# Supporting Information

## Environmentally Friendly Nafion-catalyzed Synthesis of Substituted 2-Ethyl-3-Methylquinolines from Aniline and Propionaldehyde under Microwave Irradiation

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Total Pages of Supporting Information: 107.

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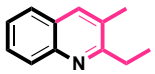
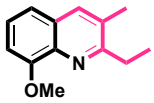
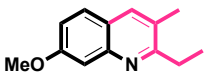
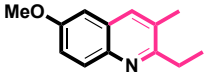
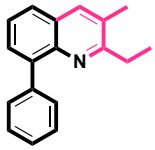
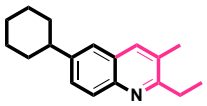
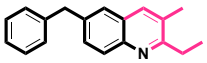
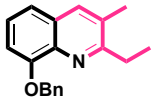
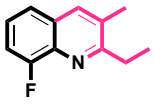
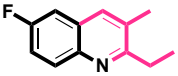
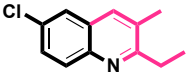
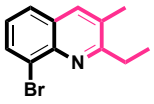
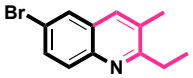
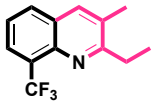
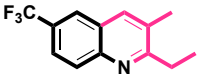
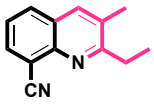
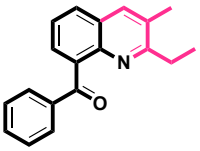
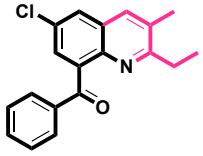
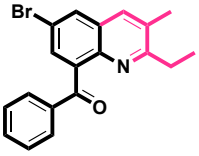
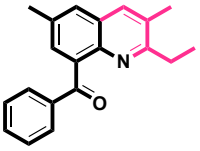
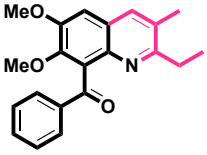
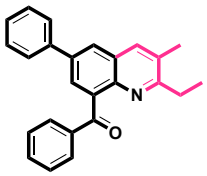
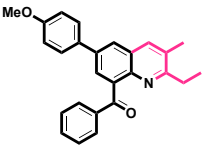
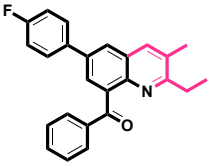
|---|---|---|---|---|---|
|  |  |  |  |  |  |
| **3g (S-32~S-33)** | **3h (S-34~S-35)** | **3i (S-36~S-37)** | **3j (S-38~S-39)** | **3k (S-40~S-41)** | **3l (S-42~S-43)** |
|  |  |  |  |  |  |
| **3m (S-44~S-45)** | **3n (S-46~S-47)** | **3o (S-48~S-49)** | **3p (S-50~S-51)** | **5a (S-52~S-53)** | **5b (S-54~S-55)** |
|  |  |  |  |  |  |
| **5c (S-56~S-57)** | **5d (S-58~S-59)** | **5e (S-60~S-61)** | **5f (S-62~S-63)** | **5g (S-64~S-65)** | **5h (S-66~S-67)** |
|  |  |  |  |  |  |
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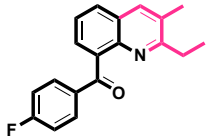
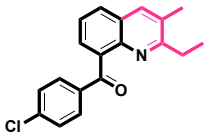
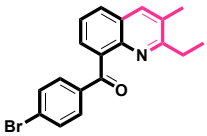
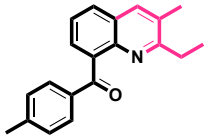
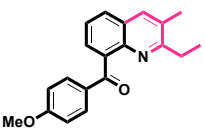
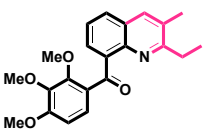
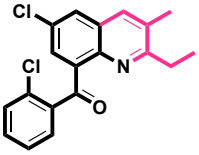
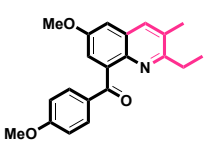
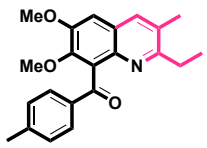
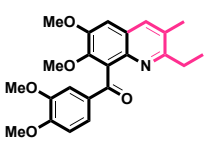
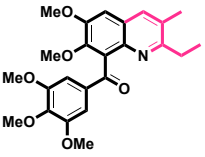
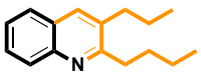
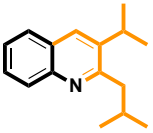
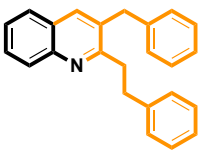
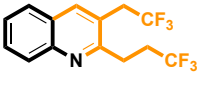
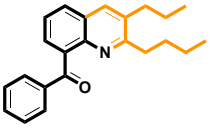
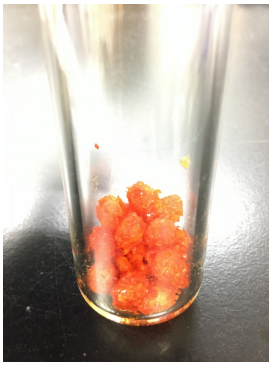
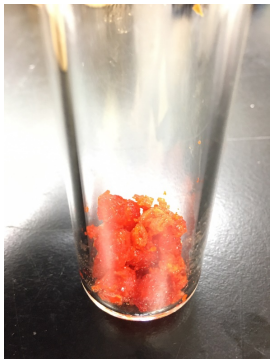
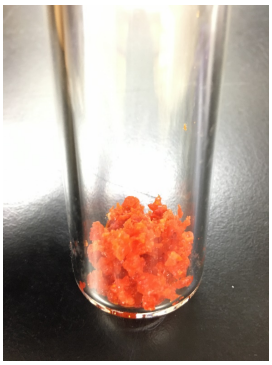
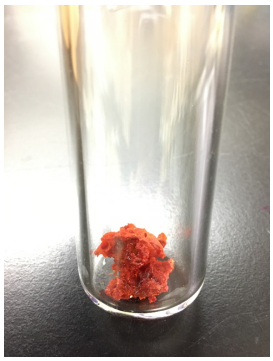
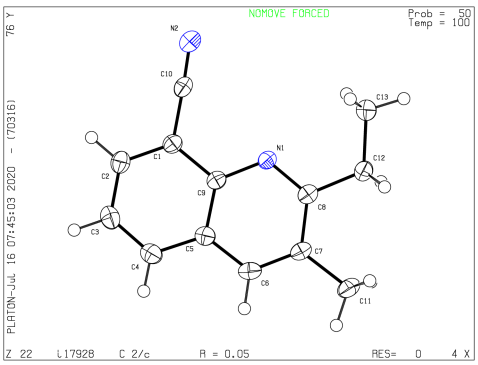
|  |  |  |  |  |  |
| **5o (S-80~S-81)** | **5p (S-82~S-83)** | **5q (S-84~S-85)** | **5r (S-86~S-87)** | **5s (S-88~S-89)** | **6a (S-90~S-91)** |
|  |  |  |  |  |  |
| **6b (S-92~S-93)** | **6c (S-94~S-95)** | **6d (S-96~S-97)** | **6e (S-98~S-99)** | **6f (S-100~S-101)** | **6g (S-102~S-103)** |
|  |  |  |  |  |  |
| **6h (S-104~S-105)** | **7 (S-106~S-107)** | | | | |
|  |  | | | | |

**Table 1.** Physical state of the recycle experiments

| Experiment 1 | Experiment 2 | Experiment 3 | Experiment 4 | Experiment 5 |
|---|---|---|---|---|
|  |  |  |  |  |
| **Experiment 6** | **Experiment 7** | **Experiment 8** | **Experiment 9** | **Experiment 10** |
|  |  |  |  |  |

Crystal data and structure refinement for compound **3p**

(the thermal ellipsoid was drawn at the 50% probability level)




| | | |
|---|---|---|
| Identification code | i17928 | |
| Empirical formula | C13 H12 N2 | |
| Formula weight | 196.25 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | C 2/c | |
| Unit cell dimensions | a = 20.8096(12) Å | a= 90°. |
| | b = 8.4535(5) Å | b= 128.6800(10)°. |
| | c = 15.3108(16) Å | g = 90°. |
| Volume | 2102.6(3) Å$^3$ | |
| Z, Density (calculated) | 8, 1.240 Mg/m$^3$ | |
| Absorption coefficient | 0.075 mm$^{-1}$ | |
| F(000) | 832 | |
| Crystal size | 0.139 x 0.103 x 0.099 mm$^3$ | |
| Theta range for data collection | 2.687 to 28.345°. | |
| Index ranges | -27<=h<=27, -11<=k<=11, -20<=l<=16 | |
| Reflections collected | 28515 | |
| Independent reflections | 2620 [R(int) = 0.1270] | |
| Completeness to theta = 25.242° | 99.8 % | |
| Absorption correction | Numerical | |
| Max. and min. transmission | 1 and 0.9039 | |
| Refinement method | Full-matrix least-squares on F$^2$ | |
| Data / restraints / parameters | 2620 / 0 / 138 | |
| Goodness-of-fit on F$^2$ | 1.022 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0459, wR2 = 0.1012 | |
| R indices (all data) | R1 = 0.0971, wR2 = 0.1285 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.260 and -0.212 e.Å$^{-3}$ | |

# checkCIF (basic structural check) running

*Checking for embedded fcf data in CIF ...*
*Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . .*

# checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) i17928

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

## Datablock: i17928

Bond precision: C-C = 0.0020 A Wavelength=0.71073
Cell: a=20.8096(12) b=8.4535(5) c=15.3108(16)
alpha=90 beta=128.680(1) gamma=90
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 2102.6(3) | 2102.6(3) |
| Space group | C 2/c | C 2/c |
| Hall group | -C 2yc | -C 2yc |
| Moiety formula | C13 H12 N2 | C13 H12 N2 |
| Sum formula | C13 H12 N2 | C13 H12 N2 |
| Mr | 196.25 | 196.25 |
| Dx,g cm-3 | 1.240 | 1.240 |
| Z | 8 | 8 |
| Mu (mm-1) | 0.075 | 0.075 |
| F000 | 832.0 | 832.0 |
| F000' | 832.27 | |
| h,k,lmax | 27,11,20 | 27,11,20 |
| Nref | 2625 | 2620 |
| Tmin,Tmax | 0.991,0.993 | 0.904,1.000 |
| Tmin' | 0.990 | |

Correction method= # Reported T Limits: Tmin=0.904
Tmax=1.000 AbsCorr = NUMERICAL
Data completeness= 0.998 Theta(max)= 28.345
R(reflections)= 0.0459( 1647) wR2(reflections)= 0.1285( 2620)
S = 1.022 Npar= 138

The following ALERTS were generated. Each ALERT has the format
**test-name_ALERT_alert-type_alert-level.**
Click on the hyperlinks for more details of the test.

**Alert level C**
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.127

```
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -6.005 Report
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.124 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         2 Report
```

**Alert level G**

```
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.127 Report
PLAT128_ALERT_4_G Alternate Setting for Input Space Group     C2/c       I2/a Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         2 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         9 Info
```

```
  0 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
  4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  7 ALERT level G = General information/check it is not something unexpected

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  1 ALERT type 2 Indicator that the structure model may be wrong or deficient
  7 ALERT type 3 Indicator that the structure quality may be low
  2 ALERT type 4 Improvement, methodology, query or suggestion
  0 ALERT type 5 Informative message, check
```

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**Publication of your CIF in IUCr journals**

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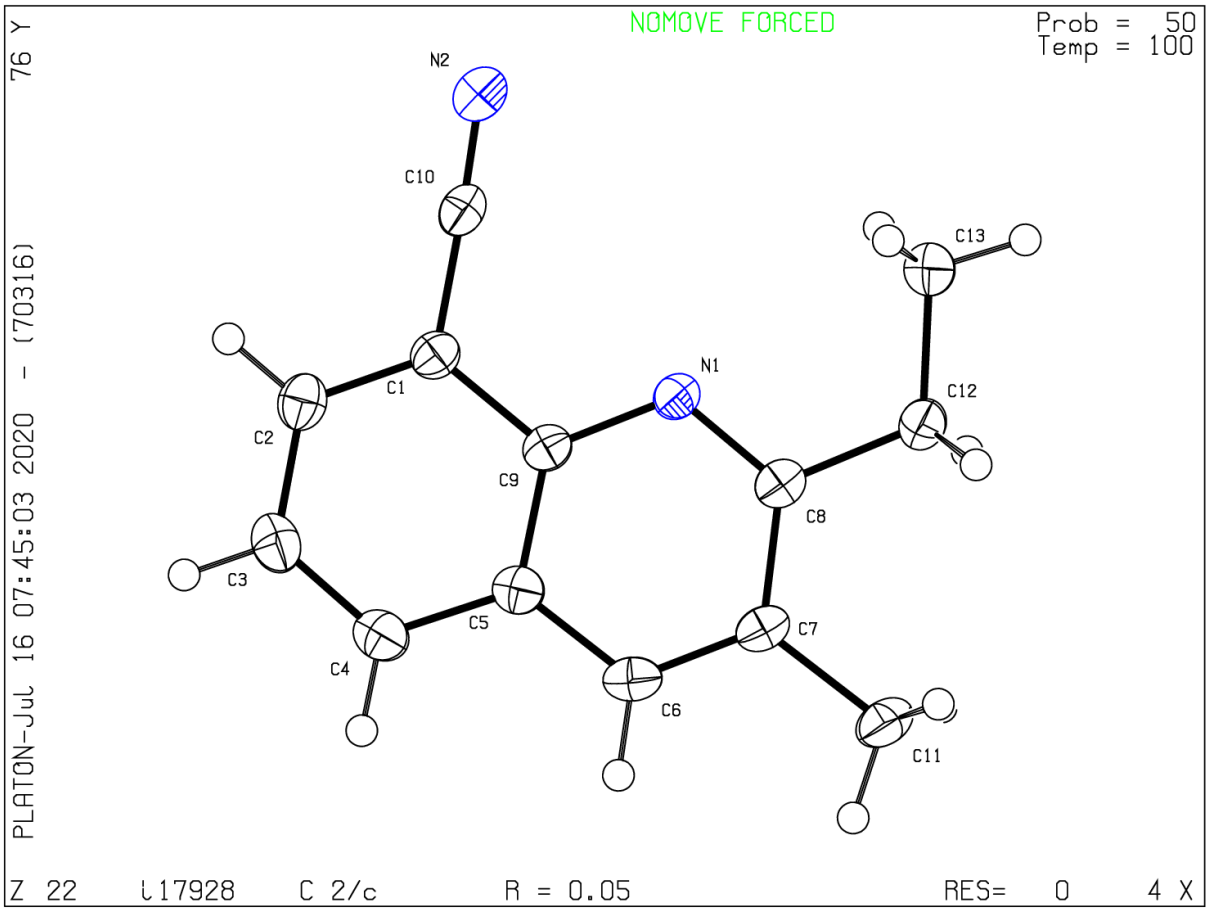
**Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

**PLATON version of 08/07/2020; check.def file version of 17/06/2020**

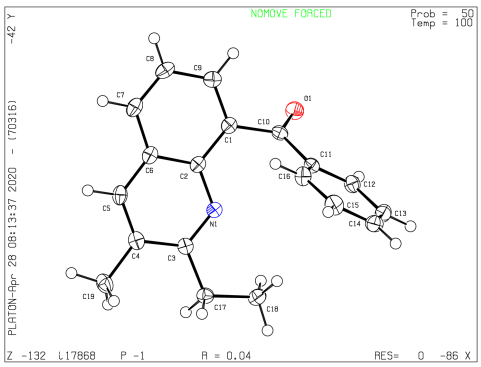
## **Datablock i17928** - ellipsoid plot




Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

Crystal data and structure refinement for compound **5a**

(the thermal ellipsoid was drawn at the 50% probability level)




| | | |
|---|---|---|
| Identification code | i17868 | |
| Empirical formula | C19 H17 N O | |
| Formula weight | 275.33 | |
| Temperature | 100.0(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P -1 | |
| Unit cell dimensions | a = 8.4108(3) Å | a= 103.454(2)°. |
| | b = 8.9126(3) Å | b= 97.603(2)°. |
| | c = 10.9019(4) Å | g = 111.8150(10)°. |
| Volume | 715.90(4) Å$^3$ | |
| Z, Density (calculated) | 2, 1.277 Mg/m$^3$ | |
| Absorption coefficient | 0.079 mm$^{-1}$ | |
| F(000) | 292 | |
| Crystal size | 0.238 x 0.208 x 0.149 mm$^3$ | |
| Theta range for data collection | 2.586 to 27.103°. | |
| Index ranges | -10<=h<=10, -11<=k<=11, -13<=l<=13 | |
| Reflections collected | 31756 | |
| Independent reflections | 3168 [R(int) = 0.0684] | |
| Completeness to theta = 25.242° | 99.9 % | |
| Absorption correction | Numerical | |
| Max. and min. transmission | 1 and 0.9107 | |
| Refinement method | Full-matrix least-squares on F$^2$ | |
| Data / restraints / parameters | 3168 / 0 / 192 | |
| Goodness-of-fit on F$^2$ | 1.027 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0387, wR2 = 0.0908 | |
| R indices (all data) | R1 = 0.0607, wR2 = 0.1047 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.234 and -0.243 e.Å$^{-3}$ | |

# checkCIF (basic structural check) running

*Checking for embedded fcf data in CIF ...*
*Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . .*

# checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) i17868

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

## Datablock: i17868

Bond precision: C-C = 0.0020 A Wavelength=0.71073
Cell: a=8.4108(3) b=8.9126(3) c=10.9019(4)
alpha=103.454(2) beta=97.603(2) gamma=111.815(1)
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 715.90(5) | 715.90(4) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C19 H17 N O | C19 H17 N O |
| Sum formula | C19 H17 N O | C19 H17 N O |
| Mr | 275.34 | 275.33 |
| Dx,g cm-3 | 1.277 | 1.277 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.079 | 0.079 |
| F000 | 292.0 | 292.0 |
| F000' | 292.11 | |
| h,k,lmax | 10,11,13 | 10,11,13 |
| Nref | 3170 | 3168 |
| Tmin,Tmax | 0.981,0.988 | 0.911,1.000 |
| Tmin' | 0.981 | |

Correction method= # Reported T Limits: Tmin=0.911
Tmax=1.000 AbsCorr = NUMERICAL
Data completeness= 0.999 Theta(max)= 27.103
R(reflections)= 0.0387( 2410) wR2(reflections)= 0.1047( 3168)
S = 1.027 Npar= 192

The following ALERTS were generated. Each ALERT has the format
**test-name_ALERT_alert-type_alert-level.**
Click on the hyperlinks for more details of the test.

**Alert level C**
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.177 Report

**Alert level G**

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 11 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 1 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

**Publication of your CIF in IUCr journals**

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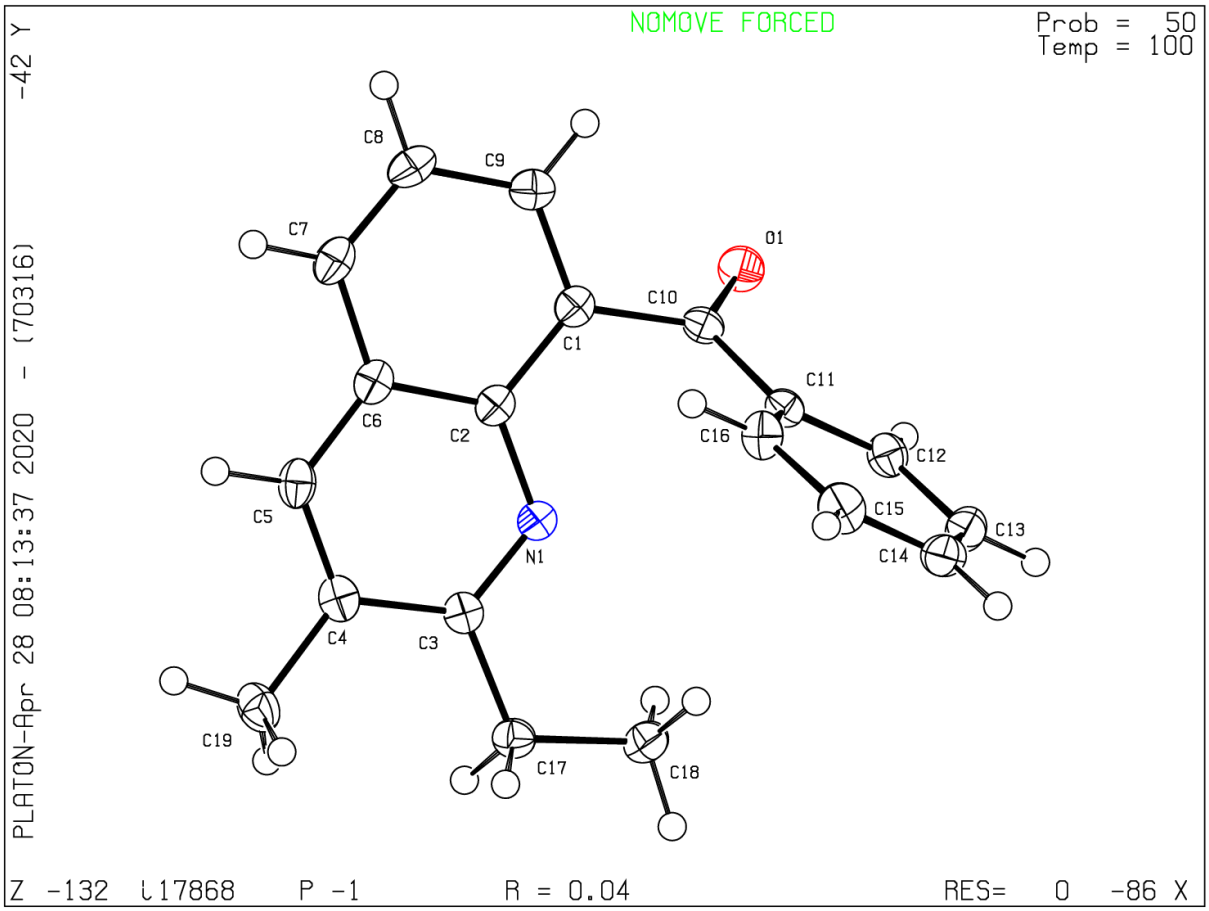
**Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

**PLATON version of 22/04/2020; check.def file version of 09/03/2020**

## **Datablock i17868** - ellipsoid plot

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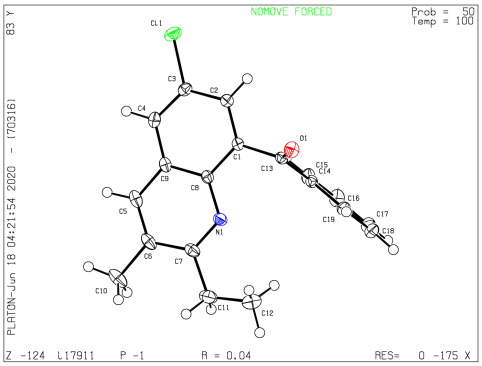
Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

Crystal data and structure refinement for compound **5b**

(the thermal ellipsoid was drawn at the 50% probability level)




| | | |
|---|---|---|
| Identification code | i17911 | |
| Empirical formula | C19 H16 Cl N O | |
| Formula weight | 309.78 | |
| Temperature | 100.0(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P -1 | |
| Unit cell dimensions | a = 7.4420(3) Å | a= 103.4120(10)°. |
| | b = 10.3406(3) Å | b= 100.533(2)°. |
| | c = 10.7949(4) Å | g = 90.7170(10)°. |
| Volume | 793.14(5) Å$^3$ | |
| Z, Density (calculated) | 2, 1.297 Mg/m$^3$ | |
| Absorption coefficient | 0.242 mm$^{-1}$ | |
| F(000) | 324 | |
| Crystal size | 0.365 x 0.351 x 0.319 mm$^3$ | |
| Theta range for data collection | 2.028 to 33.138°. | |
| Index ranges | -11<=h<=11, -15<=k<=15, -16<=l<=16 | |
| Reflections collected | 45950 | |
| Independent reflections | 6054 [R(int) = 0.0386] | |
| Completeness to theta = 25.242° | 100.0 % | |
| Absorption correction | Numerical | |
| Max. and min. transmission | 1 and 0.9445 | |
| Refinement method | Full-matrix least-squares on F$^2$ | |
| Data / restraints / parameters | 6054 / 0 / 201 | |
| Goodness-of-fit on F$^2$ | 1.092 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0383, wR2 = 0.1043 | |
| R indices (all data) | R1 = 0.0482, wR2 = 0.1123 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.453 and -0.241 e.Å$^{-3}$ | |

# checkCIF (basic structural check) running

*Checking for embedded fcf data in CIF ...*
*Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . .*

# checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) i17911

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

## Datablock: i17911

Bond precision: C-C = 0.0014 A Wavelength=0.71073
Cell: a=7.4420(3) b=10.3406(3) c=10.7949(4)
alpha=103.412(1) beta=100.533(2) gamma=90.717(1)
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 793.14(5) | 793.14(5) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C19 H16 Cl N O | C19 H16 Cl N O |
| Sum formula | C19 H16 Cl N O | C19 H16 Cl N O |
| Mr | 309.78 | 309.78 |
| Dx,g cm-3 | 1.297 | 1.297 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.242 | 0.242 |
| F000 | 324.0 | 324.0 |
| F000' | 324.41 | |
| h,k,lmax | 11,15,16 | 11,15,16 |
| Nref | 6054 | 6054 |
| Tmin,Tmax | 0.915,0.926 | 0.945,1.000 |
| Tmin' | 0.915 | |

Correction method= # Reported T Limits: Tmin=0.945
Tmax=1.000 AbsCorr = NUMERICAL
Data completeness= 1.000 Theta(max)= 33.138
R(reflections)= 0.0383( 5083) wR2(reflections)= 0.1123( 6054)
S = 1.092 Npar= 201

The following ALERTS were generated. Each ALERT has the format
**test-name_ALERT_alert-type_alert-level.**
Click on the hyperlinks for more details of the test.

