

Supporting Information

One-Pot Multicomponent Synthesis of Indole-Linked Fully Substituted Fused-Pyrroles

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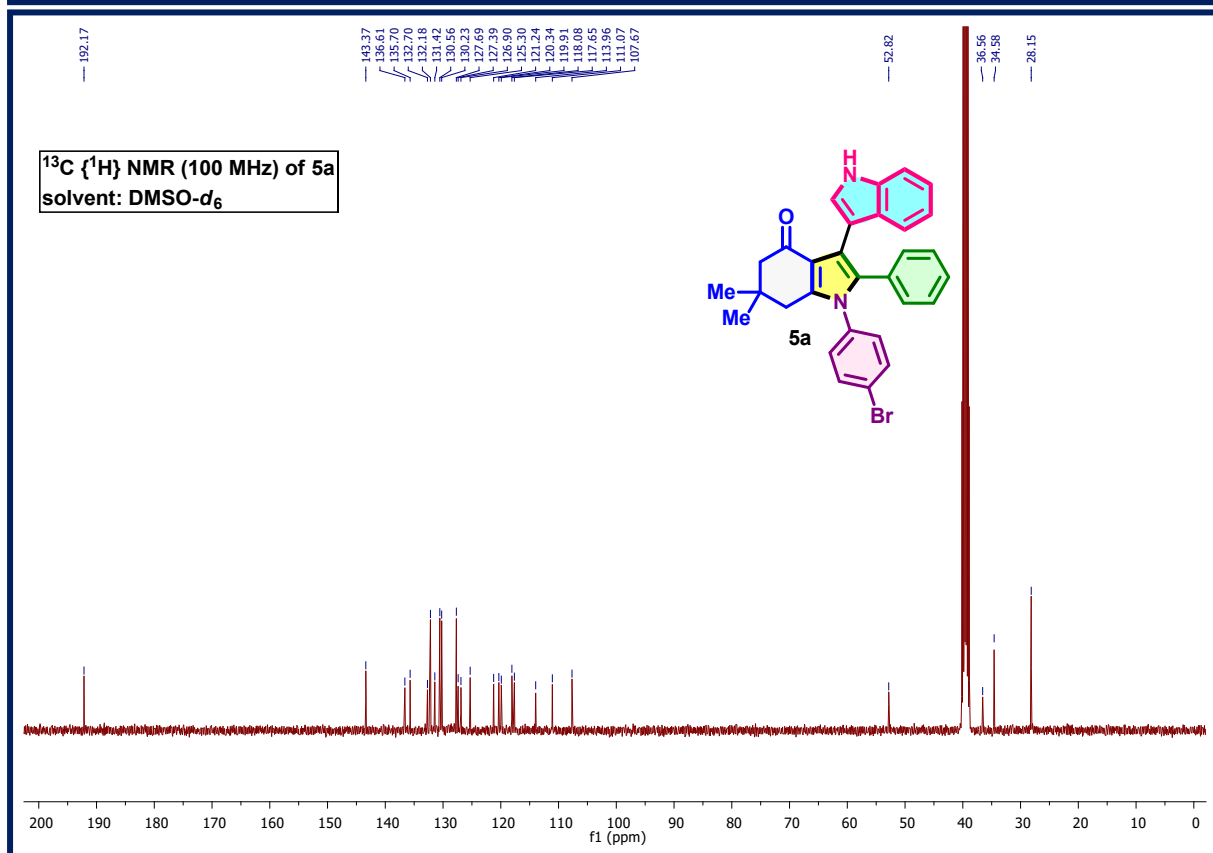
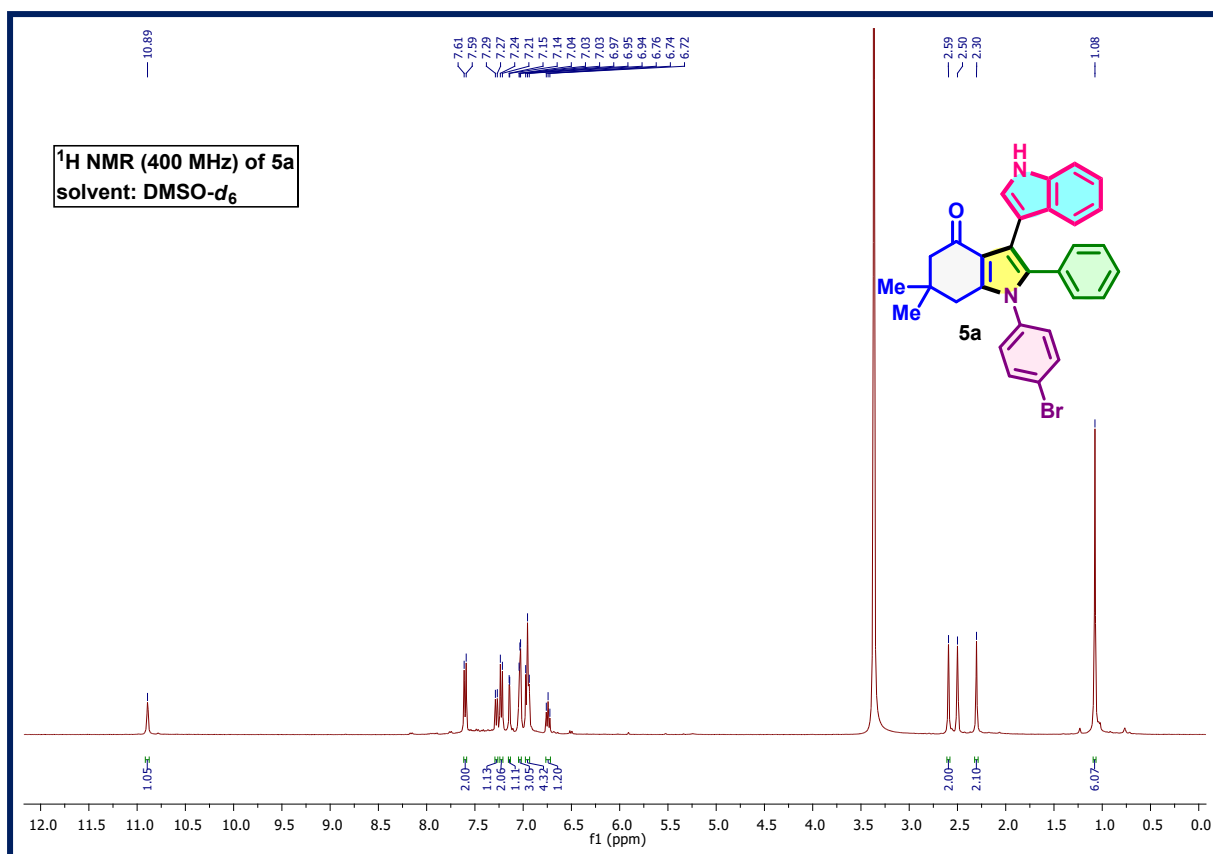
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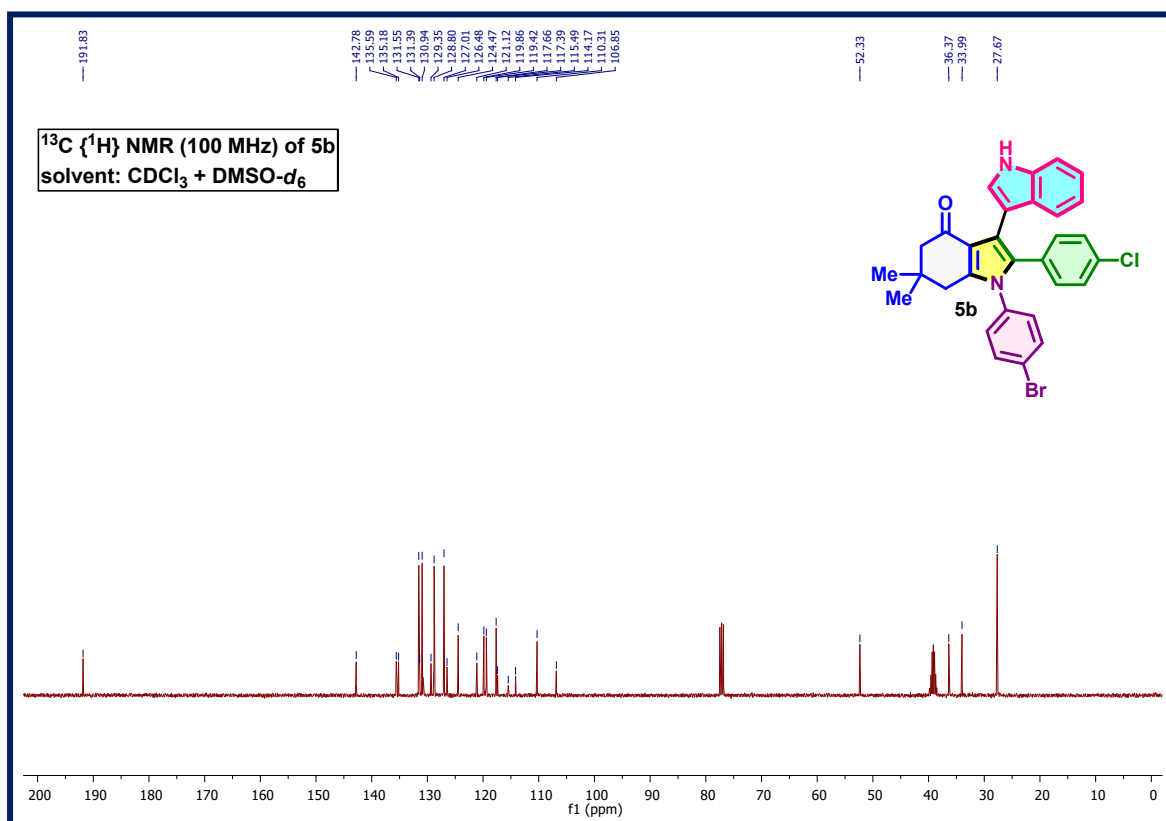
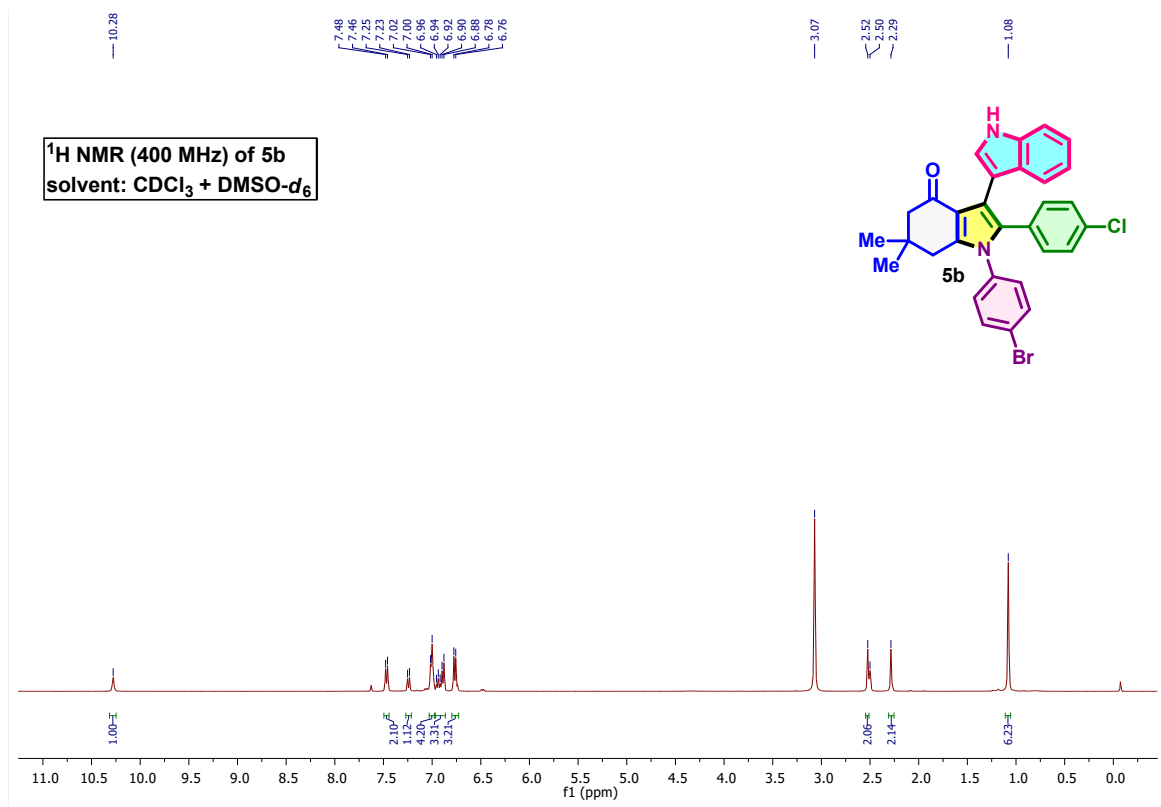
¹H, and ¹³C{¹H} NMR spectra of **5a**

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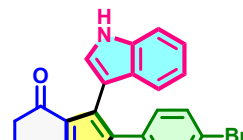
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of **5b**

