

Supporting Information

K₂CO₃-Mediated Tandem Annulation of 1,3-Acetonedicarboxylates with 2-Fluoro-1-nitroarenes: Synthesis of Indoles

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Compound 2c (¹H-NMR spectral data)

CHPr

Pulse Sequence: s2pu1

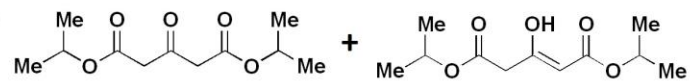
UNITYplus-400 "unity400"

Date: Aug 21 2023

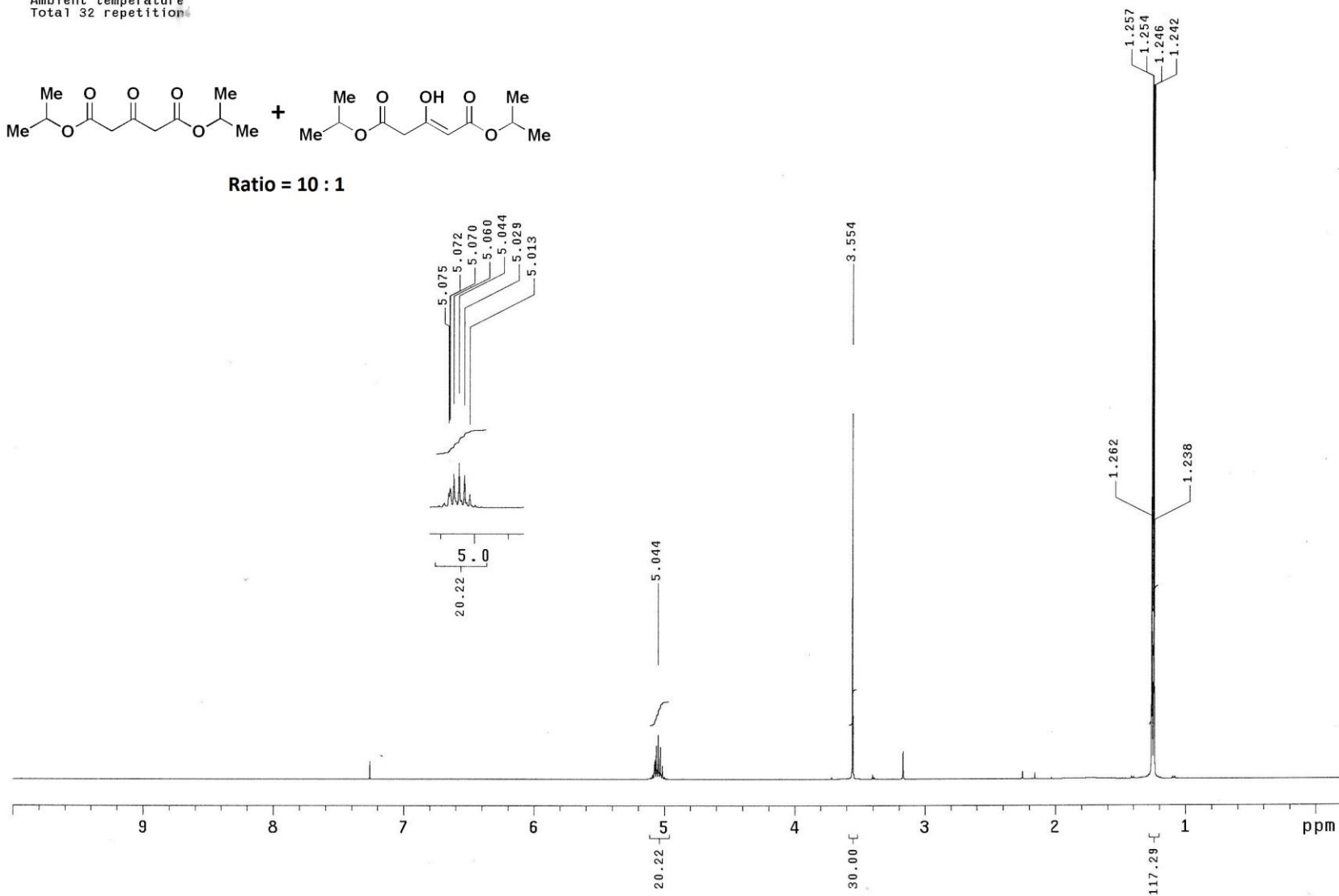
Solvent: CDCl₃

Ambient temperature

Total 32 repetition



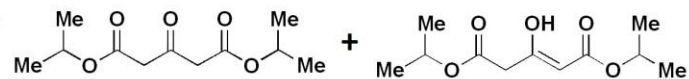
Ratio = 10 : 1



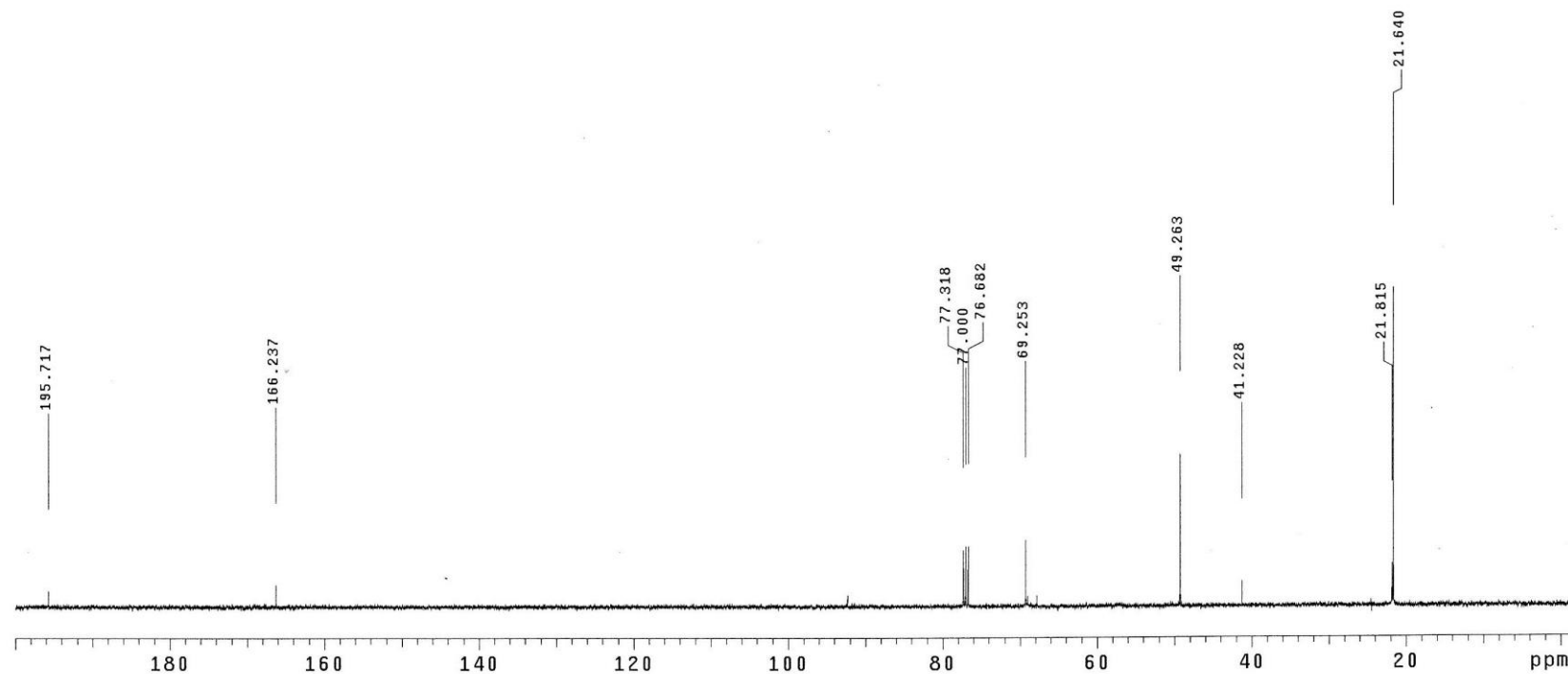
Compound 2c (¹³C-NMR spectral data)

CH1pr

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 21 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 816 repetitions



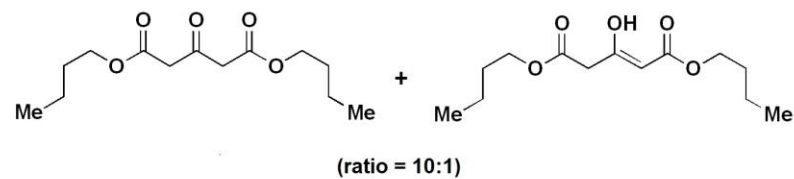
Ratio = 10 : 1



Compound 2d (¹H-NMR spectral data)

CH-nBu

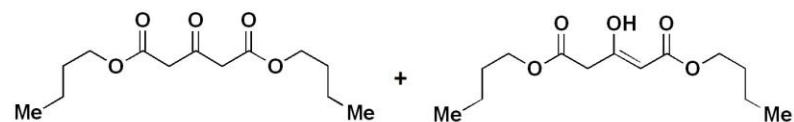
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 21 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



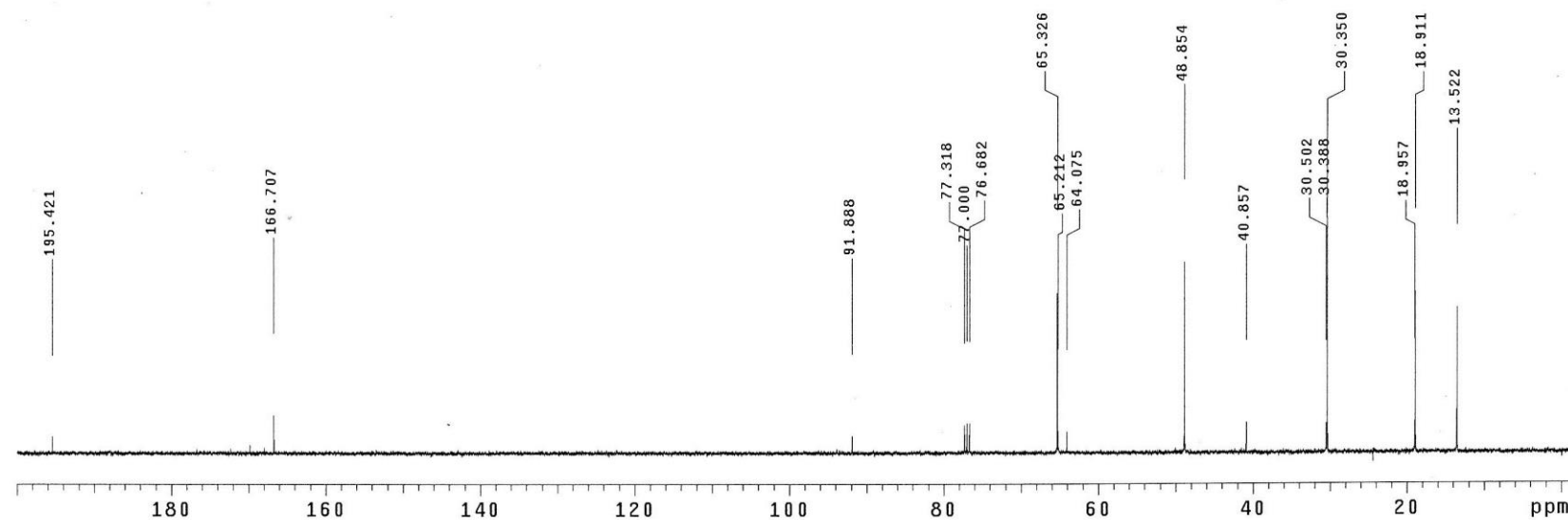
Compound 2d (¹³C-NMR spectral data)

CH-nBu

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 21 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 192 repetitions



(ratio = 10:1)



Compound 2e (¹H-NMR spectral data)

CHtBu

Pulse Sequence: s2pu1

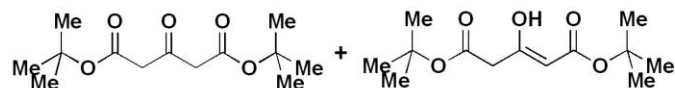
UNITYplus-400 "unity400"

Date: Aug 24 2023

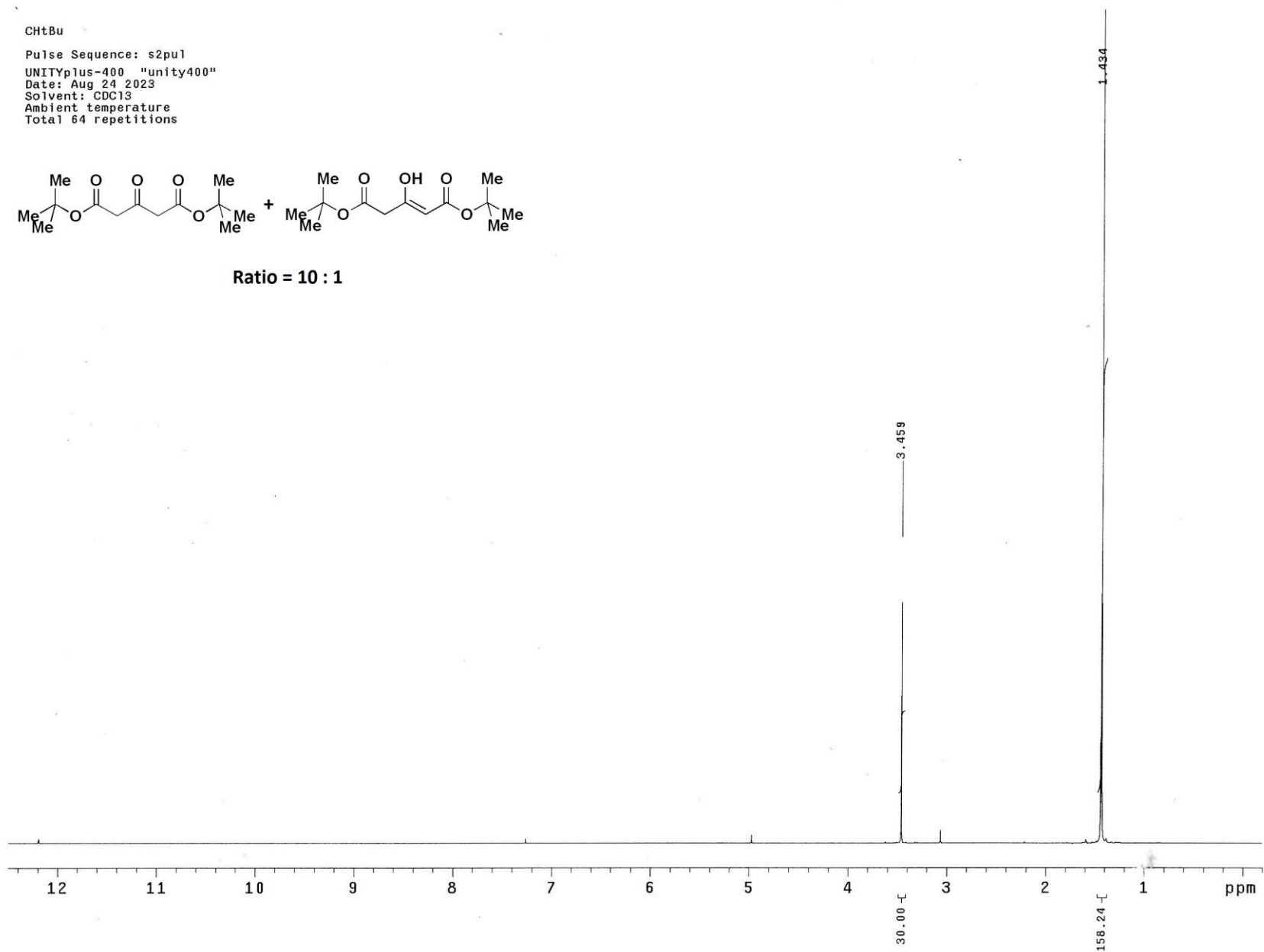
Solvent: CDCl₃

Ambient temperature

Total 64 repetitions



Ratio = 10 : 1



Compound 2e (¹³C-NMR spectral data)

CHtBu

Pulse Sequence: s2pu1

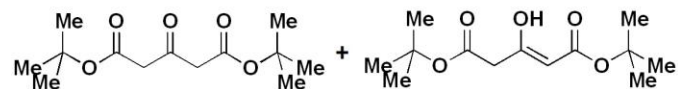
UNITYplus-400 "unity400"

Date: Aug 24 2023

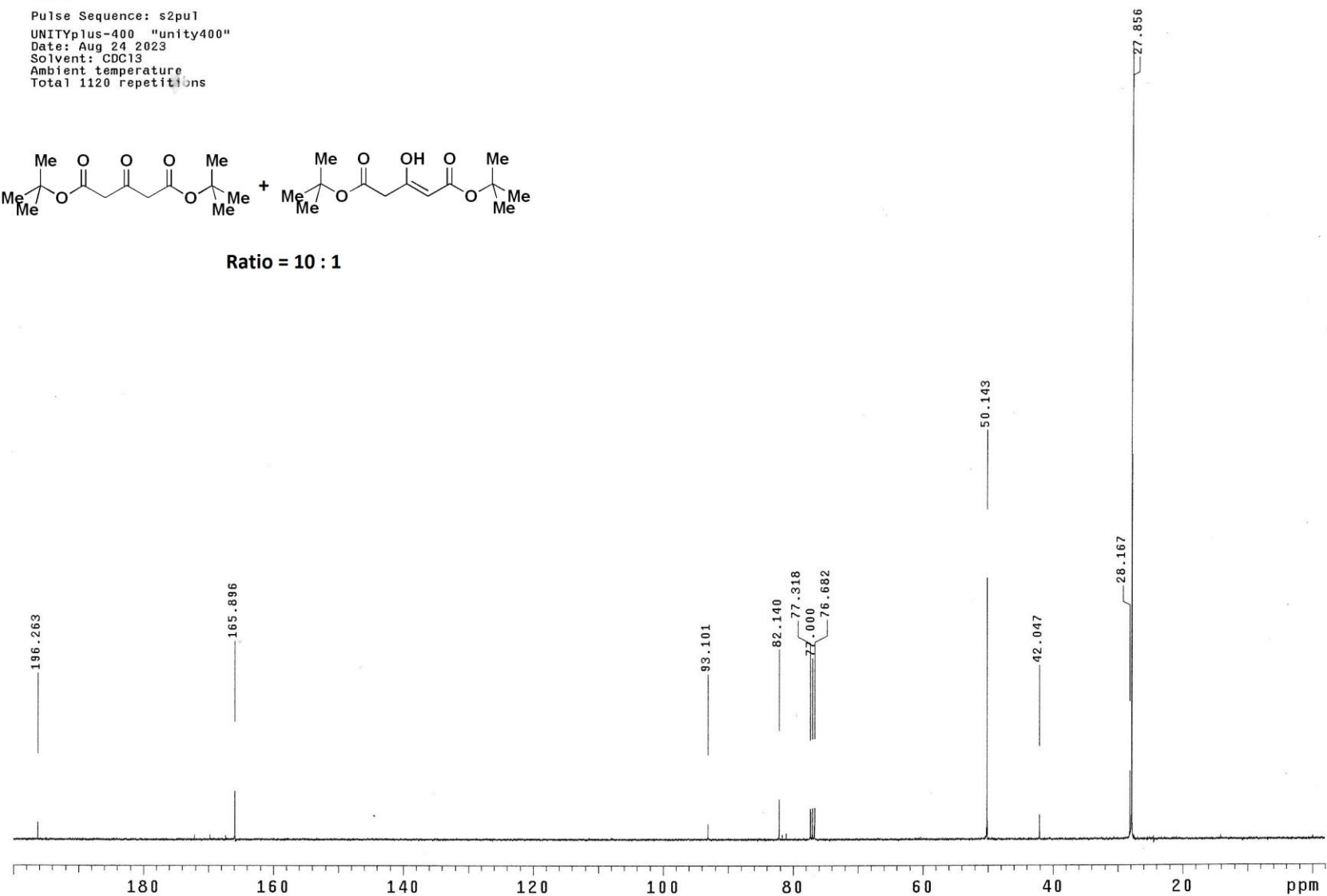
Solvent: CDCl₃

Ambient temperature

Total 1120 repetitions



Ratio = 10 : 1



Compound 3i (¹H-NMR spectral data)

A1P2Me0Ph

Pulse Sequence: s2pu1

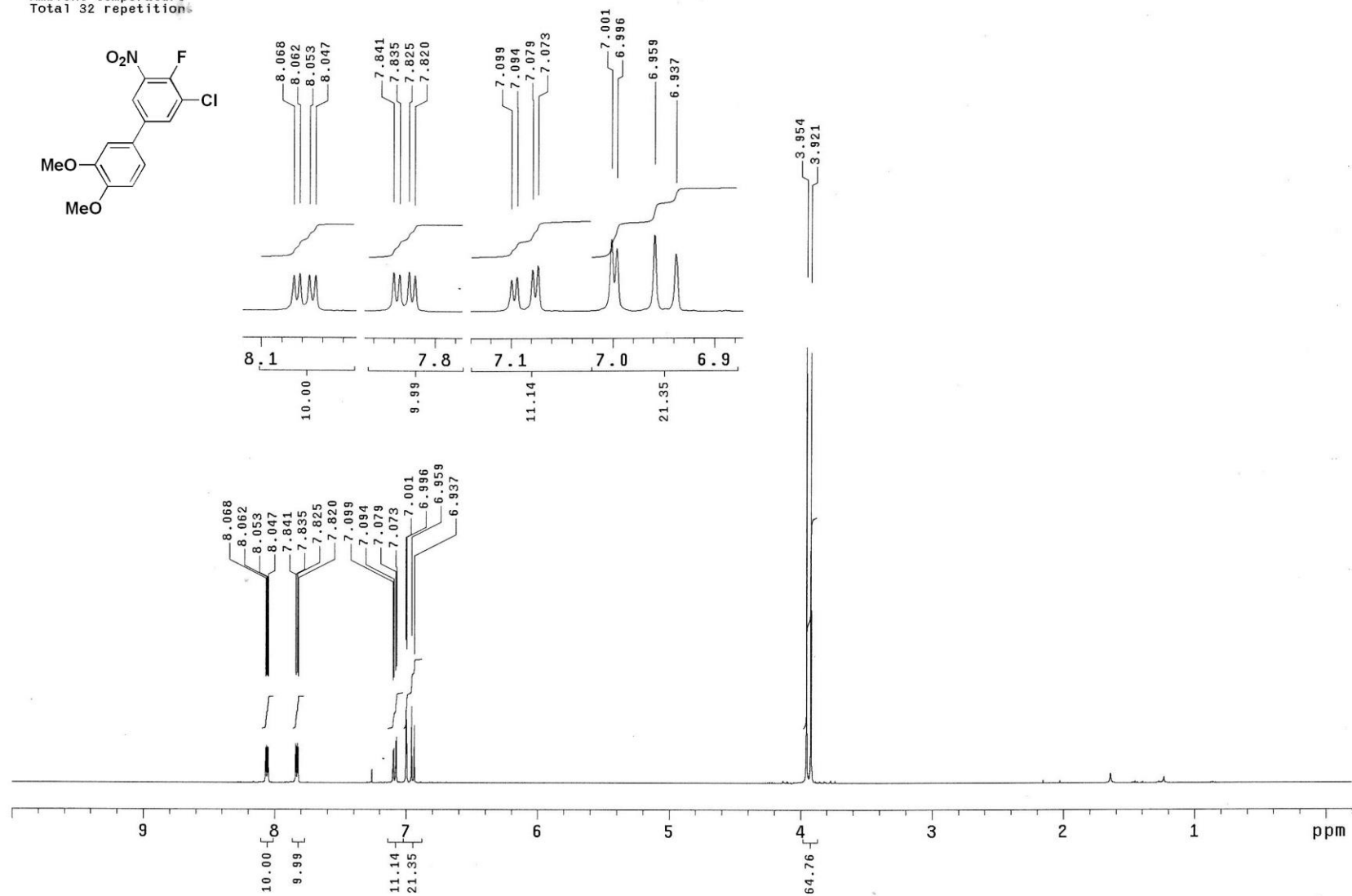
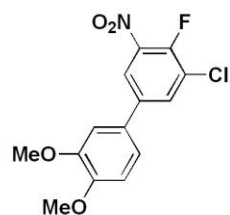
UNITYplus-400 "unity400"

Date: Jul 19 2023

Solvent: pyridine

Ambient temperature

Total 32 repetition



Compound 3i (¹³C-NMR spectral data)

A1P2Me0Ph

Pulse Sequence: s2pu1

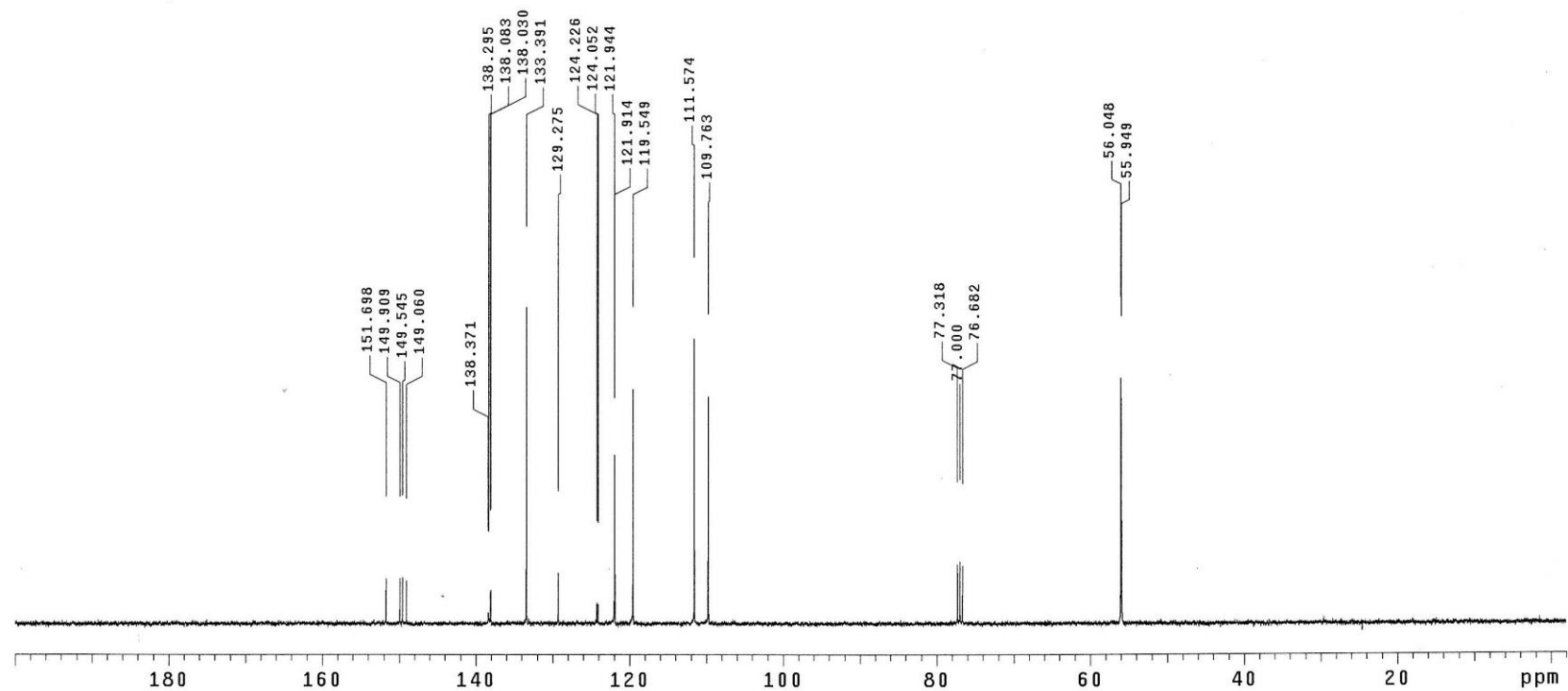
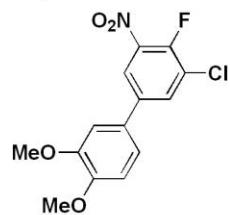
UNITYplus-400 "unity400"

Date: Jul 19 2023

Solvent: CDCl₃

Ambient temperature

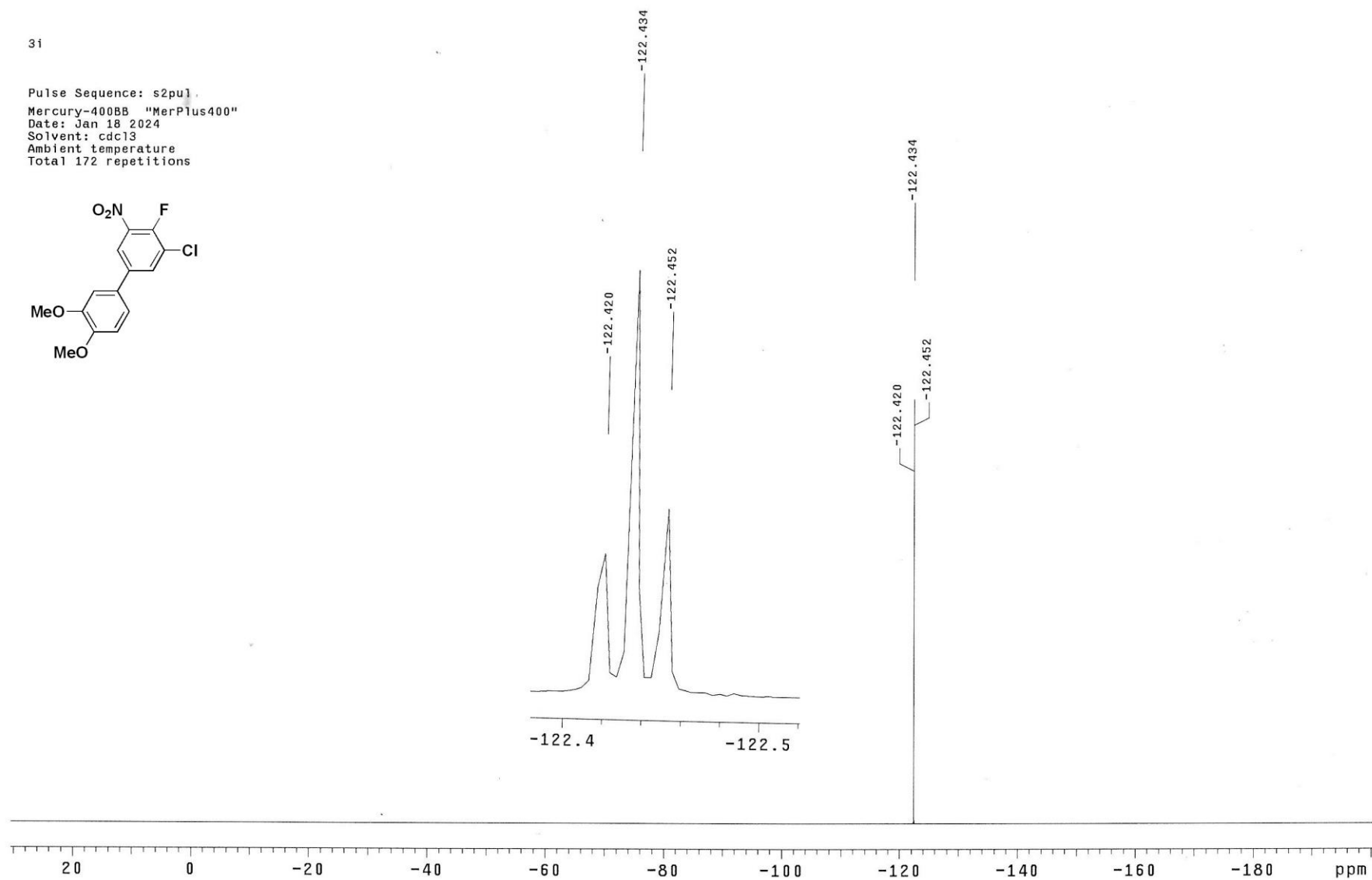
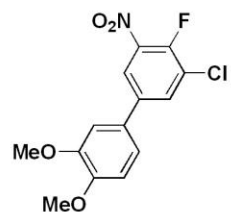
Total 1040 repetitions



Compound 3i (^{19}F -NMR spectral data)

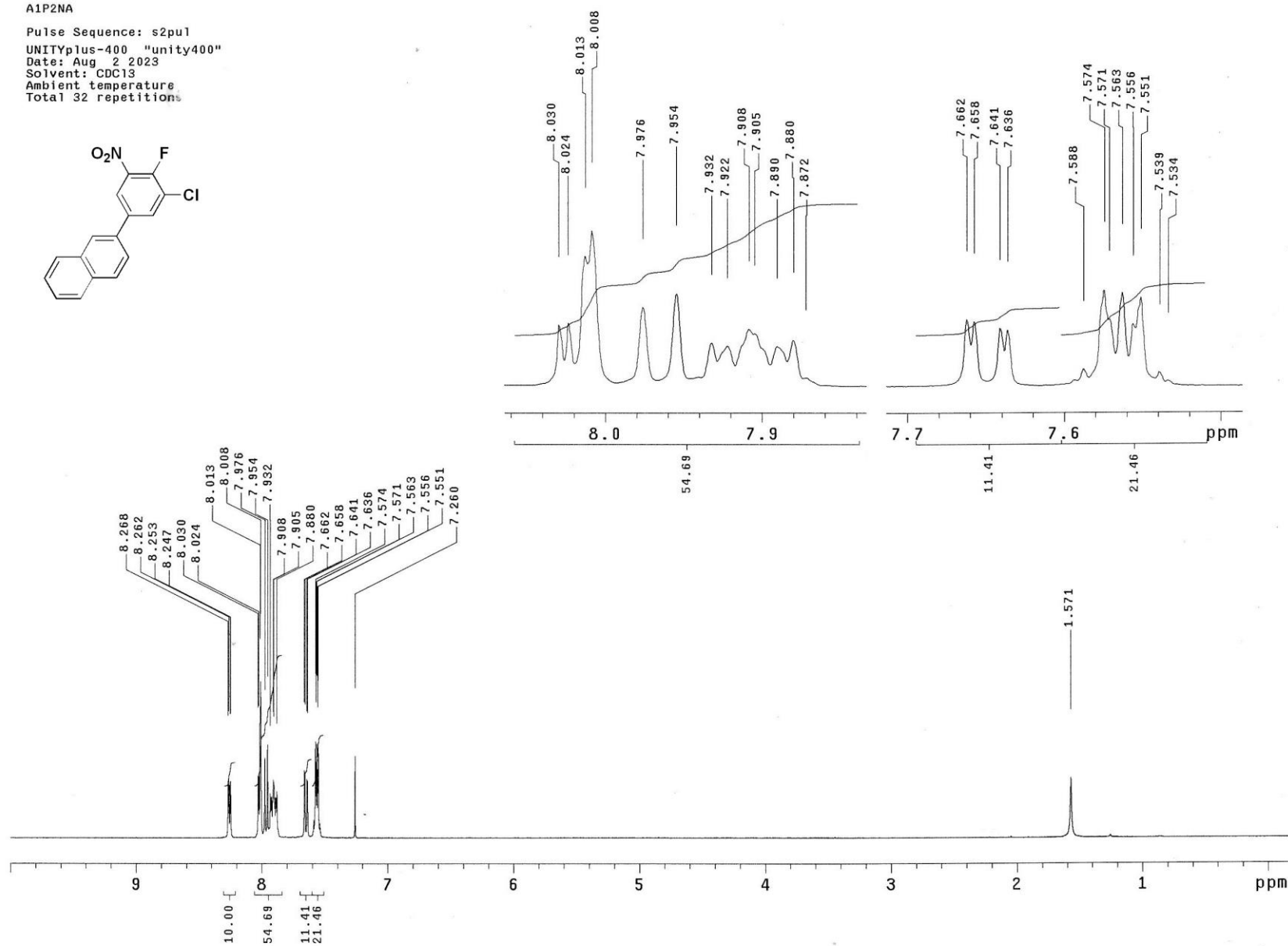
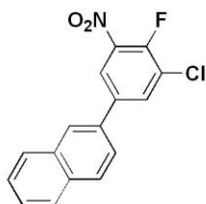
3i

Pulse Sequence: s2pu1
Mercury-400BB "MerPlus400"
Date: Jan 18 2024
Solvent: cdc13
Ambient temperature
Total 172 repetitions



A1P2NA

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Aug 2 2023
Solvent: CDC13
Ambient temperature
Total 32 repetitions



Compound 3k (¹³C-NMR spectral data)

A1P2NA

Pulse Sequence: s2pu1

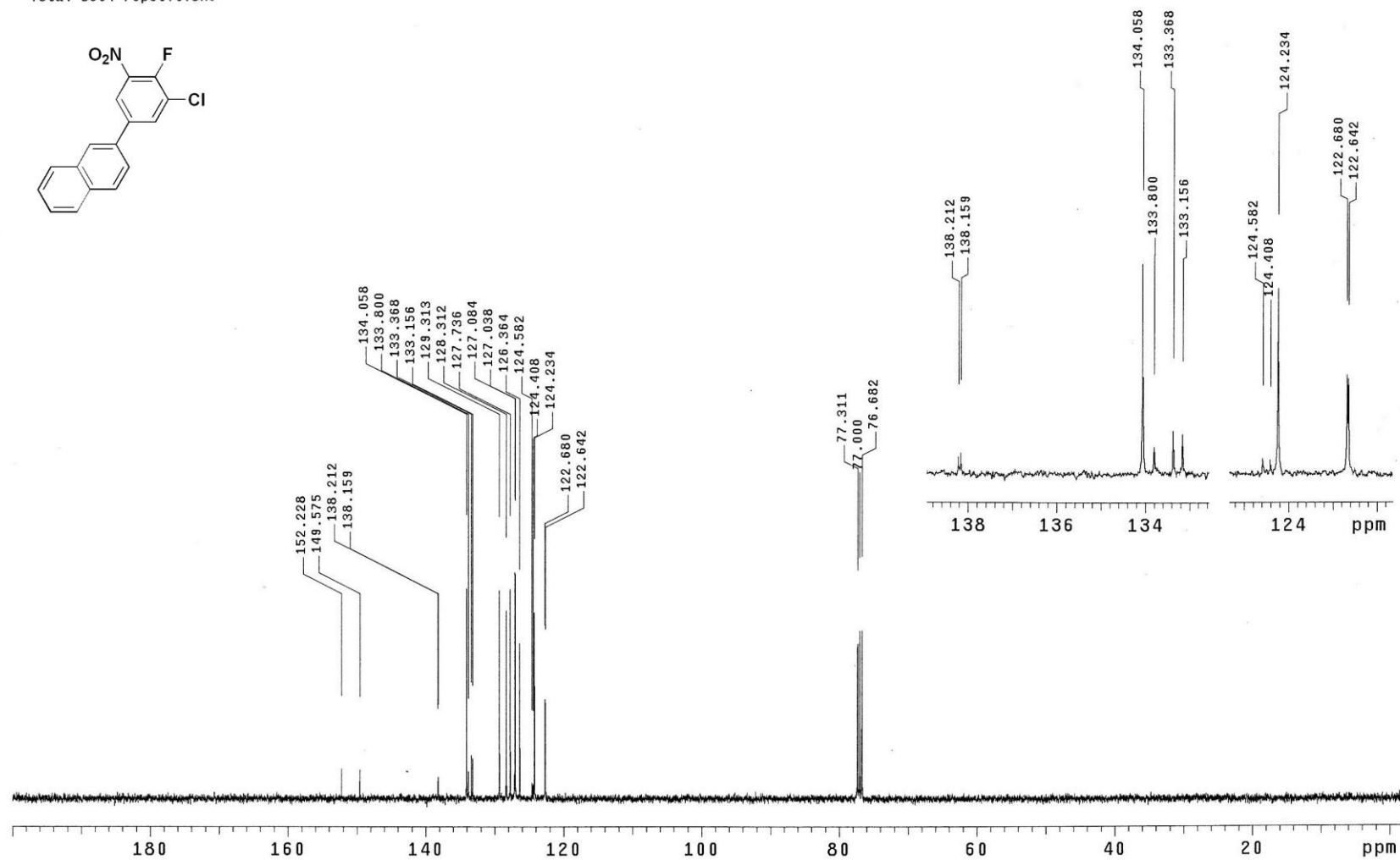
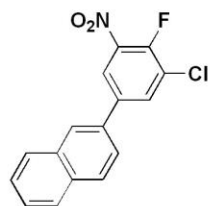
UNITYplus-400 "unity400"

Date: Aug 2 2023

Solvent: CDCl₃

Ambient temperature

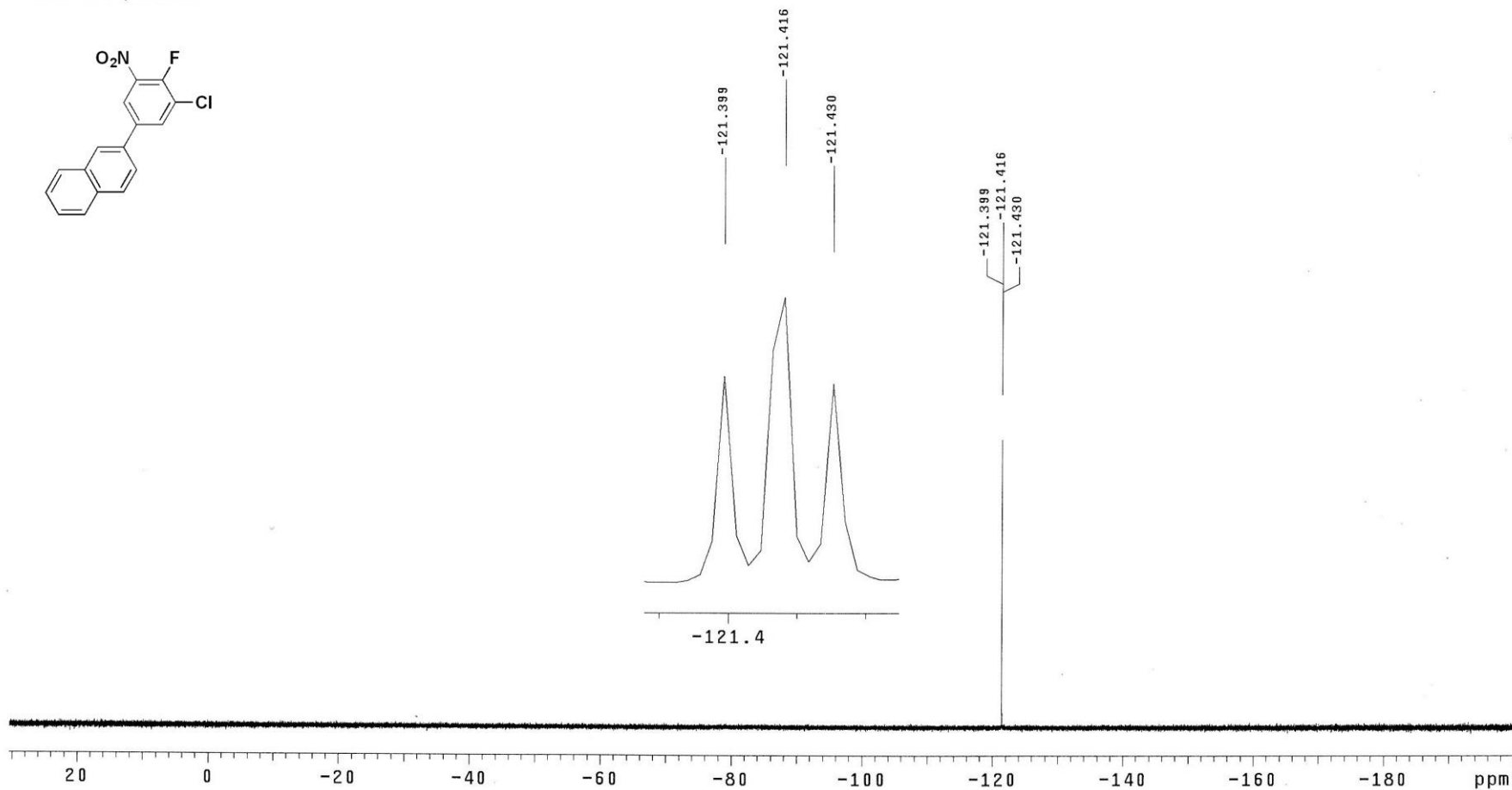
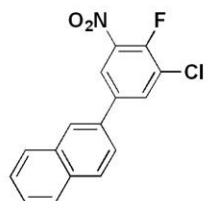
Total 3504 repetitions



Compound 3k (¹⁹F-NMR spectral data)

3k

Pulse Sequence: s2pul
Mercury-400BB "MerPlus400"
Date: Jan 18 2024
Solvent: cdcl3
Ambient temperature
Total 96 repetitions



Compound 4a (¹H-NMR spectral data)

CHNF0331

Pulse Sequence: s2pu1

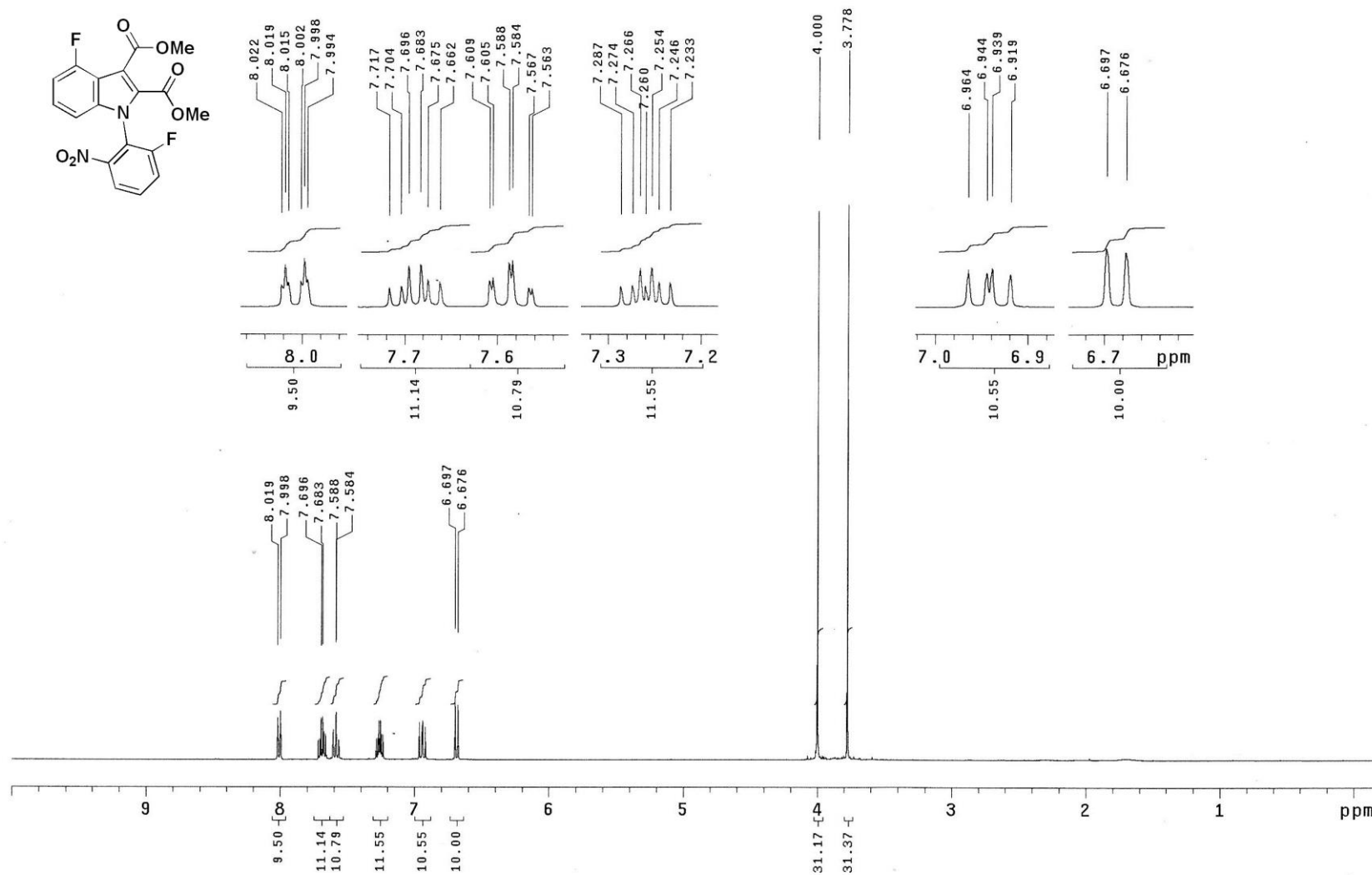
UNITYplus-400 "unity400"

Date: Apr 6 2023

Solvent: CDCl₃

Ambient temperature

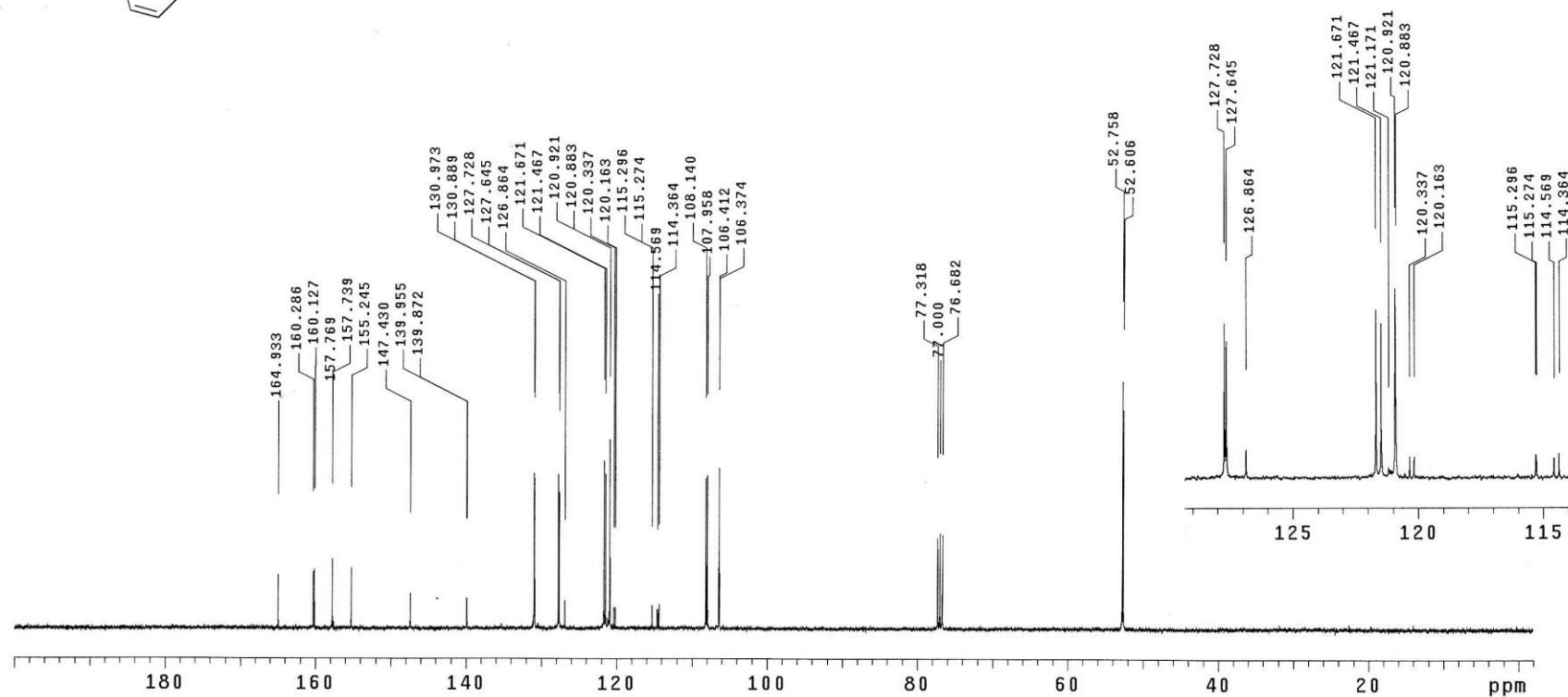
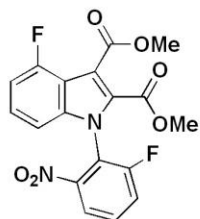
Total 32 repetitions



Compound 4a (¹³C-NMR spectral data)

CHNF0331

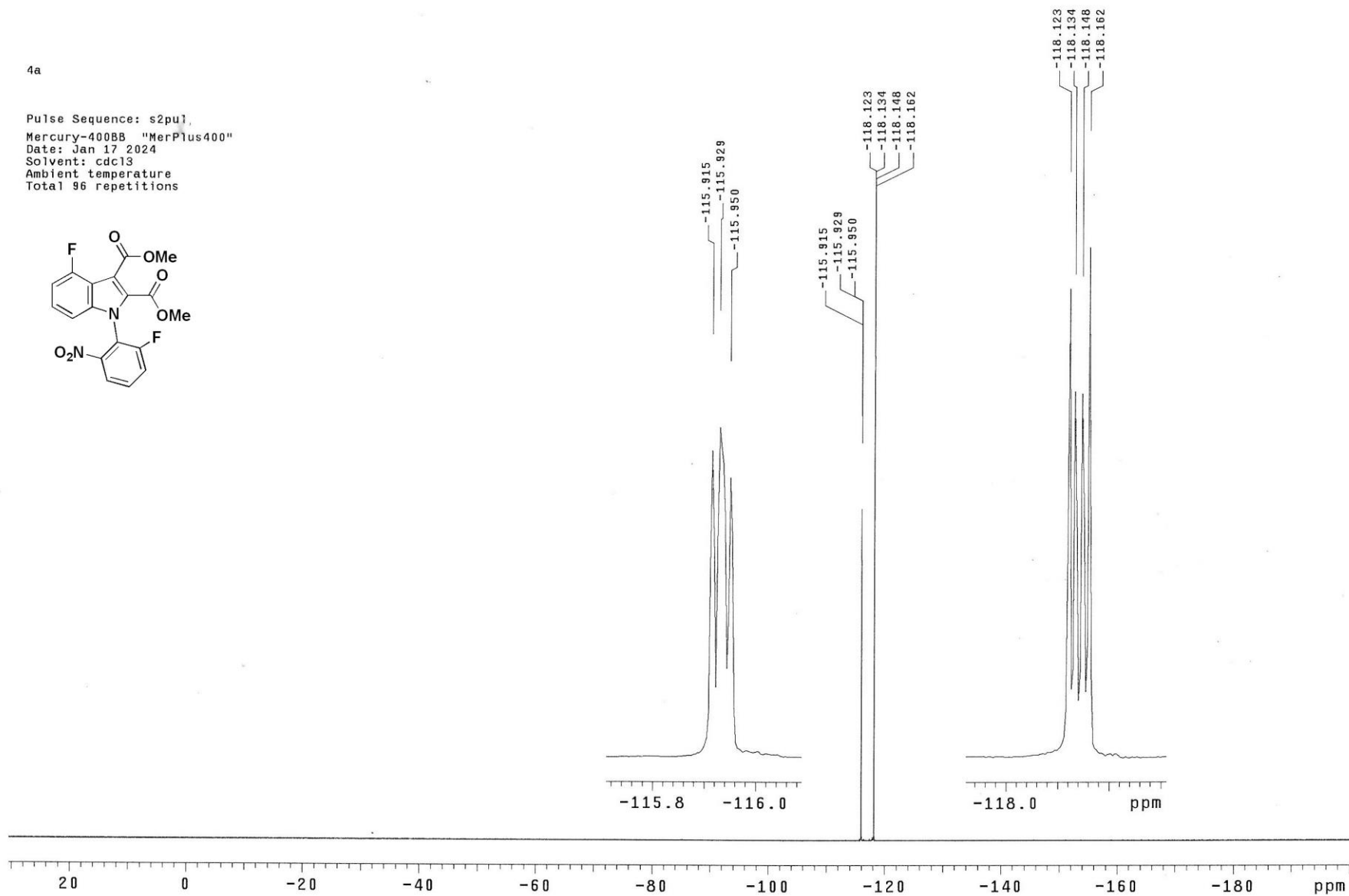
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Apr 6 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 2560 repetitions



Compound 4a (¹⁹F-NMR spectral data)

4a

Pulse Sequence: s2pu1,
Mercury-400BB "MerPlus400"
Date: Jan 17 2024
Solvent: cdcl3
Ambient temperature
Total 96 repetitions



Compound 4b (¹H-NMR spectral data)

CHNF1215

Pulse Sequence: s2pu1

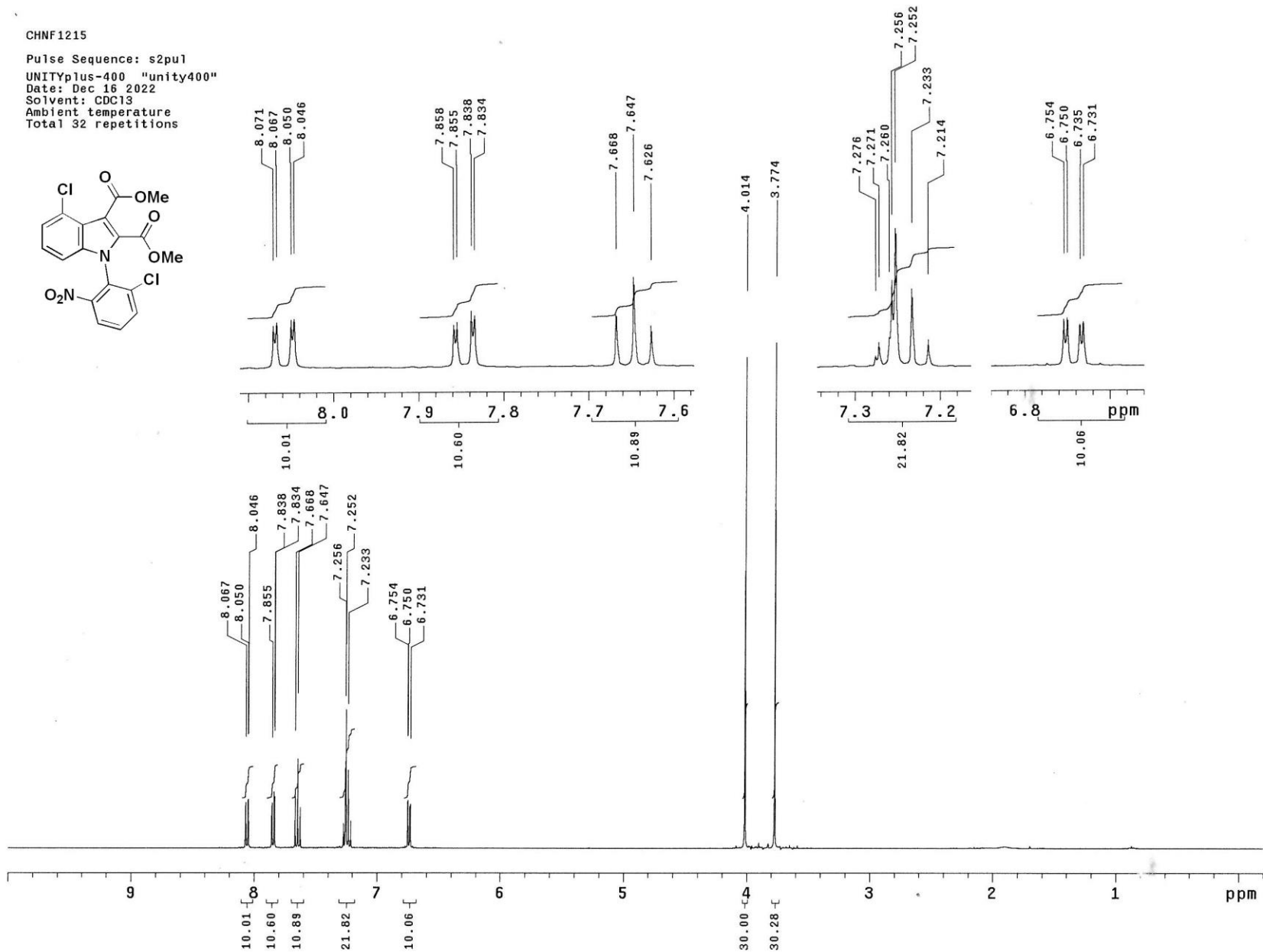
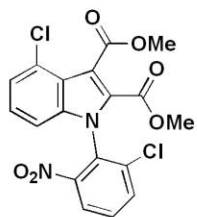
UNITYplus-400 "unity400"

Date: Dec 16 2022

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 4b (¹³C-NMR spectral data)

CHNF1215

Pulse Sequence: s2pu1

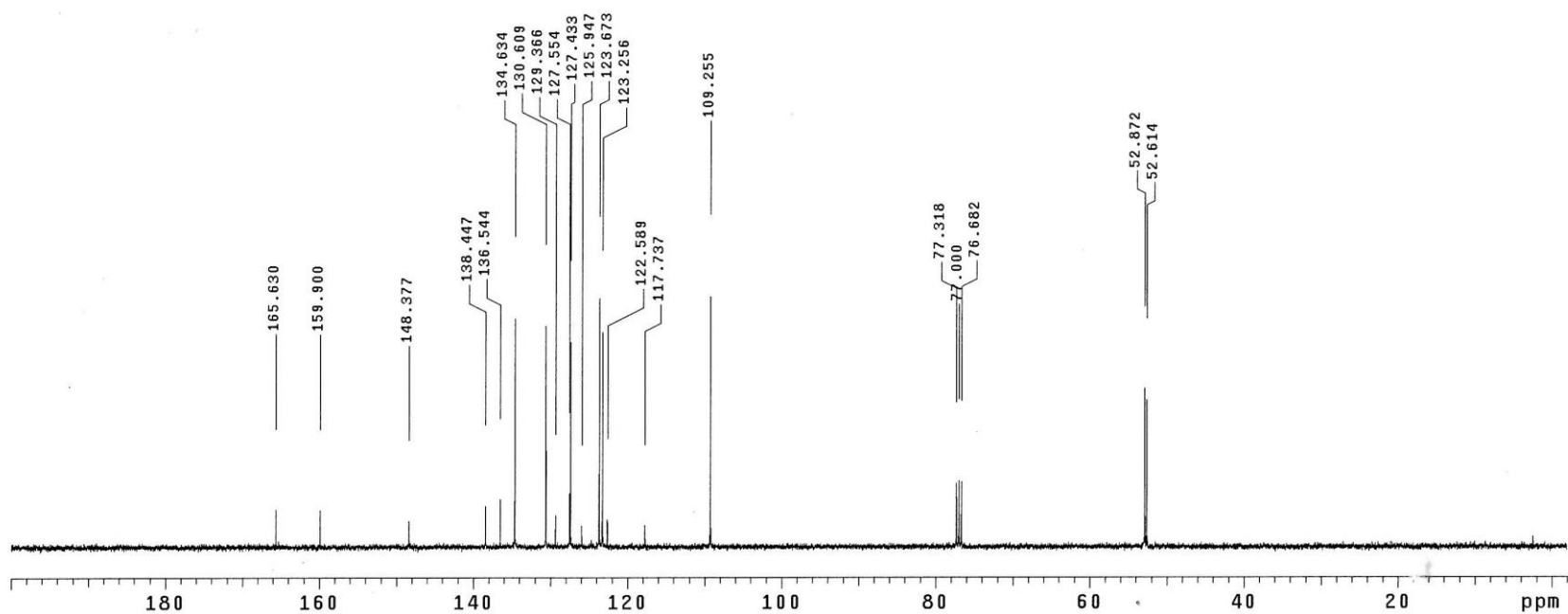
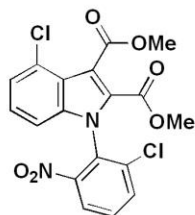
UNITYplus-400 "unity400"

