Supporting Information

for

Gold-Catalyzed Cycloisomerization of 1,6-Diyne Esters to 1*H*-Cyclopenta[*b*]naphthalenes, *cis*-Cyclopenten-2-yl δ-Diketones and Bicyclo[3.2.0]hepta-1,5-dienes

Dan Li,[†] Weidong Rao,[†] Guan Liang Tay,[†] Benjamin James Ayers,[†] and Philip Wai Hong

Chan*^{†,‡}

[‡]School of Chemistry, Monash University, Clayton 3800, Victoria, Australia

[†]Division of Chemistry and Biological Chemistry, School of Physical and Mathematical

Sciences, Nanyang Technological University, Singapore 637371, Singapore

phil.chan@monash.edu and waihong@ntu.edu.sg

Table of Contents

1. ¹ H and ¹³ C{ ¹ H	NMR spectra for compounds $1a - \lambda$ and $4a - t$	S3

1. ¹H and ¹³C{¹H} NMR spectra for compounds $1a-\lambda$ and 4a-t

Figure S1.¹H and ¹³C{¹H} NMR spectra of 1,3,7-triphenylhepta-1,6-diyn-3-yl acetate (1a)

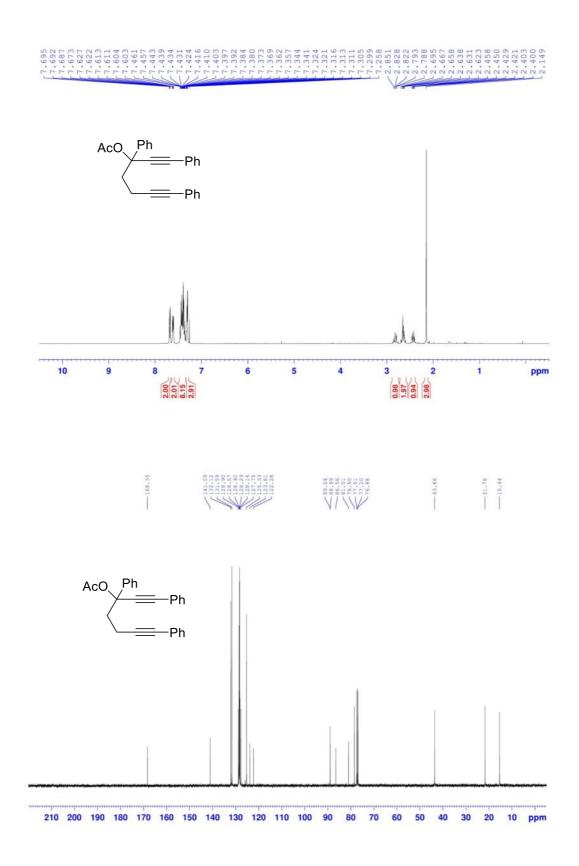


Figure S2.¹H and ¹³C{¹H} NMR spectra of 1,3,7-triphenylhepta-1,6-diyn-3-yl benzoate (1b)

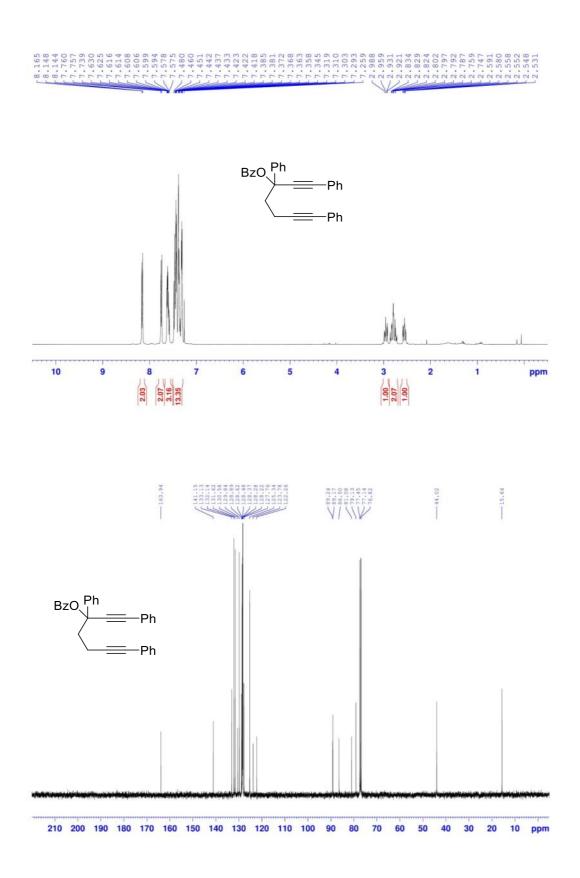


Figure S3.¹H and ¹³C{¹H} NMR spectra of 1,3,7-triphenylhepta-1,6-diyn-3-yl pivalate (1c)

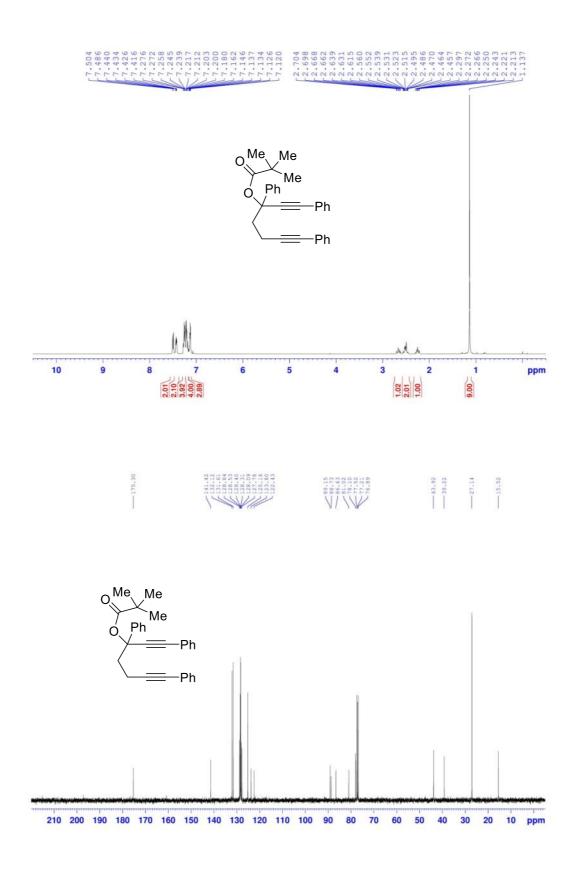


Figure S4. ¹H and ¹³C{¹H} NMR spectra of 1,3,7-triphenylhepta-1,6-diyn-3-yl cyclopropanecarboxylate (1d)

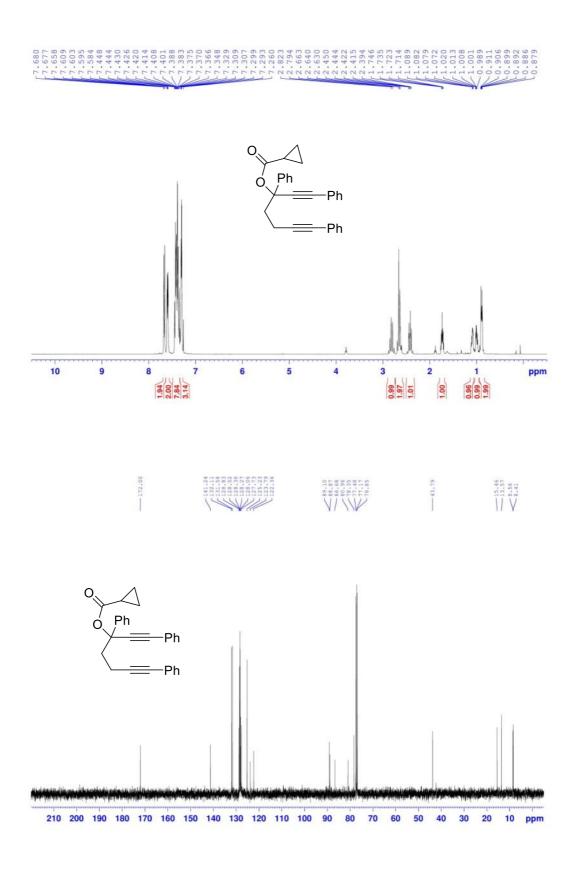


Figure S5. ¹H and ¹³C{¹H} NMR spectra of 3-methyl-1,7-diphenylhepta-1,6-diyn-3-yl acetate (1e)

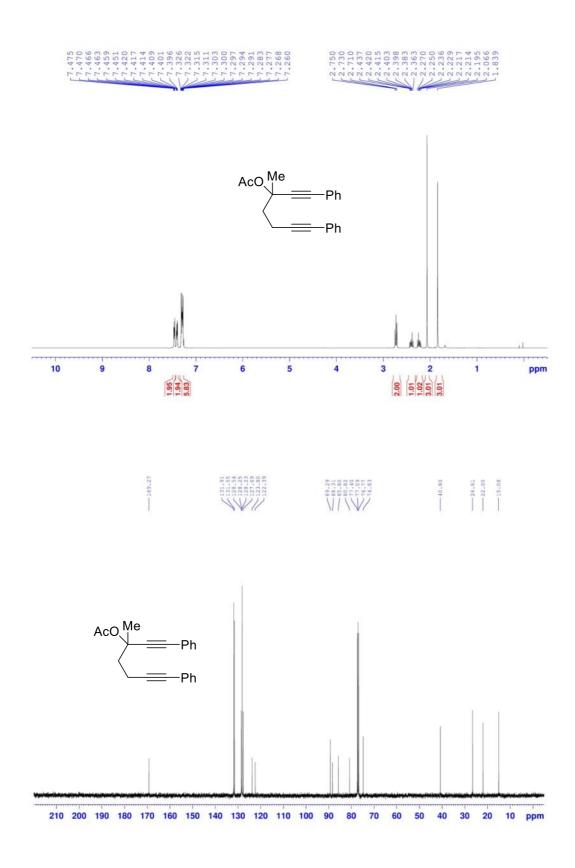


Figure S6. ¹H and ¹³C{¹H} NMR spectra of 3-cyclopropyl-1,7-diphenylhepta-1,6-diyn-3yl acetate (1f)

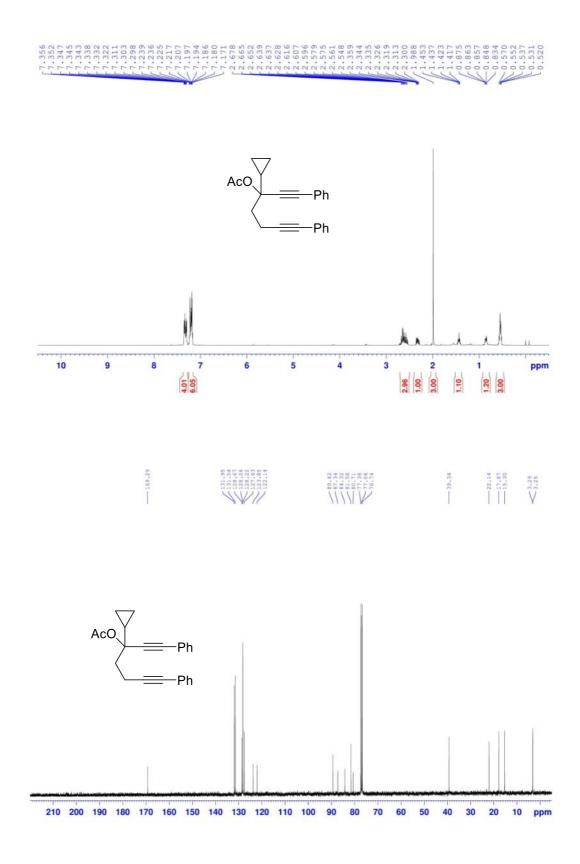


Figure S7. ¹H and ¹³C{¹H} NMR spectra of 3-(4-chlorophenyl)-1,7-diphenylhepta-1,6diyn-3-yl acetate (1g)

