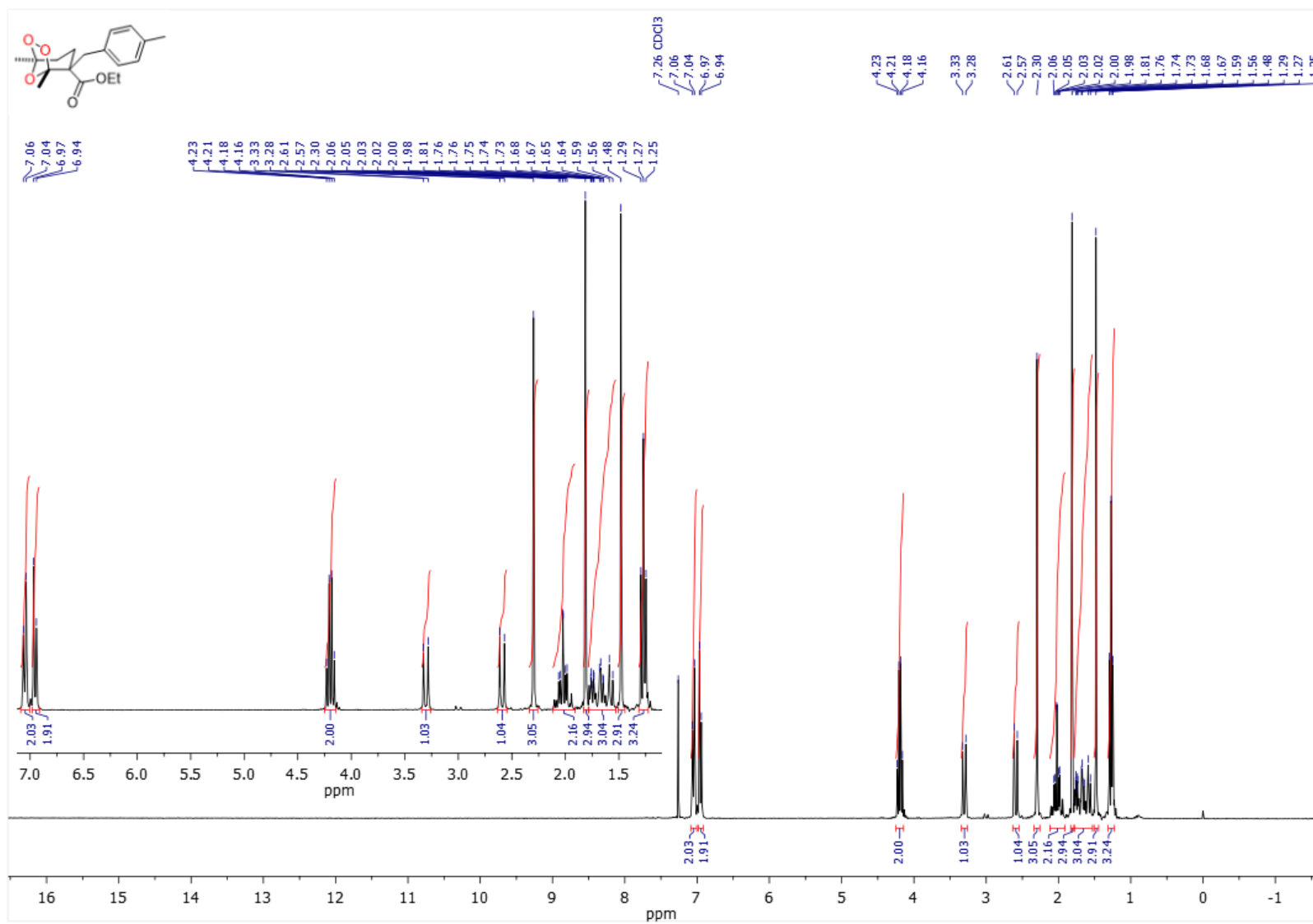
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-(4-bromobenzyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, **3c**



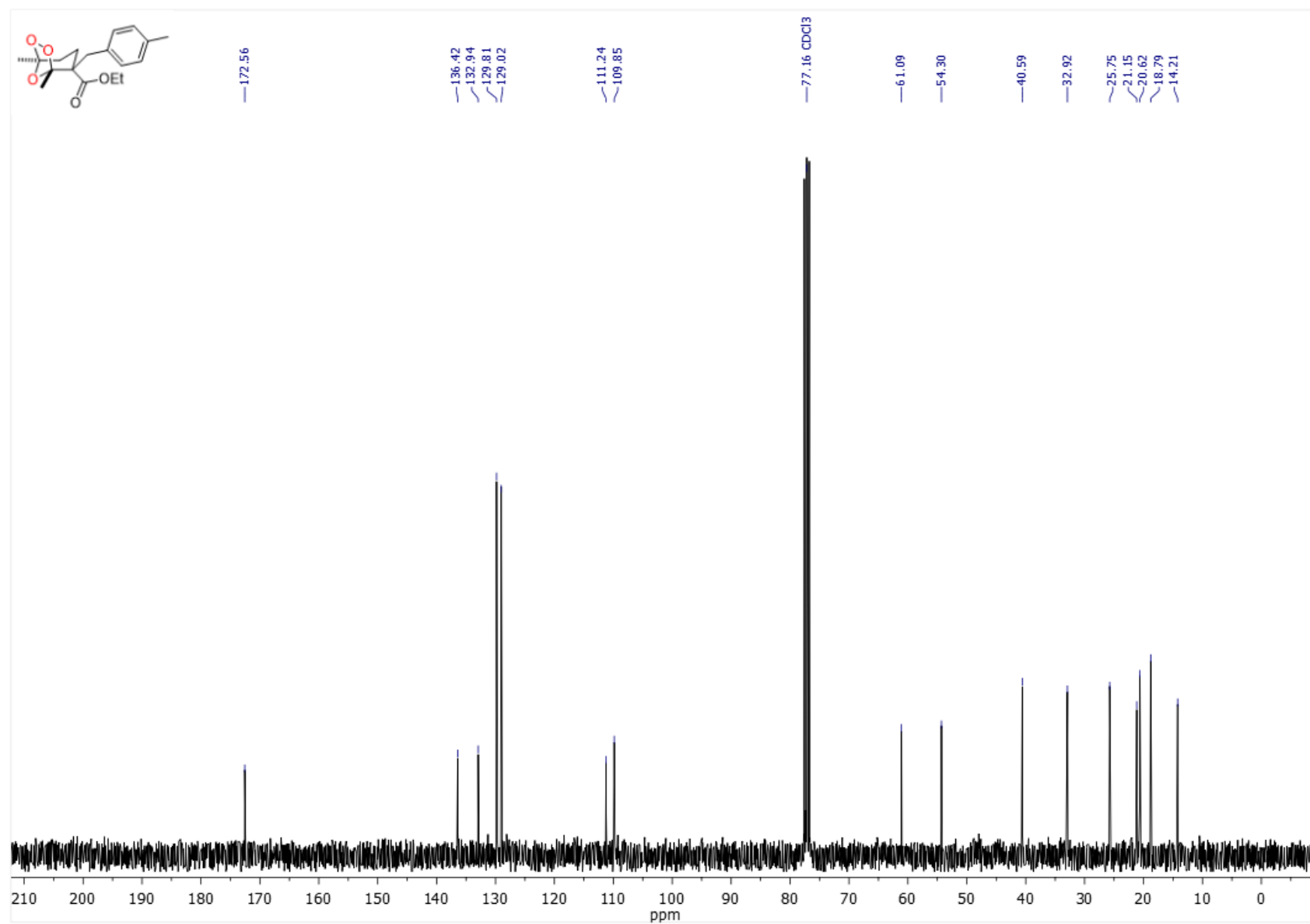
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-(4-bromobenzyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3c



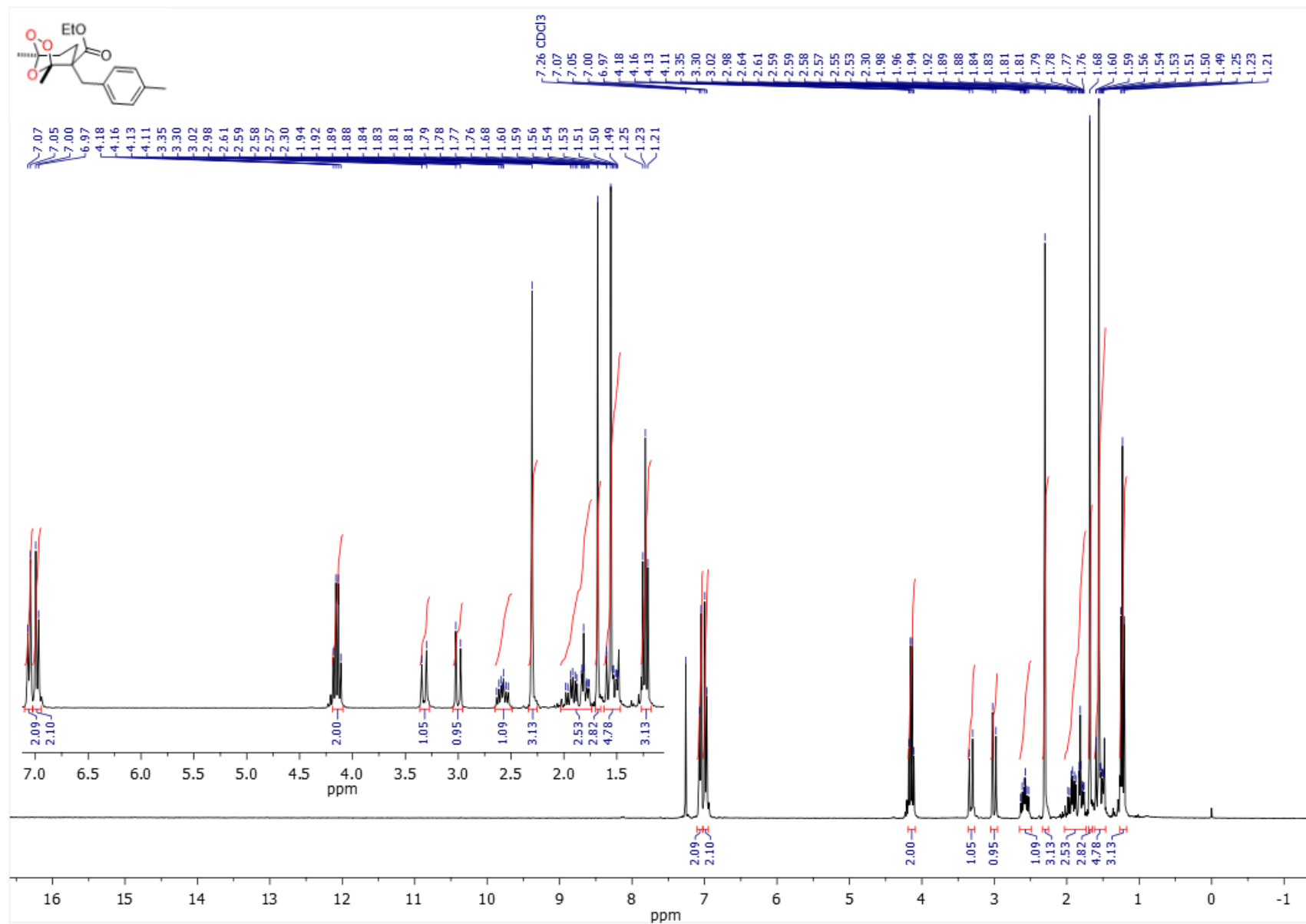
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1R*,2R*,5S*)-1,5-dimethyl-2-(4-methylbenzyl)-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2d



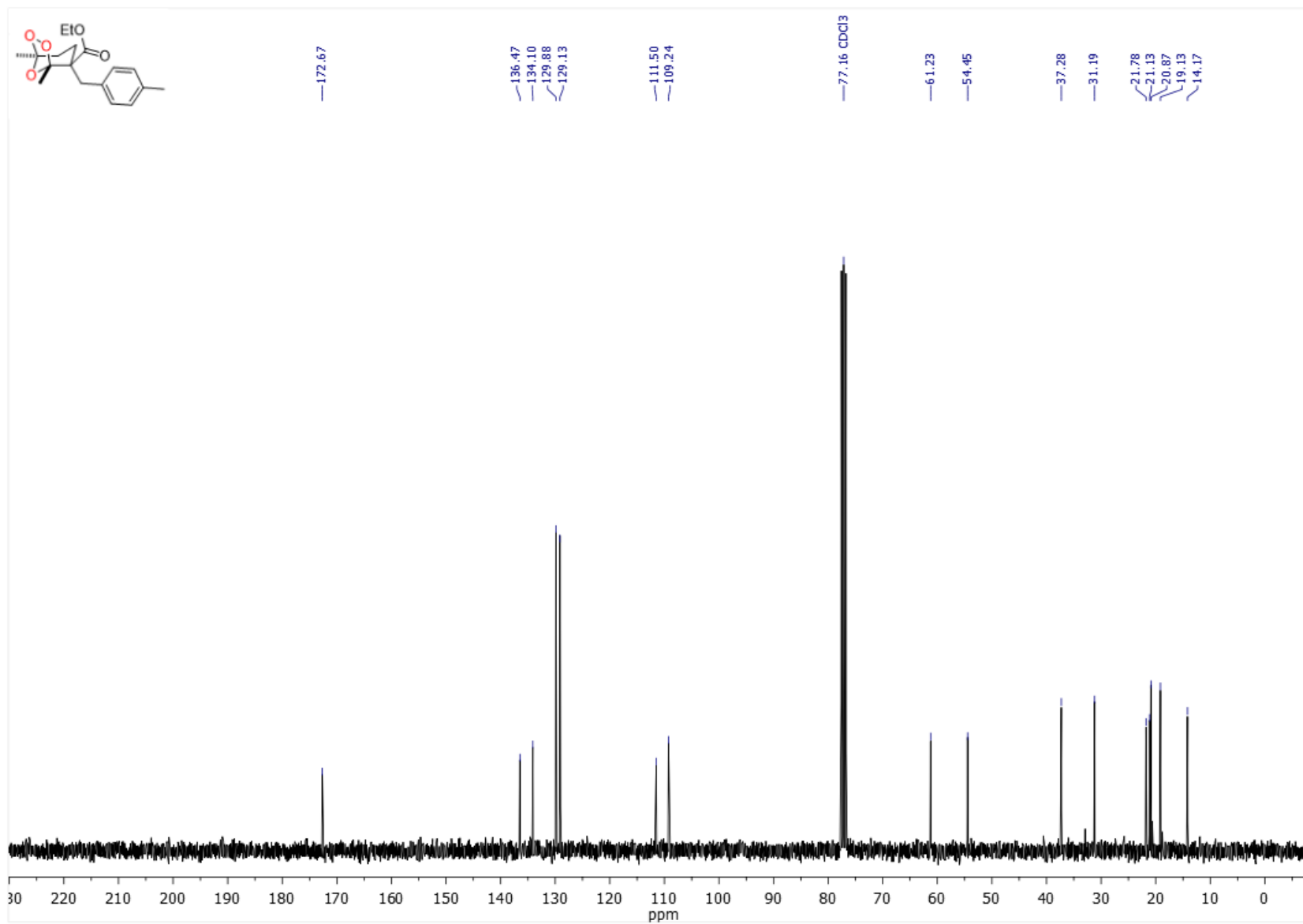
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1R*,2R*,5S*)-1,5-dimethyl-2-(4-methylbenzyl)-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2d



