

Supporting Information
for
Rapid Access to Halohydrofurans via Brønsted Acid-Catalyzed
Hydroxylation/Halocyclization of Cyclopropyl Methanols with
Water and Electrophilic Halides

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Table of Contents

	Page
¹ H and ¹³ C NMR Spectra of Substituted Cyclopropyl Methanols (1)	S3
¹ H- ¹ H NOESY Spectrum of <i>Trans</i> -diphenyl(2-phenylcyclopropyl)methanol (1t)	S22
¹ H- ¹ H NOESY Spectrum of <i>Trans</i> -(2-pentylcyclopropyl)diphenylmethanol (1u)	S24
<i>Trans</i> -1,3-diphenyl-1-(2-(thiophen-2-yl)cyclo propyl)prop-2-yn-1-ol (1v)	S26
¹ H and ¹³ C NMR Spectra of Halohydrofurans (2)	S29
NOESY Spectrum of <i>Cis</i> -tetrahydro-3-iodo-2-phenyl-2-(2-phenylethynyl)furan (2a)	S30
NOESY Spectrum of <i>Cis</i> -tetrahydro-3-iodo-2-pentyl-2-phenylfuran (2m)	S43
NOESY Spectrum of Tetrahydro-3-iodo-2-phenyl-2-(2-phenylethynyl)-5-(thiophen-2-yl) furan (2v)	S53
¹ H and ¹³ C NMR Spectra of Conjugated Enynes (3)	S61
NOESY Spectrum of (<i>Z</i>)-4,6-Diphenylhex-3-en-5-yn-1-ol (3a)	S62
NOESY Spectrum of (<i>Z</i>)-4,6-Diphenyl-1-(thiophen-2-yl)hex-3-en-5-yn-1-ol (3c)	S65
ORTEP Drawing of <i>Cis</i> -tetrahydro-3-iodo-2-phenyl-2-(2-phenylethynyl)furan (2a)	S66
ORTEP Drawing of <i>Cis</i> -3-fluoro-tetrahydro-2-phenyl-2-(2-phenylethynyl)furan (2a)	S66
References	S67

Figure S1. ^1H and ^{13}C NMR Spectra of Cyclopropyl-1,3-diphenylprop-2-yn-1-ol (**1a**)

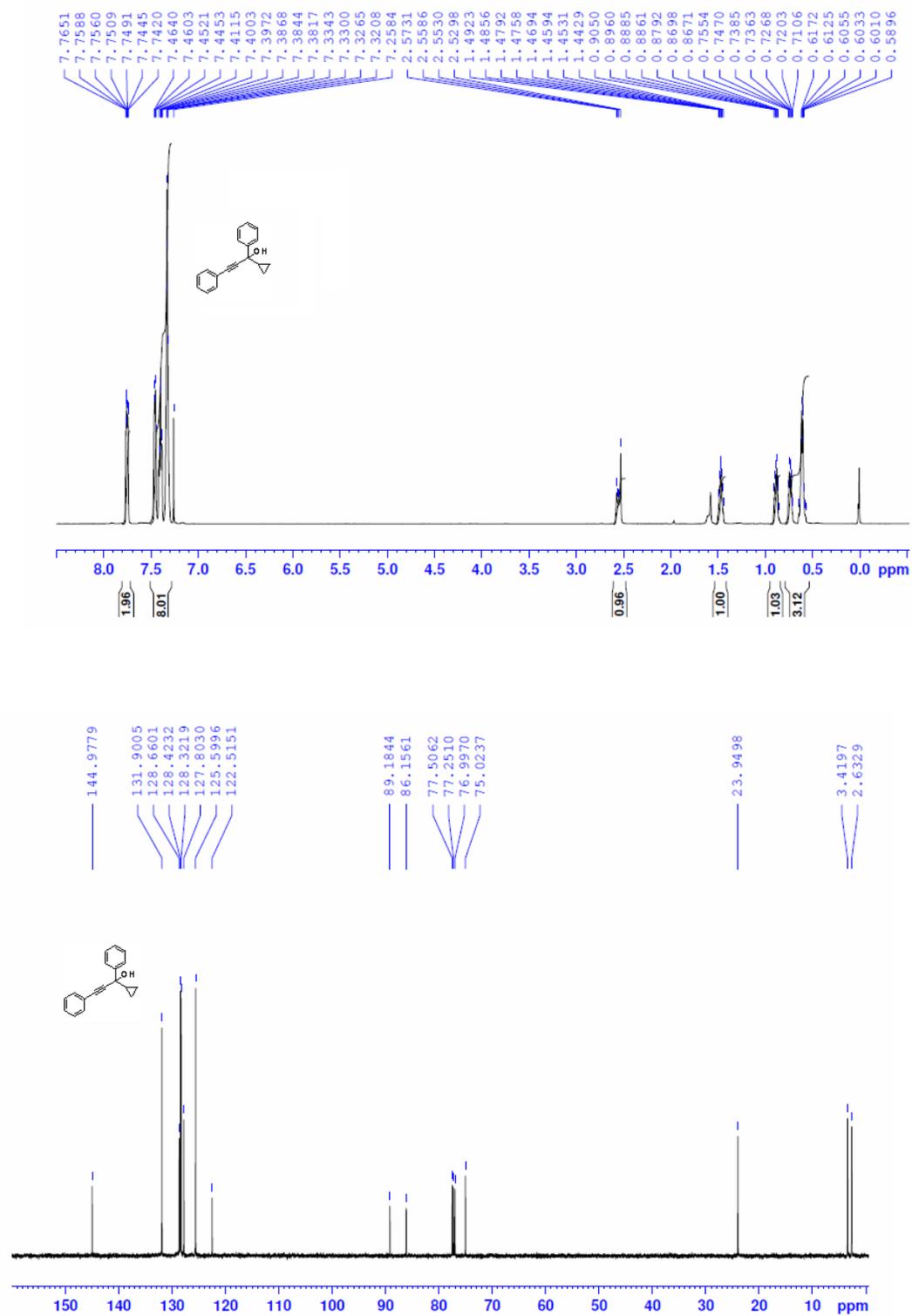


Figure S2. ^1H and ^{13}C NMR Spectra of Cyclopropylbis(4-fluorophenyl)methanol (**1b**)

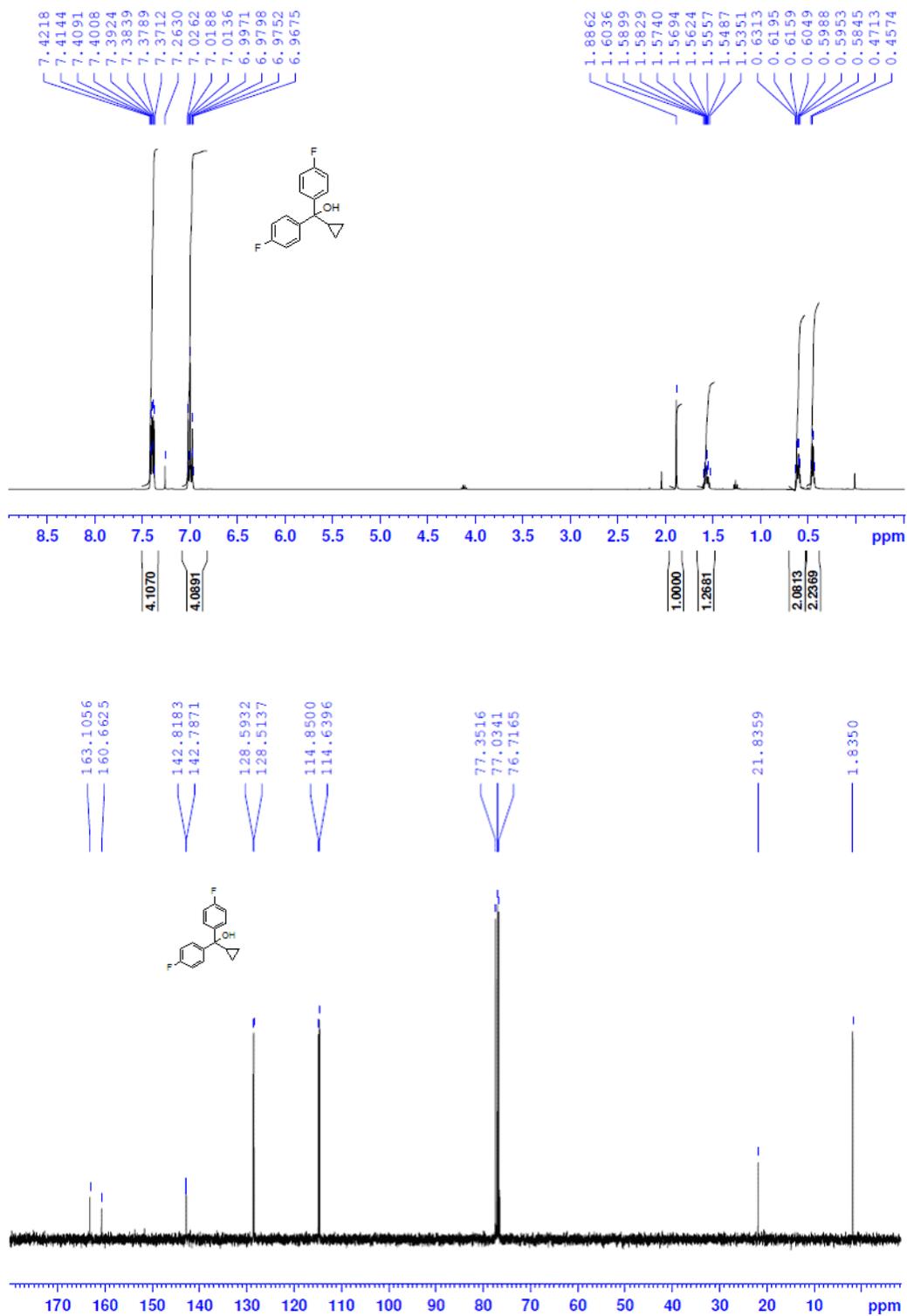


Figure S3. ^1H and ^{13}C NMR Spectra of Bis(4-chlorophenyl)(cyclopropyl)methanol (**1c**)

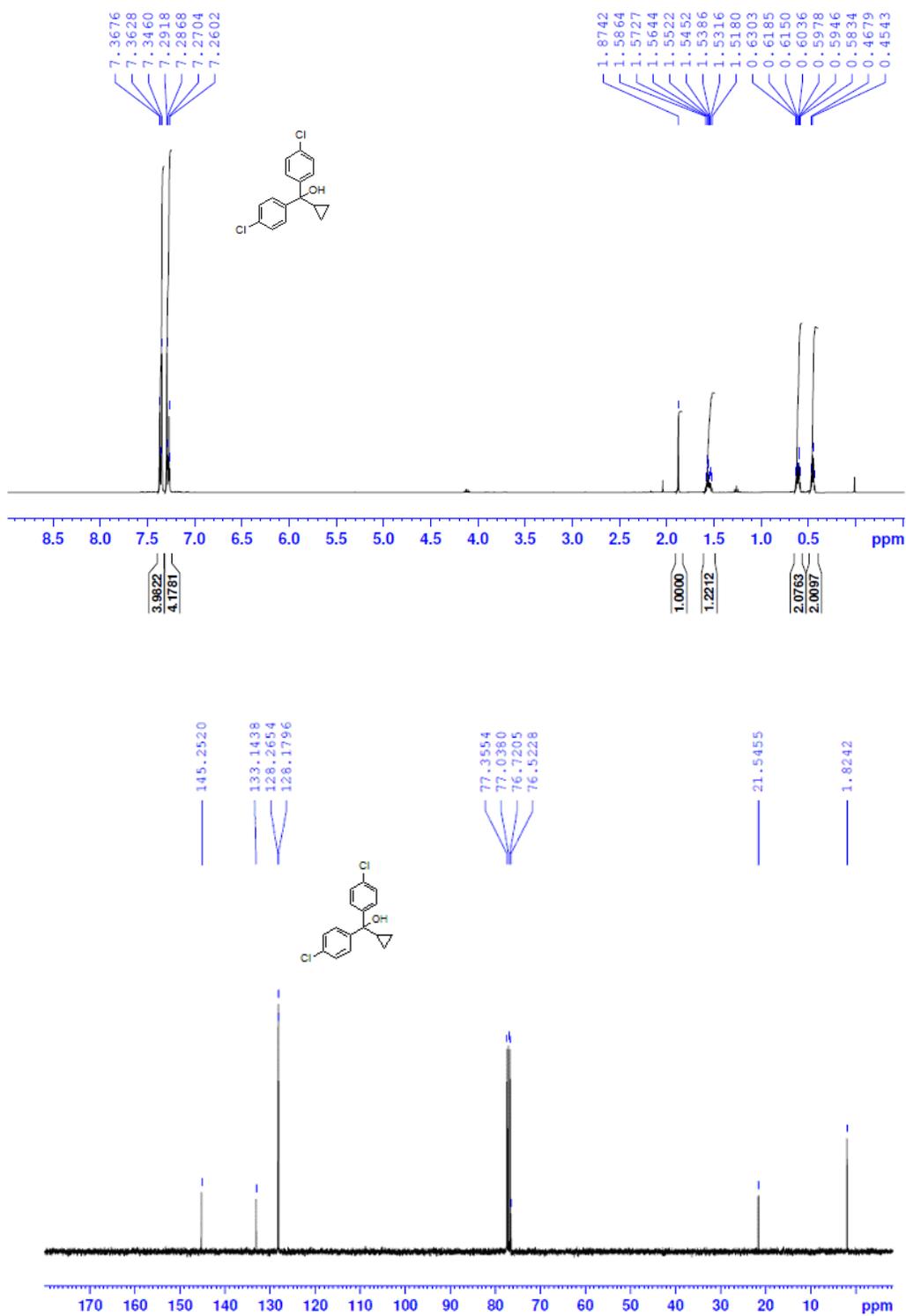


Figure S4. ^1H and ^{13}C NMR Spectra of Bis(4-bromophenyl)(cyclopropyl)methanol (**1d**)

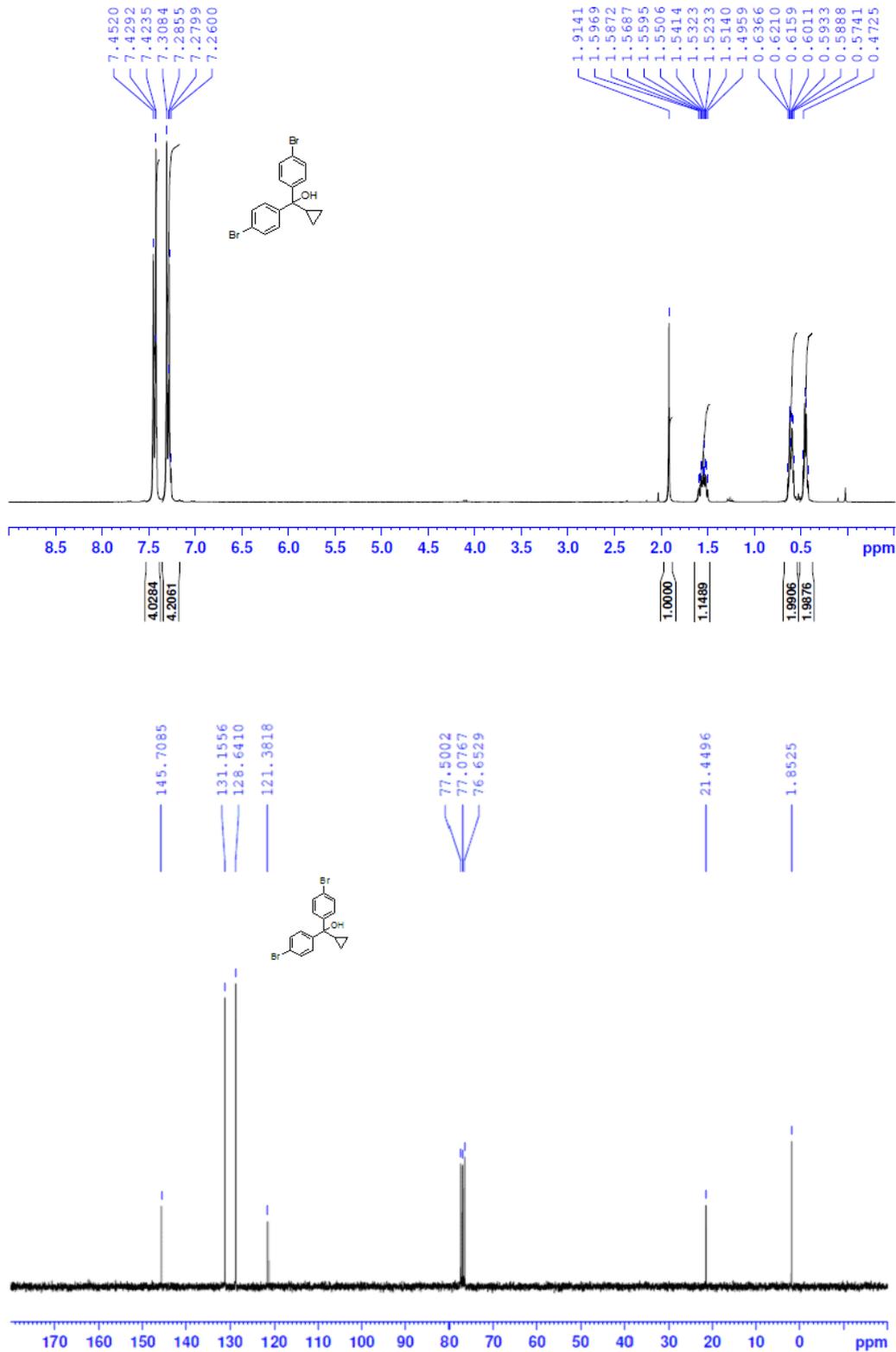


Figure S5. ^1H and ^{13}C NMR Spectra of Cyclopropyldi-*p*-tolylmethanol (**1f**)

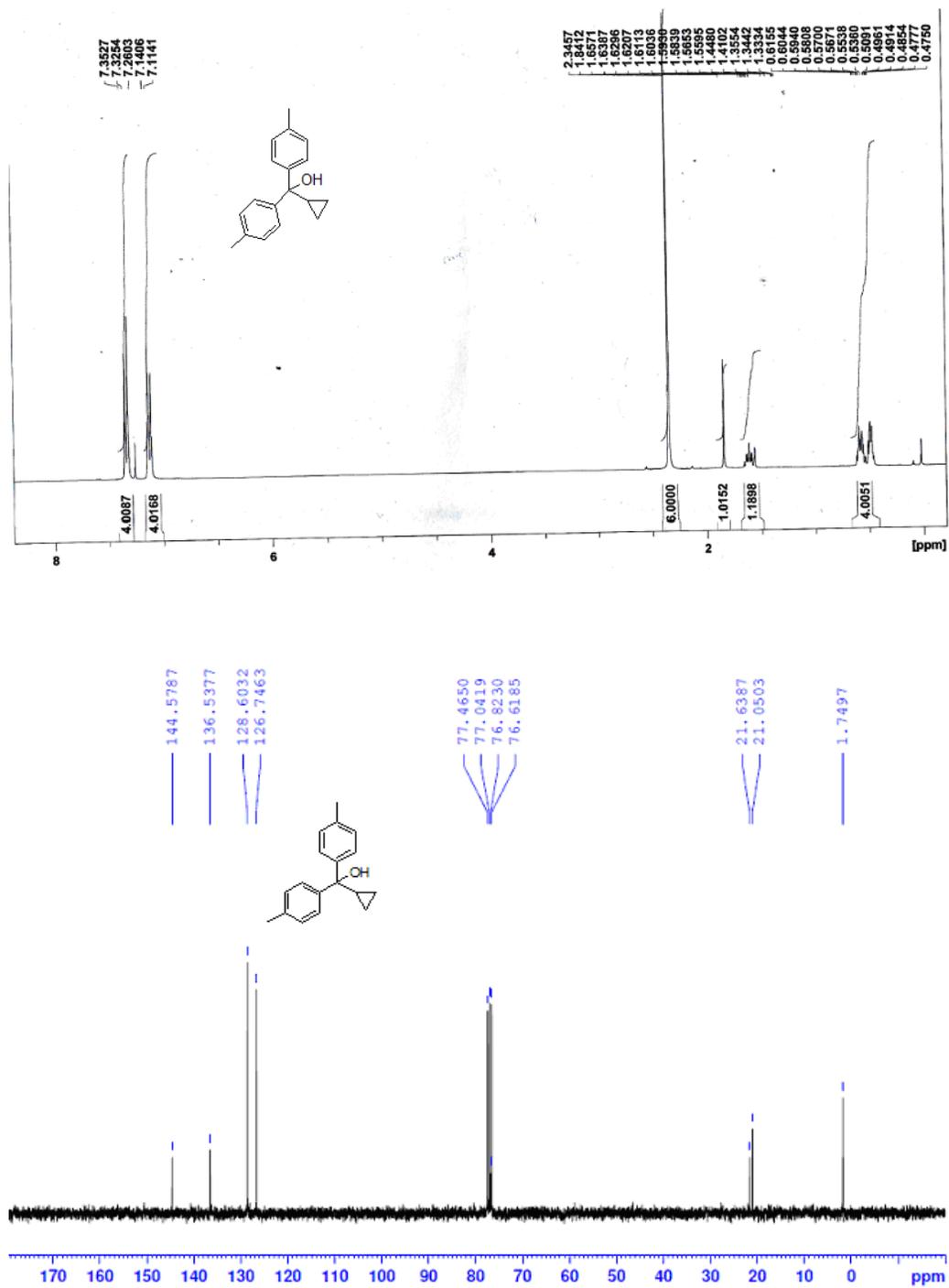


Figure S6. ^1H and ^{13}C NMR Spectra of Cyclopropylbis(4-methoxyphenyl)methanol (**1g**)

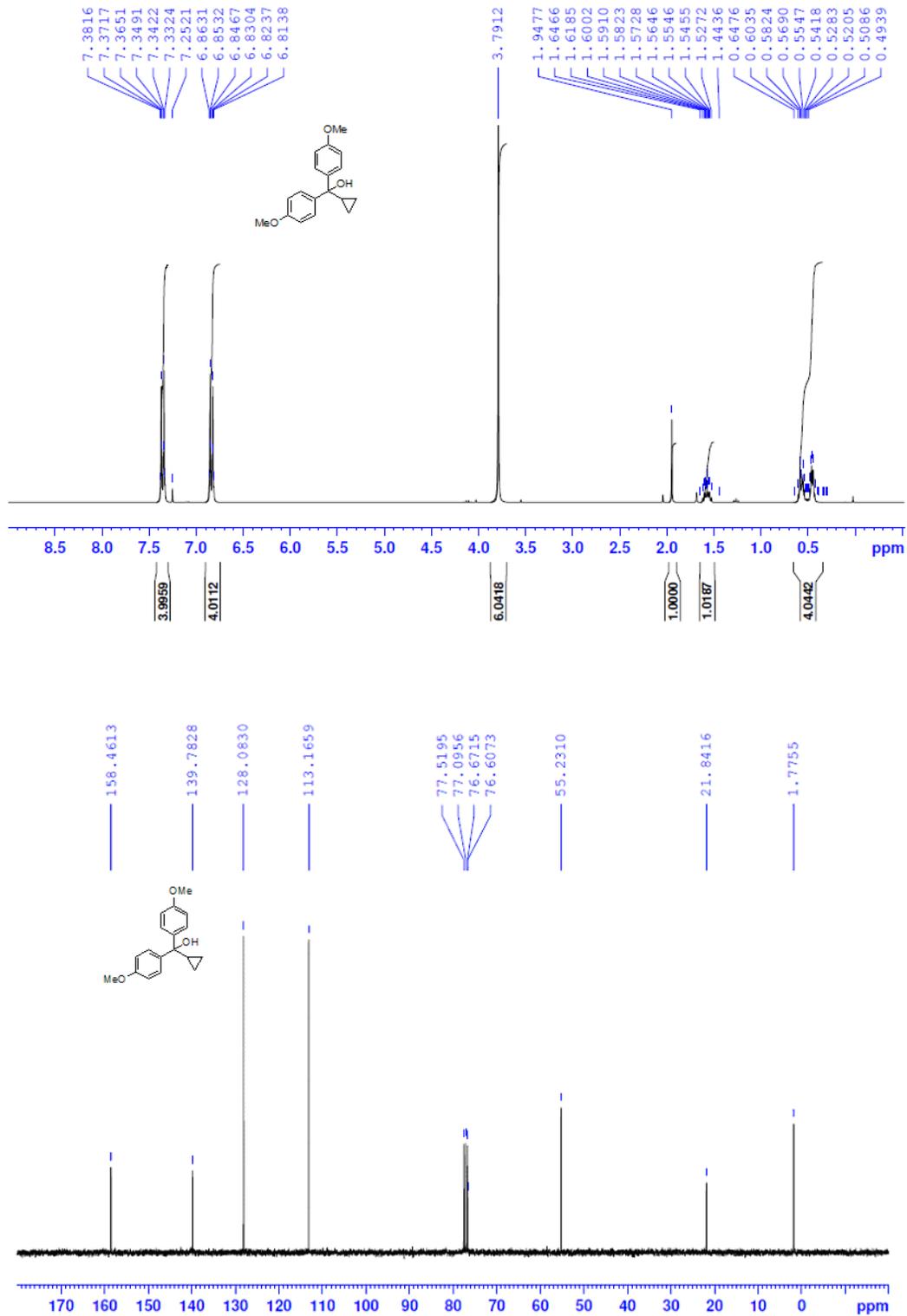


Figure S7. ^1H and ^{13}C NMR Spectra of (4-Chlorophenyl)(cyclopropyl)(*p*-tolyl)methanol

(1h)

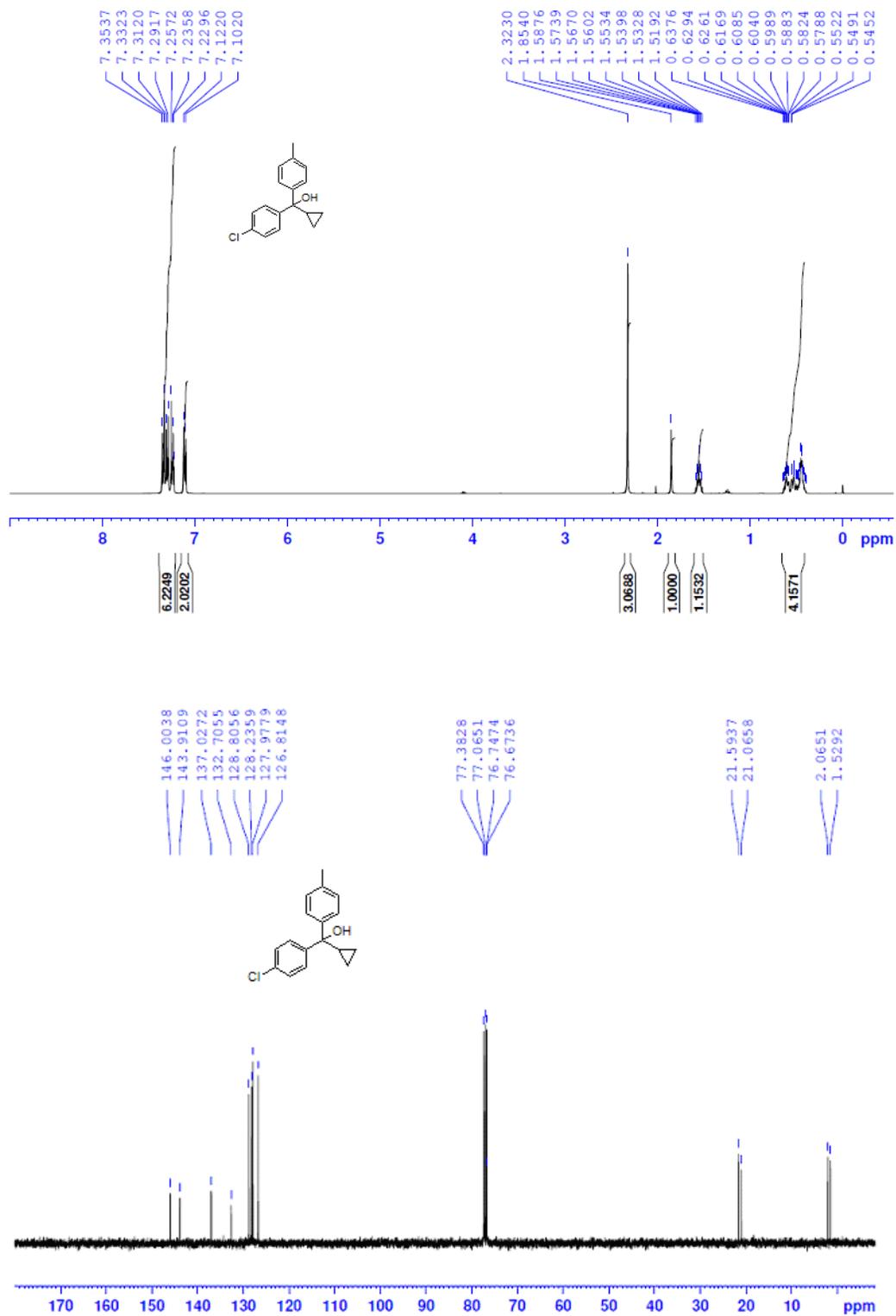


Figure S8. ^1H and ^{13}C NMR Spectra of (4-Chlorophenyl)(cyclopropyl)-(4-methoxyphenyl)

methanol (**1i**)

