

Supplementary Information

Diastereoselective Three-Component 1,3-Dipolar Cycloaddition: Concise Synthesis of Functionalized Tetrahydrocarboline-fused Spirooxindoles

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Yongchao Wang (ycwang@ynnu.edu.cn; yongchaowang126@126.com)

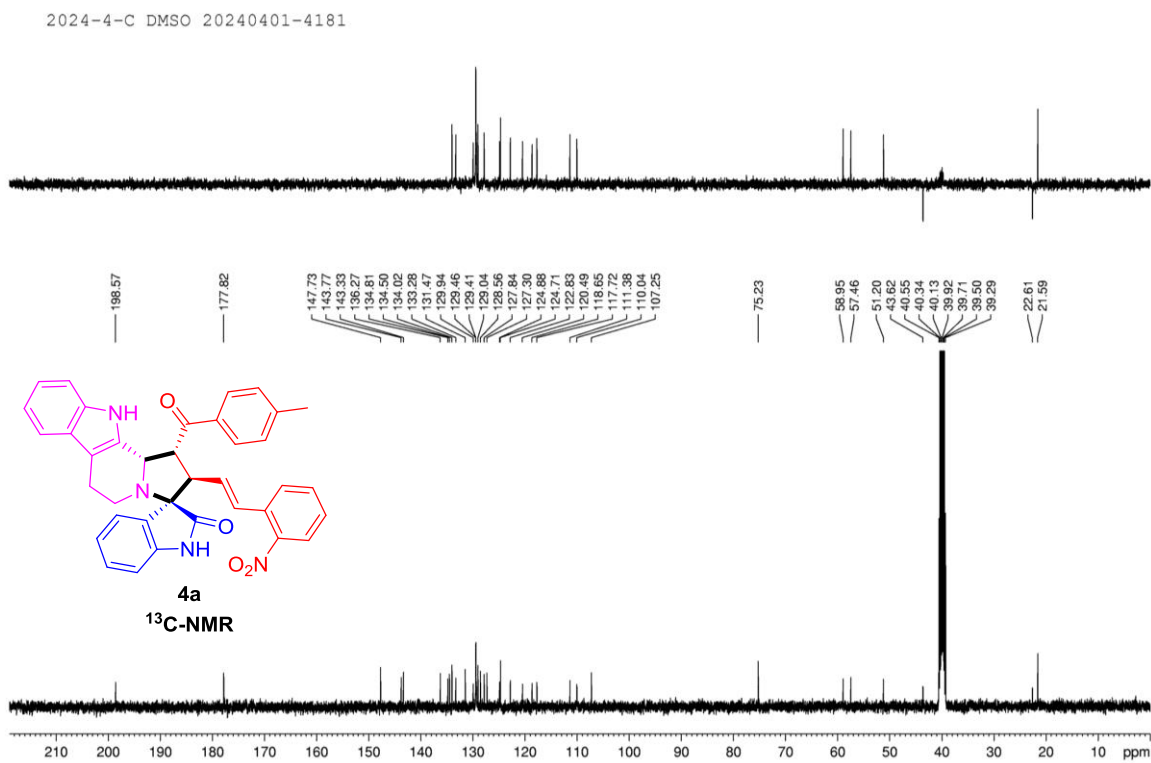
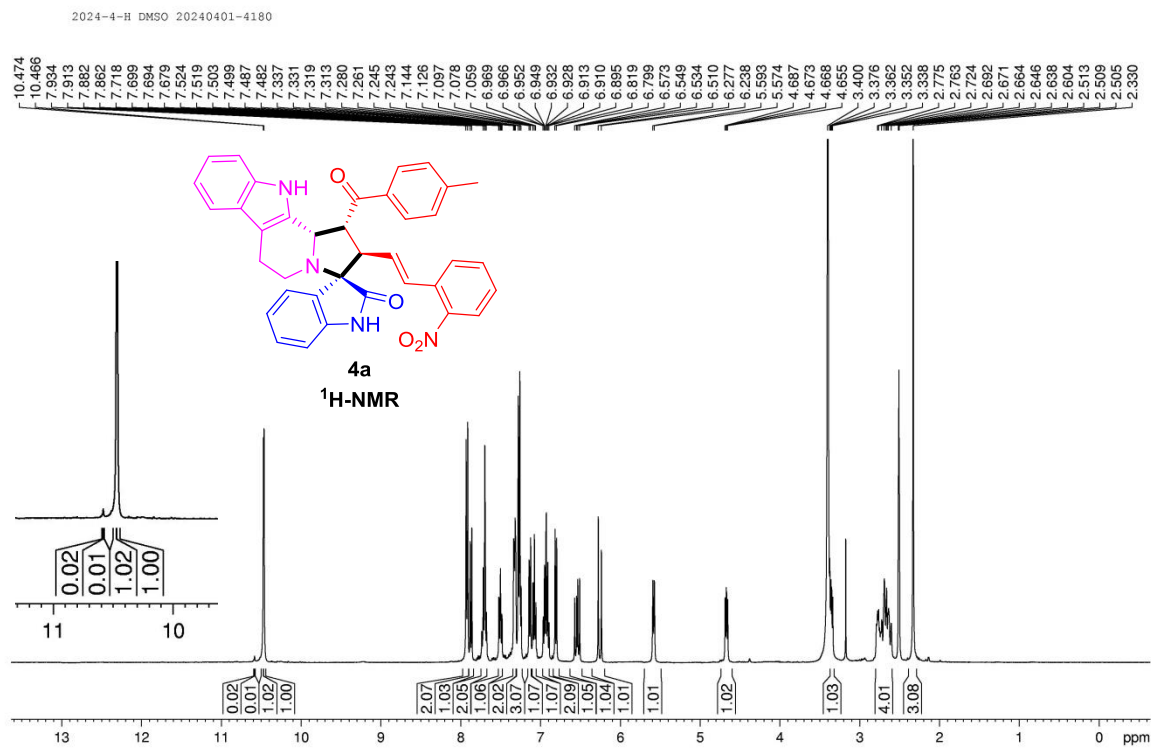
Donghua Hu (hudong-hua8888@126.com)

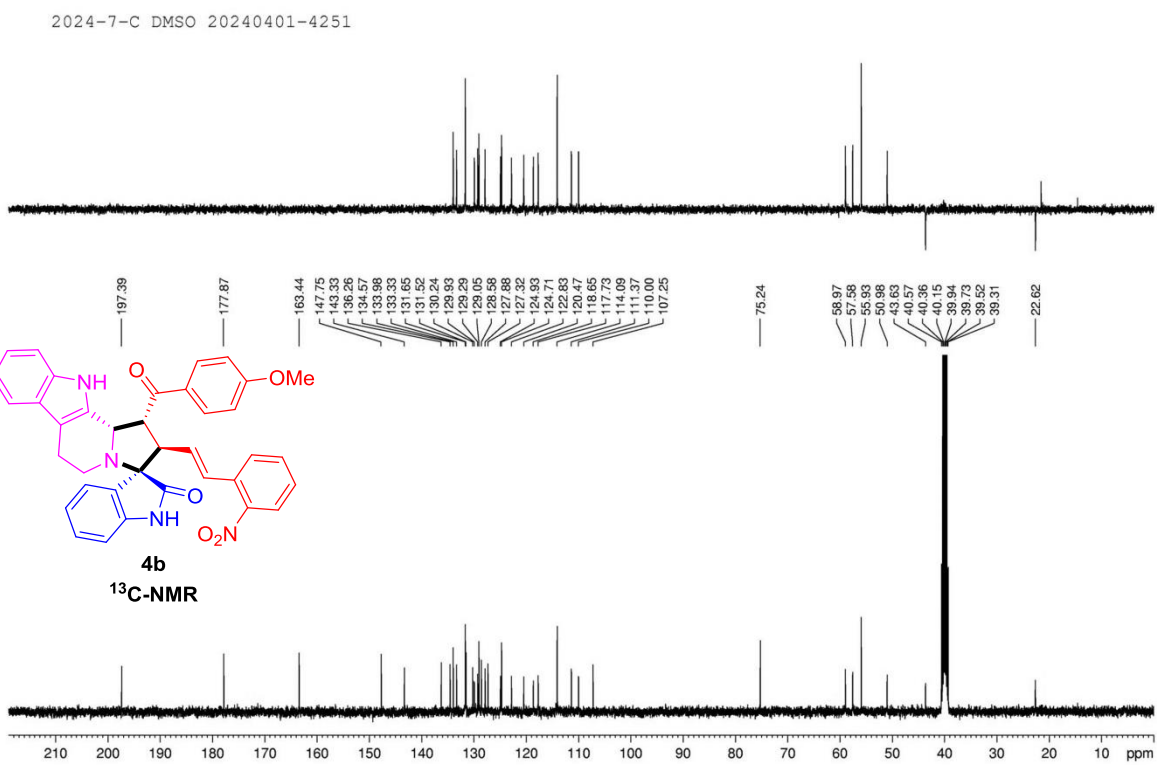
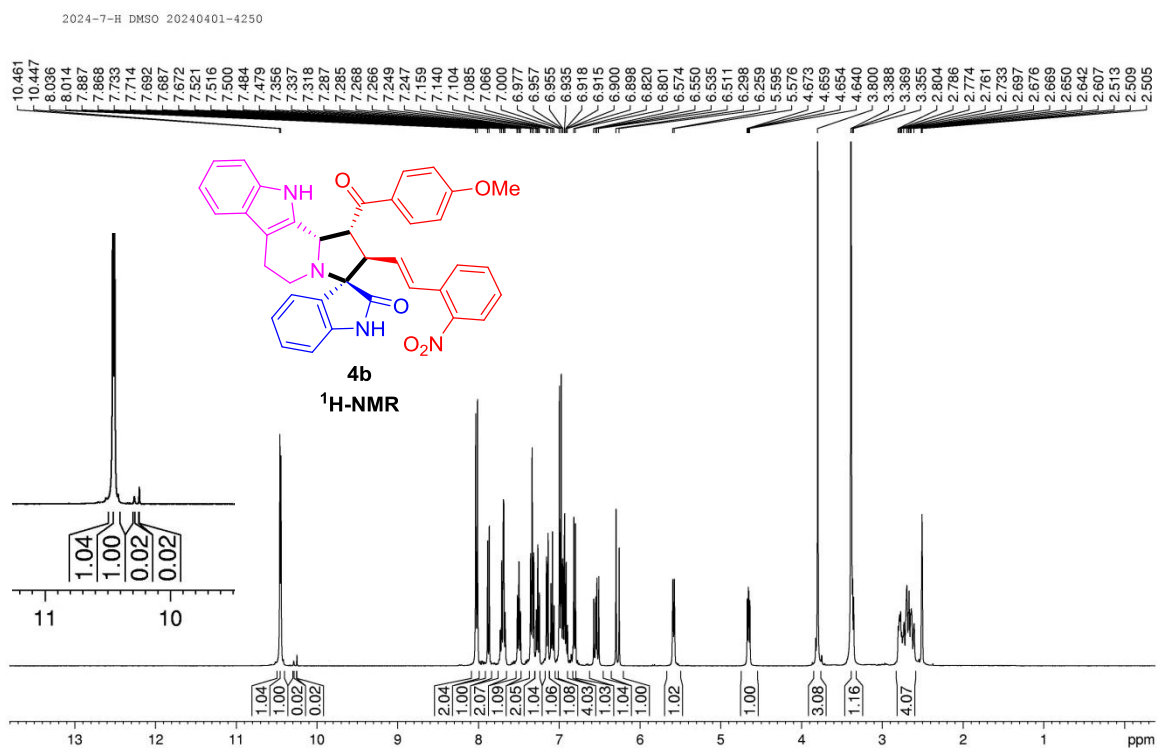
Jianwei Dong (jwdongyn@mail.qjnu.edu.cn)

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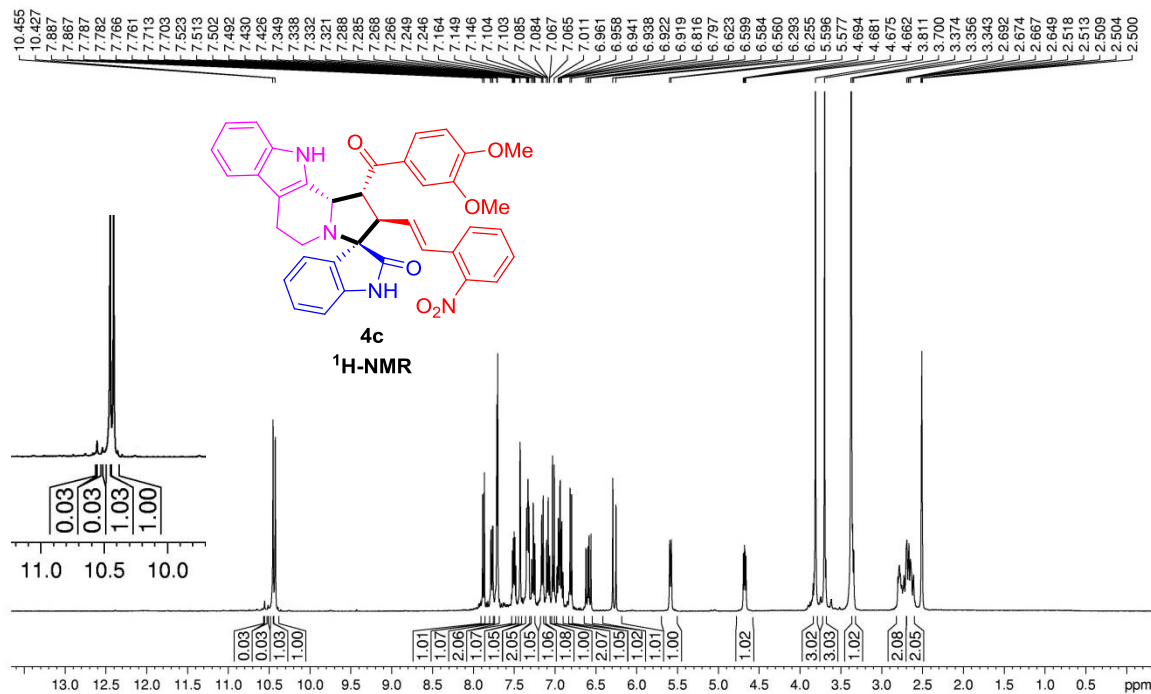
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1. ^1H and ^{13}C NMR spectra for compounds 4