Date: Dec 16 2022

Solvent: CDCl₃

Ambient temperature

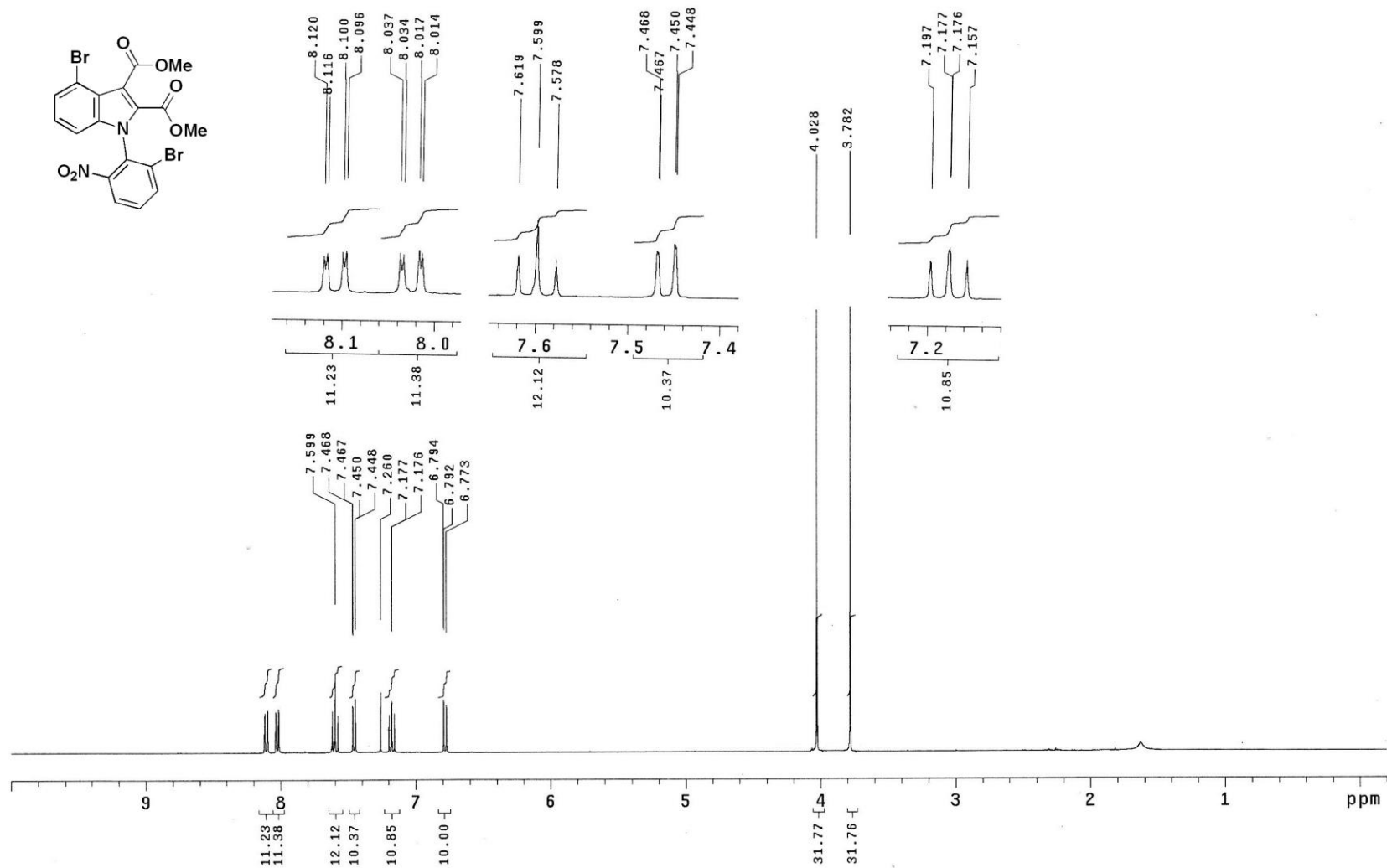
Total 640 repetitions



Compound 4c (¹H-NMR spectral data)

CHNF0222

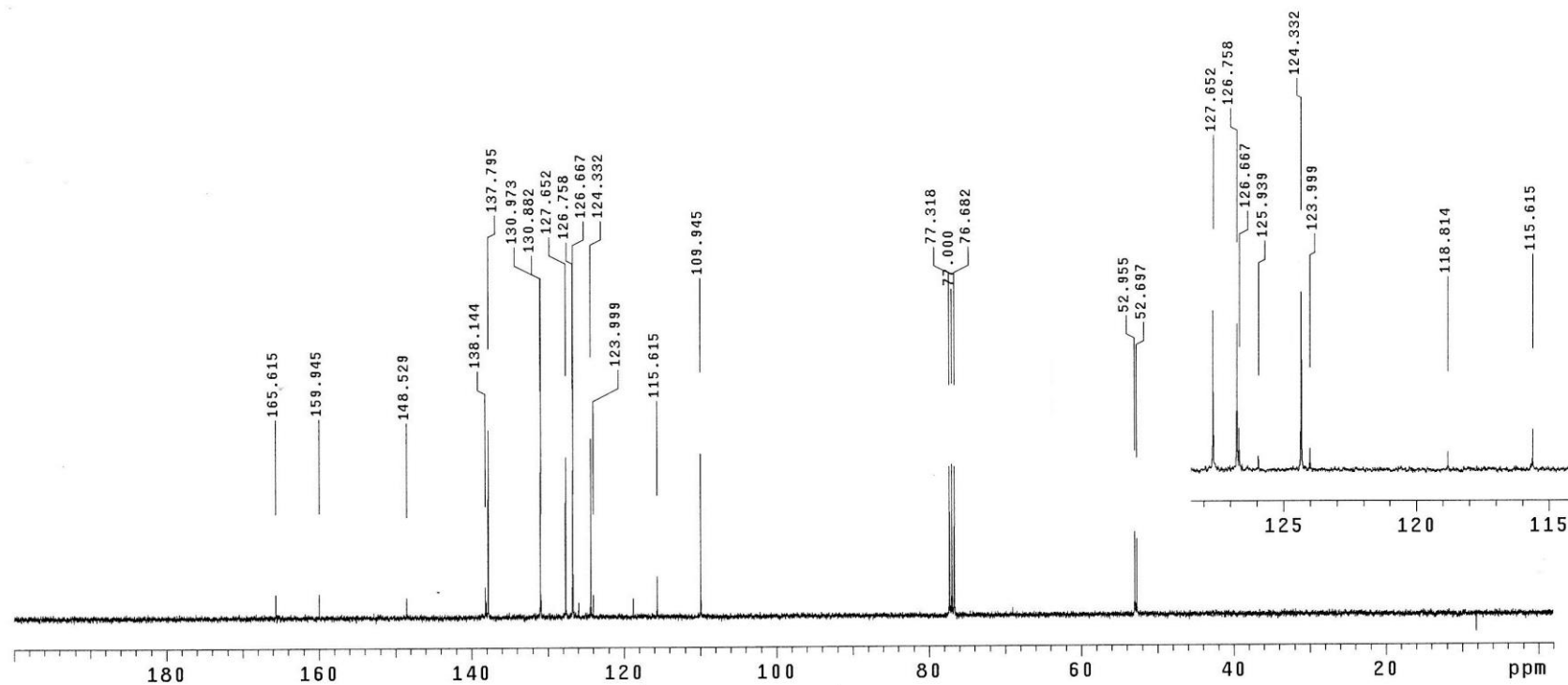
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Feb 22 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetition



Compound 4c (¹³C-NMR spectral data)

CHNF0222

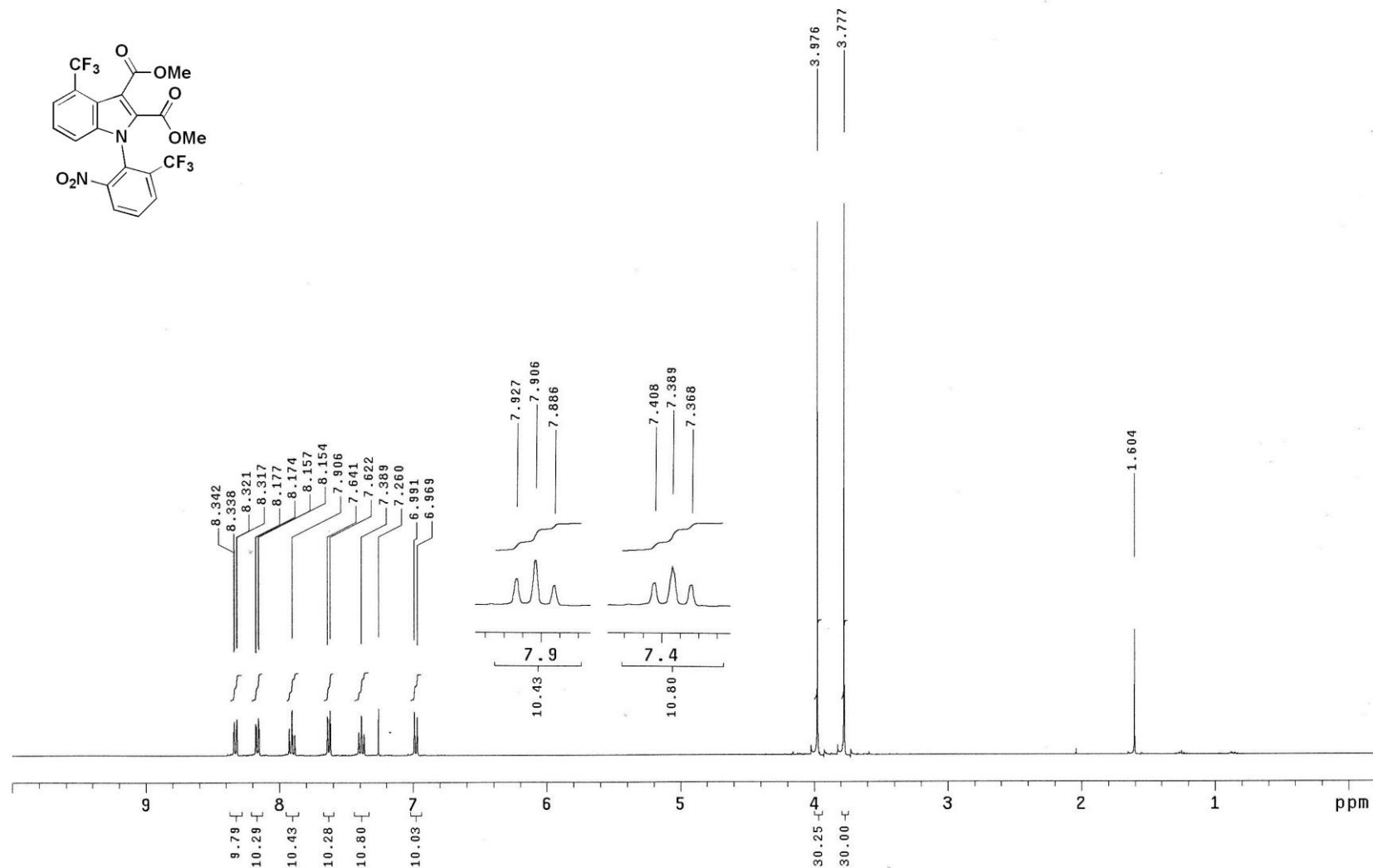
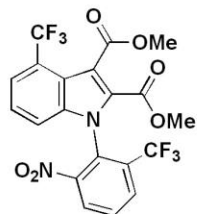
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Feb 22 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 3280 repetitions



Compound 4d (¹H-NMR spectral data)

CHNF0411

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Apr 11 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4d (¹³C-NMR spectral data)

CHNF0411

Pulse Sequence: s2pu1

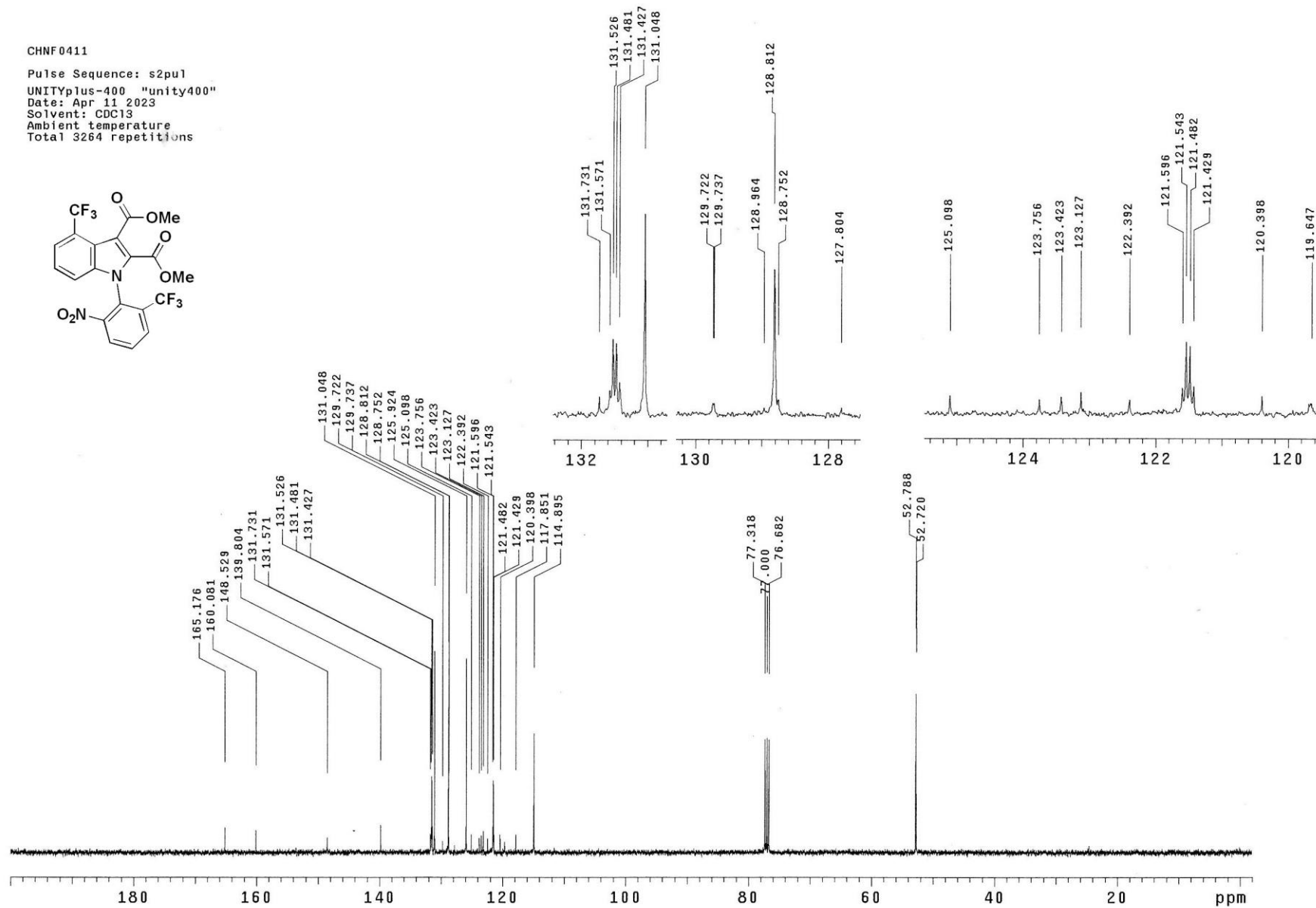
UNITYplus-400 "unity400"

Date: Apr 11 2023

Solvent: CDCl₃

Ambient temperature

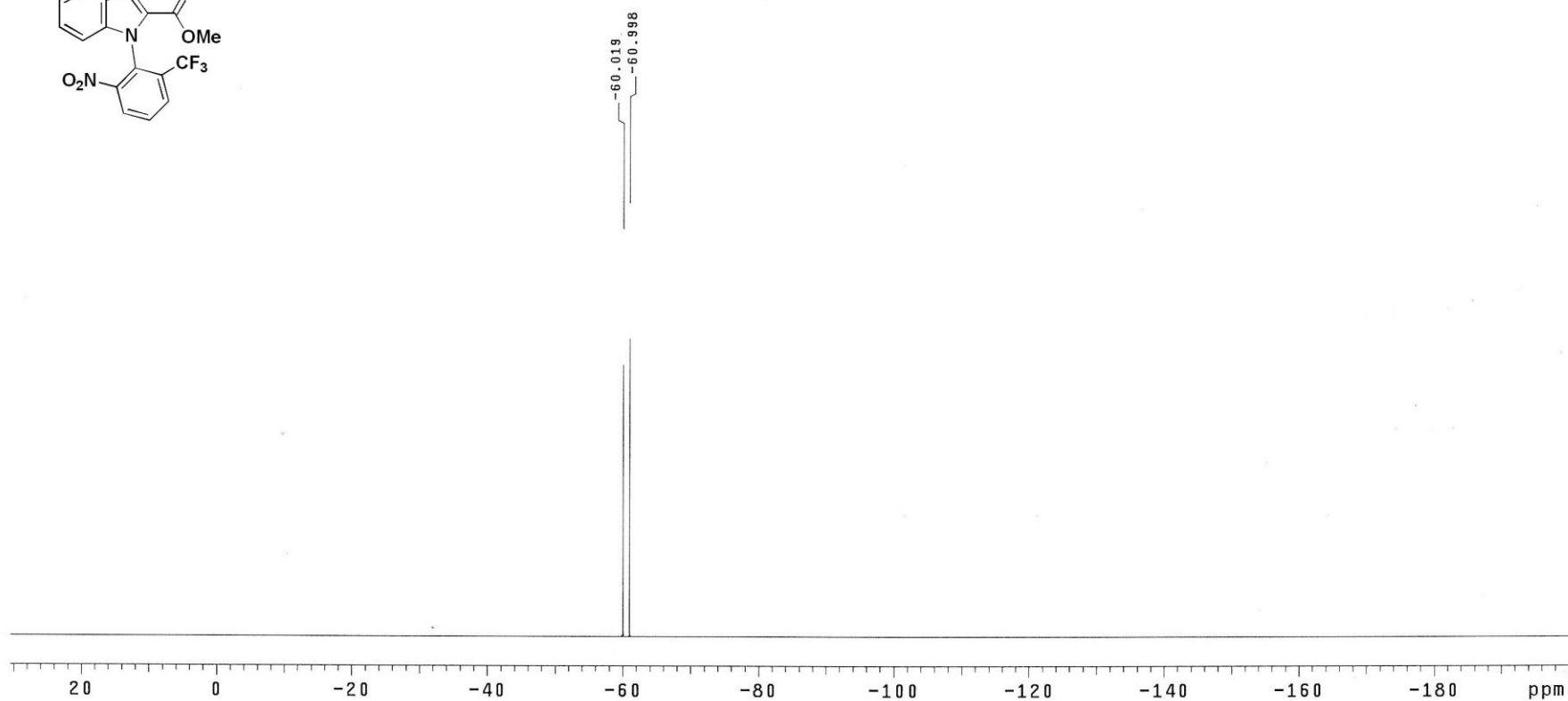
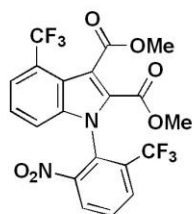
Total 3264 repetitions



Compound 4d (¹⁹F-NMR spectral data)

4d

Pulse Sequence: s2pu1
Mercury-400BB "MerPlus400"
Date: Jan 18 2024
Solvent: cdcl3
Ambient temperature
Total 64 repetitions



Compound 4e (¹H-NMR spectral data)

CHNF0406

Pulse Sequence: s2pu1

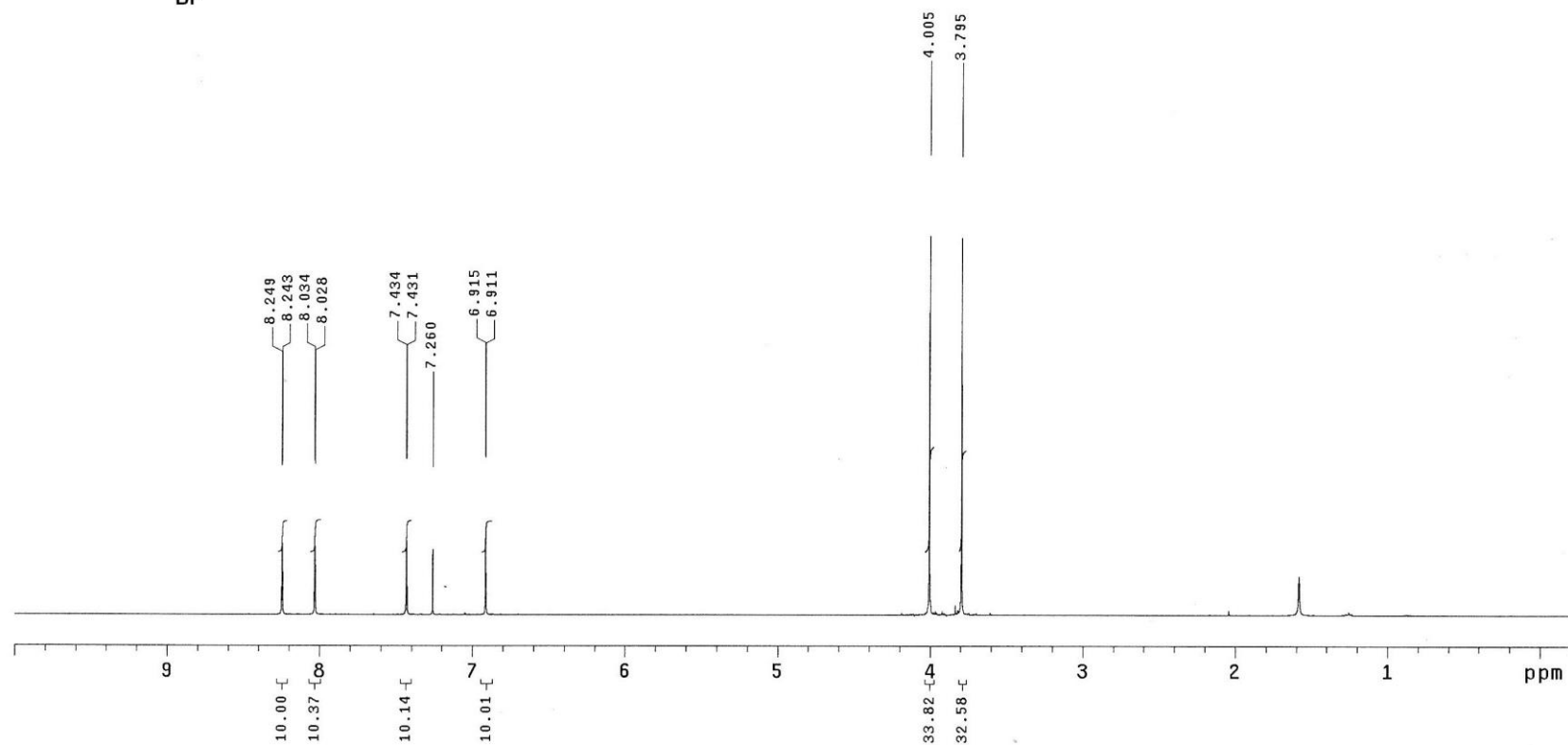
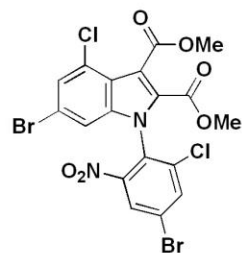
UNITYplus-400 "unity400"

Date: Apr 11 2023

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 4e (¹³C-NMR spectral data)

CHNF0406

Pulse Sequence: s2pu1

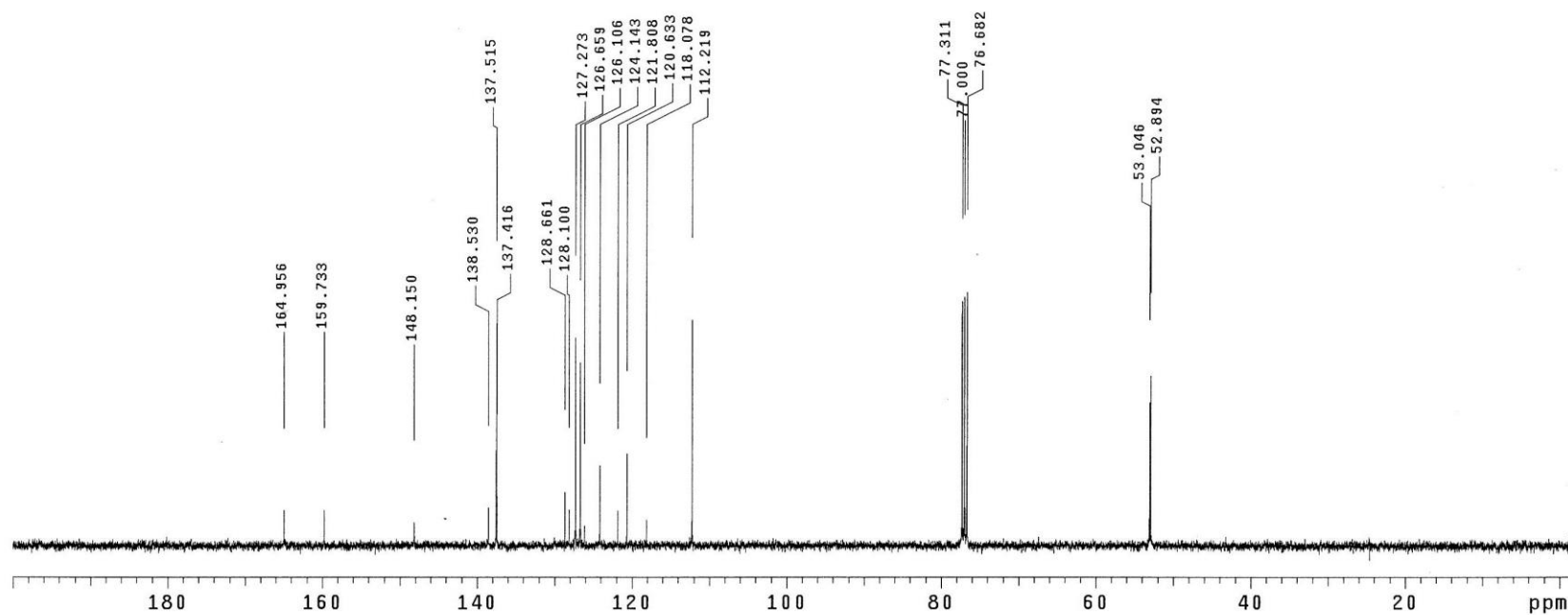
UNITYplus-400 "unity400"

Date: Apr 11 2023

Solvent: CDCl₃

Ambient temperature

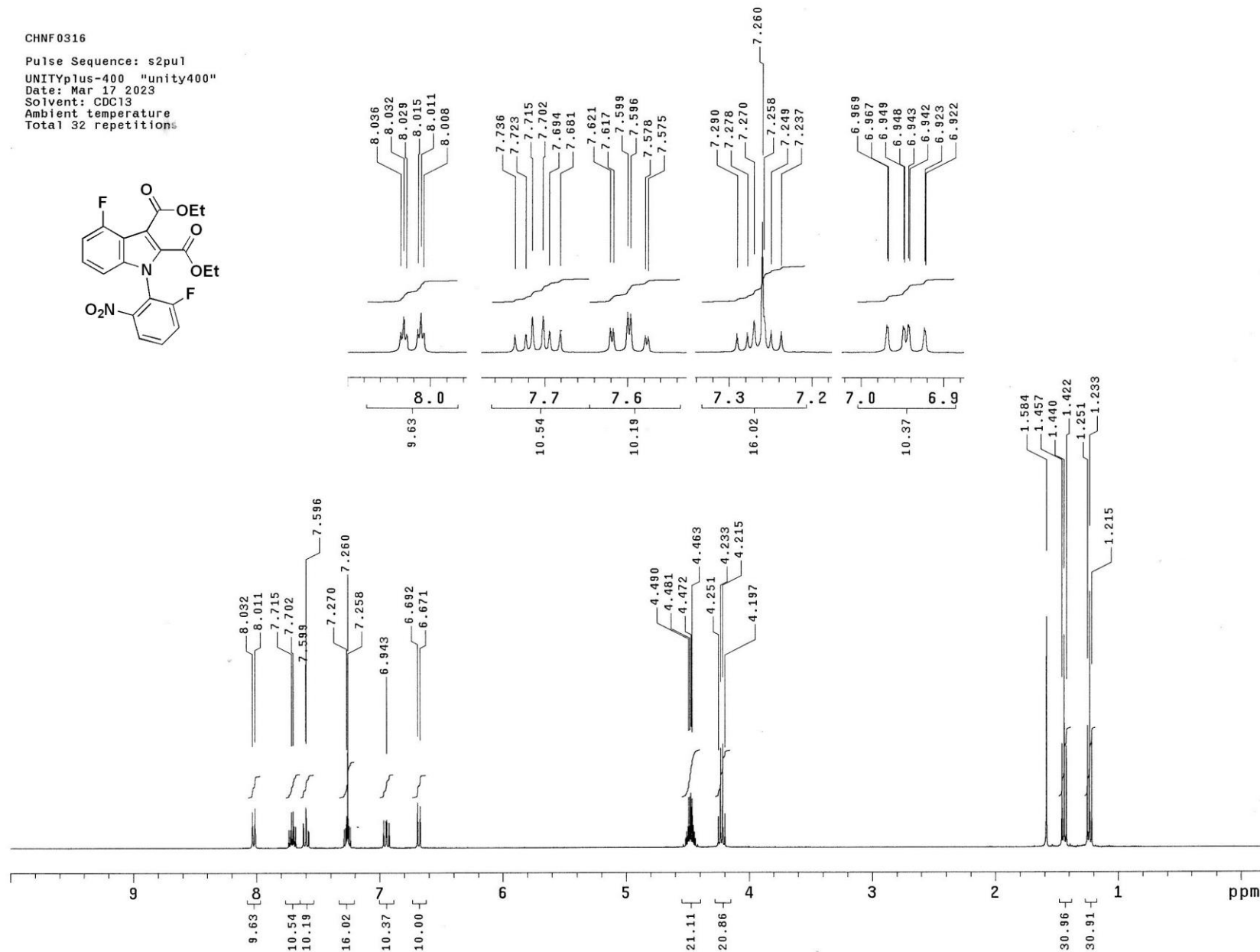
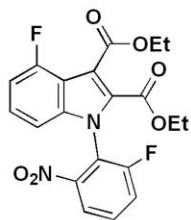
Total 4016 repetitions



Compound 4f (¹H-NMR spectral data)

CHNF0316

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Mar 17 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4f (¹³C-NMR spectral data)

CHNF0316

Pulse Sequence: s2pu1

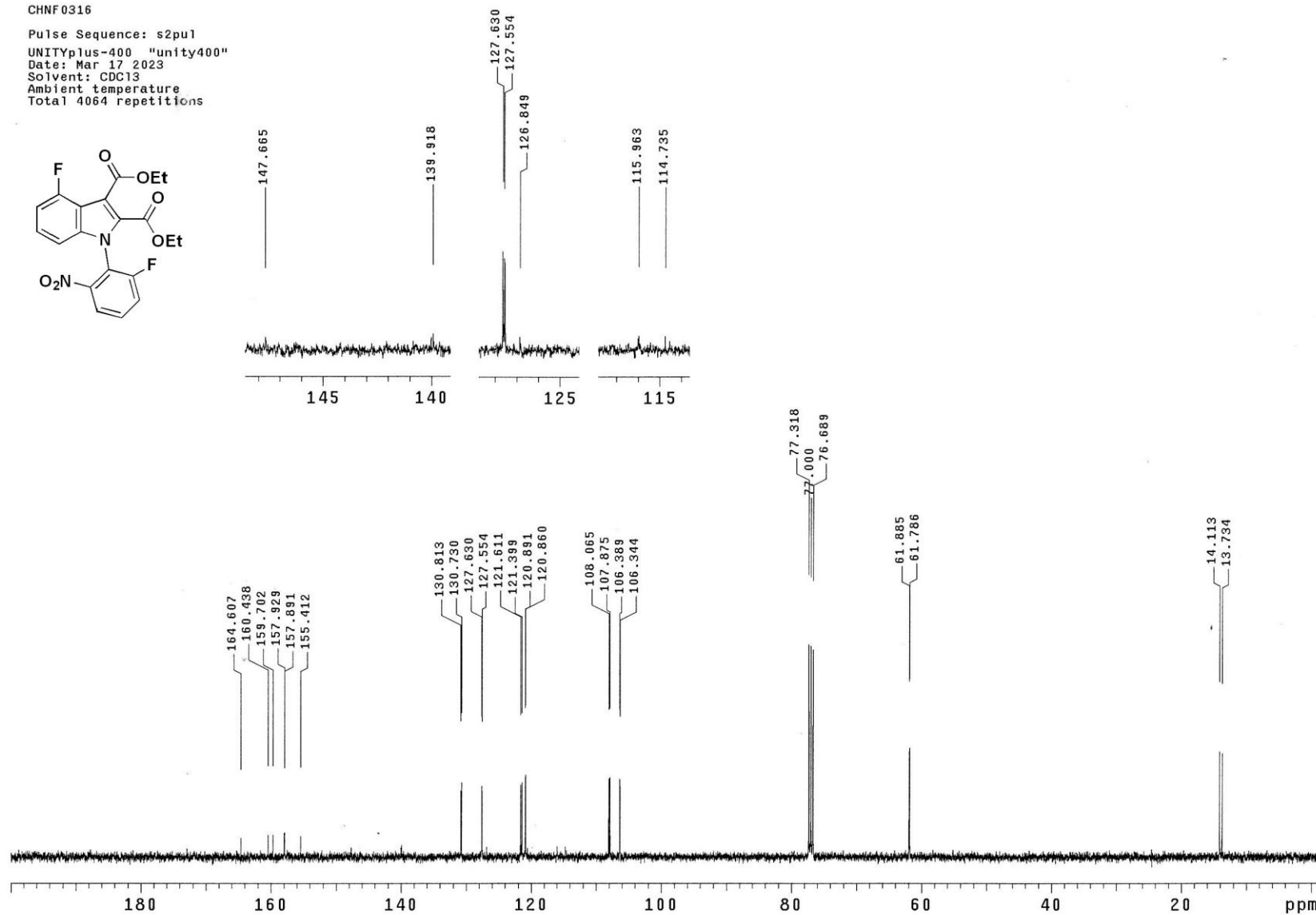
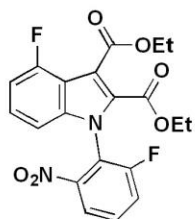
UNITYplus-400 "unity400"

Date: Mar 17 2023

Solvent: CDCl₃

Ambient temperature

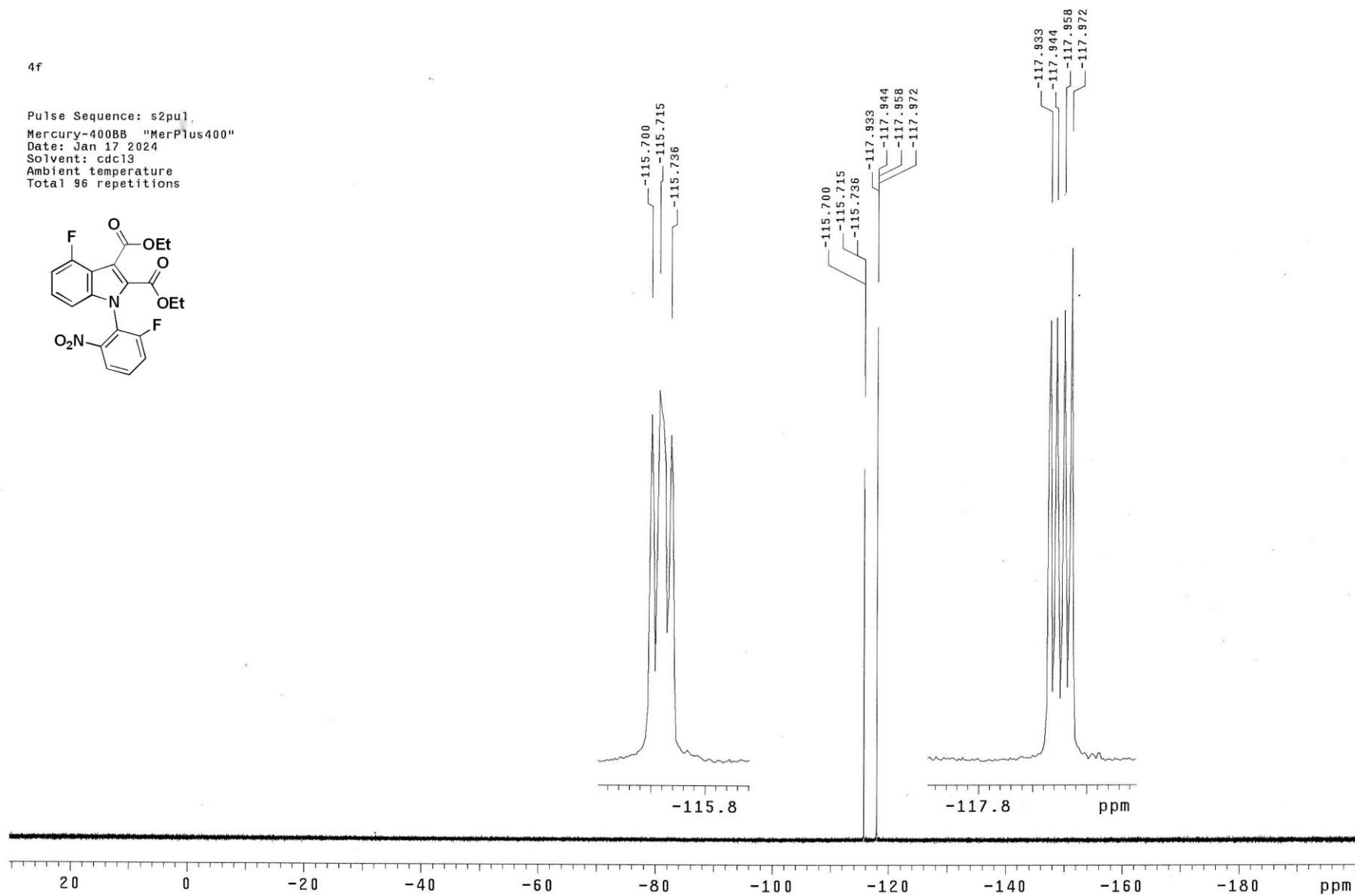
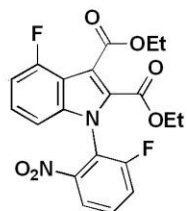
Total 4064 repetitions



Compound 4f (¹⁹F-NMR spectral data)

4f

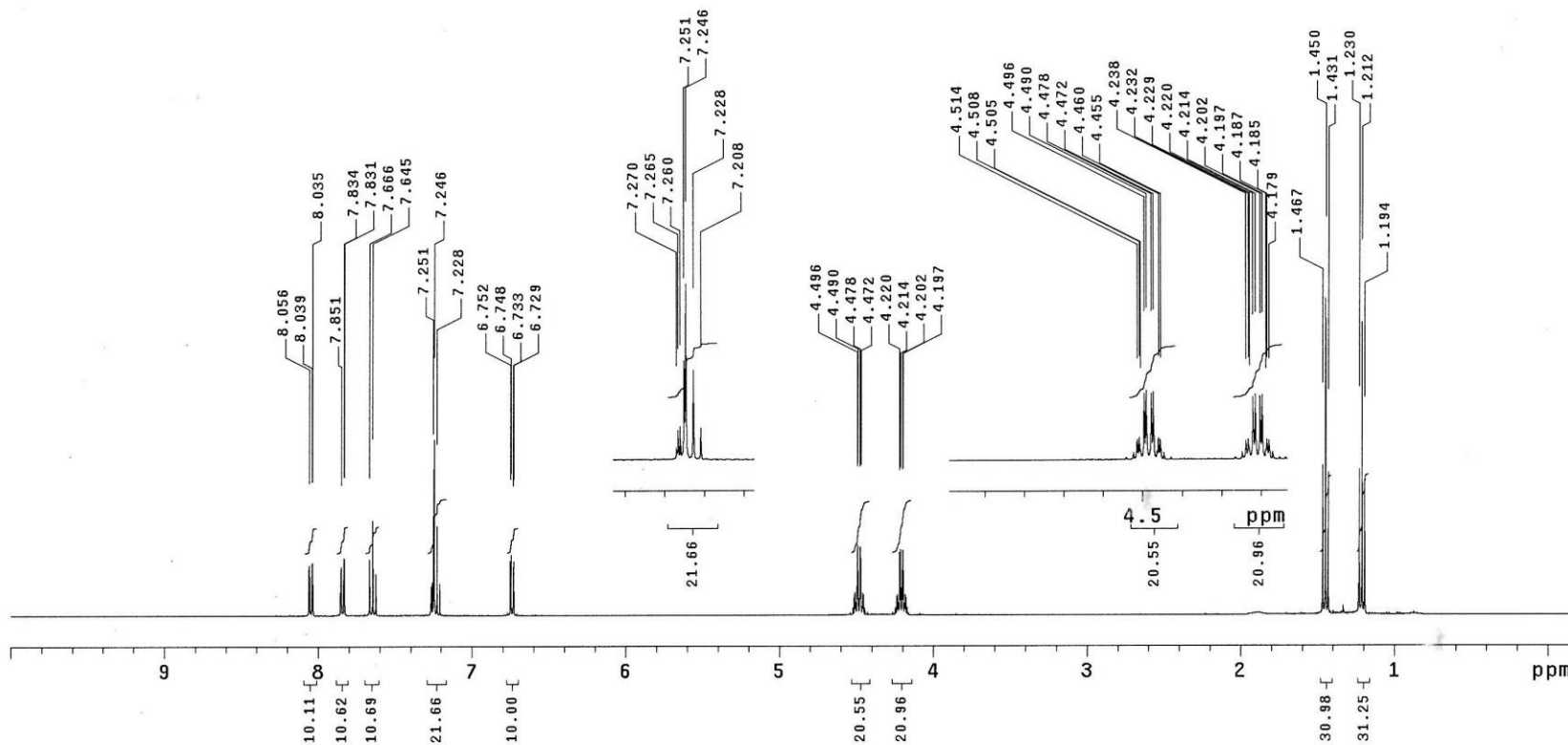
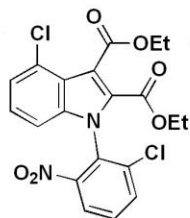
Pulse Sequence: s2pu]
Mercury-400BB "MerPlus400"
Date: Jan 17 2024
Solvent: cdcl3
Ambient temperature
Total 96 repetitions



Compound 4g (¹H-NMR spectral data)

CHQ3739

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 2 2022
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4g (¹³C-NMR spectral data)

CHQ3739

Pulse Sequence: s2pu1

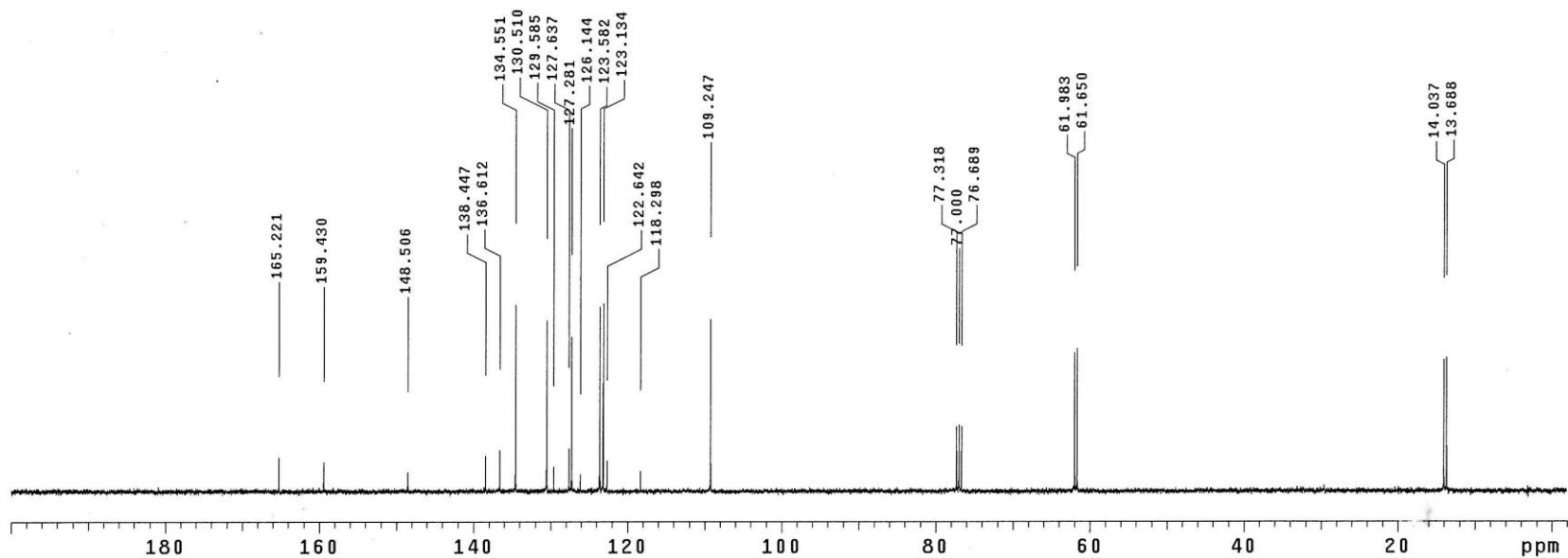
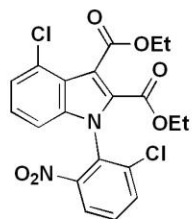
UNITYplus-400 "unity400"

Date: Nov 2 2022

Solvent: CDCl₃

Ambient temperature

Total 656 repetitions



Compound 4h (¹H-NMR spectral data)

CHNF0210

Pulse Sequence: s2pu1

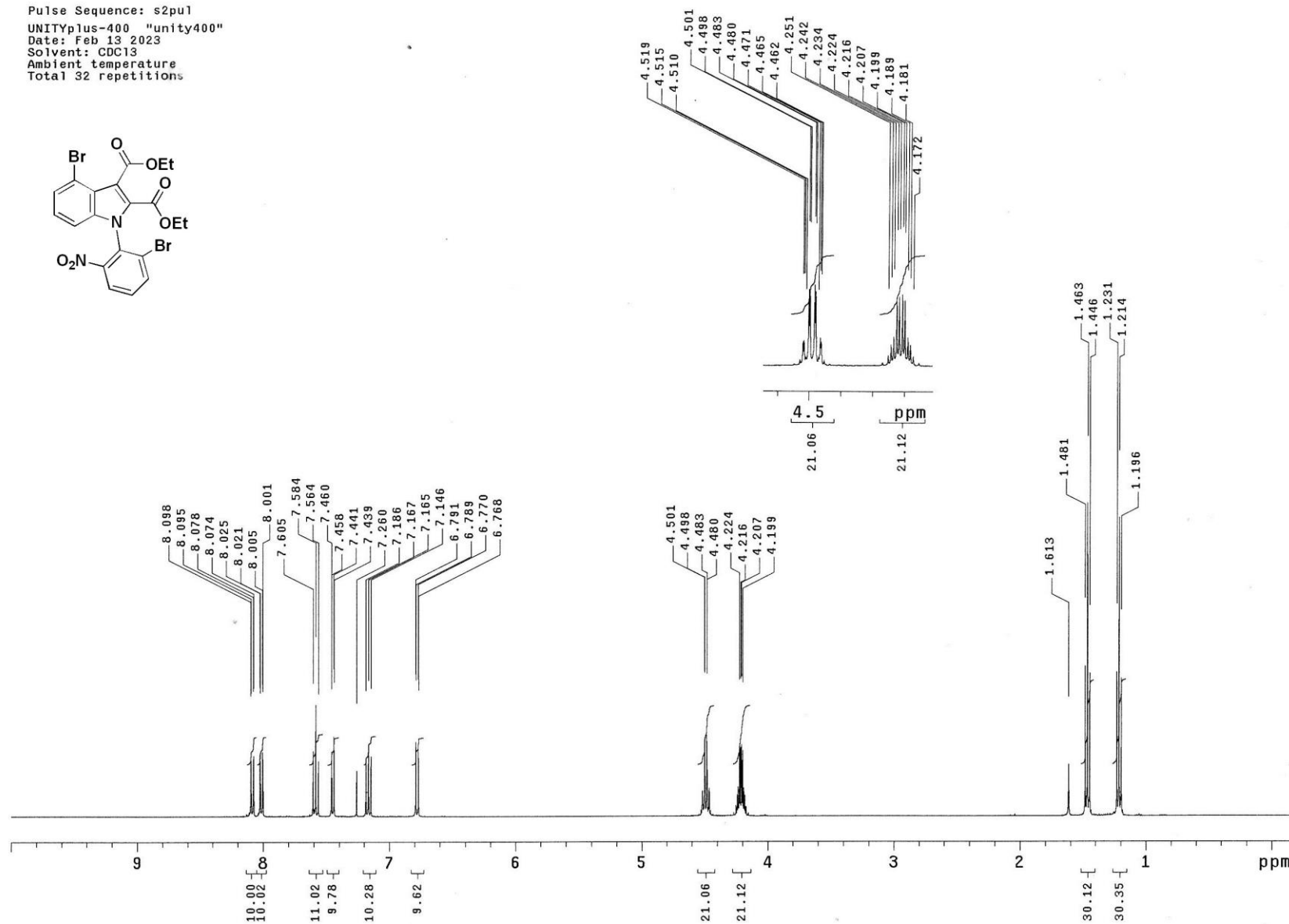
UNITYplus-400 "unity400"

Date: Feb 13 2023

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 4h (¹³C-NMR spectral data)

CHNF0210

Pulse Sequence: s2pu1

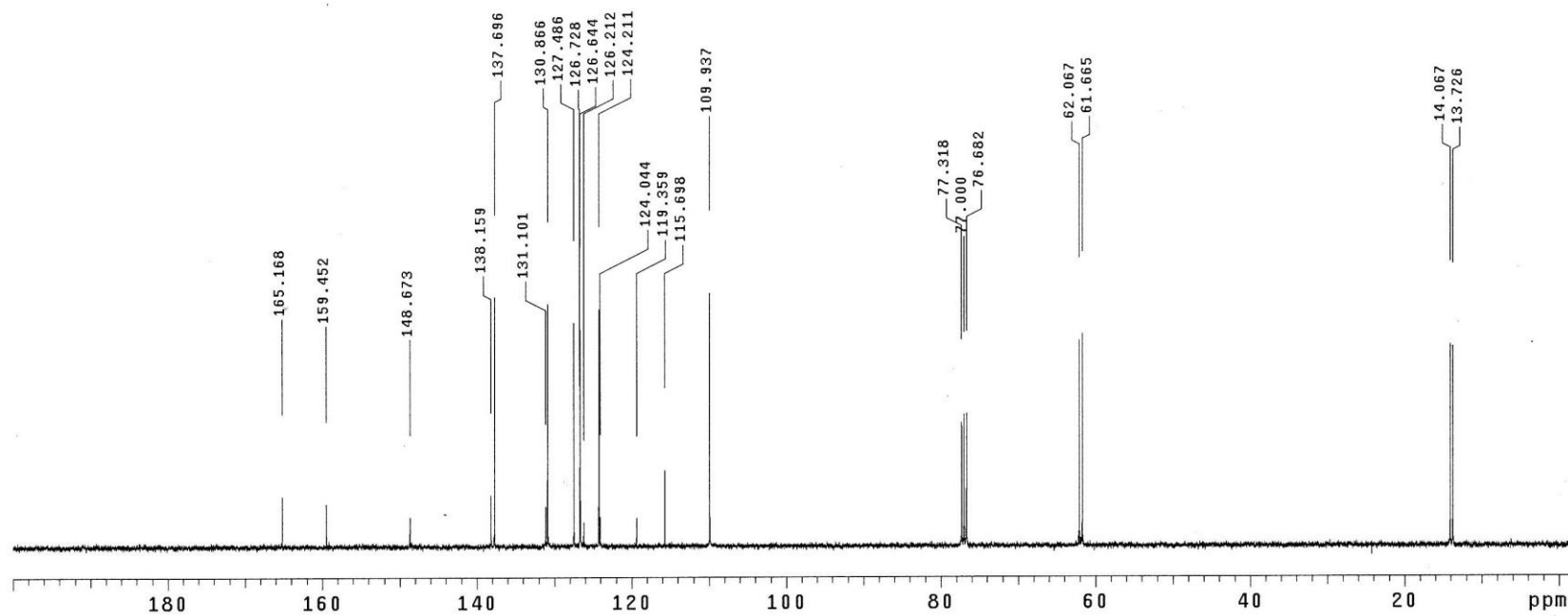
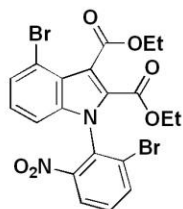
UNITYplus-400 "unity400"

Date: Feb 13 2023

Solvent: CDCl₃

Ambient temperature

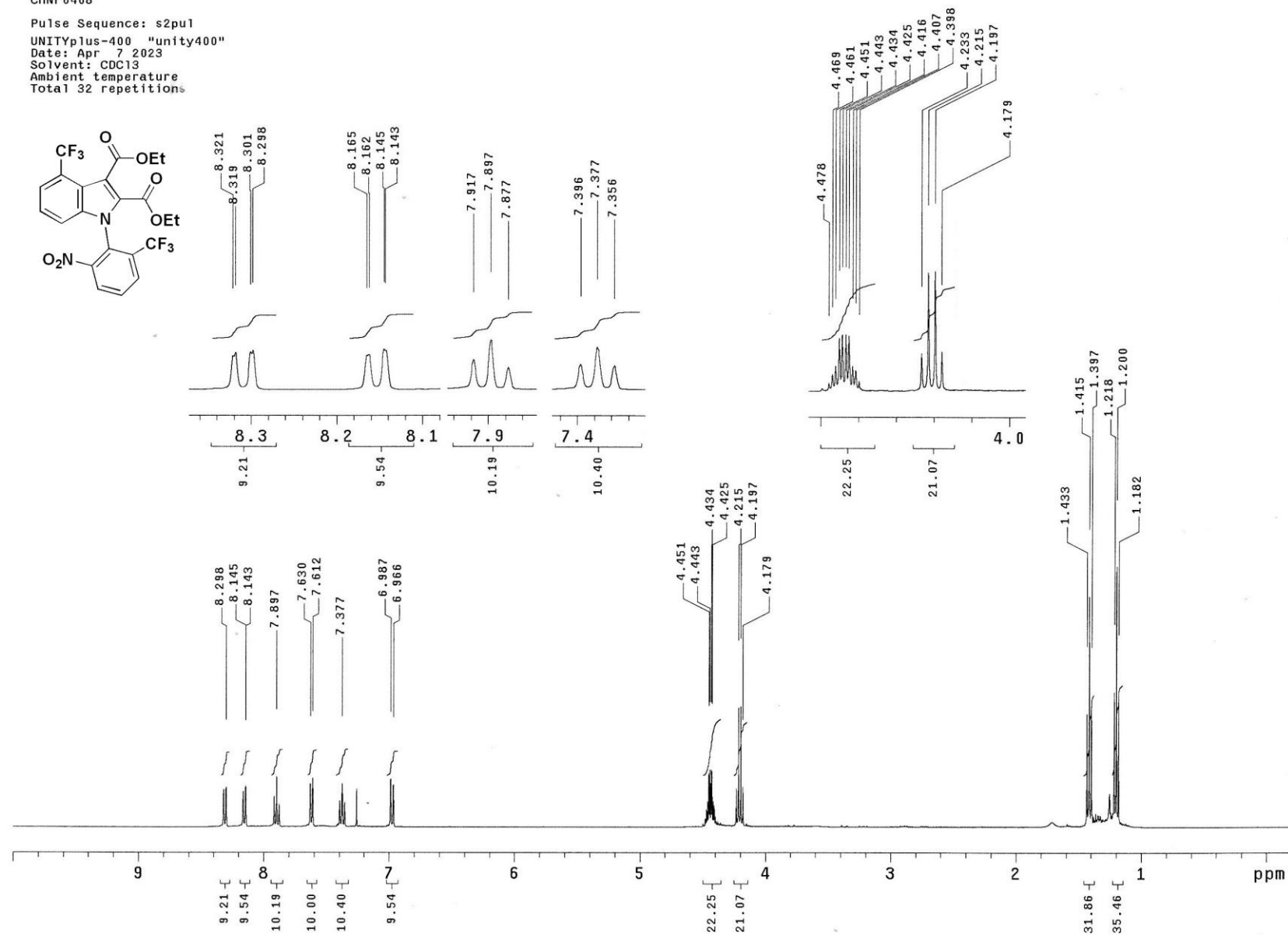
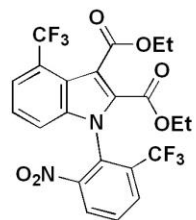
Total 4032 repetitions



Compound 4i (¹H-NMR spectral data)

CHNF0408

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Apr 7 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4i (¹³C-NMR spectral data)

CHNF0408

Pulse Sequence: s2pu1

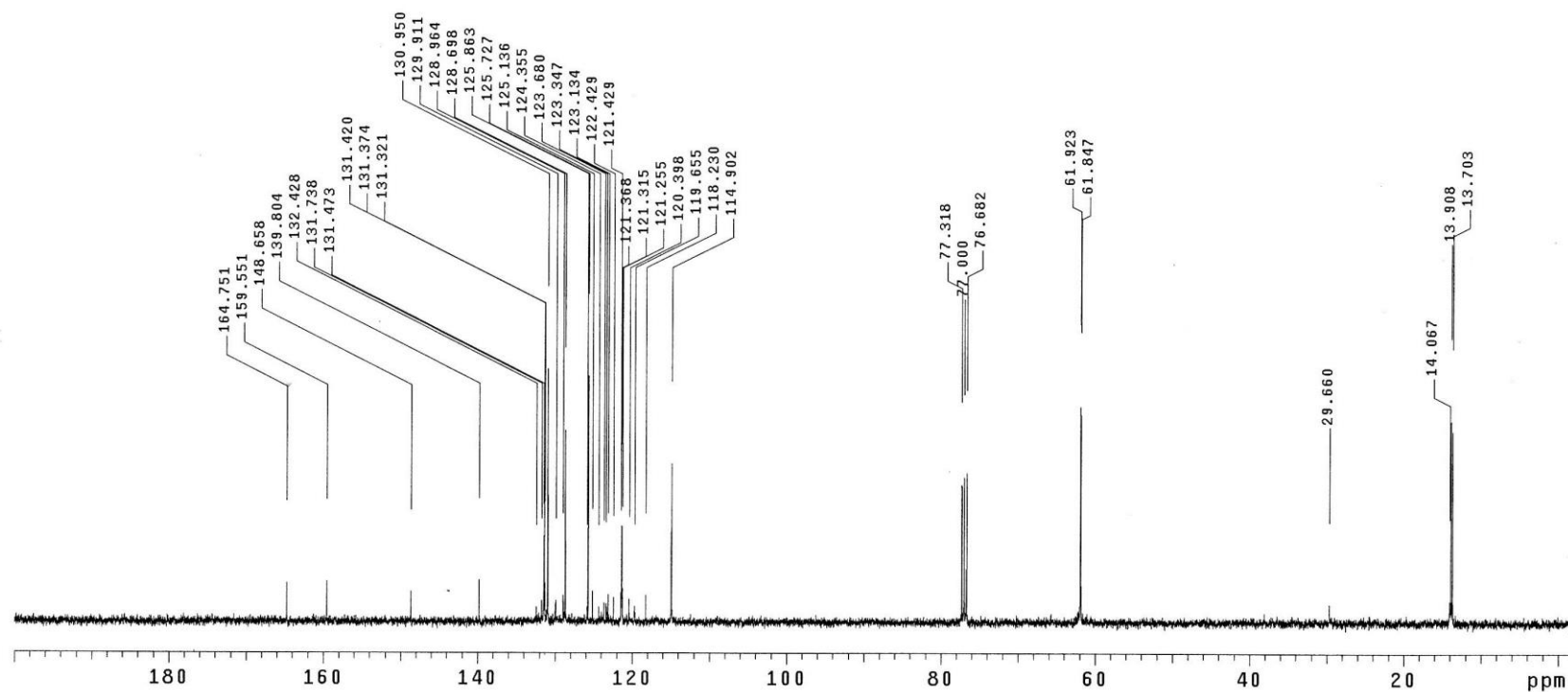
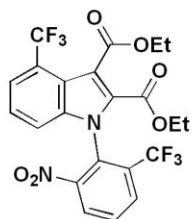
UNITYplus-400 "unity400"

Date: Apr 7 2023

Solvent: CDCl₃

Ambient temperature

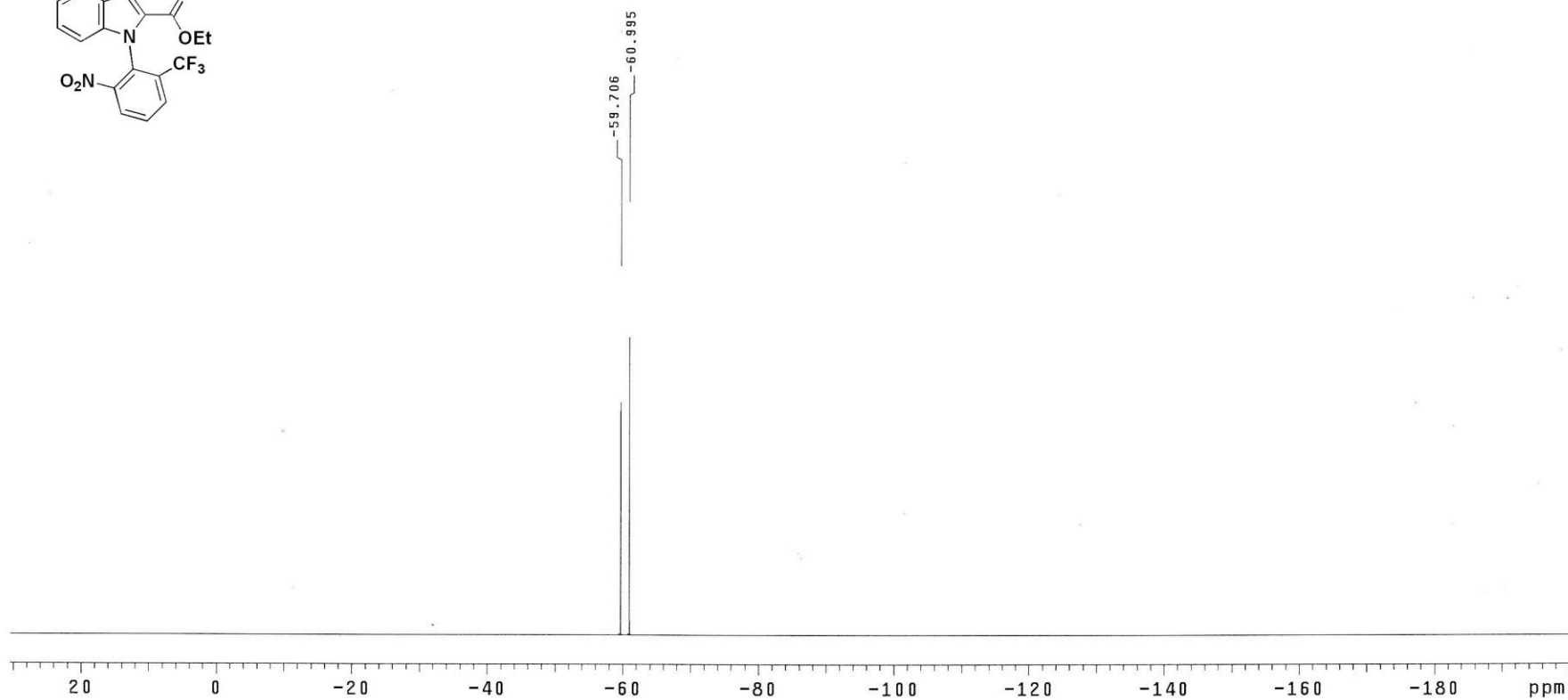
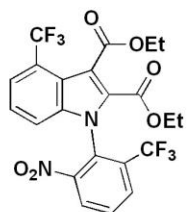
Total 2096 repetitions



Compound 4i (¹⁹F-NMR spectral data)

