

A new way to 2,3,4-Trisubstituted Benzo[h]quinolines: Synthesis, Consecutive Reactions and Cellular Activities [†]

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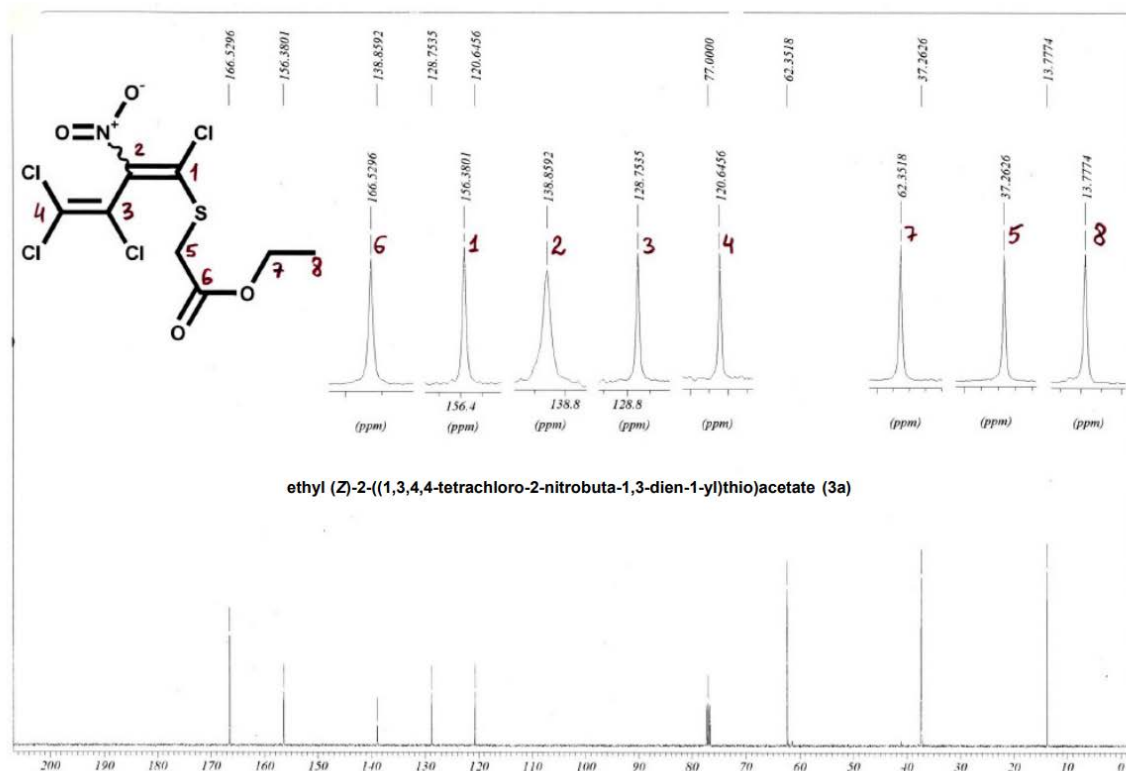
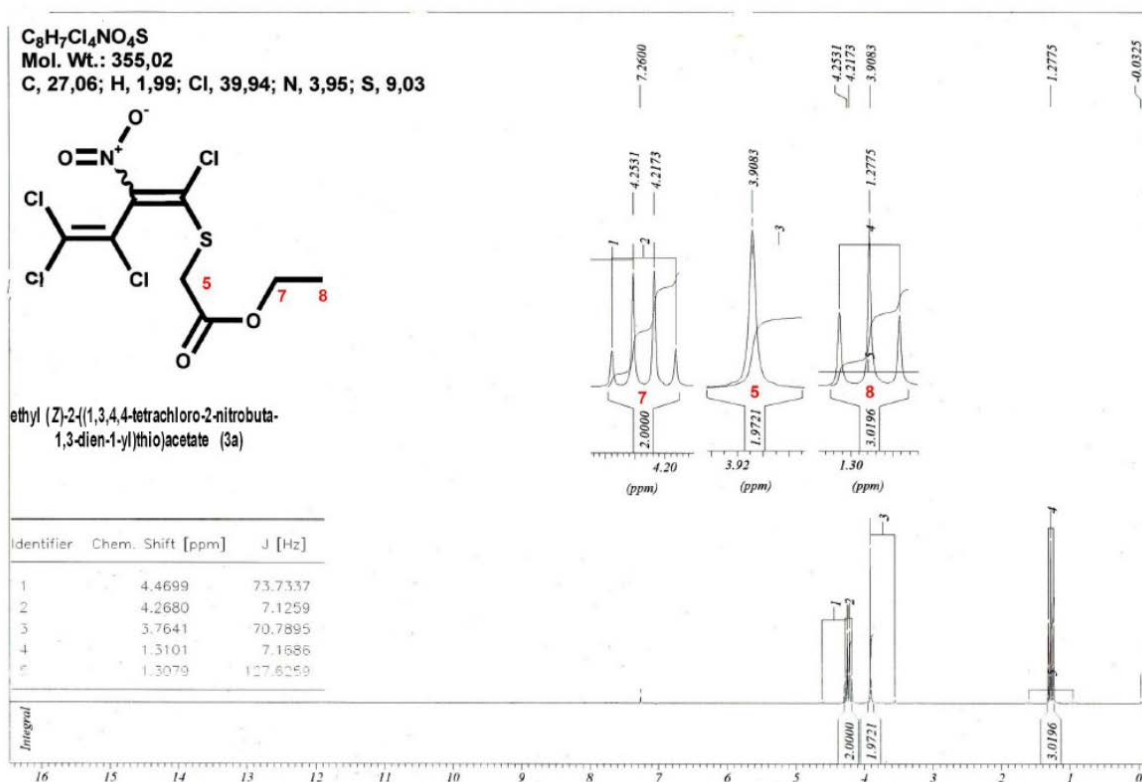
³ Department of Chemical Biology, Helmholtz Centre for Infection Research, Inhoffenstrasse 7, 38124 Braunschweig, Germany; mark.broenstrup@helmholtz-hzi.de (M.B.); bianka.karge@helmholtz-hzi.de (B.G.);

* Correspondence: dieter.kaufmann@tu-clausthal.de

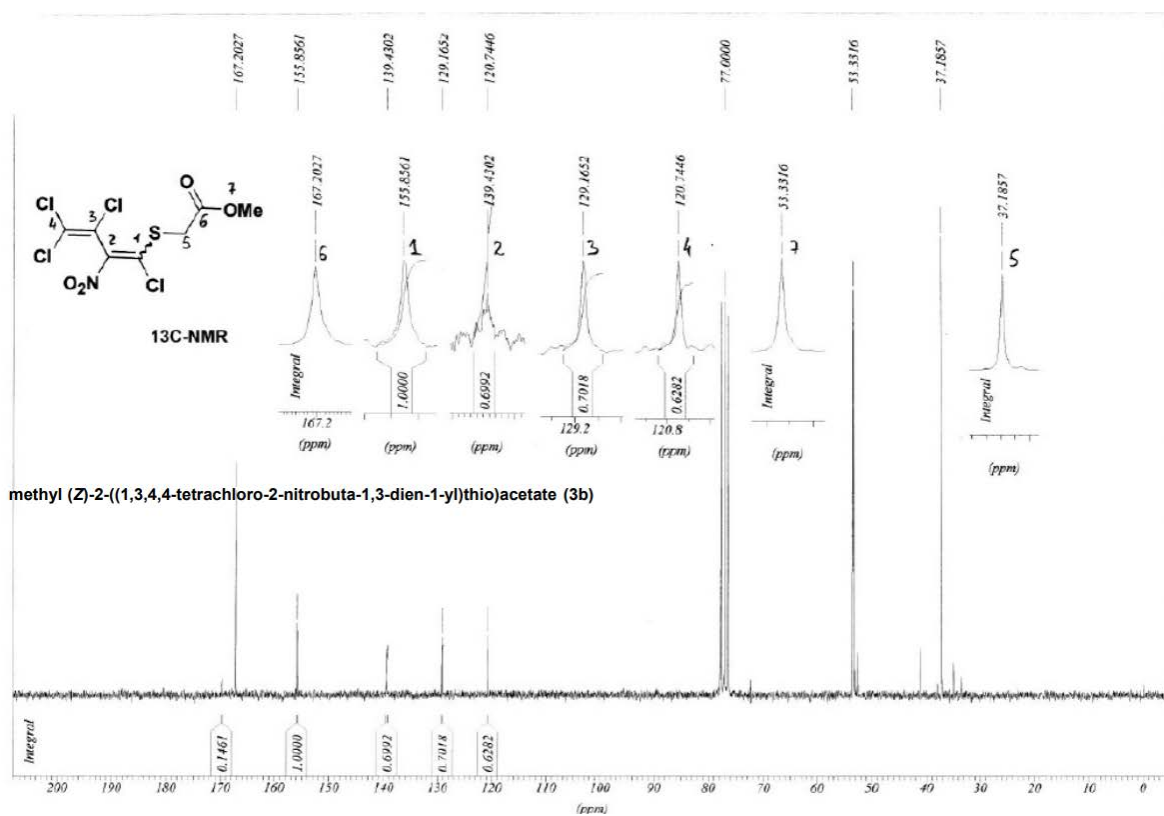
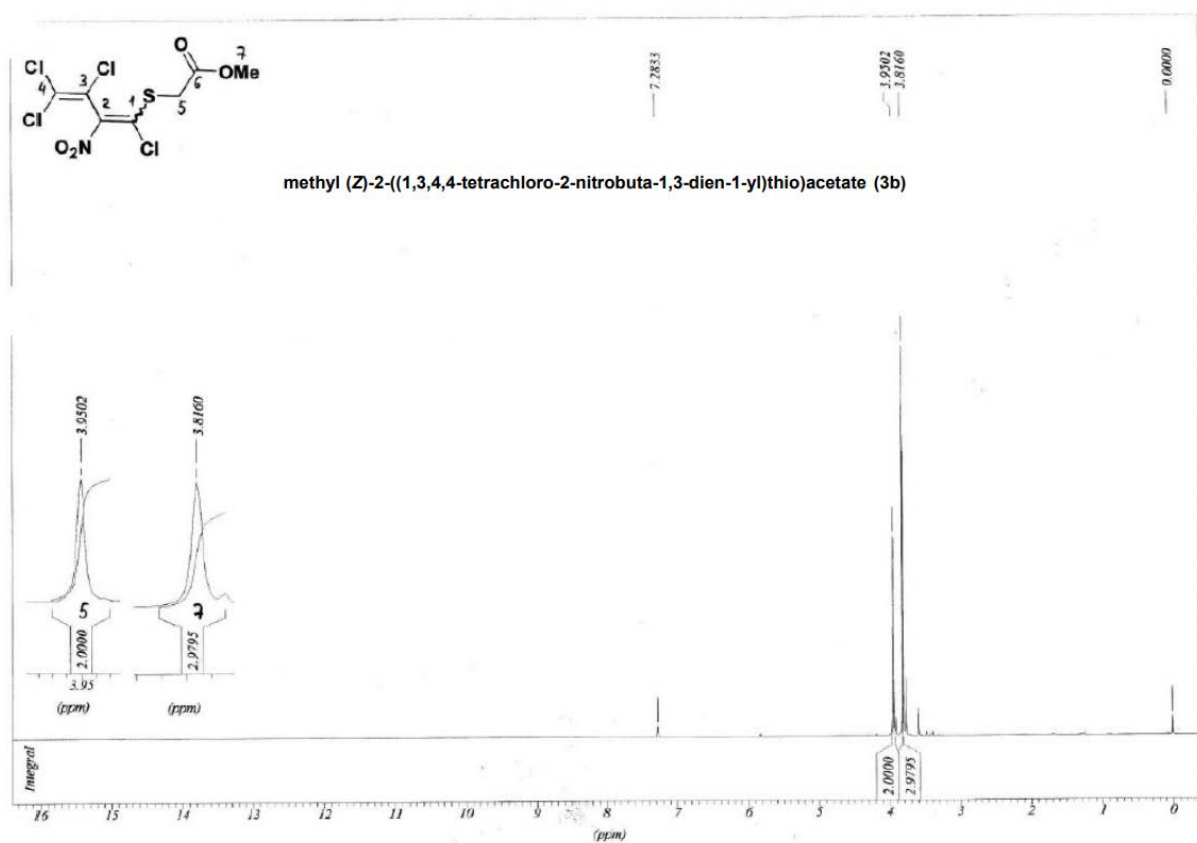
[†] Chemistry of Polyhalogenated Nitrobutadienes, 18. Chemistry of Polyhalogenated Nitrobutadienes, 17. Zapol'skii, V.A.; Berneburg, I.; Bilitewski, U.; Dillenberger, M.; Becker, K.; Jungwirth, S.; Shekhar, A. Krueger, B.; Kaufmann, D.E. Efficient synthesis of persubstituted chloroquinoliny-1H-pyrazoles and evaluation of their antimalarial, anti-SARS-CoV-2, antibacterial, and cytotoxic activities. *Beilstein J. Org. Chem.* **2022**, *18*, 524–532, doi.org/10.3762/bjoc.18.54.

Figures S2–S30: The ¹H–NMR and ¹³C–NMR-spectra of the newly synthesized compounds.

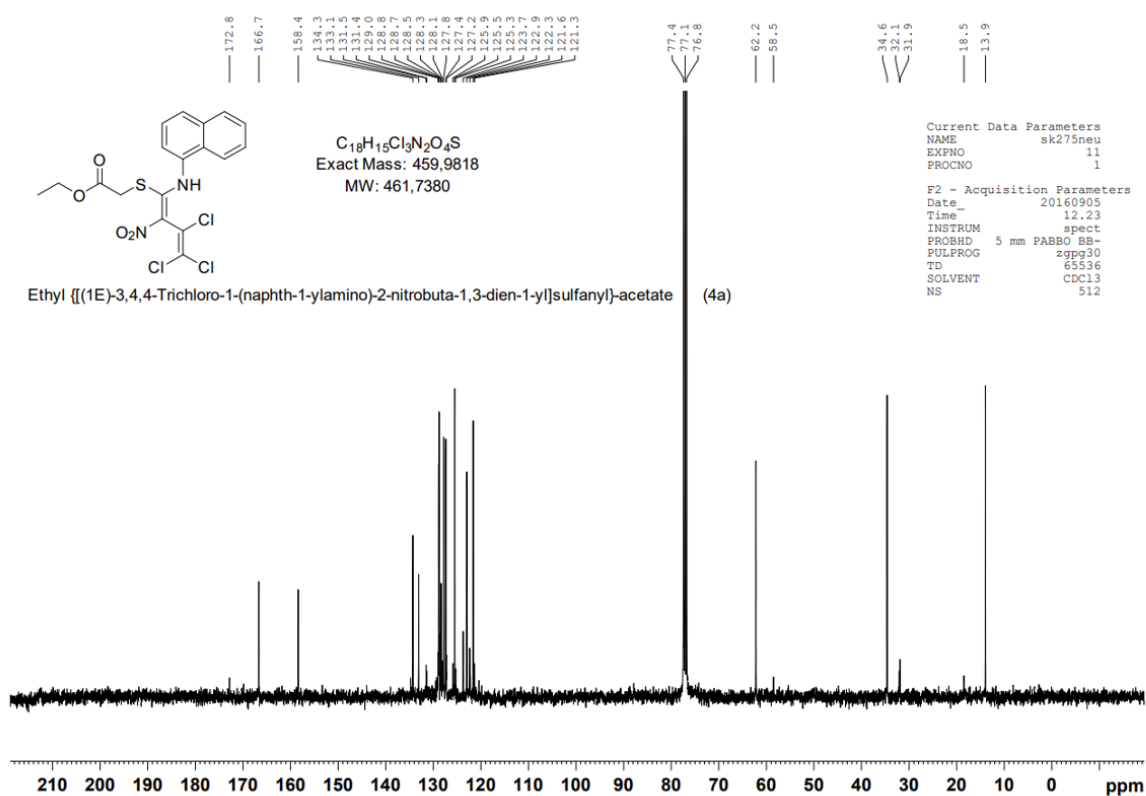
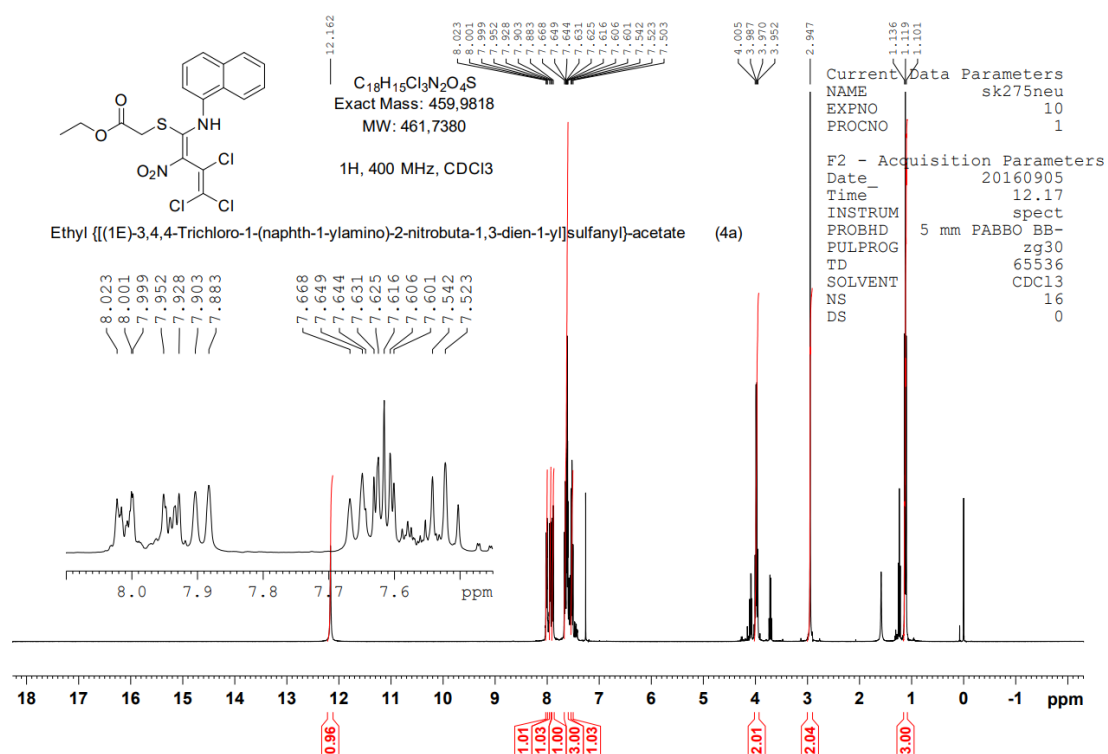
¹H and ¹³C NMR spectra of compound **3a**