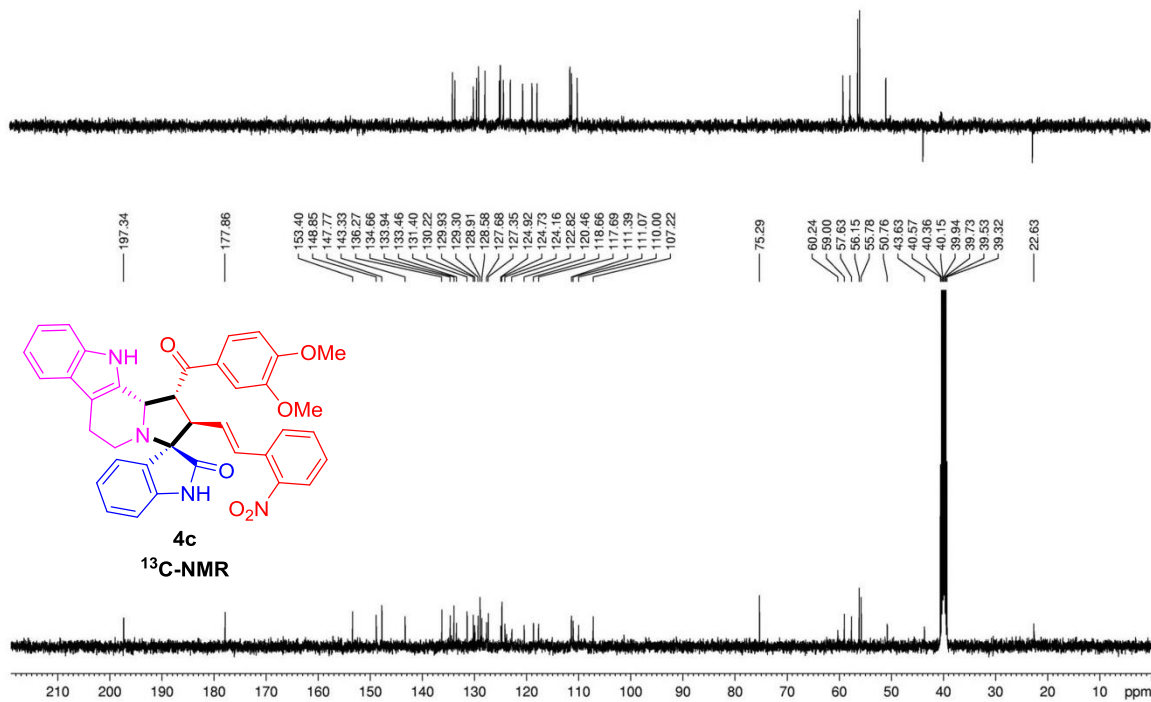




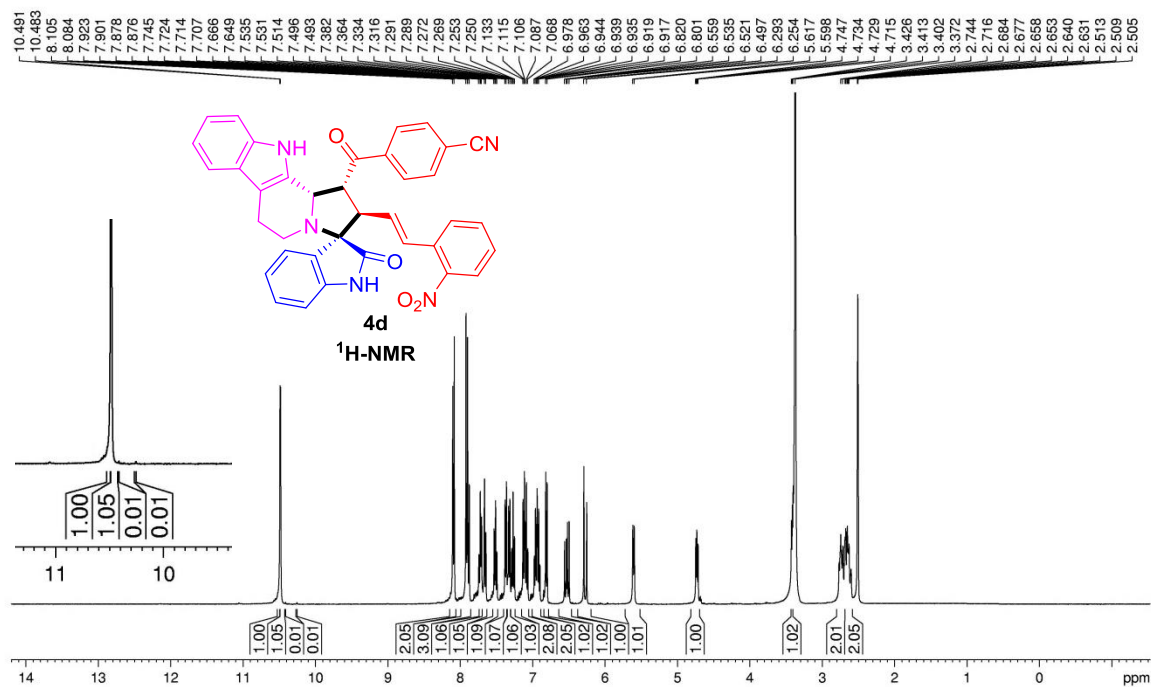
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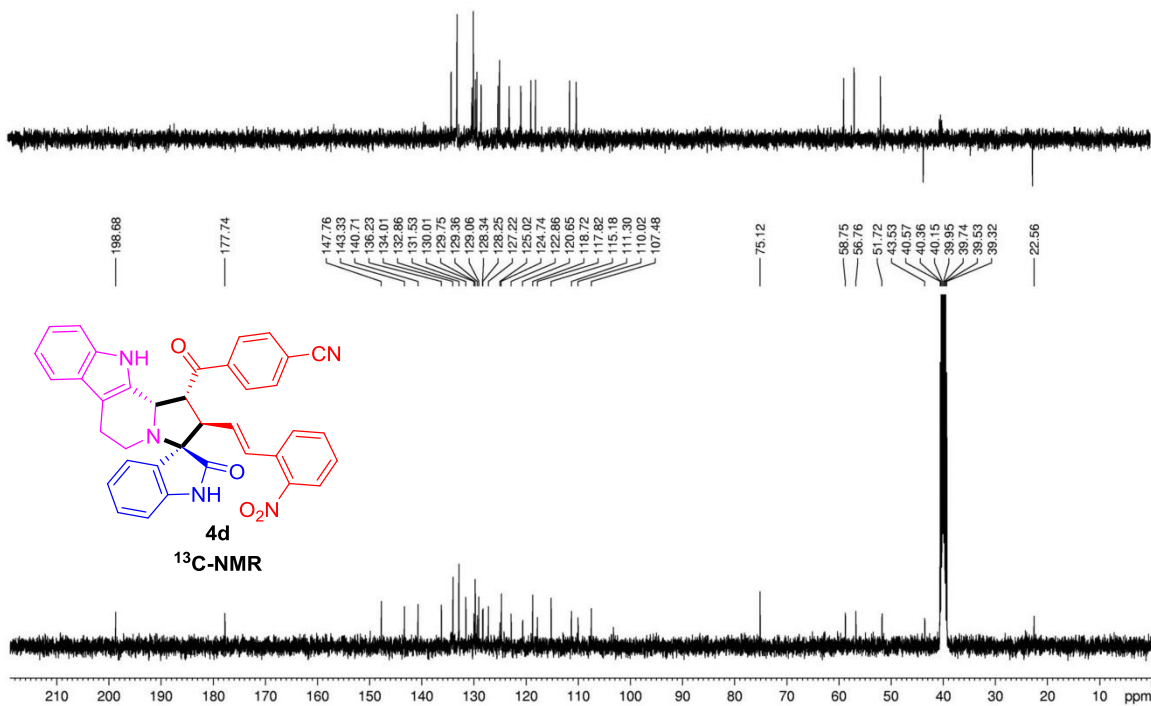
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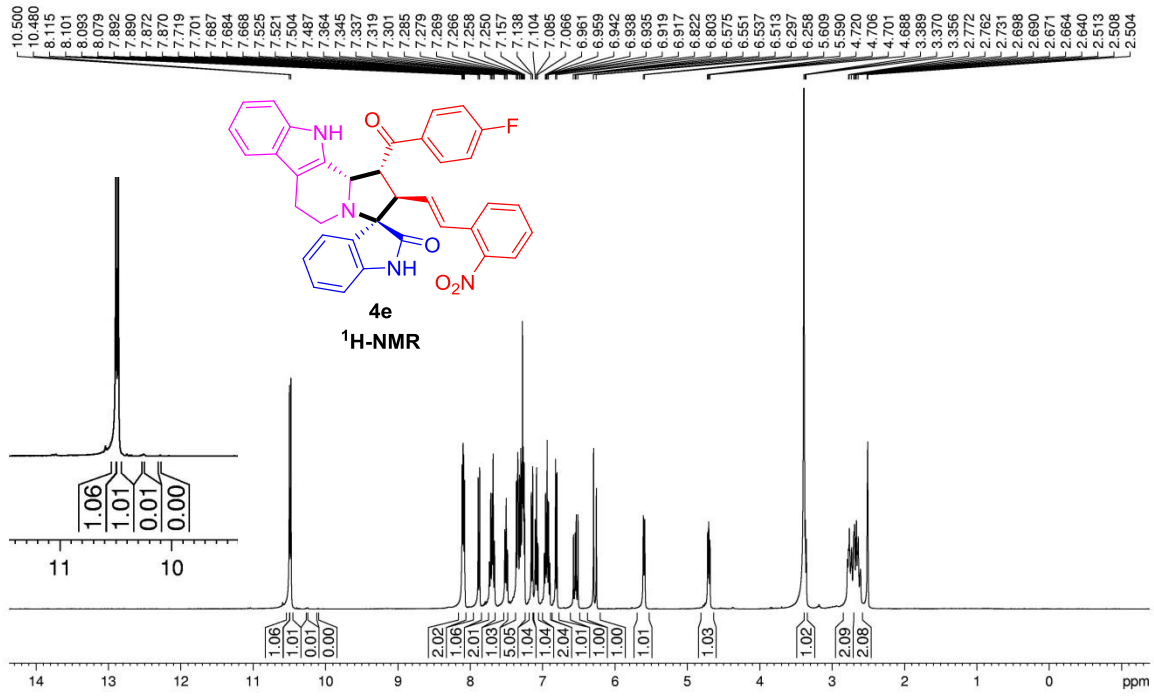
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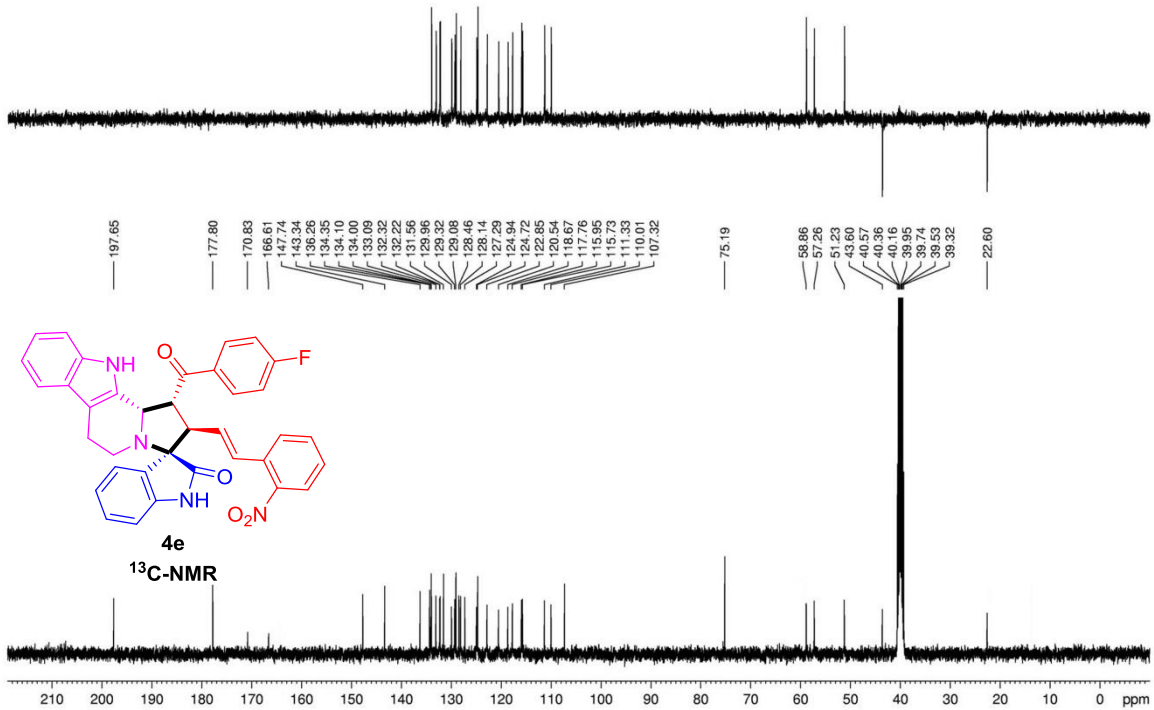
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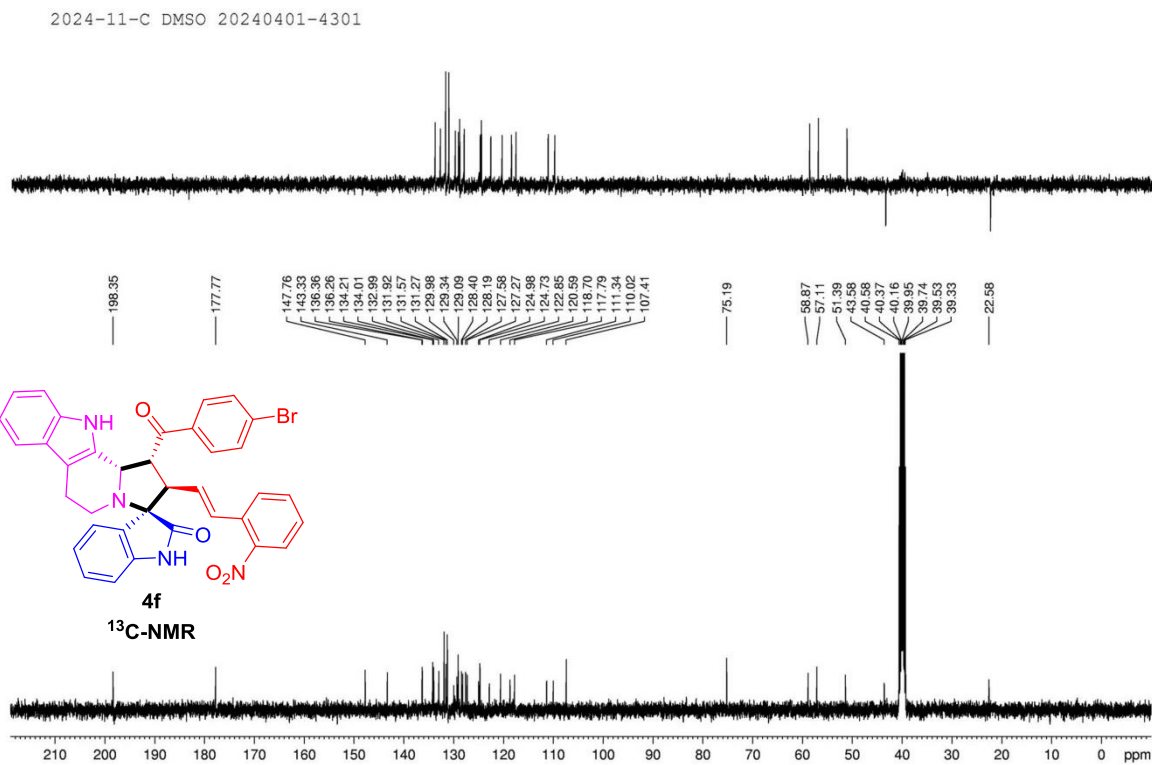
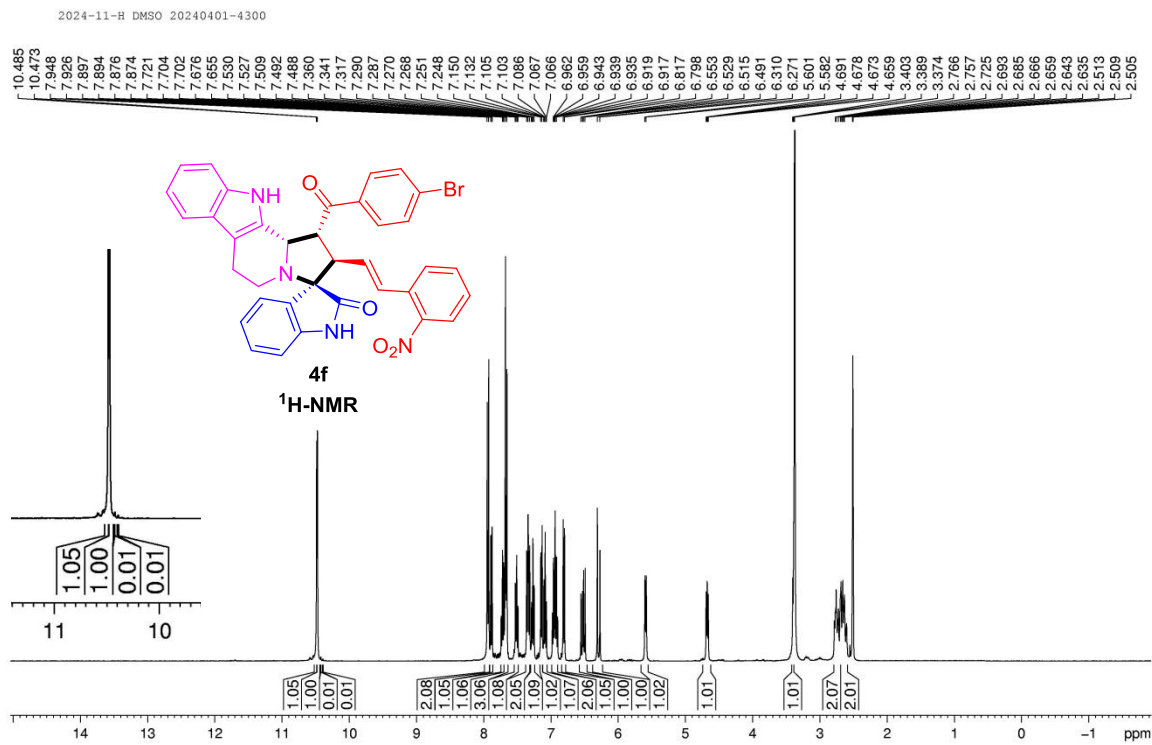


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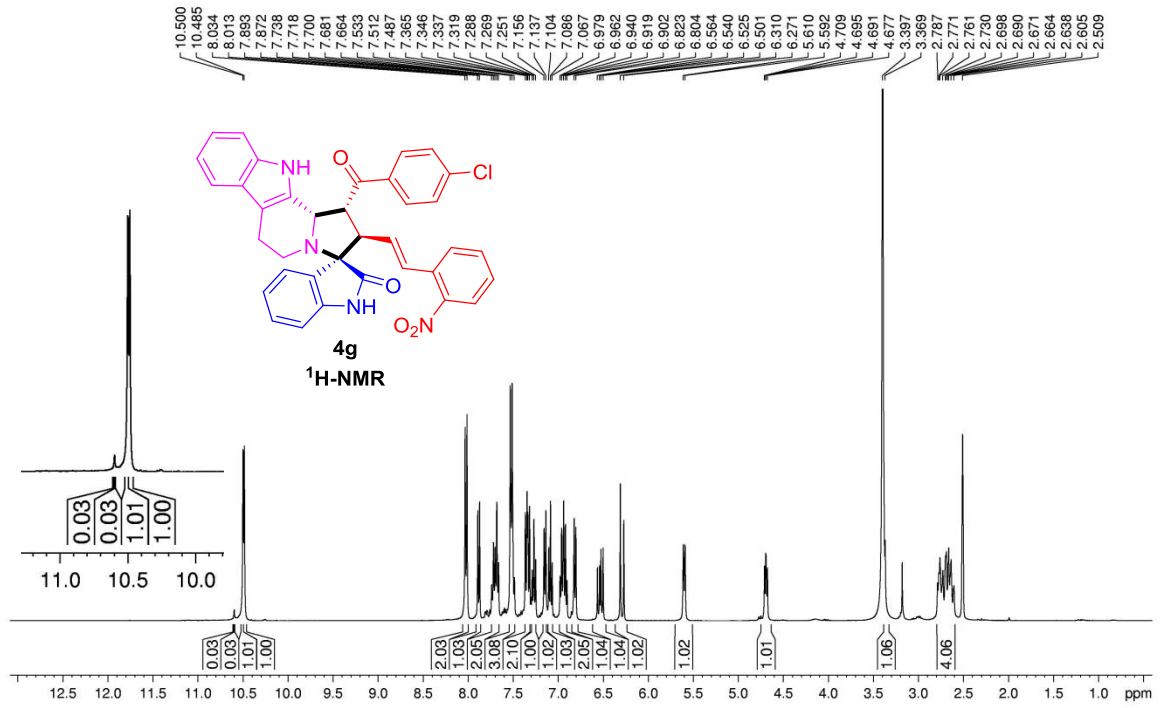


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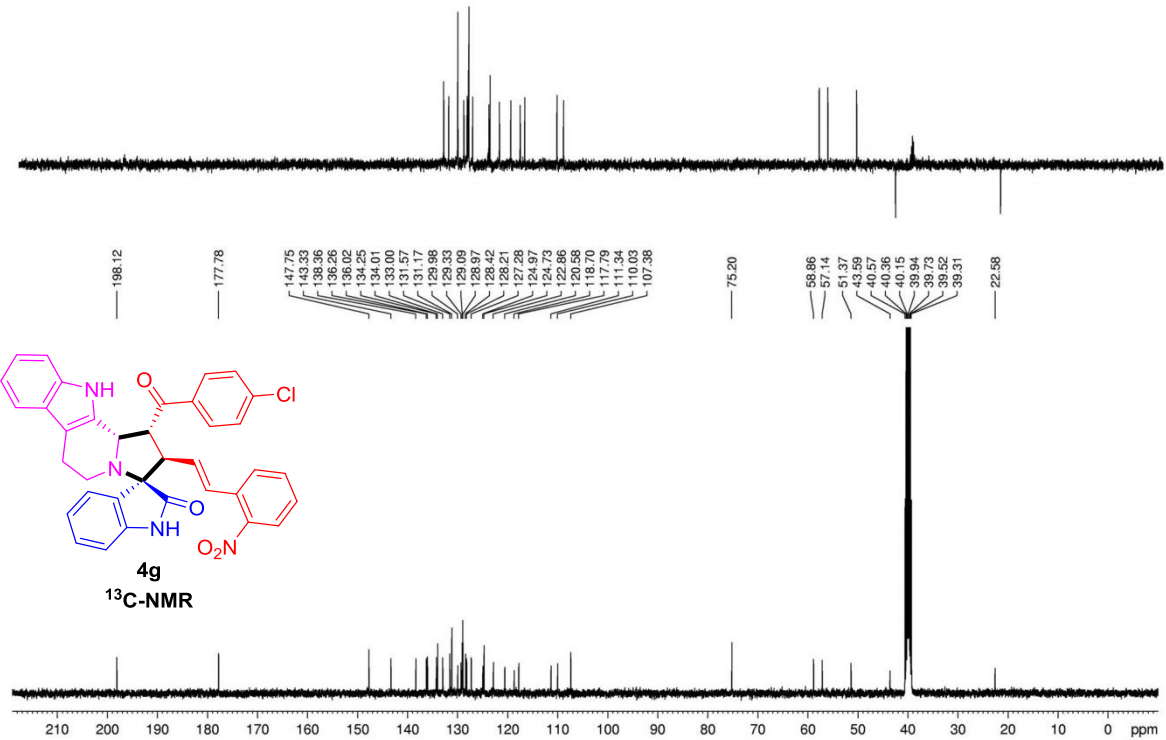




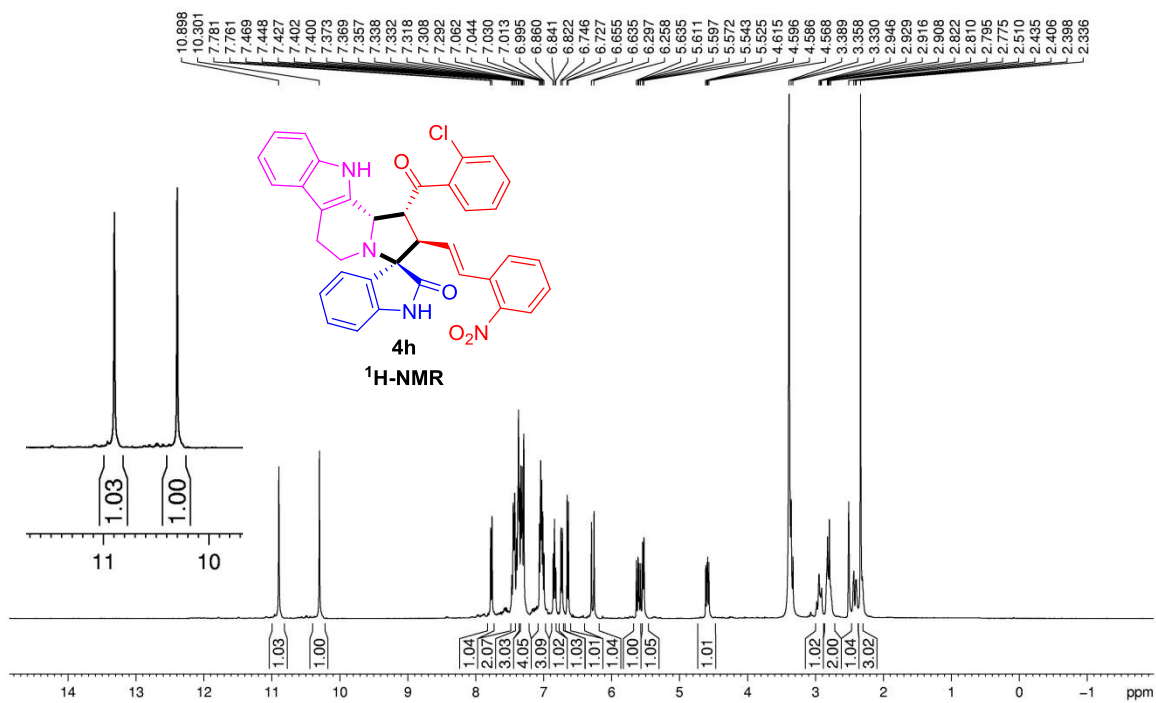
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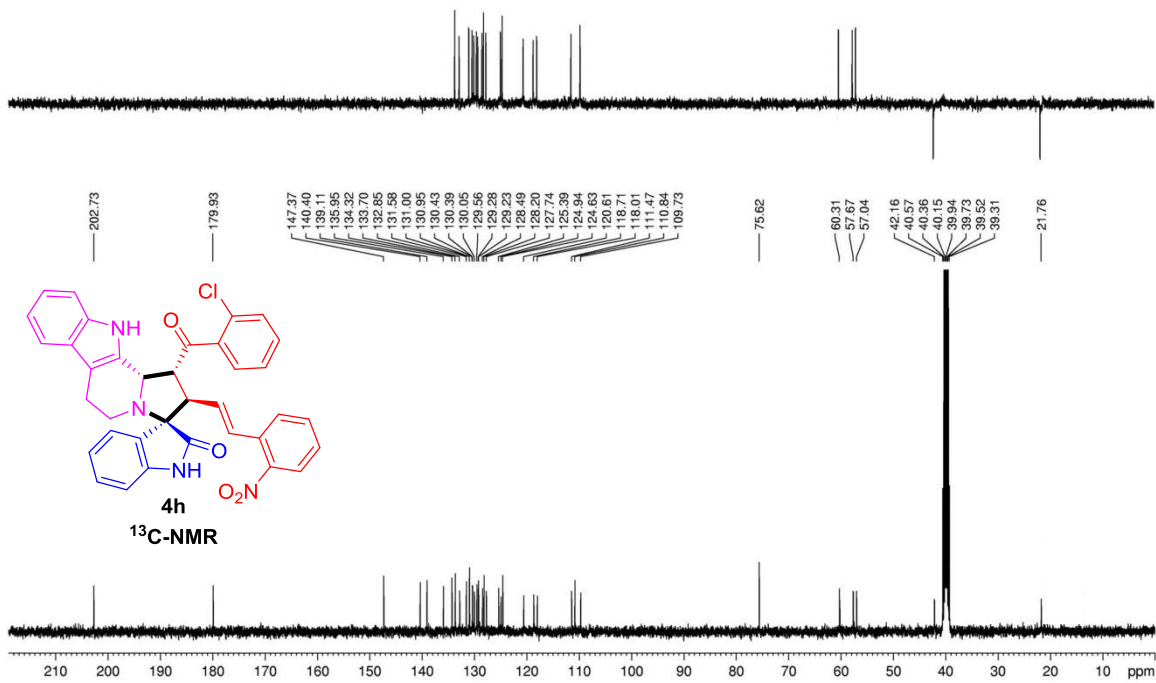
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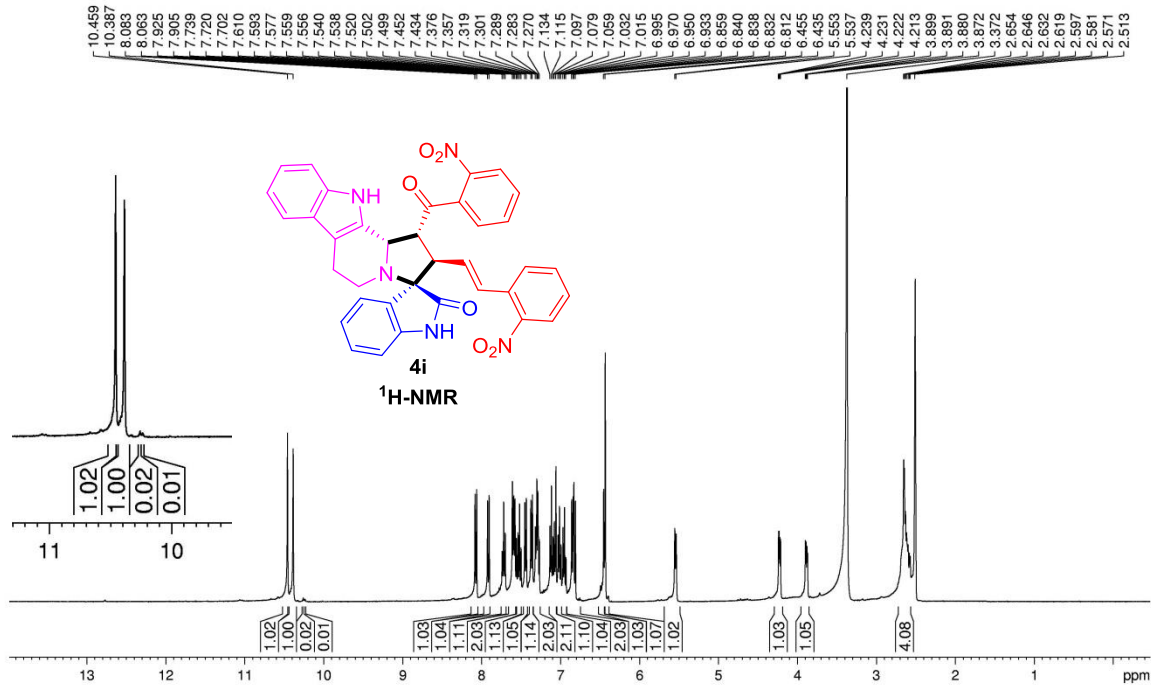
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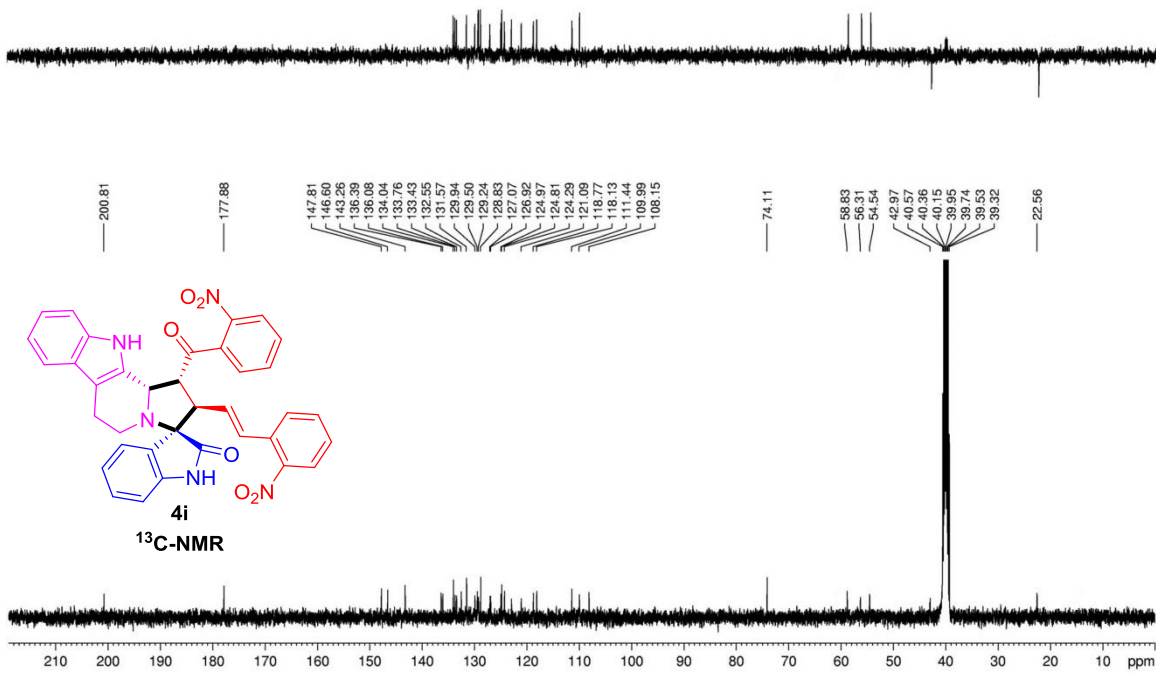
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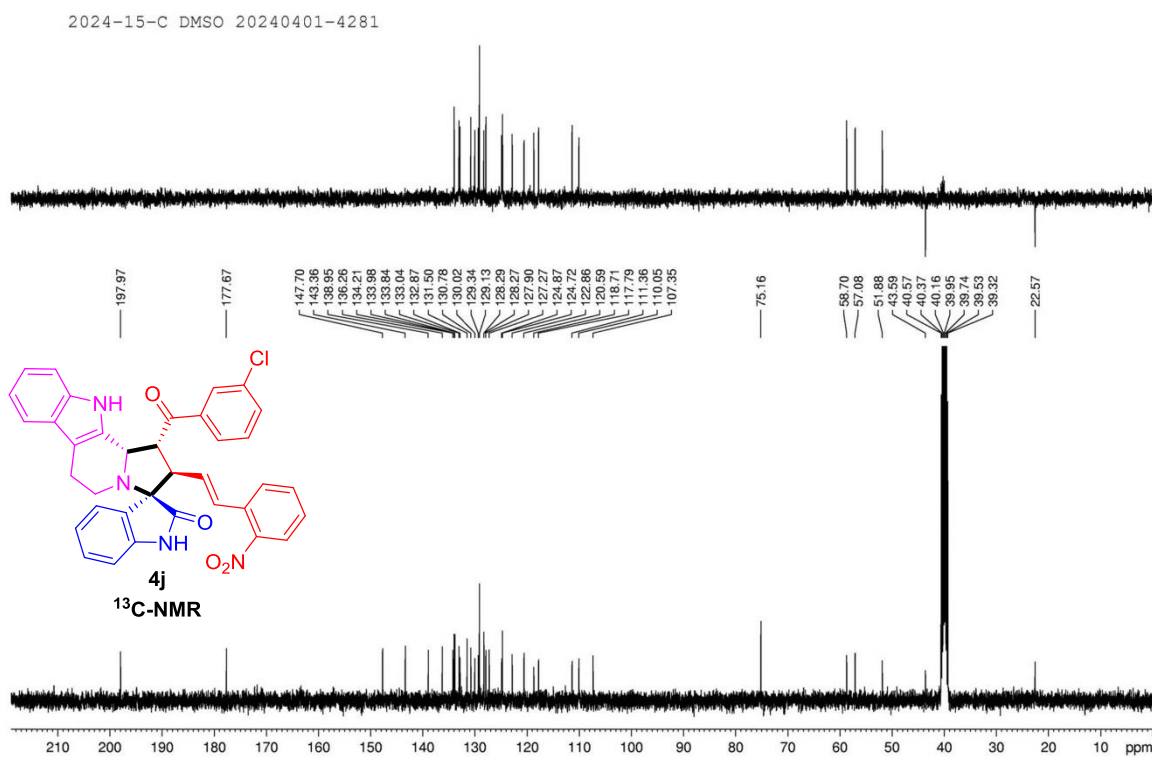
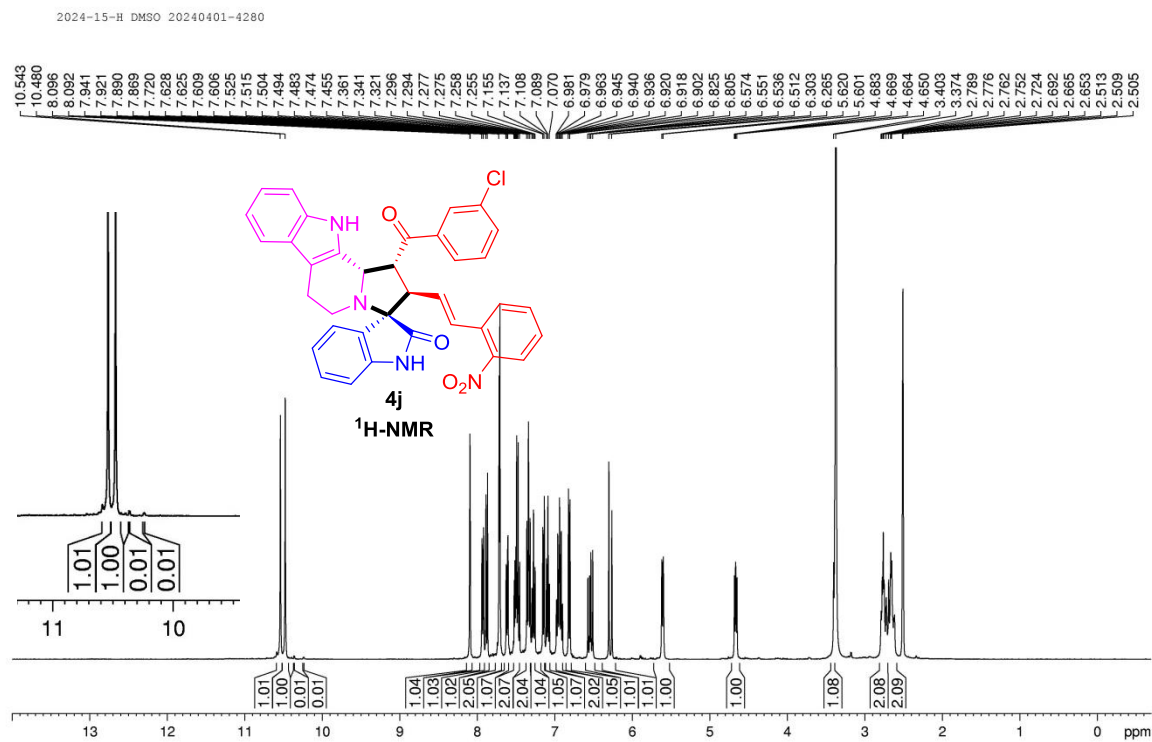