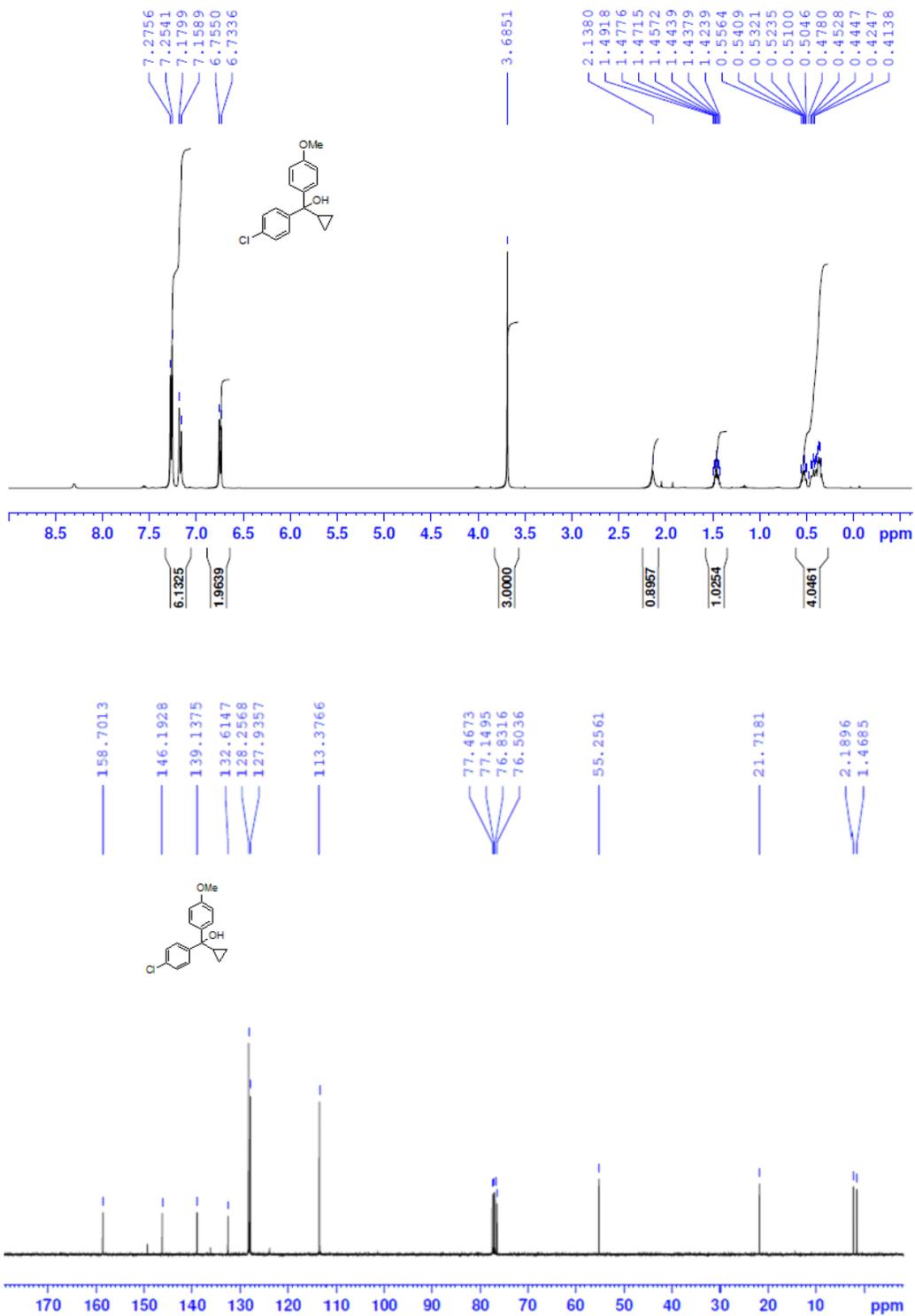


Figure S9. ^1H and ^{13}C NMR Spectra of Cyclopropyl(phenyl)(*p*-tolyl)methanol (**1j**)

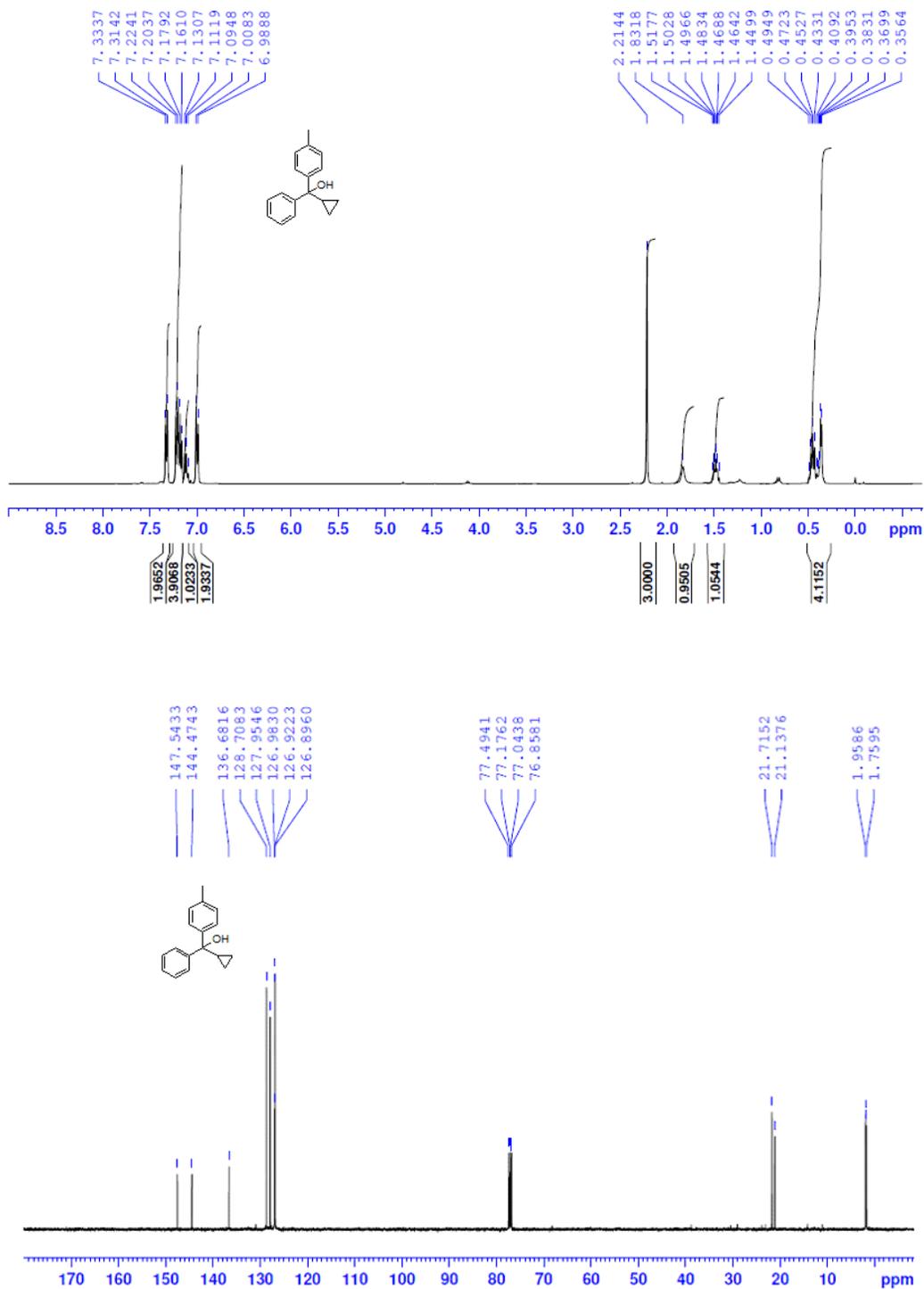


Figure S10. ^1H and ^{13}C NMR Spectra of Cyclopropyl(phenyl)(4-biphenyl)methanol (**1k**)

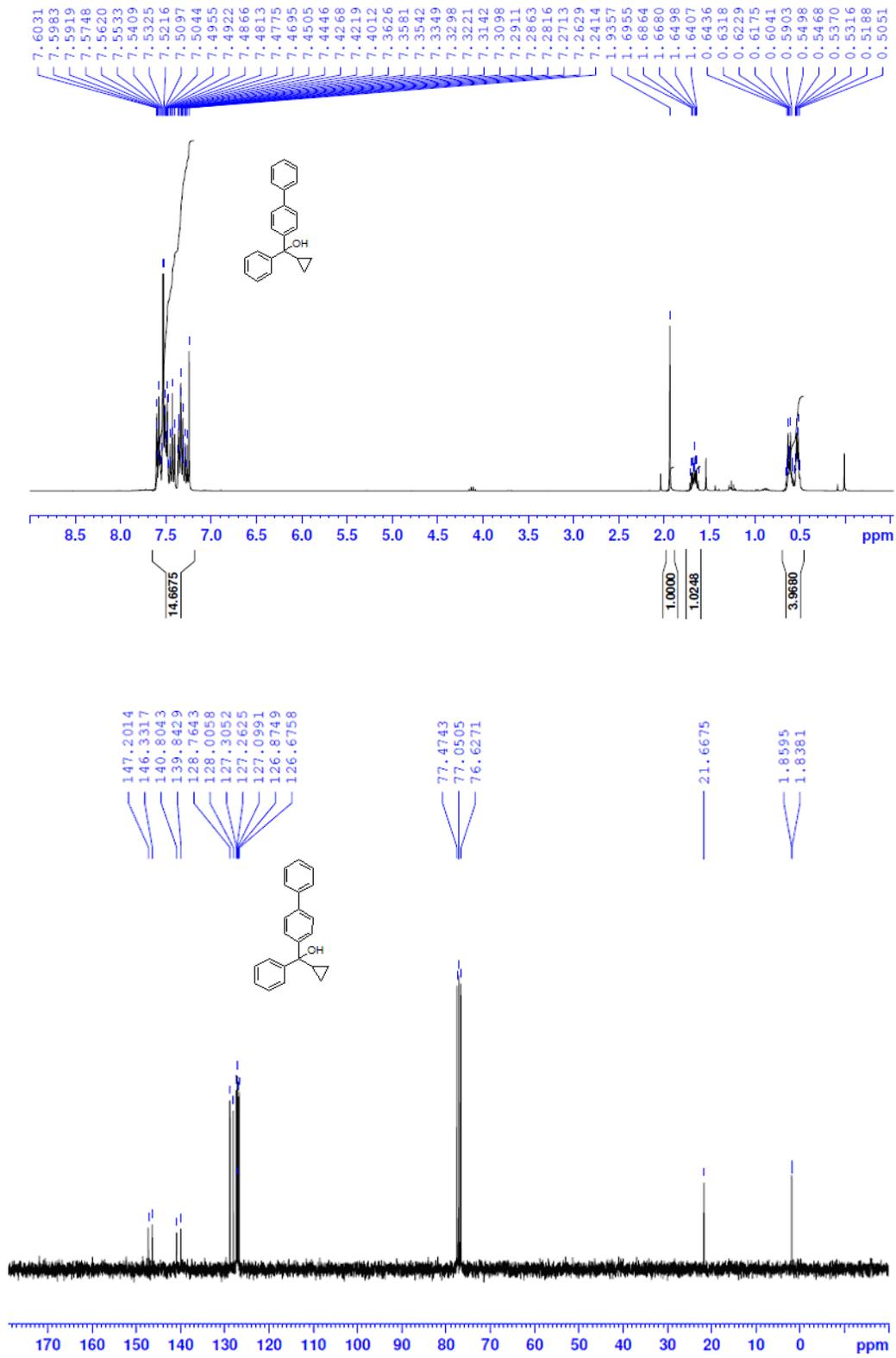


Figure S11. ^1H and ^{13}C NMR Spectra of Cyclopropyl(naphthalen-1-yl)(phenyl)methanol

(1)

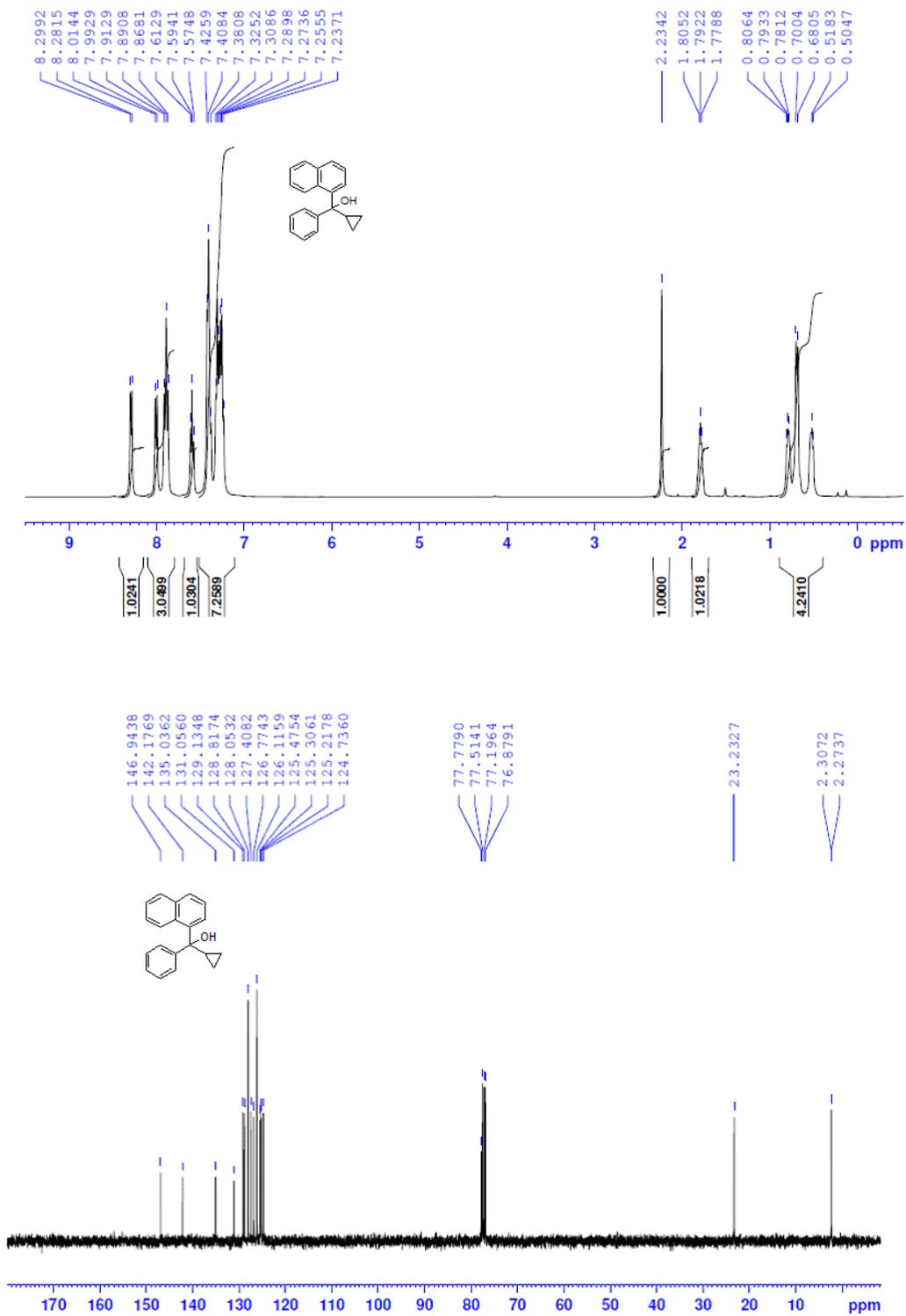


Figure S12. ^1H and ^{13}C NMR Spectra of 1-Cyclopropyl-1-phenylhexan-1-ol (**1m**)

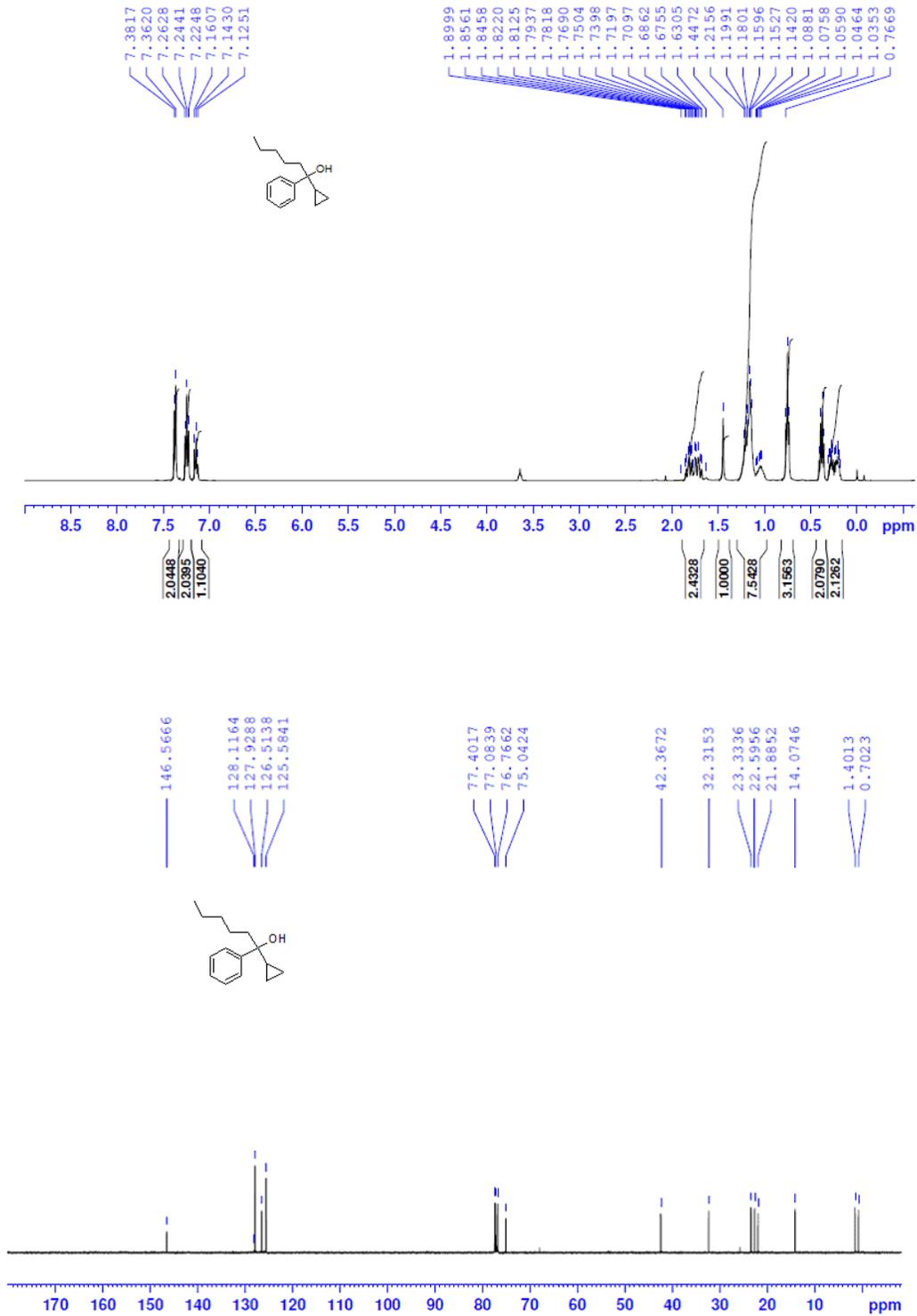


Figure S13. ^1H and ^{13}C NMR Spectra of 1-Cyclopropyl-2,2-dimethyl-1-phenylpropan-1-ol

(1n)

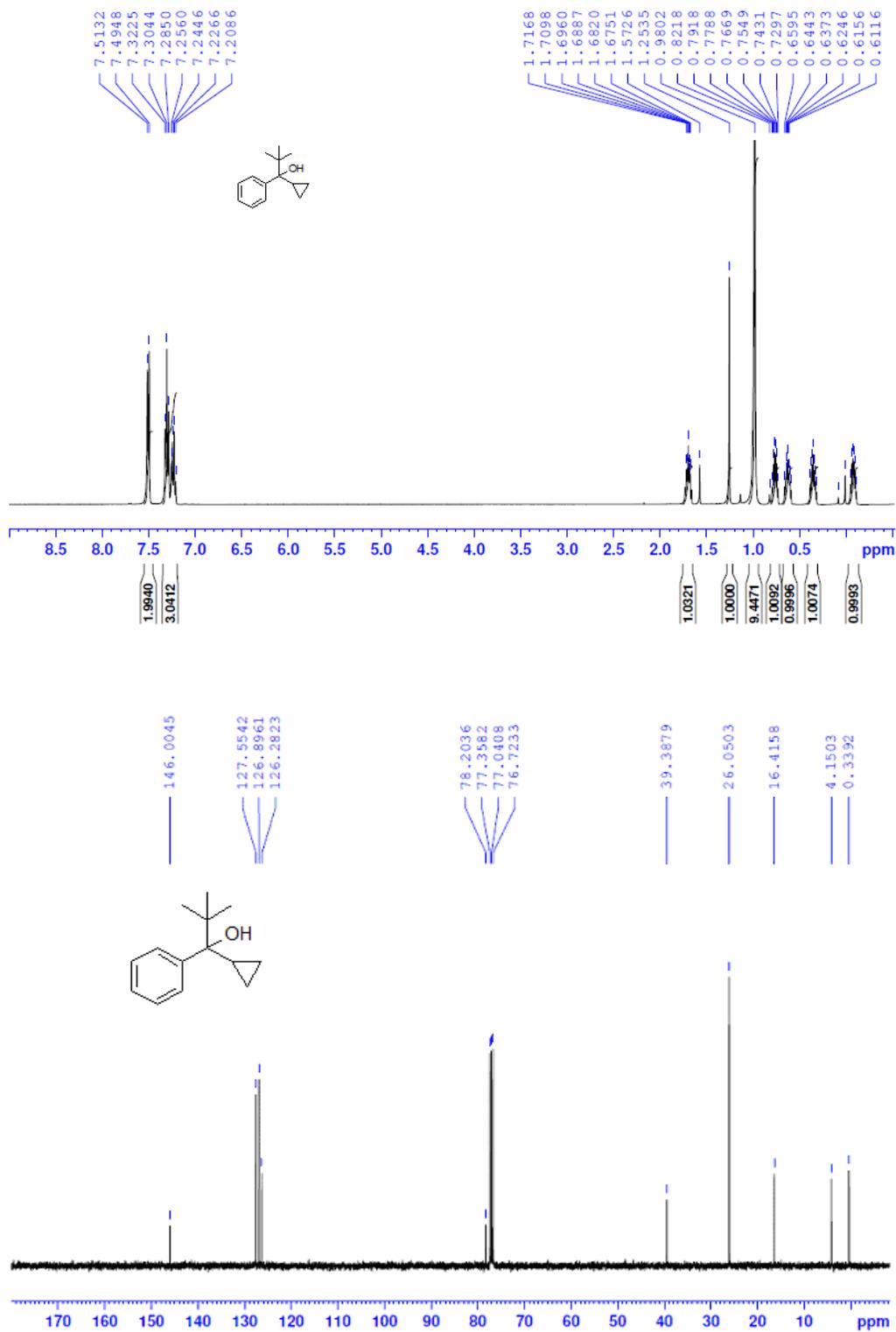


Figure S14. ^1H and ^{13}C NMR Spectra of 1-(4-Chlorophenyl)-1-cyclopropyl-3-(thiophen-2-yl)prop-2-yn-1-ol (**1o**)

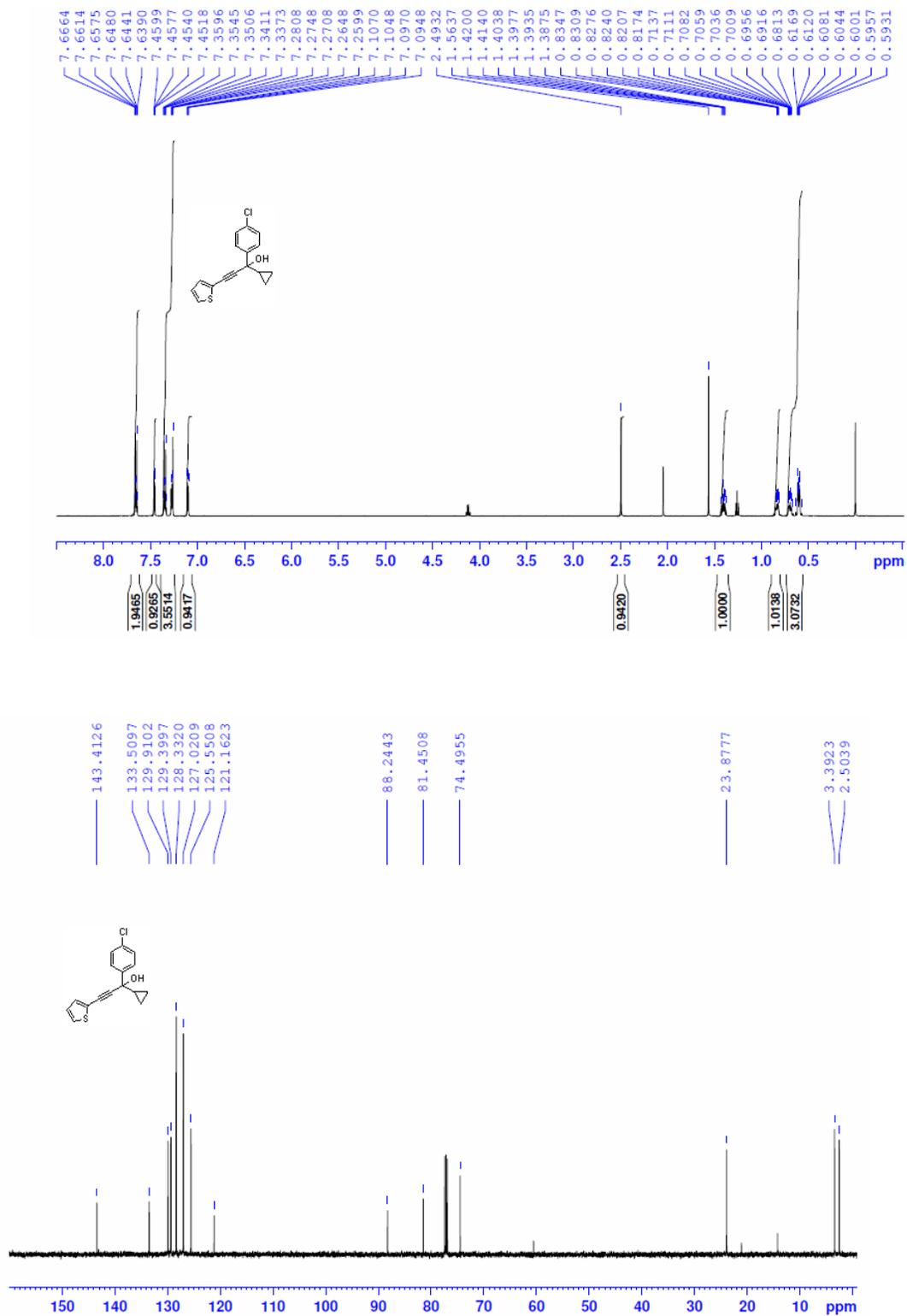


Figure S15. ^1H and ^{13}C NMR Spectra of 1-Cyclopropyl-1-(4-methoxyphenyl)-3-(pyridin-2-yl)prop-2-yn-1-ol (**1p**)

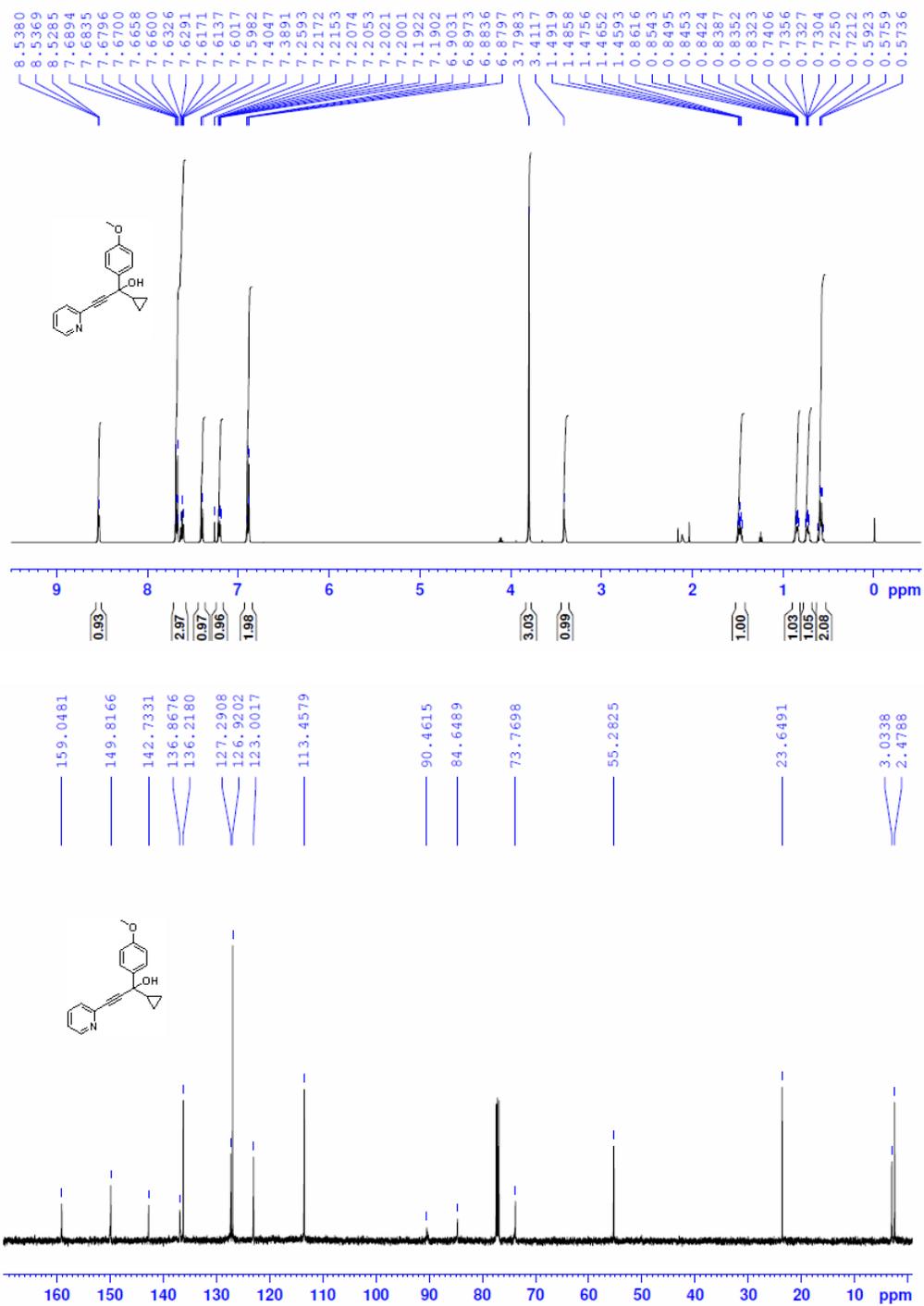


Figure S16. ^1H and ^{13}C NMR spectra of 3-Cyclopropyl-1,5-diphenylpenta-1,4-diyne-3-ol

(1q)

