Electronic Supplementary Information

Indium Triflate-Catalysed Diels-Alder Reactions of Isochromenylium Cations with Enones

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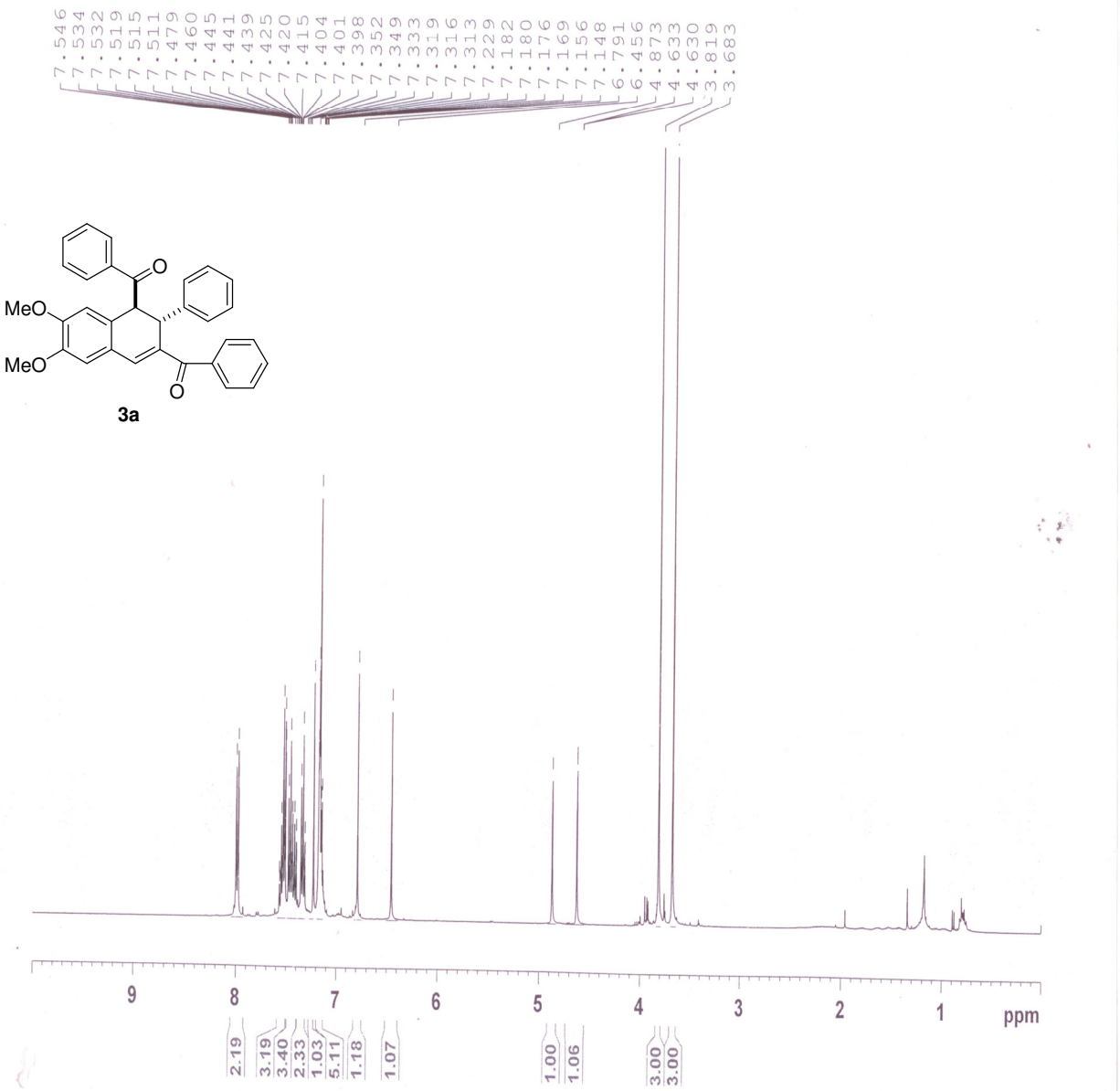
srinivasank@bdu.ac.in

Copies of ^{1}H and ^{13}C NMR spectra for compounds **3a-n** and **5a-c** and computation details and optimized geometries of transition states **TS-1** and **TS-2**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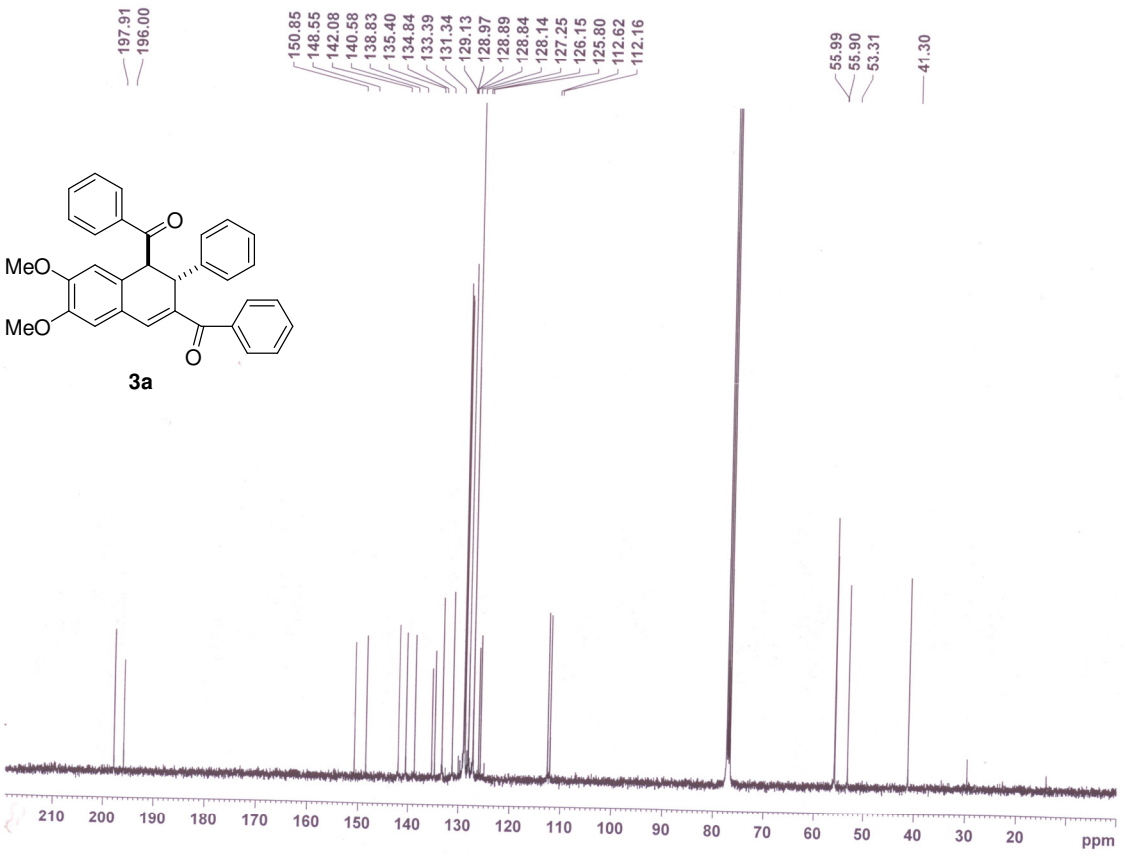
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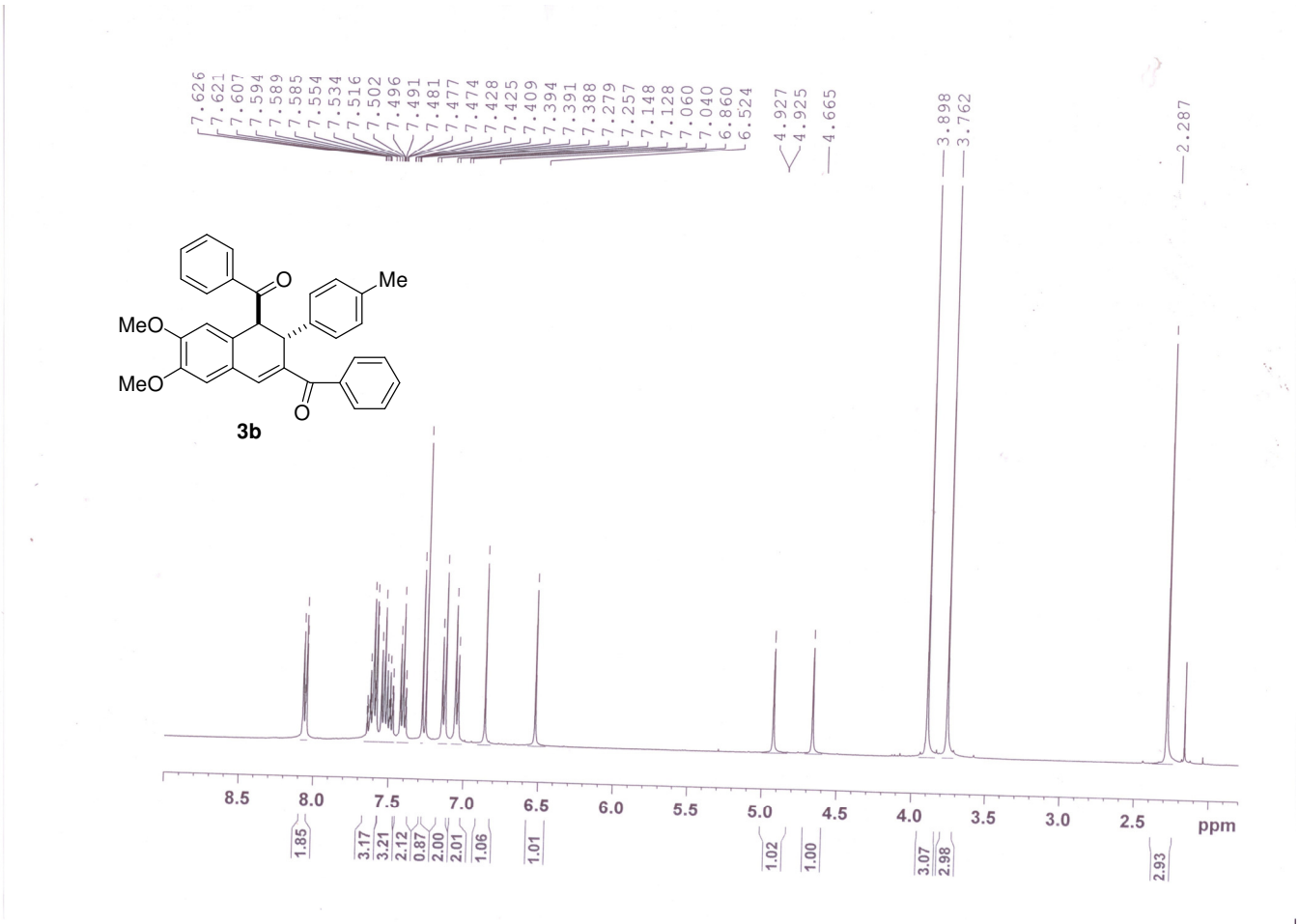