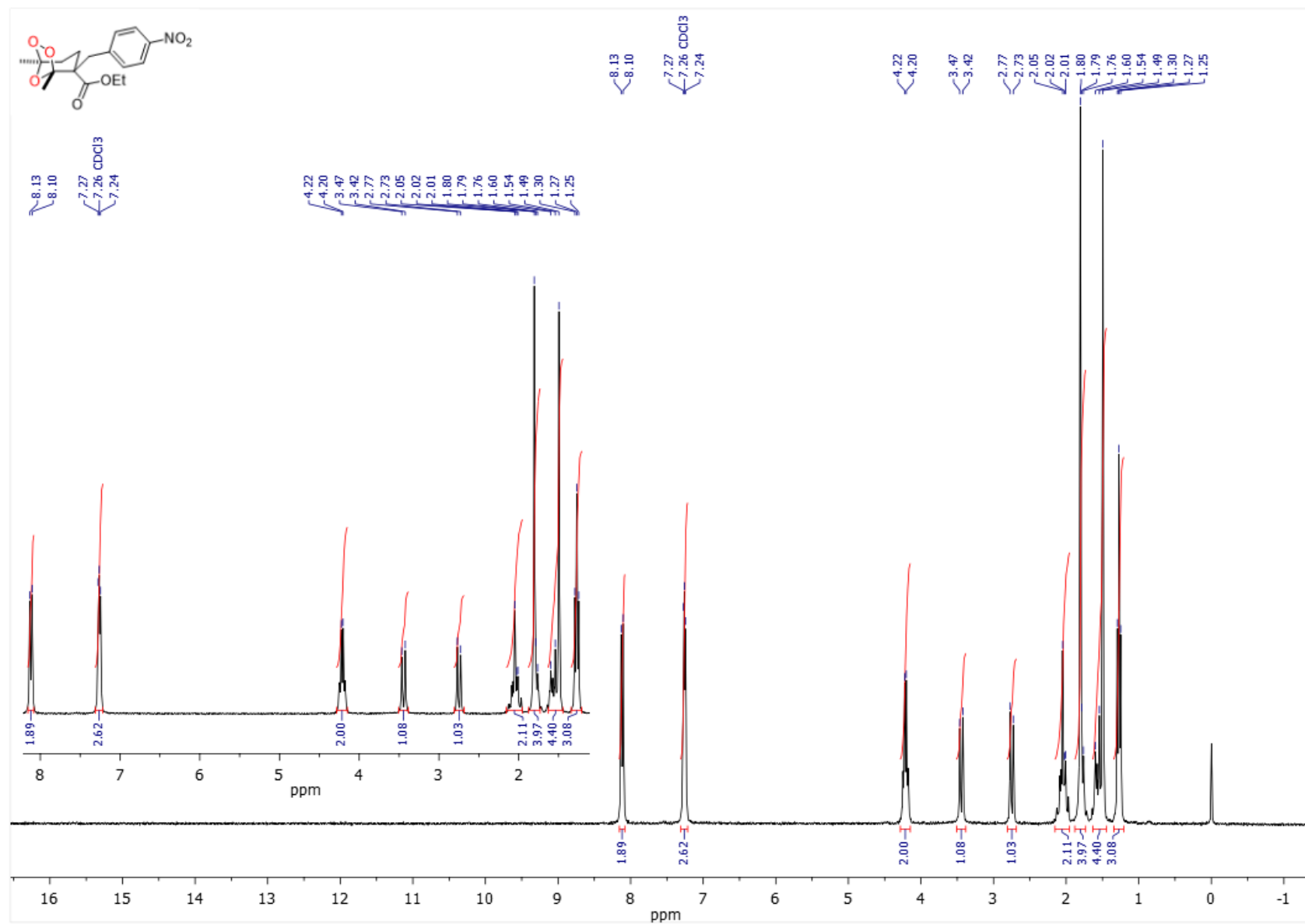
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1R*,2S*,5S*)-1,5-dimethyl-2-(4-methylbenzyl)-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3d



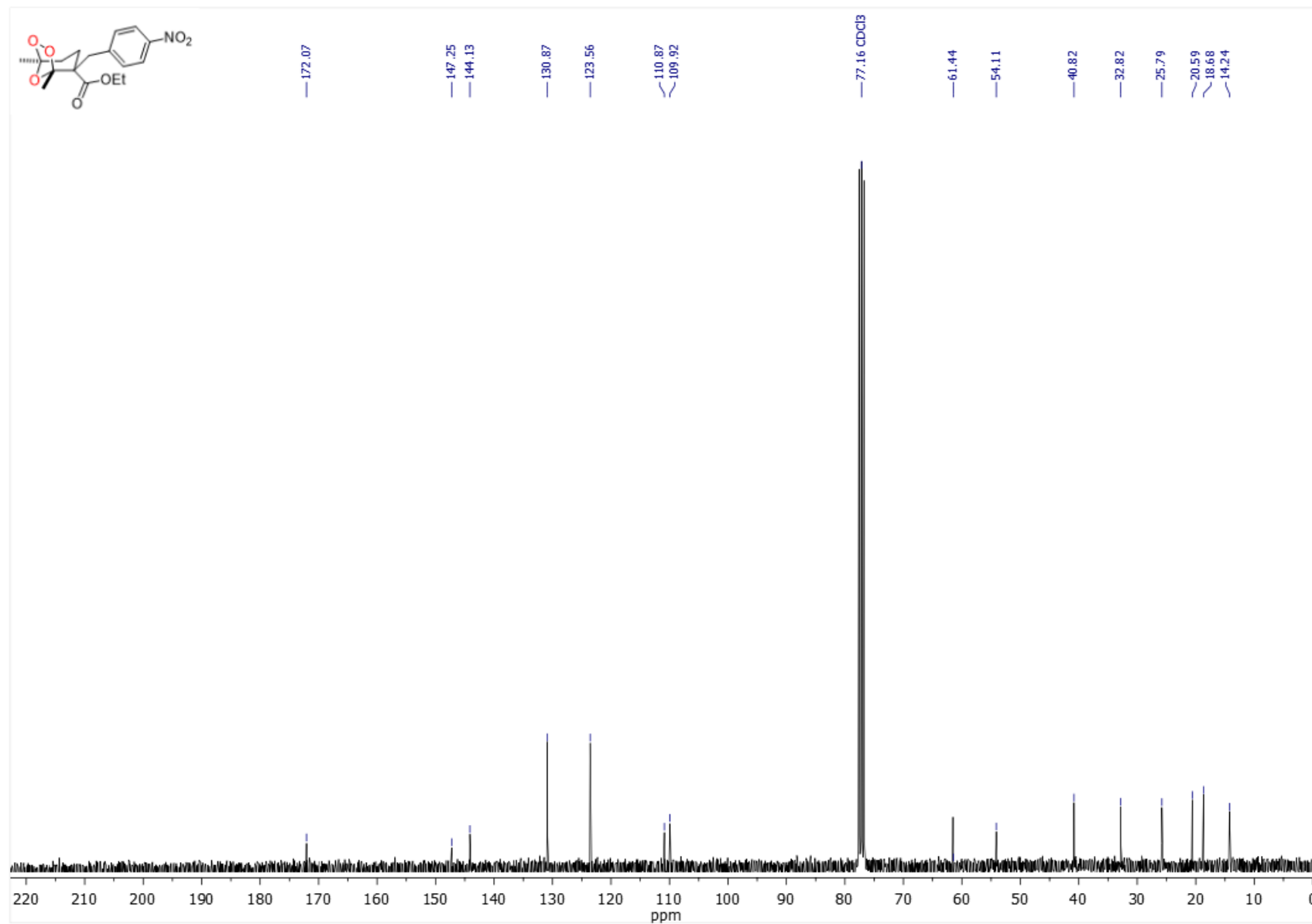
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1R*,2S*,5S*)-1,5-dimethyl-2-(4-methylbenzyl)-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3d



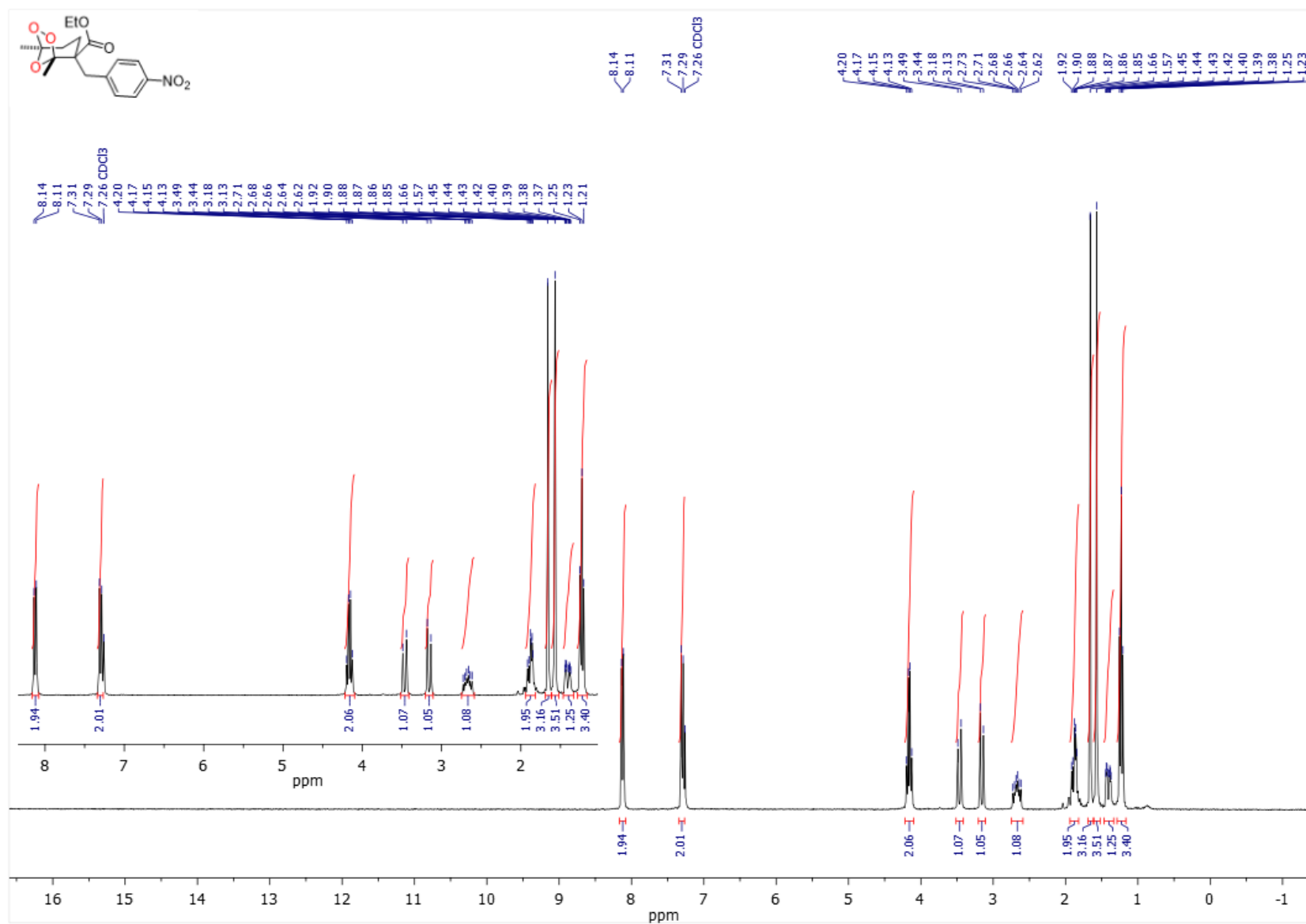
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-1,5-dimethyl-2-(4-nitrobenzyl)-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2e



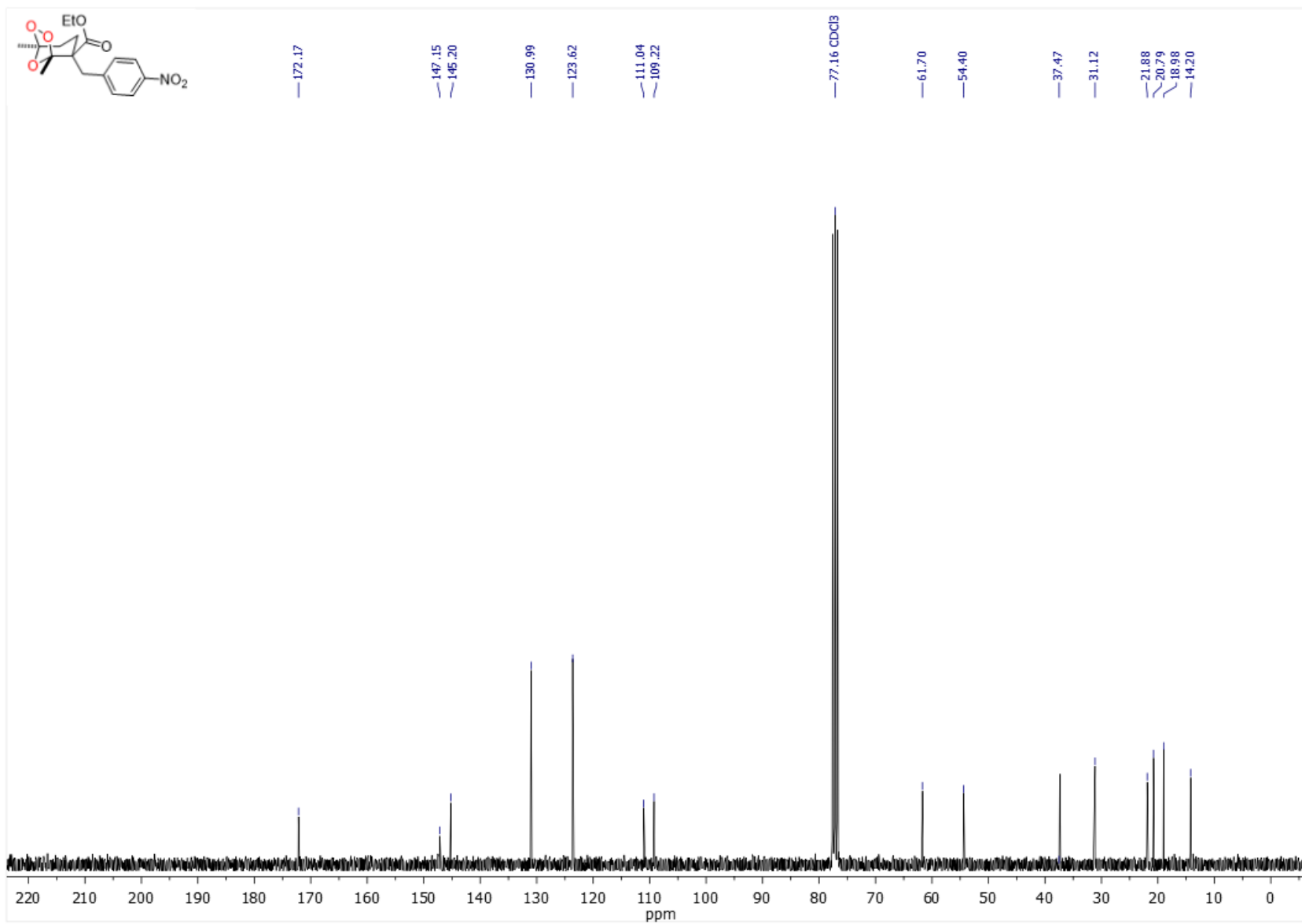
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-1,5-dimethyl-2-(4-nitrobenzyl)-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2e



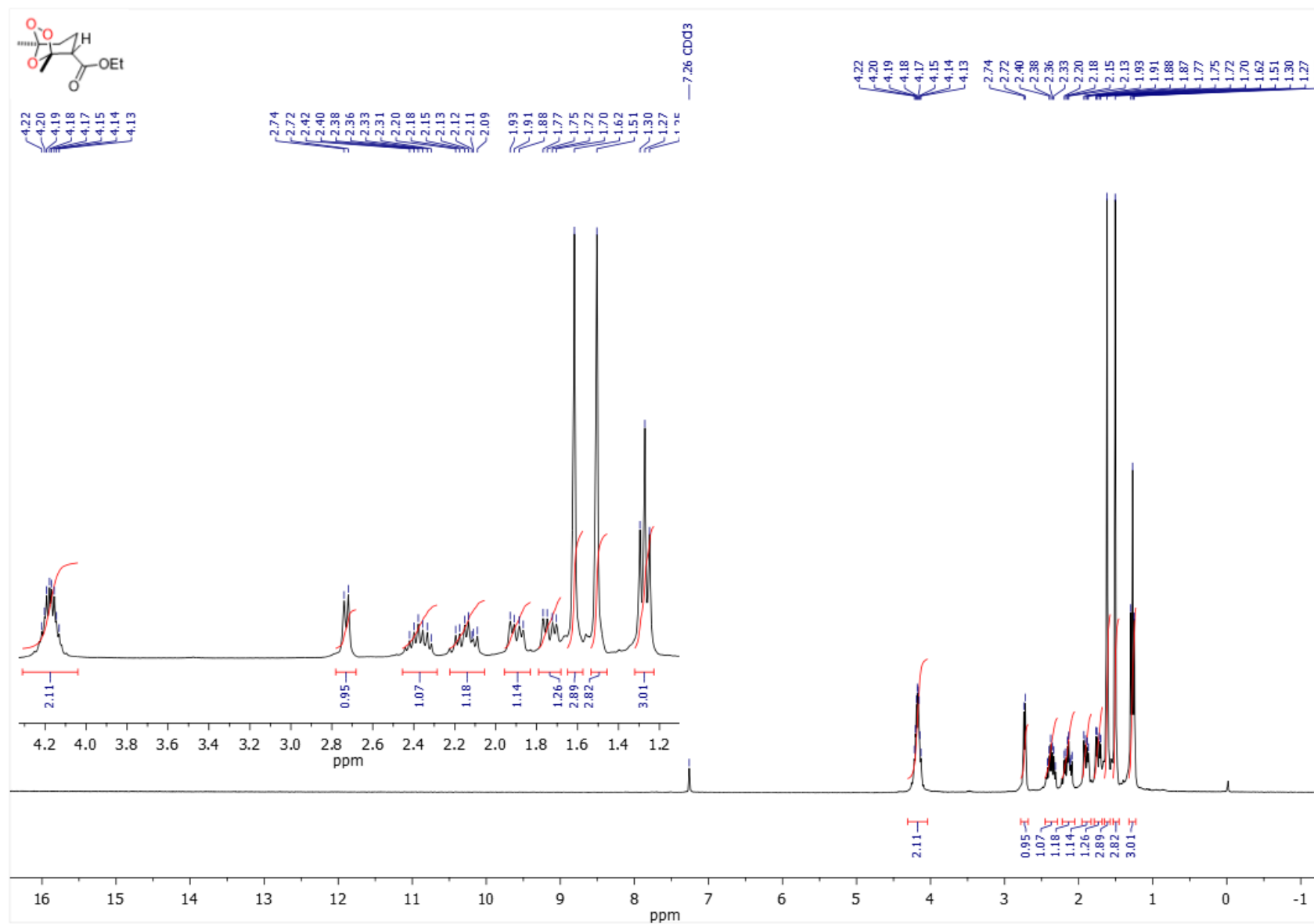
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-1,5-dimethyl-2-(4-nitrobenzyl)-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3e