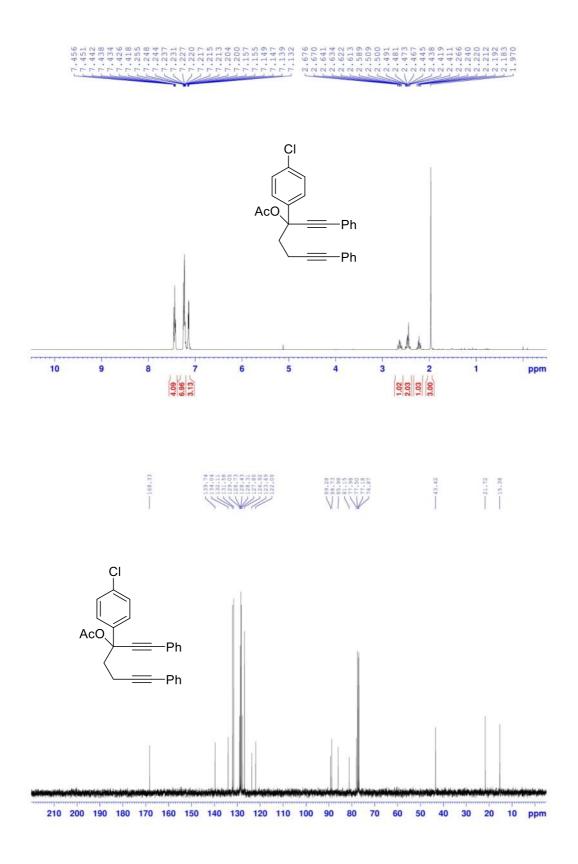


Figure S8. ¹H and ¹³C{¹H} NMR spectra of 1-(4-fluorophenyl)-3,7-diphenylhepta-1,6diyn-3-yl acetate (1h)

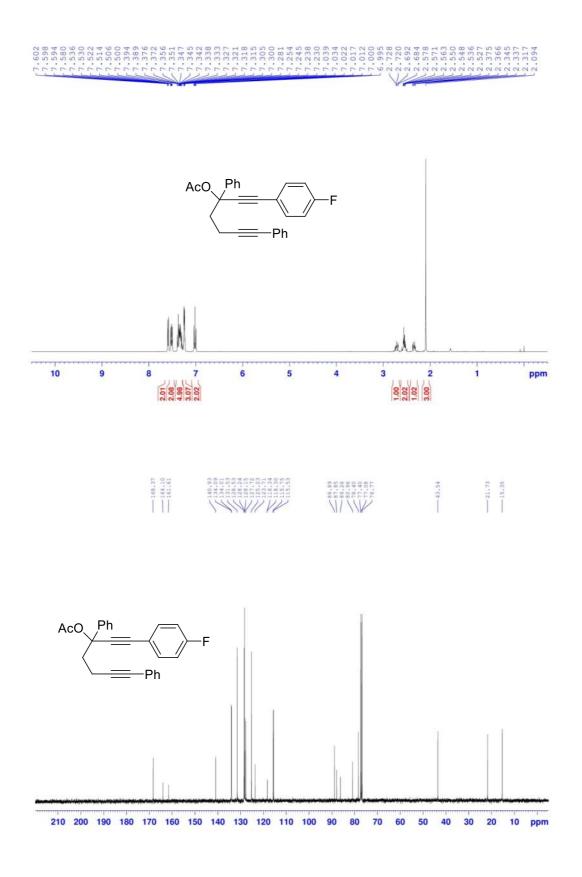


Figure S9. ¹H and ¹³C{¹H} NMR spectra of 3,7-diphenyl-1-(p-tolyl)hepta-1,6-diyn-3-yl acetate (1i)

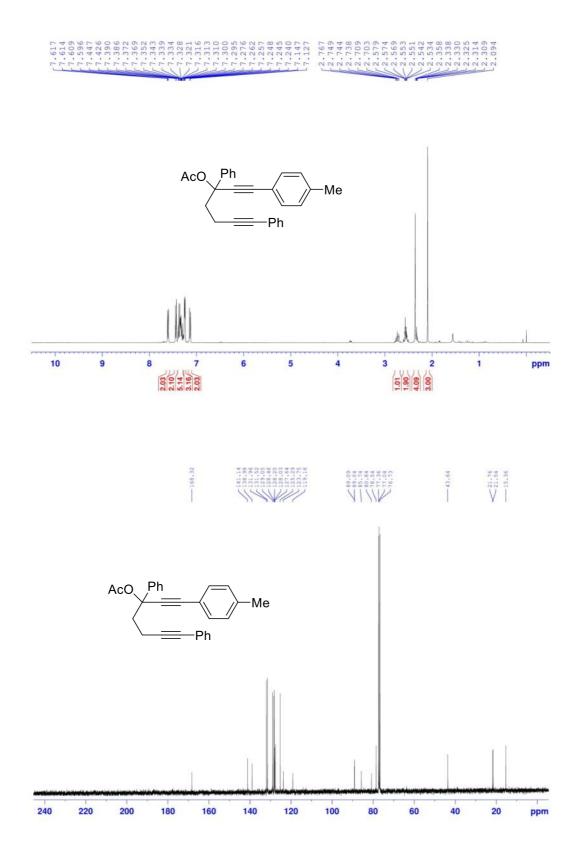


Figure S10. ¹H and ¹³C{¹H} NMR spectra of 3,7-diphenyl-1-(thiophen-3-yl)hepta-1,6diyn-3-yl acetate (1j)

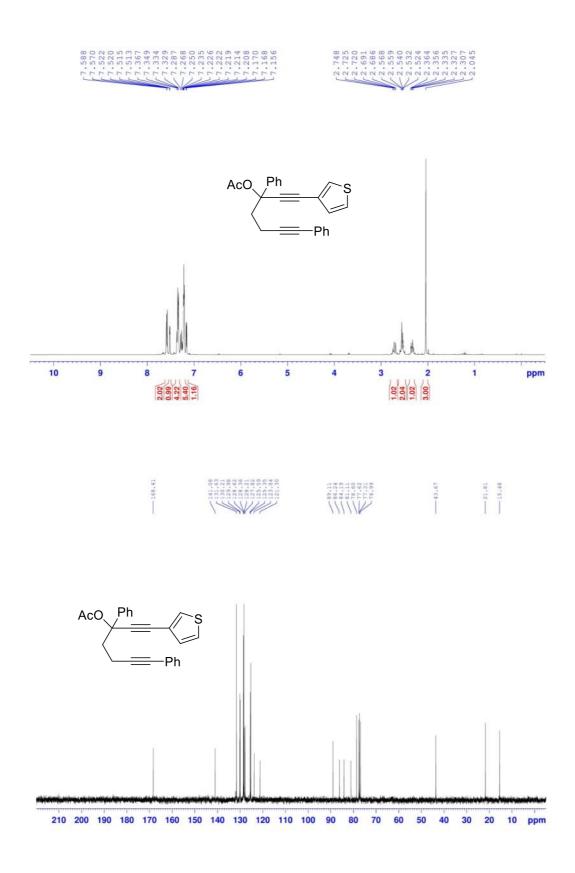


Figure S11. ¹H and ¹³C{¹H} NMR spectra of 7-(4-fluorophenyl)-1,3-diphenylhepta-1,6diyn-3-yl acetate (1k)

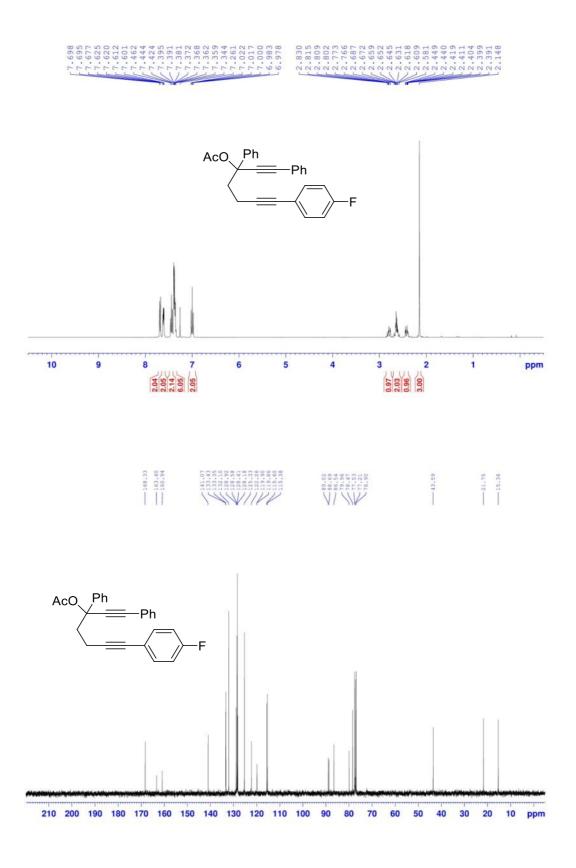


Figure S12. ¹H and ¹³C{¹H} NMR spectra of 7-(4-bromophenyl)-1,3-diphenylhepta-1,6diyn-3-yl acetate (11)

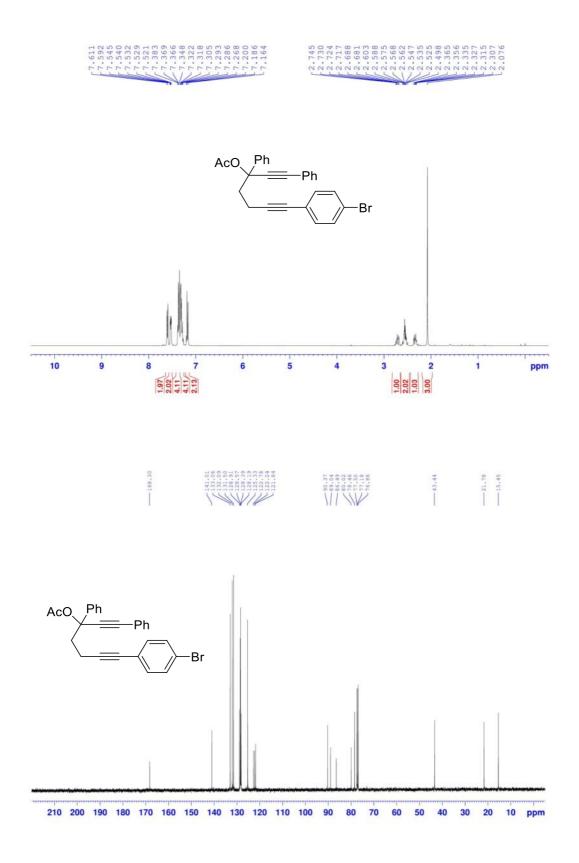


Figure S13. ¹H and ¹³C{¹H} NMR spectra of 7-(4-pentylphenyl)-1,3-diphenylhepta-1,6diyn-3-yl acetate(1m)