**Alert level G**
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note

```
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         16 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          2 Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   4 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

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**Publication of your CIF in other journals**

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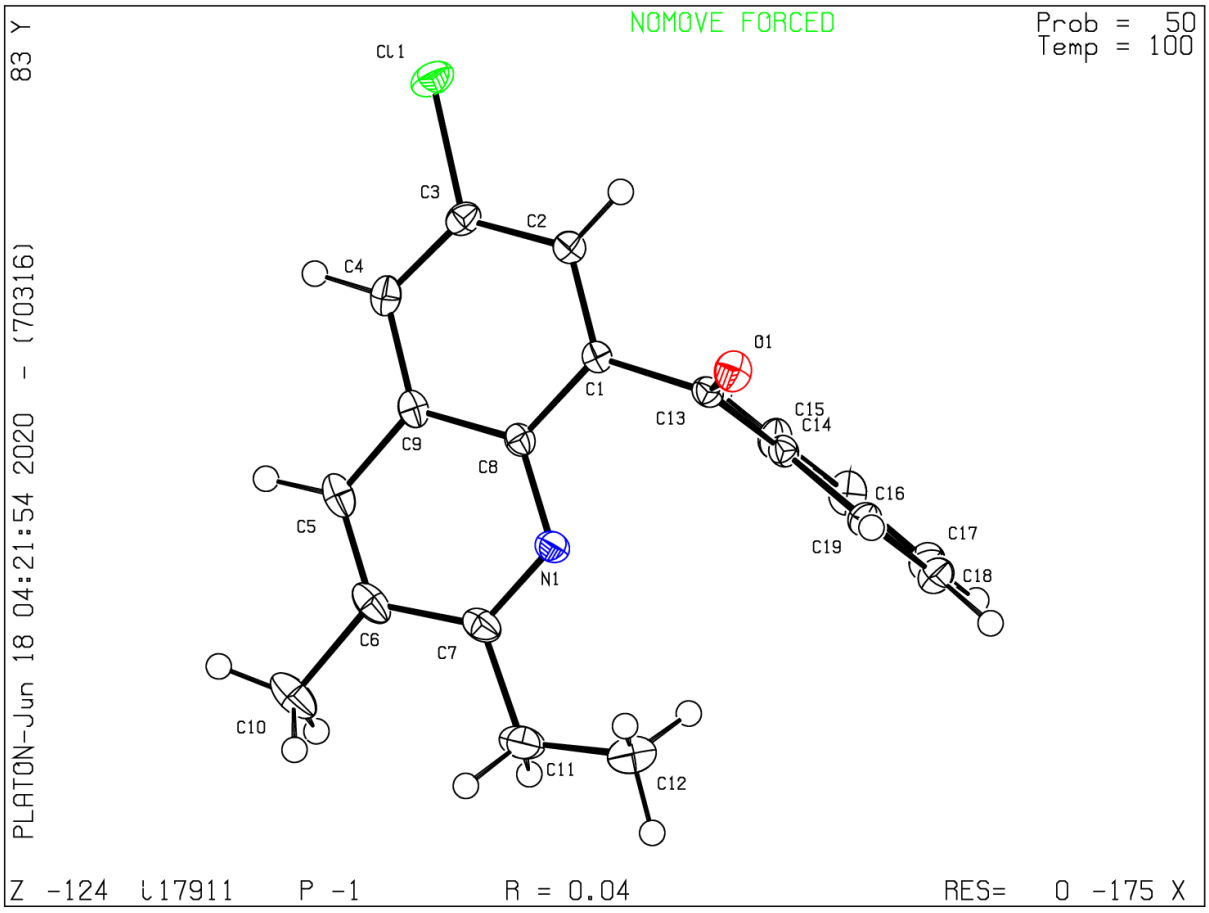
**PLATON version of 04/06/2020; check.def file version of 02/06/2020**

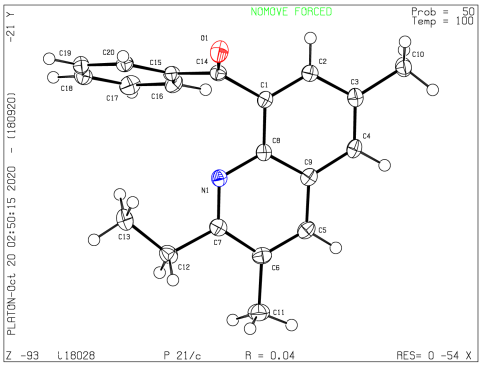
## **Datablock i17911** - ellipsoid plot




Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

Crystal data and structure refinement for compound **5d**

(the thermal ellipsoid was drawn at the 50% probability level)




| | | |
|---|---|---|
| Identification code | i18028 | |
| Empirical formula | C20 H19 N O | |
| Formula weight | 289.36 | |
| Temperature | 100.0(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21/c | |
| Unit cell dimensions | a = 13.2934(5) Å | a= 90°. |
| | b = 14.2302(5) Å | b= 108.5200(10)°. |
| | c = 8.6189(3) Å | g = 90°. |
| Volume | 1545.98(10) Å$^3$ | |
| Z, Density (calculated) | 4, 1.243 Mg/m$^3$ | |
| Absorption coefficient | 0.076 mm$^{-1}$ | |
| F(000) | 616 | |
| Crystal size | 0.214 x 0.202 x 0.094 mm$^3$ | |
| Theta range for data collection | 2.158 to 27.098°. | |
| Index ranges | -17<=h<=17, -18<=k<=18, -11<=l<=10 | |
| Reflections collected | 43540 | |
| Independent reflections | 3392 [R(int) = 0.0506] | |
| Completeness to theta = 25.242° | 99.7 % | |
| Absorption correction | Numerical | |
| Max. and min. transmission | 1 and 0.9466 | |
| Refinement method | Full-matrix least-squares on F$^2$ | |
| Data / restraints / parameters | 3392 / 0 / 202 | |
| Goodness-of-fit on F$^2$ | 1.041 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0369, wR2 = 0.0885 | |
| R indices (all data) | R1 = 0.0479, wR2 = 0.0968 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.238 and -0.177 e.Å$^-$ | |

# checkCIF (basic structural check) running

*Checking for embedded fcf data in CIF ...*
*Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . . .*

# checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) i18028

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

## Datablock: i18028

Bond precision: C-C = 0.0017 A Wavelength=0.71073
Cell: a=13.2934(5) b=14.2302(5) c=8.6189(3)
alpha=90 beta=108.520(1) gamma=90
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 1545.98(10) | 1545.98(10) |
| Space group | P 21/c | P 21/c |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C20 H19 N O | C20 H19 N O |
| Sum formula | C20 H19 N O | C20 H19 N O |
| Mr | 289.36 | 289.36 |