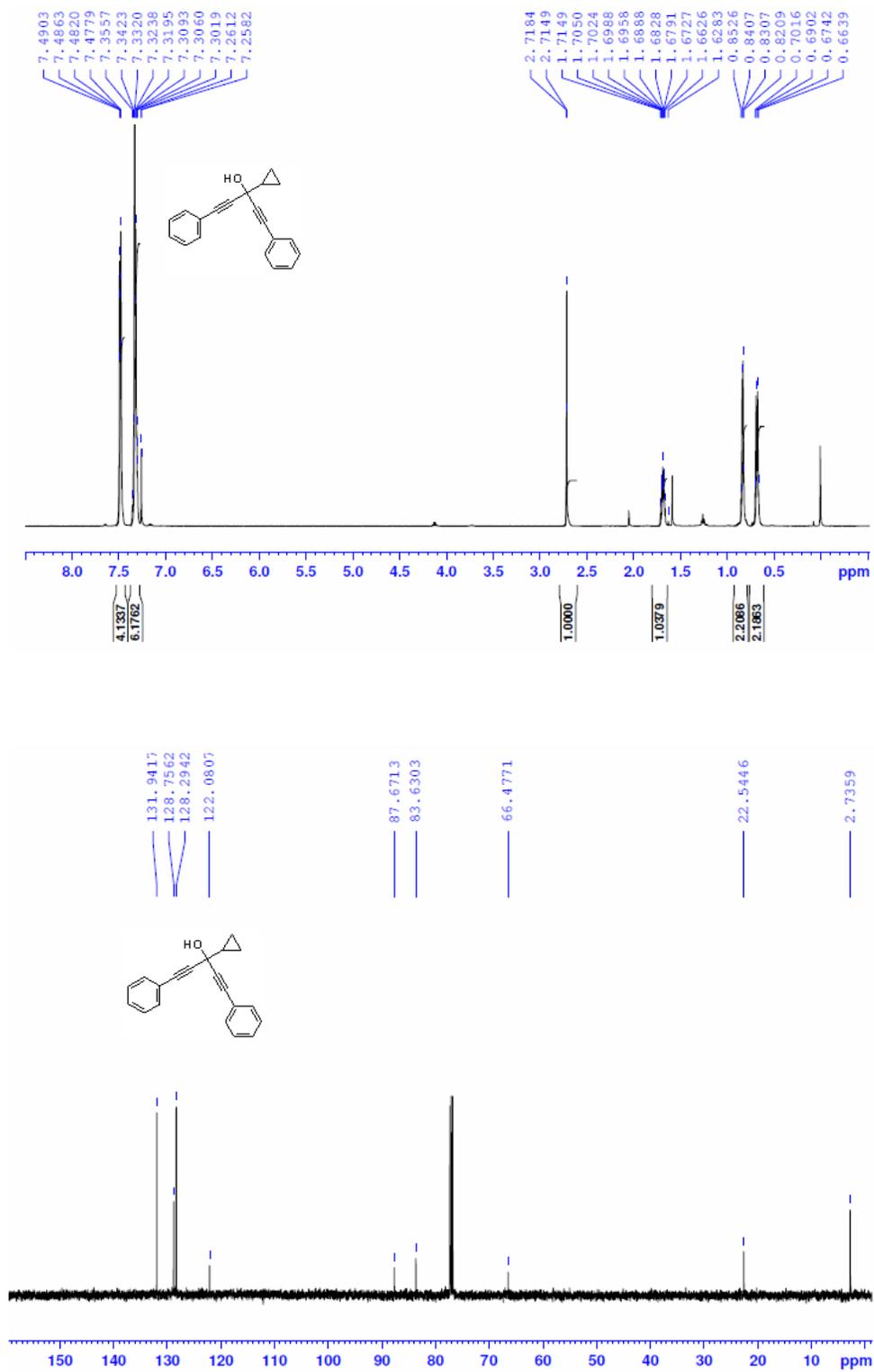


Figure S17. ^1H and ^{13}C NMR spectra of 1-Cyclopropyl-1-(1-methylcyclohexyl)-3-phenyl prop-2-yn-1-ol (**1r**)

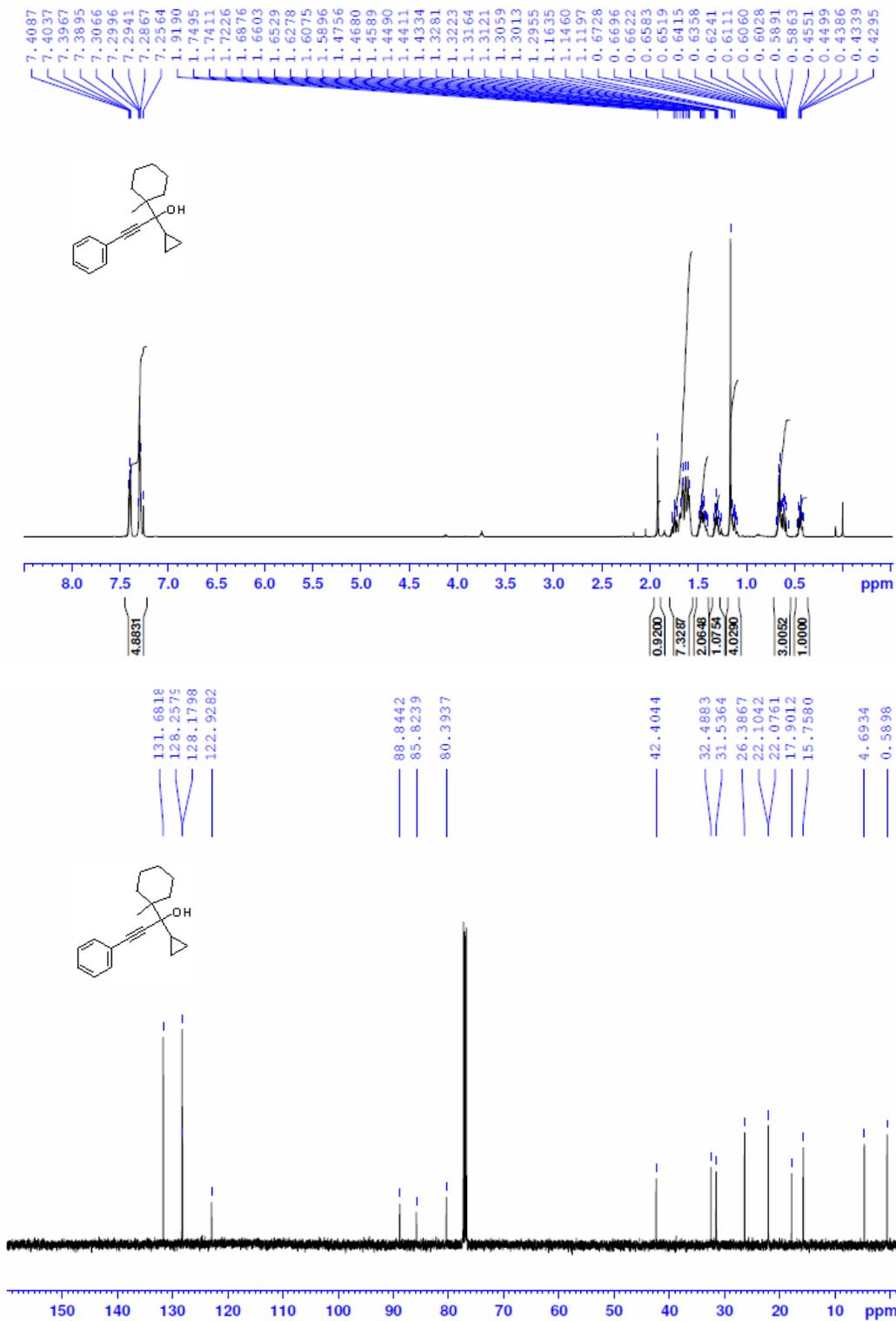


Figure S18. ^1H and ^{13}C NMR Spectra of 2-Cyclopropylbut-3-yn-2-ol (**1s**)

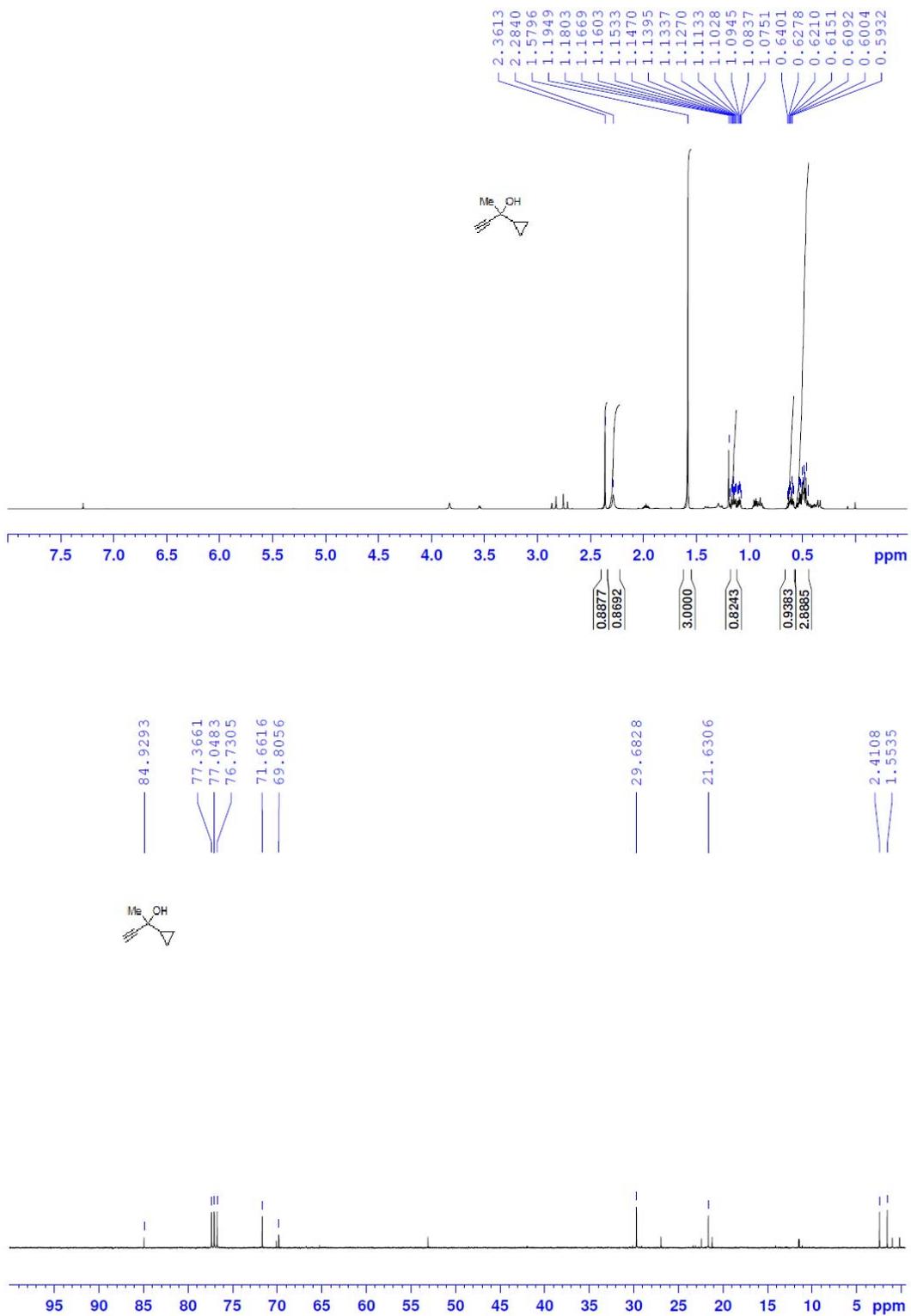


Figure S19. ^1H and ^{13}C NMR Spectra of Diphenyl(2-phenylcyclopropyl)methanol (**1t**)

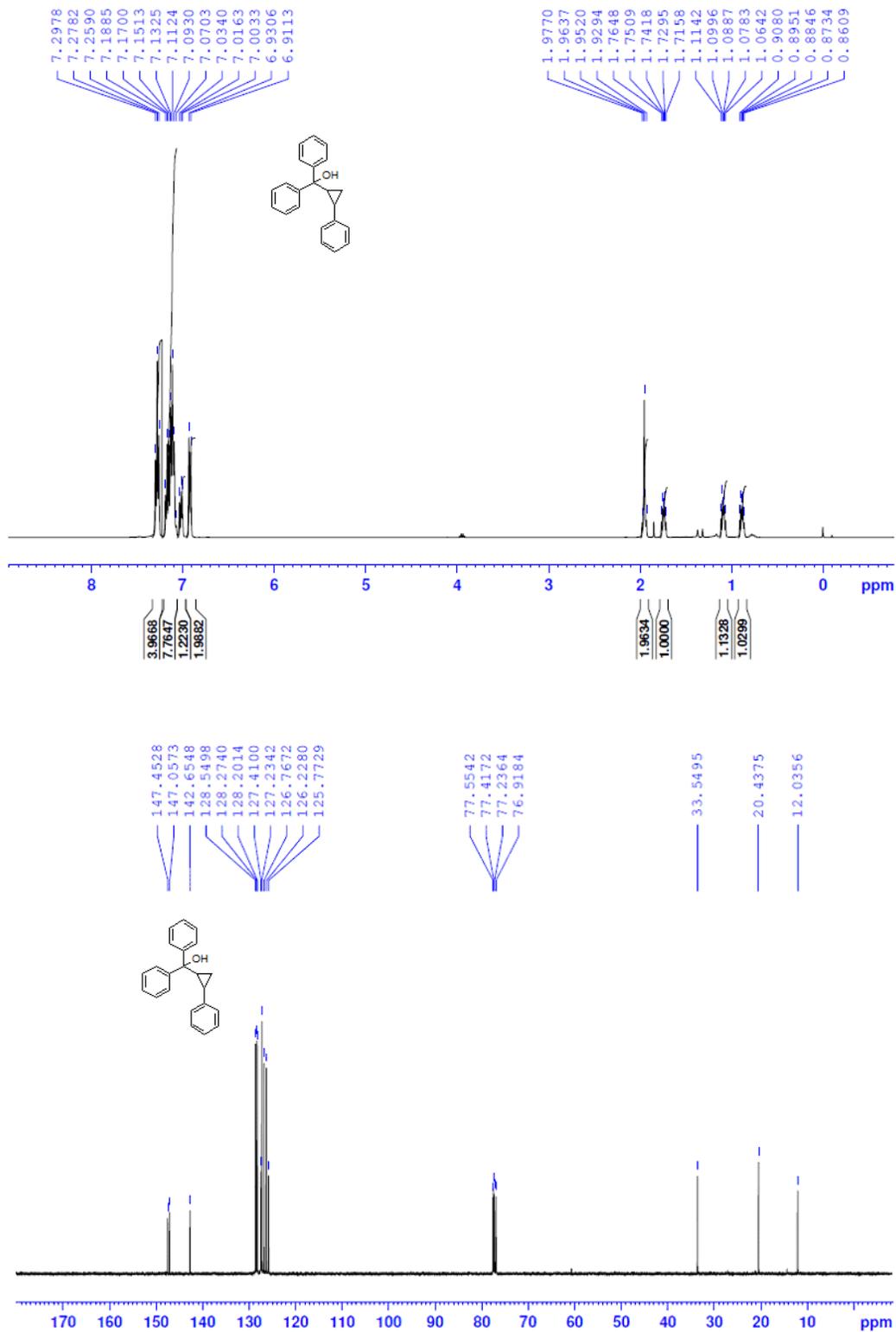
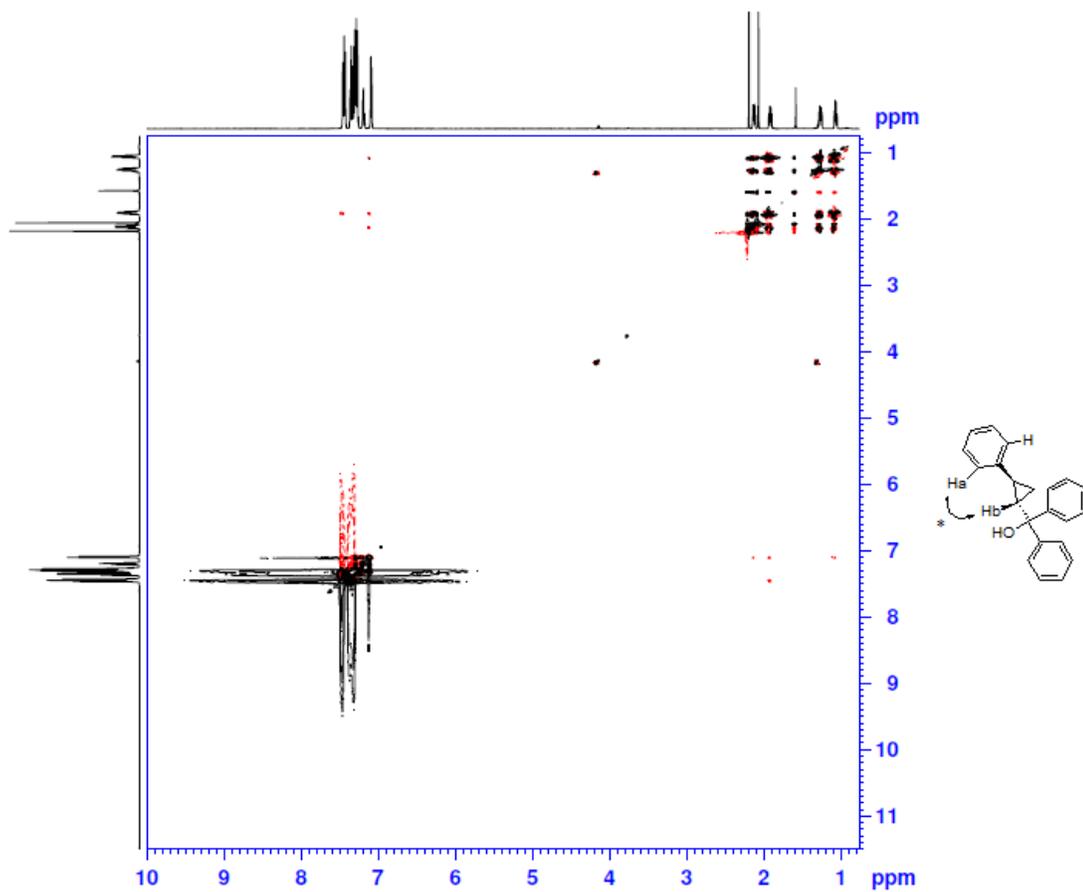


Figure S20. ^1H - ^1H NOESY Spectrum of *Trans*-diphenyl(2-phenylcyclopropyl)methanol (**1t**)



* ^1H - ^1H NOESY correlation observed between H_a at 7.27 ppm and H_b at 1.74 ppm.

Figure S21. ^1H and ^{13}C NMR Spectra of (2-Pentylcyclopropyl)diphenylmethanol (**1u**)

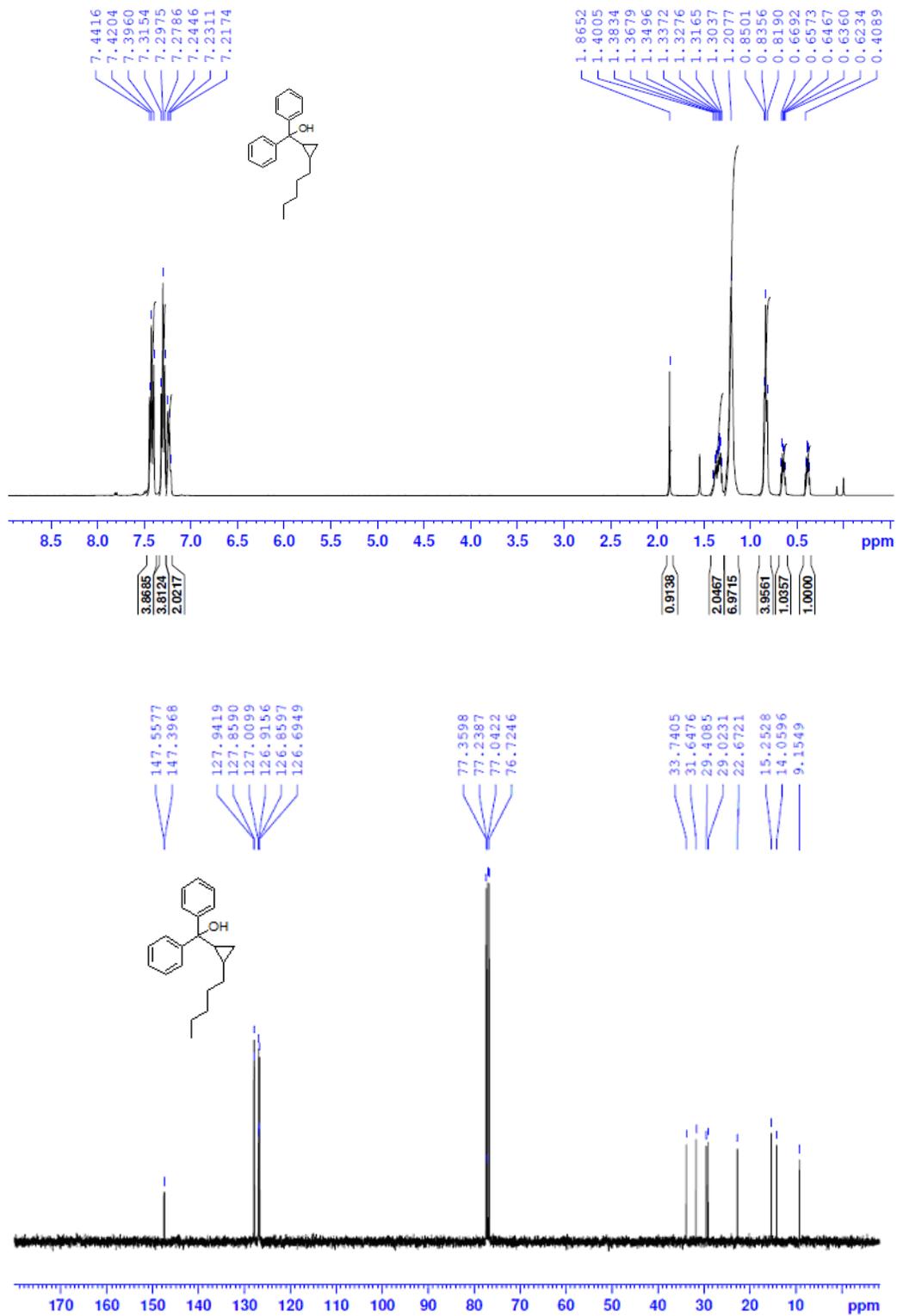
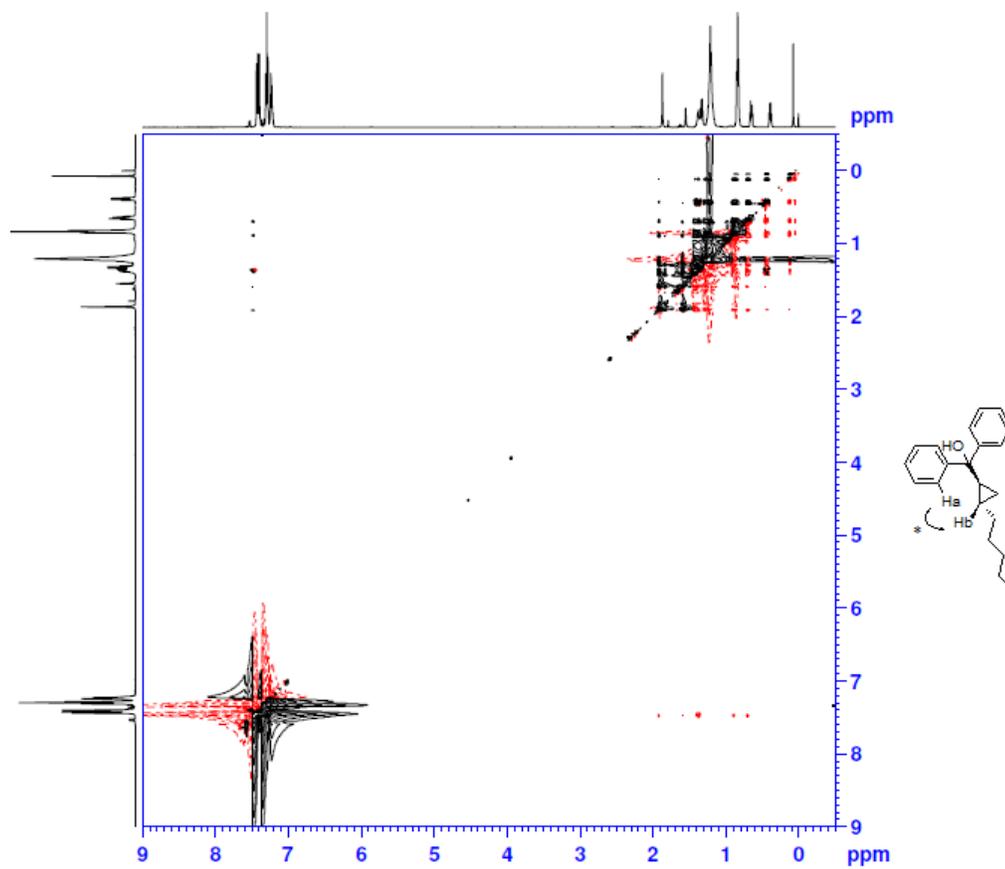


Figure S22. ^1H - ^1H NOESY Spectrum of *Trans*-(2-pentylcyclopropyl)diphenylmethanol

(1u)



* ^1H - ^1H NOESY correlation observed between H_a at 7.42 ppm and H_b at 1.32 ppm.

Figure S23. ^1H and ^{13}C NMR Spectra of 1,3-Diphenyl-1-(2-(thiophen-2-yl)cyclopropyl)prop-2-yn-1-ol (**1v**)

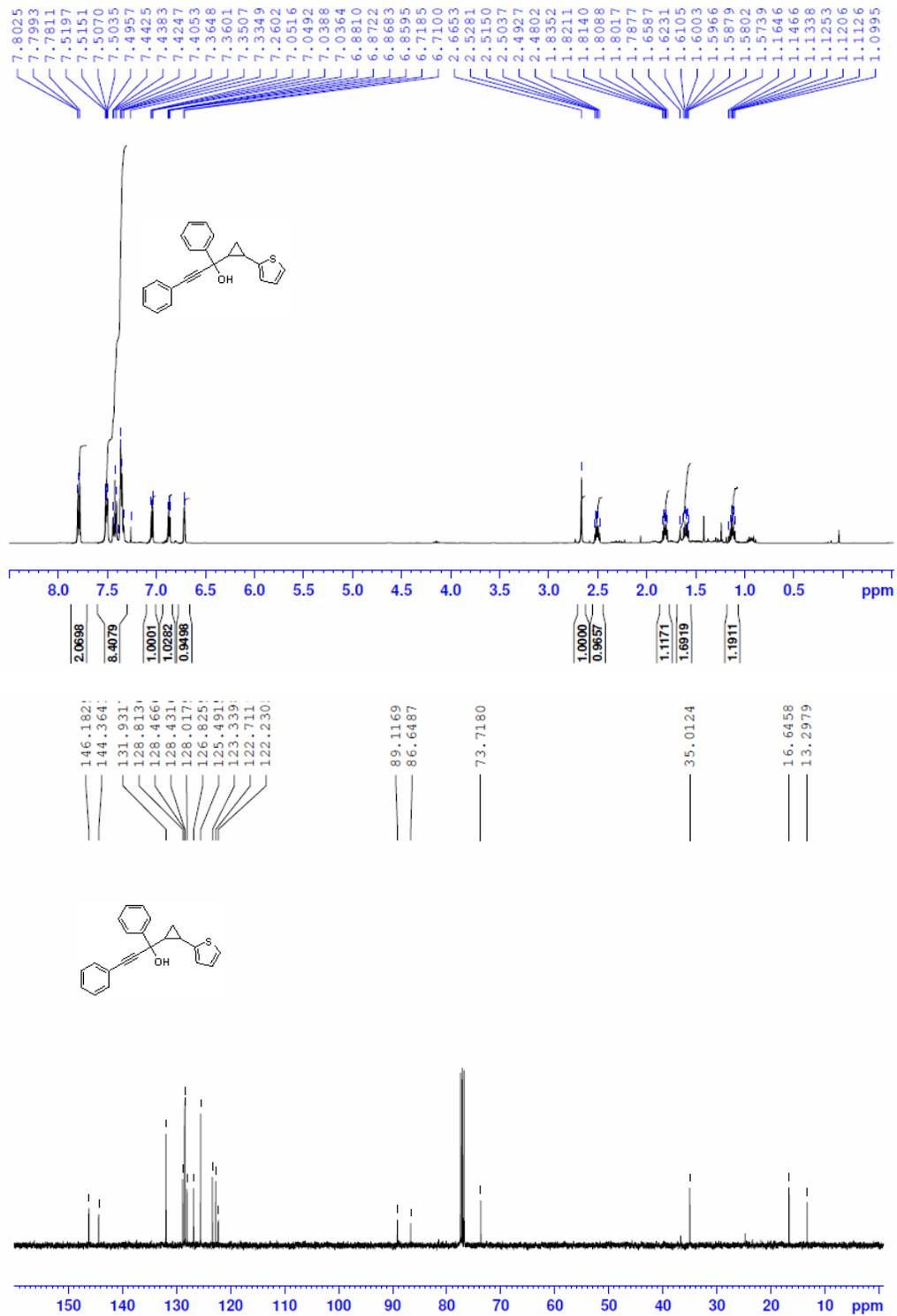
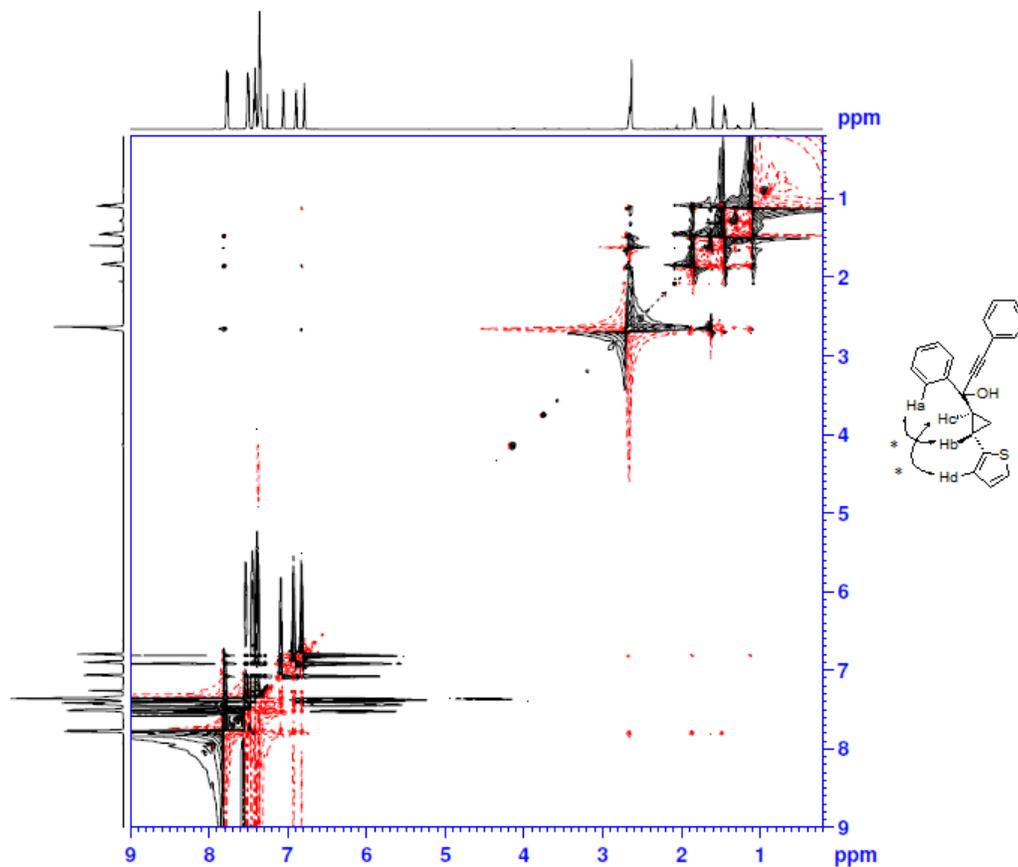


Figure S24. ^1H - ^1H NOESY Spectrum of *Trans*-1,3-diphenyl-1-(2-(thiophen-2-yl)cyclopropyl)prop-2-yn-1-ol (**1v**)



* ^1H - ^1H NOESY correlation observed between H_a at 7.79 ppm and H_b at 2.50 ppm.