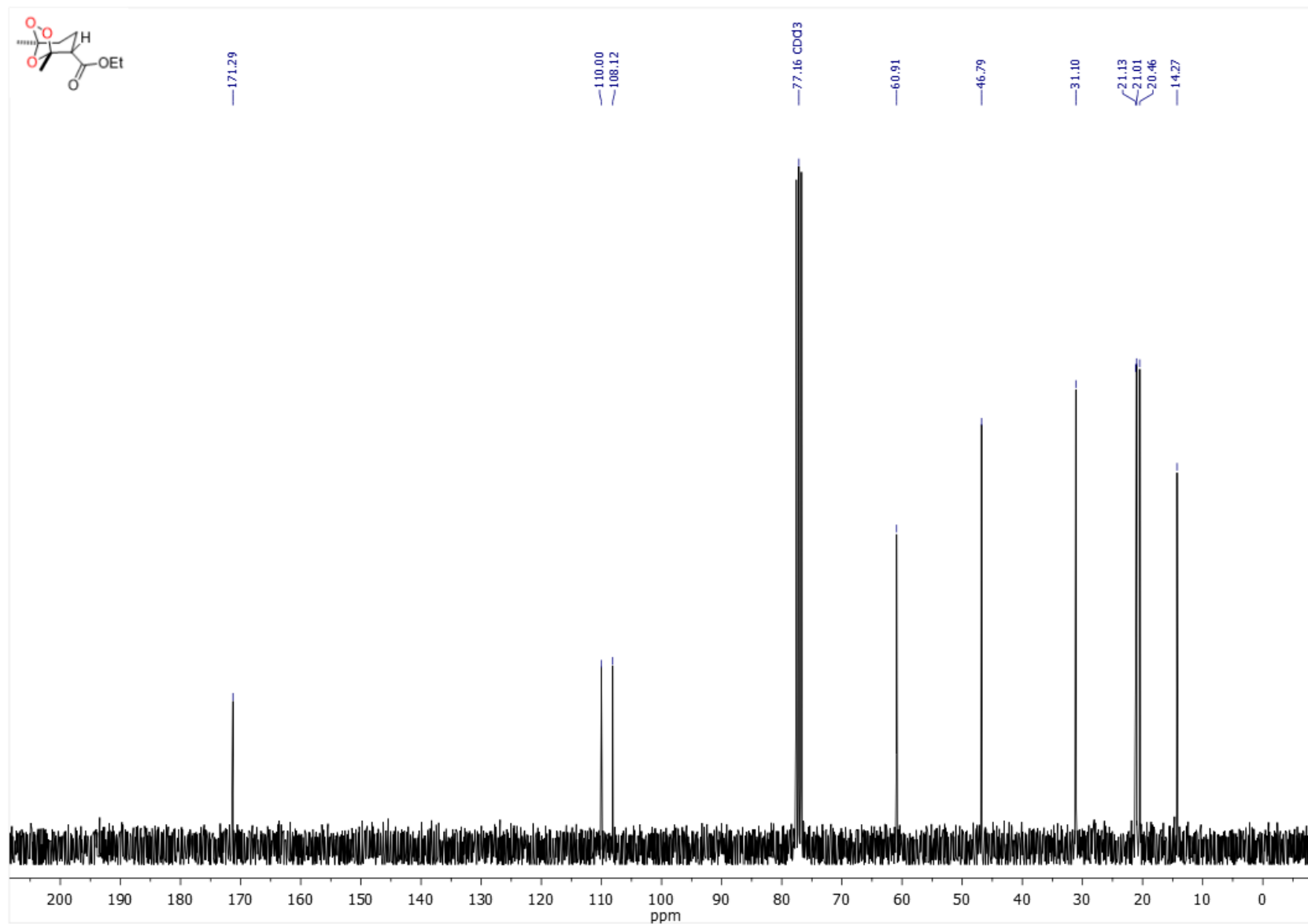
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-1,5-dimethyl-2-(4-nitrobenzyl)-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3e



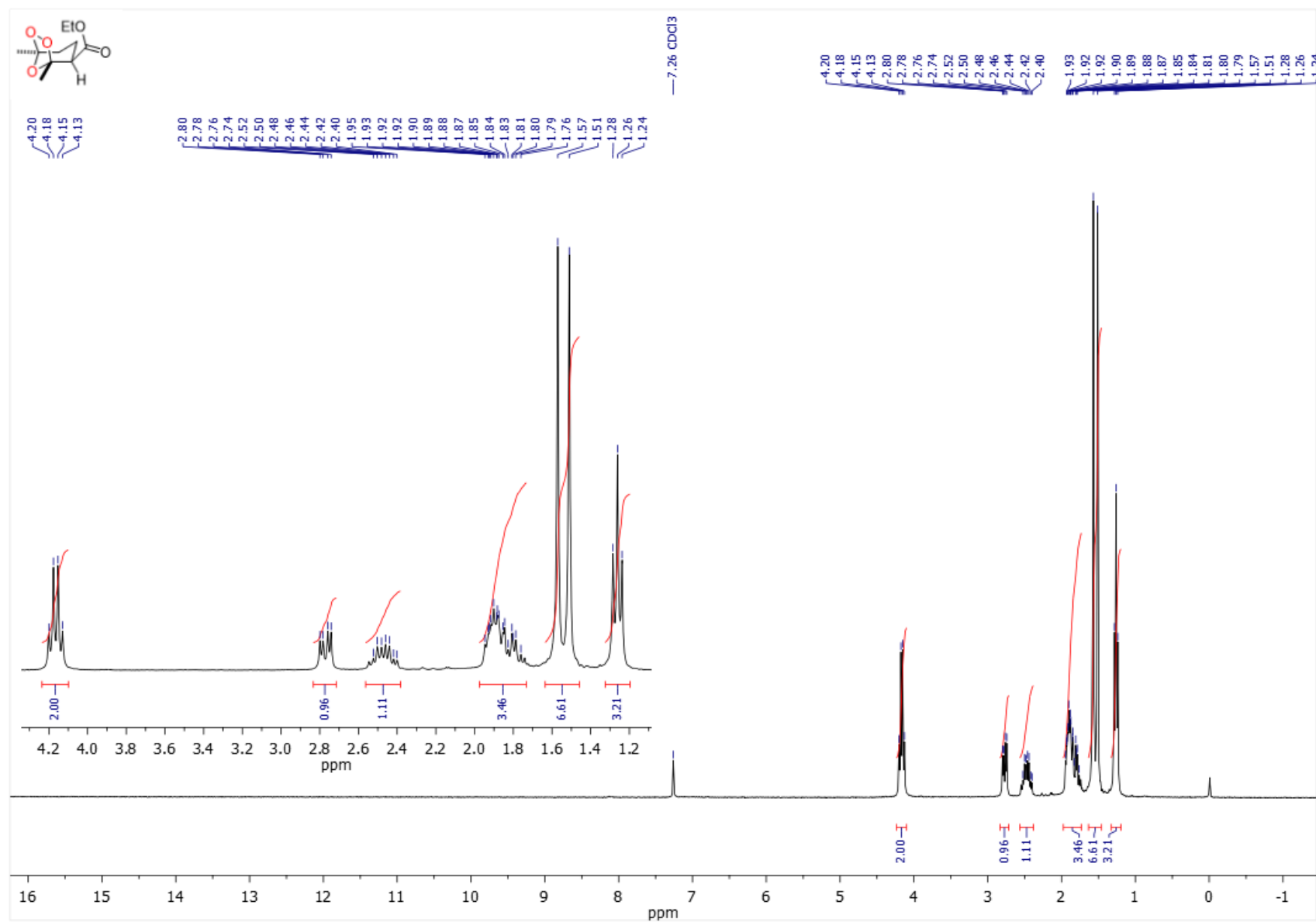
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2f



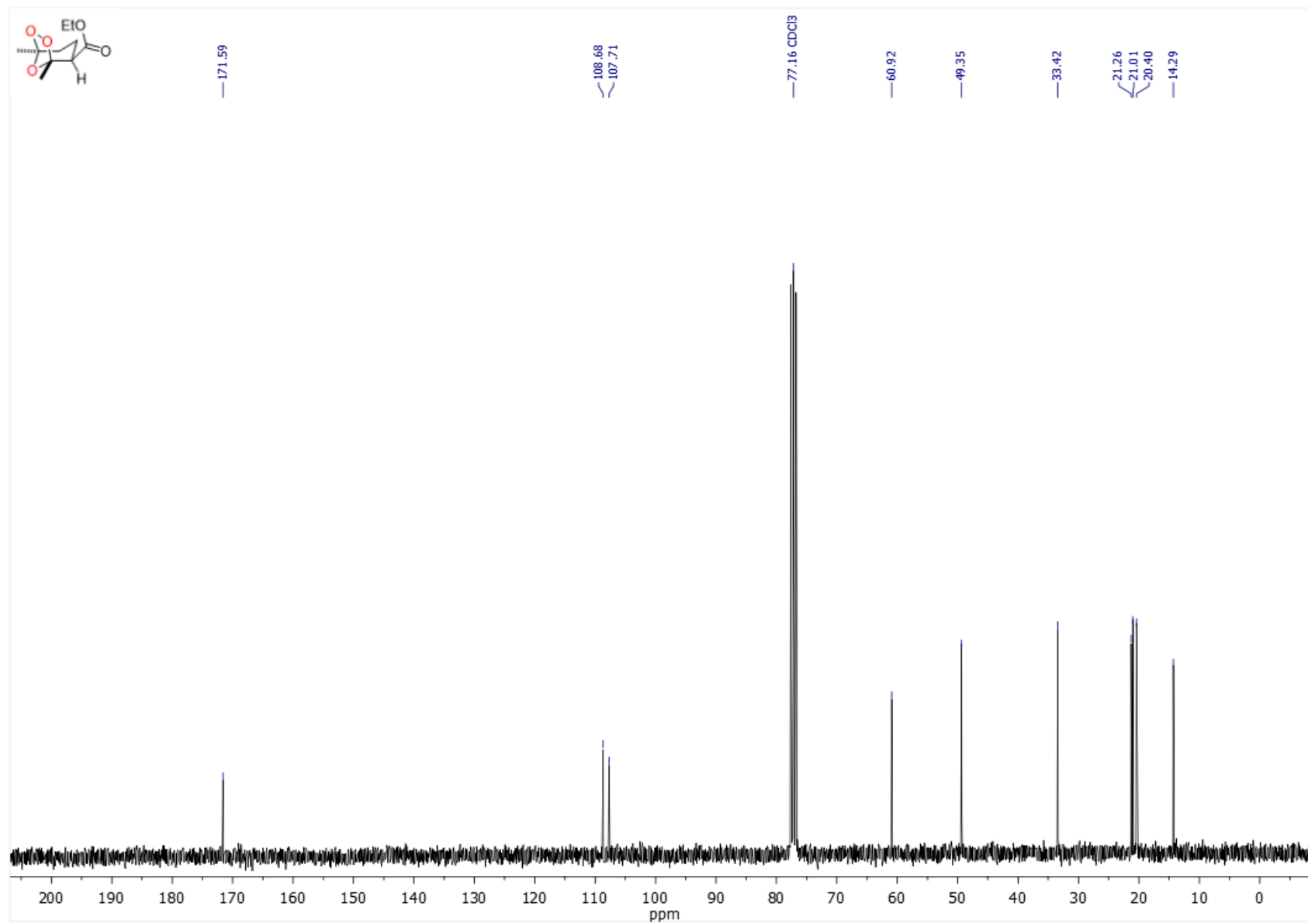
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2f



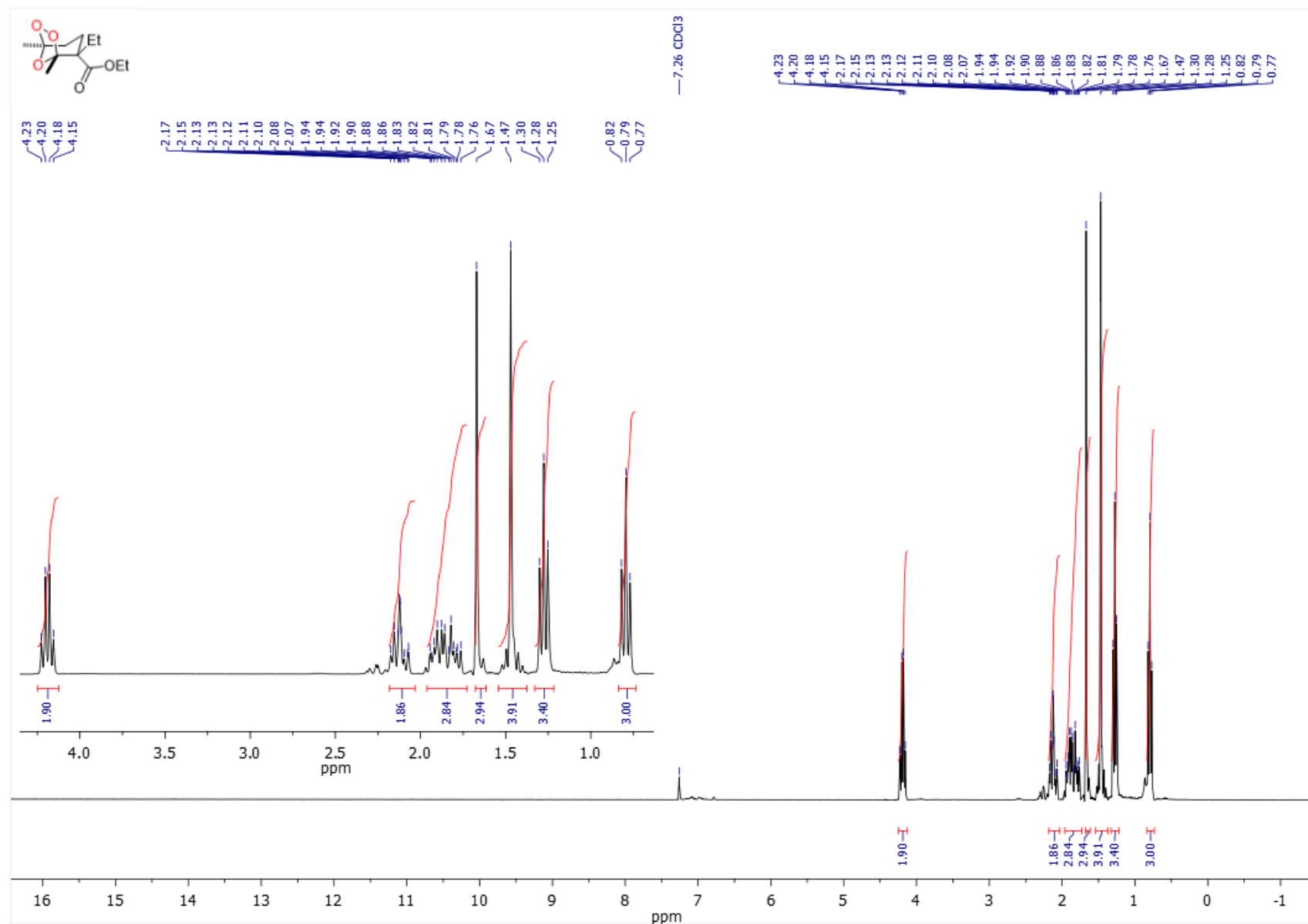
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3f



