

Supporting Information

for

Silver Acetate Catalyzed Hydroamination of 1-(2-(Sulfonylamino)phenyl)prop-2-yn-1-ols to (Z)-2-Methylene-1-sulfonylindolin-3-ols

Dewi Susanti, Fujiet Koh, Jeffrey Antonius Kusuma, Prasath Kothandaraman, and Philip Wai Hong

Chan*

*Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences,
Nanyang Technological University, Singapore 637371, Singapore*

waihong@ntu.edu.sg

Table of Contents

	Page
1. ¹ H and ¹³ C NMR Spectra of 1-(2-(Substituted-amino)phenyl)prop-2-yn-1-ols (1)	S3
2. ¹ H and ¹³ C NMR Spectra of (<i>Z</i>)-2,3-Dihydroindolin-3-ols (2)	S28
3. ¹ H and ¹³ C NMR Spectra of (<i>d₁</i> - 2a)	S51
4. ¹ H and ¹³ C NMR Spectra of Phenyl(3-phenyl-1-tosyl-1 <i>H</i> -indol-2-yl)methanol (4a)	S52
5. ¹ H and ¹³ C NMR Spectra of 2-(Fluoromethyl)-3-phenyl-1-tosyl-1 <i>H</i> -indole (5p)	S53
6. ¹ H and ¹³ C NMR Spectra of 3-(Iodomethyl)-3-phenyl-1-tosylindolin-2-one (6p)	S54
7. ¹ H and ¹³ C NMR Spectra of (<i>Z</i>)-2-Benzylidene-1-tosylindolin-3-one (7r)	S55
8. ORTEP Drawings of (5p)	S56
9. ORTEP Drawings of (6p)	S57
10. LC-MS Spectrum of (<i>d₁</i> - 2a)	S58
11. References	S59

Figure S1. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxy-1,3-diphenylprop-2-yn-1-yl)phenyl)-4-methyl benzenesulfonamide (**1a**)

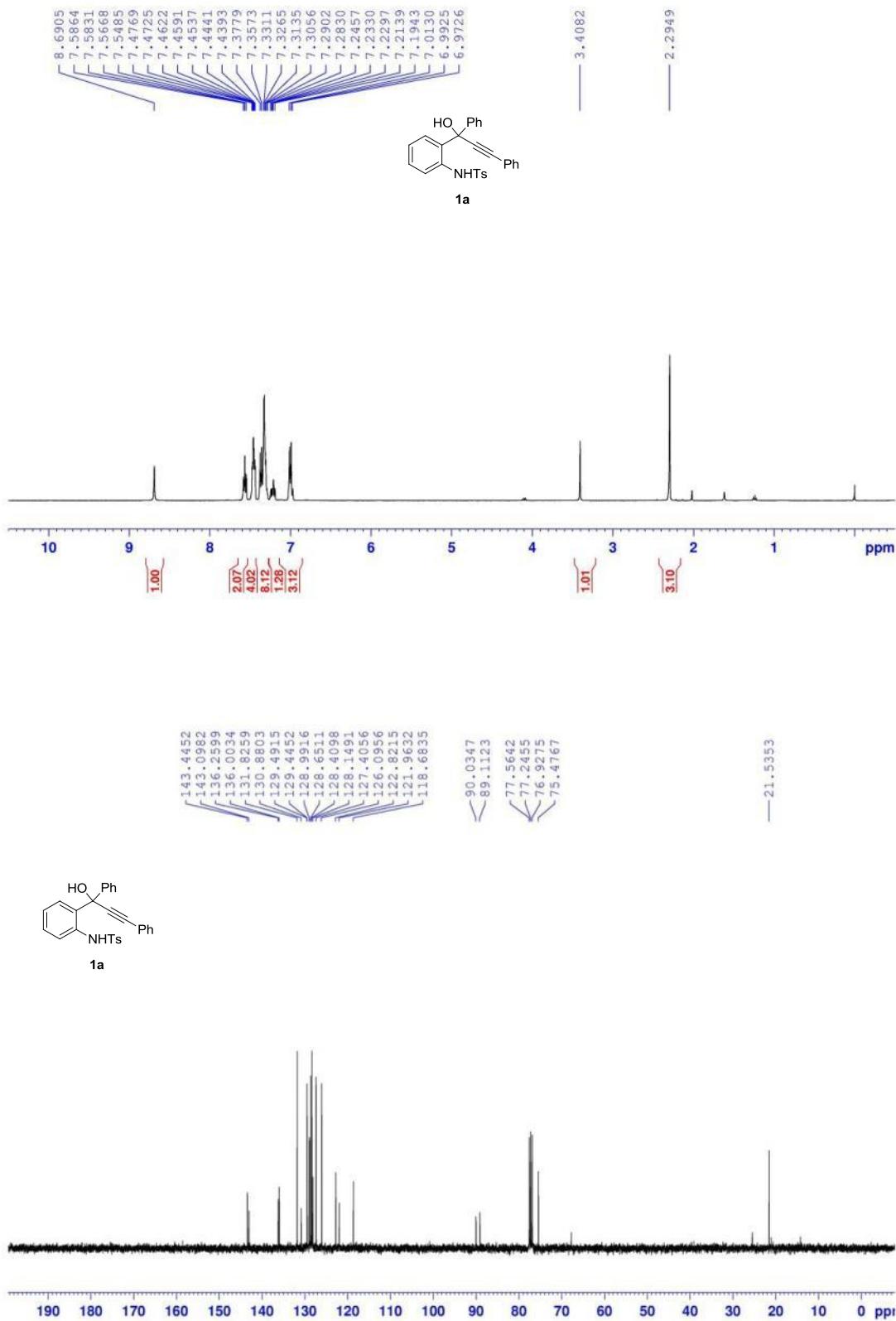


Figure S2. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxy-1,3-diphenylprop-2-yn-1-yl)-4-methylphenyl)-4-methylbenzenesulfonamide (**1b**)

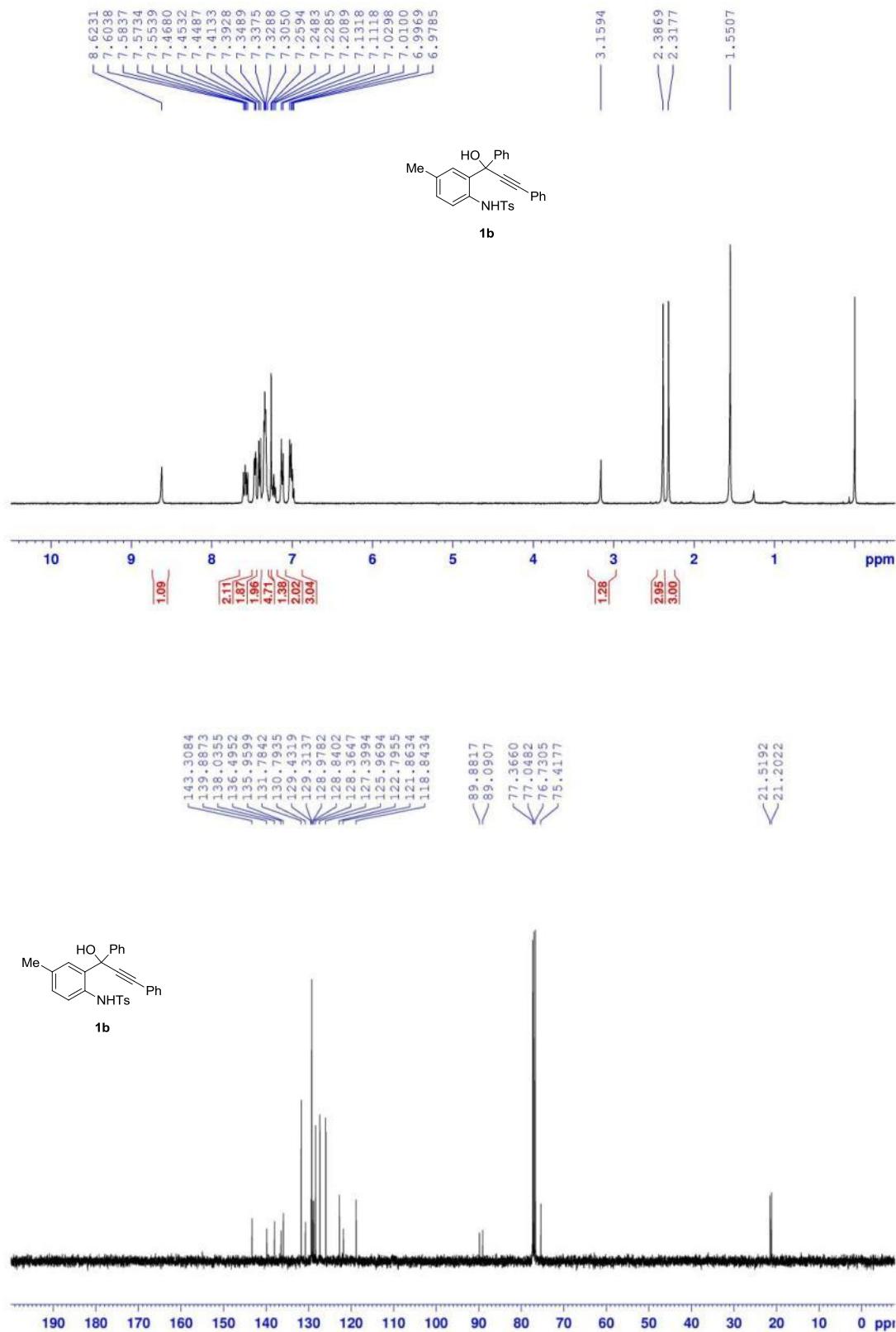


Figure S3. ^1H and ^{13}C NMR Spectra of *N*-(4-Bromo-2-(1-hydroxy-1,3-diphenylprop-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1c**)

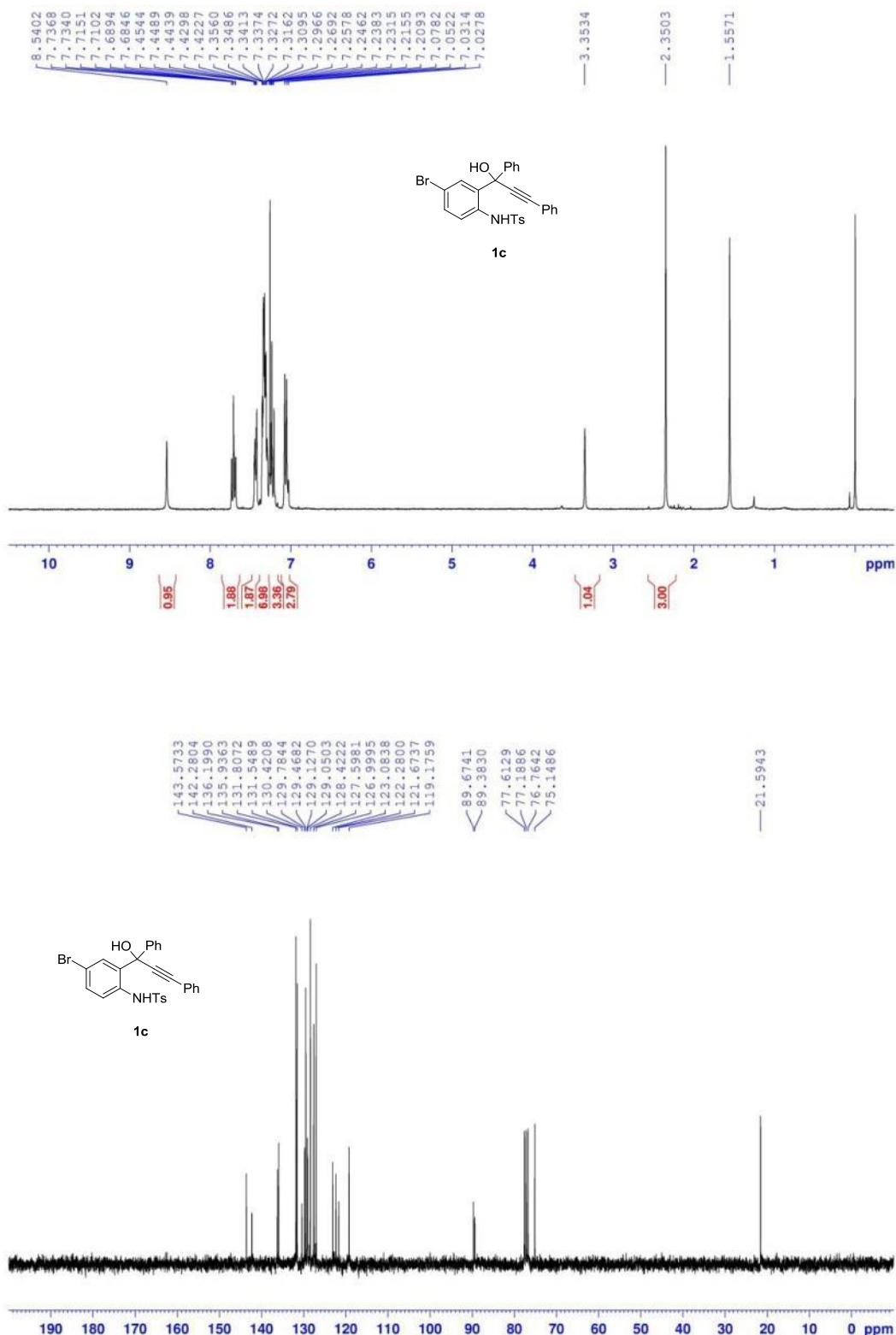


Figure S4. ^1H and ^{13}C NMR Spectra of *N*-(4-Chloro-2-(1-hydroxy-1,3-diphenylprop-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1d**)

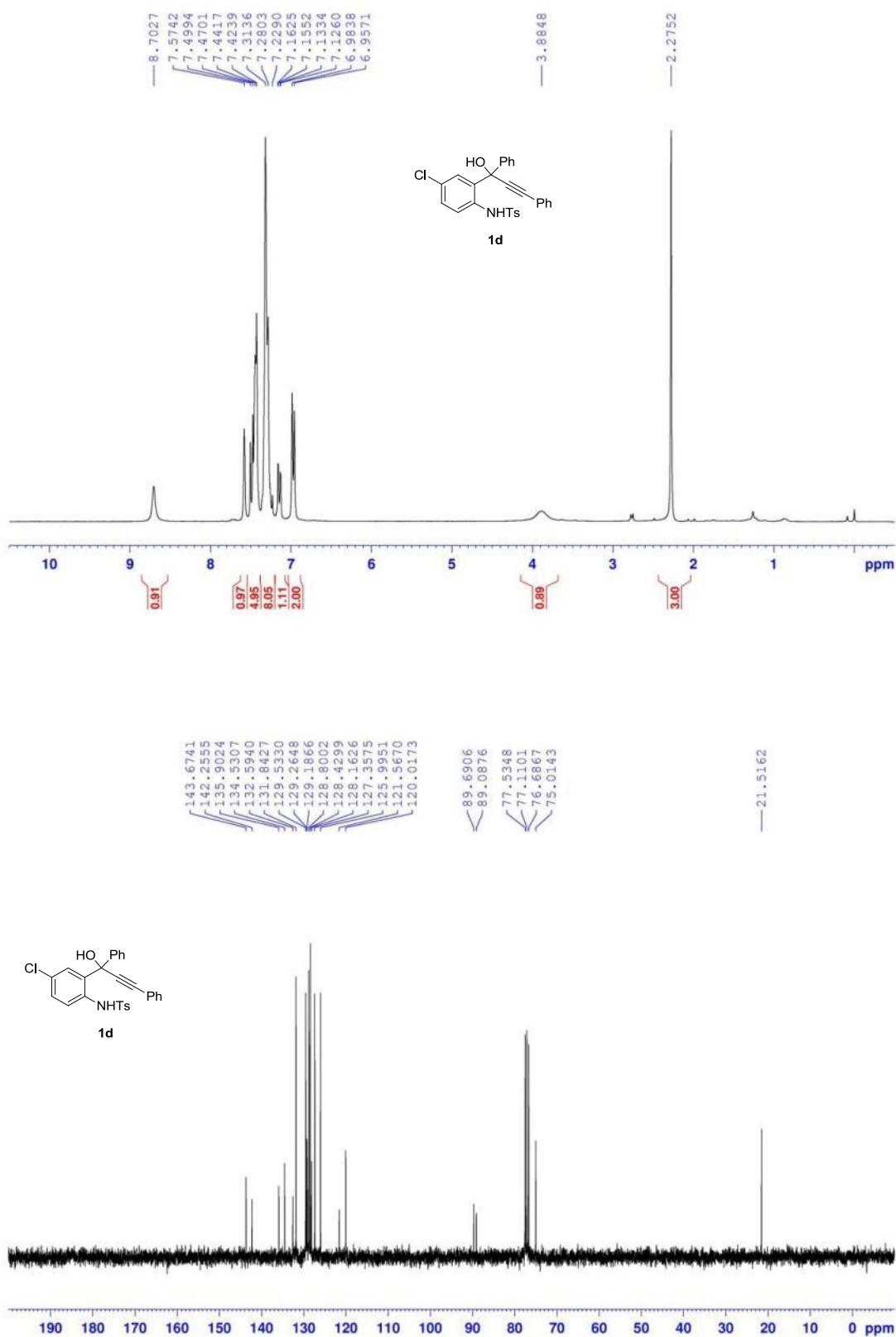


Figure S5. ^1H and ^{13}C NMR Spectra of *N*-(3-(1-Hydroxy-1,3-diphenylprop-2-yn-1-yl)naphthalen-2-yl)-4-methylbenzenesulfonamide (**1e**)

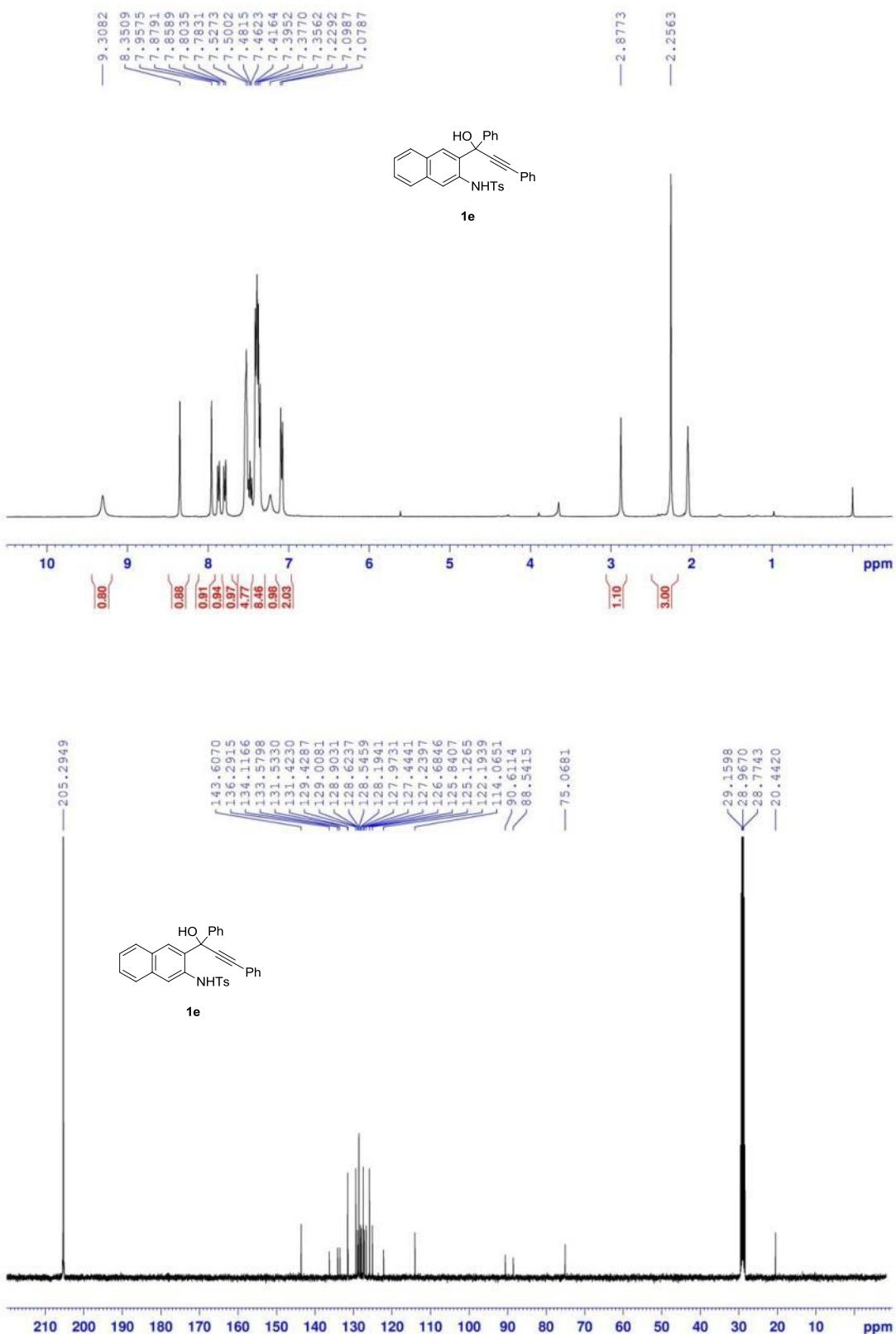


Figure S6. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxy-3-phenyl-1-(*p*-tolyl)prop-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1f**)

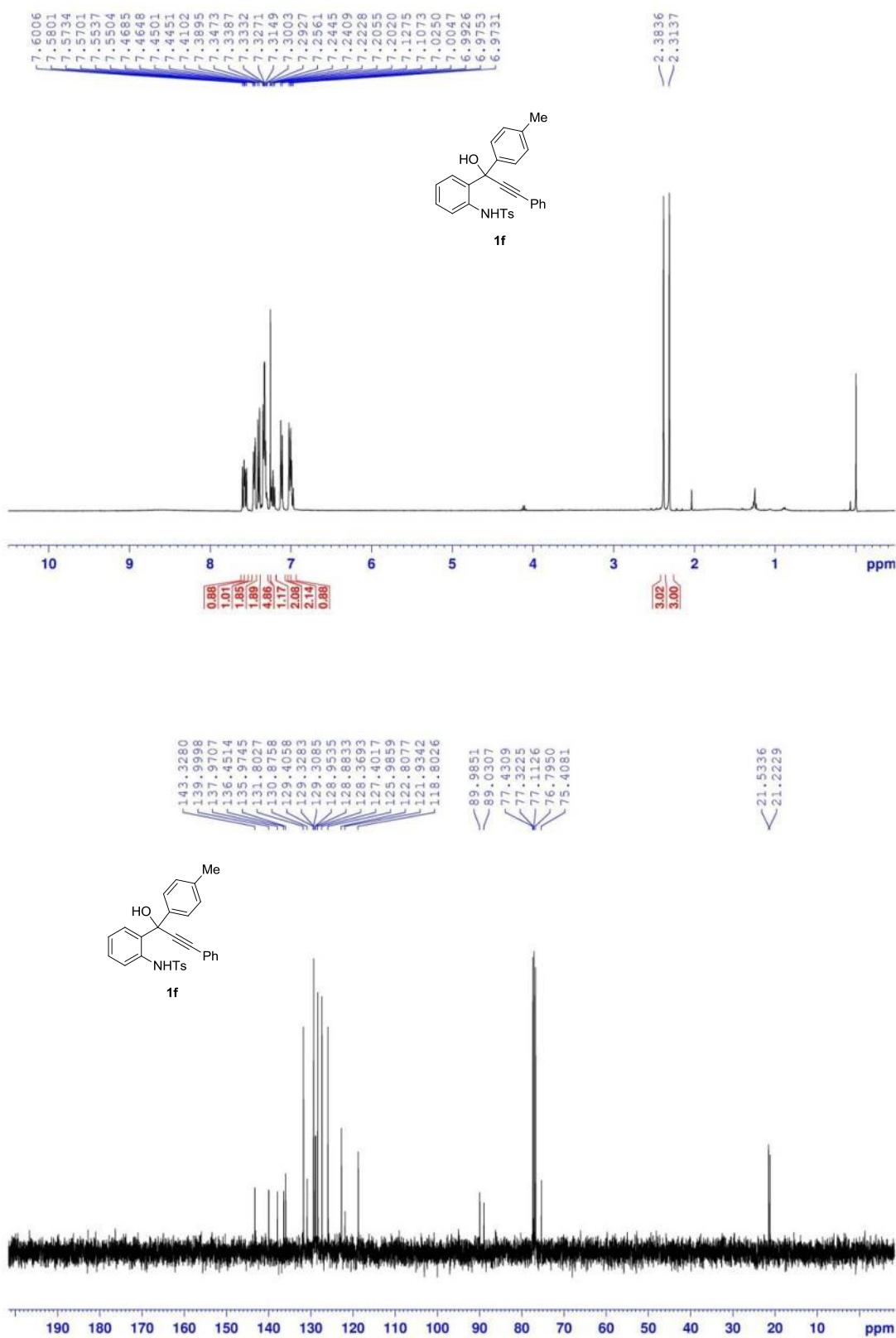


Figure S7. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-(4-Chlorophenyl)-1-hydroxy-3-phenylprop-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1g**)

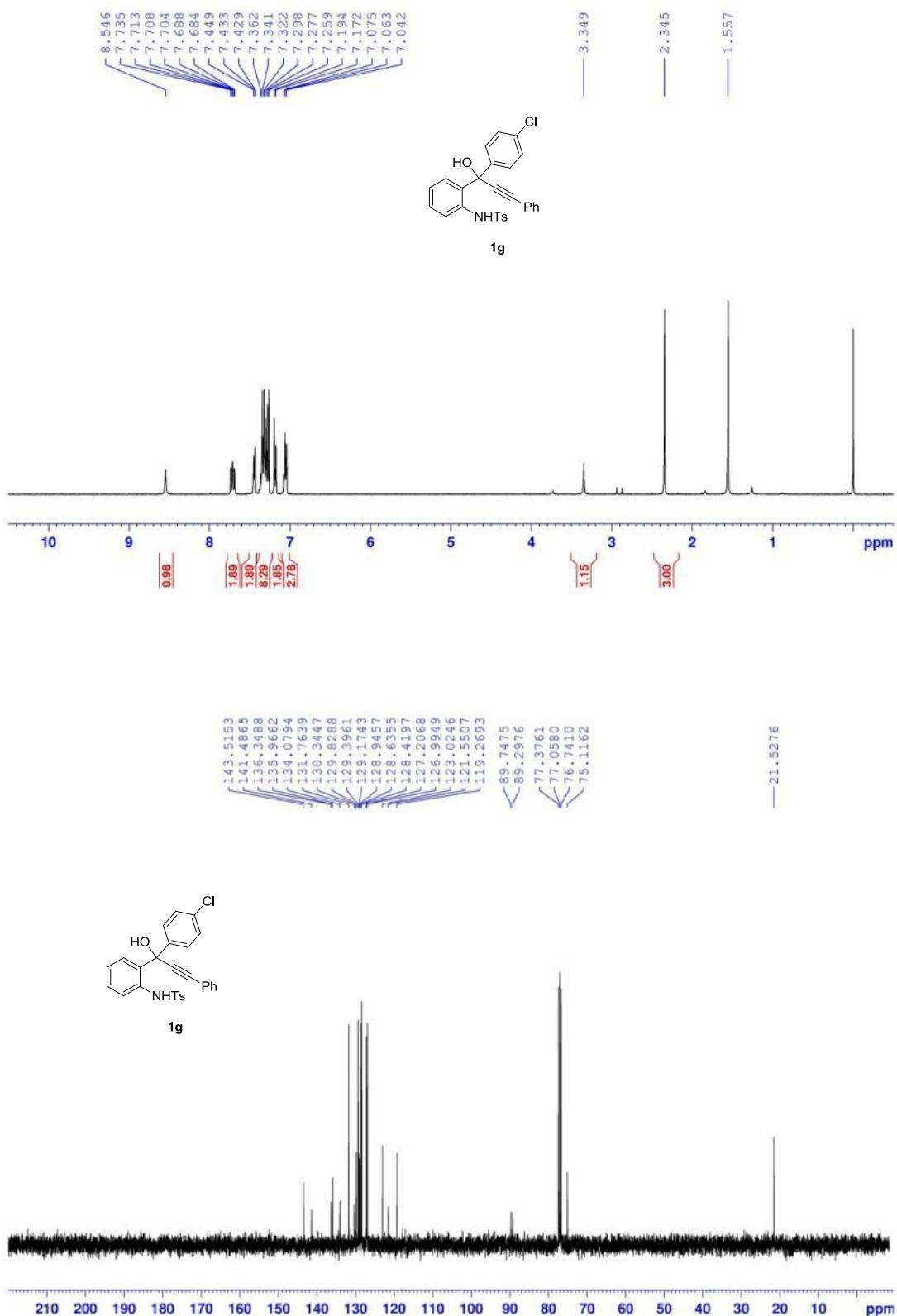


Figure S8. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-(4-Bromophenyl)-1-hydroxy-3-phenylprop-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1h**)

