

## Supporting Information

for

### **ML212: A small-molecule probe for investigating fluconazole resistance mechanisms in *Candida albicans***

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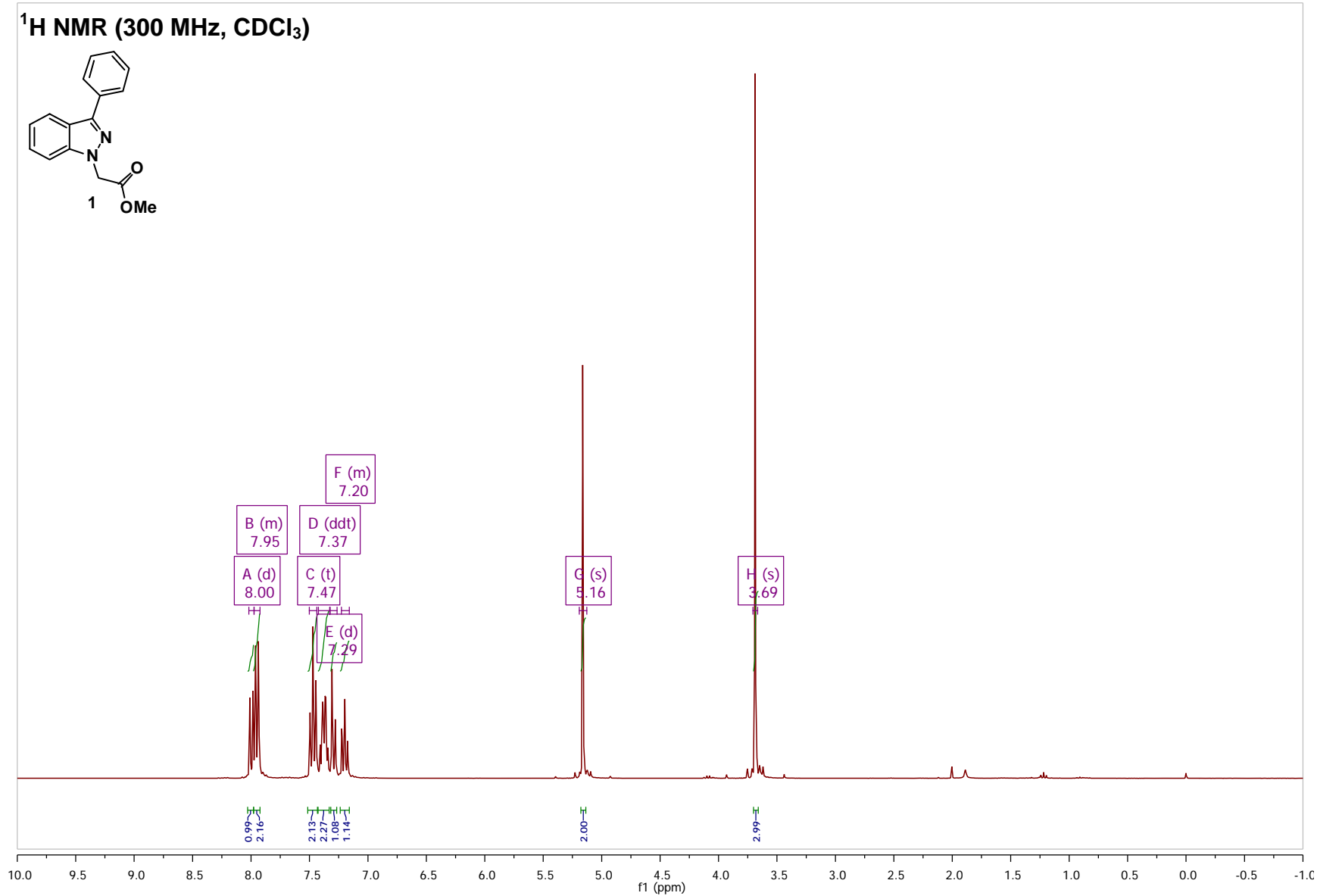
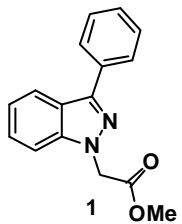
Address: <sup>1</sup>Chemical Biology Platform and Probe Development Center, Broad Institute of MIT and Harvard, 7 Cambridge Center, Cambridge, MA 02142, USA, <sup>2</sup>Whitehead Institute for Biomedical Research, 9 Cambridge Center, Cambridge, MA 02142, USA, <sup>3</sup>Microbiology Graduate Program, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA, <sup>4</sup>Department of Biology and Howard Hughes Medical Institute, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA and <sup>5</sup>Howard Hughes Medical Institute, Broad Institute of Harvard and MIT, 7 Cambridge Center, Cambridge, MA 02142, USA

Email: Benito Munoz - [bmunoz@broadinstitute.org](mailto:bmunoz@broadinstitute.org)

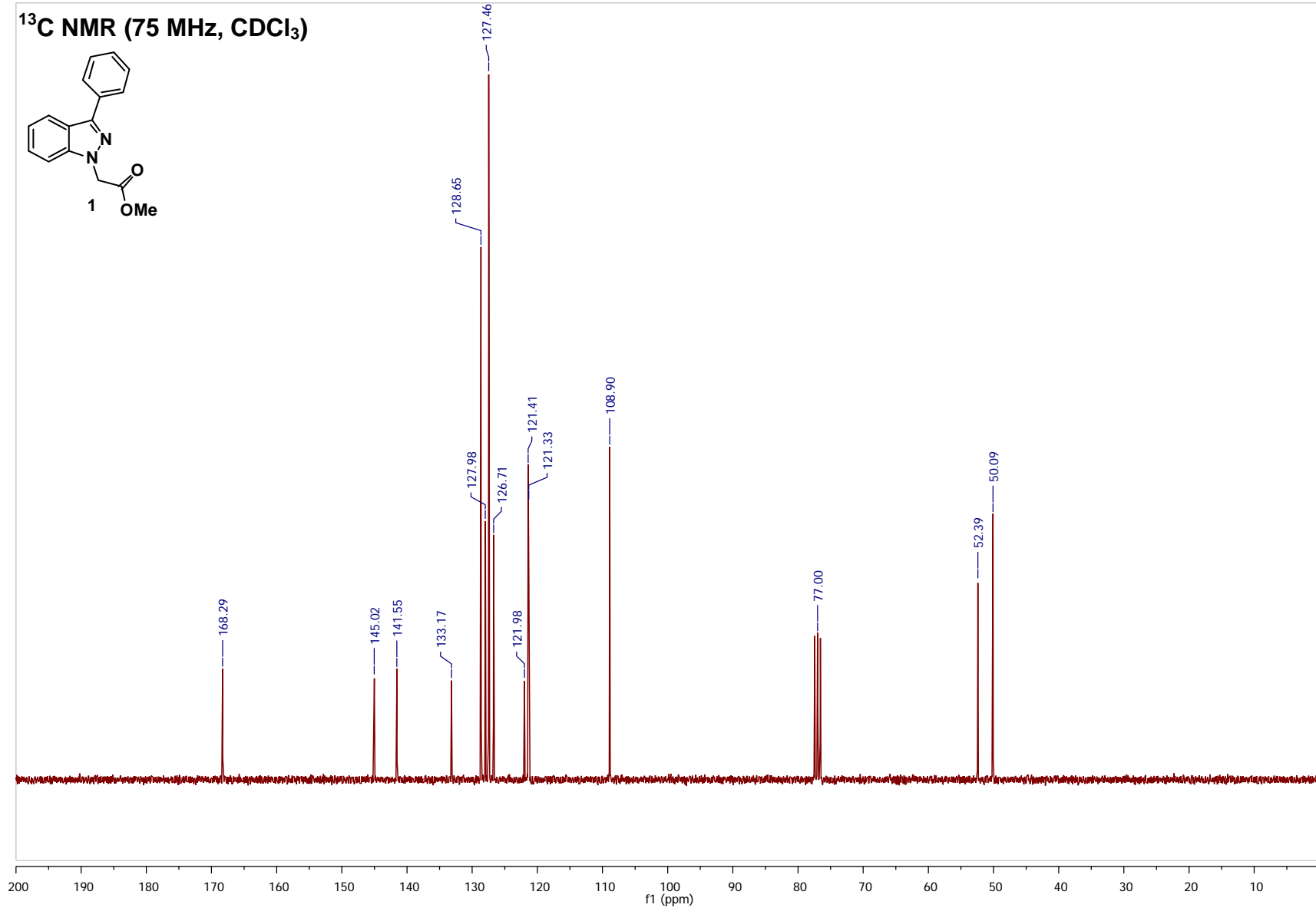
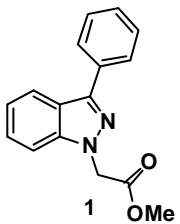
\* Corresponding author

### **NMR spectra of reported compounds**

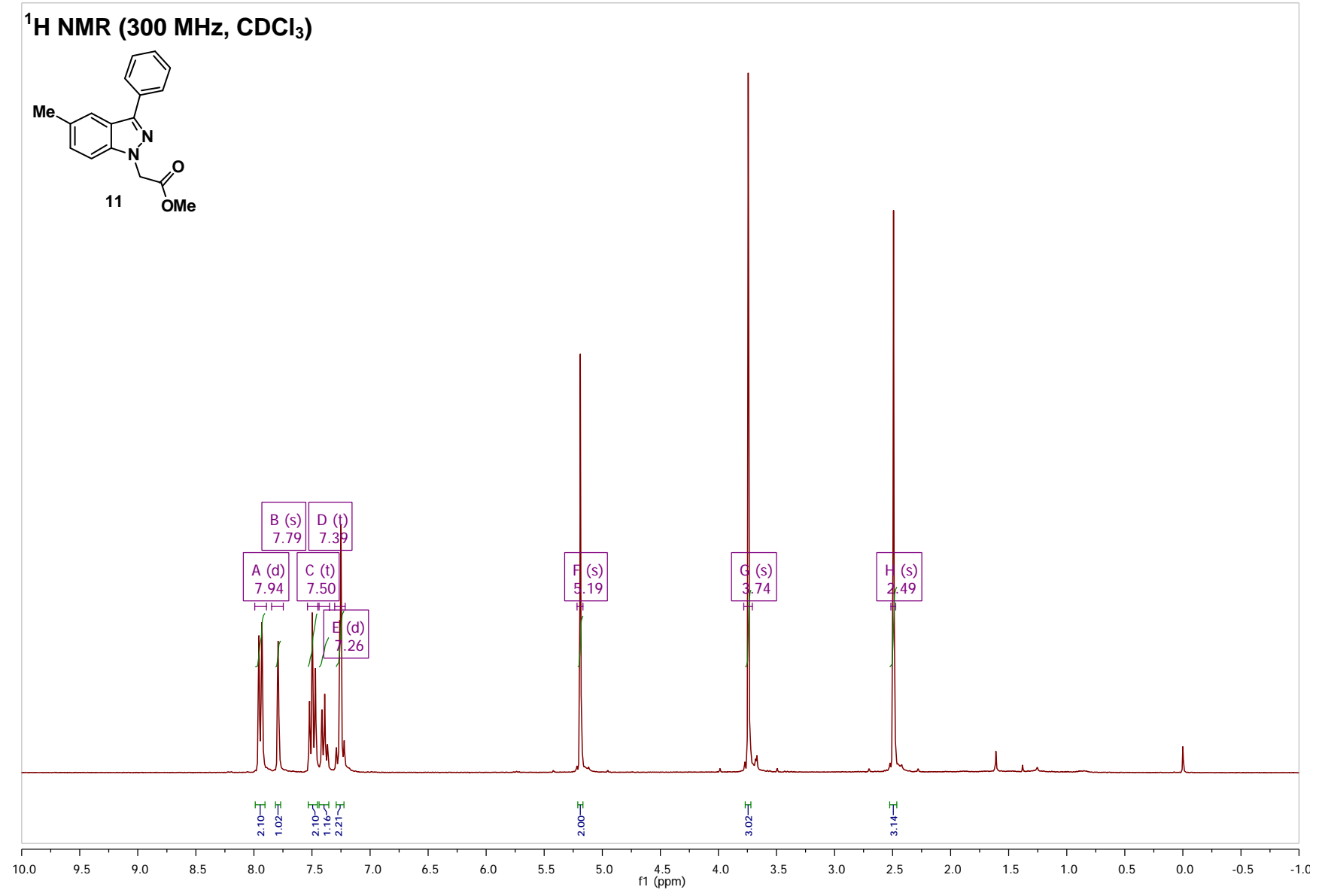
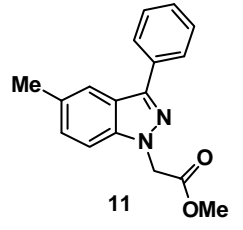
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



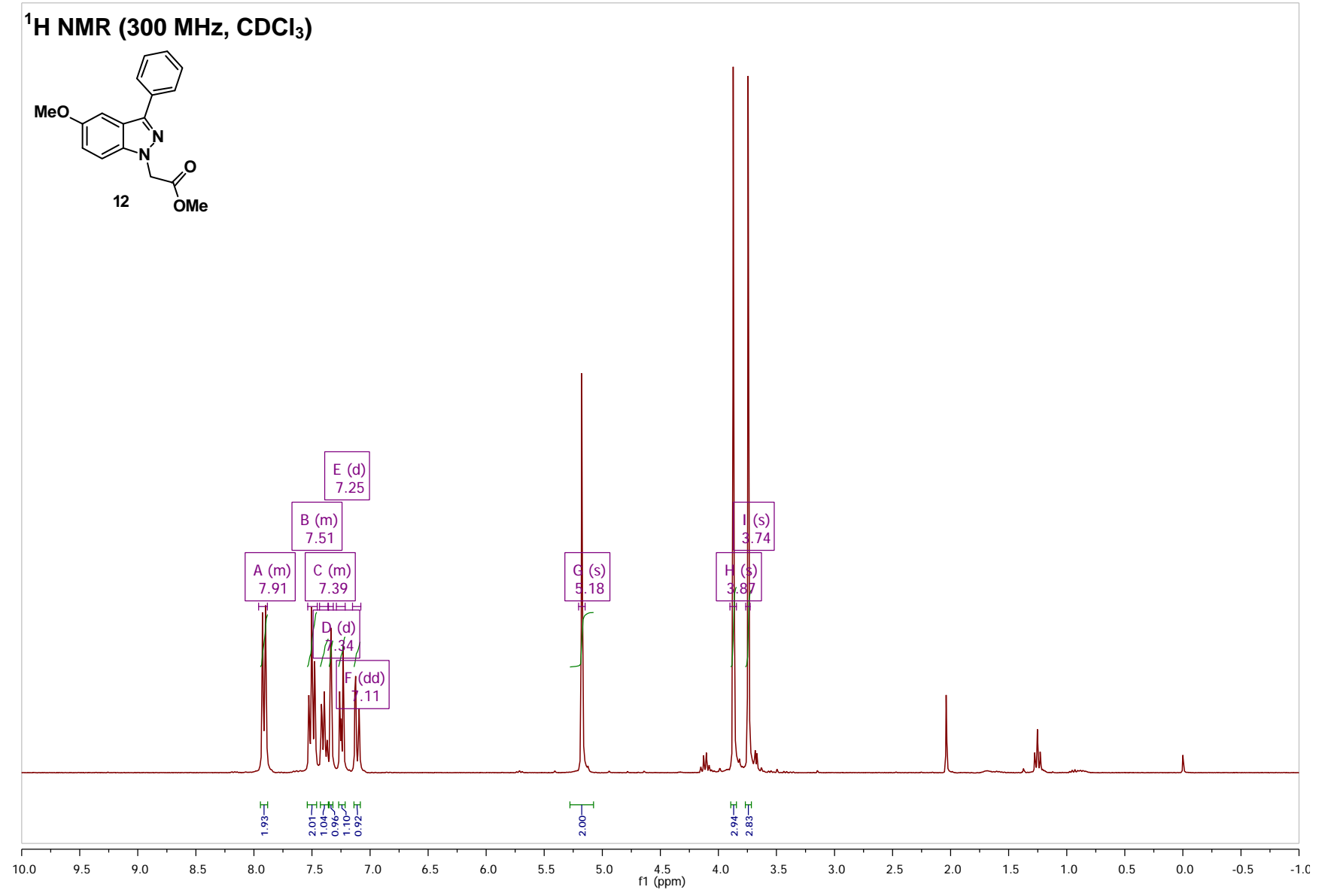
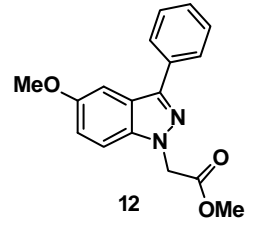
<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)



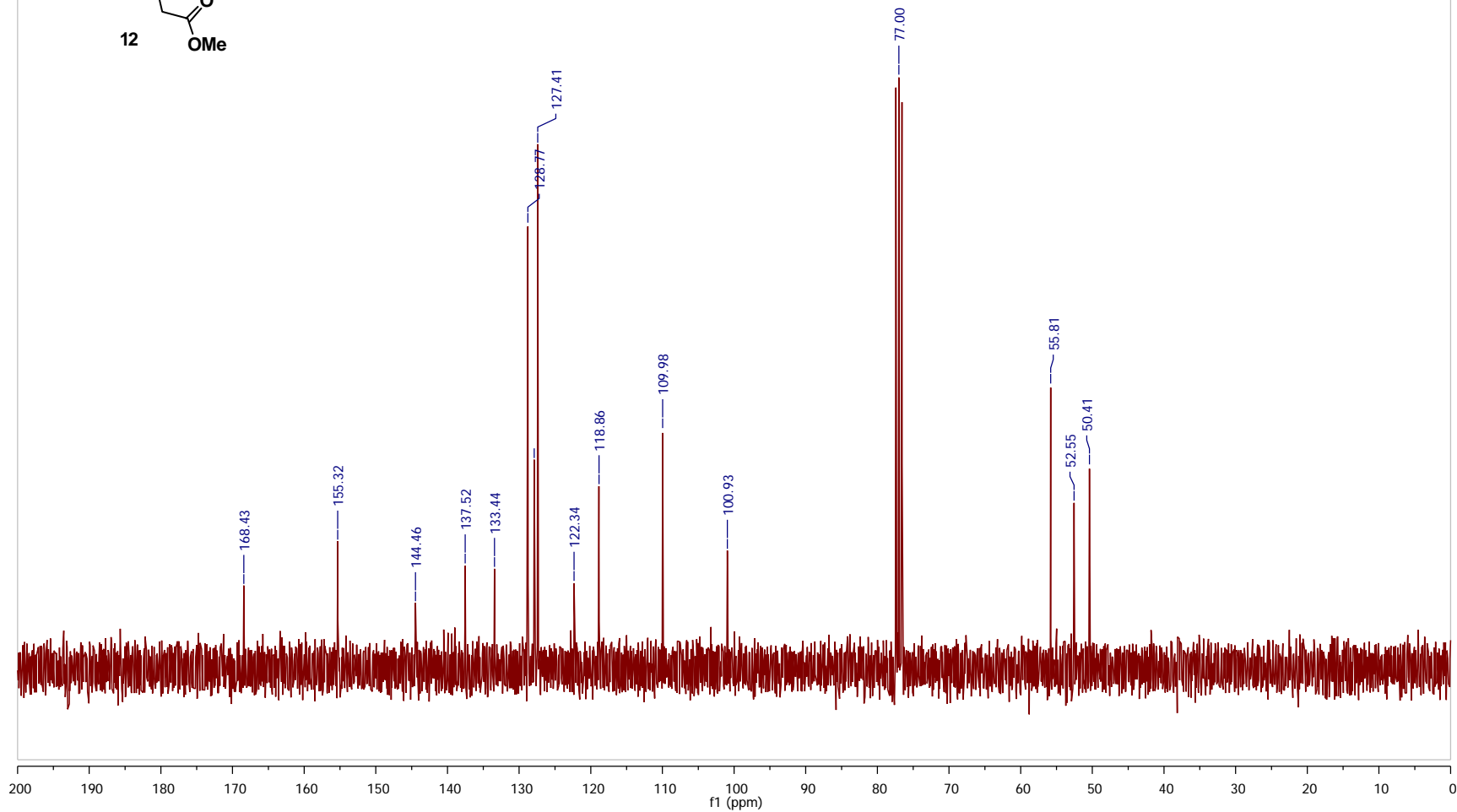
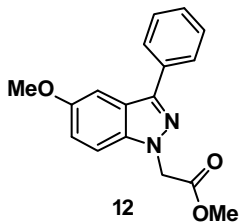
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



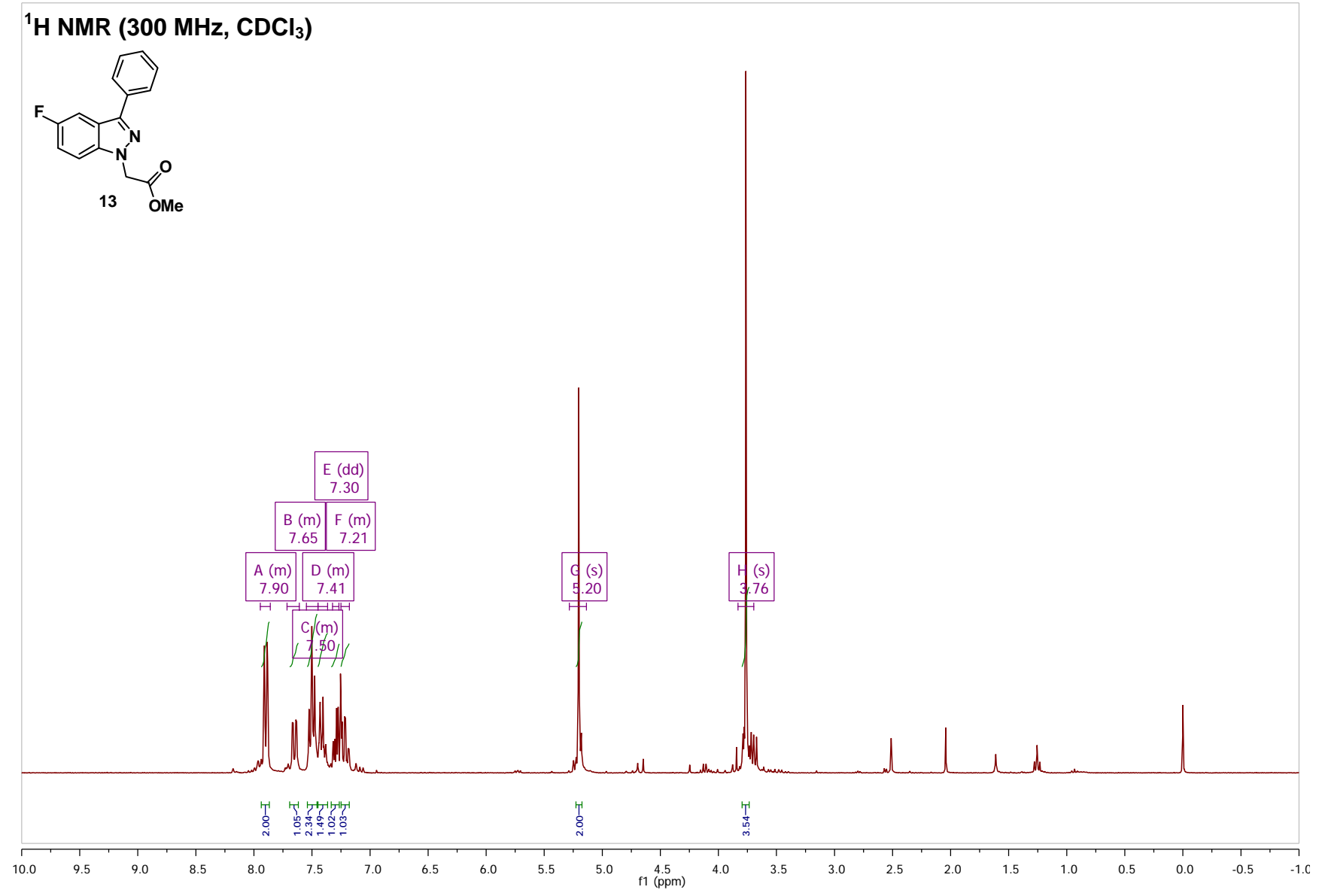
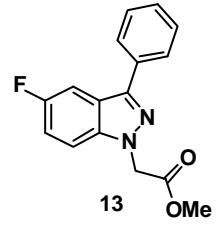
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



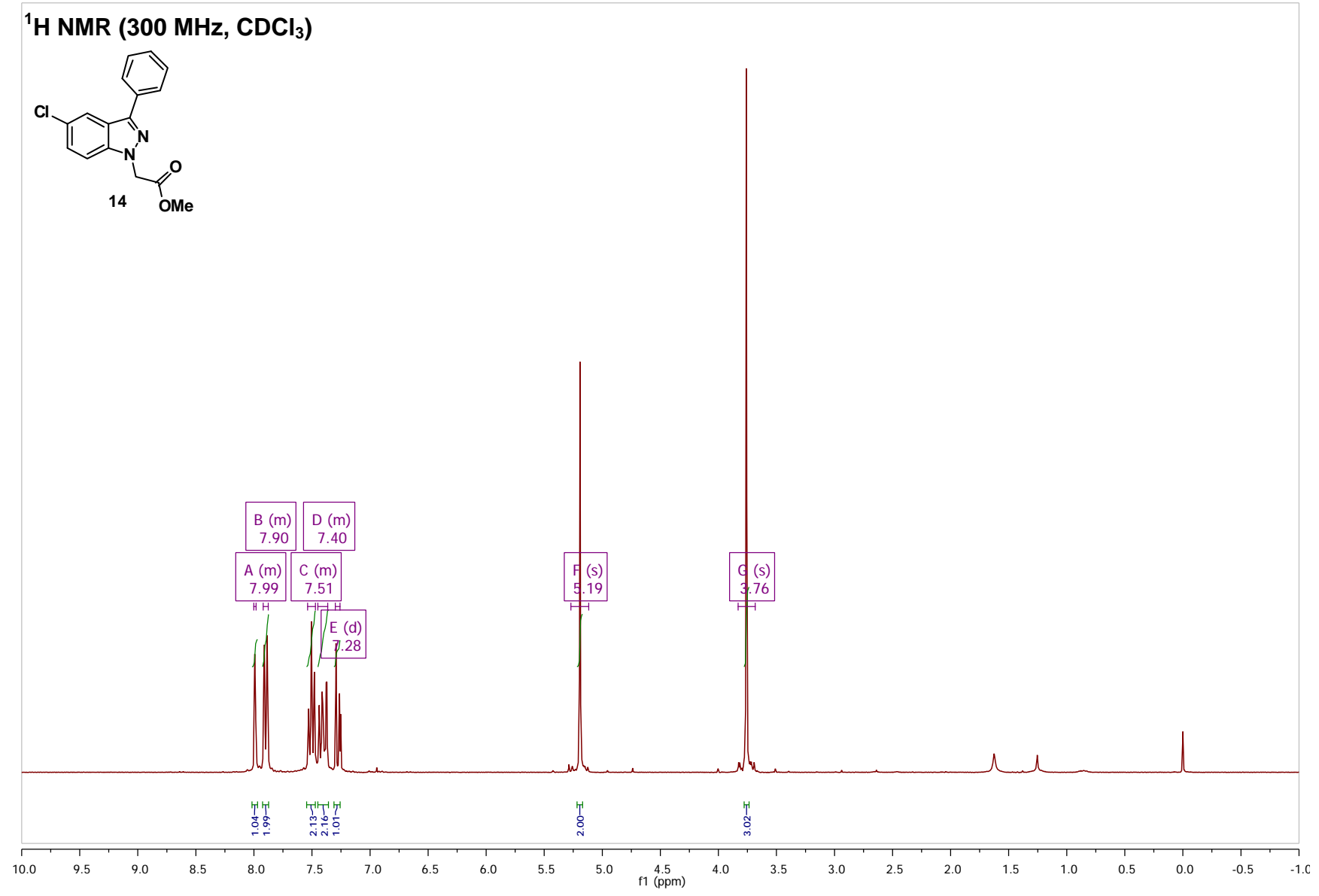
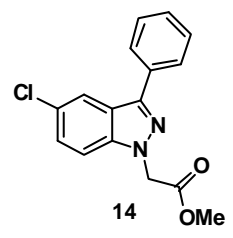
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)**