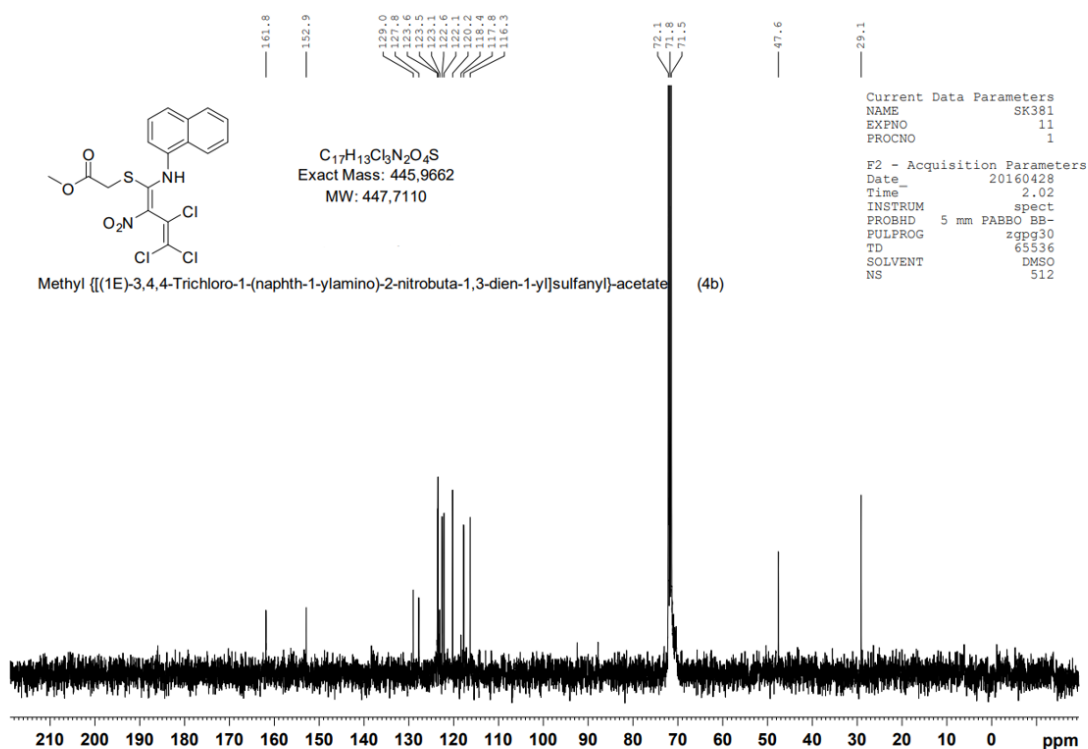
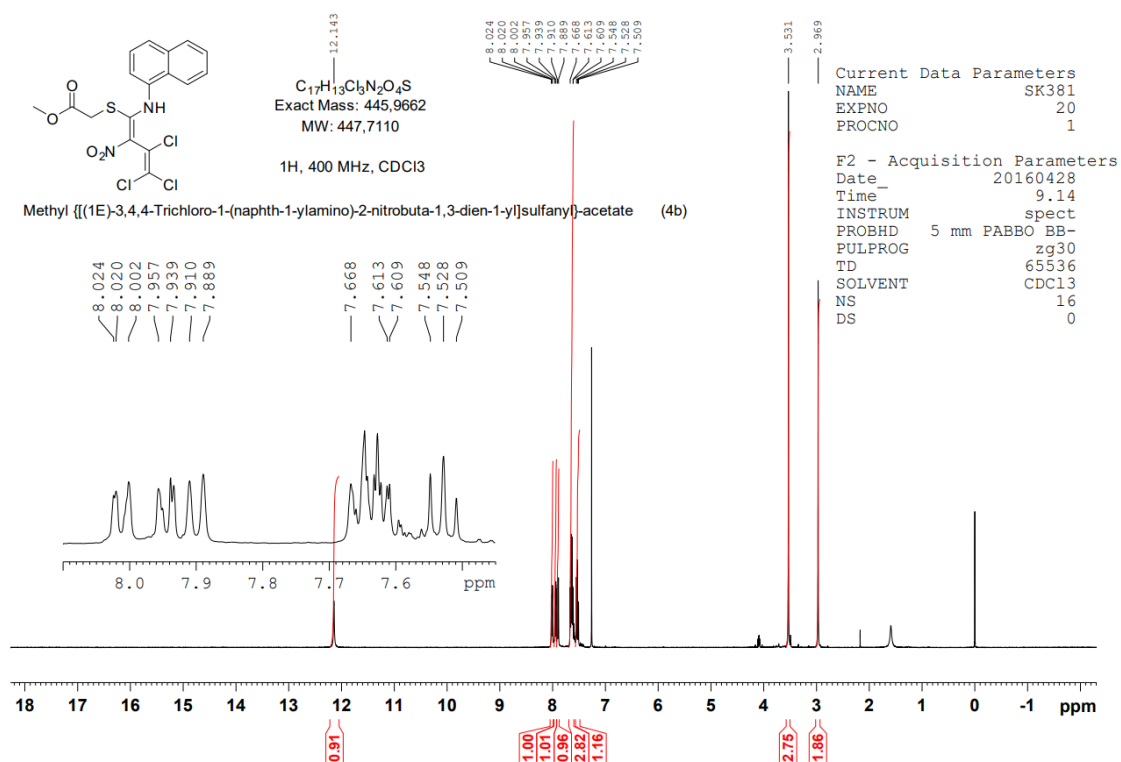
¹H and ¹³C NMR spectra of compound **3b**



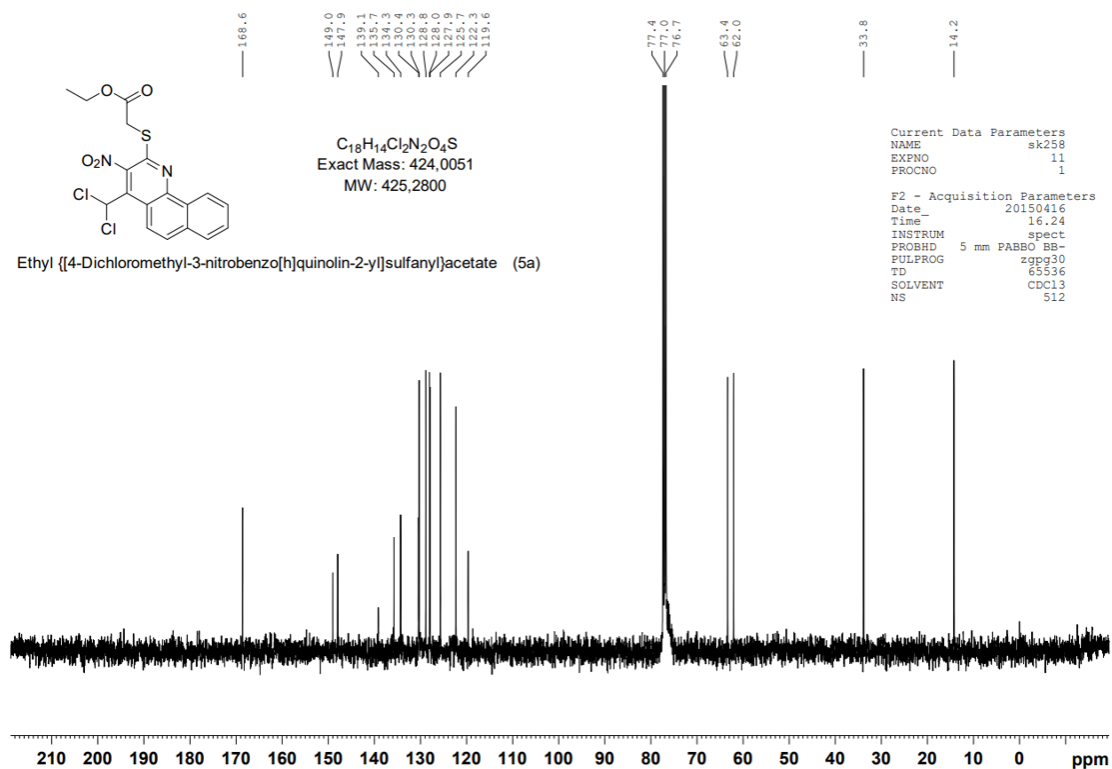
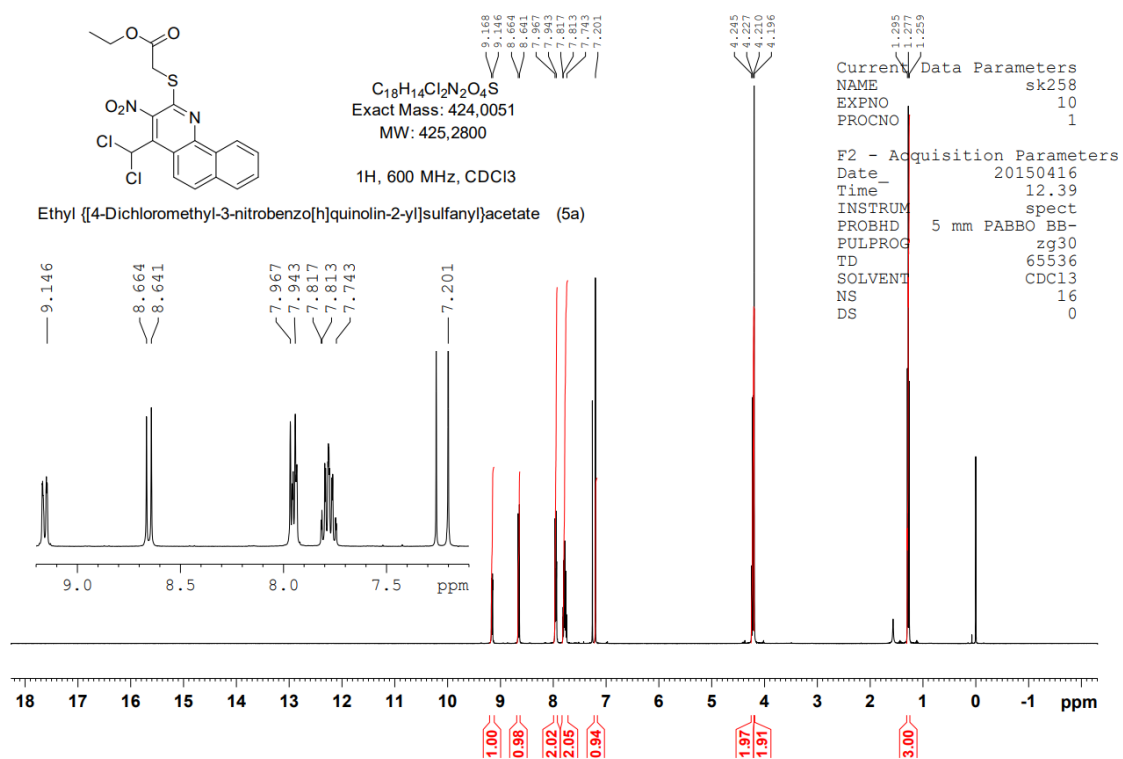
¹H and ¹³C NMR spectra of compound **4a**



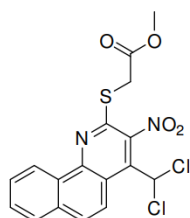
¹H and ¹³C NMR spectra of compound **4b**



¹H and ¹³C NMR spectra of compound 5a



¹H and ¹³C NMR spectra of compound **5b**

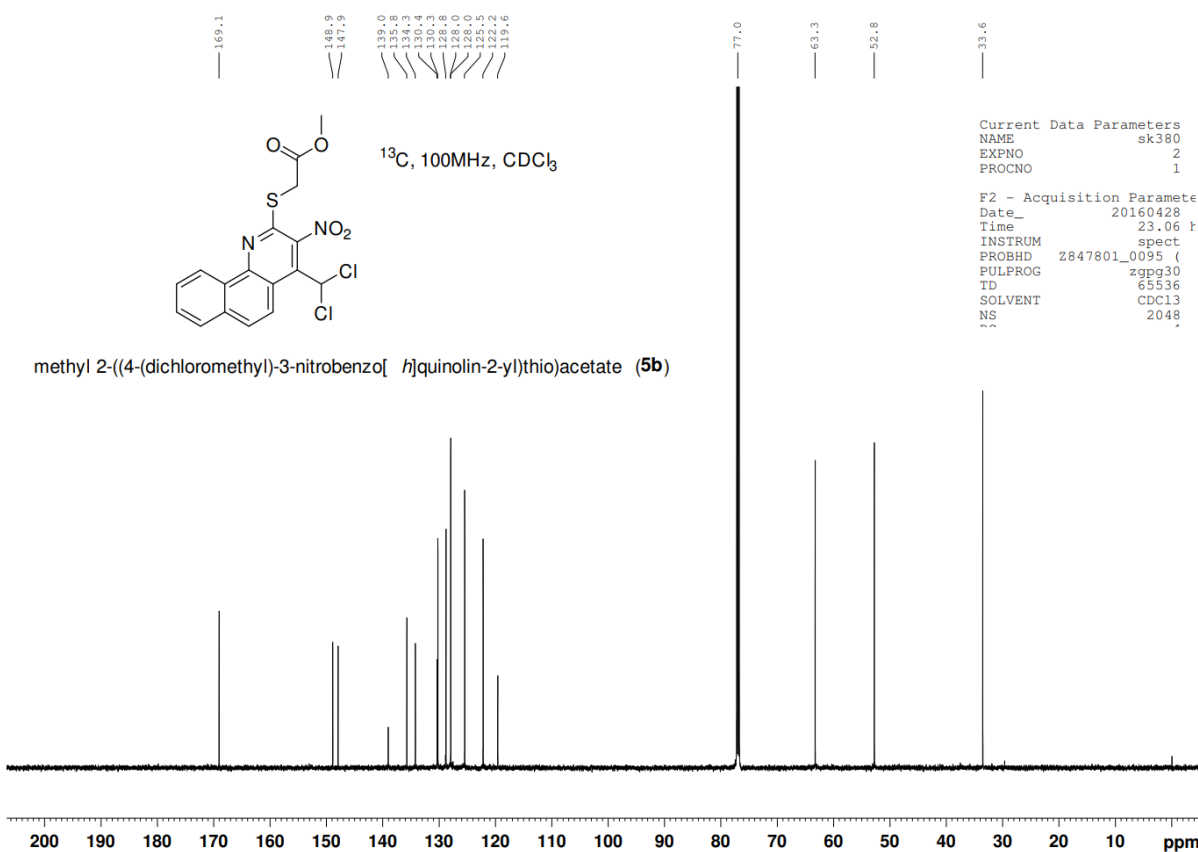
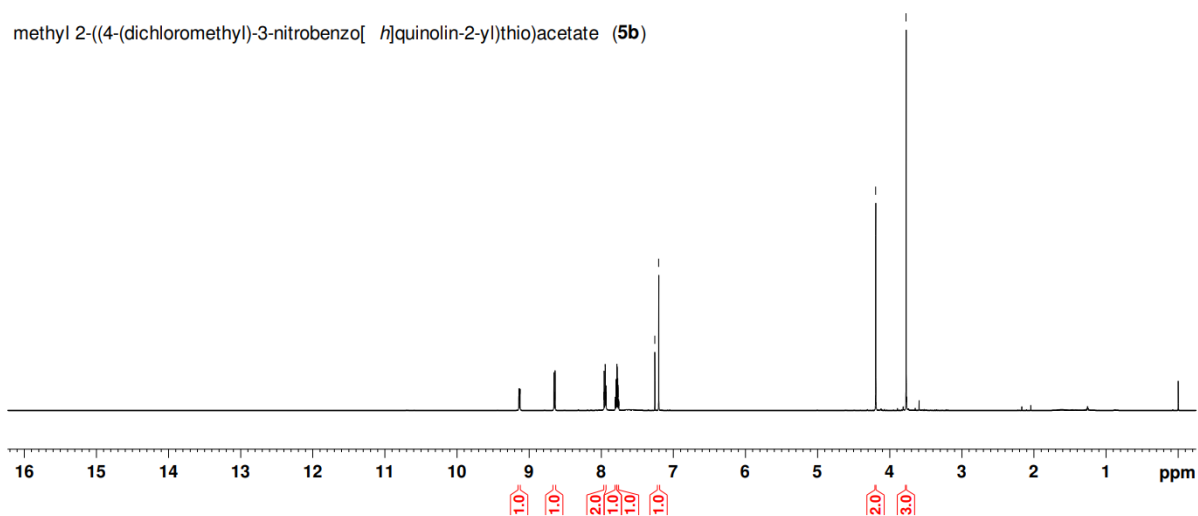


¹H, 600MHz, CDCl₃

C₁₇H₁₂Cl₂N₂O₄S
Exact 409.98948
MW 411.25

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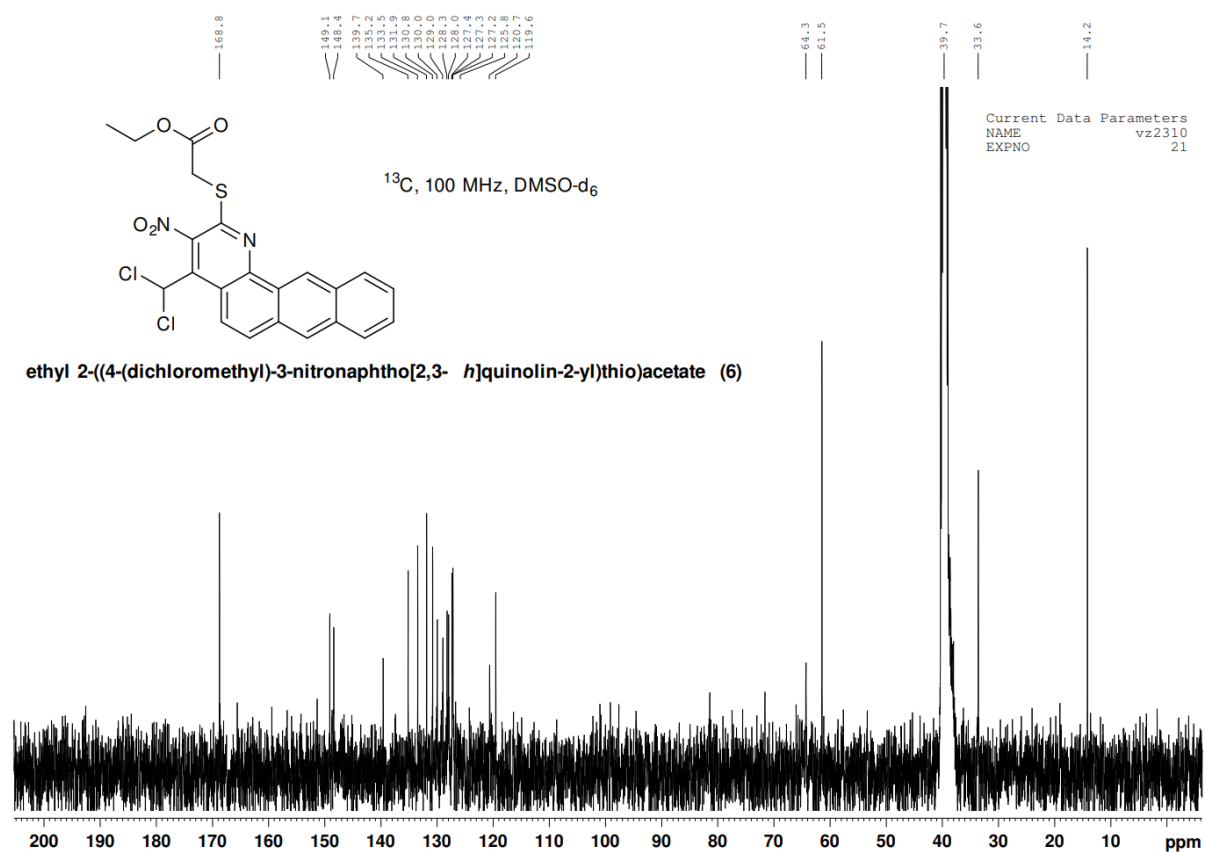
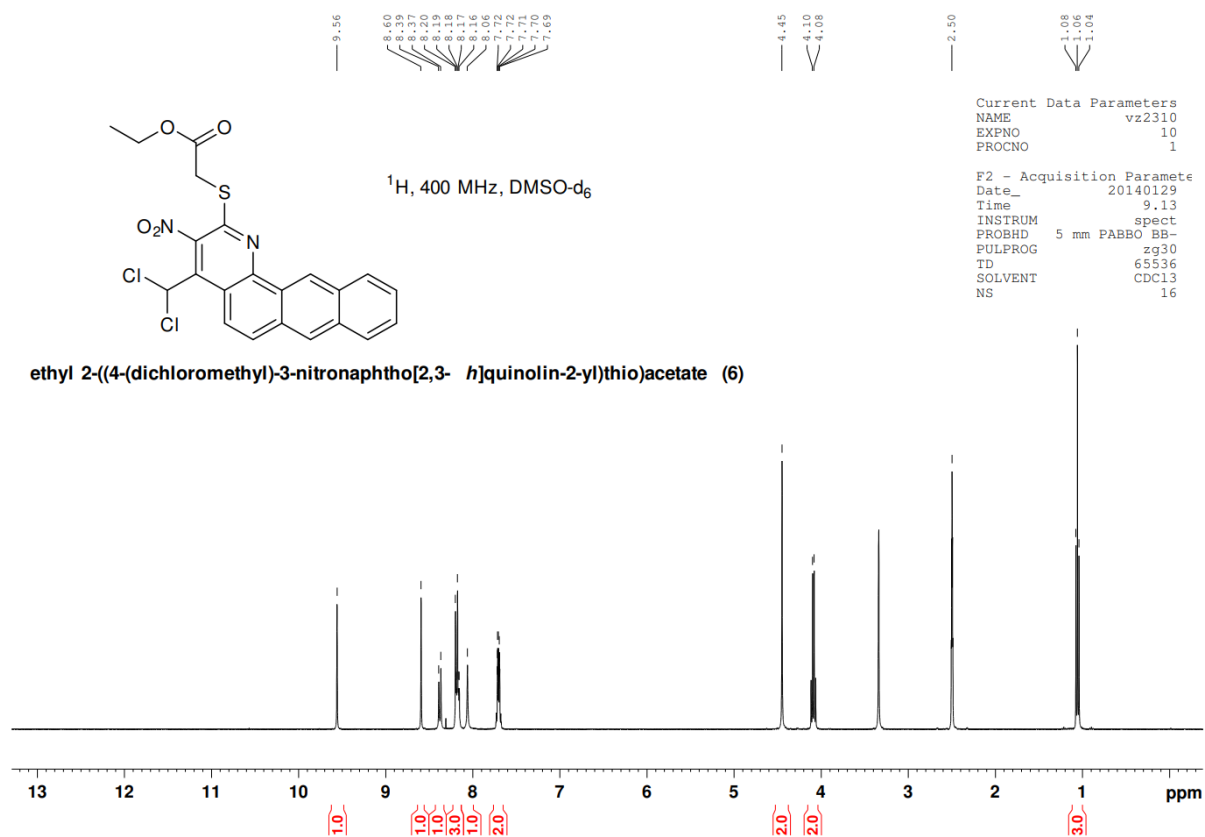


