

Electronic Supplementary Information
for
Iron(III) Chloride-Catalysed Direct Nucleophilic
 α -Substitution of Morita-Baylis-Hillman Alcohols
with Alcohols, Arenes, 1,3-Dicarbonyl Compounds,
and Thiols

Xiaoxiang Zhang, Weidong Rao, Sally, and Philip Wai Hong Chan*

Division of Chemistry and Biological Chemistry, School of Physical
and Mathematical Sciences, Nanyang Technological University,
Singapore 637616, Singapore

E-mail: waihong@ntu.edu.sg

Figure S1. ^1H and ^{13}C NMR Spectra of 2-((6-Oxocyclohex-1-enyl)(phenyl)methyl)-1,3-diphenylpropane-1,3-dione (**3a**)

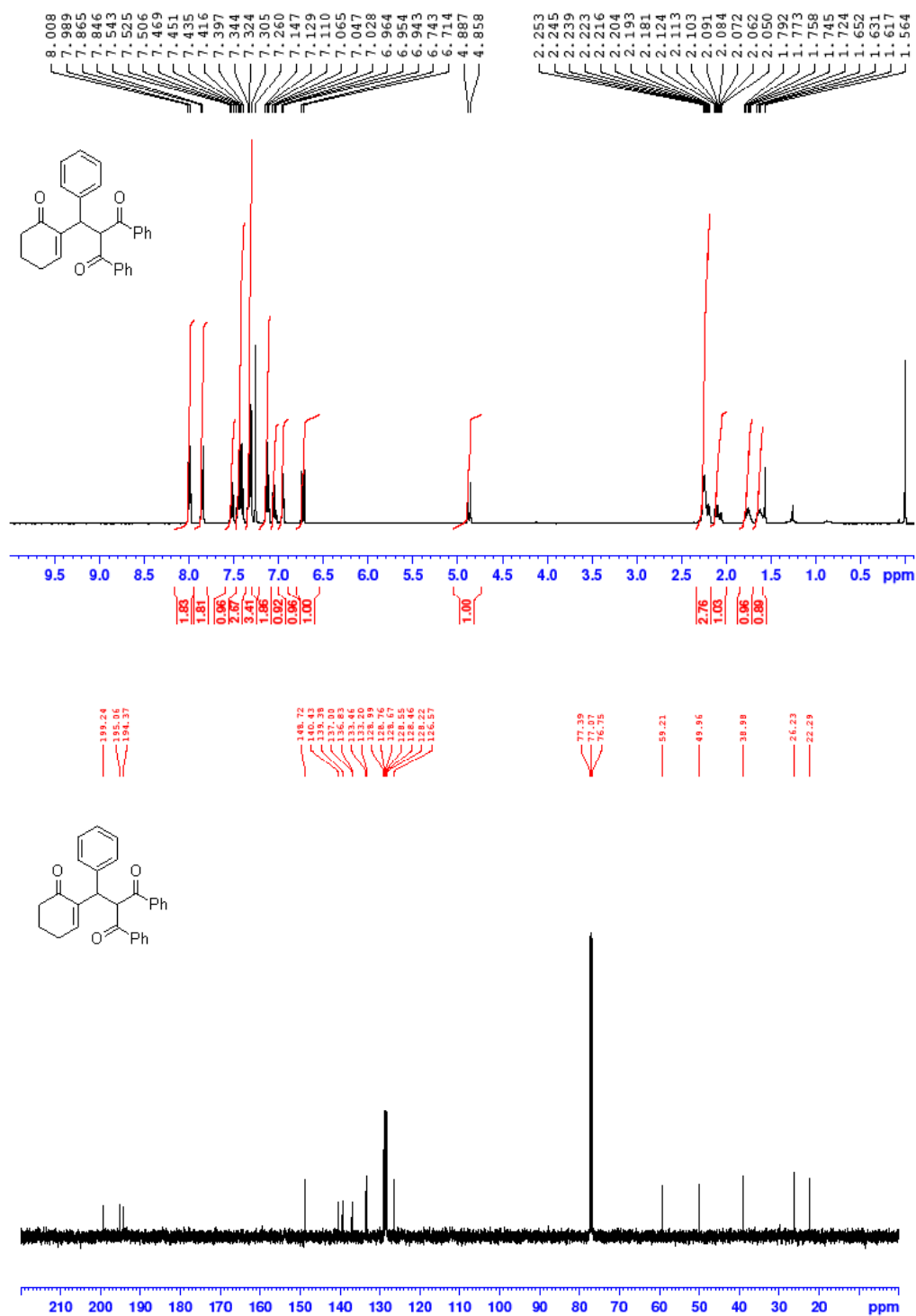


Figure S2. ^1H and ^{13}C NMR Spectra of 3-((6-Oxocyclohex-1-enyl)(phenyl)methyl)pentane-2,4-dione (**3b**)

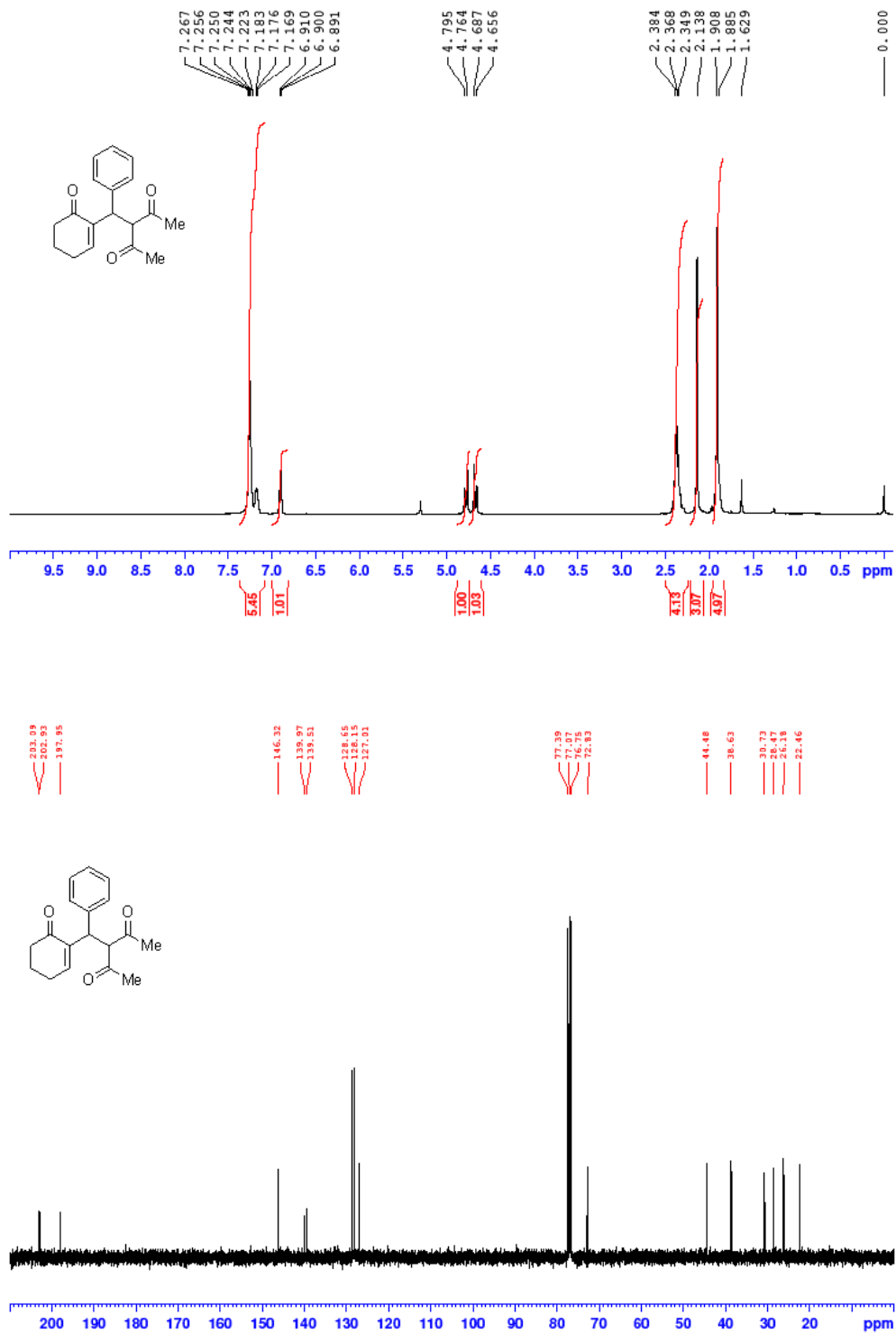


Figure S3. ^1H and ^{13}C NMR Spectra of 2-((6-Oxocyclohex-1-enyl)(phenyl)methyl)-1-phenylbutane-1,3-dione (**3c**)

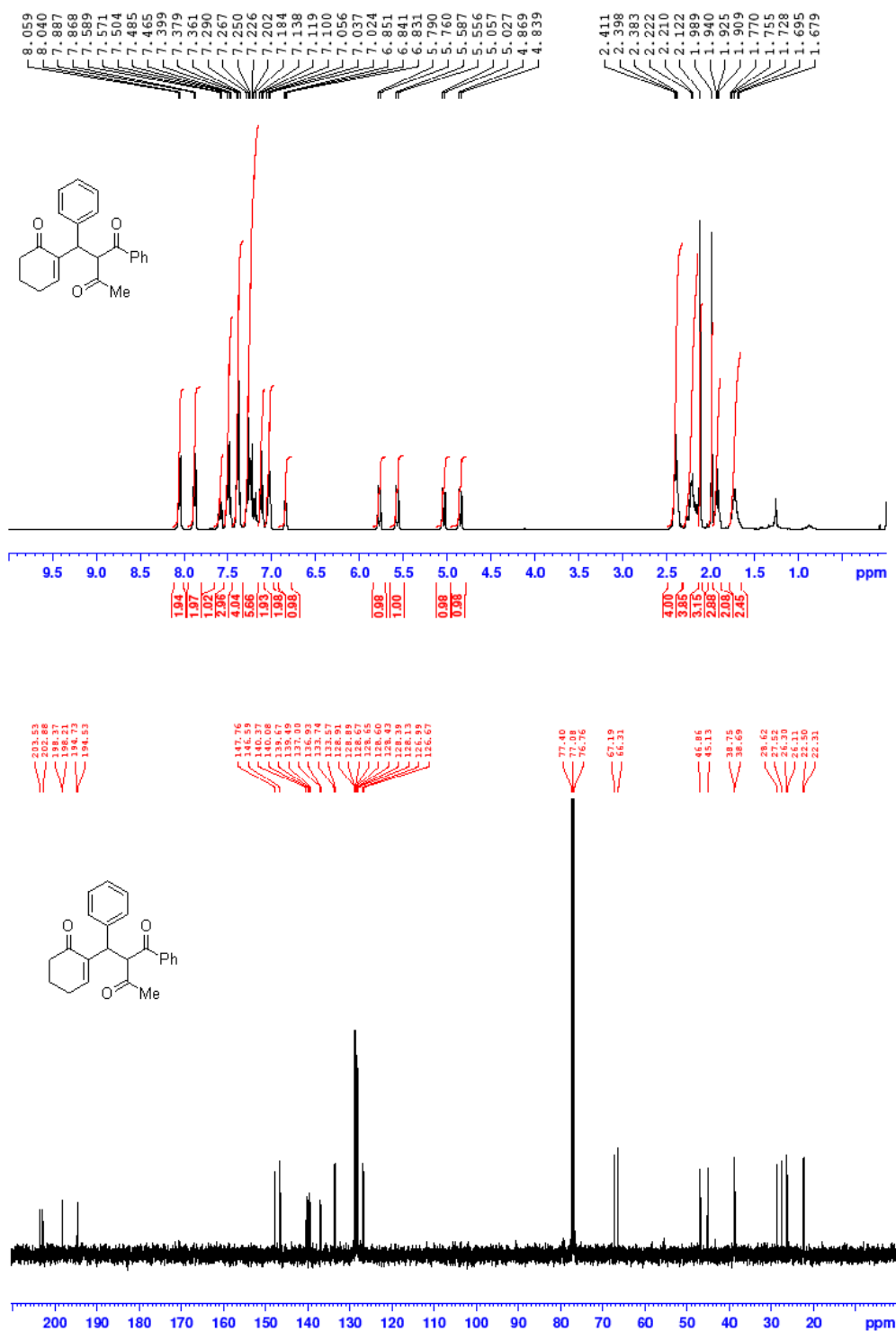


Figure S4. ^1H and ^{13}C NMR Spectra of Ethyl 2-benzoyl-3-(6-oxocyclohex-1-enyl)-3-phenylpropanoate (**3d'**) (major diastereomer)