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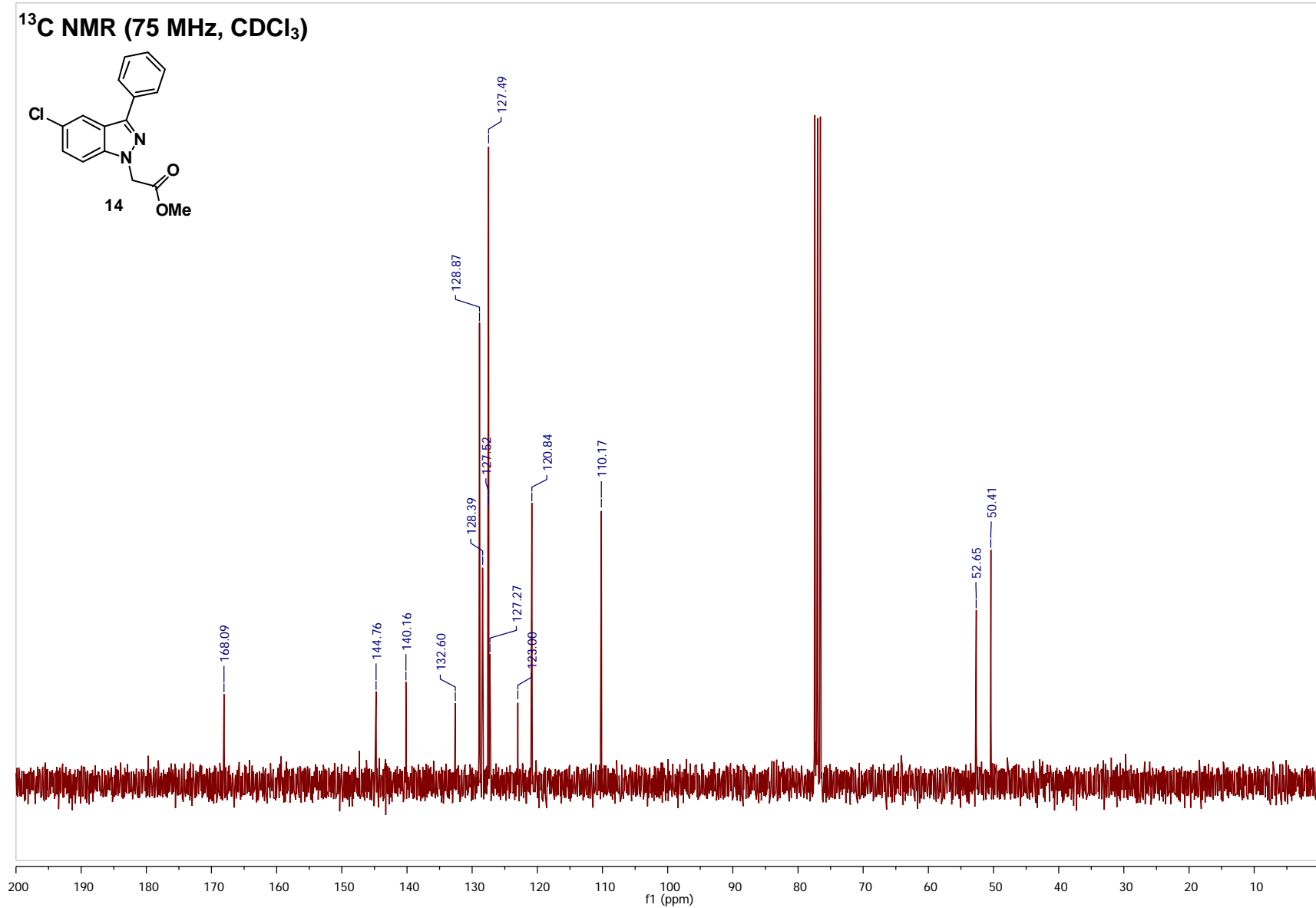
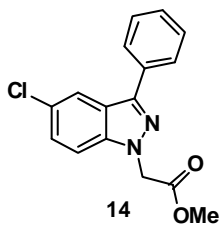


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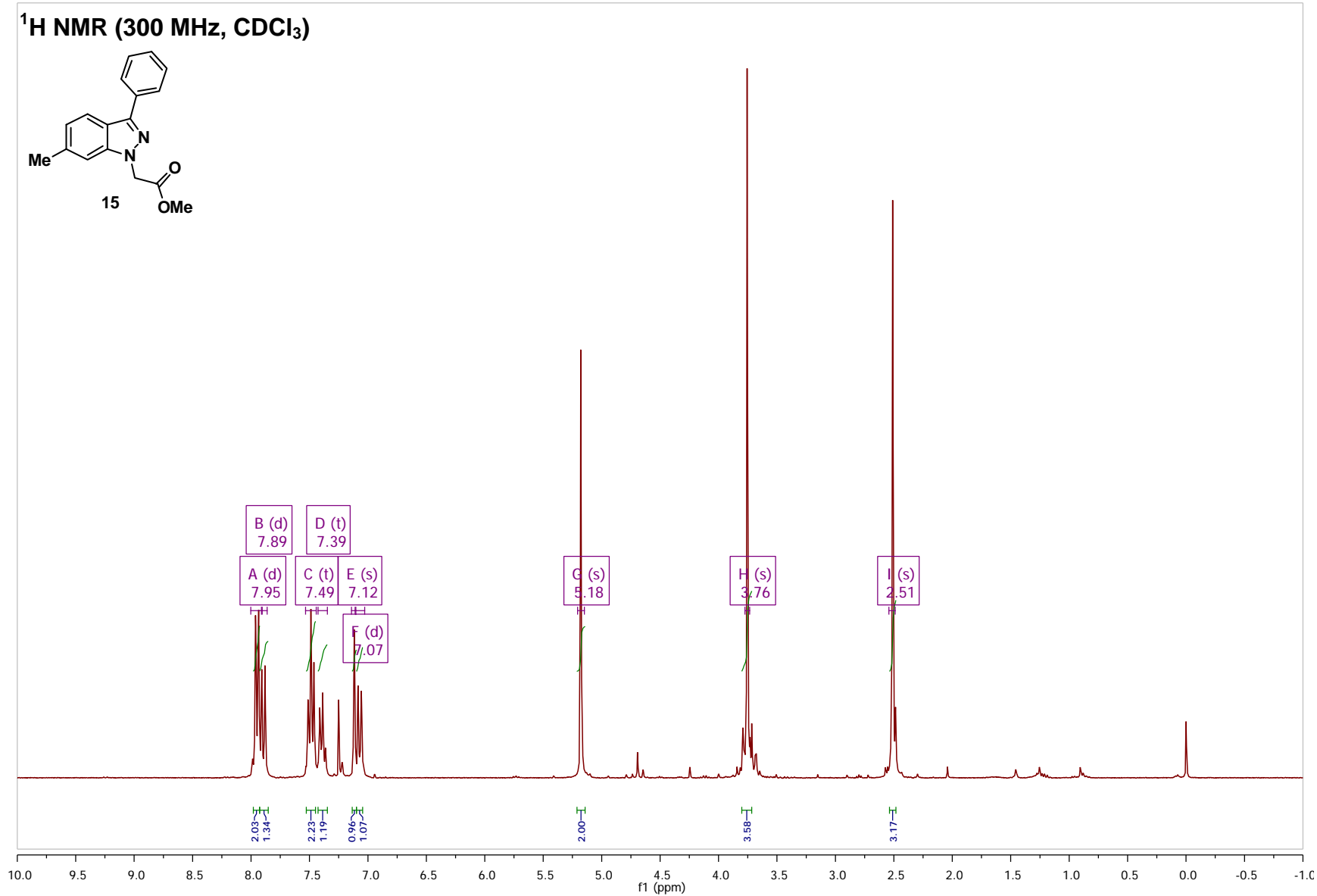
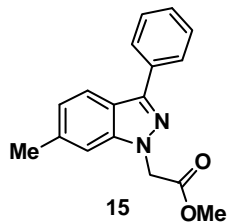




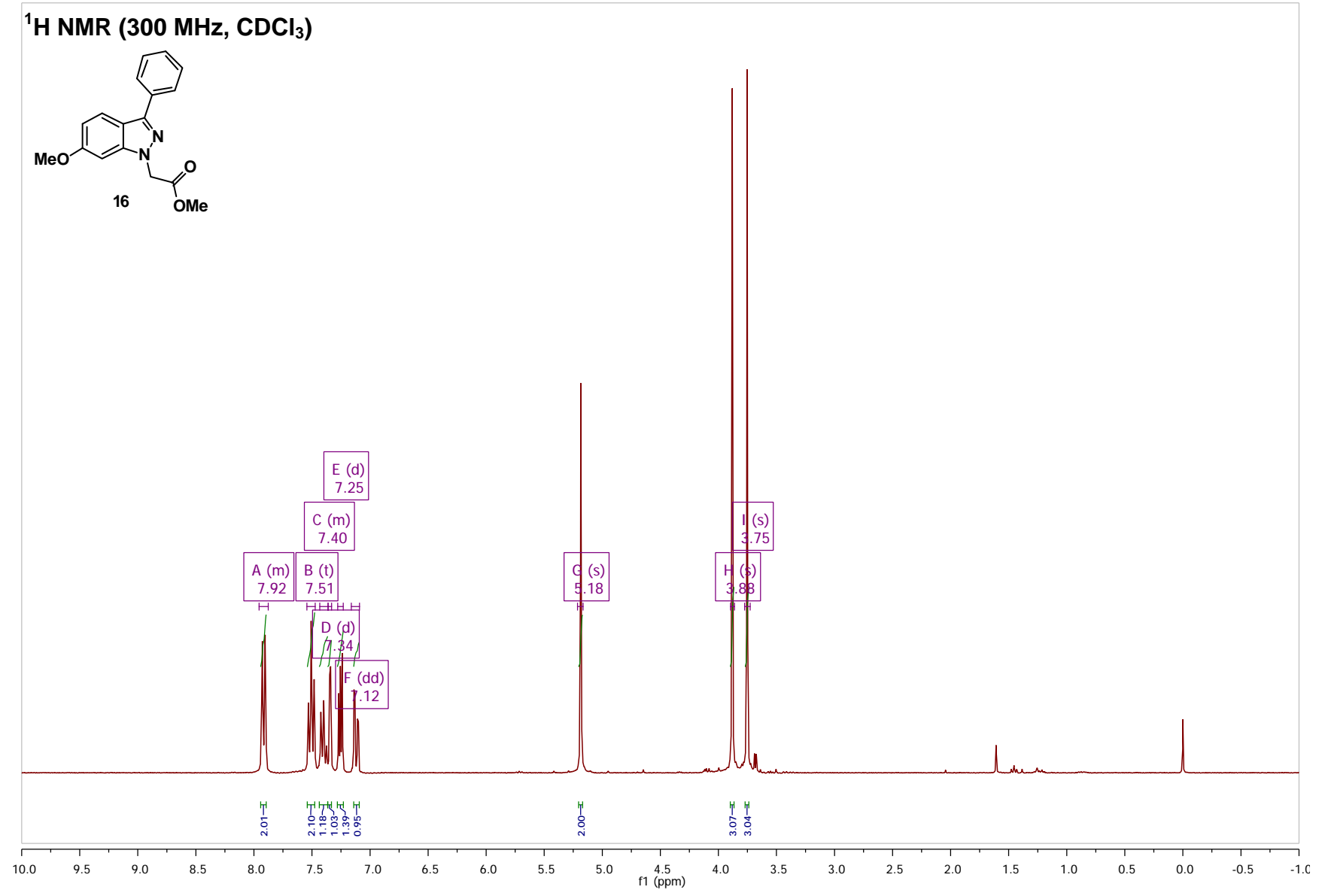
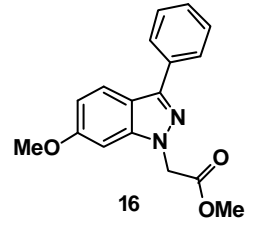
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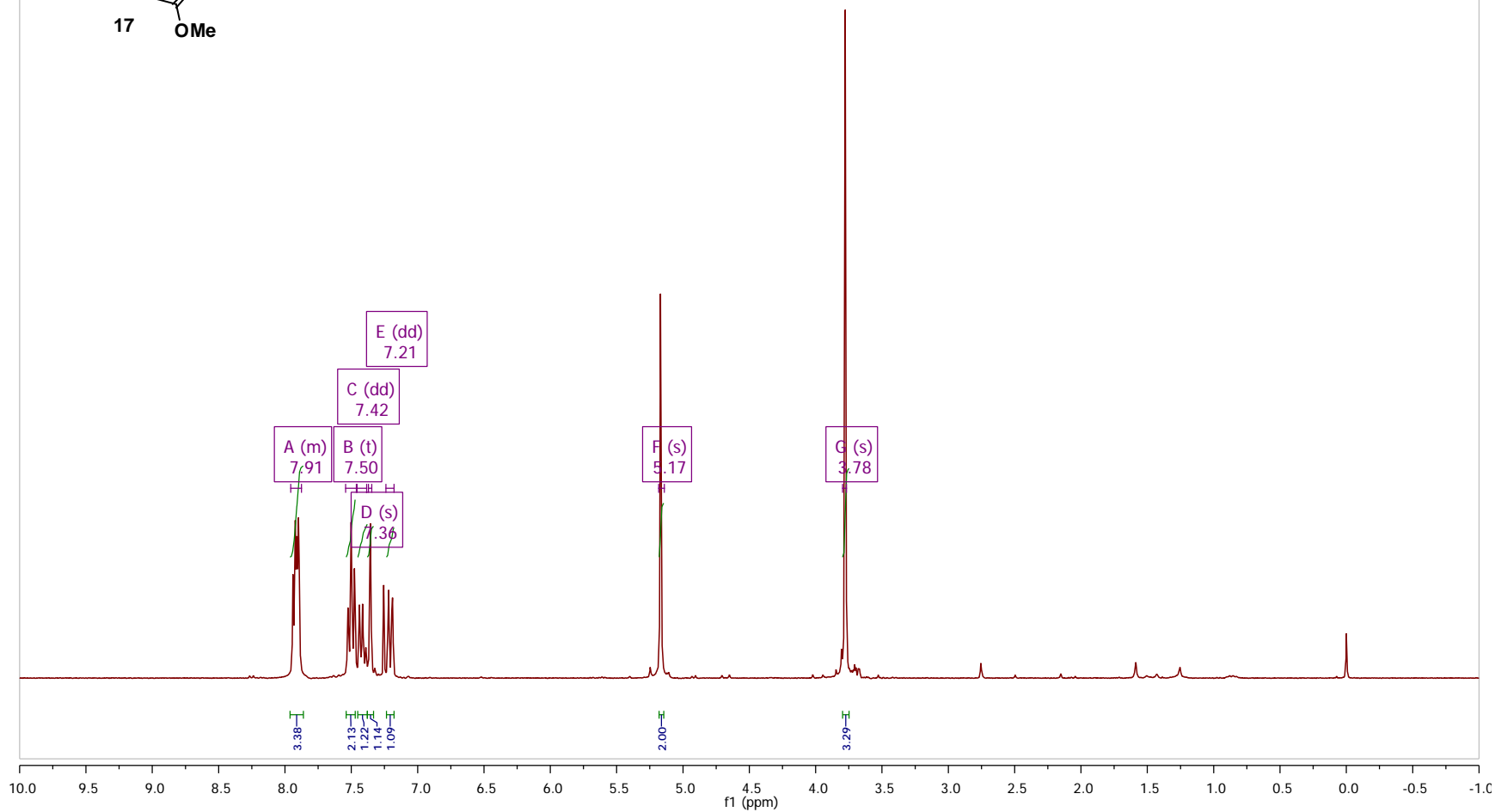
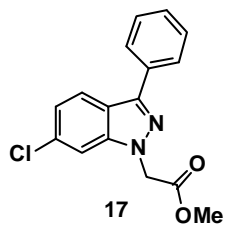
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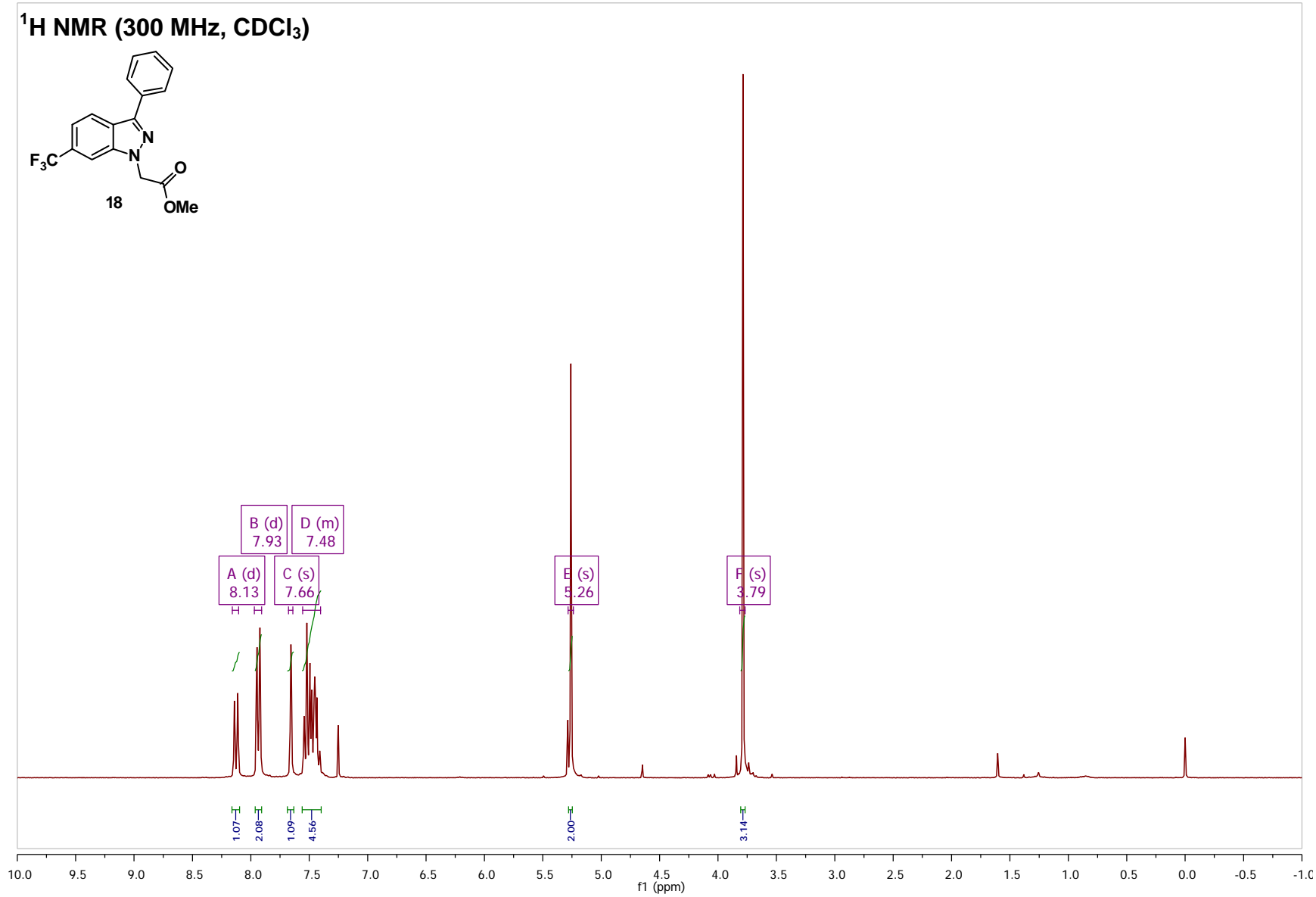
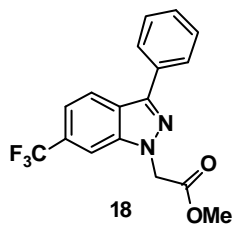
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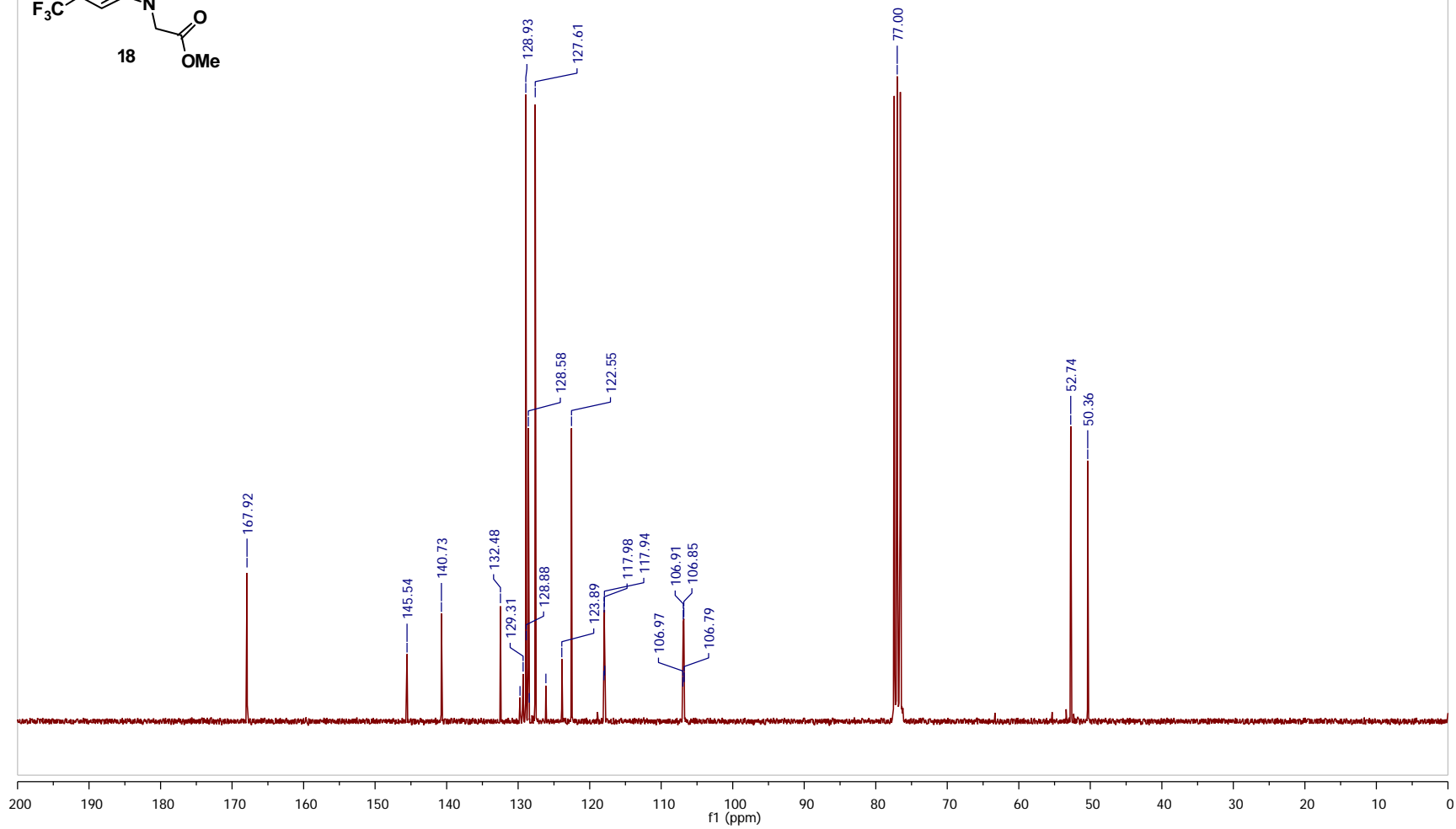
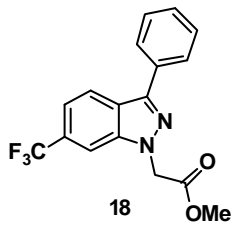
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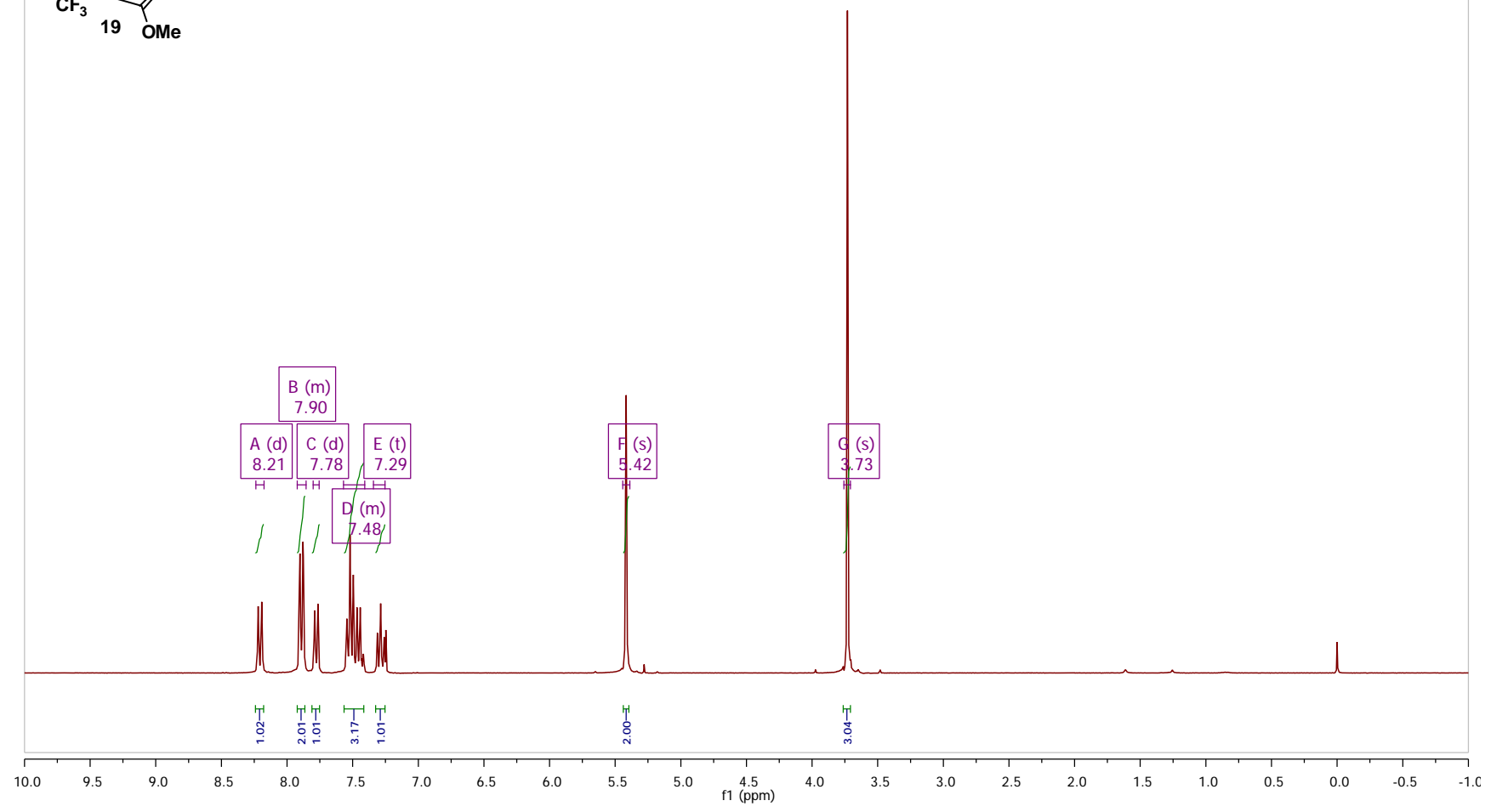
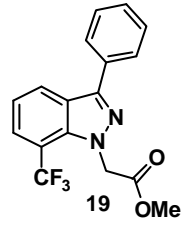
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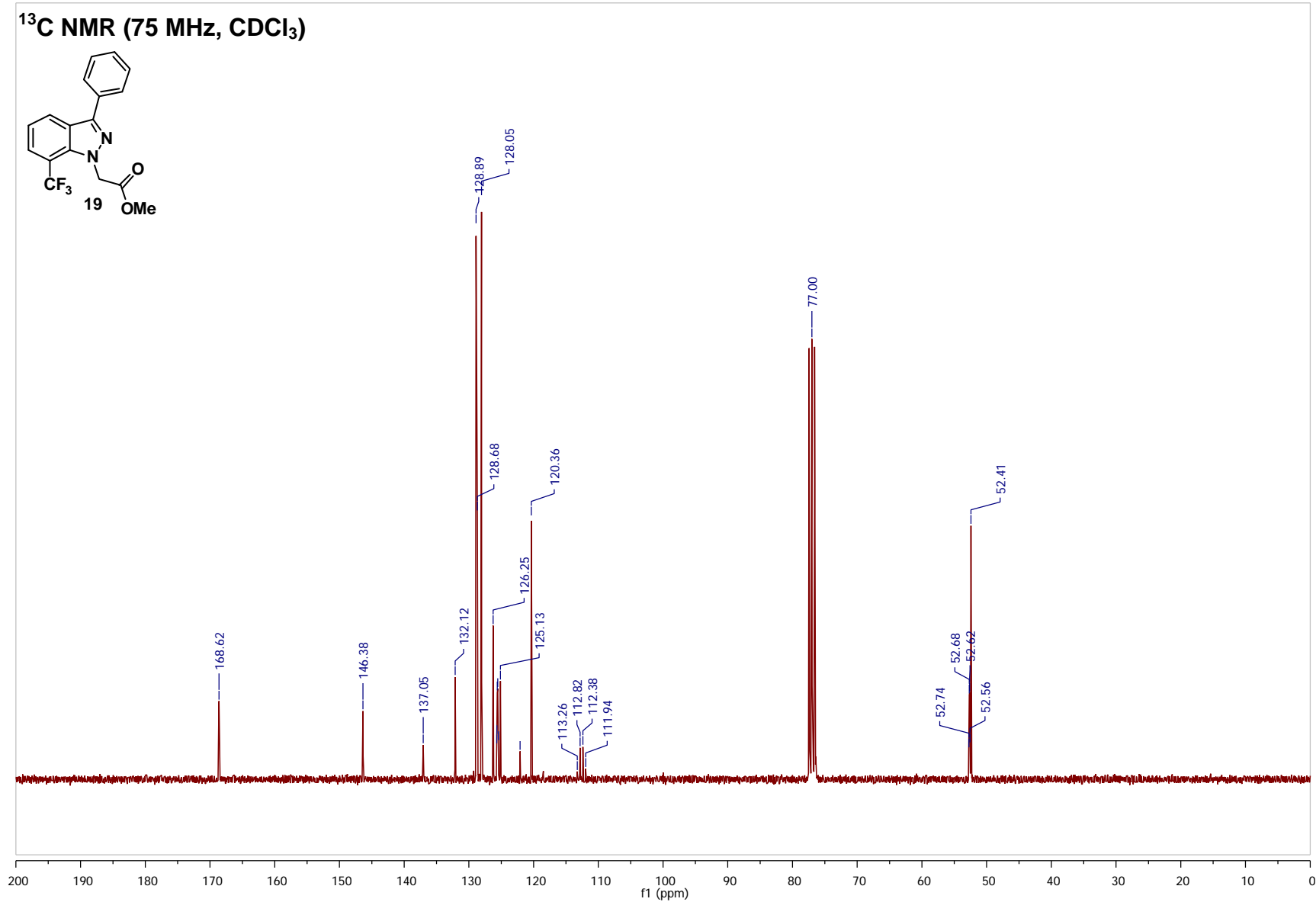
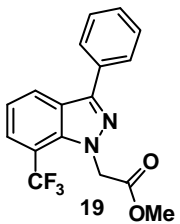
<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)