4i

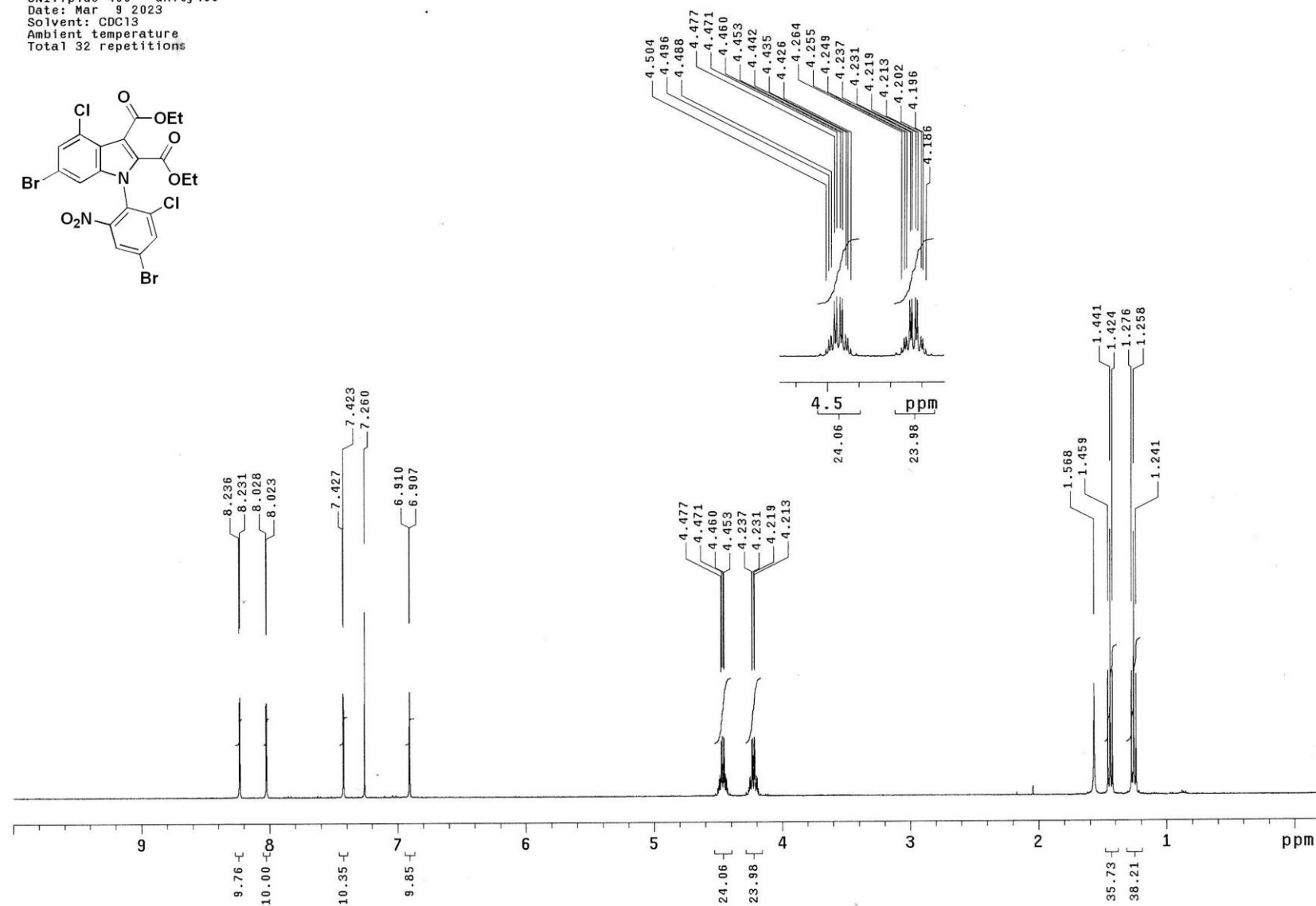
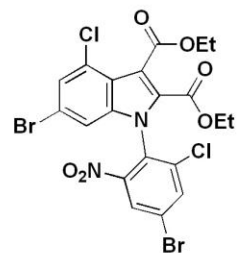
Pulse Sequence: s2pu1
Mercury-400BB "MerPlus400"
Date: Jan 18 2024
Solvent: cdcl3
Ambient temperature
Total 16 repetitions



Compound 4j (¹H-NMR spectral data)

CHNF0309

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Mar 9 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4j (¹³C-NMR spectral data)

CHNF0309

Pulse Sequence: s2pu1

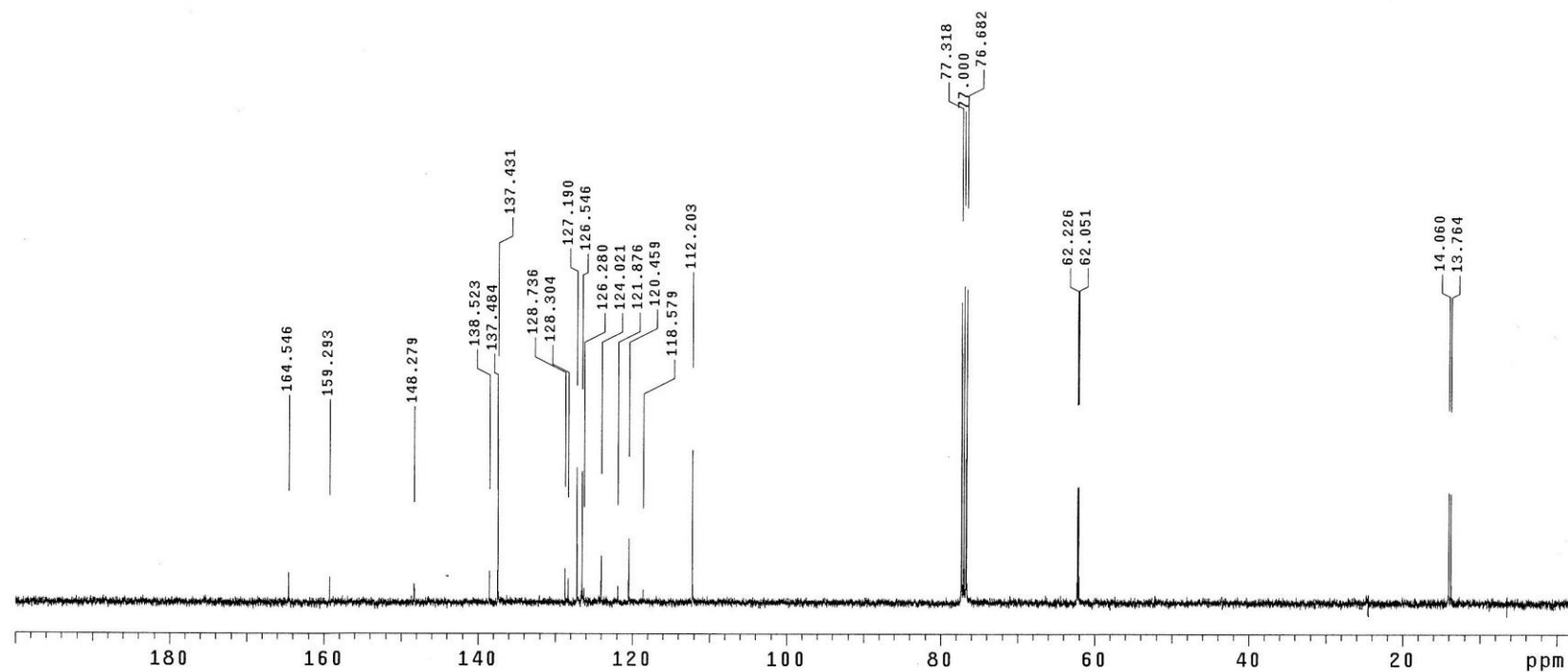
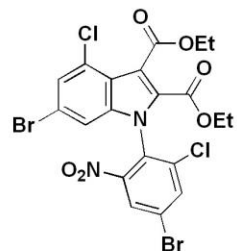
UNITYplus-400 "unity400"

Date: Mar 9 2023

Solvent: CDCl₃

Ambient temperature

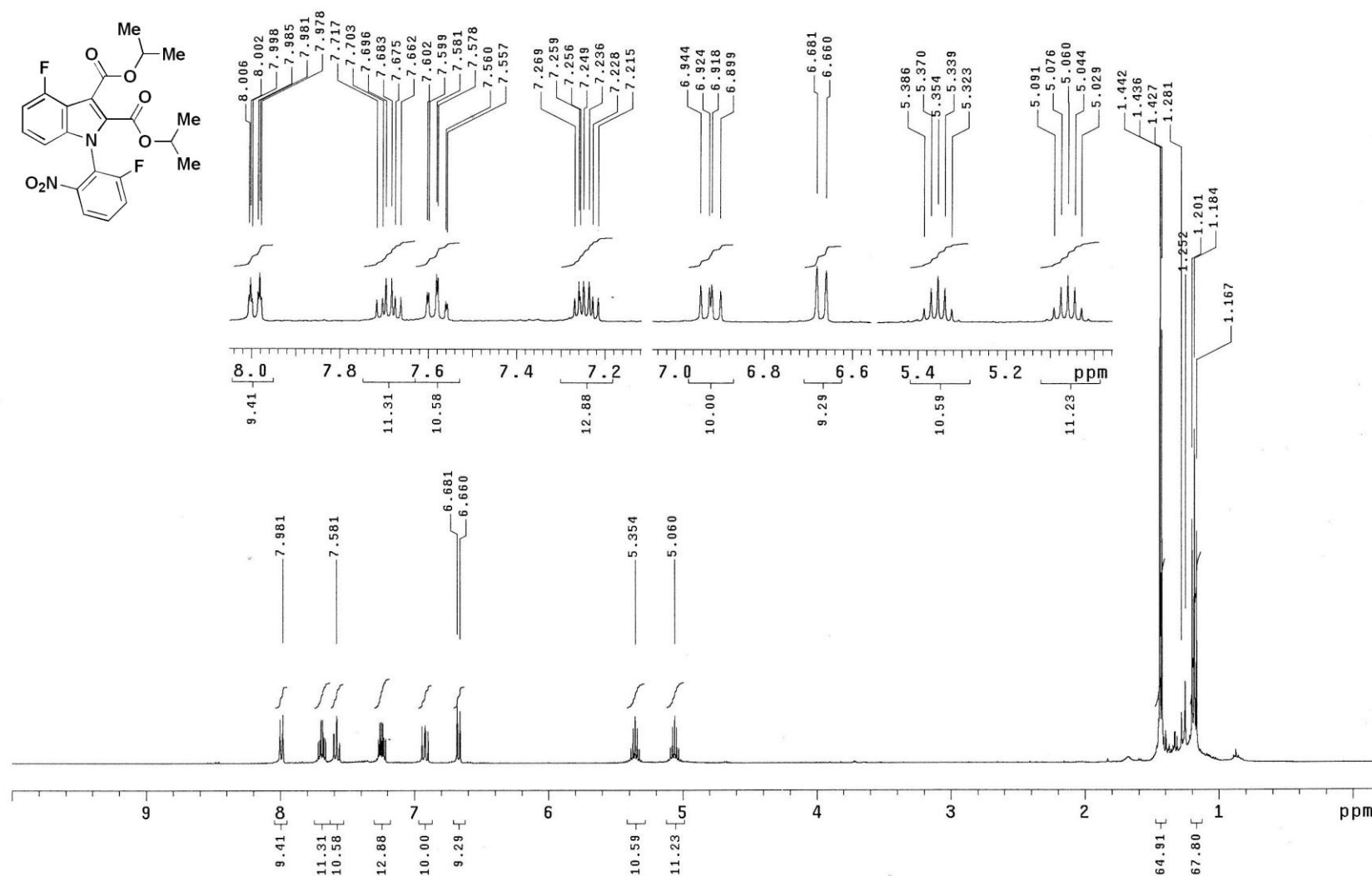
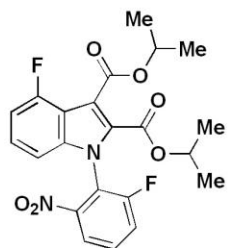
Total 8880 repetitions



Compound 4k (¹H-NMR spectral data)

CHNF0413

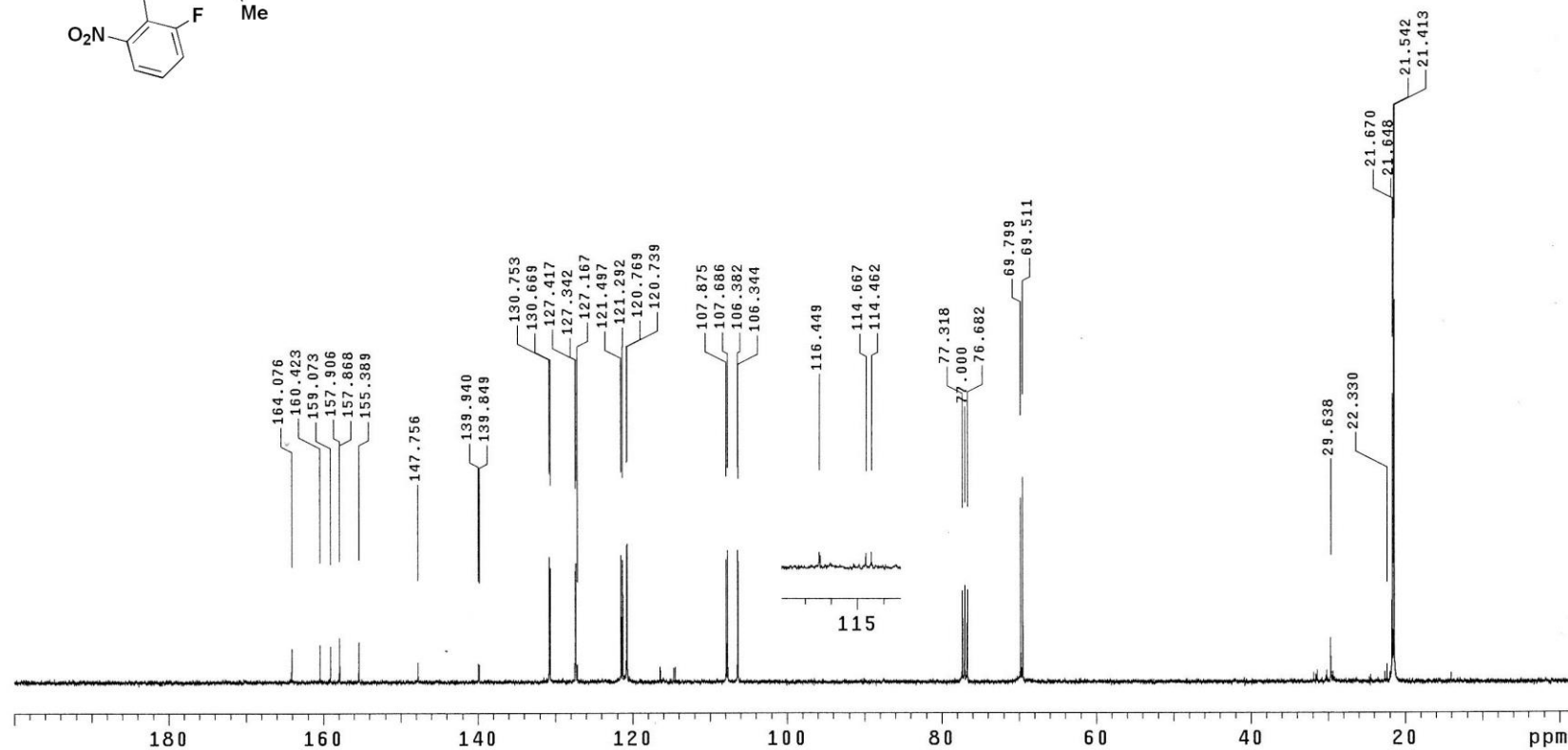
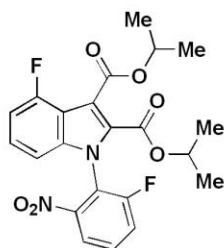
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Apr 13 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4k (¹³C-NMR spectral data)

CHNF0413

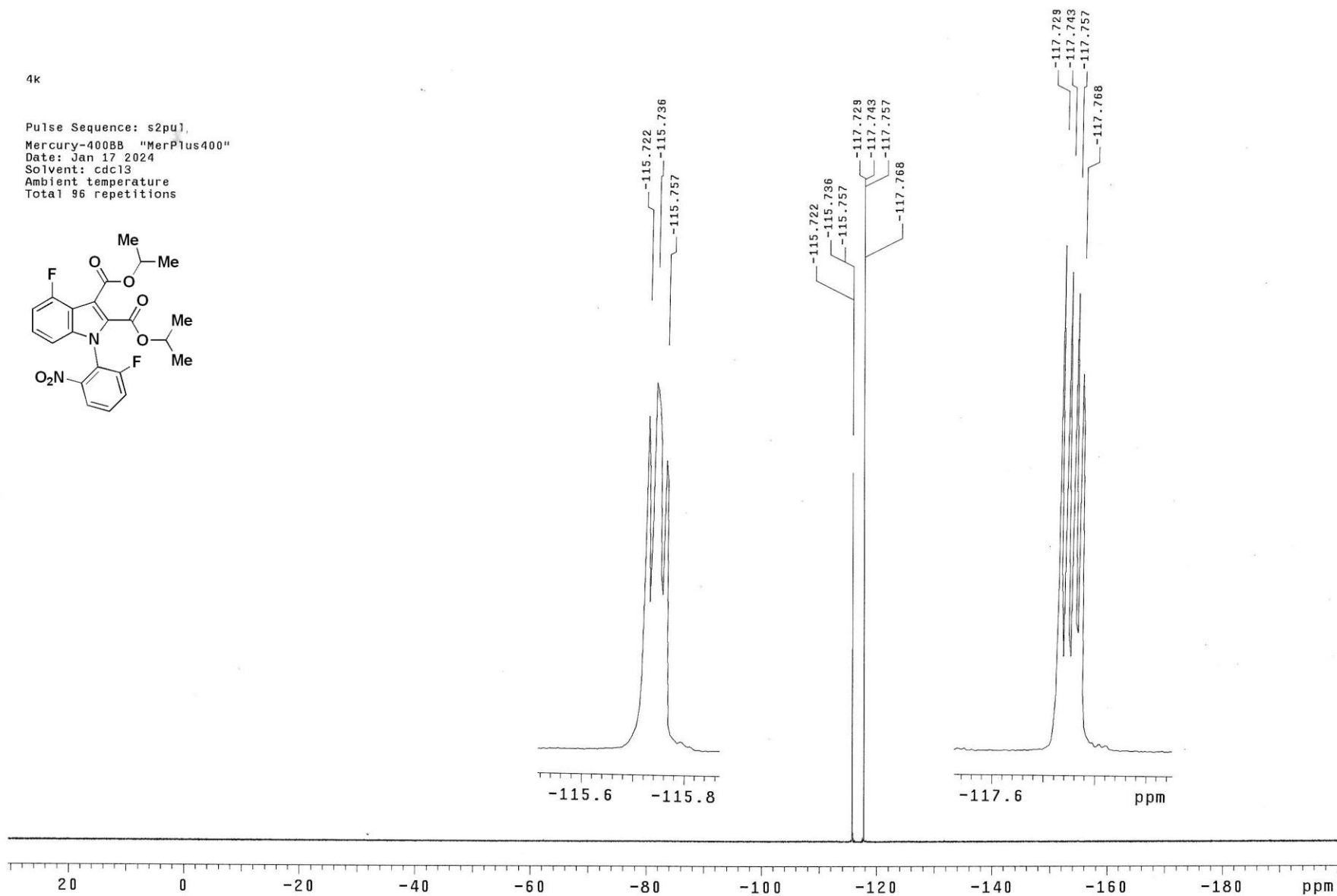
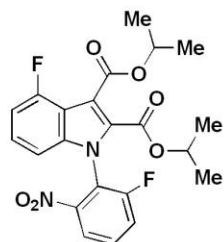
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Apr 13 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 4544 repetitions



Compound 4k (¹⁹F-NMR spectral data)

4k

Pulse Sequence: s2pu1,
Mercury-400BB "MerPlus400"
Date: Jan 17 2024
Solvent: cdc13
Ambient temperature
Total 96 repetitions



Compound 4I (¹H-NMR spectral data)

CHNF0320

Pulse Sequence: s2pu1

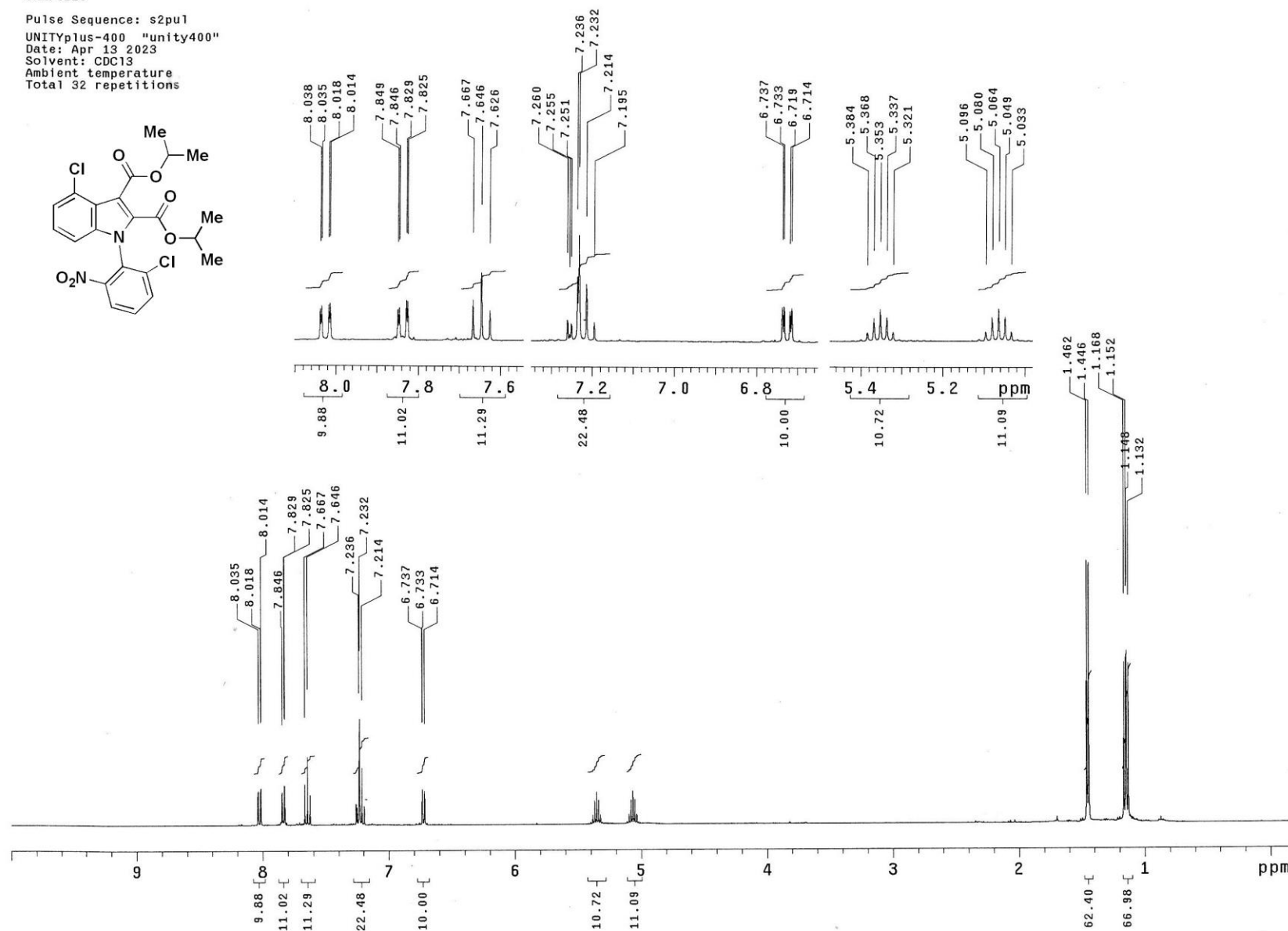
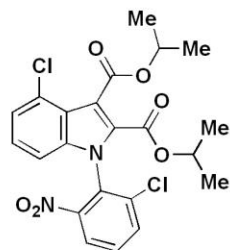
UNITYplus-400 "unity400"

Date: Apr 13 2023

Solvent: CDCl₃

Ambient temperature

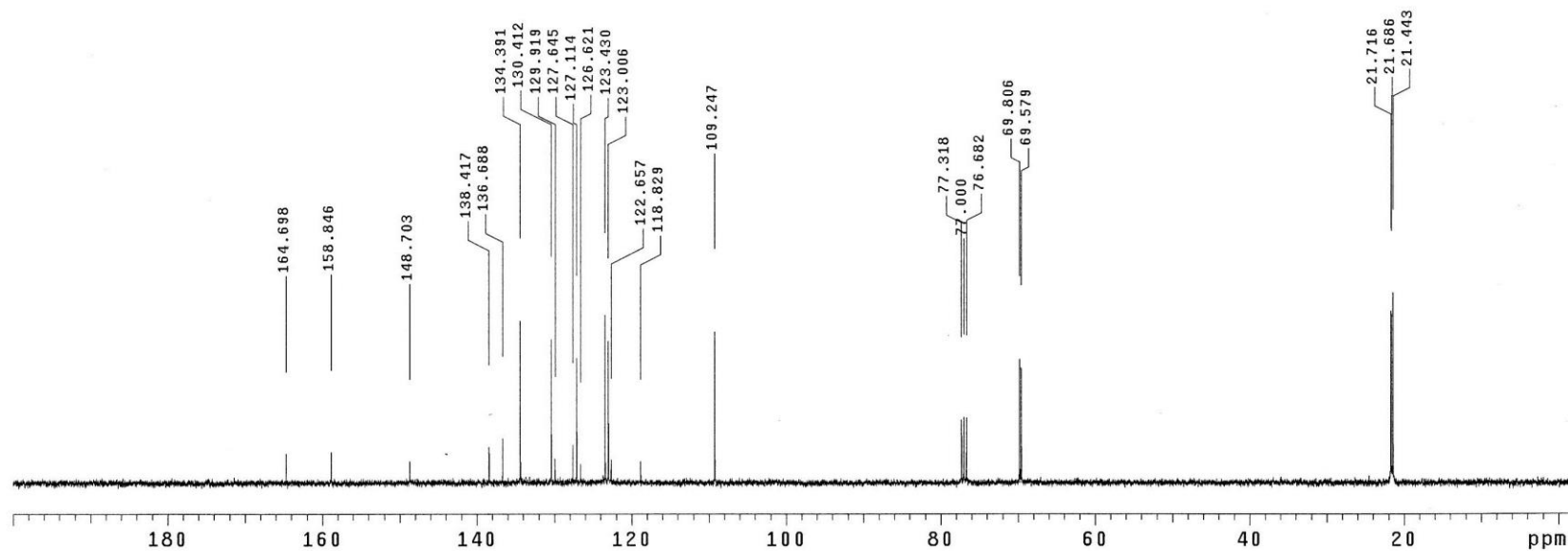
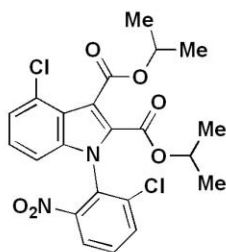
Total 32 repetitions



Compound 4I (¹³C-NMR spectral data)

CHNF0320

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Apr 13 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 512 repetitions



Compound 4m (¹H-NMR spectral data)

CHNF0506

Pulse Sequence: s2pu1

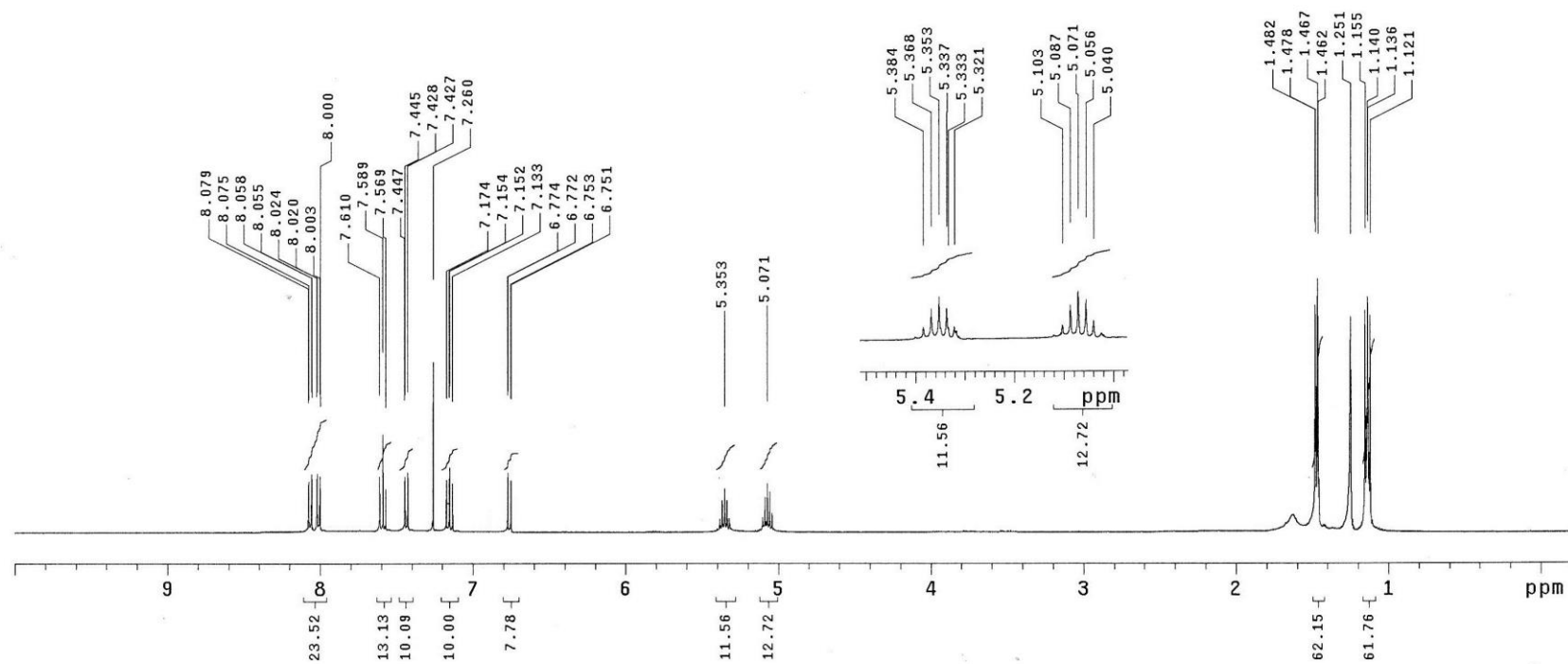
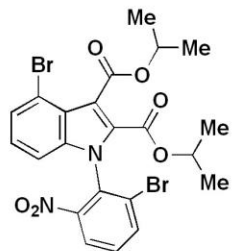
UNITYplus-400 "unity400"

Date: May 5 2023

Solvent: CDCl₃

Ambient temperature

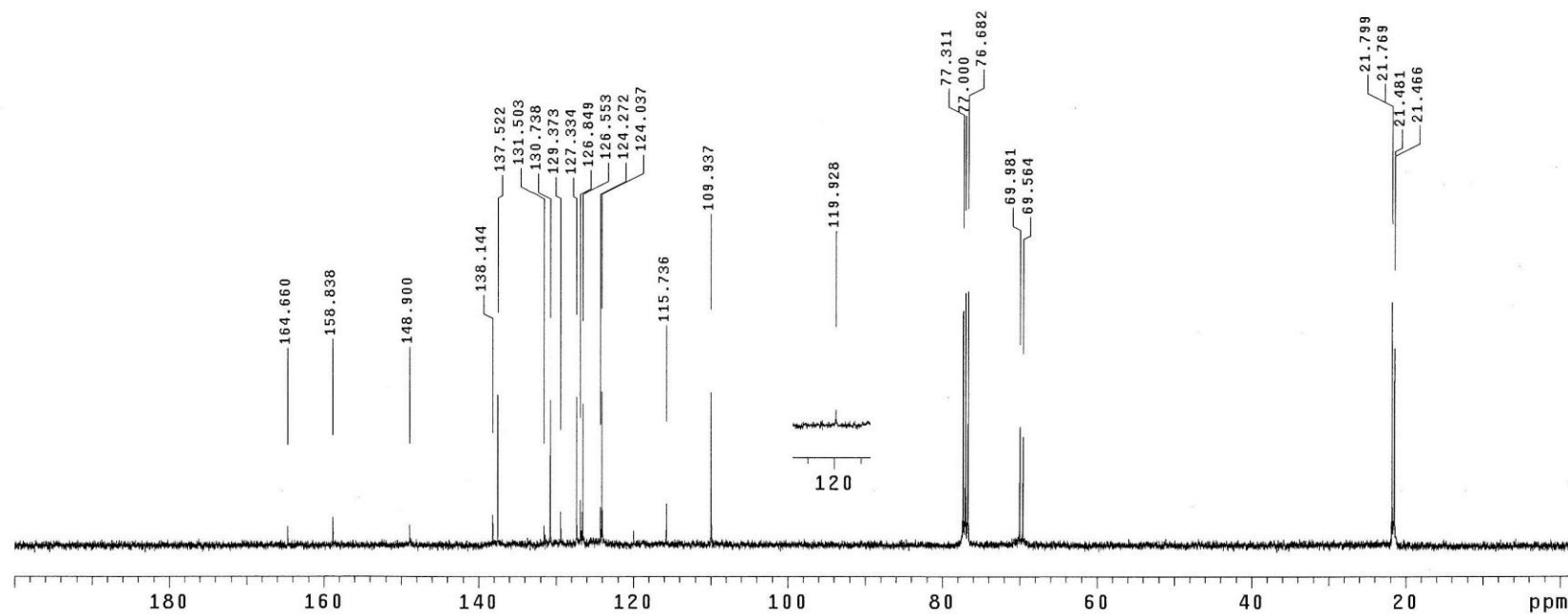
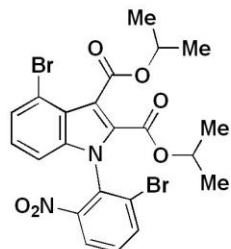
Total 32 repetitions



Compound 4m (¹³C-NMR spectral data)

CHNF0506

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: May 5 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 10256 repetitions



Compound 4n (¹H-NMR spectral data)

CHNF0425

Pulse Sequence: s2pu1

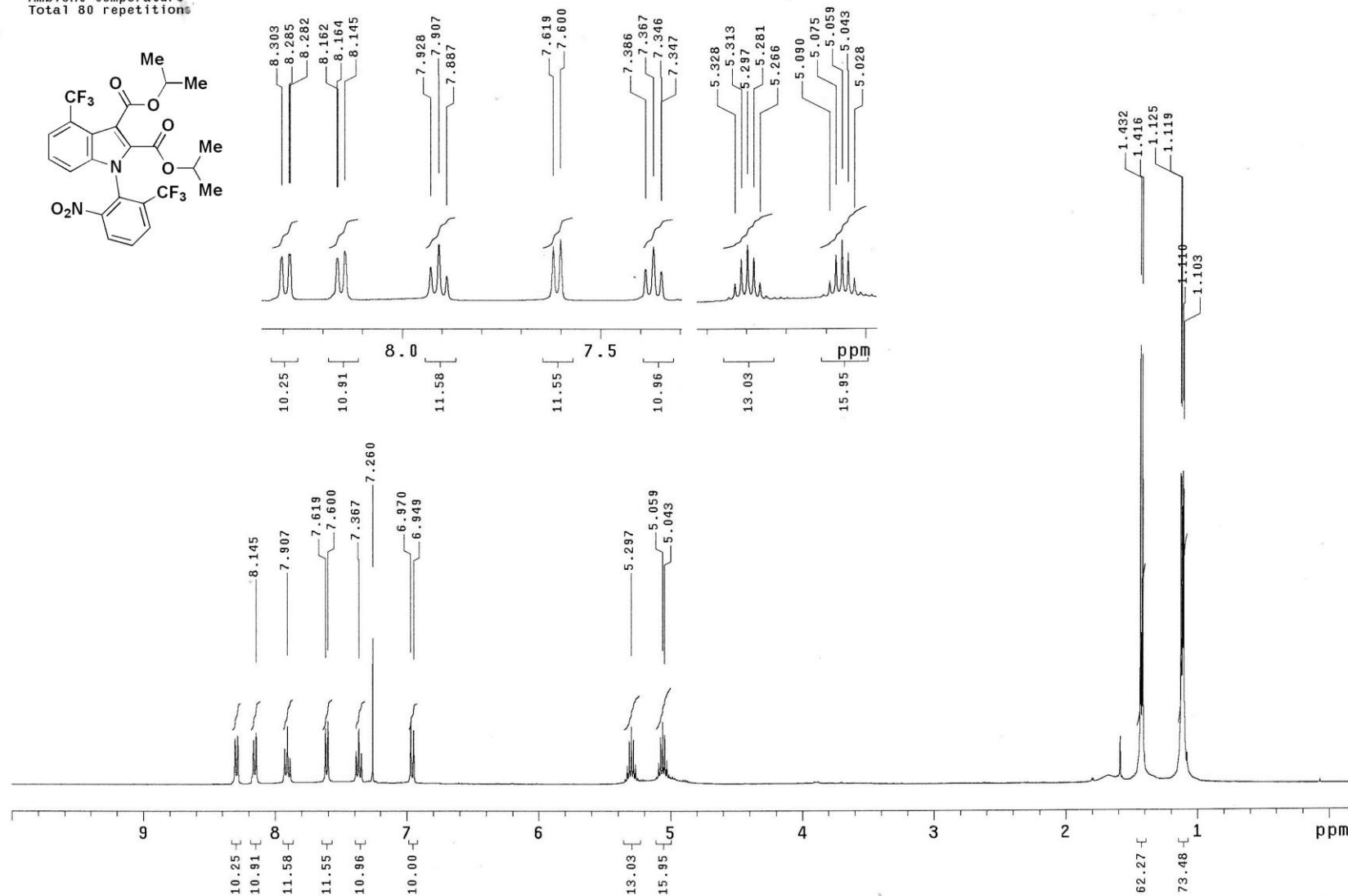
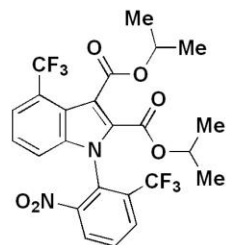
UNITYplus-400 "unity400"

Date: Aug 24 2023

Solvent: CDCl₃

Ambient temperature

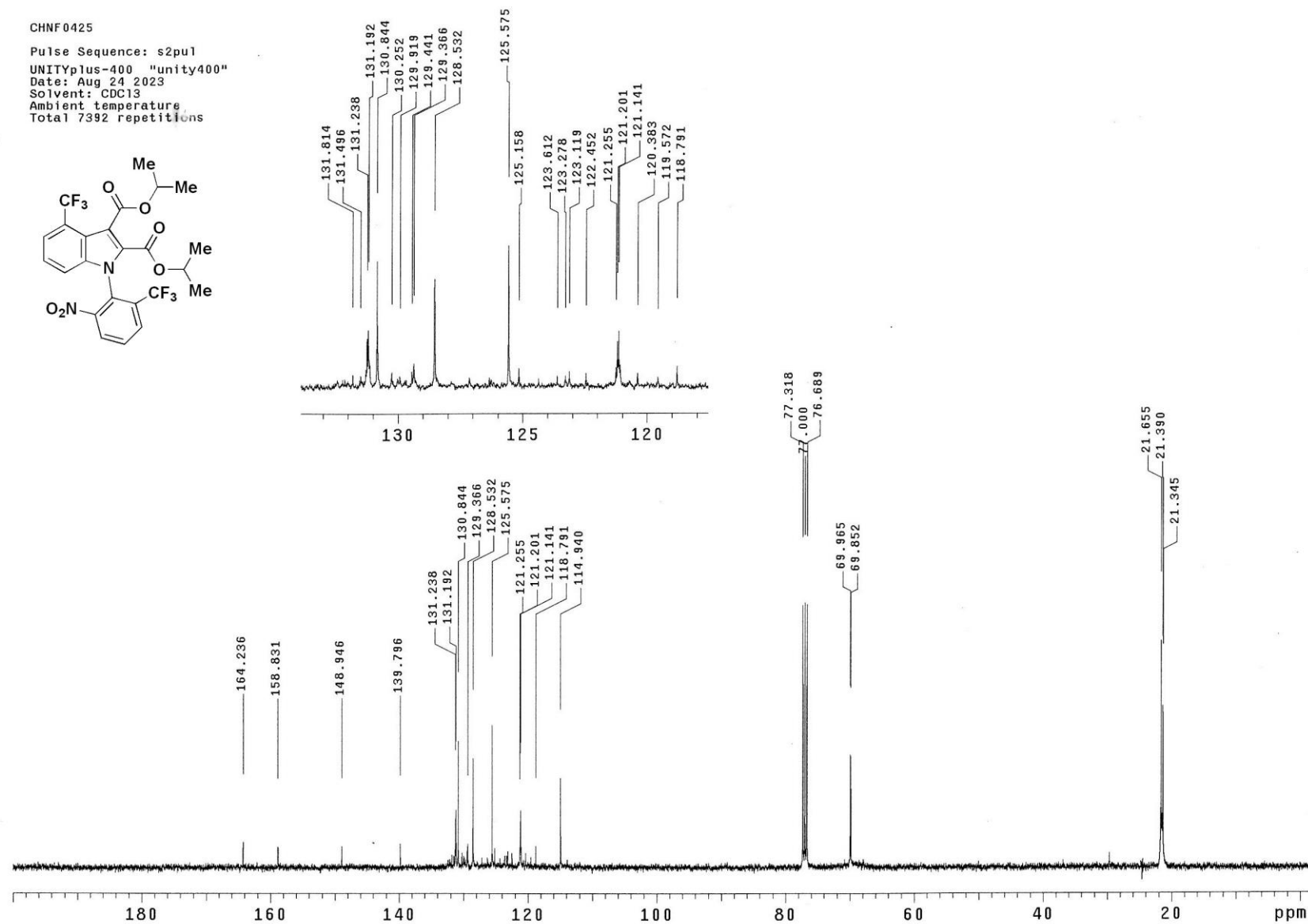
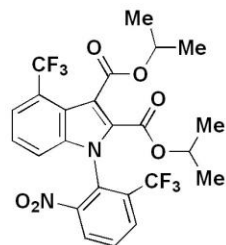
Total 80 repetitions



Compound 4n (¹³C-NMR spectral data)

CHNF0425

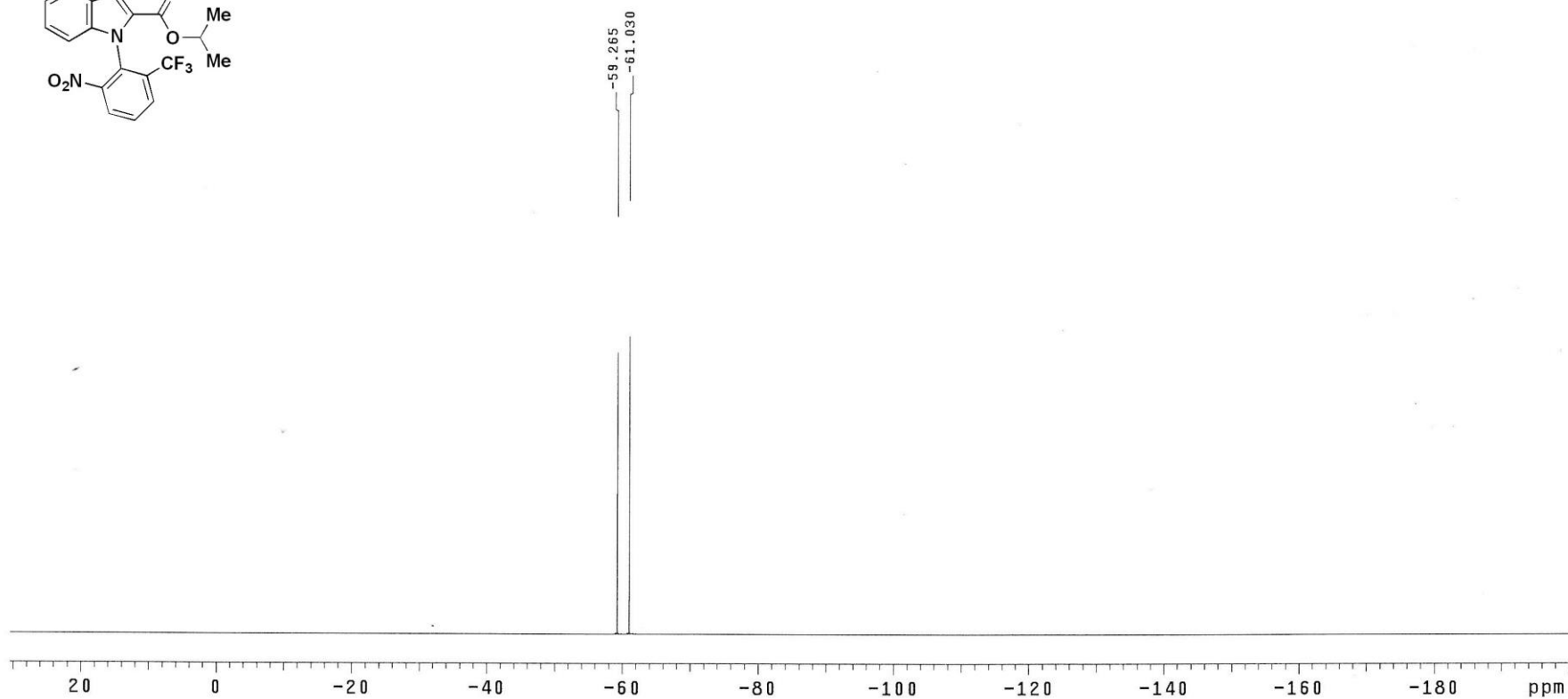
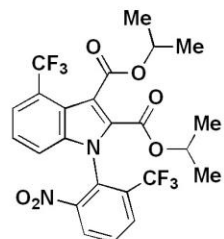
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 24 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 7392 repetitions



Compound 4n (¹⁹F-NMR spectral data)

4n

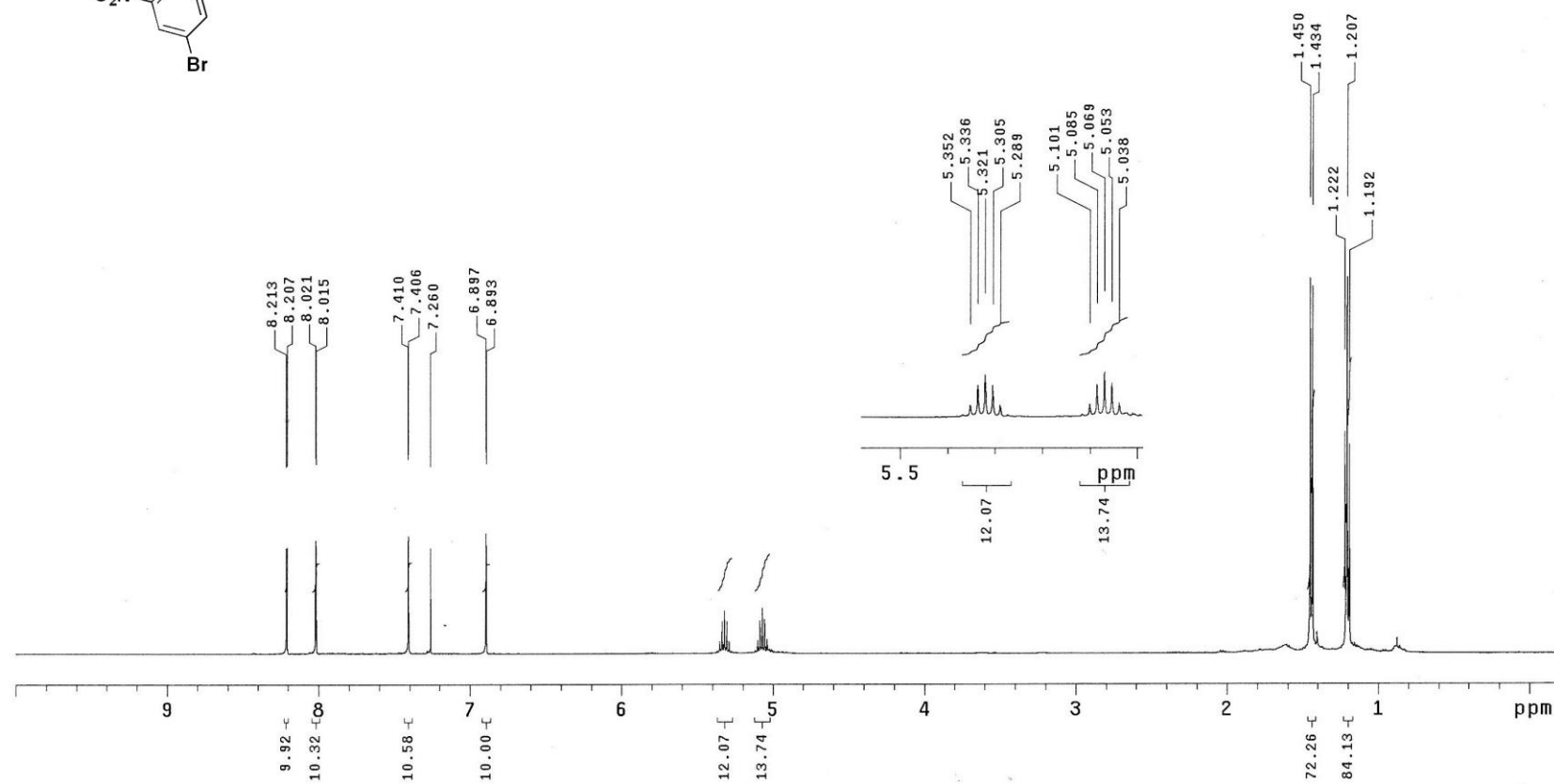
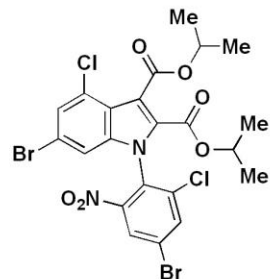
Pulse Sequence: s2pu1
Mercury-400BB "MerPlus400"
Date: Jan 18 2024
Solvent: cdcl3
Ambient temperature
Total 32 repetitions



Compound 4o (¹H-NMR spectral data)

CHNF0504

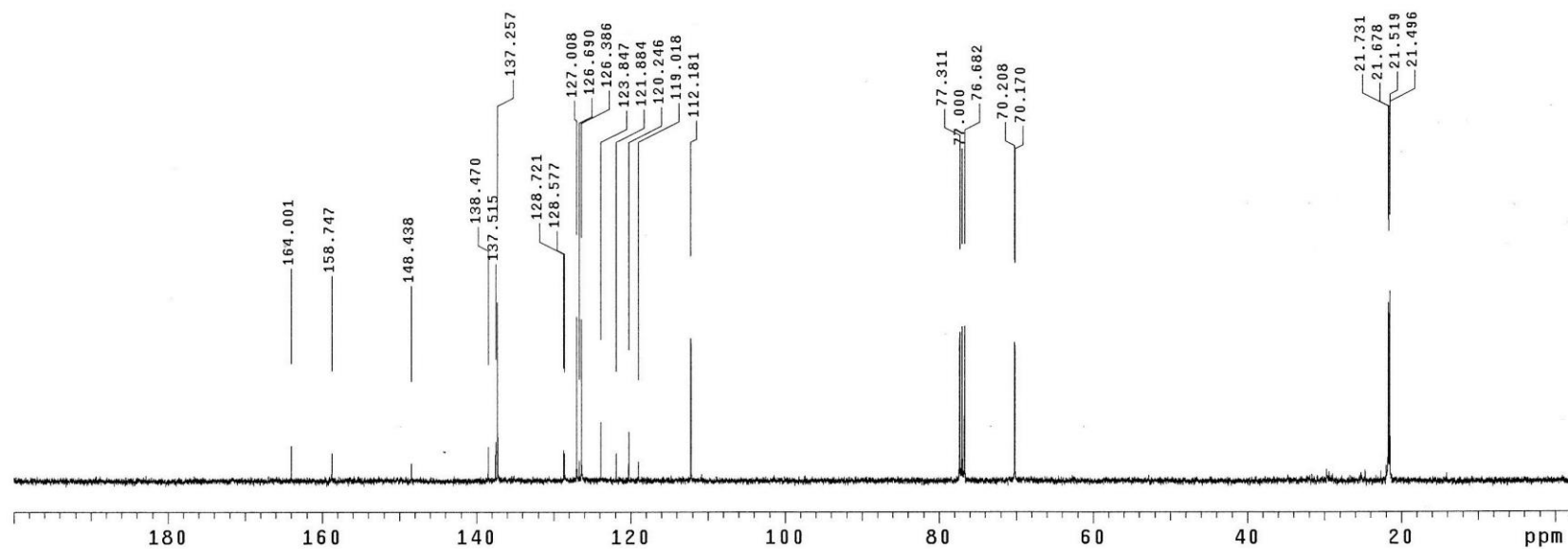
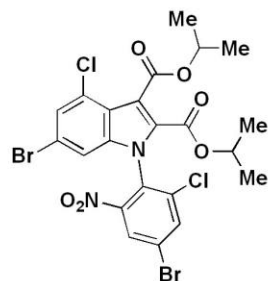
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: May 4 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4o (¹³C-NMR spectral data)

CHNF0504

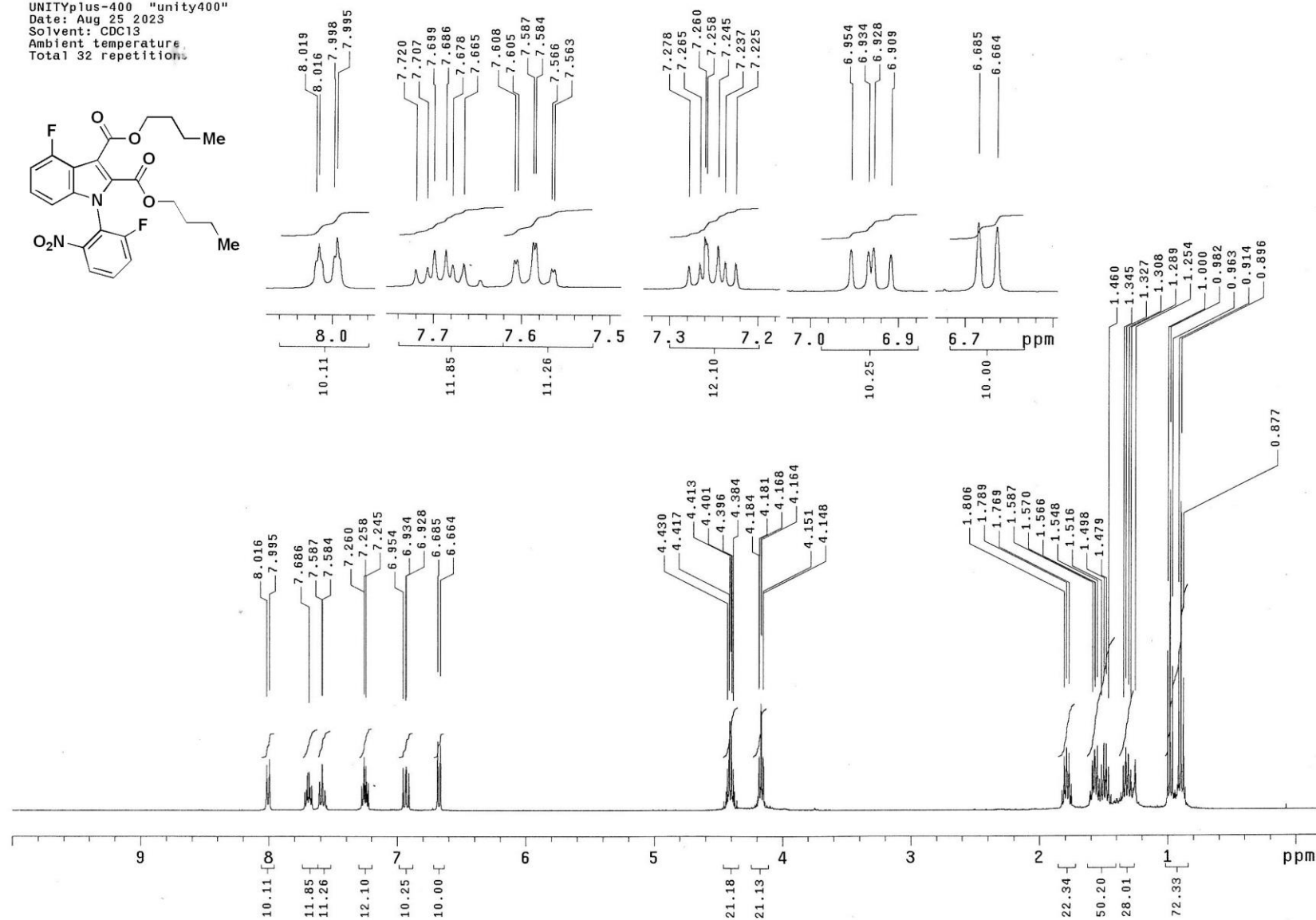
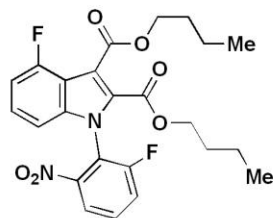
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: May 4 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 4368 repetitions



Compound 4p (¹H-NMR spectral data)

CHNF0418

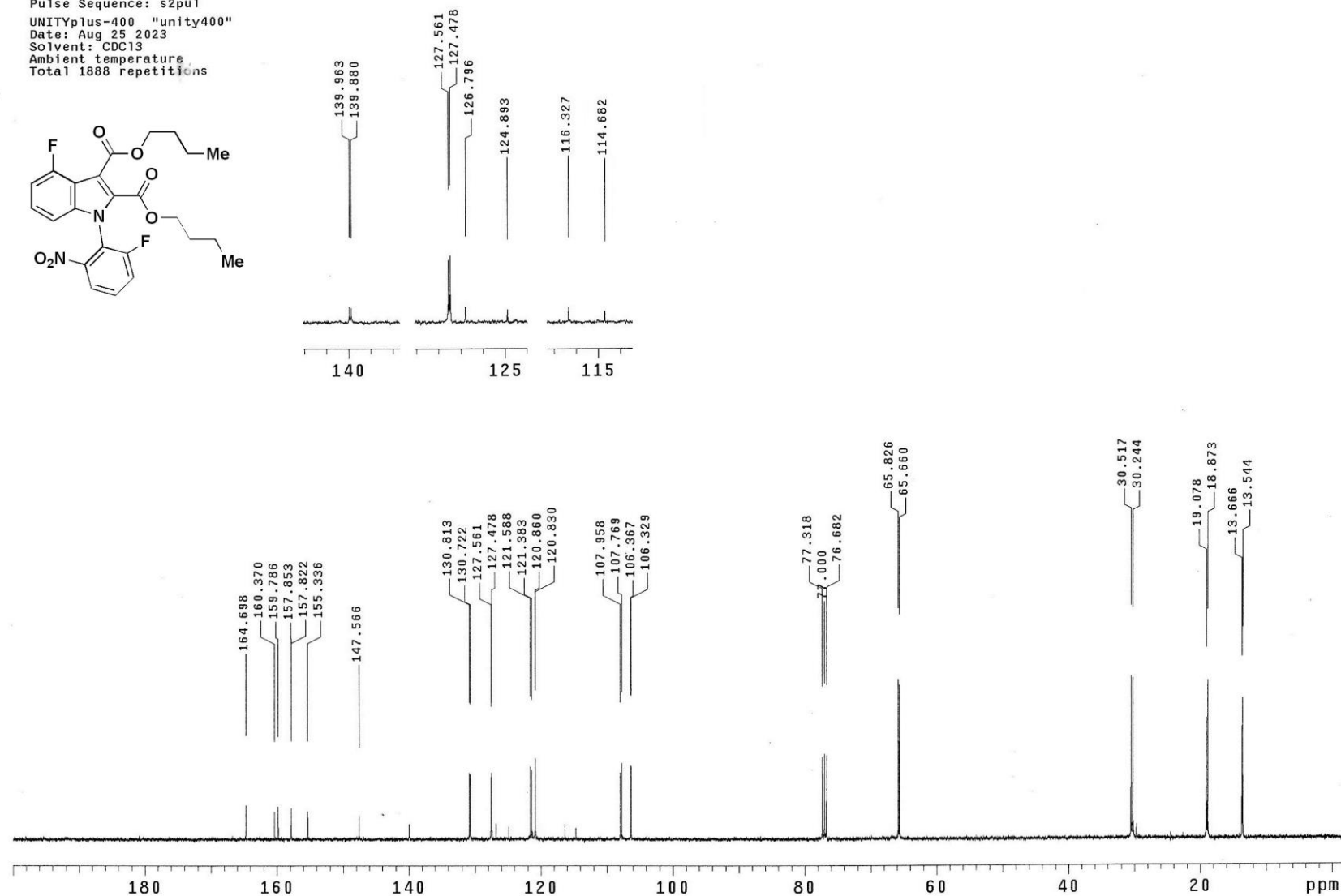
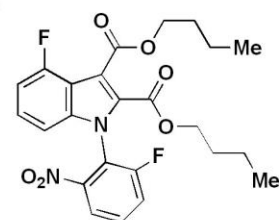
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 25 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4p (¹³C-NMR spectral data)

CHNF0418

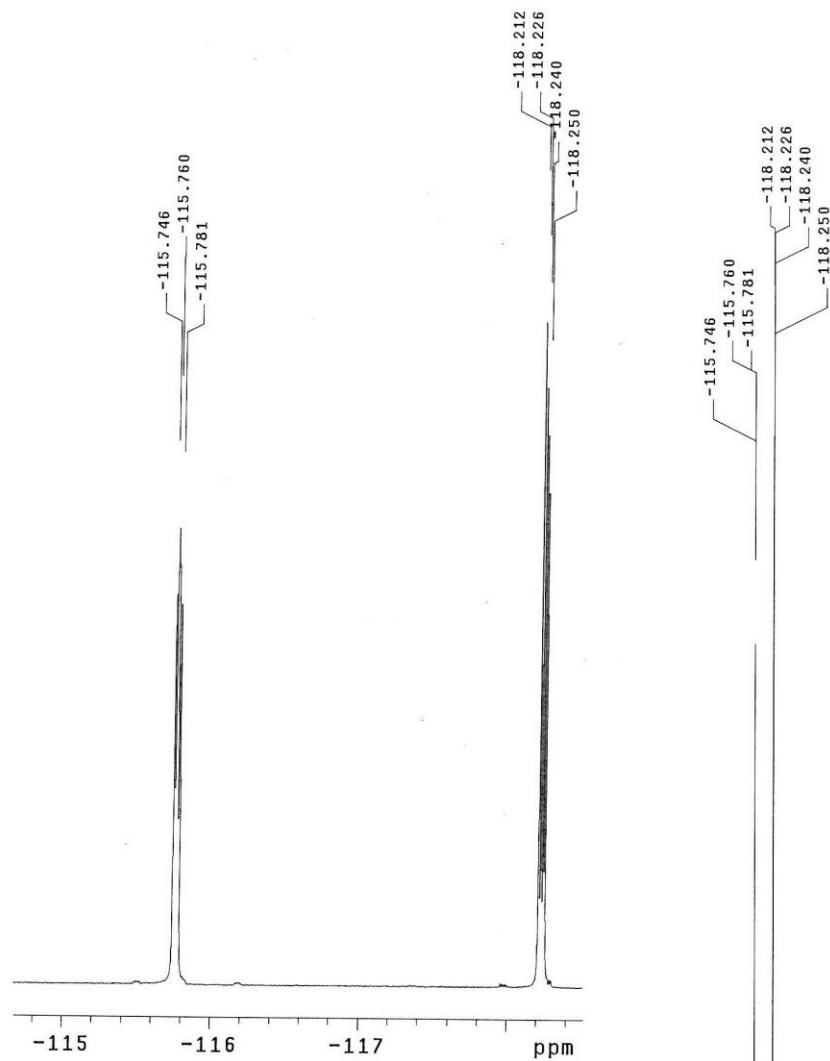
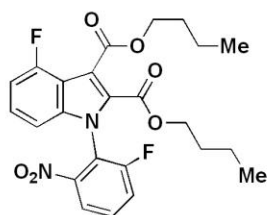
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 25 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 1888 repetitions



Compound 4p (¹⁹F-NMR spectral data)

4p

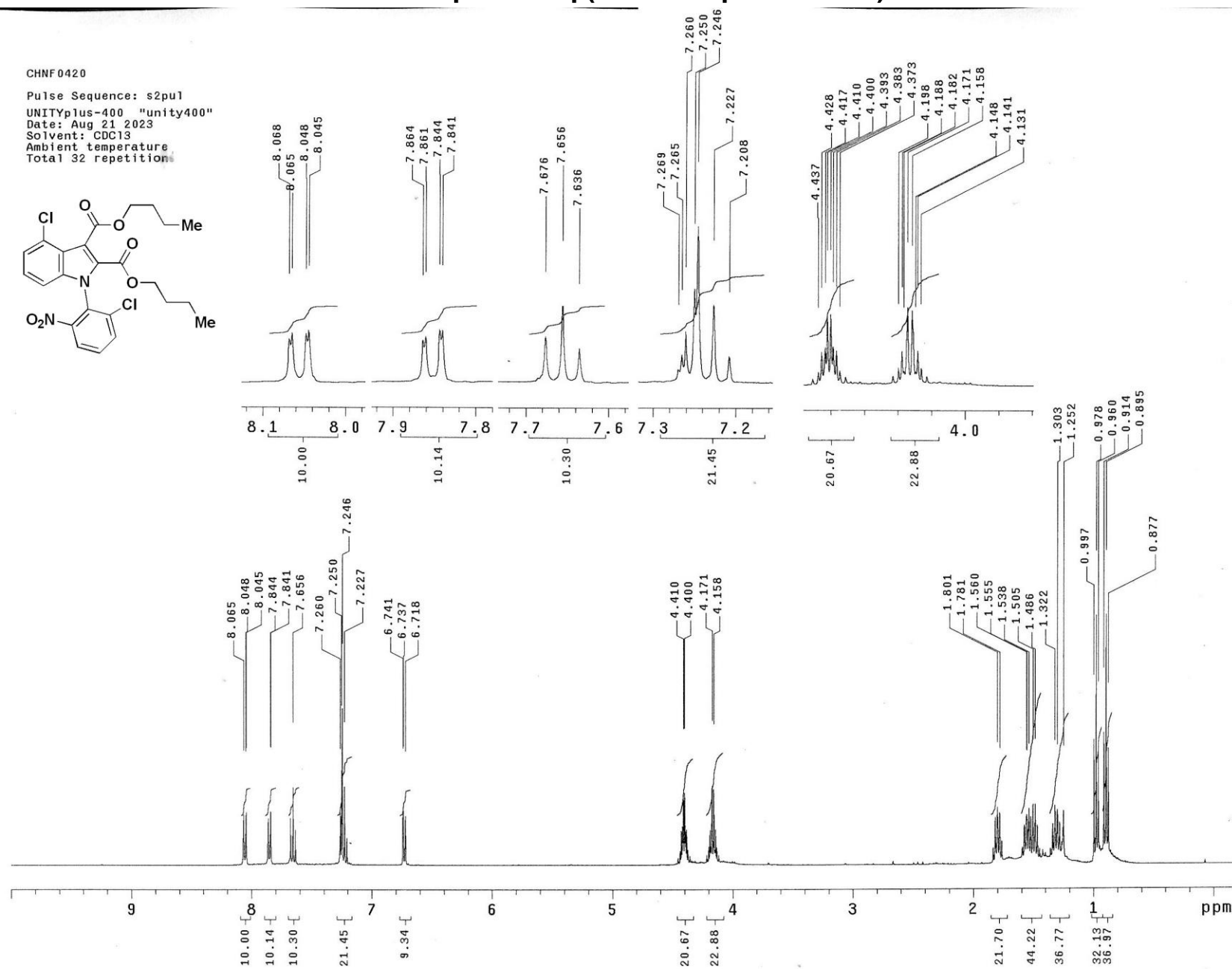
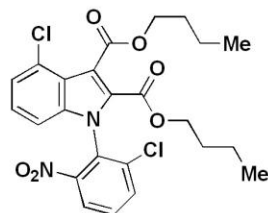
Pulse Sequence: s2pu]
Mercury-400BB "MerPlus400"
Date: Jan 17 2024
Solvent: cdcl3
Ambient temperature
Total 128 repetitions