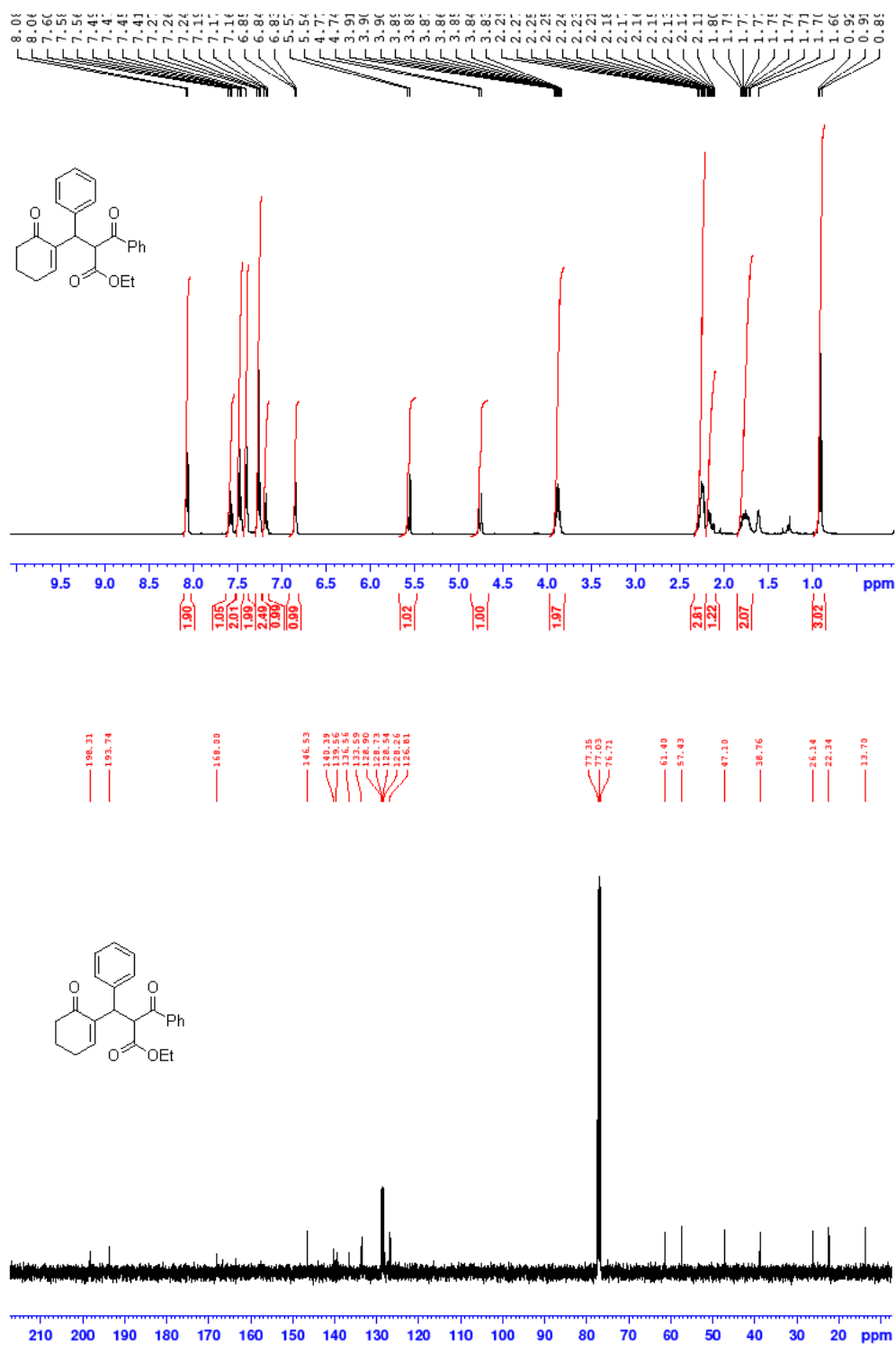


Figure S5. ^1H and ^{13}C NMR Spectra of Ethyl 2-benzoyl-3-(6-oxocyclohex-1-enyl)-3-phenylpropanoate (**3d''**) (minor diastereomer)

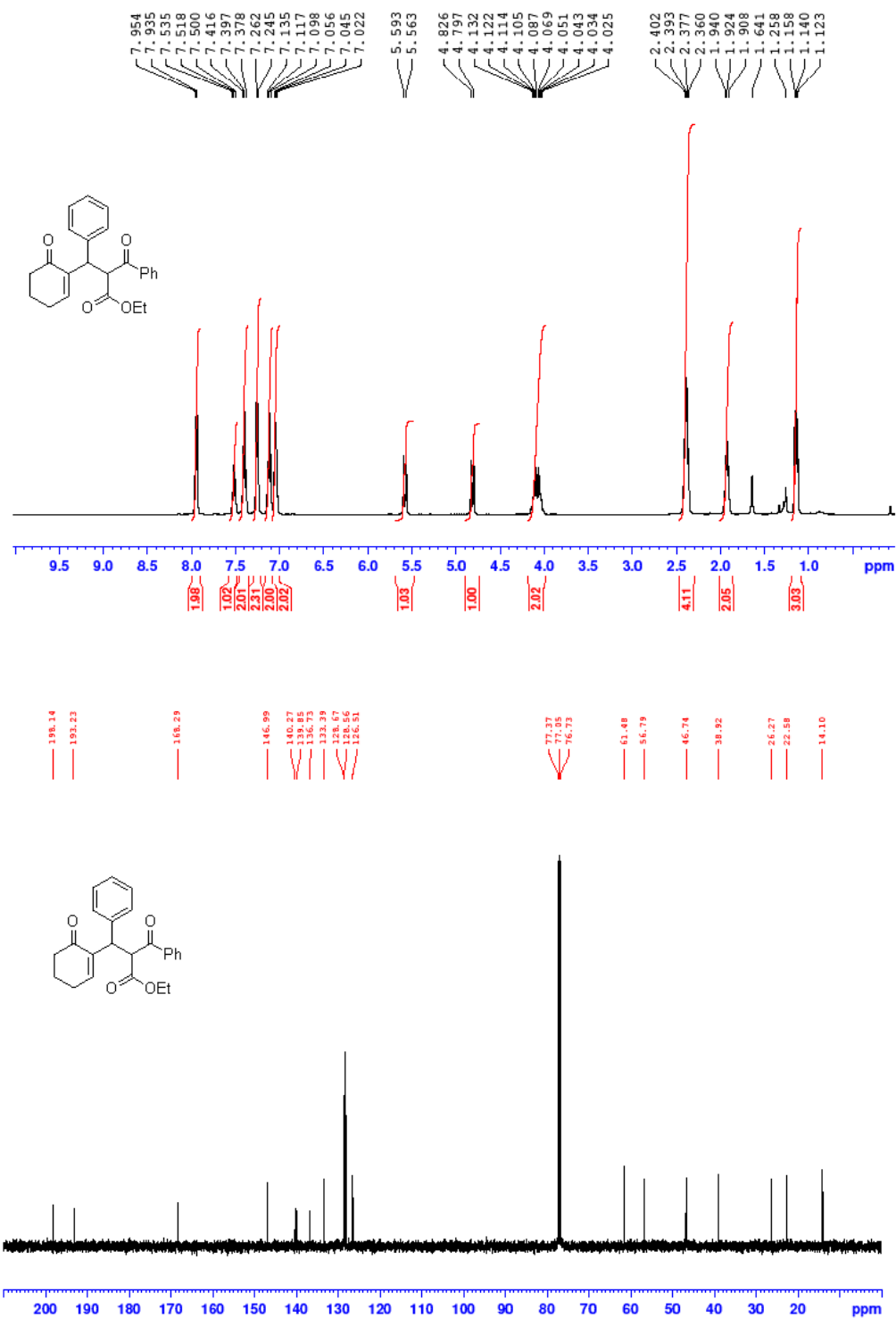


Figure S6. ^1H and ^{13}C NMR Spectra of 2-((4-Nitrophenyl)(6-oxocyclohex-1-enyl)methyl)-1,3-diphenylpropane-1,3-dione (**3e**)

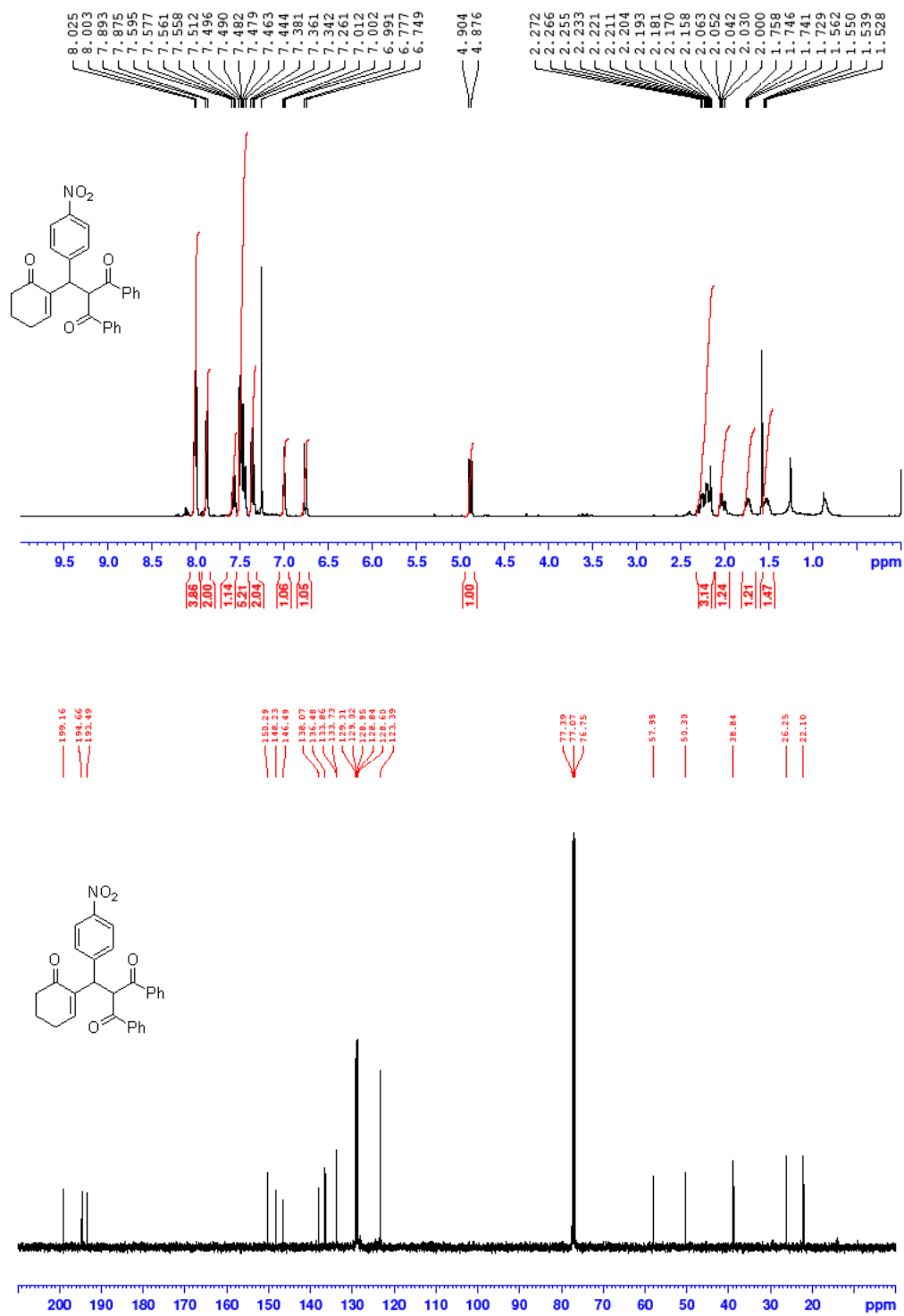


Figure S7. ^1H and ^{13}C NMR Spectra of 2-((4-Fluorophenyl)(6-oxocyclohex-1-enyl)methyl)-1,3-diphenylpropane-1,3-dione (**3f**)