**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)**

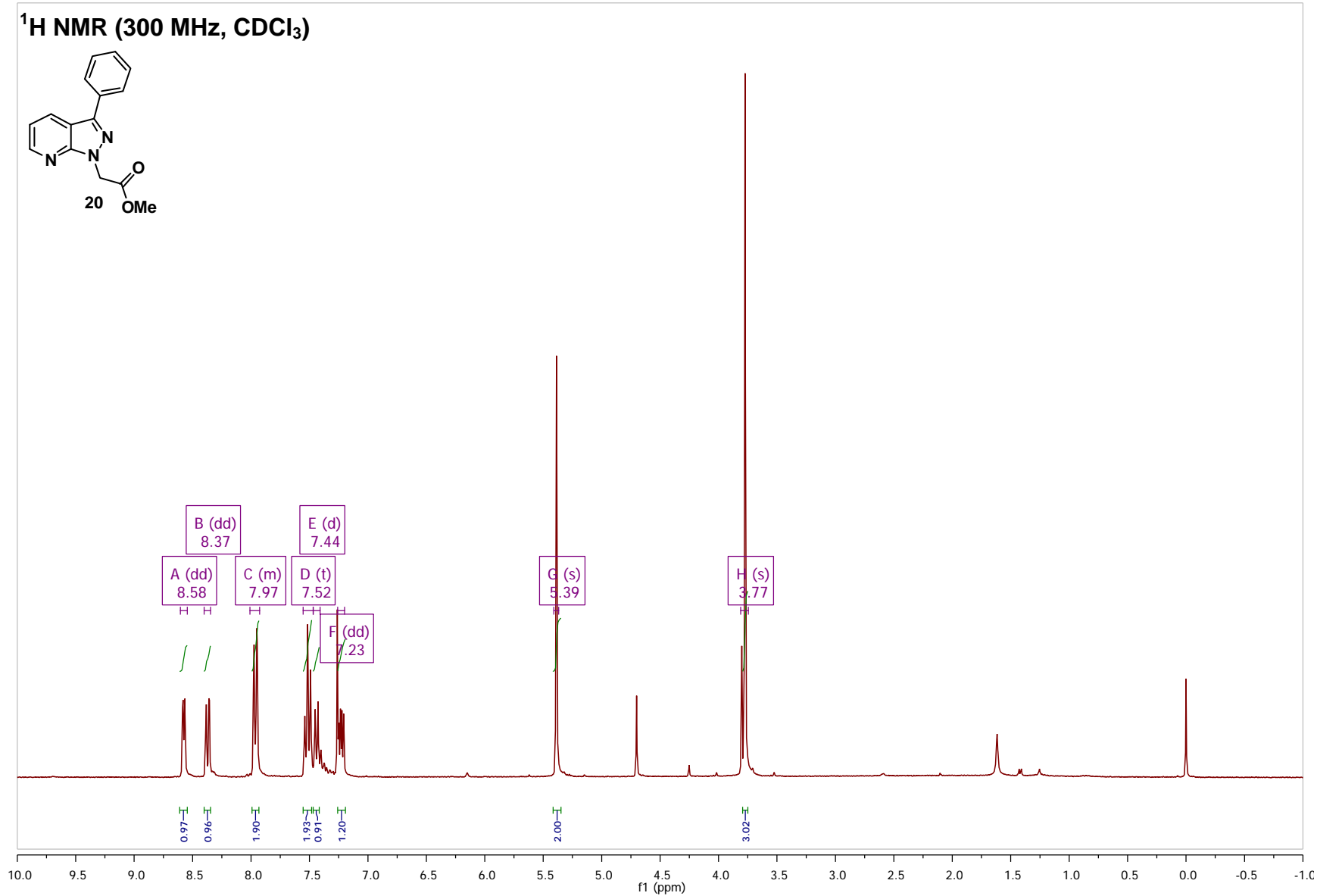
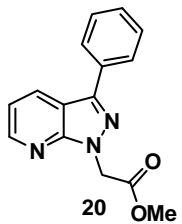


<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)

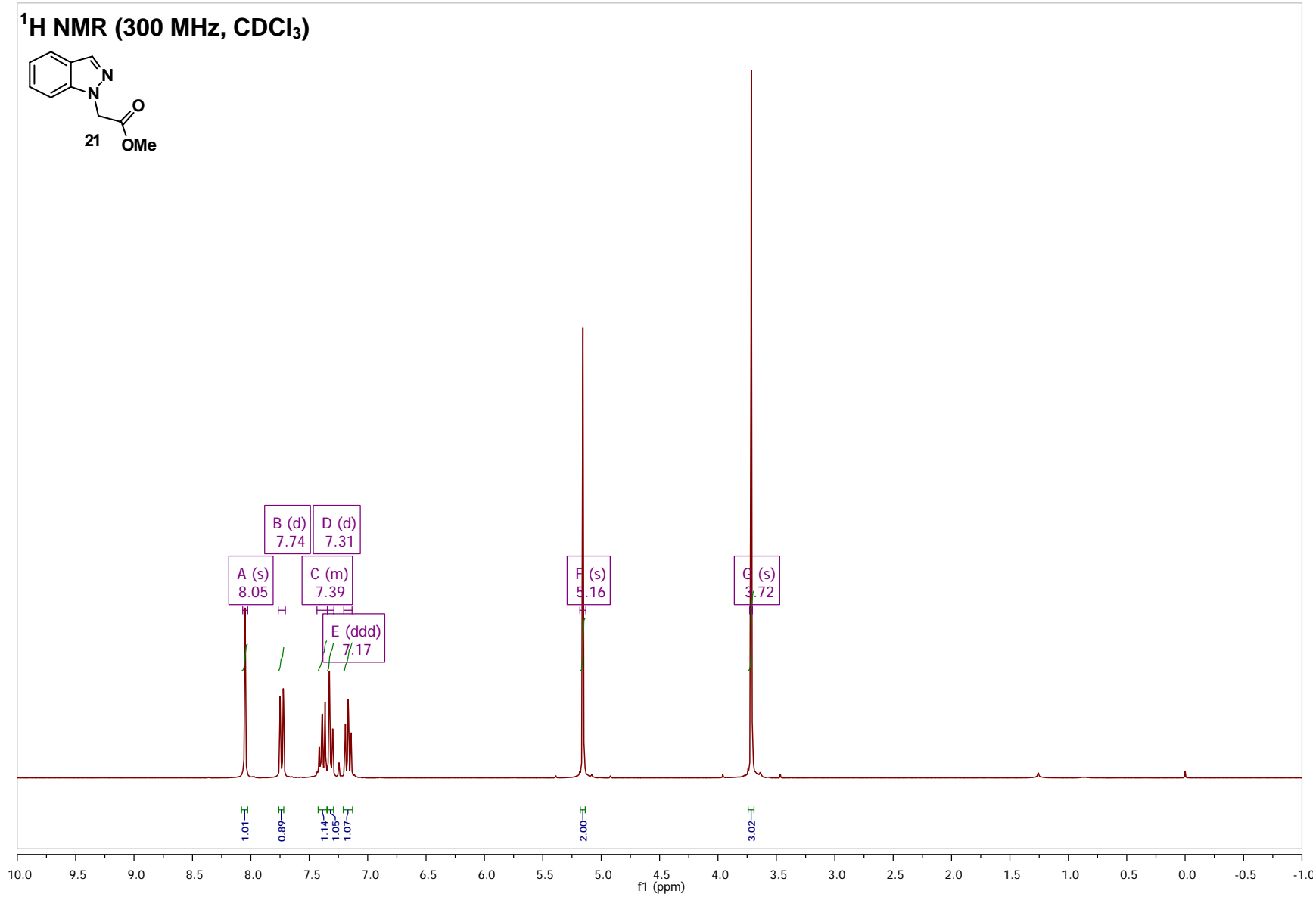
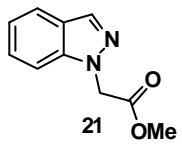




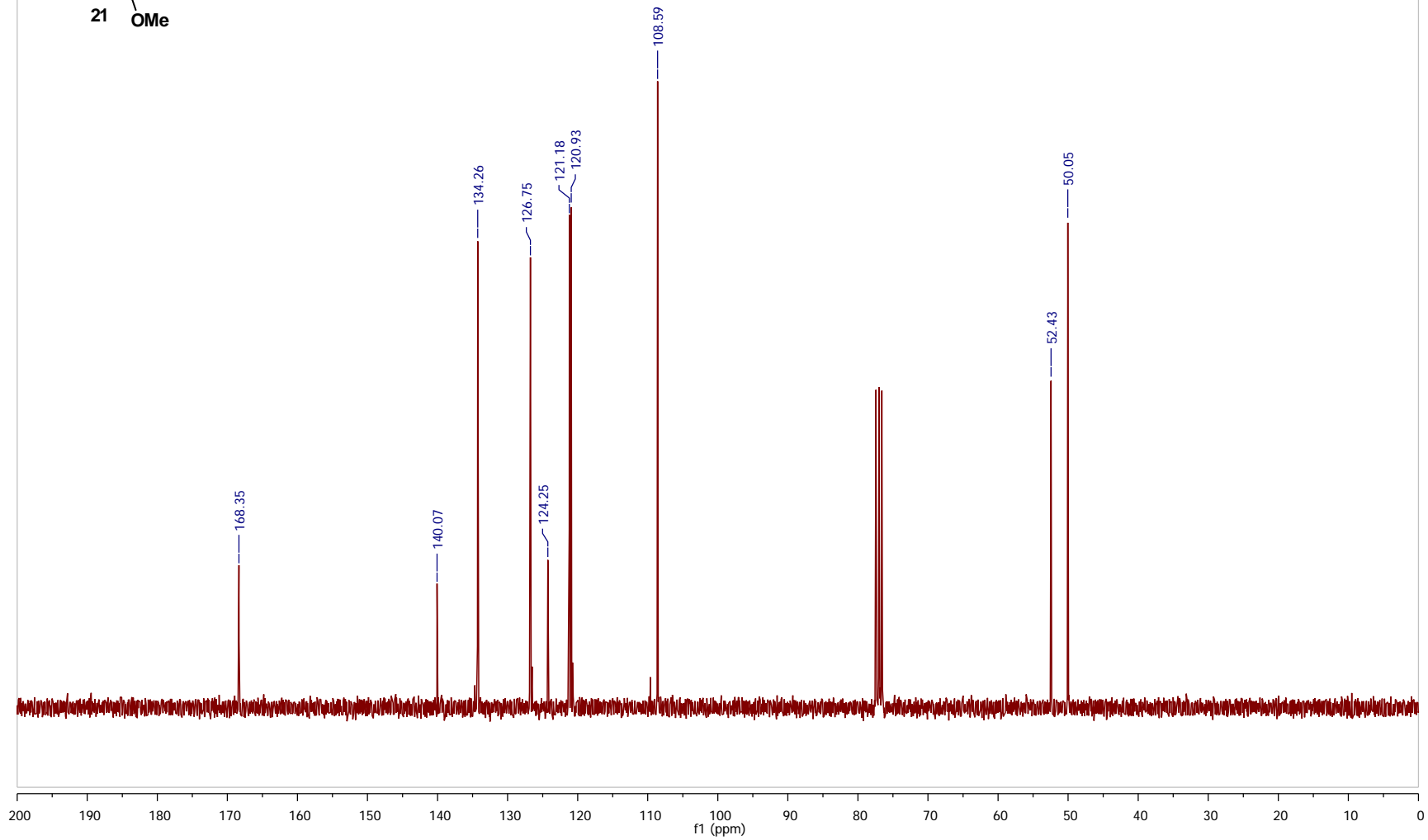
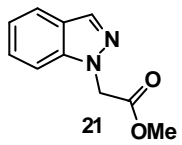
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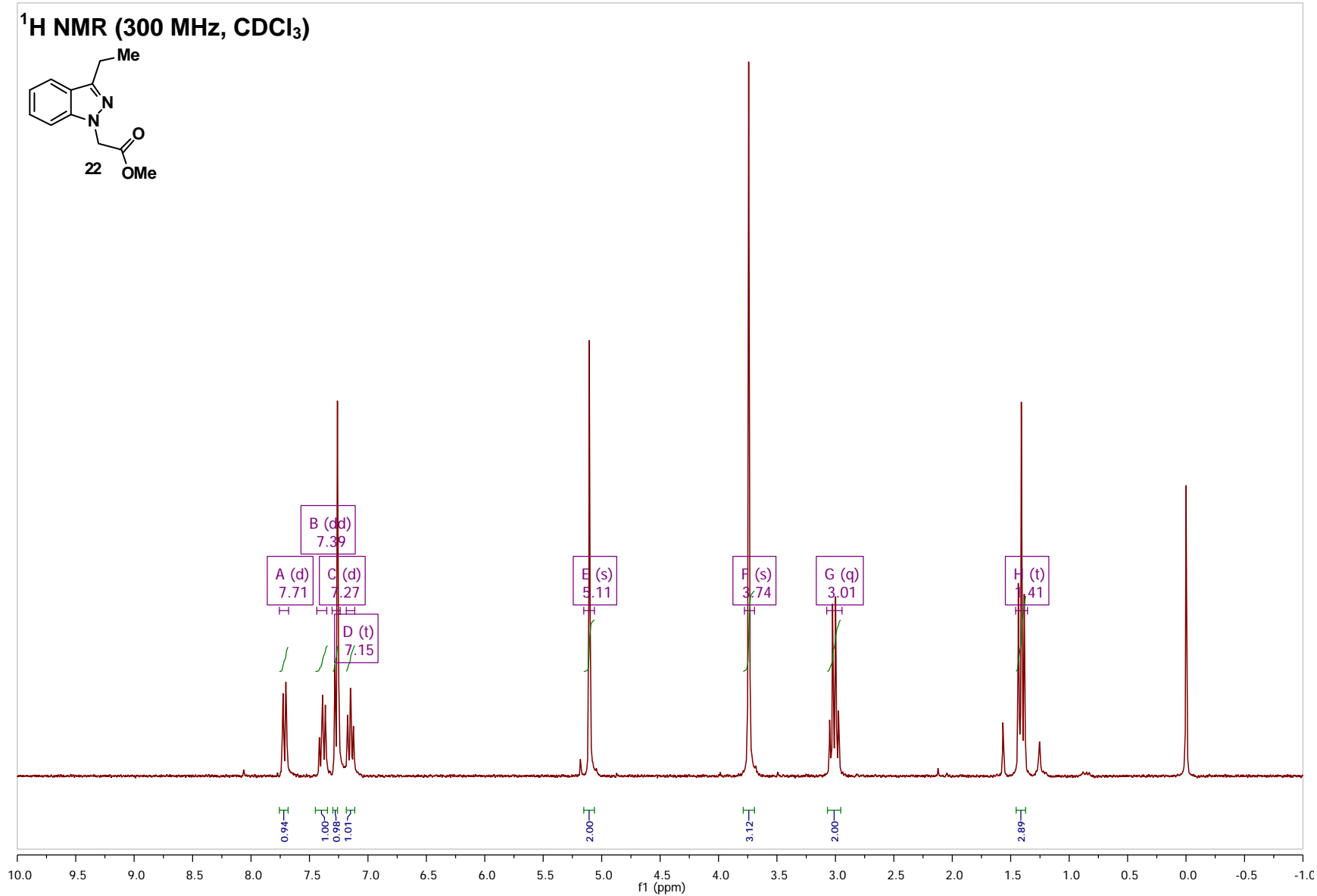
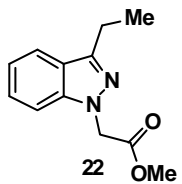
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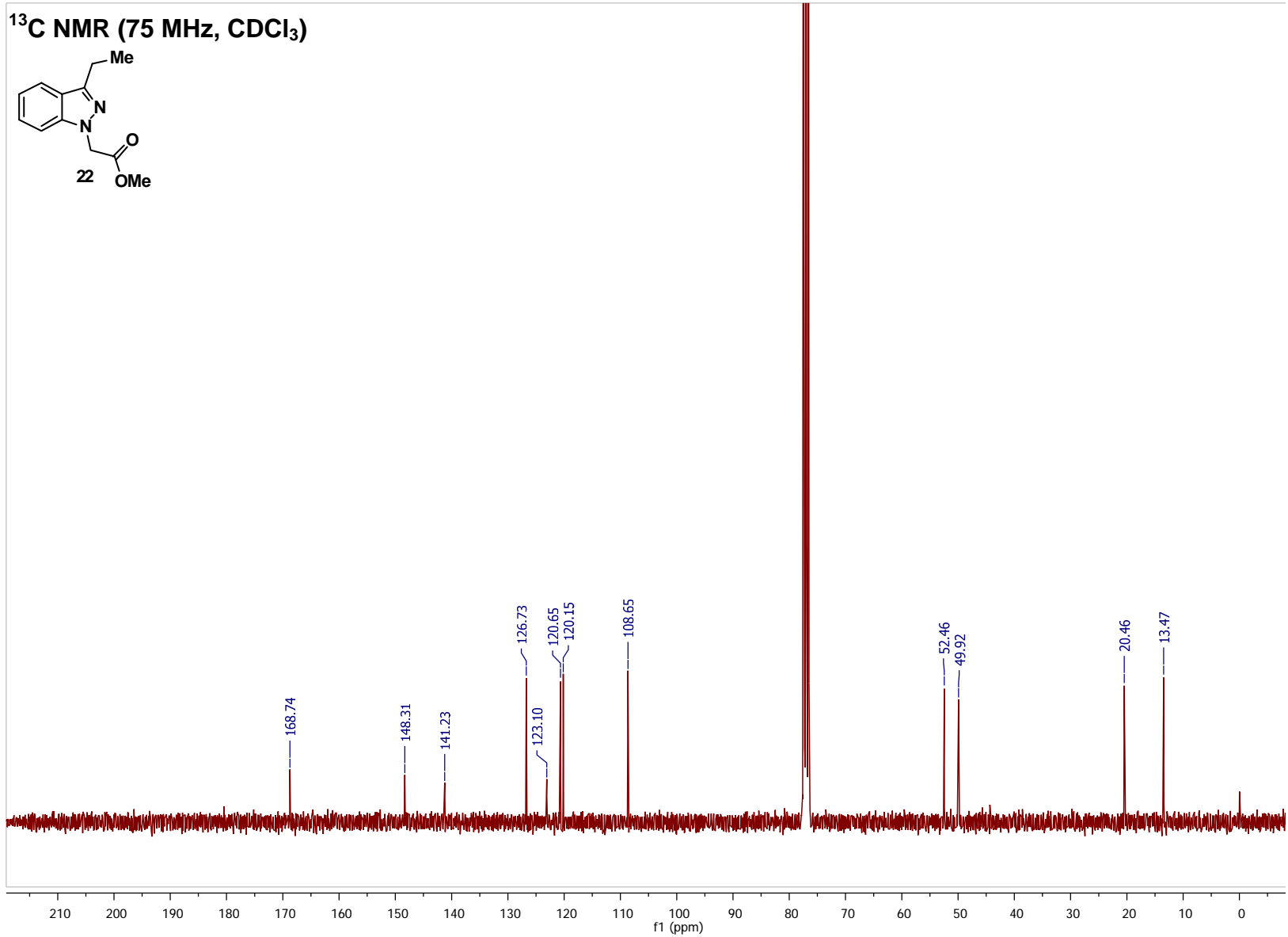
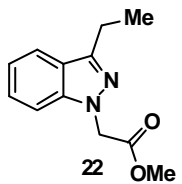
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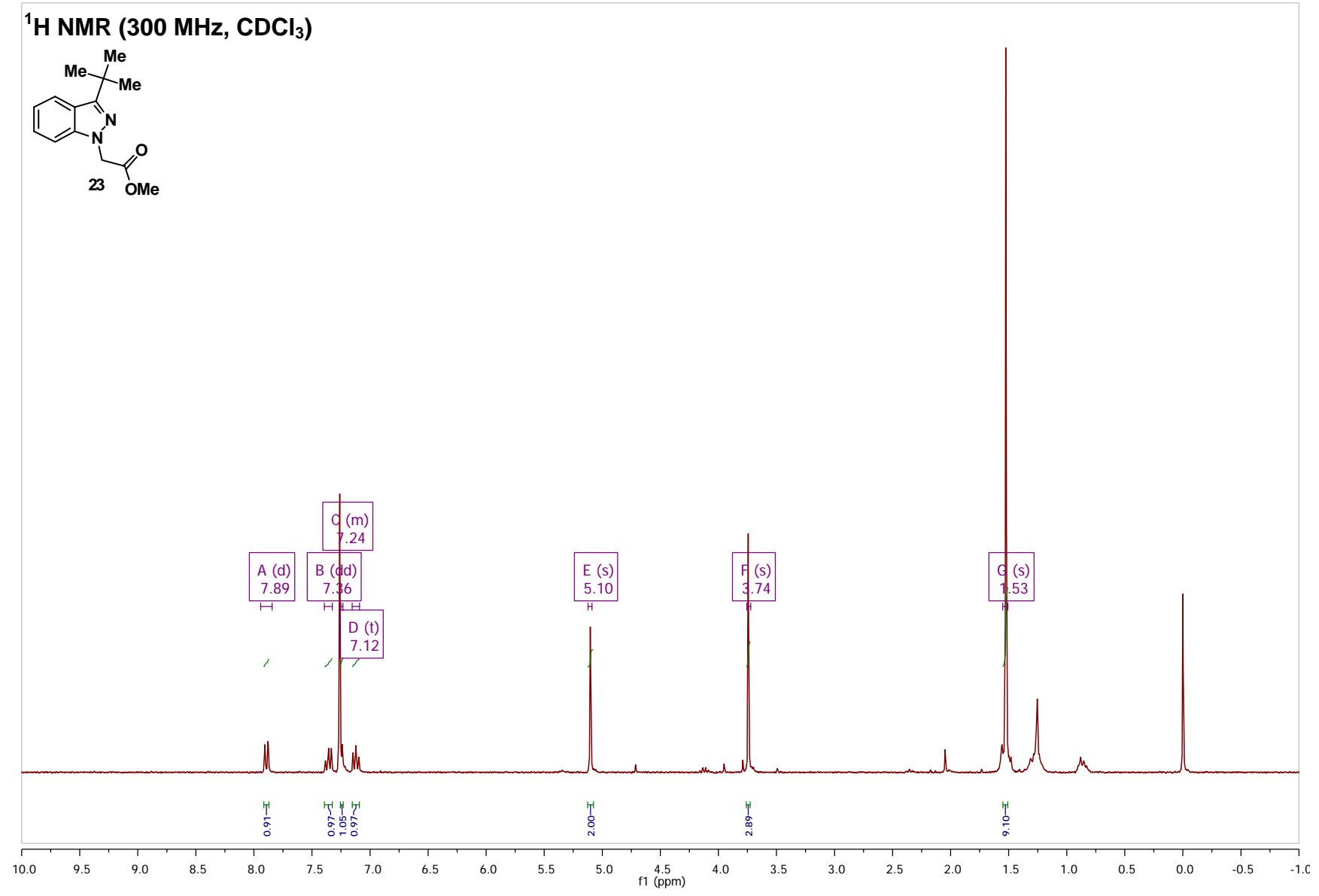
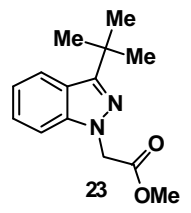
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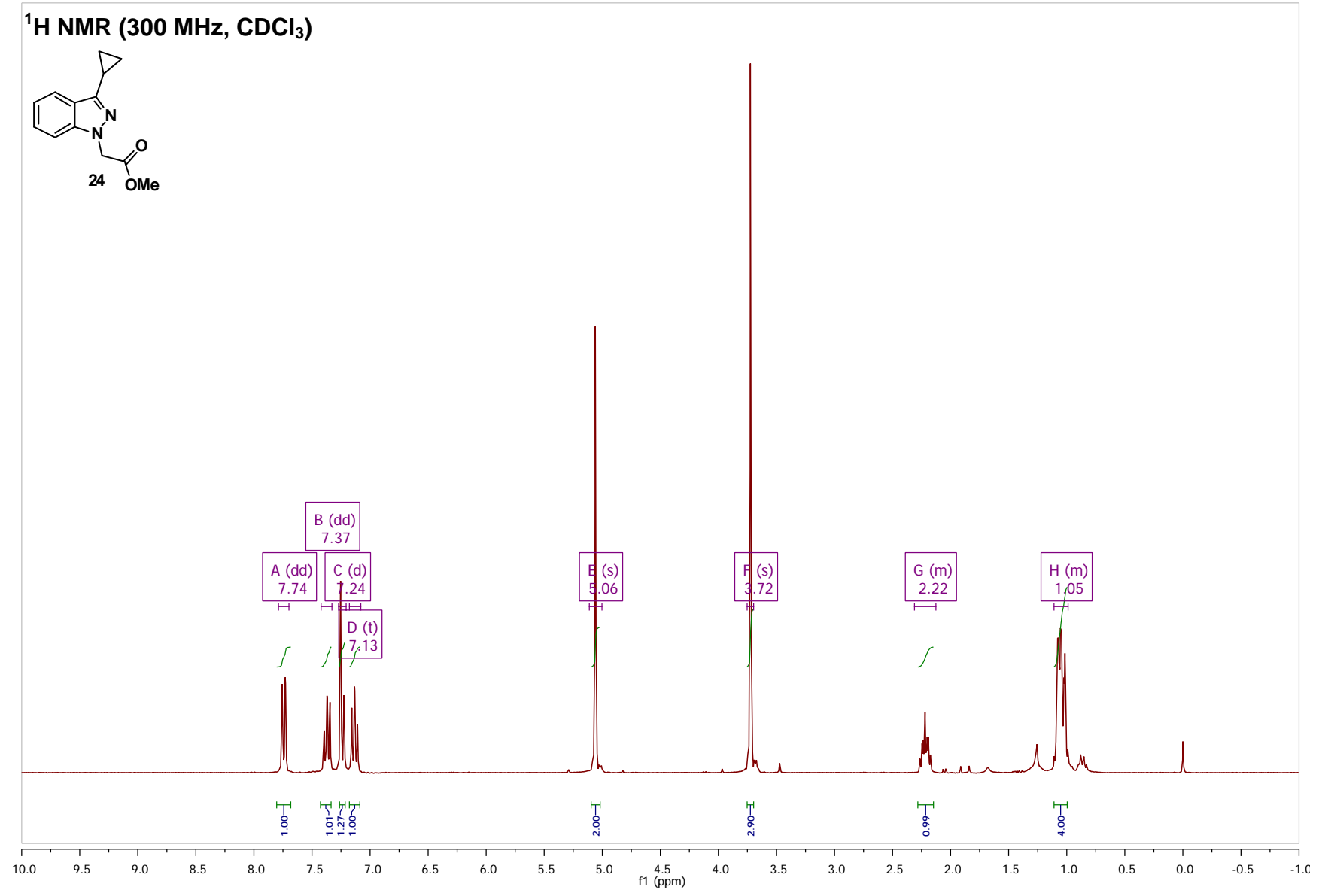
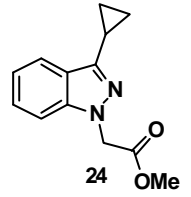
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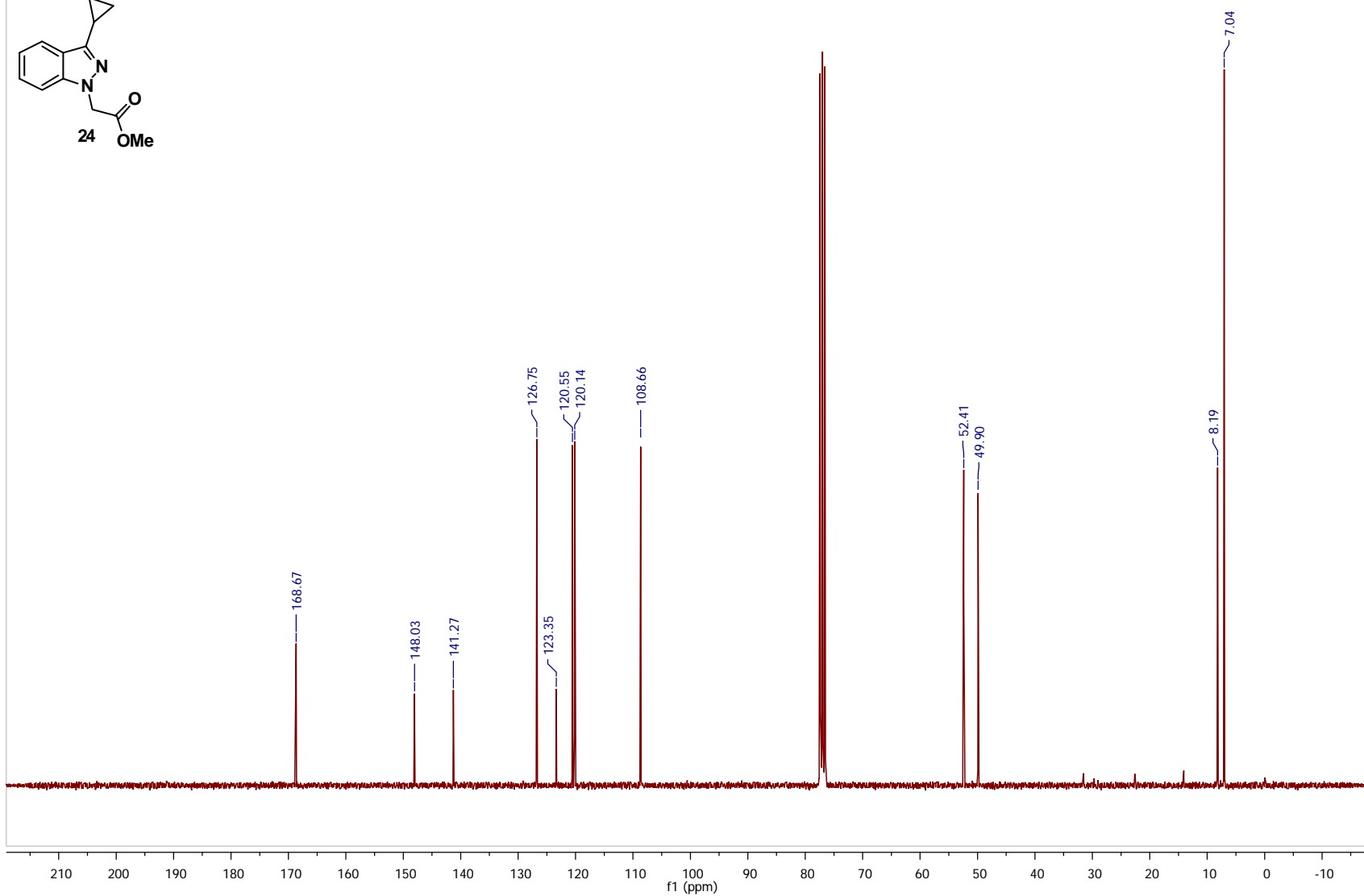
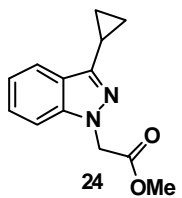
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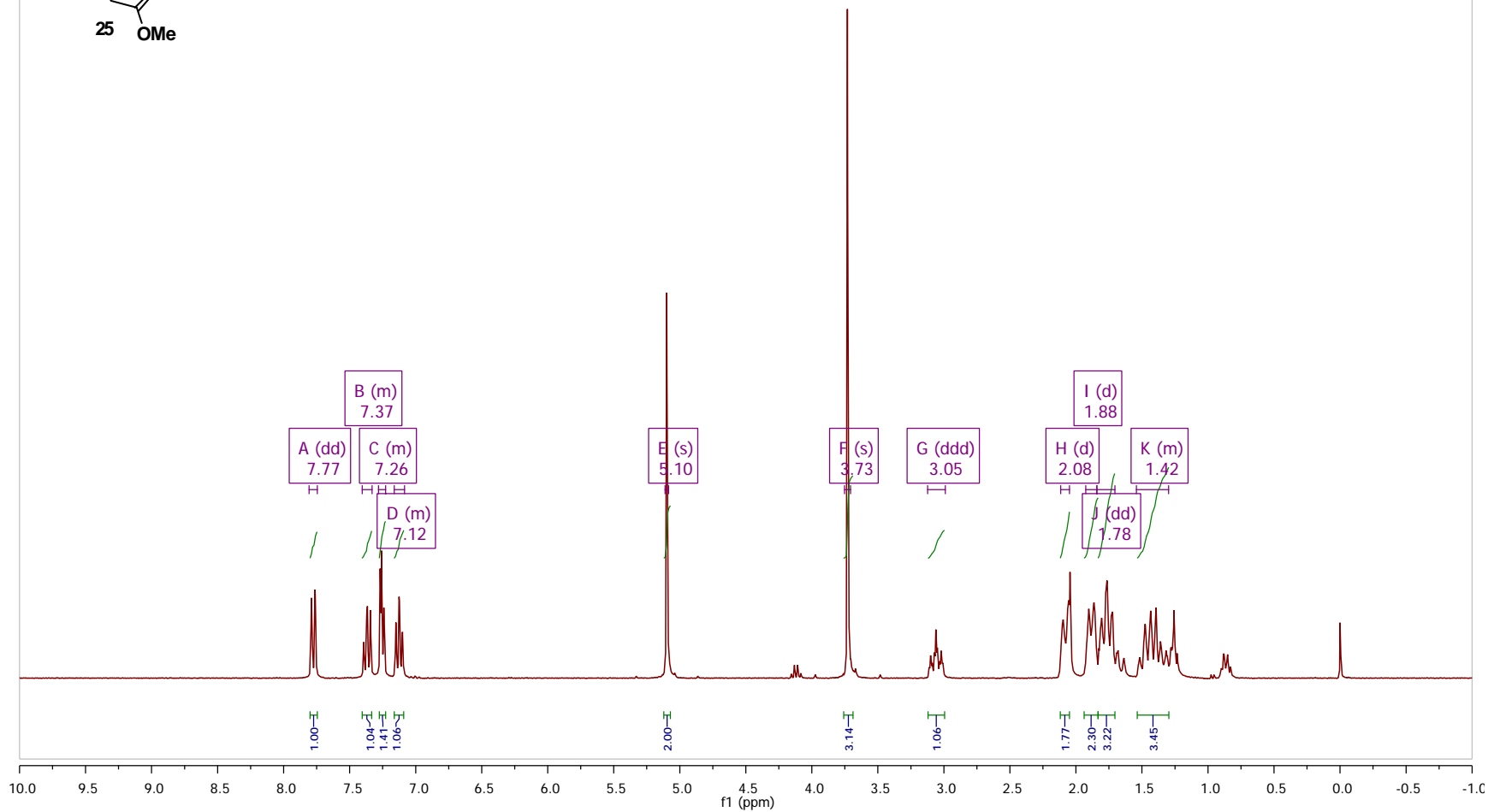
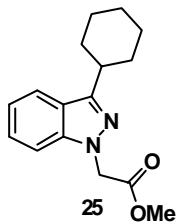