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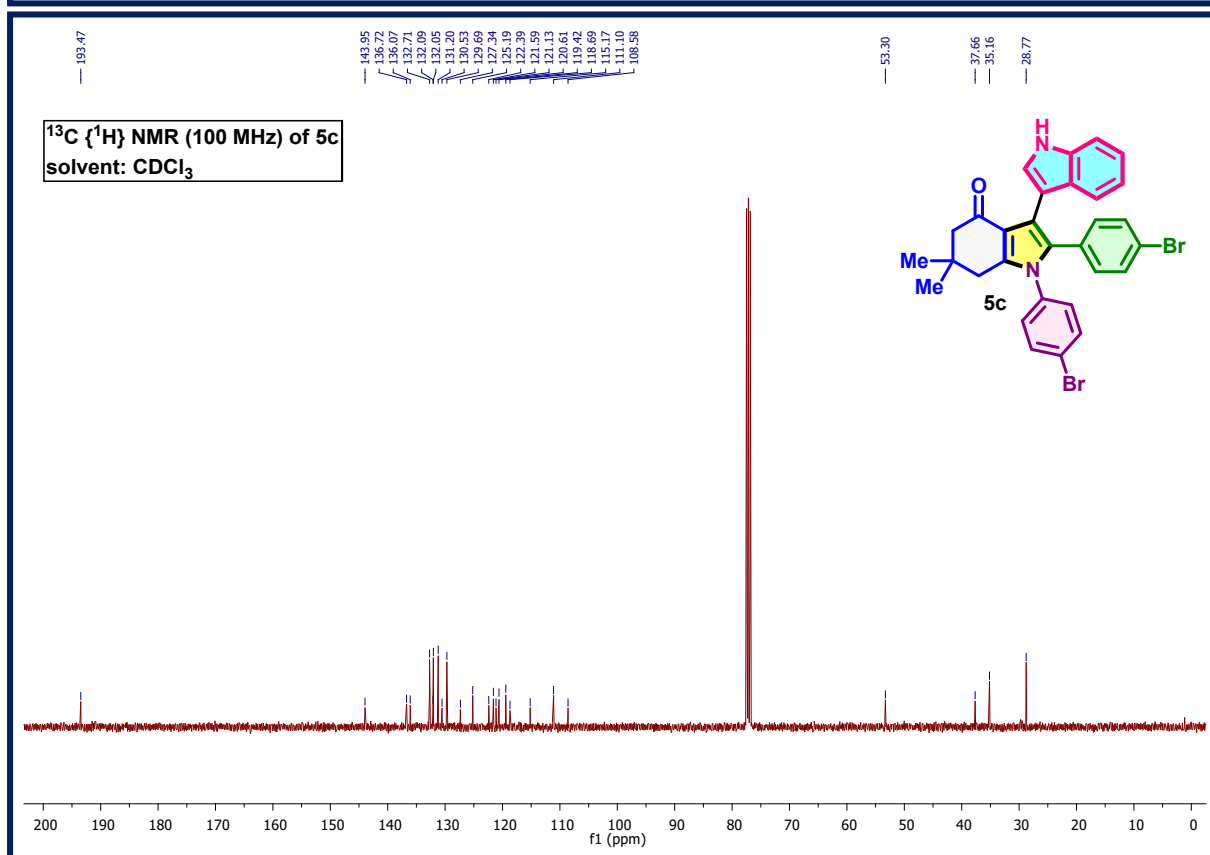
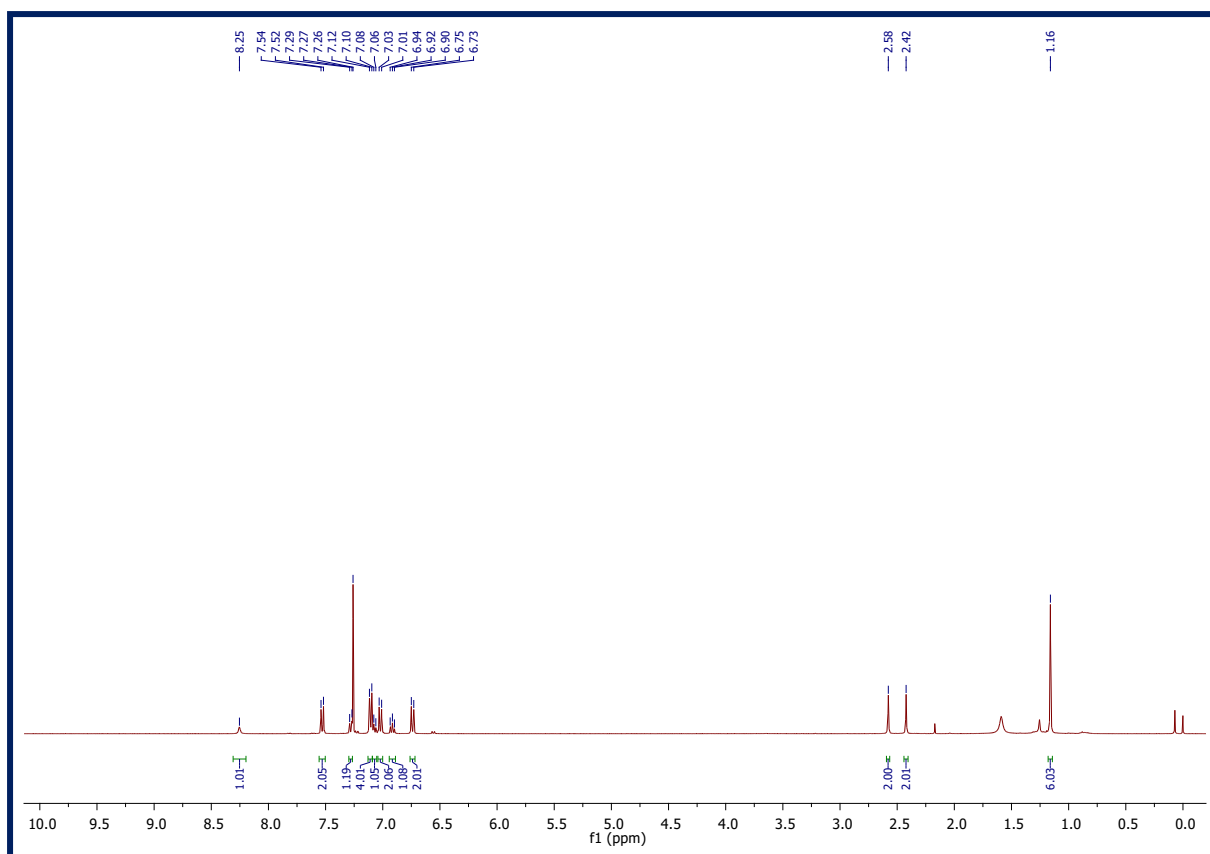


^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5c

^1H NMR (400 MHz) of 5c
solvent: CDCl_3

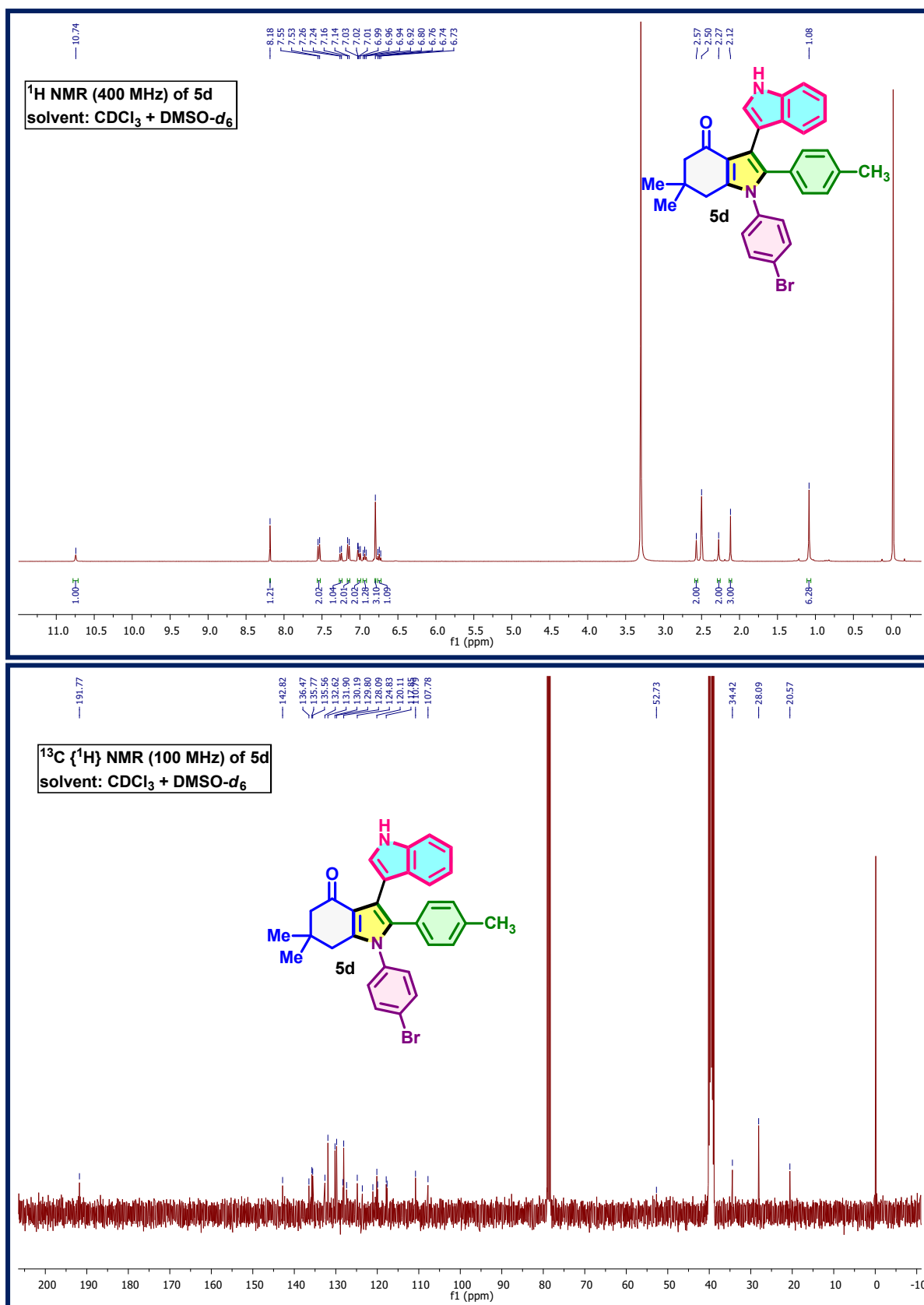


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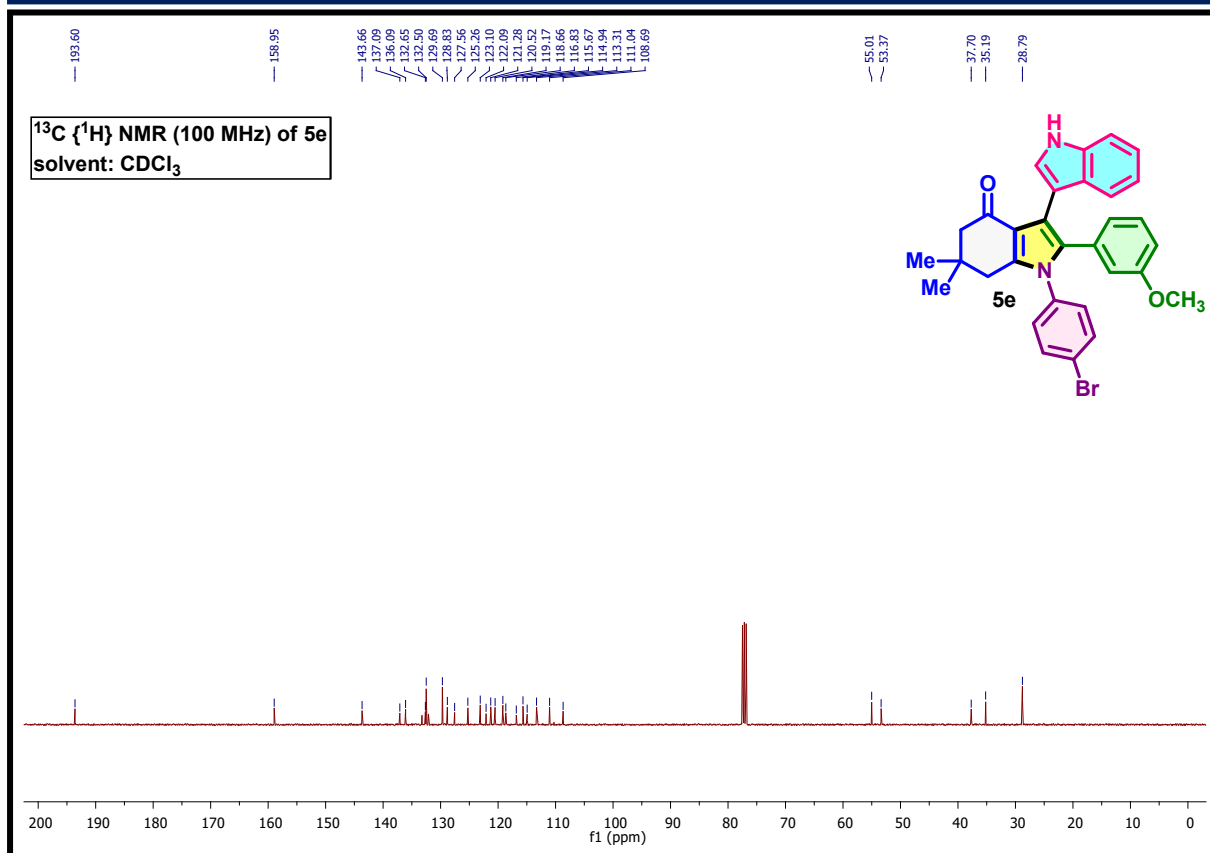
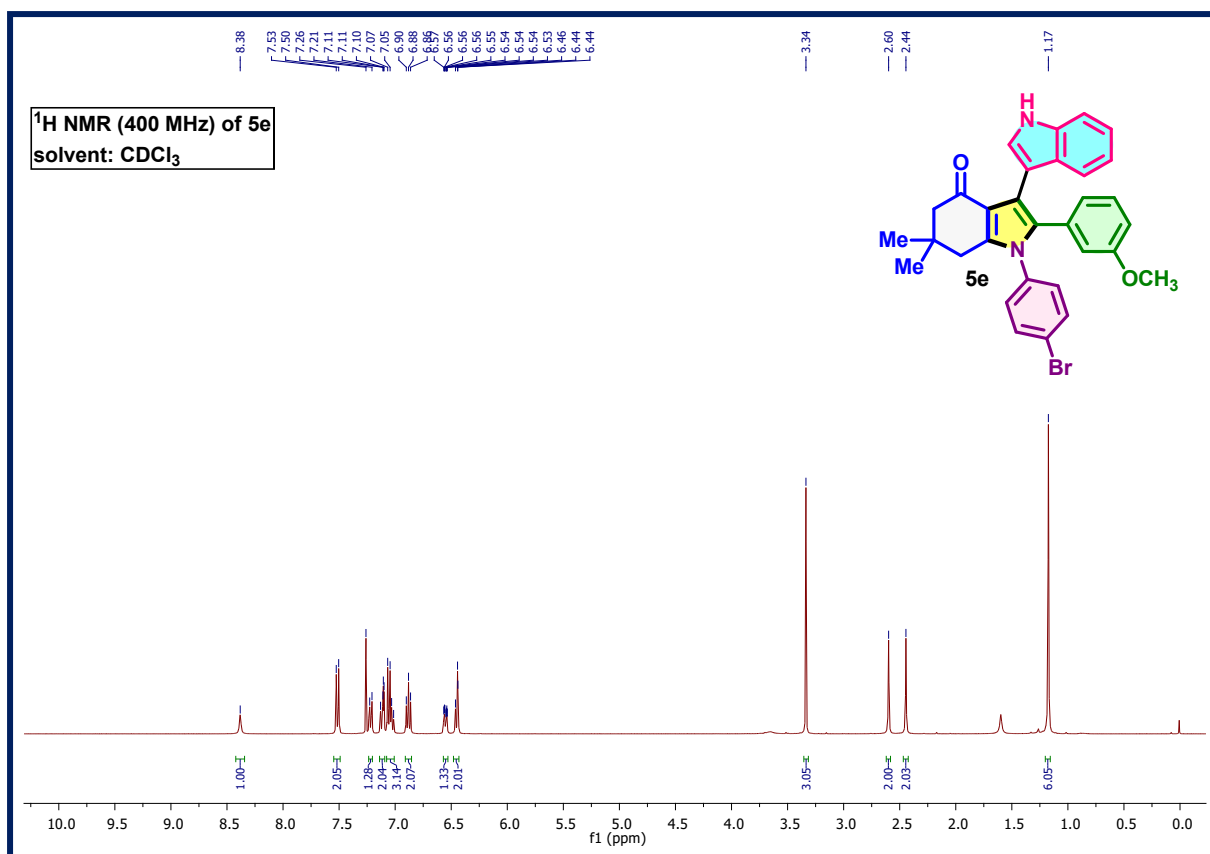
^1H , and ^{13}C { ^1H } NMR spectra of **5d**