| Dx,g cm-3 | 1.243 | 1.243 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.076 | 0.076 |
| F000 | 616.0 | 616.0 |
| F000' | 616.24 | |
| h,k,lmax | 17,18,11 | 17,18,11 |
| Nref | 3400 | 3392 |
| Tmin,Tmax | 0.984,0.993 | 0.947,1.000 |
| Tmin' | 0.984 | |

Correction method= # Reported T Limits: Tmin=0.947
Tmax=1.000 AbsCorr = NUMERICAL
Data completeness= 0.998 Theta(max)= 27.098
R(reflections)= 0.0369( 2813) wR2(reflections)= 0.0968( 3392)
S = 1.041 Npar= 202

The following ALERTS were generated. Each ALERT has the format
**test-name_ALERT_alert-type_alert-level.**
Click on the hyperlinks for more details of the test.

**Alert level C**

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 5 Note

**Alert level G**

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 16 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
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0 ALERT type 5 Informative message, check

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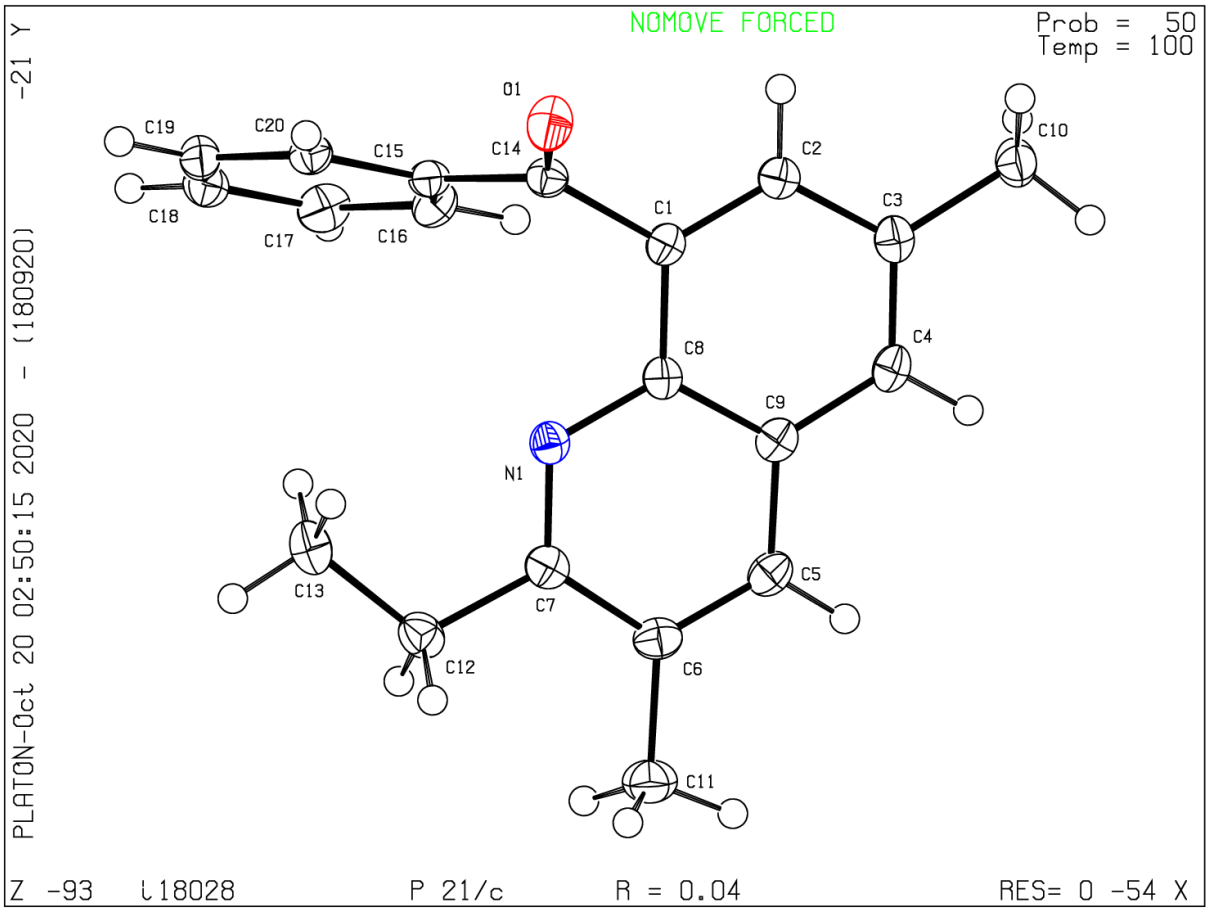
**Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

**PLATON version of 18/09/2020; check.def file version of 20/08/2020**

## **Datablock i18028** - ellipsoid plot

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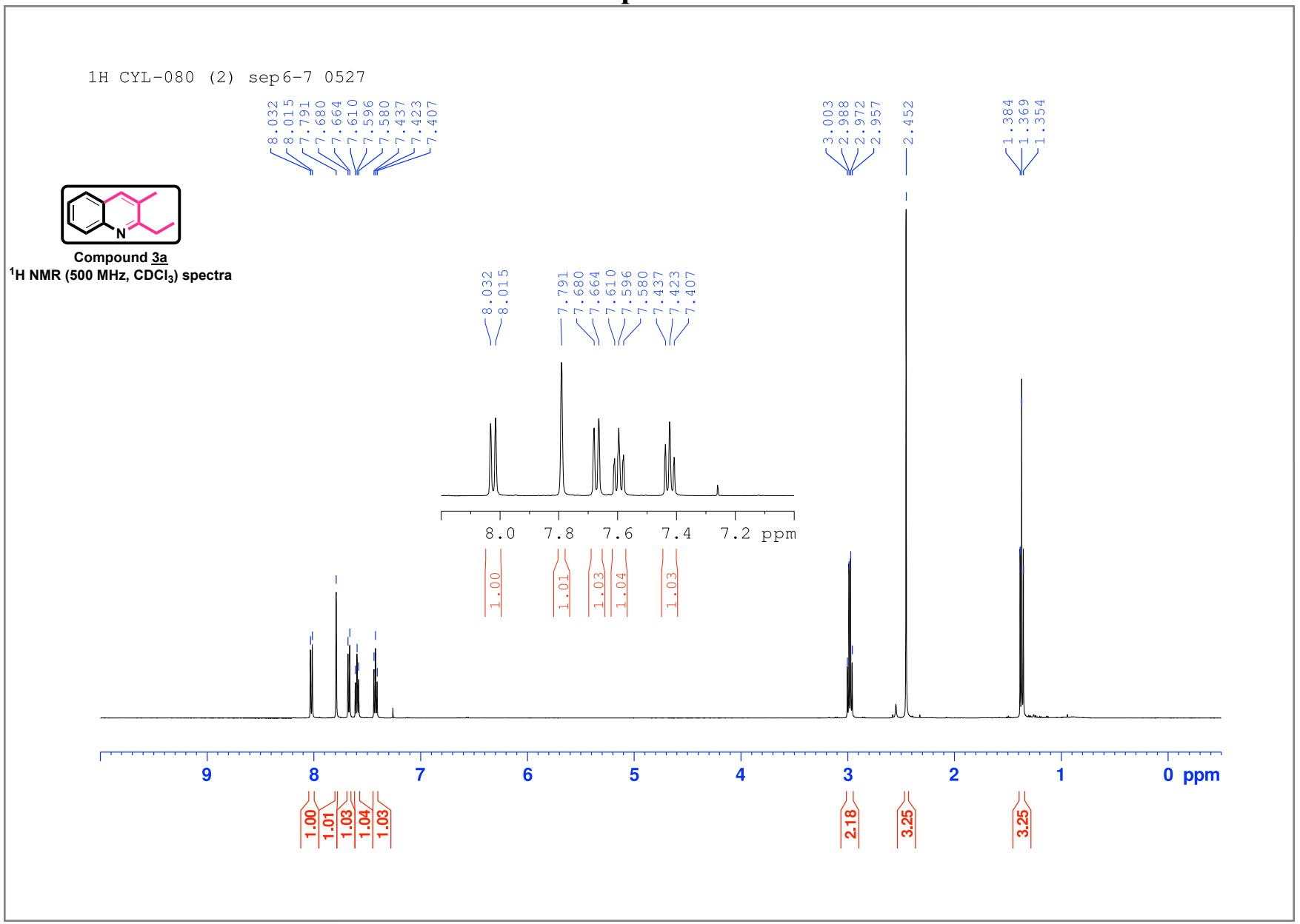
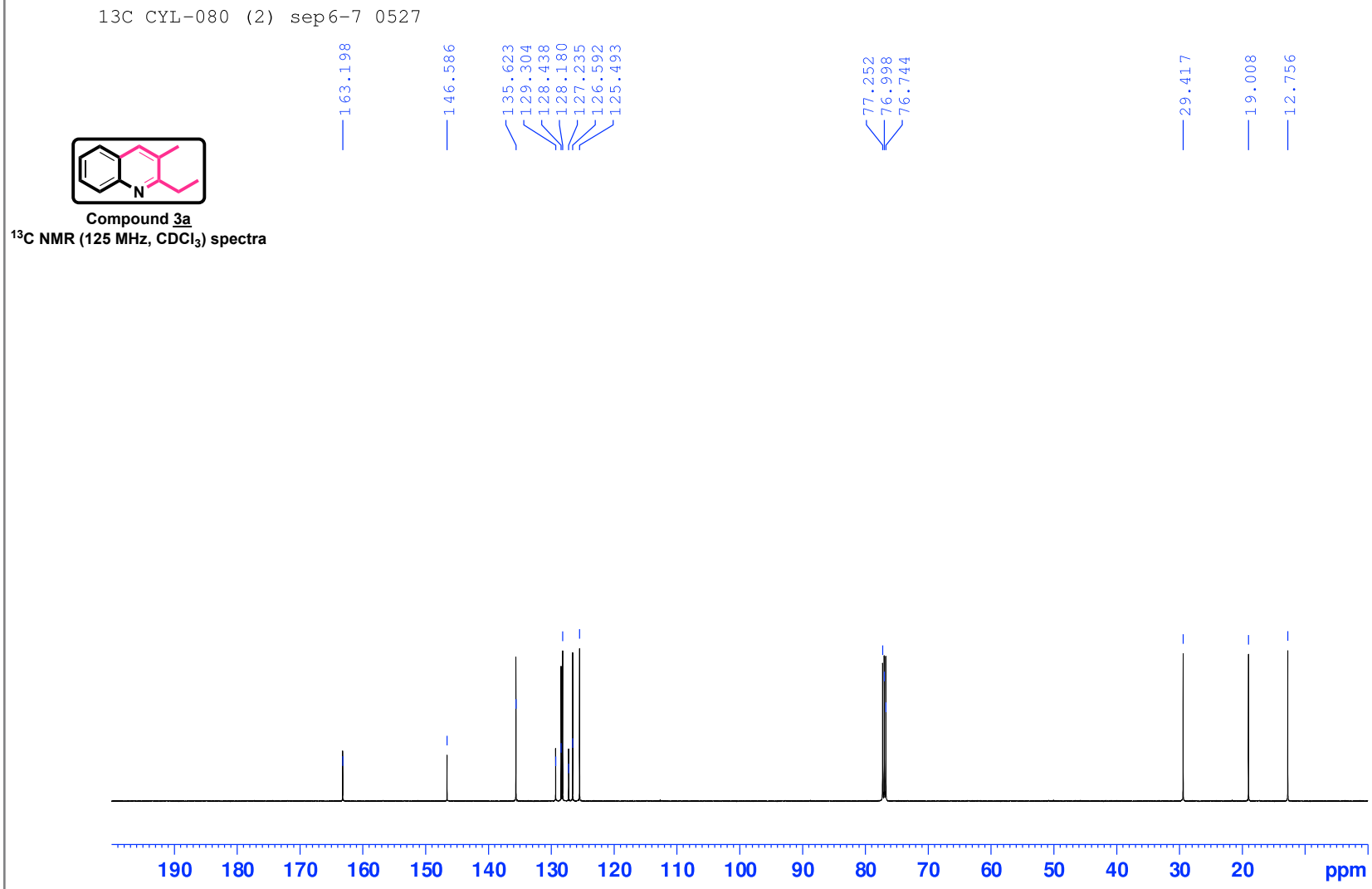
Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

# Compound 3a



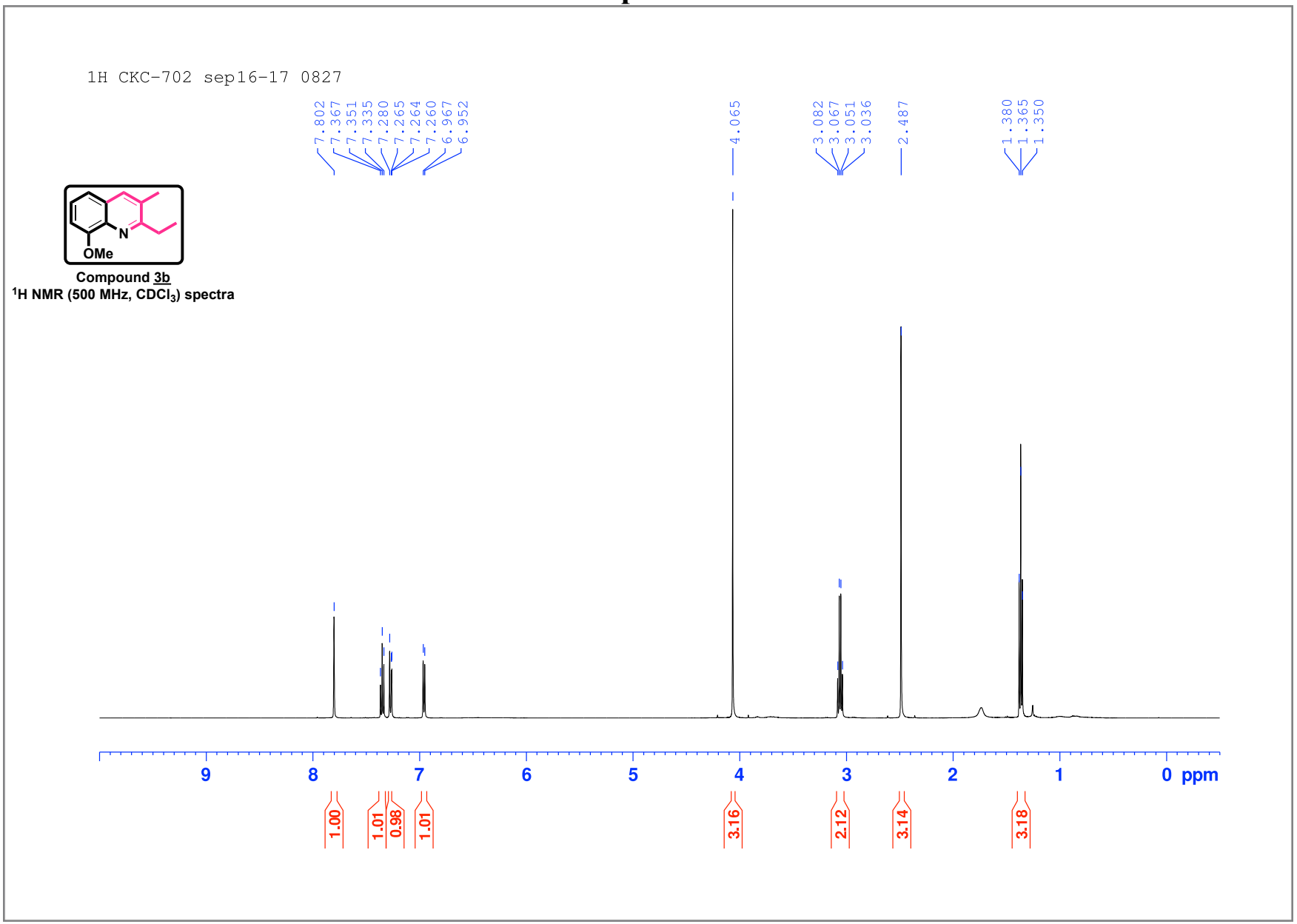

**Compound 3a**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

# Compound 3a



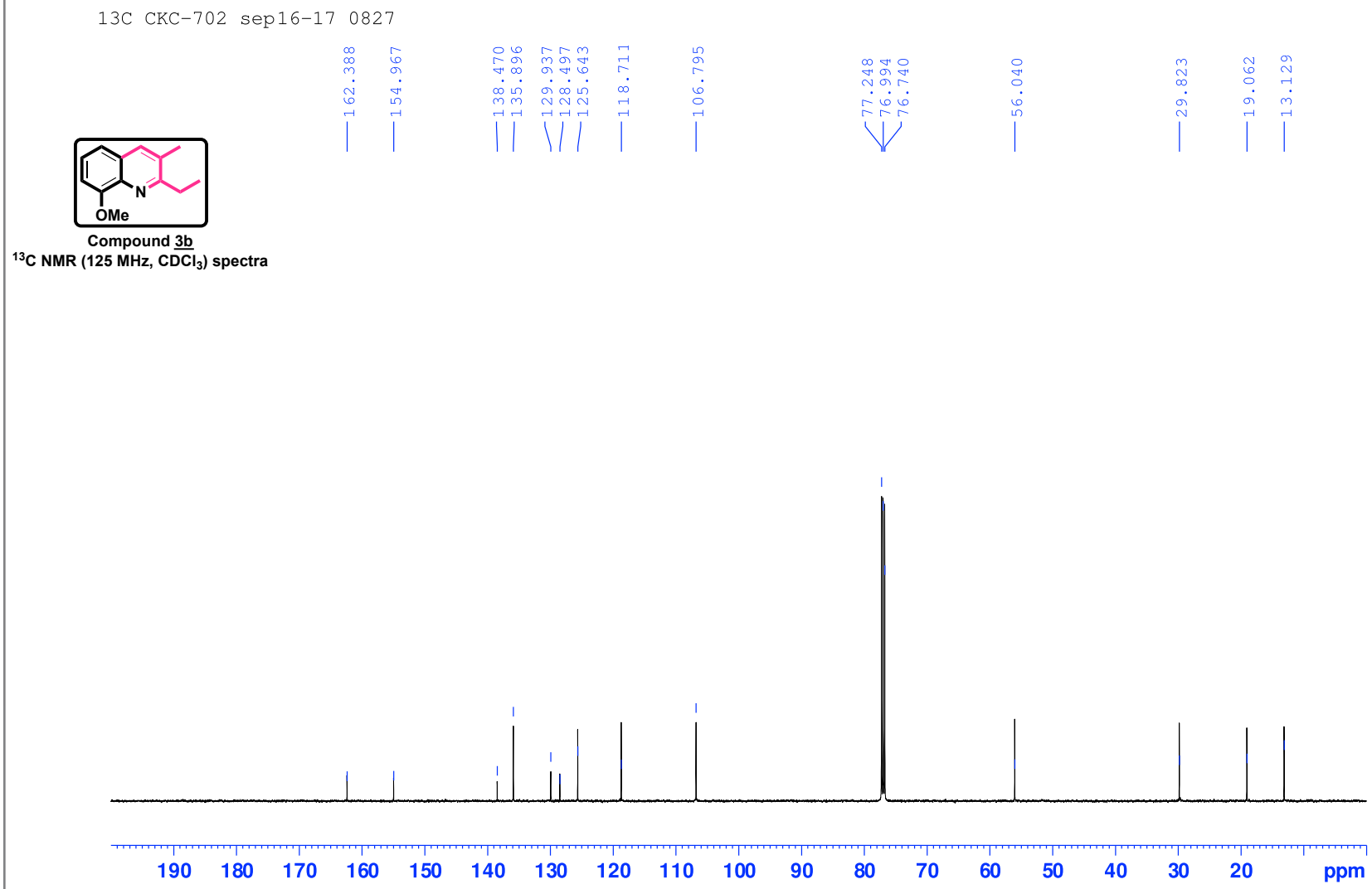

**Compound 3a**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 3b



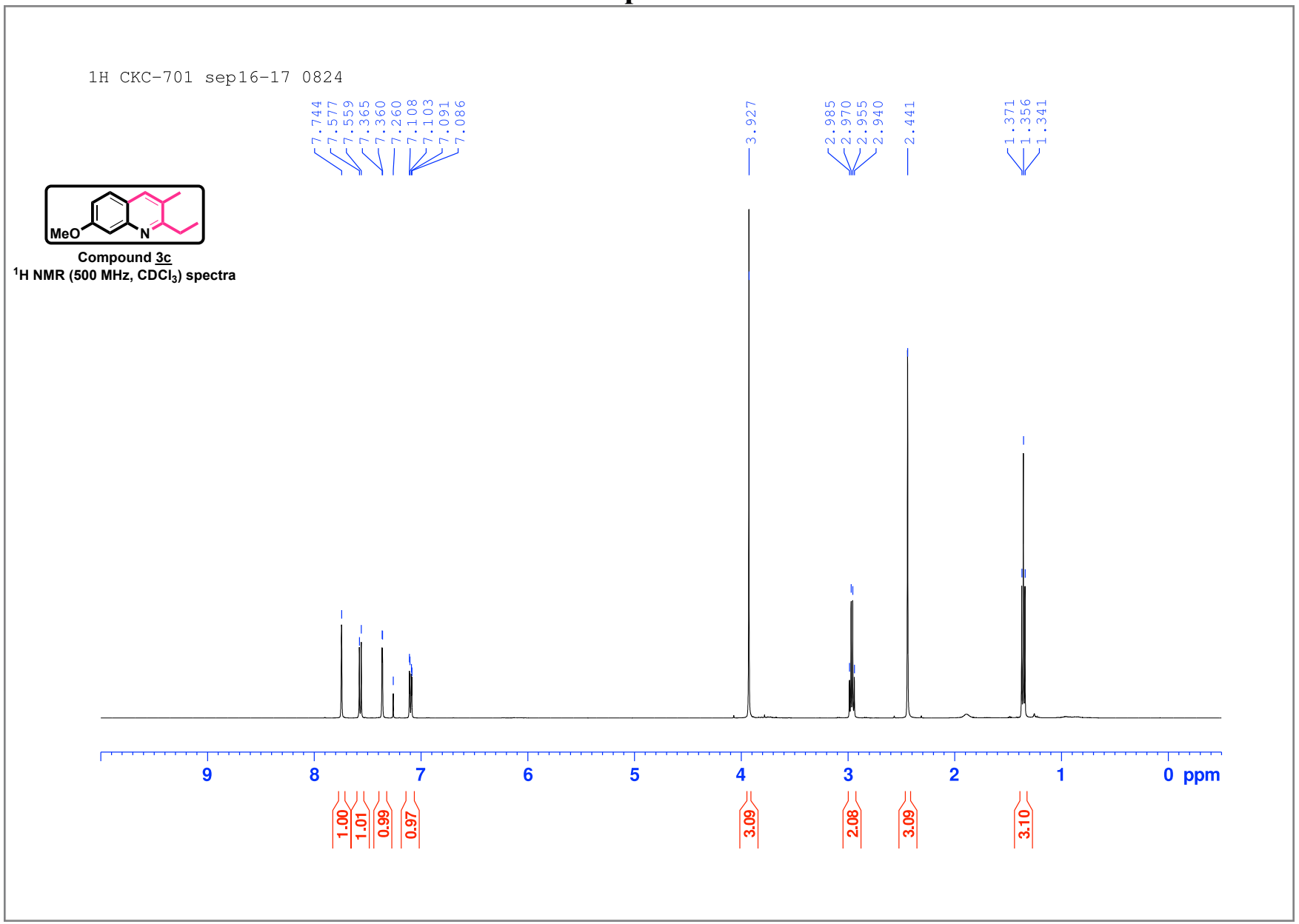

Compound 3b
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 3b



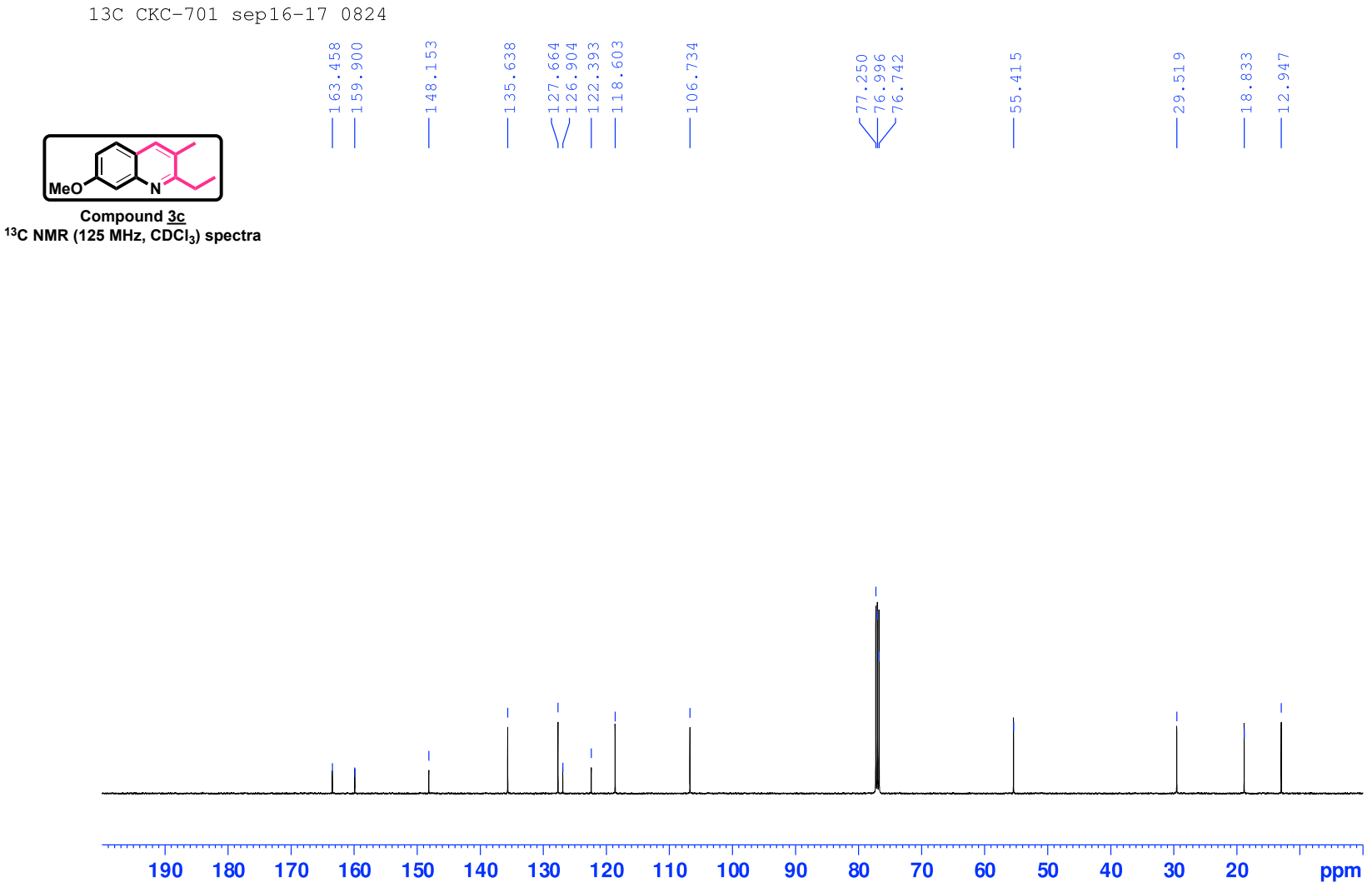

**Compound 3b**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 3c



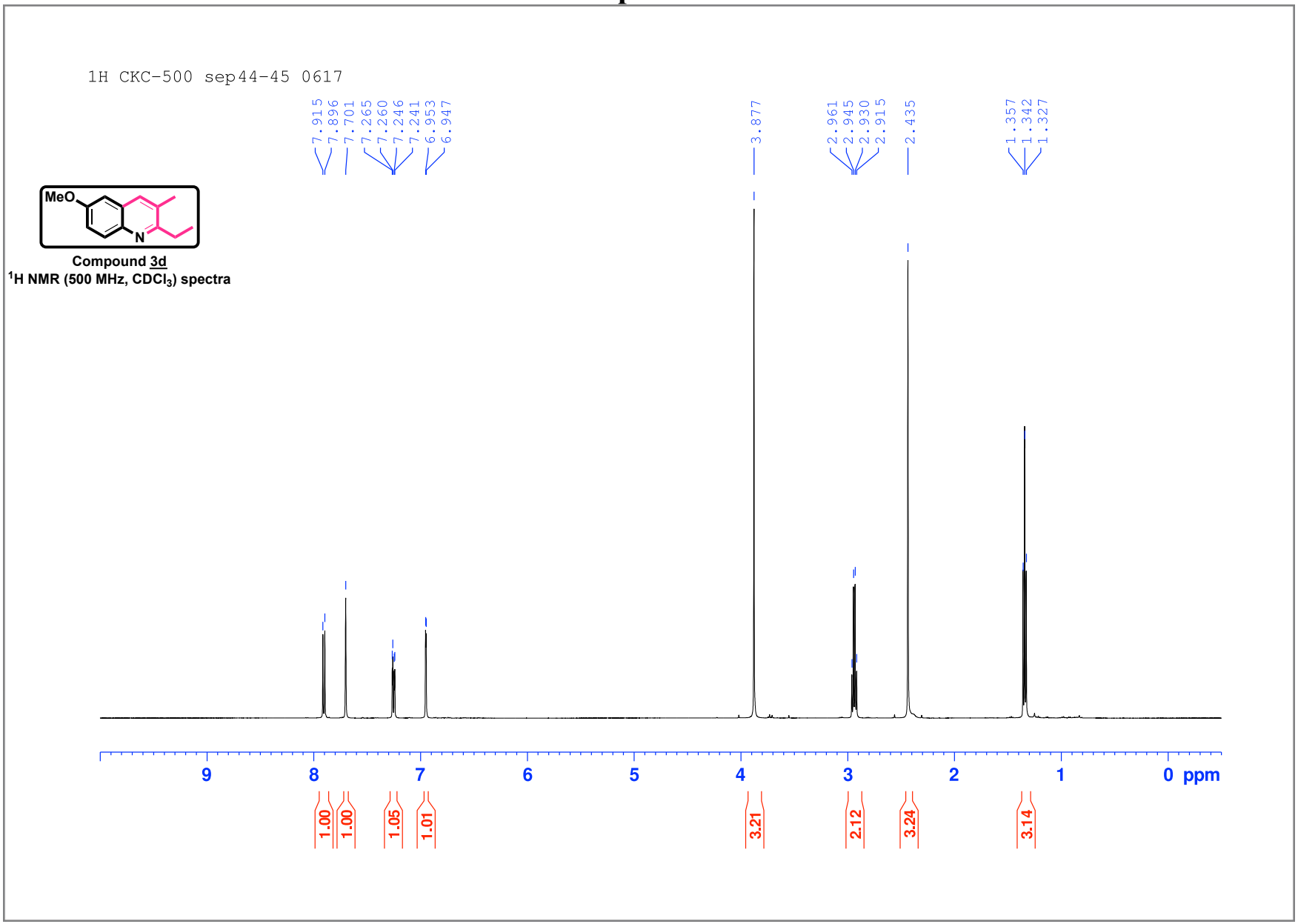

**Compound 3c**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

# Compound 3c

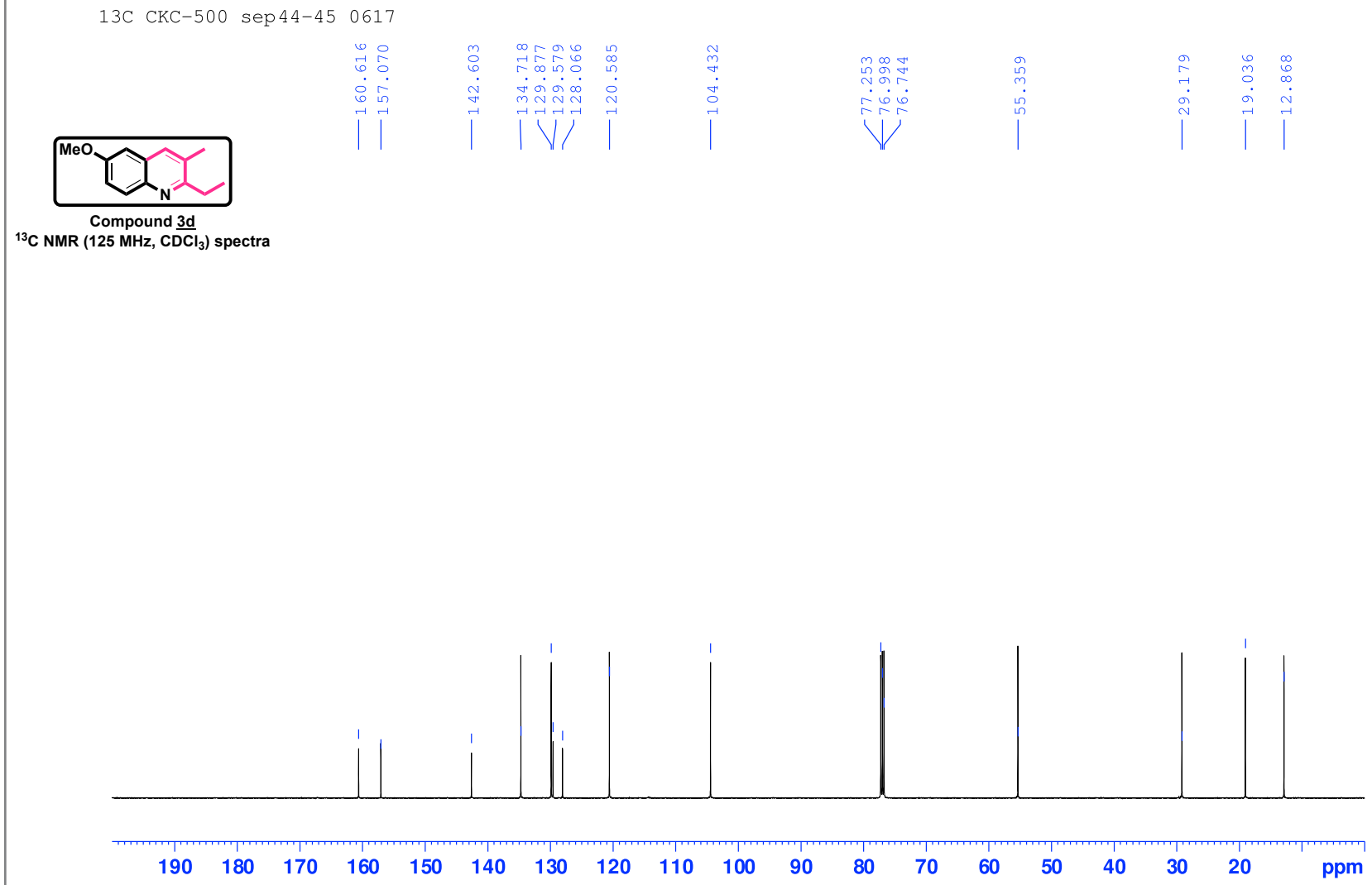



**Compound 3c**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 3d

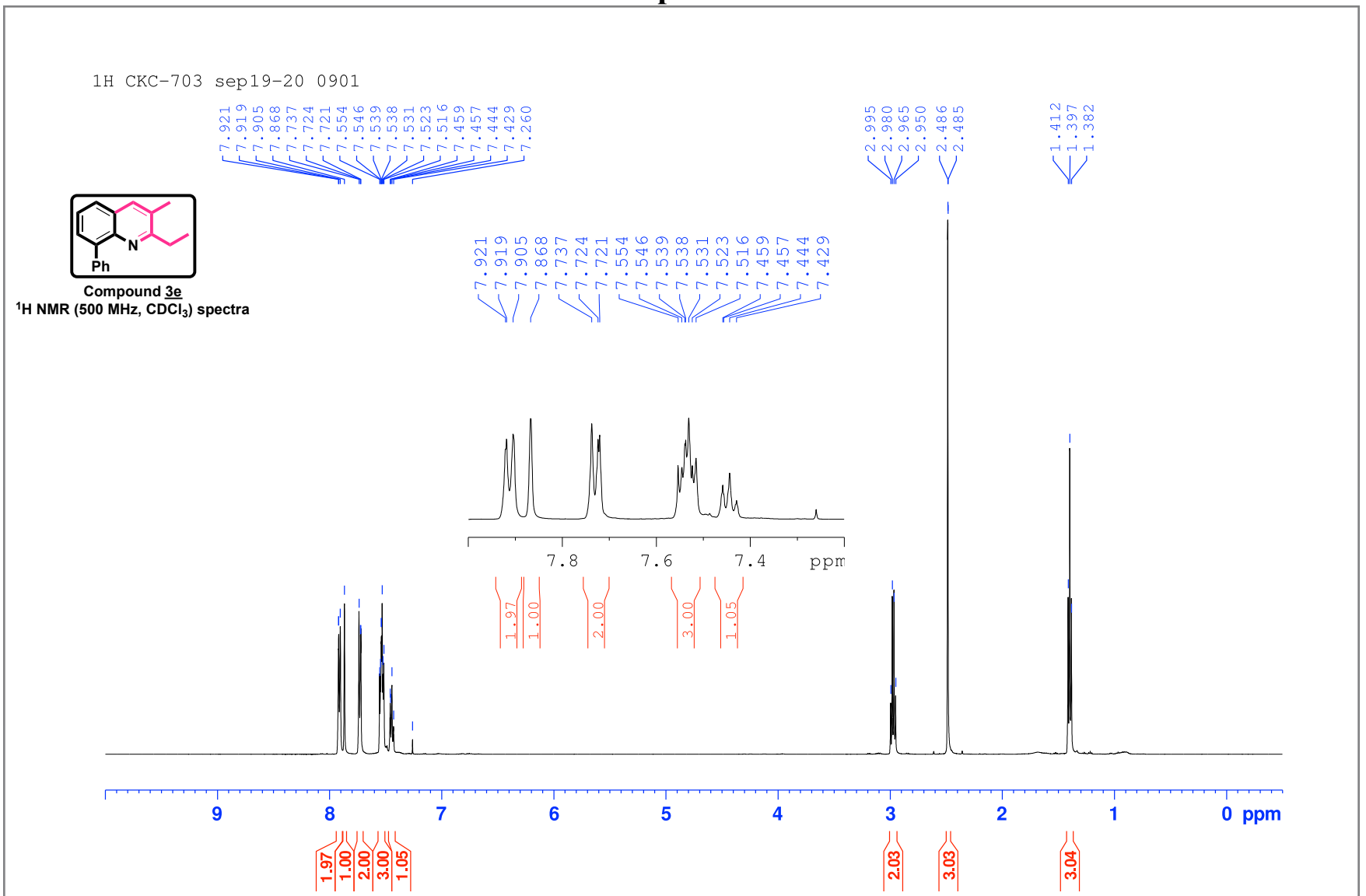

1H CKC-500 sep44-45 0617
7.915
7.896
7.701
7.265
7.260
7.246
7.241
6.953
6.947
3.877
2.961
2.945
2.930
2.915
2.435
1.357
1.342
1.327
MeO
N
Compound 3d
1H NMR (500 MHz, CDCl3) spectra
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.00
1.05
1.01
3.21
2.12
3.24
3.14

# Compound 3d

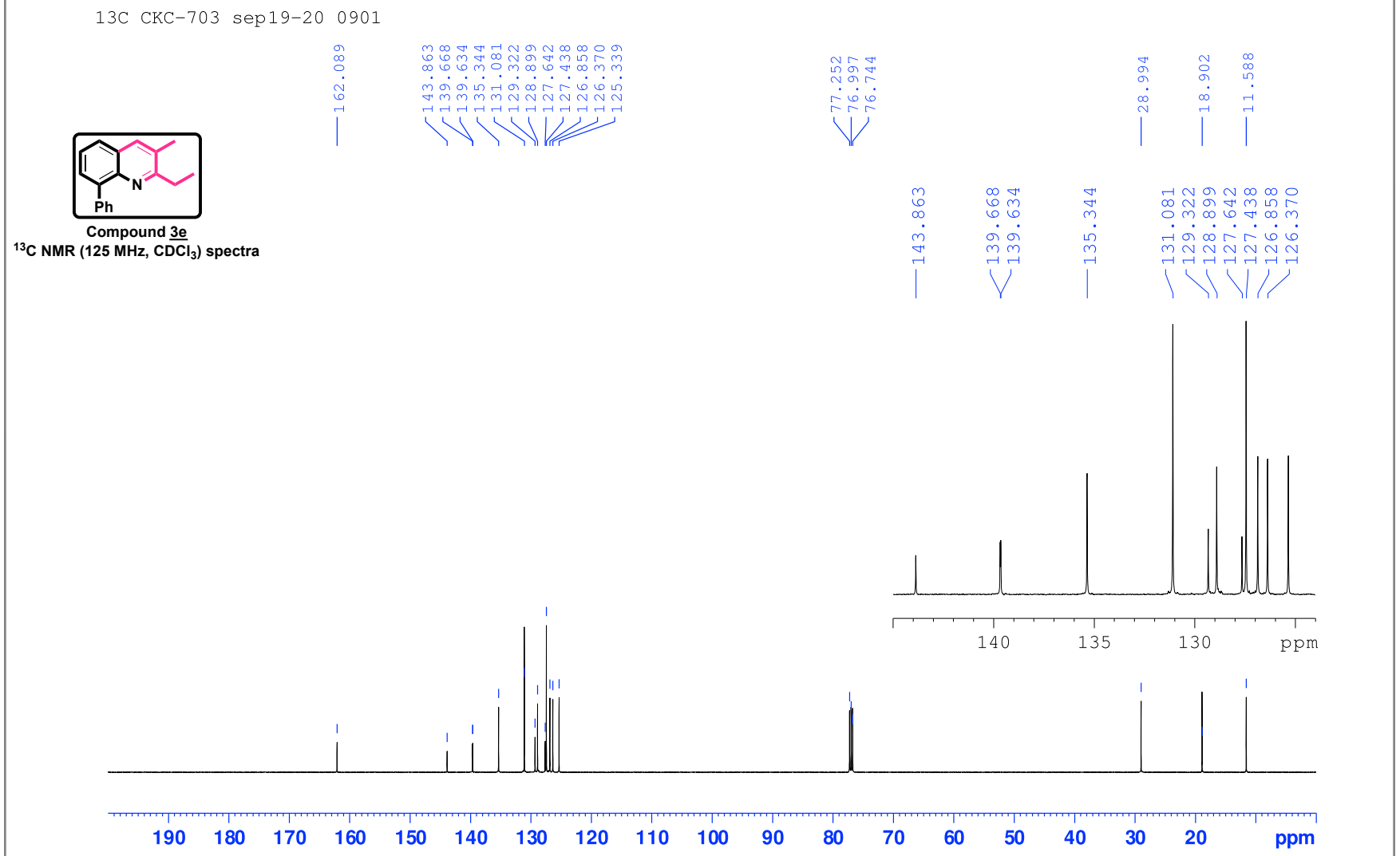



**Compound 3d**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

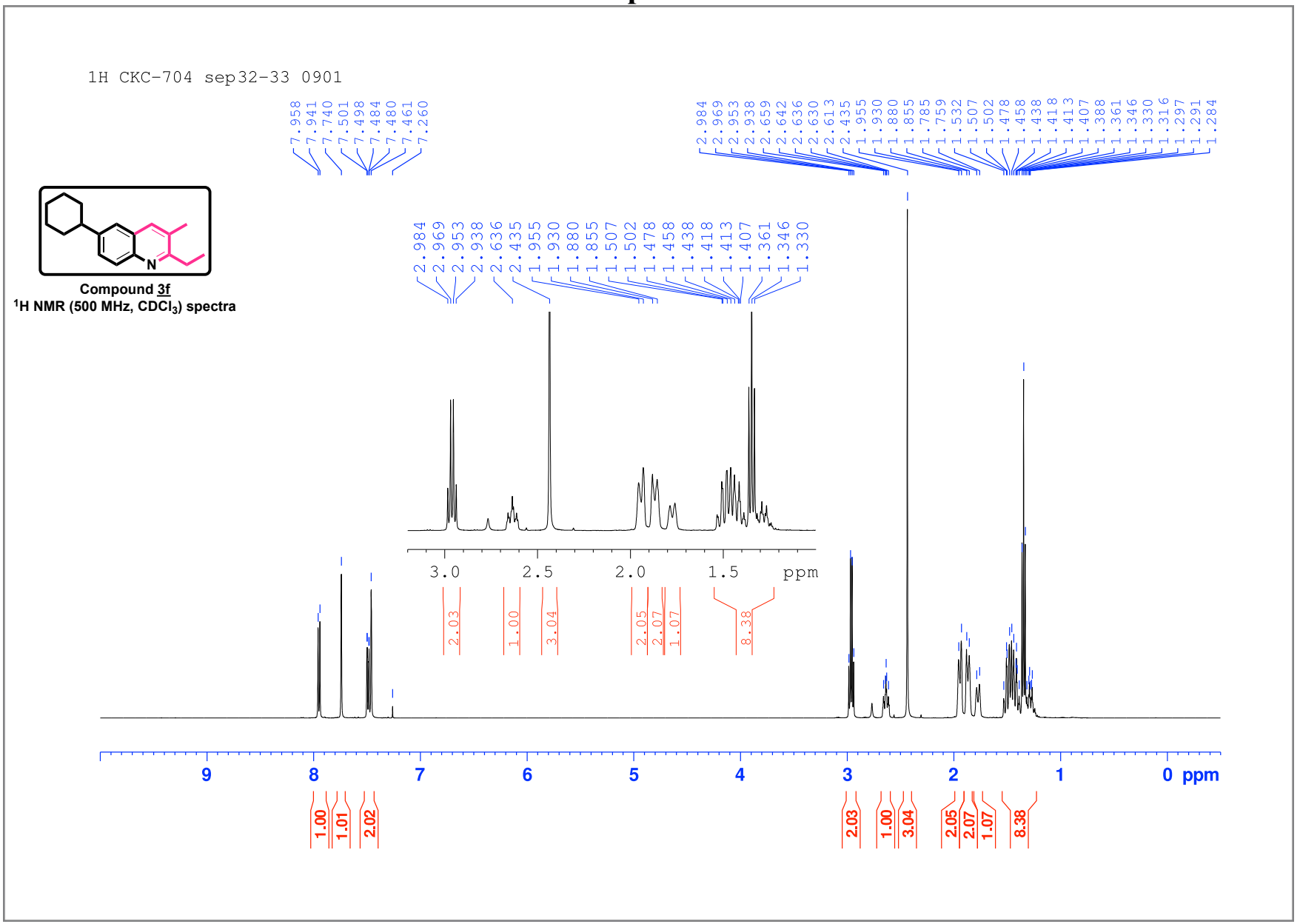
# Compound 3e


1H CKC-703 sep19-20 0901
7.921
7.919
7.905
7.868
7.737
7.724
7.721
7.554
7.546
7.539
7.538
7.531
7.523
7.516
7.459
7.457
7.444
7.429
7.260
2.995
2.980
2.965
2.950
2.486
2.485
1.412