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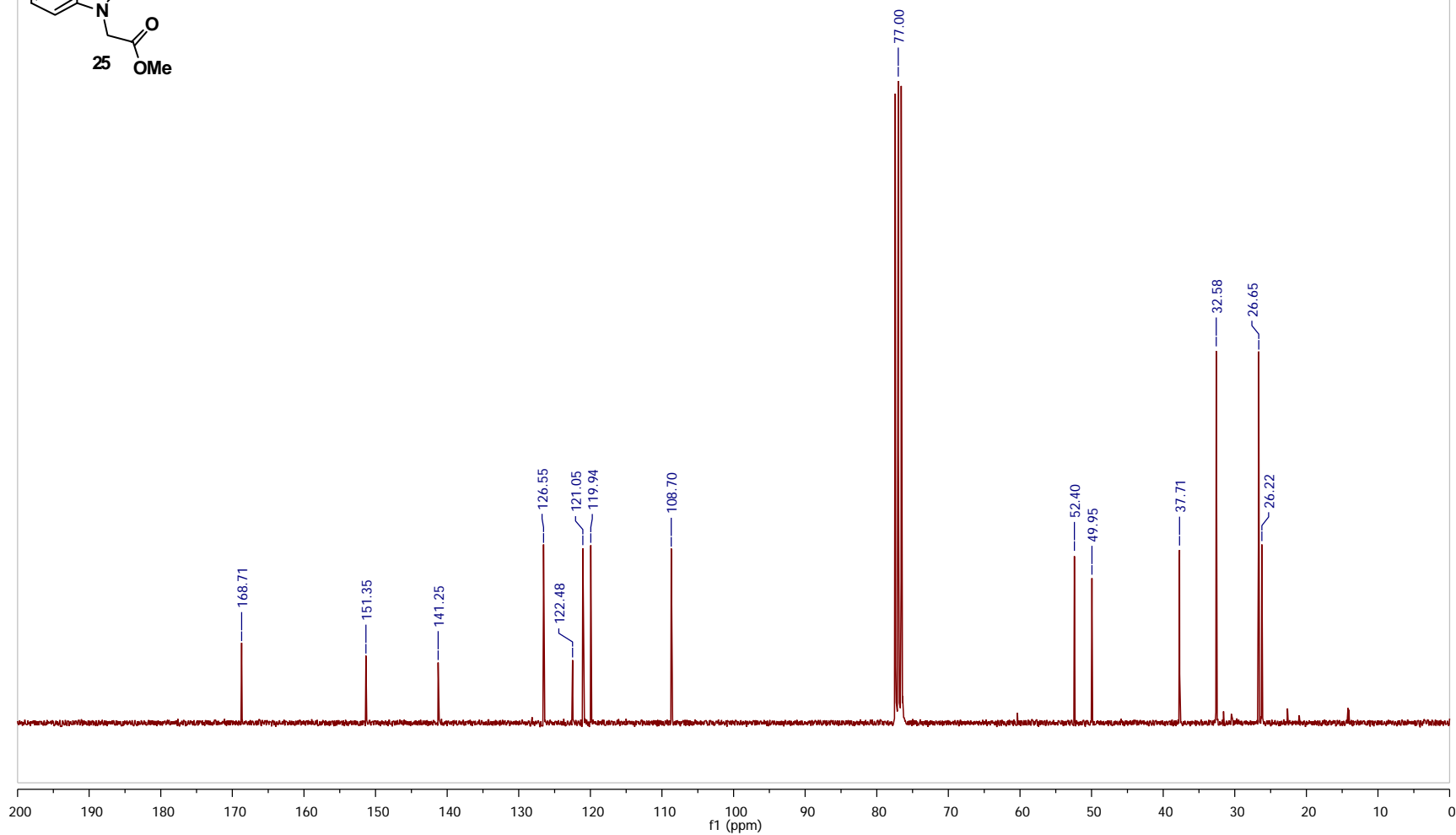
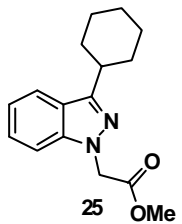




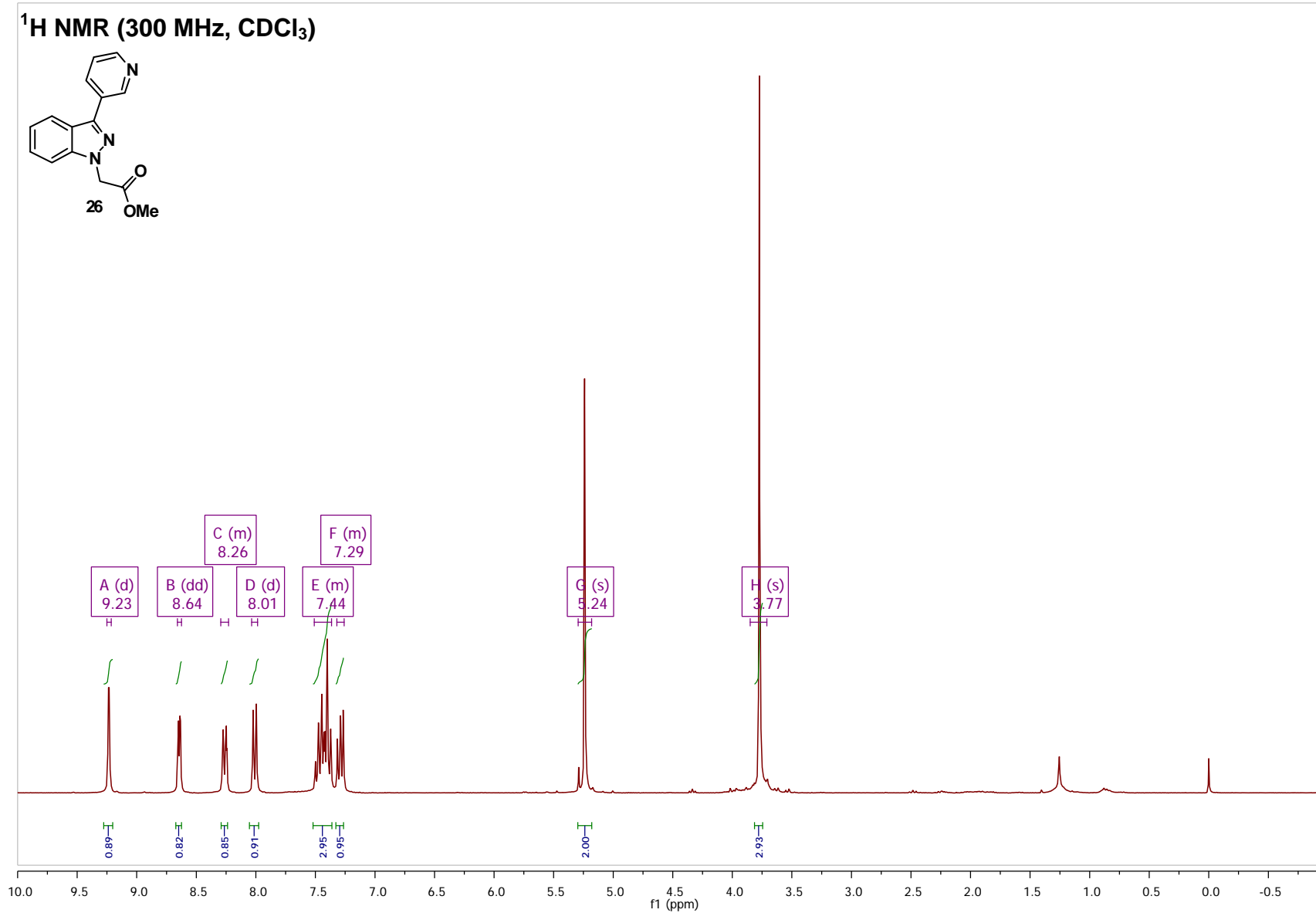
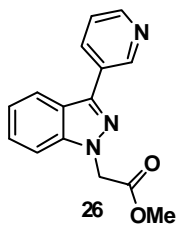
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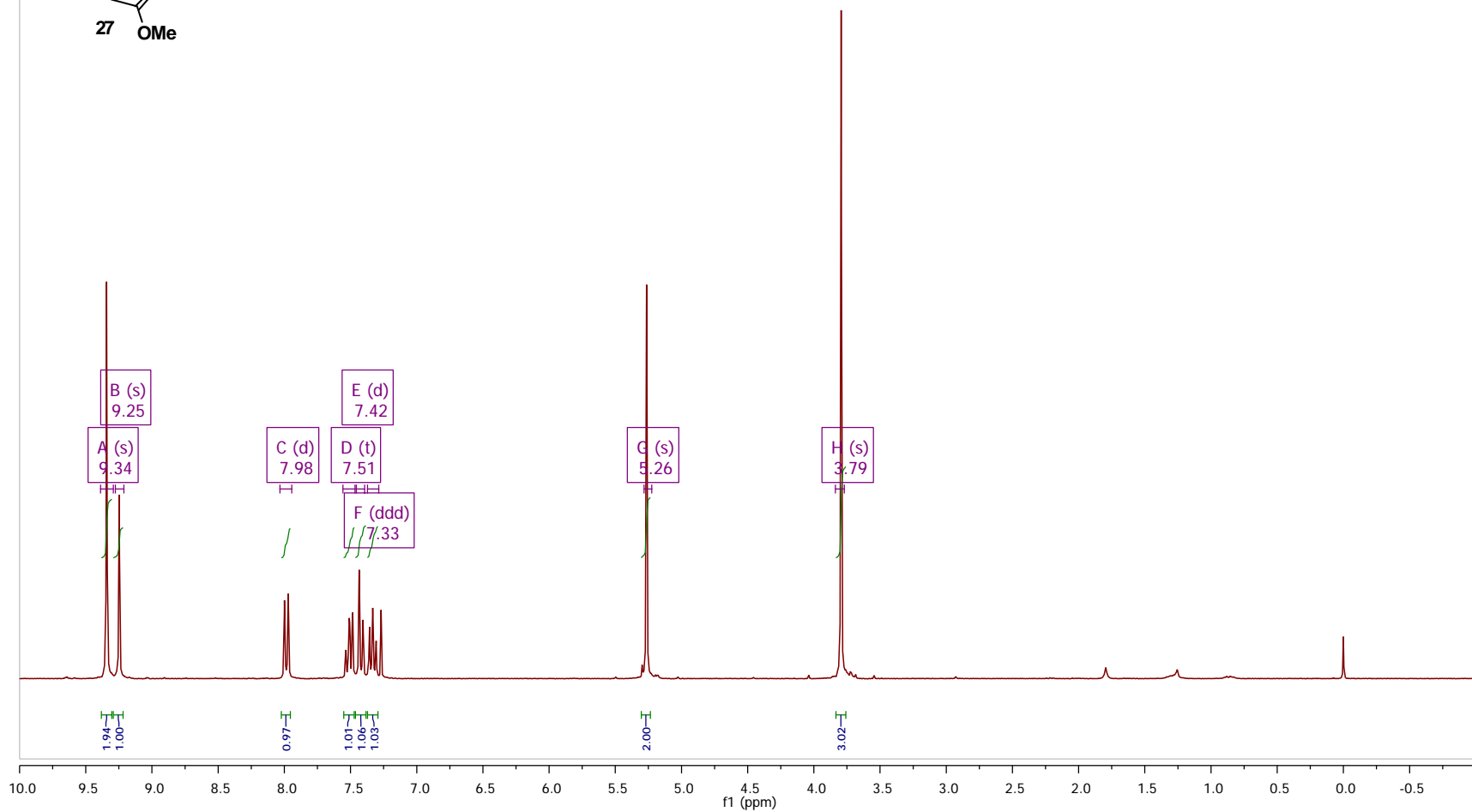
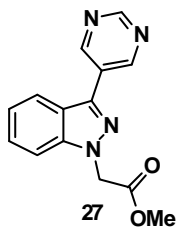
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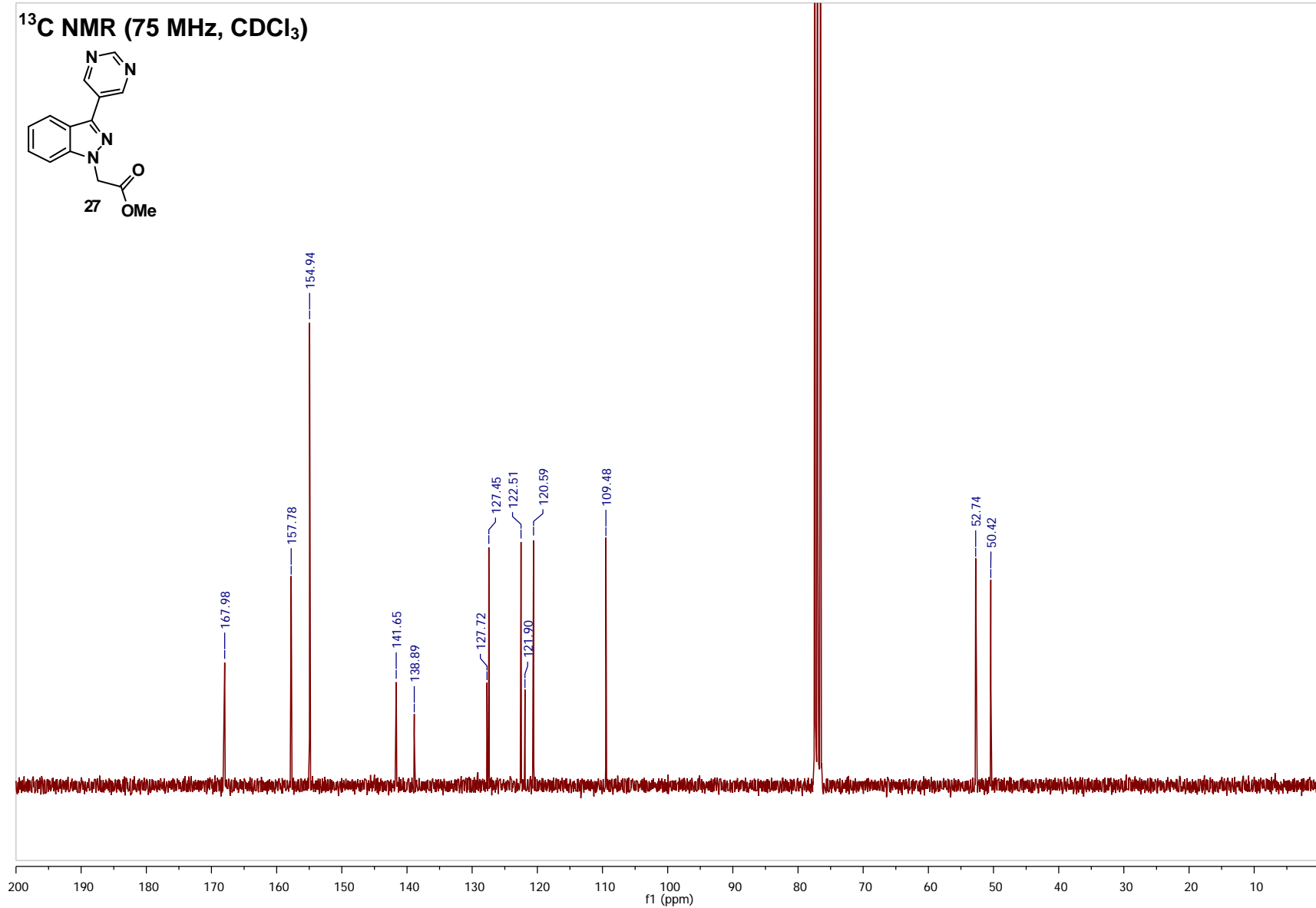
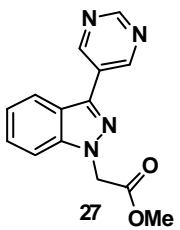
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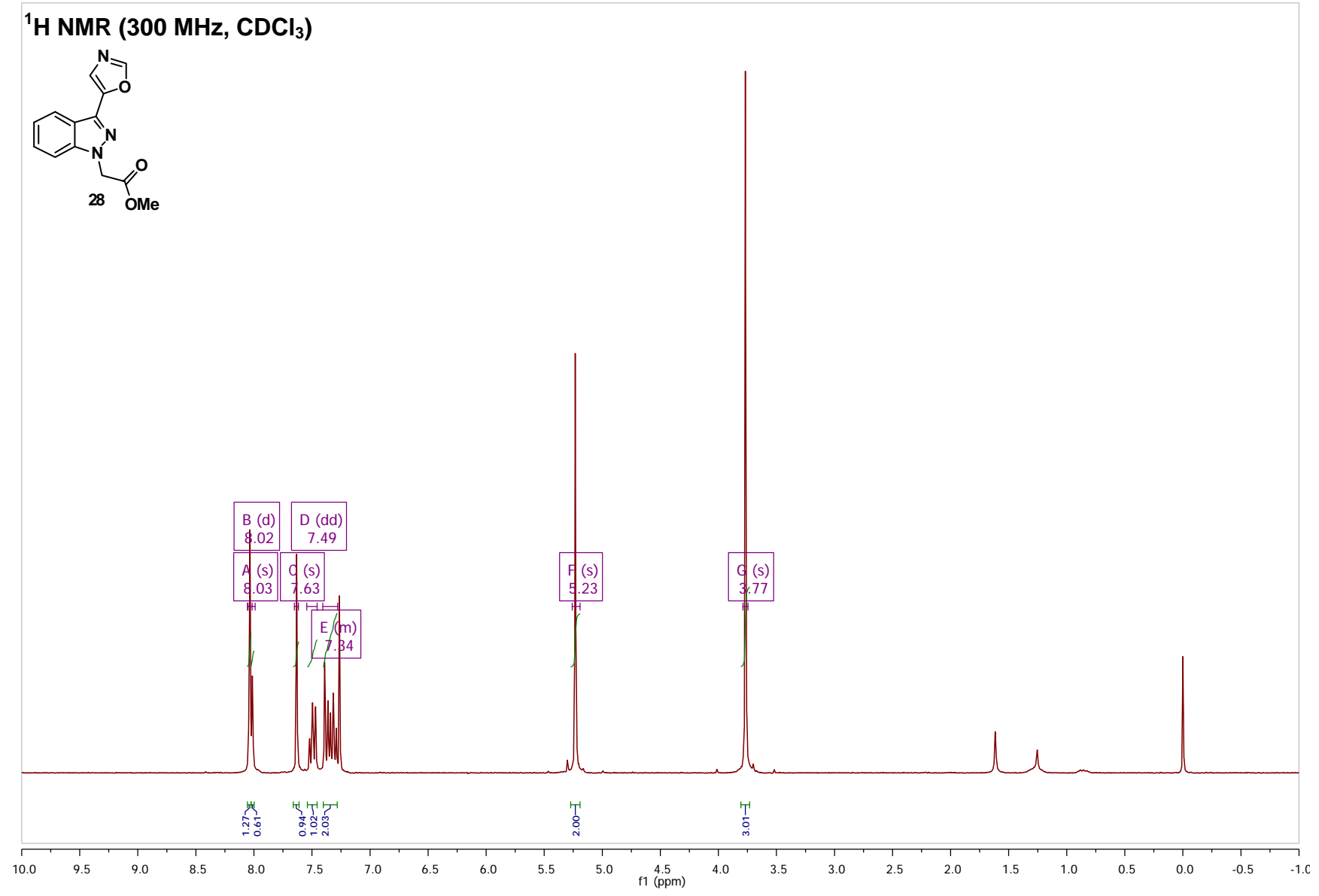
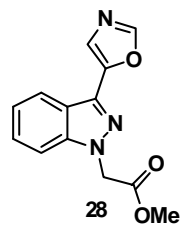
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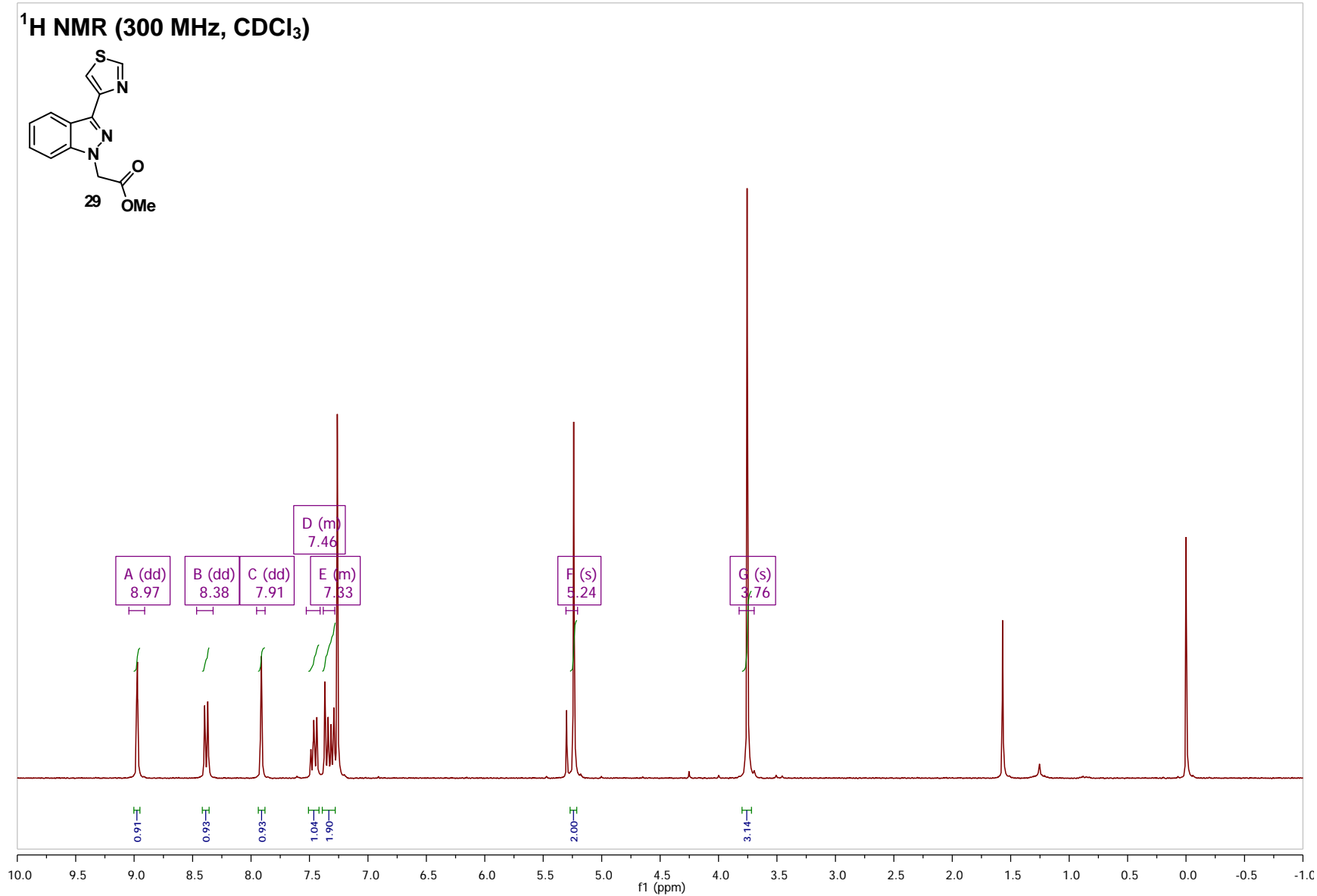
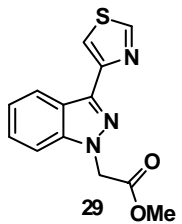
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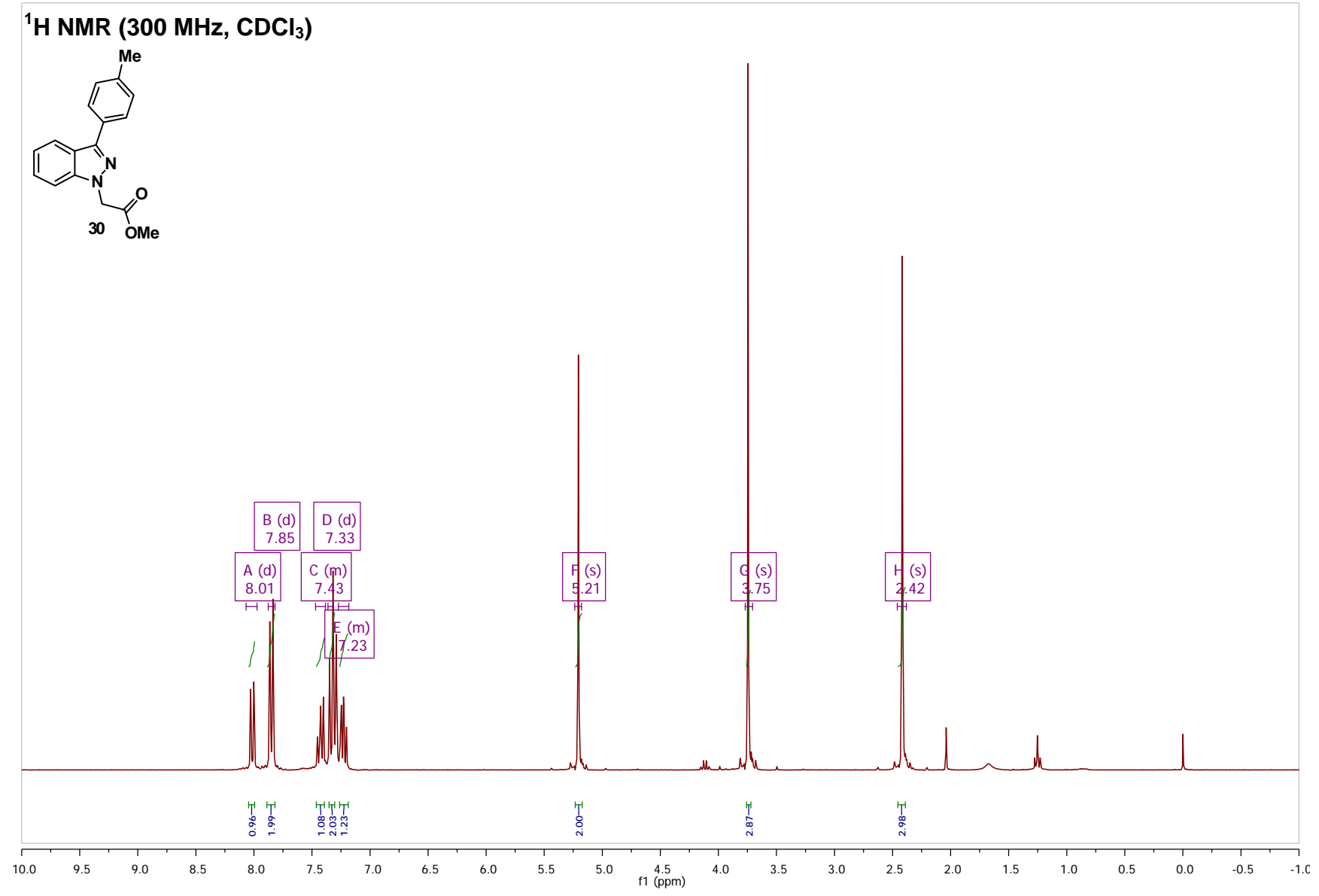
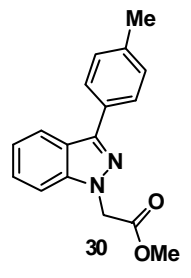
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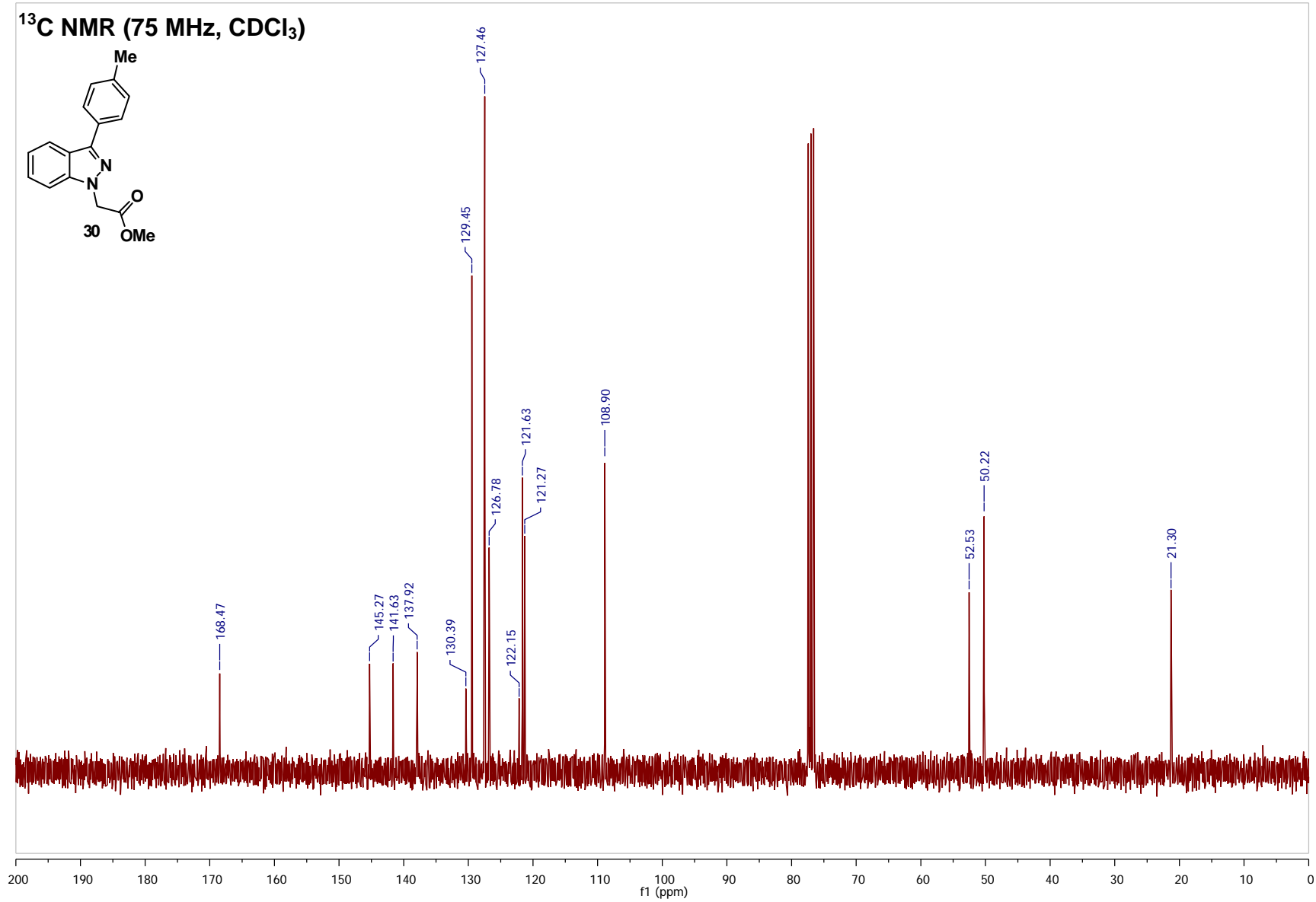
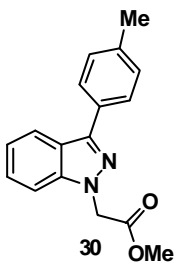