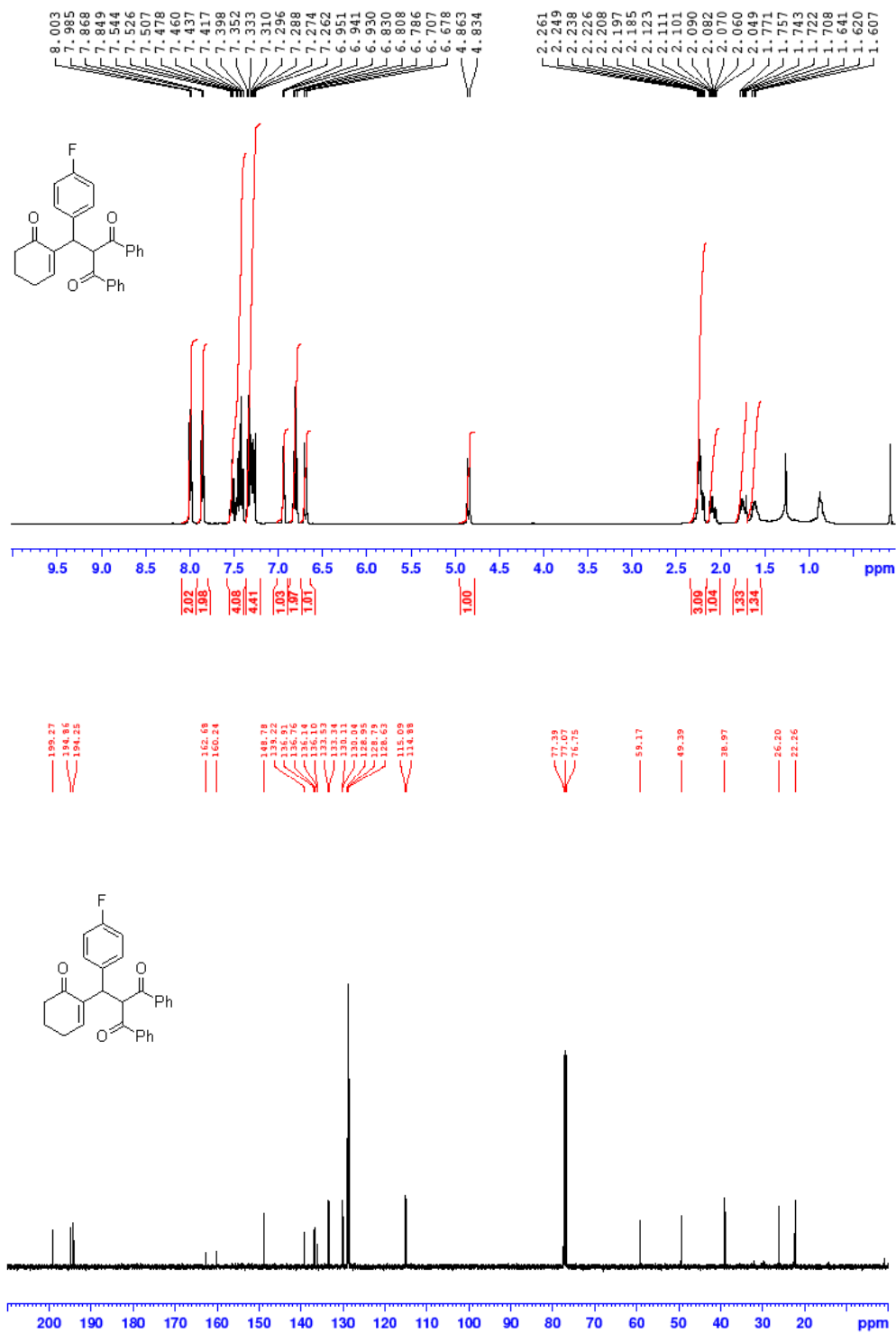


Figure S8. ^1H and ^{13}C NMR Spectra of 2-((4-Chlorophenyl)(6-oxocyclohex-1-enyl)methyl)-1,3-diphenylpropane-1,3-dione (**3g**)

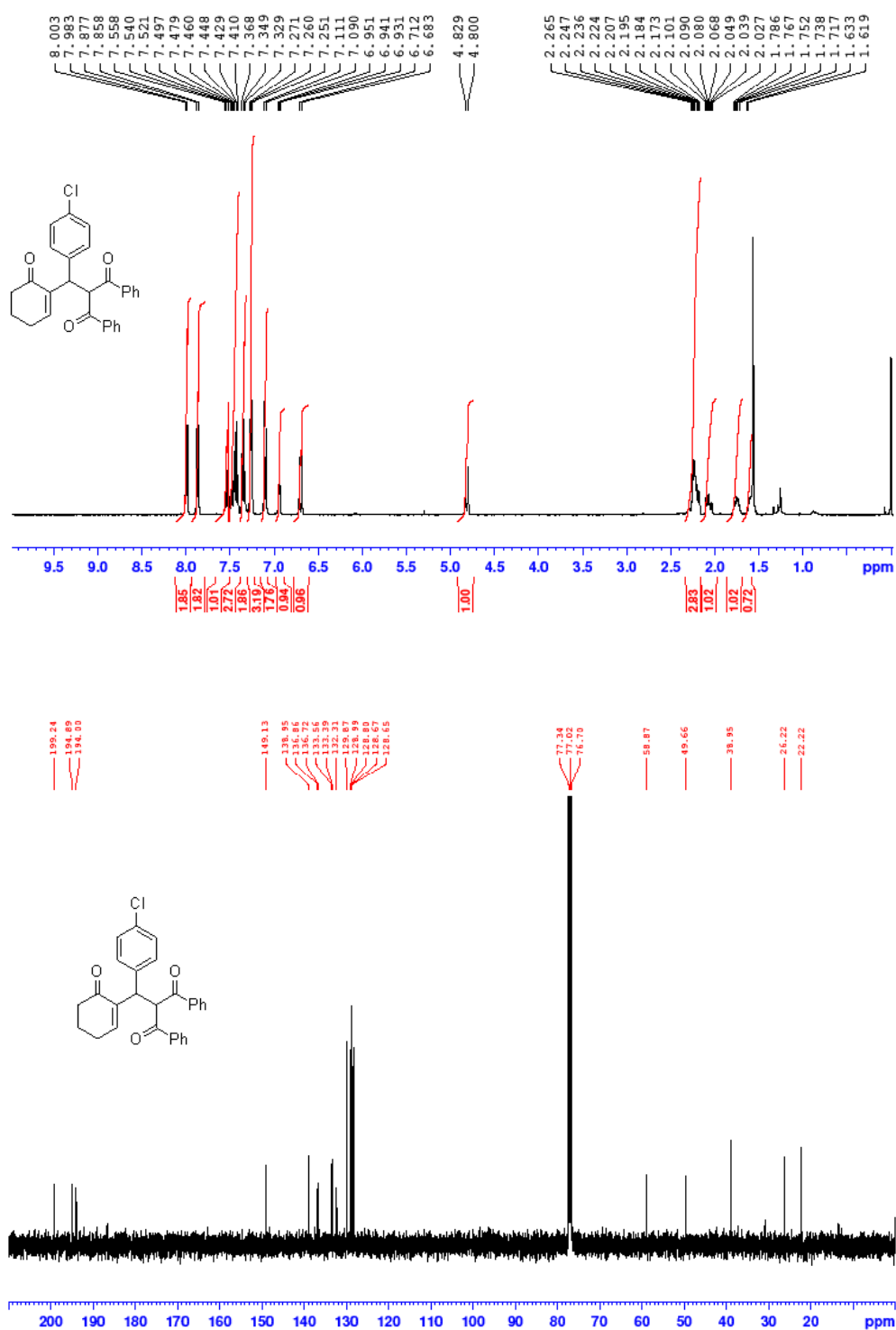


Figure S9. ^1H and ^{13}C NMR Spectra of 2-((4-Bromophenyl)(6-oxocyclohex-1-enyl)methyl)-1,3-diphenylpropane-1,3-dione (**3h**)

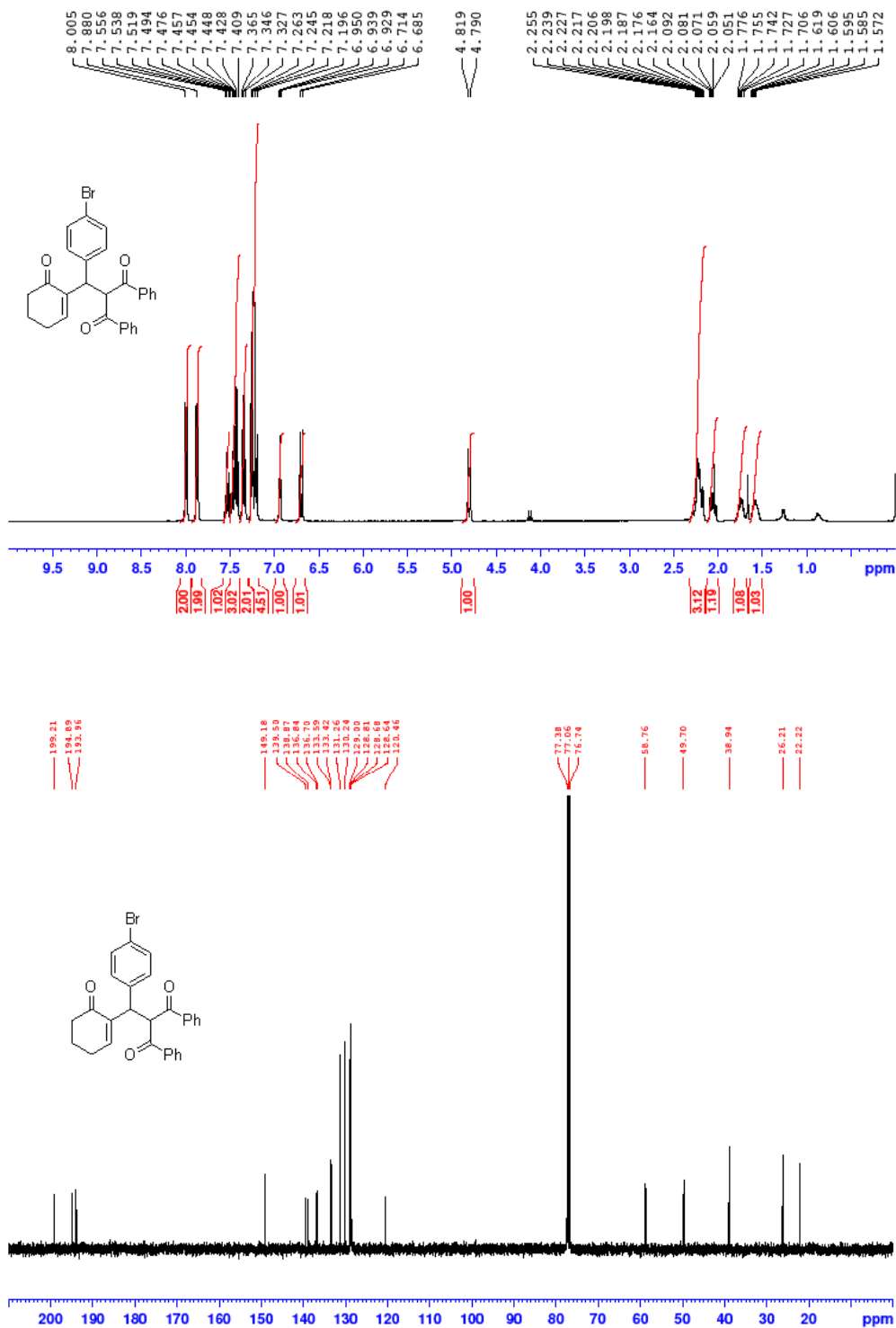


Figure S10. ^1H and ^{13}C NMR Spectra of 2-((6-Oxocyclohex-1-enyl)(*p*-tolyl)methyl)-1,3-diphenylpropane-1,3-dione (**3i**)