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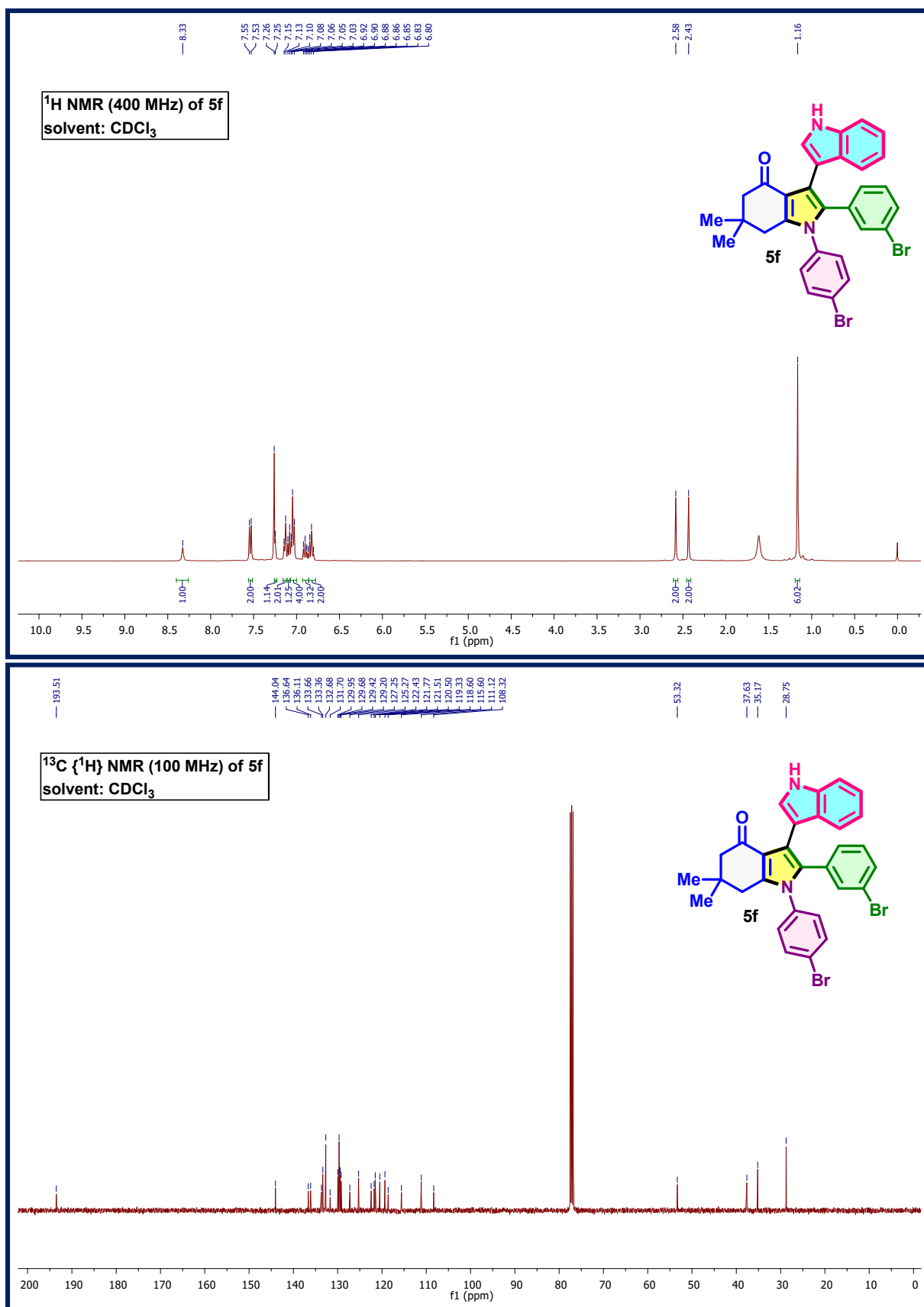
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5e

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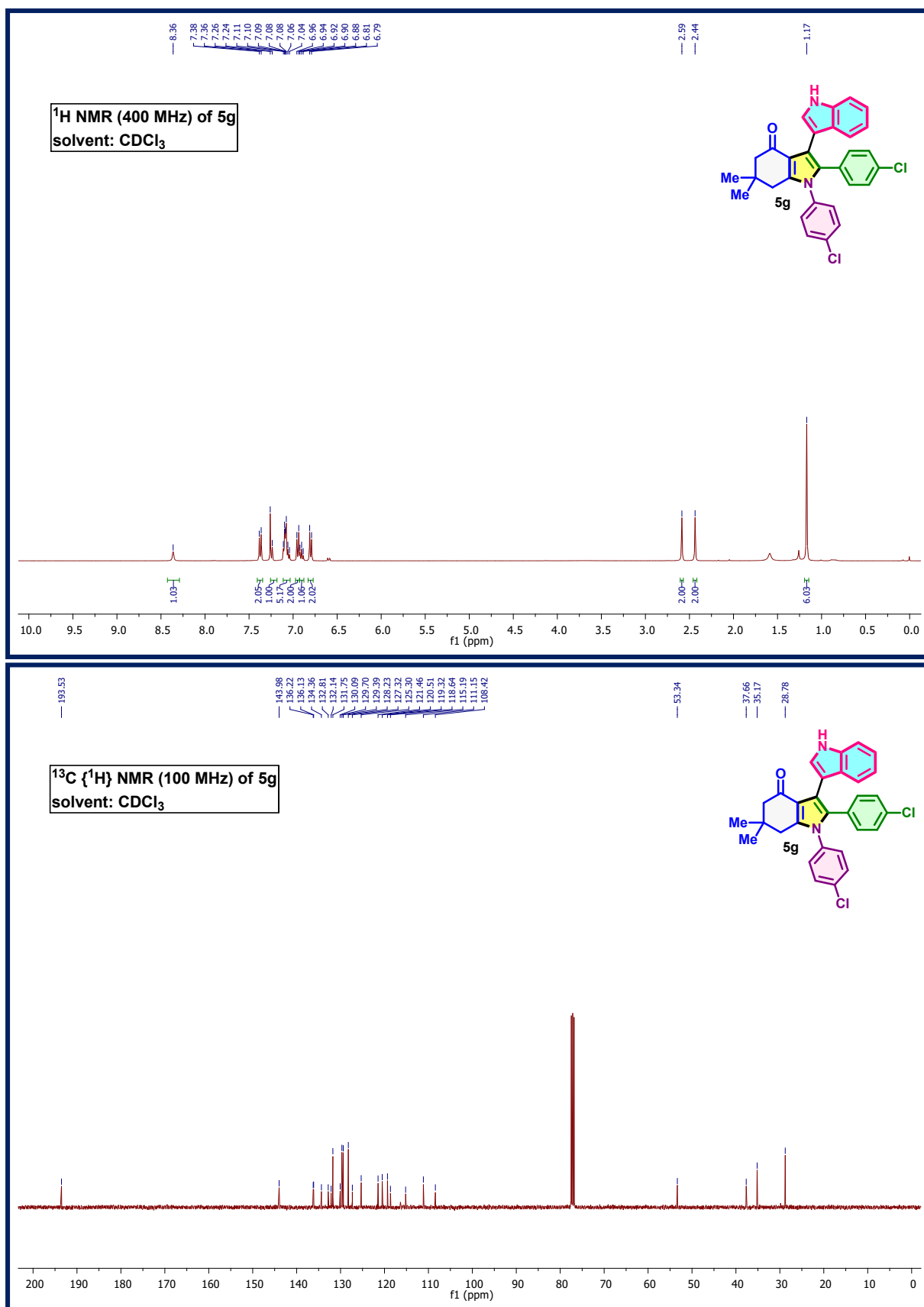
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of **5f**