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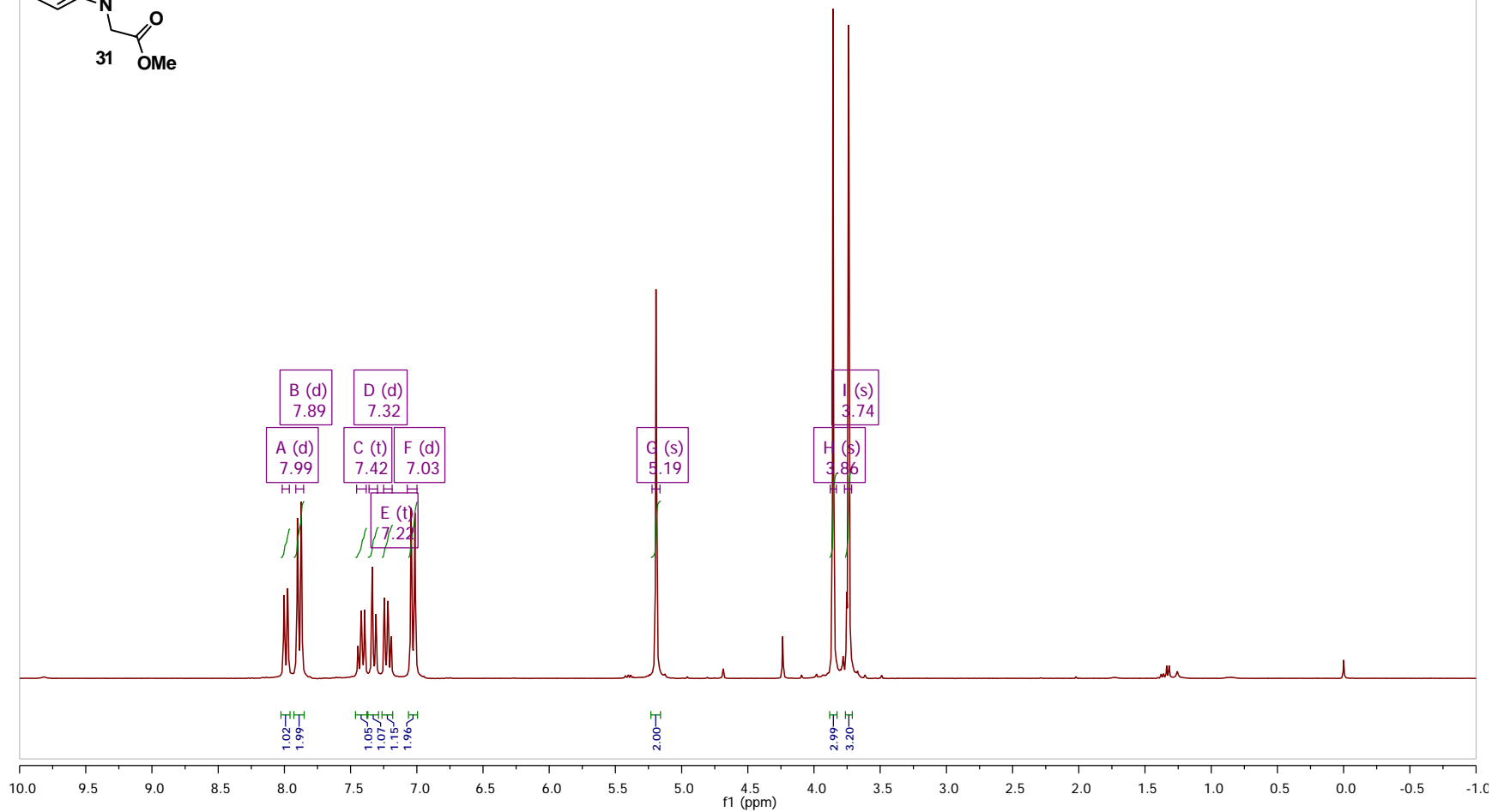
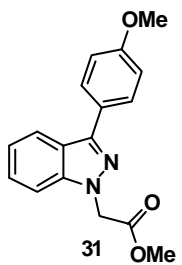