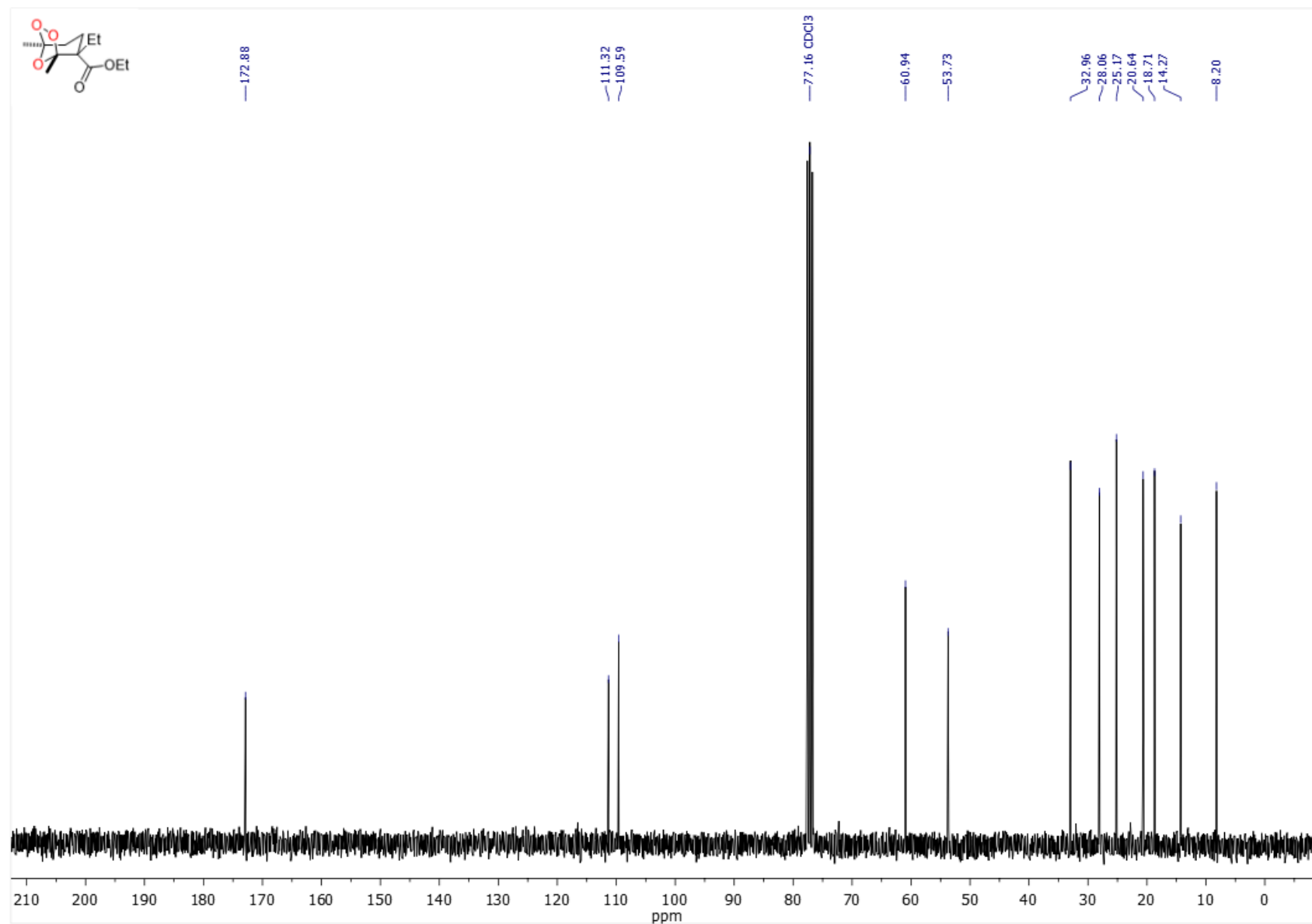
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3f



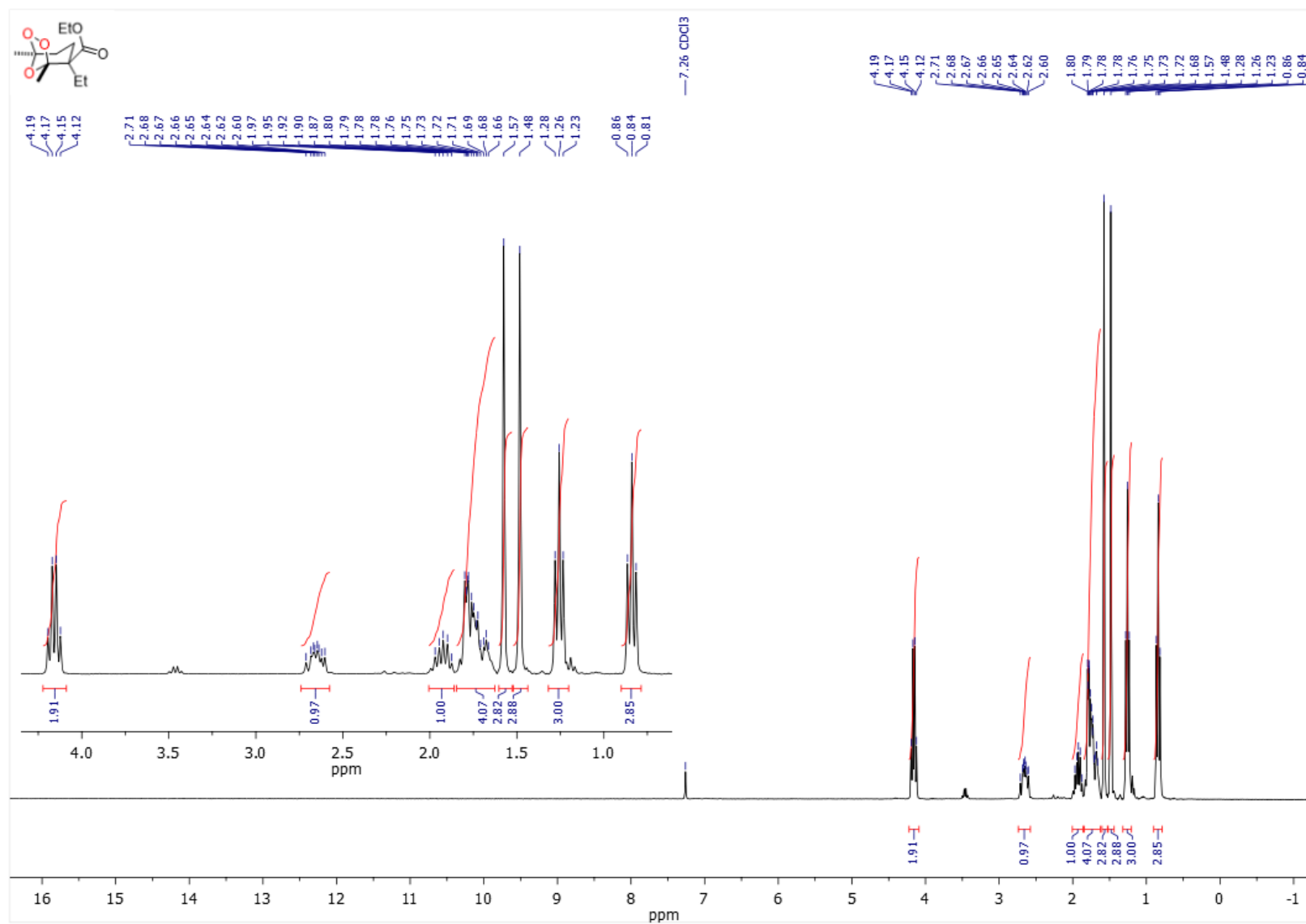
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-ethyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2g



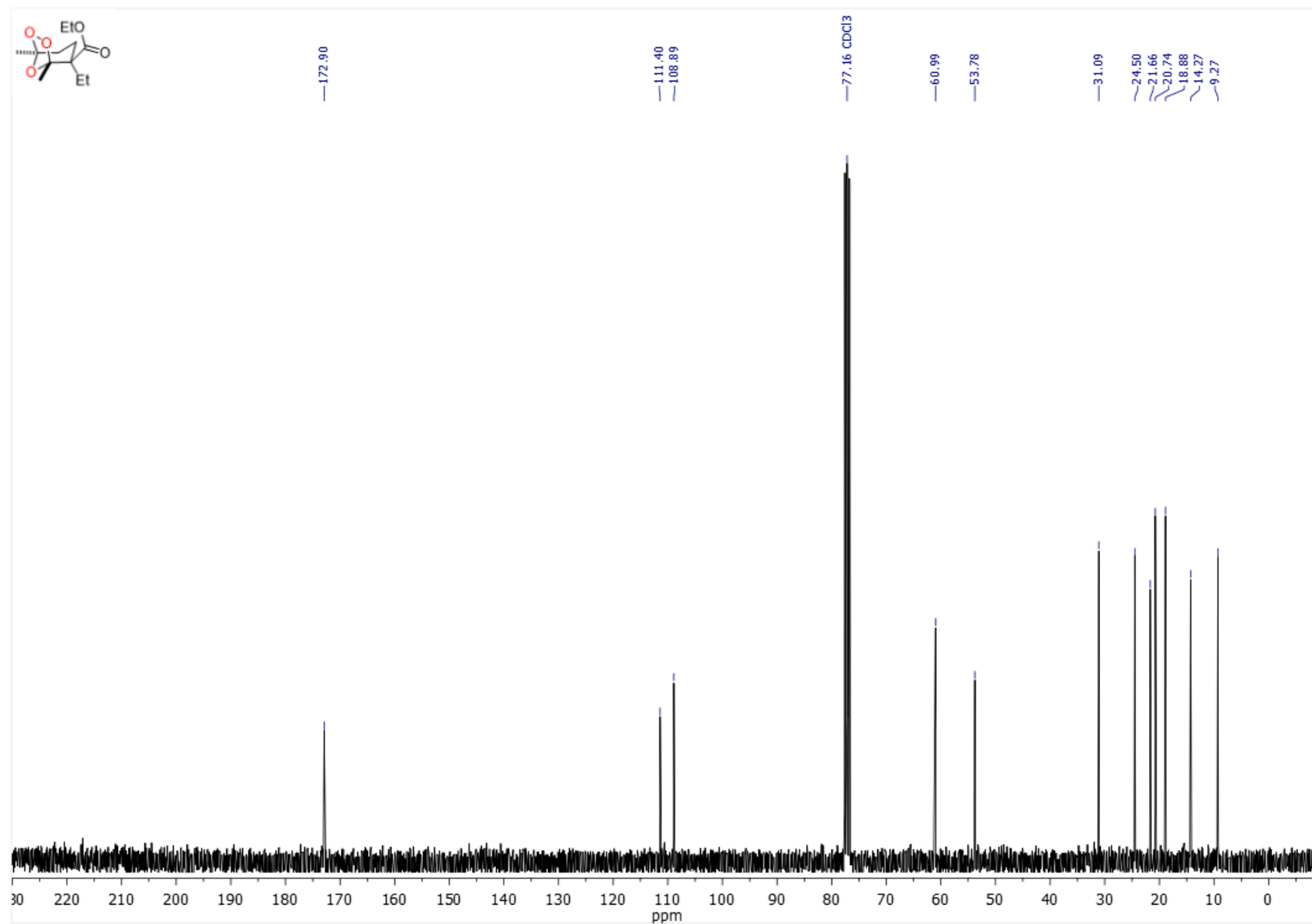
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-ethyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2g



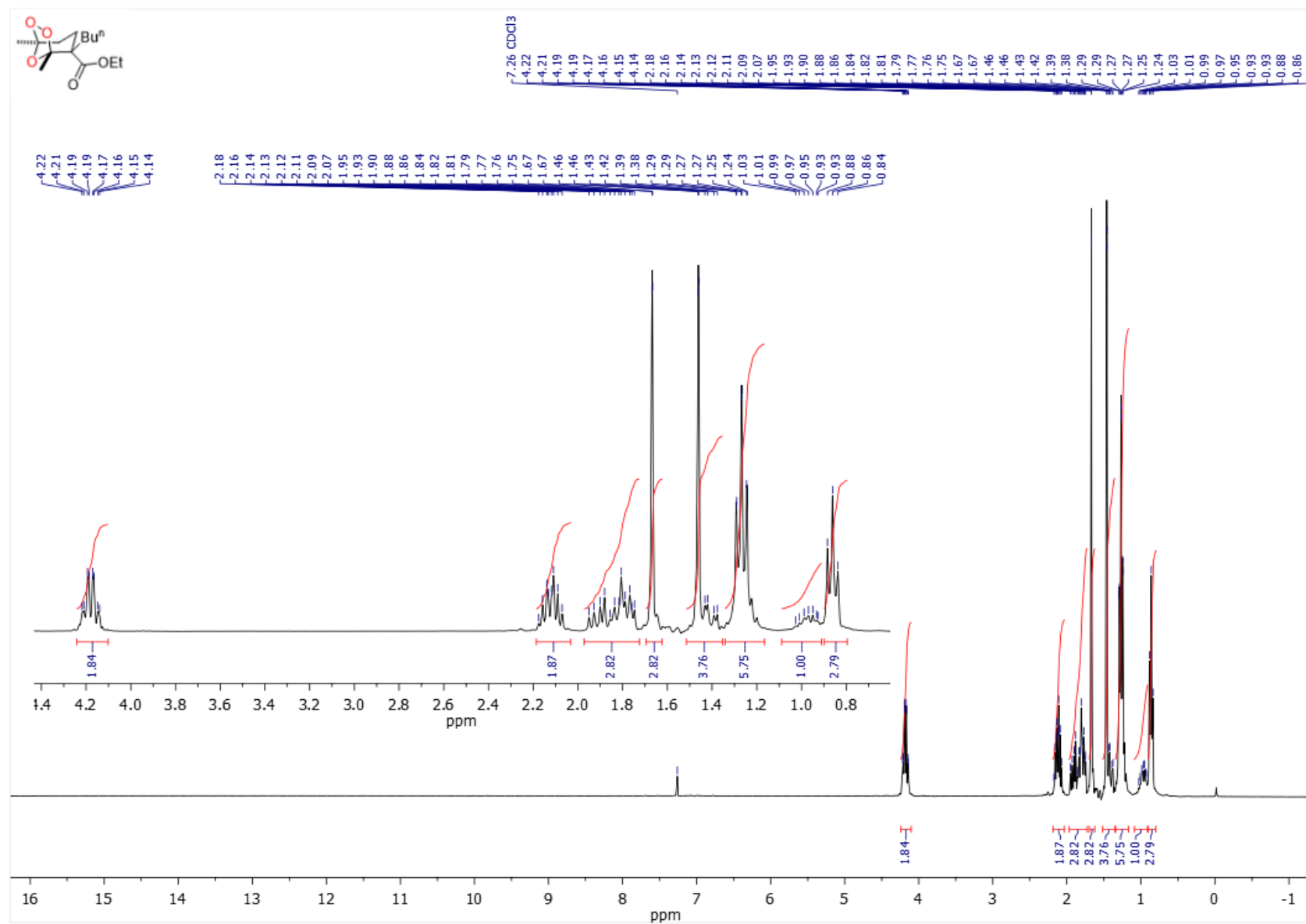
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-ethyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3g