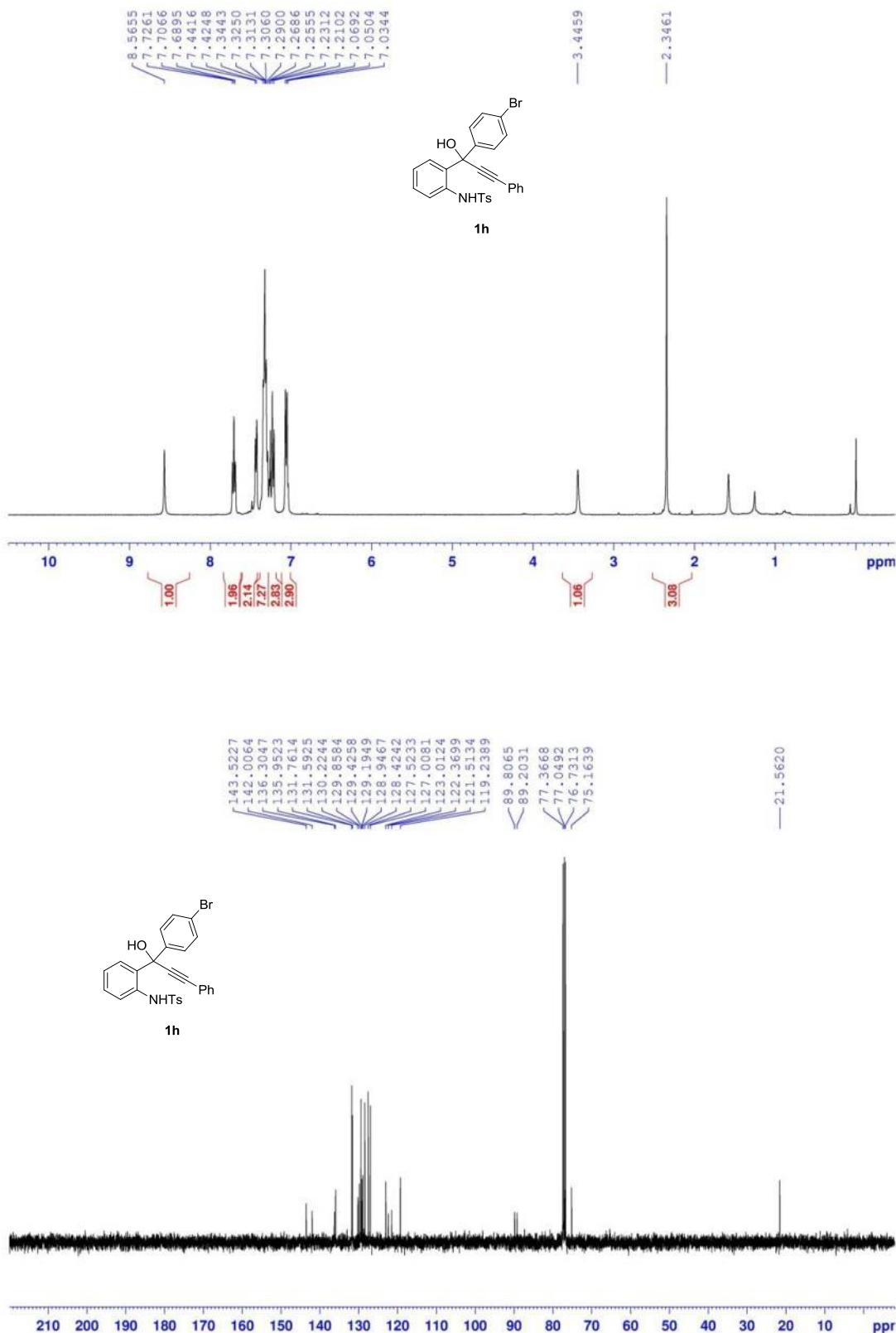


Figure S9. ^1H and ^{13}C NMR Spectra of *N*-(2-(3-(4-Fluorophenyl)-1-hydroxy-1-phenylprop-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1i**)

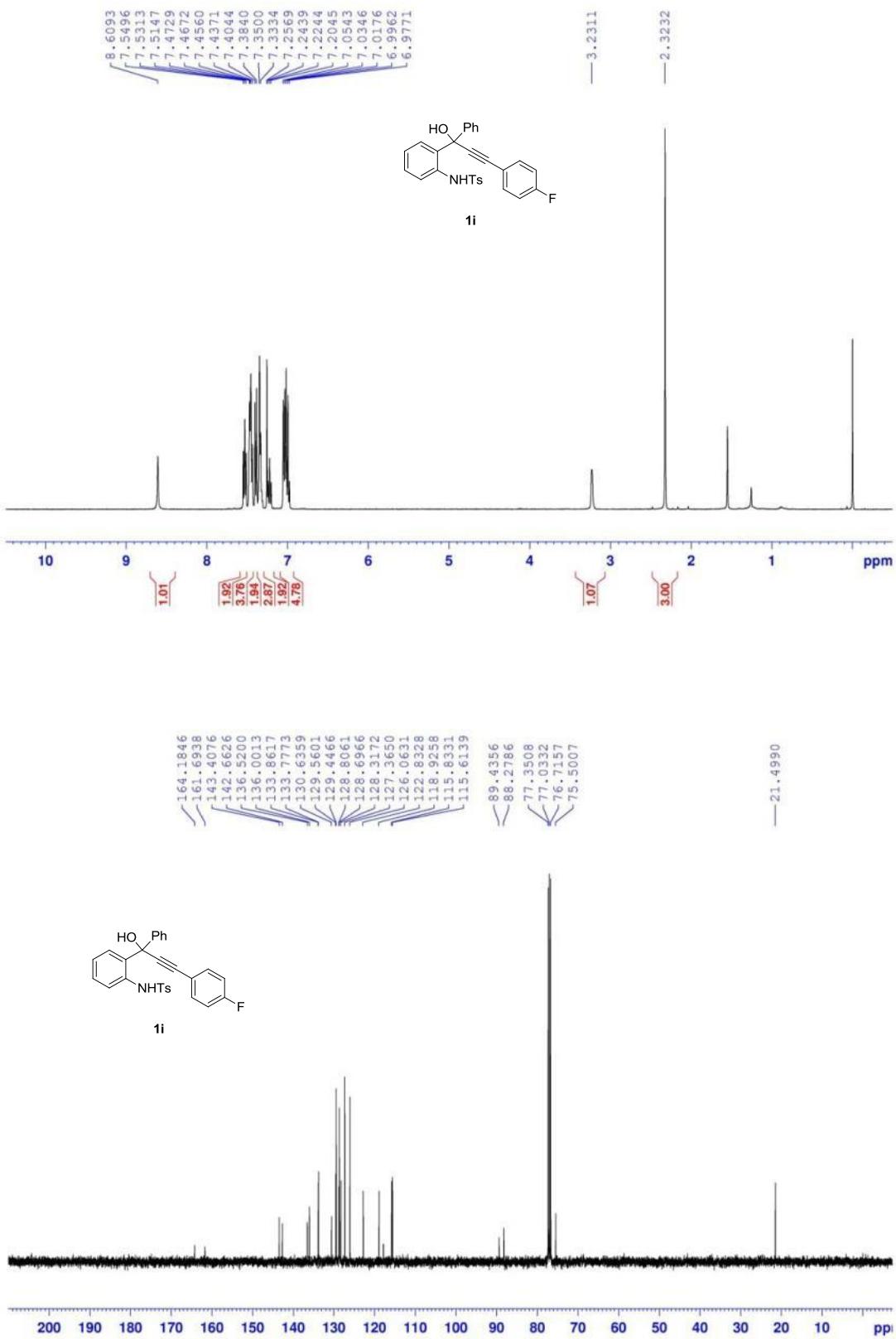


Figure S10. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxy-1-phenyl-3-(4-(trifluoromethyl)phenyl)prop-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1j**)

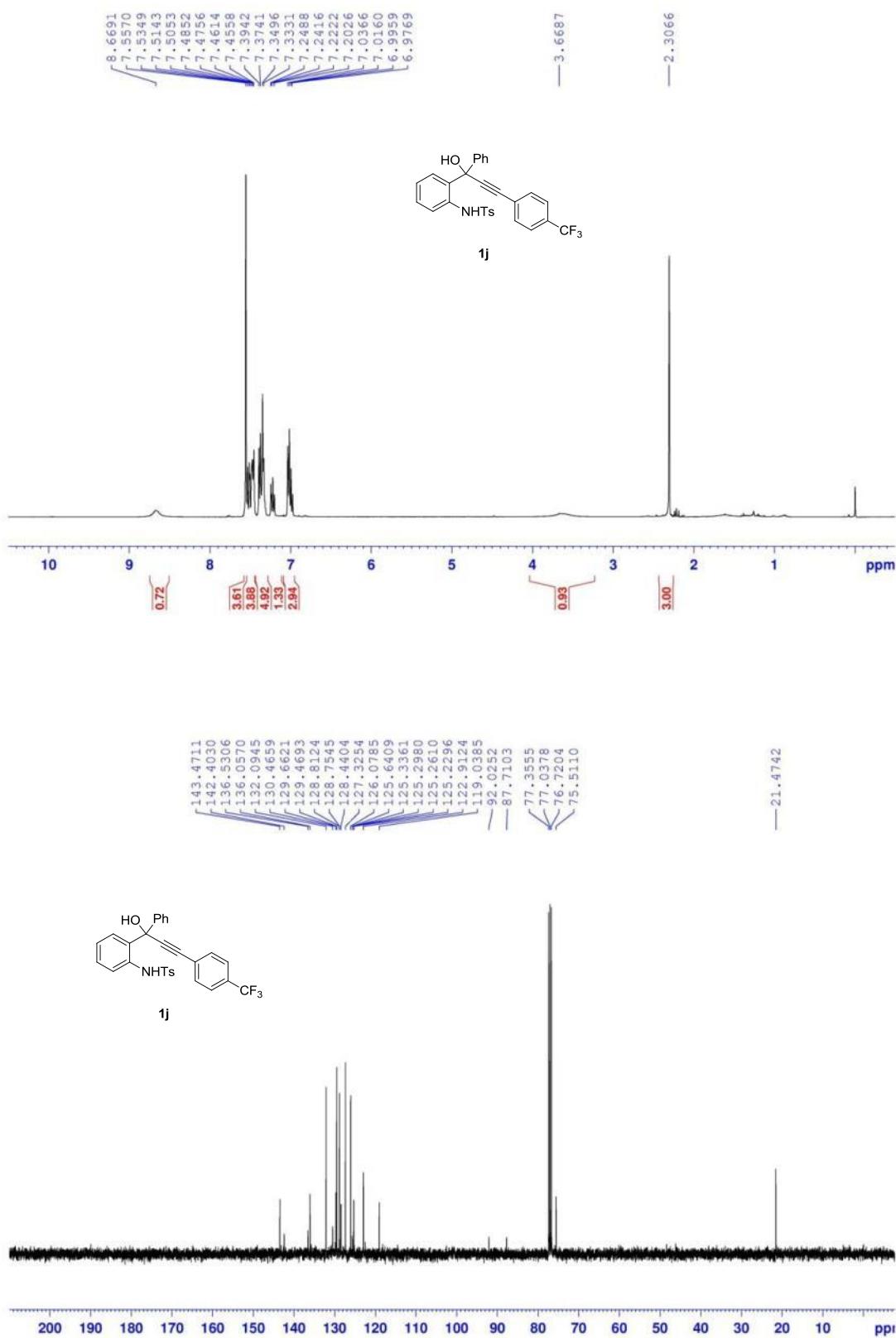


Figure S11. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxy-1-phenyl-3-(*p*-tolyl)prop-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1k**)

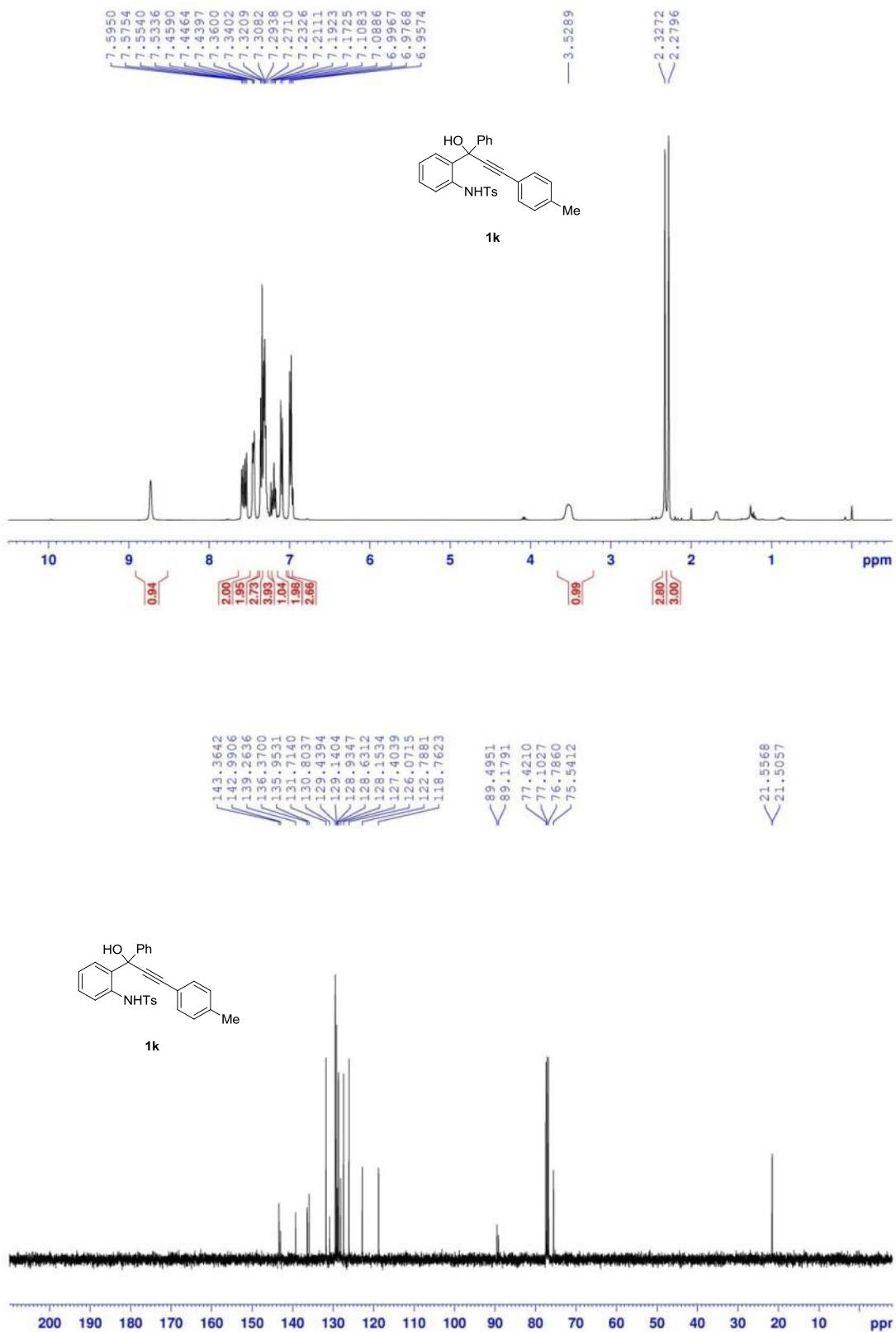


Figure S12. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxy-1-phenyl-3-(thiophen-3-yl)prop-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1l**)

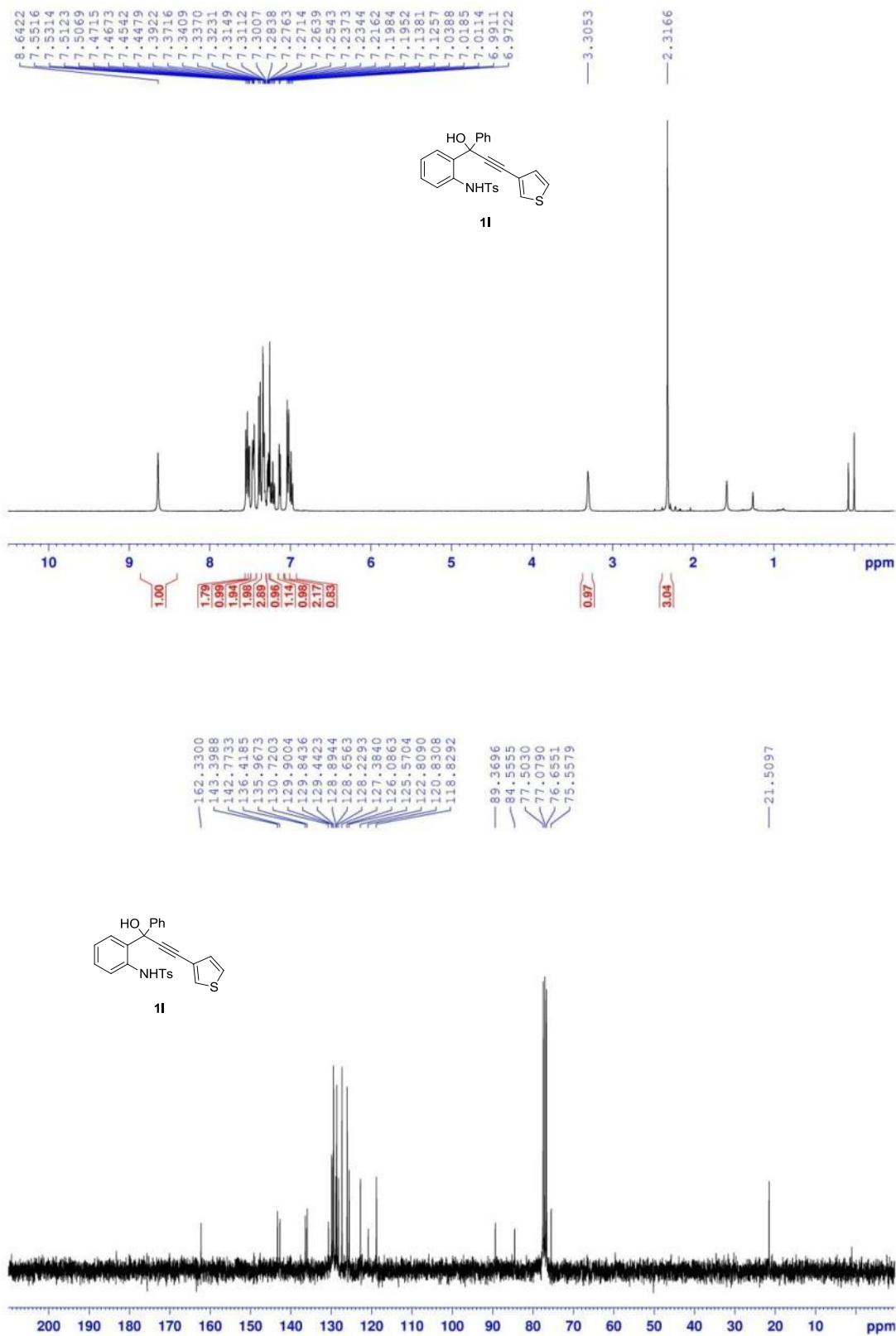


Figure S13. ^1H and ^{13}C NMR Spectra of *N*-(2-(3-Cyclopropyl-1-hydroxy-1-phenylprop-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1m**)

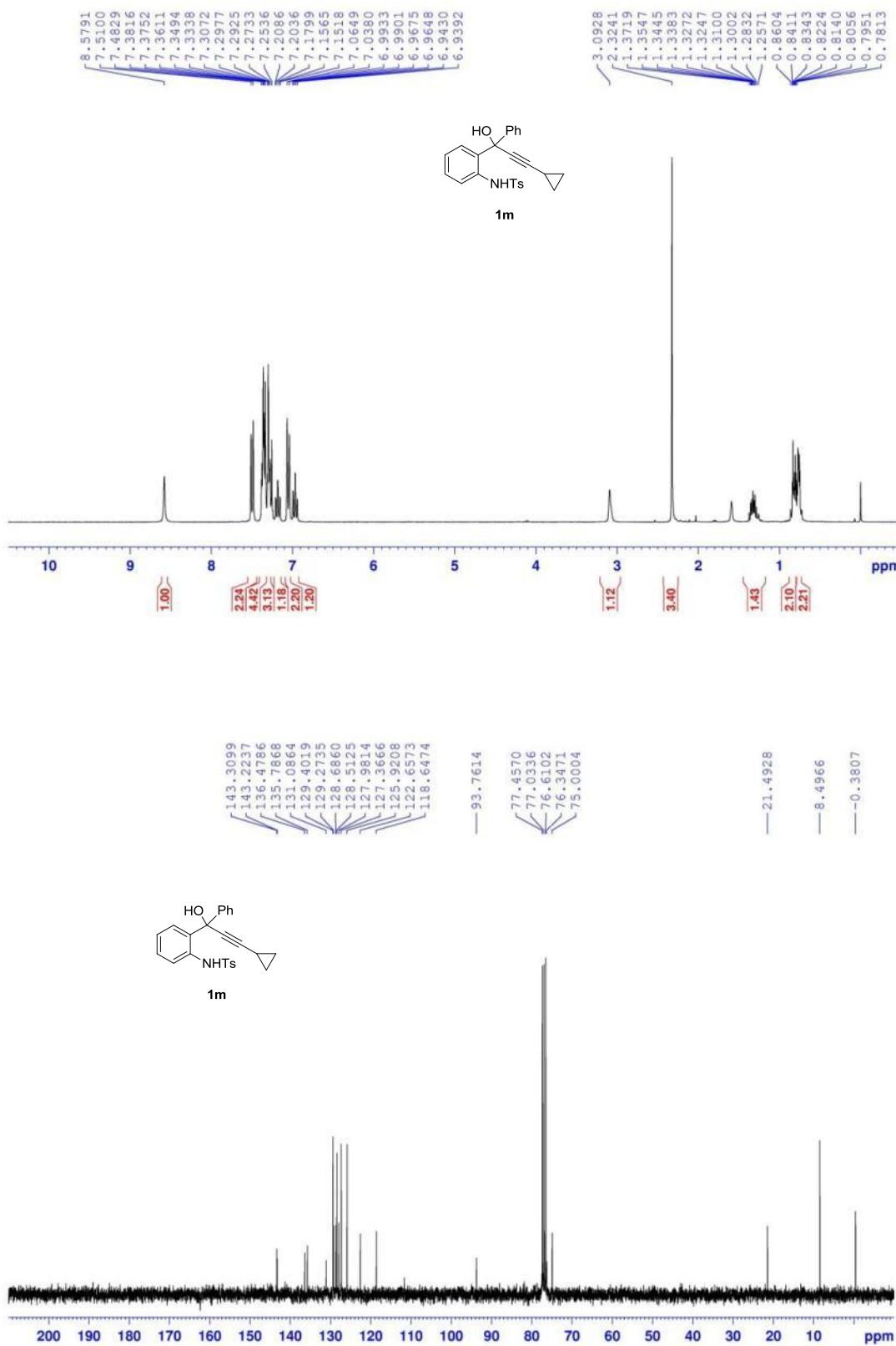


Figure S14. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxy-1-phenylhept-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1n**)

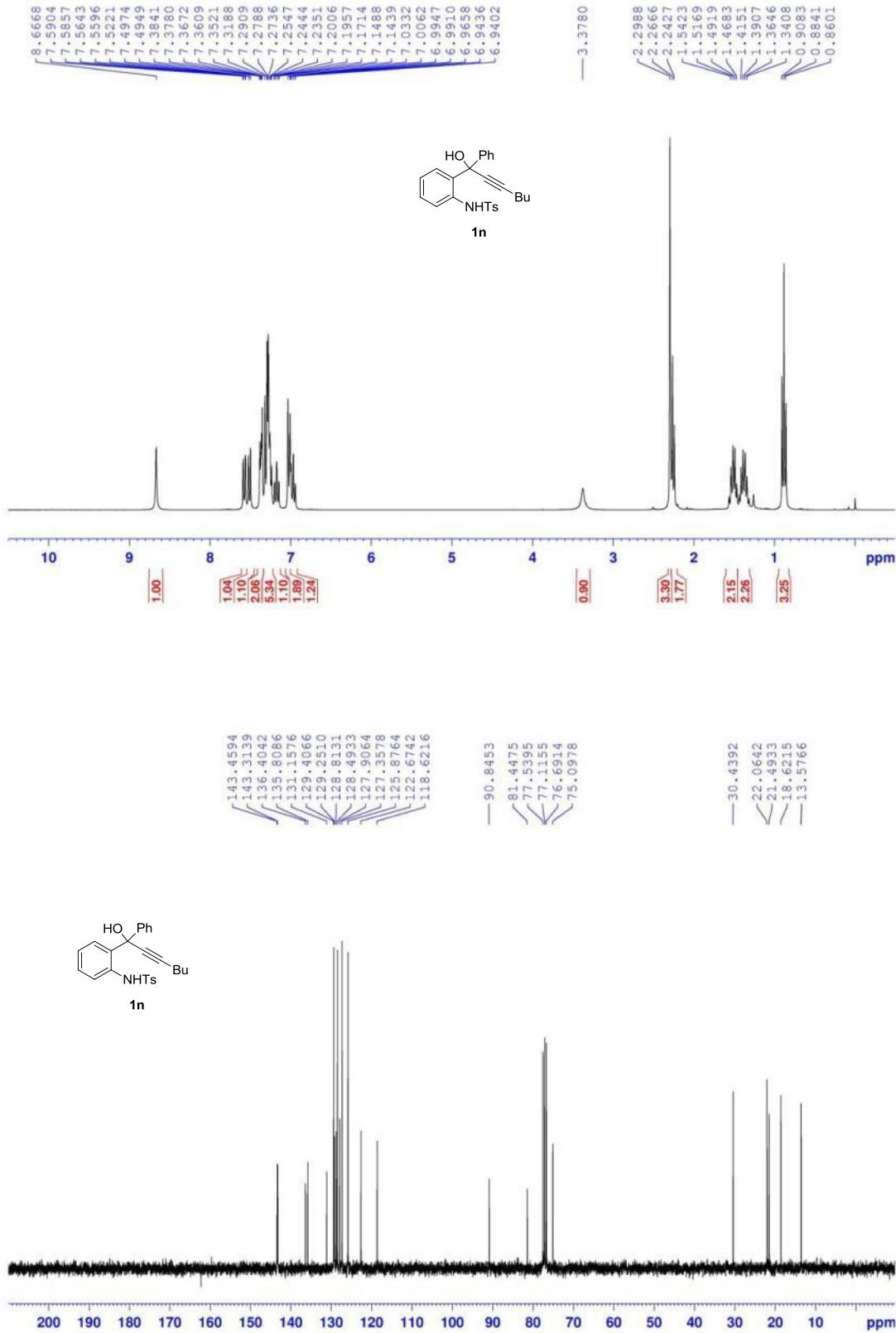


Figure S15. ^1H and ^{13}C NMR Spectra of *N*-(2-(2-Hydroxyoct-3-yn-2-yl)phenyl)-4-methylbenzenesulfonamide (**1o**)