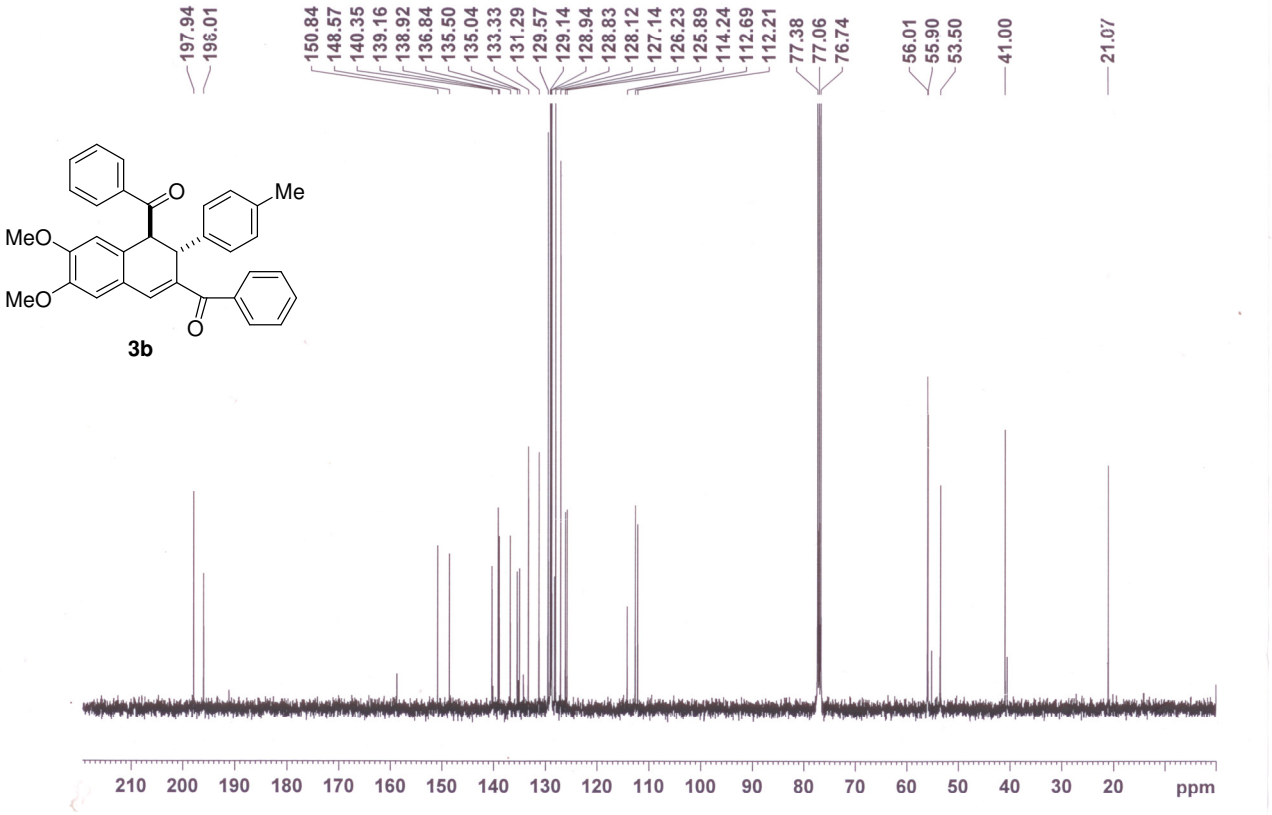

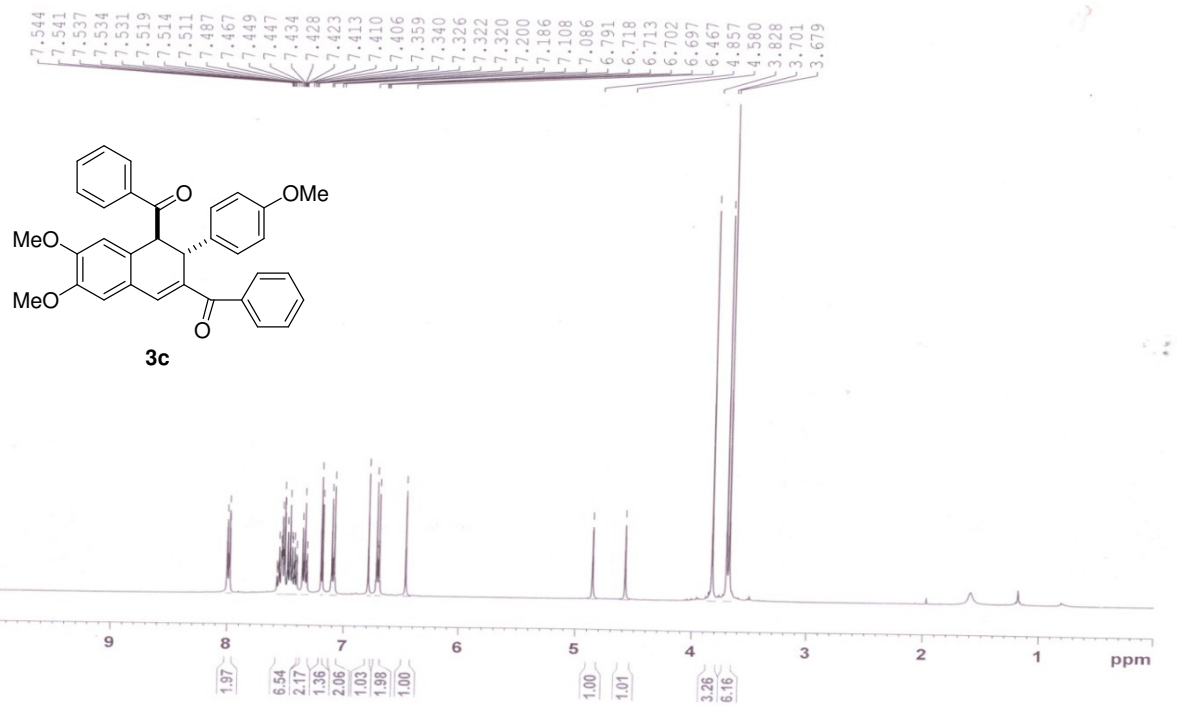

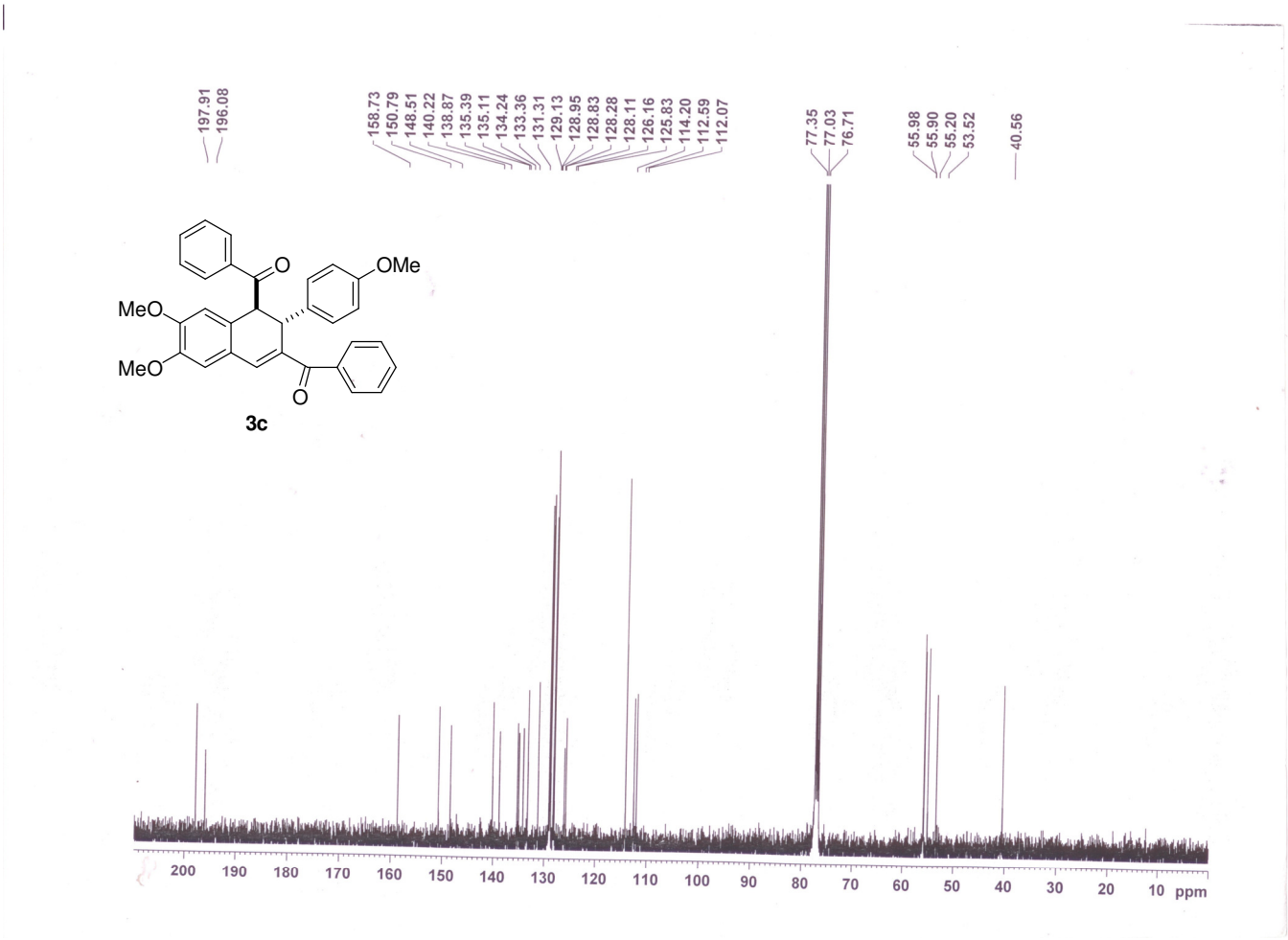
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MeO
MeO
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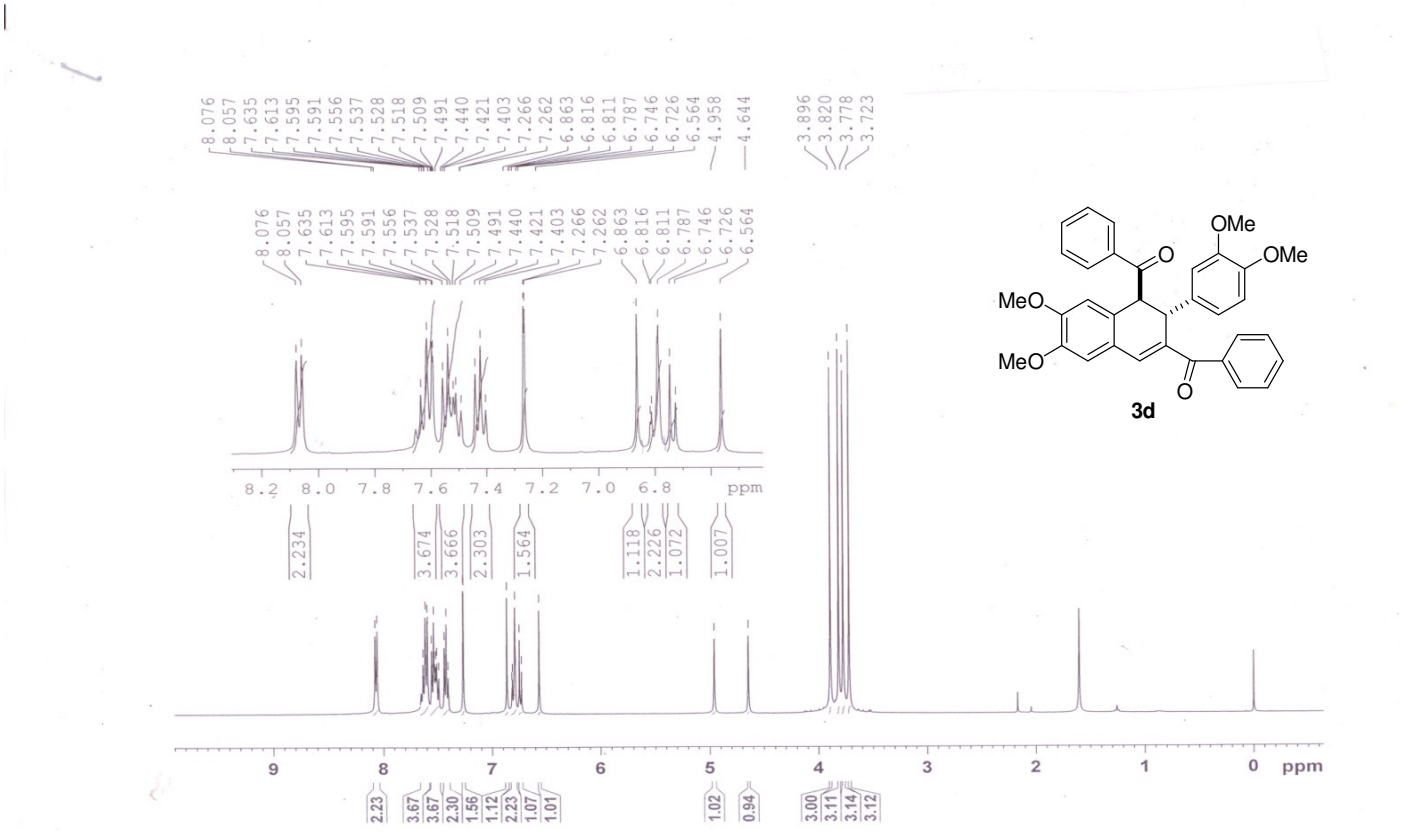