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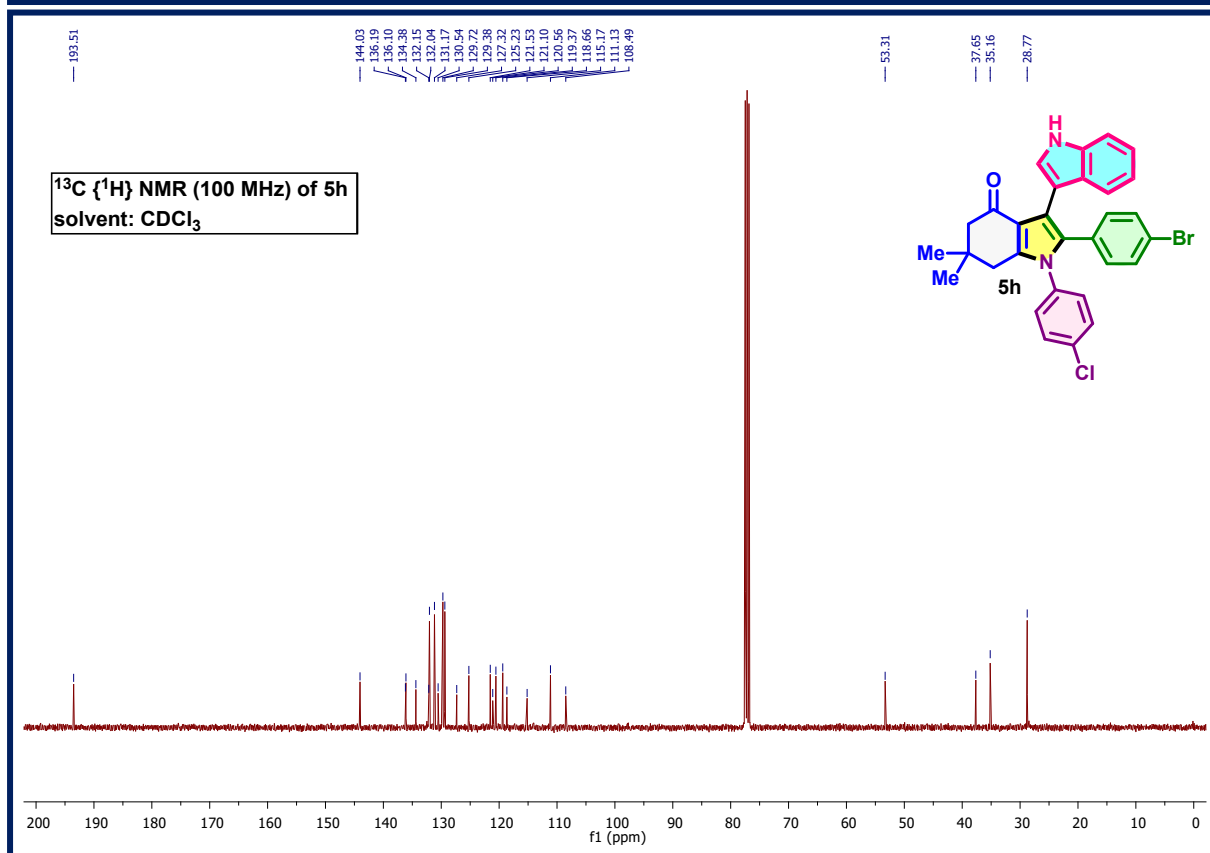
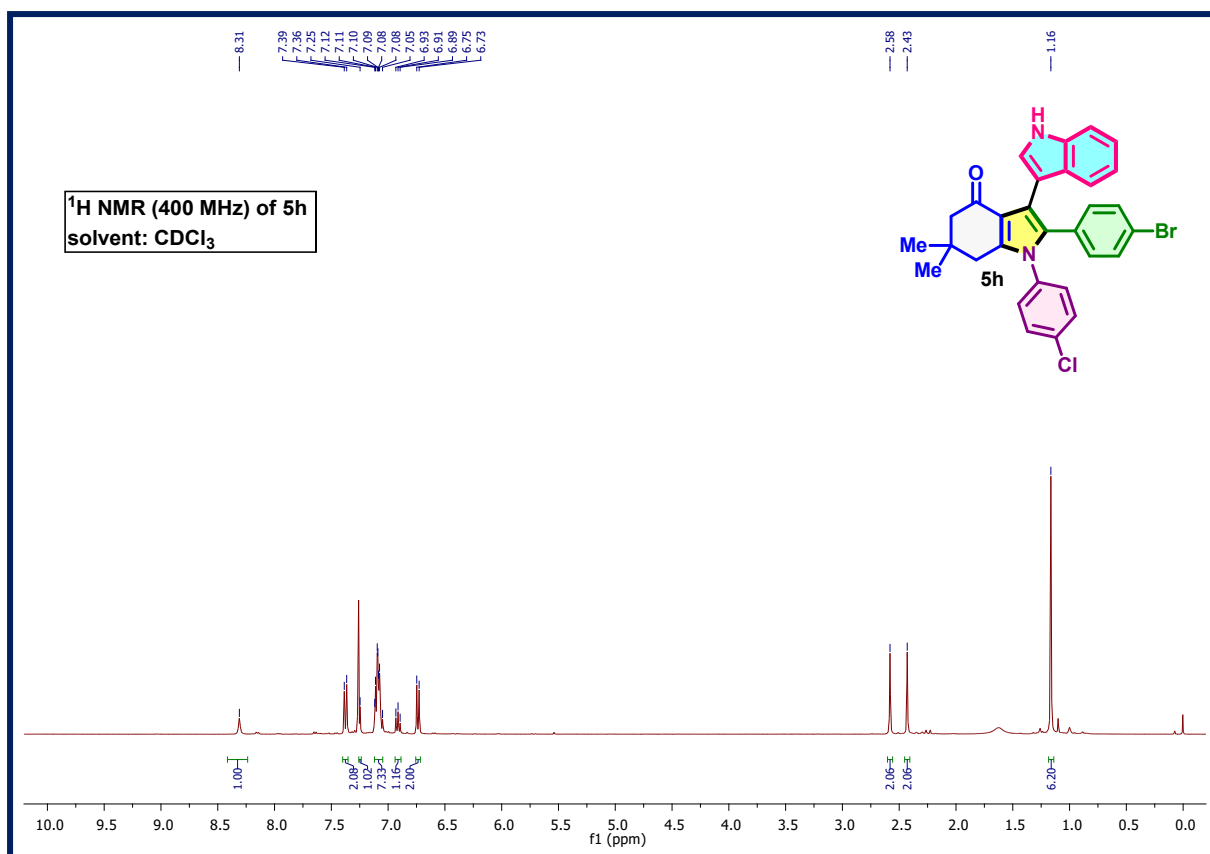
¹H, and ¹³C {¹H} NMR spectra of 5g

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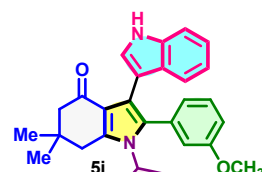
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5h

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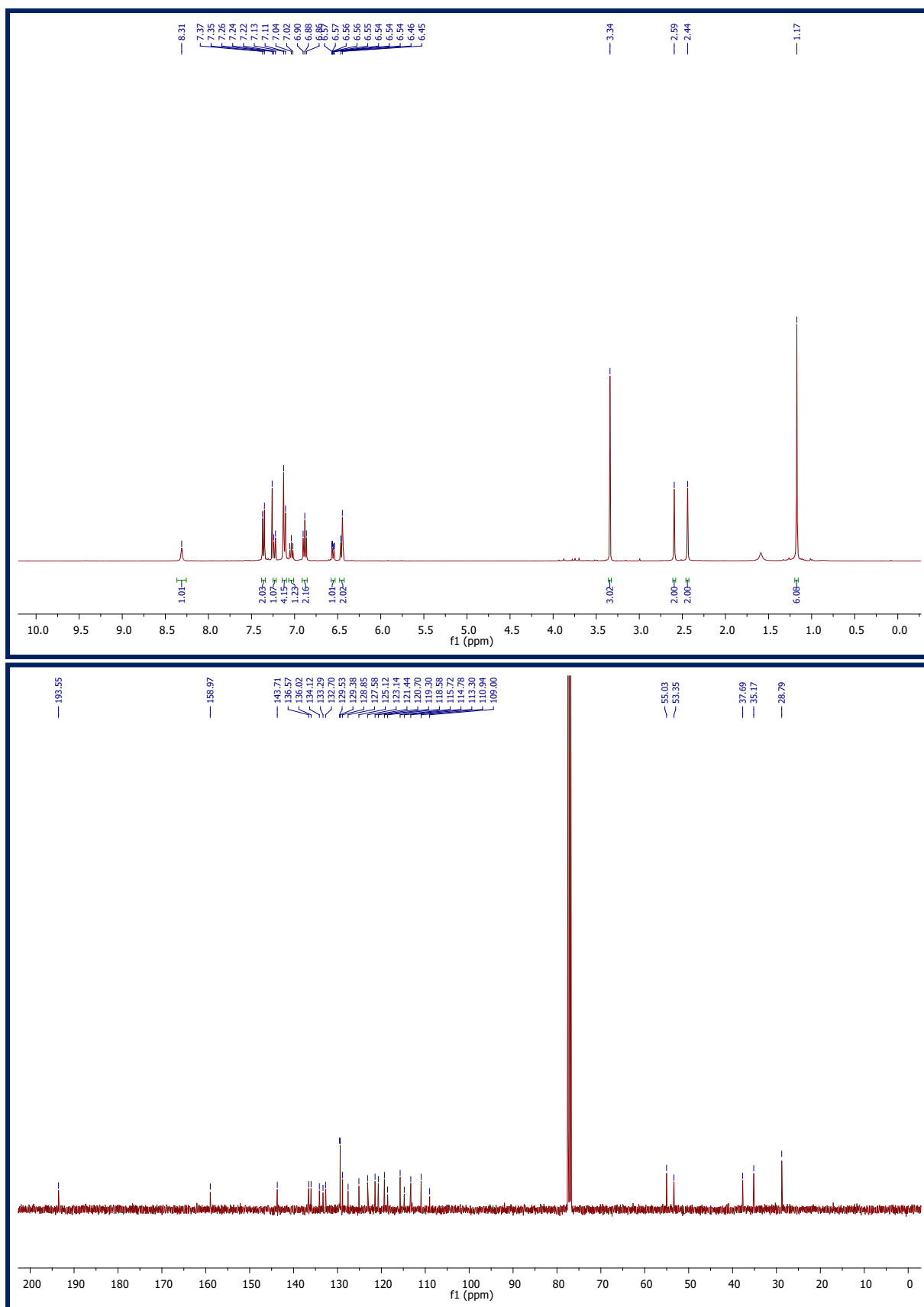