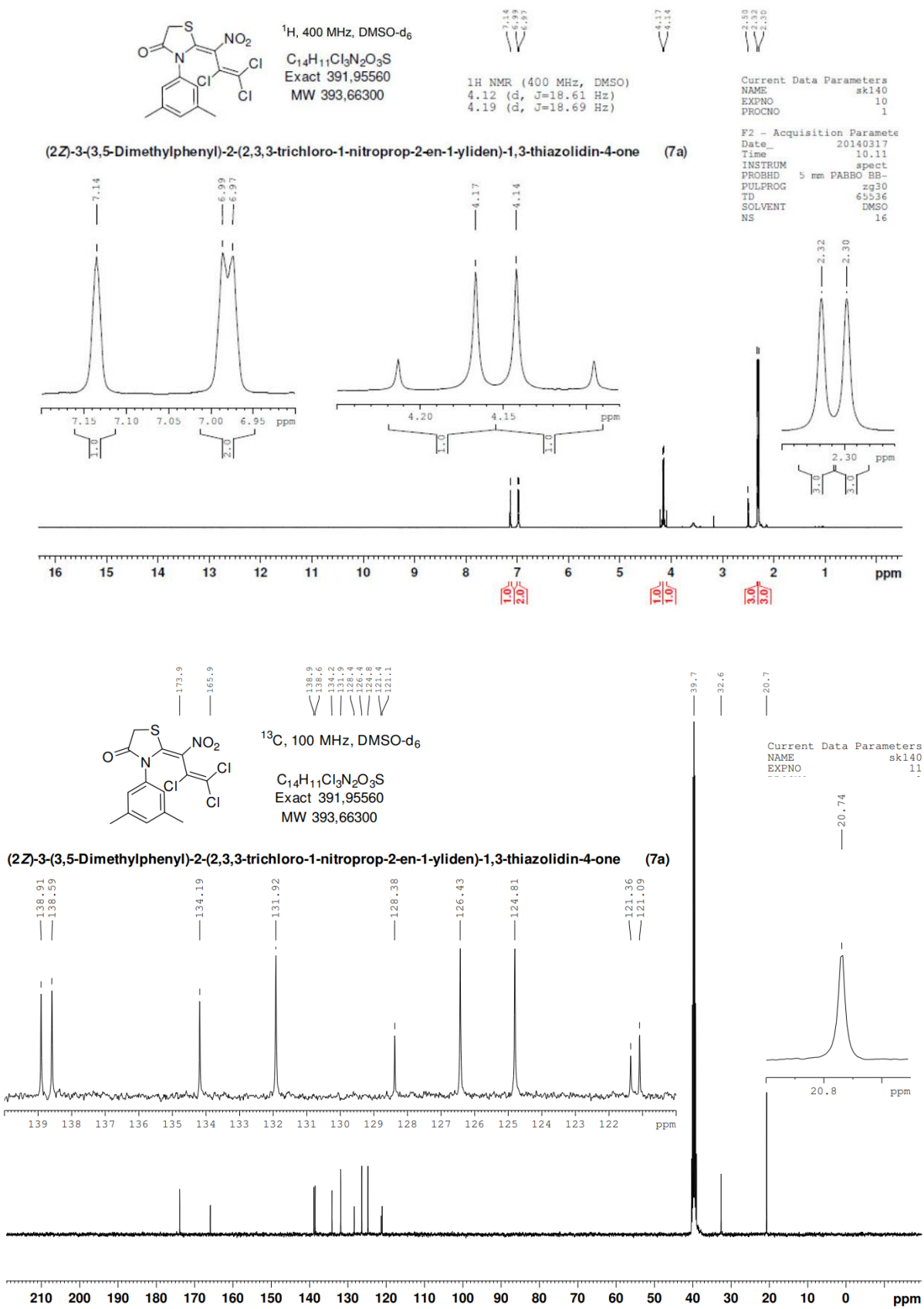
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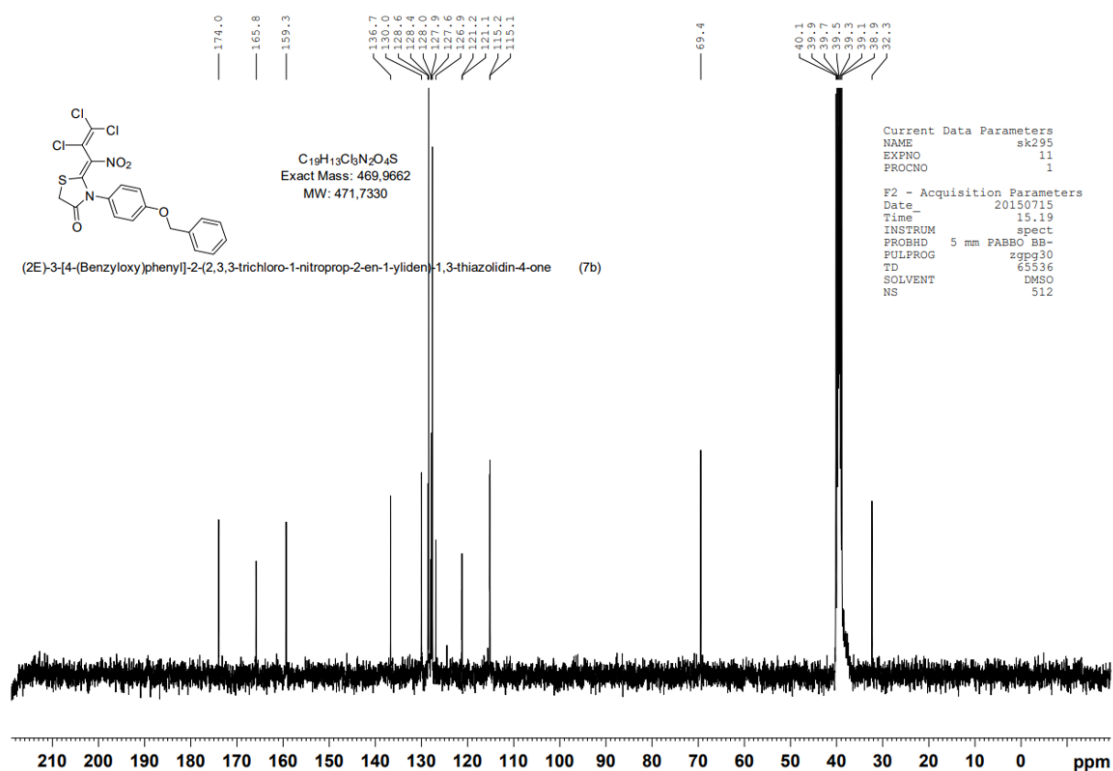
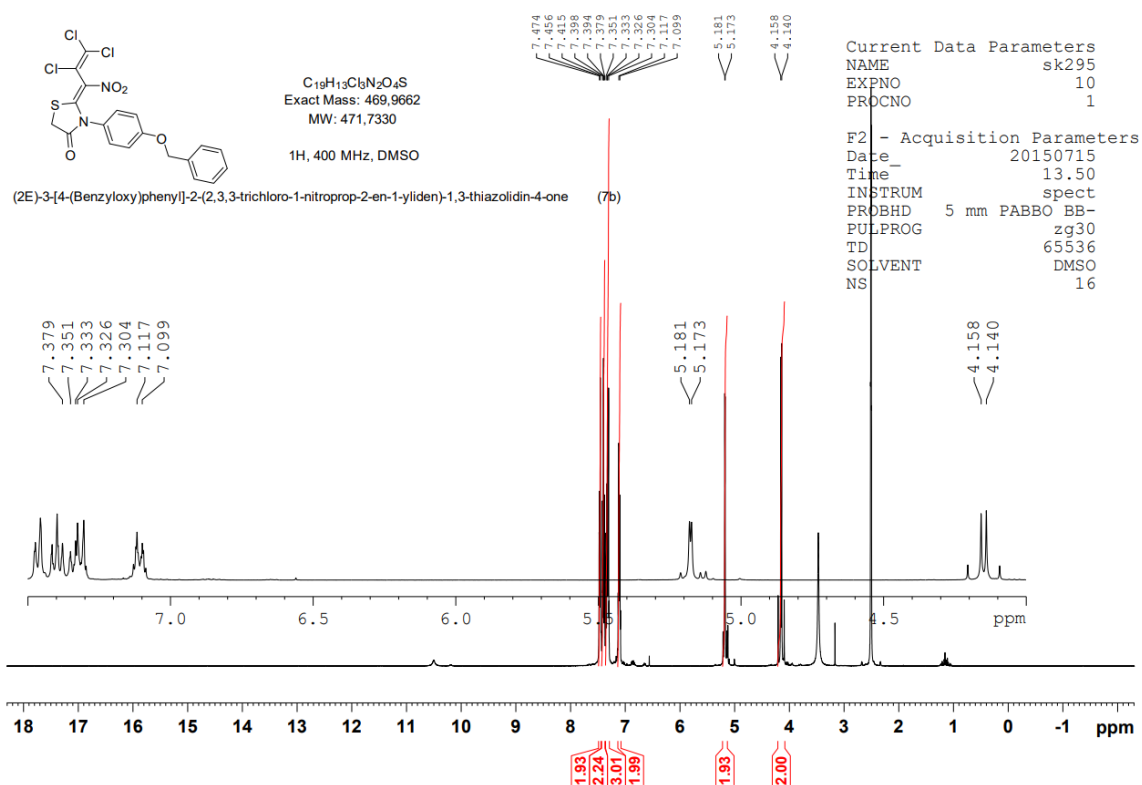
methyl 2-((4-(dichloromethyl)-3-nitrobenzo[h]quinolin-2-yl)thio)acetate (**5b**)

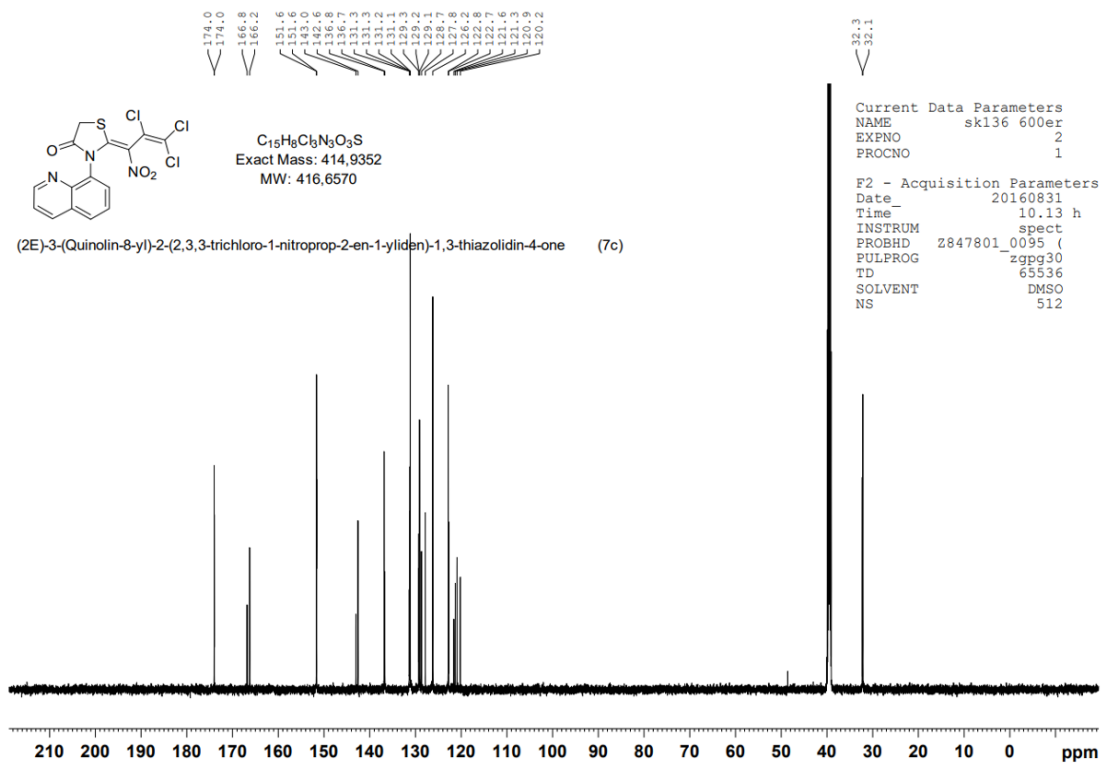
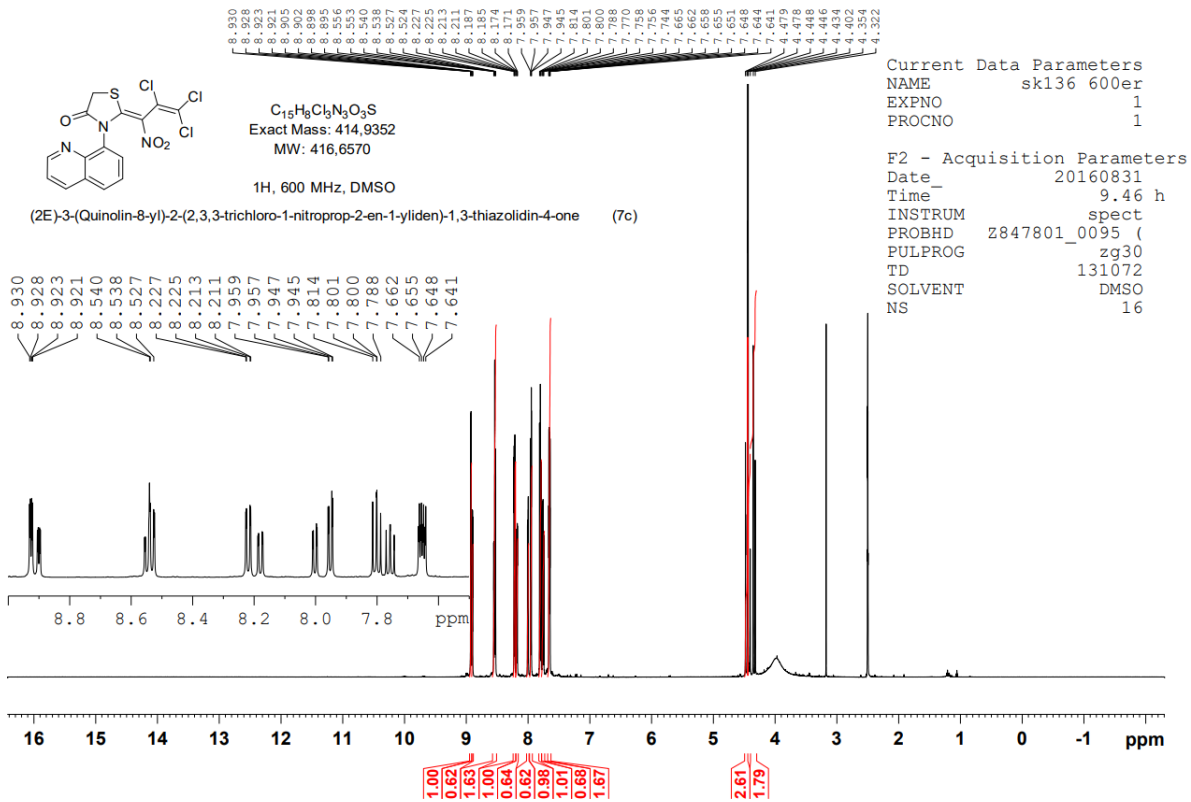
¹H and ¹³C NMR spectra of compound 6



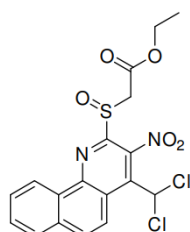
¹ H and ¹³ C NMR spectra of compound **7a**

¹H and ¹³C NMR spectra of compound **7b**



¹ H and ¹³ C NMR spectra of compound **7c**

¹H and ¹³C NMR spectra of compound **8**



¹H, 400MHz, DMSOd₆

9.21
8.69
8.40
8.39
8.13
7.96
7.92

4.64
4.41
4.08

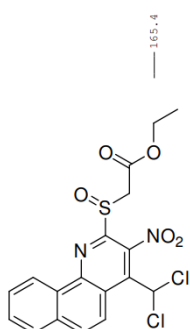
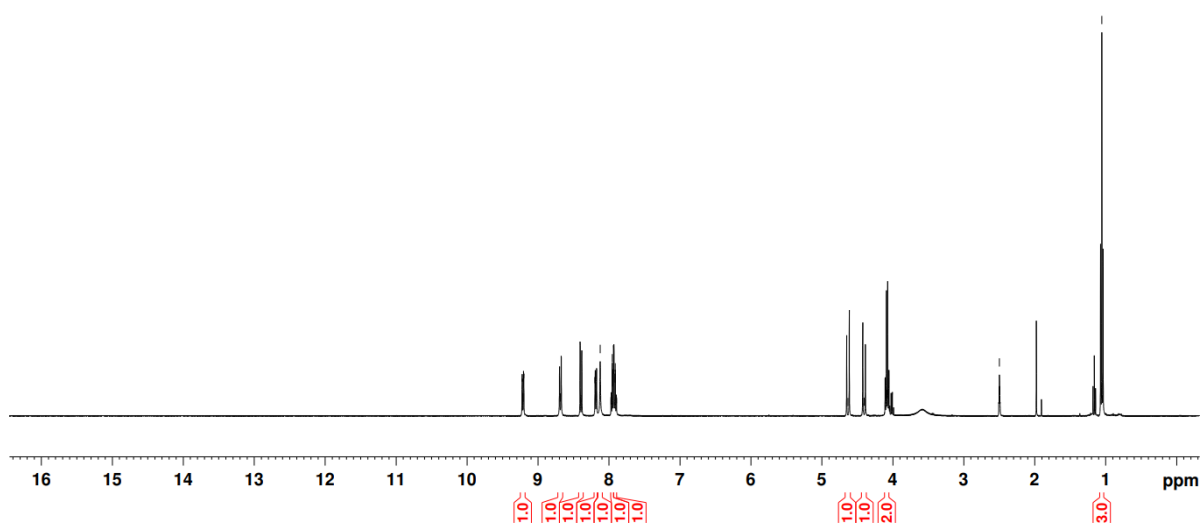
2.50

1.06

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SOLVENT DMSO

Ethyl [[4-(Dichloromethyl)-3-nitrobenzo[h]quinolin-2-yl]sulfinyl]acetate (**8**)



¹³C, 100MHz, DMSOd₆

165.4
153.5
146.9
139.4
136.3
135.2
132.2
131.3
129.8
128.4
128.4
125.4
123.1
121.7