* ^1H - ^1H NOESY correlation observed between H_c at 1.81 ppm and H_d at 6.71 ppm.

Figure S25. ^1H and ^{13}C NMR Spectra of Cyclopropyl(phenyl)methanol (**1w**)

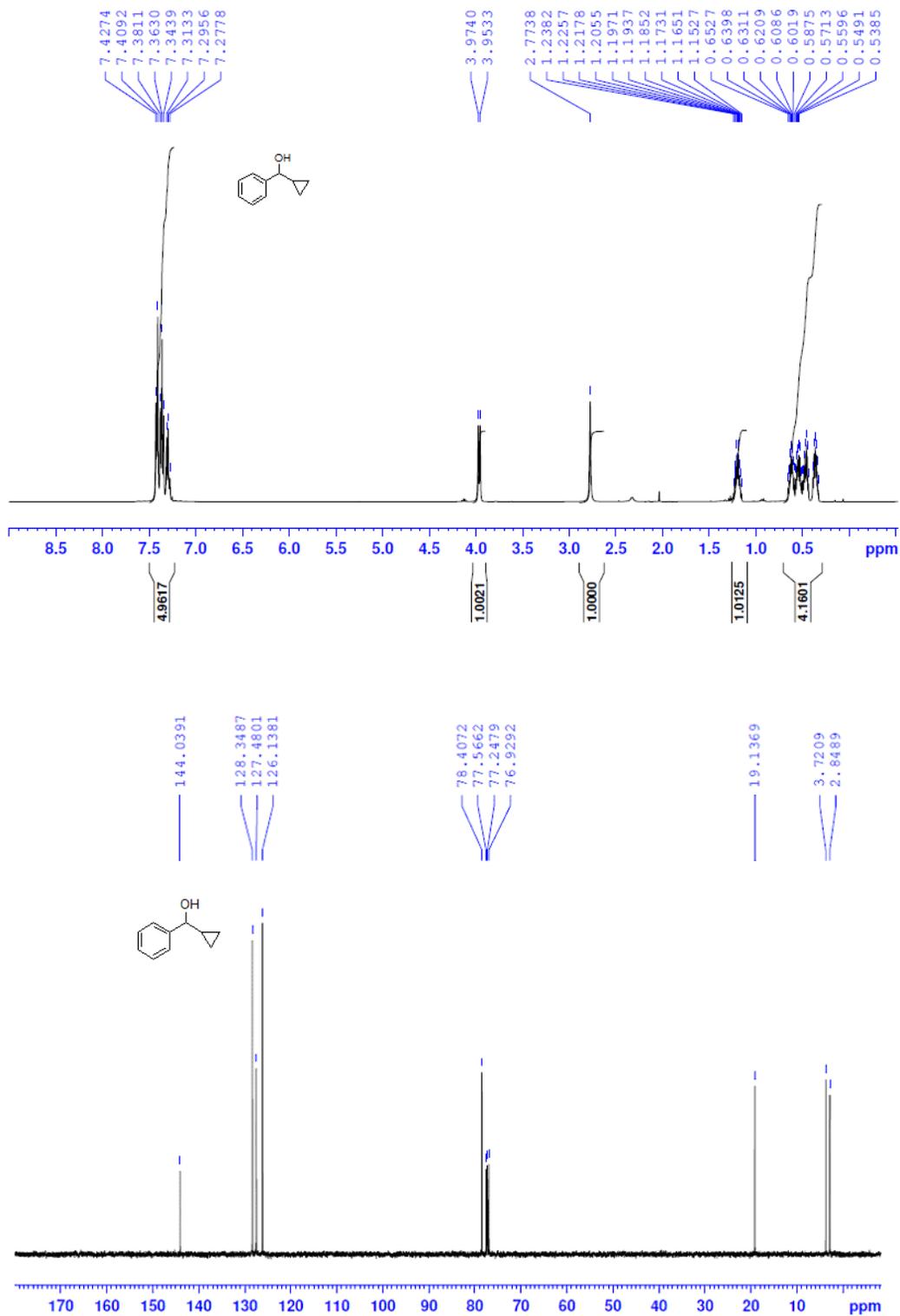


Figure S26. ^1H and ^{13}C NMR Spectra of 1-cyclopropylhexan-1-ol (**1x**)

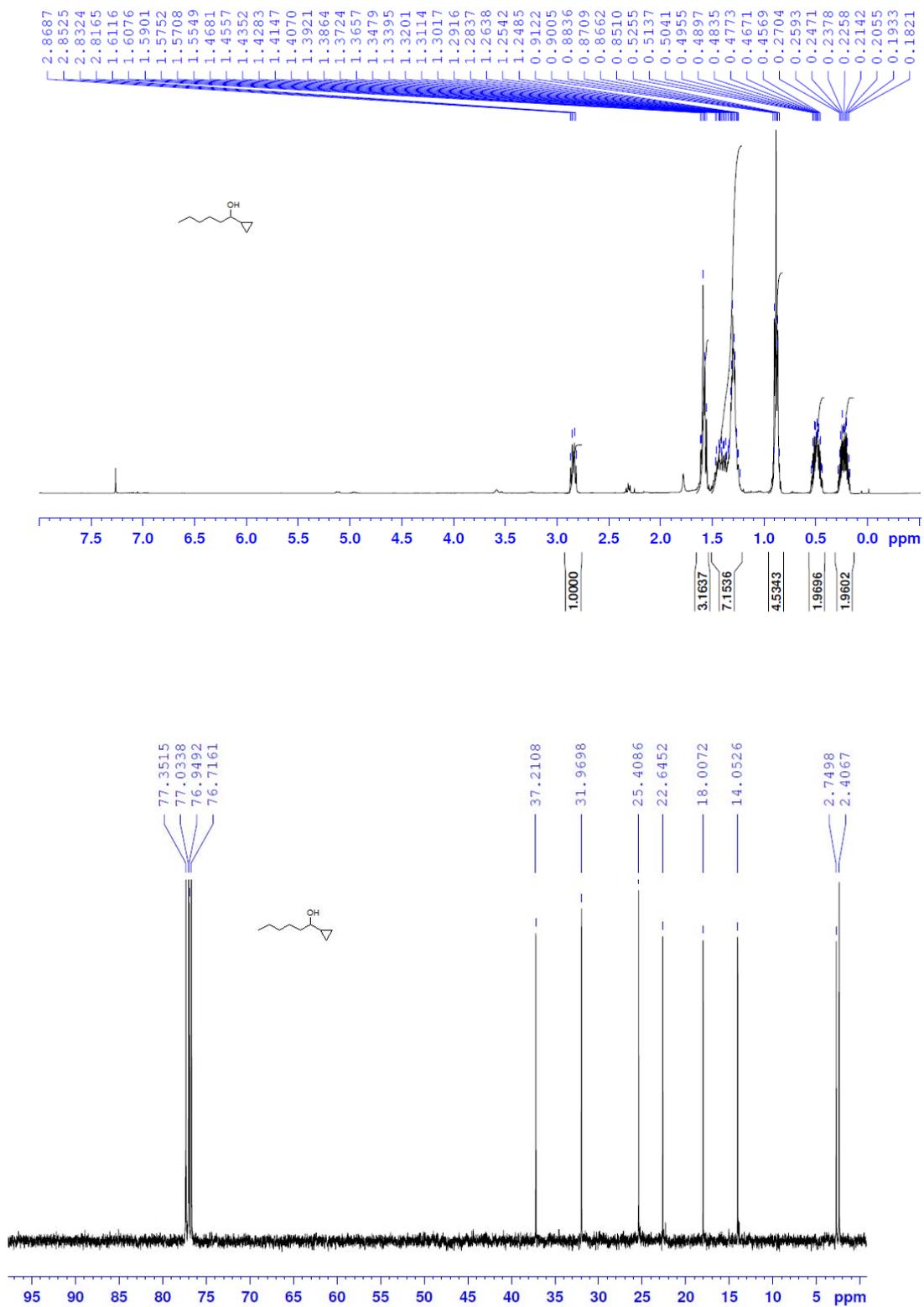


Figure S27. ^1H and ^{13}C NMR Spectra of *cis*-Tetrahydro-3-iodo-2-phenyl-2-(2-phenylethynyl)furan (**2a**)

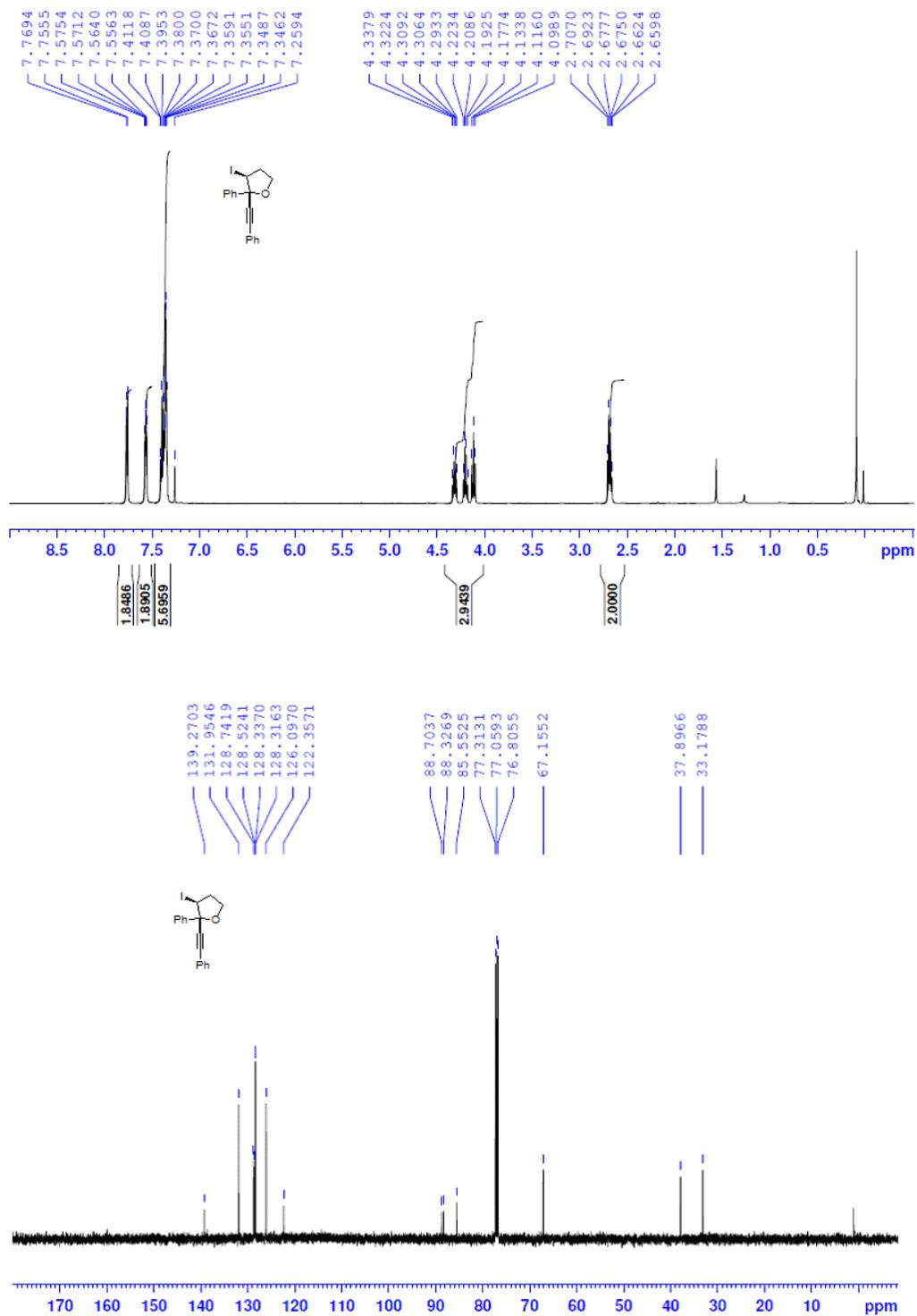
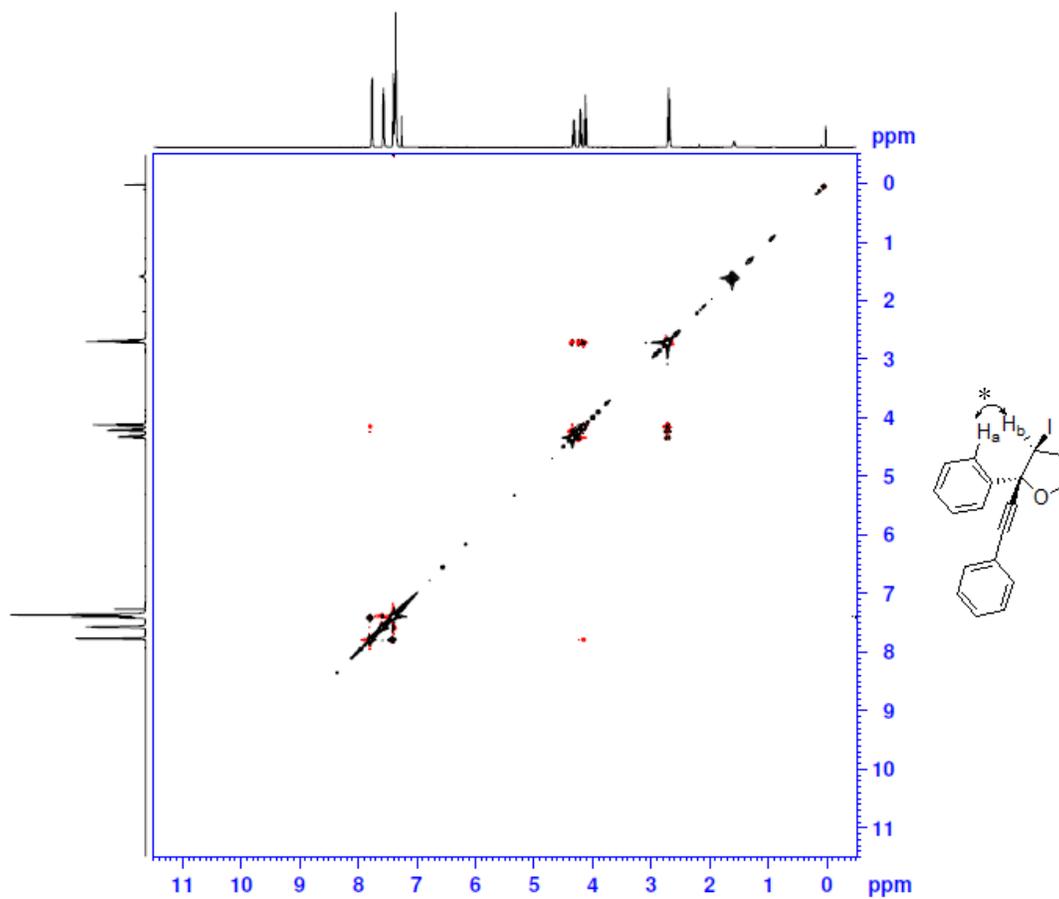


Figure S28. ^1H - ^1H NOESY Spectrum of *cis*-Tetrahydro-3-iodo-2-phenyl-2-(2-phenylethynyl)furan (**2a**)



* ^1H - ^1H NOESY correlation observed between H_a at 7.76 ppm and H_b at 4.11 ppm.

Figure S29. ^1H and ^{13}C NMR Spectra of 2,2-Bis(4-fluorophenyl)-tetrahydro-3-iodofuran

(2b)

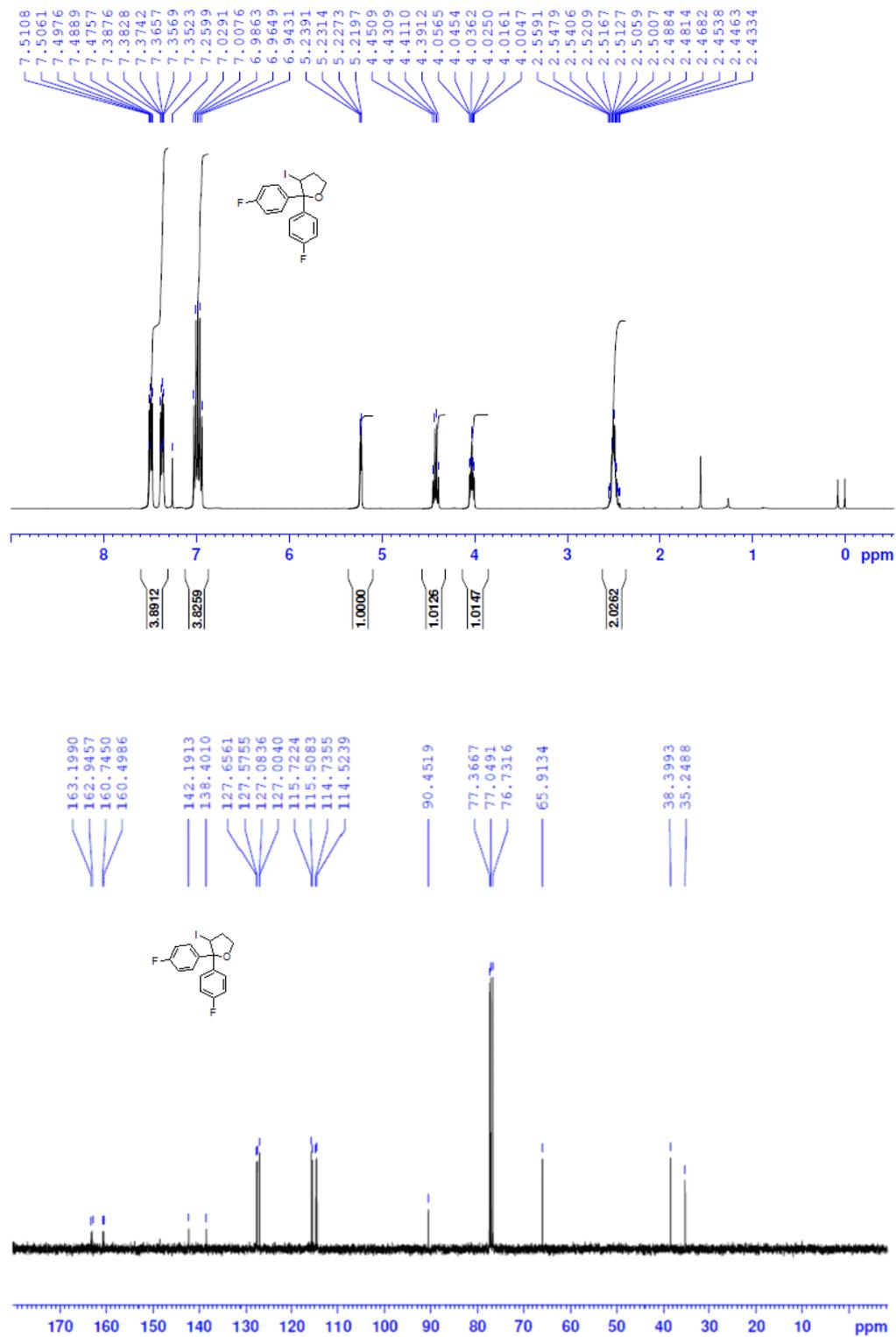


Figure S30. ^1H and ^{13}C NMR Spectra of 2,2-Bis(4-chlorophenyl)-tetrahydro-3-iodofuran

(2c)

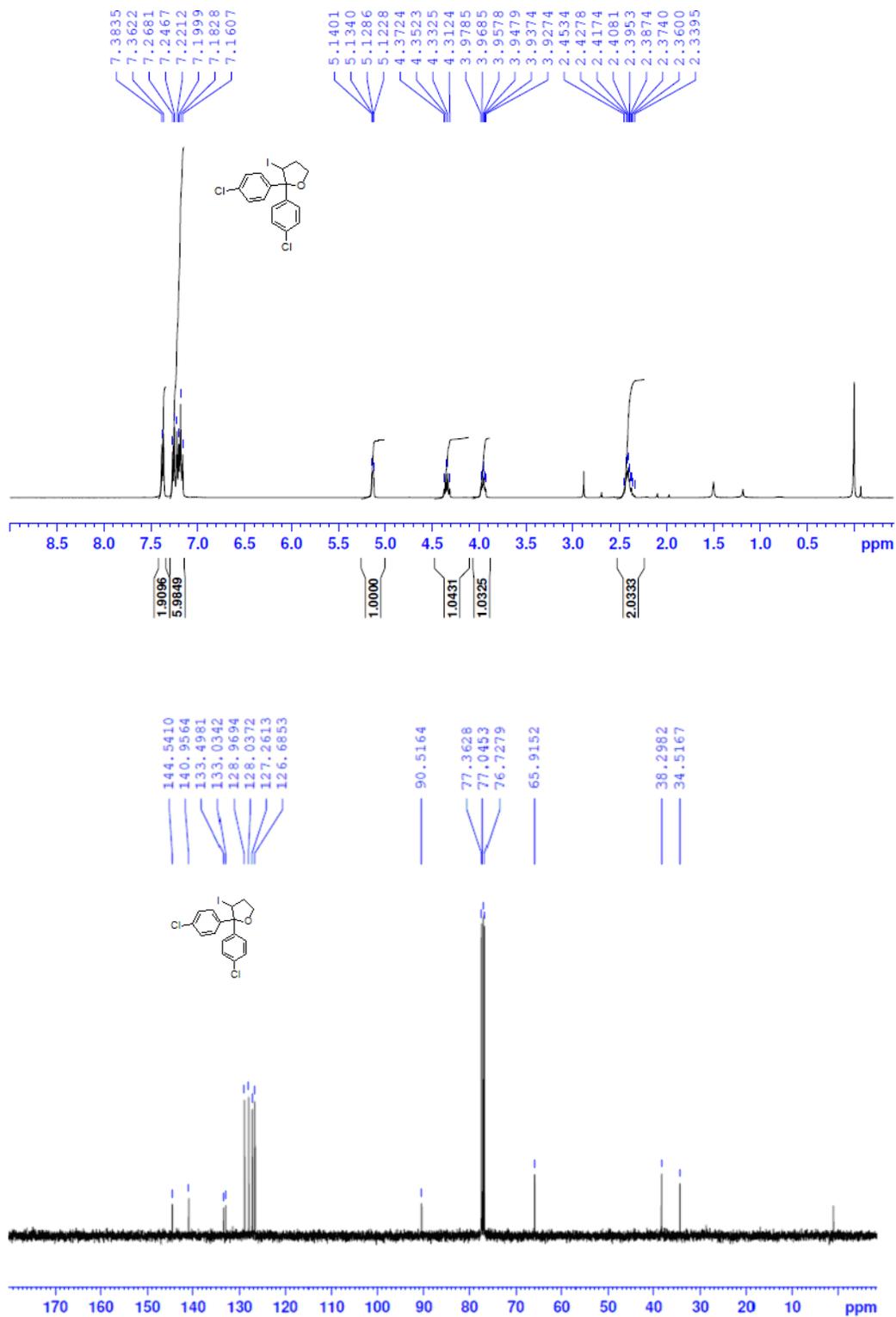


Figure S31. ^1H and ^{13}C NMR Spectra of 2,2-Bis(4-bromophenyl)-tetrahydro-3-iodofuran

(2d)

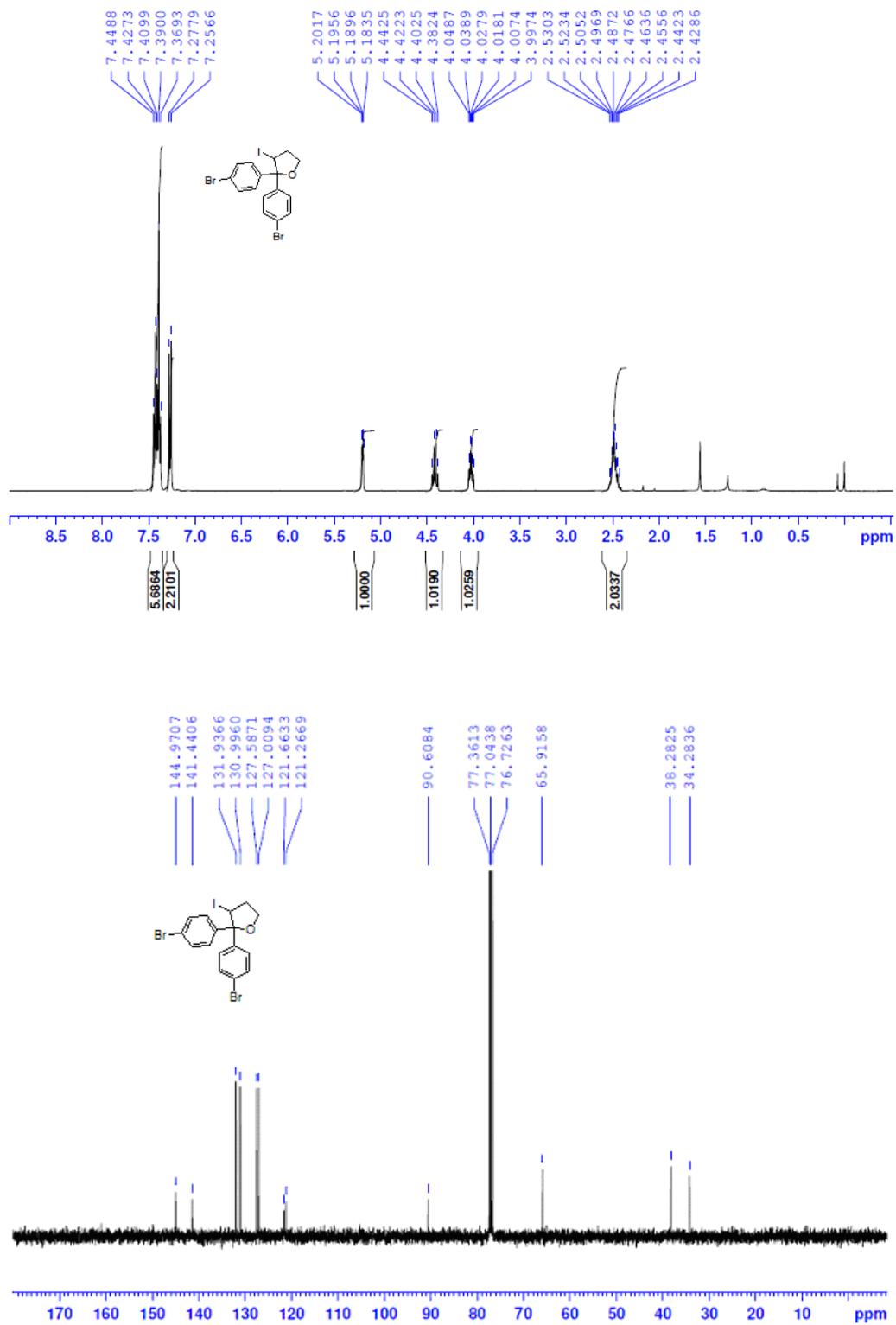


Figure S32. ^1H and ^{13}C NMR Spectra of Tetrahydro-3-iodo-2,2-diphenylfuran (**2e**)

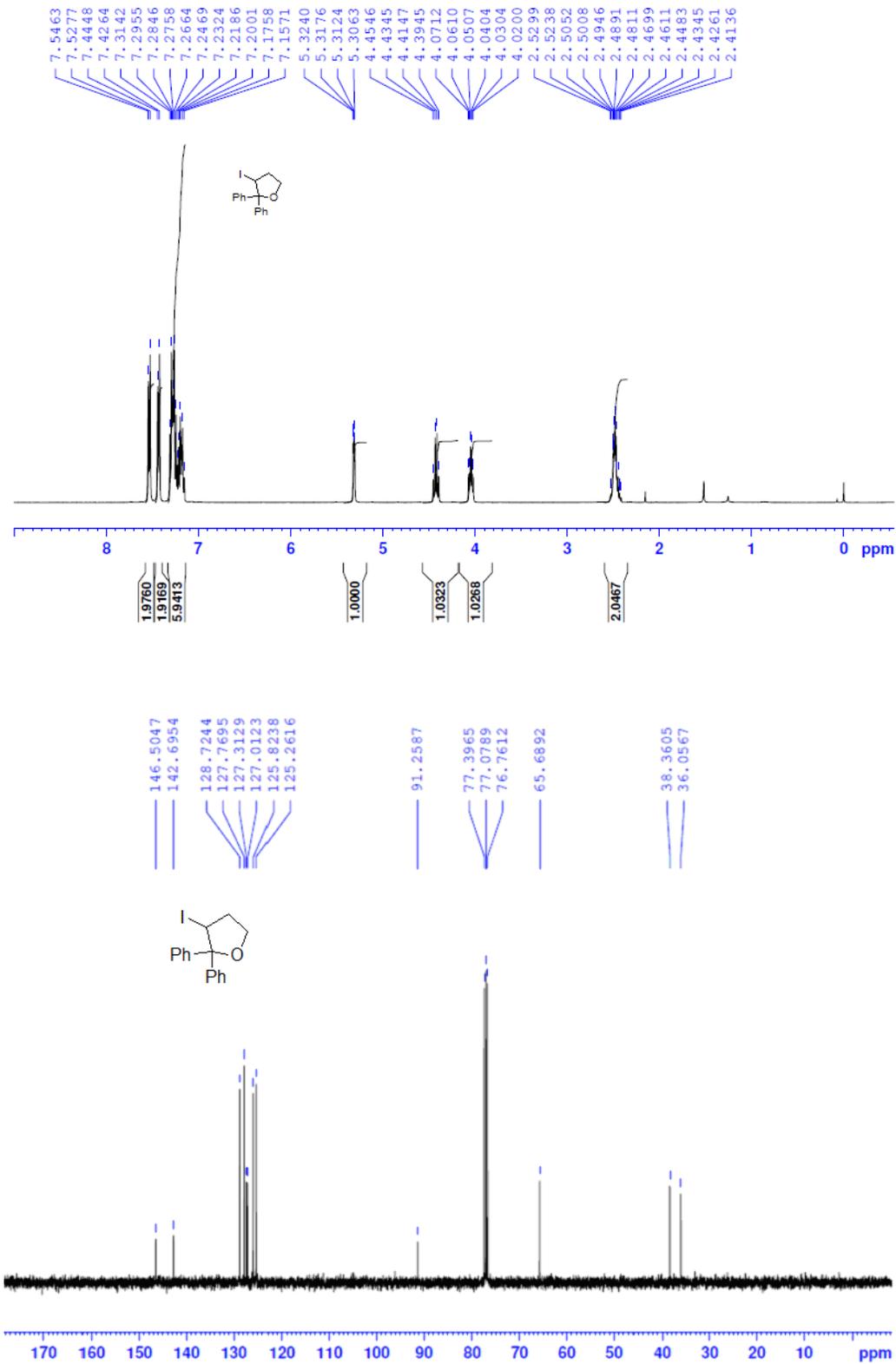


Figure S33. ^1H and ^{13}C NMR Spectra of Tetrahydro-3-iodo-2,2-dip-tolylfuran (**2f**)