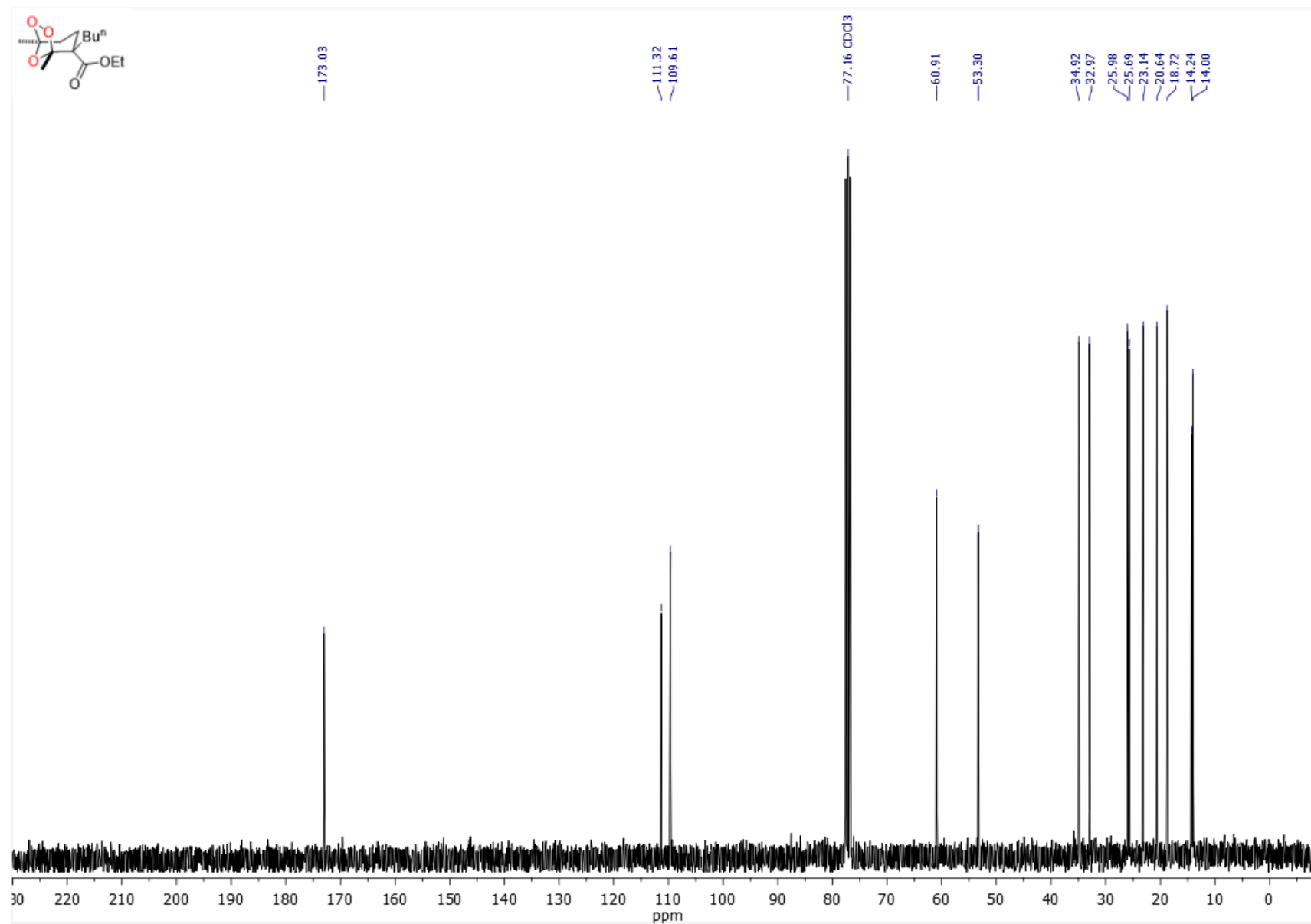
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-ethyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3g



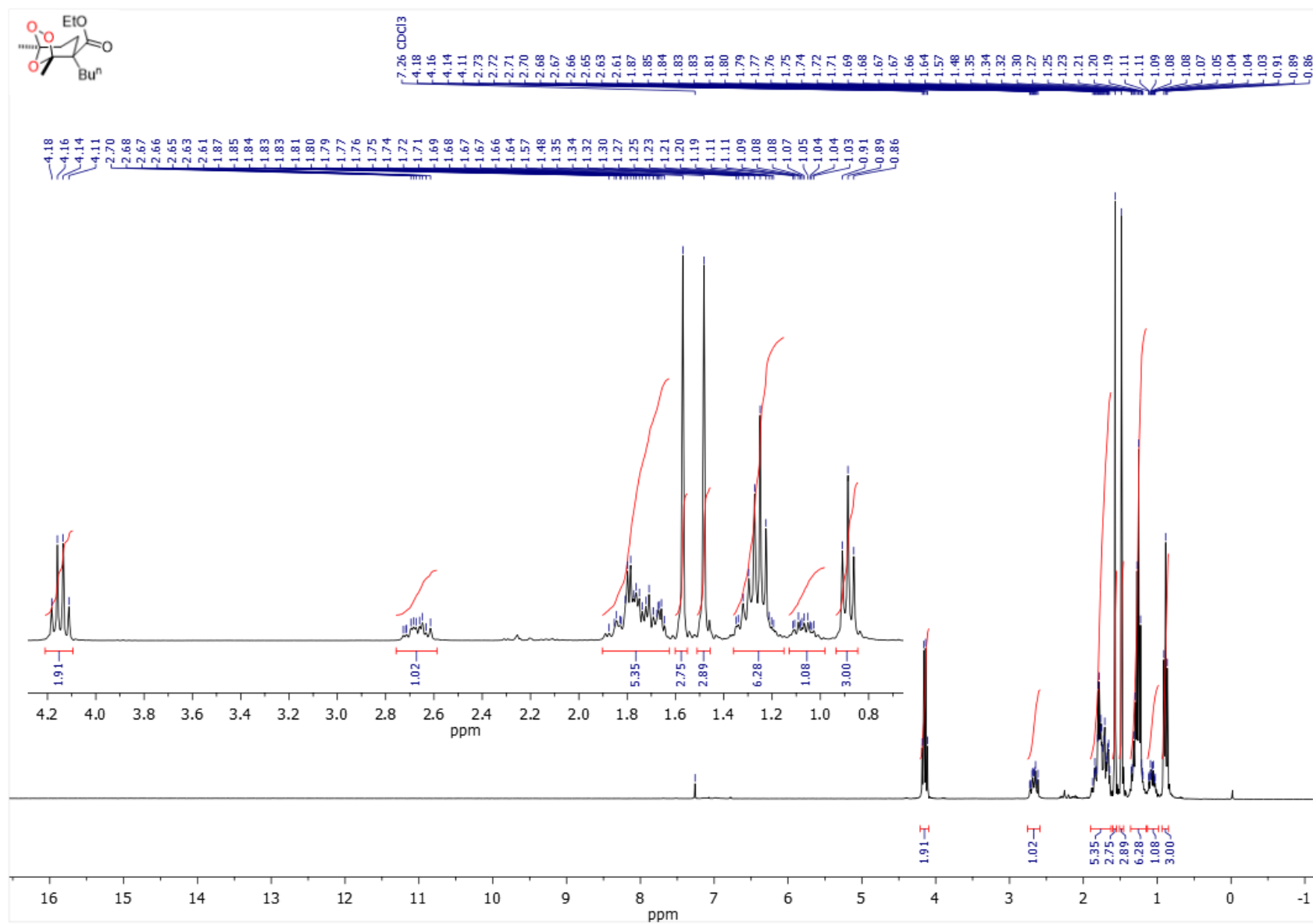
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-butyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2h



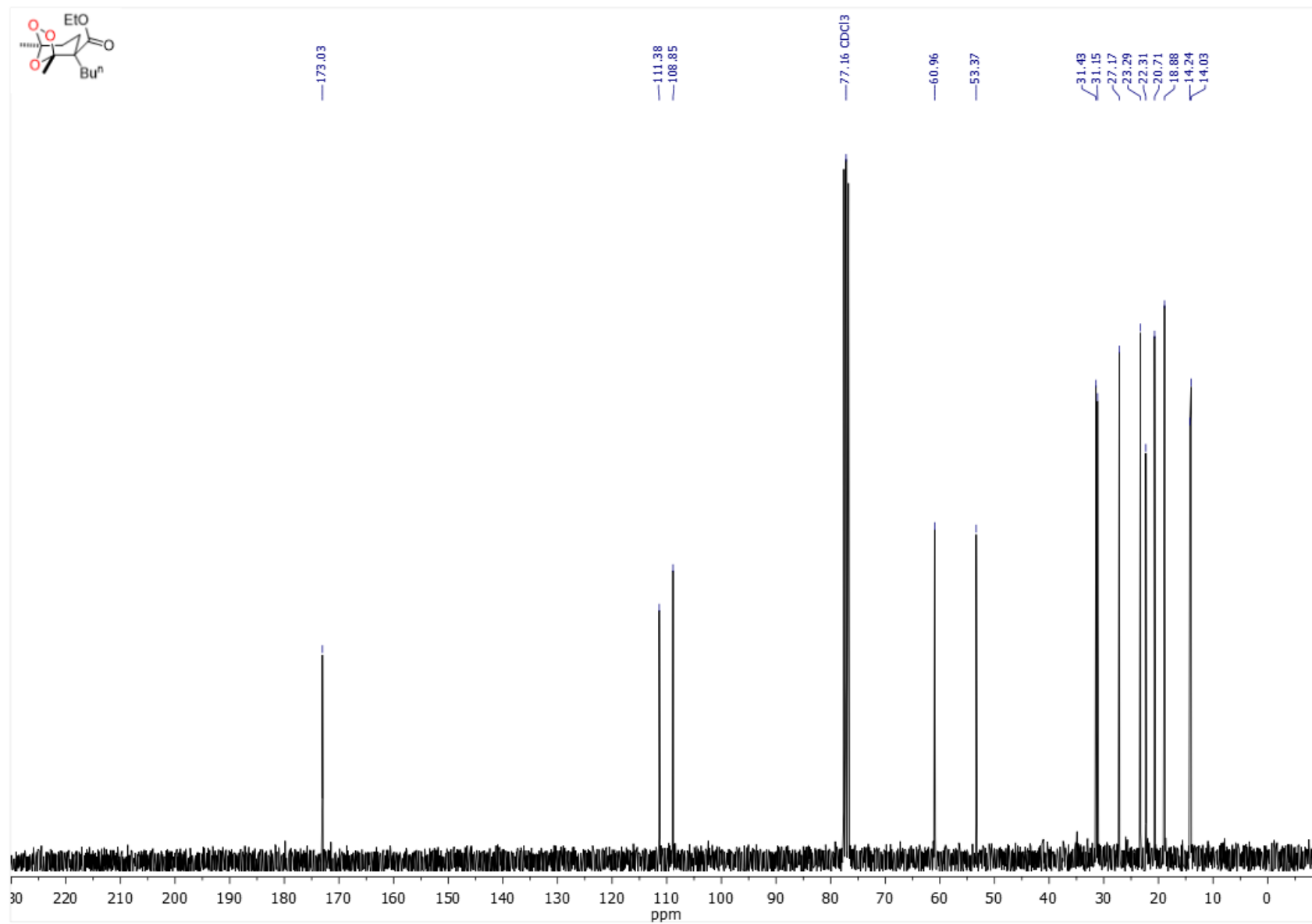
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-butyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2h



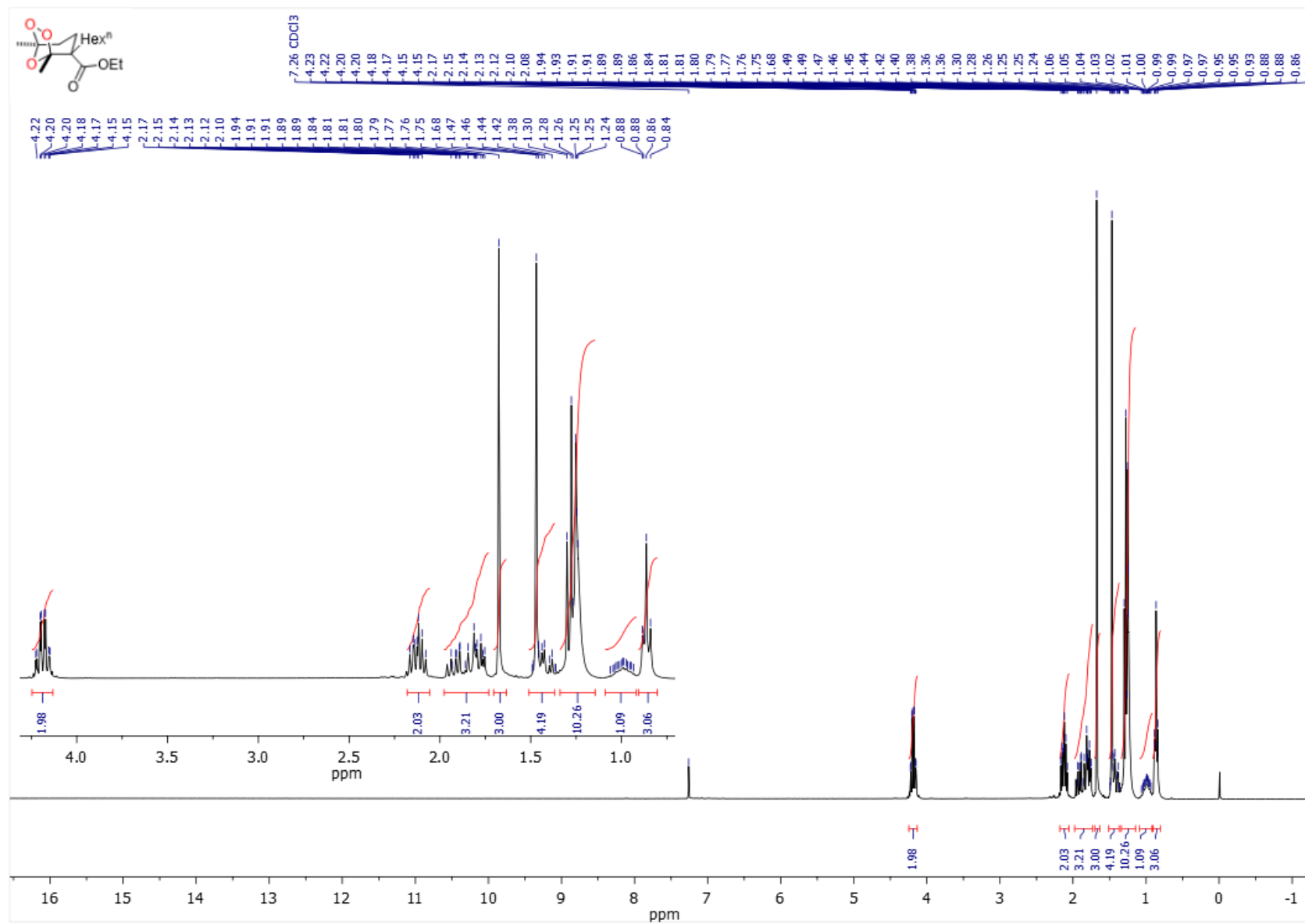
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-butyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3h