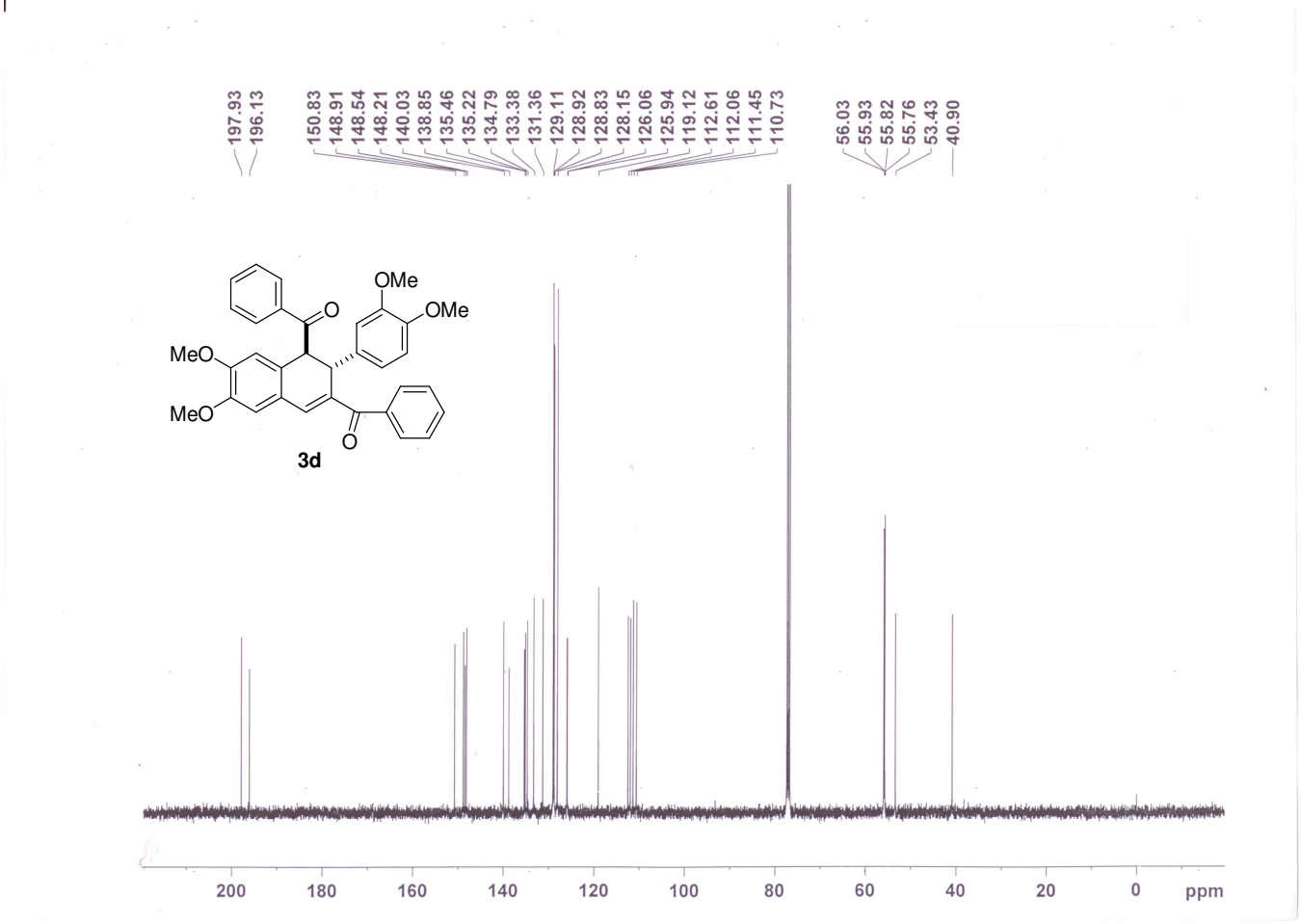

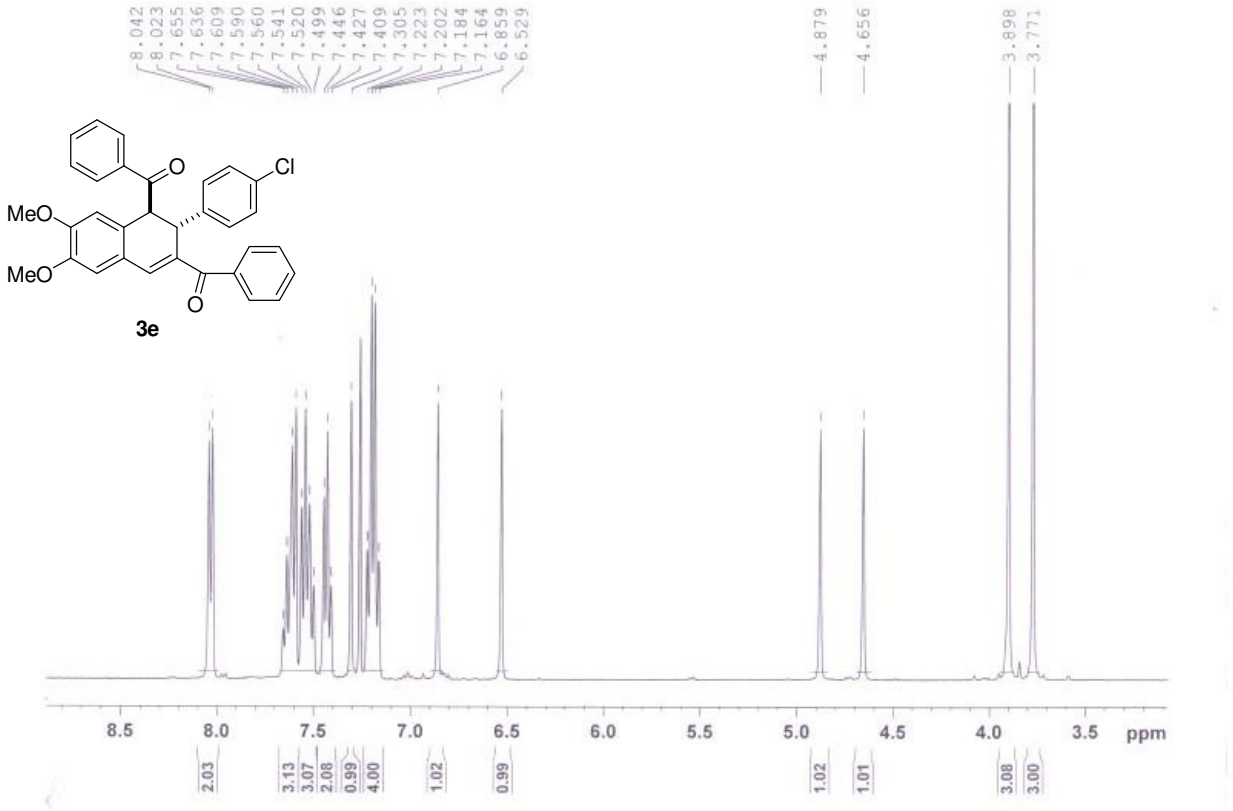

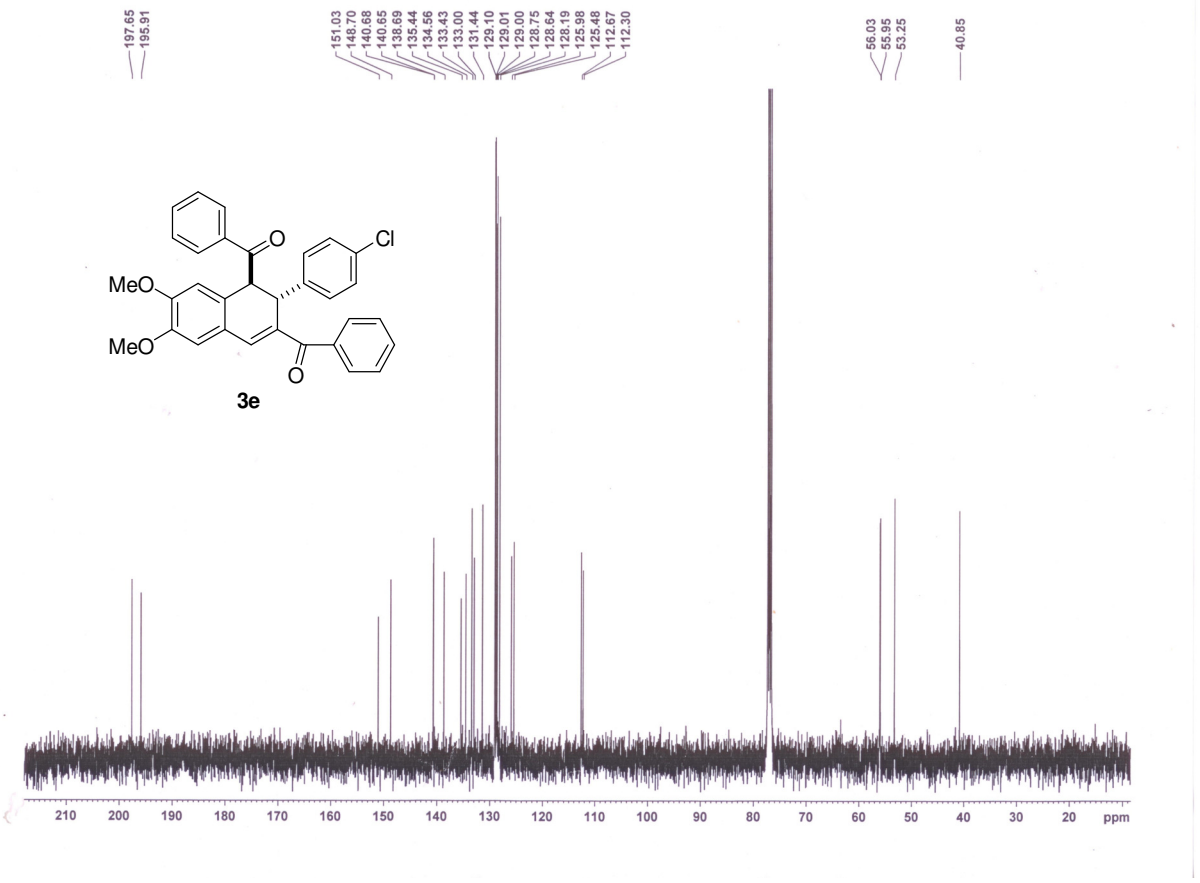
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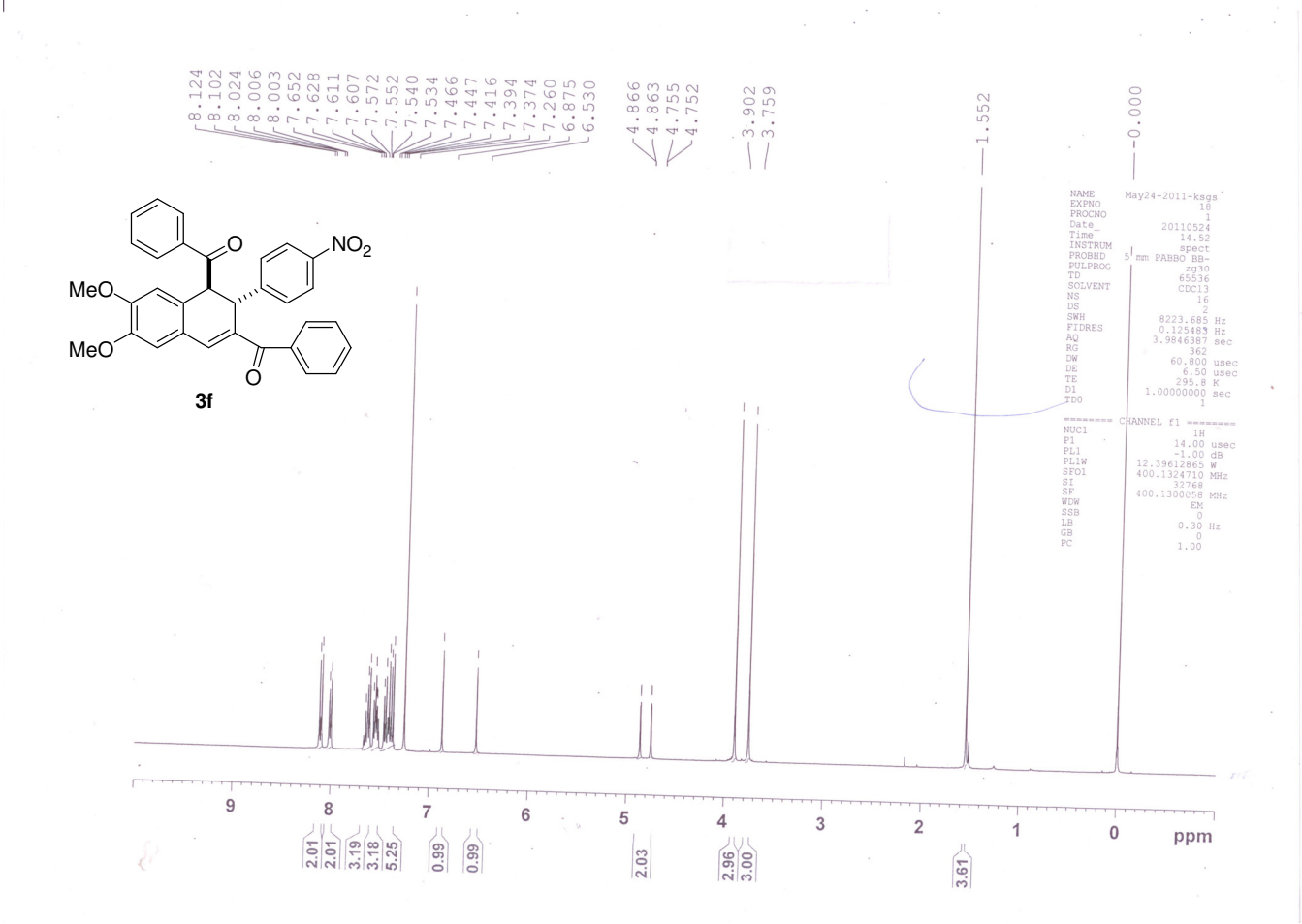