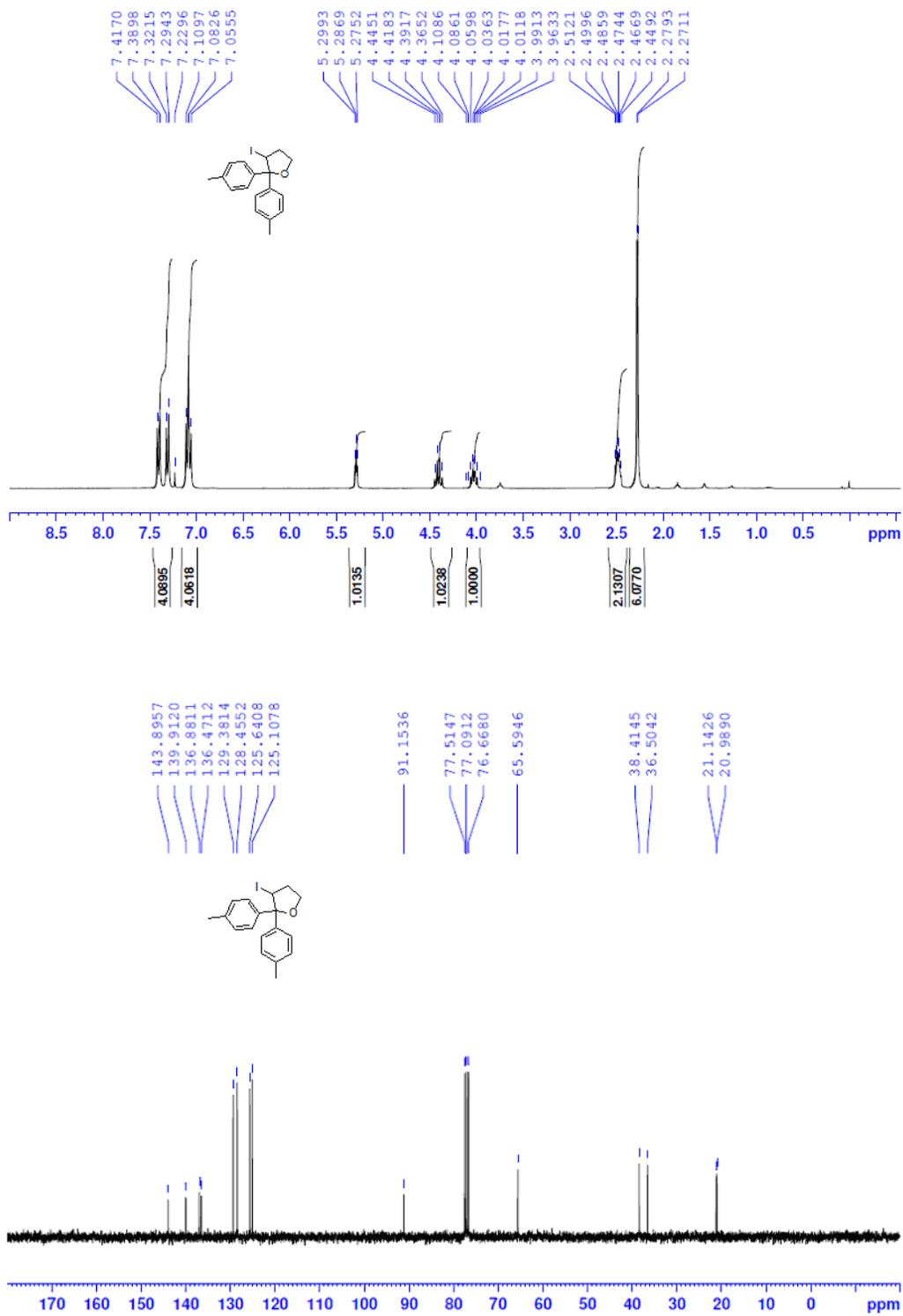


Figure S34. ^1H and ^{13}C NMR Spectra of Tetrahydro-3-iodo-2,2-bis(4-methoxyphenyl) furan (**2g**)

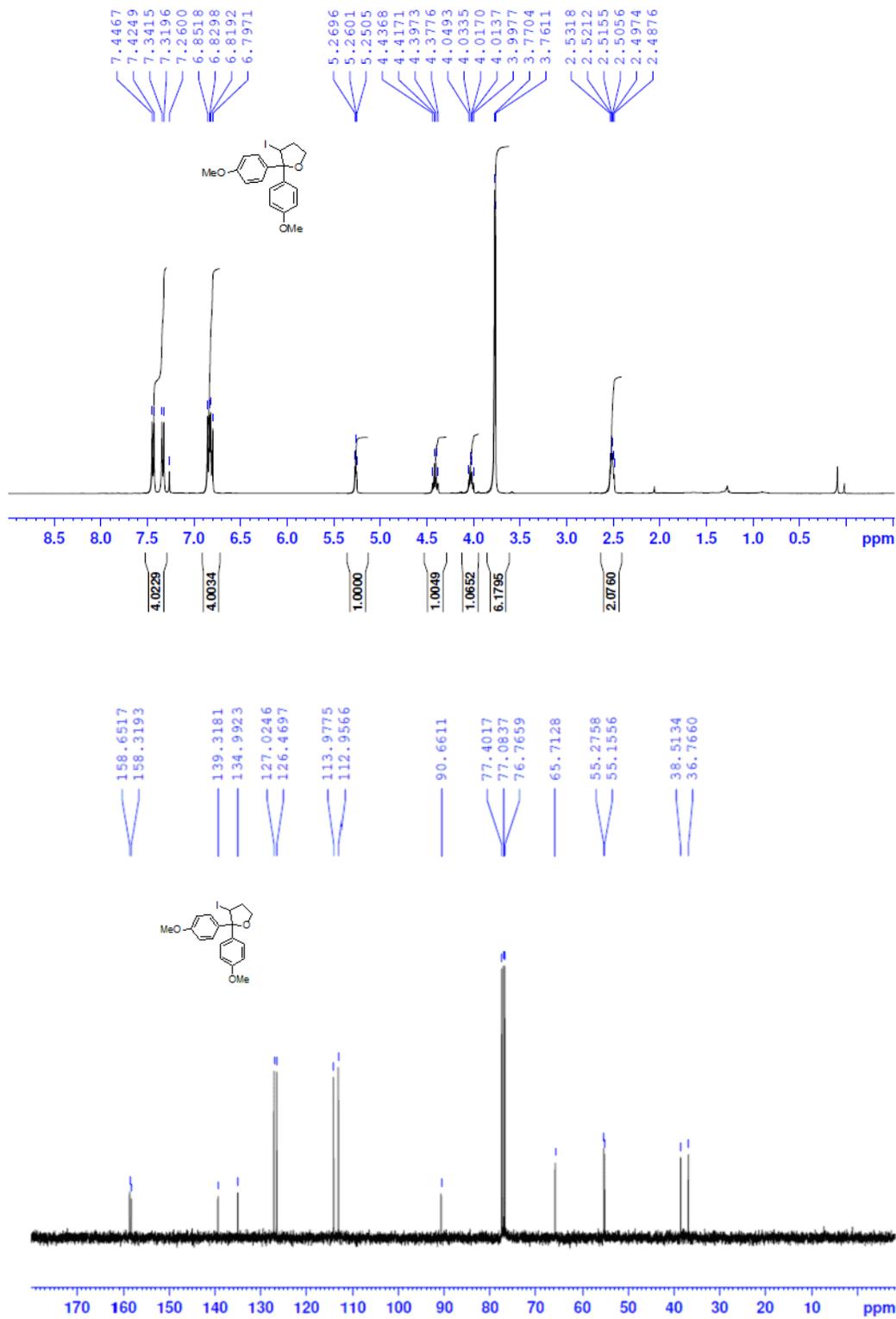


Figure S35. ^1H and ^{13}C NMR Spectra of 2-(4-Chlorophenyl)-tetrahydro-3-iodo-2-*p*-tolylfuran (**2h**)

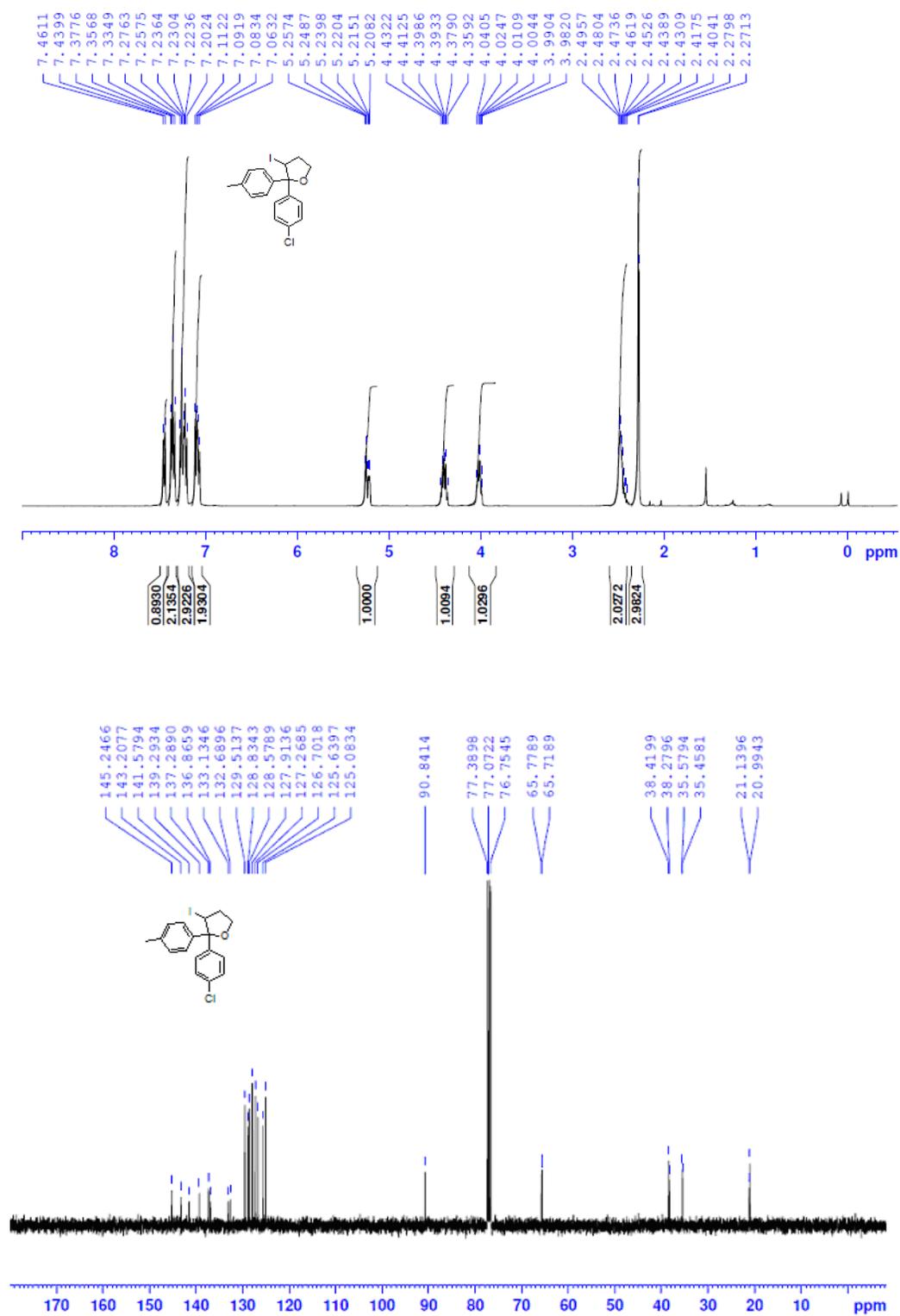


Figure S36. ^1H and ^{13}C NMR Spectra of 2-(4-Chlorophenyl)-tetrahydro-3-iodo-2-(4-methoxyphenyl)furan (**2i**)

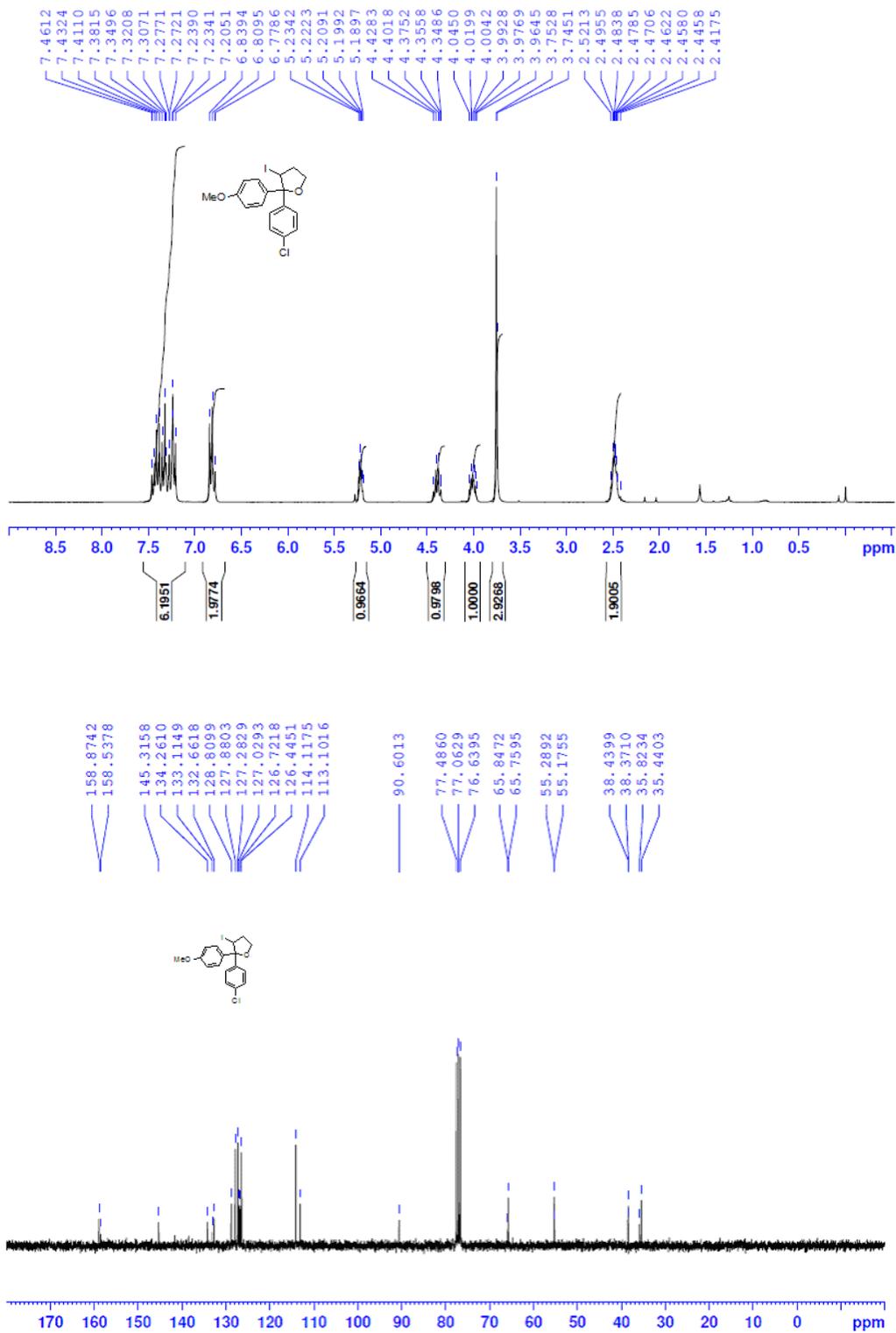


Figure S37. ^1H and ^{13}C NMR Spectra of Tetrahydro-3-iodo-2-phenyl-2-*p*-tolylfuran (**2j**)

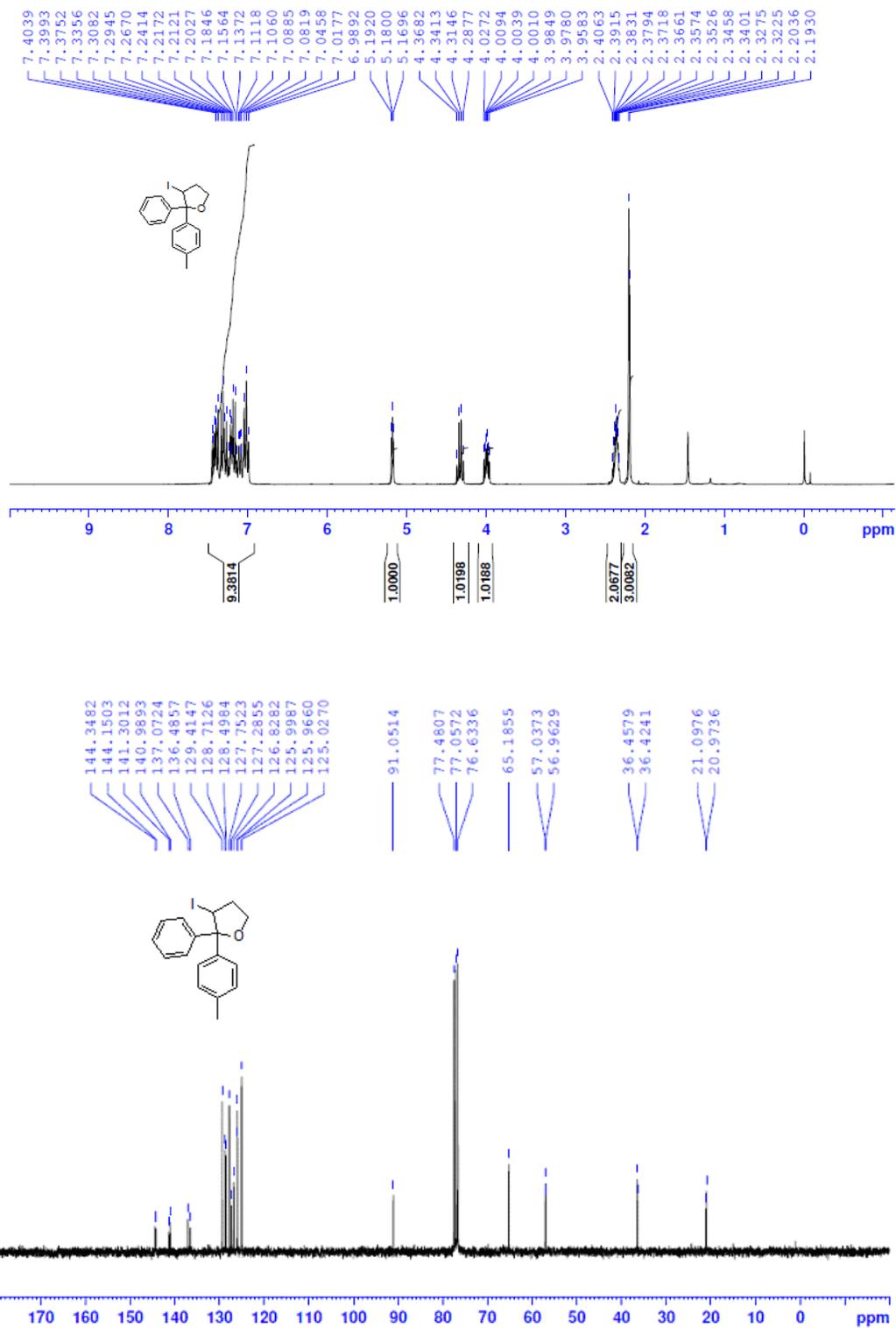


Figure S38. ^1H and ^{13}C NMR Spectra of 2-(4-Biphenyl)-tetrahydro-3-iodo-2-phenylfuran

(2k)

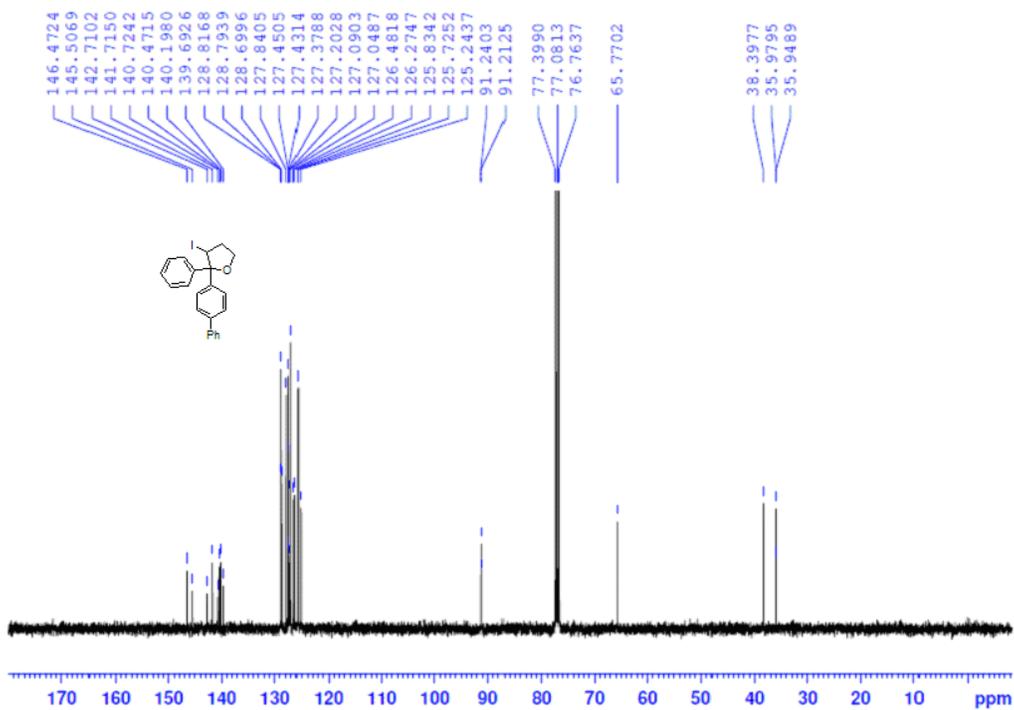
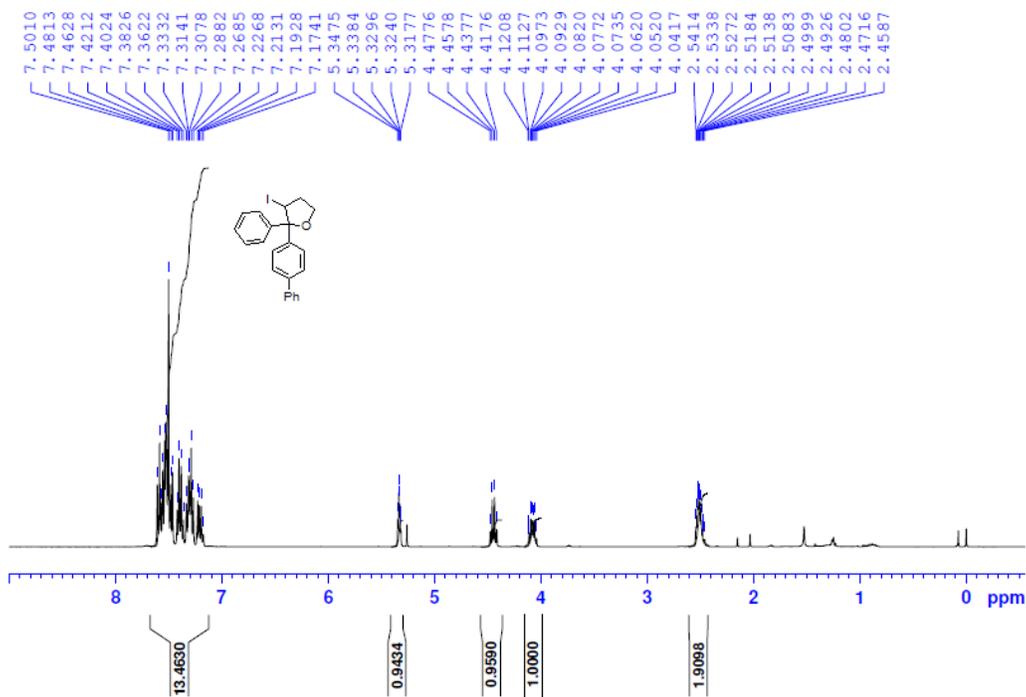


Figure S39. ^1H and ^{13}C NMR Spectra of Tetrahydro-3-iodo-2-(naphthalen-1-yl)-2-phenylfuran (**2l**)

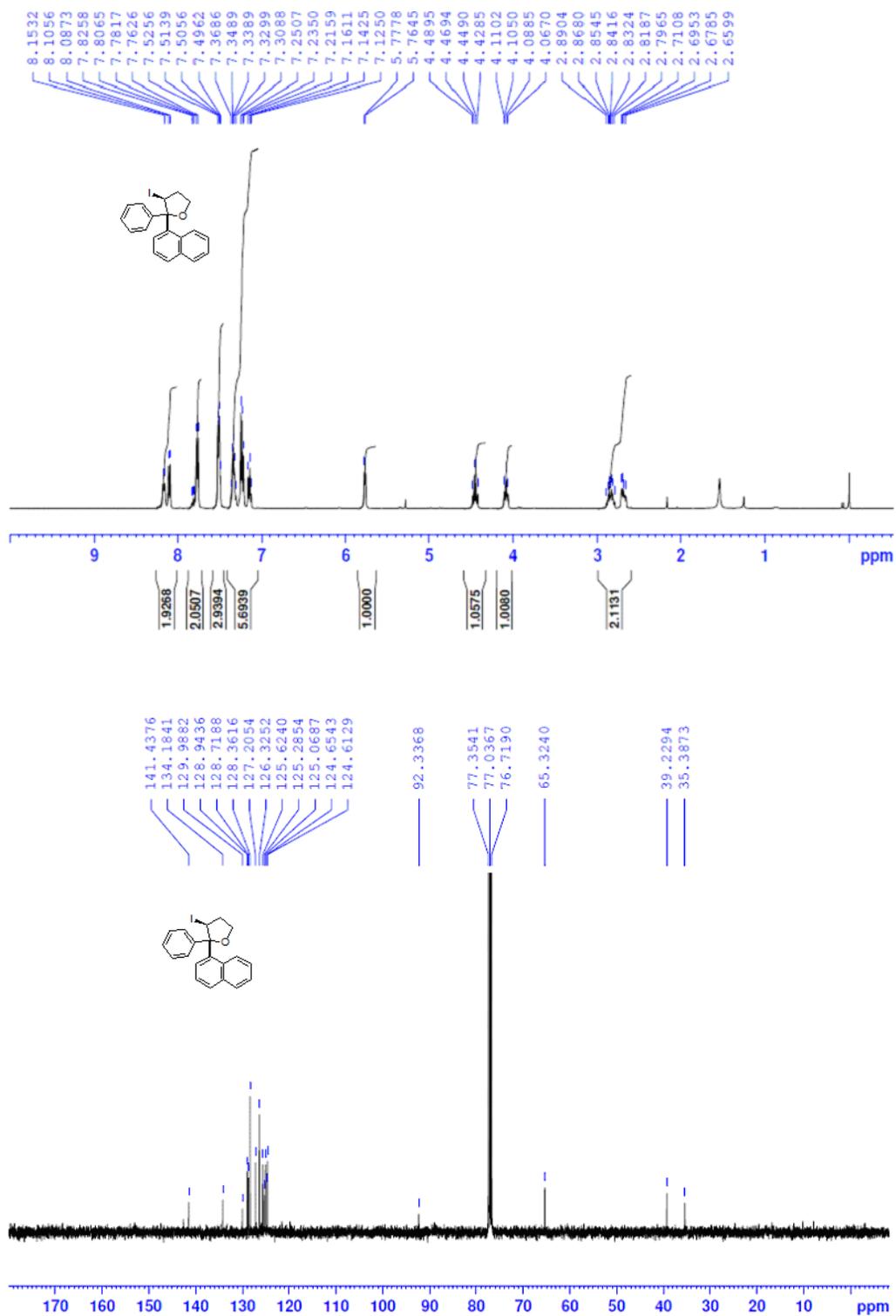


Figure S40. ¹H and ¹³C NMR Spectra of *cis*-Tetrahydro-3-iodo-2-pentyl-2-phenylfuran

(2m)

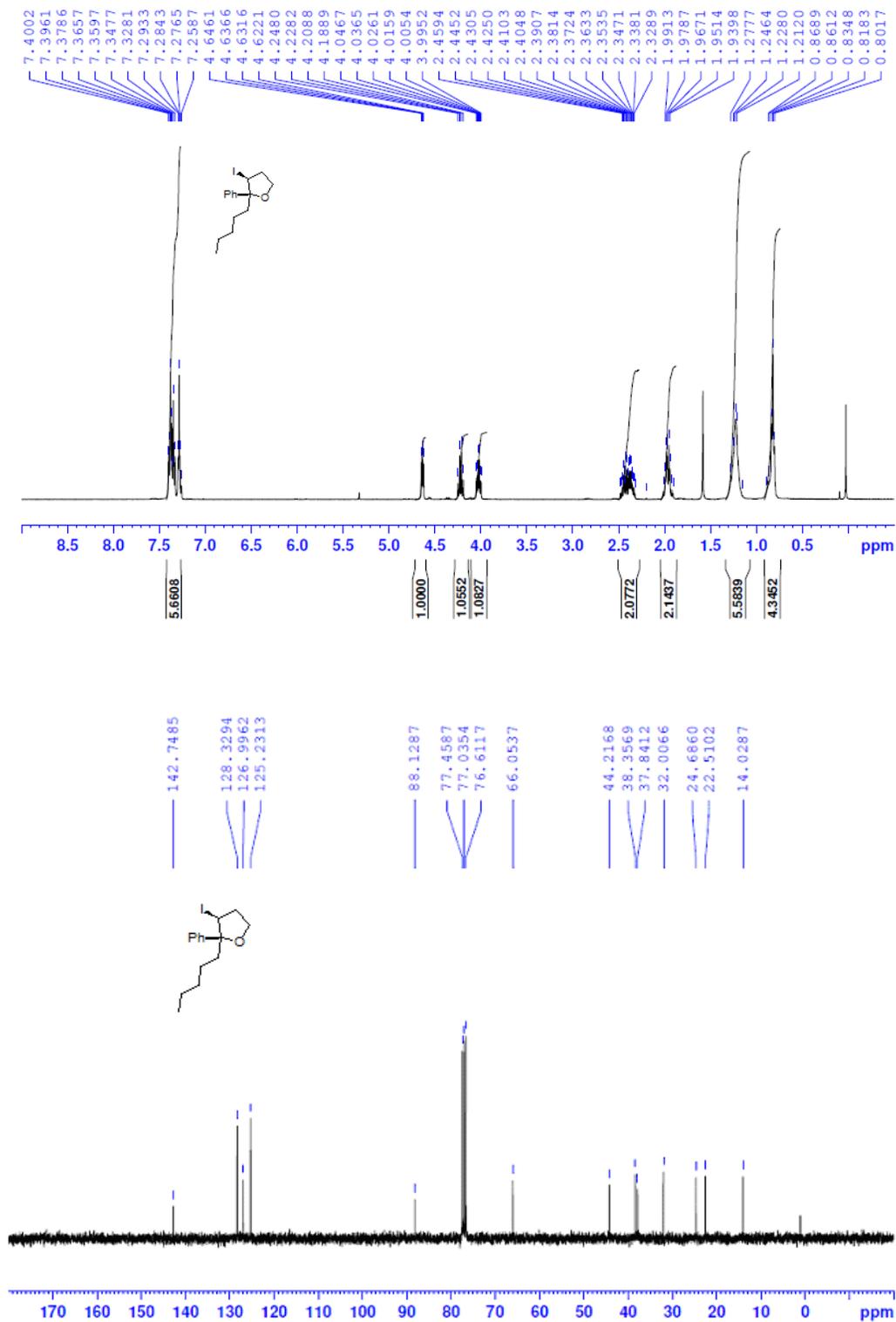
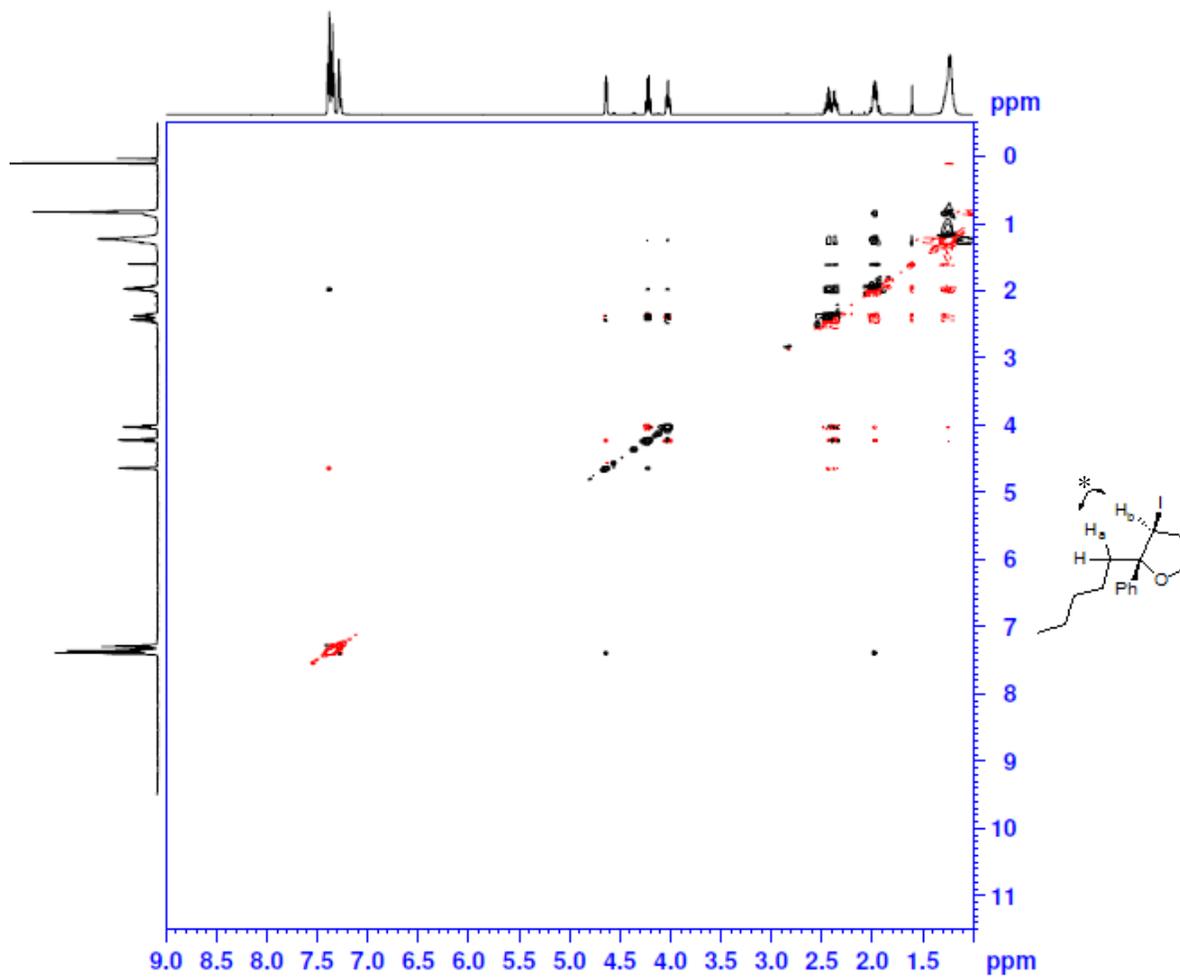


Figure S41. ^1H - ^1H NOESY Spectrum of *cis*-Tetrahydro-3-iodo-2-pentyl-2-phenylfuran

(2m)



* ^1H - ^1H NOESY correlation observed between H_a at 1.96 ppm and H_b at 4.02 ppm.