1.397
1.382
N
Ph
Compound 3e
1H NMR (500 MHz, CDCl3) spectra
7.8
7.6
7.4
ppm
1.97
1.00
2.00
3.00
1.05
9
8
7
6
5
4
3
2
1
0 ppm
2.03
3.03
3.04

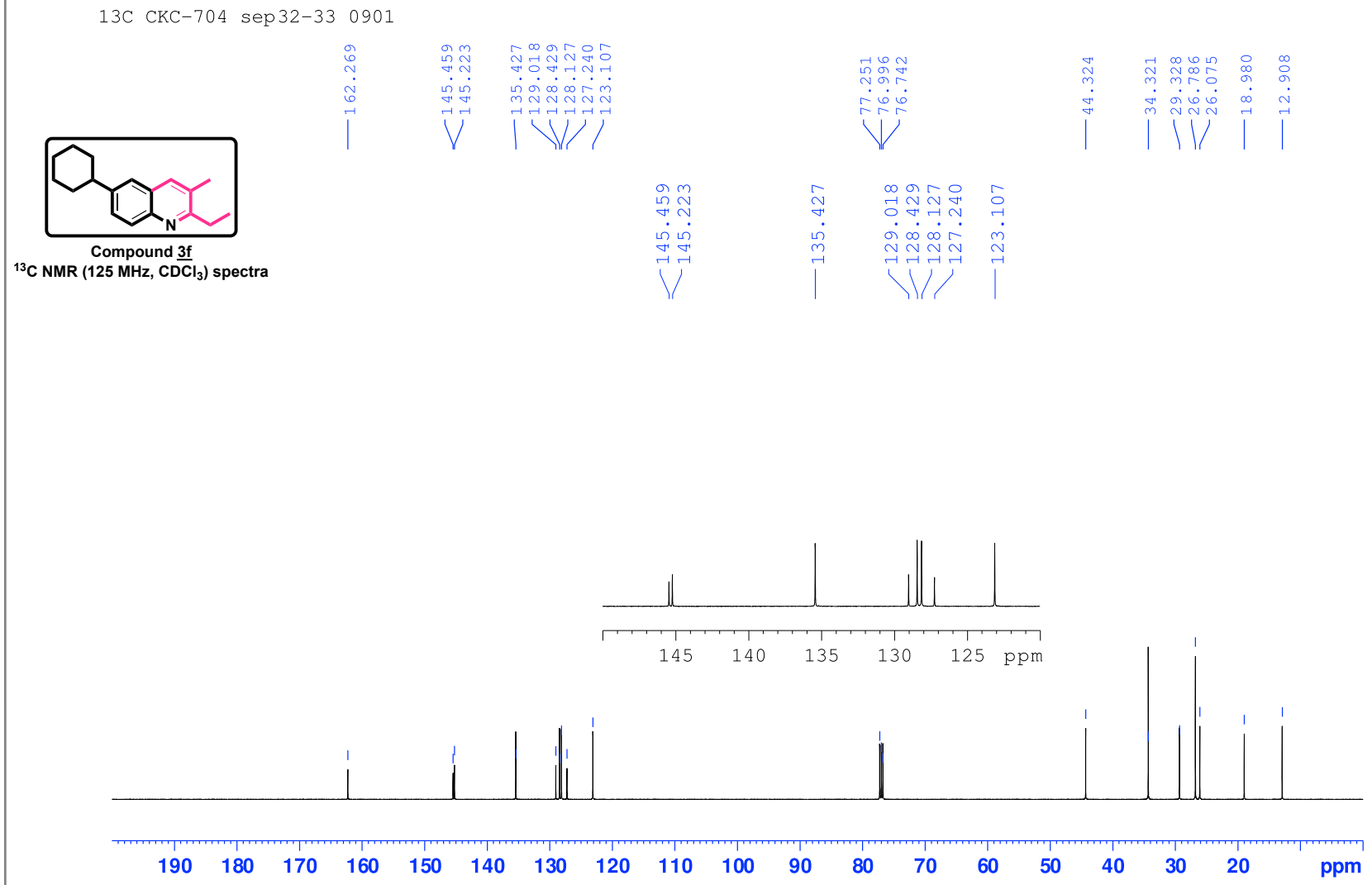
# Compound 3e


13C CKC-703 sep19-20 0901
162.089
143.863
139.668
139.634
135.344
131.081
129.322
128.899
127.642
127.438
126.858
126.370
125.339
77.252
76.997
76.744
28.994
18.902
11.588
N
Ph
Compound 3e
13C NMR (125 MHz, CDCl3) spectra
140
135
130
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

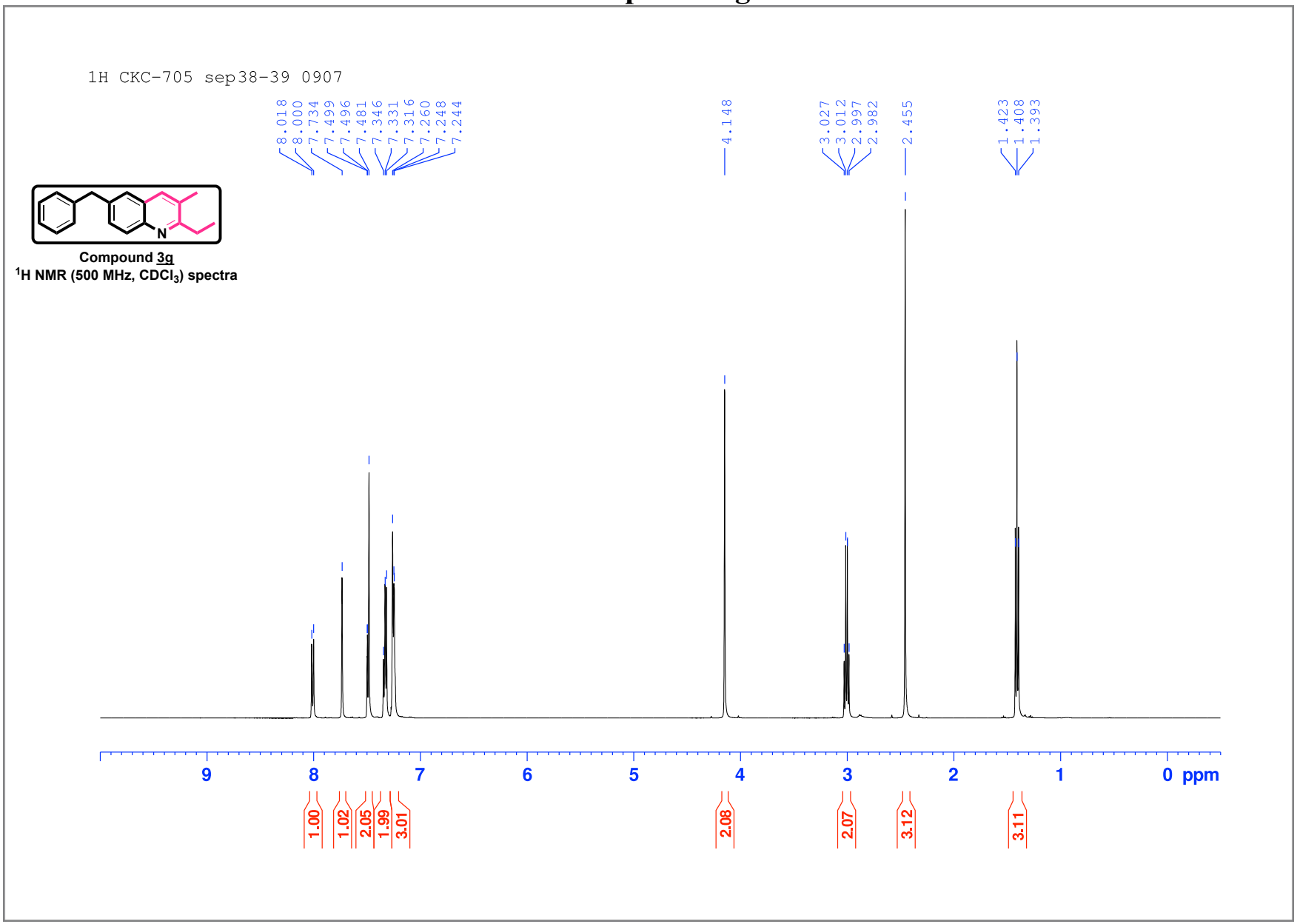
# Compound 3f


1H CKC-704 sep32-33 0901
7.958
7.941
7.740
7.501
7.498
7.484
7.480
7.461
7.260
2.984
2.969
2.953
2.938
2.659
2.642
2.636
2.630
2.613
2.435
1.955
1.930
1.880
1.785
1.759
1.532
1.507
1.502
1.478
1.458
1.438
1.418
1.413
1.407
1.388
1.361
1.346
1.330
1.316
1.297
1.291
1.284
N
Compound 3f
1H NMR (500 MHz, CDCl3) spectra
3.0
2.5
2.0
1.5
ppm
2.03
1.00
3.04
2.05
2.07
1.07
8.38
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.01
2.02
2.03
1.00
3.04
2.05
2.07
1.07
8.38

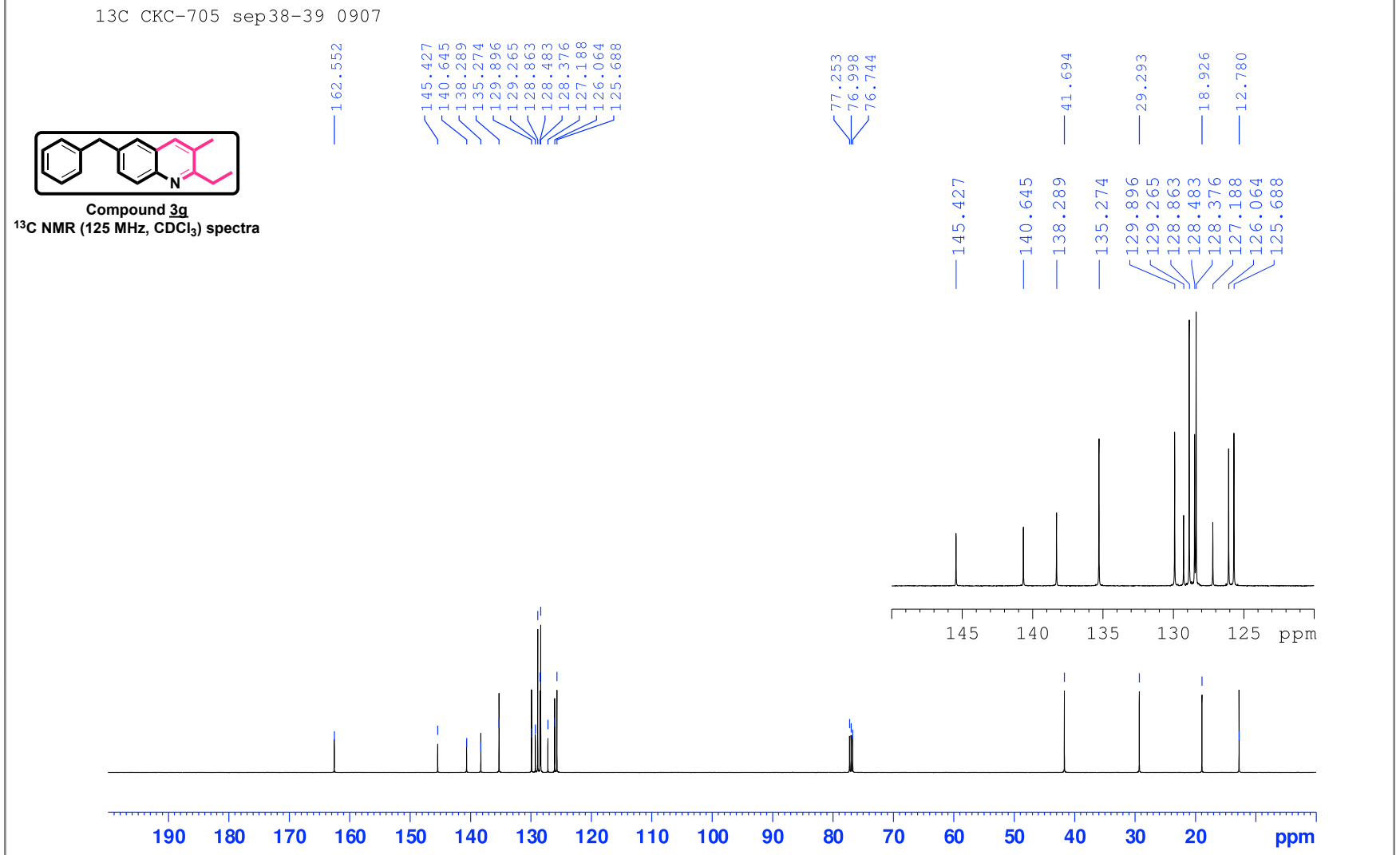
# Compound 3f


13C CKC-704 sep32-33 0901
162.269
145.459
145.223
135.427
129.018
128.429
128.127
127.240
123.107
77.251
76.996
76.742
44.324
34.321
29.328
26.786
26.075
18.980
12.908
N
Compound 3f
13C NMR (125 MHz, CDCl3) spectra
145
140
135
130
125
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

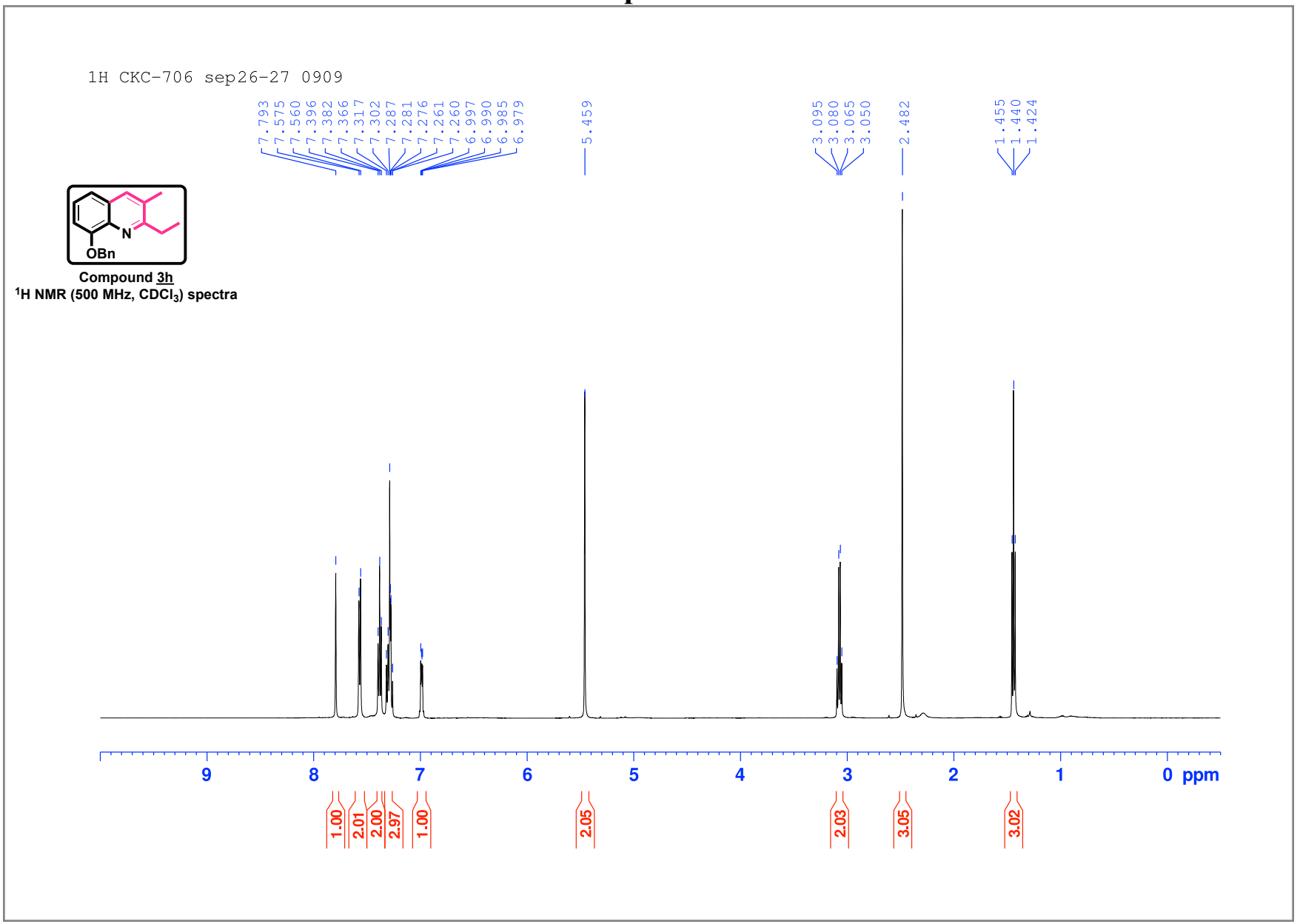
# Compound 3g


1H CKC-705 sep38-39 0907
8.018
8.000
7.734
7.499
7.496
7.481
7.346
7.331
7.316
7.260
7.248
7.244
4.148
3.027
3.012
2.997
2.982
2.455
1.423
1.408
1.393
N
Compound 3g
1H NMR (500 MHz, CDCl3) spectra
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.02
2.05
1.99
3.01
2.08
2.07
3.12
3.11

# Compound 3g

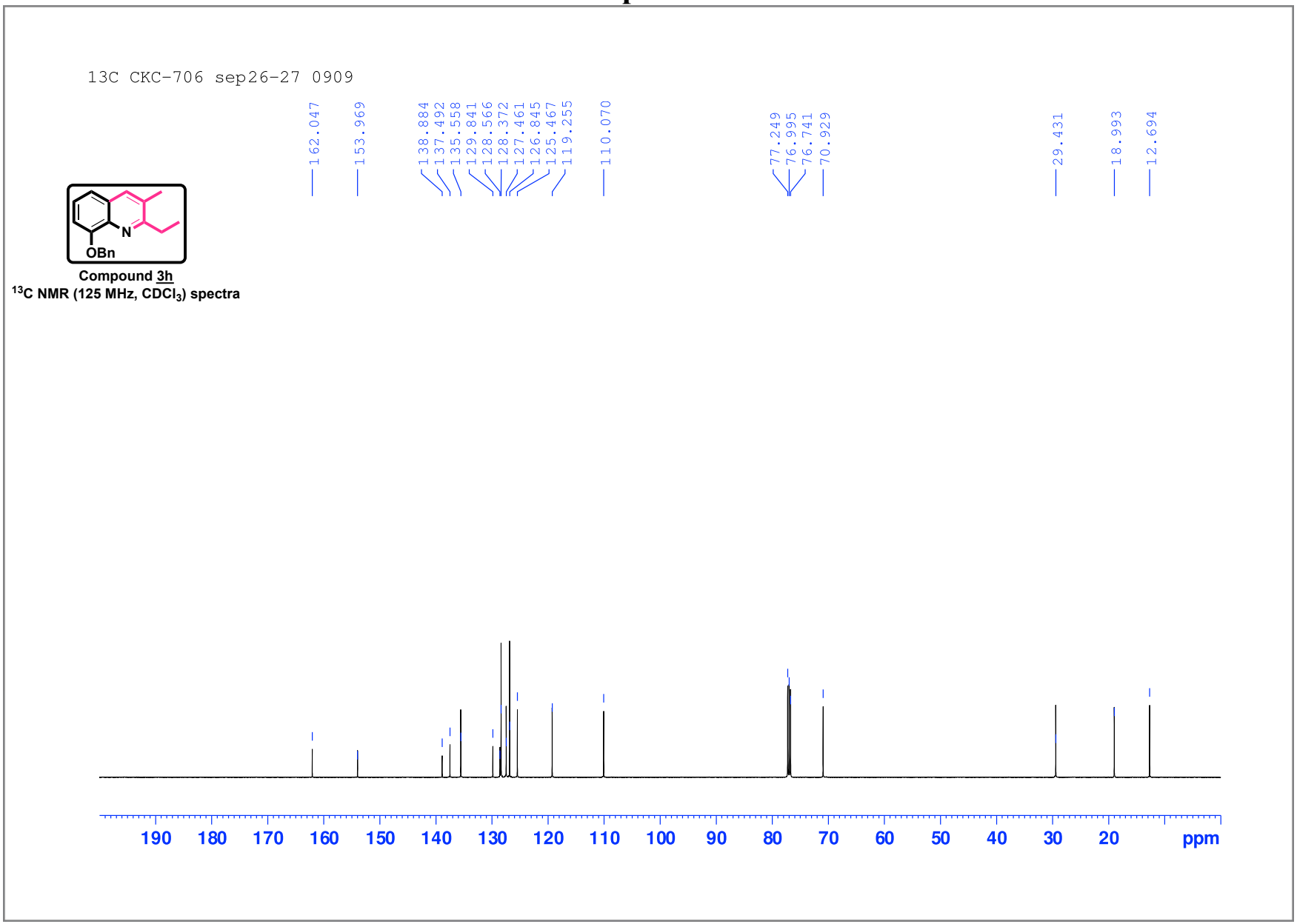

13C CKC-705 sep38-39 0907
162.552
145.427
140.645
138.289
135.274
129.896
129.265
128.863
128.483
128.376
127.188
126.064
125.688
77.253
76.998
76.744
41.694
29.293
18.926
12.780
N
Compound 3g
13C NMR (125 MHz, CDCl3) spectra
145
140
135
130
125
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

# Compound 3h




Compound 3h
$^1$H NMR (500 MHz, $CDCl_3$) spectra

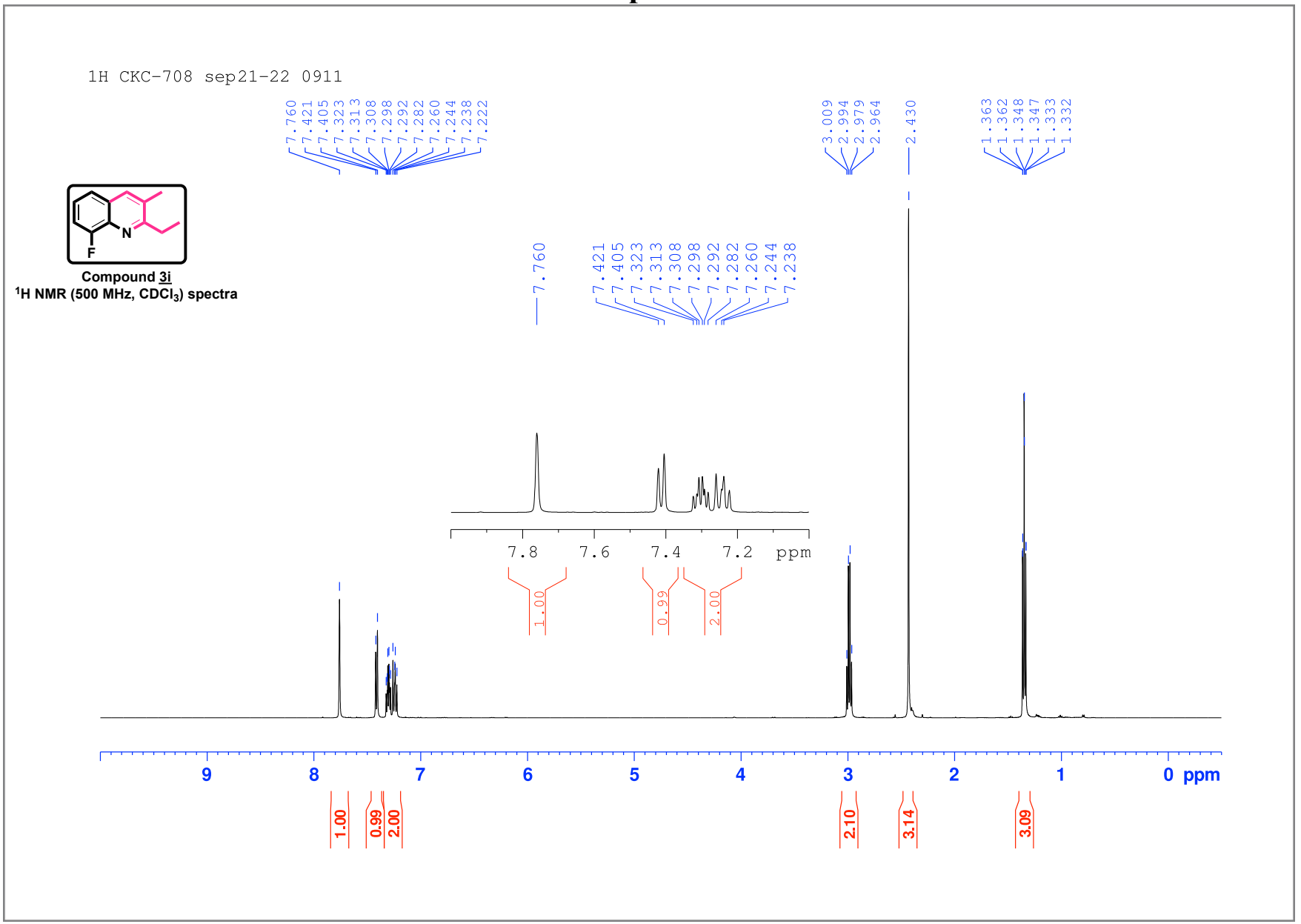
# Compound 3h



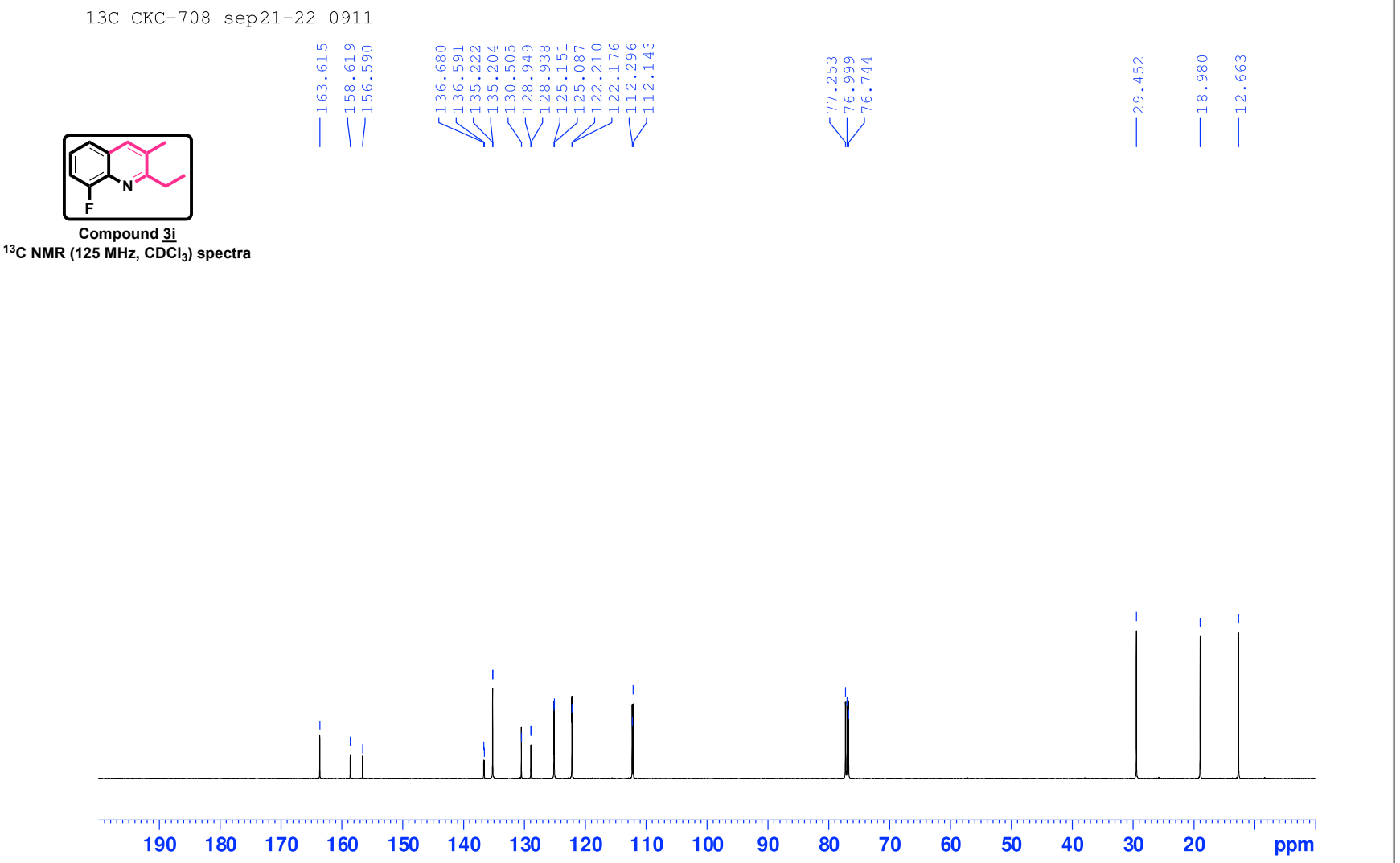

**Compound 3h**

**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 3i

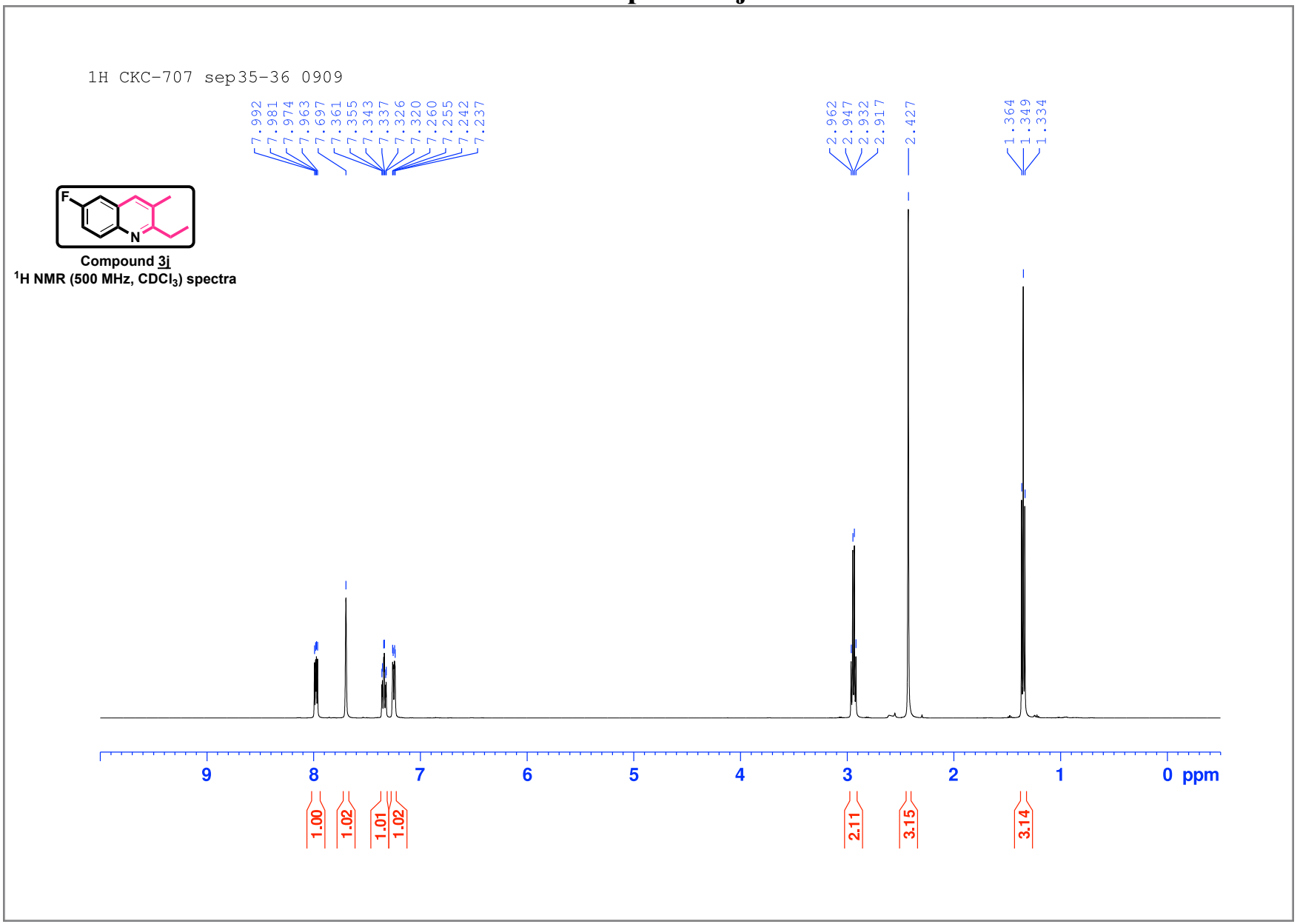

1H CKC-708 sep21-22 0911
7.760
7.421
7.405
7.323
7.313
7.308
7.298
7.292
7.282
7.260
7.244
7.238
7.222
3.009
2.994
2.979
2.964
2.430
1.363
1.362
1.348
1.347
1.333
1.332
F
N
Compound 3i
1H NMR (500 MHz, CDCl3) spectra
7.8
7.6
7.4
7.2
ppm
1.00
0.99
2.00
9
8
7
6
5
4
3
2
1
0 ppm
1.00
0.99
2.00
2.10
3.14
3.09

# Compound 3i



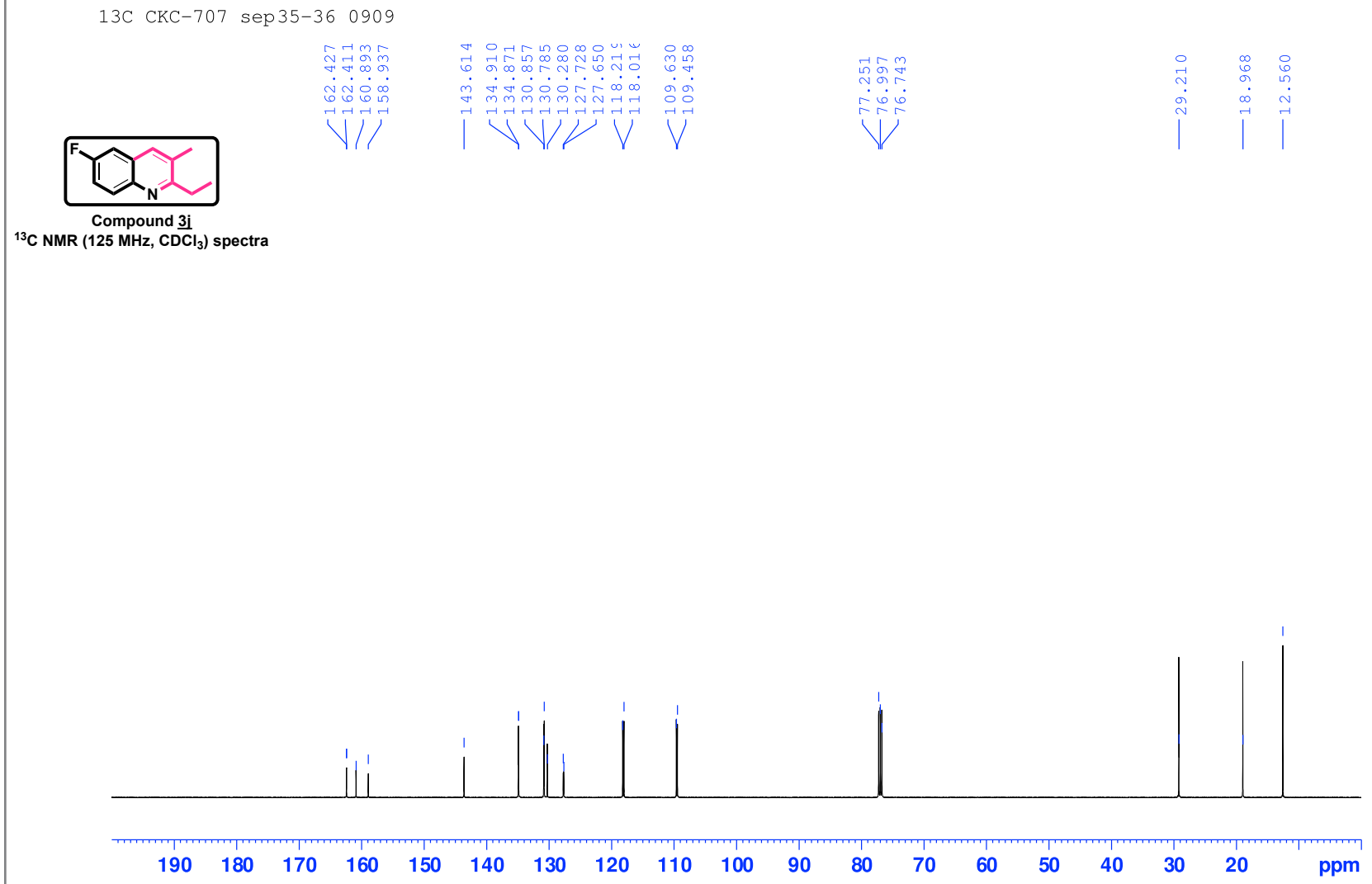

**Compound 3i**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 3j



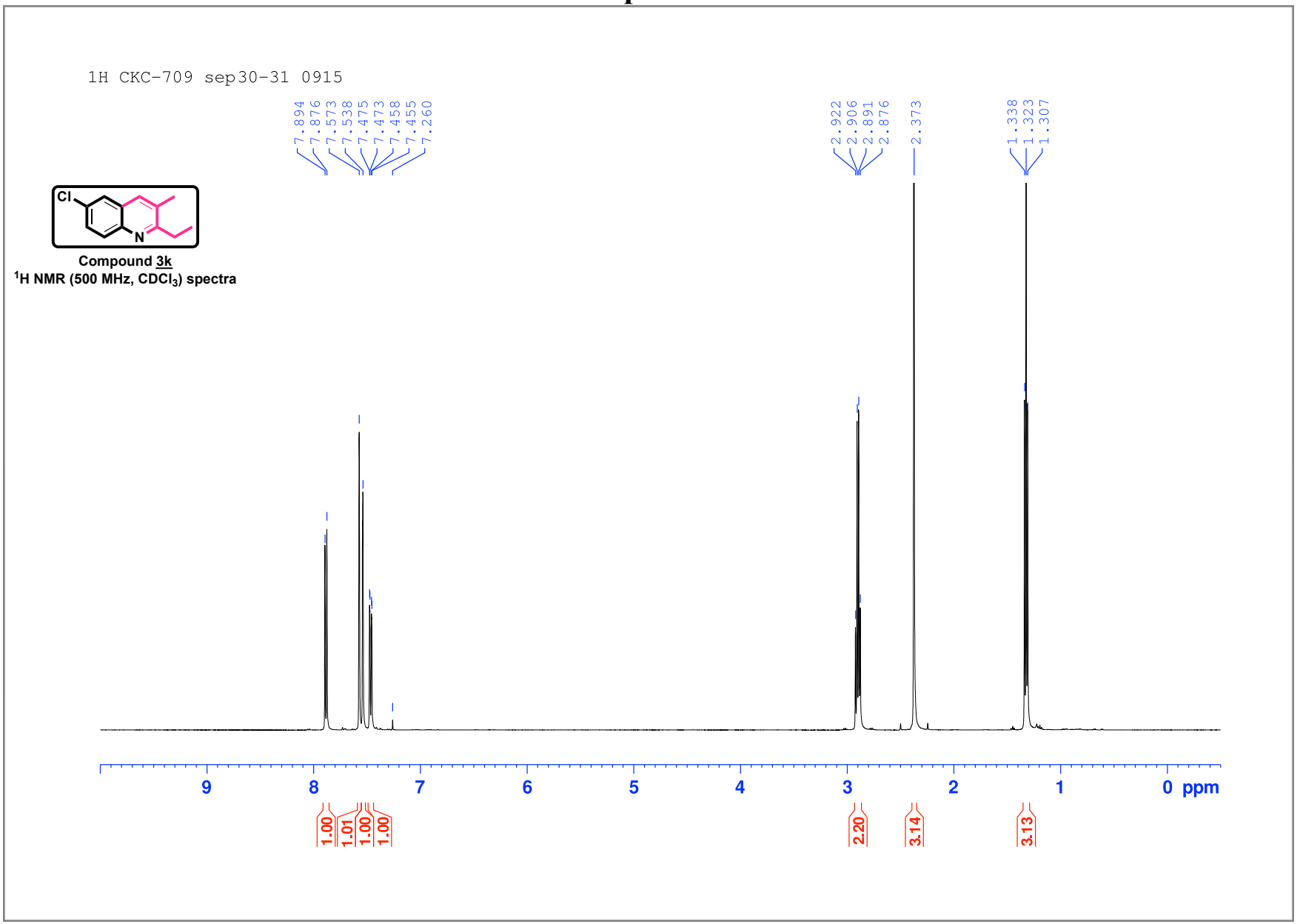