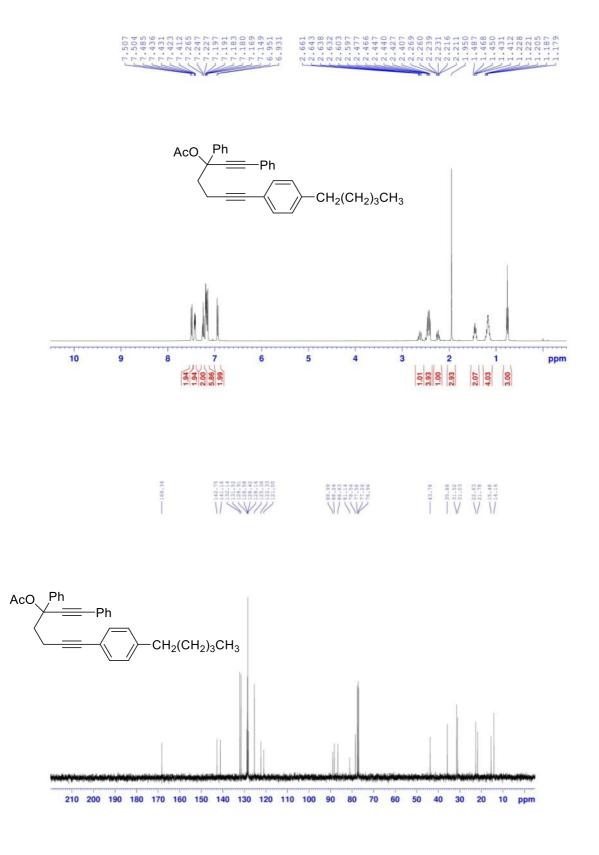


Figure S14. ¹H and ¹³C{¹H} NMR spectra of 1,3-diphenyl-7-(p-tolyl)hepta-1,6-diyn-3-yl acetate (1n)

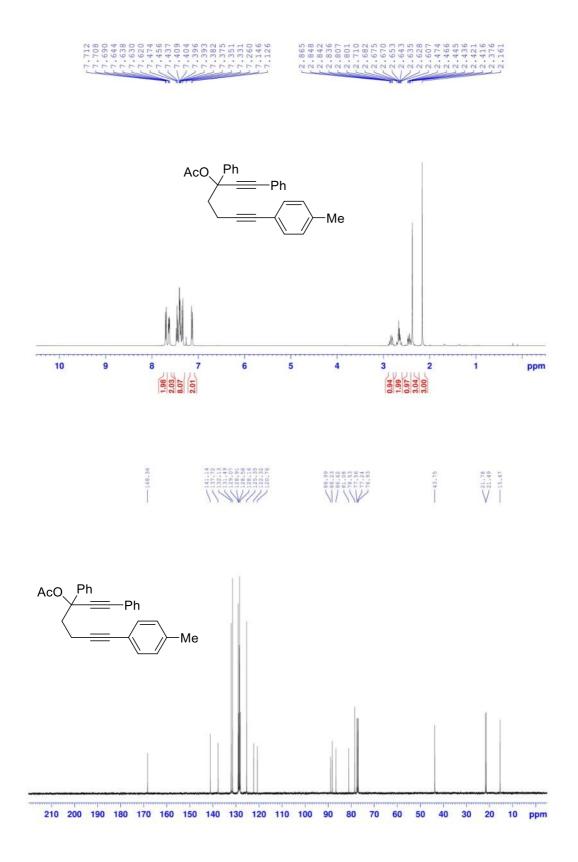


Figure S15. ¹H and ¹³C{¹H} NMR spectra of 1,3-diphenyl-7-o-tolylhepta-1,6-diyn-3-yl acetate (10)



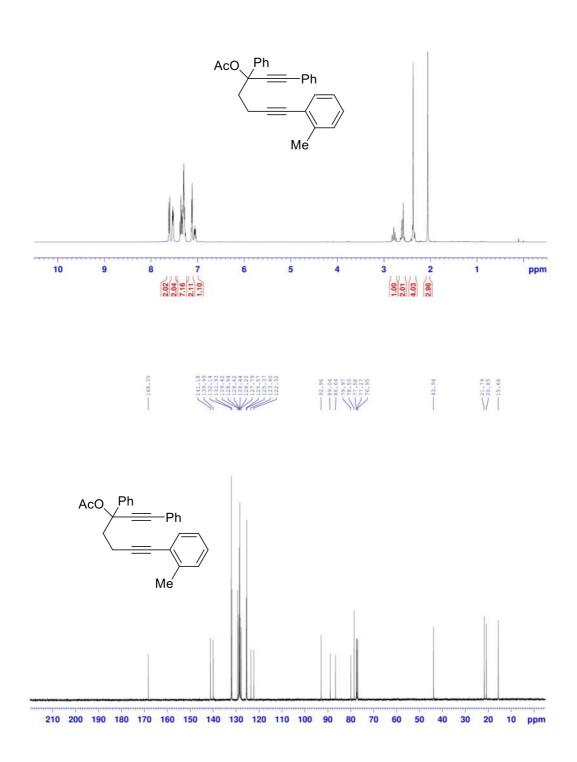


Figure S16. ¹H and ¹³C{¹H} NMR spectra of 7-(3,5-dimethylphenyl)-1,3-diphenylhepta-1,6-diyn-3-yl acetate (1p)



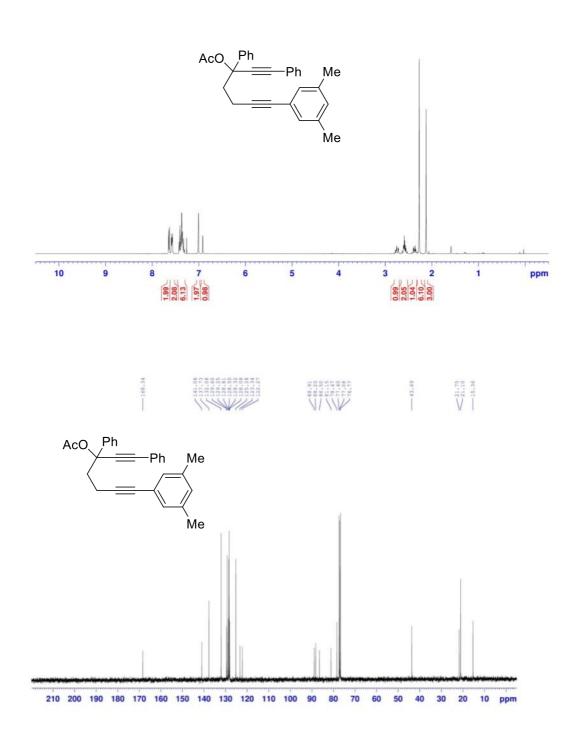


Figure S17. ¹H and ¹³C{¹H} NMR spectra of 7-mesityl-1,3-diphenylhepta-1,6-diyn-3-yl acetate (1q)



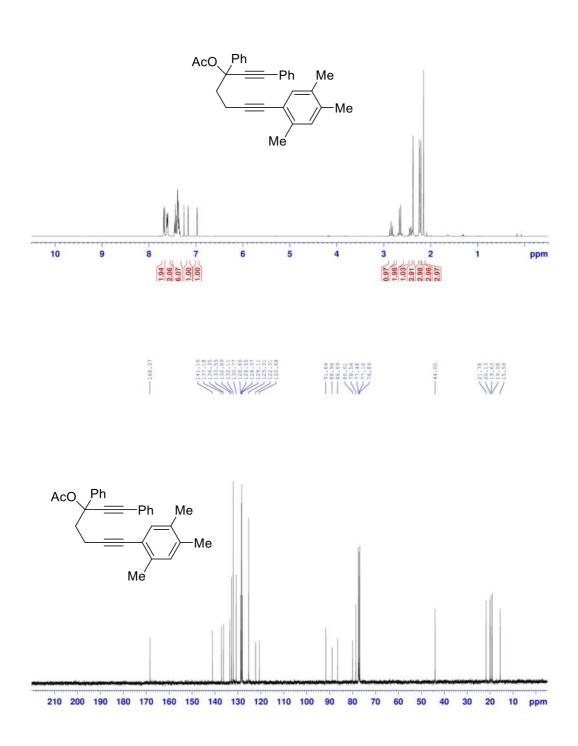


Figure S18. ¹H and ¹³C{¹H} NMR spectra of 7-(naphthalen-1-yl)-1,3-diphenylhepta-1,6diyn-3-yl acetate (1r)

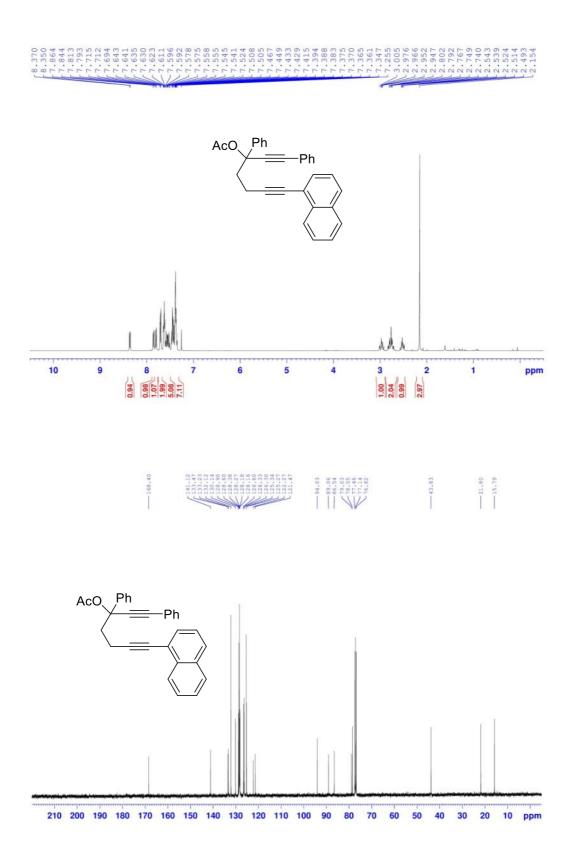


Figure S19. ¹H and ¹³C{¹H} NMR spectra of 1,3-diphenyl-7-(thiophen-3-yl)hepta-1,6diyn-3-yl acetate (1s)

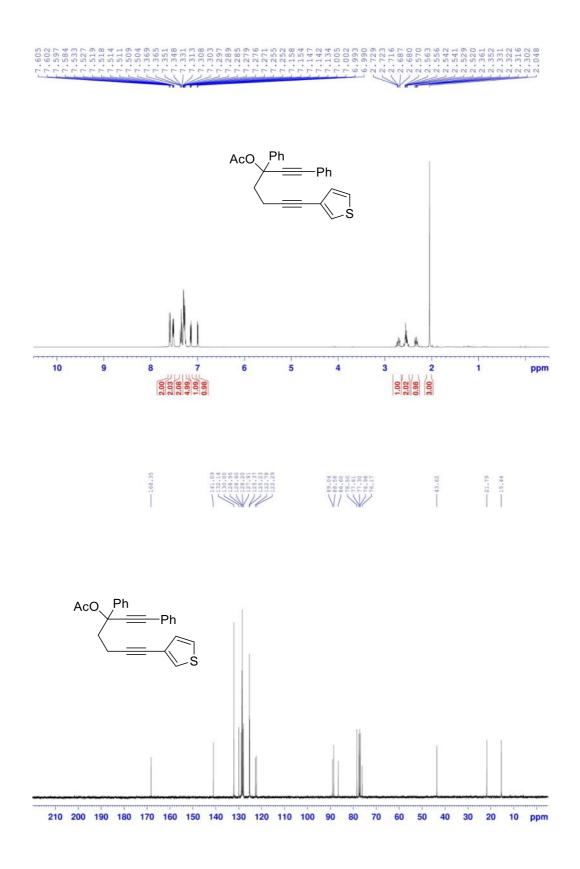


Figure S20. ¹H and ¹³C{¹H} NMR spectra of 1,3-diphenyl-7-(thiophen-2-yl)hepta-1,6diyn-3-yl acetate (1t)