Figure S42. Expansion of NOESY Spectrum of *cis*-Tetrahydro-3-iodo-2-pentyl-2-phenylfuran (**2m**)

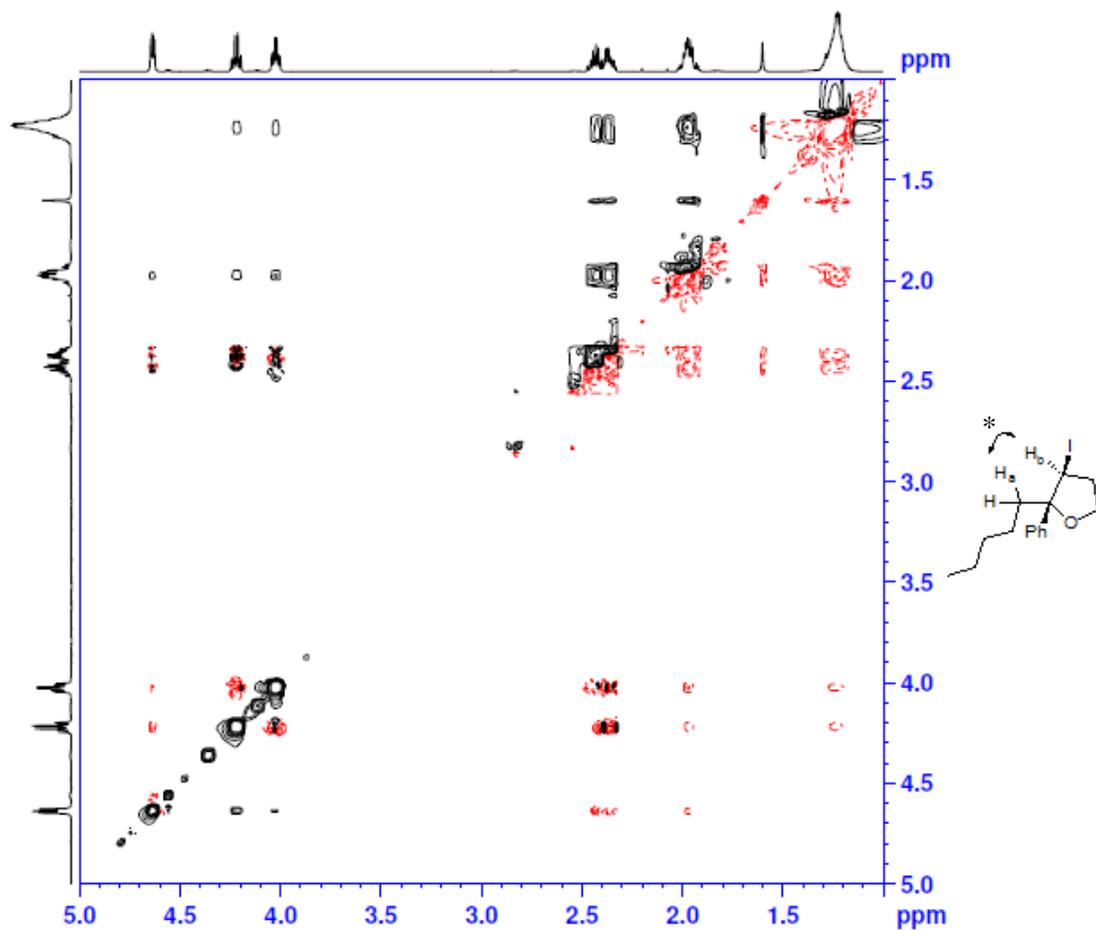


Figure S43. ^1H and ^{13}C NMR Spectra of 2-tert-Butyl-tetrahydro-3-iodo-2-phenylfuran (**2n**)

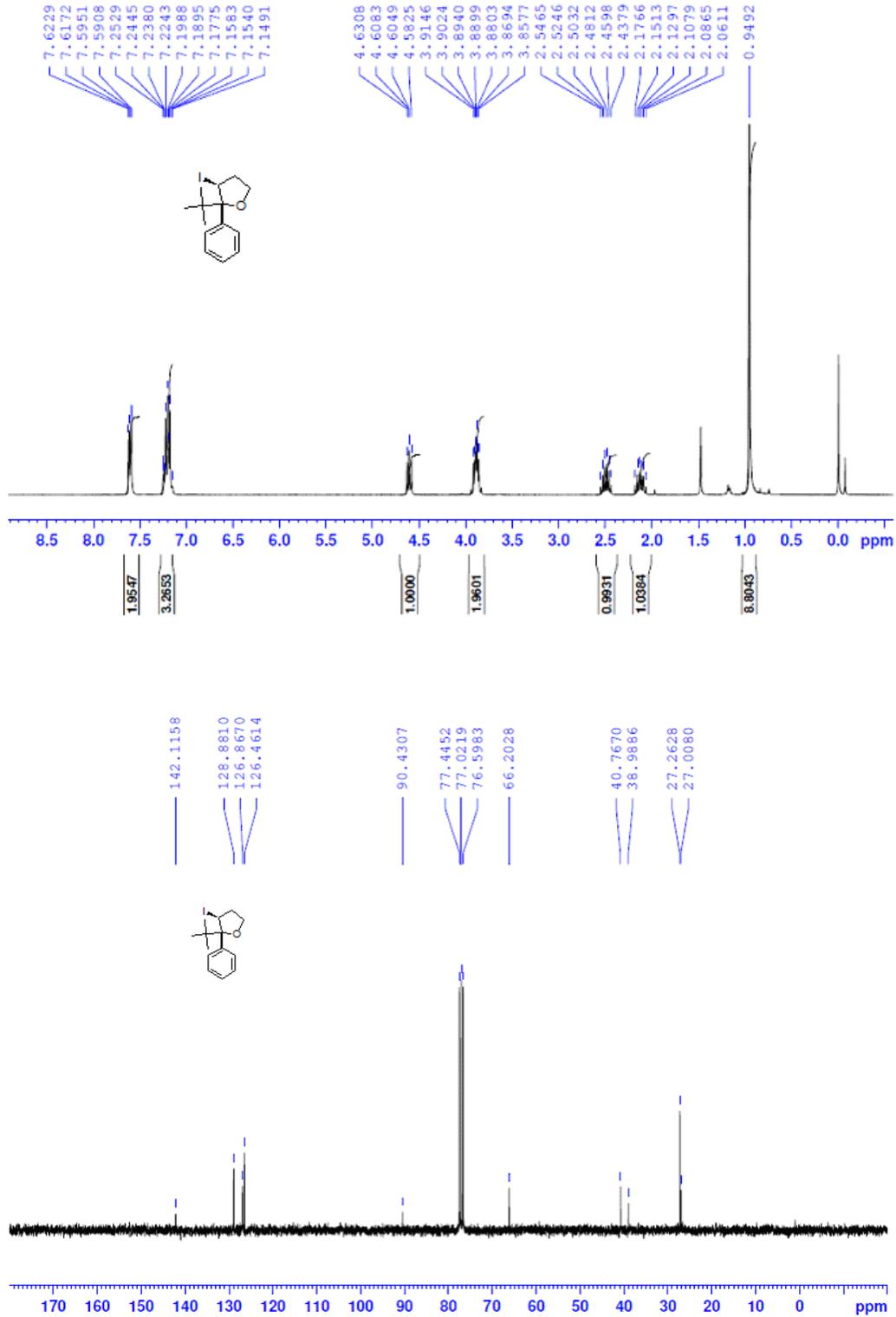


Figure S44. ^1H and ^{13}C NMR Spectra of *Cis*-2-(4-chlorophenyl)-tetrahydro-3-iodo-2-(2-(thiophen-2-yl)ethynyl)furan (**2o**)

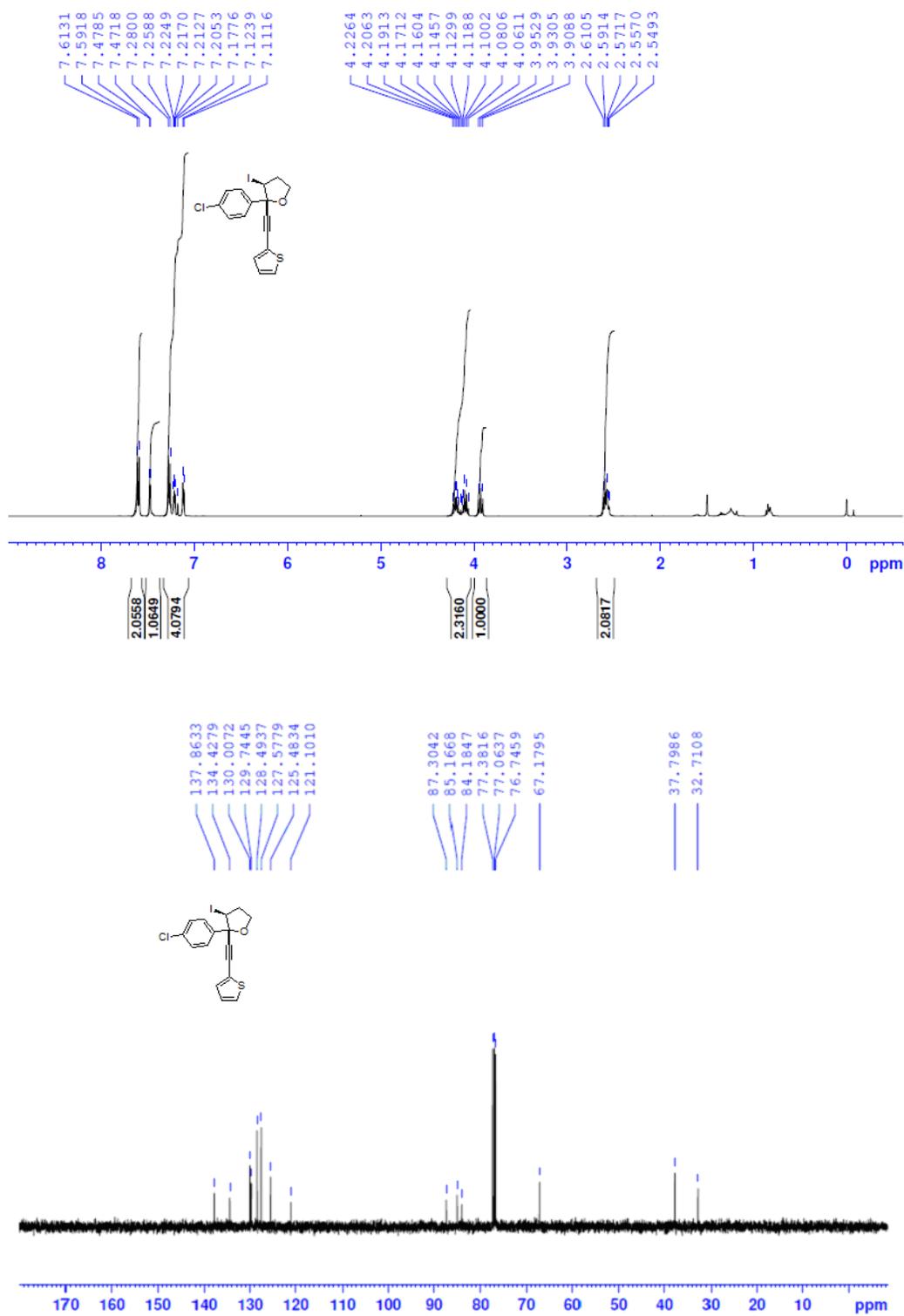


Figure S45. ^1H and ^{13}C NMR Spectra of *Cis*-2-(2-(tetrahydro-3-iodo-2-(4-methoxyphenyl)furan-2-yl)ethynyl)pyridine (**2p**)

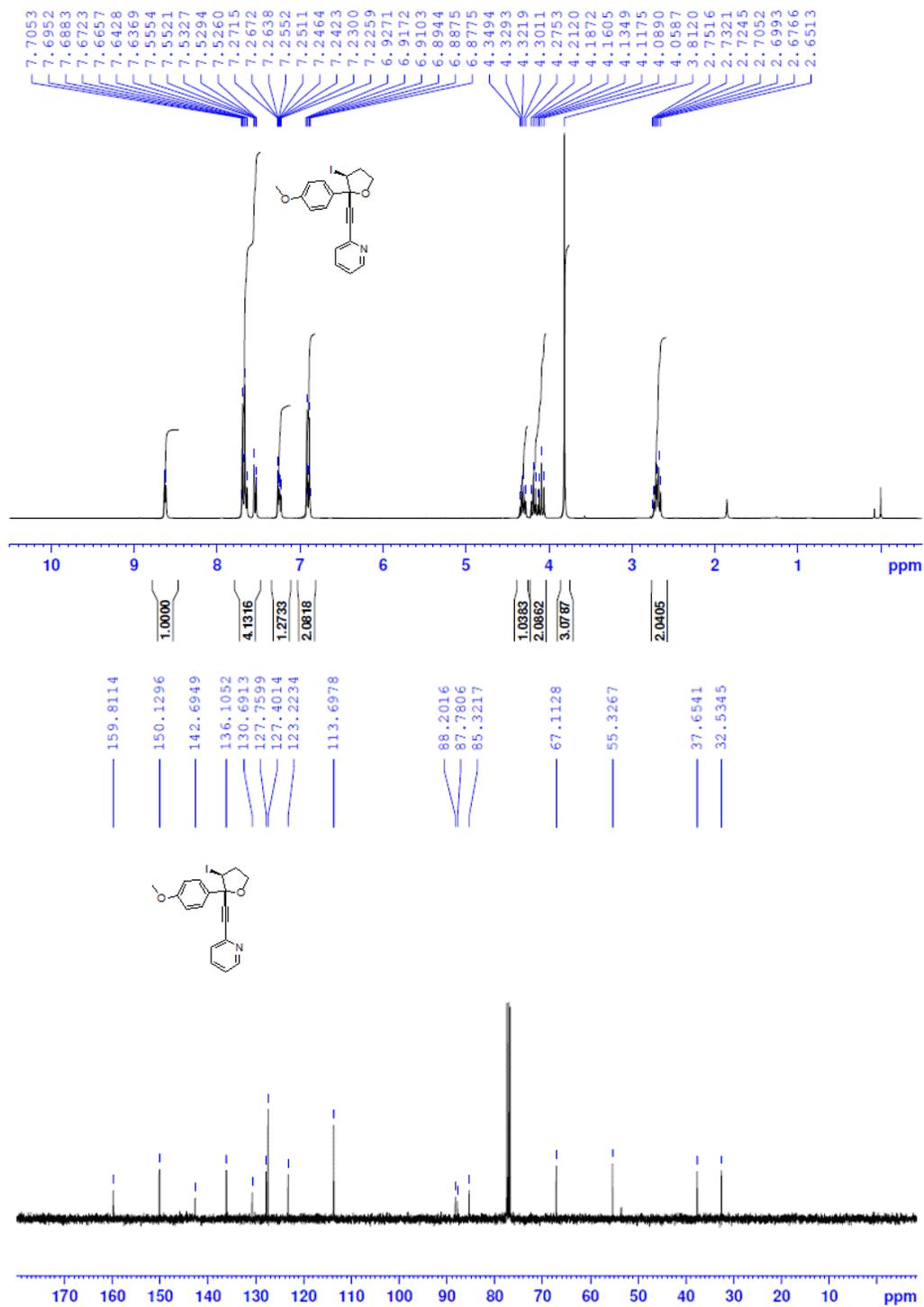


Figure S46. ^1H and ^{13}C NMR Spectra of Tetrahydro-3-iodo-2,2-bis(2-phenylethynyl)furan

(2q)

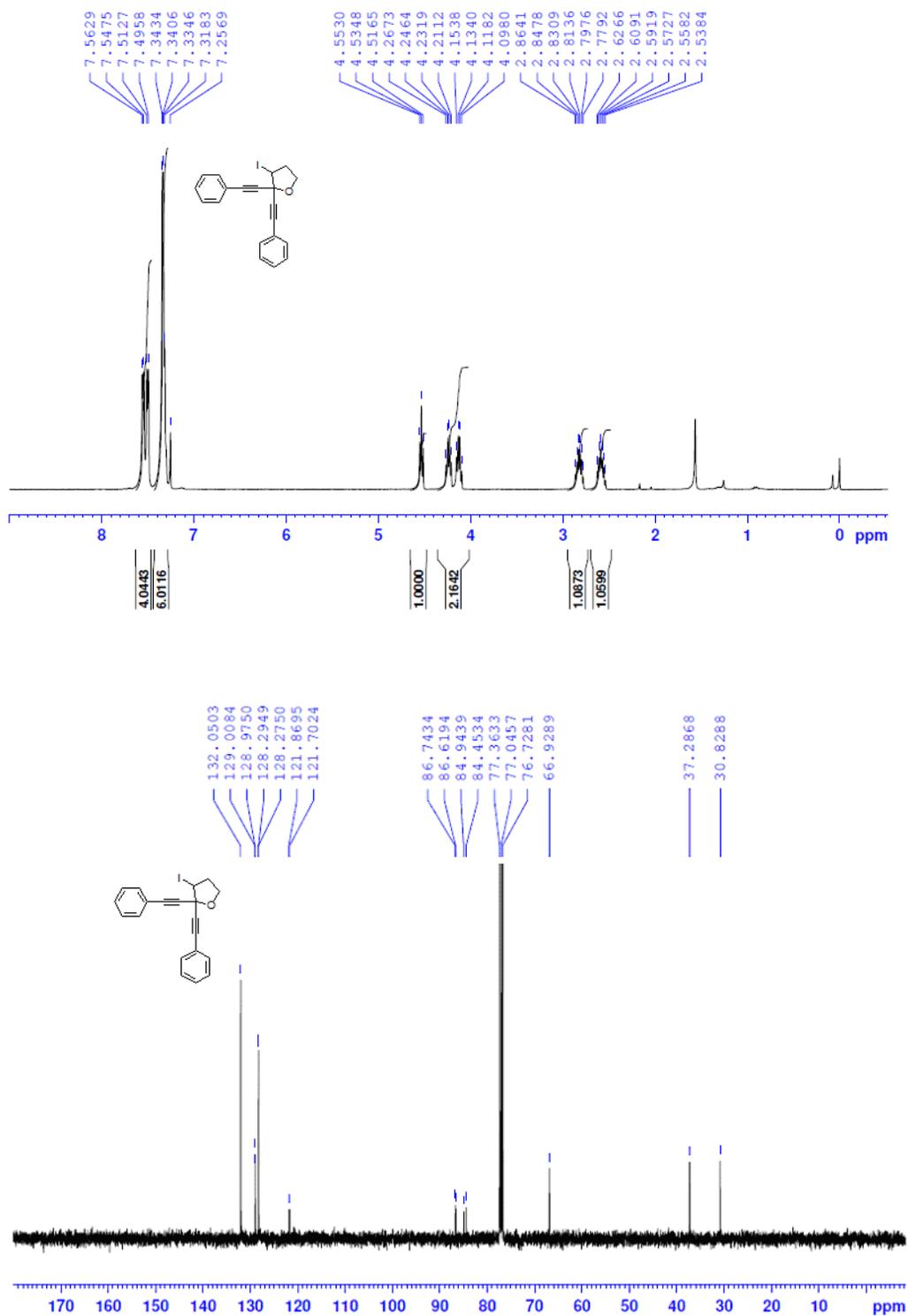


Figure S47. ^1H and ^{13}C NMR Spectra of Tetrahydro-3-iodo-2-(1-methylcyclohexyl)-2-(2-phenylethynyl)furan (**2r**)

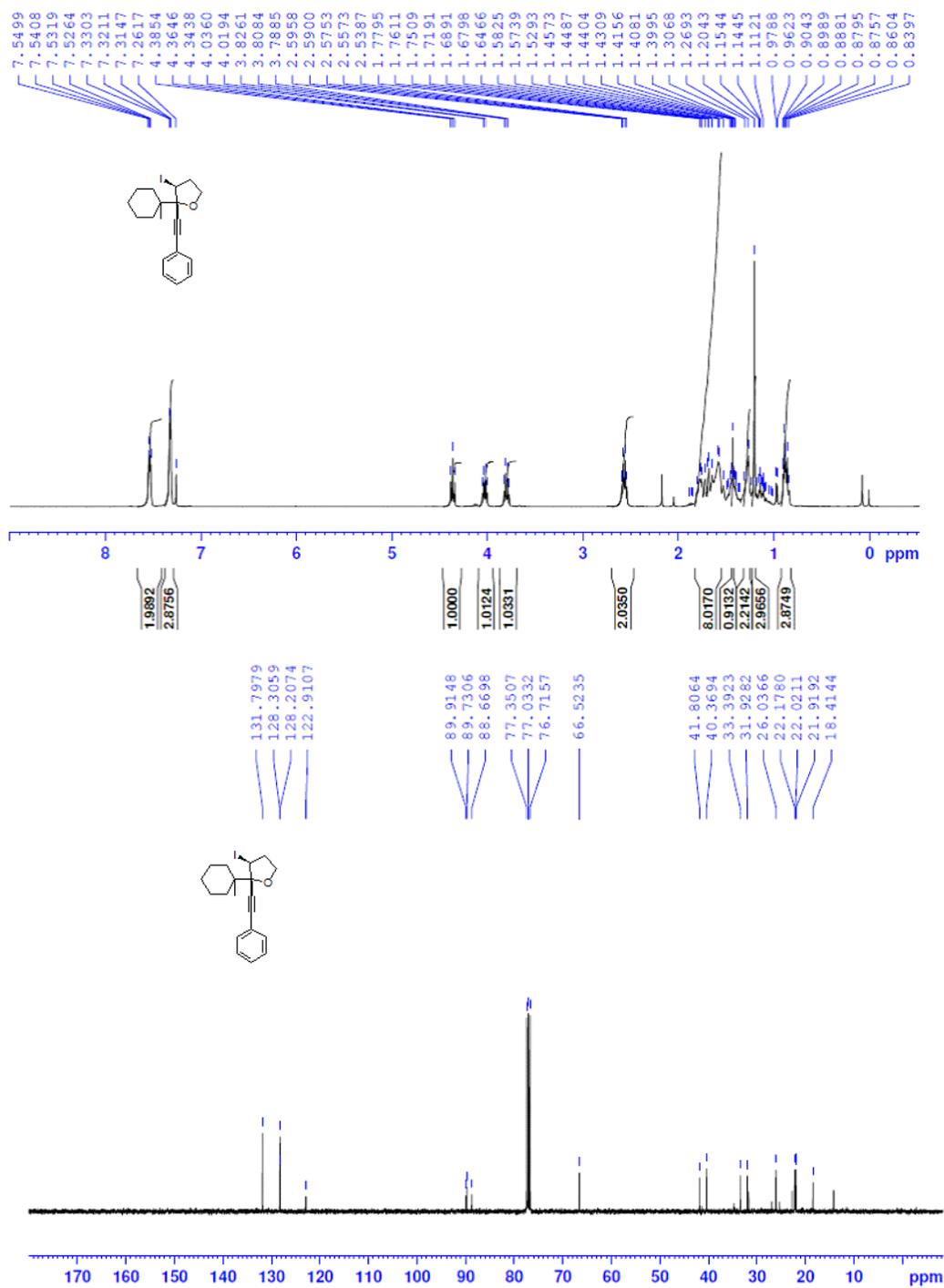


Figure S48. ^1H and ^{13}C NMR Spectra of Tetrahydro-3-iodo-2,2,5-triphenylfuran (**2t**)

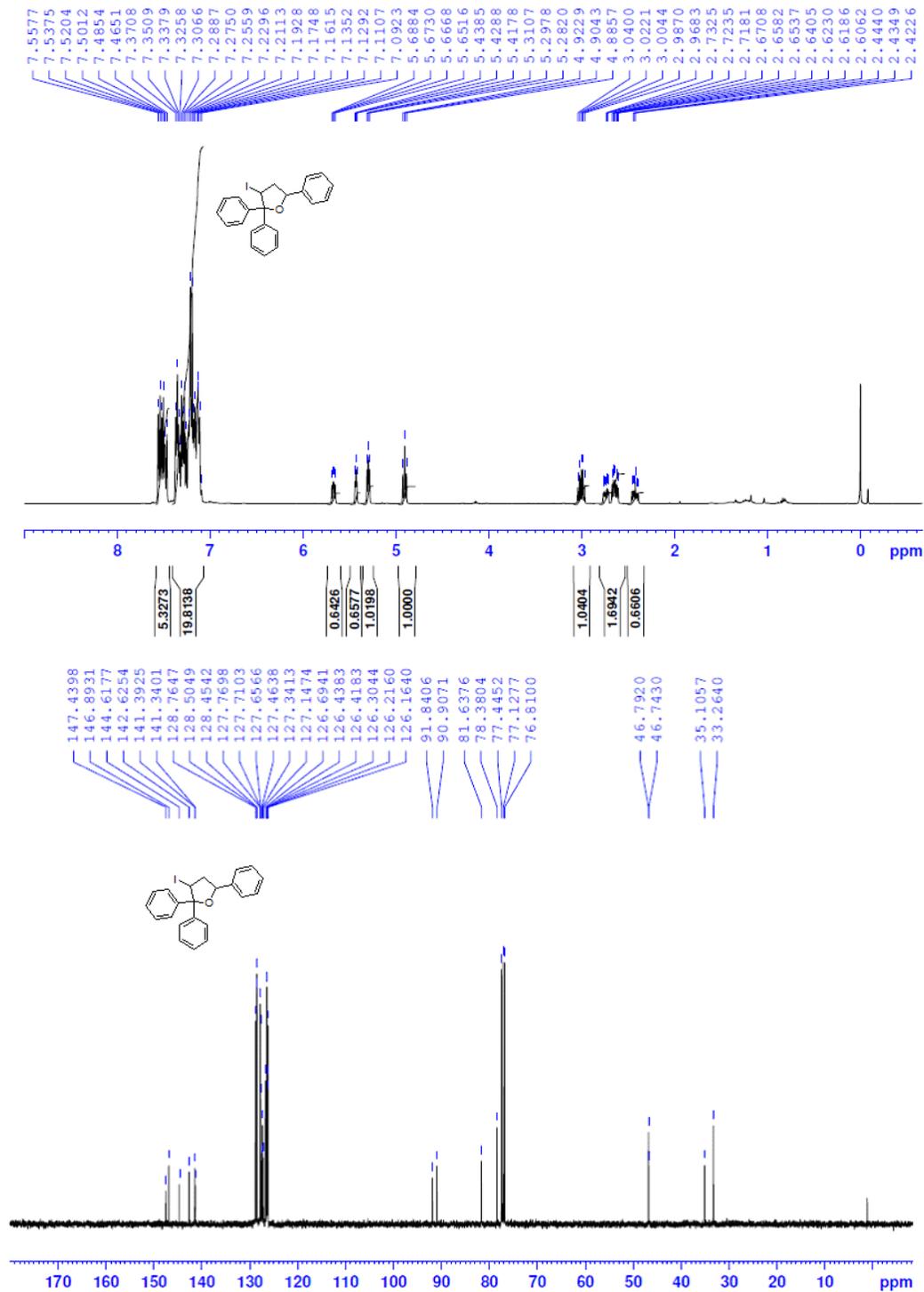


Figure S49. ^1H and ^{13}C NMR Spectra of Tetrahydro-3-iodo-5-pentyl-2,2-diphenylfuran