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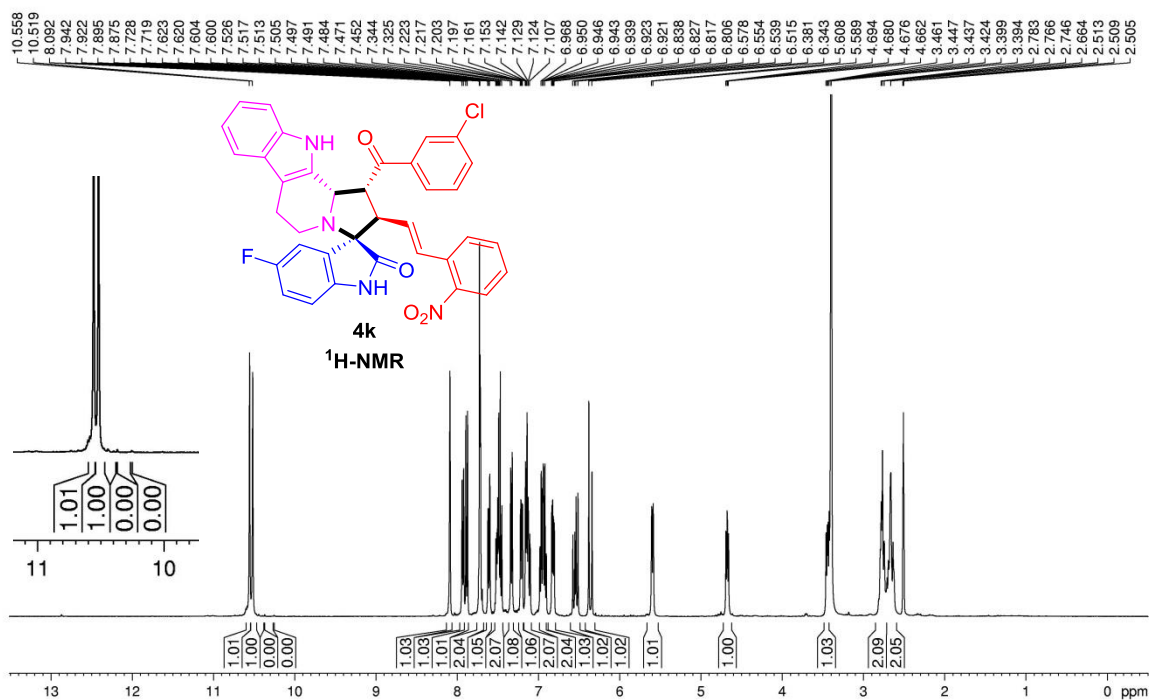


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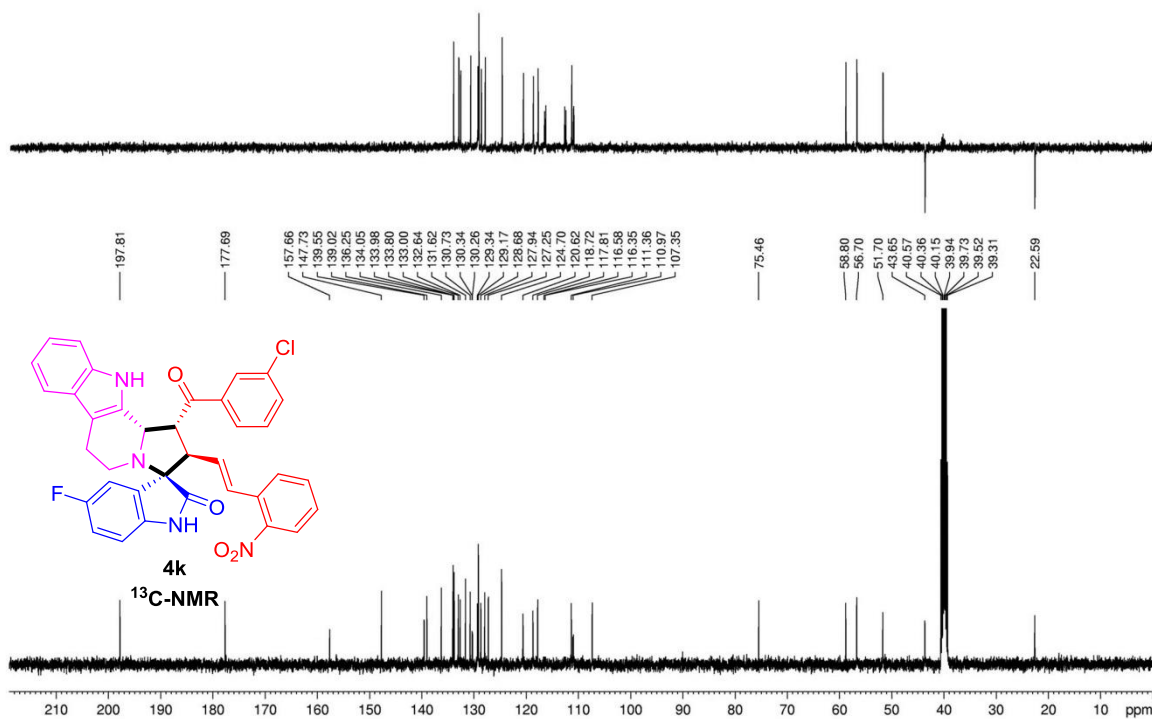




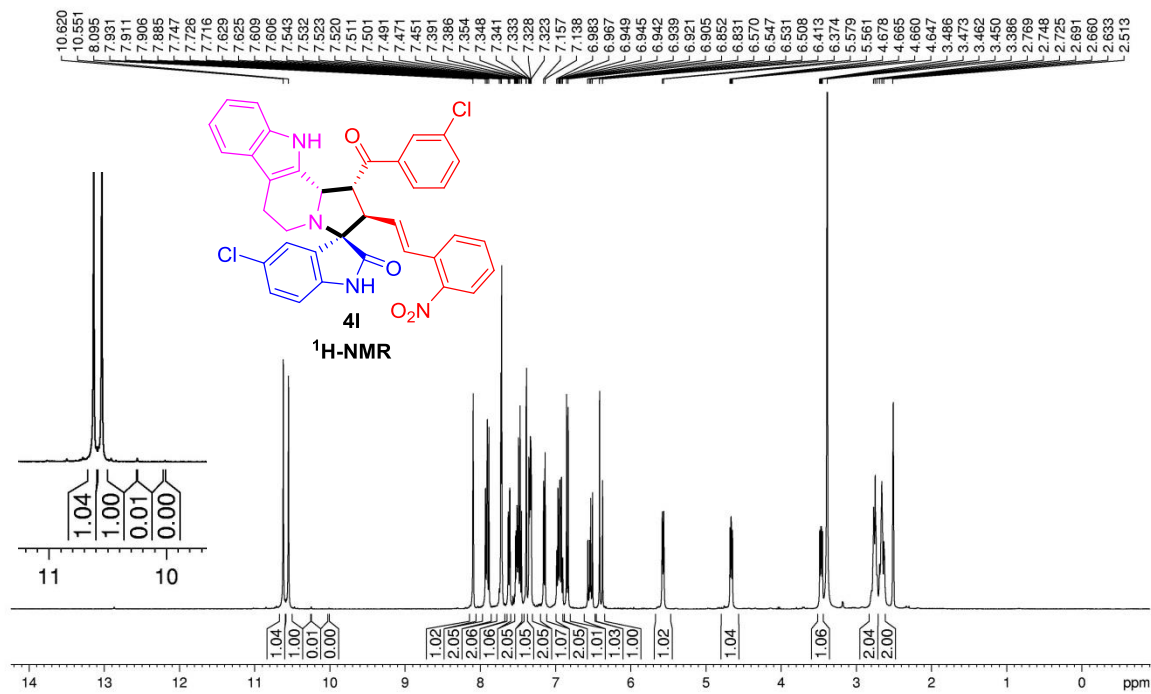
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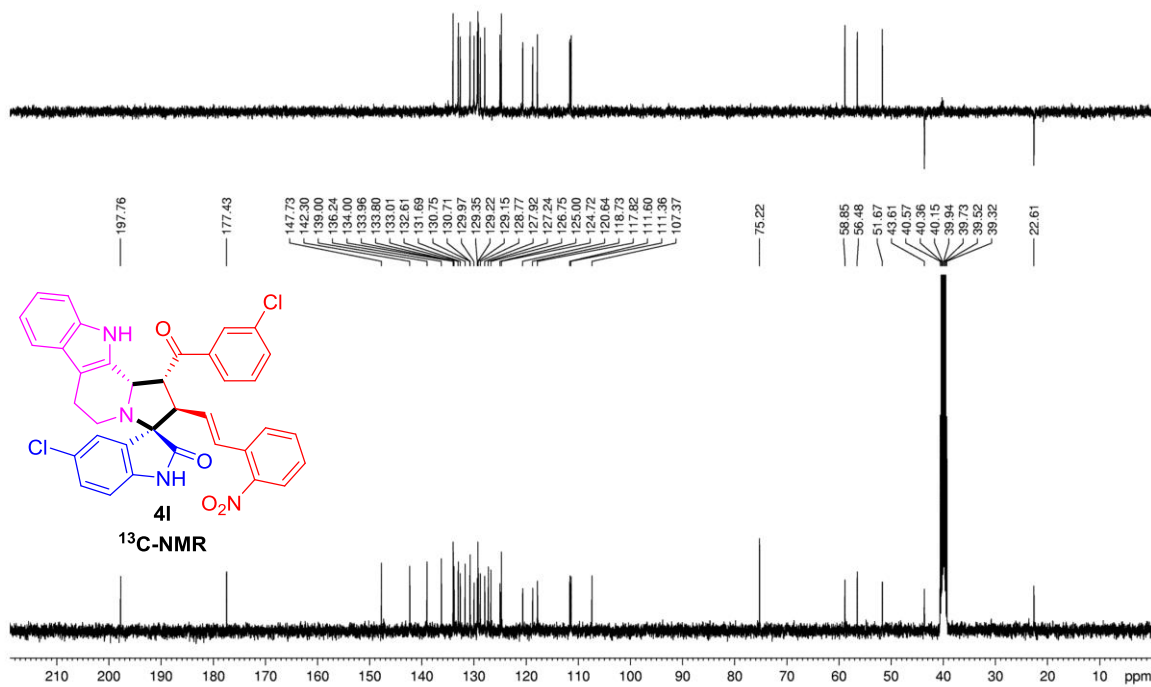
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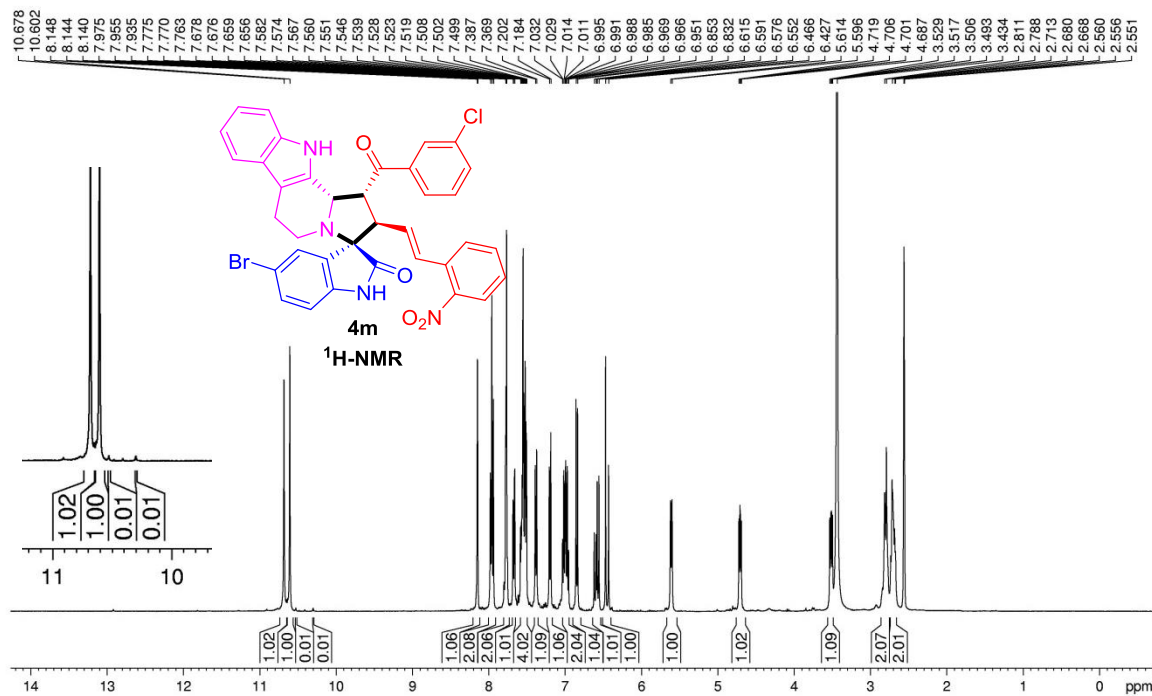
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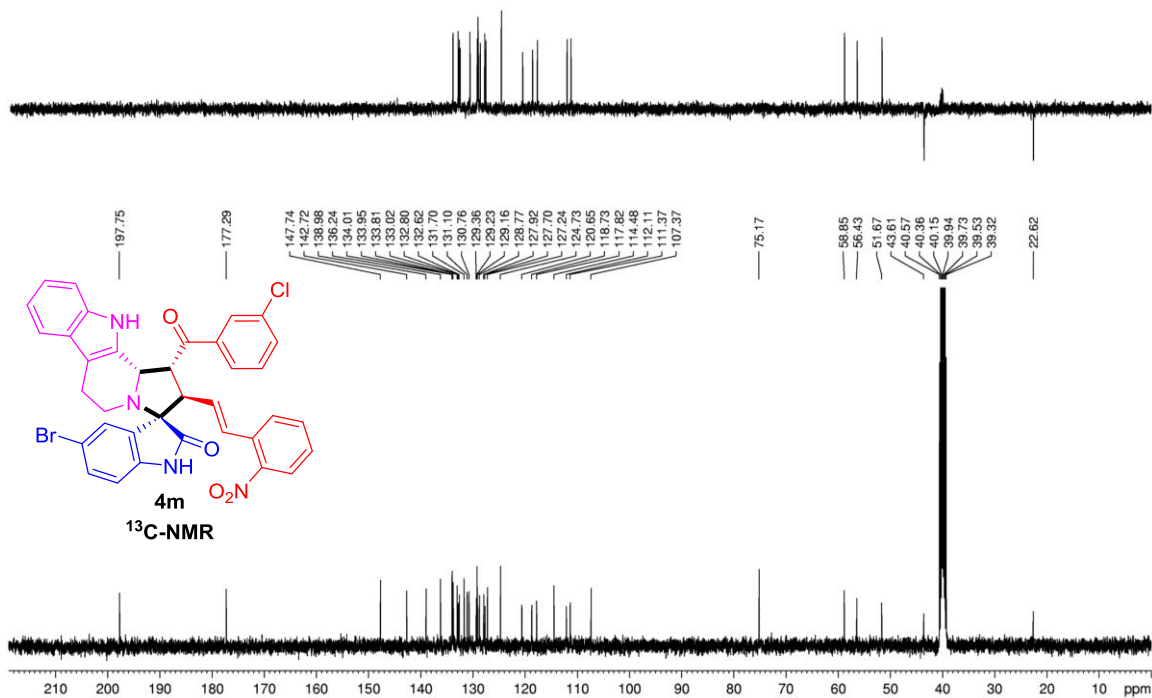
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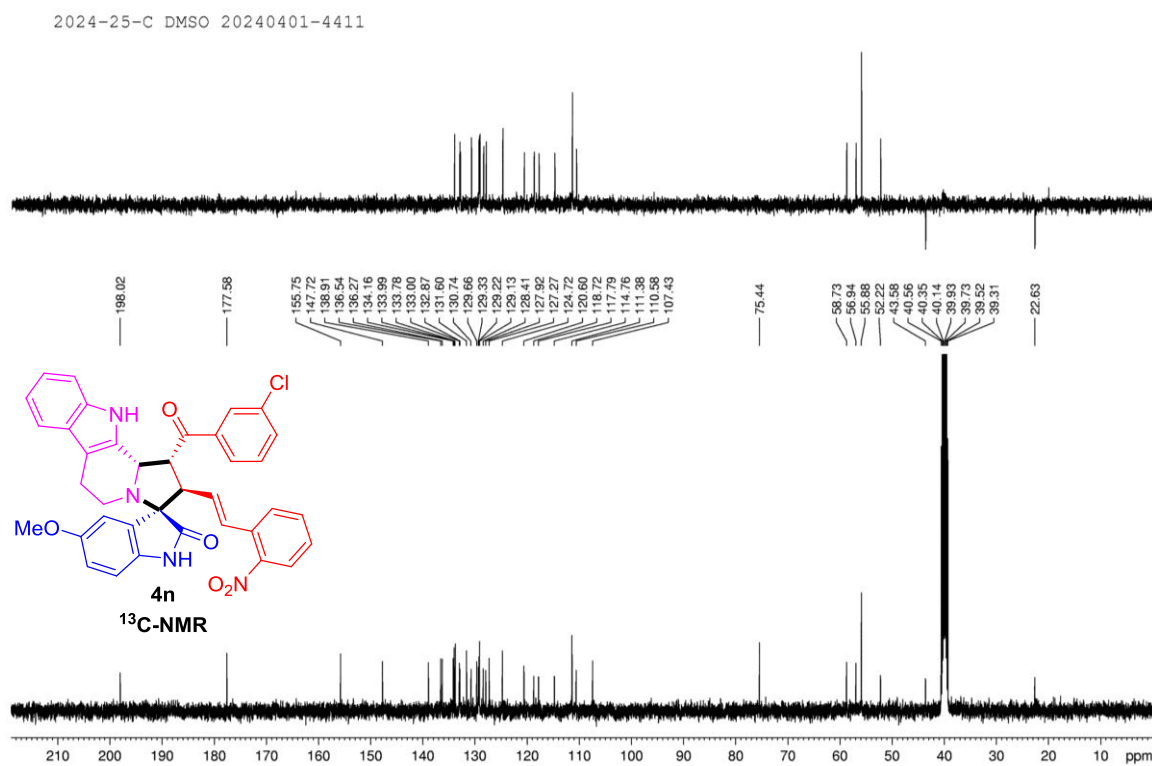
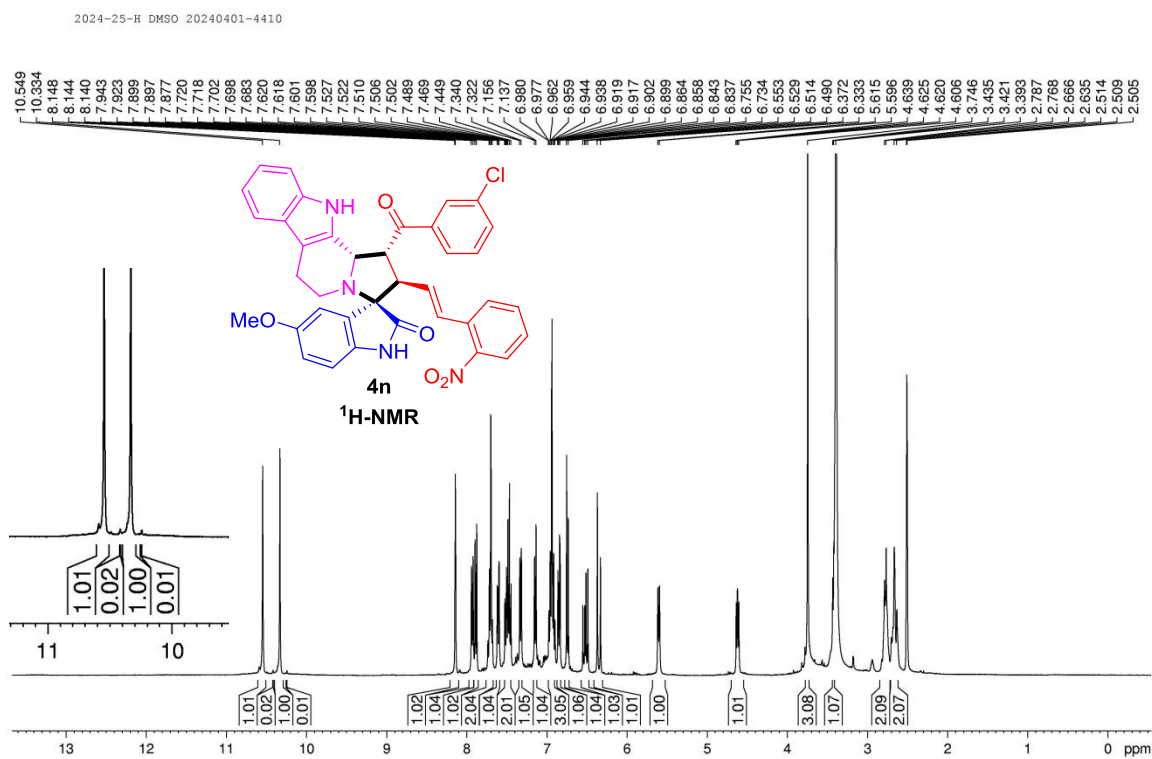