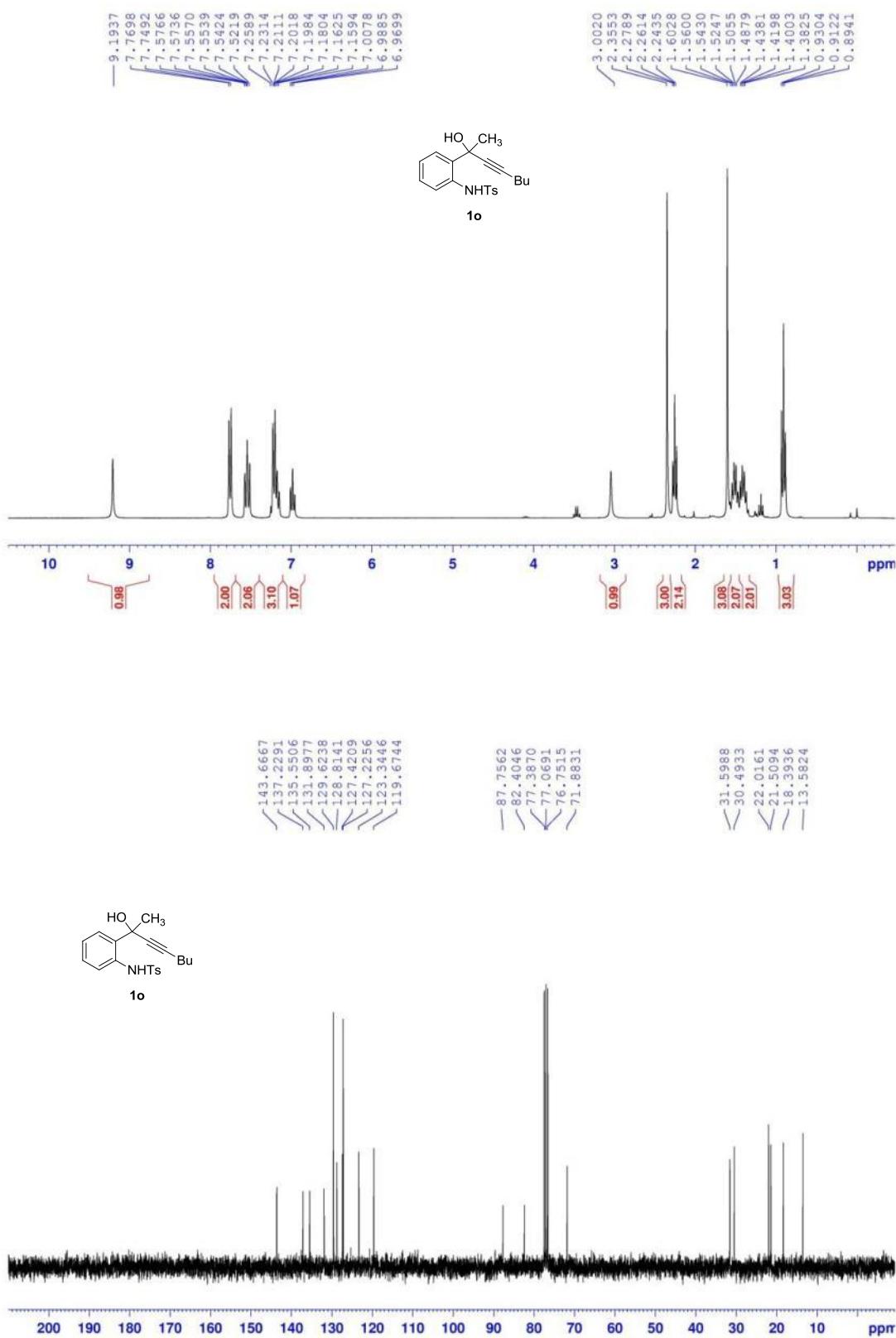


Figure S16. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxy-1-phenylprop-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1p**)

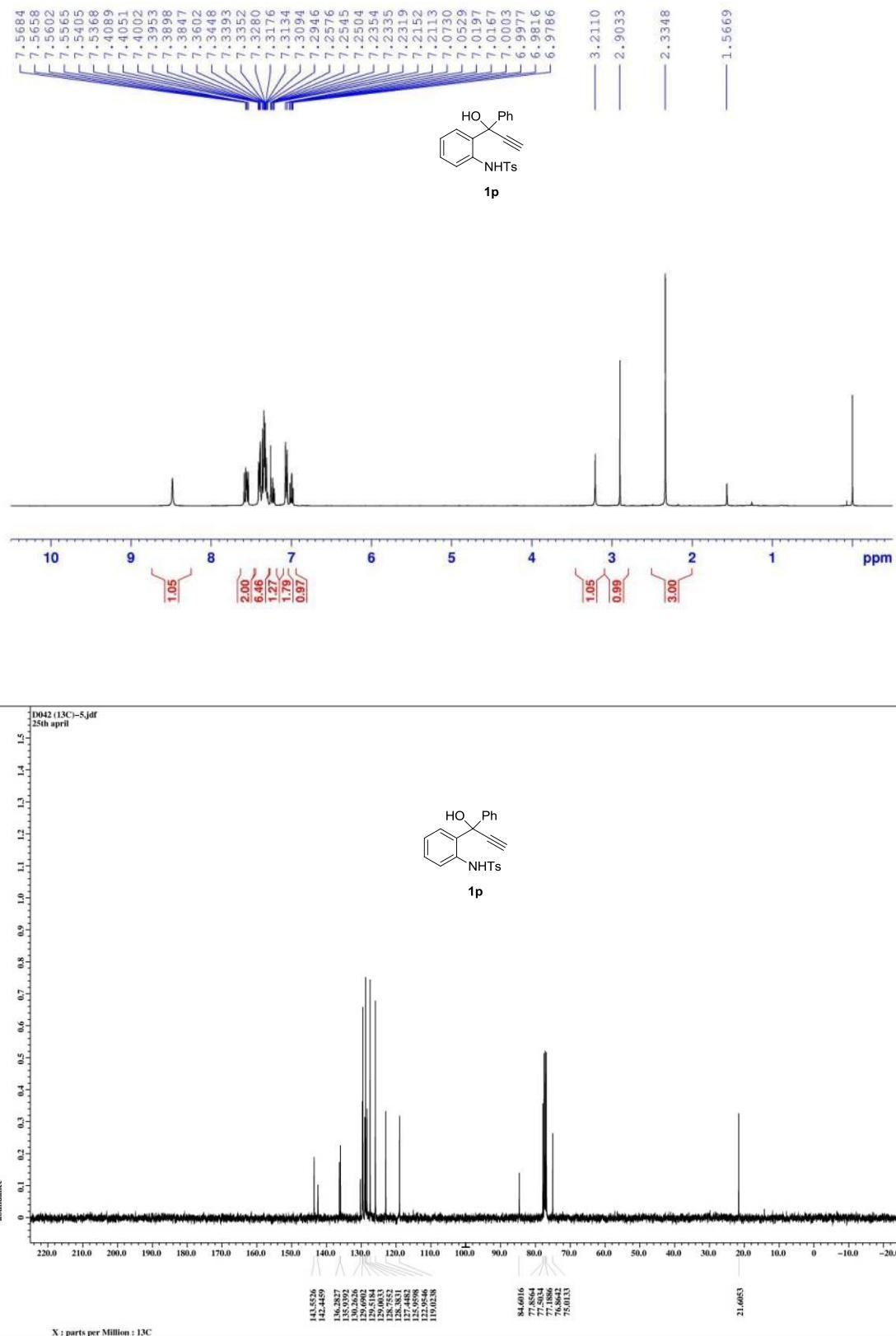


Figure S17. ^1H and ^{13}C NMR Spectra of *N*-(2-(2-Hydroxybut-3-yn-2-yl)phenyl)-4-methylbenzenesulfonamide (**1q**)

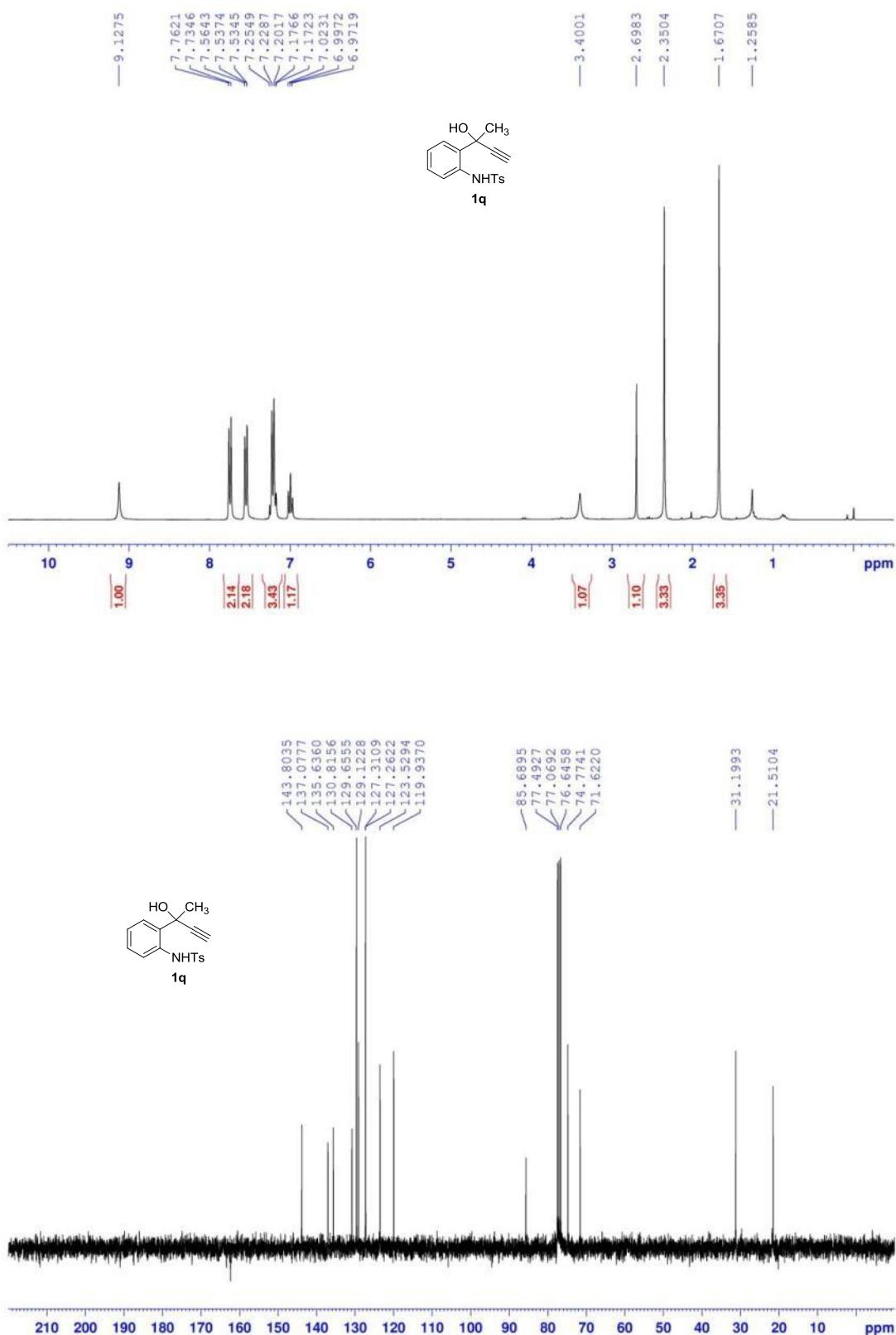


Figure S18. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxy-3-phenylprop-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1r**)

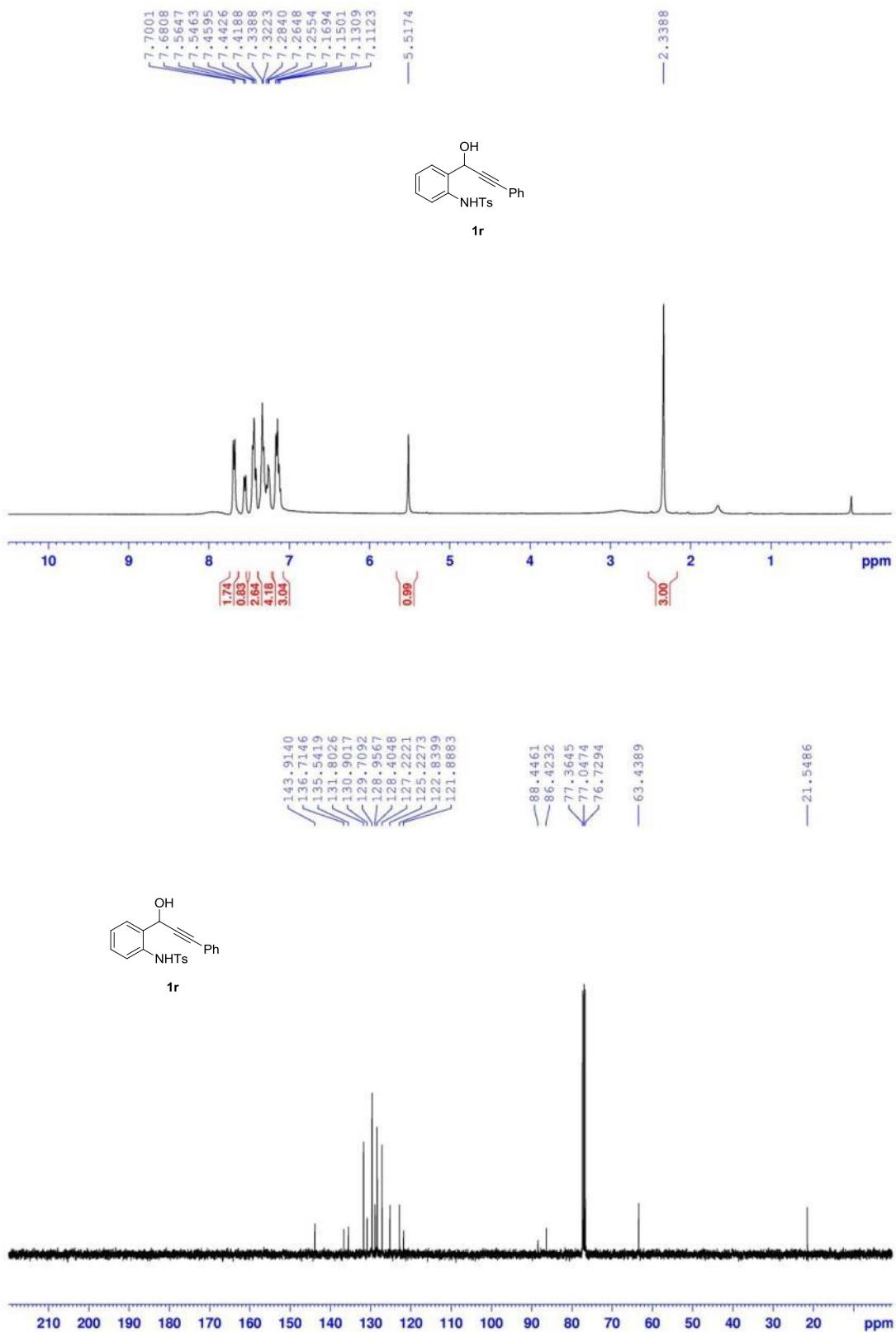


Figure S19. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxybut-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1s**)

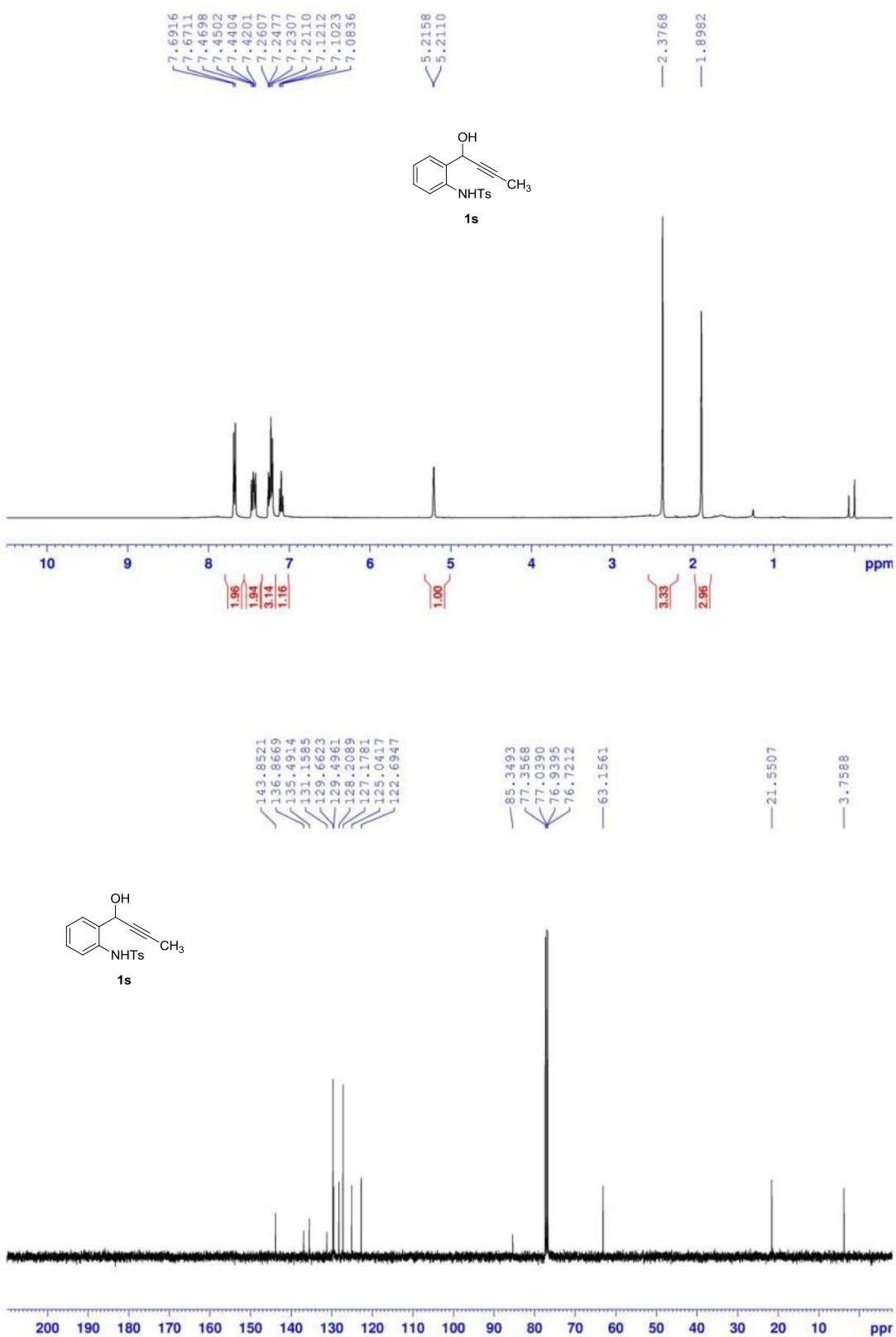


Figure S20. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxyhept-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1t**)

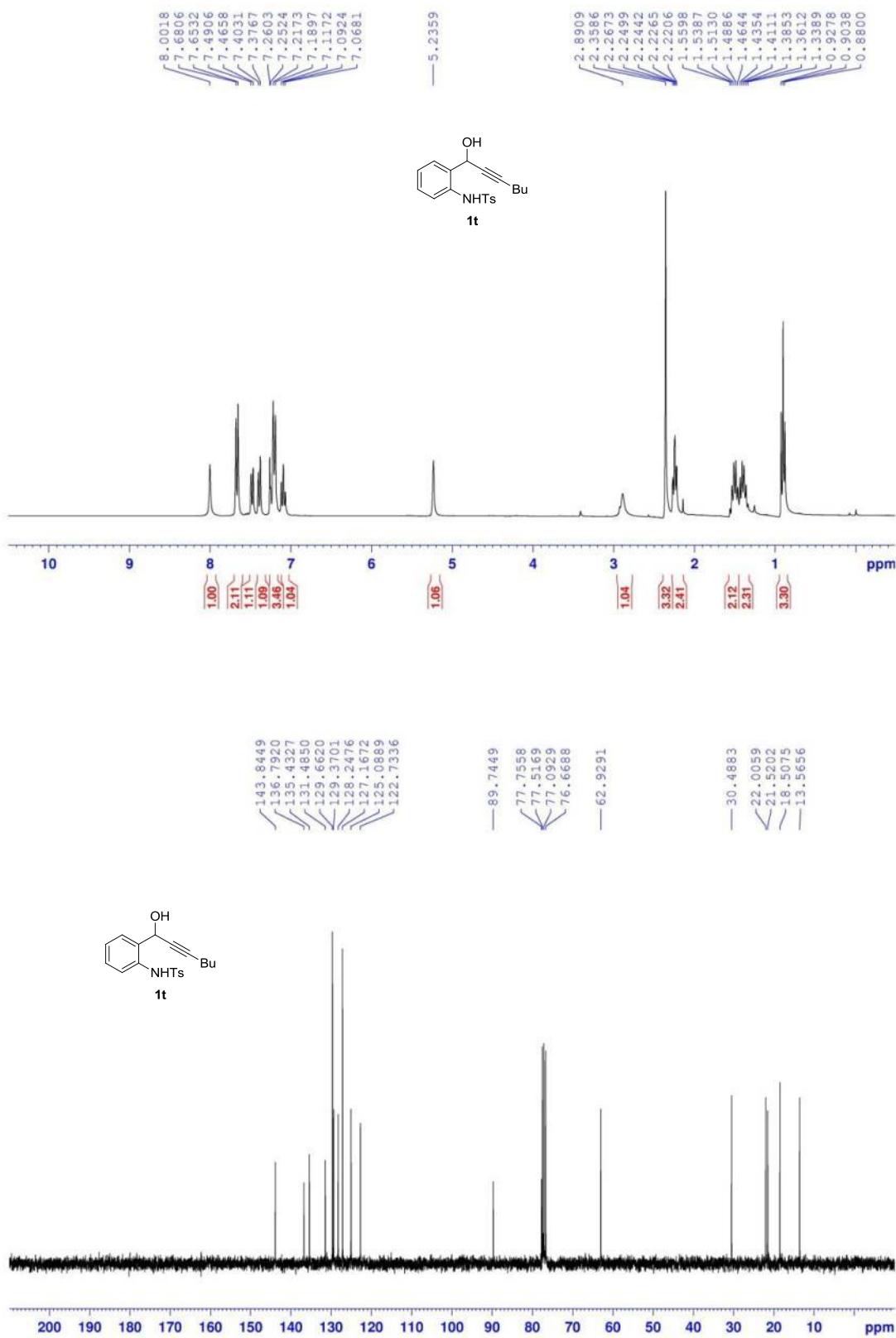


Figure S21. ^1H and ^{13}C NMR Spectra of *N*-(2-(3-Cyclopropyl-1-hydroxyprop-2-yn-1-yl)phenyl)-4-methylbenzenesulfonamide (**1u**)

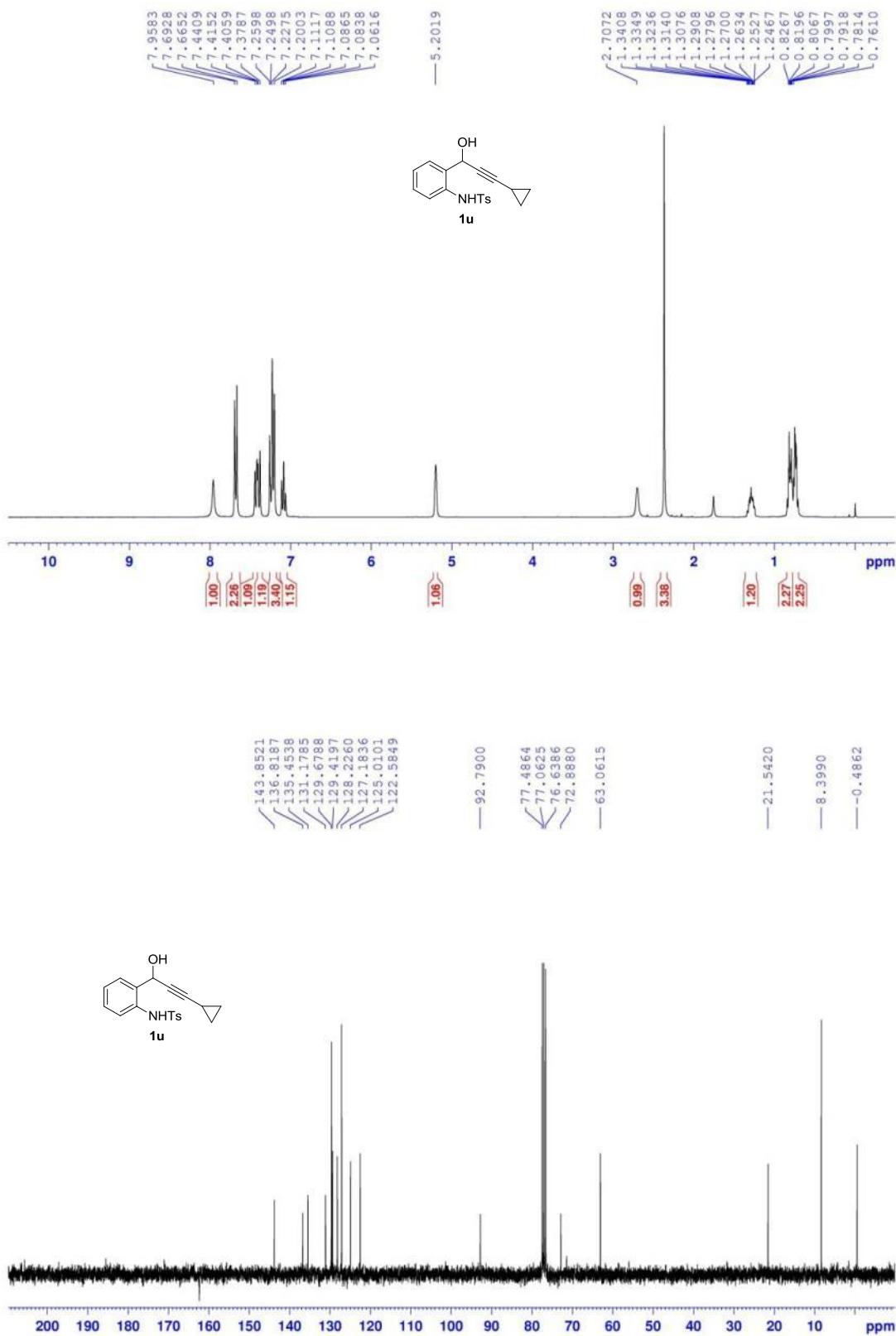


Figure S22. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxy-1,3-diphenylprop-2-yn-1-yl)phenyl)-4-nitrobenzenesulfonamide (**1v**)