^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of **5i**

^1H NMR (400 MHz) of 5i
solvent: CDCl_3

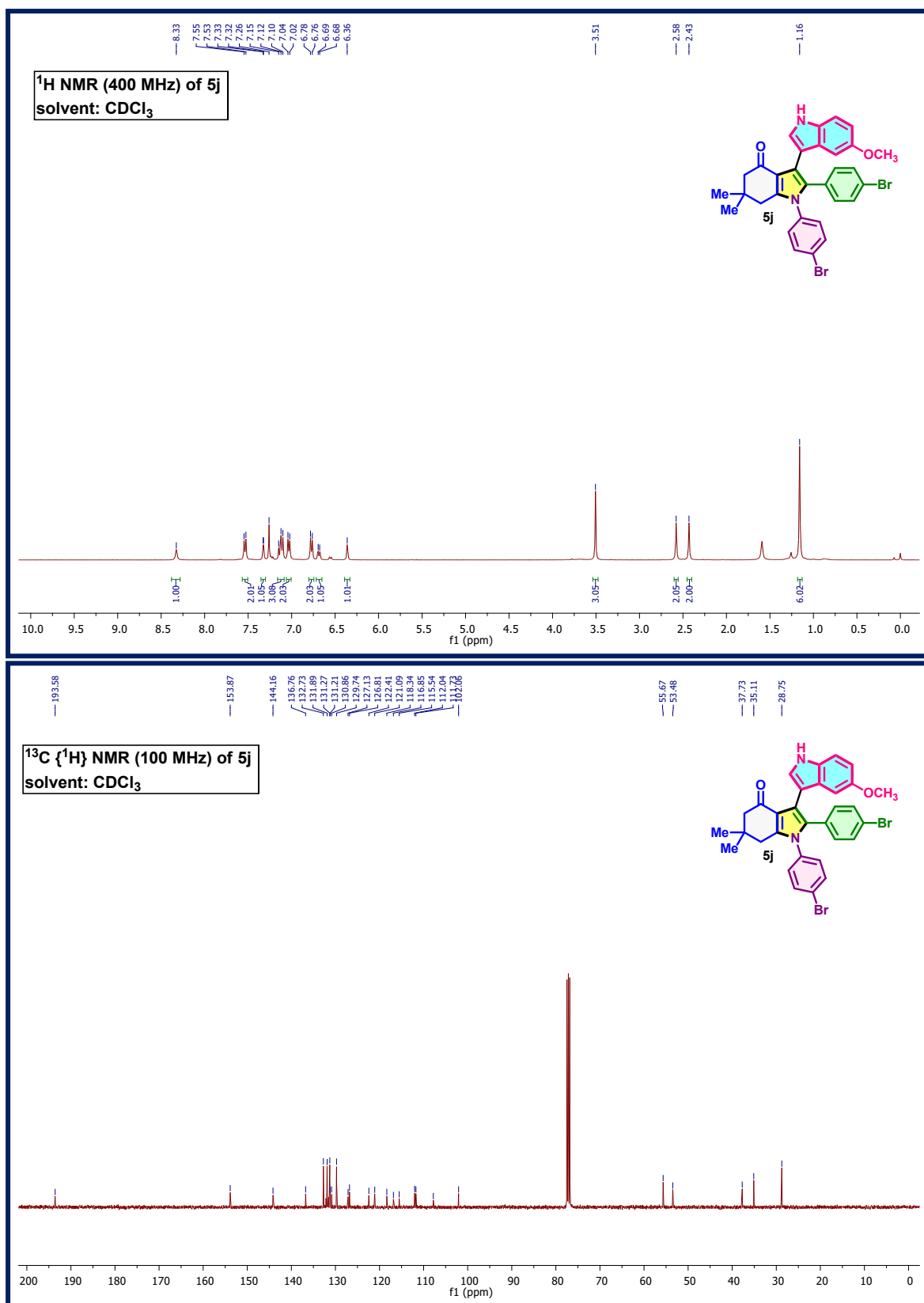


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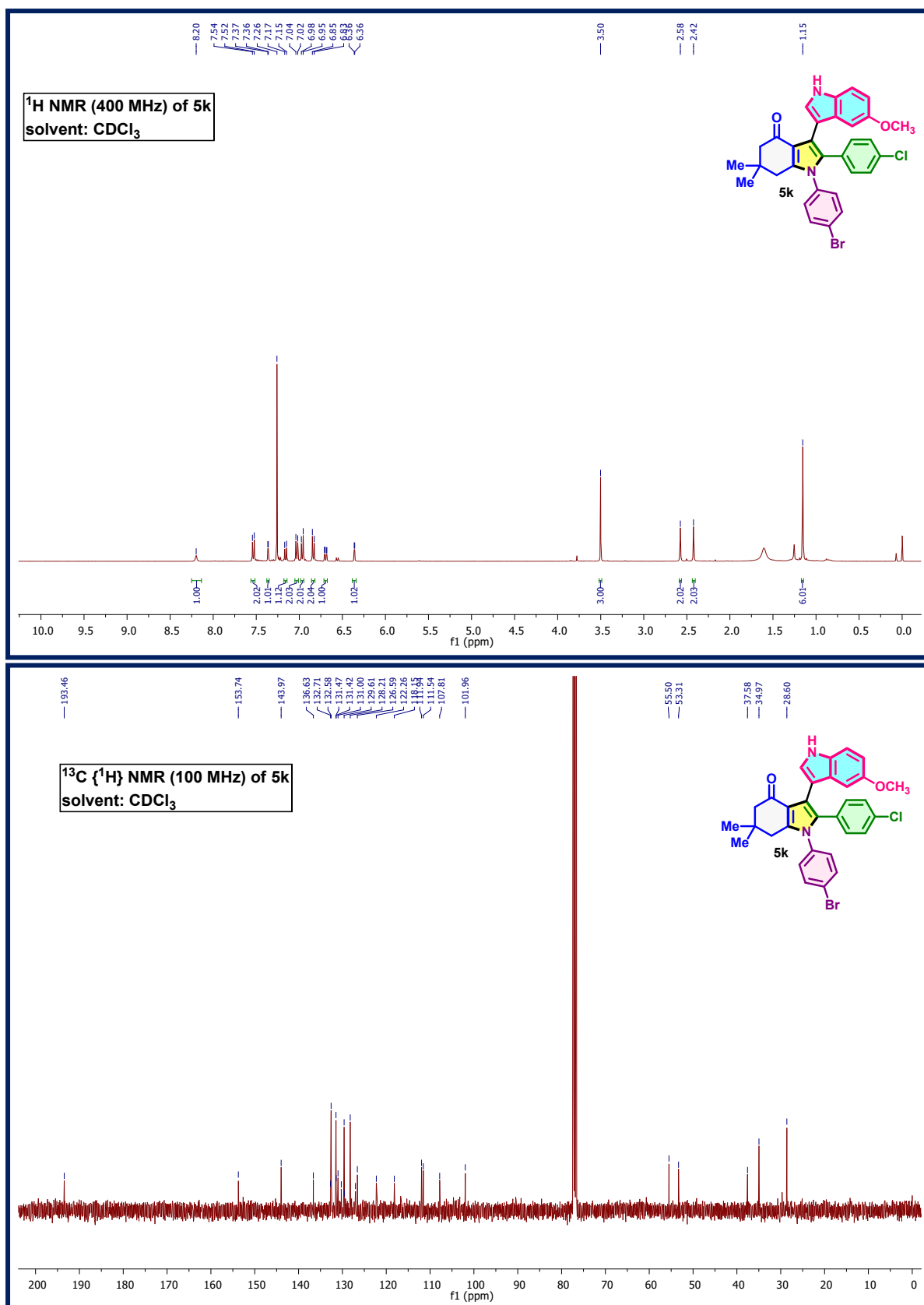
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of **5j**

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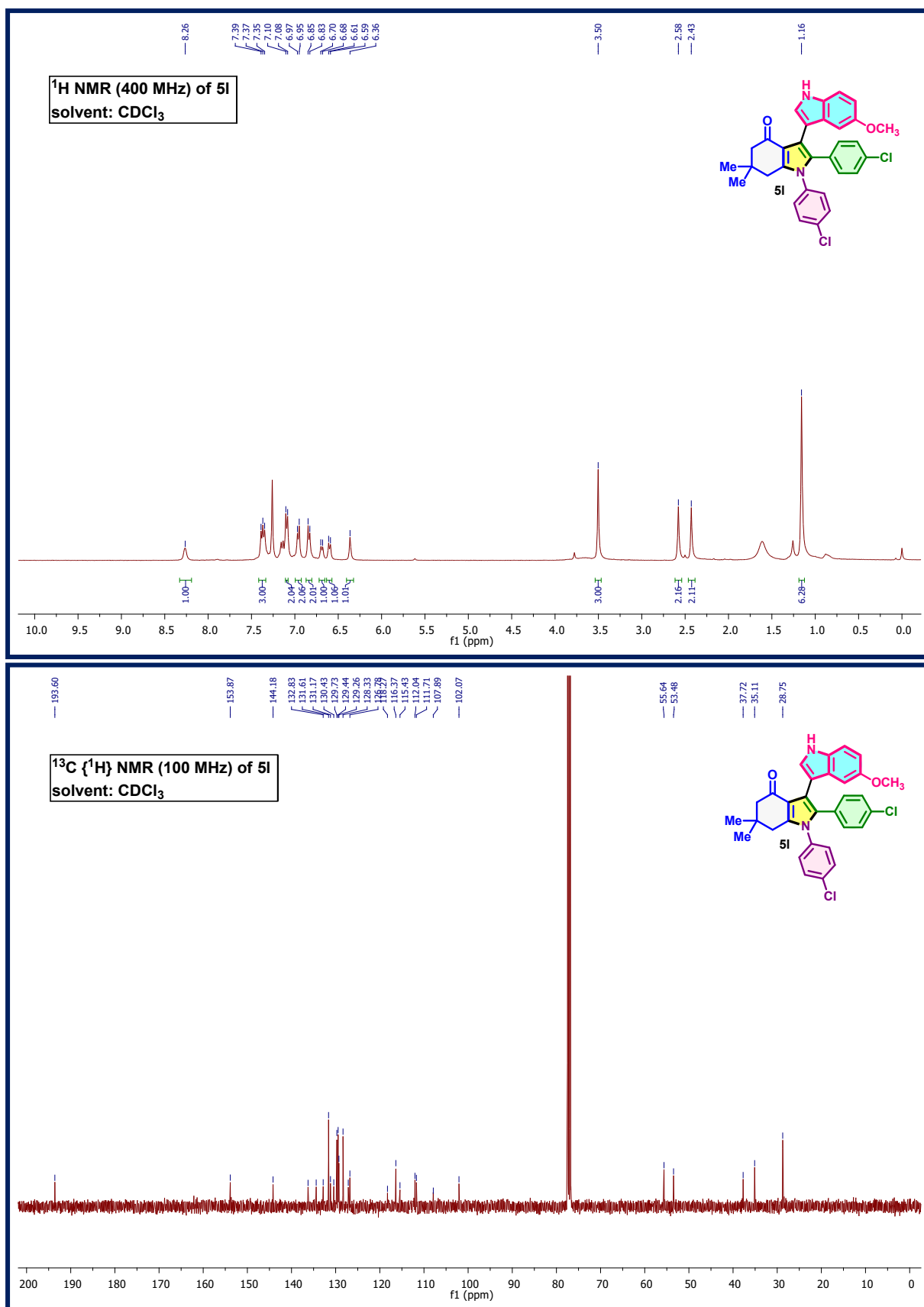
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5k

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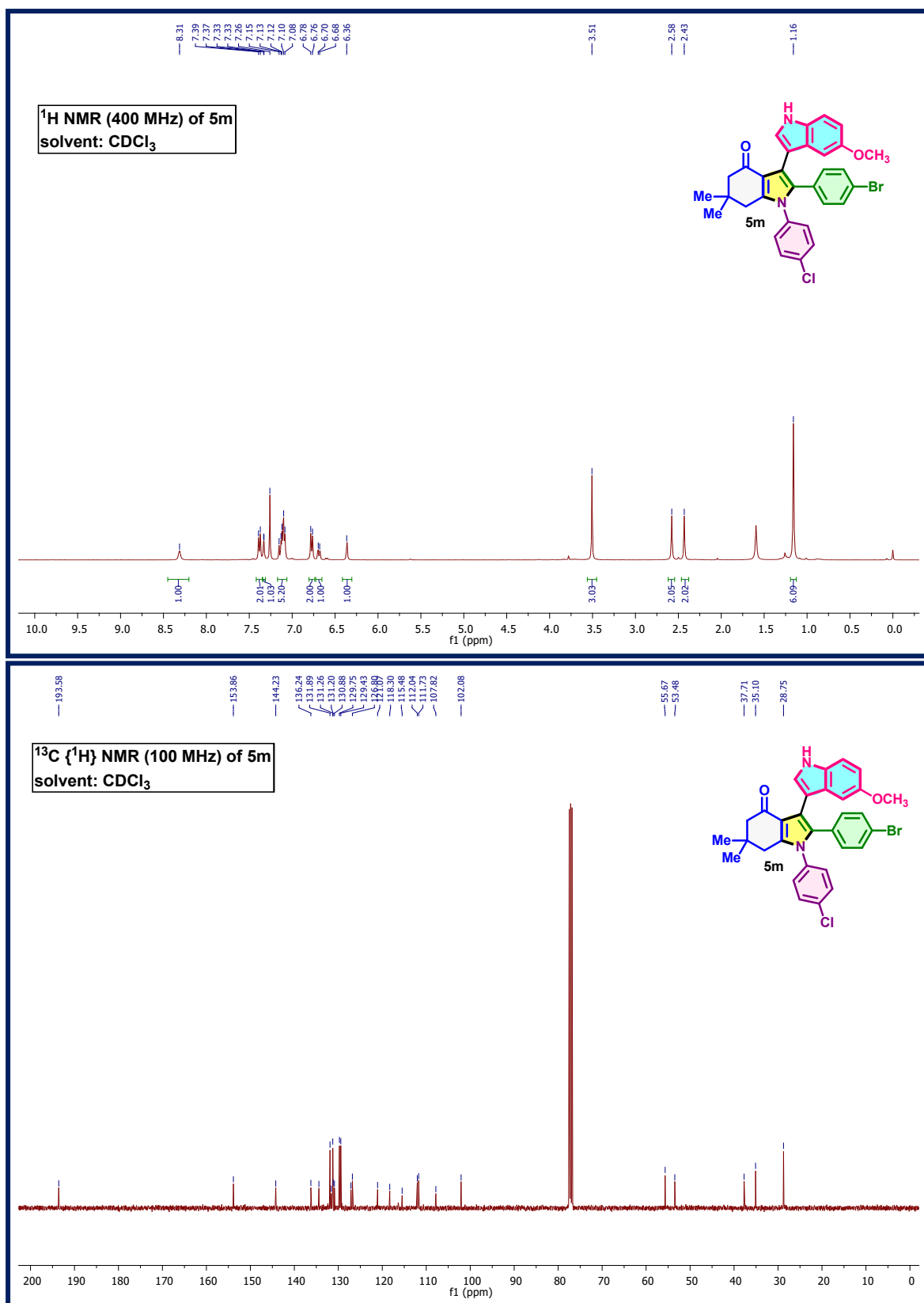
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of **5l**

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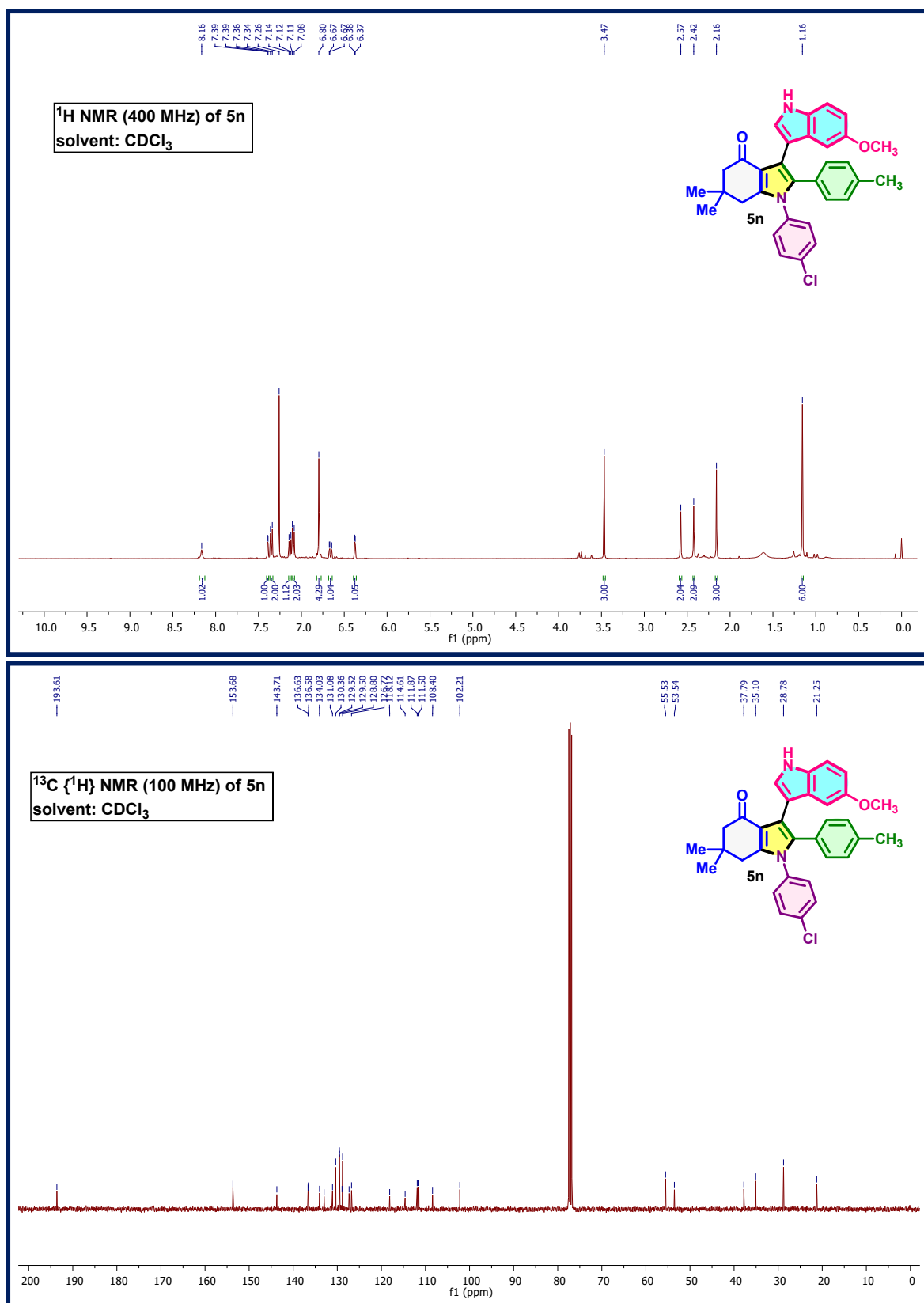
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of **5m**