Compound 3j
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 3j

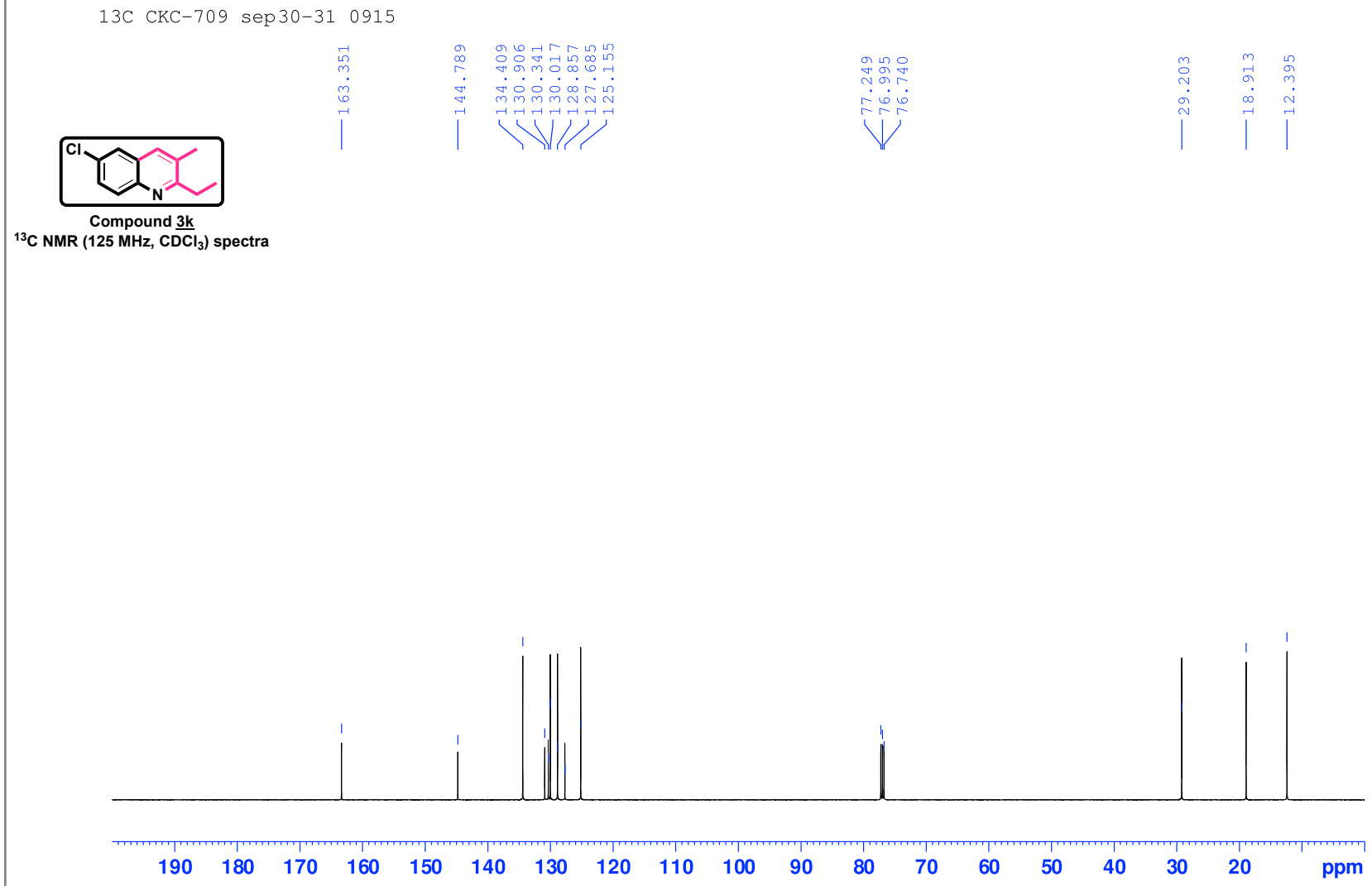



**Compound 3j**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 3k

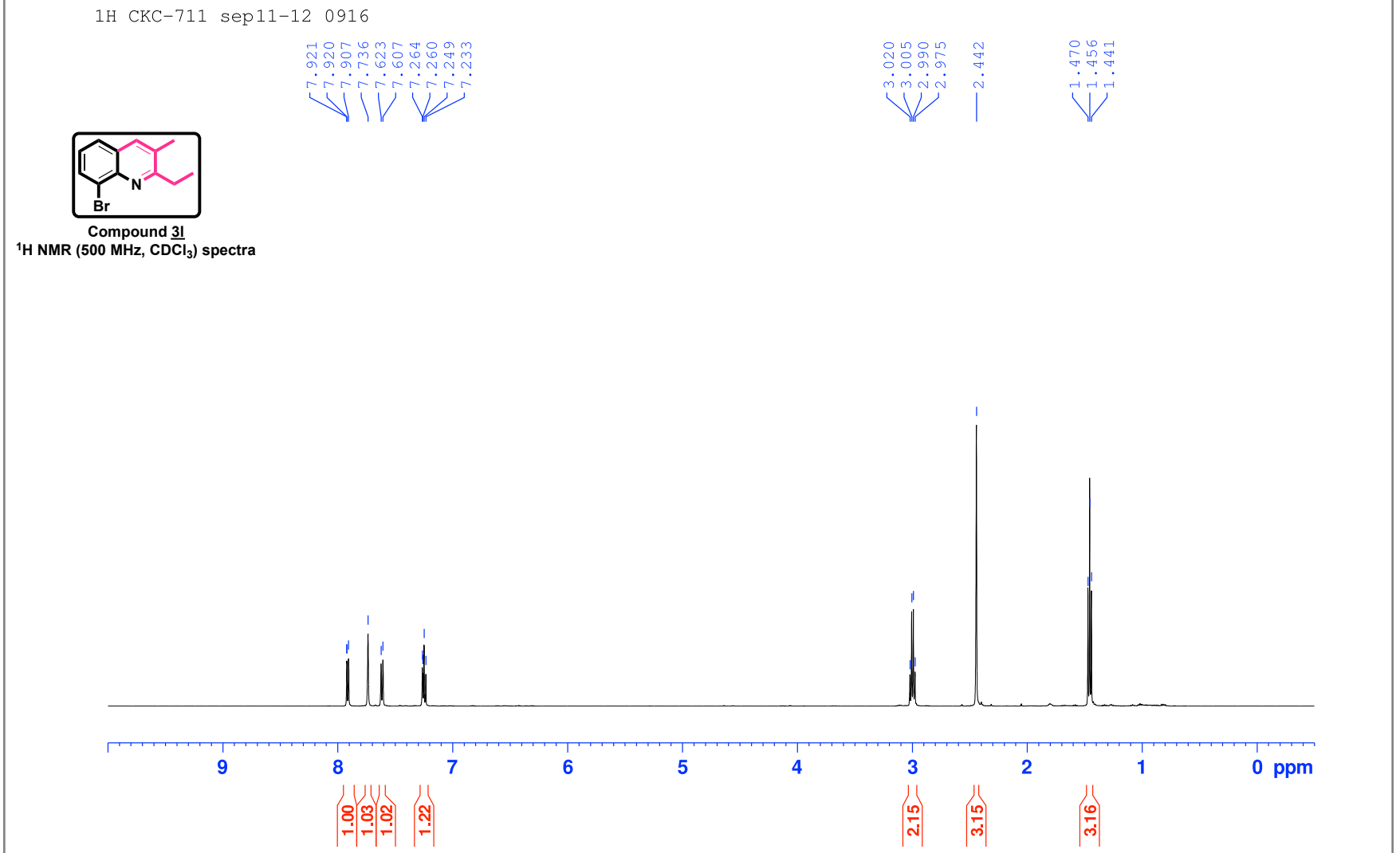

1H CKC-709 sep30-31 0915
7.894
7.876
7.573
7.538
7.475
7.473
7.458
7.455
7.260
2.922
2.906
2.891
2.876
2.373
1.338
1.323
1.307
Cl
N
Compound 3k
1H NMR (500 MHz, CDCl3) spectra
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.01
1.00
1.00
2.20
3.14
3.13

# Compound 3k




**Compound 3k**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

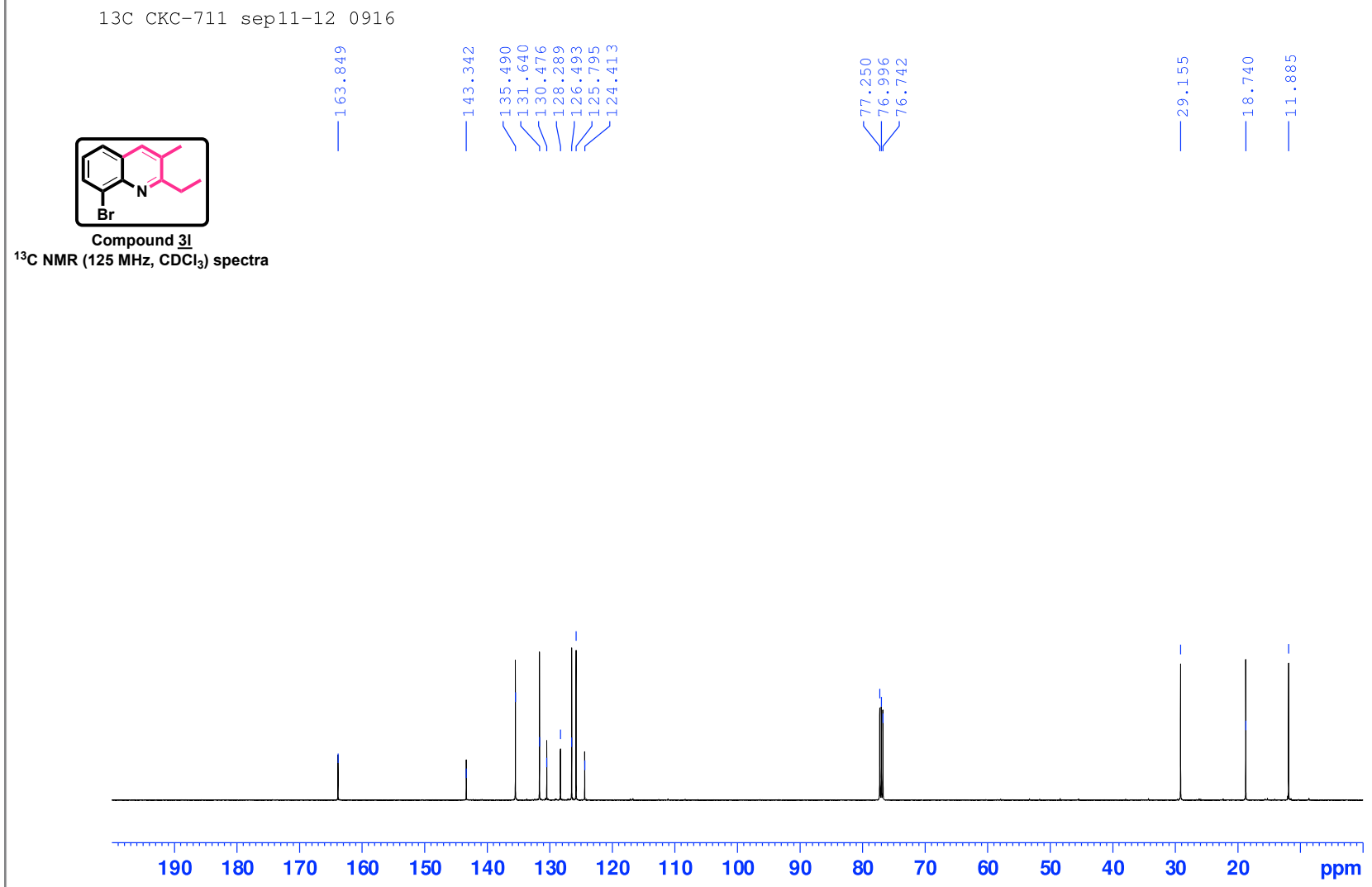
# Compound 3l




Compound 3l

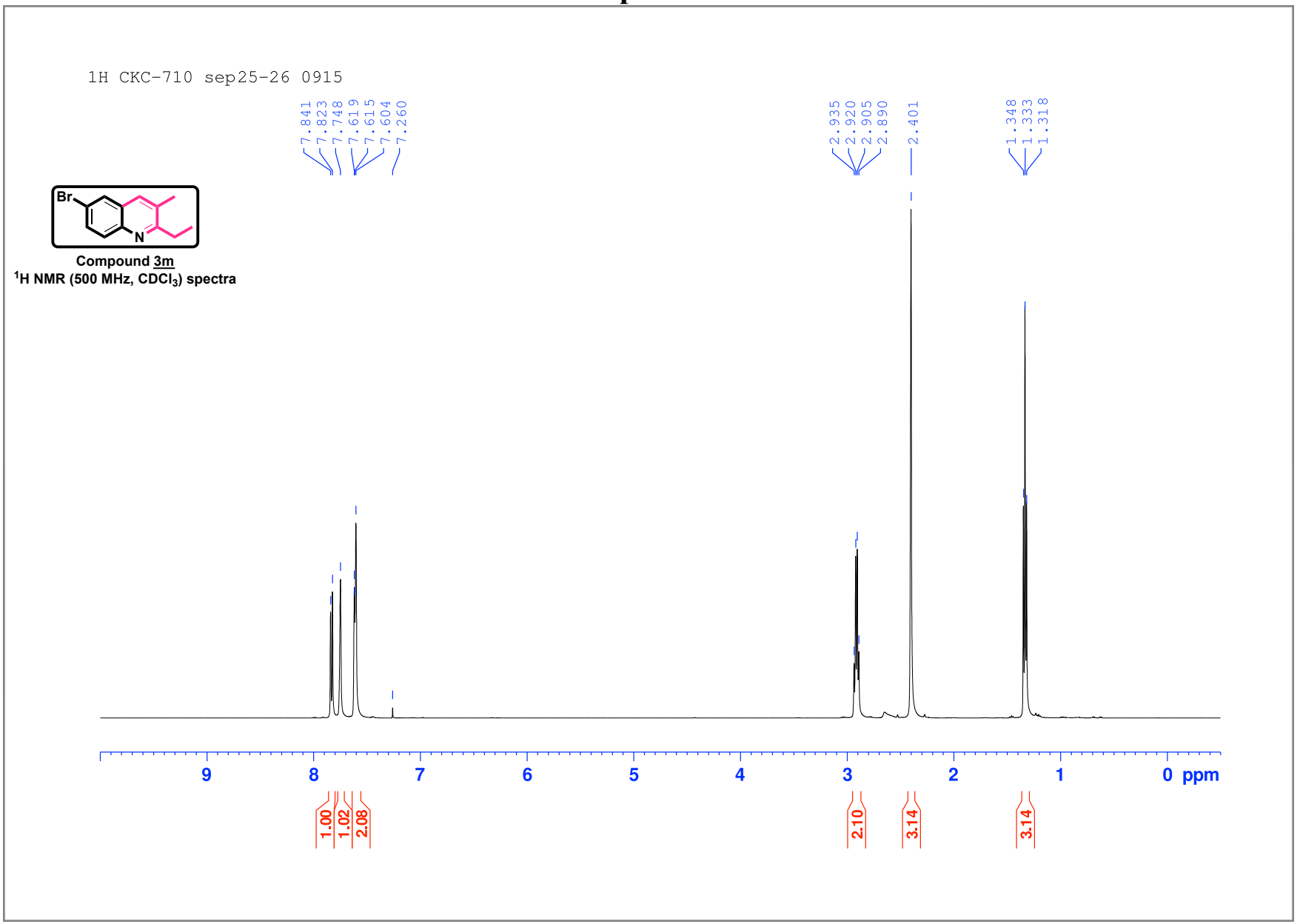
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 3l



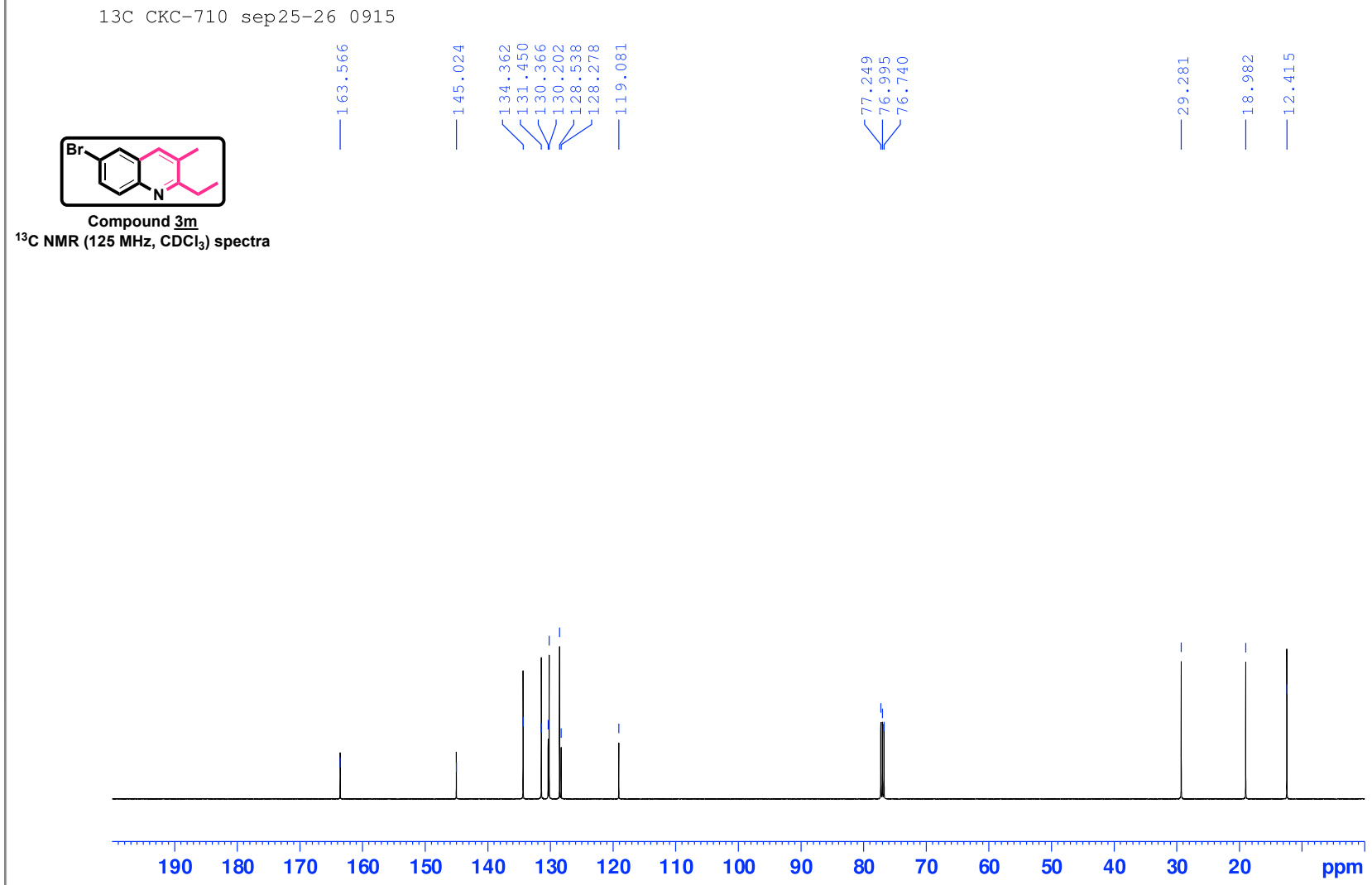

**Compound 3l**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 3m



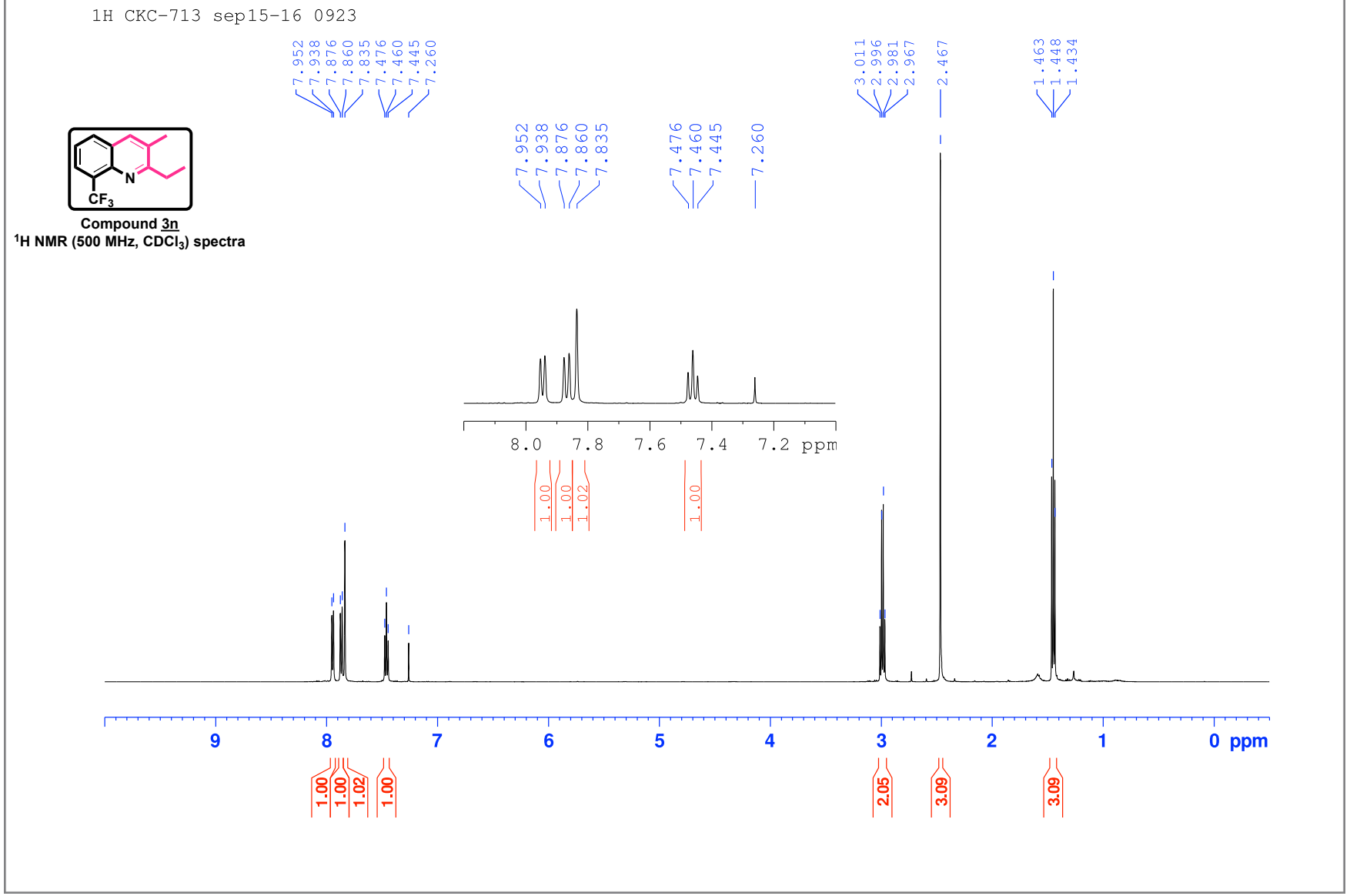

**Compound 3m**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

# Compound 3m



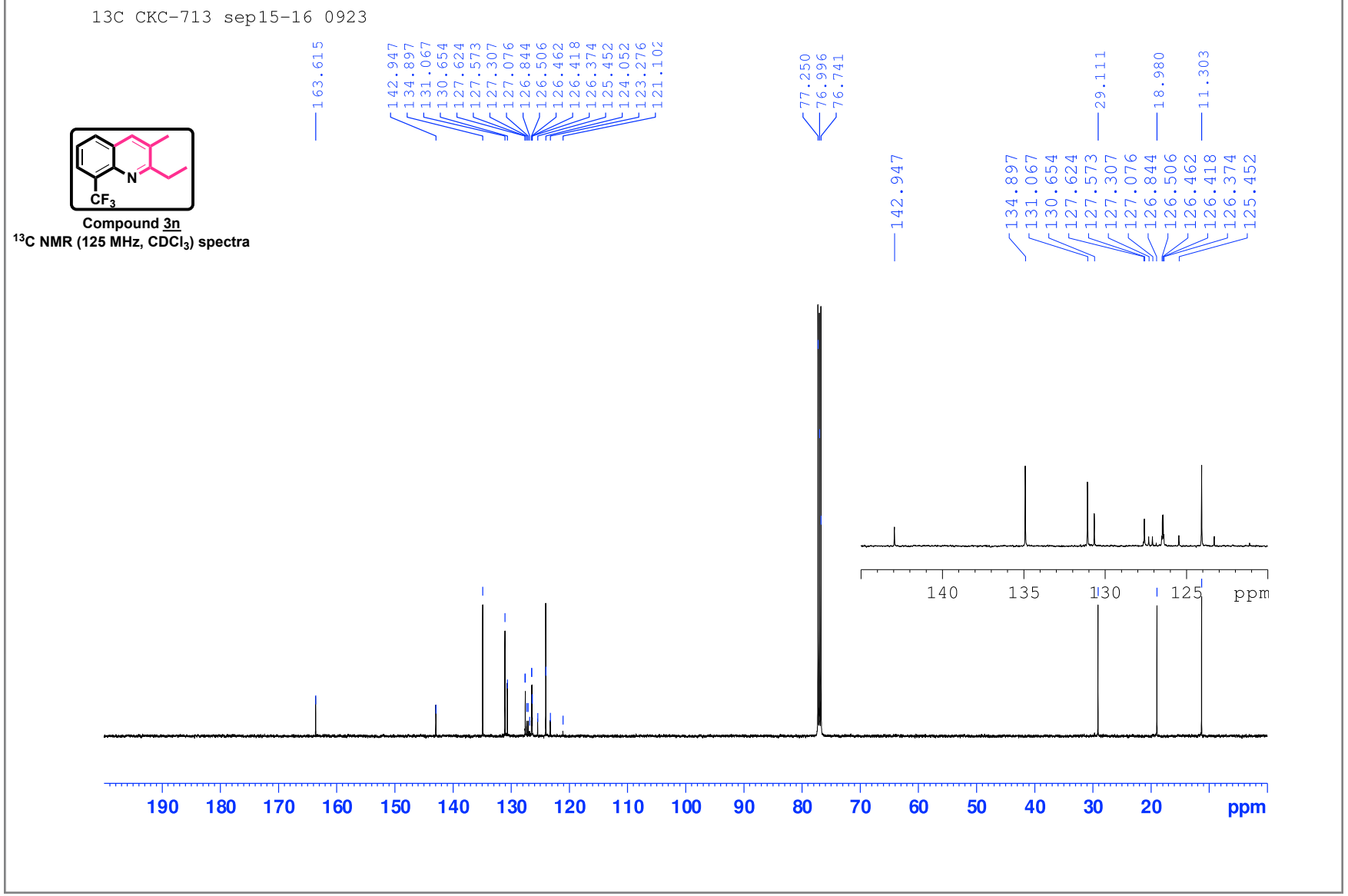

**Compound 3m**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 3n




Compound 3n
$^1$H NMR (500 MHz, $CDCl_3$) spectra

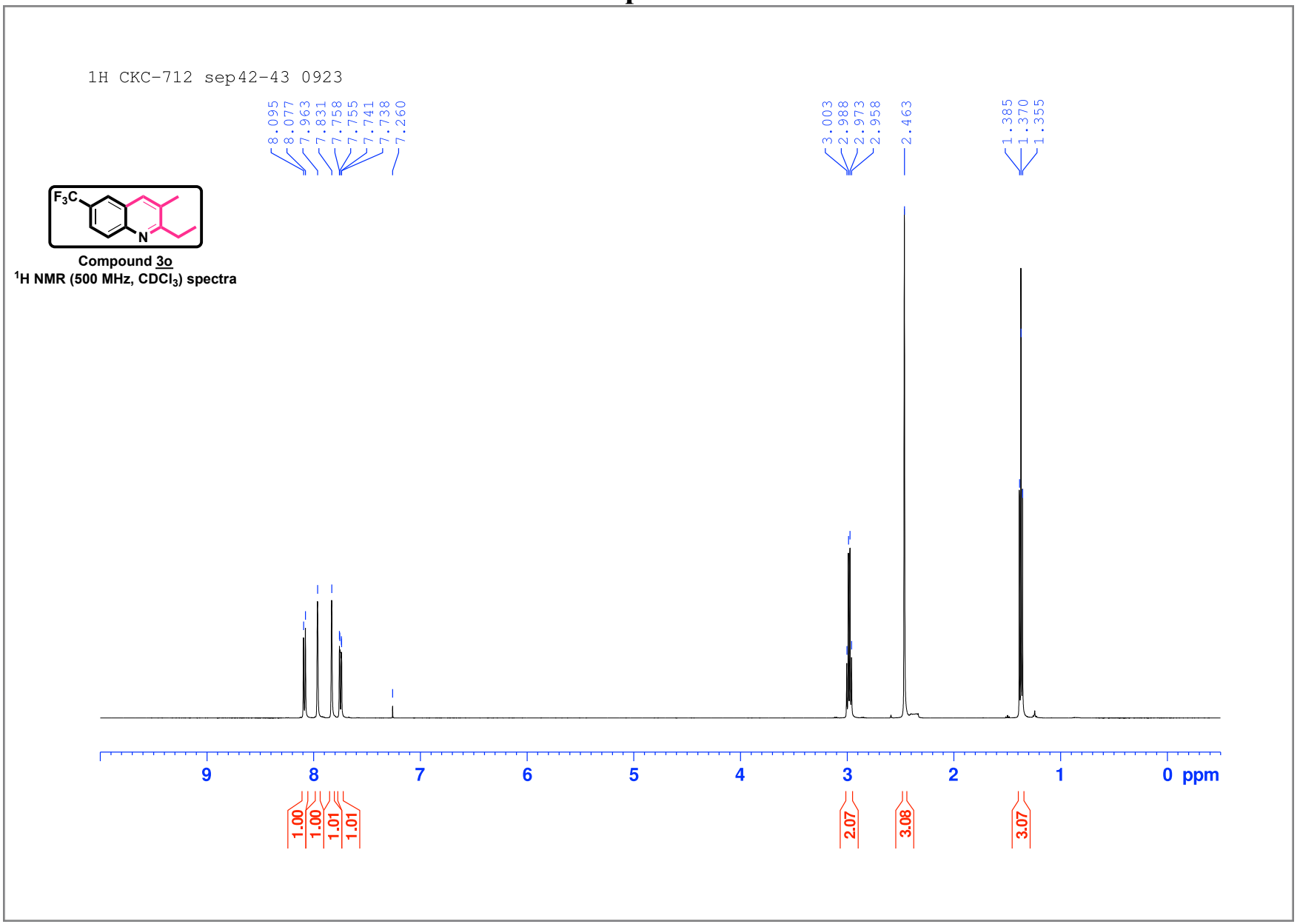
# Compound 3n




Compound 3n

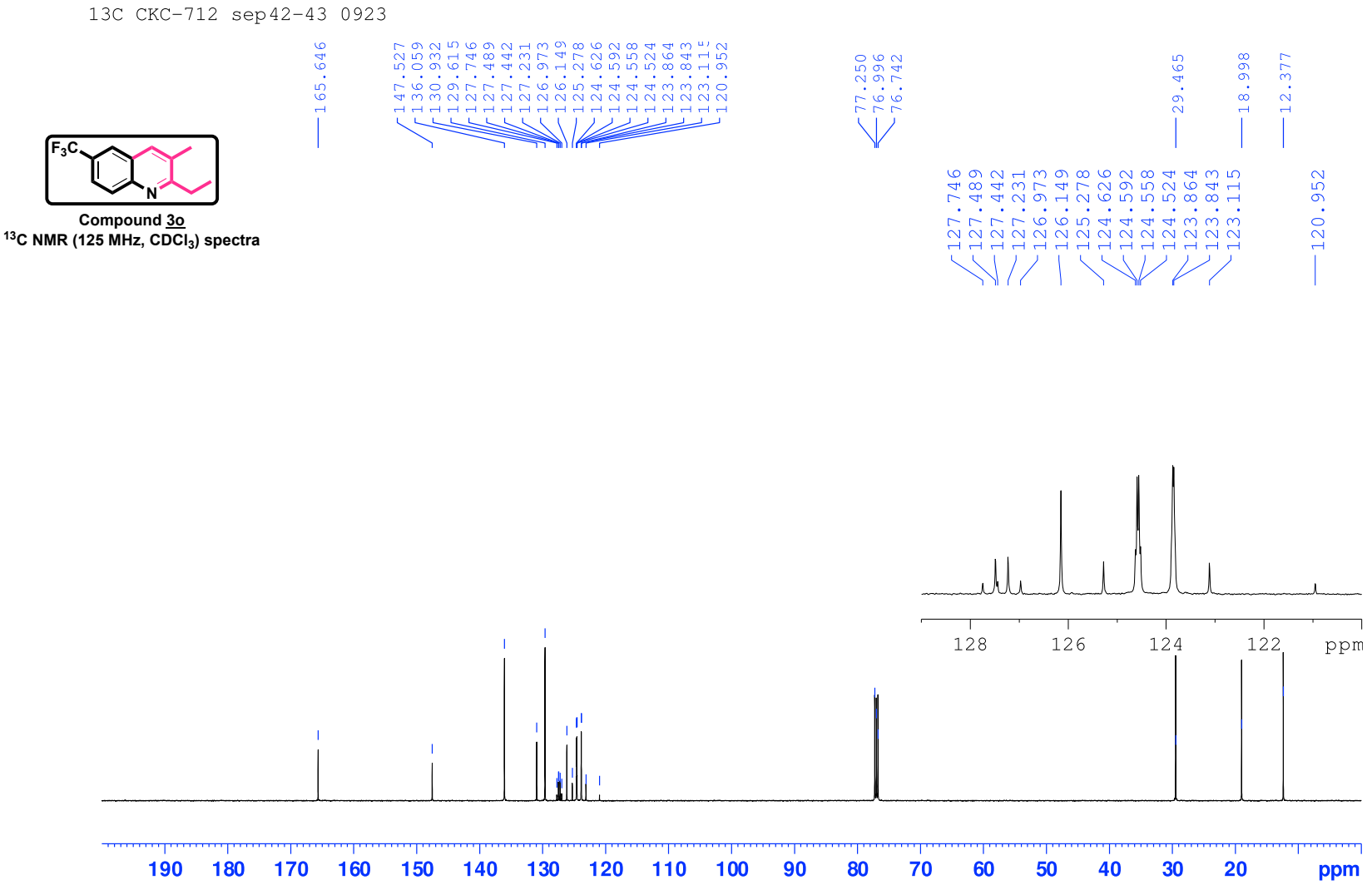
$^{13}$C NMR (125 MHz, $CDCl_3$) spectra

# Compound 3o

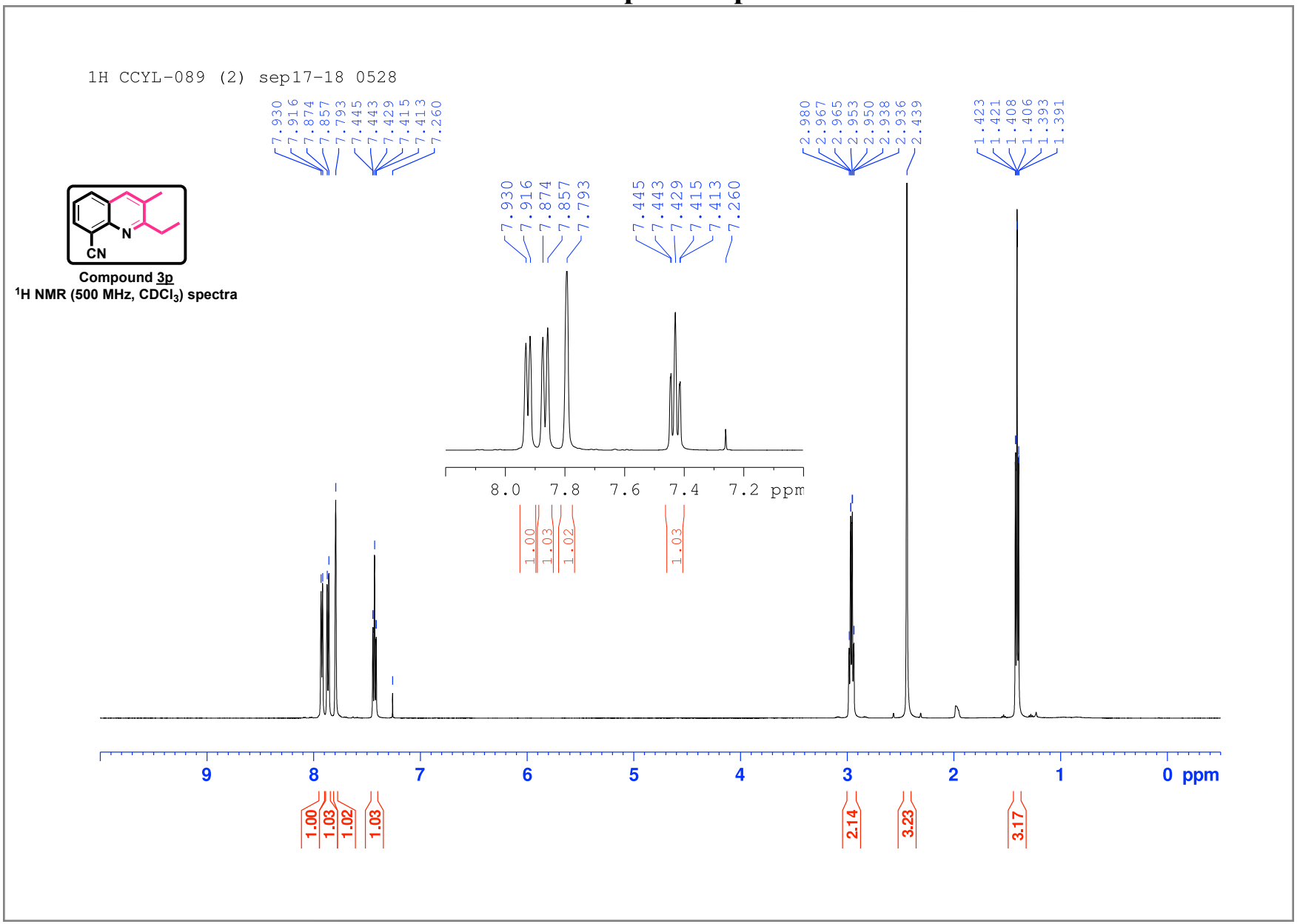



Compound 3o
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 3o

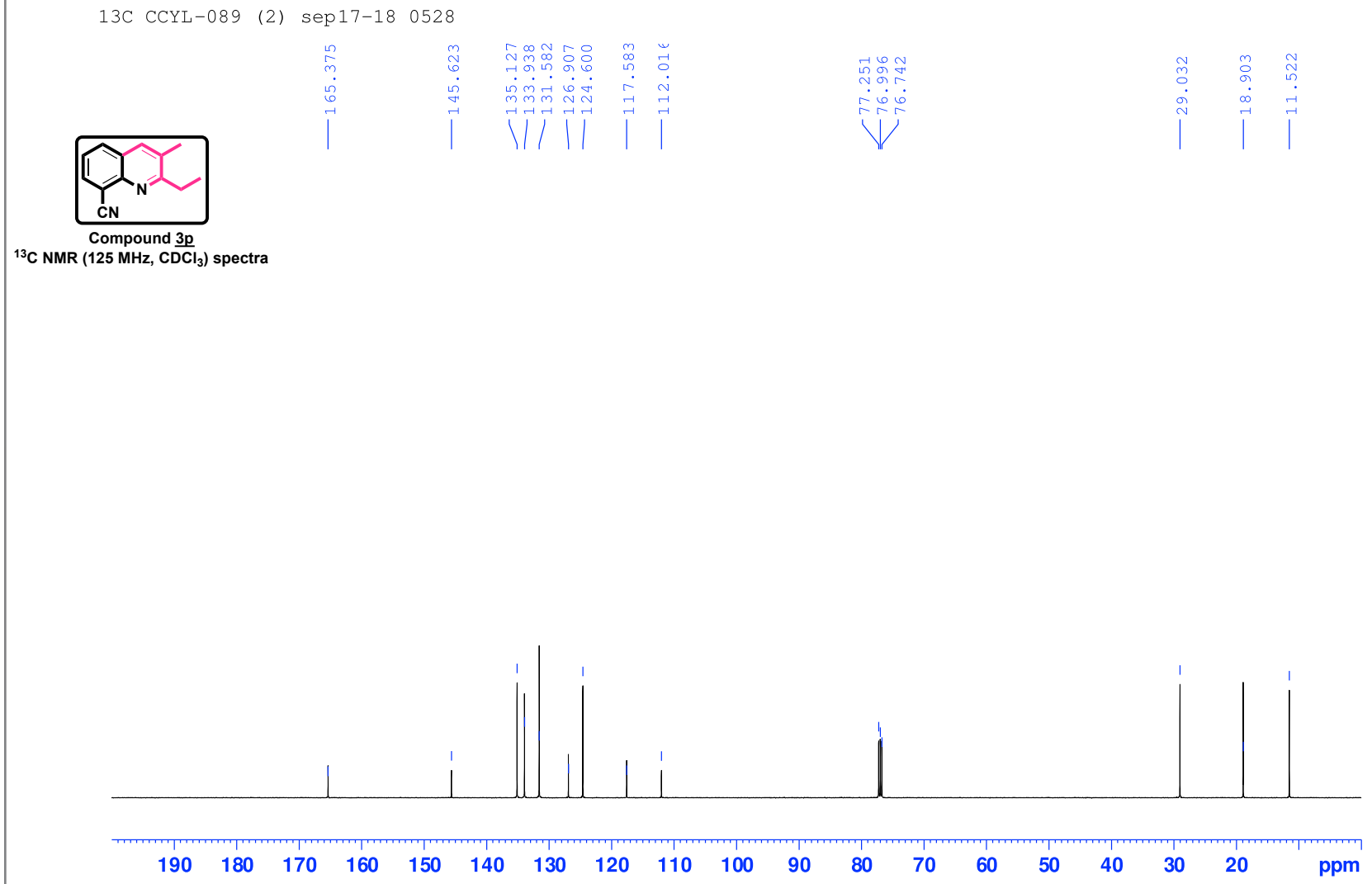

13C CKC-712 sep42-43 0923
165.646
147.527
136.059
130.932
129.615
127.746
127.489
127.442
127.231
126.973
126.149
125.278
124.626
124.592
124.558
124.524
123.864
123.843
123.115
120.952
77.250
76.996
76.742
29.465
18.998
12.377
F3C
N
Compound 3o
13C NMR (125 MHz, CDCl3) spectra
128
126
124
122
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

# Compound 3p




Compound 3p
$^1$H NMR (500 MHz, $CDCl_3$) spectra

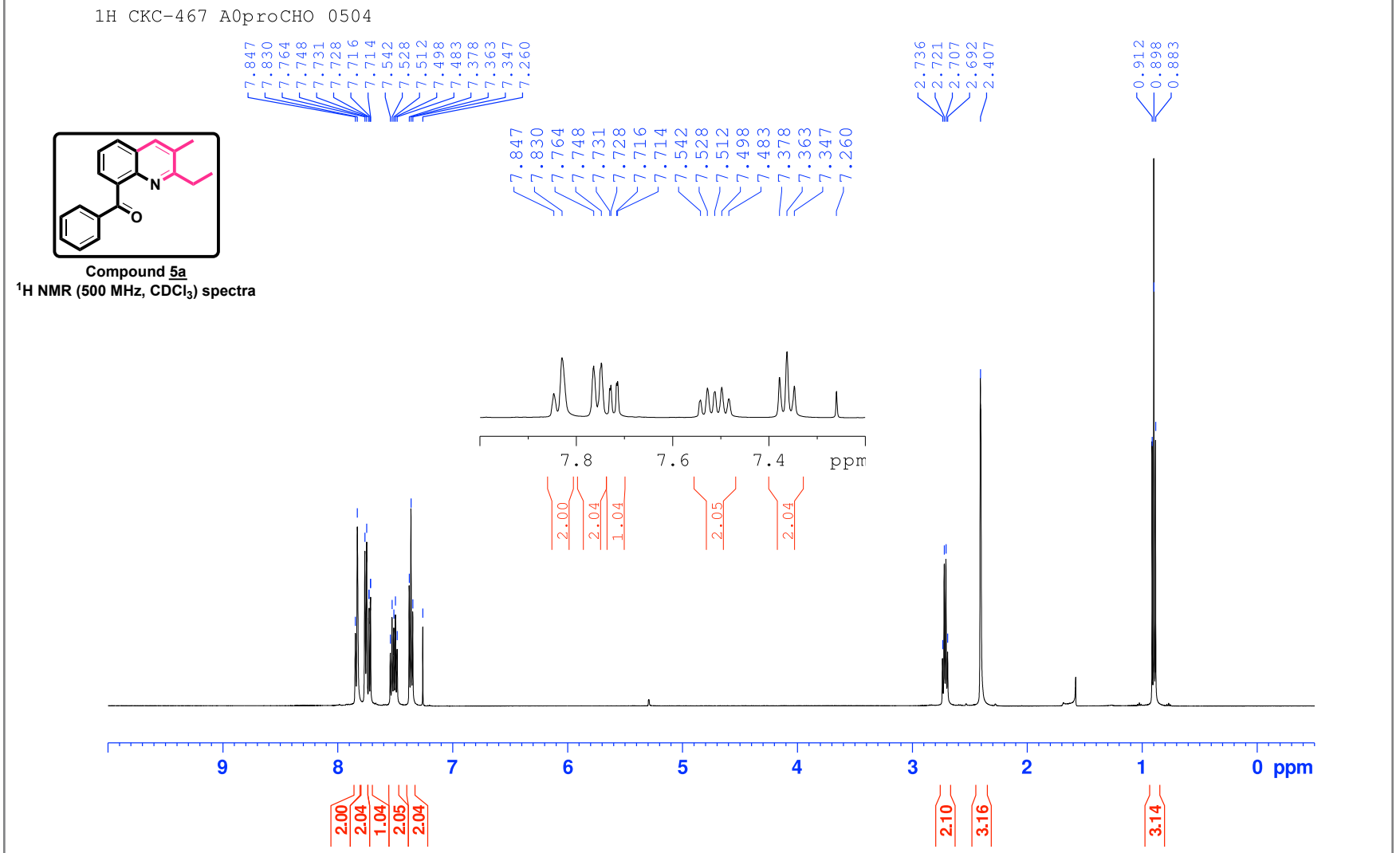
# Compound 3p




Compound 3p

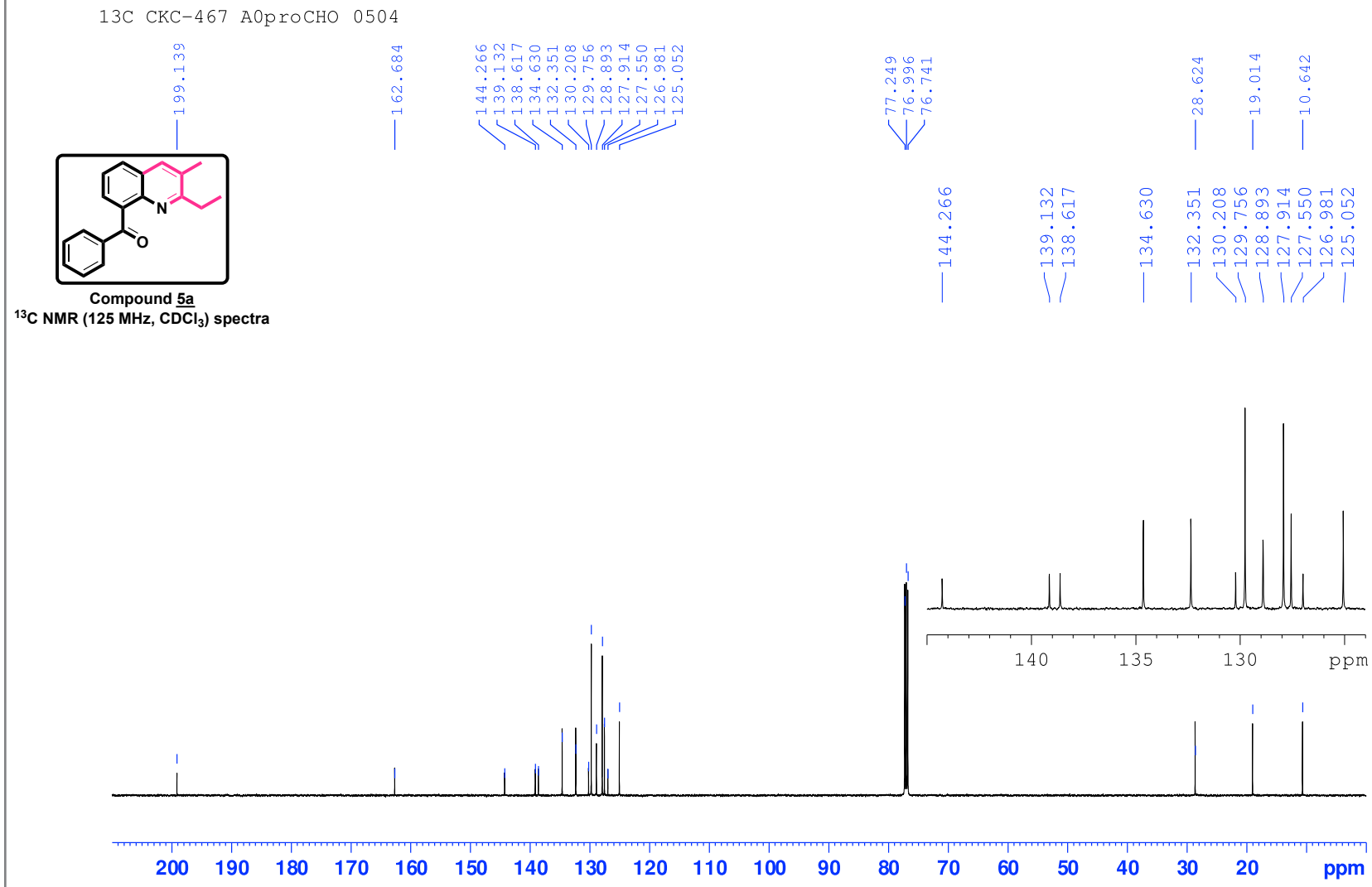
$^{13}C$ NMR (125 MHz, $CDCl_3$) spectra

# Compound 5a



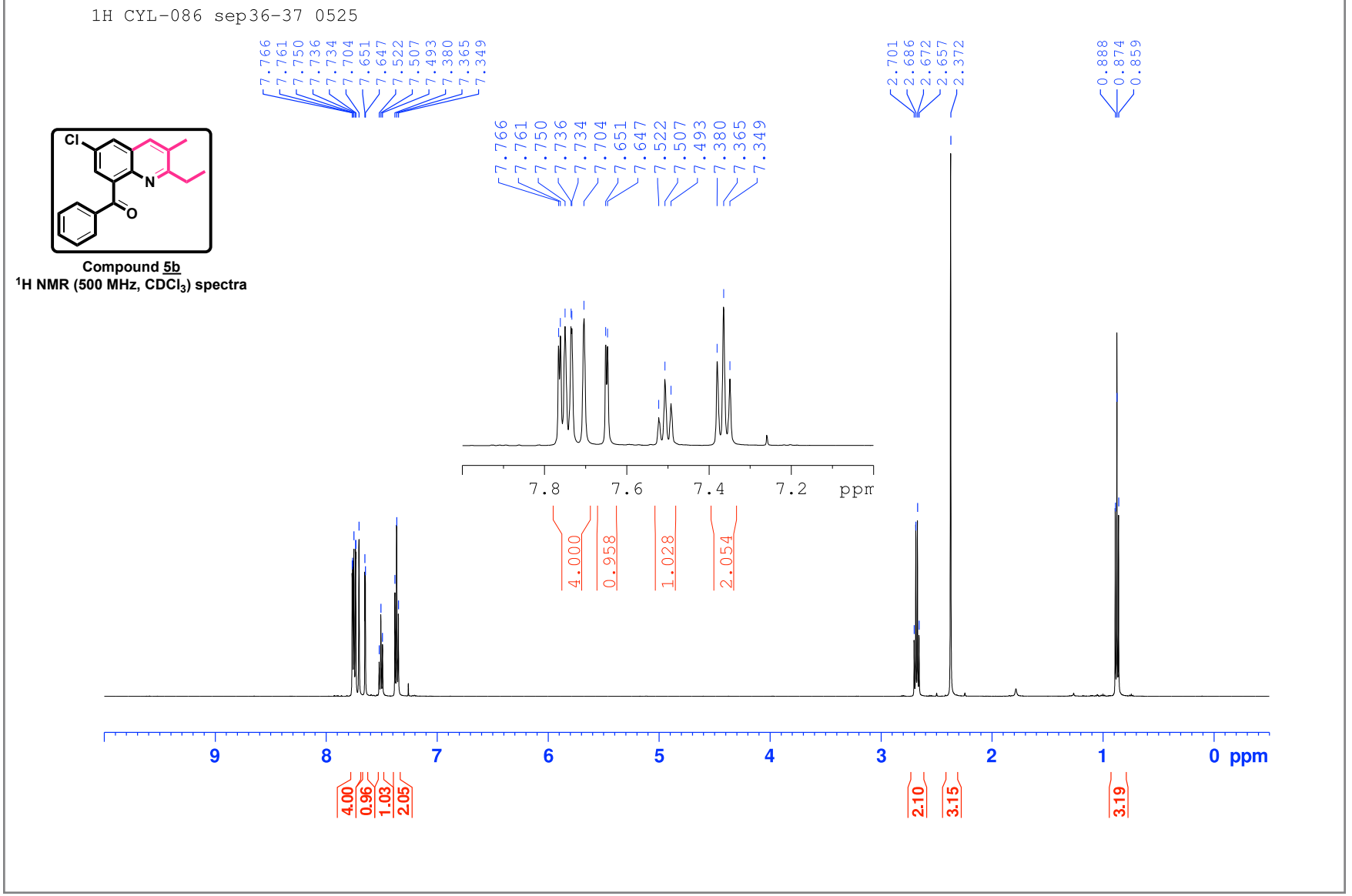

Compound 5a
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 5a



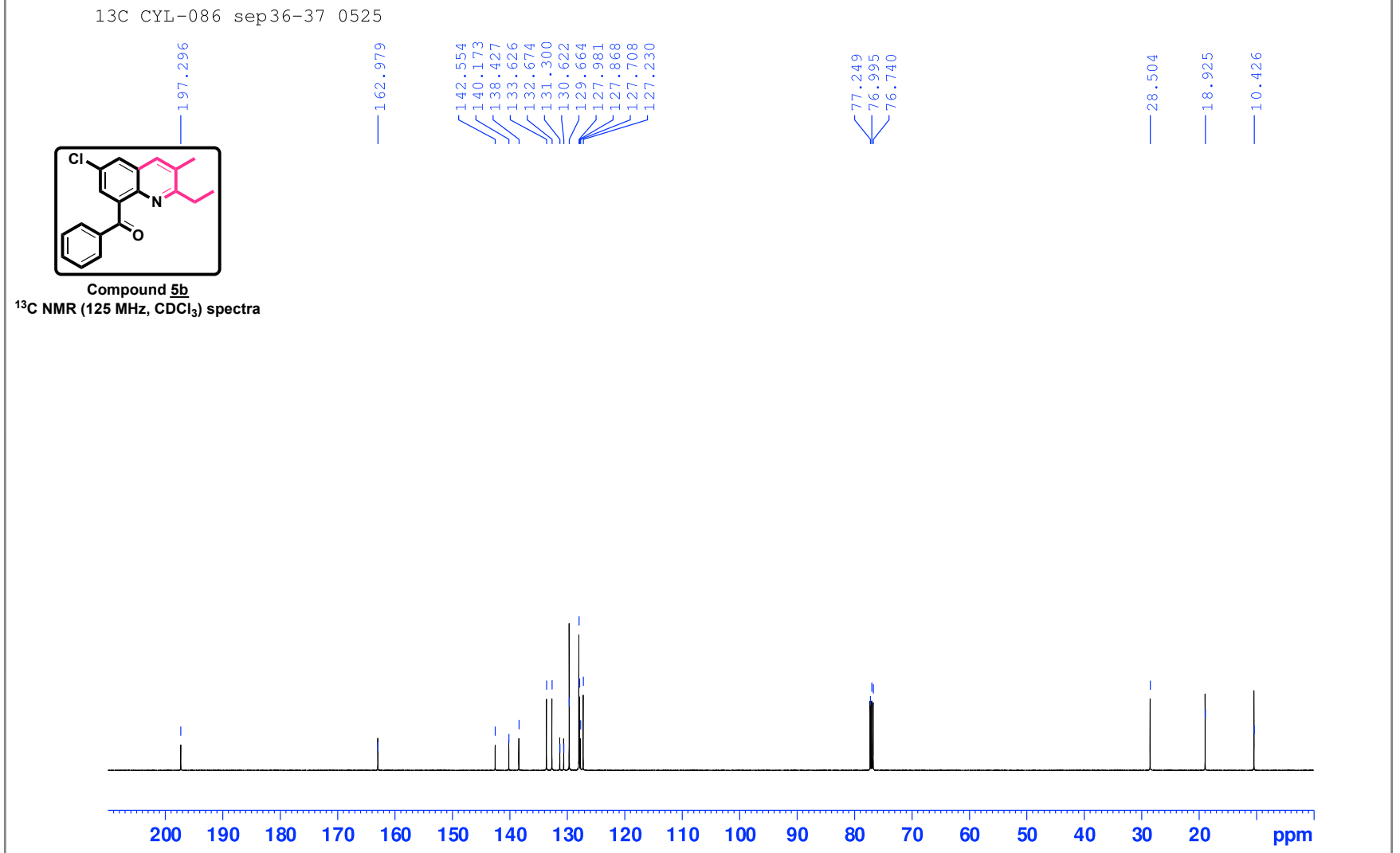

**Compound 5a**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5b




Compound 5b
$^1$H NMR (500 MHz, $CDCl_3$) spectra

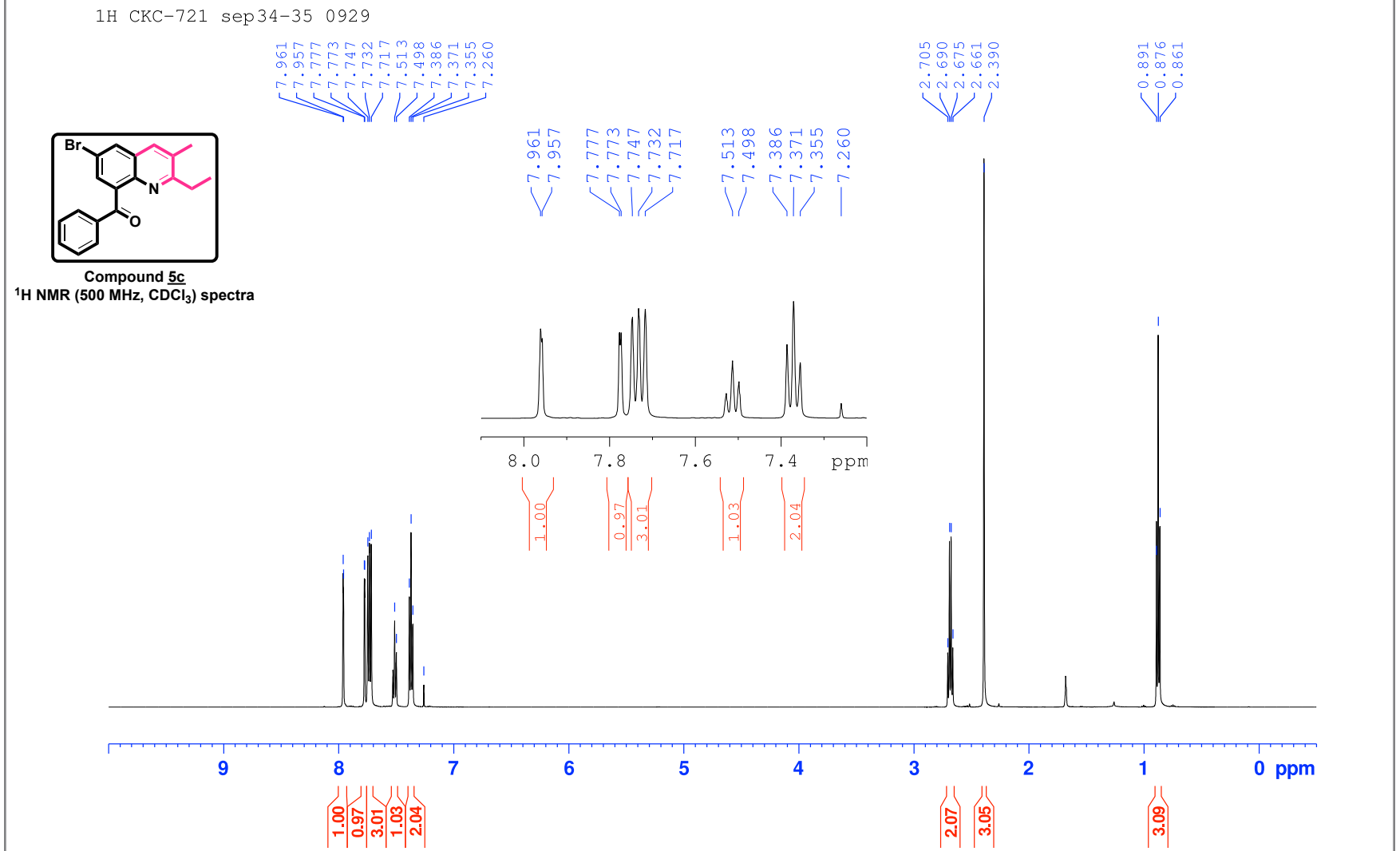
# Compound 5b




Compound 5b

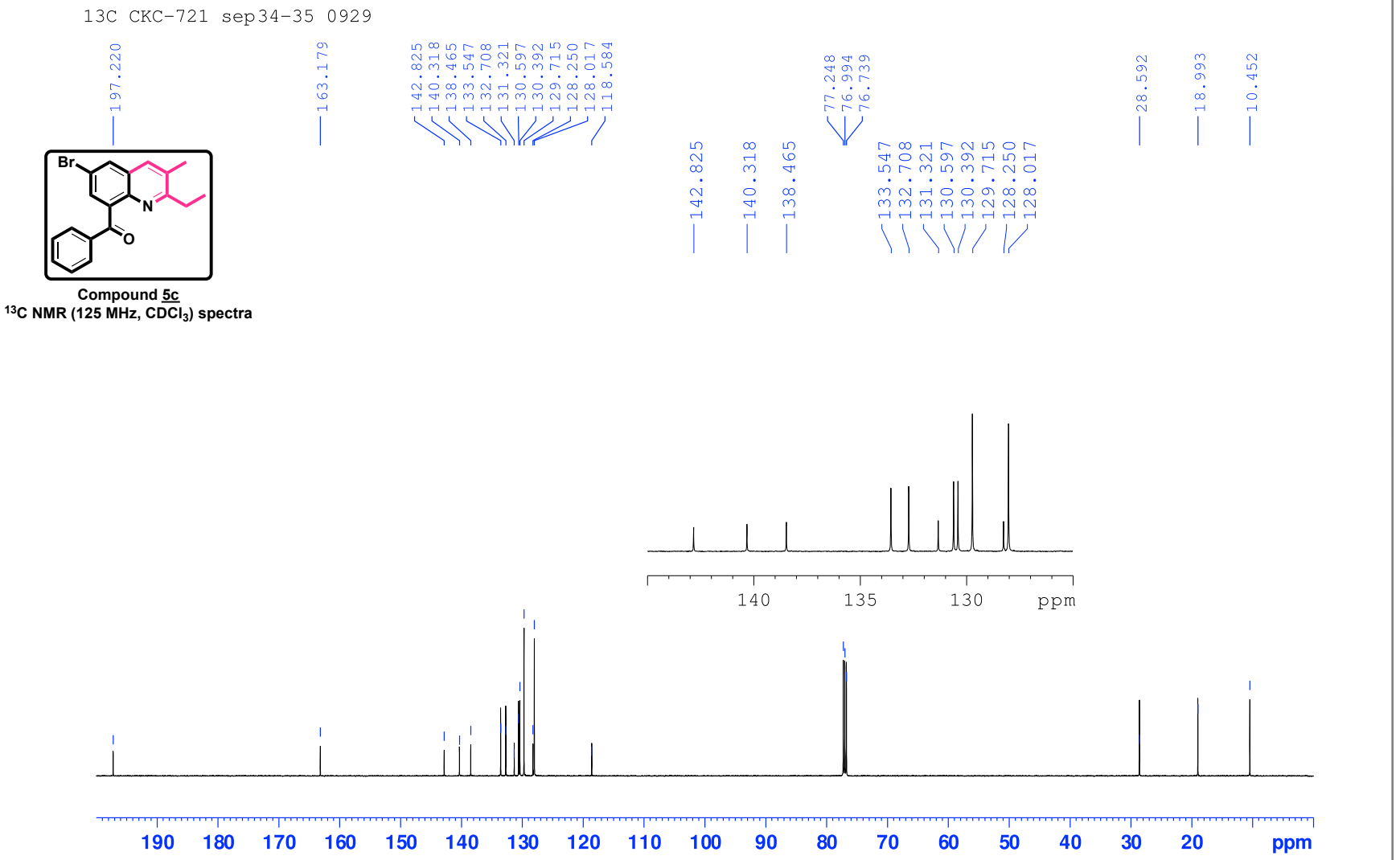
$^{13}C$ NMR (125 MHz, $CDCl_3$) spectra

# Compound 5c



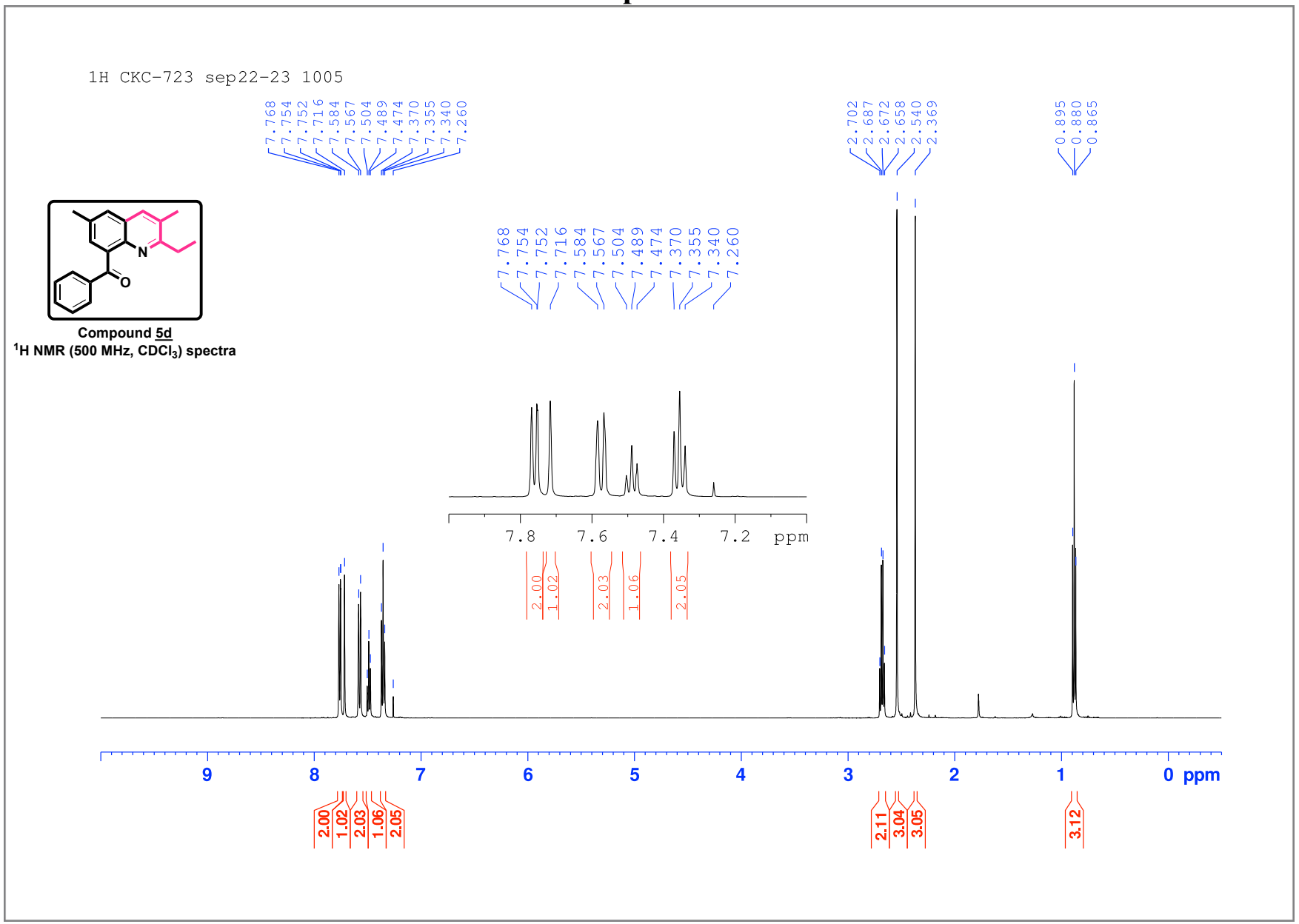

**Compound 5c**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

# Compound 5c

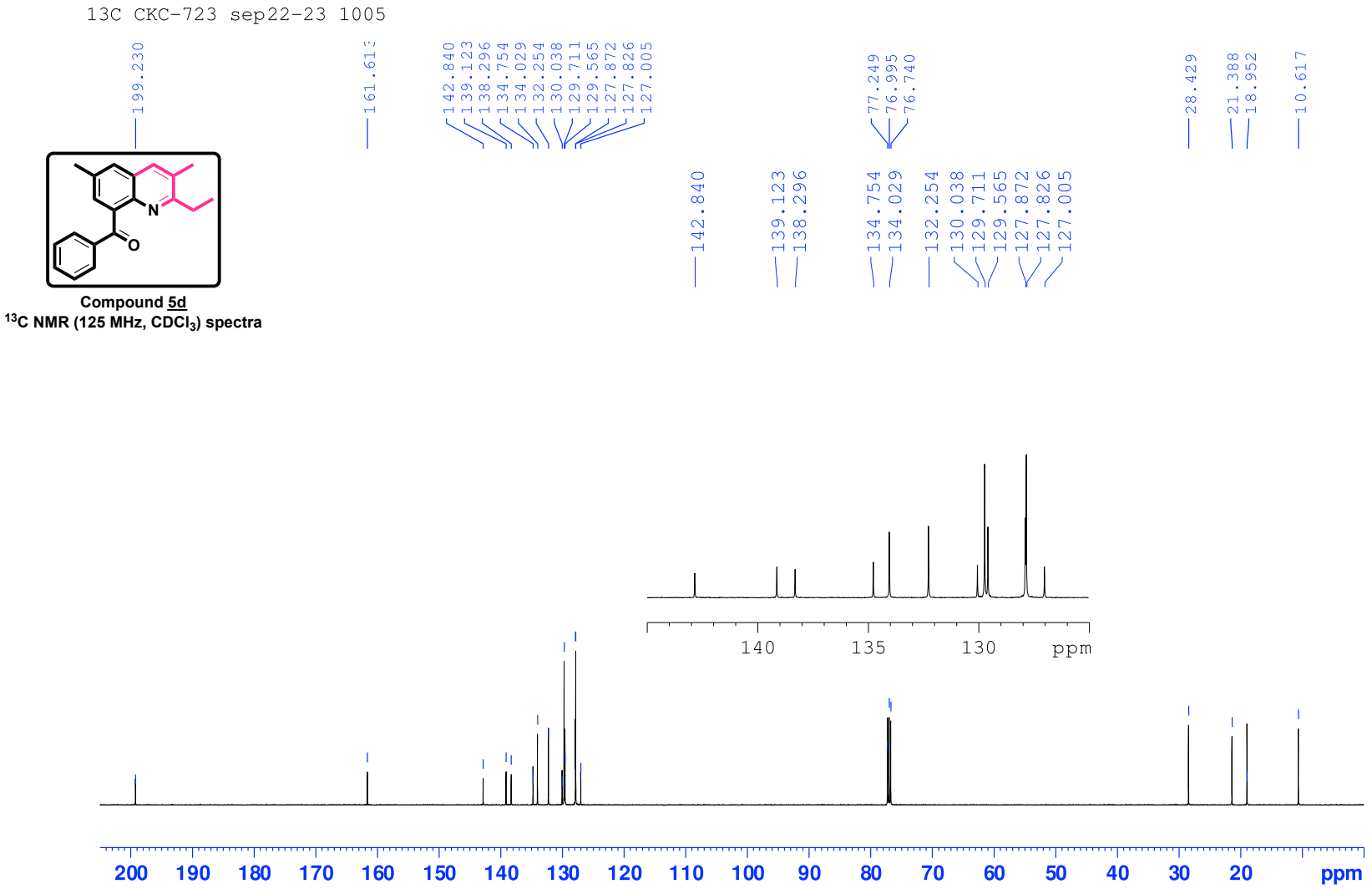