Compound 4q (¹H-NMR spectral data)

CHNF0420

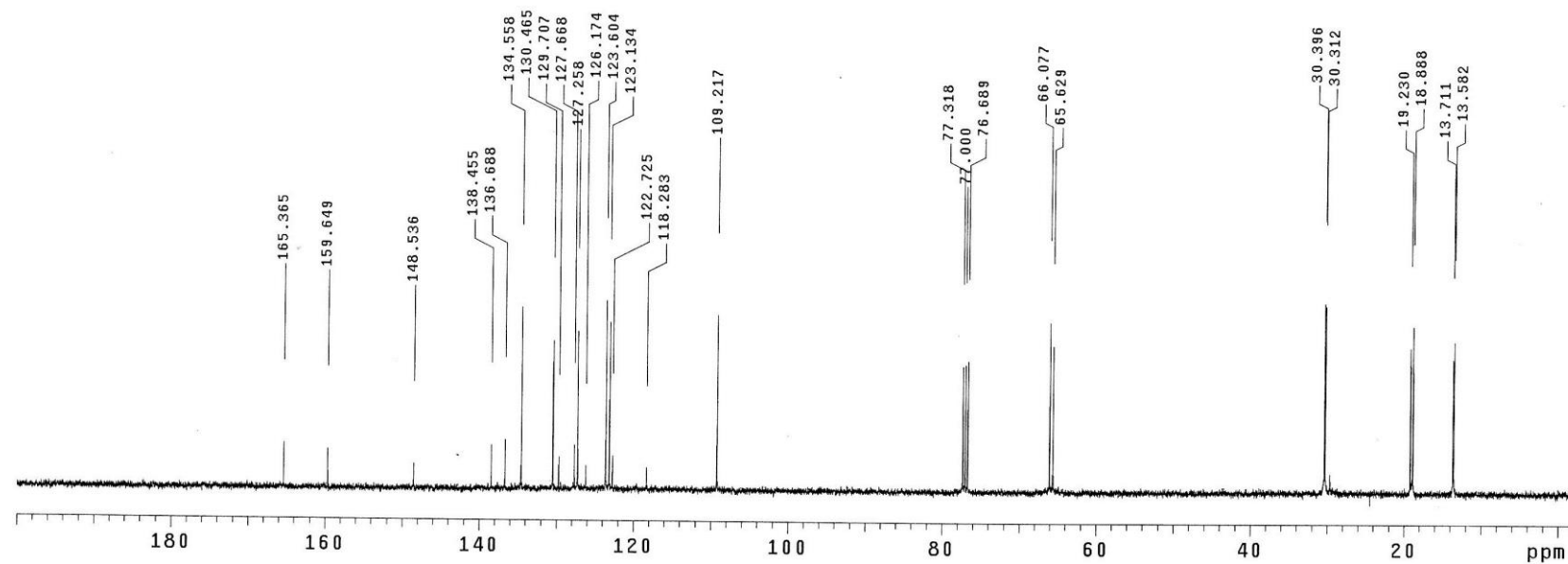
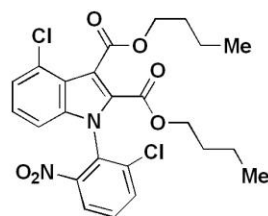
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 21 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetition



Compound 4q (¹³C-NMR spectral data)

CHNF0420

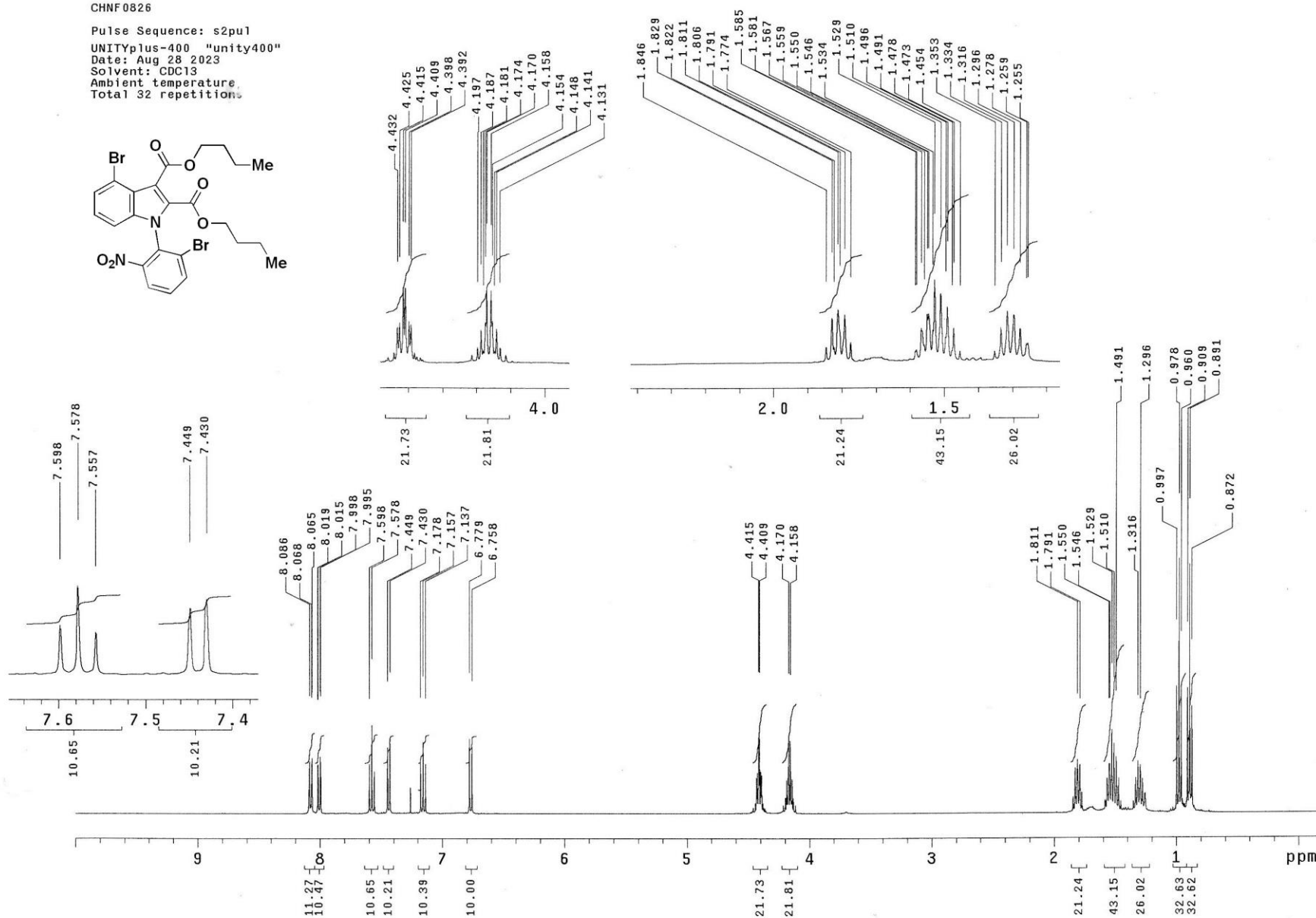
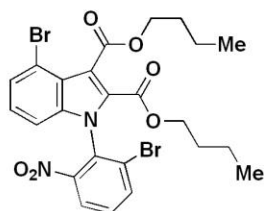
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 21 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 1872 repetitions



Compound 4r (¹H-NMR spectral data)

CHNF0826

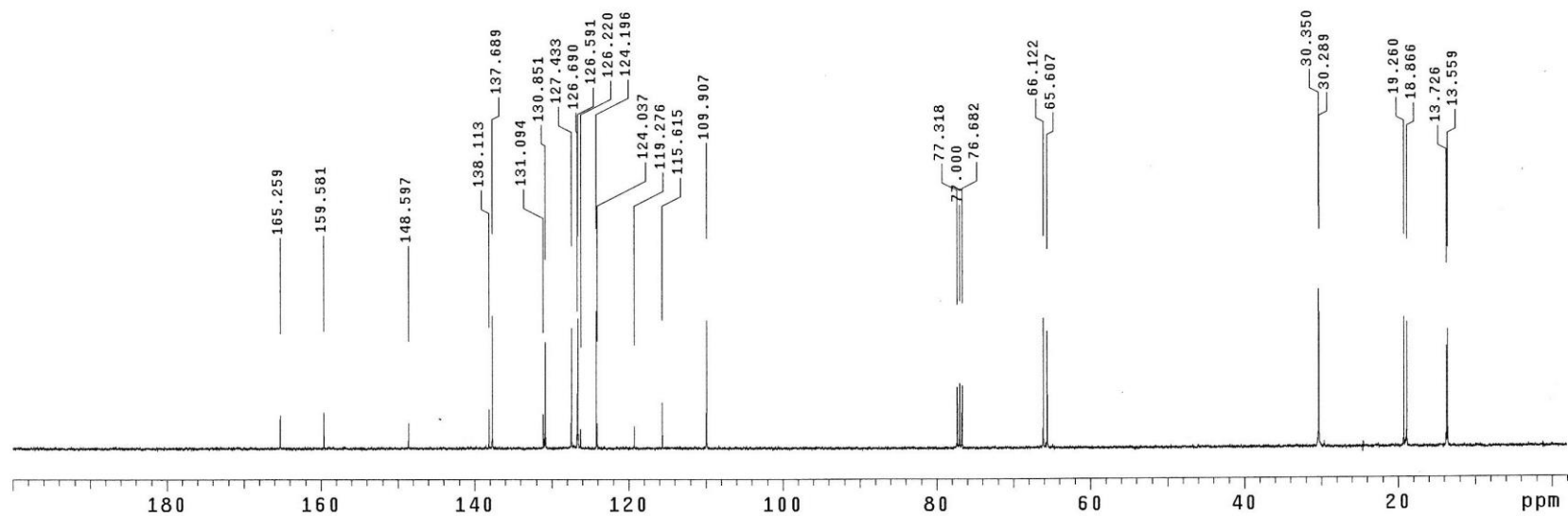
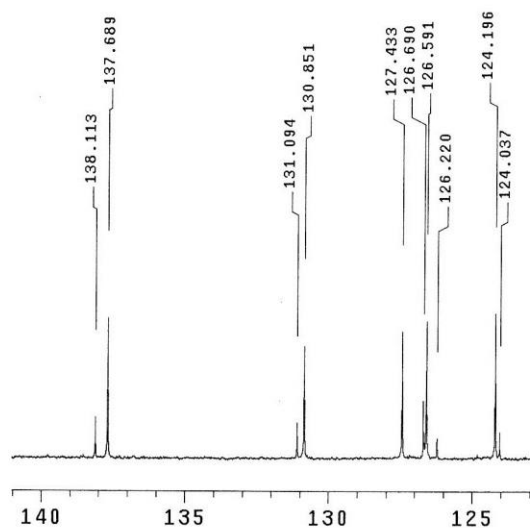
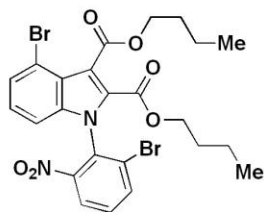
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 28 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4r (¹³C-NMR spectral data)

CHNF0826

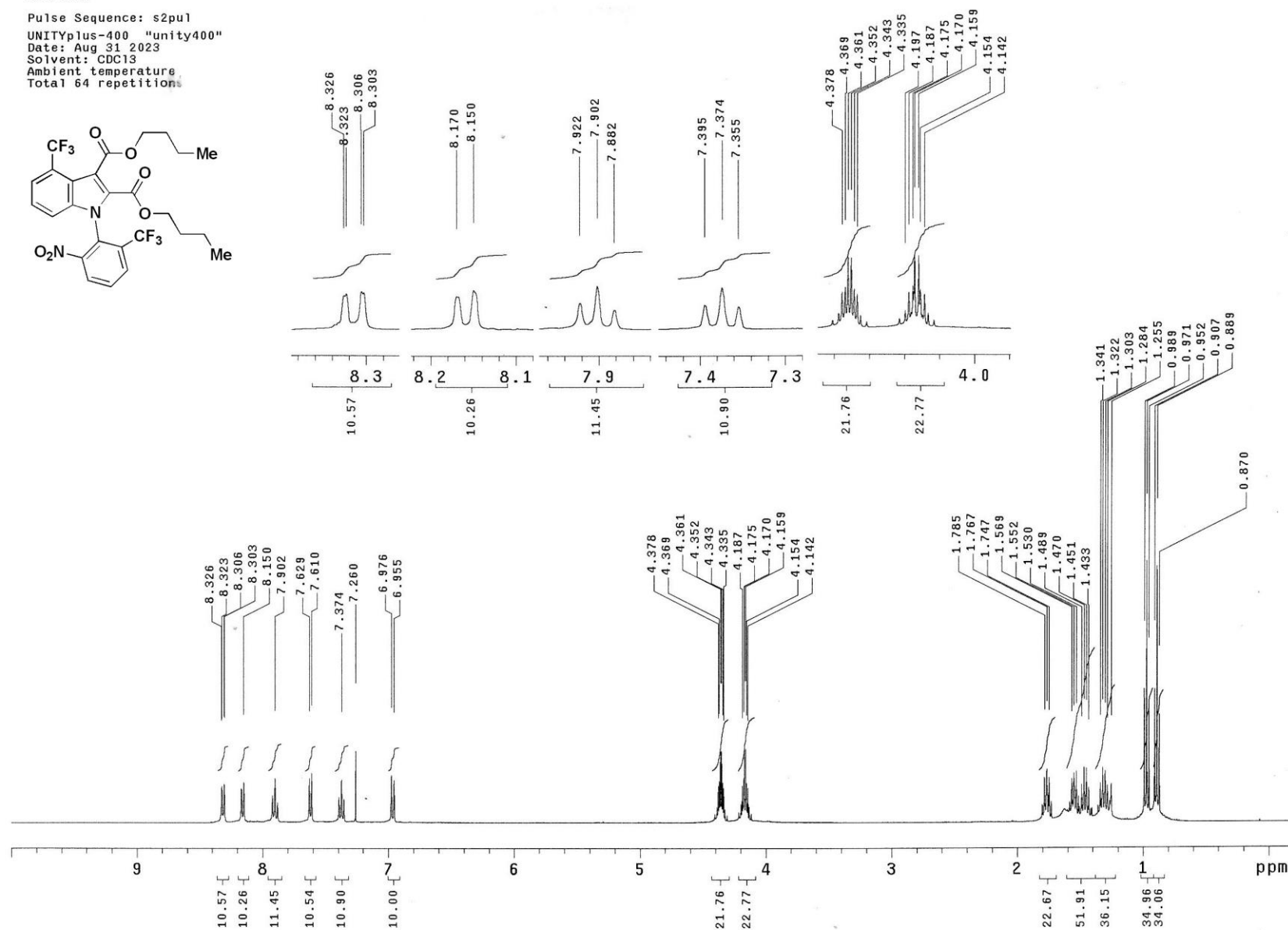
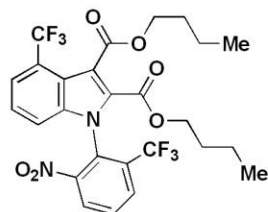
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 28 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 2256 repetitions



Compound 4s (¹H-NMR spectral data)

CHNF0831

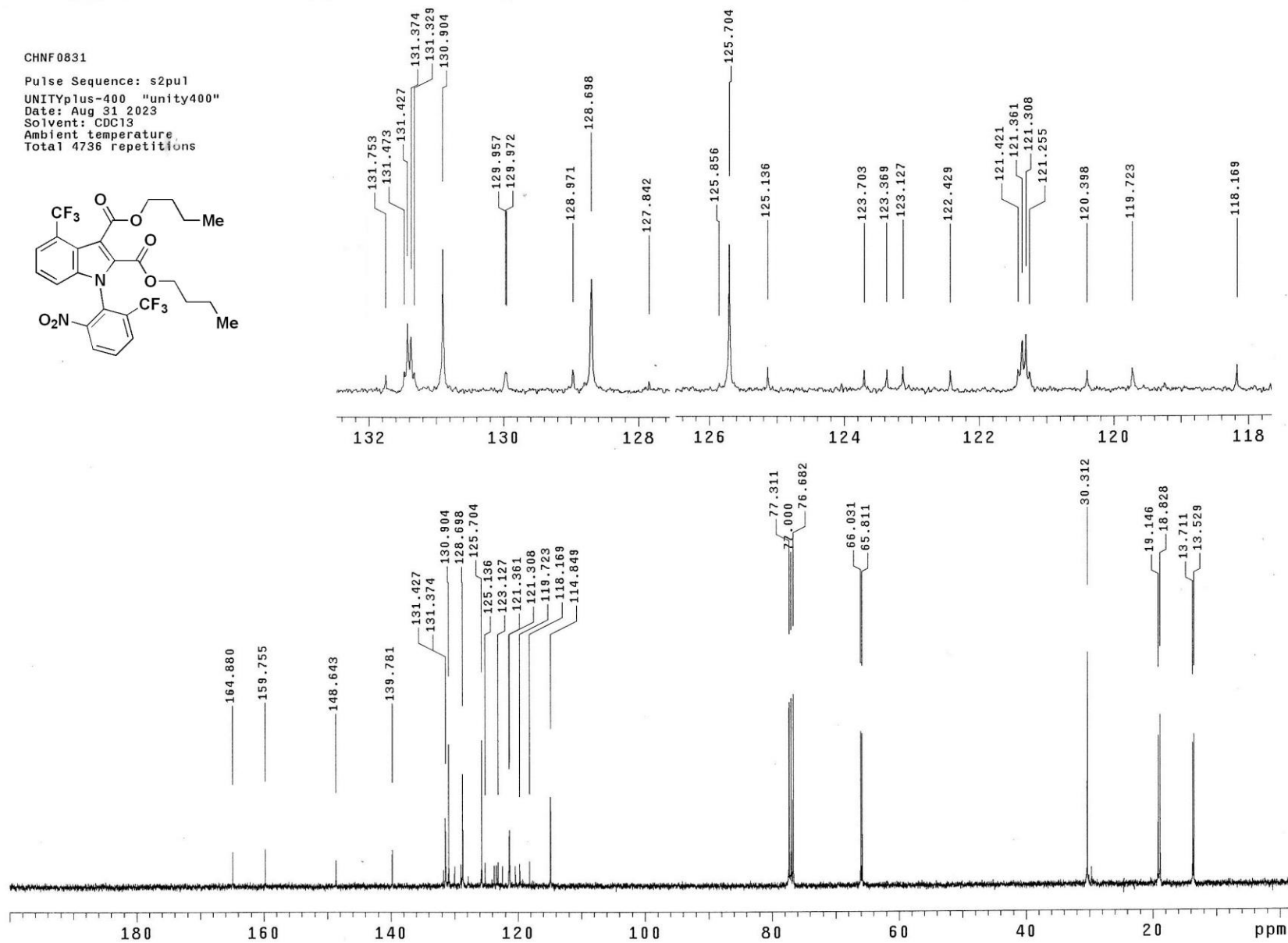
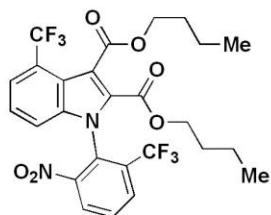
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 31 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 64 repetitions



Compound 4s (¹³C-NMR spectral data)

CHNF0831

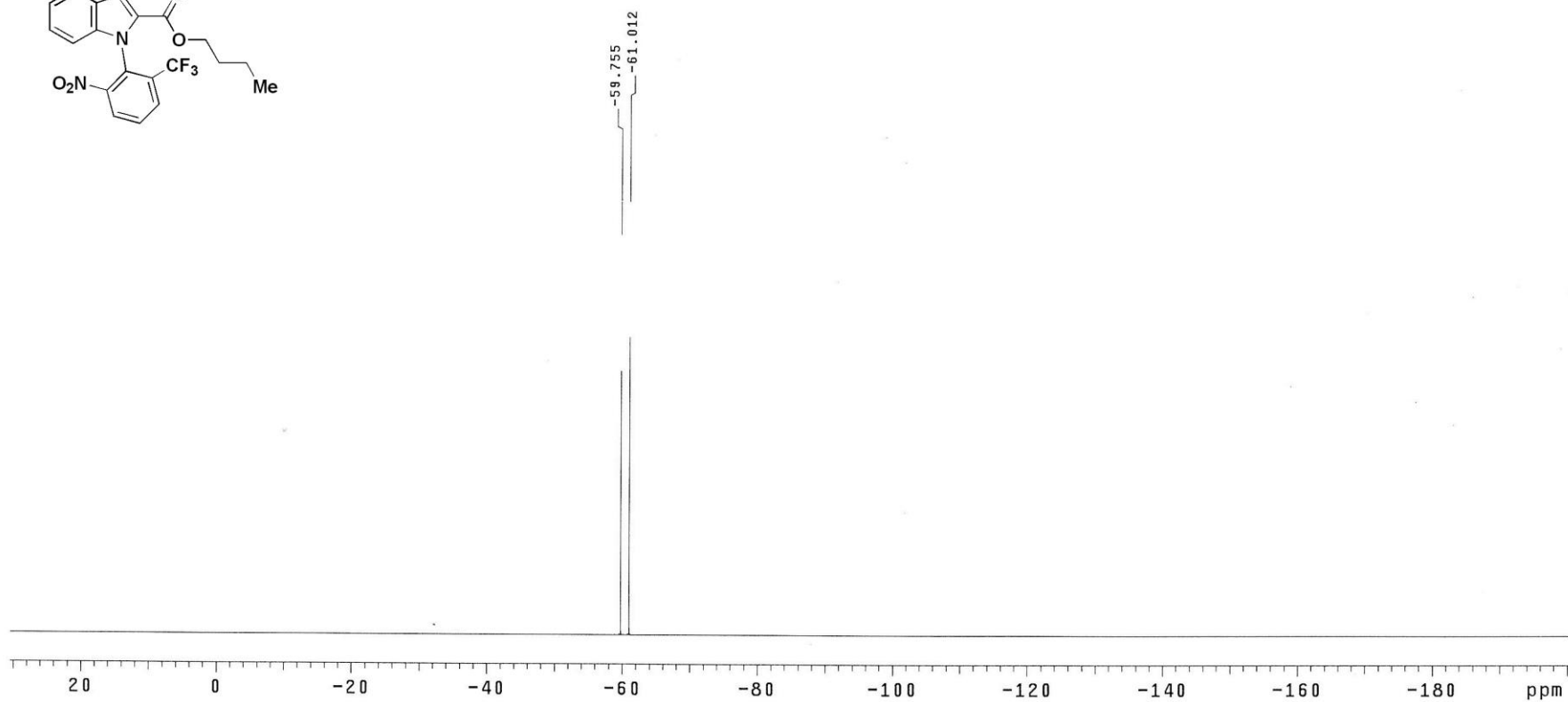
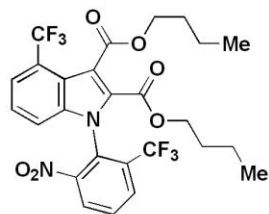
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 31 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 4736 repetitions



Compound 4s (¹⁹F-NMR spectral data)

4s

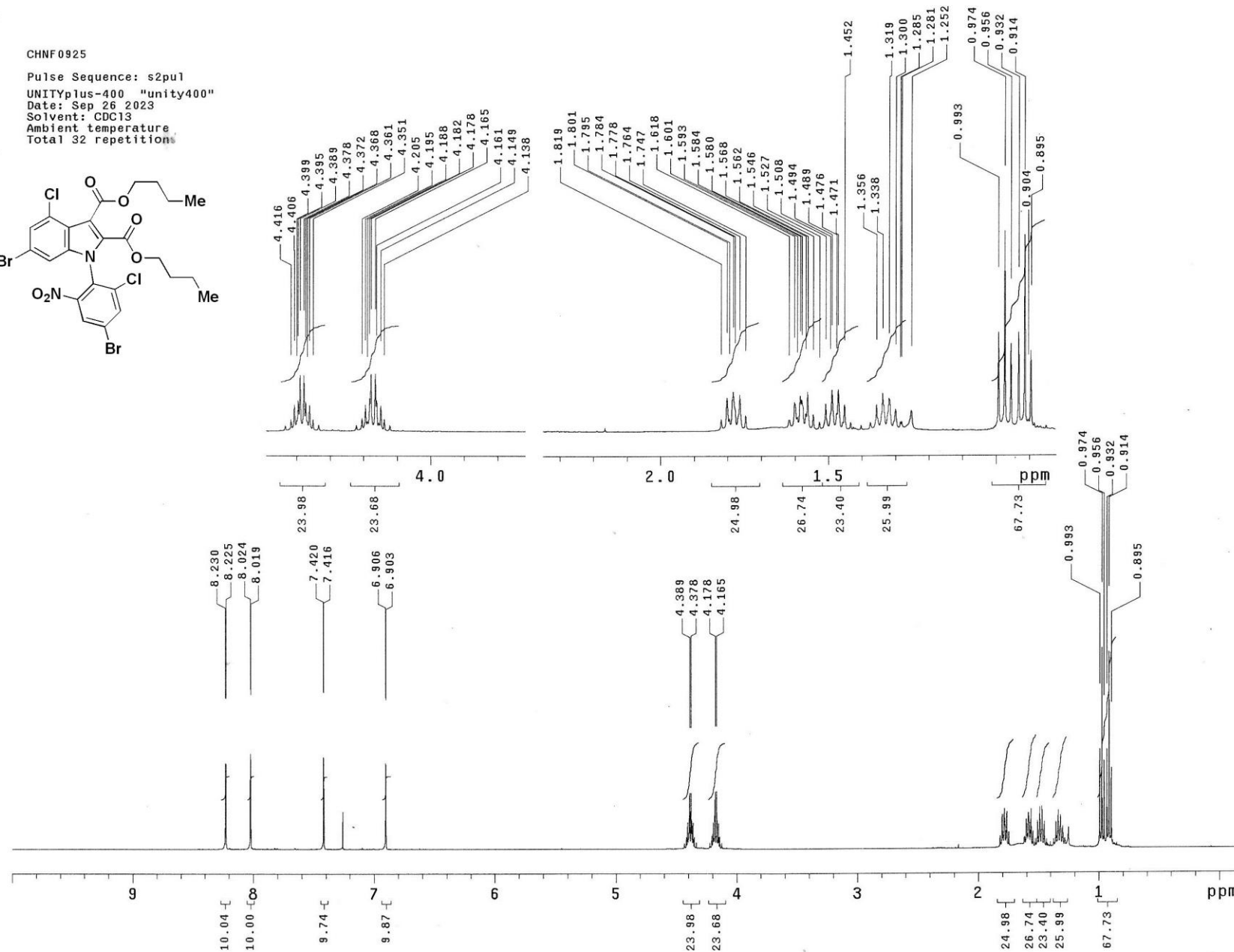
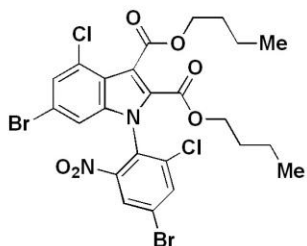
Pulse Sequence: s2pu1
Mercury-400BB "MerPlus400"
Date: Jan 18 2024
Solvent: cdcl3
Ambient temperature
Total 16 repetitions



Compound 4t (¹H-NMR spectral data)

CHNF0925

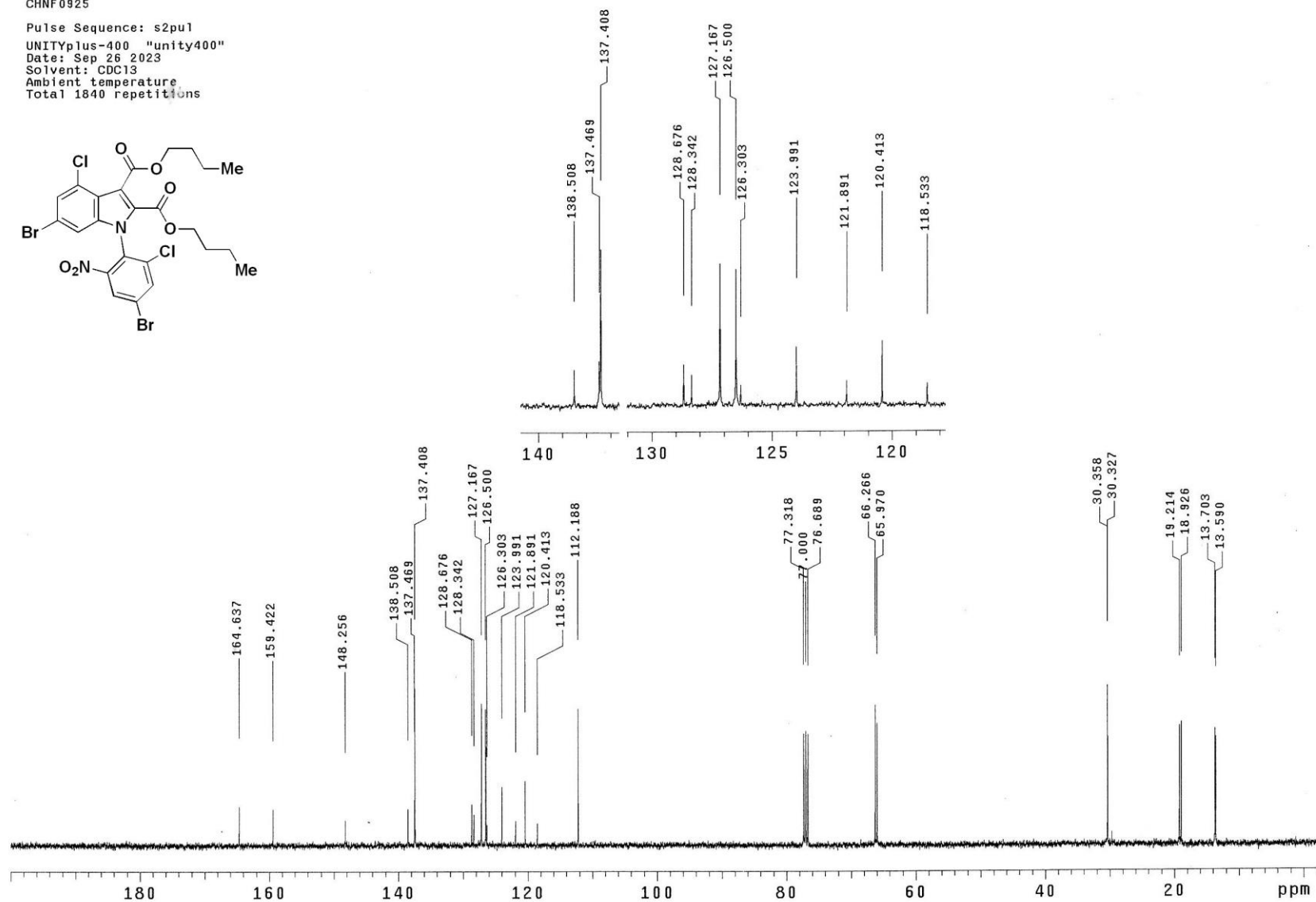
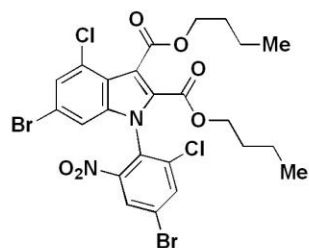
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 26 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4t (¹³C-NMR spectral data)

CHNF0925

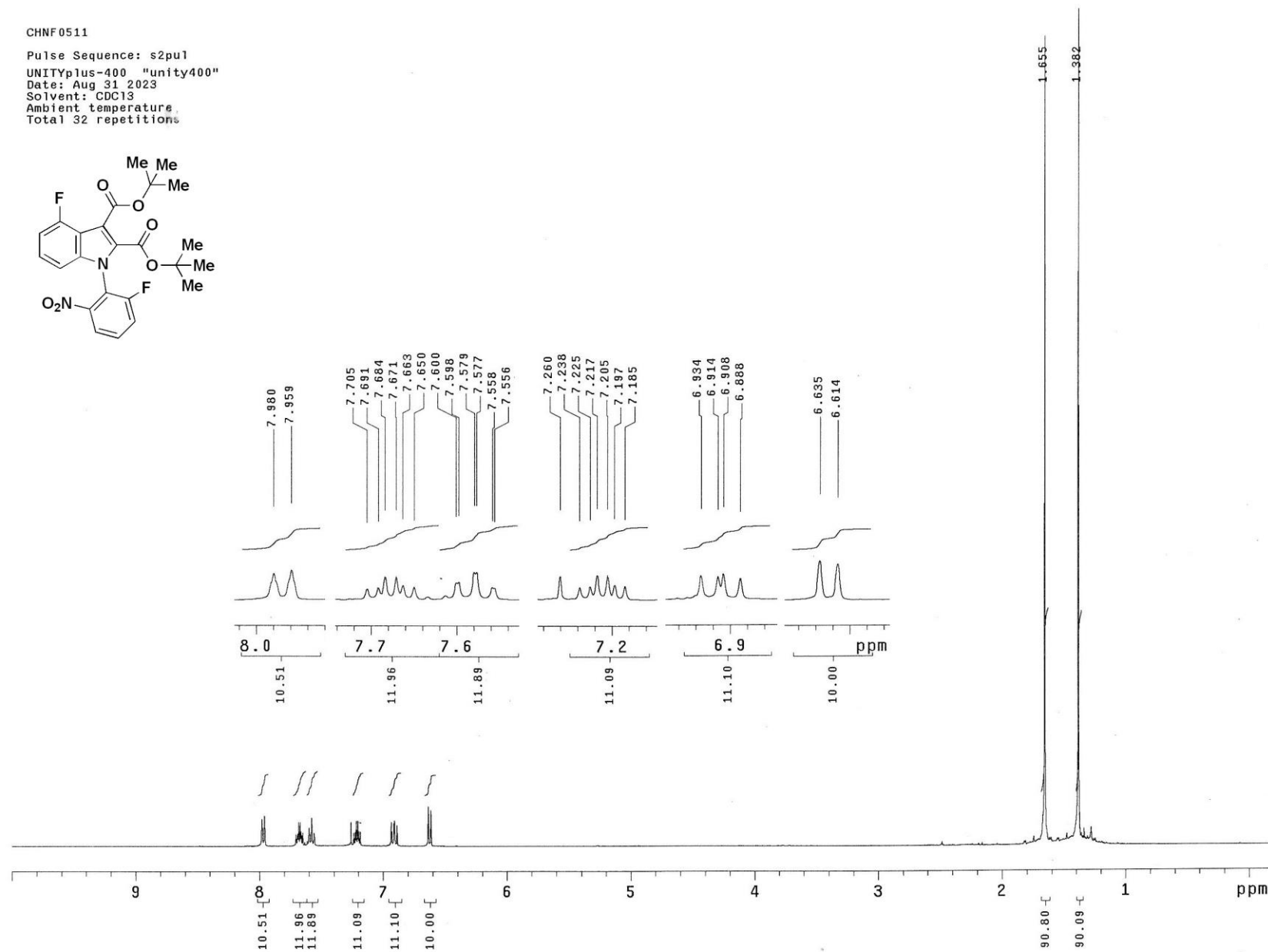
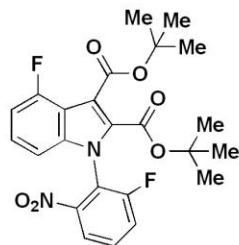
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 26 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 1840 repetitions



Compound 4u (¹H-NMR spectral data)

CHNF0511

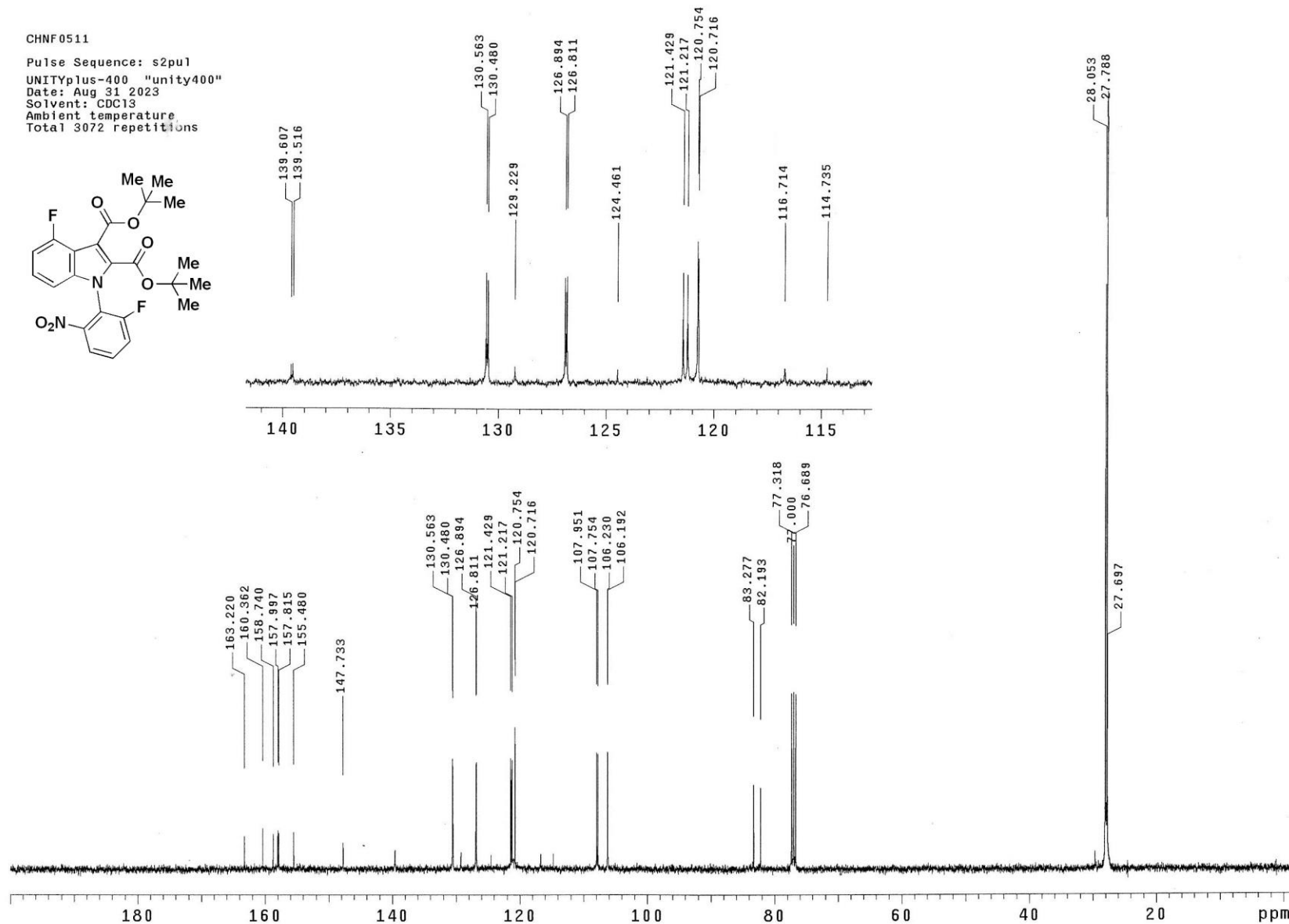
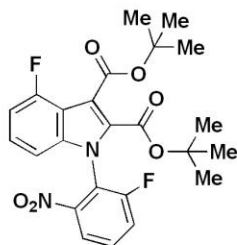
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 31 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4u (¹³C-NMR spectral data)

CHNF0511

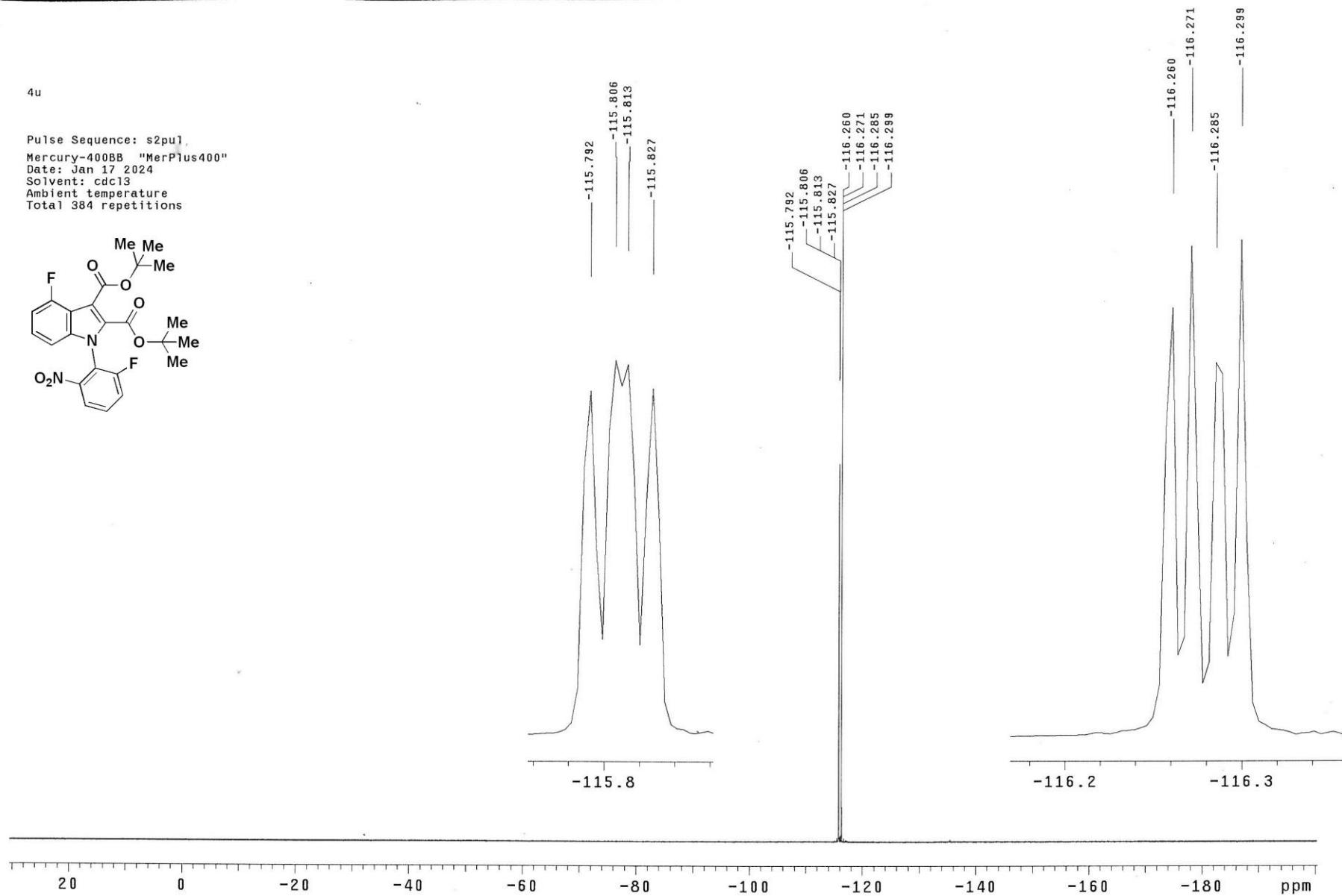
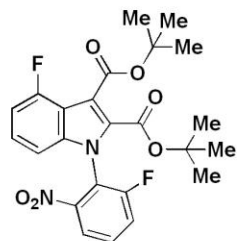
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 31 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 3072 repetitions



Compound 4u (¹⁹F-NMR spectral data)

4u

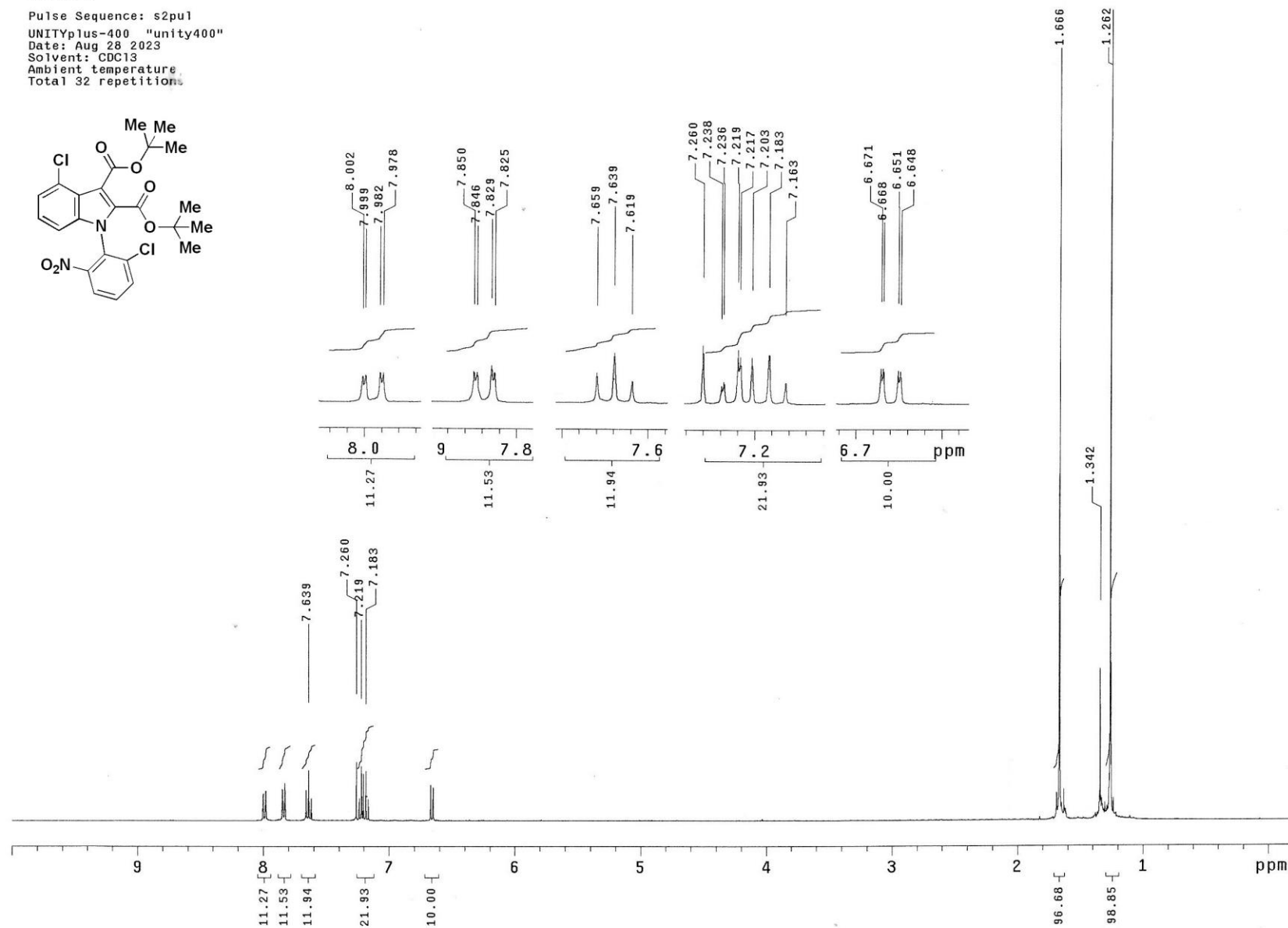
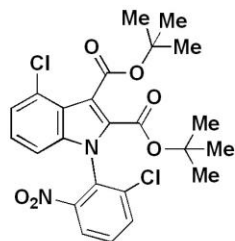
Pulse Sequence: s2pu1,
Mercury-400BB "MerPlus400"
Date: Jan 17 2024
Solvent: cdcl3
Ambient temperature
Total 384 repetitions



Compound 4v (¹H-NMR spectral data)

CHNF0512

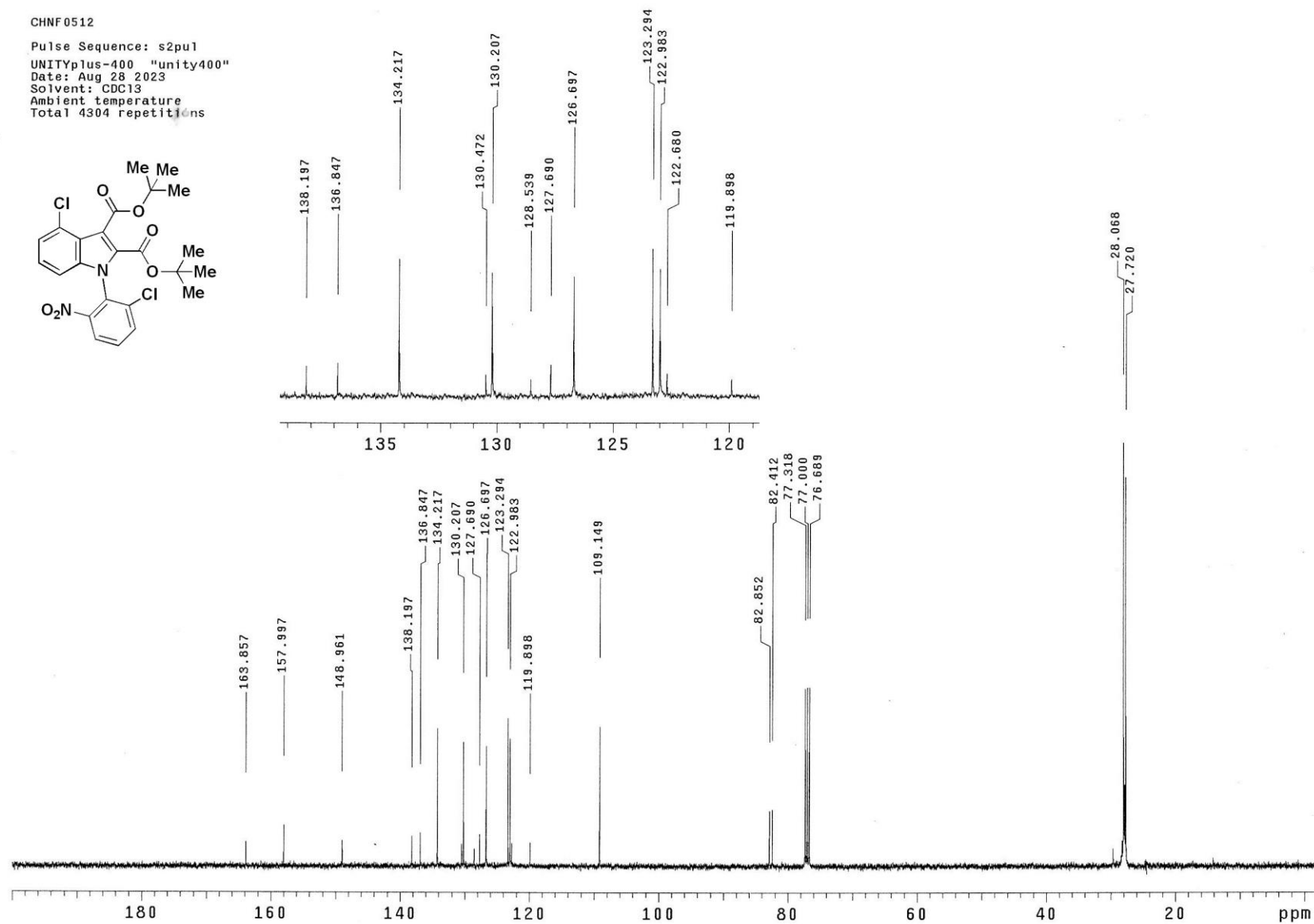
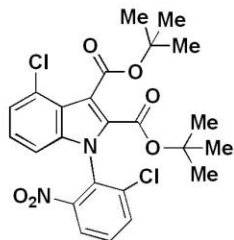
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 28 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4v (¹³C-NMR spectral data)

CHNF0512

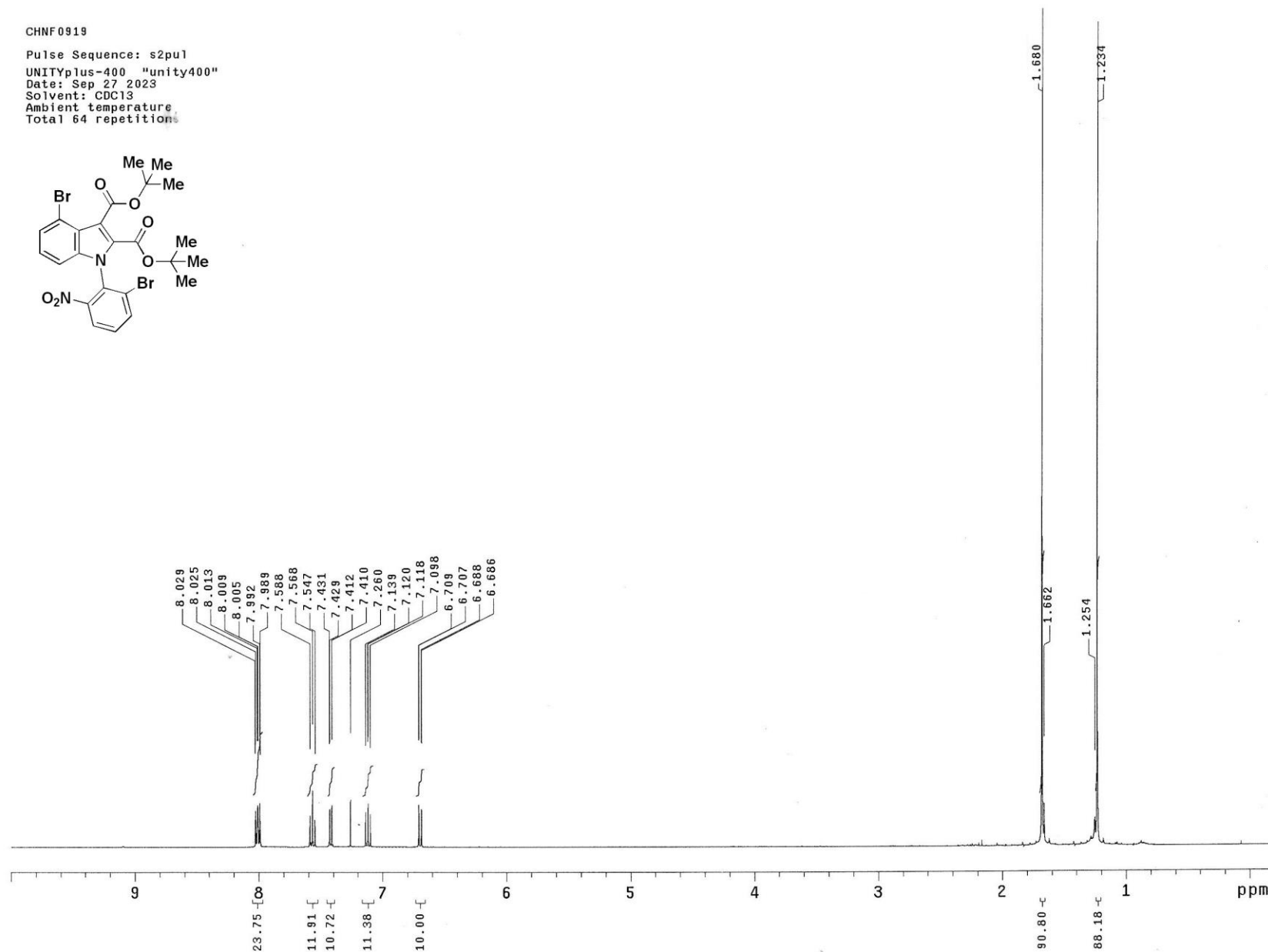
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 28 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 4304 repetitions



Compound 4w (¹H-NMR spectral data)

CHNF0919

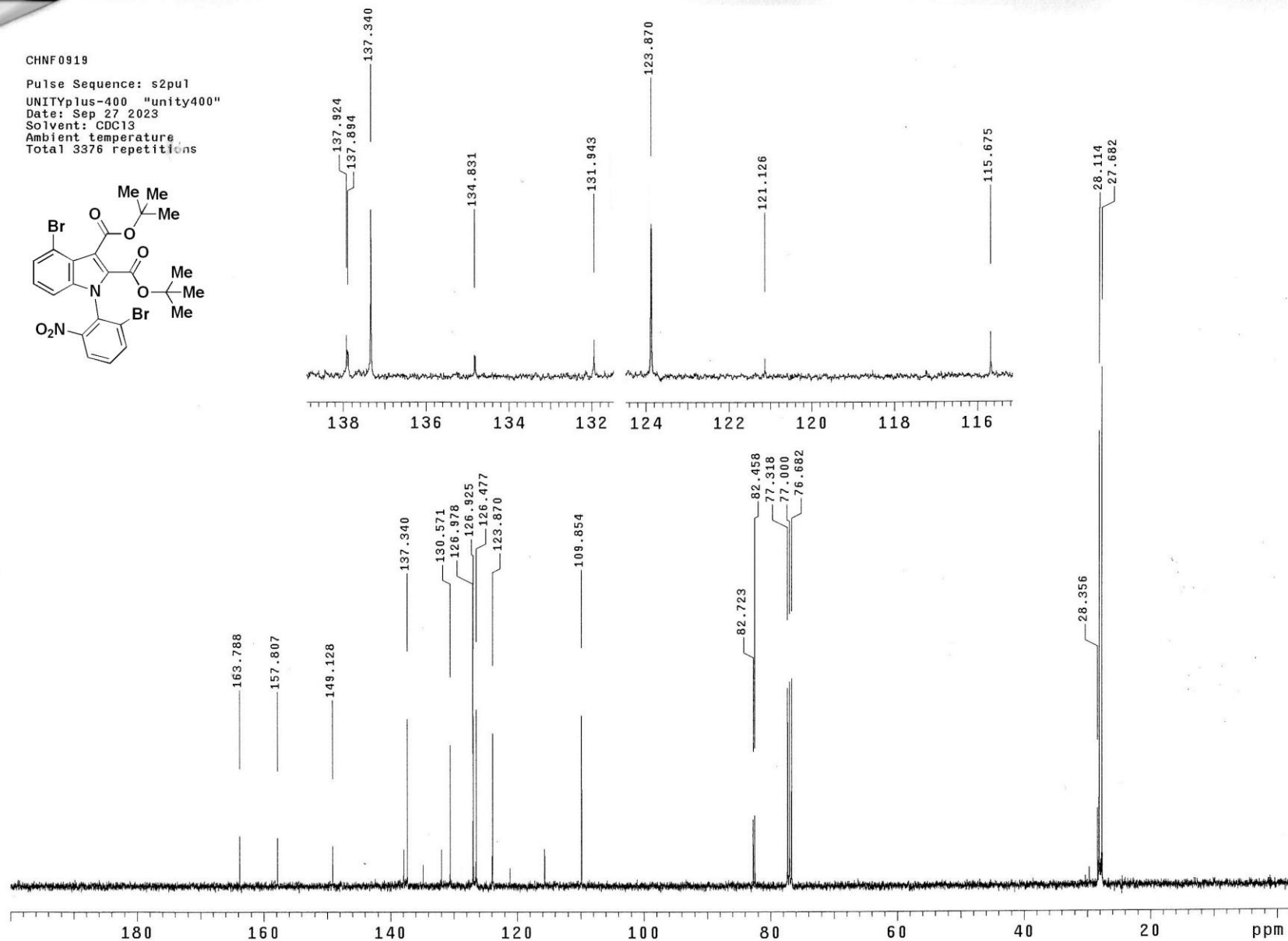
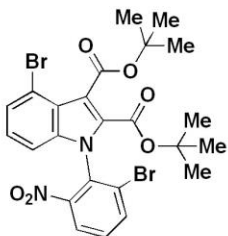
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 27 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 64 repetitions



Compound 4w (¹³C-NMR spectral data)

CHNF0919

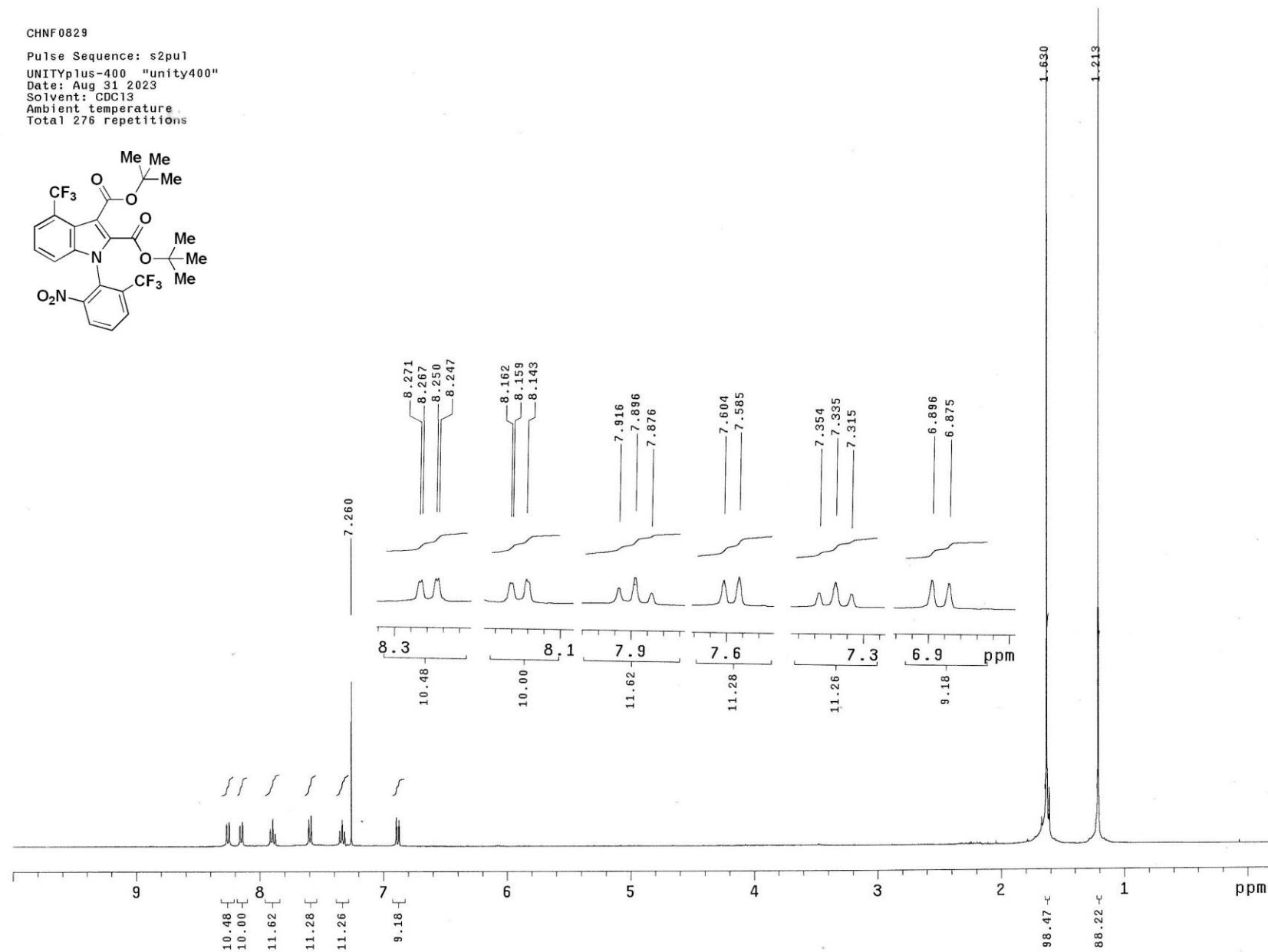
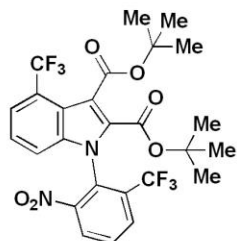
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 27 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 3376 repetitions