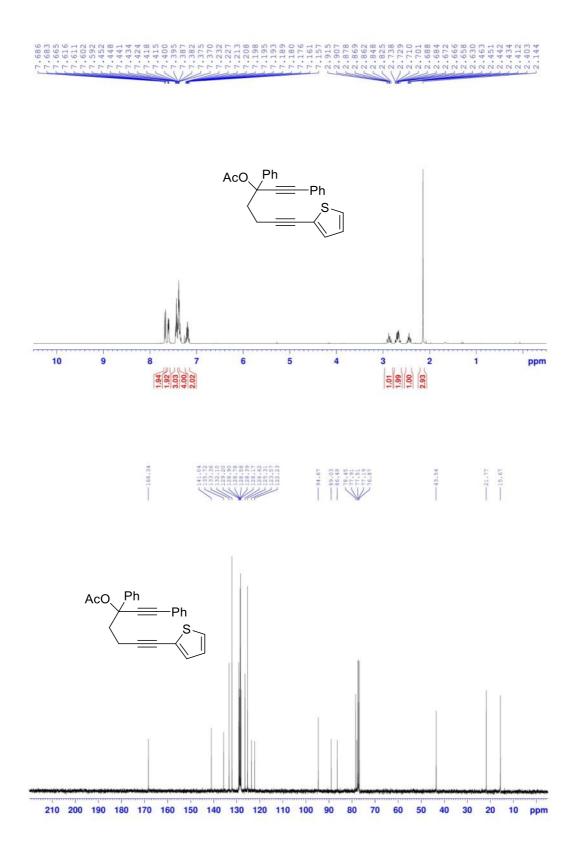


Figure S21. ¹H and ¹³C{¹H} NMR spectra of 2-methyl-5,9-diphenylnona-1-en-3,8-diyn-5-yl acetate (1u)

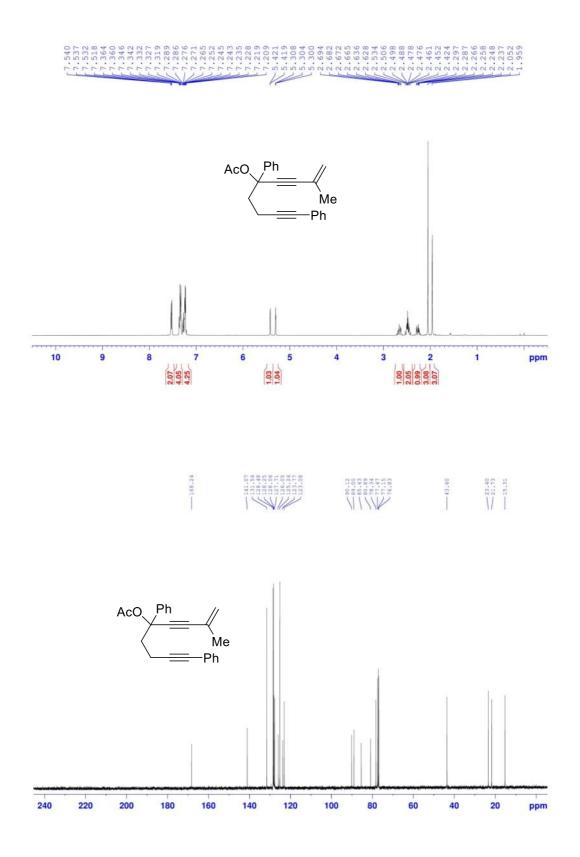


Figure S22. ¹H and ¹³C{¹H} NMR spectra of 2-methyl-5,9-diphenylnona-1-en-3,8-diyn-5-yl benzoate (1v)



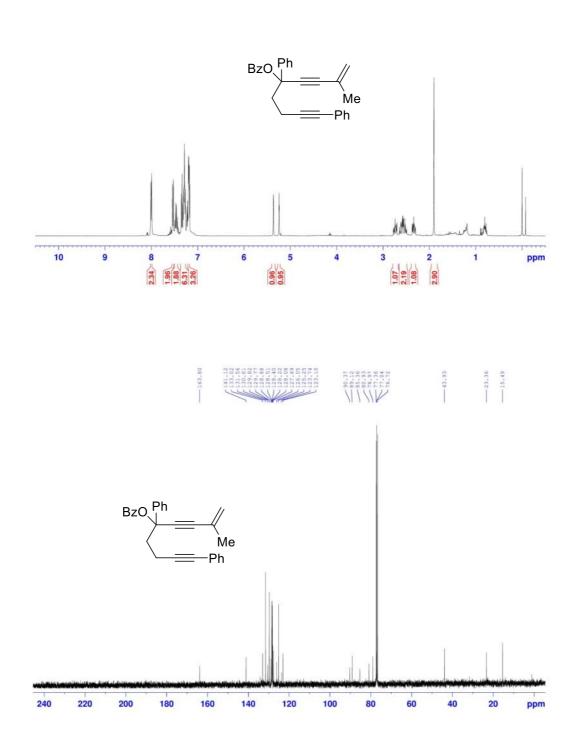


Figure S23. ¹H and ¹³C{¹H} NMR spectra of 2-methyl-5,9-diphenylnona-1-en-3,8-diyn-5-yl pivalate (1w)

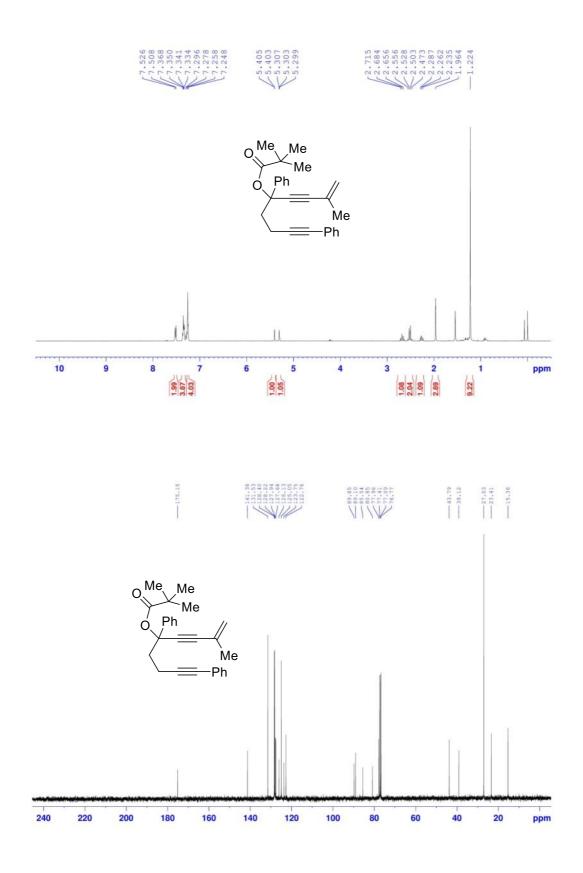


Figure S24. ¹H and ¹³C{¹H} NMR spectra of 2-methyl-5,9-diphenylnona-1-en-3,8-diyn-5-yl cyclopropanecarboxylate (1x)

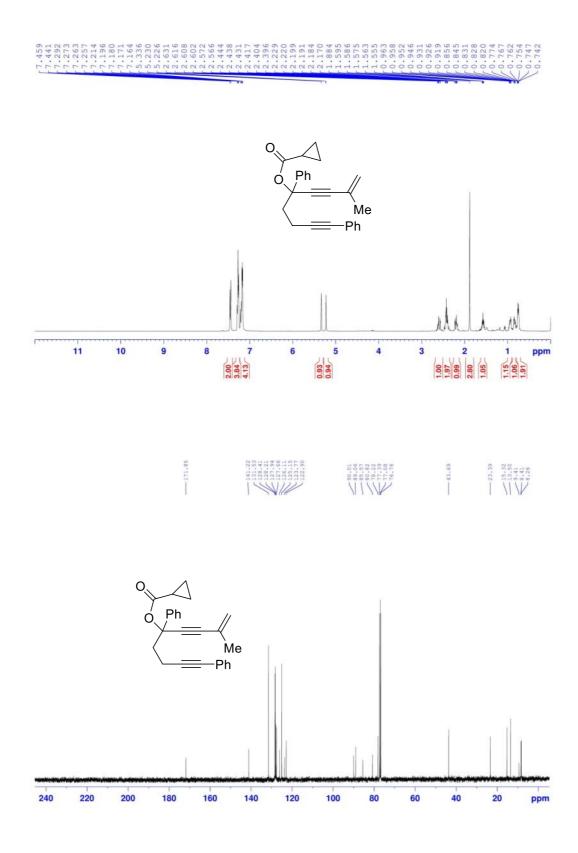


Figure S25. ¹H and ¹³C{¹H} NMR spectra of 5-(4-chlorophenyl)-2-methyl-9-phenylnona-1-en-3,8-diyn-5-yl acetate (1y)

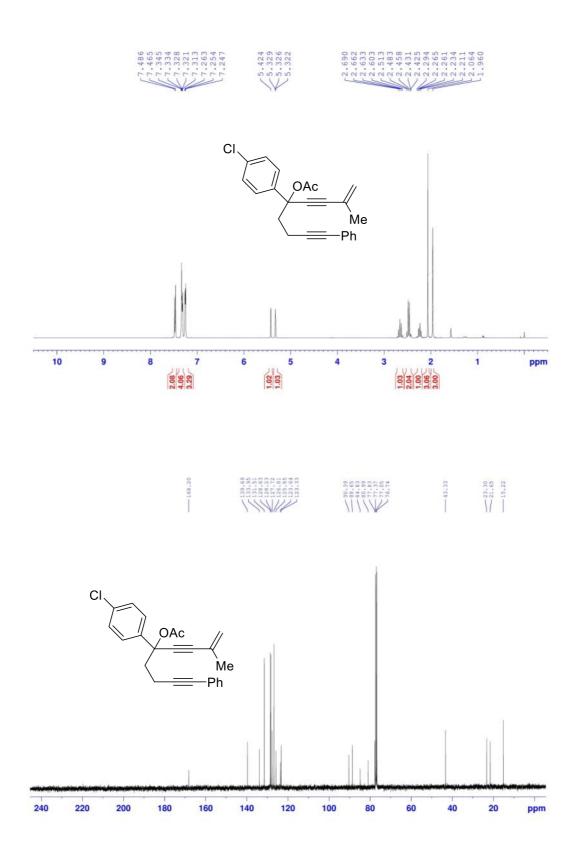


Figure S26. ¹H and ¹³C{¹H} NMR spectra of 2-methyl-9-phenyl-5-p-tolylnona-1-en-3,8diyn-5-yl acetate (1z)

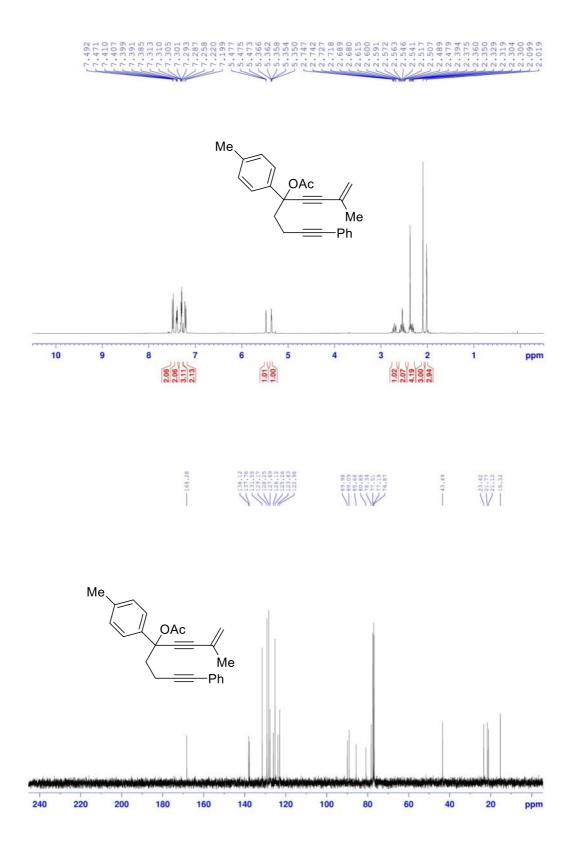


Figure S27. ¹H and ¹³C{¹H} NMR spectra of 2-methyl-5-(naphthalen-1-yl)-9phenylnona-1-en-3,8-diyn-5-yl acetate (1α)