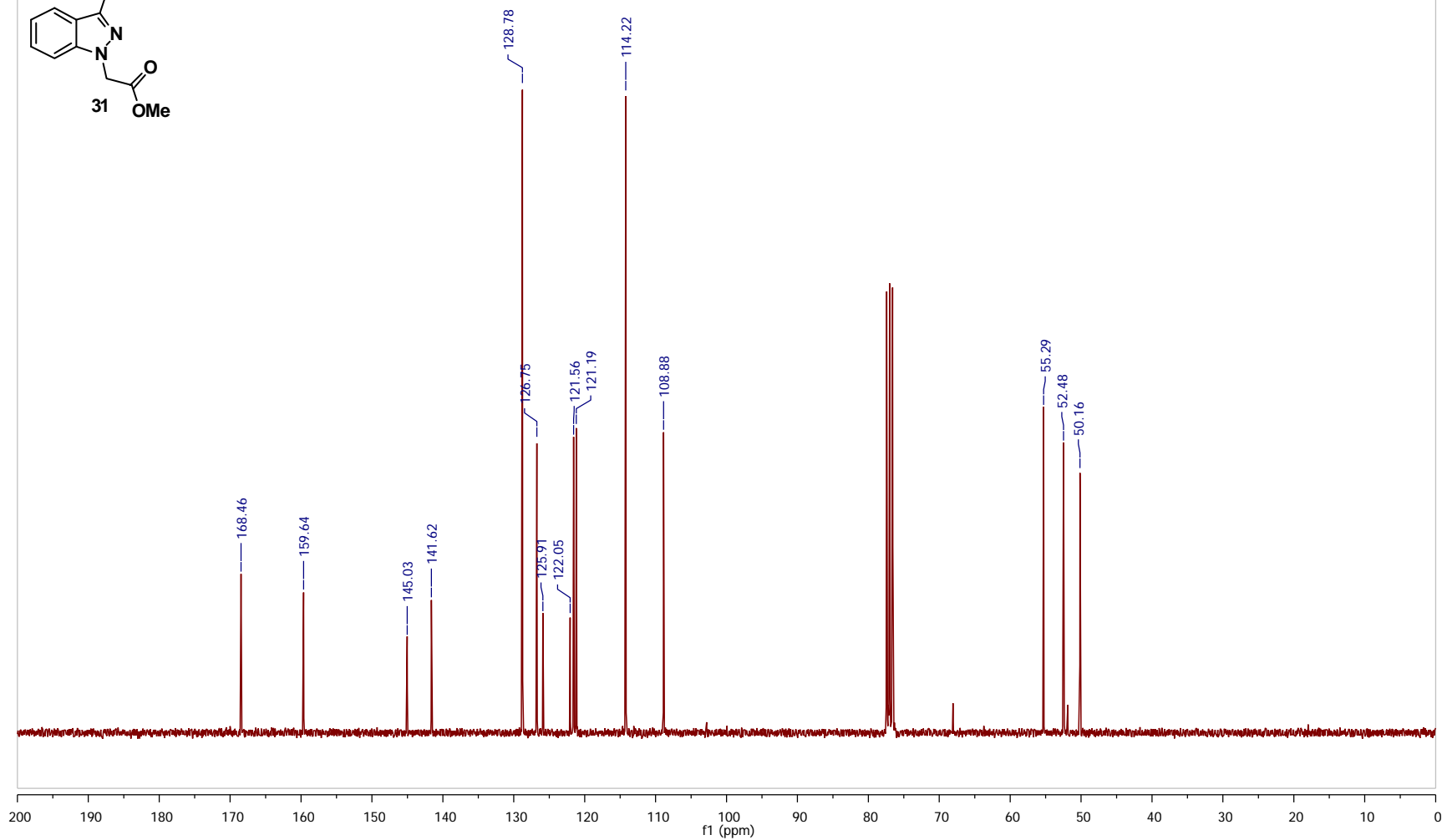
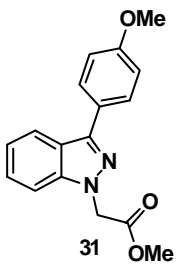
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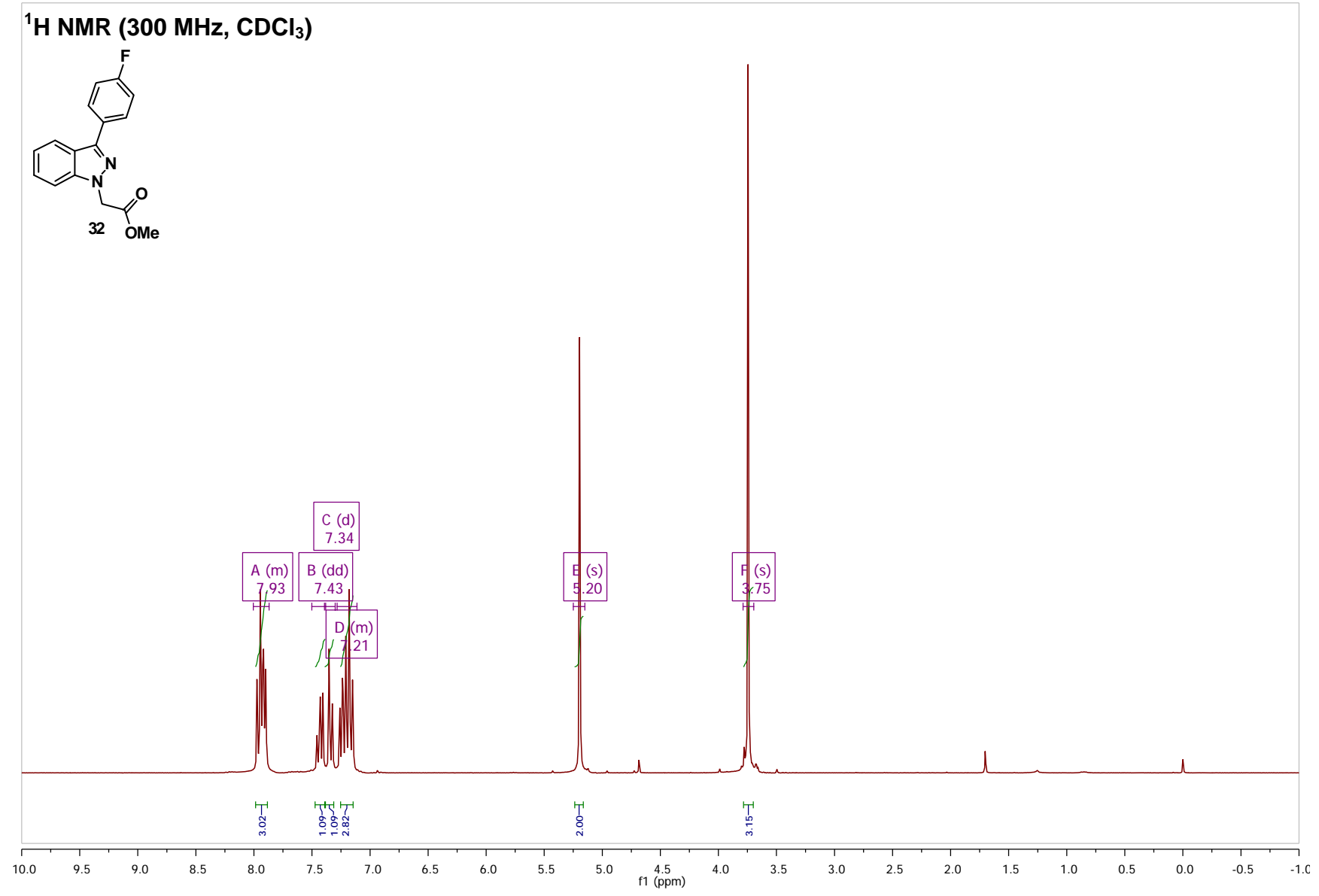
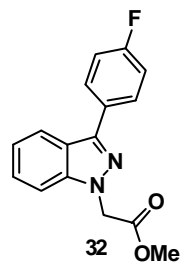
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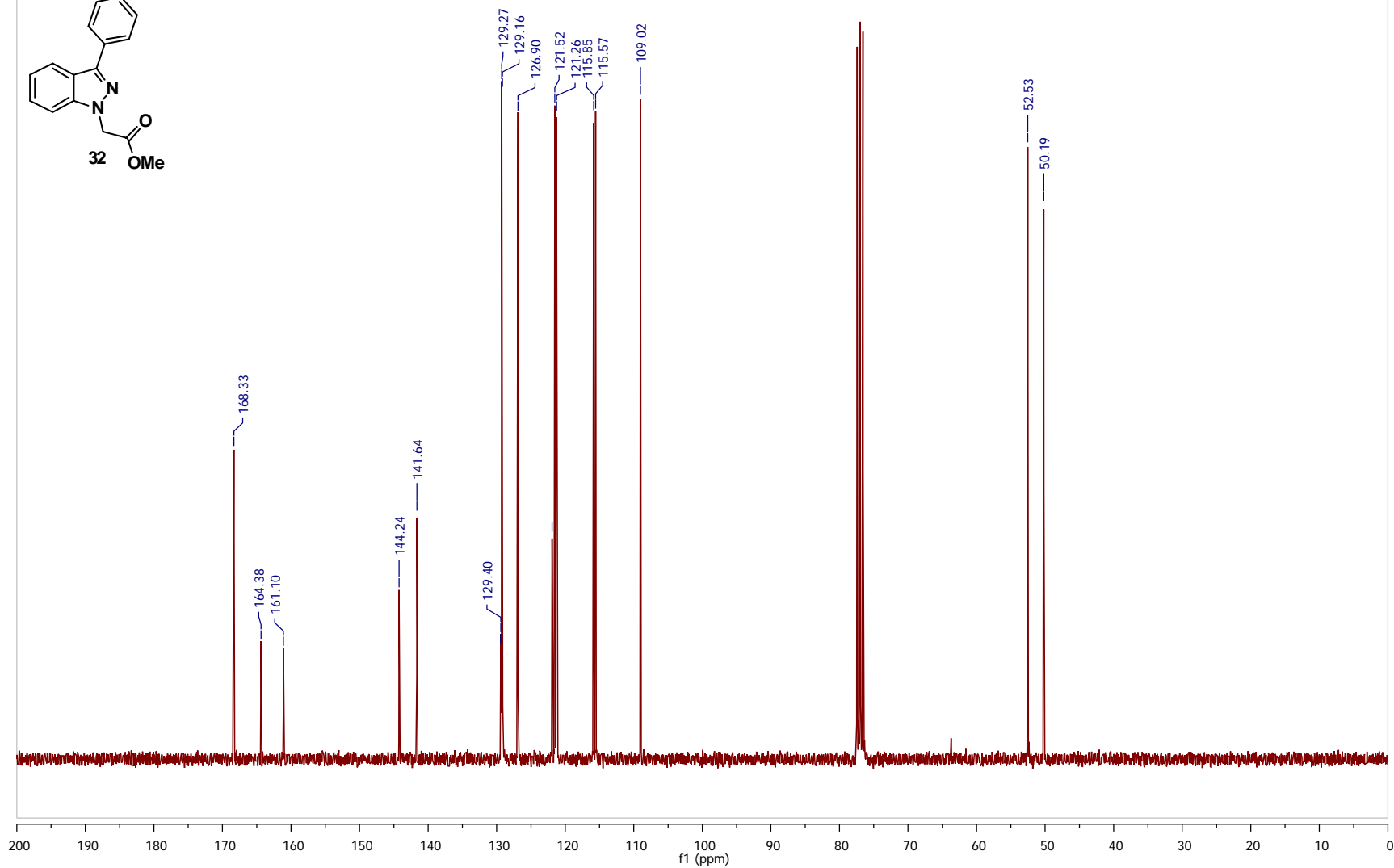
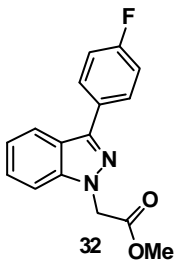
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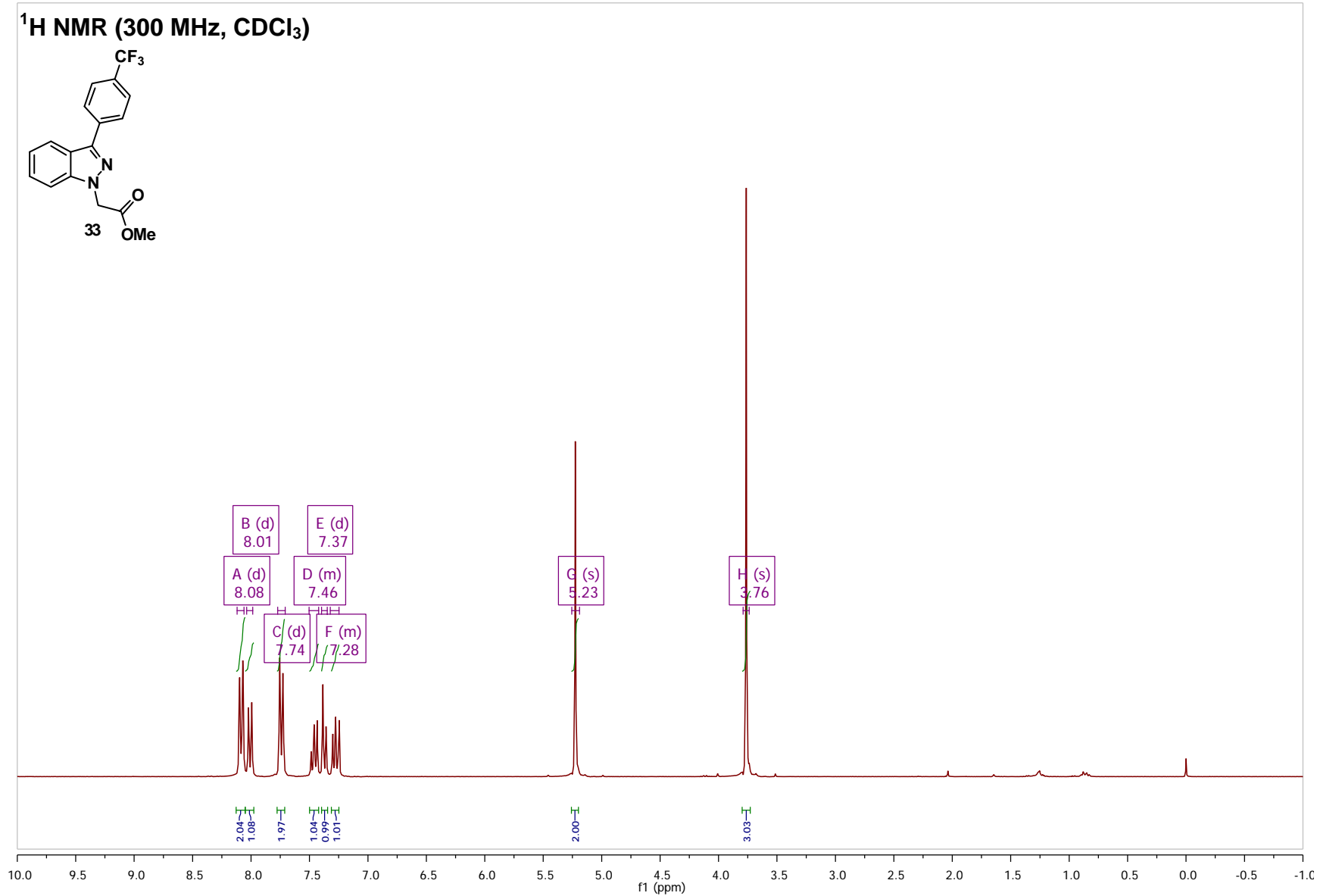
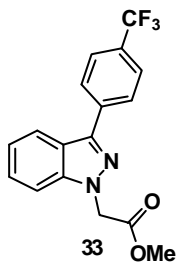
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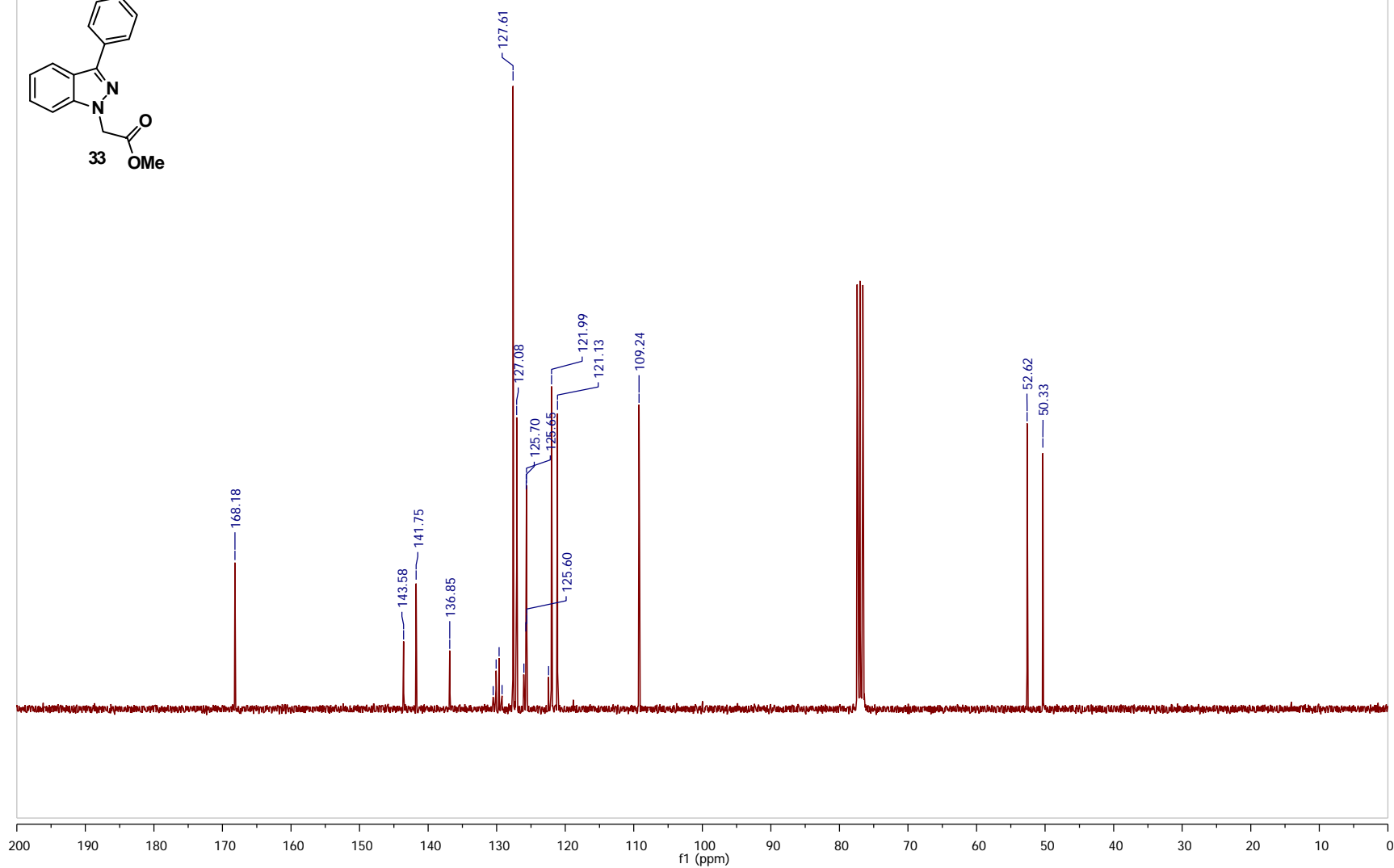
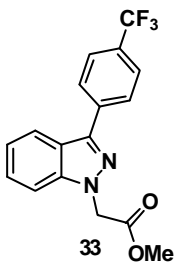
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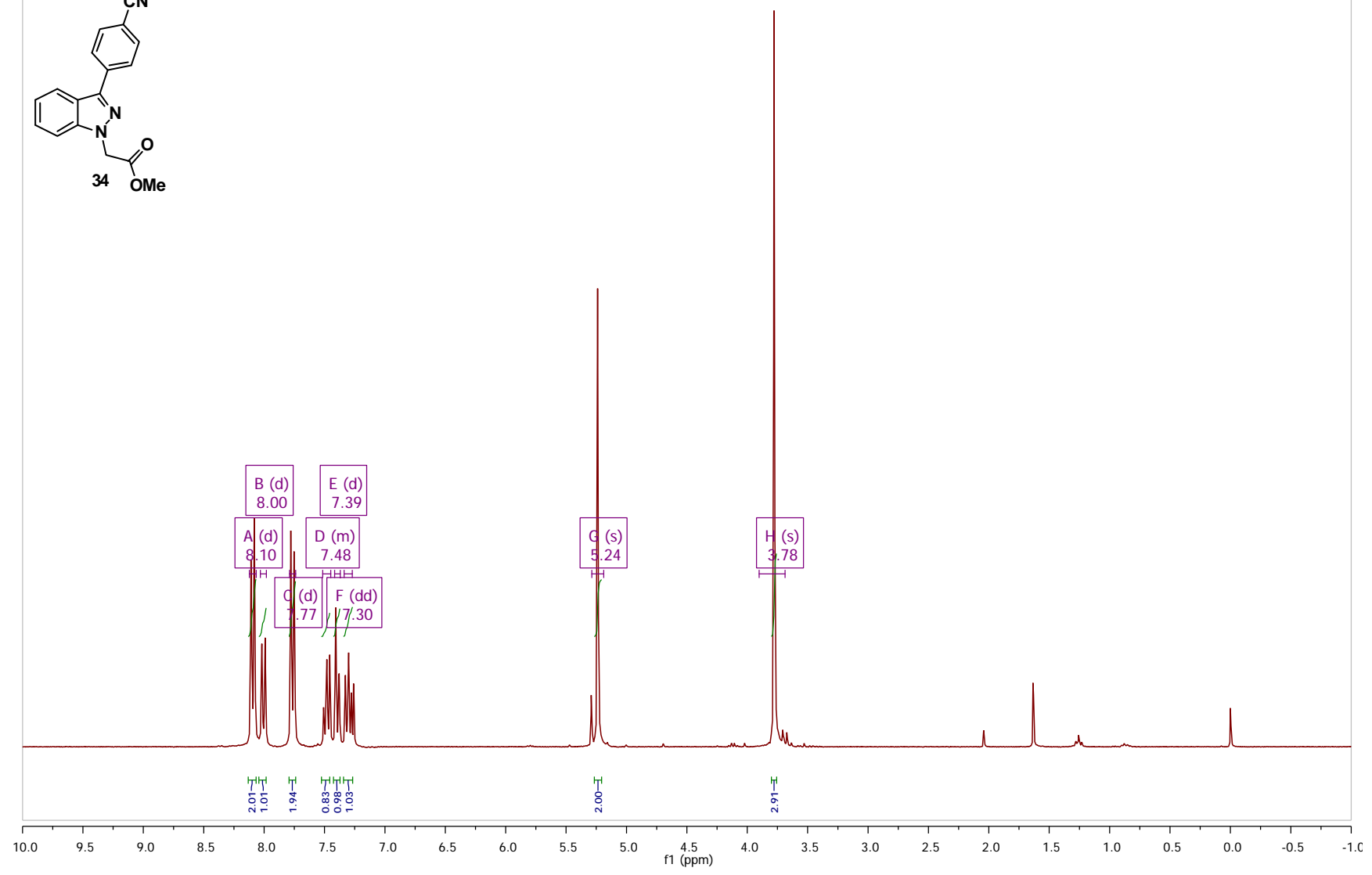
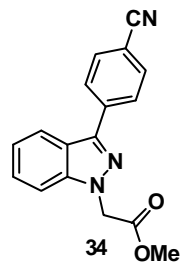
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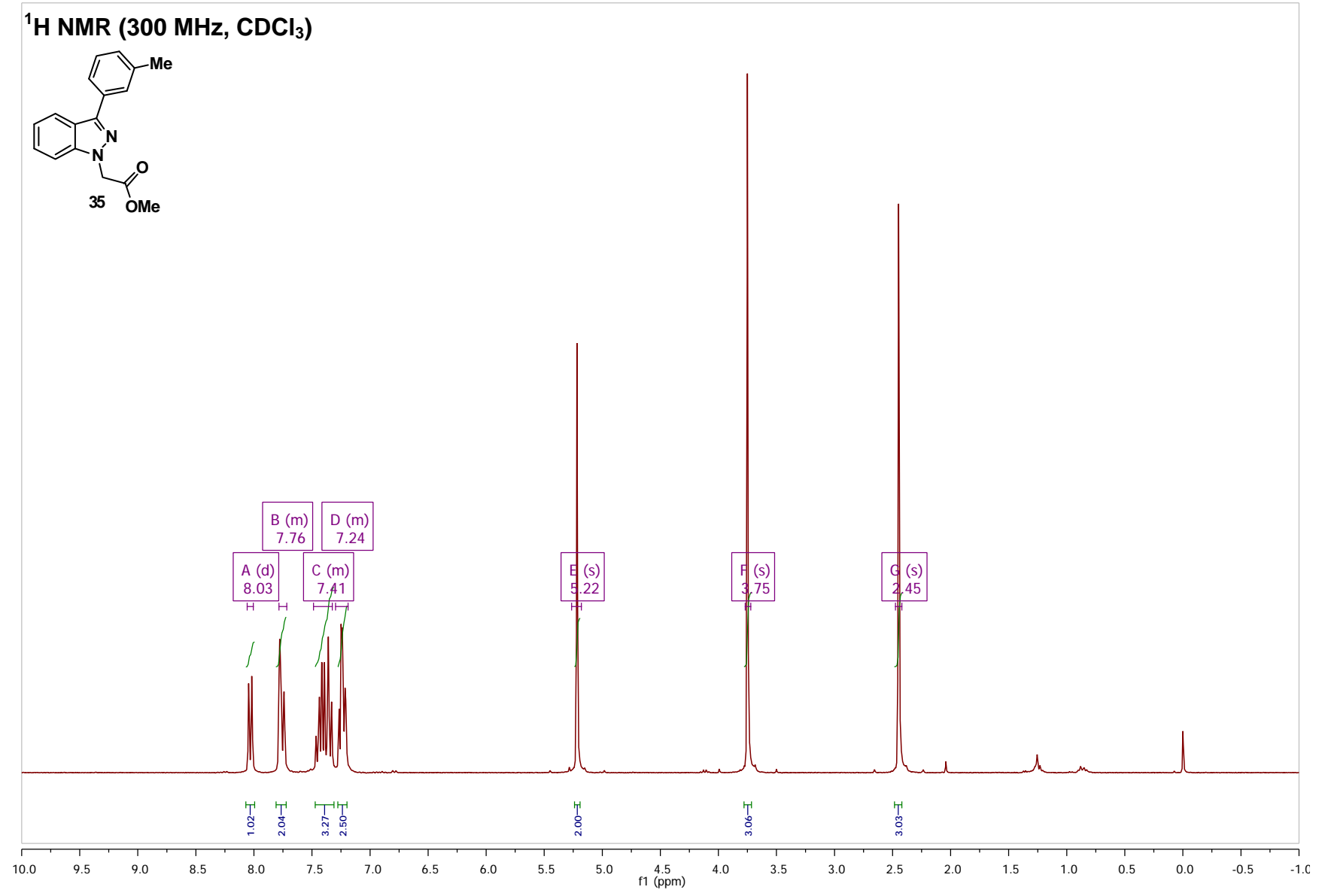
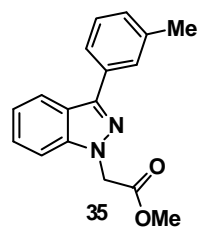


<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)

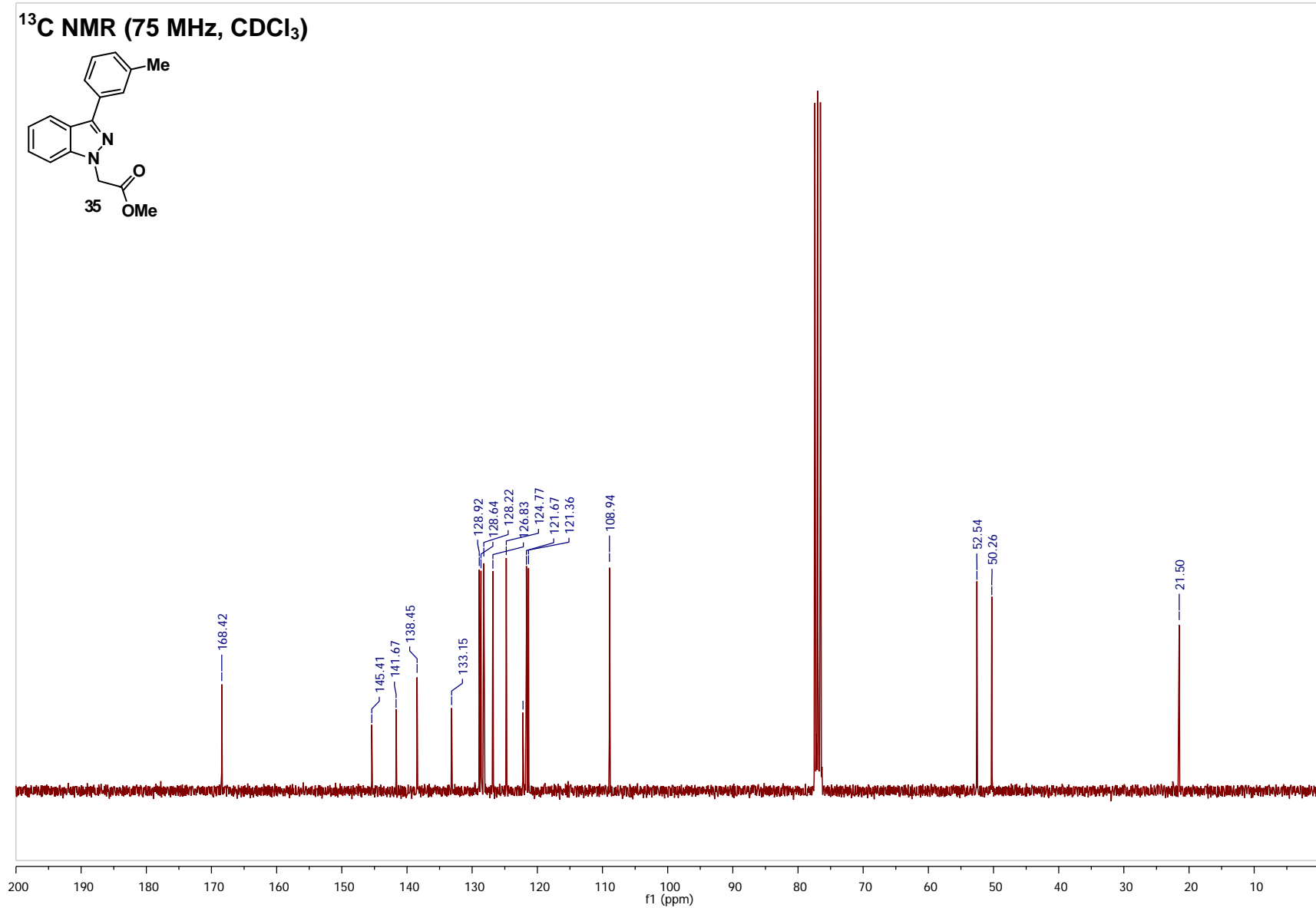
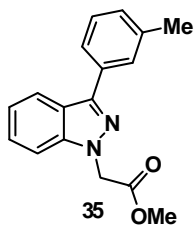




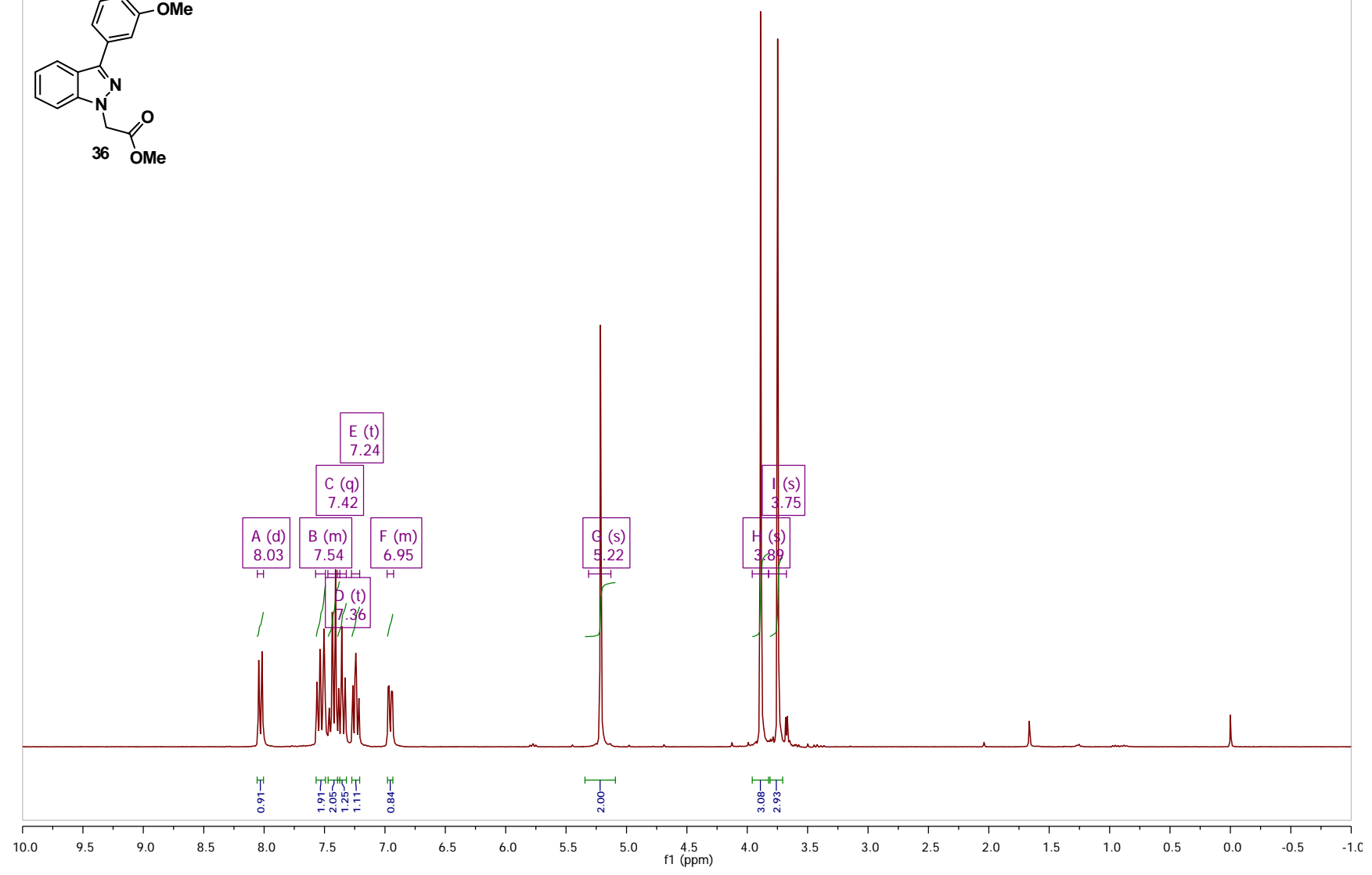
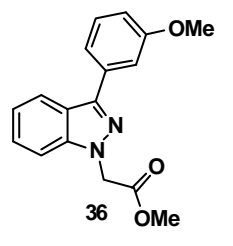
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



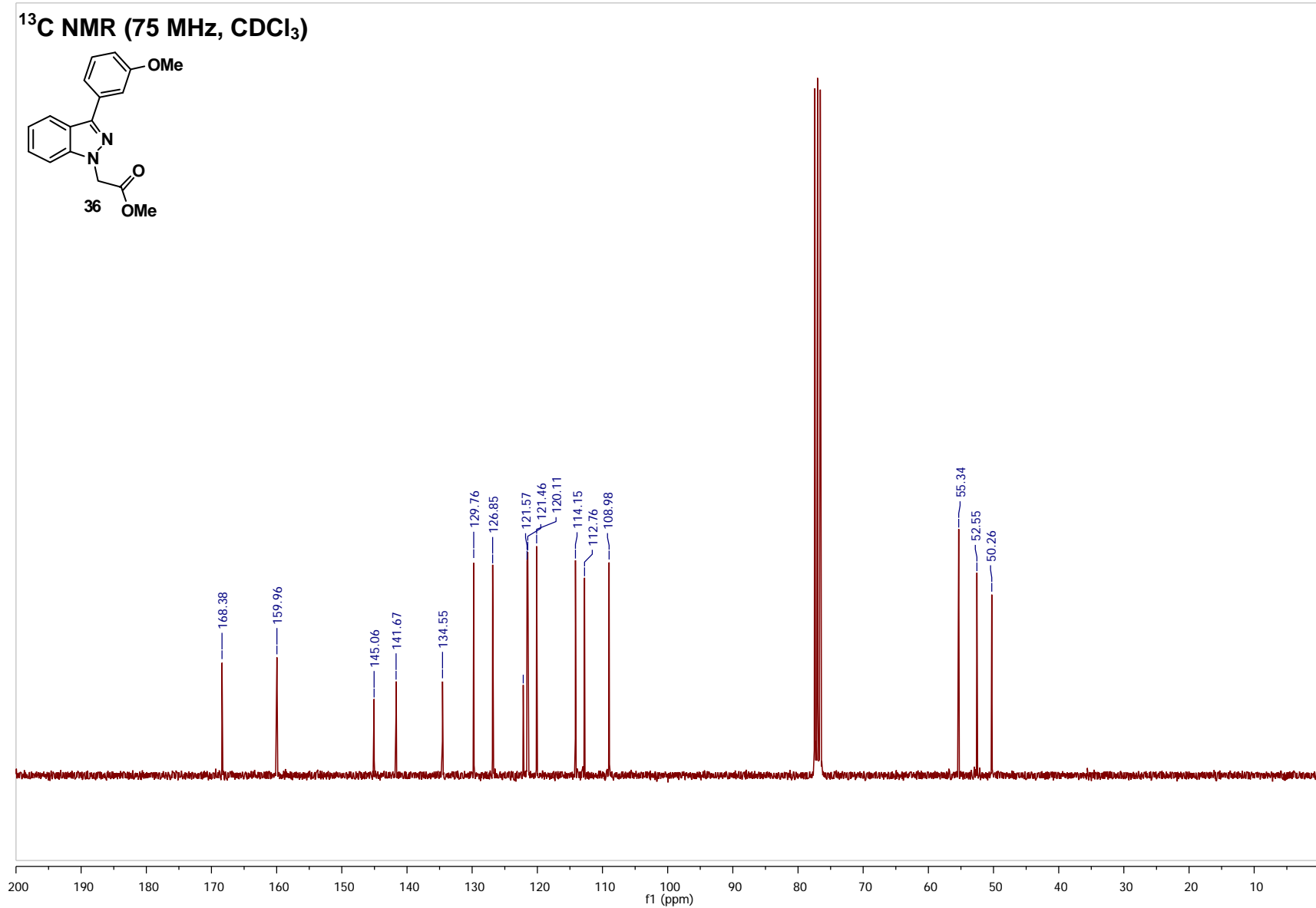
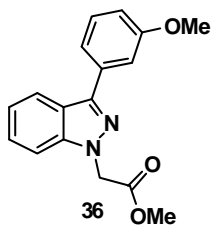
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)**