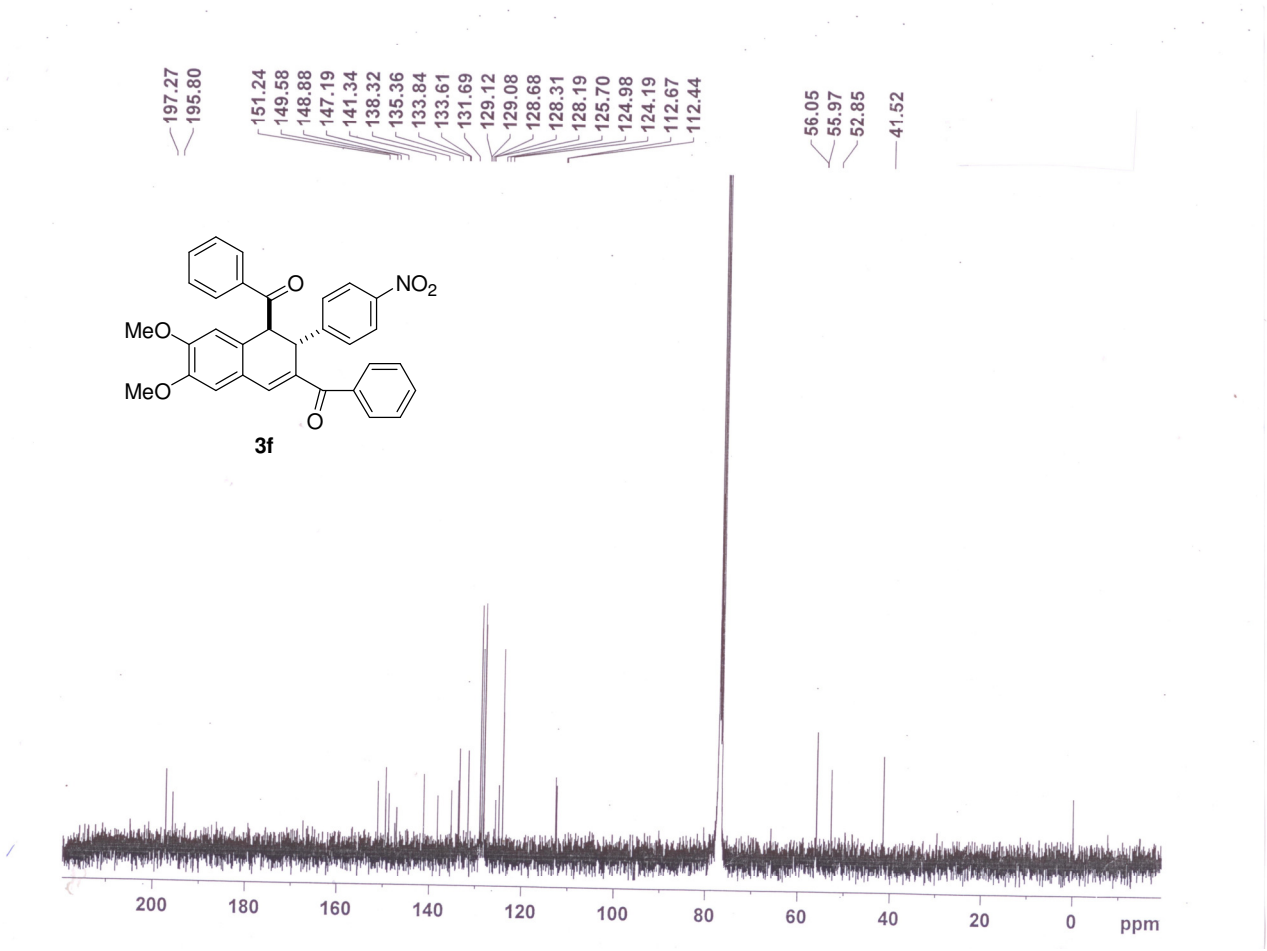

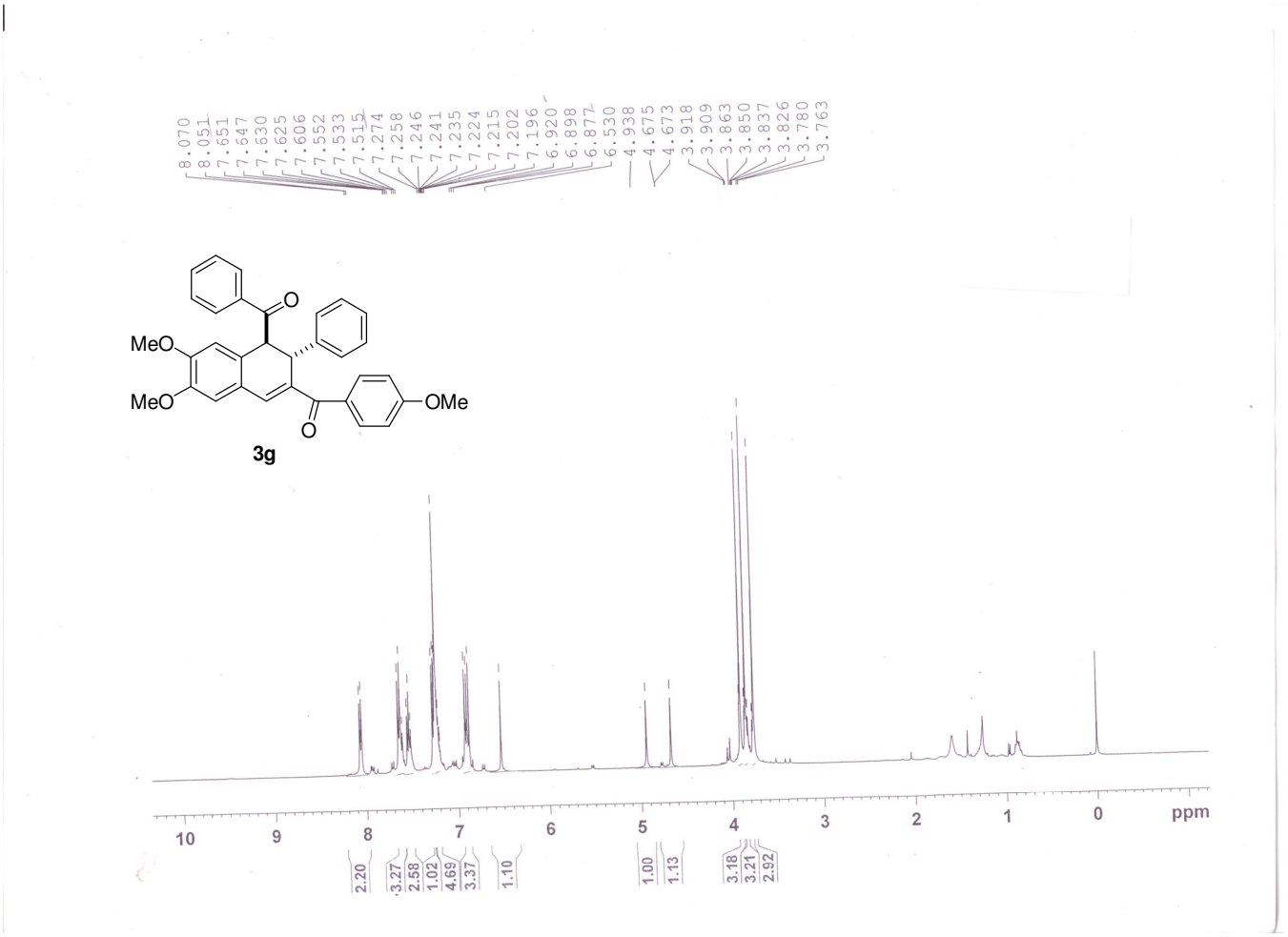

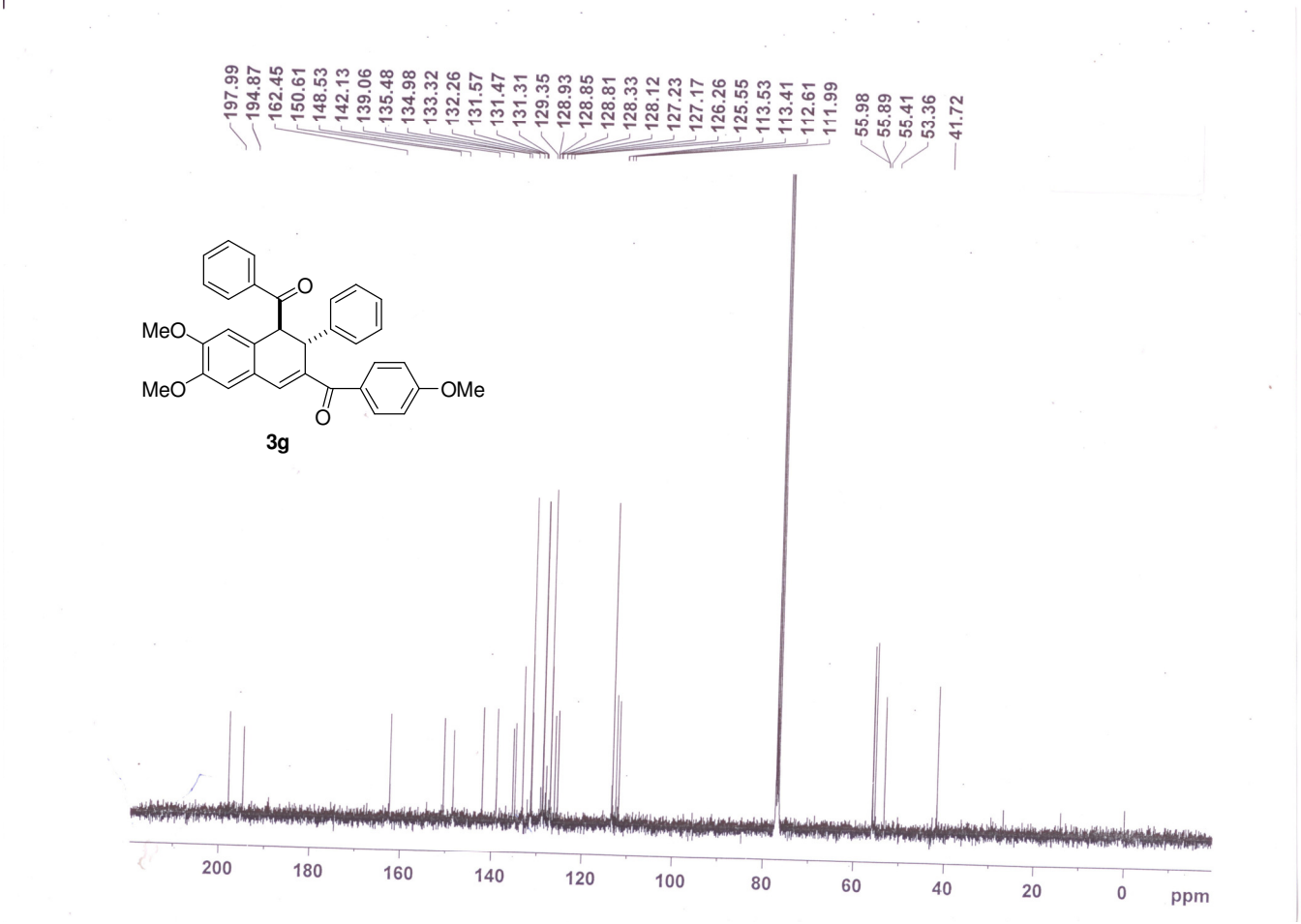
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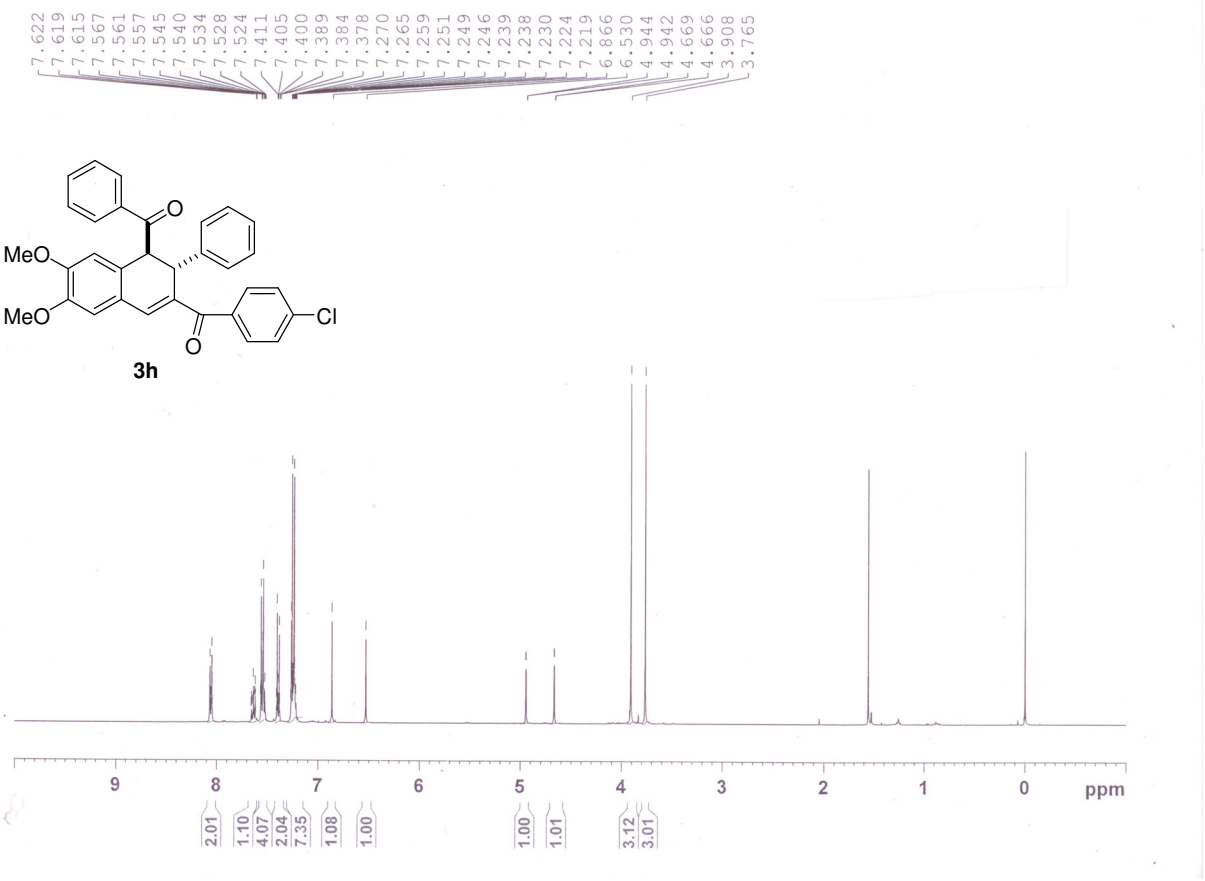
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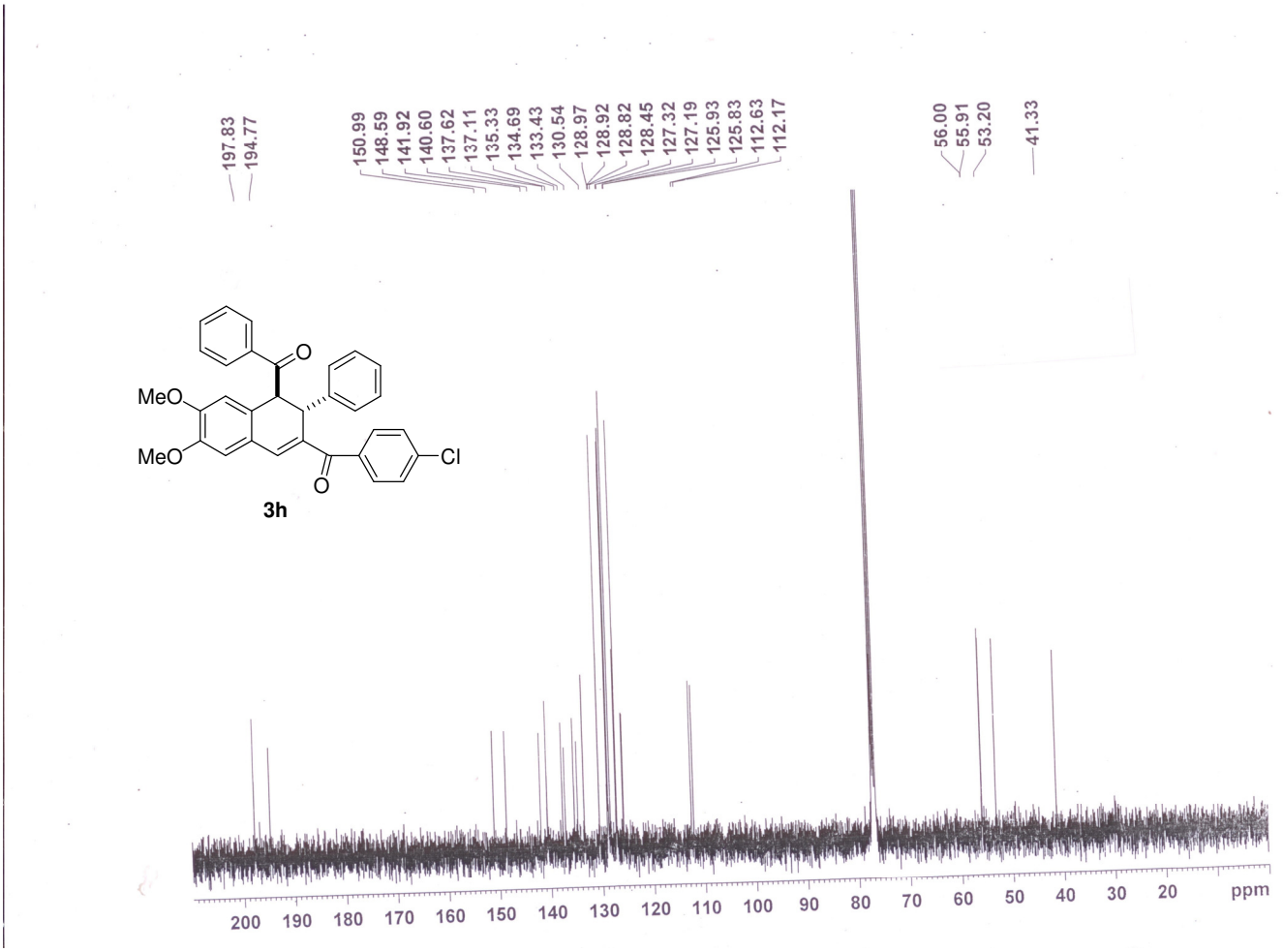