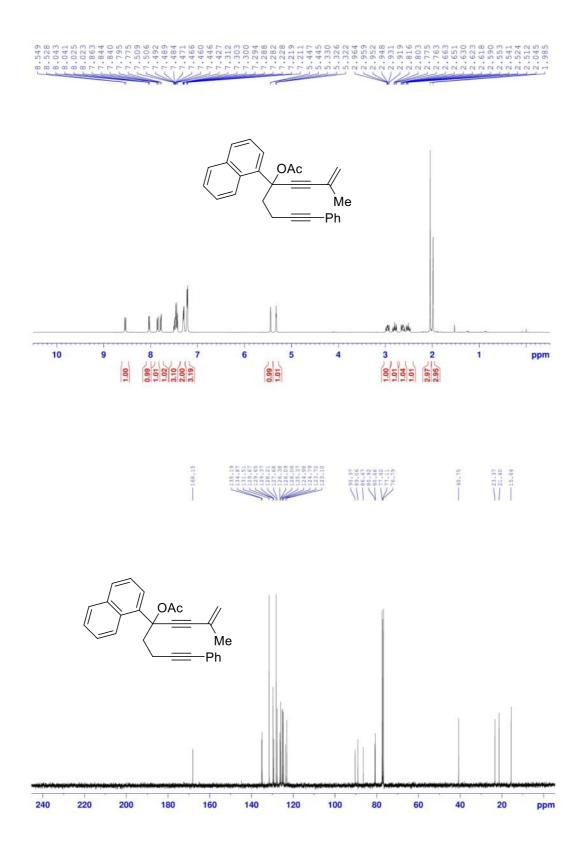


Figure S28. ¹H and ¹³C{¹H} NMR spectra of 2,5-dimethyl-9-phenylnona-1-en-3,8-diyn-5-yl acetate (1β)

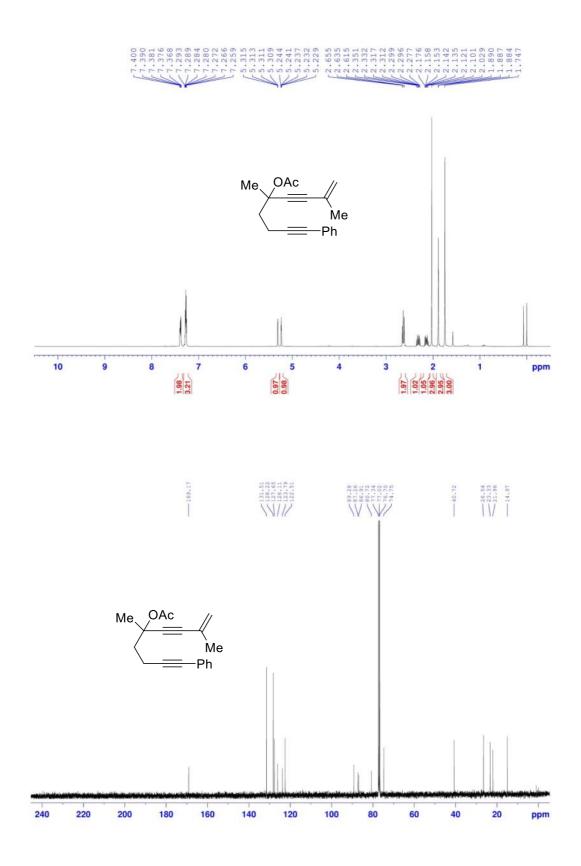


Figure S29. ¹H and ¹³C{¹H} NMR spectra of 8-methylene-1,5-diphenyltetradeca-1,6diyn-5-yl acetate (1γ)

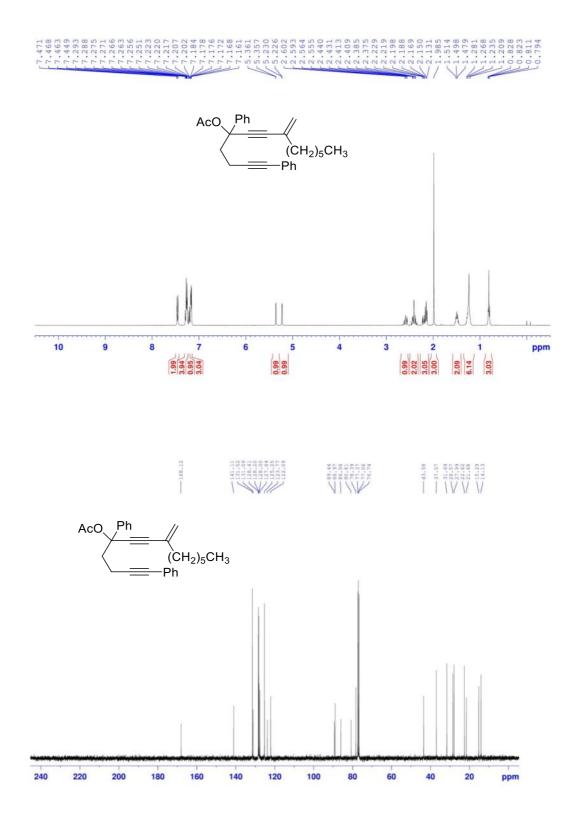


Figure S30. ¹H and ¹³C{¹H} NMR spectra of 2,5,9-triphenylnona-1-en-3,8-diyn-5-yl acetate (1δ)

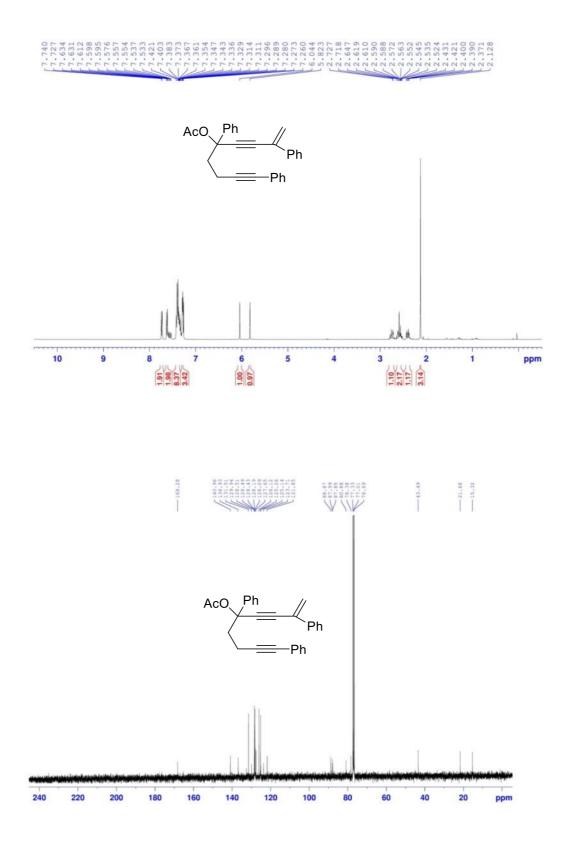


Figure S31. ¹H and ¹³C{¹H} NMR spectra of 9-(4-fluorophenyl)-2-methyl-5-phenylnona-1-en-3,8-diyn-5-yl acetate (1ε)

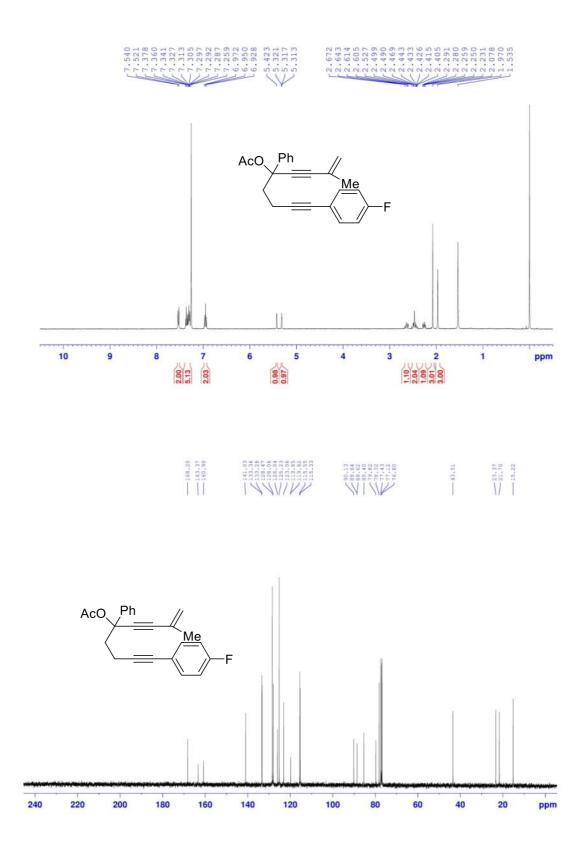


Figure S32. ¹H and ¹³C{¹H} NMR spectra of 2-methyl-5-phenyl-9-p-tolylnona-1-en-3,8diyn-5-yl acetate (1ζ)

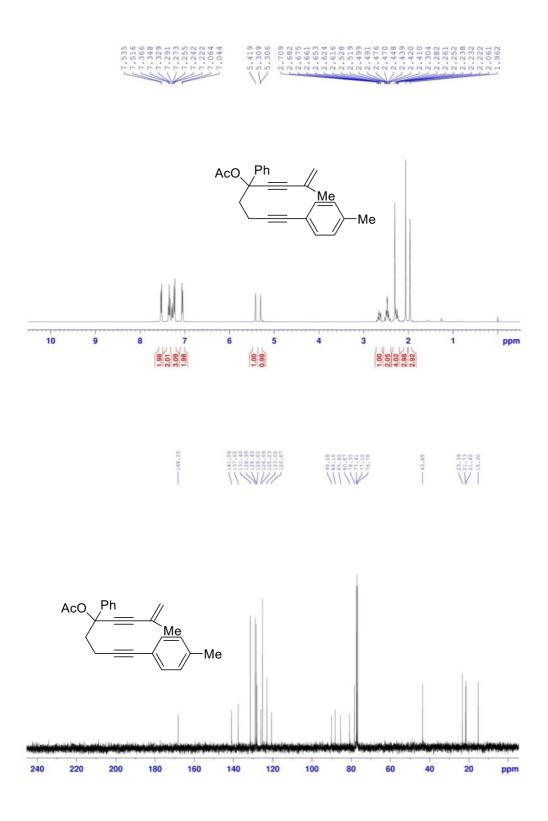


Figure S33. ¹H and ¹³C{¹H} NMR spectra of 2-methyl-9-(4-pentylphenyl)-5-phenylnona-1-en-3,8-diyn-5-yl acetate (1η)

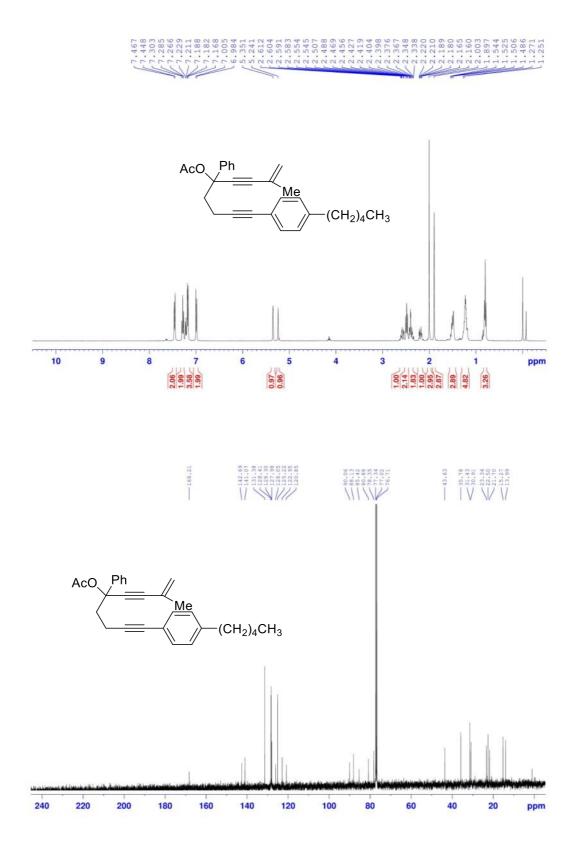


Figure S34. ¹H and ¹³C NMR spectra of 2-methyl-5-phenyl-9-o-tolylnona-1-en-3,8-diyn-5-yl acetate (1θ)