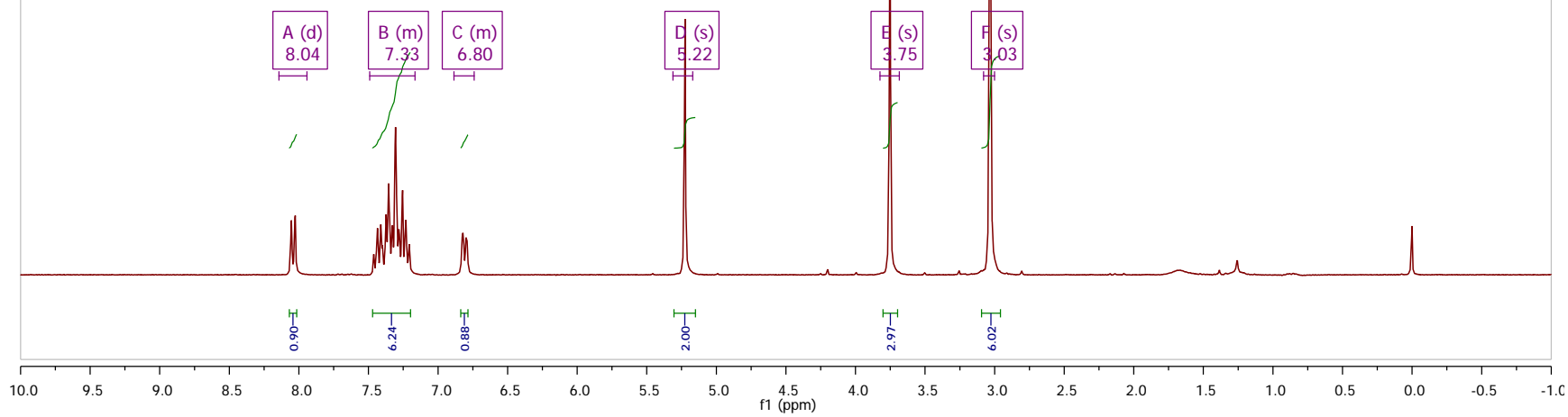
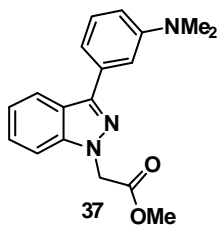
**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)**



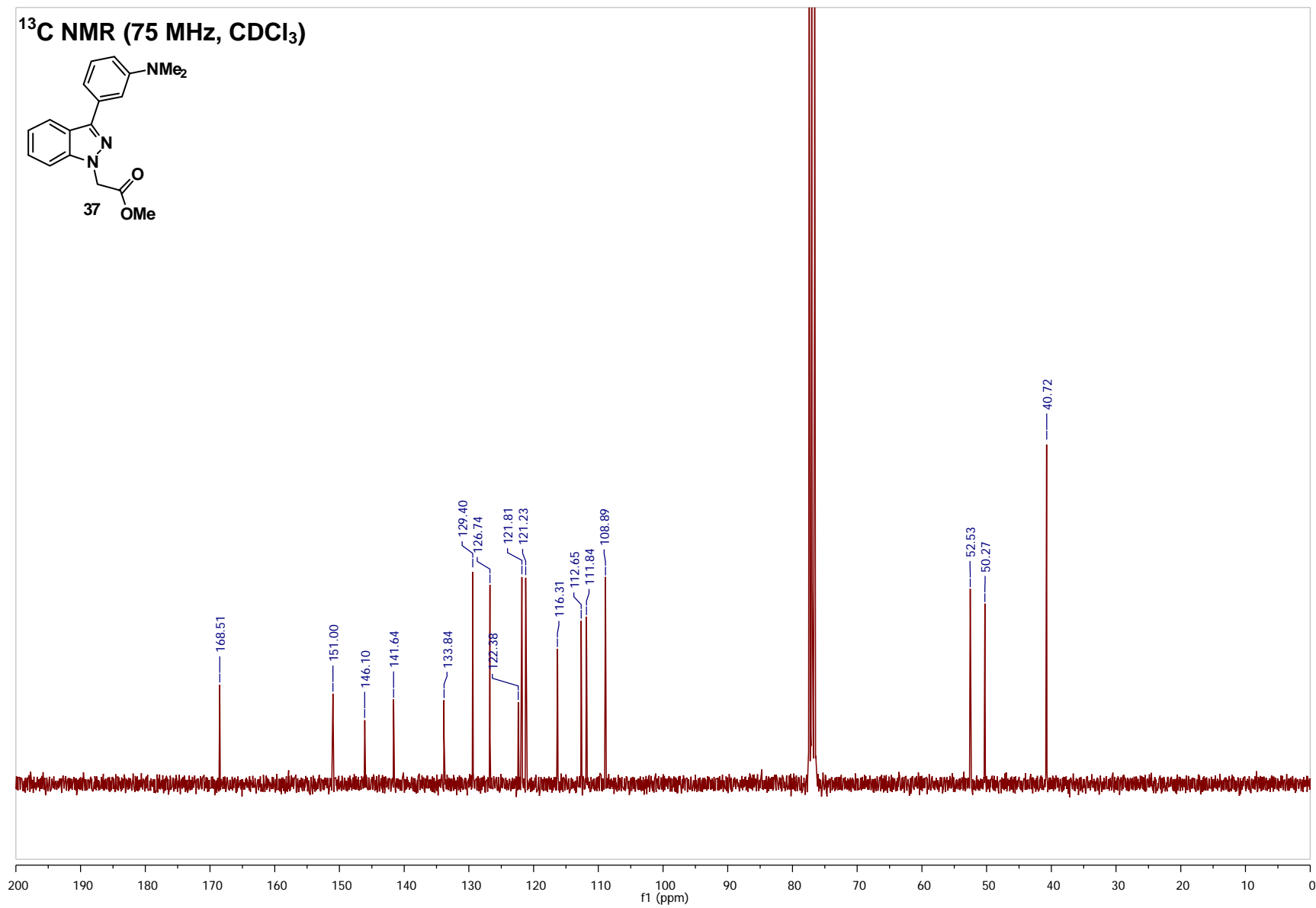
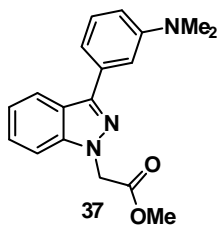
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)**



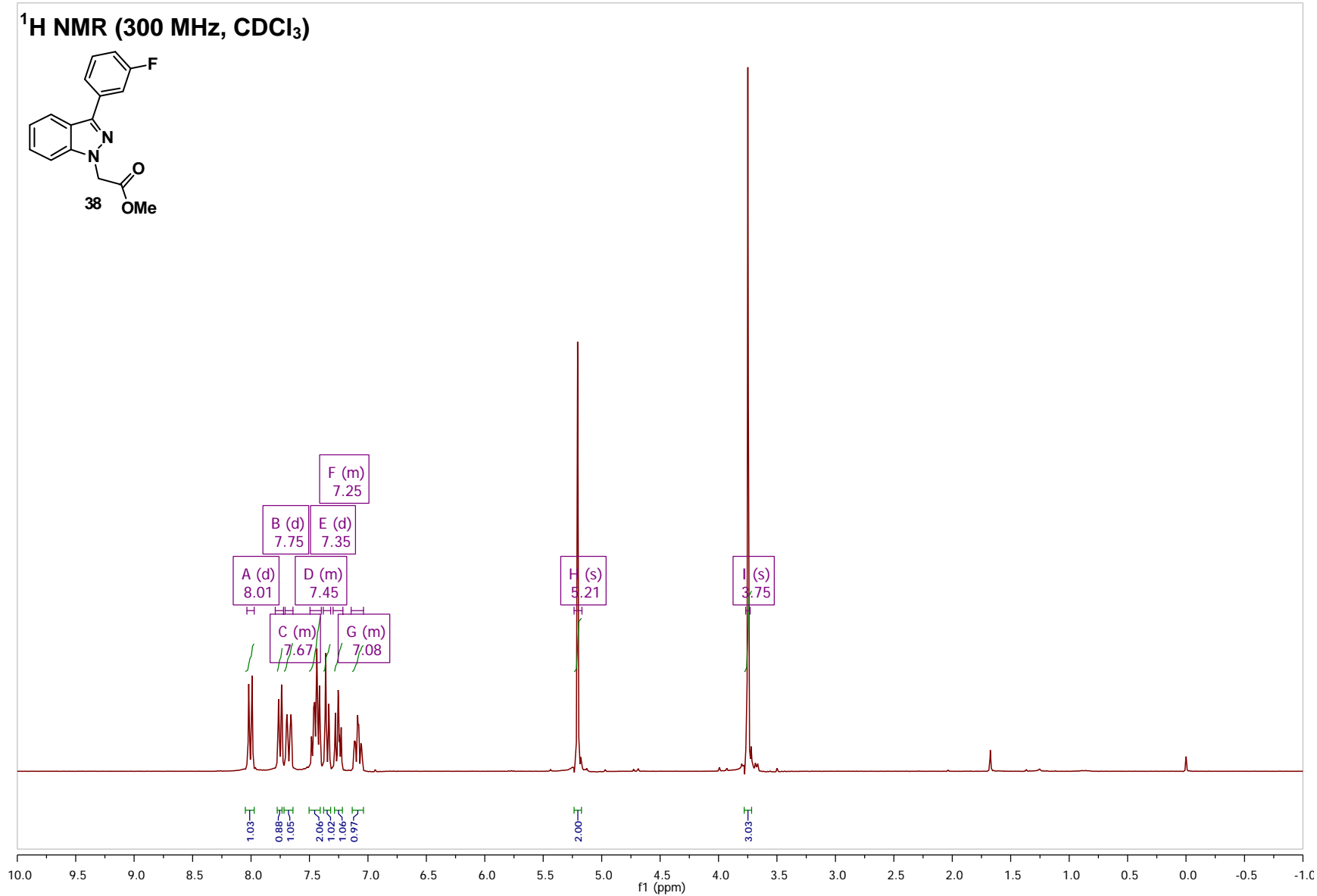
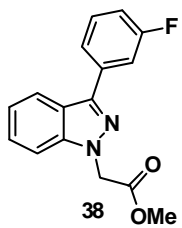
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



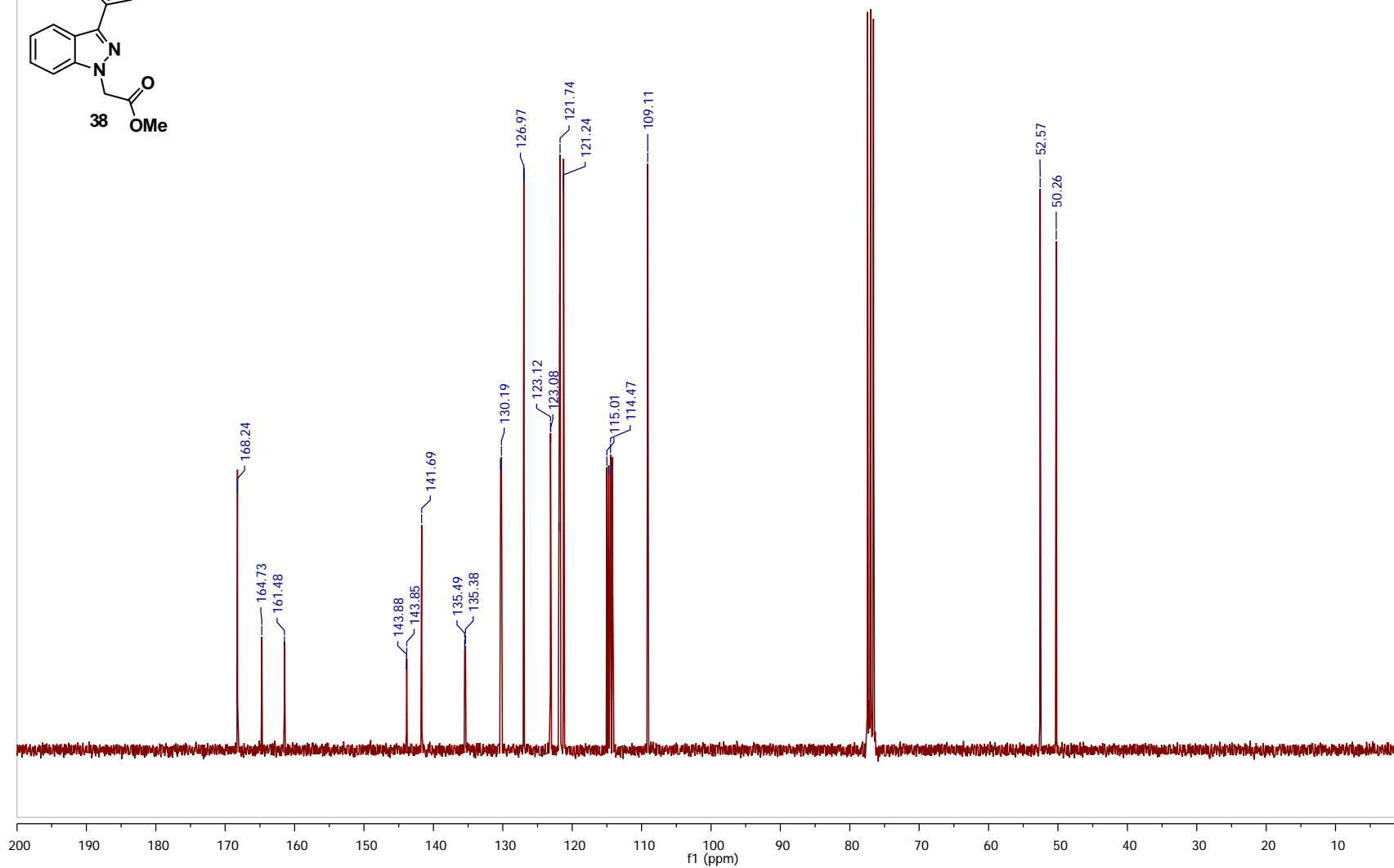
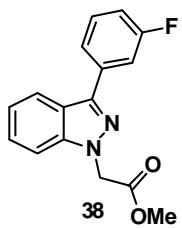
<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)



<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)

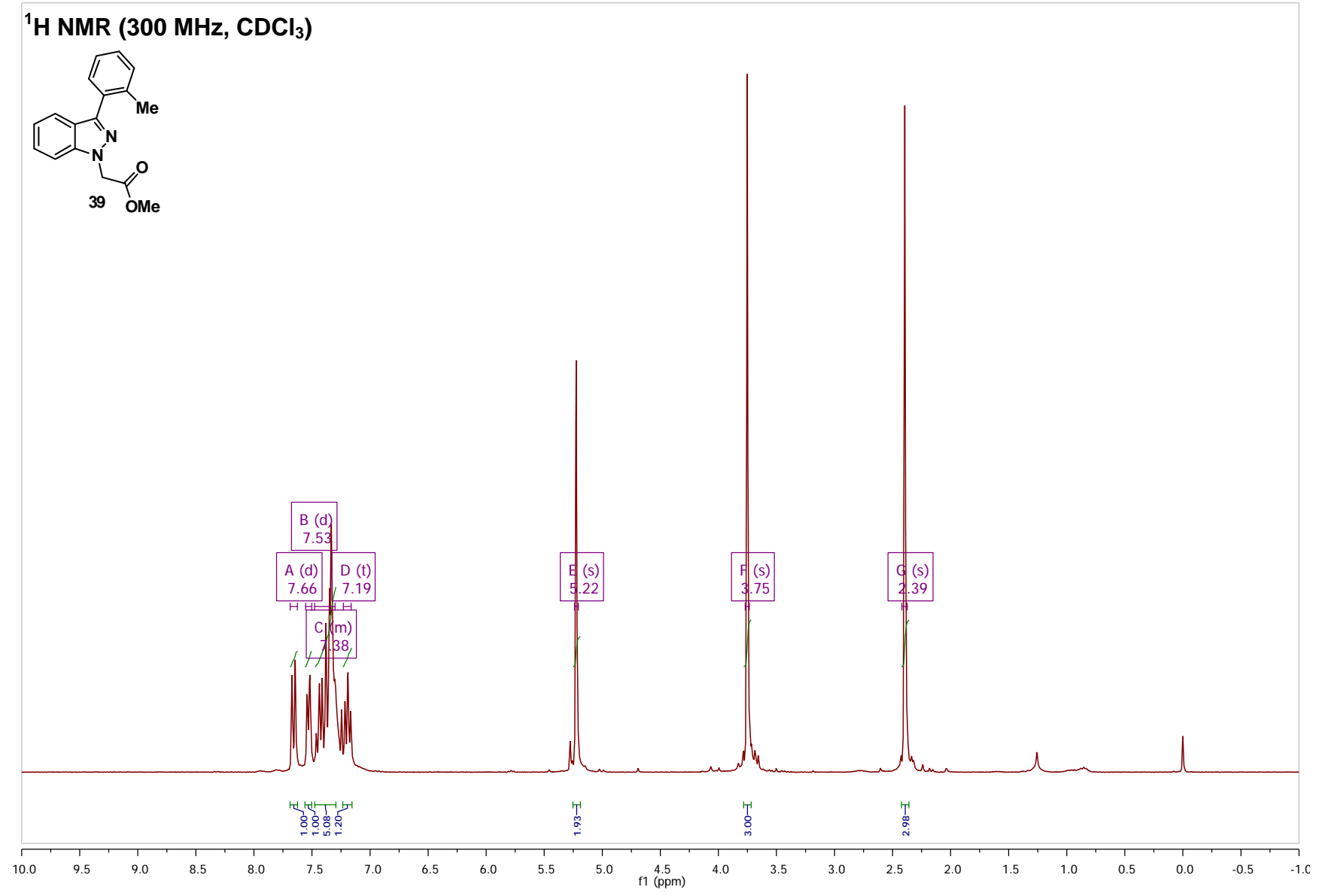
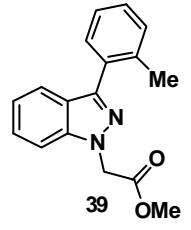


<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)

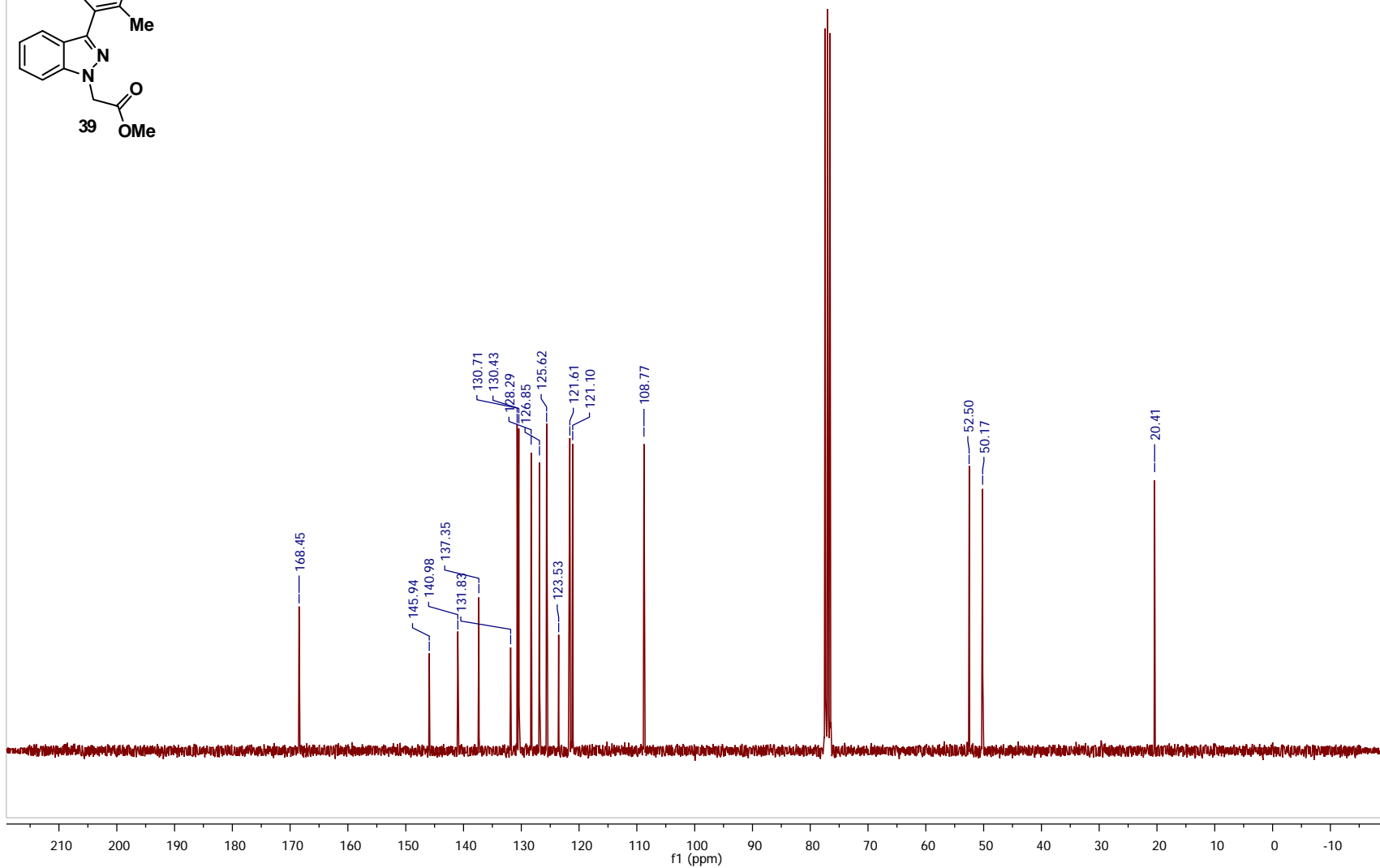
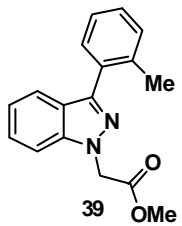




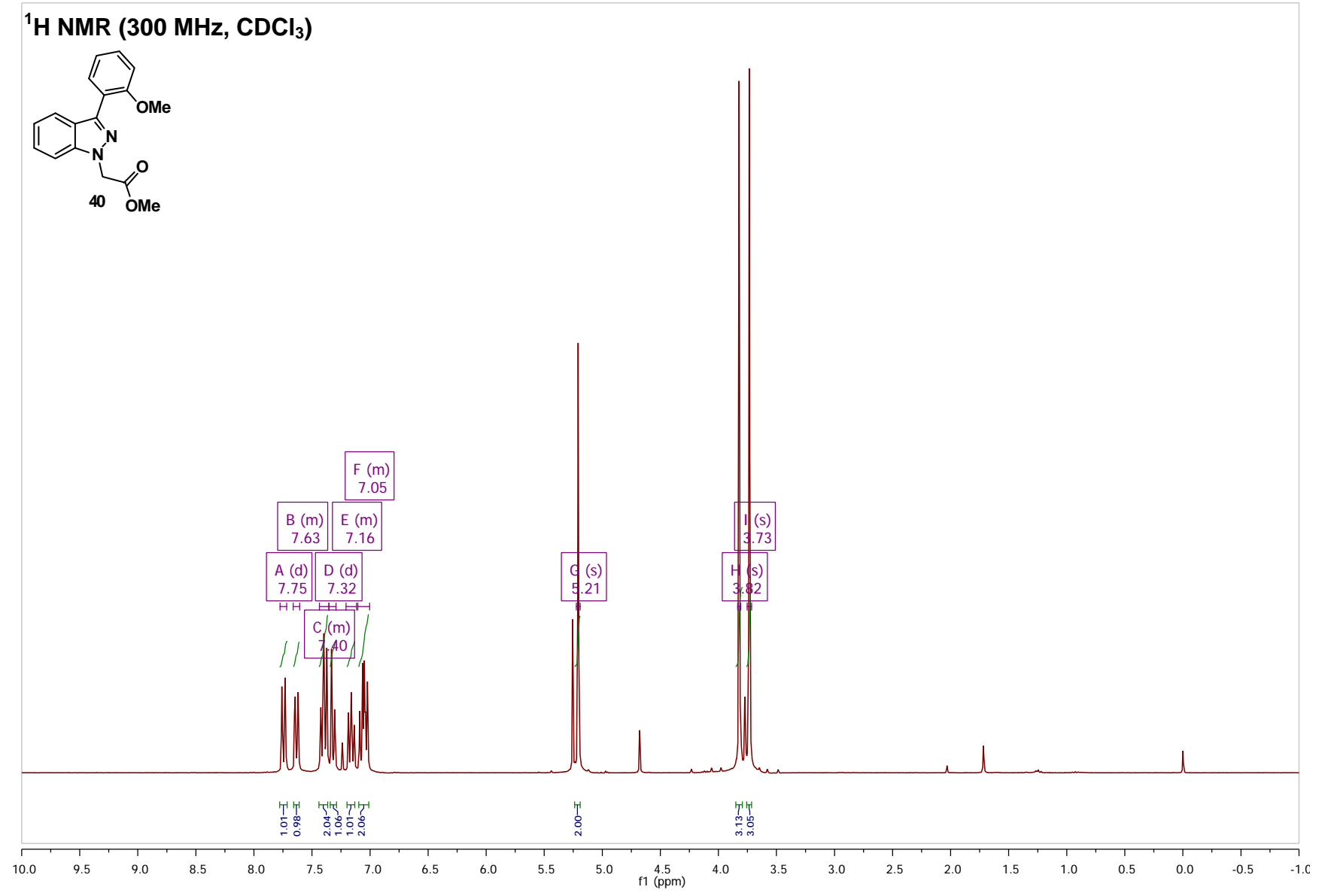
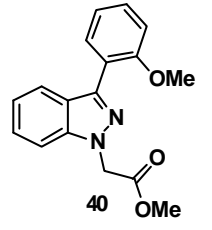
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



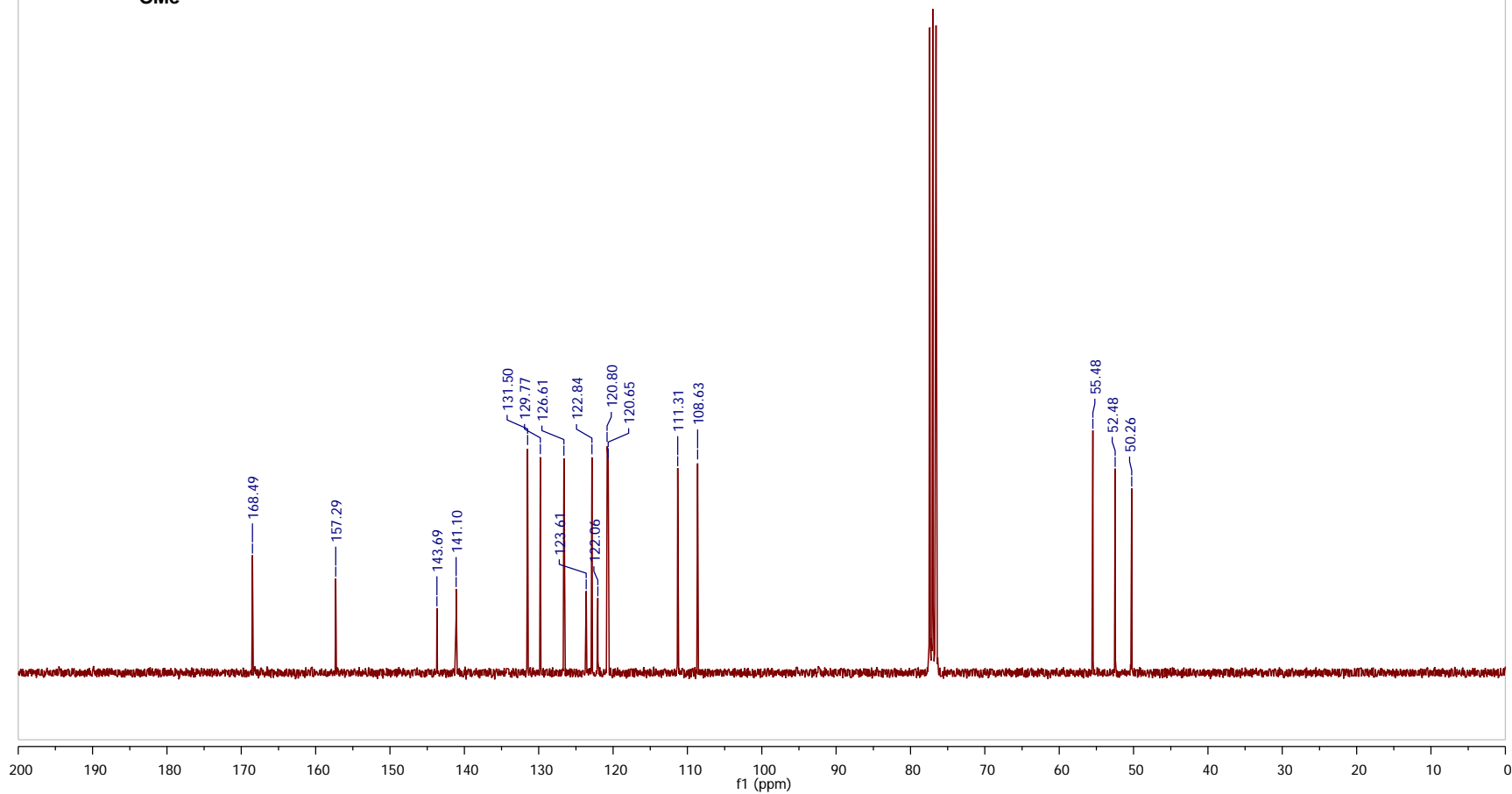
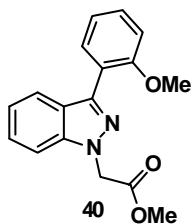
<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)