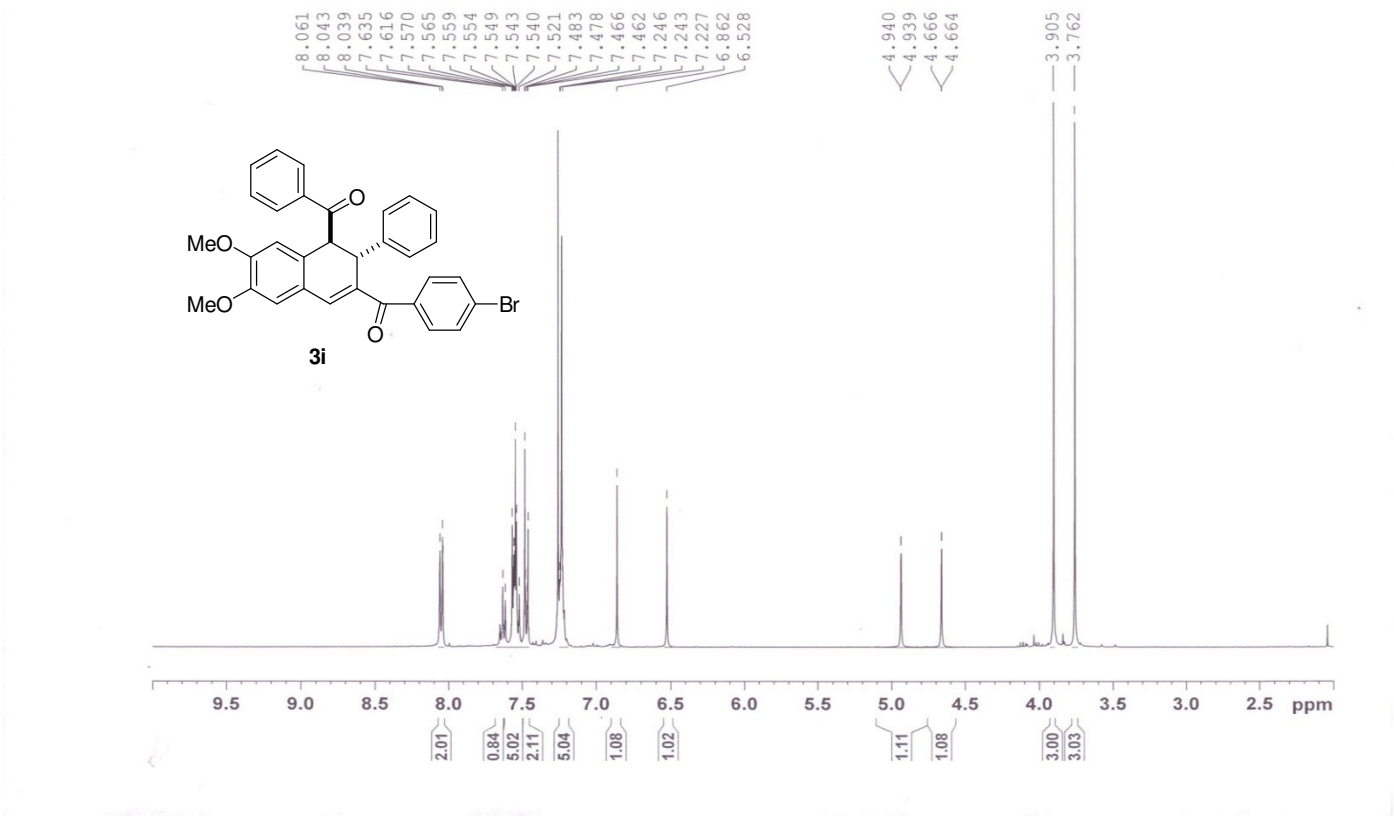

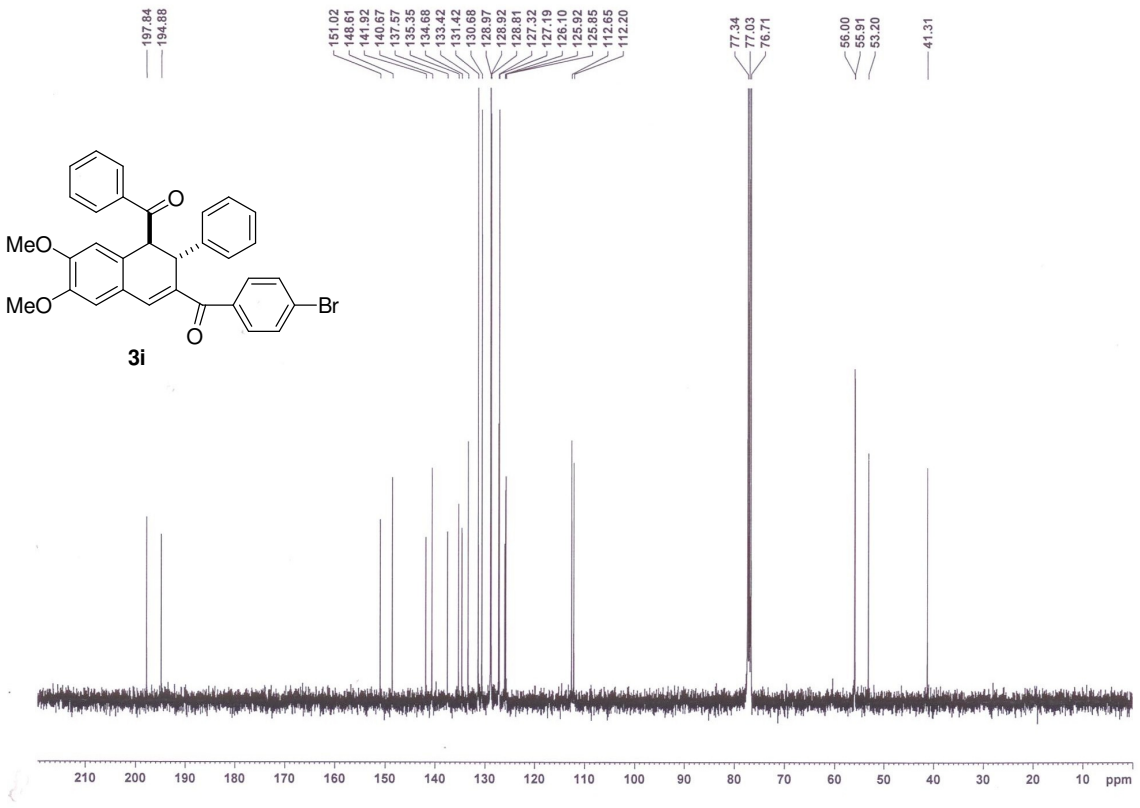
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76.71
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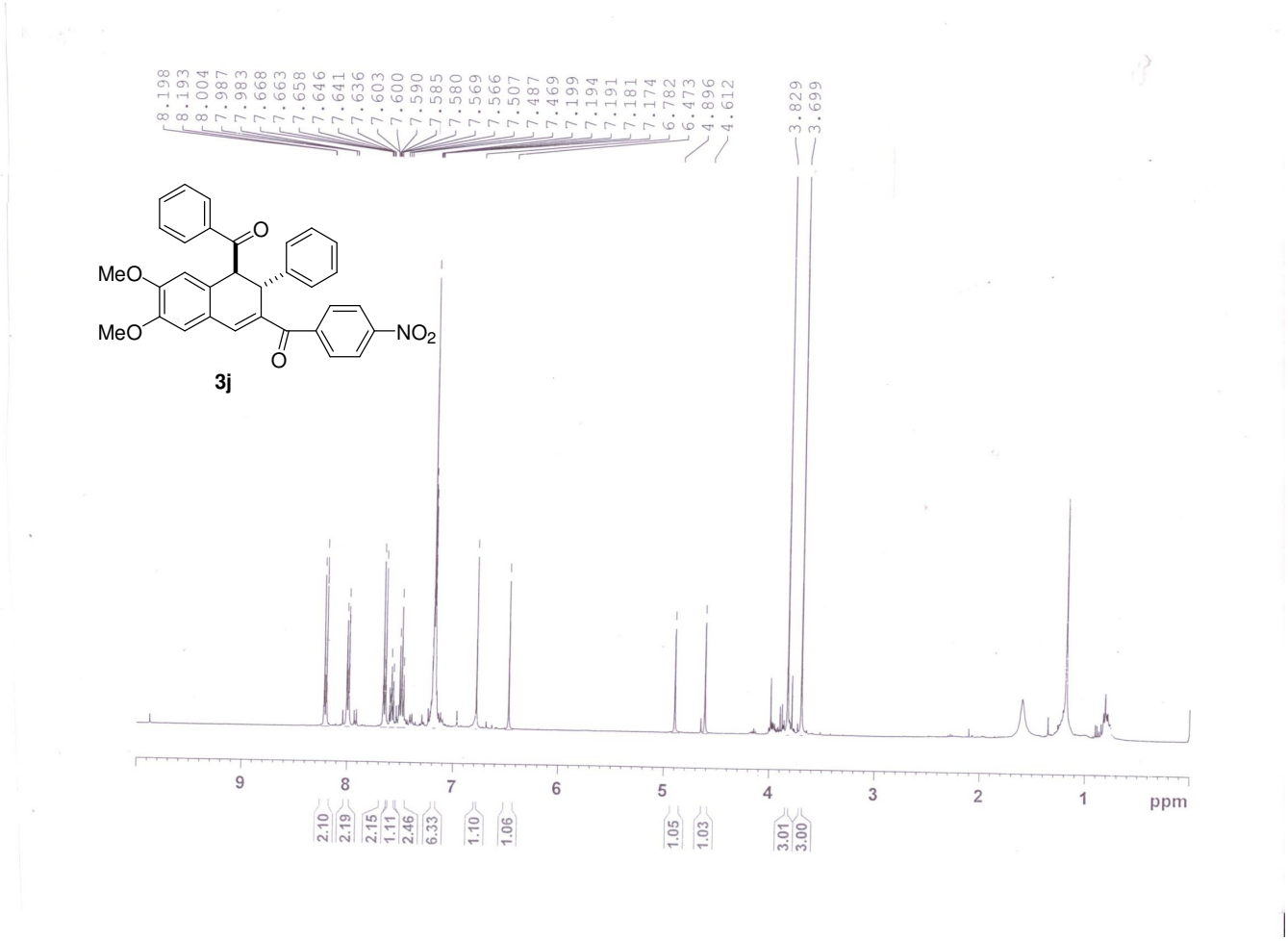
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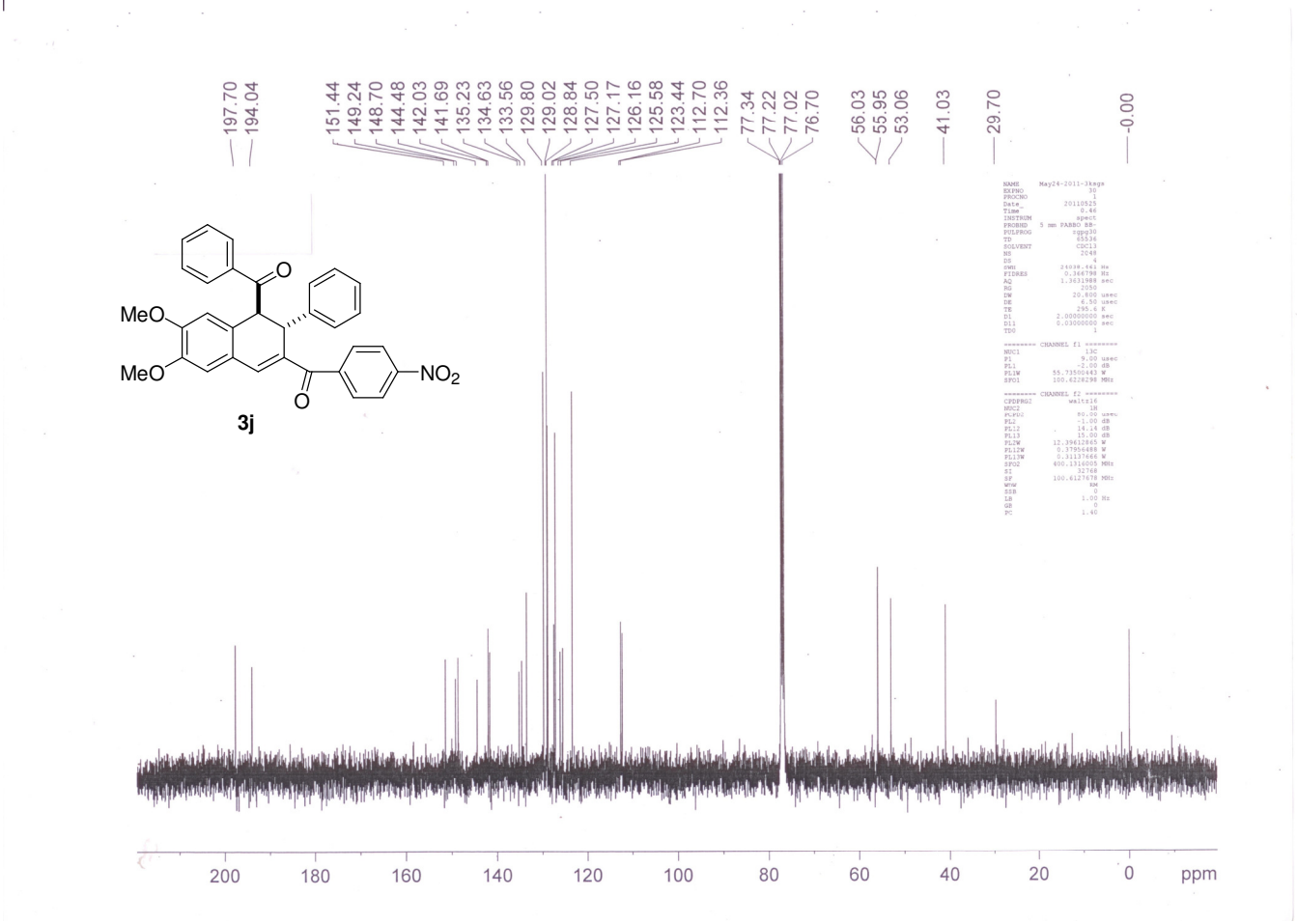
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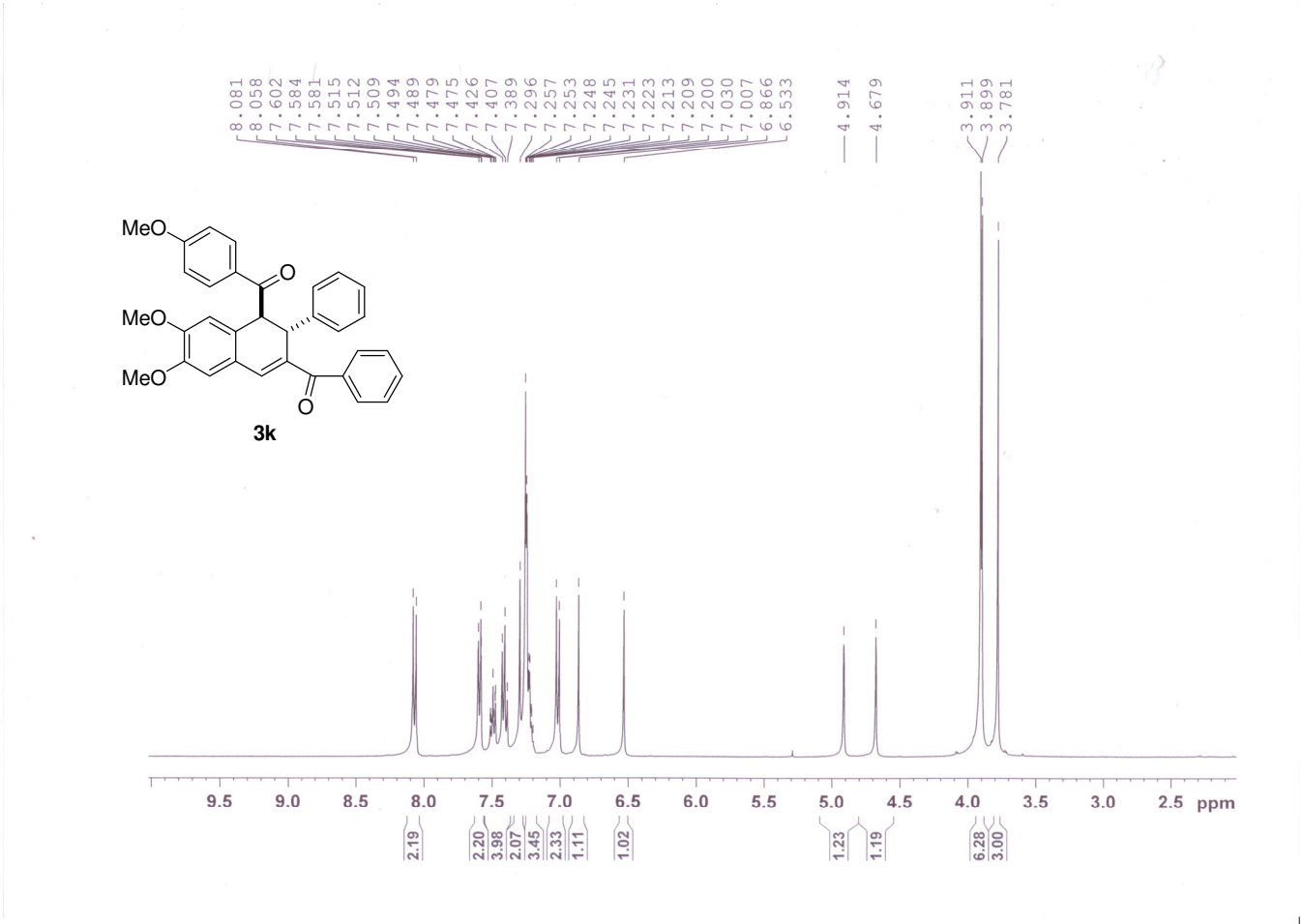
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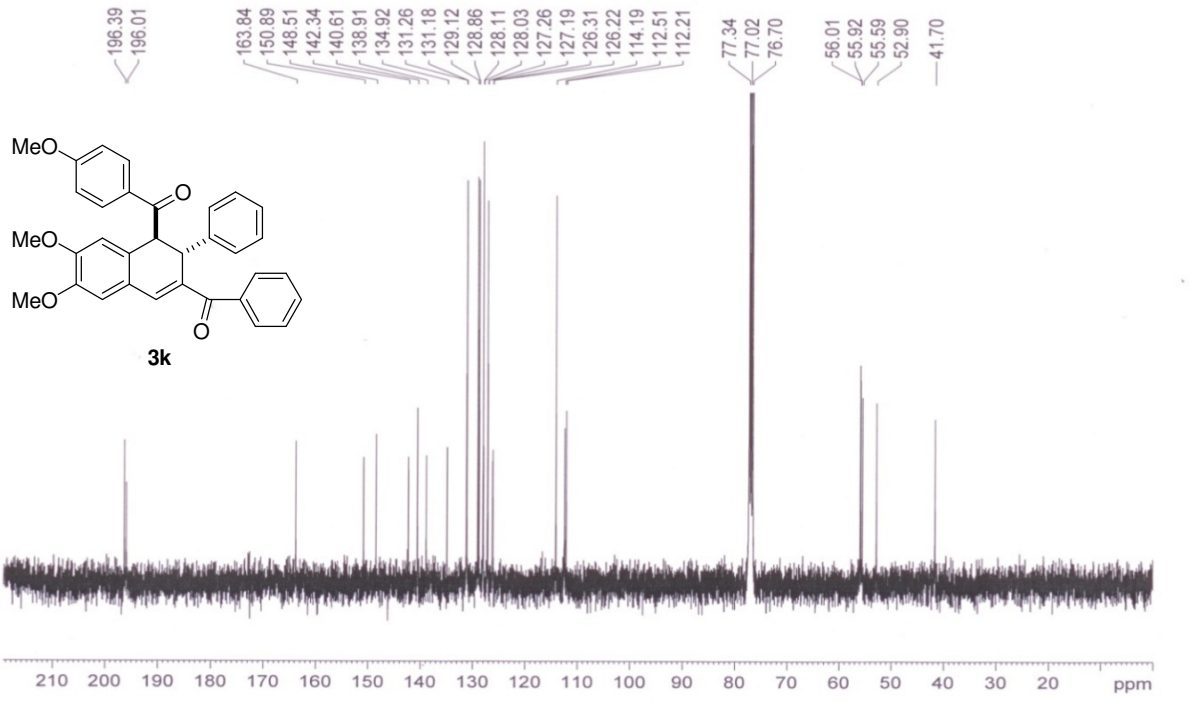