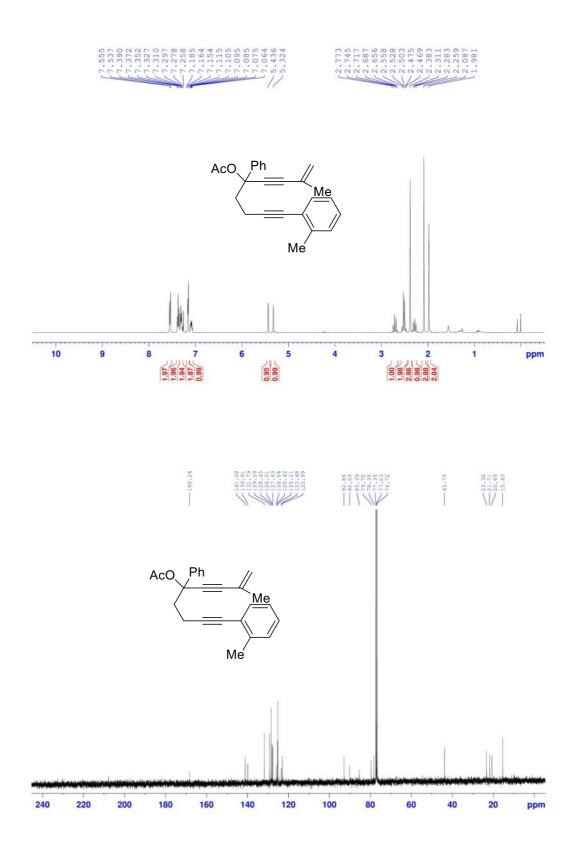


Figure S35. ¹H and ¹³C{¹H} NMR spectra of 9-(3,5-dimethylphenyl)-2-methyl-5phenylnona-1-en-3,8-diyn-5-yl acetate (1ı)

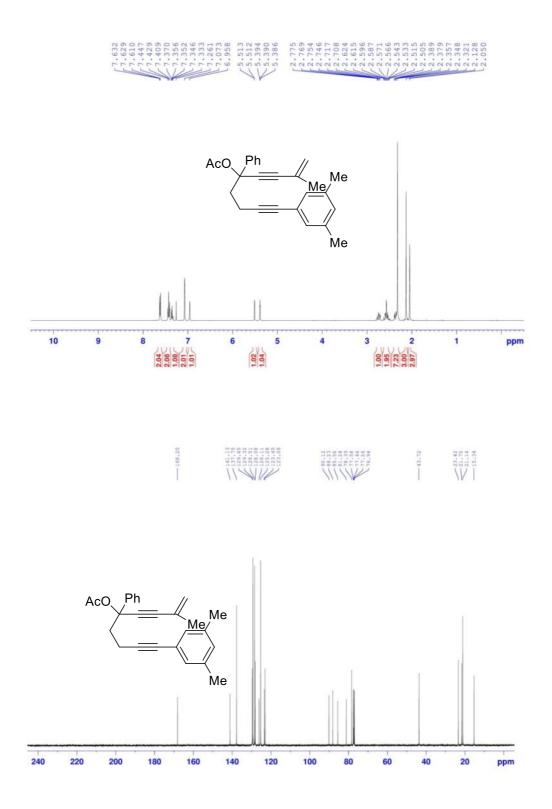


Figure S36. ¹H and ¹³C{¹H} NMR spectra of 2-methyl-5-phenyl-9-(2,4,5trimethylphenyl)nona-1-en-3,8-diyn-5-yl acetate (1κ)

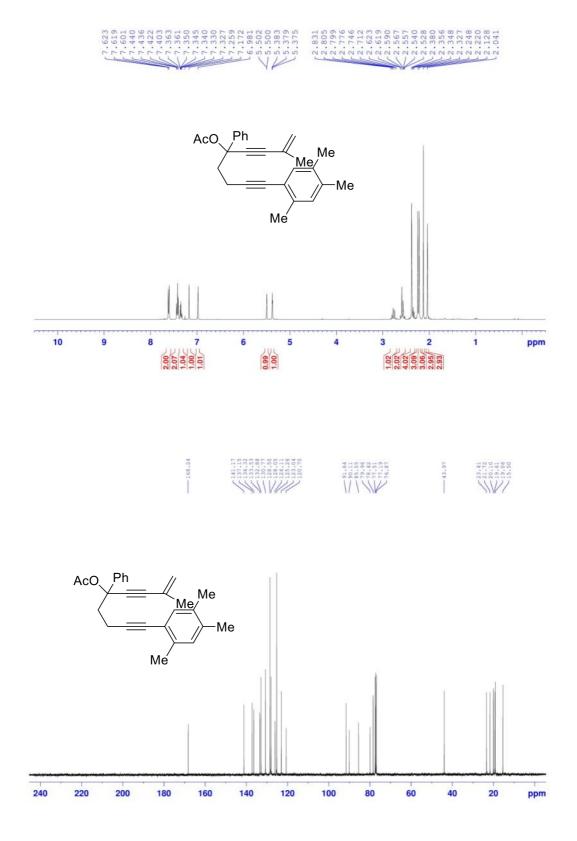


Figure S37. ¹H and ¹³C{¹H} NMR spectra of 2-methyl-5-phenyl-9-(thiophen-2-yl)nona-1-en-3,8-diyn-5-yl acetate (1λ)

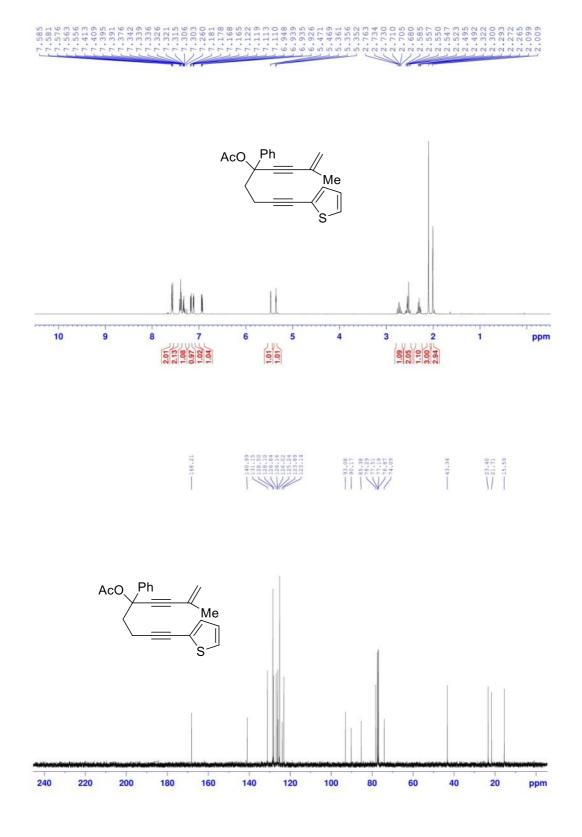


Figure S38. ¹H and ¹³C{¹H} NMR spectra of 3,4-diphenyl-1*H*-cyclopenta[*b*]naphthalene (4a)

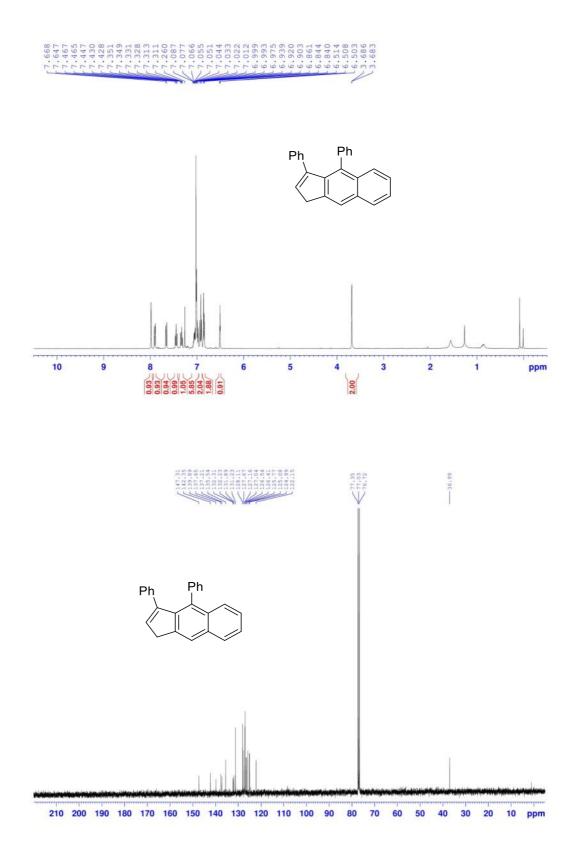


Figure S39. ¹H and ¹³C{¹H} NMR spectra of 3-methyl-4-phenyl-1*H*cyclopenta[*b*]naphthalene (4e)

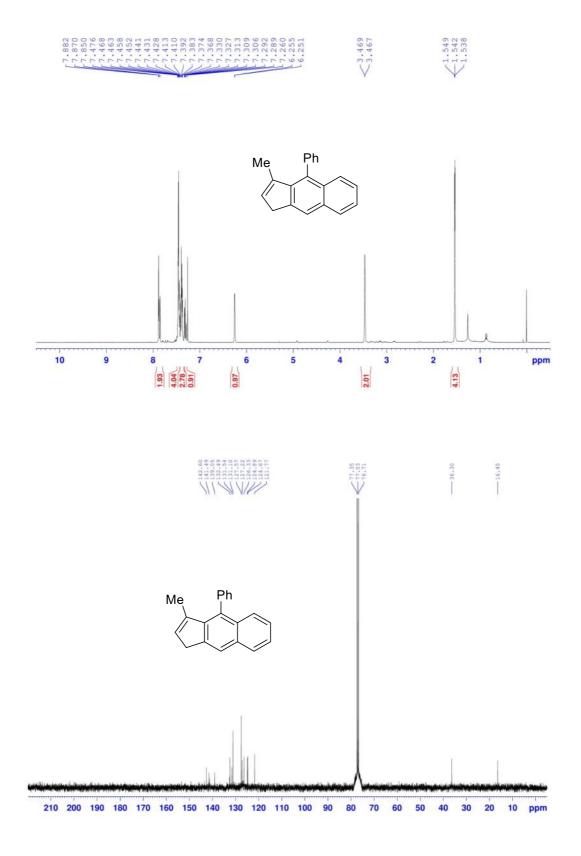


Figure S40. ¹H and ¹³C{¹H} NMR spectra of 3-cyclopropyl-4-phenyl-1*H*cyclopenta[*b*]naphthalene (4f)