**Compound 5c**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5d

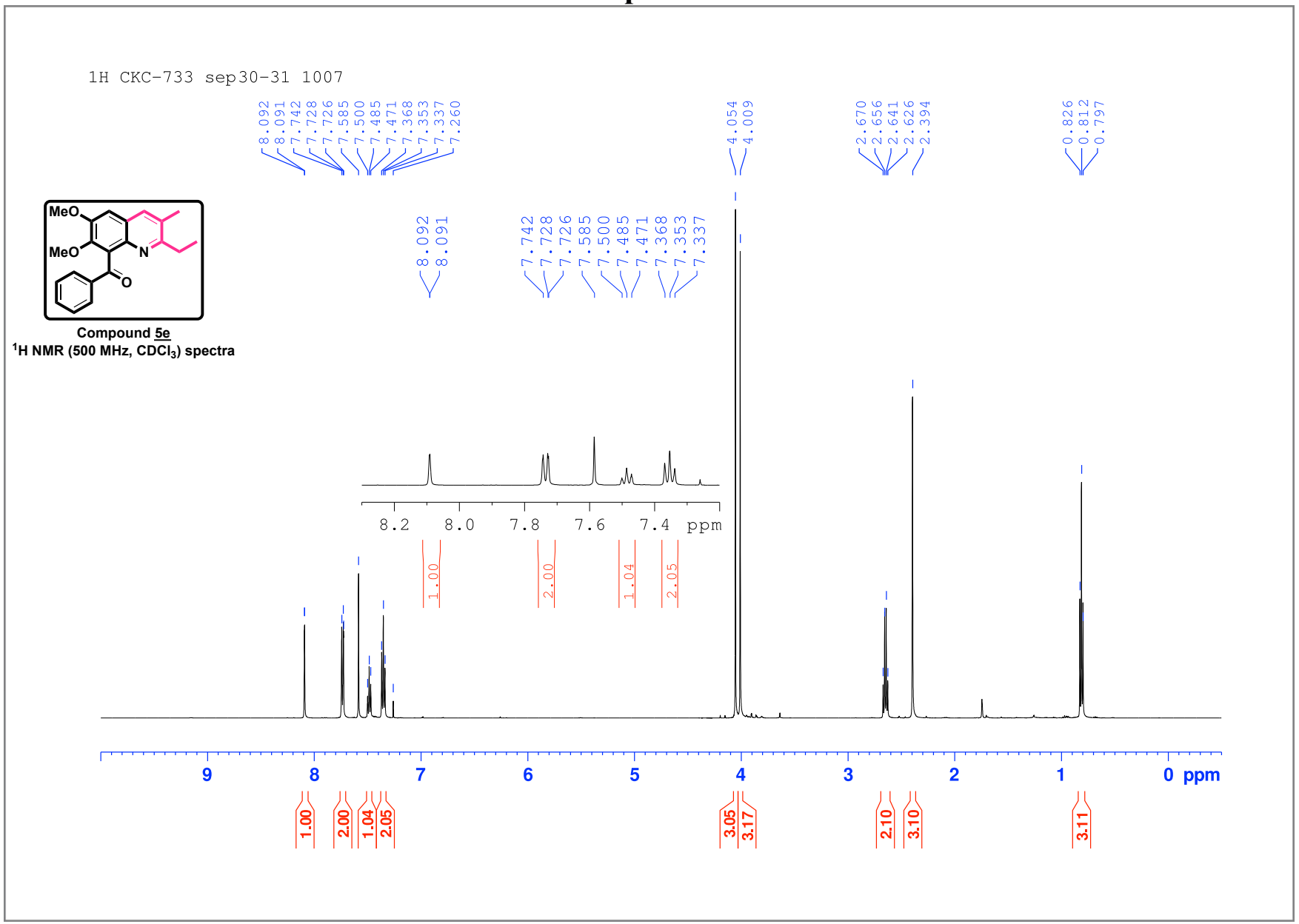

1H CKC-723 sep22-23 1005
7.768
7.754
7.752
7.716
7.584
7.567
7.504
7.489
7.474
7.370
7.355
7.340
7.260
2.702
2.687
2.672
2.658
2.540
2.369
0.895
0.880
0.865
N
O
Compound 5d
1H NMR (500 MHz, CDCl3) spectra
7.8
7.6
7.4
7.2
ppm
2.00
1.02
2.03
1.06
2.05
9
8
7
6
5
4
3
2
1
0 ppm
2.00
1.02
2.03
1.06
2.05
2.11
3.04
3.05
3.12

# Compound 5d



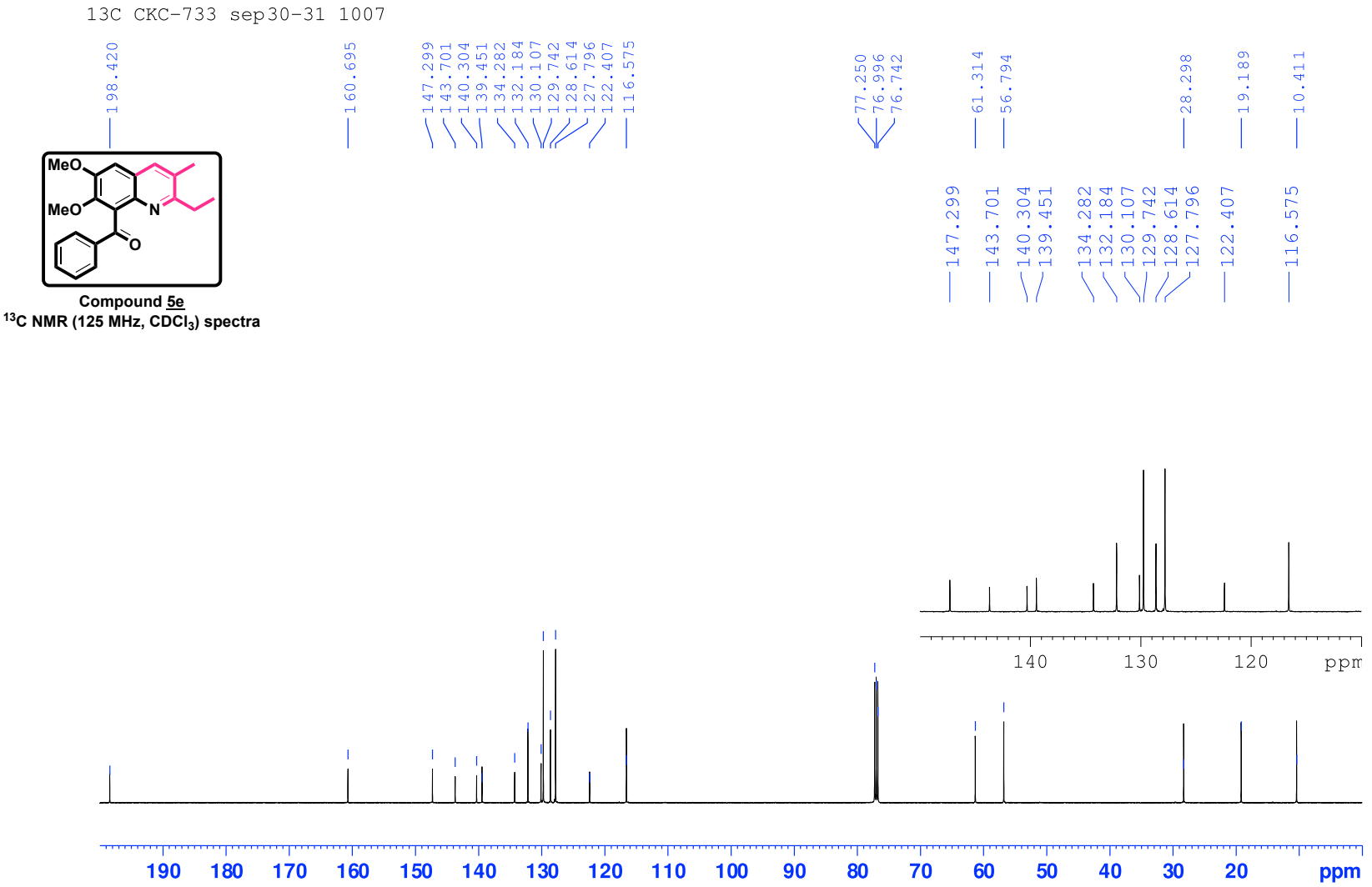

**Compound 5d**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5e



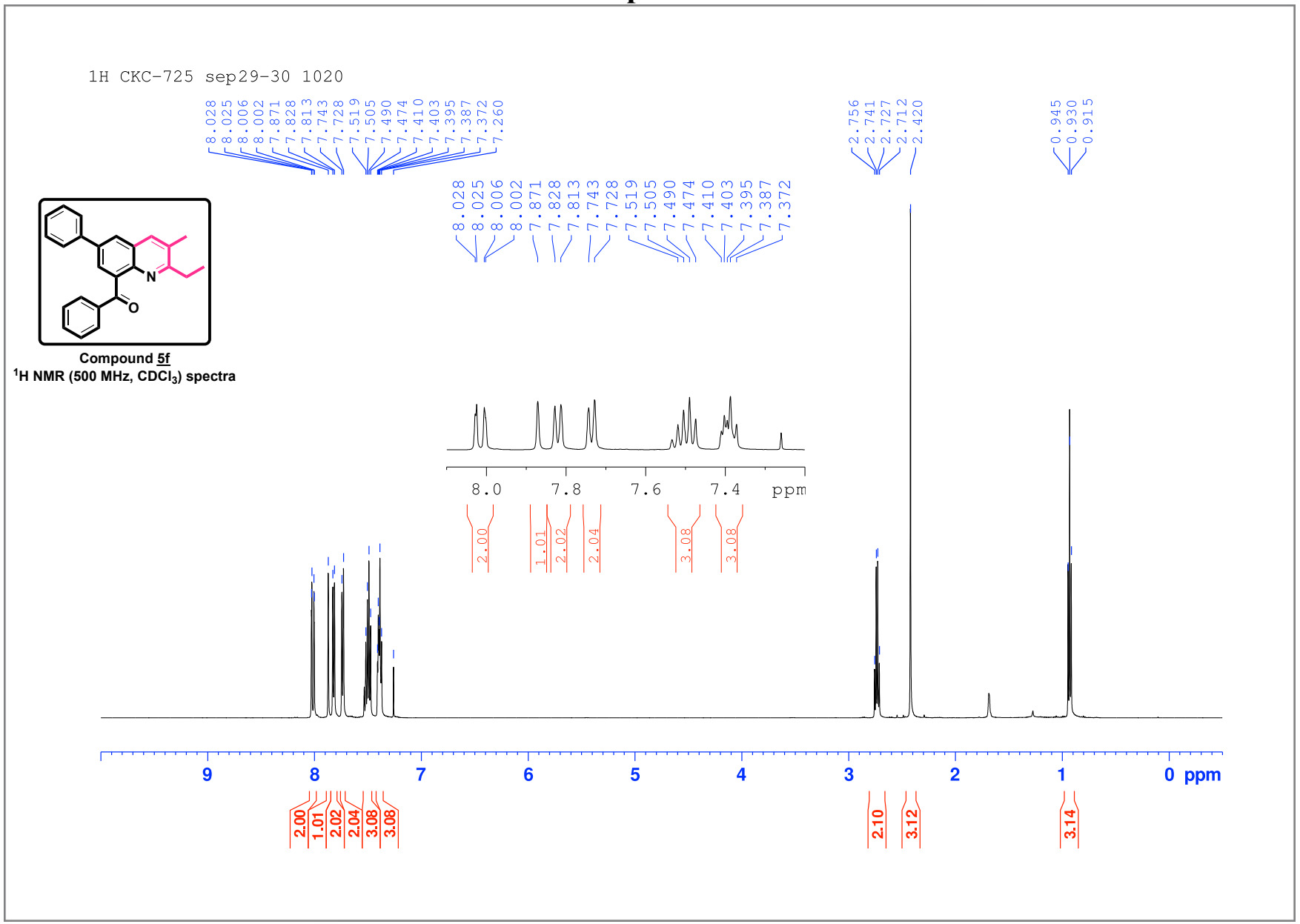

Compound 5e
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 5e



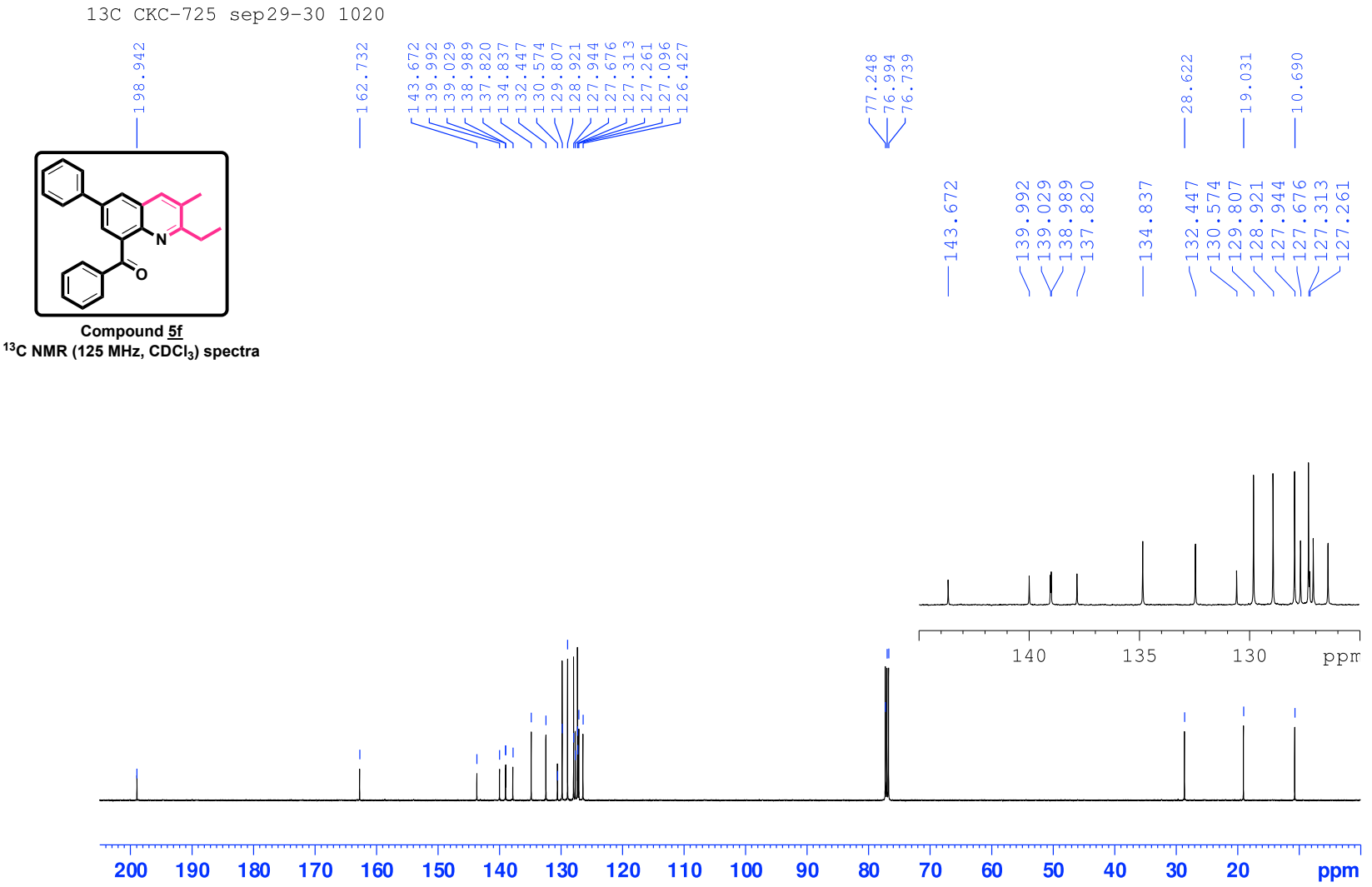

**Compound 5e**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5f



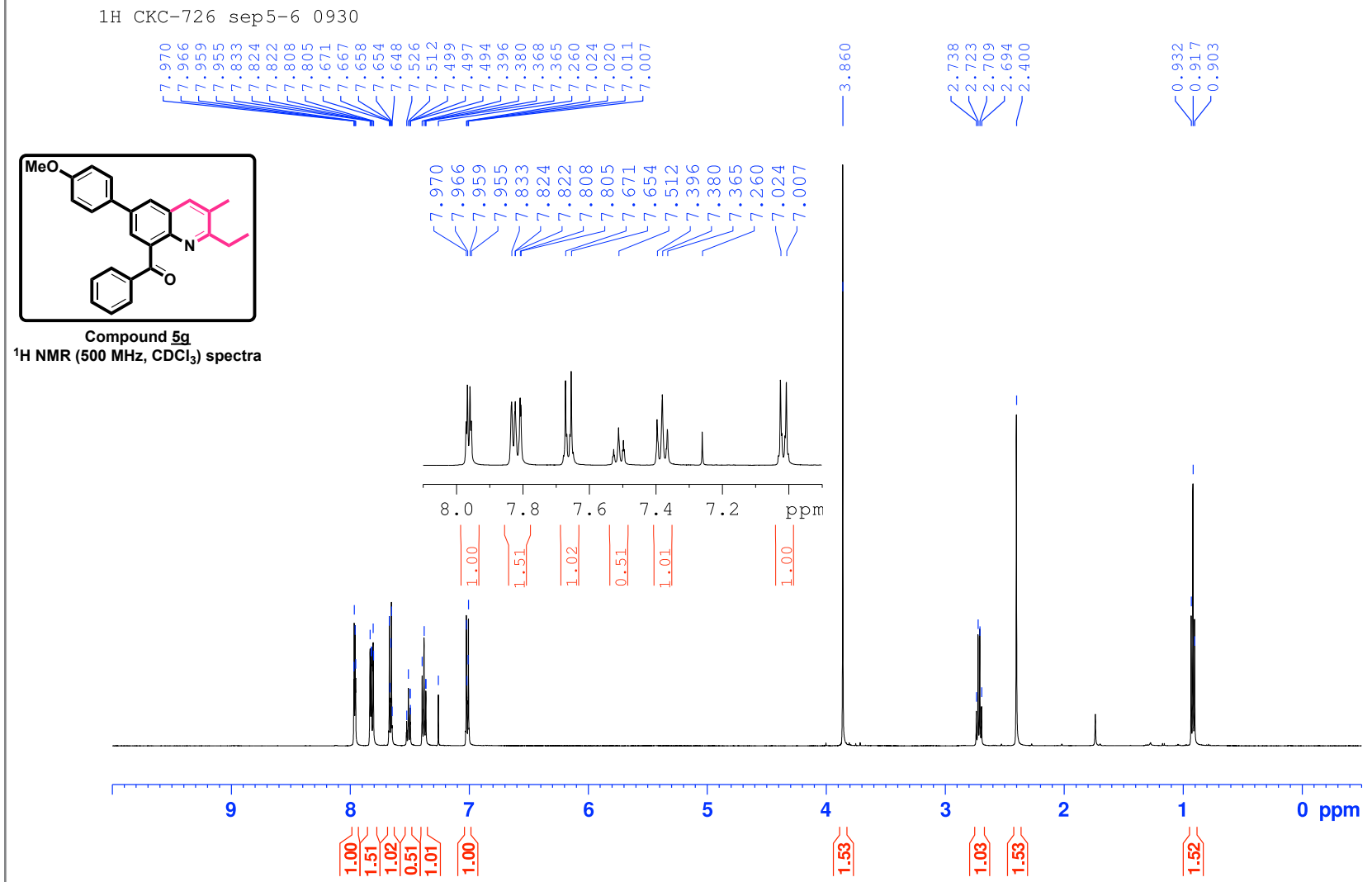

**Compound 5f**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

# Compound 5f



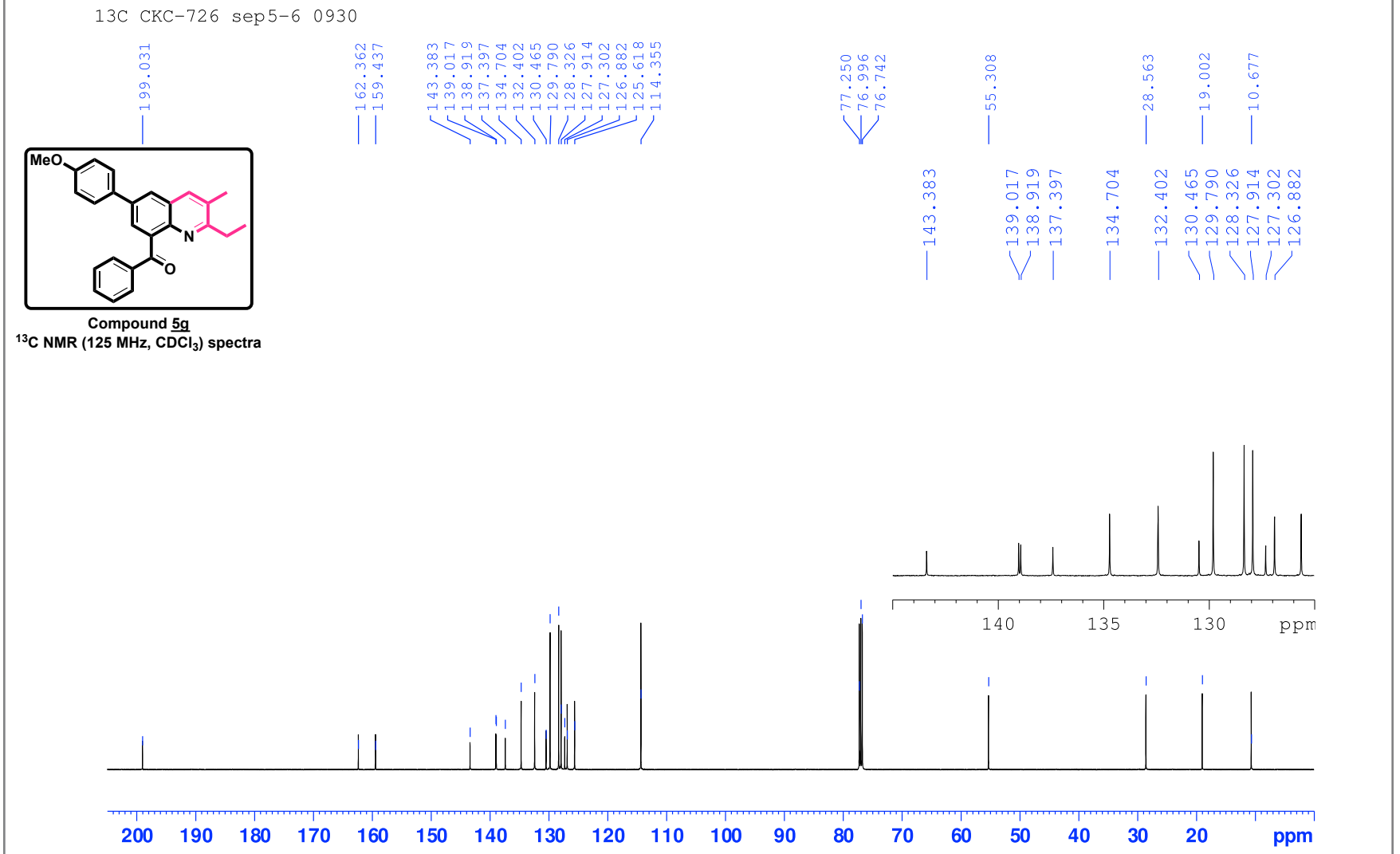

**Compound 5f**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5g




**Compound 5g**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

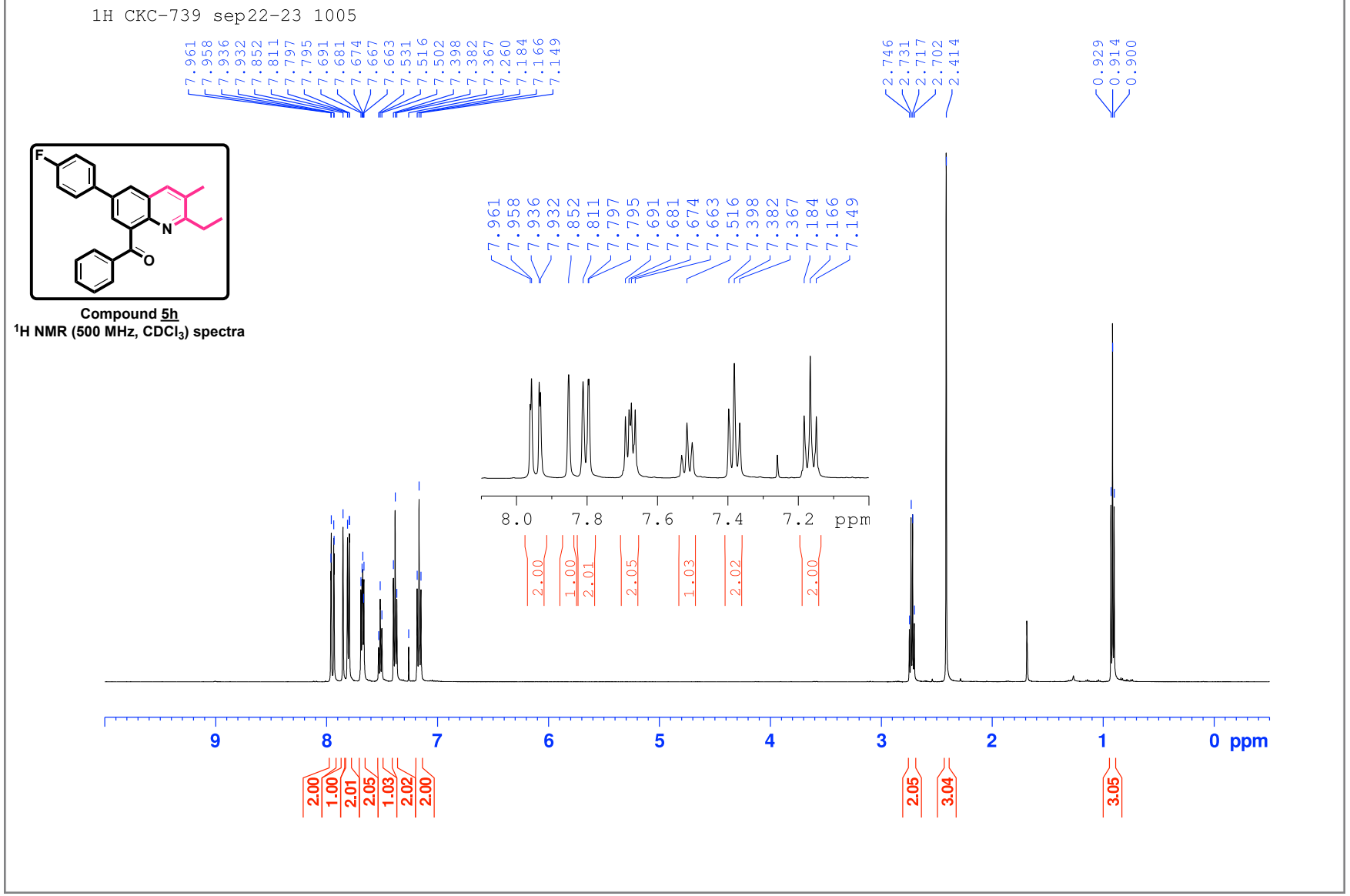
# Compound 5g




Compound 5g

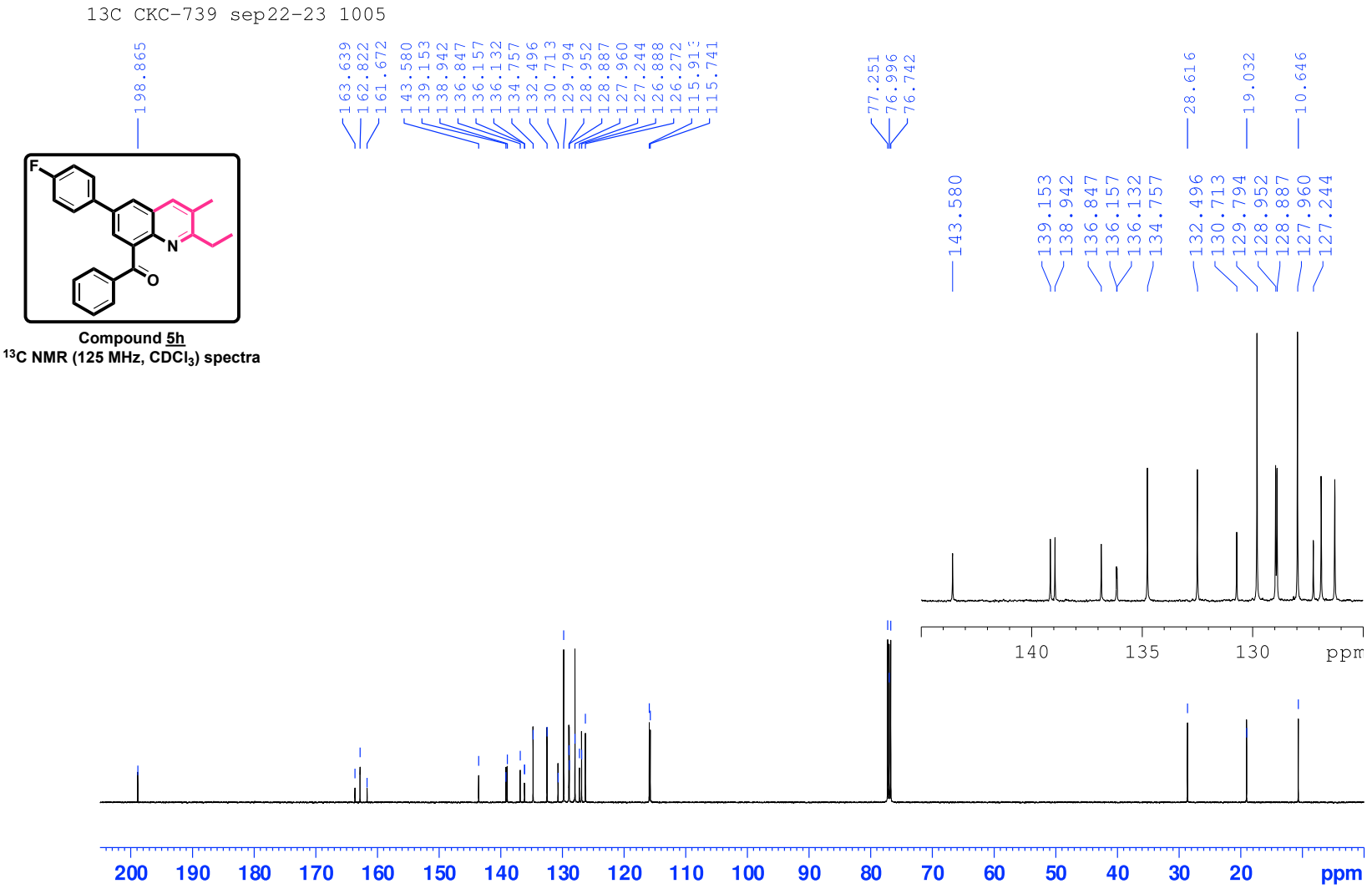
$^{13}$C NMR (125 MHz, $CDCl_3$) spectra

# Compound 5h



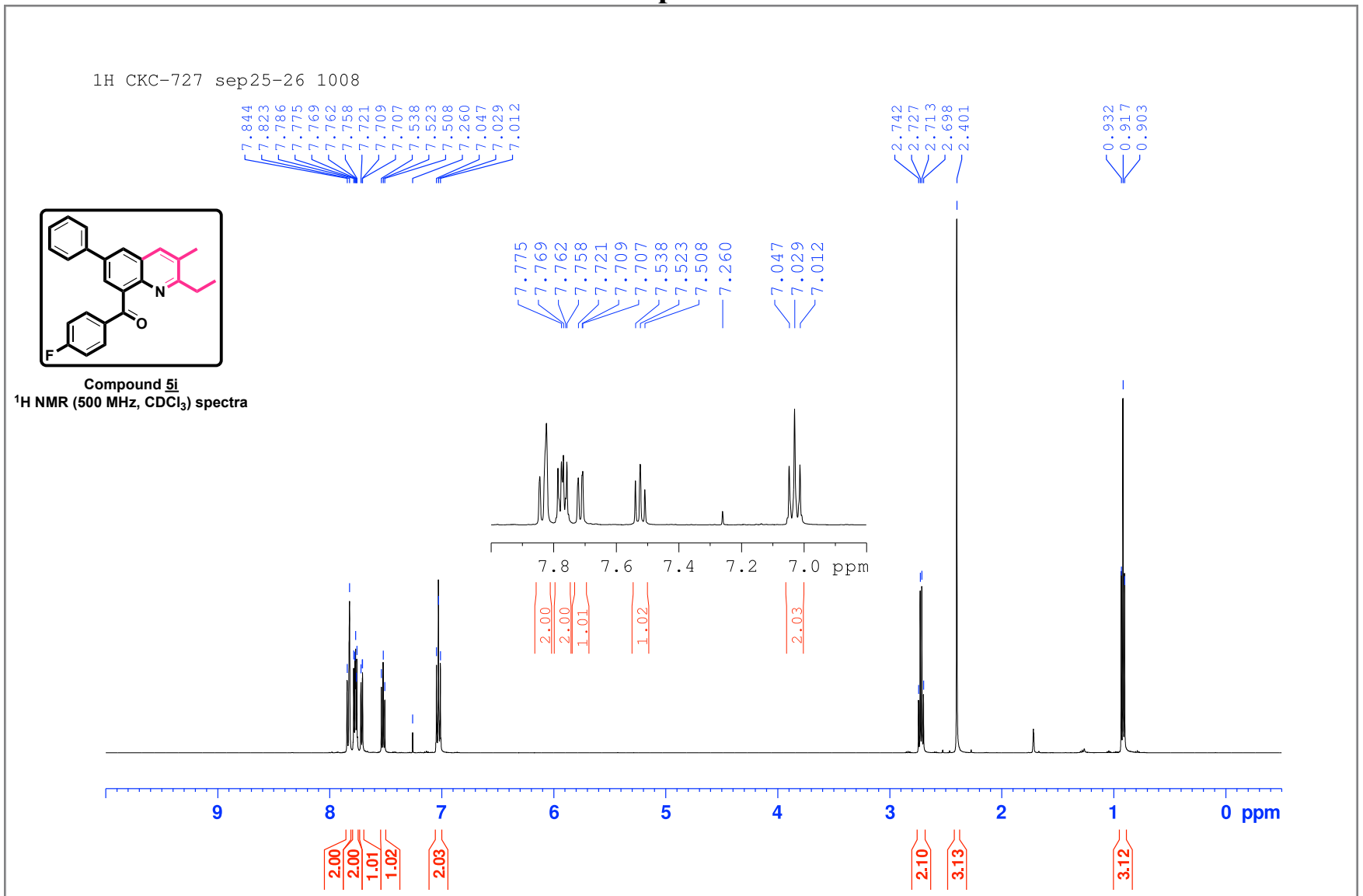

Compound 5h
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 5h



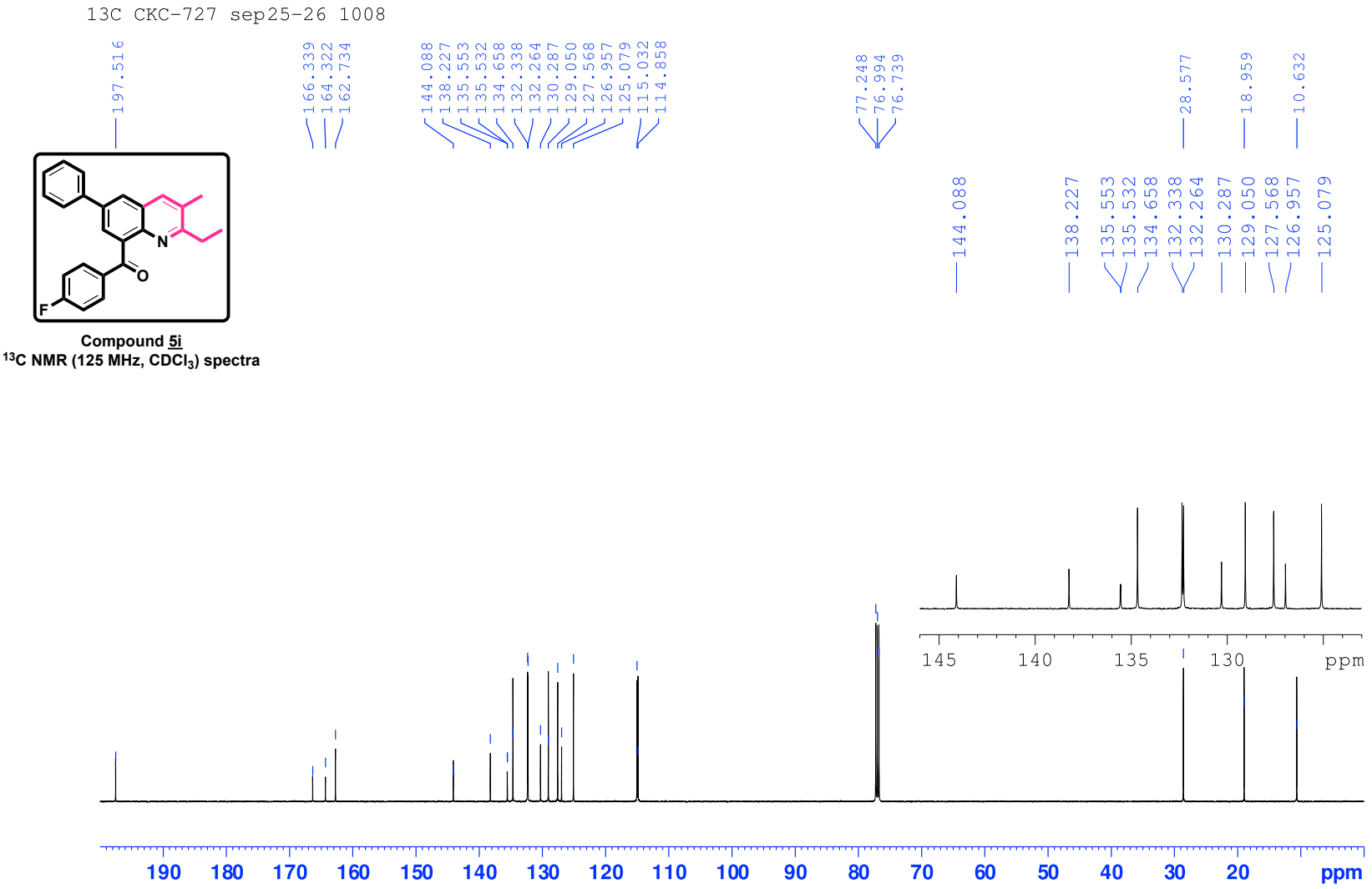

**Compound 5h**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5i



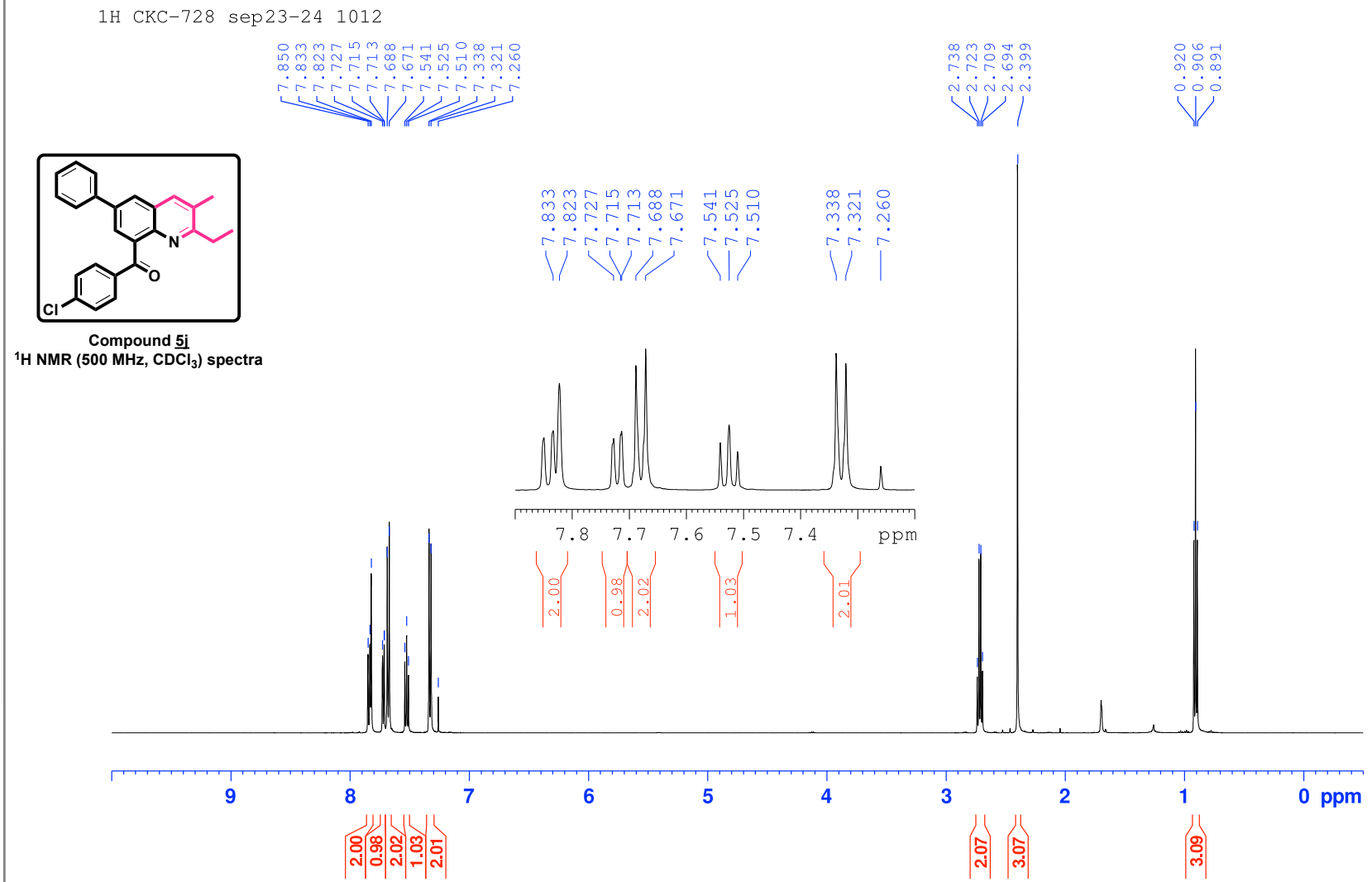

Compound 5i
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 5i



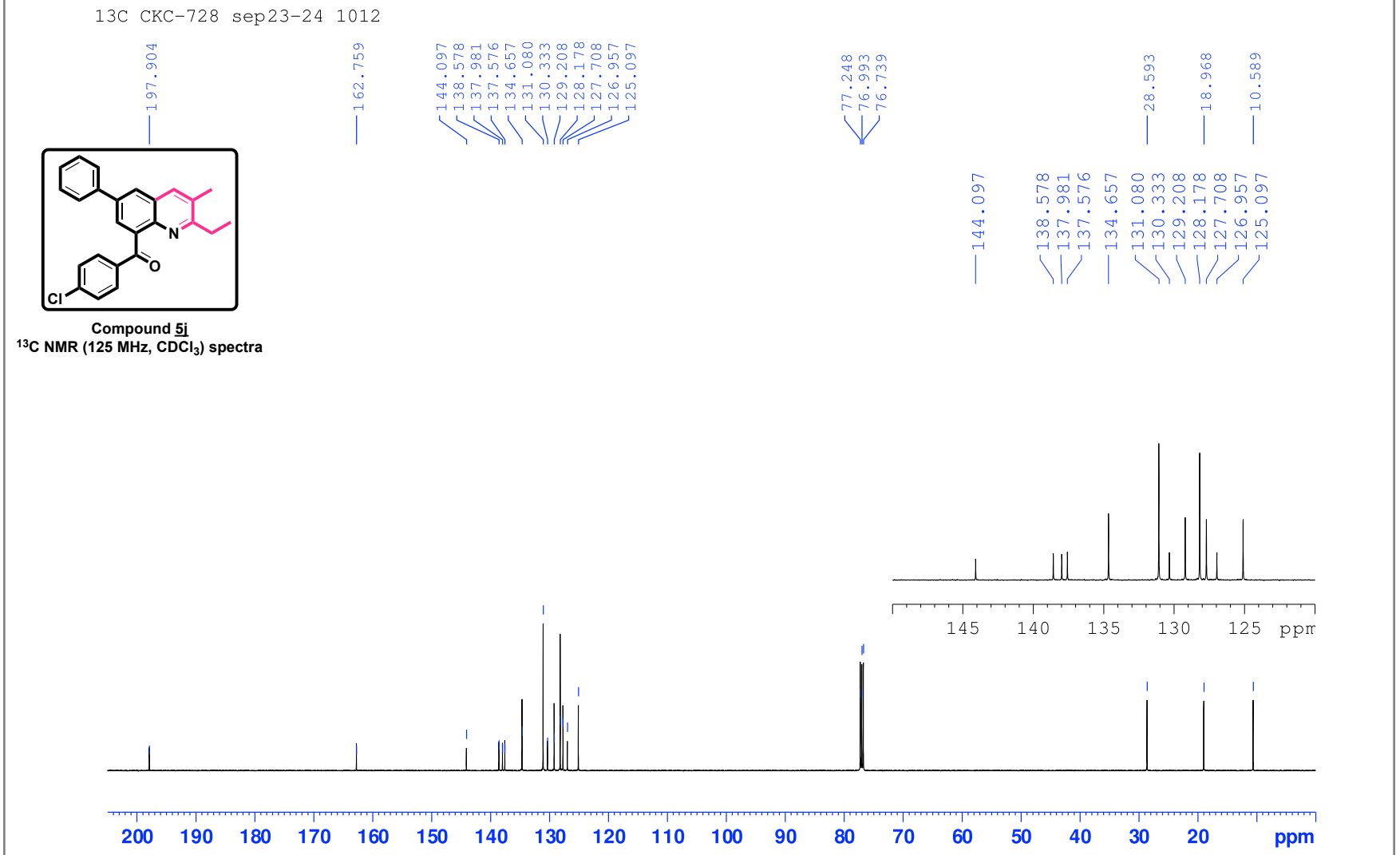

**Compound 5i**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5j



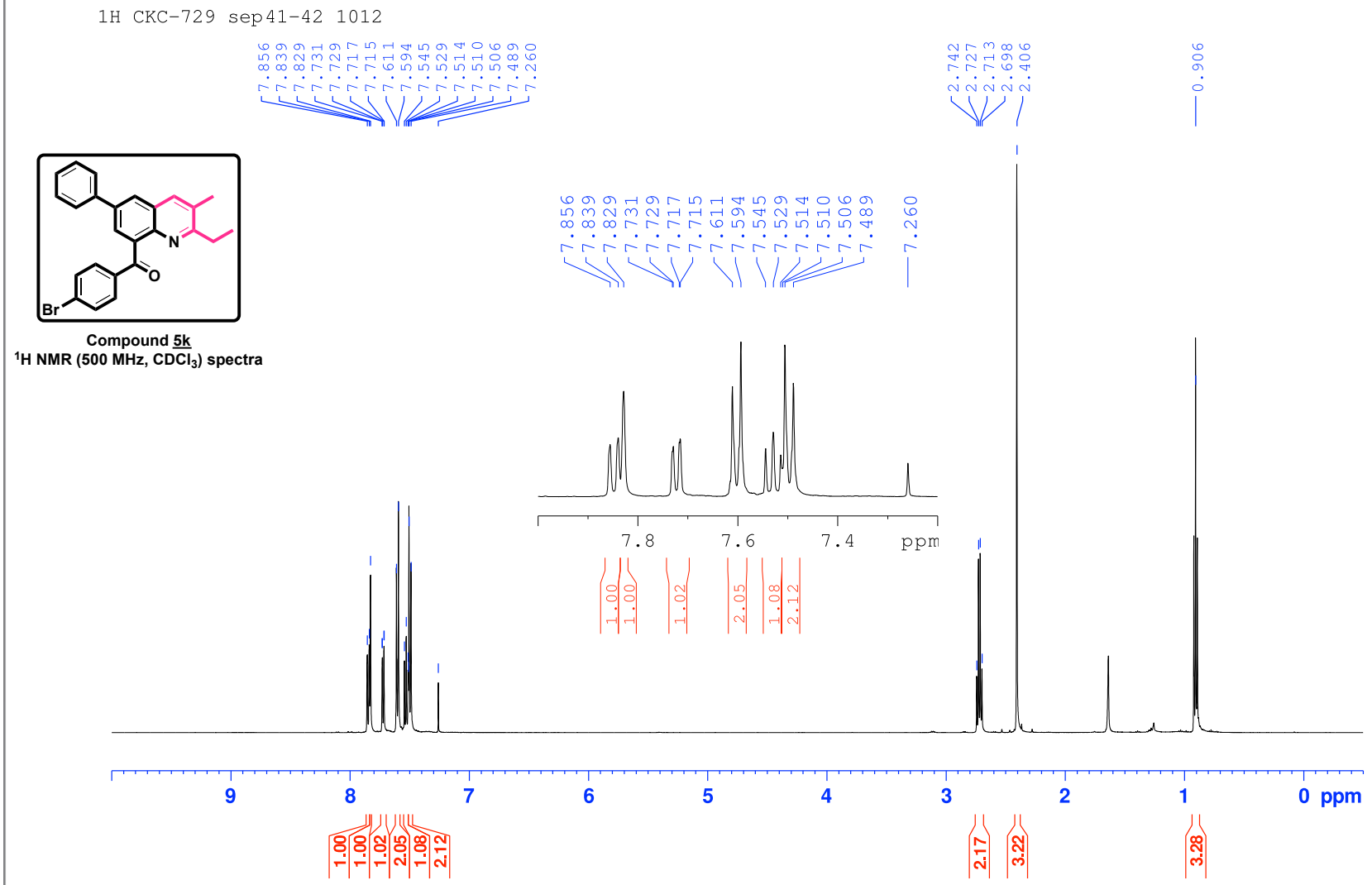

**Compound 5j**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

# Compound 5j



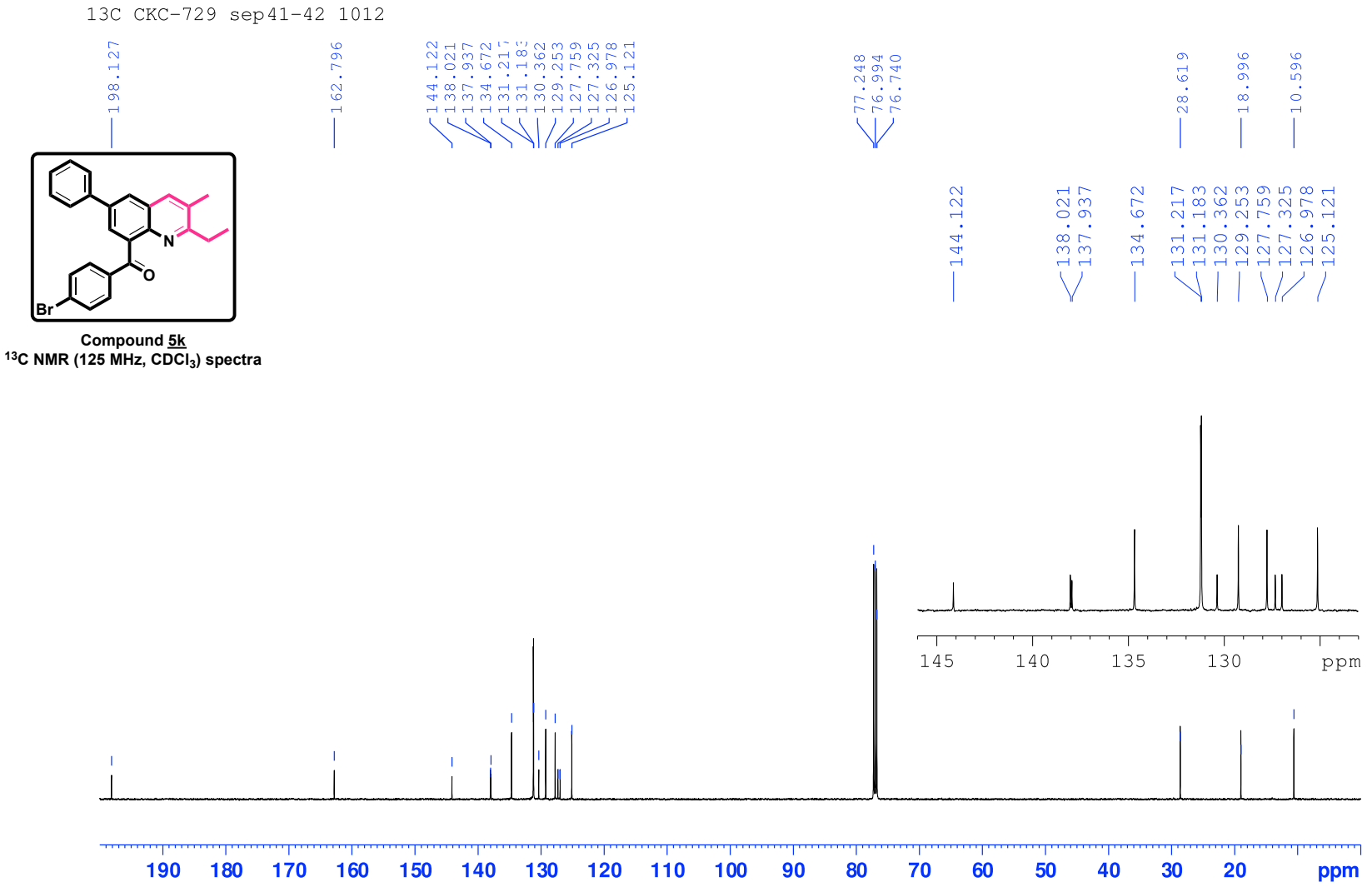

**Compound 5j**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5k



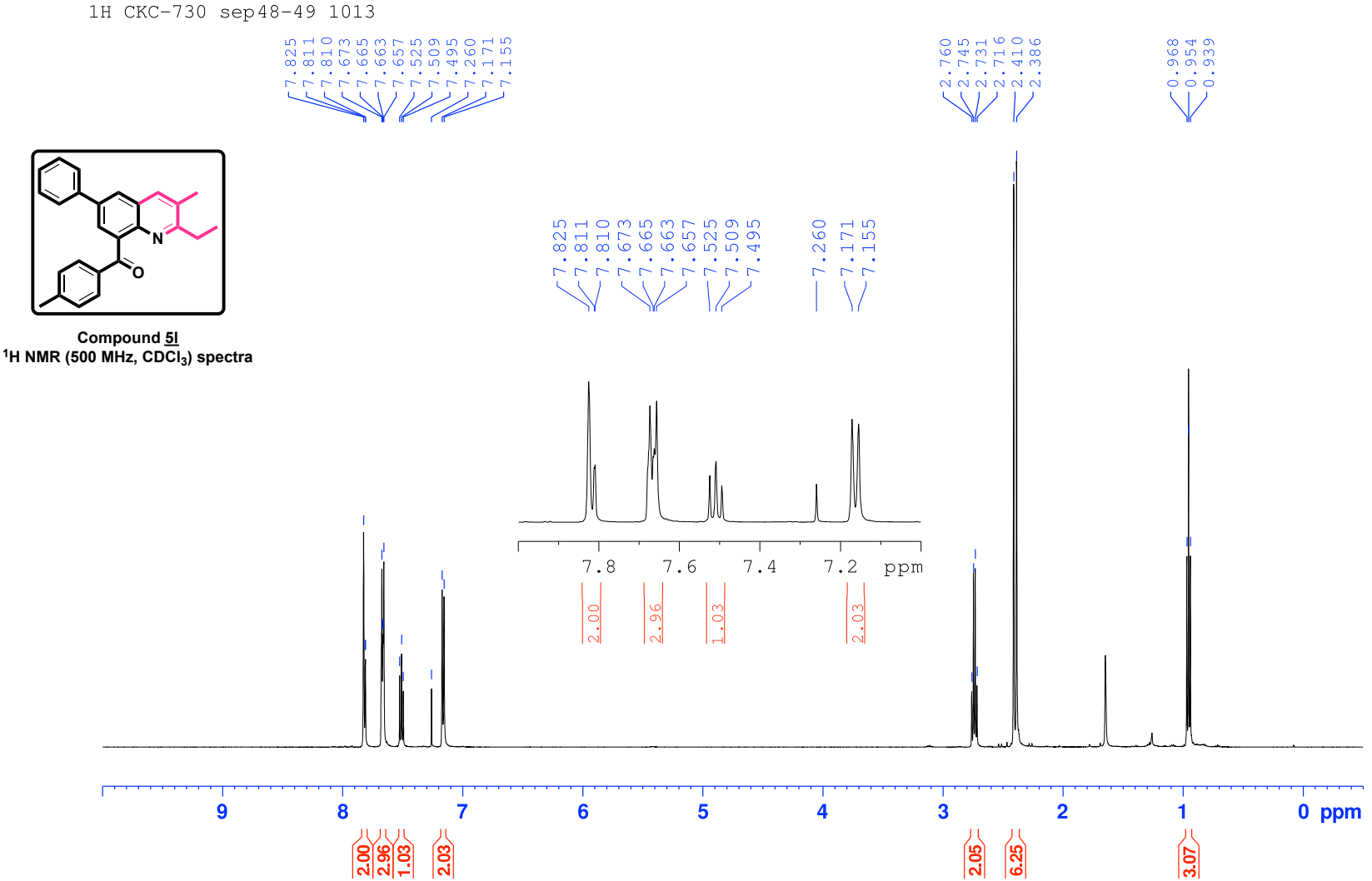

Compound 5k
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 5k



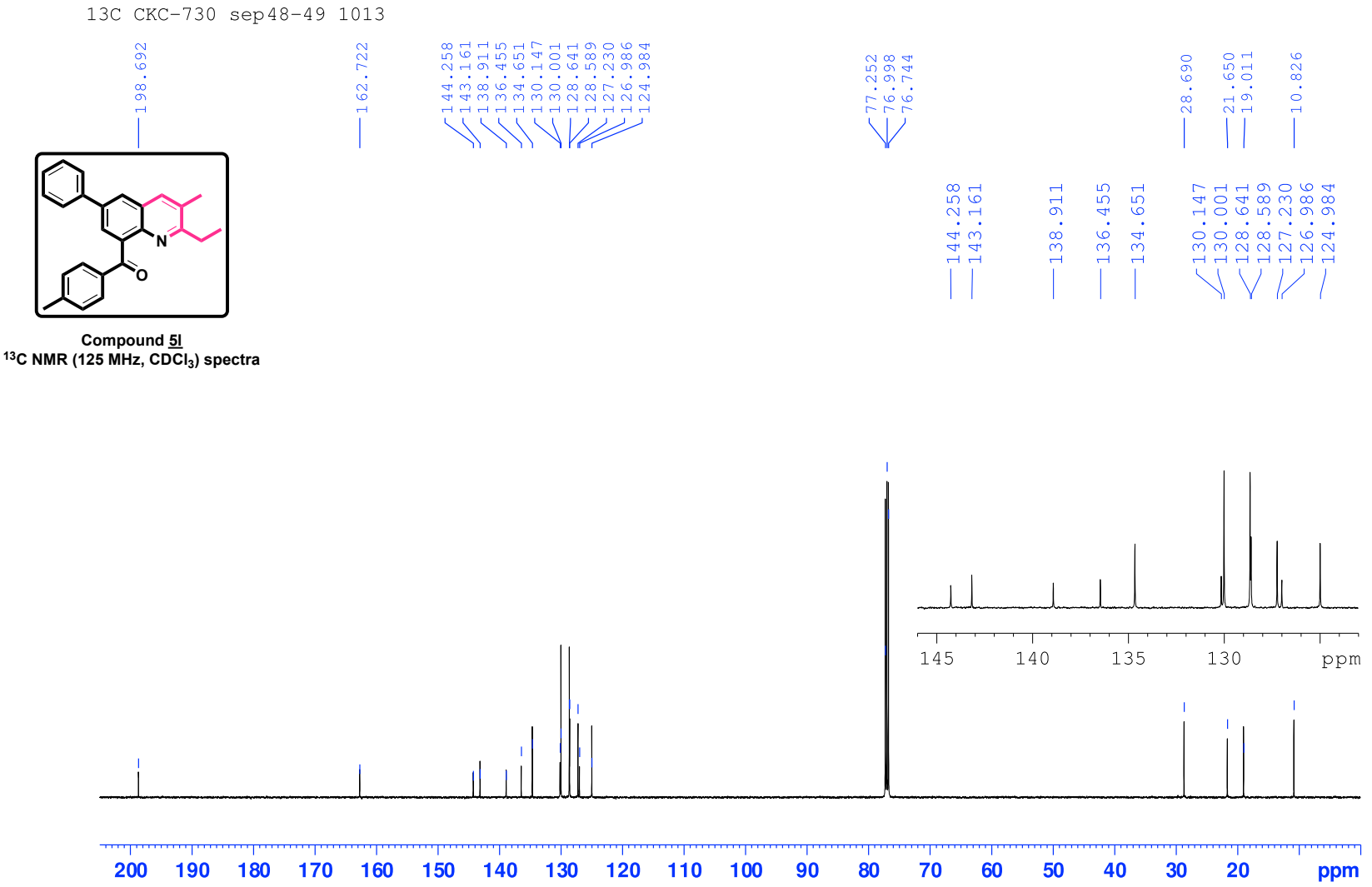

**Compound 5k**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5l



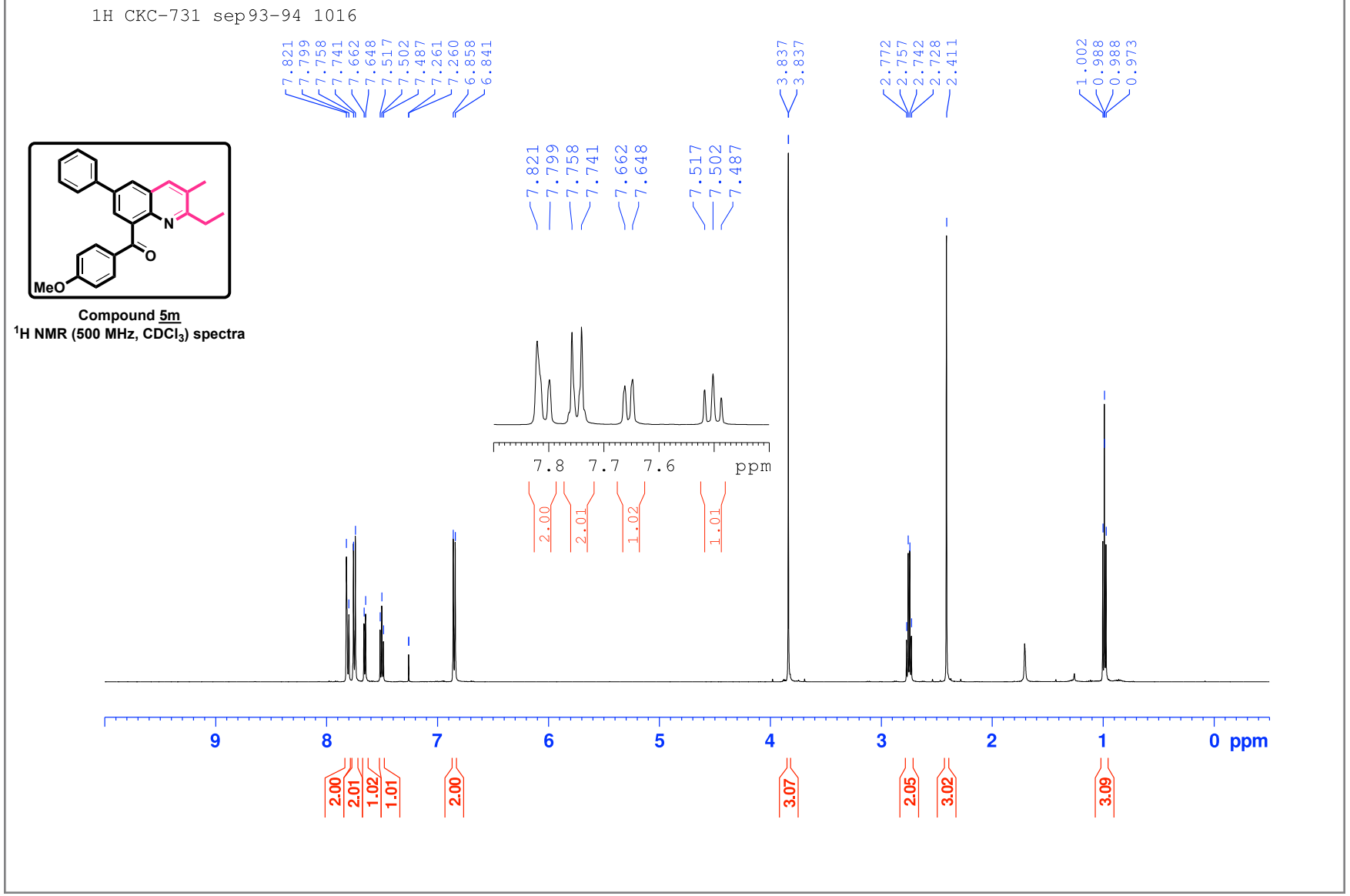

**Compound 5l**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

# Compound 5l



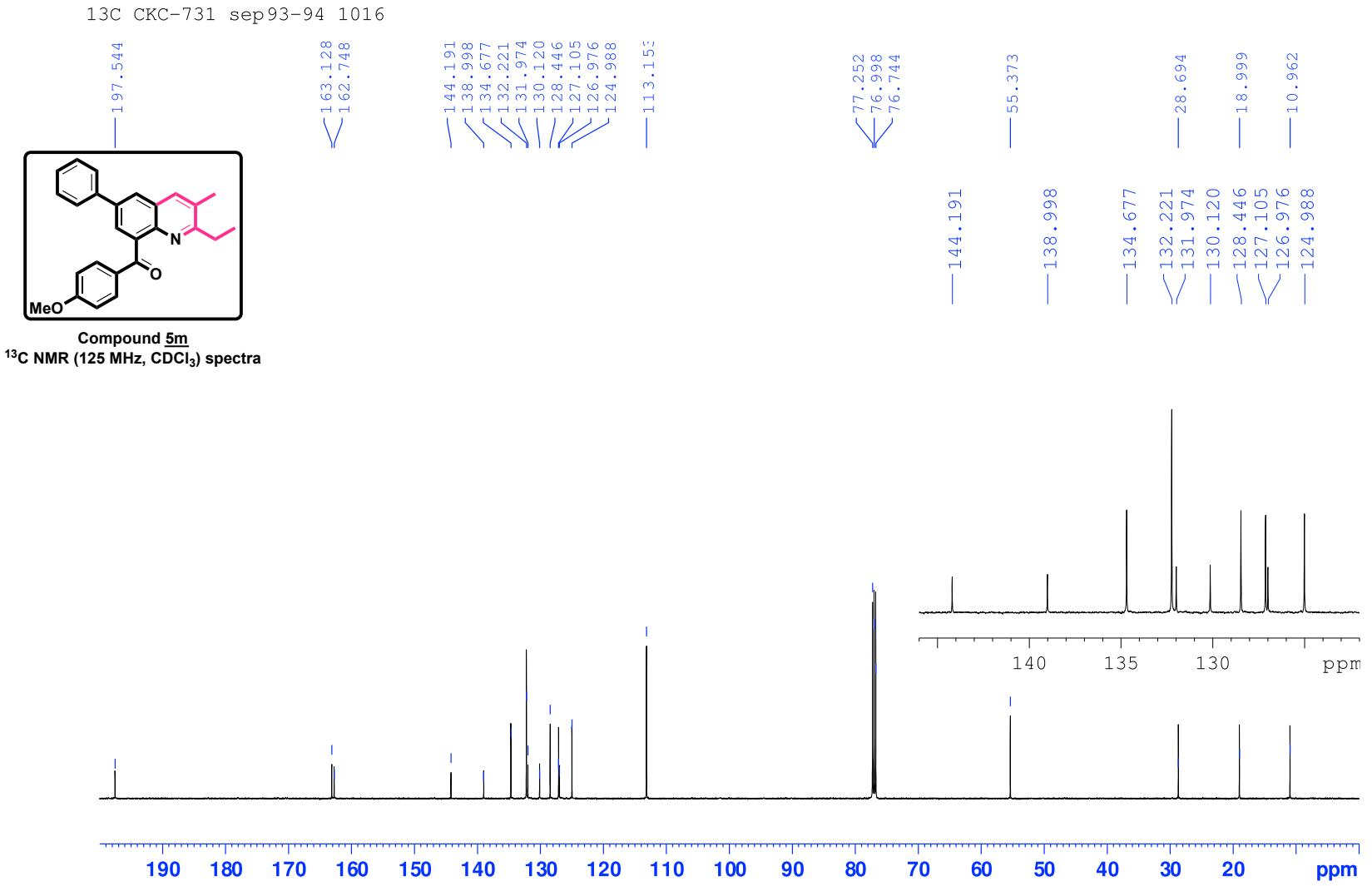

**Compound 5l**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5m



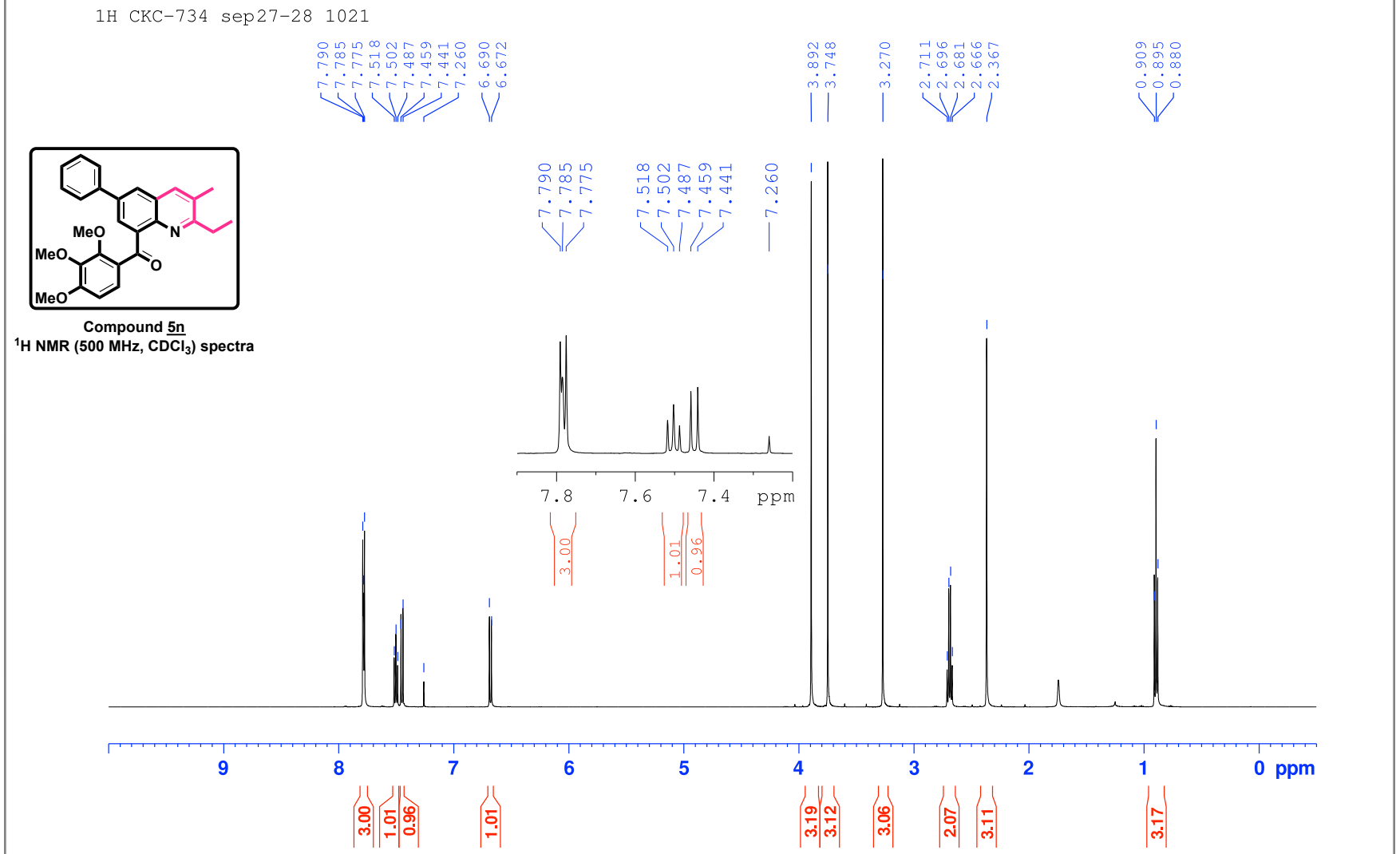

Compound 5m
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 5m



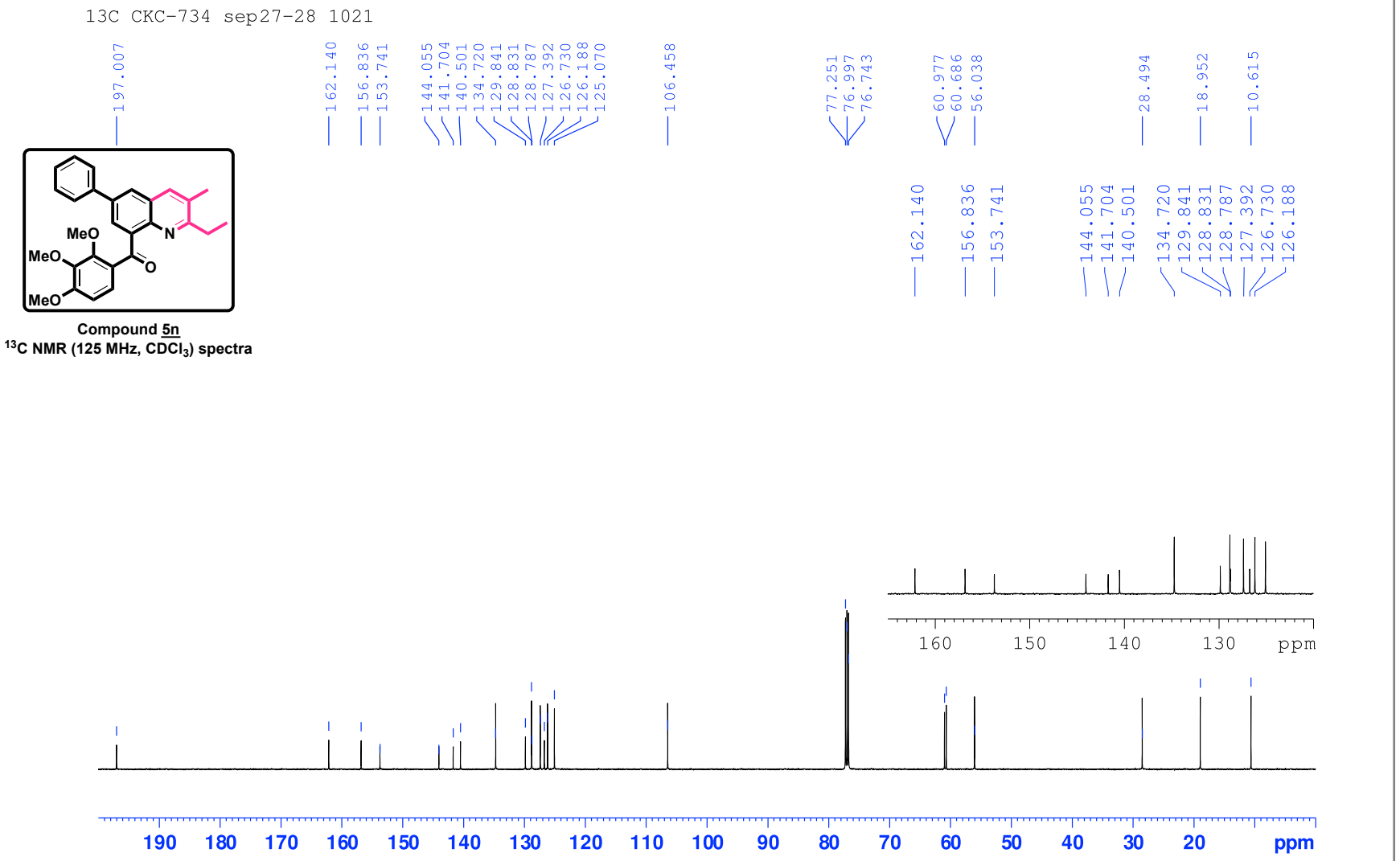

**Compound 5m**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5n



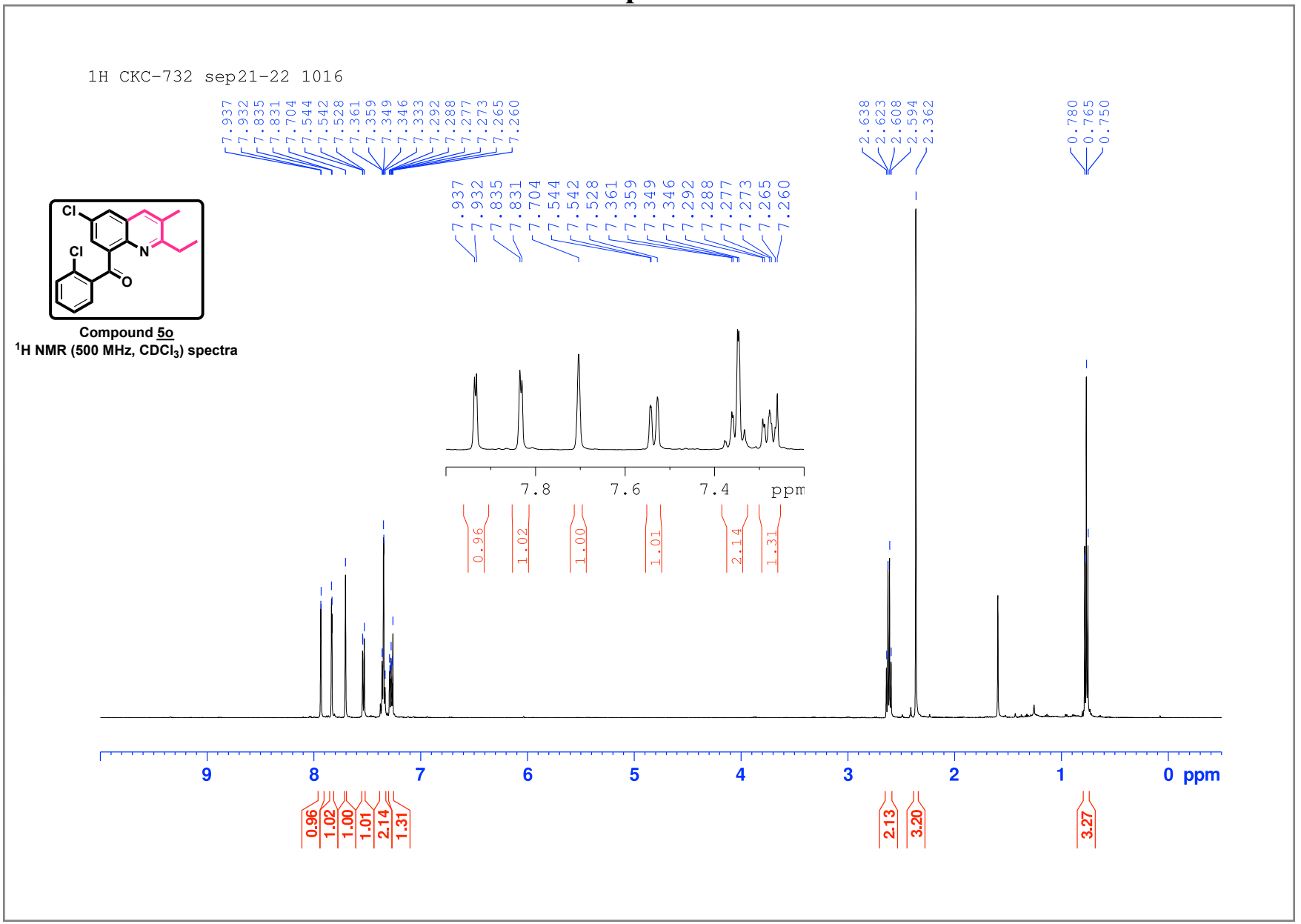

Compound 5n
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 5n



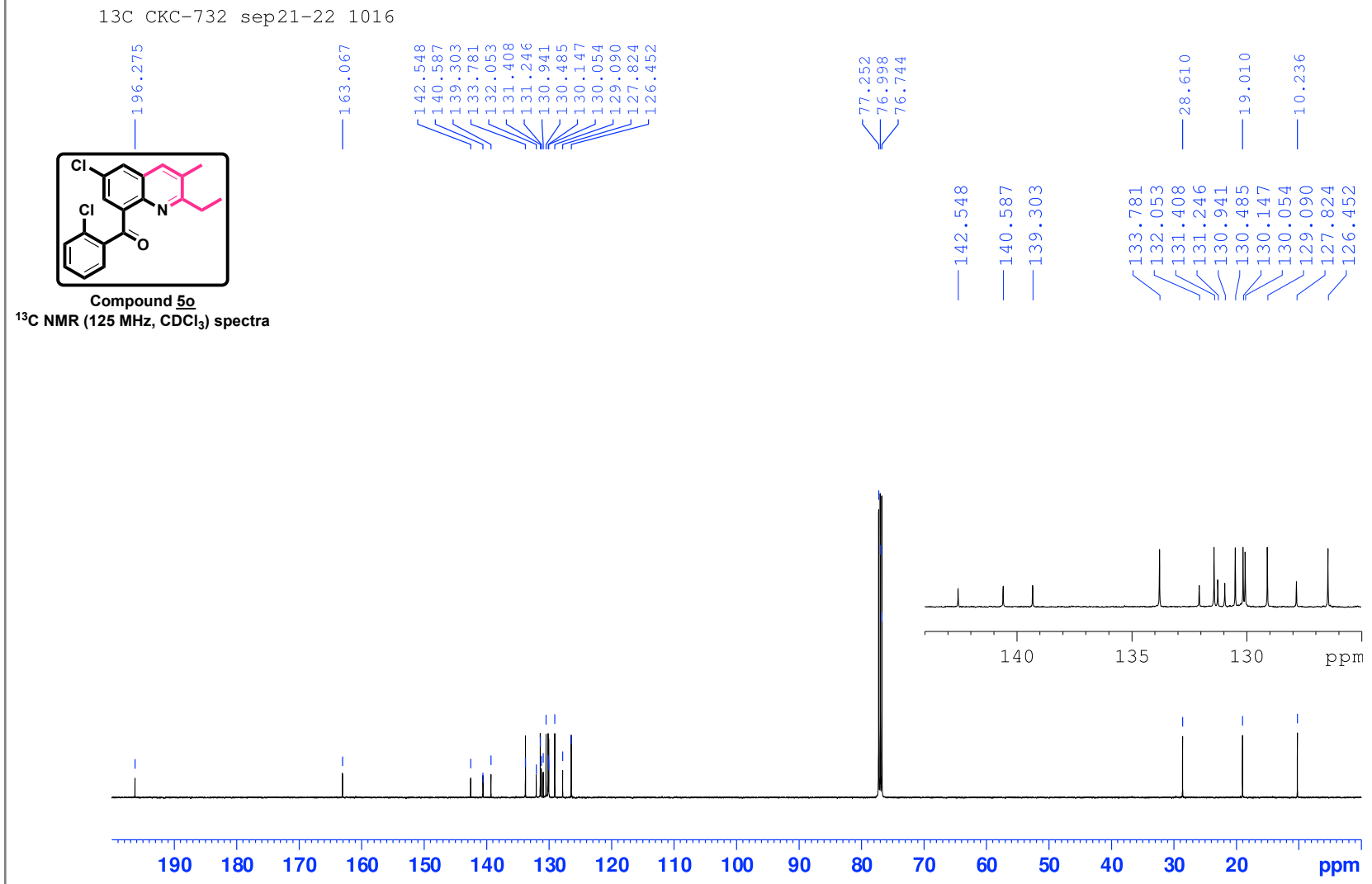