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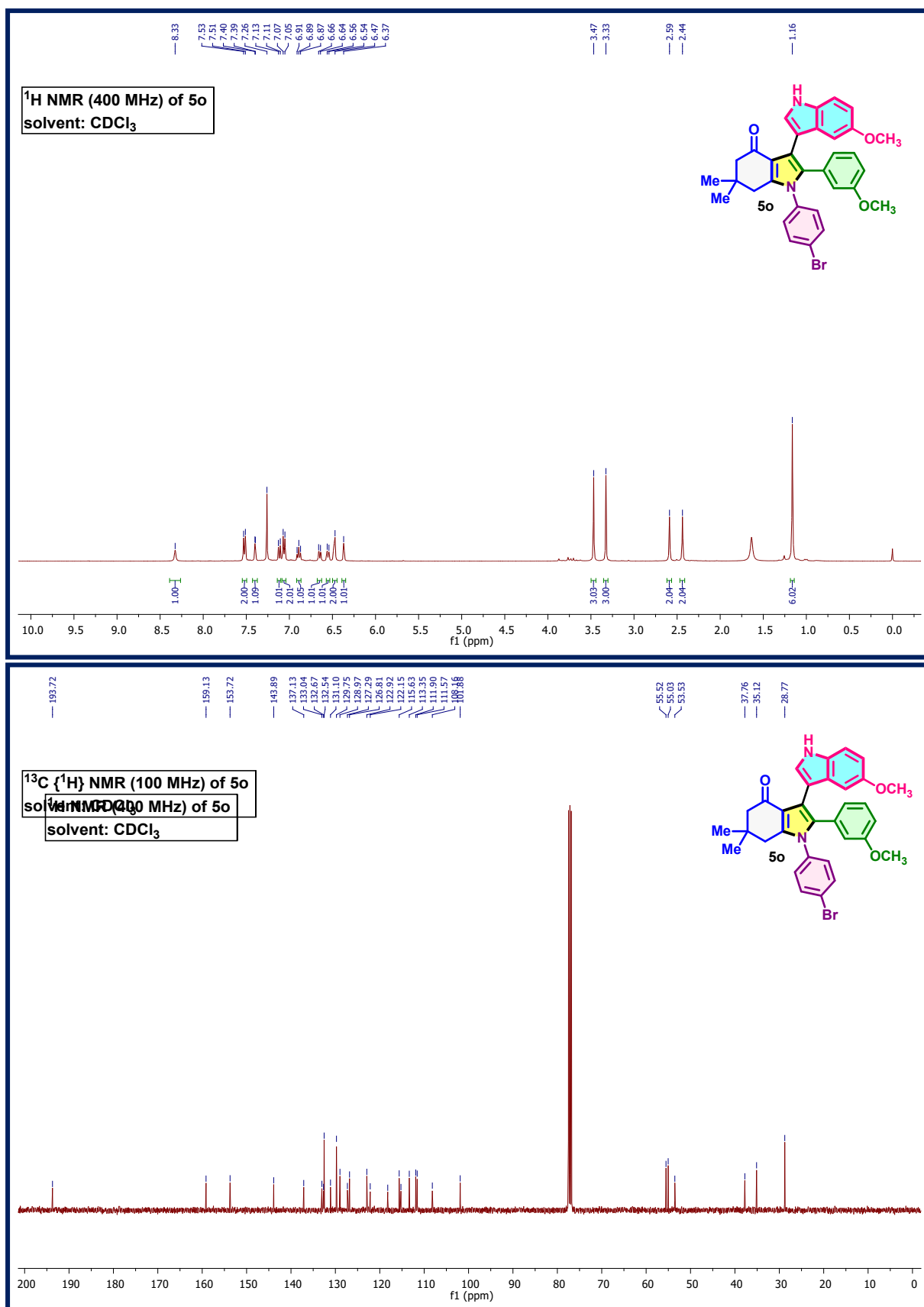
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5n

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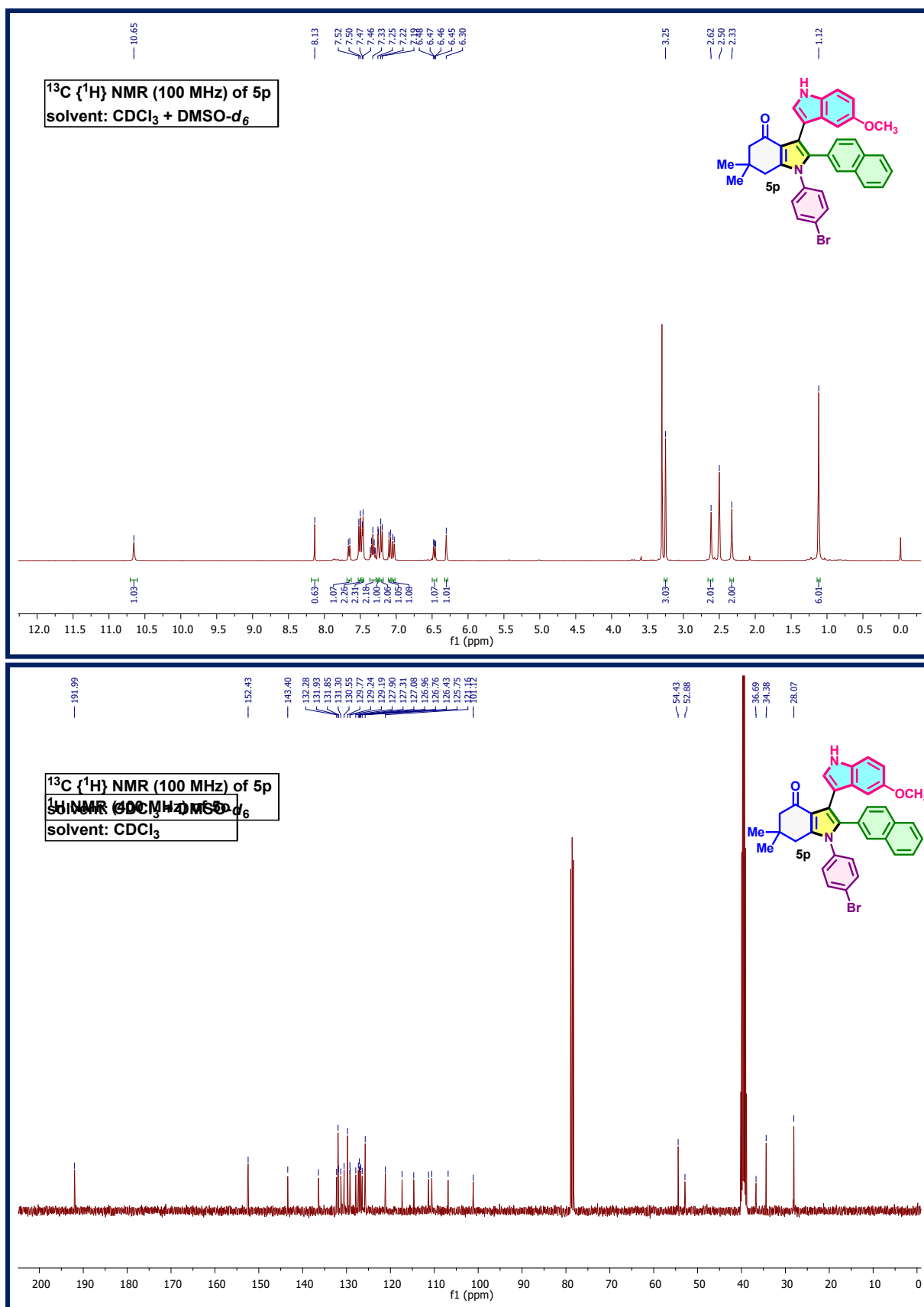
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5o

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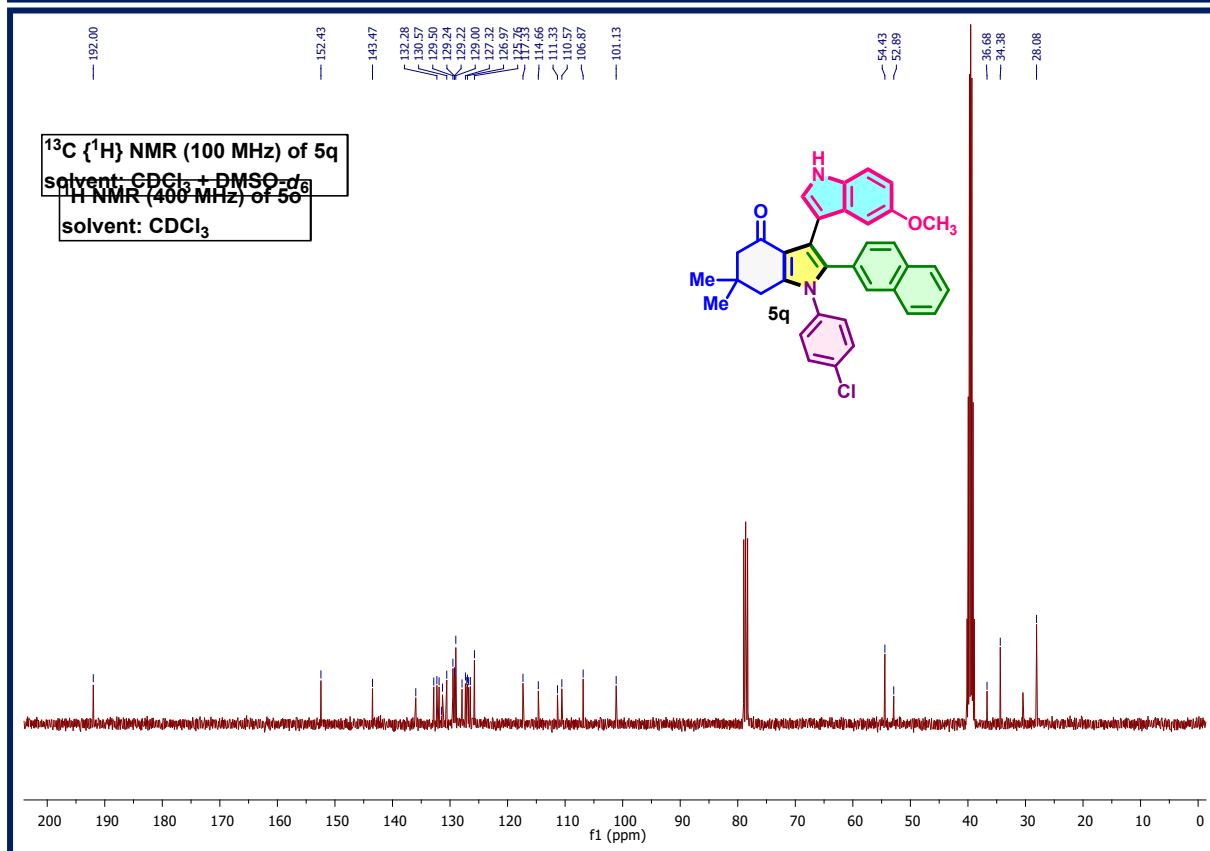
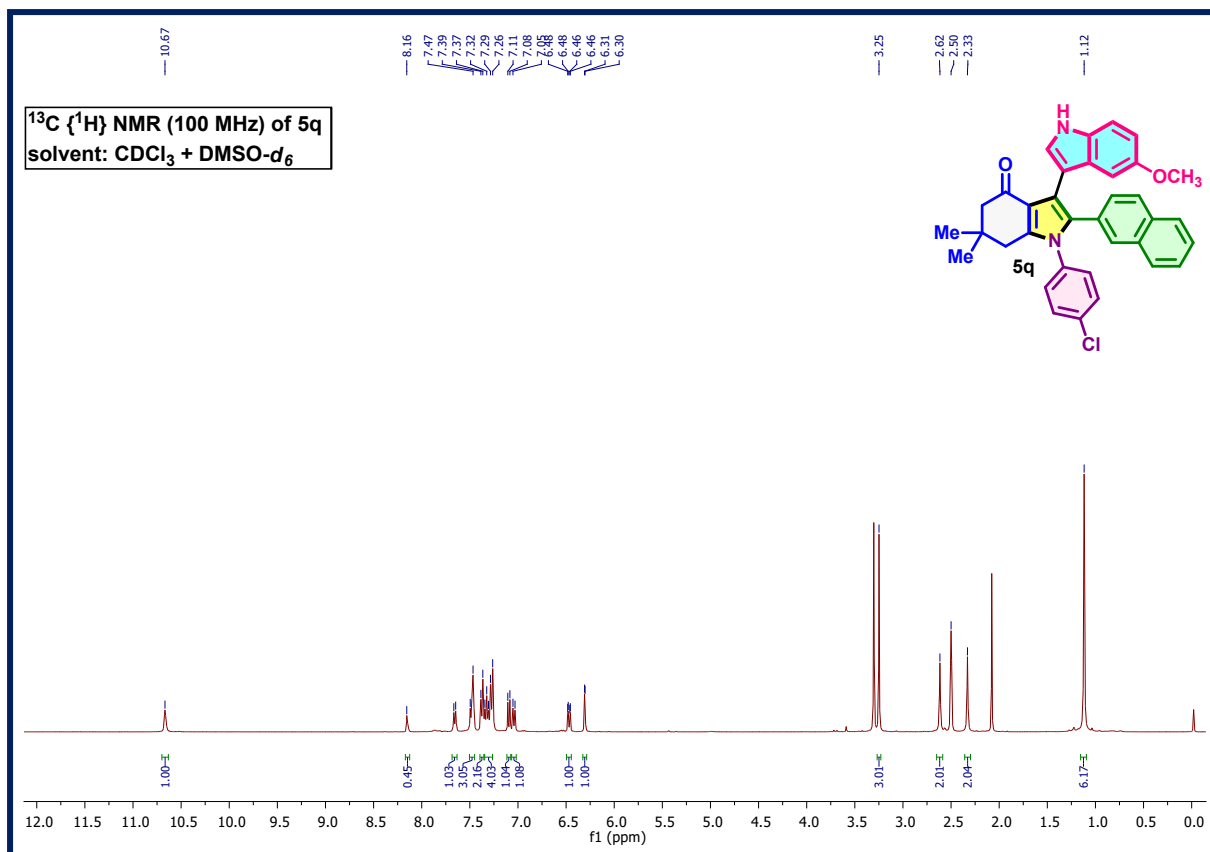
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5p