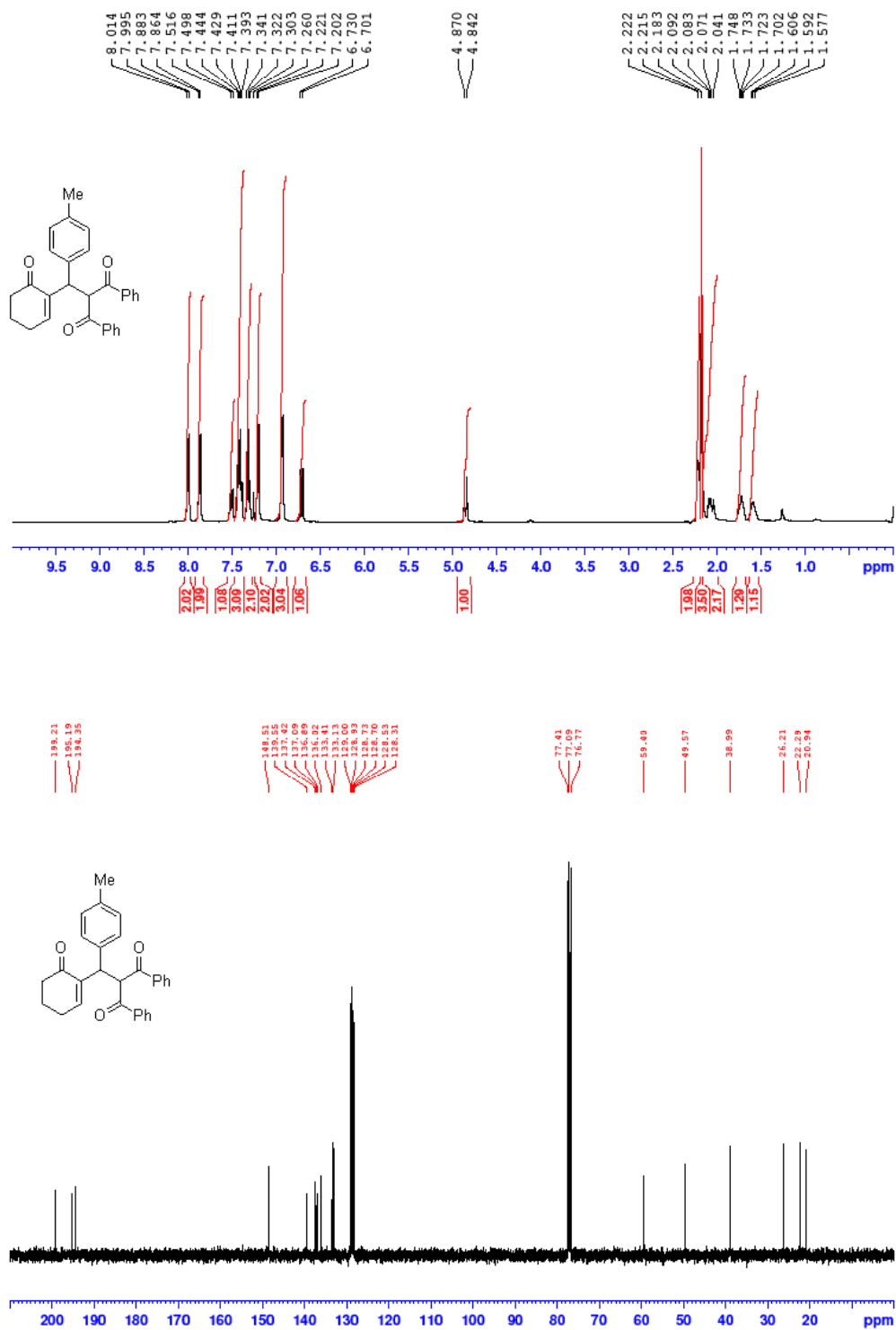


Figure 11. ^1H and ^{13}C NMR Spectra of 2-((4-Ethoxyphenyl)(6-oxocyclohex-1-enyl)methyl)-1,3-diphenylpropane-1,3-dione (**3j**)

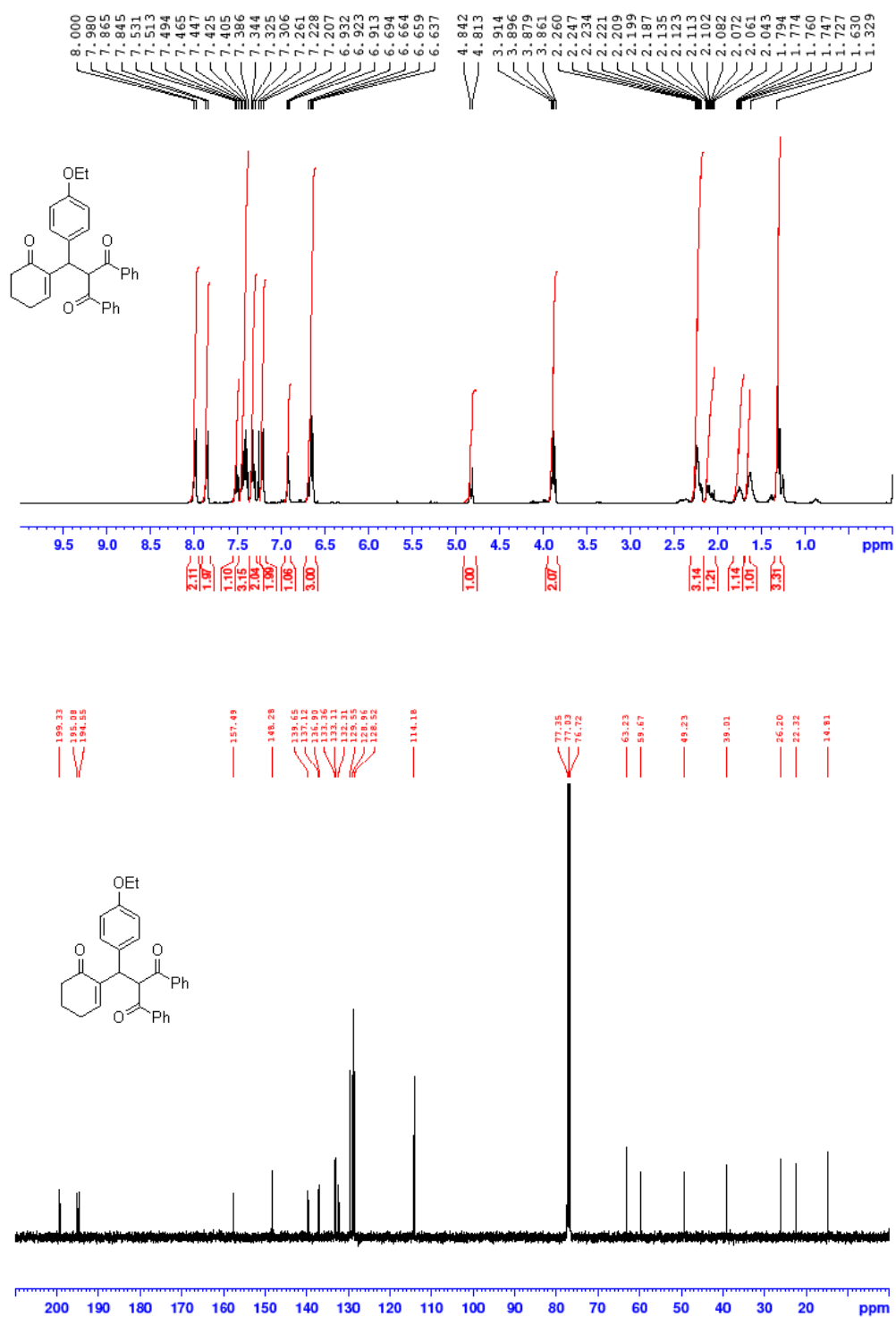


Figure S12. ^1H and ^{13}C NMR Spectra of 2-((2-Chlorophenyl)(6-oxocyclohex-1-enyl)methyl)-1,3-diphenylpropane-1,3-dione (**3I**)

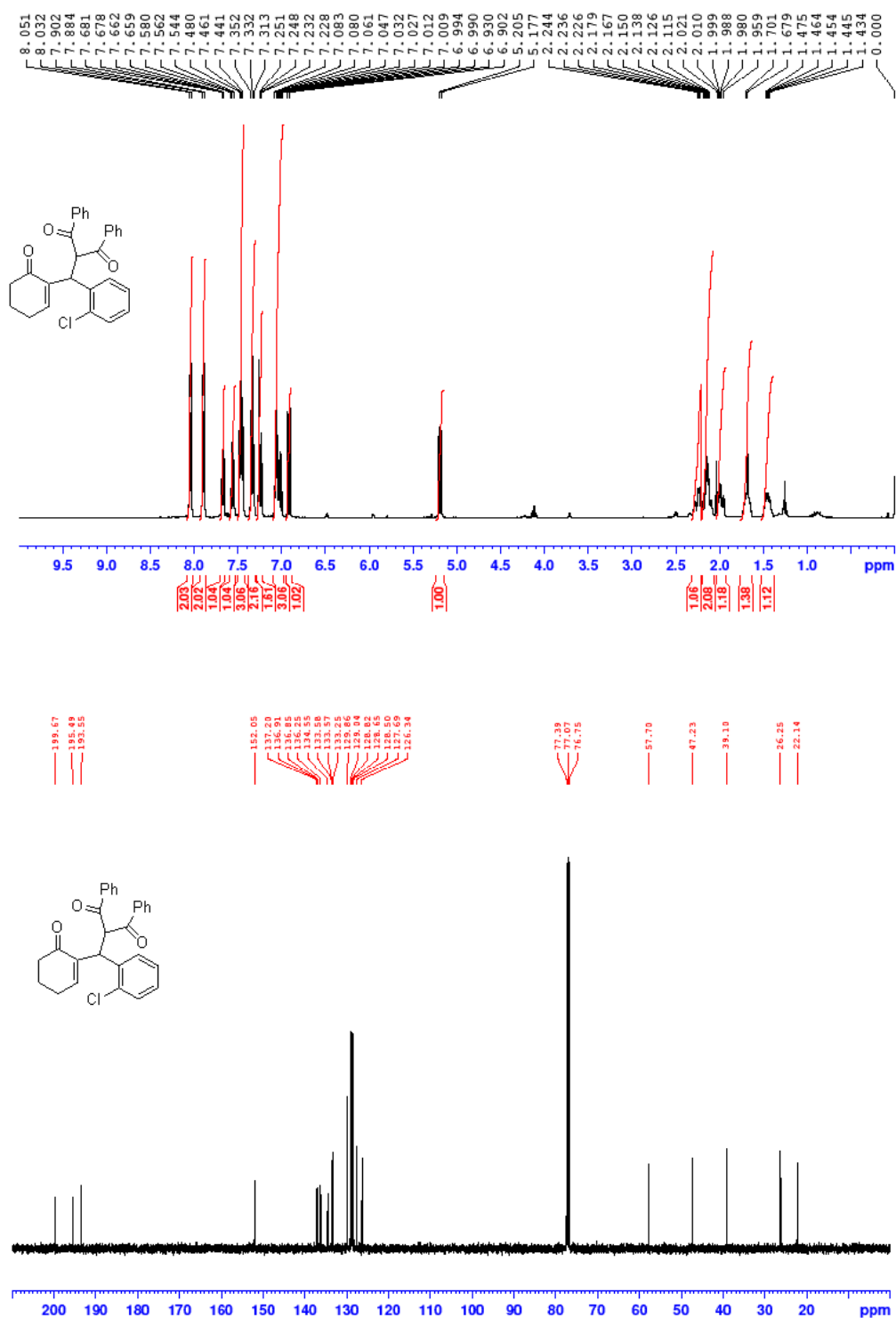


Figure S13. ^1H and ^{13}C NMR Spectra of 2-((4-Chlorophenyl)(5-oxocyclopent-1-enyl)methyl)-1,3-diphenylpropane-1,3-dione (**3m**)