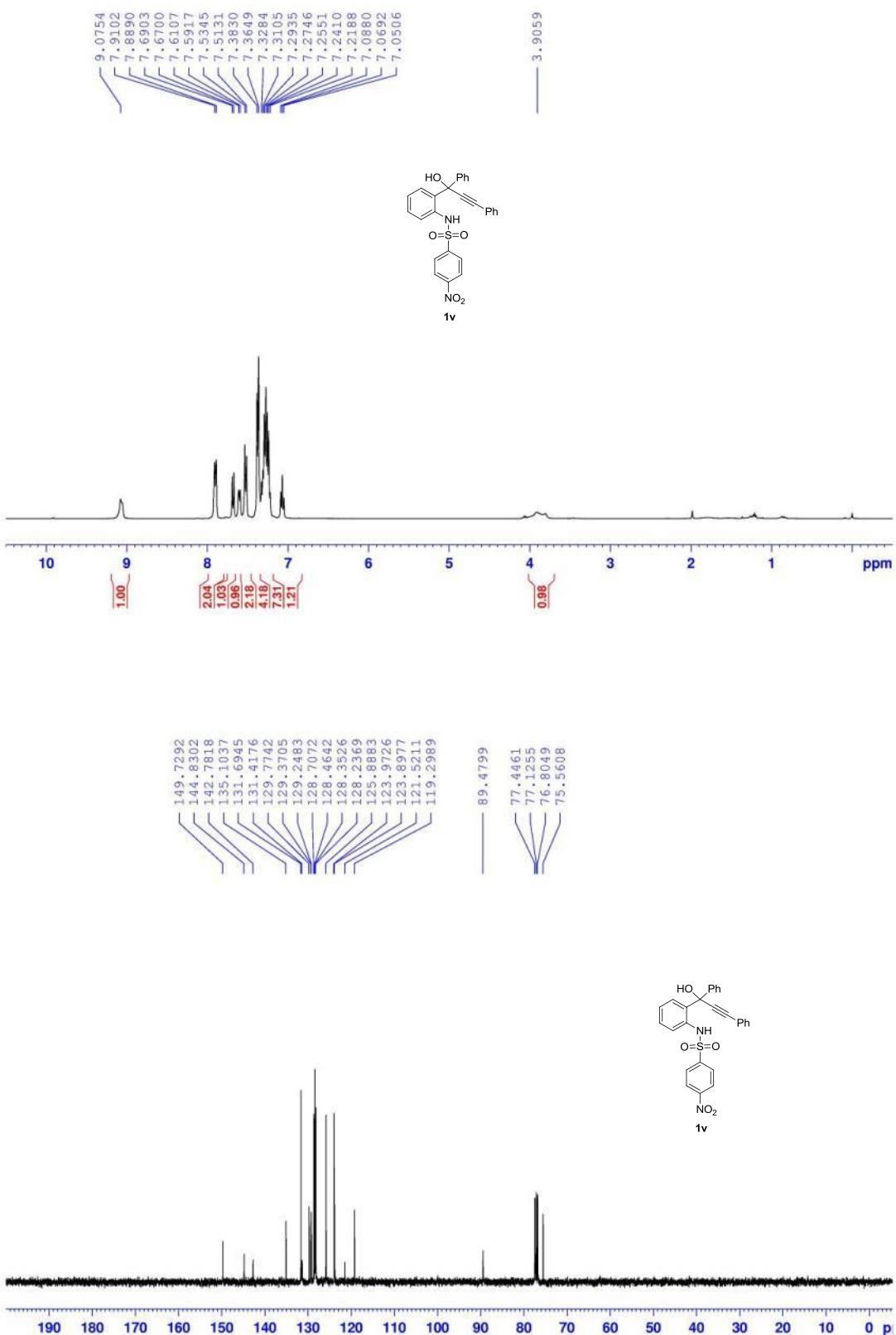


Figure S23. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxy-1,3-diphenylprop-2-yn-1-yl)phenyl) methanesulfonamide (**1w**)

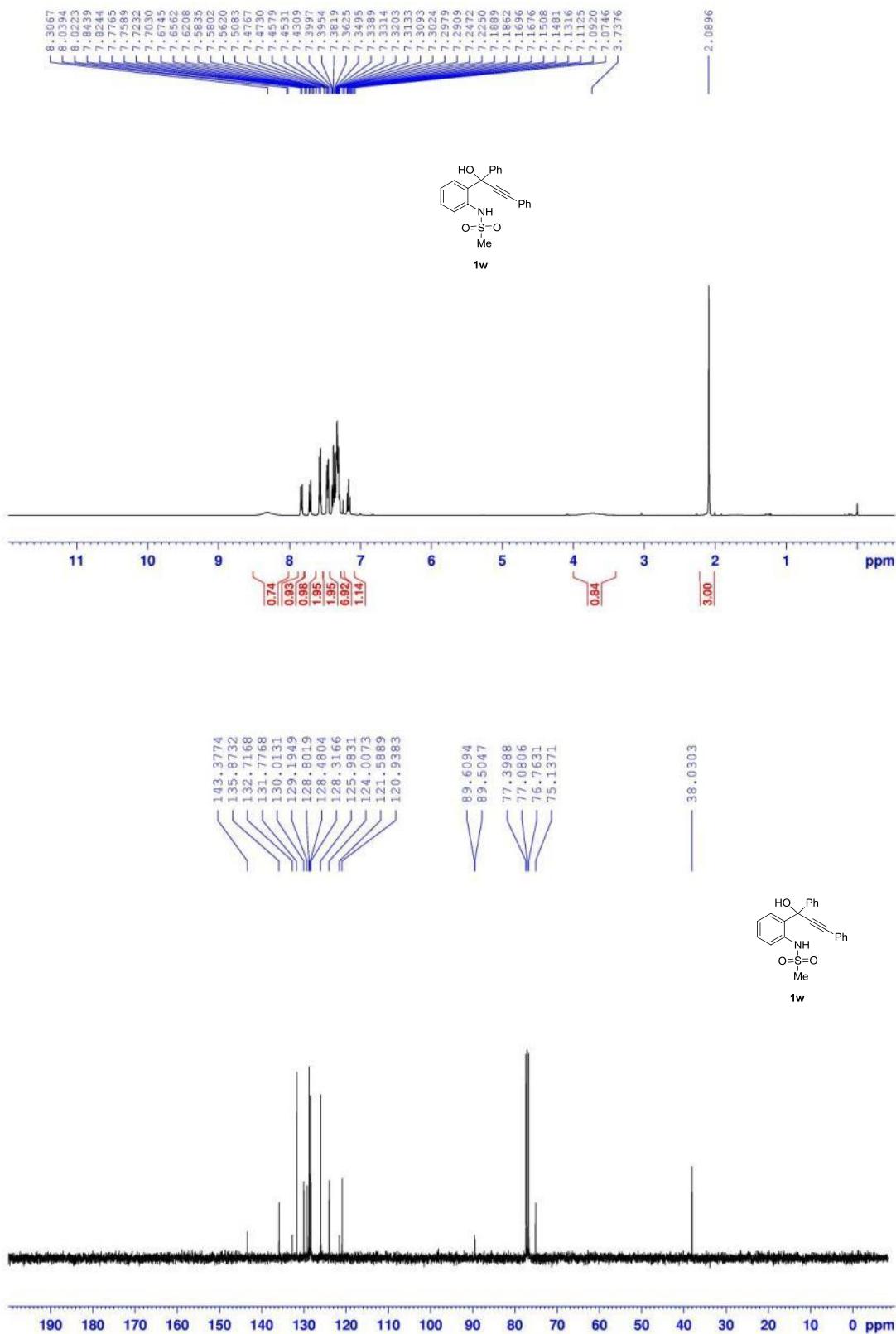


Figure S24. ^1H and ^{13}C NMR Spectra of *N*-(2-(1-Hydroxy-1,3-diphenylprop-2-yn-1-yl)phenyl) acetamide (**1x**)

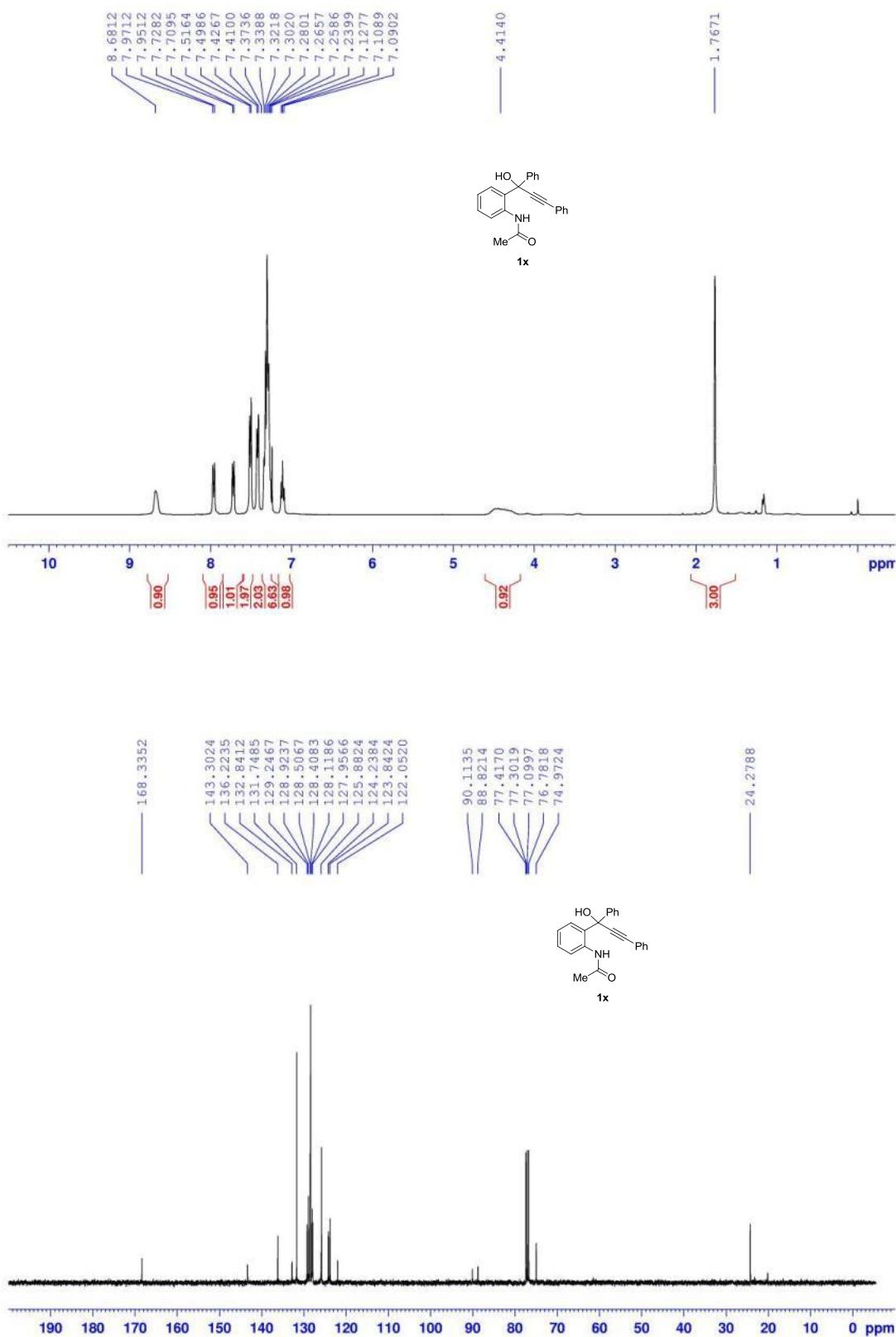


Figure S25. ^1H and ^{13}C NMR Spectra of *Tert*-butyl (2-(1-hydroxy-1,3-diphenylprop-2-yn-1-yl)phenyl)carbamate (**1y**)

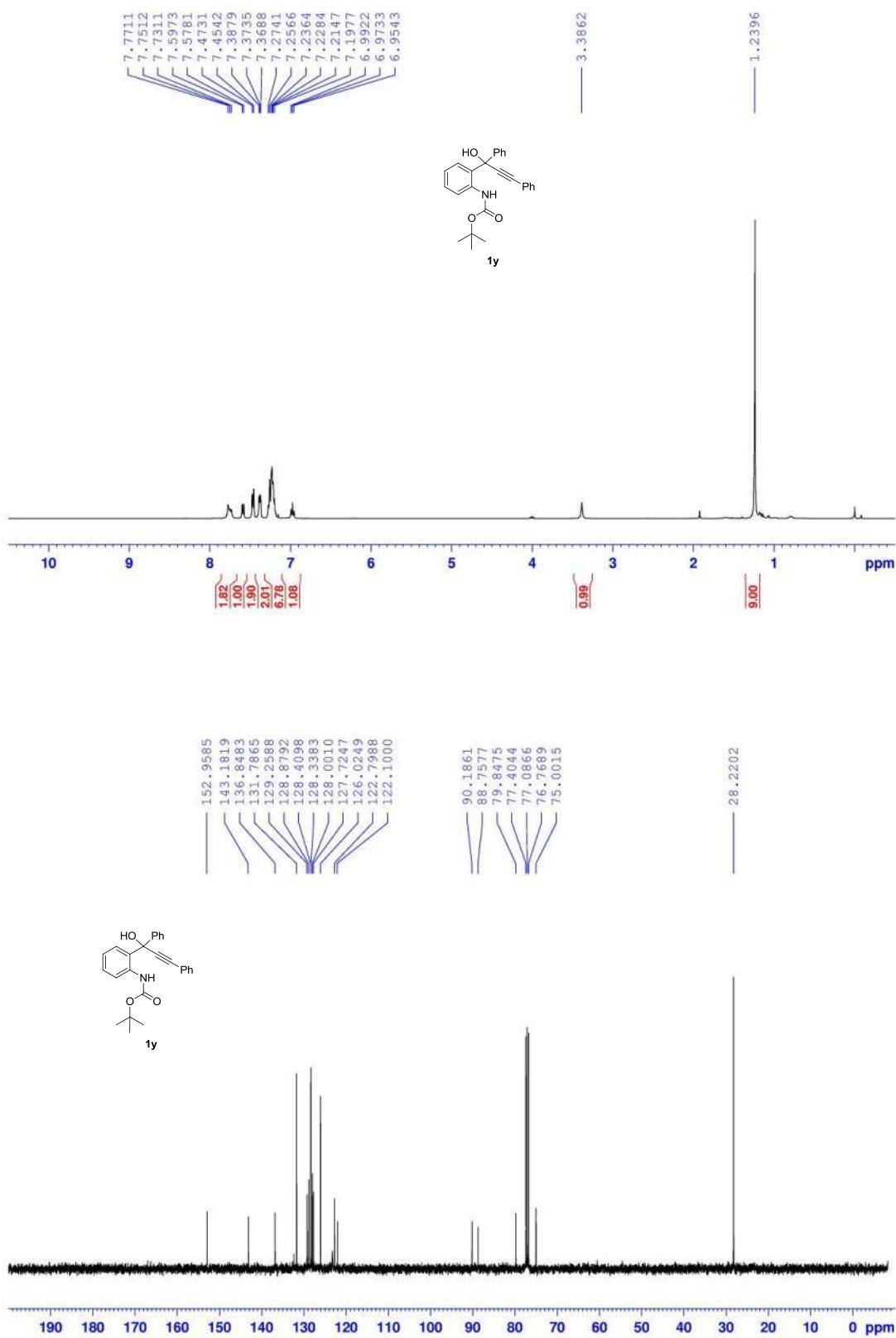


Figure S26. ^1H and ^{13}C NMR Spectra of (*Z*)-2-Benzylidene-3-phenyl-1-tosylindolin-3-ol (**2a**)^{S1}

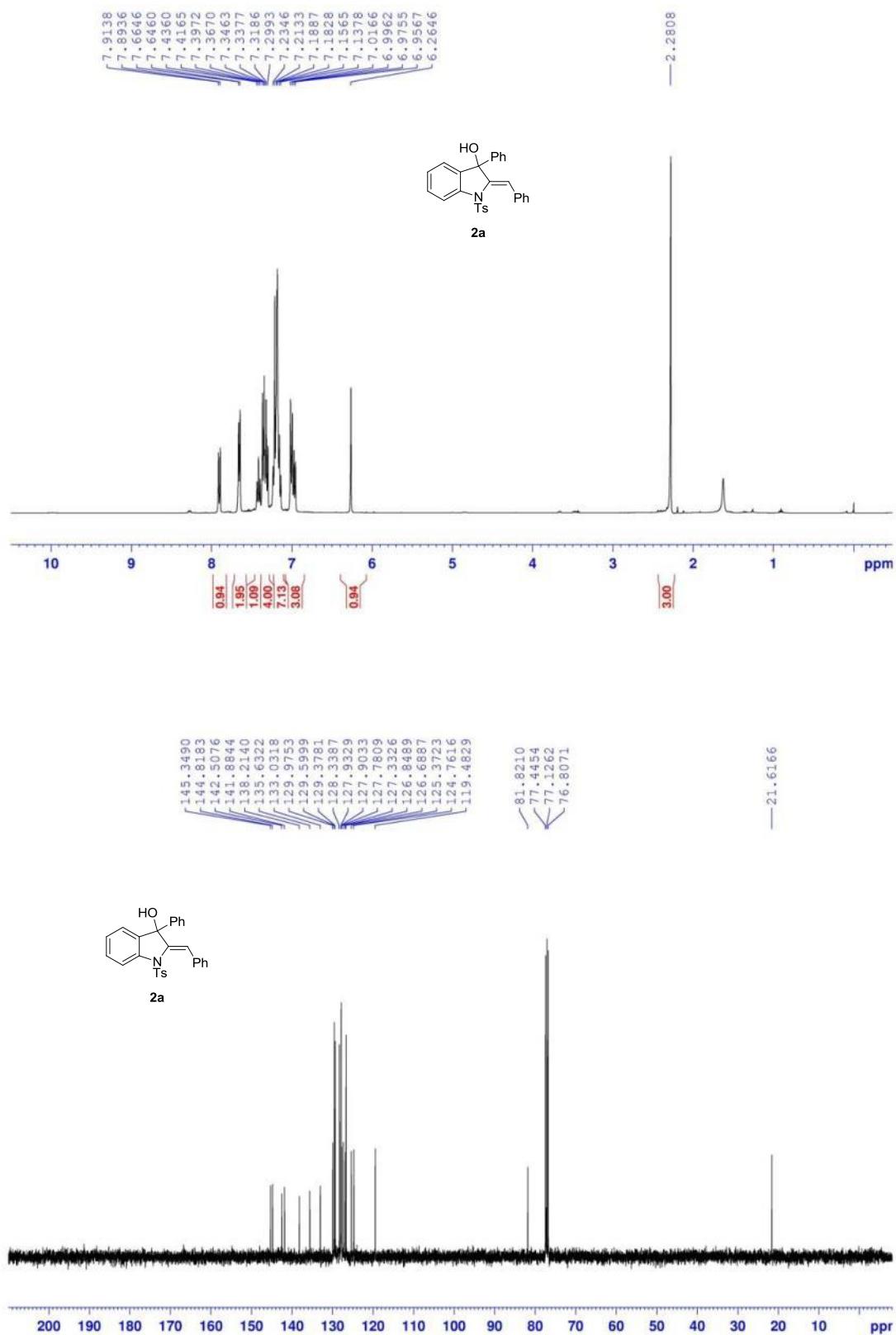


Figure S27. ^1H and ^{13}C NMR Spectra of (*Z*)-2-Benzylidene-5-methyl-3-phenyl-1-tosylindolin-3-ol (**2b**)

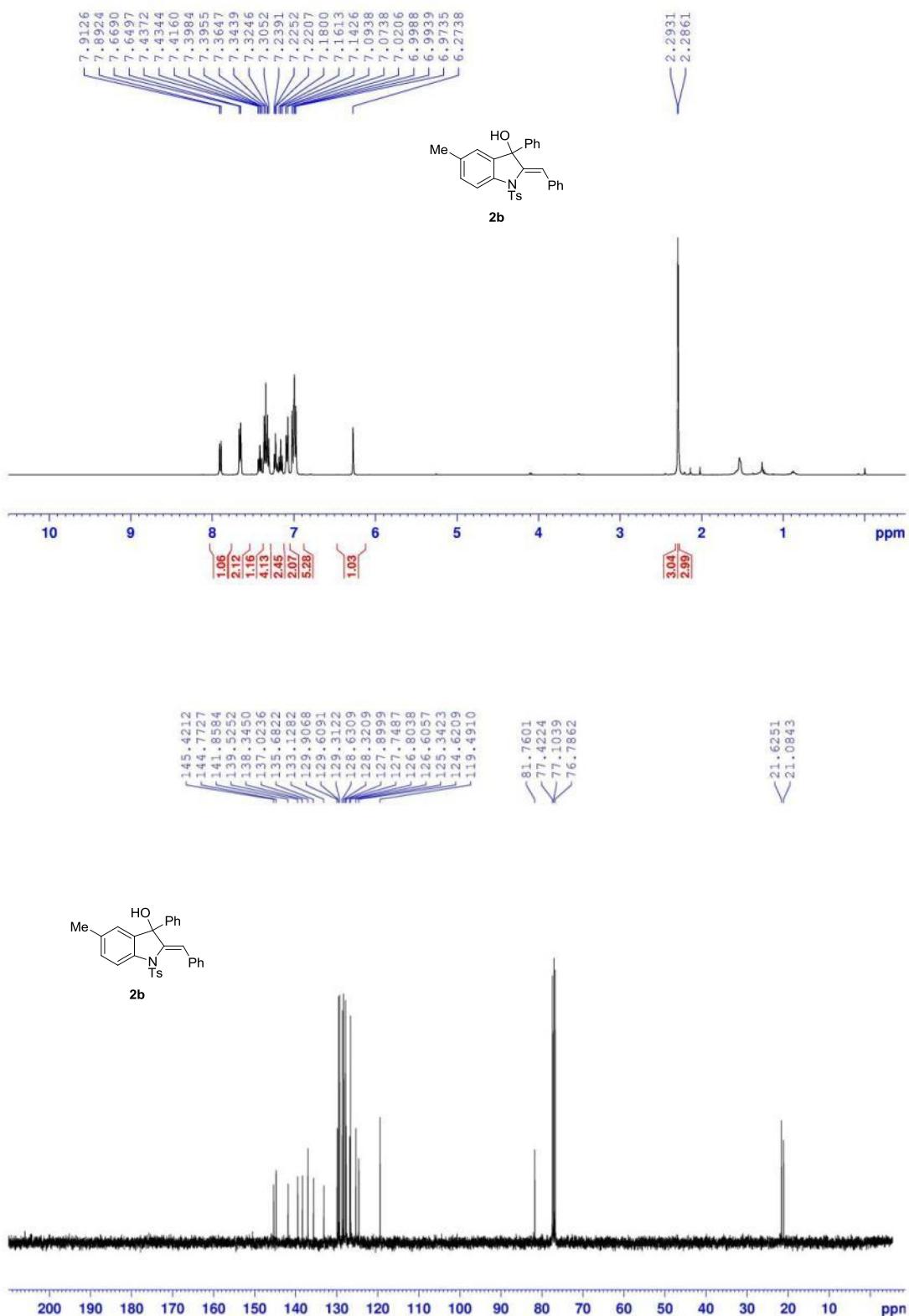


Figure S28. ^1H and ^{13}C NMR Spectra of (*Z*)-2-Benzylidene-5-bromo-3-phenyl-1-tosylindolin-3-ol (**2c**)

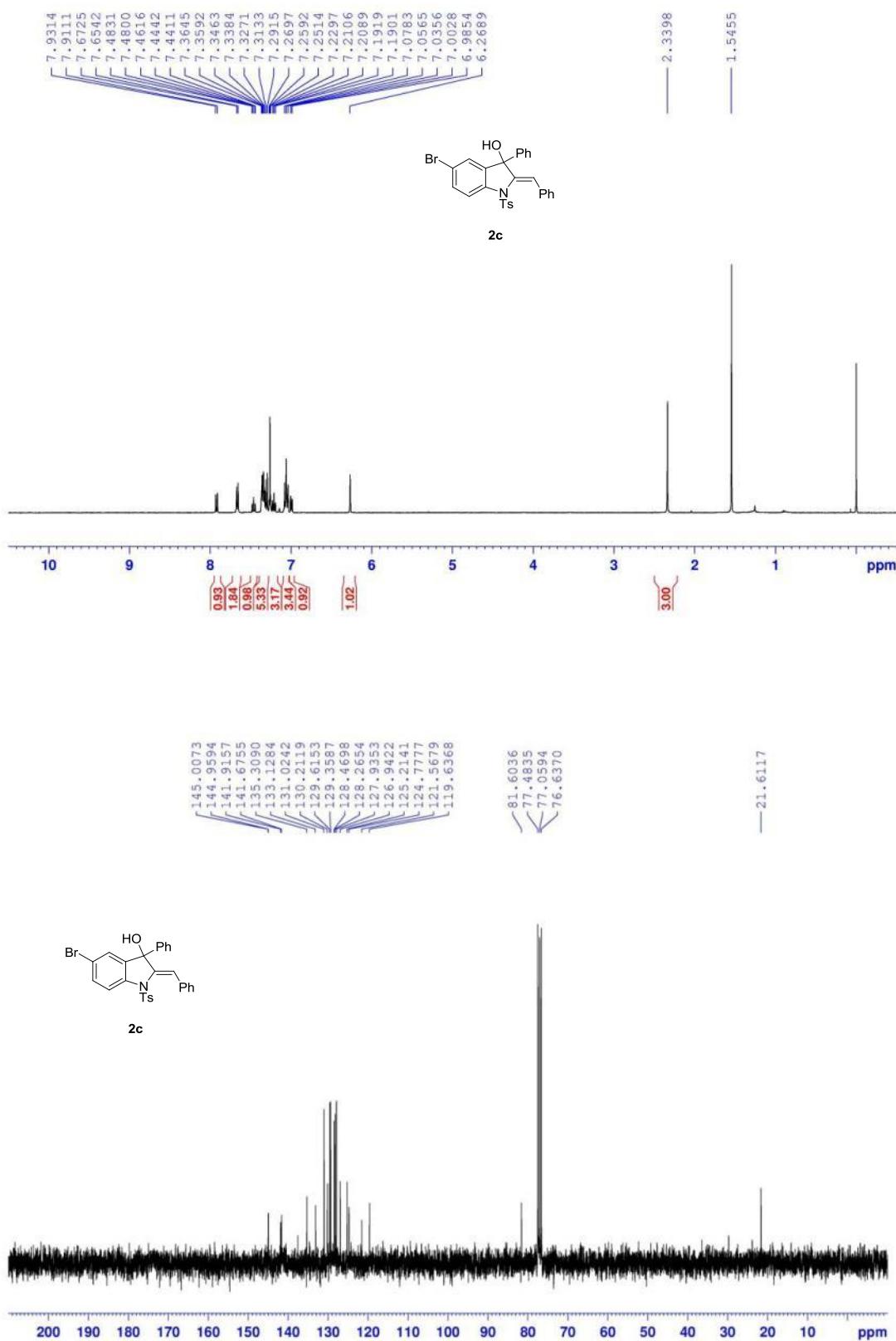


Figure S29. ^1H and ^{13}C NMR Spectra of (*Z*)-2-Benzylidene-5-chloro-3-phenyl-1-tosylindolin-3-ol (**2d**)