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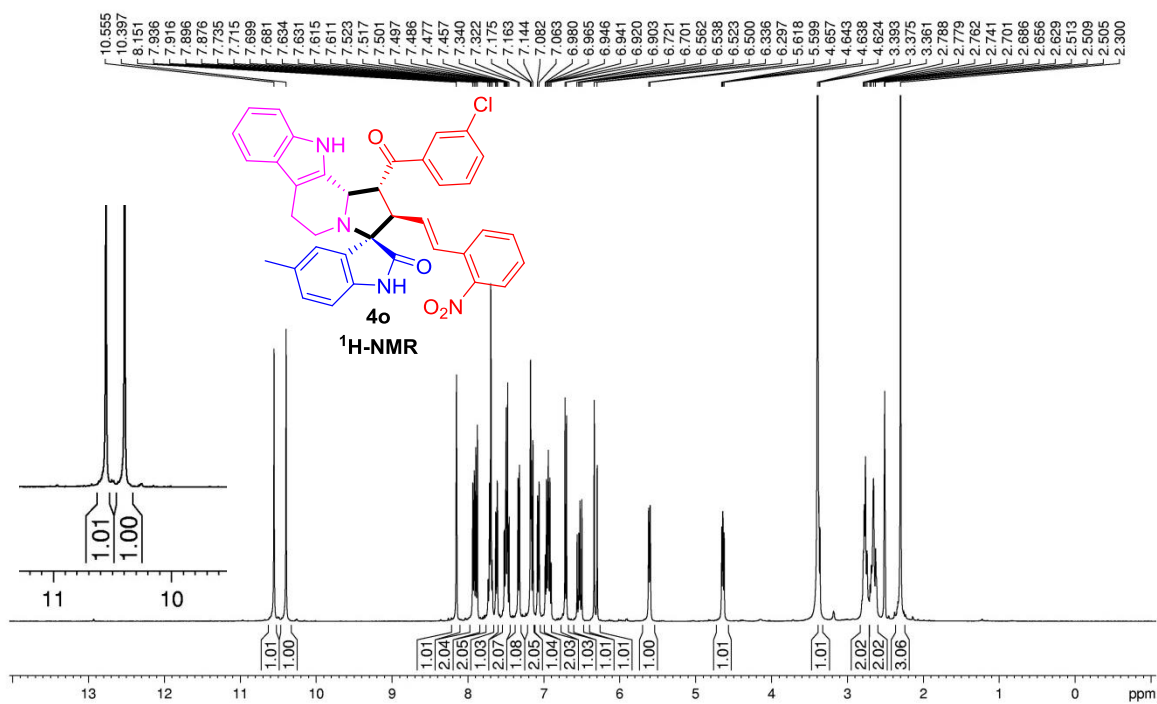


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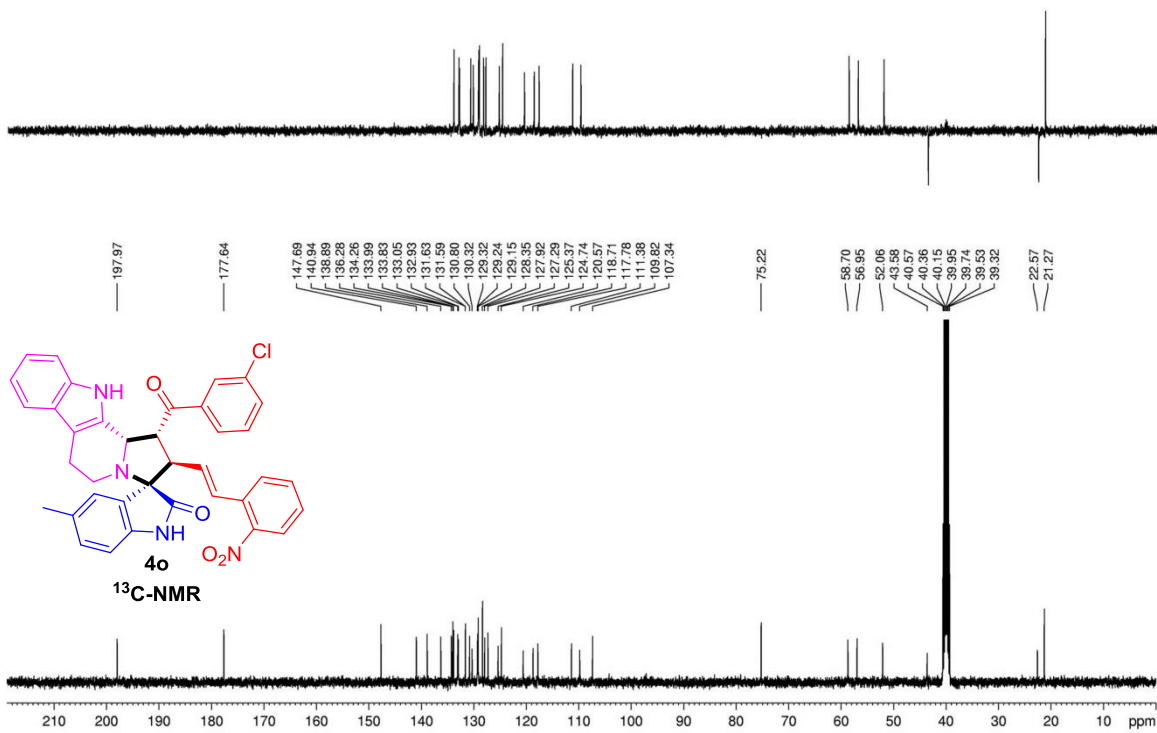




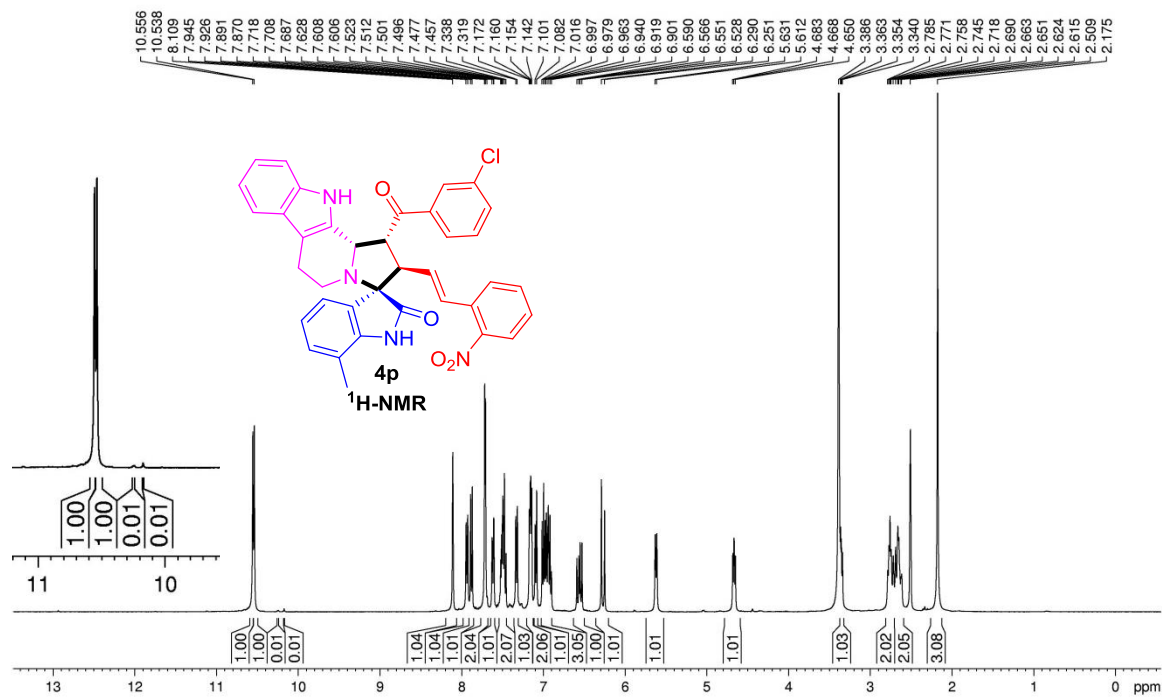
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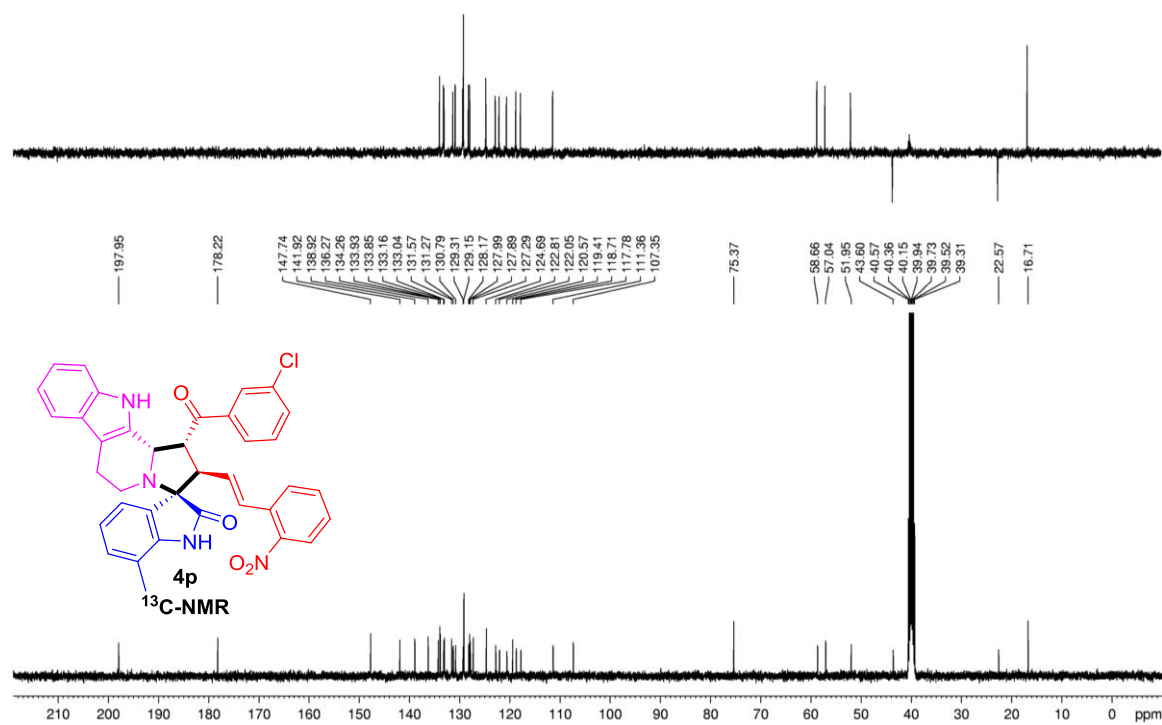
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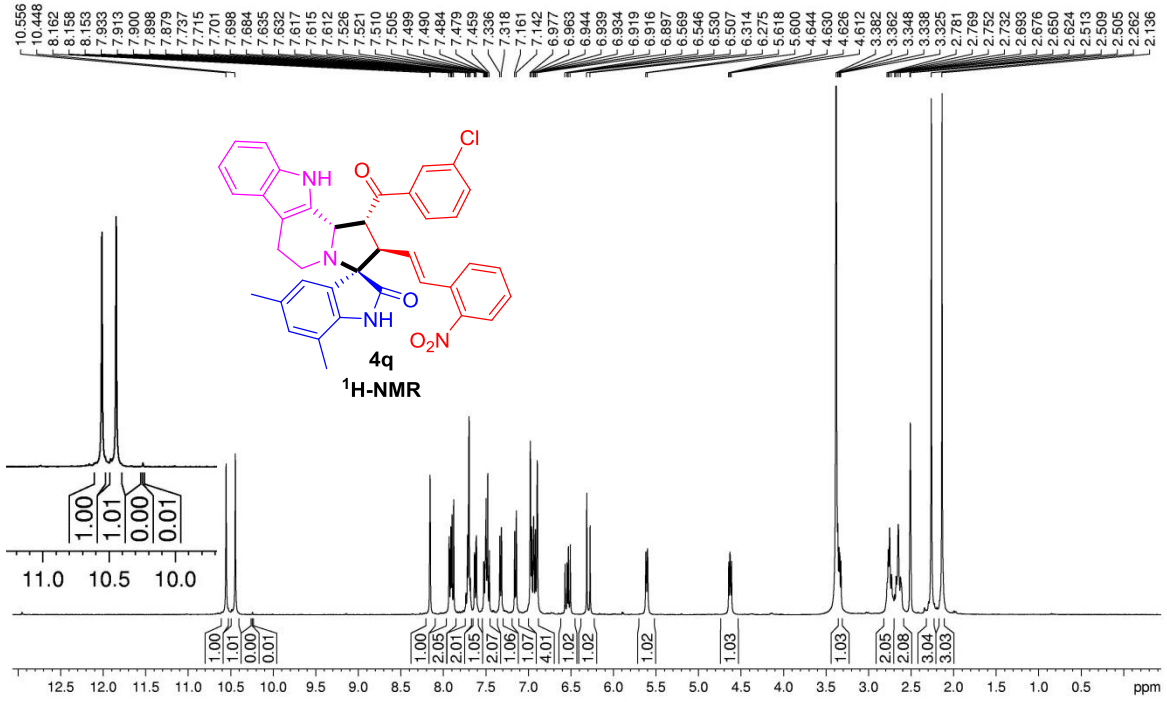
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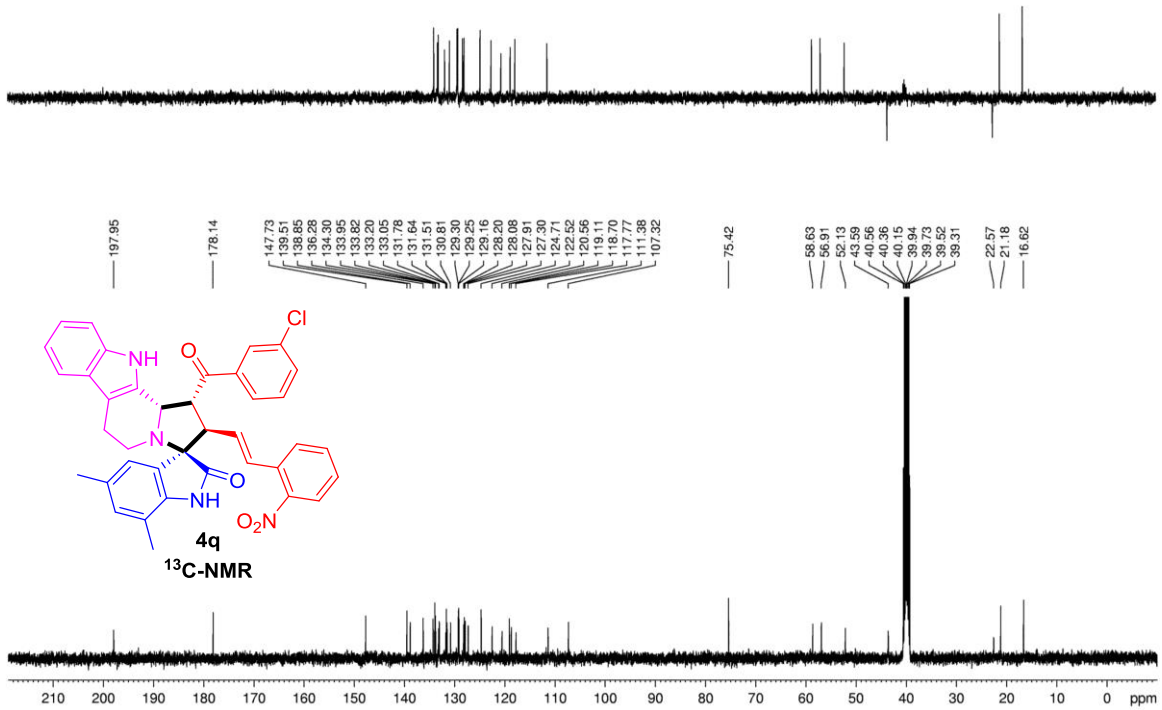
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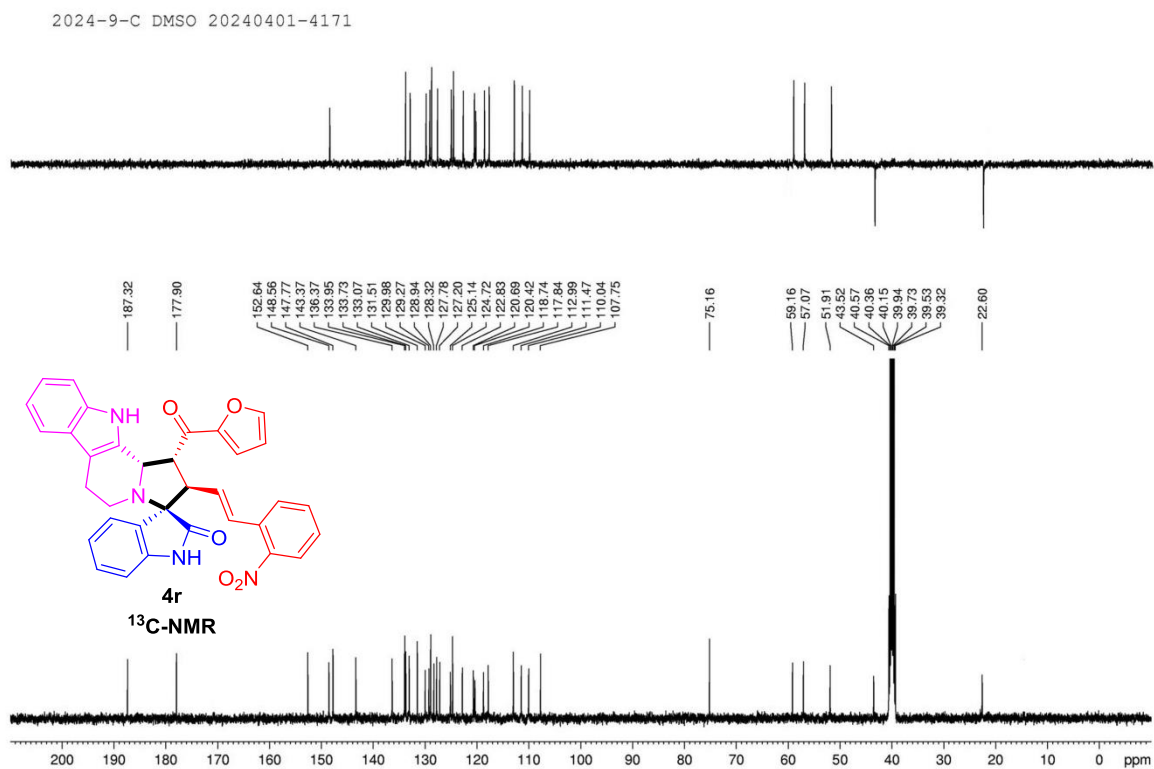
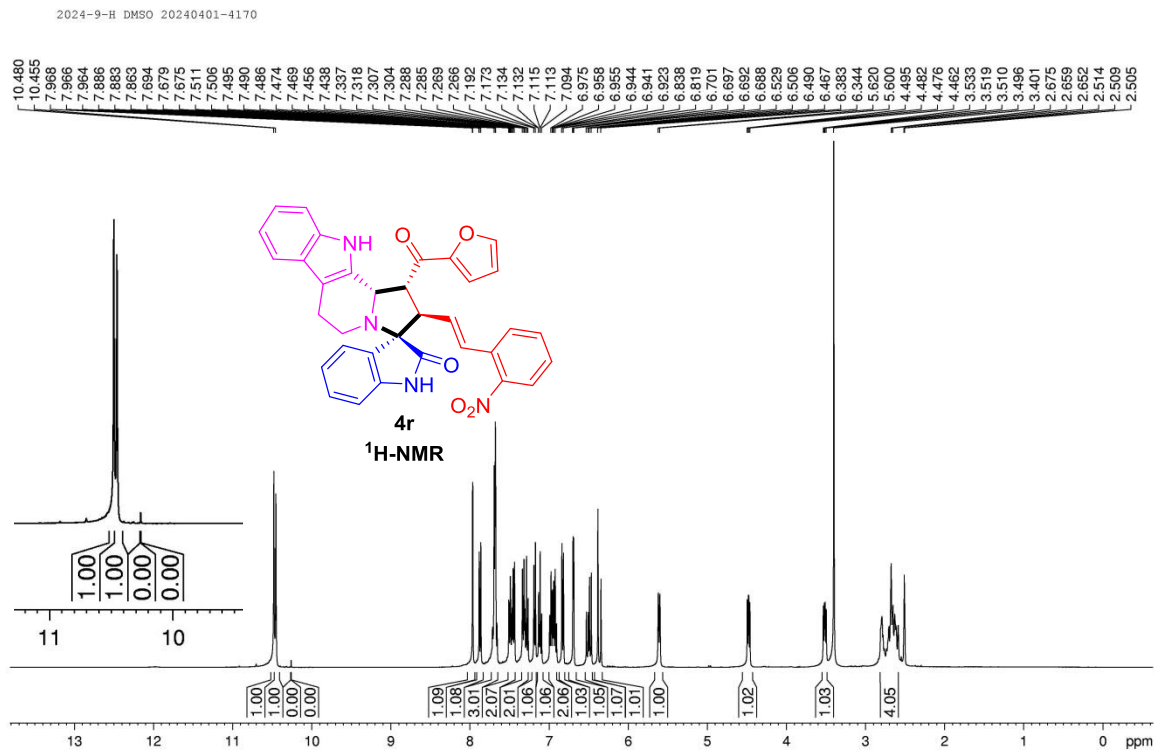