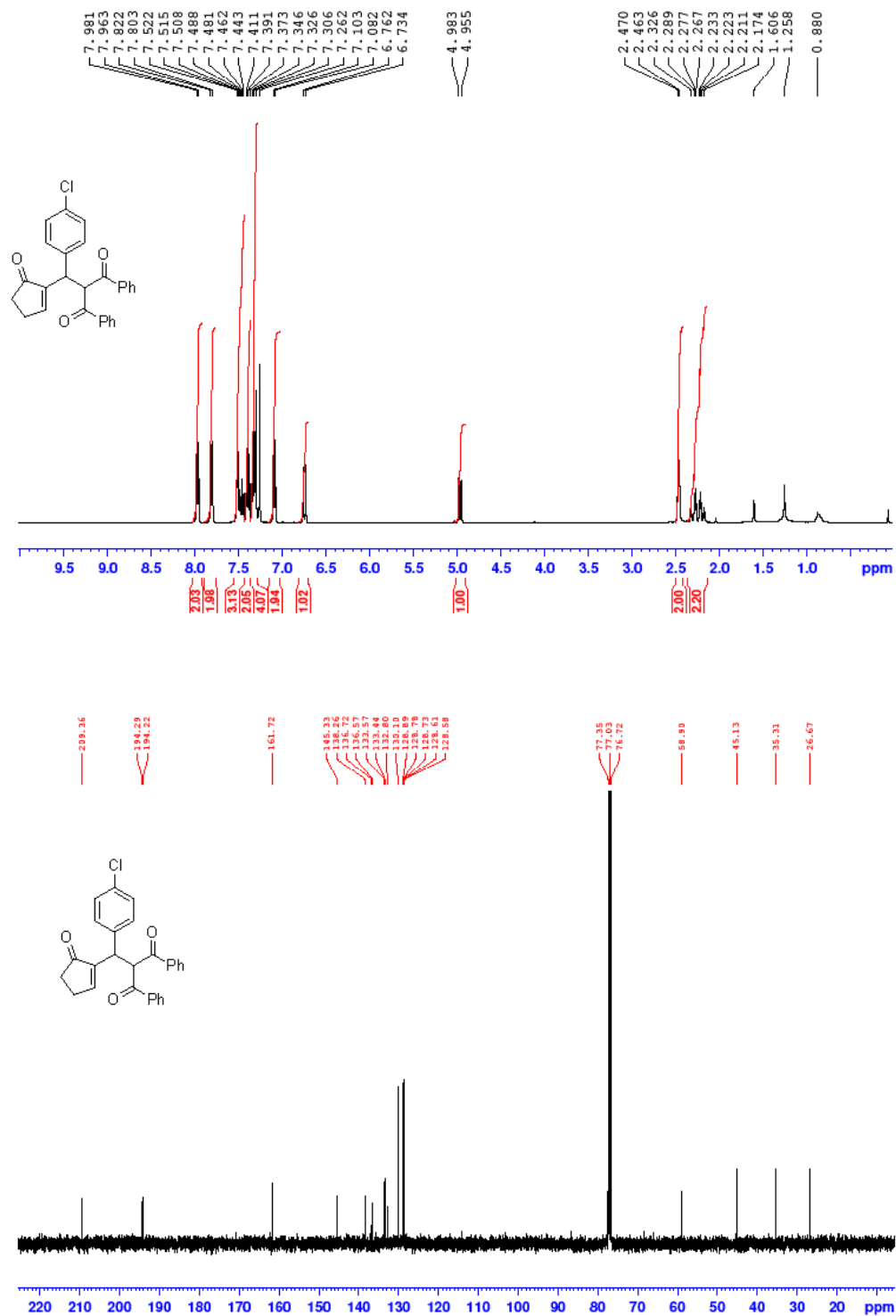


Figure S14. ^1H and ^{13}C NMR Spectra of 2-((4-Chlorophenyl)(4-oxo-4H-chromen-3-yl)methyl)-1,3-diphenylpropane-1,3-dione (**3n**)

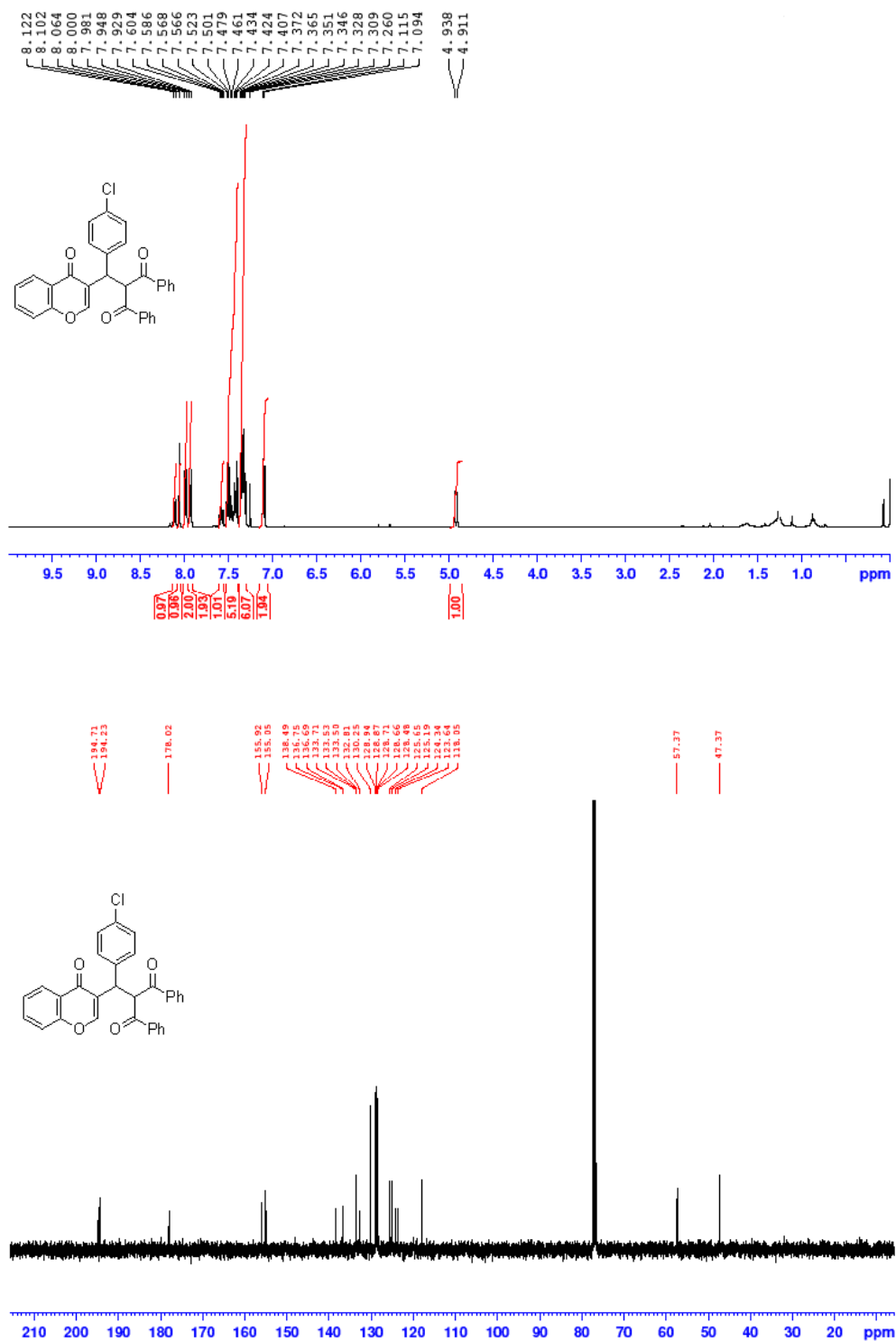


Figure S15. ^1H and ^{13}C NMR Spectra of 2-((4-hydroxy-3-methylphenyl)(phenyl)

methyl)cyclohex-2-enone (**30**)

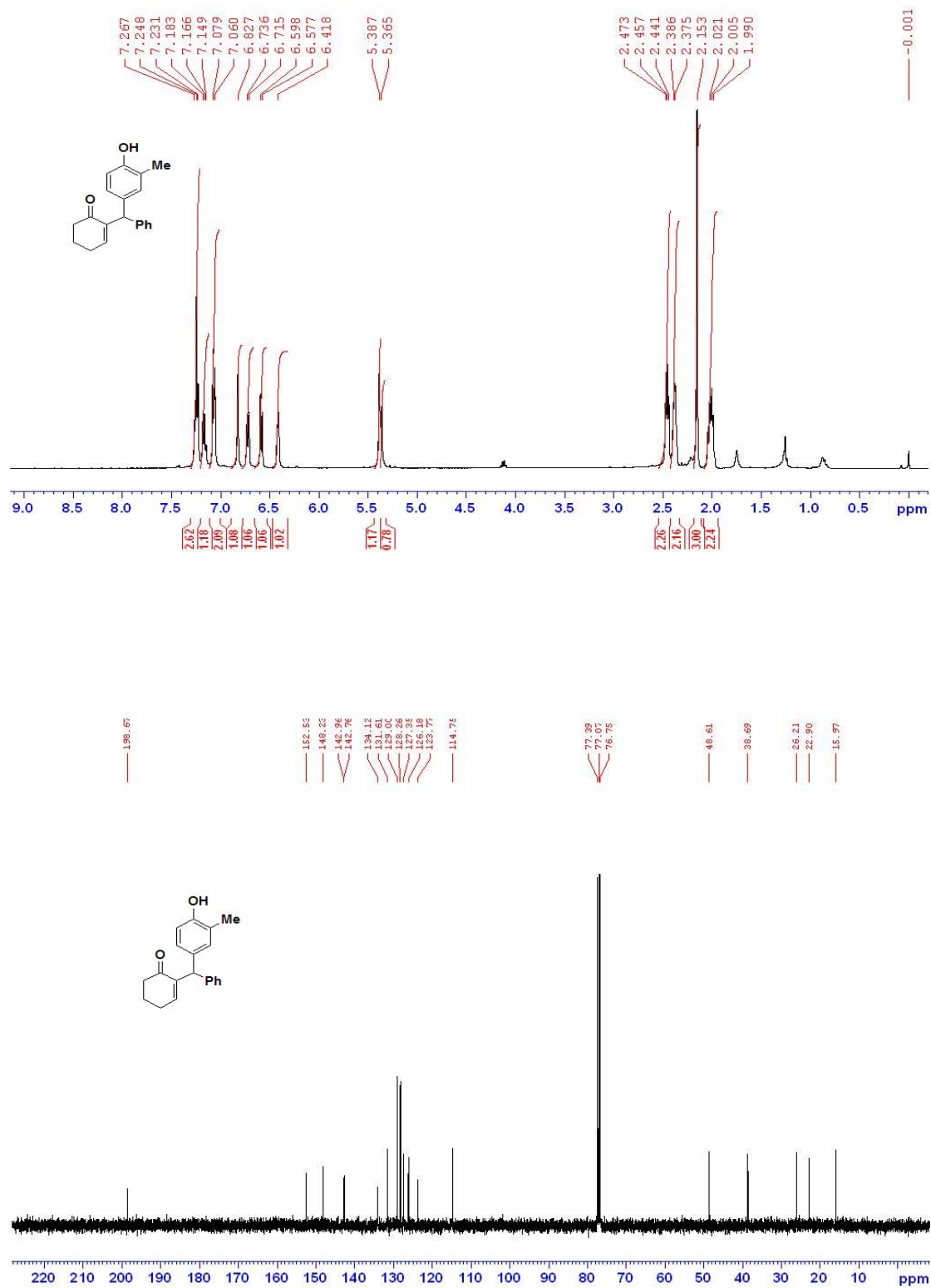


Figure S16. ^1H and ^{13}C NMR Spectra of 2-({4-Hydroxy-3,5-dimethylphenyl}(phenyl)methyl)cyclohex-2-enone (**3p**)