63.9
61.7
58.1

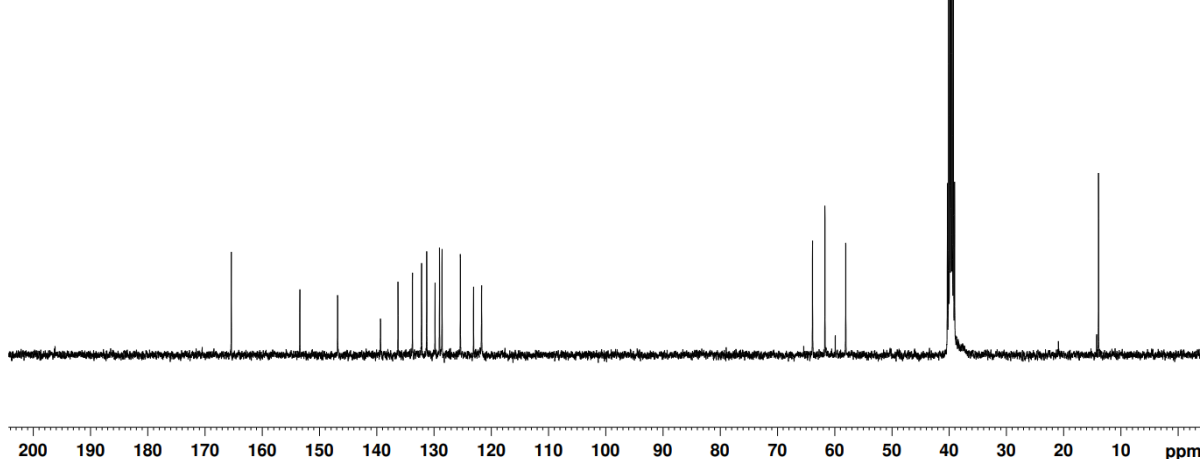
39.7

13.9

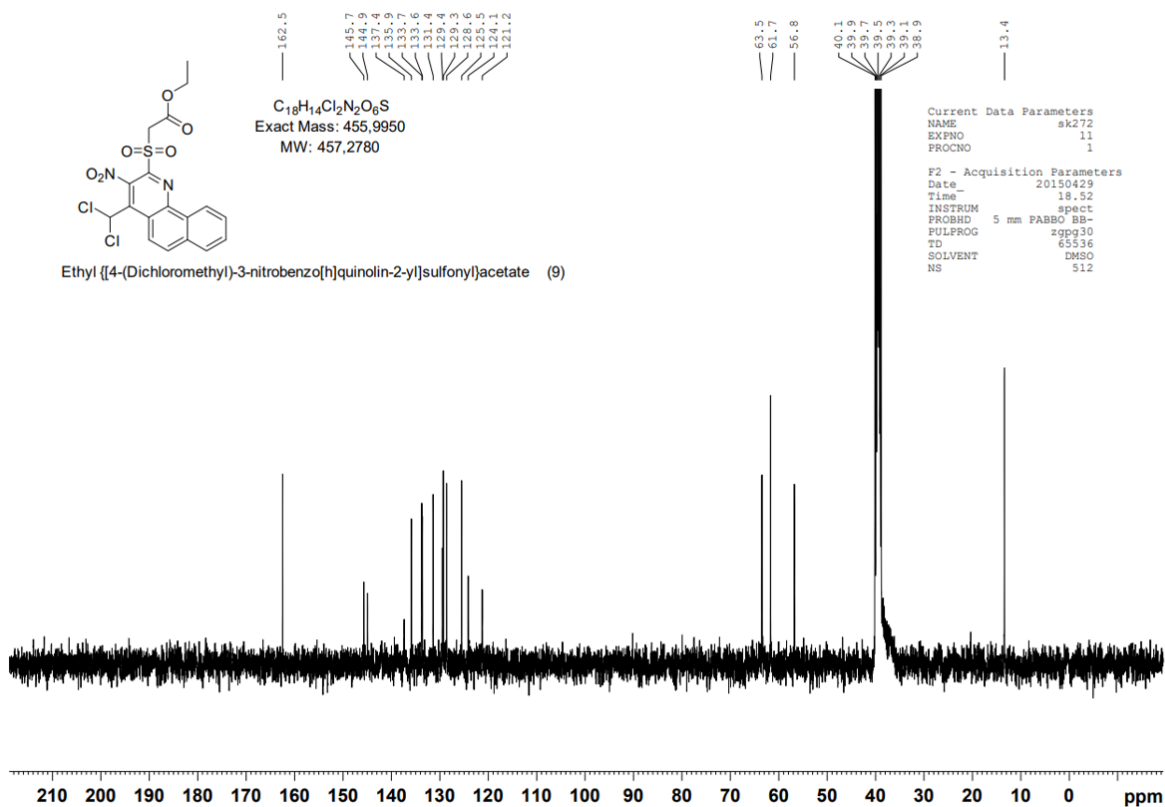
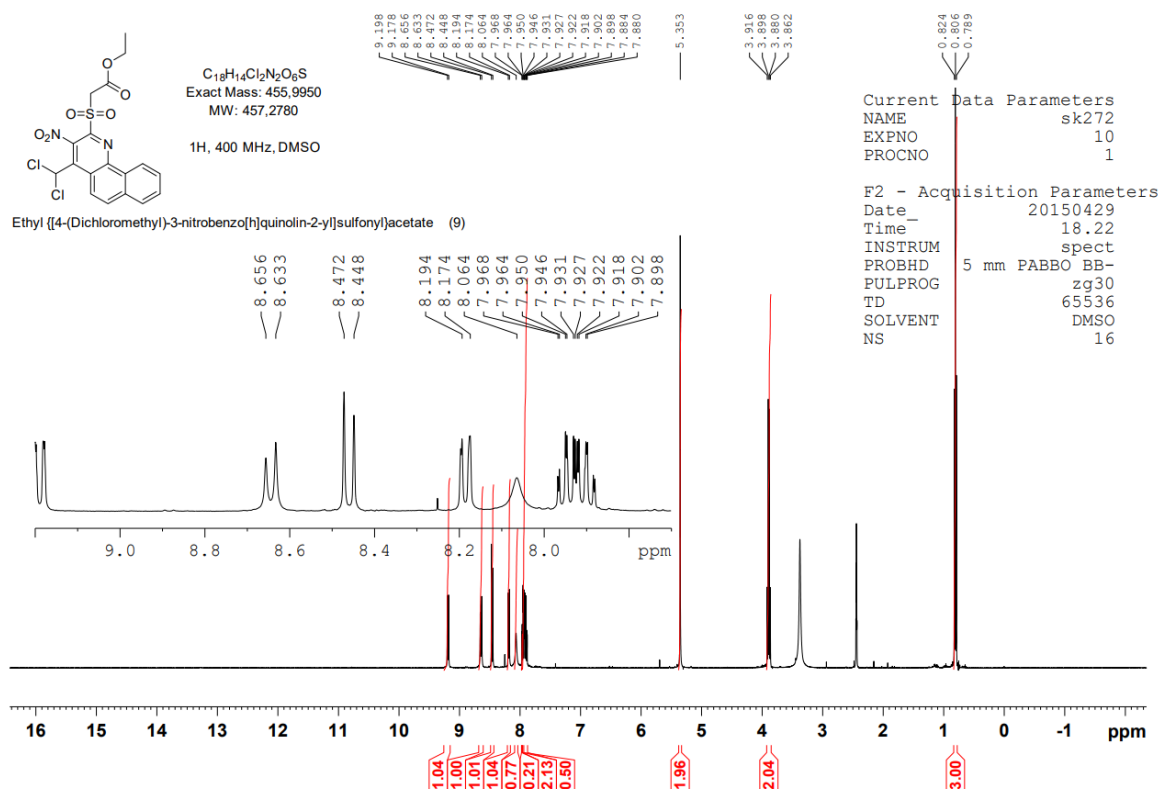
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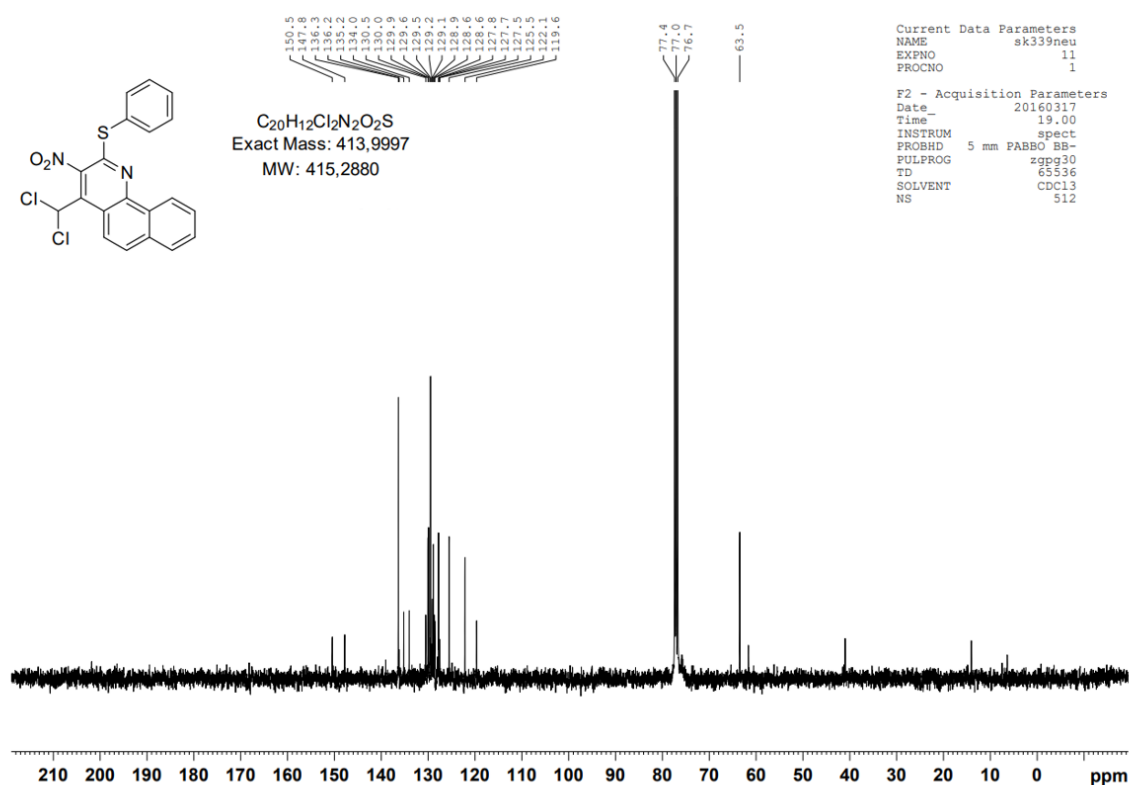
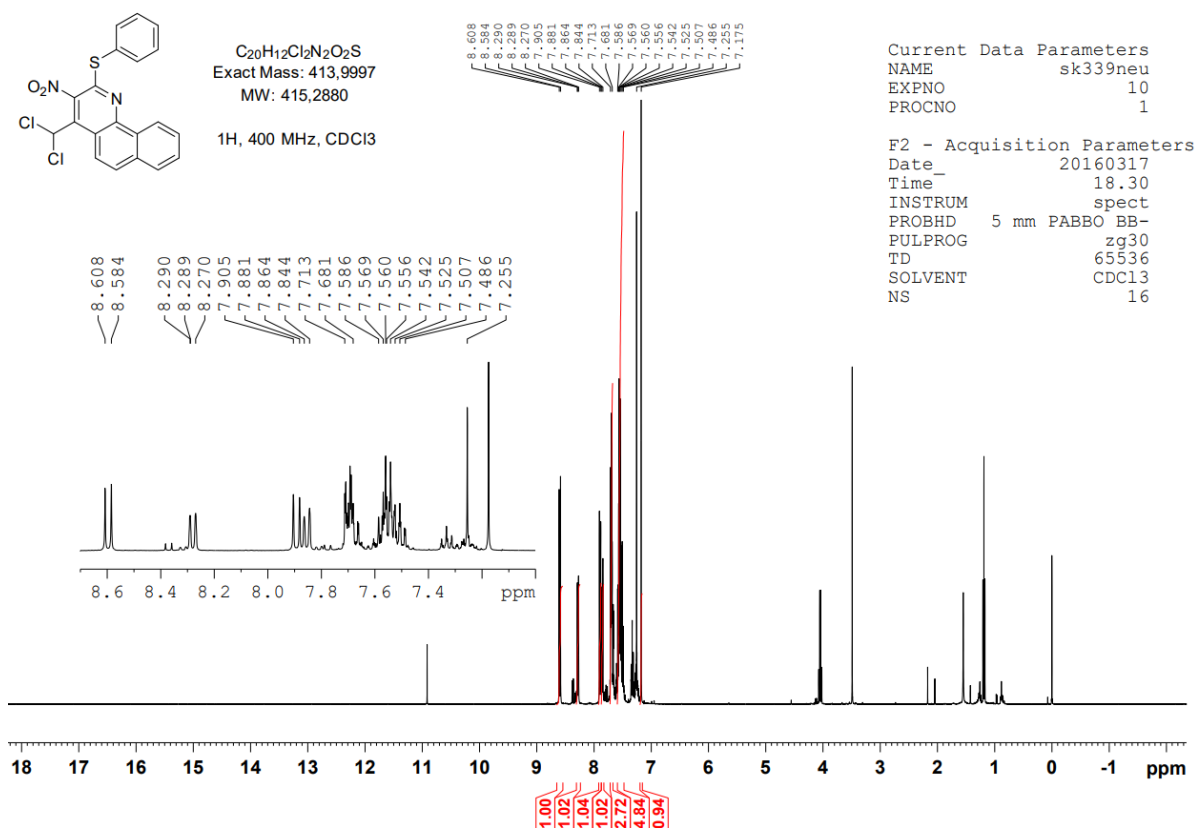
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NS 512

Ethyl [[4-(Dichloromethyl)-3-nitrobenzo[h]quinolin-2-yl]sulfinyl]acetate (**8**)

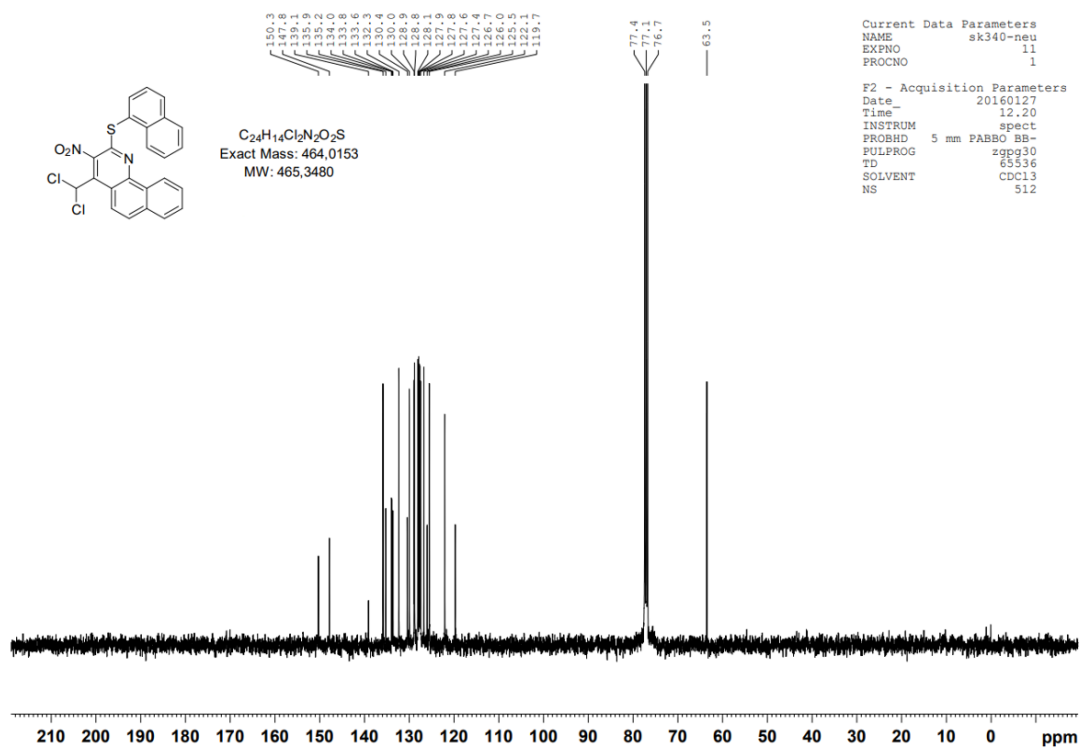
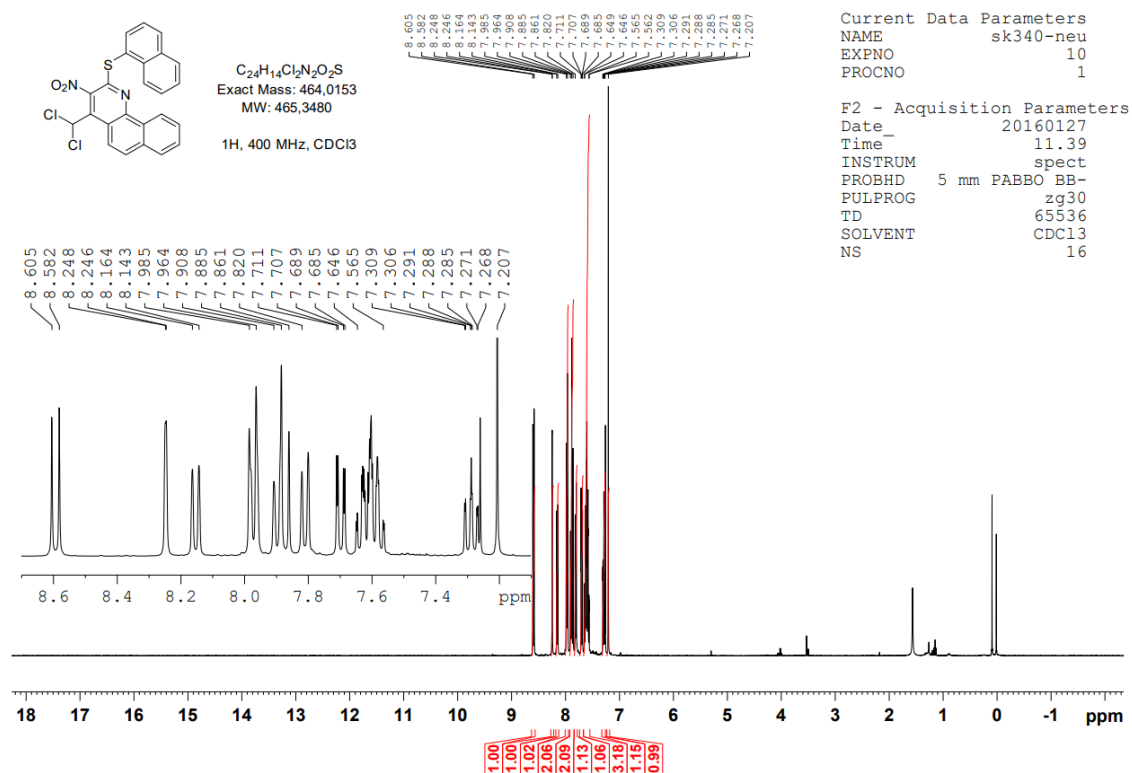