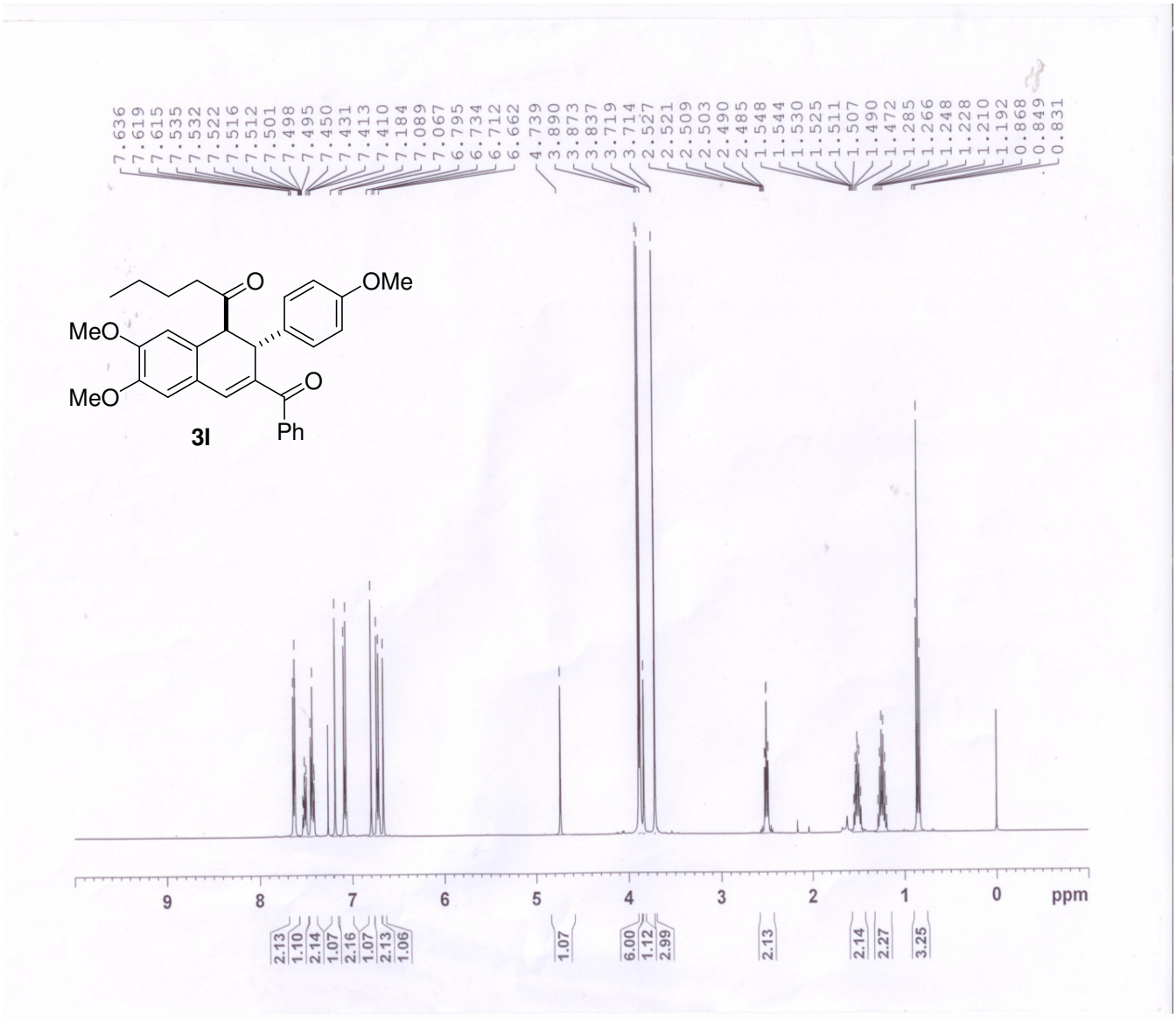

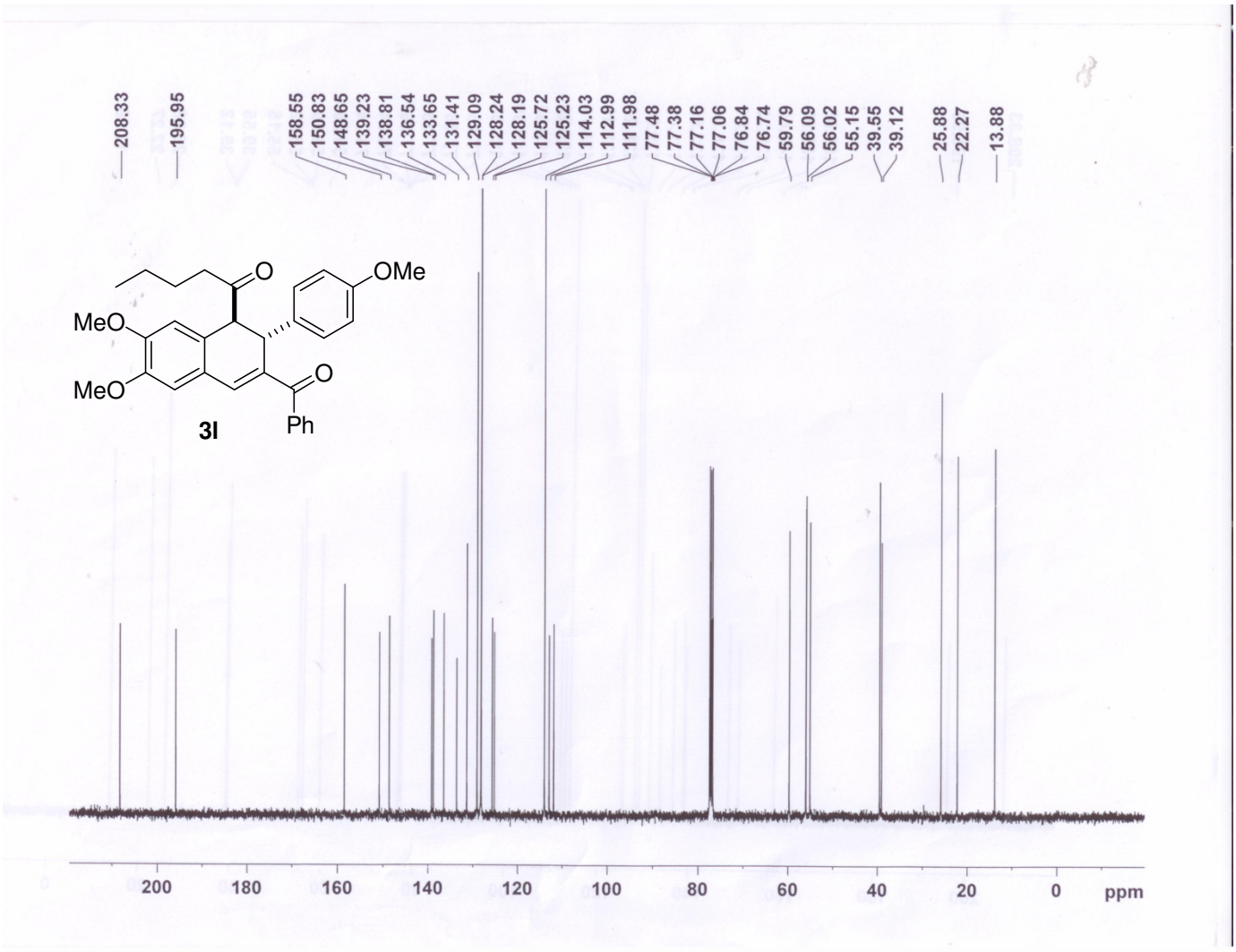

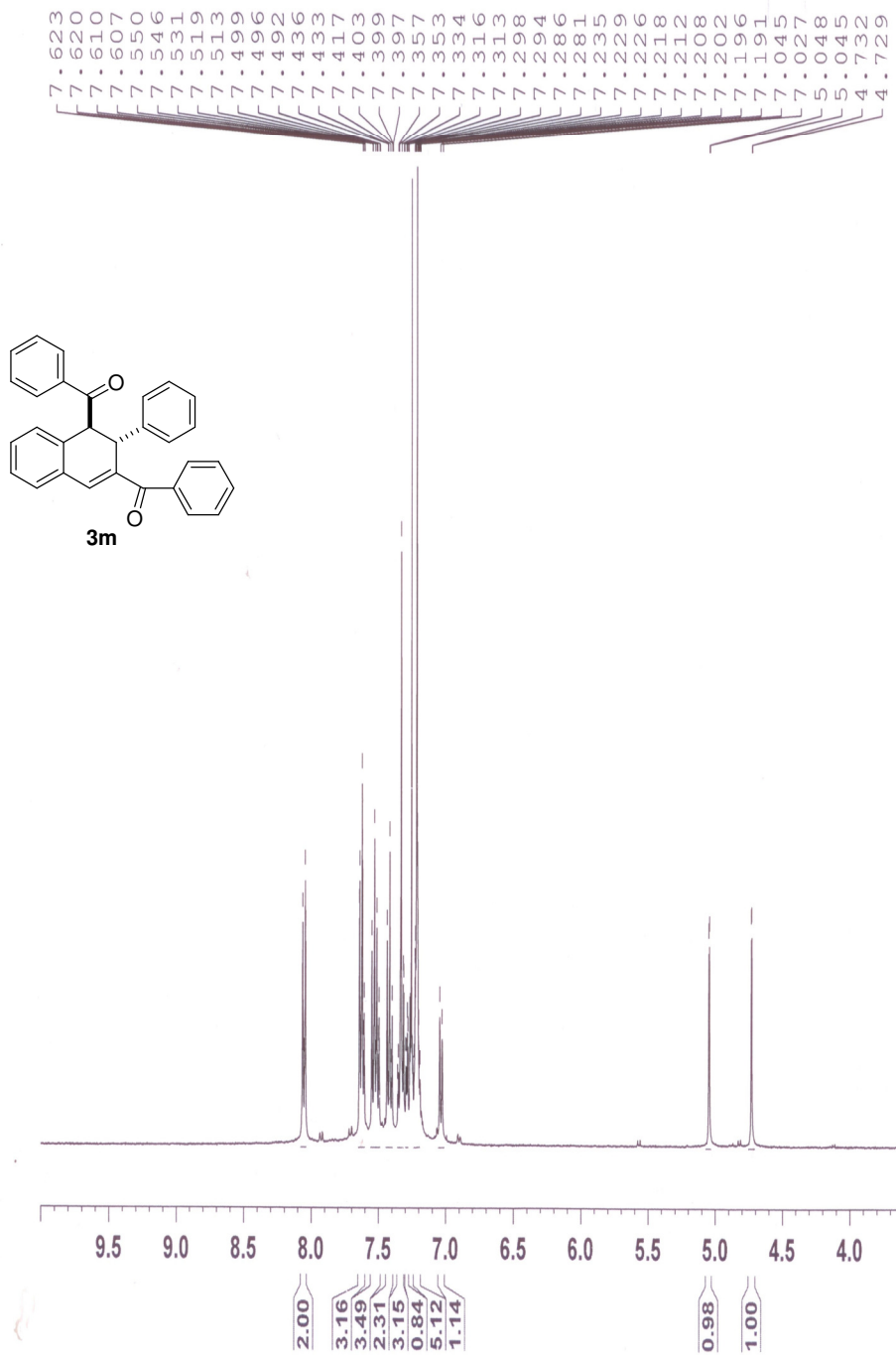

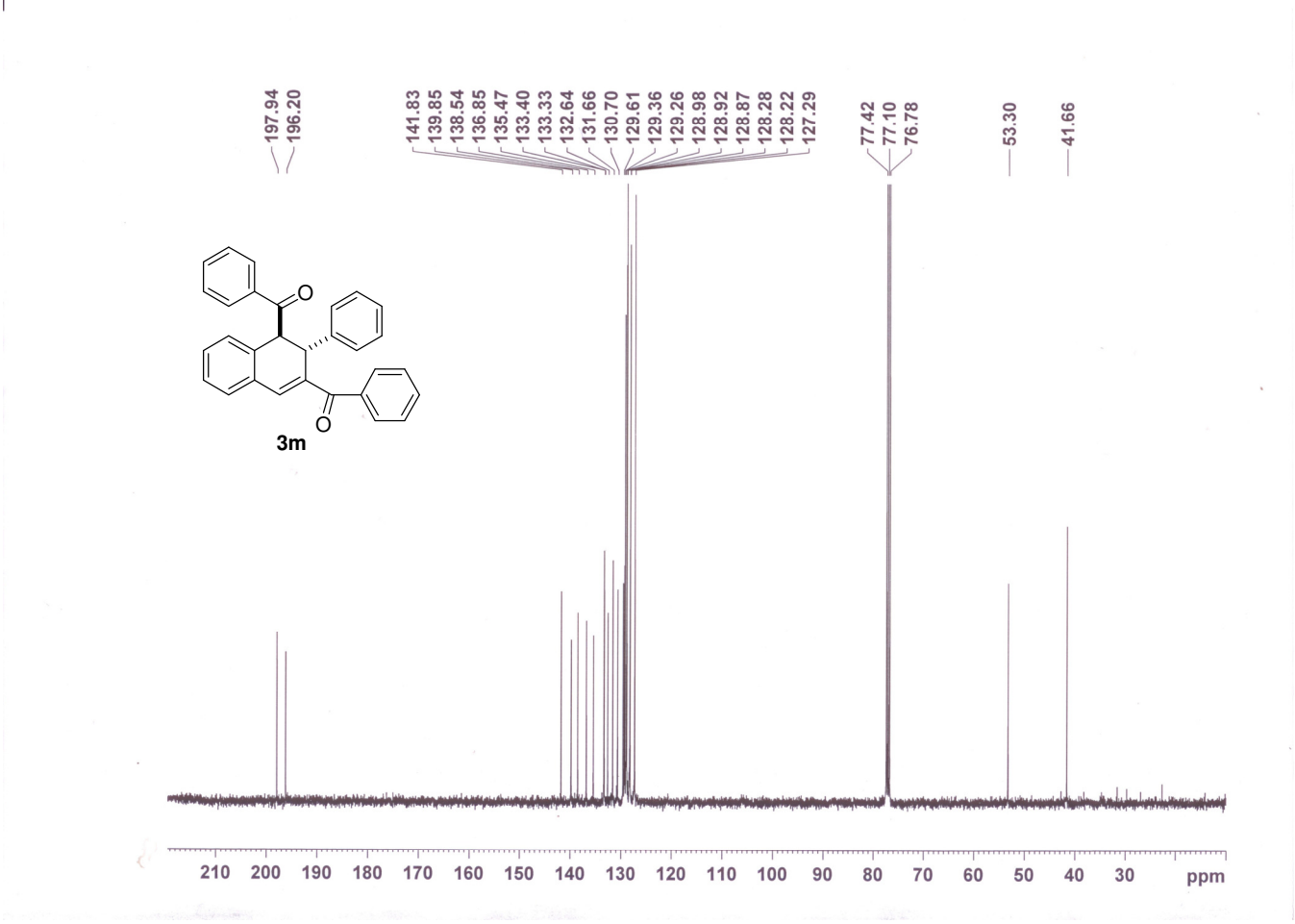
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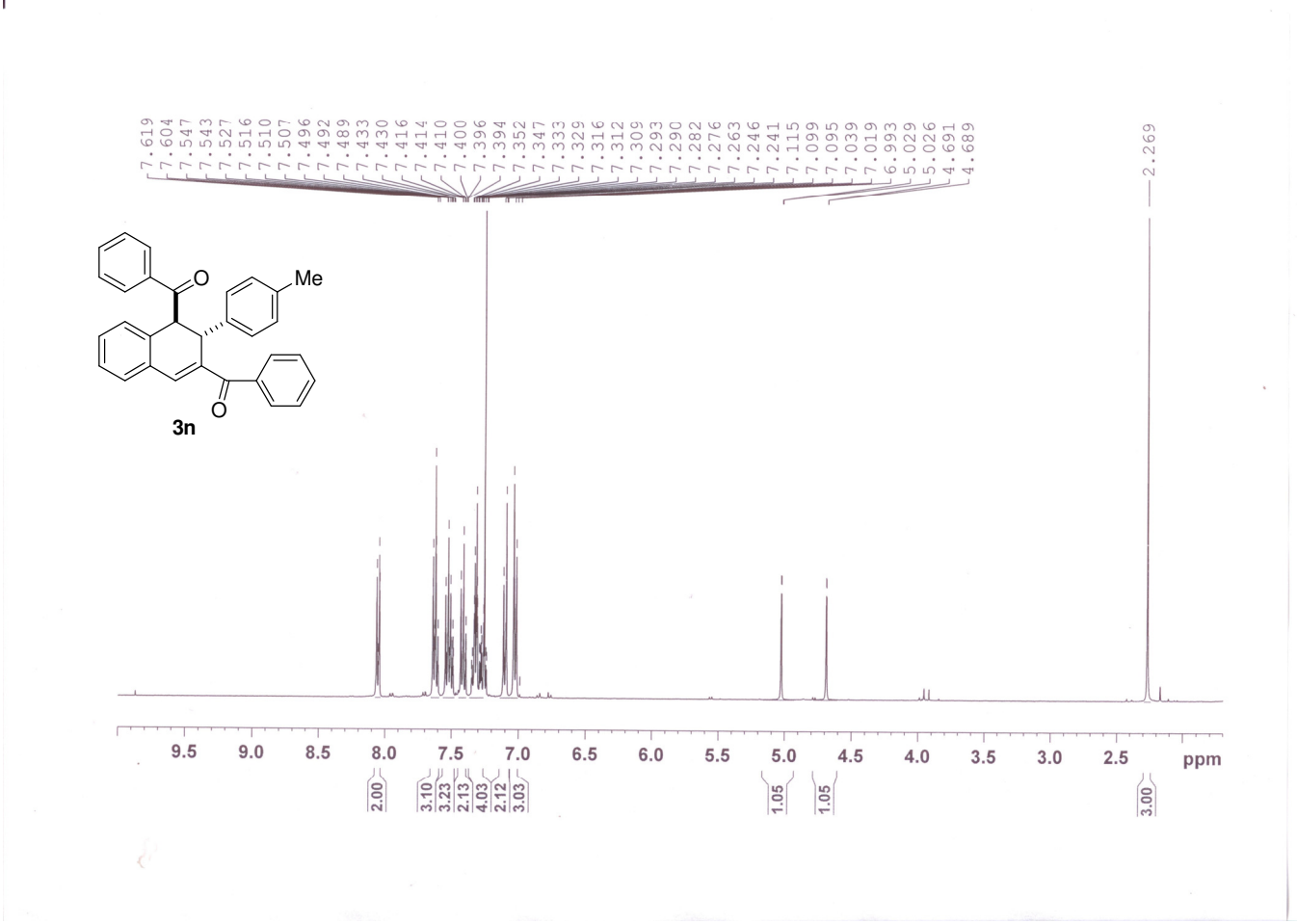
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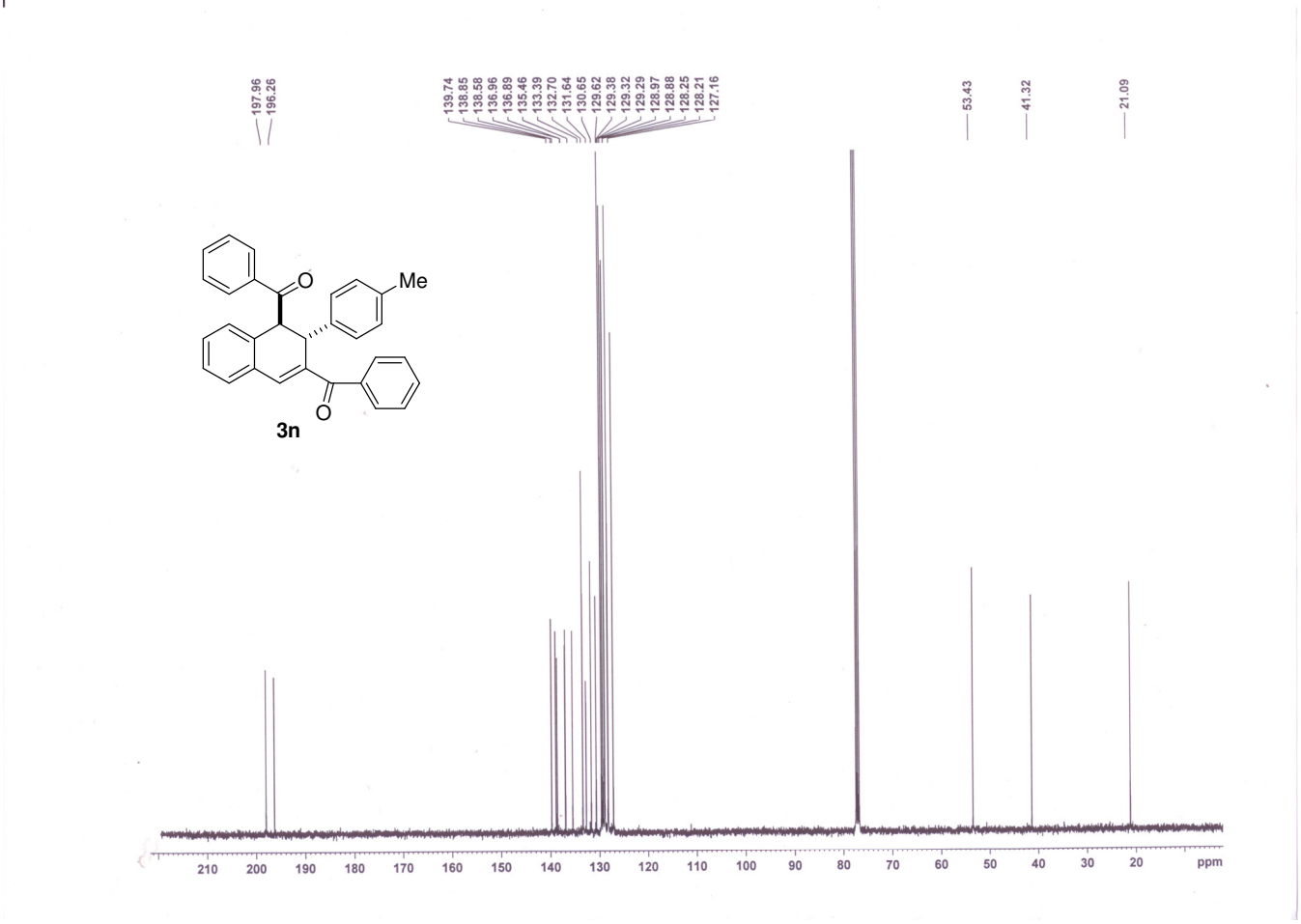