Compound 4x (¹H-NMR spectral data)

CHNF0829

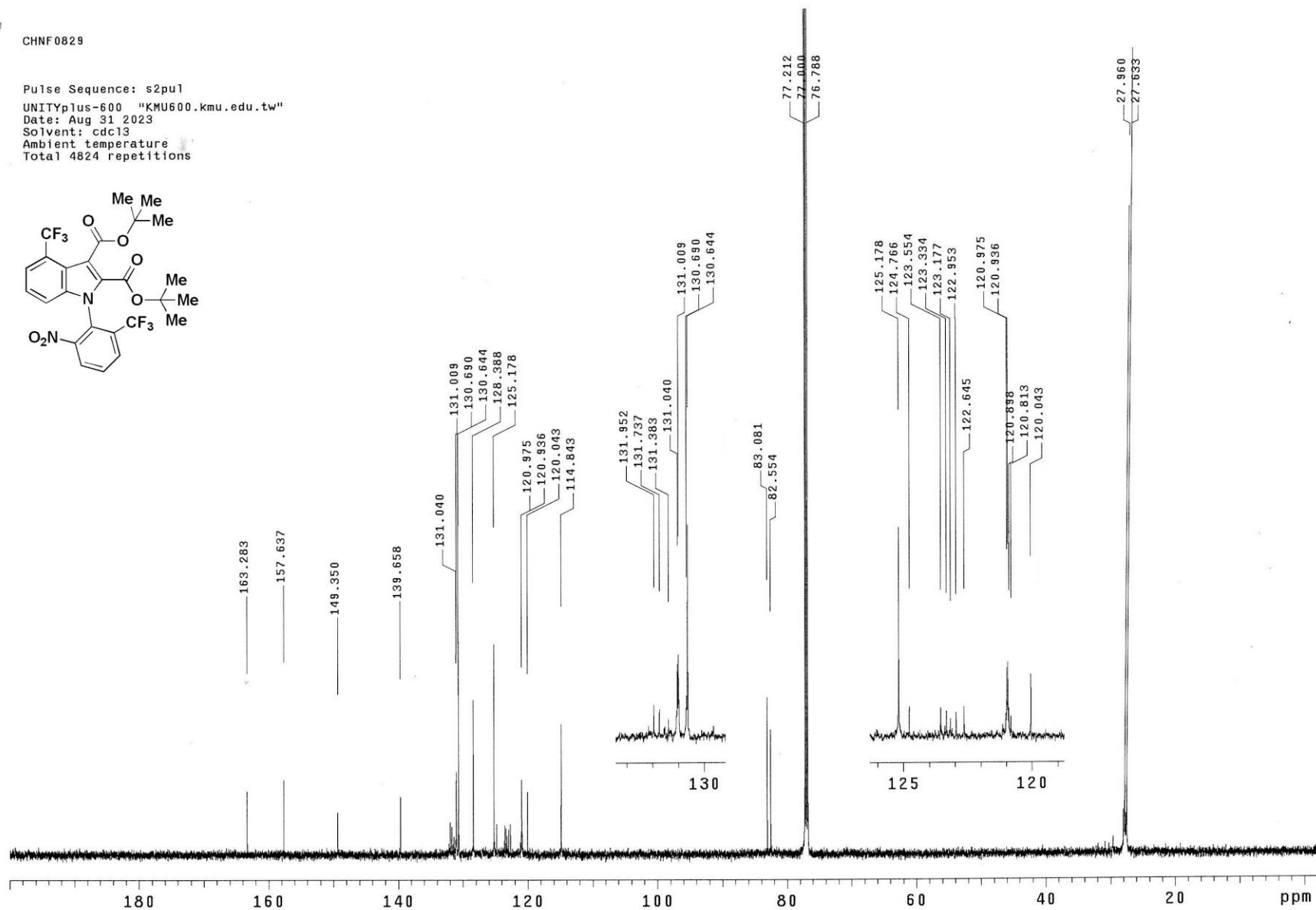
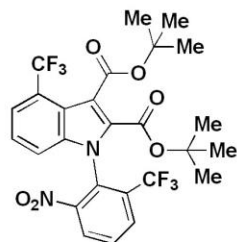
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 31 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 276 repetitions



Compound 4x (¹³C-NMR spectral data)

CHNF0829

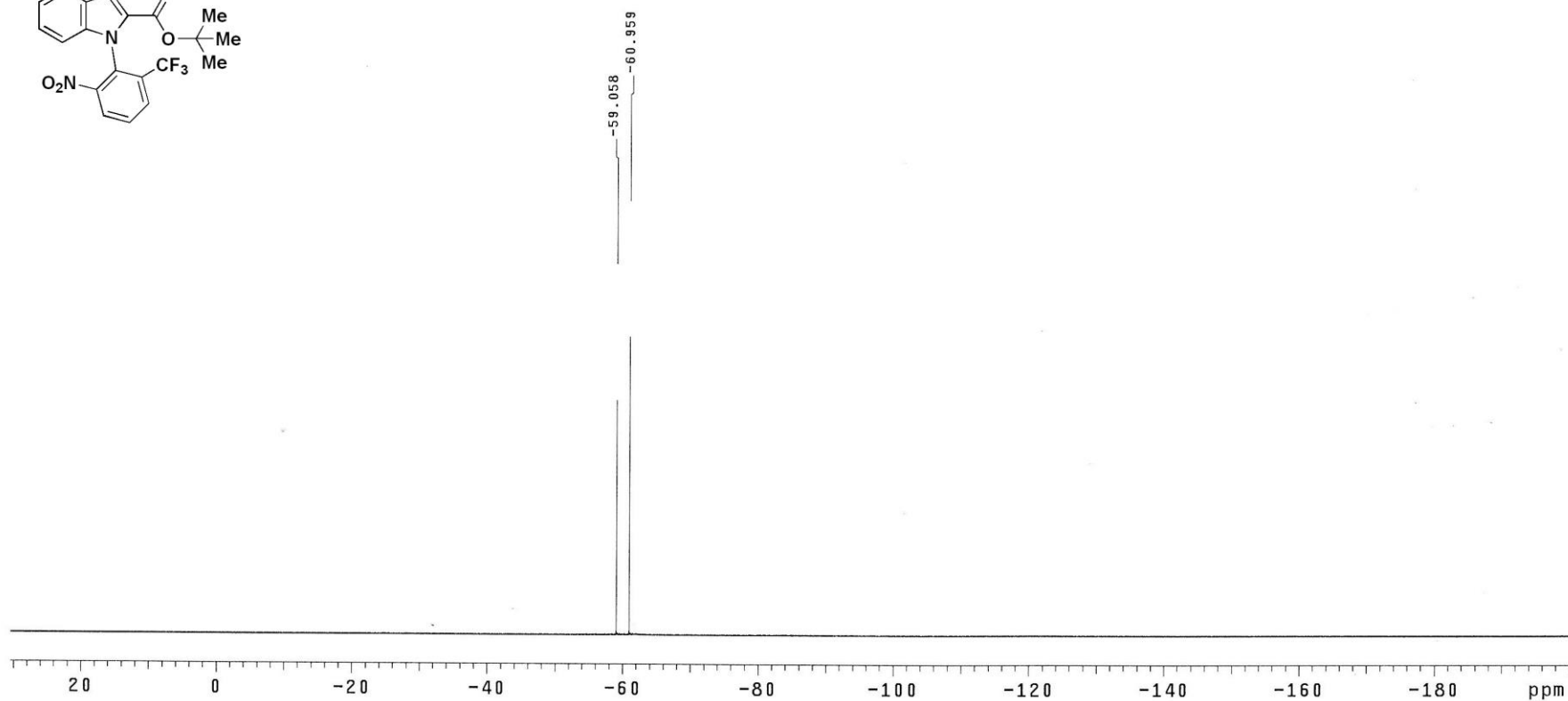
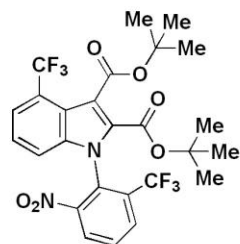
Pulse Sequence: s2pul
 UNITYplus-600 "KMU600.kmu.edu.tw"
 Date: Aug 31 2023
 Solvent: cdc13
 Ambient temperature
 Total 4824 repetitions



Compound 4x (¹⁹F-NMR spectral data)

4x

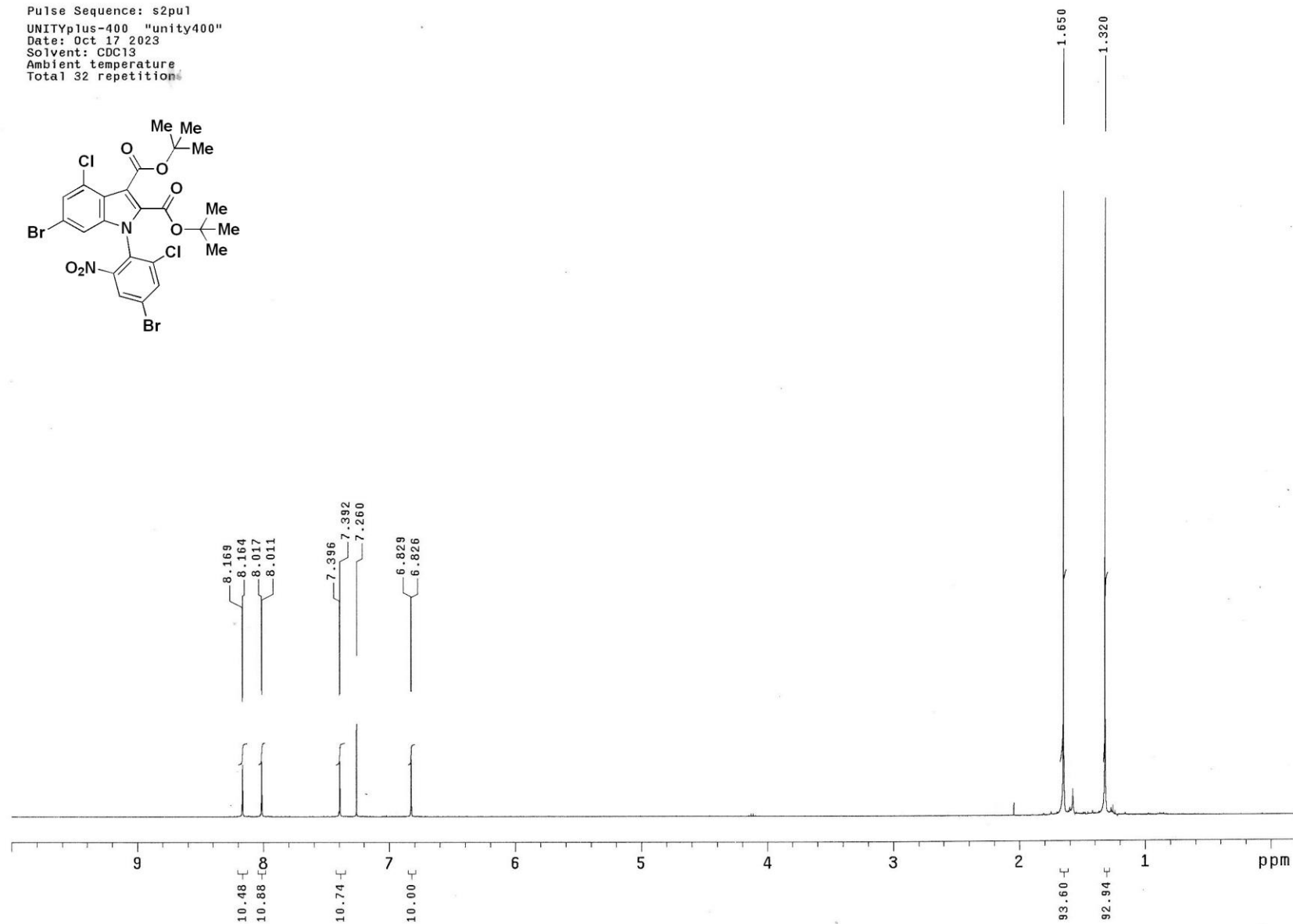
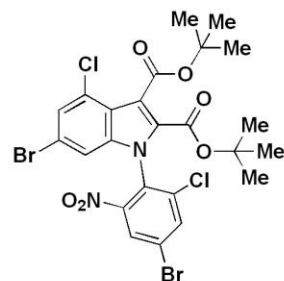
Pulse Sequence: s2pu1.
Mercury-400BB "MerPlus400"
Date: Jan 18 2024
Solvent: cdc13
Ambient temperature
Total 16 repetitions



Compound 4y (¹H-NMR spectral data)

CHNF0909

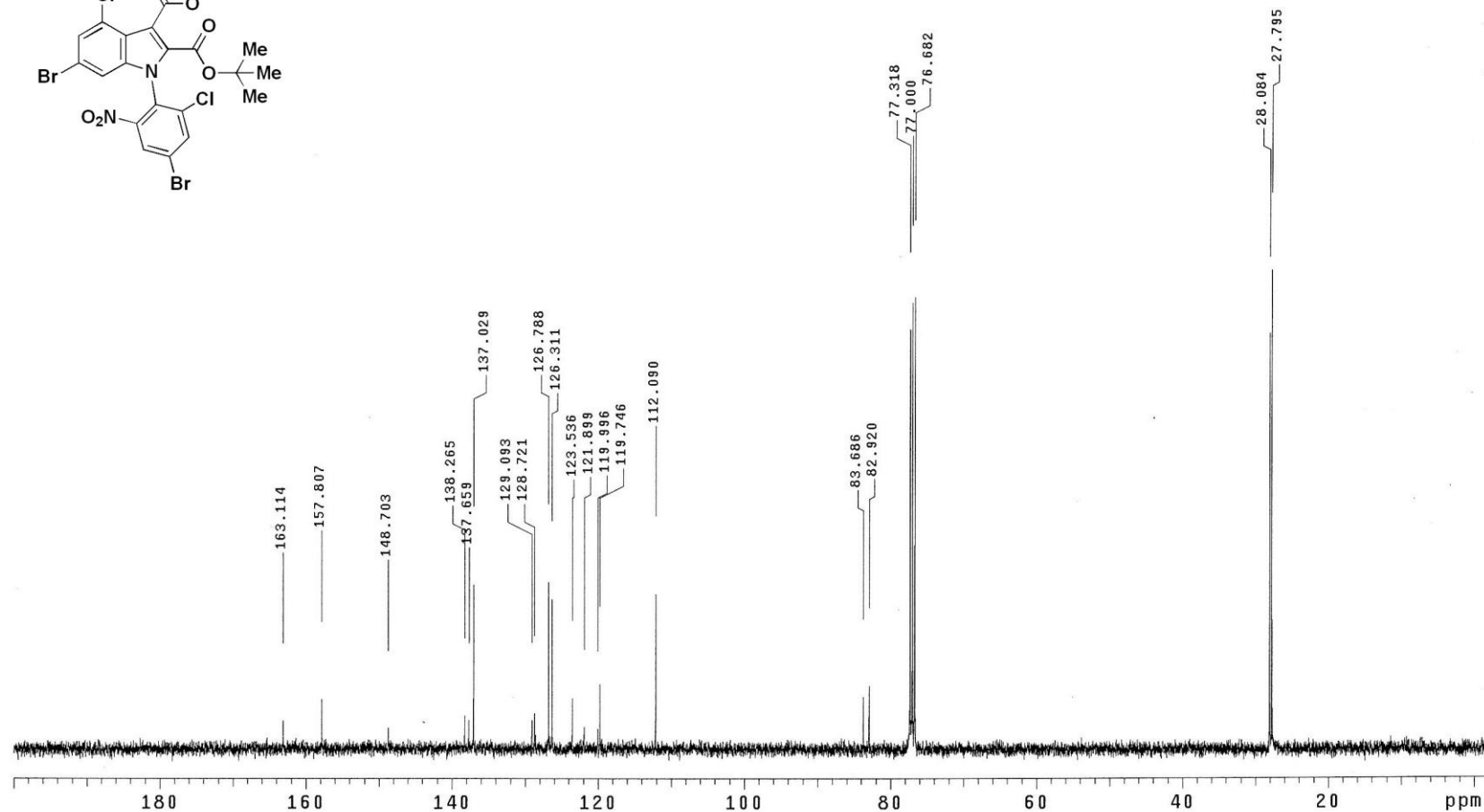
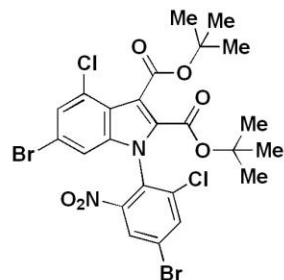
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Oct 17 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetition



Compound 4y (¹³C-NMR spectral data)

CHNF0909

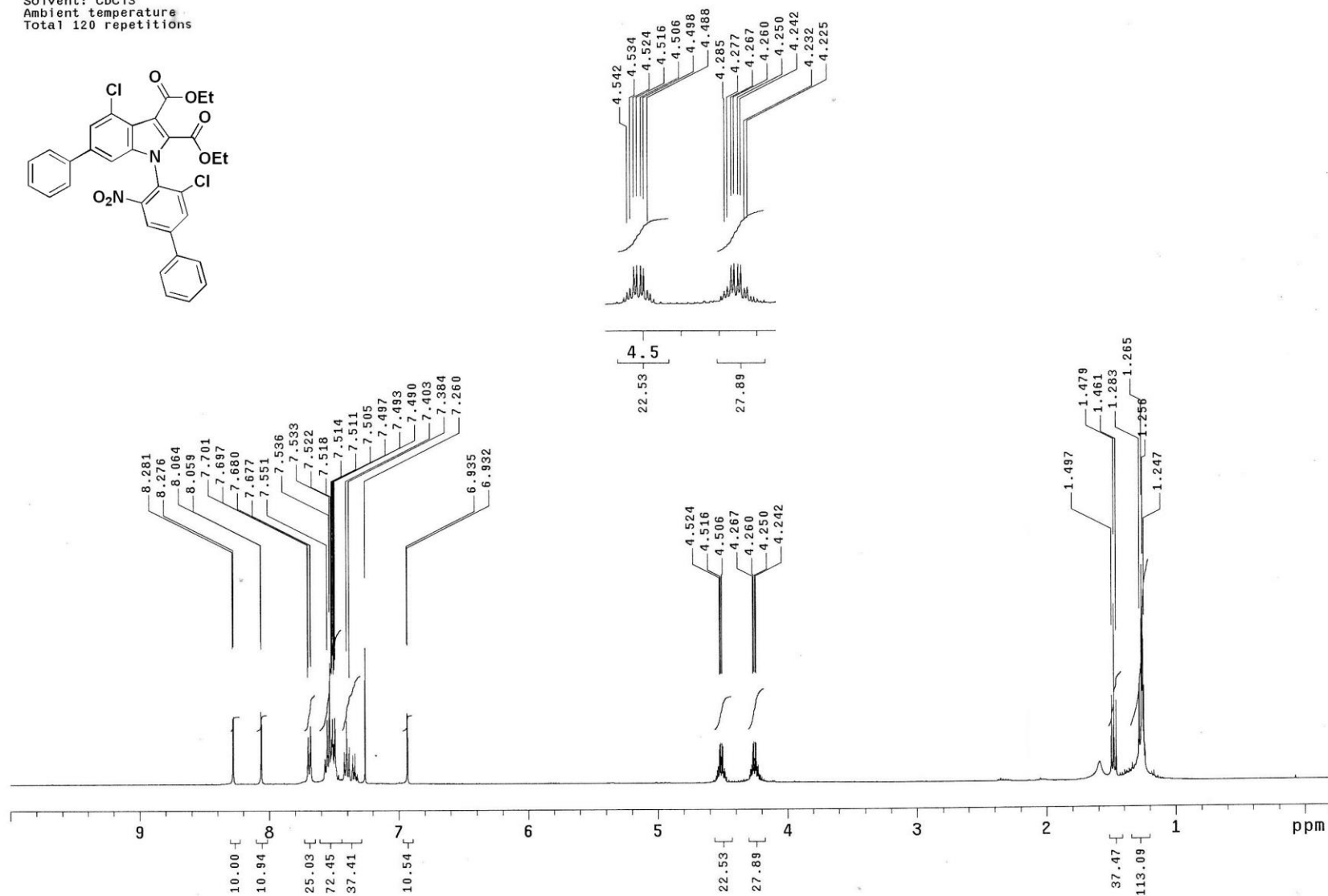
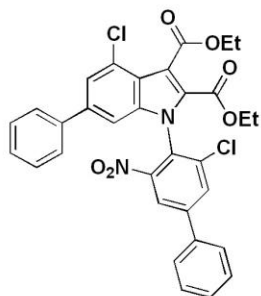
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Oct 17 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 7504 repetitions



Compound 4z (¹H-NMR spectral data)

CHNF0714

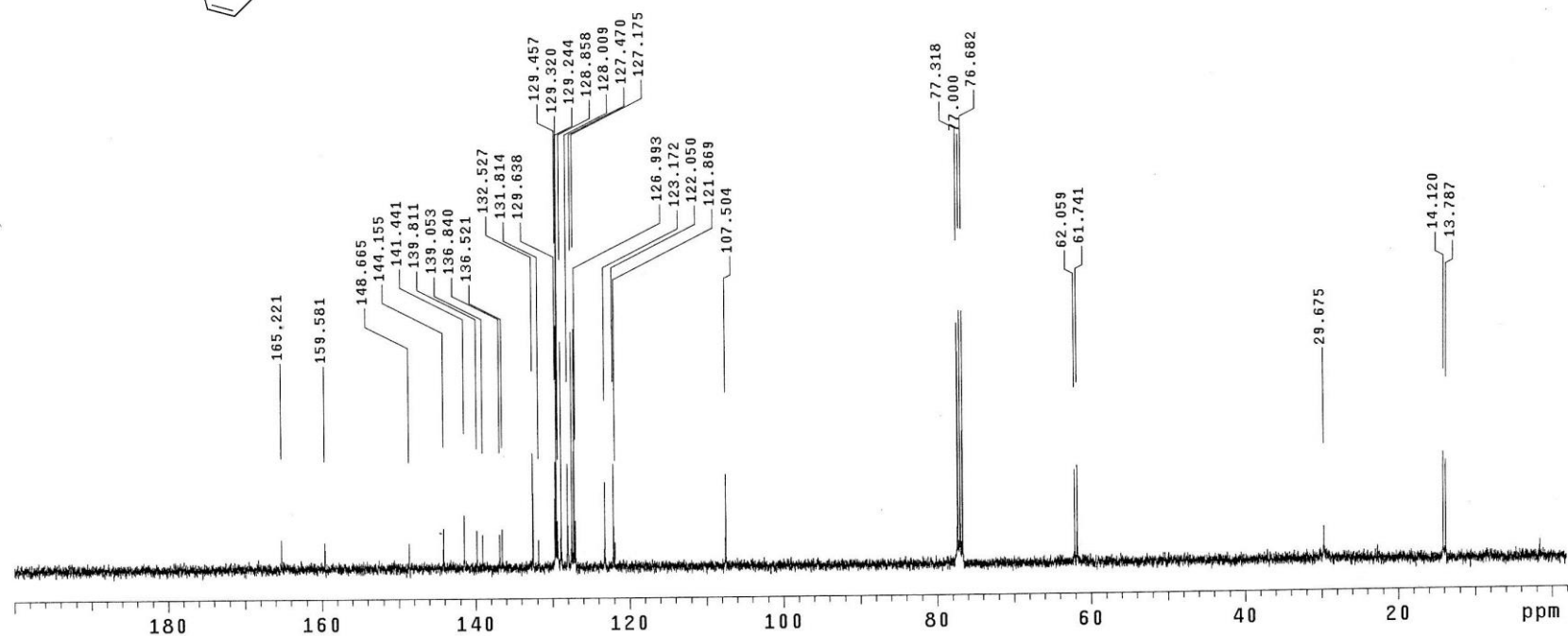
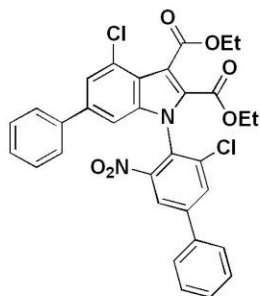
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jul 17 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 120 repetitions



Compound 4z (¹³C-NMR spectral data)

CHNF0714

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jul 17 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 4608 repetitions



Compound 4aa (¹H-NMR spectral data)

CHNF0718

Pulse Sequence: s2pu1

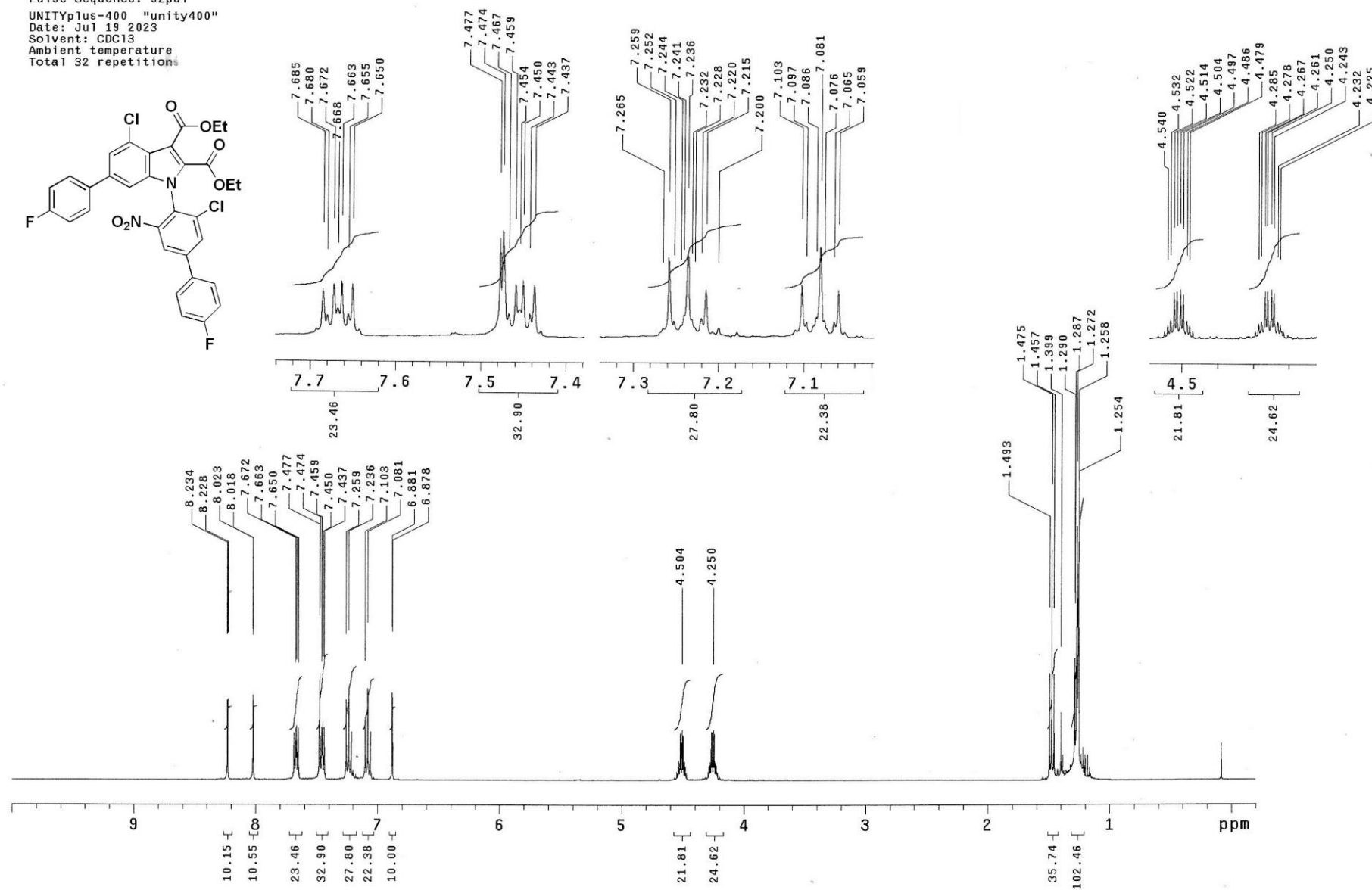
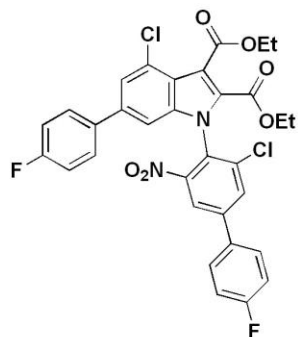
UNITYplus-400 "unity400"

Date: Jul 19 2023

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 4aa (¹³C-NMR spectral data)

CHNF0718

Pulse Sequence: s2pu1

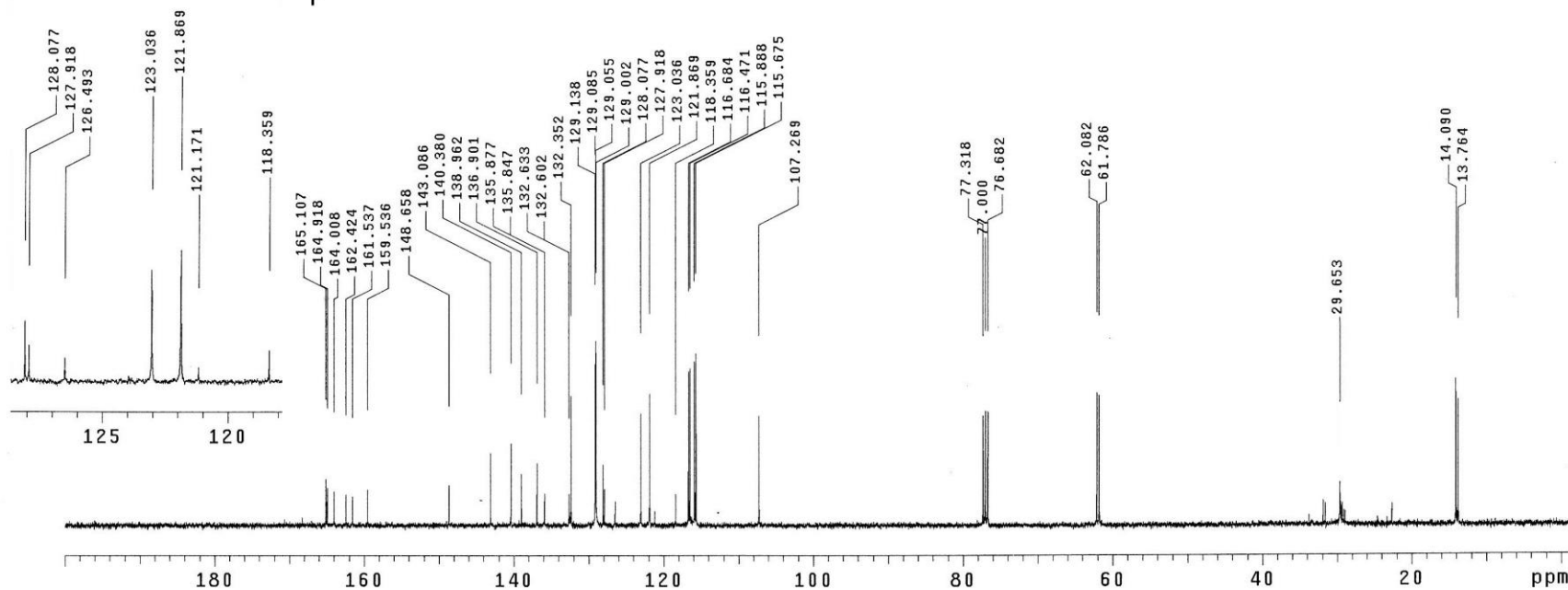
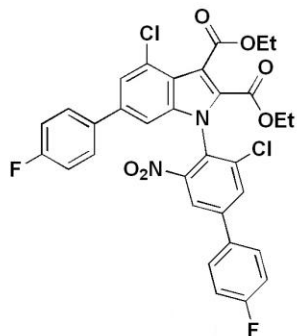
UNITYplus-400 "unity400"

Date: Jul 19 2023

Solvent: CDCl₃

Ambient temperature

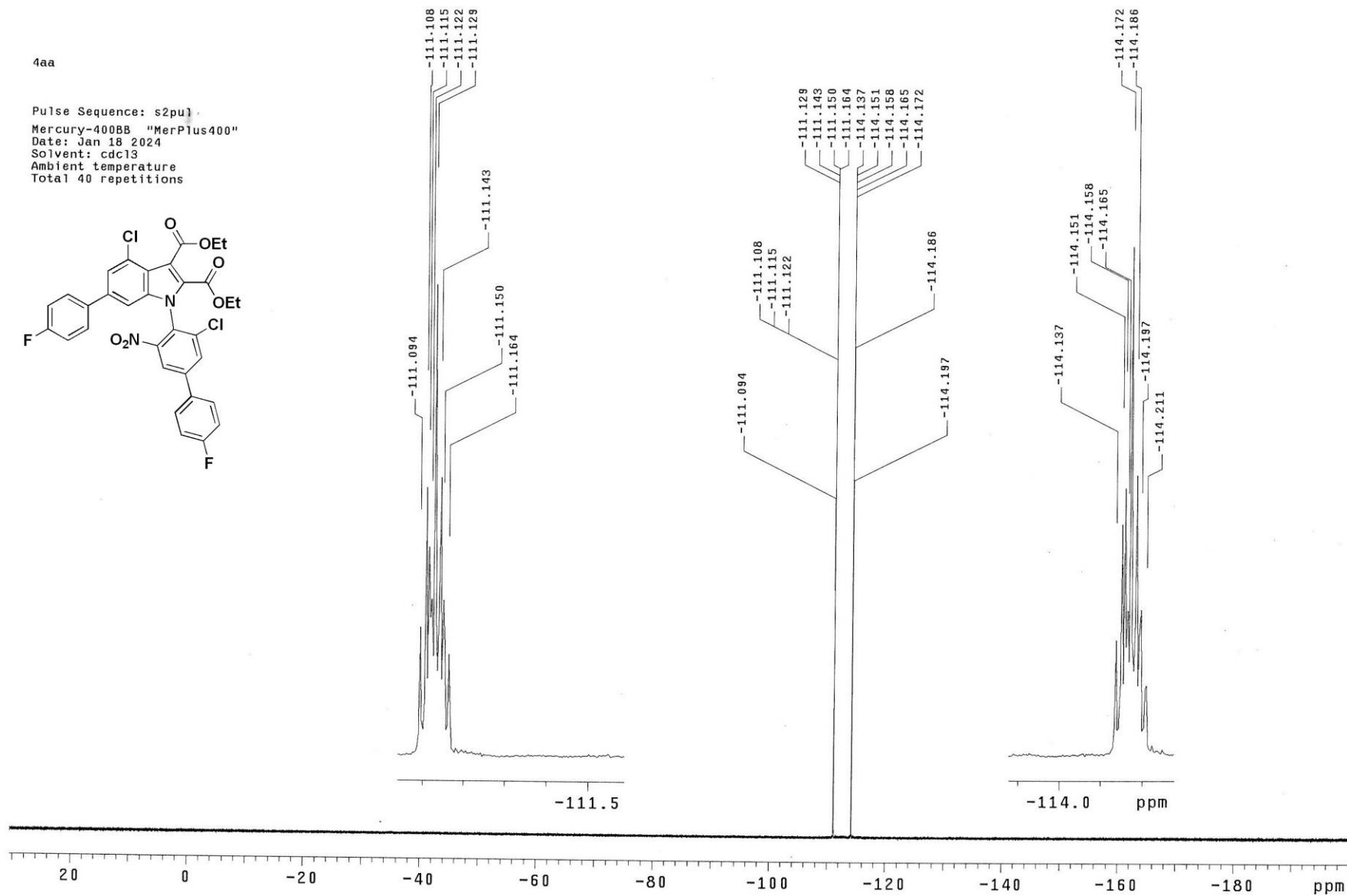
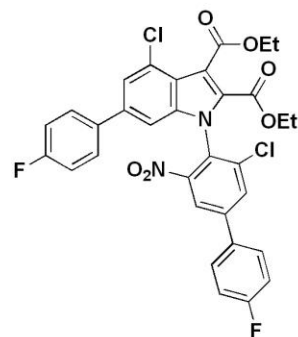
Total 2368 repetitions



Compound 4aa (¹⁹F-NMR spectral data)

4aa

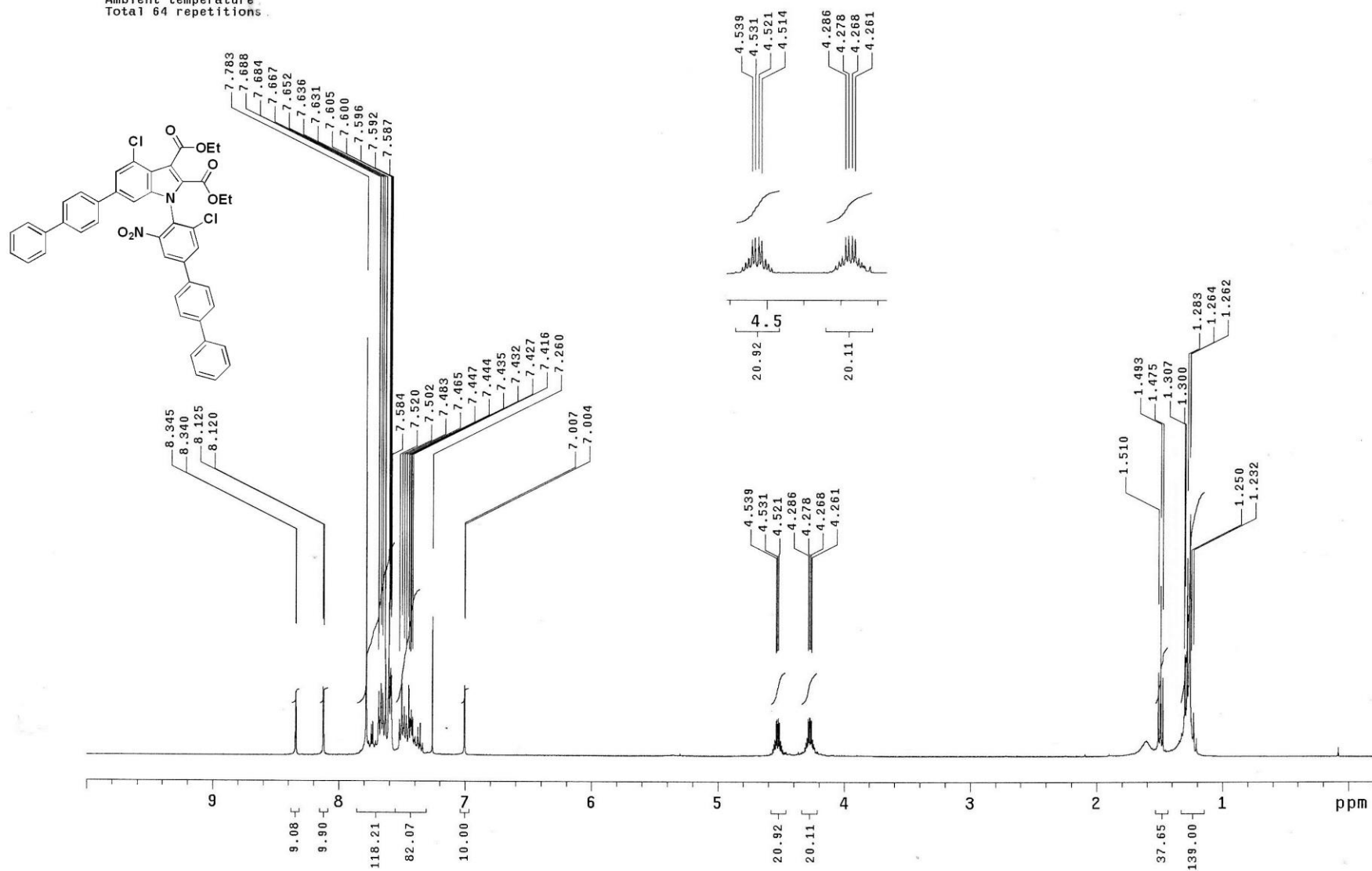
Pulse Sequence: s2pu1
Mercury-400BB "MerPlus400"
Date: Jan 18 2024
Solvent: cdc13
Ambient temperature
Total 40 repetitions



Compound 4ab (¹H-NMR spectral data)

CHNF0724

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jul 26 2023
 Solvent: pyridine
 Ambient temperature
 Total 64 repetitions



Compound 4ab (¹³C-NMR spectral data)

CHNF0724

Pulse Sequence: s2pu1

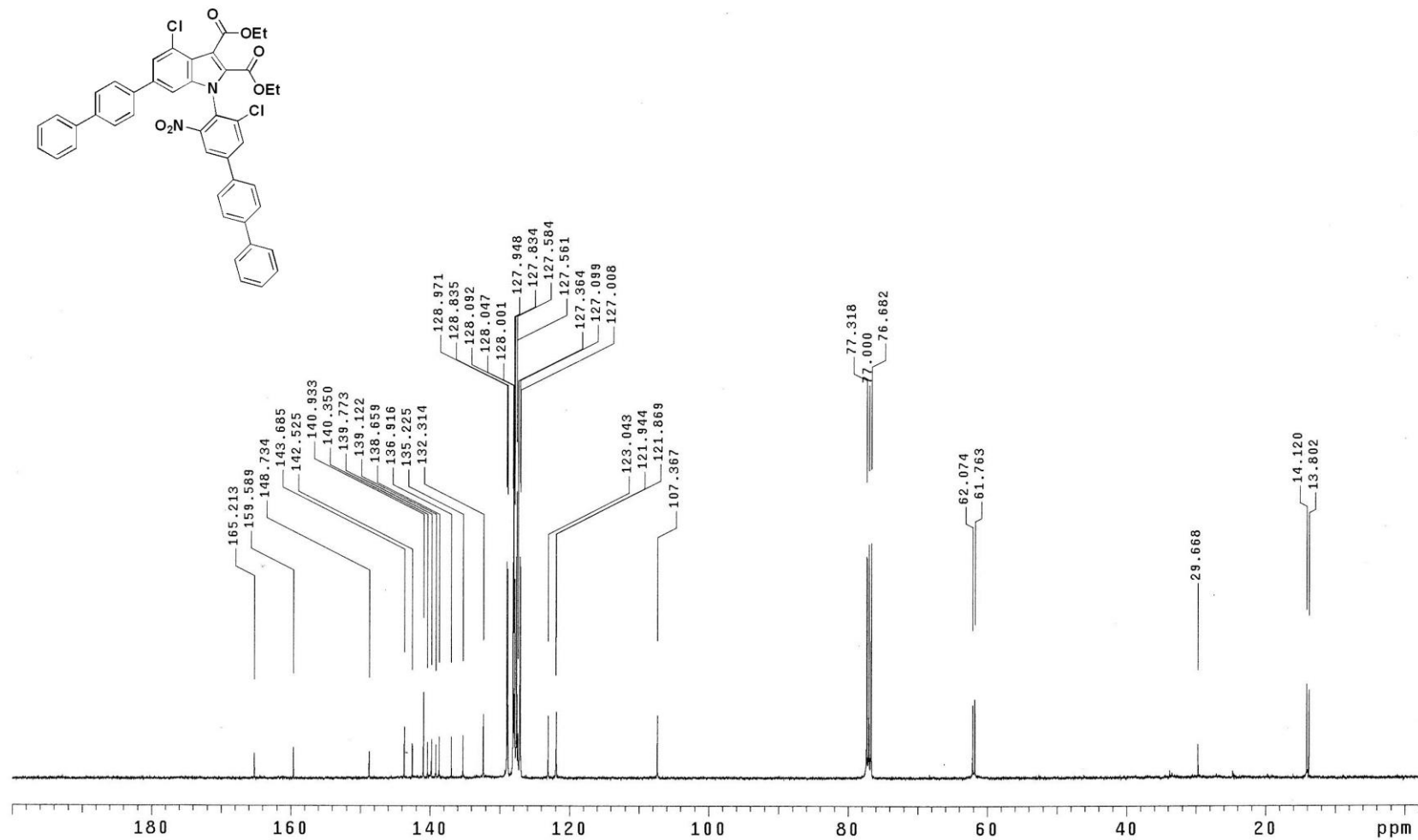
UNITYplus-400 "unity400"

Date: Jul 26 2023

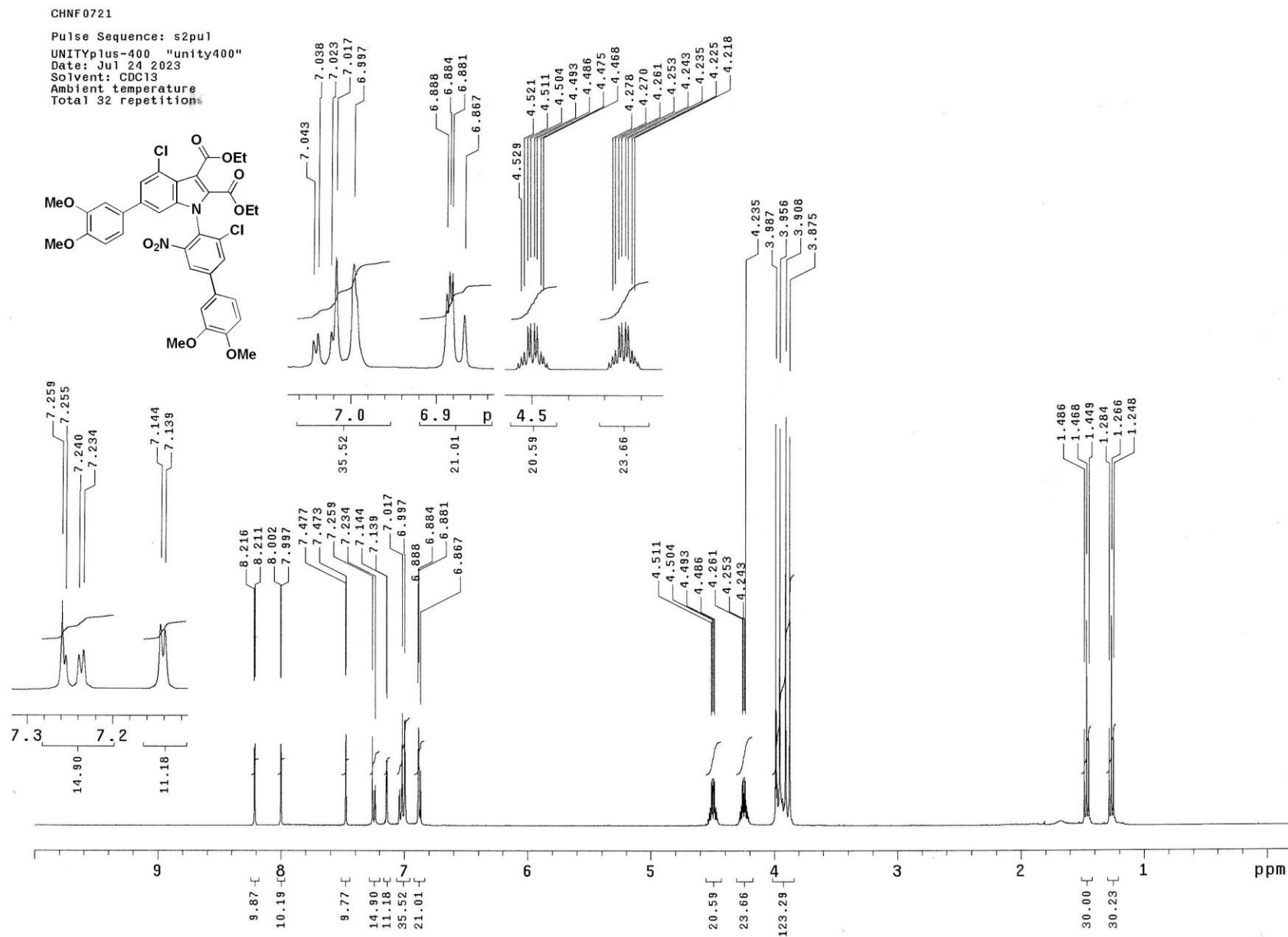
Solvent: CDCl₃

Ambient temperature

Total 64000 repetitions



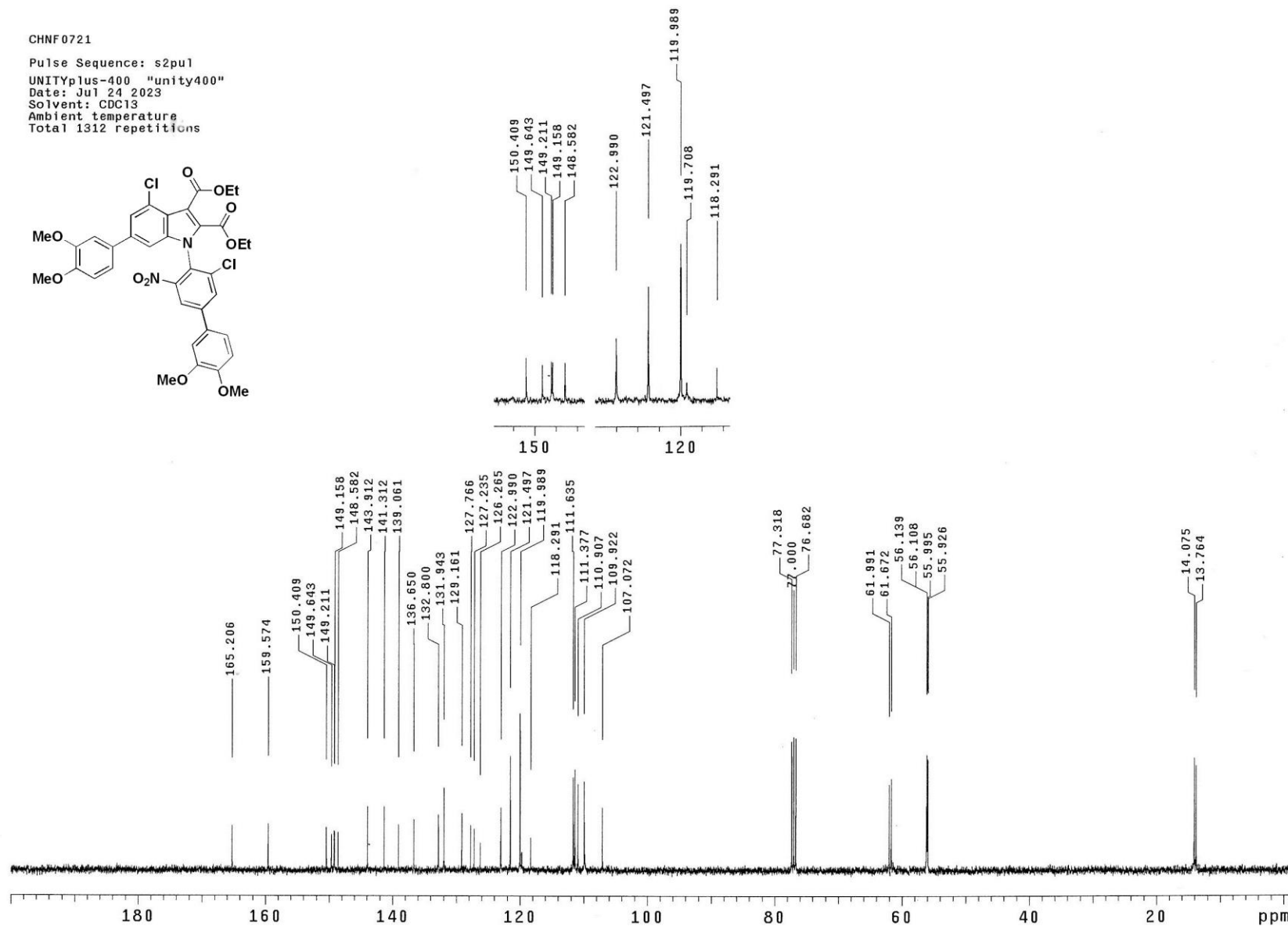
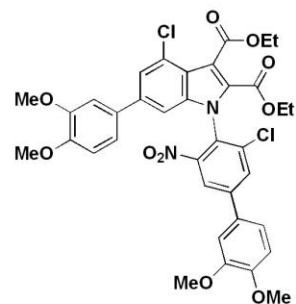
Compound 4ac (¹H-NMR spectral data)



Compound 4ac (¹³C-NMR spectral data)

CHNF0721

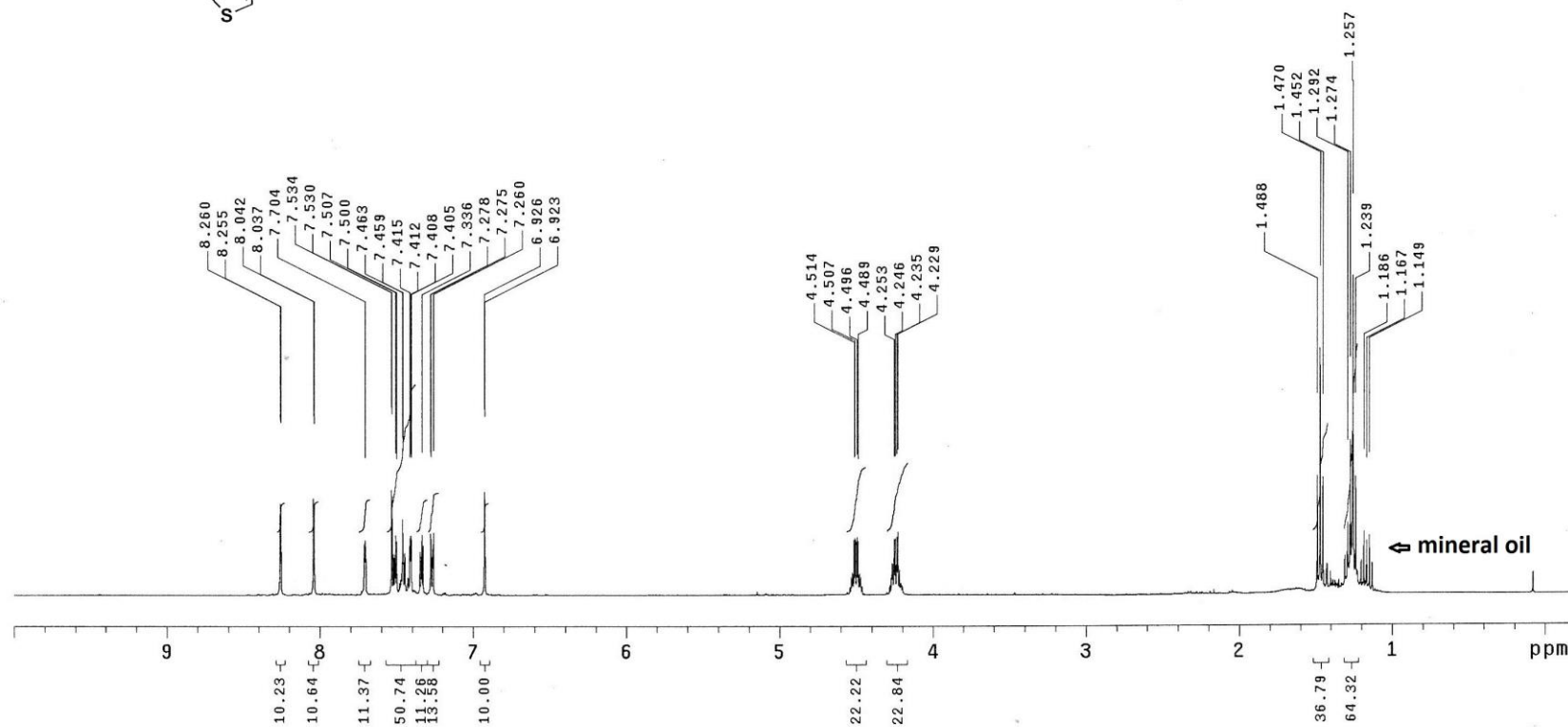
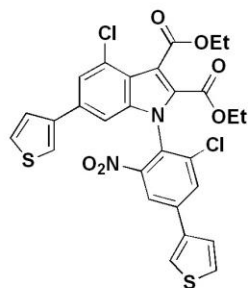
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jul 24 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 1312 repetitions



Compound 4ad (¹H-NMR spectral data)

CHNF0731

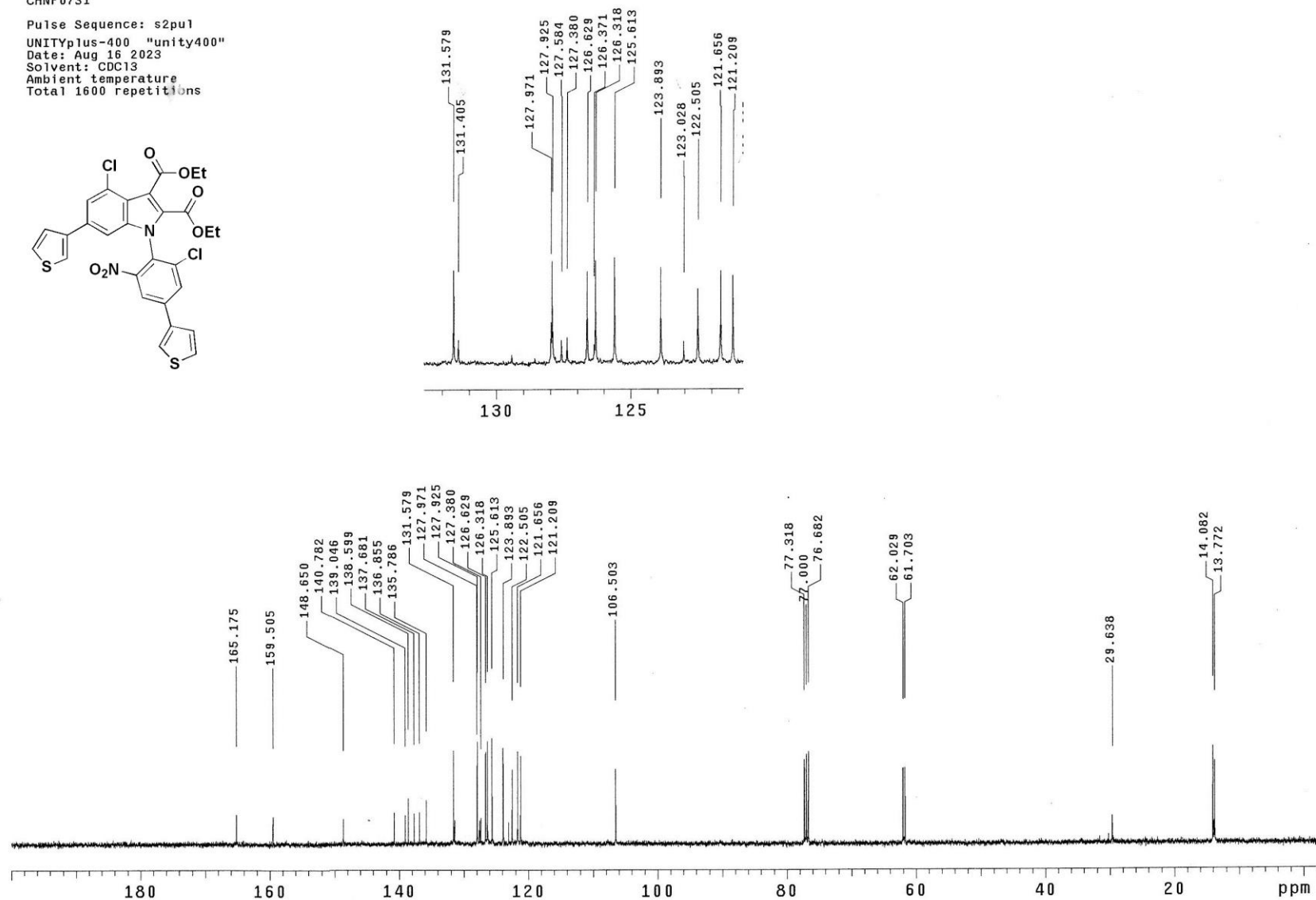
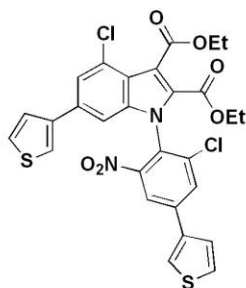
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 16 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4ad (¹³C-NMR spectral data)

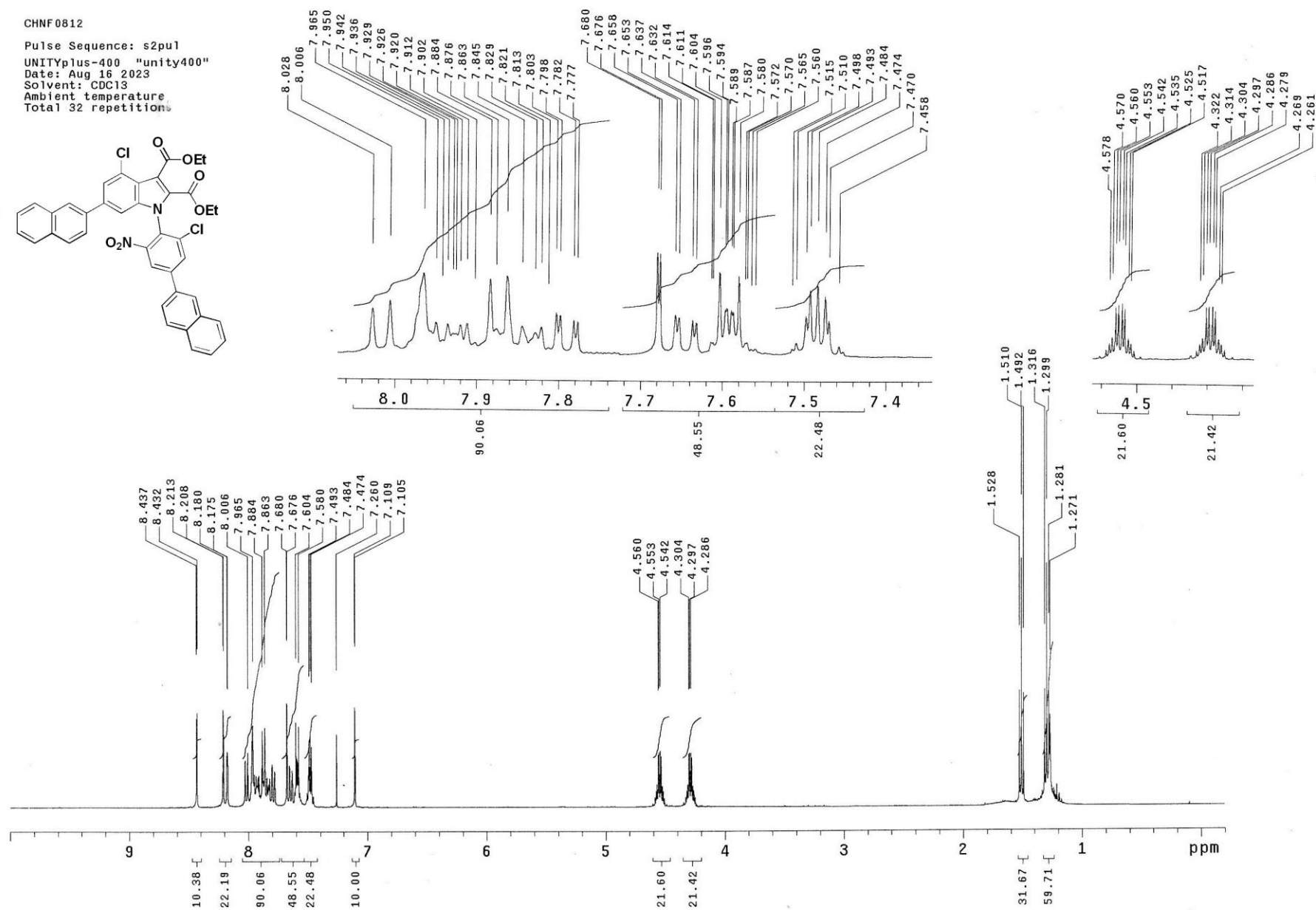
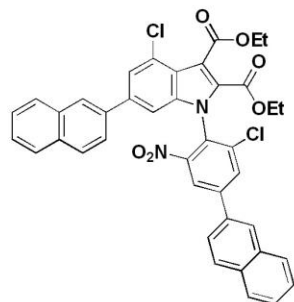
CHNF0731

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 16 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 1600 repetitions



Compound 4ae (¹H-NMR spectral data)

CHNF0812
Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Aug 16 2023
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4ae (¹³C-NMR spectral data)