¹H and ¹³C NMR spectra of compound 9

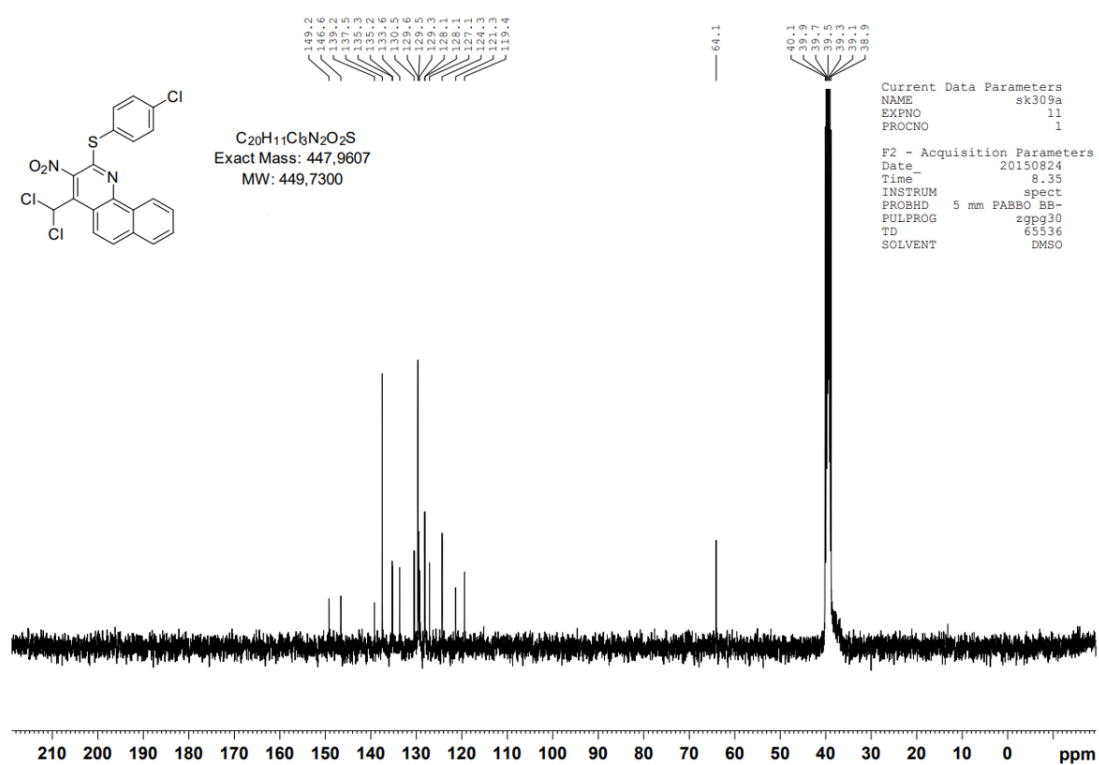
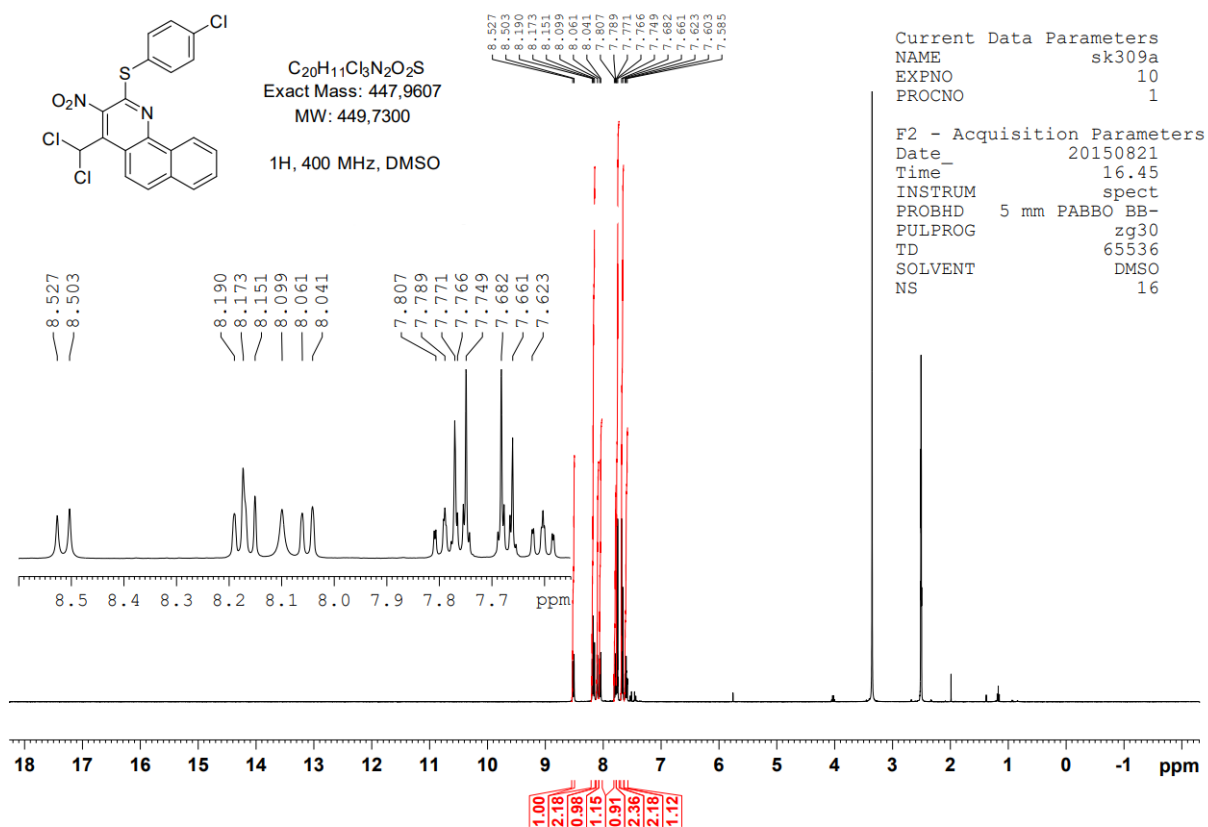




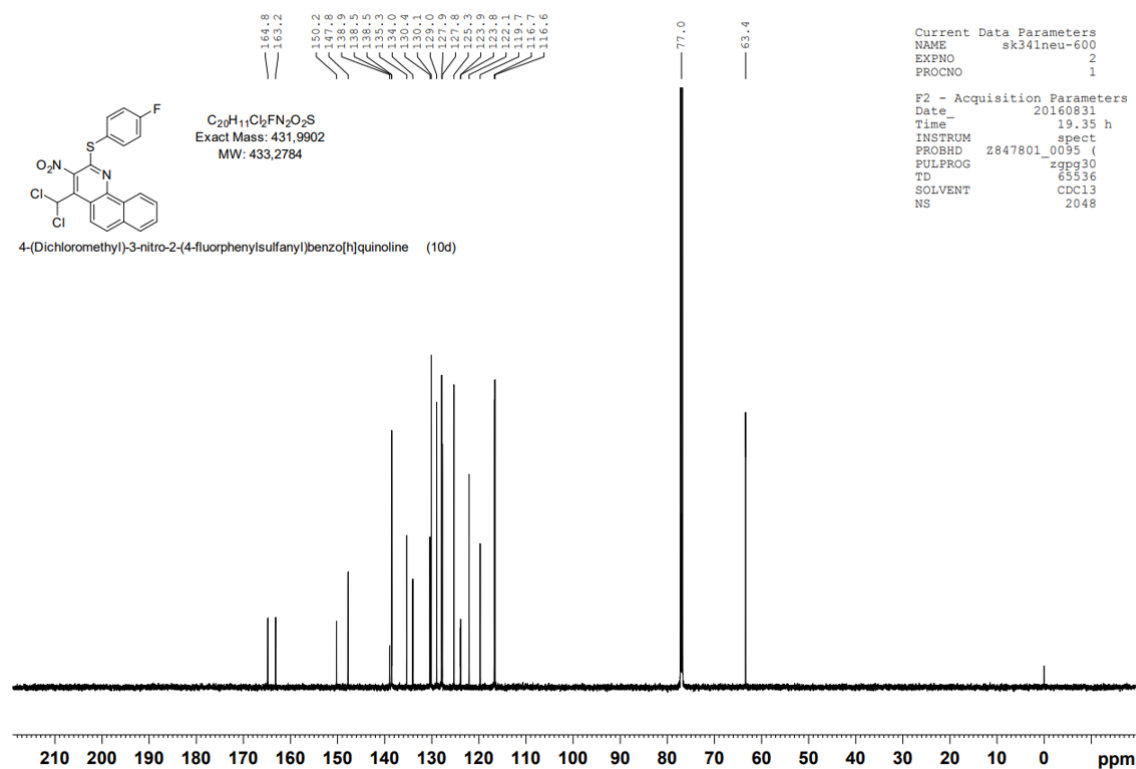
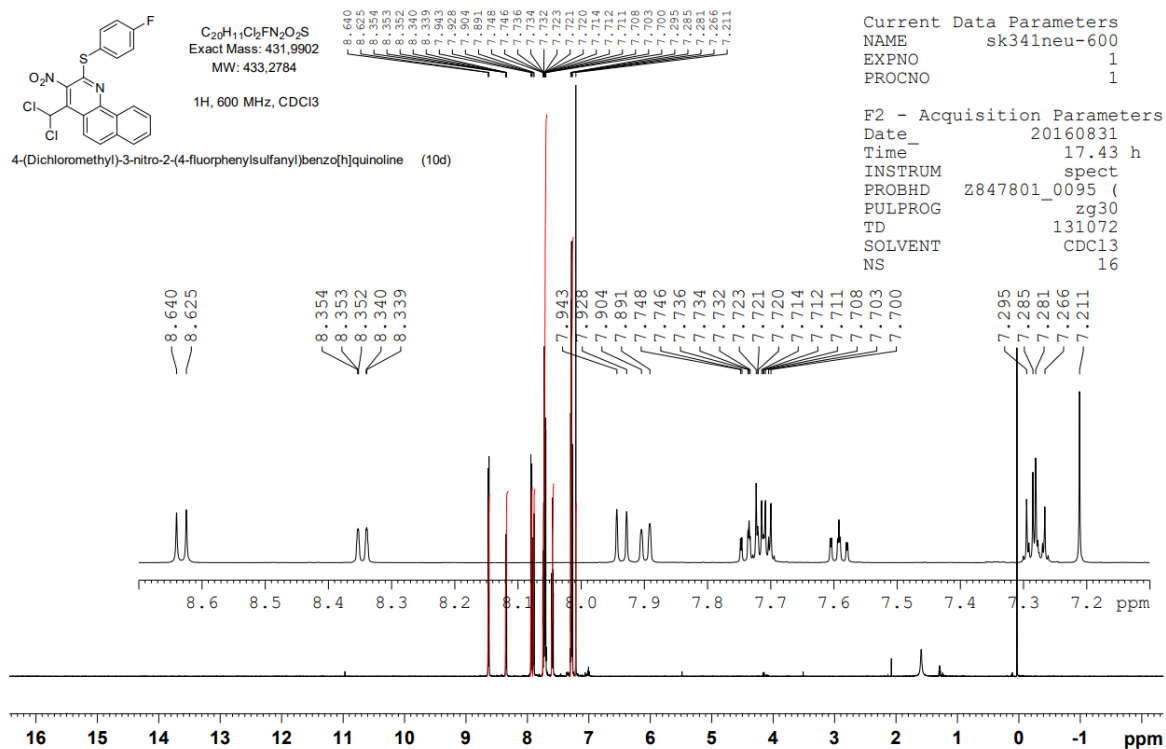
¹H and ¹³C NMR spectra of compound **10b**



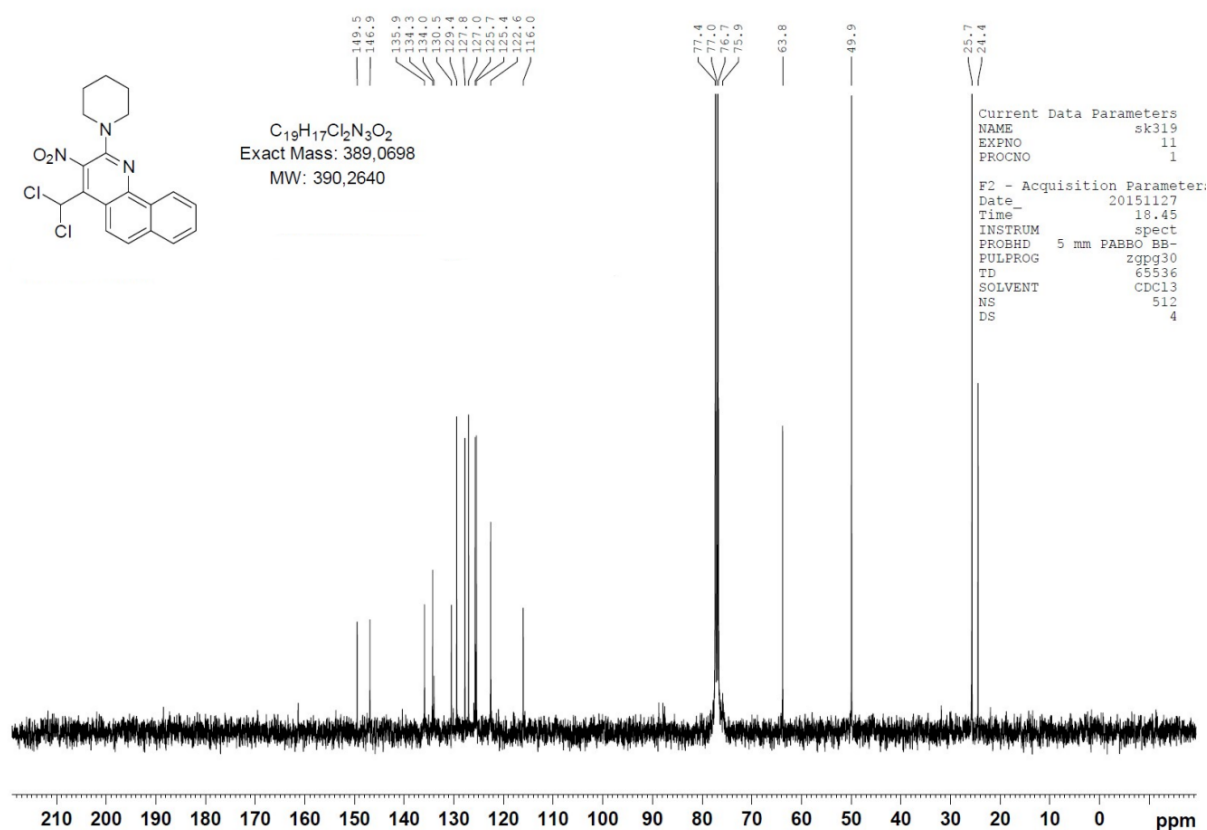
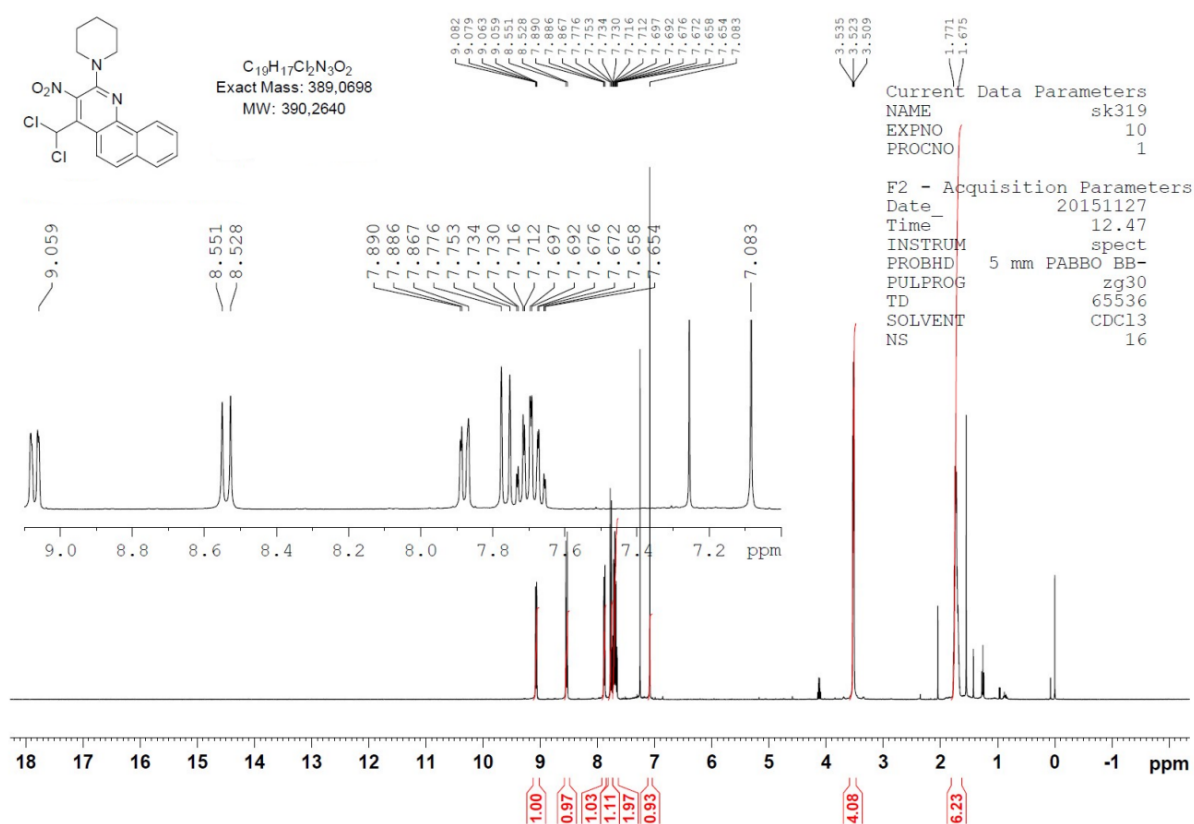
¹H and ¹³C NMR spectra of compound **10c**