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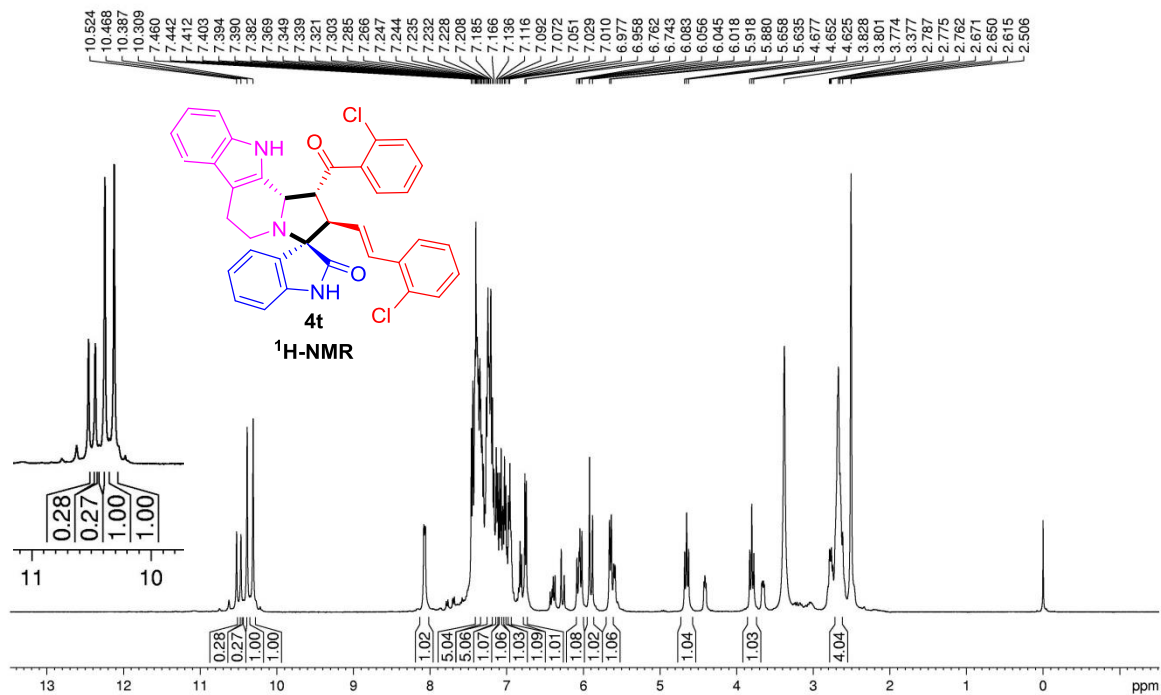


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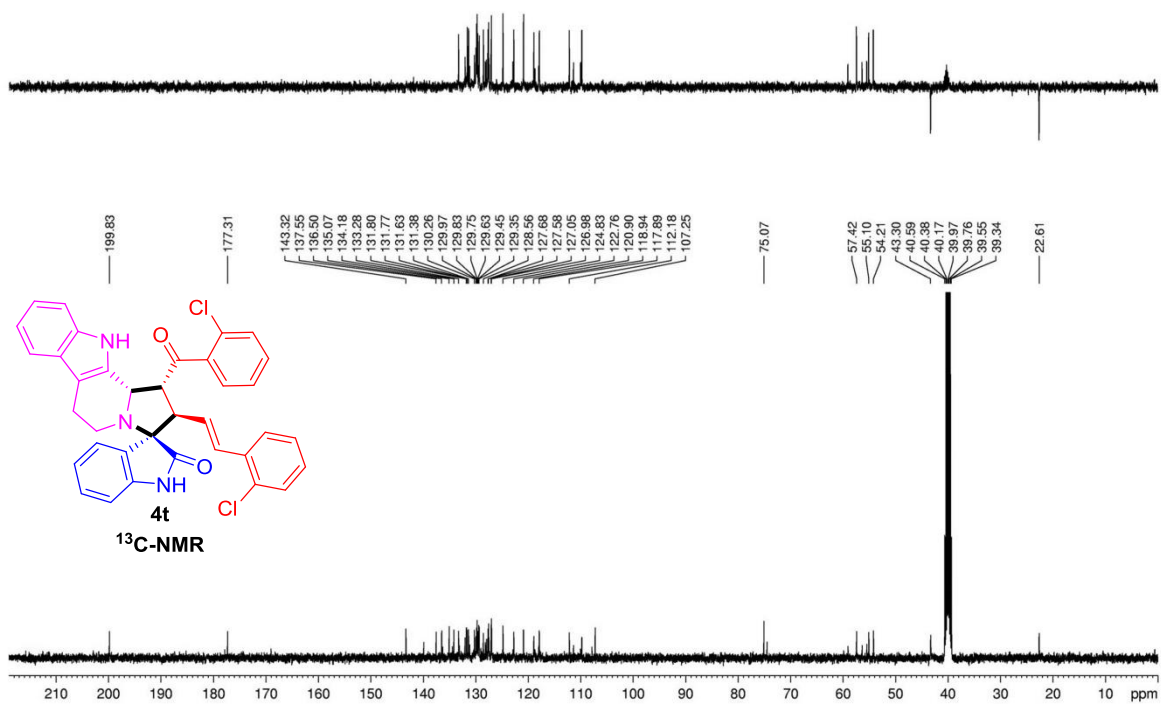




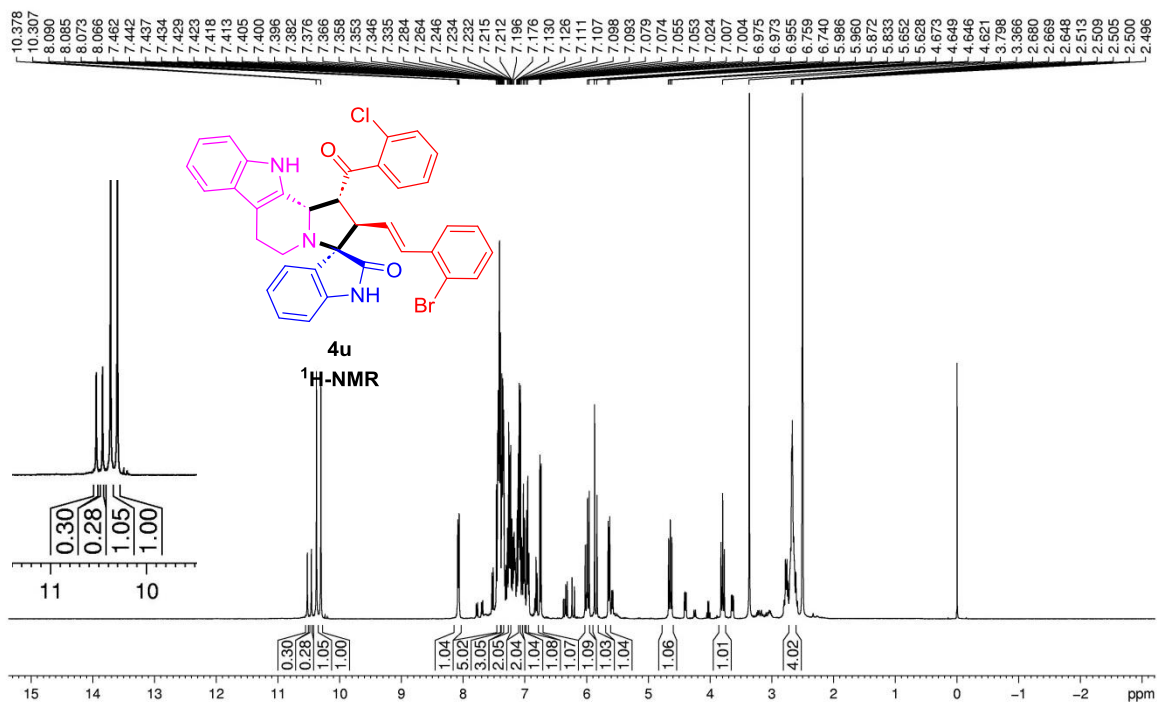
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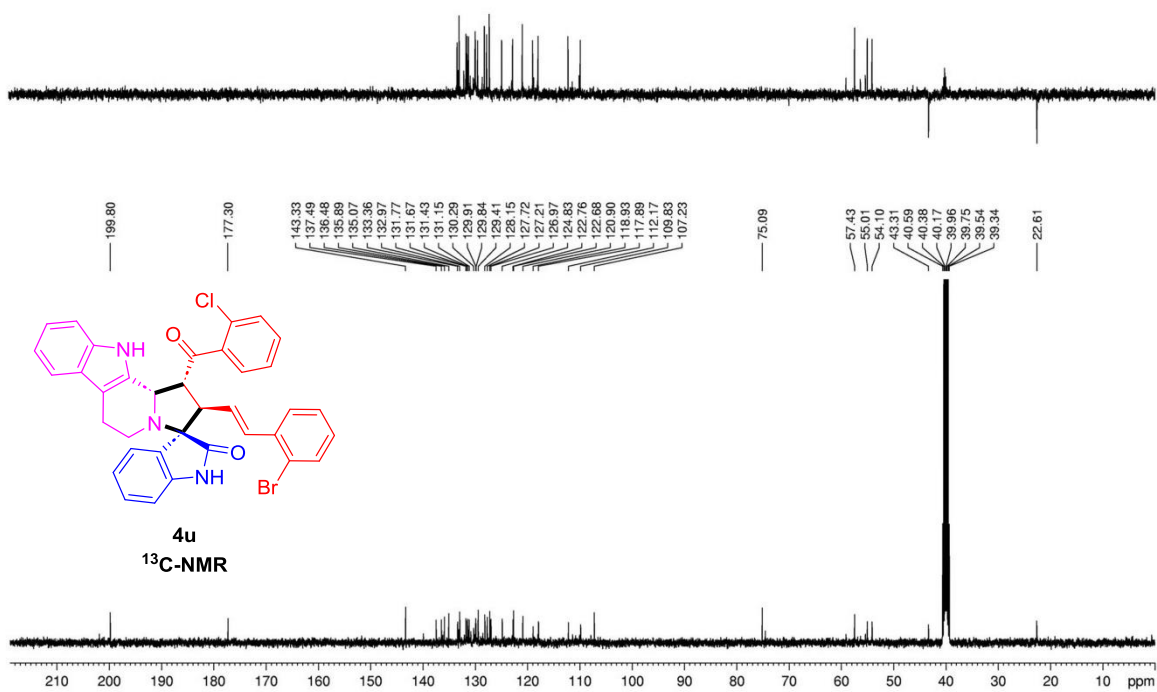
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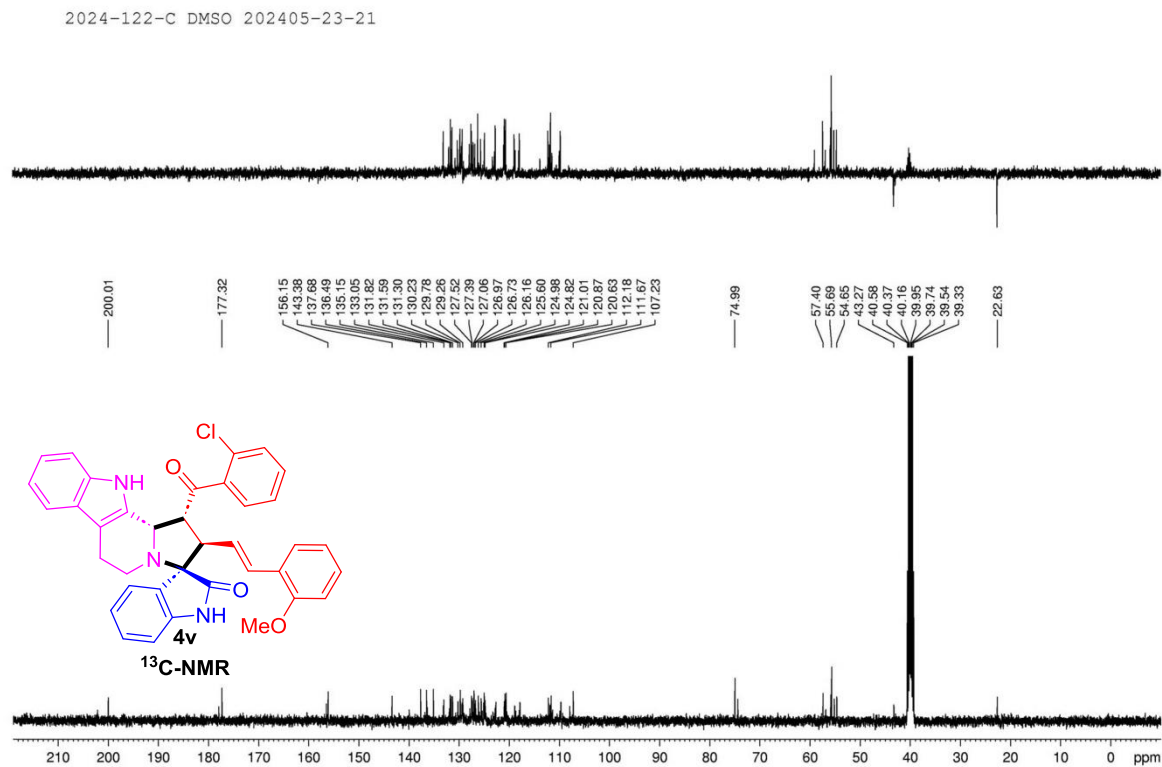
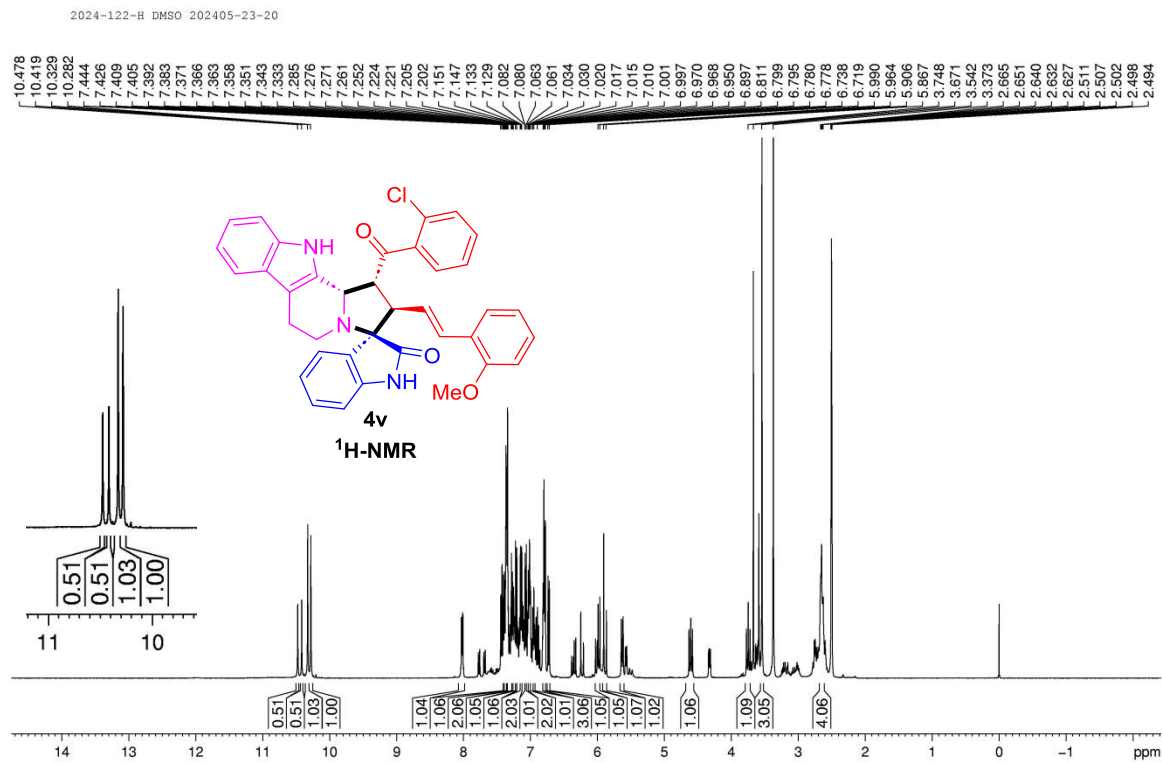


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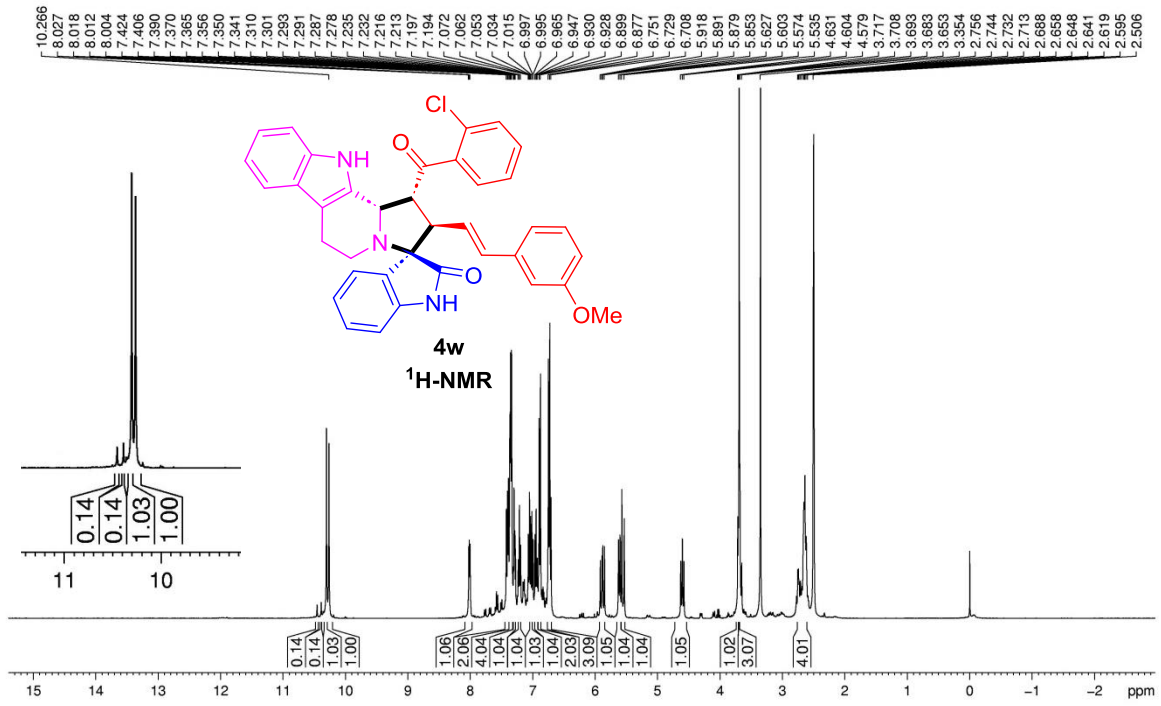


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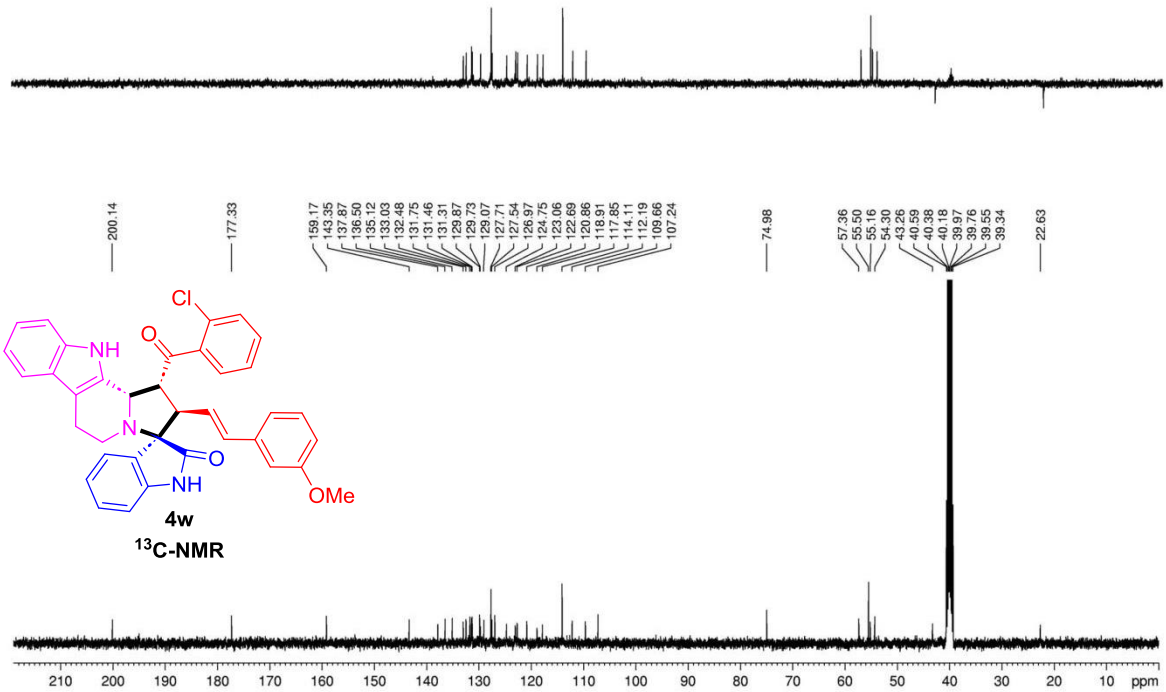


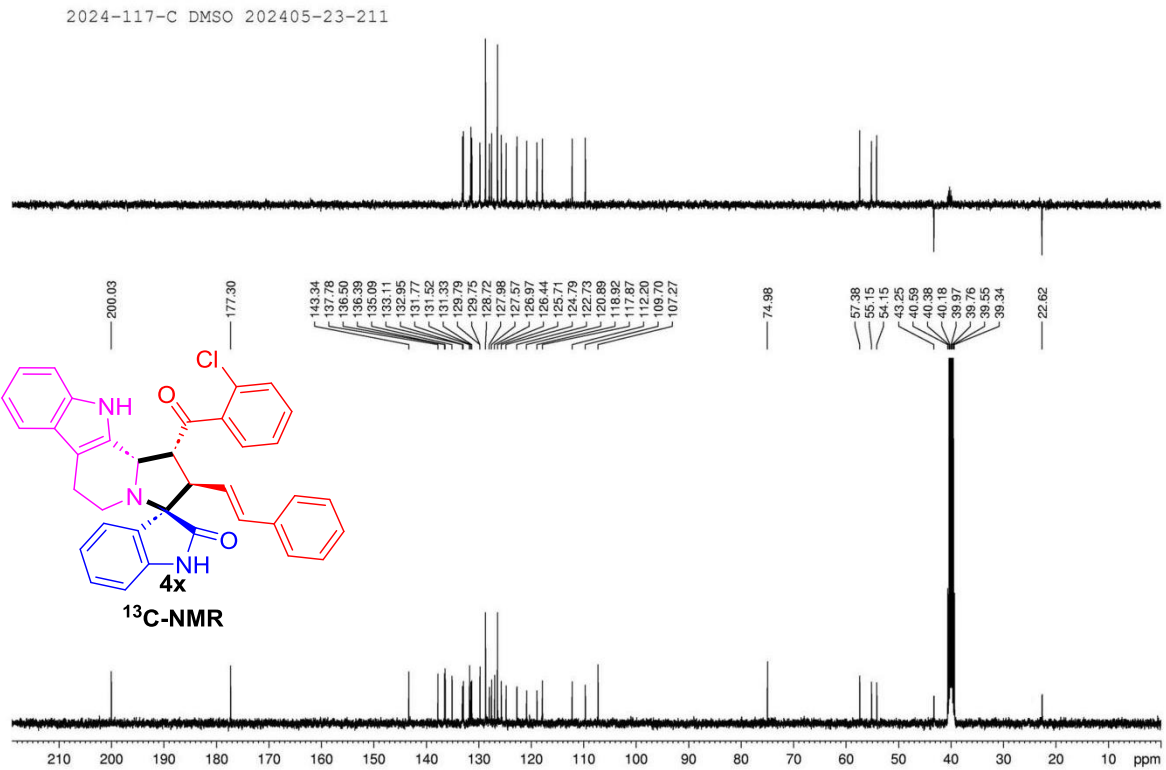
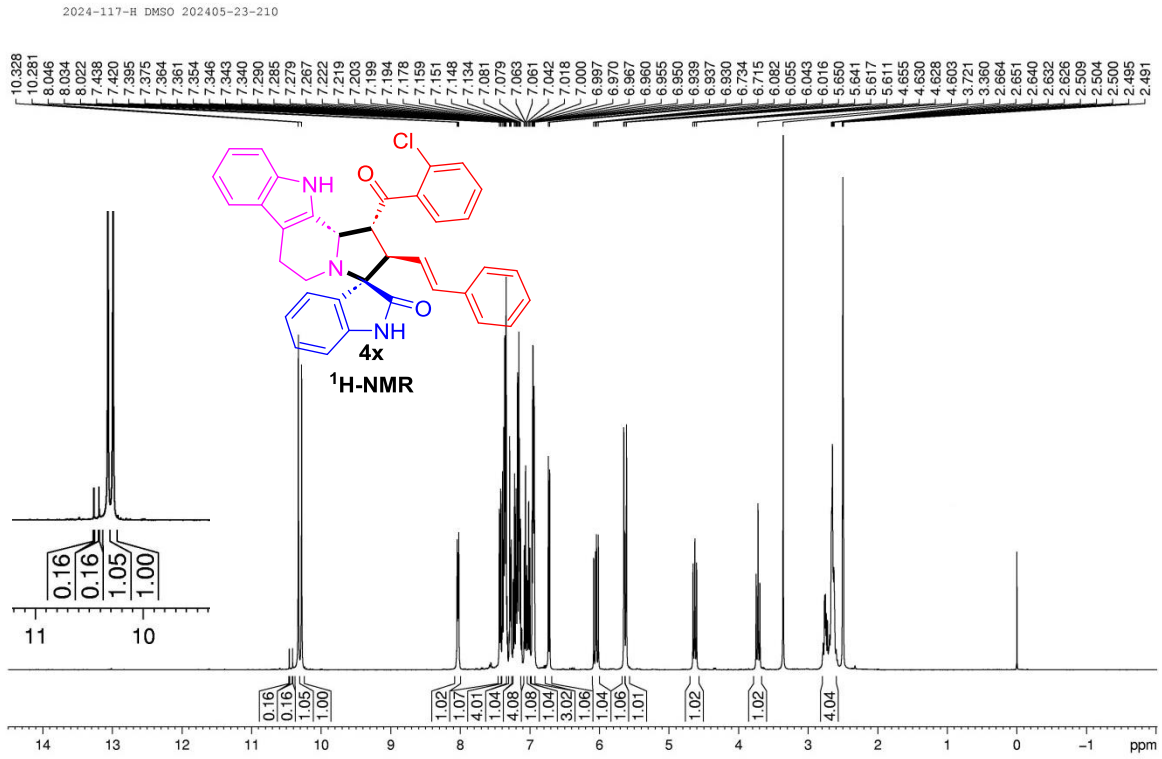