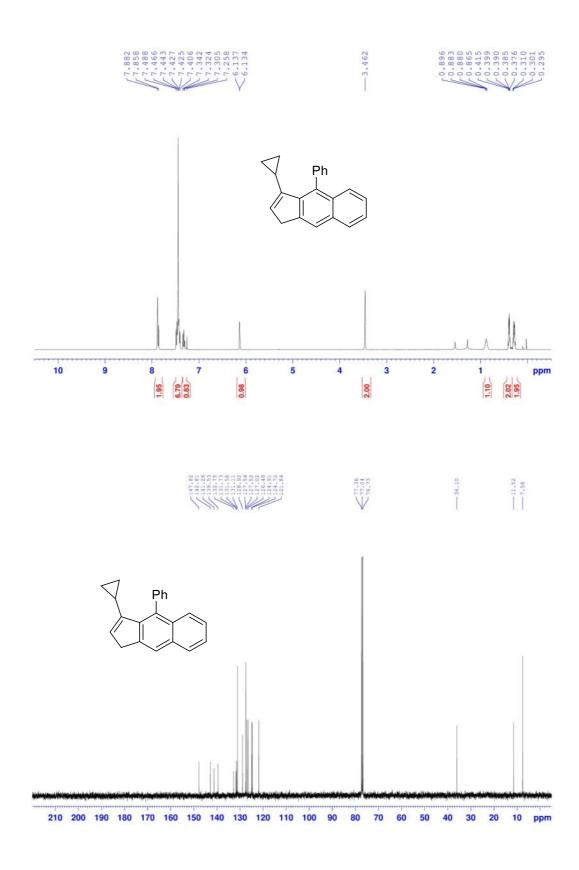


Figure S41. 1H and 13C{¹H} NMR spectra of 3-(4-chlorophenyl)-4-phenyl-1*H*cyclopenta[*b*]naphthalene(4g)

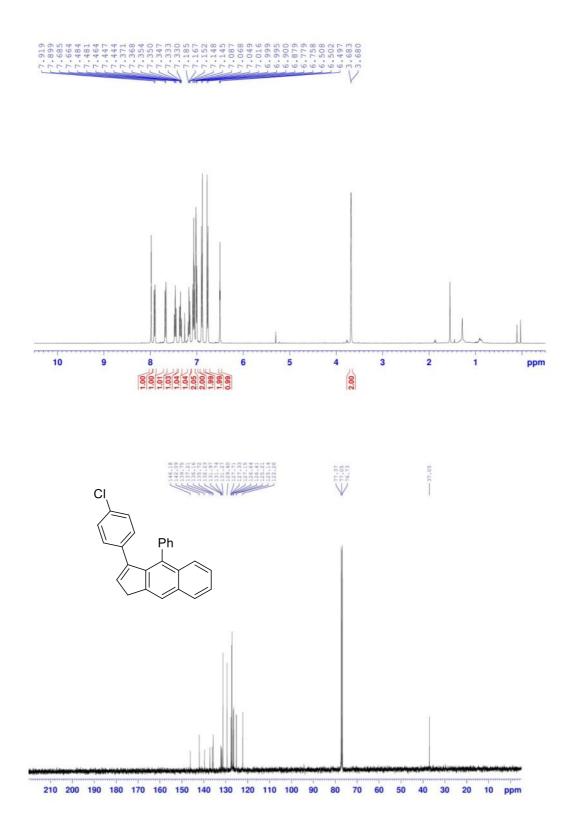


Figure S42. ¹H and ¹³C{¹H} NMR spectra of 4-(4-fluorophenyl)-3-phenyl-1*H*cyclopenta[*b*]naphthalene(4h)

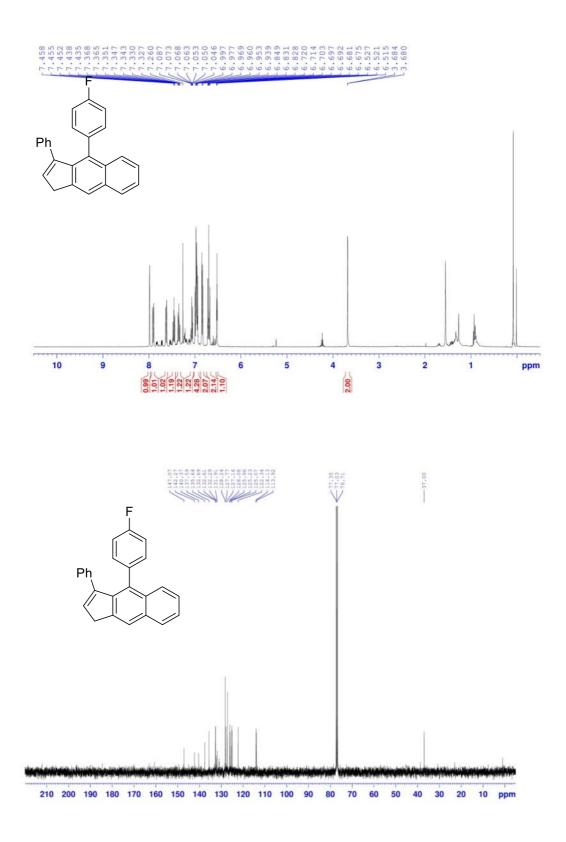


Figure S43. ¹H and ¹³C{¹H} NMR spectra of 3-phenyl-4-(p-tolyl)-1*H*cyclopenta[*b*]naphthalene (4i)



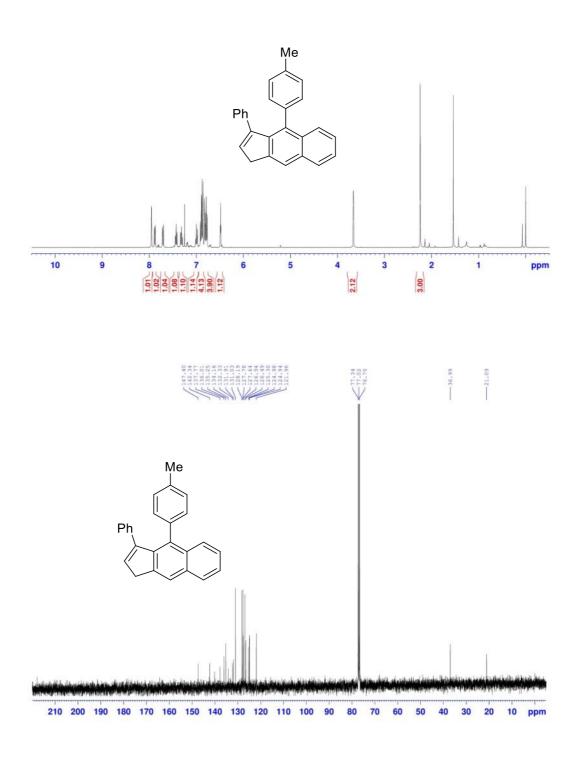


Figure S44. ¹H and ¹³C{¹H} NMR spectra of 3-(3-phenyl-1*H*-cyclopenta[*b*]naphthalen-4yl)thiophene (4j)

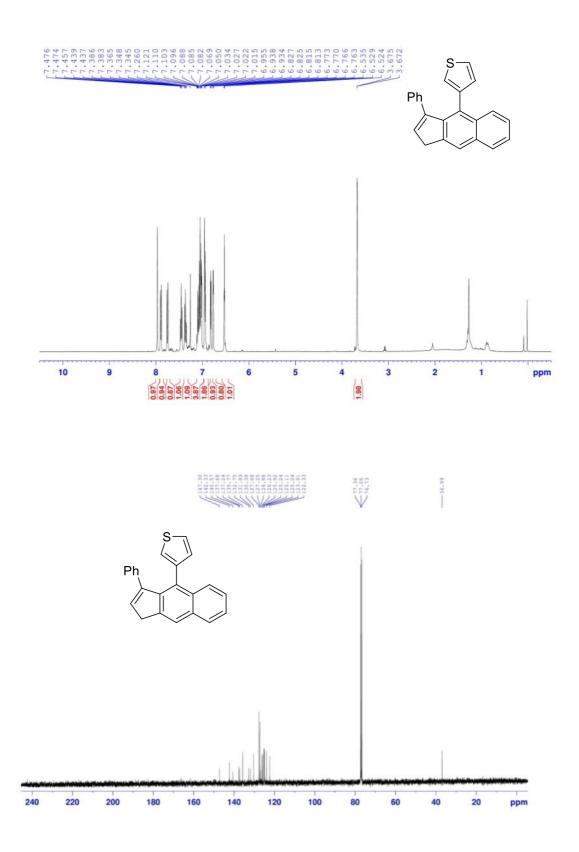


Figure S45. ¹H and ¹³C{¹H} NMR spectra of 6-fluoro-3,4-diphenyl-1*H*cyclopenta[*b*]naphthalene (4k)

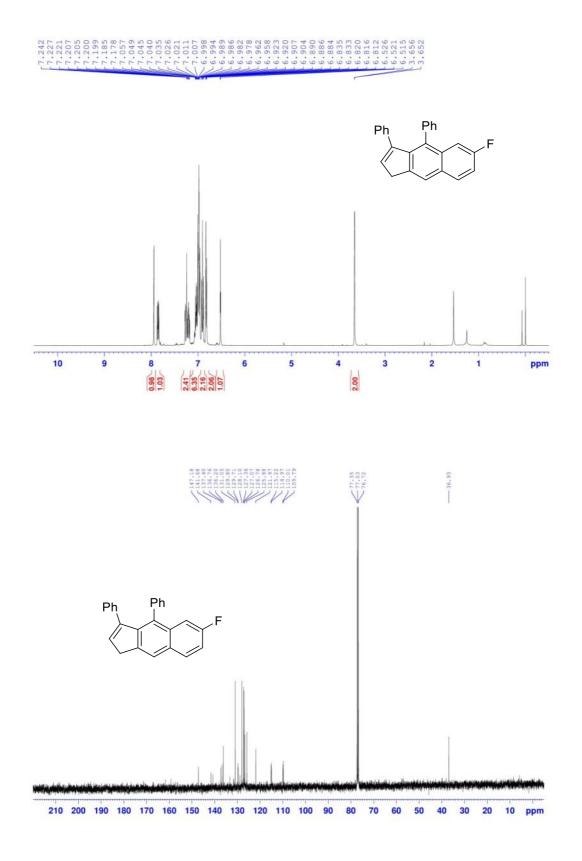


Figure S46. ¹H and ¹³C{¹H} NMR spectra of 6-bromo-3,4-diphenyl-1*H*cyclopenta[*b*]naphthalene (4l)

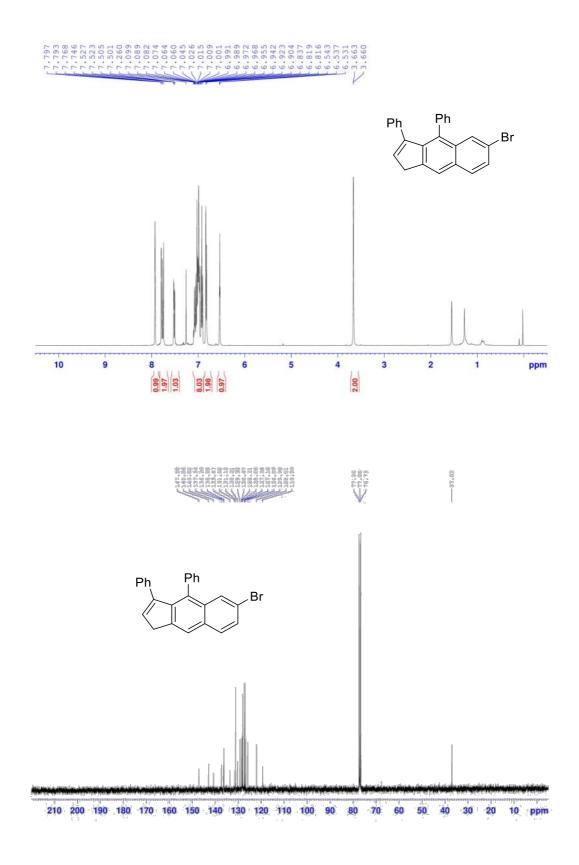


Figure S47. ¹H and ¹³C{¹H} NMR spectra of 6-pentyl-3,4-diphenyl-1*H*cyclopenta[*b*]naphthalene (4m)