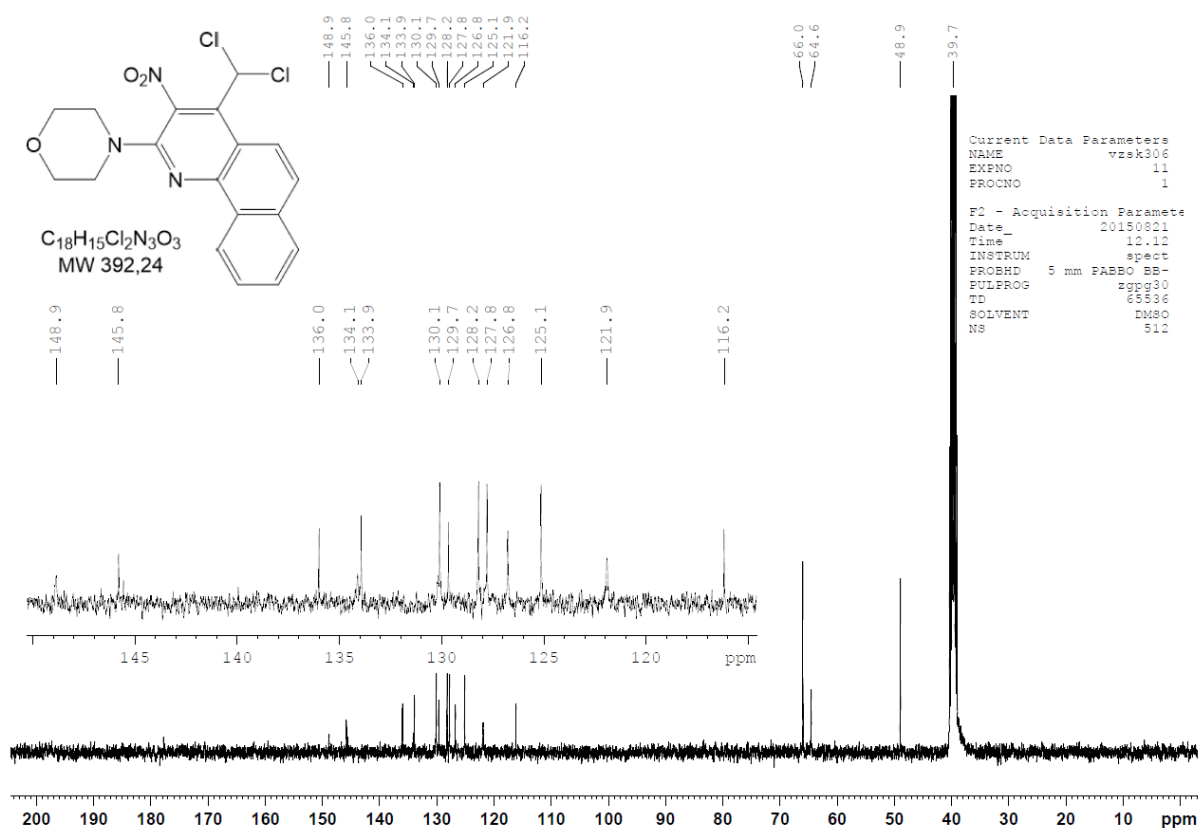
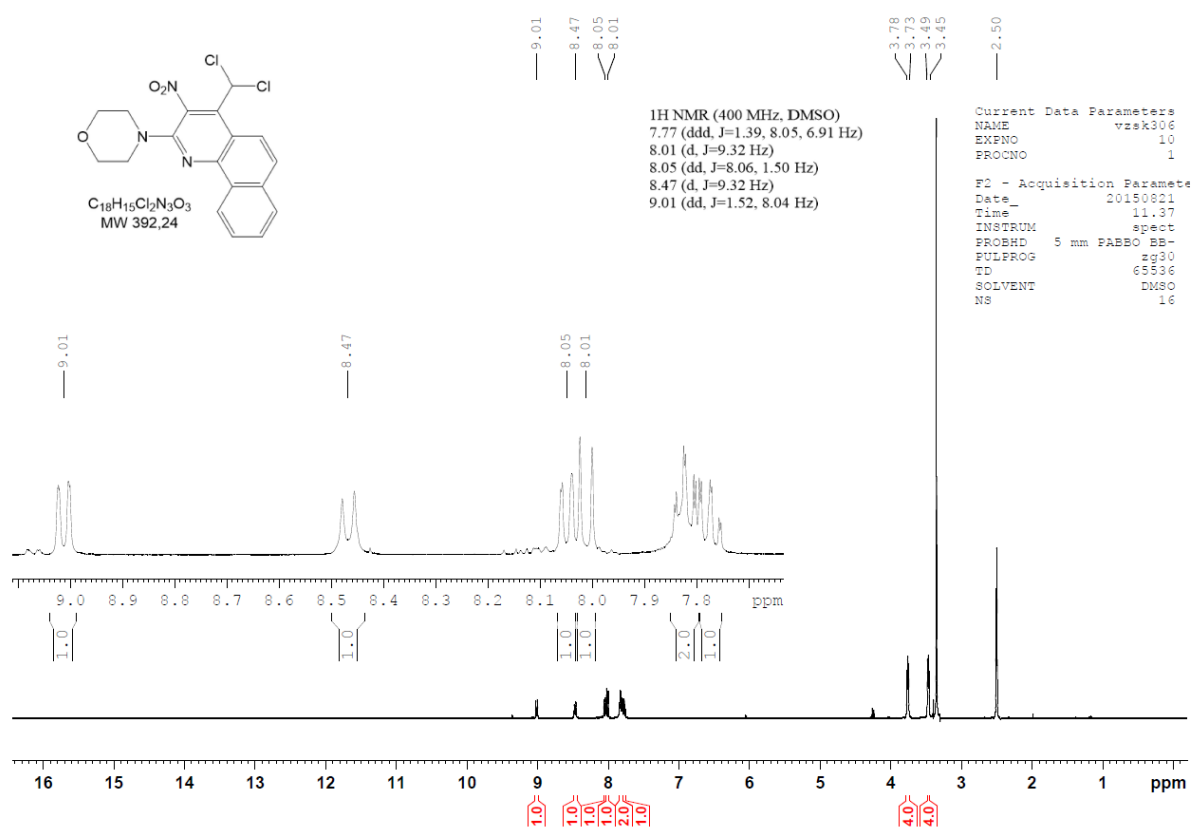
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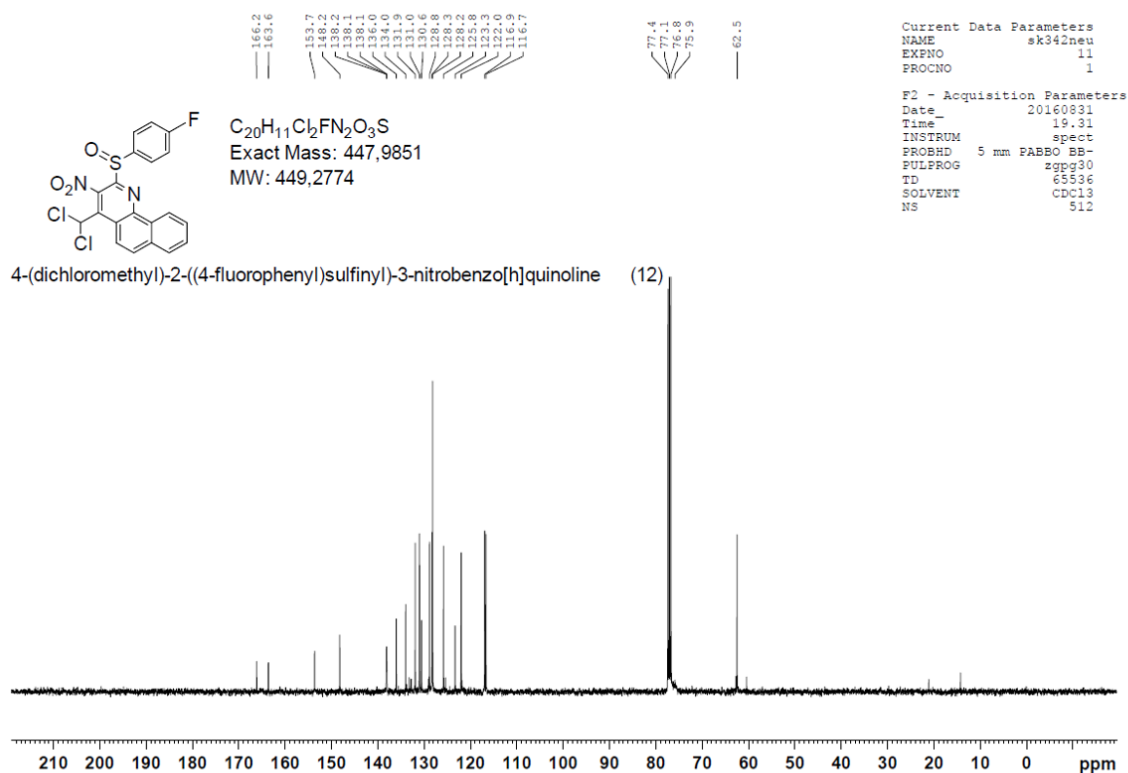
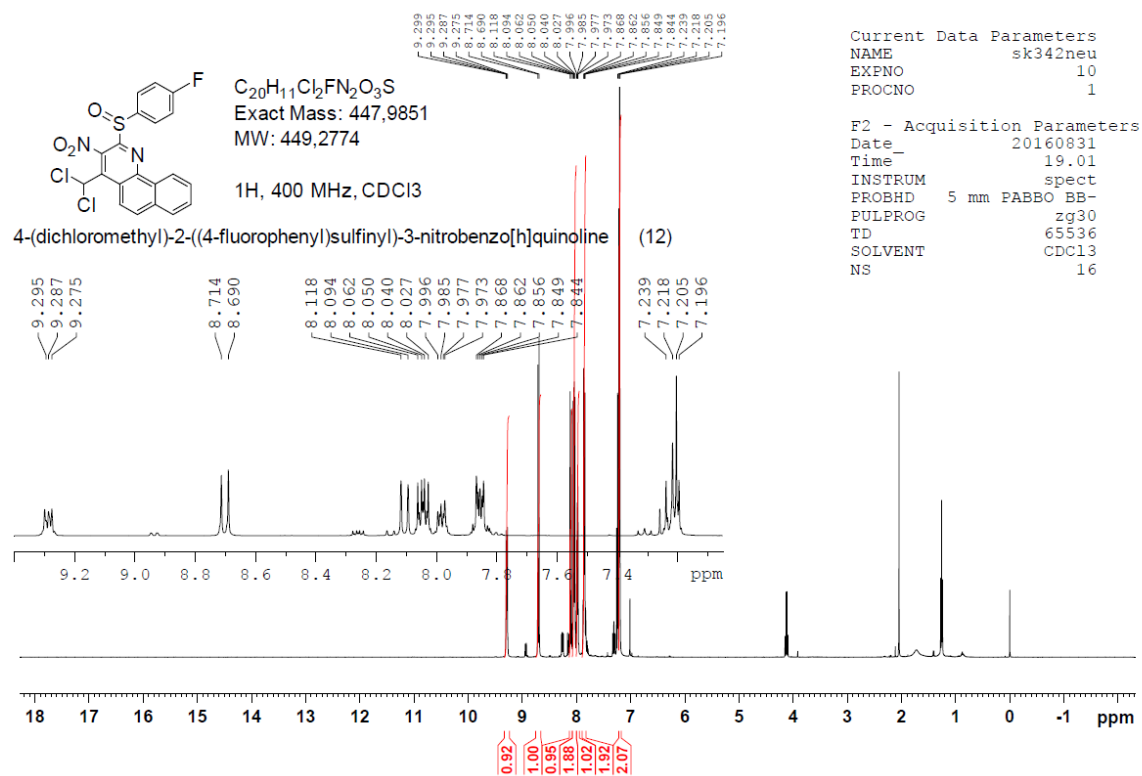
¹H and ¹³C NMR spectra of compound **11a**



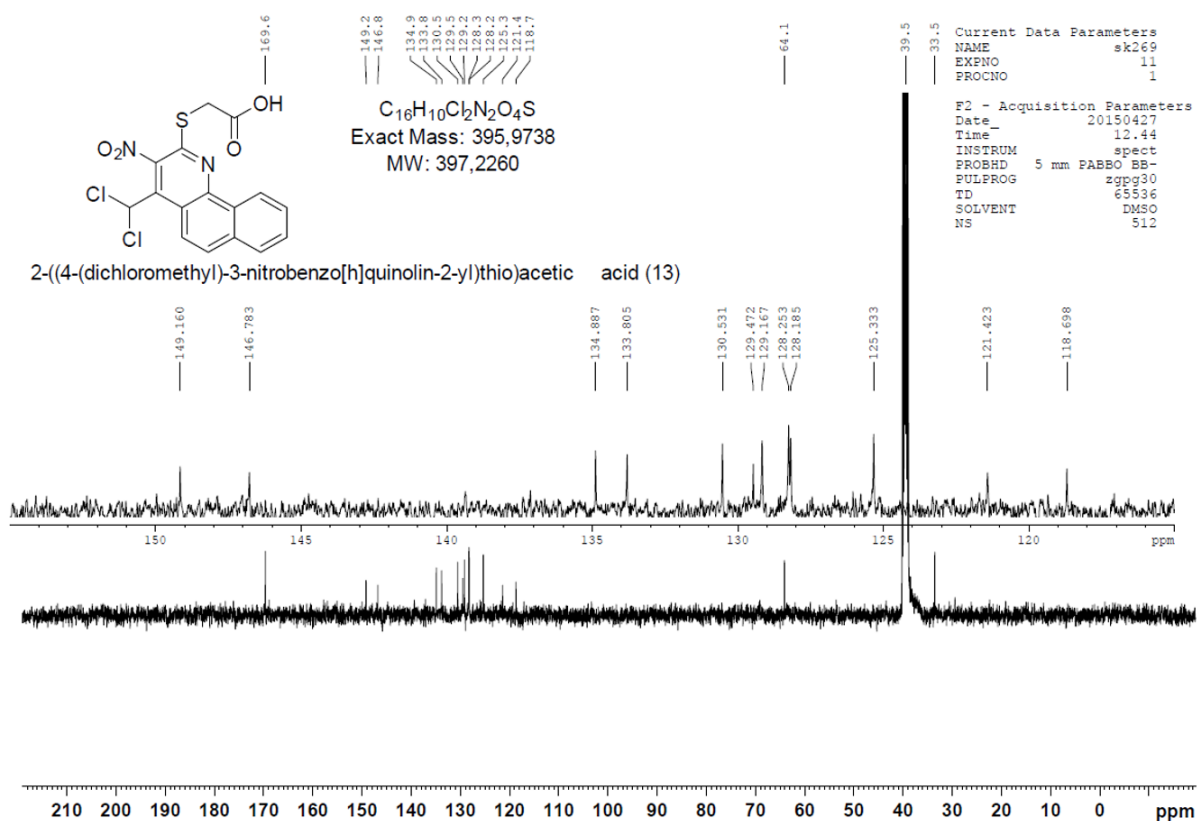
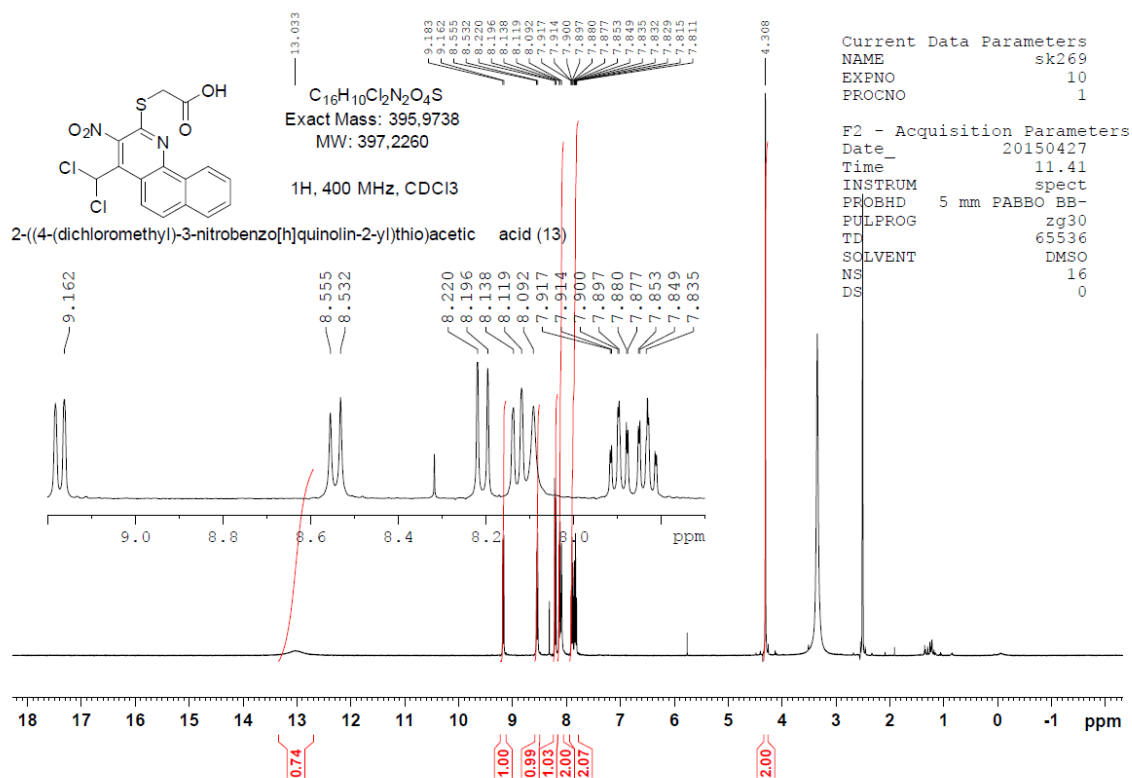
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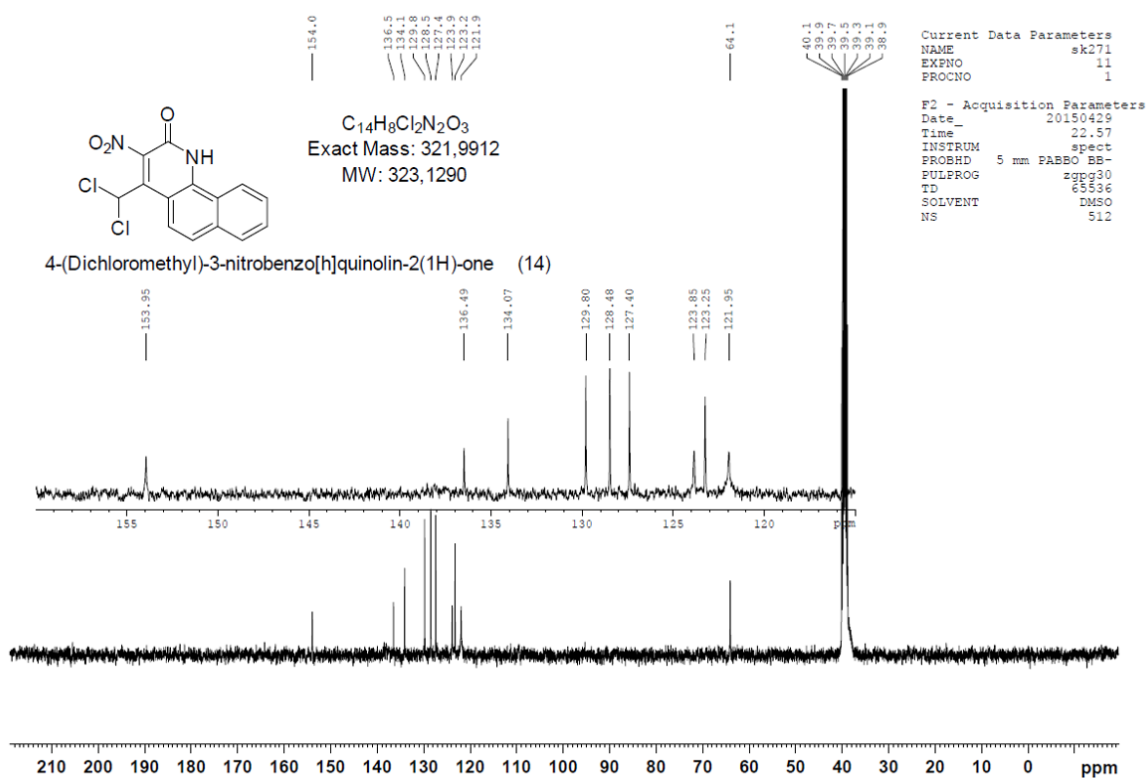
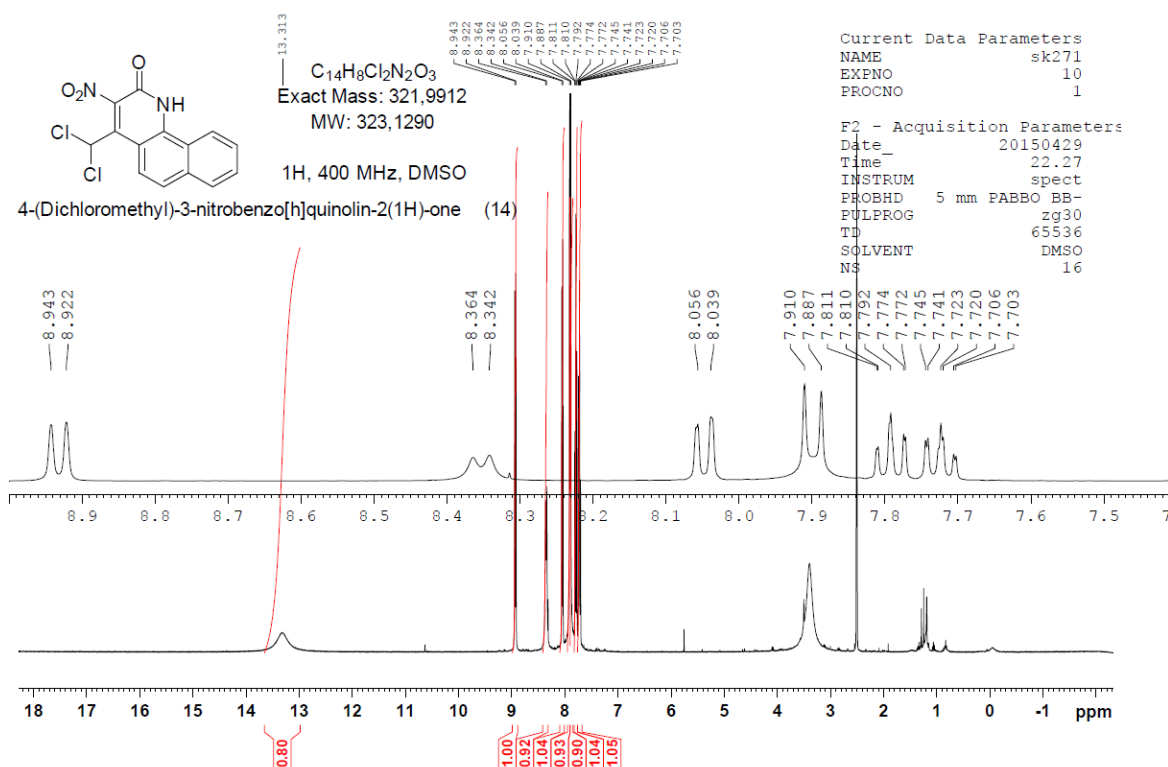
¹H and ¹³C NMR spectra of compound **12**