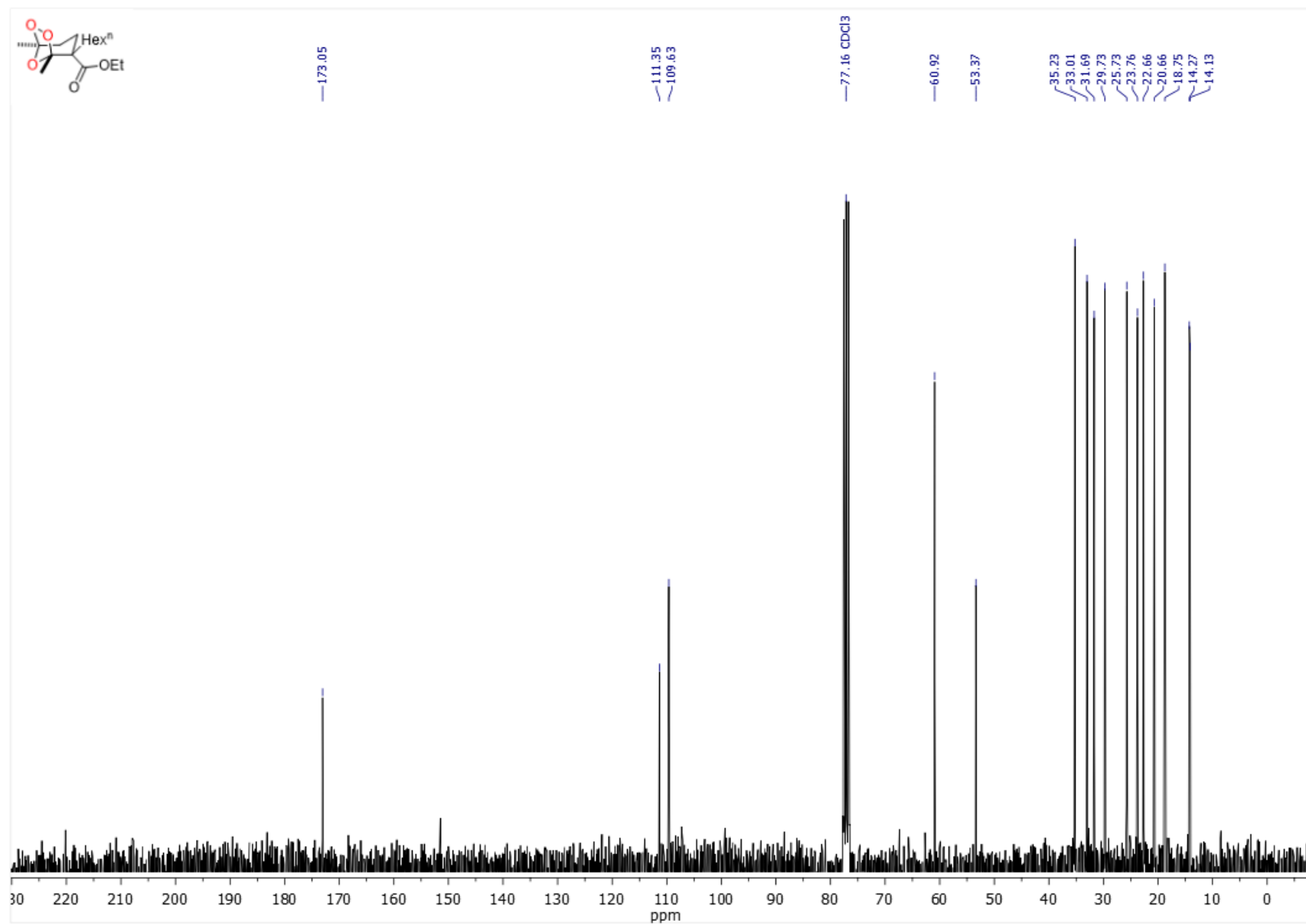
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-butyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3h



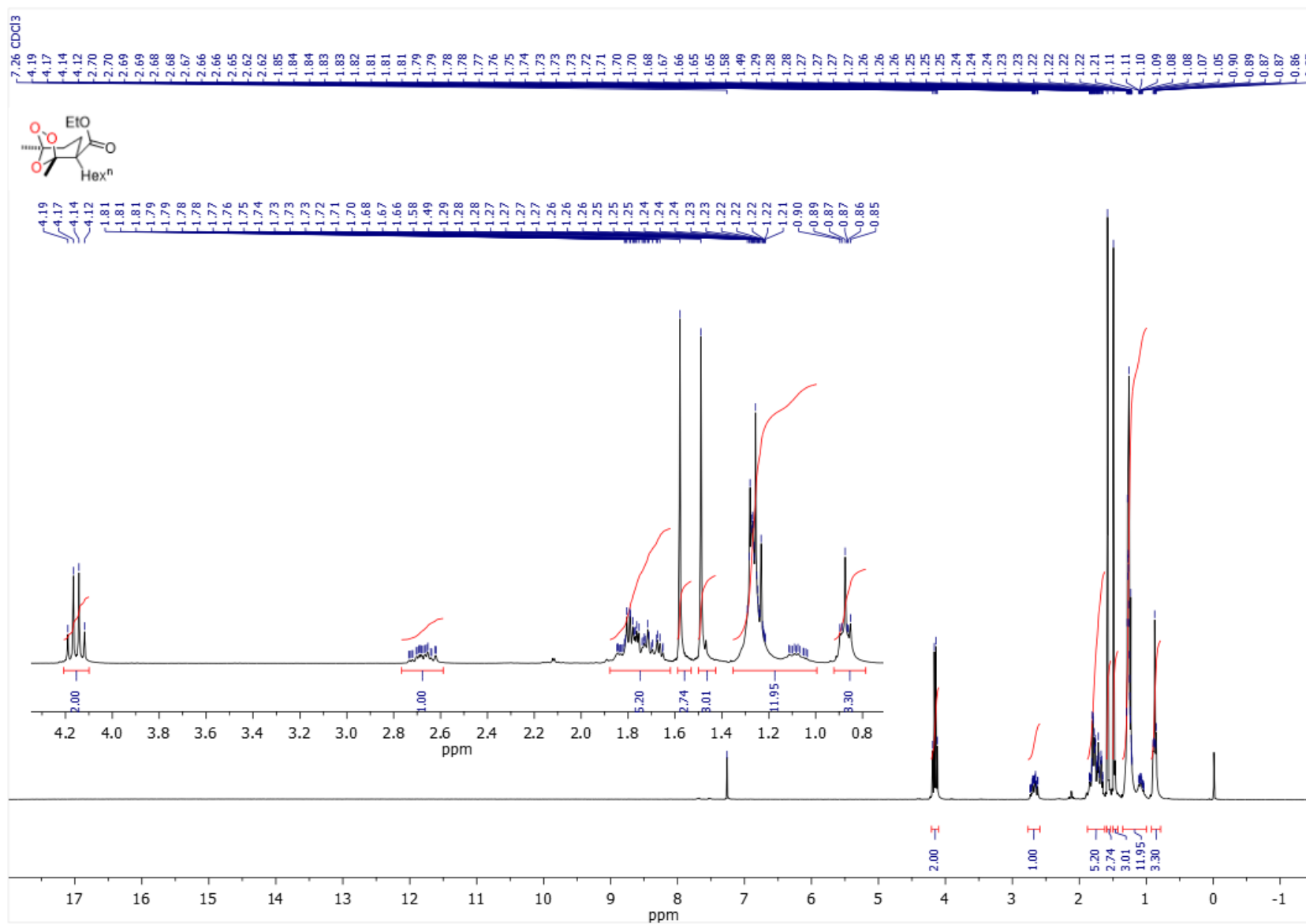
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-hexyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2i



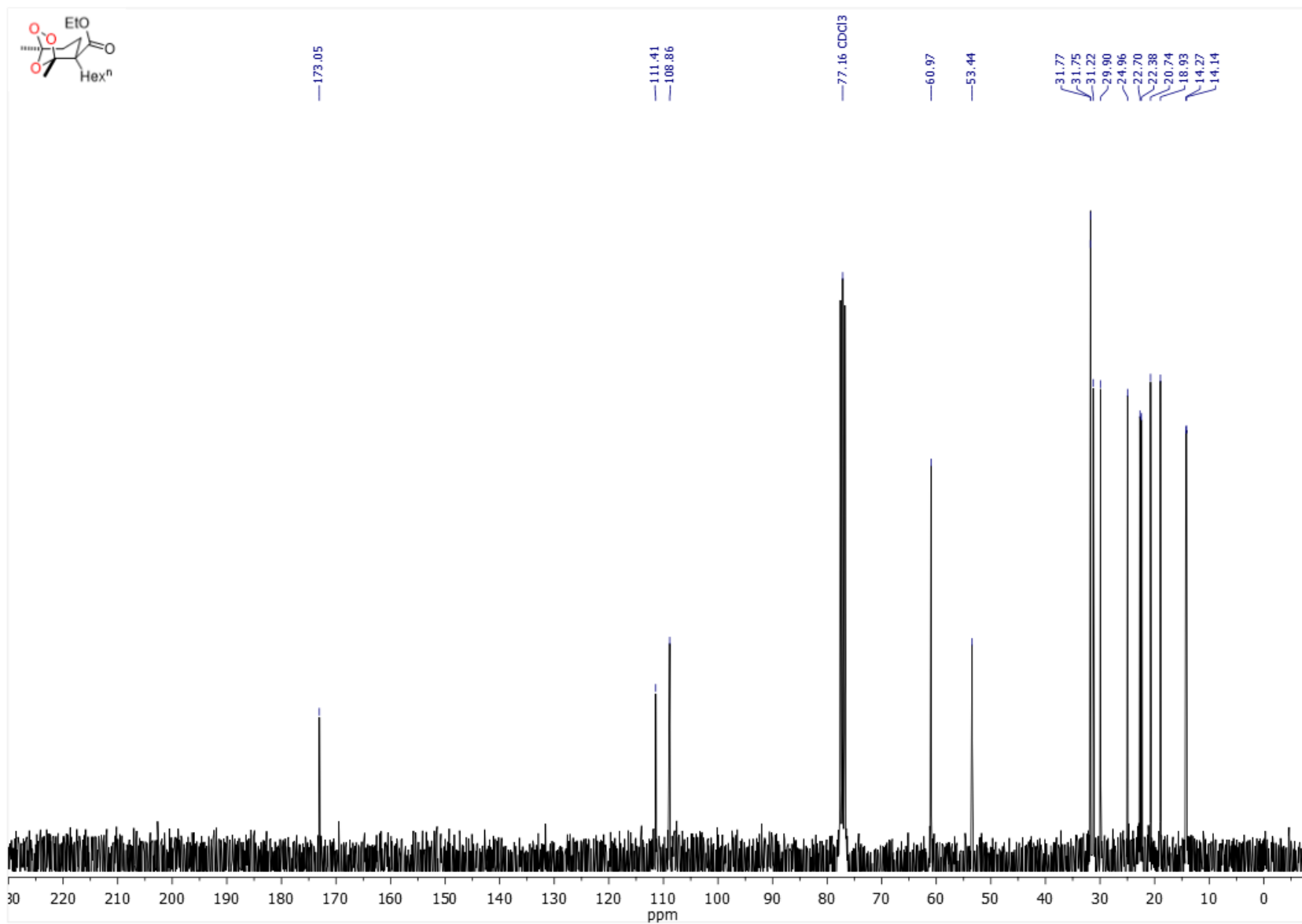
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-hexyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2i



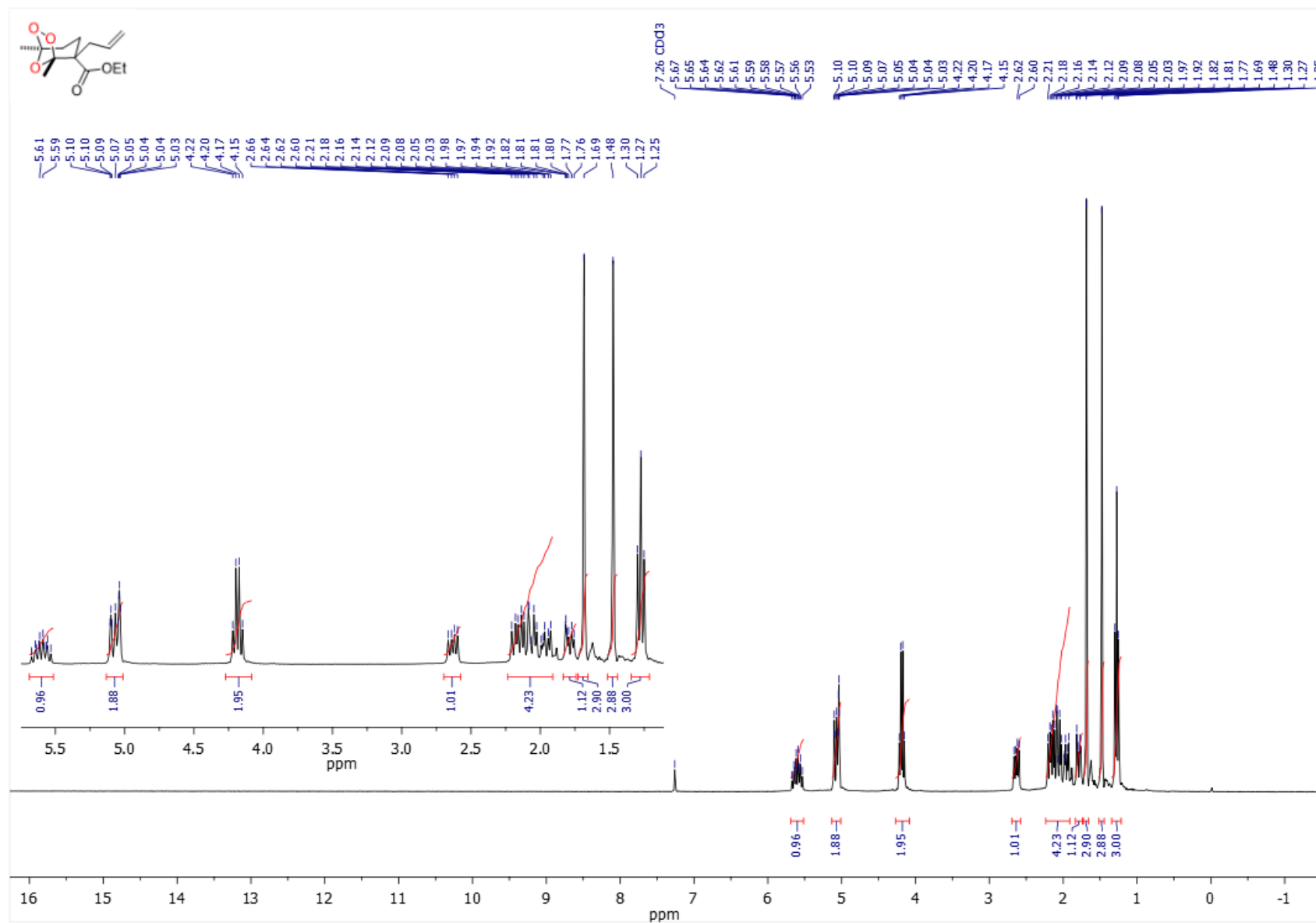
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-hexyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3i



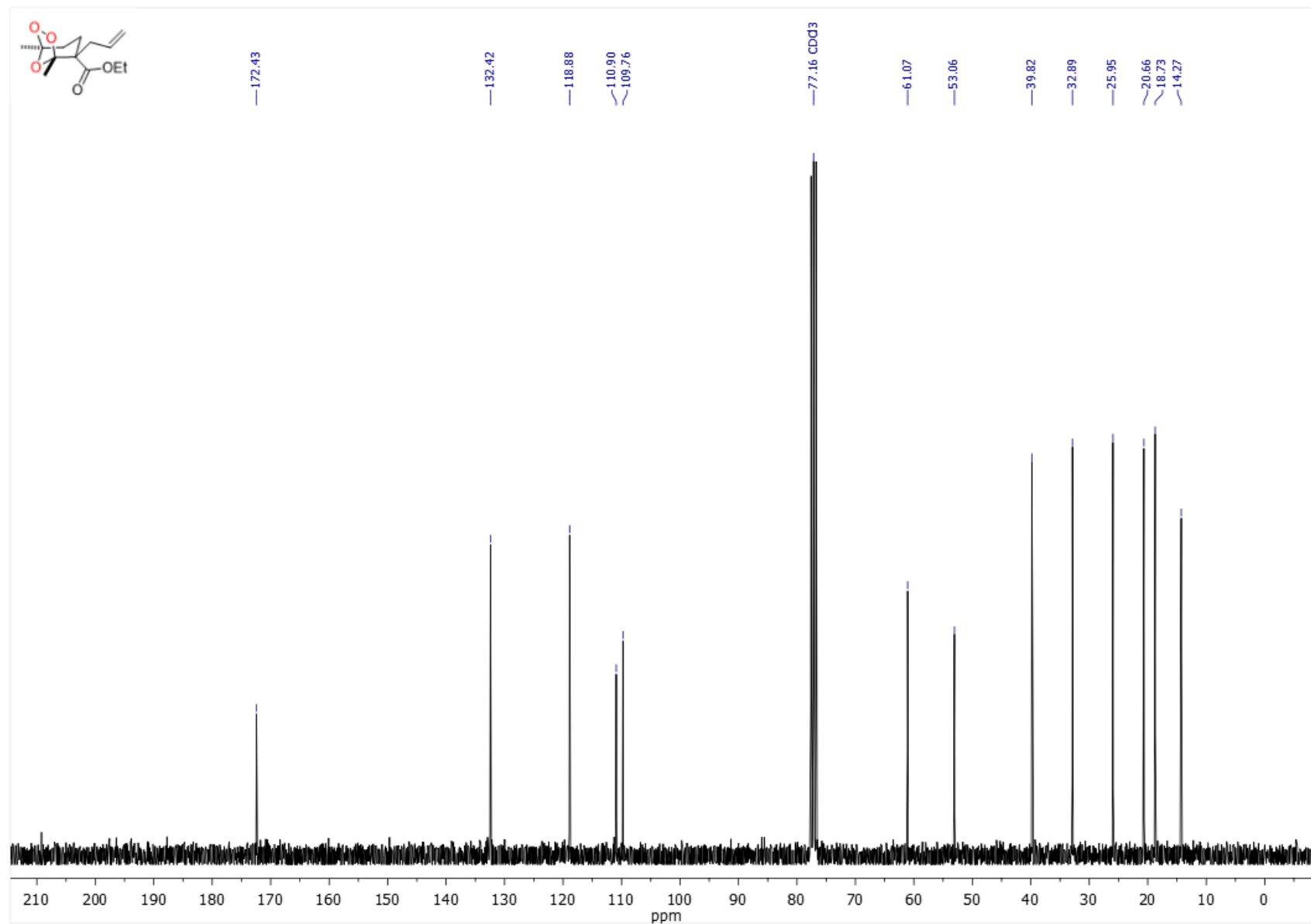
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-hexyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3i