**Compound 5n**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5o



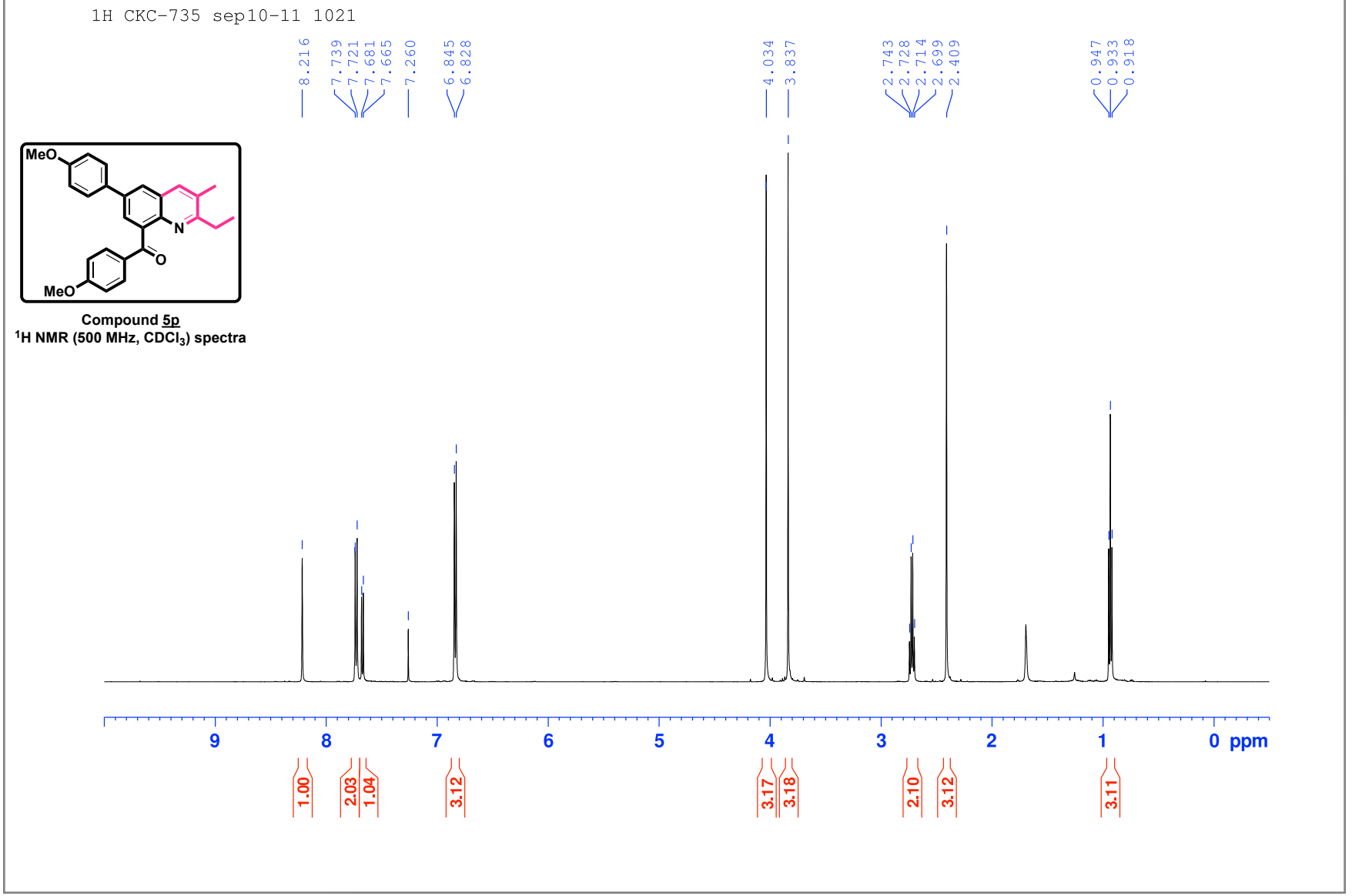

**Compound 5o**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

# Compound 5o



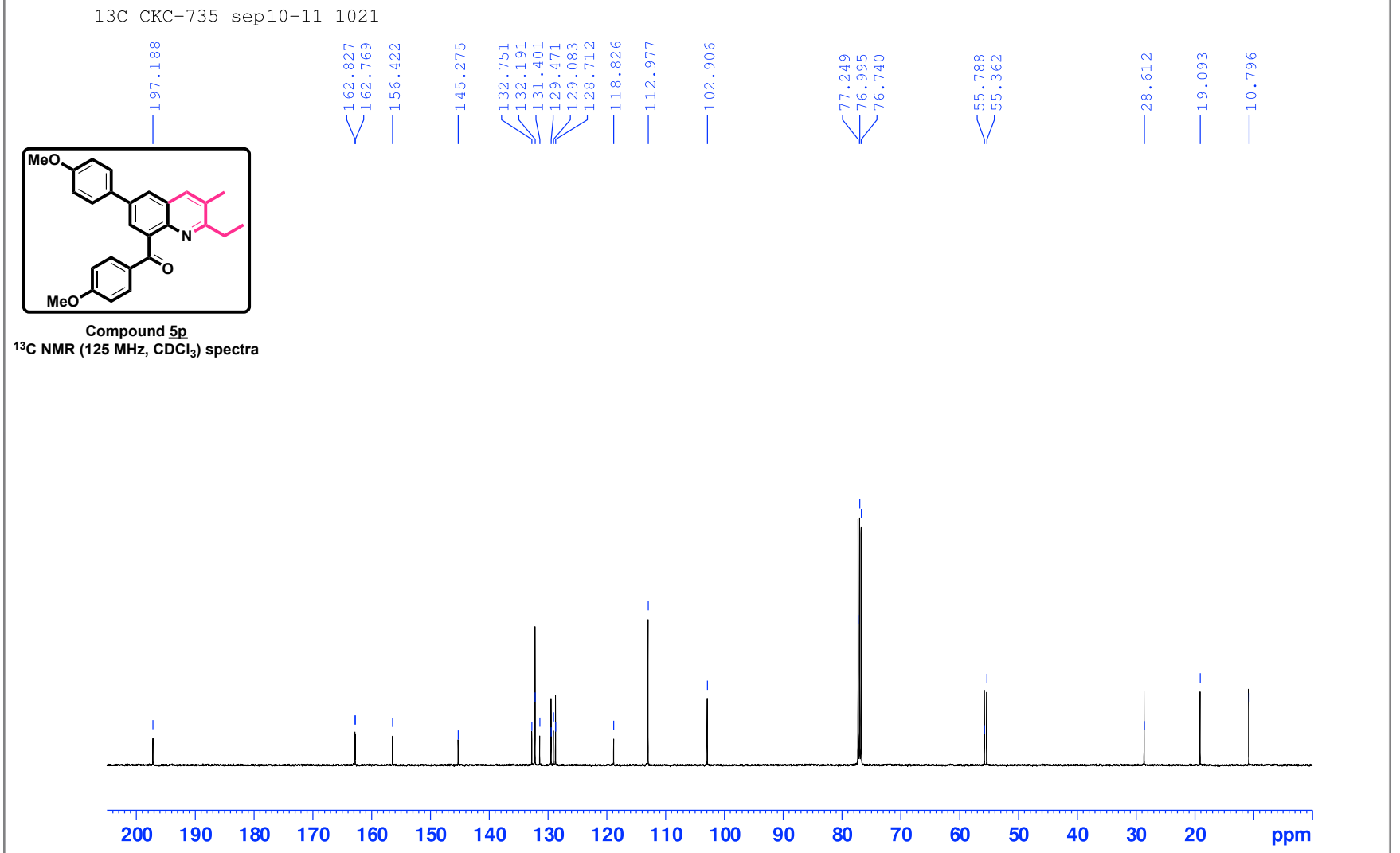

**Compound 5o**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5p



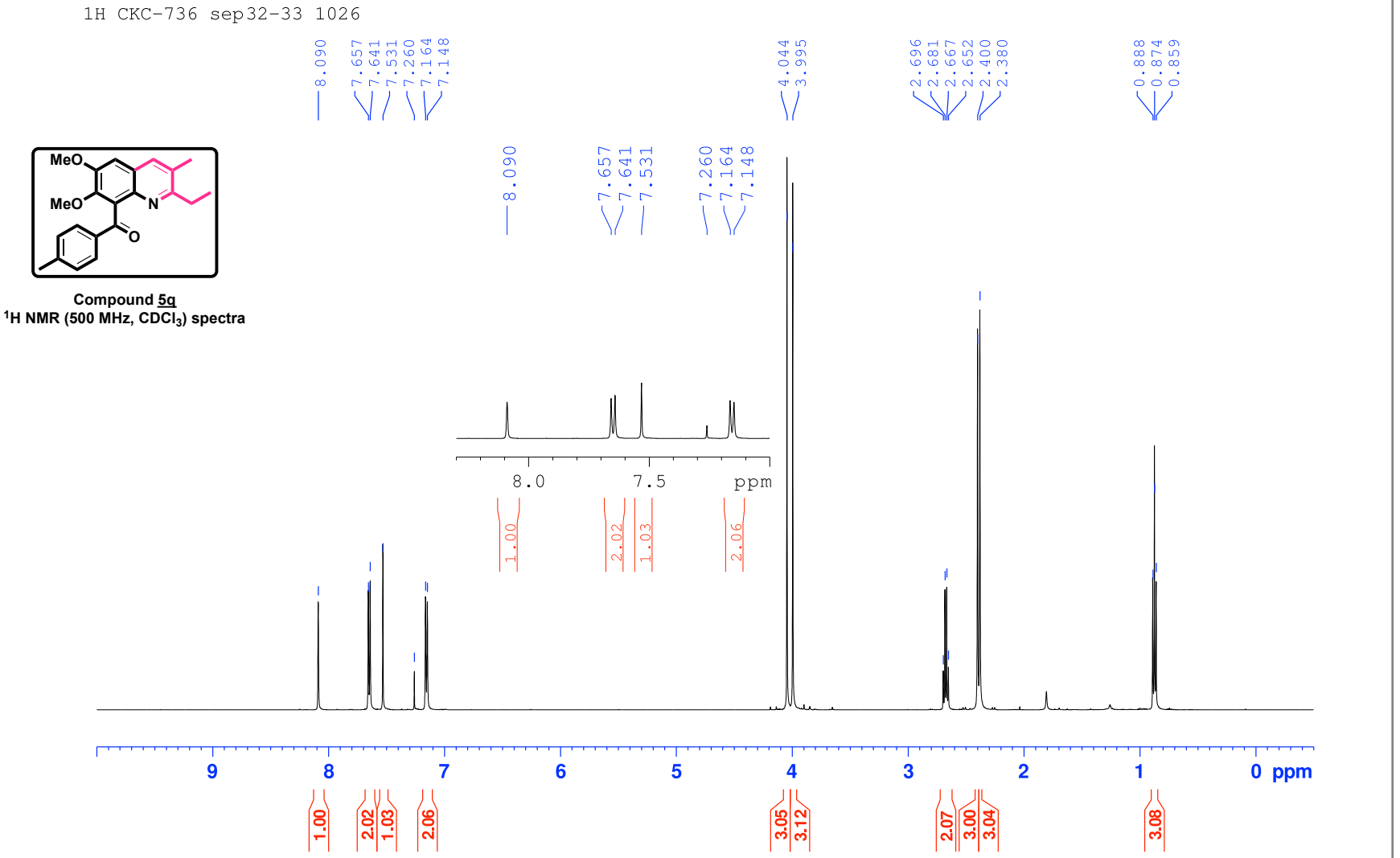

Compound 5p
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 5p



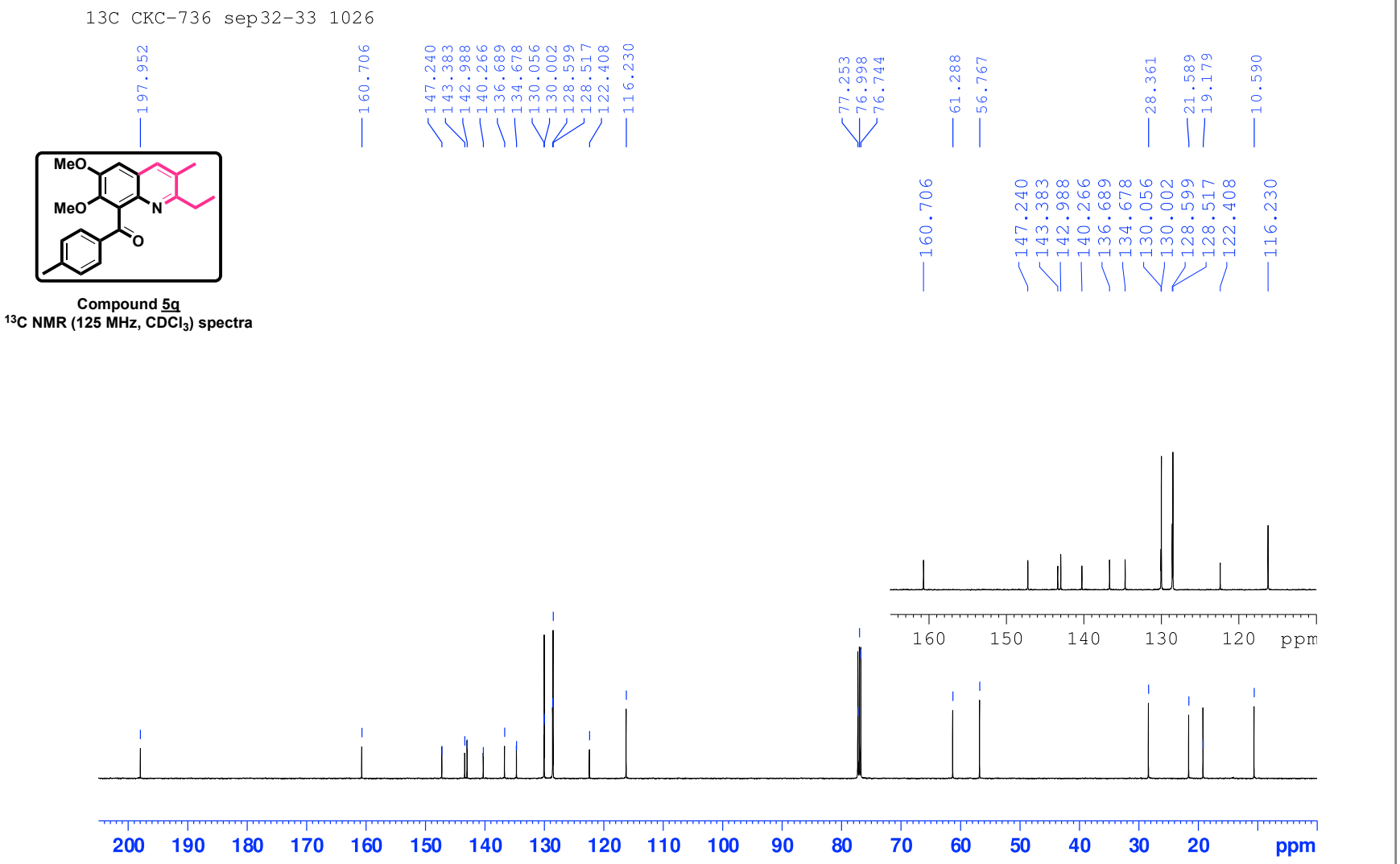

**Compound 5p**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5q



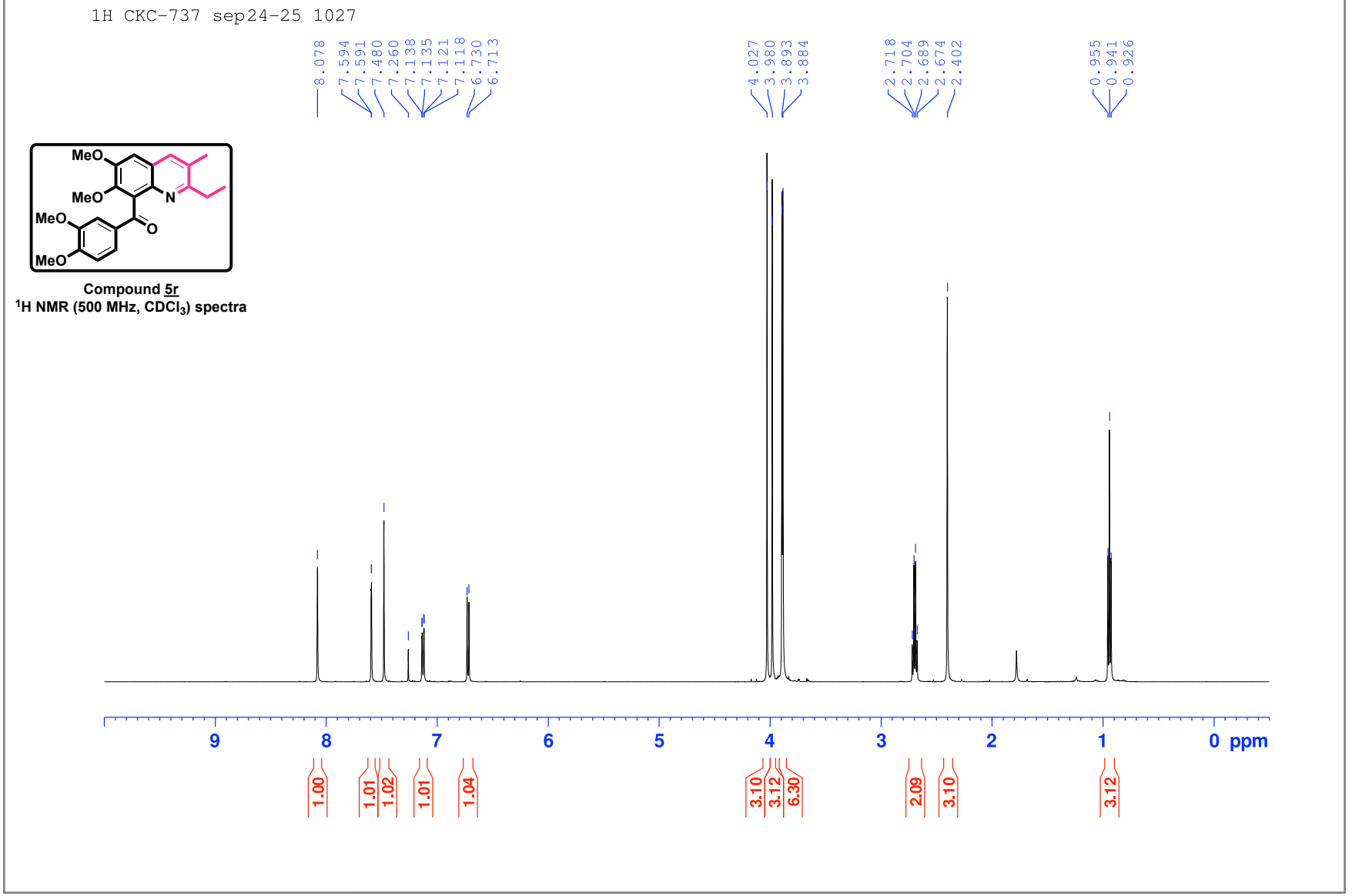

Compound 5q
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 5q



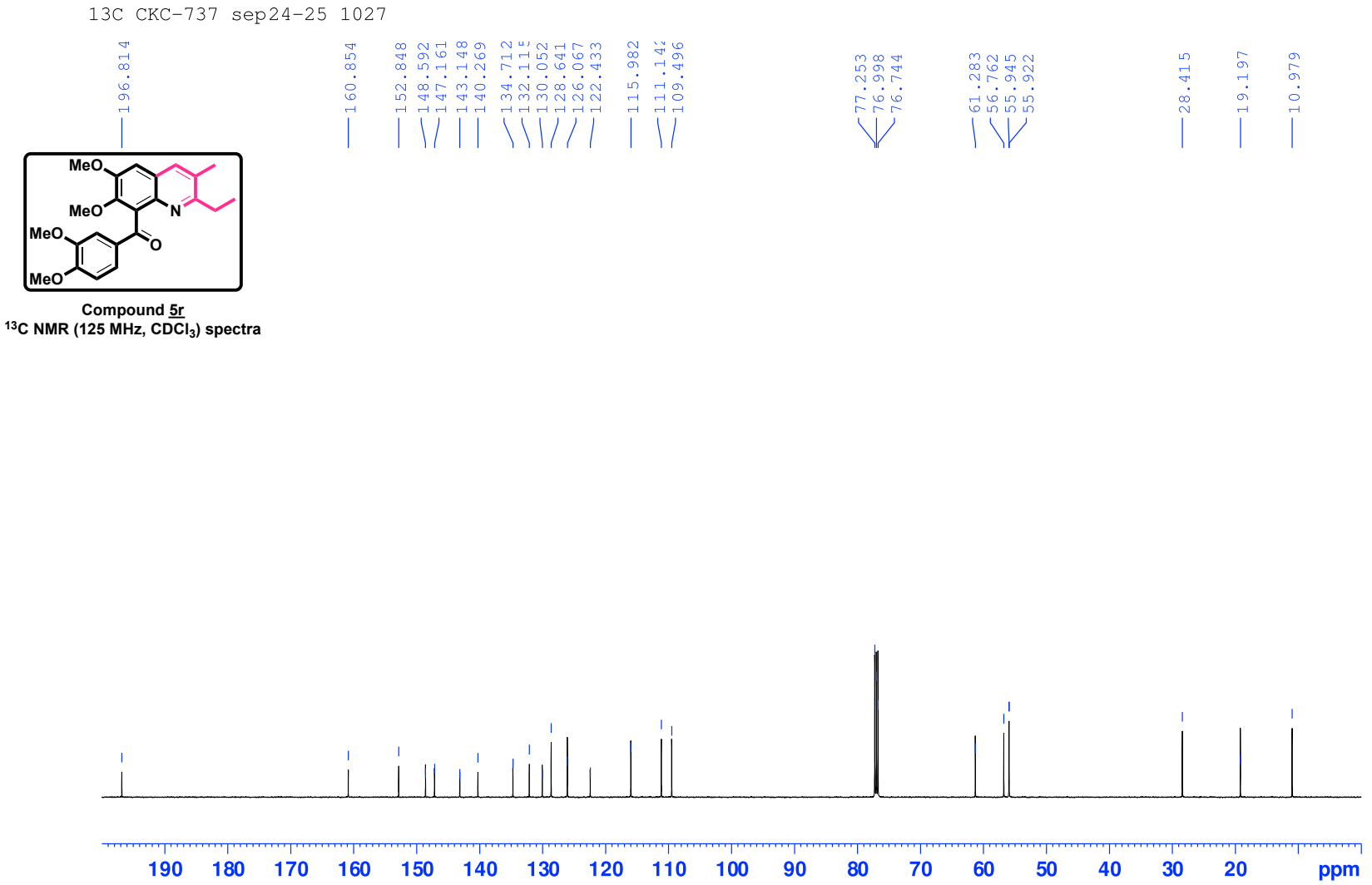

**Compound 5q**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5r



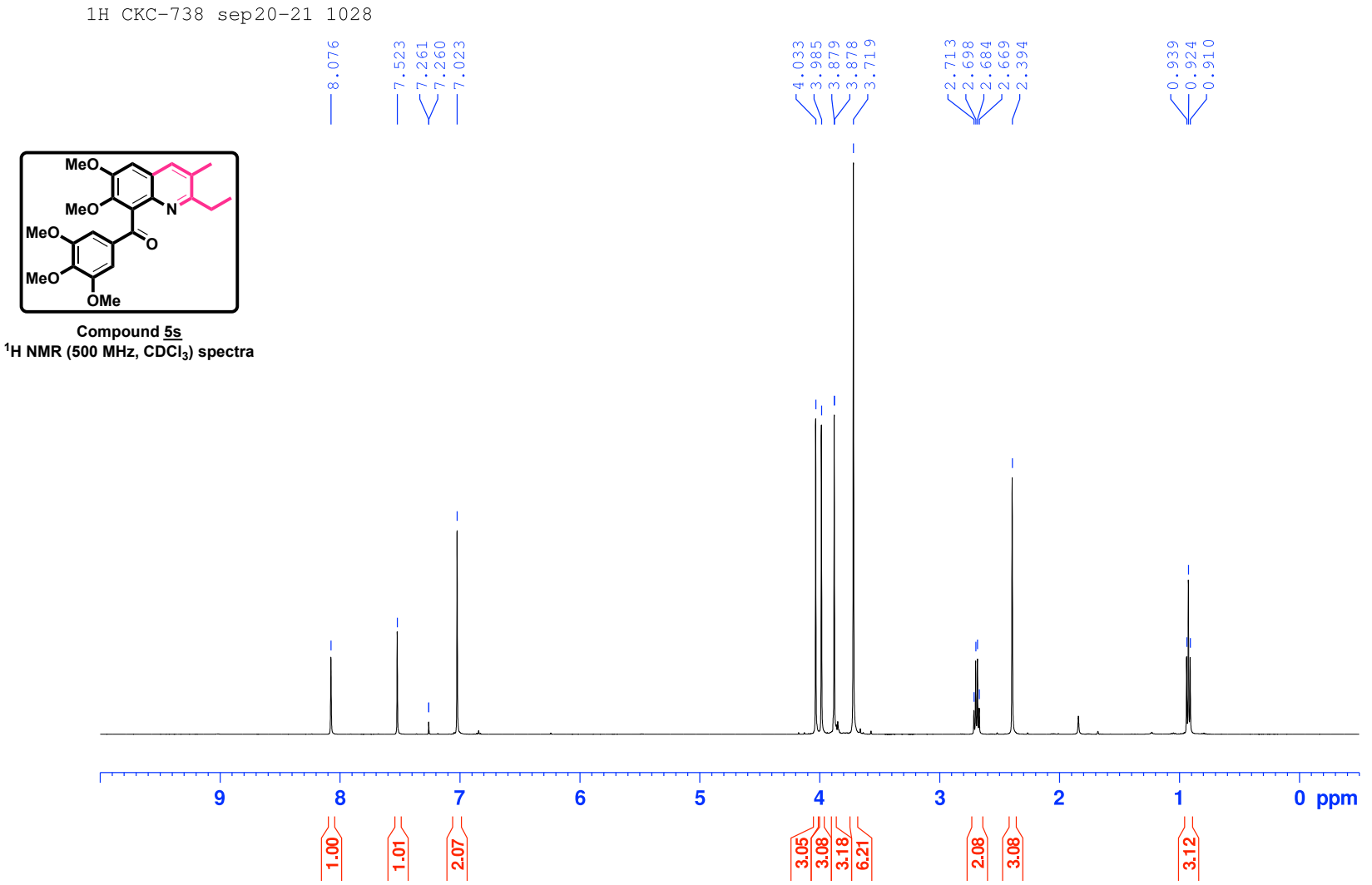

Compound 5r
$^1$H NMR (500 MHz, $CDCl_3$) spectra

# Compound 5r




**Compound 5r**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 5s

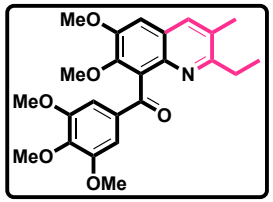



Compound 5s
$^1$H NMR (500 MHz, $CDCl_3$) spectra

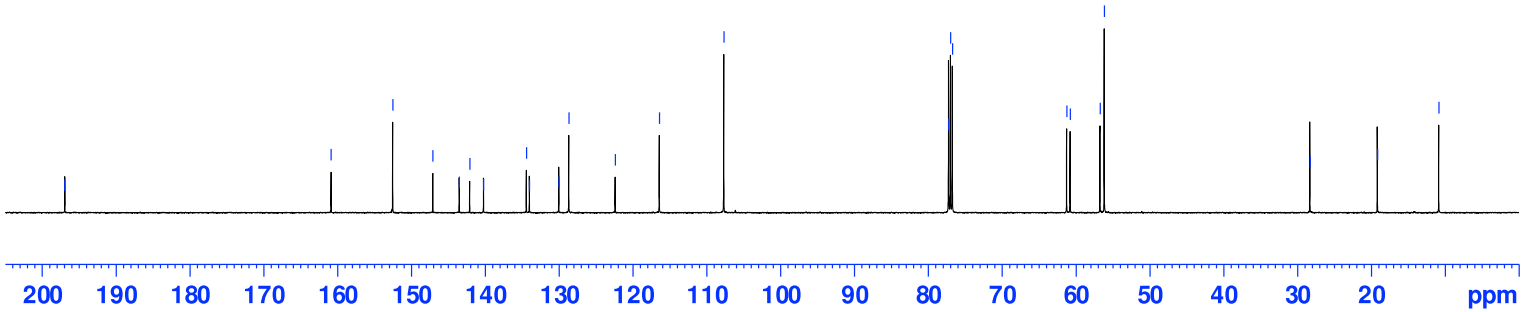
# Compound 5s

13C CKC-738 sep20-21 1028

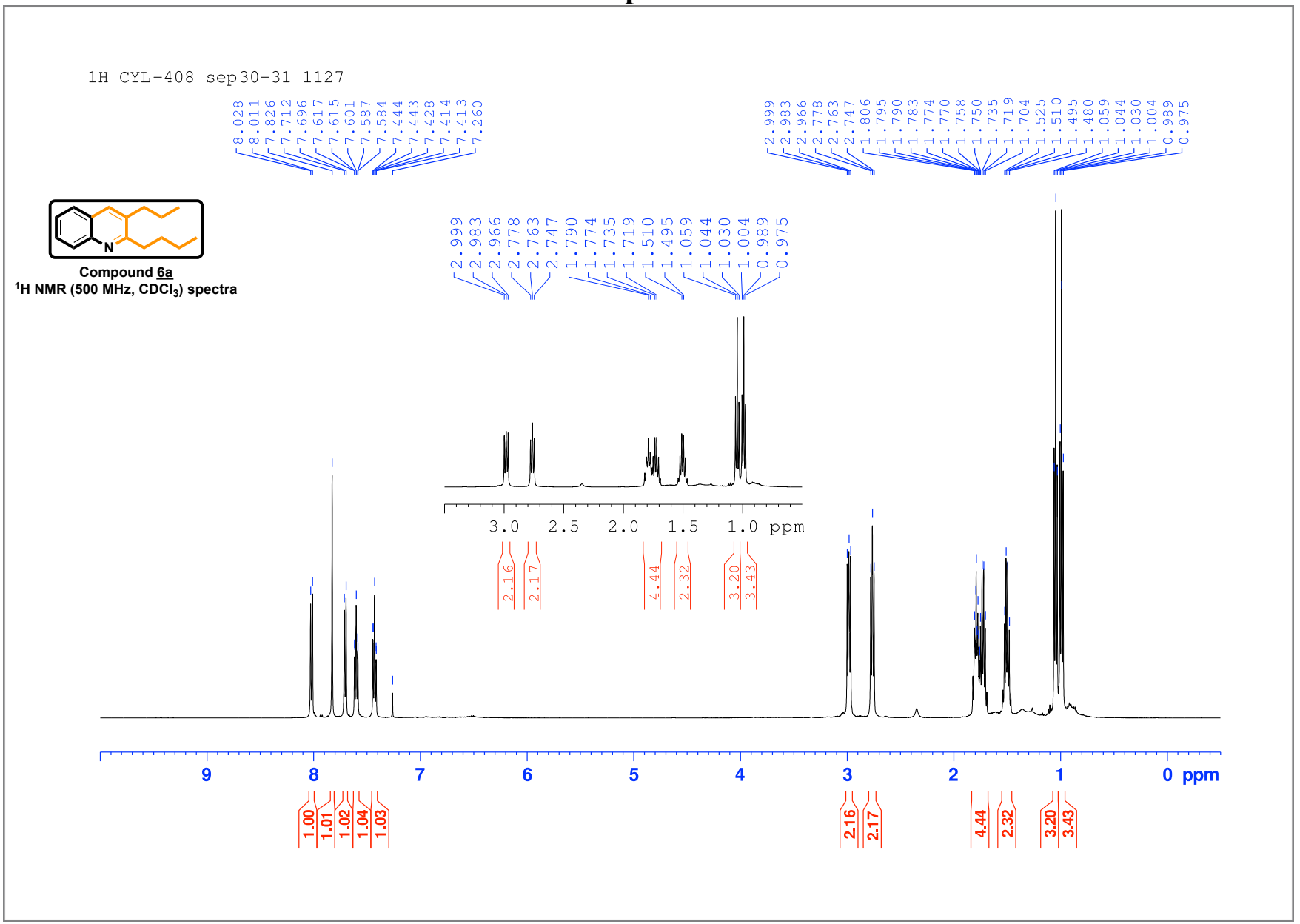
196.945
160.877
152.535
147.098
143.524
142.106
140.235
134.434
134.023
130.037
128.685
122.403
116.430
107.692
77.250
76.996
76.741
61.254
60.786
56.740
56.165
28.311
19.173
10.857



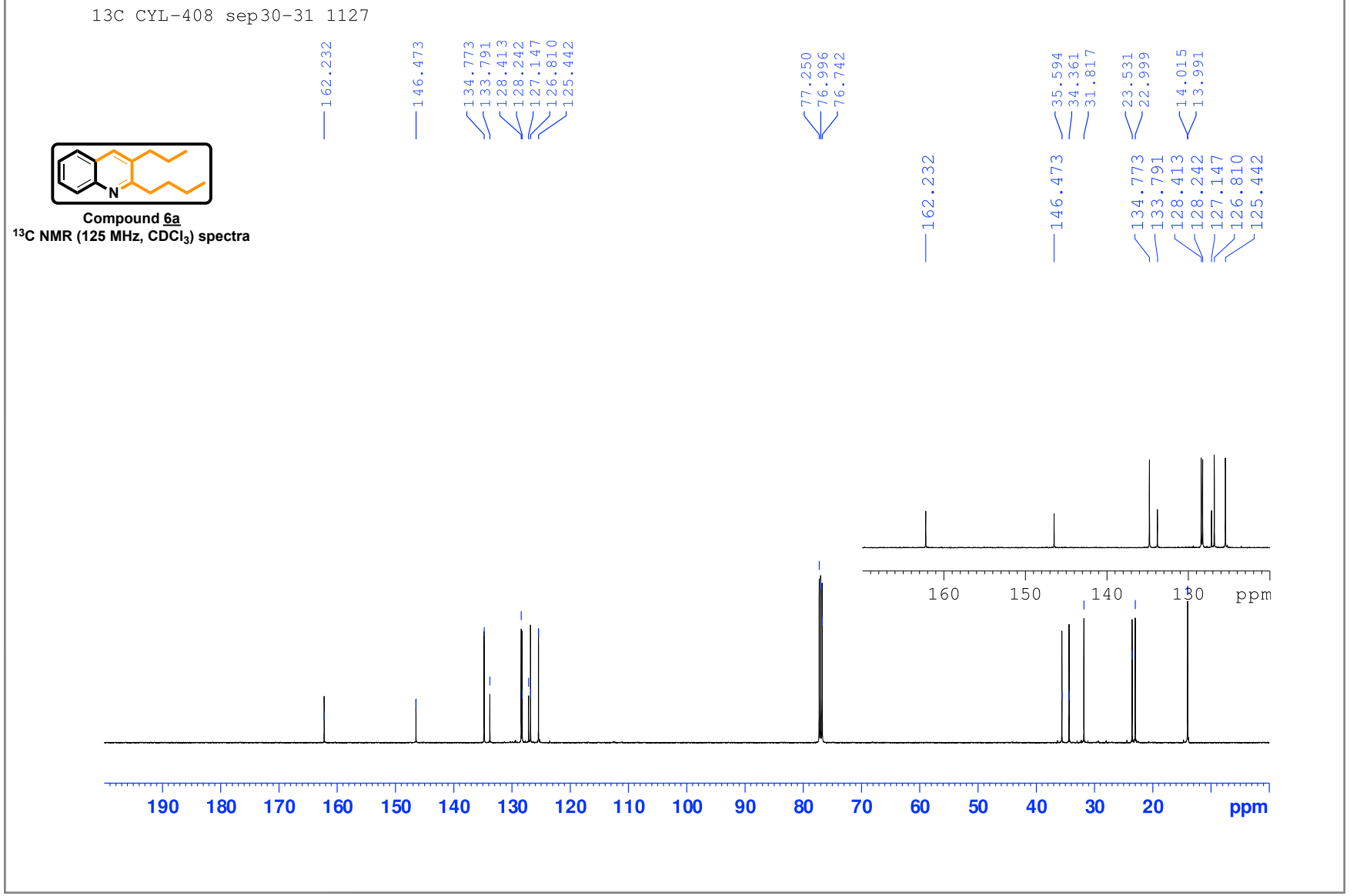

Compound 5s
$^{13}$C NMR (125 MHz, $CDCl_3$) spectra



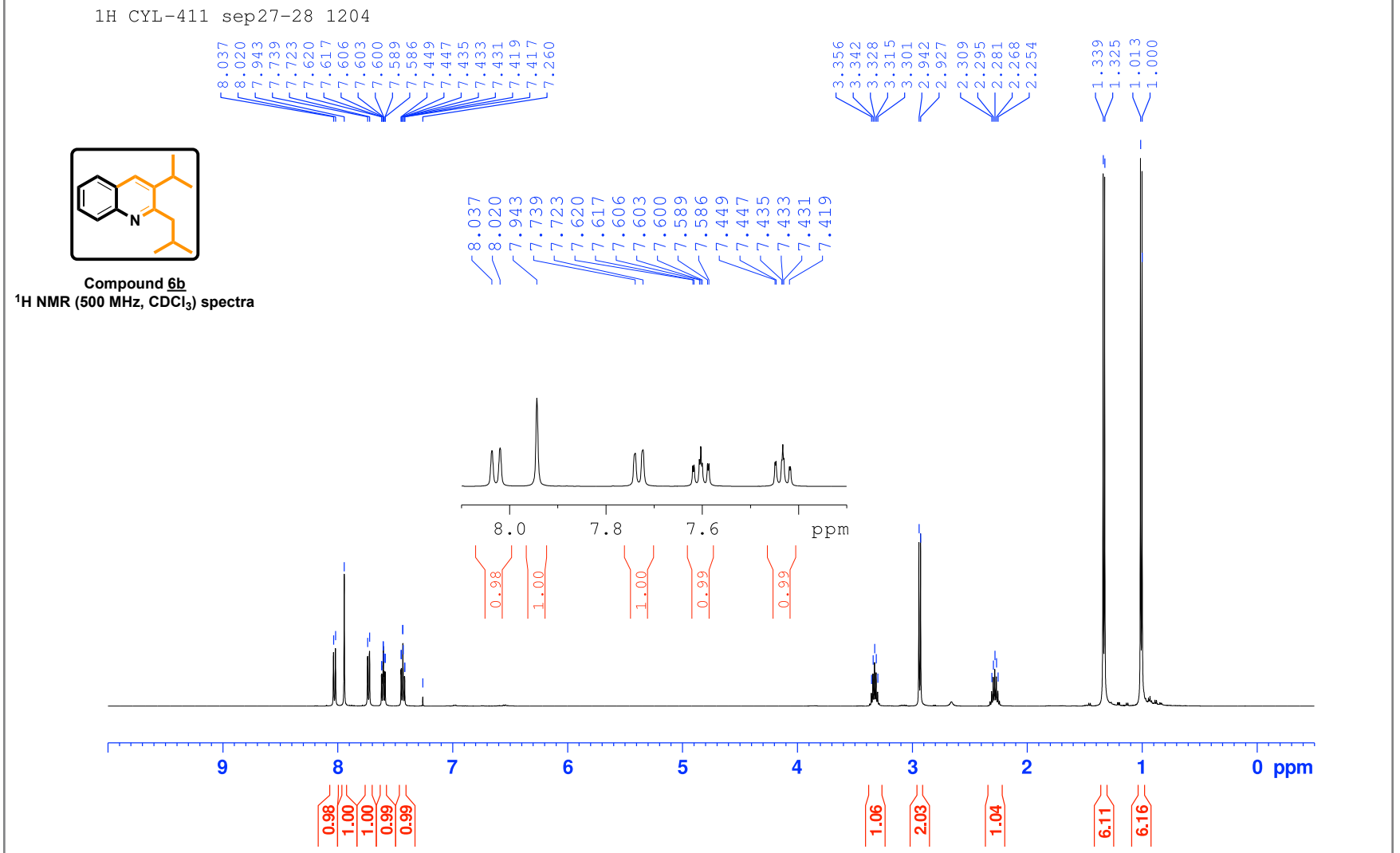
# Compound 6a


1H CYL-408 sep30-31 1127
Compound 6a
1H NMR (500 MHz, CDCl3) spectra
8.028
8.011
7.826
7.712
7.696
7.617
7.615
7.601
7.587
7.584
7.444
7.443
7.428
7.414
7.413
7.260
2.999
2.983
2.966
2.778
2.763
2.747
1.806
1.795
1.790
1.783
1.774
1.770
1.758
1.750
1.735
1.719
1.704
1.525
1.510
1.495
1.480
1.059
1.044
1.030
1.004
0.989
0.975
3.0
2.5
2.0
1.5
1.0 ppm
2.16
2.17
4.44
2.32
3.20
3.43
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.01
1.02
1.04
1.03
2.16
2.17
4.44
2.32
3.20
3.43

# Compound 6a

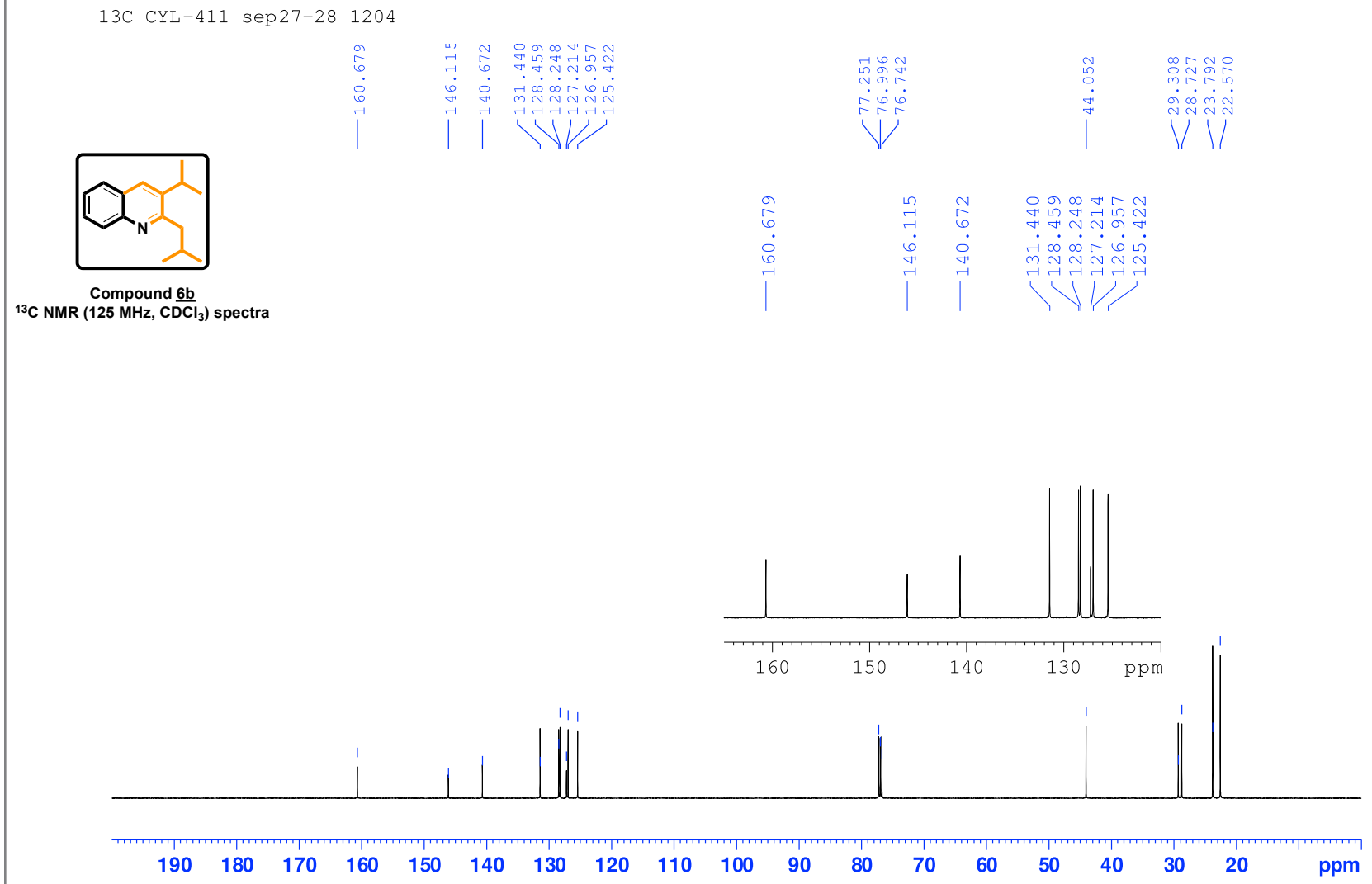

13C CYL-408 sep30-31 1127
162.232
146.473
134.773
133.791
128.413
128.242
127.147
126.810
125.442
77.250
76.996
76.742
35.594
34.361
31.817
23.531
22.999
14.015
13.991
N
Compound 6a
13C NMR (125 MHz, CDCl3) spectra
160
150
140
130
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

# Compound 6b



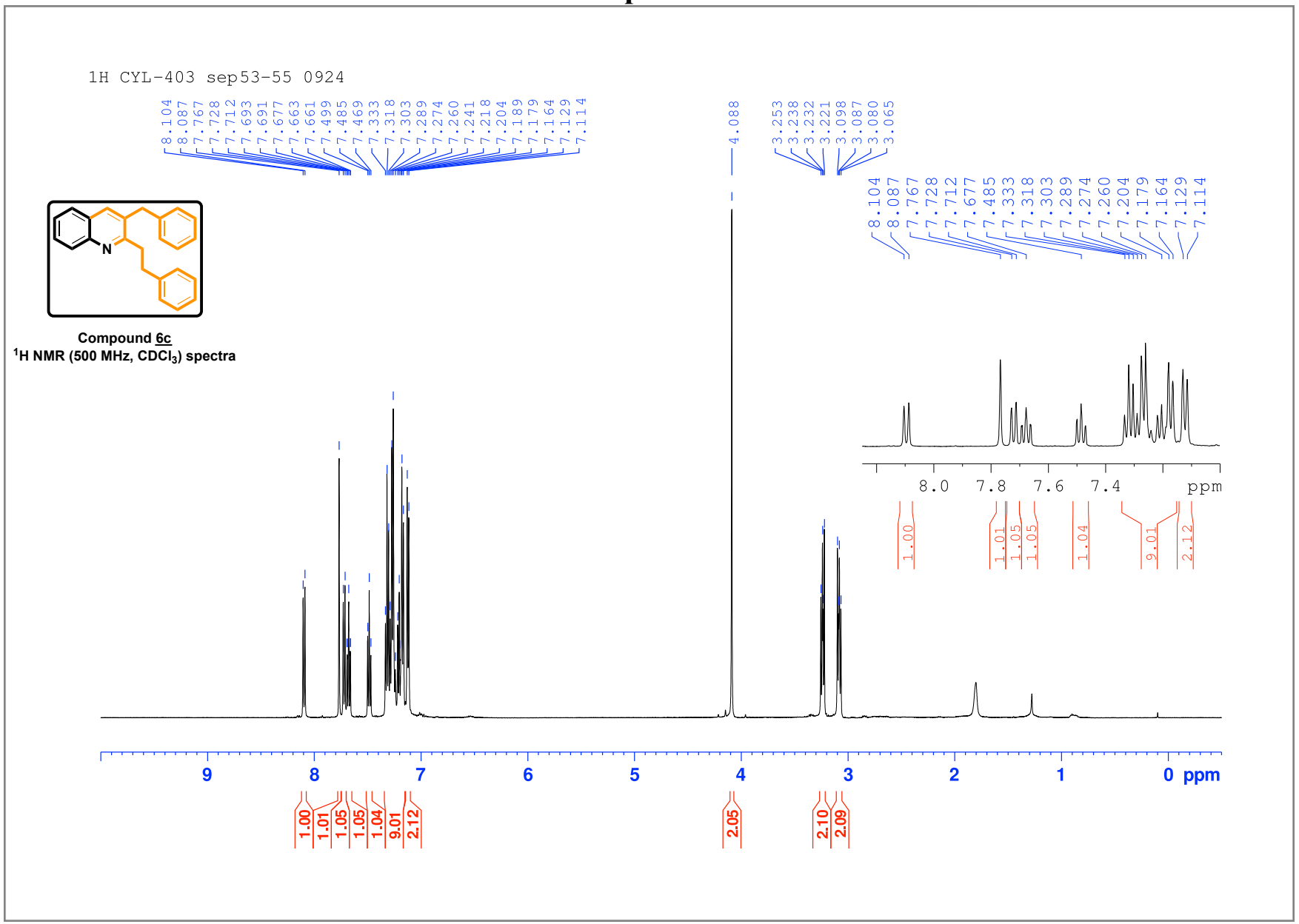

**Compound 6b**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

# Compound 6b

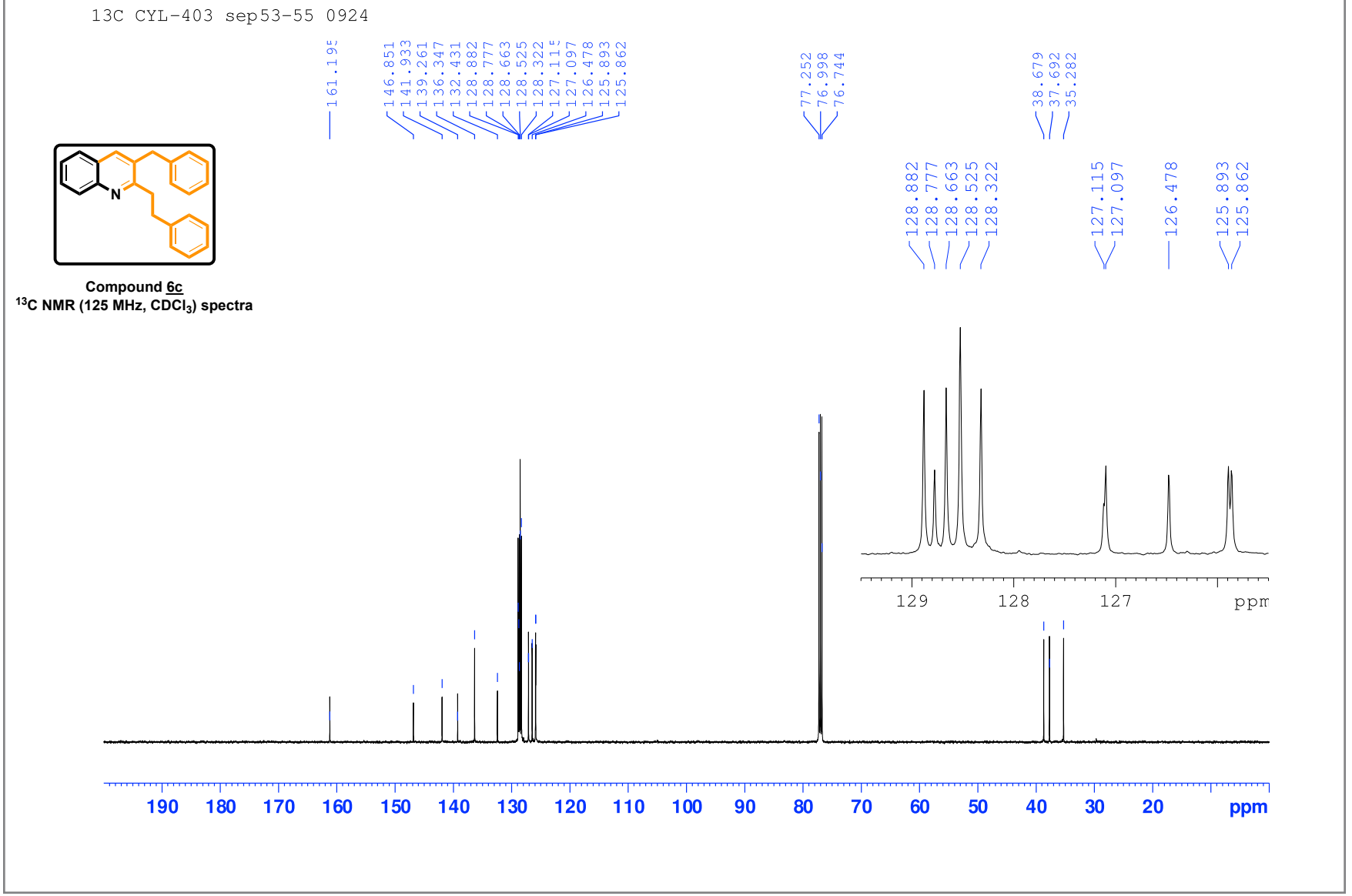



**Compound 6b**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

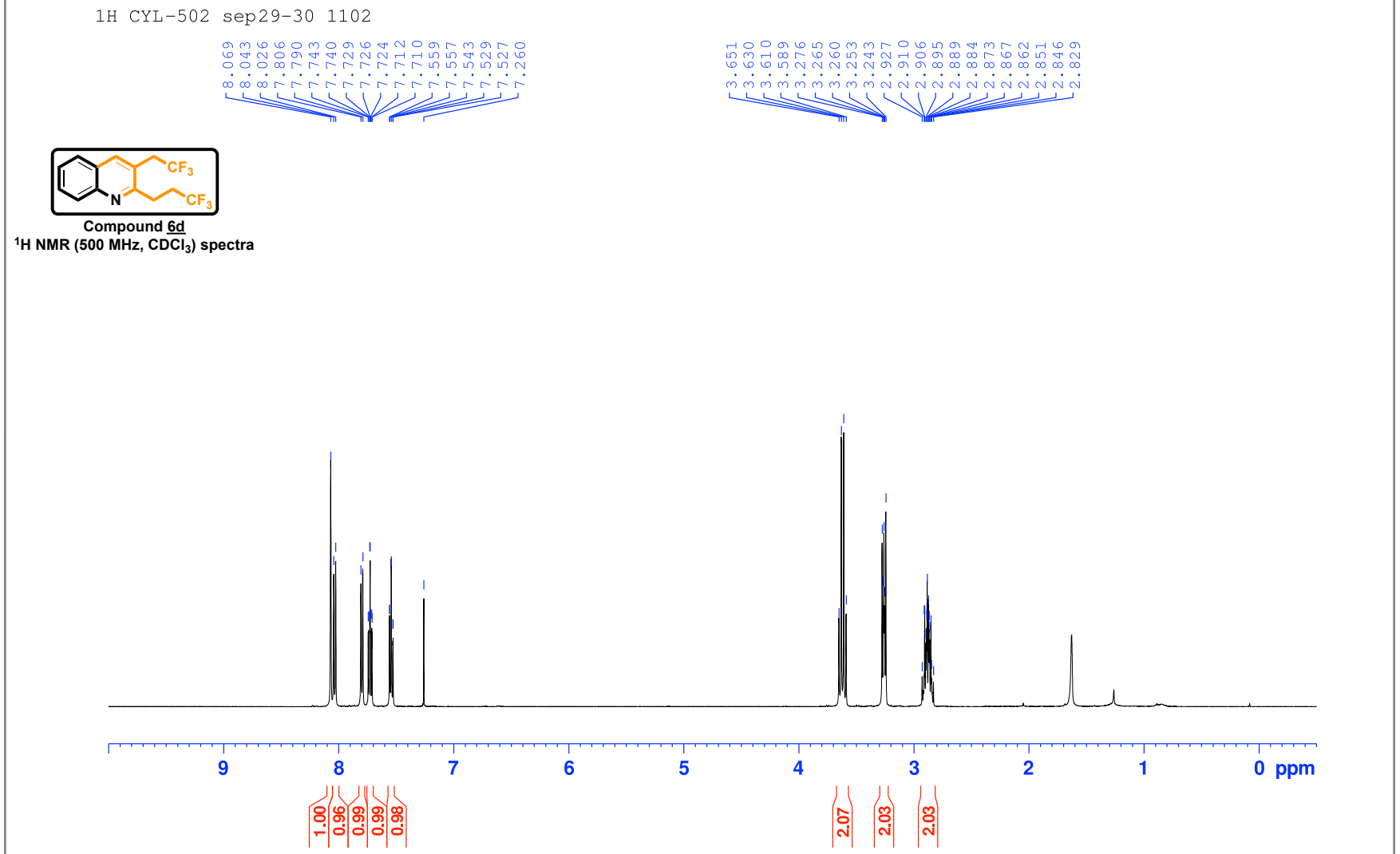
# Compound 6c


1H CYL-403 sep53-55 0924
8.104
8.087
7.767
7.728
7.712
7.693
7.691
7.677
7.663
7.661
7.499
7.485
7.469
7.333
7.318
7.303
7.289
7.274