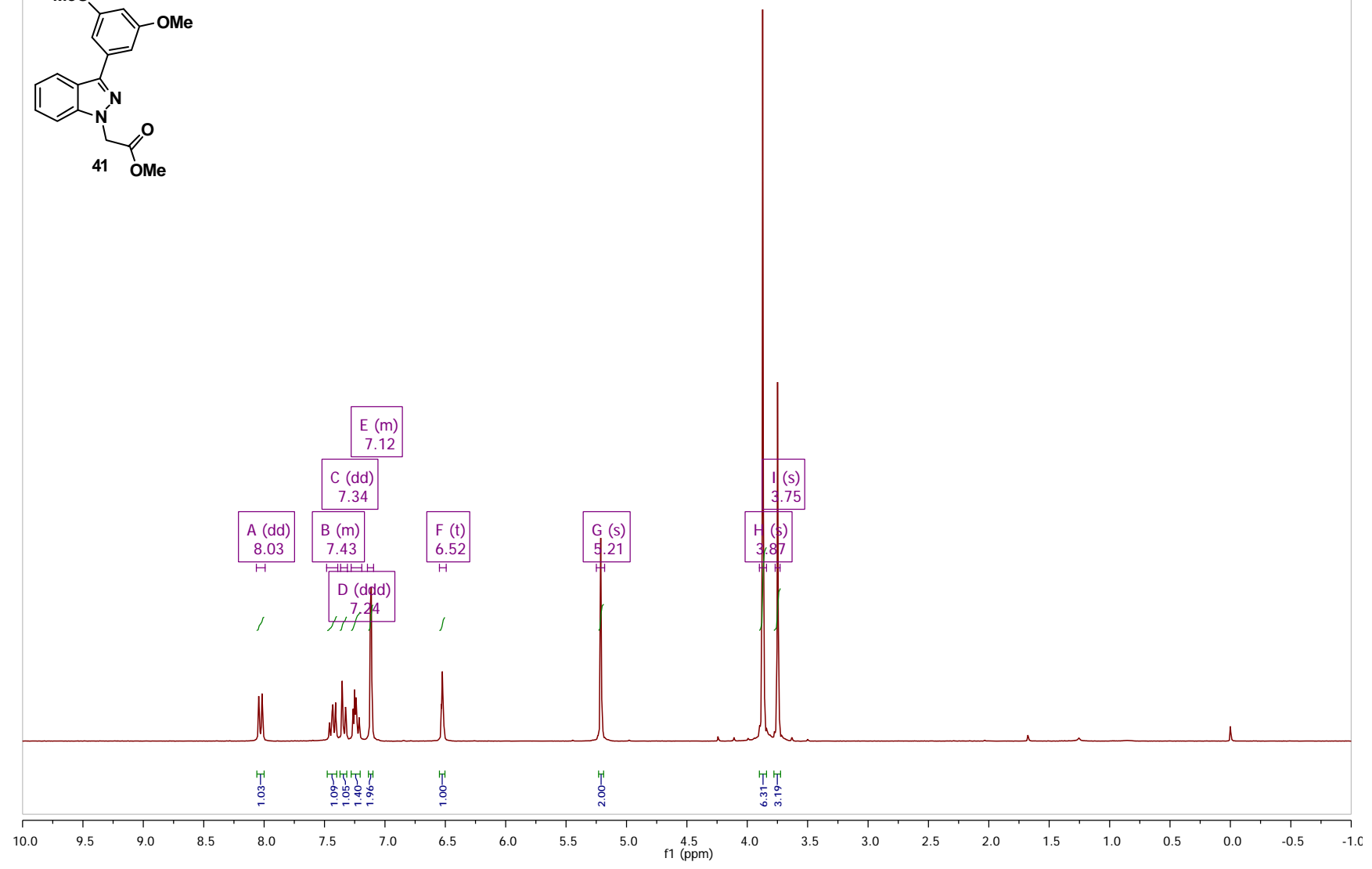
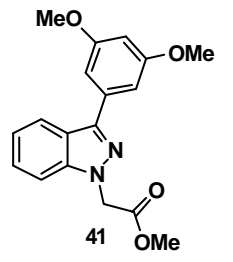
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



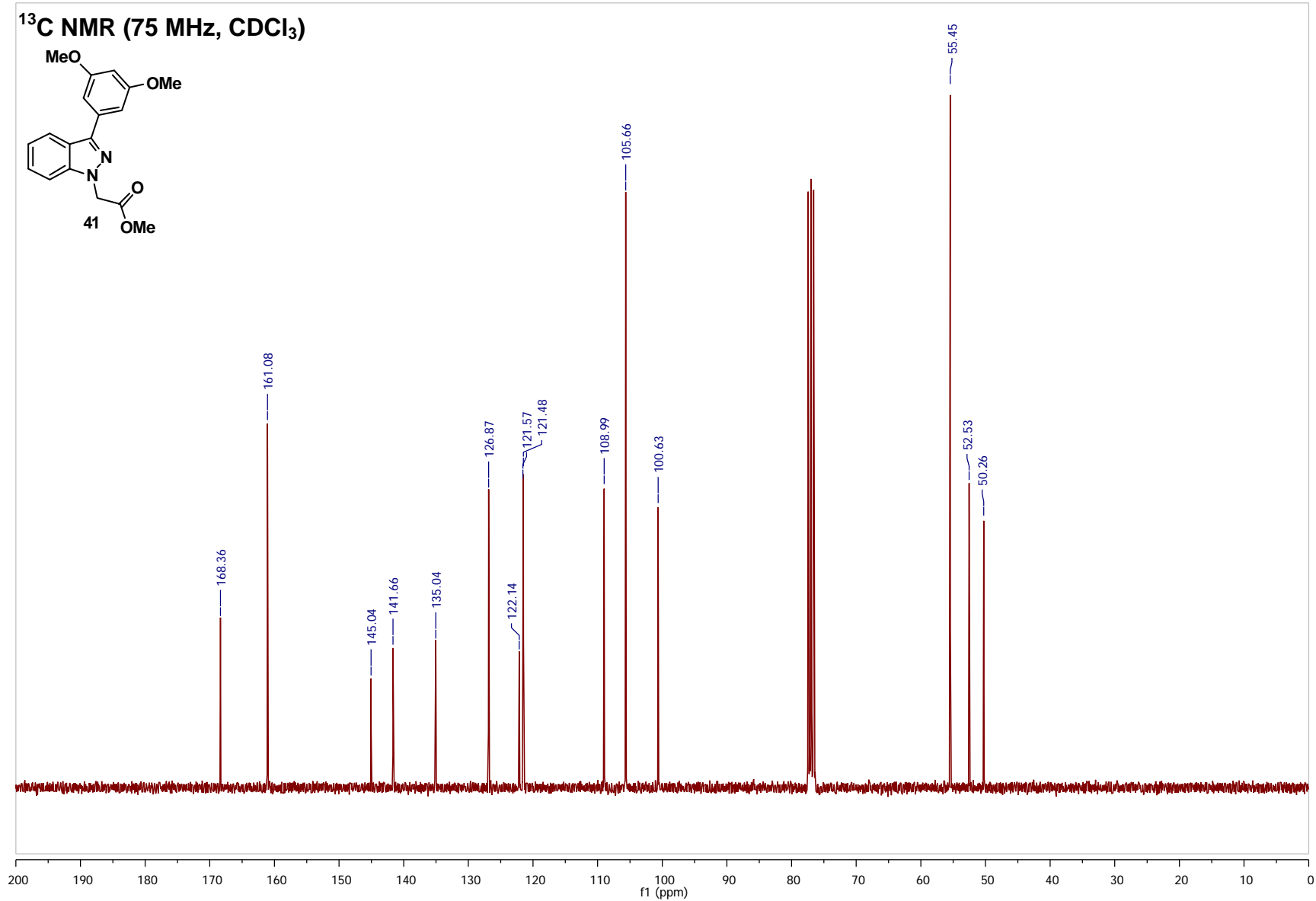
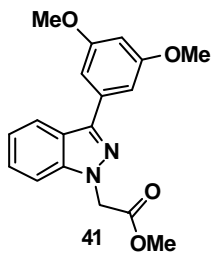
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)**



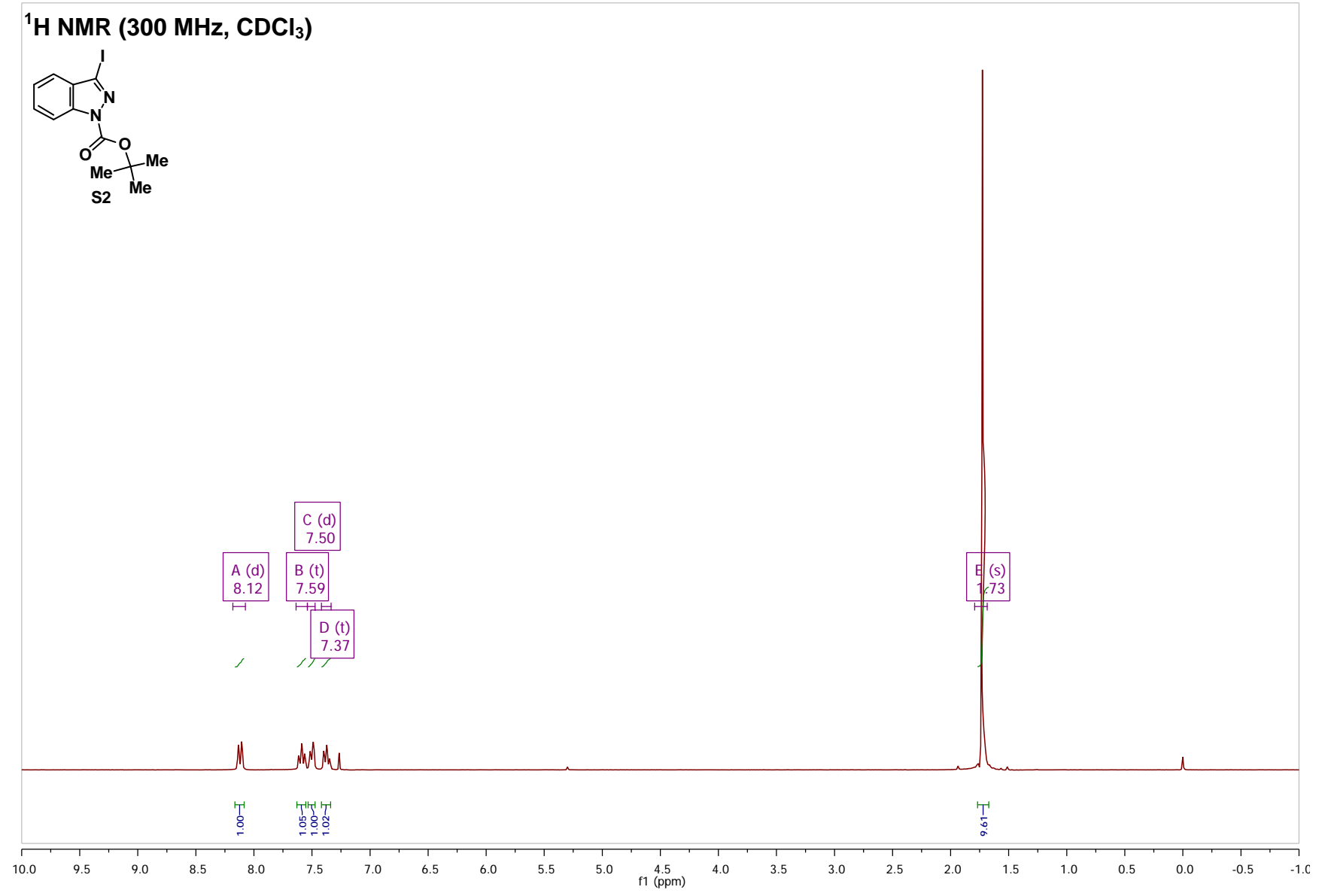
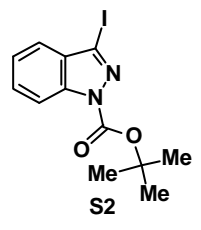
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



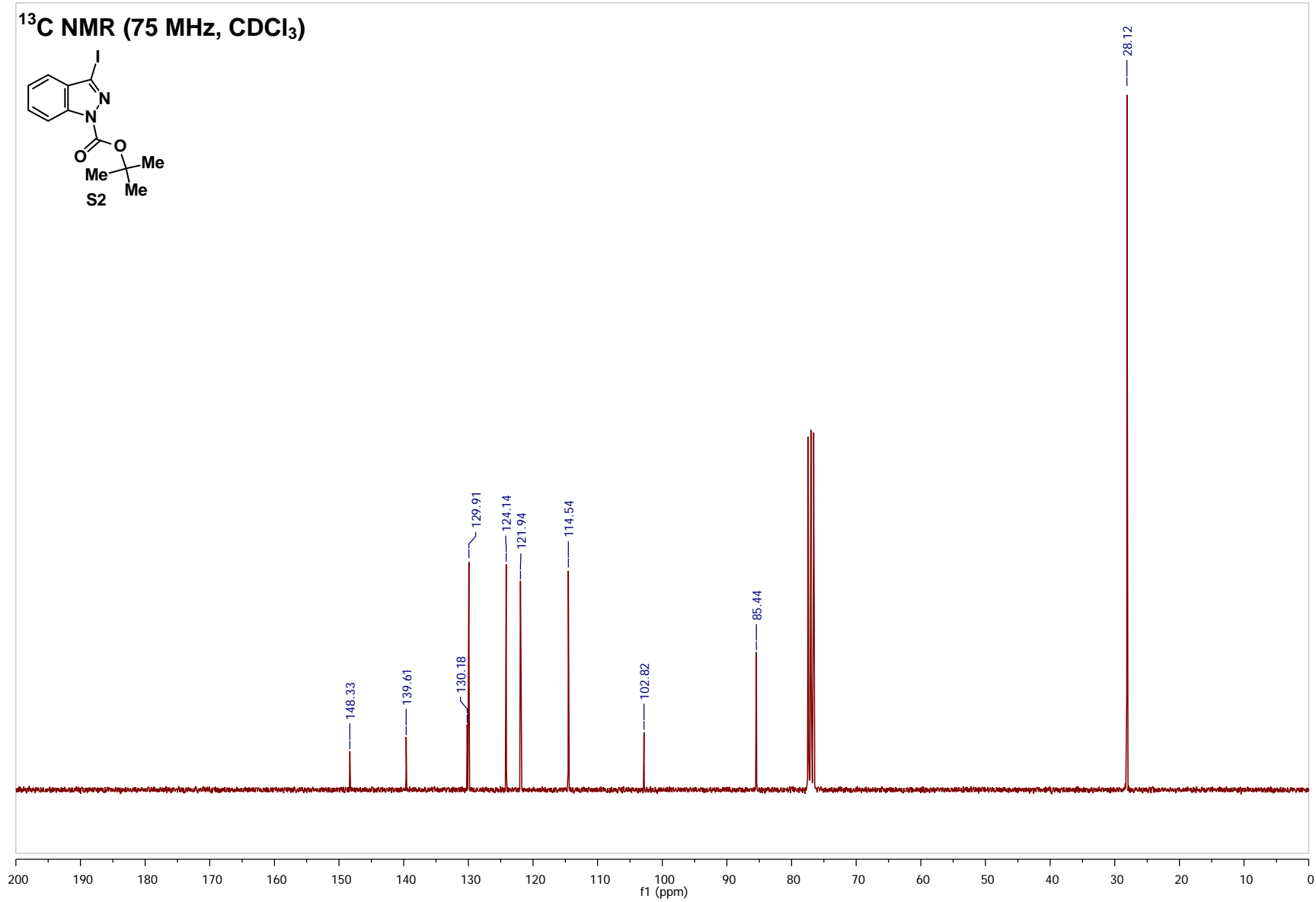
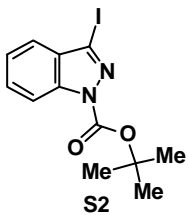
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)**



<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)

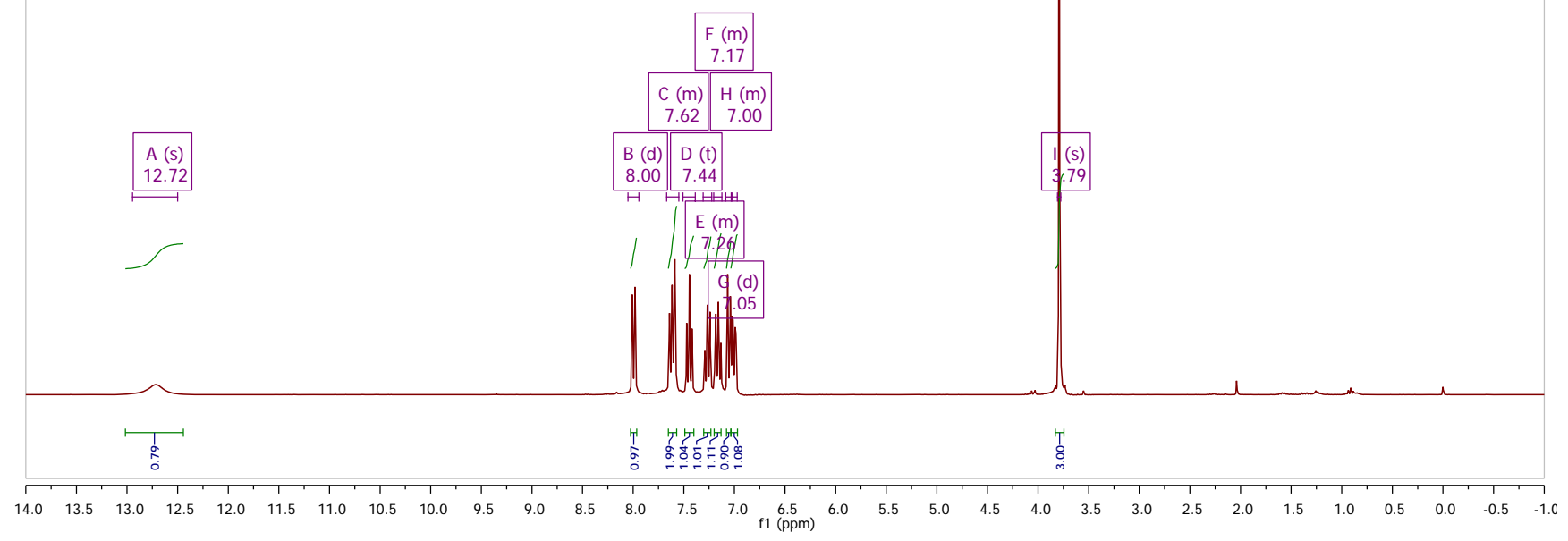
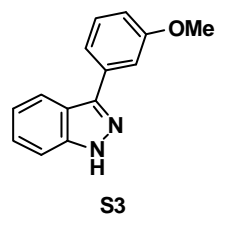


<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)

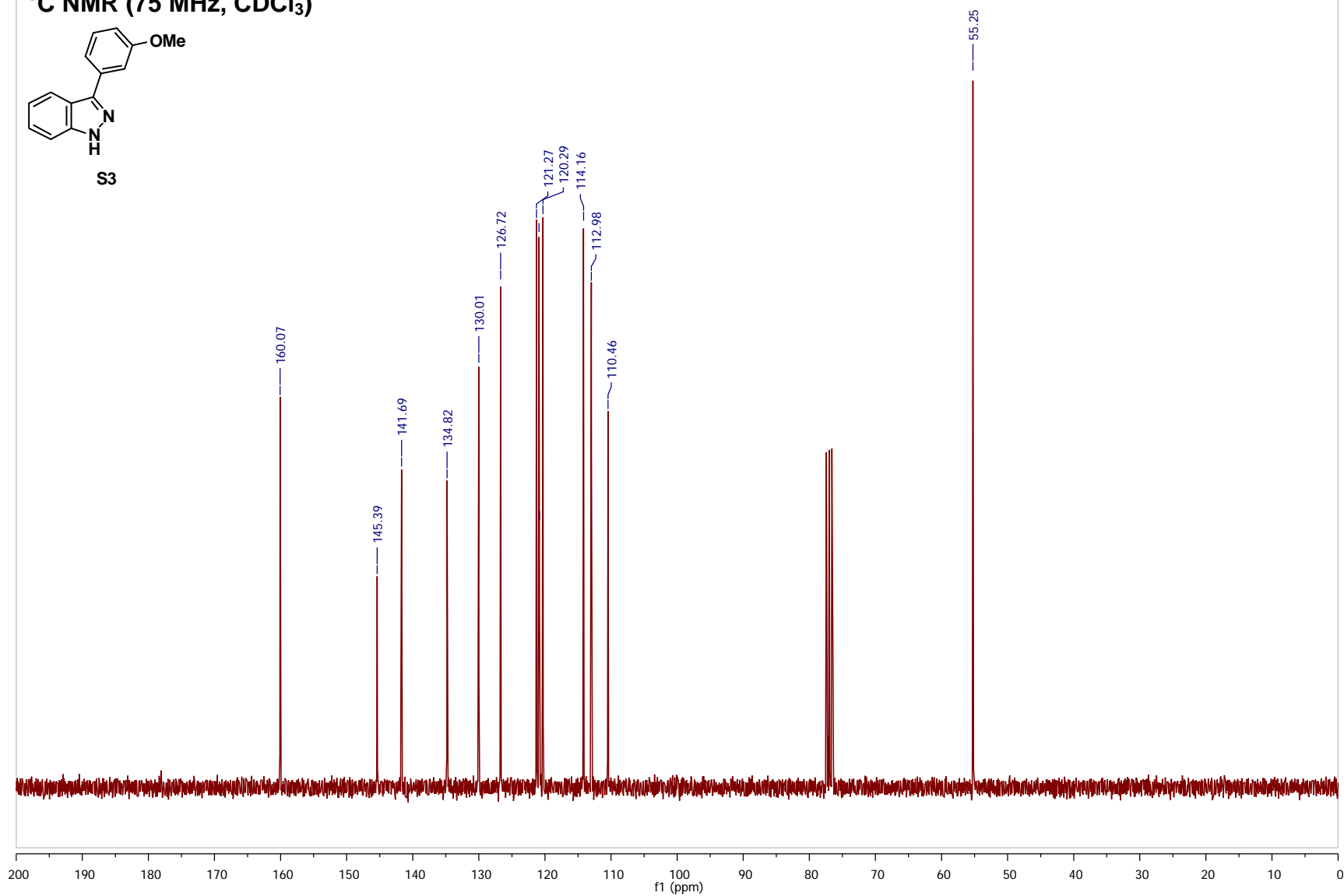
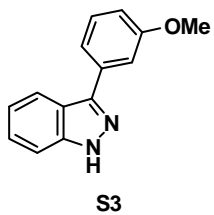




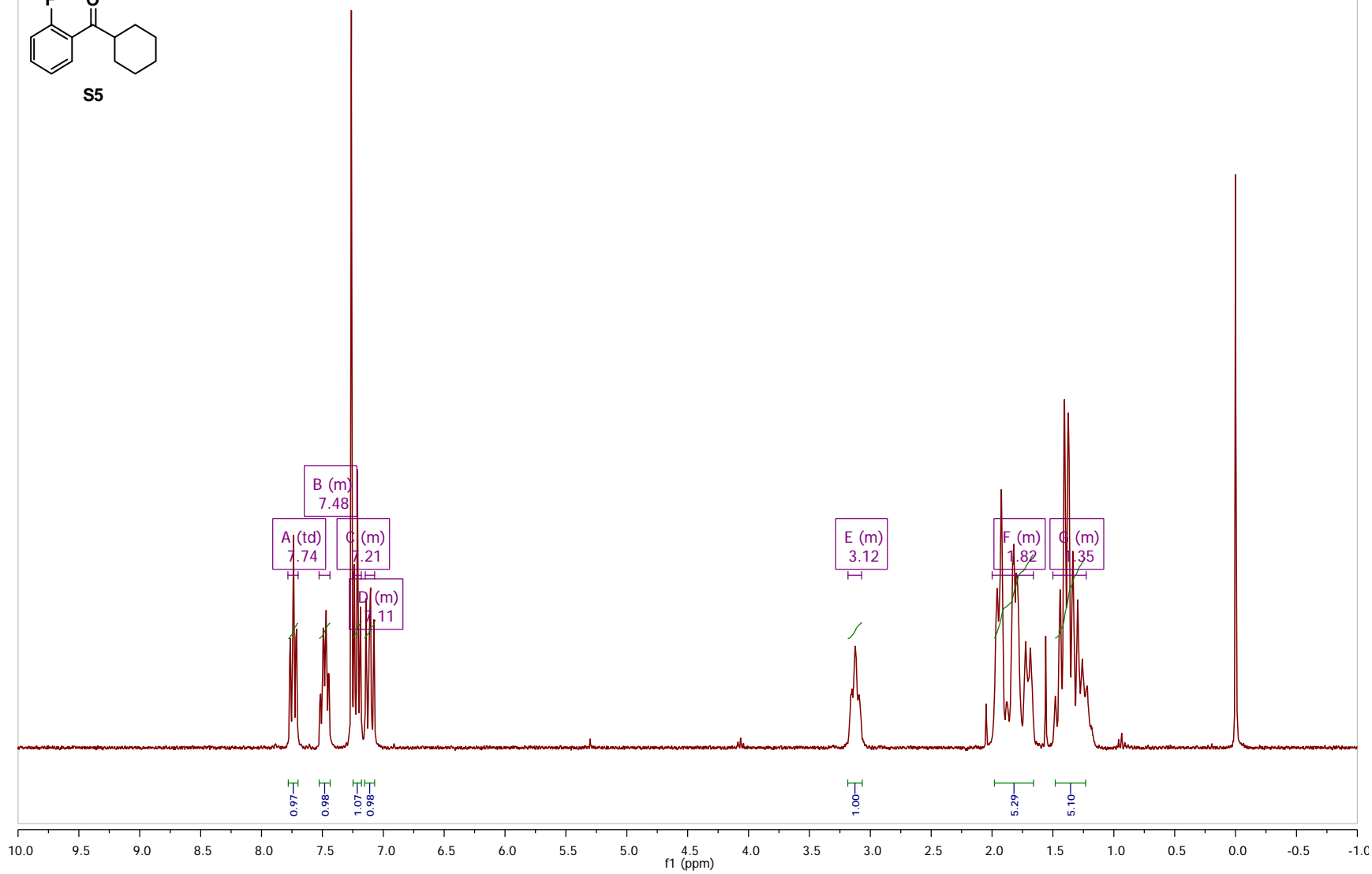
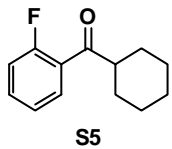
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



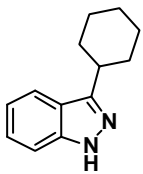
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)**



<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



S6