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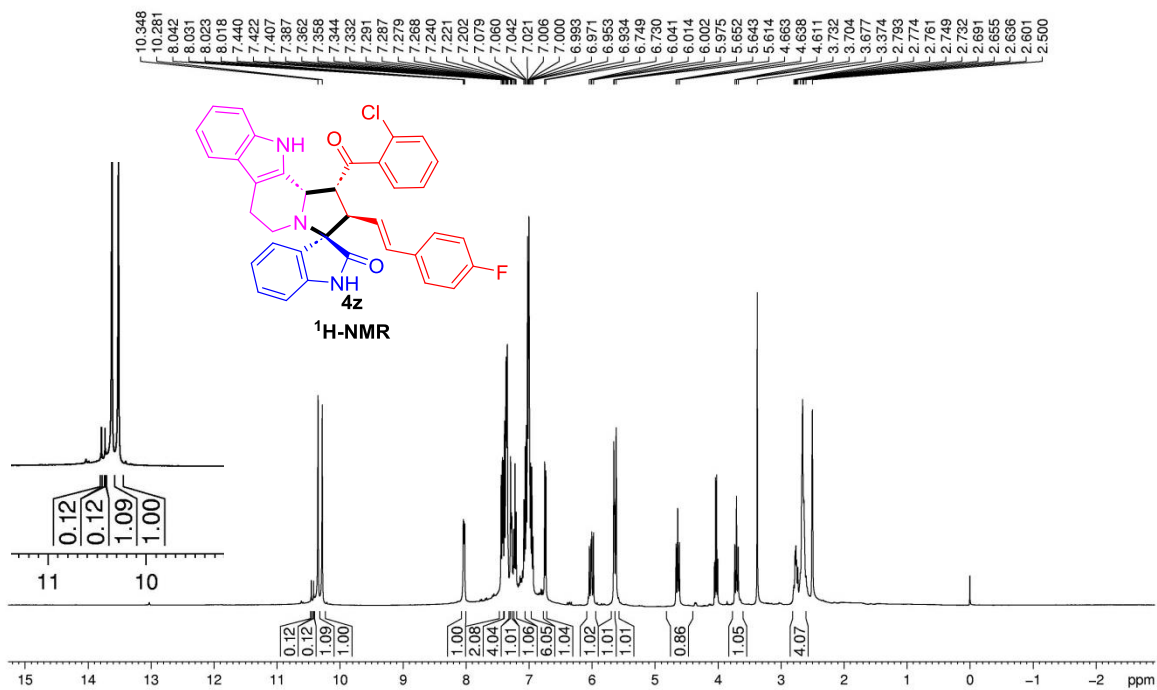


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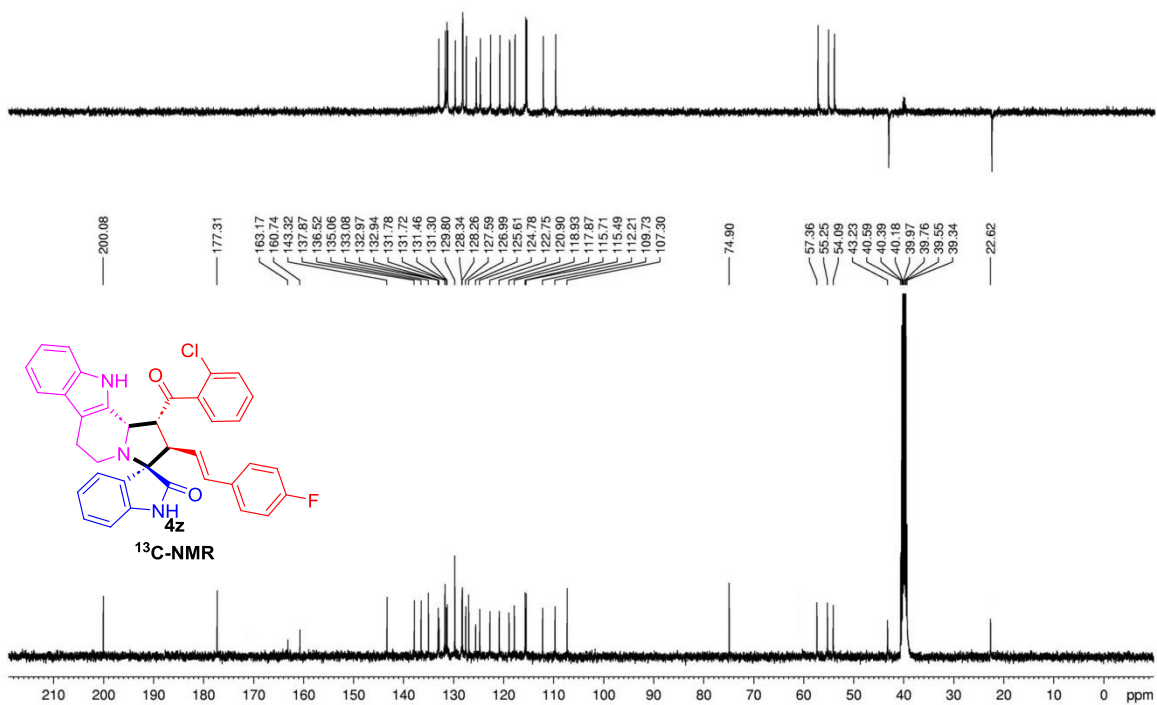




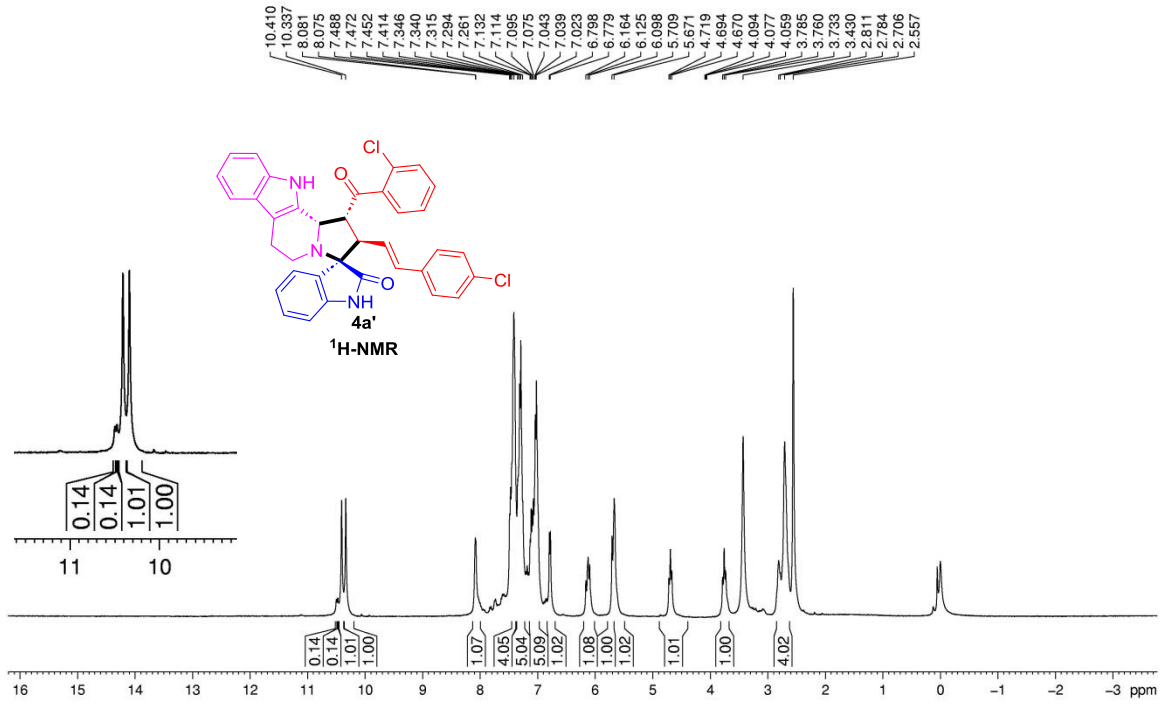
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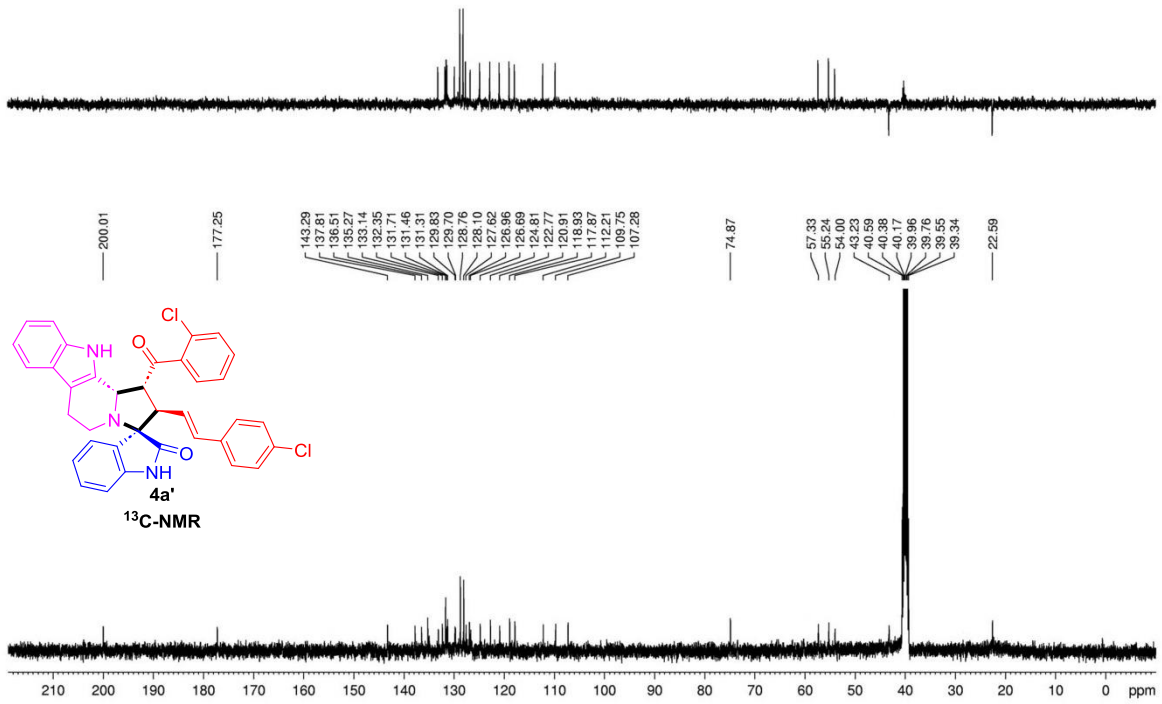
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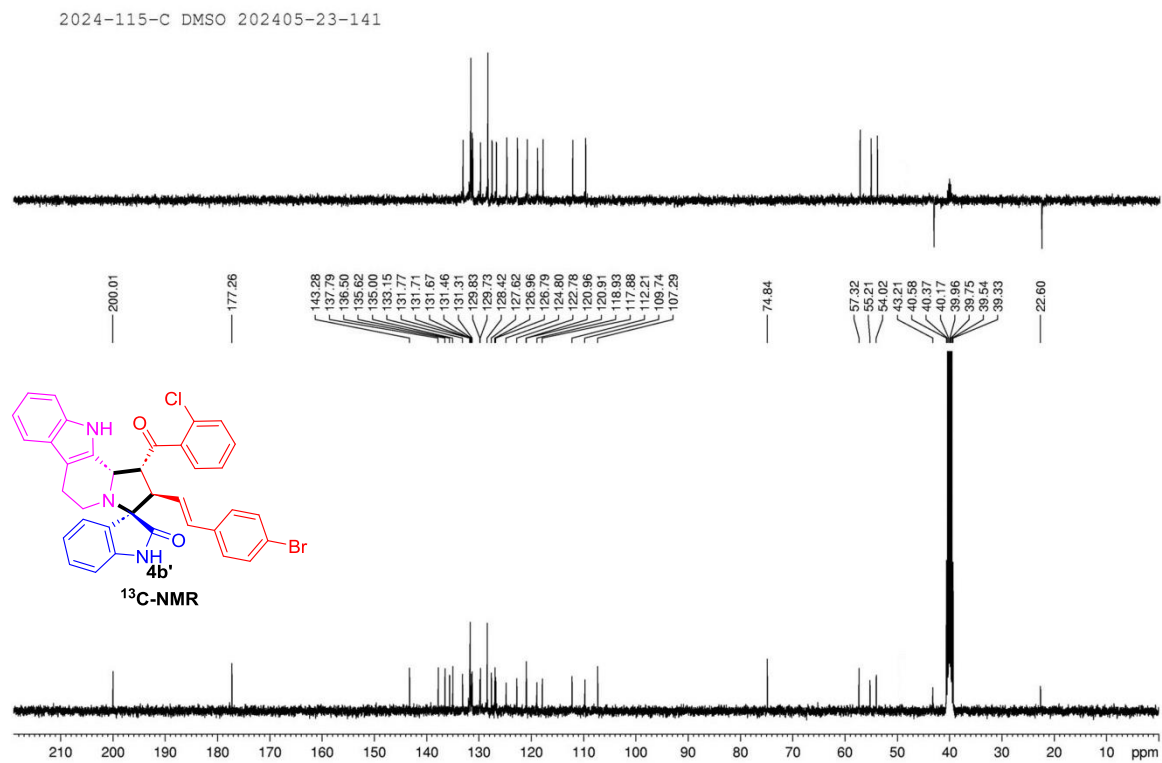
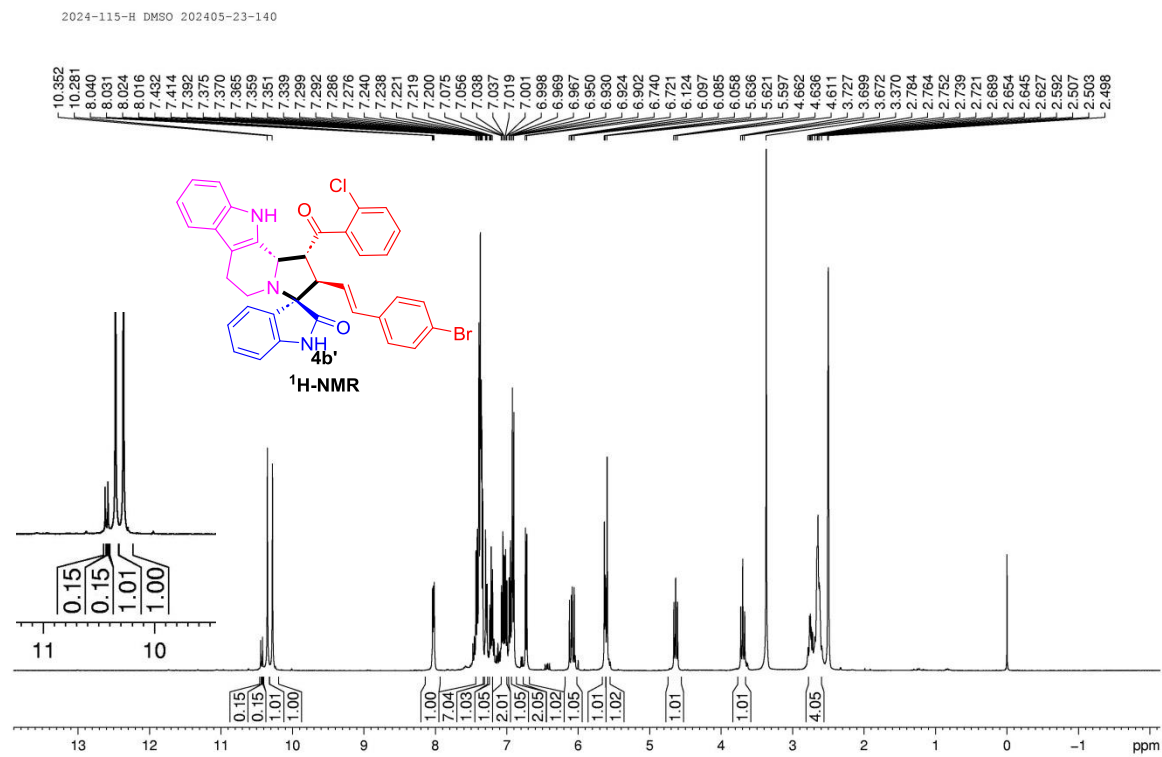


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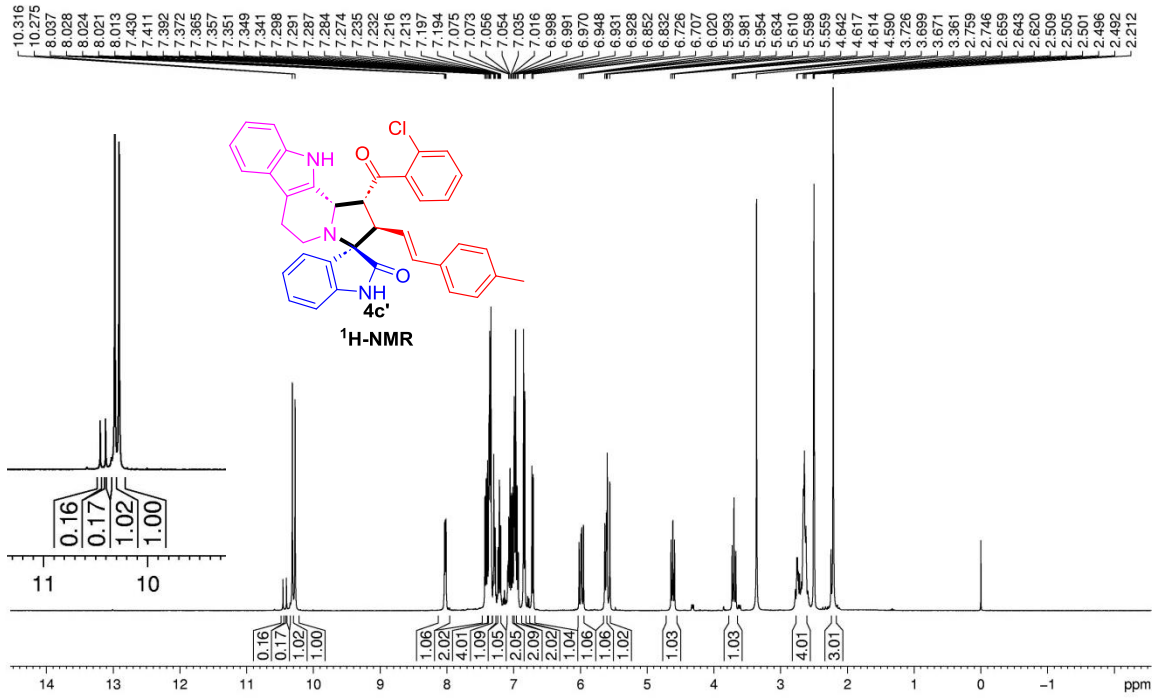


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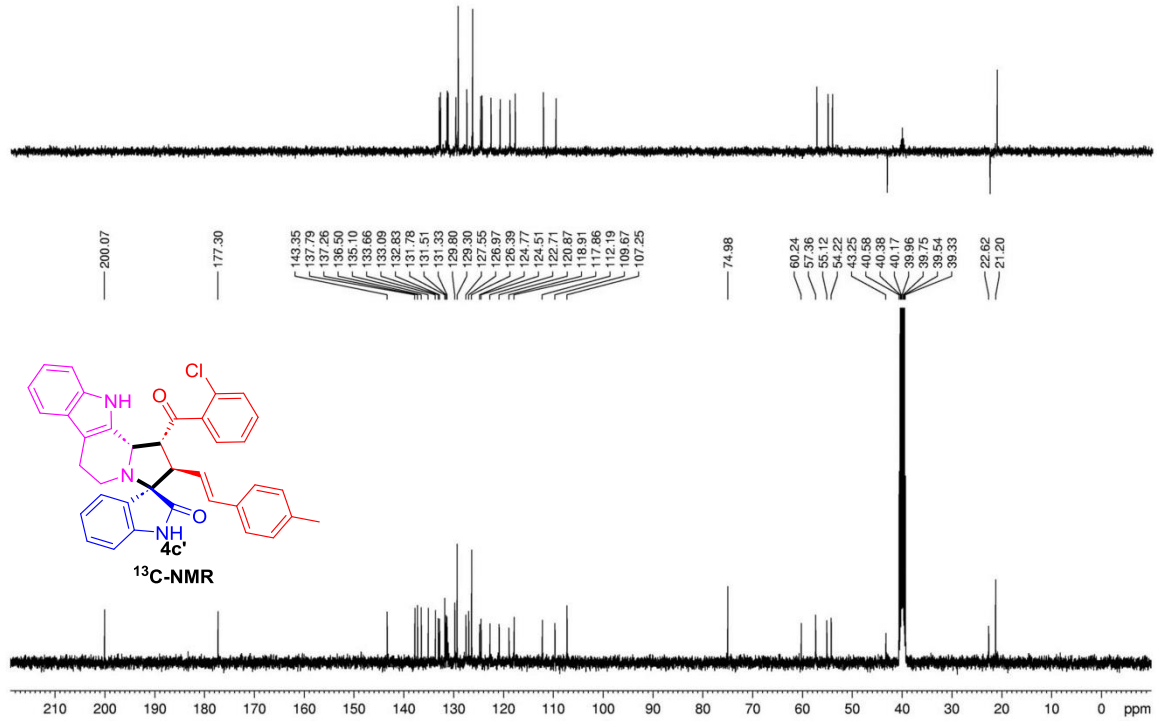