7.260
7.241
7.218
7.204
7.189
7.179
7.164
7.129
7.114
4.088
3.253
3.238
3.232
3.221
3.098
3.087
3.080
3.065
N
Compound 6c
1H NMR (500 MHz, CDCl3) spectra
8.0
7.8
7.6
7.4
ppm
1.00
1.01
1.05
1.05
1.04
9.01
2.12
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.01
1.05
1.05
1.04
9.01
2.12
2.05
2.10
2.09

# Compound 6c

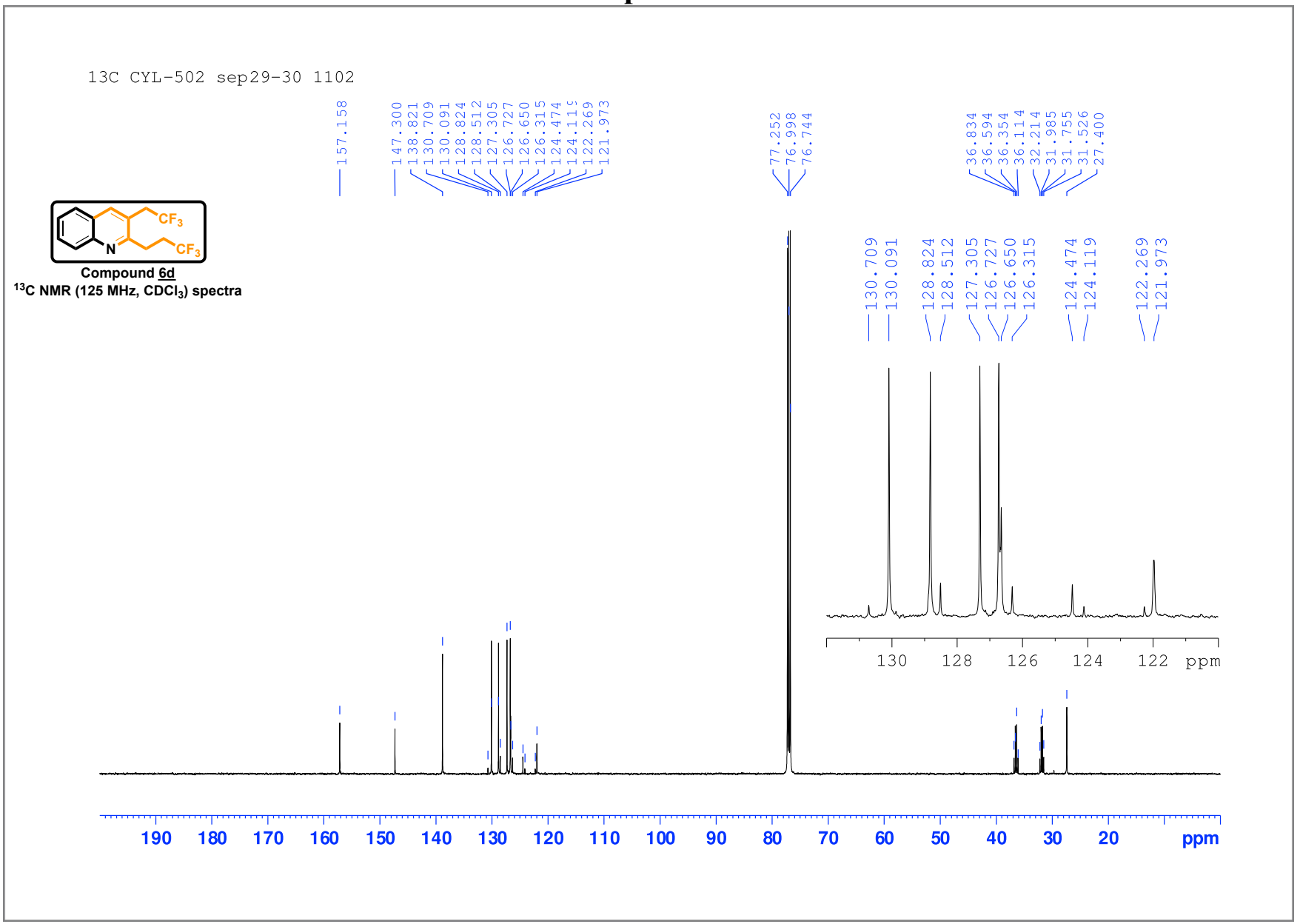

13C CYL-403 sep53-55 0924
161.19
146.851
141.933
139.261
136.347
132.431
128.882
128.777
128.663
128.525
128.322
127.11
127.097
126.478
125.893
125.862
77.252
76.998
76.744
38.679
37.692
35.282
N
Compound 6c
13C NMR (125 MHz, CDCl3) spectra
128.882
128.777
128.663
128.525
128.322
127.115
127.097
126.478
125.893
125.862
129
128
127
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

# Compound 6d




**Compound 6d**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

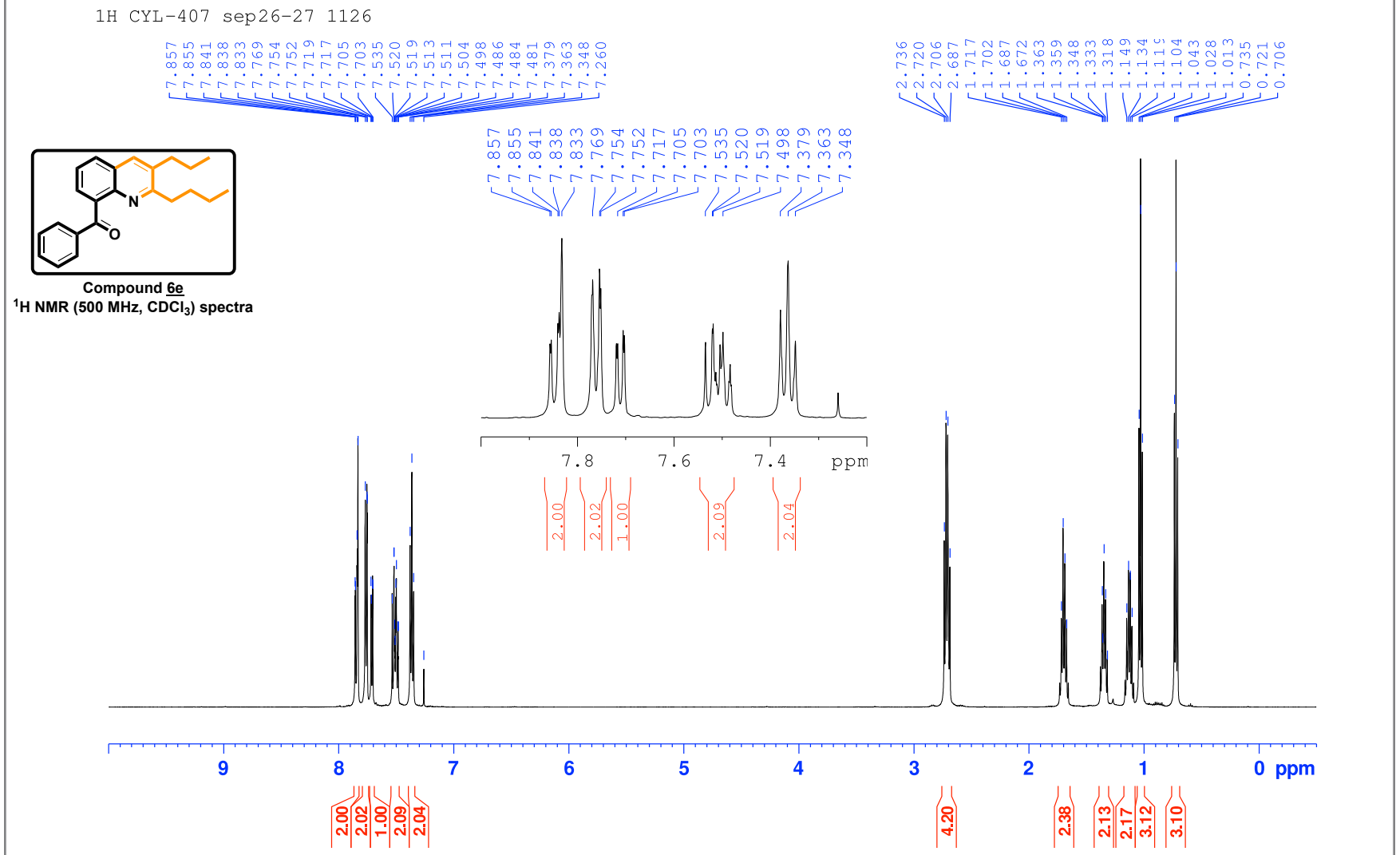
# Compound 6d




Compound 6d

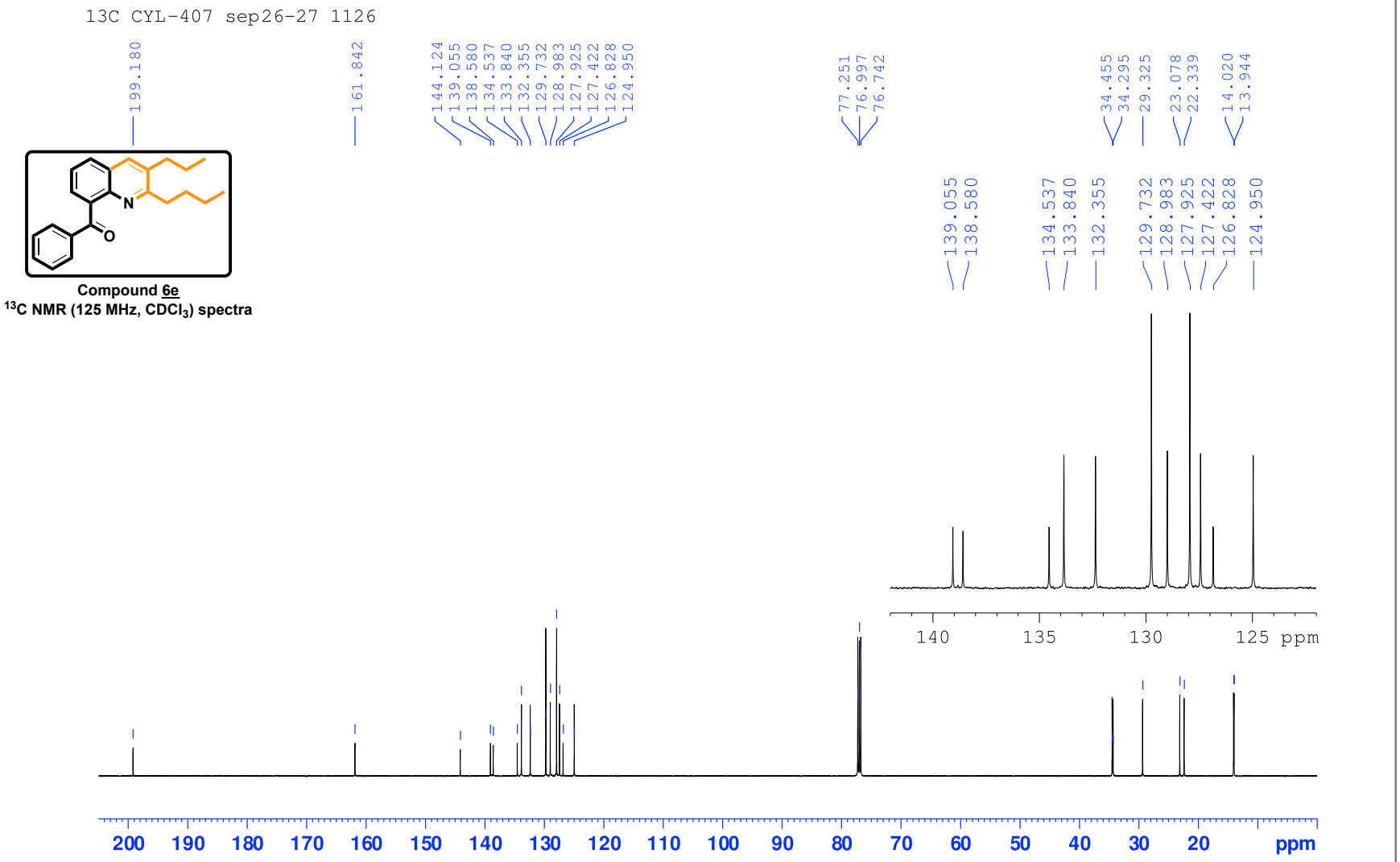
$^{13}$C NMR (125 MHz, $CDCl_3$) spectra

# Compound 6e

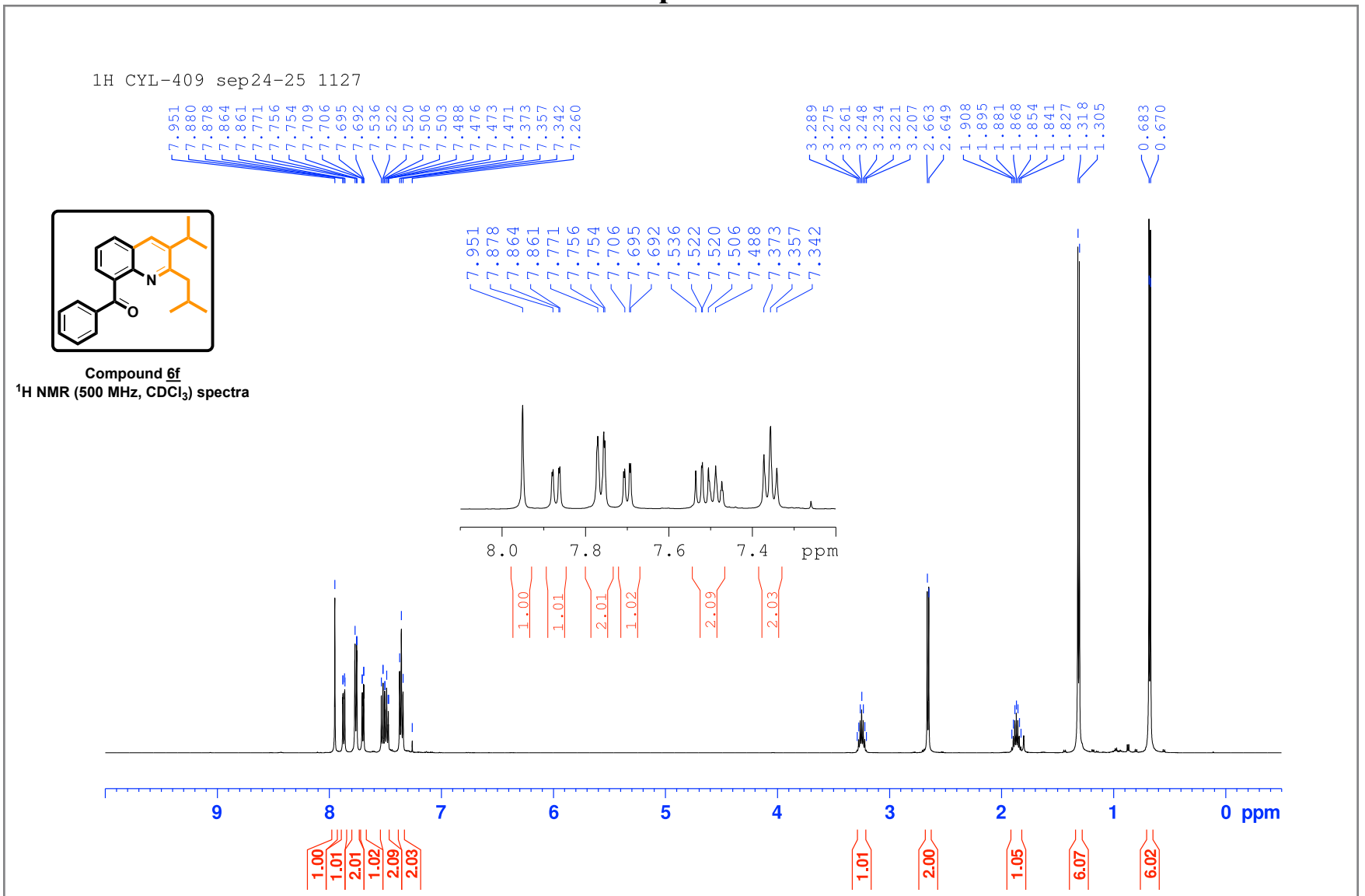



**Compound 6e**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

# Compound 6e

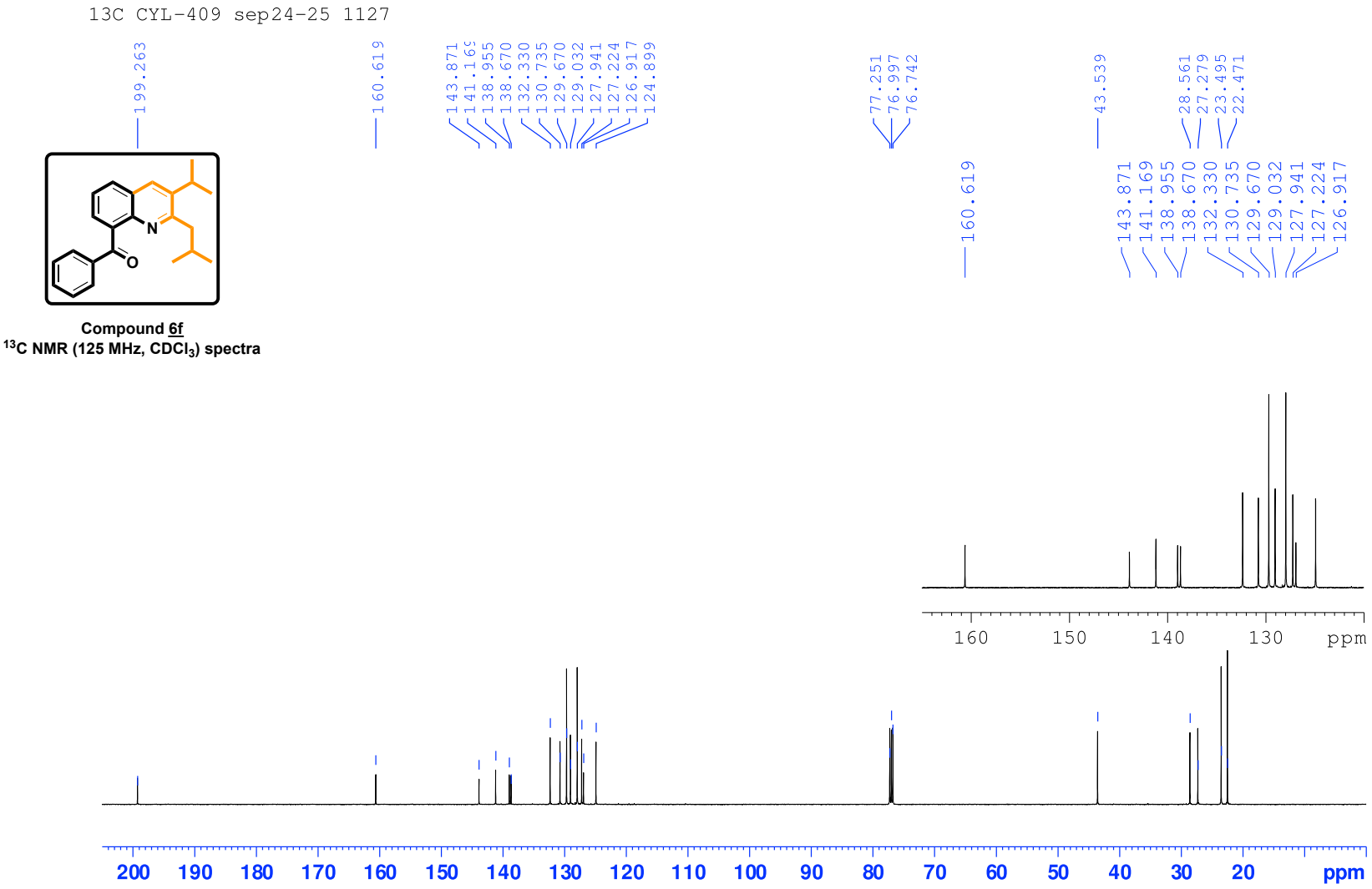

13C CYL-407 sep26-27 1126
199.180
161.842
144.124
139.055
138.580
134.537
133.840
132.355
129.732
128.983
127.925
127.422
126.828
124.950
77.251
76.997
76.742
34.455
34.295
29.325
23.078
22.339
14.020
13.944
N
O
Compound 6e
13C NMR (125 MHz, CDCl3) spectra
140
135
130
125 ppm
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

# Compound 6f



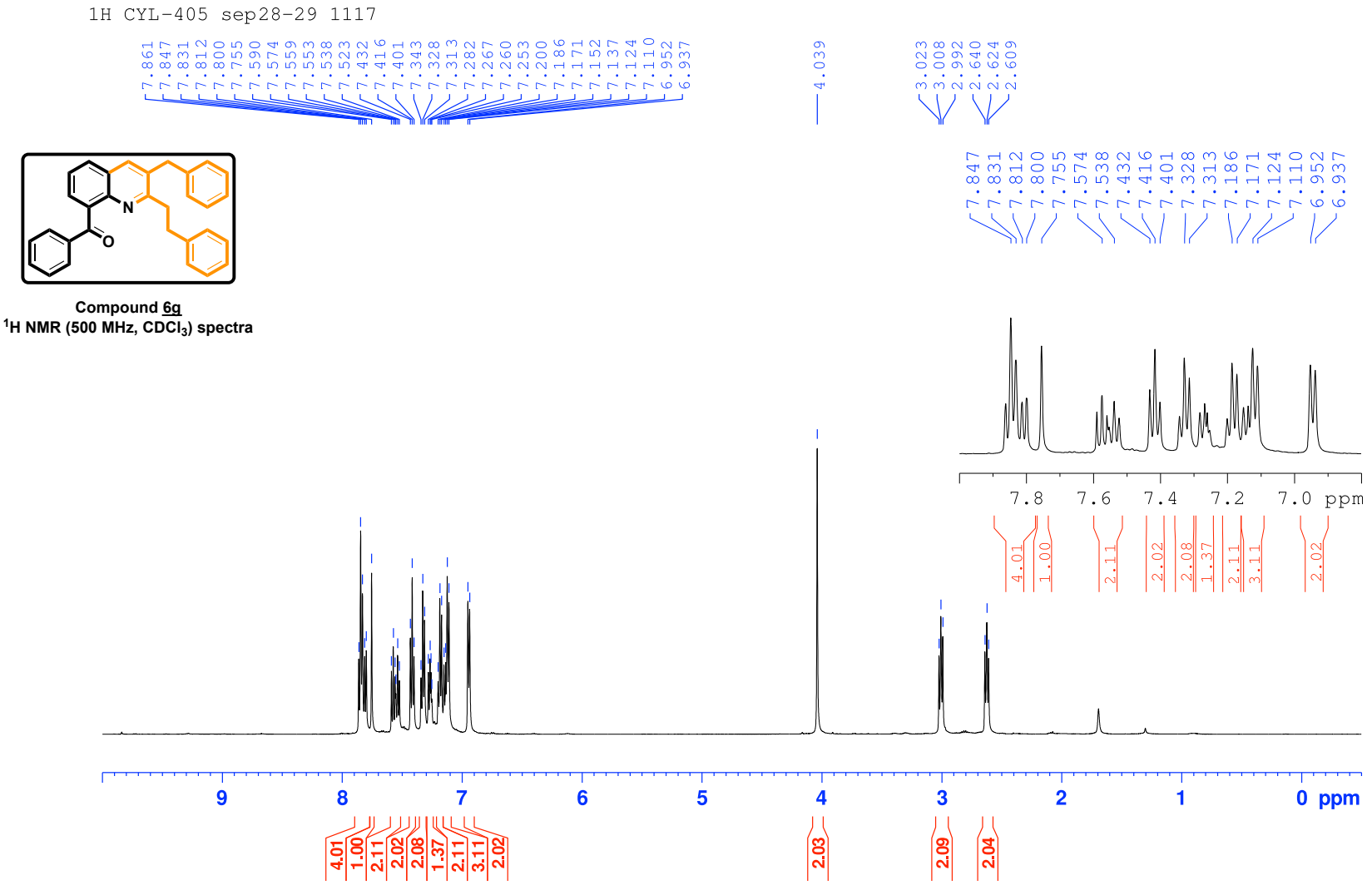

**Compound 6f**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

# Compound 6f

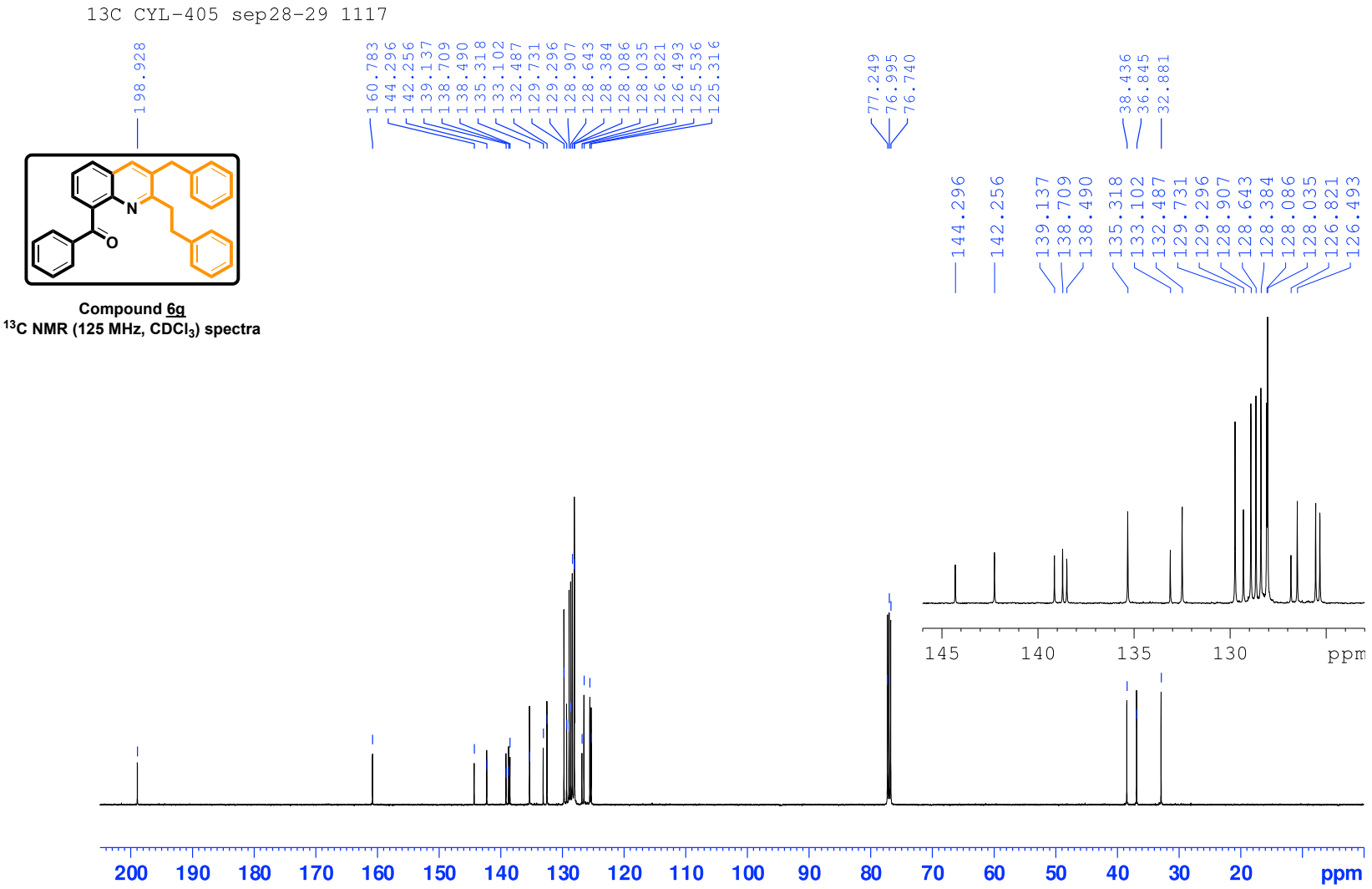



**Compound 6f**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 6g

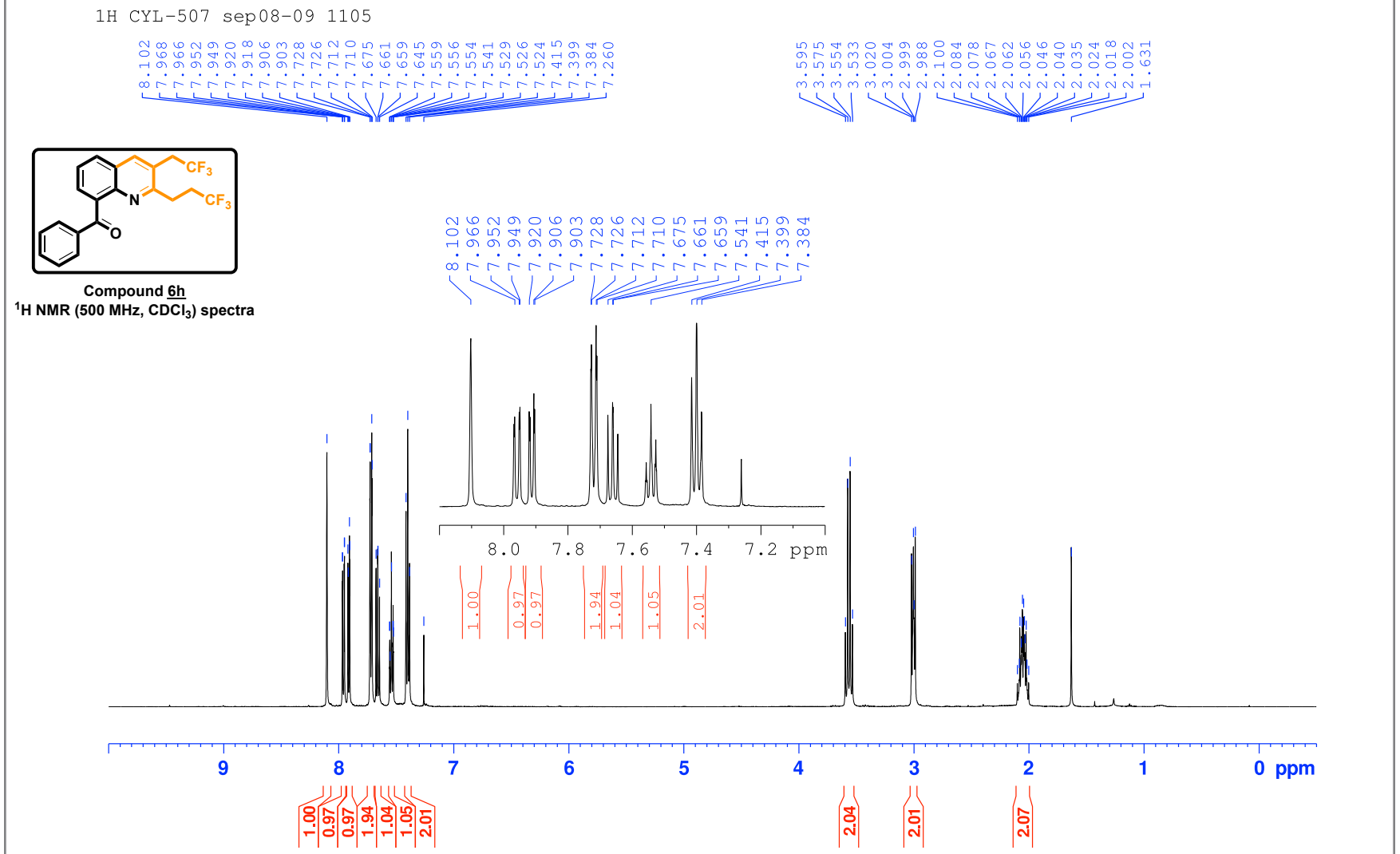

1H CYL-405 sep28-29 1117
7.861
7.847
7.831
7.812
7.800
7.755
7.590
7.574
7.559
7.553
7.538
7.523
7.432
7.416
7.401
7.343
7.328
7.313
7.282
7.267
7.260
7.253
7.200
7.186
7.171
7.152
7.137
7.124
7.110
6.952
6.937
4.039
3.023
3.008
2.992
2.640
2.624
2.609
N
O
Compound 6g
1H NMR (500 MHz, CDCl3) spectra
7.8
7.6
7.4
7.2
7.0 ppm
4.01
1.00
2.11
2.02
2.08
1.37
2.11
3.11
2.02
9
8
7
6
5
4
3
2
1
0 ppm
4.01
1.00
2.11
2.02
2.08
1.37
2.11
3.11
2.02
2.03
2.09
2.04

# Compound 6g



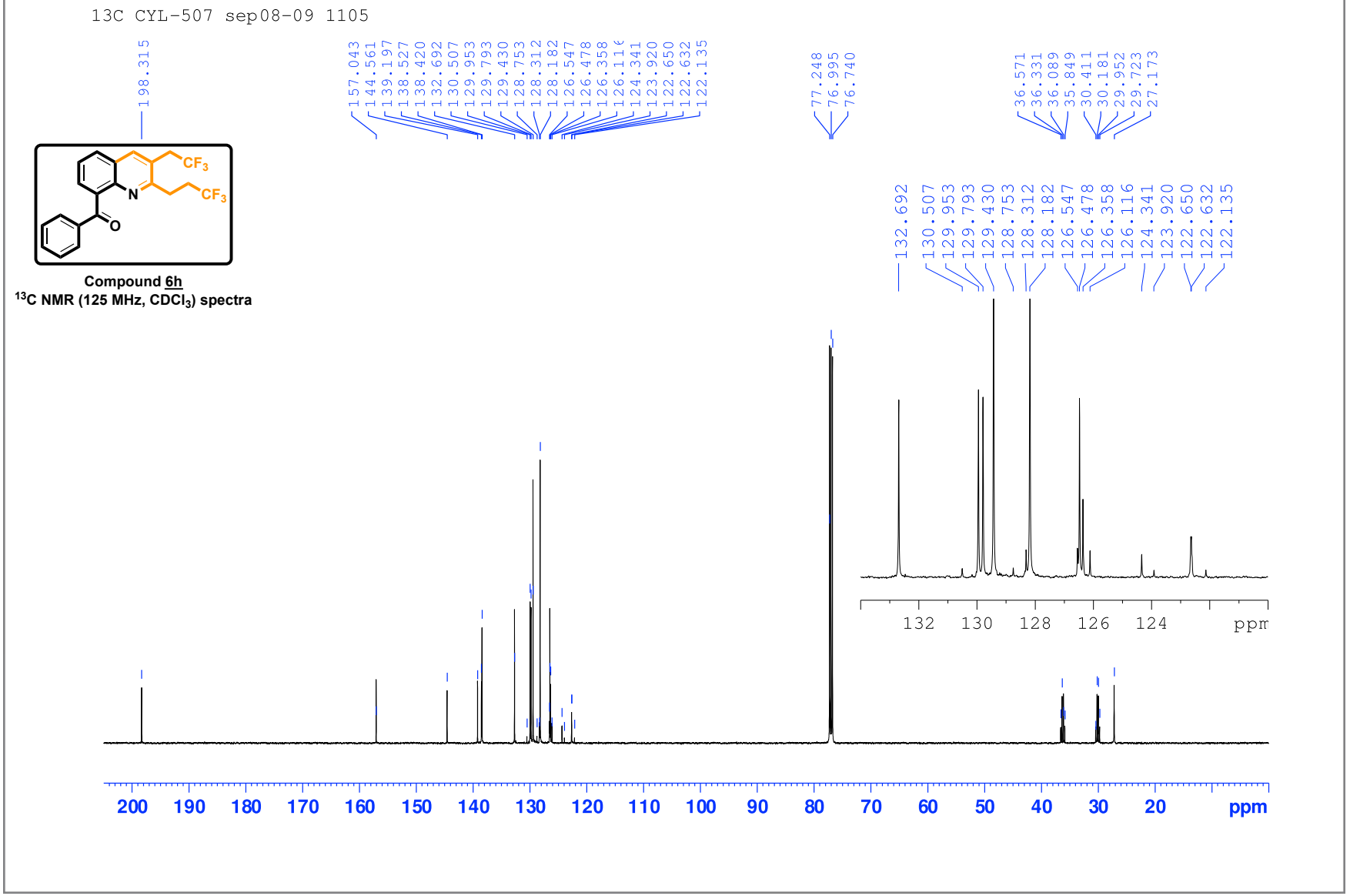

**Compound 6g**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 6h



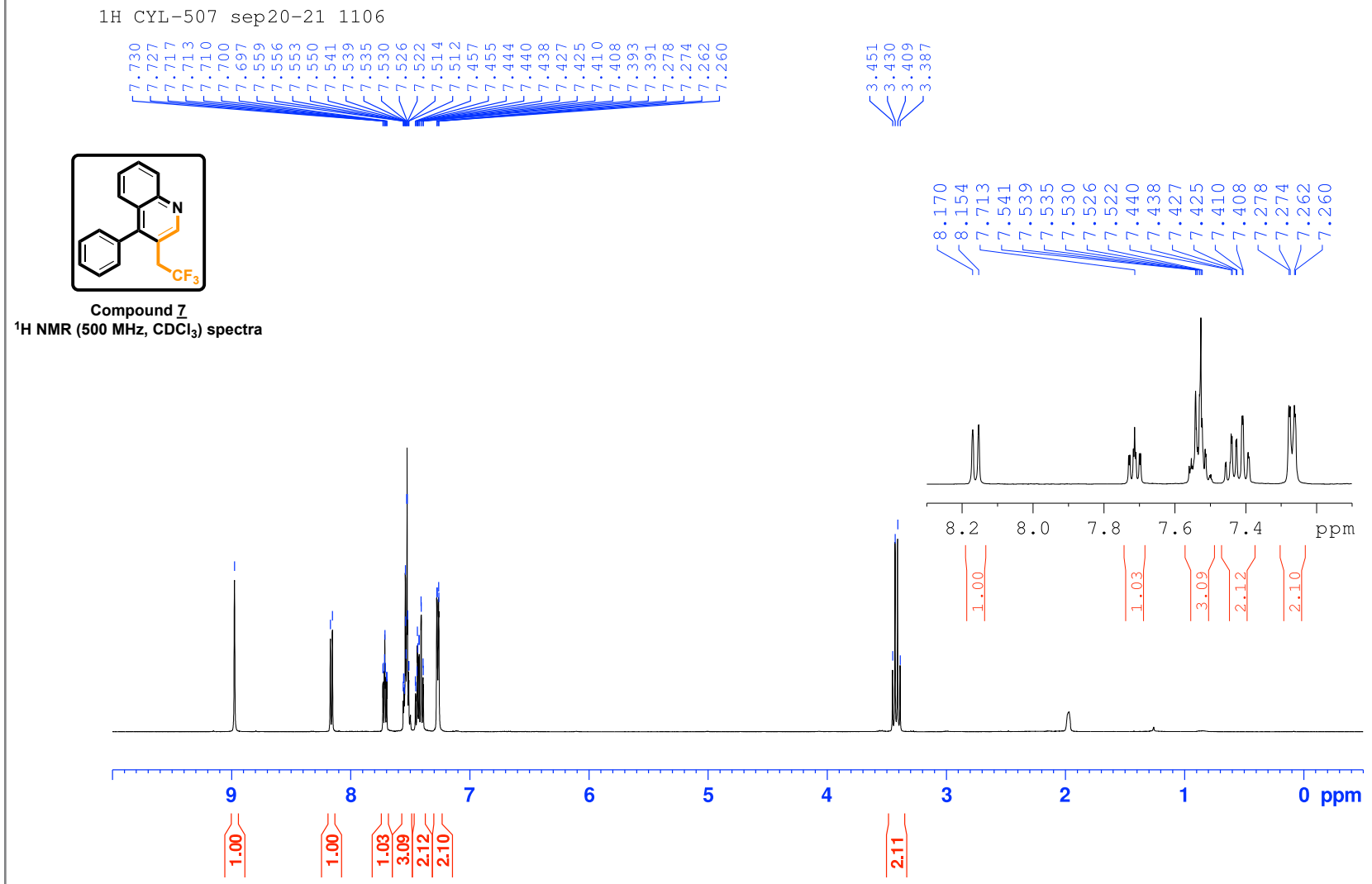

**Compound 6h**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

# Compound 6h



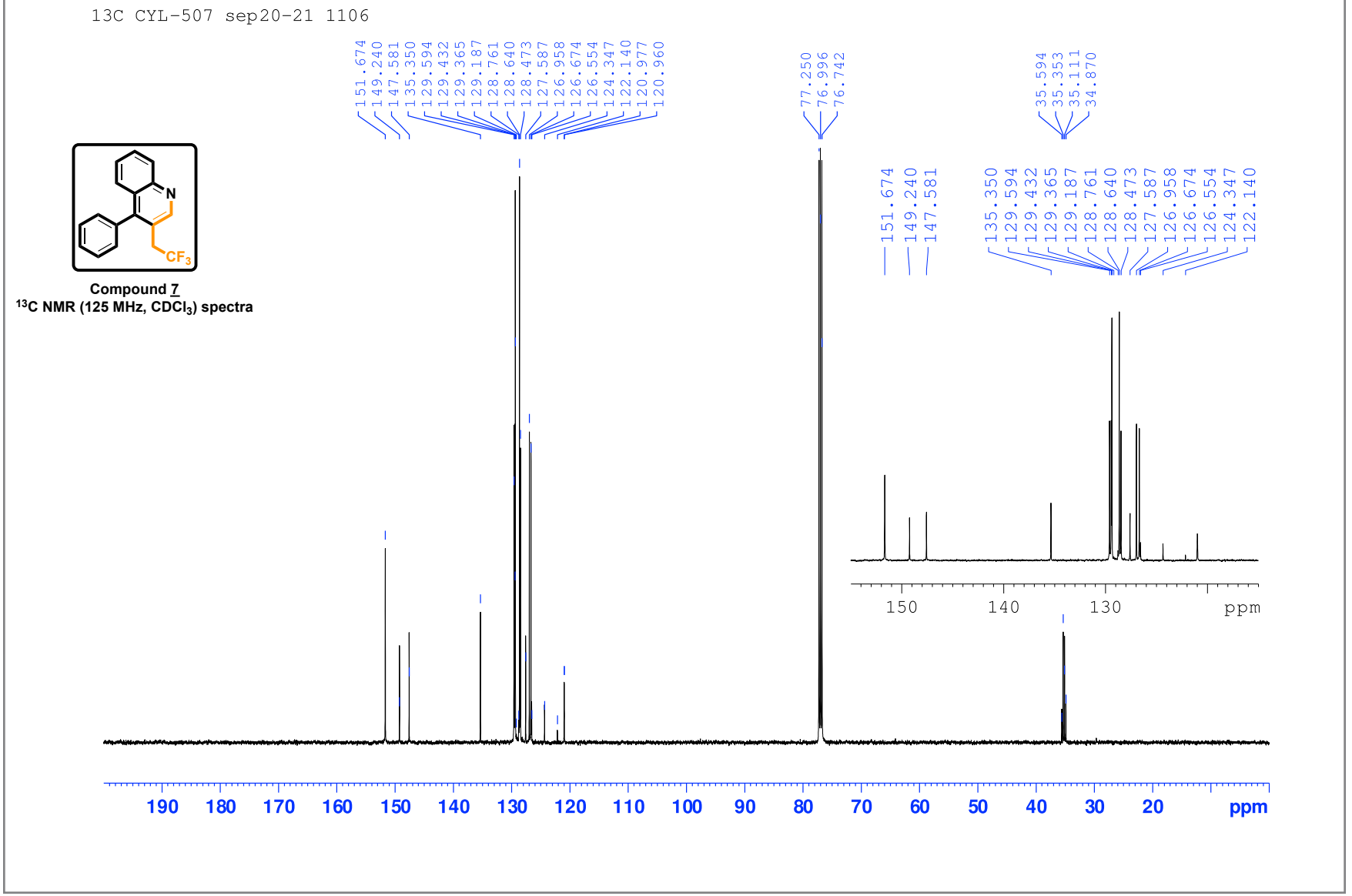

**Compound 6h**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**

# Compound 7




**Compound 7**
**$^1$H NMR (500 MHz, $CDCl_3$) spectra**

# Compound 7




**Compound 7**
**$^{13}$C NMR (125 MHz, $CDCl_3$) spectra**