(2u)

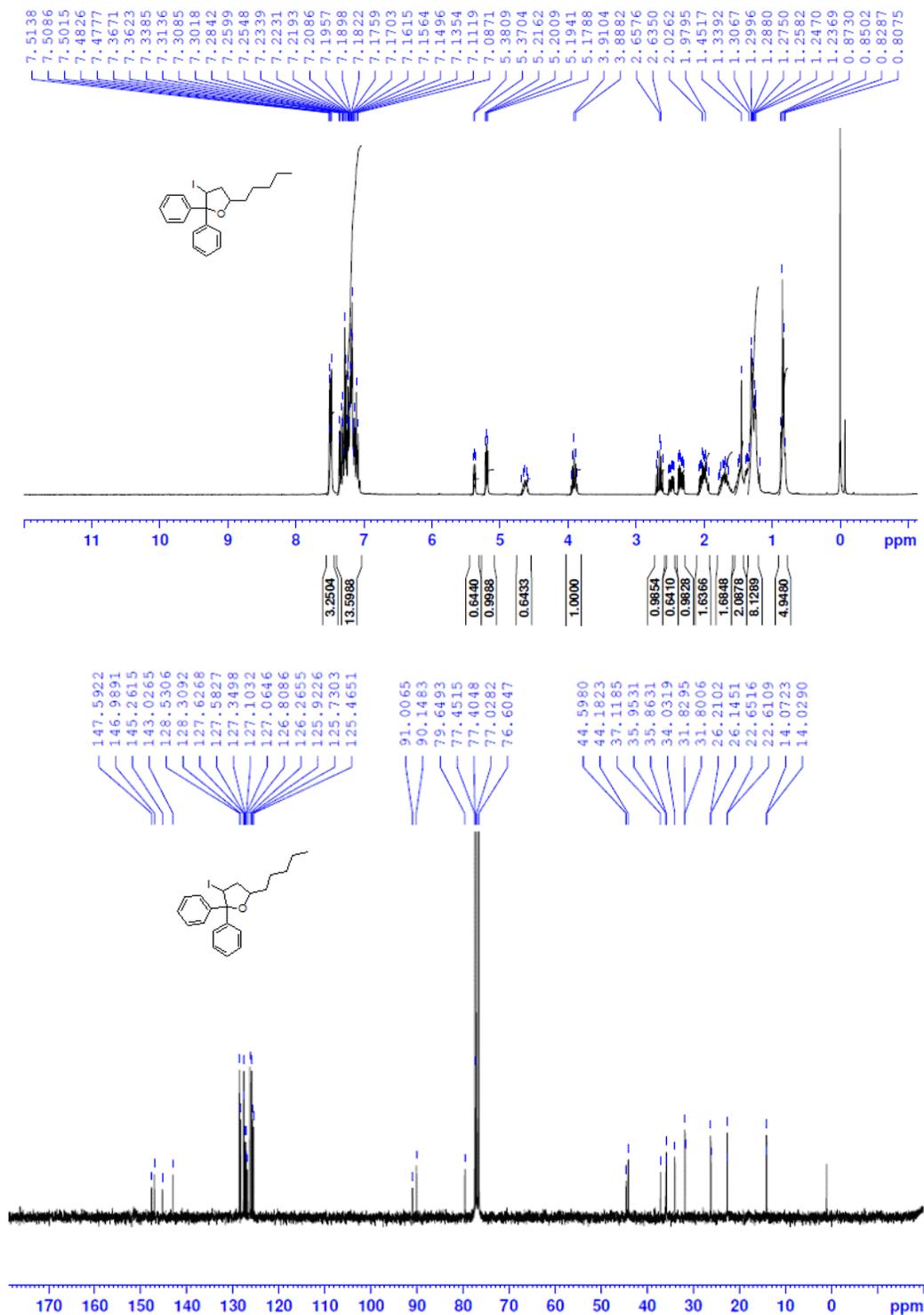


Figure S50. ^1H and ^{13}C NMR Spectra of Tetrahydro-3-iodo-2-(2-phenylethynyl)-5-(thiophen-2-yl)furan (**2v**)

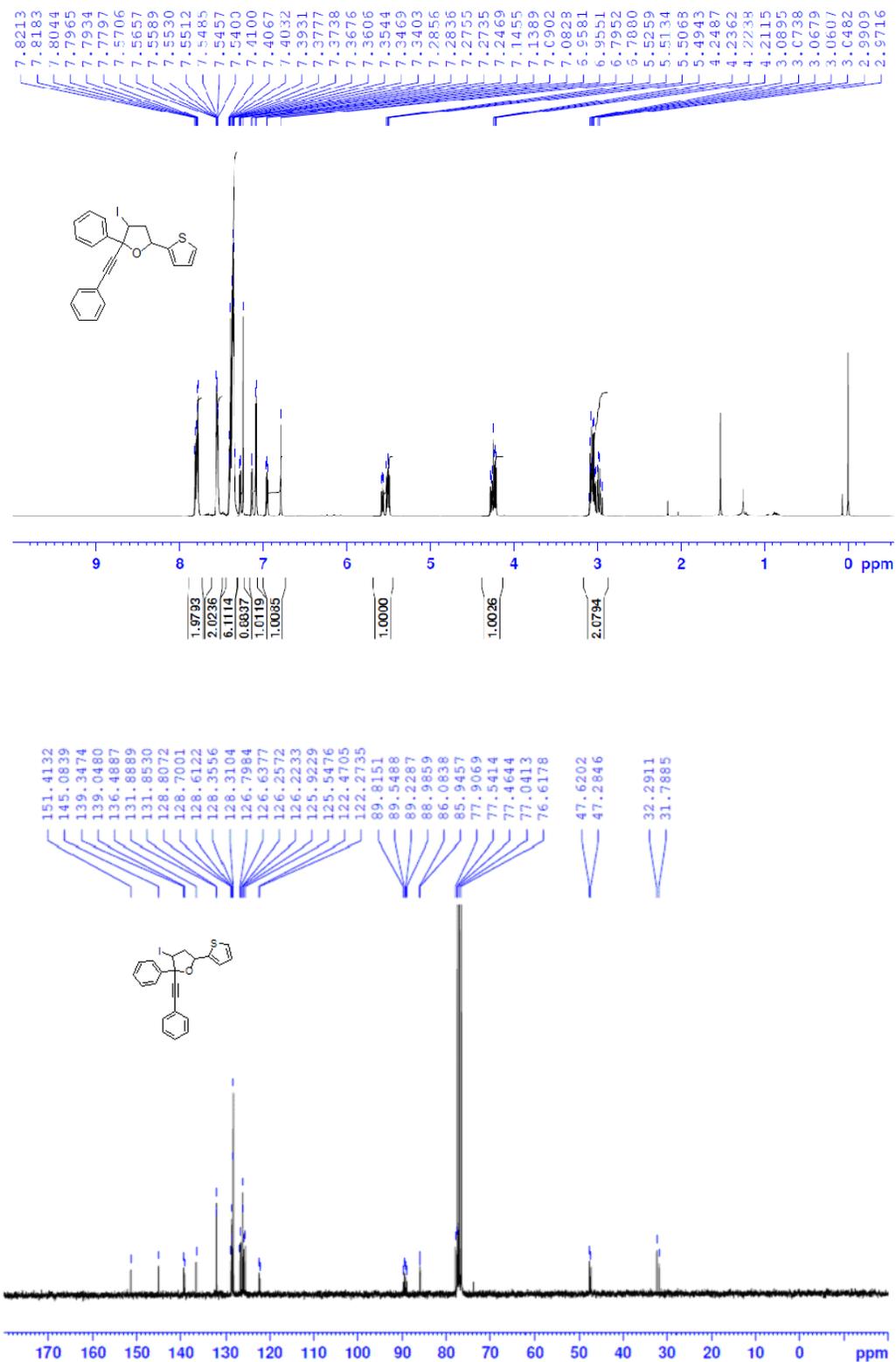
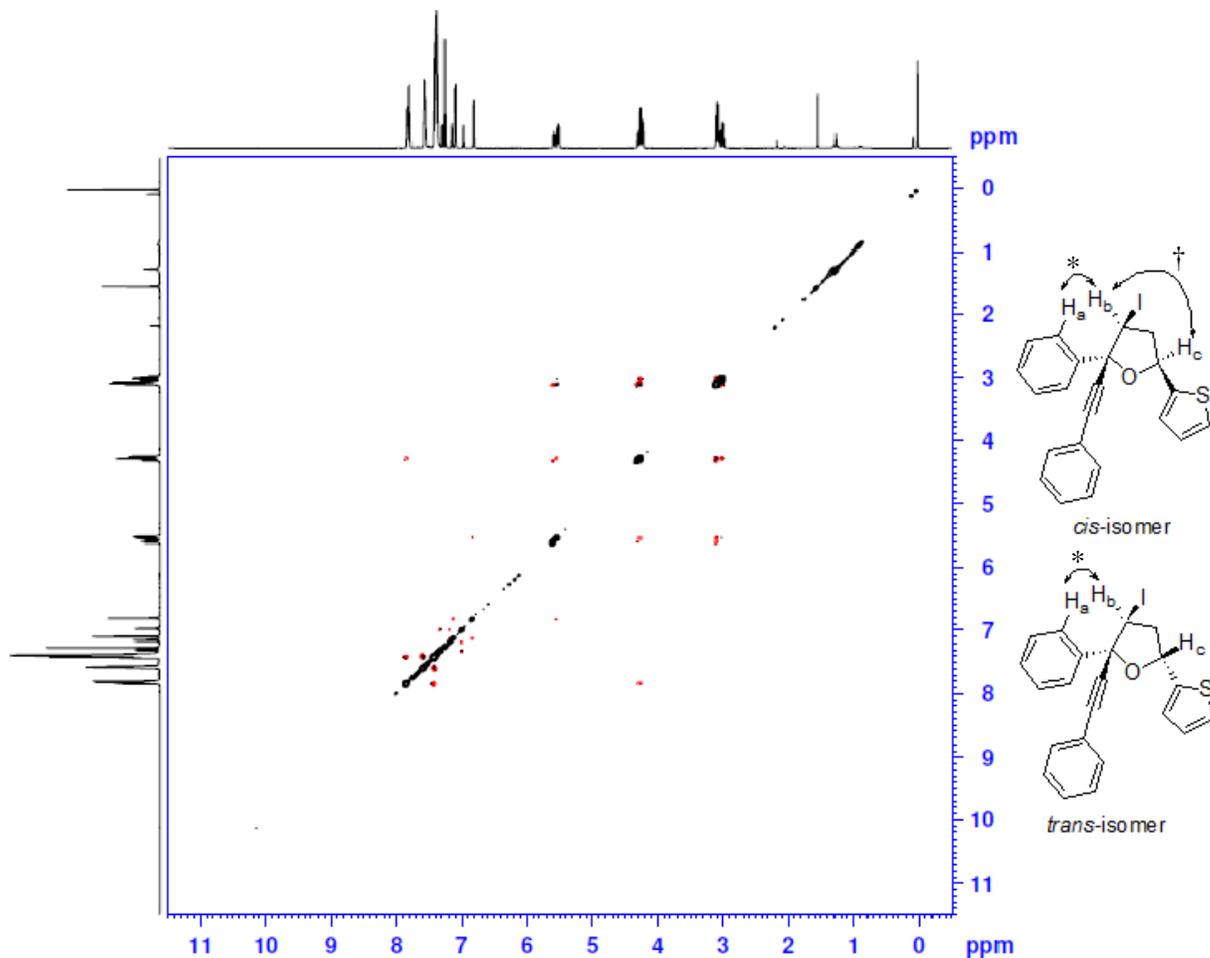


Figure S51. ^1H - ^1H NOESY Spectrum of Tetrahydro-3-iodo-2-phenyl-2-(2-phenylethynyl)-5-(thiophen-2-yl)furan (**2v**)



* ^1H - ^1H NOESY correlation observed between H_a at 7.82 ppm and H_b at 4.24 ppm.

† ^1H - ^1H NOESY correlation observed between H_c at 5.52 ppm and H_b at 4.24 ppm.

Figure S52. ^1H and ^{13}C NMR Spectra of Tetrahydro-3-iodo-2-phenylfuran (**2w**)

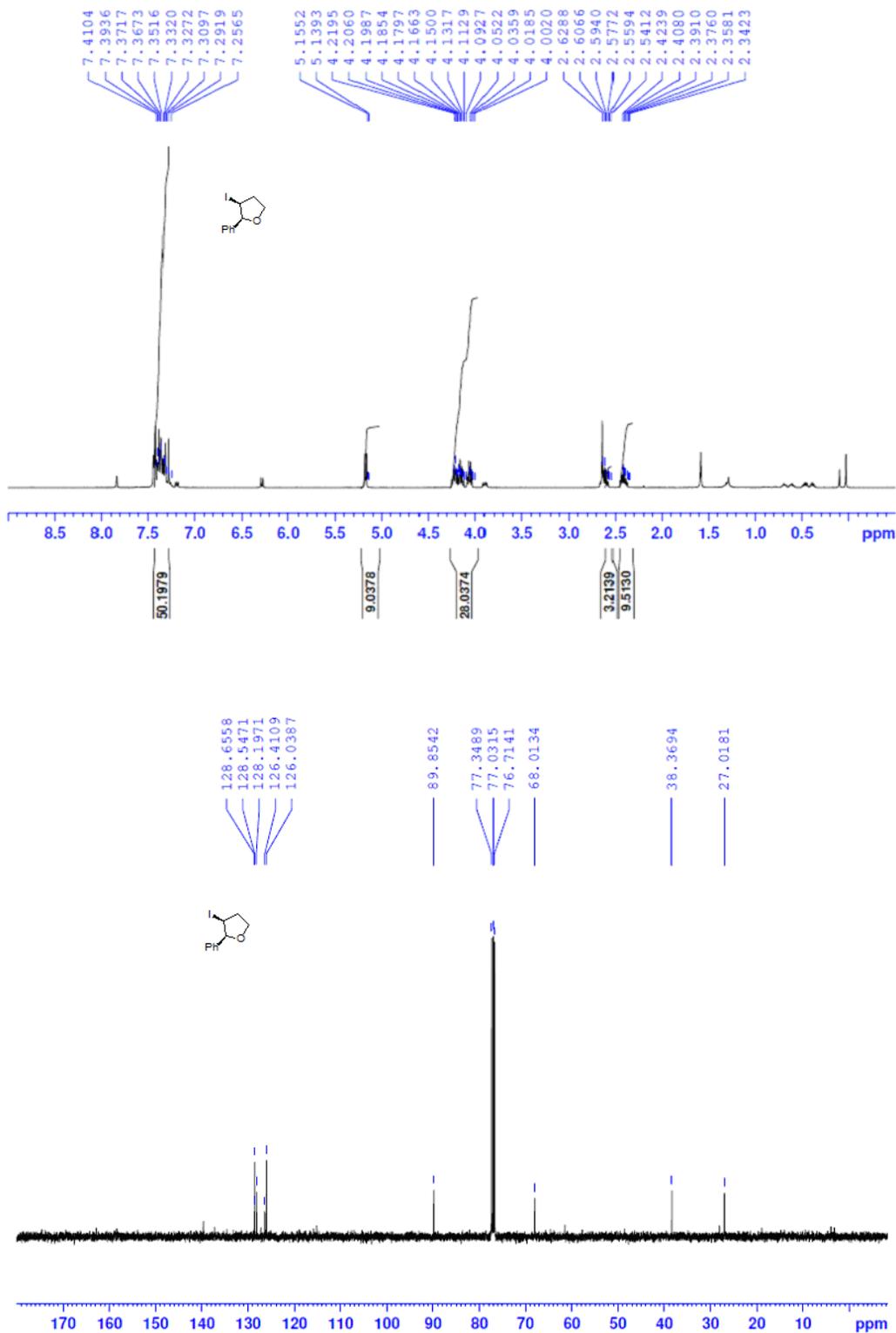


Figure S53. ^1H and ^{13}C NMR Spectra of *Cis*-3-bromo-tetrahydro-2-phenyl-2-(2-phenylethynyl)furan (**2y**)

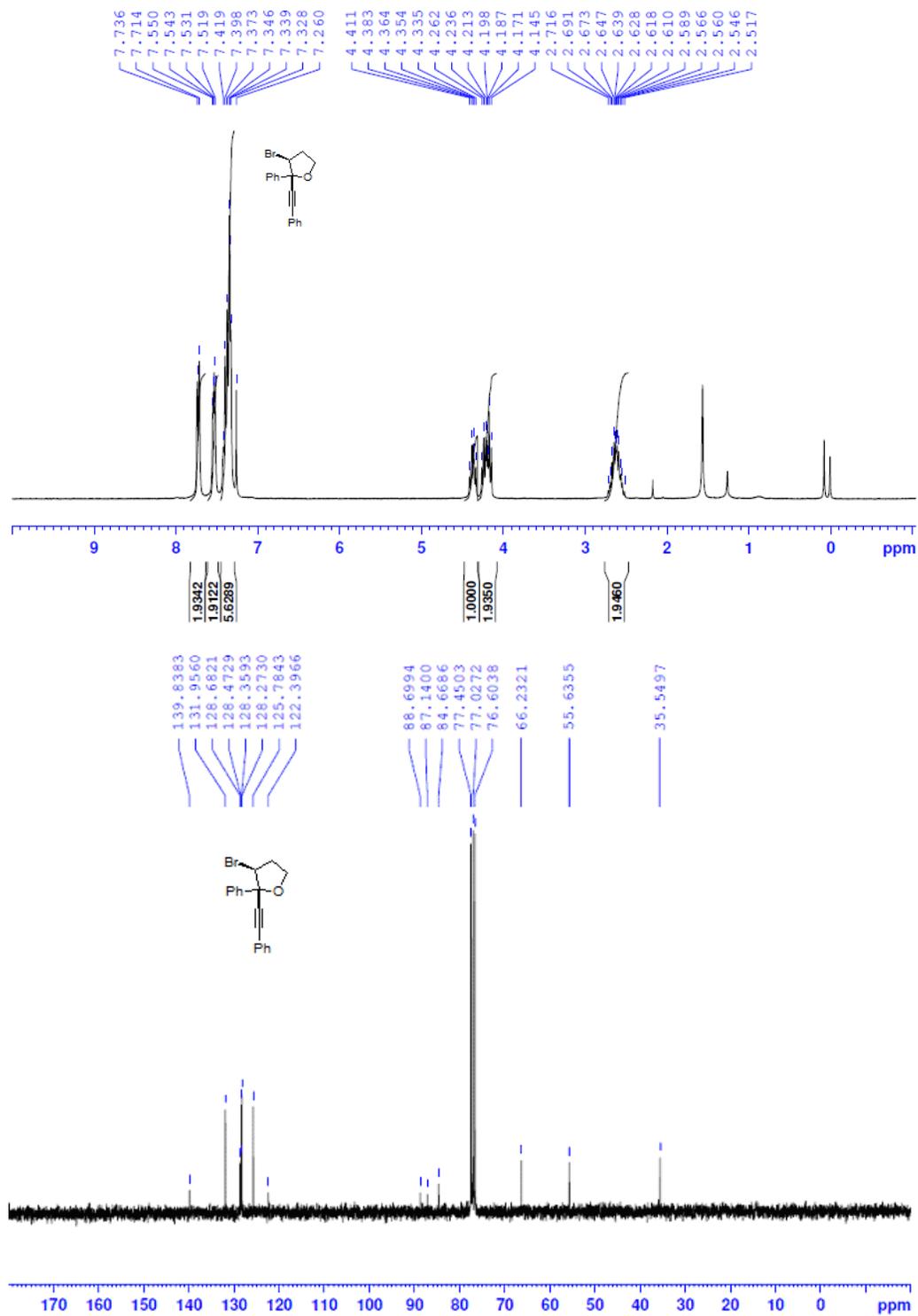


Figure S54. ^1H and ^{13}C NMR Spectra of *Cis*-3-chloro-tetrahydro-2-phenyl-2-(2-phenylethynyl)furan (**2z**)

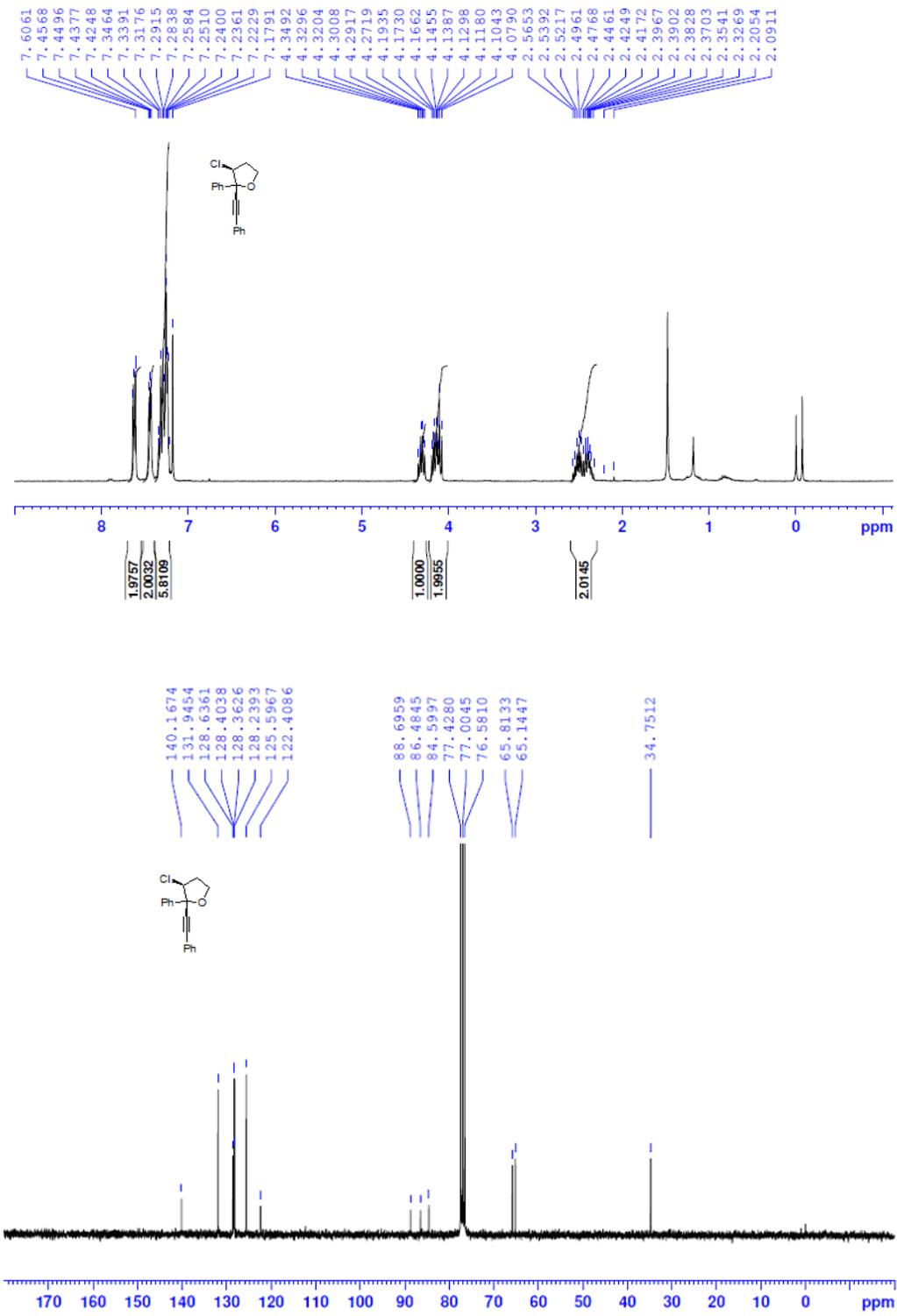


Figure S55. ^1H and ^{13}C NMR Spectra of *Cis*-3-fluoro-tetrahydro-2-phenyl-2-(2-phenylethynyl)furan (**2a**)

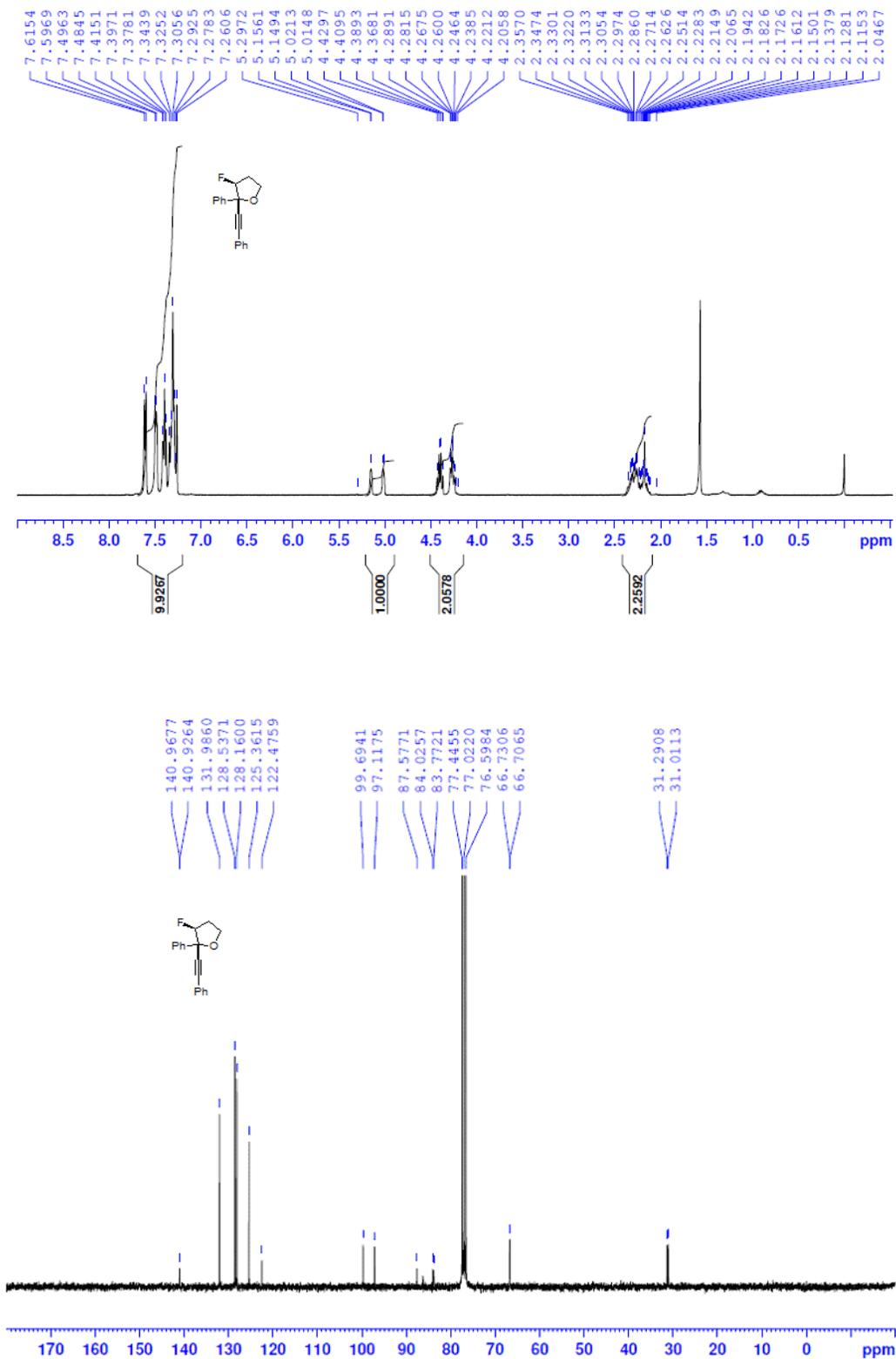


Figure S56. ^1H and ^{13}C NMR Spectra of *Cis*-3-bromo-tetrahydro-2-pentyl-2-phenylfuran

(2 β)

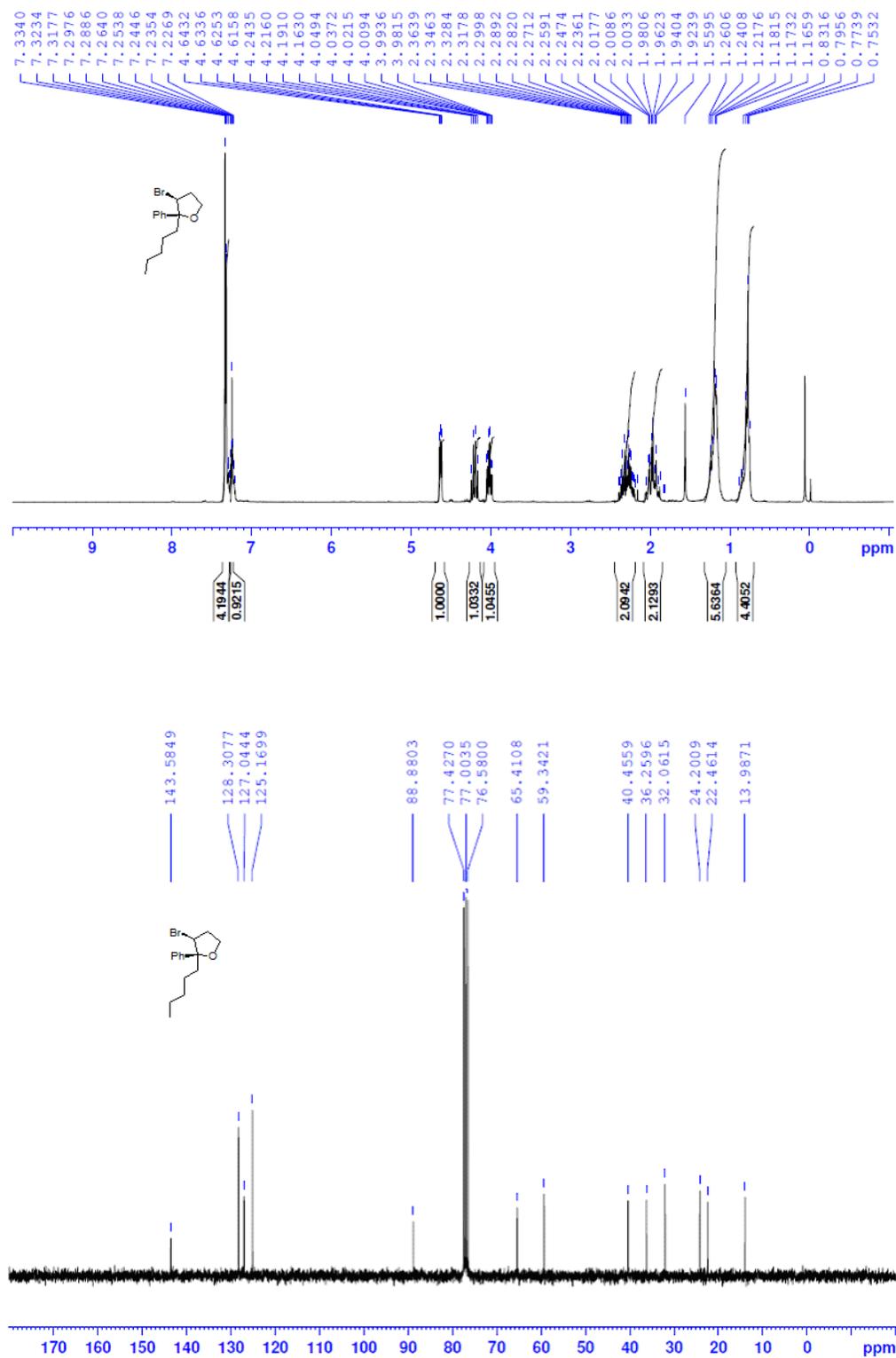


Figure S57. ^1H and ^{13}C NMR Spectra of *Cis*-3-chloro-tetrahydro-2-pentyl-2-phenylfuran