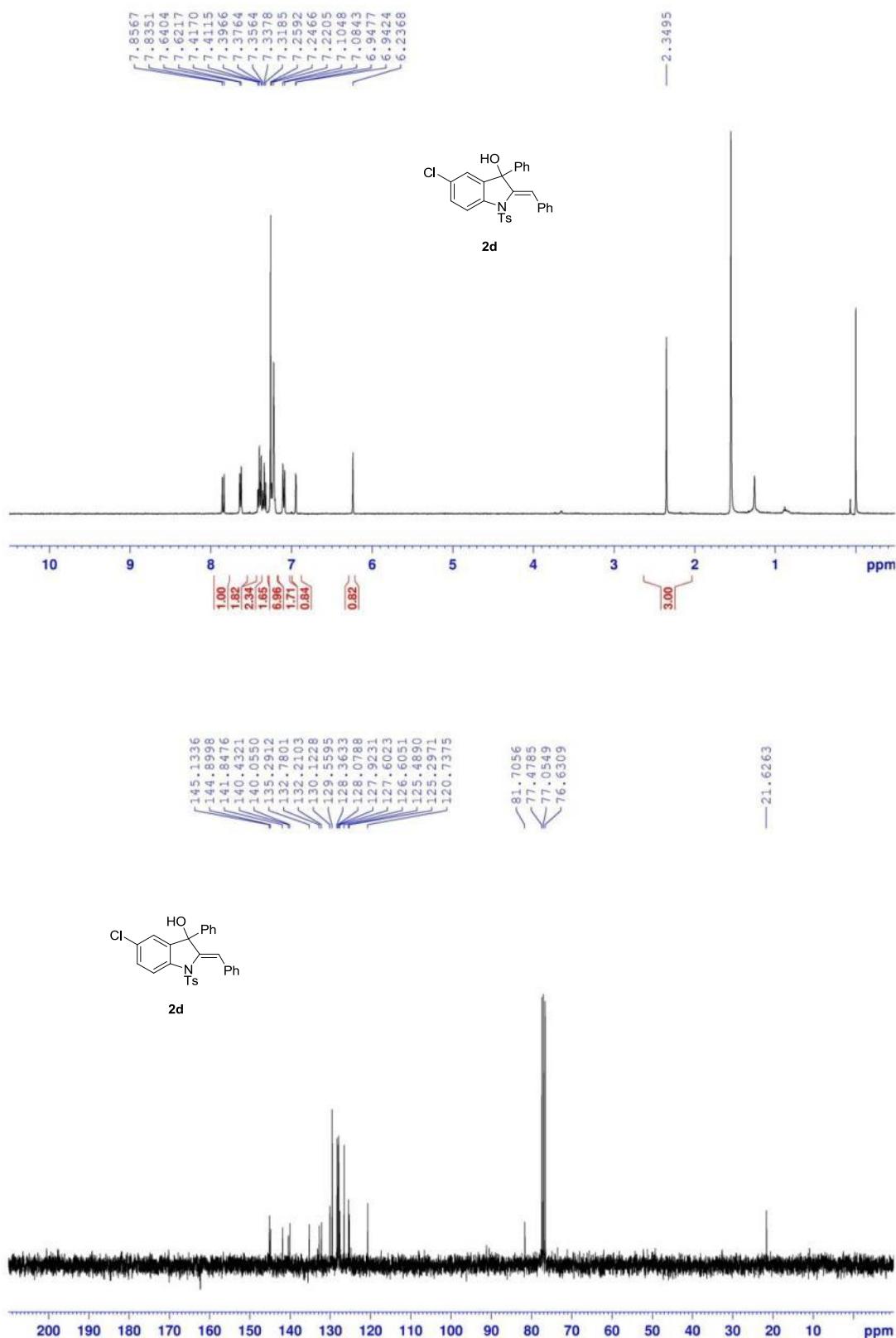


Figure S30. ^1H and ^{13}C NMR Spectra of (*Z*)-2-Benzylidene-3-phenyl-1-tosyl-2,3-dihydro-1*H*-benzo[*f*]indol-3-ol (**2e**)

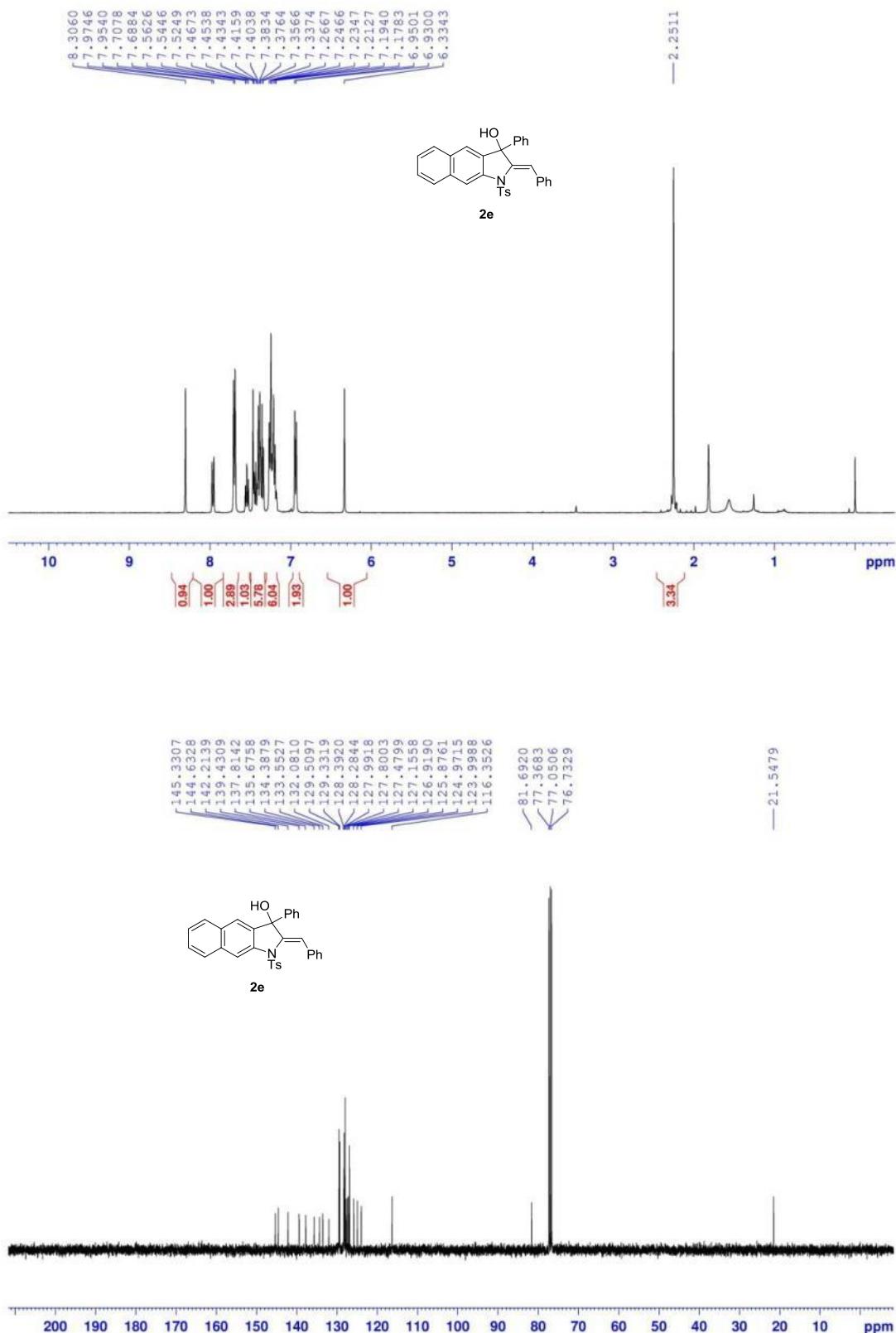


Figure S31. ^1H and ^{13}C NMR Spectra of (*Z*)-2-Benzylidene-3-(*p*-tolyl)-1-tosylindolin-3-ol (**2f**)

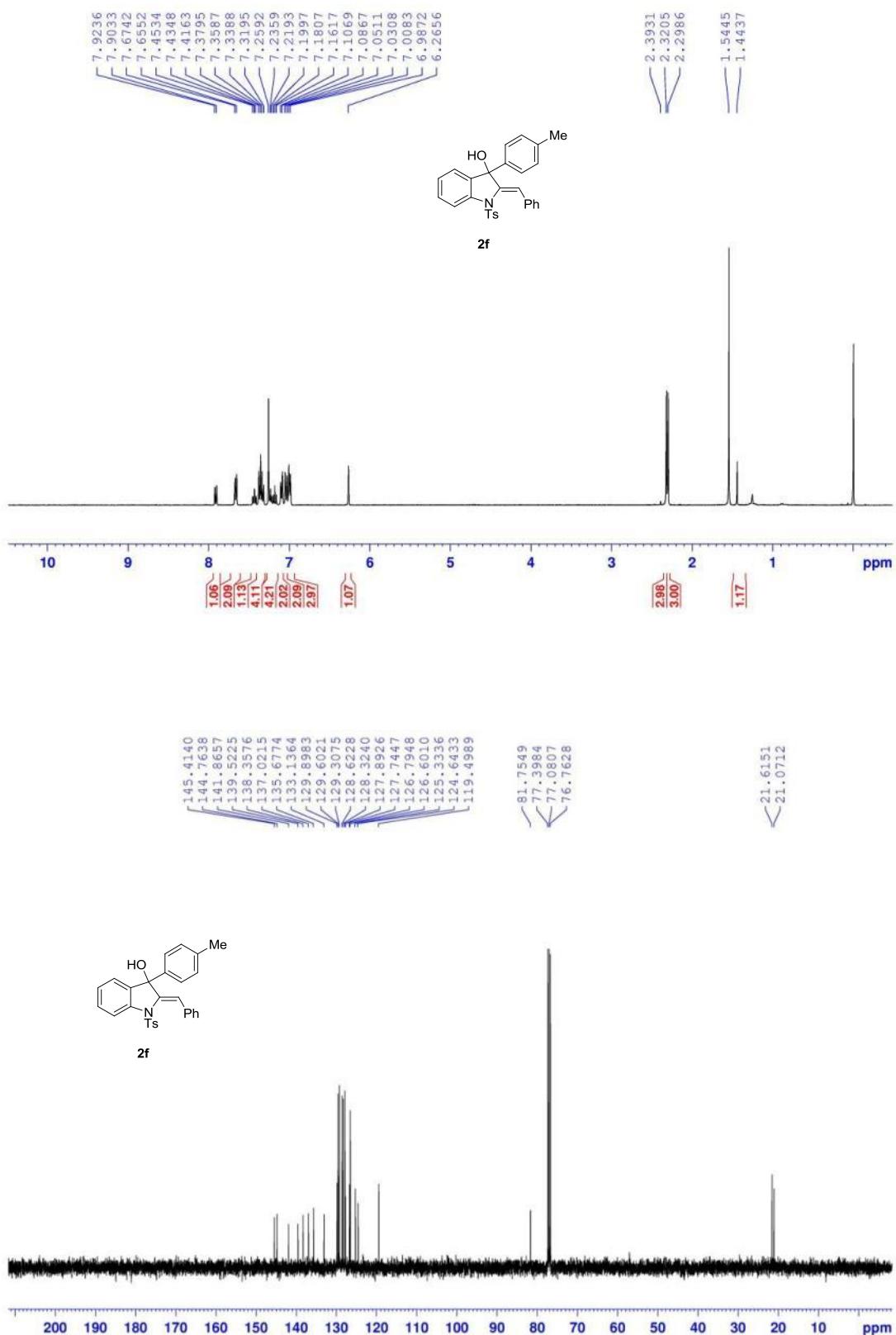


Figure S32. ^1H and ^{13}C NMR Spectra of (Z)-2-Benzylidene-3-(4-chlorophenyl)-1-tosylindolin-3-ol (**2g**)

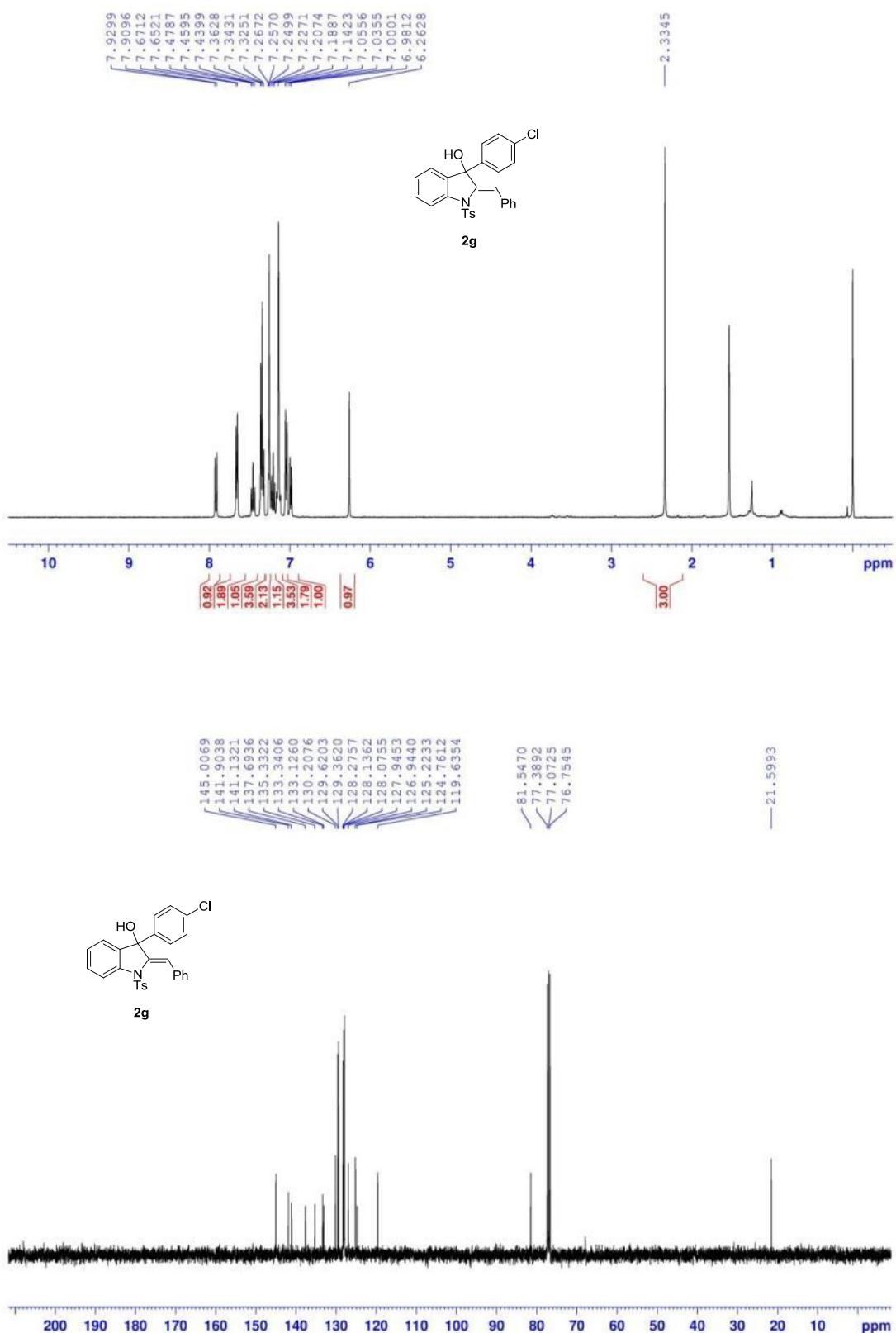


Figure S33. ^1H and ^{13}C NMR Spectra of (*Z*)-2-Benzylidene-3-(4-bromophenyl)-1-tosylindolin-3-ol (**2h**)

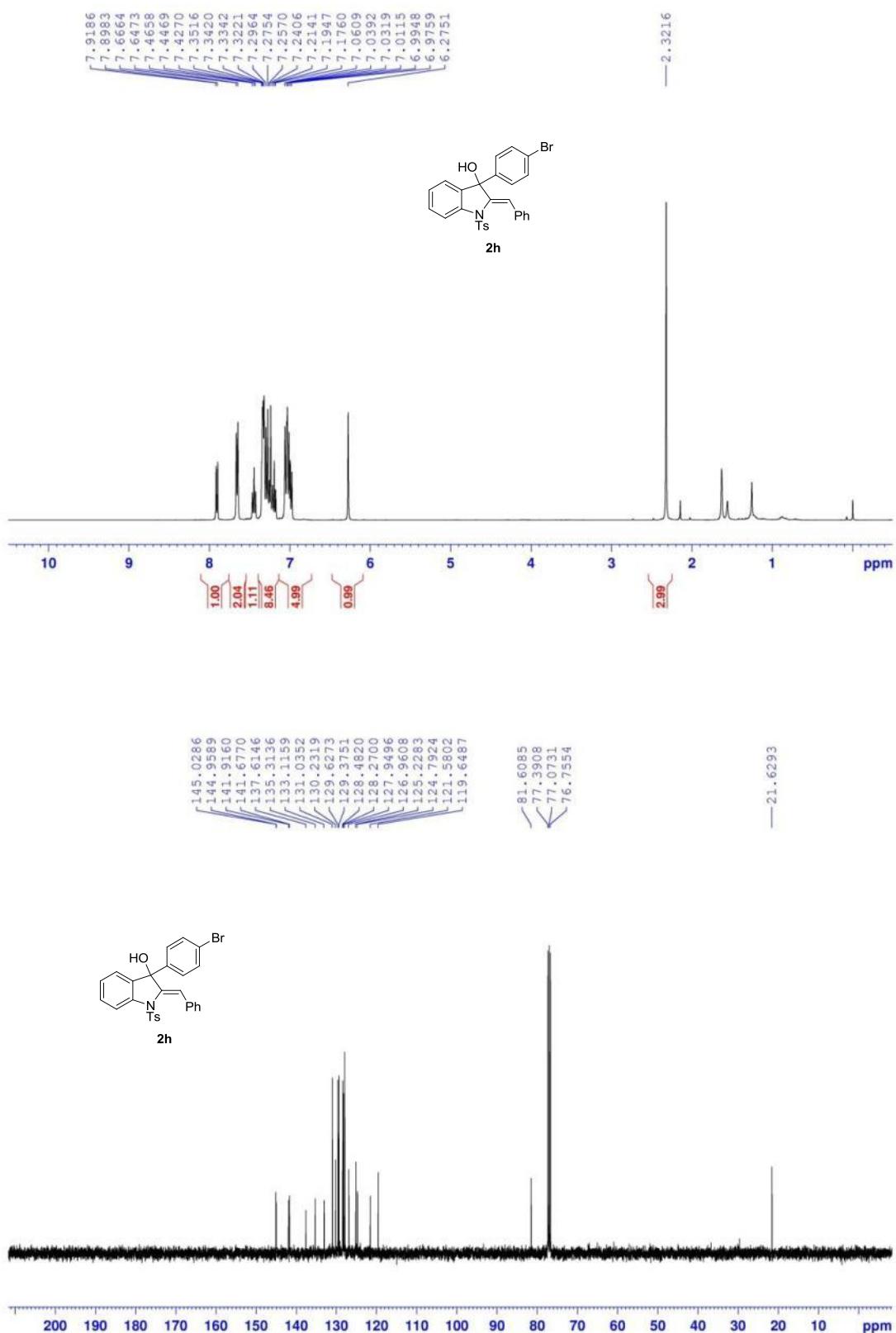


Figure S34. ^1H and ^{13}C NMR Spectra of (*Z*)-2-(4-Fluorobenzylidene)-3-phenyl-1-tosylindolin-3-ol (**2i**)

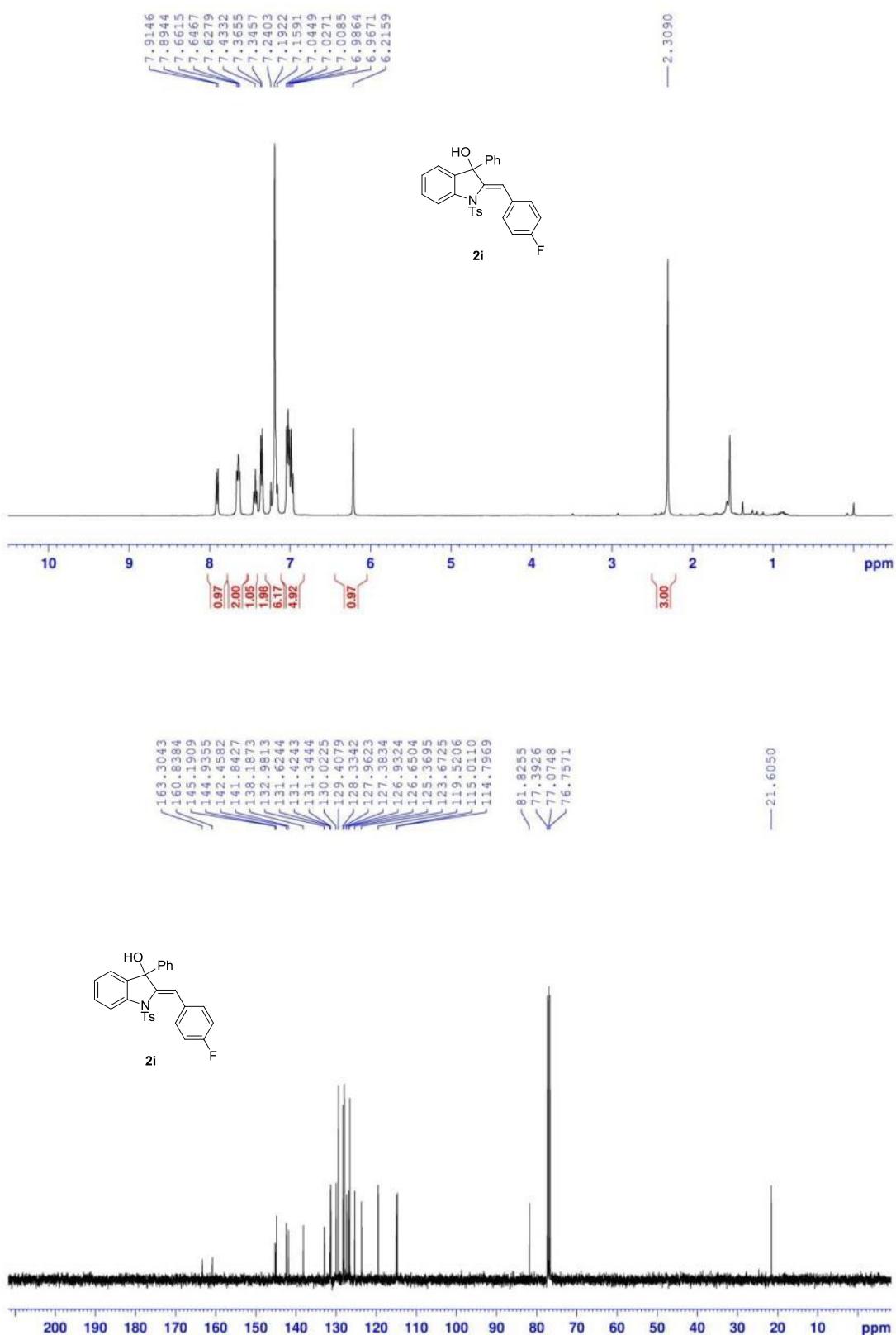


Figure S35. ^1H and ^{13}C NMR Spectra of (*Z*)-3-Phenyl-1-tosyl-2-(4-(trifluoromethyl)benzylidene)indolin-3-ol (**2j**)

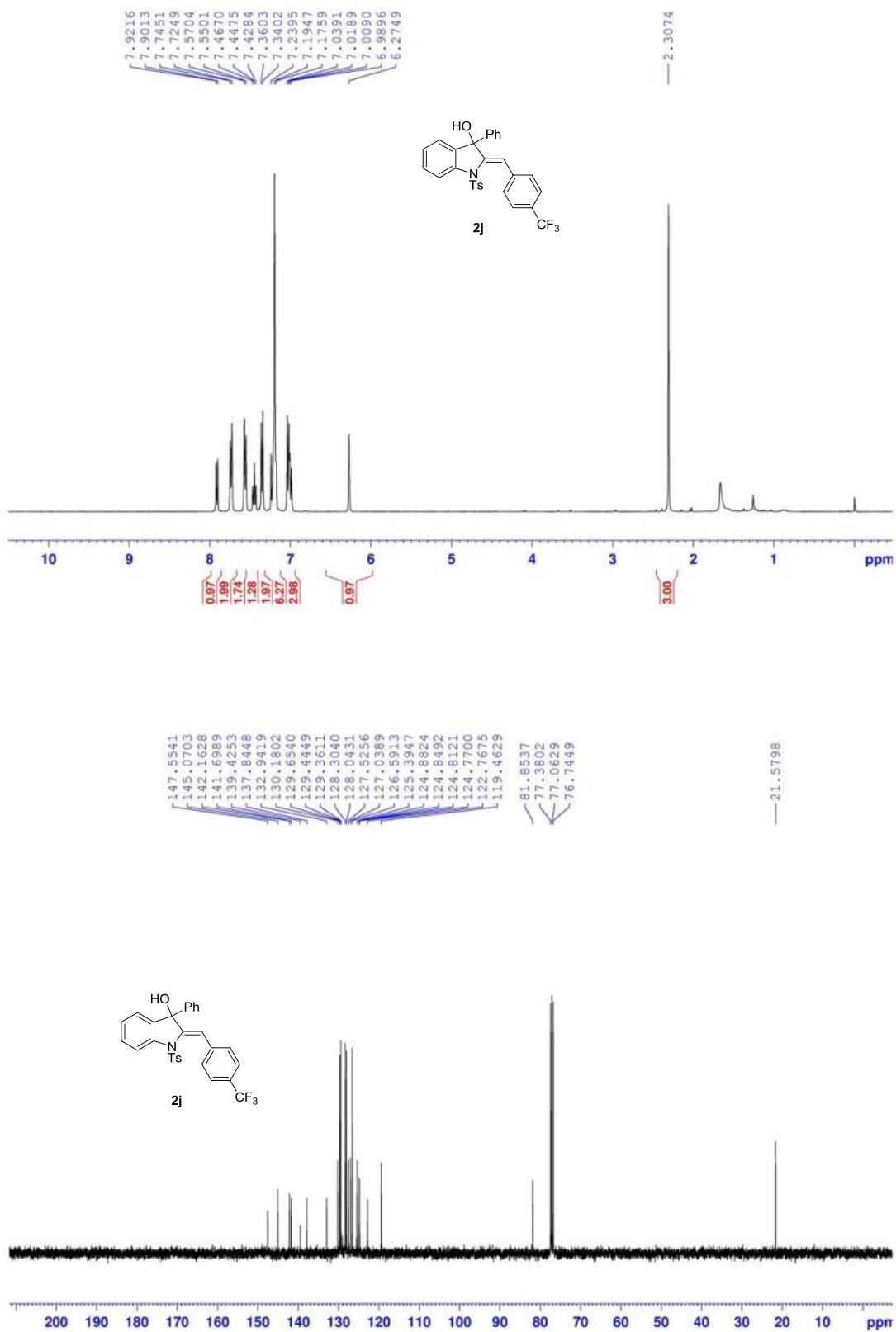


Figure S36. ^1H and ^{13}C NMR Spectra of (Z)-2-(4-Methylbenzylidene)-3-phenyl-1-tosylindolin-3-ol