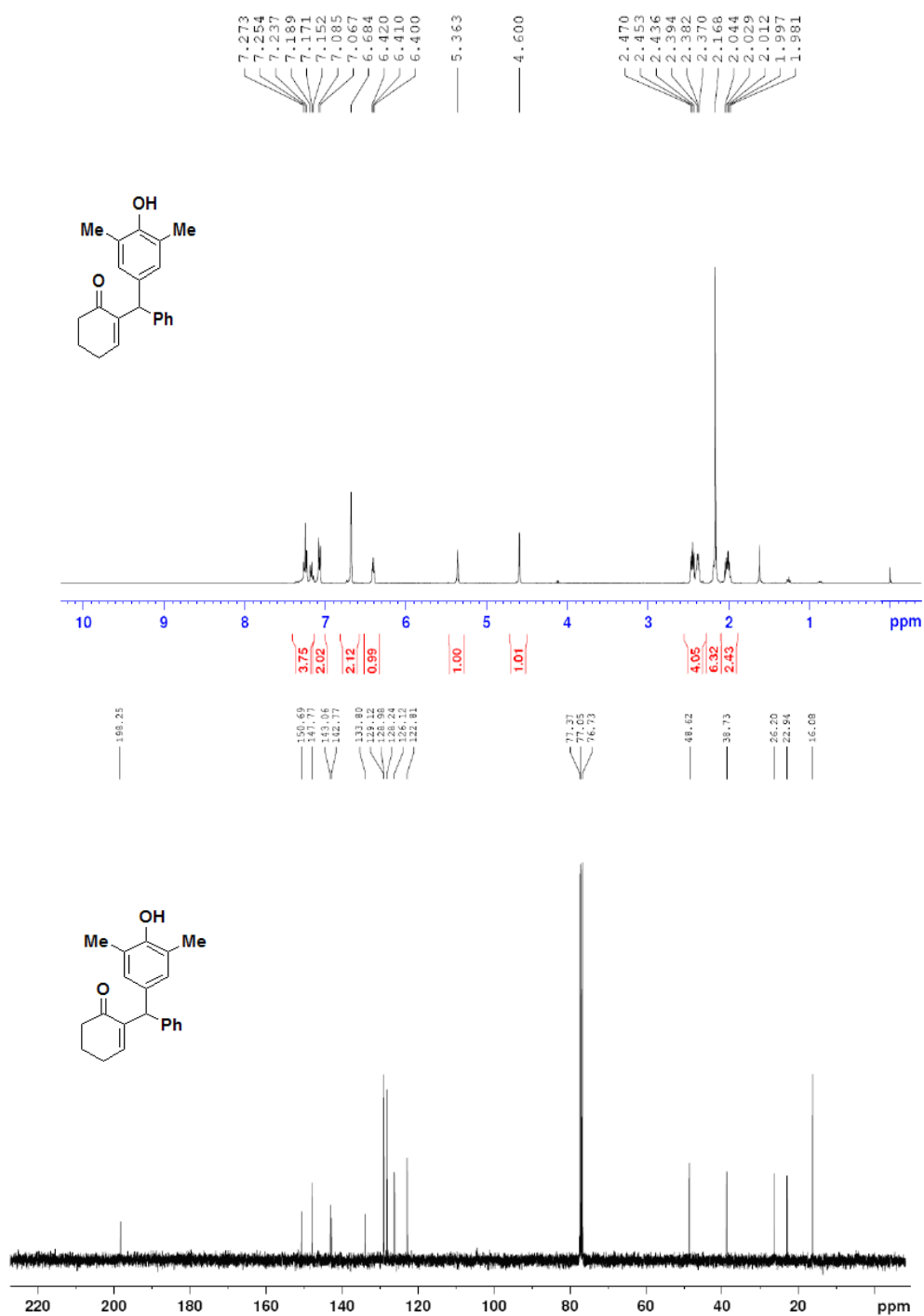


Figure S17. ^1H and ^{13}C NMR Spectra of 2-(Ethoxy(phenyl)methyl)cyclohex-2-enone

(3q)

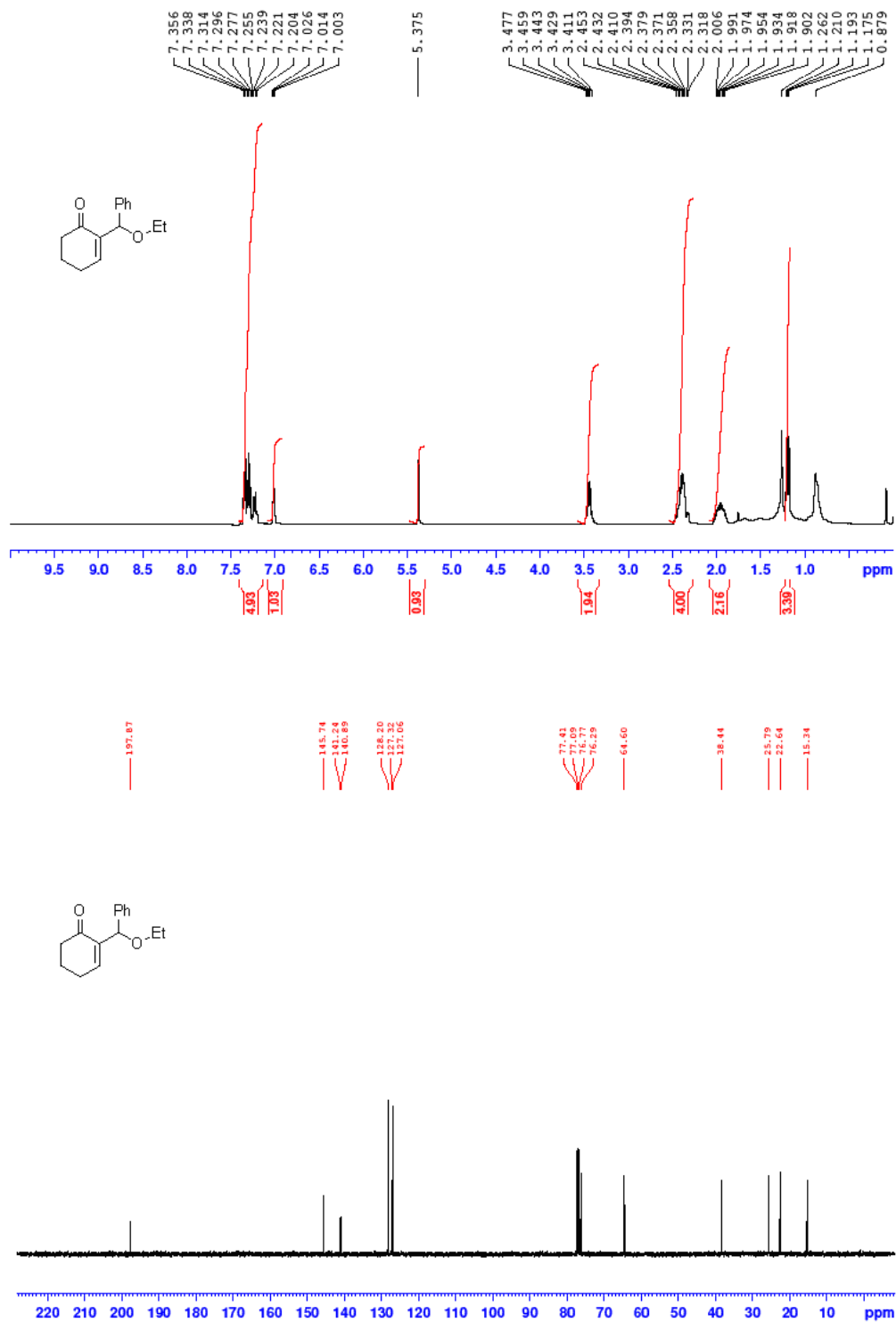


Figure S18. ^1H and ^{13}C NMR Spectra of 2-(Benzyloxy(phenyl)methyl)cyclohex-2-enone (**3r**)

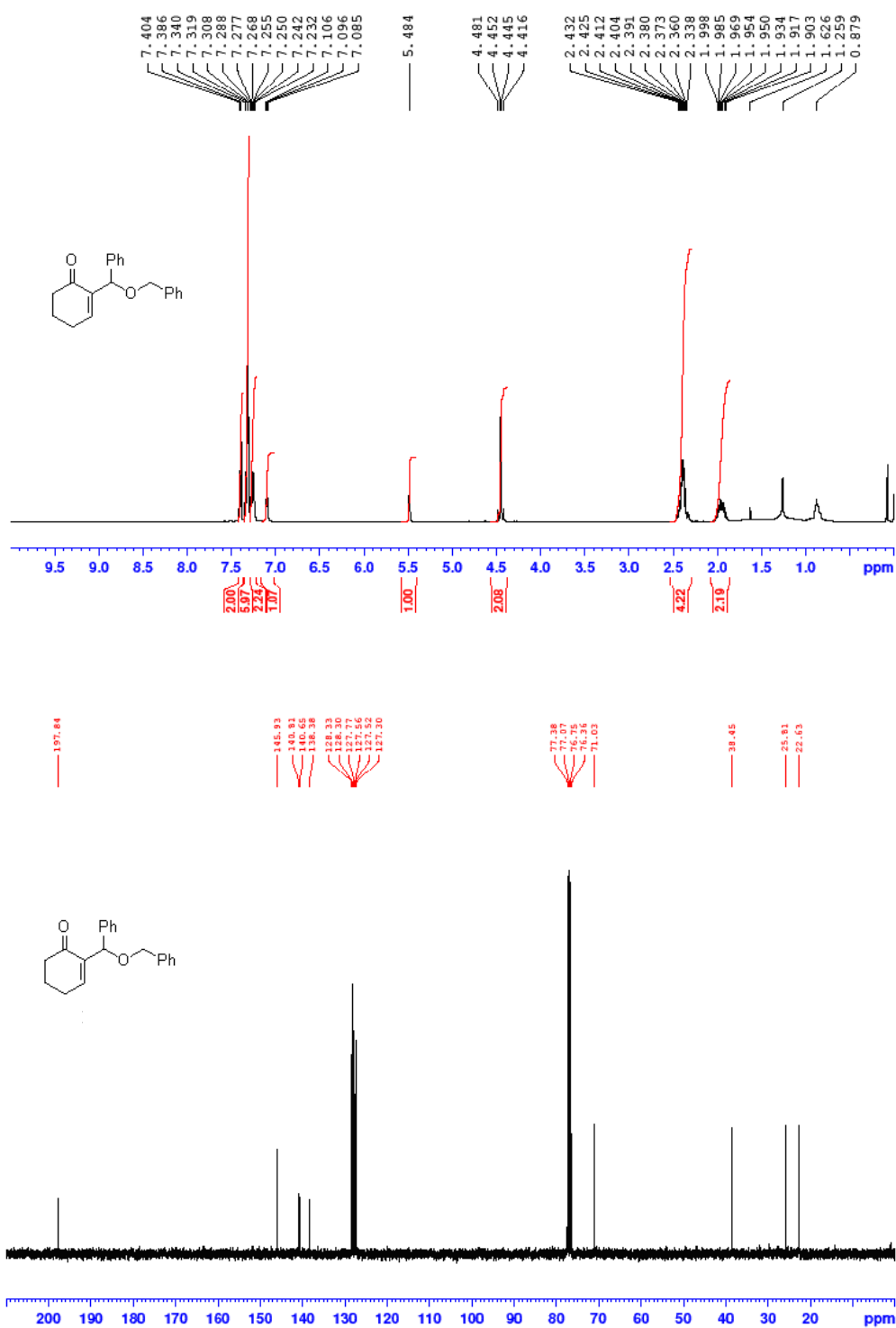


Figure 19. ^1H and ^{13}C NMR Spectra of 2-((But-3-enyloxy)(phenyl)methyl)cyclohex-2-enone (**3s**)