(2γ)

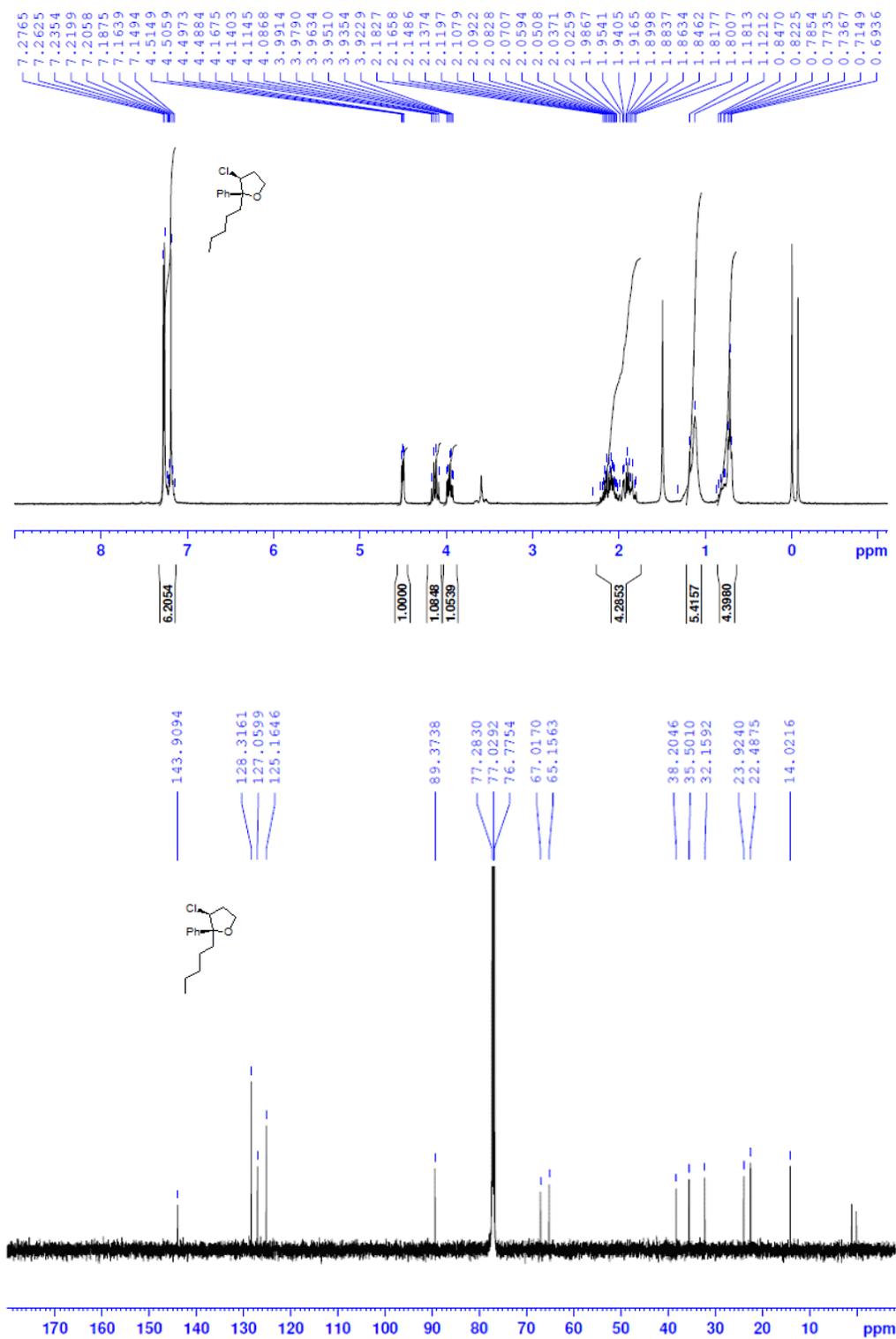


Figure S58. ¹H and ¹³C NMR Spectra of *Cis*-3-fluoro-tetrahydro-2-pentyl-2-phenylfuran

(2d)

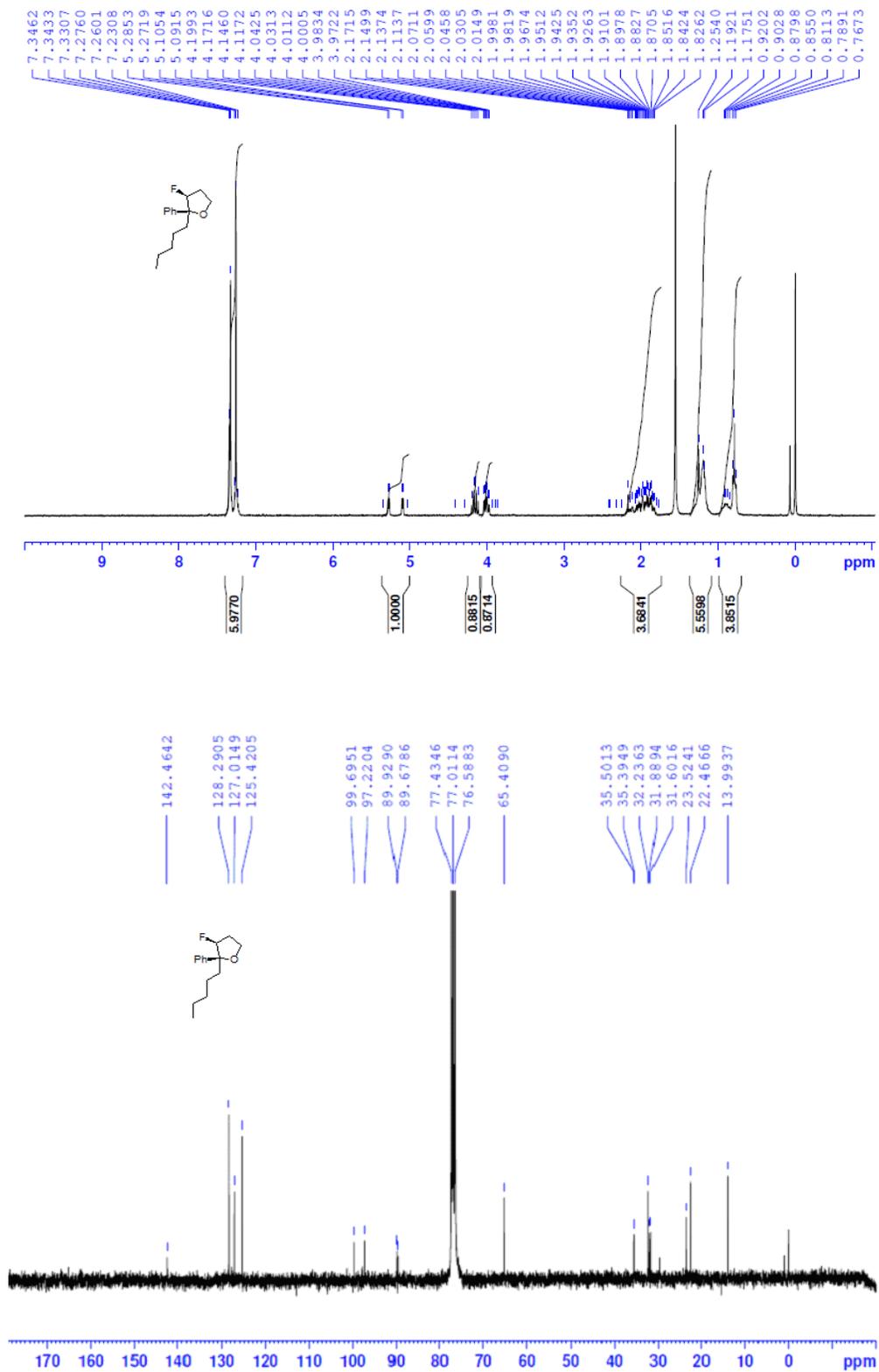


Figure S59. ^1H and ^{13}C NMR Spectra of (Z)-4,6-Diphenylhex-3-en-5-yn-1-ol (**3a**)

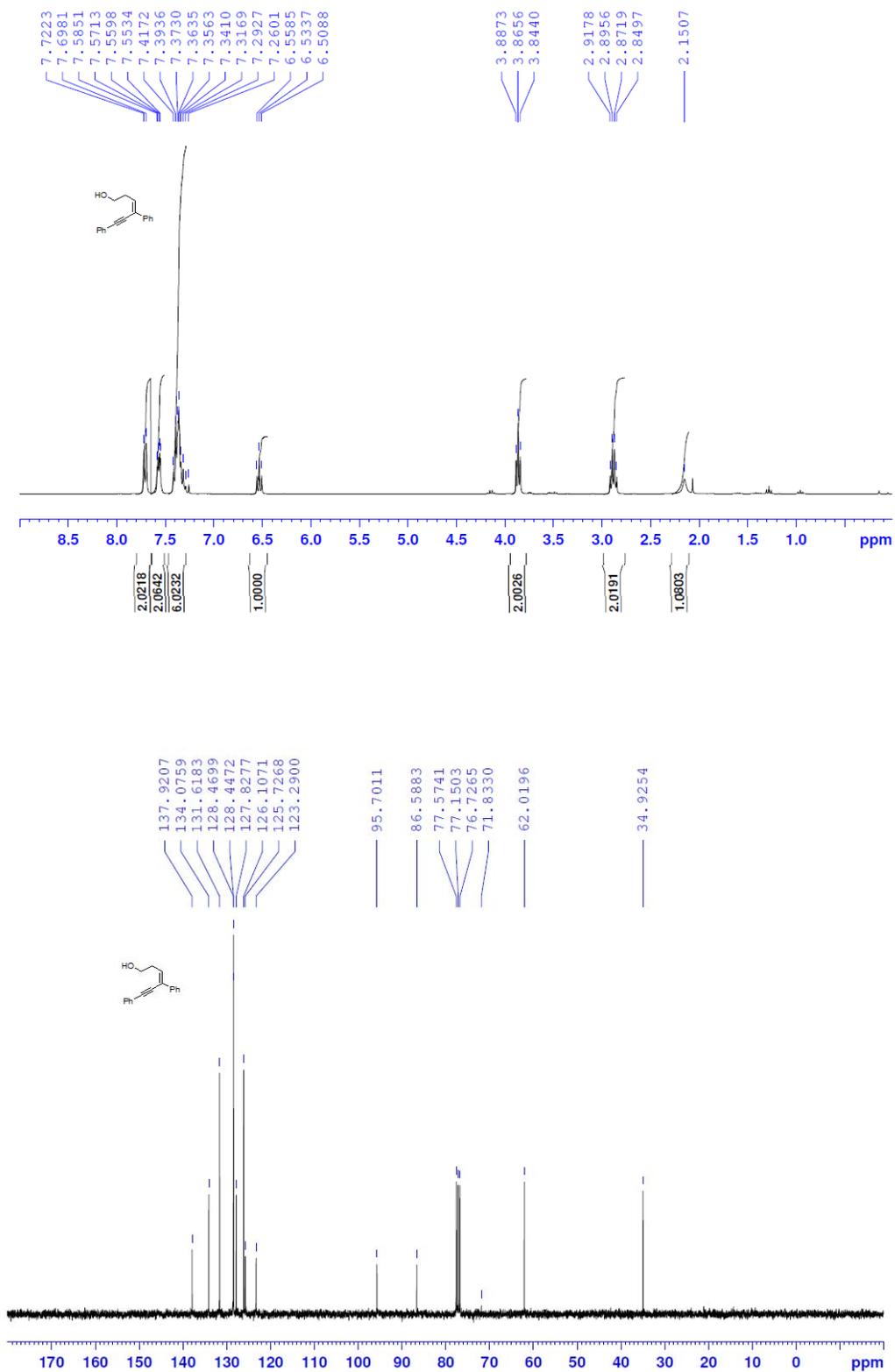
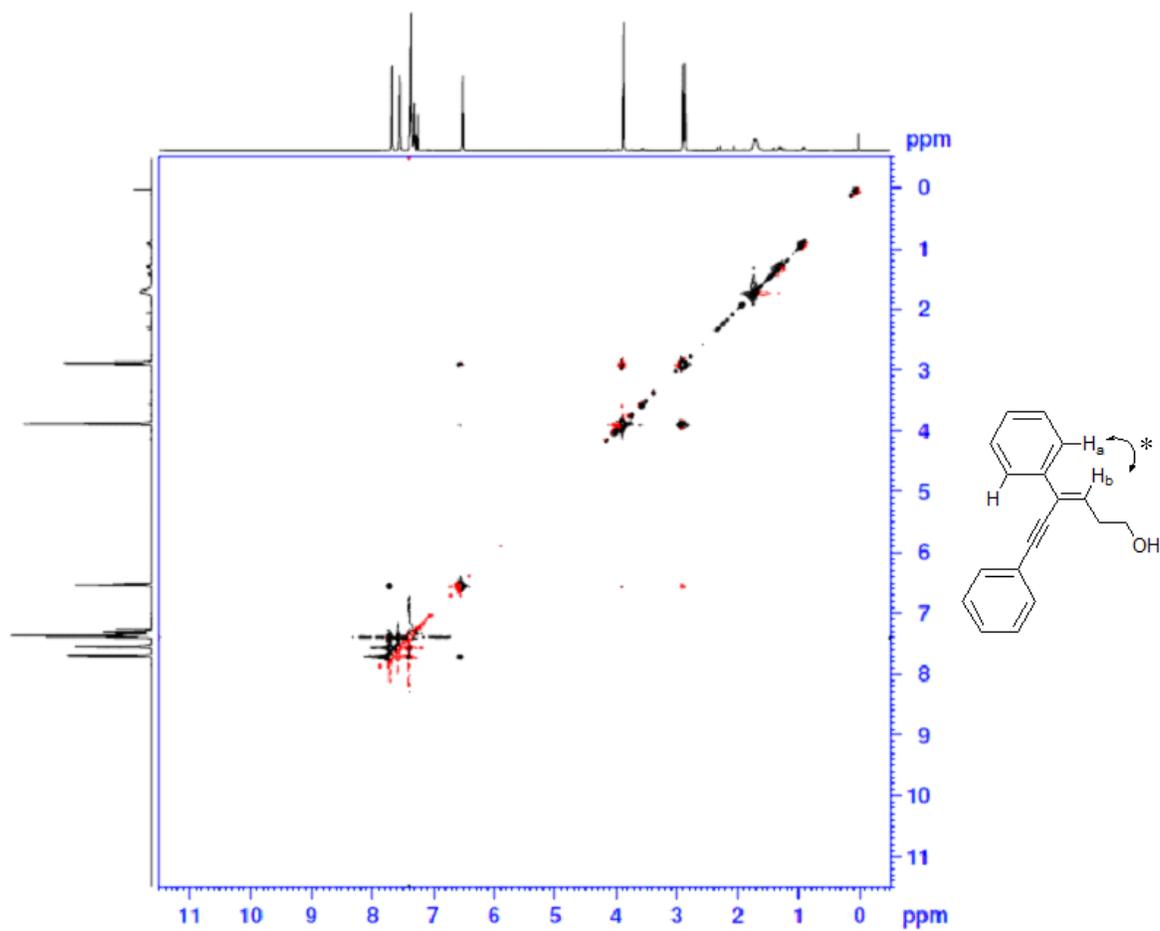


Figure S60. ^1H - ^1H NOESY Spectrum of (Z)-4,6-Diphenylhex-3-en-5-yn-1-ol (**3a**)



* ^1H - ^1H NOESY correlation observed between H_a at 7.72 ppm and H_b at 6.53 ppm.

Figure S61. ^1H and ^{13}C NMR Spectra of 4-Phenyl-4-*p*-tolylbut-3-en-1-ol (**3b**)

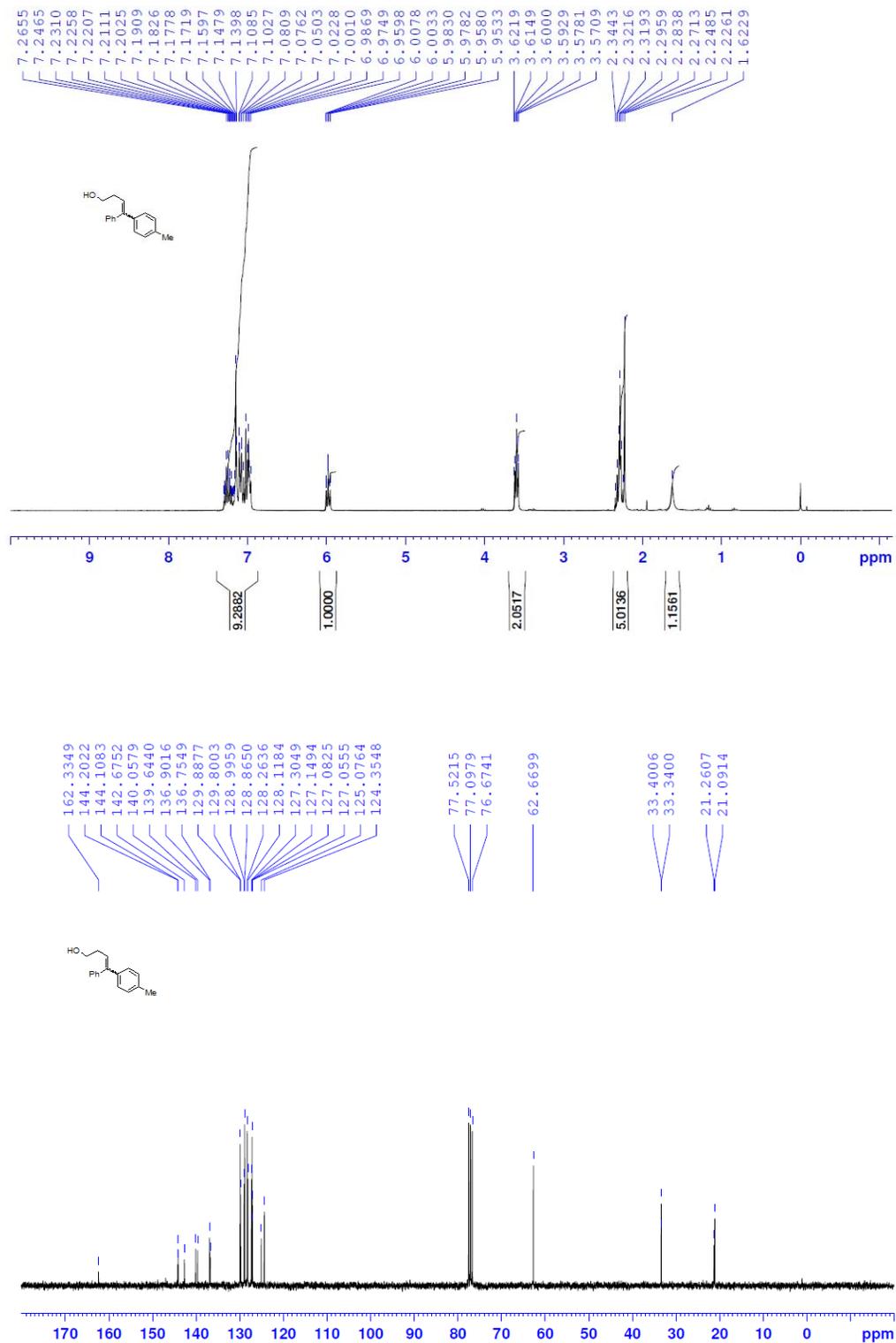


Figure S62. ^1H and ^{13}C NMR Spectra of (Z)-4,6-diphenyl-1-(thiophen-2-yl)hex-3-en-5-yn-1-ol (**3c**)

1-ol (**3c**)

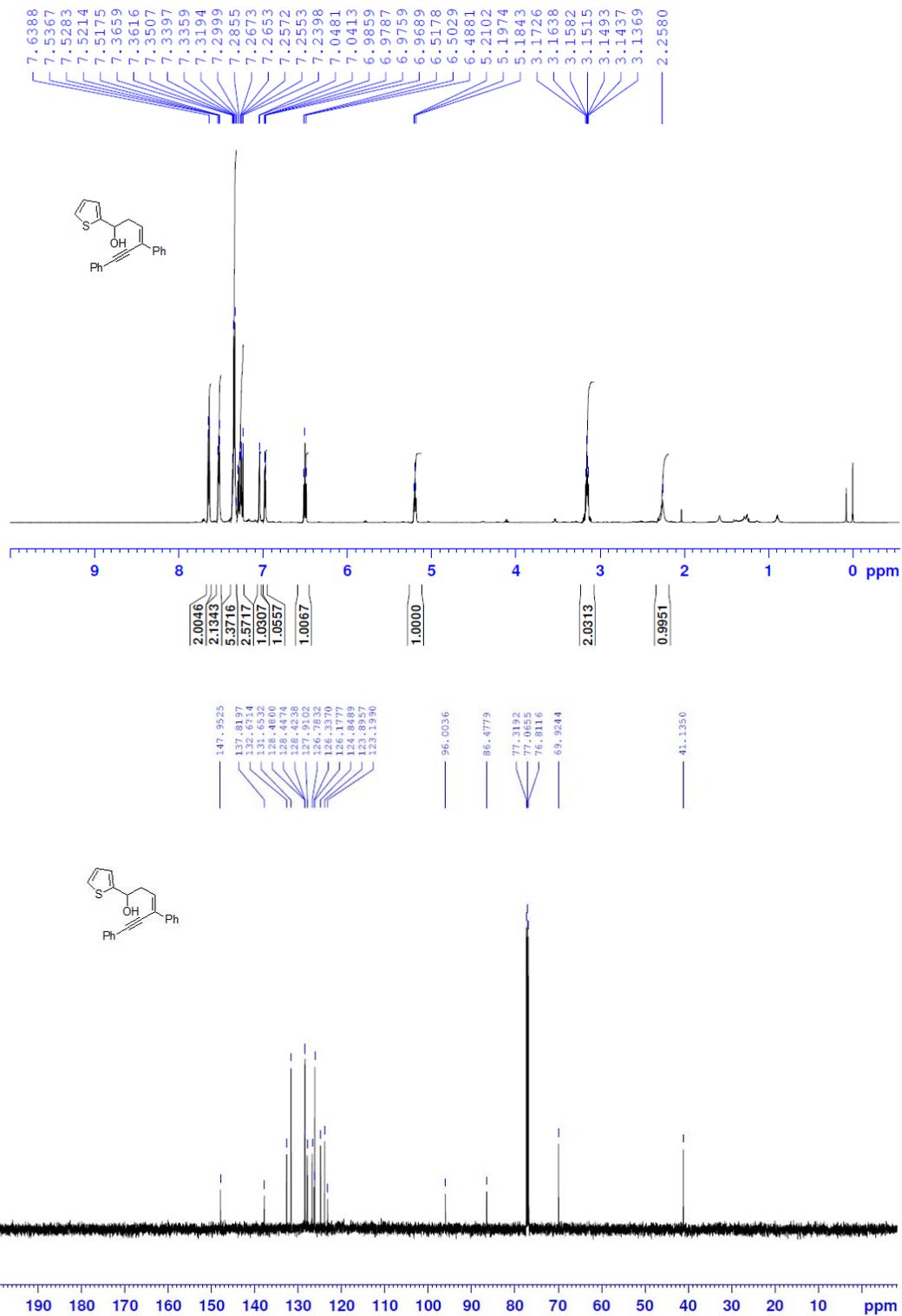
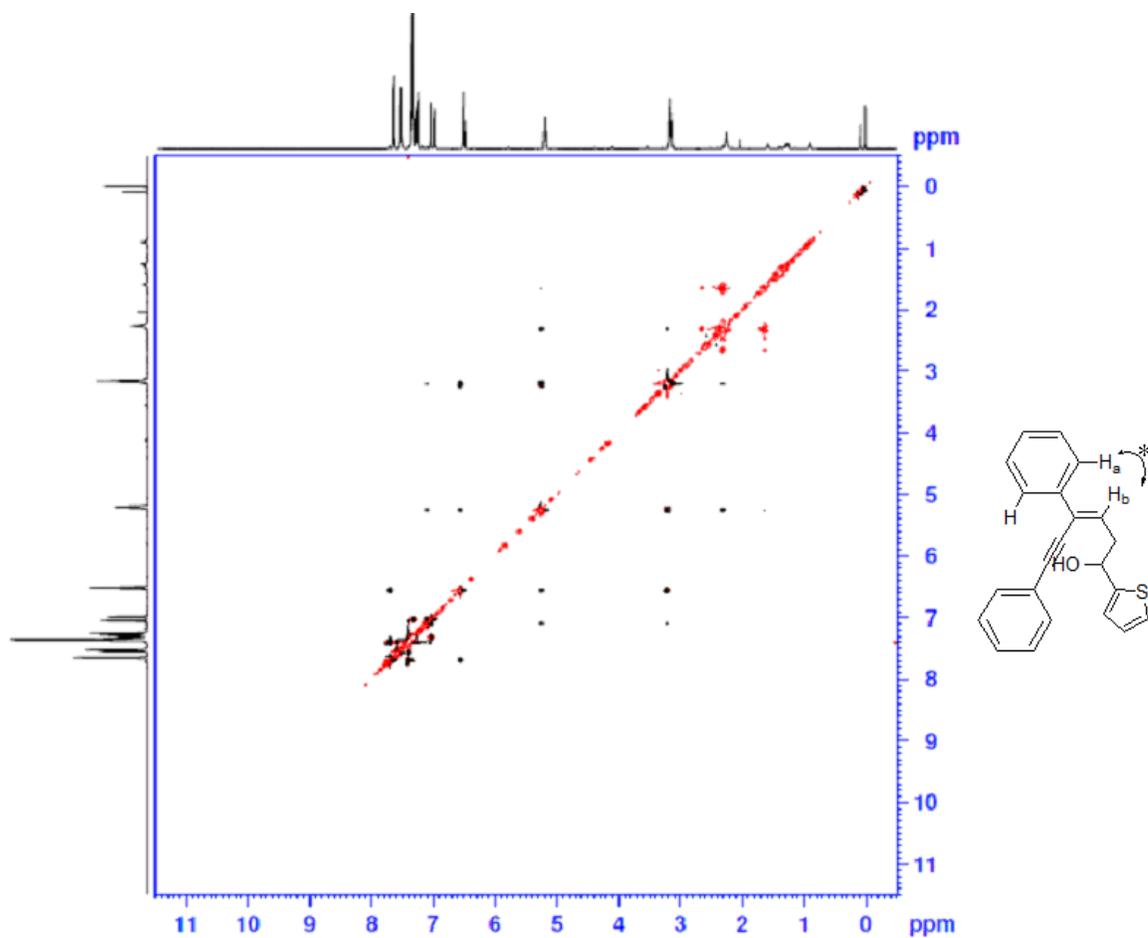


Figure S63. NOESY Spectrum of (Z)-4,6-diphenyl-1-(thiophen-2-yl)hex-3-en-5-yn-1-ol

(3c)



*¹H-¹H NOESY correlation observed between H_a at 7.63 ppm and H_b at 6.50 ppm.

Figure S64. ORTEP Drawing of *Cis*-tetrahydro-3-iodo-2-phenyl-2-(2-phenylethynyl)furan

(**2a**) with Thermal Ellipsoids at 50% Probability Levels^{S1}

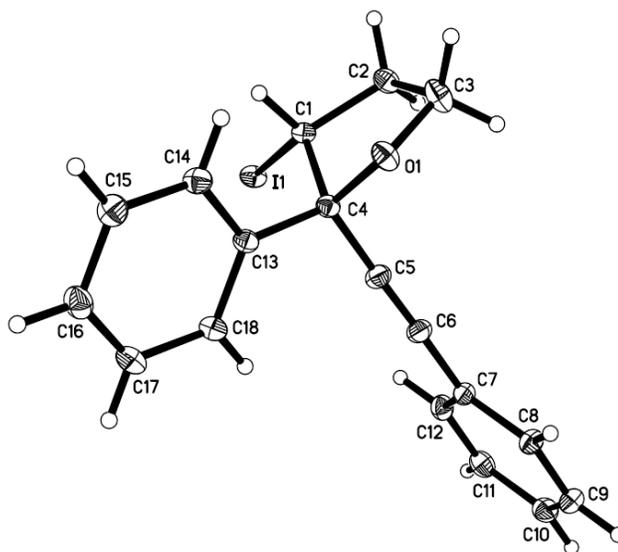
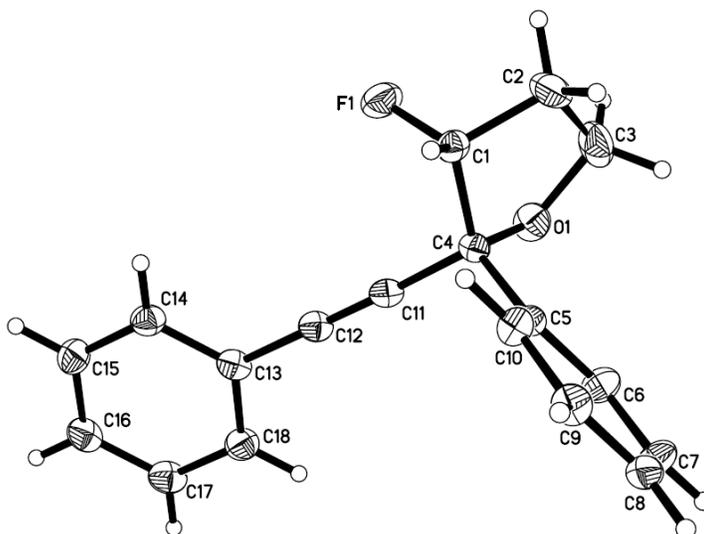


Figure S65. ORTEP Drawing of *Cis*-3-fluoro-tetrahydro-2-phenyl-2-(2-phenylethynyl)

furan (**2a**) with Thermal Ellipsoids at 50% Probability Levels^{S1}



References

S1. CCDC 720922 and 791026 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.