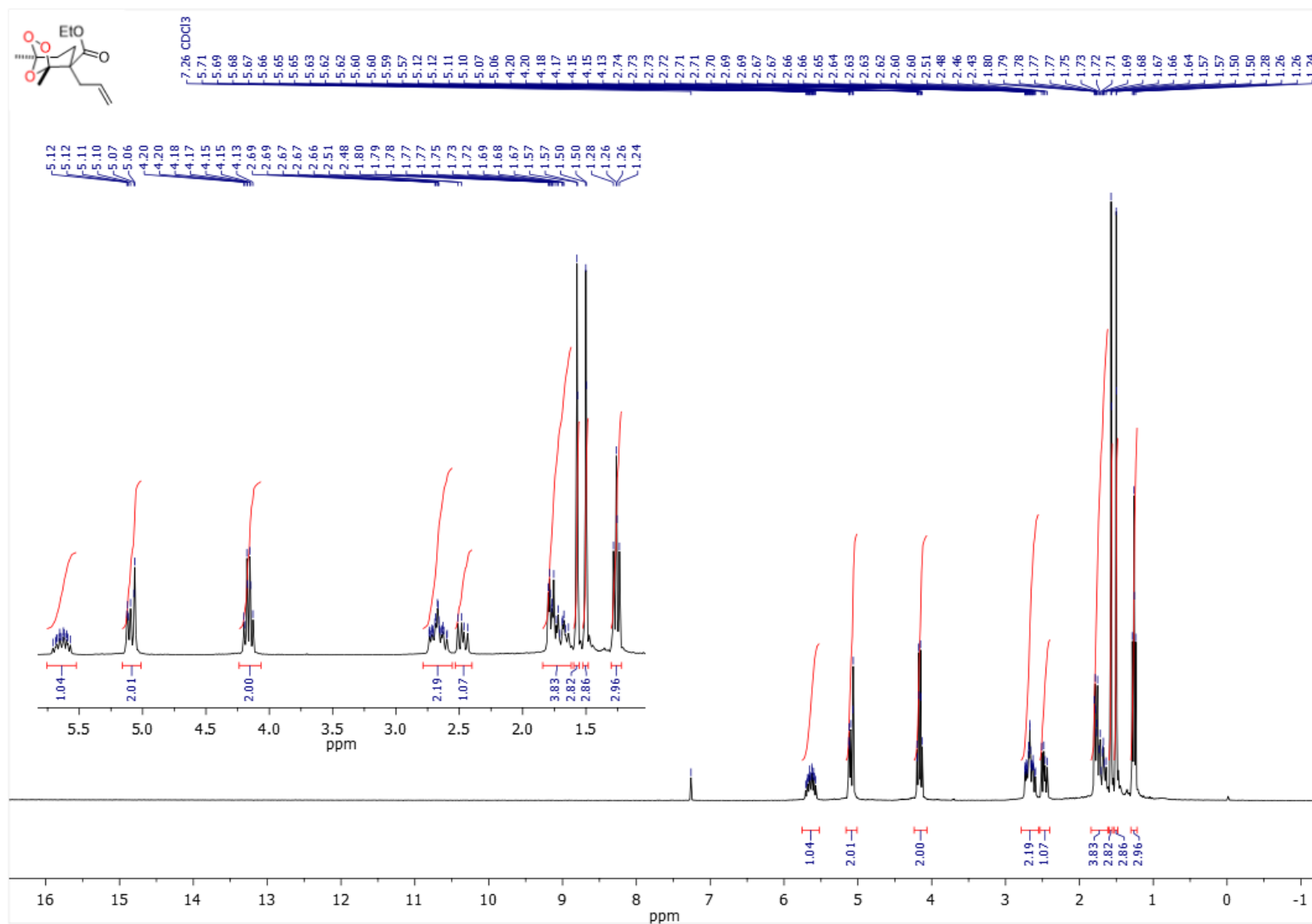
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-allyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2j



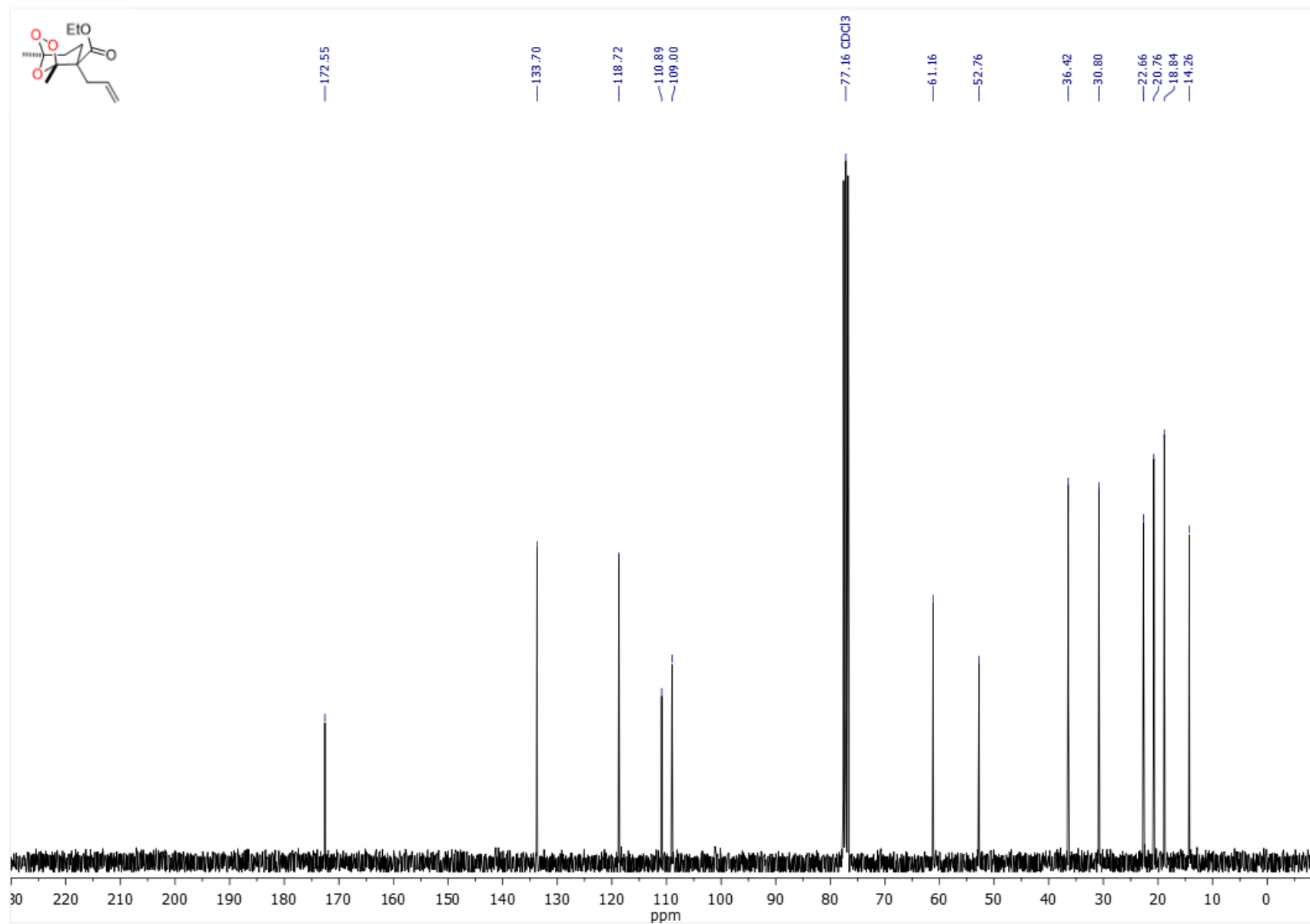
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-allyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2j



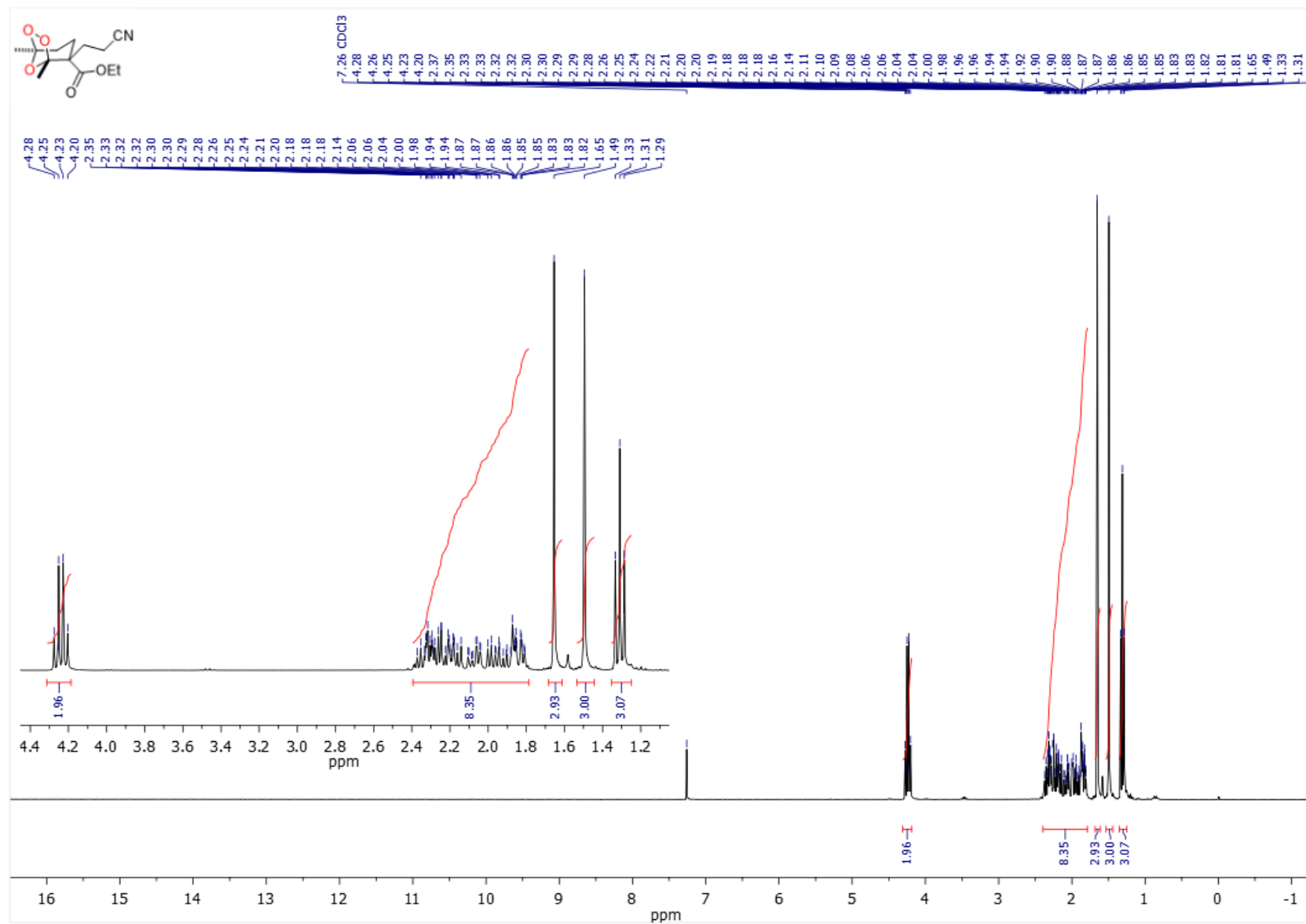
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-allyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3j



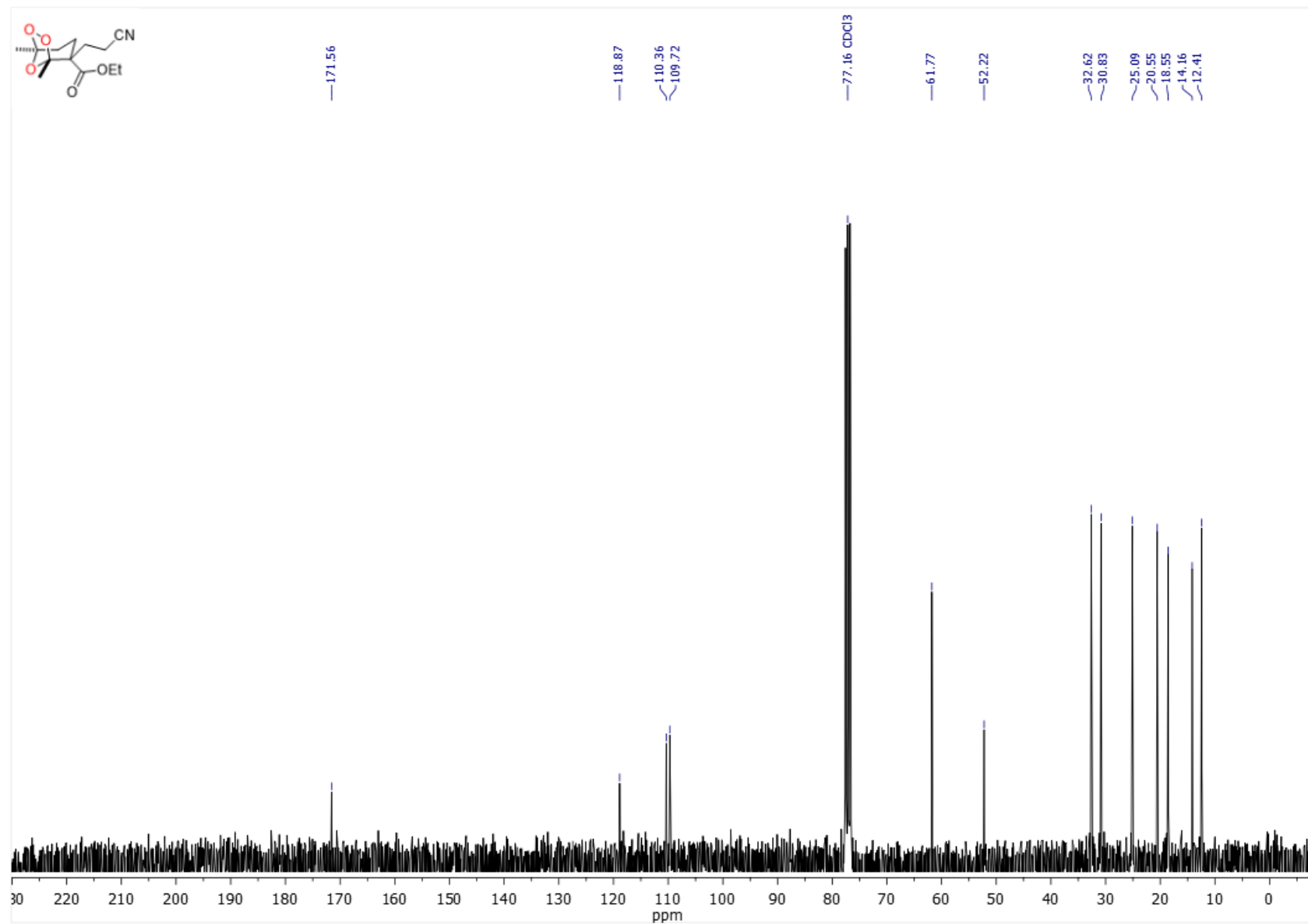
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*S**,5*S**)-2-allyl-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3j