(2k)

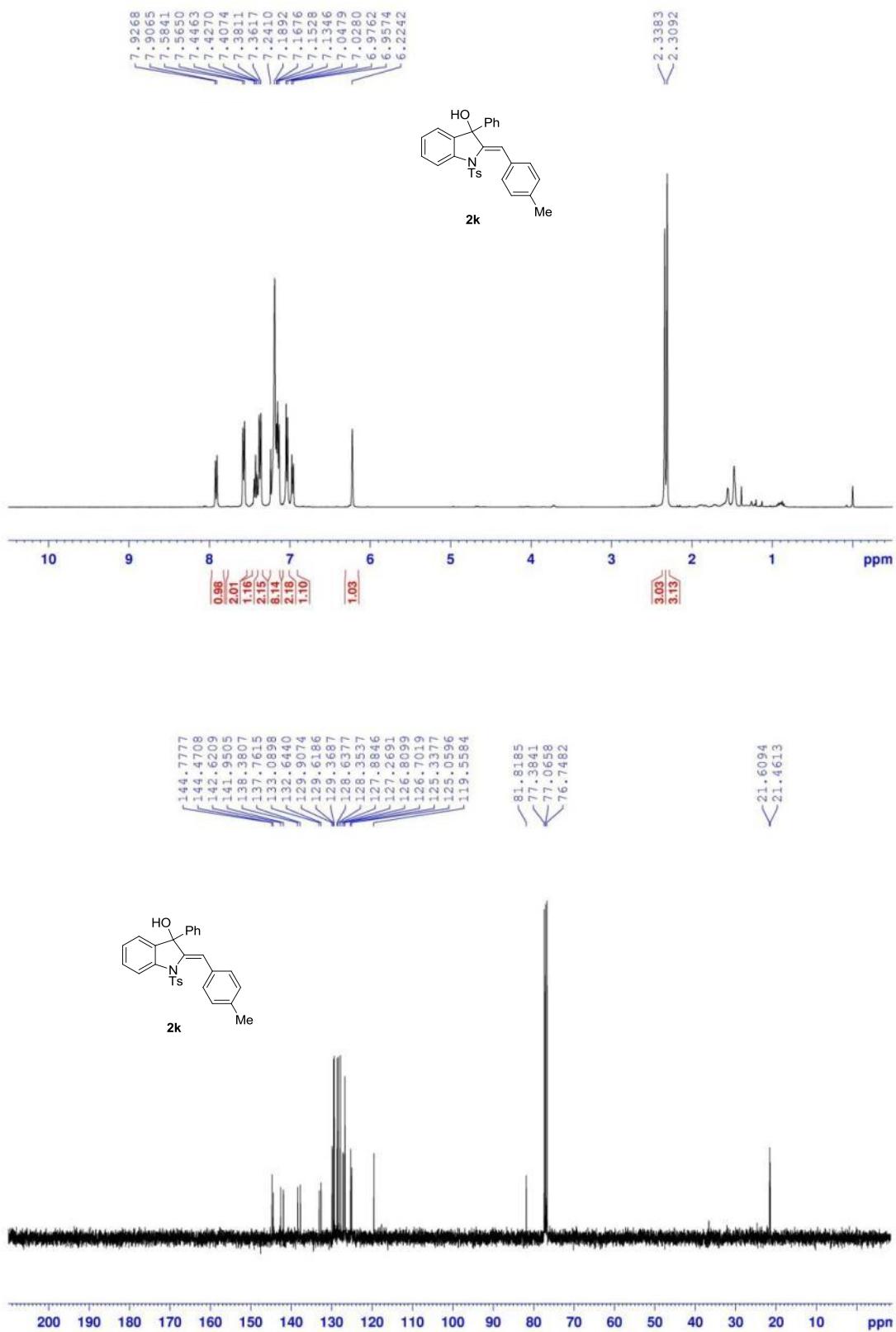


Figure S37. ^1H and ^{13}C NMR Spectra of (Z)-3-Phenyl-2-(thiophen-3-ylmethylene)-1-tosylindolin-3-ol

(**2l**)

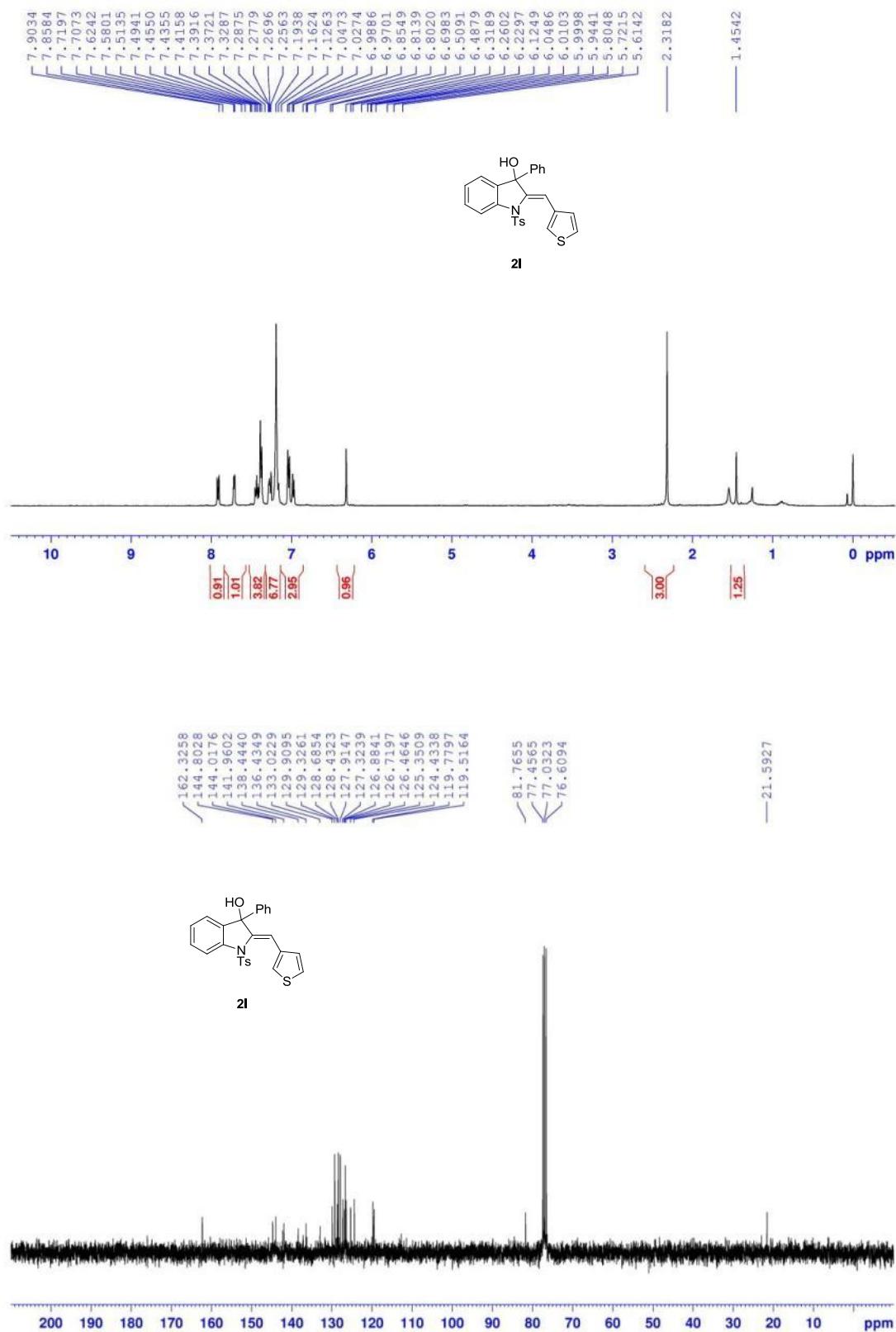


Figure S38. ^1H and ^{13}C NMR Spectra of (Z)-2-(Cyclopropylmethylene)-3-phenyl-1-tosylindolin-3-ol (**2m**)

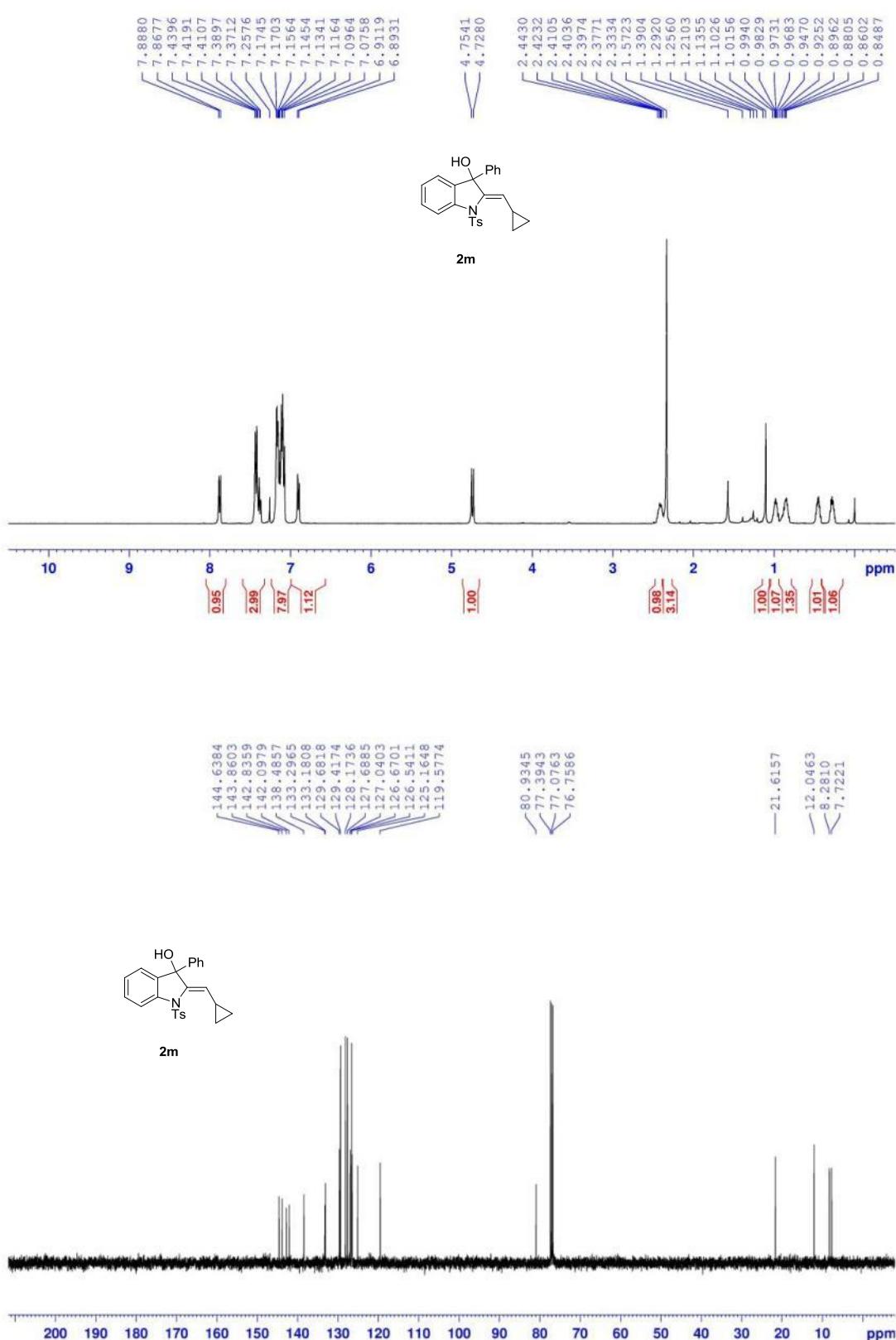


Figure S39. ^1H and ^{13}C NMR Spectra of (*Z*)-2-Pentylidene-3-phenyl-1-tosylindolin-3-ol (**2n**)

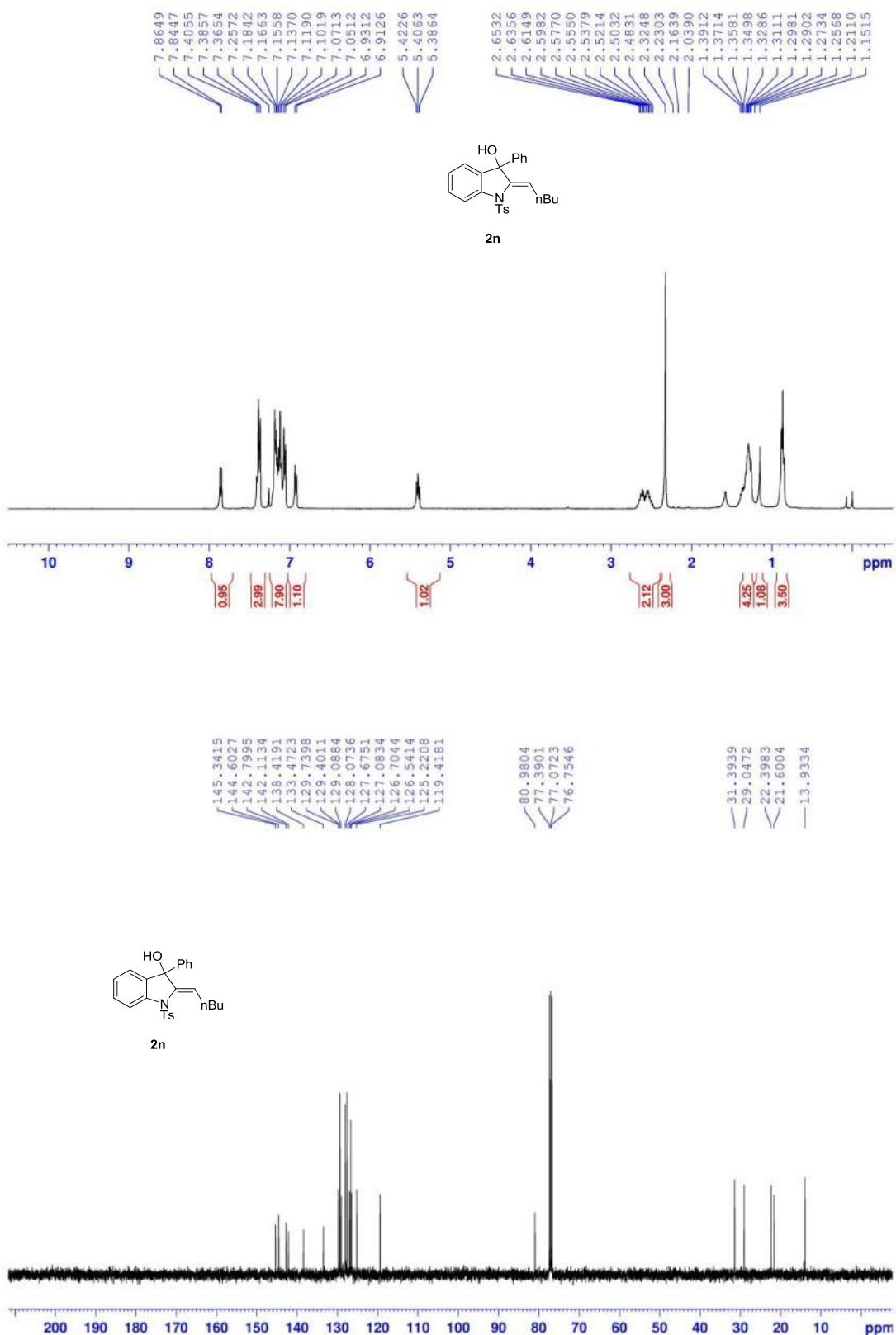


Figure S40. ^1H and ^{13}C NMR Spectra of (*Z*)-3-Methyl-2-pentylidene-1-tosylinolin-3-ol (**2o**)

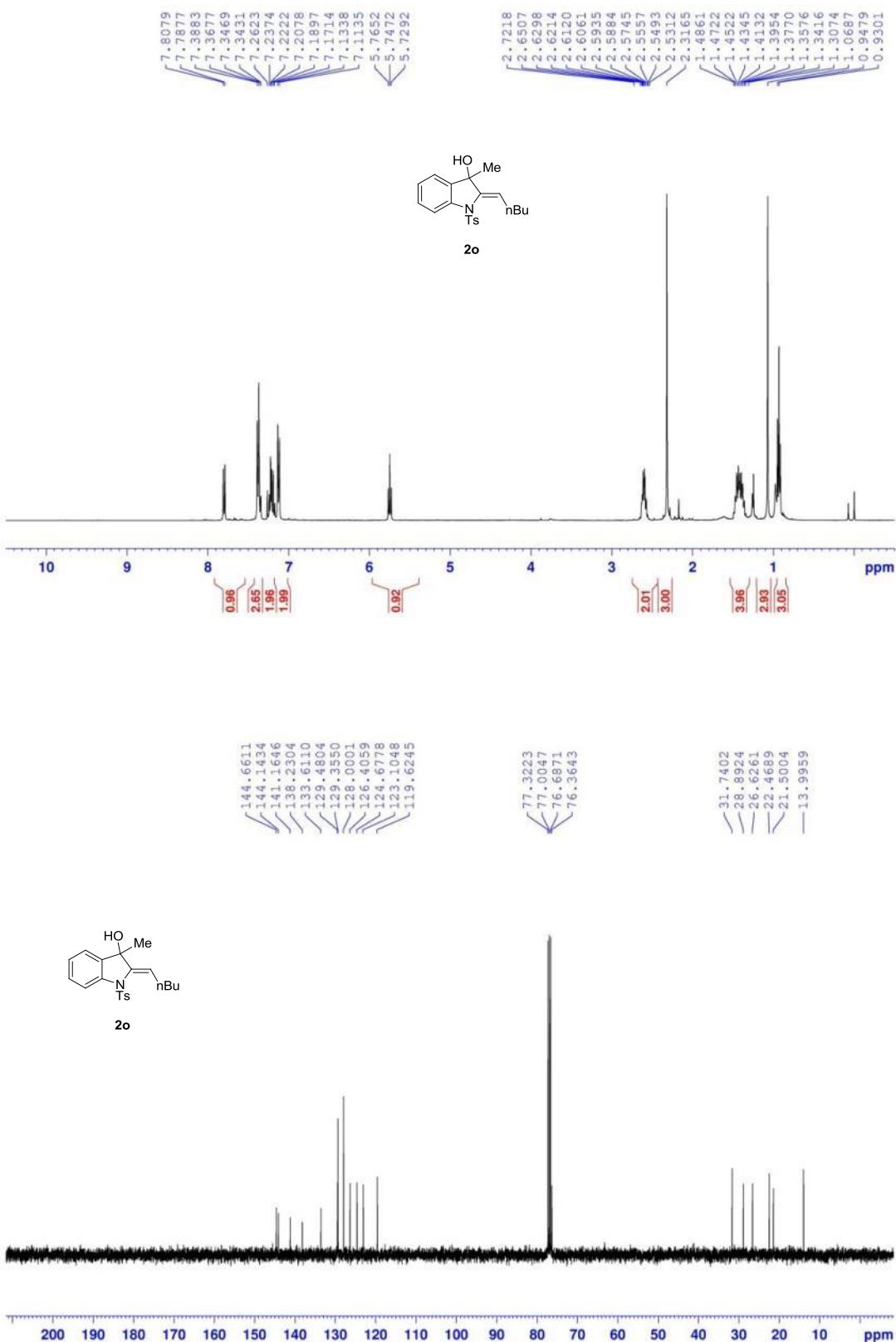


Figure S41. ^1H and ^{13}C NMR Spectra of 2-Methylene-3-phenyl-1-tosylindolin-3-ol (**2p**)

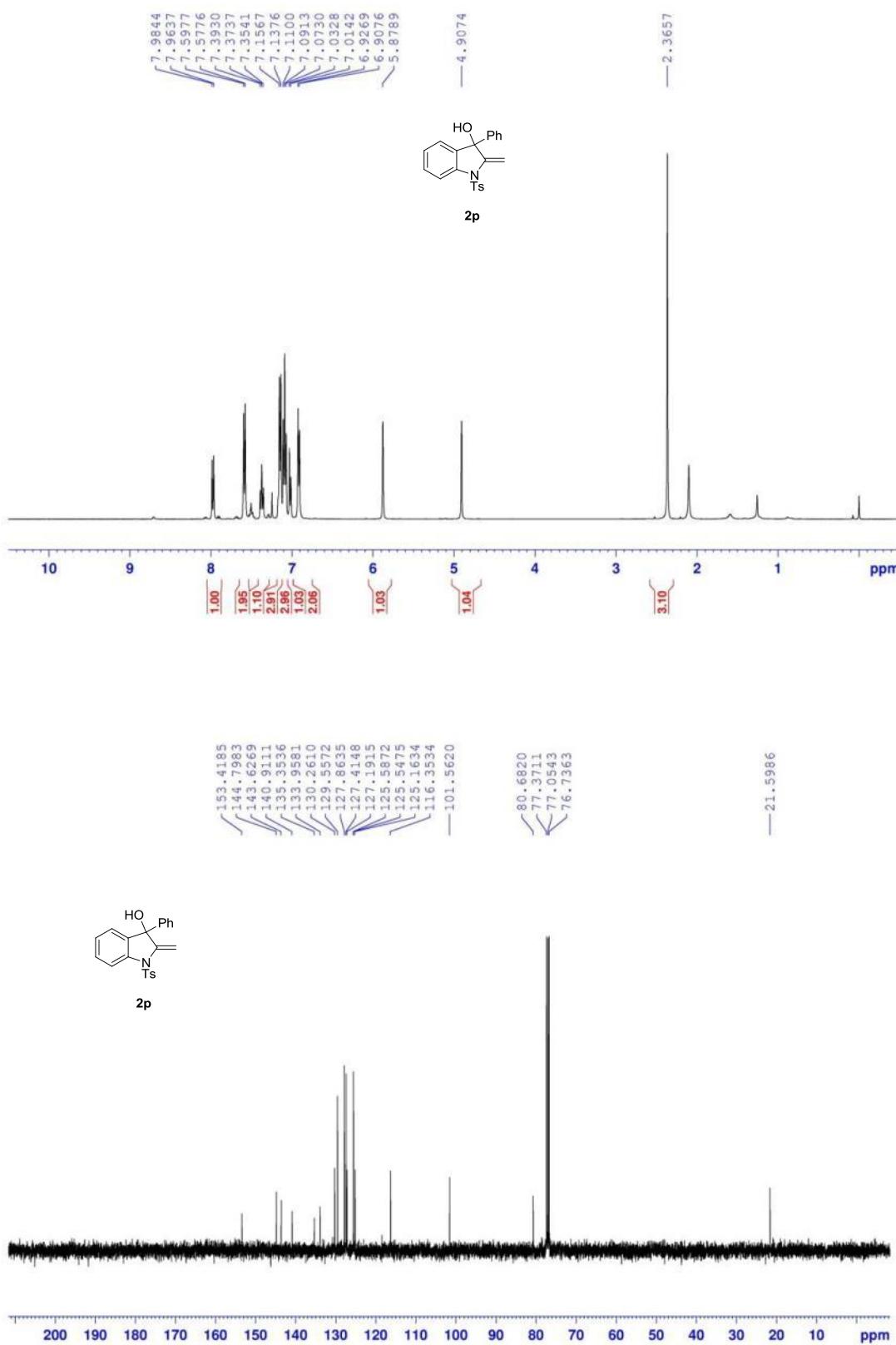


Figure S42. ^1H and ^{13}C NMR Spectra of 3-Methyl-2-methylene-1-tosylindolin-3-ol (**2q**)

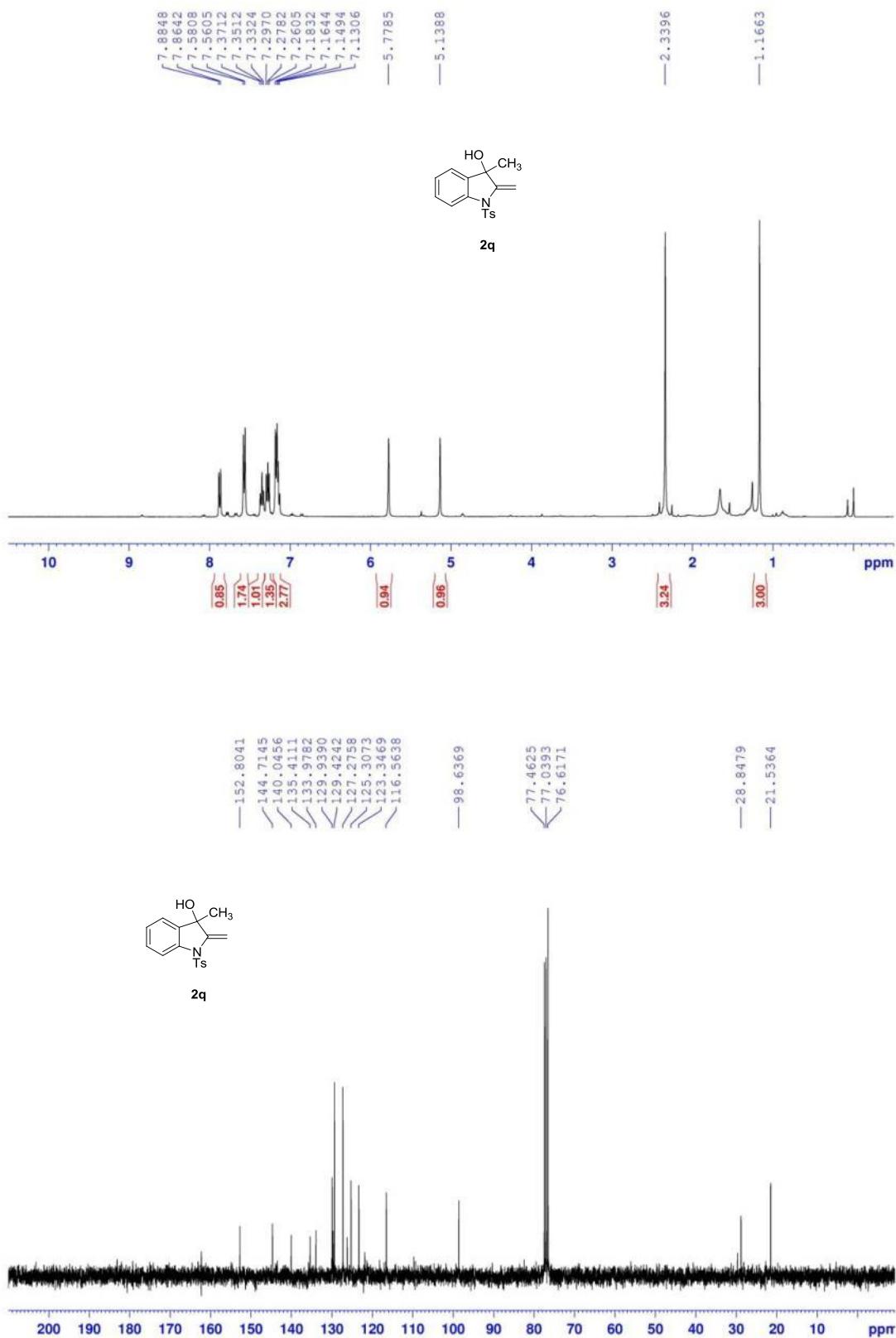


Figure S43. ^1H and ^{13}C NMR Spectra of (*Z*)-2-Benzylidene-1-tosylindolin-3-ol (**2r**)