CHNF0812

Pulse Sequence: s2pu1

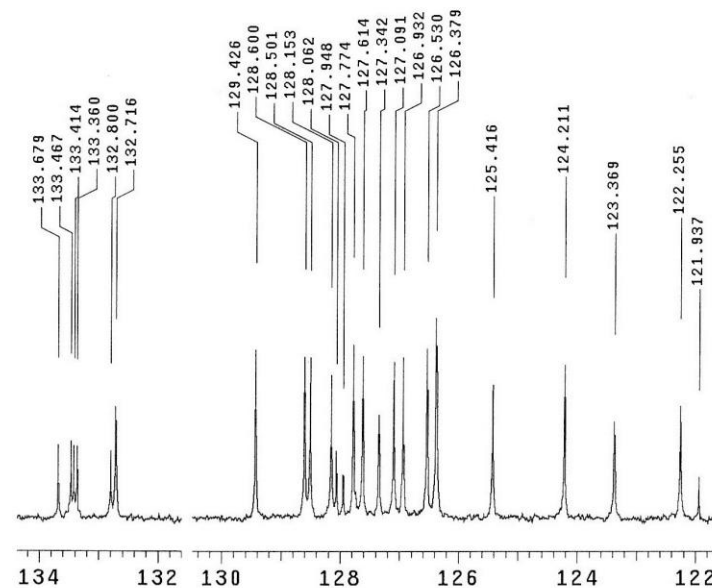
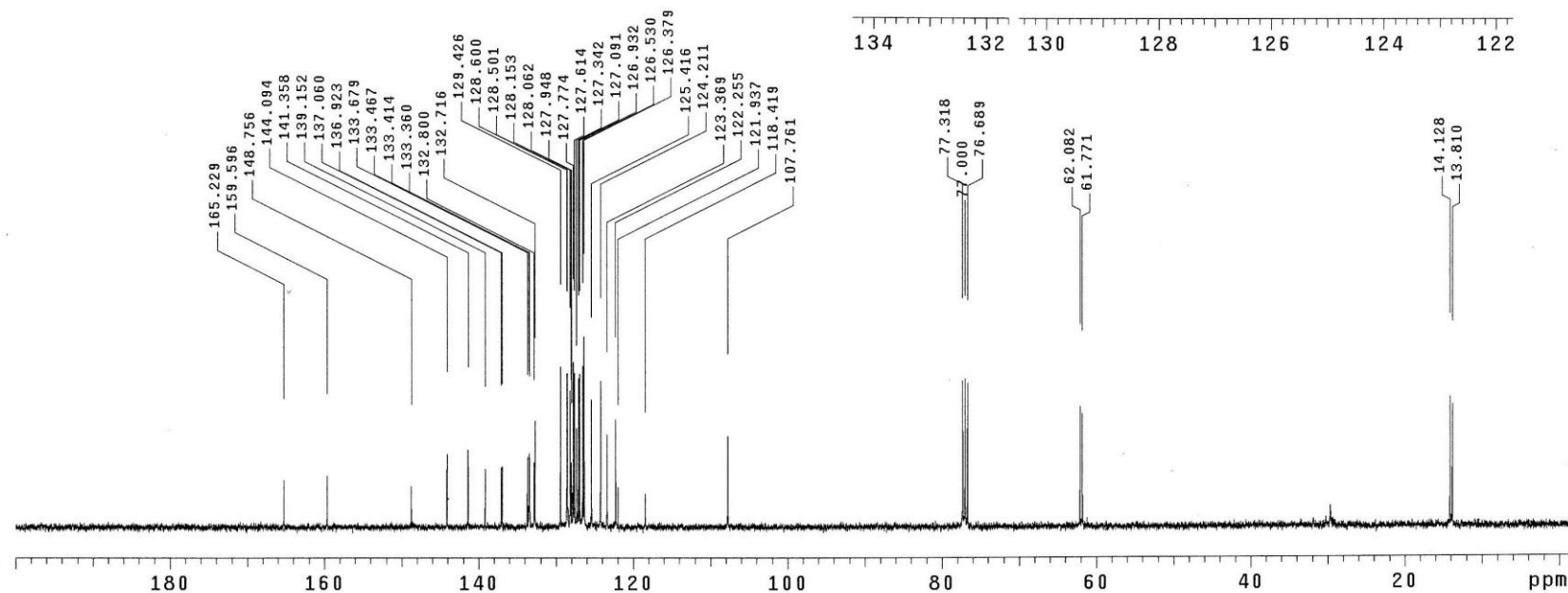
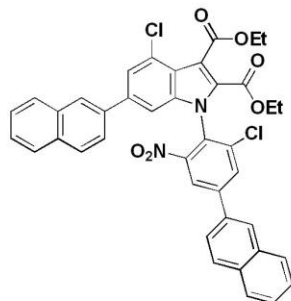
UNITYplus-400 "unity400"

Date: Aug 16 2023

Solvent: CDCl₃

Ambient temperature

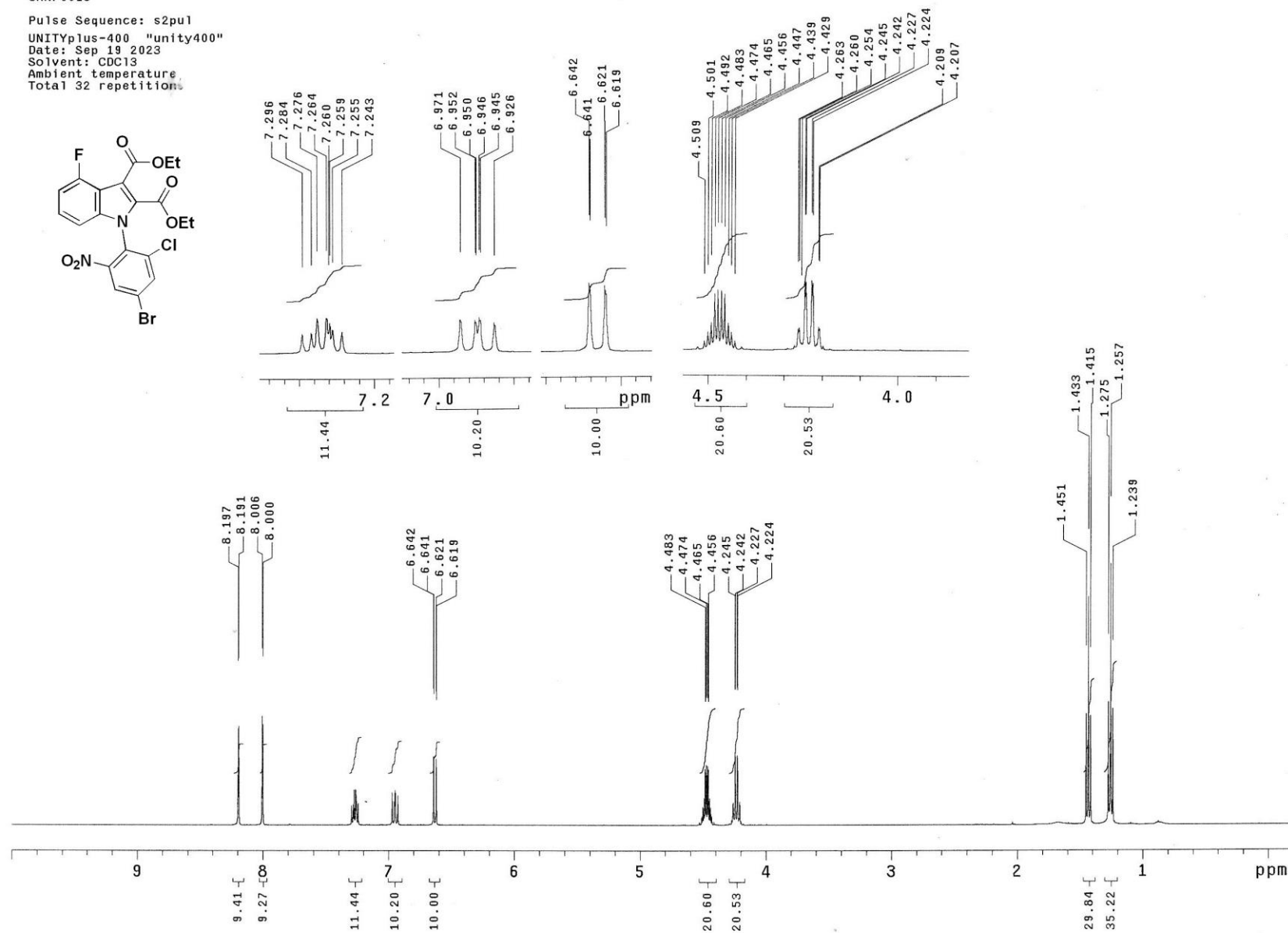
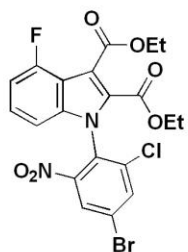
Total 2960 repetitions



Compound 4af (¹H-NMR spectral data)

CHNF0918

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 19 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetition



Compound 4af (¹³C-NMR spectral data)

CHNF0918

Pulse Sequence: s2pu1

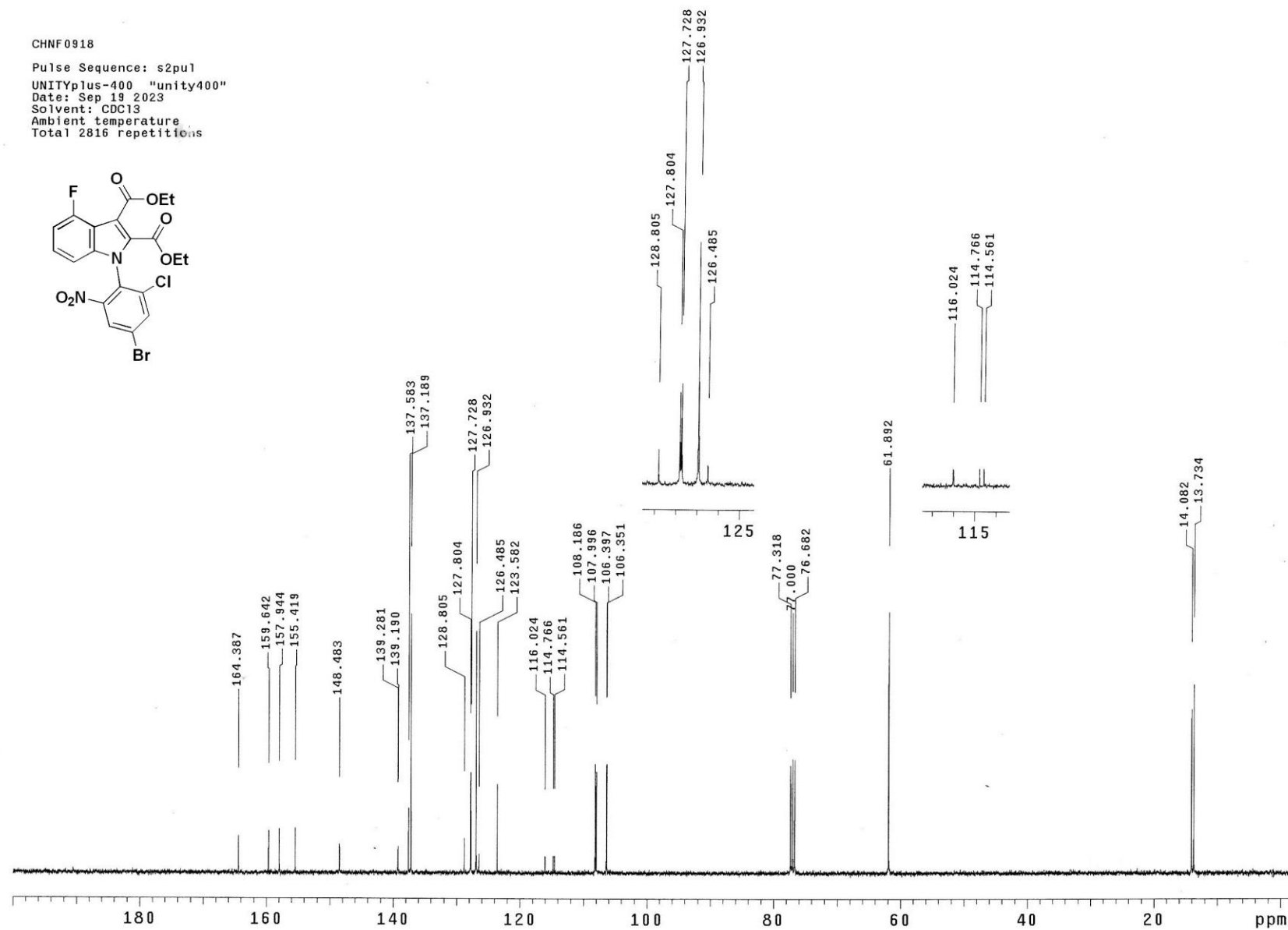
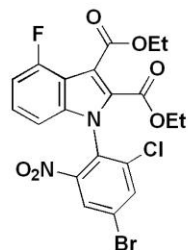
UNITYplus-400 "unity400"

Date: Sep 19 2023

Solvent: CDCl₃

Ambient temperature

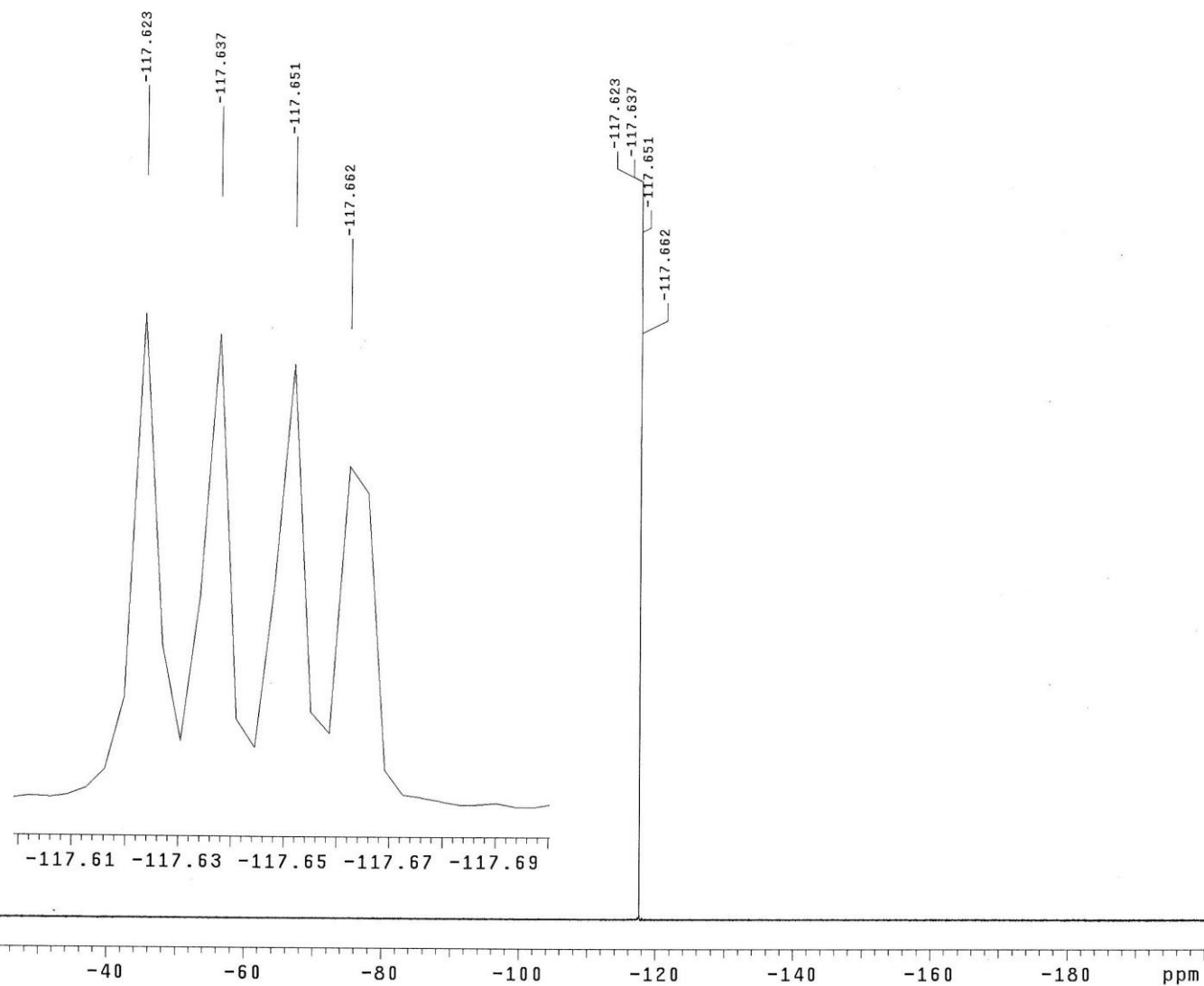
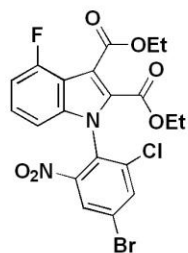
Total 2816 repetitions



Compound 4af (¹⁹F-NMR spectral data)

4af

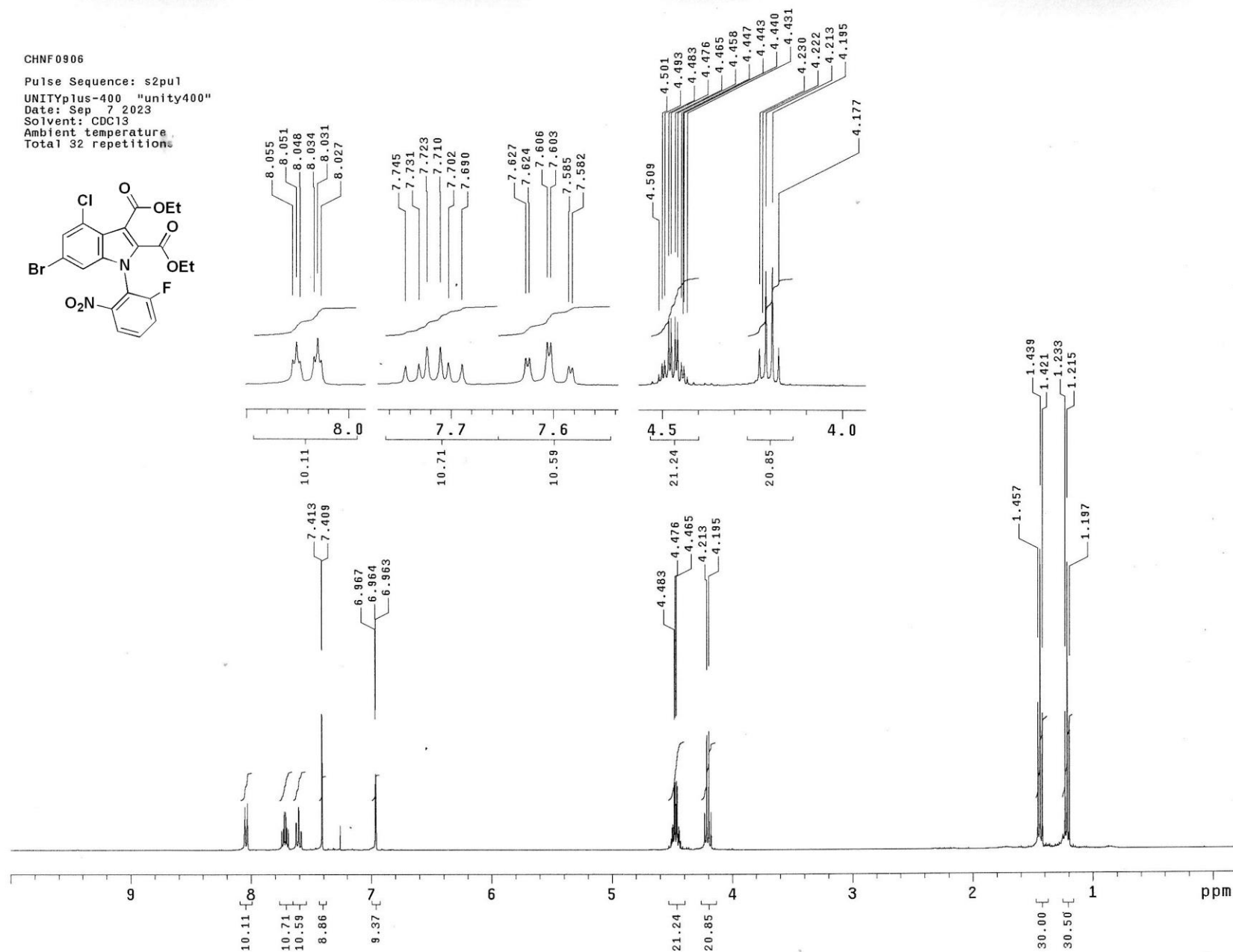
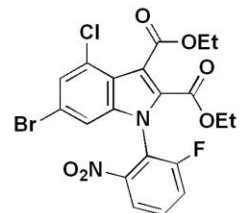
Pulse Sequence: s2pu1
Mercury-400BB "MerPlus400"
Date: Jan 19 2024
Solvent: cdcl3
Ambient temperature
Total 44 repetitions



Compound 4ag (¹H-NMR spectral data)

CHNF0906

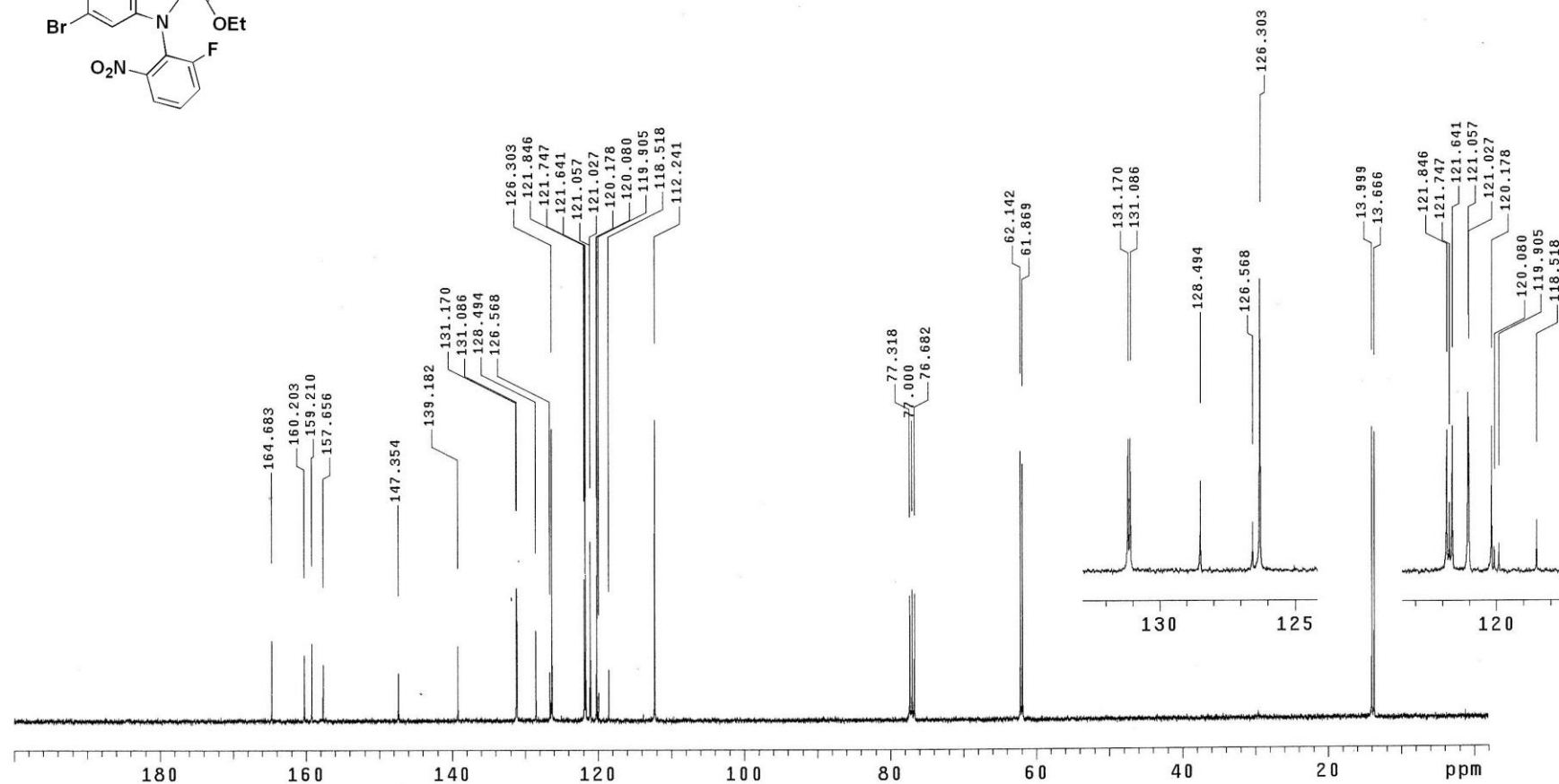
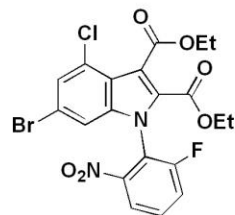
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 7 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4ag (¹³C-NMR spectral data)

CHNF0906

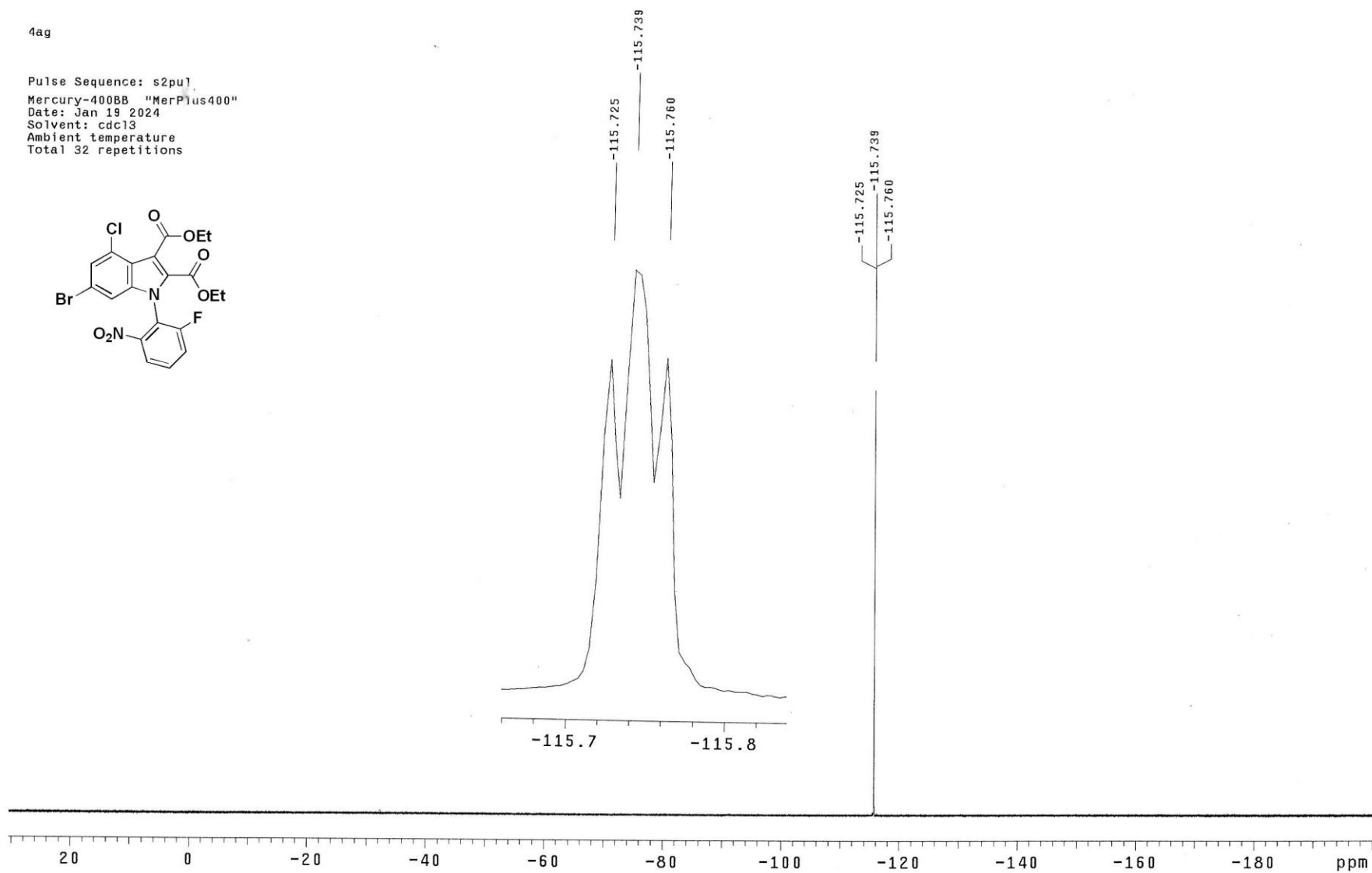
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 7 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 3120 repetitions



Compound 4ag (¹⁹F-NMR spectral data)

4ag

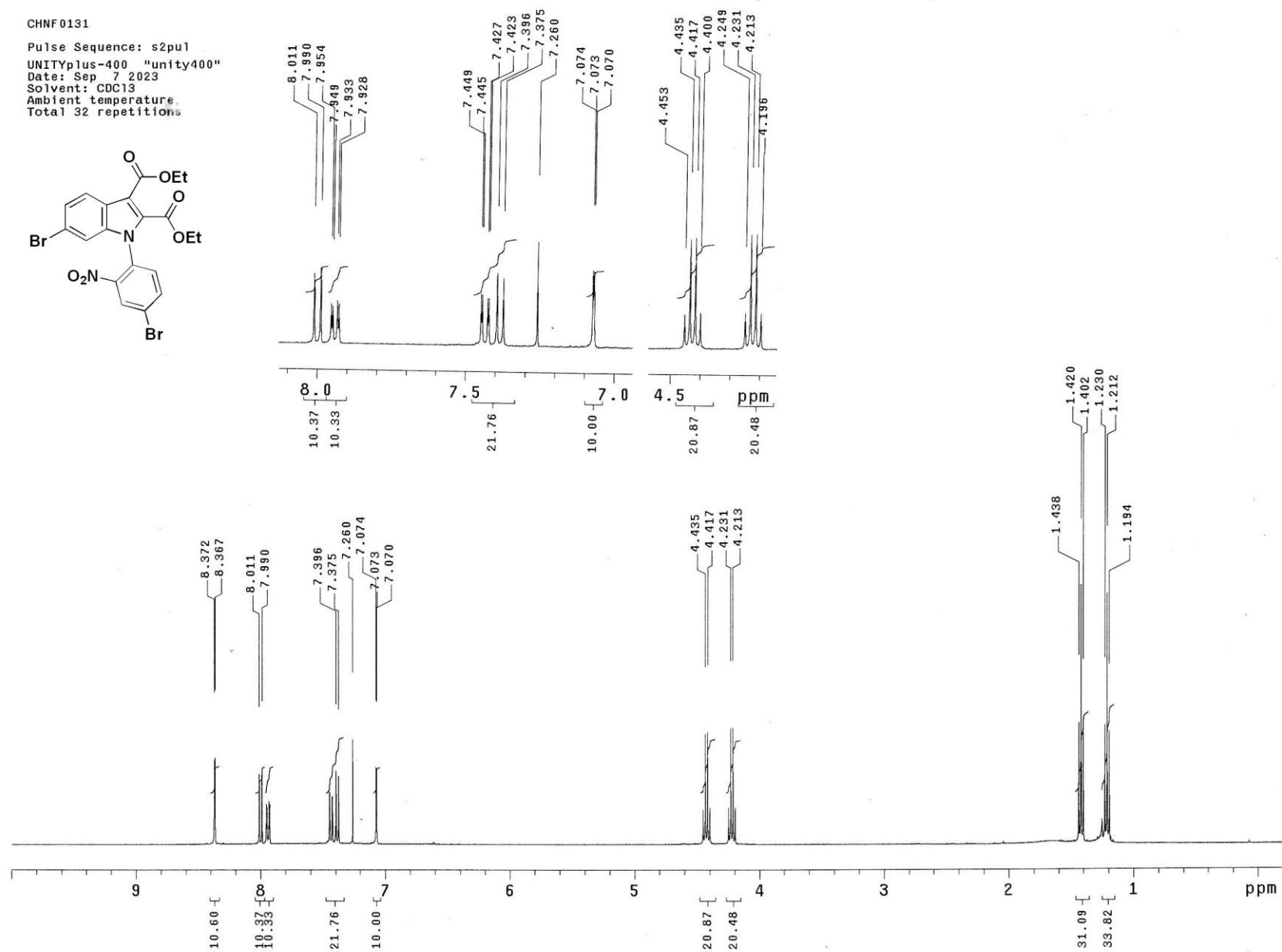
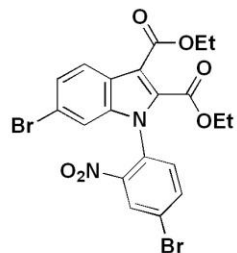
Pulse Sequence: s2pu1
Mercury-400BB "MerPlus400"
Date: Jan 19 2024
Solvent: cdcl3
Ambient temperature
Total 32 repetitions



Compound 4ah (¹H-NMR spectral data)

CHNF0131

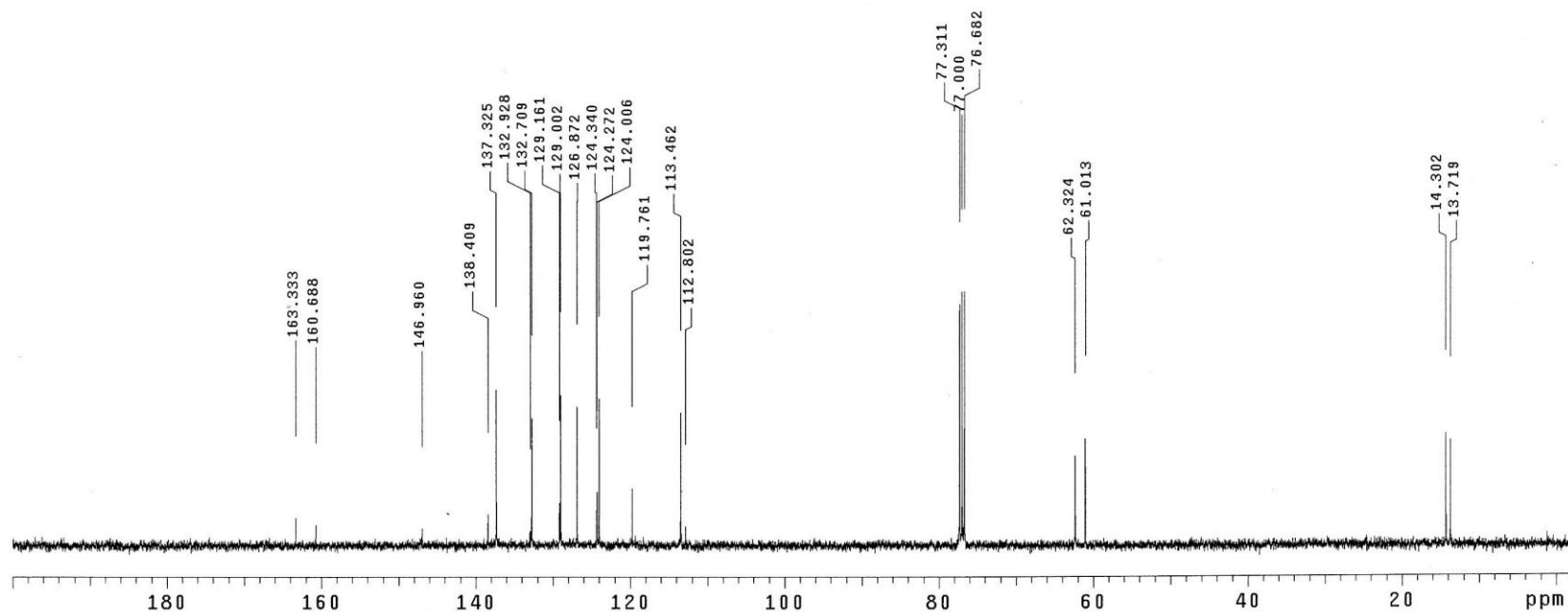
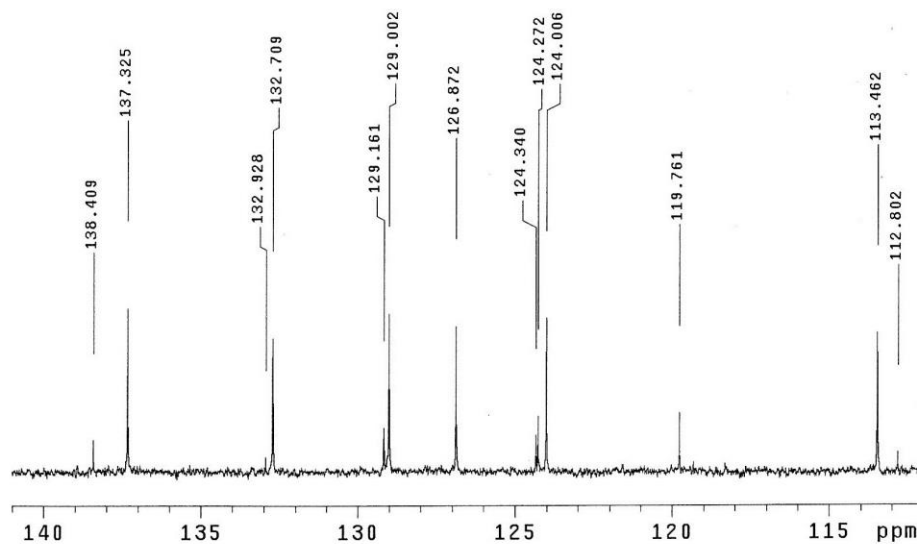
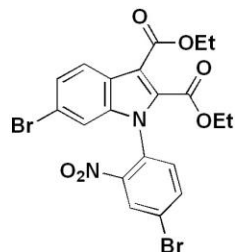
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 7 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4ah (¹³C-NMR spectral data)

CHNF0131

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 7 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 3056 repetitions



Compound 5a (¹H-NMR spectral data)

CHNF0317

Pulse Sequence: s2pu1

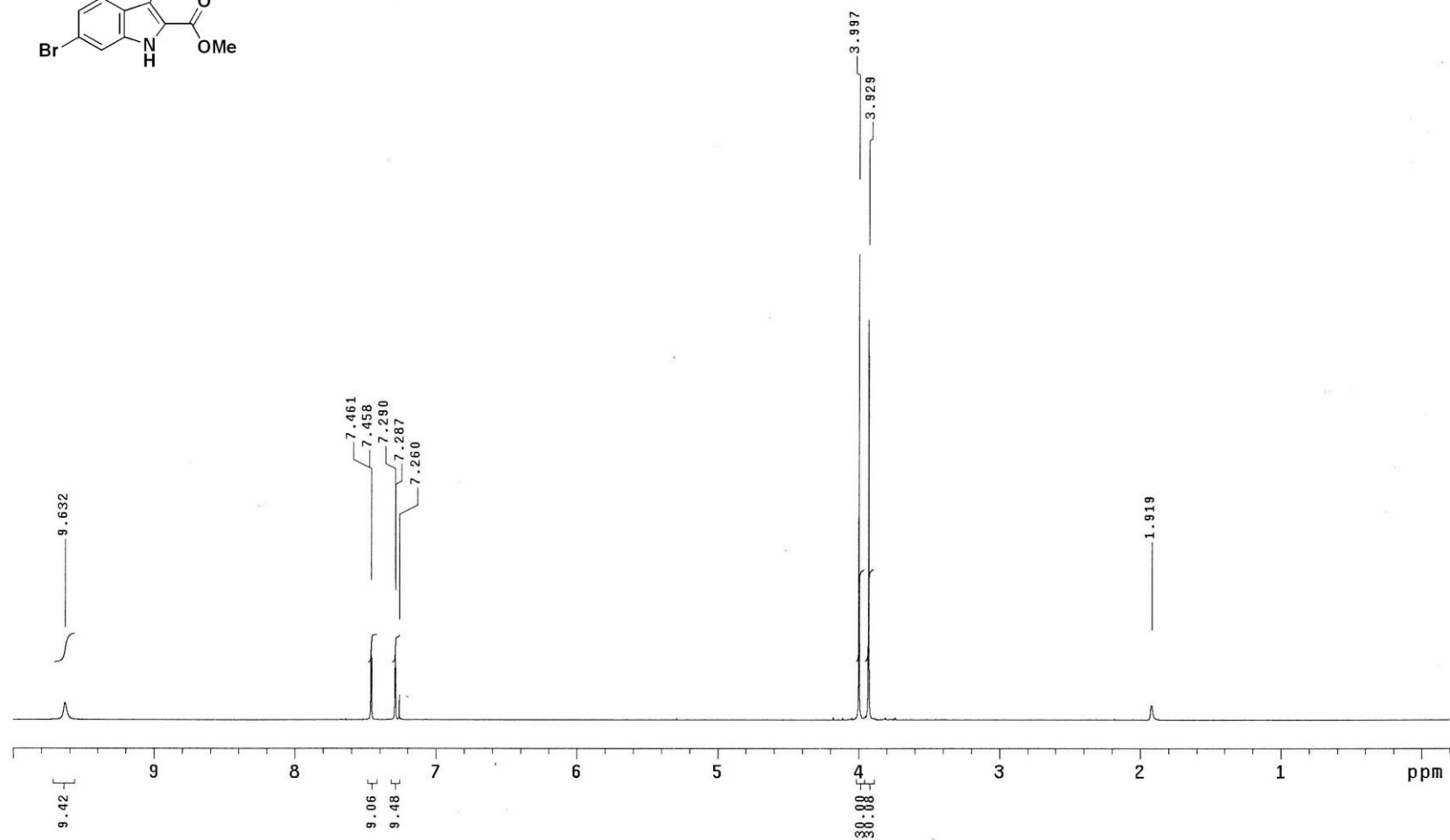
UNITYplus-400 "unity400"

Date: Mar 17 2023

Solvent: CDCl₃

Ambient temperature

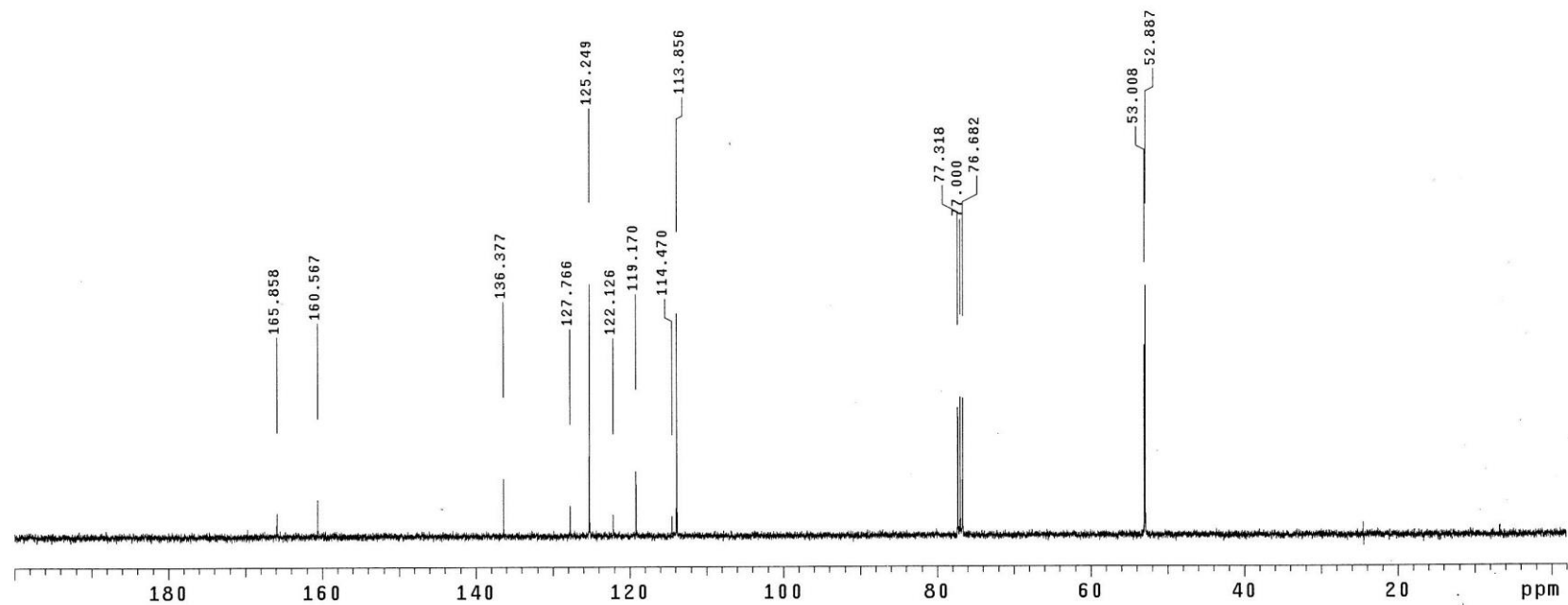
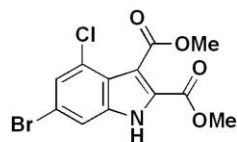
Total 32 repetitions



Compound 5a (^{13}C -NMR spectral data)

CHNF0317

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 17 2023
Solvent: CDCl₃
Ambient temperature
Total 2720 repetitions



Compound 5b (¹H-NMR spectral data)

CHNF0315

Pulse Sequence: s2pu1

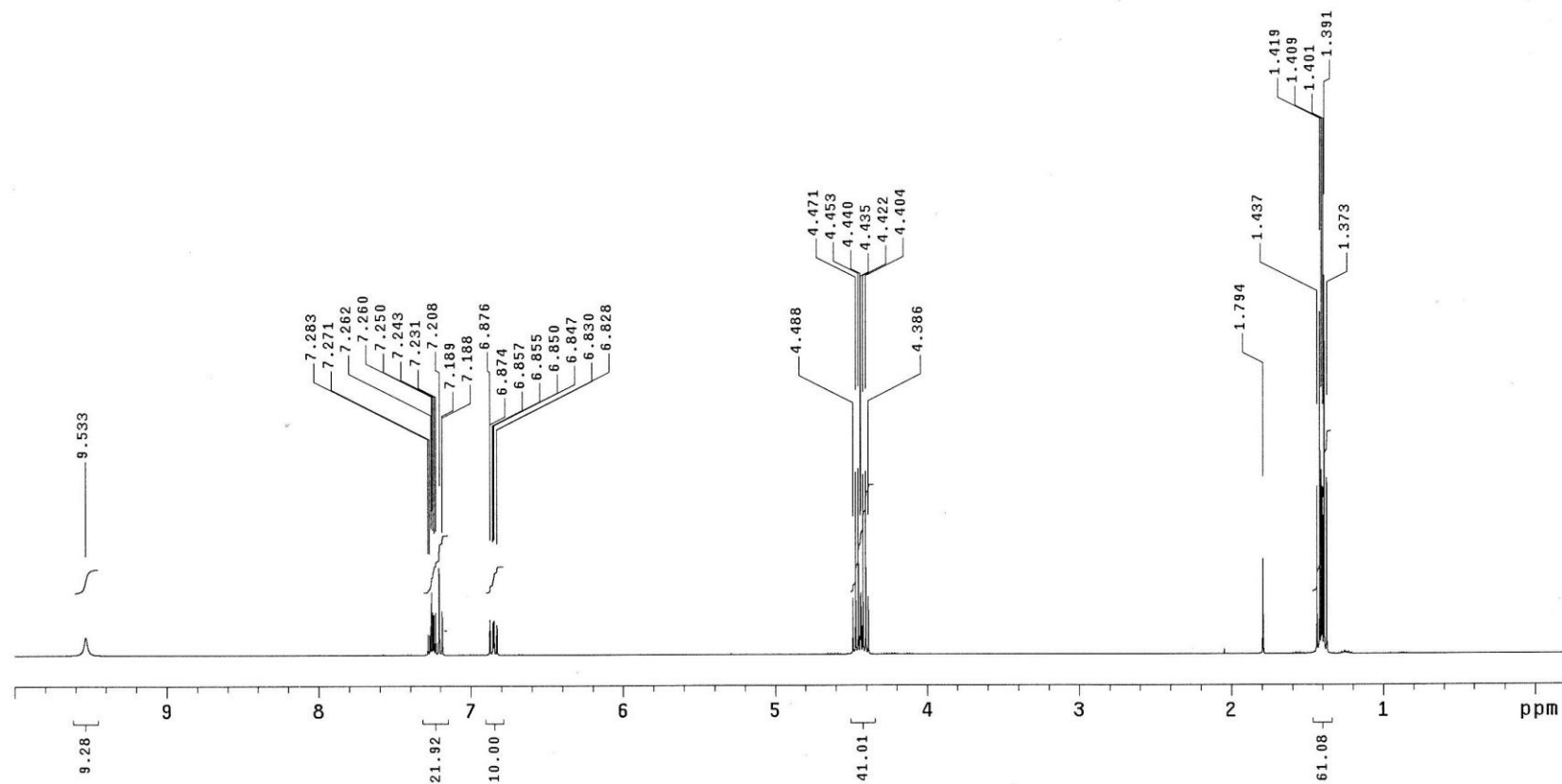
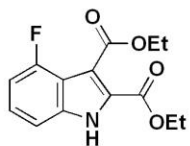
UNITYplus-400 "unity400"

Date: Mar 16 2023

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5b (¹³C-NMR spectral data)

CHNF0315

Pulse Sequence: s2pu1

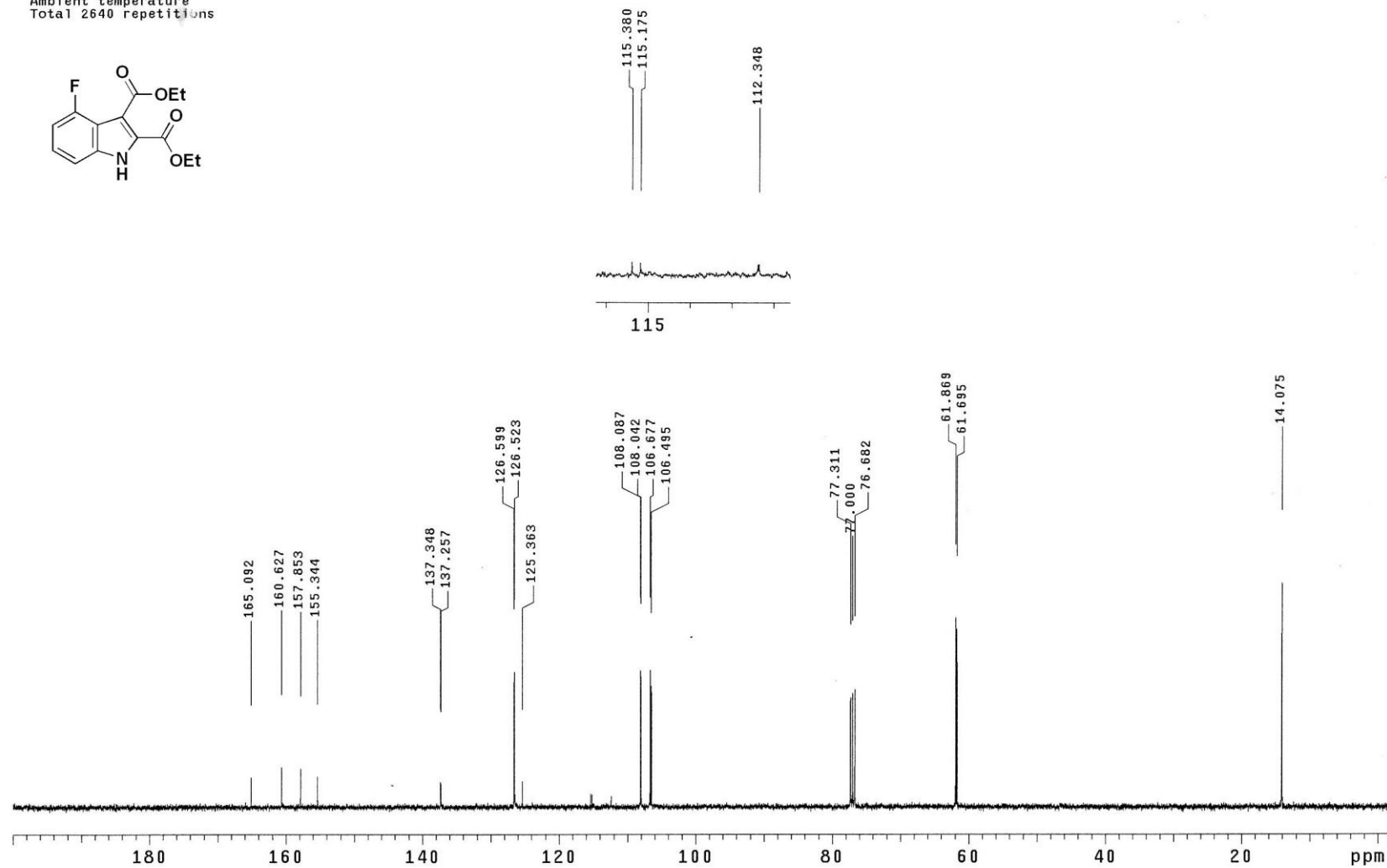
UNITYplus-400 "unity400"

Date: Mar 16 2023

Solvent: CDCl₃

Ambient temperature

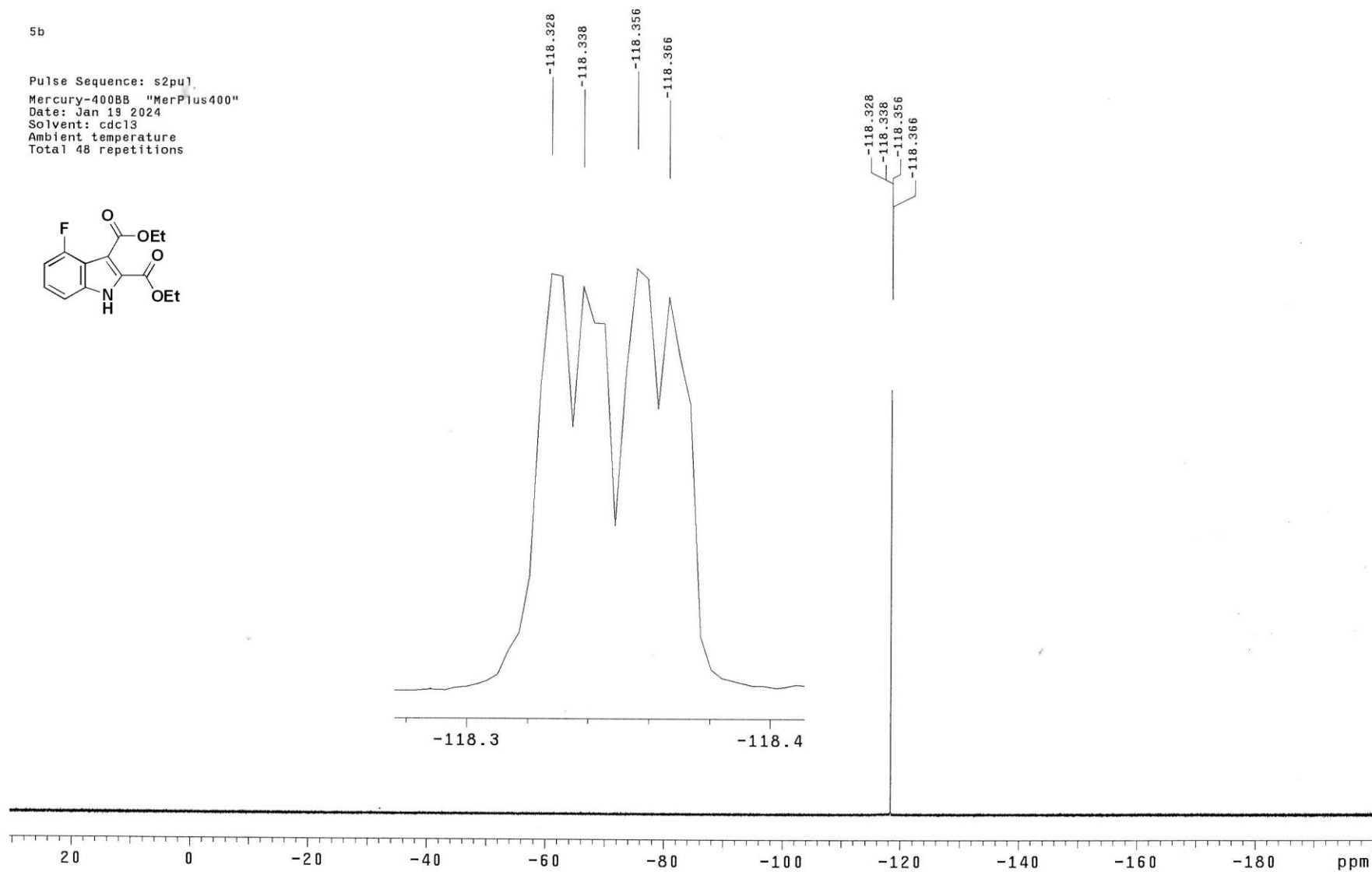
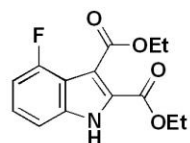
Total 2640 repetitions



Compound 5b (^{19}F -NMR spectral data)

5b

Pulse Sequence: s2pu1
Mercury-400BB "MerPlus400"
Date: Jan 19 2024
Solvent: cdcl3
Ambient temperature
Total 48 repetitions



Compound 5c (¹H-NMR spectral data)

CHQ4148

Pulse Sequence: s2pu1

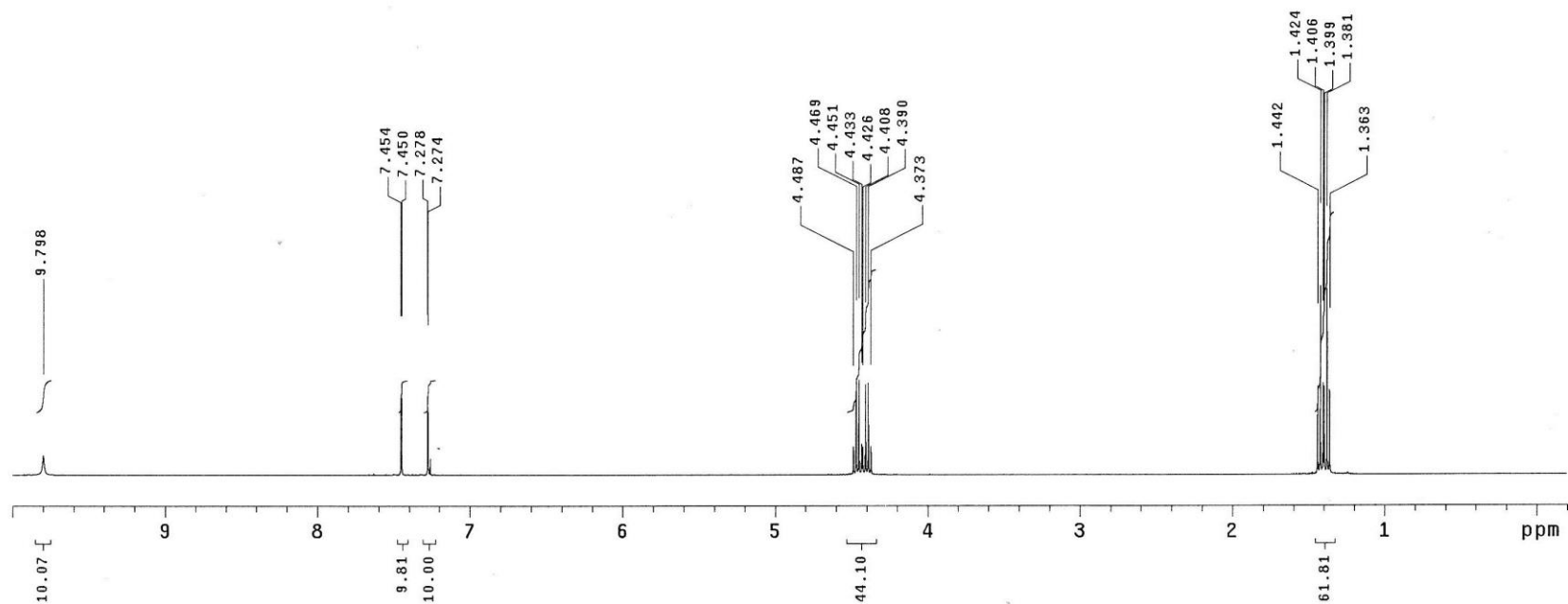
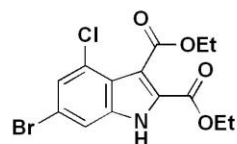
UNITYplus-400 "unity400"

Date: Mar 9 2023

Solvent: CDCl₃

Ambient temperature

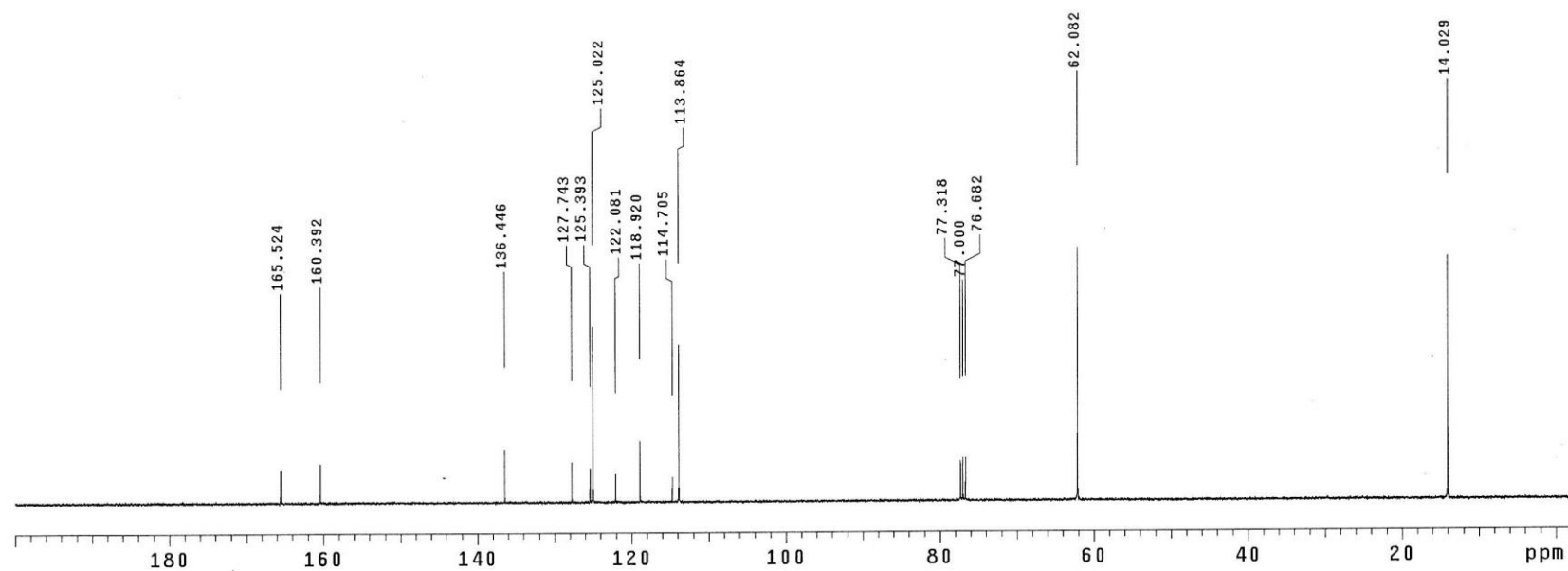
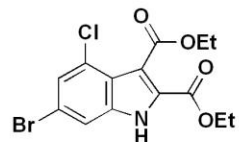
Total 32 repetitions



Compound 5c (¹³C-NMR spectral data)