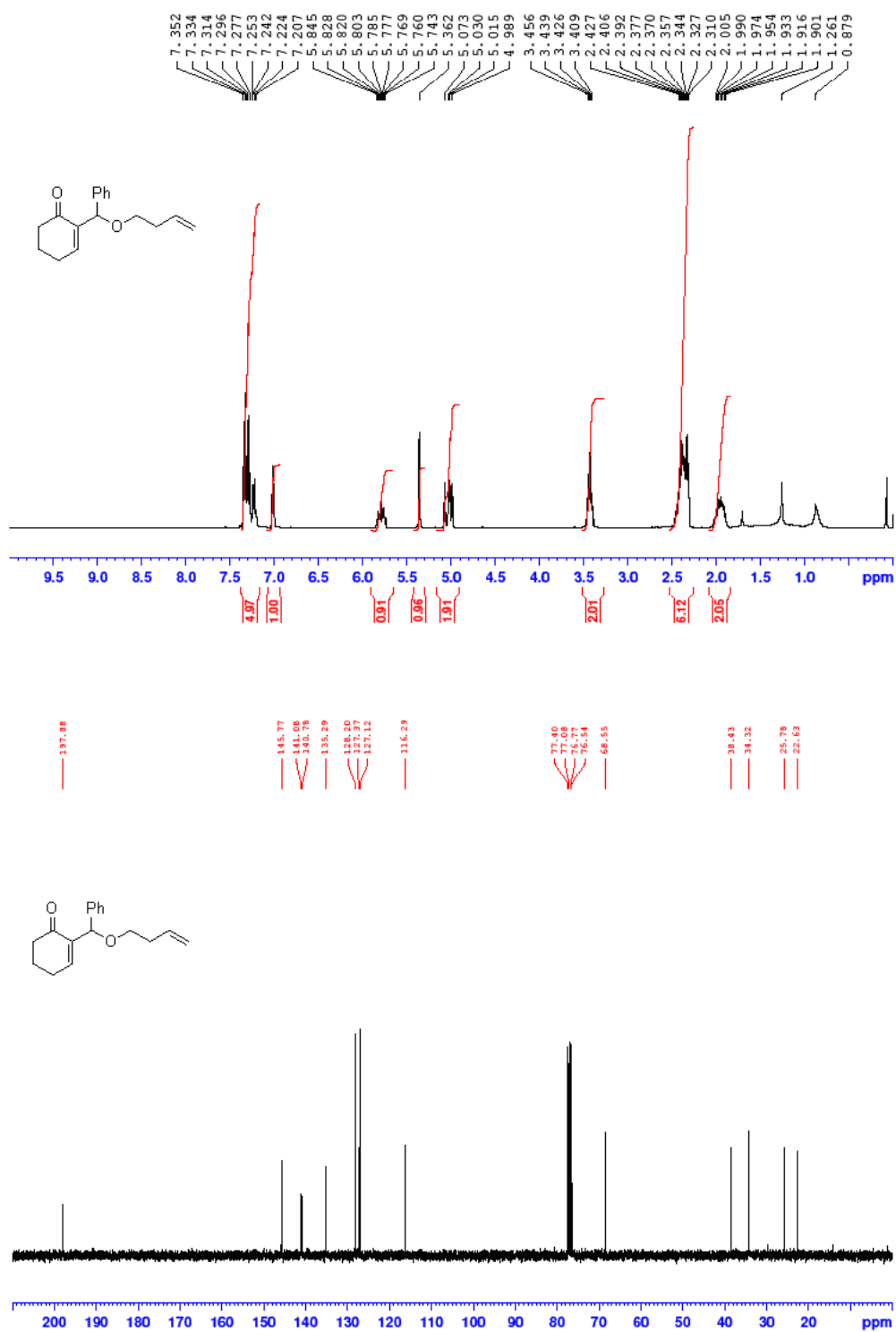


Figure S20. ^1H and ^{13}C NMR Spectra of 2-(Ethylthio(phenyl) methyl)cyclohex-2-enone (**3t**)

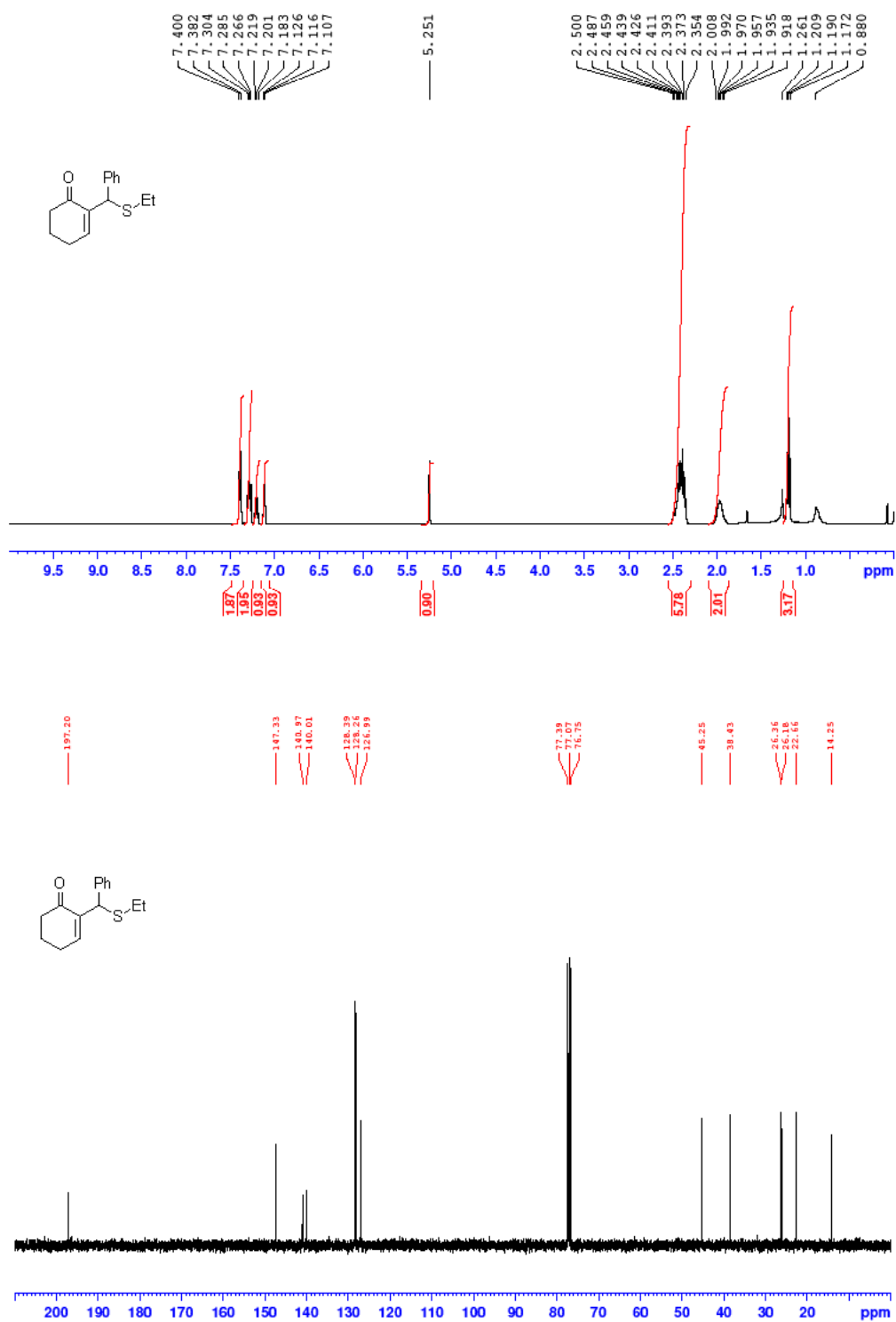


Figure S21. ^1H and ^{13}C NMR Spectra of 2-((4-Chlorophenylthio)(phenyl)methyl)cyclohex-2-enone (**3u**)

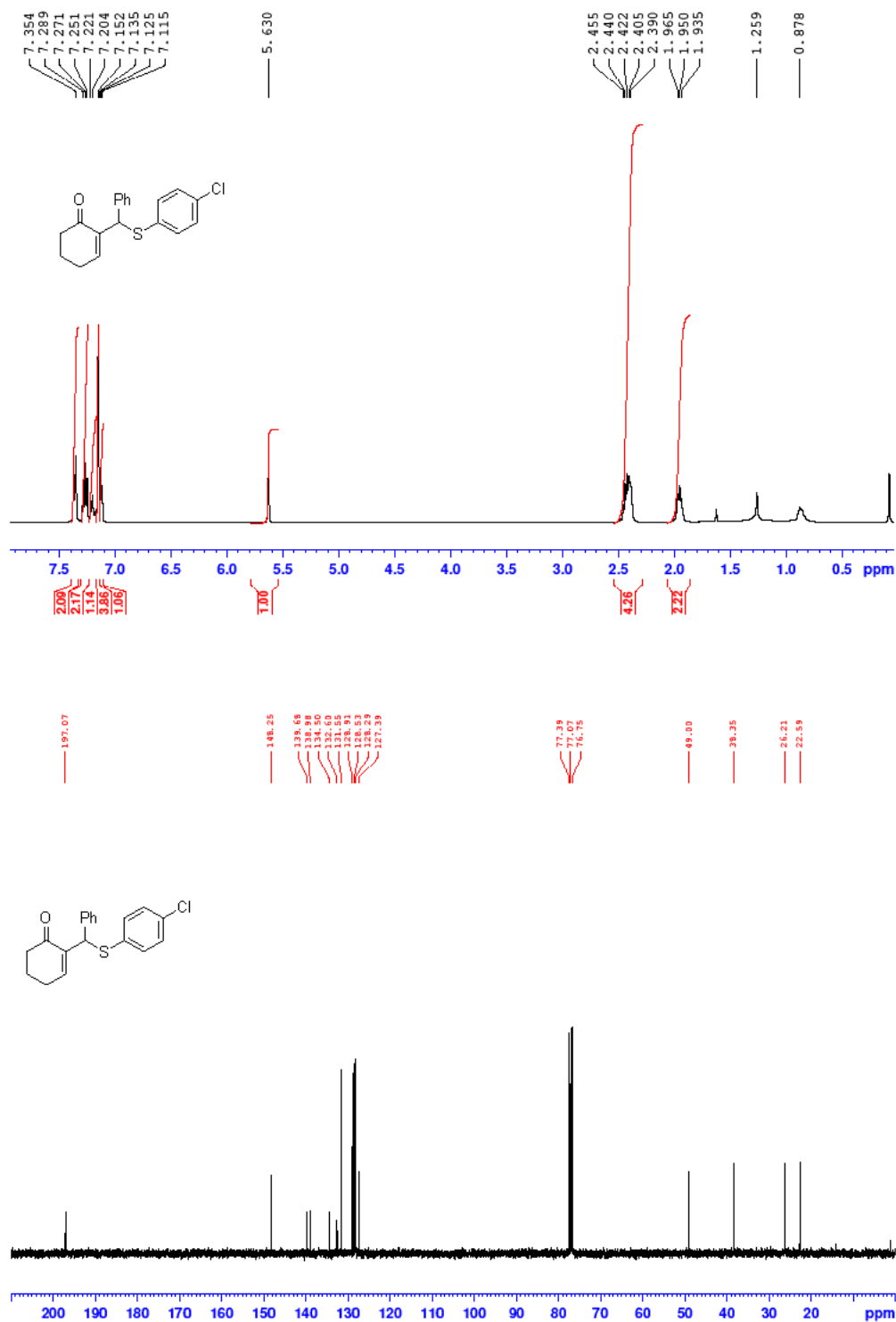


Figure S22. ^1H and ^{13}C NMR Spectra of 2-(Phenyl(*p*-tolylthio)methyl)cyclohex-2-enone (**3v**)