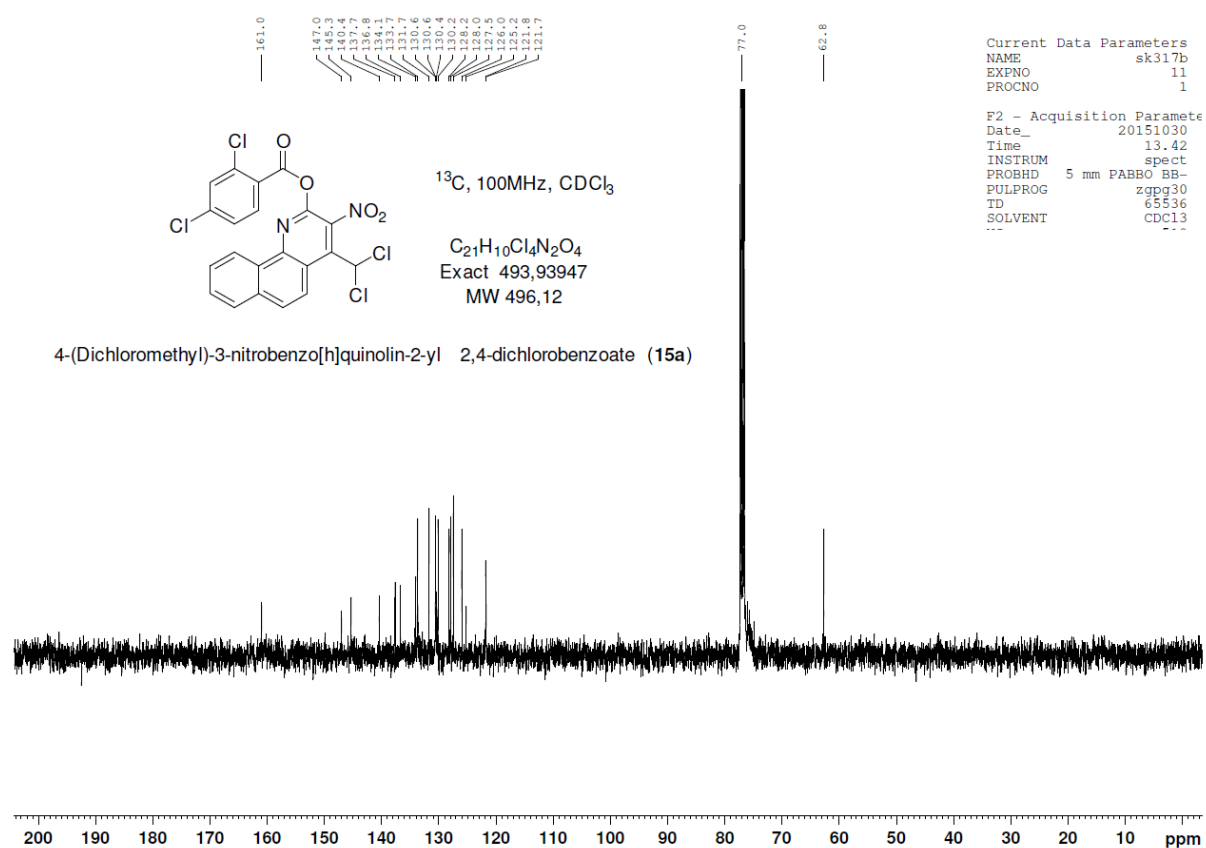
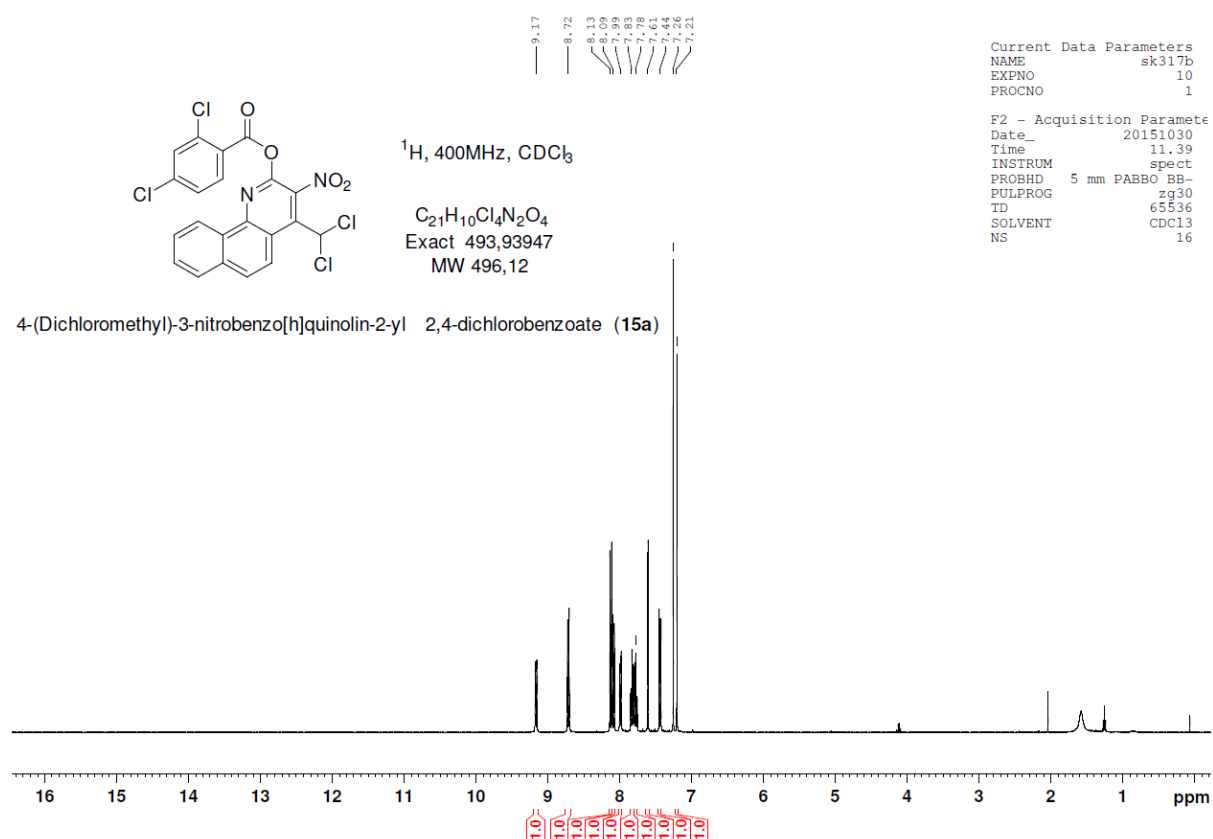
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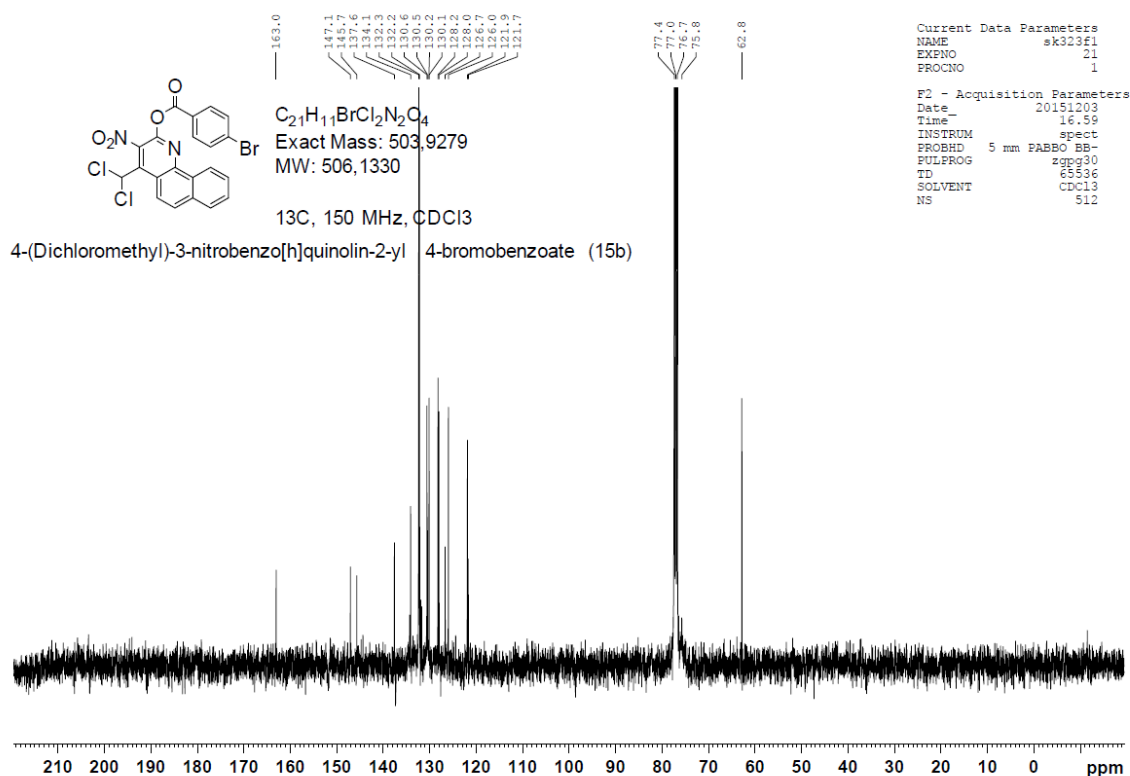
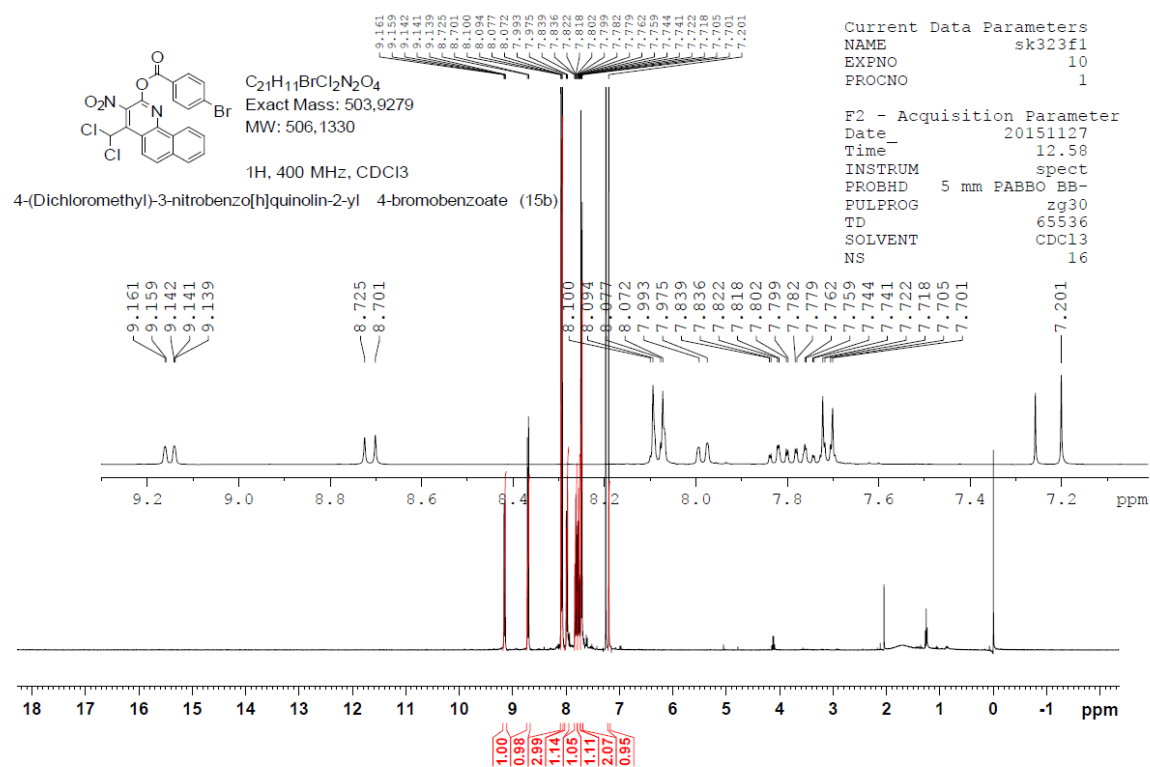
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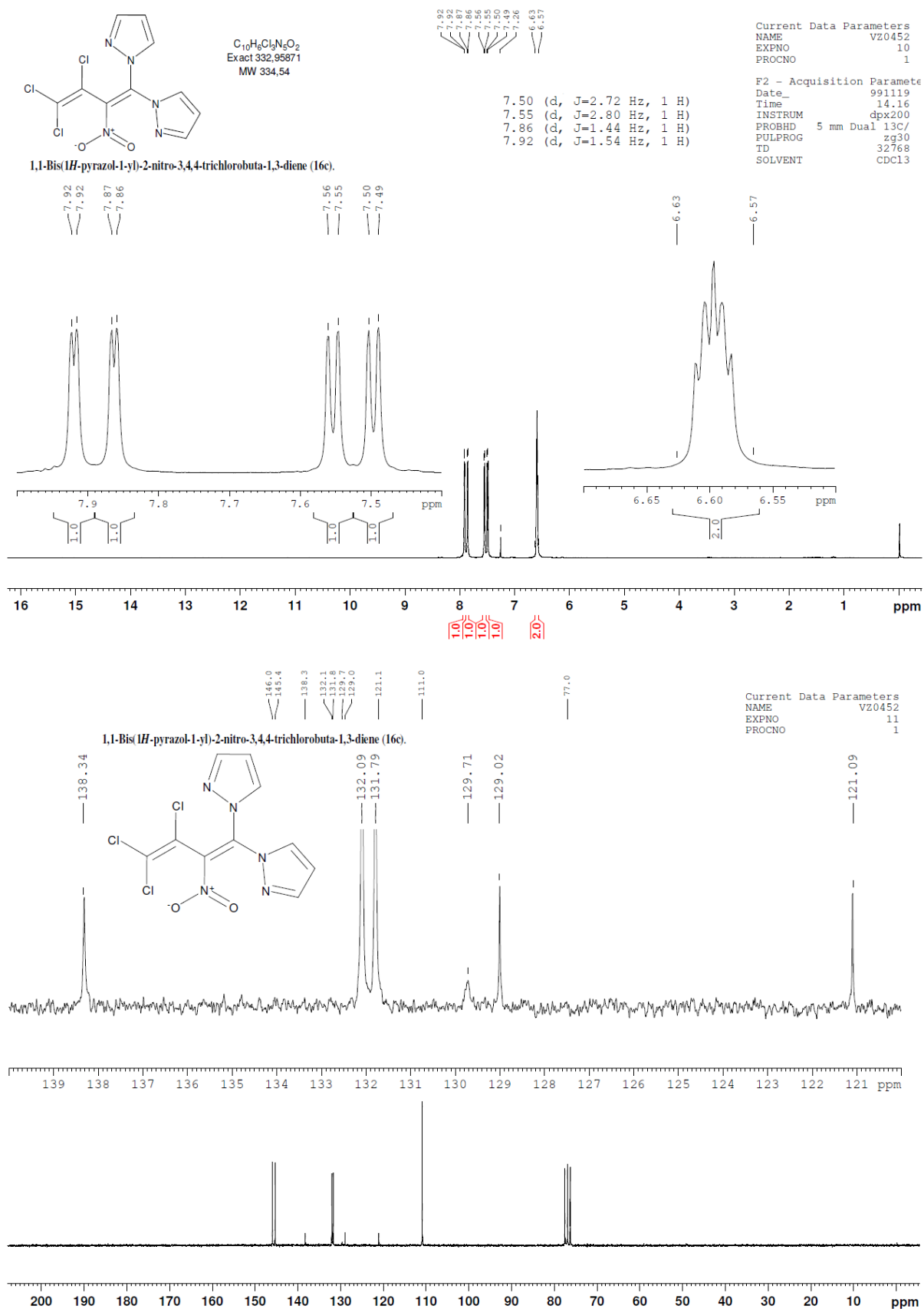
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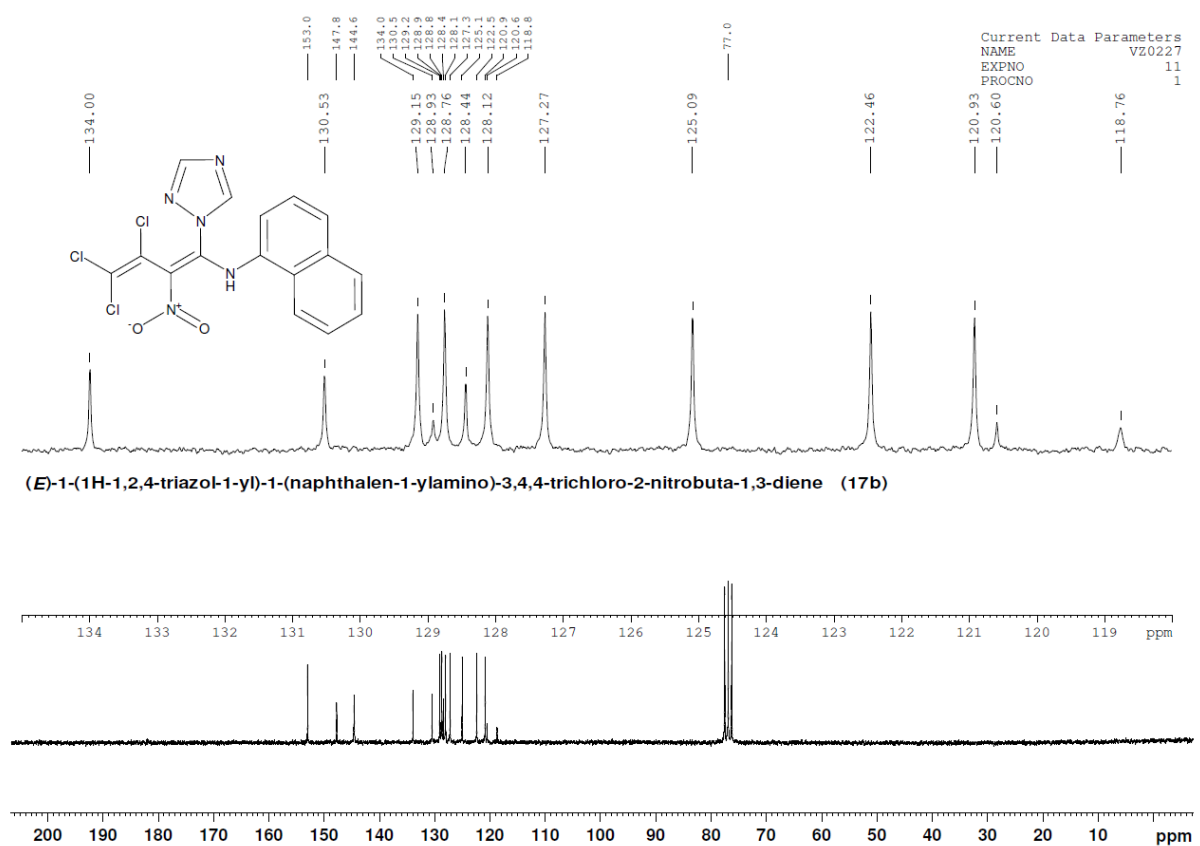
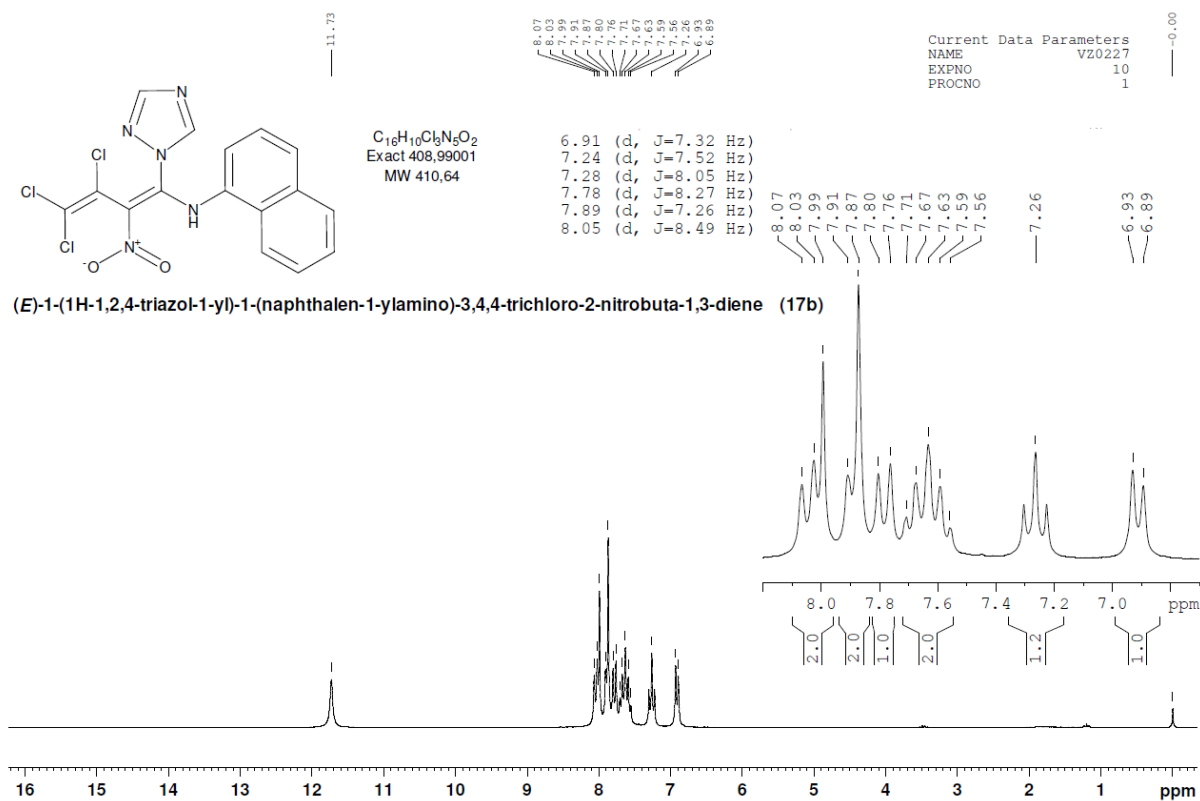
¹H and ¹³C NMR spectra of compound **15b**