CHQ4148

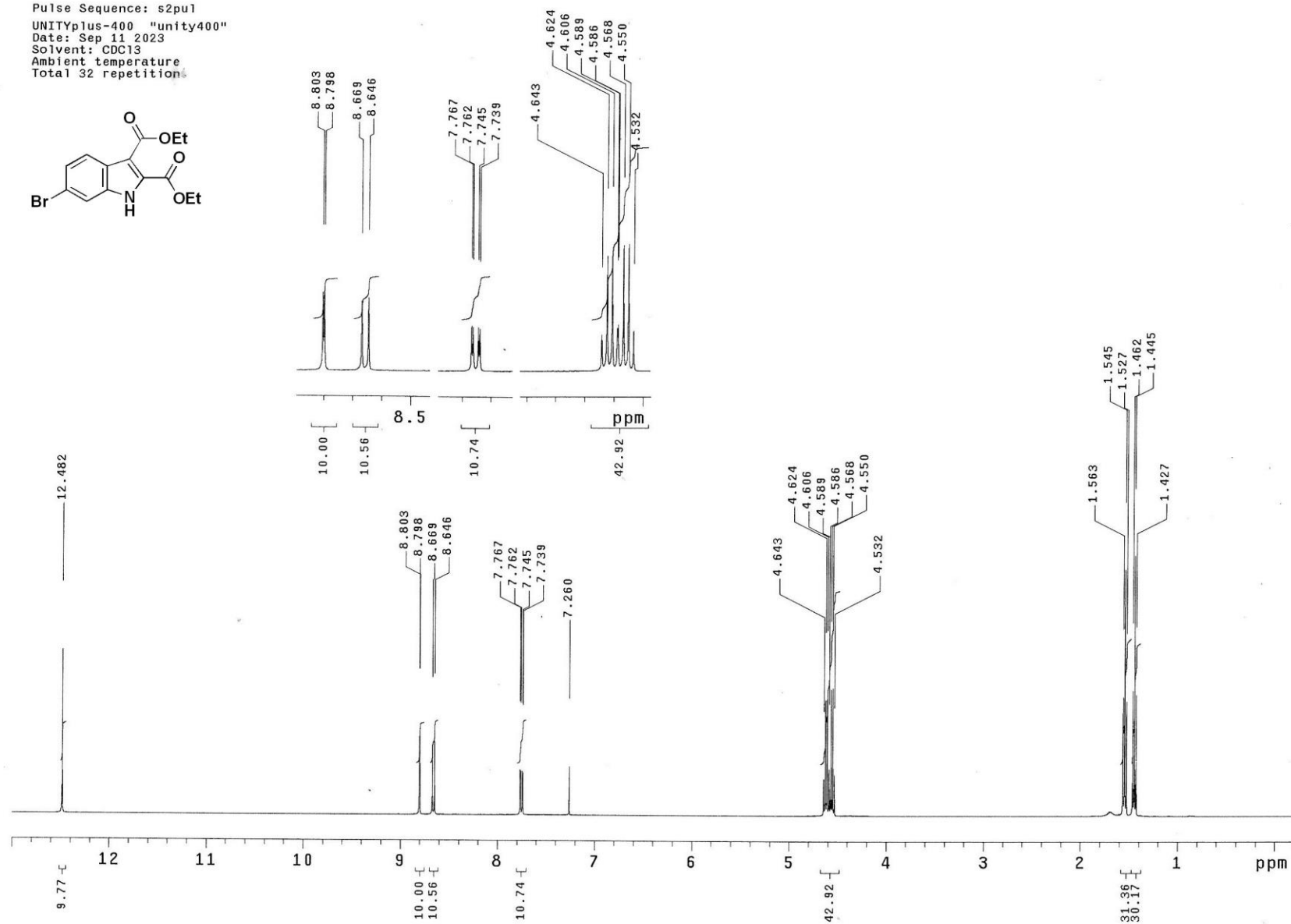
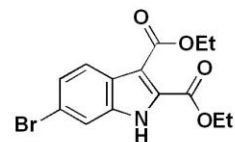
Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 9 2023
Solvent: CDCl₃
Ambient temperature
Total 2032 repetitions



Compound 5d (¹H-NMR spectral data)

CHNF0908

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 11 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetition



Compound 5d (¹³C-NMR spectral data)

CHNF0908

Pulse Sequence: s2pu1

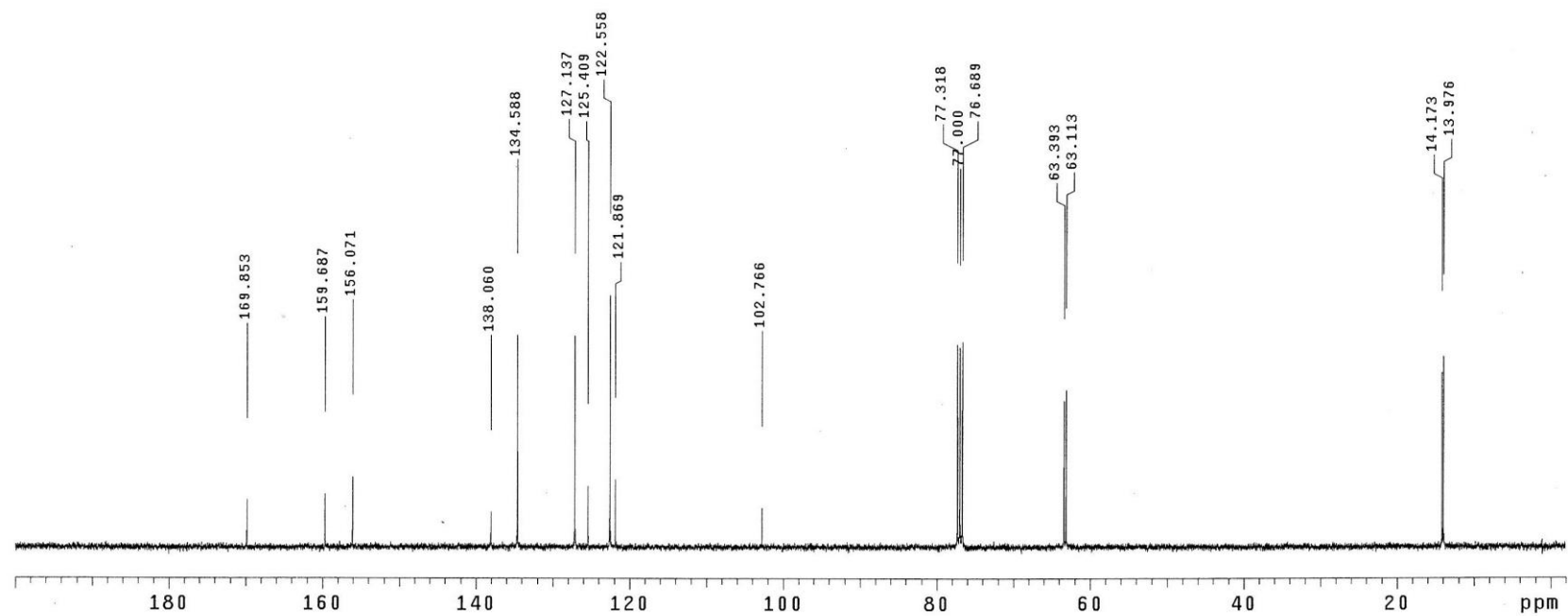
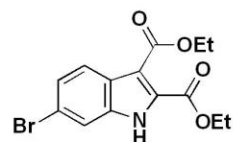
UNITYplus-400 "unity400"

Date: Sep 11 2023

Solvent: CDCl₃

Ambient temperature

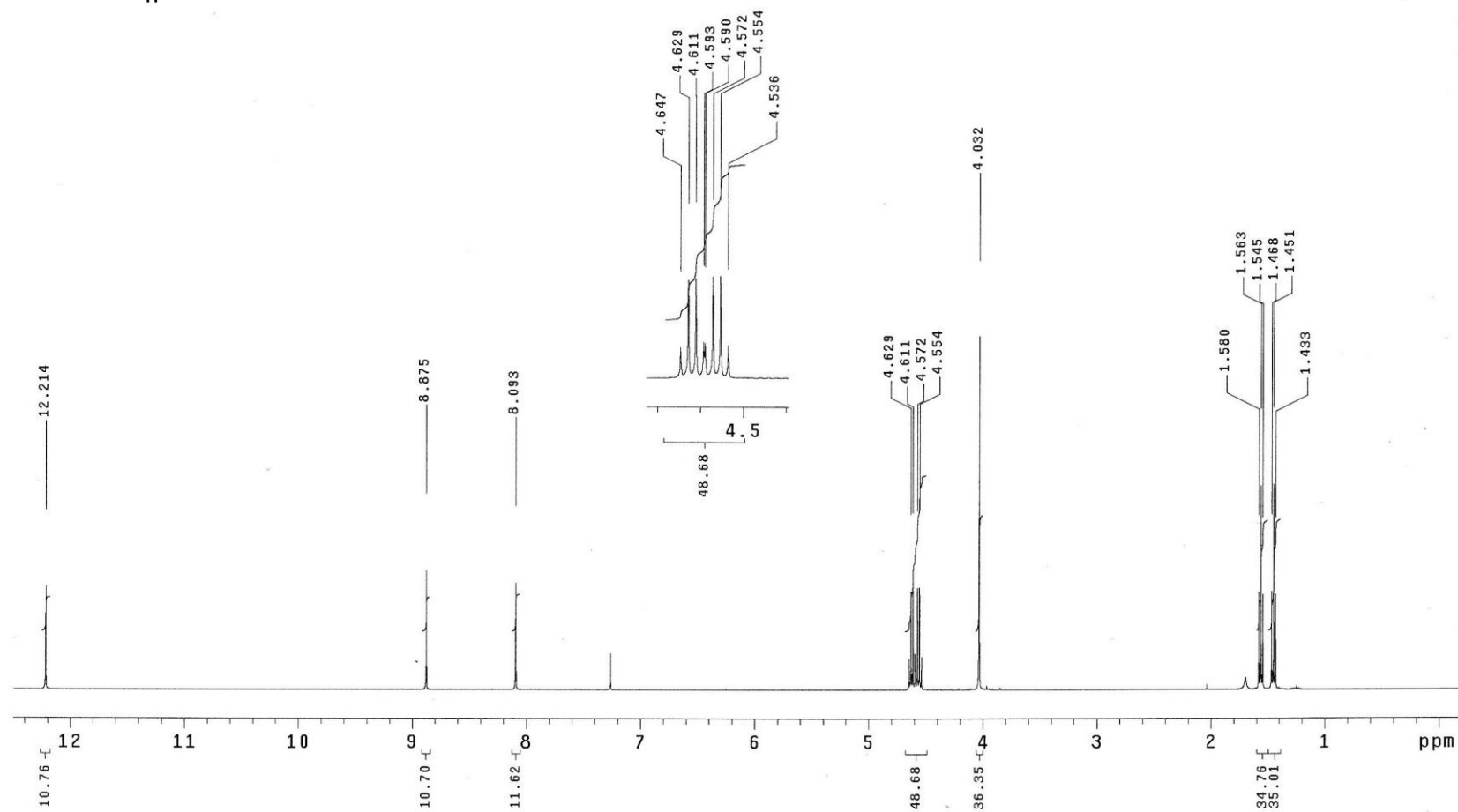
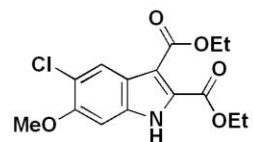
Total 4688 repetitions



Compound 5e (¹H-NMR spectral data)

CHNF1016

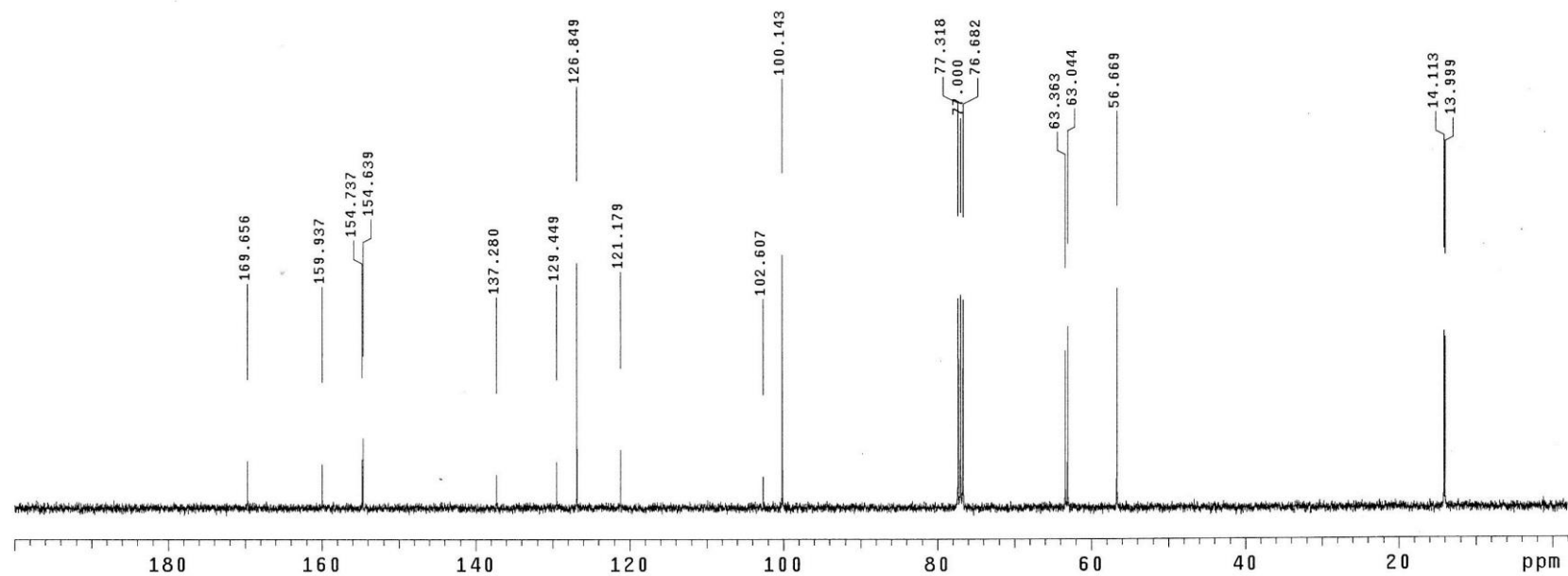
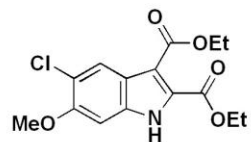
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Oct 17 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 5e (¹³C-NMR spectral data)

CHNF1016

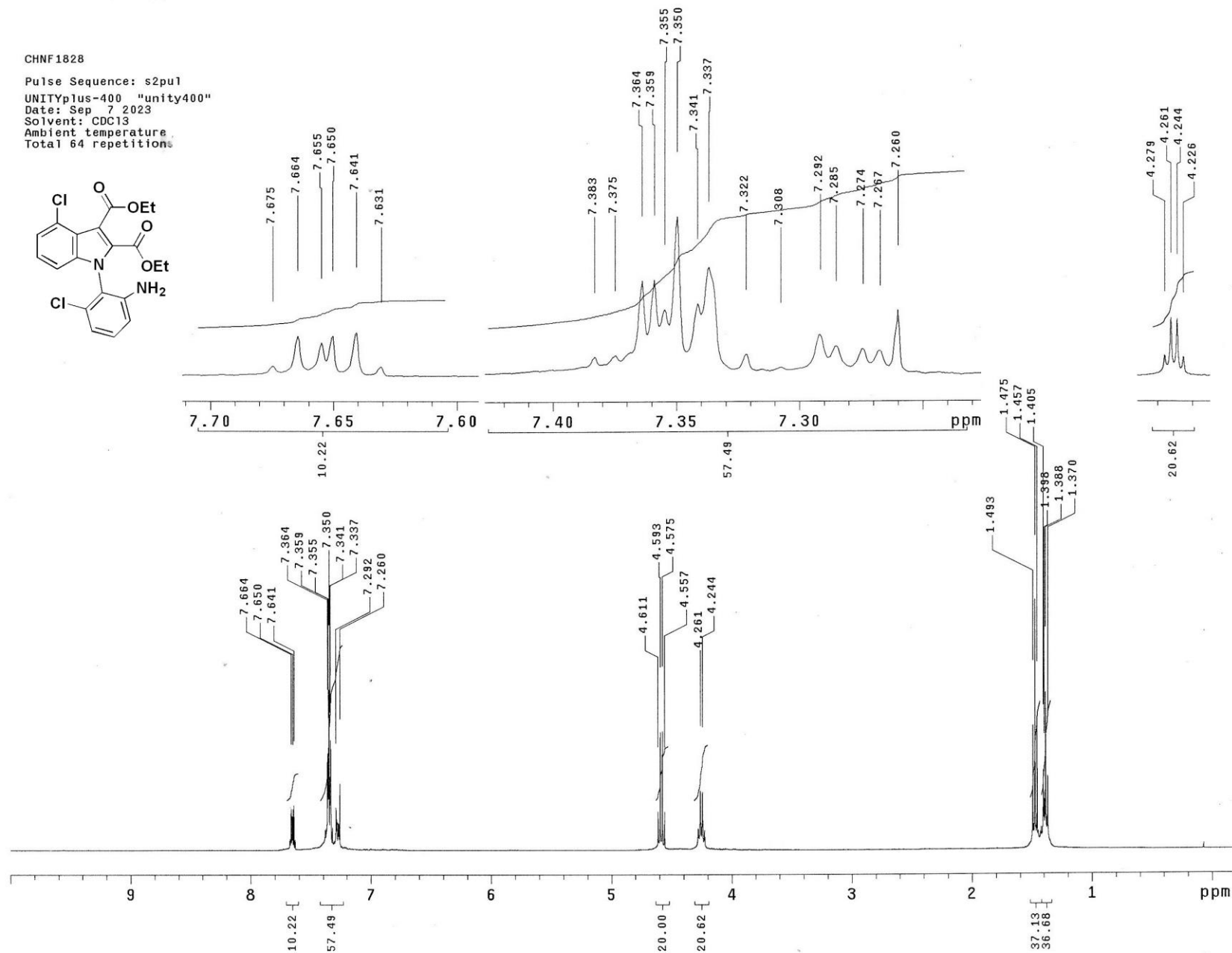
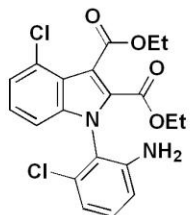
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Oct 17 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 3072 repetitions



Compound 6a (¹H-NMR spectral data)

CHNF1828

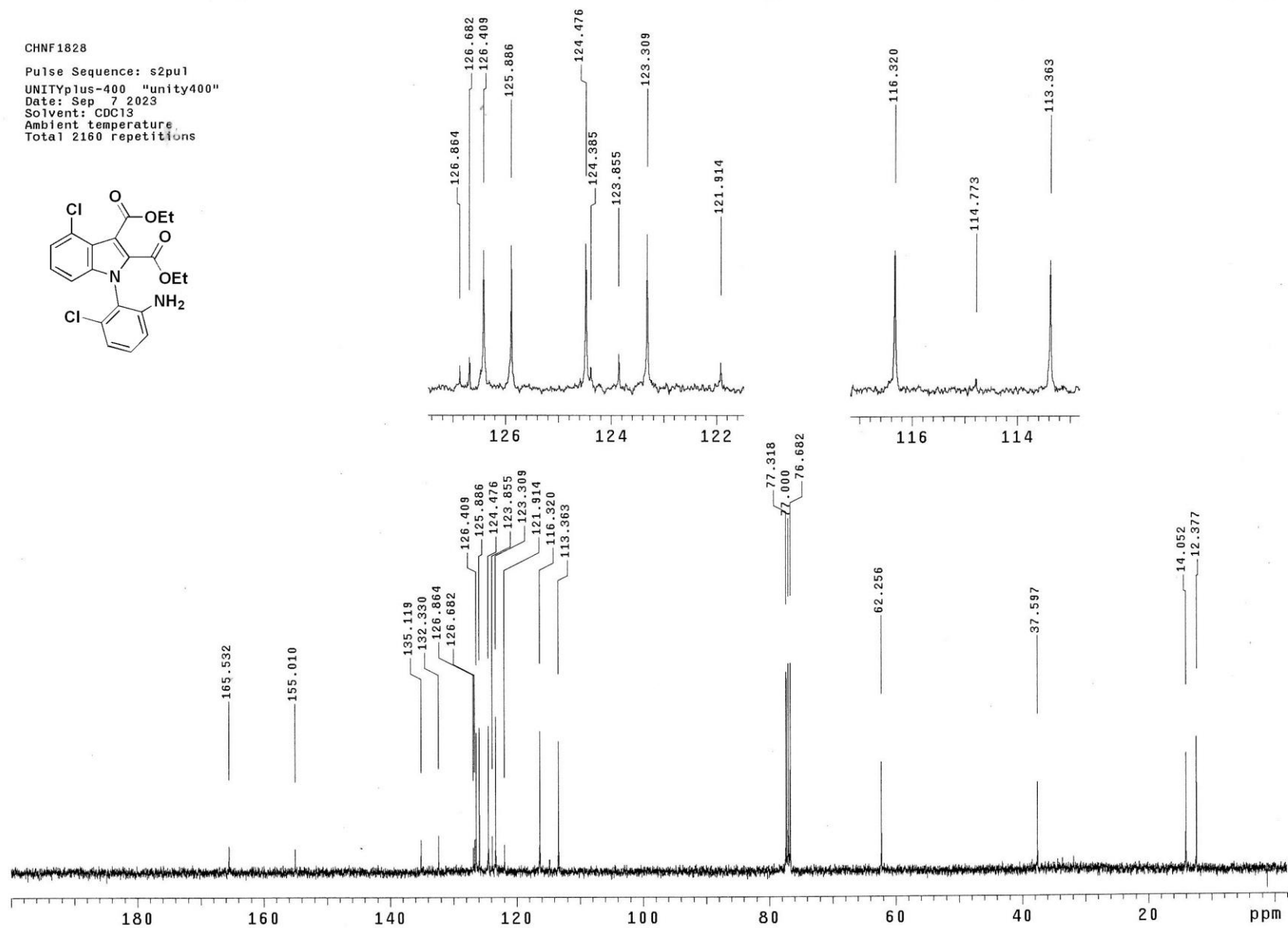
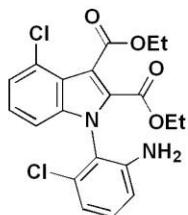
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 7 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 64 repetitions



Compound 6a (¹³C-NMR spectral data)

CHNF1828

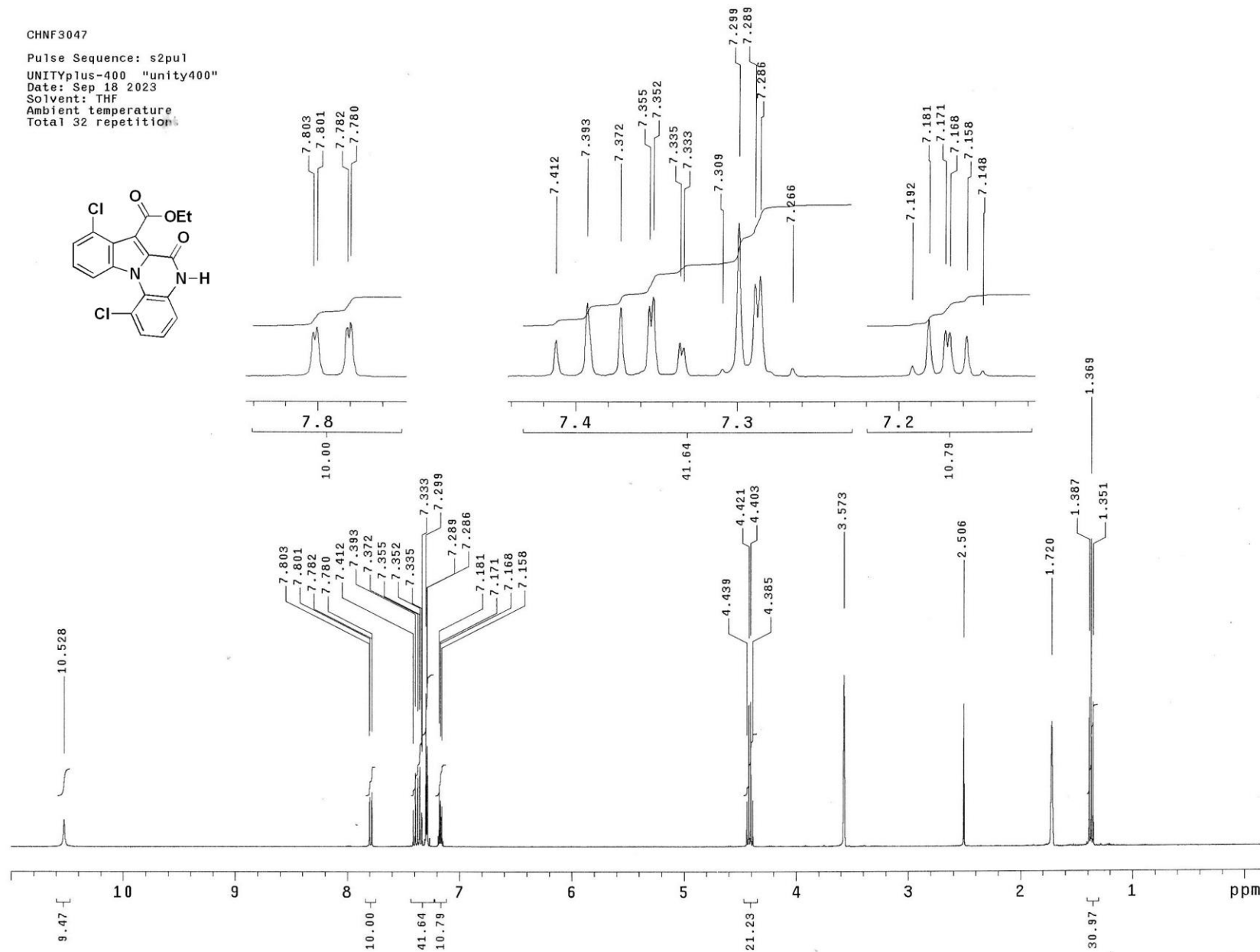
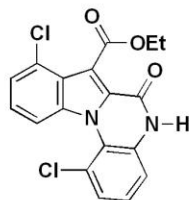
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 7 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 2160 repetitions



Compound 6b (¹H-NMR spectral data)

CHNF3047

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 18 2023
 Solvent: THF
 Ambient temperature
 Total 32 repetitions



Compound 6b (¹³C-NMR spectral data)

CHNF3047

Pulse Sequence: s2pu1

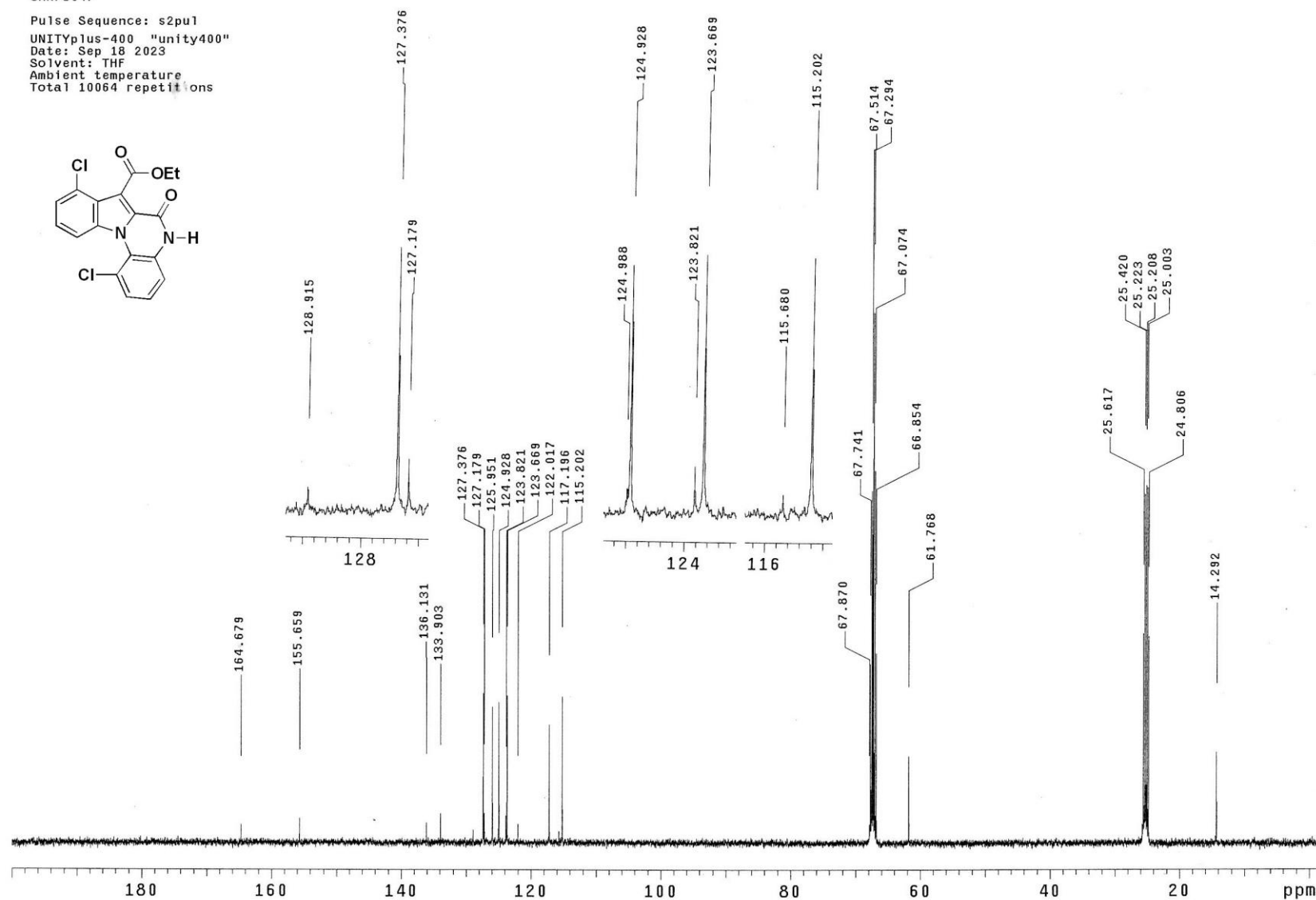
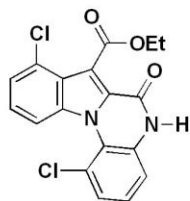
UNITYplus-400 "unity400"

Date: Sep 18 2023

Solvent: THF

Ambient temperature

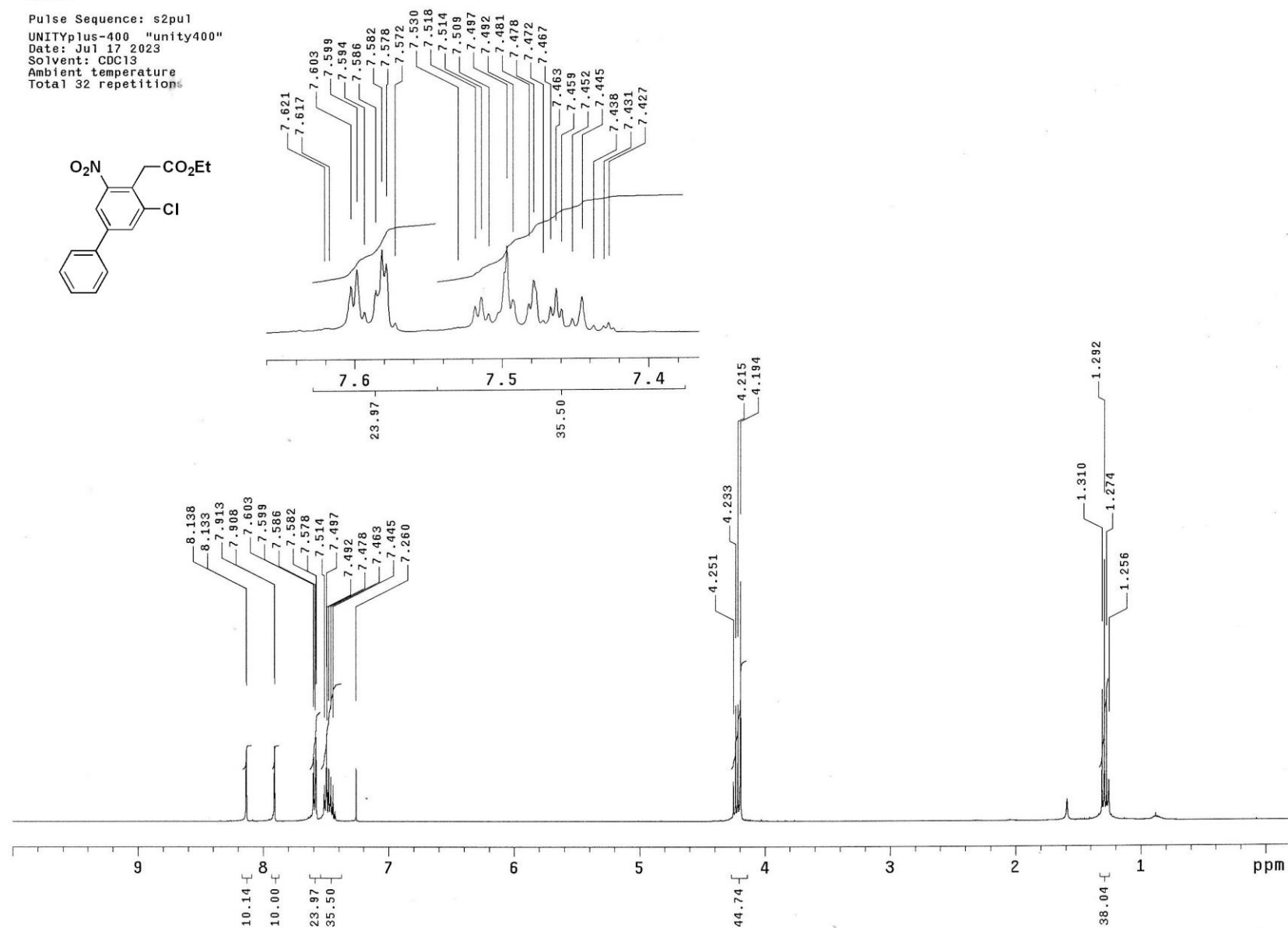
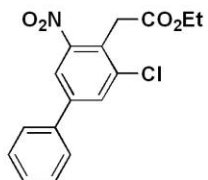
Total 10064 repetitions



Compound 7a (¹H-NMR spectral data)

CH3238

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jul 17 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 7a (¹³C-NMR spectral data)

CH3238

Pulse Sequence: s2pu1

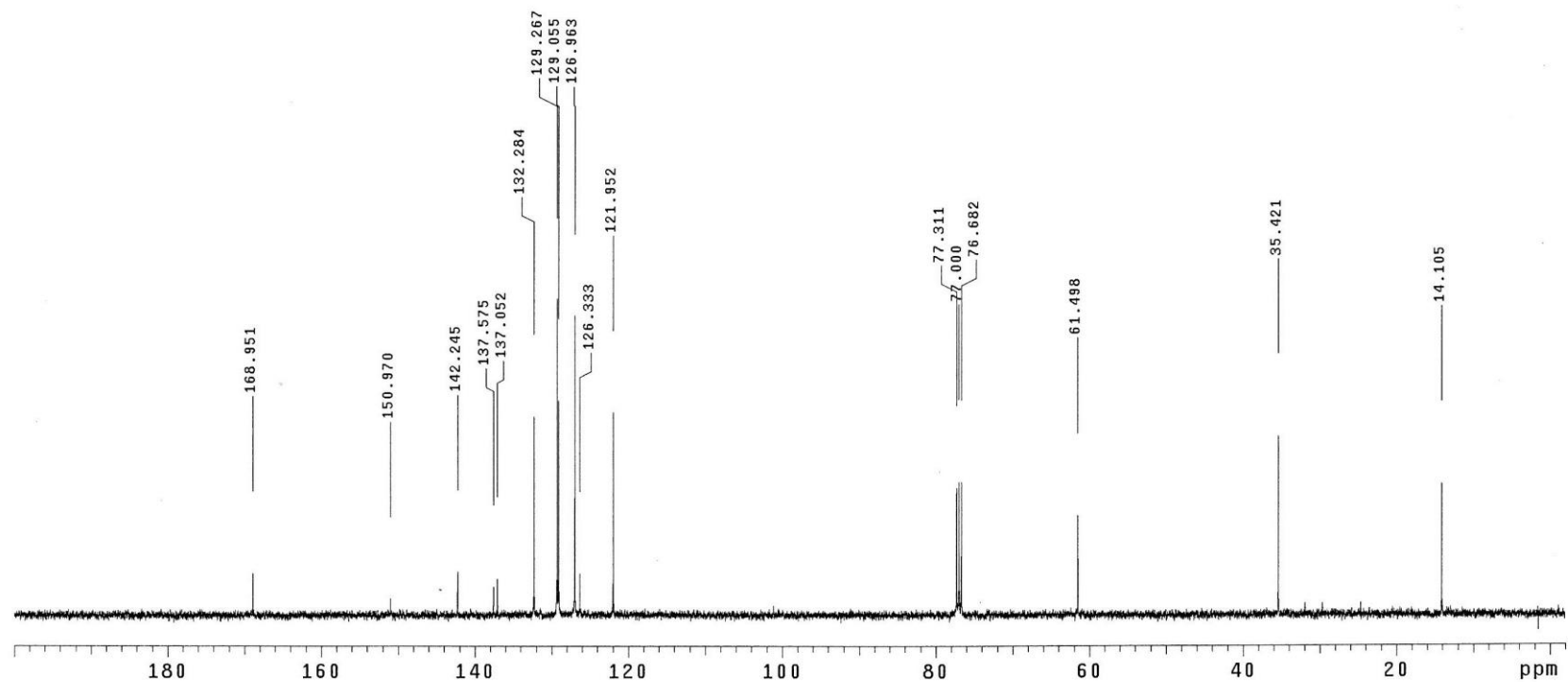
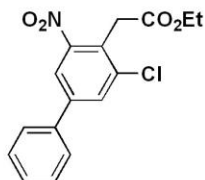
UNITYplus-400 "unity400"

Date: Jul 17 2023

Solvent: CDCl₃

Ambient temperature

Total 2368 repetitions



Compound 7b (¹H-NMR spectral data)

CH2734

Pulse Sequence: s2pu1

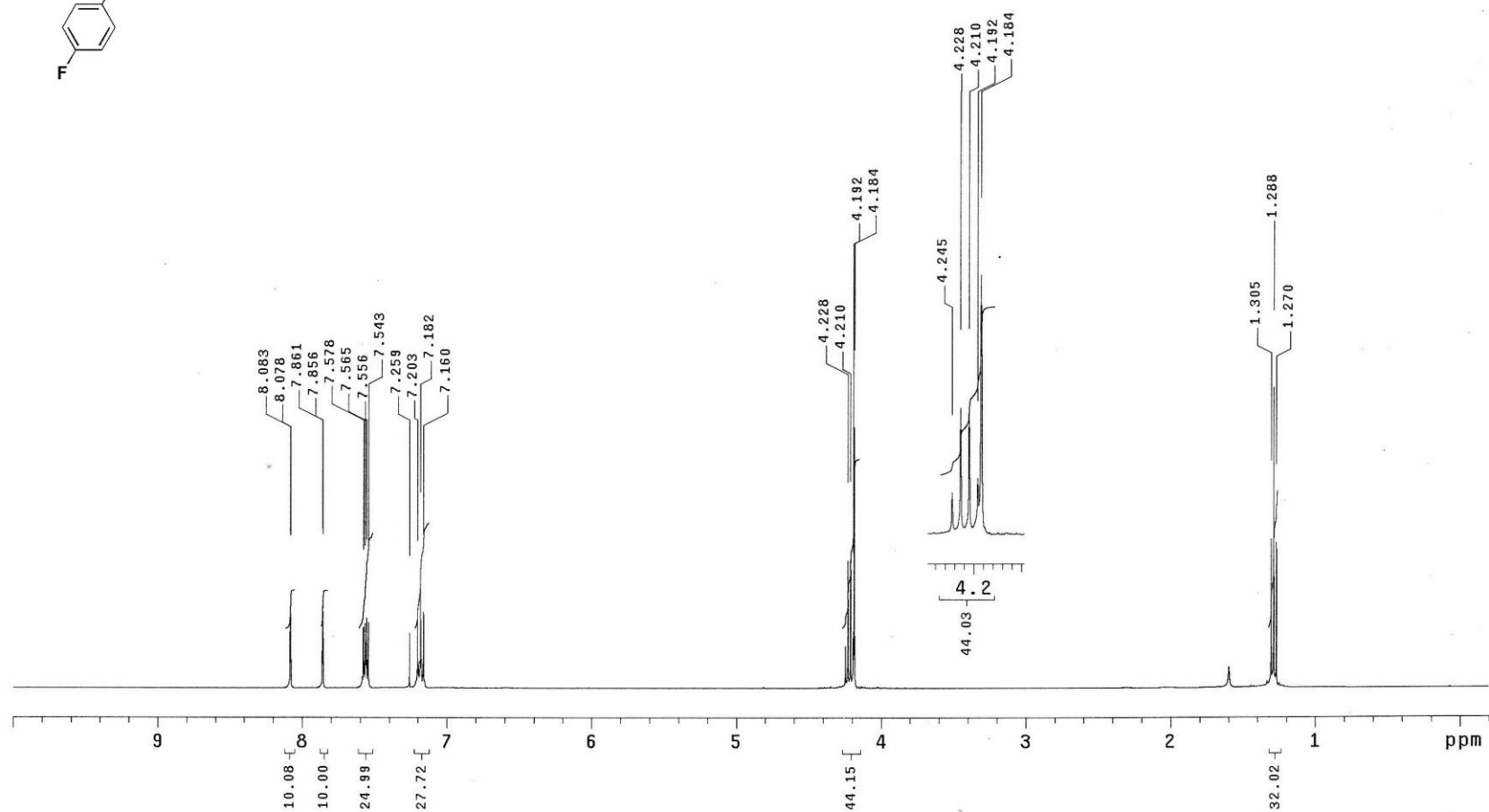
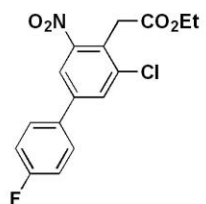
UNITYplus-400 "unity400"

Date: Jul 19 2023

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 7b (¹³C-NMR spectral data)

CH2734

Pulse Sequence: s2pu1

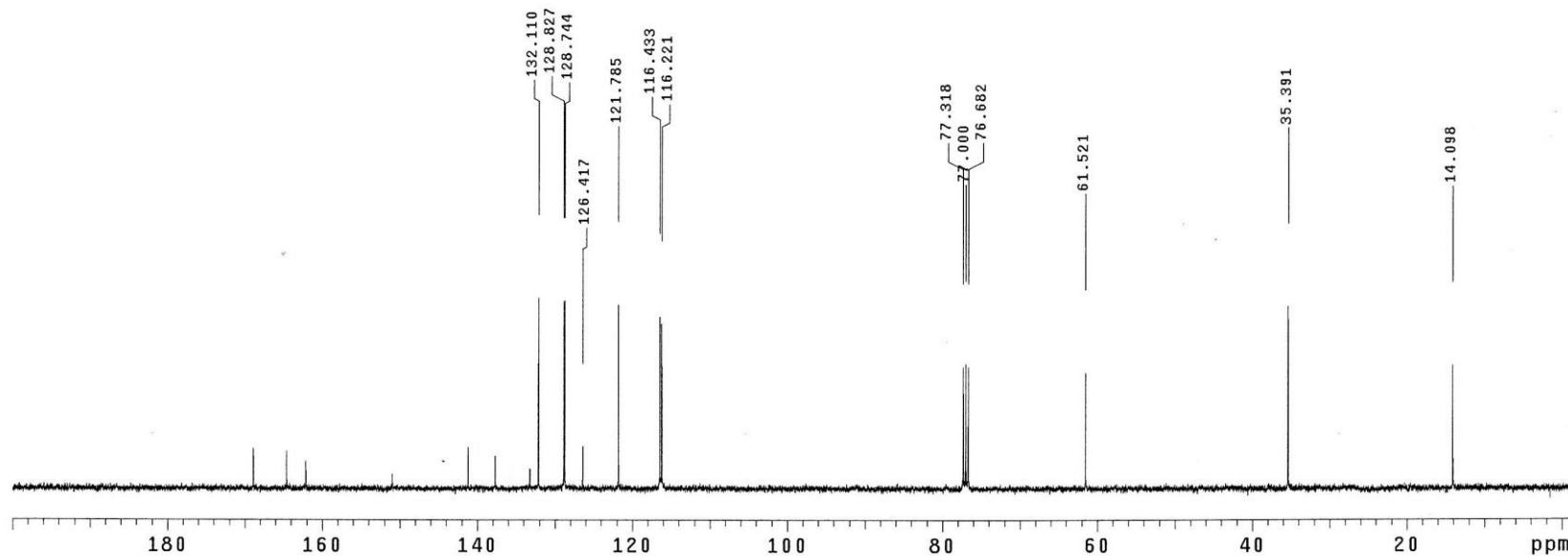
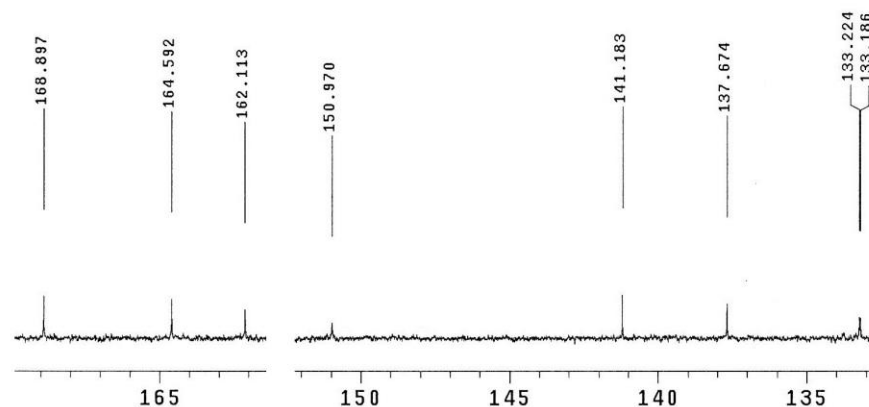
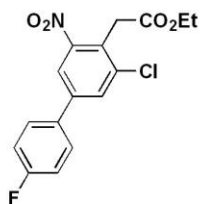
UNITYplus-400 "unity400"

Date: Jul 19 2023

Solvent: CDCl₃

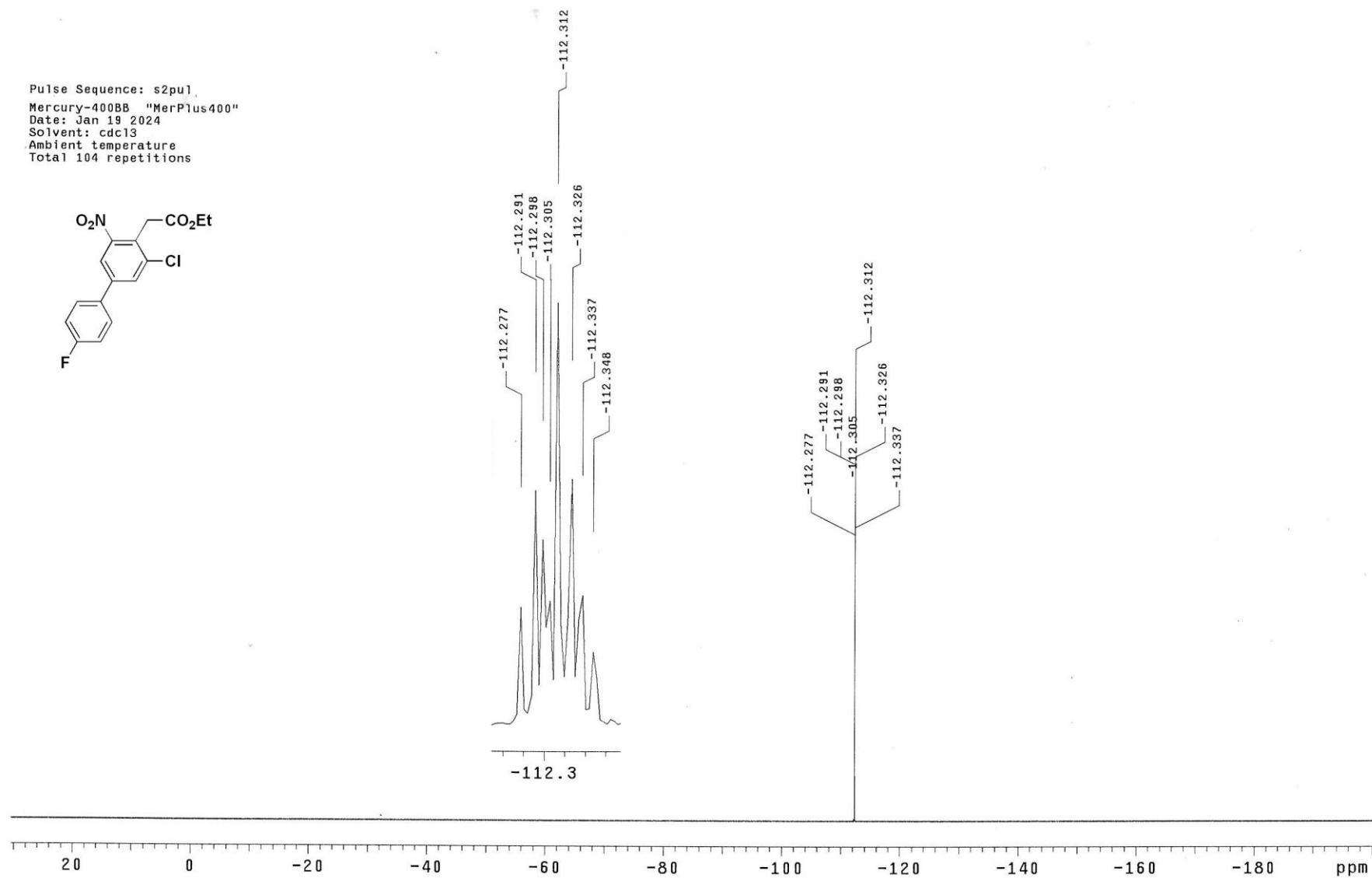
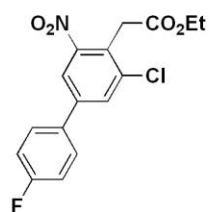
Ambient temperature

Total 2240 repetitions



Compound 7b (^{19}F -NMR spectral data)

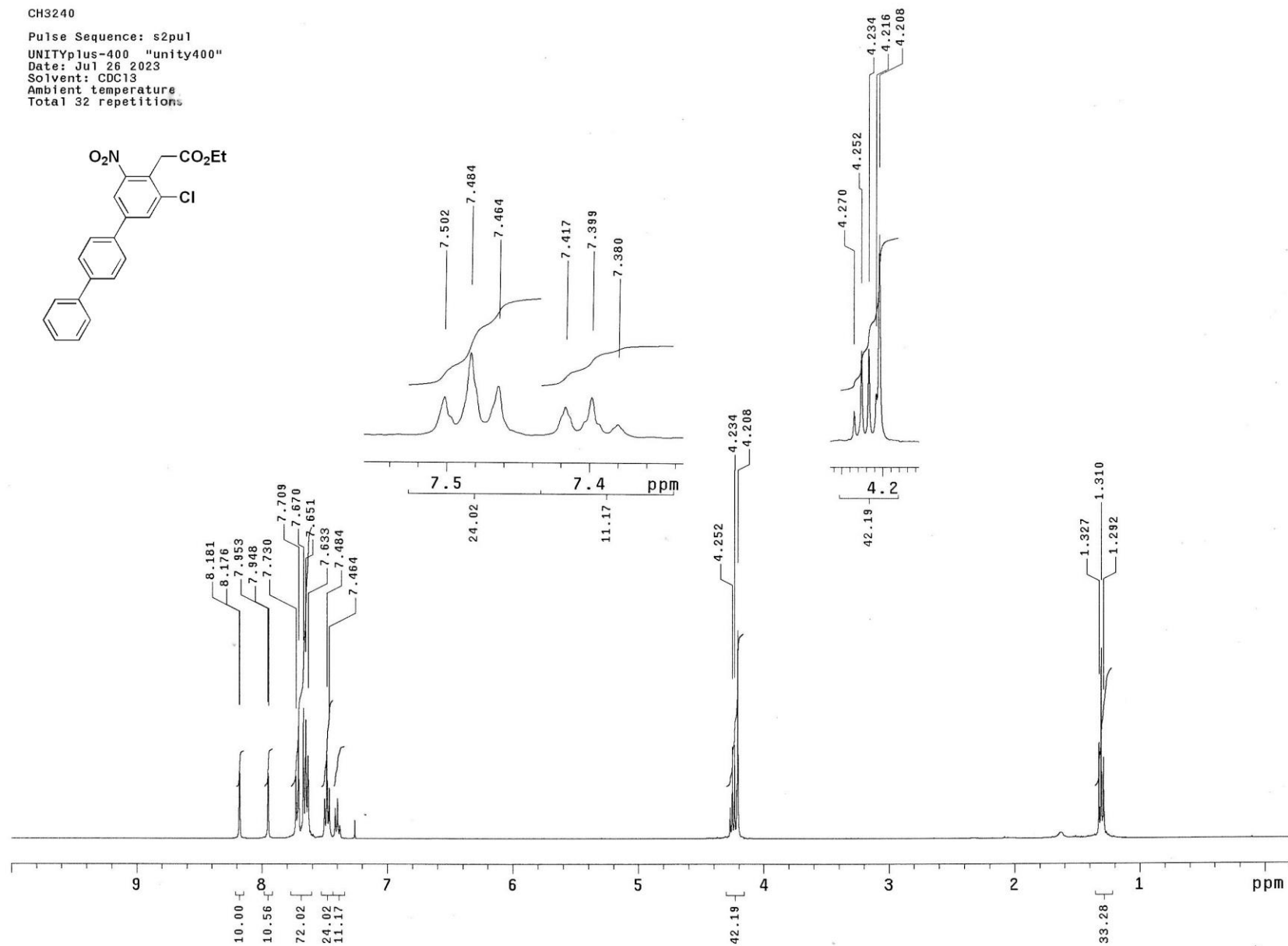
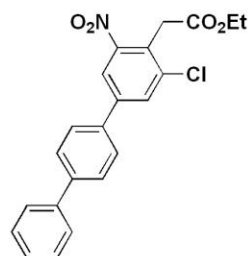
Pulse Sequence: s2pu1
Mercury-400BB "MerPlus400"
Date: Jan 19 2024
Solvent: cdcl3
Ambient temperature
Total 104 repetitions



Compound 7c (¹H-NMR spectral data)

CH3240

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jul 26 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 7c (¹³C-NMR spectral data)

CH3240

Pulse Sequence: s2pu1

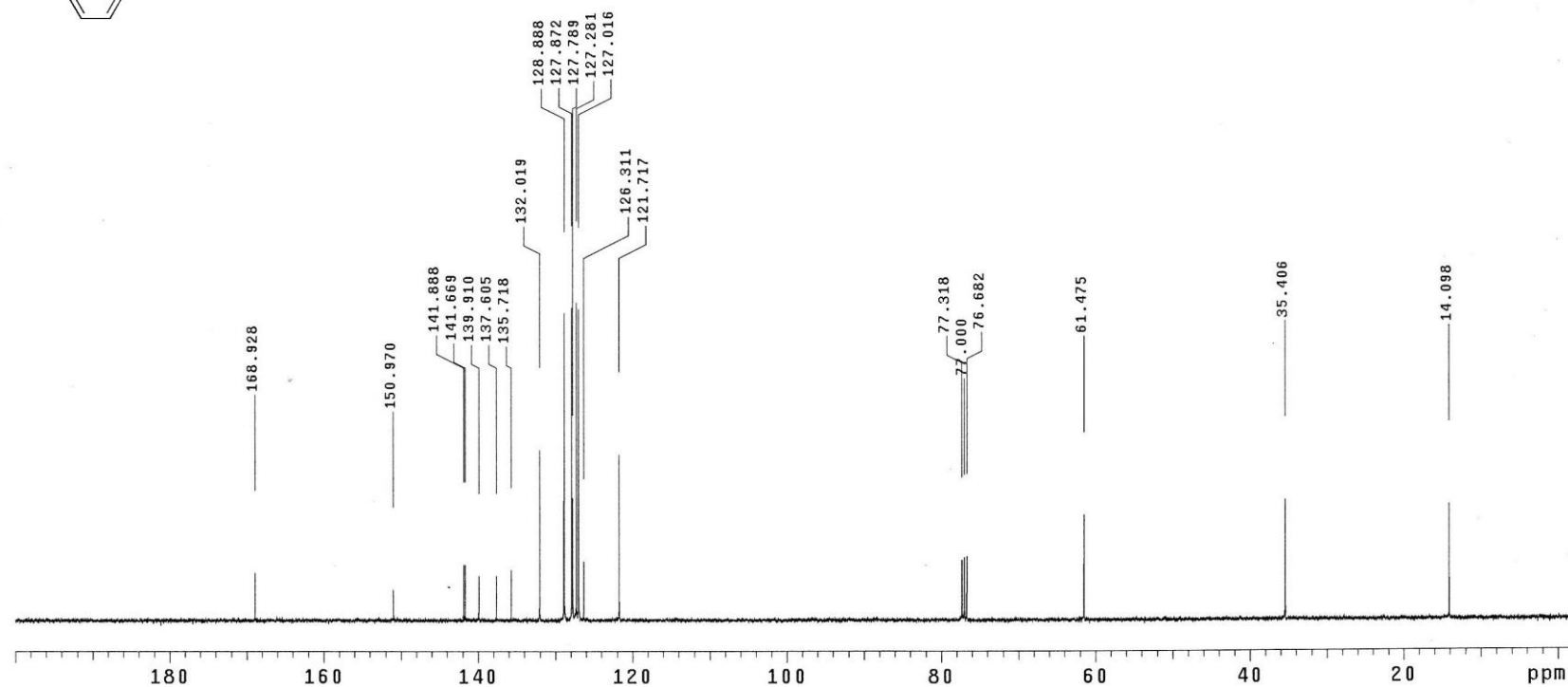
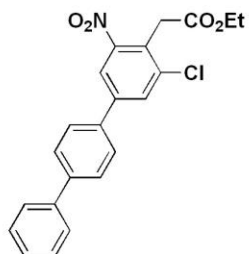
UNITYplus-400 "unity400"

Date: Jul 26 2023

Solvent: CDCl₃

Ambient temperature

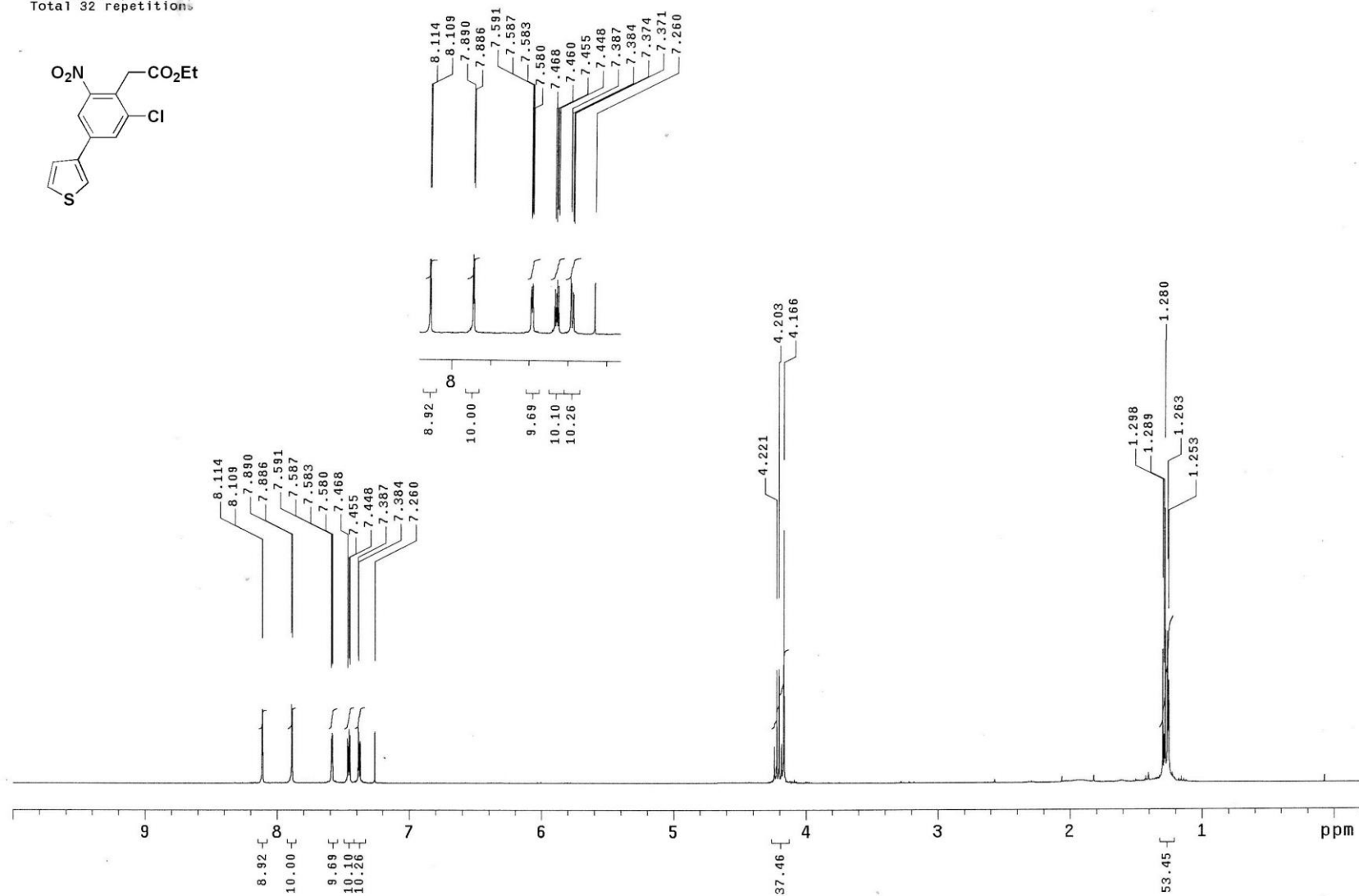
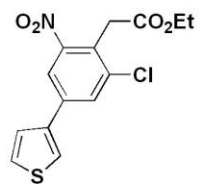
Total 1200 repetitions



Compound 7d (¹H-NMR spectral data)

CH3742

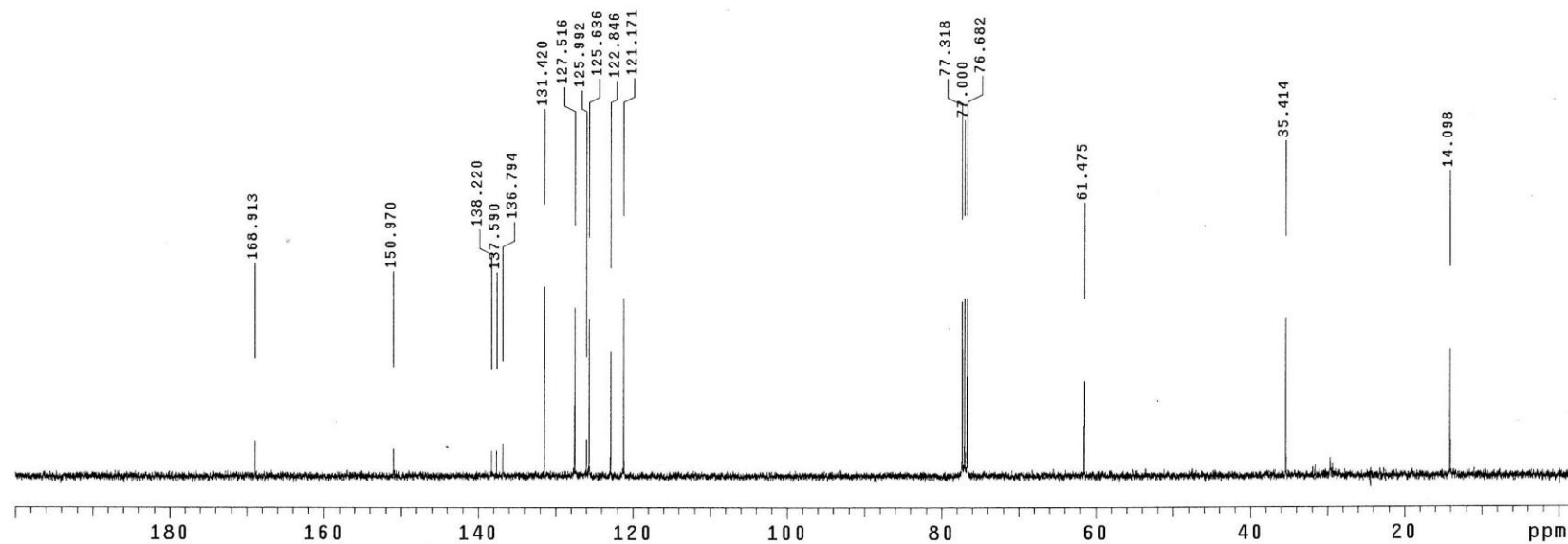
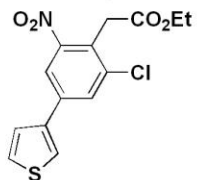
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 17 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 7d (¹³C-NMR spectral data)