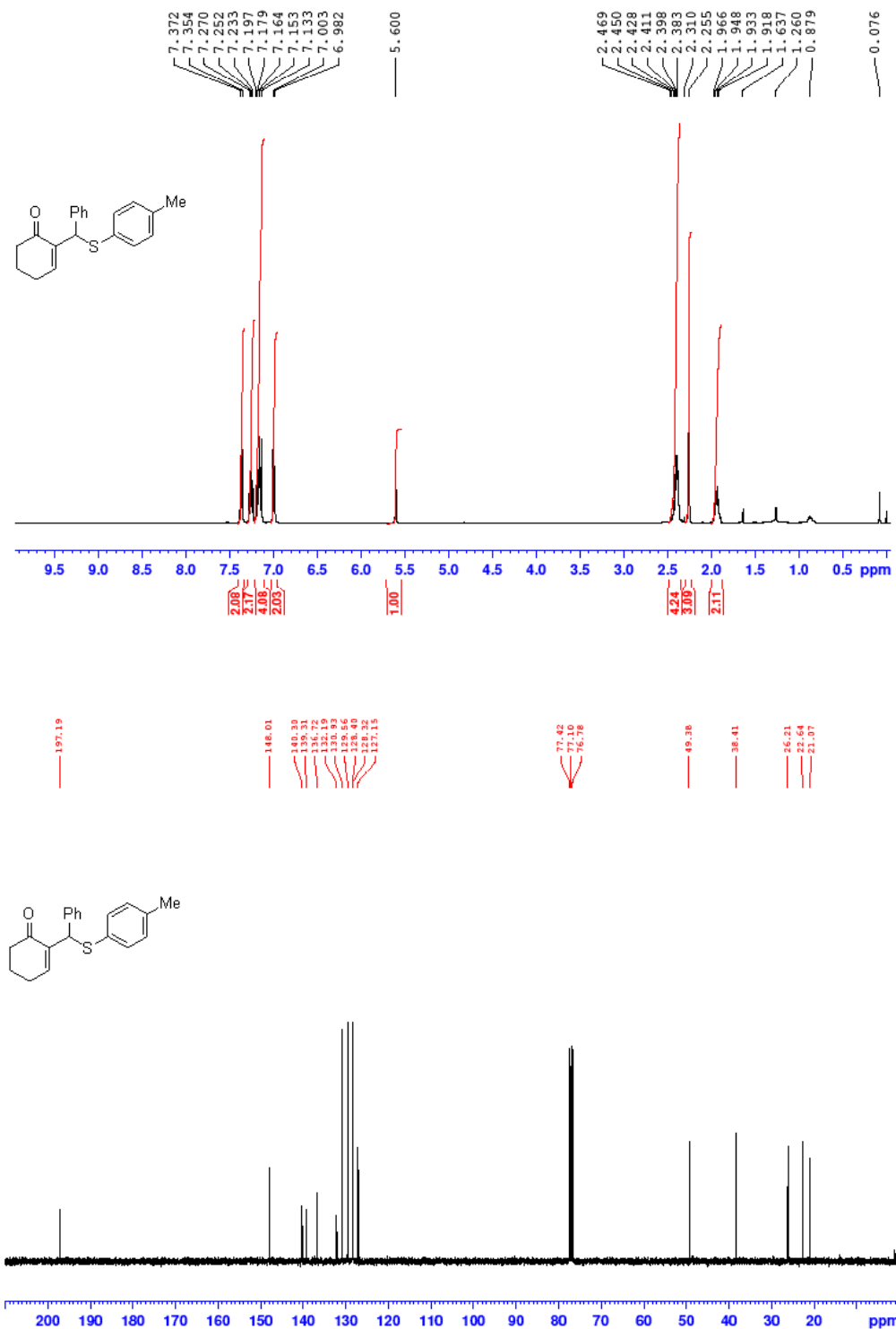


Figure S23. HPLC Spectrum of Racemic **1a**^{S1,S2}

Chiralcel OJ-H Column, *n*-hexane/*i*-PrOH = 90/10, flow rate 1 mL/min, λ = 254 nm.

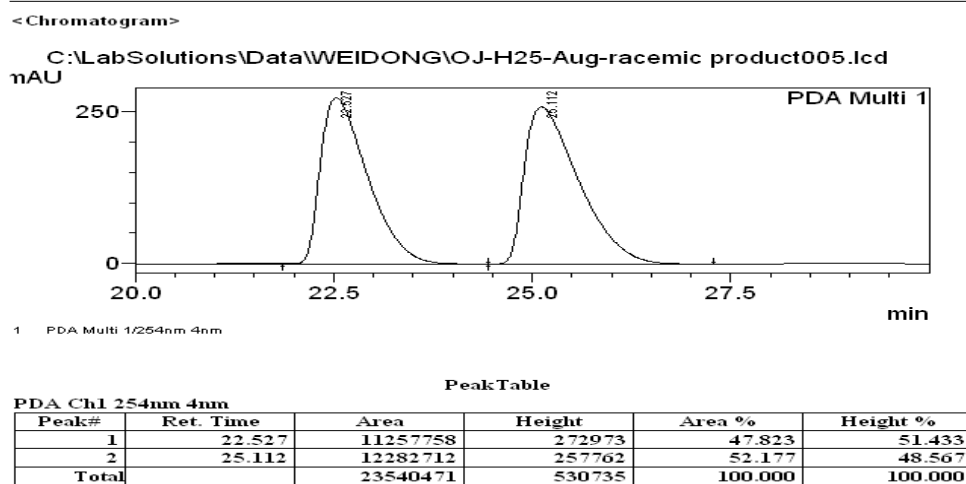


Figure S24. HPLC Spectrum of Chiral **1a**^{S1,S2}

Chiralcel OJ-H column, *n*-hexane/*i*-PrOH = 90/10, flow rate 1 mL/min, λ = 254 nm.

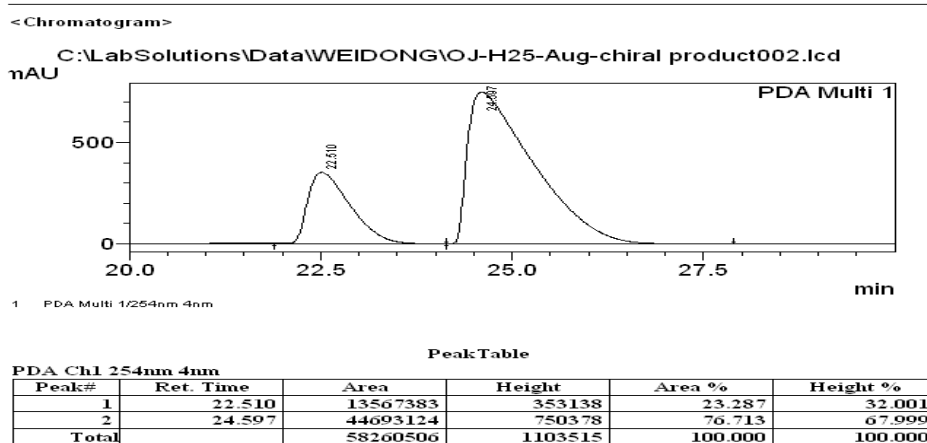


Figure S25. HPLC Spectrum of Racemic **3a** obtained from Racemic **1a**

Chiralcel AD-H column, *n*-hexane/*i*-PrOH = 80/20, flow rate 1 mL/min, λ = 254 nm.

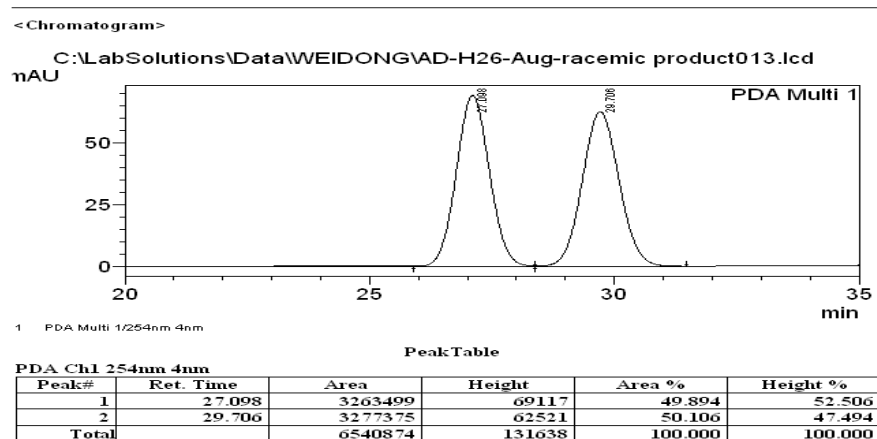
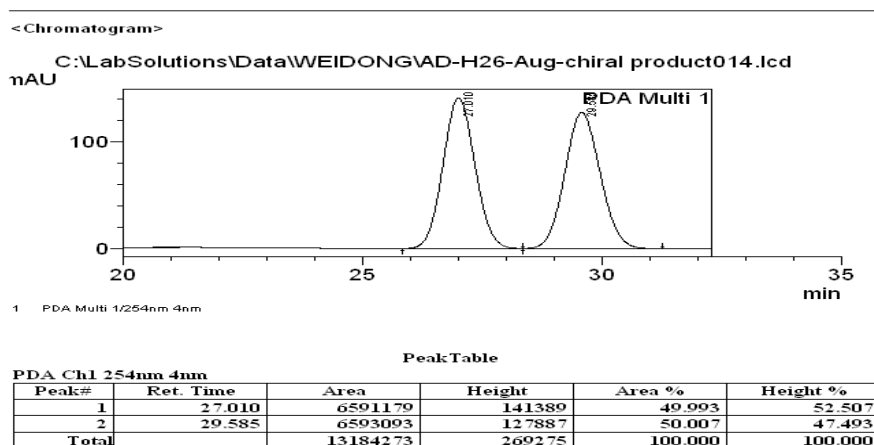


Figure S26. HPLC Spectrum of Racemic **3a** obtained from Chiral **1a**

Chiralcel AD-H column, *n*-hexane/*i*-PrOH = 80/20, flow rate 1 mL/min, λ = 254 nm.



References

- S1 S. Sohtome, A. Tanatani and K. Nagasawa *Tetrahedron Lett.*, 2004, **45**, 5589.
- S2 T. M. Nolan and E. S. Scott *J. Am. Chem. Soc.* 2003, **125**, 12094.