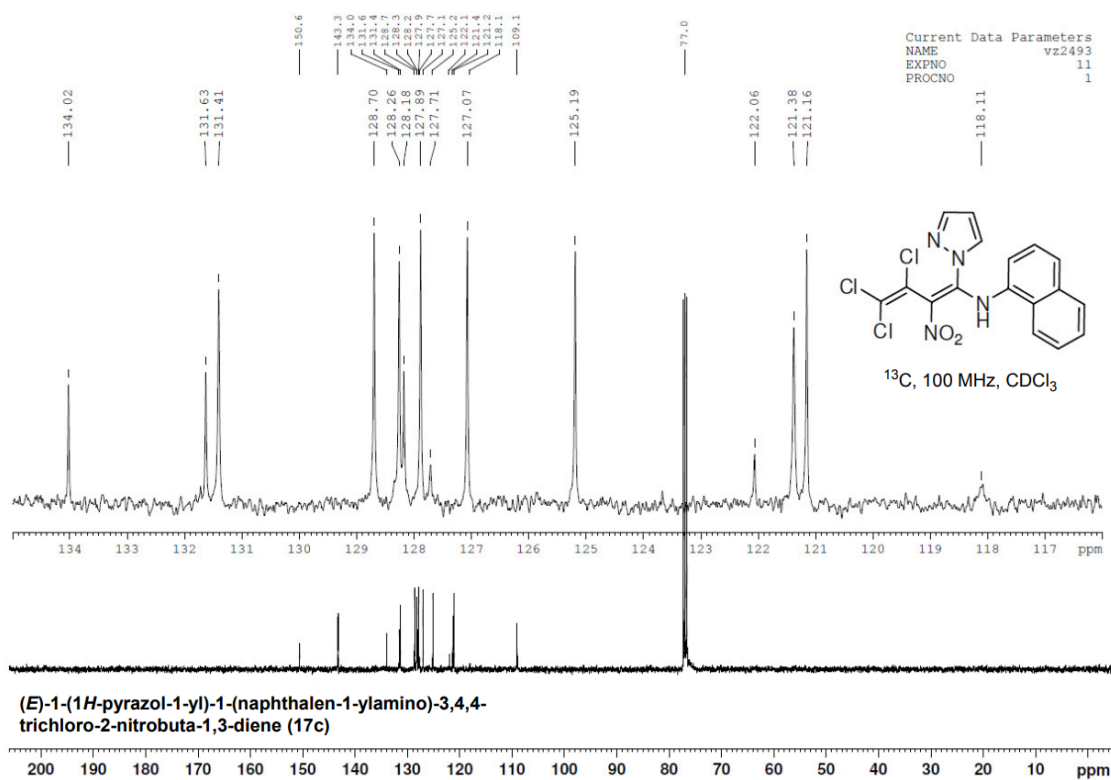
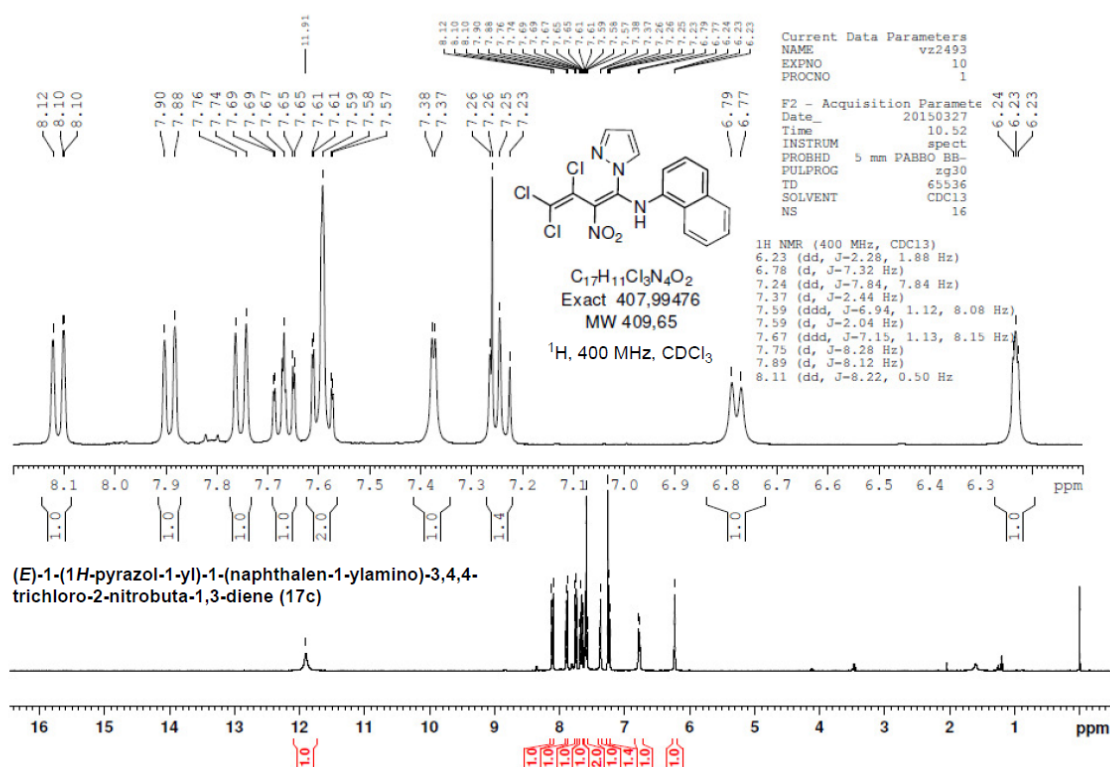


¹H and ¹³C NMR spectra of compound **16c**

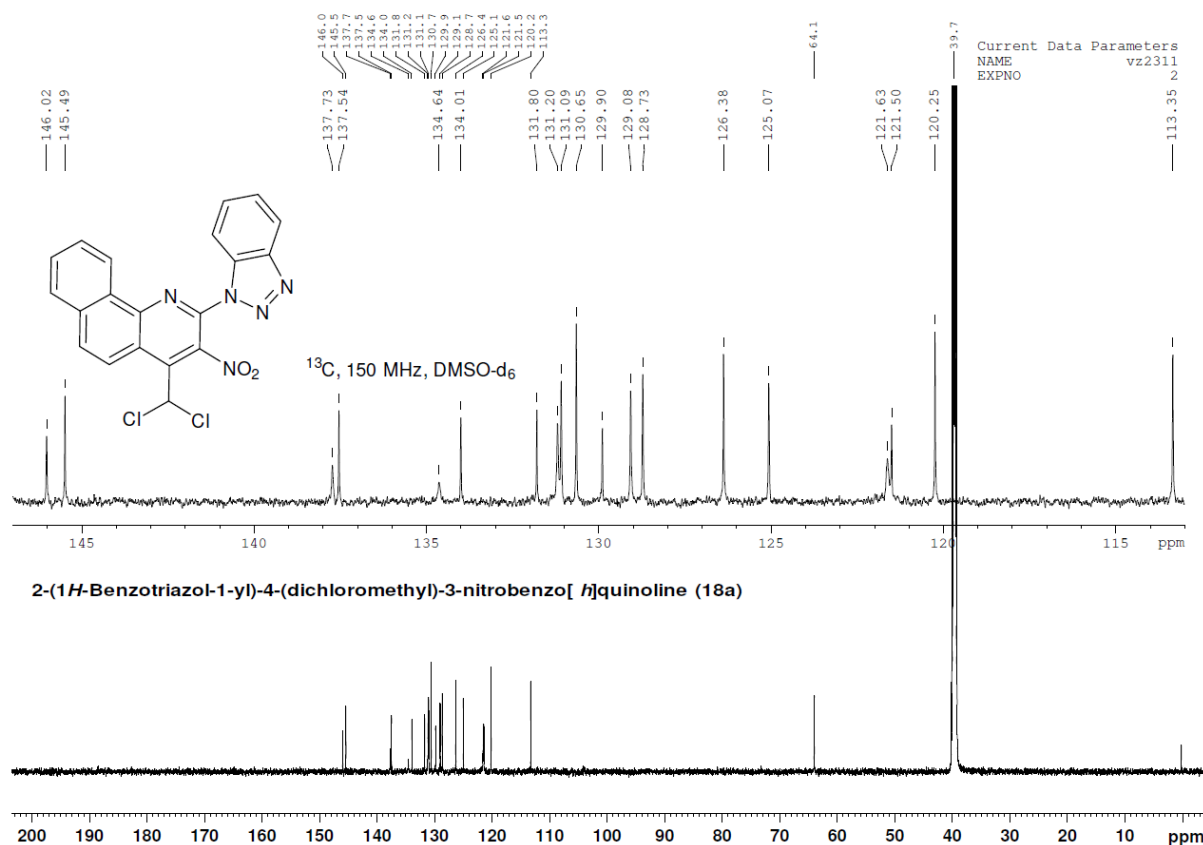
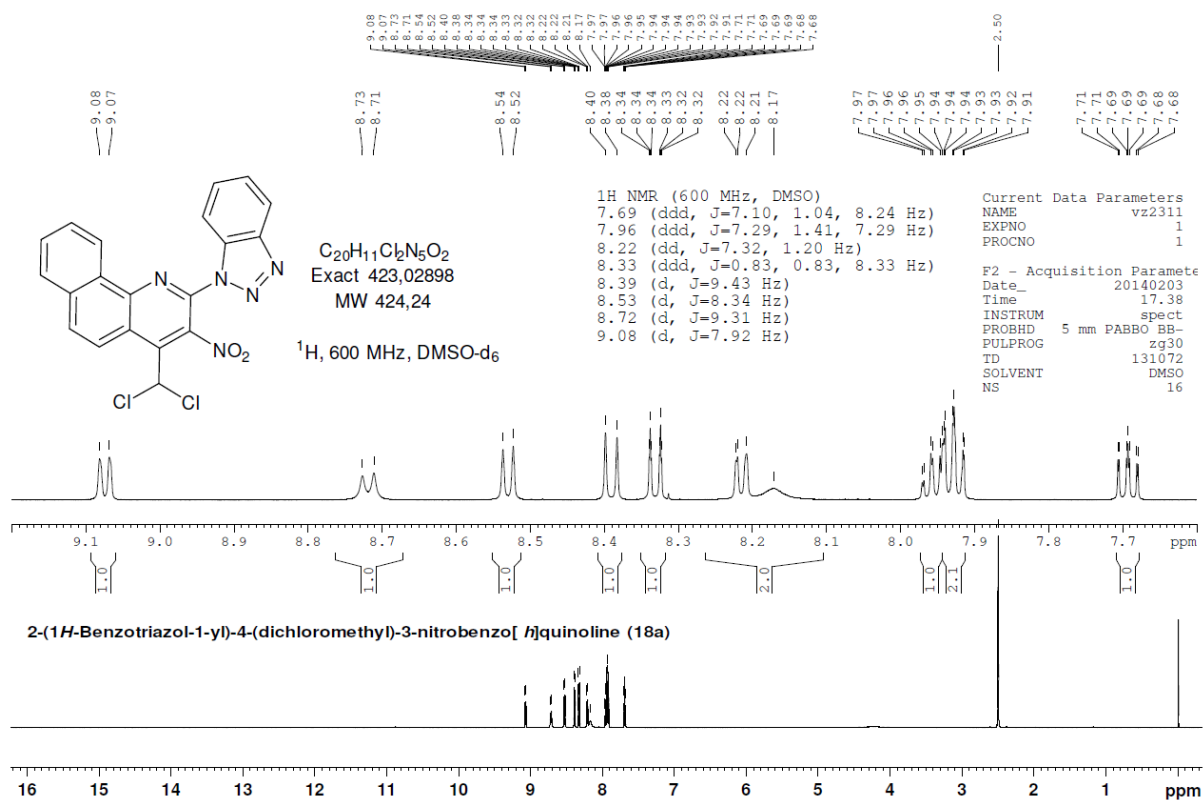


¹H and ¹³C NMR spectra of compound **17b**

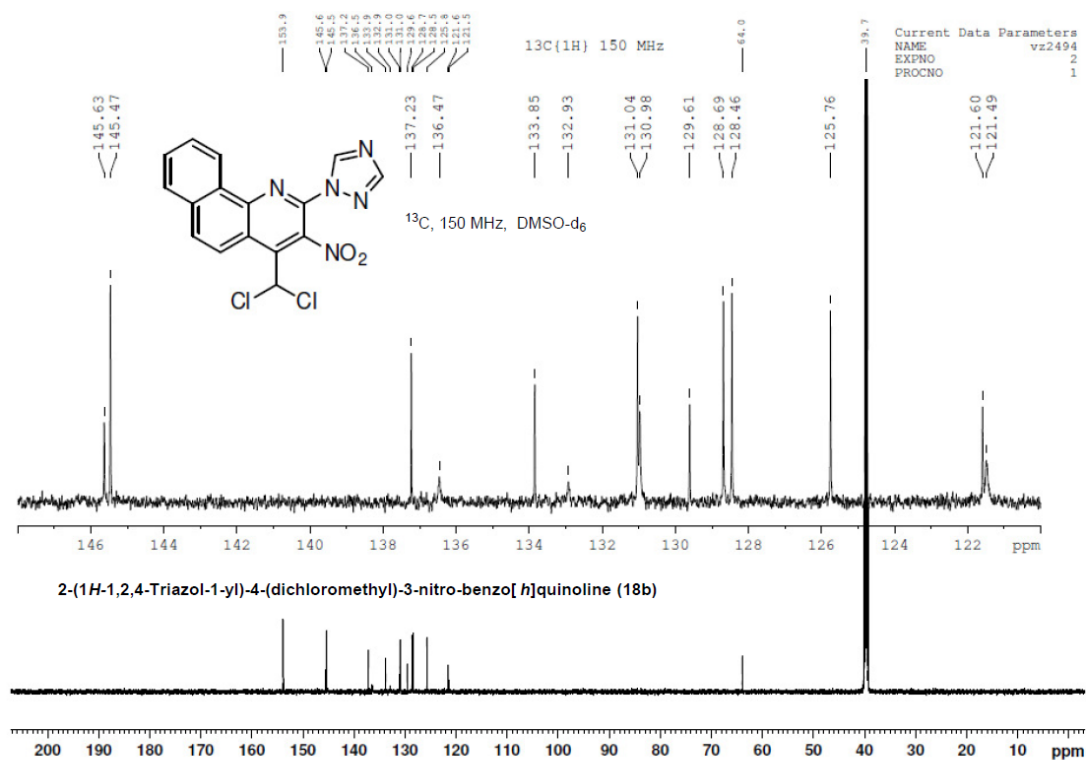
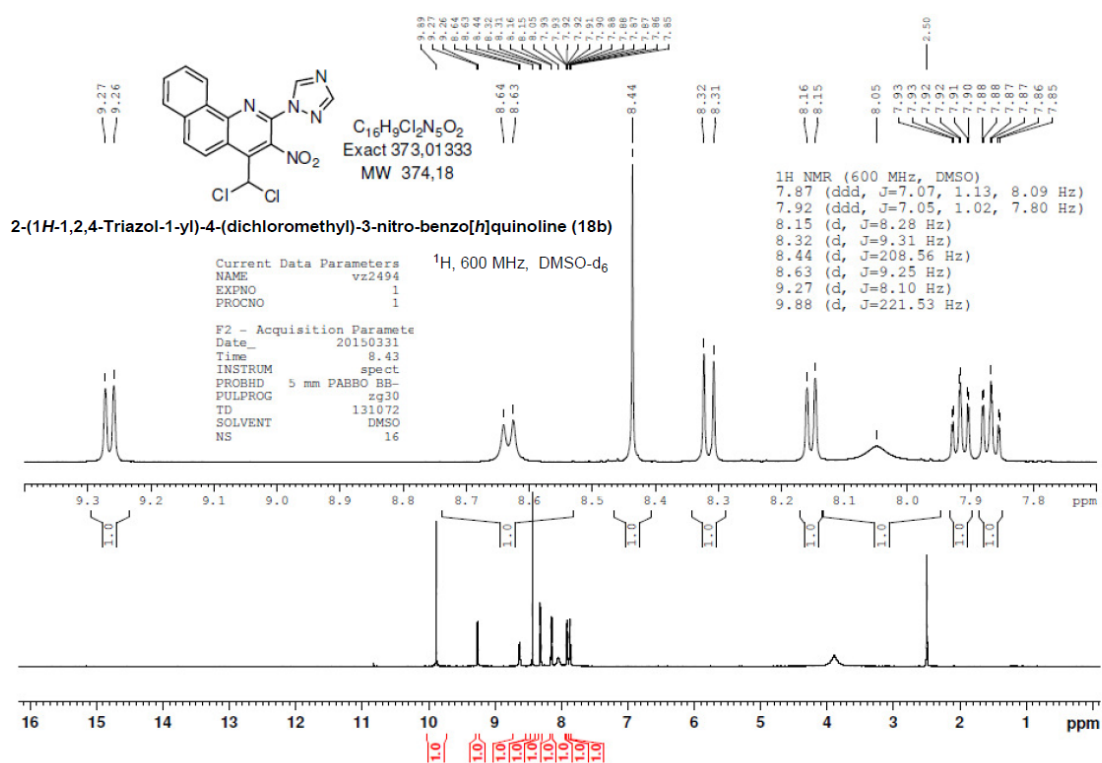


¹ H and ¹³ C NMR spectra of compound **17c**

¹H and ¹³C NMR spectra of compound **18a**



¹H and ¹³C NMR spectra of compound **18b**



¹ H and ¹³ C NMR spectra of compound **18c**