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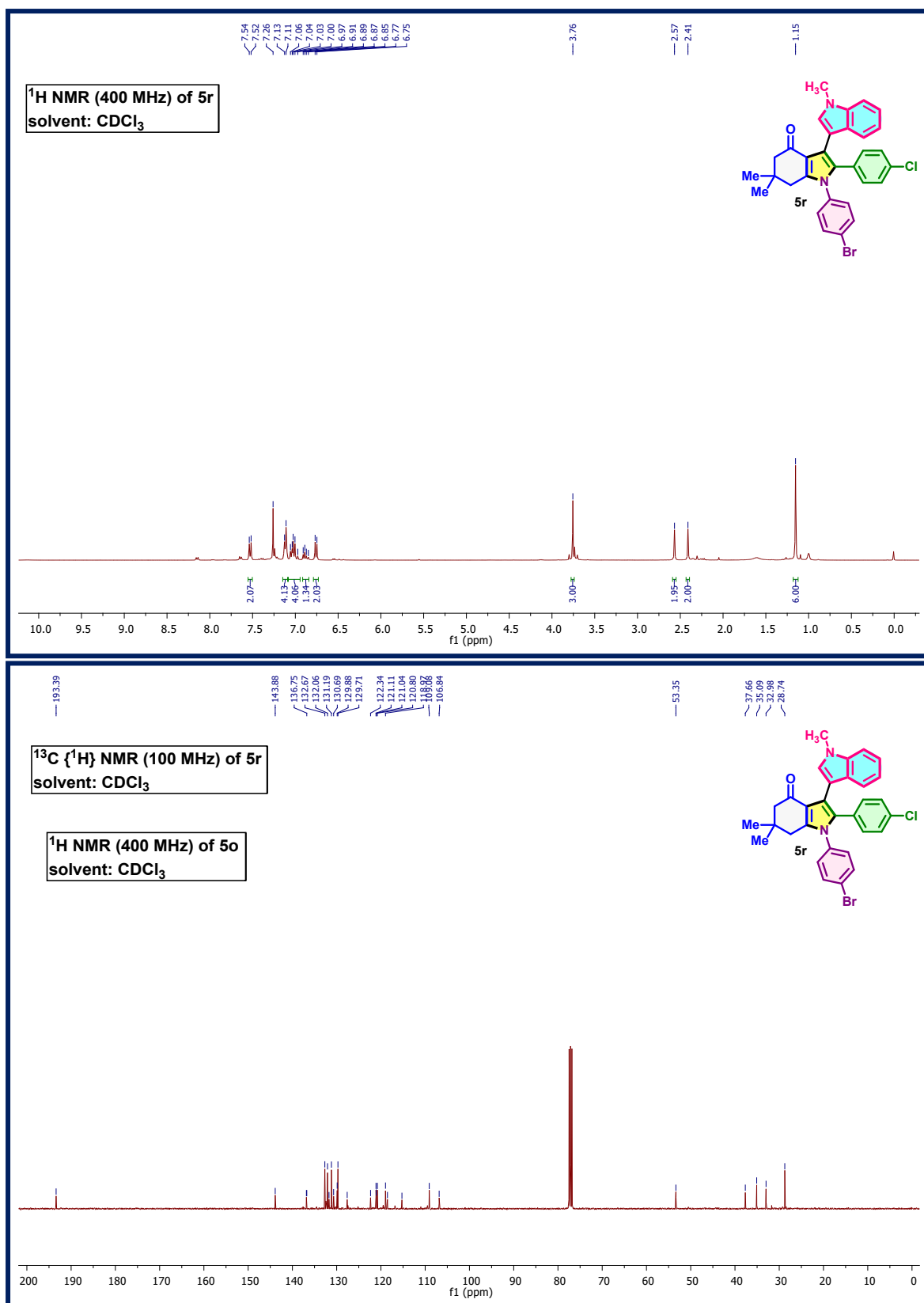
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5q

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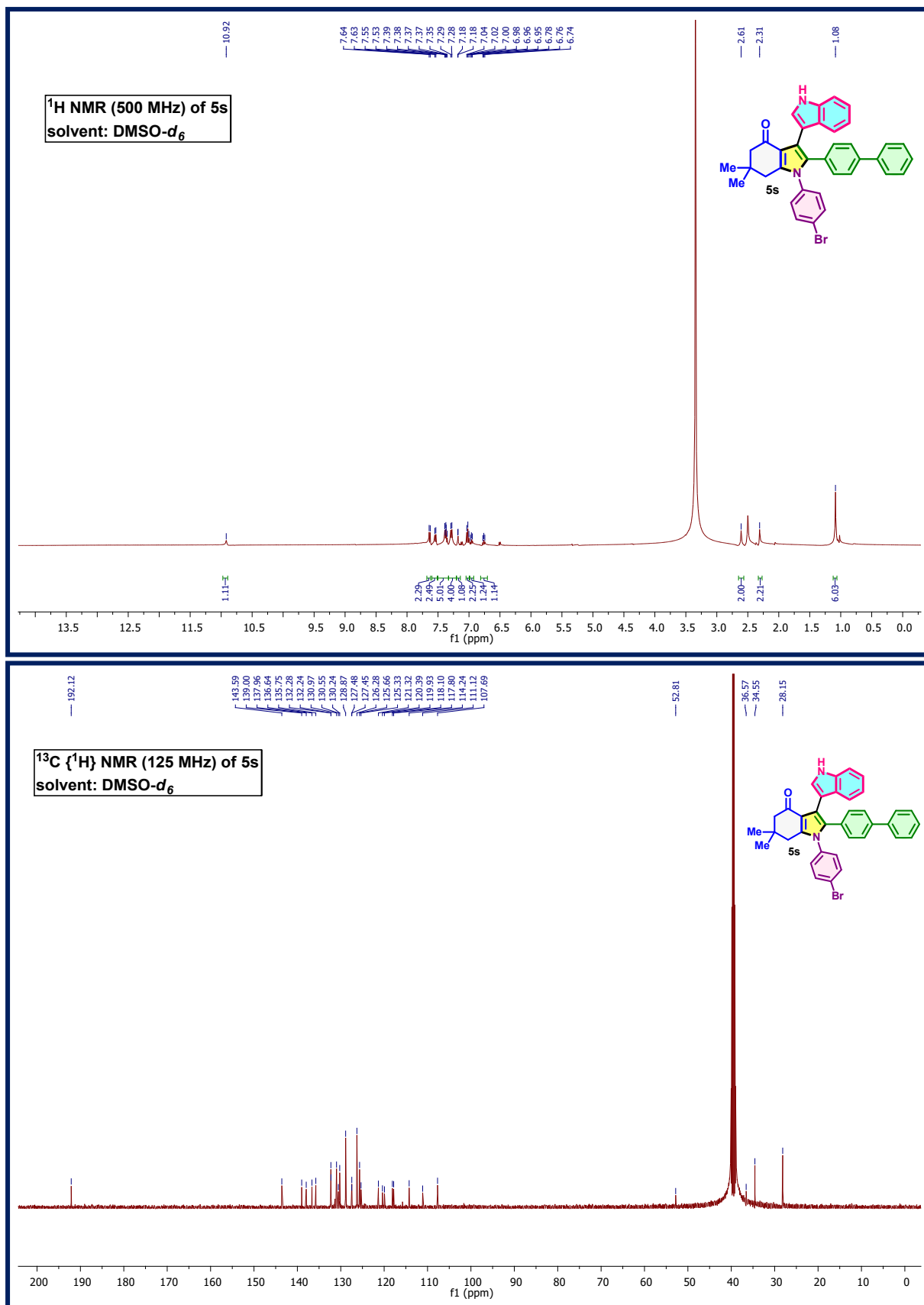
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of **5r**

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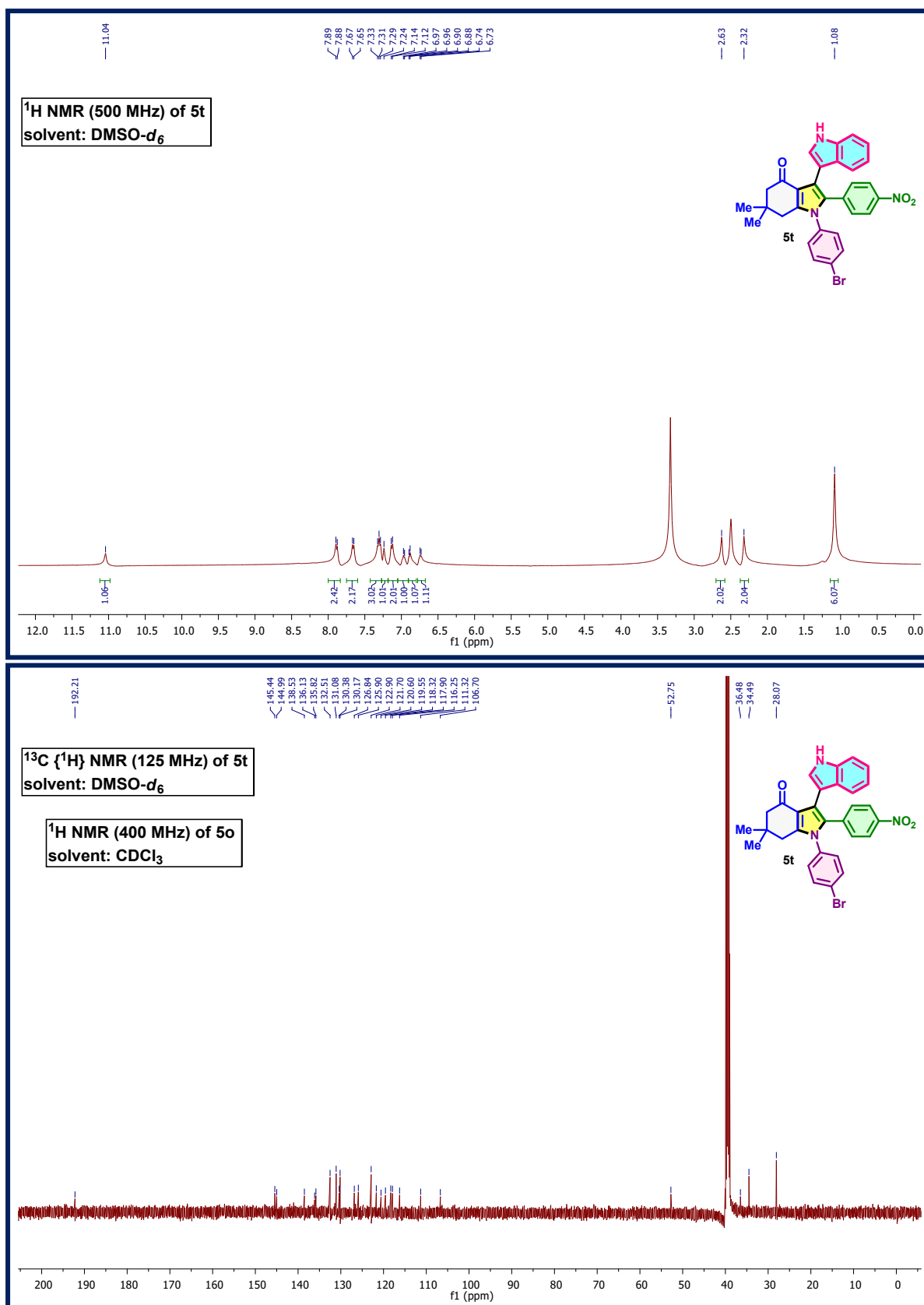
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5s