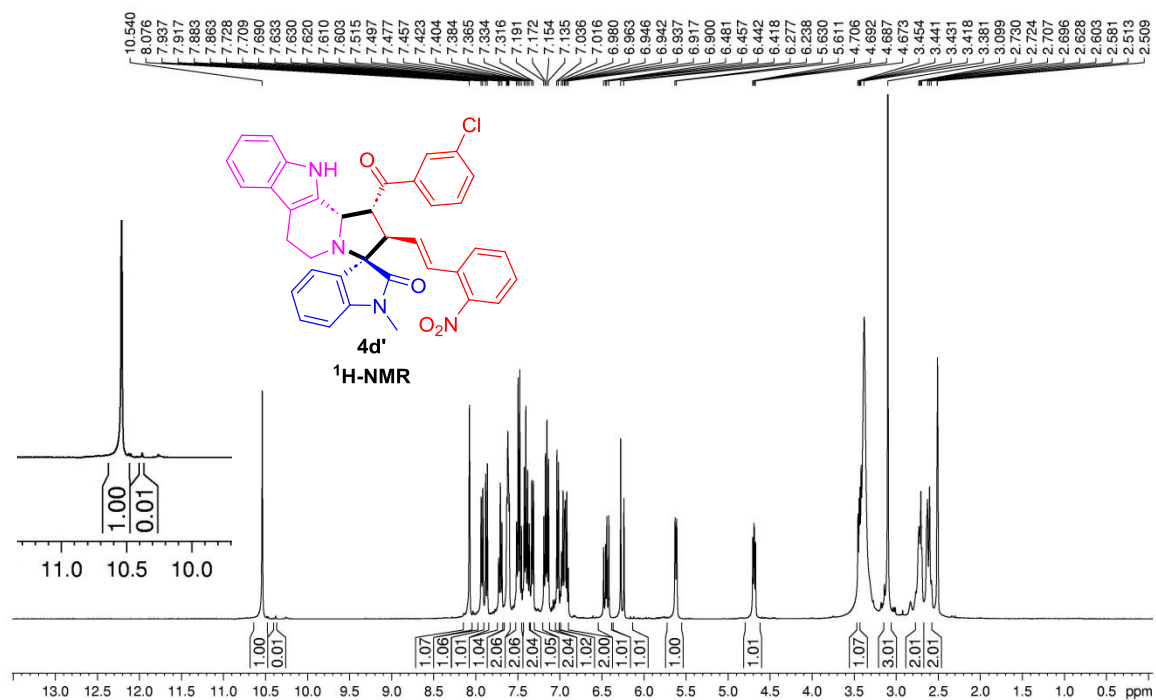
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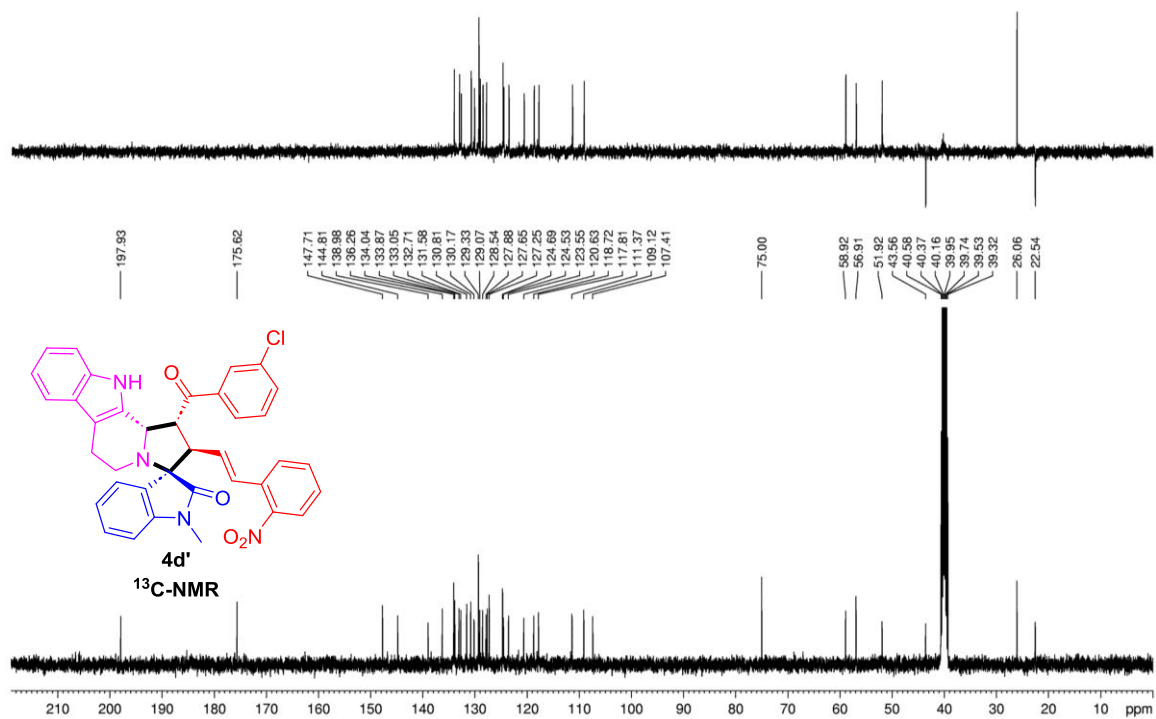
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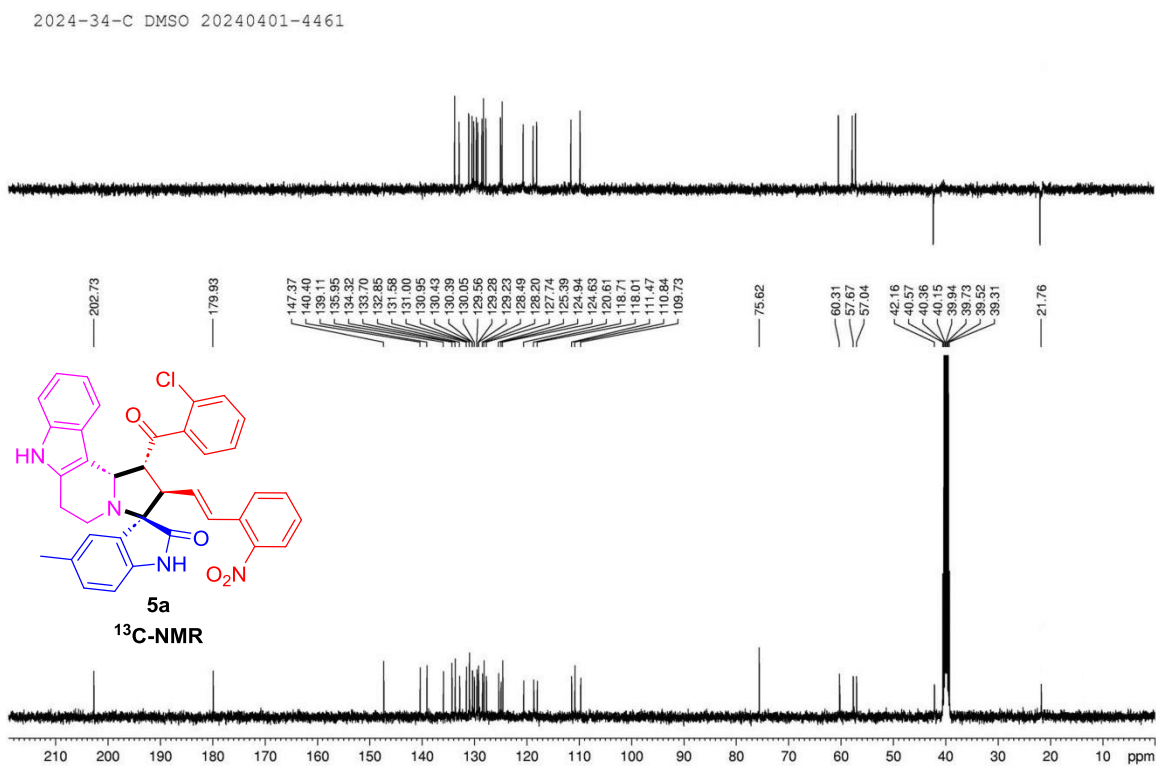
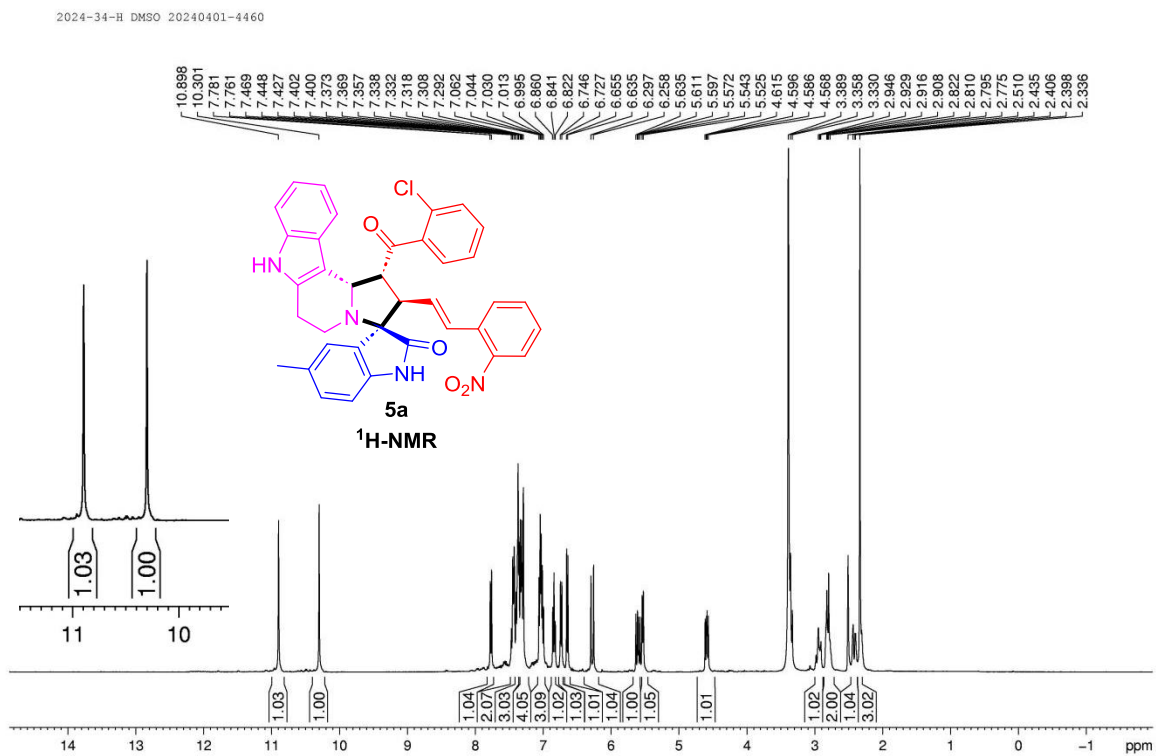
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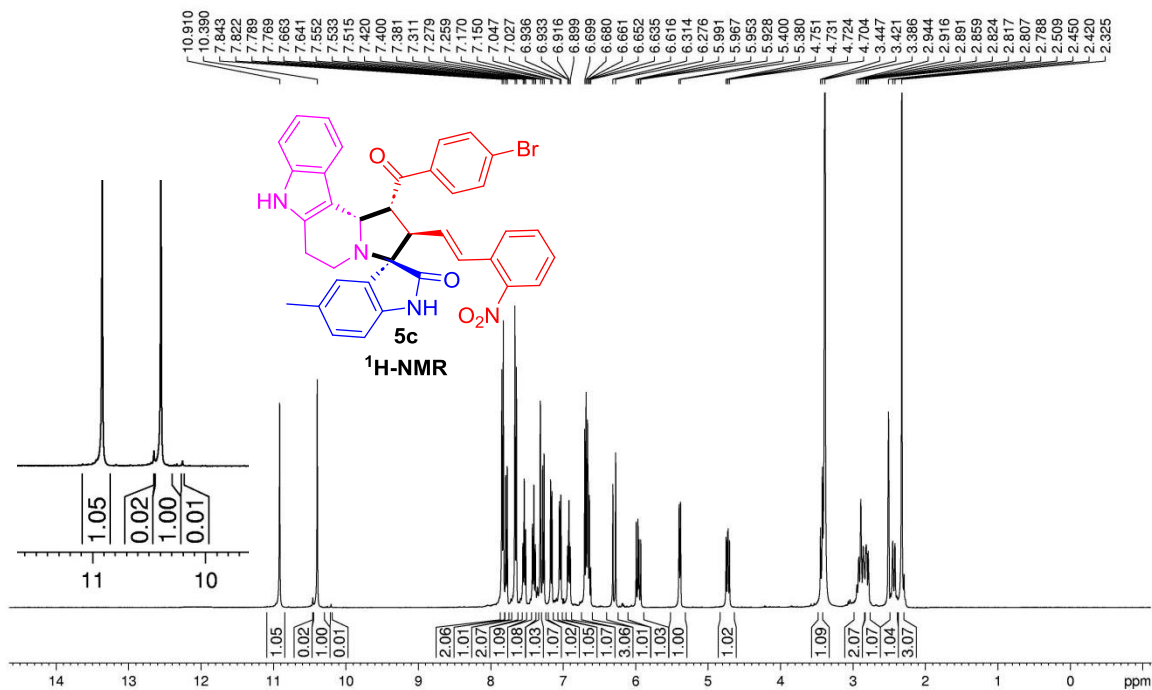
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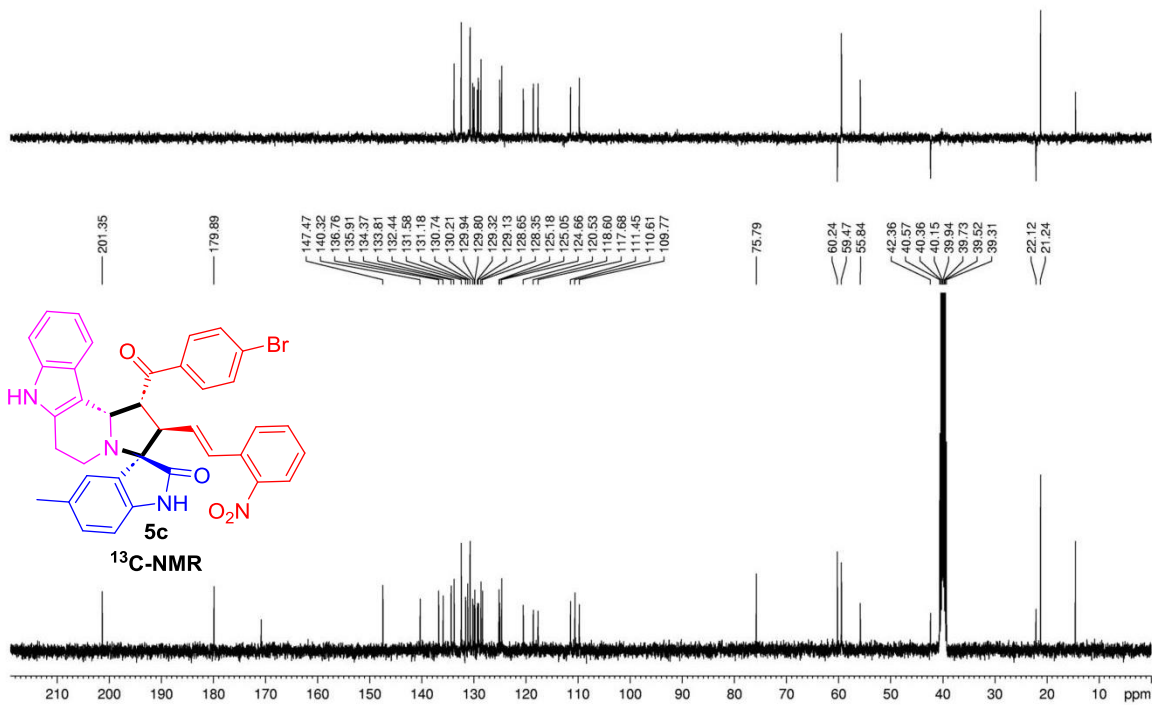
2. ^1H and ^{13}C NMR spectra for compounds 5