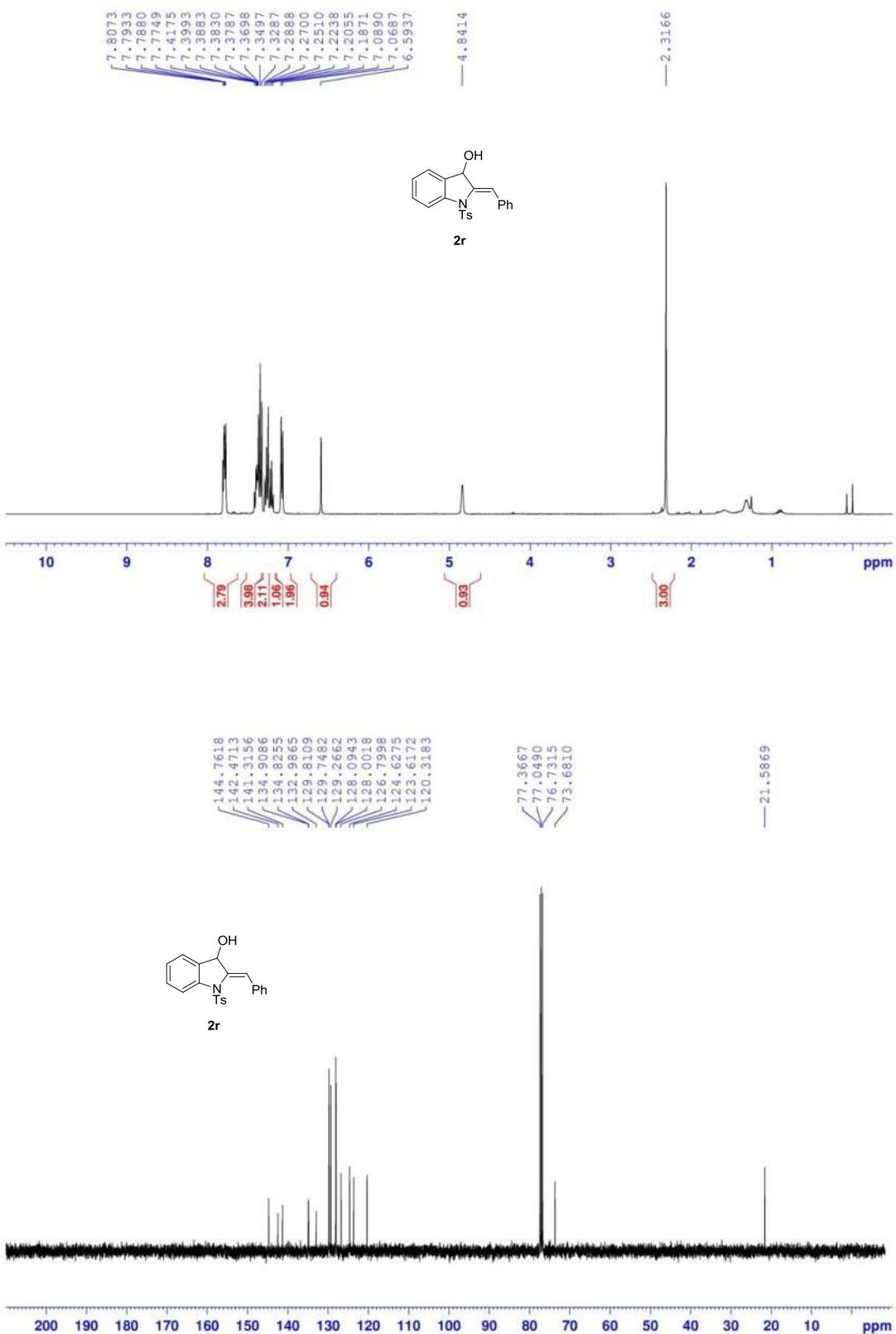


Figure S44. ^1H and ^{13}C NMR Spectra of (Z)-2-Ethylidene-1-tosylindolin-3-ol (**2s**)

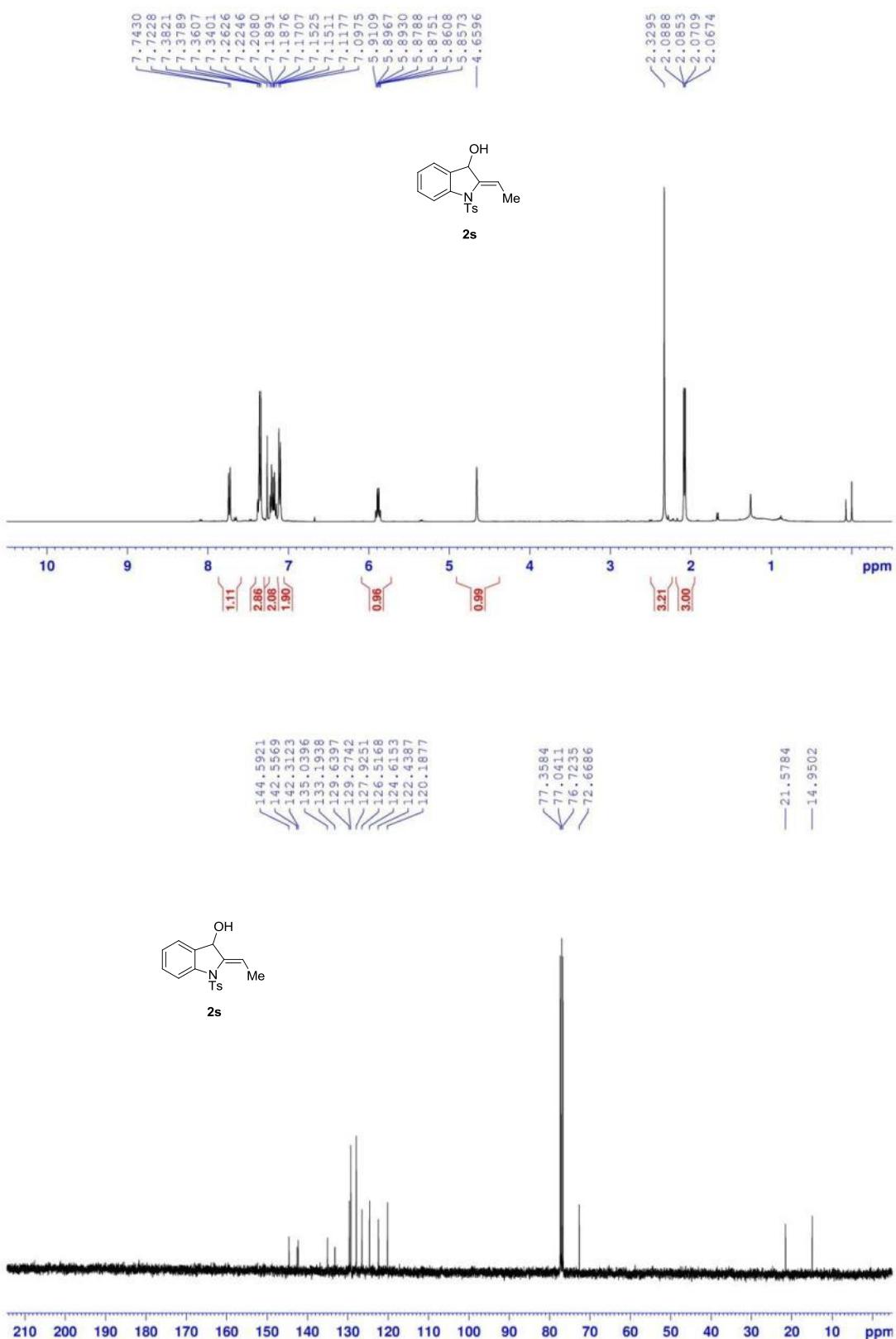


Figure S45. ^1H and ^{13}C NMR Spectra of (*Z*)-2-Pentylidene-1-tosylindolin-3-ol (**2t**)

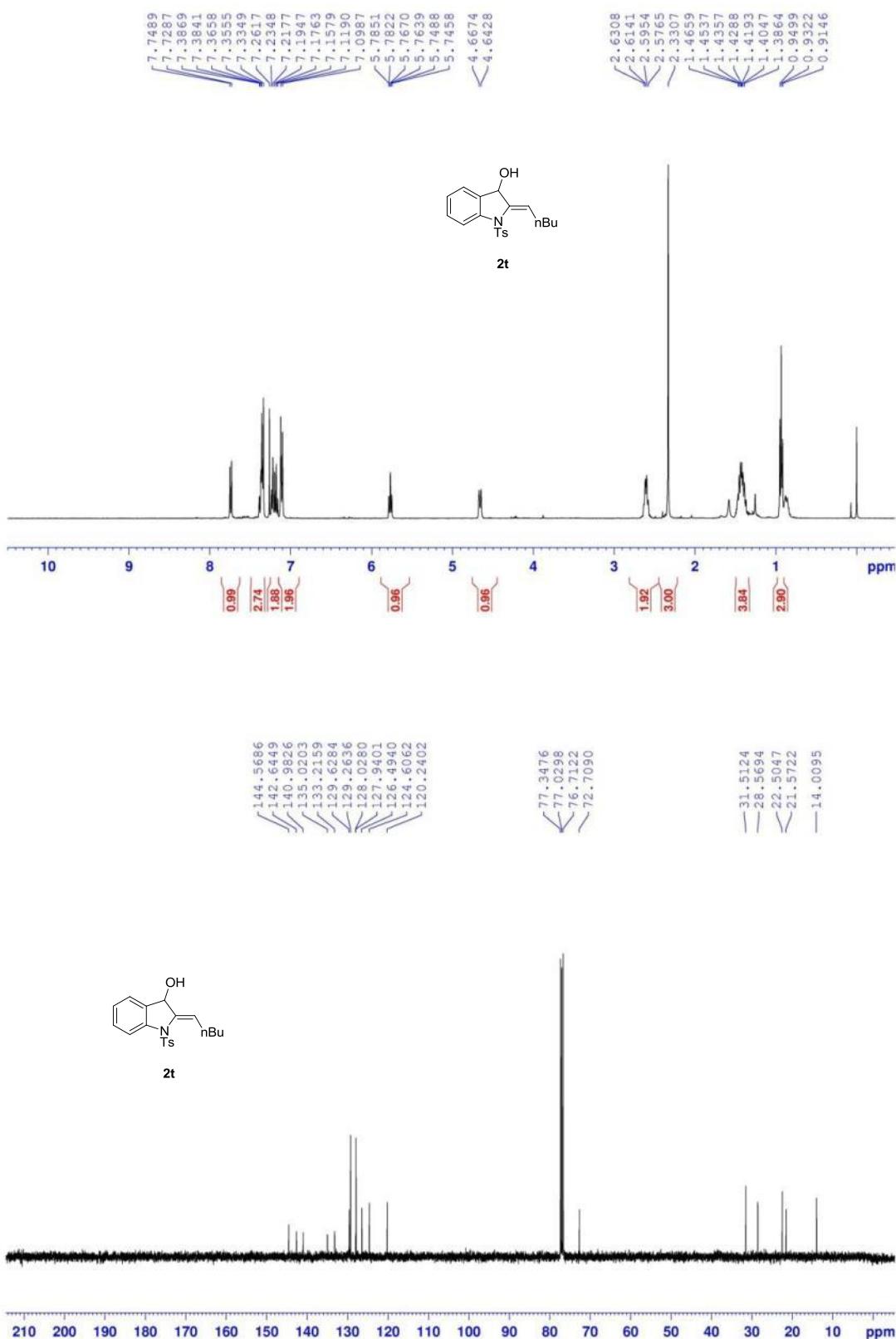


Figure S46. ^1H and ^{13}C NMR Spectra of (*Z*)-2-(Cyclopropylmethylene)-1-tosylindolin-3-ol (**2u**)

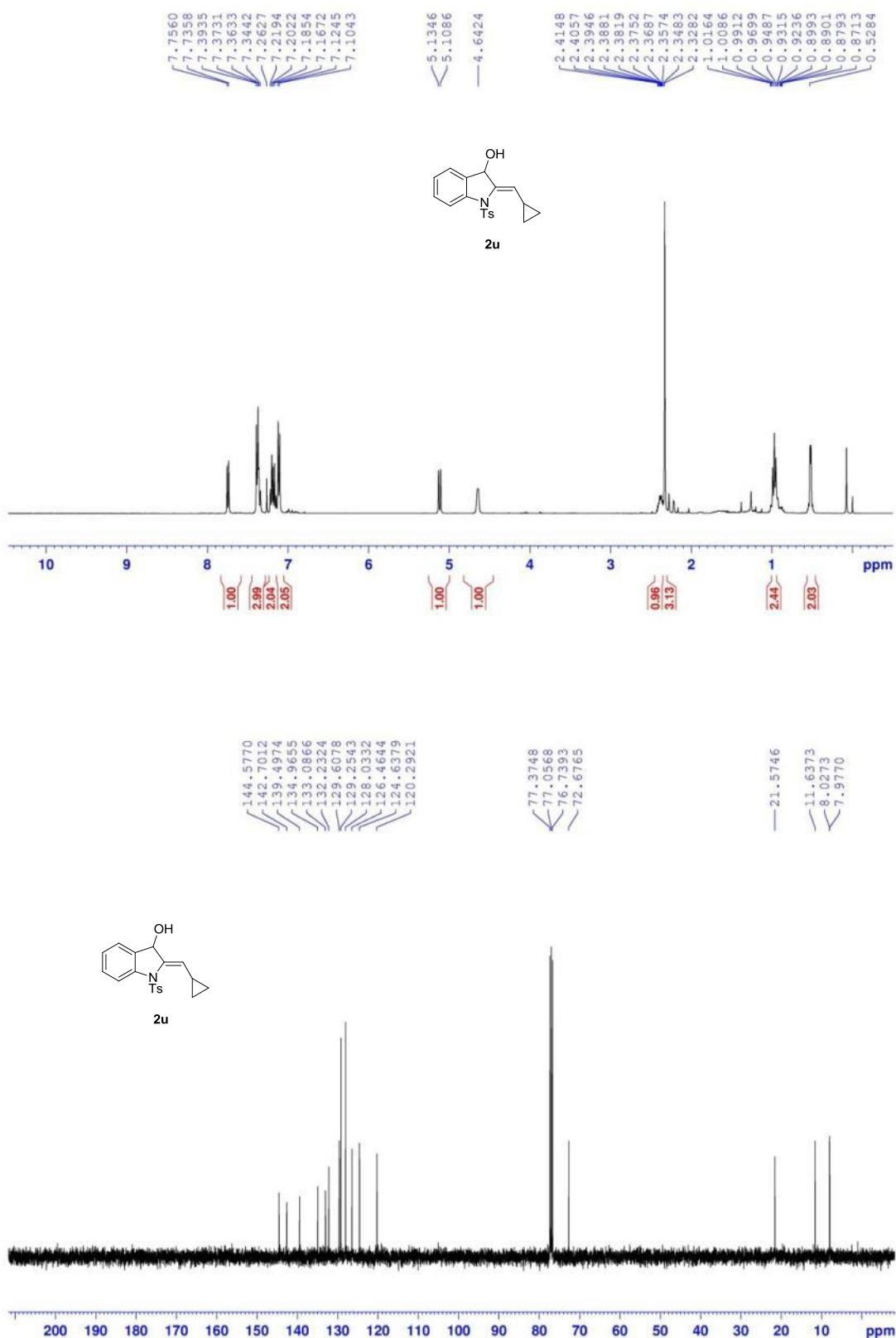


Figure S47. ^1H and ^{13}C NMR Spectra of (Z)-2-Benzylidene-1-((4-nitrophenyl)sulfonyl)-3-phenylindolin-3-ol (**2v**)

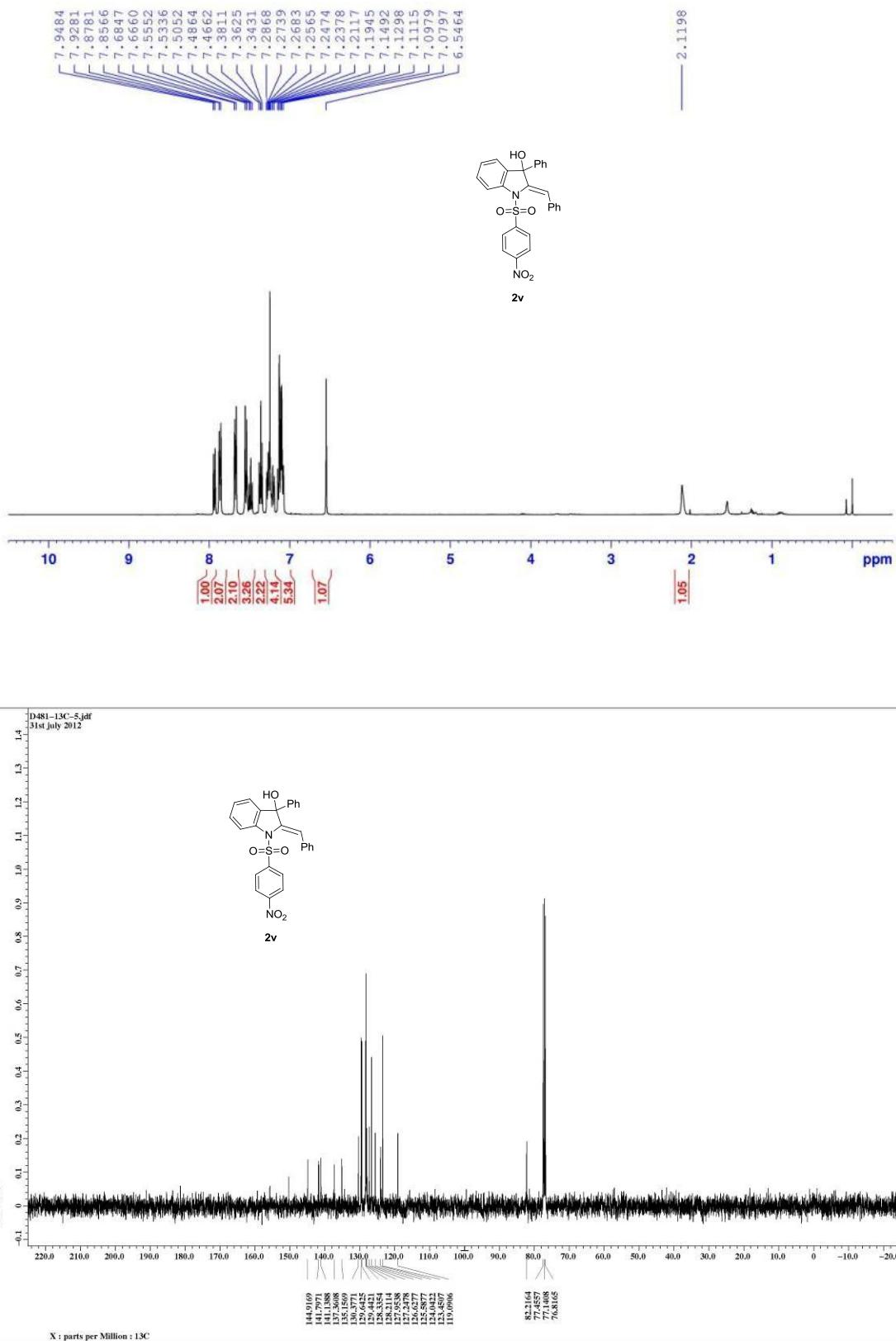


Figure S48. ^1H and ^{13}C NMR Spectra of (*Z*)-2-Benzylidene-1-(methylsulfonyl)-3-phenylindolin-3-ol

(**2w**)

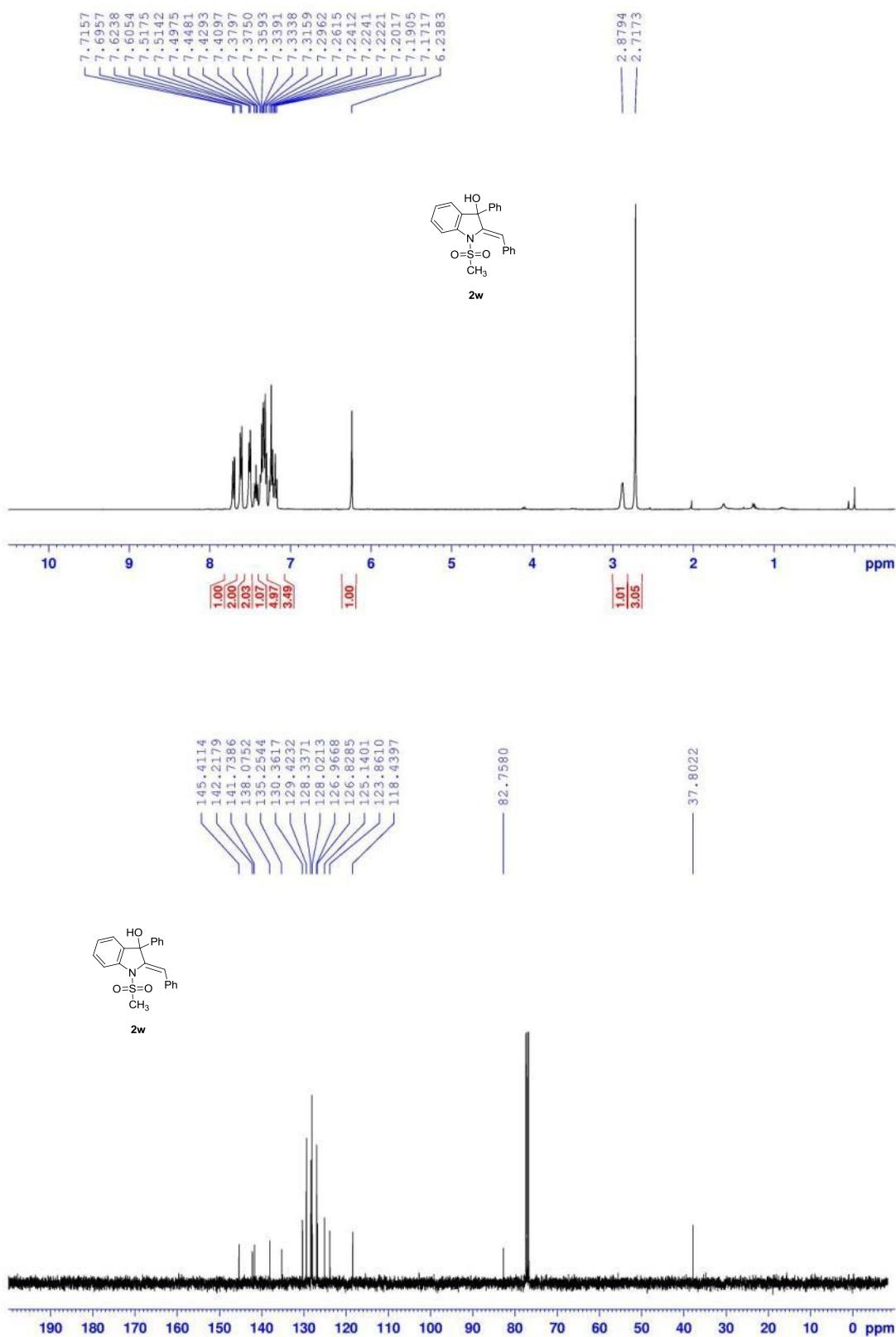


Figure S49. ^1H and ^{13}C NMR Spectra of (*Z*)-2-Benzylidene-3-phenyl-1-tosylindolin-3-ol (d_7 -**2a**)

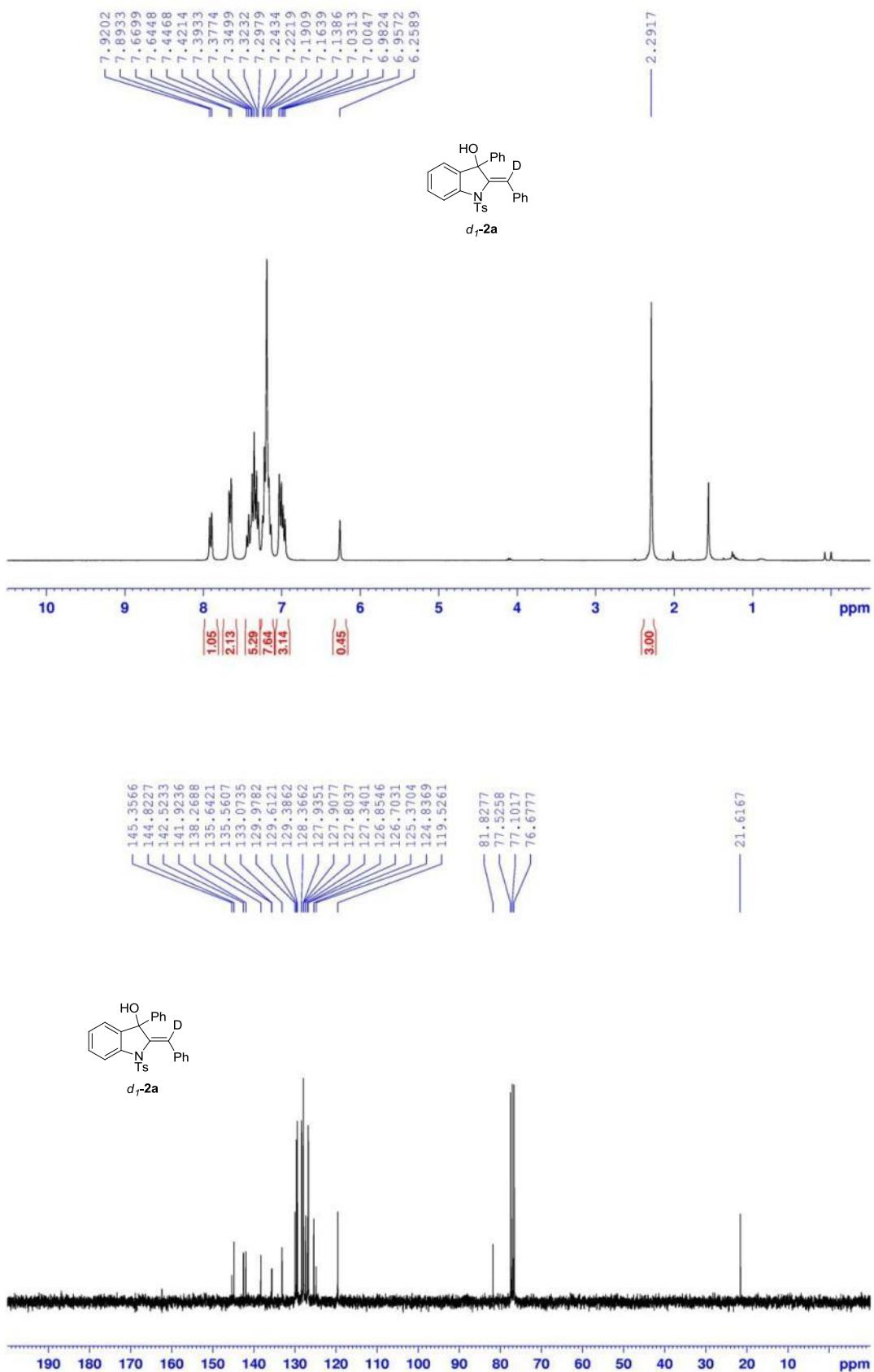


Figure S50. ^1H and ^{13}C NMR Spectra of Phenyl(3-phenyl-1-tosyl-1*H*-indol-2-yl)methanol (**4a**)