CH3742

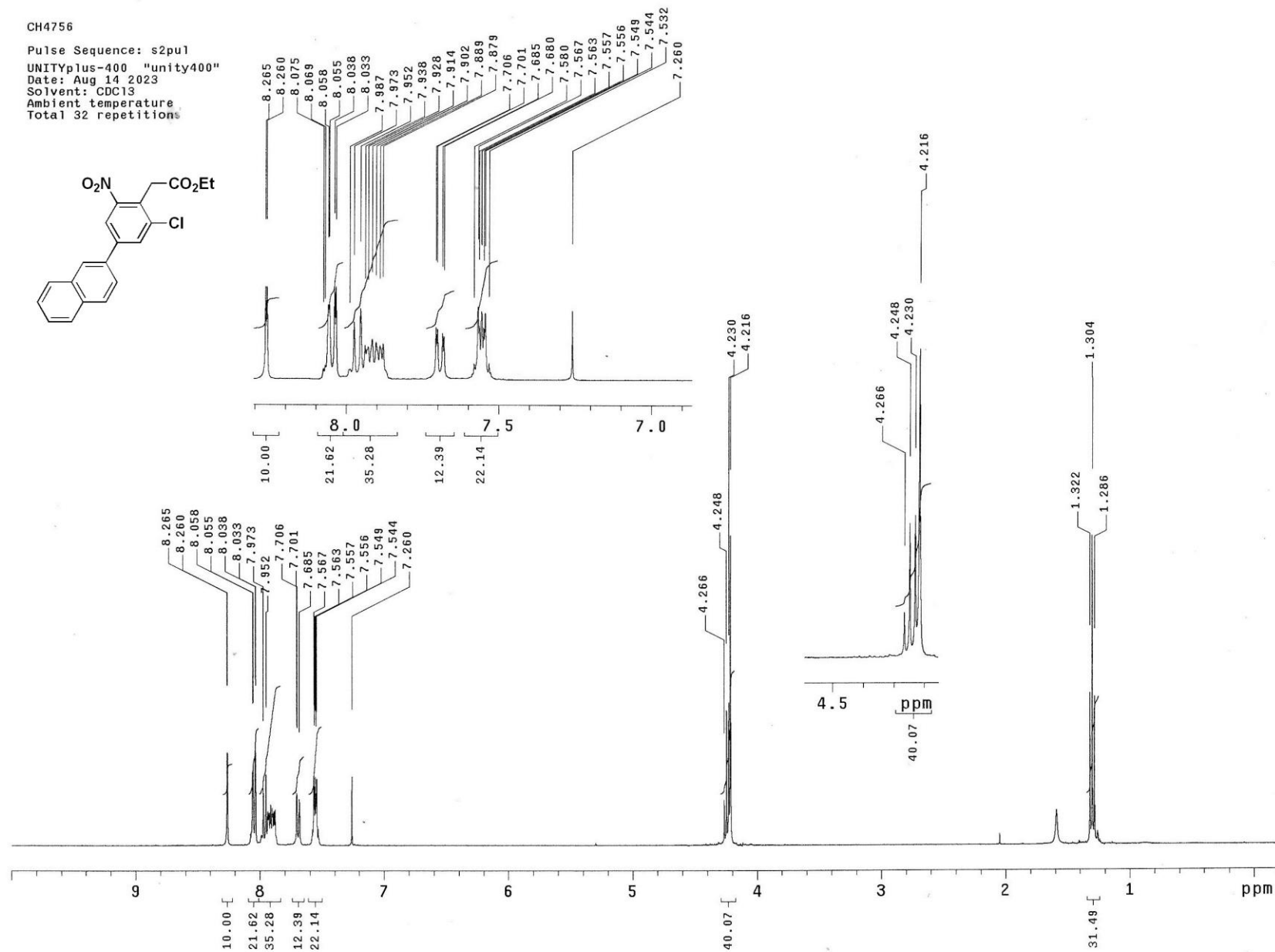
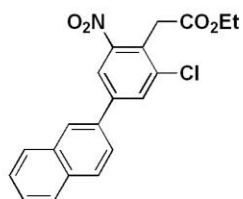
Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Aug 17 2023
Solvent: CDCl₃
Ambient temperature
Total 2048 repetitions



Compound 7e (¹H-NMR spectral data)

CH4756

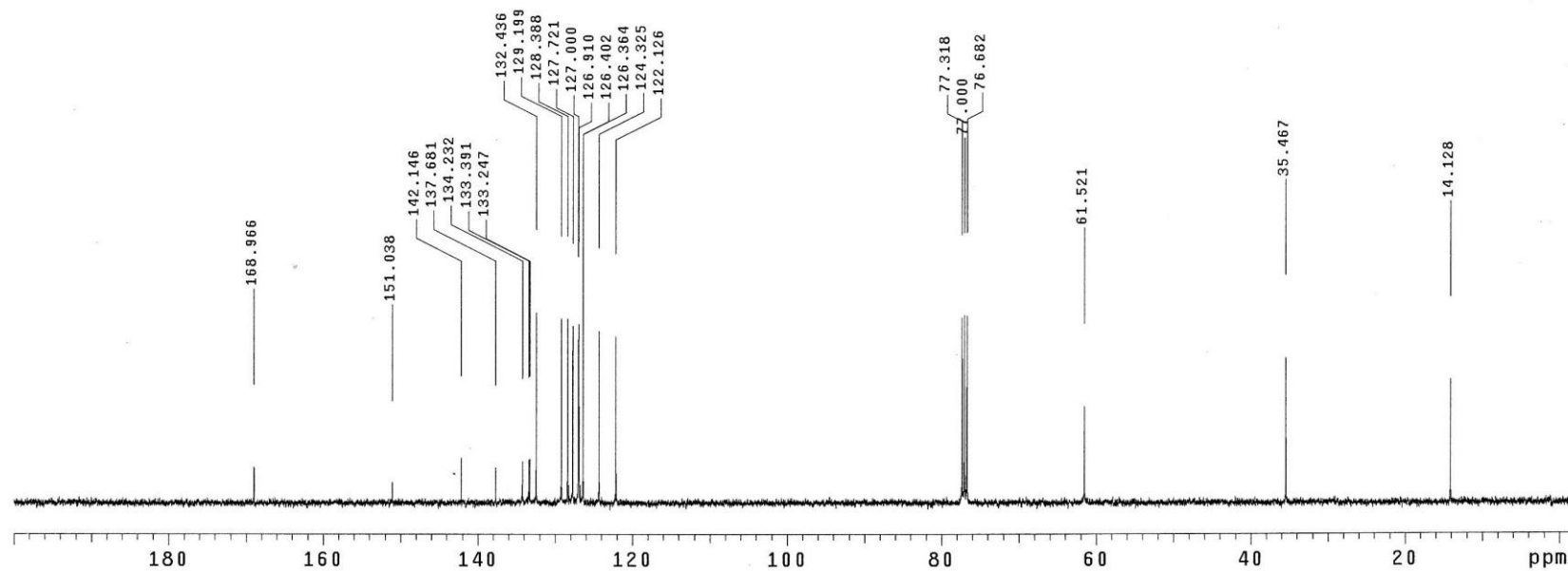
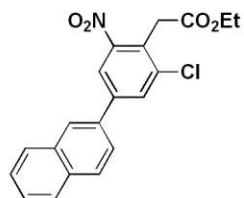
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 14 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 7e (¹³C-NMR spectral data)

CH4756

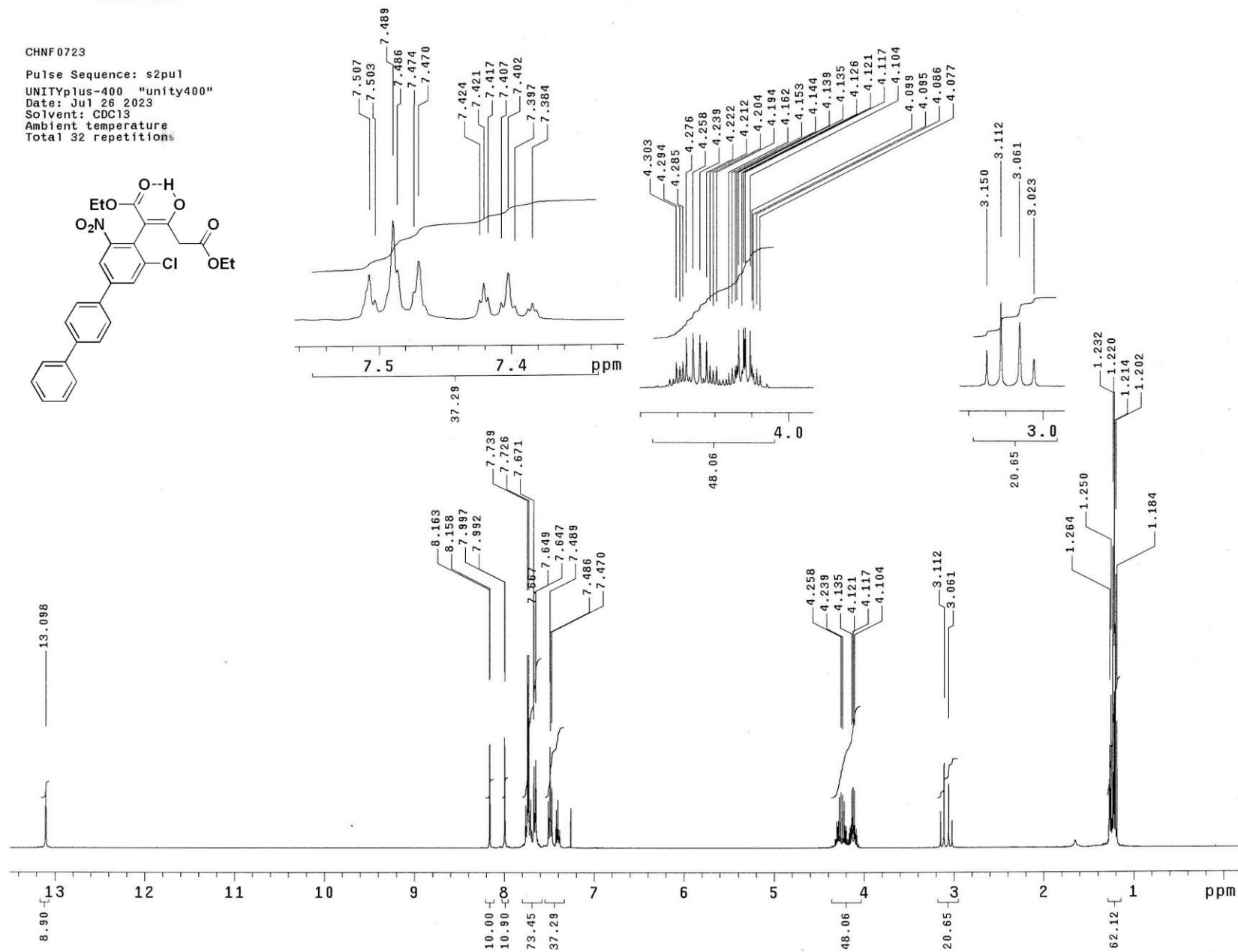
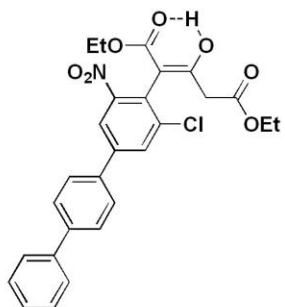
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 14 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 3888 repetitions



Compound 8a (¹H-NMR spectral data)

CHNF0723

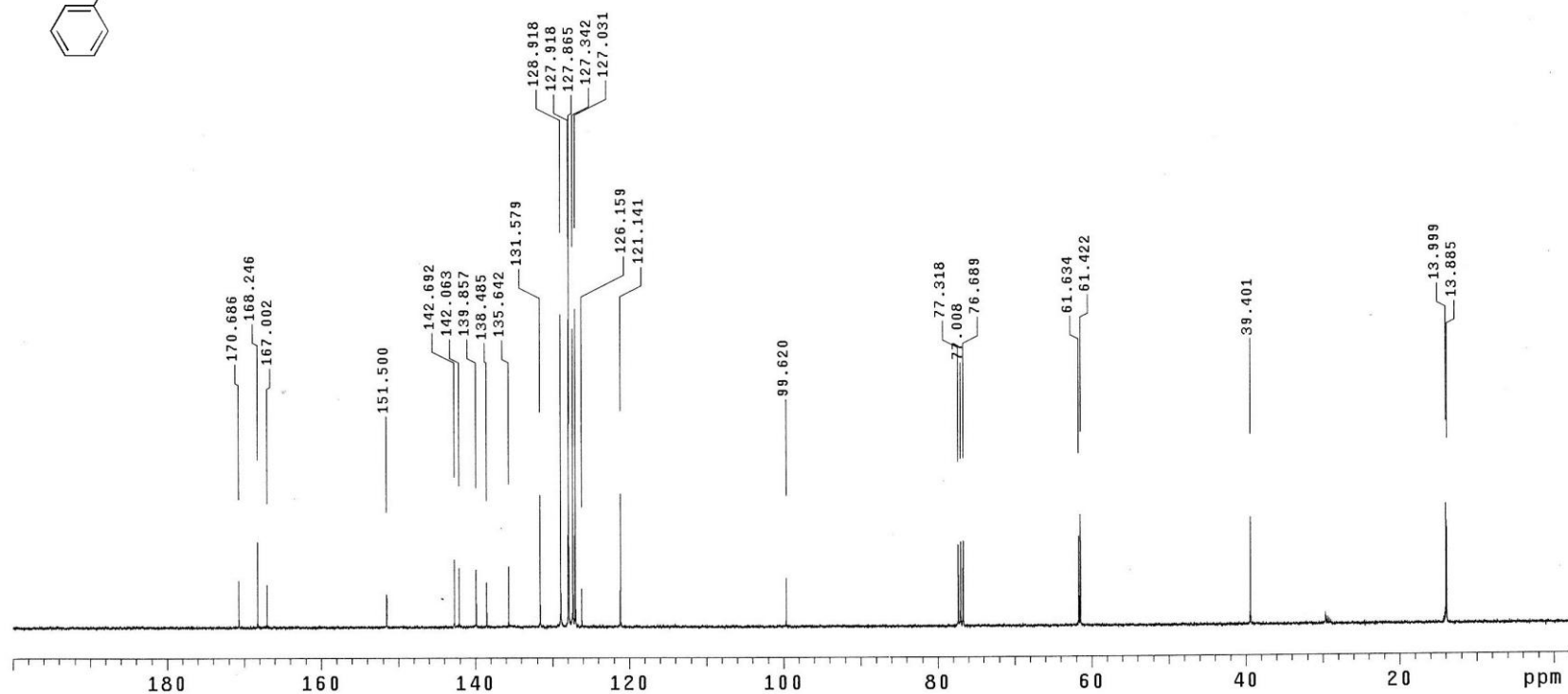
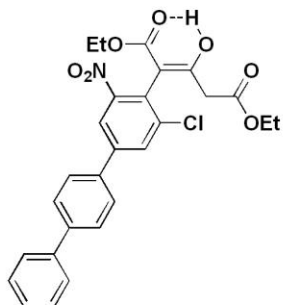
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jul 26 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 8a (¹³C-NMR spectral data)

CHNF0723

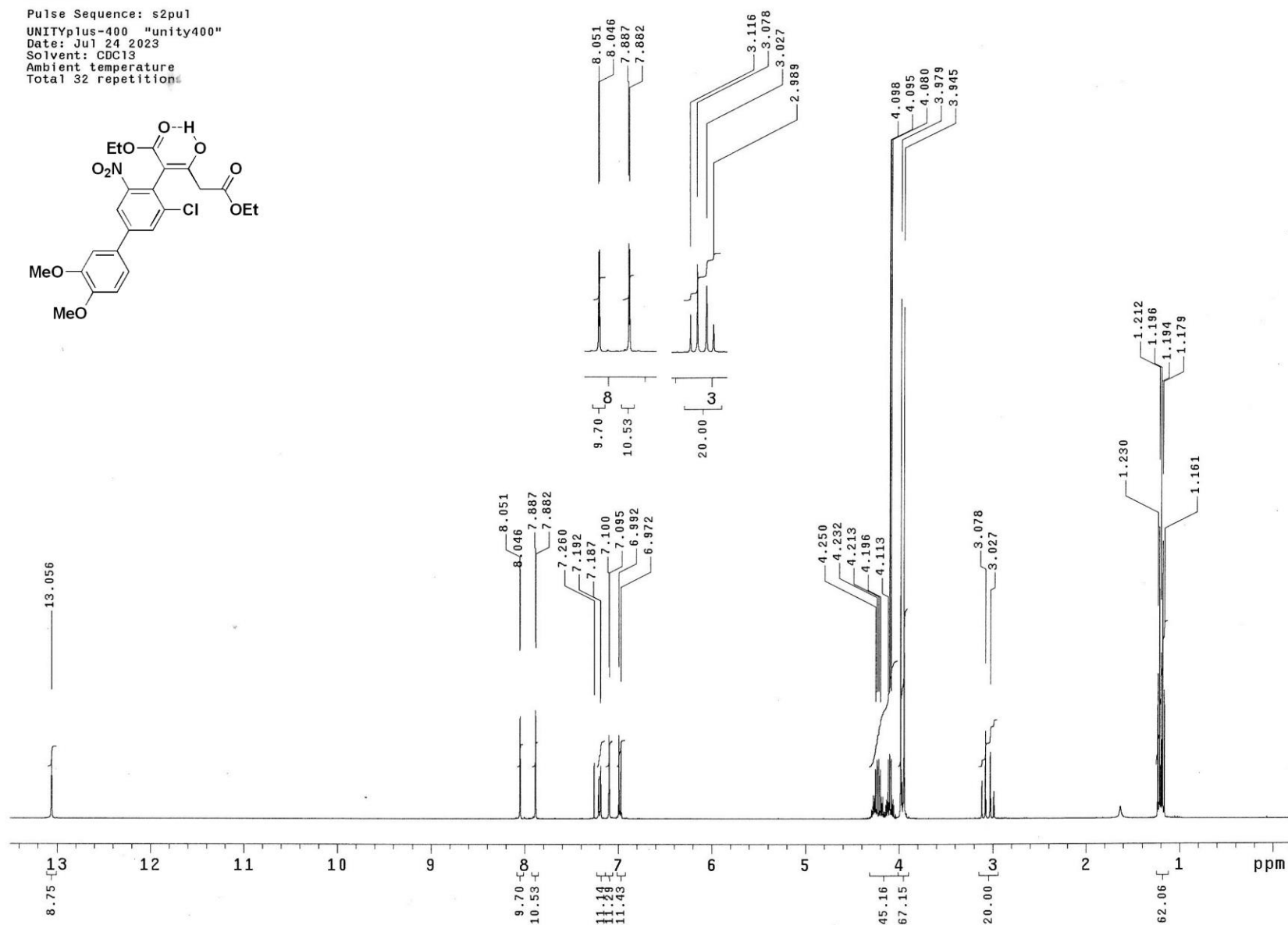
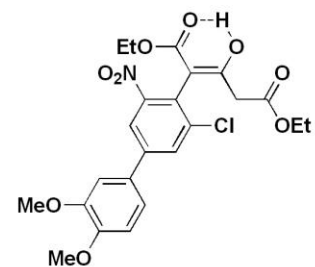
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jul 26 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 3824 repetitions



Compound 8b (¹H-NMR spectral data)

CHNF0720

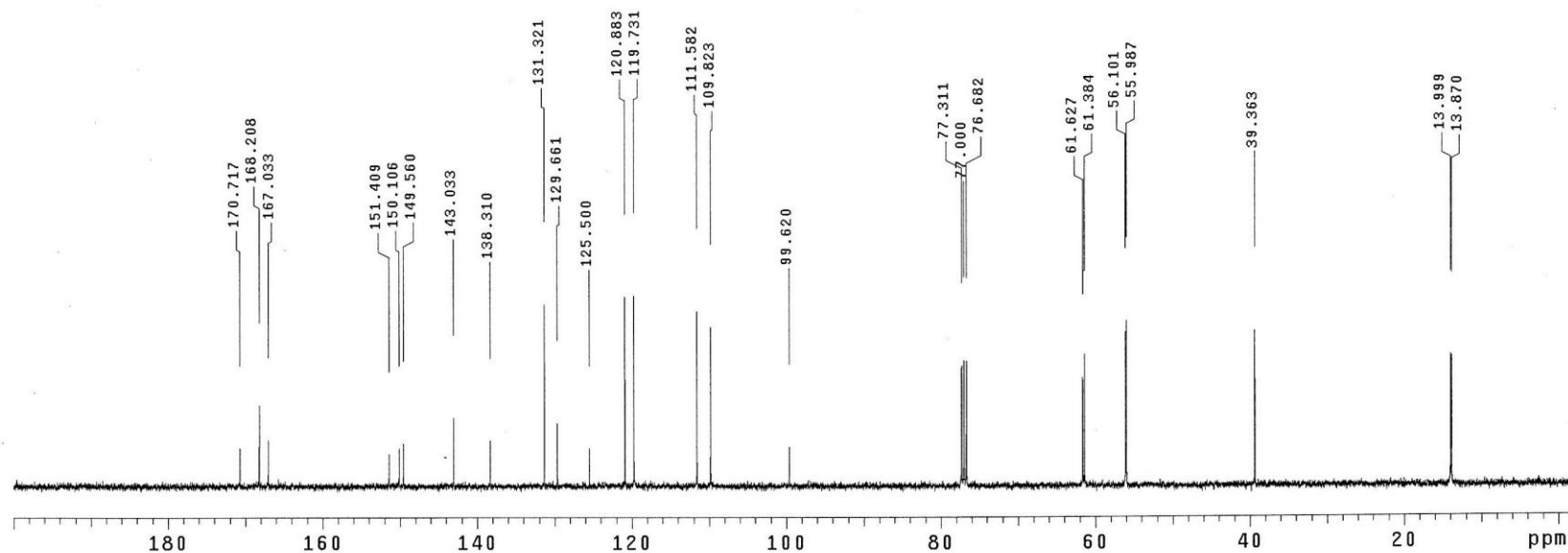
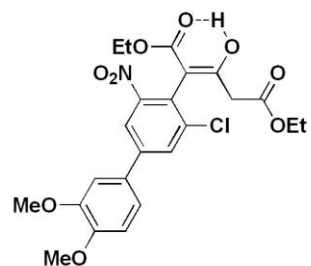
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jul 24 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 8b (¹³C-NMR spectral data)

CHNF0720

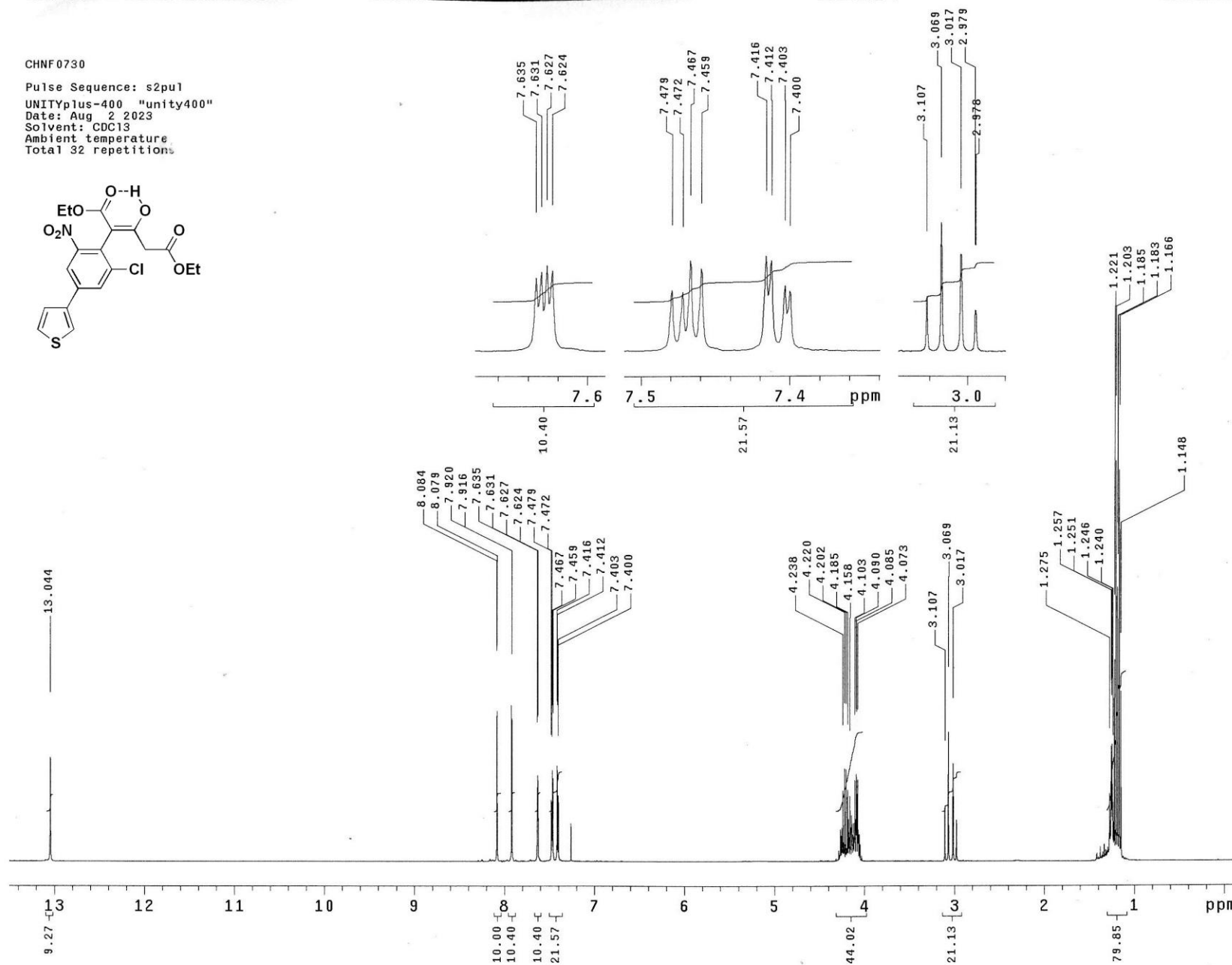
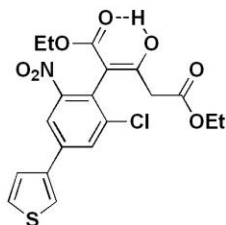
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jul 24 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 1648 repetitions



Compound 8c (¹H-NMR spectral data)

CHNF0730

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Aug 2 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 8c (¹³C-NMR spectral data)

CHNF0730

Pulse Sequence: s2pu1

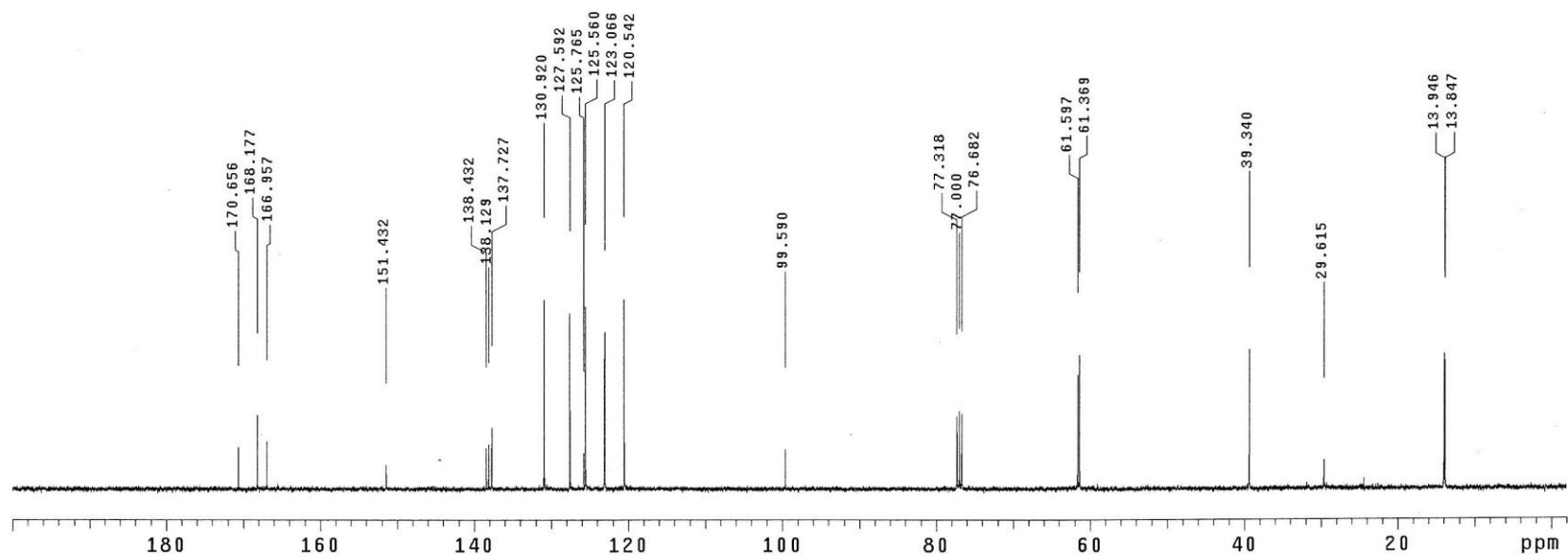
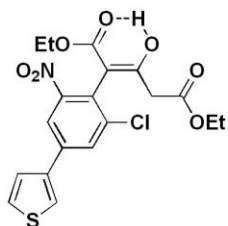
UNITYplus-400 "unity400"

Date: Aug 2 2023

Solvent: CDCl₃

Ambient temperature

Total 1072 repetitions



Compound 8d (¹H-NMR spectral data)

CHNF0811

Pulse Sequence: s2pu1

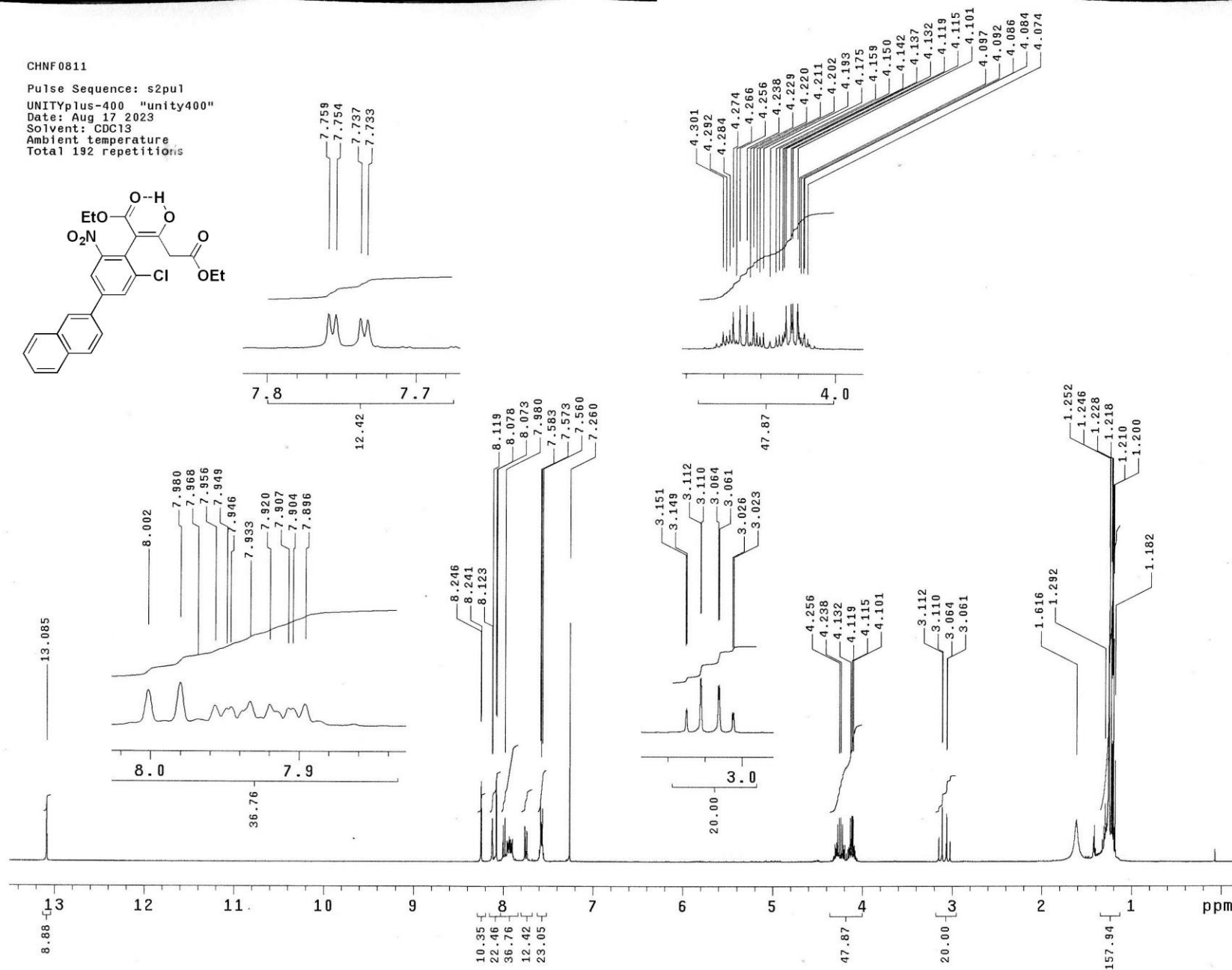
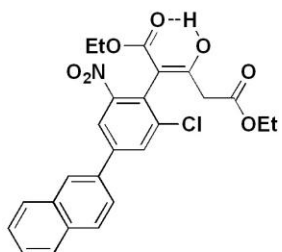
UNITYplus-400 "unity400"

Date: Aug 17 2023

Solvent: CDCl₃

Ambient temperature

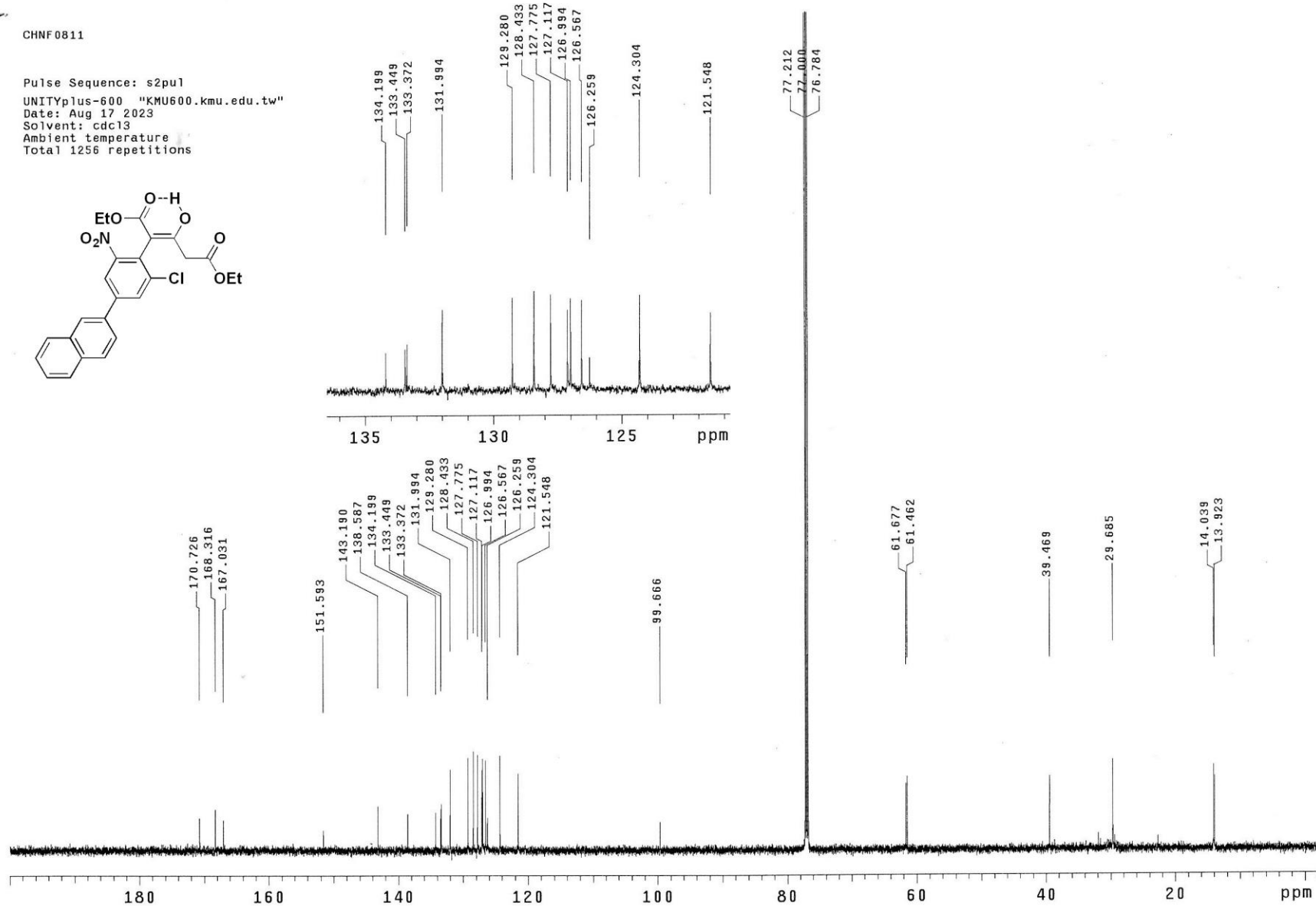
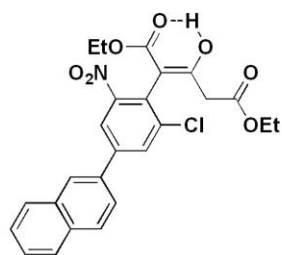
Total 192 repetitions



Compound 8d (¹³C-NMR spectral data)

CHNF0811

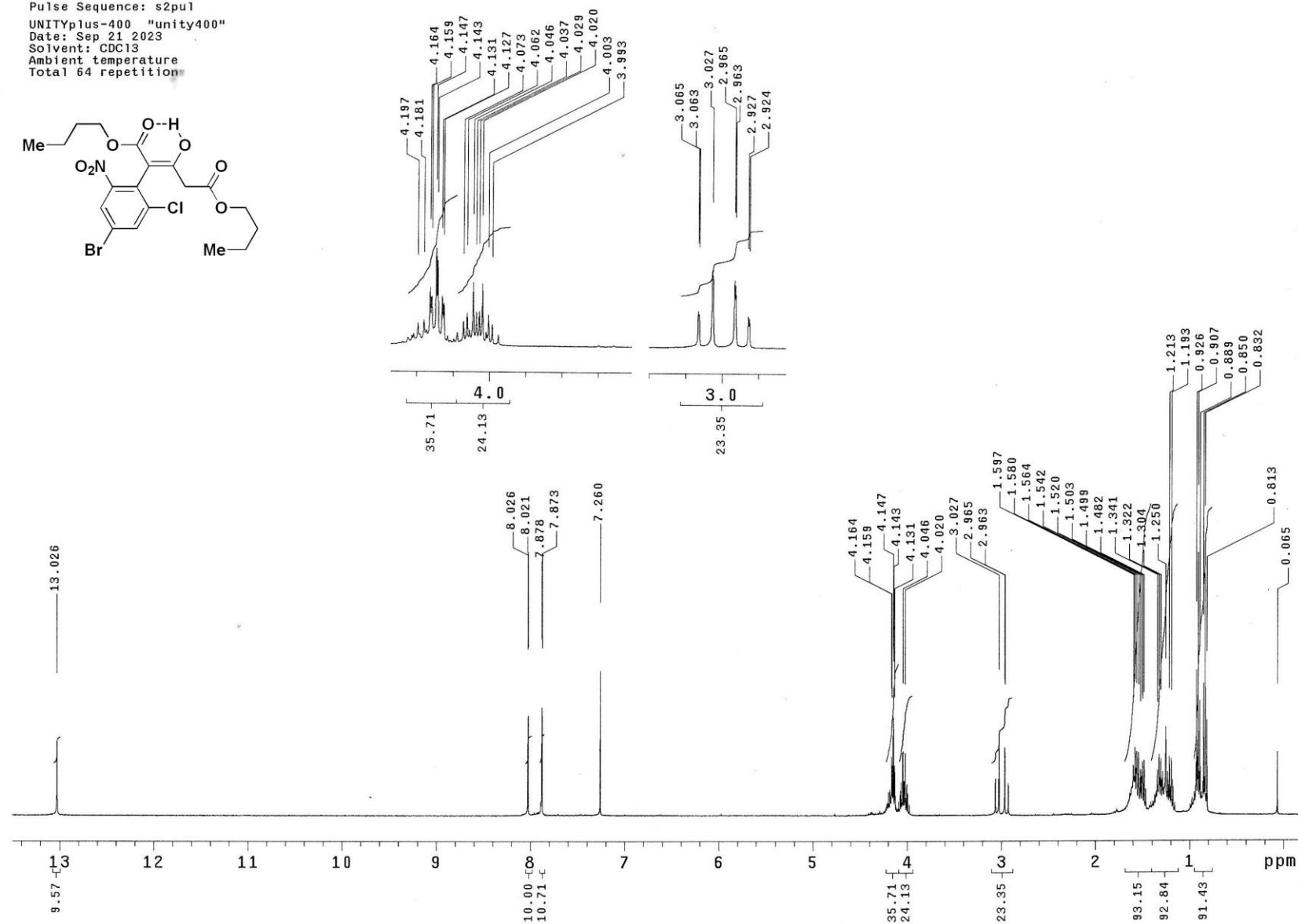
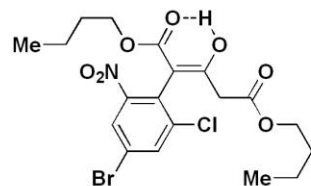
Pulse Sequence: s2pu1
 UNITYplus-600 "KMU600.kmu.edu.tw"
 Date: Aug 17 2023
 Solvent: cdc13
 Ambient temperature
 Total 1256 repetitions



Compound 8e (¹H-NMR spectral data)

CHNF0921

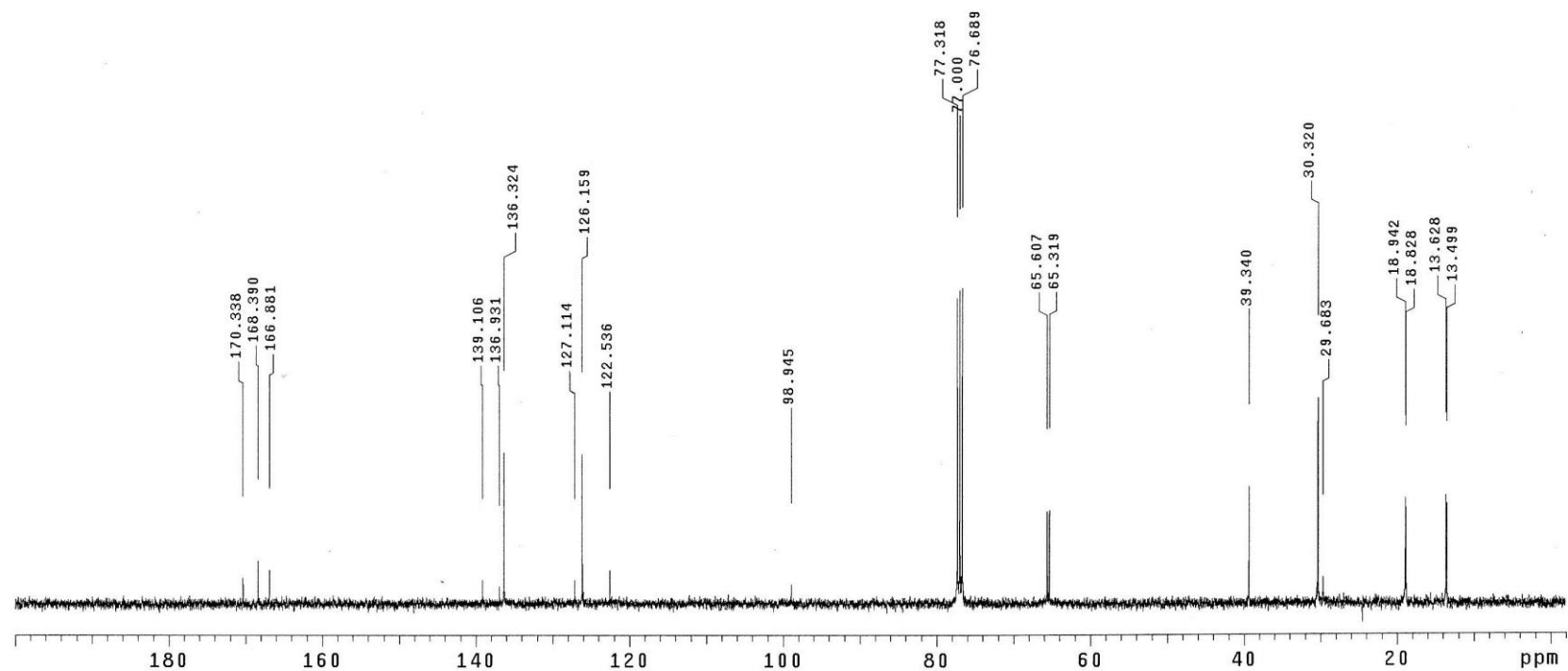
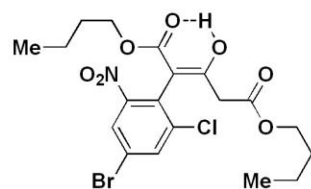
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 21 2023
 Solvent: CDCl₃
 Ambient temperature
 Total 64 repetition



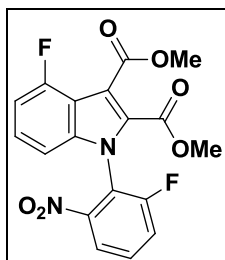
Compound 8e (¹³C-NMR spectral data)

CHNF0921

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 21 2023
 Solvent: CDCl₃
 Ambient temperature
 File: U0315-4
 Total 8672 repetitions

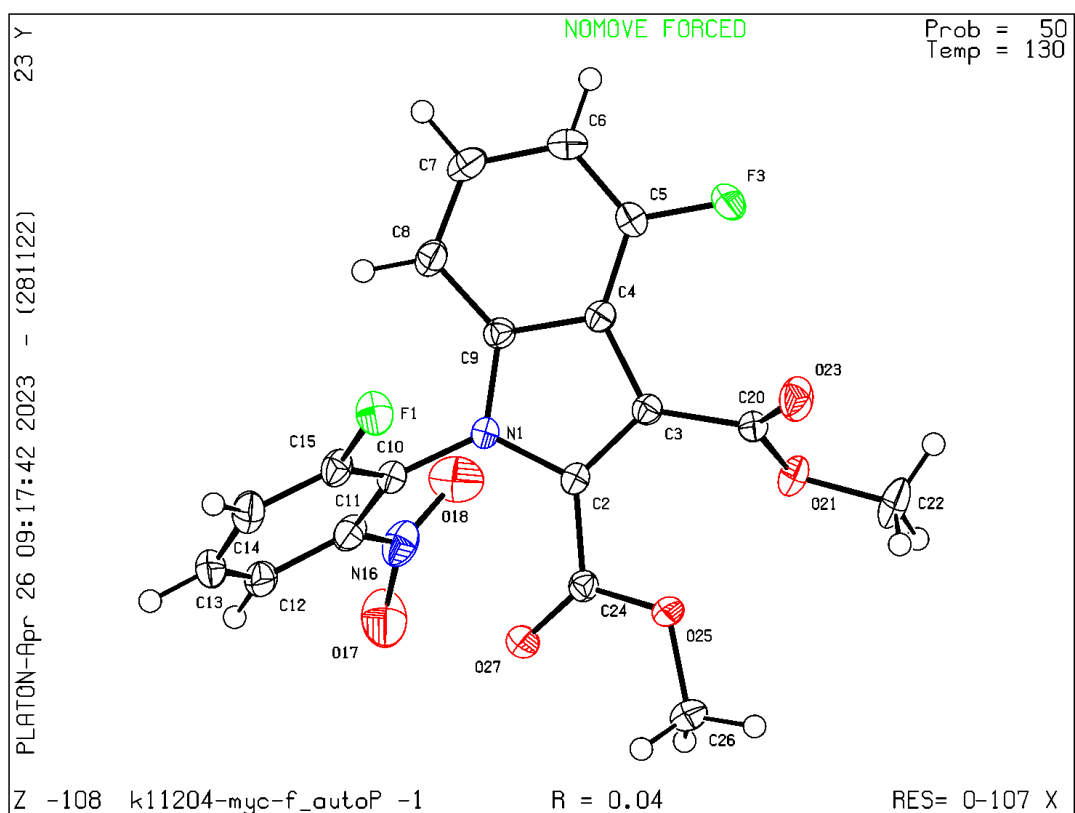


X-ray crystal data of compound 4a



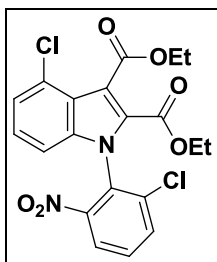
Sample preparation : A solution of compound **4a** (30 mg) in CH₂Cl₂ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

Crystal measurement : X-ray crystal structures were determined with a Bruker Enraf-Nonius single-crystal diffractometer (CAD4, Kappa CCD). Thermal ellipsoids are drawn at 50% probability level.



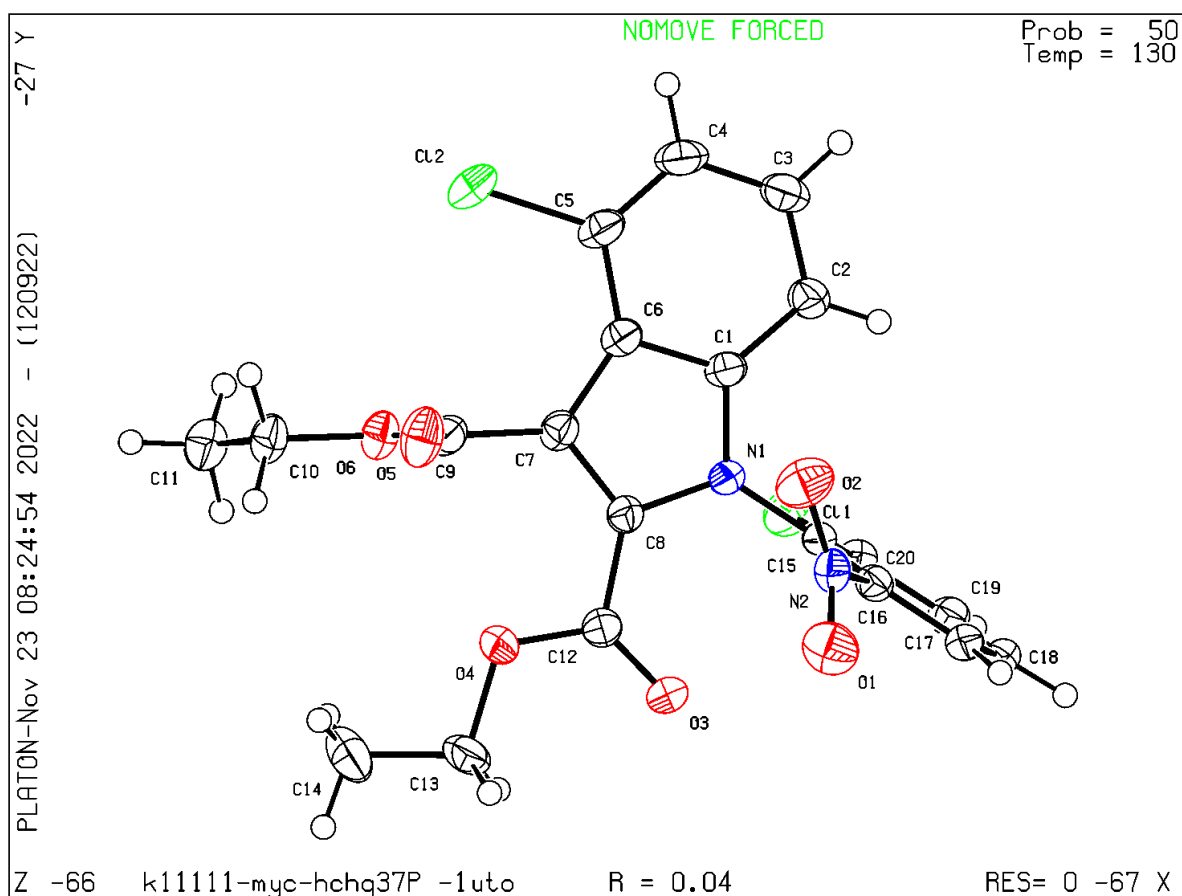
Empirical formula	C ₁₈ H ₁₂ F ₂ N ₂ O ₆
Formula weight	390.30
Temperature/K	130(2)
Crystal system	triclinic
Space group	P-1
a/Å	7.8953(2)
b/Å	10.6880(2)
c/Å	10.9838(2)
α/°	68.919(2)
β/°	77.025(2)
γ/°	82.949(2)
Volume/Å ³	841.86(3)
Z	2
ρ _{calc} /cm ³	1.540
μ/mm ⁻¹	0.131
F(000)	400.0
Crystal size/mm ³	0.5 × 0.4 × 0.4
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.052 to 53.942
Index ranges	-9 ≤ h ≤ 9, -13 ≤ k ≤ 13, -13 ≤ l ≤ 13
Reflections collected	22714
Independent reflections	3516 [R _{int} = 0.0359, R _{sigma} = 0.0240]
Data/restraints/parameters	3516/0/256
Goodness-of-fit on F ²	1.068
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0389, wR ₂ = 0.0995
Final R indexes [all data]	R ₁ = 0.0456, wR ₂ = 0.1035
Largest diff. peak/hole / e Å ⁻³	0.44/-0.23

X-ray crystal data of compound 4g



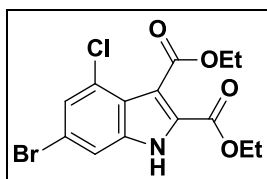
Sample preparation : A solution of compound **4g** (30 mg) in CH₂Cl₂ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

Crystal measurement : X-ray crystal structures were determined with a Bruker Enraf-Nonius single-crystal diffractometer (CAD4, Kappa CCD). Thermal ellipsoids are drawn at 50% probability level.



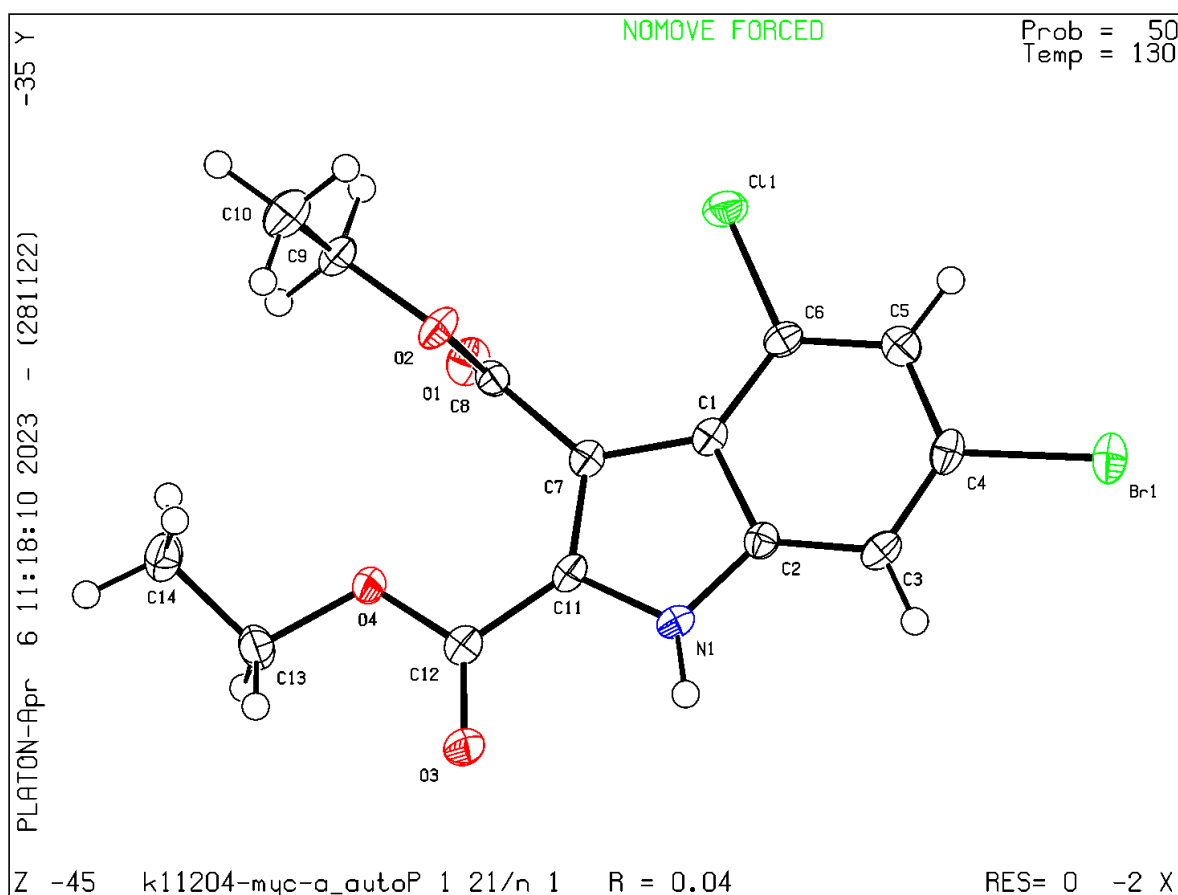
Empirical formula	C ₂₀ H ₁₆ Cl ₂ N ₂ O ₆
Formula weight	451.25
Temperature/K	130(2)
Crystal system	triclinic
Space group	P-1
a/Å	8.0746(2)
b/Å	8.2867(3)
c/Å	16.9277(3)
α /°	95.590(2)
β /°	98.647(2)
γ /°	114.340(3)
Volume/Å ³	1004.16(5)
Z	2
ρ_{calc} /cm ³	1.492
μ /mm ⁻¹	0.365
F(000)	464.0
Crystal size/mm ³	0.5 × 0.4 × 0.4
Radiation	Mo K α (λ = 0.71073)
2 Θ range for data collection/°	4.946 to 49.98
Index ranges	-9 ≤ h ≤ 9, -9 ≤ k ≤ 9, -20 ≤ l ≤ 20
Reflections collected	25407
Independent reflections	3539 [R_{int} = 0.0369, R_{sigma} = 0.0228]
Data/restraints/parameters	3539/1/273
Goodness-of-fit on F ²	1.055
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0397, wR_2 = 0.1030
Final R indexes [all data]	R_1 = 0.0464, wR_2 = 0.1073
Largest diff. peak/hole / e Å ⁻³	0.63/-0.36

X-ray crystal data of compound 5c



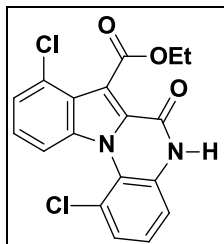
Sample preparation : A solution of compound **5c** (30 mg) in CH₂Cl₂ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

Crystal measurement : X-ray crystal structures were determined with a Bruker Enraf-Nonius single-crystal diffractometer (CAD4, Kappa CCD). Thermal ellipsoids are drawn at 50% probability level.



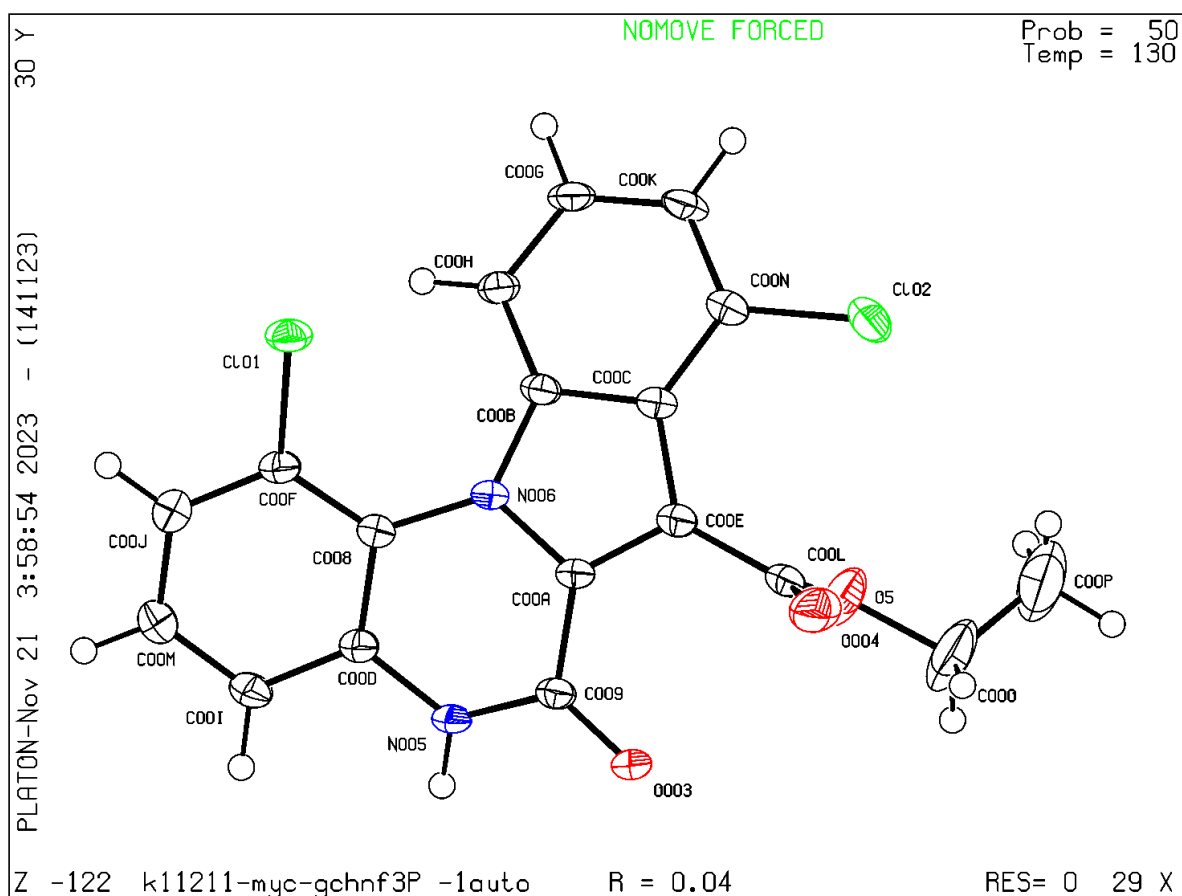
Empirical formula	C ₁₄ H ₁₃ BrClNO ₄
Formula weight	374.61
Temperature/K	130(2)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	7.4292(3)
b/Å	16.5544(8)
c/Å	12.3299(5)
α/°	90
β/°	96.297(4)
γ/°	90
Volume/Å ³	1507.26(11)
Z	4
ρ _{calc} /cm ³	1.651
μ/mm ⁻¹	2.918
F(000)	752.0
Crystal size/mm ³	0.5 × 0.4 × 0.2
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.136 to 54.166
Index ranges	-9 ≤ h ≤ 8, -21 ≤ k ≤ 21, -15 ≤ l ≤ 15
Reflections collected	20549
Independent reflections	3138 [R _{int} = 0.0520, R _{sigma} = 0.0447]
Data/restraints/parameters	3138/0/192
Goodness-of-fit on F ²	1.024
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0387, wR ₂ = 0.0854
Final R indexes [all data]	R ₁ = 0.0478, wR ₂ = 0.0884
Largest diff. peak/hole / e Å ⁻³	1.25/-0.96

X-ray crystal data of compound 6b



Sample preparation : A solution of compound **6b** (30 mg) in CH₂Cl₂ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

Crystal measurement : X-ray crystal structures were determined with a Bruker Enraf-Nonius single-crystal diffractometer (CAD4, Kappa CCD). Thermal ellipsoids are drawn at 50% probability level.



Empirical formula	C ₁₈ H ₁₂ Cl ₂ N ₂ O ₃
Formula weight	375.20
Temperature/K	130(2)
Crystal system	triclinic
Space group	P-1
a/Å	8.2481(2)
b/Å	10.2725(2)
c/Å	10.6752(2)
α/°	68.739(2)
β/°	77.265(2)
γ/°	87.293(2)
Volume/Å ³	821.67(3)
Z	2
ρ _{calc} /g/cm ³	1.516
μ/mm ⁻¹	0.416
F(000)	384.0
Crystal size/mm ³	0.5 × 0.5 × 0.5
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.196 to 54.088
Index ranges	-10 ≤ h ≤ 10, -13 ≤ k ≤ 13, -13 ≤ l ≤ 13
Reflections collected	22394
Independent reflections	3443 [R _{int} = 0.0419, R _{sigma} = 0.0245]
Data/restraints/parameters	3443/402/227
Goodness-of-fit on F ²	1.067
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0382, wR ₂ = 0.0997
Final R indexes [all data]	R ₁ = 0.0431, wR ₂ = 0.1031
Largest diff. peak/hole / e Å ⁻³	0.58/-0.43

Figure S1. Free energy profile from **INT-3** to **INT-4**.