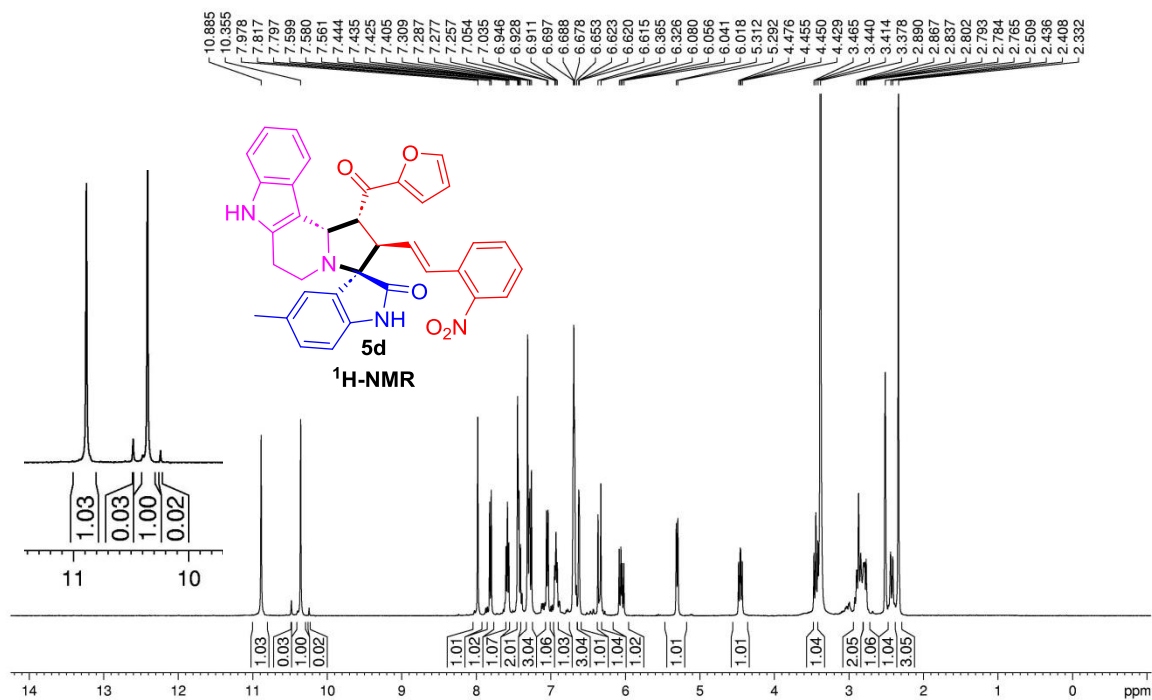
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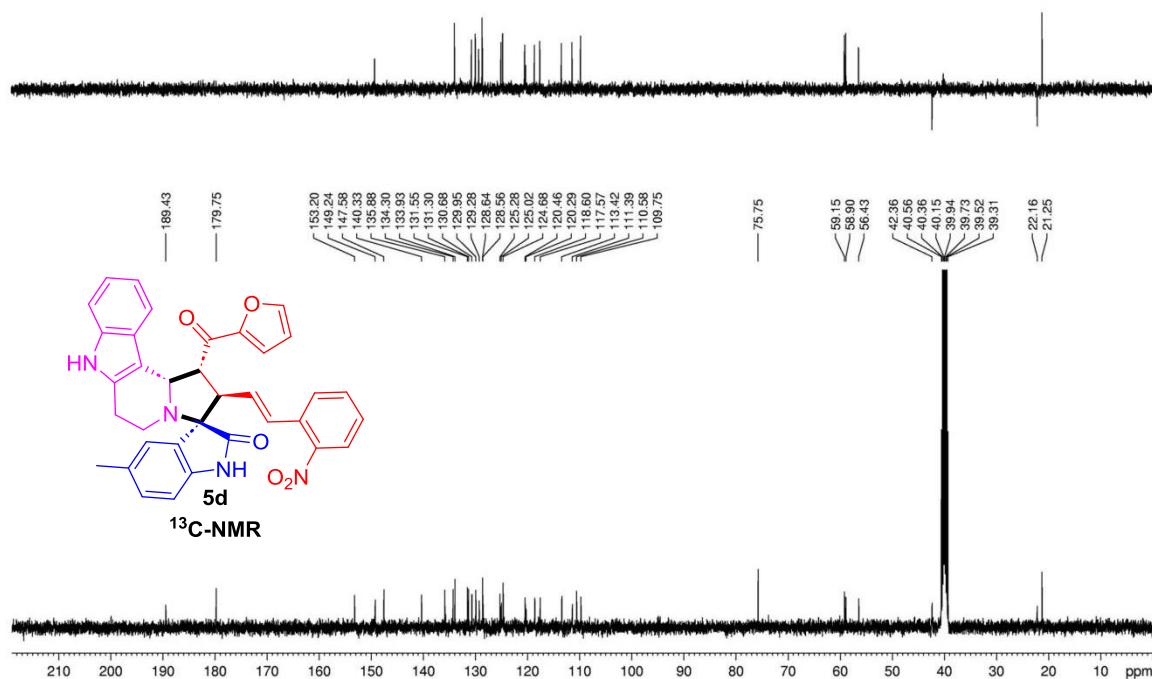
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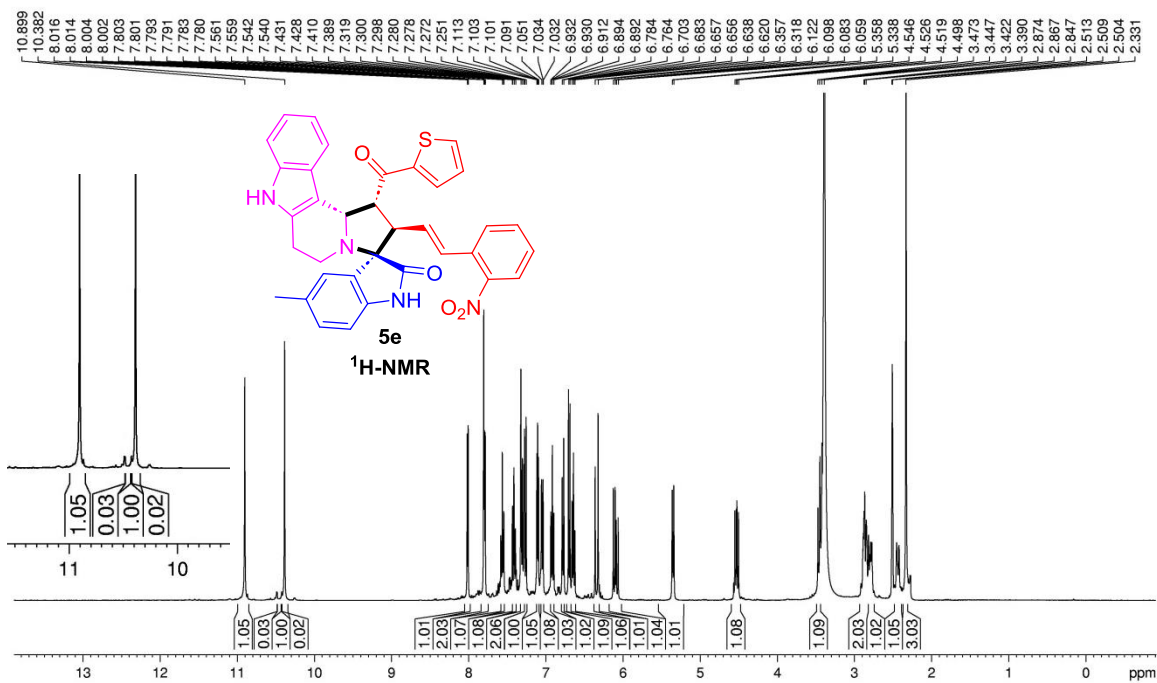
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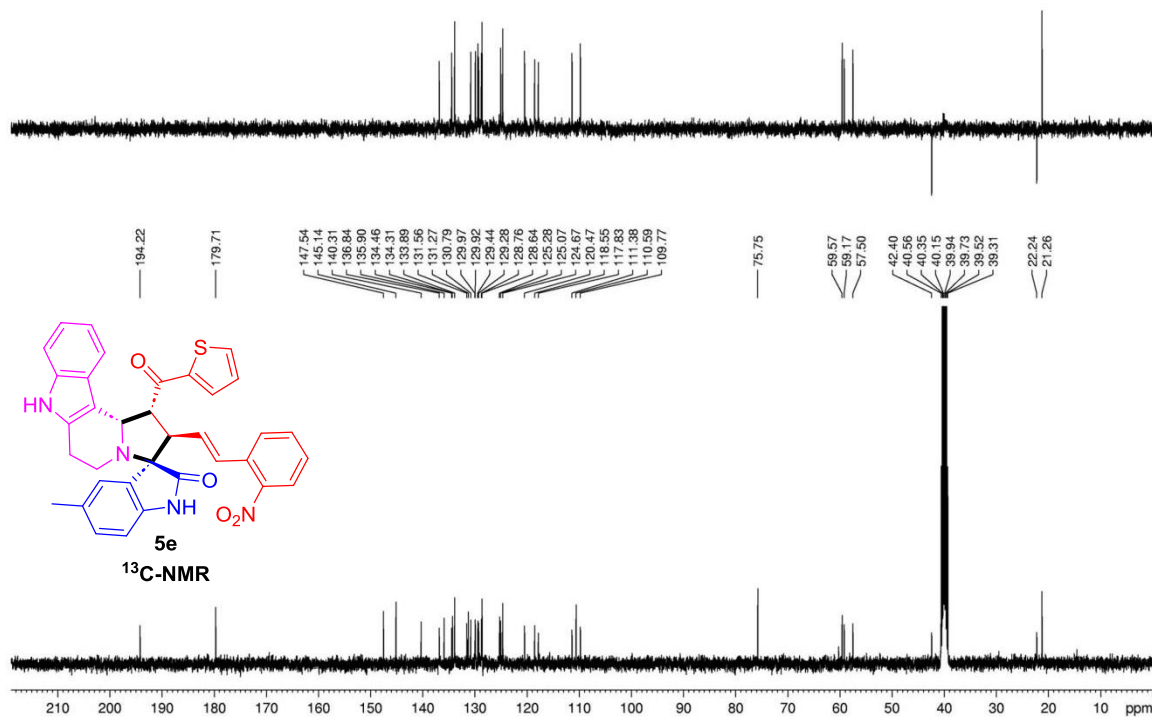
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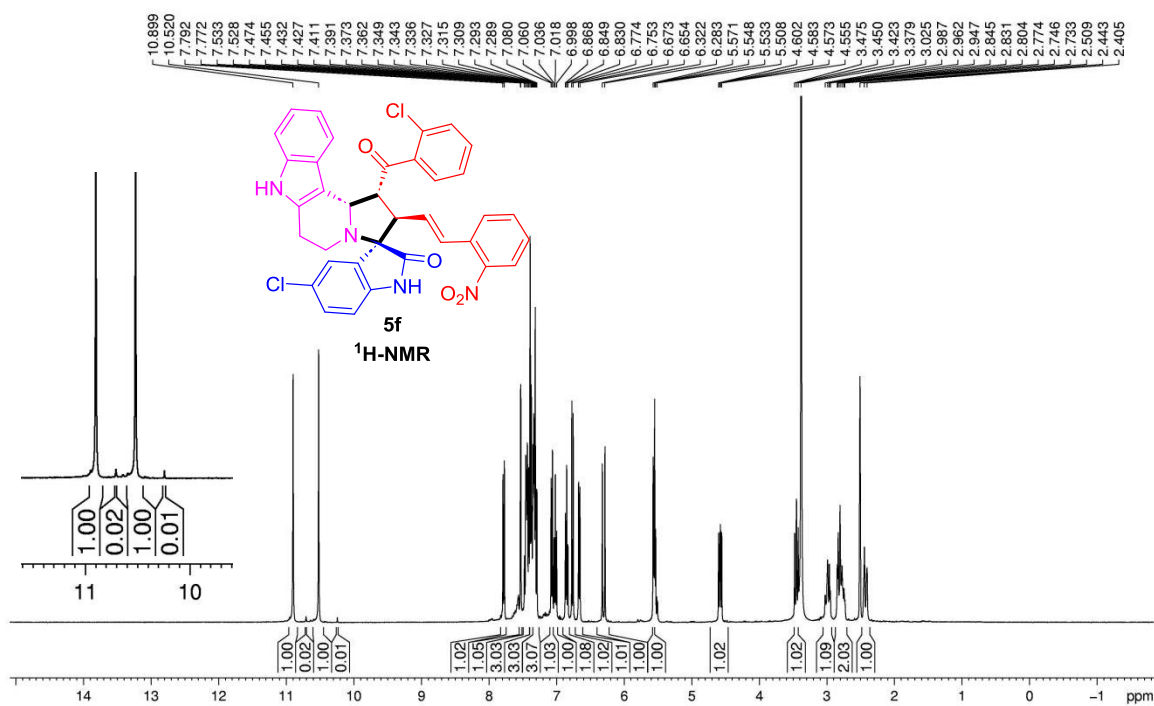
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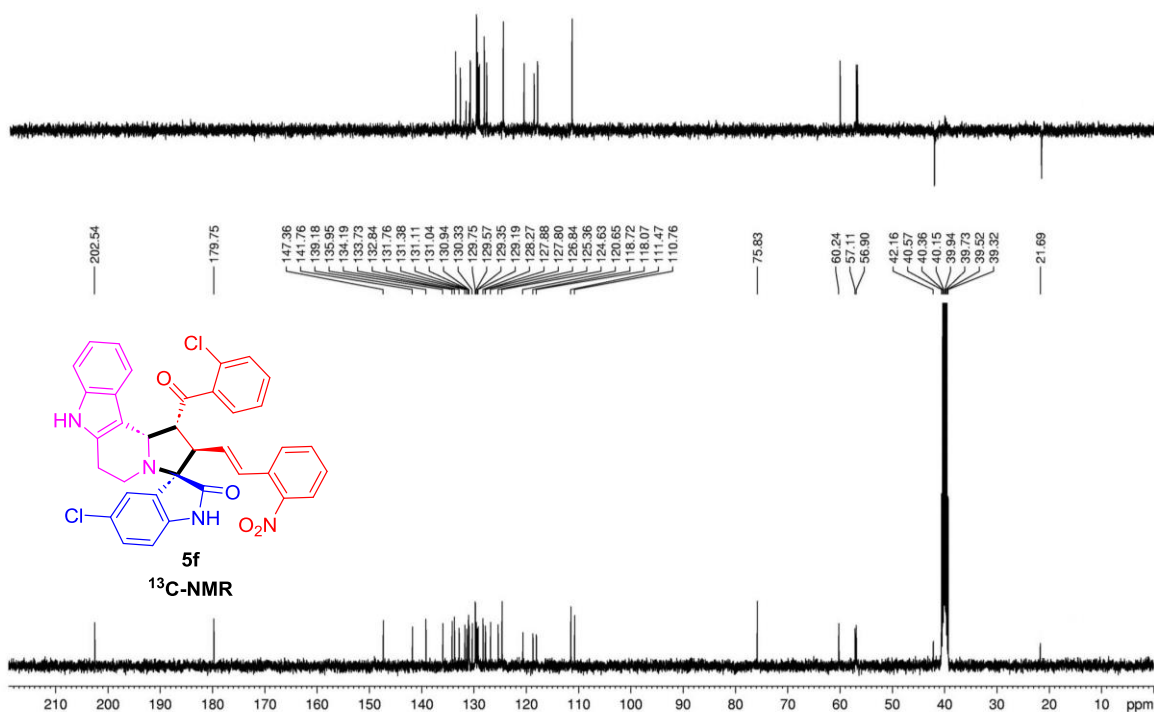
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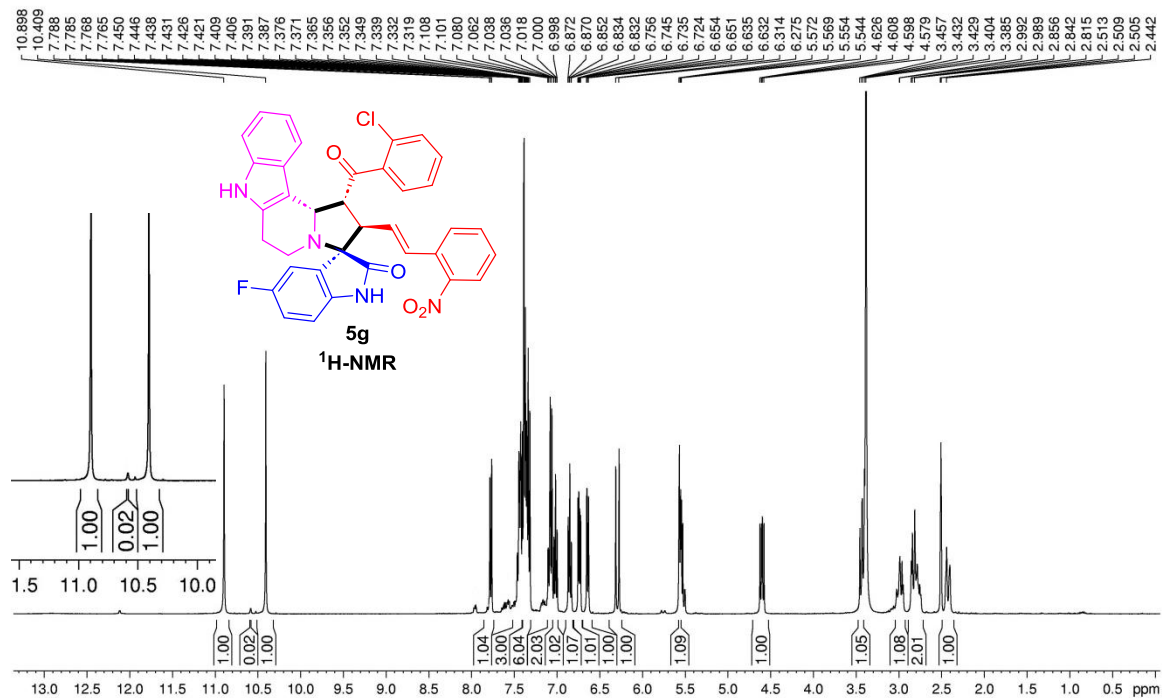
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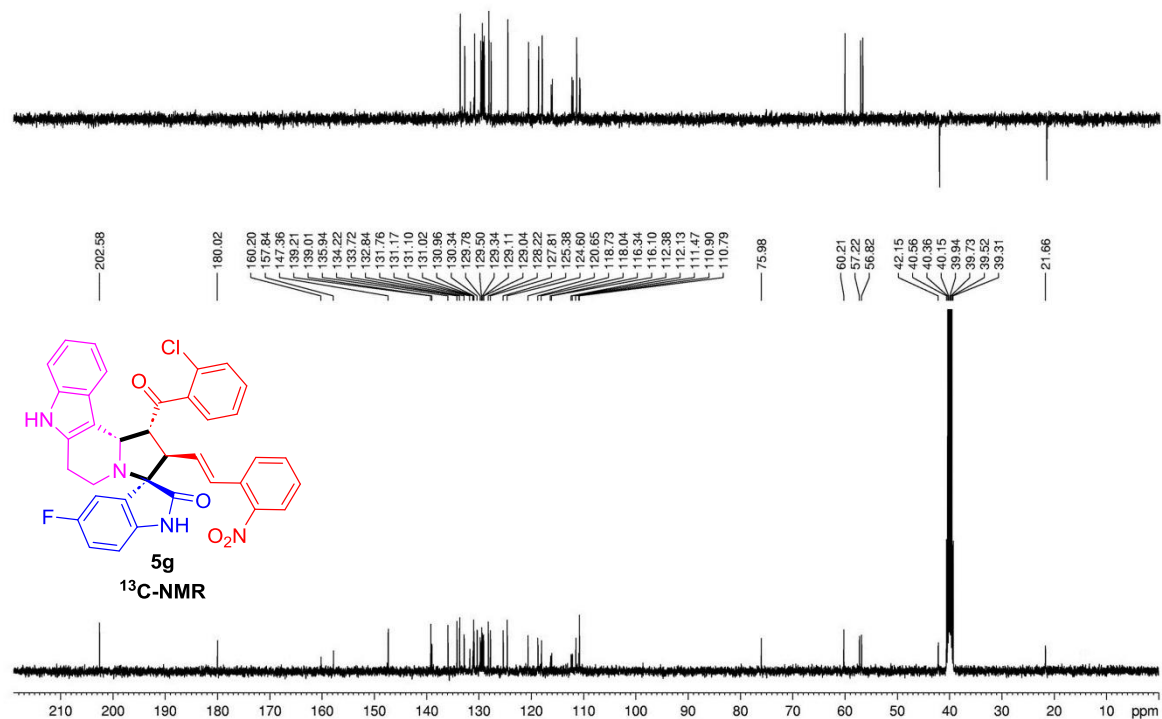
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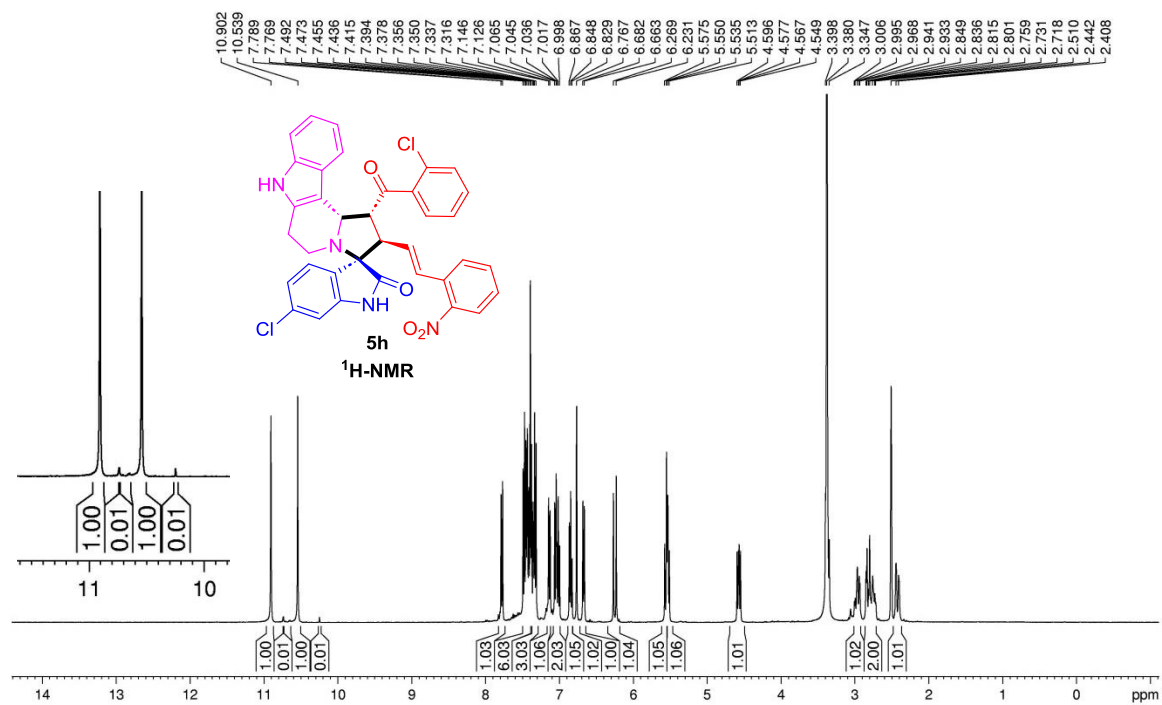
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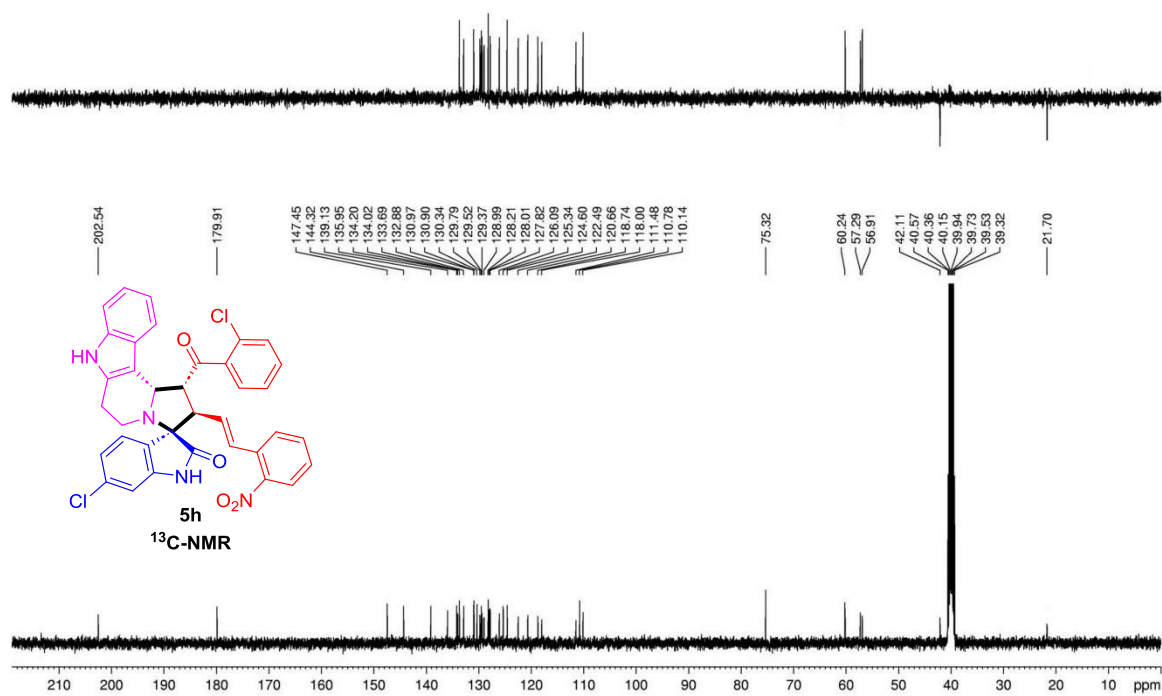
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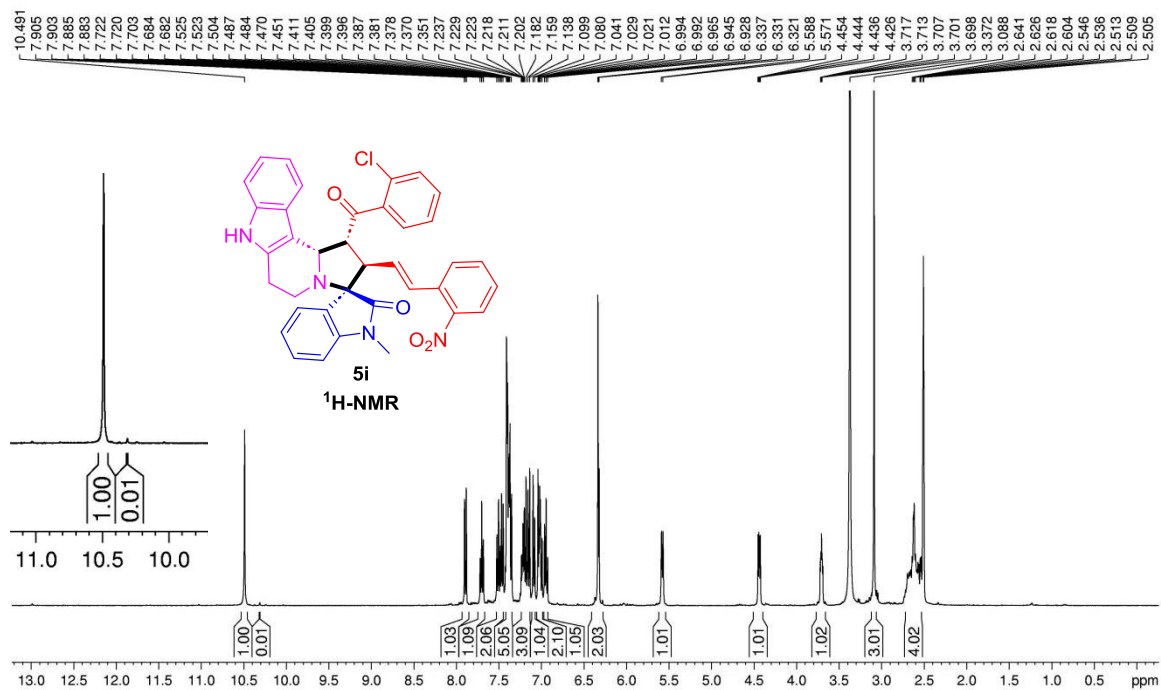
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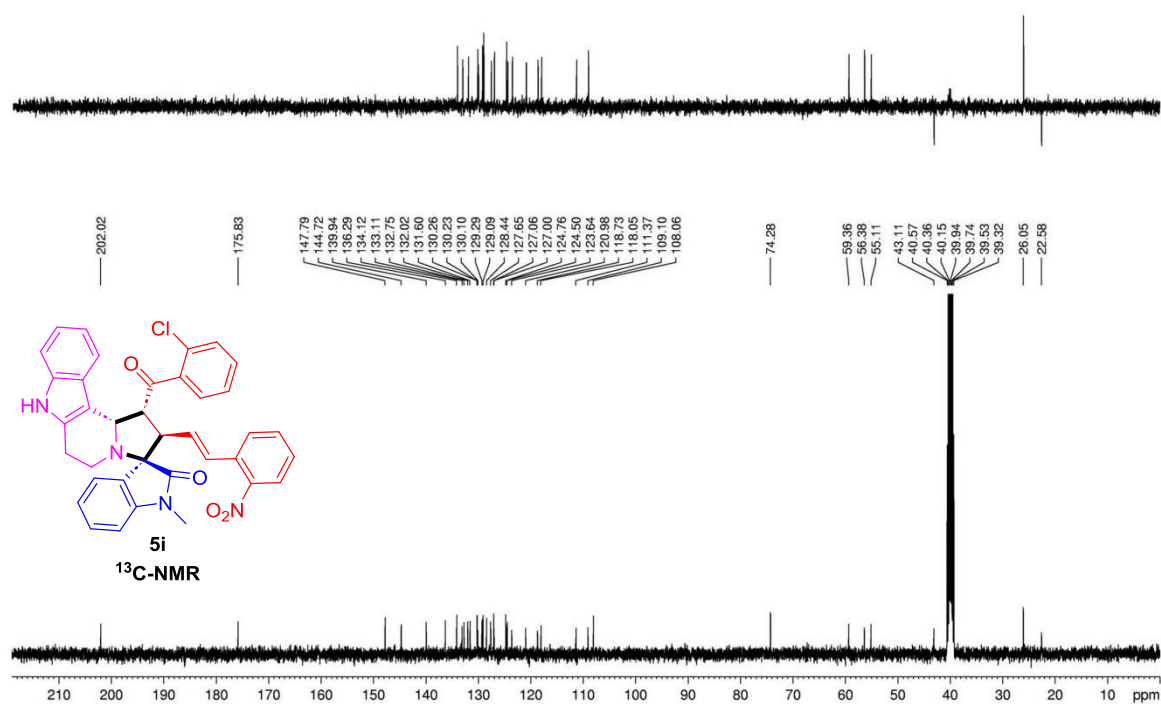
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE. 293 Degree

Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.966 Why?
PLAT220_ALERT_2_C NonSolvent Resd 1 0 Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for N42 --C30 . 5.5 s.u.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N42 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.957 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 9 Report
-8 2 9, 0 10 12, 8 11 12, -5 -3 13, 0 10 13, -4 -2 14,
5 10 14, 6 10 14, 5 9 15,

Alert level G

PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report
PLAT073_ALERT_1_G H-atoms ref, but _hydrogen_treatment Reported as constr Check
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 4 Note
PLAT769_ALERT_4_G CIF Embedded Explicitly Supplied Scattering Data Please Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 229 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.8 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 4.04 Note
Predicted wR2: Based on SigI**2 4.55 or SHELX Weight 18.24
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 9 Info
PLAT982_ALERT_1_G The C-f' = 0.0192 Deviates from IT-value = 0.0181 Check
PLAT982_ALERT_1_G The N-f' = 0.0326 Deviates from IT-value = 0.0311 Check
PLAT982_ALERT_1_G The O-f' = 0.0524 Deviates from IT-value = 0.0492 Check
PLAT983_ALERT_1_G The O-f" = 0.0338 Deviates from IT-Value = 0.0322 Check

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
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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

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

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.

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Datablock b - ellipsoid plot