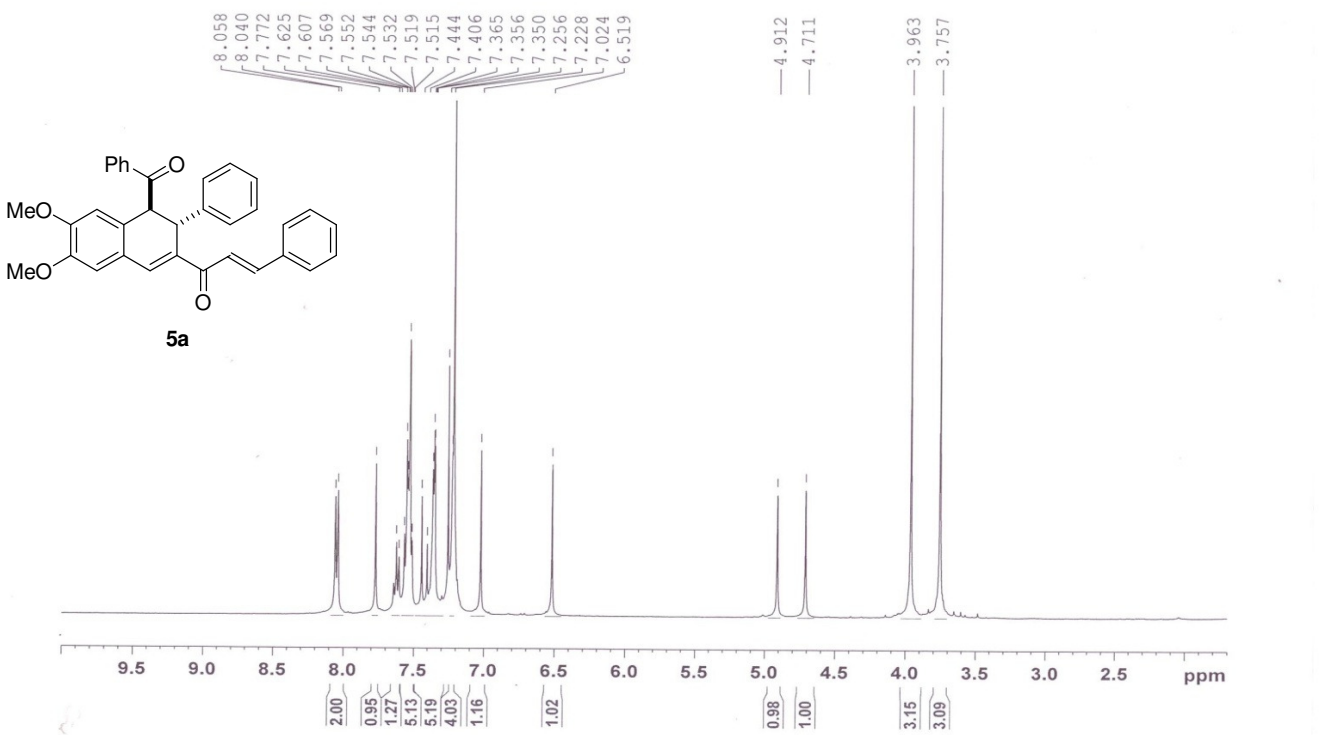

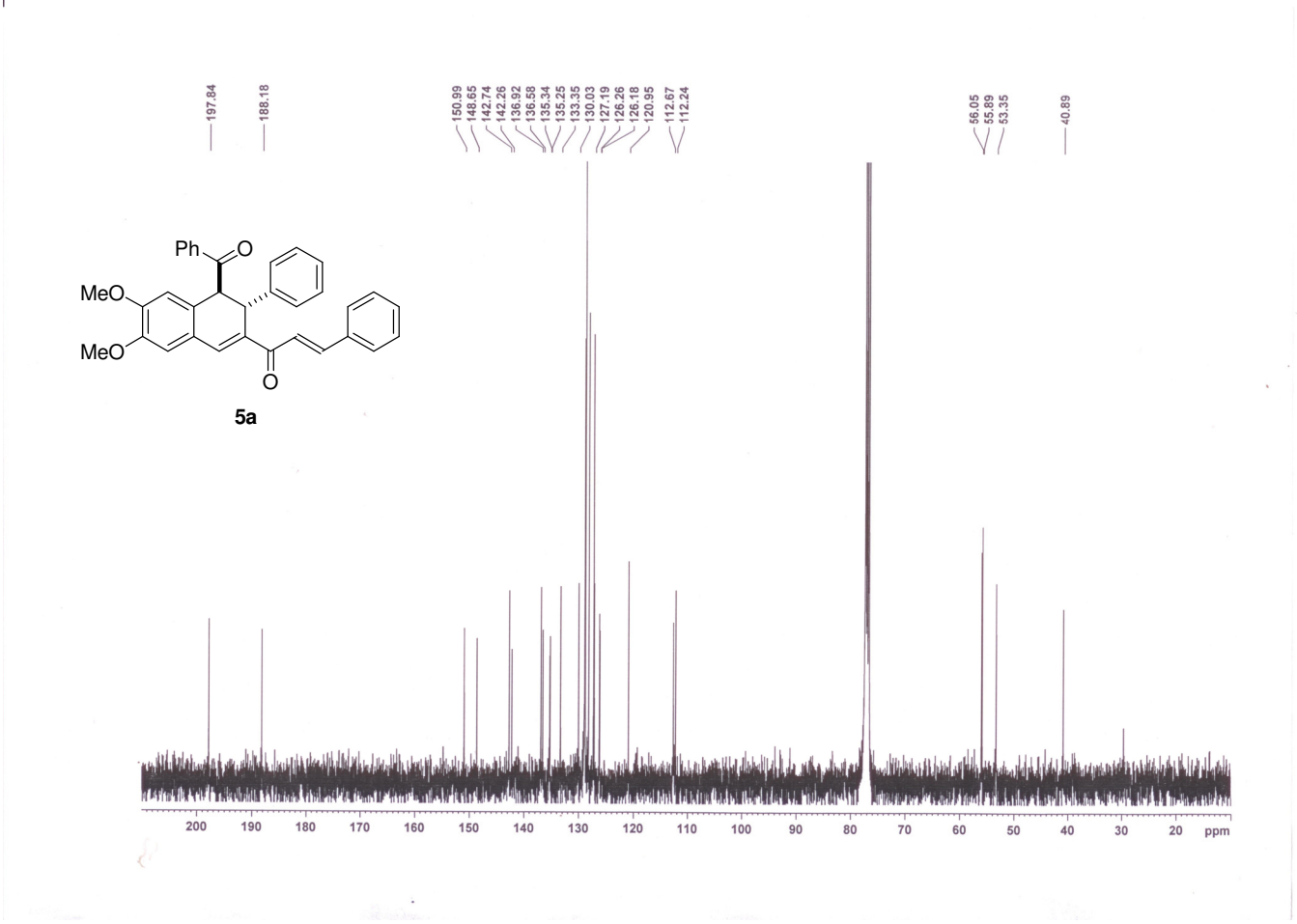

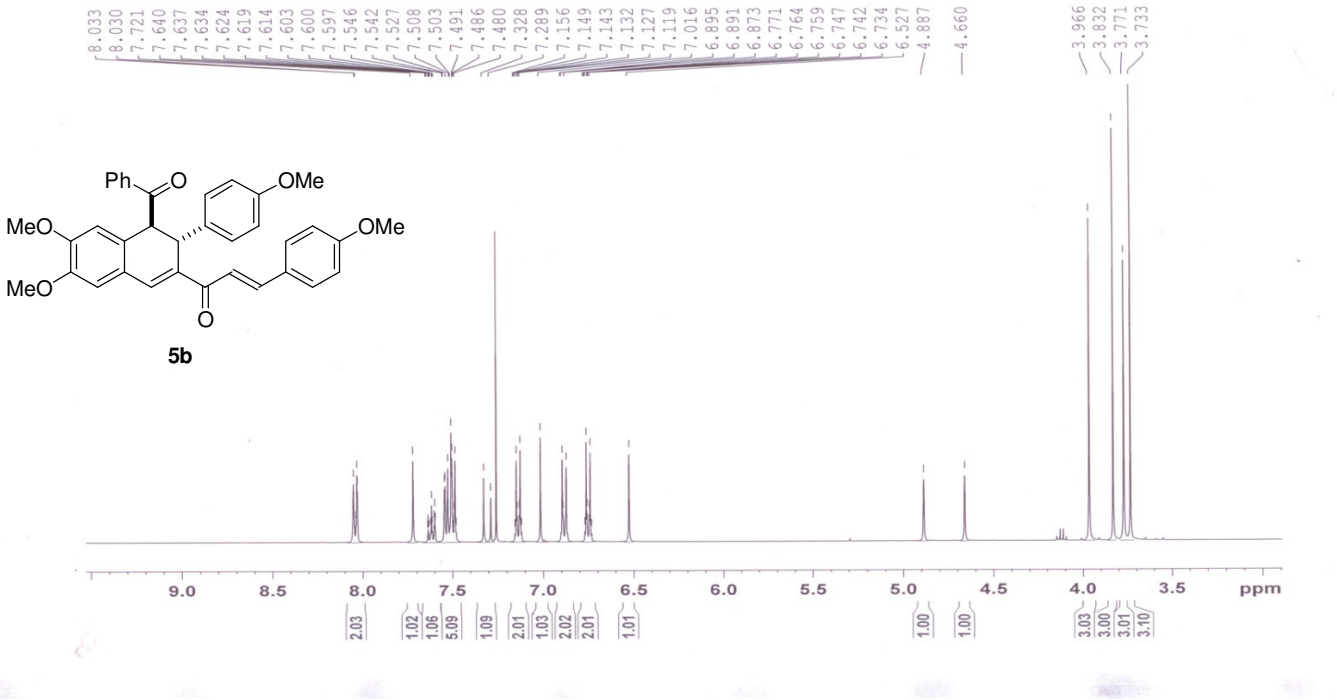
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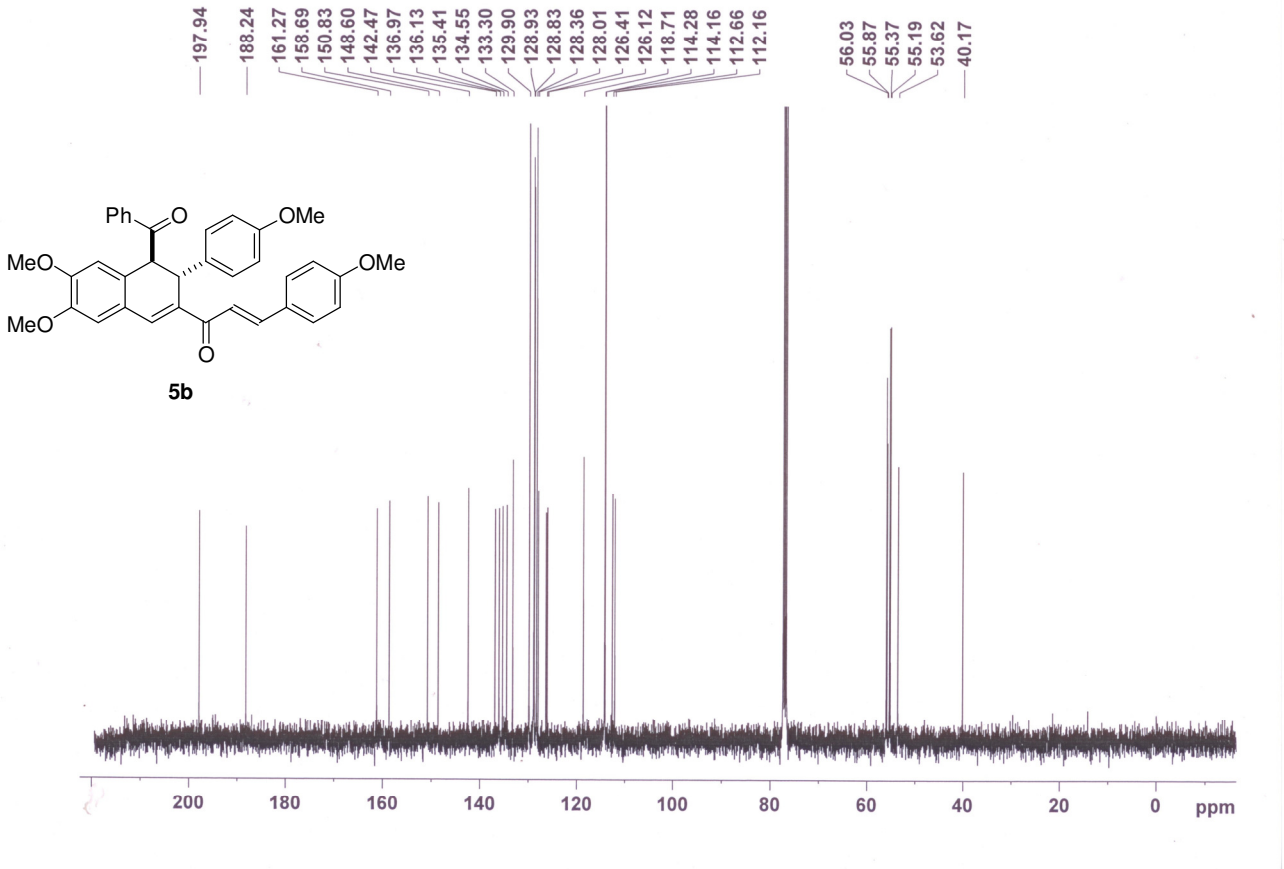
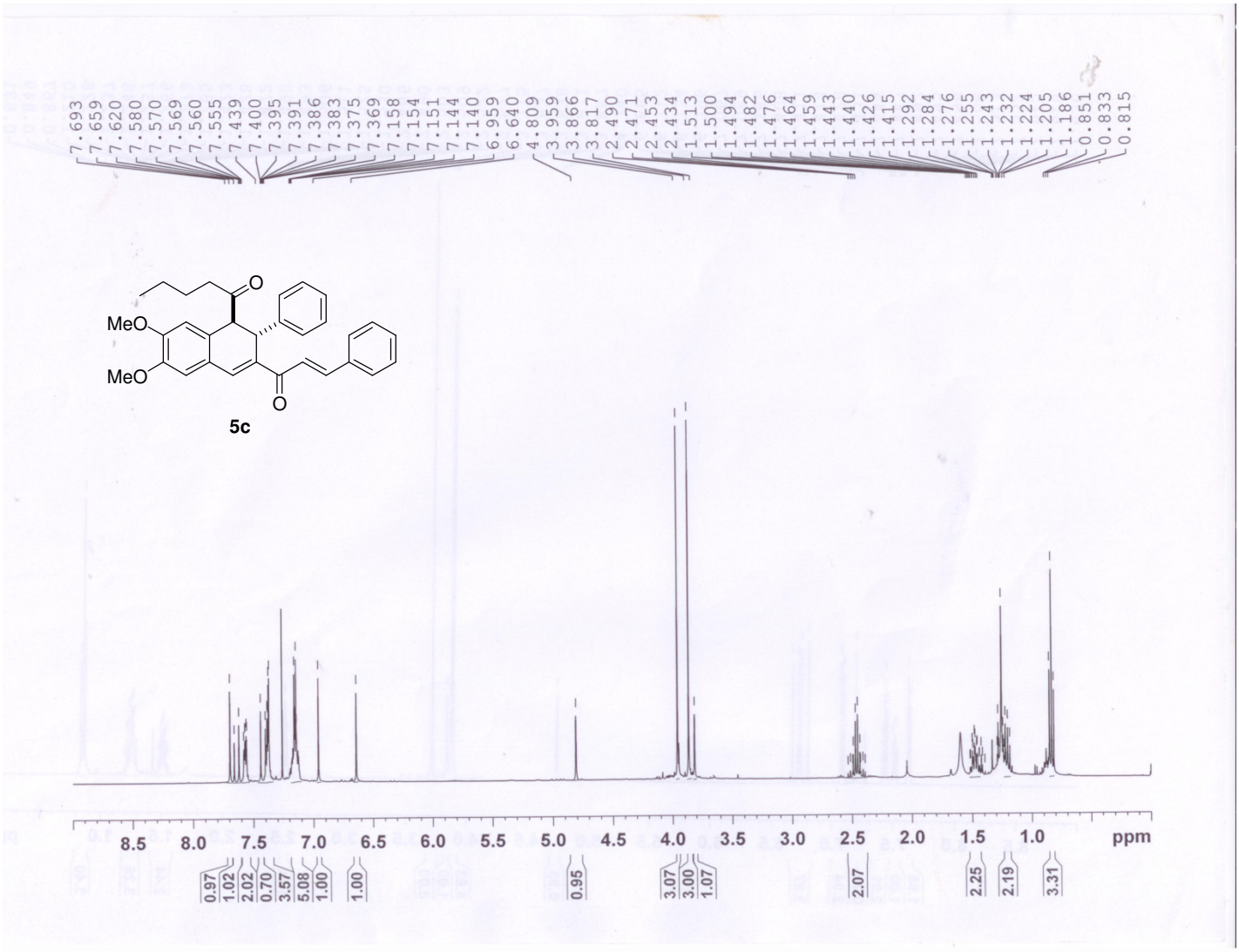
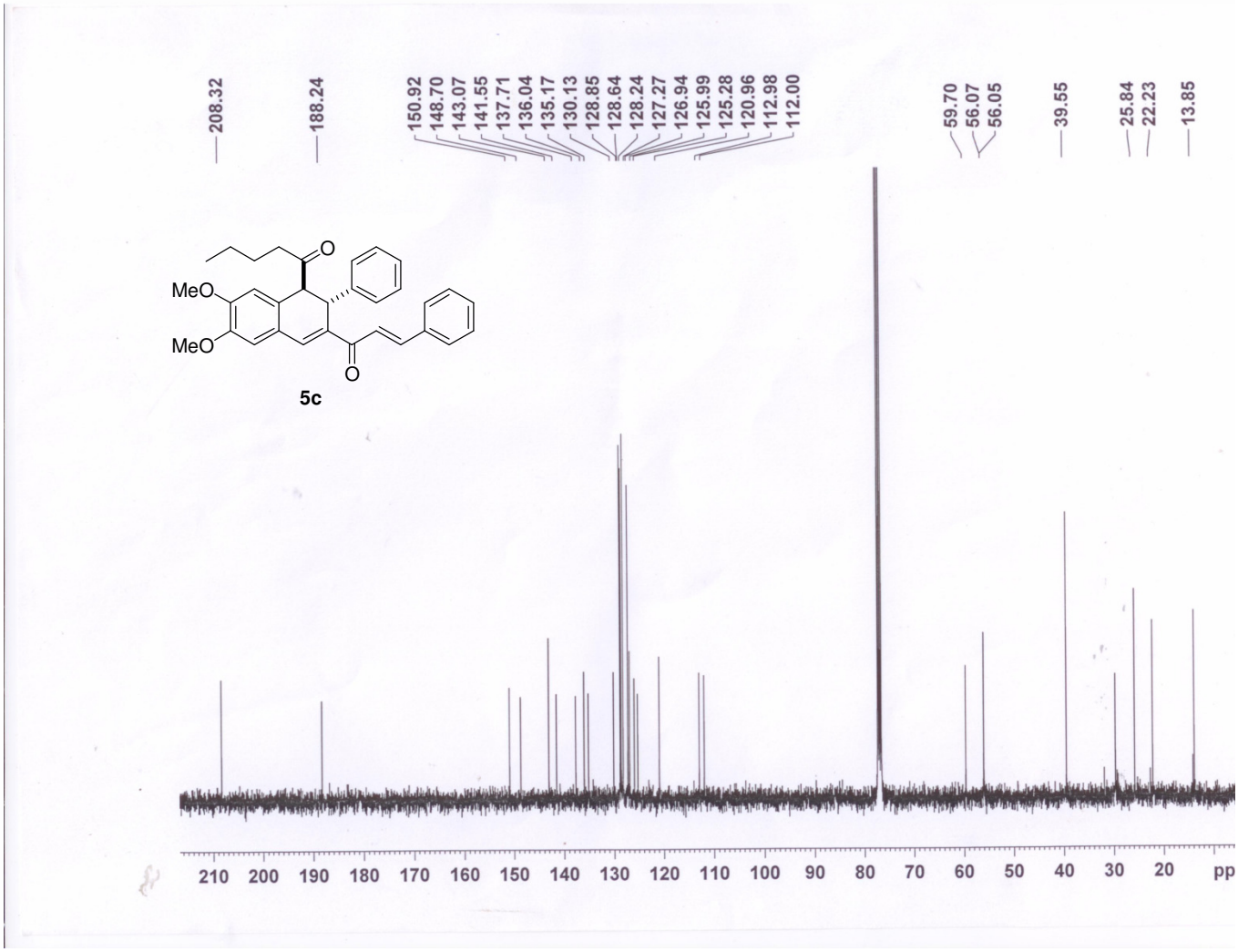
5b







Computation details and optimised geometries of transition states TS-1 and TS-2:

The Density Functional Theory (DFT) calculation was performed using the