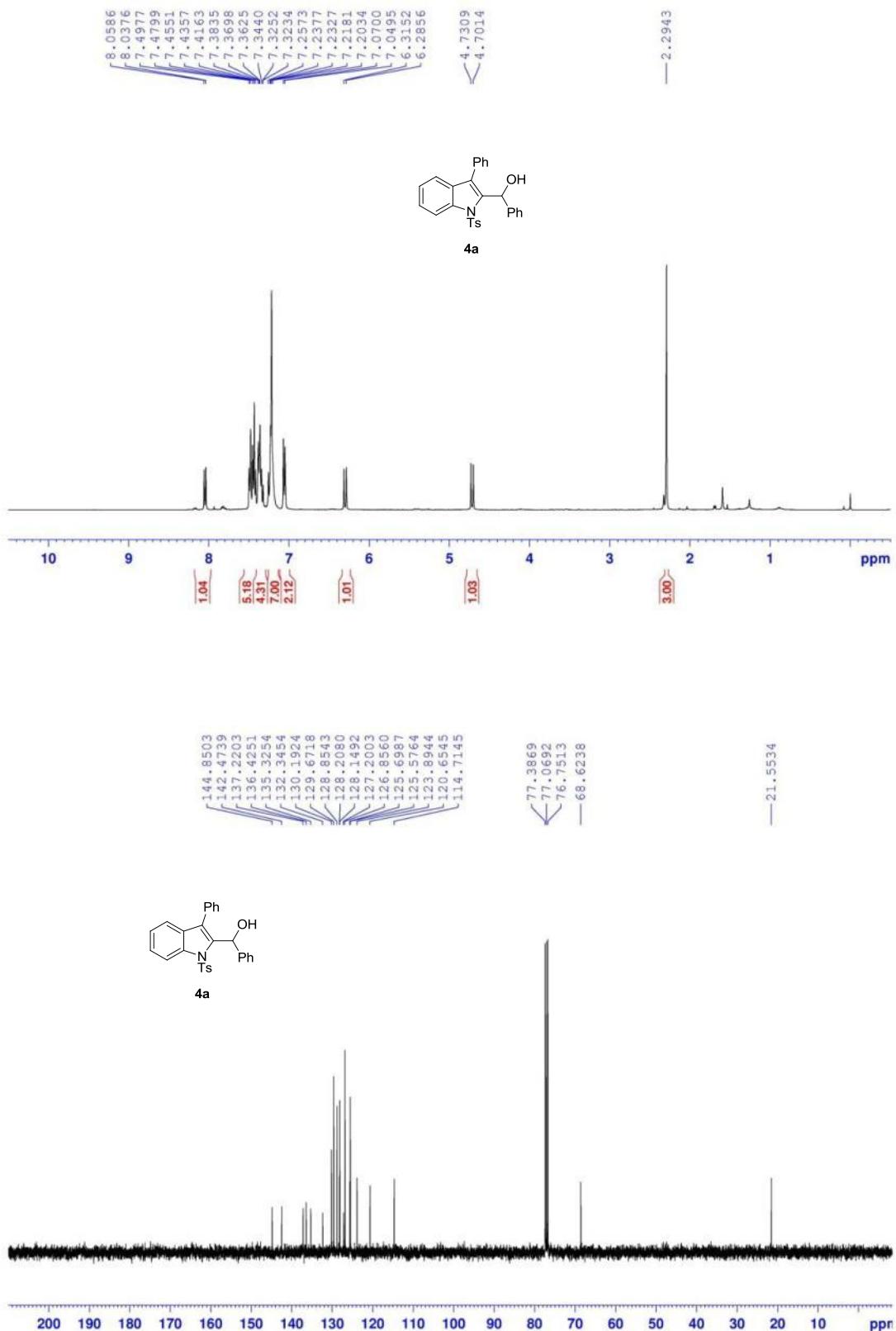


Figure S51. ^1H and ^{13}C NMR Spectra of 2-(Fluoromethyl)-3-phenyl-1-tosyl-1*H*-indole (**5p**)

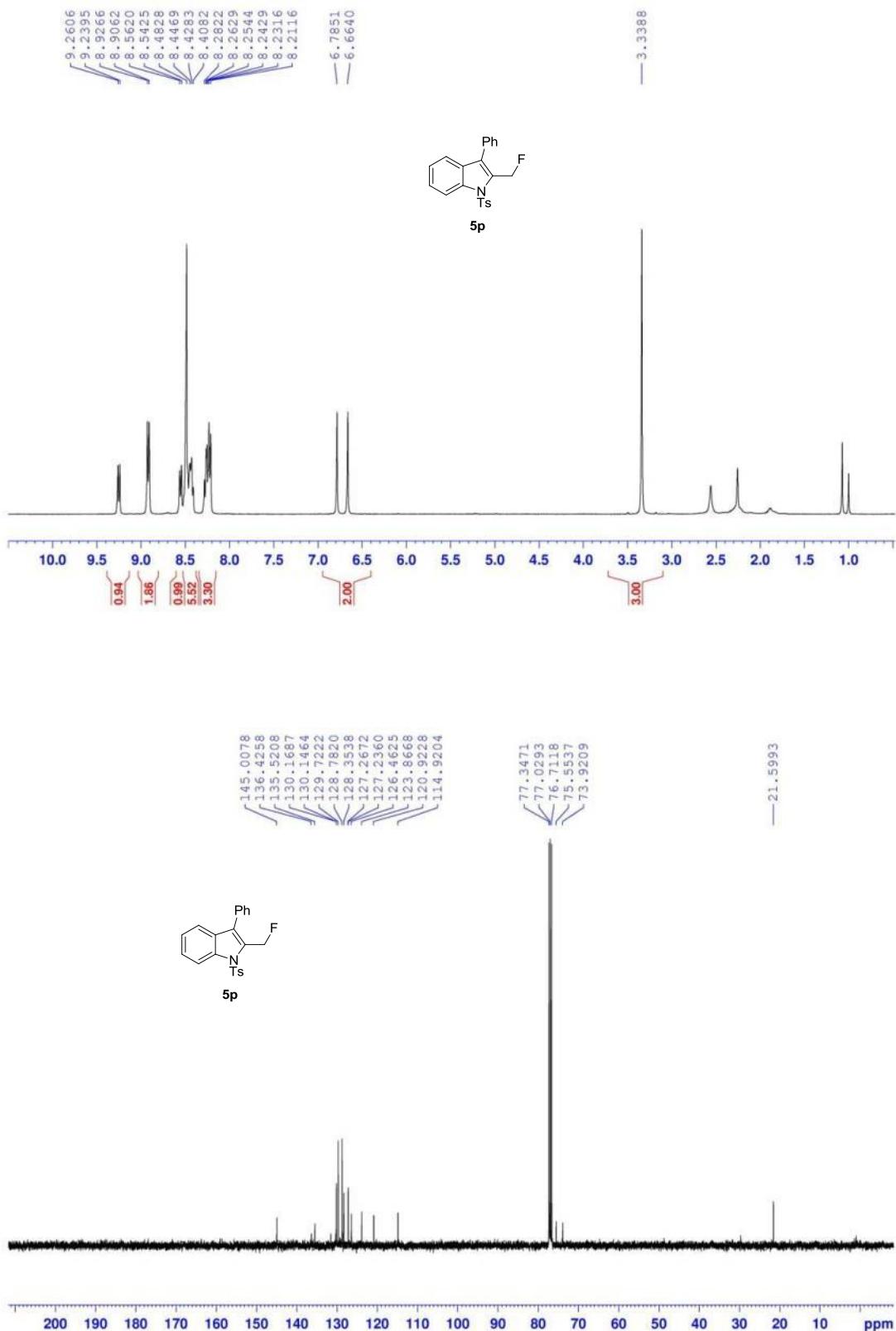


Figure S52. ^1H and ^{13}C NMR Spectra of 3-(Iodomethyl)-3-phenyl-1-tosylindolin-2-one (**6p**)

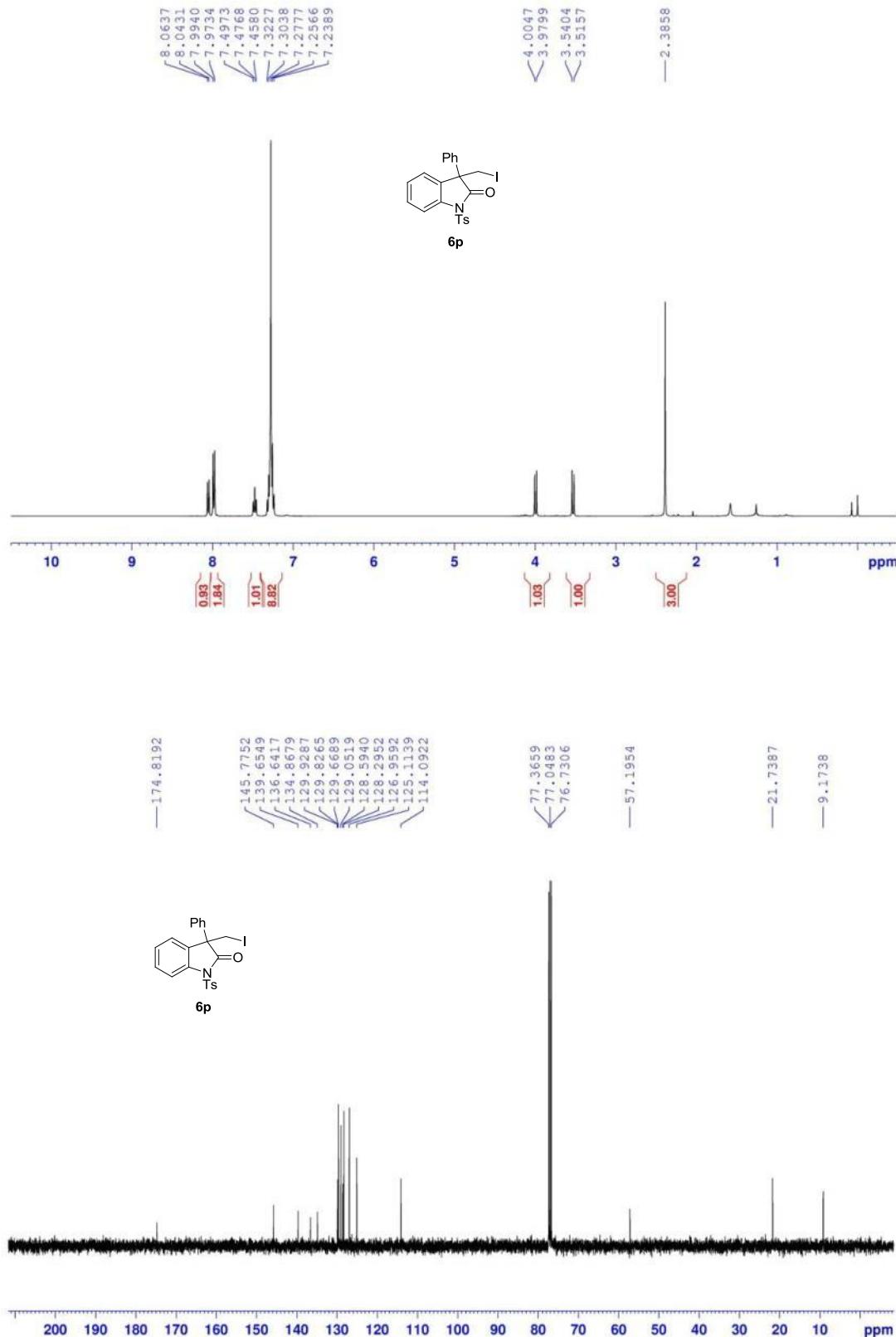


Figure S53. ^1H and ^{13}C NMR Spectra of (*Z*)-2-Benzylidene-1-tosylindolin-3-one (**7r**)

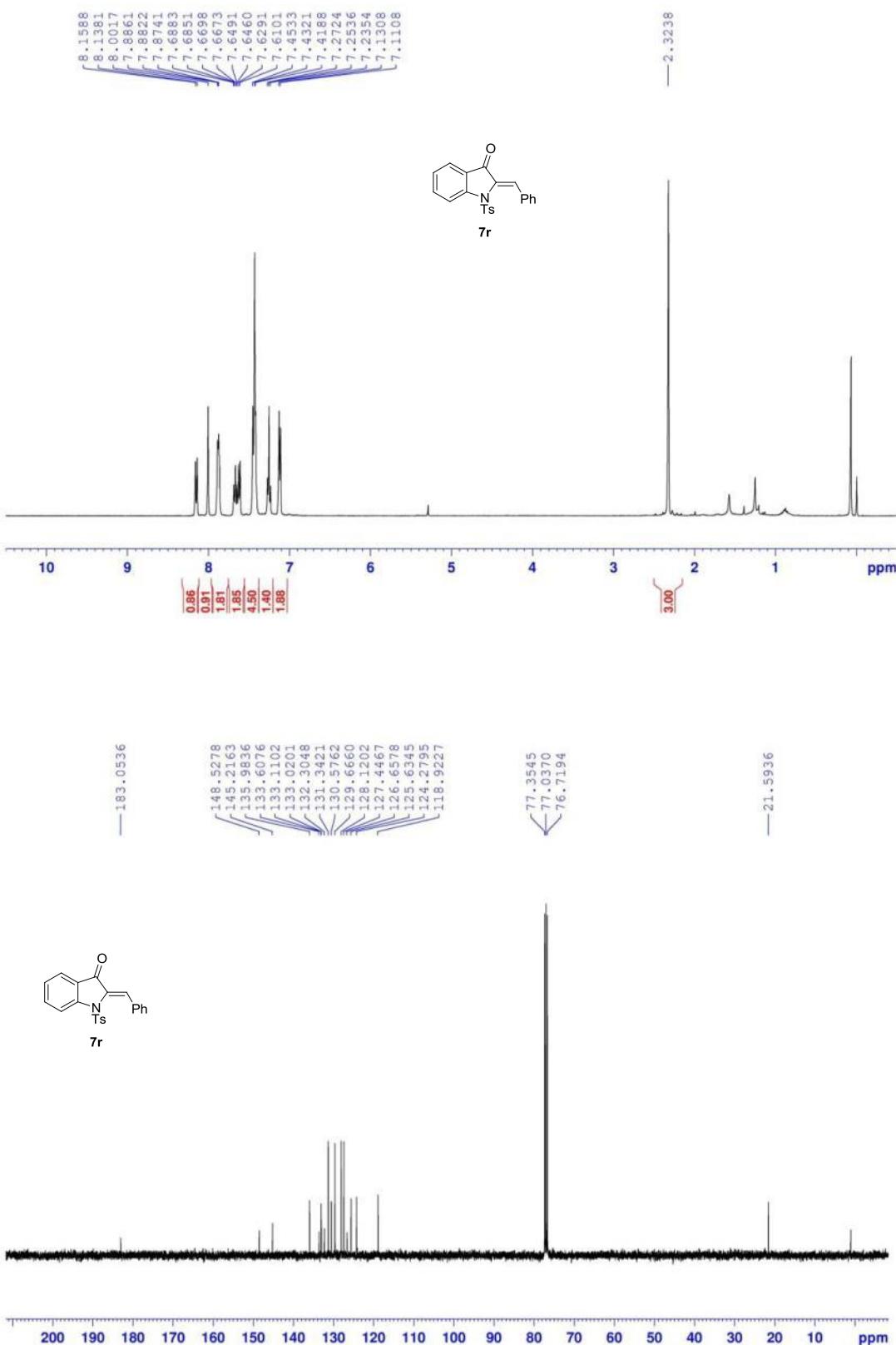


Figure S54. ORTEP Drawing of 2-(Fluoromethyl)-3-phenyl-1-tosyl-1*H*-indole (**5p**) with Thermal Ellipsoids at 50% Probability Levels^{S2}

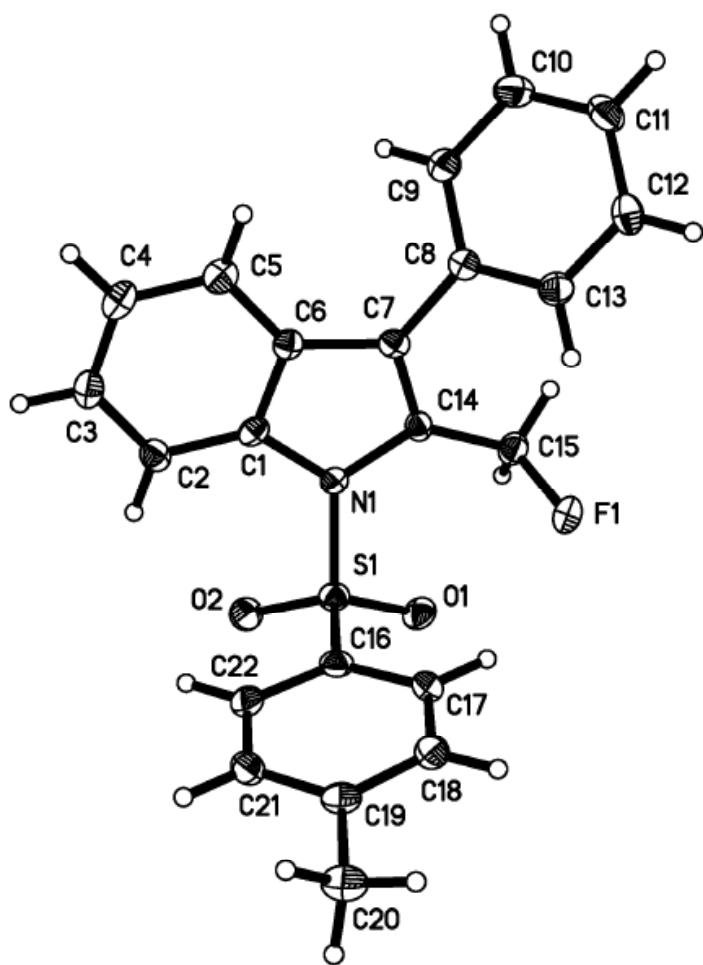


Figure S55. ORTEP Drawing of 3-(Iodomethyl)-3-phenyl-1-tosylindolin-2-one (**6p**) with Thermal Ellipsoids at 50% Probability Levels^{S3}

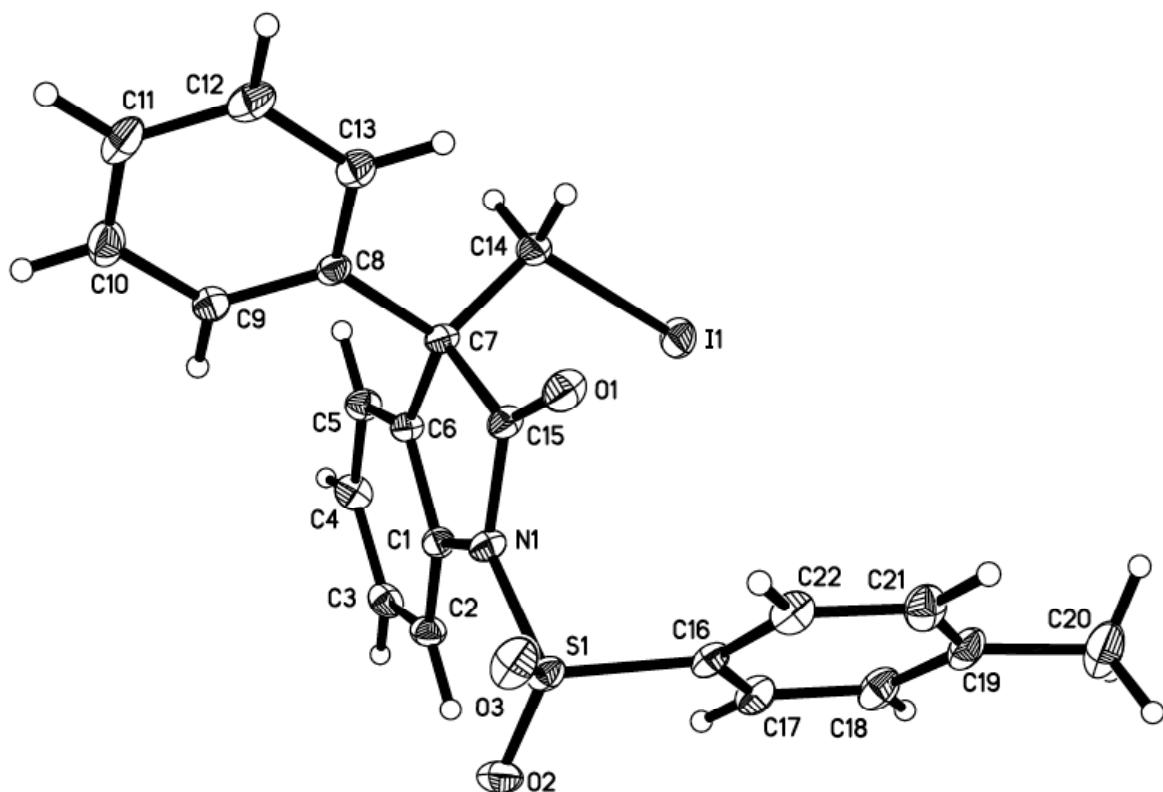
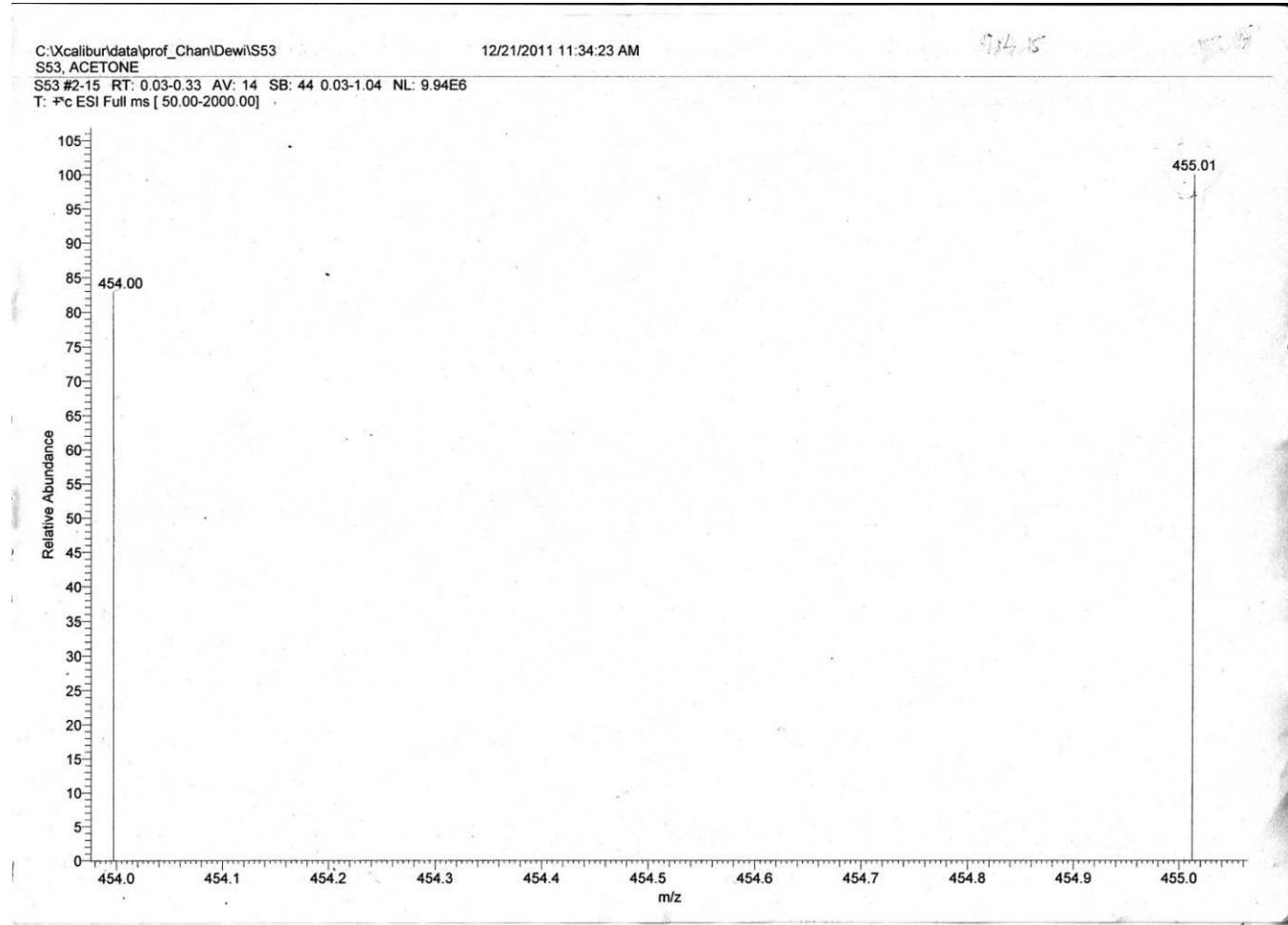


Figure S56. LC-MS Spectrum of (*d*₁-2a)



References

- S1. For X-Ray crystal structure of **2a**, refer to: Kothandaraman, P.; Rao, W.; Foo, S. J.; Chan, P. W. H. *Angew. Chem. Int. Ed.* **2010**, *49*, 4619
- S2. CCDC 883977 (**5p**) 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.
- S3. CCDC 884750 (**6p**) 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.