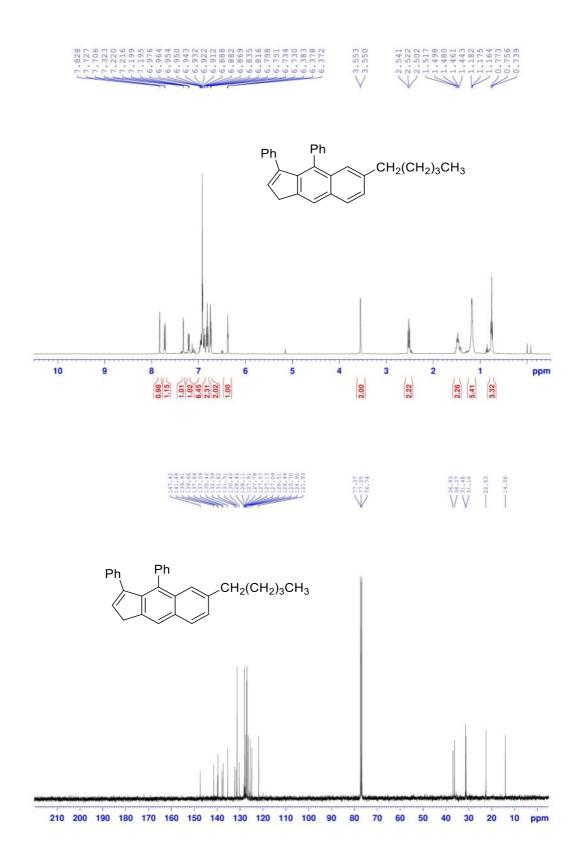


Figure S48. ¹H and ¹³C{¹H} NMR spectra of 6-methyl-3,4-diphenyl-1*H*cyclopenta[*b*]naphthalene (4n)

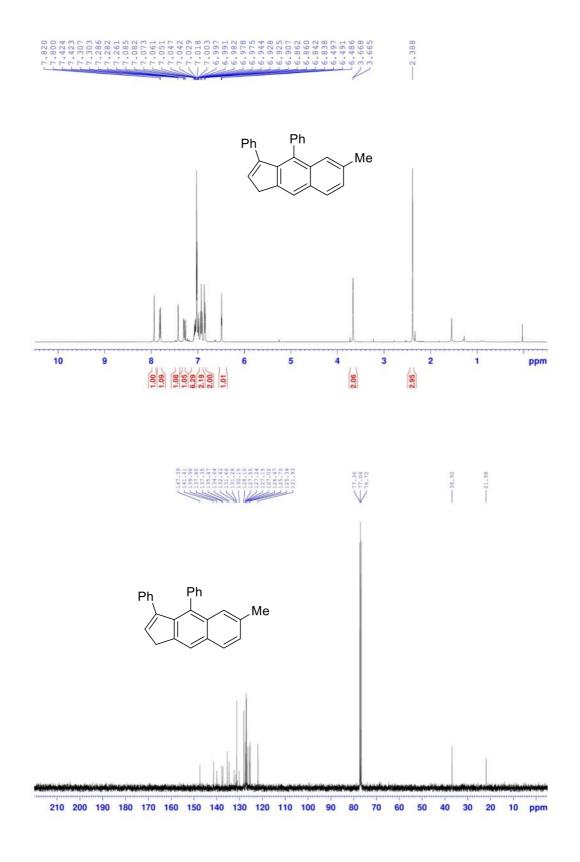


Figure S49. ¹H and ¹³C{¹H} NMR spectra of 8-methyl-3,4-diphenyl-1*H*cyclopenta[*b*]naphthalene (40)



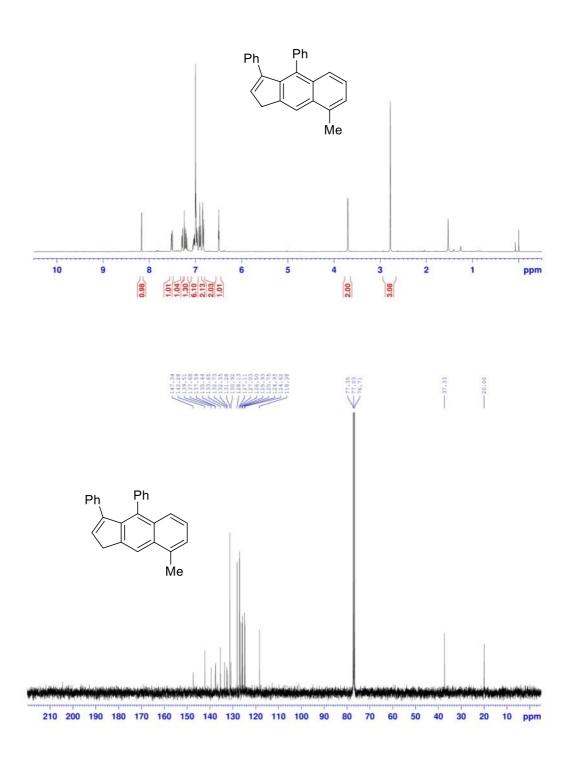


Figure S50. ¹H and ¹³C{¹H} NMR spectra of 5,7-dimethyl-3,4-diphenyl-1*H*cyclopenta[*b*]naphthalene (4p)

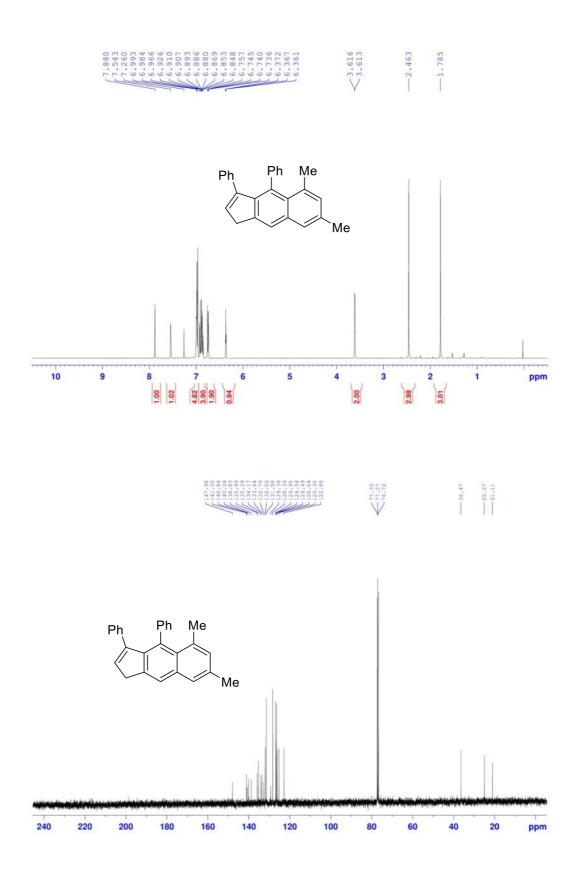


Figure S51. ¹H and ¹³C{¹H} NMR spectra of 5,6,8-trimethyl-3,4-diphenyl-1*H*cyclopenta[*b*]naphthalene (4q)

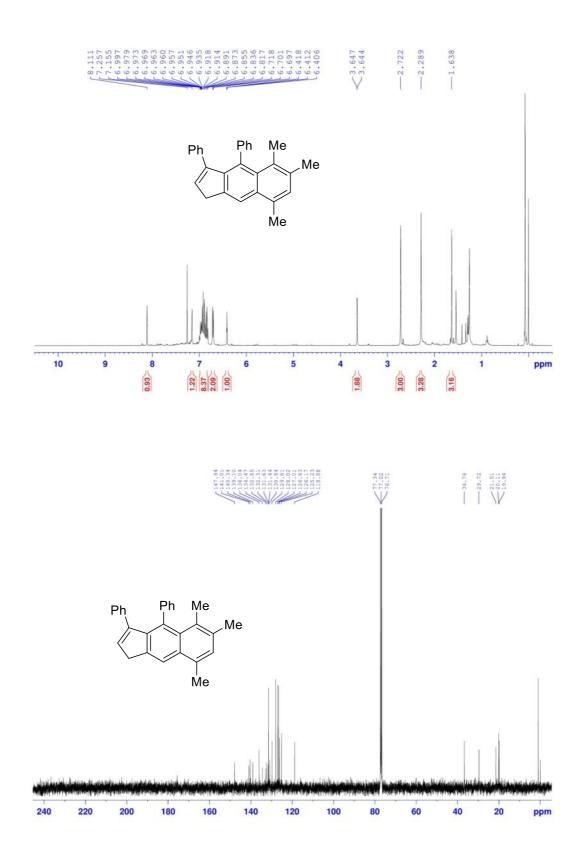
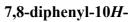


Figure S52. ¹H and ¹³C{¹H} NMR spectra of 7,8-dipho cyclopenta[*b*]phenanthrene (4r)





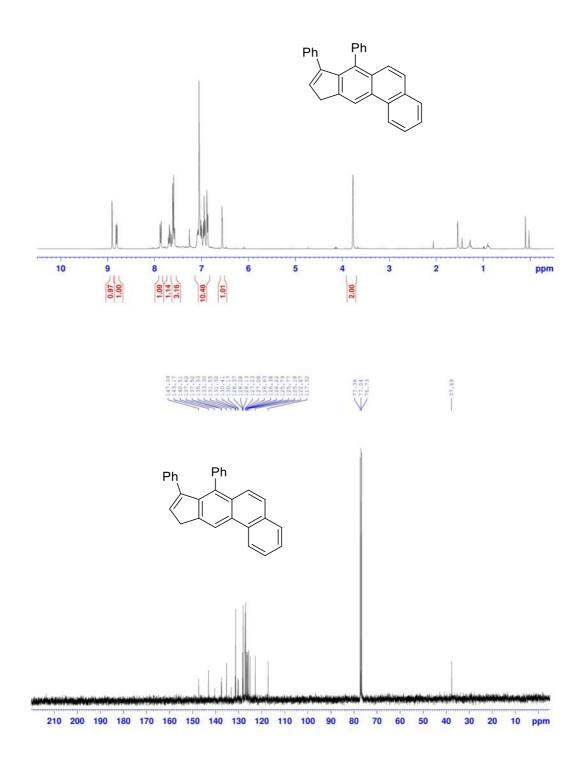


Figure S53. ¹H and ¹³C{¹H} NMR spectra of 7,8-diphenyl-5*H*-indeno[5,6-*b*]thiophene (4s)

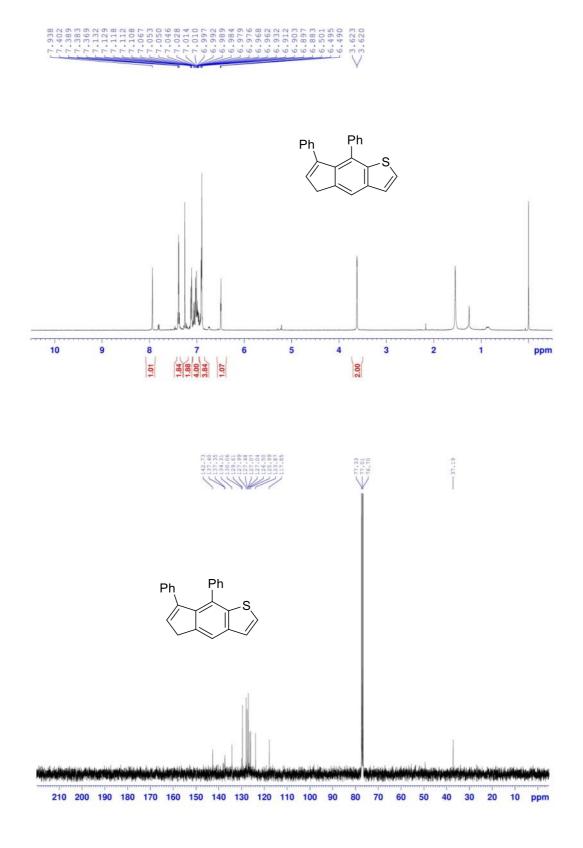


Figure S54. ¹H and ¹³C{¹H} NMR spectra of 4,5-diphenyl-7*H*-indeno[5,6-*b*]thiophene (4t)