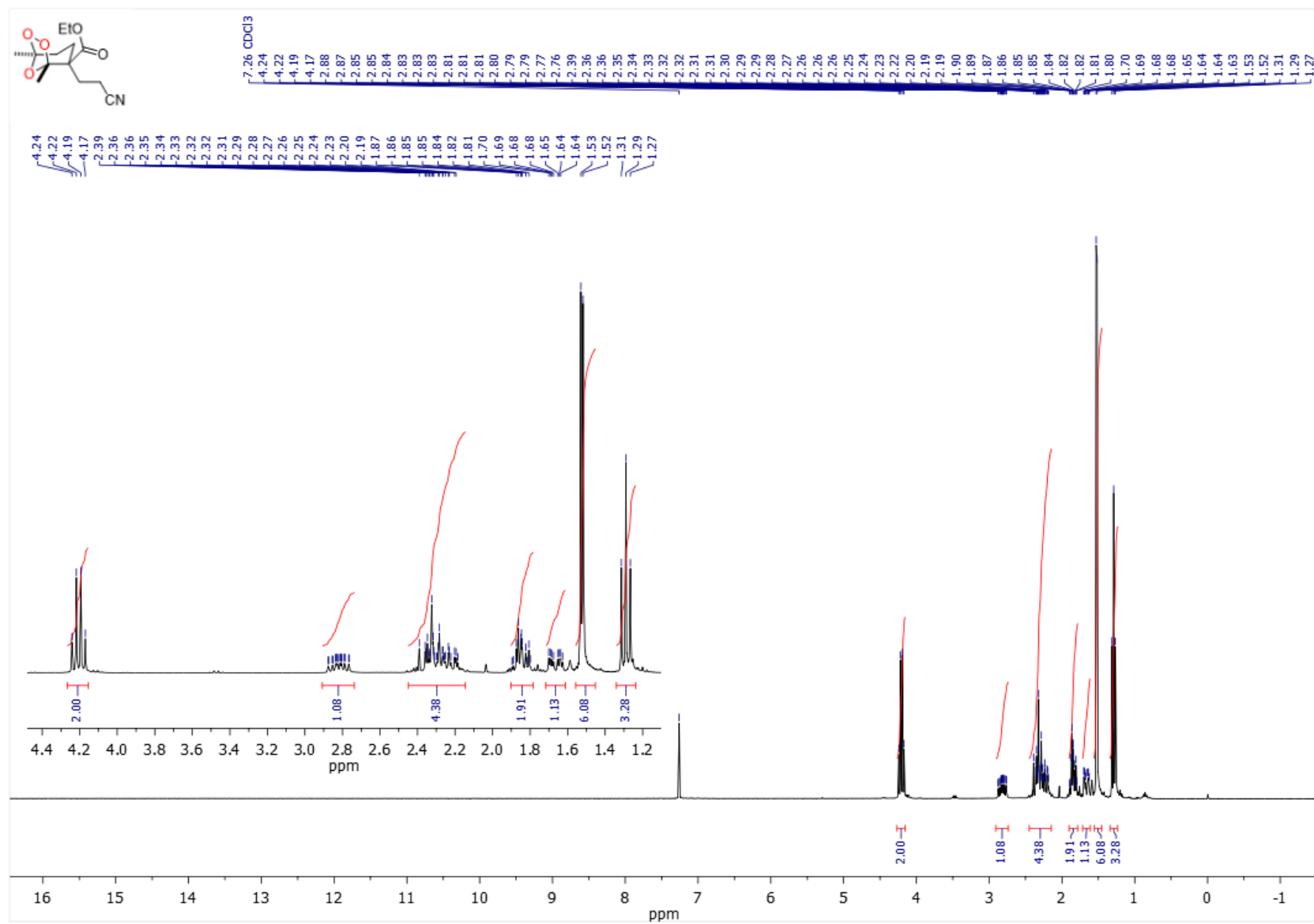
^1H NMR (300.13 MHz, CDCl_3). Ethyl(1*R**,2*S**,5*S**)-2-(2-cyanoethyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2k



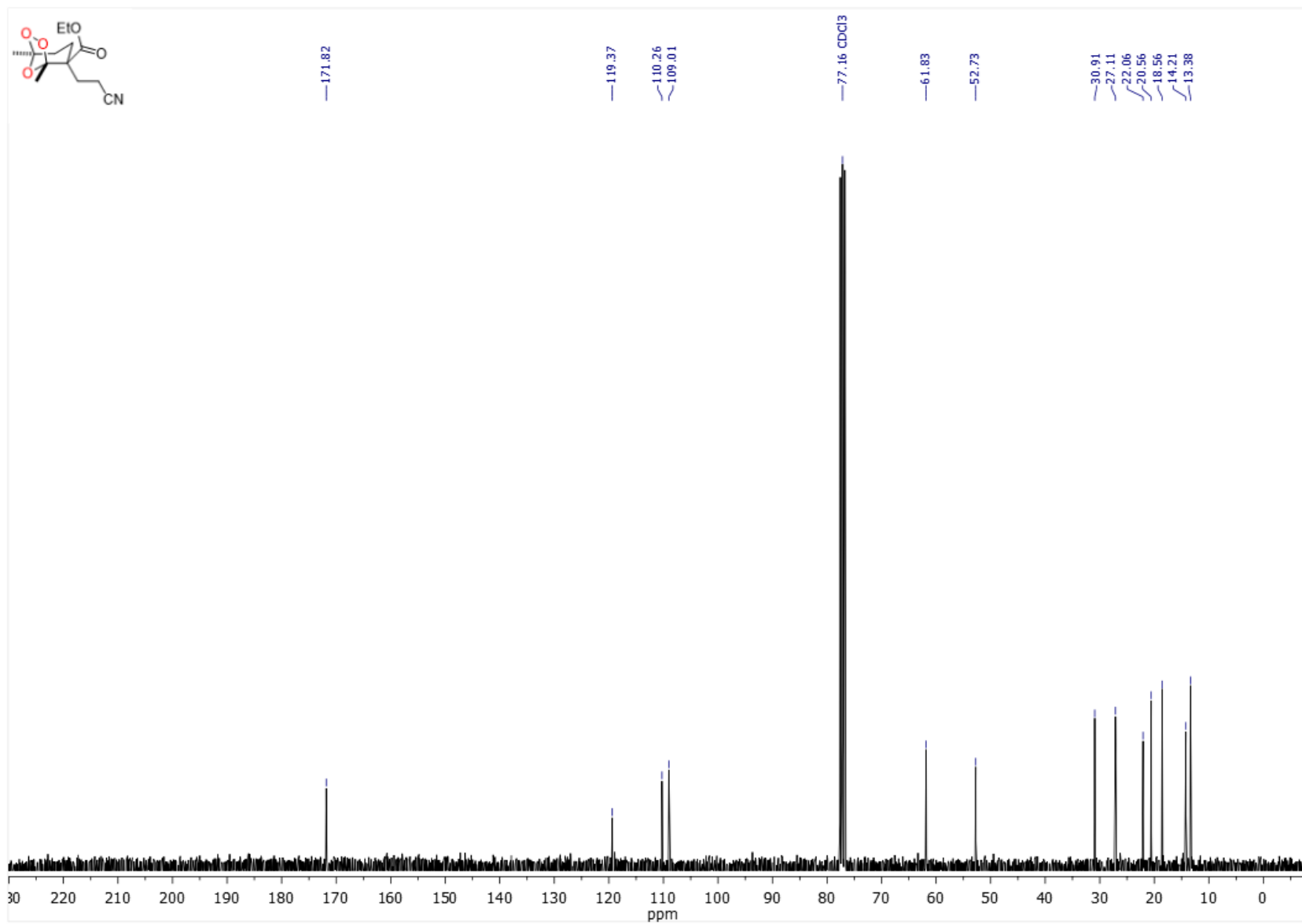
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl(1*R**,2*S**,5*S**)-2-(2-cyanoethyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 2k



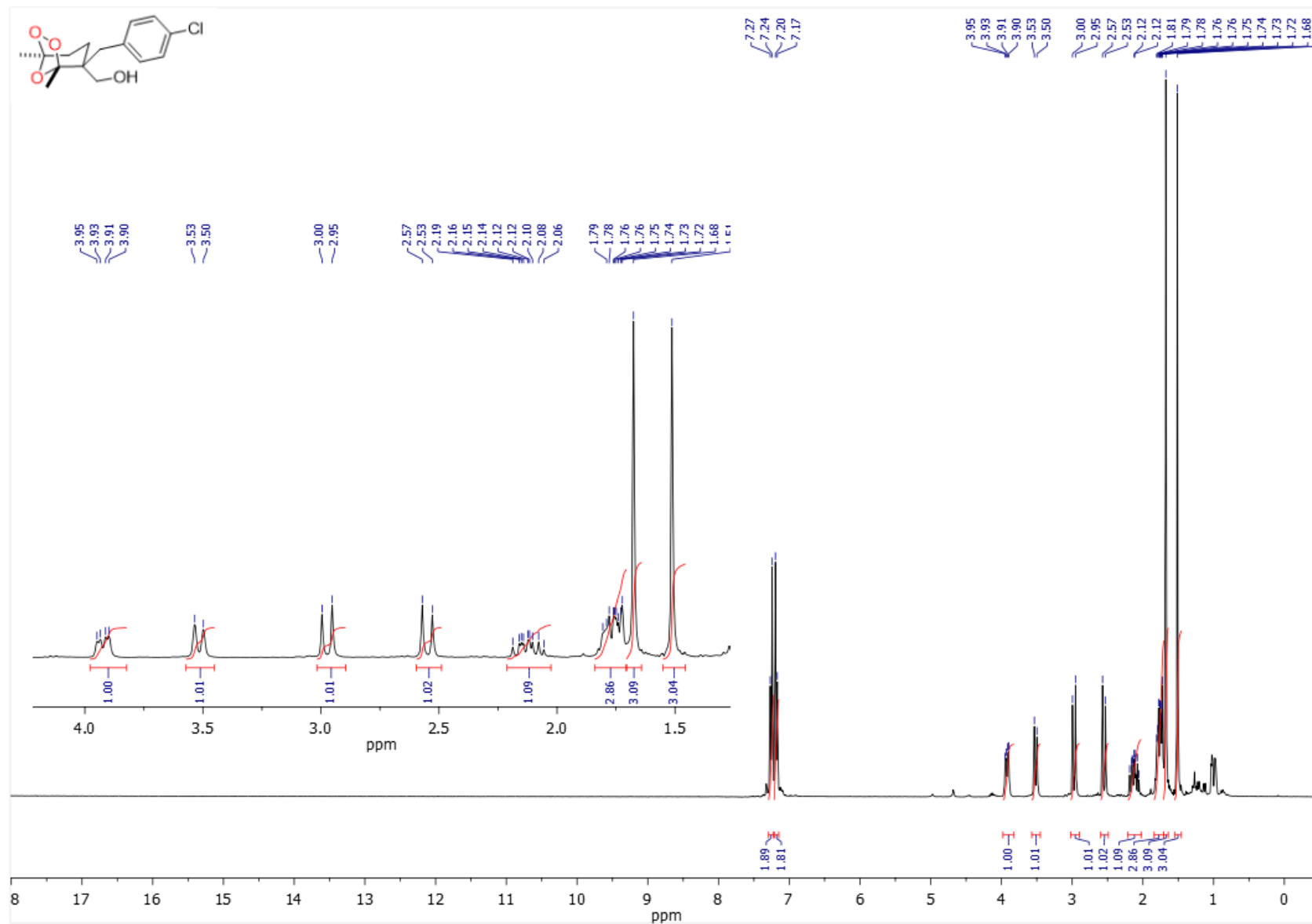
^1H NMR (300.13 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-(2-cyanoethyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3k



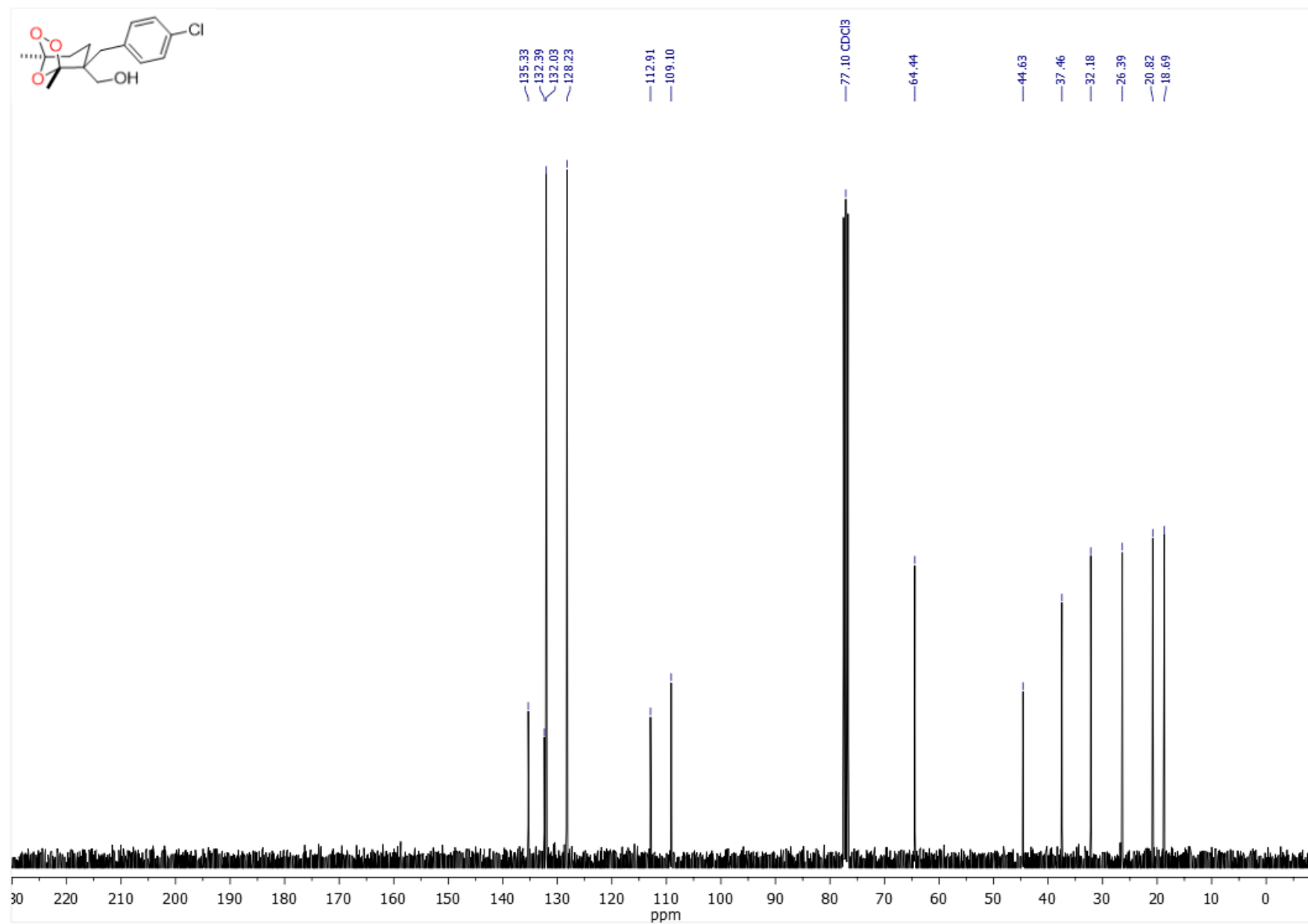
^{13}C NMR (75.48 MHz, CDCl_3). Ethyl (1*R**,2*R**,5*S**)-2-(2-cyanoethyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octane-2-carboxylate, 3k



^1H NMR (300.13 MHz, CDCl_3). (1*R**,2*S**,5*S**)-2-(4-chlorobenzyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octan-2-yl)methanol, 4

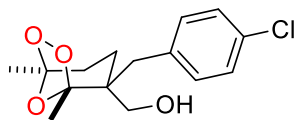


^{13}C NMR (75.48 MHz, CDCl_3). (1*R**,2*S**,5*S**)-2-(4-chlorobenzyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octan-2-ylmethanol, 4



HRMS spectra of peroxide 4

(1*R**,2*S**,5*S**)-2-(4-chlorobenzyl)-1,5-dimethyl-6,7,8-trioxabicyclo[3.2.1]octan-2-yl)methanol, 4



4

Display Report

Analysis Info

Analysis Name D:\Data\Chizhov\Terentiev\Radulov\rd1052_&clblow.d
Method tune_low.m
Sample Name /TERN Rd1052
Comment CH3CN 100 %, dil. 200, calibrant added

Acquisition Date 21.02.2020 16:25:21

Operator BDAL@DE
Instrument / Ser# microTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