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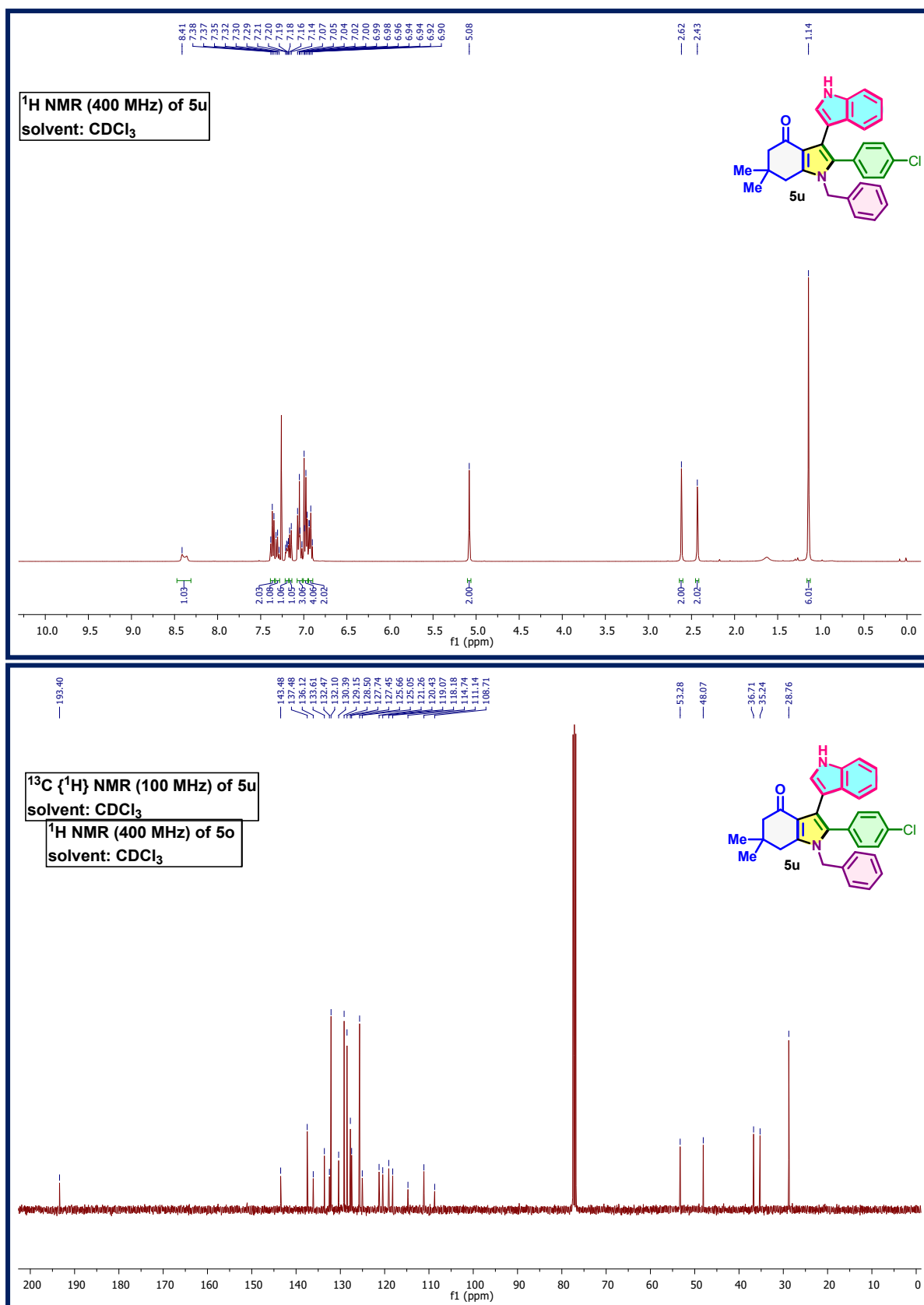
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5t

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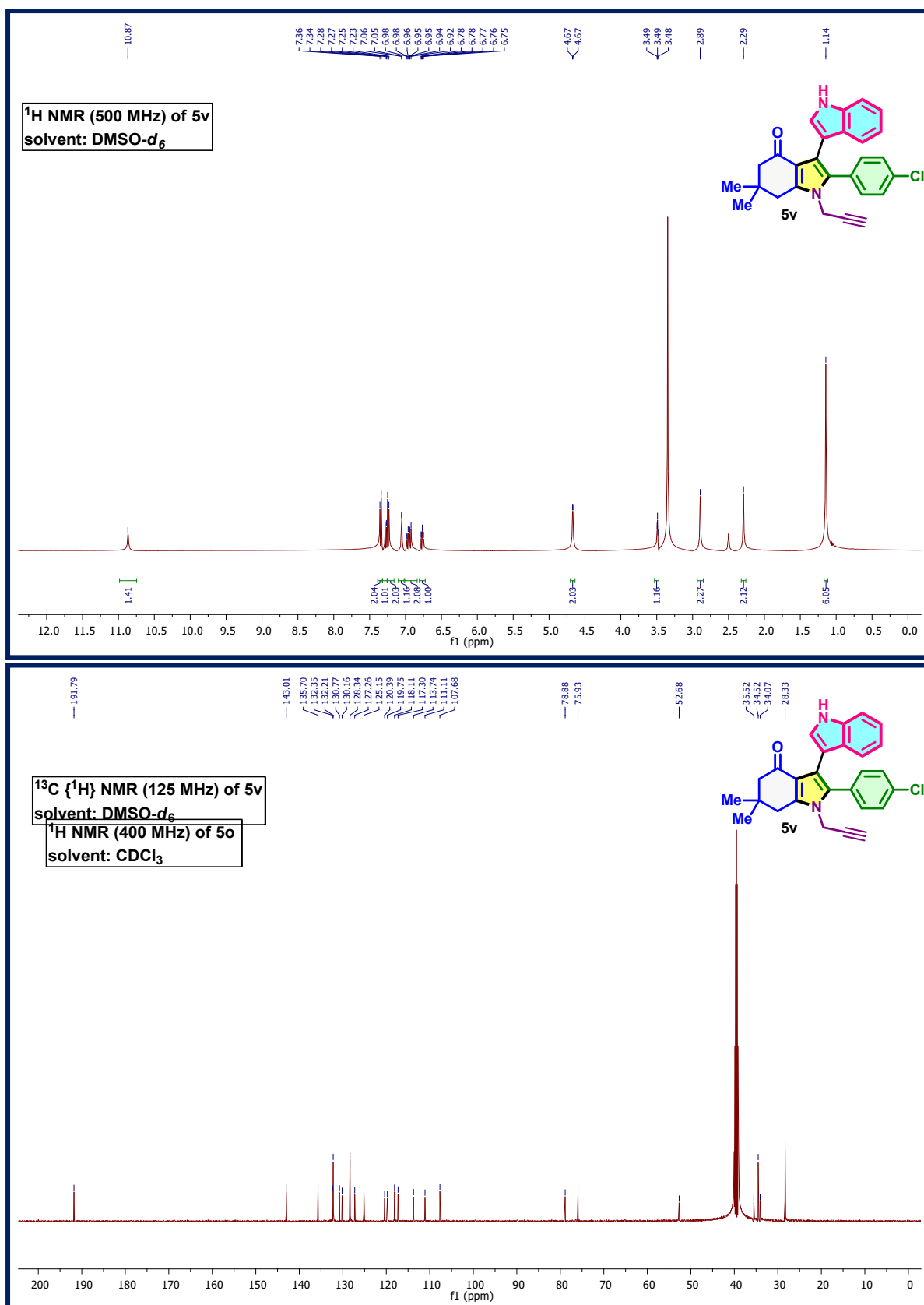
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5u

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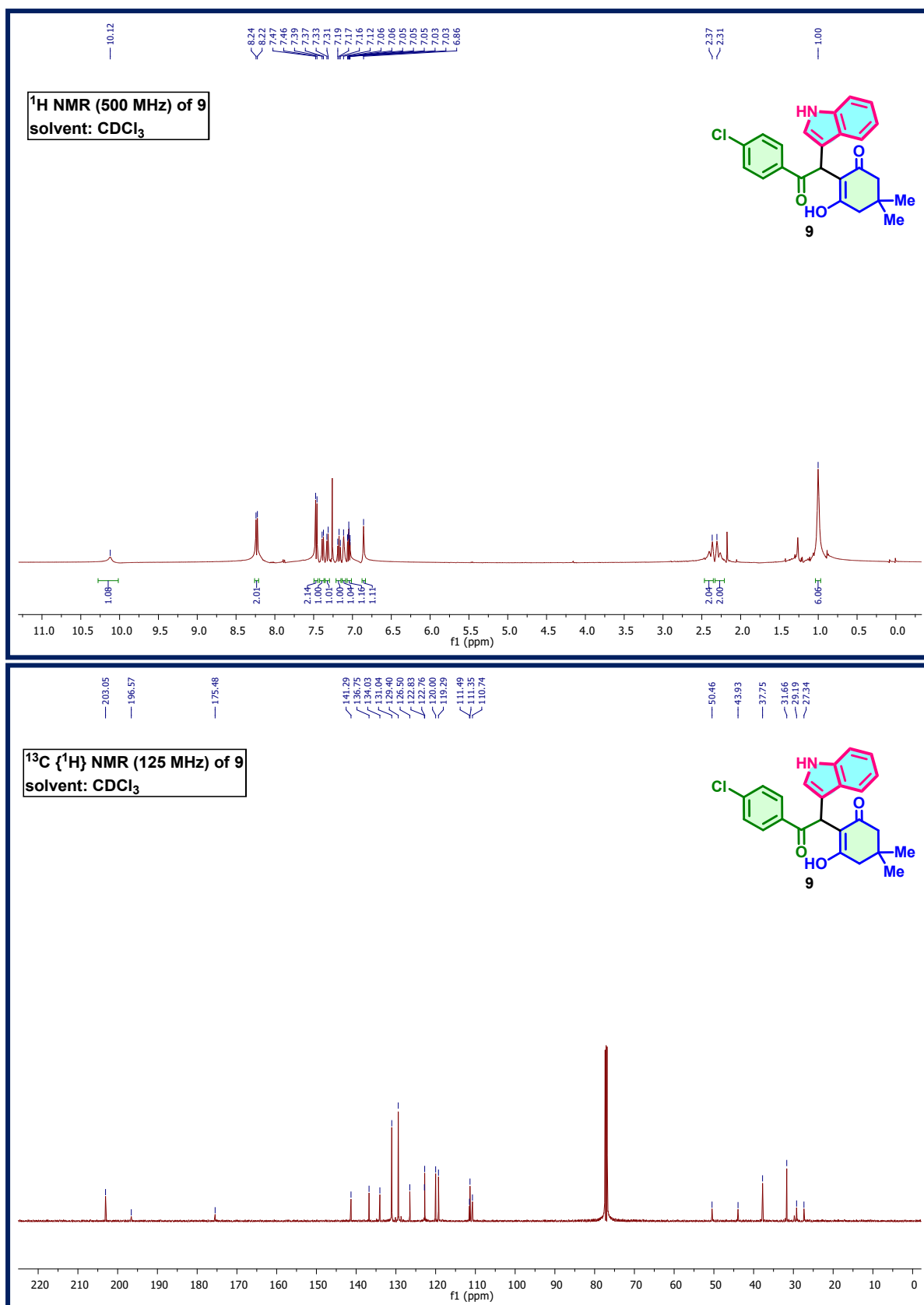
^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 5v

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^1H , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of **9**

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2. Green parameters^[1] of the protocol of representative compound 5b

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$$\text{Effective Mass Yield (EMY)} = \frac{\text{Mass of product}}{\text{Mass of non benign reagent}} \times 100$$

$$= \frac{0.132 \text{ g}}{0.04662 \text{ g} + 0.03502 \text{ g} + 0.02927 \text{ g} + 0.043 \text{ g}} \times 100 = 85.76 \%$$

$$\text{Atom Economy (AE)} = \frac{\text{Molecular weight of product}}{\text{Total molecular weight of reactants}} \times 100$$

$$= \frac{543.88}{186.59 + 140.17 + 117.14 + 172.02} \times 100 = 88.30\%$$

$$\text{Atom Efficiency (AEf)} = \text{AE} \times \text{Yield}\% = 88.30 \times 97 = 85.65\%$$

$$\text{Carbon Economy (CE)} = \frac{\text{Amount of carbon in the product}}{\text{Total carbon present in the reactants}} \times 100$$

$$= \frac{30 \times 0.00024}{8 \times 0.00025 + 8 \times 0.00025 + 8 \times 0.00025 + 6 \times 0.00025} \times 100 = 96\%$$

$$\text{Reaction Mass Efficiency (RME)} = \frac{\text{Mass of isolated the product}}{\text{Total mass of reactants}} \times 100$$

$$= \frac{0.132 \text{ g}}{0.04662 \text{ g} + 0.03502 \text{ g} + 0.02927 \text{ g} + 0.043 \text{ g}} \times 100 = 85.76 \%$$

$$\text{Optimum Efficiency (OE)} = \frac{\text{RME}}{\text{AE}} \times 100 = \frac{85.76}{88.30} \times 100 = 97.12\%$$

$$\text{E factor} = \frac{\text{Mass of raw materials} - \text{Mass of product}}{\text{Mass of product}}$$

$$= \frac{(0.04662 \text{ g} + 0.3502 \text{ g} + 0.02927 \text{ g}) - 0.132 \text{ g}}{0.132 \text{ g}} = 0.16 \text{ (g/g)}$$

Eco score (E-score) calculation:^{2,3}

Sl. No.	Parameter	Values	Penalty points
1	yield	(100-97)/2	1.5
2	Price of the reaction components	Inexpensive	0
3	Technical setup	Common setup	0
4	Temperature/time	heating, <1	2
5	Workup and purification	Simple filtration	0
6	Safety*	5+5	10
Total penalty point			13.5

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*Based on the hazard warning symbols

E-score = 100 – the sum of the individual penalties

E-score = 100 – 13.5 = **86.5** (>75, excellent synthesis).

3. References:

1 G. Brahmachari, N. Nayek, I. Karmakar, K. Nurjamal, S. K. Chandra, A. Bhowmick, *J. Org. Chem.*, 2020, **85**, 8405–8414.

2 K. V. Aken, L. Streckowski, L. Patiny, *Beilstein J. Org. Chem.*, 2006, **2**, 3.

3 S. Teli, S. Soni, P. Teli, N. Sahiba, S. Agarwal, *Res. Chem. Intermed.*, 2024, **50**, 1475–1495.