Gaussian 03 package. The level of approximation used was B3LYP with a basis set LanL2DZ in dichloroethane medium. The electronic energy of TS-1 is – 3026.85489823 a.u. and that of TS-2 is – 3026.79516153 a.u. This implies that **TS-1** is 37.4856 kcal mol^{-1} more stable than **TS-2**.

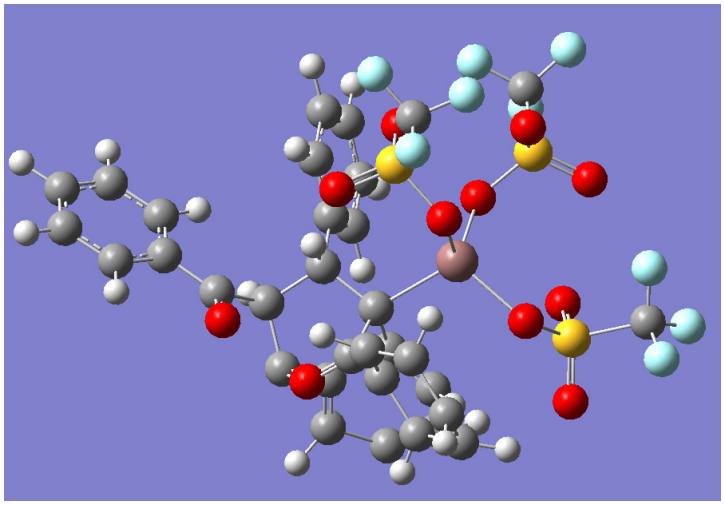


Figure 1. The optimised geometry of **TS-1**

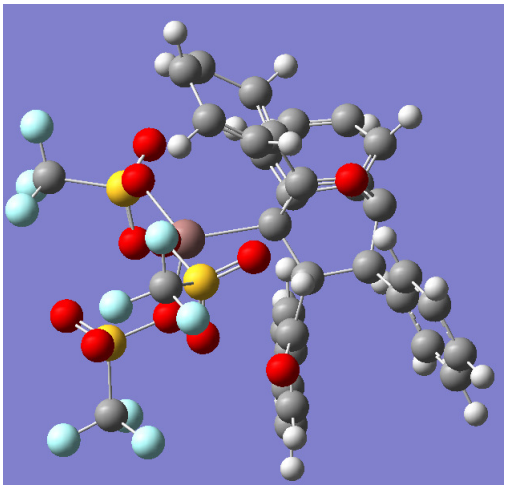


Figure 2. The optimised geometry of **TS-2**